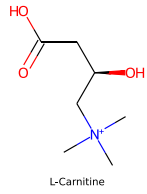
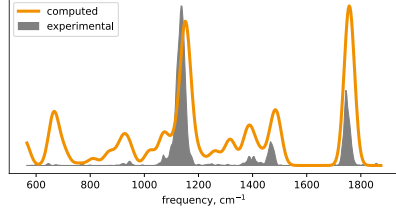


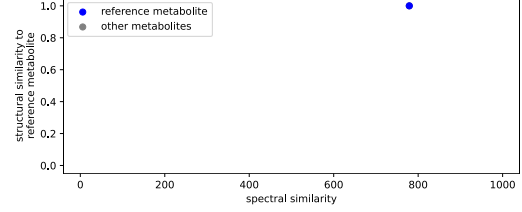
1 protonated HMDB0000062



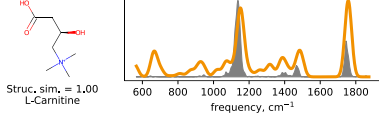
Spectra of protonated HMDB0000062, spectral sim. = 779, #1



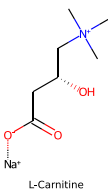
Structural similarity plot of protonated HMDB0000062



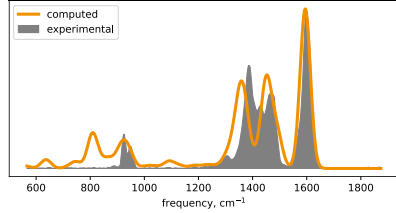
protonated HMDB0000062, spectral sim. = 779, #1



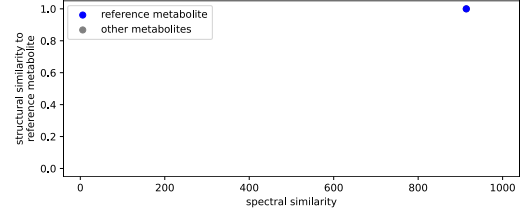
2 sodiated HMDB0000062



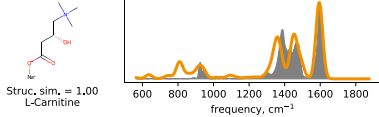
Spectra of sodiated HMDB0000062, spectral sim. = 914, #1



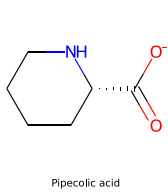
Structural similarity plot of sodiated HMDB0000062



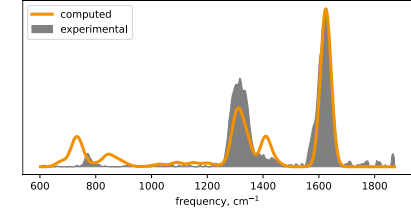
sodiated HMDB0000062, spectral sim. = 914, #1



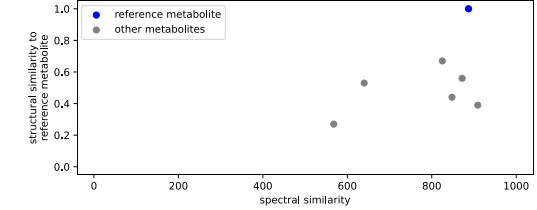
3 deprotonated HMDB0000070



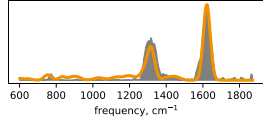
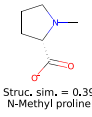
Spectra of deprotonated HMDB0000070, spectral sim. = 887, #2



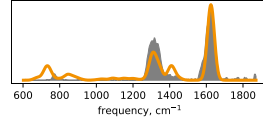
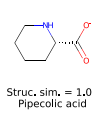
Structural similarity plot of deprotonated HMDB0000070



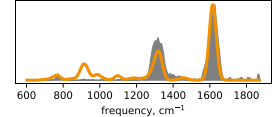
deprotonated HMDB0094696, spectral sim. = 909, #1



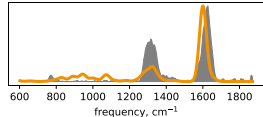
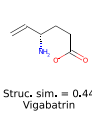
deprotonated HMDB0000070, spectral sim. = 887, #2



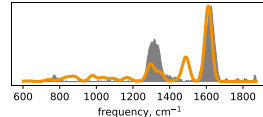
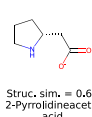
deprotonated HMDB0062225, spectral sim. = 872, #3



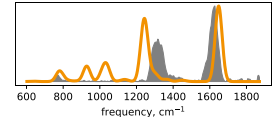
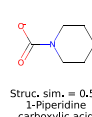
deprotonated HMDB0015212, spectral sim. = 848, #4



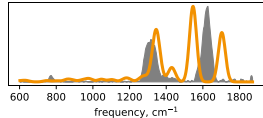
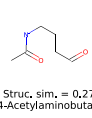
deprotonated HMDB0029444, spectral sim. = 825, #5



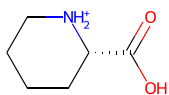
deprotonated HMDB0094697, spectral sim. = 640, #6



deprotonated HMDB0004226, spectral sim. = 568, #7

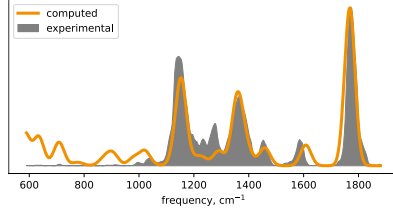


4 protonated HMDB0000070

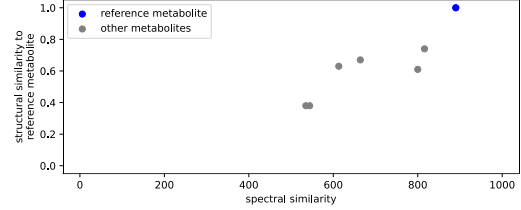


Pipecolic acid

Spectra of protonated HMDB0000070, spectral sim. = 890, #1



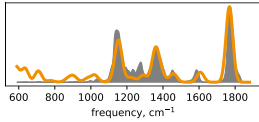
Structural similarity plot of protonated HMDB0000070



protonated HMDB0000070, spectral sim. = 890, #1



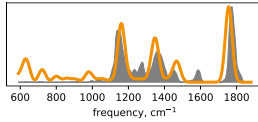
Struc. sim. = 1.00  
Pipecolic acid



protonated HMDB0094696, spectral sim. = 816, #2



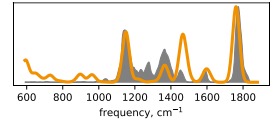
Struc. sim. = 0.74  
N-Methyl proline



protonated HMDB0062225, spectral sim. = 800, #3



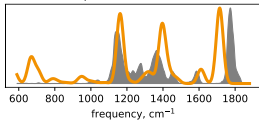
Struc. sim. = 0.61  
(2E)-Decenoyl-ACP



protonated HMDB0029444, spectral sim. = 664, #4



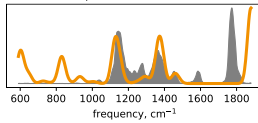
Struc. sim. = 0.67  
2-Pyrrolidineacetic acid



protonated HMDB0094697, spectral sim. = 613, #5



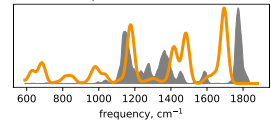
Struc. sim. = 0.63  
1-Piperidine carboxylic acid



protonated HMDB0015212, spectral sim. = 544, #6



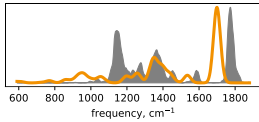
Struc. sim. = 0.38  
Vigabatrin



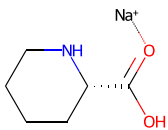
protonated HMDB0004226, spectral sim. = 535, #7



Struc. sim. = 0.38  
N4-Acetylaminobutanal

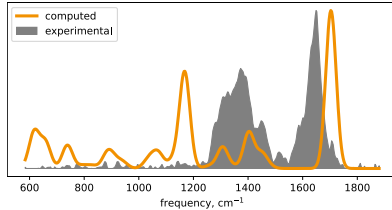


5 sodiated HMDB0000070

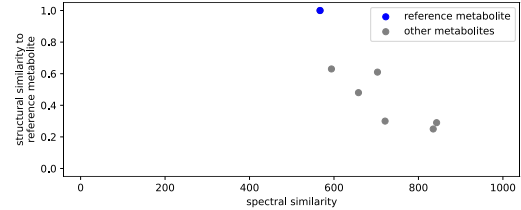


Pipecolic acid

Spectra of sodiated HMDB0000070, spectral sim. = 567, #7



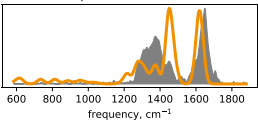
Structural similarity plot of sodiated HMDB0000070



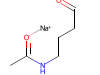
sodiated HMDB0029444, spectral sim. = 843, #1



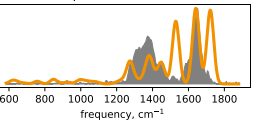
Struc. sim. = 0.29  
2-Pyrrolidineacetic acid



sodiated HMDB0004226, spectral sim. = 835, #2



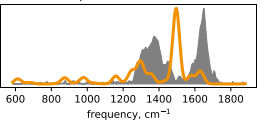
Struc. sim. = 0.25  
N4-Acetylaminobutanal



sodiated HMDB0015212, spectral sim. = 721, #3



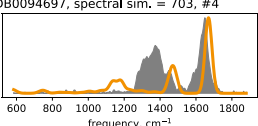
Struc. sim. = 0.30  
Vigabatrin



sodiated HMDB0094697, spectral sim. = 703, #4



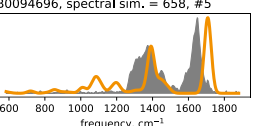
Struc. sim. = 0.61  
1-Piperidine carboxylic acid



sodiated HMDB0094696, spectral sim. = 658, #5



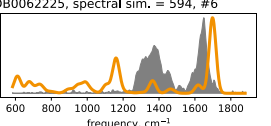
Struc. sim. = 0.48  
N-Methyl proline



sodiated HMDB0062225, spectral sim. = 594, #6



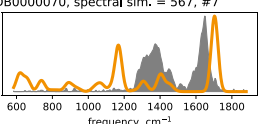
Struc. sim. = 0.63  
(2E)-Decenoyl-ACP



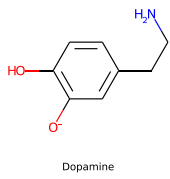
sodiated HMDB0000070, spectral sim. = 567, #7



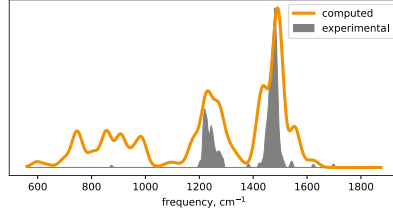
Struc. sim. = 1.00  
Pipecolic acid



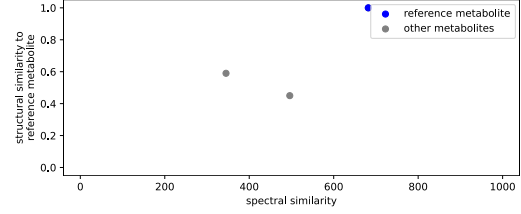
6 deprotonated HMDB0000073



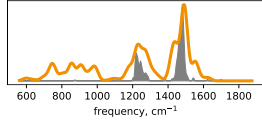
Spectra of deprotonated HMDB0000073, spectral sim. = 682, #1



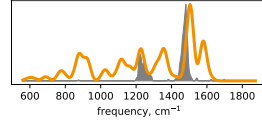
Structural similarity plot of deprotonated HMDB0000073



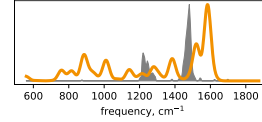
deprotonated HMDB0000073, spectral sim. = 682, #1



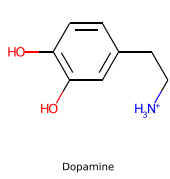
deprotonated HMDB0012309, spectral sim. = 496, #2



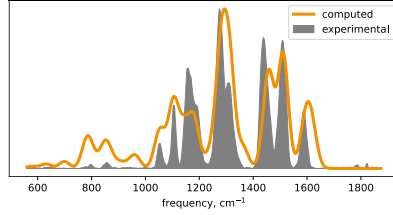
deprotonated HMDB0004825, spectral sim. = 345, #3



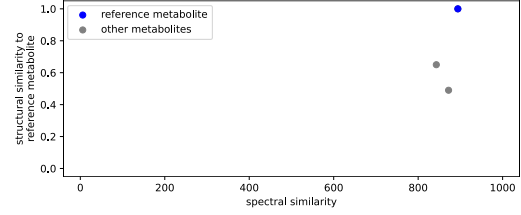
7 protonated HMDB0000073



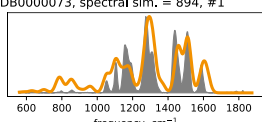
Spectra of protonated HMDB0000073, spectral sim. = 894, #1



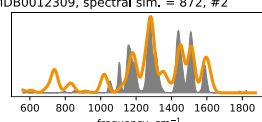
Structural similarity plot of protonated HMDB0000073



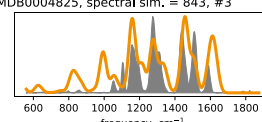
protonated HMDB0000073, spectral sim. = 894, #1



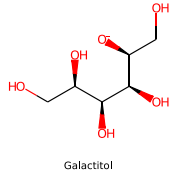
protonated HMDB0012309, spectral sim. = 872, #2



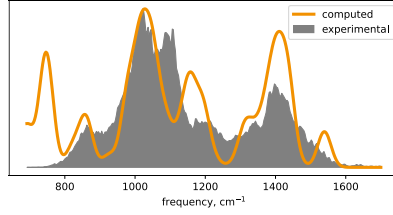
protonated HMDB0004825, spectral sim. = 843, #3



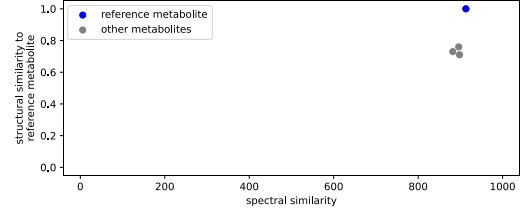
8 deprotonated HMDB0000107



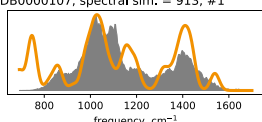
Spectra of deprotonated HMDB0000107, spectral sim. = 913, #1



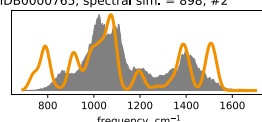
Structural similarity plot of deprotonated HMDB0000107



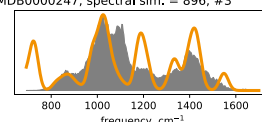
deprotonated HMDB0000107, spectral sim. = 913, #1



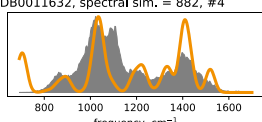
deprotonated HMDB0000765, spectral sim. = 898, #2



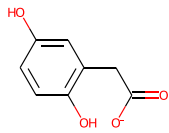
deprotonated HMDB0000247, spectral sim. = 896, #3



deprotonated HMDB0011632, spectral sim. = 882, #4

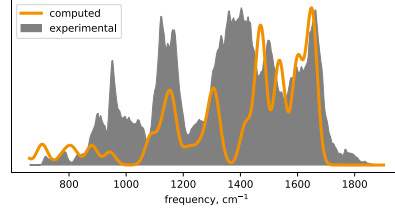


9 deprotonated HMDB0000130

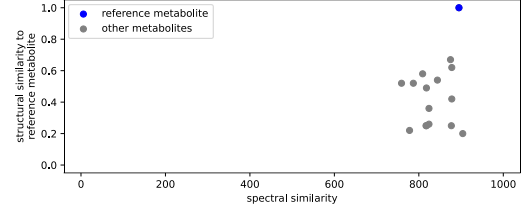


Homogentisic acid

Spectra of deprotonated HMDB0000130, spectral sim. = 895, #2



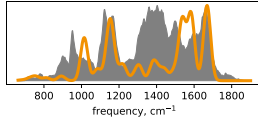
Structural similarity plot of deprotonated HMDB0000130



deprotonated HMDB0000484, spectral sim. = 904, #1



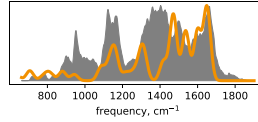
Struc. sim. = 0.20  
Vanillic acid



deprotonated HMDB0000130, spectral sim. = 895, #2



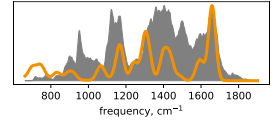
Struc. sim. = 1.00  
Homogentisic acid



deprotonated HMDB0000750, spectral sim. = 878, #3



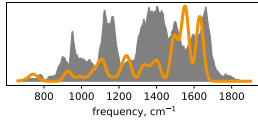
Struc. sim. = 0.62  
3-Hydroxymandelic acid



deprotonated HMDB0029644, spectral sim. = 878, #4



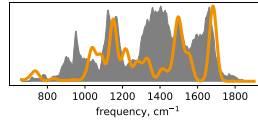
Struc. sim. = 0.42  
2',4',6'-  
Trihydroxyacetophenone



deprotonated HMDB0060003, spectral sim. = 877, #5



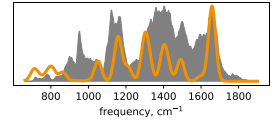
Struc. sim. = 0.25  
Isovanillic acid



deprotonated HMDB0000822, spectral sim. = 875, #6



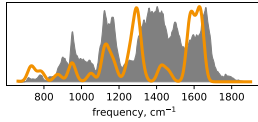
Struc. sim. = 0.67  
p-Hydroxymandelic acid



deprotonated HMDB0125536, spectral sim. = 844, #7



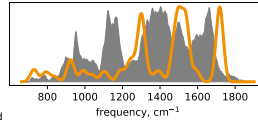
Struc. sim. = 0.54  
3-hydroxy-5-  
methoxybenzoic acid



deprotonated HMDB0006242, spectral sim. = 824, #8



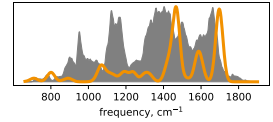
Struc. sim. = 0.36  
3,4-  
Dihydroxymandelaldehyd  
e



deprotonated HMDB0001868, spectral sim. = 824, #9



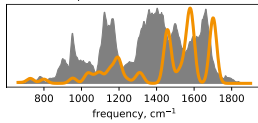
Struc. sim. = 0.26  
5-Methoxysalicylic acid



deprotonated HMDB0131176, spectral sim. = 818, #10



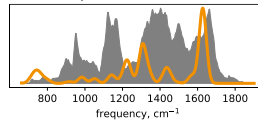
Struc. sim. = 0.25  
2-hydroxy-4-  
methoxybenzoic acid



deprotonated HMDB0140902, spectral sim. = 818, #11



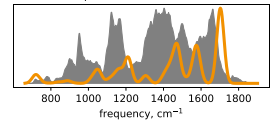
Struc. sim. = 0.49  
3-hydroxy-2-  
methoxybenzoic acid



deprotonated HMDB0059713, spectral sim. = 817, #12



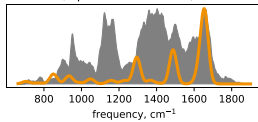
Struc. sim. = 0.25  
3-Methoxysalicylic acid



deprotonated HMDB0240257, spectral sim. = 809, #13



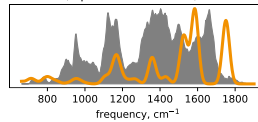
Struc. sim. = 0.58  
Quinolacetic acid



deprotonated HMDB0094709, spectral sim. = 787, #14



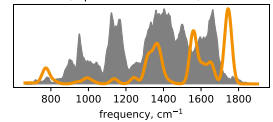
Struc. sim. = 0.52  
3-  
5-  
Dihydroxyphenylacetic acid



deprotonated HMDB0033129, spectral sim. = 778, #15



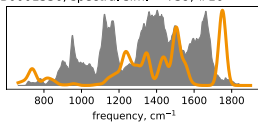
Struc. sim. = 0.22  
3-Acetyl-4-hydroxy-6-  
methyl-2H-pyran-2-one



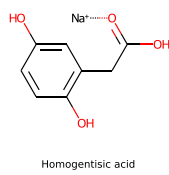
deprotonated HMDB0001336, spectral sim. = 759, #16



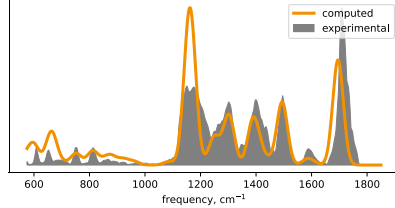
Struc. sim. = 0.52  
3,4-  
Dihydroxybenzeneacetic acid



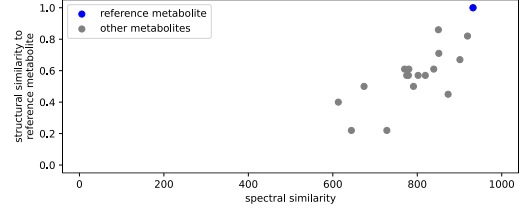
10 sodiated HMDB0000130



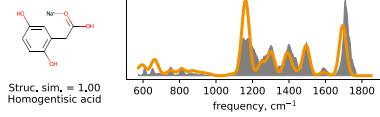
Spectra of sodiated HMDB0000130, spectral sim. = 932, #1



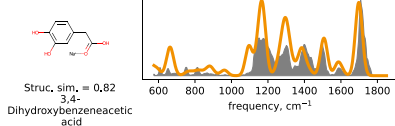
Structural similarity plot of sodiated HMDB0000130



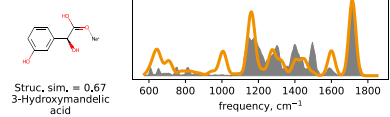
sodiated HMDB0000130, spectral sim. = 932, #1



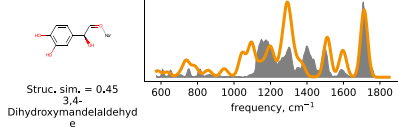
sodiated HMDB0001336, spectral sim. = 919, #2



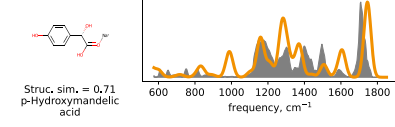
sodiated HMDB0000750, spectral sim. = 901, #3



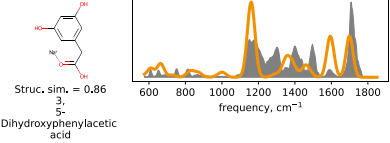
sodiated HMDB0006242, spectral sim. = 873, #4



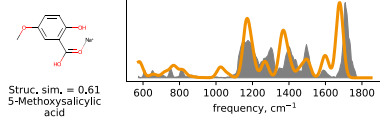
sodiated HMDB0000822, spectral sim. = 851, #5



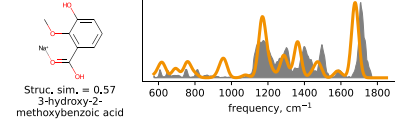
sodiated HMDB0094709, spectral sim. = 850, #6



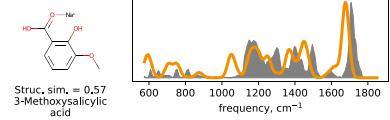
sodiated HMDB0001868, spectral sim. = 839, #7



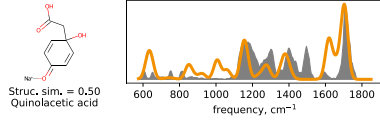
sodiated HMDB0140902, spectral sim. = 819, #8



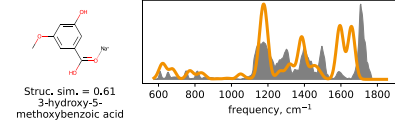
sodiated HMDB0059713, spectral sim. = 802, #9



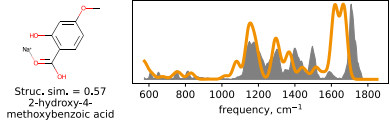
sodiated HMDB0240257, spectral sim. = 791, #10



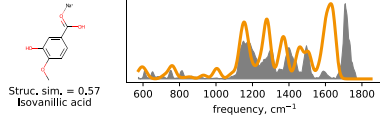
sodiated HMDB0125536, spectral sim. = 780, #11



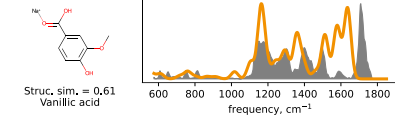
sodiated HMDB0131176, spectral sim. = 779, #12



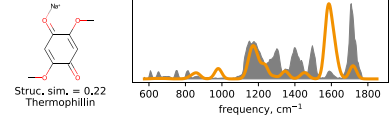
sodiated HMDB0060003, spectral sim. = 775, #13



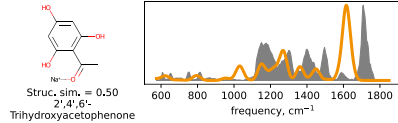
sodiated HMDB0000484, spectral sim. = 770, #14



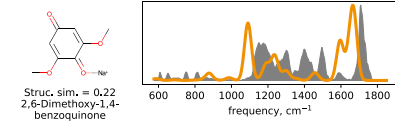
sodiated HMDB0034335, spectral sim. = 728, #15



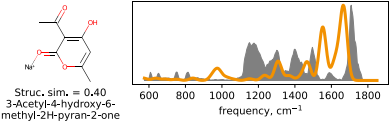
sodiated HMDB0029644, spectral sim. = 674, #16



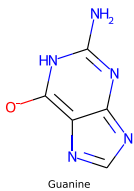
sodiated HMDB0029673, spectral sim. = 644, #17



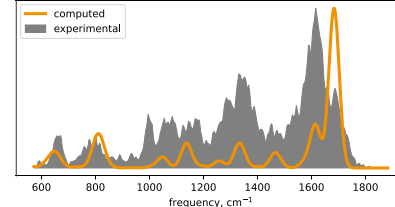
sodiated HMDB0033129, spectral sim. = 613, #18



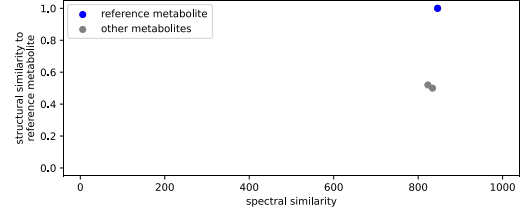
11 deprotonated HMDB0000132



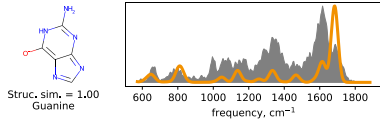
Spectra of deprotonated HMDB0000132, spectral sim. = 846, #1



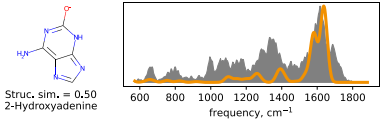
Structural similarity plot of deprotonated HMDB0000132



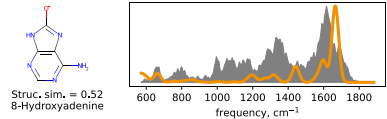
deprotonated HMDB0000132, spectral sim. = 846, #1



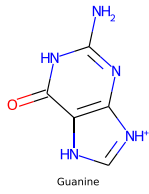
deprotonated HMDB0000403, spectral sim. = 834, #2



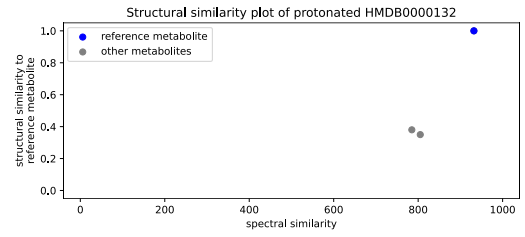
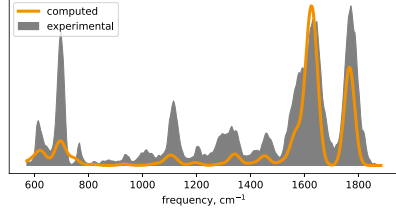
deprotonated HMDB0000542, spectral sim. = 823, #3



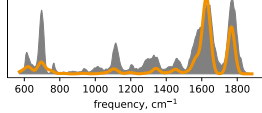
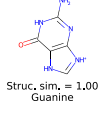
12 protonated HMDB0000132



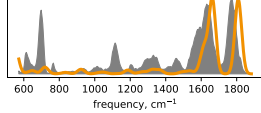
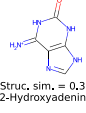
Spectra of protonated HMDB0000132, spectral sim. = 932, #1



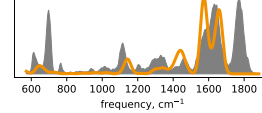
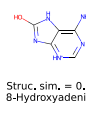
protonated HMDB0000132, spectral sim. = 932, #1



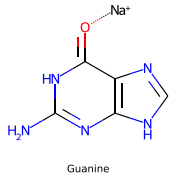
protonated HMDB0000403, spectral sim. = 805, #2



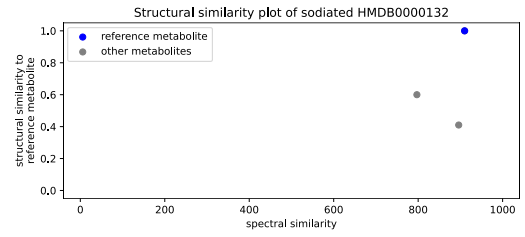
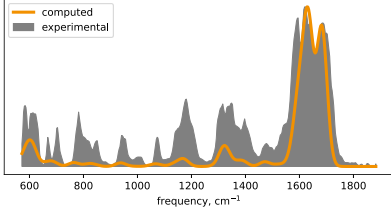
protonated HMDB0000542, spectral sim. = 785, #3



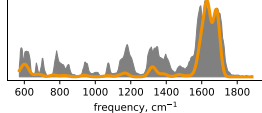
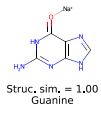
13 sodiated HMDB0000132



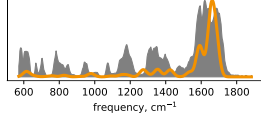
Spectra of sodiated HMDB0000132, spectral sim. = 910, #1



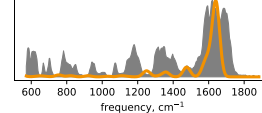
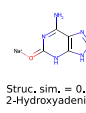
sodiated HMDB0000132, spectral sim. = 910, #1



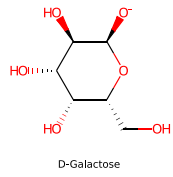
sodiated HMDB0000542, spectral sim. = 896, #2



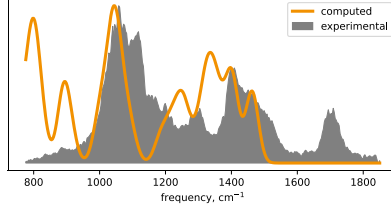
sodiated HMDB0000403, spectral sim. = 797, #3



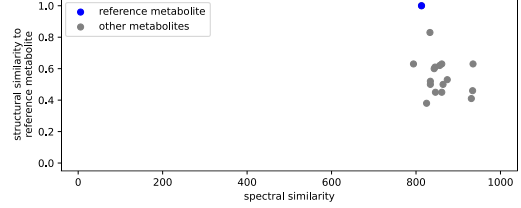
14 deprotonated HMDB0000143



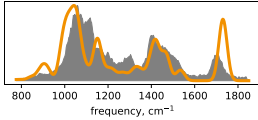
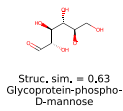
Spectra of deprotonated HMDB0000143, spectral sim. = 813, #16



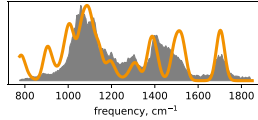
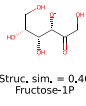
Structural similarity plot of deprotonated HMDB0000143



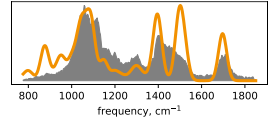
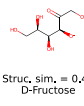
deprotonated HMDB0062473, spectral sim. = 935, #1



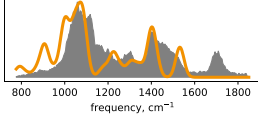
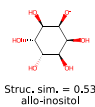
deprotonated HMDB0062538, spectral sim. = 934, #2



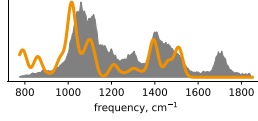
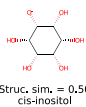
deprotonated HMDB0000660, spectral sim. = 931, #3



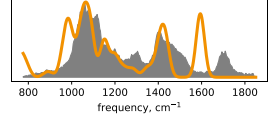
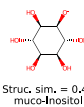
deprotonated HMDB0240211, spectral sim. = 874, #4



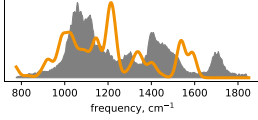
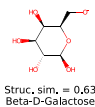
deprotonated HMDB0240210, spectral sim. = 864, #5



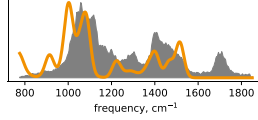
deprotonated HMDB0062138, spectral sim. = 861, #6



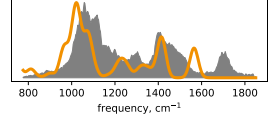
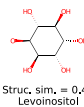
deprotonated HMDB0003449, spectral sim. = 861, #7



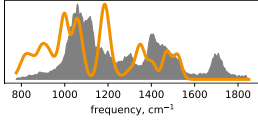
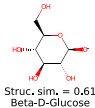
deprotonated HMDB0000211, spectral sim. = 856, #8



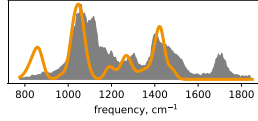
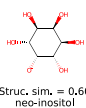
deprotonated HMDB0034220, spectral sim. = 846, #9



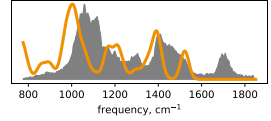
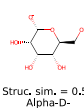
deprotonated HMDB0000516, spectral sim. = 845, #10



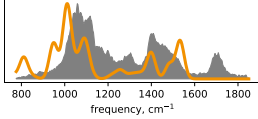
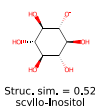
deprotonated HMDB0240208, spectral sim. = 843, #11



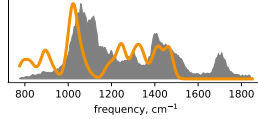
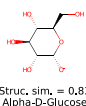
deprotonated HMDB0061922, spectral sim. = 834, #12



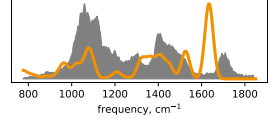
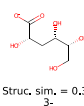
deprotonated HMDB0006088, spectral sim. = 834, #13



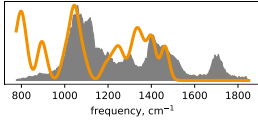
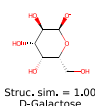
deprotonated HMDB0003345, spectral sim. = 833, #14



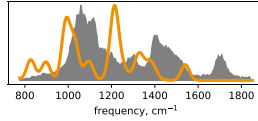
deprotonated HMDB0000346, spectral sim. = 825, #15



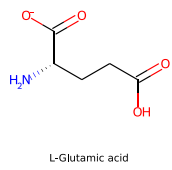
deprotonated HMDB0000143, spectral sim. = 813, #16



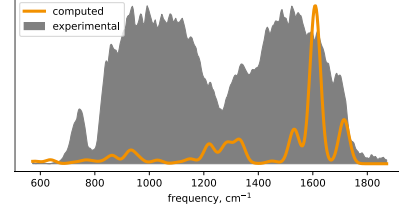
deprotonated HMDB0062202, spectral sim. = 794, #17



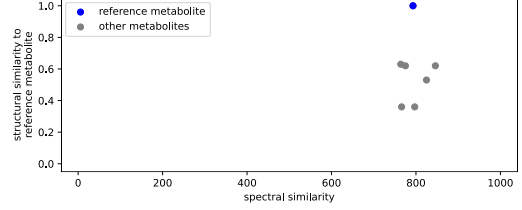
15 deprotonated HMDB0000148



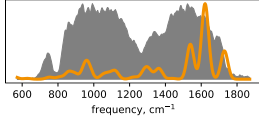
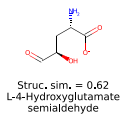
Spectra of deprotonated HMDB0000148, spectral sim. = 793, #4



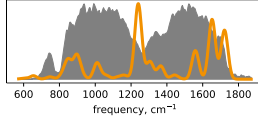
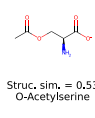
Structural similarity plot of deprotonated HMDB0000148



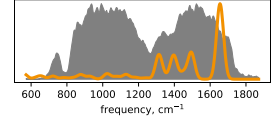
deprotonated HMDB0006556, spectral sim. = 846, #1



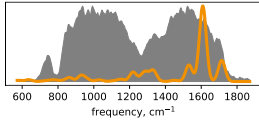
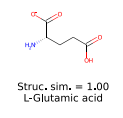
deprotonated HMDB0003011, spectral sim. = 825, #2



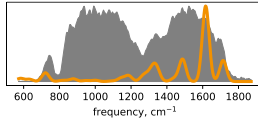
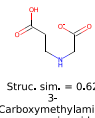
deprotonated HMDB0062183, spectral sim. = 797, #3



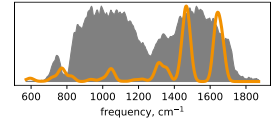
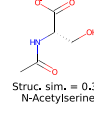
deprotonated HMDB0000148, spectral sim. = 793, #4



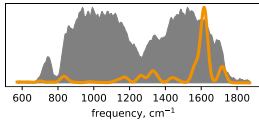
deprotonated HMDB0003350, spectral sim. = 775, #5



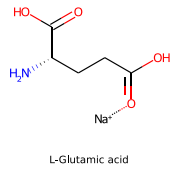
deprotonated HMDB0002931, spectral sim. = 766, #6



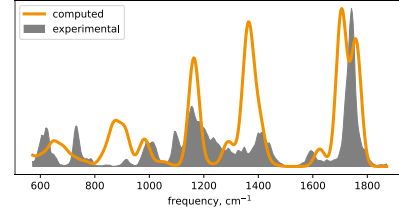
deprotonated HMDB0002393, spectral sim. = 764, #7



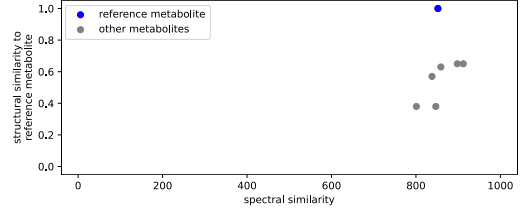
16 sodiated HMDB0000148



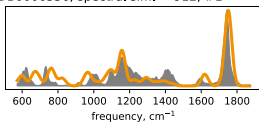
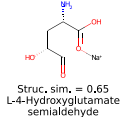
Spectra of sodiated HMDB0000148, spectral sim. = 852, #4



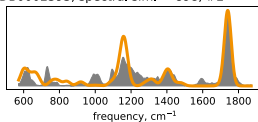
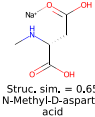
Structural similarity plot of sodiated HMDB0000148



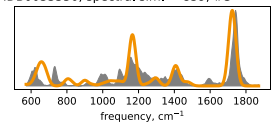
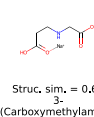
sodiated HMDB0006556, spectral sim. = 912, #1



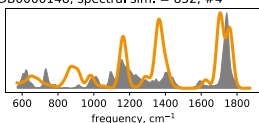
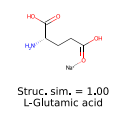
sodiated HMDB0002393, spectral sim. = 898, #2



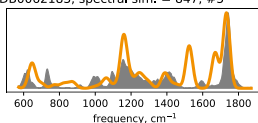
sodiated HMDB0003350, spectral sim. = 859, #3



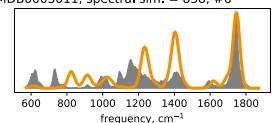
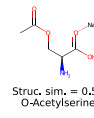
sodiated HMDB0000148, spectral sim. = 852, #4



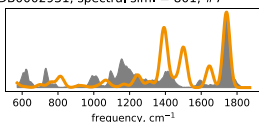
sodiated HMDB0062183, spectral sim. = 847, #5



sodiated HMDB0003011, spectral sim. = 838, #6

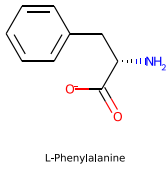


sodiated HMDB0002931, spectral sim. = 801, #7

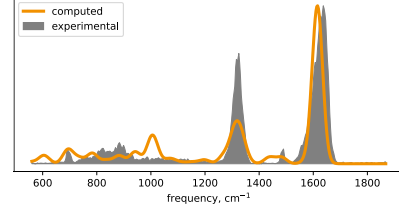




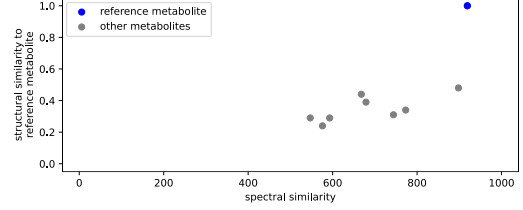
17 deprotonated HMDB0000159



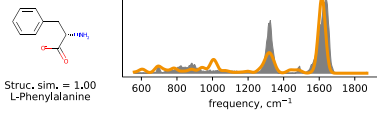
Spectra of deprotonated HMDB0000159, spectral sim. = 919, #1



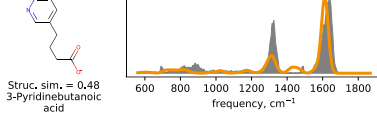
Structural similarity plot of deprotonated HMDB0000159



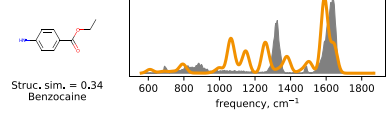
deprotonated HMDB0000159, spectral sim. = 919, #1



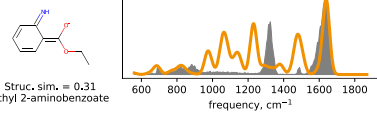
deprotonated HMDB0001007, spectral sim. = 898, #2



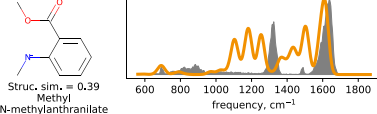
deprotonated HMDB0004992, spectral sim. = 773, #3



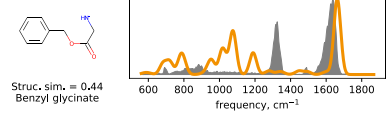
deprotonated HMDB0003589, spectral sim. = 744, #4



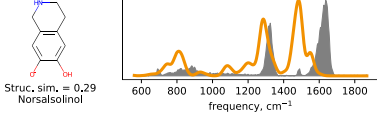
deprotonated HMDB0034169, spectral sim. = 679, #5



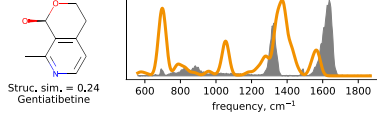
deprotonated HMDB0059934, spectral sim. = 668, #6



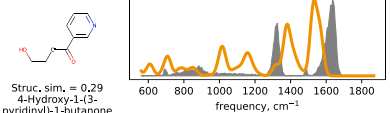
deprotonated HMDB0006044, spectral sim. = 593, #7



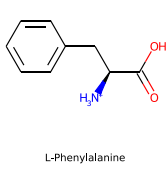
deprotonated HMDB0033485, spectral sim. = 576, #8



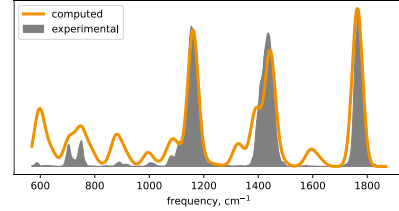
deprotonated HMDB0062402, spectral sim. = 547, #9



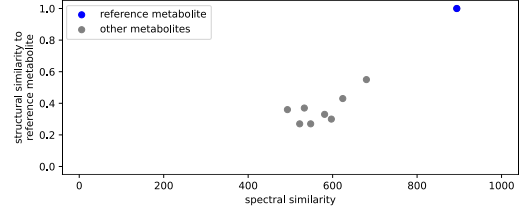
18 protonated HMDB0000159



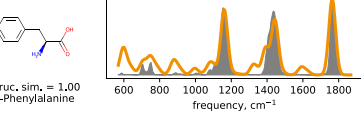
Spectra of protonated HMDB0000159, spectral sim. = 894, #1



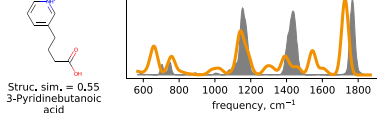
Structural similarity plot of protonated HMDB0000159



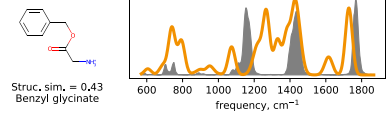
protonated HMDB0000159, spectral sim. = 894, #1



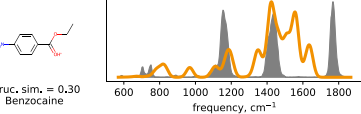
protonated HMDB0001007, spectral sim. = 680, #2



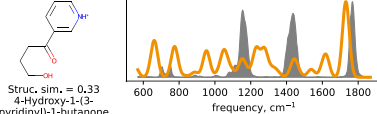
protonated HMDB0059934, spectral sim. = 624, #3



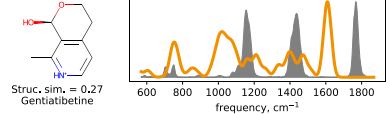
protonated HMDB0004992, spectral sim. = 597, #4



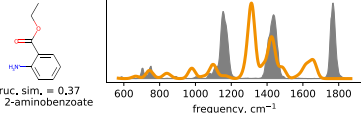
protonated HMDB0062402, spectral sim. = 581, #5



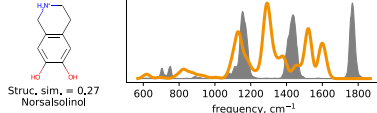
protonated HMDB0033485, spectral sim. = 548, #6



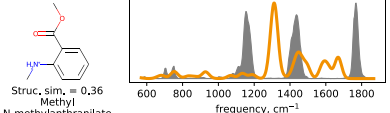
protonated HMDB0003589, spectral sim. = 533, #7



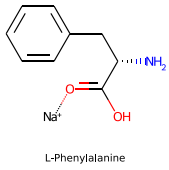
protonated HMDB0006044, spectral sim. = 522, #8



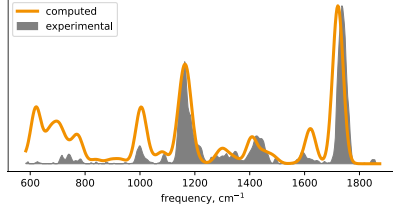
protonated HMDB0034169, spectral sim. = 493, #9



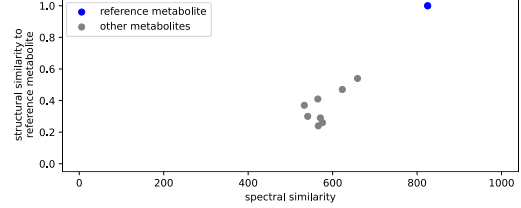
19 sodiated HMDB0000159



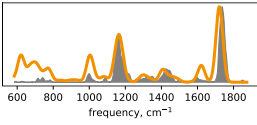
Spectra of sodiated HMDB0000159, spectral sim. = 825, #1



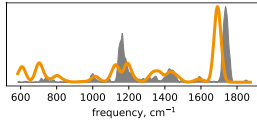
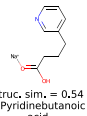
Structural similarity plot of sodiated HMDB0000159



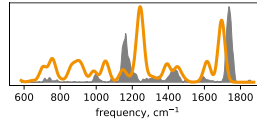
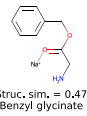
sodiated HMDB0000159, spectral sim. = 825, #1



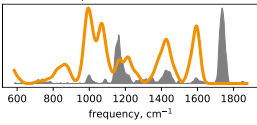
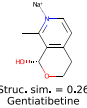
sodiated HMDB0001007, spectral sim. = 659, #2



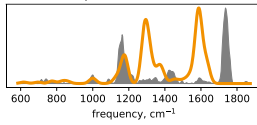
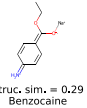
sodiated HMDB0059934, spectral sim. = 623, #3



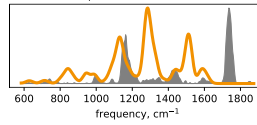
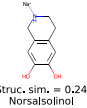
sodiated HMDB0033485, spectral sim. = 576, #4



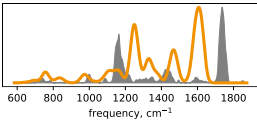
sodiated HMDB0004992, spectral sim. = 571, #5



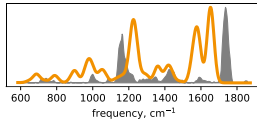
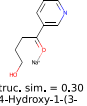
sodiated HMDB0006044, spectral sim. = 566, #6



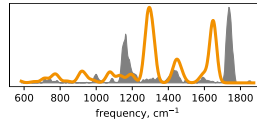
sodiated HMDB0033589, spectral sim. = 565, #7



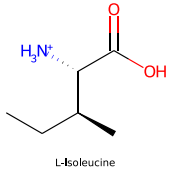
sodiated HMDB0062402, spectral sim. = 541, #8



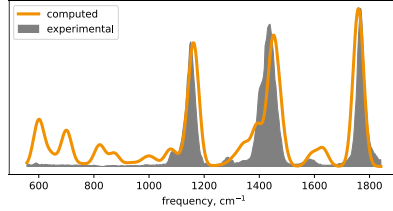
sodiated HMDB0034169, spectral sim. = 533, #9



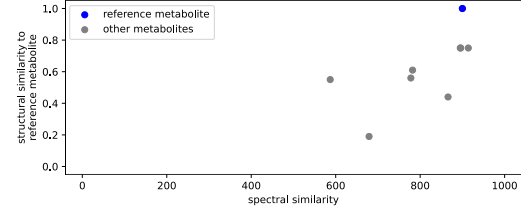
20 protonated HMDB0000172



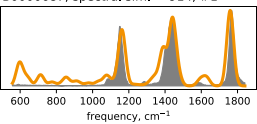
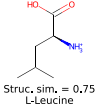
Spectra of protonated HMDB0000172, spectral sim. = 900, #2



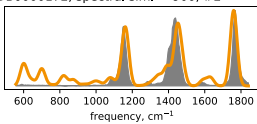
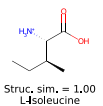
Structural similarity plot of protonated HMDB0000172



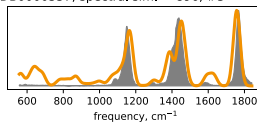
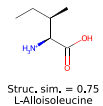
protonated HMDB0000687, spectral sim. = 914, #1



