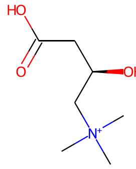
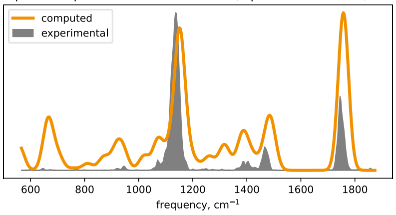
1 protonated HMDB0000062

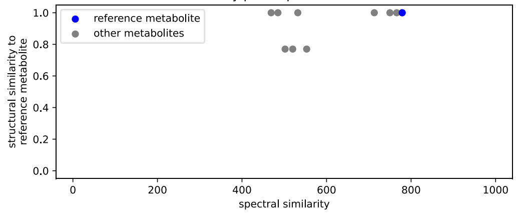


L-Carnitine

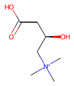
Spectra of protonated HMDB0000062, spectral sim. = 779, #1



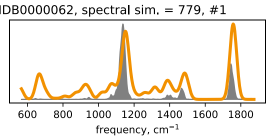
Structural similarity plot of protonated HMDB0000062



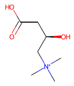
protonated HMDB0000062, spectral sim. = 779, #1



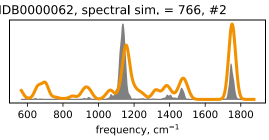
0.0 kJ/mol
L-Carnitine



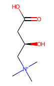
protonated HMDB0000062, spectral sim. = 766, #2



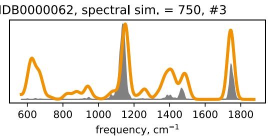
21.8 kJ/mol
L-Carnitine



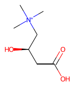
protonated HMDB0000062, spectral sim. = 750, #3



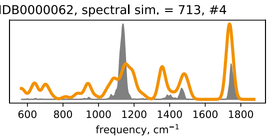
9.3 kJ/mol
L-Carnitine



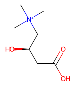
protonated HMDB0000062, spectral sim. = 713, #4



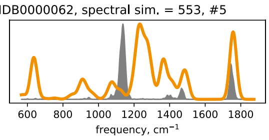
10.2 kJ/mol
L-Carnitine



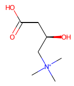
protonated HMDB0000062, spectral sim. = 553, #5



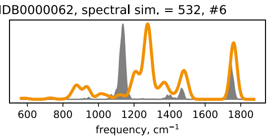
24.8 kJ/mol
L-Carnitine



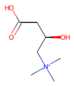
protonated HMDB0000062, spectral sim. = 532, #6



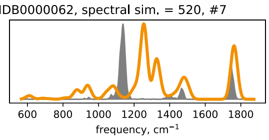
50.9 kJ/mol
L-Carnitine



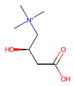
protonated HMDB0000062, spectral sim. = 520, #7



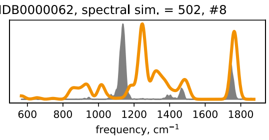
39.3 kJ/mol
L-Carnitine



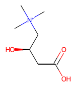
protonated HMDB0000062, spectral sim. = 502, #8



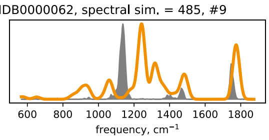
48.8 kJ/mol
L-Carnitine



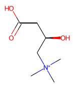
protonated HMDB0000062, spectral sim. = 485, #9



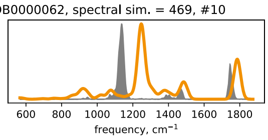
20.1 kJ/mol
L-Carnitine



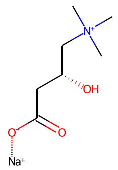
protonated HMDB0000062, spectral sim. = 469, #10



32.0 kJ/mol
L-Carnitine

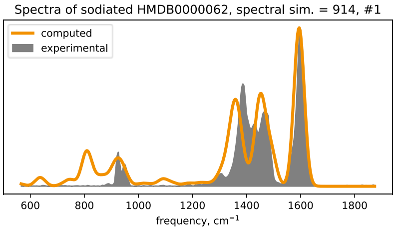


2 sodiated HMDB0000062

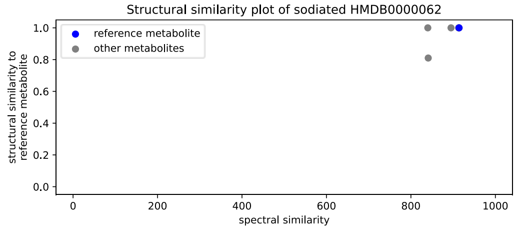


L-Carnitine

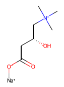
Spectra of sodiated HMDB0000062, spectral sim. = 914, #1



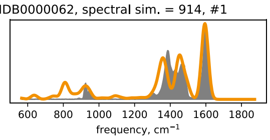
Structural similarity plot of sodiated HMDB0000062



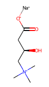
sodiated HMDB0000062, spectral sim. = 914, #1



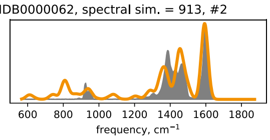
0.0 kJ/mol
L-Carnitine



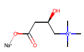
sodiated HMDB0000062, spectral sim. = 913, #2



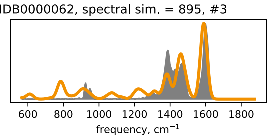
16.2 kJ/mol
L-Carnitine



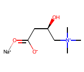
sodiated HMDB0000062, spectral sim. = 895, #3



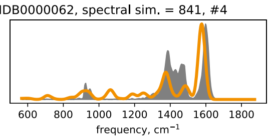
5.5 kJ/mol
L-Carnitine



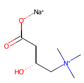
sodiated HMDB0000062, spectral sim. = 841, #4



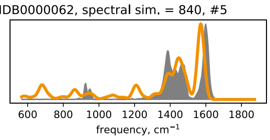
12.7 kJ/mol
L-Carnitine

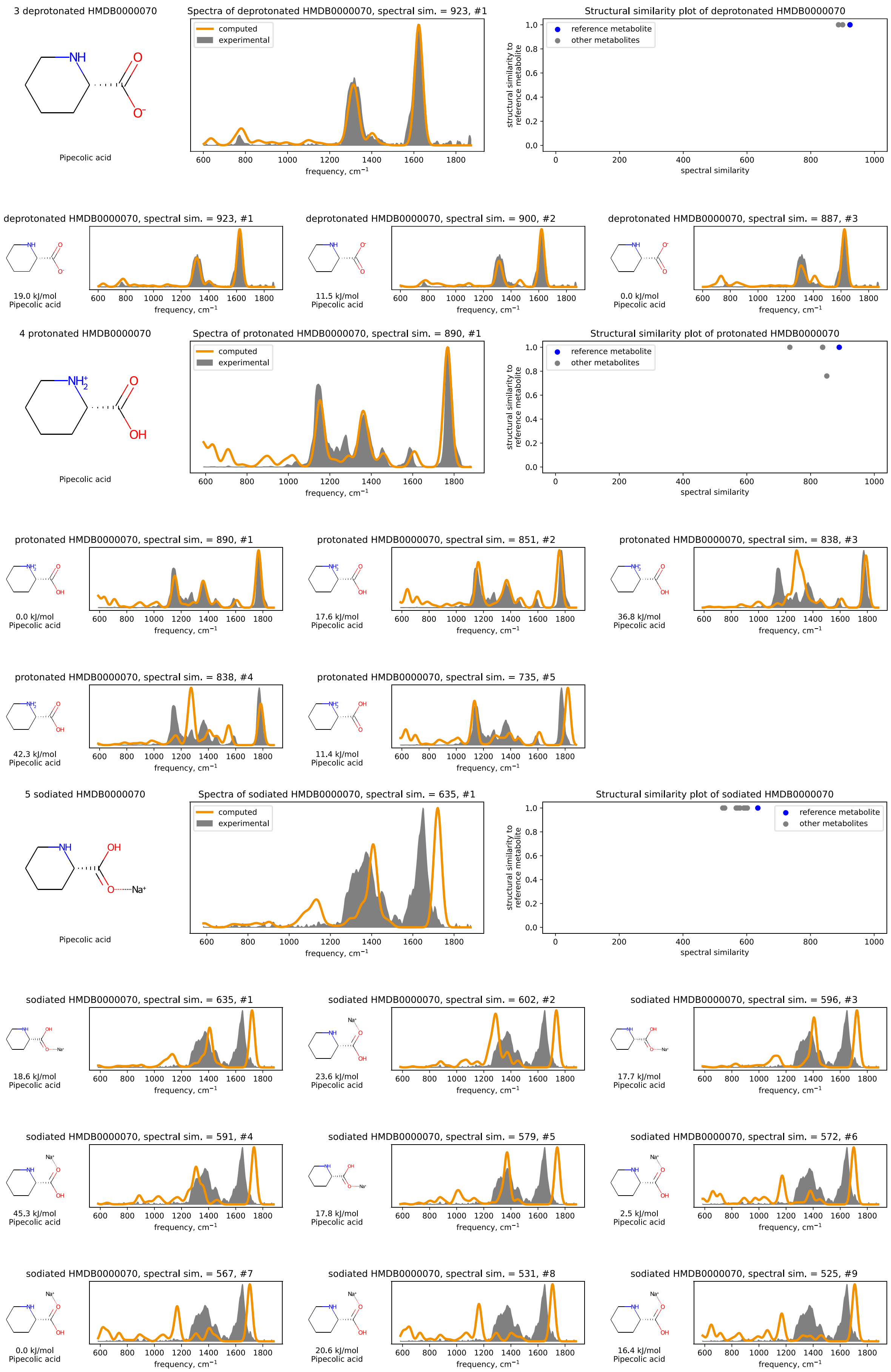


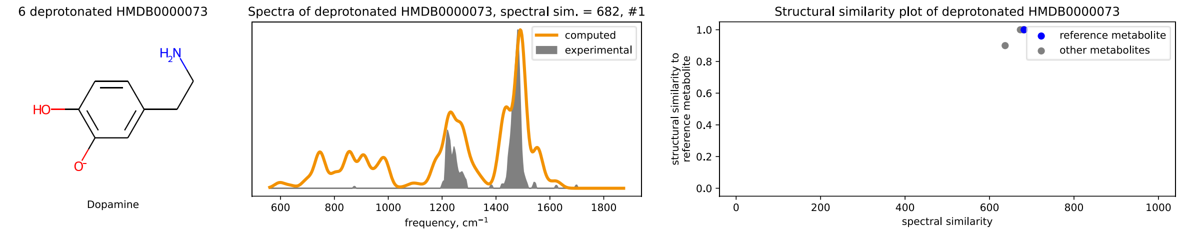
sodiated HMDB0000062, spectral sim. = 840, #5



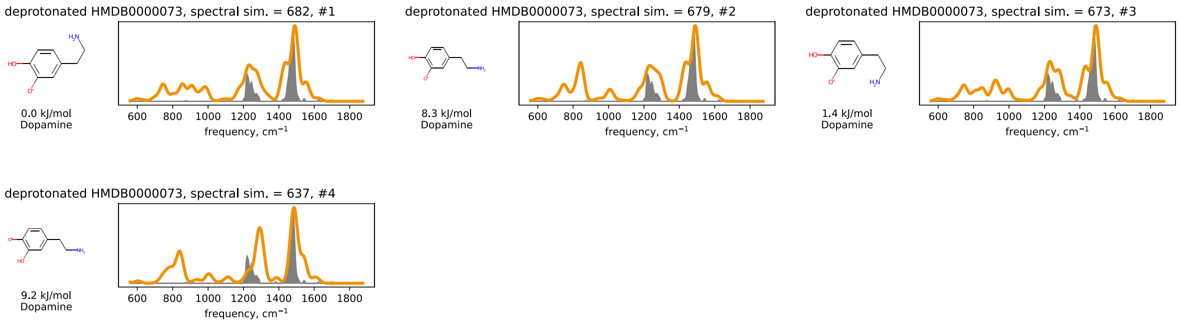
28.1 kJ/mol
L-Carnitine



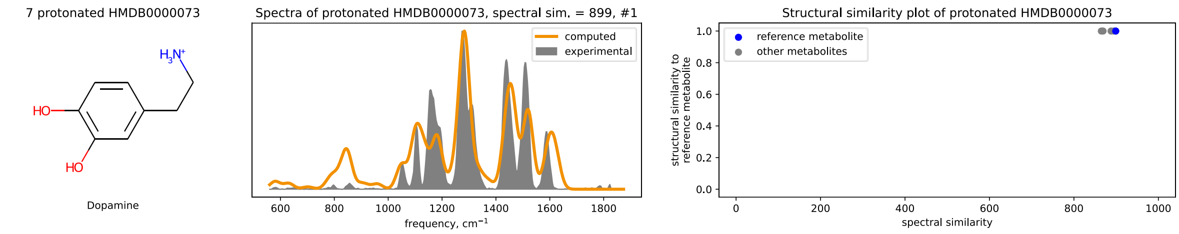

3 deprotonated HMDB0000070
Pipecolic acid
Spectra of deprotonated HMDB0000070, spectral sim. = 923, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of deprotonated HMDB0000070
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0000070, spectral sim. = 923, #1
19.0 kJ/mol
Pipecolic acid
deprotonated HMDB0000070, spectral sim. = 900, #2
11.5 kJ/mol
Pipecolic acid
deprotonated HMDB0000070, spectral sim. = 887, #3
0.0 kJ/mol
Pipecolic acid
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
0.0 kJ/mol
Pipecolic acid
protonated HMDB0000070, spectral sim. = 851, #2
17.6 kJ/mol
Pipecolic acid
protonated HMDB0000070, spectral sim. = 838, #3
36.8 kJ/mol
Pipecolic acid
protonated HMDB0000070, spectral sim. = 838, #4
42.3 kJ/mol
Pipecolic acid
protonated HMDB0000070, spectral sim. = 735, #5
11.4 kJ/mol
Pipecolic acid
5 sodiated HMDB0000070
Pipecolic acid
Spectra of sodiated HMDB0000070, spectral sim. = 635, #1
Structural similarity plot of sodiated HMDB0000070
sodiated HMDB0000070, spectral sim. = 635, #1
18.6 kJ/mol
Pipecolic acid
sodiated HMDB0000070, spectral sim. = 602, #2
23.6 kJ/mol
Pipecolic acid
sodiated HMDB0000070, spectral sim. = 596, #3
17.7 kJ/mol
Pipecolic acid
sodiated HMDB0000070, spectral sim. = 591, #4
45.3 kJ/mol
Pipecolic acid
sodiated HMDB0000070, spectral sim. = 579, #5
17.8 kJ/mol
Pipecolic acid
sodiated HMDB0000070, spectral sim. = 572, #6
2.5 kJ/mol
Pipecolic acid
sodiated HMDB0000070, spectral sim. = 567, #7
0.0 kJ/mol
Pipecolic acid
sodiated HMDB0000070, spectral sim. = 531, #8
20.6 kJ/mol
Pipecolic acid
sodiated HMDB0000070, spectral sim. = 525, #9
16.4 kJ/mol
Pipecolic acid



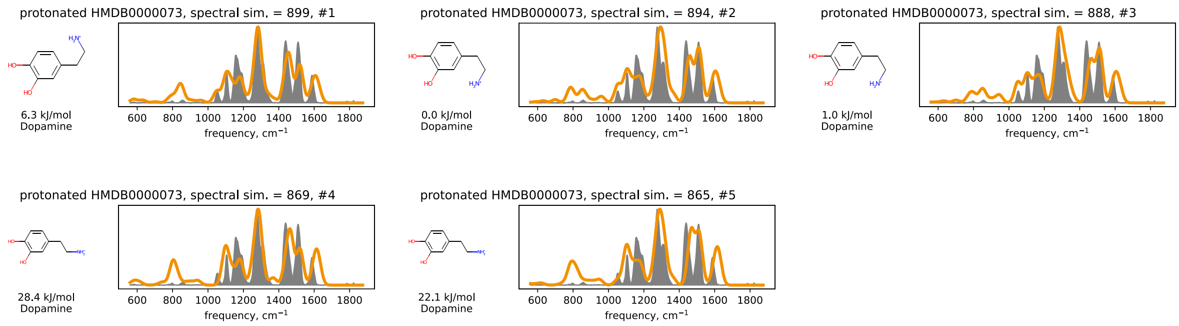
6 deprotonated HMDB0000073
Dopamine
Spectra of deprotonated HMDB0000073, spectral sim. = 682, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of deprotonated HMDB0000073
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity



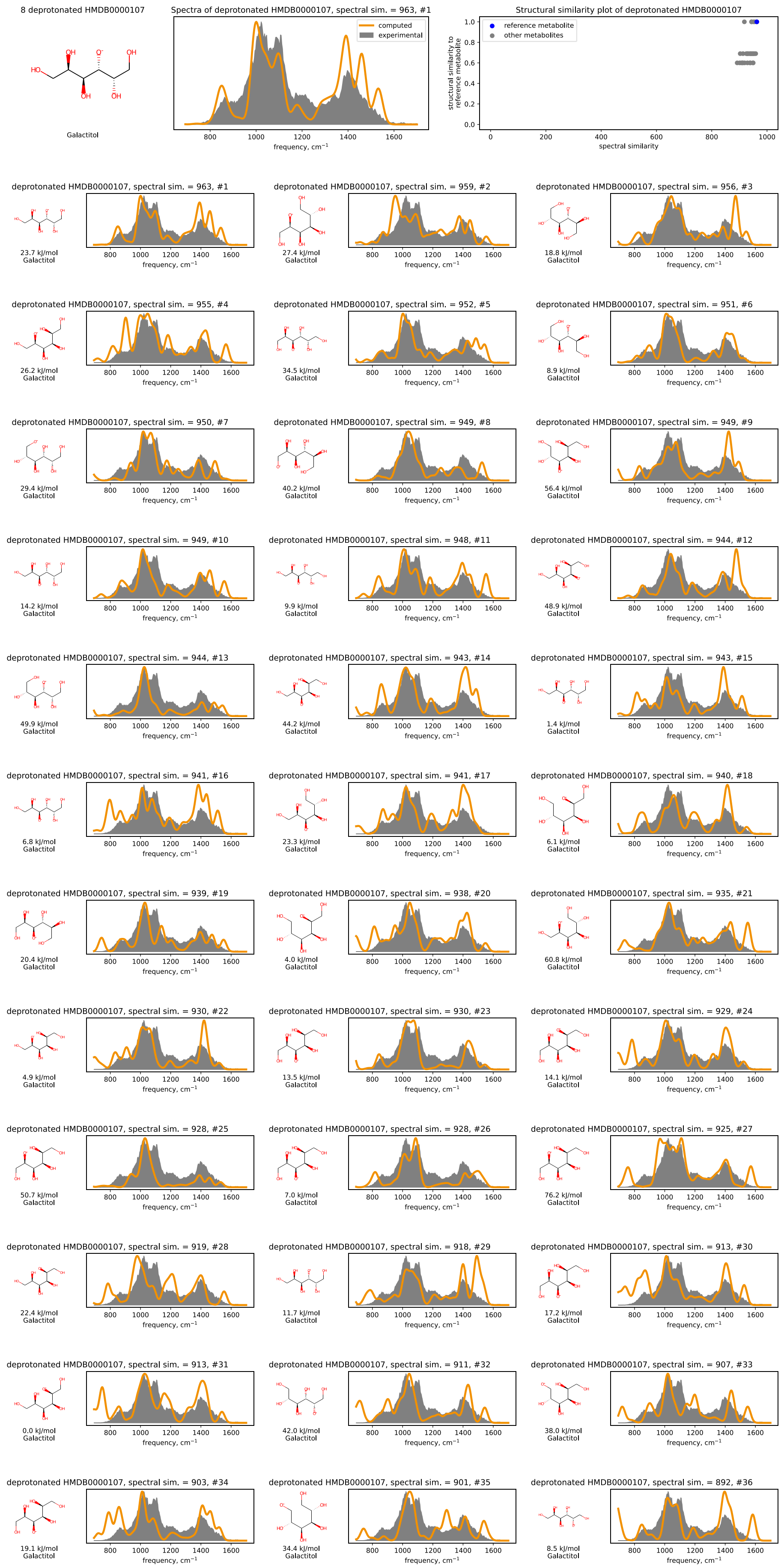
deprotonated HMDB0000073, spectral sim. = 682, #1
0.0 kJ/mol
Dopamine
deprotonated HMDB0000073, spectral sim. = 679, #2
8.3 kJ/mol
Dopamine
deprotonated HMDB0000073, spectral sim. = 673, #3
1.4 kJ/mol
Dopamine
deprotonated HMDB0000073, spectral sim. = 637, #4
9.2 kJ/mol
Dopamine
frequency, cm⁻¹



7 protonated HMDB0000073
Dopamine
Spectra of protonated HMDB0000073, spectral sim. = 899, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of protonated HMDB0000073
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

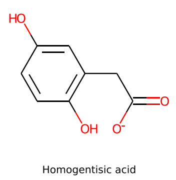


protonated HMDB0000073, spectral sim. = 899, #1
6.3 kJ/mol
Dopamine
protonated HMDB0000073, spectral sim. = 894, #2
0.0 kJ/mol
Dopamine
protonated HMDB0000073, spectral sim. = 888, #3
1.0 kJ/mol
Dopamine
protonated HMDB0000073, spectral sim. = 869, #4
28.4 kJ/mol
Dopamine
protonated HMDB0000073, spectral sim. = 865, #5
22.1 kJ/mol
Dopamine
frequency, cm⁻¹

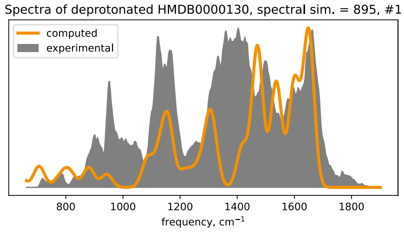


8 deprotonated HMDB0000107
Galactitol
Spectra of deprotonated HMDB0000107, spectral sim. = 963, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of deprotonated HMDB0000107
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0000107, spectral sim. = 963, #1
23.7 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 959, #2
27.4 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 956, #3
18.8 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 955, #4
26.2 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 952, #5
34.5 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 951, #6
8.9 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 950, #7
29.4 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 949, #8
40.2 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 949, #9
56.4 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 949, #10
14.2 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 948, #11
9.9 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 944, #12
48.9 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 944, #13
49.9 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 943, #14
44.2 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 943, #15
1.4 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 941, #16
6.8 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 941, #17
23.3 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 940, #18
6.1 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 939, #19
20.4 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 938, #20
4.0 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 935, #21
60.8 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 930, #22
4.9 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 930, #23
13.5 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 929, #24
14.1 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 928, #25
50.7 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 928, #26
7.0 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 925, #27
76.2 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 919, #28
22.4 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 918, #29
11.7 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 913, #30
17.2 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 913, #31
0.0 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 911, #32
42.0 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 907, #33
38.0 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 903, #34
19.1 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 901, #35
34.4 kJ/mol Galactitol
deprotonated HMDB0000107, spectral sim. = 892, #36
8.5 kJ/mol Galactitol

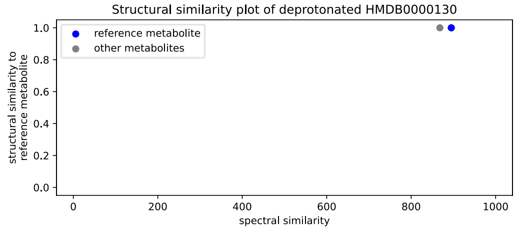
9 deprotonated HMDB0000130



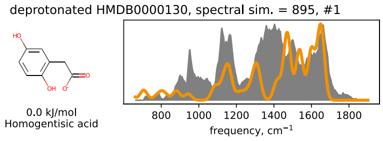
Spectra of deprotonated HMDB0000130, spectral sim. = 895, #1



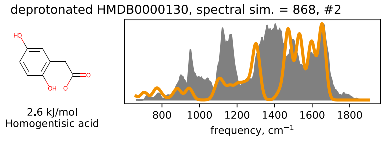
Structural similarity plot of deprotonated HMDB0000130



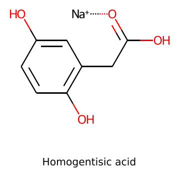
deprotonated HMDB0000130, spectral sim. = 895, #1



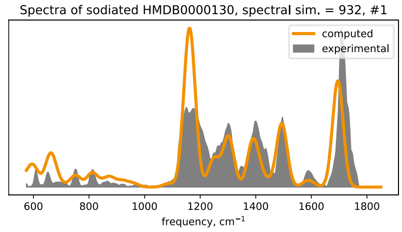
deprotonated HMDB0000130, spectral sim. = 868, #2



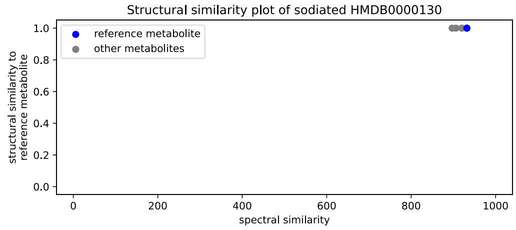
10 sodiated HMDB0000130



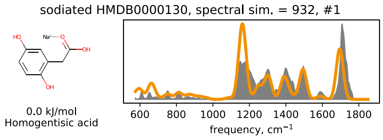
Spectra of sodiated HMDB0000130, spectral sim. = 932, #1



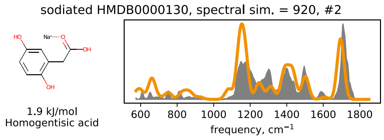
Structural similarity plot of sodiated HMDB0000130



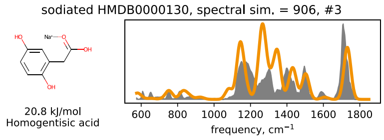
sodiated HMDB0000130, spectral sim. = 932, #1



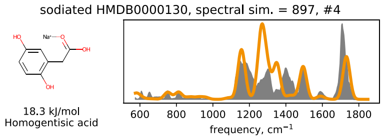
sodiated HMDB0000130, spectral sim. = 920, #2



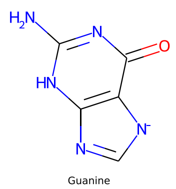
sodiated HMDB0000130, spectral sim. = 906, #3



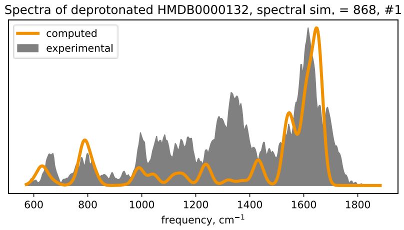
sodiated HMDB0000130, spectral sim. = 897, #4



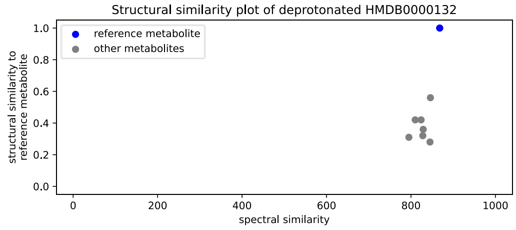
11 deprotonated HMDB0000132



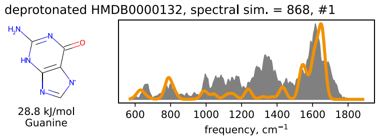
Spectra of deprotonated HMDB0000132, spectral sim. = 868, #1



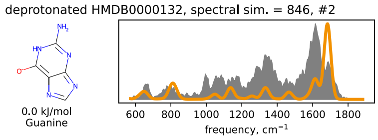
Structural similarity plot of deprotonated HMDB0000132



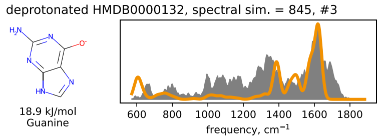
deprotonated HMDB0000132, spectral sim. = 868, #1



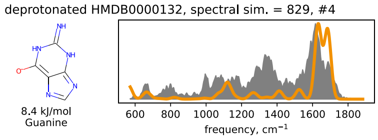
deprotonated HMDB0000132, spectral sim. = 846, #2



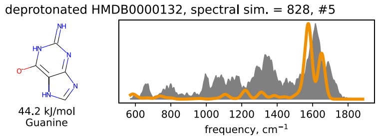
deprotonated HMDB0000132, spectral sim. = 845, #3



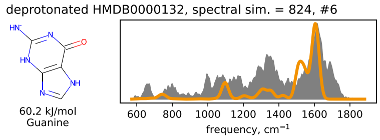
deprotonated HMDB0000132, spectral sim. = 829, #4



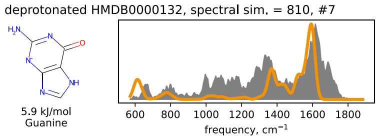
deprotonated HMDB0000132, spectral sim. = 828, #5



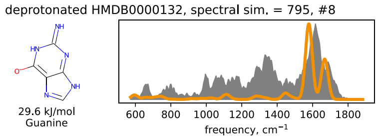
deprotonated HMDB0000132, spectral sim. = 824, #6



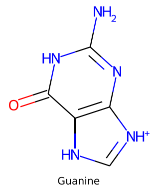
deprotonated HMDB0000132, spectral sim. = 810, #7



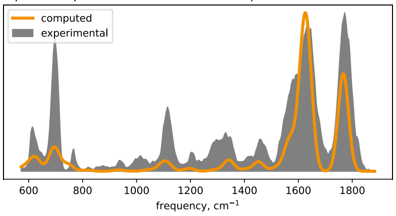
deprotonated HMDB0000132, spectral sim. = 795, #8



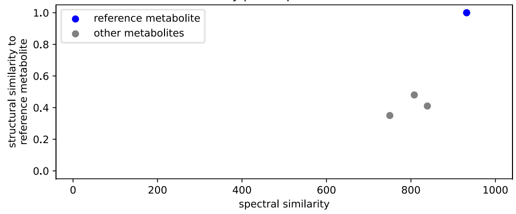
12 protonated HMDB0000132



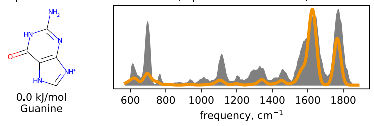
Spectra of protonated HMDB0000132, spectral sim. = 932, #1



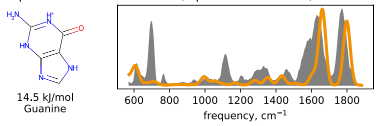
Structural similarity plot of protonated HMDB0000132



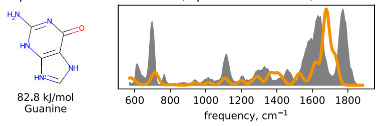
protonated HMDB0000132, spectral sim. = 932, #1



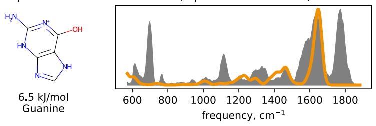
protonated HMDB0000132, spectral sim. = 839, #2



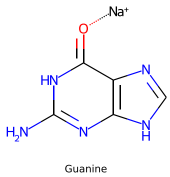
protonated HMDB0000132, spectral sim. = 808, #3



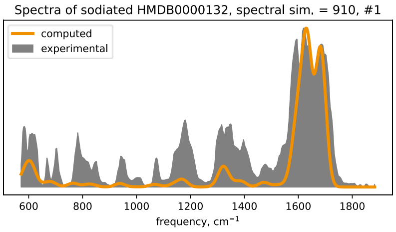
protonated HMDB0000132, spectral sim. = 750, #4



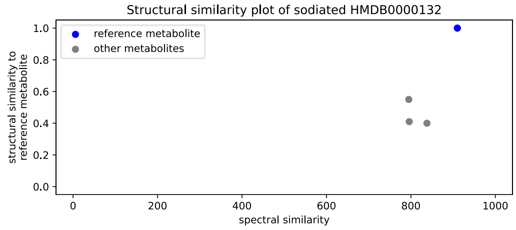
13 sodiated HMDB0000132



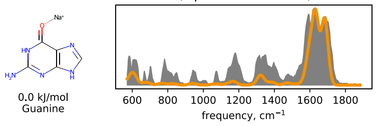
Spectra of sodiated HMDB0000132, spectral sim. = 910, #1



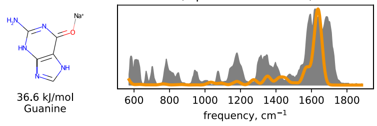
Structural similarity plot of sodiated HMDB0000132



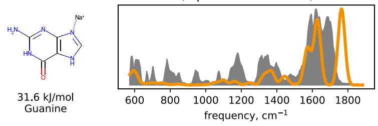
sodiated HMDB0000132, spectral sim. = 910, #1



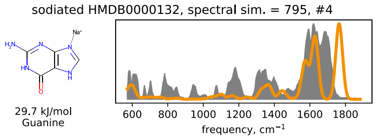
sodiated HMDB0000132, spectral sim. = 838, #2



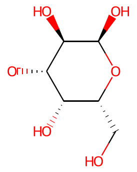
sodiated HMDB0000132, spectral sim. = 796, #3



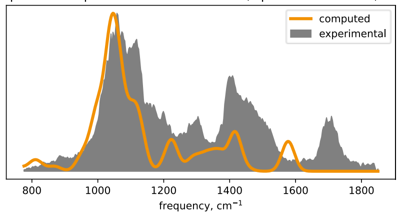
sodiated HMDB0000132, spectral sim. = 795, #4



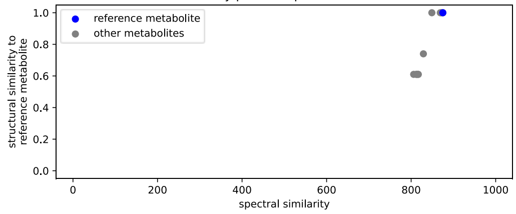
14 deprotonated HMDB0000143



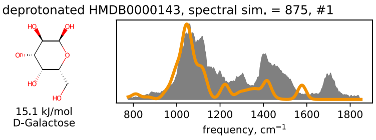
Spectra of deprotonated HMDB0000143, spectral sim. = 875, #1



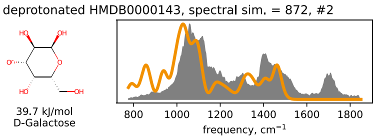
Structural similarity plot of deprotonated HMDB0000143



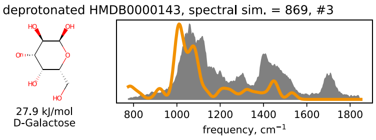
deprotonated HMDB0000143, spectral sim. = 875, #1



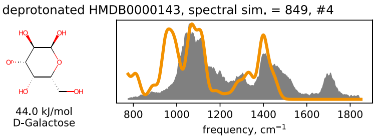
deprotonated HMDB0000143, spectral sim. = 872, #2



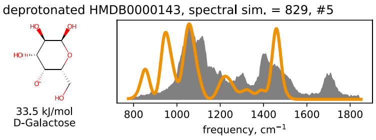
deprotonated HMDB0000143, spectral sim. = 869, #3



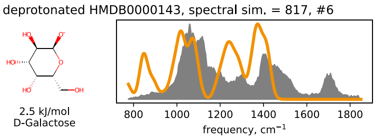
deprotonated HMDB0000143, spectral sim. = 849, #4



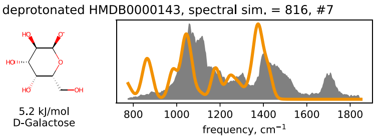
deprotonated HMDB0000143, spectral sim. = 829, #5



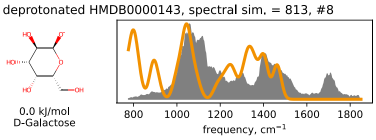
deprotonated HMDB0000143, spectral sim. = 817, #6



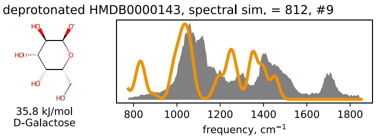
deprotonated HMDB0000143, spectral sim. = 816, #7



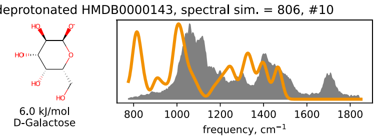
deprotonated HMDB0000143, spectral sim. = 813, #8



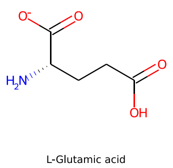
deprotonated HMDB0000143, spectral sim. = 812, #9



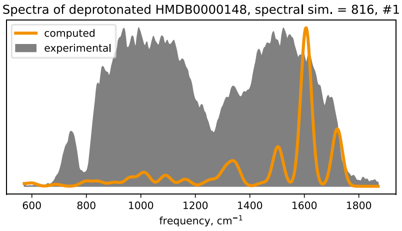
deprotonated HMDB0000143, spectral sim. = 806, #10



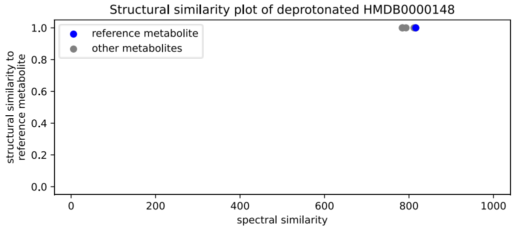
15 deprotonated HMDB0000148



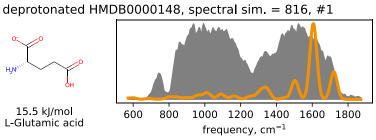
Spectra of deprotonated HMDB0000148, spectral sim. = 816, #1



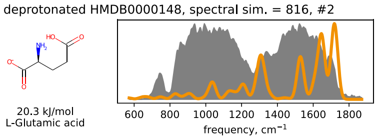
Structural similarity plot of deprotonated HMDB0000148



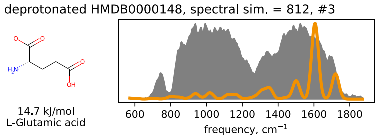
deprotonated HMDB0000148, spectral sim. = 816, #1



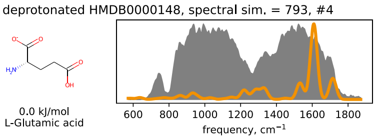
deprotonated HMDB0000148, spectral sim. = 816, #2



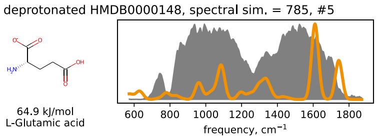
deprotonated HMDB0000148, spectral sim. = 812, #3



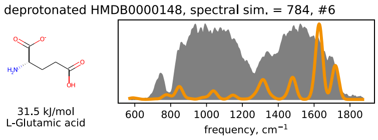
deprotonated HMDB0000148, spectral sim. = 793, #4



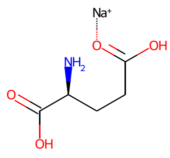
deprotonated HMDB0000148, spectral sim. = 785, #5



deprotonated HMDB0000148, spectral sim. = 784, #6

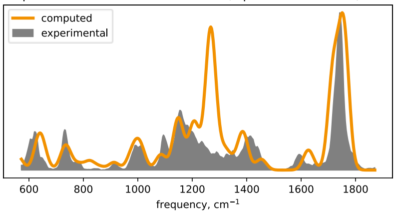


16 sodiated HMDB0000148

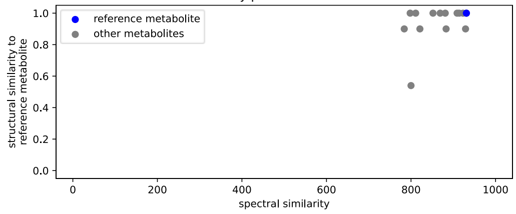


L-Glutamic acid

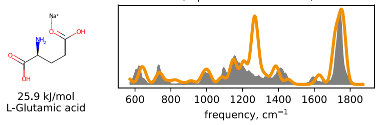
Spectra of sodiated HMDB0000148, spectral sim. = 931, #1



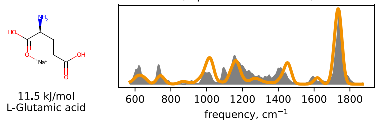
Structural similarity plot of sodiated HMDB0000148



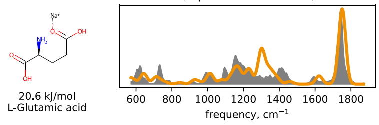
sodiated HMDB0000148, spectral sim. = 931, #1



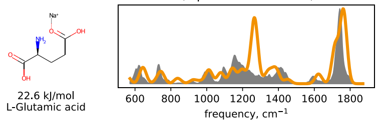
sodiated HMDB0000148, spectral sim. = 929, #2



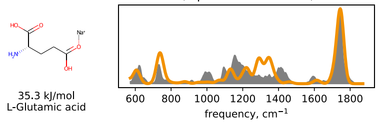
sodiated HMDB0000148, spectral sim. = 923, #3



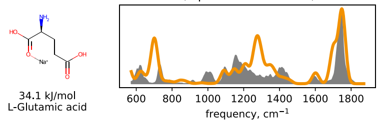
sodiated HMDB0000148, spectral sim. = 914, #4



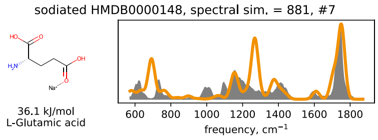
sodiated HMDB0000148, spectral sim. = 909, #5



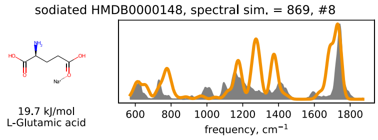
sodiated HMDB0000148, spectral sim. = 883, #6



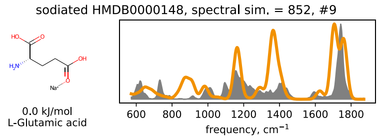
sodiated HMDB0000148, spectral sim. = 881, #7



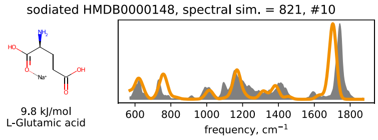
sodiated HMDB0000148, spectral sim. = 869, #8



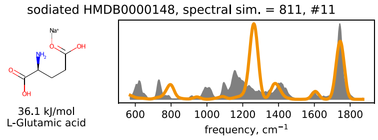
sodiated HMDB0000148, spectral sim. = 852, #9



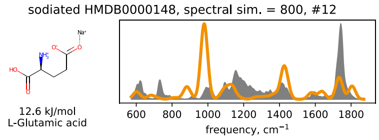
sodiated HMDB0000148, spectral sim. = 821, #10



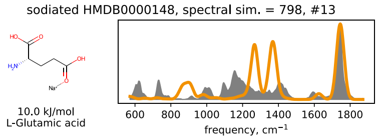
sodiated HMDB0000148, spectral sim. = 811, #11



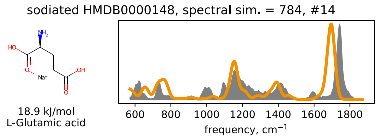
sodiated HMDB0000148, spectral sim. = 800, #12



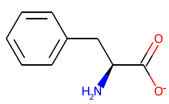
sodiated HMDB0000148, spectral sim. = 798, #13



sodiated HMDB0000148, spectral sim. = 784, #14

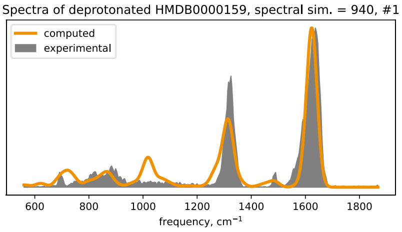


17 deprotonated HMDB0000159

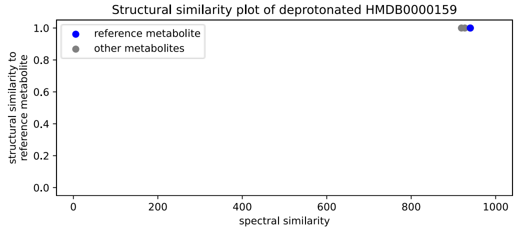


L-Phenylalanine

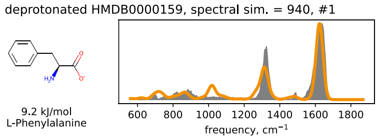
Spectra of deprotonated HMDB0000159, spectral sim. = 940, #1



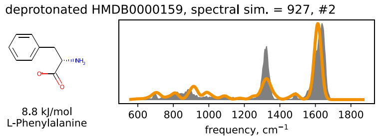
Structural similarity plot of deprotonated HMDB0000159



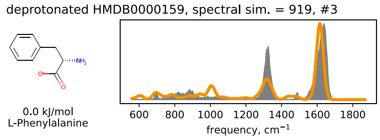
deprotonated HMDB0000159, spectral sim. = 940, #1

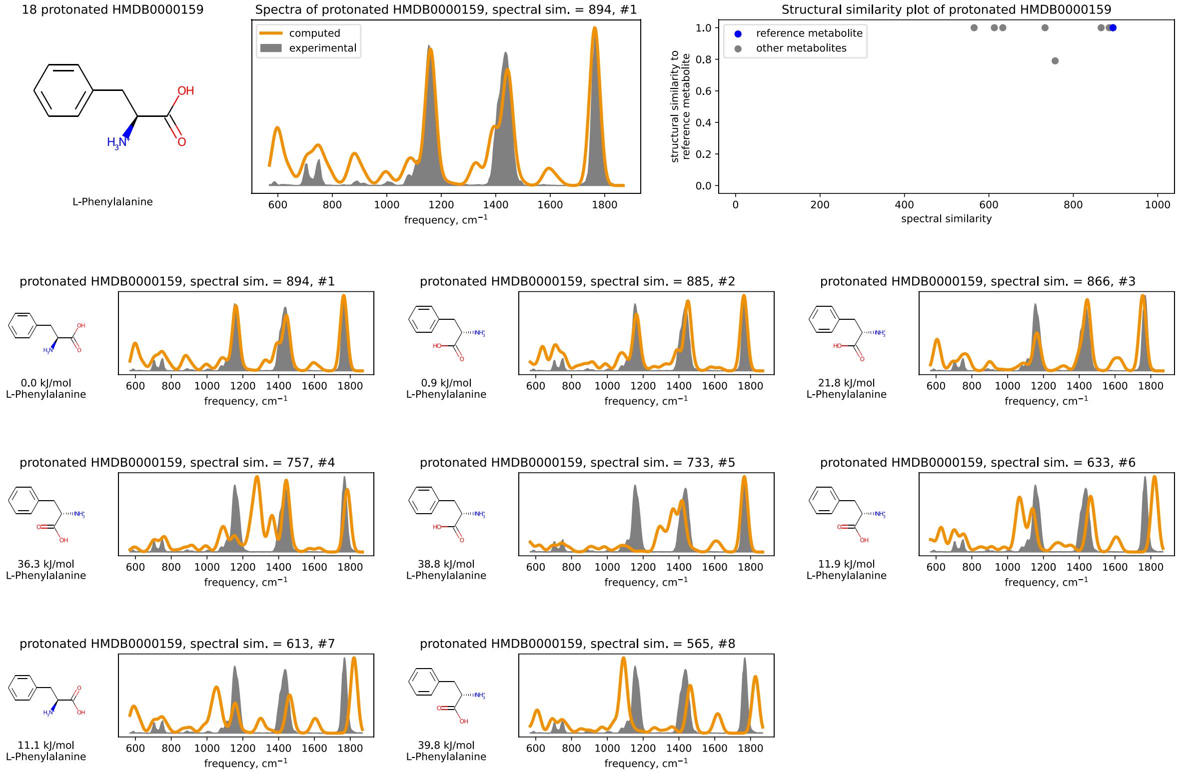


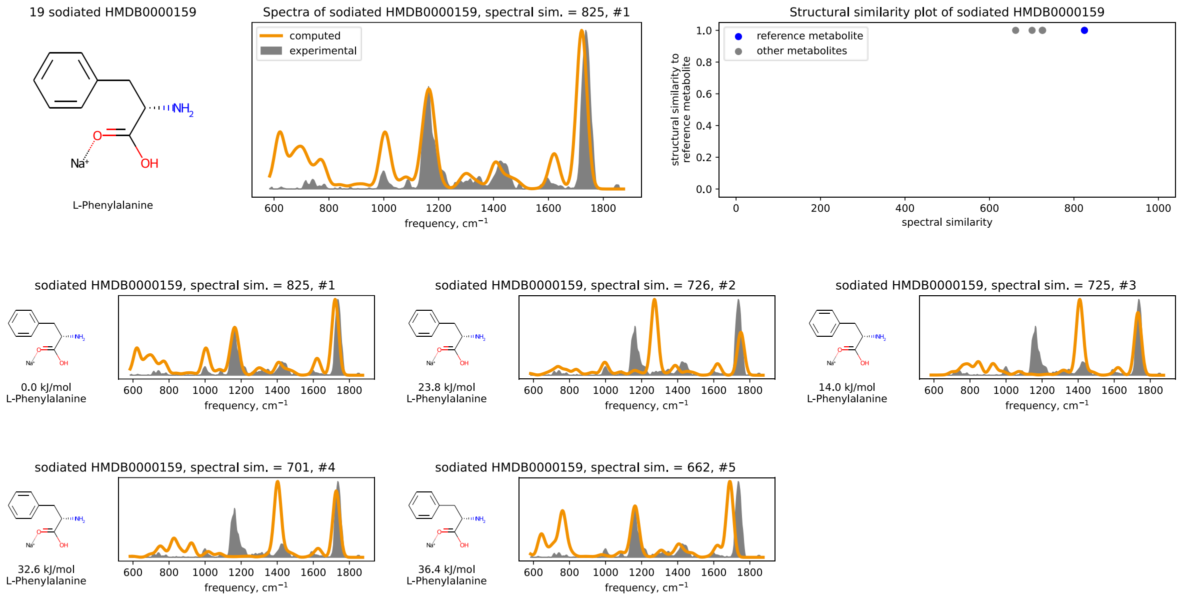
deprotonated HMDB0000159, spectral sim. = 927, #2

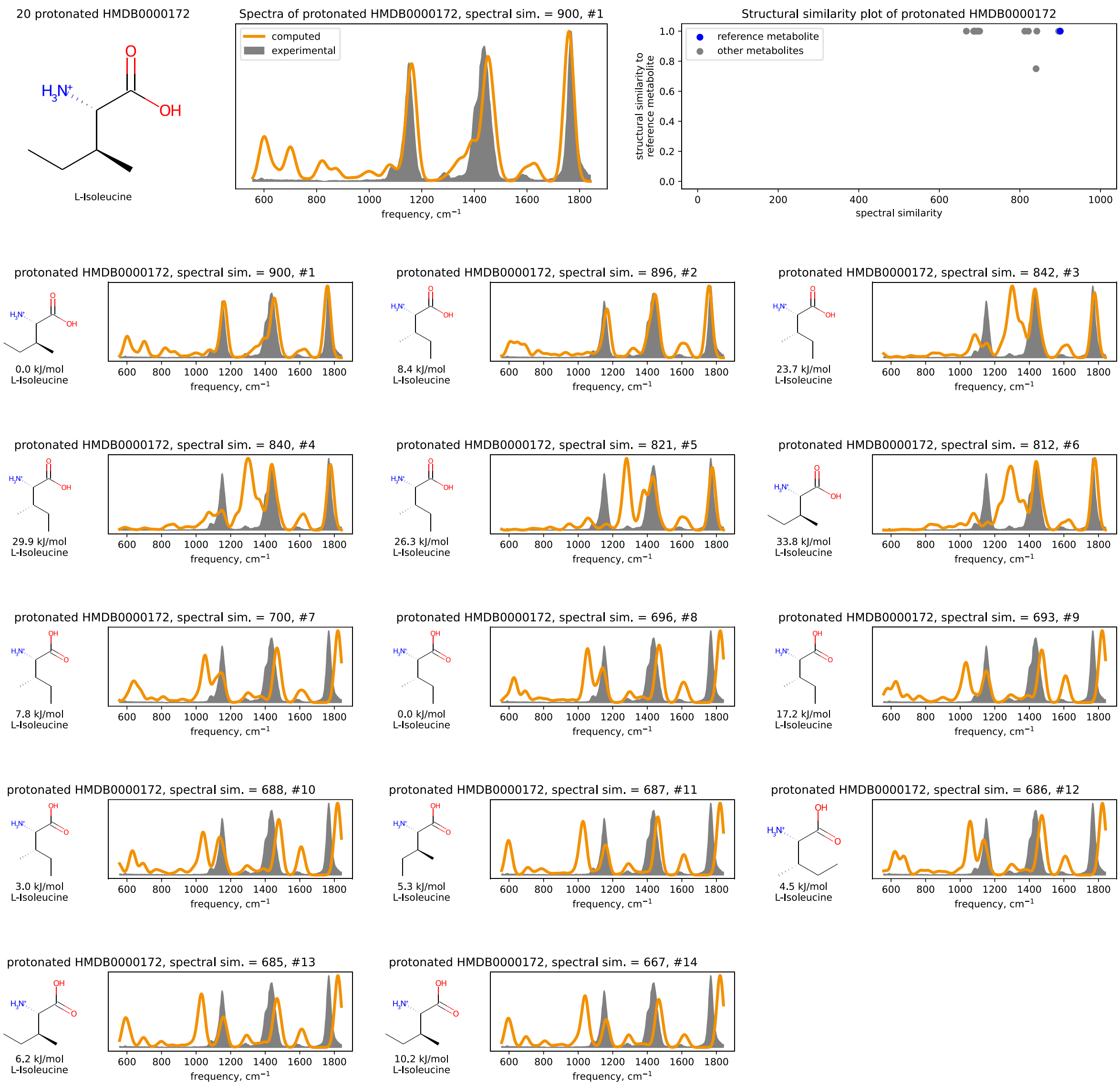


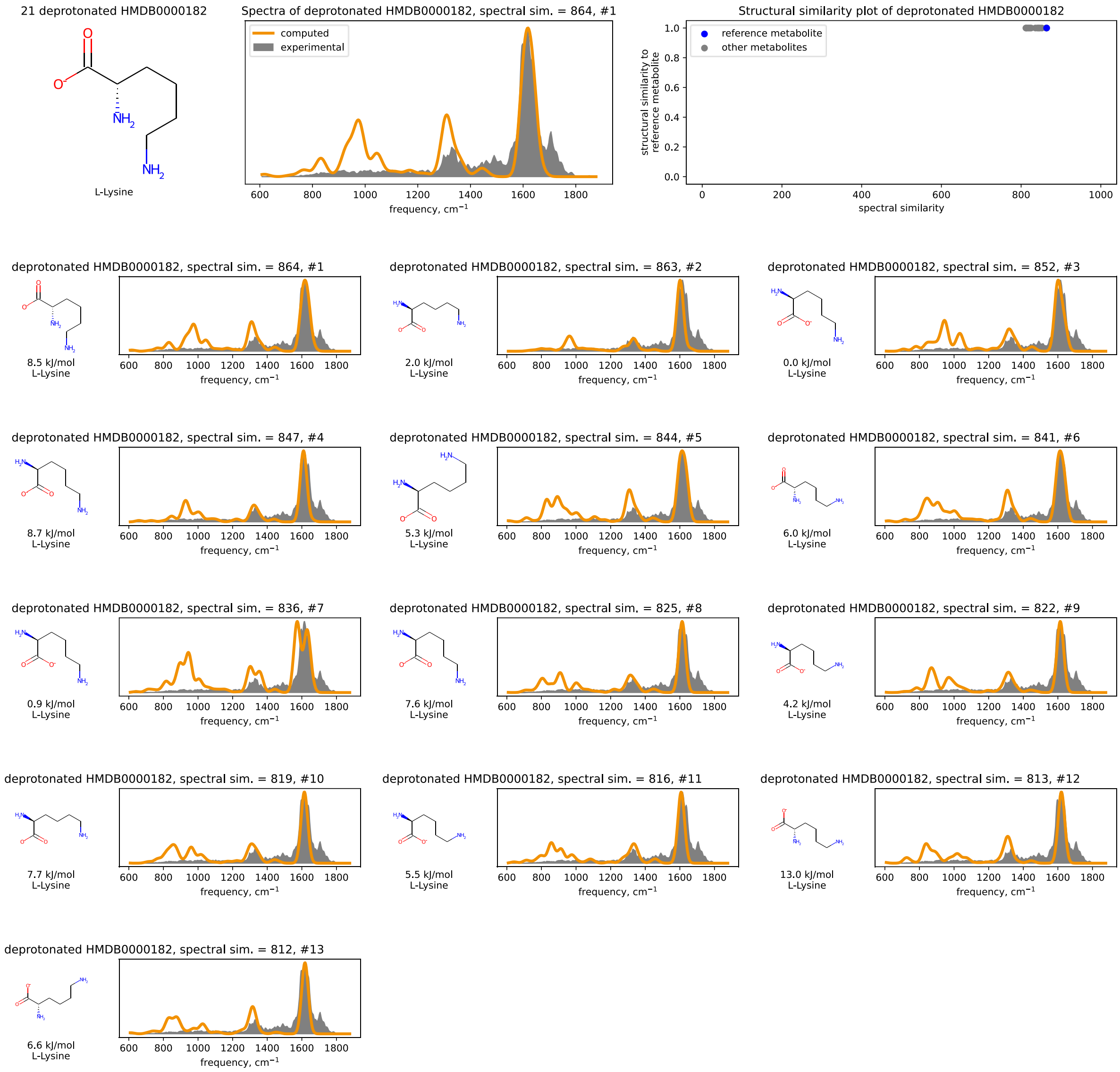
deprotonated HMDB0000159, spectral sim. = 919, #3




18 protonated HMDB0000159
L-Phenylalanine
Spectra of protonated HMDB0000159, spectral sim. = 894, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of protonated HMDB0000159
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
protonated HMDB0000159, spectral sim. = 894, #1
0.0 kJ/mol
L-Phenylalanine
protonated HMDB0000159, spectral sim. = 885, #2
0.9 kJ/mol
L-Phenylalanine
protonated HMDB0000159, spectral sim. = 866, #3
21.8 kJ/mol
L-Phenylalanine
protonated HMDB0000159, spectral sim. = 757, #4
36.3 kJ/mol
L-Phenylalanine
protonated HMDB0000159, spectral sim. = 733, #5
38.8 kJ/mol
L-Phenylalanine
protonated HMDB0000159, spectral sim. = 633, #6
11.9 kJ/mol
L-Phenylalanine
protonated HMDB0000159, spectral sim. = 613, #7
11.1 kJ/mol
L-Phenylalanine
protonated HMDB0000159, spectral sim. = 565, #8
39.8 kJ/mol
L-Phenylalanine

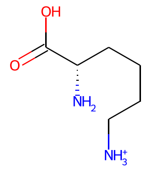

19 sodiated HMDB0000159
L-Phenylalanine
Spectra of sodiated HMDB0000159, spectral sim. = 825, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of sodiated HMDB0000159
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
sodiated HMDB0000159, spectral sim. = 825, #1
0.0 kJ/mol
L-Phenylalanine
sodiated HMDB0000159, spectral sim. = 726, #2
23.8 kJ/mol
L-Phenylalanine
sodiated HMDB0000159, spectral sim. = 725, #3
14.0 kJ/mol
L-Phenylalanine
sodiated HMDB0000159, spectral sim. = 701, #4
32.6 kJ/mol
L-Phenylalanine
sodiated HMDB0000159, spectral sim. = 662, #5
36.4 kJ/mol
L-Phenylalanine


20 protonated HMDB0000172
L-Isoleucine
Spectra of protonated HMDB0000172, spectral sim. = 900, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of protonated HMDB0000172
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
protonated HMDB0000172, spectral sim. = 900, #1
0.0 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 896, #2
8.4 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 842, #3
23.7 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 840, #4
29.9 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 821, #5
26.3 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 812, #6
33.8 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 700, #7
7.8 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 696, #8
0.0 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 693, #9
17.2 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 688, #10
3.0 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 687, #11
5.3 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 686, #12
4.5 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 685, #13
6.2 kJ/mol
L-Isoleucine
protonated HMDB0000172, spectral sim. = 667, #14
10.2 kJ/mol
L-Isoleucine



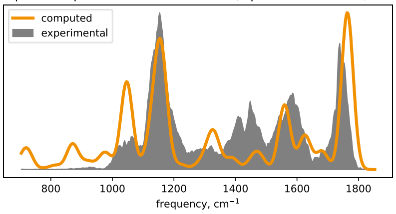
21 deprotonated HMDB0000182
L-Lysine
Spectra of deprotonated HMDB0000182, spectral sim. = 864, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of deprotonated HMDB0000182
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0000182, spectral sim. = 864, #1
8.5 kJ/mol
L-Lysine
deprotonated HMDB0000182, spectral sim. = 863, #2
2.0 kJ/mol
L-Lysine
deprotonated HMDB0000182, spectral sim. = 852, #3
0.0 kJ/mol
L-Lysine
deprotonated HMDB0000182, spectral sim. = 847, #4
8.7 kJ/mol
L-Lysine
deprotonated HMDB0000182, spectral sim. = 844, #5
5.3 kJ/mol
L-Lysine
deprotonated HMDB0000182, spectral sim. = 841, #6
6.0 kJ/mol
L-Lysine
deprotonated HMDB0000182, spectral sim. = 836, #7
0.9 kJ/mol
L-Lysine
deprotonated HMDB0000182, spectral sim. = 825, #8
7.6 kJ/mol
L-Lysine
deprotonated HMDB0000182, spectral sim. = 822, #9
4.2 kJ/mol
L-Lysine
deprotonated HMDB0000182, spectral sim. = 819, #10
7.7 kJ/mol
L-Lysine
deprotonated HMDB0000182, spectral sim. = 816, #11
5.5 kJ/mol
L-Lysine
deprotonated HMDB0000182, spectral sim. = 813, #12
13.0 kJ/mol
L-Lysine
deprotonated HMDB0000182, spectral sim. = 812, #13
6.6 kJ/mol
L-Lysine

22 protonated HMDB0000182

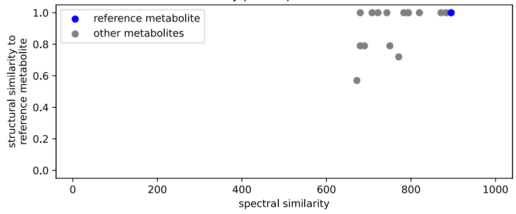


L-Lysine

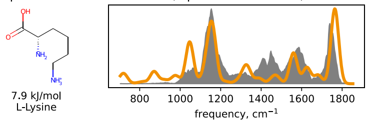
Spectra of protonated HMDB0000182, spectral sim. = 895, #1



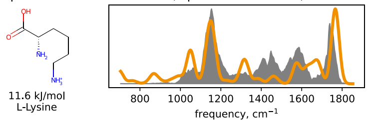
Structural similarity plot of protonated HMDB0000182



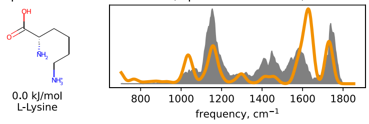
protonated HMDB0000182, spectral sim. = 895, #1



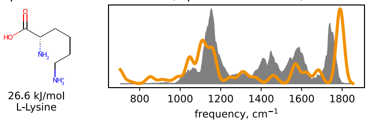
protonated HMDB0000182, spectral sim. = 883, #2



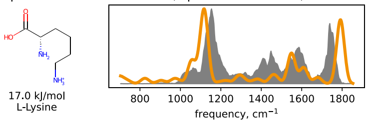
protonated HMDB0000182, spectral sim. = 871, #3



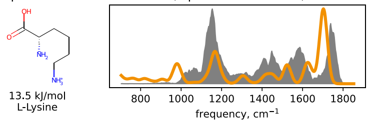
protonated HMDB0000182, spectral sim. = 820, #4



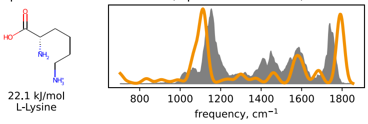
protonated HMDB0000182, spectral sim. = 794, #5



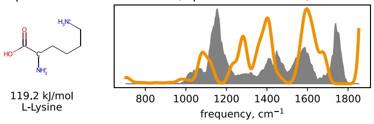
protonated HMDB0000182, spectral sim. = 793, #6



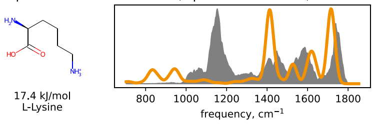
protonated HMDB0000182, spectral sim. = 783, #7



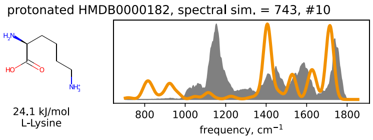
protonated HMDB0000182, spectral sim. = 771, #8



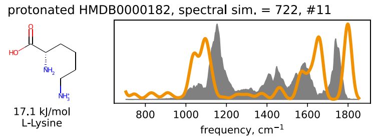
protonated HMDB0000182, spectral sim. = 750, #9



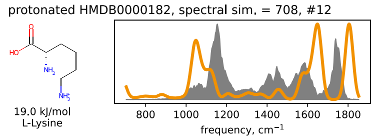
protonated HMDB0000182, spectral sim. = 743, #10



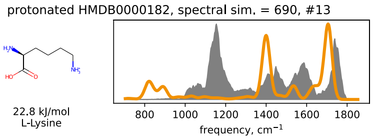
protonated HMDB0000182, spectral sim. = 722, #11



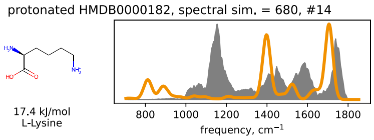
protonated HMDB0000182, spectral sim. = 708, #12



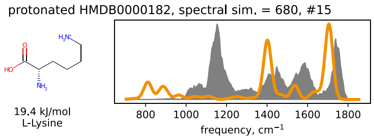
protonated HMDB0000182, spectral sim. = 690, #13



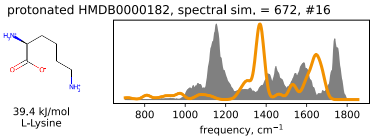
protonated HMDB0000182, spectral sim. = 680, #14



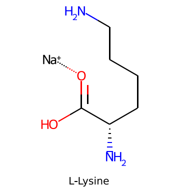
protonated HMDB0000182, spectral sim. = 680, #15



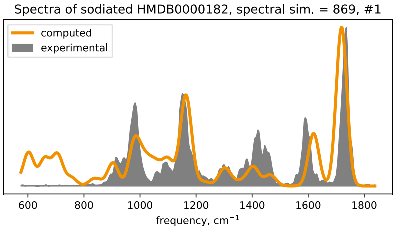
protonated HMDB0000182, spectral sim. = 672, #16



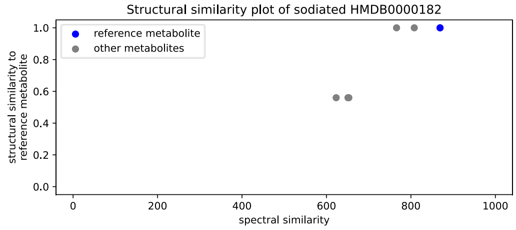
23 sodiated HMDB0000182



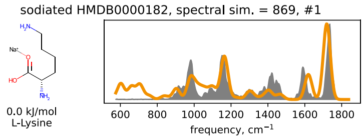
Spectra of sodiated HMDB0000182, spectral sim. = 869, #1



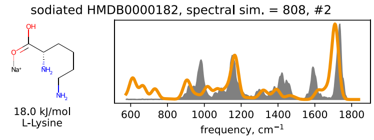
Structural similarity plot of sodiated HMDB0000182



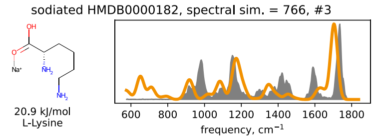
sodiated HMDB0000182, spectral sim. = 869, #1



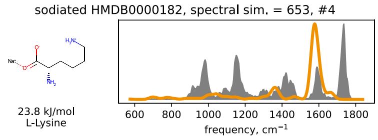
sodiated HMDB0000182, spectral sim. = 808, #2



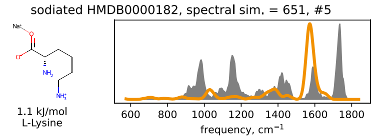
sodiated HMDB0000182, spectral sim. = 766, #3



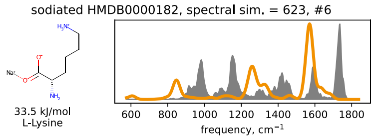
sodiated HMDB0000182, spectral sim. = 653, #4



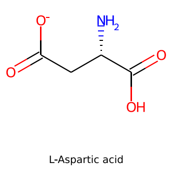
sodiated HMDB0000182, spectral sim. = 651, #5



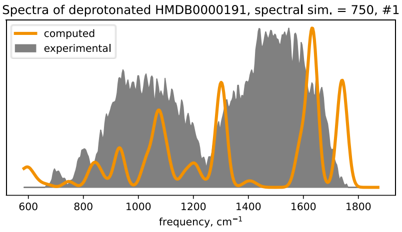
sodiated HMDB0000182, spectral sim. = 623, #6



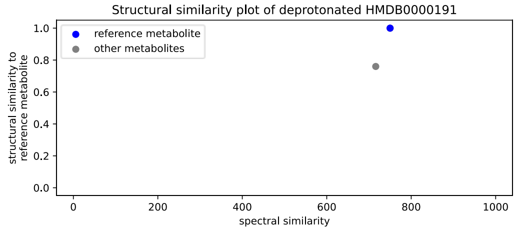
24 deprotonated HMDB0000191



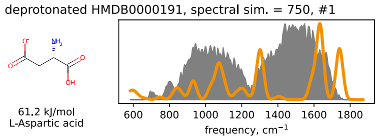
Spectra of deprotonated HMDB0000191, spectral sim. = 750, #1



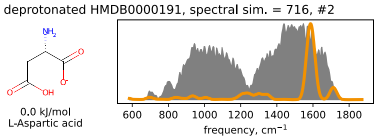
Structural similarity plot of deprotonated HMDB0000191



