

## JESS Thermodynamic Database v8.9

## Chemical species in reactions with C18

24-Jan-23

Charge	CAS	Count	Molecular formula	Mol. mass
<b>[14]N2O2:DiBenz</b>				
3,4:9,10-Dibenzo-1,12-diaza-5,8-dioxacyclotetradecane; O-en-N-enH4; 6,7:12,13-Dibenzo-1,4-diaza-8,11-dioxacyclotetradecane				
0	65639-47-6	6	C(18)H(22)N(2)O(2)	298.385
<b>[14]N4:2OHEt*4</b>				
N,N',N'',N'''-Tetrakis(2-hydroxyethyl)-1,4,8,11-tetraazacyclotetradecane; Tetrakis(2-hydroxyethyl)-1,4,8-11-tetraazacyclotetradecane				
0	---	18	C(18)H(40)N(4)O(4)	376.540
<b>[14]N4:Acet*4-4</b>				
1,4,8,11-Tetraazacyclotetradecane-1,4,8,11-tetraacetate; TETA ("cyclo"); 1,4,8,11-Tetraazacyclotetradecane-N,N',N'',N'''-tetraacetate				
-4	---	112	C(18)H(28)N(4)O(8)	428.442
<b>[18]dieneN6dipyo</b>				
3,6,14,17,23,24-Hexaazotricyclo[17.3.1.1[8,12]]tetracos-1(23),8,10,12(24),19,21				
0	---	11	C(18)H(26)N(6)	326.445
<b>[18]N2O4:DiIsoPr</b>				
7,16-Diisopropyl-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane				
0	---	3	C(18)H(38)N(2)O(4)	346.511
<b>[18]N2O4:DiMalon-4</b>				
-4	---	13	C(18)H(26)N(2)O(12)	462.411
<b>[18]N2O4:EtCOO*2-2</b>				
1,10-Diaza-4,7,13,16-tetraoxacyclooctadecane-N,N'-di-b-propionate; K22DP; oddp				
-2	---	23	C(18)H(32)N(2)O(8)	404.461
<b>[18]N2O4:Meox*2</b>				
7,16-Bis(2-methoxyethyl)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane; BME-K22				
0	---	11	C(18)H(38)N(2)O(6)	378.510

<b>[18]N3O3:Acet*3-3</b>				
-3	---	46	C(18)H(30)N(3)O(9)	432.451
<b>[2.2.2]crypt</b> [2.2.2]cryptand; 4,7,13,16,21,24-Hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane; Kryptofix 222; Cryptand 2,2,2; 1,10-Diaza-4,7,13,16,21,24-hexaoxabicyclo[8.8.8]hexacosane				
0	23978-09-8	48	C(18)H(36)N(2)O(6)	376.494
<b>[2.2.2]crypt_Gly-1</b>				
-1	---	1	C(20)H(40)N(3)O(8)	450.553
<b>[2.2.2]crypt_Phe-1</b>				
-1	---	1	C(27)H(46)N(3)O(8)	540.678
<b>[2.2.2]crypt:DiLactam</b> Cryptate 2,2,2 dilactam; 2,9-Oxo-4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane				
0	---	9	C(18)H(32)N(2)O(8)	404.461
<b>[24]N6</b> 1,5,9,13,17,21-Hexaazacyclotetracosane; [24]aneN6				
0	---	51	C(18)H(42)N(6)	342.572
<b>[27]N6O3</b> 1,10,19-Trioxa-4,7,13,16,22,25-hexaazacycloheptacosane; [27]aneN6O3				
0	---	21	C(18)H(42)N(6)O(3)	390.570
<b>[27]N9</b> 1,4,7,10,13,16,19,22,25-Nonazacycloheptacosane; Nonazacycloheptacosane:1,4,7,10,13,16,19,22,25; [27]aneN9				
0	57970-53-3	71	C(18)H(45)N(9)	387.616
<b>1238910HexMe47Phenanth</b> 1,2,3,8,9,10-Hexamethyl-4,7-phenanthroline				
0	---	1	C(18)H(20)N(2)	264.370
<b>135BenzTriCOO-3</b> 1,3,5-Benzenetricarboxylate ion				
-3	---	13	C(9)H(3)O(6)	207.119

<b>246Tri2Pyrid135Triazine</b> 2,4,6-Tri(2'-pyridyl)-1,3,5-triazine				
0	---	7	C(18)H(12)N(6)	312.334
<b>262Dpa</b> 2,6,2-dpa; N,N'-Bis(2-pyridylmethyl)-1,6-diaminohexane				
0	---	5	C(18)H(26)N(4)	298.431
<b>4LICAMS-6</b> LICAMS-4 ion				
-6	---	10	C(18)H(14)N(2)O(12)S(2)	514.435
<b>5ADP-3</b> Adenosine-5'-(trihydrogendiphosphate) ion; ADP ion				
-3	52322-03-9	111	C(10)H(12)N(5)O(10)P(2)	424.181
<b>5AMP-2</b> Adenosine-5'-monophosphate ion				
-2	6042-43-9	105	C(10)H(12)N(5)O(7)P(1)	345.209
<b>5ATP-4</b> Adenosine-5'-(tetrahydrogentriphosphate) ion; ATP ion; Adenosine-5'-triphosphate ion				
-4	13265-06-0	481	C(10)H(12)N(5)O(13)P(3)	503.153
<b>Adipic-2</b> Adipate ion				
-2	18667-07-7	94	C(6)H(8)O(4)	144.127
<b>Ag+1</b> Silver(I) ion				
1	14701-21-4	1534	Ag(1)	107.870
<b>Ag+1_[18]N2O4:Meox*2</b>				
1	---	1	C(18)H(38)Ag(1)N(2)O(6)	486.380
<b>Ag+1_[2.2.2]crypt</b>				
1	57692-62-3	1	C(18)H(36)Ag(1)N(2)O(6)	484.364
<b>Ag+1_[2.2.2]crypt_ClO4-1_(s)</b>				

0	---	1	C (18) H (36) Ag (1) Cl (1) N (2) O (10)	583.814
<b>Ag+1_H+1_TTHA-6</b>				
-4	---	2	C (18) H (25) Ag (1) N (4) O (12)	597.286
<b>Ag+1_H+1 (2)_TTHA-6</b>				
-3	---	1	C (18) H (26) Ag (1) N (4) O (12)	598.294
<b>Ag+1_Tri2PicAm</b>				
1	---	2	C (18) H (18) Ag (1) N (4)	398.238
<b>Ag+1_Tri2PicAm_OH-1</b>				
0	---	1	C (18) H (19) Ag (1) N (4) O (1)	415.245
<b>Ag+1_Triphenylarsine</b>				
1	---	2	C (18) H (15) Ag (1) As (1)	414.109
<b>Ag+1_Triphenylarsine (2)</b>				
1	---	3	C (36) H (30) Ag (1) As (2)	720.348
<b>Ag+1_Triphenylarsine (3)</b>				
1	---	2	C (54) H (45) Ag (1) As (3)	1026.59
<b>Ag+1_TTHA-6</b>				
-5	---	3	C (18) H (24) Ag (1) N (4) O (12)	596.278
<b>Ag+1 (2)_ [2.2.2]crypt</b>				
2	---	1	C (18) H (36) Ag (2) N (2) O (6)	592.234
<b>Ag+1 (2)_H+1_TTHA-6</b>				
-3	---	1	C (18) H (25) Ag (2) N (4) O (12)	705.156
<b>Ag+1 (2)_H+1 (2)_TTHA-6</b>				
-2	---	1	C (18) H (26) Ag (2) N (4) O (12)	706.164
<b>Ag+1 (2)_TTHA-6</b>				
-4	---	2	C (18) H (24) Ag (2) N (4) O (12)	704.148