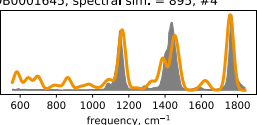
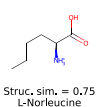
protonated HMDB0000172, spectral sim. = 900, #2



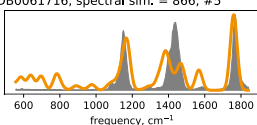
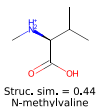
protonated HMDB0000557, spectral sim. = 896, #3



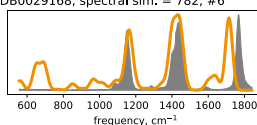
protonated HMDB0001645, spectral sim. = 895, #4



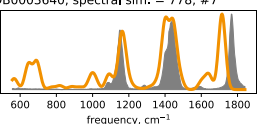
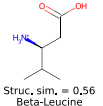
protonated HMDB0061716, spectral sim. = 866, #5



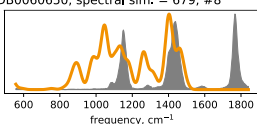
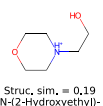
protonated HMDB0029168, spectral sim. = 782, #6



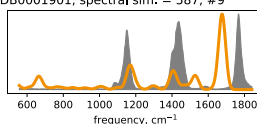
protonated HMDB0003640, spectral sim. = 778, #7



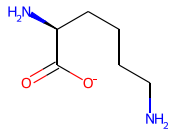
protonated HMDB0060650, spectral sim. = 679, #8



protonated HMDB0001901, spectral sim. = 587, #9

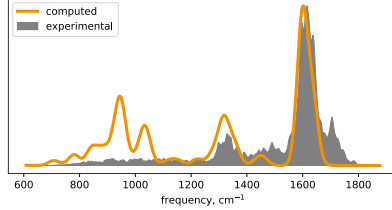


21 deprotonated HMDB0000182

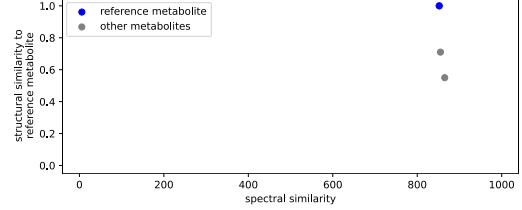


L-Lysine

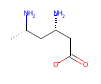
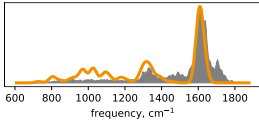
Spectra of deprotonated HMDB0000182, spectral sim. = 852, #3



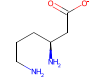
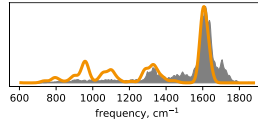
Structural similarity plot of deprotonated HMDB0000182



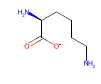
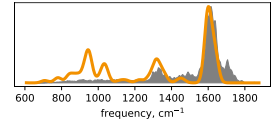
deprotonated HMDB0012115, spectral sim. = 865, #1

Struc. sim. = 0.55  
(3S,5S)-3,5-Diaminohexanoate

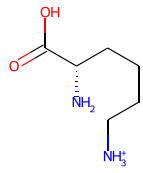
deprotonated HMDB0012114, spectral sim. = 855, #2

Struc. sim. = 0.71  
(3S)-3,6-Diaminohexanoate

deprotonated HMDB0000182, spectral sim. = 852, #3

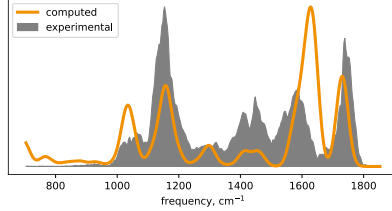
Struc. sim. = 1.00  
L-Lysine

22 protonated HMDB0000182

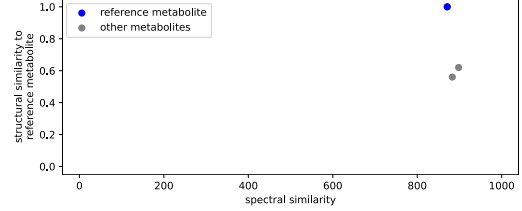


L-Lysine

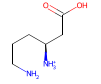
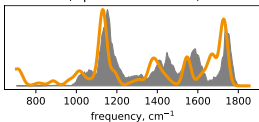
Spectra of protonated HMDB0000182, spectral sim. = 871, #3



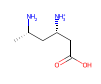
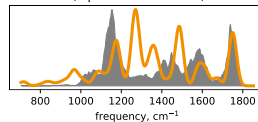
Structural similarity plot of protonated HMDB0000182



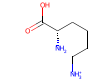
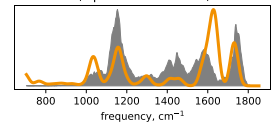
protonated HMDB0012114, spectral sim. = 898, #1

Struc. sim. = 0.62  
(3S)-3,6-Diaminohexanoate

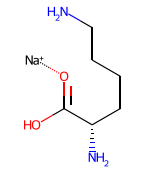
protonated HMDB0012115, spectral sim. = 883, #2

Struc. sim. = 0.56  
(3S,5S)-3,5-Diaminohexanoate

protonated HMDB0000182, spectral sim. = 871, #3

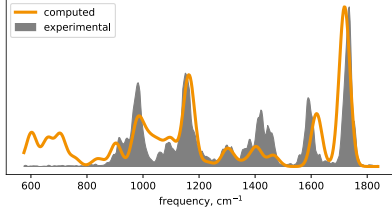
Struc. sim. = 1.00  
L-Lysine

23 sodiated HMDB0000182

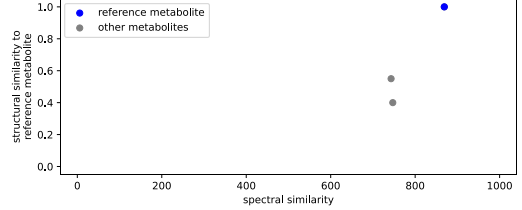


L-Lysine

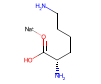
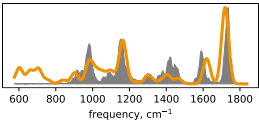
Spectra of sodiated HMDB0000182, spectral sim. = 869, #1



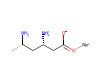
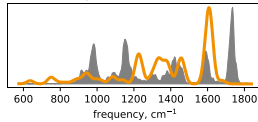
Structural similarity plot of sodiated HMDB0000182



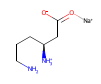
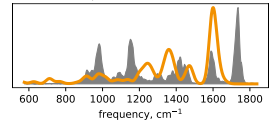
sodiated HMDB0000182, spectral sim. = 869, #1

Struc. sim. = 1.00  
L-Lysine

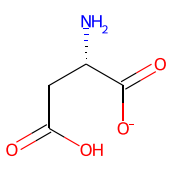
sodiated HMDB0012115, spectral sim. = 747, #2

Struc. sim. = 0.40  
(3S,5S)-3,5-Diaminohexanoate

sodiated HMDB0012114, spectral sim. = 743, #3

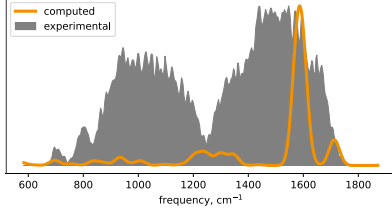
Struc. sim. = 0.55  
(3S)-3,6-Diaminohexanoate

24 deprotonated HMDB0000191

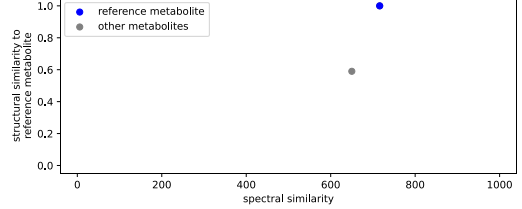


L-Aspartic acid

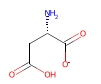
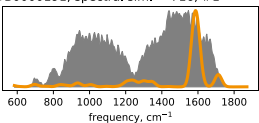
Spectra of deprotonated HMDB0000191, spectral sim. = 716, #1



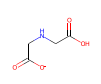
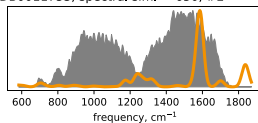
Structural similarity plot of deprotonated HMDB0000191



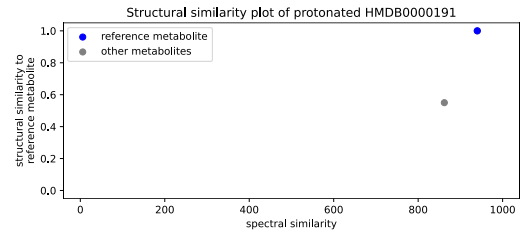
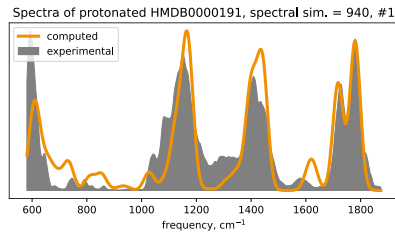
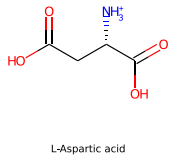
deprotonated HMDB0000191, spectral sim. = 716, #1

Struc. sim. = 1.00  
L-Aspartic acid

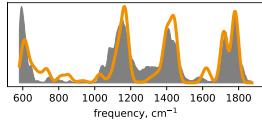
deprotonated HMDB0011753, spectral sim. = 650, #2

Struc. sim. = 0.59  
lminodiacetic acid

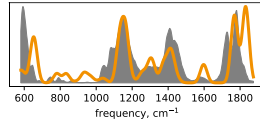
25 protonated HMDB0000191



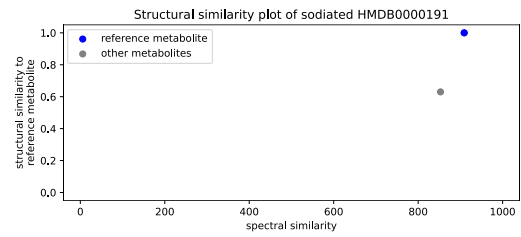
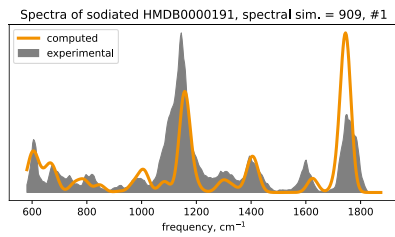
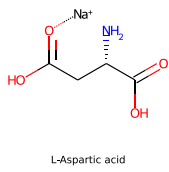
protonated HMDB0000191, spectral sim. = 940, #1



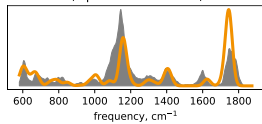
protonated HMDB0011753, spectral sim. = 862, #2



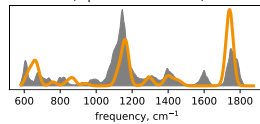
26 sodiated HMDB0000191



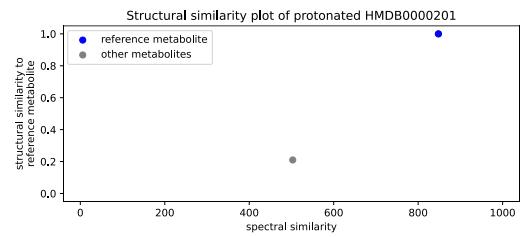
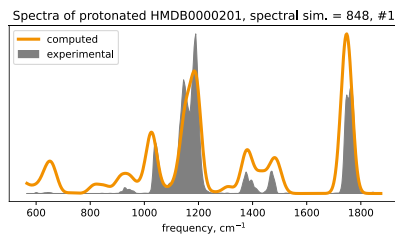
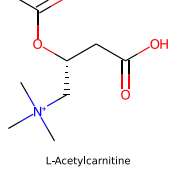
sodiated HMDB0000191, spectral sim. = 909, #1



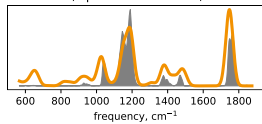
sodiated HMDB0011753, spectral sim. = 853, #2



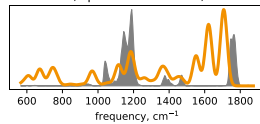
27 protonated HMDB0000201



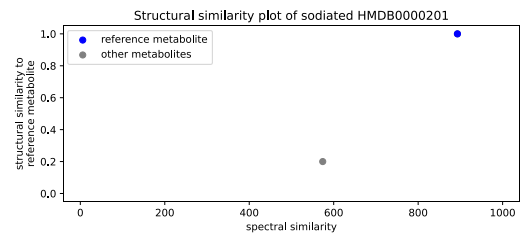
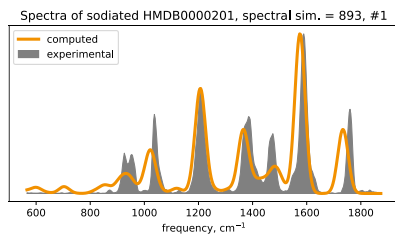
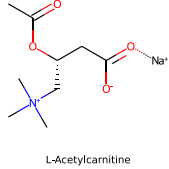
protonated HMDB0000201, spectral sim. = 848, #1



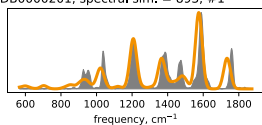
protonated HMDB0062176, spectral sim. = 503, #2



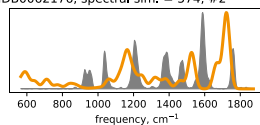
28 sodiated HMDB0000201



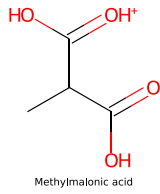
sodiated HMDB0000201, spectral sim. = 893, #1



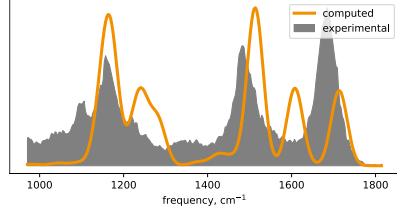
sodiated HMDB0062176, spectral sim. = 574, #2



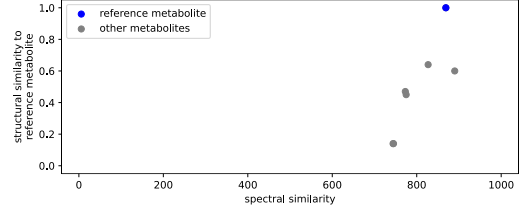
29 protonated HMDB0000202



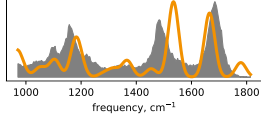
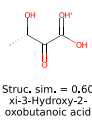
Spectra of protonated HMDB0000202, spectral sim. = 869, #2



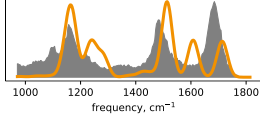
Structural similarity plot of protonated HMDB0000202



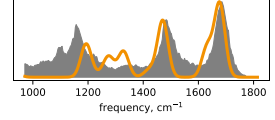
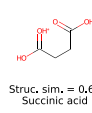
protonated HMDB0039324, spectral sim. = 890, #1



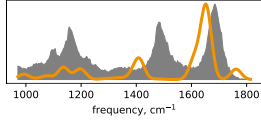
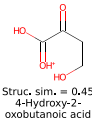
protonated HMDB0000202, spectral sim. = 869, #2



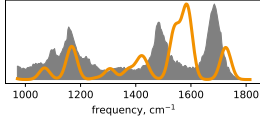
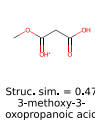
protonated HMDB0000254, spectral sim. = 827, #3



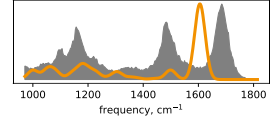
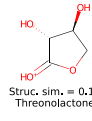
protonated HMDB0031204, spectral sim. = 775, #4



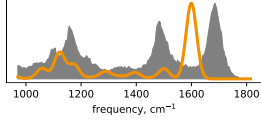
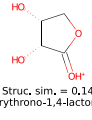
protonated HMDB0130020, spectral sim. = 773, #5



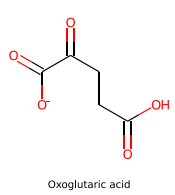
protonated HMDB0000940, spectral sim. = 745, #6



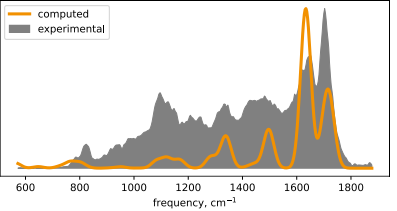
protonated HMDB0000349, spectral sim. = 744, #7



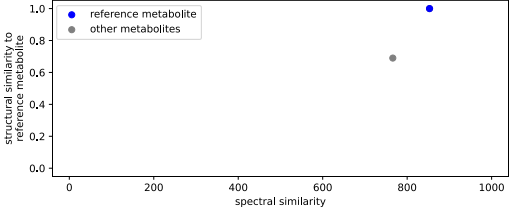
30 deprotonated HMDB0000208



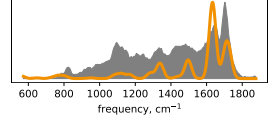
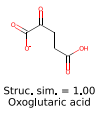
Spectra of deprotonated HMDB0000208, spectral sim. = 853, #1



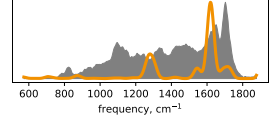
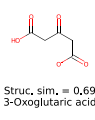
Structural similarity plot of deprotonated HMDB0000208



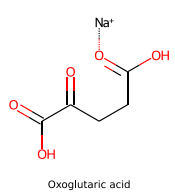
deprotonated HMDB0000208, spectral sim. = 853, #1



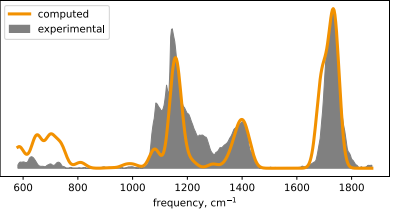
deprotonated HMDB0013701, spectral sim. = 766, #2



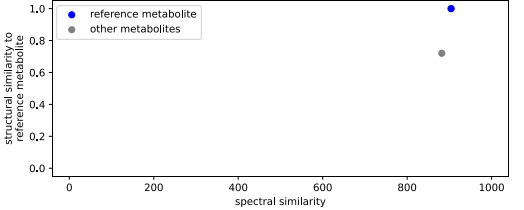
31 sodiated HMDB0000208



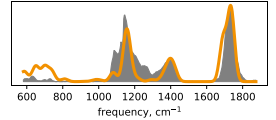
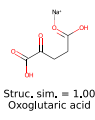
Spectra of sodiated HMDB0000208, spectral sim. = 904, #1



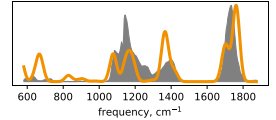
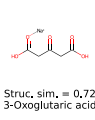
Structural similarity plot of sodiated HMDB0000208



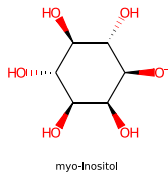
sodiated HMDB0000208, spectral sim. = 904, #1



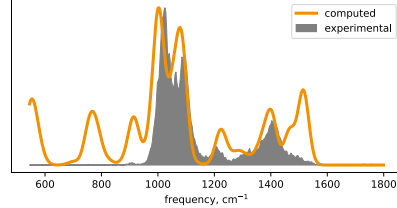
sodiated HMDB0013701, spectral sim. = 882, #2



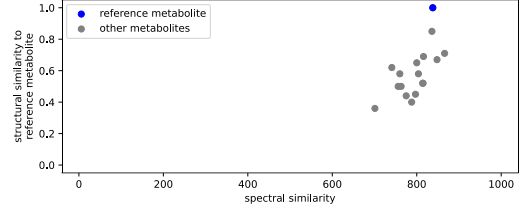
32 deprotonated HMDB0000211



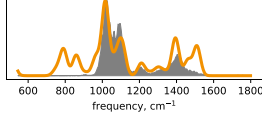
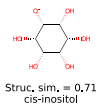
Spectra of deprotonated HMDB0000211, spectral sim. = 838, #3



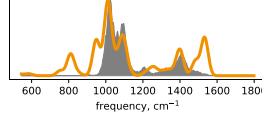
Structural similarity plot of deprotonated HMDB0000211



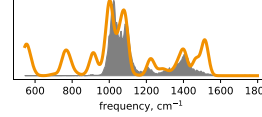
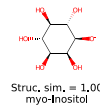
deprotonated HMDB0240210, spectral sim. = 866, #1



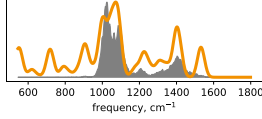
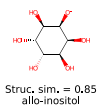
deprotonated HMDB0006088, spectral sim. = 848, #2



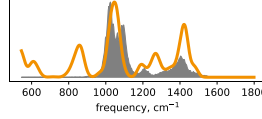
deprotonated HMDB0000211, spectral sim. = 838, #3



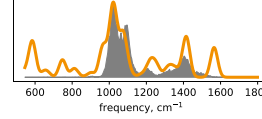
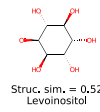
deprotonated HMDB0240211, spectral sim. = 836, #4



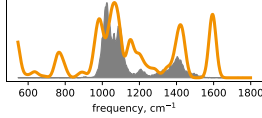
deprotonated HMDB0240208, spectral sim. = 816, #5



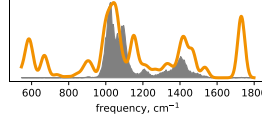
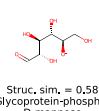
deprotonated HMDB0034220, spectral sim. = 815, #6



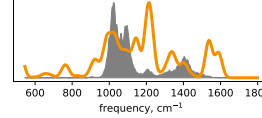
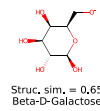
deprotonated HMDB0062138, spectral sim. = 814, #7



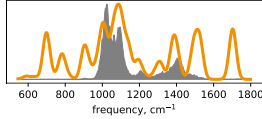
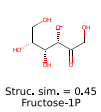
deprotonated HMDB0062473, spectral sim. = 804, #8



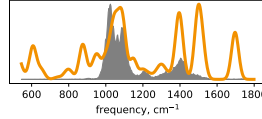
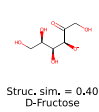
deprotonated HMDB0003449, spectral sim. = 800, #9



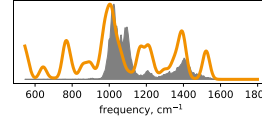
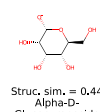
deprotonated HMDB0062538, spectral sim. = 797, #10



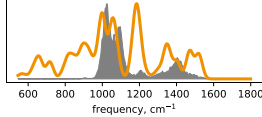
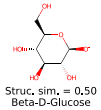
deprotonated HMDB000660, spectral sim. = 788, #11



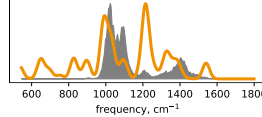
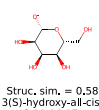
deprotonated HMDB0061922, spectral sim. = 775, #12



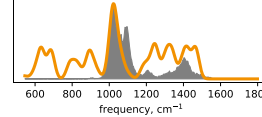
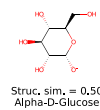
deprotonated HMDB0000516, spectral sim. = 763, #13



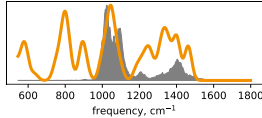
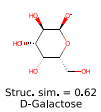
deprotonated HMDB0062202, spectral sim. = 760, #14



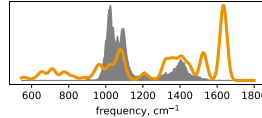
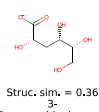
deprotonated HMDB0003345, spectral sim. = 756, #15



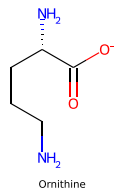
deprotonated HMDB0000143, spectral sim. = 741, #16



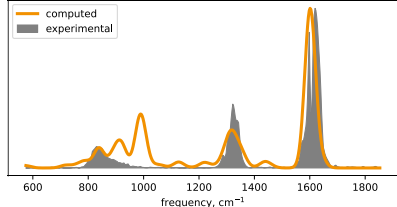
deprotonated HMDB0000346, spectral sim. = 701, #17



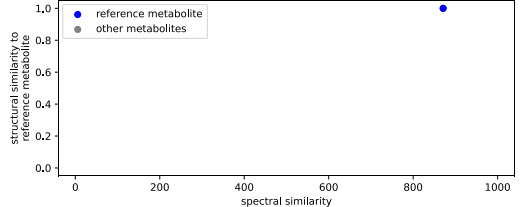
33 deprotonated HMDB0000214



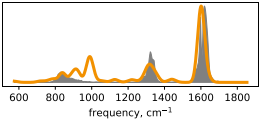
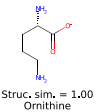
Spectra of deprotonated HMDB0000214, spectral sim. = 871, #1



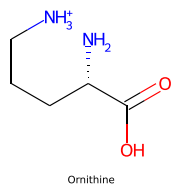
Structural similarity plot of deprotonated HMDB0000214



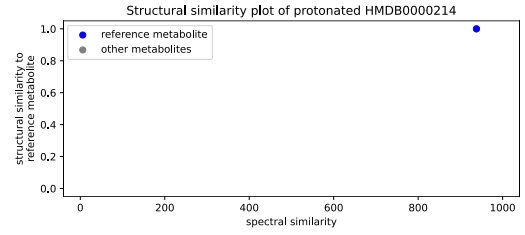
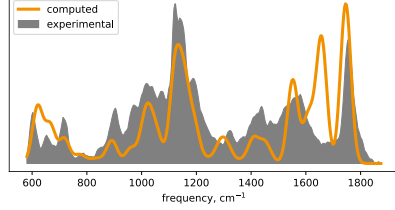
deprotonated HMDB0000214, spectral sim. = 871, #1



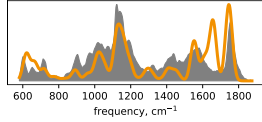
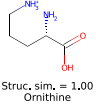
34 protonated HMDB0000214



Spectra of protonated HMDB0000214, spectral sim. = 938, #1

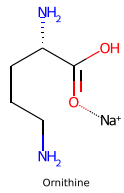


protonated HMDB0000214, spectral sim. = 938, #1

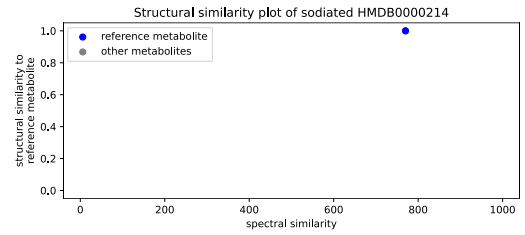
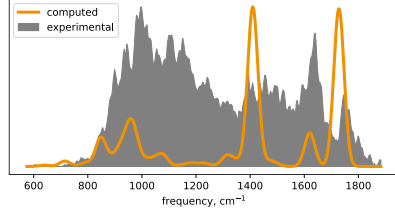


Struc. sim. = 1.00

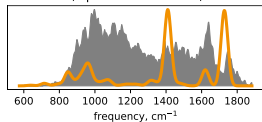
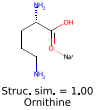
35 sodiated HMDB0000214



Spectra of sodiated HMDB0000214, spectral sim. = 770, #1

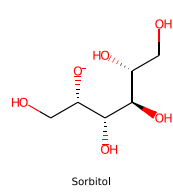


sodiated HMDB0000214, spectral sim. = 770, #1

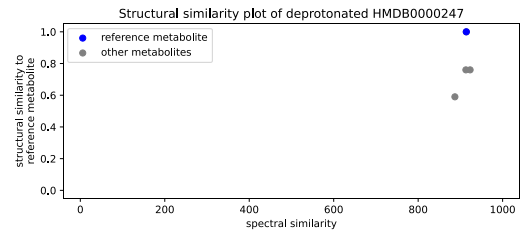
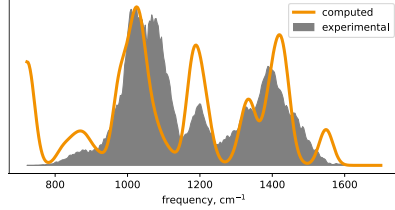


Struc. sim. = 1.00

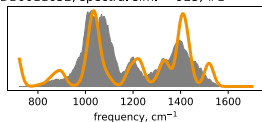
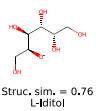
36 deprotonated HMDB0000247



Spectra of deprotonated HMDB0000247, spectral sim. = 914, #2

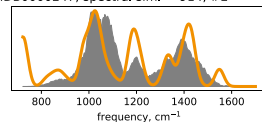
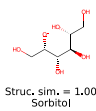


deprotonated HMDB0011632, spectral sim. = 923, #1



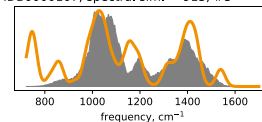
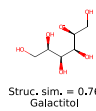
Struc. sim. = 0.76

deprotonated HMDB0000247, spectral sim. = 914, #2



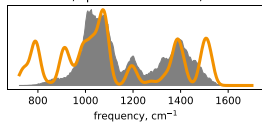
Struc. sim. = 1.00

deprotonated HMDB0000107, spectral sim. = 913, #3



Struc. sim. = 0.76

deprotonated HMDB0000765, spectral sim. = 887, #4

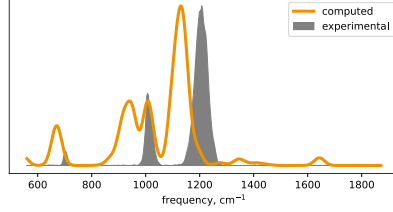


Struc. sim. = 0.59

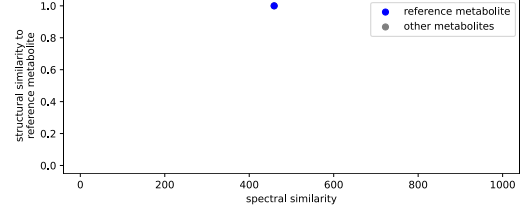
37 deprotonated HMDB0000251



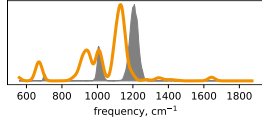
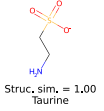
Spectra of deprotonated HMDB0000251, spectral sim. = 459, #1



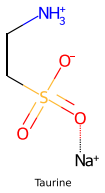
Structural similarity plot of deprotonated HMDB0000251



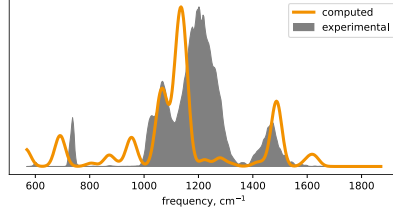
deprotonated HMDB0000251, spectral sim. = 459, #1



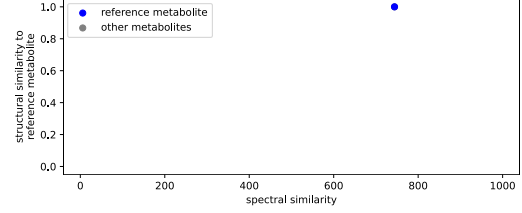
38 sodiated HMDB0000251



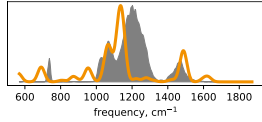
Spectra of sodiated HMDB0000251, spectral sim. = 744, #1



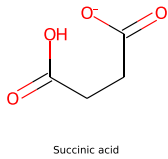
Structural similarity plot of sodiated HMDB0000251



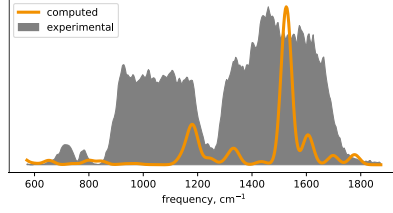
sodiated HMDB0000251, spectral sim. = 744, #1



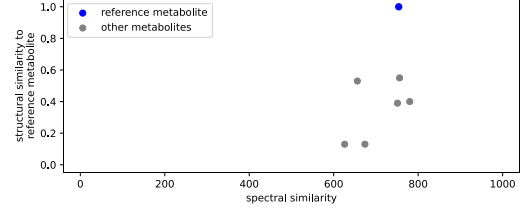
39 deprotonated HMDB0000254



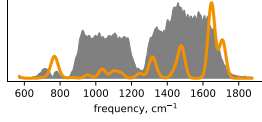
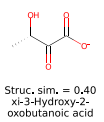
Spectra of deprotonated HMDB0000254, spectral sim. = 754, #3



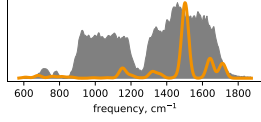
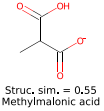
Structural similarity plot of deprotonated HMDB0000254



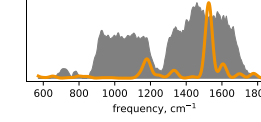
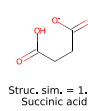
deprotonated HMDB0039324, spectral sim. = 780, #1



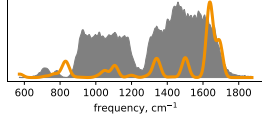
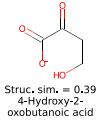
deprotonated HMDB0000202, spectral sim. = 756, #2



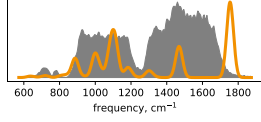
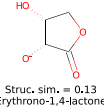
deprotonated HMDB0000254, spectral sim. = 754, #3



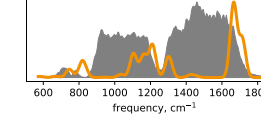
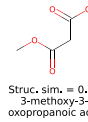
deprotonated HMDB0031204, spectral sim. = 751, #4



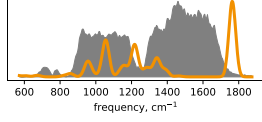
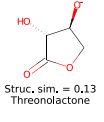
deprotonated HMDB0000349, spectral sim. = 674, #5



deprotonated HMDB0130020, spectral sim. = 656, #6

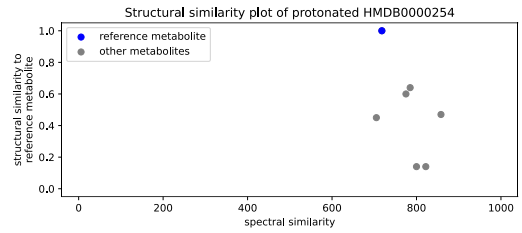
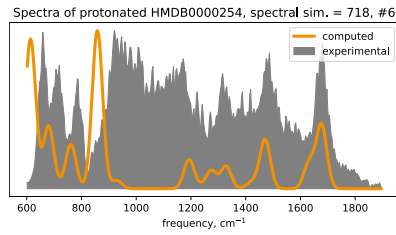
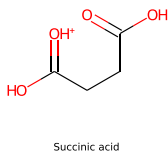


deprotonated HMDB0000940, spectral sim. = 626, #7

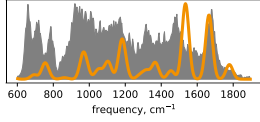
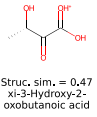




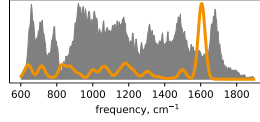
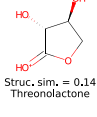
40 protonated HMDB0000254



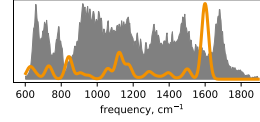
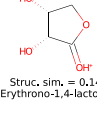
protonated HMDB0039324, spectral sim. = 858, #1



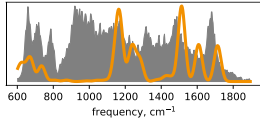
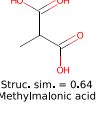
protonated HMDB0000940, spectral sim. = 822, #2



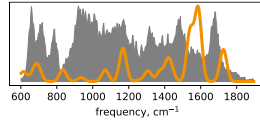
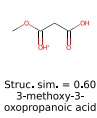
protonated HMDB0000349, spectral sim. = 800, #3



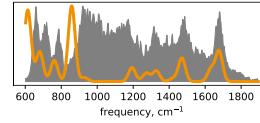
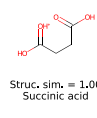
protonated HMDB0000202, spectral sim. = 785, #4



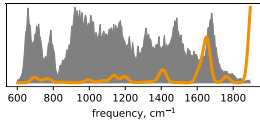
protonated HMDB0130020, spectral sim. = 775, #5



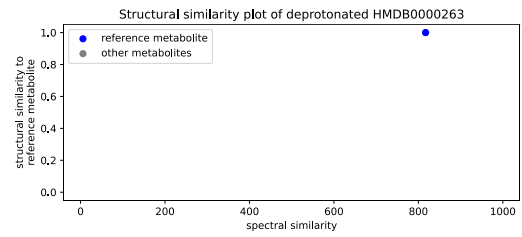
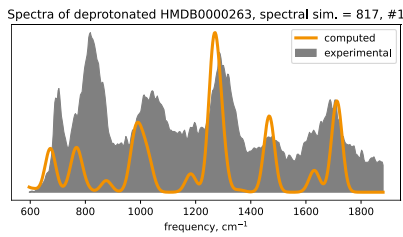
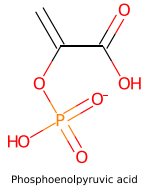
protonated HMDB0000254, spectral sim. = 718, #6



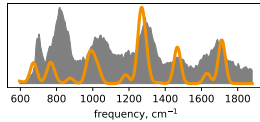
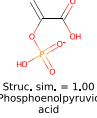
protonated HMDB0031204, spectral sim. = 705, #7



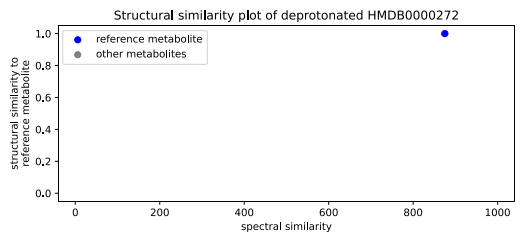
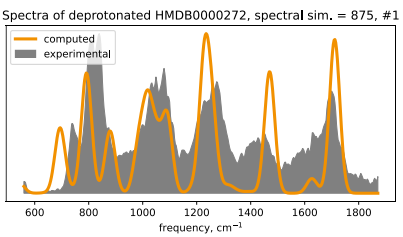
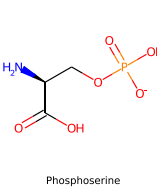
41 deprotonated HMDB0000263



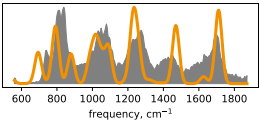
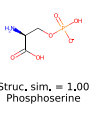
deprotonated HMDB0000263, spectral sim. = 817, #1



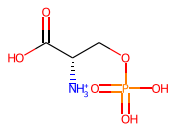
42 deprotonated HMDB0000272



deprotonated HMDB0000272, spectral sim. = 875, #1

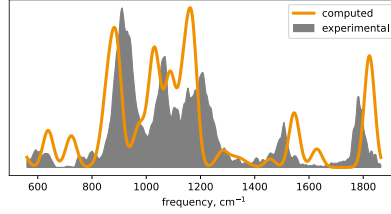


43 protonated HMDB0000272

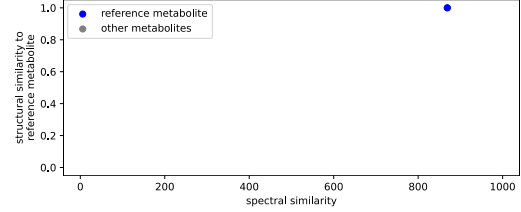


Phosphoserine

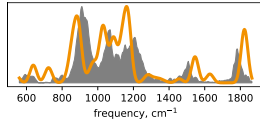
Spectra of protonated HMDB0000272, spectral sim. = 869, #1



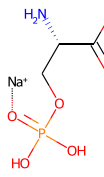
Structural similarity plot of protonated HMDB0000272



protonated HMDB0000272, spectral sim. = 869, #1

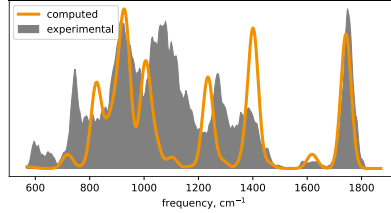
Struc. sim. = 1.00  
Phosphoserine

44 sodiated HMDB0000272

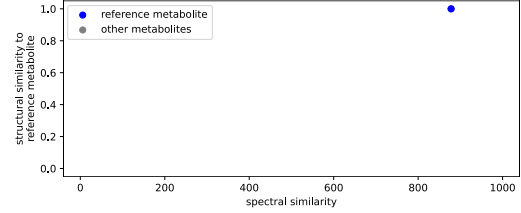


Phosphoserine

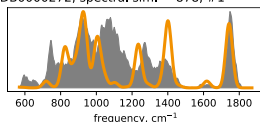
Spectra of sodiated HMDB0000272, spectral sim. = 878, #1



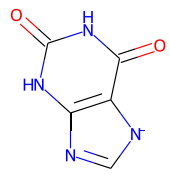
Structural similarity plot of sodiated HMDB0000272



sodiated HMDB0000272, spectral sim. = 878, #1

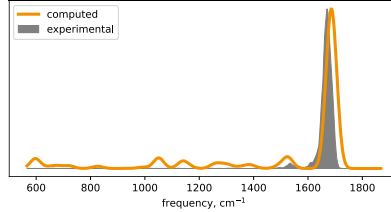
Struc. sim. = 1.00  
Phosphoserine

45 deprotonated HMDB0000292

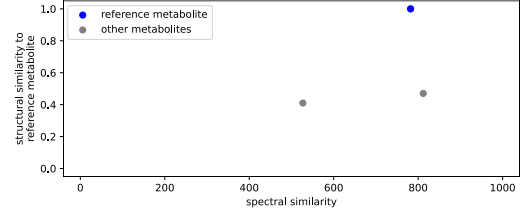


Xanthine

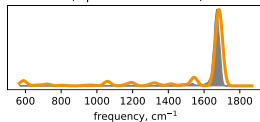
Spectra of deprotonated HMDB0000292, spectral sim. = 782, #2



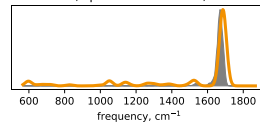
Structural similarity plot of deprotonated HMDB0000292



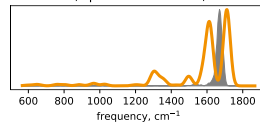
deprotonated HMDB0000786, spectral sim. = 812, #1

Struc. sim. = 0.47  
Oxypurinol

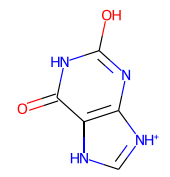
deprotonated HMDB0000292, spectral sim. = 782, #2

Struc. sim. = 1.00  
Xanthine

deprotonated HMDB0001182, spectral sim. = 527, #3

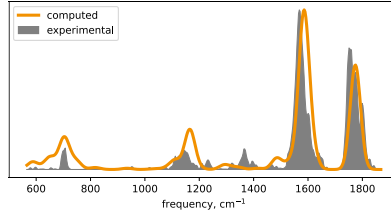
Struc. sim. = 0.41  
6,8-Dihydroxypurine

46 protonated HMDB0000292

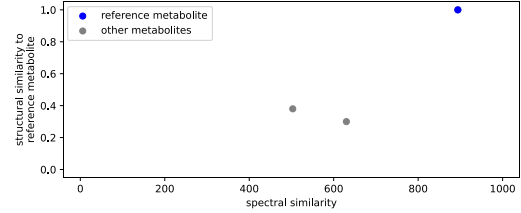


Xanthine

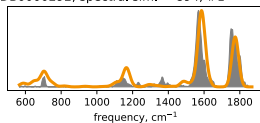
Spectra of protonated HMDB0000292, spectral sim. = 894, #1



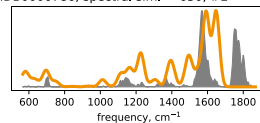
Structural similarity plot of protonated HMDB0000292



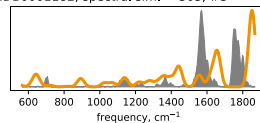
protonated HMDB0000292, spectral sim. = 894, #1

Struc. sim. = 1.00  
Xanthine

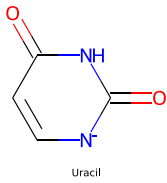
protonated HMDB0000786, spectral sim. = 630, #2

Struc. sim. = 0.30  
Oxypurinol

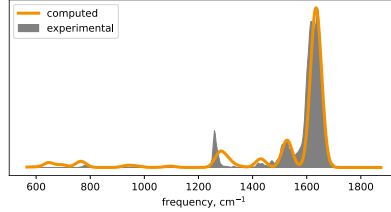
protonated HMDB0001182, spectral sim. = 503, #3

Struc. sim. = 0.38  
6,8-Dihydroxypurine

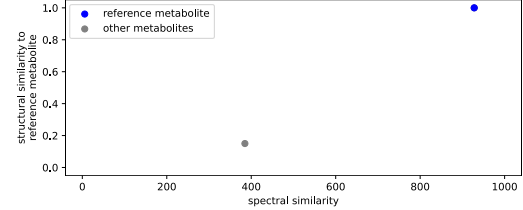
47 deprotonated HMDB0000300



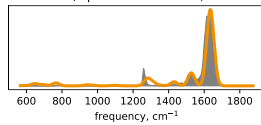
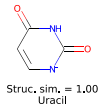
Spectra of deprotonated HMDB0000300, spectral sim. = 928, #1



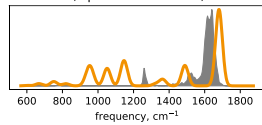
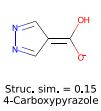
Structural similarity plot of deprotonated HMDB0000300



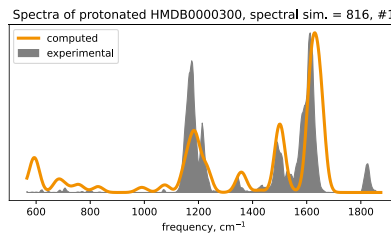
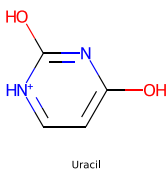
deprotonated HMDB0000300, spectral sim. = 928, #1



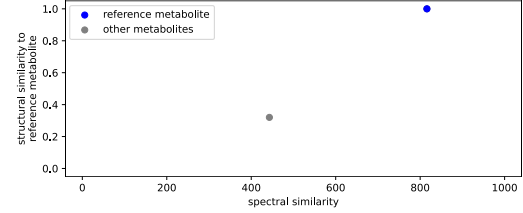
deprotonated HMDB0060760, spectral sim. = 385, #2



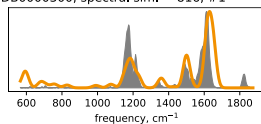
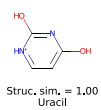
48 protonated HMDB0000300



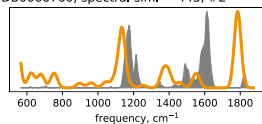
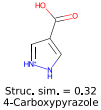
Structural similarity plot of protonated HMDB0000300



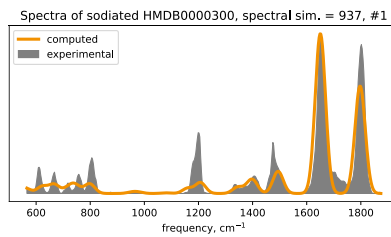
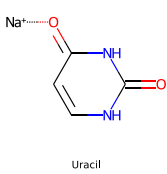
protonated HMDB0000300, spectral sim. = 816, #1



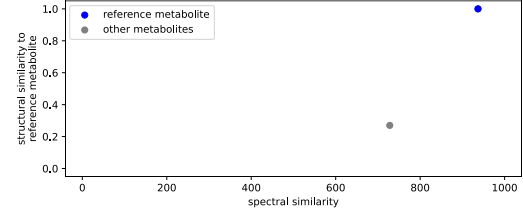
protonated HMDB0060760, spectral sim. = 443, #2



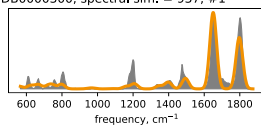
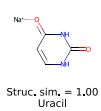
49 sodiated HMDB0000300



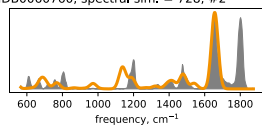
Structural similarity plot of sodiated HMDB0000300



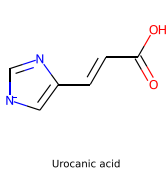
sodiated HMDB0000300, spectral sim. = 937, #1



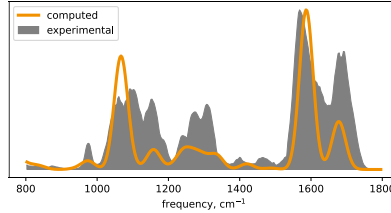
sodiated HMDB0060760, spectral sim. = 728, #2



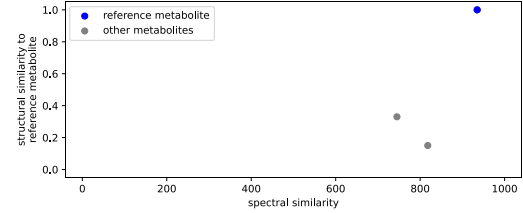
50 deprotonated HMDB0000301



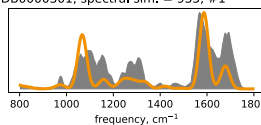
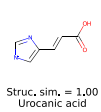
Spectra of deprotonated HMDB0000301, spectral sim. = 935, #1



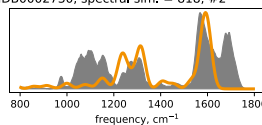
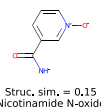
Structural similarity plot of deprotonated HMDB0000301



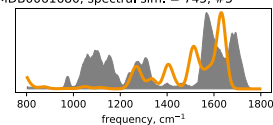
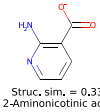
deprotonated HMDB0000301, spectral sim. = 935, #1



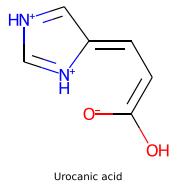
deprotonated HMDB0002730, spectral sim. = 818, #2



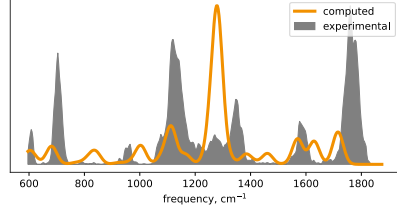
deprotonated HMDB0061680, spectral sim. = 745, #3



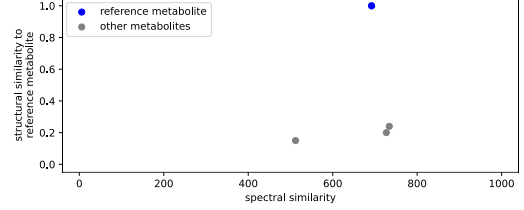
51 protonated HMDB0000301



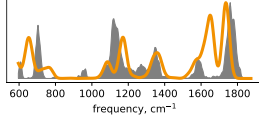
Spectra of protonated HMDB0000301, spectral sim. = 692, #3