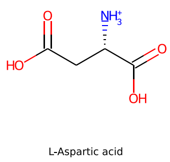
deprotonated HMDB0000191, spectral sim. = 750, #1



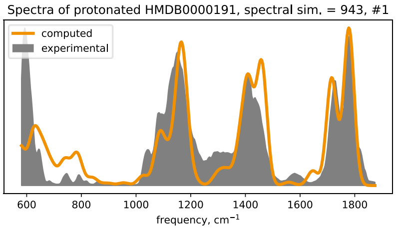
deprotonated HMDB0000191, spectral sim. = 716, #2



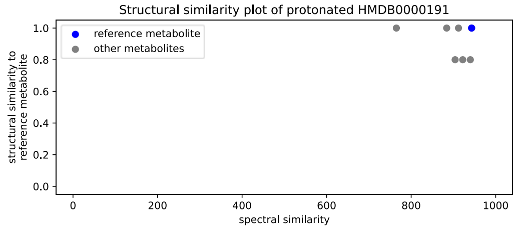
25 protonated HMDB0000191



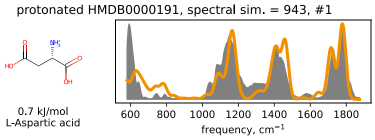
Spectra of protonated HMDB0000191, spectral sim. = 943, #1



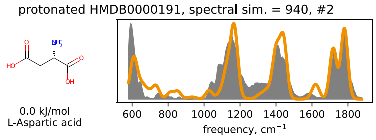
Structural similarity plot of protonated HMDB0000191



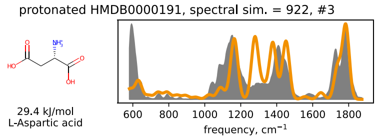
protonated HMDB0000191, spectral sim. = 943, #1



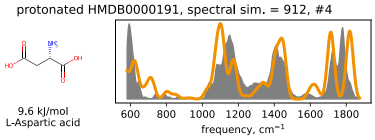
protonated HMDB0000191, spectral sim. = 940, #2



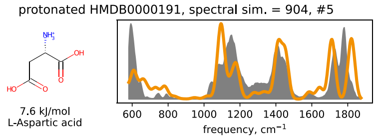
protonated HMDB0000191, spectral sim. = 922, #3



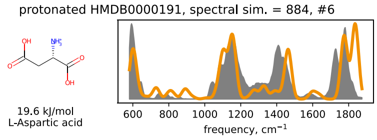
protonated HMDB0000191, spectral sim. = 912, #4



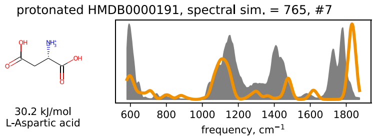
protonated HMDB0000191, spectral sim. = 904, #5



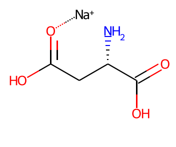
protonated HMDB0000191, spectral sim. = 884, #6



protonated HMDB0000191, spectral sim. = 765, #7

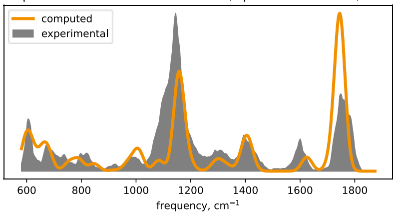


26 sodiated HMDB0000191

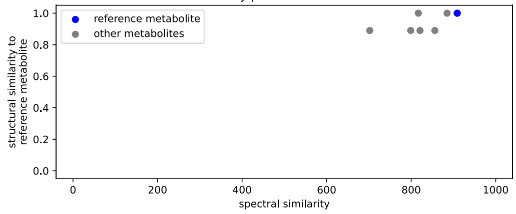


L-Aspartic acid

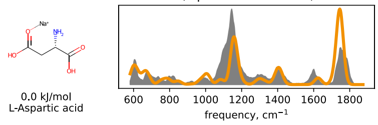
Spectra of sodiated HMDB0000191, spectral sim. = 909, #1



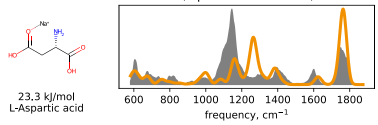
Structural similarity plot of sodiated HMDB0000191



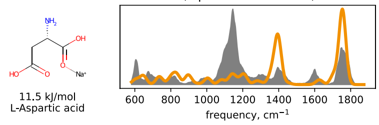
sodiated HMDB0000191, spectral sim. = 909, #1



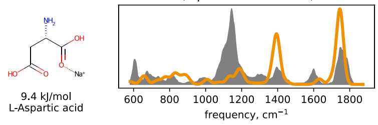
sodiated HMDB0000191, spectral sim. = 885, #2



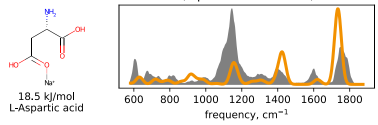
sodiated HMDB0000191, spectral sim. = 856, #3



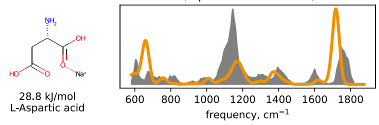
sodiated HMDB0000191, spectral sim. = 821, #4



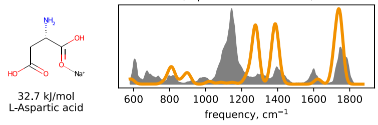
sodiated HMDB0000191, spectral sim. = 817, #5



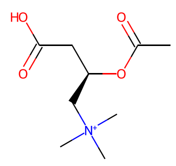
sodiated HMDB0000191, spectral sim. = 799, #6



sodiated HMDB0000191, spectral sim. = 702, #7

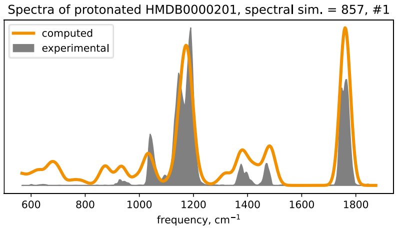


27 protonated HMDB0000201

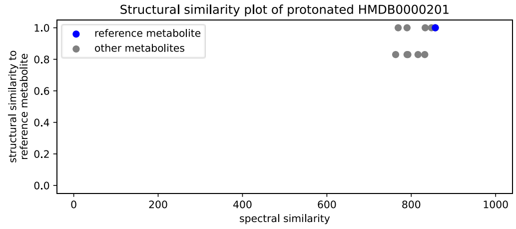


L-Acetylcarnitine

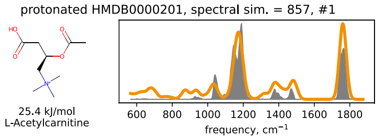
Spectra of protonated HMDB0000201, spectral sim. = 857, #1



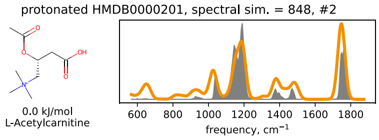
Structural similarity plot of protonated HMDB0000201



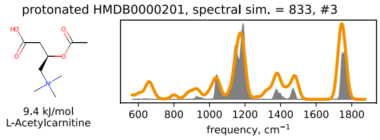
protonated HMDB0000201, spectral sim. = 857, #1



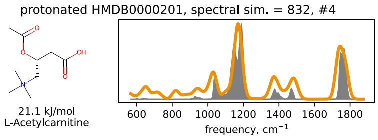
protonated HMDB0000201, spectral sim. = 848, #2



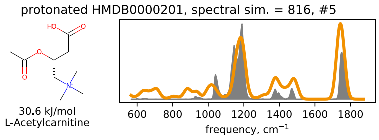
protonated HMDB0000201, spectral sim. = 833, #3



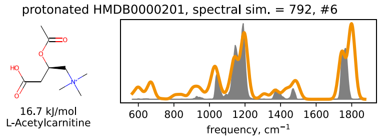
protonated HMDB0000201, spectral sim. = 832, #4



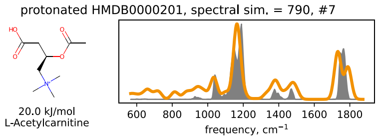
protonated HMDB0000201, spectral sim. = 816, #5



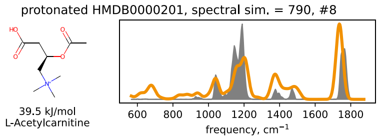
protonated HMDB0000201, spectral sim. = 792, #6



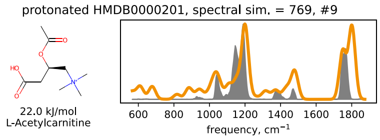
protonated HMDB0000201, spectral sim. = 790, #7



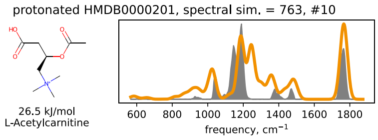
protonated HMDB0000201, spectral sim. = 790, #8



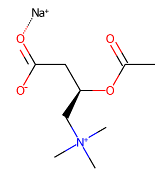
protonated HMDB0000201, spectral sim. = 769, #9



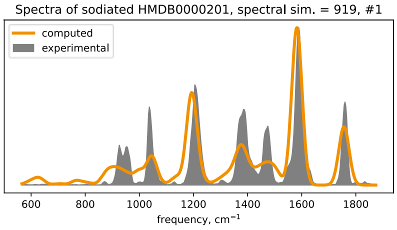
protonated HMDB0000201, spectral sim. = 763, #10



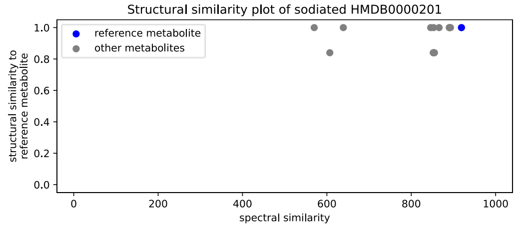
28 sodiated HMDB0000201



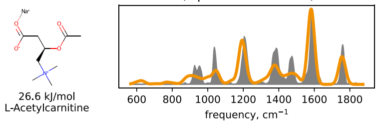
Spectra of sodiated HMDB0000201, spectral sim. = 919, #1



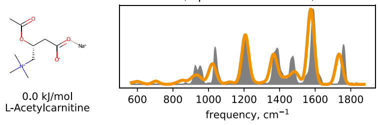
Structural similarity plot of sodiated HMDB0000201



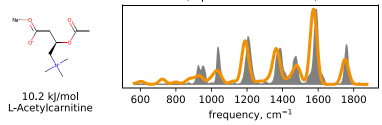
sodiated HMDB0000201, spectral sim. = 919, #1



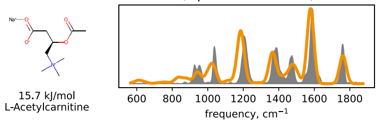
sodiated HMDB0000201, spectral sim. = 893, #2



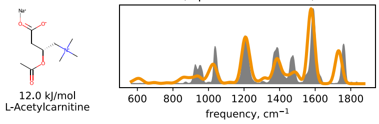
sodiated HMDB0000201, spectral sim. = 891, #3



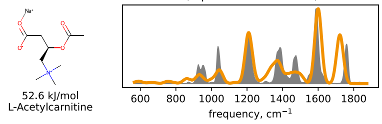
sodiated HMDB0000201, spectral sim. = 891, #4



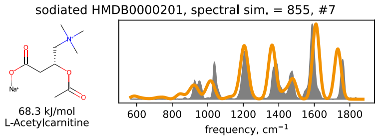
sodiated HMDB0000201, spectral sim. = 890, #5



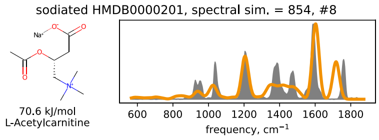
sodiated HMDB0000201, spectral sim. = 866, #6



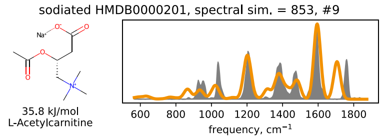
sodiated HMDB0000201, spectral sim. = 855, #7



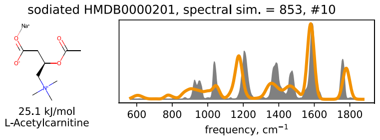
sodiated HMDB0000201, spectral sim. = 854, #8



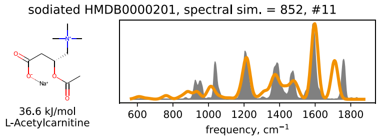
sodiated HMDB0000201, spectral sim. = 853, #9



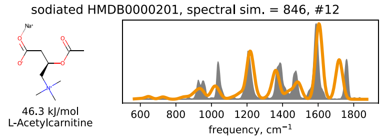
sodiated HMDB0000201, spectral sim. = 853, #10



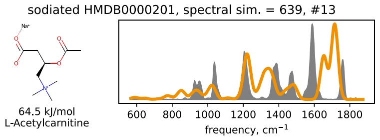
sodiated HMDB0000201, spectral sim. = 852, #11



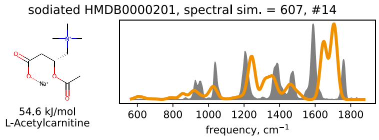
sodiated HMDB0000201, spectral sim. = 846, #12



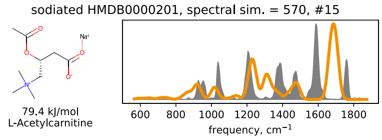
sodiated HMDB0000201, spectral sim. = 639, #13



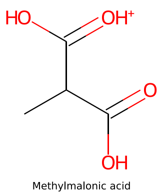
sodiated HMDB0000201, spectral sim. = 607, #14



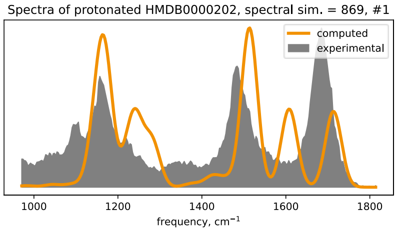
sodiated HMDB0000201, spectral sim. = 570, #15



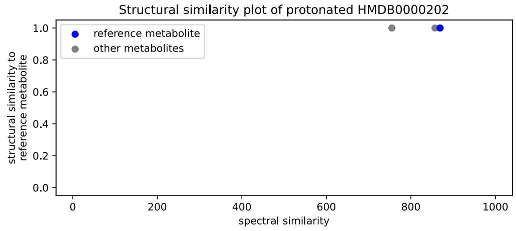
29 protonated HMDB0000202



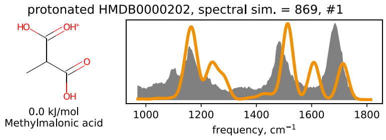
Spectra of protonated HMDB0000202, spectral sim. = 869, #1



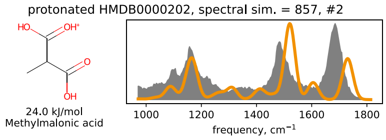
Structural similarity plot of protonated HMDB0000202



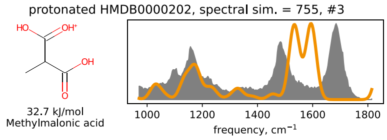
protonated HMDB0000202, spectral sim. = 869, #1



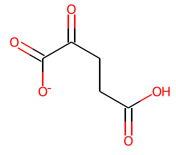
protonated HMDB0000202, spectral sim. = 857, #2



protonated HMDB0000202, spectral sim. = 755, #3

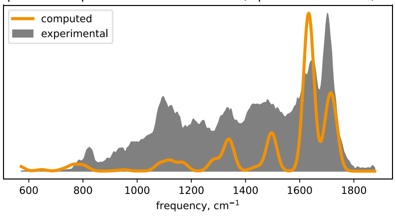


30 deprotonated HMDB0000208

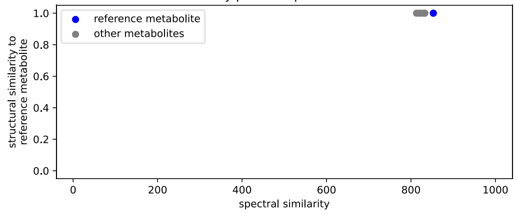


Oxoglutaric acid

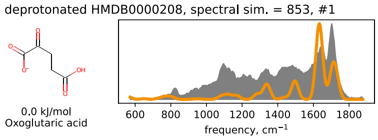
Spectra of deprotonated HMDB0000208, spectral sim. = 853, #1



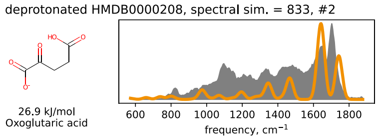
Structural similarity plot of deprotonated HMDB0000208



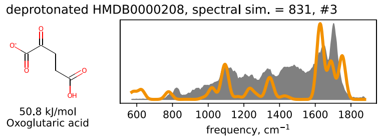
deprotonated HMDB0000208, spectral sim. = 853, #1



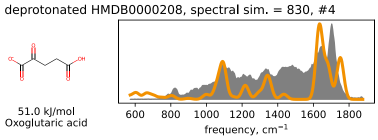
deprotonated HMDB0000208, spectral sim. = 833, #2



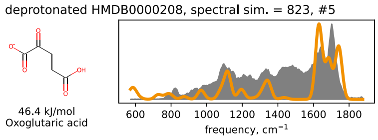
deprotonated HMDB0000208, spectral sim. = 831, #3



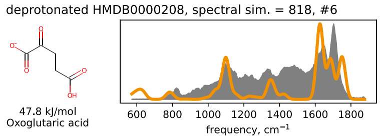
deprotonated HMDB0000208, spectral sim. = 830, #4



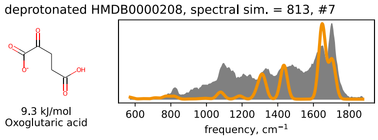
deprotonated HMDB0000208, spectral sim. = 823, #5



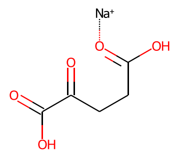
deprotonated HMDB0000208, spectral sim. = 818, #6



deprotonated HMDB0000208, spectral sim. = 813, #7

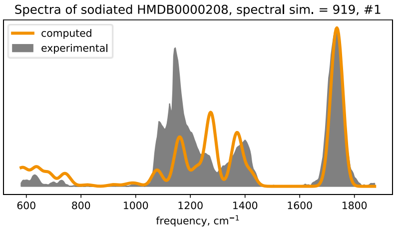


31 sodiated HMDB0000208

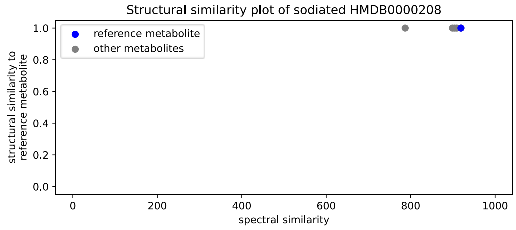


Oxoglutaric acid

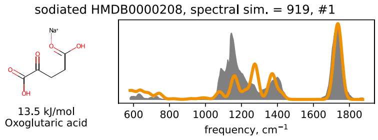
Spectra of sodiated HMDB0000208, spectral sim. = 919, #1



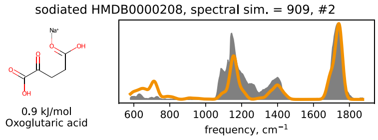
Structural similarity plot of sodiated HMDB0000208



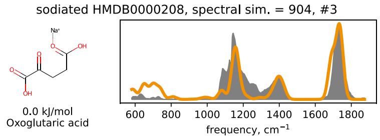
sodiated HMDB0000208, spectral sim. = 919, #1



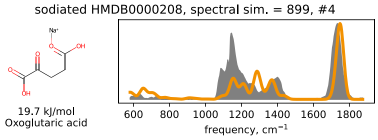
sodiated HMDB0000208, spectral sim. = 909, #2



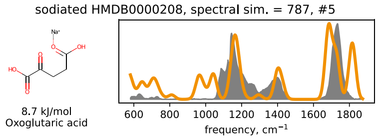
sodiated HMDB0000208, spectral sim. = 904, #3

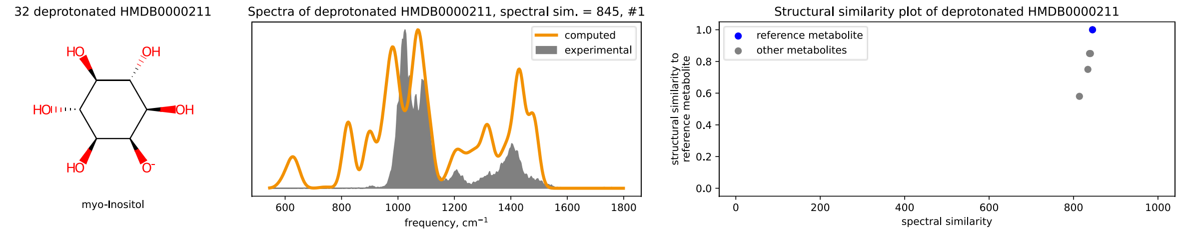


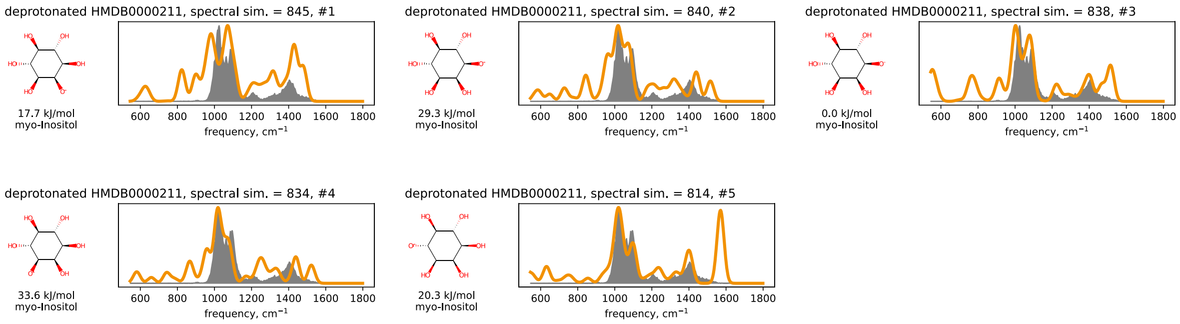
sodiated HMDB0000208, spectral sim. = 899, #4

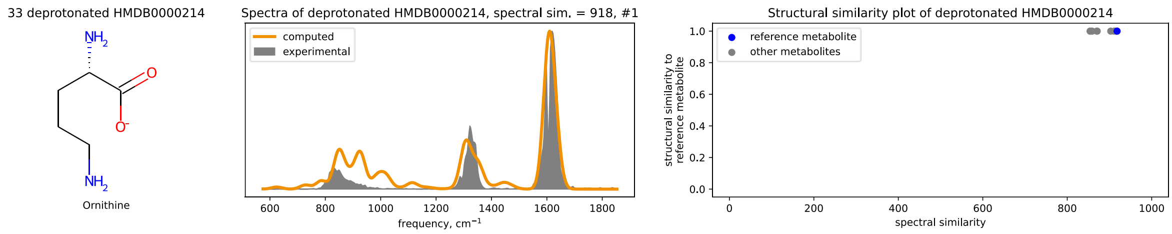


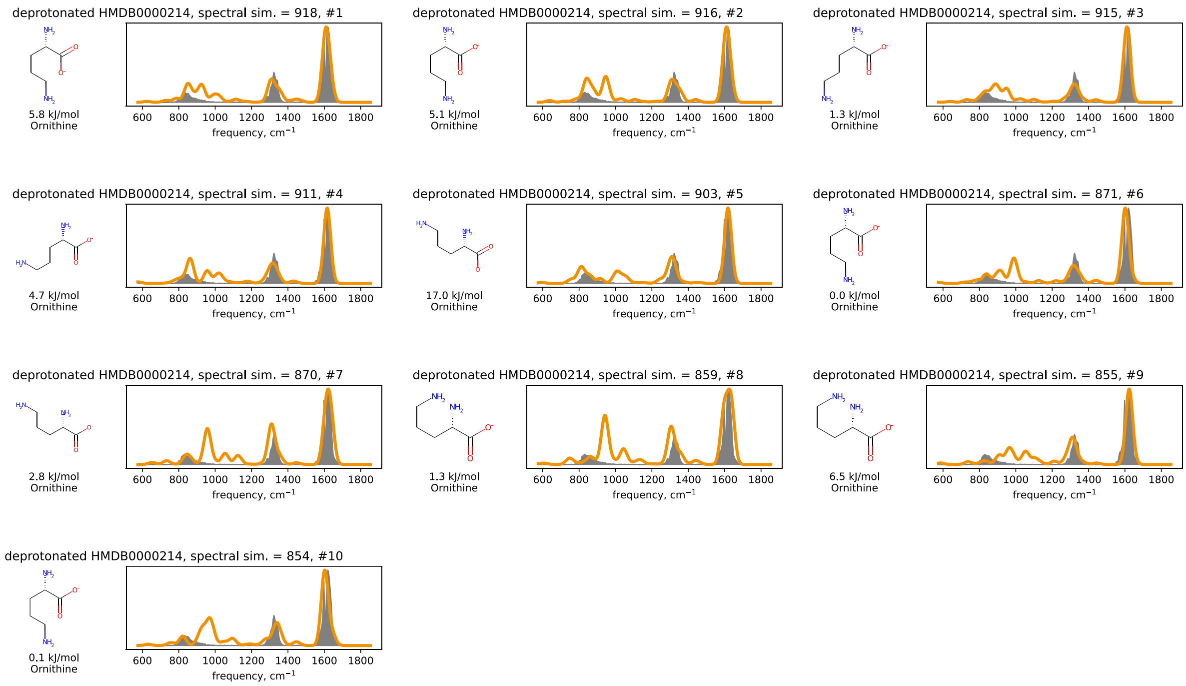
sodiated HMDB0000208, spectral sim. = 787, #5



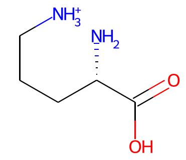

32 deprotonated HMDB0000211
myo-Inositol
Spectra of deprotonated HMDB0000211, spectral sim. = 845, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0000211
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity


deprotonated HMDB0000211, spectral sim. = 845, #1
17.7 kJ/mol
myo-Inositol
deprotonated HMDB0000211, spectral sim. = 840, #2
29.3 kJ/mol
myo-Inositol
deprotonated HMDB0000211, spectral sim. = 838, #3
0.0 kJ/mol
myo-Inositol
deprotonated HMDB0000211, spectral sim. = 834, #4
33.6 kJ/mol
myo-Inositol
deprotonated HMDB0000211, spectral sim. = 814, #5
20.3 kJ/mol
myo-Inositol
frequency, cm^{-1}


33 deprotonated HMDB0000214
Ornithine
Spectra of deprotonated HMDB0000214, spectral sim. = 918, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0000214
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

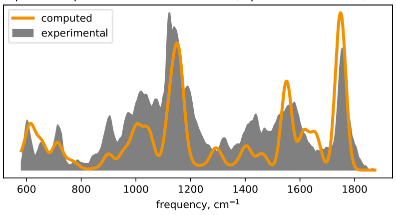

deprotonated HMDB0000214, spectral sim. = 918, #1
5.8 kJ/mol
Ornithine
deprotonated HMDB0000214, spectral sim. = 916, #2
5.1 kJ/mol
Ornithine
deprotonated HMDB0000214, spectral sim. = 915, #3
1.3 kJ/mol
Ornithine
deprotonated HMDB0000214, spectral sim. = 911, #4
4.7 kJ/mol
Ornithine
deprotonated HMDB0000214, spectral sim. = 903, #5
17.0 kJ/mol
Ornithine
deprotonated HMDB0000214, spectral sim. = 871, #6
0.0 kJ/mol
Ornithine
deprotonated HMDB0000214, spectral sim. = 870, #7
2.8 kJ/mol
Ornithine
deprotonated HMDB0000214, spectral sim. = 859, #8
1.3 kJ/mol
Ornithine
deprotonated HMDB0000214, spectral sim. = 855, #9
6.5 kJ/mol
Ornithine
deprotonated HMDB0000214, spectral sim. = 854, #10
0.1 kJ/mol
Ornithine
frequency, cm^{-1}

34 protonated HMDB0000214

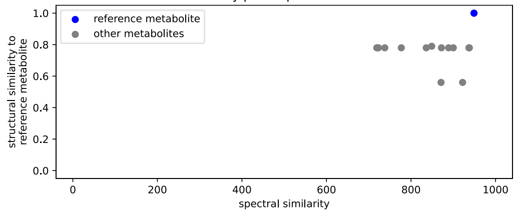


Ornithine

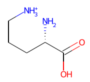
Spectra of protonated HMDB0000214, spectral sim. = 949, #1



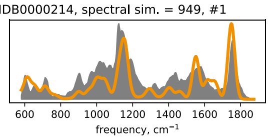
Structural similarity plot of protonated HMDB0000214



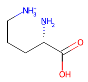
protonated HMDB0000214, spectral sim. = 949, #1



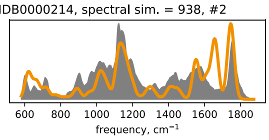
13.4 kJ/mol
Ornithine



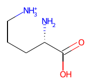
protonated HMDB0000214, spectral sim. = 938, #2



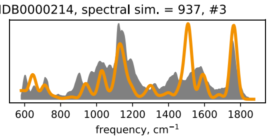
0.0 kJ/mol
Ornithine



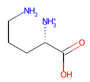
protonated HMDB0000214, spectral sim. = 937, #3



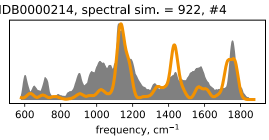
17.1 kJ/mol
Ornithine



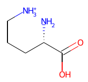
protonated HMDB0000214, spectral sim. = 922, #4



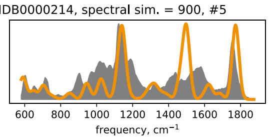
20.6 kJ/mol
Ornithine



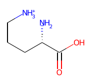
protonated HMDB0000214, spectral sim. = 900, #5



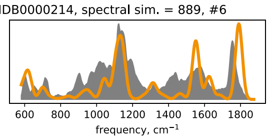
22.0 kJ/mol
Ornithine



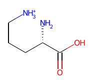
protonated HMDB0000214, spectral sim. = 889, #6



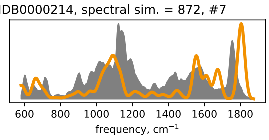
30.1 kJ/mol
Ornithine



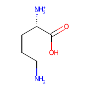
protonated HMDB0000214, spectral sim. = 872, #7



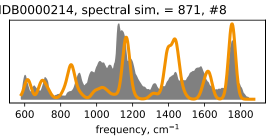
15.0 kJ/mol
Ornithine



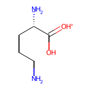
protonated HMDB0000214, spectral sim. = 871, #8



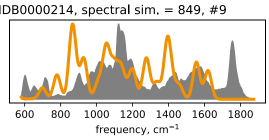
81.6 kJ/mol
Ornithine



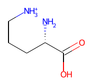
protonated HMDB0000214, spectral sim. = 849, #9



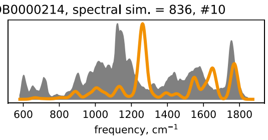
59.4 kJ/mol
Ornithine



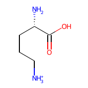
protonated HMDB0000214, spectral sim. = 836, #10



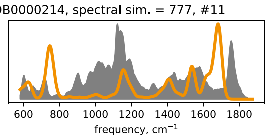
28.7 kJ/mol
Ornithine



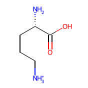
protonated HMDB0000214, spectral sim. = 777, #11



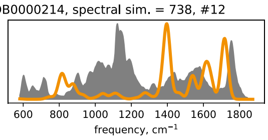
51.7 kJ/mol
Ornithine



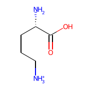
protonated HMDB0000214, spectral sim. = 738, #12



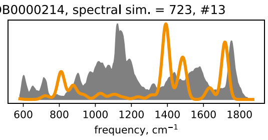
42.4 kJ/mol
Ornithine



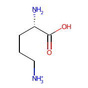
protonated HMDB0000214, spectral sim. = 723, #13



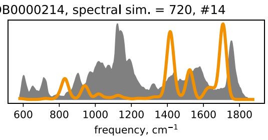
42.7 kJ/mol
Ornithine



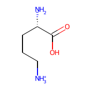
protonated HMDB0000214, spectral sim. = 720, #14



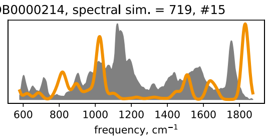
37.6 kJ/mol
Ornithine

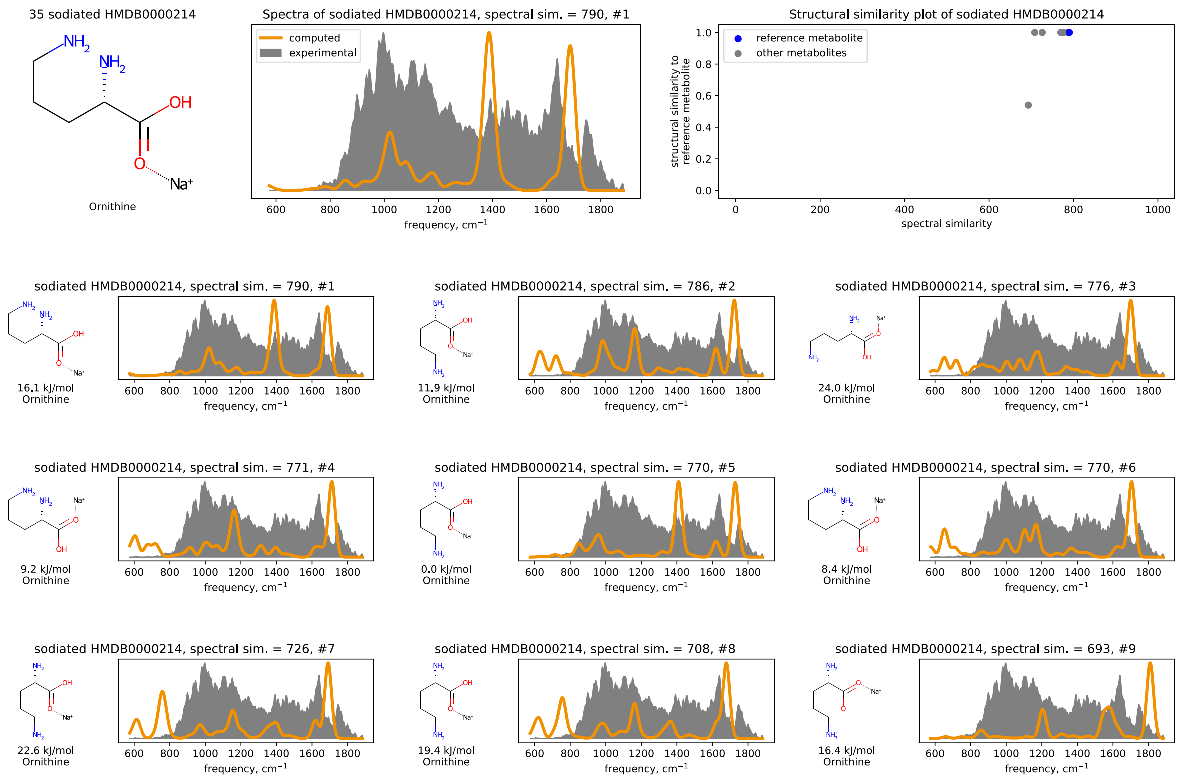


protonated HMDB0000214, spectral sim. = 719, #15

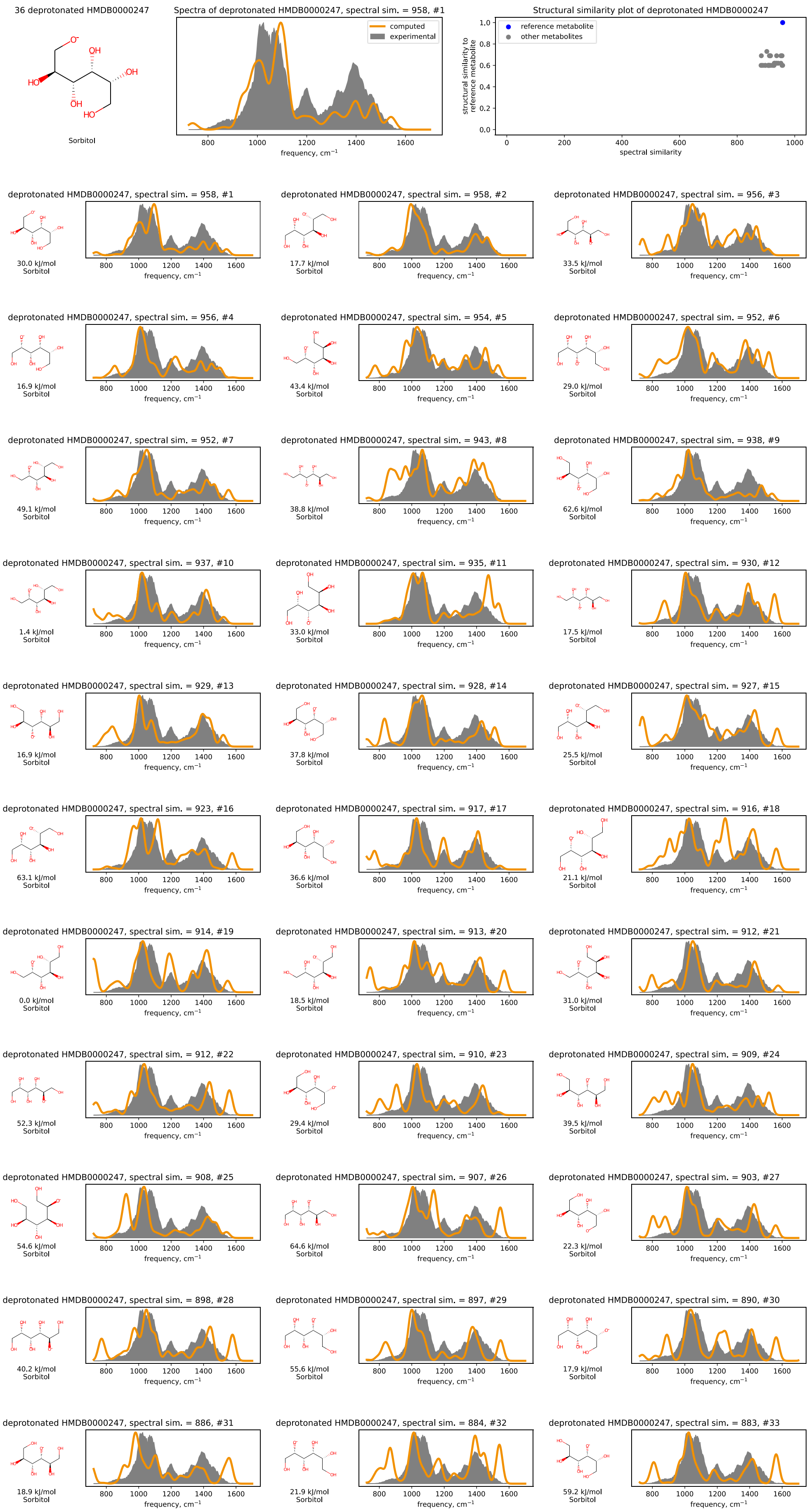


73.1 kJ/mol
Ornithine

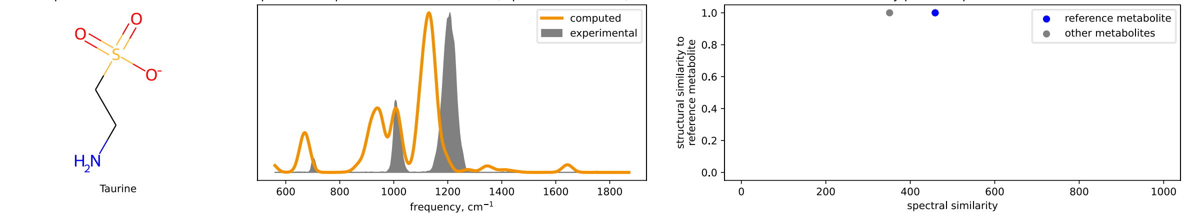




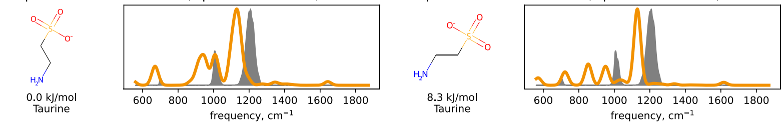
35 sodiated HMDB0000214
Ornithine
Spectra of sodiated HMDB0000214, spectral sim. = 790, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of sodiated HMDB0000214
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
sodiated HMDB0000214, spectral sim. = 790, #1
16.1 kJ/mol
Ornithine
sodiated HMDB0000214, spectral sim. = 786, #2
11.9 kJ/mol
Ornithine
sodiated HMDB0000214, spectral sim. = 776, #3
24.0 kJ/mol
Ornithine
sodiated HMDB0000214, spectral sim. = 771, #4
9.2 kJ/mol
Ornithine
sodiated HMDB0000214, spectral sim. = 770, #5
0.0 kJ/mol
Ornithine
sodiated HMDB0000214, spectral sim. = 770, #6
8.4 kJ/mol
Ornithine
sodiated HMDB0000214, spectral sim. = 726, #7
22.6 kJ/mol
Ornithine
sodiated HMDB0000214, spectral sim. = 708, #8
19.4 kJ/mol
Ornithine
sodiated HMDB0000214, spectral sim. = 693, #9
16.4 kJ/mol
Ornithine


36 deprotonated HMDB0000247
Sorbitol
Spectra of deprotonated HMDB0000247, spectral sim. = 958, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of deprotonated HMDB0000247
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0000247, spectral sim. = 958, #1
30.0 kJ/mol
deprotonated HMDB0000247, spectral sim. = 958, #2
17.7 kJ/mol
deprotonated HMDB0000247, spectral sim. = 956, #3
33.5 kJ/mol
deprotonated HMDB0000247, spectral sim. = 956, #4
16.9 kJ/mol
deprotonated HMDB0000247, spectral sim. = 954, #5
43.4 kJ/mol
deprotonated HMDB0000247, spectral sim. = 952, #6
29.0 kJ/mol
deprotonated HMDB0000247, spectral sim. = 952, #7
49.1 kJ/mol
deprotonated HMDB0000247, spectral sim. = 943, #8
38.8 kJ/mol
deprotonated HMDB0000247, spectral sim. = 938, #9
62.6 kJ/mol
deprotonated HMDB0000247, spectral sim. = 937, #10
1.4 kJ/mol
deprotonated HMDB0000247, spectral sim. = 935, #11
33.0 kJ/mol
deprotonated HMDB0000247, spectral sim. = 930, #12
17.5 kJ/mol
deprotonated HMDB0000247, spectral sim. = 929, #13
16.9 kJ/mol
deprotonated HMDB0000247, spectral sim. = 928, #14
37.8 kJ/mol
deprotonated HMDB0000247, spectral sim. = 927, #15
25.5 kJ/mol
deprotonated HMDB0000247, spectral sim. = 923, #16
63.1 kJ/mol
deprotonated HMDB0000247, spectral sim. = 917, #17
36.6 kJ/mol
deprotonated HMDB0000247, spectral sim. = 916, #18
21.1 kJ/mol
deprotonated HMDB0000247, spectral sim. = 914, #19
0.0 kJ/mol
deprotonated HMDB0000247, spectral sim. = 913, #20
18.5 kJ/mol
deprotonated HMDB0000247, spectral sim. = 912, #21
31.0 kJ/mol
deprotonated HMDB0000247, spectral sim. = 912, #22
52.3 kJ/mol
deprotonated HMDB0000247, spectral sim. = 910, #23
29.4 kJ/mol
deprotonated HMDB0000247, spectral sim. = 909, #24
39.5 kJ/mol
deprotonated HMDB0000247, spectral sim. = 908, #25
54.6 kJ/mol
deprotonated HMDB0000247, spectral sim. = 907, #26
64.6 kJ/mol
deprotonated HMDB0000247, spectral sim. = 903, #27
22.3 kJ/mol
deprotonated HMDB0000247, spectral sim. = 898, #28
40.2 kJ/mol
deprotonated HMDB0000247, spectral sim. = 897, #29
55.6 kJ/mol
deprotonated HMDB0000247, spectral sim. = 890, #30
17.9 kJ/mol
deprotonated HMDB0000247, spectral sim. = 886, #31
18.9 kJ/mol
deprotonated HMDB0000247, spectral sim. = 884, #32
21.9 kJ/mol
deprotonated HMDB0000247, spectral sim. = 883, #33
59.2 kJ/mol

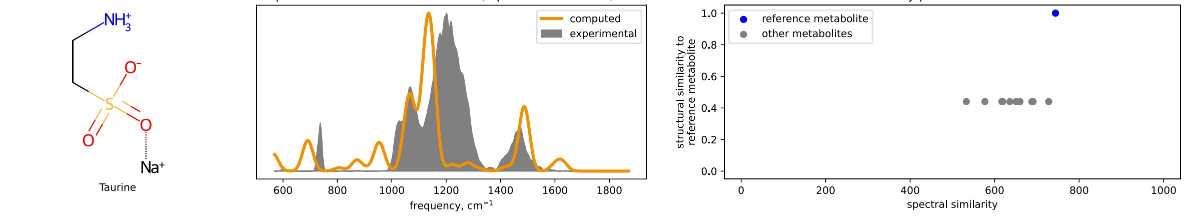
37 deprotonated HMDB0000251 | Spectra of deprotonated HMDB0000251, spectral sim. = 459, #1 | Structural similarity plot of deprotonated HMDB0000251



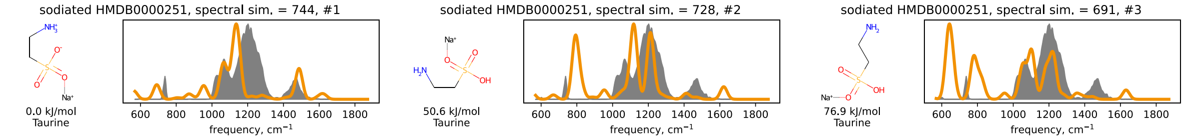
deprotonated HMDB0000251, spectral sim. = 459, #1 | deprotonated HMDB0000251, spectral sim. = 351, #2



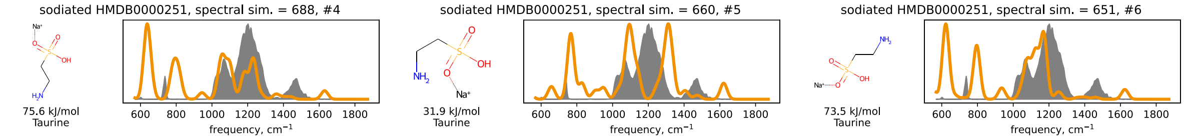
38 sodiated HMDB0000251 | Spectra of sodiated HMDB0000251, spectral sim. = 744, #1 | Structural similarity plot of sodiated HMDB0000251



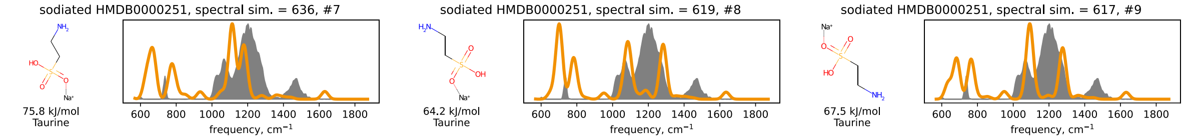
sodiated HMDB0000251, spectral sim. = 744, #1 | sodiated HMDB0000251, spectral sim. = 728, #2 | sodiated HMDB0000251, spectral sim. = 691, #3



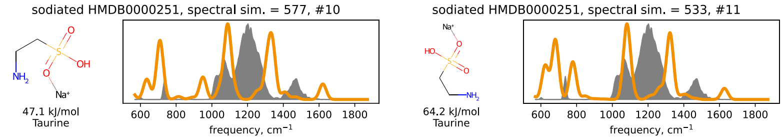
sodiated HMDB0000251, spectral sim. = 688, #4 | sodiated HMDB0000251, spectral sim. = 660, #5 | sodiated HMDB0000251, spectral sim. = 651, #6



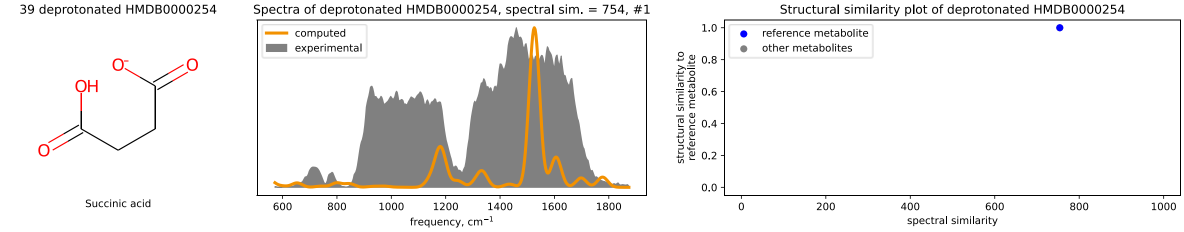
sodiated HMDB0000251, spectral sim. = 636, #7 | sodiated HMDB0000251, spectral sim. = 619, #8 | sodiated HMDB0000251, spectral sim. = 617, #9



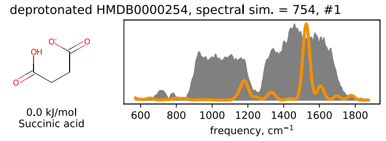
sodiated HMDB0000251, spectral sim. = 577, #10 | sodiated HMDB0000251, spectral sim. = 533, #11



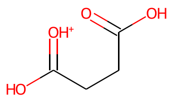
39 deprotonated HMDB0000254 | Spectra of deprotonated HMDB0000254, spectral sim. = 754, #1 | Structural similarity plot of deprotonated HMDB0000254



deprotonated HMDB0000254, spectral sim. = 754, #1

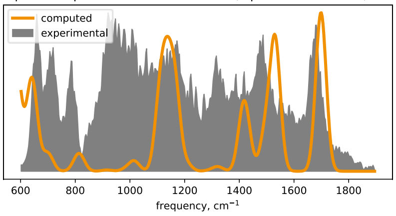


40 protonated HMDB0000254

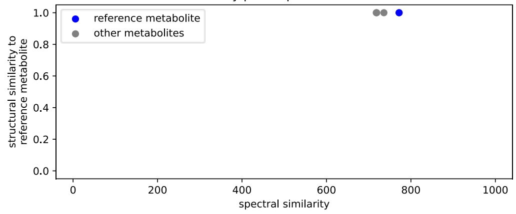


Succinic acid

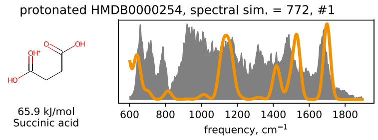
Spectra of protonated HMDB0000254, spectral sim. = 772, #1



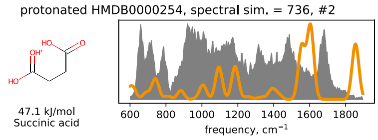
Structural similarity plot of protonated HMDB0000254



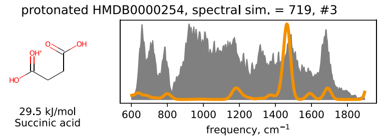
protonated HMDB0000254, spectral sim. = 772, #1



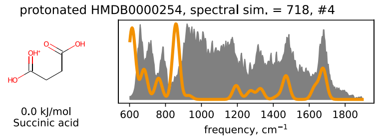
protonated HMDB0000254, spectral sim. = 736, #2



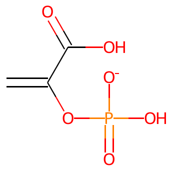
protonated HMDB0000254, spectral sim. = 719, #3



protonated HMDB0000254, spectral sim. = 718, #4

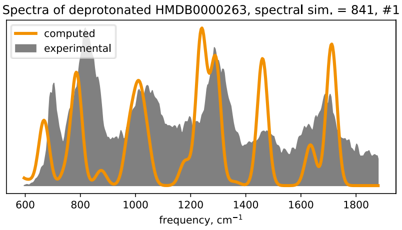


41 deprotonated HMDB0000263

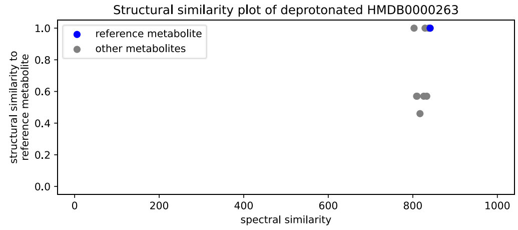


Phosphoenolpyruvic acid

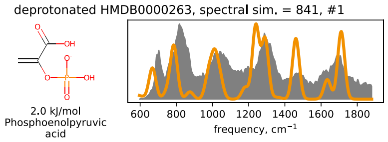
Spectra of deprotonated HMDB0000263, spectral sim. = 841, #1



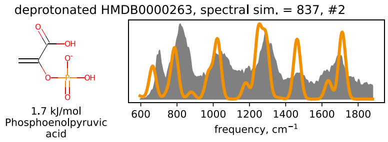
Structural similarity plot of deprotonated HMDB0000263



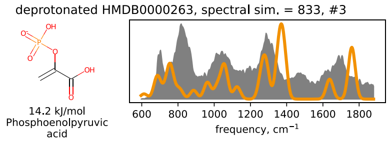
deprotonated HMDB0000263, spectral sim. = 841, #1



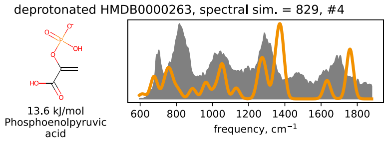
deprotonated HMDB0000263, spectral sim. = 837, #2



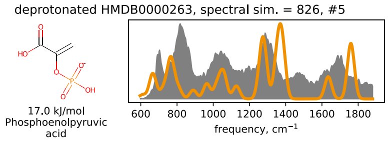
deprotonated HMDB0000263, spectral sim. = 833, #3



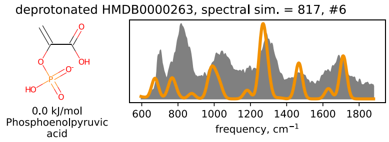
deprotonated HMDB0000263, spectral sim. = 829, #4



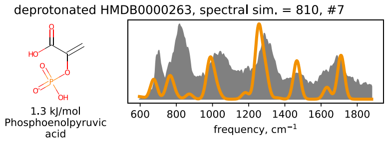
deprotonated HMDB0000263, spectral sim. = 826, #5



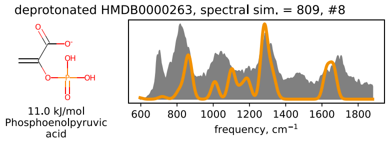
deprotonated HMDB0000263, spectral sim. = 817, #6



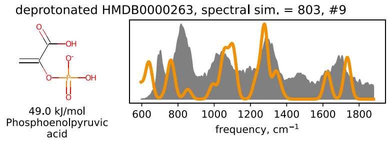
deprotonated HMDB0000263, spectral sim. = 810, #7

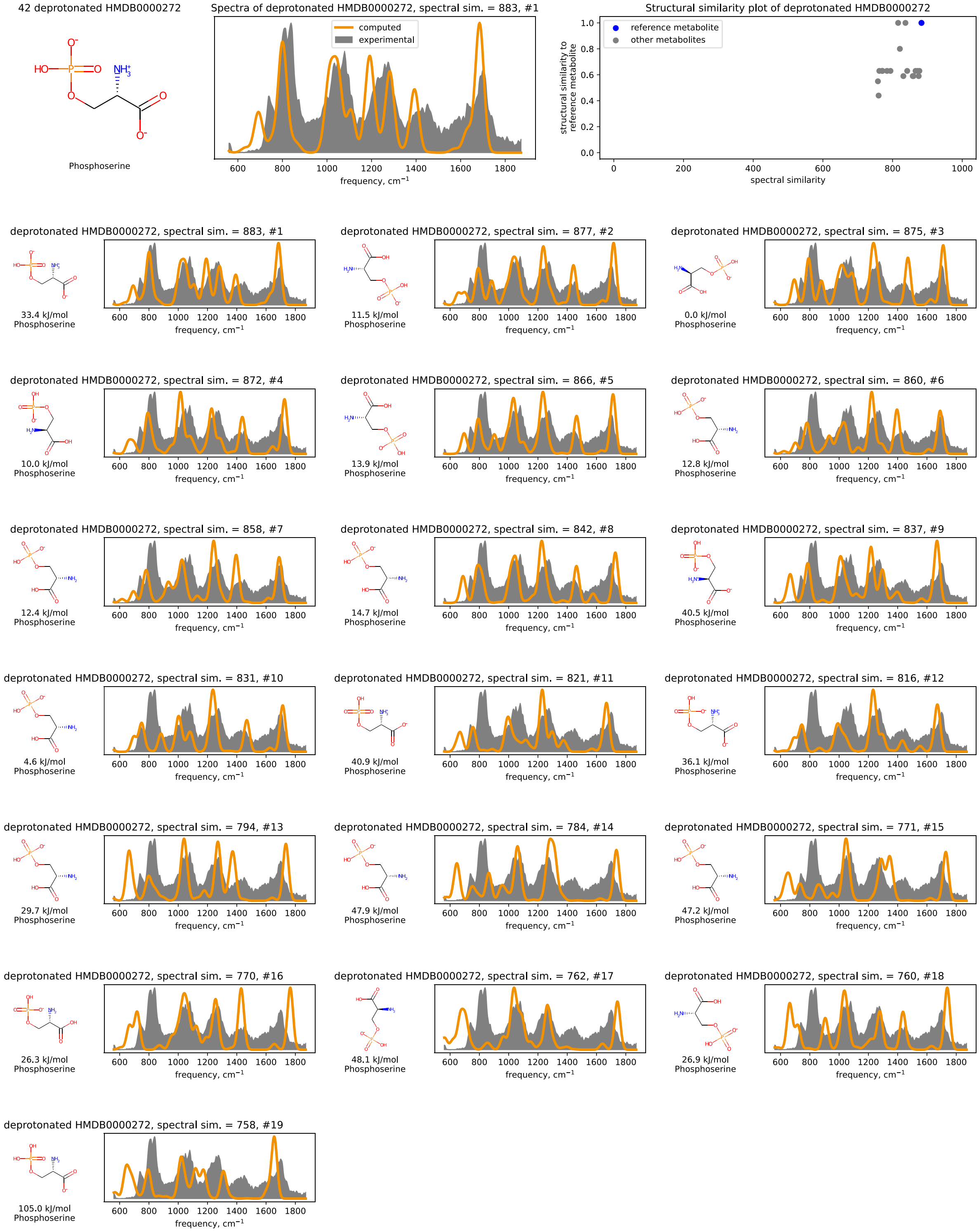


deprotonated HMDB0000263, spectral sim. = 809, #8

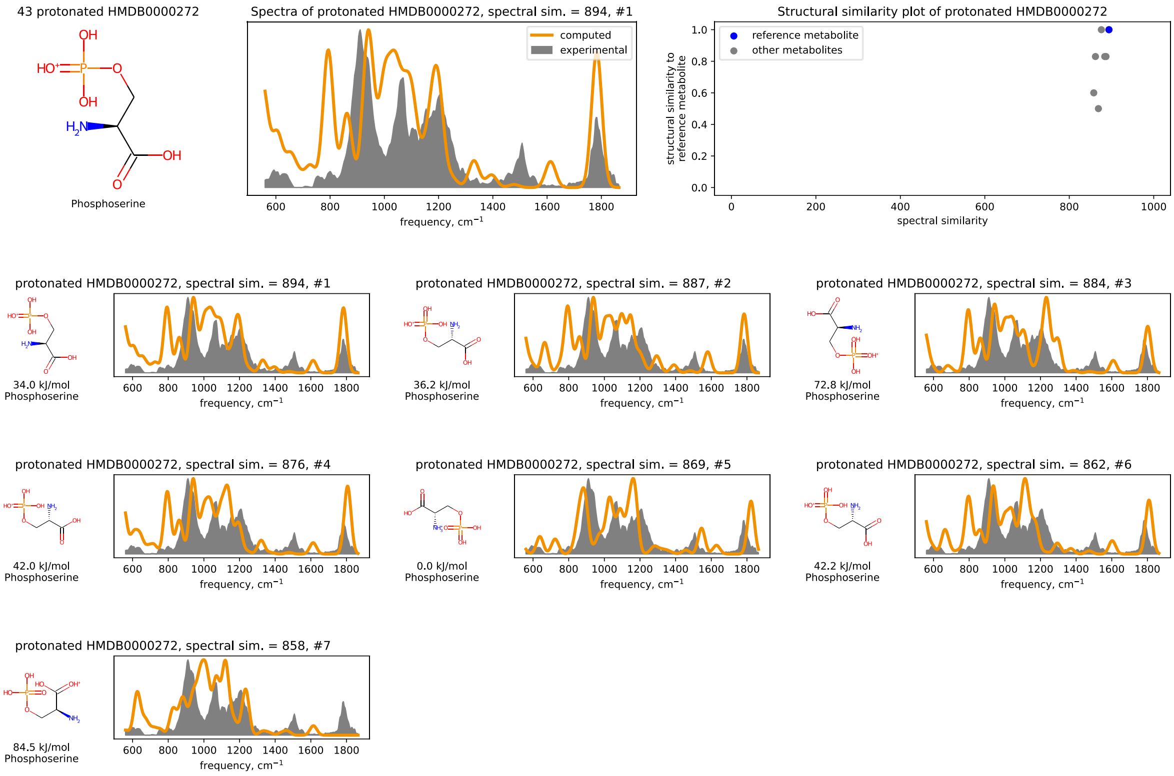


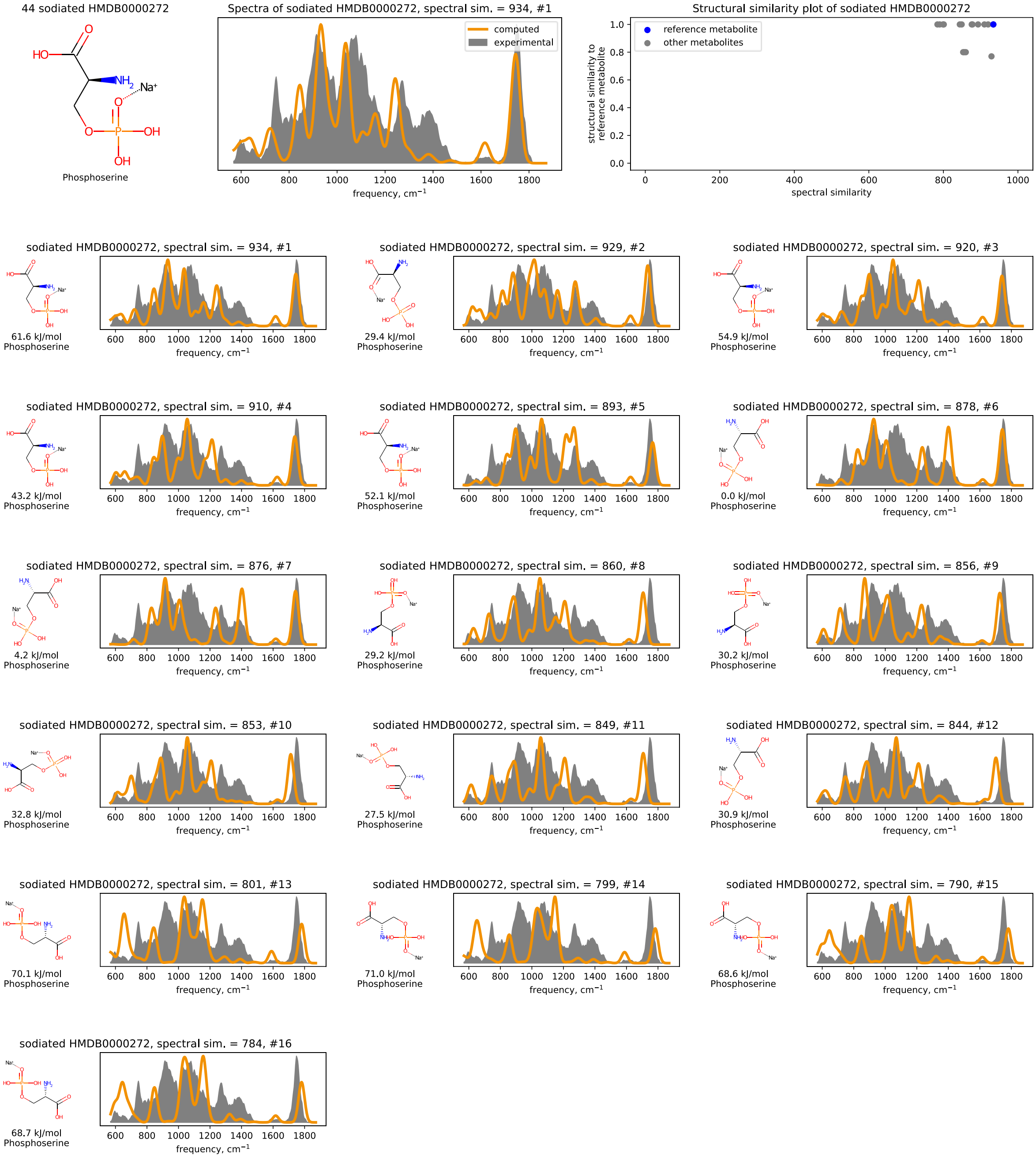
deprotonated HMDB0000263, spectral sim. = 803, #9



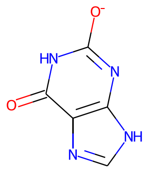


42 deprotonated HMDB0000272
Phosphoserine
Spectra of deprotonated HMDB0000272, spectral sim. = 883, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0000272
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0000272, spectral sim. = 883, #1
33.4 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 877, #2
11.5 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 875, #3
0.0 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 872, #4
10.0 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 866, #5
13.9 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 860, #6
12.8 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 858, #7
12.4 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 842, #8
14.7 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 837, #9
40.5 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 831, #10
4.6 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 821, #11
40.9 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 816, #12
36.1 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 794, #13
29.7 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 784, #14
47.9 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 771, #15
47.2 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 770, #16
26.3 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 762, #17
48.1 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 760, #18
26.9 kJ/mol
Phosphoserine
deprotonated HMDB0000272, spectral sim. = 758, #19
105.0 kJ/mol
Phosphoserine


43 protonated HMDB0000272
Phosphoserine
Spectra of protonated HMDB0000272, spectral sim. = 894, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of protonated HMDB0000272
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
protonated HMDB0000272, spectral sim. = 894, #1
34.0 kJ/mol
Phosphoserine
protonated HMDB0000272, spectral sim. = 887, #2
36.2 kJ/mol
Phosphoserine
protonated HMDB0000272, spectral sim. = 884, #3
72.8 kJ/mol
Phosphoserine
protonated HMDB0000272, spectral sim. = 876, #4
42.0 kJ/mol
Phosphoserine
protonated HMDB0000272, spectral sim. = 869, #5
0.0 kJ/mol
Phosphoserine
protonated HMDB0000272, spectral sim. = 862, #6
42.2 kJ/mol
Phosphoserine
protonated HMDB0000272, spectral sim. = 858, #7
84.5 kJ/mol
Phosphoserine

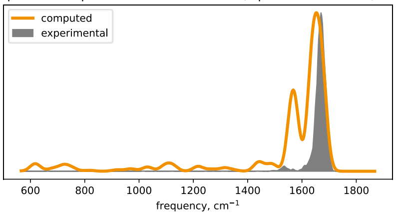

44 sodiated HMDB0000272
Phosphoserine
Spectra of sodiated HMDB0000272, spectral sim. = 934, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of sodiated HMDB0000272
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
sodiated HMDB0000272, spectral sim. = 934, #1
61.6 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 929, #2
29.4 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 920, #3
54.9 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 910, #4
43.2 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 893, #5
52.1 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 878, #6
0.0 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 876, #7
4.2 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 860, #8
29.2 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 856, #9
30.2 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 853, #10
32.8 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 849, #11
27.5 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 844, #12
30.9 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 801, #13
70.1 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 799, #14
71.0 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 790, #15
68.6 kJ/mol
Phosphoserine
sodiated HMDB0000272, spectral sim. = 784, #16
68.7 kJ/mol
Phosphoserine

45 deprotonated HMDB0000292

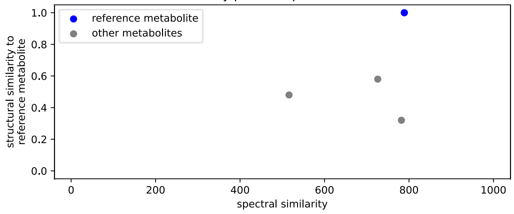


Xanthine

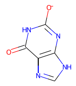
Spectra of deprotonated HMDB0000292, spectral sim. = 789, #1



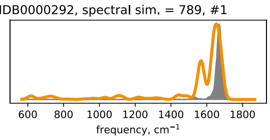
Structural similarity plot of deprotonated HMDB0000292



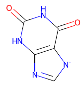
deprotonated HMDB0000292, spectral sim. = 789, #1



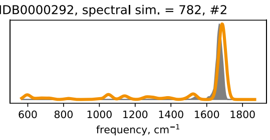
35.4 kJ/mol
Xanthine



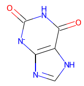
deprotonated HMDB0000292, spectral sim. = 782, #2



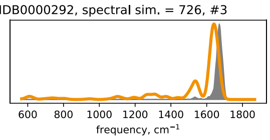
0.0 kJ/mol
Xanthine



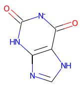
deprotonated HMDB0000292, spectral sim. = 726, #3