<b>Ag+1 (3) _TTHA-6</b>				
-3	---	1	C (18) H (24) Ag (3) N (4) O (12)	812.018
<b>Ag+2</b> Silver(II) ion				
2	15046-91-0	47	Ag (1)	107.870
<b>Ag+2 _[14]N4:Acet*4-4</b>				
-2	---	1	C (18) H (28) Ag (1) N (4) O (8)	536.312
<b>Al+3</b> Aluminium(III) ion; Aluminum(III) ion				
3	22537-23-1	1518	Al (1)	26.9820
<b>Al+3 _BAMTPH-3</b>				
0	---	1	C (18) H (21) Al (1) N (6) O (9)	492.382
<b>Al+3 _EDOHPhen*2Me*2DPI-4</b>				
-1	---	1	C (18) H (22) Al (1) N (2) O (6) P (2)	451.313
<b>Al+3 _EHPG-4</b>				
-1	---	1	C (18) H (16) Al (1) N (2) O (6)	383.317
<b>Al+3 _H+1 _EDOHPhen*2Me*2DPI-4</b>				
0	---	1	C (18) H (23) Al (1) N (2) O (6) P (2)	452.320
<b>Al+3 _H+1 _HPEDDA-4</b>				
0	---	1	C (18) H (17) Al (1) N (2) O (6)	384.325
<b>Al+3 _H+1 _TTHA-6</b>				
-2	---	1	C (18) H (25) Al (1) N (4) O (12)	516.398
<b>Al+3 _HPEDDA-4</b>				
-1	---	2	C (18) H (16) Al (1) N (2) O (6)	383.317
<b>Al+3 _TTHA-6</b>				
-3	---	3	C (18) H (24) Al (1) N (4) O (12)	515.390

<b>Al+3 (2) _OH-1 (2) _TTHA-6</b>				
-2	---	1	C (18) H (26) Al (2) N (4) O (14)	576.387
<b>Al+3 (2) _TTHA-6</b>				
0	---	3	C (18) H (24) Al (2) N (4) O (12)	542.372
<b>Am+3</b> Americium(III) ion				
3	22541-46-4	376	Am (1)	243.000
<b>Am+3 _TTHA-6</b>				
-3	---	1	C (18) H (24) Am (1) N (4) O (12)	731.408
<b>Ba+2</b> Barium(II) ion				
2	22541-12-4	584	Ba (1)	137.330
<b>Ba+2 _[14]N4:Acet*4-4</b>				
-2	---	2	C (18) H (28) Ba (1) N (4) O (8)	565.772
<b>Ba+2 _[18]N2O4:DiMalon-4</b>				
-2	---	1	C (18) H (26) Ba (1) N (2) O (12)	599.741
<b>Ba+2 _[2.2.2]crypt</b>				
2	---	1	C (18) H (36) Ba (1) N (2) O (6)	513.824
<b>Ba+2 _[2.2.2]crypt:DiLactam</b>				
2	---	1	C (18) H (32) Ba (1) N (2) O (8)	541.791
<b>Ba+2 _H+1 _[14]N4:Acet*4-4</b>				
-1	---	2	C (18) H (29) Ba (1) N (4) O (8)	566.780
<b>Ba+2 _H+1 _TTHA-6</b>				
-3	---	3	C (18) H (25) Ba (1) N (4) O (12)	626.746
<b>Ba+2 _H+1 (2) _TTHA-6</b>				
-2	---	2	C (18) H (26) Ba (1) N (4) O (12)	627.754

<b>Ba+2_TTHA-6</b>				
-4	---	3	C(18)H(24)Ba(1)N(4)O(12)	625.738
<b>Ba+2(2)_TTHA-6</b>				
-2	---	1	C(18)H(24)Ba(2)N(4)O(12)	763.068
<b>BAMTPH-3</b> BAMTPH ion				
-3	---	18	C(18)H(21)N(6)O(9)	465.400
<b>Be+2</b> Beryllium(II) ion				
2	22537-20-8	665	Be(1)	9.01220
<b>Be+2_[14]N4:Acet*4-4</b>				
-2	---	2	C(18)H(28)Be(1)N(4)O(8)	437.455
<b>Be+2_H+1_[14]N4:Acet*4-4</b>				
-1	---	3	C(18)H(29)Be(1)N(4)O(8)	438.463
<b>Be+2_H+1(2)_[14]N4:Acet*4-4</b>				
0	---	2	C(18)H(30)Be(1)N(4)O(8)	439.470
<b>BEATA-4</b> BEATA anion				
-4	---	18	C(18)H(21)N(3)O(8)	407.380
<b>Bi+3</b> Bismuth(III) ion				
3	23713-46-4	335	Bi(1)	208.980
<b>Bi+3_H+1_TTHA-6</b>				
-2	---	3	C(18)H(25)Bi(1)N(4)O(12)	698.396
<b>Bi+3_H+1(2)_TTHA-6</b>				
-1	---	2	C(18)H(26)Bi(1)N(4)O(12)	699.404
<b>Bi+3_H+1(3)_TTHA-6</b>				

0	---	3	C(18)H(27)Bi(1)N(4)O(12)	700.412
<b>Bi+3_H+1(4)_TTHA-6</b>				
1	---	2	C(18)H(28)Bi(1)N(4)O(12)	701.420
<b>Bi+3_TTHA-6</b>				
-3	---	2	C(18)H(24)Bi(1)N(4)O(12)	697.388
<b>Bipy</b> 2,2'-Bipyridyl; Bipyridine; 2,2'-Bipyridine; Dipyrldyl; 2,2'-Dipyrldyl; 2-(2-Pyridyl)pyridine; bipy; bpy; dip; dipy; alpha-alpha'-Bipyridyl				
0	366-18-7	823	C(10)H(8)N(2)	156.187
<b>Ca+2</b> Calcium(II) ion				
2	14127-61-8	2161	Ca(1)	40.0780
<b>Ca+2_[14]N4:Acet*4-4</b>				
-2	---	2	C(18)H(28)Ca(1)N(4)O(8)	468.520
<b>Ca+2_[18]dieneN6dipyo</b>				
2	---	1	C(18)H(26)Ca(1)N(6)	366.523
<b>Ca+2_[18]N2O4:DiMalon-4</b>				
-2	---	1	C(18)H(26)Ca(1)N(2)O(12)	502.489
<b>Ca+2_[18]N2O4:EtCOO*2-2</b>				
0	---	1	C(18)H(32)Ca(1)N(2)O(8)	444.539
<b>Ca+2_[2.2.2]crypt</b>				
2	---	1	C(18)H(36)Ca(1)N(2)O(6)	416.572
<b>Ca+2_[2.2.2]crypt:DiLactam</b>				
2	---	1	C(18)H(32)Ca(1)N(2)O(8)	444.539
<b>Ca+2_EHPG-4</b>				
-2	---	1	C(18)H(16)Ca(1)N(2)O(6)	396.413



<b>Ca+2_H+1_[14]N4:Acet*4-4</b>				
-1	---	2	C (18) H (29) Ca (1) N (4) O (8)	469.528
<b>Ca+2_H+1_EHPG-4</b>				
-1	---	1	C (18) H (17) Ca (1) N (2) O (6)	397.421
<b>Ca+2_H+1_HBEDPO-6</b>				
-3	---	2	C (18) H (21) Ca (1) N (2) O (8) P (2)	495.399
<b>Ca+2_H+1_HPEDDA-4</b>				
-1	---	3	C (18) H (17) Ca (1) N (2) O (6)	397.421
<b>Ca+2_H+1_TTHA-6</b>				
-3	---	3	C (18) H (25) Ca (1) N (4) O (12)	529.494
<b>Ca+2_H+1 (2)_EHPG-4</b>				
0	---	1	C (18) H (18) Ca (1) N (2) O (6)	398.429
<b>Ca+2_H+1 (2)_HBEDPO-6</b>				
-2	---	2	C (18) H (22) Ca (1) N (2) O (8) P (2)	496.407
<b>Ca+2_H+1 (2)_HPEDDA-4</b>				
0	---	2	C (18) H (18) Ca (1) N (2) O (6)	398.429
<b>Ca+2_H+1 (2)_TTHA-6</b>				
-2	---	2	C (18) H (26) Ca (1) N (4) O (12)	530.502
<b>Ca+2_HBEDPO-6</b>				
-4	---	2	C (18) H (20) Ca (1) N (2) O (8) P (2)	494.391
<b>Ca+2_HPEDDA-4</b>				
-2	---	2	C (18) H (16) Ca (1) N (2) O (6)	396.413
<b>Ca+2_TTHA-6</b>				
-4	---	3	C (18) H (24) Ca (1) N (4) O (12)	528.486