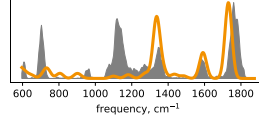
Structural similarity plot of protonated HMDB0000301



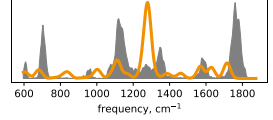
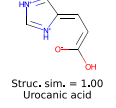
protonated HMDB0061680, spectral sim. = 734, #1



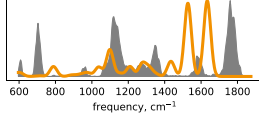
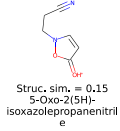
protonated HMDB0002730, spectral sim. = 727, #2



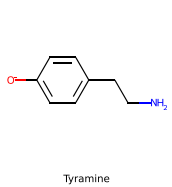
protonated HMDB0000301, spectral sim. = 692, #3



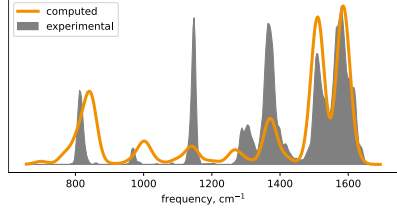
protonated HMDB0031338, spectral sim. = 512, #4



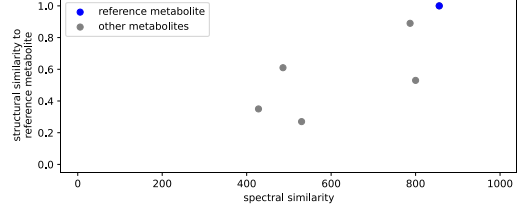
52 deprotonated HMDB0000306



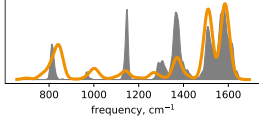
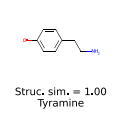
Spectra of deprotonated HMDB0000306, spectral sim. = 856, #1



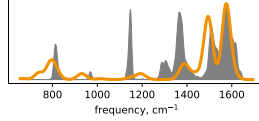
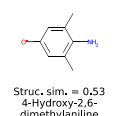
Structural similarity plot of deprotonated HMDB0000306



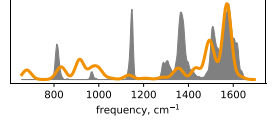
deprotonated HMDB0000306, spectral sim. = 856, #1



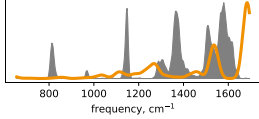
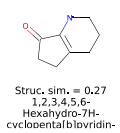
deprotonated HMDB0060681, spectral sim. = 800, #2



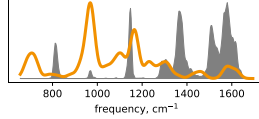
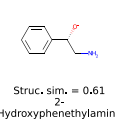
deprotonated HMDB0004989, spectral sim. = 787, #3



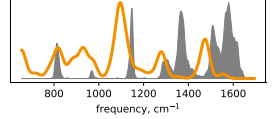
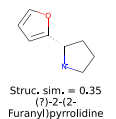
deprotonated HMDB0039657, spectral sim. = 530, #4



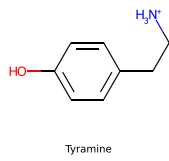
deprotonated HMDB0001065, spectral sim. = 486, #5



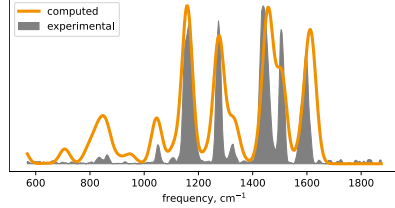
deprotonated HMDB0040059, spectral sim. = 428, #6



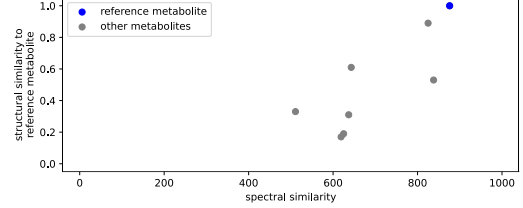
53 protonated HMDB0000306



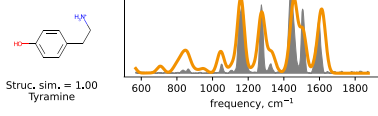
Spectra of protonated HMDB0000306, spectral sim. = 876, #1



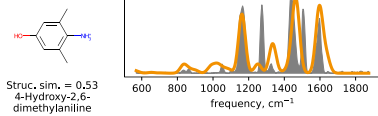
Structural similarity plot of protonated HMDB0000306



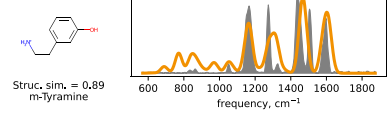
protonated HMDB0000306, spectral sim. = 876, #1



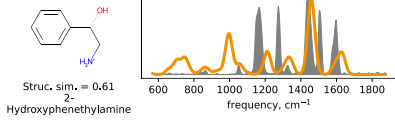
protonated HMDB0060681, spectral sim. = 838, #2



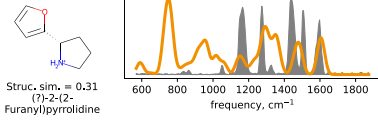
protonated HMDB0004989, spectral sim. = 825, #3



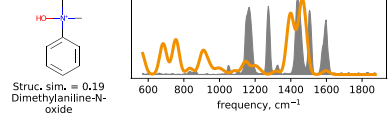
protonated HMDB0001065, spectral sim. = 643, #4



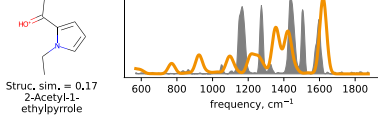
protonated HMDB0040059, spectral sim. = 637, #5



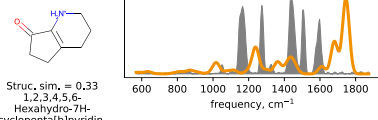
protonated HMDB0001466, spectral sim. = 625, #6



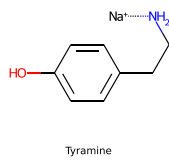
protonated HMDB0029759, spectral sim. = 619, #7



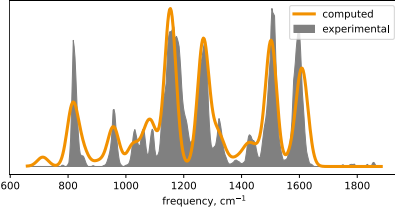
protonated HMDB0039657, spectral sim. = 511, #8



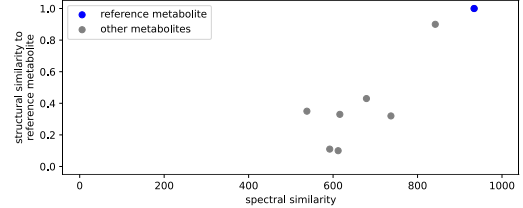
54 sodiated HMDB0000306



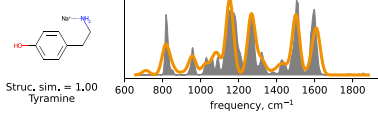
Spectra of sodiated HMDB0000306, spectral sim. = 934, #1



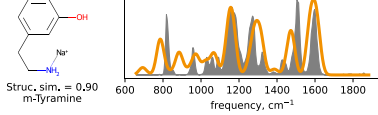
Structural similarity plot of sodiated HMDB0000306



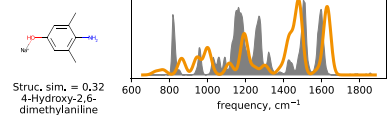
sodiated HMDB0000306, spectral sim. = 934, #1



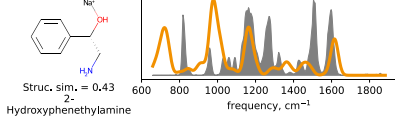
sodiated HMDB0004989, spectral sim. = 842, #2



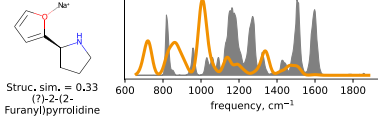
sodiated HMDB0060681, spectral sim. = 737, #3



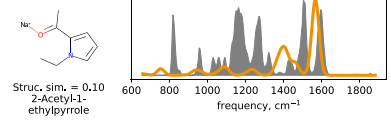
sodiated HMDB0001065, spectral sim. = 679, #4



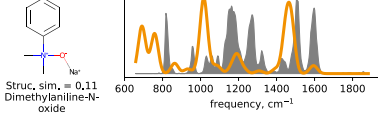
sodiated HMDB0040059, spectral sim. = 616, #5



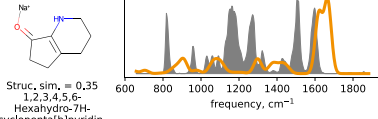
sodiated HMDB0029759, spectral sim. = 612, #6



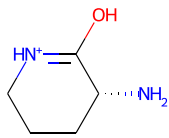
sodiated HMDB0001466, spectral sim. = 592, #7



sodiated HMDB0039657, spectral sim. = 538, #8

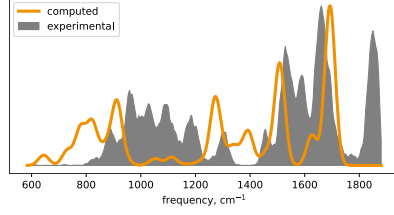


55 protonated HMDB0000323

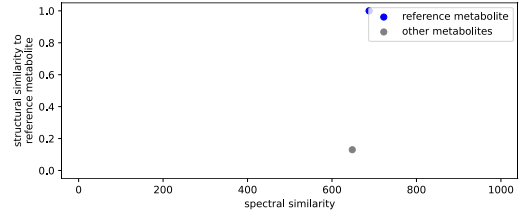


3-Amino-2-piperidone

Spectra of protonated HMDB0000323, spectral sim. = 688, #1



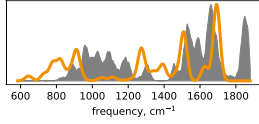
Structural similarity plot of protonated HMDB0000323



protonated HMDB0000323, spectral sim. = 688, #1



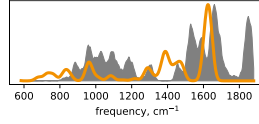
Struc. sim. = 1.00  
3-Amino-2-piperidone



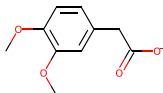
protonated HMDB0061162, spectral sim. = 648, #2



Struc. sim. = 0.13  
Mononitrosopiperazine

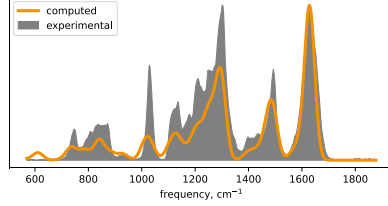


56 deprotonated HMDB0000434

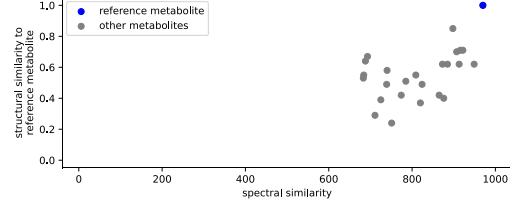


Homoveratric acid

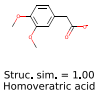
Spectra of deprotonated HMDB0000434, spectral sim. = 970, #1



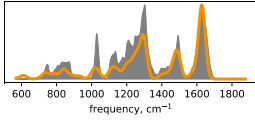
Structural similarity plot of deprotonated HMDB0000434



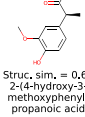
deprotonated HMDB0000434, spectral sim. = 970, #1



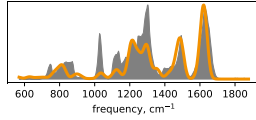
Struc. sim. = 1.00  
Homoveratric acid



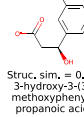
deprotonated HMDB0130895, spectral sim. = 949, #2



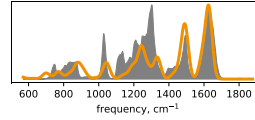
Struc. sim. = 0.62  
2-(4-hydroxy-3-methoxyphenyl) propanoic acid



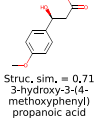
deprotonated HMDB0133490, spectral sim. = 922, #3



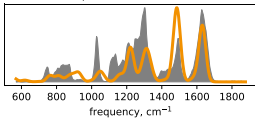
Struc. sim. = 0.71  
3-hydroxy-3-(3-methoxyphenyl) propanoic acid



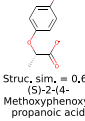
deprotonated HMDB0140293, spectral sim. = 916, #4



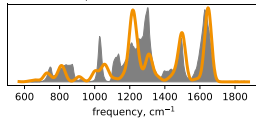
Struc. sim. = 0.71  
3-hydroxy-3-(4-methoxyphenyl) propanoic acid



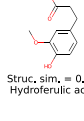
deprotonated HMDB0040256, spectral sim. = 913, #5



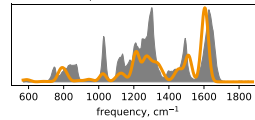
Struc. sim. = 0.62  
(S)-2-(4-Methoxyphenoxy) propanoic acid



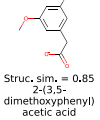
deprotonated HMDB0062121, spectral sim. = 907, #6



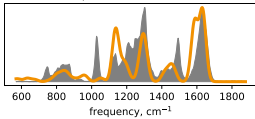
Struc. sim. = 0.70  
Hydroferulic acid



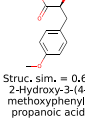
deprotonated HMDB0131427, spectral sim. = 898, #7



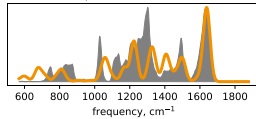
Struc. sim. = 0.85  
2-(3,5-dimethoxyphenyl) acetic acid



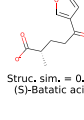
deprotonated HMDB0039427, spectral sim. = 885, #8



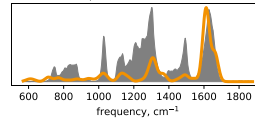
Struc. sim. = 0.62  
2-Hydroxy-3-(4-methoxyphenyl) propanoic acid



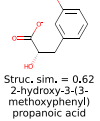
deprotonated HMDB0035721, spectral sim. = 876, #9



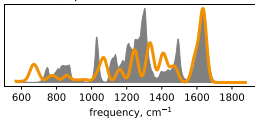
Struc. sim. = 0.40  
(S)-Baticic acid



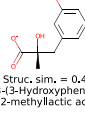
deprotonated HMDB0133530, spectral sim. = 873, #10



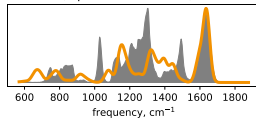
Struc. sim. = 0.62  
2-hydroxy-3-(3-methoxyphenyl) propanoic acid



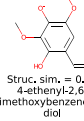
deprotonated HMDB0060733, spectral sim. = 865, #11



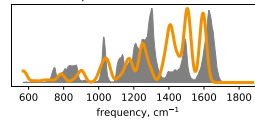
Struc. sim. = 0.42  
3-(3-Hydroxyphenyl)-2-methylactic acid



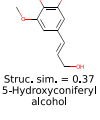
deprotonated HMDB0135753, spectral sim. = 824, #12



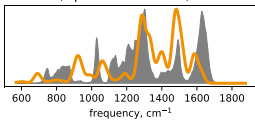
Struc. sim. = 0.49  
4-ethyl-2,6-dimethoxybenzene-1,3-diol



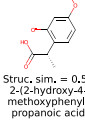
deprotonated HMDB0060398, spectral sim. = 820, #13



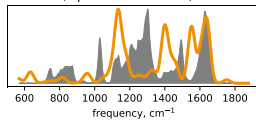
Struc. sim. = 0.37  
5-Hydroxyconiferyl alcohol



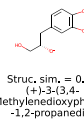
deprotonated HMDB0133782, spectral sim. = 809, #14



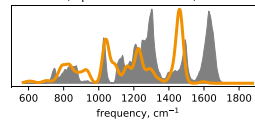
Struc. sim. = 0.55  
2-(2-hydroxy-4-methoxyphenyl) propanoic acid



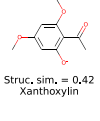
deprotonated HMDB0030571, spectral sim. = 785, #15



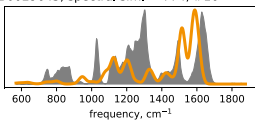
Struc. sim. = 0.51  
(+)-3-(3,4-Methylenedioxyphenyl)-1,2-propanediol



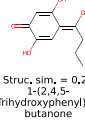
deprotonated HMDB0029645, spectral sim. = 774, #16



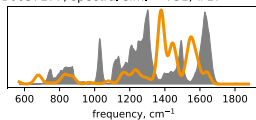
Struc. sim. = 0.42  
Xanthoxilin



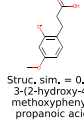
deprotonated HMDB0037177, spectral sim. = 751, #17



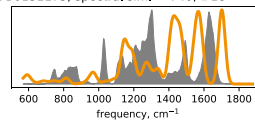
Struc. sim. = 0.24  
1-(2,4,5-Trihydroxyphenyl)-1-butanone



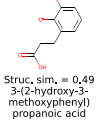
deprotonated HMDB0131175, spectral sim. = 740, #18



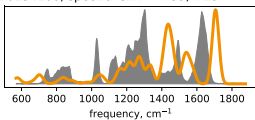
Struc. sim. = 0.58  
3-(2-hydroxy-4-methoxyphenyl) propanoic acid



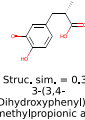
deprotonated HMDB0134100, spectral sim. = 739, #19



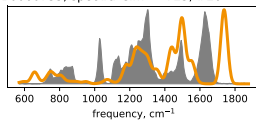
Struc. sim. = 0.49  
3-(2-hydroxy-3-methoxyphenyl) propanoic acid



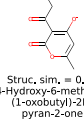
deprotonated HMDB0060735, spectral sim. = 725, #20



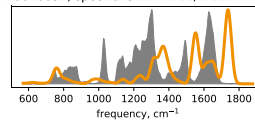
Struc. sim. = 0.39  
3-(3,4-Dihydroxyphenyl)-2-methylpropionic acid



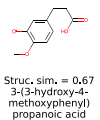
deprotonated HMDB0040637, spectral sim. = 711, #21



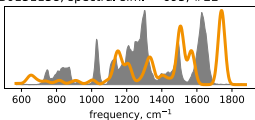
Struc. sim. = 0.29  
4-Hydroxy-6-methyl-3-(1-oxobutyl)-2H-pyran-2-one



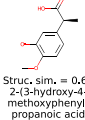
deprotonated HMDB0131138, spectral sim. = 693, #22



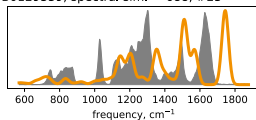
Struc. sim. = 0.67  
3-(3-hydroxy-4-methoxyphenyl) propanoic acid



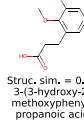
deprotonated HMDB0129339, spectral sim. = 688, #23



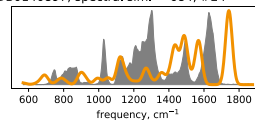
Struc. sim. = 0.64  
2-(3-hydroxy-4-methoxyphenyl) propanoic acid



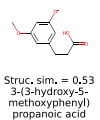
deprotonated HMDB0140897, spectral sim. = 684, #24



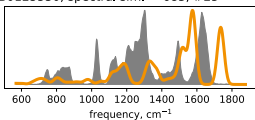
Struc. sim. = 0.55  
3-(3-hydroxy-2-methoxyphenyl) propanoic acid



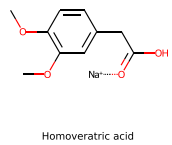
deprotonated HMDB0125530, spectral sim. = 683, #25



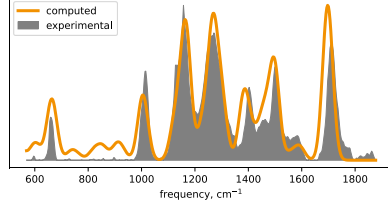
Struc. sim. = 0.53  
3-(3-hydroxy-5-methoxyphenyl) propanoic acid



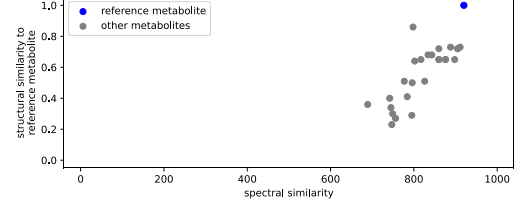
57 sodiated HMDB0000434



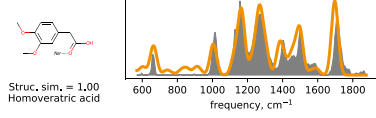
Spectra of sodiated HMDB0000434, spectral sim. = 920, #1



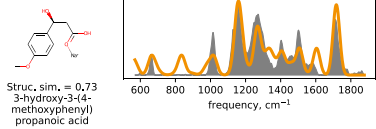
Structural similarity plot of sodiated HMDB0000434



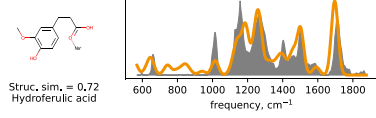
sodiated HMDB0000434, spectral sim. = 920, #1



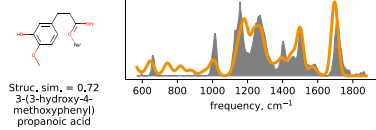
sodiated HMDB0140293, spectral sim. = 911, #2



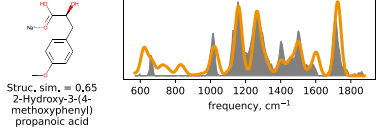
sodiated HMDB0062121, spectral sim. = 905, #3



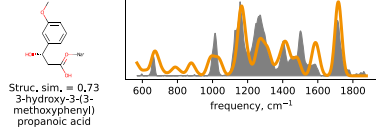
sodiated HMDB0131138, spectral sim. = 905, #4



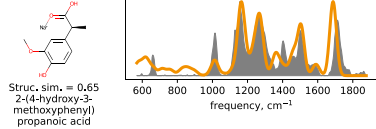
sodiated HMDB0039427, spectral sim. = 898, #5



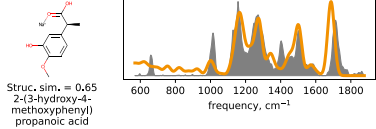
sodiated HMDB0133490, spectral sim. = 888, #6



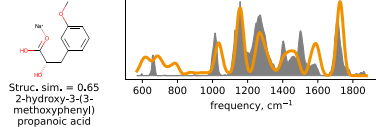
sodiated HMDB0130895, spectral sim. = 876, #7



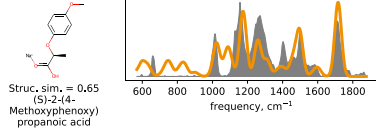
sodiated HMDB0129339, spectral sim. = 876, #8



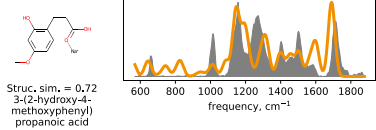
sodiated HMDB0133530, spectral sim. = 860, #9



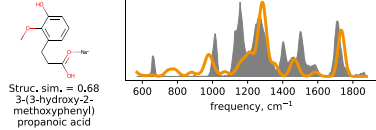
sodiated HMDB0040256, spectral sim. = 860, #10



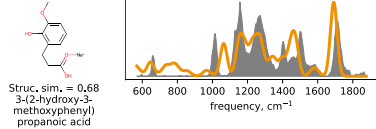
sodiated HMDB0131175, spectral sim. = 860, #11



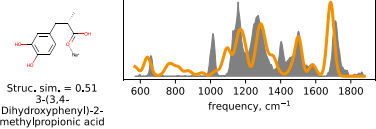
sodiated HMDB0140897, spectral sim. = 843, #12



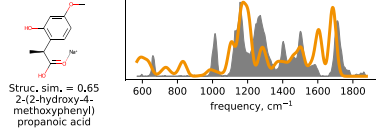
sodiated HMDB0134100, spectral sim. = 834, #13



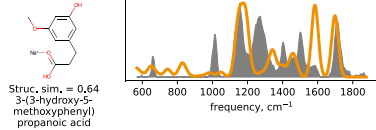
sodiated HMDB0060735, spectral sim. = 826, #14



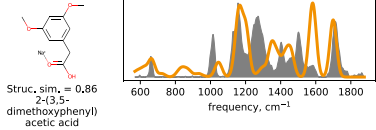
sodiated HMDB0133782, spectral sim. = 817, #15



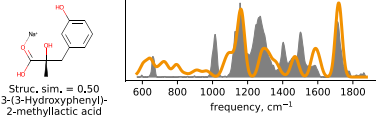
sodiated HMDB0125530, spectral sim. = 802, #16



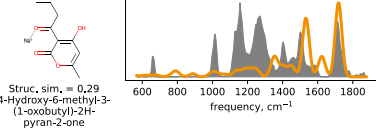
sodiated HMDB0131427, spectral sim. = 798, #17



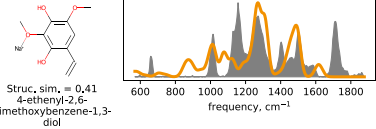
sodiated HMDB0060733, spectral sim. = 796, #18



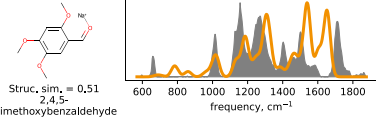
sodiated HMDB0040637, spectral sim. = 795, #19



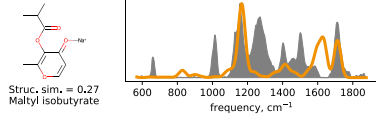
sodiated HMDB0135753, spectral sim. = 784, #20



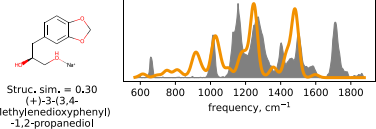
sodiated HMDB0029648, spectral sim. = 777, #21



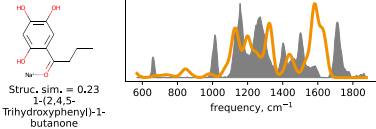
sodiated HMDB0032365, spectral sim. = 756, #22



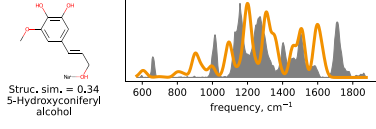
sodiated HMDB0030571, spectral sim. = 749, #23



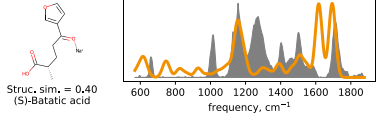
sodiated HMDB0037177, spectral sim. = 747, #24



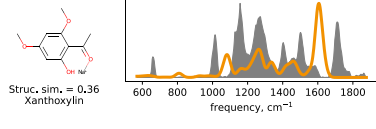
sodiated HMDB0060398, spectral sim. = 745, #25



sodiated HMDB0035721, spectral sim. = 742, #26

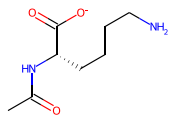


sodiated HMDB0029645, spectral sim. = 689, #27



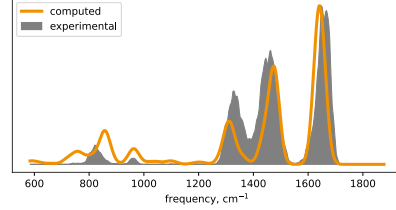


58 deprotonated HMDB0000446

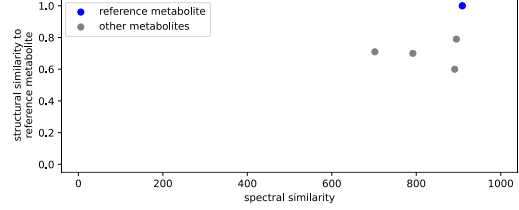


N-Alpha-acetylylsine

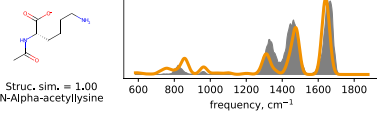
Spectra of deprotonated HMDB0000446, spectral sim. = 909, #1



Structural similarity plot of deprotonated HMDB0000446

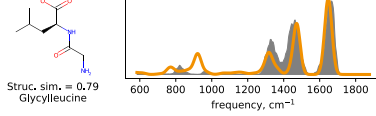


deprotonated HMDB0000446, spectral sim. = 909, #1



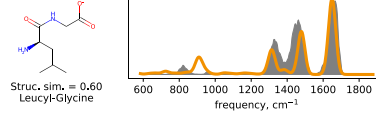
Struc. sim. = 1.00  
N-Alpha-acetylylsine

deprotonated HMDB0000759, spectral sim. = 895, #2



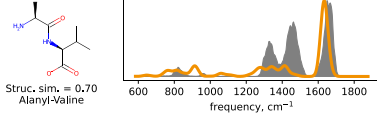
Struc. sim. = 0.79  
Glycylleucine

deprotonated HMDB0028929, spectral sim. = 891, #3



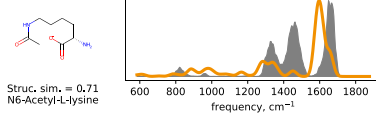
Struc. sim. = 0.60  
Leucyl-Glycine

deprotonated HMDB0028700, spectral sim. = 792, #4



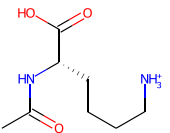
Struc. sim. = 0.70  
Alanyl-Valine

deprotonated HMDB0000206, spectral sim. = 702, #5



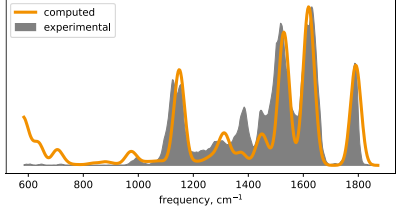
Struc. sim. = 0.71  
N6-Acetyl-L-lysine

59 protonated HMDB0000446

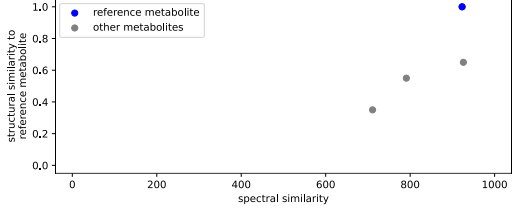


N-Alpha-acetylylsine

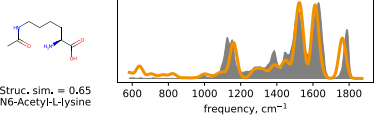
Spectra of protonated HMDB0000446, spectral sim. = 923, #2



Structural similarity plot of protonated HMDB0000446

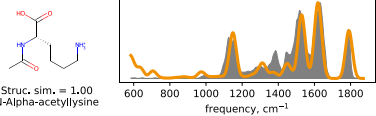


protonated HMDB0000206, spectral sim. = 926, #1



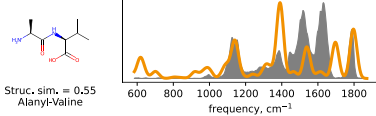
Struc. sim. = 0.65  
N6-Acetyl-L-lysine

protonated HMDB0000446, spectral sim. = 923, #2



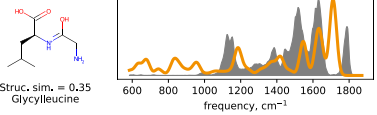
Struc. sim. = 1.00  
N-Alpha-acetylylsine

protonated HMDB0028700, spectral sim. = 791, #3



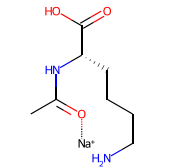
Struc. sim. = 0.55  
Alanyl-Valine

protonated HMDB0000759, spectral sim. = 711, #4



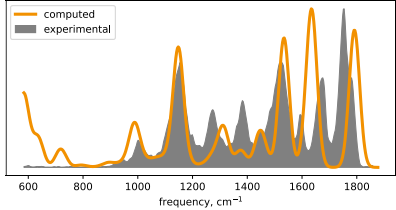
Struc. sim. = 0.35  
Glycylleucine

60 sodiated HMDB0000446

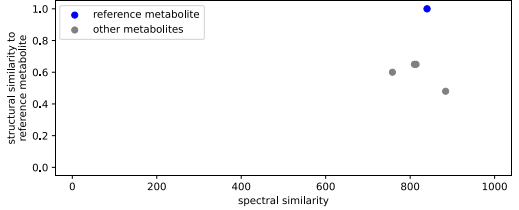


N-Alpha-acetylylsine

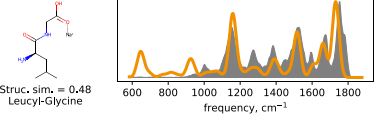
Spectra of sodiated HMDB0000446, spectral sim. = 840, #2



Structural similarity plot of sodiated HMDB0000446

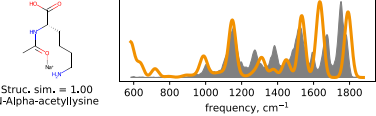


sodiated HMDB0028929, spectral sim. = 884, #1



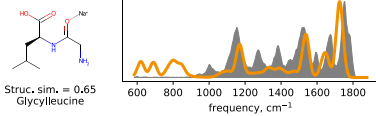
Struc. sim. = 0.48  
Leucyl-Glycine

sodiated HMDB0000446, spectral sim. = 840, #2



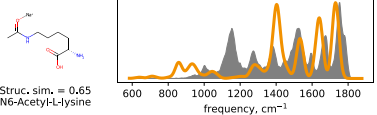
Struc. sim. = 1.00  
N-Alpha-acetylylsine

sodiated HMDB0000759, spectral sim. = 814, #3



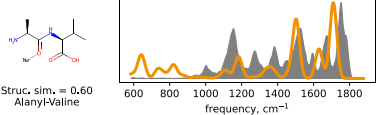
Struc. sim. = 0.65  
Glycylleucine

sodiated HMDB0000206, spectral sim. = 810, #4



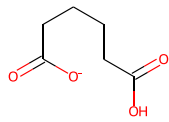
Struc. sim. = 0.65  
N6-Acetyl-L-lysine

sodiated HMDB0028700, spectral sim. = 758, #5



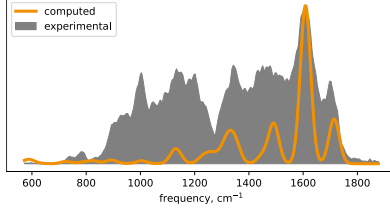
Struc. sim. = 0.60  
Alanyl-Valine

61 deprotonated HMDB0000448

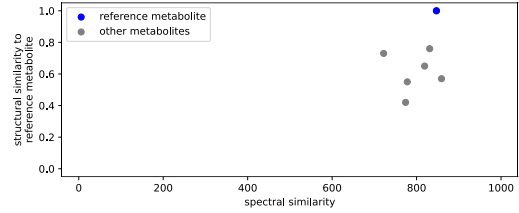


Adipic acid

Spectra of deprotonated HMDB0000448, spectral sim. = 847, #2



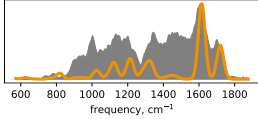
Structural similarity plot of deprotonated HMDB0000448



deprotonated HMDB0061930, spectral sim. = 859, #1



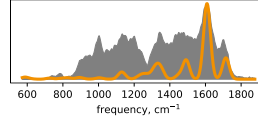
Struc. sim. = 0.57  
4-Ethoxy-4-oxobutanoic acid



deprotonated HMDB0000448, spectral sim. = 847, #2



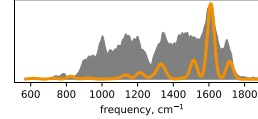
Struc. sim. = 1.00  
Adipic acid



deprotonated HMDB0000422, spectral sim. = 831, #3



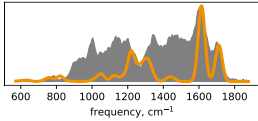
Struc. sim. = 0.76  
2-Methylglutaric acid



deprotonated HMDB0000858, spectral sim. = 819, #4



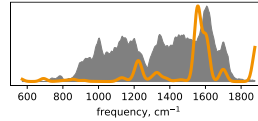
Struc. sim. = 0.65  
Monomethyl glutaric acid



deprotonated HMDB0002074, spectral sim. = 778, #5



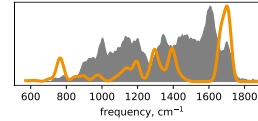
Struc. sim. = 0.55  
2,2-Dimethylsuccinic acid



deprotonated HMDB0006900, spectral sim. = 774, #6



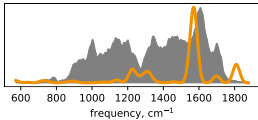
Struc. sim. = 0.42  
(S)-2-Aceto-2-hydroxybutanoic acid



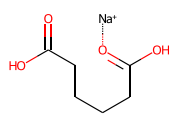
deprotonated HMDB0000752, spectral sim. = 722, #7



Struc. sim. = 0.73  
Methylglutaric acid

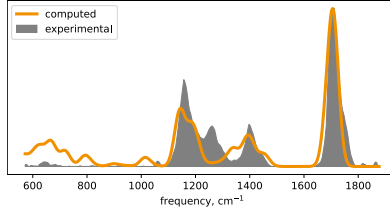


62 sodiated HMDB0000448

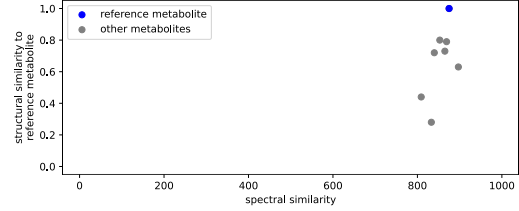


Adipic acid

Spectra of sodiated HMDB0000448, spectral sim. = 875, #2



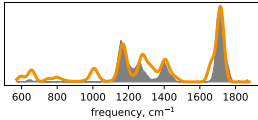
Structural similarity plot of sodiated HMDB0000448



sodiated HMDB0061930, spectral sim. = 897, #1



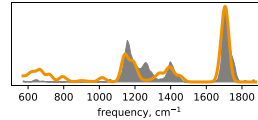
Struc. sim. = 0.63  
4-Ethoxy-4-oxobutanoic acid



sodiated HMDB0000448, spectral sim. = 875, #2



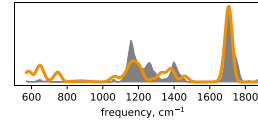
Struc. sim. = 1.00  
Adipic acid



sodiated HMDB0000752, spectral sim. = 869, #3



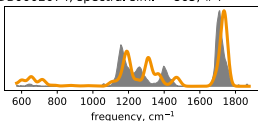
Struc. sim. = 0.79  
Methylglutaric acid



sodiated HMDB0002074, spectral sim. = 865, #4



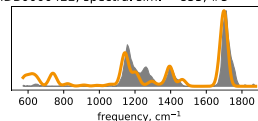
Struc. sim. = 0.73  
2,2-Dimethylsuccinic acid



sodiated HMDB0000422, spectral sim. = 853, #5



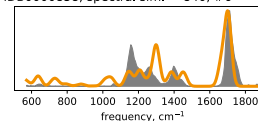
Struc. sim. = 0.80  
2-Methylglutaric acid



sodiated HMDB0000858, spectral sim. = 840, #6



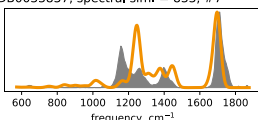
Struc. sim. = 0.72  
Monomethyl glutaric acid



sodiated HMDB0033837, spectral sim. = 833, #7



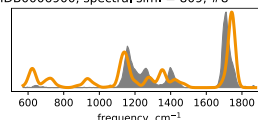
Struc. sim. = 0.28  
Dimethyl succinate



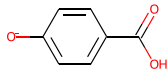
sodiated HMDB0006900, spectral sim. = 809, #8



Struc. sim. = 0.44  
(S)-2-Aceto-2-hydroxybutanoic acid

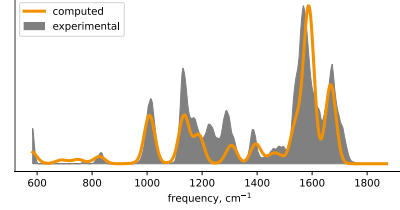


63 deprotonated HMDB0000500

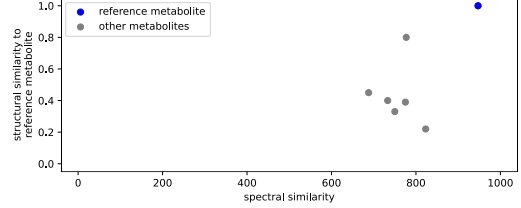


4-Hydroxybenzoic acid

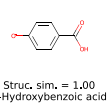
Spectra of deprotonated HMDB0000500, spectral sim. = 947, #1



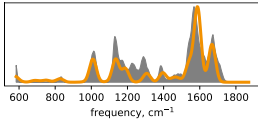
Structural similarity plot of deprotonated HMDB0000500



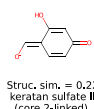
deprotonated HMDB0000500, spectral sim. = 947, #1



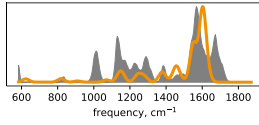
Struc. sim. = 1.00  
4-Hydroxybenzoic acid



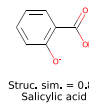
deprotonated HMDB0062484, spectral sim. = 823, #2



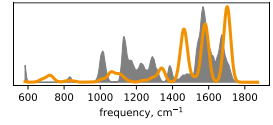
Struc. sim. = 0.22  
keratan sulfate II  
(core 2-linked),  
degradation product 1



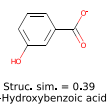
deprotonated HMDB0001895, spectral sim. = 777, #3



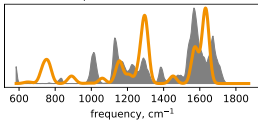
Struc. sim. = 0.80  
Salicylic acid



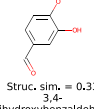
deprotonated HMDB0002466, spectral sim. = 775, #4



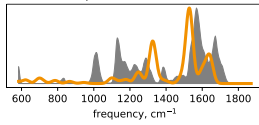
Struc. sim. = 0.39  
3-Hydroxybenzoic acid



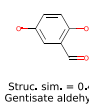
deprotonated HMDB0059965, spectral sim. = 750, #5



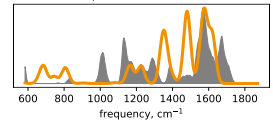
Struc. sim. = 0.33  
Dihydroxybenzaldehyde



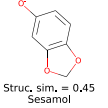
deprotonated HMDB0004062, spectral sim. = 733, #6



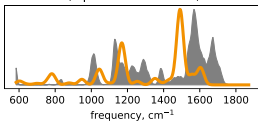
Struc. sim. = 0.40  
Gentisate aldehyde



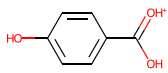
deprotonated HMDB0033812, spectral sim. = 688, #7



Struc. sim. = 0.45  
Sesamol

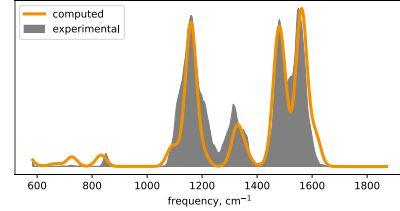


64 protonated HMDB0000500

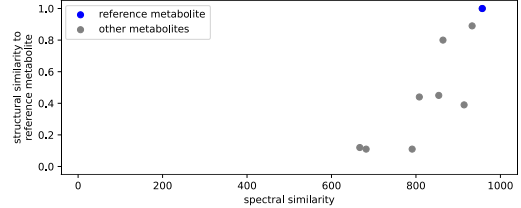


4-Hydroxybenzoic acid

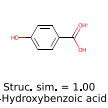
Spectra of protonated HMDB0000500, spectral sim. = 957, #1



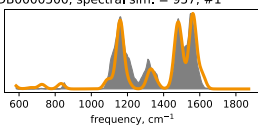
Structural similarity plot of protonated HMDB0000500



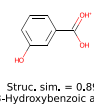
protonated HMDB0000500, spectral sim. = 957, #1



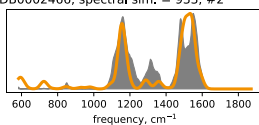
Struc. sim. = 1.00  
4-Hydroxybenzoic acid



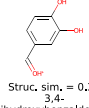
protonated HMDB0002466, spectral sim. = 933, #2



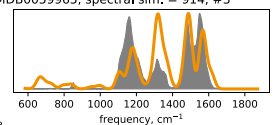
Struc. sim. = 0.89  
3-Hydroxybenzoic acid



protonated HMDB0059965, spectral sim. = 914, #3



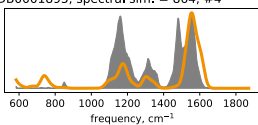
Struc. sim. = 0.39  
Dihydroxybenzaldehyde



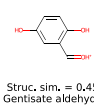
protonated HMDB0001895, spectral sim. = 864, #4



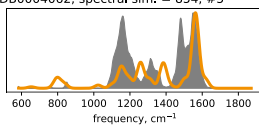
Struc. sim. = 0.80  
Salicylic acid



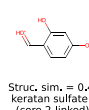
protonated HMDB0004062, spectral sim. = 854, #5



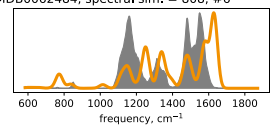
Struc. sim. = 0.45  
Gentisate aldehyde



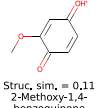
protonated HMDB0062484, spectral sim. = 808, #6



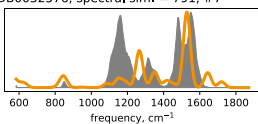
Struc. sim. = 0.44  
keratan sulfate II  
(core 2-linked),  
degradation product 1



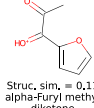
protonated HMDB0032576, spectral sim. = 791, #7



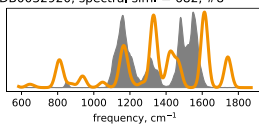
Struc. sim. = 0.11  
2-Methoxy-1,4-  
benzoquinone



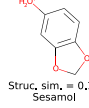
protonated HMDB0032920, spectral sim. = 682, #8



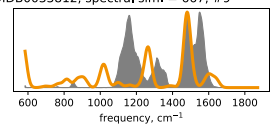
Struc. sim. = 0.11  
alpha-Furyl methyl  
diketone



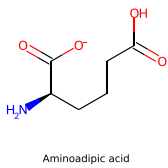
protonated HMDB0033812, spectral sim. = 667, #9



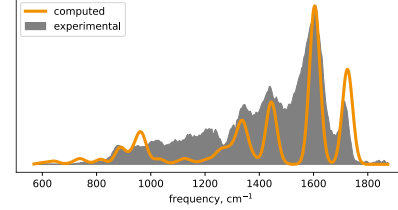
Struc. sim. = 0.12  
Sesamol



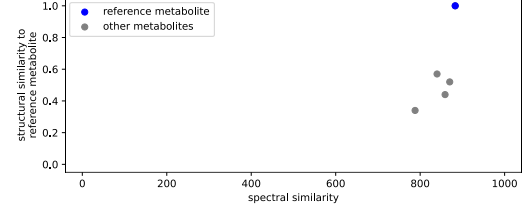
65 deprotonated HMDB0000510



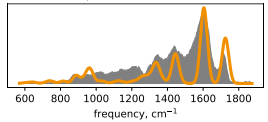
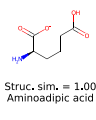
Spectra of deprotonated HMDB0000510, spectral sim. = 883, #1



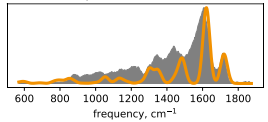
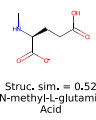
Structural similarity plot of deprotonated HMDB0000510



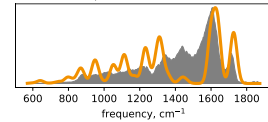
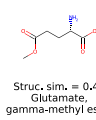
deprotonated HMDB0000510, spectral sim. = 883, #1



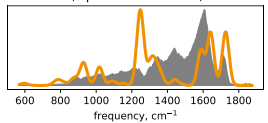
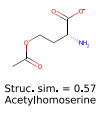
deprotonated HMDB0062660, spectral sim. = 870, #2



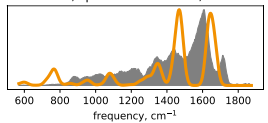
deprotonated HMDB0061715, spectral sim. = 859, #3



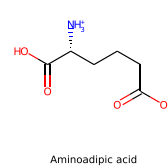
deprotonated HMDB0029423, spectral sim. = 840, #4



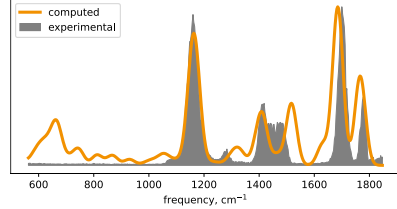
deprotonated HMDB0062557, spectral sim. = 788, #5



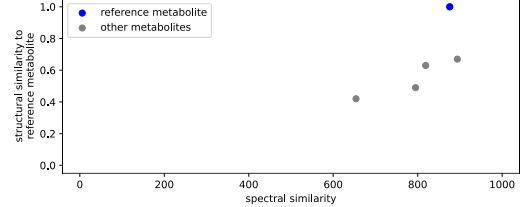
66 protonated HMDB0000510



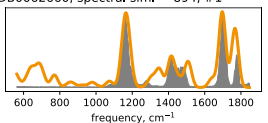
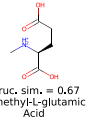
Spectra of protonated HMDB0000510, spectral sim. = 876, #2



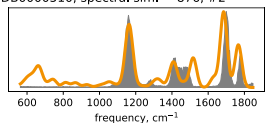
Structural similarity plot of protonated HMDB0000510



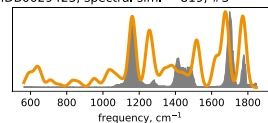
protonated HMDB0062660, spectral sim. = 894, #1



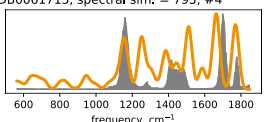
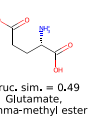
protonated HMDB0000510, spectral sim. = 876, #2



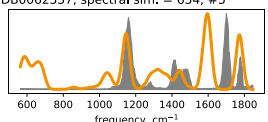
protonated HMDB0029423, spectral sim. = 819, #3



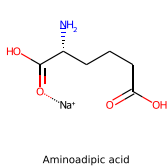
protonated HMDB0061715, spectral sim. = 795, #4



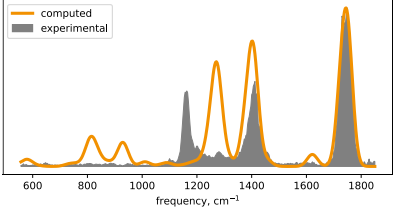
protonated HMDB0062557, spectral sim. = 654, #5