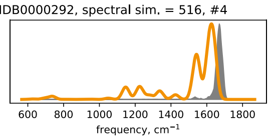
51.5 kJ/mol
Xanthine



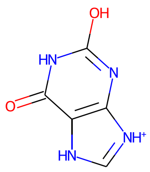
deprotonated HMDB0000292, spectral sim. = 516, #4



74.6 kJ/mol
Xanthine

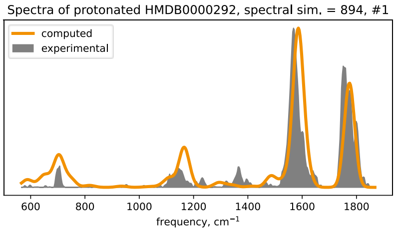


46 protonated HMDB0000292

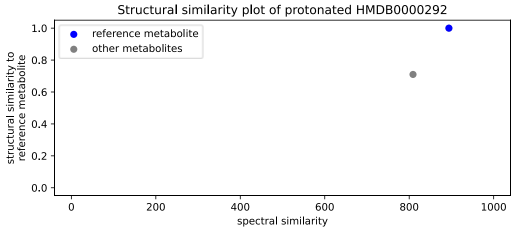


Xanthine

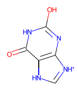
Spectra of protonated HMDB0000292, spectral sim. = 894, #1



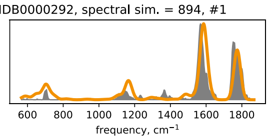
Structural similarity plot of protonated HMDB0000292



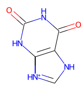
protonated HMDB0000292, spectral sim. = 894, #1



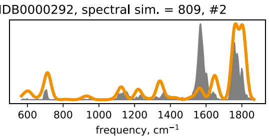
0.0 kJ/mol
Xanthine



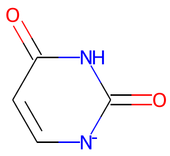
protonated HMDB0000292, spectral sim. = 809, #2



15.2 kJ/mol
Xanthine

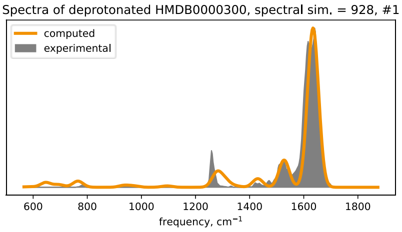


47 deprotonated HMDB0000300

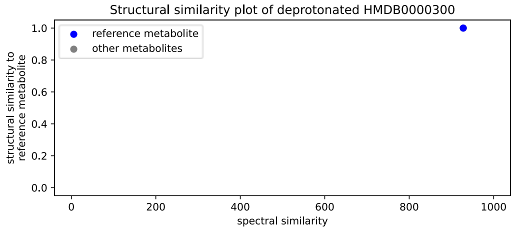


Uracil

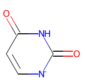
Spectra of deprotonated HMDB0000300, spectral sim. = 928, #1



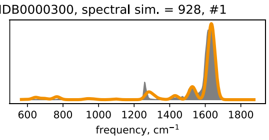
Structural similarity plot of deprotonated HMDB0000300



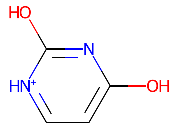
deprotonated HMDB0000300, spectral sim. = 928, #1



0.0 kJ/mol
Uracil

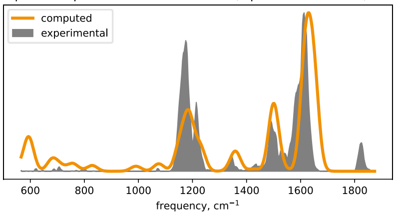


48 protonated HMDB0000300

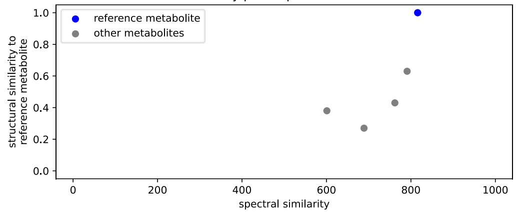


Uracil

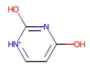
Spectra of protonated HMDB0000300, spectral sim. = 816, #1



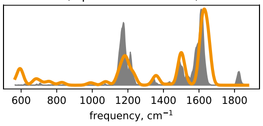
Structural similarity plot of protonated HMDB0000300



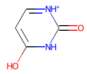
protonated HMDB0000300, spectral sim. = 816, #1



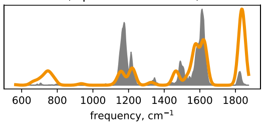
0.0 kJ/mol
Uracil



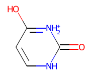
protonated HMDB0000300, spectral sim. = 791, #2



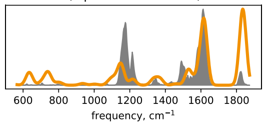
8.9 kJ/mol
Uracil



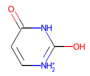
protonated HMDB0000300, spectral sim. = 762, #3



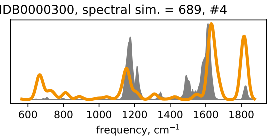
20.8 kJ/mol
Uracil



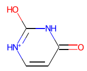
protonated HMDB0000300, spectral sim. = 689, #4



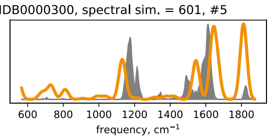
40.3 kJ/mol
Uracil



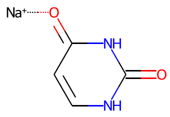
protonated HMDB0000300, spectral sim. = 601, #5



45.5 kJ/mol
Uracil

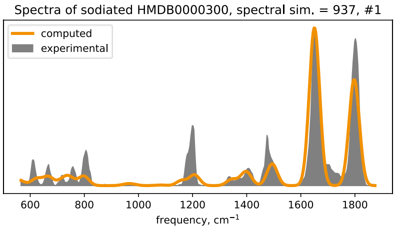


49 sodiated HMDB0000300

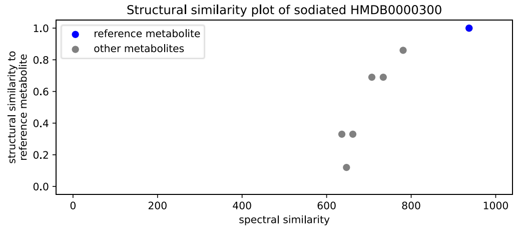


Uracil

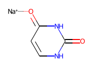
Spectra of sodiated HMDB0000300, spectral sim. = 937, #1



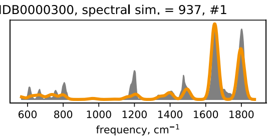
Structural similarity plot of sodiated HMDB0000300



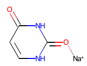
sodiated HMDB0000300, spectral sim. = 937, #1



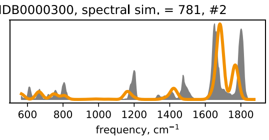
0.0 kJ/mol
Uracil



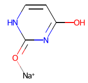
sodiated HMDB0000300, spectral sim. = 781, #2



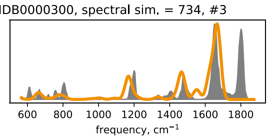
12.3 kJ/mol
Uracil



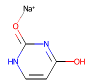
sodiated HMDB0000300, spectral sim. = 734, #3



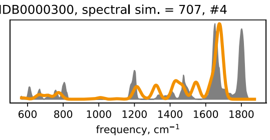
12.8 kJ/mol
Uracil



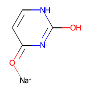
sodiated HMDB0000300, spectral sim. = 707, #4



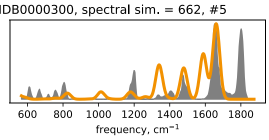
16.0 kJ/mol
Uracil



sodiated HMDB0000300, spectral sim. = 662, #5

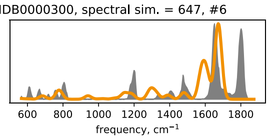


47.9 kJ/mol
Uracil

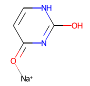


sodiated HMDB0000300, spectral sim. = 647, #6

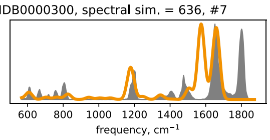
31.6 kJ/mol
Uracil



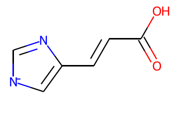
sodiated HMDB0000300, spectral sim. = 636, #7



29.3 kJ/mol
Uracil

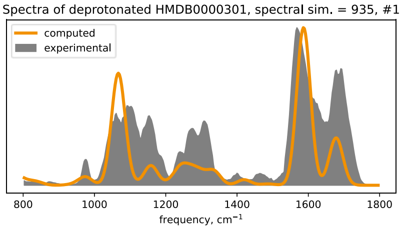


50 deprotonated HMDB0000301

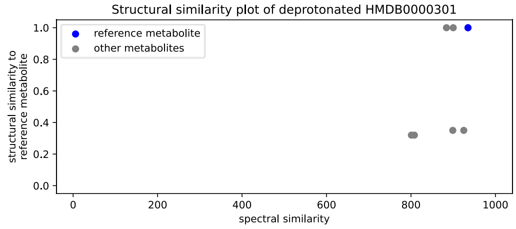


Urocanic acid

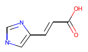
Spectra of deprotonated HMDB0000301, spectral sim. = 935, #1



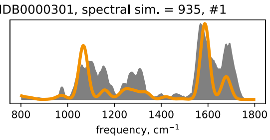
Structural similarity plot of deprotonated HMDB0000301



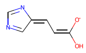
deprotonated HMDB0000301, spectral sim. = 935, #1



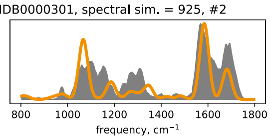
0.0 kJ/mol
Urocanic acid



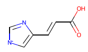
deprotonated HMDB0000301, spectral sim. = 925, #2



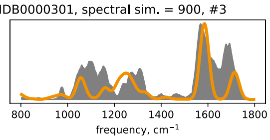
5.0 kJ/mol
Urocanic acid



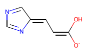
deprotonated HMDB0000301, spectral sim. = 900, #3



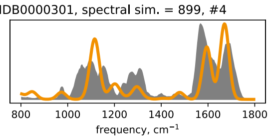
10.4 kJ/mol
Urocanic acid



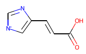
deprotonated HMDB0000301, spectral sim. = 899, #4



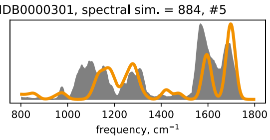
0.8 kJ/mol
Urocanic acid



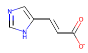
deprotonated HMDB0000301, spectral sim. = 884, #5



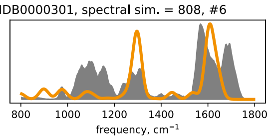
9.8 kJ/mol
Urocanic acid



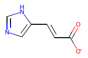
deprotonated HMDB0000301, spectral sim. = 808, #6



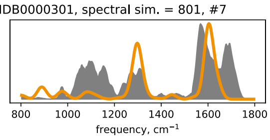
33.4 kJ/mol
Urocanic acid



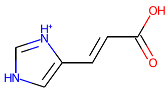
deprotonated HMDB0000301, spectral sim. = 801, #7



40.7 kJ/mol
Urocanic acid

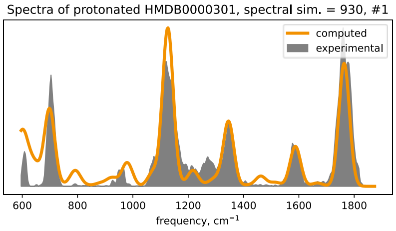


51 protonated HMDB0000301

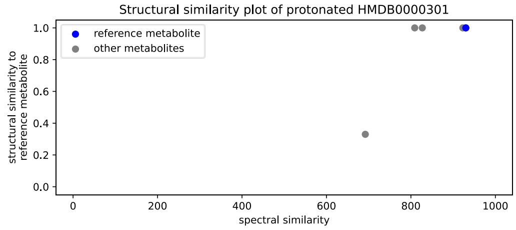


Urocanic acid

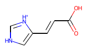
Spectra of protonated HMDB0000301, spectral sim. = 930, #1



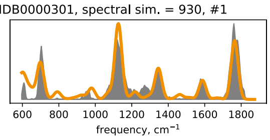
Structural similarity plot of protonated HMDB0000301



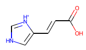
protonated HMDB0000301, spectral sim. = 930, #1



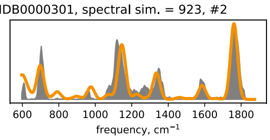
8.7 kJ/mol
Urocanic acid



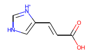
protonated HMDB0000301, spectral sim. = 923, #2



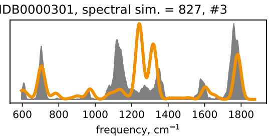
12.0 kJ/mol
Urocanic acid



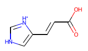
protonated HMDB0000301, spectral sim. = 827, #3



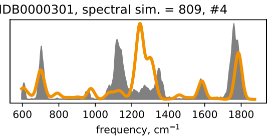
43.5 kJ/mol
Urocanic acid



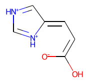
protonated HMDB0000301, spectral sim. = 809, #4



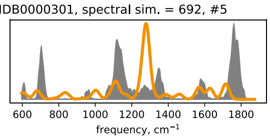
46.5 kJ/mol
Urocanic acid



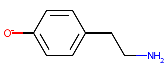
protonated HMDB0000301, spectral sim. = 692, #5



0.0 kJ/mol
Urocanic acid

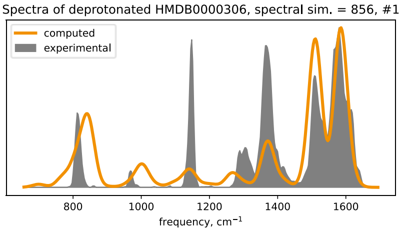


52 deprotonated HMDB0000306

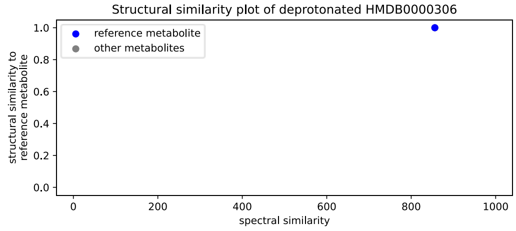


Tyramine

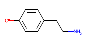
Spectra of deprotonated HMDB0000306, spectral sim. = 856, #1



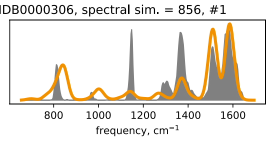
Structural similarity plot of deprotonated HMDB0000306

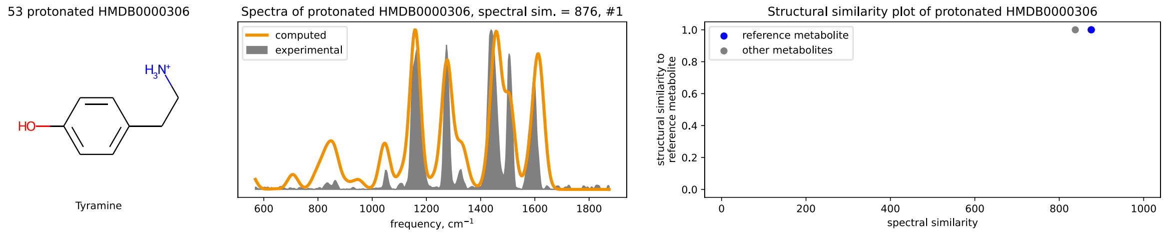


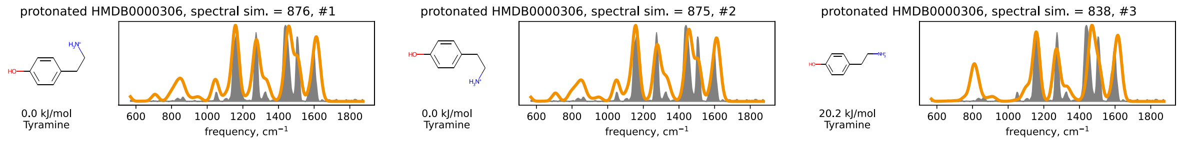
deprotonated HMDB0000306, spectral sim. = 856, #1

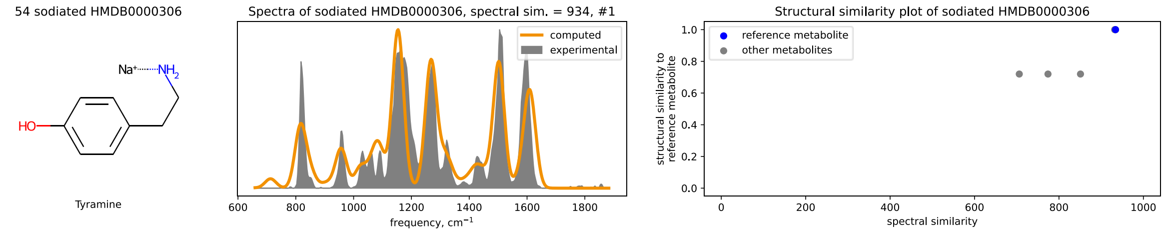


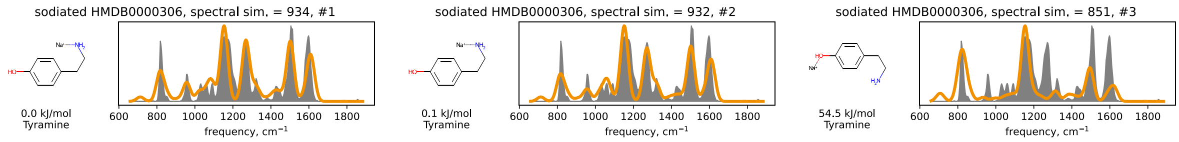
0.0 kJ/mol
Tyramine

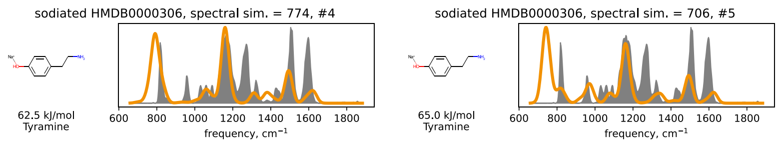


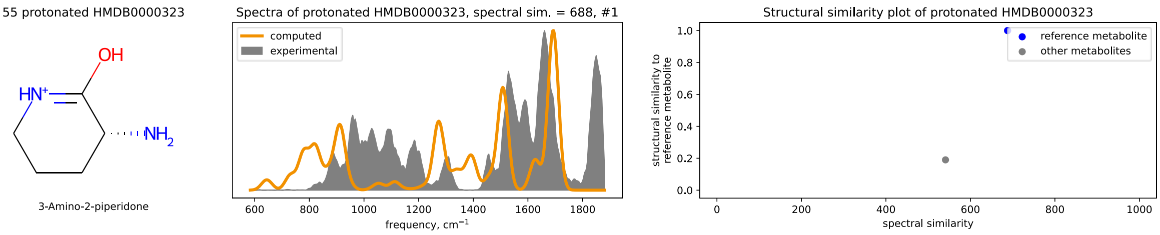

53 protonated HMDB0000306
Tyramine
Spectra of protonated HMDB0000306, spectral sim. = 876, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of protonated HMDB0000306
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

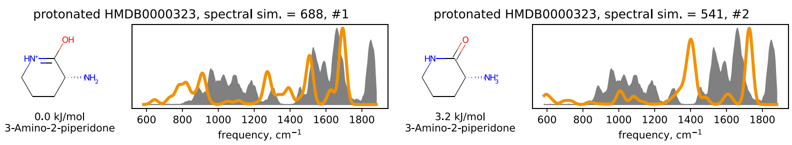

protonated HMDB0000306, spectral sim. = 876, #1
0.0 kJ/mol
Tyramine
protonated HMDB0000306, spectral sim. = 875, #2
0.0 kJ/mol
Tyramine
protonated HMDB0000306, spectral sim. = 838, #3
20.2 kJ/mol
Tyramine
frequency, cm^{-1}

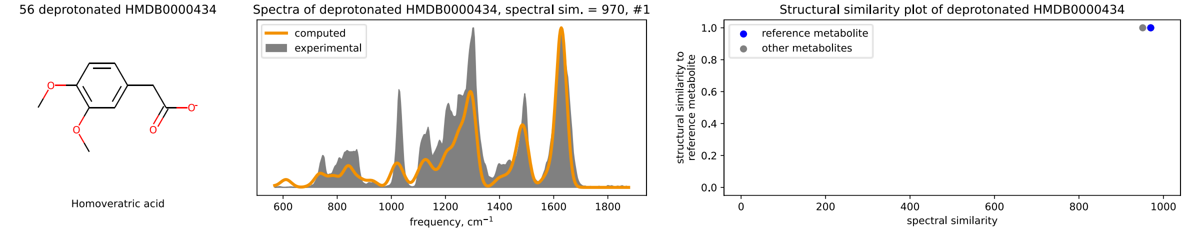

54 sodiated HMDB0000306
Tyramine
Spectra of sodiated HMDB0000306, spectral sim. = 934, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of sodiated HMDB0000306
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

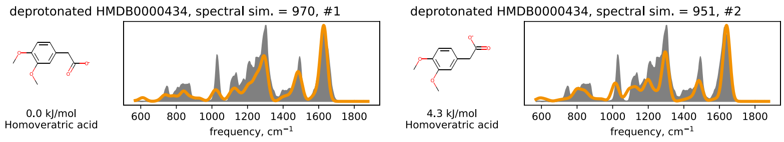

sodiated HMDB0000306, spectral sim. = 934, #1
0.0 kJ/mol
Tyramine
sodiated HMDB0000306, spectral sim. = 932, #2
0.1 kJ/mol
Tyramine
sodiated HMDB0000306, spectral sim. = 851, #3
54.5 kJ/mol
Tyramine
frequency, cm^{-1}

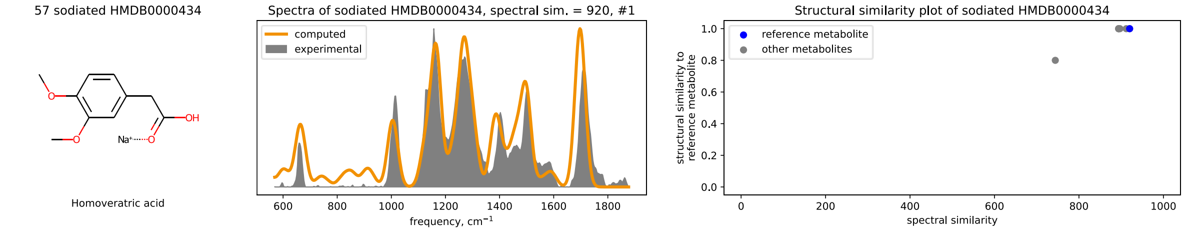

sodiated HMDB0000306, spectral sim. = 774, #4
62.5 kJ/mol
Tyramine
sodiated HMDB0000306, spectral sim. = 706, #5
65.0 kJ/mol
Tyramine
frequency, cm^{-1}

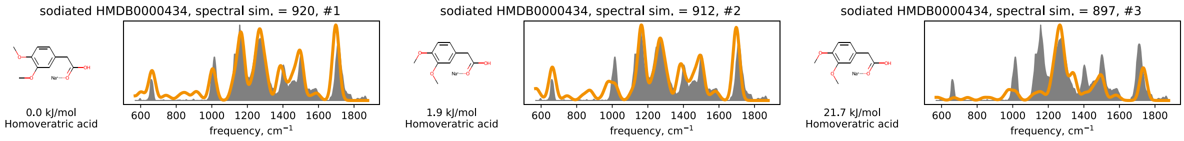

55 protonated HMDB0000323
3-Amino-2-piperidone
Spectra of protonated HMDB0000323, spectral sim. = 688, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of protonated HMDB0000323
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

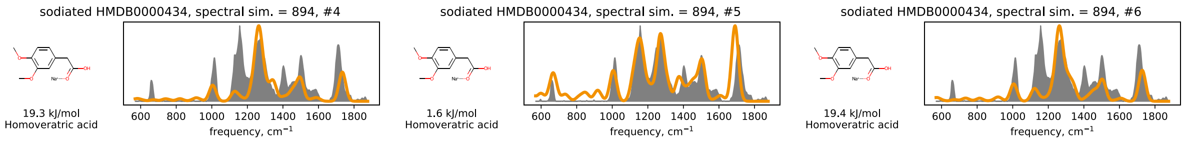

protonated HMDB0000323, spectral sim. = 688, #1
0.0 kJ/mol
3-Amino-2-piperidone
protonated HMDB0000323, spectral sim. = 541, #2
3.2 kJ/mol
3-Amino-2-piperidone
frequency, cm^{-1}

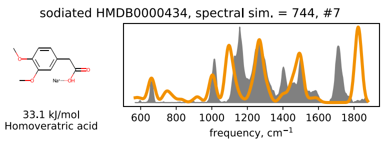

56 deprotonated HMDB0000434
Homoveratric acid
Spectra of deprotonated HMDB0000434, spectral sim. = 970, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0000434
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

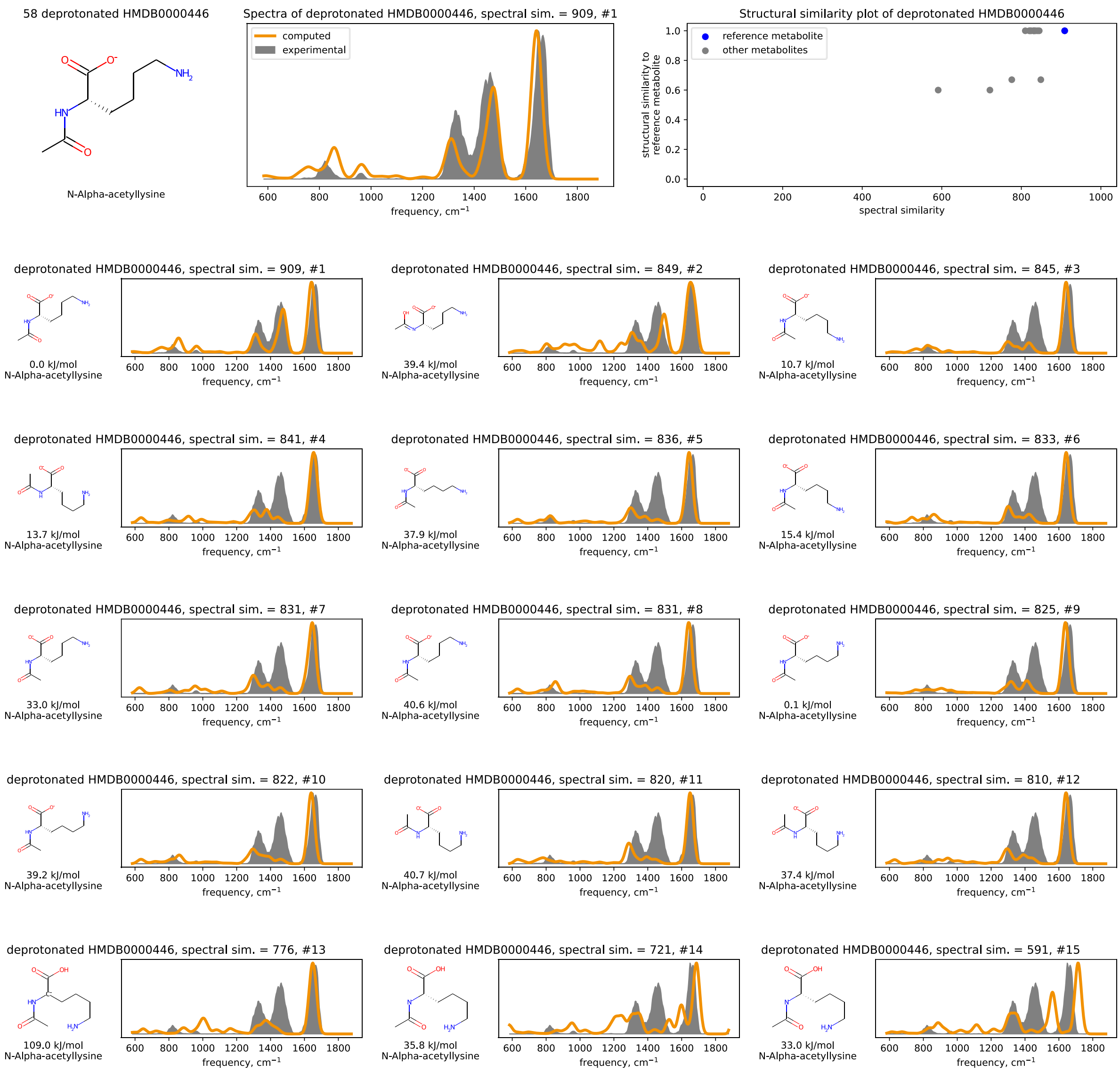

deprotonated HMDB0000434, spectral sim. = 970, #1
0.0 kJ/mol
Homoveratric acid
deprotonated HMDB0000434, spectral sim. = 951, #2
4.3 kJ/mol
Homoveratric acid
frequency, cm^{-1}


57 sodiated HMDB0000434
Homoveratric acid
Spectra of sodiated HMDB0000434, spectral sim. = 920, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of sodiated HMDB0000434
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity


sodiated HMDB0000434, spectral sim. = 920, #1
0.0 kJ/mol
Homoveratric acid
sodiated HMDB0000434, spectral sim. = 912, #2
1.9 kJ/mol
Homoveratric acid
sodiated HMDB0000434, spectral sim. = 897, #3
21.7 kJ/mol
Homoveratric acid
frequency, cm^{-1}

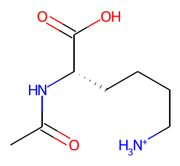

sodiated HMDB0000434, spectral sim. = 894, #4
19.3 kJ/mol
Homoveratric acid
sodiated HMDB0000434, spectral sim. = 894, #5
1.6 kJ/mol
Homoveratric acid
sodiated HMDB0000434, spectral sim. = 894, #6
19.4 kJ/mol
Homoveratric acid
frequency, cm^{-1}


sodiated HMDB0000434, spectral sim. = 744, #7
33.1 kJ/mol
Homoveratric acid
frequency, cm^{-1}



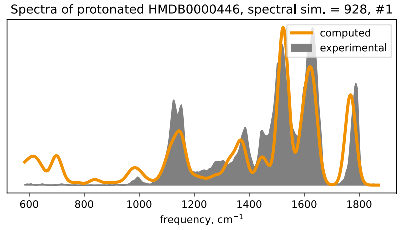
58 deprotonated HMDB0000446
N-Alpha-acetyllysine
Spectra of deprotonated HMDB0000446, spectral sim. = 909, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0000446
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0000446, spectral sim. = 909, #1
0.0 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 849, #2
39.4 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 845, #3
10.7 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 841, #4
13.7 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 836, #5
37.9 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 833, #6
15.4 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 831, #7
33.0 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 831, #8
40.6 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 825, #9
0.1 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 822, #10
39.2 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 820, #11
40.7 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 810, #12
37.4 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 776, #13
109.0 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 721, #14
35.8 kJ/mol
N-Alpha-acetyllysine
deprotonated HMDB0000446, spectral sim. = 591, #15
33.0 kJ/mol
N-Alpha-acetyllysine
frequency, cm^{-1}

59 protonated HMDB0000446

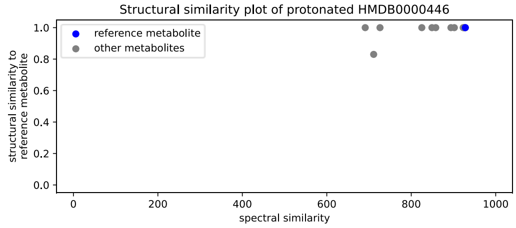


N-Alpha-acetyllysine

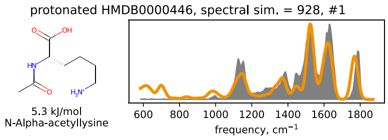
Spectra of protonated HMDB0000446, spectral sim. = 928, #1



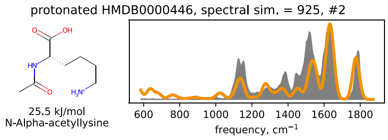
Structural similarity plot of protonated HMDB0000446



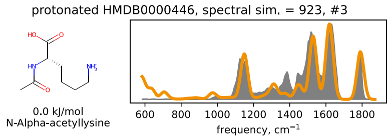
protonated HMDB0000446, spectral sim. = 928, #1



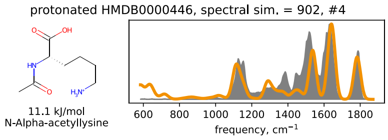
protonated HMDB0000446, spectral sim. = 925, #2



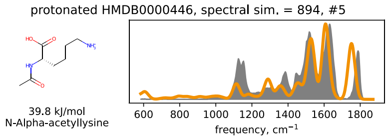
protonated HMDB0000446, spectral sim. = 923, #3



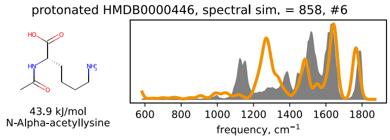
protonated HMDB0000446, spectral sim. = 902, #4



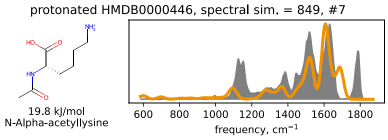
protonated HMDB0000446, spectral sim. = 894, #5



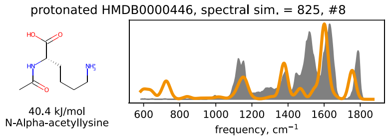
protonated HMDB0000446, spectral sim. = 858, #6



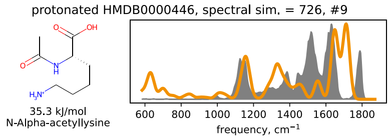
protonated HMDB0000446, spectral sim. = 849, #7



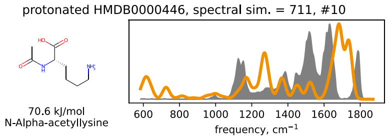
protonated HMDB0000446, spectral sim. = 825, #8



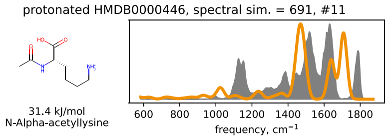
protonated HMDB0000446, spectral sim. = 726, #9



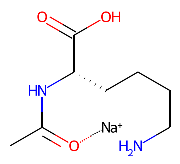
protonated HMDB0000446, spectral sim. = 711, #10



protonated HMDB0000446, spectral sim. = 691, #11

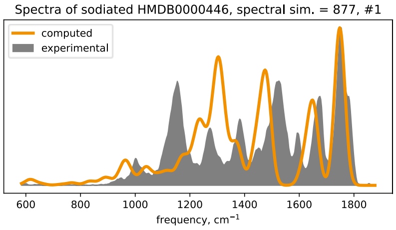


60 sodiated HMDB0000446

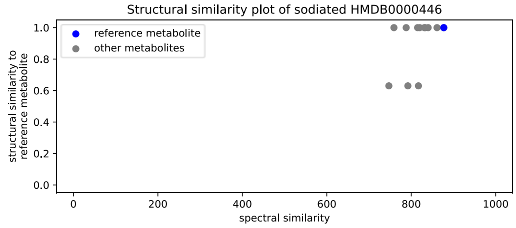


N-Alpha-acetyllysine

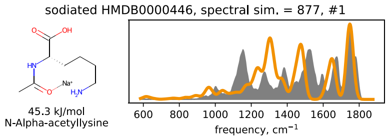
Spectra of sodiated HMDB0000446, spectral sim. = 877, #1



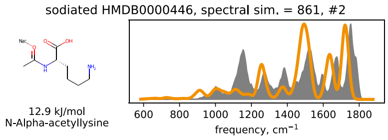
Structural similarity plot of sodiated HMDB0000446



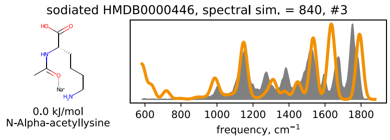
sodiated HMDB0000446, spectral sim. = 877, #1



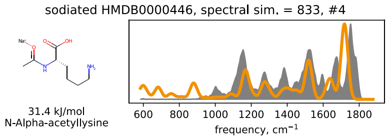
sodiated HMDB0000446, spectral sim. = 861, #2



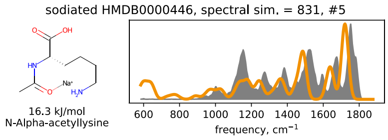
sodiated HMDB0000446, spectral sim. = 840, #3



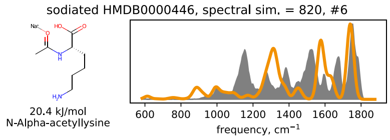
sodiated HMDB0000446, spectral sim. = 833, #4



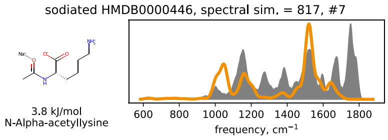
sodiated HMDB0000446, spectral sim. = 831, #5



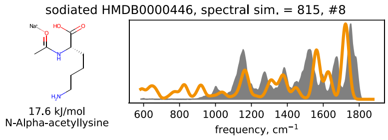
sodiated HMDB0000446, spectral sim. = 820, #6



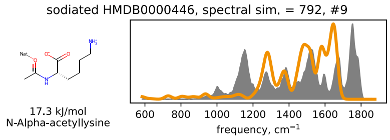
sodiated HMDB0000446, spectral sim. = 817, #7



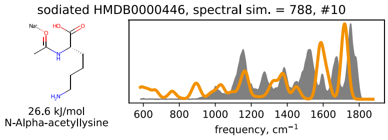
sodiated HMDB0000446, spectral sim. = 815, #8



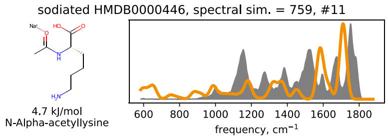
sodiated HMDB0000446, spectral sim. = 792, #9



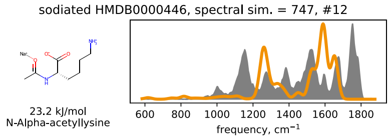
sodiated HMDB0000446, spectral sim. = 788, #10



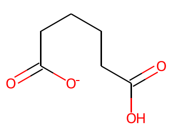
sodiated HMDB0000446, spectral sim. = 759, #11



sodiated HMDB0000446, spectral sim. = 747, #12

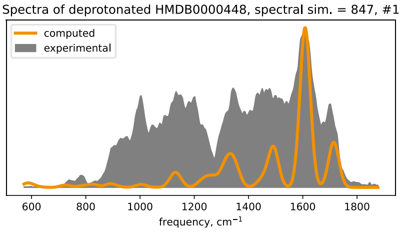


61 deprotonated HMDB0000448

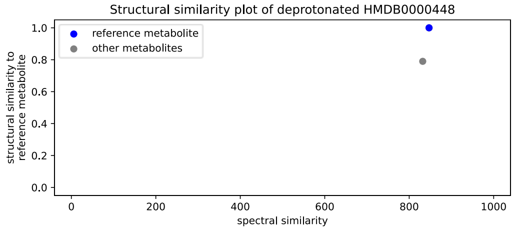


Adipic acid

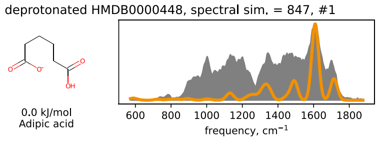
Spectra of deprotonated HMDB0000448, spectral sim. = 847, #1



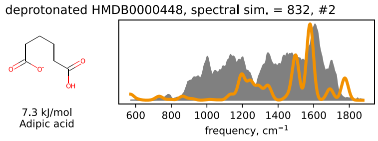
Structural similarity plot of deprotonated HMDB0000448



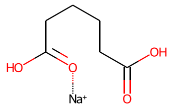
deprotonated HMDB0000448, spectral sim. = 847, #1



deprotonated HMDB0000448, spectral sim. = 832, #2

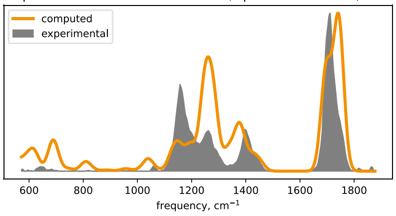


62 sodiated HMDB0000448

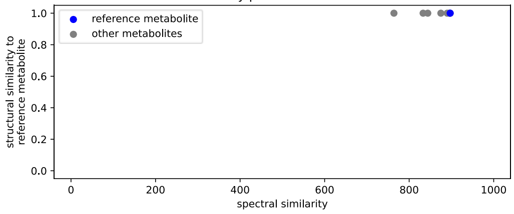


Adipic acid

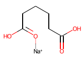
Spectra of sodiated HMDB0000448, spectral sim. = 897, #1



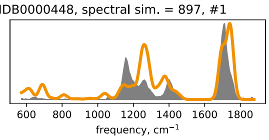
Structural similarity plot of sodiated HMDB0000448



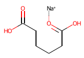
sodiated HMDB0000448, spectral sim. = 897, #1



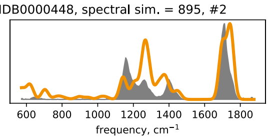
16.7 kJ/mol
Adipic acid



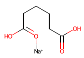
sodiated HMDB0000448, spectral sim. = 895, #2



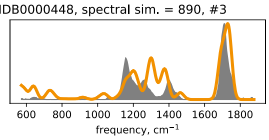
8.9 kJ/mol
Adipic acid



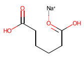
sodiated HMDB0000448, spectral sim. = 890, #3



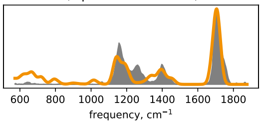
15.6 kJ/mol
Adipic acid



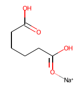
sodiated HMDB0000448, spectral sim. = 875, #4



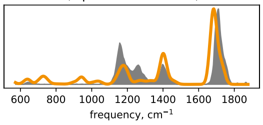
0.0 kJ/mol
Adipic acid



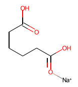
sodiated HMDB0000448, spectral sim. = 844, #5



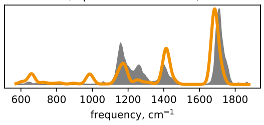
30.5 kJ/mol
Adipic acid



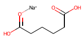
sodiated HMDB0000448, spectral sim. = 833, #6



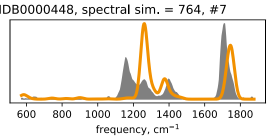
17.8 kJ/mol
Adipic acid



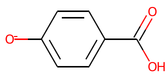
sodiated HMDB0000448, spectral sim. = 764, #7



14.2 kJ/mol
Adipic acid

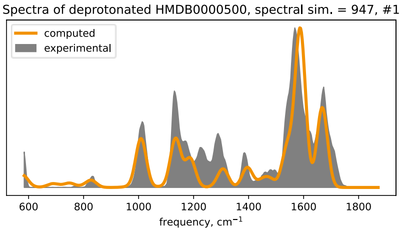


63 deprotonated HMDB0000500

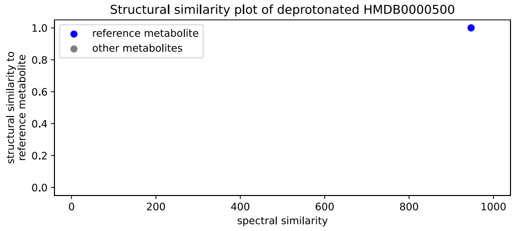


4-Hydroxybenzoic acid

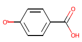
Spectra of deprotonated HMDB0000500, spectral sim. = 947, #1



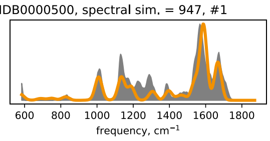
Structural similarity plot of deprotonated HMDB0000500



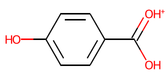
deprotonated HMDB0000500, spectral sim. = 947, #1



0.0 kJ/mol
4-Hydroxybenzoic acid

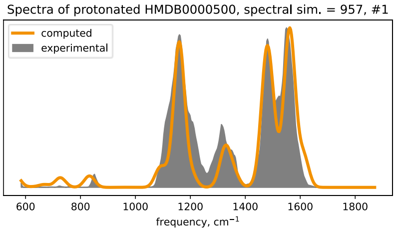


64 protonated HMDB0000500

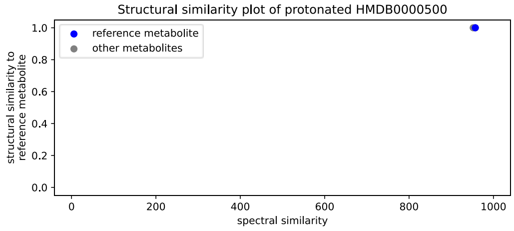


4-Hydroxybenzoic acid

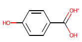
Spectra of protonated HMDB0000500, spectral sim. = 957, #1



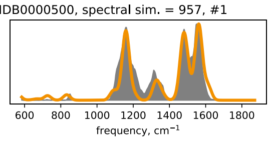
Structural similarity plot of protonated HMDB0000500



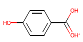
protonated HMDB0000500, spectral sim. = 957, #1



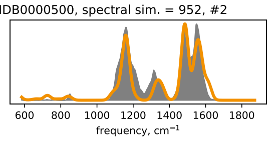
0.0 kJ/mol
4-Hydroxybenzoic acid



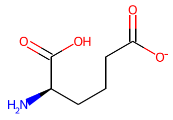
protonated HMDB0000500, spectral sim. = 952, #2



0.6 kJ/mol
4-Hydroxybenzoic acid

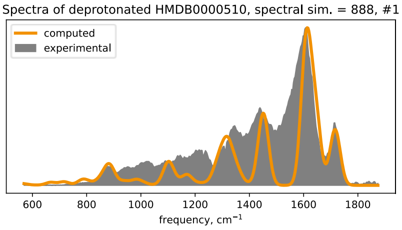


65 deprotonated HMDB0000510

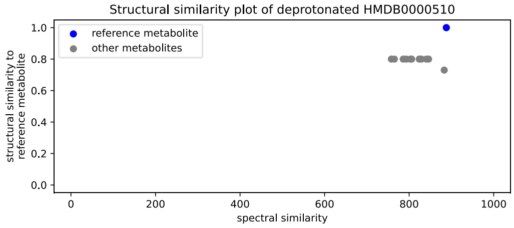


Aminoadipic acid

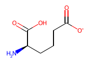
Spectra of deprotonated HMDB0000510, spectral sim. = 888, #1



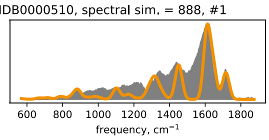
Structural similarity plot of deprotonated HMDB0000510



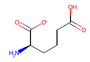
deprotonated HMDB0000510, spectral sim. = 888, #1



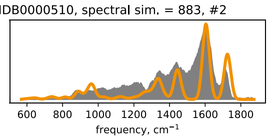
17.1 kJ/mol
Aminoadipic acid



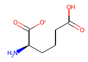
deprotonated HMDB0000510, spectral sim. = 883, #2



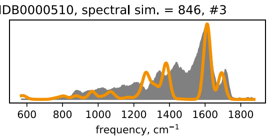
0.0 kJ/mol
Aminoadipic acid



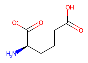
deprotonated HMDB0000510, spectral sim. = 846, #3



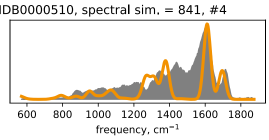
10.1 kJ/mol
Aminoadipic acid



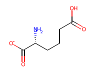
deprotonated HMDB0000510, spectral sim. = 841, #4



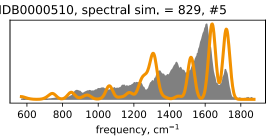
9.7 kJ/mol
Aminoadipic acid



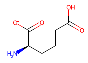
deprotonated HMDB0000510, spectral sim. = 829, #5



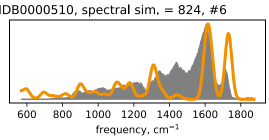
15.8 kJ/mol
Aminoadipic acid



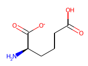
deprotonated HMDB0000510, spectral sim. = 824, #6



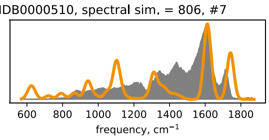
47.4 kJ/mol
Aminoadipic acid



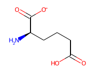
deprotonated HMDB0000510, spectral sim. = 806, #7



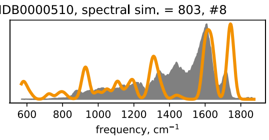
44.8 kJ/mol
Aminoadipic acid



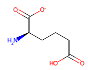
deprotonated HMDB0000510, spectral sim. = 803, #8



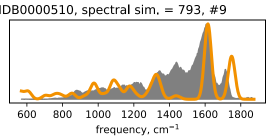
45.1 kJ/mol
Aminoadipic acid



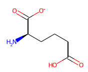
deprotonated HMDB0000510, spectral sim. = 793, #9



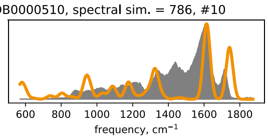
50.8 kJ/mol
Aminoadipic acid



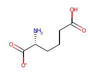
deprotonated HMDB0000510, spectral sim. = 786, #10



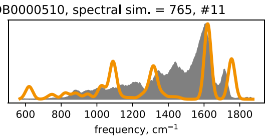
49.0 kJ/mol
Aminoadipic acid



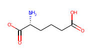
deprotonated HMDB0000510, spectral sim. = 765, #11



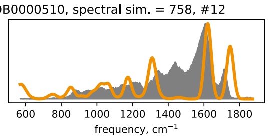
48.9 kJ/mol
Aminoadipic acid



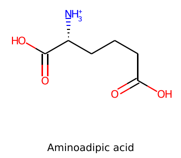
deprotonated HMDB0000510, spectral sim. = 758, #12



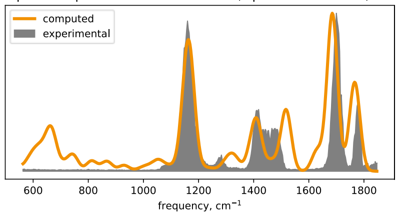
51.0 kJ/mol
Aminoadipic acid



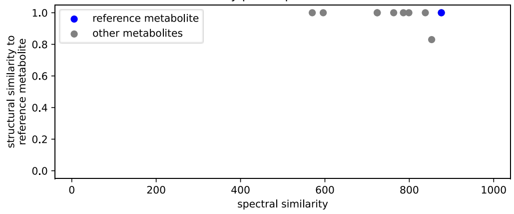
66 protonated HMDB0000510



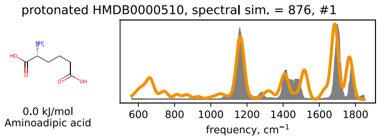
Spectra of protonated HMDB0000510, spectral sim. = 876, #1



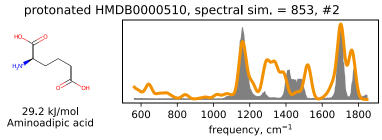
Structural similarity plot of protonated HMDB0000510



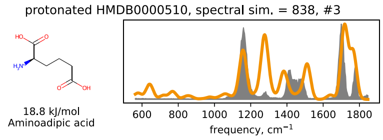
protonated HMDB0000510, spectral sim. = 876, #1



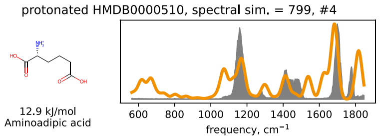
protonated HMDB0000510, spectral sim. = 853, #2



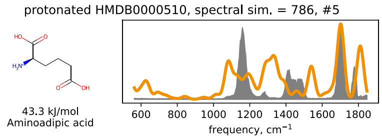
protonated HMDB0000510, spectral sim. = 838, #3



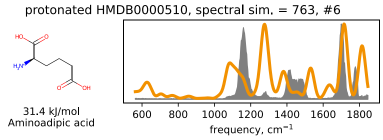
protonated HMDB0000510, spectral sim. = 799, #4



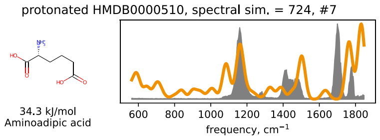
protonated HMDB0000510, spectral sim. = 786, #5



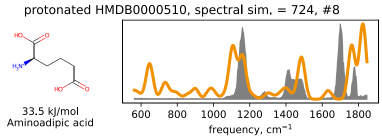
protonated HMDB0000510, spectral sim. = 763, #6



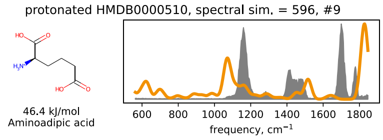
protonated HMDB0000510, spectral sim. = 724, #7



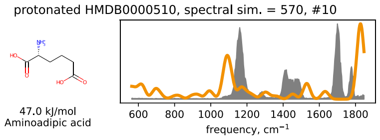
protonated HMDB0000510, spectral sim. = 724, #8



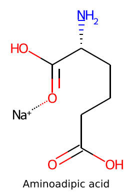
protonated HMDB0000510, spectral sim. = 596, #9



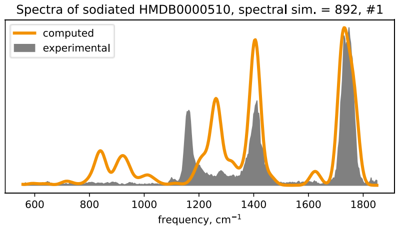
protonated HMDB0000510, spectral sim. = 570, #10



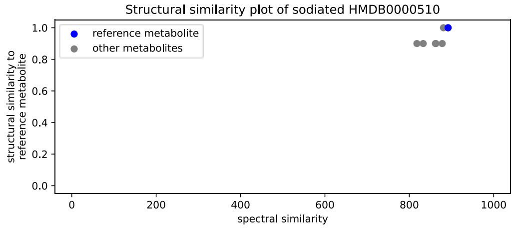
67 sodiated HMDB0000510



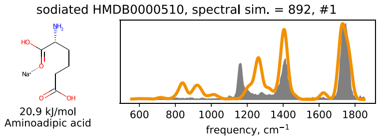
Spectra of sodiated HMDB0000510, spectral sim. = 892, #1



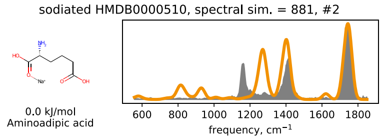
Structural similarity plot of sodiated HMDB0000510



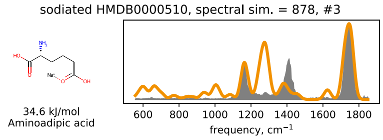
sodiated HMDB0000510, spectral sim. = 892, #1



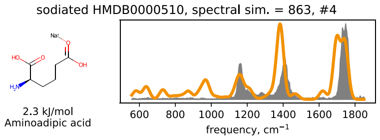
sodiated HMDB0000510, spectral sim. = 881, #2



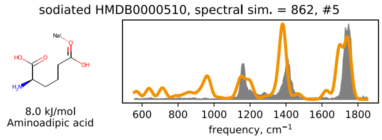
sodiated HMDB0000510, spectral sim. = 878, #3



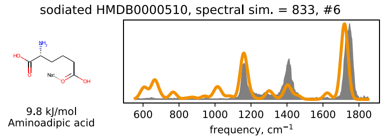
sodiated HMDB0000510, spectral sim. = 863, #4



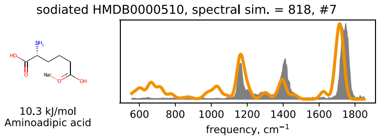
sodiated HMDB0000510, spectral sim. = 862, #5



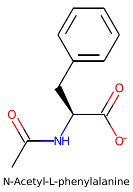
sodiated HMDB0000510, spectral sim. = 833, #6



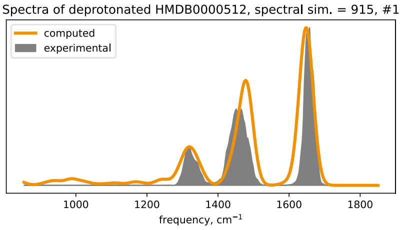
sodiated HMDB0000510, spectral sim. = 818, #7



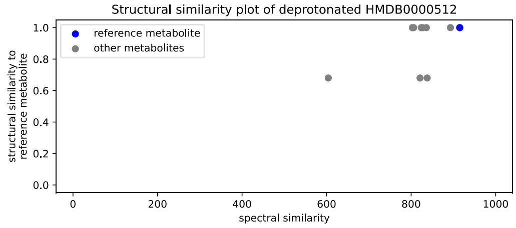
68 deprotonated HMDB0000512



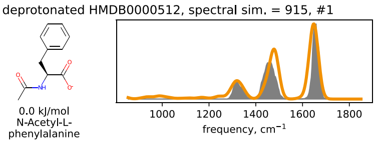
Spectra of deprotonated HMDB0000512, spectral sim. = 915, #1



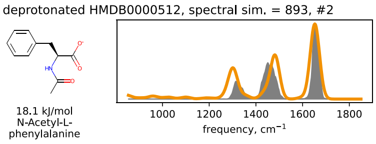
Structural similarity plot of deprotonated HMDB0000512



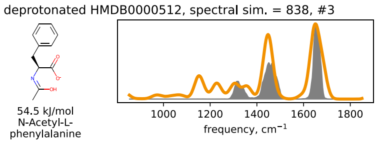
deprotonated HMDB0000512, spectral sim. = 915, #1



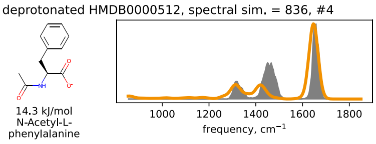
deprotonated HMDB0000512, spectral sim. = 893, #2



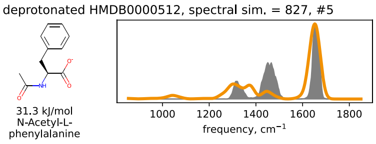
deprotonated HMDB0000512, spectral sim. = 838, #3



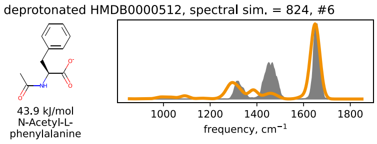
deprotonated HMDB0000512, spectral sim. = 836, #4



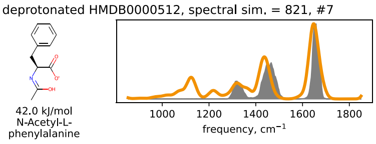
deprotonated HMDB0000512, spectral sim. = 827, #5



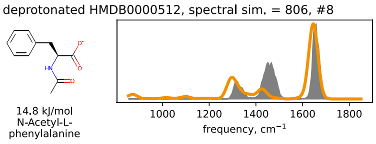
deprotonated HMDB0000512, spectral sim. = 824, #6



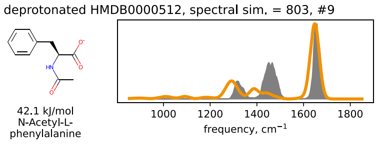
deprotonated HMDB0000512, spectral sim. = 821, #7



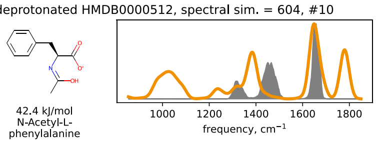
deprotonated HMDB0000512, spectral sim. = 806, #8



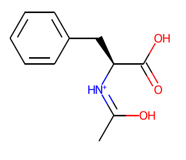
deprotonated HMDB0000512, spectral sim. = 803, #9



deprotonated HMDB0000512, spectral sim. = 604, #10

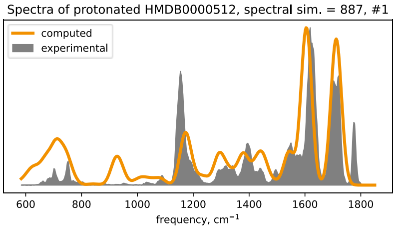


69 protonated HMDB0000512

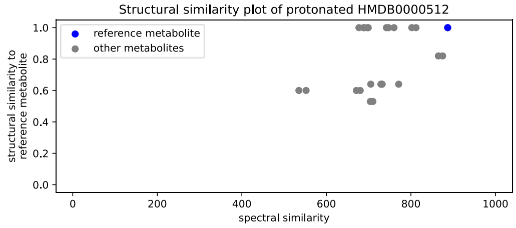


N-Acetyl-L-phenylalanine

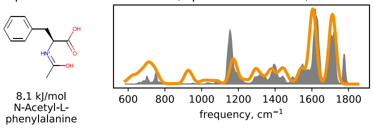
Spectra of protonated HMDB0000512, spectral sim. = 887, #1



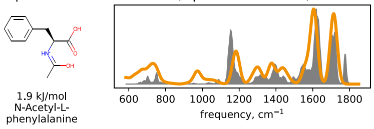
Structural similarity plot of protonated HMDB0000512



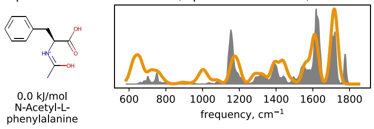
protonated HMDB0000512, spectral sim. = 887, #1



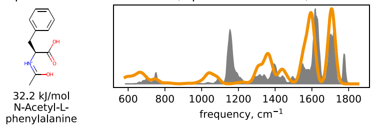
protonated HMDB0000512, spectral sim. = 875, #2



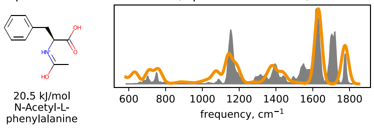
protonated HMDB0000512, spectral sim. = 865, #3



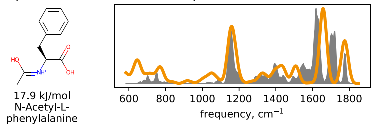
protonated HMDB0000512, spectral sim. = 812, #4



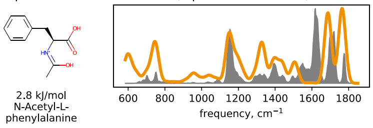
protonated HMDB0000512, spectral sim. = 802, #5



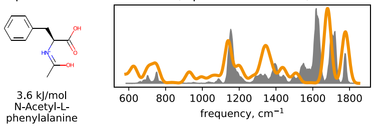
protonated HMDB0000512, spectral sim. = 771, #6



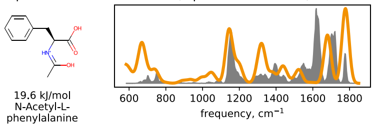
protonated HMDB0000512, spectral sim. = 760, #7



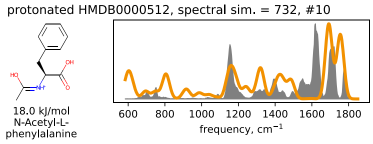
protonated HMDB0000512, spectral sim. = 747, #8



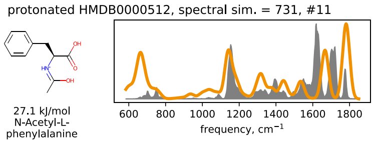
protonated HMDB0000512, spectral sim. = 742, #9



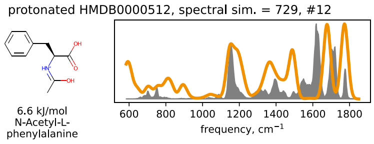
protonated HMDB0000512, spectral sim. = 732, #10



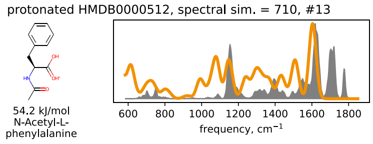
protonated HMDB0000512, spectral sim. = 731, #11



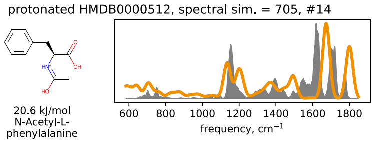
protonated HMDB0000512, spectral sim. = 729, #12



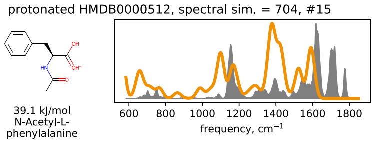
protonated HMDB0000512, spectral sim. = 710, #13



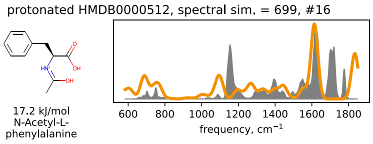
protonated HMDB0000512, spectral sim. = 705, #14



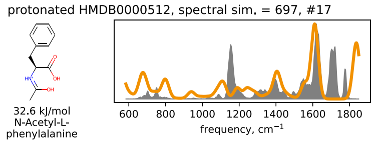
protonated HMDB0000512, spectral sim. = 704, #15



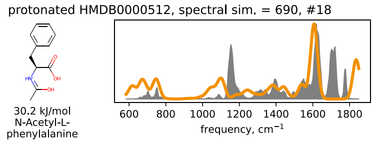
protonated HMDB0000512, spectral sim. = 699, #16



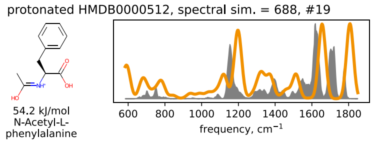
protonated HMDB0000512, spectral sim. = 697, #17



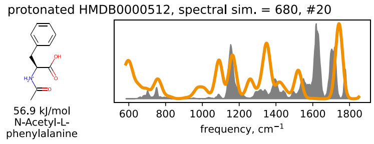
protonated HMDB0000512, spectral sim. = 690, #18



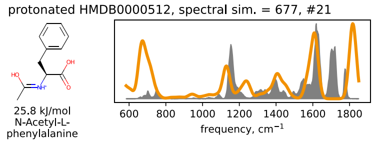
protonated HMDB0000512, spectral sim. = 688, #19



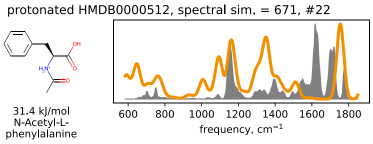
protonated HMDB0000512, spectral sim. = 680, #20



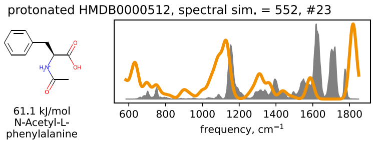
protonated HMDB0000512, spectral sim. = 677, #21



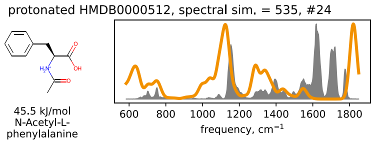
protonated HMDB0000512, spectral sim. = 671, #22

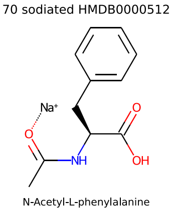


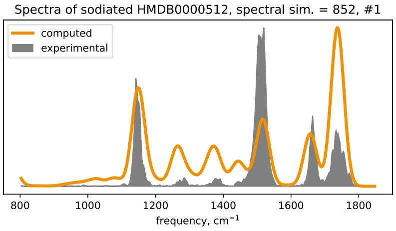
protonated HMDB0000512, spectral sim. = 552, #23

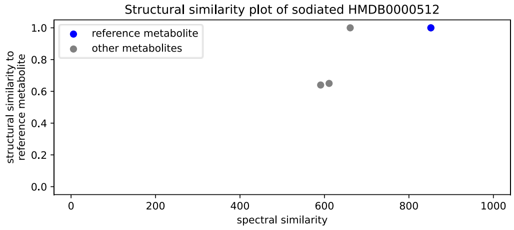


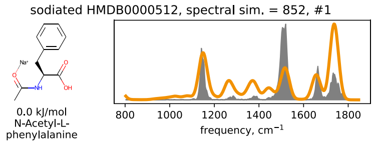
protonated HMDB0000512, spectral sim. = 535, #24

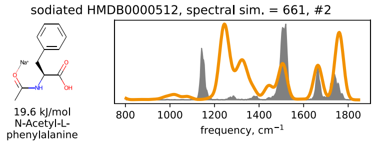


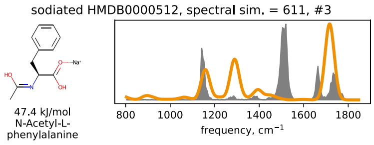

70 sodiated HMDB0000512
Na+
O
NH
O
OH
N-Acetyl-L-phenylalanine

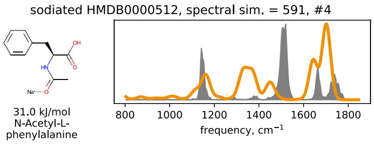

Spectra of sodiated HMDB0000512, spectral sim. = 852, #1
computed
experimental
800
1000
1200
1400
1600
1800
frequency, cm^{-1}


Structural similarity plot of sodiated HMDB0000512
reference metabolite
other metabolites
structural similarity to reference metabolite
1.0
0.8
0.6
0.4
0.2
0.0
0
200
400
600
800
1000
spectral similarity

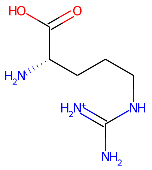

sodiated HMDB0000512, spectral sim. = 852, #1
0.0 kJ/mol
N-Acetyl-L-phenylalanine
800
1000
1200
1400
1600
1800
frequency, cm^{-1}


sodiated HMDB0000512, spectral sim. = 661, #2
19.6 kJ/mol
N-Acetyl-L-phenylalanine
800
1000
1200
1400
1600
1800
frequency, cm^{-1}


sodiated HMDB0000512, spectral sim. = 611, #3
47.4 kJ/mol
N-Acetyl-L-phenylalanine
800
1000
1200
1400
1600
1800
frequency, cm^{-1}

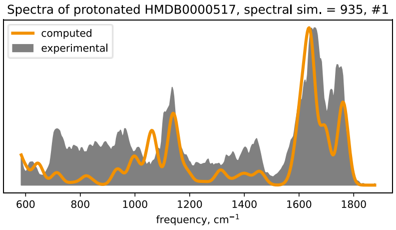

sodiated HMDB0000512, spectral sim. = 591, #4
31.0 kJ/mol
N-Acetyl-L-phenylalanine
800
1000
1200
1400
1600
1800
frequency, cm^{-1}