<b>Ca+2 (2) _TTHA-6</b>				
-2	---	3	C (18) H (24) Ca (2) N (4) O (12)	568.564
<b>Ca+2 (3) _TTHA-6</b>				
0	---	1	C (18) H (24) Ca (3) N (4) O (12)	608.642
<b>Cd+2</b> Cadmium(II) ion				
2	22537-48-0	3554	Cd (1)	112.410
<b>Cd+2 _[14]N4:2OHEt*4</b>				
2	---	1	C (18) H (40) Cd (1) N (4) O (4)	488.950
<b>Cd+2 _[14]N4:Acet*4-4</b>				
-2	---	3	C (18) H (28) Cd (1) N (4) O (8)	540.852
<b>Cd+2 _[18]dieneN6dipyo</b>				
2	---	1	C (18) H (26) Cd (1) N (6)	438.855
<b>Cd+2 _[18]N2O4:DiMalon-4</b>				
-2	---	1	C (18) H (26) Cd (1) N (2) O (12)	574.821
<b>Cd+2 _[18]N2O4:EtCOO*2-2</b>				
0	---	1	C (18) H (32) Cd (1) N (2) O (8)	516.871
<b>Cd+2 _[18]N2O4:Meox*2</b>				
2	---	1	C (18) H (38) Cd (1) N (2) O (6)	490.920
<b>Cd+2 _[18]N3O3:Acet*3-3</b>				
-1	---	3	C (18) H (30) Cd (1) N (3) O (9)	544.861
<b>Cd+2 _[2.2.2]crypt</b>				
2	---	1	C (18) H (36) Cd (1) N (2) O (6)	488.904
<b>Cd+2 _[24]N6</b>				
2	---	1	C (18) H (42) Cd (1) N (6)	454.982

<b>Cd+2_Co+2_TTHA-6</b>				
-2	---	2	C(18)H(24)Cd(1)Co(1)N(4)O(12)	659.751
<b>Cd+2_EHPG-4</b>				
-2	---	1	C(18)H(16)Cd(1)N(2)O(6)	468.745
<b>Cd+2_H+1_[14]N4:Acet*4-4</b>				
-1	---	3	C(18)H(29)Cd(1)N(4)O(8)	541.860
<b>Cd+2_H+1_[18]N3O3:Acet*3-3</b>				
0	---	1	C(18)H(31)Cd(1)N(3)O(9)	545.869
<b>Cd+2_H+1_EHPG-4</b>				
-1	---	1	C(18)H(17)Cd(1)N(2)O(6)	469.753
<b>Cd+2_H+1_HPEDDA-4</b>				
-1	---	3	C(18)H(17)Cd(1)N(2)O(6)	469.753
<b>Cd+2_H+1_TTHA-6</b>				
-3	---	4	C(18)H(25)Cd(1)N(4)O(12)	601.826
<b>Cd+2_H+1(2)_[14]N4:Acet*4-4</b>				
0	---	2	C(18)H(30)Cd(1)N(4)O(8)	542.868
<b>Cd+2_H+1(2)_EHPG-4</b>				
0	---	1	C(18)H(18)Cd(1)N(2)O(6)	470.761
<b>Cd+2_H+1(2)_HPEDDA-4</b>				
0	---	2	C(18)H(18)Cd(1)N(2)O(6)	470.761
<b>Cd+2_H+1(2)_TTHA-6</b>				
-2	---	2	C(18)H(26)Cd(1)N(4)O(12)	602.834
<b>Cd+2_H+1(3)_TTHA-6</b>				
-1	---	1	C(18)H(27)Cd(1)N(4)O(12)	603.842

<b>Cd+2_HPEDDA-4</b>				
-2	---	2	C(18)H(16)Cd(1)N(2)O(6)	468.745
<b>Cd+2_Ni+2_TTHA-6</b>				
-2	---	1	C(18)H(24)Cd(1)N(4)Ni(1)O(12)	659.511
<b>Cd+2_OH-1_[18]N3O3:Acet*3-3</b>				
-2	---	1	C(18)H(31)Cd(1)N(3)O(10)	561.868
<b>Cd+2_Tri2PicAm</b>				
2	---	2	C(18)H(18)Cd(1)N(4)	402.778
<b>Cd+2_Tri2PicAm_OH-1</b>				
1	---	1	C(18)H(19)Cd(1)N(4)O(1)	419.785
<b>Cd+2_Tri2PicAm(2)</b>				
2	---	1	C(36)H(36)Cd(1)N(8)	693.145
<b>Cd+2_TTHA-6</b>				
-4	---	3	C(18)H(24)Cd(1)N(4)O(12)	600.818
<b>Cd+2(2)_[14]N4:Acet*4-4</b>				
0	---	2	C(18)H(28)Cd(2)N(4)O(8)	653.262
<b>Cd+2(2)_[18]N3O3:Acet*3-3</b>				
1	---	2	C(18)H(30)Cd(2)N(3)O(9)	657.271
<b>Cd+2(2)_[27]N9</b>				
4	---	1	C(18)H(45)Cd(2)N(9)	612.436
<b>Cd+2(2)_H+1_[14]N4:Acet*4-4</b>				
1	---	1	C(18)H(29)Cd(2)N(4)O(8)	654.270
<b>Cd+2(2)_H+1_[18]N3O3:Acet*3-3</b>				
2	---	1	C(18)H(31)Cd(2)N(3)O(9)	658.279

<b>Cd+2 (2) _H+1 _[27]N9</b>				
5	---	1	C (18) H (46) Cd (2) N (9)	613.444
<b>Cd+2 (2) _H+1 (2) _[27]N9</b>				
6	---	1	C (18) H (47) Cd (2) N (9)	614.452
<b>Cd+2 (2) _TTHA-6</b>				
-2	---	2	C (18) H (24) Cd (2) N (4) O (12)	713.228
<b>Ce+2</b>				
2	---	7	Ce (1)	140.120
<b>Ce+2 _[2.2.2] crypt</b>				
2	---	1	C (18) H (36) Ce (1) N (2) O (6)	516.614
<b>Ce+3</b> Cerium(III) ion				
3	18923-26-7	627	Ce (1)	140.120
<b>Ce+3 _[18]N2O4:DiMalon-4</b>				
-1	---	1	C (18) H (26) Ce (1) N (2) O (12)	602.531
<b>Ce+3 _[18]N2O4:EtCOO*2-2</b>				
1	---	1	C (18) H (32) Ce (1) N (2) O (8)	544.581
<b>Ce+3 _[2.2.2] crypt</b>				
3	---	1	C (18) H (36) Ce (1) N (2) O (6)	516.614
<b>Ce+3 _BEATA-4</b>				
-1	---	1	C (18) H (21) Ce (1) N (3) O (8)	547.500
<b>Ce+3 _TTHA-6</b>				
-3	---	1	C (18) H (24) Ce (1) N (4) O (12)	628.528
<b>Ce+3 (2) _TTHA-6</b>				
0	---	1	C (18) H (24) Ce (2) N (4) O (12)	768.648