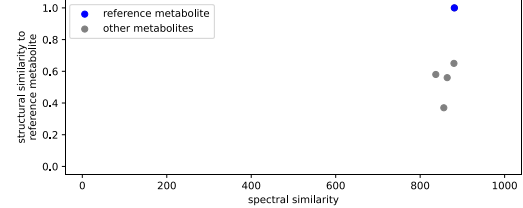
67 sodiated HMDB0000510



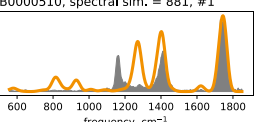
Spectra of sodiated HMDB0000510, spectral sim. = 881, #1



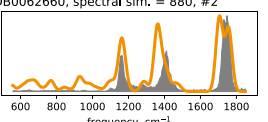
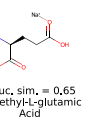
Structural similarity plot of sodiated HMDB0000510



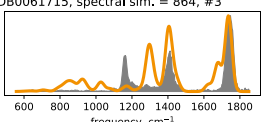
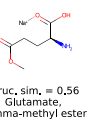
sodiated HMDB0000510, spectral sim. = 881, #1



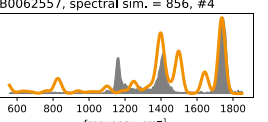
sodiated HMDB0062660, spectral sim. = 880, #2



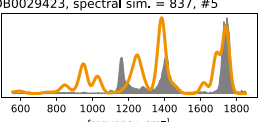
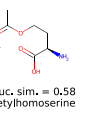
sodiated HMDB0061715, spectral sim. = 864, #3



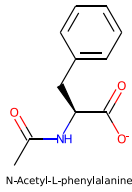
sodiated HMDB0062557, spectral sim. = 856, #4



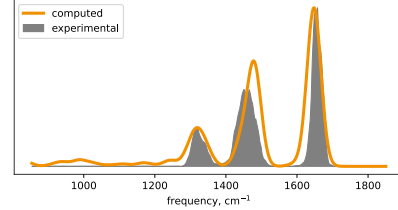
sodiated HMDB0029423, spectral sim. = 837, #5



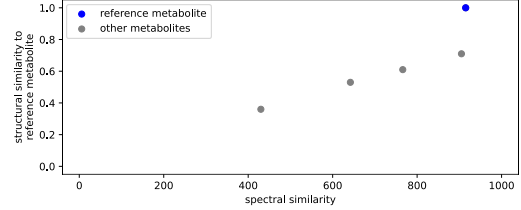
68 deprotonated HMDB0000512



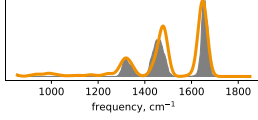
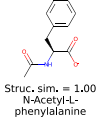
Spectra of deprotonated HMDB0000512, spectral sim. = 915, #1



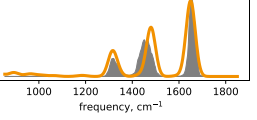
Structural similarity plot of deprotonated HMDB0000512



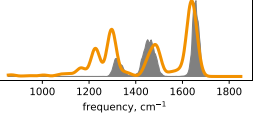
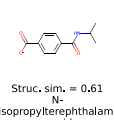
deprotonated HMDB0000512, spectral sim. = 915, #1



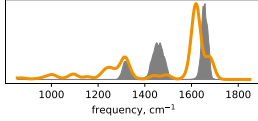
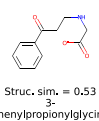
deprotonated HMDB0000860, spectral sim. = 905, #2



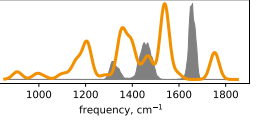
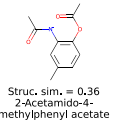
deprotonated HMDB0060608, spectral sim. = 766, #3



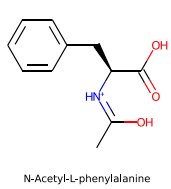
deprotonated HMDB0002042, spectral sim. = 642, #4



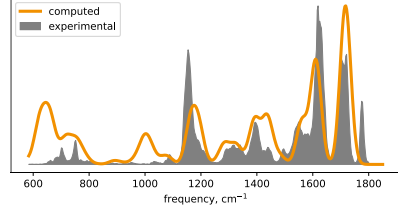
deprotonated HMDB0061682, spectral sim. = 430, #5



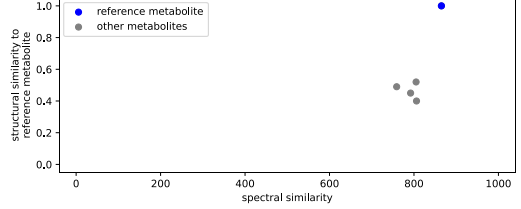
69 protonated HMDB0000512



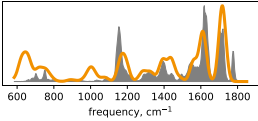
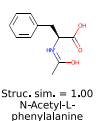
Spectra of protonated HMDB0000512, spectral sim. = 865, #1



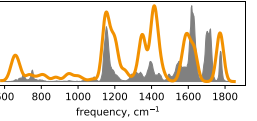
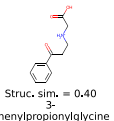
Structural similarity plot of protonated HMDB0000512



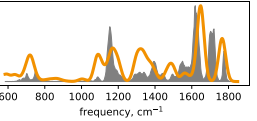
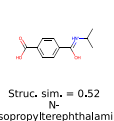
protonated HMDB0000512, spectral sim. = 865, #1



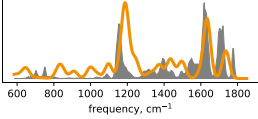
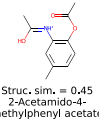
protonated HMDB0002042, spectral sim. = 806, #2



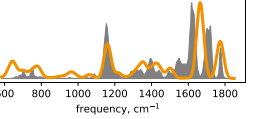
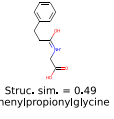
protonated HMDB0060608, spectral sim. = 805, #3



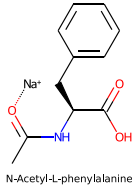
protonated HMDB0061682, spectral sim. = 792, #4



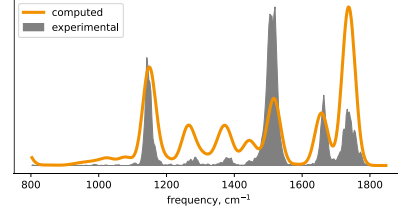
protonated HMDB0000860, spectral sim. = 759, #5



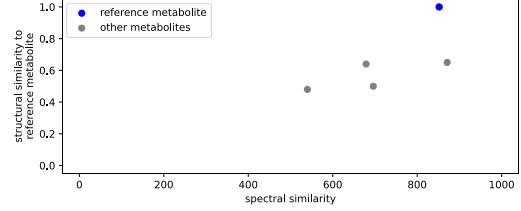
70 sodiated HMDB0000512



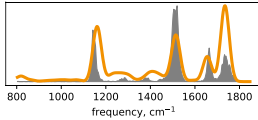
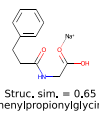
Spectra of sodiated HMDB0000512, spectral sim. = 852, #2



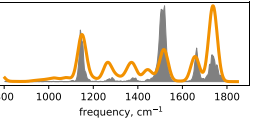
Structural similarity plot of sodiated HMDB0000512



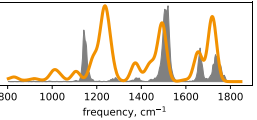
sodiated HMDB0000860, spectral sim. = 871, #1



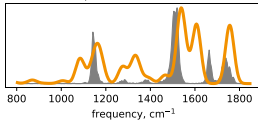
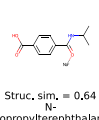
sodiated HMDB0000512, spectral sim. = 852, #2



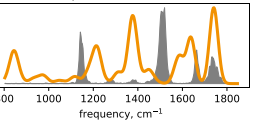
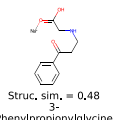
sodiated HMDB0061682, spectral sim. = 696, #3



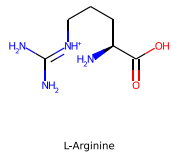
sodiated HMDB0060608, spectral sim. = 679, #4



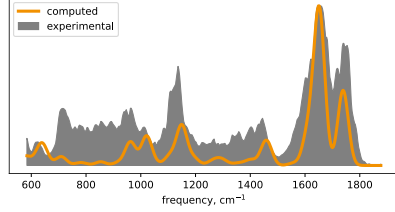
sodiated HMDB0002042, spectral sim. = 540, #5



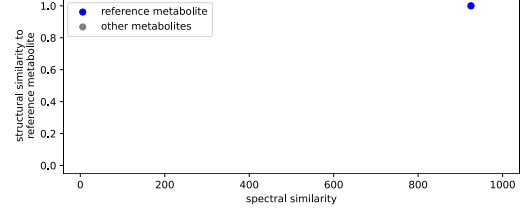
71 protonated HMDB0000517



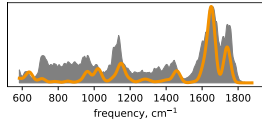
Spectra of protonated HMDB0000517, spectral sim. = 925, #1



Structural similarity plot of protonated HMDB0000517

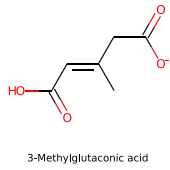


protonated HMDB0000517, spectral sim. = 925, #1

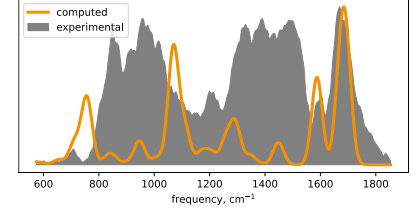


Struc. sim. = 1.00

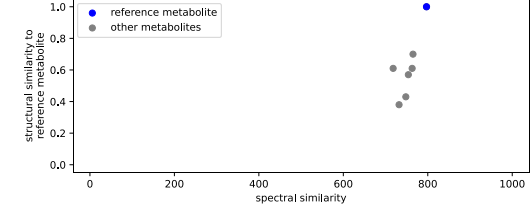
72 deprotonated HMDB0000522



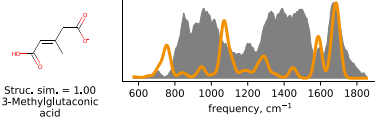
Spectra of deprotonated HMDB0000522, spectral sim. = 797, #1



Structural similarity plot of deprotonated HMDB0000522



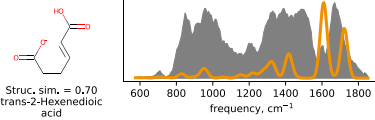
deprotonated HMDB0000522, spectral sim. = 797, #1



Struc. sim. = 1.00

3-Methylglutaconic acid

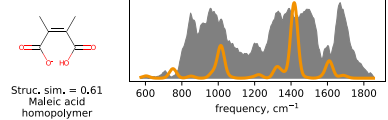
deprotonated HMDB0013311, spectral sim. = 765, #2



Struc. sim. = 0.70

trans-2-Hexenedioic acid

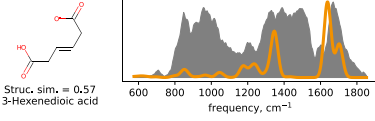
deprotonated HMDB0036232, spectral sim. = 763, #3



Struc. sim. = 0.61

Maleic acid homopolymer

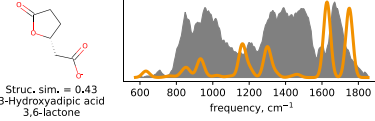
deprotonated HMDB0000393, spectral sim. = 754, #4



Struc. sim. = 0.57

3-Hexenedioic acid

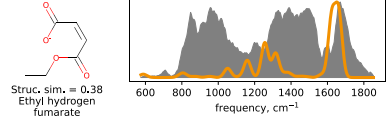
deprotonated HMDB0029171, spectral sim. = 748, #5



Struc. sim. = 0.43

3-Hydroxyadipic acid 3,6-lactone

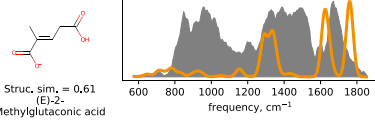
deprotonated HMDB0040207, spectral sim. = 732, #6



Struc. sim. = 0.38

Ethyl hydrogen fumarate

deprotonated HMDB0002266, spectral sim. = 718, #7

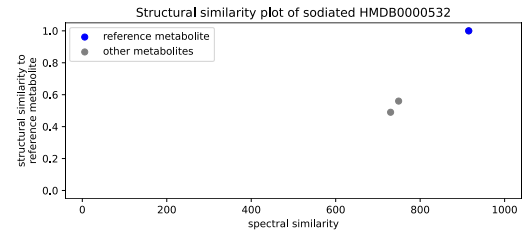
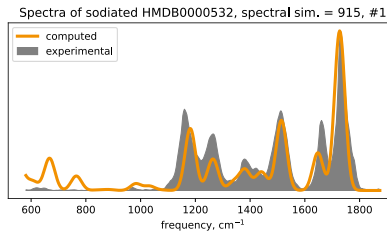
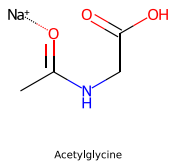


Struc. sim. = 0.61

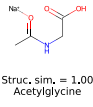
(E)-2-Methylglutaconic acid



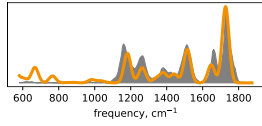
76 sodiated HMDB0000532



sodiated HMDB0000532, spectral sim. = 915, #1



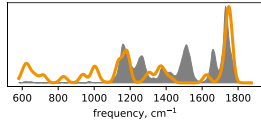
Struc. sim. = 1.00



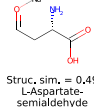
sodiated HMDB0006454, spectral sim. = 749, #2



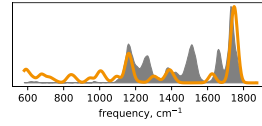
Struc. sim. = 0.56



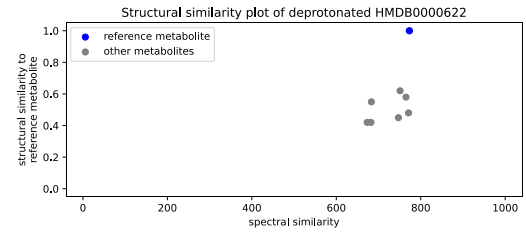
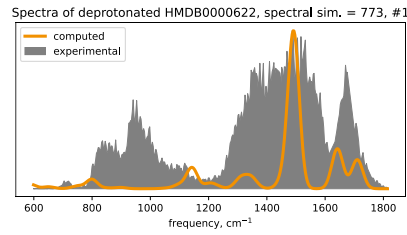
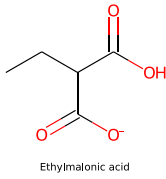
sodiated HMDB0012249, spectral sim. = 730, #3



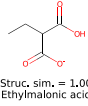
Struc. sim. = 0.49



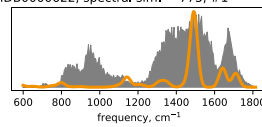
77 deprotonated HMDB0000622



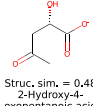
deprotonated HMDB0000622, spectral sim. = 773, #1



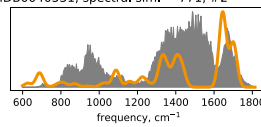
Struc. sim. = 1.00



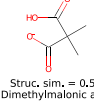
deprotonated HMDB0040531, spectral sim. = 771, #2



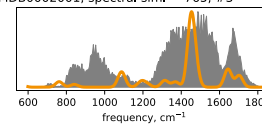
Struc. sim. = 0.48



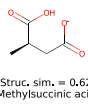
deprotonated HMDB0002001, spectral sim. = 765, #3



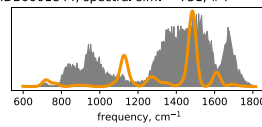
Struc. sim. = 0.58



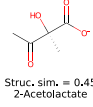
deprotonated HMDB0001844, spectral sim. = 751, #4



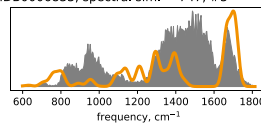
Struc. sim. = 0.62



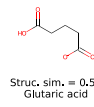
deprotonated HMDB0006833, spectral sim. = 747, #5



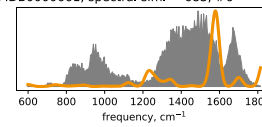
Struc. sim. = 0.45



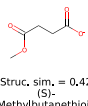
deprotonated HMDB0000661, spectral sim. = 683, #6



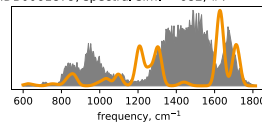
Struc. sim. = 0.55



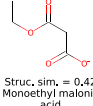
deprotonated HMDB0061879, spectral sim. = 682, #7



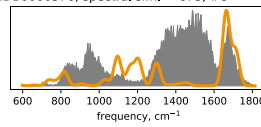
Struc. sim. = 0.42



deprotonated HMDB0000576, spectral sim. = 673, #8

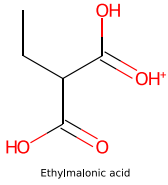


Struc. sim. = 0.42

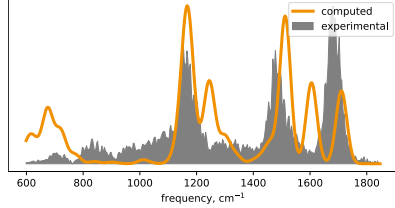




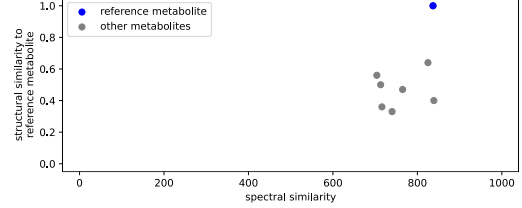
78 protonated HMDB0000622



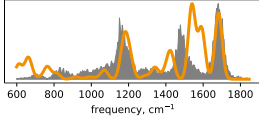
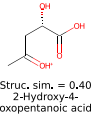
Spectra of protonated HMDB0000622, spectral sim. = 837, #2



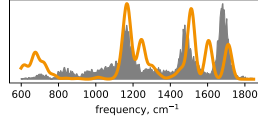
Structural similarity plot of protonated HMDB0000622



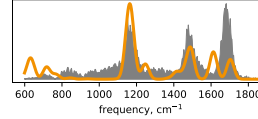
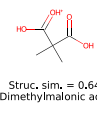
protonated HMDB0040531, spectral sim. = 839, #1



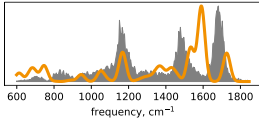
protonated HMDB0000622, spectral sim. = 837, #2



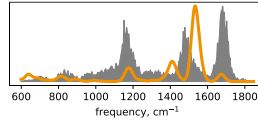
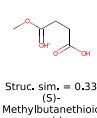
protonated HMDB0002001, spectral sim. = 825, #3



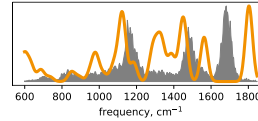
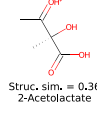
protonated HMDB0000576, spectral sim. = 765, #4



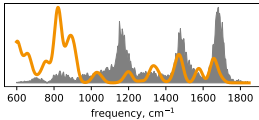
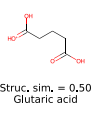
protonated HMDB0061879, spectral sim. = 740, #5



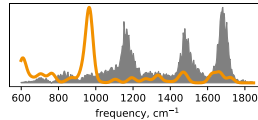
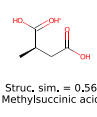
protonated HMDB0006833, spectral sim. = 716, #6



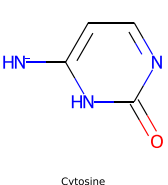
protonated HMDB0000661, spectral sim. = 713, #7



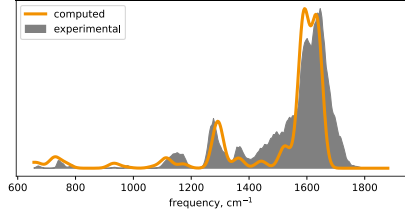
protonated HMDB0001844, spectral sim. = 704, #8



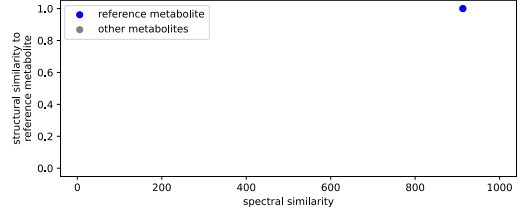
79 deprotonated HMDB0000630



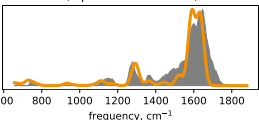
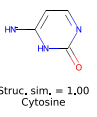
Spectra of deprotonated HMDB0000630, spectral sim. = 913, #1



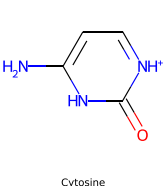
Structural similarity plot of deprotonated HMDB0000630



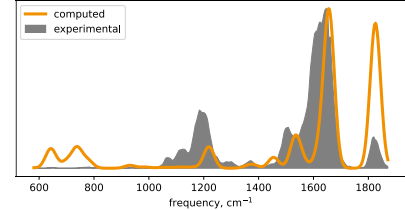
deprotonated HMDB0000630, spectral sim. = 913, #1



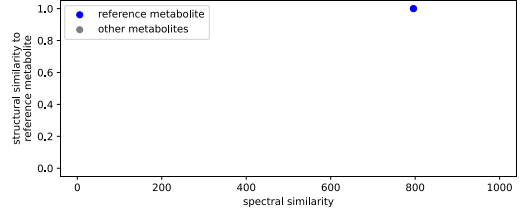
80 protonated HMDB0000630



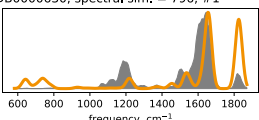
Spectra of protonated HMDB0000630, spectral sim. = 796, #1



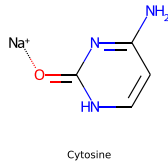
Structural similarity plot of protonated HMDB0000630



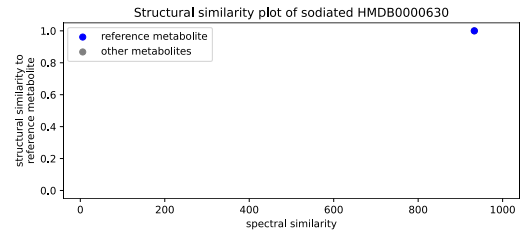
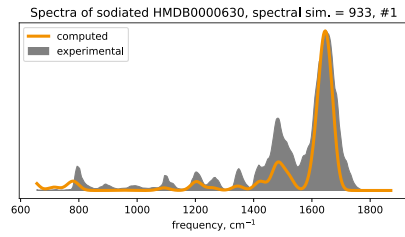
protonated HMDB0000630, spectral sim. = 796, #1



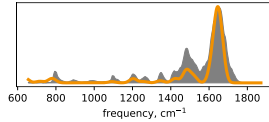
81 sodiated HMDB0000630



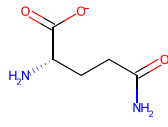
Cytosine



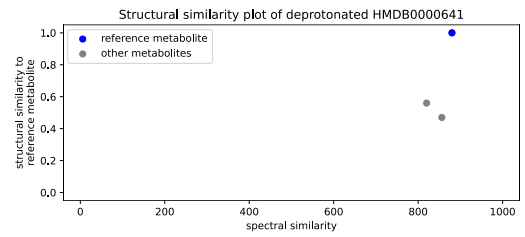
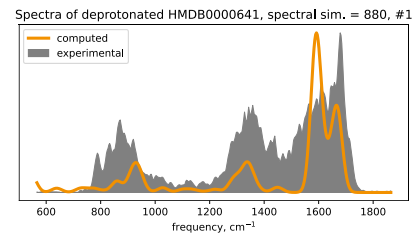
sodiated HMDB0000630, spectral sim. = 933, #1

Struc. sim. = 1.00  
Cytosine

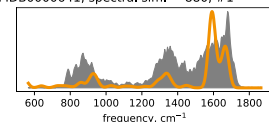
82 deprotonated HMDB0000641



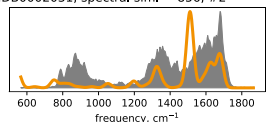
L-Glutamine



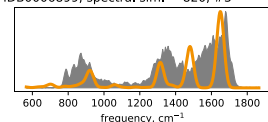
deprotonated HMDB0000641, spectral sim. = 880, #1

Struc. sim. = 1.00  
L-Glutamine

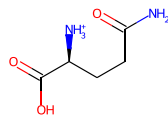
deprotonated HMDB0002031, spectral sim. = 856, #2

Struc. sim. = 0.47  
Ureidoisobutyric acid

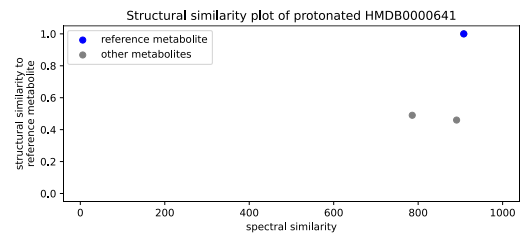
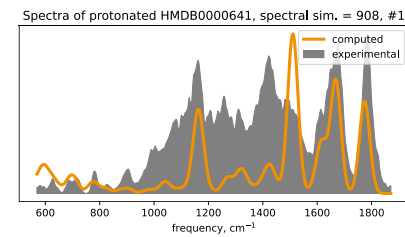
deprotonated HMDB0006899, spectral sim. = 820, #3

Struc. sim. = 0.56  
Alanylglycine

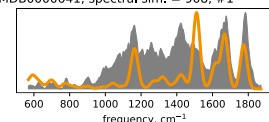
83 protonated HMDB0000641



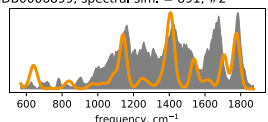
L-Glutamine



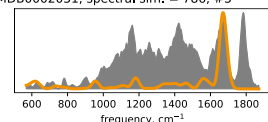
protonated HMDB0000641, spectral sim. = 908, #1

Struc. sim. = 1.00  
L-Glutamine

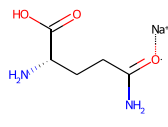
protonated HMDB0006899, spectral sim. = 891, #2

Struc. sim. = 0.46  
Alanylglycine

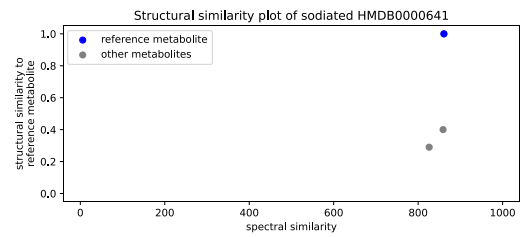
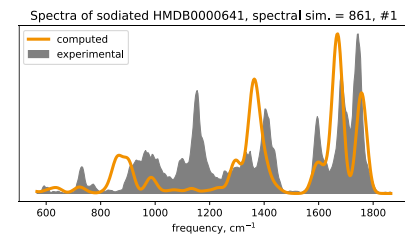
protonated HMDB0002031, spectral sim. = 786, #3

Struc. sim. = 0.49  
Ureidoisobutyric acid

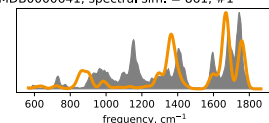
84 sodiated HMDB0000641



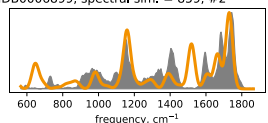
L-Glutamine



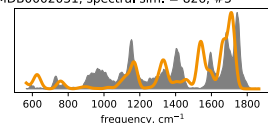
sodiated HMDB0000641, spectral sim. = 861, #1

Struc. sim. = 1.00  
L-Glutamine

sodiated HMDB0006899, spectral sim. = 859, #2

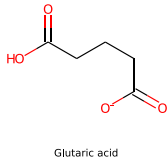
Struc. sim. = 0.40  
Alanylglycine

sodiated HMDB0002031, spectral sim. = 826, #3

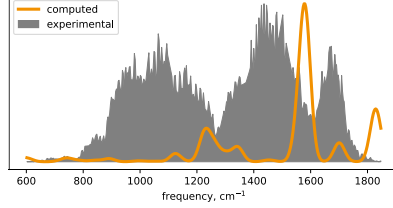
Struc. sim. = 0.29  
Ureidoisobutyric acid



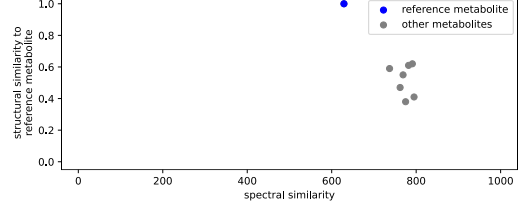
86 deprotonated HMDB0000661



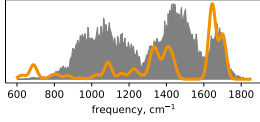
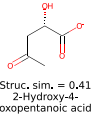
Spectra of deprotonated HMDB0000661, spectral sim. = 629, #8



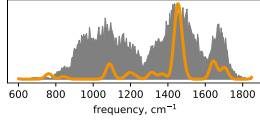
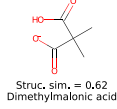
Structural similarity plot of deprotonated HMDB0000661



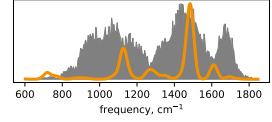
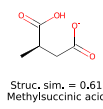
deprotonated HMDB0040531, spectral sim. = 795, #1



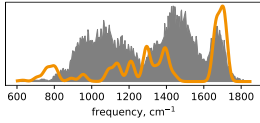
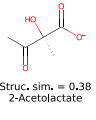
deprotonated HMDB0002001, spectral sim. = 791, #2



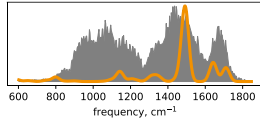
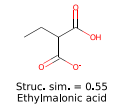
deprotonated HMDB0001844, spectral sim. = 782, #3



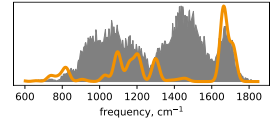
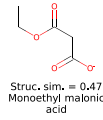
deprotonated HMDB0006833, spectral sim. = 775, #4



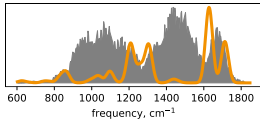
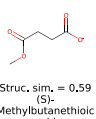
deprotonated HMDB0000622, spectral sim. = 769, #5



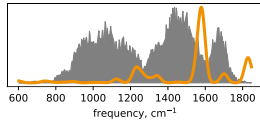
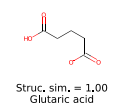
deprotonated HMDB0000576, spectral sim. = 762, #6



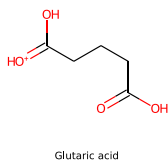
deprotonated HMDB0061879, spectral sim. = 737, #7



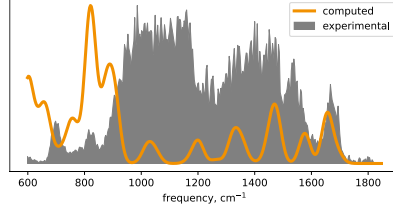
deprotonated HMDB0000661, spectral sim. = 629, #8



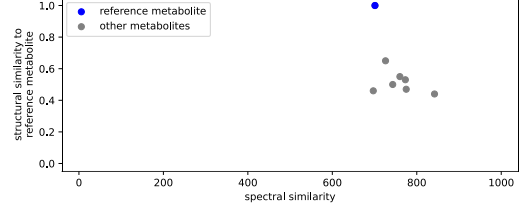
87 protonated HMDB0000661



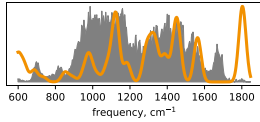
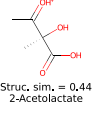
Spectra of protonated HMDB0000661, spectral sim. = 701, #7



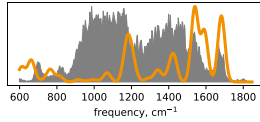
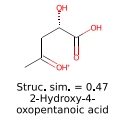
Structural similarity plot of protonated HMDB0000661



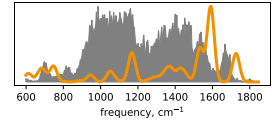
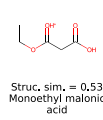
protonated HMDB0006833, spectral sim. = 842, #1



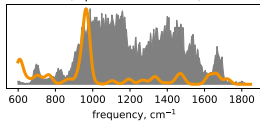
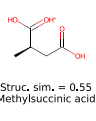
protonated HMDB0040531, spectral sim. = 775, #2



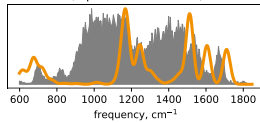
protonated HMDB0000576, spectral sim. = 773, #3



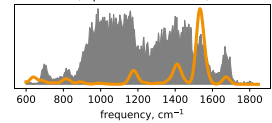
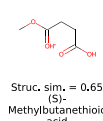
protonated HMDB0001844, spectral sim. = 760, #4



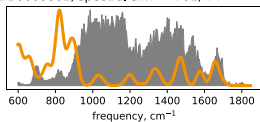
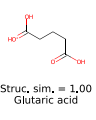
protonated HMDB0000622, spectral sim. = 743, #5



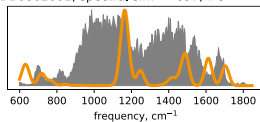
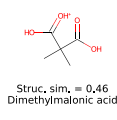
protonated HMDB0061879, spectral sim. = 726, #6



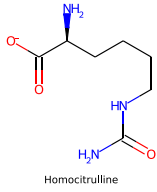
protonated HMDB0000661, spectral sim. = 701, #7



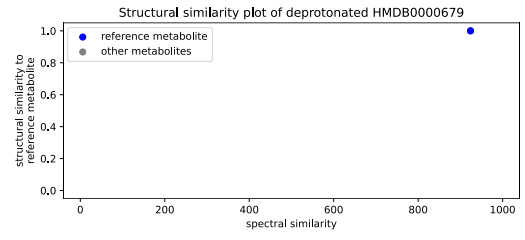
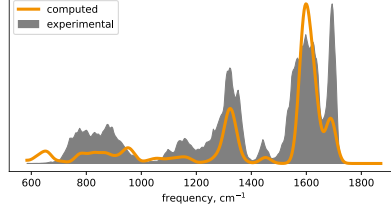
protonated HMDB0002001, spectral sim. = 697, #8



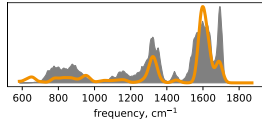
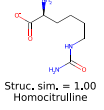
88 deprotonated HMDB0000679



Spectra of deprotonated HMDB0000679, spectral sim. = 924, #1

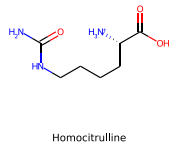


deprotonated HMDB0000679, spectral sim. = 924, #1

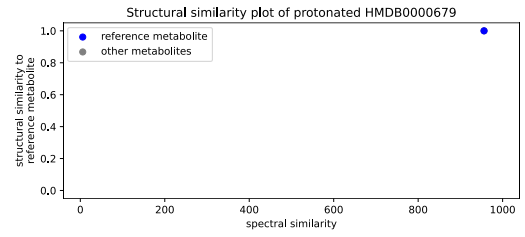
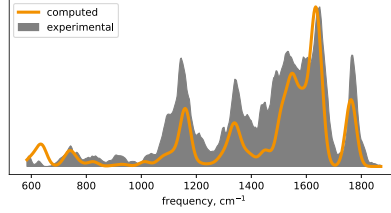


Struc. sim. = 1.00

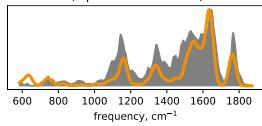
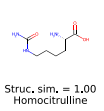
89 protonated HMDB0000679



Spectra of protonated HMDB0000679, spectral sim. = 956, #1

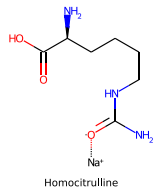


protonated HMDB0000679, spectral sim. = 956, #1

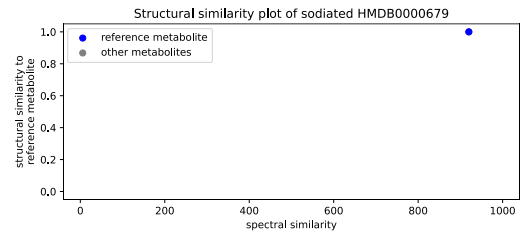
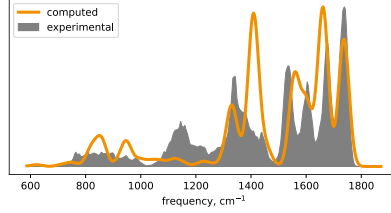


Struc. sim. = 1.00

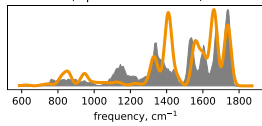
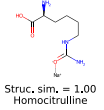
90 sodiated HMDB0000679



Spectra of sodiated HMDB0000679, spectral sim. = 920, #1

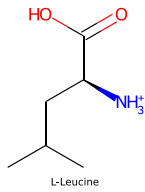


sodiated HMDB0000679, spectral sim. = 920, #1

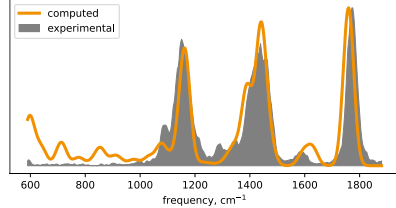


Struc. sim. = 1.00

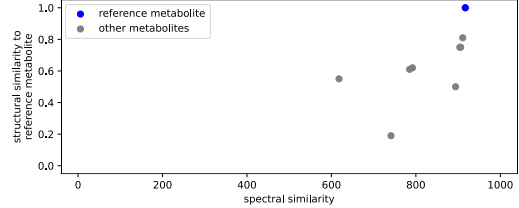
91 protonated HMDB0000687



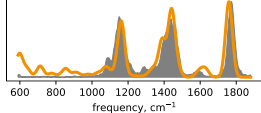
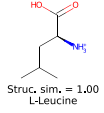
Spectra of protonated HMDB0000687, spectral sim. = 917, #1



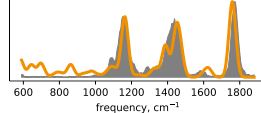
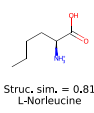
Structural similarity plot of protonated HMDB0000687



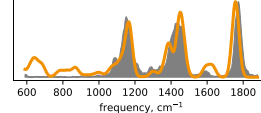
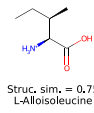
protonated HMDB0000687, spectral sim. = 917, #1



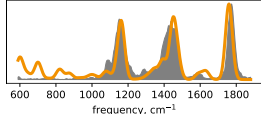
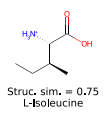
protonated HMDB0001645, spectral sim. = 911, #2



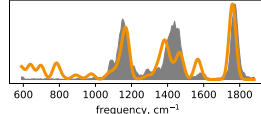
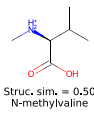
protonated HMDB0000557, spectral sim. = 906, #3



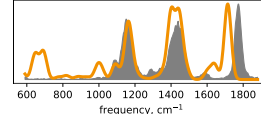
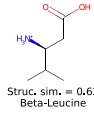
protonated HMDB0000172, spectral sim. = 904, #4



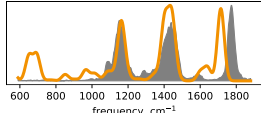
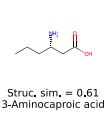
protonated HMDB0061716, spectral sim. = 894, #5



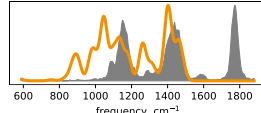
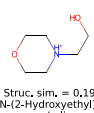
protonated HMDB0003640, spectral sim. = 792, #6



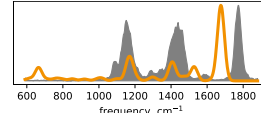
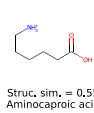
protonated HMDB0029168, spectral sim. = 785, #7



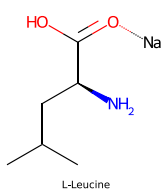
protonated HMDB0060650, spectral sim. = 741, #8



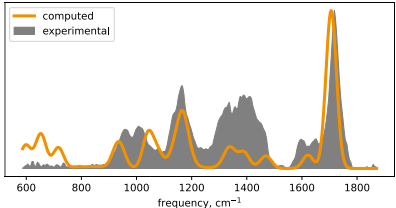
protonated HMDB0001901, spectral sim. = 618, #9



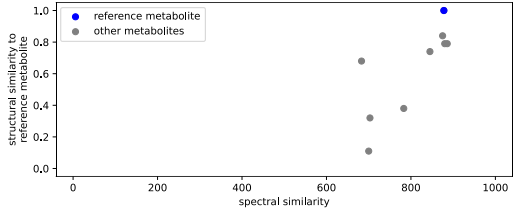
92 sodiated HMDB0000687



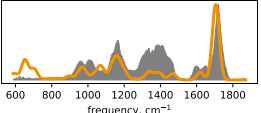
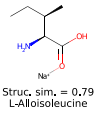
Spectra of sodiated HMDB0000687, spectral sim. = 878, #3



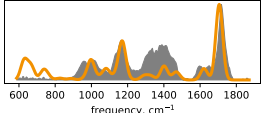
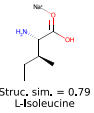
Structural similarity plot of sodiated HMDB0000687



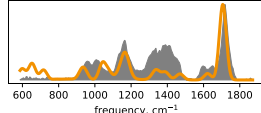
sodiated HMDB0000557, spectral sim. = 886, #1



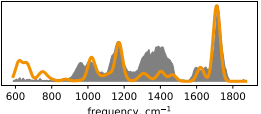
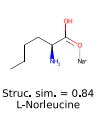
sodiated HMDB0000172, spectral sim. = 880, #2



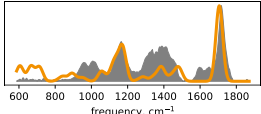
sodiated HMDB0000687, spectral sim. = 878, #3



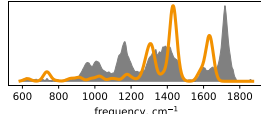
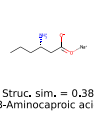
sodiated HMDB0001645, spectral sim. = 875, #4



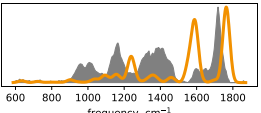
sodiated HMDB0061716, spectral sim. = 845, #5



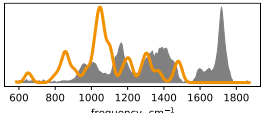
sodiated HMDB0029168, spectral sim. = 783, #6



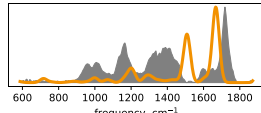
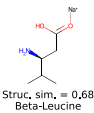
sodiated HMDB0001901, spectral sim. = 703, #7



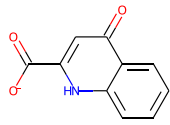
sodiated HMDB0060650, spectral sim. = 700, #8



sodiated HMDB0003640, spectral sim. = 683, #9

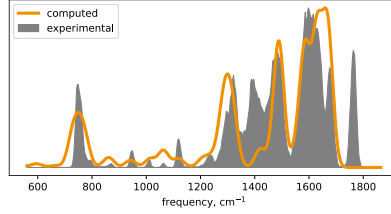


93 deprotonated HMDB0000715

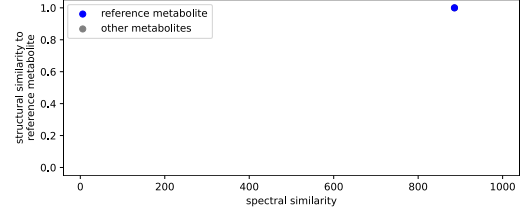


Kynurenic acid

Spectra of deprotonated HMDB0000715, spectral sim. = 886, #1



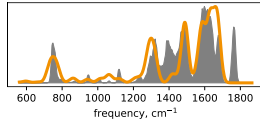
Structural similarity plot of deprotonated HMDB0000715



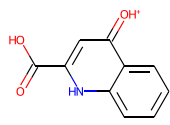
deprotonated HMDB0000715, spectral sim. = 886, #1



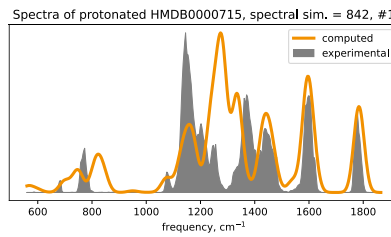
Struc. sim. = 1.00  
Kynurenic acid



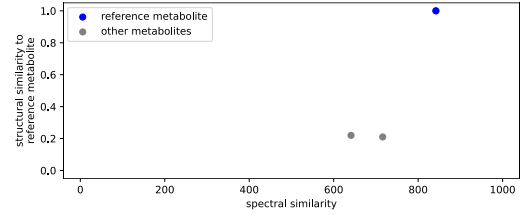
94 protonated HMDB0000715



Kynurenic acid



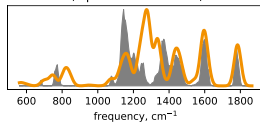
Structural similarity plot of protonated HMDB0000715



protonated HMDB0000715, spectral sim. = 842, #1



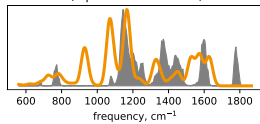
Struc. sim. = 1.00  
Kynurenic acid



protonated HMDB0060331, spectral sim. = 716, #2



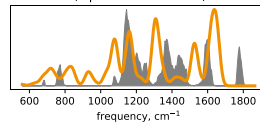
Struc. sim. = 0.21  
1-Nitronaphthalene-5,6-oxide



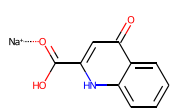
protonated HMDB0060332, spectral sim. = 641, #3



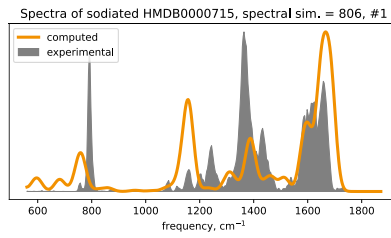
Struc. sim. = 0.22  
1-Nitronaphthalene-7,8-oxide



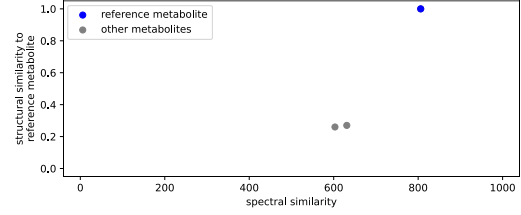
95 sodiated HMDB0000715



Kynurenic acid



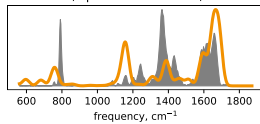
Structural similarity plot of sodiated HMDB0000715



sodiated HMDB0000715, spectral sim. = 806, #1



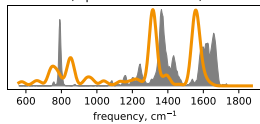
Struc. sim. = 1.00  
Kynurenic acid



sodiated HMDB0060332, spectral sim. = 631, #2



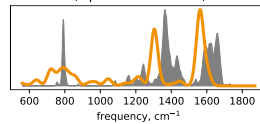
Struc. sim. = 0.27  
1-Nitronaphthalene-7,8-oxide



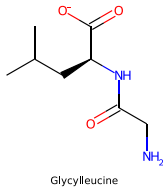
sodiated HMDB0060331, spectral sim. = 603, #3



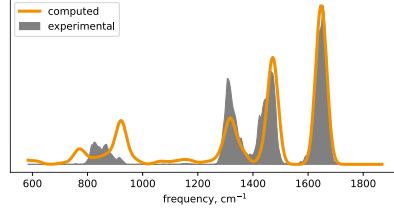
Struc. sim. = 0.26  
1-Nitronaphthalene-5,6-oxide



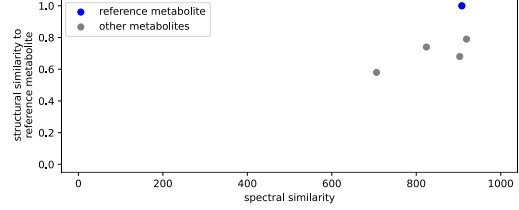
96 deprotonated HMDB0000759



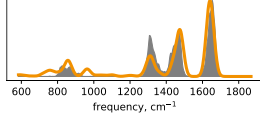
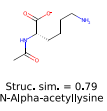
Spectra of deprotonated HMDB0000759, spectral sim. = 908, #2



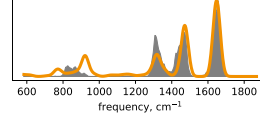
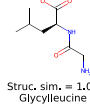
Structural similarity plot of deprotonated HMDB0000759



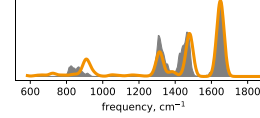
deprotonated HMDB0000446, spectral sim. = 919, #1



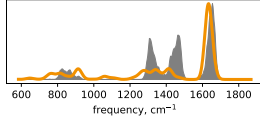
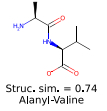
deprotonated HMDB0000759, spectral sim. = 908, #2



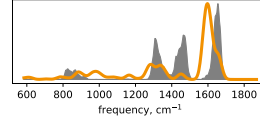
deprotonated HMDB0028929, spectral sim. = 903, #3



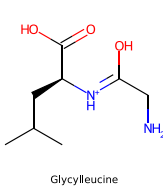
deprotonated HMDB0028700, spectral sim. = 824, #4



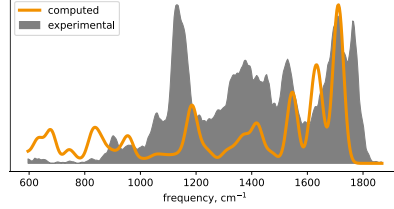
deprotonated HMDB0000206, spectral sim. = 706, #5



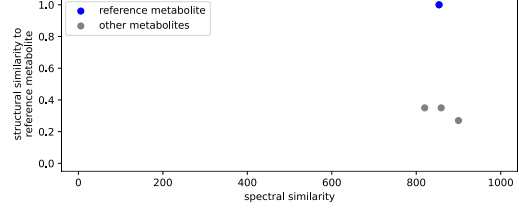
97 protonated HMDB0000759



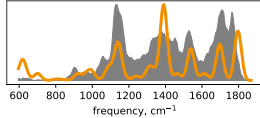
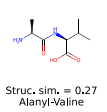
Spectra of protonated HMDB0000759, spectral sim. = 854, #3



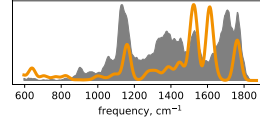
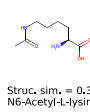
Structural similarity plot of protonated HMDB0000759



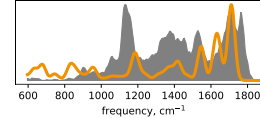
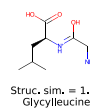
protonated HMDB0028700, spectral sim. = 900, #1