71 protonated HMDB0000517

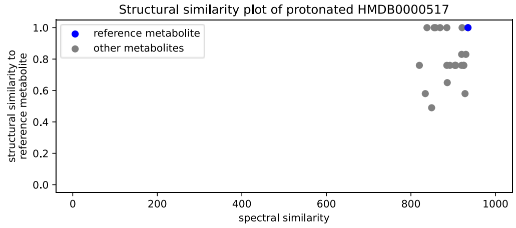


L-Arginine

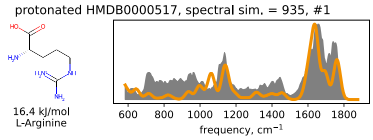
Spectra of protonated HMDB0000517, spectral sim. = 935, #1



Structural similarity plot of protonated HMDB0000517

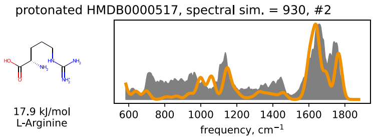


protonated HMDB0000517, spectral sim. = 935, #1



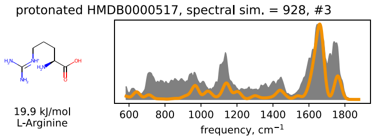
16.4 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 930, #2



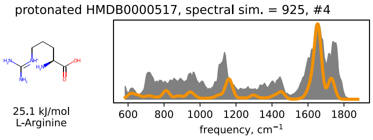
17.9 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 928, #3



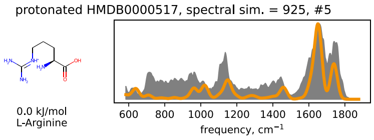
19.9 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 925, #4



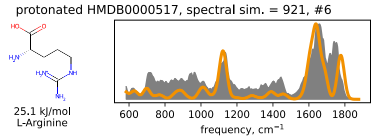
25.1 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 925, #5



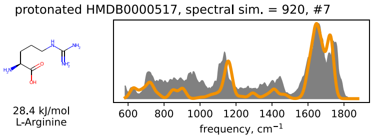
0.0 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 921, #6



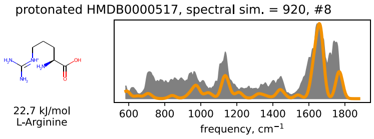
25.1 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 920, #7



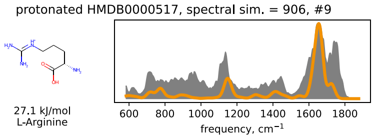
28.4 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 920, #8



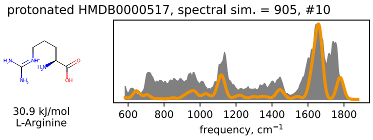
22.7 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 906, #9



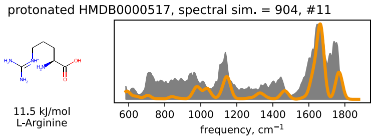
27.1 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 905, #10



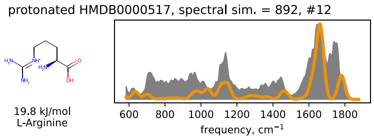
30.9 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 904, #11



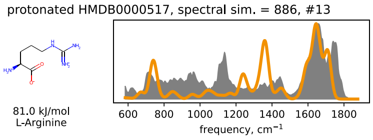
11.5 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 892, #12



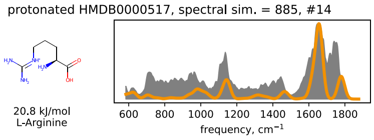
19.8 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 886, #13



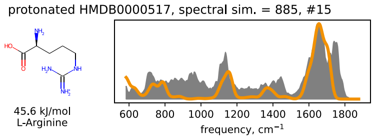
81.0 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 885, #14



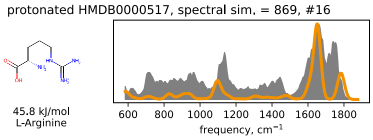
20.8 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 885, #15



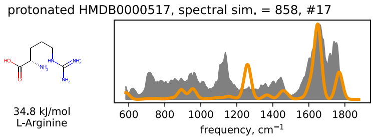
45.6 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 869, #16



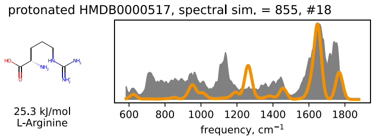
45.8 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 858, #17



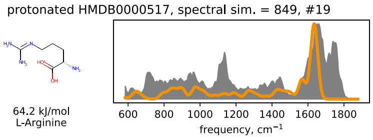
34.8 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 855, #18



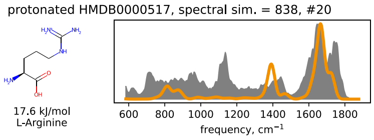
25.3 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 849, #19



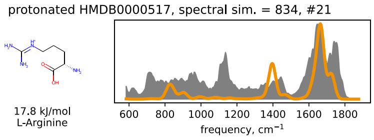
64.2 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 838, #20



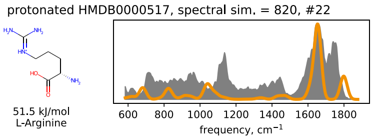
17.6 kJ/mol
L-Arginine

protonated HMDB0000517, spectral sim. = 834, #21

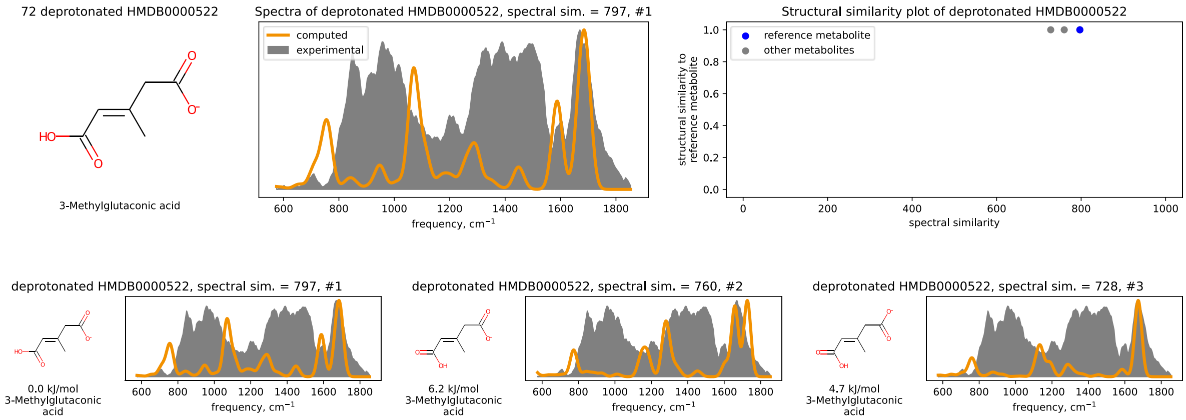


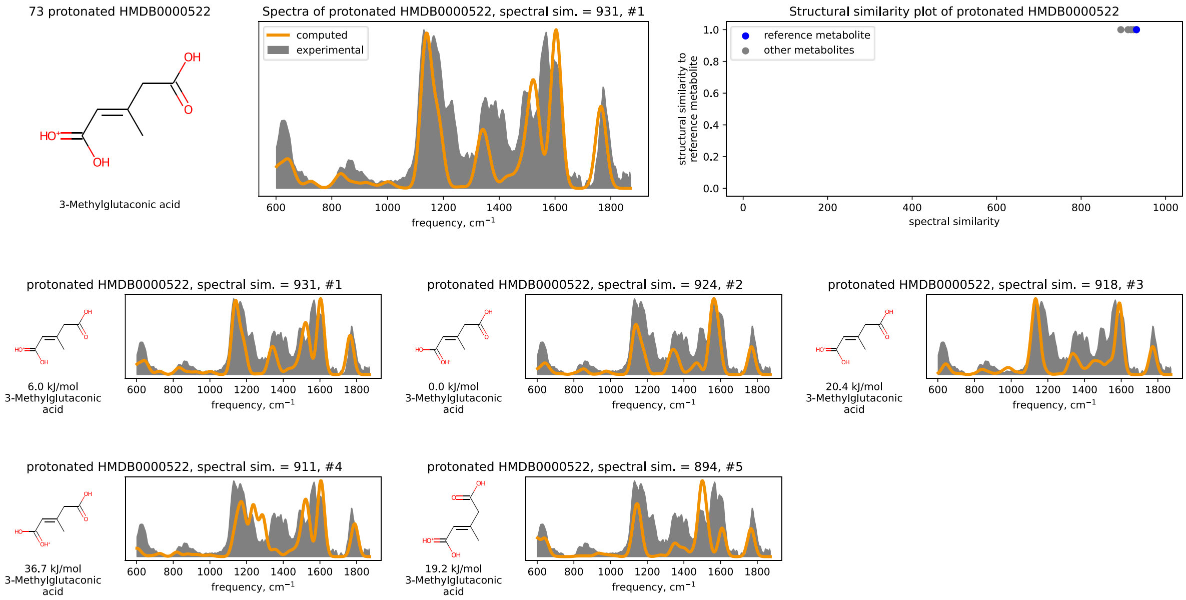
17.8 kJ/mol
L-Arginine

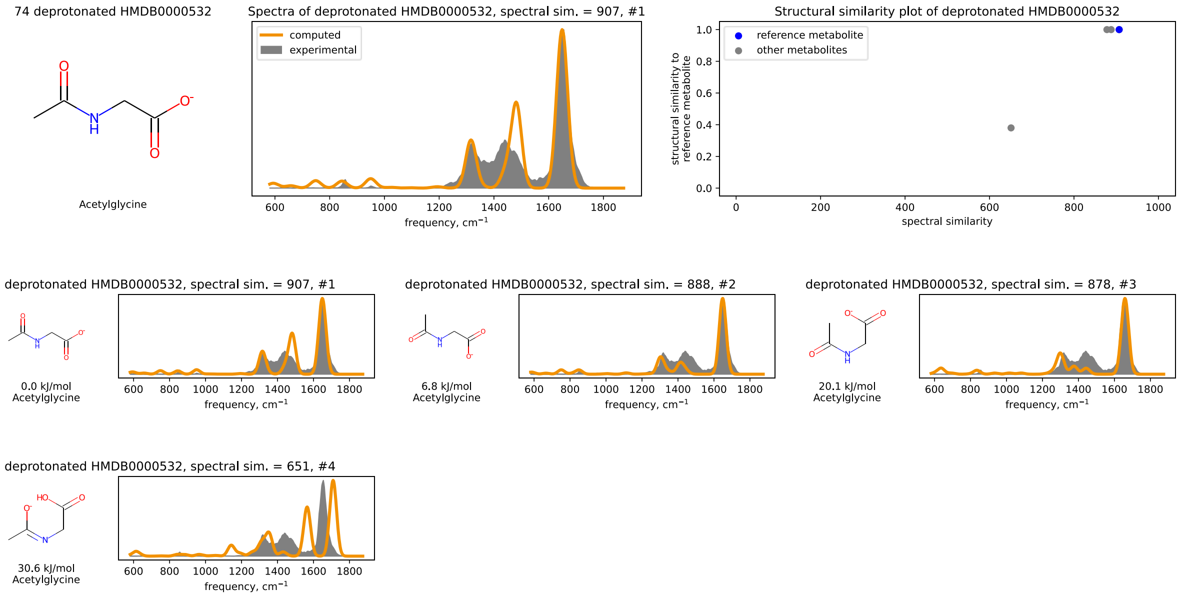
protonated HMDB0000517, spectral sim. = 820, #22

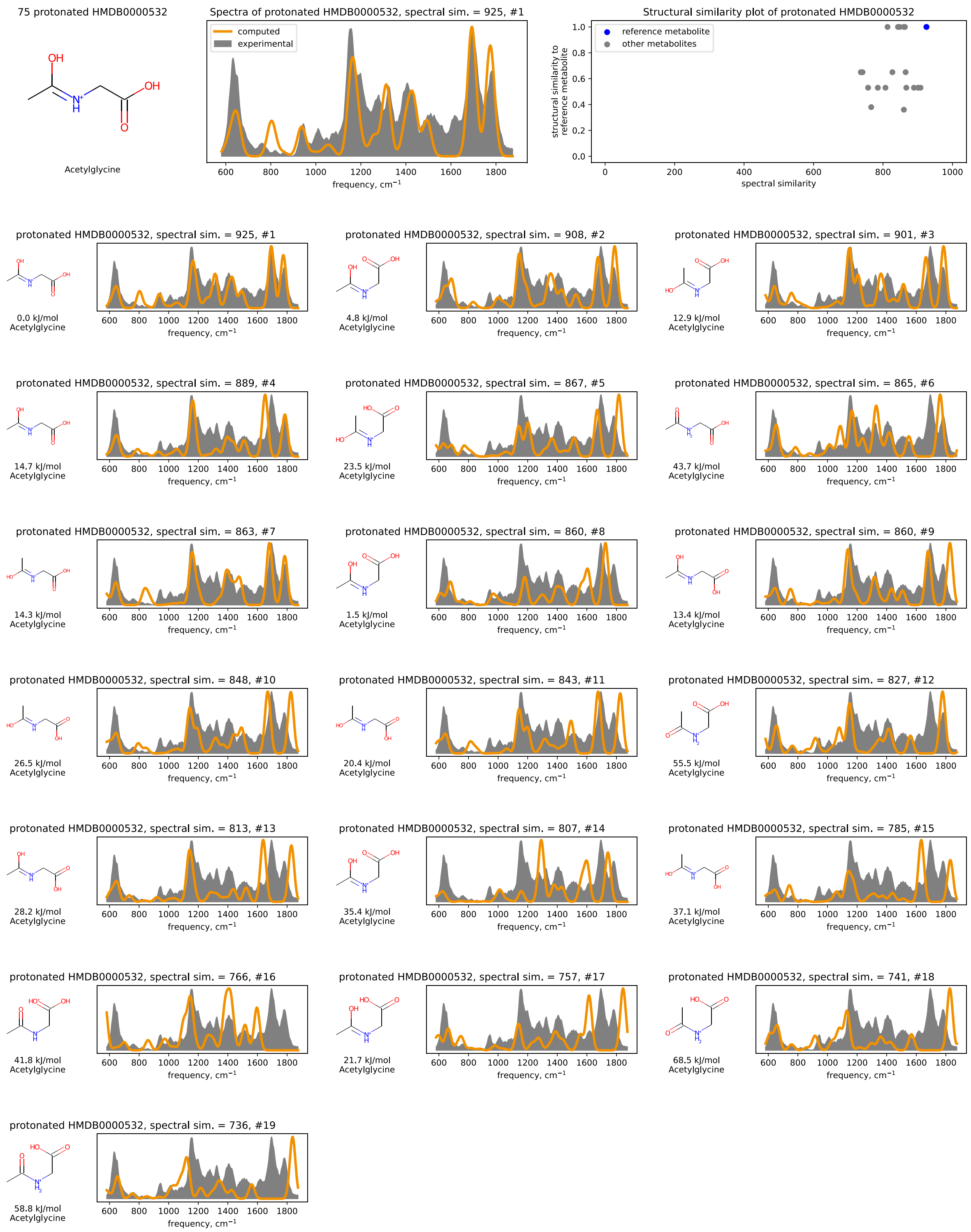


51.5 kJ/mol
L-Arginine

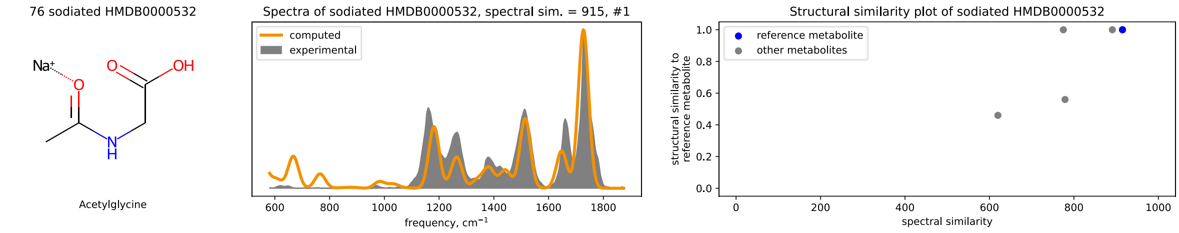

72 deprotonated HMDB0000522
3-Methylglutaconic acid
Spectra of deprotonated HMDB0000522, spectral sim. = 797, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0000522
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0000522, spectral sim. = 797, #1
0.0 kJ/mol
3-Methylglutaconic acid
deprotonated HMDB0000522, spectral sim. = 760, #2
6.2 kJ/mol
3-Methylglutaconic acid
deprotonated HMDB0000522, spectral sim. = 728, #3
4.7 kJ/mol
3-Methylglutaconic acid

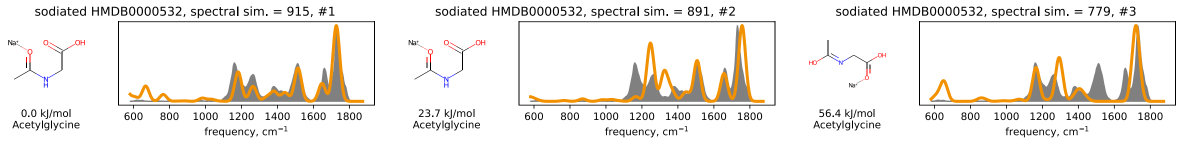

73 protonated HMDB0000522
3-Methylglutaconic acid
Spectra of protonated HMDB0000522, spectral sim. = 931, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of protonated HMDB0000522
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
protonated HMDB0000522, spectral sim. = 931, #1
6.0 kJ/mol
3-Methylglutaconic acid
protonated HMDB0000522, spectral sim. = 924, #2
0.0 kJ/mol
3-Methylglutaconic acid
protonated HMDB0000522, spectral sim. = 918, #3
20.4 kJ/mol
3-Methylglutaconic acid
protonated HMDB0000522, spectral sim. = 911, #4
36.7 kJ/mol
3-Methylglutaconic acid
protonated HMDB0000522, spectral sim. = 894, #5
19.2 kJ/mol
3-Methylglutaconic acid

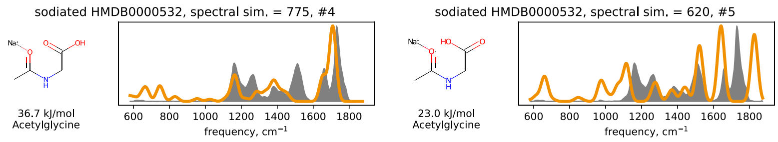

74 deprotonated HMDB0000532
Acetylglycine
Spectra of deprotonated HMDB0000532, spectral sim. = 907, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0000532
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0000532, spectral sim. = 907, #1
0.0 kJ/mol
Acetylglycine
deprotonated HMDB0000532, spectral sim. = 888, #2
6.8 kJ/mol
Acetylglycine
deprotonated HMDB0000532, spectral sim. = 878, #3
20.1 kJ/mol
Acetylglycine
deprotonated HMDB0000532, spectral sim. = 651, #4
30.6 kJ/mol
Acetylglycine

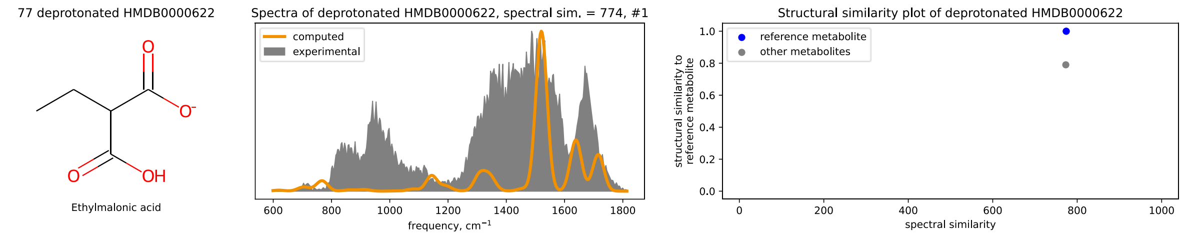


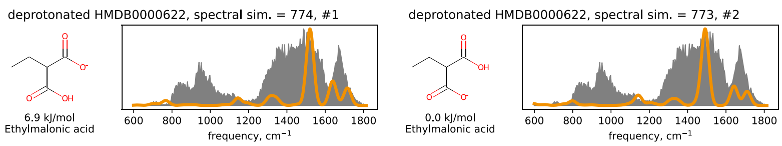
75 protonated HMDB0000532
Acetylglycine
Spectra of protonated HMDB0000532, spectral sim. = 925, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of protonated HMDB0000532
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
protonated HMDB0000532, spectral sim. = 925, #1
0.0 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 908, #2
4.8 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 901, #3
12.9 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 889, #4
14.7 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 867, #5
23.5 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 865, #6
43.7 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 863, #7
14.3 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 860, #8
1.5 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 860, #9
13.4 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 848, #10
26.5 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 843, #11
20.4 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 827, #12
55.5 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 813, #13
28.2 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 807, #14
35.4 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 785, #15
37.1 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 766, #16
41.8 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 757, #17
21.7 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 741, #18
68.5 kJ/mol Acetylglycine
protonated HMDB0000532, spectral sim. = 736, #19
58.8 kJ/mol Acetylglycine

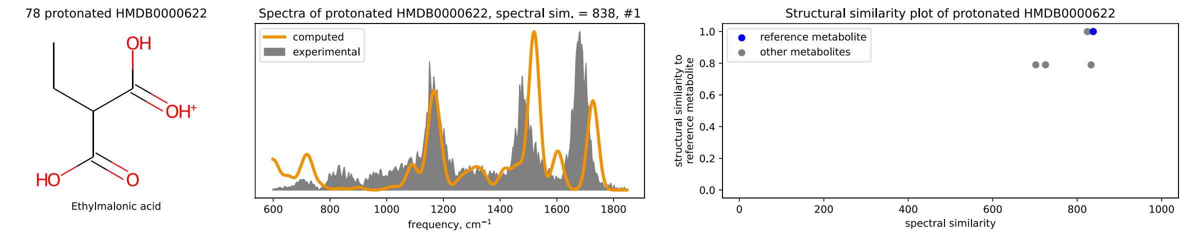

76 sodiated HMDB0000532
Acetylglycine
Spectra of sodiated HMDB0000532, spectral sim. = 915, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of sodiated HMDB0000532
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

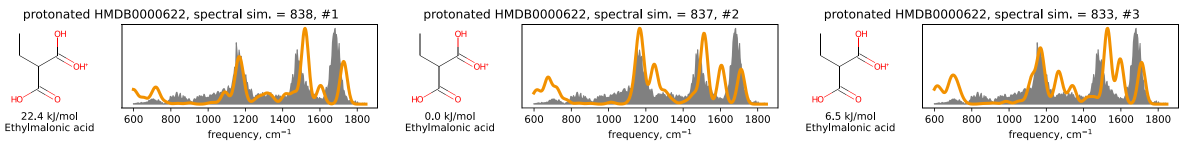

sodiated HMDB0000532, spectral sim. = 915, #1
0.0 kJ/mol
Acetylglycine
sodiated HMDB0000532, spectral sim. = 891, #2
23.7 kJ/mol
Acetylglycine
sodiated HMDB0000532, spectral sim. = 779, #3
56.4 kJ/mol
Acetylglycine
frequency, cm^{-1}

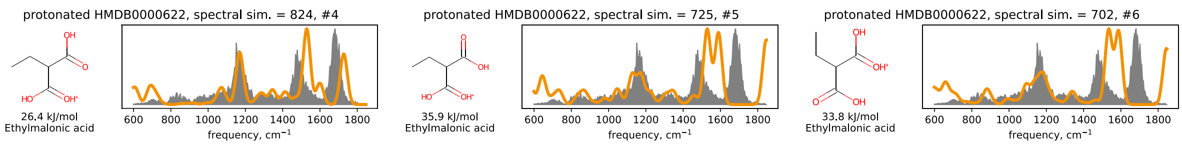

sodiated HMDB0000532, spectral sim. = 775, #4
36.7 kJ/mol
Acetylglycine
sodiated HMDB0000532, spectral sim. = 620, #5
23.0 kJ/mol
Acetylglycine
frequency, cm^{-1}


77 deprotonated HMDB0000622
Ethylmalonic acid
Spectra of deprotonated HMDB0000622, spectral sim. = 774, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0000622
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

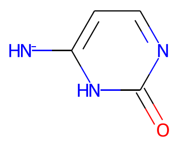

deprotonated HMDB0000622, spectral sim. = 774, #1
6.9 kJ/mol
Ethylmalonic acid
deprotonated HMDB0000622, spectral sim. = 773, #2
0.0 kJ/mol
Ethylmalonic acid
frequency, cm^{-1}


78 protonated HMDB0000622
Ethylmalonic acid
Spectra of protonated HMDB0000622, spectral sim. = 838, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of protonated HMDB0000622
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity


protonated HMDB0000622, spectral sim. = 838, #1
22.4 kJ/mol
Ethylmalonic acid
protonated HMDB0000622, spectral sim. = 837, #2
0.0 kJ/mol
Ethylmalonic acid
protonated HMDB0000622, spectral sim. = 833, #3
6.5 kJ/mol
Ethylmalonic acid
frequency, cm^{-1}

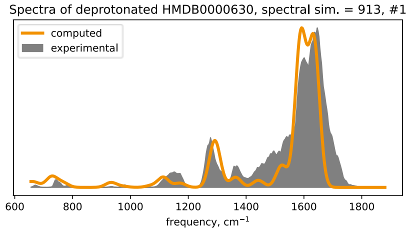

protonated HMDB0000622, spectral sim. = 824, #4
26.4 kJ/mol
Ethylmalonic acid
protonated HMDB0000622, spectral sim. = 725, #5
35.9 kJ/mol
Ethylmalonic acid
protonated HMDB0000622, spectral sim. = 702, #6
33.8 kJ/mol
Ethylmalonic acid
frequency, cm^{-1}

79 deprotonated HMDB0000630

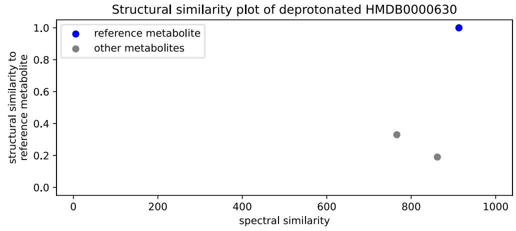


Cytosine

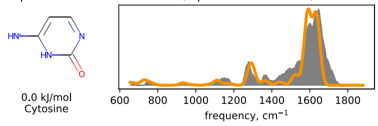
Spectra of deprotonated HMDB0000630, spectral sim. = 913, #1



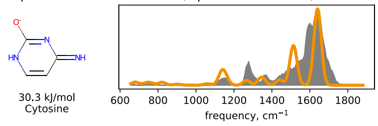
Structural similarity plot of deprotonated HMDB0000630



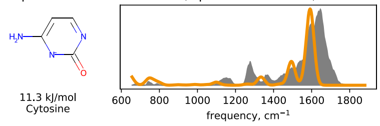
deprotonated HMDB0000630, spectral sim. = 913, #1



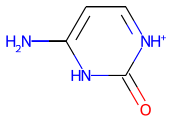
deprotonated HMDB0000630, spectral sim. = 862, #2



deprotonated HMDB0000630, spectral sim. = 766, #3

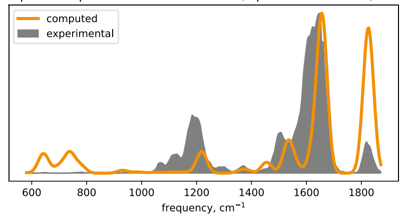


80 protonated HMDB0000630

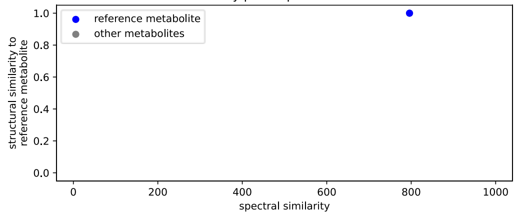


Cytosine

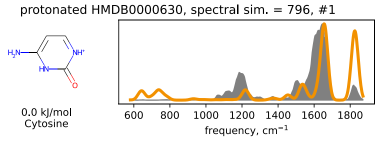
Spectra of protonated HMDB0000630, spectral sim. = 796, #1



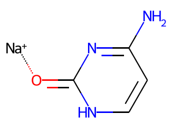
Structural similarity plot of protonated HMDB0000630



protonated HMDB0000630, spectral sim. = 796, #1

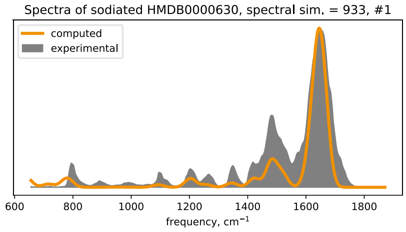


81 sodiated HMDB0000630

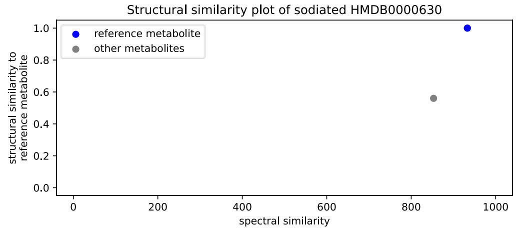


Cytosine

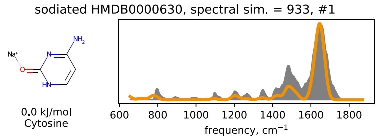
Spectra of sodiated HMDB0000630, spectral sim. = 933, #1



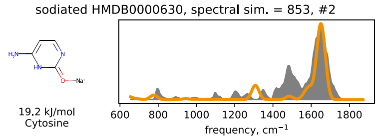
Structural similarity plot of sodiated HMDB0000630

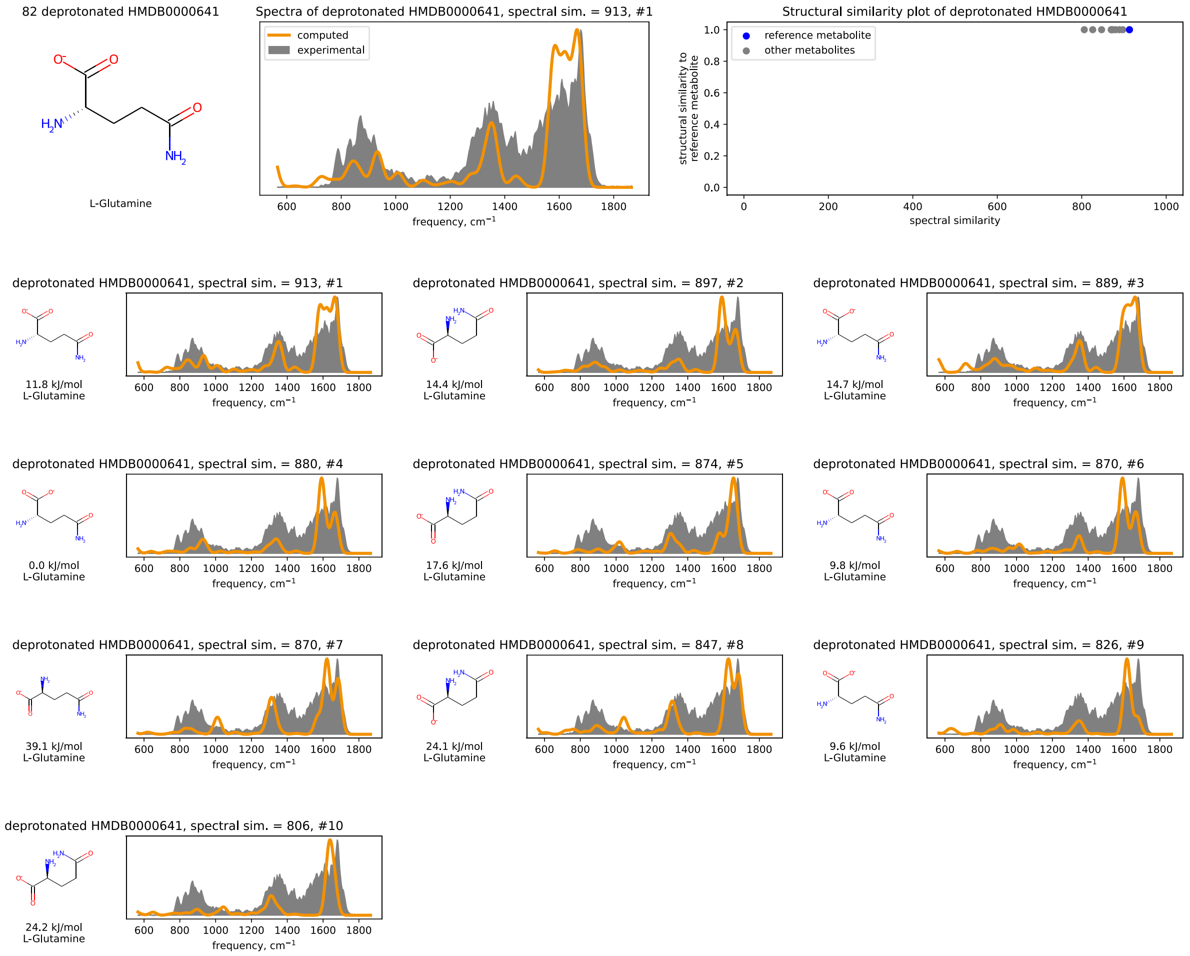


sodiated HMDB0000630, spectral sim. = 933, #1

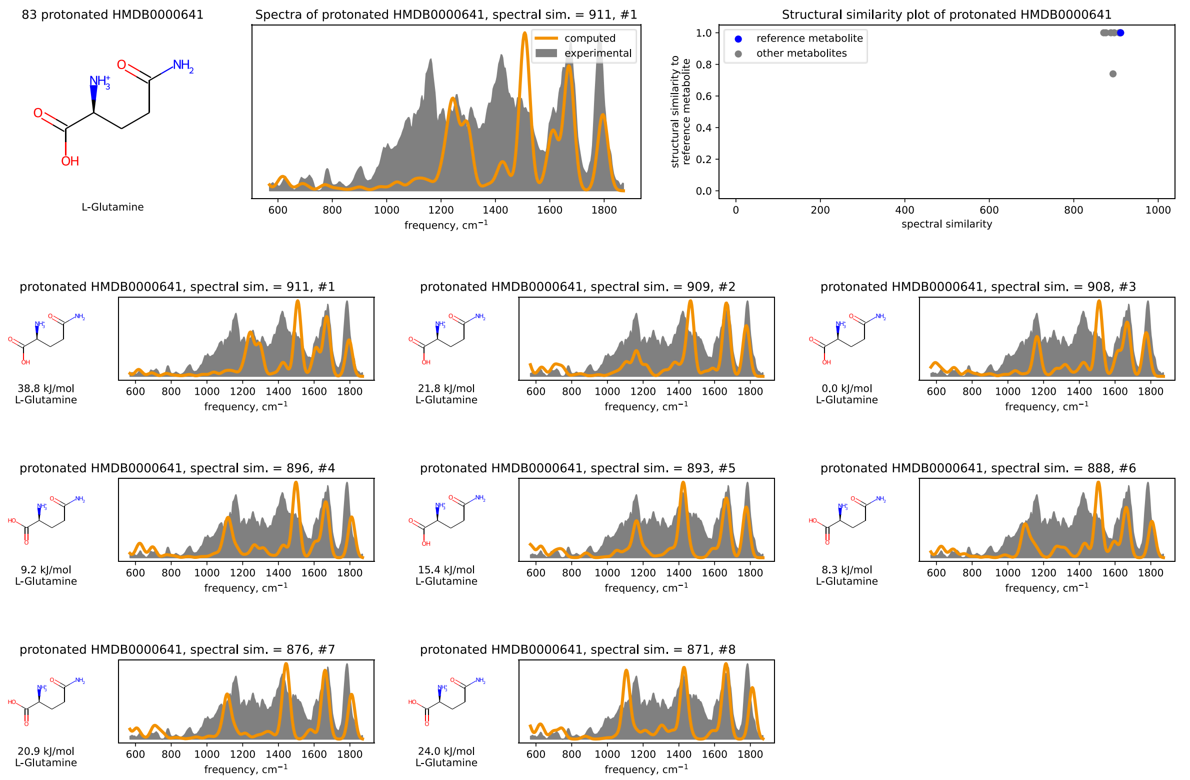


sodiated HMDB0000630, spectral sim. = 853, #2

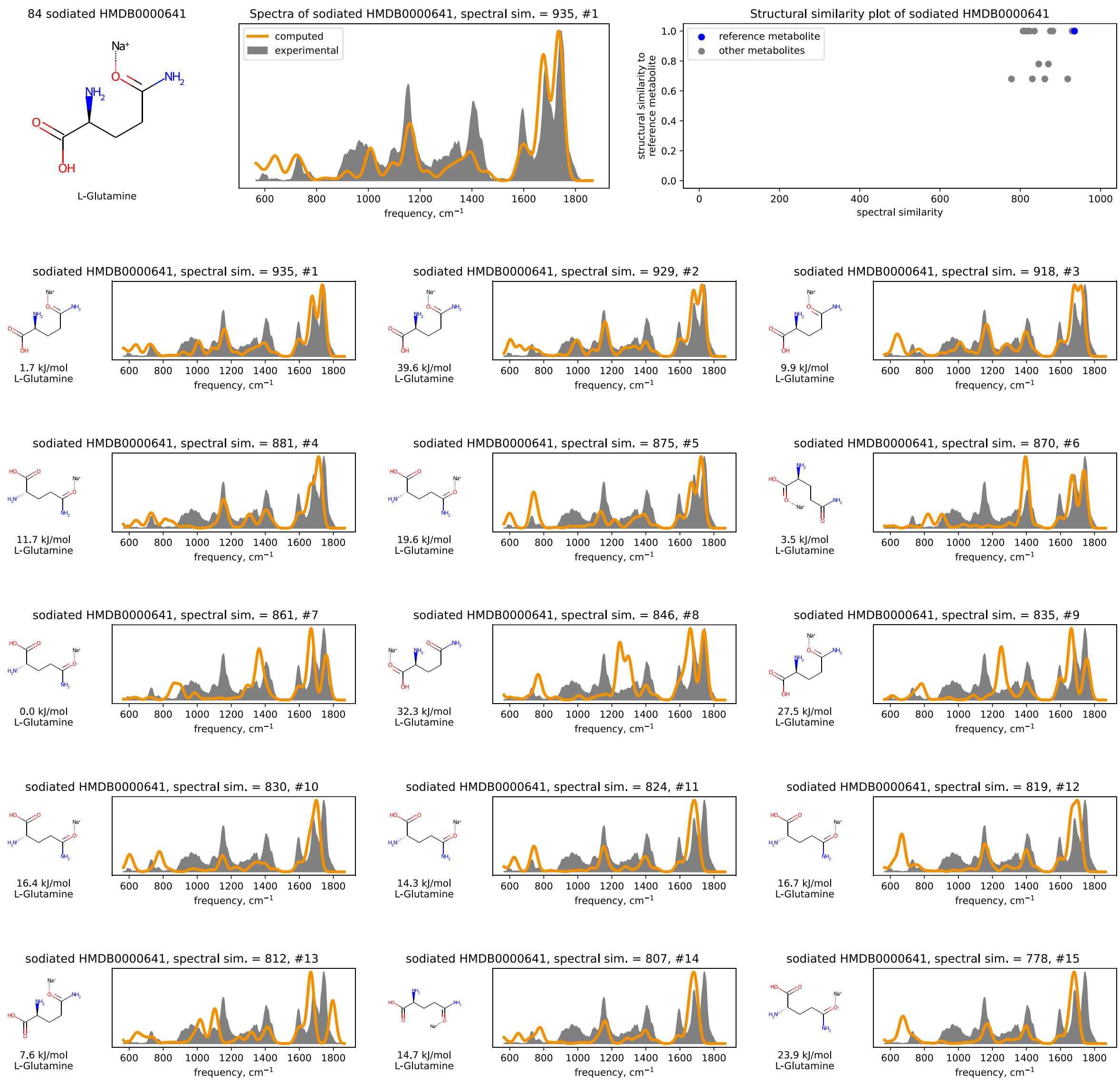




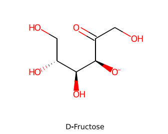
82 deprotonated HMDB0000641
L-Glutamine
Spectra of deprotonated HMDB0000641, spectral sim. = 913, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of deprotonated HMDB0000641
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0000641, spectral sim. = 913, #1
11.8 kJ/mol
L-Glutamine
deprotonated HMDB0000641, spectral sim. = 897, #2
14.4 kJ/mol
L-Glutamine
deprotonated HMDB0000641, spectral sim. = 889, #3
14.7 kJ/mol
L-Glutamine
deprotonated HMDB0000641, spectral sim. = 880, #4
0.0 kJ/mol
L-Glutamine
deprotonated HMDB0000641, spectral sim. = 874, #5
17.6 kJ/mol
L-Glutamine
deprotonated HMDB0000641, spectral sim. = 870, #6
9.8 kJ/mol
L-Glutamine
deprotonated HMDB0000641, spectral sim. = 870, #7
39.1 kJ/mol
L-Glutamine
deprotonated HMDB0000641, spectral sim. = 847, #8
24.1 kJ/mol
L-Glutamine
deprotonated HMDB0000641, spectral sim. = 826, #9
9.6 kJ/mol
L-Glutamine
deprotonated HMDB0000641, spectral sim. = 806, #10
24.2 kJ/mol
L-Glutamine



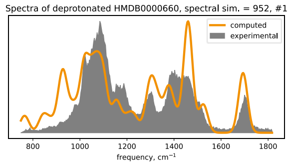
83 protonated HMDB0000641
L-Glutamine
Spectra of protonated HMDB0000641, spectral sim. = 911, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of protonated HMDB0000641
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
protonated HMDB0000641, spectral sim. = 911, #1
38.8 kJ/mol
L-Glutamine
protonated HMDB0000641, spectral sim. = 909, #2
21.8 kJ/mol
L-Glutamine
protonated HMDB0000641, spectral sim. = 908, #3
0.0 kJ/mol
L-Glutamine
protonated HMDB0000641, spectral sim. = 896, #4
9.2 kJ/mol
L-Glutamine
protonated HMDB0000641, spectral sim. = 893, #5
15.4 kJ/mol
L-Glutamine
protonated HMDB0000641, spectral sim. = 888, #6
8.3 kJ/mol
L-Glutamine
protonated HMDB0000641, spectral sim. = 876, #7
20.9 kJ/mol
L-Glutamine
protonated HMDB0000641, spectral sim. = 871, #8
24.0 kJ/mol
L-Glutamine


84 sodiated HMDB0000641
L-Glutamine
Spectra of sodiated HMDB0000641, spectral sim. = 935, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of sodiated HMDB0000641
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
sodiated HMDB0000641, spectral sim. = 935, #1
1.7 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 929, #2
39.6 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 918, #3
9.9 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 881, #4
11.7 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 875, #5
19.6 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 870, #6
3.5 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 861, #7
0.0 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 846, #8
32.3 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 835, #9
27.5 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 830, #10
16.4 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 824, #11
14.3 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 819, #12
16.7 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 812, #13
7.6 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 807, #14
14.7 kJ/mol
L-Glutamine
sodiated HMDB0000641, spectral sim. = 778, #15
23.9 kJ/mol
L-Glutamine

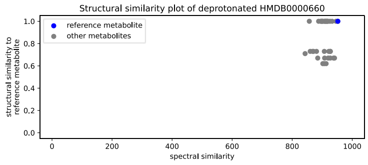
85 deprotonated HMDB0000660



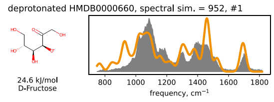
Spectra of deprotonated HMDB0000660, spectral sim. = 952, #1



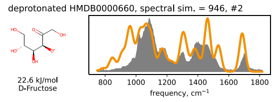
Structural similarity plot of deprotonated HMDB0000660



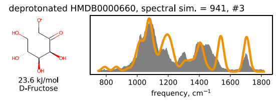
deprotonated HMDB0000660, spectral sim. = 952, #1



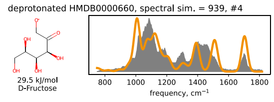
deprotonated HMDB0000660, spectral sim. = 946, #2



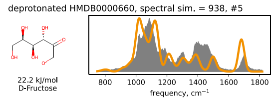
deprotonated HMDB0000660, spectral sim. = 941, #3



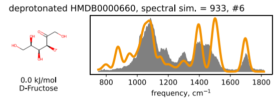
deprotonated HMDB0000660, spectral sim. = 939, #4



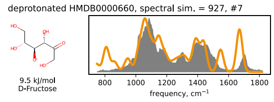
deprotonated HMDB0000660, spectral sim. = 938, #5



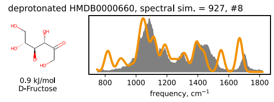
deprotonated HMDB0000660, spectral sim. = 933, #6



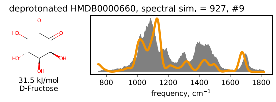
deprotonated HMDB0000660, spectral sim. = 927, #7



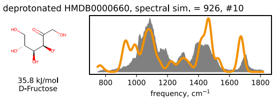
deprotonated HMDB0000660, spectral sim. = 927, #8



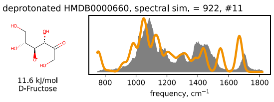
deprotonated HMDB0000660, spectral sim. = 927, #9



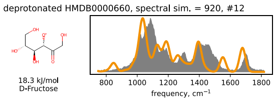
deprotonated HMDB0000660, spectral sim. = 926, #10



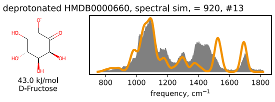
deprotonated HMDB0000660, spectral sim. = 922, #11



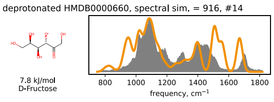
deprotonated HMDB0000660, spectral sim. = 920, #12



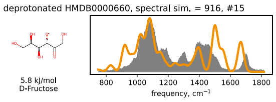
deprotonated HMDB0000660, spectral sim. = 920, #13



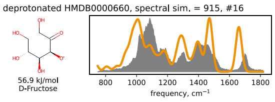
deprotonated HMDB0000660, spectral sim. = 916, #14



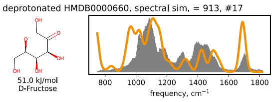
deprotonated HMDB0000660, spectral sim. = 916, #15



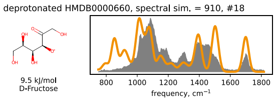
deprotonated HMDB0000660, spectral sim. = 915, #16



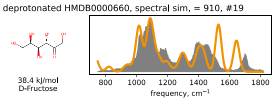
deprotonated HMDB0000660, spectral sim. = 913, #17



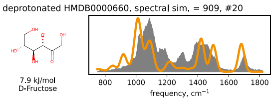
deprotonated HMDB0000660, spectral sim. = 910, #18



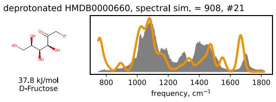
deprotonated HMDB0000660, spectral sim. = 910, #19



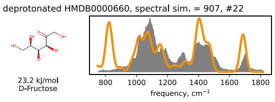
deprotonated HMDB0000660, spectral sim. = 909, #20



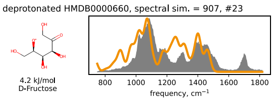
deprotonated HMDB0000660, spectral sim. = 908, #21



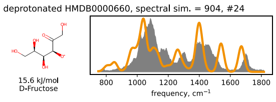
deprotonated HMDB0000660, spectral sim. = 907, #22



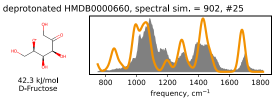
deprotonated HMDB0000660, spectral sim. = 907, #23



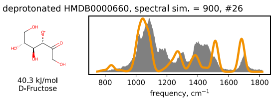
deprotonated HMDB0000660, spectral sim. = 904, #24



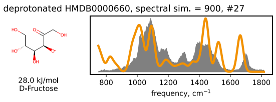
deprotonated HMDB0000660, spectral sim. = 902, #25



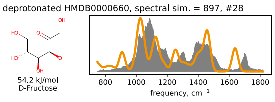
deprotonated HMDB0000660, spectral sim. = 900, #26



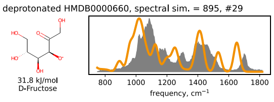
deprotonated HMDB0000660, spectral sim. = 900, #27



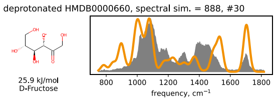
deprotonated HMDB0000660, spectral sim. = 897, #28



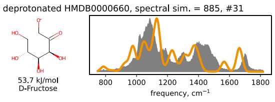
deprotonated HMDB0000660, spectral sim. = 895, #29



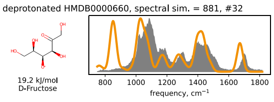
deprotonated HMDB0000660, spectral sim. = 888, #30



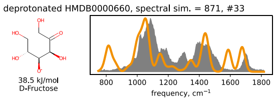
deprotonated HMDB0000660, spectral sim. = 885, #31



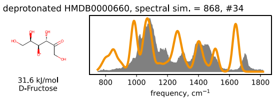
deprotonated HMDB0000660, spectral sim. = 881, #32



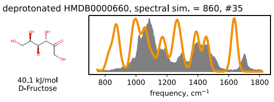
deprotonated HMDB0000660, spectral sim. = 871, #33



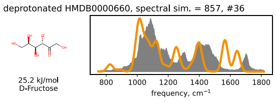
deprotonated HMDB0000660, spectral sim. = 868, #34



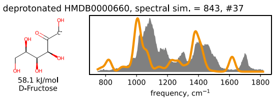
deprotonated HMDB0000660, spectral sim. = 860, #35



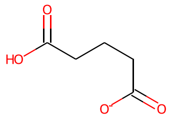
deprotonated HMDB0000660, spectral sim. = 857, #36



deprotonated HMDB0000660, spectral sim. = 843, #37

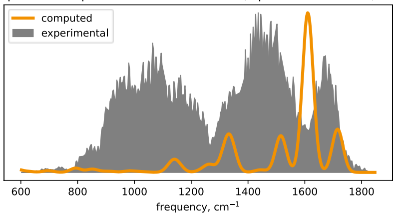


86 deprotonated HMDB0000661

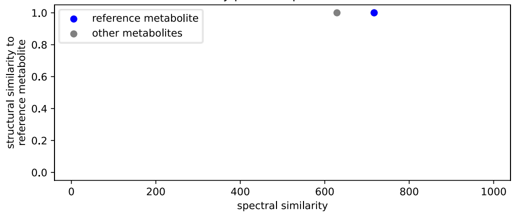


Glutaric acid

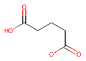
Spectra of deprotonated HMDB0000661, spectral sim. = 717, #1



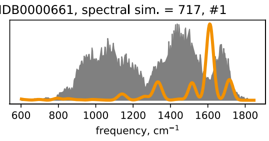
Structural similarity plot of deprotonated HMDB0000661



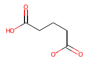
deprotonated HMDB0000661, spectral sim. = 717, #1



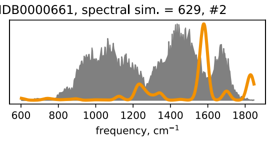
11.1 kJ/mol
Glutaric acid



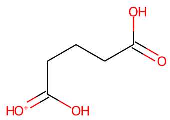
deprotonated HMDB0000661, spectral sim. = 629, #2



0.0 kJ/mol
Glutaric acid

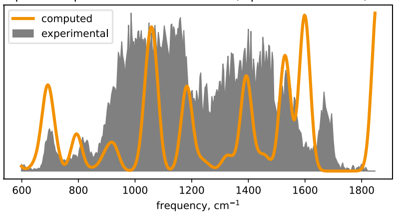


87 protonated HMDB0000661

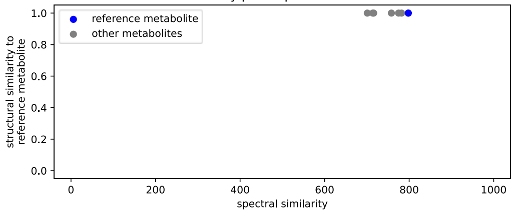


Glutaric acid

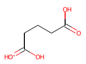
Spectra of protonated HMDB0000661, spectral sim. = 798, #1



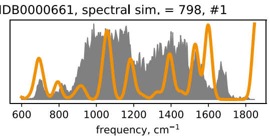
Structural similarity plot of protonated HMDB0000661



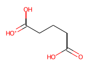
protonated HMDB0000661, spectral sim. = 798, #1



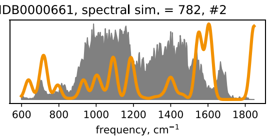
48.6 kJ/mol
Glutaric acid



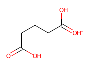
protonated HMDB0000661, spectral sim. = 782, #2



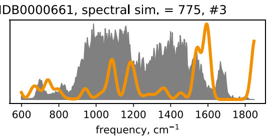
47.2 kJ/mol
Glutaric acid



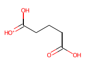
protonated HMDB0000661, spectral sim. = 775, #3



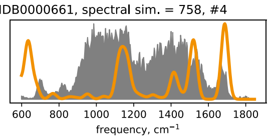
44.0 kJ/mol
Glutaric acid



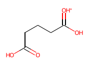
protonated HMDB0000661, spectral sim. = 758, #4



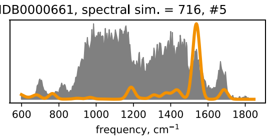
56.9 kJ/mol
Glutaric acid



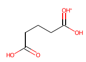
protonated HMDB0000661, spectral sim. = 716, #5



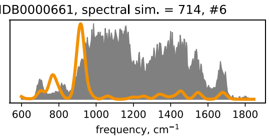
22.8 kJ/mol
Glutaric acid



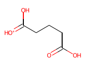
protonated HMDB0000661, spectral sim. = 714, #6



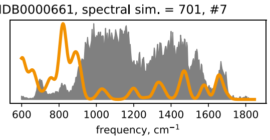
1.9 kJ/mol
Glutaric acid

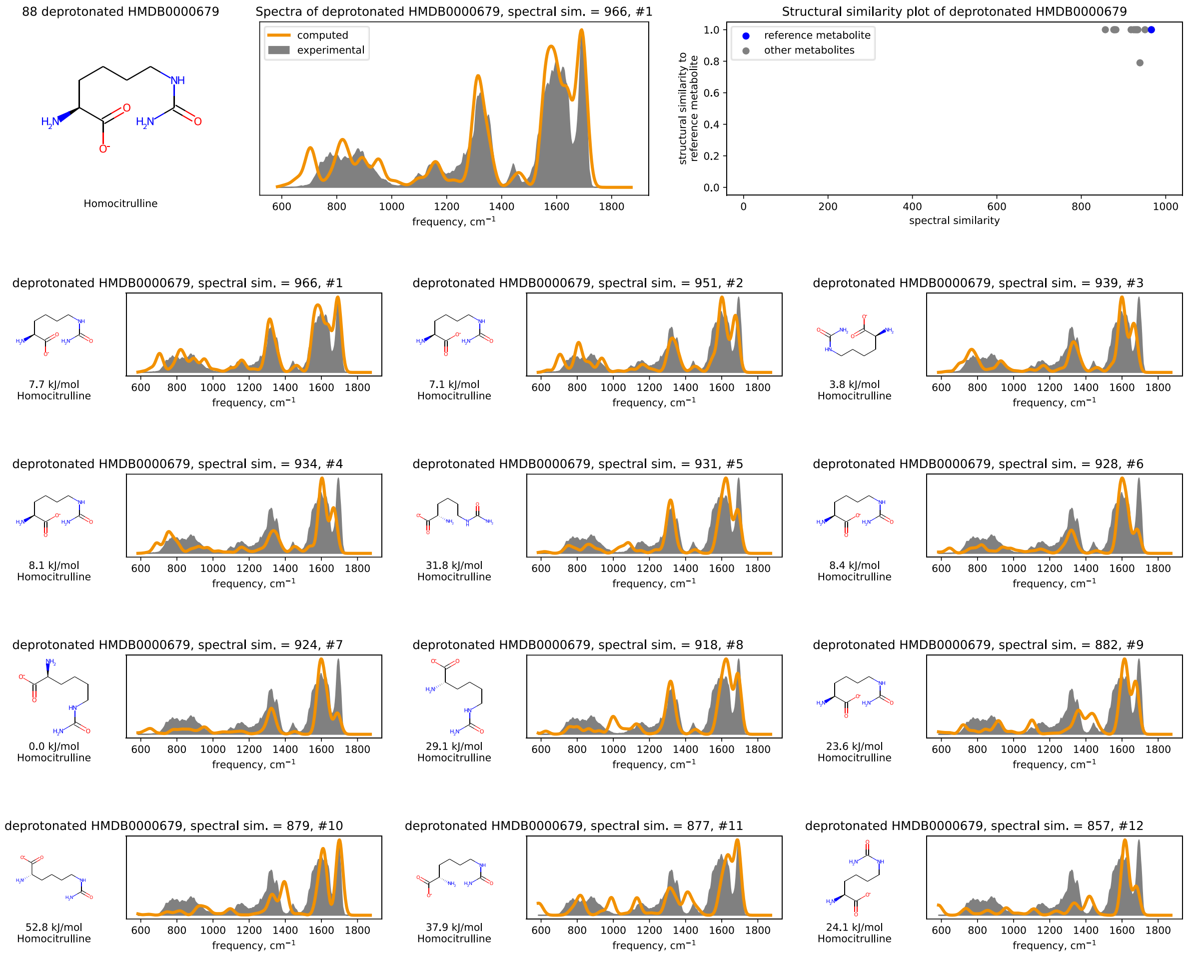


protonated HMDB0000661, spectral sim. = 701, #7



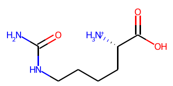
0.0 kJ/mol
Glutaric acid





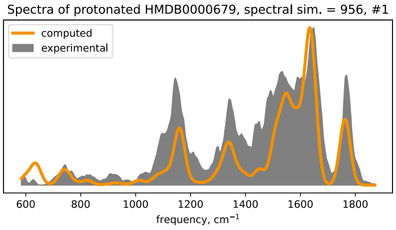
88 deprotonated HMDB0000679
Homocitrulline
Spectra of deprotonated HMDB0000679, spectral sim. = 966, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of deprotonated HMDB0000679
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0000679, spectral sim. = 966, #1
7.7 kJ/mol Homocitrulline
deprotonated HMDB0000679, spectral sim. = 951, #2
7.1 kJ/mol Homocitrulline
deprotonated HMDB0000679, spectral sim. = 939, #3
3.8 kJ/mol Homocitrulline
deprotonated HMDB0000679, spectral sim. = 934, #4
8.1 kJ/mol Homocitrulline
deprotonated HMDB0000679, spectral sim. = 931, #5
31.8 kJ/mol Homocitrulline
deprotonated HMDB0000679, spectral sim. = 928, #6
8.4 kJ/mol Homocitrulline
deprotonated HMDB0000679, spectral sim. = 924, #7
0.0 kJ/mol Homocitrulline
deprotonated HMDB0000679, spectral sim. = 918, #8
29.1 kJ/mol Homocitrulline
deprotonated HMDB0000679, spectral sim. = 882, #9
23.6 kJ/mol Homocitrulline
deprotonated HMDB0000679, spectral sim. = 879, #10
52.8 kJ/mol Homocitrulline
deprotonated HMDB0000679, spectral sim. = 877, #11
37.9 kJ/mol Homocitrulline
deprotonated HMDB0000679, spectral sim. = 857, #12
24.1 kJ/mol Homocitrulline

89 protonated HMDB0000679

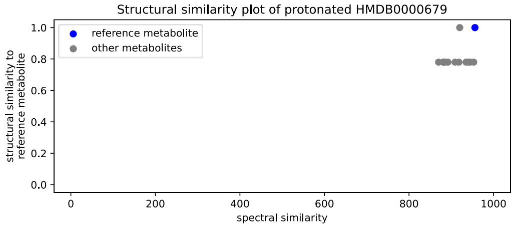


Homocitrulline

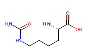
Spectra of protonated HMDB0000679, spectral sim. = 956, #1



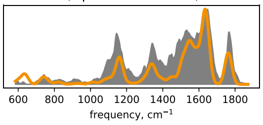
Structural similarity plot of protonated HMDB0000679



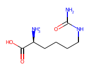
protonated HMDB0000679, spectral sim. = 956, #1



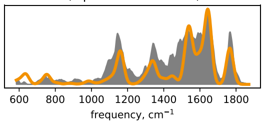
0.0 kJ/mol
Homocitrulline



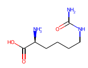
protonated HMDB0000679, spectral sim. = 953, #2



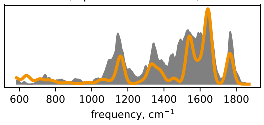
10.0 kJ/mol
Homocitrulline



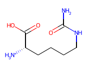
protonated HMDB0000679, spectral sim. = 945, #3



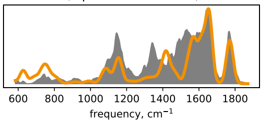
21.4 kJ/mol
Homocitrulline



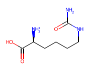
protonated HMDB0000679, spectral sim. = 940, #4



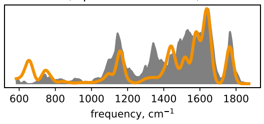
44.6 kJ/mol
Homocitrulline



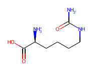
protonated HMDB0000679, spectral sim. = 935, #5



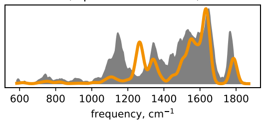
34.6 kJ/mol
Homocitrulline



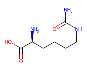
protonated HMDB0000679, spectral sim. = 920, #6



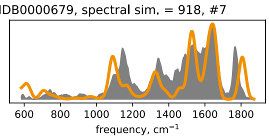
32.9 kJ/mol
Homocitrulline



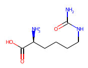
protonated HMDB0000679, spectral sim. = 918, #7



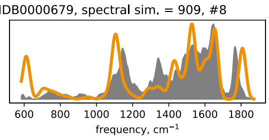
36.2 kJ/mol
Homocitrulline



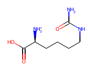
protonated HMDB0000679, spectral sim. = 909, #8



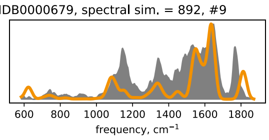
42.4 kJ/mol
Homocitrulline



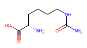
protonated HMDB0000679, spectral sim. = 892, #9



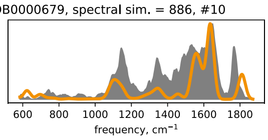
14.3 kJ/mol
Homocitrulline



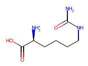
protonated HMDB0000679, spectral sim. = 886, #10



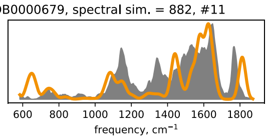
20.7 kJ/mol
Homocitrulline



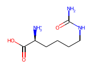
protonated HMDB0000679, spectral sim. = 882, #11



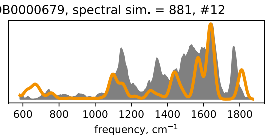
47.7 kJ/mol
Homocitrulline



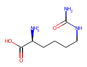
protonated HMDB0000679, spectral sim. = 881, #12



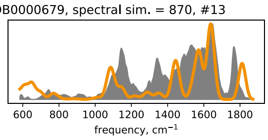
45.2 kJ/mol
Homocitrulline

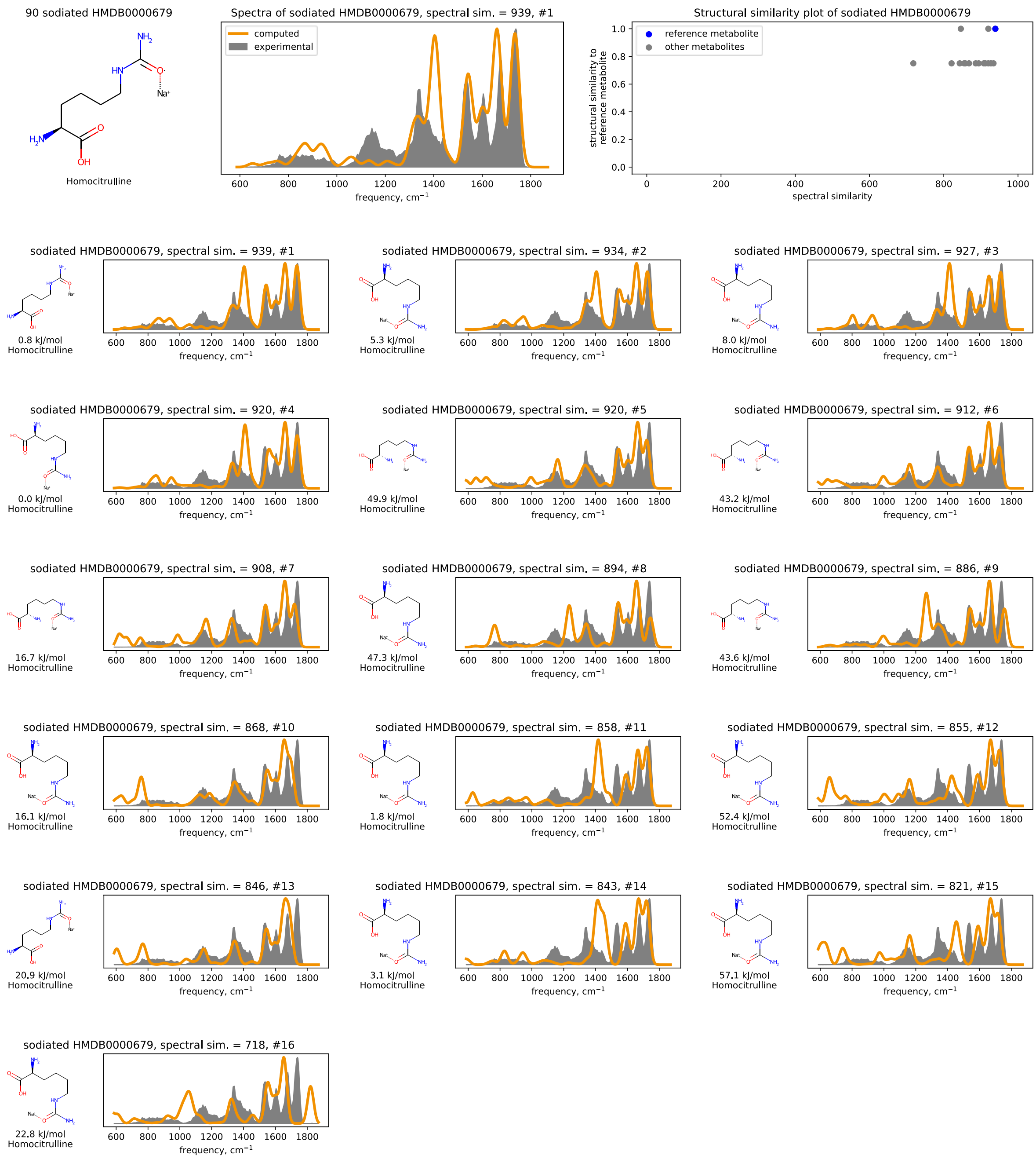


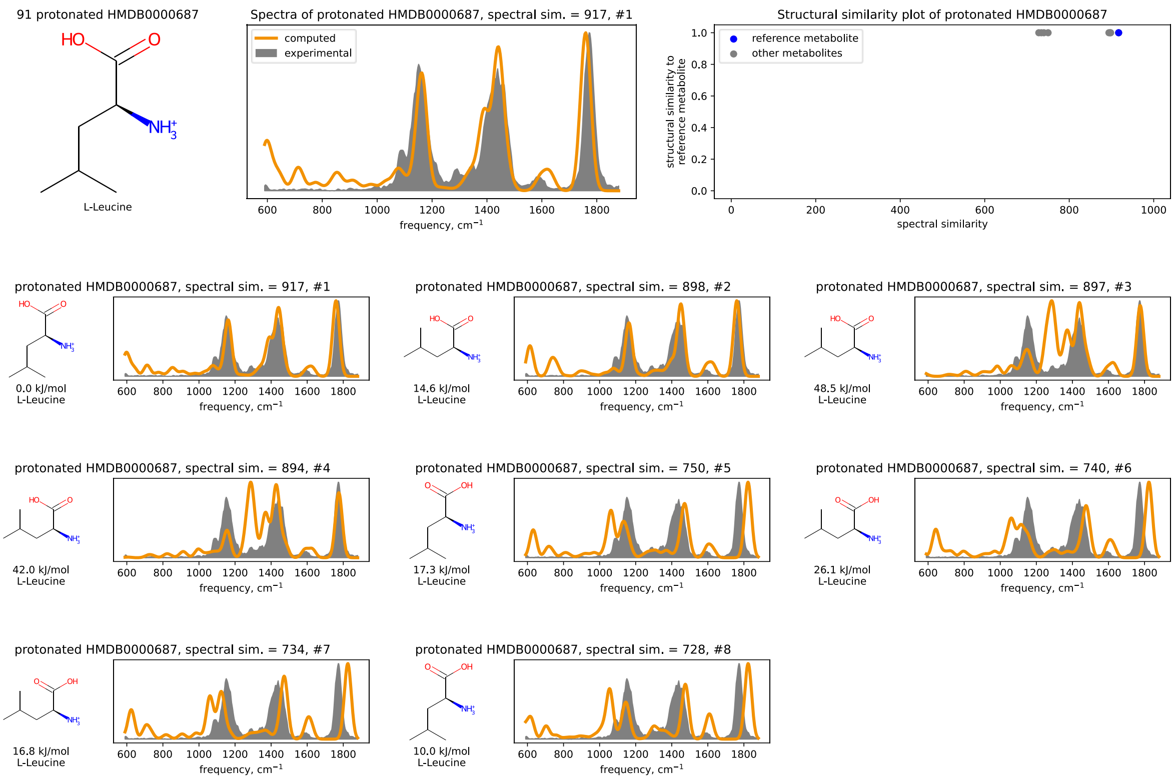
protonated HMDB0000679, spectral sim. = 870, #13