<b>Citric-3</b> Citrate ion				
-3	126-44-3	1347	C(6)H(5)O(7)	189.102
<b>Cl-1</b> Chloride ion				
-1	16887-00-6	2242	Cl(1)	35.4530
<b>ClO4-1</b> Perchlorate ion				
-1	14797-73-0	114	Cl(1)O(4)	99.4506
<b>Co+2</b> Cobalt(II) ion				
2	22541-53-3	2857	Co(1)	58.9330
<b>Co+2_[14]N2O2:DiBenz</b>				
2	---	1	C(18)H(22)Co(1)N(2)O(2)	357.318
<b>Co+2_[14]N4:2OHEt*4</b>				
2	---	2	C(18)H(40)Co(1)N(4)O(4)	435.473
<b>Co+2_[14]N4:Acet*4-4</b>				
-2	---	4	C(18)H(28)Co(1)N(4)O(8)	487.375
<b>Co+2_[18]N3O3:Acet*3-3</b>				
-1	---	3	C(18)H(30)Co(1)N(3)O(9)	491.384
<b>Co+2_[2.2.2]crypt</b>				
2	---	1	C(18)H(36)Co(1)N(2)O(6)	435.427
<b>Co+2_[27]N9</b>				
2	---	1	C(18)H(45)Co(1)N(9)	446.549
<b>Co+2_246Tri2Pyrid135Triazine</b>				
2	---	2	C(18)H(12)Co(1)N(6)	371.266
<b>Co+2_246Tri2Pyrid135Triazine(2)</b>				

2	---	1	C (36) H (24) Co (1) N (12)	683.600
<b>Co+2_4LICAMS-6</b>				
-4	---	1	C (18) H (14) Co (1) N (2) O (12) S (2)	573.368
<b>Co+2_BAMTPH-3</b>				
-1	---	2	C (18) H (21) Co (1) N (6) O (9)	524.333
<b>Co+2_H+1_[14]N4:2OHEt*4</b>				
3	---	1	C (18) H (41) Co (1) N (4) O (4)	436.481
<b>Co+2_H+1_[14]N4:Acet*4-4</b>				
-1	---	4	C (18) H (29) Co (1) N (4) O (8)	488.383
<b>Co+2_H+1_[18]N3O3:Acet*3-3</b>				
0	---	1	C (18) H (31) Co (1) N (3) O (9)	492.392
<b>Co+2_H+1_[27]N9</b>				
3	---	1	C (18) H (46) Co (1) N (9)	447.557
<b>Co+2_H+1_BAMTPH-3</b>				
0	---	2	C (18) H (22) Co (1) N (6) O (9)	525.341
<b>Co+2_H+1_HBEDPO-6</b>				
-3	---	2	C (18) H (21) Co (1) N (2) O (8) P (2)	514.254
<b>Co+2_H+1_HPEDDA-4</b>				
-1	---	3	C (18) H (17) Co (1) N (2) O (6)	416.276
<b>Co+2_H+1_TTHA-6</b>				
-3	---	3	C (18) H (25) Co (1) N (4) O (12)	548.349
<b>Co+2_H+1(2)_[14]N4:Acet*4-4</b>				
0	---	2	C (18) H (30) Co (1) N (4) O (8)	489.391
<b>Co+2_H+1(2)_[27]N9</b>				
4	---	1	C (18) H (47) Co (1) N (9)	448.565

<b>Co+2_H+1 (2) _BAMTPH-3</b>				
1	---	1	C (18) H (23) Co (1) N (6) O (9)	526.348
<b>Co+2_H+1 (2) _HBEDPO-6</b>				
-2	---	3	C (18) H (22) Co (1) N (2) O (8) P (2)	515.262
<b>Co+2_H+1 (2) _HPEDDA-4</b>				
0	---	2	C (18) H (18) Co (1) N (2) O (6)	417.284
<b>Co+2_H+1 (2) _TTHA-6</b>				
-2	---	2	C (18) H (26) Co (1) N (4) O (12)	549.357
<b>Co+2_H+1 (3) _HBEDPO-6</b>				
-1	---	2	C (18) H (23) Co (1) N (2) O (8) P (2)	516.270
<b>Co+2_H+1 (3) _TTHA-6</b>				
-1	---	2	C (18) H (27) Co (1) N (4) O (12)	550.365
<b>Co+2_H+1 (4) _HBEDPO-6</b>				
0	---	1	C (18) H (24) Co (1) N (2) O (8) P (2)	517.278
<b>Co+2_H+1 (4) _TTHA-6</b>				
0	---	1	C (18) H (28) Co (1) N (4) O (12)	551.373
<b>Co+2 _HBEDPO-6</b>				
-4	---	2	C (18) H (20) Co (1) N (2) O (8) P (2)	513.246
<b>Co+2 _HPEDDA-4</b>				
-2	---	2	C (18) H (16) Co (1) N (2) O (6)	415.268
<b>Co+2 _OH-1 _[14]N4:Acet*4-4</b>				
-3	---	1	C (18) H (29) Co (1) N (4) O (9)	504.383
<b>Co+2 _OH-1 _[18]N3O3:Acet*3-3</b>				
-2	---	1	C (18) H (31) Co (1) N (3) O (10)	508.391



<b>Co+2_Tri2PicAm</b>				
2	---	2	C (18) H (18) Co (1) N (4)	349.301
<b>Co+2_Tri2PicAm_OH-1</b>				
1	---	1	C (18) H (19) Co (1) N (4) O (1)	366.308
<b>Co+2_TTHA-6</b>				
-4	---	4	C (18) H (24) Co (1) N (4) O (12)	547.341
<b>Co+2 (2)_[14]N4:Acet*4-4</b>				
0	---	2	C (18) H (28) Co (2) N (4) O (8)	546.308
<b>Co+2 (2)_[18]N3O3:Acet*3-3</b>				
1	---	2	C (18) H (30) Co (2) N (3) O (9)	550.317
<b>Co+2 (2)_[27]N9</b>				
4	---	2	C (18) H (45) Co (2) N (9)	505.482
<b>Co+2 (2)_[27]N9_OH-1</b>				
3	---	2	C (18) H (46) Co (2) N (9) O (1)	522.489
<b>Co+2 (2)_H+1_[14]N4:Acet*4-4</b>				
1	---	1	C (18) H (29) Co (2) N (4) O (8)	547.316
<b>Co+2 (2)_H+1_[18]N3O3:Acet*3-3</b>				
2	---	1	C (18) H (31) Co (2) N (3) O (9)	551.325
<b>Co+2 (2)_H+1_[27]N9</b>				
5	---	1	C (18) H (46) Co (2) N (9)	506.490
<b>Co+2 (2)_H+1_TTHA-6</b>				
-1	---	2	C (18) H (25) Co (2) N (4) O (12)	607.282
<b>Co+2 (2)_H+1 (2)_TTHA-6</b>				
0	---	1	C (18) H (26) Co (2) N (4) O (12)	608.290

<b>Co+2 (2) _TTHA-6</b>				
-2	---	3	C (18) H (24) Co (2) N (4) O (12)	606.274
<b>Co+3</b> Cobalt(III) ion				
3	22541-63-5	697	Co (1)	58.9330
<b>Co+3 _CN-1 (6)</b>				
-3	---	52	C (6) Co (1) N (6)	215.039
<b>Co+3 _H+1 (4) _[27]N9 _CN-1 (6)</b>				
1	---	1	C (24) H (49) Co (1) N (15)	606.687
<b>Co+3 _H+1 (5) _[27]N9 _CN-1 (6)</b>				
2	---	1	C (24) H (50) Co (1) N (15)	607.695
<b>Co+3 _H+1 (6) _[24]N6 _CN-1 (6)</b>				
3	---	1	C (24) H (48) Co (1) N (12)	563.659
<b>Co+3 _H+1 (6) _[27]N6O3 _CN-1 (6)</b>				
3	---	1	C (24) H (48) Co (1) N (12) O (3)	611.657
<b>Co+3 _H+1 (6) _[27]N9 _CN-1 (6)</b>				
3	---	1	C (24) H (51) Co (1) N (15)	608.702
<b>Co+3 _H+1 (7) _[27]N9 _CN-1 (6)</b>				
4	---	1	C (24) H (52) Co (1) N (15)	609.710
<b>Co+3 _H+1 (8) _[27]N9 _CN-1 (6)</b>				
5	---	1	C (24) H (53) Co (1) N (15)	610.718
<b>Co+3 _TTHA-6</b>				
-3	---	1	C (18) H (24) Co (1) N (4) O (12)	547.341
<b>Codeine</b> Codeine				
0	76-57-3	1	C (18) H (21) N (1) O (3)	299.370