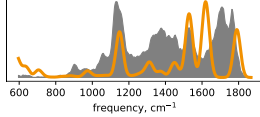
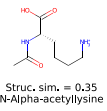
protonated HMDB0000206, spectral sim. = 859, #2



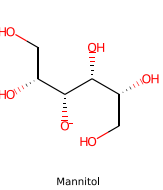
protonated HMDB0000759, spectral sim. = 854, #3



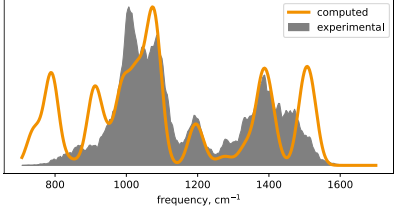
protonated HMDB0000446, spectral sim. = 820, #4



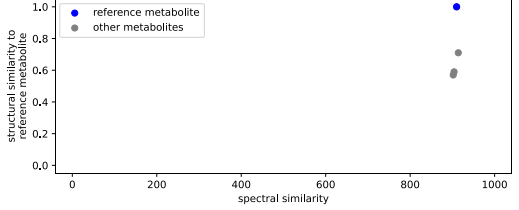
98 deprotonated HMDB0000765



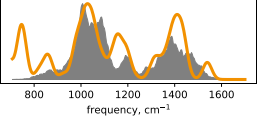
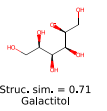
Spectra of deprotonated HMDB0000765, spectral sim. = 910, #2



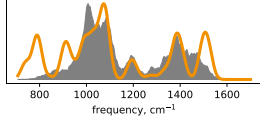
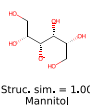
Structural similarity plot of deprotonated HMDB0000765



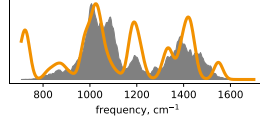
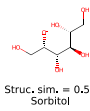
deprotonated HMDB0000107, spectral sim. = 914, #1



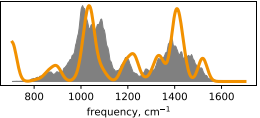
deprotonated HMDB0000765, spectral sim. = 910, #2



deprotonated HMDB0000247, spectral sim. = 904, #3

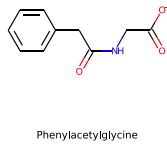


deprotonated HMDB0011632, spectral sim. = 902, #4

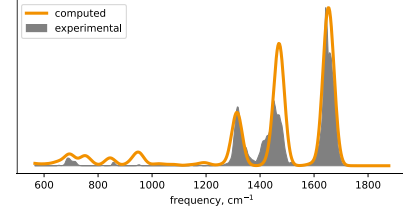




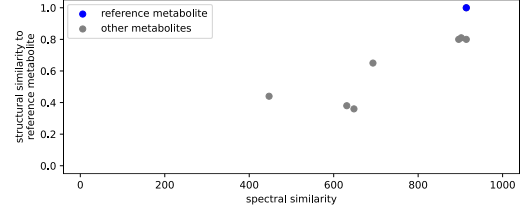
99 deprotonated HMDB0000821



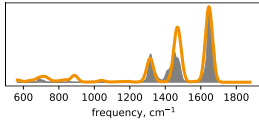
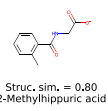
Spectra of deprotonated HMDB0000821, spectral sim. = 914, #2



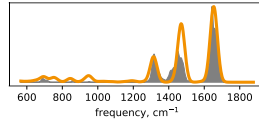
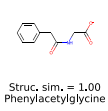
Structural similarity plot of deprotonated HMDB0000821



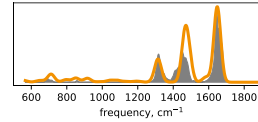
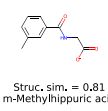
deprotonated HMDB0011723, spectral sim. = 914, #1



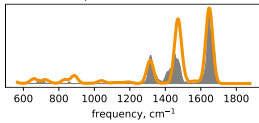
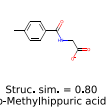
deprotonated HMDB0000821, spectral sim. = 914, #2



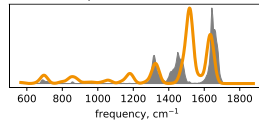
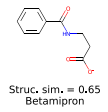
deprotonated HMDB0013245, spectral sim. = 902, #3



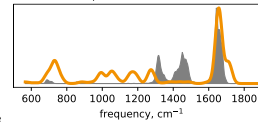
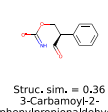
deprotonated HMDB0013292, spectral sim. = 896, #4



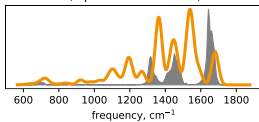
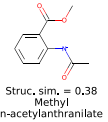
deprotonated HMDB0034250, spectral sim. = 693, #5



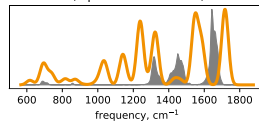
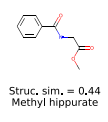
deprotonated HMDB0060366, spectral sim. = 648, #6



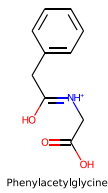
deprotonated HMDB0032388, spectral sim. = 631, #7



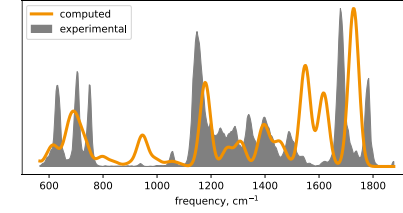
deprotonated HMDB0000859, spectral sim. = 447, #8



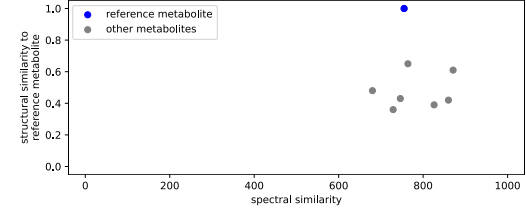
100 protonated HMDB0000821



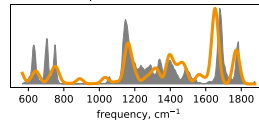
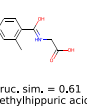
Spectra of protonated HMDB0000821, spectral sim. = 755, #5



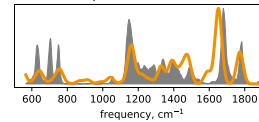
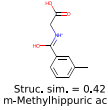
Structural similarity plot of protonated HMDB0000821



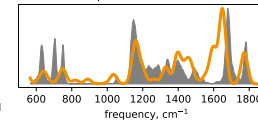
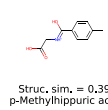
protonated HMDB0011723, spectral sim. = 871, #1



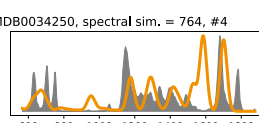
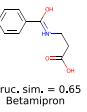
protonated HMDB0013245, spectral sim. = 860, #2



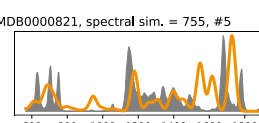
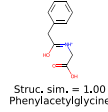
protonated HMDB0013292, spectral sim. = 826, #3



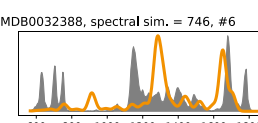
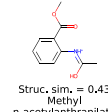
protonated HMDB0034250, spectral sim. = 764, #4



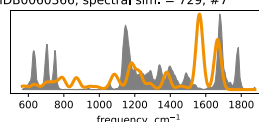
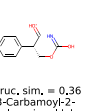
protonated HMDB0000821, spectral sim. = 755, #5



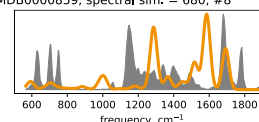
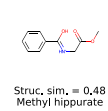
protonated HMDB0032388, spectral sim. = 746, #6



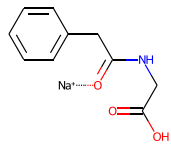
protonated HMDB0060366, spectral sim. = 729, #7



protonated HMDB0000859, spectral sim. = 680, #8

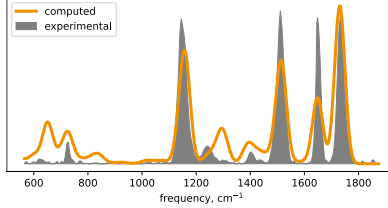


101 sodiated HMDB0000821

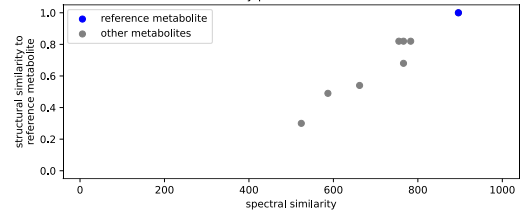


Phenylacetylglycine

Spectra of sodiated HMDB0000821, spectral sim. = 896, #1



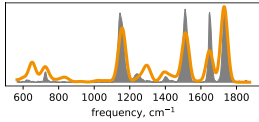
Structural similarity plot of sodiated HMDB0000821



sodiated HMDB0000821, spectral sim. = 896, #1



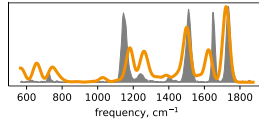
Struc. sim. = 1.00  
Phenylacetylglycine



sodiated HMDB0011723, spectral sim. = 783, #2



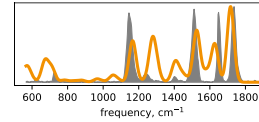
Struc. sim. = 0.82  
2-Methylhippuric acid



sodiated HMDB0034250, spectral sim. = 766, #3



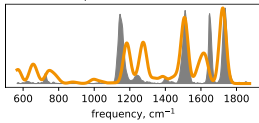
Struc. sim. = 0.68  
Betamipron



sodiated HMDB0013245, spectral sim. = 766, #4



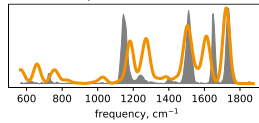
Struc. sim. = 0.82  
m-Methylhippuric acid



sodiated HMDB0013292, spectral sim. = 755, #5



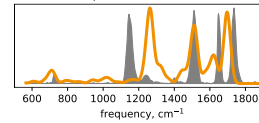
Struc. sim. = 0.82  
p-Methylhippuric acid



sodiated HMDB0000859, spectral sim. = 662, #6



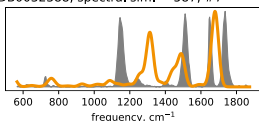
Struc. sim. = 0.54  
Methyl hippurate



sodiated HMDB0032388, spectral sim. = 587, #7



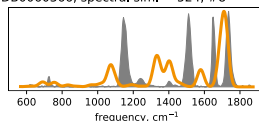
Struc. sim. = 0.49  
Methyl  
n-acetylanthranilate



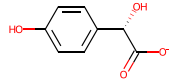
sodiated HMDB0060366, spectral sim. = 524, #8



Struc. sim. = 0.30  
3-Carbamoyl-2-  
phenylpropionaldehyde

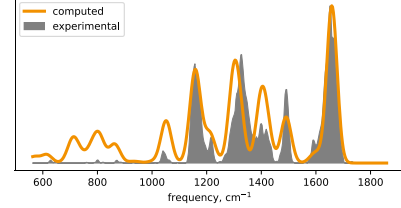


102 deprotonated HMDB0000822

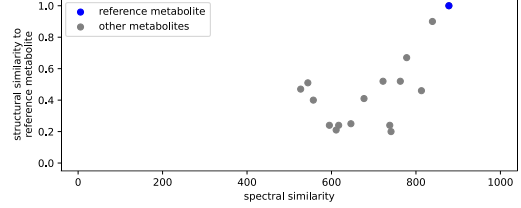


p-Hydroxymandelic acid

Spectra of deprotonated HMDB0000822, spectral sim. = 878, #1



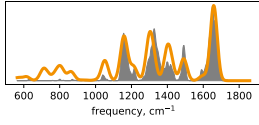
Structural similarity plot of deprotonated HMDB0000822



deprotonated HMDB0000822, spectral sim. = 878, #1



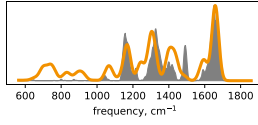
Struc. sim. = 1.00  
p-Hydroxymandelic acid



deprotonated HMDB0000750, spectral sim. = 839, #2



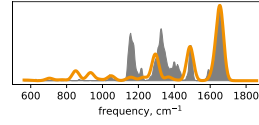
Struc. sim. = 0.90  
3-Hydroxymandelic acid



deprotonated HMDB0240257, spectral sim. = 813, #3



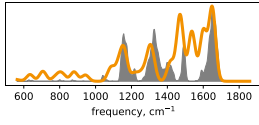
Struc. sim. = 0.46  
Quinolacetic acid



deprotonated HMDB0000130, spectral sim. = 778, #4



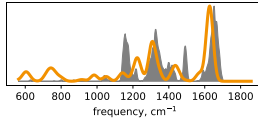
Struc. sim. = 0.67  
Homogentisic acid



deprotonated HMDB0140902, spectral sim. = 763, #5



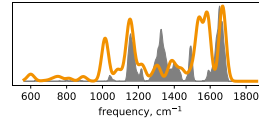
Struc. sim. = 0.52  
3-hydroxy-2-methoxybenzoic acid



deprotonated HMDB0000484, spectral sim. = 741, #6



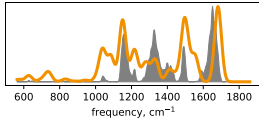
Struc. sim. = 0.20  
Vanillic acid



deprotonated HMDB0060003, spectral sim. = 738, #7



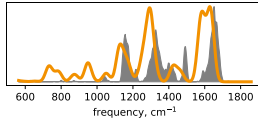
Struc. sim. = 0.24  
Isovanillic acid



deprotonated HMDB0125536, spectral sim. = 722, #8



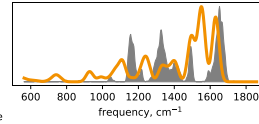
Struc. sim. = 0.52  
3-hydroxy-5-methoxybenzoic acid



deprotonated HMDB0029644, spectral sim. = 677, #9



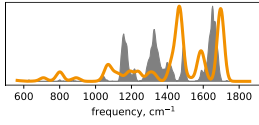
Struc. sim. = 0.41  
Trihydroxyacetophenone



deprotonated HMDB0001868, spectral sim. = 646, #10



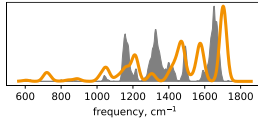
Struc. sim. = 0.25  
5-Methoxysalicylic acid



deprotonated HMDB0059713, spectral sim. = 617, #11



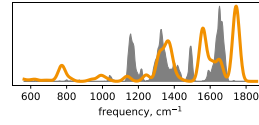
Struc. sim. = 0.24  
3-Methoxysalicylic acid



deprotonated HMDB0033129, spectral sim. = 611, #12



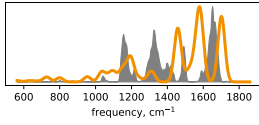
Struc. sim. = 0.21  
3-Acetyl-4-hydroxy-6-methyl-2H-pyran-2-one



deprotonated HMDB0131176, spectral sim. = 595, #13



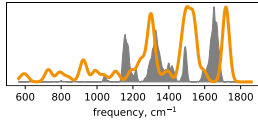
Struc. sim. = 0.24  
2-hydroxy-4-methoxybenzoic acid



deprotonated HMDB0006242, spectral sim. = 557, #14



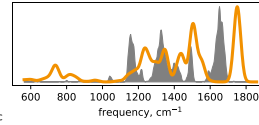
Struc. sim. = 0.40  
3,4-Dihydroxymandelaldehyde



deprotonated HMDB0001336, spectral sim. = 544, #15



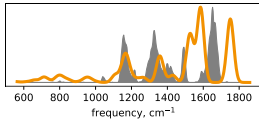
Struc. sim. = 0.51  
3,4-Dihydroxybenzeneacetic acid



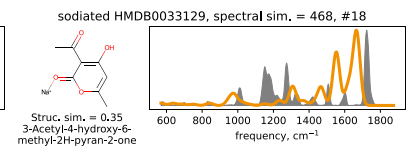
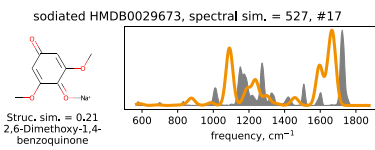
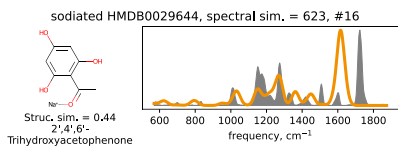
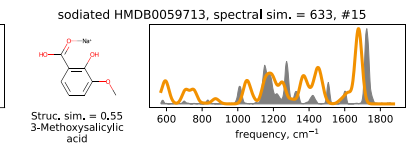
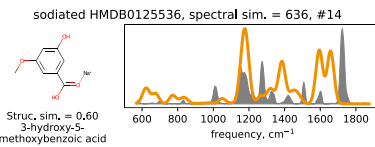
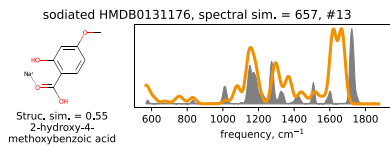
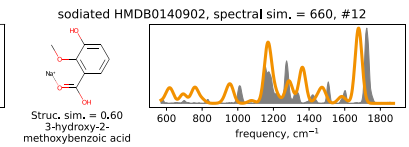
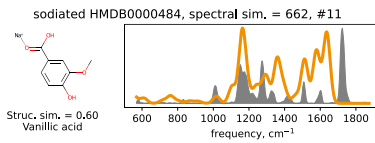
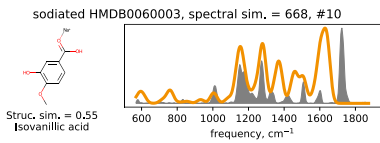
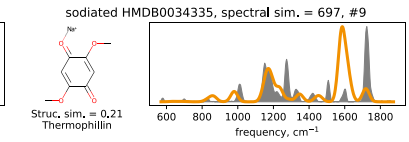
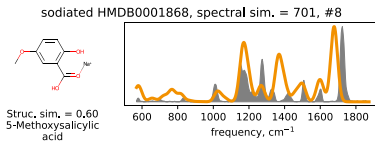
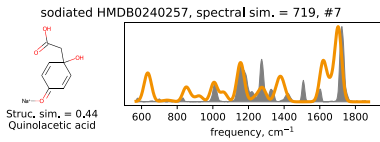
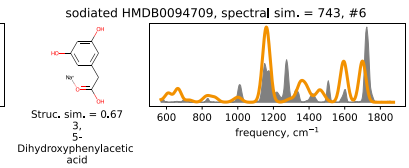
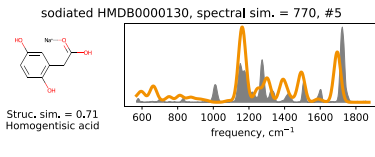
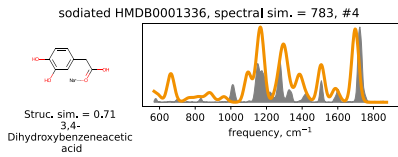
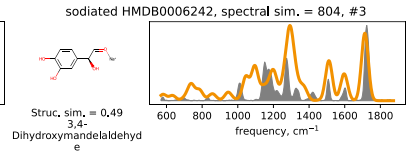
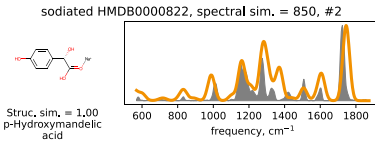
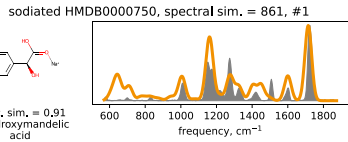
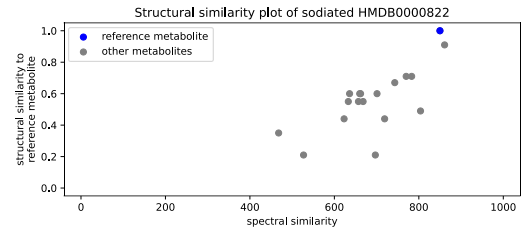
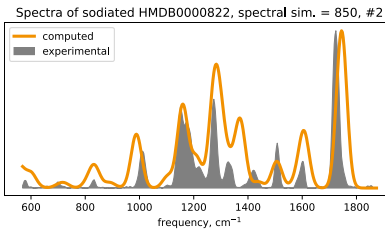
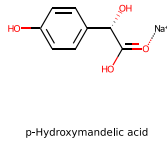
deprotonated HMDB0094709, spectral sim. = 527, #16



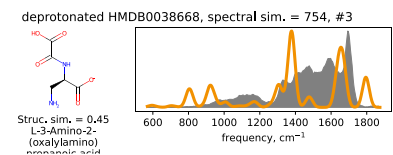
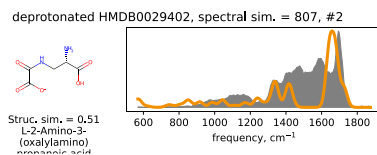
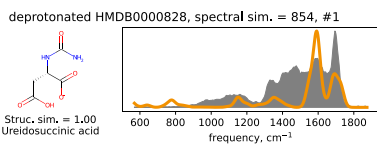
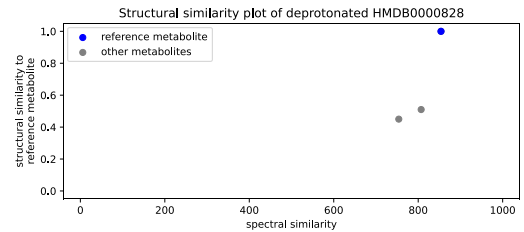
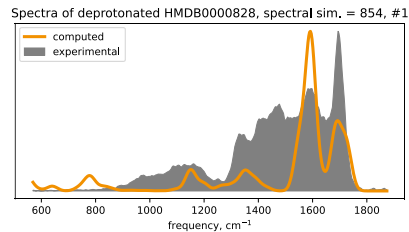
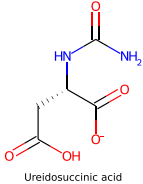
Struc. sim. = 0.47  
3,5-Dihydroxyphenylacetic acid



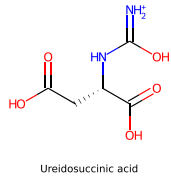
103 sodiated HMDB0000822



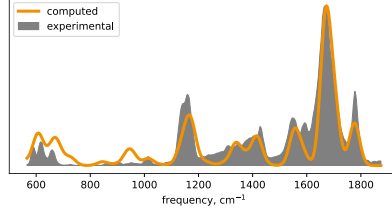
104 deprotonated HMDB0000828



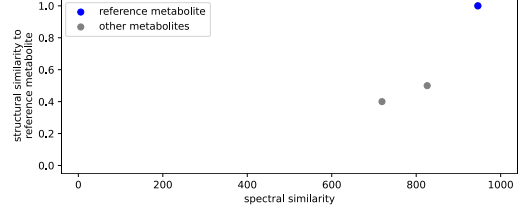
105 protonated HMDB0000828



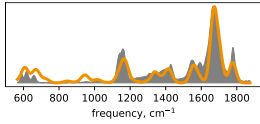
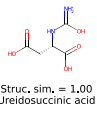
Spectra of protonated HMDB0000828, spectral sim. = 946, #1



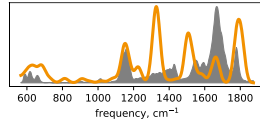
Structural similarity plot of protonated HMDB0000828



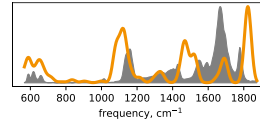
protonated HMDB0000828, spectral sim. = 946, #1



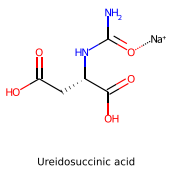
protonated HMDB0029402, spectral sim. = 826, #2



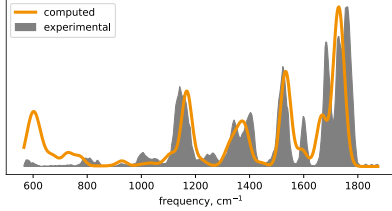
protonated HMDB0038668, spectral sim. = 719, #3



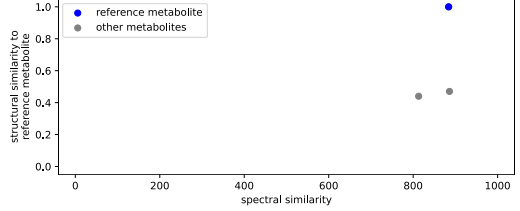
106 sodiated HMDB0000828



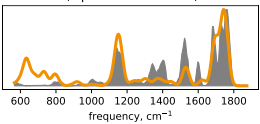
Spectra of sodiated HMDB0000828, spectral sim. = 884, #2



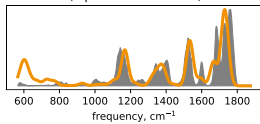
Structural similarity plot of sodiated HMDB0000828



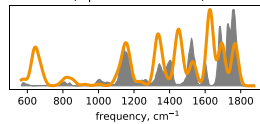
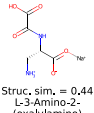
sodiated HMDB0029402, spectral sim. = 886, #1



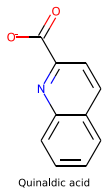
sodiated HMDB0000828, spectral sim. = 884, #2



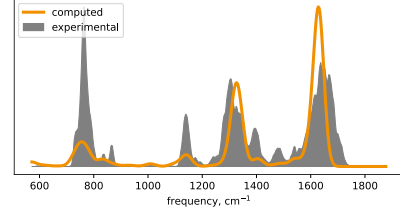
sodiated HMDB0038668, spectral sim. = 813, #3



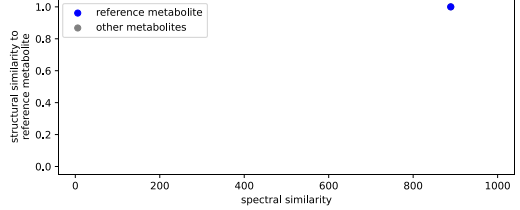
107 deprotonated HMDB0000842



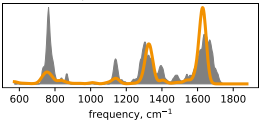
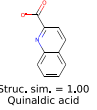
Spectra of deprotonated HMDB0000842, spectral sim. = 889, #1



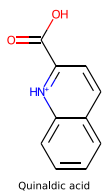
Structural similarity plot of deprotonated HMDB0000842



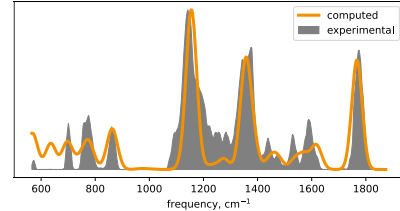
deprotonated HMDB0000842, spectral sim. = 889, #1



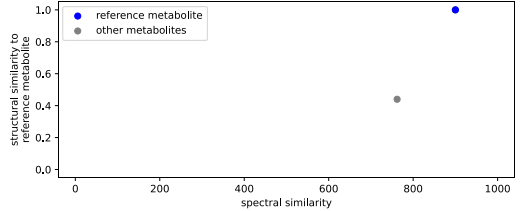
108 protonated HMDB0000842



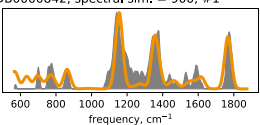
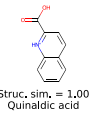
Spectra of protonated HMDB0000842, spectral sim. = 900, #1



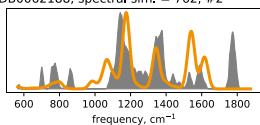
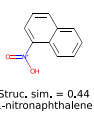
Structural similarity plot of protonated HMDB0000842



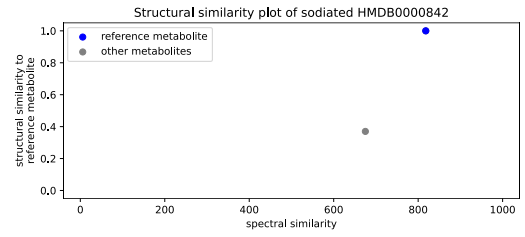
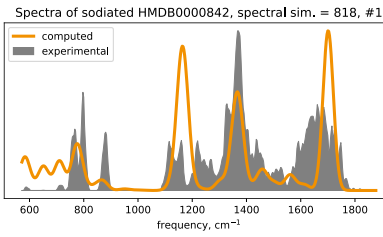
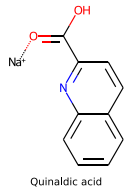
protonated HMDB0000842, spectral sim. = 900, #1



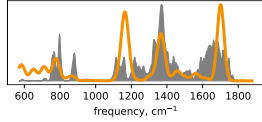
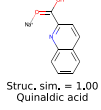
protonated HMDB0062188, spectral sim. = 762, #2



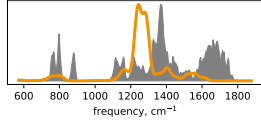
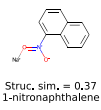
109 sodiated HMDB0000842



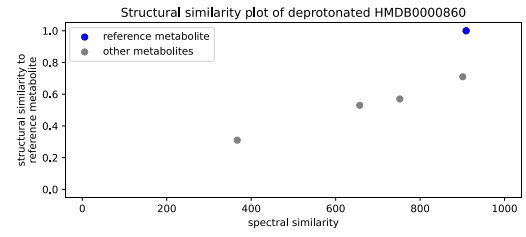
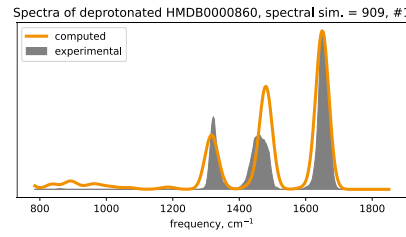
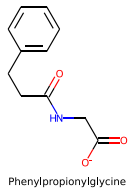
sodiated HMDB0000842, spectral sim. = 818, #1



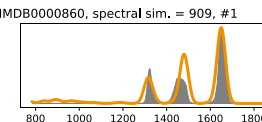
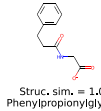
sodiated HMDB0062188, spectral sim. = 675, #2



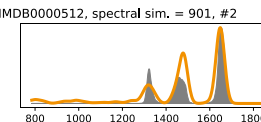
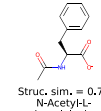
110 deprotonated HMDB0000860



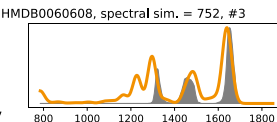
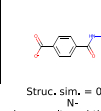
deprotonated HMDB0000860, spectral sim. = 909, #1



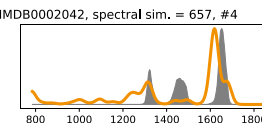
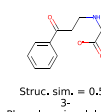
deprotonated HMDB0000512, spectral sim. = 901, #2



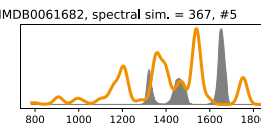
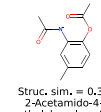
deprotonated HMDB0060608, spectral sim. = 752, #3



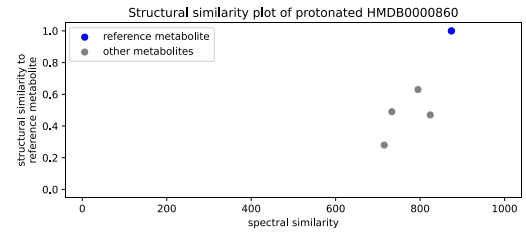
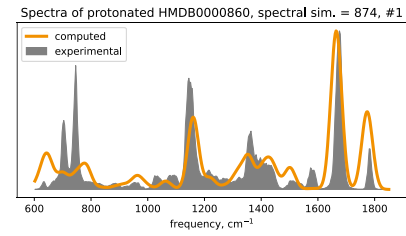
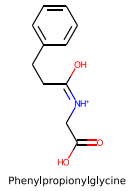
deprotonated HMDB0002042, spectral sim. = 657, #4



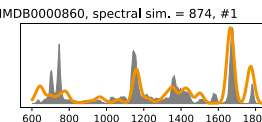
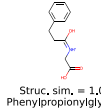
deprotonated HMDB0061682, spectral sim. = 367, #5



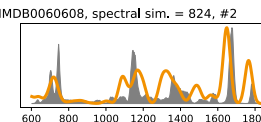
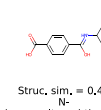
111 protonated HMDB0000860



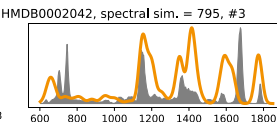
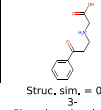
protonated HMDB0000860, spectral sim. = 874, #1



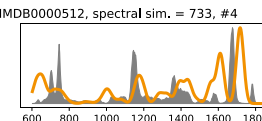
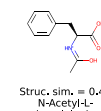
protonated HMDB0060608, spectral sim. = 824, #2



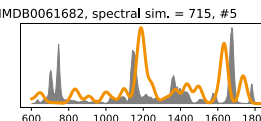
protonated HMDB0002042, spectral sim. = 795, #3



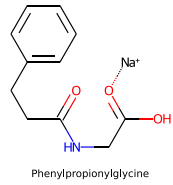
protonated HMDB0000512, spectral sim. = 733, #4



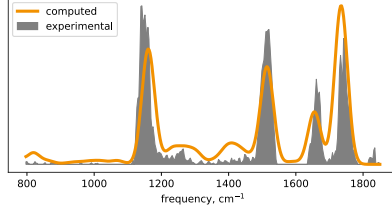
protonated HMDB0061682, spectral sim. = 715, #5



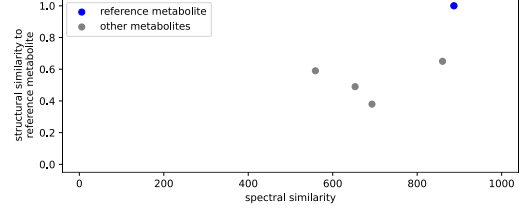
112 sodiated HMDB0000860



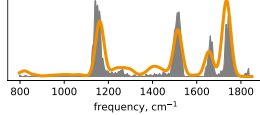
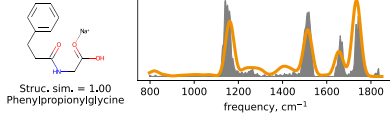
Spectra of sodiated HMDB0000860, spectral sim. = 887, #1



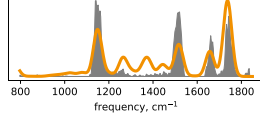
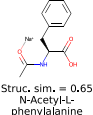
Structural similarity plot of sodiated HMDB0000860



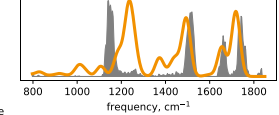
sodiated HMDB0000860, spectral sim. = 887, #1



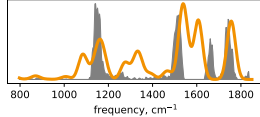
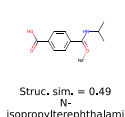
sodiated HMDB0000512, spectral sim. = 860, #2



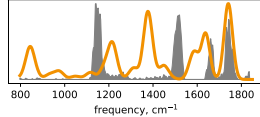
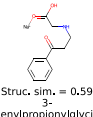
sodiated HMDB0061682, spectral sim. = 693, #3



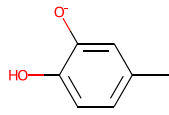
sodiated HMDB0060608, spectral sim. = 653, #4



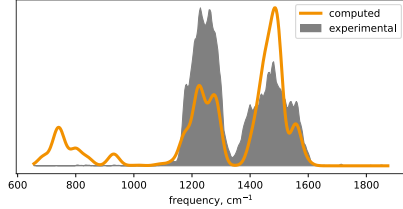
sodiated HMDB0002042, spectral sim. = 559, #5



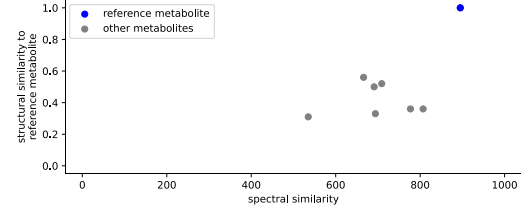
113 deprotonated HMDB0000873



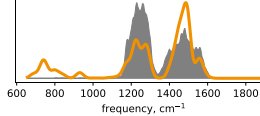
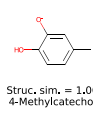
Spectra of deprotonated HMDB0000873, spectral sim. = 895, #1



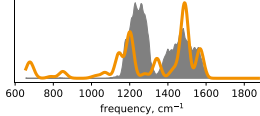
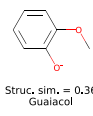
Structural similarity plot of deprotonated HMDB0000873



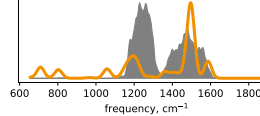
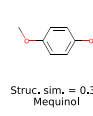
deprotonated HMDB0000873, spectral sim. = 895, #1



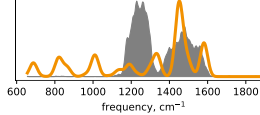
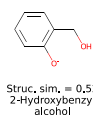
deprotonated HMDB0001398, spectral sim. = 807, #2



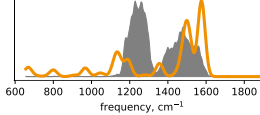
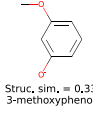
deprotonated HMDB0029696, spectral sim. = 777, #3



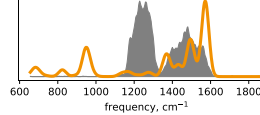
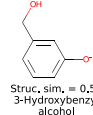
deprotonated HMDB0059709, spectral sim. = 709, #4



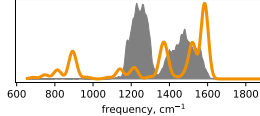
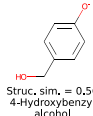
deprotonated HMDB0135619, spectral sim. = 694, #5



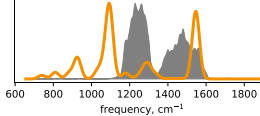
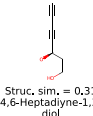
deprotonated HMDB0059712, spectral sim. = 691, #6



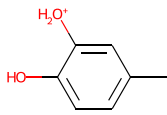
deprotonated HMDB0011724, spectral sim. = 666, #7



deprotonated HMDB0038963, spectral sim. = 535, #8

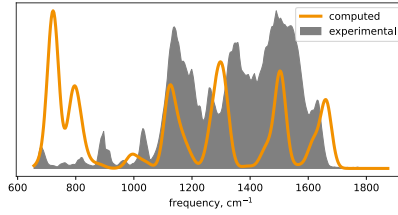


114 protonated HMDB0000873

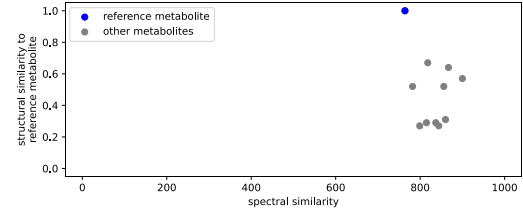


4-Methylcatechol

Spectra of protonated HMDB0000873, spectral sim. = 764, #11



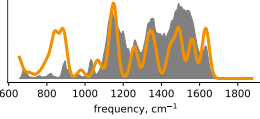
Structural similarity plot of protonated HMDB0000873



protonated HMDB0135619, spectral sim. = 900, #1



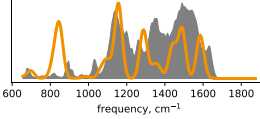
Struc. sim. = 0.57  
3-methoxyphenol



protonated HMDB0029696, spectral sim. = 867, #2



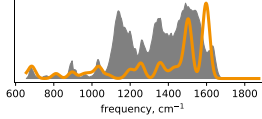
Struc. sim. = 0.64  
Mequinol



protonated HMDB0035226, spectral sim. = 860, #3



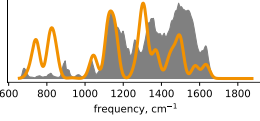
Struc. sim. = 0.31  
2-Acetyl-5-methylfuran



protonated HMDB0001398, spectral sim. = 856, #4



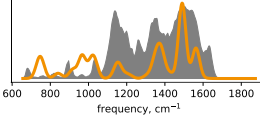
Struc. sim. = 0.52  
Guaiacol



protonated HMDB0032917, spectral sim. = 844, #5



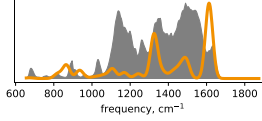
Struc. sim. = 0.27  
1-(2-Furanyl)-2-propanone



protonated HMDB0034877, spectral sim. = 837, #6



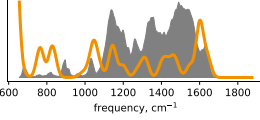
Struc. sim. = 0.29  
2-Acetyl-3-methylfuran



protonated HMDB0059712, spectral sim. = 818, #7



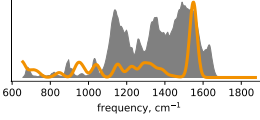
Struc. sim. = 0.67  
3-Hydroxybenzyl alcohol



protonated HMDB0038963, spectral sim. = 815, #8



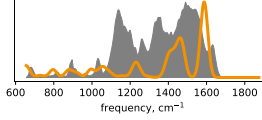
Struc. sim. = 0.29  
4,6-Heptadiyne-1,3-diol



protonated HMDB0040280, spectral sim. = 799, #9



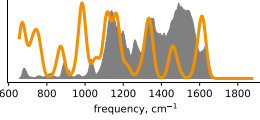
Struc. sim. = 0.27  
1-(2-Furanyl)-1-propanone



protonated HMDB0059709, spectral sim. = 782, #10



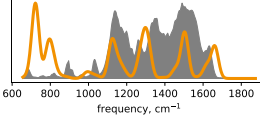
Struc. sim. = 0.52  
2-Hydroxybenzyl alcohol



protonated HMDB0000873, spectral sim. = 764, #11

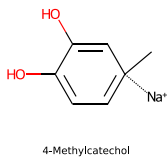


Struc. sim. = 1.00  
4-Methylcatechol

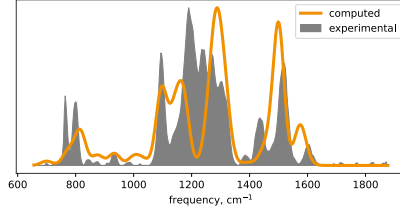




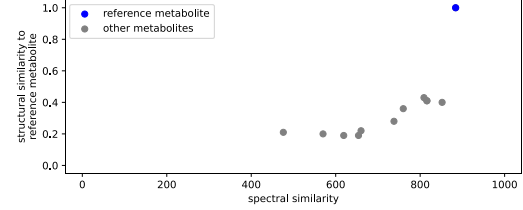
115 sodiated HMDB0000873



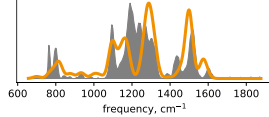
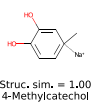
Spectra of sodiated HMDB0000873, spectral sim. = 884, #1



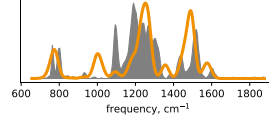
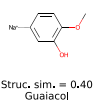
Structural similarity plot of sodiated HMDB0000873



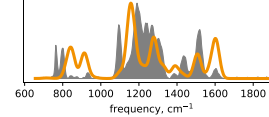
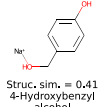
sodiated HMDB0000873, spectral sim. = 884, #1



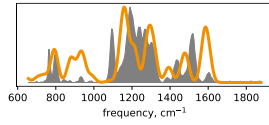
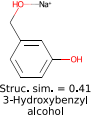
sodiated HMDB0001398, spectral sim. = 852, #2



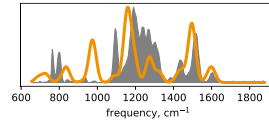
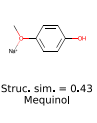
sodiated HMDB0011724, spectral sim. = 816, #3



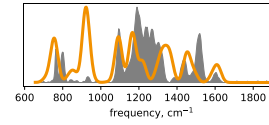
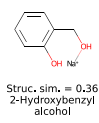
sodiated HMDB0059712, spectral sim. = 816, #4



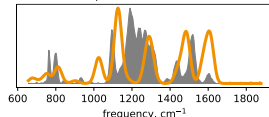
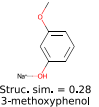
sodiated HMDB0029696, spectral sim. = 809, #5



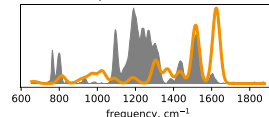
sodiated HMDB0059709, spectral sim. = 760, #6



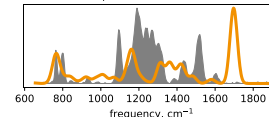
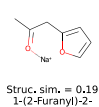
sodiated HMDB0135619, spectral sim. = 738, #7



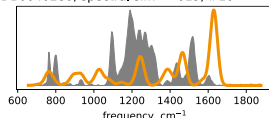
sodiated HMDB0035226, spectral sim. = 660, #8



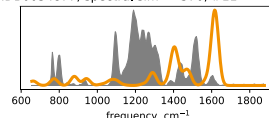
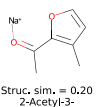
sodiated HMDB0032917, spectral sim. = 654, #9



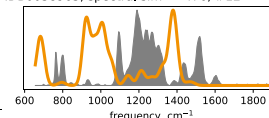
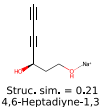
sodiated HMDB0040280, spectral sim. = 619, #10



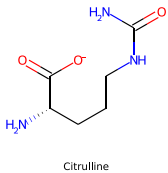
sodiated HMDB0034877, spectral sim. = 570, #11



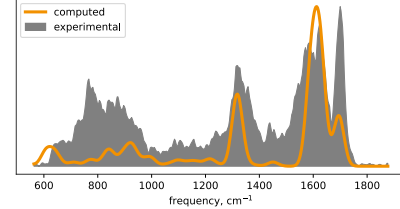
sodiated HMDB0038963, spectral sim. = 476, #12



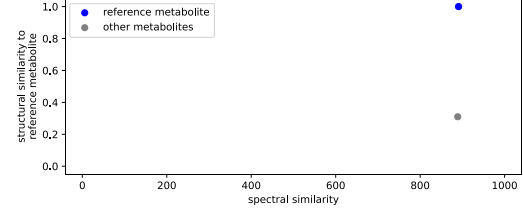
116 deprotonated HMDB0000904



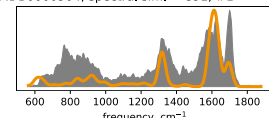
Spectra of deprotonated HMDB0000904, spectral sim. = 891, #1



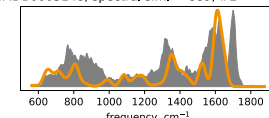
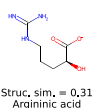
Structural similarity plot of deprotonated HMDB0000904



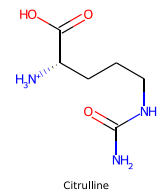
deprotonated HMDB0000904, spectral sim. = 891, #1



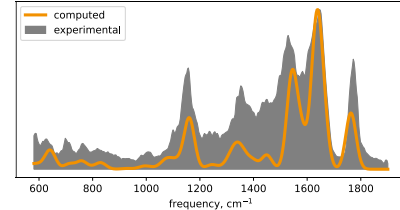
deprotonated HMDB0003148, spectral sim. = 889, #2



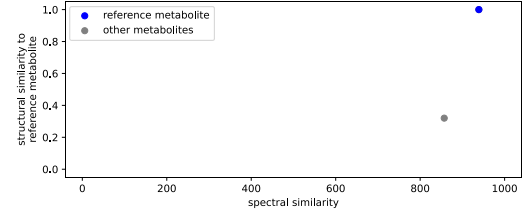
117 protonated HMDB0000904



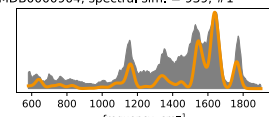
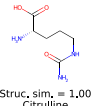
Spectra of protonated HMDB0000904, spectral sim. = 939, #1



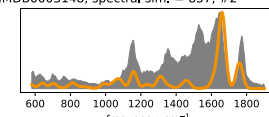
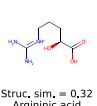
Structural similarity plot of protonated HMDB0000904



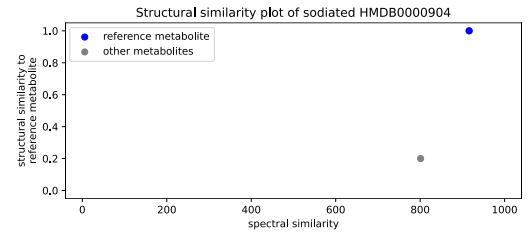
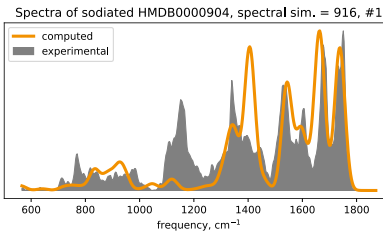
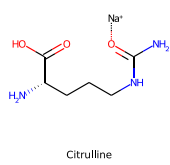
protonated HMDB0000904, spectral sim. = 939, #1



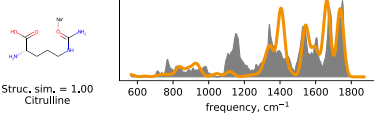
protonated HMDB0003148, spectral sim. = 857, #2



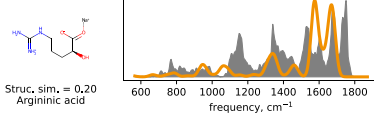
118 sodiated HMDB0000904



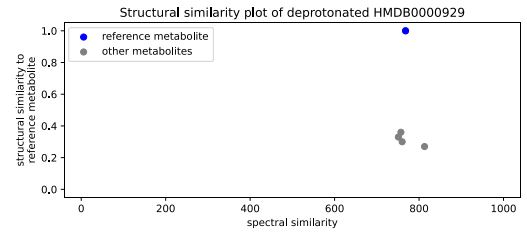
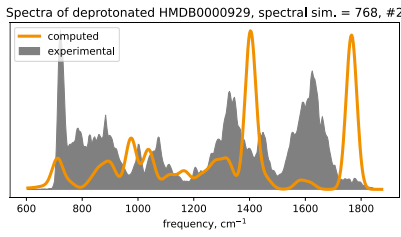
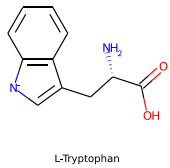
sodiated HMDB0000904, spectral sim. = 916, #1



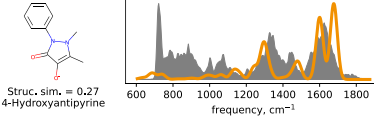
sodiated HMDB0003148, spectral sim. = 801, #2



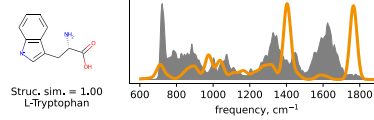
119 deprotonated HMDB0000929



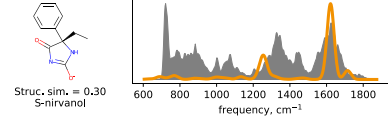
deprotonated HMDB0060878, spectral sim. = 813, #1