48.4 kJ/mol
Homocitrulline

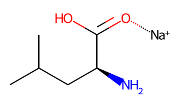



90 sodiated HMDB0000679
Homocitrulline
Spectra of sodiated HMDB0000679, spectral sim. = 939, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of sodiated HMDB0000679
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
sodiated HMDB0000679, spectral sim. = 939, #1
0.8 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 934, #2
5.3 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 927, #3
8.0 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 920, #4
0.0 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 920, #5
49.9 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 912, #6
43.2 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 908, #7
16.7 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 894, #8
47.3 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 886, #9
43.6 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 868, #10
16.1 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 858, #11
1.8 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 855, #12
52.4 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 846, #13
20.9 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 843, #14
3.1 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 821, #15
57.1 kJ/mol
Homocitrulline
sodiated HMDB0000679, spectral sim. = 718, #16
22.8 kJ/mol
Homocitrulline
frequency, cm⁻¹



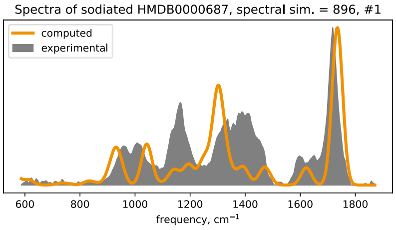
91 protonated HMDB0000687
HO
O
NH3+
L-Leucine
Spectra of protonated HMDB0000687, spectral sim. = 917, #1
computed
experimental
frequency, cm−1
Structural similarity plot of protonated HMDB0000687
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
protonated HMDB0000687, spectral sim. = 917, #1
0.0 kJ/mol
L-Leucine
protonated HMDB0000687, spectral sim. = 898, #2
14.6 kJ/mol
L-Leucine
protonated HMDB0000687, spectral sim. = 897, #3
48.5 kJ/mol
L-Leucine
protonated HMDB0000687, spectral sim. = 894, #4
42.0 kJ/mol
L-Leucine
protonated HMDB0000687, spectral sim. = 750, #5
17.3 kJ/mol
L-Leucine
protonated HMDB0000687, spectral sim. = 740, #6
26.1 kJ/mol
L-Leucine
protonated HMDB0000687, spectral sim. = 734, #7
16.8 kJ/mol
L-Leucine
protonated HMDB0000687, spectral sim. = 728, #8
10.0 kJ/mol
L-Leucine

92 sodiated HMDB0000687

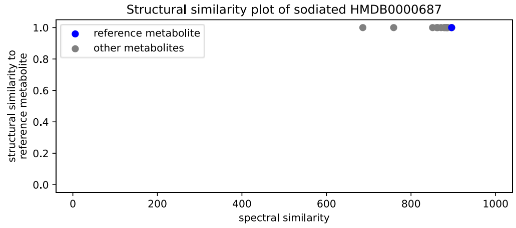


L-Leucine

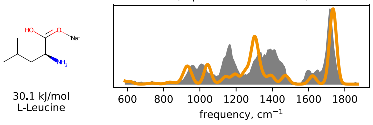
Spectra of sodiated HMDB0000687, spectral sim. = 896, #1



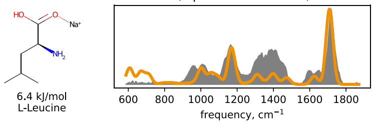
Structural similarity plot of sodiated HMDB0000687



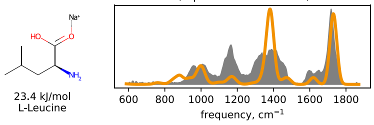
sodiated HMDB0000687, spectral sim. = 896, #1



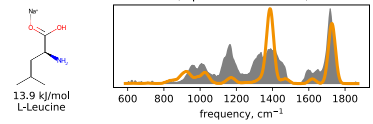
sodiated HMDB0000687, spectral sim. = 896, #2



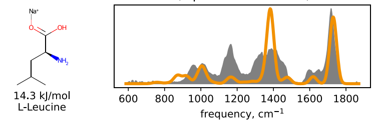
sodiated HMDB0000687, spectral sim. = 887, #3



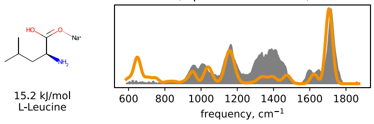
sodiated HMDB0000687, spectral sim. = 886, #4



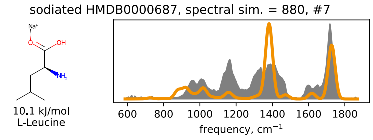
sodiated HMDB0000687, spectral sim. = 885, #5



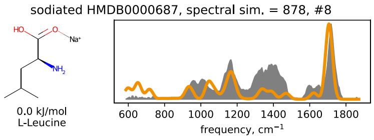
sodiated HMDB0000687, spectral sim. = 883, #6



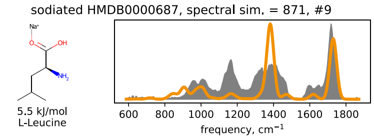
sodiated HMDB0000687, spectral sim. = 880, #7



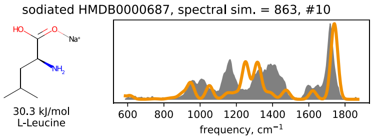
sodiated HMDB0000687, spectral sim. = 878, #8



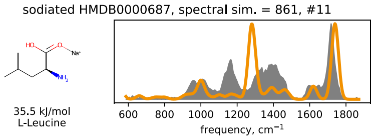
sodiated HMDB0000687, spectral sim. = 871, #9



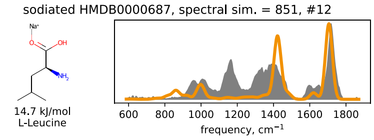
sodiated HMDB0000687, spectral sim. = 863, #10



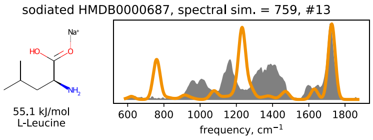
sodiated HMDB0000687, spectral sim. = 861, #11



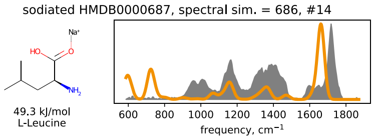
sodiated HMDB0000687, spectral sim. = 851, #12



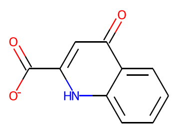
sodiated HMDB0000687, spectral sim. = 759, #13



sodiated HMDB0000687, spectral sim. = 686, #14

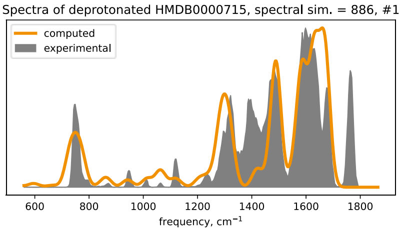


93 deprotonated HMDB0000715

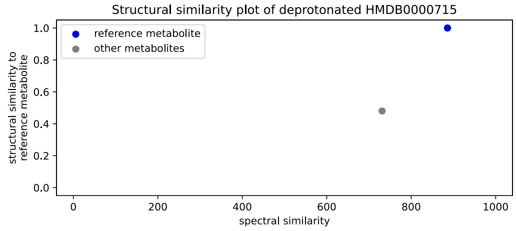


Kynurenic acid

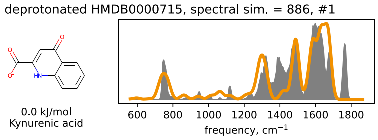
Spectra of deprotonated HMDB0000715, spectral sim. = 886, #1



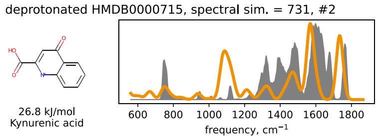
Structural similarity plot of deprotonated HMDB0000715



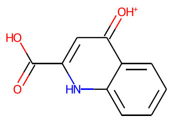
deprotonated HMDB0000715, spectral sim. = 886, #1



deprotonated HMDB0000715, spectral sim. = 731, #2

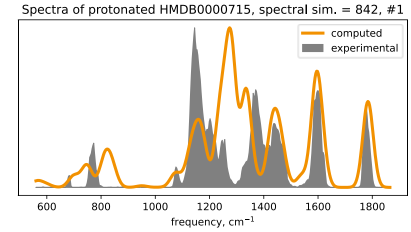


94 protonated HMDB0000715

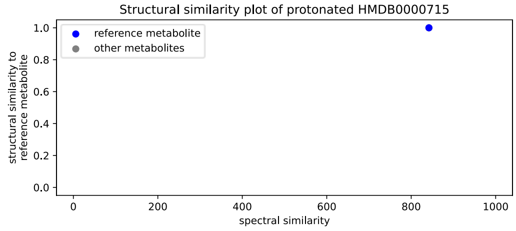


Kynurenic acid

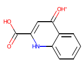
Spectra of protonated HMDB0000715, spectral sim. = 842, #1



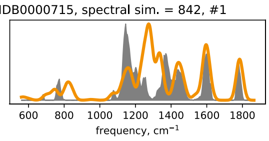
Structural similarity plot of protonated HMDB0000715



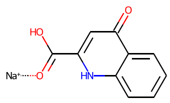
protonated HMDB0000715, spectral sim. = 842, #1



0.0 kJ/mol
Kynurenic acid

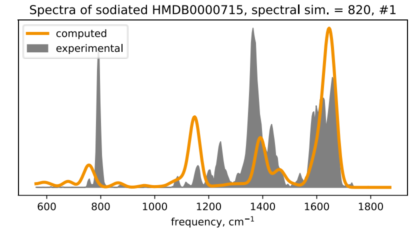


95 sodiated HMDB0000715

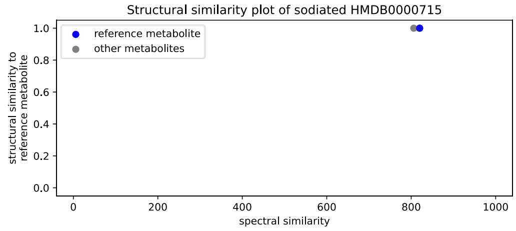


Kynurenic acid

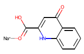
Spectra of sodiated HMDB0000715, spectral sim. = 820, #1



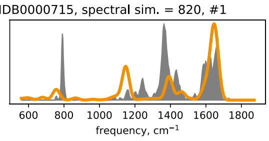
Structural similarity plot of sodiated HMDB0000715



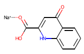
sodiated HMDB0000715, spectral sim. = 820, #1



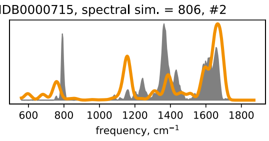
21.6 kJ/mol
Kynurenic acid



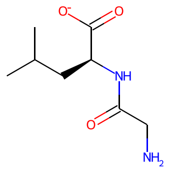
sodiated HMDB0000715, spectral sim. = 806, #2



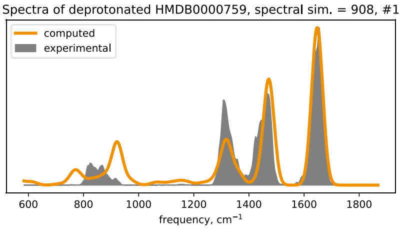
0.0 kJ/mol
Kynurenic acid



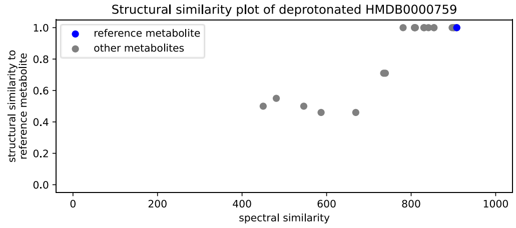
96 deprotonated HMDB0000759



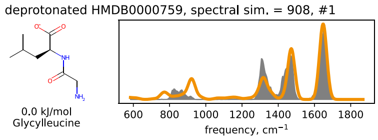
Spectra of deprotonated HMDB0000759, spectral sim. = 908, #1



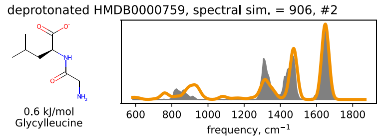
Structural similarity plot of deprotonated HMDB0000759



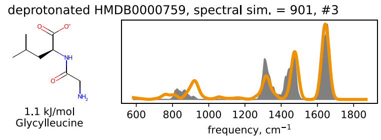
deprotonated HMDB0000759, spectral sim. = 908, #1



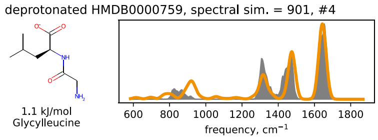
deprotonated HMDB0000759, spectral sim. = 906, #2



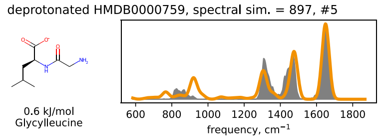
deprotonated HMDB0000759, spectral sim. = 901, #3



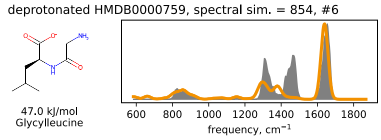
deprotonated HMDB0000759, spectral sim. = 901, #4



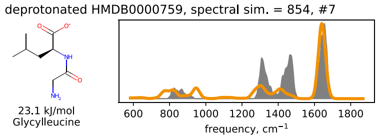
deprotonated HMDB0000759, spectral sim. = 897, #5



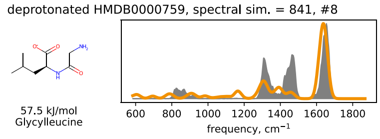
deprotonated HMDB0000759, spectral sim. = 854, #6



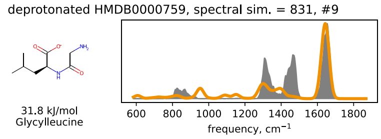
deprotonated HMDB0000759, spectral sim. = 854, #7



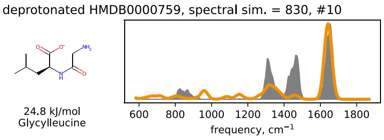
deprotonated HMDB0000759, spectral sim. = 841, #8



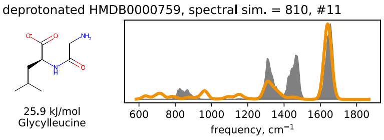
deprotonated HMDB0000759, spectral sim. = 831, #9



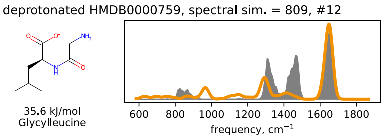
deprotonated HMDB0000759, spectral sim. = 830, #10



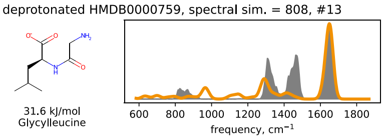
deprotonated HMDB0000759, spectral sim. = 810, #11



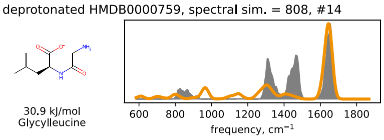
deprotonated HMDB0000759, spectral sim. = 809, #12



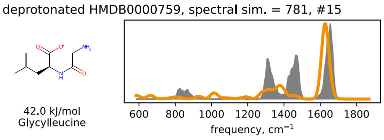
deprotonated HMDB0000759, spectral sim. = 808, #13



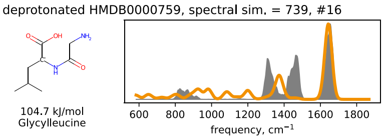
deprotonated HMDB0000759, spectral sim. = 808, #14



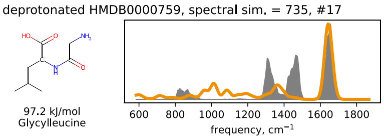
deprotonated HMDB0000759, spectral sim. = 781, #15



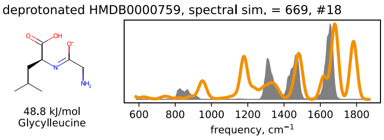
deprotonated HMDB0000759, spectral sim. = 739, #16



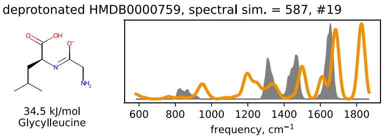
deprotonated HMDB0000759, spectral sim. = 735, #17



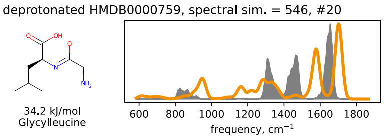
deprotonated HMDB0000759, spectral sim. = 669, #18



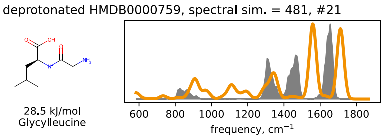
deprotonated HMDB0000759, spectral sim. = 587, #19



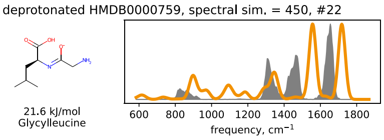
deprotonated HMDB0000759, spectral sim. = 546, #20



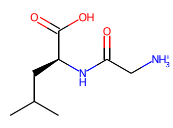
deprotonated HMDB0000759, spectral sim. = 481, #21



deprotonated HMDB0000759, spectral sim. = 450, #22

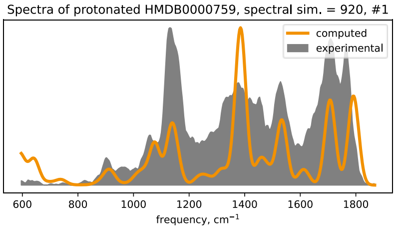


97 protonated HMDB0000759

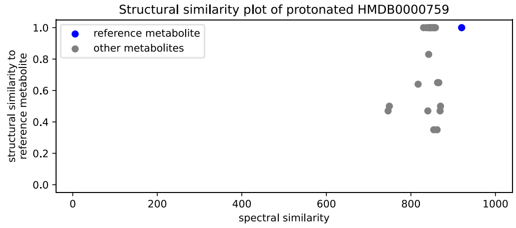


Glycylleucine

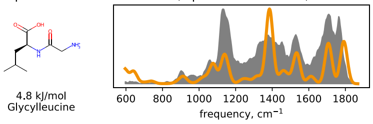
Spectra of protonated HMDB0000759, spectral sim. = 920, #1



Structural similarity plot of protonated HMDB0000759

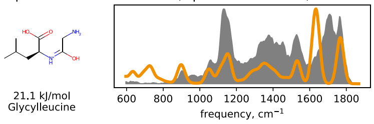


protonated HMDB0000759, spectral sim. = 920, #1



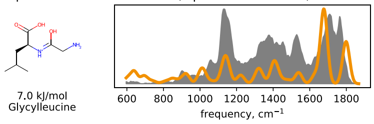
4.8 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 870, #2



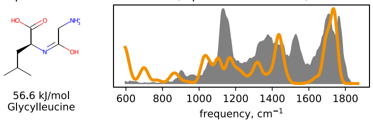
21.1 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 869, #3



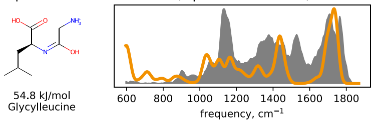
7.0 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 866, #4



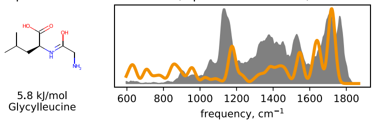
56.6 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 863, #5



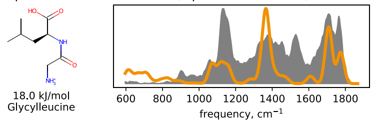
54.8 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 862, #6



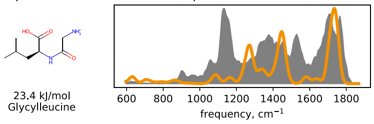
5.8 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 858, #7



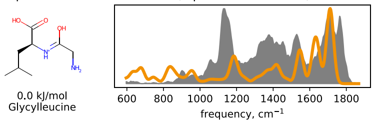
18.0 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 856, #8



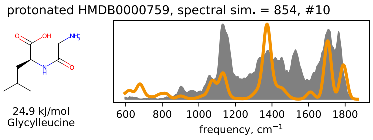
23.4 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 854, #9



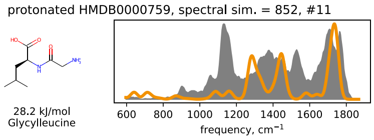
0.0 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 854, #10



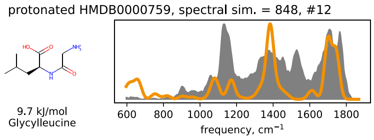
24.9 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 852, #11



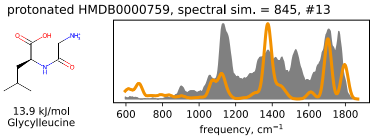
28.2 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 848, #12



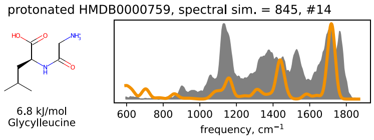
9.7 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 845, #13



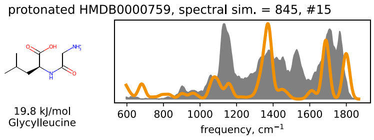
13.9 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 845, #14



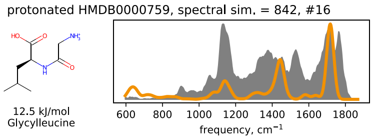
6.8 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 845, #15



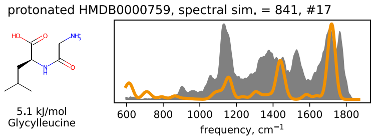
19.8 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 842, #16



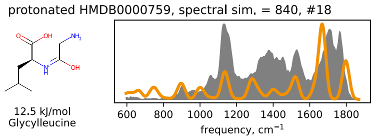
12.5 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 841, #17



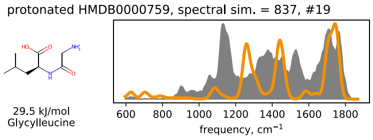
5.1 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 840, #18



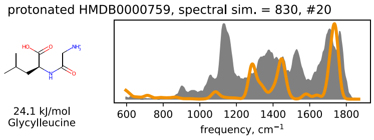
12.5 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 837, #19



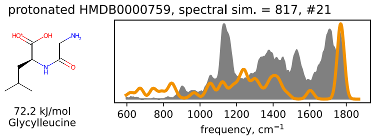
29.5 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 830, #20



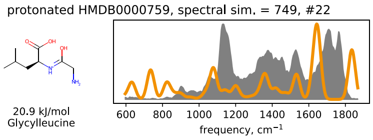
24.1 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 817, #21



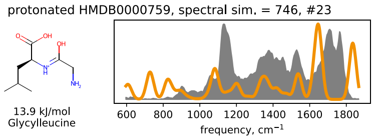
72.2 kJ/mol
Glycylleucine

protonated HMDB0000759, spectral sim. = 749, #22

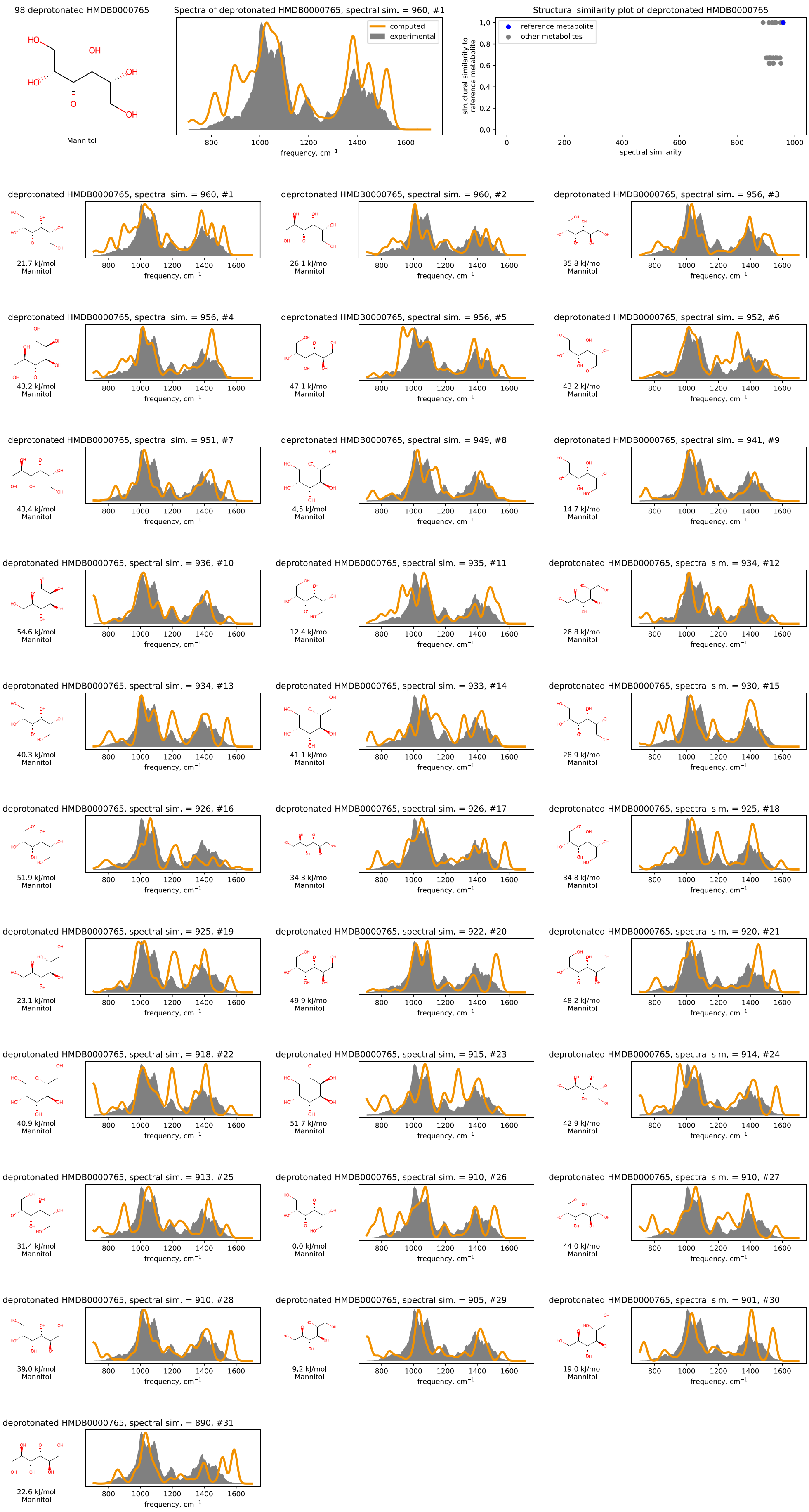


20.9 kJ/mol
Glycylleucine

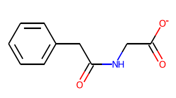
protonated HMDB0000759, spectral sim. = 746, #23



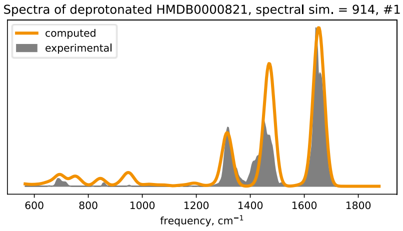
13.9 kJ/mol
Glycylleucine


98 deprotonated HMDB0000765
Mannitol
Spectra of deprotonated HMDB0000765, spectral sim. = 960, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0000765
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0000765, spectral sim. = 960, #1
21.7 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 960, #2
26.1 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 956, #3
35.8 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 956, #4
43.2 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 956, #5
47.1 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 952, #6
43.2 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 951, #7
43.4 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 949, #8
4.5 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 941, #9
14.7 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 936, #10
54.6 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 935, #11
12.4 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 934, #12
26.8 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 934, #13
40.3 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 933, #14
41.1 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 930, #15
28.9 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 926, #16
51.9 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 926, #17
34.3 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 925, #18
34.8 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 925, #19
23.1 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 922, #20
49.9 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 920, #21
48.2 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 918, #22
40.9 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 915, #23
51.7 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 914, #24
42.9 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 913, #25
31.4 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 910, #26
0.0 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 910, #27
44.0 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 910, #28
39.0 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 905, #29
9.2 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 901, #30
19.0 kJ/mol
Mannitol
deprotonated HMDB0000765, spectral sim. = 890, #31
22.6 kJ/mol
Mannitol

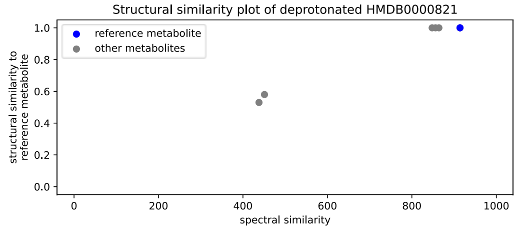
99 deprotonated HMDB0000821



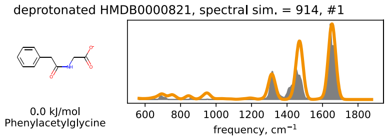
Spectra of deprotonated HMDB0000821, spectral sim. = 914, #1



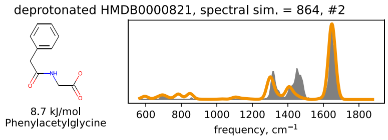
Structural similarity plot of deprotonated HMDB0000821



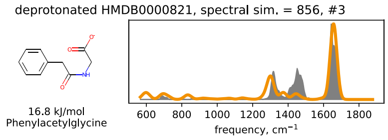
deprotonated HMDB0000821, spectral sim. = 914, #1



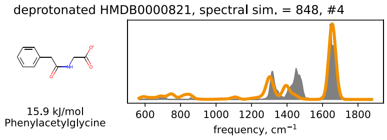
deprotonated HMDB0000821, spectral sim. = 864, #2



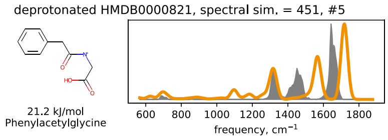
deprotonated HMDB0000821, spectral sim. = 856, #3



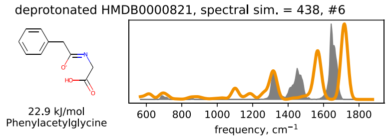
deprotonated HMDB0000821, spectral sim. = 848, #4



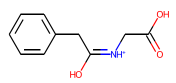
deprotonated HMDB0000821, spectral sim. = 451, #5



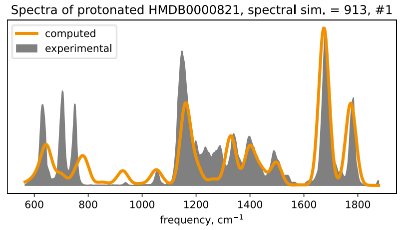
deprotonated HMDB0000821, spectral sim. = 438, #6



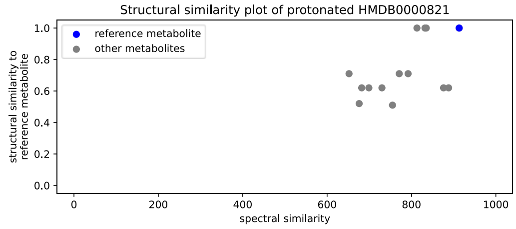
100 protonated HMDB0000821



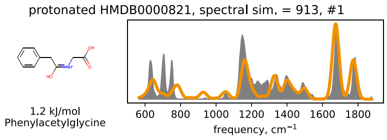
Spectra of protonated HMDB0000821, spectral sim. = 913, #1



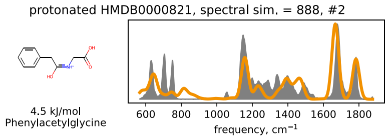
Structural similarity plot of protonated HMDB0000821



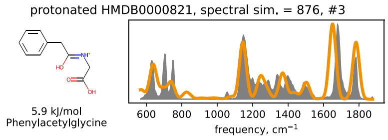
protonated HMDB0000821, spectral sim. = 913, #1



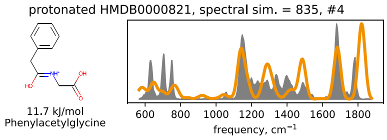
protonated HMDB0000821, spectral sim. = 888, #2



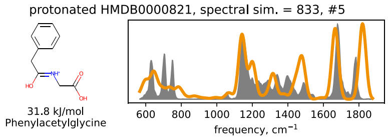
protonated HMDB0000821, spectral sim. = 876, #3



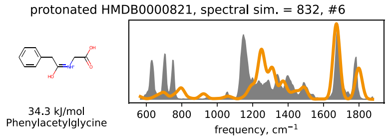
protonated HMDB0000821, spectral sim. = 835, #4



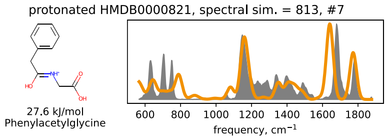
protonated HMDB0000821, spectral sim. = 833, #5



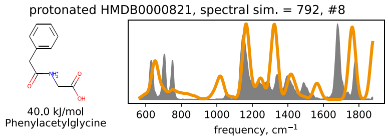
protonated HMDB0000821, spectral sim. = 832, #6



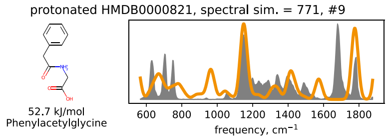
protonated HMDB0000821, spectral sim. = 813, #7



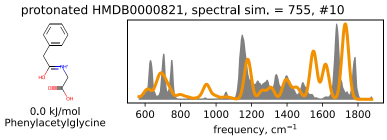
protonated HMDB0000821, spectral sim. = 792, #8



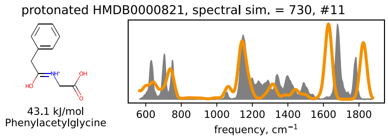
protonated HMDB0000821, spectral sim. = 771, #9



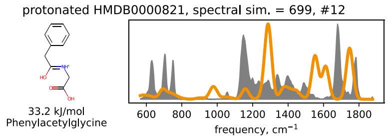
protonated HMDB0000821, spectral sim. = 755, #10



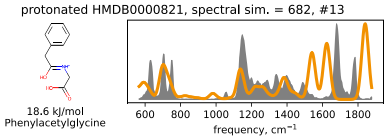
protonated HMDB0000821, spectral sim. = 730, #11



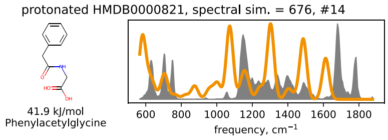
protonated HMDB0000821, spectral sim. = 699, #12



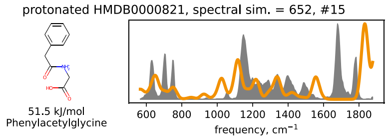
protonated HMDB0000821, spectral sim. = 682, #13



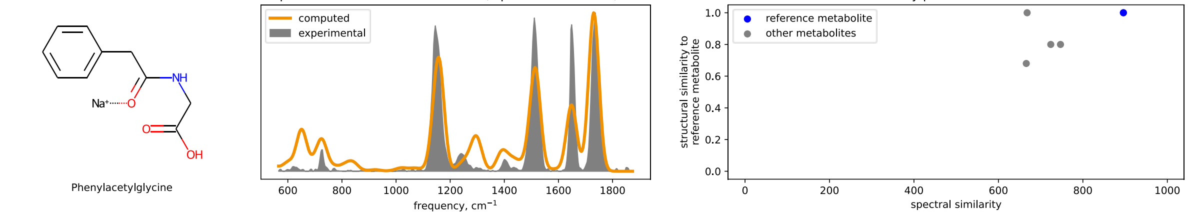
protonated HMDB0000821, spectral sim. = 676, #14



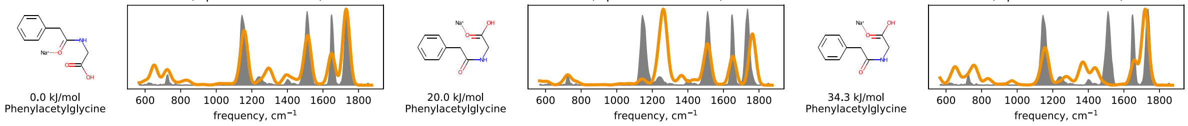
protonated HMDB0000821, spectral sim. = 652, #15



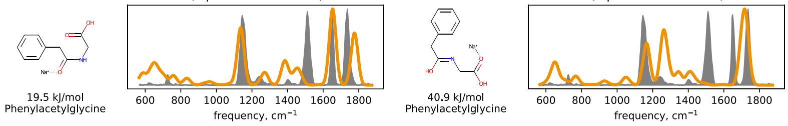
101 sodiated HMDB0000821 | Spectra of sodiated HMDB0000821, spectral sim. = 896, #1 | Structural similarity plot of sodiated HMDB0000821



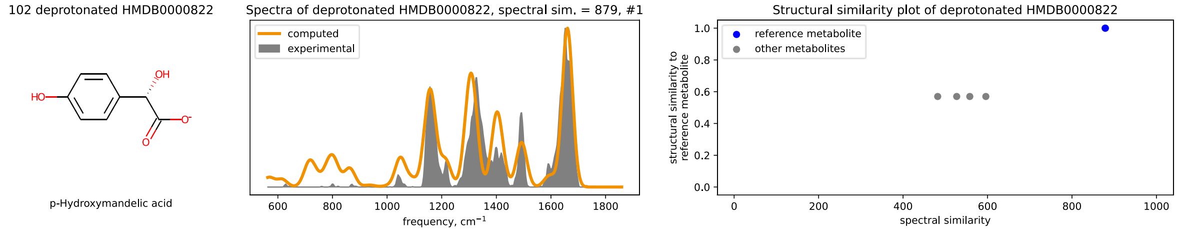
sodiated HMDB0000821, spectral sim. = 896, #1 | sodiated HMDB0000821, spectral sim. = 747, #2 | sodiated HMDB0000821, spectral sim. = 724, #3



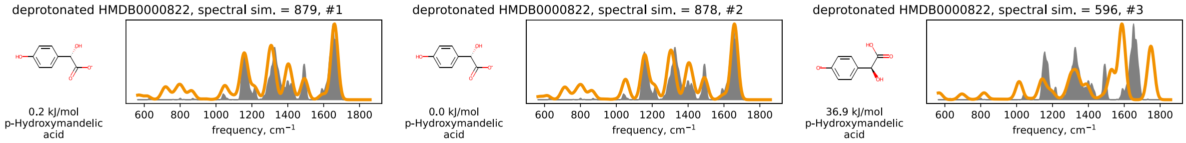
sodiated HMDB0000821, spectral sim. = 668, #4 | sodiated HMDB0000821, spectral sim. = 666, #5



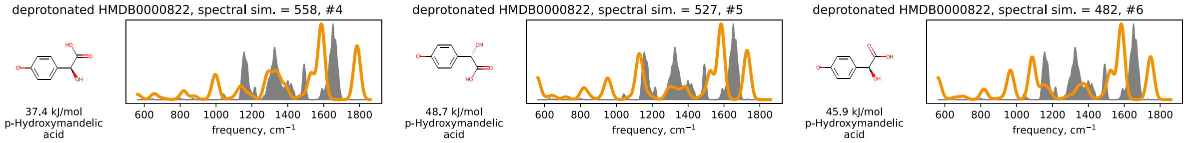
102 deprotonated HMDB0000822 | Spectra of deprotonated HMDB0000822, spectral sim. = 879, #1 | Structural similarity plot of deprotonated HMDB0000822



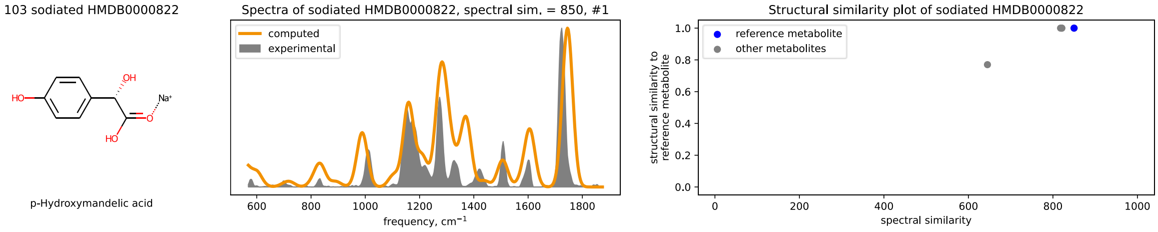
deprotonated HMDB0000822, spectral sim. = 879, #1 | deprotonated HMDB0000822, spectral sim. = 878, #2 | deprotonated HMDB0000822, spectral sim. = 596, #3



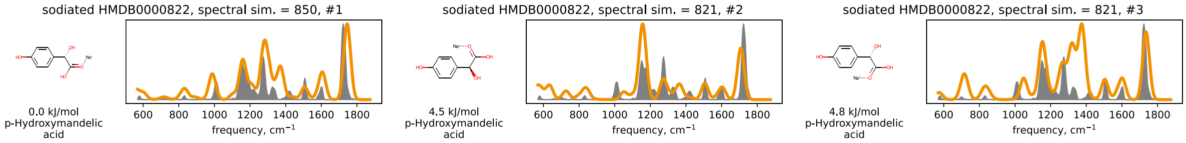
deprotonated HMDB0000822, spectral sim. = 558, #4 | deprotonated HMDB0000822, spectral sim. = 527, #5 | deprotonated HMDB0000822, spectral sim. = 482, #6



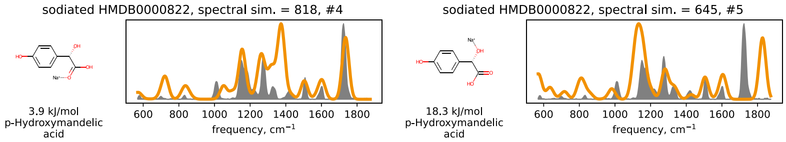
103 sodiated HMDB0000822 | Spectra of sodiated HMDB0000822, spectral sim. = 850, #1 | Structural similarity plot of sodiated HMDB0000822



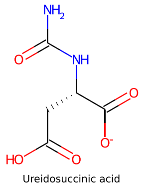
sodiated HMDB0000822, spectral sim. = 850, #1 | sodiated HMDB0000822, spectral sim. = 821, #2 | sodiated HMDB0000822, spectral sim. = 821, #3



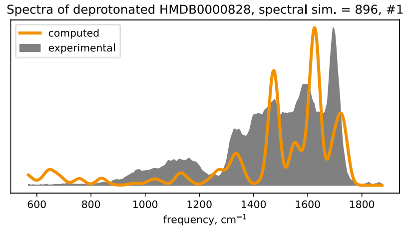
sodiated HMDB0000822, spectral sim. = 818, #4 | sodiated HMDB0000822, spectral sim. = 645, #5



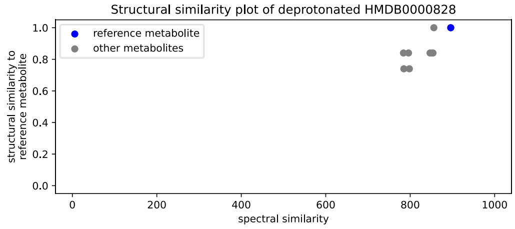
104 deprotonated HMDB0000828



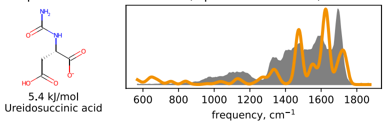
Spectra of deprotonated HMDB0000828, spectral sim. = 896, #1



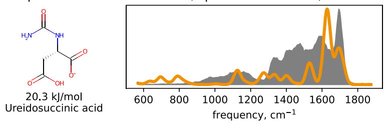
Structural similarity plot of deprotonated HMDB0000828



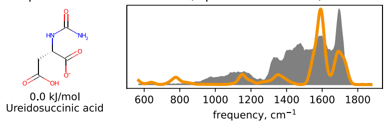
deprotonated HMDB0000828, spectral sim. = 896, #1



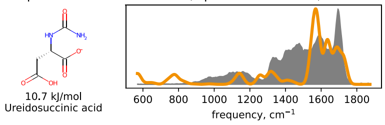
deprotonated HMDB0000828, spectral sim. = 856, #2



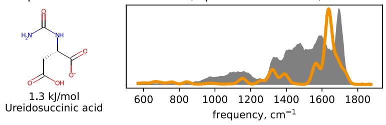
deprotonated HMDB0000828, spectral sim. = 854, #3



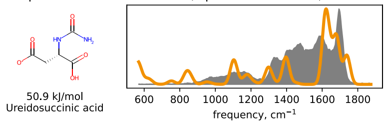
deprotonated HMDB0000828, spectral sim. = 851, #4



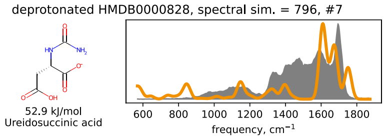
deprotonated HMDB0000828, spectral sim. = 847, #5



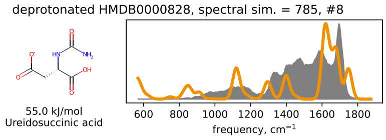
deprotonated HMDB0000828, spectral sim. = 798, #6



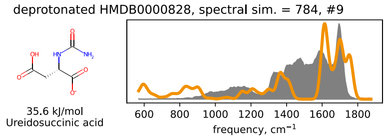
deprotonated HMDB0000828, spectral sim. = 796, #7

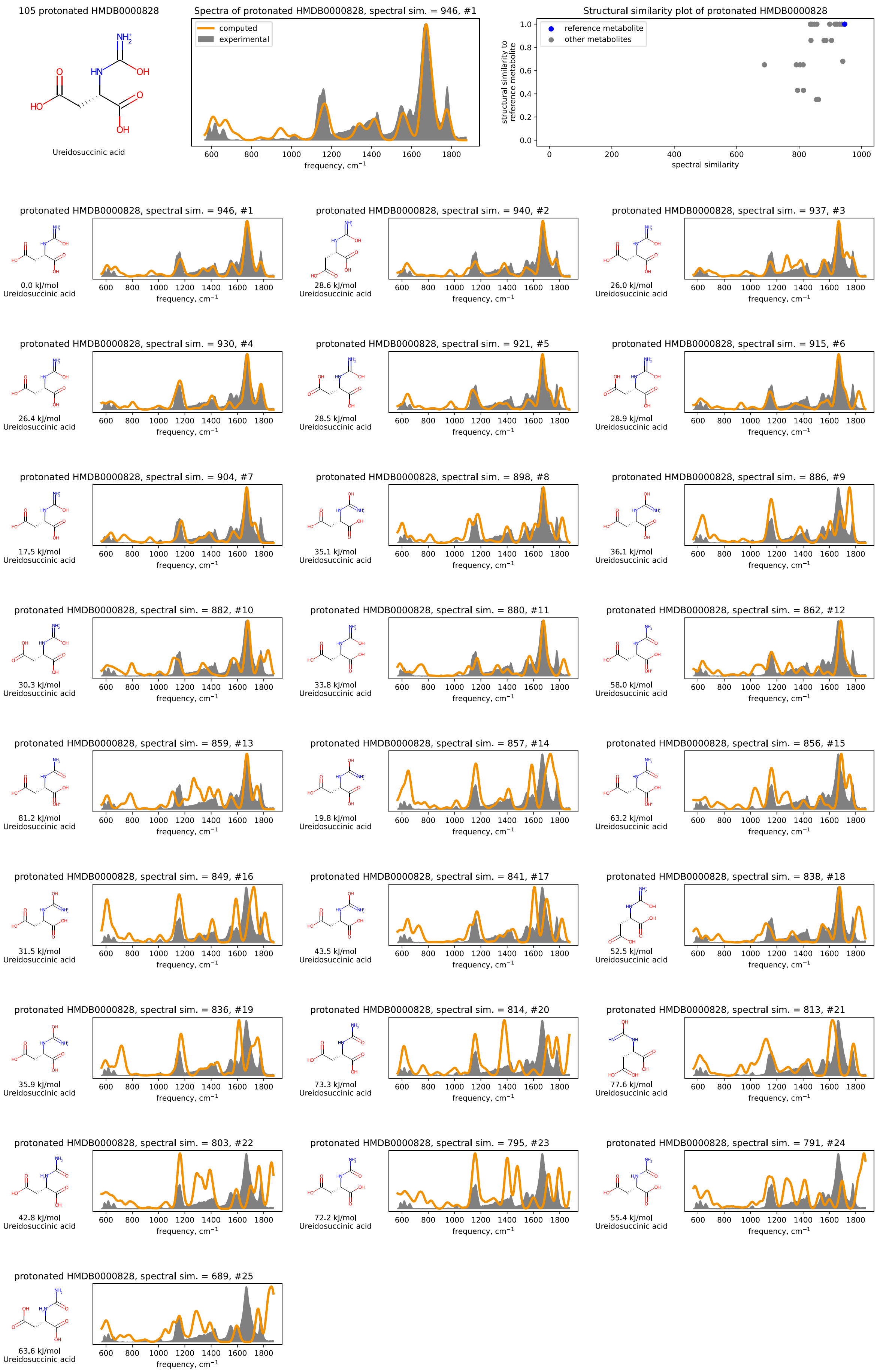


deprotonated HMDB0000828, spectral sim. = 785, #8



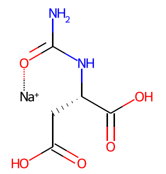
deprotonated HMDB0000828, spectral sim. = 784, #9





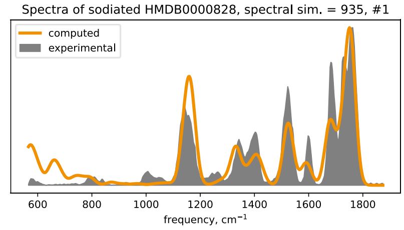
105 protonated HMDB0000828
Ureidosuccinic acid
Spectra of protonated HMDB0000828, spectral sim. = 946, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of protonated HMDB0000828
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
protonated HMDB0000828, spectral sim. = 946, #1
0.0 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 940, #2
28.6 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 937, #3
26.0 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 930, #4
26.4 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 921, #5
28.5 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 915, #6
28.9 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 904, #7
17.5 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 898, #8
35.1 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 886, #9
36.1 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 882, #10
30.3 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 880, #11
33.8 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 862, #12
58.0 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 859, #13
81.2 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 857, #14
19.8 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 856, #15
63.2 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 849, #16
31.5 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 841, #17
43.5 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 838, #18
52.5 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 836, #19
35.9 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 814, #20
73.3 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 813, #21
77.6 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 803, #22
42.8 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 795, #23
72.2 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 791, #24
55.4 kJ/mol
Ureidosuccinic acid
protonated HMDB0000828, spectral sim. = 689, #25
63.6 kJ/mol
Ureidosuccinic acid

106 sodiated HMDB0000828

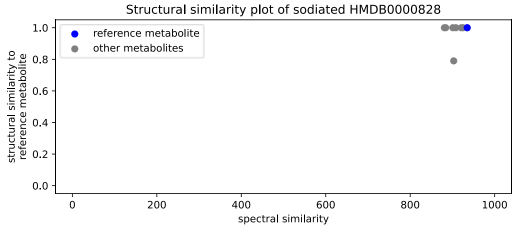


Ureidosuccinic acid

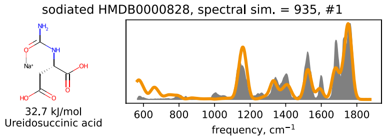
Spectra of sodiated HMDB0000828, spectral sim. = 935, #1



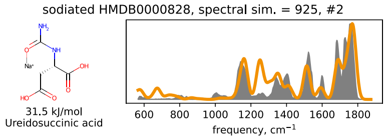
Structural similarity plot of sodiated HMDB0000828



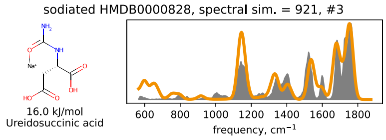
sodiated HMDB0000828, spectral sim. = 935, #1



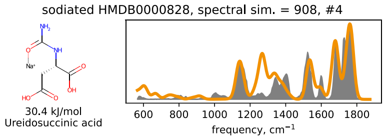
sodiated HMDB0000828, spectral sim. = 925, #2



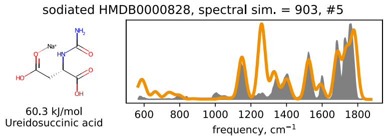
sodiated HMDB0000828, spectral sim. = 921, #3



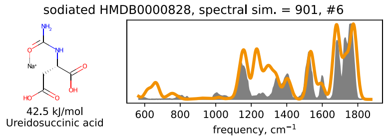
sodiated HMDB0000828, spectral sim. = 908, #4



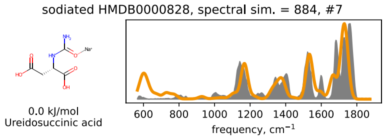
sodiated HMDB0000828, spectral sim. = 903, #5



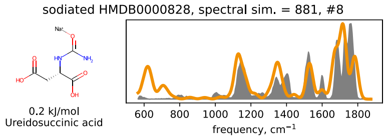
sodiated HMDB0000828, spectral sim. = 901, #6



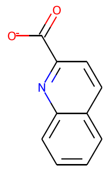
sodiated HMDB0000828, spectral sim. = 884, #7



sodiated HMDB0000828, spectral sim. = 881, #8

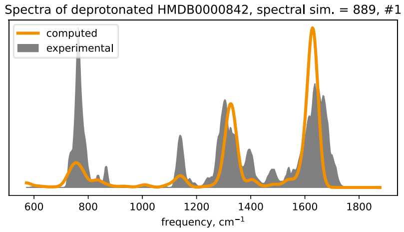


107 deprotonated HMDB0000842

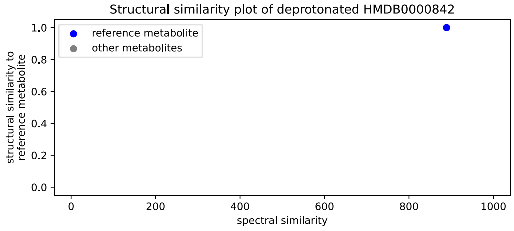


Quinaldic acid

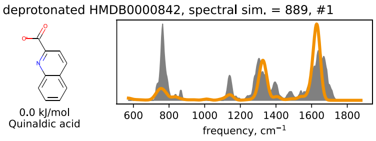
Spectra of deprotonated HMDB0000842, spectral sim. = 889, #1



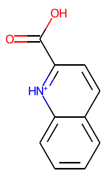
Structural similarity plot of deprotonated HMDB0000842



deprotonated HMDB0000842, spectral sim. = 889, #1

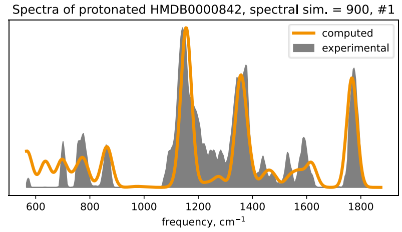


108 protonated HMDB0000842

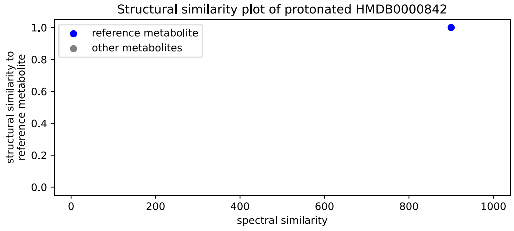


Quinaldic acid

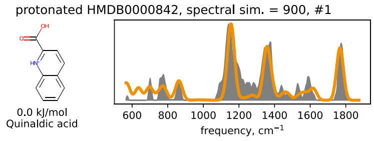
Spectra of protonated HMDB0000842, spectral sim. = 900, #1



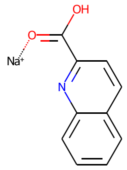
Structural similarity plot of protonated HMDB0000842



protonated HMDB0000842, spectral sim. = 900, #1

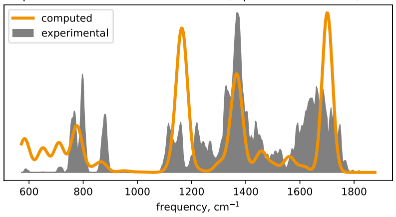


109 sodiated HMDB0000842

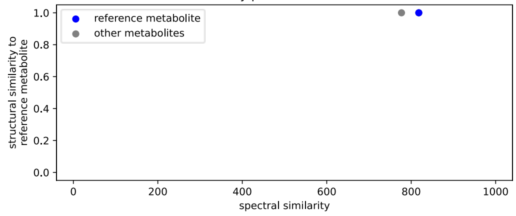


Quinaldic acid

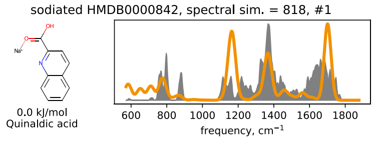
Spectra of sodiated HMDB0000842, spectral sim. = 818, #1



Structural similarity plot of sodiated HMDB0000842

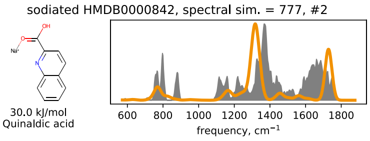


sodiated HMDB0000842, spectral sim. = 818, #1



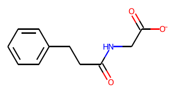
0.0 kJ/mol
Quinaldic acid

sodiated HMDB0000842, spectral sim. = 777, #2



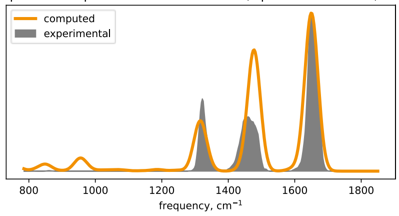
30.0 kJ/mol
Quinaldic acid

110 deprotonated HMDB0000860

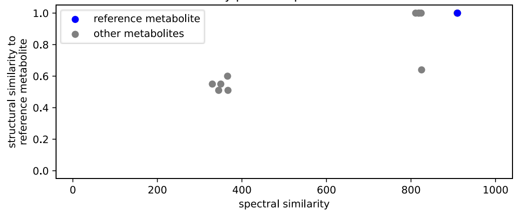


Phenylpropionylglycine

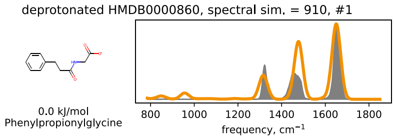
Spectra of deprotonated HMDB0000860, spectral sim. = 910, #1



Structural similarity plot of deprotonated HMDB0000860

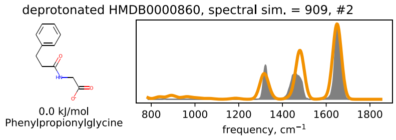


deprotonated HMDB0000860, spectral sim. = 910, #1



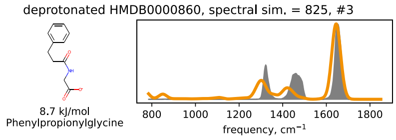
0.0 kJ/mol
Phenylpropionylglycine

deprotonated HMDB0000860, spectral sim. = 909, #2



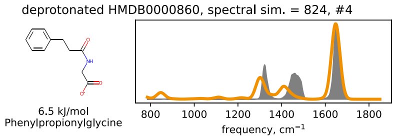
0.0 kJ/mol
Phenylpropionylglycine

deprotonated HMDB0000860, spectral sim. = 825, #3



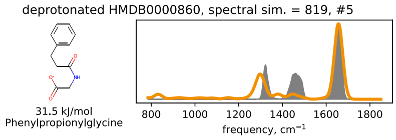
8.7 kJ/mol
Phenylpropionylglycine

deprotonated HMDB0000860, spectral sim. = 824, #4



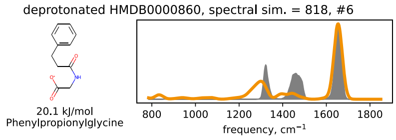
6.5 kJ/mol
Phenylpropionylglycine

deprotonated HMDB0000860, spectral sim. = 819, #5



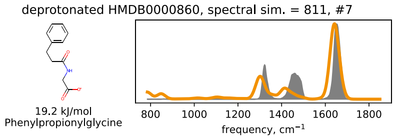
31.5 kJ/mol
Phenylpropionylglycine

deprotonated HMDB0000860, spectral sim. = 818, #6



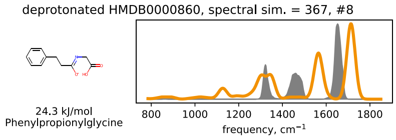
20.1 kJ/mol
Phenylpropionylglycine

deprotonated HMDB0000860, spectral sim. = 811, #7



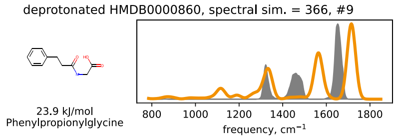
19.2 kJ/mol
Phenylpropionylglycine

deprotonated HMDB0000860, spectral sim. = 367, #8



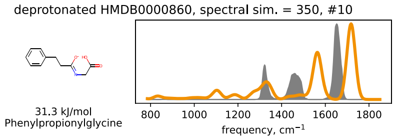
24.3 kJ/mol
Phenylpropionylglycine

deprotonated HMDB0000860, spectral sim. = 366, #9



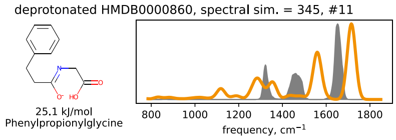
23.9 kJ/mol
Phenylpropionylglycine

deprotonated HMDB0000860, spectral sim. = 350, #10



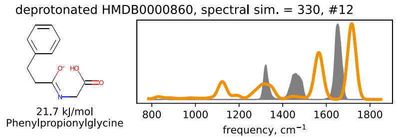
31.3 kJ/mol
Phenylpropionylglycine

deprotonated HMDB0000860, spectral sim. = 345, #11



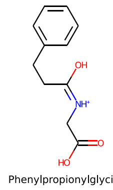
25.1 kJ/mol
Phenylpropionylglycine

deprotonated HMDB0000860, spectral sim. = 330, #12

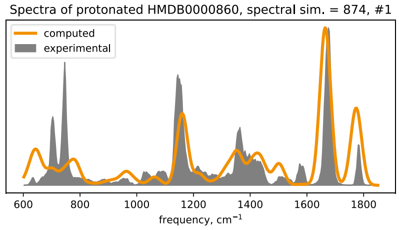


21.7 kJ/mol
Phenylpropionylglycine

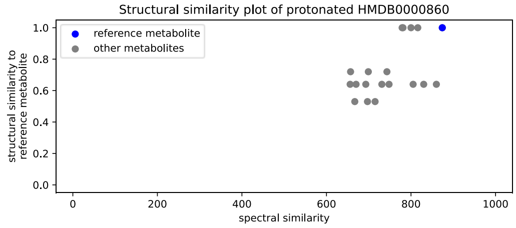
111 protonated HMDB0000860



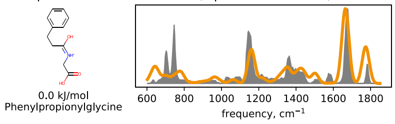
Spectra of protonated HMDB0000860, spectral sim. = 874, #1



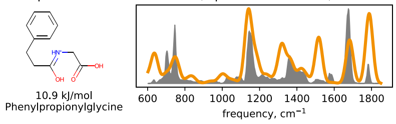
Structural similarity plot of protonated HMDB0000860



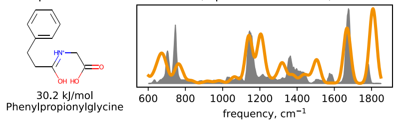
protonated HMDB0000860, spectral sim. = 874, #1



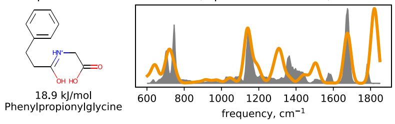
protonated HMDB0000860, spectral sim. = 860, #2



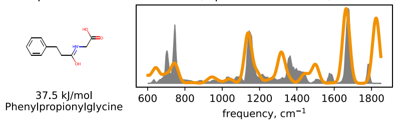
protonated HMDB0000860, spectral sim. = 830, #3



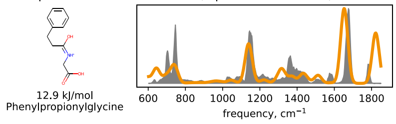
protonated HMDB0000860, spectral sim. = 816, #4



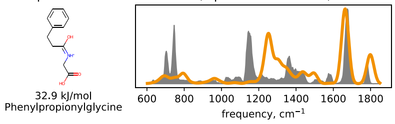
protonated HMDB0000860, spectral sim. = 805, #5



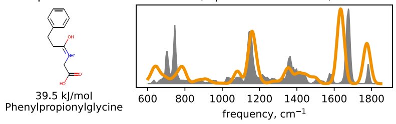
protonated HMDB0000860, spectral sim. = 800, #6



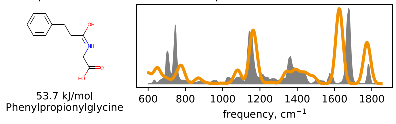
protonated HMDB0000860, spectral sim. = 781, #7



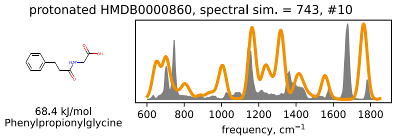
protonated HMDB0000860, spectral sim. = 779, #8



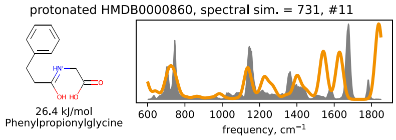
protonated HMDB0000860, spectral sim. = 748, #9



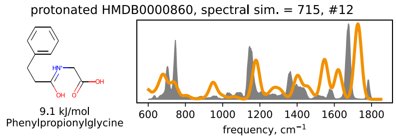
protonated HMDB0000860, spectral sim. = 743, #10



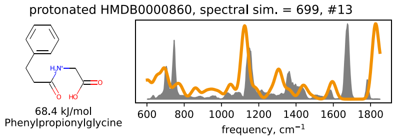
protonated HMDB0000860, spectral sim. = 731, #11



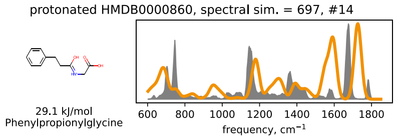
protonated HMDB0000860, spectral sim. = 715, #12



protonated HMDB0000860, spectral sim. = 699, #13



protonated HMDB0000860, spectral sim. = 697, #14



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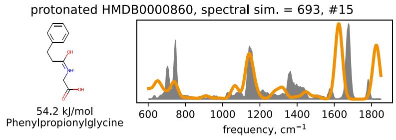

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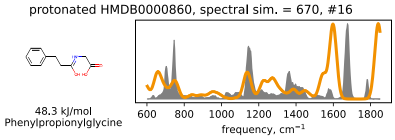
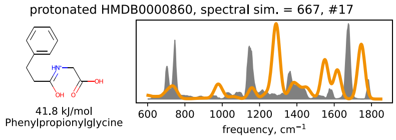
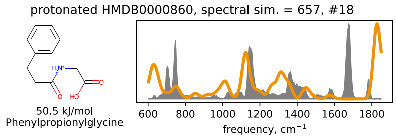


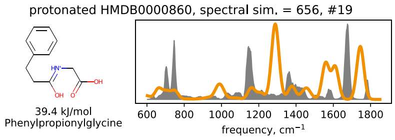
protonated HMDB0000860, spectral sim. = 667, #17



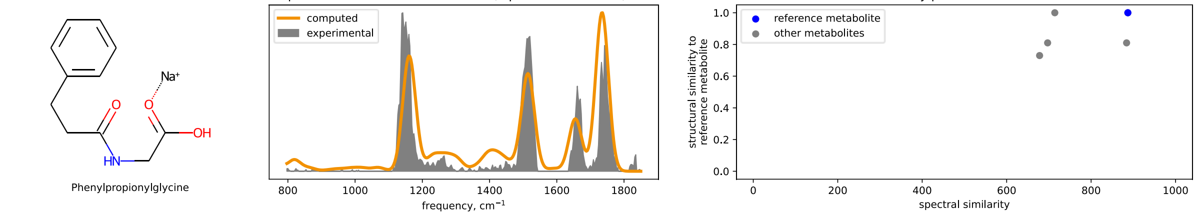
protonated HMDB0000860, spectral sim. = 657, #18



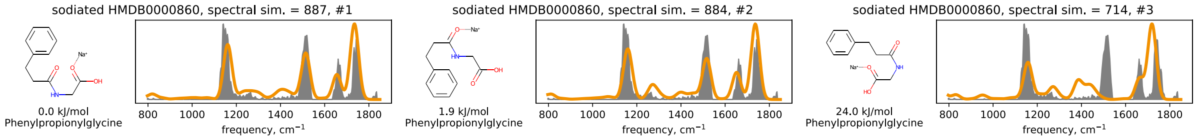
protonated HMDB0000860, spectral sim. = 656, #19



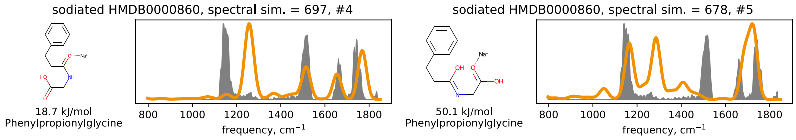
112 sodiated HMDB0000860 | Spectra of sodiated HMDB0000860, spectral sim. = 887, #1 | Structural similarity plot of sodiated HMDB0000860