<b>Cs+1</b> Caesium(I) ion; Cesium(I) ion				
1	18459-37-5	246	Cs (1)	132.910
<b>Cs+1_[18]N2O4:Meox*2</b>				
1	---	1	C (18) H (38) Cs (1) N (2) O (6)	511.420
<b>Cs+1_[2.2.2]crypt</b>				
1	---	1	C (18) H (36) Cs (1) N (2) O (6)	509.404
<b>Cs+1_[2.2.2]crypt:DiLactam</b>				
1	---	1	C (18) H (32) Cs (1) N (2) O (8)	537.371
<b>Cu+1</b> Copper(I) ion; Cuprous ion				
1	17493-86-6	491	Cu (1)	63.5460
<b>Cu+1_[2.2.2]crypt</b>				
1	---	1	C (18) H (36) Cu (1) N (2) O (6)	440.040
<b>Cu+1_Triphenylarsine</b>				
1	---	1	C (18) H (15) As (1) Cu (1)	369.785
<b>Cu+1_Triphenylarsine (2)</b>				
1	---	1	C (36) H (30) As (2) Cu (1)	676.024
<b>Cu+2</b> Copper(II) ion; Cupric ion				
2	15158-11-9	9346	Cu (1)	63.5460
<b>Cu+2_[14]N2O2:DiBenz</b>				
2	---	1	C (18) H (22) Cu (1) N (2) O (2)	361.931
<b>Cu+2_[14]N4:2OHEt*4</b>				
2	---	2	C (18) H (40) Cu (1) N (4) O (4)	440.086
<b>Cu+2_[14]N4:Acet*4-4</b>				

-2	---	4	C (18) H (28) Cu (1) N (4) O (8)	491.988
<b>Cu+2_[18]dieneN6dipyo</b>				
2	---	1	C (18) H (26) Cu (1) N (6)	389.991
<b>Cu+2_[18]N2O4:EtCOO*2-2</b>				
0	---	1	C (18) H (32) Cu (1) N (2) O (8)	468.007
<b>Cu+2_[18]N3O3:Acet*3-3</b>				
-1	---	3	C (18) H (30) Cu (1) N (3) O (9)	495.997
<b>Cu+2_[2.2.2]crypt</b>				
2	---	1	C (18) H (36) Cu (1) N (2) O (6)	440.040
<b>Cu+2_[24]N6</b>				
2	---	1	C (18) H (42) Cu (1) N (6)	406.118
<b>Cu+2_[27]N9_OH-1</b>				
1	---	1	C (18) H (46) Cu (1) N (9) O (1)	468.169
<b>Cu+2_4LICAMS-6</b>				
-4	---	1	C (18) H (14) Cu (1) N (2) O (12) S (2)	577.981
<b>Cu+2_Bipy_TyrPhe-2</b>				
0	---	1	C (28) H (26) Cu (1) N (4) O (4)	546.085
<b>Cu+2_Bipy_TyrTyr-3</b>				
-1	---	1	C (28) H (25) Cu (1) N (4) O (5)	561.076
<b>Cu+2_EDOHPhen*2Me*2DPI-4</b>				
-2	---	2	C (18) H (22) Cu (1) N (2) O (6) P (2)	487.877
<b>Cu+2_EDPhen*2Me*2DPI-2</b>				
0	---	1	C (18) H (24) Cu (1) N (2) O (4) P (2)	457.894
<b>Cu+2_EHPG-4</b>				
-2	---	2	C (18) H (16) Cu (1) N (2) O (6)	419.881

<b>Cu+2_Enalaprilat-2</b>				
0	---	2	C (18) H (22) Cu (1) N (2) O (5)	409.929
<b>Cu+2_Enalaprilat-2 (2)</b>				
-2	---	2	C (36) H (44) Cu (1) N (4) O (10)	756.312
<b>Cu+2_Enalaprilat-2 (3)</b>				
-4	---	1	C (54) H (66) Cu (1) N (6) O (15)	1102.70
<b>Cu+2_EtDiAm_TyrPhe-2</b>				
0	---	1	C (20) H (26) Cu (1) N (4) O (4)	449.997
<b>Cu+2_GlyProDPheGly-1</b>				
1	---	2	C (18) H (23) Cu (1) N (4) O (5)	438.950
<b>Cu+2_GlyProGlyPhe-1</b>				
1	---	2	C (18) H (23) Cu (1) N (4) O (5)	438.950
<b>Cu+2_GlyProPheGly-1</b>				
1	---	2	C (18) H (23) Cu (1) N (4) O (5)	438.950
<b>Cu+2_H+1_[14]N4:2OHEt*4</b>				
3	---	1	C (18) H (41) Cu (1) N (4) O (4)	441.094
<b>Cu+2_H+1_[14]N4:Acet*4-4</b>				
-1	---	4	C (18) H (29) Cu (1) N (4) O (8)	492.996
<b>Cu+2_H+1_[18]N3O3:Acet*3-3</b>				
0	---	2	C (18) H (31) Cu (1) N (3) O (9)	497.005
<b>Cu+2_H+1_[24]N6</b>				
3	---	1	C (18) H (43) Cu (1) N (6)	407.126
<b>Cu+2_H+1_BAMTPH-3</b>				
0	---	2	C (18) H (22) Cu (1) N (6) O (9)	529.954

<b>Cu+2_H+1_Bipy_TyrPhe-2</b>				
1	---	1	C (28) H (27) Cu (1) N (4) O (4)	547.093
<b>Cu+2_H+1_Bipy_TyrTyr-3</b>				
0	---	1	C (28) H (26) Cu (1) N (4) O (5)	562.084
<b>Cu+2_H+1_EDOHPhen*2Me*2DPI-4</b>				
-1	---	2	C (18) H (23) Cu (1) N (2) O (6) P (2)	488.884
<b>Cu+2_H+1_EHPG-4</b>				
-1	---	3	C (18) H (17) Cu (1) N (2) O (6)	420.889
<b>Cu+2_H+1_EtDiAm_TyrPhe-2</b>				
1	---	1	C (20) H (27) Cu (1) N (4) O (4)	451.005
<b>Cu+2_H+1_EtDiAm_TyrTyr-3</b>				
0	---	1	C (20) H (26) Cu (1) N (4) O (5)	465.996
<b>Cu+2_H+1_HBEDPO-6</b>				
-3	---	2	C (18) H (21) Cu (1) N (2) O (8) P (2)	518.867
<b>Cu+2_H+1_HPEDDA-4</b>				
-1	---	3	C (18) H (17) Cu (1) N (2) O (6)	420.889
<b>Cu+2_H+1_mEHPG-4</b>				
-1	---	2	C (18) H (17) Cu (1) N (2) O (6)	420.889
<b>Cu+2_H+1_Phenanth_TyrPhe-2</b>				
1	---	1	C (30) H (27) Cu (1) N (4) O (4)	571.115
<b>Cu+2_H+1_Phenanth_TyrTyr-3</b>				
0	---	1	C (30) H (26) Cu (1) N (4) O (5)	586.106
<b>Cu+2_H+1_PheTyr-2</b>				
1	---	1	C (18) H (19) Cu (1) N (2) O (4)	390.906