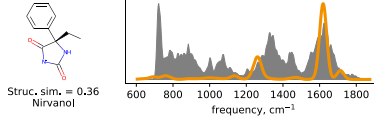
deprotonated HMDB0000929, spectral sim. = 768, #2



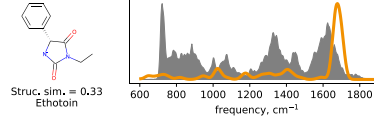
deprotonated HMDB0060967, spectral sim. = 760, #3



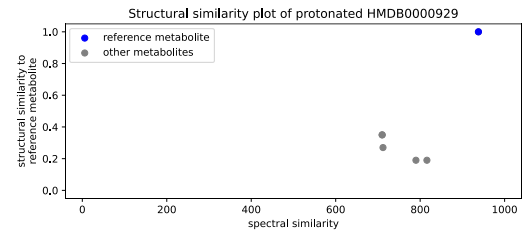
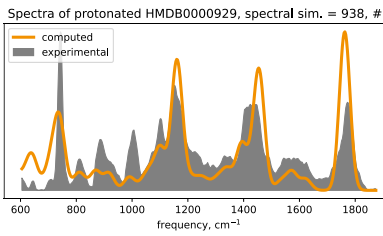
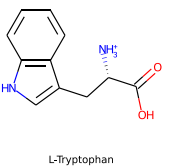
deprotonated HMDB0060533, spectral sim. = 757, #4



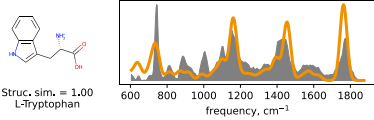
deprotonated HMDB0014892, spectral sim. = 751, #5



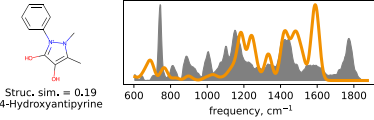
120 protonated HMDB0000929



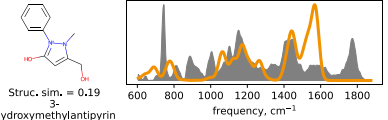
protonated HMDB0000929, spectral sim. = 938, #1



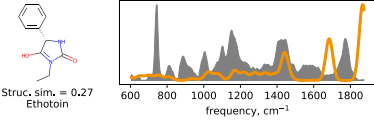
protonated HMDB0060878, spectral sim. = 816, #2



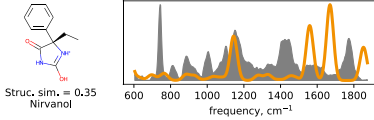
protonated HMDB0013840, spectral sim. = 790, #3



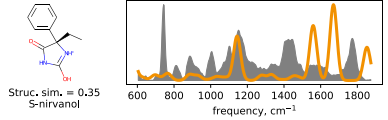
protonated HMDB0014892, spectral sim. = 712, #4



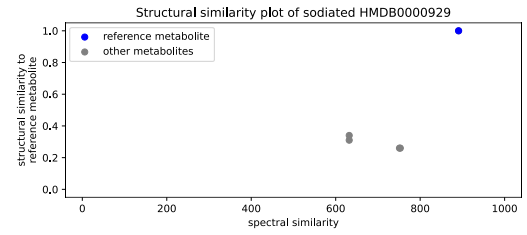
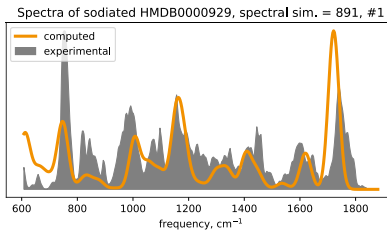
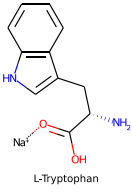
protonated HMDB0060533, spectral sim. = 710, #5



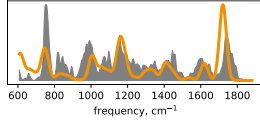
protonated HMDB0060967, spectral sim. = 710, #6



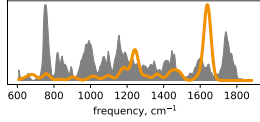
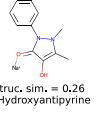
121 sodiated HMDB0000929



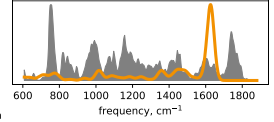
sodiated HMDB0000929, spectral sim. = 891, #1



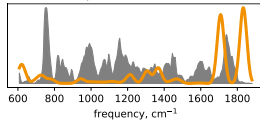
sodiated HMDB0060878, spectral sim. = 753, #2



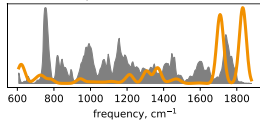
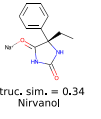
sodiated HMDB0013840, spectral sim. = 751, #3



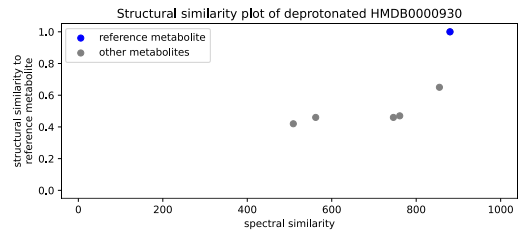
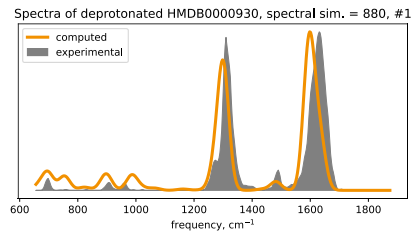
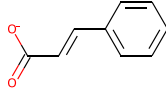
sodiated HMDB0060967, spectral sim. = 632, #4



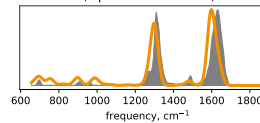
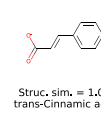
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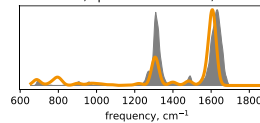
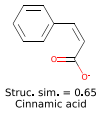
122 deprotonated HMDB0000930



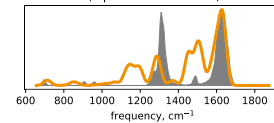
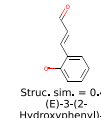
deprotonated HMDB0000930, spectral sim. = 880, #1



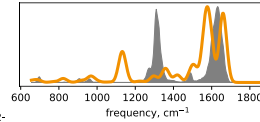
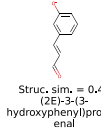
deprotonated HMDB0000567, spectral sim. = 855, #2



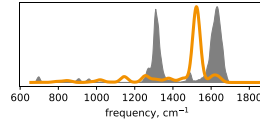
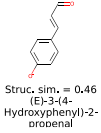
deprotonated HMDB0031725, spectral sim. = 761, #3



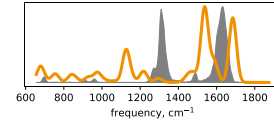
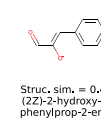
deprotonated HMDB0135274, spectral sim. = 746, #4



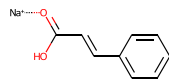
deprotonated HMDB0040986, spectral sim. = 562, #5



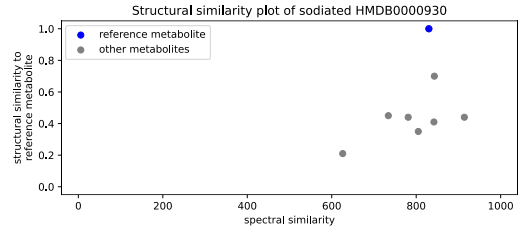
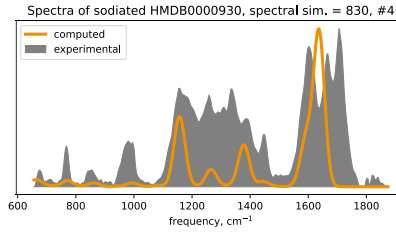
deprotonated HMDB0135273, spectral sim. = 509, #6



123 sodiated HMDB0000930



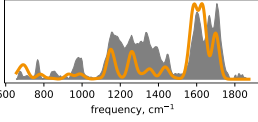
trans-Cinnamic acid



sodiated HMDB0035243, spectral sim. = 914, #1



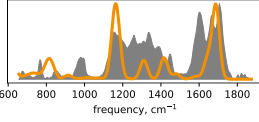
Struc. sim. = 0.44  
1-Phenyl-1,2-propanedione



sodiated HMDB0000567, spectral sim. = 843, #2



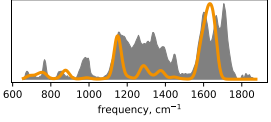
Struc. sim. = 0.70  
Cinnamic acid



sodiated HMDB0135273, spectral sim. = 842, #3



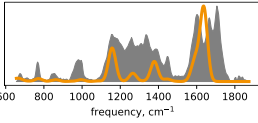
Struc. sim. = 0.41  
(2Z)-2-hydroxy-3-phenylprop-2-enal



sodiated HMDB0000930, spectral sim. = 830, #4



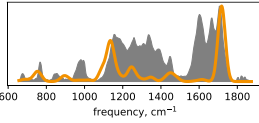
Struc. sim. = 1.00  
trans-Cinnamic acid



sodiated HMDB0036626, spectral sim. = 805, #5



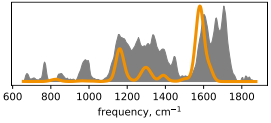
Struc. sim. = 0.35  
3,4-Dihydro-2H-1-benzopyran-2-one



sodiated HMDB0040986, spectral sim. = 781, #6



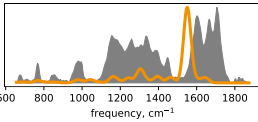
Struc. sim. = 0.44  
(E)-3-(4-Hydroxyphenyl)-2-propenal



sodiated HMDB0135274, spectral sim. = 734, #7



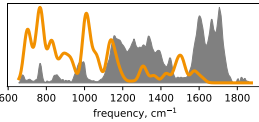
Struc. sim. = 0.45  
(2E)-3-(3-hydroxyphenyl)prop-2-enal



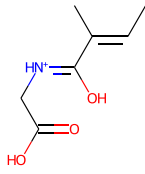
sodiated HMDB0032947, spectral sim. = 626, #8



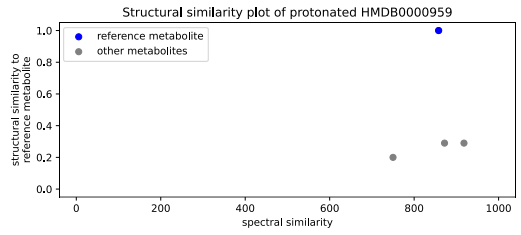
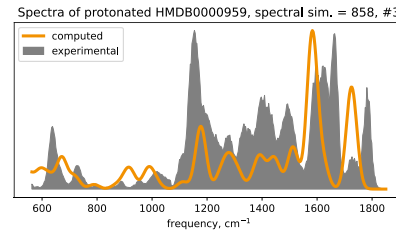
Struc. sim. = 0.21  
Di-2-furanylmethane



124 protonated HMDB0000959



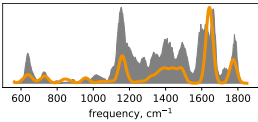
Tiglylglycine



protonated HMDB0000459, spectral sim. = 918, #1



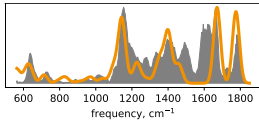
Struc. sim. = 0.29  
Methylcrotonylglycine



protonated HMDB0094701, spectral sim. = 872, #2



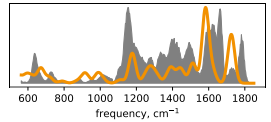
Struc. sim. = 0.29  
N-Acetylproline



protonated HMDB0000959, spectral sim. = 858, #3



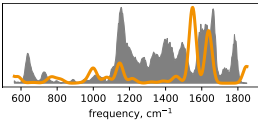
Struc. sim. = 1.00  
Tiglylglycine



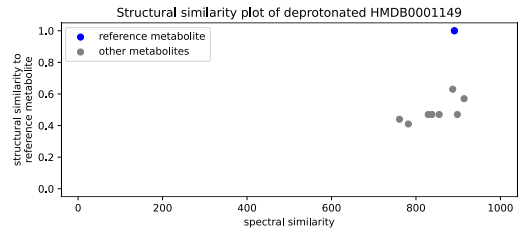
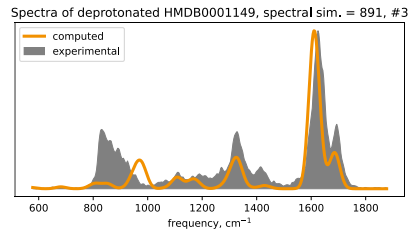
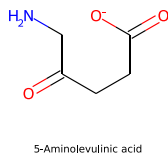
protonated HMDB0014755, spectral sim. = 750, #4



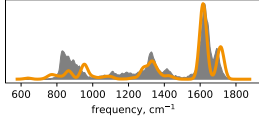
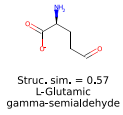
Struc. sim. = 0.20  
Paramethadione



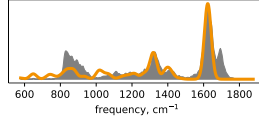
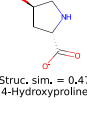
125 deprotonated HMDB0001149



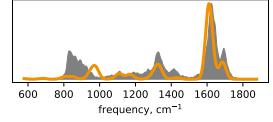
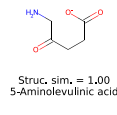
deprotonated HMDB0002104, spectral sim. = 914, #1



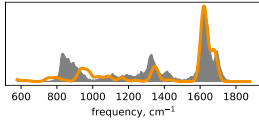
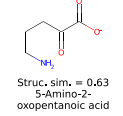
deprotonated HMDB0000725, spectral sim. = 898, #2



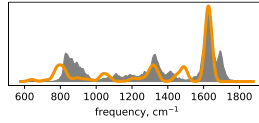
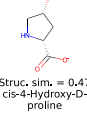
deprotonated HMDB0001149, spectral sim. = 891, #3



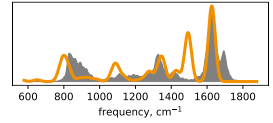
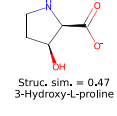
deprotonated HMDB0006272, spectral sim. = 887, #4



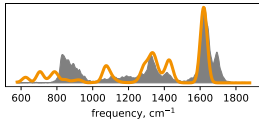
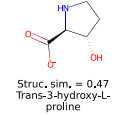
deprotonated HMDB0006460, spectral sim. = 855, #5



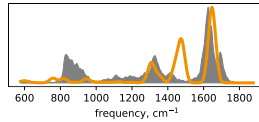
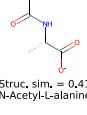
deprotonated HMDB0002113, spectral sim. = 838, #6



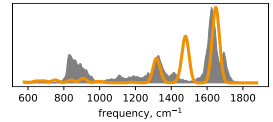
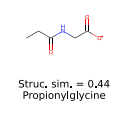
deprotonated HMDB0059659, spectral sim. = 829, #7



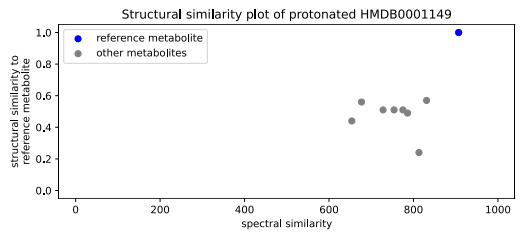
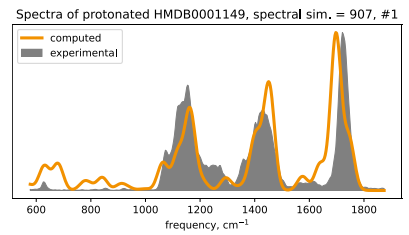
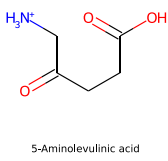
deprotonated HMDB0000766, spectral sim. = 782, #8



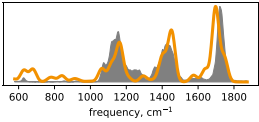
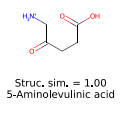
deprotonated HMDB0000783, spectral sim. = 761, #9



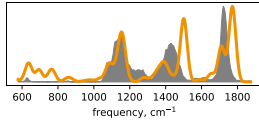
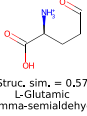
126 protonated HMDB0001149



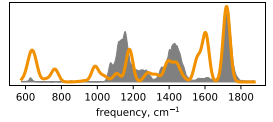
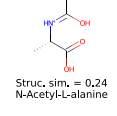
protonated HMDB0001149, spectral sim. = 907, #1



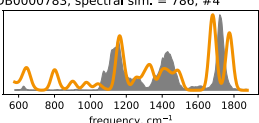
protonated HMDB0002104, spectral sim. = 831, #2



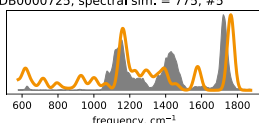
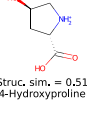
protonated HMDB0000766, spectral sim. = 813, #3



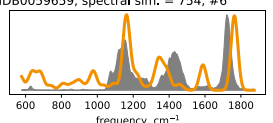
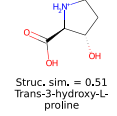
protonated HMDB0000783, spectral sim. = 786, #4



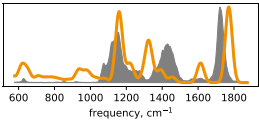
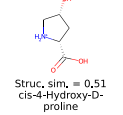
protonated HMDB0000725, spectral sim. = 775, #5



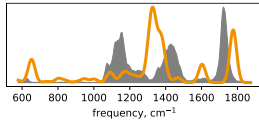
protonated HMDB0059659, spectral sim. = 754, #6



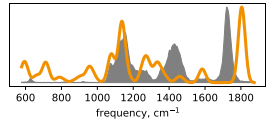
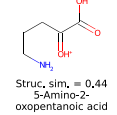
protonated HMDB0006460, spectral sim. = 728, #7



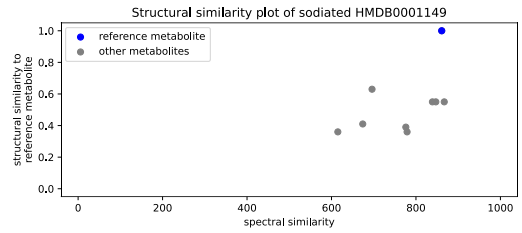
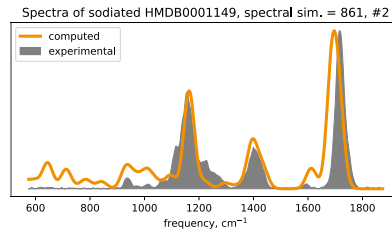
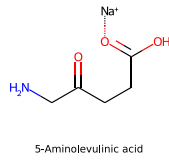
protonated HMDB0002113, spectral sim. = 677, #8



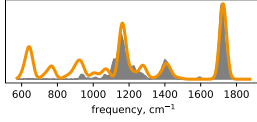
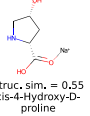
protonated HMDB0006272, spectral sim. = 654, #9



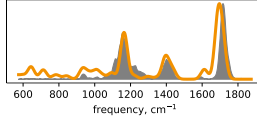
127 sodiated HMDB0001149



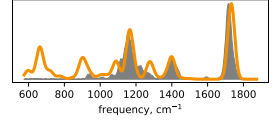
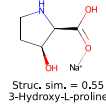
sodiated HMDB0060460, spectral sim. = 867, #1



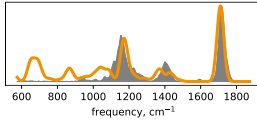
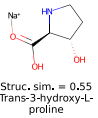
sodiated HMDB0001149, spectral sim. = 861, #2



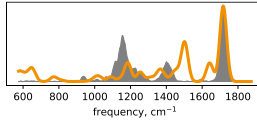
sodiated HMDB0002113, spectral sim. = 847, #3



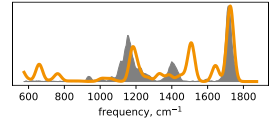
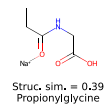
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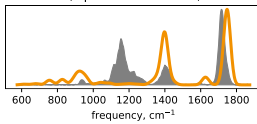
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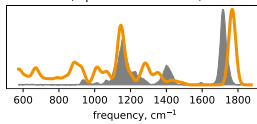
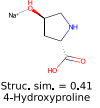
sodiated HMDB0000783, spectral sim. = 776, #6



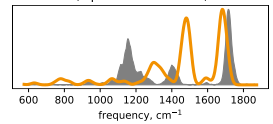
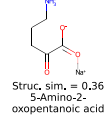
sodiated HMDB0002104, spectral sim. = 696, #7



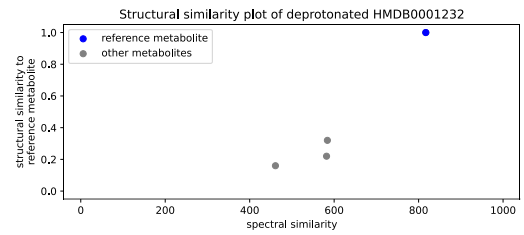
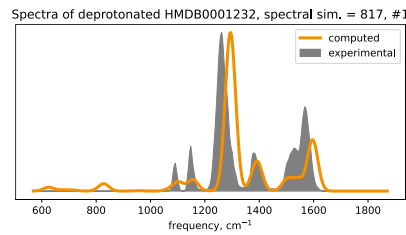
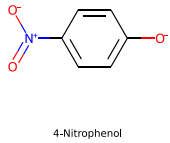
sodiated HMDB0000725, spectral sim. = 674, #8



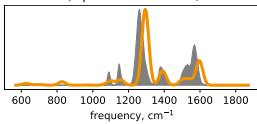
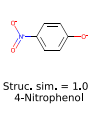
sodiated HMDB0006272, spectral sim. = 615, #9



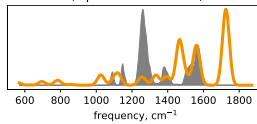
128 deprotonated HMDB0001232



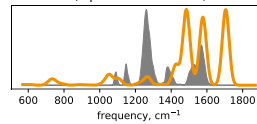
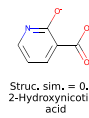
deprotonated HMDB0001232, spectral sim. = 817, #1



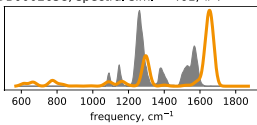
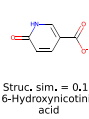
deprotonated HMDB0013188, spectral sim. = 584, #2



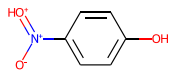
deprotonated HMDB0059710, spectral sim. = 582, #3



deprotonated HMDB0002658, spectral sim. = 461, #4

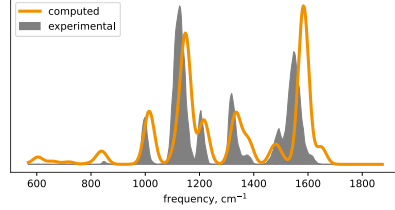


129 protonated HMDB0001232

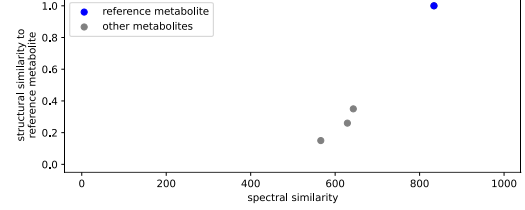


4-Nitrophenol

Spectra of protonated HMDB0001232, spectral sim. = 834, #1



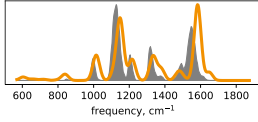
Structural similarity plot of protonated HMDB0001232



protonated HMDB0001232, spectral sim. = 834, #1



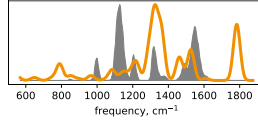
Struc. sim. = 1.00  
4-Nitrophenol



protonated HMDB0013188, spectral sim. = 643, #2



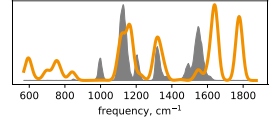
Struc. sim. = 0.25  
3-Hydroxypicolinic acid



protonated HMDB0002658, spectral sim. = 629, #3



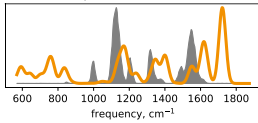
Struc. sim. = 0.26  
6-Hydroxynicotinic acid



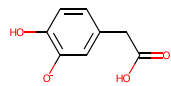
protonated HMDB0059710, spectral sim. = 566, #4



Struc. sim. = 0.15  
2-Hydroxynicotinic acid

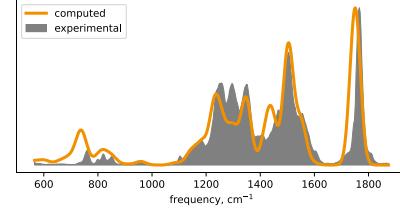


130 deprotonated HMDB0001336

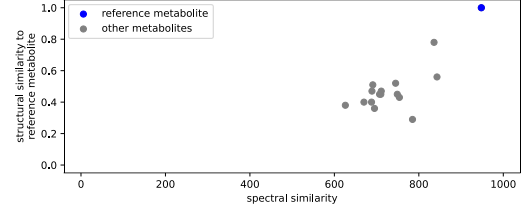


3,4-Dihydroxybenzeneacetic acid

Spectra of deprotonated HMDB0001336, spectral sim. = 948, #1



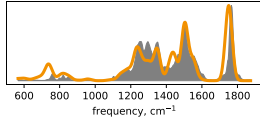
Structural similarity plot of deprotonated HMDB0001336



deprotonated HMDB0001336, spectral sim. = 948, #1



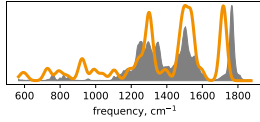
Struc. sim. = 1.00  
3,4-Dihydroxybenzeneacetic acid



deprotonated HMDB0006242, spectral sim. = 843, #2



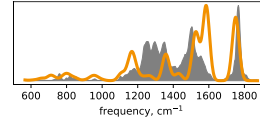
Struc. sim. = 0.56  
3,4-Dihydroxymandelaldehyde



deprotonated HMDB0094709, spectral sim. = 836, #3



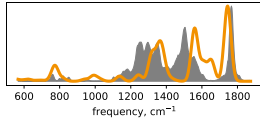
Struc. sim. = 0.78  
3,5-Dihydroxyphenylacetic acid



deprotonated HMDB0033129, spectral sim. = 785, #4



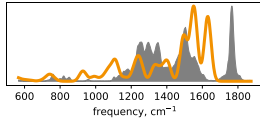
Struc. sim. = 0.29  
3-Acetyl-4-hydroxy-6-methyl-2H-pyran-2-one



deprotonated HMDB0029644, spectral sim. = 754, #5



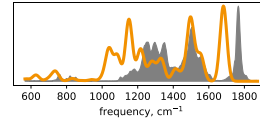
Struc. sim. = 0.43  
Trihydroxyacetophenone



deprotonated HMDB0060003, spectral sim. = 749, #6



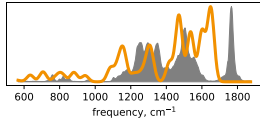
Struc. sim. = 0.45  
Isovanillic acid



deprotonated HMDB0000130, spectral sim. = 745, #7



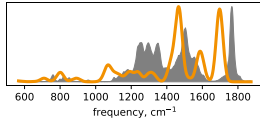
Struc. sim. = 0.52  
Homogentisic acid



deprotonated HMDB0001868, spectral sim. = 711, #8



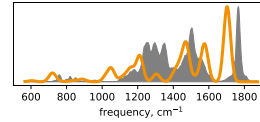
Struc. sim. = 0.47  
5-Methoxysalicylic acid



deprotonated HMDB0059713, spectral sim. = 710, #9



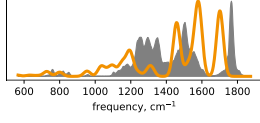
Struc. sim. = 0.45  
3-Methoxysalicylic acid



deprotonated HMDB0131176, spectral sim. = 707, #10



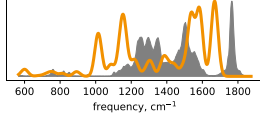
Struc. sim. = 0.45  
2-hydroxy-4-methoxybenzoic acid



deprotonated HMDB0000484, spectral sim. = 695, #11



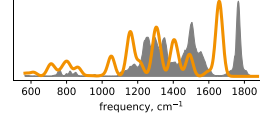
Struc. sim. = 0.36  
Vanillic acid



deprotonated HMDB0000822, spectral sim. = 691, #12



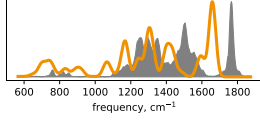
Struc. sim. = 0.51  
p-Hydroxymandelic acid



deprotonated HMDB0000750, spectral sim. = 689, #13



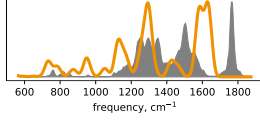
Struc. sim. = 0.47  
3-Hydroxymandelic acid



deprotonated HMDB0125536, spectral sim. = 688, #14



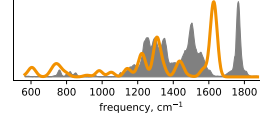
Struc. sim. = 0.40  
3-hydroxy-5-methoxybenzoic acid



deprotonated HMDB0140902, spectral sim. = 670, #15



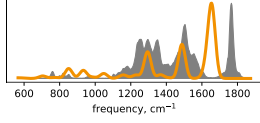
Struc. sim. = 0.40  
3-hydroxy-2-methoxybenzoic acid



deprotonated HMDB0240257, spectral sim. = 626, #16

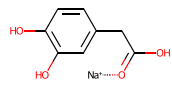


Struc. sim. = 0.38  
Quinolacetic acid



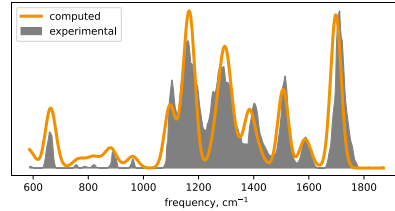


131 sodiated HMDB0001336

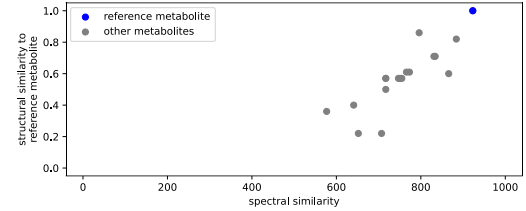


3,4-Dihydroxybenzeneacetic acid

Spectra of sodiated HMDB0001336, spectral sim. = 923, #1



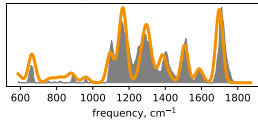
Structural similarity plot of sodiated HMDB0001336



sodiated HMDB0001336, spectral sim. = 923, #1



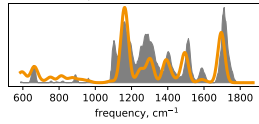
Struc. sim. = 1.00  
3,4-Dihydroxybenzeneacetic acid



sodiated HMDB0000130, spectral sim. = 884, #2



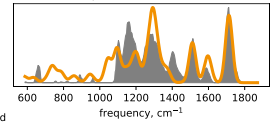
Struc. sim. = 0.82  
Homogentisic acid



sodiated HMDB0006242, spectral sim. = 866, #3



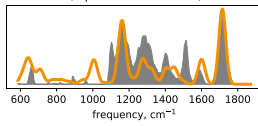
Struc. sim. = 0.60  
3,4-Dihydroxymandelaldehyde



sodiated HMDB0000750, spectral sim. = 834, #4



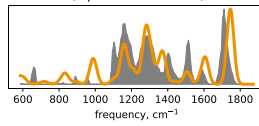
Struc. sim. = 0.71  
3-Hydroxymandelic acid



sodiated HMDB0000822, spectral sim. = 831, #5



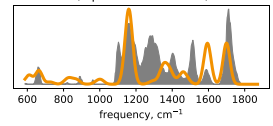
Struc. sim. = 0.71  
p-Hydroxymandelic acid



sodiated HMDB00094709, spectral sim. = 796, #6



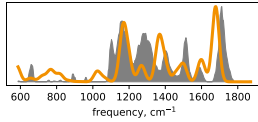
Struc. sim. = 0.86  
3,5-Dihydroxyphenylacetic acid



sodiated HMDB0001868, spectral sim. = 773, #7



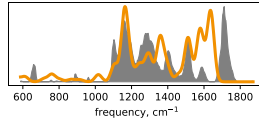
Struc. sim. = 0.61  
5-Methoxysalicylic acid



sodiated HMDB0000484, spectral sim. = 766, #8



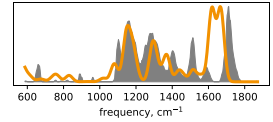
Struc. sim. = 0.61  
Vanillic acid



sodiated HMDB0131176, spectral sim. = 755, #9



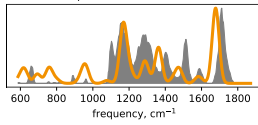
Struc. sim. = 0.57  
2-Hydroxy-4-methoxybenzoic acid



sodiated HMDB0140902, spectral sim. = 751, #10



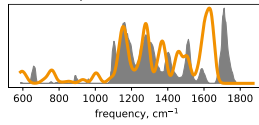
Struc. sim. = 0.57  
3-Hydroxy-2-methoxybenzoic acid



sodiated HMDB0060003, spectral sim. = 747, #11



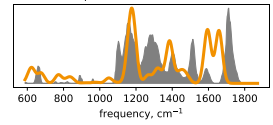
Struc. sim. = 0.57  
Isovanillic acid



sodiated HMDB0125536, spectral sim. = 717, #12



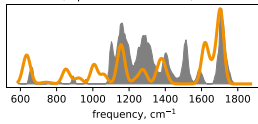
Struc. sim. = 0.57  
3-Hydroxy-5-methoxybenzoic acid



sodiated HMDB0240257, spectral sim. = 717, #13



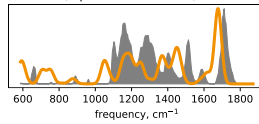
Struc. sim. = 0.50  
Quinolacetic acid



sodiated HMDB0059713, spectral sim. = 717, #14



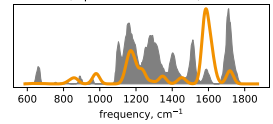
Struc. sim. = 0.57  
3-Methoxysalicylic acid



sodiated HMDB0034335, spectral sim. = 707, #15



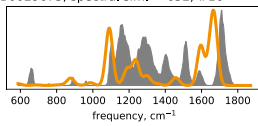
Struc. sim. = 0.22  
Thermophilin



sodiated HMDB0029673, spectral sim. = 652, #16



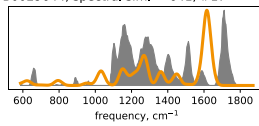
Struc. sim. = 0.22  
2,6-Dimethoxy-1,4-benzoquinone



sodiated HMDB0029644, spectral sim. = 641, #17



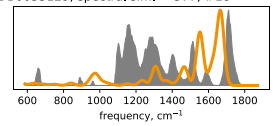
Struc. sim. = 0.40  
2,4,6-Trihydroxyacetophenone



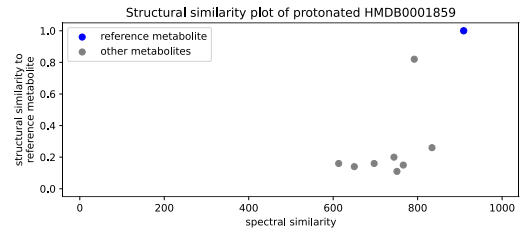
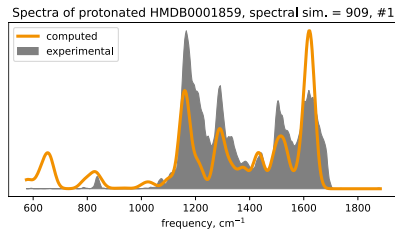
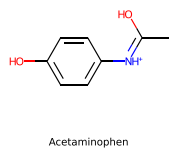
sodiated HMDB0033129, spectral sim. = 577, #18



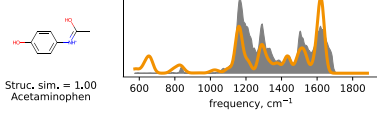
Struc. sim. = 0.36  
3-Acetyl-4-hydroxy-6-methyl-2H-pyran-2-one



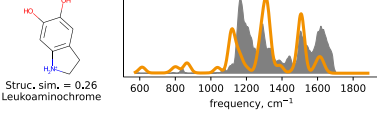
132 protonated HMDB0001859



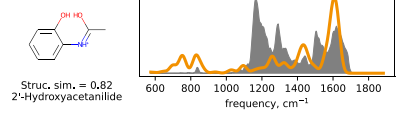
protonated HMDB0001859, spectral sim. = 909, #1



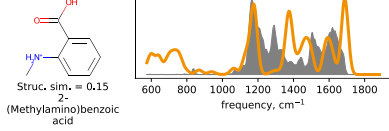
protonated HMDB0012992, spectral sim. = 834, #2



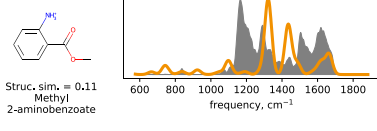
protonated HMDB0061919, spectral sim. = 792, #3



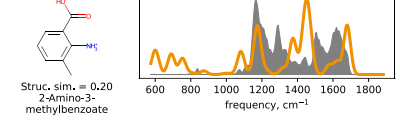
protonated HMDB0032609, spectral sim. = 766, #4



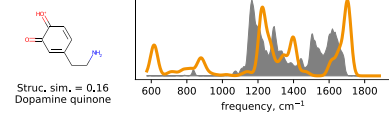
protonated HMDB0029703, spectral sim. = 751, #5



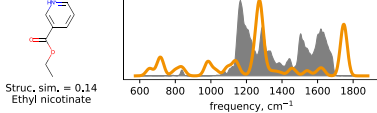
protonated HMDB0060680, spectral sim. = 744, #6



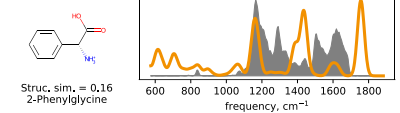
protonated HMDB0012219, spectral sim. = 697, #7



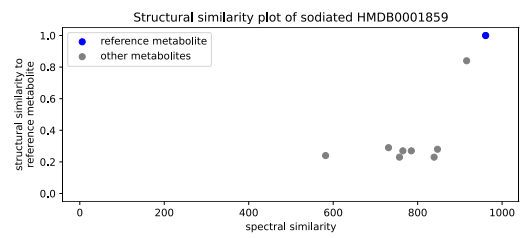
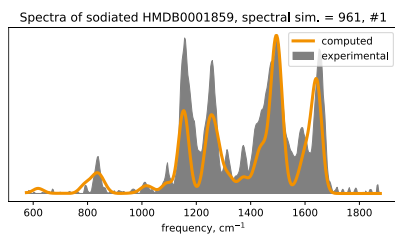
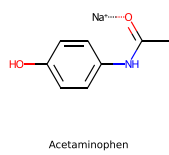
protonated HMDB0059846, spectral sim. = 650, #8



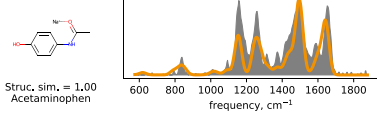
protonated HMDB0002210, spectral sim. = 613, #9



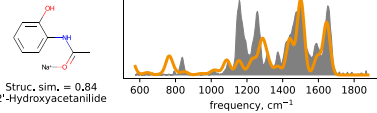
133 sodiated HMDB0001859



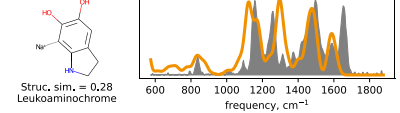
sodiated HMDB0001859, spectral sim. = 961, #1



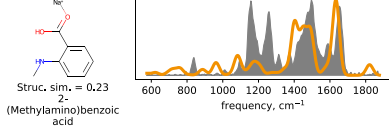
sodiated HMDB0061919, spectral sim. = 916, #2



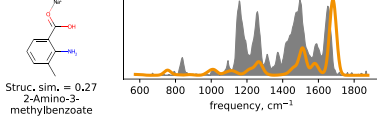
sodiated HMDB0012992, spectral sim. = 847, #3



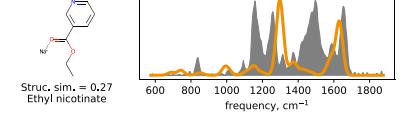
sodiated HMDB0032609, spectral sim. = 839, #4



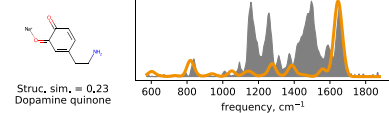
sodiated HMDB0060680, spectral sim. = 785, #5



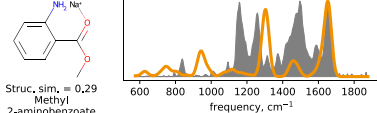
sodiated HMDB0059846, spectral sim. = 765, #6



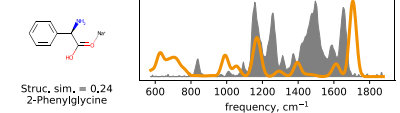
sodiated HMDB0012219, spectral sim. = 757, #7



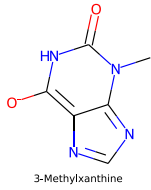
sodiated HMDB0029703, spectral sim. = 731, #8



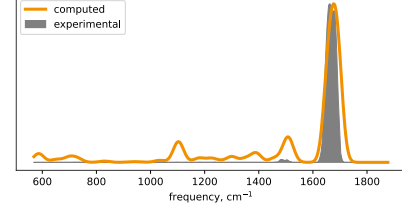
sodiated HMDB0002210, spectral sim. = 582, #9



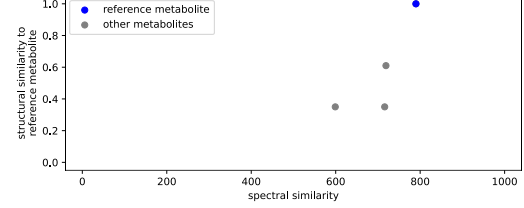
134 deprotonated HMDB0001886



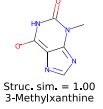
Spectra of deprotonated HMDB0001886, spectral sim. = 790, #1



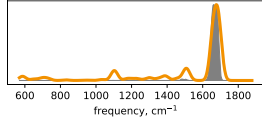
Structural similarity plot of deprotonated HMDB0001886



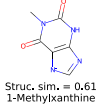
deprotonated HMDB0001886, spectral sim. = 790, #1



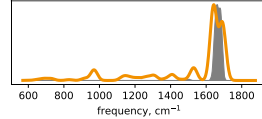
Struc. sim. = 1.00



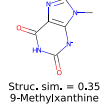
deprotonated HMDB0010738, spectral sim. = 719, #2



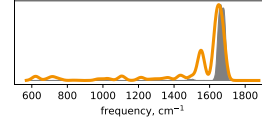
Struc. sim. = 0.61



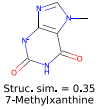
deprotonated HMDB0059716, spectral sim. = 716, #3



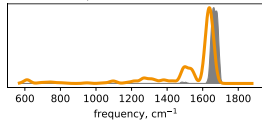
Struc. sim. = 0.35



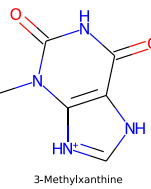
deprotonated HMDB0001991, spectral sim. = 599, #4



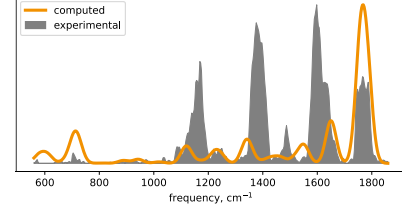
Struc. sim. = 0.35



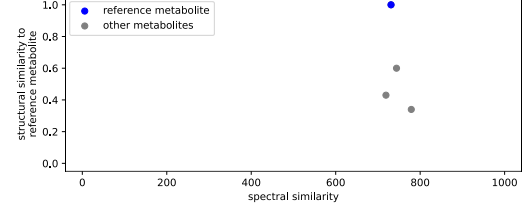
135 protonated HMDB0001886



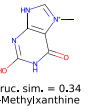
Spectra of protonated HMDB0001886, spectral sim. = 731, #3



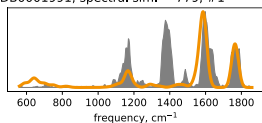
Structural similarity plot of protonated HMDB0001886



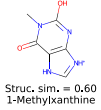
protonated HMDB0001991, spectral sim. = 779, #1



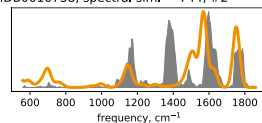
Struc. sim. = 0.34



protonated HMDB0010738, spectral sim. = 744, #2



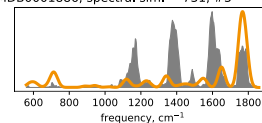
Struc. sim. = 0.60



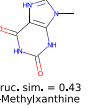
protonated HMDB0001886, spectral sim. = 731, #3



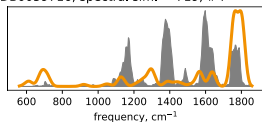
Struc. sim. = 1.00



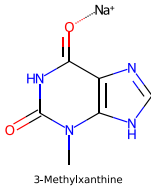
protonated HMDB0059716, spectral sim. = 719, #4



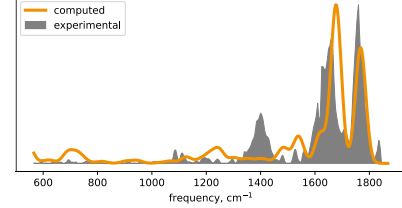
Struc. sim. = 0.43



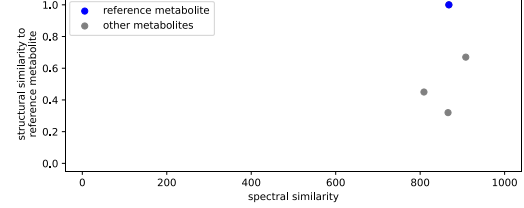
136 sodiated HMDB0001886



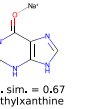
Spectra of sodiated HMDB0001886, spectral sim. = 868, #2



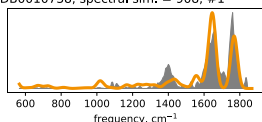
Structural similarity plot of sodiated HMDB0001886



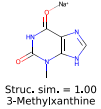
sodiated HMDB0010738, spectral sim. = 908, #1



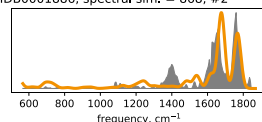
Struc. sim. = 0.67



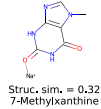
sodiated HMDB0001886, spectral sim. = 868, #2



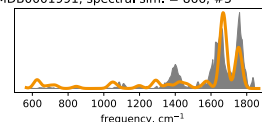
Struc. sim. = 1.00



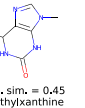
sodiated HMDB0001991, spectral sim. = 866, #3



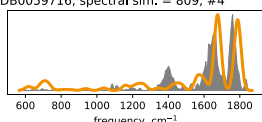
Struc. sim. = 0.32



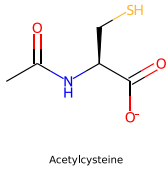
sodiated HMDB0059716, spectral sim. = 809, #4



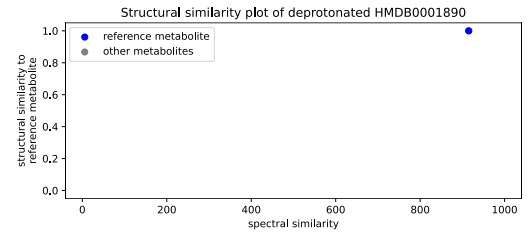
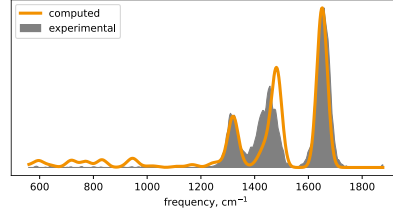
Struc. sim. = 0.45



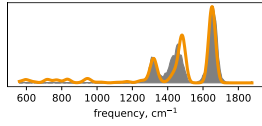
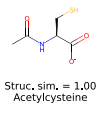
137 deprotonated HMDB0001890



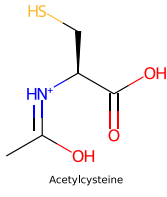
Spectra of deprotonated HMDB0001890, spectral sim. = 915, #1



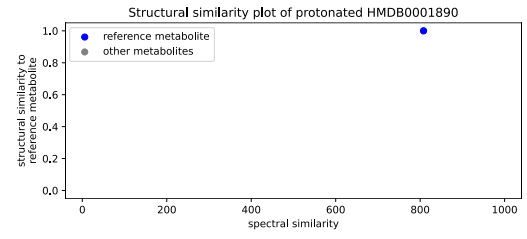
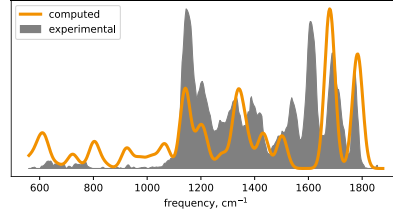
deprotonated HMDB0001890, spectral sim. = 915, #1



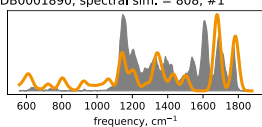
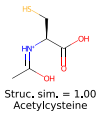
138 protonated HMDB0001890



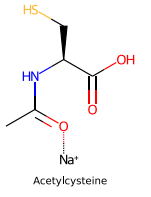
Spectra of protonated HMDB0001890, spectral sim. = 808, #1



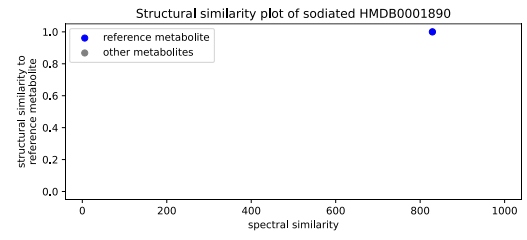
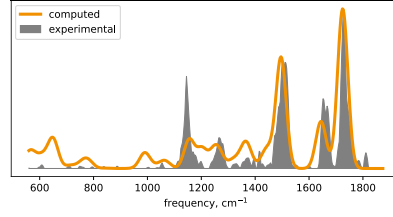
protonated HMDB0001890, spectral sim. = 808, #1



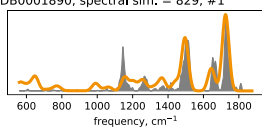
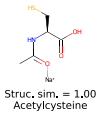
139 sodiated HMDB0001890