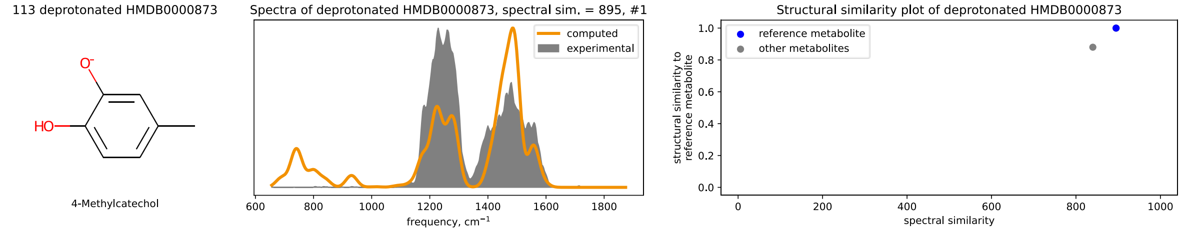
sodiated HMDB0000860, spectral sim. = 887, #1 | sodiated HMDB0000860, spectral sim. = 884, #2 | sodiated HMDB0000860, spectral sim. = 714, #3



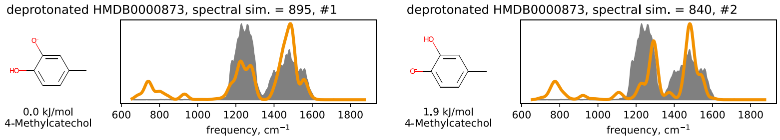
sodiated HMDB0000860, spectral sim. = 697, #4 | sodiated HMDB0000860, spectral sim. = 678, #5



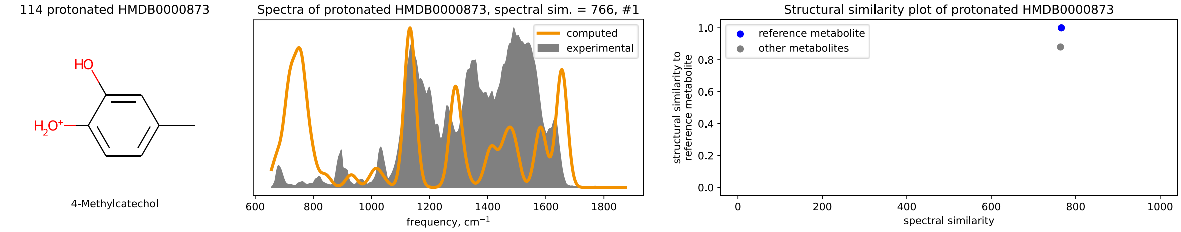
113 deprotonated HMDB0000873 | Spectra of deprotonated HMDB0000873, spectral sim. = 895, #1 | Structural similarity plot of deprotonated HMDB0000873



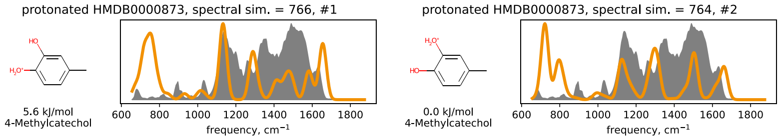
deprotonated HMDB0000873, spectral sim. = 895, #1 | deprotonated HMDB0000873, spectral sim. = 840, #2



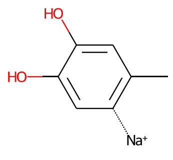
114 protonated HMDB0000873 | Spectra of protonated HMDB0000873, spectral sim. = 766, #1 | Structural similarity plot of protonated HMDB0000873



protonated HMDB0000873, spectral sim. = 766, #1 | protonated HMDB0000873, spectral sim. = 764, #2

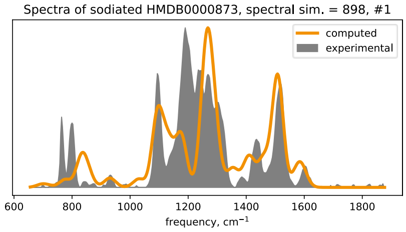


115 sodiated HMDB0000873

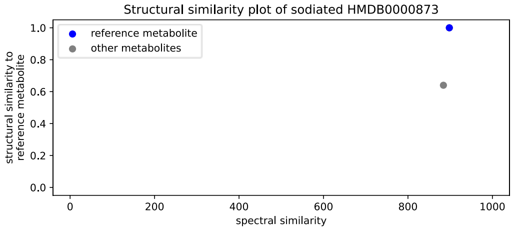


4-Methylcatechol

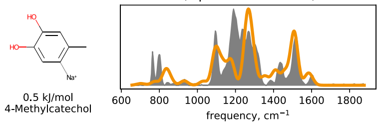
Spectra of sodiated HMDB0000873, spectral sim. = 898, #1



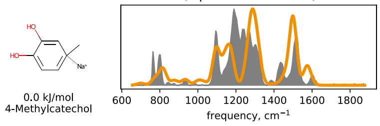
Structural similarity plot of sodiated HMDB0000873



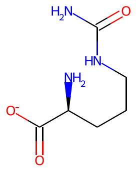
sodiated HMDB0000873, spectral sim. = 898, #1



sodiated HMDB0000873, spectral sim. = 884, #2

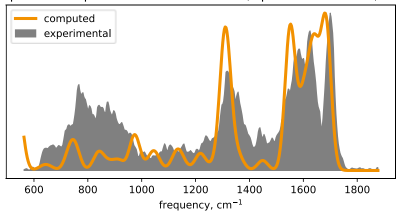


116 deprotonated HMDB0000904

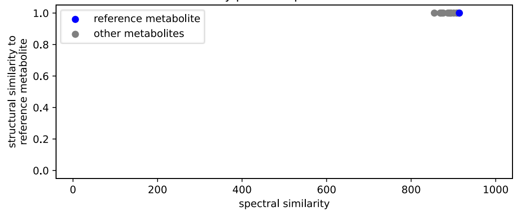


Citrulline

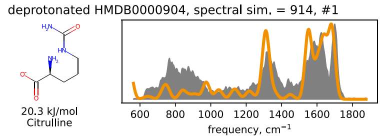
Spectra of deprotonated HMDB0000904, spectral sim. = 914, #1



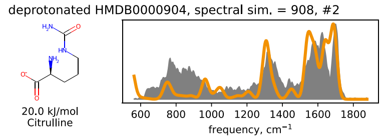
Structural similarity plot of deprotonated HMDB0000904



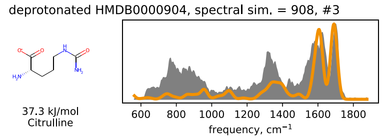
deprotonated HMDB0000904, spectral sim. = 914, #1



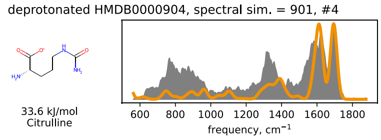
deprotonated HMDB0000904, spectral sim. = 908, #2



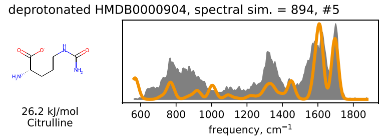
deprotonated HMDB0000904, spectral sim. = 908, #3



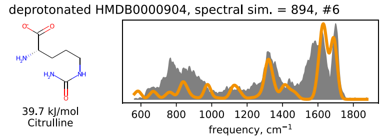
deprotonated HMDB0000904, spectral sim. = 901, #4



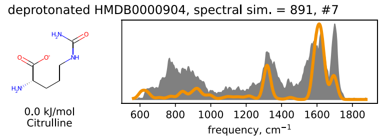
deprotonated HMDB0000904, spectral sim. = 894, #5



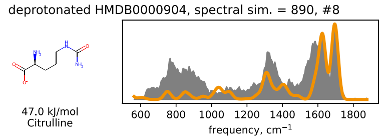
deprotonated HMDB0000904, spectral sim. = 894, #6



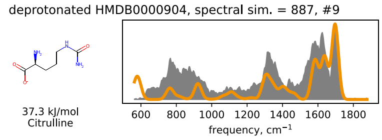
deprotonated HMDB0000904, spectral sim. = 891, #7



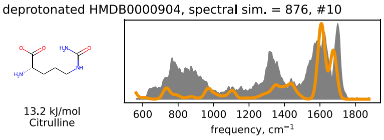
deprotonated HMDB0000904, spectral sim. = 890, #8



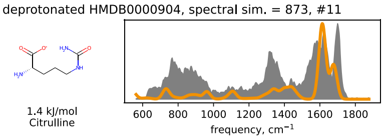
deprotonated HMDB0000904, spectral sim. = 887, #9



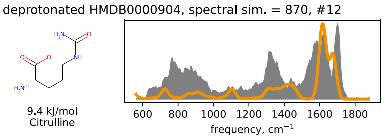
deprotonated HMDB0000904, spectral sim. = 876, #10



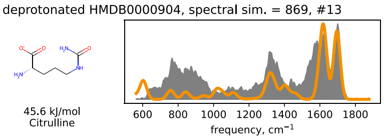
deprotonated HMDB0000904, spectral sim. = 873, #11



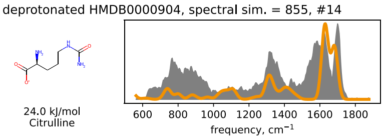
deprotonated HMDB0000904, spectral sim. = 870, #12



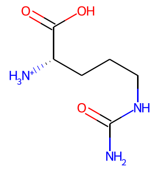
deprotonated HMDB0000904, spectral sim. = 869, #13



deprotonated HMDB0000904, spectral sim. = 855, #14

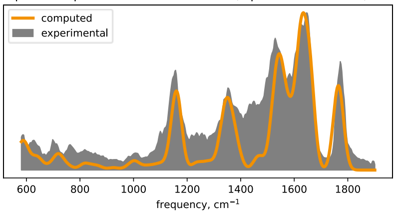


117 protonated HMDB0000904

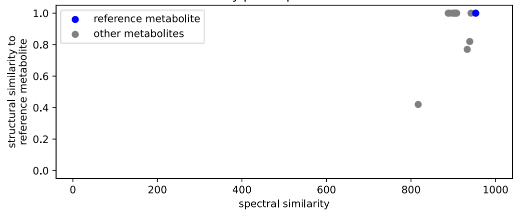


Citrulline

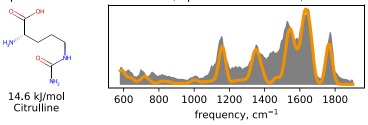
Spectra of protonated HMDB0000904, spectral sim. = 953, #1



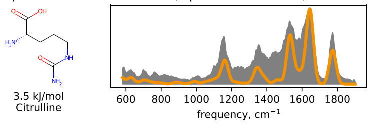
Structural similarity plot of protonated HMDB0000904



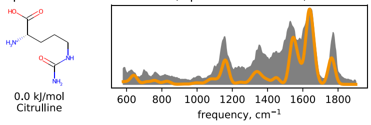
protonated HMDB0000904, spectral sim. = 953, #1



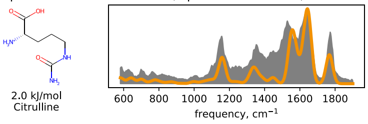
protonated HMDB0000904, spectral sim. = 942, #2



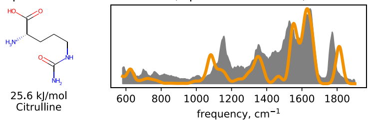
protonated HMDB0000904, spectral sim. = 939, #3



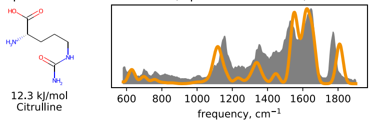
protonated HMDB0000904, spectral sim. = 933, #4



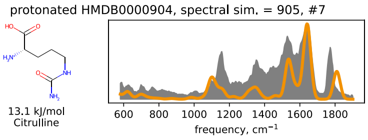
protonated HMDB0000904, spectral sim. = 908, #5



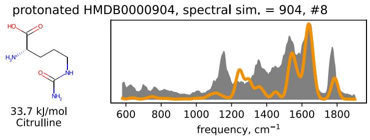
protonated HMDB0000904, spectral sim. = 907, #6



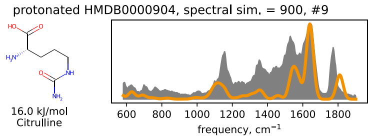
protonated HMDB0000904, spectral sim. = 905, #7



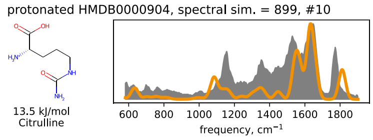
protonated HMDB0000904, spectral sim. = 904, #8



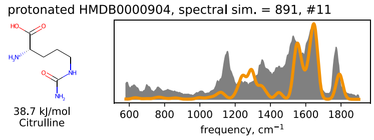
protonated HMDB0000904, spectral sim. = 900, #9



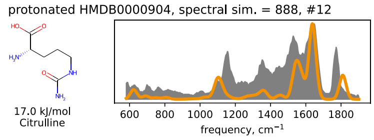
protonated HMDB0000904, spectral sim. = 899, #10



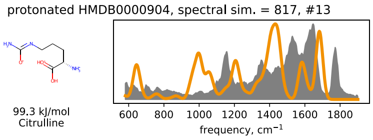
protonated HMDB0000904, spectral sim. = 891, #11



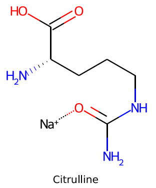
protonated HMDB0000904, spectral sim. = 888, #12



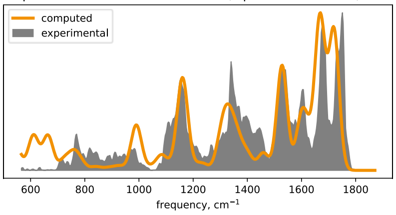
protonated HMDB0000904, spectral sim. = 817, #13



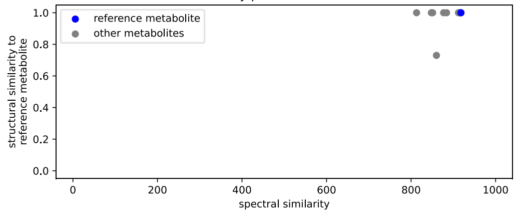
118 sodiated HMDB0000904



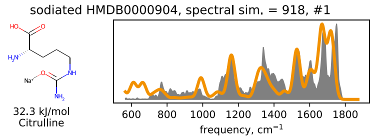
Spectra of sodiated HMDB0000904, spectral sim. = 918, #1



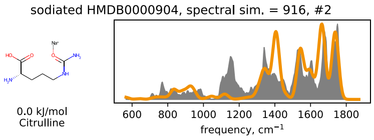
Structural similarity plot of sodiated HMDB0000904



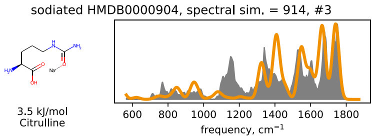
sodiated HMDB0000904, spectral sim. = 918, #1



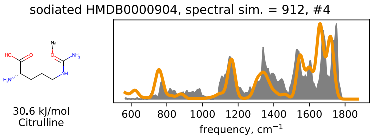
sodiated HMDB0000904, spectral sim. = 916, #2



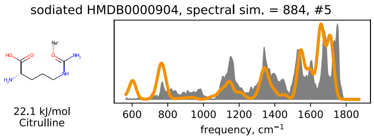
sodiated HMDB0000904, spectral sim. = 914, #3



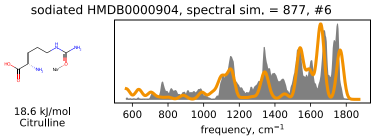
sodiated HMDB0000904, spectral sim. = 912, #4



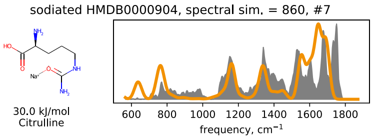
sodiated HMDB0000904, spectral sim. = 884, #5



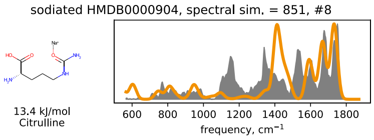
sodiated HMDB0000904, spectral sim. = 877, #6



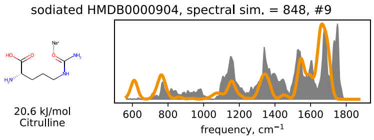
sodiated HMDB0000904, spectral sim. = 860, #7



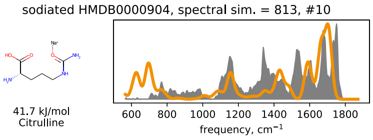
sodiated HMDB0000904, spectral sim. = 851, #8

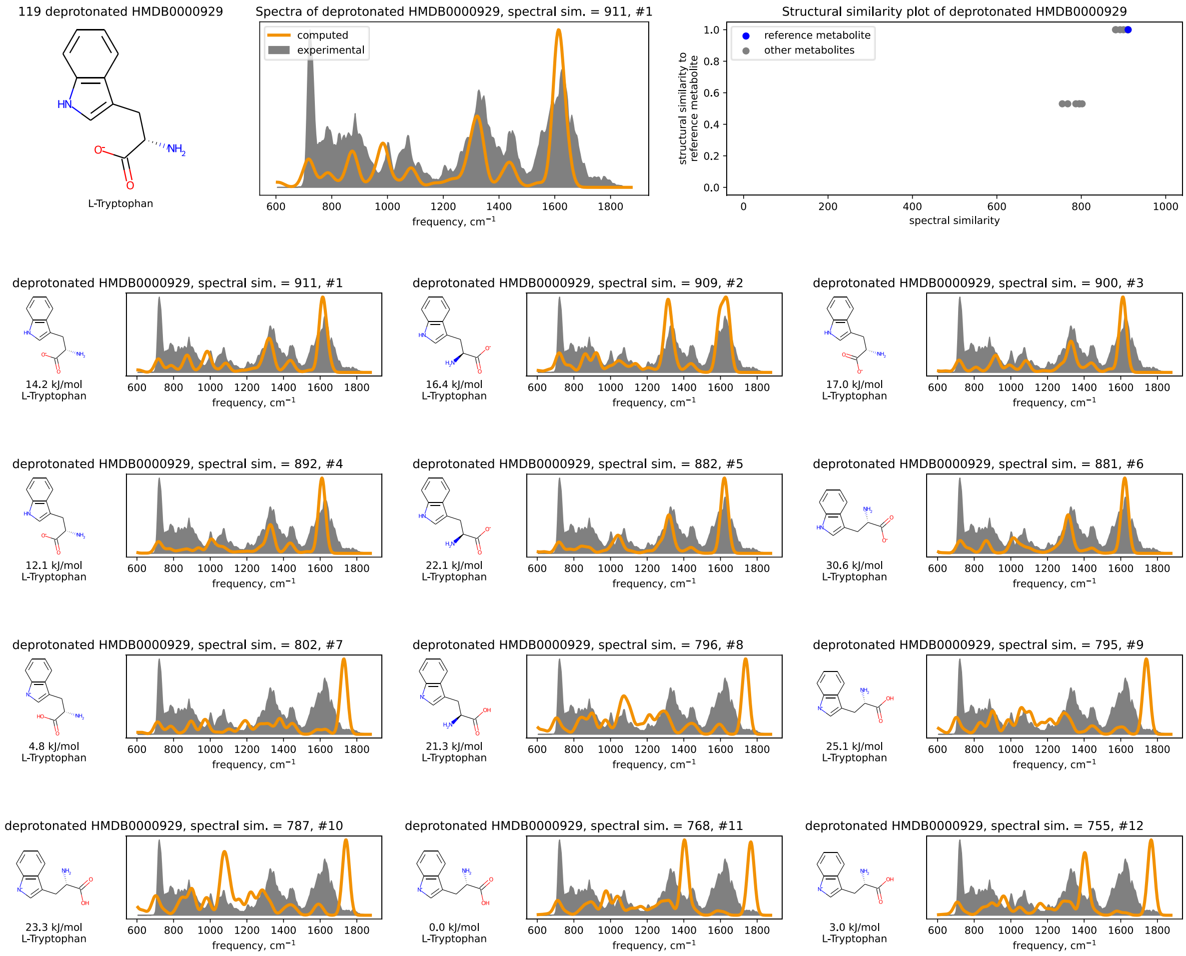


sodiated HMDB0000904, spectral sim. = 848, #9

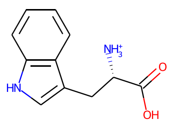


sodiated HMDB0000904, spectral sim. = 813, #10

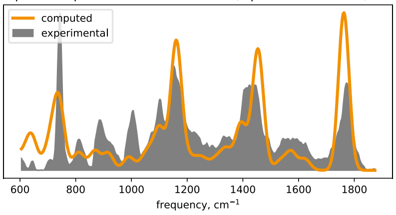



119 deprotonated HMDB0000929
L-Tryptophan
Spectra of deprotonated HMDB0000929, spectral sim. = 911, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0000929
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0000929, spectral sim. = 911, #1
14.2 kJ/mol
L-Tryptophan
deprotonated HMDB0000929, spectral sim. = 909, #2
16.4 kJ/mol
L-Tryptophan
deprotonated HMDB0000929, spectral sim. = 900, #3
17.0 kJ/mol
L-Tryptophan
deprotonated HMDB0000929, spectral sim. = 892, #4
12.1 kJ/mol
L-Tryptophan
deprotonated HMDB0000929, spectral sim. = 882, #5
22.1 kJ/mol
L-Tryptophan
deprotonated HMDB0000929, spectral sim. = 881, #6
30.6 kJ/mol
L-Tryptophan
deprotonated HMDB0000929, spectral sim. = 802, #7
4.8 kJ/mol
L-Tryptophan
deprotonated HMDB0000929, spectral sim. = 796, #8
21.3 kJ/mol
L-Tryptophan
deprotonated HMDB0000929, spectral sim. = 795, #9
25.1 kJ/mol
L-Tryptophan
deprotonated HMDB0000929, spectral sim. = 787, #10
23.3 kJ/mol
L-Tryptophan
deprotonated HMDB0000929, spectral sim. = 768, #11
0.0 kJ/mol
L-Tryptophan
deprotonated HMDB0000929, spectral sim. = 755, #12
3.0 kJ/mol
L-Tryptophan
frequency, cm^{-1}

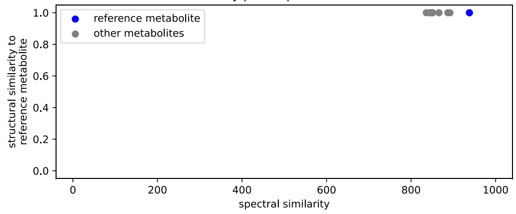
120 protonated HMDB0000929


L-Tryptophan

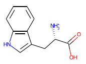
Spectra of protonated HMDB0000929, spectral sim. = 938, #1

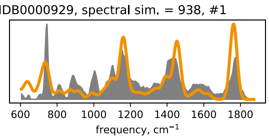


Structural similarity plot of protonated HMDB0000929

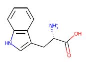


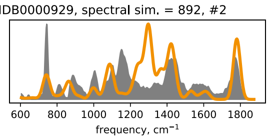
protonated HMDB0000929, spectral sim. = 938, #1


0.0 kJ/mol
L-Tryptophan

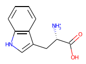


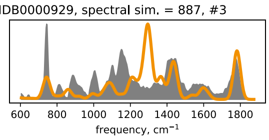
protonated HMDB0000929, spectral sim. = 892, #2


37.6 kJ/mol
L-Tryptophan

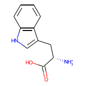


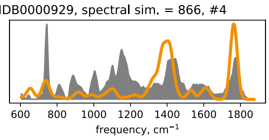
protonated HMDB0000929, spectral sim. = 887, #3


37.7 kJ/mol
L-Tryptophan

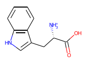


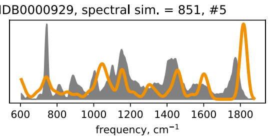
protonated HMDB0000929, spectral sim. = 866, #4


40.6 kJ/mol
L-Tryptophan

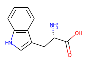


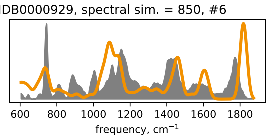
protonated HMDB0000929, spectral sim. = 851, #5


13.2 kJ/mol
L-Tryptophan

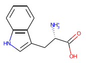


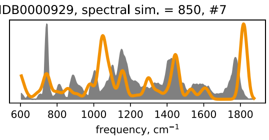
protonated HMDB0000929, spectral sim. = 850, #6


10.2 kJ/mol
L-Tryptophan

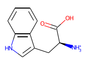


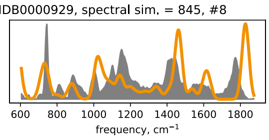
protonated HMDB0000929, spectral sim. = 850, #7


14.4 kJ/mol
L-Tryptophan

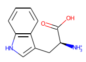


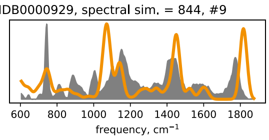
protonated HMDB0000929, spectral sim. = 845, #8


43.9 kJ/mol
L-Tryptophan

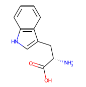


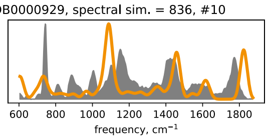
protonated HMDB0000929, spectral sim. = 844, #9


17.3 kJ/mol
L-Tryptophan

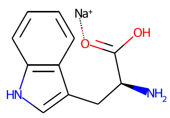


protonated HMDB0000929, spectral sim. = 836, #10

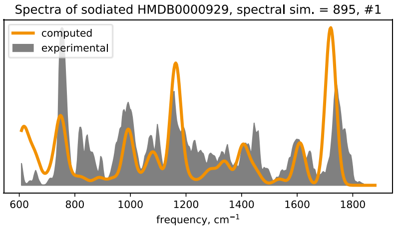

45.9 kJ/mol
L-Tryptophan



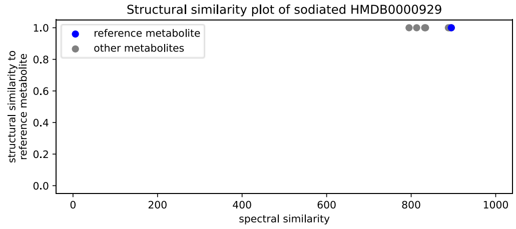
121 sodiated HMDB0000929


L-Tryptophan

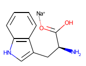
Spectra of sodiated HMDB0000929, spectral sim. = 895, #1

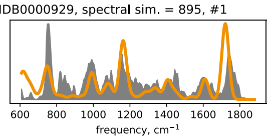


Structural similarity plot of sodiated HMDB0000929

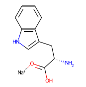


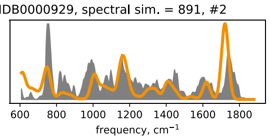
sodiated HMDB0000929, spectral sim. = 895, #1


10.2 kJ/mol
L-Tryptophan

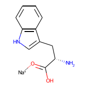


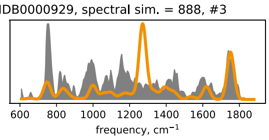
sodiated HMDB0000929, spectral sim. = 891, #2


0.0 kJ/mol
L-Tryptophan

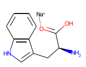


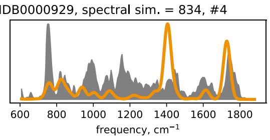
sodiated HMDB0000929, spectral sim. = 888, #3


23.0 kJ/mol
L-Tryptophan

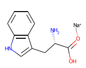


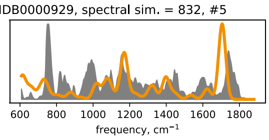
sodiated HMDB0000929, spectral sim. = 834, #4


18.0 kJ/mol
L-Tryptophan

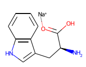


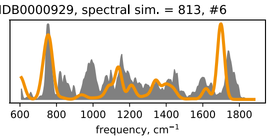
sodiated HMDB0000929, spectral sim. = 832, #5


27.7 kJ/mol
L-Tryptophan

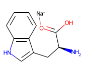


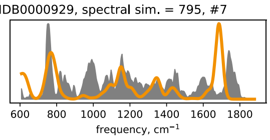
sodiated HMDB0000929, spectral sim. = 813, #6


36.1 kJ/mol
L-Tryptophan

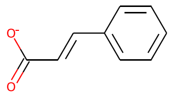


sodiated HMDB0000929, spectral sim. = 795, #7


33.6 kJ/mol
L-Tryptophan

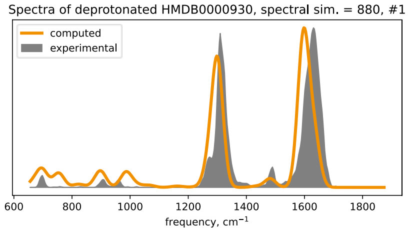


122 deprotonated HMDB0000930

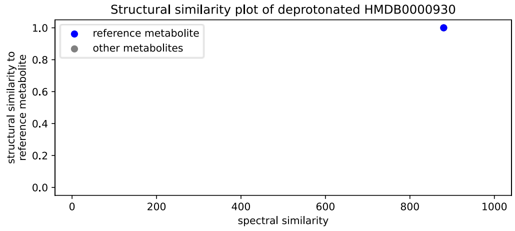


trans-Cinnamic acid

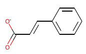
Spectra of deprotonated HMDB0000930, spectral sim. = 880, #1



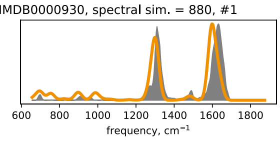
Structural similarity plot of deprotonated HMDB0000930



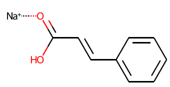
deprotonated HMDB0000930, spectral sim. = 880, #1



0.0 kJ/mol
trans-Cinnamic acid

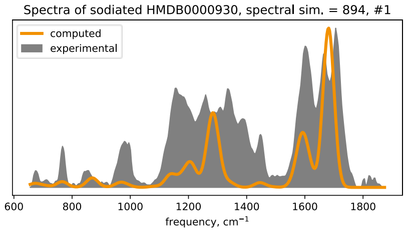


123 sodiated HMDB0000930

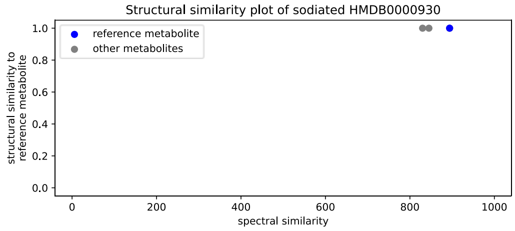


trans-Cinnamic acid

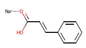
Spectra of sodiated HMDB0000930, spectral sim. = 894, #1



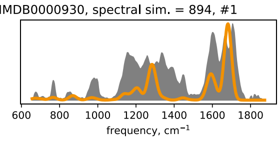
Structural similarity plot of sodiated HMDB0000930



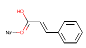
sodiated HMDB0000930, spectral sim. = 894, #1



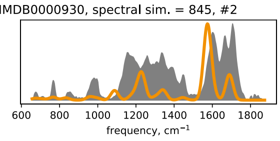
5.1 kJ/mol
trans-Cinnamic acid



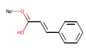
sodiated HMDB0000930, spectral sim. = 845, #2



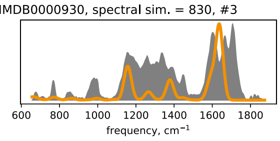
2.1 kJ/mol
trans-Cinnamic acid



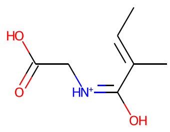
sodiated HMDB0000930, spectral sim. = 830, #3



0.0 kJ/mol
trans-Cinnamic acid

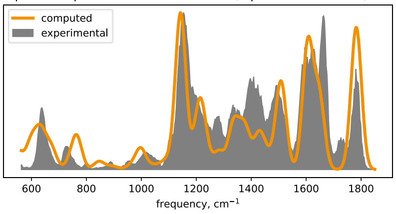


124 protonated HMDB0000959

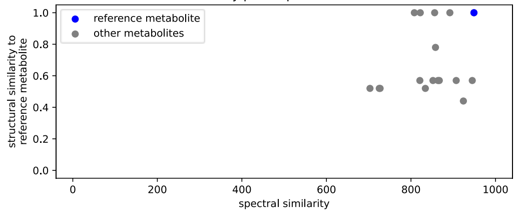


Tiglylglycine

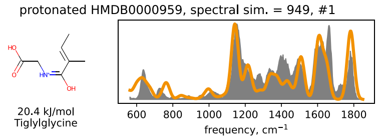
Spectra of protonated HMDB0000959, spectral sim. = 949, #1



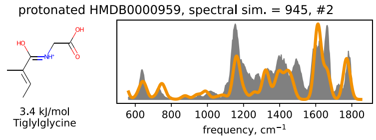
Structural similarity plot of protonated HMDB0000959



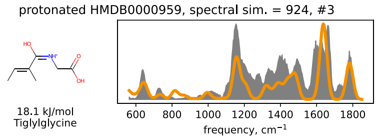
protonated HMDB0000959, spectral sim. = 949, #1



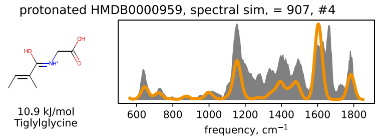
protonated HMDB0000959, spectral sim. = 945, #2



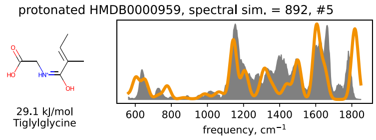
protonated HMDB0000959, spectral sim. = 924, #3



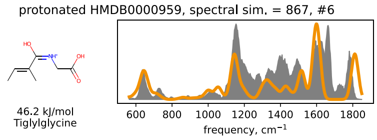
protonated HMDB0000959, spectral sim. = 907, #4



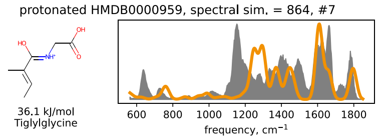
protonated HMDB0000959, spectral sim. = 892, #5



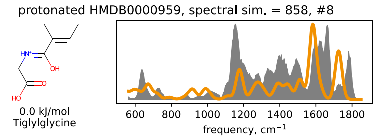
protonated HMDB0000959, spectral sim. = 867, #6



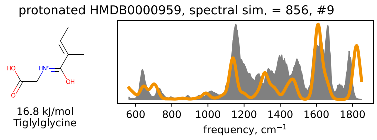
protonated HMDB0000959, spectral sim. = 864, #7



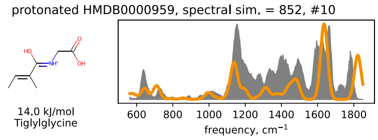
protonated HMDB0000959, spectral sim. = 858, #8



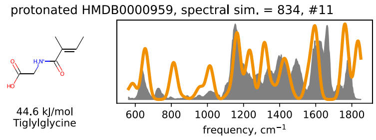
protonated HMDB0000959, spectral sim. = 856, #9



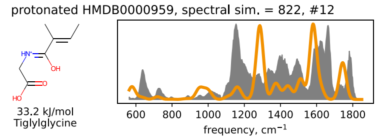
protonated HMDB0000959, spectral sim. = 852, #10



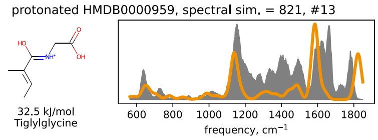
protonated HMDB0000959, spectral sim. = 834, #11



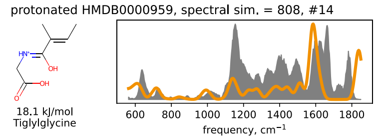
protonated HMDB0000959, spectral sim. = 822, #12



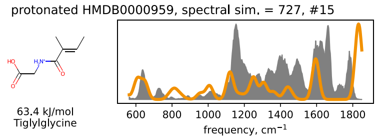
protonated HMDB0000959, spectral sim. = 821, #13



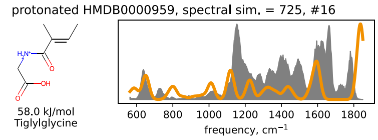
protonated HMDB0000959, spectral sim. = 808, #14



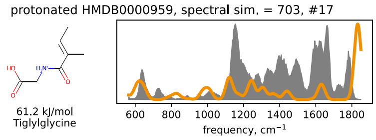
protonated HMDB0000959, spectral sim. = 727, #15



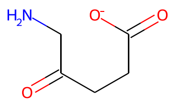
protonated HMDB0000959, spectral sim. = 725, #16



protonated HMDB0000959, spectral sim. = 703, #17

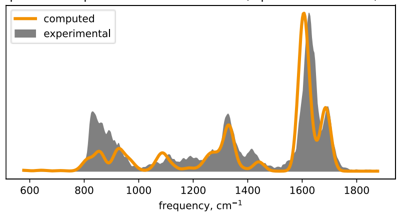


125 deprotonated HMDB0001149

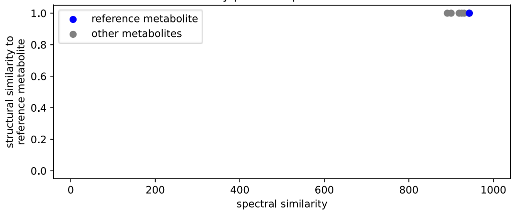


5-Aminolevulinic acid

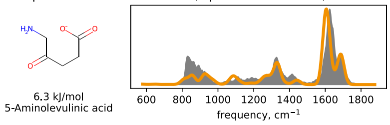
Spectra of deprotonated HMDB0001149, spectral sim. = 943, #1



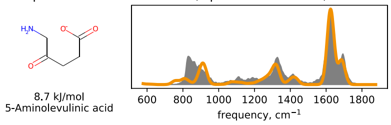
Structural similarity plot of deprotonated HMDB0001149



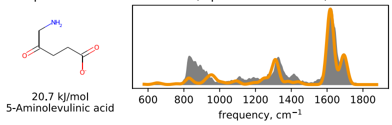
deprotonated HMDB0001149, spectral sim. = 943, #1



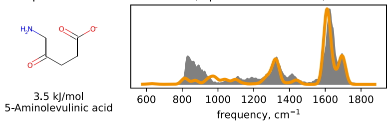
deprotonated HMDB0001149, spectral sim. = 943, #2



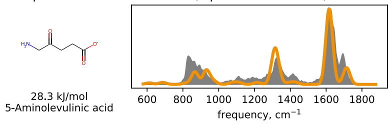
deprotonated HMDB0001149, spectral sim. = 931, #3



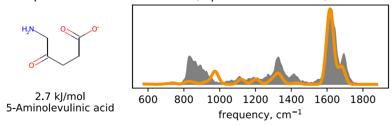
deprotonated HMDB0001149, spectral sim. = 925, #4



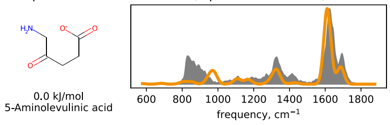
deprotonated HMDB0001149, spectral sim. = 919, #5



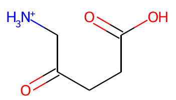
deprotonated HMDB0001149, spectral sim. = 900, #6



deprotonated HMDB0001149, spectral sim. = 891, #7

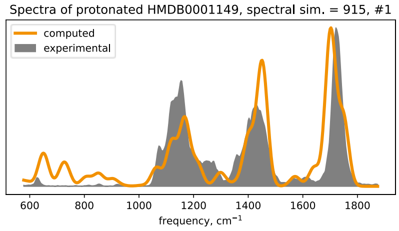


126 protonated HMDB0001149

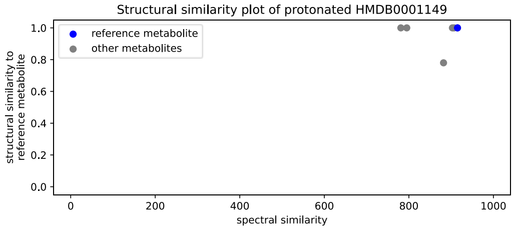


5-Aminolevulinic acid

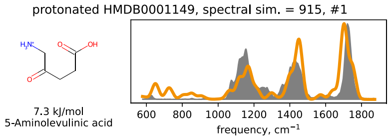
Spectra of protonated HMDB0001149, spectral sim. = 915, #1



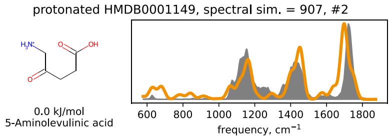
Structural similarity plot of protonated HMDB0001149



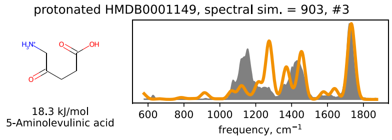
protonated HMDB0001149, spectral sim. = 915, #1



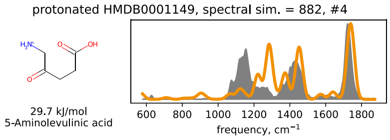
protonated HMDB0001149, spectral sim. = 907, #2



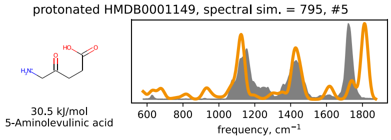
protonated HMDB0001149, spectral sim. = 903, #3



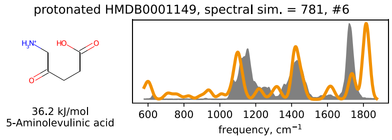
protonated HMDB0001149, spectral sim. = 882, #4

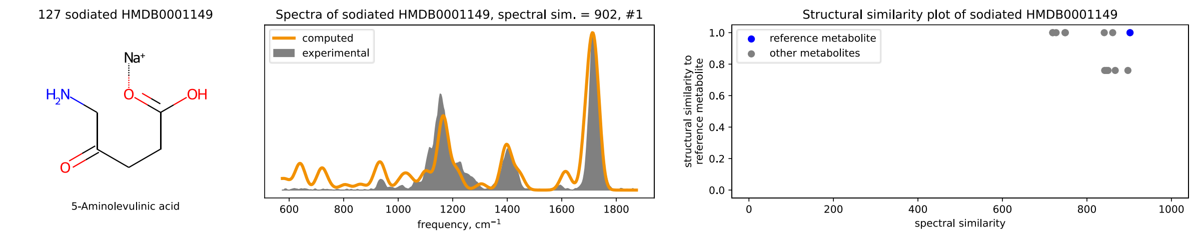


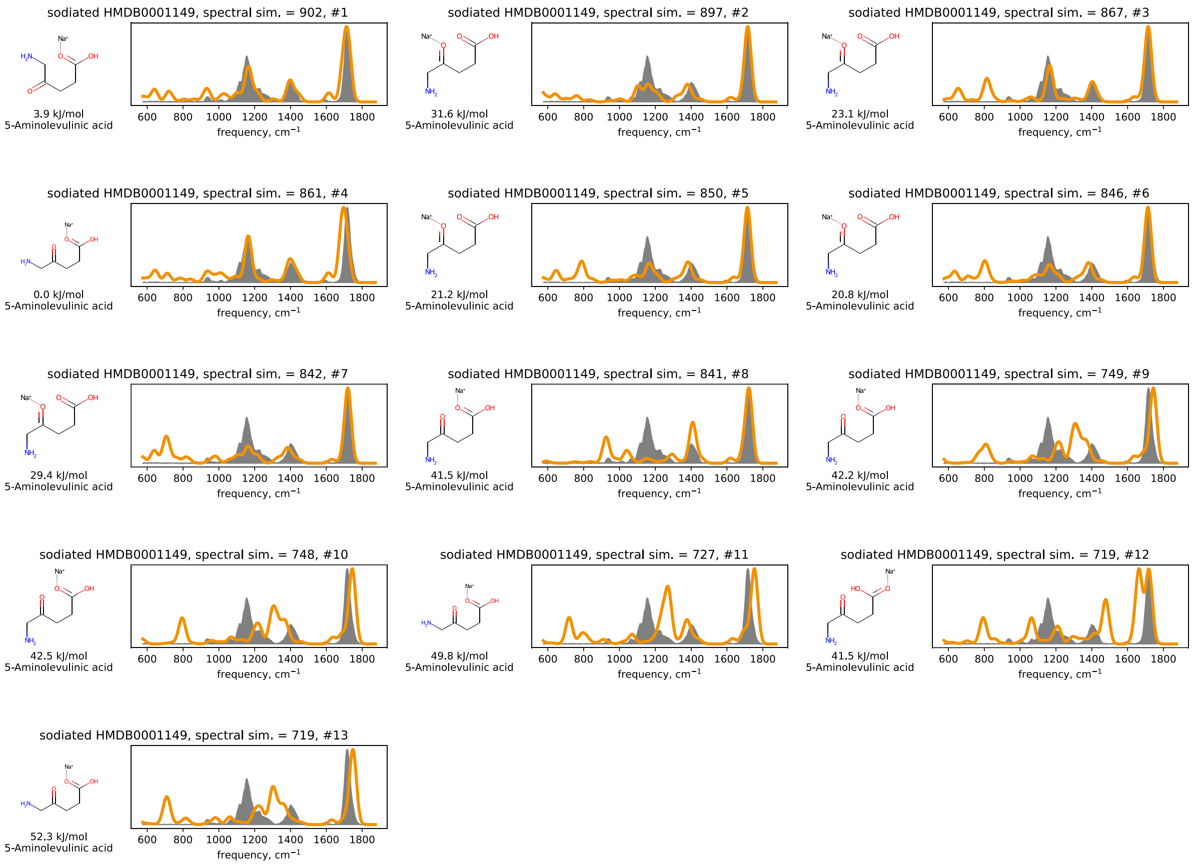
protonated HMDB0001149, spectral sim. = 795, #5

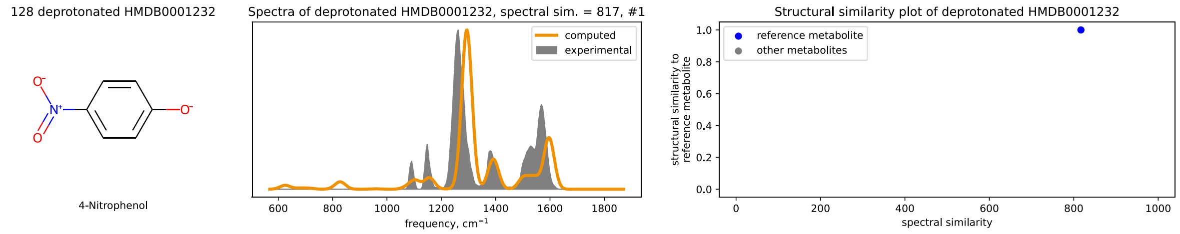


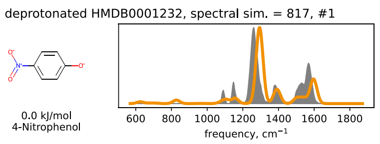
protonated HMDB0001149, spectral sim. = 781, #6

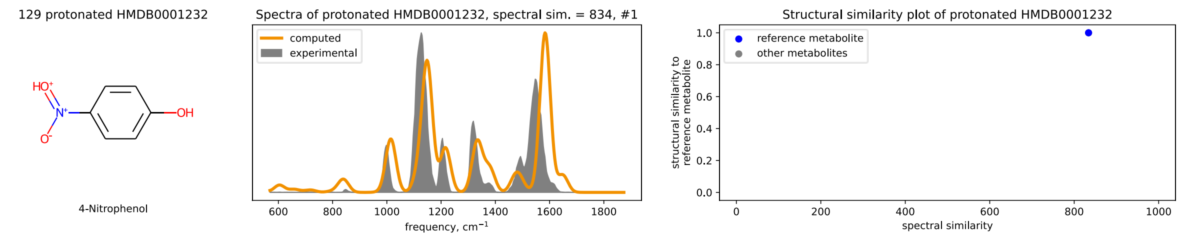


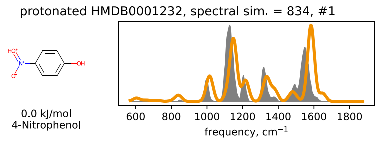

127 sodiated HMDB0001149
Na+
H2N
O
OH
O
5-Aminolevulinic acid
Spectra of sodiated HMDB0001149, spectral sim. = 902, #1
computed
experimental
frequency, cm−1
Structural similarity plot of sodiated HMDB0001149
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

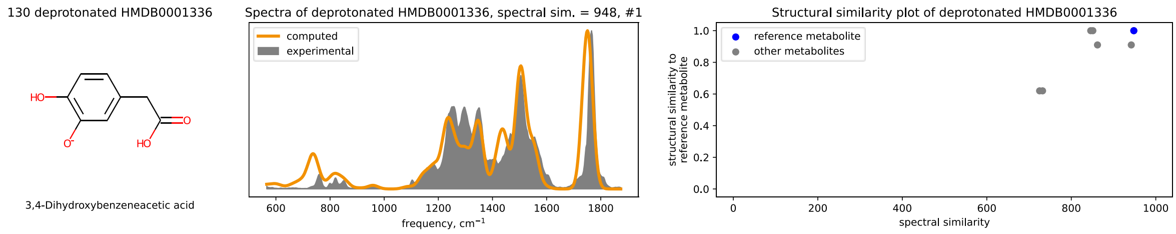

sodiated HMDB0001149, spectral sim. = 902, #1
3.9 kJ/mol
5-Aminolevulinic acid
sodiated HMDB0001149, spectral sim. = 897, #2
31.6 kJ/mol
5-Aminolevulinic acid
sodiated HMDB0001149, spectral sim. = 867, #3
23.1 kJ/mol
5-Aminolevulinic acid
sodiated HMDB0001149, spectral sim. = 861, #4
0.0 kJ/mol
5-Aminolevulinic acid
sodiated HMDB0001149, spectral sim. = 850, #5
21.2 kJ/mol
5-Aminolevulinic acid
sodiated HMDB0001149, spectral sim. = 846, #6
20.8 kJ/mol
5-Aminolevulinic acid
sodiated HMDB0001149, spectral sim. = 842, #7
29.4 kJ/mol
5-Aminolevulinic acid
sodiated HMDB0001149, spectral sim. = 841, #8
41.5 kJ/mol
5-Aminolevulinic acid
sodiated HMDB0001149, spectral sim. = 749, #9
42.2 kJ/mol
5-Aminolevulinic acid
sodiated HMDB0001149, spectral sim. = 748, #10
42.5 kJ/mol
5-Aminolevulinic acid
sodiated HMDB0001149, spectral sim. = 727, #11
49.8 kJ/mol
5-Aminolevulinic acid
sodiated HMDB0001149, spectral sim. = 719, #12
41.5 kJ/mol
5-Aminolevulinic acid
sodiated HMDB0001149, spectral sim. = 719, #13
52.3 kJ/mol
5-Aminolevulinic acid
frequency, cm−1

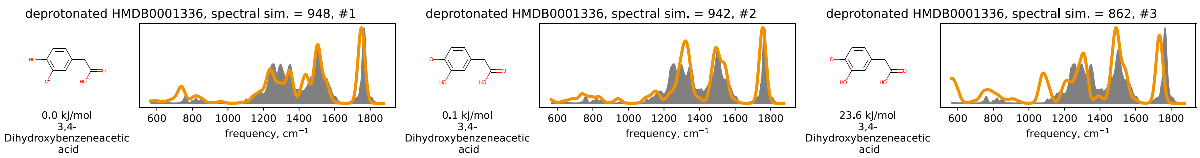

128 deprotonated HMDB0001232
O-
N+
O
O-
4-Nitrophenol
Spectra of deprotonated HMDB0001232, spectral sim. = 817, #1
computed
experimental
frequency, cm−1
Structural similarity plot of deprotonated HMDB0001232
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

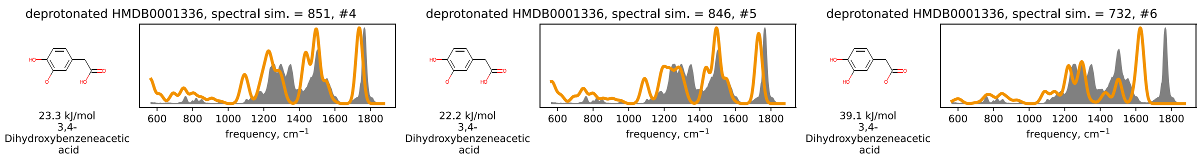

deprotonated HMDB0001232, spectral sim. = 817, #1
0.0 kJ/mol
4-Nitrophenol
frequency, cm−1

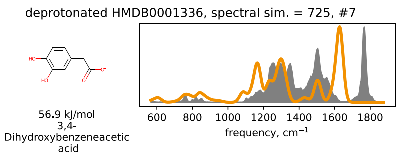

129 protonated HMDB0001232
4-Nitrophenol
Spectra of protonated HMDB0001232, spectral sim. = 834, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of protonated HMDB0001232
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

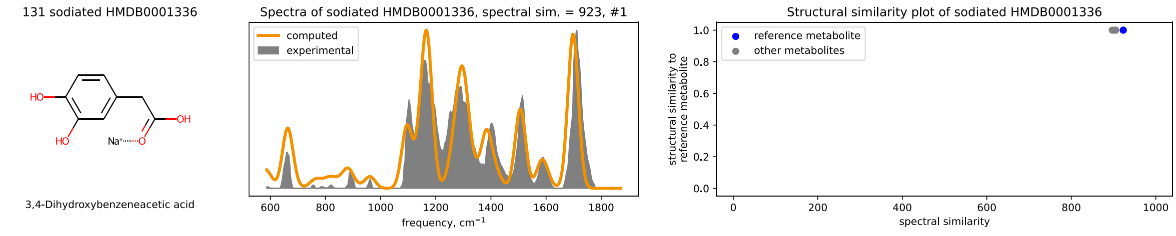

protonated HMDB0001232, spectral sim. = 834, #1
0.0 kJ/mol
4-Nitrophenol
frequency, cm^{-1}

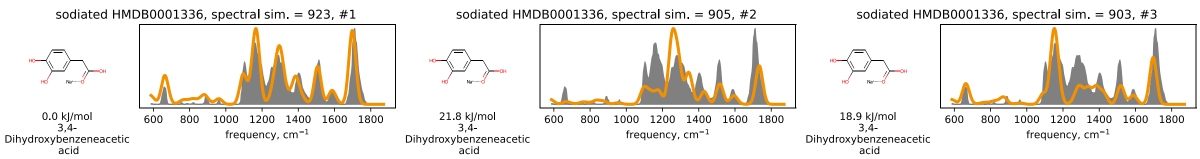

130 deprotonated HMDB0001336
3,4-Dihydroxybenzeneacetic acid
Spectra of deprotonated HMDB0001336, spectral sim. = 948, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0001336
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

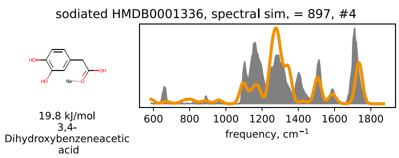

deprotonated HMDB0001336, spectral sim. = 948, #1
0.0 kJ/mol
3,4-Dihydroxybenzeneacetic acid
deprotonated HMDB0001336, spectral sim. = 942, #2
0.1 kJ/mol
3,4-Dihydroxybenzeneacetic acid
deprotonated HMDB0001336, spectral sim. = 862, #3
23.6 kJ/mol
3,4-Dihydroxybenzeneacetic acid
frequency, cm^{-1}


deprotonated HMDB0001336, spectral sim. = 851, #4
23.3 kJ/mol
3,4-Dihydroxybenzeneacetic acid
deprotonated HMDB0001336, spectral sim. = 846, #5
22.2 kJ/mol
3,4-Dihydroxybenzeneacetic acid
deprotonated HMDB0001336, spectral sim. = 732, #6
39.1 kJ/mol
3,4-Dihydroxybenzeneacetic acid
frequency, cm^{-1}

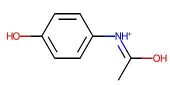

deprotonated HMDB0001336, spectral sim. = 725, #7
56.9 kJ/mol
3,4-Dihydroxybenzeneacetic acid
frequency, cm^{-1}


131 sodiated HMDB0001336
3,4-Dihydroxybenzeneacetic acid
Spectra of sodiated HMDB0001336, spectral sim. = 923, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of sodiated HMDB0001336
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity


sodiated HMDB0001336, spectral sim. = 923, #1
0.0 kJ/mol
3,4-Dihydroxybenzeneacetic acid
sodiated HMDB0001336, spectral sim. = 905, #2
21.8 kJ/mol
3,4-Dihydroxybenzeneacetic acid
sodiated HMDB0001336, spectral sim. = 903, #3
18.9 kJ/mol
3,4-Dihydroxybenzeneacetic acid
frequency, cm^{-1}

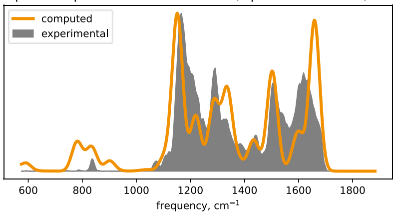

sodiated HMDB0001336, spectral sim. = 897, #4
19.8 kJ/mol
3,4-Dihydroxybenzeneacetic acid
frequency, cm^{-1}

132 protonated HMDB0001859

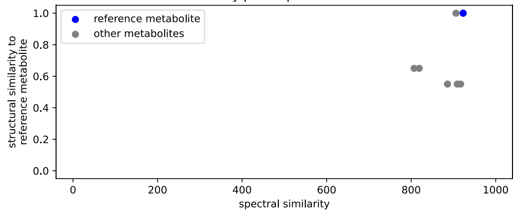


Acetaminophen

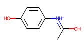
Spectra of protonated HMDB0001859, spectral sim. = 923, #1



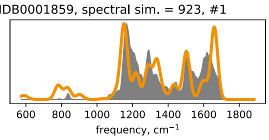
Structural similarity plot of protonated HMDB0001859



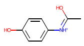
protonated HMDB0001859, spectral sim. = 923, #1



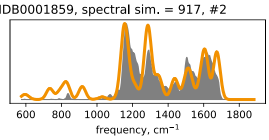
10.5 kJ/mol
Acetaminophen



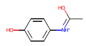
protonated HMDB0001859, spectral sim. = 917, #2



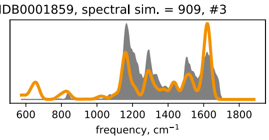
18.1 kJ/mol
Acetaminophen



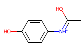
protonated HMDB0001859, spectral sim. = 909, #3



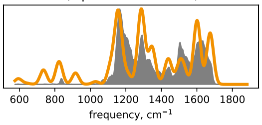
0.0 kJ/mol
Acetaminophen



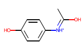
protonated HMDB0001859, spectral sim. = 906, #4



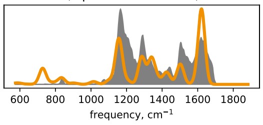
17.0 kJ/mol
Acetaminophen



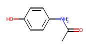
protonated HMDB0001859, spectral sim. = 886, #5



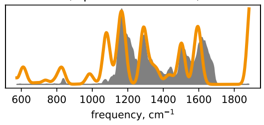
21.5 kJ/mol
Acetaminophen



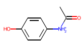
protonated HMDB0001859, spectral sim. = 819, #6



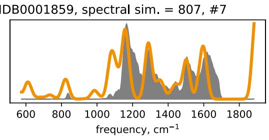
54.3 kJ/mol
Acetaminophen



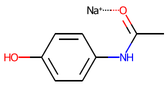
protonated HMDB0001859, spectral sim. = 807, #7



54.2 kJ/mol
Acetaminophen

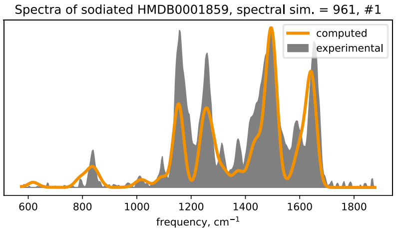


133 sodiated HMDB0001859

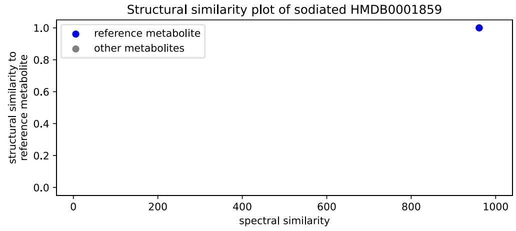


Acetaminophen

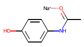
Spectra of sodiated HMDB0001859, spectral sim. = 961, #1



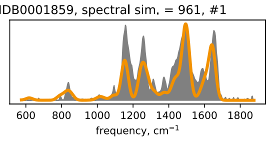
Structural similarity plot of sodiated HMDB0001859



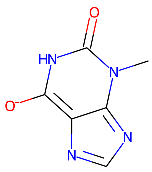
sodiated HMDB0001859, spectral sim. = 961, #1



0.0 kJ/mol
Acetaminophen

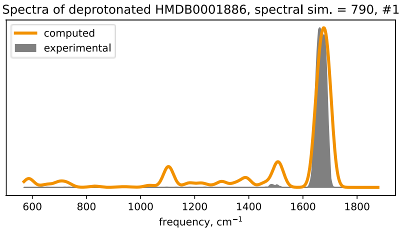


134 deprotonated HMDB0001886

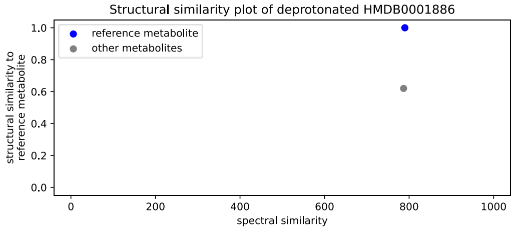


3-Methylxanthine

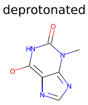
Spectra of deprotonated HMDB0001886, spectral sim. = 790, #1



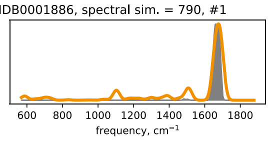
Structural similarity plot of deprotonated HMDB0001886



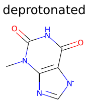
deprotonated HMDB0001886, spectral sim. = 790, #1



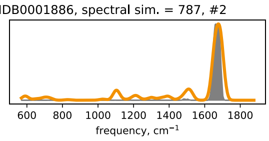
0.0 kJ/mol
3-Methylxanthine

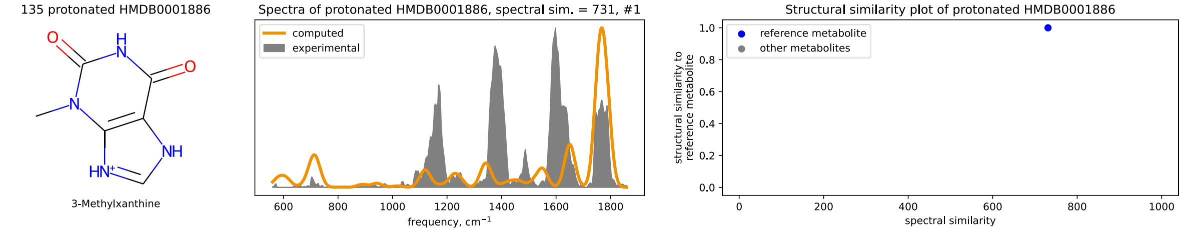


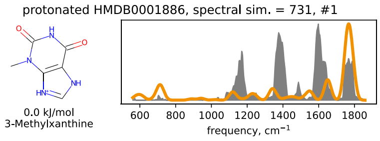
deprotonated HMDB0001886, spectral sim. = 787, #2

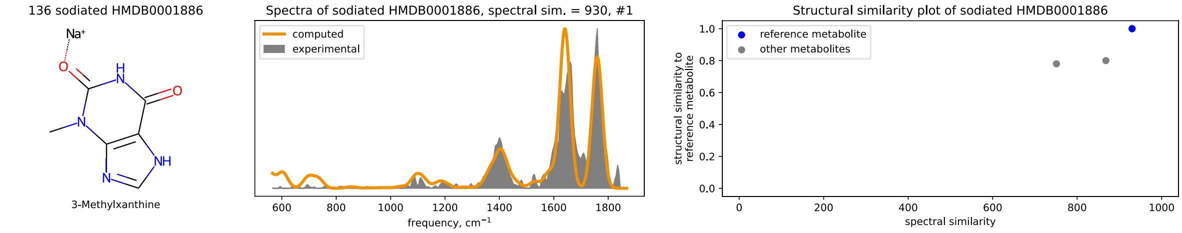


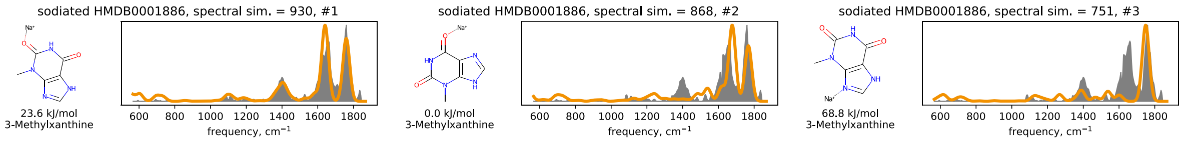
3.5 kJ/mol
3-Methylxanthine

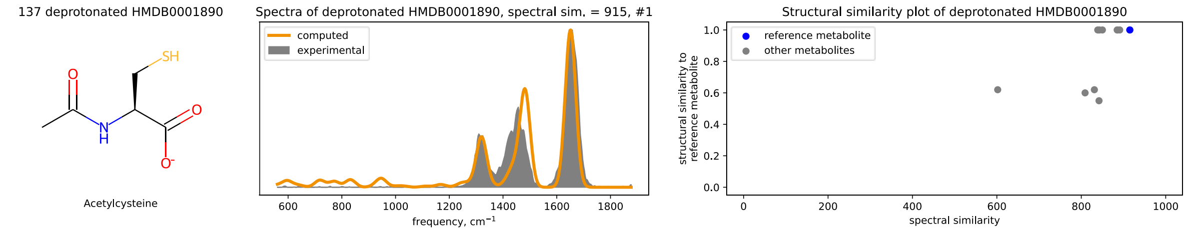


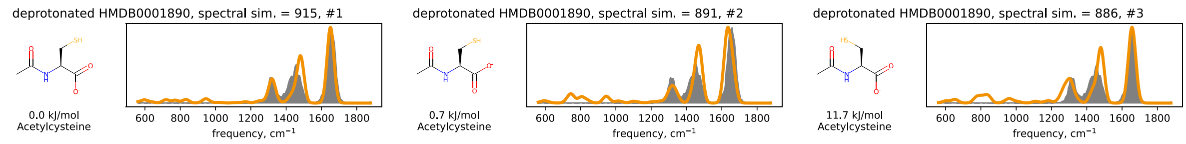

135 protonated HMDB0001886
3-Methylxanthine
Spectra of protonated HMDB0001886, spectral sim. = 731, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of protonated HMDB0001886
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

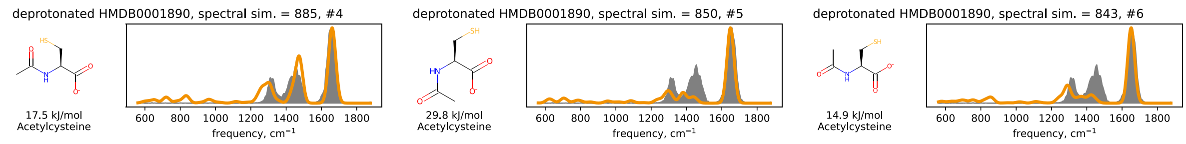

protonated HMDB0001886, spectral sim. = 731, #1
0.0 kJ/mol
3-Methylxanthine
frequency, cm⁻¹

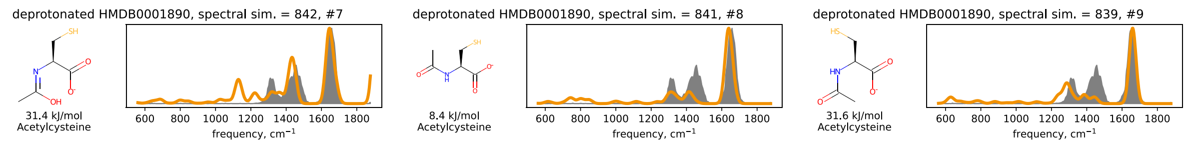

136 sodiated HMDB0001886
3-Methylxanthine
Spectra of sodiated HMDB0001886, spectral sim. = 930, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of sodiated HMDB0001886
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

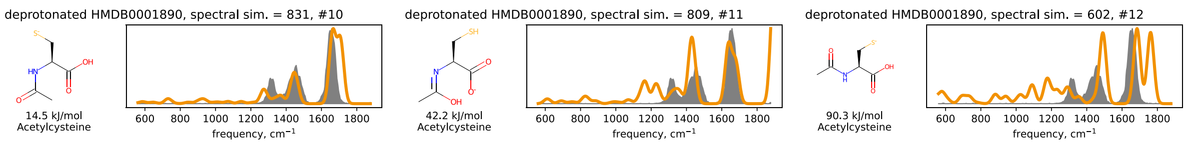

sodiated HMDB0001886, spectral sim. = 930, #1
23.6 kJ/mol
3-Methylxanthine
sodiated HMDB0001886, spectral sim. = 868, #2
0.0 kJ/mol
3-Methylxanthine
sodiated HMDB0001886, spectral sim. = 751, #3
68.8 kJ/mol
3-Methylxanthine
frequency, cm⁻¹


137 deprotonated HMDB0001890
Acetylcysteine
Spectra of deprotonated HMDB0001890, spectral sim. = 915, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of deprotonated HMDB0001890
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

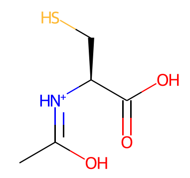

deprotonated HMDB0001890, spectral sim. = 915, #1
0.0 kJ/mol
Acetylcysteine
deprotonated HMDB0001890, spectral sim. = 891, #2
0.7 kJ/mol
Acetylcysteine
deprotonated HMDB0001890, spectral sim. = 886, #3
11.7 kJ/mol
Acetylcysteine
frequency, cm⁻¹


deprotonated HMDB0001890, spectral sim. = 885, #4
17.5 kJ/mol
Acetylcysteine
deprotonated HMDB0001890, spectral sim. = 850, #5
29.8 kJ/mol
Acetylcysteine
deprotonated HMDB0001890, spectral sim. = 843, #6
14.9 kJ/mol
Acetylcysteine
frequency, cm⁻¹