<b>Cu+2_H+1_PheTyr-2 (2)</b>				
-1	---	1	C (36) H (37) Cu (1) N (4) O (8)	717.258
<b>Cu+2_H+1_Trigalacturonic-3</b>				
0	---	1	C (18) H (24) Cu (1) O (19)	607.923
<b>Cu+2_H+1_TTHA-6</b>				
-3	---	2	C (18) H (25) Cu (1) N (4) O (12)	552.962
<b>Cu+2_H+1_TyrPhe-2</b>				
1	---	1	C (18) H (19) Cu (1) N (2) O (4)	390.906
<b>Cu+2_H+1_TyrPhe-2 (2)</b>				
-1	---	1	C (36) H (37) Cu (1) N (4) O (8)	717.258
<b>Cu+2_H+1_TyrTyr-3</b>				
0	---	1	C (18) H (18) Cu (1) N (2) O (5)	405.897
<b>Cu+2_H+1 (-1)_Bipy_TyrPhe-2</b>				
-1	---	1	C (28) H (25) Cu (1) N (4) O (4)	545.077
<b>Cu+2_H+1 (-1)_EtDiAm_TyrPhe-2</b>				
-1	---	1	C (20) H (25) Cu (1) N (4) O (4)	448.989
<b>Cu+2_H+1 (-1)_GlyProDPheGly-1</b>				
0	---	2	C (18) H (22) Cu (1) N (4) O (5)	437.943
<b>Cu+2_H+1 (-1)_GlyProGlyPhe-1</b>				
0	---	2	C (18) H (22) Cu (1) N (4) O (5)	437.943
<b>Cu+2_H+1 (-1)_GlyProPheGly-1</b>				
0	---	3	C (18) H (22) Cu (1) N (4) O (5)	437.943
<b>Cu+2_H+1 (-1)_Phenanth_TyrPhe-2</b>				
-1	---	1	C (30) H (25) Cu (1) N (4) O (4)	569.099

<b>Cu+2_H+1 (-1) _PhePhe-1</b>				
0	---	1	C (18) H (18) Cu (1) N (2) O (3)	373.899
<b>Cu+2_H+1 (-1) _PhePhe-1 (2)</b>				
-1	---	1	C (36) H (37) Cu (1) N (4) O (6)	685.259
<b>Cu+2_H+1 (-1) _PheProGlyGly-1</b>				
0	---	3	C (18) H (22) Cu (1) N (4) O (5)	437.943
<b>Cu+2_H+1 (-1) _PheTyr-2</b>				
-1	---	1	C (18) H (17) Cu (1) N (2) O (4)	388.890
<b>Cu+2_H+1 (-1) _TyrPhe-2</b>				
-1	---	1	C (18) H (17) Cu (1) N (2) O (4)	388.890
<b>Cu+2_H+1 (-1) _TyrTyr-3</b>				
-2	---	1	C (18) H (16) Cu (1) N (2) O (5)	403.881
<b>Cu+2_H+1 (-2) _GlyProPheGly-1</b>				
-1	---	2	C (18) H (21) Cu (1) N (4) O (5)	436.935
<b>Cu+2_H+1 (-2) _PhePhe-1</b>				
-1	---	1	C (18) H (17) Cu (1) N (2) O (3)	372.891
<b>Cu+2_H+1 (-2) _PheProGlyGly-1</b>				
-1	---	2	C (18) H (21) Cu (1) N (4) O (5)	436.935
<b>Cu+2_H+1 (-2) _PheTyr-2</b>				
-2	---	1	C (18) H (16) Cu (1) N (2) O (4)	387.882
<b>Cu+2_H+1 (-2) _TyrPhe-2</b>				
-2	---	1	C (18) H (16) Cu (1) N (2) O (4)	387.882
<b>Cu+2_H+1 (-2) _TyrTyr-3</b>				
-3	---	1	C (18) H (15) Cu (1) N (2) O (5)	402.874



<b>Cu+2_H+1 (-3) _PheTyr-2</b>				
-3	---	1	C (18) H (15) Cu (1) N (2) O (4)	386.874
<b>Cu+2_H+1 (-3) _TyrPhe-2</b>				
-3	---	1	C (18) H (15) Cu (1) N (2) O (4)	386.874
<b>Cu+2_H+1 (2) _[14]N4:Acet*4-4</b>				
0	---	2	C (18) H (30) Cu (1) N (4) O (8)	494.004
<b>Cu+2_H+1 (2) _[18]N3O3:Acet*3-3</b>				
1	---	1	C (18) H (32) Cu (1) N (3) O (9)	498.013
<b>Cu+2_H+1 (2) _[24]N6</b>				
4	---	1	C (18) H (44) Cu (1) N (6)	408.134
<b>Cu+2_H+1 (2) _BAMTPH-3</b>				
1	---	1	C (18) H (23) Cu (1) N (6) O (9)	530.961
<b>Cu+2_H+1 (2) _Bipy_TyrTyr-3</b>				
1	---	1	C (28) H (27) Cu (1) N (4) O (5)	563.092
<b>Cu+2_H+1 (2) _EDOHPhen*2Me*2DPI-4</b>				
0	---	1	C (18) H (24) Cu (1) N (2) O (6) P (2)	489.892
<b>Cu+2_H+1 (2) _EHPG-4</b>				
0	---	2	C (18) H (18) Cu (1) N (2) O (6)	421.897
<b>Cu+2_H+1 (2) _EtDiAm_TyrTyr-3</b>				
1	---	1	C (20) H (27) Cu (1) N (4) O (5)	467.004
<b>Cu+2_H+1 (2) _HBEDPO-6</b>				
-2	---	3	C (18) H (22) Cu (1) N (2) O (8) P (2)	519.875
<b>Cu+2_H+1 (2) _HPEDDA-4</b>				
0	---	2	C (18) H (18) Cu (1) N (2) O (6)	421.897

<b>Cu+2_H+1 (2) _mEHGP-4</b>				
0	---	1	C (18) H (18) Cu (1) N (2) O (6)	421.897
<b>Cu+2_H+1 (2) _Phenanth_TyrTyr-3</b>				
1	---	1	C (30) H (27) Cu (1) N (4) O (5)	587.114
<b>Cu+2_H+1 (2) _TTHA-6</b>				
-2	---	2	C (18) H (26) Cu (1) N (4) O (12)	553.970
<b>Cu+2_H+1 (2) _TyrTyr-3</b>				
1	---	1	C (18) H (19) Cu (1) N (2) O (5)	406.905
<b>Cu+2_H+1 (3) _[24]N6</b>				
5	---	1	C (18) H (45) Cu (1) N (6)	409.142
<b>Cu+2_H+1 (3) _HBEDPO-6</b>				
-1	---	2	C (18) H (23) Cu (1) N (2) O (8) P (2)	520.883
<b>Cu+2_H+1 (3) _TTHA-6</b>				
-1	---	2	C (18) H (27) Cu (1) N (4) O (12)	554.978
<b>Cu+2_H+1 (3) _TyrTyr-3 (2)</b>				
-1	---	1	C (36) H (37) Cu (1) N (4) O (10)	749.257
<b>Cu+2_H+1 (4) _[24]N6</b>				
6	---	1	C (18) H (46) Cu (1) N (6)	410.149
<b>Cu+2_H+1 (4) _HBEDPO-6</b>				
0	---	1	C (18) H (24) Cu (1) N (2) O (8) P (2)	521.891
<b>Cu+2_H+1 (4) _TTHA-6</b>				
0	---	1	C (18) H (28) Cu (1) N (4) O (12)	555.986
<b>Cu+2_HBEDPO-6</b>				
-4	---	2	C (18) H (20) Cu (1) N (2) O (8) P (2)	517.859

<b>Cu+2_HPEDDA-4</b>				
-2	---	2	C (18) H (16) Cu (1) N (2) O (6)	419.881
<b>Cu+2_mEHPPG-4</b>				
-2	---	2	C (18) H (16) Cu (1) N (2) O (6)	419.881
<b>Cu+2_Ni+2_TTHA-6</b>				
-2	---	1	C (18) H (24) Cu (1) N (4) Ni (1) O (12)	610.647
<b>Cu+2_OH-1_[14]N4:Acet*4-4</b>				
-3	---	1	C (18) H (29) Cu (1) N (4) O (9)	508.996
<b>Cu+2_OH-1_[18]N3O3:Acet*3-3</b>				
-2	---	1	C (18) H (31) Cu (1) N (3) O (10)	513.004
<b>Cu+2_OH-1_Enalaprilat-2</b>				
-1	---	1	C (18) H (23) Cu (1) N (2) O (6)	426.936
<b>Cu+2_OH-1_Enalaprilat-2(2)</b>				
-3	---	2	C (36) H (45) Cu (1) N (4) O (11)	773.320
<b>Cu+2_Phenanth_TyrPhe-2</b>				
0	---	1	C (30) H (26) Cu (1) N (4) O (4)	570.107
<b>Cu+2_Phenanth_TyrTyr-3</b>				
-1	---	1	C (30) H (25) Cu (1) N (4) O (5)	585.098
<b>Cu+2_PhePhe-1</b>				
1	---	1	C (18) H (19) Cu (1) N (2) O (3)	374.907
<b>Cu+2_PheProGlyGly-1</b>				
1	---	2	C (18) H (23) Cu (1) N (4) O (5)	438.950
<b>Cu+2_PheProGlyGly-1(2)</b>				
0	---	1	C (36) H (46) Cu (1) N (8) O (10)	814.355