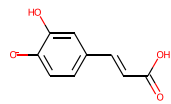
Spectra of sodiated HMDB0001890, spectral sim. = 829, #1



sodiated HMDB0001890, spectral sim. = 829, #1

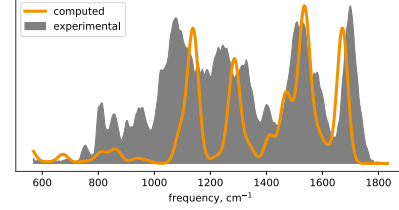


140 deprotonated HMDB0001964

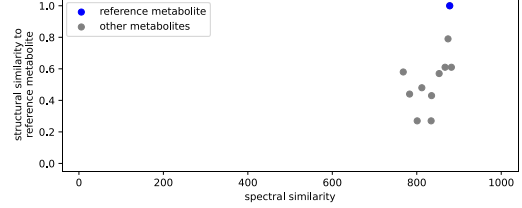


Caffeic acid

Spectra of deprotonated HMDB0001964, spectral sim. = 878, #2



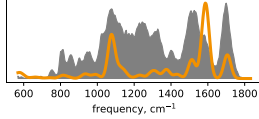
Structural similarity plot of deprotonated HMDB0001964



deprotonated HMDB0125527, spectral sim. = 882, #1



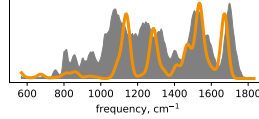
Struc. sim. = 0.61  
(2E)-3-(3,5-dihydroxyphenyl)prop-2-enoic acid



deprotonated HMDB0001964, spectral sim. = 878, #2



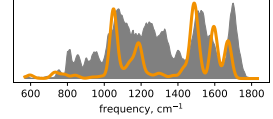
Struc. sim. = 1.00  
Caffeic acid



deprotonated HMDB0140956, spectral sim. = 874, #3



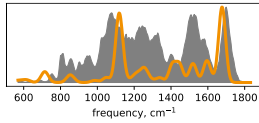
Struc. sim. = 0.79  
(2E)-3-(2,5-dihydroxyphenyl)prop-2-enoic acid



deprotonated HMDB0140954, spectral sim. = 867, #4



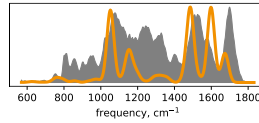
Struc. sim. = 0.61  
(2E)-3-(2,3-dihydroxyphenyl)prop-2-enoic acid



deprotonated HMDB0126377, spectral sim. = 853, #5



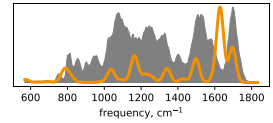
Struc. sim. = 0.57  
(2E)-3-(2,4-dihydroxyphenyl)prop-2-enoic acid



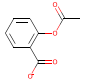
deprotonated HMDB0000707, spectral sim. = 835, #6



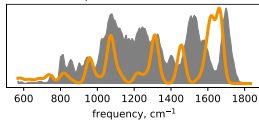
Struc. sim. = 0.43  
4-Hydroxyphenylpyruvic acid



deprotonated HMDB0001879, spectral sim. = 834, #7



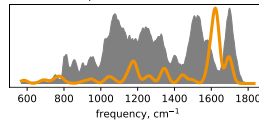
Struc. sim. = 0.27  
Aspirin



deprotonated HMDB0011663, spectral sim. = 812, #8



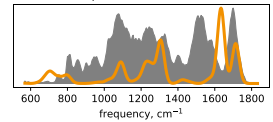
Struc. sim. = 0.48  
3-Hydroxyphenylpyruvic acid



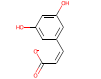
deprotonated HMDB0002130, spectral sim. = 801, #9



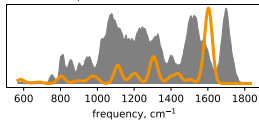
Struc. sim. = 0.27  
Monomethyl phthalate



deprotonated HMDB0032131, spectral sim. = 783, #10



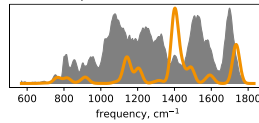
Struc. sim. = 0.44  
3-(3,5-Dihydroxyphenyl)-2-propenoic acid



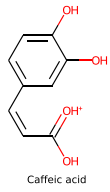
deprotonated HMDB0006915, spectral sim. = 768, #11



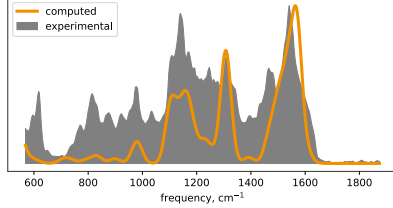
Struc. sim. = 0.58  
2-Hydroxy-3-(4-hydroxyphenyl)propenoic acid



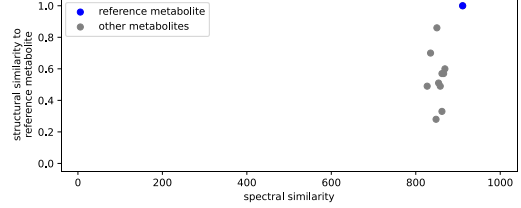
141 protonated HMDB0001964



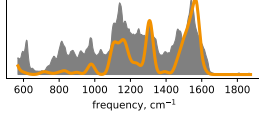
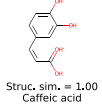
Spectra of protonated HMDB0001964, spectral sim. = 911, #1



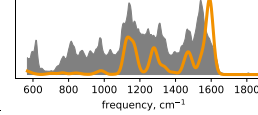
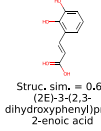
Structural similarity plot of protonated HMDB0001964



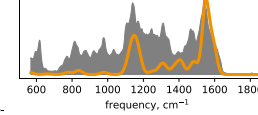
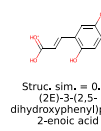
protonated HMDB0001964, spectral sim. = 911, #1



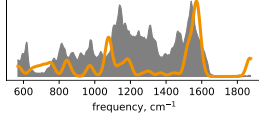
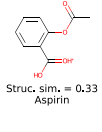
protonated HMDB0140954, spectral sim. = 869, #2



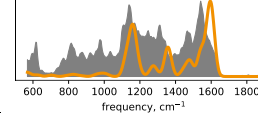
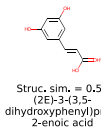
protonated HMDB0140956, spectral sim. = 866, #3



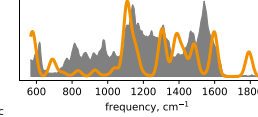
protonated HMDB0001879, spectral sim. = 862, #4



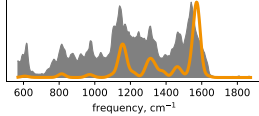
protonated HMDB0125527, spectral sim. = 862, #5



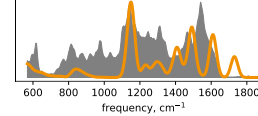
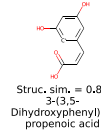
protonated HMDB0000707, spectral sim. = 858, #6



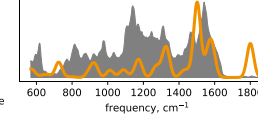
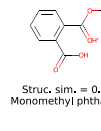
protonated HMDB0126377, spectral sim. = 854, #7



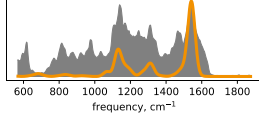
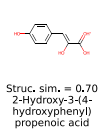
protonated HMDB0032131, spectral sim. = 850, #8



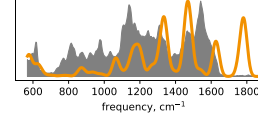
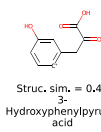
protonated HMDB0002130, spectral sim. = 848, #9



protonated HMDB0006915, spectral sim. = 835, #10

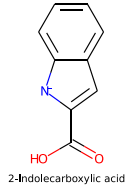


protonated HMDB0011663, spectral sim. = 827, #11

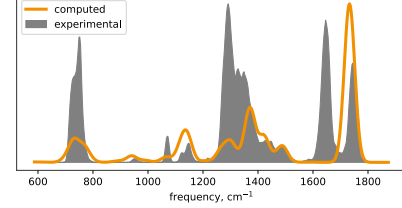




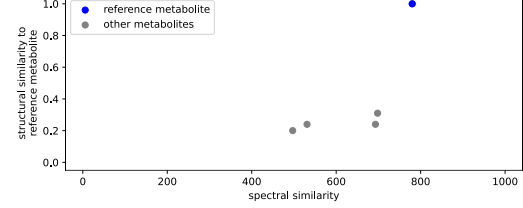
144 deprotonated HMDB0002285



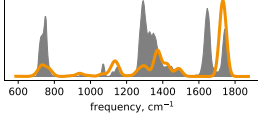
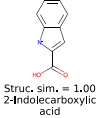
Spectra of deprotonated HMDB0002285, spectral sim. = 780, #1



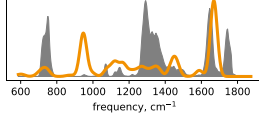
Structural similarity plot of deprotonated HMDB0002285



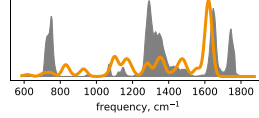
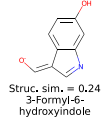
deprotonated HMDB0002285, spectral sim. = 780, #1



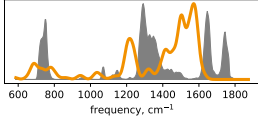
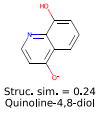
deprotonated HMDB0003320, spectral sim. = 698, #2



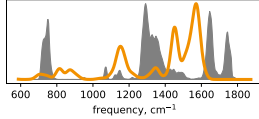
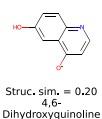
deprotonated HMDB00031172, spectral sim. = 693, #3



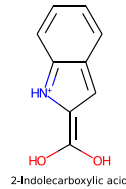
deprotonated HMDB00060289, spectral sim. = 531, #4



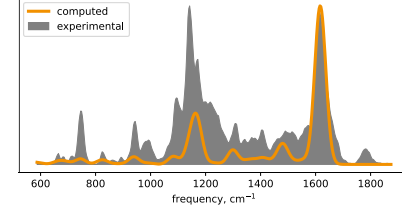
deprotonated HMDB0004077, spectral sim. = 497, #5



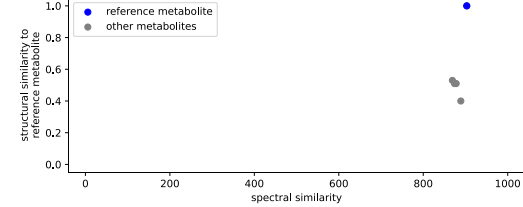
145 protonated HMDB0002285



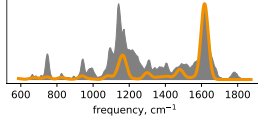
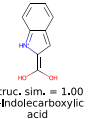
Spectra of protonated HMDB0002285, spectral sim. = 903, #1



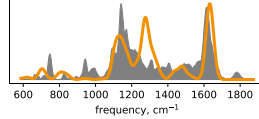
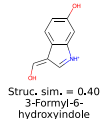
Structural similarity plot of protonated HMDB0002285



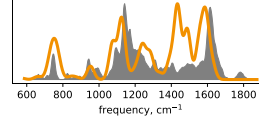
protonated HMDB0002285, spectral sim. = 903, #1



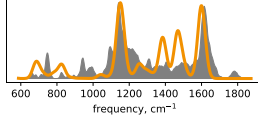
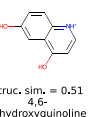
protonated HMDB00031172, spectral sim. = 889, #2



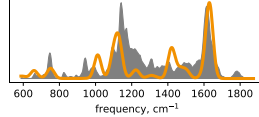
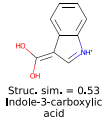
protonated HMDB00060289, spectral sim. = 878, #3



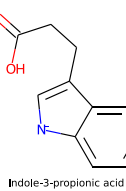
protonated HMDB0004077, spectral sim. = 874, #4



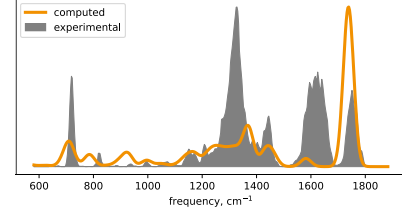
protonated HMDB0003320, spectral sim. = 869, #5



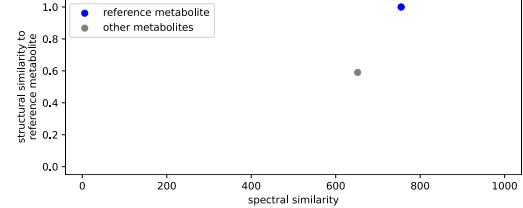
146 deprotonated HMDB0002302



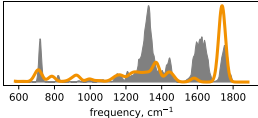
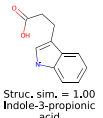
Spectra of deprotonated HMDB0002302, spectral sim. = 755, #1



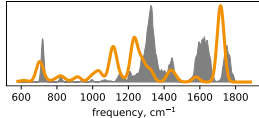
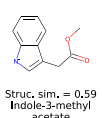
Structural similarity plot of deprotonated HMDB0002302



deprotonated HMDB0002302, spectral sim. = 755, #1

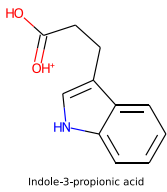


deprotonated HMDB0029738, spectral sim. = 652, #2

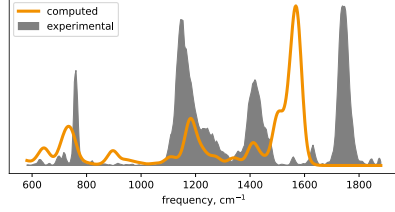




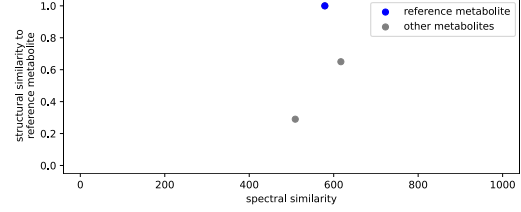
147 protonated HMDB0002302



Spectra of protonated HMDB0002302, spectral sim. = 579, #2



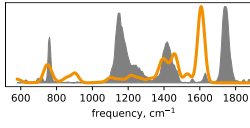
Structural similarity plot of protonated HMDB0002302



protonated HMDB0029738, spectral sim. = 617, #1



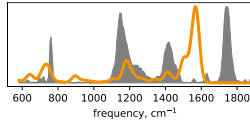
Struc. sim. = 0.65



protonated HMDB0002302, spectral sim. = 579, #2



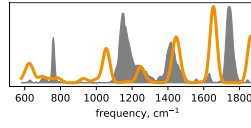
Struc. sim. = 1.00



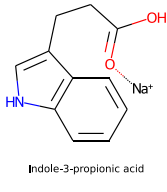
protonated HMDB0014970, spectral sim. = 509, #3



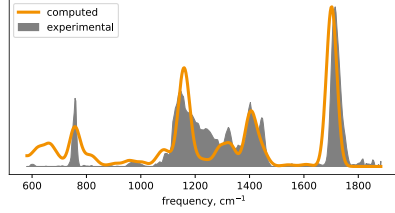
Struc. sim. = 0.29



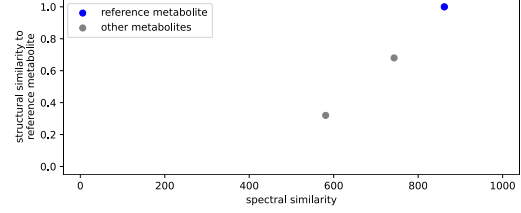
148 sodiated HMDB0002302



Spectra of sodiated HMDB0002302, spectral sim. = 862, #1



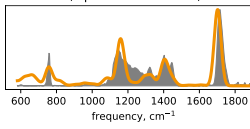
Structural similarity plot of sodiated HMDB0002302



sodiated HMDB0002302, spectral sim. = 862, #1



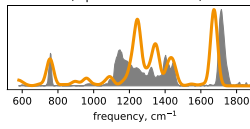
Struc. sim. = 1.00



sodiated HMDB0029738, spectral sim. = 743, #2



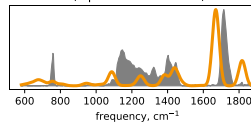
Struc. sim. = 0.68



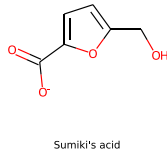
sodiated HMDB0014970, spectral sim. = 581, #3



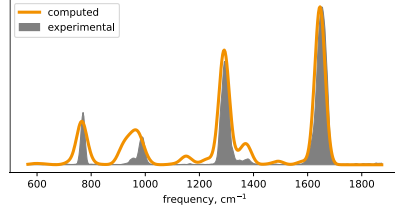
Struc. sim. = 0.32



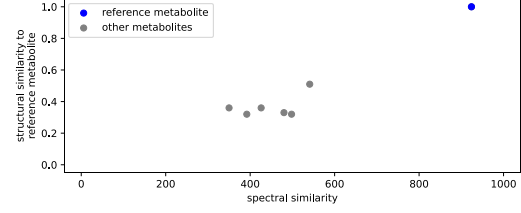
149 deprotonated HMDB0002432



Spectra of deprotonated HMDB0002432, spectral sim. = 924, #1



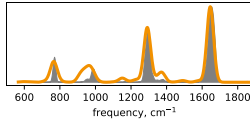
Structural similarity plot of deprotonated HMDB0002432



deprotonated HMDB0002432, spectral sim. = 924, #1



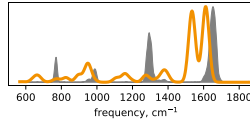
Struc. sim. = 1.00



deprotonated HMDB0032923, spectral sim. = 541, #2



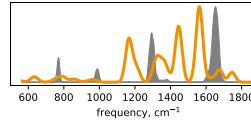
Struc. sim. = 0.51



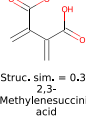
deprotonated HMDB0002349, spectral sim. = 498, #3



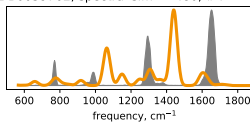
Struc. sim. = 0.32



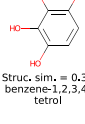
deprotonated HMDB0059762, spectral sim. = 480, #4



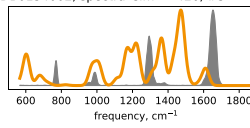
Struc. sim. = 0.33



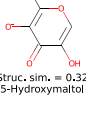
deprotonated HMDB0134002, spectral sim. = 426, #5



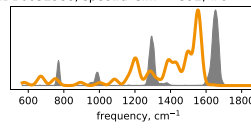
Struc. sim. = 0.36



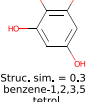
deprotonated HMDB0032988, spectral sim. = 392, #6



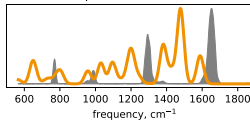
Struc. sim. = 0.32



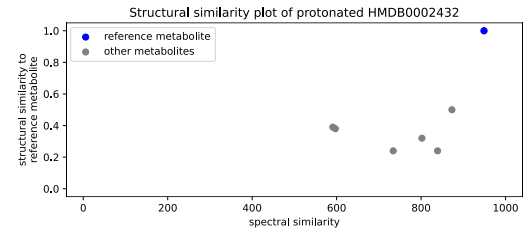
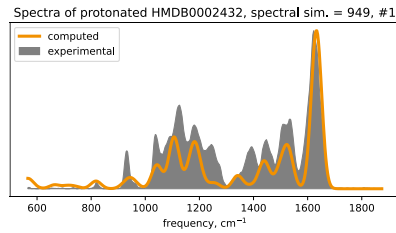
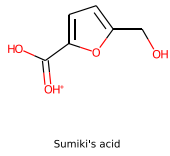
deprotonated HMDB0125218, spectral sim. = 350, #7



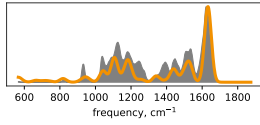
Struc. sim. = 0.36



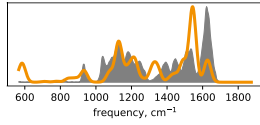
150 protonated HMDB0002432



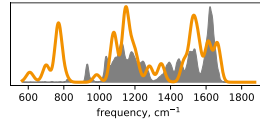
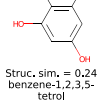
protonated HMDB0002432, spectral sim. = 949, #1



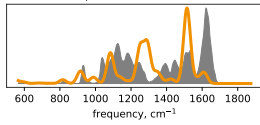
protonated HMDB0032923, spectral sim. = 873, #2



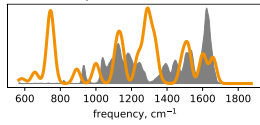
protonated HMDB0125218, spectral sim. = 839, #3



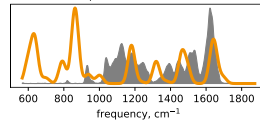
protonated HMDB0032988, spectral sim. = 802, #4



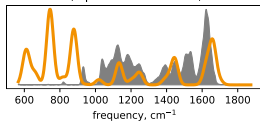
protonated HMDB0134002, spectral sim. = 734, #5



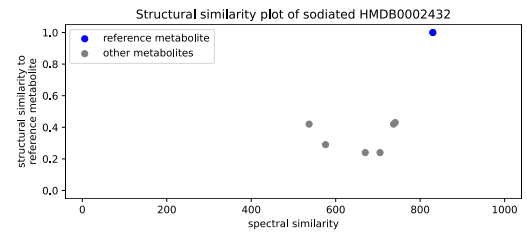
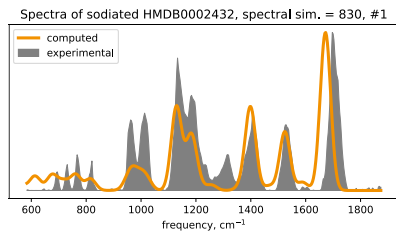
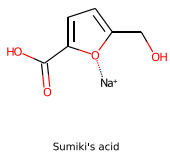
protonated HMDB0002349, spectral sim. = 597, #6



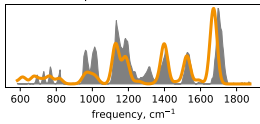
protonated HMDB0059762, spectral sim. = 591, #7



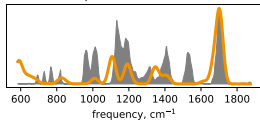
151 sodiated HMDB0002432



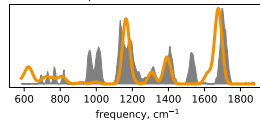
sodiated HMDB0002432, spectral sim. = 830, #1



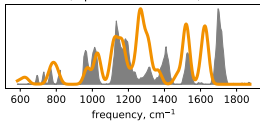
sodiated HMDB0059762, spectral sim. = 741, #2



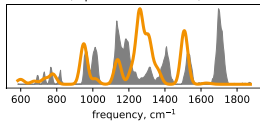
sodiated HMDB0002349, spectral sim. = 737, #3



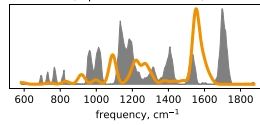
sodiated HMDB0125218, spectral sim. = 705, #4



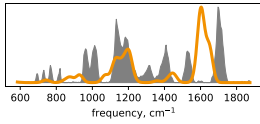
sodiated HMDB0134002, spectral sim. = 670, #5



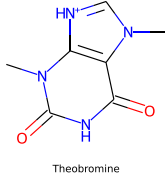
sodiated HMDB0032988, spectral sim. = 576, #6



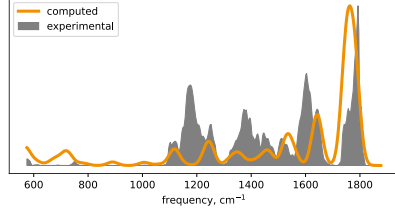
sodiated HMDB0032923, spectral sim. = 537, #7



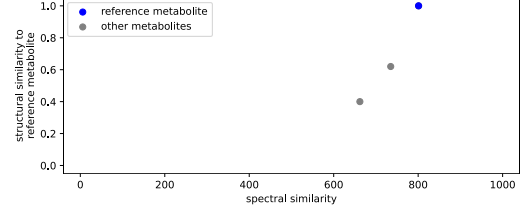
152 protonated HMDB0002825



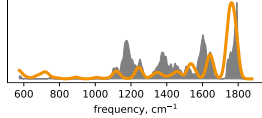
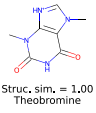
Spectra of protonated HMDB0002825, spectral sim. = 801, #1



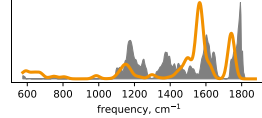
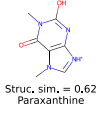
Structural similarity plot of protonated HMDB0002825



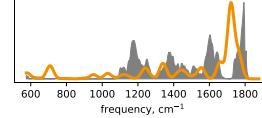
protonated HMDB0002825, spectral sim. = 801, #1



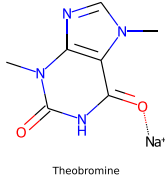
protonated HMDB0001860, spectral sim. = 735, #2



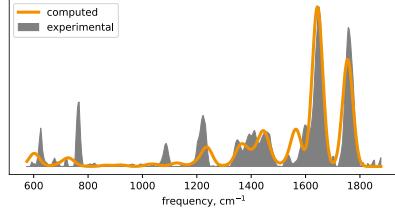
protonated HMDB0001889, spectral sim. = 662, #3



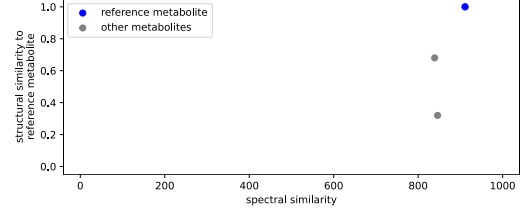
153 sodiated HMDB0002825



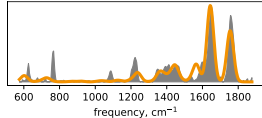
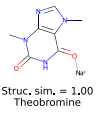
Spectra of sodiated HMDB0002825, spectral sim. = 911, #1



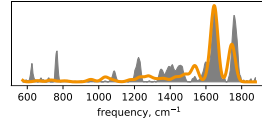
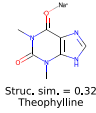
Structural similarity plot of sodiated HMDB0002825



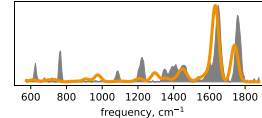
sodiated HMDB0002825, spectral sim. = 911, #1



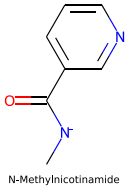
sodiated HMDB0001889, spectral sim. = 846, #2



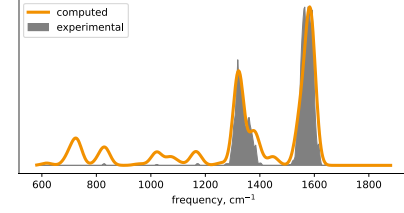
sodiated HMDB0001860, spectral sim. = 839, #3



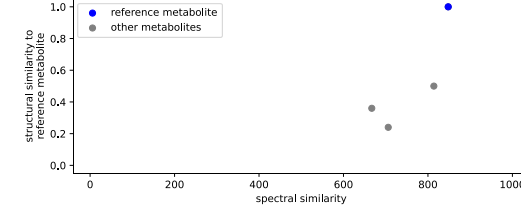
154 deprotonated HMDB0003152



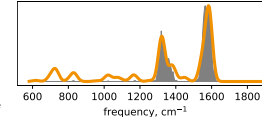
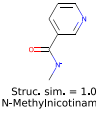
Spectra of deprotonated HMDB0003152, spectral sim. = 848, #1



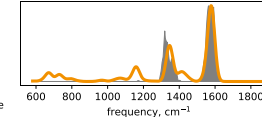
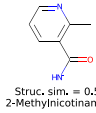
Structural similarity plot of deprotonated HMDB0003152



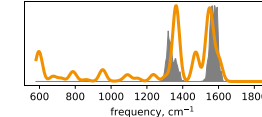
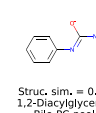
deprotonated HMDB0003152, spectral sim. = 848, #1



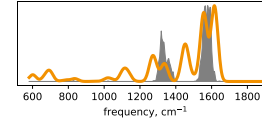
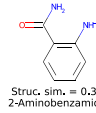
deprotonated HMDB0059711, spectral sim. = 814, #2



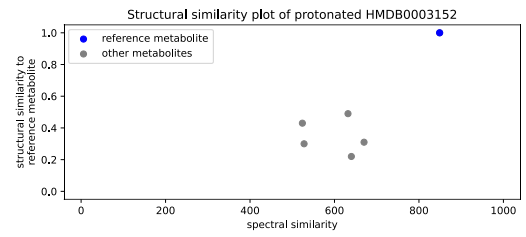
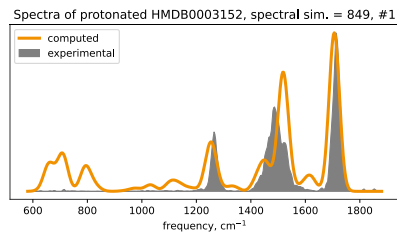
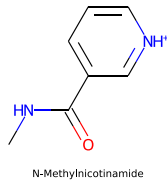
deprotonated HMDB0062267, spectral sim. = 706, #3



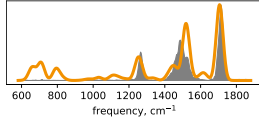
deprotonated HMDB0033947, spectral sim. = 667, #4



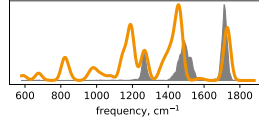
155 protonated HMDB0003152



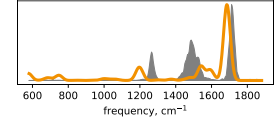
protonated HMDB0003152, spectral sim. = 849, #1



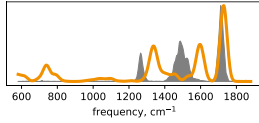
protonated HMDB0030001, spectral sim. = 670, #2



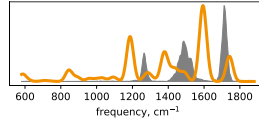
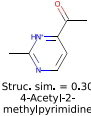
protonated HMDB0062267, spectral sim. = 640, #3



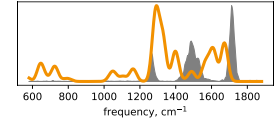
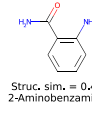
protonated HMDB0059711, spectral sim. = 632, #4



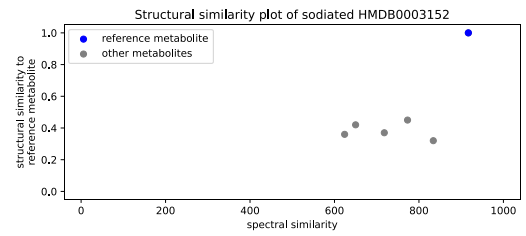
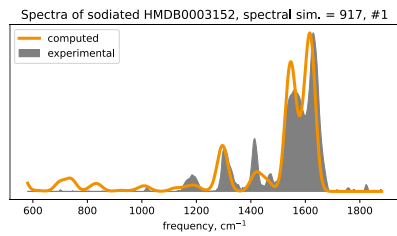
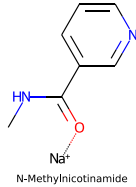
protonated HMDB0037819, spectral sim. = 528, #5



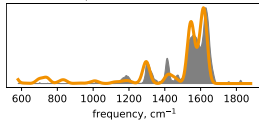
protonated HMDB0033947, spectral sim. = 524, #6



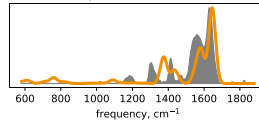
156 sodiated HMDB0003152



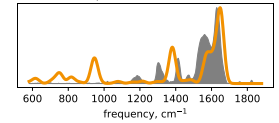
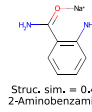
sodiated HMDB0003152, spectral sim. = 917, #1



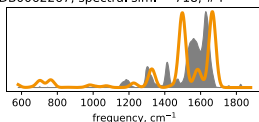
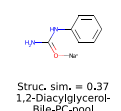
sodiated HMDB0059711, spectral sim. = 834, #2



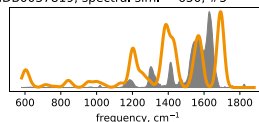
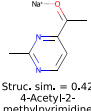
sodiated HMDB0033947, spectral sim. = 773, #3



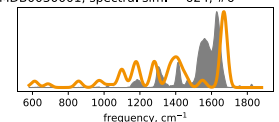
sodiated HMDB0062267, spectral sim. = 718, #4



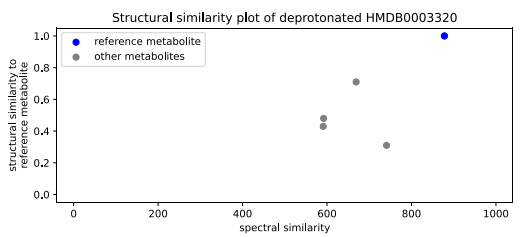
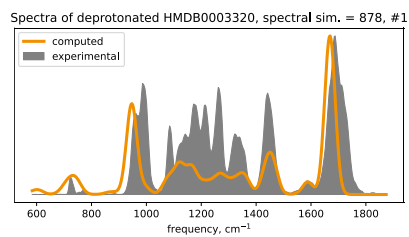
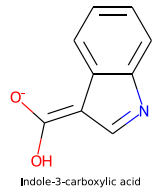
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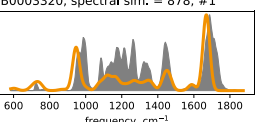
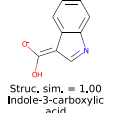
sodiated HMDB0030001, spectral sim. = 624, #6



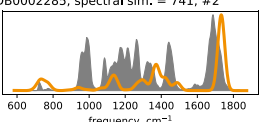
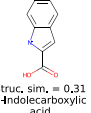
157 deprotonated HMDB0003320



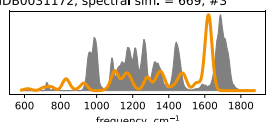
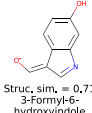
deprotonated HMDB0003320, spectral sim. = 878, #1



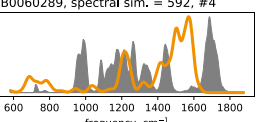
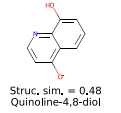
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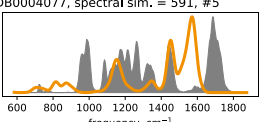
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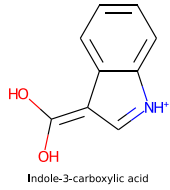
deprotonated HMDB0060289, spectral sim. = 592, #4



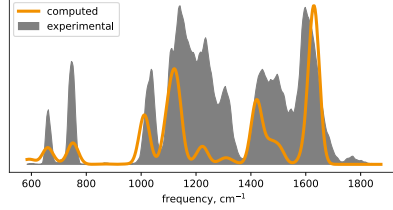
deprotonated HMDB0004077, spectral sim. = 591, #5



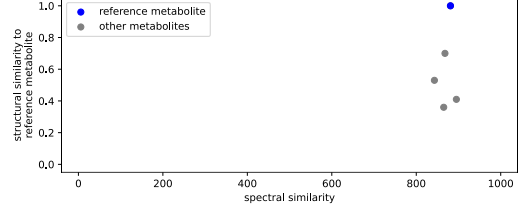
158 protonated HMDB0003320



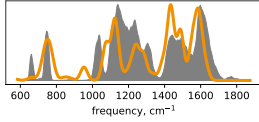
Spectra of protonated HMDB0003320, spectral sim. = 881, #2



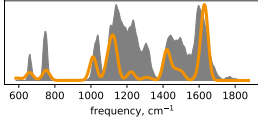
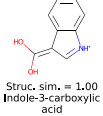
Structural similarity plot of protonated HMDB0003320



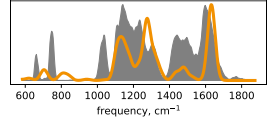
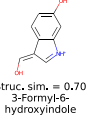
protonated HMDB0060289, spectral sim. = 895, #1



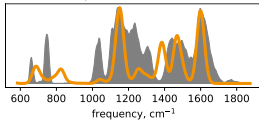
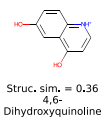
protonated HMDB0003320, spectral sim. = 881, #2



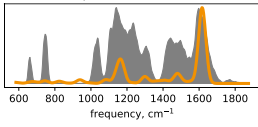
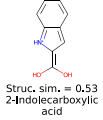
protonated HMDB00031172, spectral sim. = 868, #3



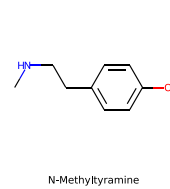
protonated HMDB0004077, spectral sim. = 865, #4



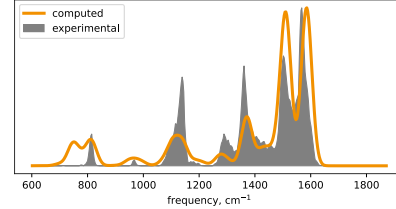
protonated HMDB0002285, spectral sim. = 843, #5



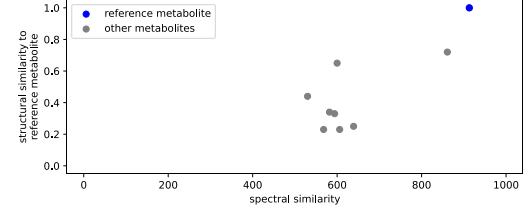
159 deprotonated HMDB0003633



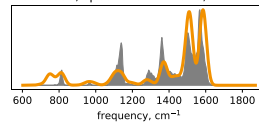
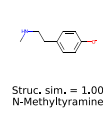
Spectra of deprotonated HMDB0003633, spectral sim. = 913, #1



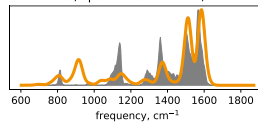
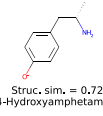
Structural similarity plot of deprotonated HMDB0003633



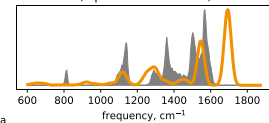
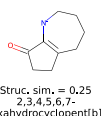
deprotonated HMDB0003633, spectral sim. = 913, #1



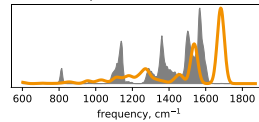
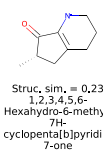
deprotonated HMDB0060765, spectral sim. = 861, #2



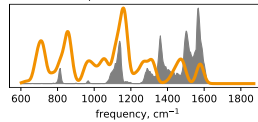
deprotonated HMDB0039663, spectral sim. = 639, #3



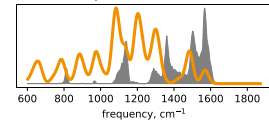
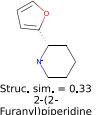
deprotonated HMDB0039659, spectral sim. = 606, #4



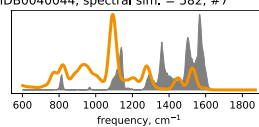
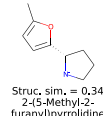
deprotonated HMDB0001387, spectral sim. = 600, #5



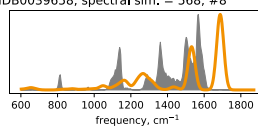
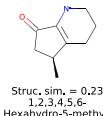
deprotonated HMDB0039835, spectral sim. = 594, #6



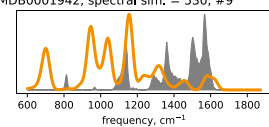
deprotonated HMDB0040044, spectral sim. = 582, #7



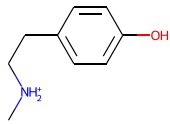
deprotonated HMDB0039658, spectral sim. = 568, #8



deprotonated HMDB0001942, spectral sim. = 530, #9

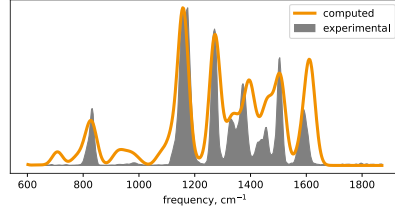


160 protonated HMDB0003633

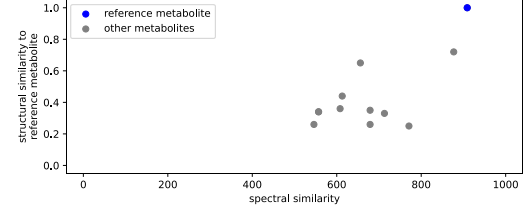


N-Methyltyramine

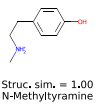
Spectra of protonated HMDB0003633, spectral sim. = 909, #1



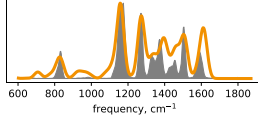
Structural similarity plot of protonated HMDB0003633



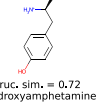
protonated HMDB0003633, spectral sim. = 909, #1



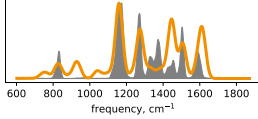
Struc. sim. = 1.00  
N-Methyltyramine



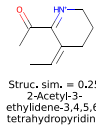
protonated HMDB0060765, spectral sim. = 877, #2



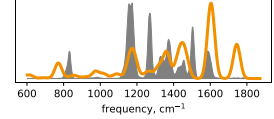
Struc. sim. = 0.72  
4-Hydroxyamphetamine



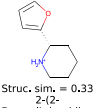
protonated HMDB0040039, spectral sim. = 771, #3



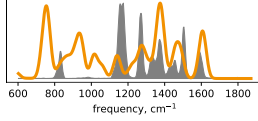
Struc. sim. = 0.25  
2-Acetyl-3-ethylidene-3,4,5,6-tetrahydropyridine



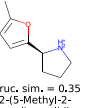
protonated HMDB0039835, spectral sim. = 713, #4



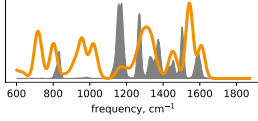
Struc. sim. = 0.33  
Furanylpiperidine



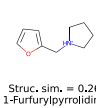
protonated HMDB0040044, spectral sim. = 679, #5



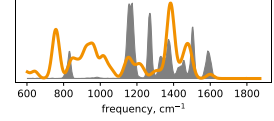
Struc. sim. = 0.35  
2-(5-Methyl-2-furanyl)pyrrolidine



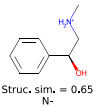
protonated HMDB0040037, spectral sim. = 679, #6



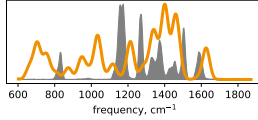
Struc. sim. = 0.26  
1-Furanylpiperidine



protonated HMDB0001387, spectral sim. = 656, #7



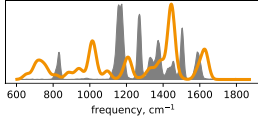
Struc. sim. = 0.65  
N-Methylphenylethanolamine



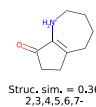
protonated HMDB0001942, spectral sim. = 613, #8



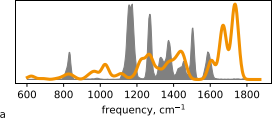
Struc. sim. = 0.44  
Phenylpropanolamine



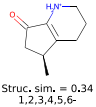
protonated HMDB0039663, spectral sim. = 608, #9



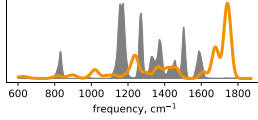
Struc. sim. = 0.36  
2,3,4,5,6,7-Hexahydrocyclopent[b]azepin-8(1H)-one



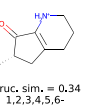
protonated HMDB0039658, spectral sim. = 557, #10



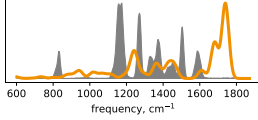
Struc. sim. = 0.34  
1,2,3,4,5,6-Hexahydro-5-methyl-7H-



protonated HMDB0039659, spectral sim. = 557, #11



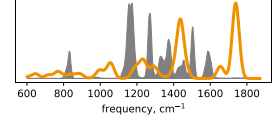
Struc. sim. = 0.34  
1,2,3,4,5,6-Hexahydro-6-methyl-7H-



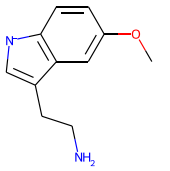
protonated HMDB0039674, spectral sim. = 546, #12



Struc. sim. = 0.26  
2-(1-Pyrrolidinyl)-2-cyclopenten-1-one

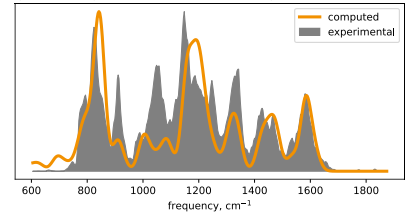


161 deprotonated HMDB0004095

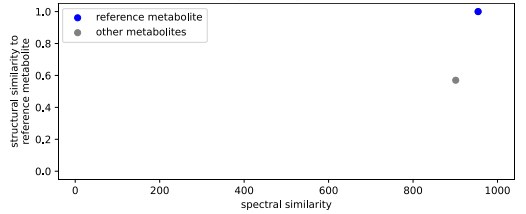


5-Methoxytryptamine

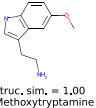
Spectra of deprotonated HMDB0004095, spectral sim. = 954, #1



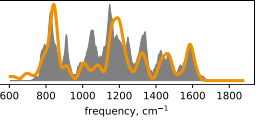
Structural similarity plot of deprotonated HMDB0004095



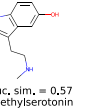
deprotonated HMDB0004095, spectral sim. = 954, #1



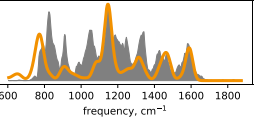
Struc. sim. = 1.00  
5-Methoxytryptamine



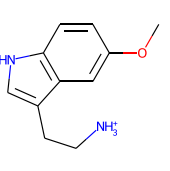
deprotonated HMDB0004369, spectral sim. = 901, #2



Struc. sim. = 0.57  
N-Methylserotonin

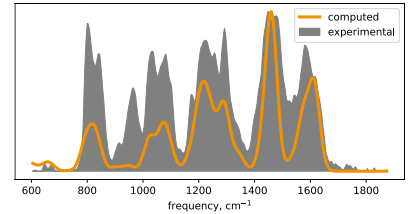


162 protonated HMDB0004095

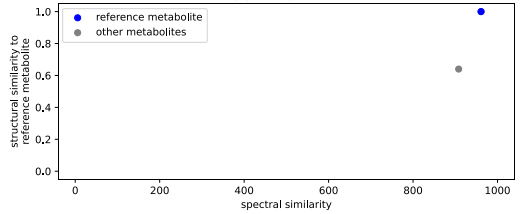


5-Methoxytryptamine

Spectra of protonated HMDB0004095, spectral sim. = 961, #1



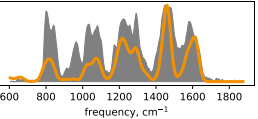
Structural similarity plot of protonated HMDB0004095



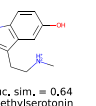
protonated HMDB0004095, spectral sim. = 961, #1



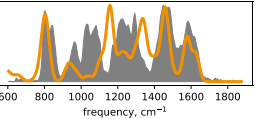
Struc. sim. = 1.00  
5-Methoxytryptamine



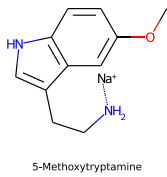
protonated HMDB0004369, spectral sim. = 908, #2



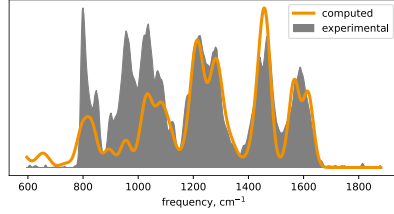
Struc. sim. = 0.64  
N-Methylserotonin



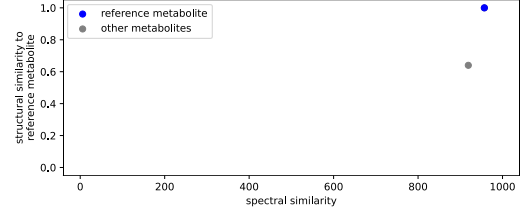
163 sodiated HMDB0004095



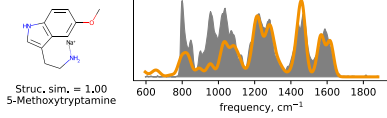
Spectra of sodiated HMDB0004095, spectral sim. = 957, #1



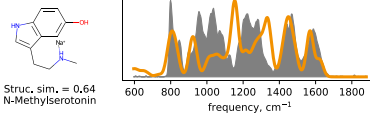
Structural similarity plot of sodiated HMDB0004095



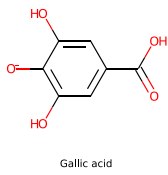
sodiated HMDB0004095, spectral sim. = 957, #1



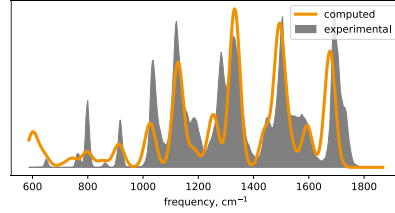
sodiated HMDB0004369, spectral sim. = 919, #2



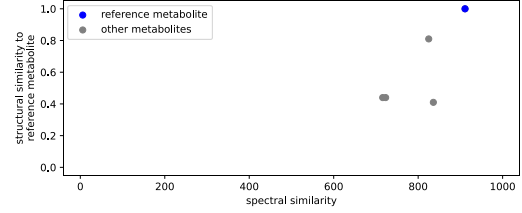
164 deprotonated HMDB0005807



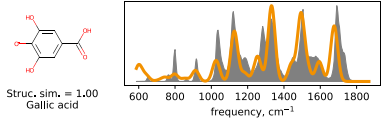
Spectra of deprotonated HMDB0005807, spectral sim. = 911, #1



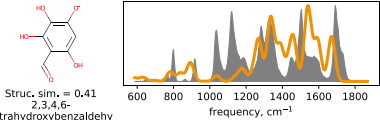
Structural similarity plot of deprotonated HMDB0005807



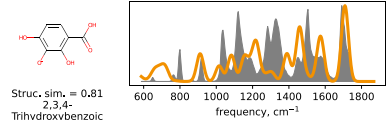
deprotonated HMDB0005807, spectral sim. = 911, #1



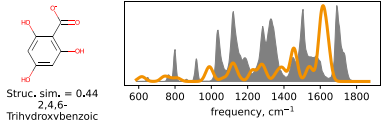
deprotonated HMDB0130402, spectral sim. = 836, #2



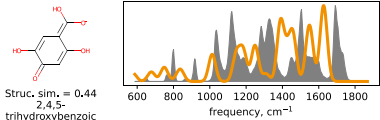
deprotonated HMDB0059964, spectral sim. = 825, #3



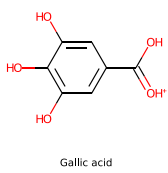
deprotonated HMDB0029649, spectral sim. = 723, #4