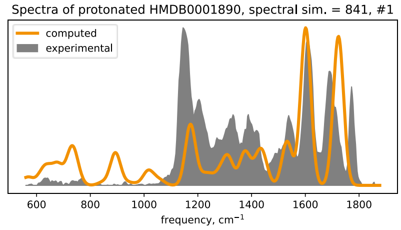

deprotonated HMDB0001890, spectral sim. = 842, #7
31.4 kJ/mol
Acetylcysteine
deprotonated HMDB0001890, spectral sim. = 841, #8
8.4 kJ/mol
Acetylcysteine
deprotonated HMDB0001890, spectral sim. = 839, #9
31.6 kJ/mol
Acetylcysteine
frequency, cm⁻¹


deprotonated HMDB0001890, spectral sim. = 831, #10
14.5 kJ/mol
Acetylcysteine
deprotonated HMDB0001890, spectral sim. = 809, #11
42.2 kJ/mol
Acetylcysteine
deprotonated HMDB0001890, spectral sim. = 602, #12
90.3 kJ/mol
Acetylcysteine
frequency, cm⁻¹

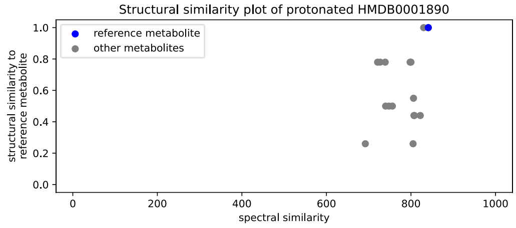
138 protonated HMDB0001890



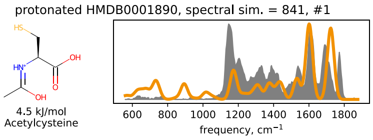
Spectra of protonated HMDB0001890, spectral sim. = 841, #1



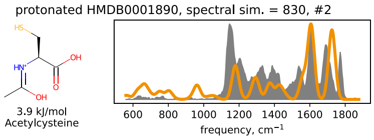
Structural similarity plot of protonated HMDB0001890



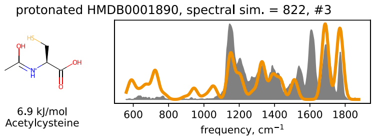
protonated HMDB0001890, spectral sim. = 841, #1



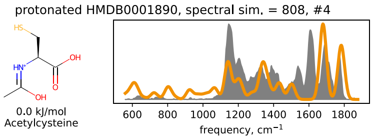
protonated HMDB0001890, spectral sim. = 830, #2



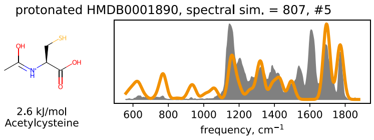
protonated HMDB0001890, spectral sim. = 822, #3



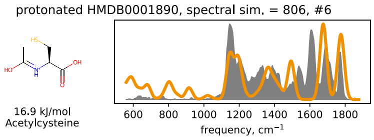
protonated HMDB0001890, spectral sim. = 808, #4



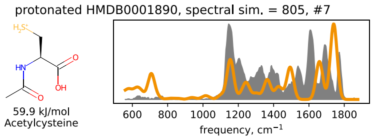
protonated HMDB0001890, spectral sim. = 807, #5



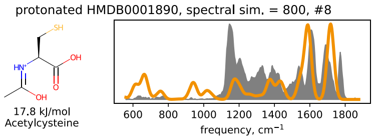
protonated HMDB0001890, spectral sim. = 806, #6



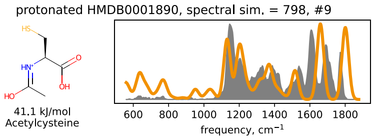
protonated HMDB0001890, spectral sim. = 805, #7



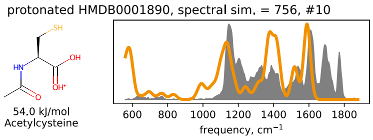
protonated HMDB0001890, spectral sim. = 800, #8



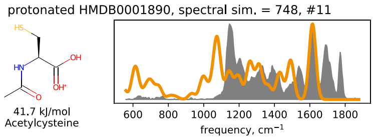
protonated HMDB0001890, spectral sim. = 798, #9



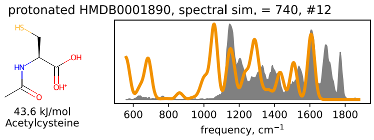
protonated HMDB0001890, spectral sim. = 756, #10



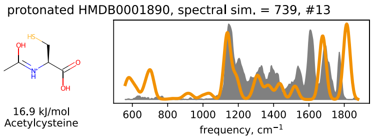
protonated HMDB0001890, spectral sim. = 748, #11



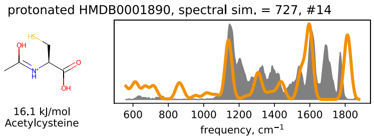
protonated HMDB0001890, spectral sim. = 740, #12



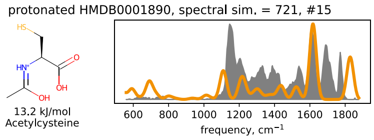
protonated HMDB0001890, spectral sim. = 739, #13



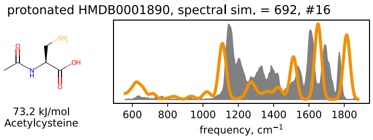
protonated HMDB0001890, spectral sim. = 727, #14

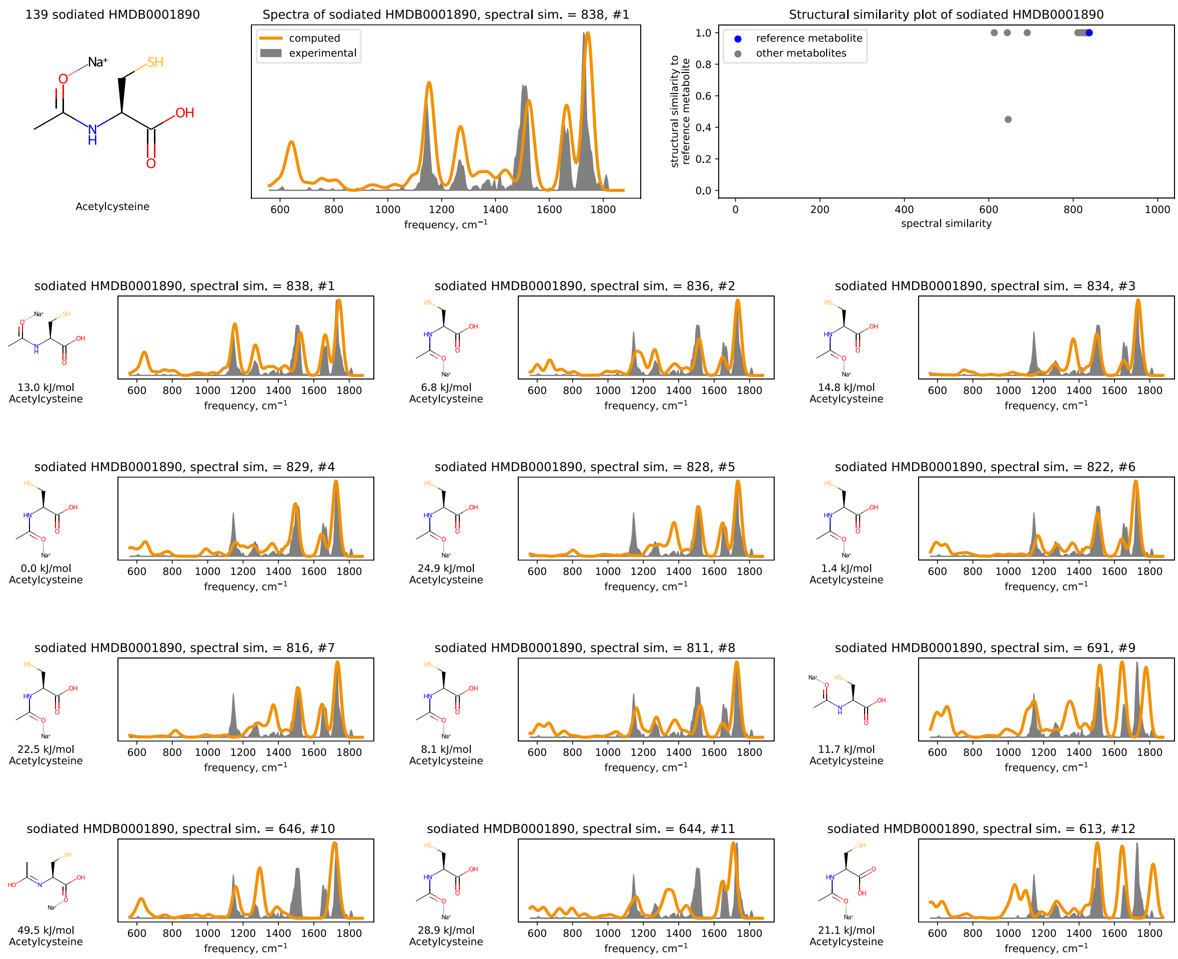


protonated HMDB0001890, spectral sim. = 721, #15

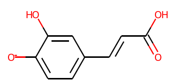


protonated HMDB0001890, spectral sim. = 692, #16



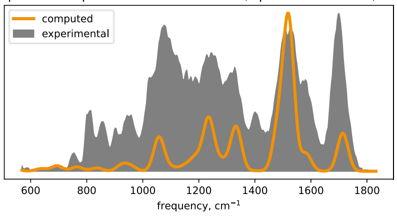

139 sodiated HMDB0001890
Na⁺
SH
OH
Acetylcysteine
Spectra of sodiated HMDB0001890, spectral sim. = 838, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of sodiated HMDB0001890
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
sodiated HMDB0001890, spectral sim. = 838, #1
13.0 kJ/mol
Acetylcysteine
sodiated HMDB0001890, spectral sim. = 836, #2
6.8 kJ/mol
Acetylcysteine
sodiated HMDB0001890, spectral sim. = 834, #3
14.8 kJ/mol
Acetylcysteine
sodiated HMDB0001890, spectral sim. = 829, #4
0.0 kJ/mol
Acetylcysteine
sodiated HMDB0001890, spectral sim. = 828, #5
24.9 kJ/mol
Acetylcysteine
sodiated HMDB0001890, spectral sim. = 822, #6
1.4 kJ/mol
Acetylcysteine
sodiated HMDB0001890, spectral sim. = 816, #7
22.5 kJ/mol
Acetylcysteine
sodiated HMDB0001890, spectral sim. = 811, #8
8.1 kJ/mol
Acetylcysteine
sodiated HMDB0001890, spectral sim. = 691, #9
11.7 kJ/mol
Acetylcysteine
sodiated HMDB0001890, spectral sim. = 646, #10
49.5 kJ/mol
Acetylcysteine
sodiated HMDB0001890, spectral sim. = 644, #11
28.9 kJ/mol
Acetylcysteine
sodiated HMDB0001890, spectral sim. = 613, #12
21.1 kJ/mol
Acetylcysteine
frequency, cm⁻¹

140 deprotonated HMDB0001964

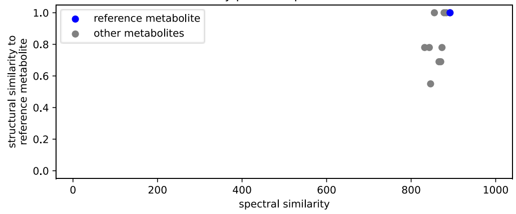


Caffeic acid

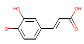
Spectra of deprotonated HMDB0001964, spectral sim. = 892, #1



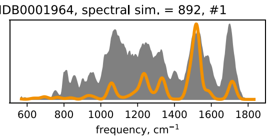
Structural similarity plot of deprotonated HMDB0001964



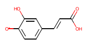
deprotonated HMDB0001964, spectral sim. = 892, #1



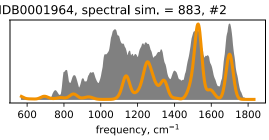
9.1 kJ/mol
Caffeic acid



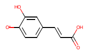
deprotonated HMDB0001964, spectral sim. = 883, #2



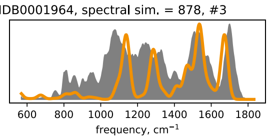
12.0 kJ/mol
Caffeic acid



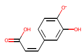
deprotonated HMDB0001964, spectral sim. = 878, #3



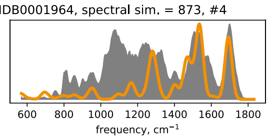
0.0 kJ/mol
Caffeic acid



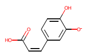
deprotonated HMDB0001964, spectral sim. = 873, #4



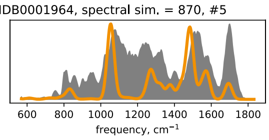
18.9 kJ/mol
Caffeic acid



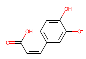
deprotonated HMDB0001964, spectral sim. = 870, #5



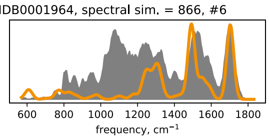
46.1 kJ/mol
Caffeic acid



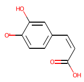
deprotonated HMDB0001964, spectral sim. = 866, #6



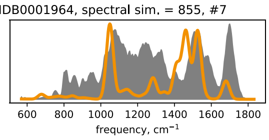
23.8 kJ/mol
Caffeic acid



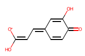
deprotonated HMDB0001964, spectral sim. = 855, #7



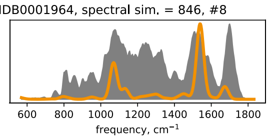
29.0 kJ/mol
Caffeic acid



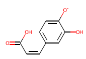
deprotonated HMDB0001964, spectral sim. = 846, #8



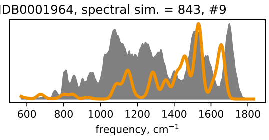
43.6 kJ/mol
Caffeic acid



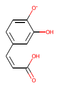
deprotonated HMDB0001964, spectral sim. = 843, #9



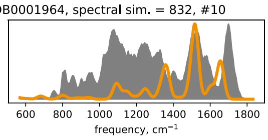
34.0 kJ/mol
Caffeic acid



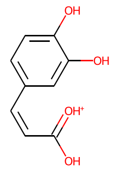
deprotonated HMDB0001964, spectral sim. = 832, #10



31.4 kJ/mol
Caffeic acid

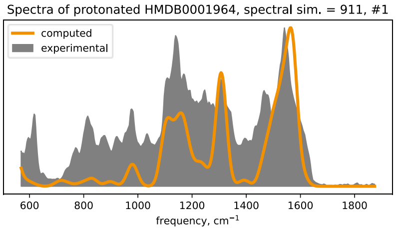


141 protonated HMDB0001964

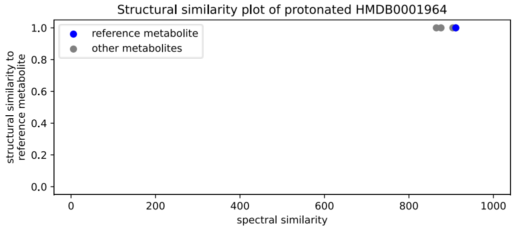


Caffeic acid

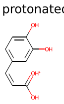
Spectra of protonated HMDB0001964, spectral sim. = 911, #1



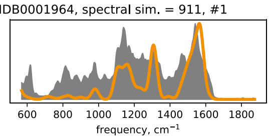
Structural similarity plot of protonated HMDB0001964



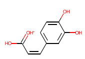
protonated HMDB0001964, spectral sim. = 911, #1



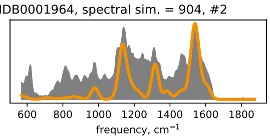
0.0 kJ/mol
Caffeic acid



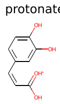
protonated HMDB0001964, spectral sim. = 904, #2



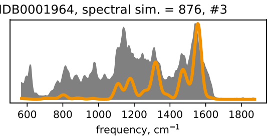
3.2 kJ/mol
Caffeic acid



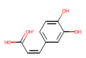
protonated HMDB0001964, spectral sim. = 876, #3



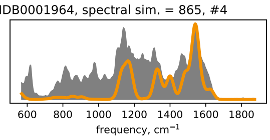
12.9 kJ/mol
Caffeic acid



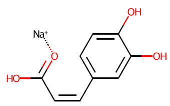
protonated HMDB0001964, spectral sim. = 865, #4



14.3 kJ/mol
Caffeic acid

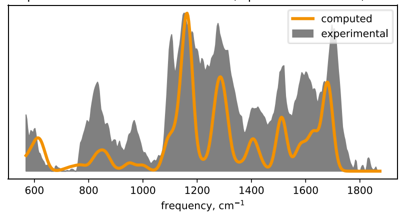


142 sodiated HMDB0001964

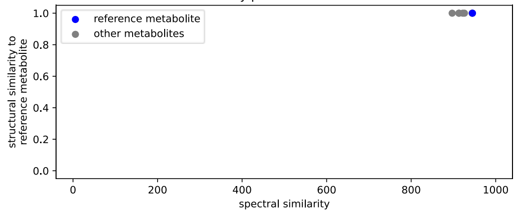


Caffeic acid

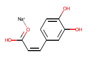
Spectra of sodiated HMDB0001964, spectral sim. = 945, #1



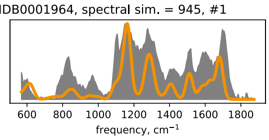
Structural similarity plot of sodiated HMDB0001964



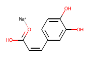
sodiated HMDB0001964, spectral sim. = 945, #1



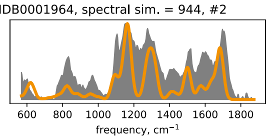
0.5 kJ/mol
Caffeic acid



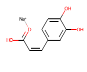
sodiated HMDB0001964, spectral sim. = 944, #2



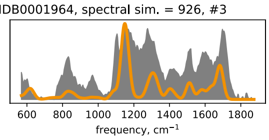
0.0 kJ/mol
Caffeic acid



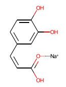
sodiated HMDB0001964, spectral sim. = 926, #3



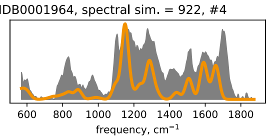
17.5 kJ/mol
Caffeic acid



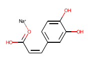
sodiated HMDB0001964, spectral sim. = 922, #4



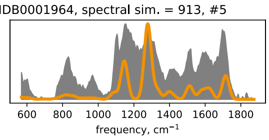
0.7 kJ/mol
Caffeic acid



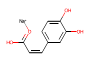
sodiated HMDB0001964, spectral sim. = 913, #5



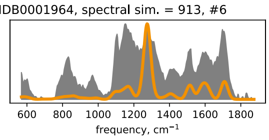
34.4 kJ/mol
Caffeic acid



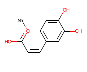
sodiated HMDB0001964, spectral sim. = 913, #6



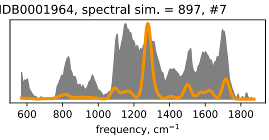
19.6 kJ/mol
Caffeic acid



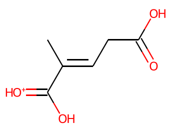
sodiated HMDB0001964, spectral sim. = 897, #7



16.9 kJ/mol
Caffeic acid

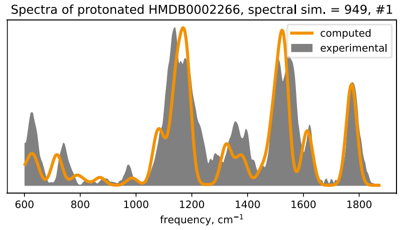


143 protonated HMDB0002266

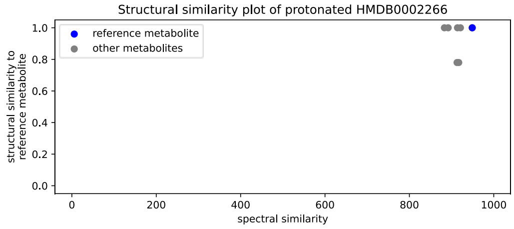


(E)-2-Methylglutaconic acid

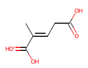
Spectra of protonated HMDB0002266, spectral sim. = 949, #1



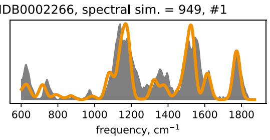
Structural similarity plot of protonated HMDB0002266



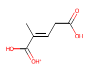
protonated HMDB0002266, spectral sim. = 949, #1



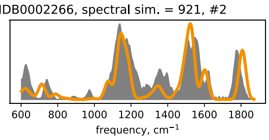
0.0 kJ/mol
(E)-2-
Methylglutaconic acid



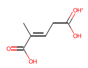
protonated HMDB0002266, spectral sim. = 921, #2



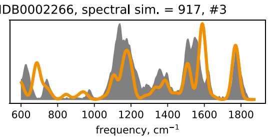
17.4 kJ/mol
(E)-2-
Methylglutaconic acid



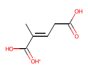
protonated HMDB0002266, spectral sim. = 917, #3



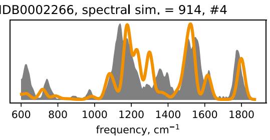
11.1 kJ/mol
(E)-2-
Methylglutaconic acid



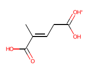
protonated HMDB0002266, spectral sim. = 914, #4



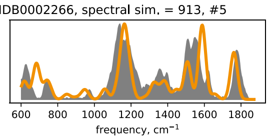
32.7 kJ/mol
(E)-2-
Methylglutaconic acid



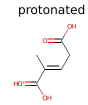
protonated HMDB0002266, spectral sim. = 913, #5



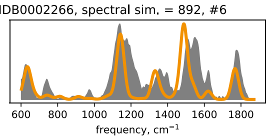
10.9 kJ/mol
(E)-2-
Methylglutaconic acid



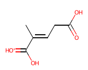
protonated HMDB0002266, spectral sim. = 892, #6



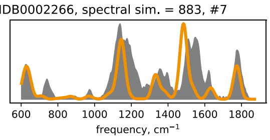
9.1 kJ/mol
(E)-2-
Methylglutaconic acid



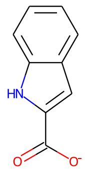
protonated HMDB0002266, spectral sim. = 883, #7



7.6 kJ/mol
(E)-2-
Methylglutaconic acid

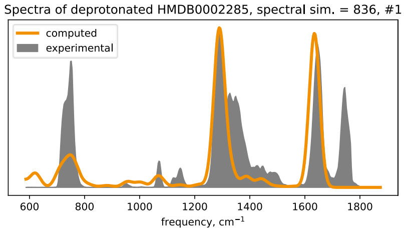


144 deprotonated HMDB0002285

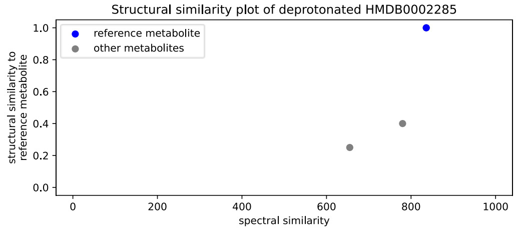


2-Indolecarboxylic acid

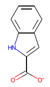
Spectra of deprotonated HMDB0002285, spectral sim. = 836, #1



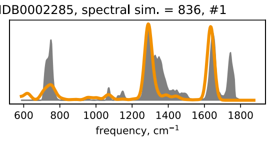
Structural similarity plot of deprotonated HMDB0002285



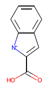
deprotonated HMDB0002285, spectral sim. = 836, #1



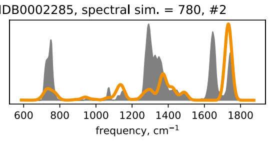
10.4 kJ/mol
2-Indolecarboxylic acid



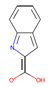
deprotonated HMDB0002285, spectral sim. = 780, #2



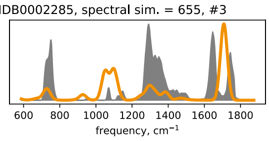
0.0 kJ/mol
2-Indolecarboxylic acid



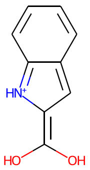
deprotonated HMDB0002285, spectral sim. = 655, #3



36.3 kJ/mol
2-Indolecarboxylic acid

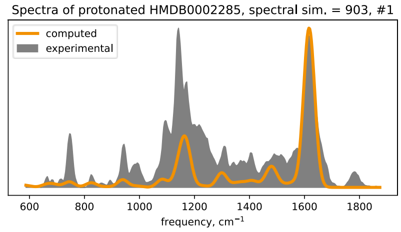


145 protonated HMDB0002285

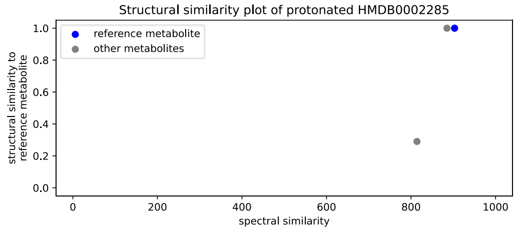


2-Indolecarboxylic acid

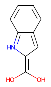
Spectra of protonated HMDB0002285, spectral sim. = 903, #1



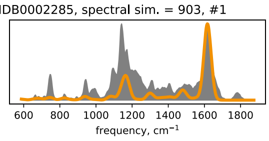
Structural similarity plot of protonated HMDB0002285



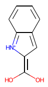
protonated HMDB0002285, spectral sim. = 903, #1



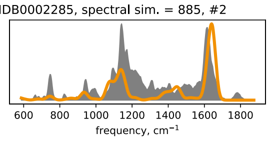
0.0 kJ/mol
2-Indolecarboxylic acid



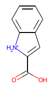
protonated HMDB0002285, spectral sim. = 885, #2



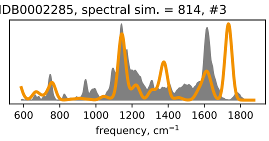
16.4 kJ/mol
2-Indolecarboxylic acid



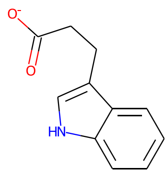
protonated HMDB0002285, spectral sim. = 814, #3



17.0 kJ/mol
2-Indolecarboxylic acid

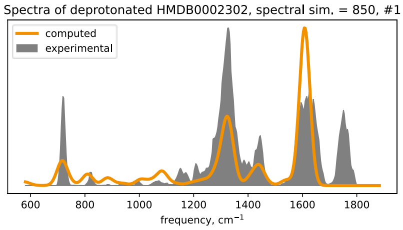


146 deprotonated HMDB0002302

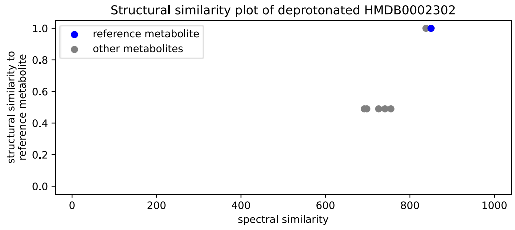


Indole-3-propionic acid

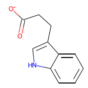
Spectra of deprotonated HMDB0002302, spectral sim. = 850, #1



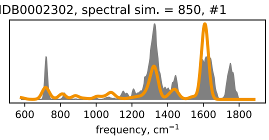
Structural similarity plot of deprotonated HMDB0002302



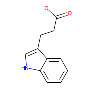
deprotonated HMDB0002302, spectral sim. = 850, #1



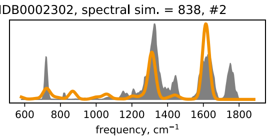
22.7 kJ/mol
Indole-3-propionic acid



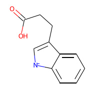
deprotonated HMDB0002302, spectral sim. = 838, #2



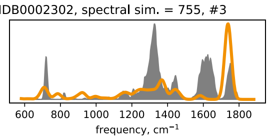
32.6 kJ/mol
Indole-3-propionic acid



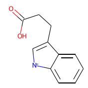
deprotonated HMDB0002302, spectral sim. = 755, #3



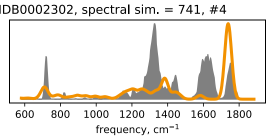
0.0 kJ/mol
Indole-3-propionic acid



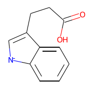
deprotonated HMDB0002302, spectral sim. = 741, #4



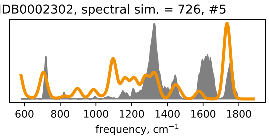
4.0 kJ/mol
Indole-3-propionic acid



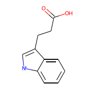
deprotonated HMDB0002302, spectral sim. = 726, #5



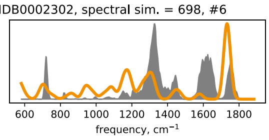
29.1 kJ/mol
Indole-3-propionic acid



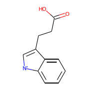
deprotonated HMDB0002302, spectral sim. = 698, #6



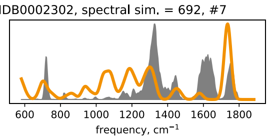
25.1 kJ/mol
Indole-3-propionic acid

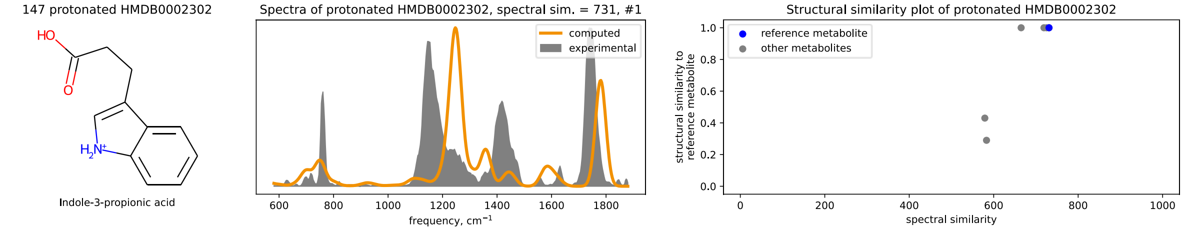


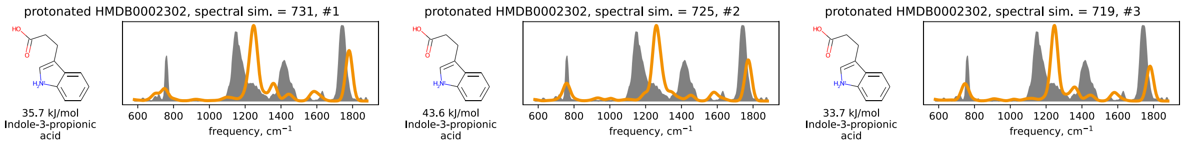
deprotonated HMDB0002302, spectral sim. = 692, #7

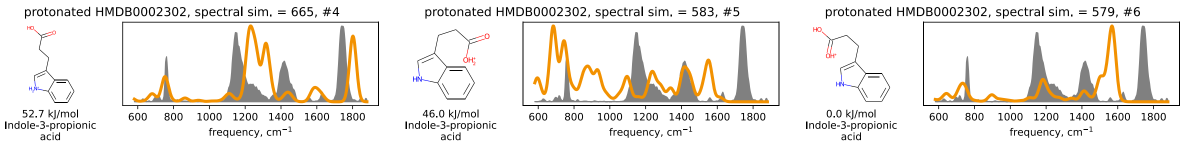


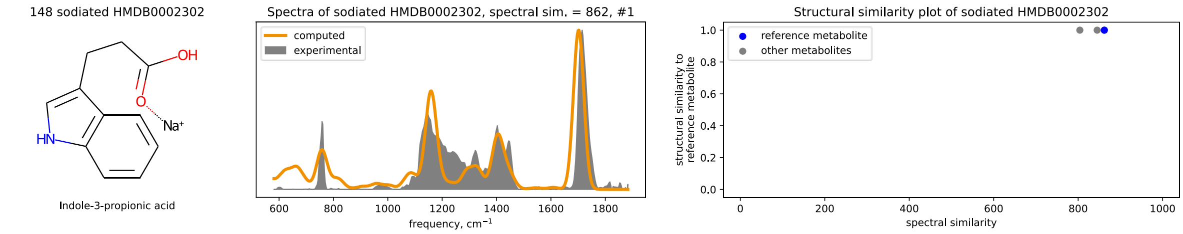
25.5 kJ/mol
Indole-3-propionic acid

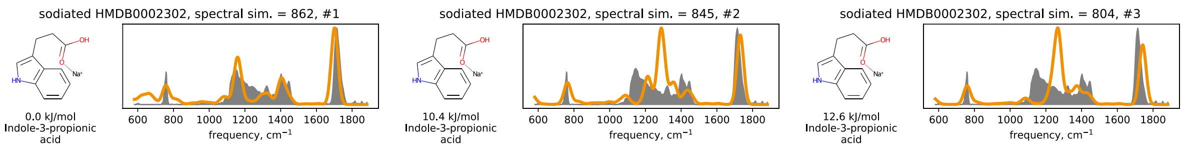


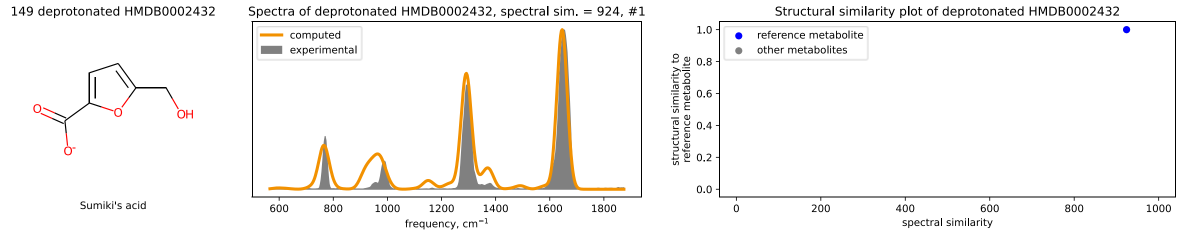

147 protonated HMDB0002302
Indole-3-propionic acid
Spectra of protonated HMDB0002302, spectral sim. = 731, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of protonated HMDB0002302
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

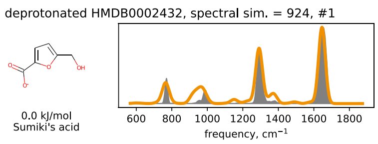

protonated HMDB0002302, spectral sim. = 731, #1
35.7 kJ/mol
Indole-3-propionic acid
protonated HMDB0002302, spectral sim. = 725, #2
43.6 kJ/mol
Indole-3-propionic acid
protonated HMDB0002302, spectral sim. = 719, #3
33.7 kJ/mol
Indole-3-propionic acid
frequency, cm^{-1}


protonated HMDB0002302, spectral sim. = 665, #4
52.7 kJ/mol
Indole-3-propionic acid
protonated HMDB0002302, spectral sim. = 583, #5
46.0 kJ/mol
Indole-3-propionic acid
protonated HMDB0002302, spectral sim. = 579, #6
0.0 kJ/mol
Indole-3-propionic acid
frequency, cm^{-1}

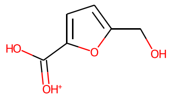

148 sodiated HMDB0002302
Indole-3-propionic acid
Spectra of sodiated HMDB0002302, spectral sim. = 862, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of sodiated HMDB0002302
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity


sodiated HMDB0002302, spectral sim. = 862, #1
0.0 kJ/mol
Indole-3-propionic acid
sodiated HMDB0002302, spectral sim. = 845, #2
10.4 kJ/mol
Indole-3-propionic acid
sodiated HMDB0002302, spectral sim. = 804, #3
12.6 kJ/mol
Indole-3-propionic acid
frequency, cm^{-1}


149 deprotonated HMDB0002432
Sumiki's acid
Spectra of deprotonated HMDB0002432, spectral sim. = 924, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0002432
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

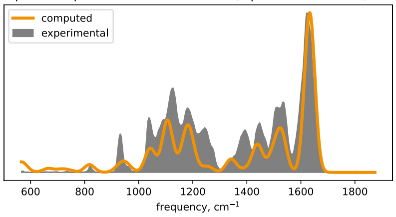

deprotonated HMDB0002432, spectral sim. = 924, #1
0.0 kJ/mol
Sumiki's acid
frequency, cm^{-1}

150 protonated HMDB0002432

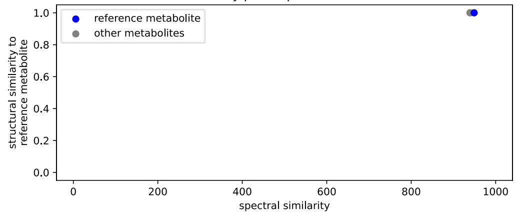


Sumiki's acid

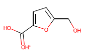
Spectra of protonated HMDB0002432, spectral sim. = 949, #1



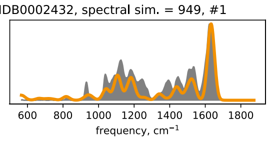
Structural similarity plot of protonated HMDB0002432



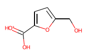
protonated HMDB0002432, spectral sim. = 949, #1



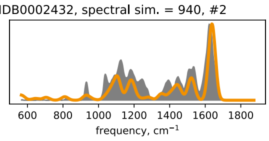
0.0 kJ/mol
Sumiki's acid



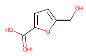
protonated HMDB0002432, spectral sim. = 940, #2



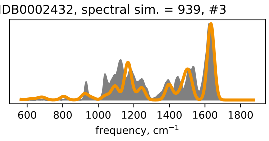
1.9 kJ/mol
Sumiki's acid



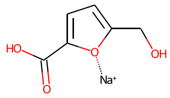
protonated HMDB0002432, spectral sim. = 939, #3



8.5 kJ/mol
Sumiki's acid

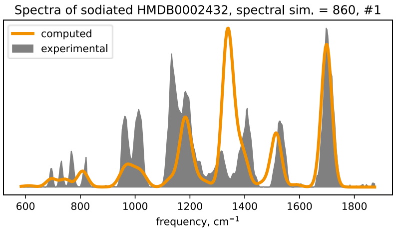


151 sodiated HMDB0002432

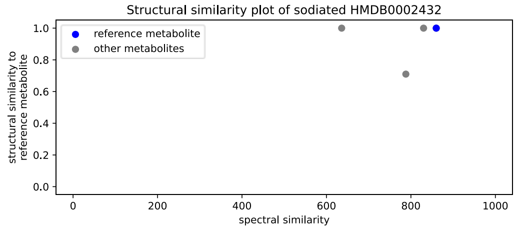


Sumiki's acid

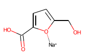
Spectra of sodiated HMDB0002432, spectral sim. = 860, #1



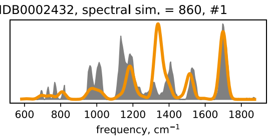
Structural similarity plot of sodiated HMDB0002432



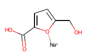
sodiated HMDB0002432, spectral sim. = 860, #1



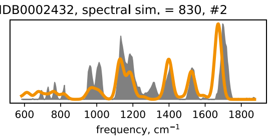
34.3 kJ/mol
Sumiki's acid



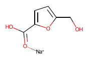
sodiated HMDB0002432, spectral sim. = 830, #2



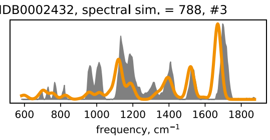
0.0 kJ/mol
Sumiki's acid



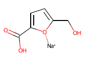
sodiated HMDB0002432, spectral sim. = 788, #3



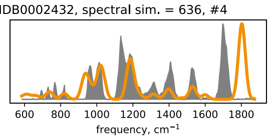
30.3 kJ/mol
Sumiki's acid



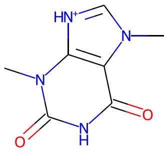
sodiated HMDB0002432, spectral sim. = 636, #4



11.9 kJ/mol
Sumiki's acid

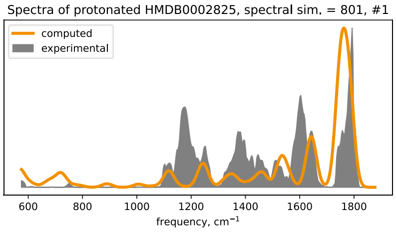


152 protonated HMDB0002825

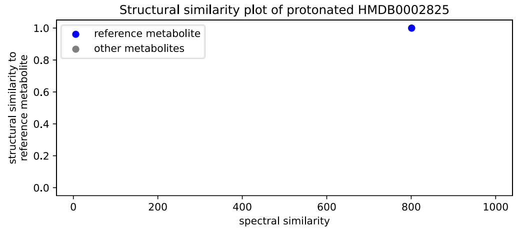


Theobromine

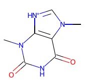
Spectra of protonated HMDB0002825, spectral sim. = 801, #1



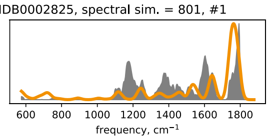
Structural similarity plot of protonated HMDB0002825



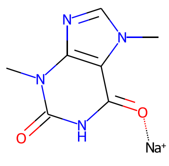
protonated HMDB0002825, spectral sim. = 801, #1



0.0 kJ/mol
Theobromine

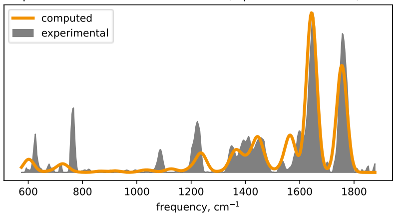


153 sodiated HMDB0002825

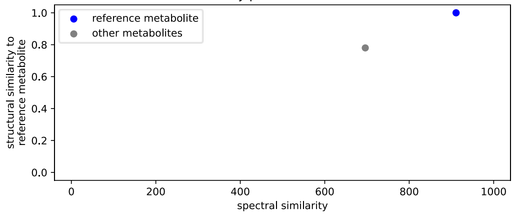


Theobromine

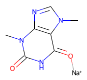
Spectra of sodiated HMDB0002825, spectral sim. = 911, #1



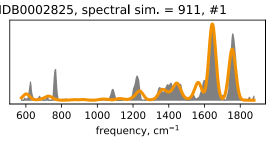
Structural similarity plot of sodiated HMDB0002825



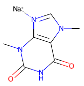
sodiated HMDB0002825, spectral sim. = 911, #1



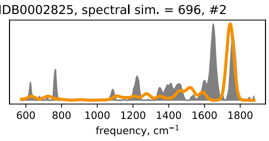
0.0 kJ/mol
Theobromine



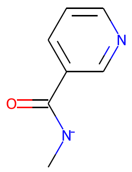
sodiated HMDB0002825, spectral sim. = 696, #2



24.2 kJ/mol
Theobromine

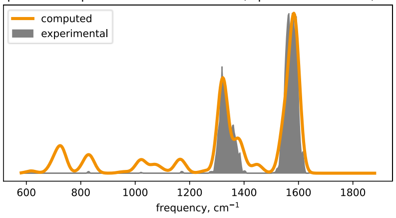


154 deprotonated HMDB0003152

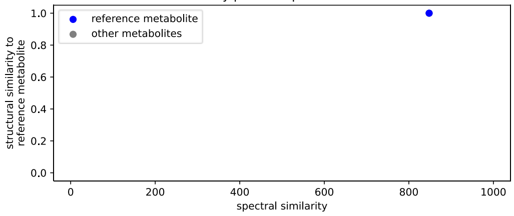


N-Methylnicotinamide

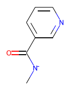
Spectra of deprotonated HMDB0003152, spectral sim. = 848, #1



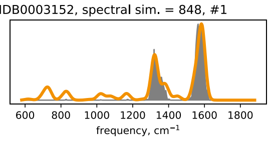
Structural similarity plot of deprotonated HMDB0003152



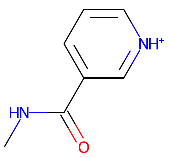
deprotonated HMDB0003152, spectral sim. = 848, #1



0.0 kJ/mol
N-Methylnicotinamide

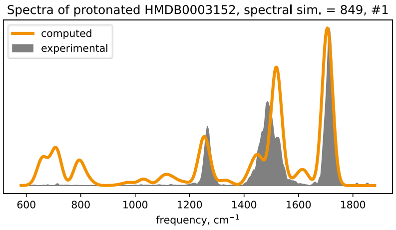


155 protonated HMDB0003152

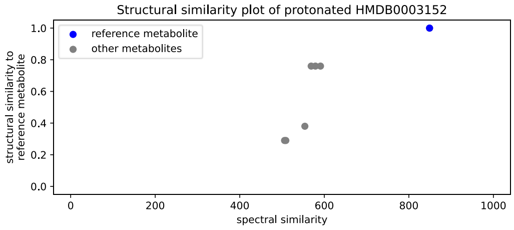


N-Methylnicotinamide

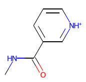
Spectra of protonated HMDB0003152, spectral sim. = 849, #1



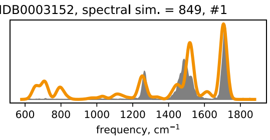
Structural similarity plot of protonated HMDB0003152



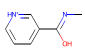
protonated HMDB0003152, spectral sim. = 849, #1



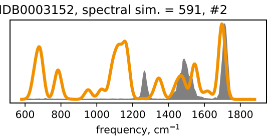
0.0 kJ/mol
N-Methylnicotinamide



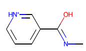
protonated HMDB0003152, spectral sim. = 591, #2



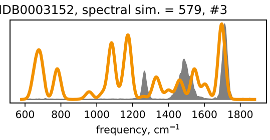
45.6 kJ/mol
N-Methylnicotinamide



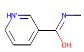
protonated HMDB0003152, spectral sim. = 579, #3



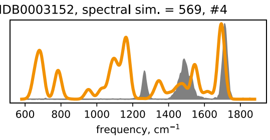
45.1 kJ/mol
N-Methylnicotinamide



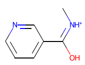
protonated HMDB0003152, spectral sim. = 569, #4



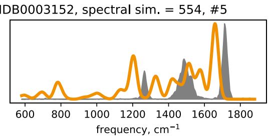
40.9 kJ/mol
N-Methylnicotinamide



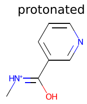
protonated HMDB0003152, spectral sim. = 554, #5



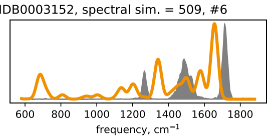
50.8 kJ/mol
N-Methylnicotinamide



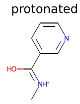
protonated HMDB0003152, spectral sim. = 509, #6



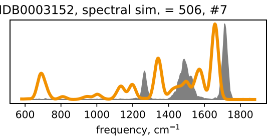
41.8 kJ/mol
N-Methylnicotinamide

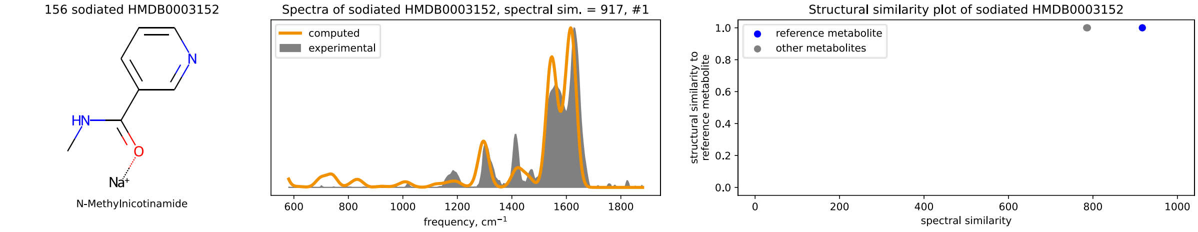


protonated HMDB0003152, spectral sim. = 506, #7

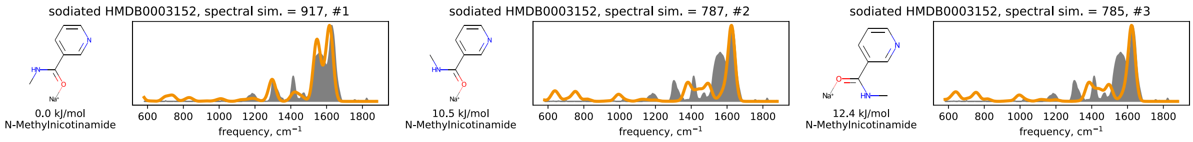


40.8 kJ/mol
N-Methylnicotinamide

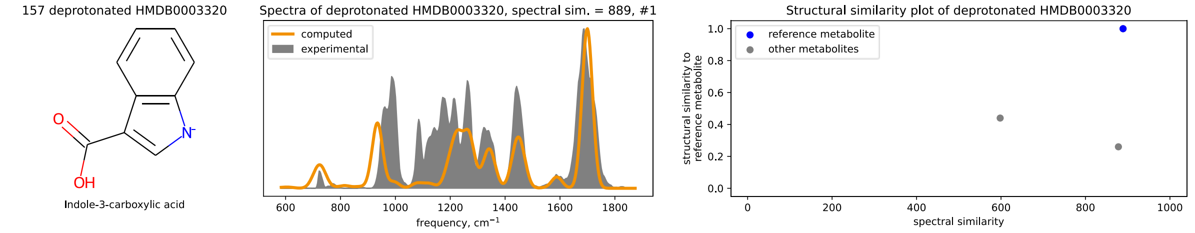




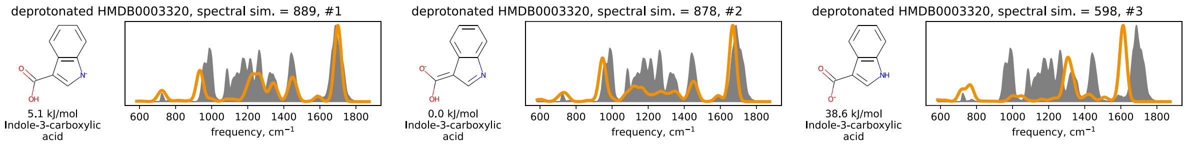
156 sodiated HMDB0003152
N-Methylnicotinamide
Spectra of sodiated HMDB0003152, spectral sim. = 917, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of sodiated HMDB0003152
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity



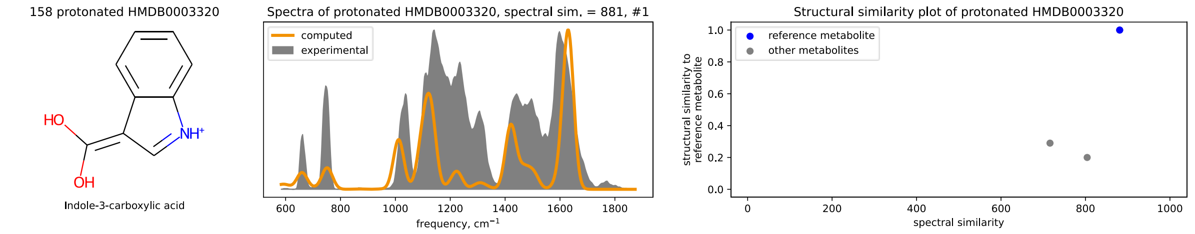
sodiated HMDB0003152, spectral sim. = 917, #1
0.0 kJ/mol
N-Methylnicotinamide
sodiated HMDB0003152, spectral sim. = 787, #2
10.5 kJ/mol
N-Methylnicotinamide
sodiated HMDB0003152, spectral sim. = 785, #3
12.4 kJ/mol
N-Methylnicotinamide
frequency, cm⁻¹



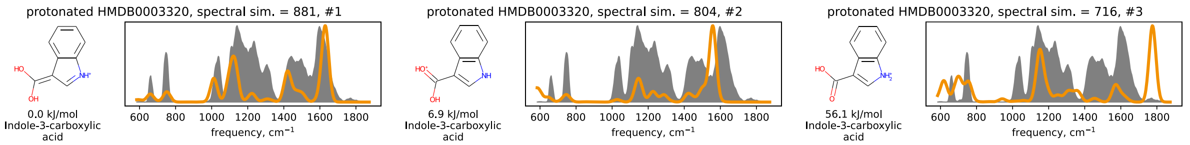
157 deprotonated HMDB0003320
Indole-3-carboxylic acid
Spectra of deprotonated HMDB0003320, spectral sim. = 889, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of deprotonated HMDB0003320
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity



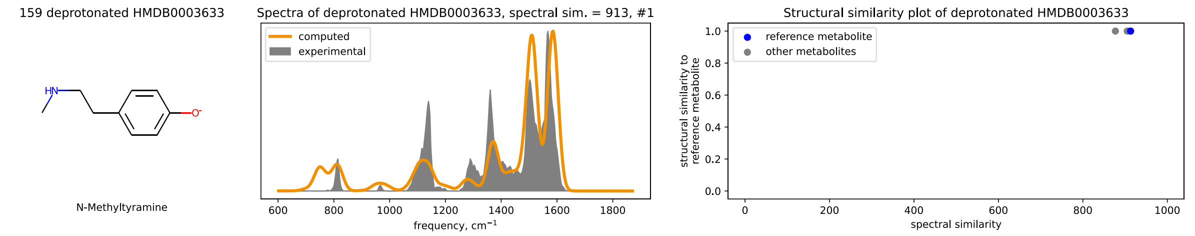
deprotonated HMDB0003320, spectral sim. = 889, #1
5.1 kJ/mol
Indole-3-carboxylic acid
deprotonated HMDB0003320, spectral sim. = 878, #2
0.0 kJ/mol
Indole-3-carboxylic acid
deprotonated HMDB0003320, spectral sim. = 598, #3
38.6 kJ/mol
Indole-3-carboxylic acid
frequency, cm⁻¹



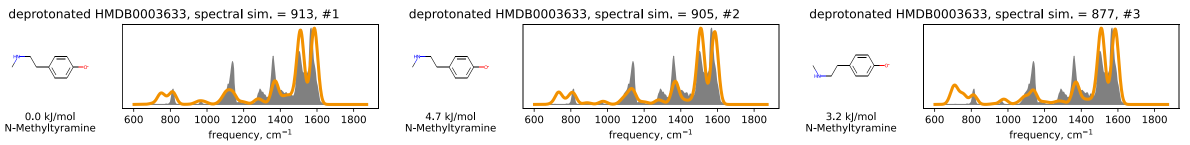
158 protonated HMDB0003320
Indole-3-carboxylic acid
Spectra of protonated HMDB0003320, spectral sim. = 881, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of protonated HMDB0003320
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity



protonated HMDB0003320, spectral sim. = 881, #1
0.0 kJ/mol
Indole-3-carboxylic acid
protonated HMDB0003320, spectral sim. = 804, #2
6.9 kJ/mol
Indole-3-carboxylic acid
protonated HMDB0003320, spectral sim. = 716, #3
56.1 kJ/mol
Indole-3-carboxylic acid
frequency, cm⁻¹

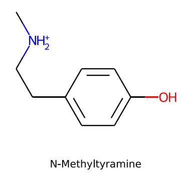


159 deprotonated HMDB0003633
N-Methyltyramine
Spectra of deprotonated HMDB0003633, spectral sim. = 913, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of deprotonated HMDB0003633
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

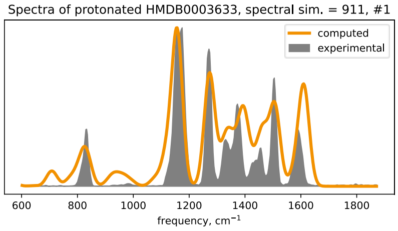


deprotonated HMDB0003633, spectral sim. = 913, #1
0.0 kJ/mol
N-Methyltyramine
deprotonated HMDB0003633, spectral sim. = 905, #2
4.7 kJ/mol
N-Methyltyramine
deprotonated HMDB0003633, spectral sim. = 877, #3
3.2 kJ/mol
N-Methyltyramine
frequency, cm⁻¹

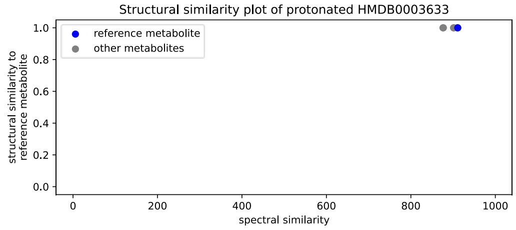
160 protonated HMDB0003633



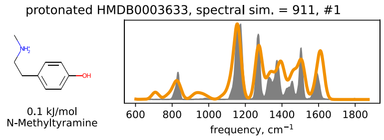
Spectra of protonated HMDB0003633, spectral sim. = 911, #1



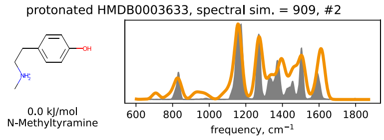
Structural similarity plot of protonated HMDB0003633



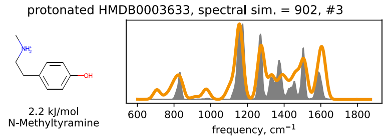
protonated HMDB0003633, spectral sim. = 911, #1



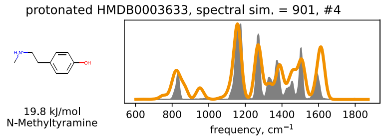
protonated HMDB0003633, spectral sim. = 909, #2



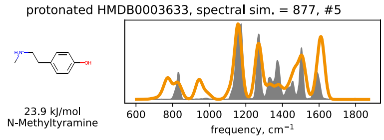
protonated HMDB0003633, spectral sim. = 902, #3



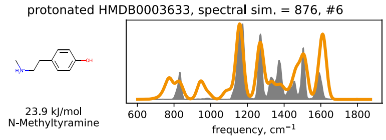
protonated HMDB0003633, spectral sim. = 901, #4



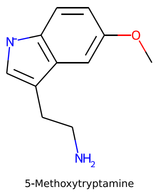
protonated HMDB0003633, spectral sim. = 877, #5



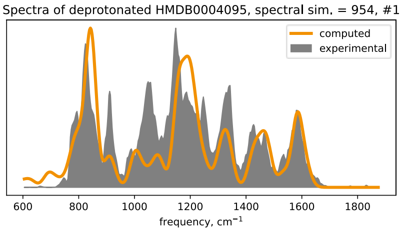
protonated HMDB0003633, spectral sim. = 876, #6



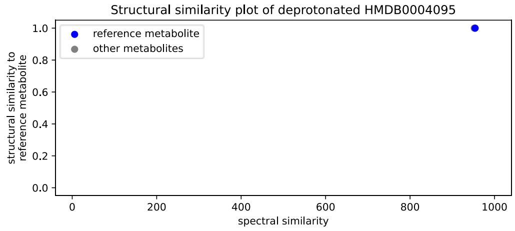
161 deprotonated HMDB0004095



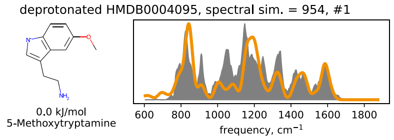
Spectra of deprotonated HMDB0004095, spectral sim. = 954, #1



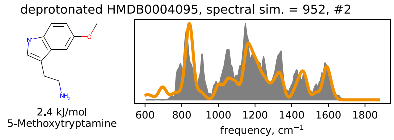
Structural similarity plot of deprotonated HMDB0004095



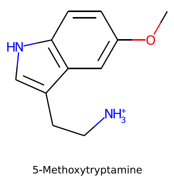
deprotonated HMDB0004095, spectral sim. = 954, #1



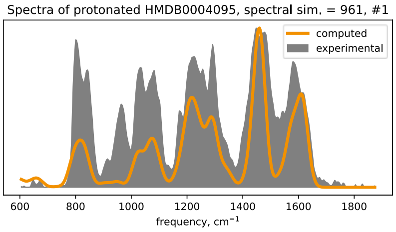
deprotonated HMDB0004095, spectral sim. = 952, #2



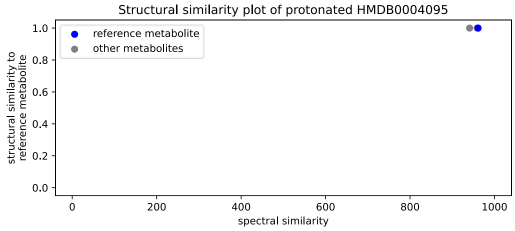
162 protonated HMDB0004095



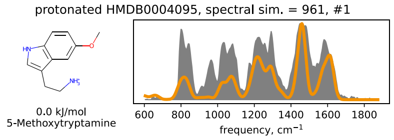
Spectra of protonated HMDB0004095, spectral sim. = 961, #1



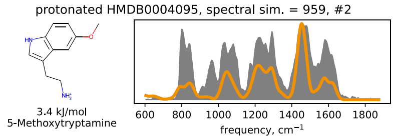
Structural similarity plot of protonated HMDB0004095



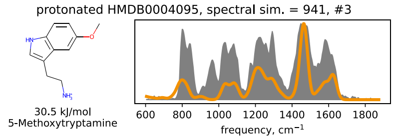
protonated HMDB0004095, spectral sim. = 961, #1



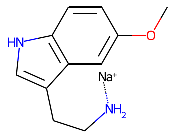
protonated HMDB0004095, spectral sim. = 959, #2



protonated HMDB0004095, spectral sim. = 941, #3

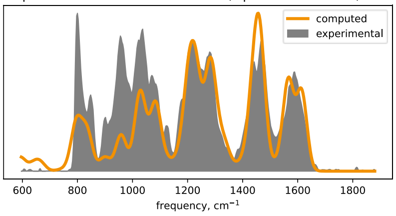


163 sodiated HMDB0004095

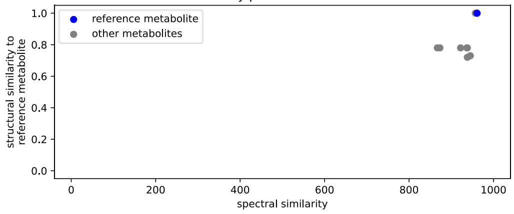


5-Methoxytryptamine

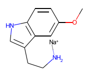
Spectra of sodiated HMDB0004095, spectral sim. = 961, #1



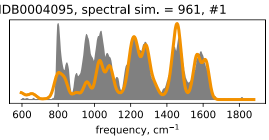
Structural similarity plot of sodiated HMDB0004095



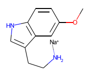
sodiated HMDB0004095, spectral sim. = 961, #1



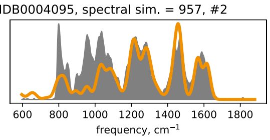
1.6 kJ/mol
5-Methoxytryptamine



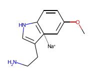
sodiated HMDB0004095, spectral sim. = 957, #2



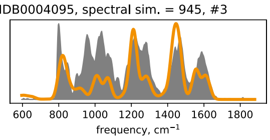
0.0 kJ/mol
5-Methoxytryptamine



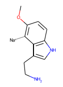
sodiated HMDB0004095, spectral sim. = 945, #3



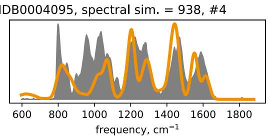
53.8 kJ/mol
5-Methoxytryptamine



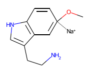
sodiated HMDB0004095, spectral sim. = 938, #4



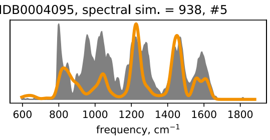
55.9 kJ/mol
5-Methoxytryptamine



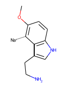
sodiated HMDB0004095, spectral sim. = 938, #5



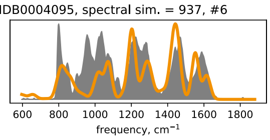
50.5 kJ/mol
5-Methoxytryptamine



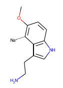
sodiated HMDB0004095, spectral sim. = 937, #6



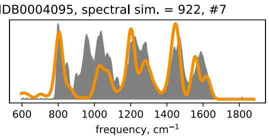
57.4 kJ/mol
5-Methoxytryptamine



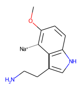
sodiated HMDB0004095, spectral sim. = 922, #7



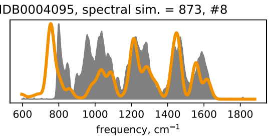
65.2 kJ/mol
5-Methoxytryptamine



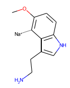
sodiated HMDB0004095, spectral sim. = 873, #8



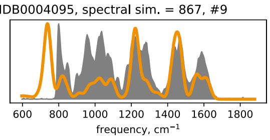
63.0 kJ/mol
5-Methoxytryptamine



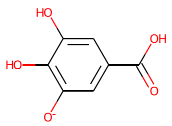
sodiated HMDB0004095, spectral sim. = 867, #9



62.0 kJ/mol
5-Methoxytryptamine

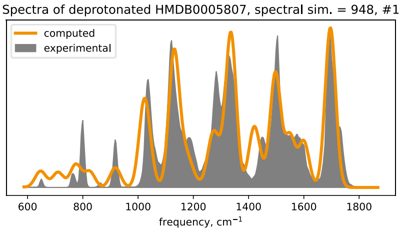


164 deprotonated HMDB0005807

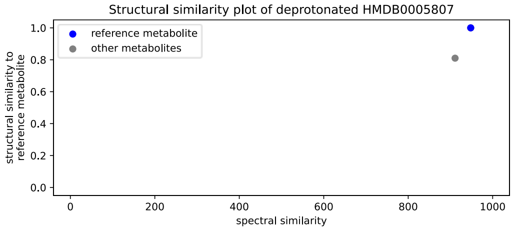


Gallic acid

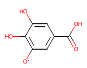
Spectra of deprotonated HMDB0005807, spectral sim. = 948, #1



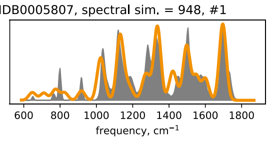
Structural similarity plot of deprotonated HMDB0005807



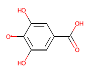
deprotonated HMDB0005807, spectral sim. = 948, #1



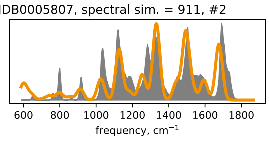
47.6 kJ/mol
Gallic acid



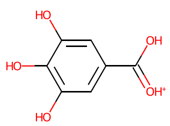
deprotonated HMDB0005807, spectral sim. = 911, #2



0.0 kJ/mol
Gallic acid

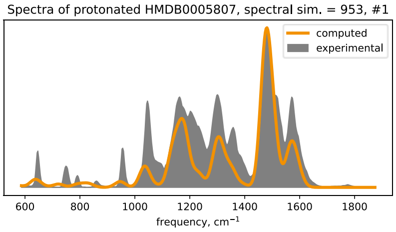


165 protonated HMDB0005807

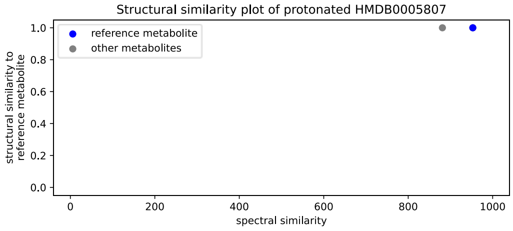


Gallic acid

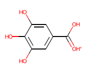
Spectra of protonated HMDB0005807, spectral sim. = 953, #1



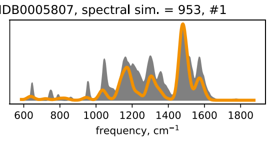
Structural similarity plot of protonated HMDB0005807



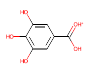
protonated HMDB0005807, spectral sim. = 953, #1



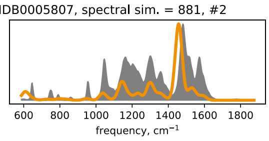
0.0 kJ/mol
Gallic acid



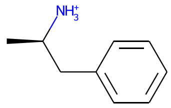
protonated HMDB0005807, spectral sim. = 881, #2



22.2 kJ/mol
Gallic acid

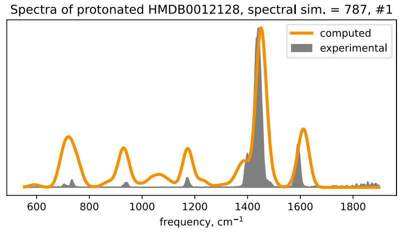


166 protonated HMDB0012128

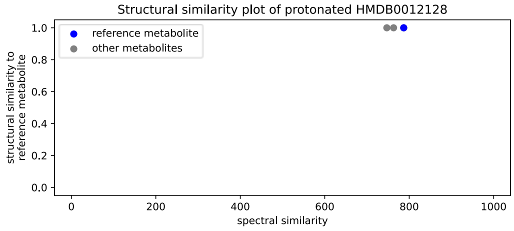


(R)-Amphetamine

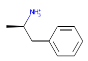
Spectra of protonated HMDB0012128, spectral sim. = 787, #1



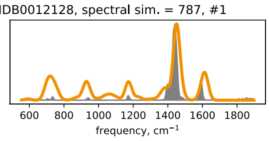
Structural similarity plot of protonated HMDB0012128



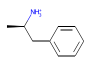
protonated HMDB0012128, spectral sim. = 787, #1



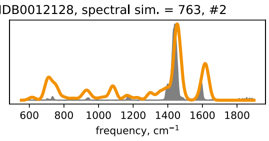
0.0 kJ/mol
(R)-Amphetamine



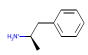
protonated HMDB0012128, spectral sim. = 763, #2



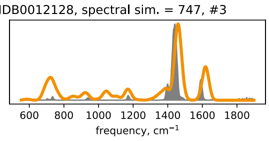
6.5 kJ/mol
(R)-Amphetamine



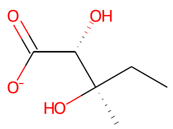
protonated HMDB0012128, spectral sim. = 747, #3