<b>Cu+2_PheTyr-2</b>				
0	---	1	C (18) H (18) Cu (1) N (2) O (4)	389.898
<b>Cu+2_Tri2PicAm</b>				
2	---	2	C (18) H (18) Cu (1) N (4)	353.914
<b>Cu+2_Tri2PicAm_OH-1</b>				
1	---	1	C (18) H (19) Cu (1) N (4) O (1)	370.921
<b>Cu+2_Trigalacturonic-3</b>				
-1	---	1	C (18) H (23) Cu (1) O (19)	606.915
<b>Cu+2_TTHA-6</b>				
-4	---	3	C (18) H (24) Cu (1) N (4) O (12)	551.954
<b>Cu+2_TyrPhe-2</b>				
0	---	1	C (18) H (18) Cu (1) N (2) O (4)	389.898
<b>Cu+2_TyrTyr-3</b>				
-1	---	1	C (18) H (17) Cu (1) N (2) O (5)	404.889
<b>Cu+2 (2)_ [14]N4:Acet*4-4</b>				
0	---	3	C (18) H (28) Cu (2) N (4) O (8)	555.534
<b>Cu+2 (2)_ [18]N3O3:Acet*3-3</b>				
1	---	3	C (18) H (30) Cu (2) N (3) O (9)	559.543
<b>Cu+2 (2)_ [2.2.2]crypt</b>				
4	---	1	C (18) H (36) Cu (2) N (2) O (6)	503.586
<b>Cu+2 (2)_ [27]N9</b>				
4	---	5	C (18) H (45) Cu (2) N (9)	514.708
<b>Cu+2 (2)_ [27]N9_OH-1</b>				
3	---	1	C (18) H (46) Cu (2) N (9) O (1)	531.715

<b>Cu+2 (2) _Enalaprilat-2 (3)</b>				
-2	---	1	C (54) H (66) Cu (2) N (6) O (15)	1166.24
<b>Cu+2 (2) _H+1 _[14]N4:Acet*4-4</b>				
1	---	2	C (18) H (29) Cu (2) N (4) O (8)	556.542
<b>Cu+2 (2) _H+1 _[18]N3O3:Acet*3-3</b>				
2	---	1	C (18) H (31) Cu (2) N (3) O (9)	560.551
<b>Cu+2 (2) _H+1 _[27]N9</b>				
5	---	2	C (18) H (46) Cu (2) N (9)	515.716
<b>Cu+2 (2) _H+1 _TTHA-6</b>				
-1	---	2	C (18) H (25) Cu (2) N (4) O (12)	616.508
<b>Cu+2 (2) _H+1 (-1) _Enalaprilat-2 (2)</b>				
-1	---	1	C (36) H (43) Cu (2) N (4) O (10)	818.850
<b>Cu+2 (2) _H+1 (-1) _PheTyr-2 (2)</b>				
-1	---	1	C (36) H (35) Cu (2) N (4) O (8)	778.788
<b>Cu+2 (2) _H+1 (-1) _Trigalacturonic-3 (2)</b>				
-3	---	1	C (36) H (45) Cu (2) O (38)	1212.82
<b>Cu+2 (2) _H+1 (-1) _TyrTyr-3 (2)</b>				
-3	---	1	C (36) H (33) Cu (2) N (4) O (10)	808.771
<b>Cu+2 (2) _H+1 (-2) _PheTyr-2 (2)</b>				
-2	---	1	C (36) H (34) Cu (2) N (4) O (8)	777.780
<b>Cu+2 (2) _H+1 (-2) _TyrPhe-2 (2)</b>				
-2	---	1	C (36) H (34) Cu (2) N (4) O (8)	777.780
<b>Cu+2 (2) _H+1 (2) _[27]N9</b>				
6	---	2	C (18) H (47) Cu (2) N (9)	516.723

<b>Cu+2 (2) _H+1 (2) _TTHA-6</b>				
0	---	1	C (18) H (26) Cu (2) N (4) O (12)	617.516
<b>Cu+2 (2) _H+1 (3) _[27]N9</b>				
7	---	2	C (18) H (48) Cu (2) N (9)	517.731
<b>Cu+2 (2) _OH-1 _[18]N3O3:Acet*3-3</b>				
0	---	2	C (18) H (31) Cu (2) N (3) O (10)	576.550
<b>Cu+2 (2) _OH-1 (2) _[18]N3O3:Acet*3-3</b>				
-1	---	1	C (18) H (32) Cu (2) N (3) O (11)	593.558
<b>Cu+2 (2) _Sulfox-2 _TTHA-6</b>				
-4	---	2	C (27) H (29) Cu (2) N (5) O (16) S (1)	838.703
<b>Cu+2 (2) _Sulfox-2 (2) _TTHA-6</b>				
-6	---	2	C (36) H (34) Cu (2) N (6) O (20) S (2)	1061.91
<b>Cu+2 (2) _Tiron-4 (2) _TTHA-6</b>				
-10	---	1	C (30) H (28) Cu (2) N (4) O (28) S (4)	1147.89
<b>Cu+2 (2) _TTHA-6</b>				
-2	---	6	C (18) H (24) Cu (2) N (4) O (12)	615.500
<b>Cu+2 (2) _TyrTyr-3 (2)</b>				
-2	---	1	C (36) H (34) Cu (2) N (4) O (10)	809.779
<b>Cu+2 (3) _[18]N3O3:Acet*3-3</b>				
3	---	1	C (18) H (30) Cu (3) N (3) O (9)	623.089
<b>Dy+3</b> Dysprosium(III) ion				
3	22541-21-5	592	Dy (1)	162.500
<b>Dy+3 _[14]N4:Acet*4-4</b>				
-1	---	2	C (18) H (28) Dy (1) N (4) O (8)	590.942

<b>Dy+3_[18]N2O4:EtCOO*2-2</b>				
1	---	1	C (18) H (32) Dy (1) N (2) O (8)	566.961
<b>Dy+3_[2.2.2]crypt</b>				
3	---	1	C (18) H (36) Dy (1) N (2) O (6)	538.994
<b>Dy+3_BEATA-4</b>				
-1	---	1	C (18) H (21) Dy (1) N (3) O (8)	569.880
<b>Dy+3_H+1_[14]N4:Acet*4-4</b>				
0	---	1	C (18) H (29) Dy (1) N (4) O (8)	591.950
<b>Dy+3_H+1_TTHA-6</b>				
-2	---	2	C (18) H (25) Dy (1) N (4) O (12)	651.916
<b>Dy+3_H+1 (2)_TTHA-6</b>				
-1	---	1	C (18) H (26) Dy (1) N (4) O (12)	652.924
<b>Dy+3_TTHA-6</b>				
-3	---	2	C (18) H (24) Dy (1) N (4) O (12)	650.908
<b>EDOHPhen*2Me*2DPI-4</b>				
-4	---	13	C (18) H (22) N (2) O (6) P (2)	424.331
<b>EDPhen*2Me*2DPI-2</b>				
-2	---	4	C (18) H (24) N (2) O (4) P (2)	394.348
<b>EHPG-4</b> EHPG ion				
-4	---	41	C (18) H (16) N (2) O (6)	356.335
<b>Enalaprilat-2</b> Enalaprilat anion				
-2	---	23	C (18) H (22) N (2) O (5)	346.383
<b>Er+3</b> Erbium(III) ion				