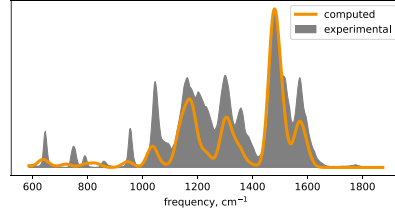
deprotonated HMDB0126491, spectral sim. = 716, #5



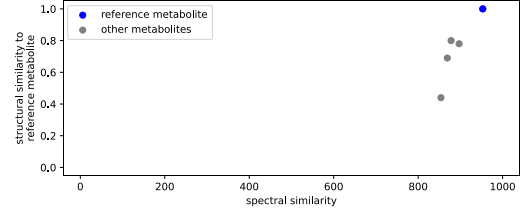
165 protonated HMDB0005807



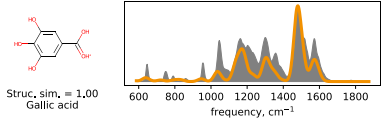
Spectra of protonated HMDB0005807, spectral sim. = 953, #1



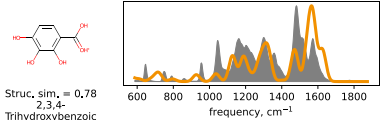
Structural similarity plot of protonated HMDB0005807



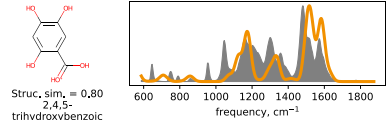
protonated HMDB0005807, spectral sim. = 953, #1



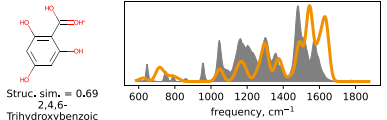
protonated HMDB0059964, spectral sim. = 897, #2



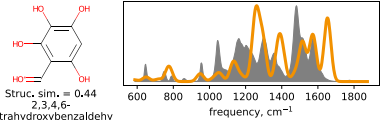
protonated HMDB0126491, spectral sim. = 878, #3



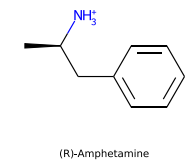
protonated HMDB0029649, spectral sim. = 869, #4



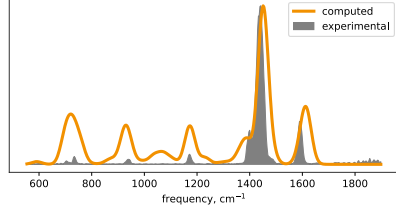
protonated HMDB0130402, spectral sim. = 854, #5



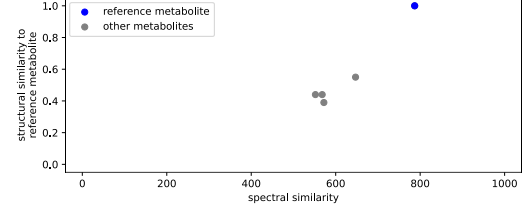
166 protonated HMDB0012128



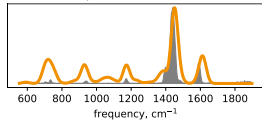
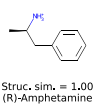
Spectra of protonated HMDB0012128, spectral sim. = 787, #1



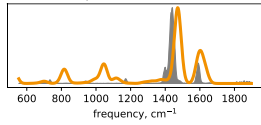
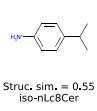
Structural similarity plot of protonated HMDB0012128



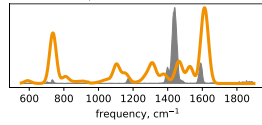
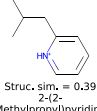
protonated HMDB0012128, spectral sim. = 787, #1



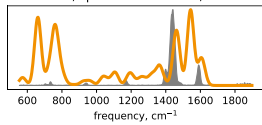
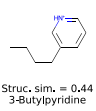
protonated HMDB0062481, spectral sim. = 647, #2



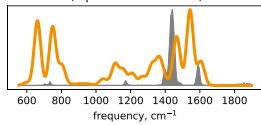
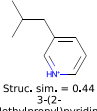
protonated HMDB0037291, spectral sim. = 572, #3



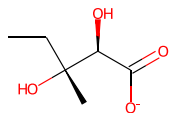
protonated HMDB0032934, spectral sim. = 568, #4



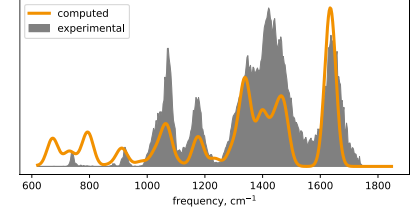
protonated HMDB0037287, spectral sim. = 552, #5



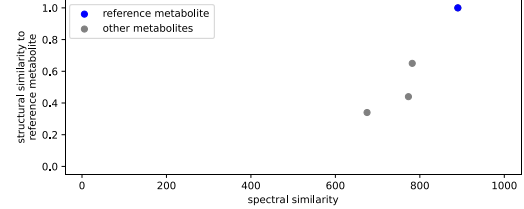
167 deprotonated HMDB0012140



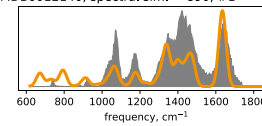
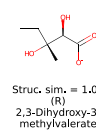
Spectra of deprotonated HMDB0012140, spectral sim. = 890, #1



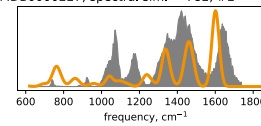
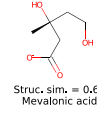
Structural similarity plot of deprotonated HMDB0012140



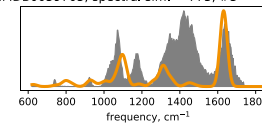
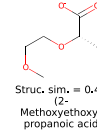
deprotonated HMDB0012140, spectral sim. = 890, #1



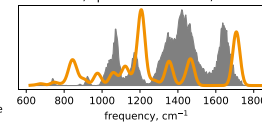
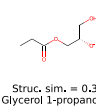
deprotonated HMDB0000227, spectral sim. = 782, #2



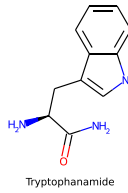
deprotonated HMDB0059705, spectral sim. = 773, #3



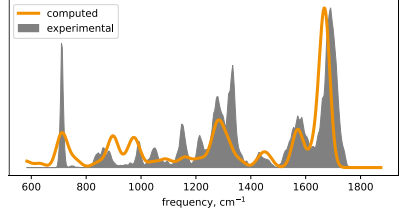
deprotonated HMDB0031639, spectral sim. = 675, #4



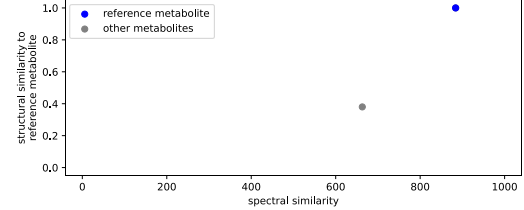
168 deprotonated HMDB0013318



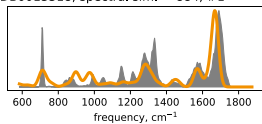
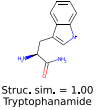
Spectra of deprotonated HMDB0013318, spectral sim. = 884, #1



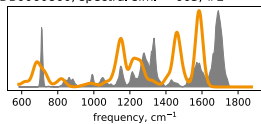
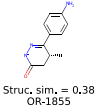
Structural similarity plot of deprotonated HMDB0013318



deprotonated HMDB0013318, spectral sim. = 884, #1

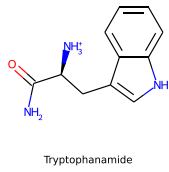


deprotonated HMDB0060860, spectral sim. = 663, #2

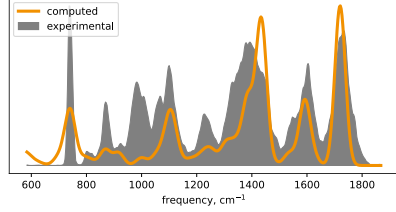




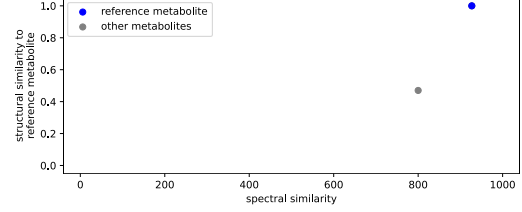
169 protonated HMDB0013318



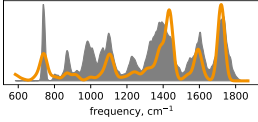
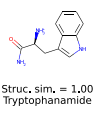
Spectra of protonated HMDB0013318, spectral sim. = 927, #1



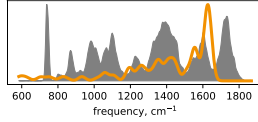
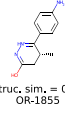
Structural similarity plot of protonated HMDB0013318



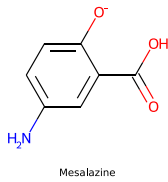
protonated HMDB0013318, spectral sim. = 927, #1



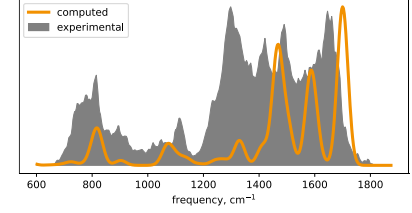
protonated HMDB0060860, spectral sim. = 800, #2



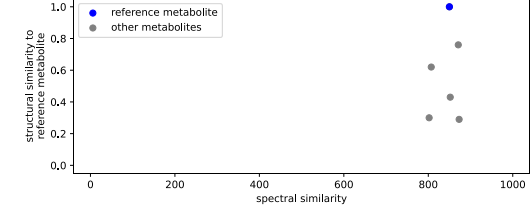
170 deprotonated HMDB0014389



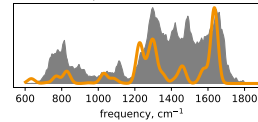
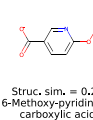
Spectra of deprotonated HMDB0014389, spectral sim. = 850, #4



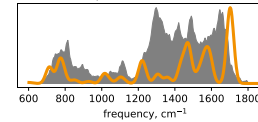
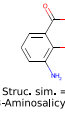
Structural similarity plot of deprotonated HMDB0014389



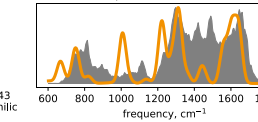
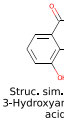
deprotonated HMDB0059749, spectral sim. = 873, #1



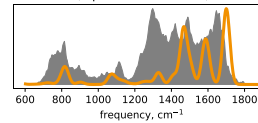
deprotonated HMDB0001972, spectral sim. = 871, #2



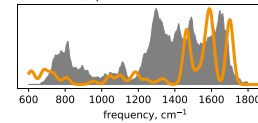
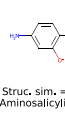
deprotonated HMDB0001476, spectral sim. = 852, #3



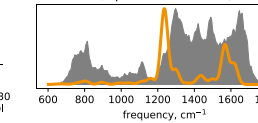
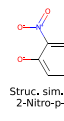
deprotonated HMDB0014389, spectral sim. = 850, #4



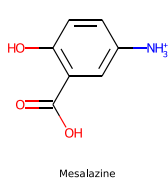
deprotonated HMDB0014378, spectral sim. = 807, #5



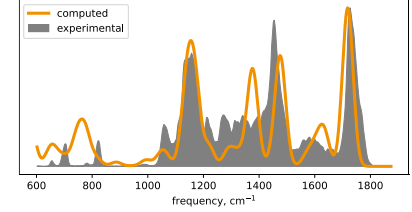
deprotonated HMDB0059811, spectral sim. = 802, #6



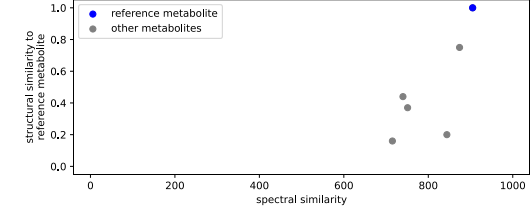
171 protonated HMDB0014389



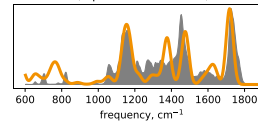
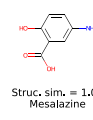
Spectra of protonated HMDB0014389, spectral sim. = 905, #1



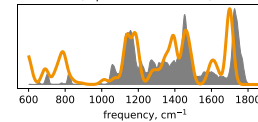
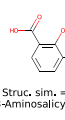
Structural similarity plot of protonated HMDB0014389



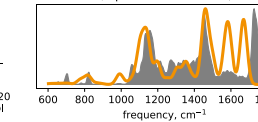
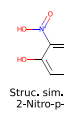
protonated HMDB0014389, spectral sim. = 905, #1



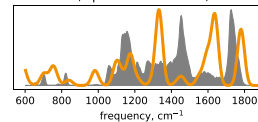
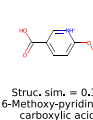
protonated HMDB0001972, spectral sim. = 874, #2



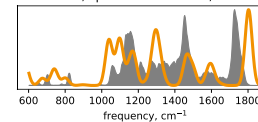
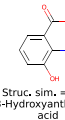
protonated HMDB0059811, spectral sim. = 844, #3



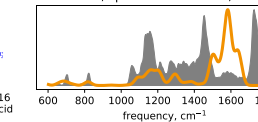
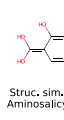
protonated HMDB0059749, spectral sim. = 751, #4



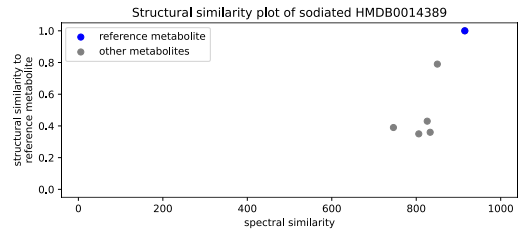
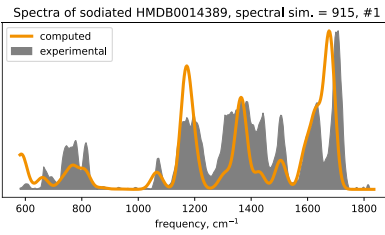
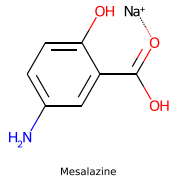
protonated HMDB0001476, spectral sim. = 740, #5



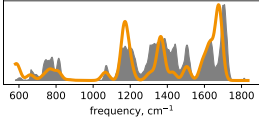
protonated HMDB0014378, spectral sim. = 715, #6



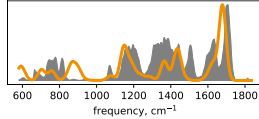
172 sodiated HMDB0014389



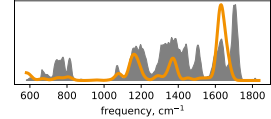
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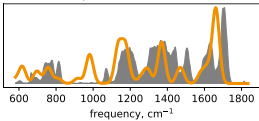
sodiated HMDB0001972, spectral sim. = 850, #2



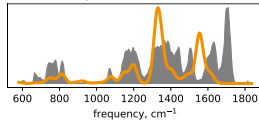
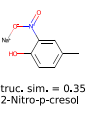
sodiated HMDB0014378, spectral sim. = 833, #3



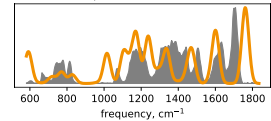
sodiated HMDB0001476, spectral sim. = 826, #4



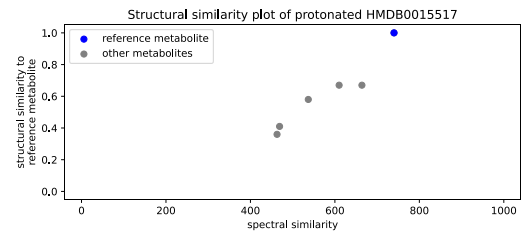
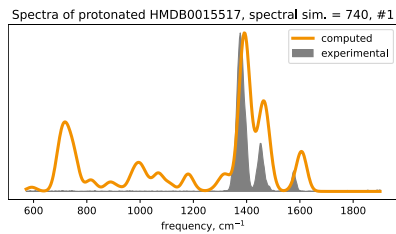
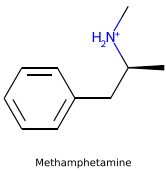
sodiated HMDB0059811, spectral sim. = 806, #5



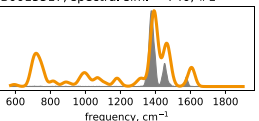
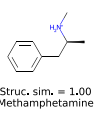
sodiated HMDB0059749, spectral sim. = 746, #6



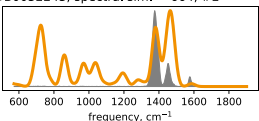
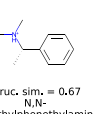
173 protonated HMDB0015517



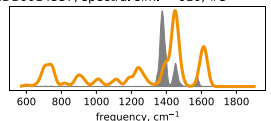
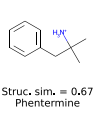
protonated HMDB0015517, spectral sim. = 740, #1



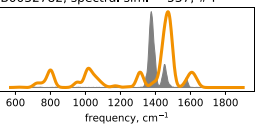
protonated HMDB0032243, spectral sim. = 664, #2



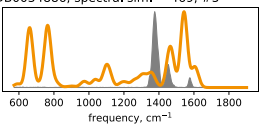
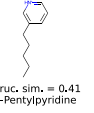
protonated HMDB0014337, spectral sim. = 610, #3



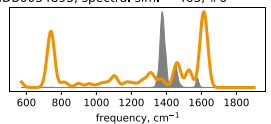
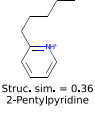
protonated HMDB0032782, spectral sim. = 537, #4



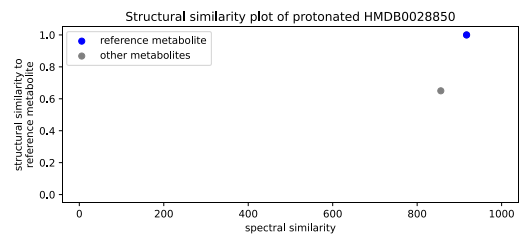
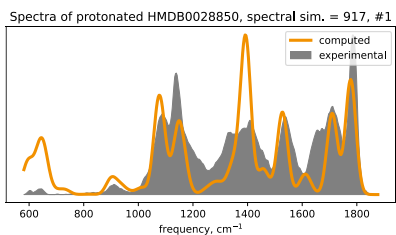
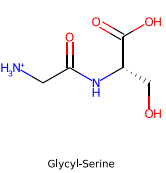
protonated HMDB0034886, spectral sim. = 469, #5



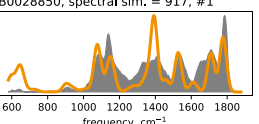
protonated HMDB0034893, spectral sim. = 463, #6



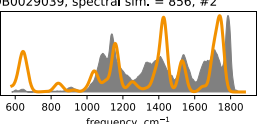
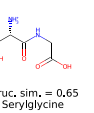
174 protonated HMDB0028850



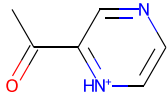
protonated HMDB0028850, spectral sim. = 917, #1



protonated HMDB0029039, spectral sim. = 856, #2

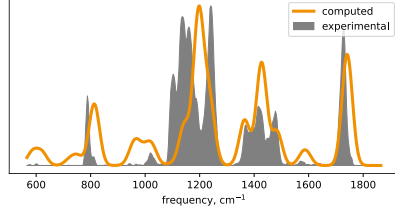


175 protonated HMDB0031861

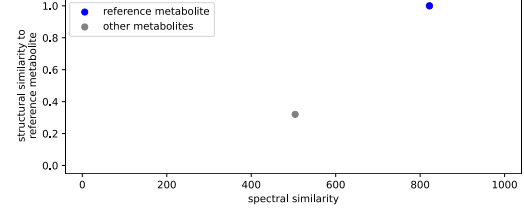


2-Acetylpyrazine

Spectra of protonated HMDB0031861, spectral sim. = 822, #1



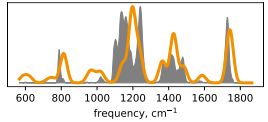
Structural similarity plot of protonated HMDB0031861



protonated HMDB0031861, spectral sim. = 822, #1



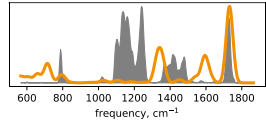
Struc. sim. = 1.00  
2-Acetylpyrazine



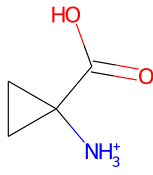
protonated HMDB0001406, spectral sim. = 504, #2



Struc. sim. = 0.32  
Niacinamide

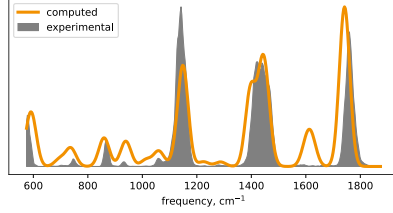


176 protonated HMDB0036458

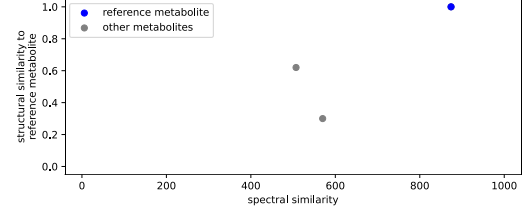


1-Aminocyclopropanecarboxylic acid

Spectra of protonated HMDB0036458, spectral sim. = 874, #1



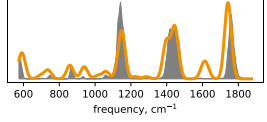
Structural similarity plot of protonated HMDB0036458



protonated HMDB0036458, spectral sim. = 874, #1



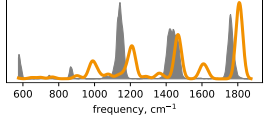
Struc. sim. = 1.00  
1-Aminocyclopropanecarbo



protonated HMDB0029387, spectral sim. = 570, #2



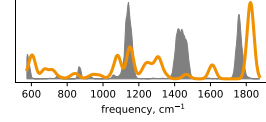
Struc. sim. = 0.30  
L-3-Aminodihydro-2(3H)-furanone



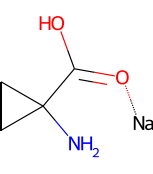
protonated HMDB0029615, spectral sim. = 507, #3



Struc. sim. = 0.62  
(S)-2-Azetidinecarboxylic

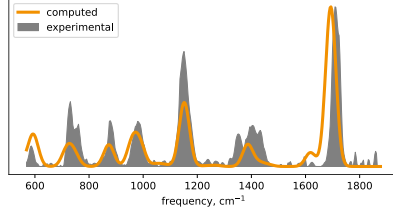


177 sodiated HMDB0036458

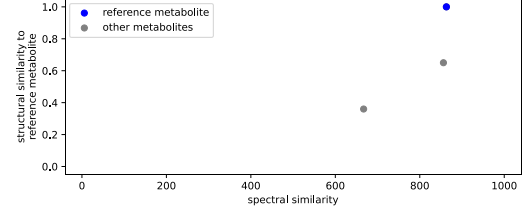


1-Aminocyclopropanecarboxylic acid

Spectra of sodiated HMDB0036458, spectral sim. = 863, #1



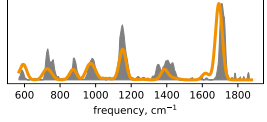
Structural similarity plot of sodiated HMDB0036458



sodiated HMDB0036458, spectral sim. = 863, #1



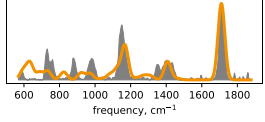
Struc. sim. = 1.00  
1-Aminocyclopropanecarbo



sodiated HMDB0029615, spectral sim. = 856, #2



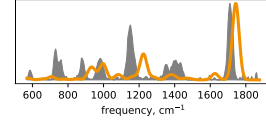
Struc. sim. = 0.65  
(S)-2-Azetidinecarboxylic



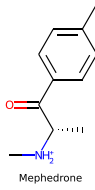
sodiated HMDB0029387, spectral sim. = 667, #3



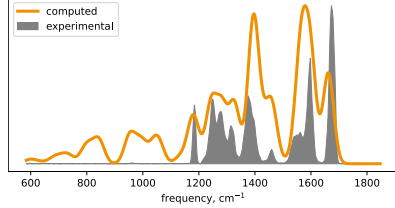
Struc. sim. = 0.36  
L-3-Aminodihydro-2(3H)-furanone



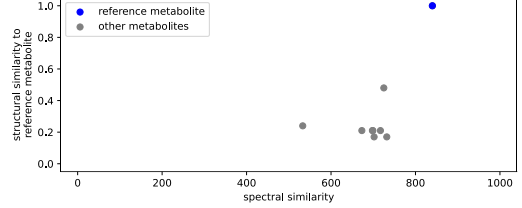
178 protonated HMDB0041923



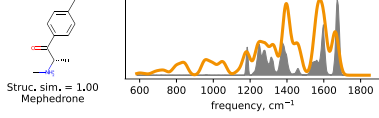
Spectra of protonated HMDB0041923, spectral sim. = 840, #1



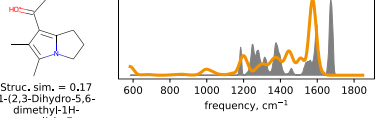
Structural similarity plot of protonated HMDB0041923



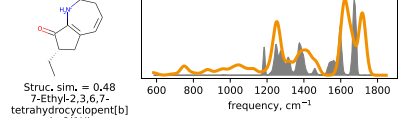
protonated HMDB0041923, spectral sim. = 840, #1



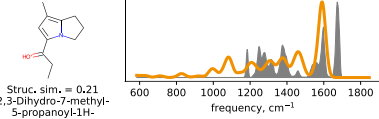
protonated HMDB0040027, spectral sim. = 732, #2



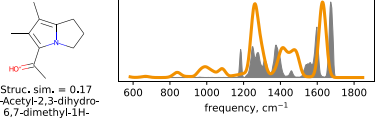
protonated HMDB0039664, spectral sim. = 725, #3



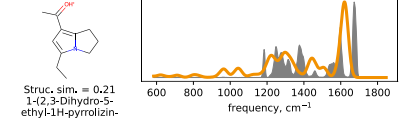
protonated HMDB0040017, spectral sim. = 717, #4



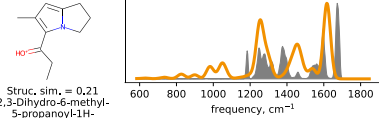
protonated HMDB0040020, spectral sim. = 702, #5



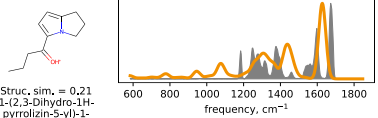
protonated HMDB0040019, spectral sim. = 699, #6



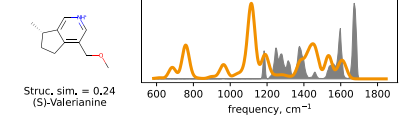
protonated HMDB0040018, spectral sim. = 698, #7



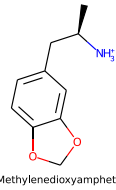
protonated HMDB0040014, spectral sim. = 673, #8



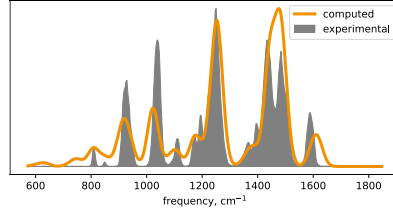
protonated HMDB0033484, spectral sim. = 533, #9



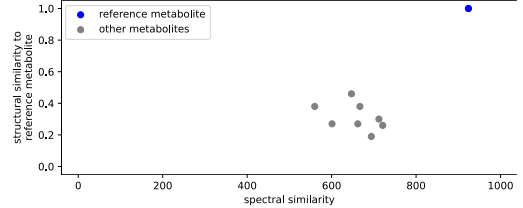
179 protonated HMDB0041931



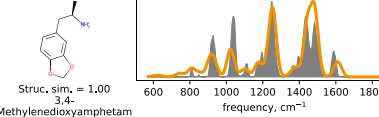
Spectra of protonated HMDB0041931, spectral sim. = 924, #1



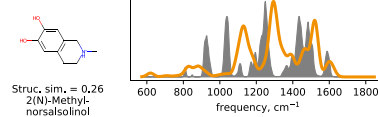
Structural similarity plot of protonated HMDB0041931



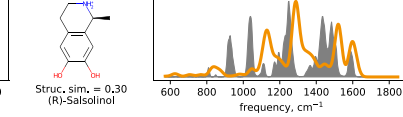
protonated HMDB0041931, spectral sim. = 924, #1



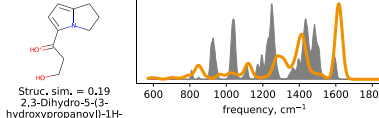
protonated HMDB0001189, spectral sim. = 721, #2



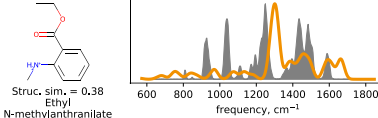
protonated HMDB0005199, spectral sim. = 712, #3



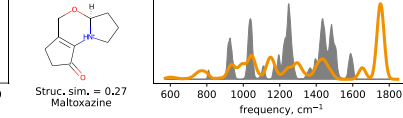
protonated HMDB0040021, spectral sim. = 694, #4



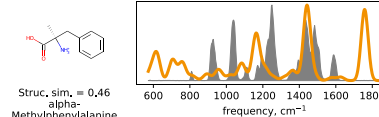
protonated HMDB0033763, spectral sim. = 667, #5



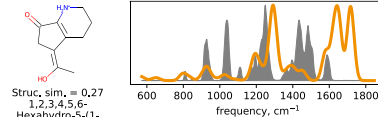
protonated HMDB0030372, spectral sim. = 662, #6



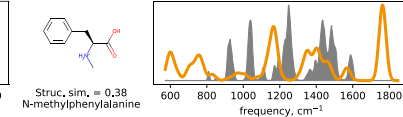
protonated HMDB0029223, spectral sim. = 647, #7



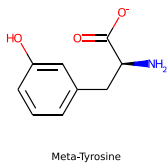
protonated HMDB0039655, spectral sim. = 601, #8



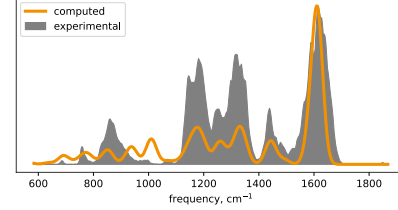
protonated HMDB0029224, spectral sim. = 560, #9



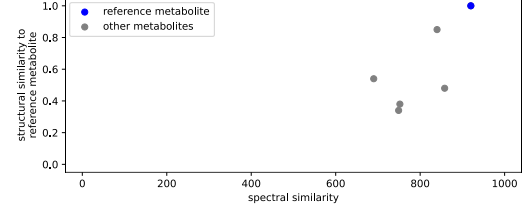
180 deprotonated HMDB0059720



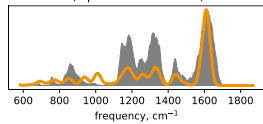
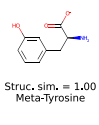
Spectra of deprotonated HMDB0059720, spectral sim. = 920, #1



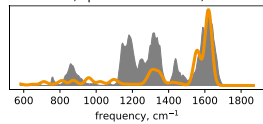
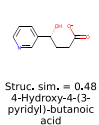
Structural similarity plot of deprotonated HMDB0059720



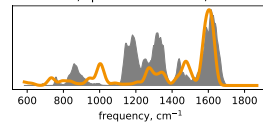
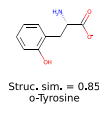
deprotonated HMDB0059720, spectral sim. = 920, #1



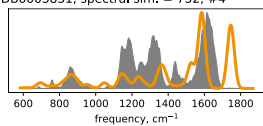
deprotonated HMDB0001119, spectral sim. = 858, #2



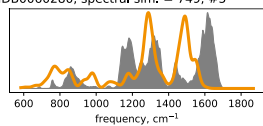
deprotonated HMDB0006050, spectral sim. = 840, #3



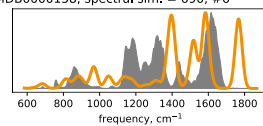
deprotonated HMDB0003831, spectral sim. = 752, #4



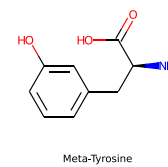
deprotonated HMDB0060280, spectral sim. = 749, #5



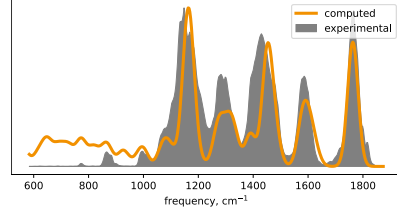
deprotonated HMDB0000158, spectral sim. = 690, #6



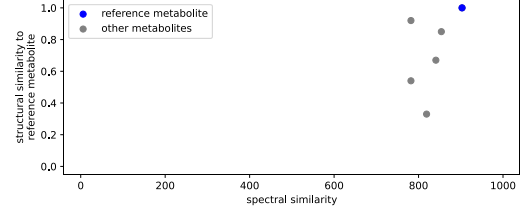
181 protonated HMDB0059720



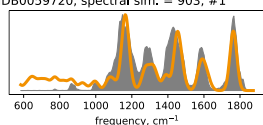
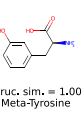
Spectra of protonated HMDB0059720, spectral sim. = 903, #1



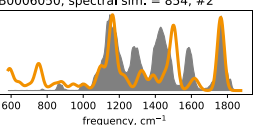
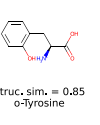
Structural similarity plot of protonated HMDB0059720



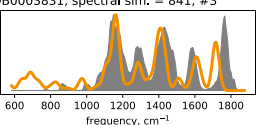
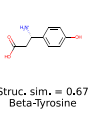
protonated HMDB0059720, spectral sim. = 903, #1



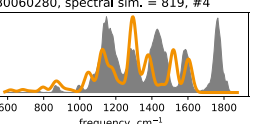
protonated HMDB0006050, spectral sim. = 854, #2



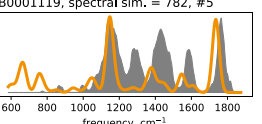
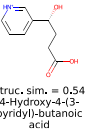
protonated HMDB0003831, spectral sim. = 841, #3



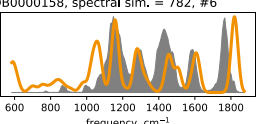
protonated HMDB0060280, spectral sim. = 819, #4



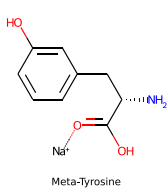
protonated HMDB0001119, spectral sim. = 782, #5



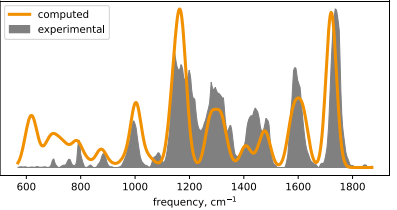
protonated HMDB0000158, spectral sim. = 782, #6



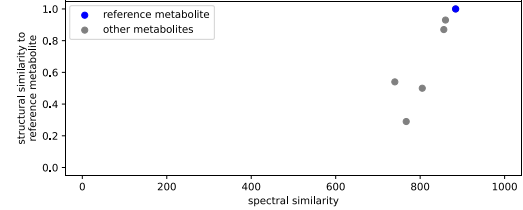
182 sodiated HMDB0059720



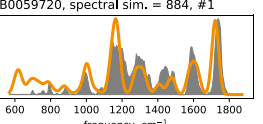
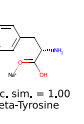
Spectra of sodiated HMDB0059720, spectral sim. = 884, #1



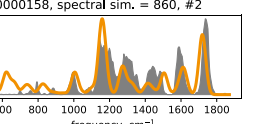
Structural similarity plot of sodiated HMDB0059720



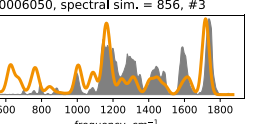
sodiated HMDB0059720, spectral sim. = 884, #1



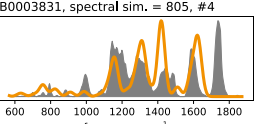
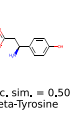
sodiated HMDB0000158, spectral sim. = 860, #2



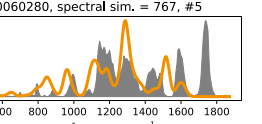
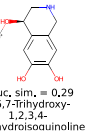
sodiated HMDB0006050, spectral sim. = 856, #3



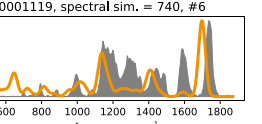
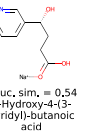
sodiated HMDB0003831, spectral sim. = 805, #4



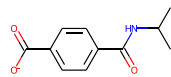
sodiated HMDB0060280, spectral sim. = 767, #5



sodiated HMDB0001119, spectral sim. = 740, #6

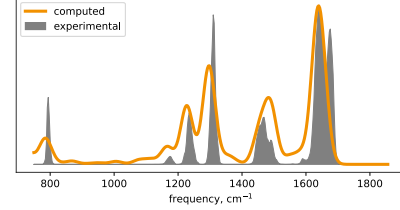


183 deprotonated HMDB0060608

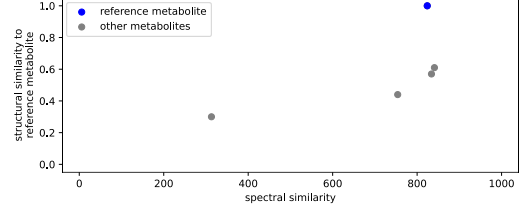


N-isopropylterephthalamide

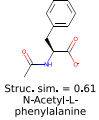
Spectra of deprotonated HMDB0060608, spectral sim. = 824, #3



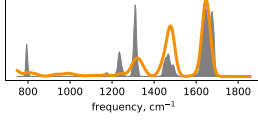
Structural similarity plot of deprotonated HMDB0060608



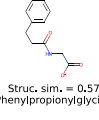
deprotonated HMDB0000512, spectral sim. = 841, #1



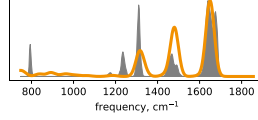
Struc. sim. = 0.61  
N-Acetyl-L-phenylalanine



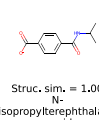
deprotonated HMDB0000860, spectral sim. = 834, #2



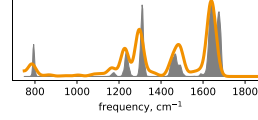
Struc. sim. = 0.57  
Phenylpropionylglycine



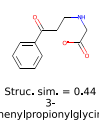
deprotonated HMDB0060608, spectral sim. = 824, #3



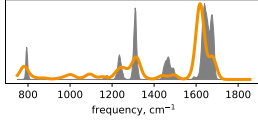
Struc. sim. = 1.00  
N-isopropylterephthalamide



deprotonated HMDB0002042, spectral sim. = 754, #4



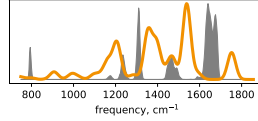
Struc. sim. = 0.44  
3-Phenylpropionylglycine



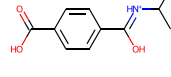
deprotonated HMDB0061682, spectral sim. = 313, #5



Struc. sim. = 0.30  
2-Acetamido-4-methylphenyl acetate

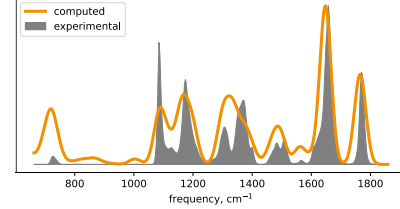


184 protonated HMDB0060608

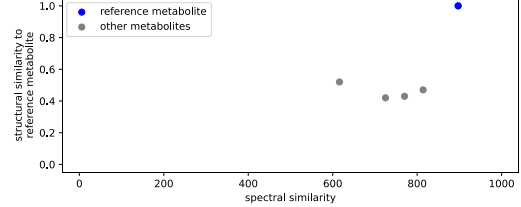


N-isopropylterephthalamide

Spectra of protonated HMDB0060608, spectral sim. = 897, #1



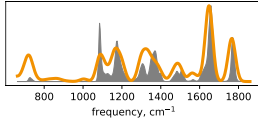
Structural similarity plot of protonated HMDB0060608



protonated HMDB0060608, spectral sim. = 897, #1



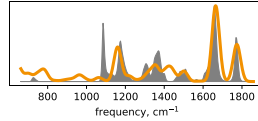
Struc. sim. = 1.00  
N-isopropylterephthalamide



protonated HMDB0000860, spectral sim. = 814, #2



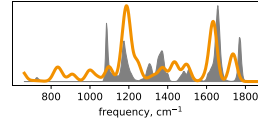
Struc. sim. = 0.47  
Phenylpropionylglycine



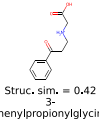
protonated HMDB0061682, spectral sim. = 770, #3



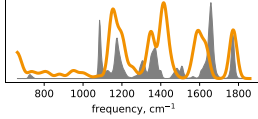
Struc. sim. = 0.43  
2-Acetamido-4-methylphenyl acetate



protonated HMDB0002042, spectral sim. = 725, #4



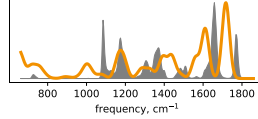
Struc. sim. = 0.42  
3-Phenylpropionylglycine



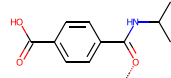
protonated HMDB0000512, spectral sim. = 616, #5



Struc. sim. = 0.52  
N-Acetyl-L-phenylalanine

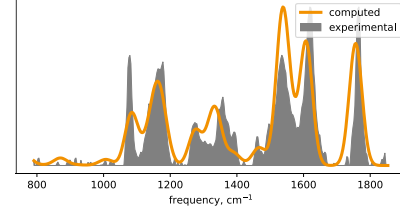


185 sodiated HMDB0060608

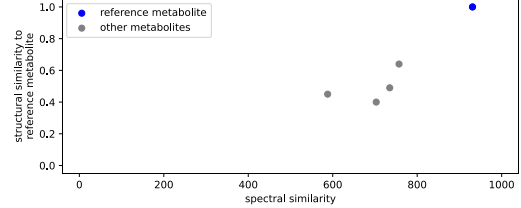


N-isopropylterephthalamide

Spectra of sodiated HMDB0060608, spectral sim. = 931, #1



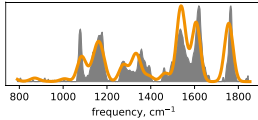
Structural similarity plot of sodiated HMDB0060608



sodiated HMDB0060608, spectral sim. = 931, #1



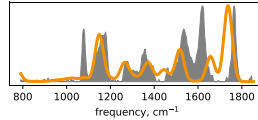
Struc. sim. = 1.00  
N-isopropylterephthalamide



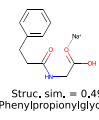
sodiated HMDB0000512, spectral sim. = 757, #2



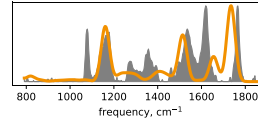
Struc. sim. = 0.64  
N-Acetyl-L-phenylalanine



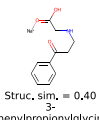
sodiated HMDB0000860, spectral sim. = 735, #3



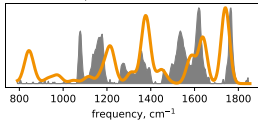
Struc. sim. = 0.49  
Phenylpropionylglycine



sodiated HMDB0002042, spectral sim. = 703, #4



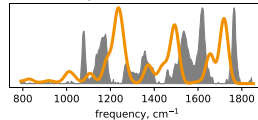
Struc. sim. = 0.40  
3-Phenylpropionylglycine



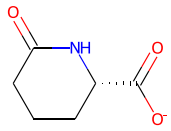
sodiated HMDB0061682, spectral sim. = 588, #5



Struc. sim. = 0.45  
2-Acetamido-4-methylphenyl acetate

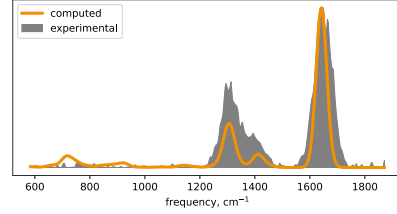


186 deprotonated HMDB0061705

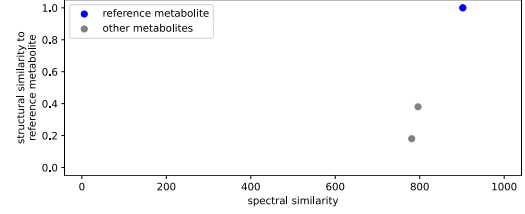


6-Oxopiperidine-2-carboxylic acid

Spectra of deprotonated HMDB0061705, spectral sim. = 902, #1



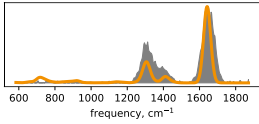
Structural similarity plot of deprotonated HMDB0061705



deprotonated HMDB0061705, spectral sim. = 902, #1



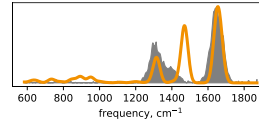
Struc. sim. = 1.00  
6-Oxopiperidine-2-carboxylic acid



deprotonated HMDB0000894, spectral sim. = 796, #2



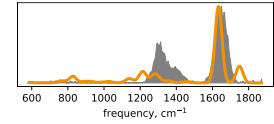
Struc. sim. = 0.38  
Vinylacetylglycine



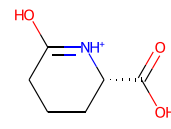
deprotonated HMDB0061082, spectral sim. = 781, #3



Struc. sim. = 0.18  
5-ethyl-5-methyl-2,4-oxazolidinedione

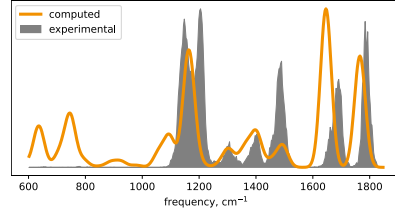


187 protonated HMDB0061705

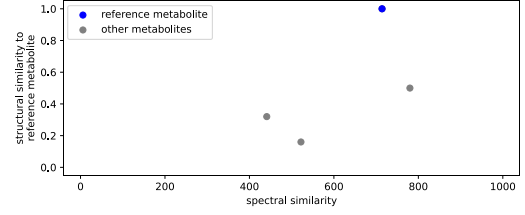


6-Oxopiperidine-2-carboxylic acid

Spectra of protonated HMDB0061705, spectral sim. = 714, #2



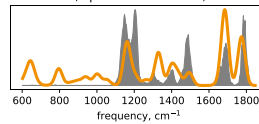
Structural similarity plot of protonated HMDB0061705



protonated HMDB0000894, spectral sim. = 780, #1



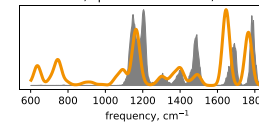
Struc. sim. = 0.50  
Vinylacetylglycine



protonated HMDB0061705, spectral sim. = 714, #2



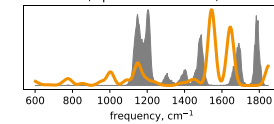
Struc. sim. = 1.00  
6-Oxopiperidine-2-carboxylic acid



protonated HMDB0014491, spectral sim. = 522, #3



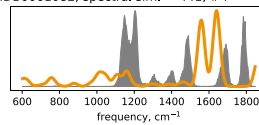
Struc. sim. = 0.16  
Trimethadione



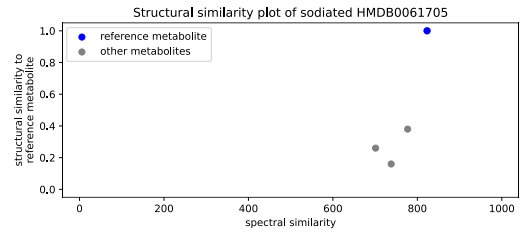
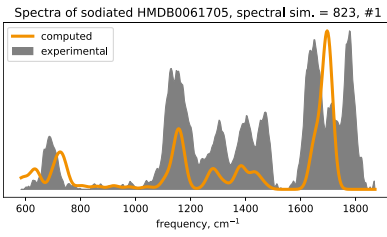
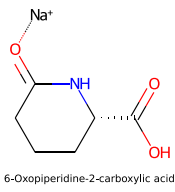
protonated HMDB0061082, spectral sim. = 441, #4



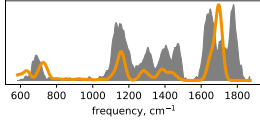
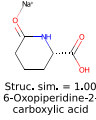
Struc. sim. = 0.32  
5-ethyl-5-methyl-2,4-oxazolidinedione



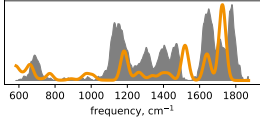
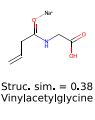
188 sodiated HMDB0061705



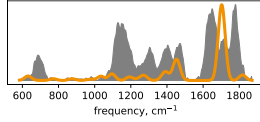
sodiated HMDB0061705, spectral sim. = 823, #1



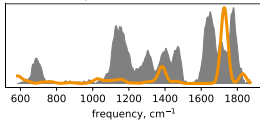
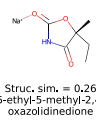
sodiated HMDB0000894, spectral sim. = 777, #2



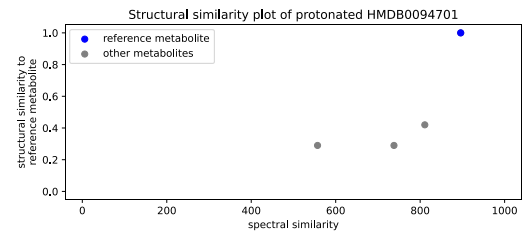
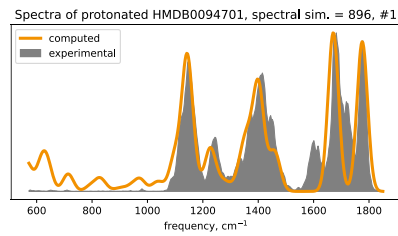
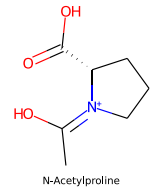
sodiated HMDB0014491, spectral sim. = 738, #3



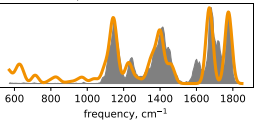
sodiated HMDB0061082, spectral sim. = 701, #4



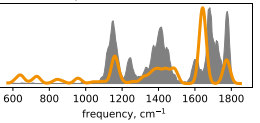
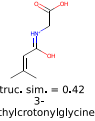
189 protonated HMDB0094701



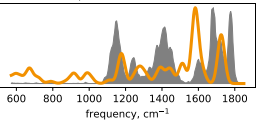
protonated HMDB0094701, spectral sim. = 896, #1



protonated HMDB0000459, spectral sim. = 811, #2



protonated HMDB0000959, spectral sim. = 738, #3



protonated HMDB0014755, spectral sim. = 557, #4