19.1 kJ/mol
(R)-Amphetamine

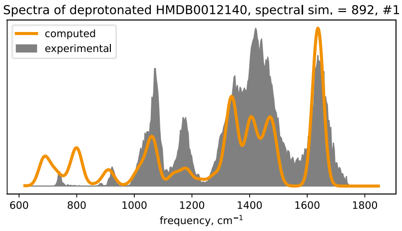


167 deprotonated HMDB0012140

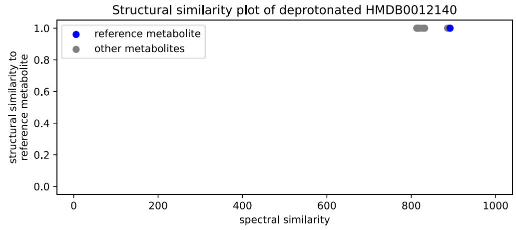


(R) 2,3-Dihydroxy-3-methylvalerate

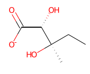
Spectra of deprotonated HMDB0012140, spectral sim. = 892, #1



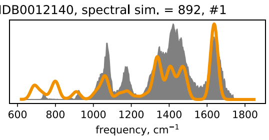
Structural similarity plot of deprotonated HMDB0012140



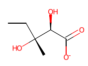
deprotonated HMDB0012140, spectral sim. = 892, #1



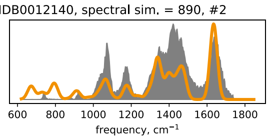
6.7 kJ/mol
(R)
2,3-Dihydroxy-3-methylvalerate



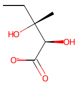
deprotonated HMDB0012140, spectral sim. = 890, #2



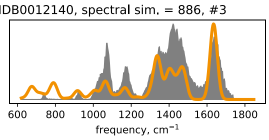
0.0 kJ/mol
(R)
2,3-Dihydroxy-3-methylvalerate



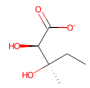
deprotonated HMDB0012140, spectral sim. = 886, #3



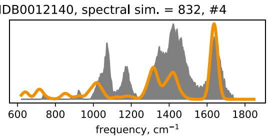
2.2 kJ/mol
(R)
2,3-Dihydroxy-3-methylvalerate



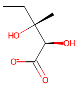
deprotonated HMDB0012140, spectral sim. = 832, #4



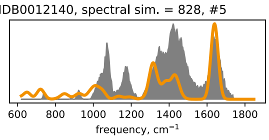
24.7 kJ/mol
(R)
2,3-Dihydroxy-3-methylvalerate



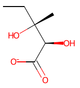
deprotonated HMDB0012140, spectral sim. = 828, #5



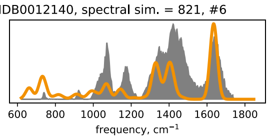
25.7 kJ/mol
(R)
2,3-Dihydroxy-3-methylvalerate



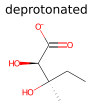
deprotonated HMDB0012140, spectral sim. = 821, #6



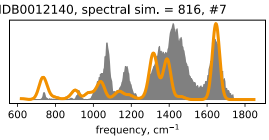
28.2 kJ/mol
(R)
2,3-Dihydroxy-3-methylvalerate



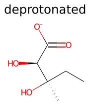
deprotonated HMDB0012140, spectral sim. = 816, #7



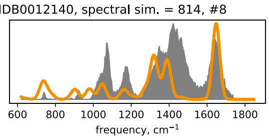
22.0 kJ/mol
(R)
2,3-Dihydroxy-3-methylvalerate



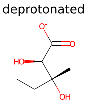
deprotonated HMDB0012140, spectral sim. = 814, #8



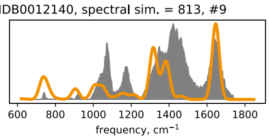
17.9 kJ/mol
(R)
2,3-Dihydroxy-3-methylvalerate

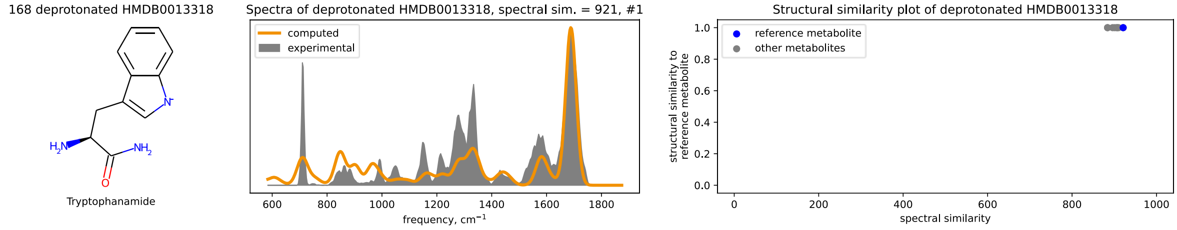


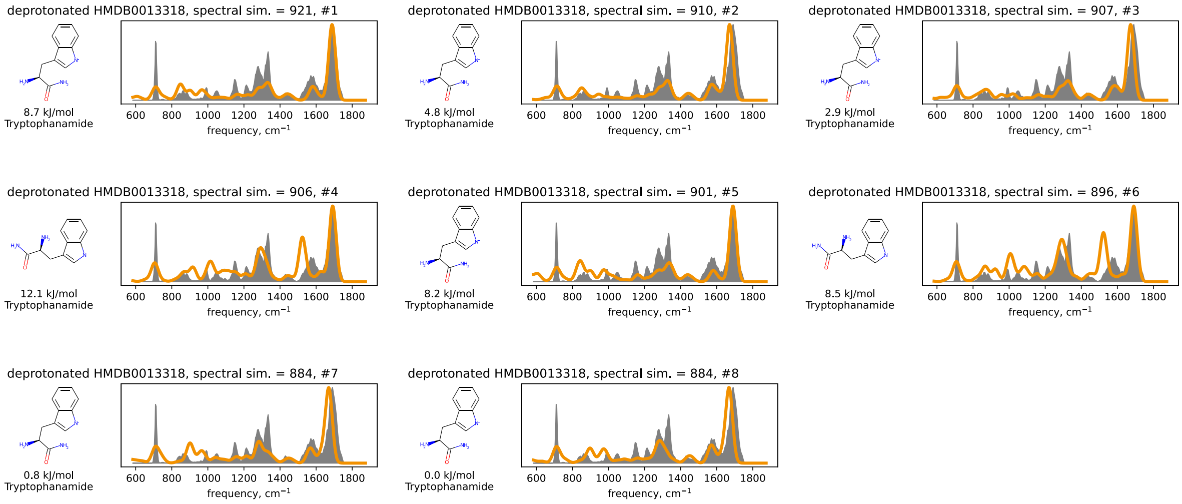
deprotonated HMDB0012140, spectral sim. = 813, #9

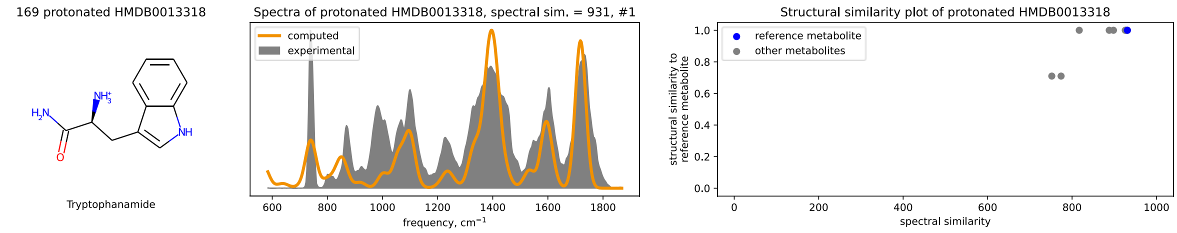


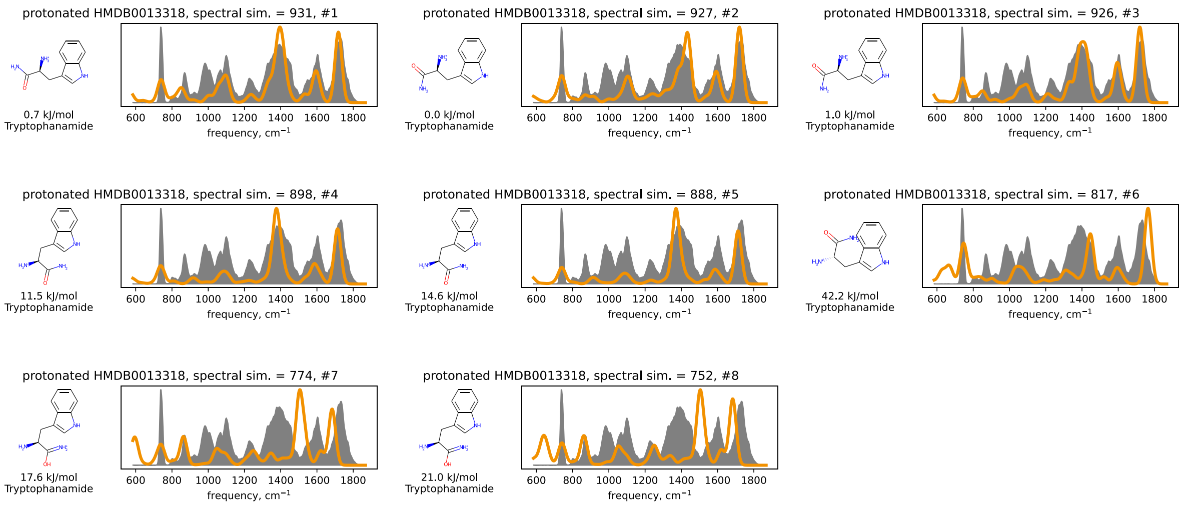
21.1 kJ/mol
(R)
2,3-Dihydroxy-3-methylvalerate



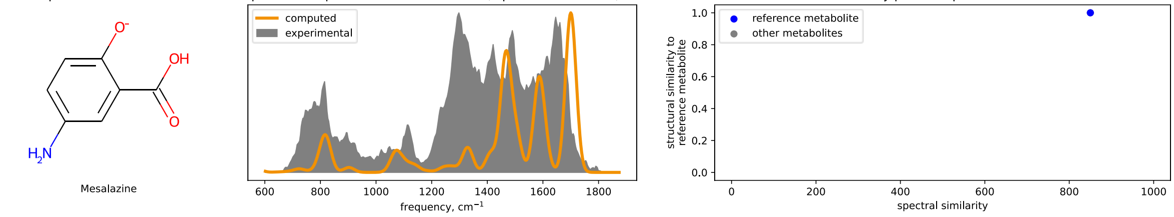

168 deprotonated HMDB0013318
Tryptophanamide
Spectra of deprotonated HMDB0013318, spectral sim. = 921, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of deprotonated HMDB0013318
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity


deprotonated HMDB0013318, spectral sim. = 921, #1
8.7 kJ/mol
Tryptophanamide
deprotonated HMDB0013318, spectral sim. = 910, #2
4.8 kJ/mol
Tryptophanamide
deprotonated HMDB0013318, spectral sim. = 907, #3
2.9 kJ/mol
Tryptophanamide
deprotonated HMDB0013318, spectral sim. = 906, #4
12.1 kJ/mol
Tryptophanamide
deprotonated HMDB0013318, spectral sim. = 901, #5
8.2 kJ/mol
Tryptophanamide
deprotonated HMDB0013318, spectral sim. = 896, #6
8.5 kJ/mol
Tryptophanamide
deprotonated HMDB0013318, spectral sim. = 884, #7
0.8 kJ/mol
Tryptophanamide
deprotonated HMDB0013318, spectral sim. = 884, #8
0.0 kJ/mol
Tryptophanamide
frequency, cm⁻¹

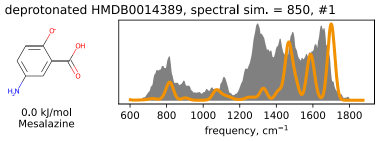

169 protonated HMDB0013318
Tryptophanamide
Spectra of protonated HMDB0013318, spectral sim. = 931, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of protonated HMDB0013318
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity


protonated HMDB0013318, spectral sim. = 931, #1
0.7 kJ/mol
Tryptophanamide
protonated HMDB0013318, spectral sim. = 927, #2
0.0 kJ/mol
Tryptophanamide
protonated HMDB0013318, spectral sim. = 926, #3
1.0 kJ/mol
Tryptophanamide
protonated HMDB0013318, spectral sim. = 898, #4
11.5 kJ/mol
Tryptophanamide
protonated HMDB0013318, spectral sim. = 888, #5
14.6 kJ/mol
Tryptophanamide
protonated HMDB0013318, spectral sim. = 817, #6
42.2 kJ/mol
Tryptophanamide
protonated HMDB0013318, spectral sim. = 774, #7
17.6 kJ/mol
Tryptophanamide
protonated HMDB0013318, spectral sim. = 752, #8
21.0 kJ/mol
Tryptophanamide
frequency, cm⁻¹

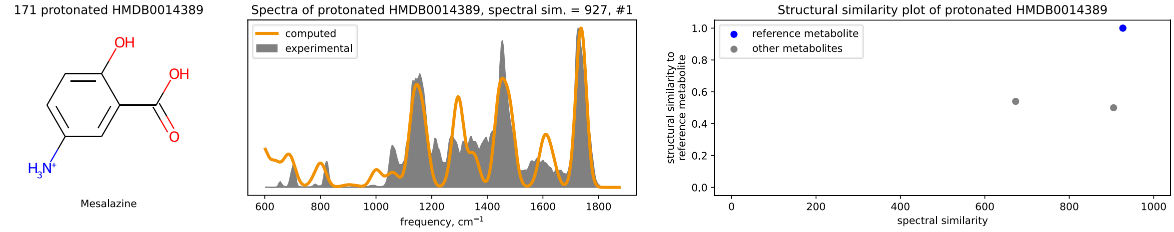
170 deprotonated HMDB0014389 | Spectra of deprotonated HMDB0014389, spectral sim. = 850, #1 | Structural similarity plot of deprotonated HMDB0014389



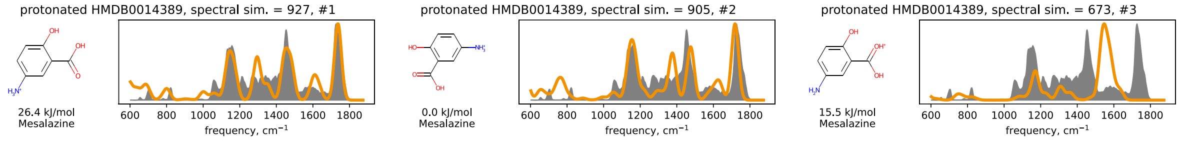
deprotonated HMDB0014389, spectral sim. = 850, #1



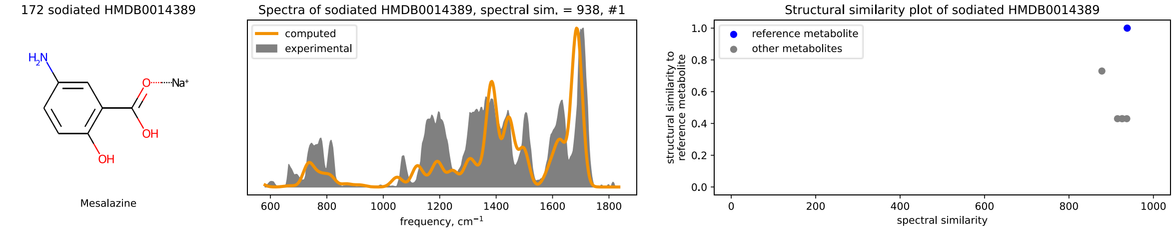
171 protonated HMDB0014389 | Spectra of protonated HMDB0014389, spectral sim. = 927, #1 | Structural similarity plot of protonated HMDB0014389



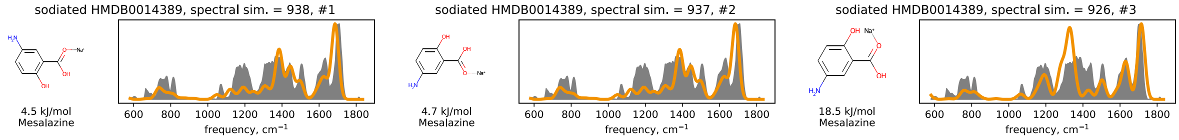
protonated HMDB0014389, spectral sim. = 927, #1 | protonated HMDB0014389, spectral sim. = 905, #2 | protonated HMDB0014389, spectral sim. = 673, #3



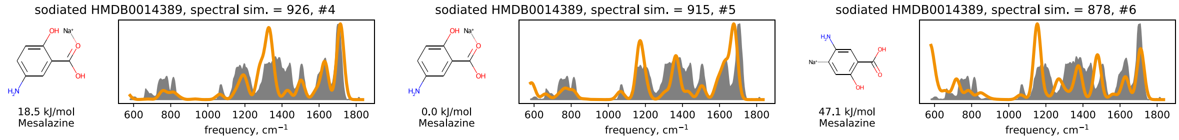
172 sodiated HMDB0014389 | Spectra of sodiated HMDB0014389, spectral sim. = 938, #1 | Structural similarity plot of sodiated HMDB0014389

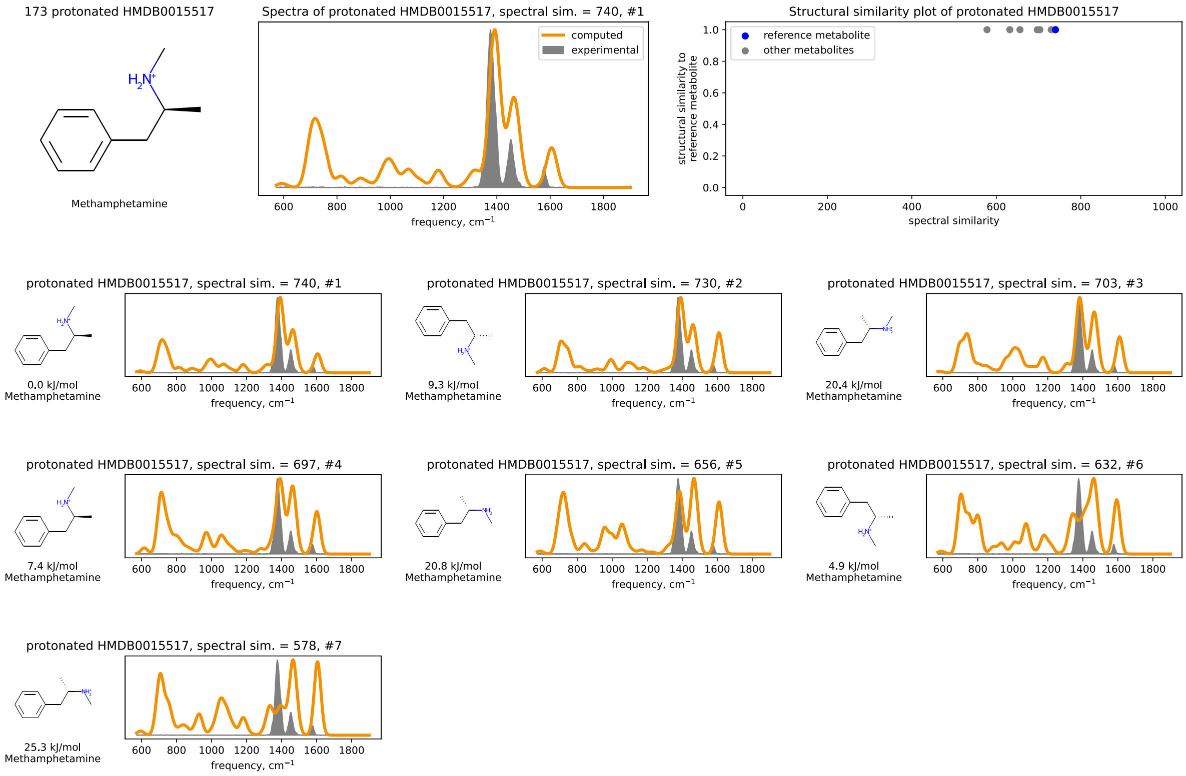


sodiated HMDB0014389, spectral sim. = 938, #1 | sodiated HMDB0014389, spectral sim. = 937, #2 | sodiated HMDB0014389, spectral sim. = 926, #3



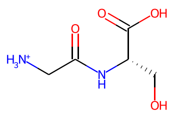
sodiated HMDB0014389, spectral sim. = 926, #4 | sodiated HMDB0014389, spectral sim. = 915, #5 | sodiated HMDB0014389, spectral sim. = 878, #6





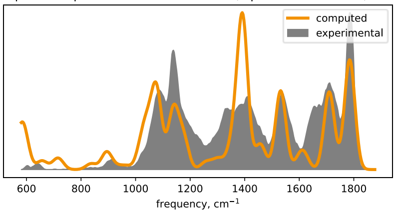
173 protonated HMDB0015517
Methamphetamine
Spectra of protonated HMDB0015517, spectral sim. = 740, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of protonated HMDB0015517
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
protonated HMDB0015517, spectral sim. = 740, #1
0.0 kJ/mol
Methamphetamine
protonated HMDB0015517, spectral sim. = 730, #2
9.3 kJ/mol
Methamphetamine
protonated HMDB0015517, spectral sim. = 703, #3
20.4 kJ/mol
Methamphetamine
protonated HMDB0015517, spectral sim. = 697, #4
7.4 kJ/mol
Methamphetamine
protonated HMDB0015517, spectral sim. = 656, #5
20.8 kJ/mol
Methamphetamine
protonated HMDB0015517, spectral sim. = 632, #6
4.9 kJ/mol
Methamphetamine
protonated HMDB0015517, spectral sim. = 578, #7
25.3 kJ/mol
Methamphetamine

174 protonated HMDB0028850

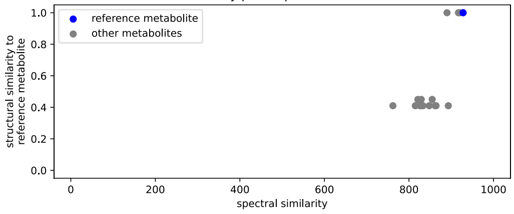


Glycyl-Serine

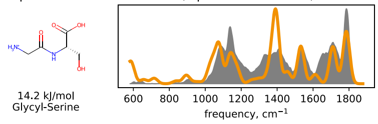
Spectra of protonated HMDB0028850, spectral sim. = 928, #1



Structural similarity plot of protonated HMDB0028850

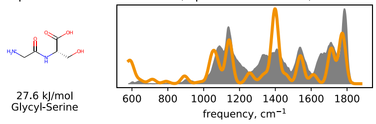


protonated HMDB0028850, spectral sim. = 928, #1



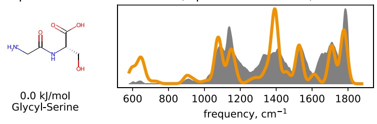
14.2 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 920, #2



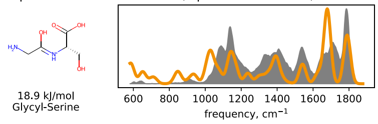
27.6 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 917, #3



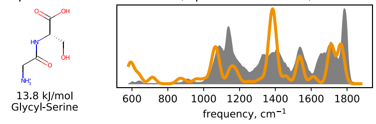
0.0 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 893, #4



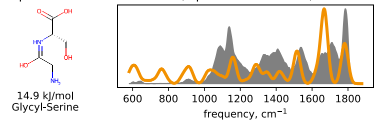
18.9 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 890, #5



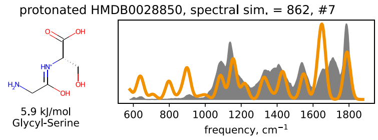
13.8 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 864, #6



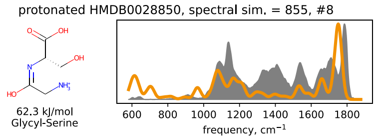
14.9 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 862, #7



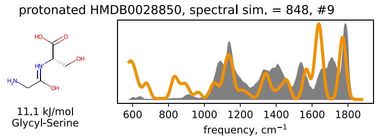
5.9 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 855, #8



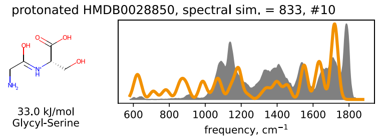
62.3 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 848, #9



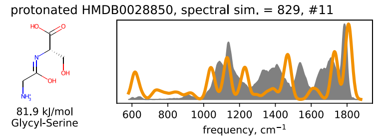
11.1 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 833, #10



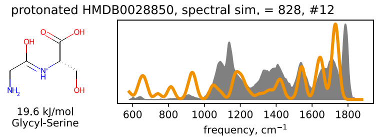
33.0 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 829, #11



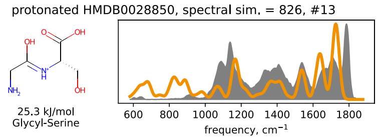
81.9 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 828, #12



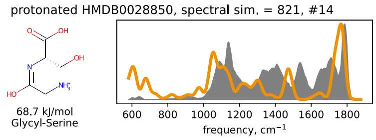
19.6 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 826, #13



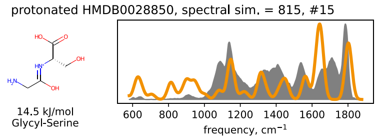
25.3 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 821, #14



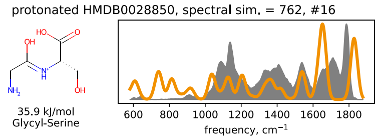
68.7 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 815, #15



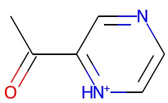
14.5 kJ/mol
Glycyl-Serine

protonated HMDB0028850, spectral sim. = 762, #16



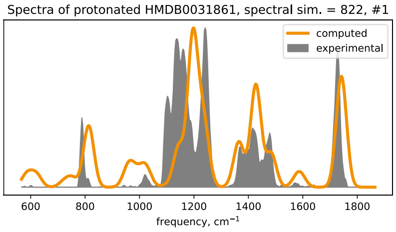
35.9 kJ/mol
Glycyl-Serine

175 protonated HMDB0031861

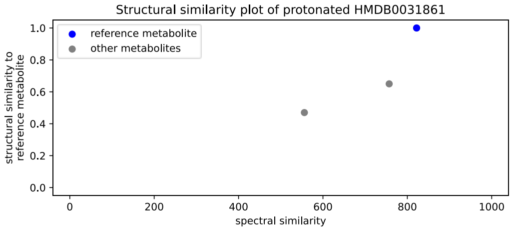


2-Acetylpyrazine

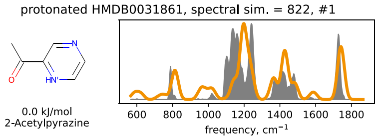
Spectra of protonated HMDB0031861, spectral sim. = 822, #1



Structural similarity plot of protonated HMDB0031861

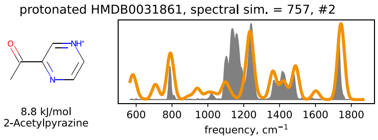


protonated HMDB0031861, spectral sim. = 822, #1



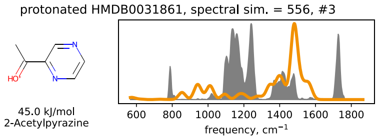
0.0 kJ/mol
2-Acetylpyrazine

protonated HMDB0031861, spectral sim. = 757, #2

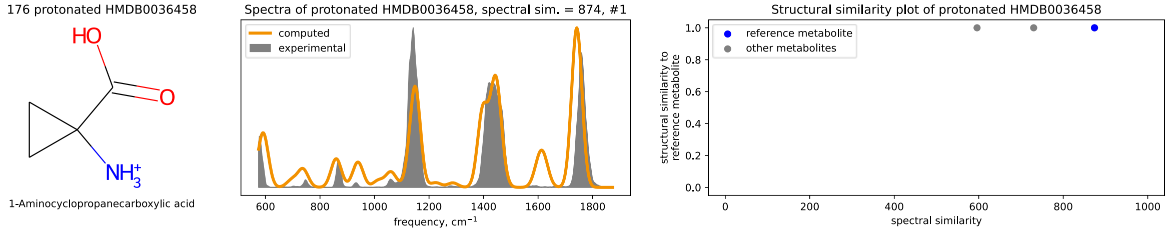


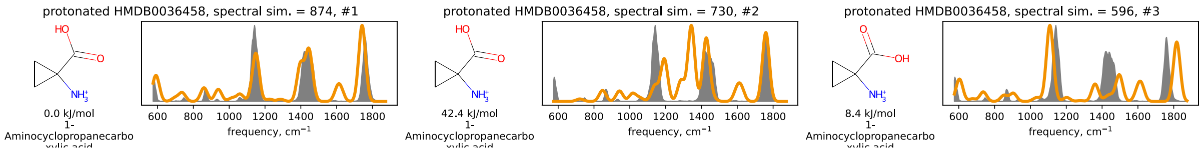
8.8 kJ/mol
2-Acetylpyrazine

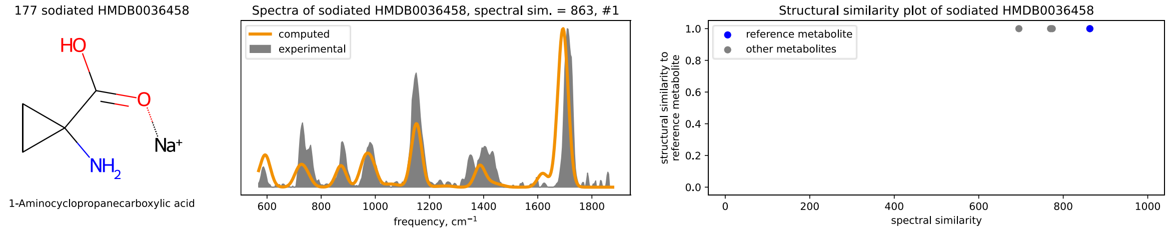
protonated HMDB0031861, spectral sim. = 556, #3

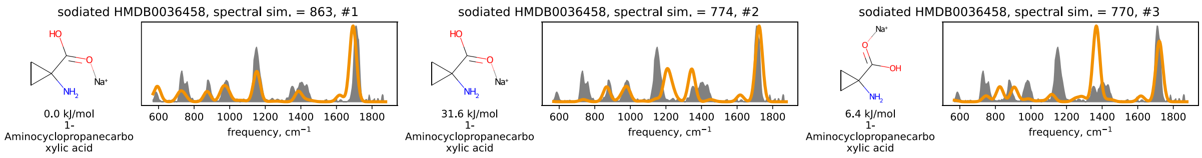


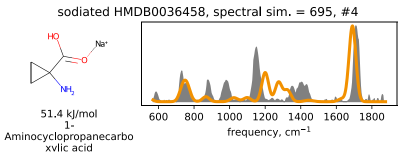
45.0 kJ/mol
2-Acetylpyrazine

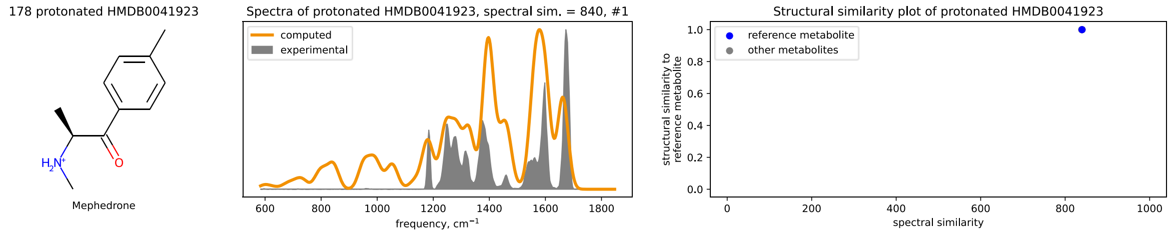

176 protonated HMDB0036458
HO
O
NH3+
1-Aminocyclopropanecarboxylic acid
Spectra of protonated HMDB0036458, spectral sim. = 874, #1
computed
experimental
frequency, cm−1
Structural similarity plot of protonated HMDB0036458
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

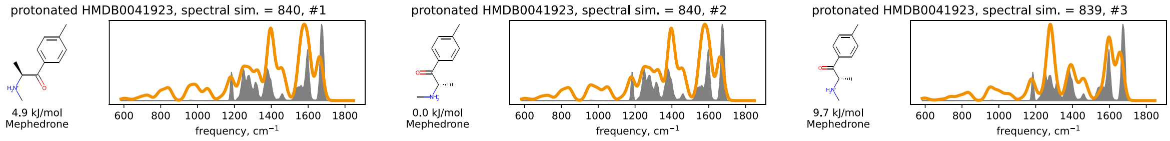

protonated HMDB0036458, spectral sim. = 874, #1
0.0 kJ/mol
1-Aminocyclopropanecarbo
frequency, cm−1
protonated HMDB0036458, spectral sim. = 730, #2
42.4 kJ/mol
1-Aminocyclopropanecarbo
frequency, cm−1
protonated HMDB0036458, spectral sim. = 596, #3
8.4 kJ/mol
1-Aminocyclopropanecarbo
frequency, cm−1


177 sodiated HMDB0036458
HO
O
Na+
NH2
1-Aminocyclopropanecarboxylic acid
Spectra of sodiated HMDB0036458, spectral sim. = 863, #1
computed
experimental
frequency, cm−1
Structural similarity plot of sodiated HMDB0036458
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

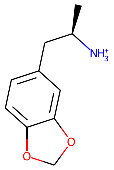

sodiated HMDB0036458, spectral sim. = 863, #1
0.0 kJ/mol
1-Aminocyclopropanecarboxylic acid
frequency, cm−1
sodiated HMDB0036458, spectral sim. = 774, #2
31.6 kJ/mol
1-Aminocyclopropanecarboxylic acid
frequency, cm−1
sodiated HMDB0036458, spectral sim. = 770, #3
6.4 kJ/mol
1-Aminocyclopropanecarboxylic acid
frequency, cm−1


sodiated HMDB0036458, spectral sim. = 695, #4
51.4 kJ/mol
1-Aminocyclopropanecarboxylic acid
frequency, cm−1


178 protonated HMDB0041923
H2N+
O
Mephedrone
Spectra of protonated HMDB0041923, spectral sim. = 840, #1
computed
experimental
frequency, cm−1
Structural similarity plot of protonated HMDB0041923
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

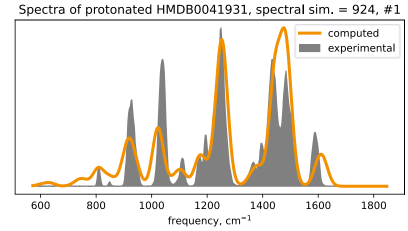

protonated HMDB0041923, spectral sim. = 840, #1
4.9 kJ/mol
Mephedrone
frequency, cm−1
protonated HMDB0041923, spectral sim. = 840, #2
0.0 kJ/mol
Mephedrone
frequency, cm−1
protonated HMDB0041923, spectral sim. = 839, #3
9.7 kJ/mol
Mephedrone
frequency, cm−1

179 protonated HMDB0041931

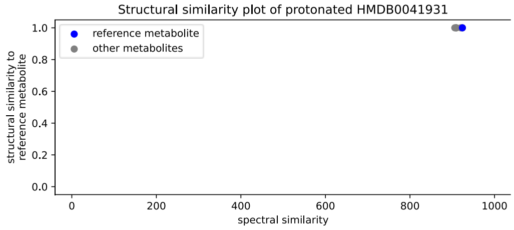


3,4-Methylenedioxyamphetamine

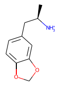
Spectra of protonated HMDB0041931, spectral sim. = 924, #1



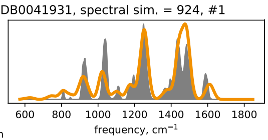
Structural similarity plot of protonated HMDB0041931



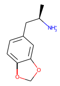
protonated HMDB0041931, spectral sim. = 924, #1



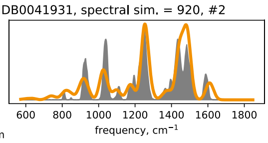
0.0 kJ/mol
3,4-Methylenedioxyamphetamine



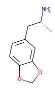
protonated HMDB0041931, spectral sim. = 920, #2



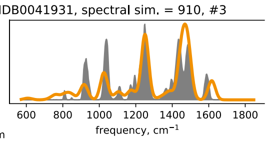
0.8 kJ/mol
3,4-Methylenedioxyamphetamine



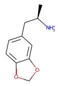
protonated HMDB0041931, spectral sim. = 910, #3



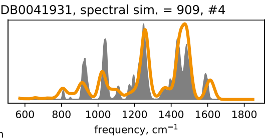
20.7 kJ/mol
3,4-Methylenedioxyamphetamine



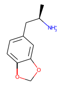
protonated HMDB0041931, spectral sim. = 909, #4



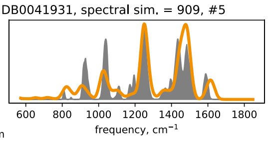
5.8 kJ/mol
3,4-Methylenedioxyamphetamine



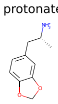
protonated HMDB0041931, spectral sim. = 909, #5



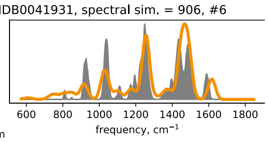
7.3 kJ/mol
3,4-Methylenedioxyamphetamine

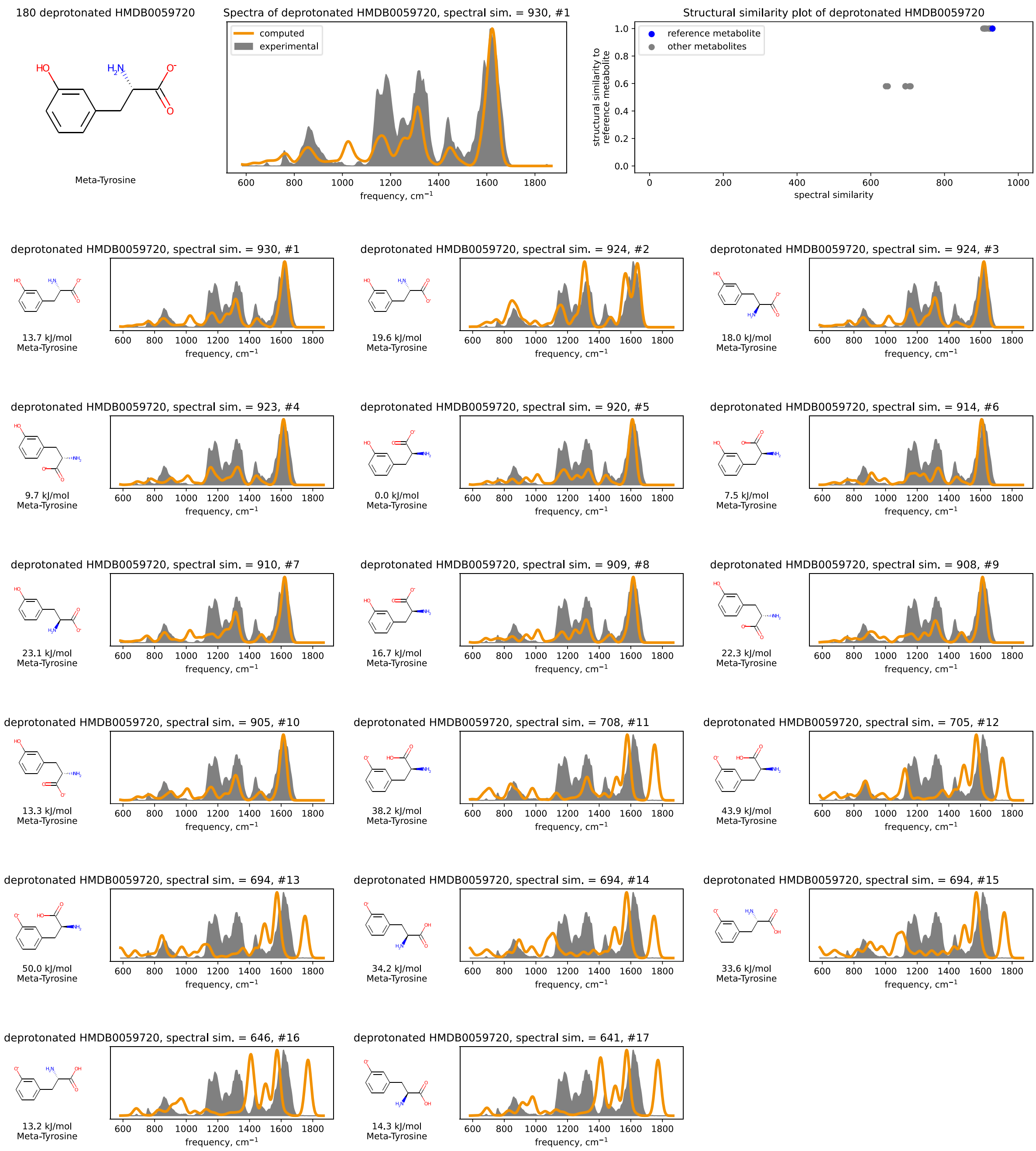


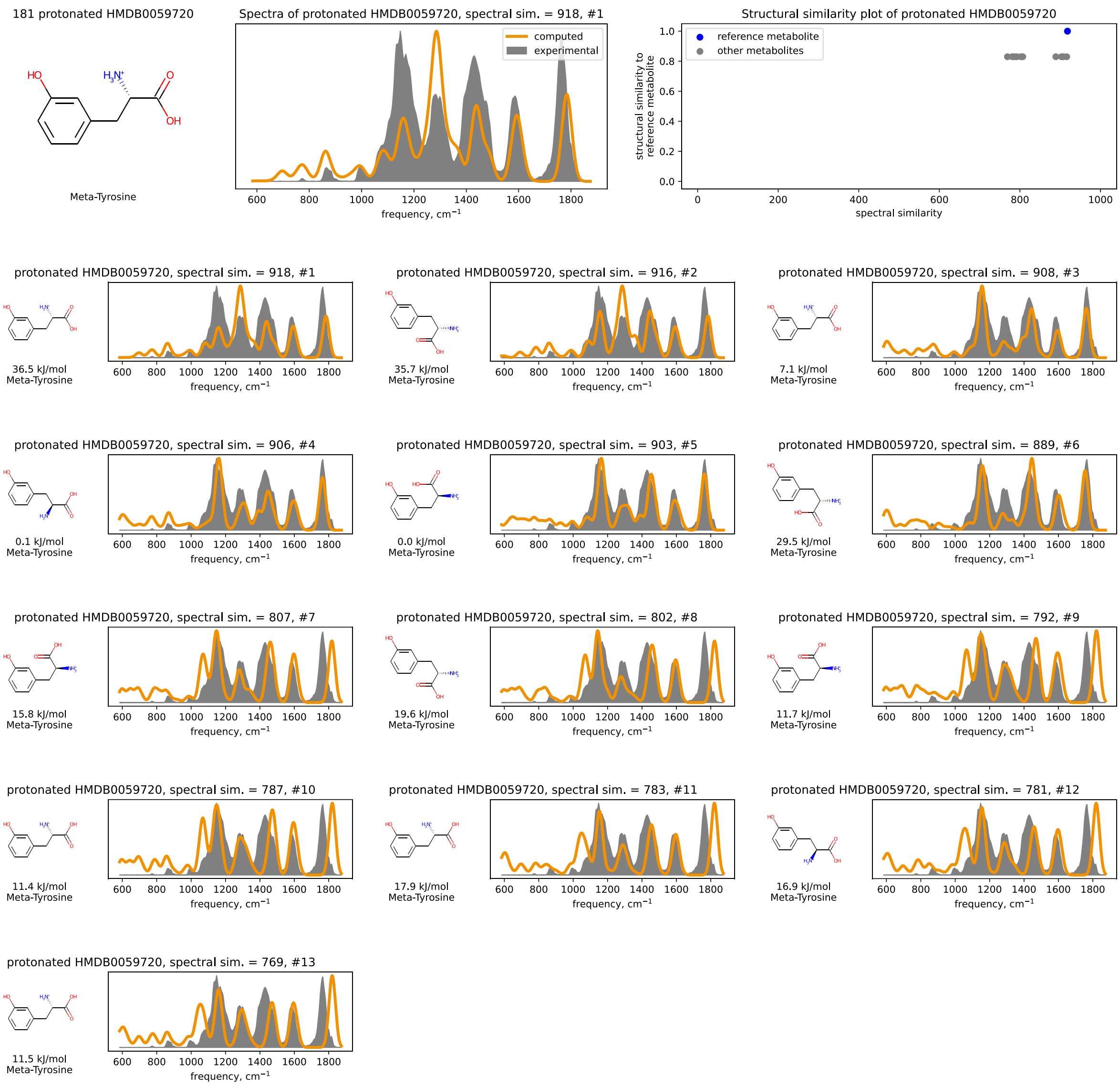
protonated HMDB0041931, spectral sim. = 906, #6



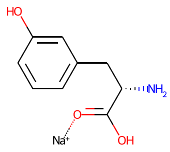
21.2 kJ/mol
3,4-Methylenedioxyamphetamine




180 deprotonated HMDB0059720
Meta-Tyrosine
Spectra of deprotonated HMDB0059720, spectral sim. = 930, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of deprotonated HMDB0059720
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
deprotonated HMDB0059720, spectral sim. = 930, #1
13.7 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 924, #2
19.6 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 924, #3
18.0 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 923, #4
9.7 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 920, #5
0.0 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 914, #6
7.5 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 910, #7
23.1 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 909, #8
16.7 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 908, #9
22.3 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 905, #10
13.3 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 708, #11
38.2 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 705, #12
43.9 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 694, #13
50.0 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 694, #14
34.2 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 694, #15
33.6 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 646, #16
13.2 kJ/mol
Meta-Tyrosine
deprotonated HMDB0059720, spectral sim. = 641, #17
14.3 kJ/mol
Meta-Tyrosine

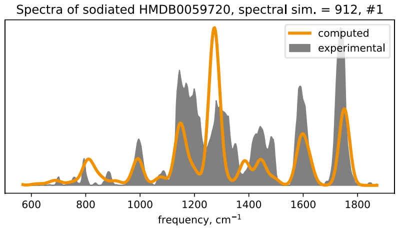

181 protonated HMDB0059720
Meta-Tyrosine
Spectra of protonated HMDB0059720, spectral sim. = 918, #1
computed
experimental
frequency, cm⁻¹
Structural similarity plot of protonated HMDB0059720
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity
protonated HMDB0059720, spectral sim. = 918, #1
36.5 kJ/mol
Meta-Tyrosine
protonated HMDB0059720, spectral sim. = 916, #2
35.7 kJ/mol
Meta-Tyrosine
protonated HMDB0059720, spectral sim. = 908, #3
7.1 kJ/mol
Meta-Tyrosine
protonated HMDB0059720, spectral sim. = 906, #4
0.1 kJ/mol
Meta-Tyrosine
protonated HMDB0059720, spectral sim. = 903, #5
0.0 kJ/mol
Meta-Tyrosine
protonated HMDB0059720, spectral sim. = 889, #6
29.5 kJ/mol
Meta-Tyrosine
protonated HMDB0059720, spectral sim. = 807, #7
15.8 kJ/mol
Meta-Tyrosine
protonated HMDB0059720, spectral sim. = 802, #8
19.6 kJ/mol
Meta-Tyrosine
protonated HMDB0059720, spectral sim. = 792, #9
11.7 kJ/mol
Meta-Tyrosine
protonated HMDB0059720, spectral sim. = 787, #10
11.4 kJ/mol
Meta-Tyrosine
protonated HMDB0059720, spectral sim. = 783, #11
17.9 kJ/mol
Meta-Tyrosine
protonated HMDB0059720, spectral sim. = 781, #12
16.9 kJ/mol
Meta-Tyrosine
protonated HMDB0059720, spectral sim. = 769, #13
11.5 kJ/mol
Meta-Tyrosine

182 sodiated HMDB0059720

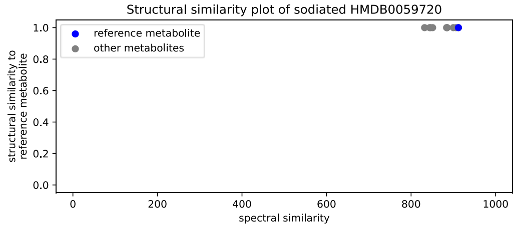


Meta-Tyrosine

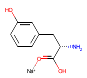
Spectra of sodiated HMDB0059720, spectral sim. = 912, #1



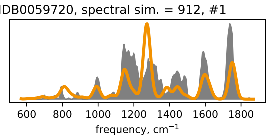
Structural similarity plot of sodiated HMDB0059720



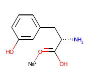
sodiated HMDB0059720, spectral sim. = 912, #1



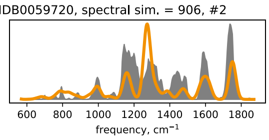
28.9 kJ/mol
Meta-Tyrosine



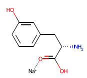
sodiated HMDB0059720, spectral sim. = 906, #2



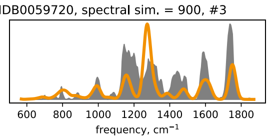
25.2 kJ/mol
Meta-Tyrosine



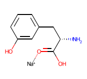
sodiated HMDB0059720, spectral sim. = 900, #3



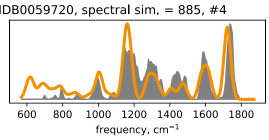
24.1 kJ/mol
Meta-Tyrosine



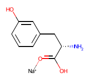
sodiated HMDB0059720, spectral sim. = 885, #4



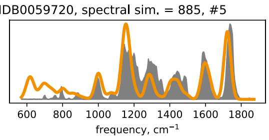
0.2 kJ/mol
Meta-Tyrosine



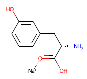
sodiated HMDB0059720, spectral sim. = 885, #5



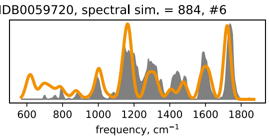
4.7 kJ/mol
Meta-Tyrosine



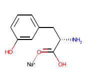
sodiated HMDB0059720, spectral sim. = 884, #6



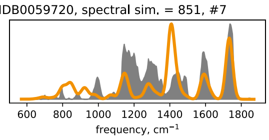
0.0 kJ/mol
Meta-Tyrosine



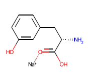
sodiated HMDB0059720, spectral sim. = 851, #7



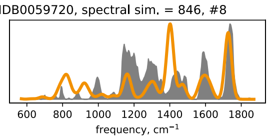
16.8 kJ/mol
Meta-Tyrosine



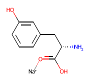
sodiated HMDB0059720, spectral sim. = 846, #8



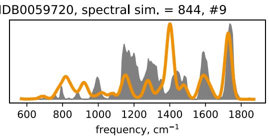
33.5 kJ/mol
Meta-Tyrosine



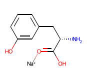
sodiated HMDB0059720, spectral sim. = 844, #9



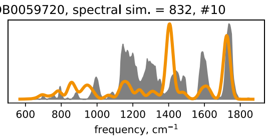
34.2 kJ/mol
Meta-Tyrosine



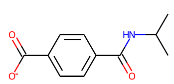
sodiated HMDB0059720, spectral sim. = 832, #10



13.6 kJ/mol
Meta-Tyrosine

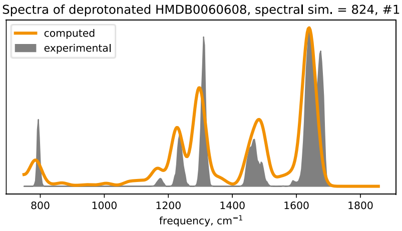


183 deprotonated HMDB0060608

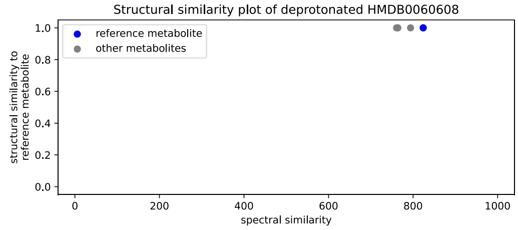


N-isopropylterephthalamic acid

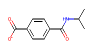
Spectra of deprotonated HMDB0060608, spectral sim. = 824, #1



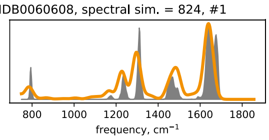
Structural similarity plot of deprotonated HMDB0060608



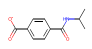
deprotonated HMDB0060608, spectral sim. = 824, #1



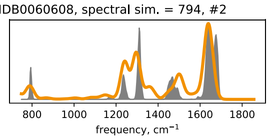
0.0 kJ/mol
N-isopropylterephthalamic acid



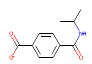
deprotonated HMDB0060608, spectral sim. = 794, #2



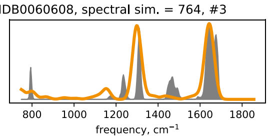
8.9 kJ/mol
N-isopropylterephthalamic acid



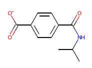
deprotonated HMDB0060608, spectral sim. = 764, #3



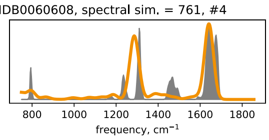
11.0 kJ/mol
N-isopropylterephthalamic acid



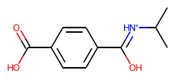
deprotonated HMDB0060608, spectral sim. = 761, #4



29.7 kJ/mol
N-isopropylterephthalamic acid

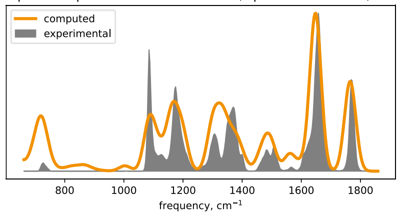


184 protonated HMDB0060608

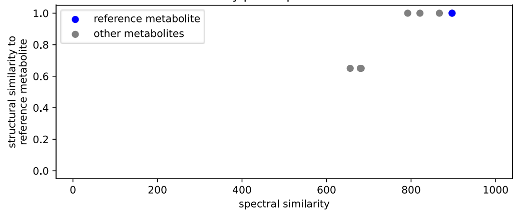


N-isopropylterephthalamic acid

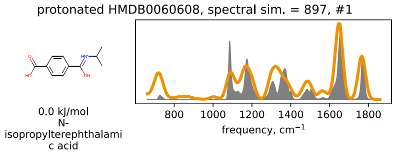
Spectra of protonated HMDB0060608, spectral sim. = 897, #1



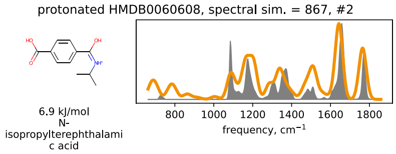
Structural similarity plot of protonated HMDB0060608



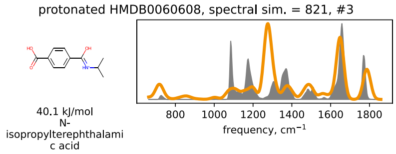
protonated HMDB0060608, spectral sim. = 897, #1



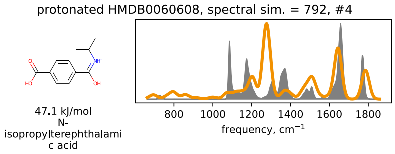
protonated HMDB0060608, spectral sim. = 867, #2



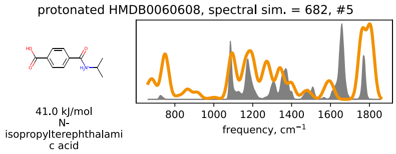
protonated HMDB0060608, spectral sim. = 821, #3



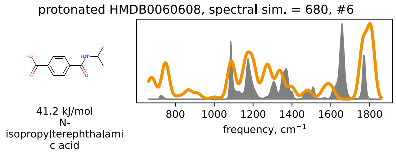
protonated HMDB0060608, spectral sim. = 792, #4



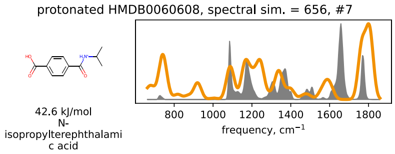
protonated HMDB0060608, spectral sim. = 682, #5



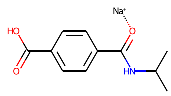
protonated HMDB0060608, spectral sim. = 680, #6



protonated HMDB0060608, spectral sim. = 656, #7

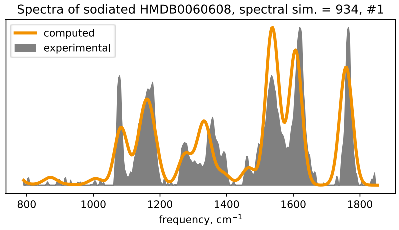


185 sodiated HMDB0060608

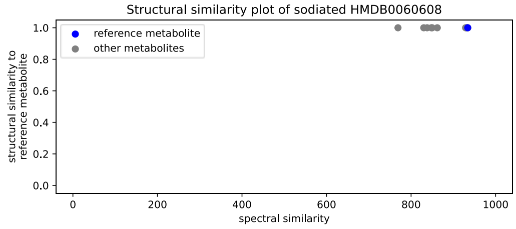


N-isopropylterephthalamic acid

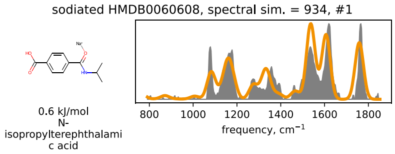
Spectra of sodiated HMDB0060608, spectral sim. = 934, #1



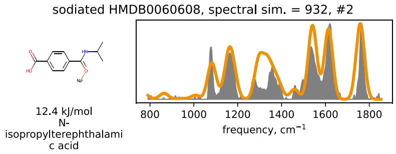
Structural similarity plot of sodiated HMDB0060608



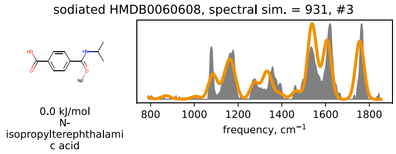
sodiated HMDB0060608, spectral sim. = 934, #1



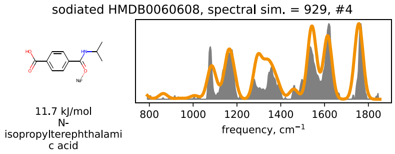
sodiated HMDB0060608, spectral sim. = 932, #2



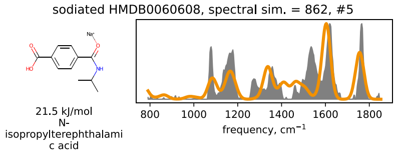
sodiated HMDB0060608, spectral sim. = 931, #3



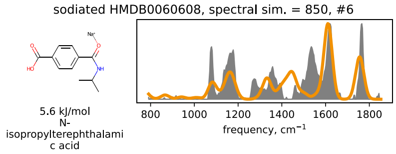
sodiated HMDB0060608, spectral sim. = 929, #4



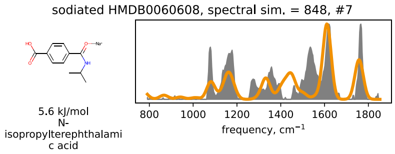
sodiated HMDB0060608, spectral sim. = 862, #5



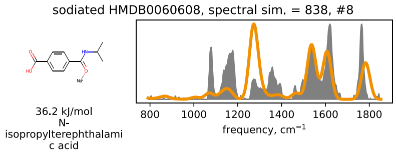
sodiated HMDB0060608, spectral sim. = 850, #6



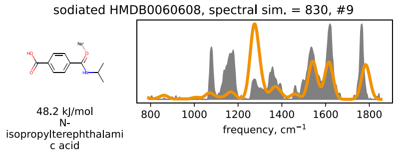
sodiated HMDB0060608, spectral sim. = 848, #7



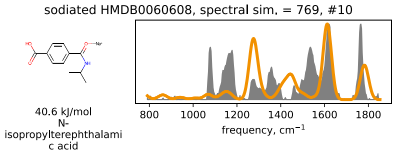
sodiated HMDB0060608, spectral sim. = 838, #8

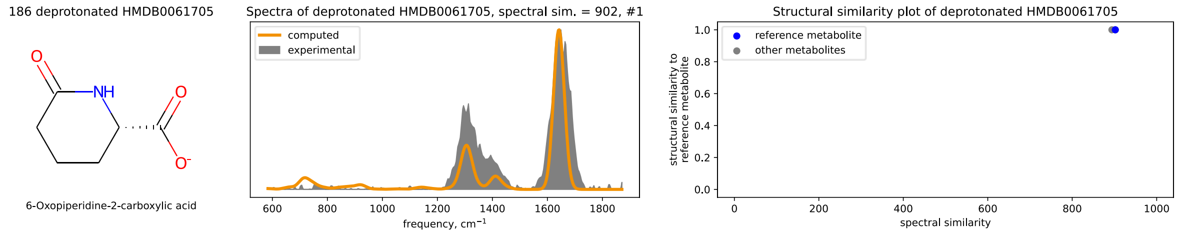


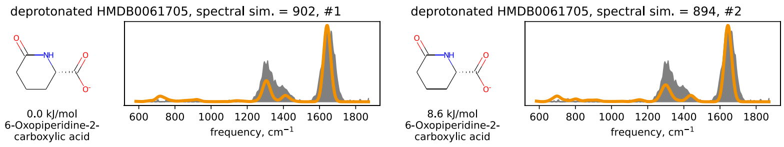
sodiated HMDB0060608, spectral sim. = 830, #9

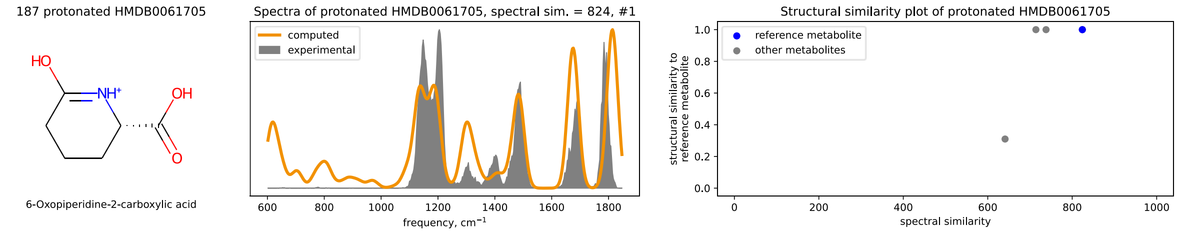


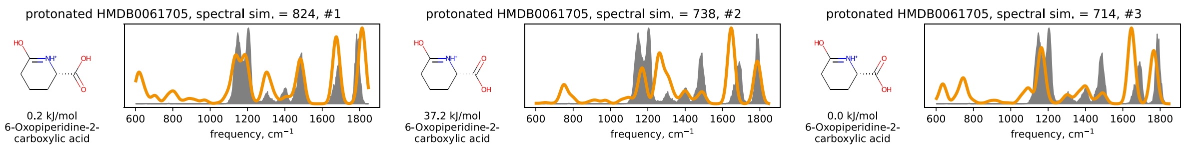
sodiated HMDB0060608, spectral sim. = 769, #10

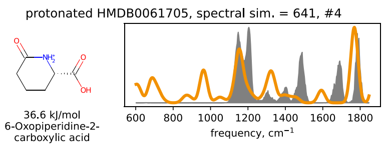



186 deprotonated HMDB0061705
6-Oxopiperidine-2-carboxylic acid
Spectra of deprotonated HMDB0061705, spectral sim. = 902, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of deprotonated HMDB0061705
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

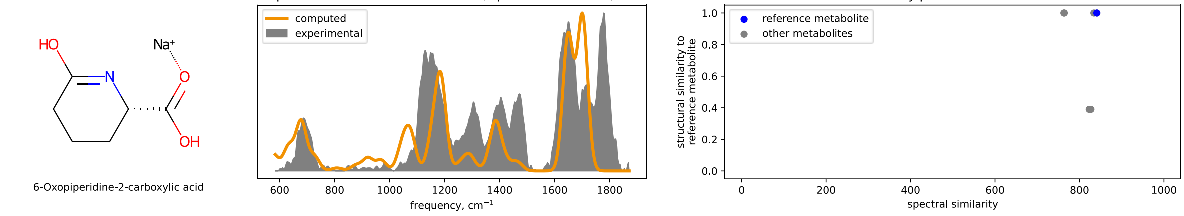

deprotonated HMDB0061705, spectral sim. = 902, #1
0.0 kJ/mol
6-Oxopiperidine-2-carboxylic acid
frequency, cm^{-1}
deprotonated HMDB0061705, spectral sim. = 894, #2
8.6 kJ/mol
6-Oxopiperidine-2-carboxylic acid
frequency, cm^{-1}


187 protonated HMDB0061705
6-Oxopiperidine-2-carboxylic acid
Spectra of protonated HMDB0061705, spectral sim. = 824, #1
computed
experimental
frequency, cm^{-1}
Structural similarity plot of protonated HMDB0061705
reference metabolite
other metabolites
structural similarity to reference metabolite
spectral similarity

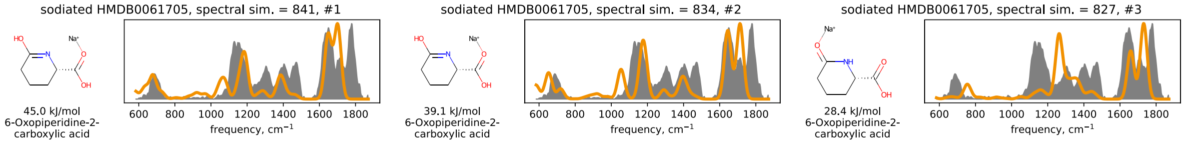

protonated HMDB0061705, spectral sim. = 824, #1
0.2 kJ/mol
6-Oxopiperidine-2-carboxylic acid
frequency, cm^{-1}
protonated HMDB0061705, spectral sim. = 738, #2
37.2 kJ/mol
6-Oxopiperidine-2-carboxylic acid
frequency, cm^{-1}
protonated HMDB0061705, spectral sim. = 714, #3
0.0 kJ/mol
6-Oxopiperidine-2-carboxylic acid
frequency, cm^{-1}


protonated HMDB0061705, spectral sim. = 641, #4
36.6 kJ/mol
6-Oxopiperidine-2-carboxylic acid
frequency, cm^{-1}

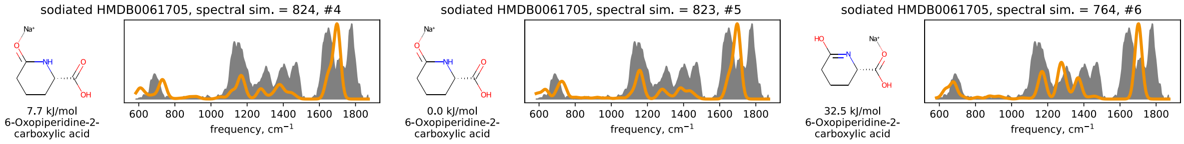
188 sodiated HMDB0061705 | Spectra of sodiated HMDB0061705, spectral sim. = 841, #1 | Structural similarity plot of sodiated HMDB0061705



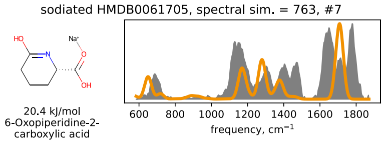
sodiated HMDB0061705, spectral sim. = 841, #1 | sodiated HMDB0061705, spectral sim. = 834, #2 | sodiated HMDB0061705, spectral sim. = 827, #3



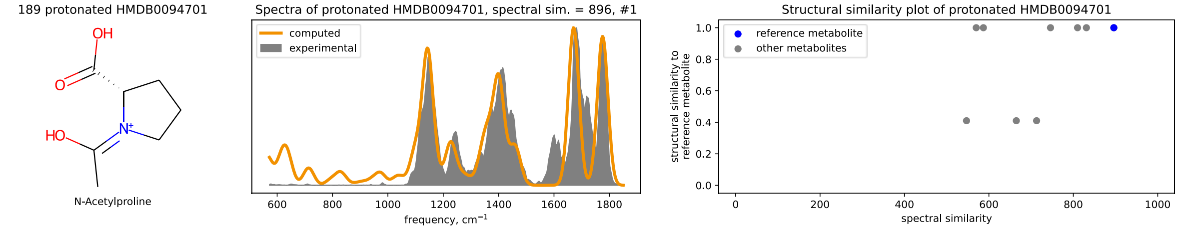
sodiated HMDB0061705, spectral sim. = 824, #4 | sodiated HMDB0061705, spectral sim. = 823, #5 | sodiated HMDB0061705, spectral sim. = 764, #6



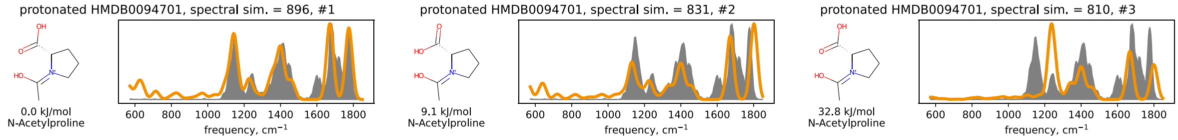
sodiated HMDB0061705, spectral sim. = 763, #7



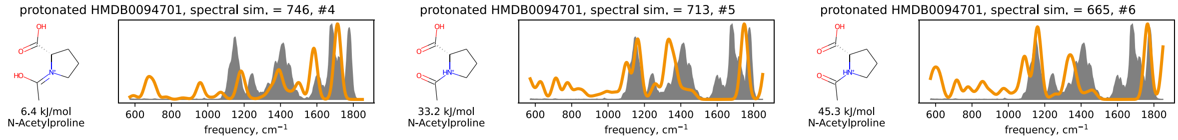
189 protonated HMDB0094701 | Spectra of protonated HMDB0094701, spectral sim. = 896, #1 | Structural similarity plot of protonated HMDB0094701



protonated HMDB0094701, spectral sim. = 896, #1 | protonated HMDB0094701, spectral sim. = 831, #2 | protonated HMDB0094701, spectral sim. = 810, #3



protonated HMDB0094701, spectral sim. = 746, #4 | protonated HMDB0094701, spectral sim. = 713, #5 | protonated HMDB0094701, spectral sim. = 665, #6



protonated HMDB0094701, spectral sim. = 587, #7 | protonated HMDB0094701, spectral sim. = 570, #8 | protonated HMDB0094701, spectral sim. = 547, #9