3	18472-30-5	620	Er (1)	167.260
<b>Er+3_[14]N4:Acet*4-4</b>				
-1	---	2	C (18)H (28)Er (1)N (4)O (8)	595.702
<b>Er+3_[18]N2O4:EtCOO*2-2</b>				
1	---	1	C (18)H (32)Er (1)N (2)O (8)	571.721
<b>Er+3_[2.2.2]crypt</b>				
3	---	1	C (18)H (36)Er (1)N (2)O (6)	543.754
<b>Er+3_BEATA-4</b>				
-1	---	1	C (18)H (21)Er (1)N (3)O (8)	574.640
<b>Er+3_H+1_[14]N4:Acet*4-4</b>				
0	---	1	C (18)H (29)Er (1)N (4)O (8)	596.710
<b>Er+3_H+1_TTHA-6</b>				
-2	---	1	C (18)H (25)Er (1)N (4)O (12)	656.676
<b>Er+3_TTHA-6</b>				
-3	---	2	C (18)H (24)Er (1)N (4)O (12)	655.668
<b>Er+3 (2)_OH-1 (2)_TTHA-6</b>				
-2	---	1	C (18)H (26)Er (2)N (4)O (14)	856.943
<b>Er+3 (2)_TTHA-6</b>				
0	---	1	C (18)H (24)Er (2)N (4)O (12)	822.928
<b>EtDiAm</b> Ethylenediamine; 1,2-Ethanediamine; 1,2-Diaminoethane; en !				
0	107-15-3	879	C (2)H (8)N (2)	60.0989
<b>Eu+2</b> Europium(II) ion				
2	---	37	Eu (1)	151.960
<b>Eu+2_[2.2.2]crypt</b>				



2	---	1	C(18)H(36)Eu(1)N(2)O(6)	528.454
<b>Eu+3</b> Europium(III) ion				
3	22541-18-0	683	Eu(1)	151.960
<b>Eu+3_[14]N4:Acet*4-4</b>				
-1	---	2	C(18)H(28)Eu(1)N(4)O(8)	580.402
<b>Eu+3_[18]N2O4:EtCOO*2-2</b>				
1	---	1	C(18)H(32)Eu(1)N(2)O(8)	556.421
<b>Eu+3_[2.2.2]crypt</b>				
3	---	1	C(18)H(36)Eu(1)N(2)O(6)	528.454
<b>Eu+3_BEATA-4</b>				
-1	---	1	C(18)H(21)Eu(1)N(3)O(8)	559.340
<b>Eu+3_H+1_[14]N4:Acet*4-4</b>				
0	---	1	C(18)H(29)Eu(1)N(4)O(8)	581.410
<b>Eu+3_H+1_TTHA-6</b>				
-2	---	2	C(18)H(25)Eu(1)N(4)O(12)	641.376
<b>Eu+3_H+1(2)_TTHA-6</b>				
-1	---	1	C(18)H(26)Eu(1)N(4)O(12)	642.384
<b>Eu+3_TTHA-6</b>				
-3	---	2	C(18)H(24)Eu(1)N(4)O(12)	640.368
<b>Fe+2</b> Iron(II) ion; Ferrous ion				
2	15438-31-0	1769	Fe(1)	55.8452
<b>Fe+2_[14]N4:Acet*4-4</b>				
-2	---	3	C(18)H(28)Fe(1)N(4)O(8)	484.288
<b>Fe+2_246Tri2Pyrid135Triazine</b>				

2	---	1	C (18) H (12) Fe (1) N (6)	368.179
<b>Fe+2_246Tri2Pyrid135Triazine (2)</b>				
2	---	2	C (36) H (24) Fe (1) N (12)	680.512
<b>Fe+2_4LICAMS-6</b>				
-4	---	1	C (18) H (14) Fe (1) N (2) O (12) S (2)	570.281
<b>Fe+2_CN-1 (6)</b> Ferrocyanide ion				
-4	---	100	C (6) Fe (1) N (6)	211.951
<b>Fe+2_H+1_246Tri2Pyrid135Triazine (2)</b>				
3	---	1	C (36) H (25) Fe (1) N (12)	681.520
<b>Fe+2_H+1_4LICAMS-6 (2)</b>				
-9	---	1	C (36) H (29) Fe (1) N (4) O (24) S (4)	1085.72
<b>Fe+2_H+1_TTHA-6</b>				
-3	---	2	C (18) H (25) Fe (1) N (4) O (12)	545.261
<b>Fe+2_H+1 (2)_4LICAMS-6 (2)</b>				
-8	---	1	C (36) H (30) Fe (1) N (4) O (24) S (4)	1086.73
<b>Fe+2_H+1 (2)_TTHA-6</b>				
-2	---	1	C (18) H (26) Fe (1) N (4) O (12)	546.269
<b>Fe+2_H+1 (4)_[27]N9_CN-1 (6)</b>				
0	---	1	C (24) H (49) Fe (1) N (15)	603.599
<b>Fe+2_H+1 (5)_[27]N9_CN-1 (6)</b>				
1	---	1	C (24) H (50) Fe (1) N (15)	604.607
<b>Fe+2_H+1 (6)_[24]N6_CN-1 (6)</b>				
2	---	1	C (24) H (48) Fe (1) N (12)	560.571
<b>Fe+2_H+1 (6)_[27]N6O3_CN-1 (6)</b>				

2	---	1	C(24)H(48)Fe(1)N(12)O(3)	608.569
<b>Fe+2_H+1(6)_[27]N9_CN-1(6)</b>				
2	---	1	C(24)H(51)Fe(1)N(15)	605.615
<b>Fe+2_H+1(7)_[27]N9_CN-1(6)</b>				
3	---	1	C(24)H(52)Fe(1)N(15)	606.623
<b>Fe+2_OH-1_[14]N4:Acet*4-4</b>				
-3	---	2	C(18)H(29)Fe(1)N(4)O(9)	501.295
<b>Fe+2_OH-1_TTHA-6</b>				
-5	---	2	C(18)H(25)Fe(1)N(4)O(13)	561.261
<b>Fe+2_OH-1(2)_TTHA-6</b>				
-6	---	1	C(18)H(26)Fe(1)N(4)O(14)	578.268
<b>Fe+2_Tri2PicAm</b>				
2	---	2	C(18)H(18)Fe(1)N(4)	346.213
<b>Fe+2_Tri2PicAm_OH-1</b>				
1	---	1	C(18)H(19)Fe(1)N(4)O(1)	363.220
<b>Fe+2_TTHA-6</b>				
-4	---	5	C(18)H(24)Fe(1)N(4)O(12)	544.253
<b>Fe+2_TTHA-6(2)</b>				
-10	---	2	C(36)H(48)Fe(1)N(8)O(24)	1032.66
<b>Fe+2_TTHA-6(3)</b>				
-16	---	1	C(54)H(72)Fe(1)N(12)O(36)	1521.07
<b>Fe+2_TTHA-6(4)</b>				
-22	---	1	C(72)H(96)Fe(1)N(16)O(48)	2009.48
<b>Fe+2_TTHA-6(5)</b>				
-28	---	1	C(90)H(120)Fe(1)N(20)O(60)	2497.89

<b>Fe+2_TTHA-6(6)</b>				
-34	---	1	C(108)H(144)Fe(1)N(24)O(72)	2986.29
<b>Fe+2(2)_[14]N4:Acet*4-4</b>				
0	---	2	C(18)H(28)Fe(2)N(4)O(8)	540.133
<b>Fe+2(2)_4LICAMS-6(3)</b>				
-14	---	1	C(54)H(42)Fe(2)N(6)O(36)S(6)	1655.00
<b>Fe+2(2)_OH-1_TTHA-6</b>				
-3	---	2	C(18)H(25)Fe(2)N(4)O(13)	617.106
<b>Fe+2(2)_OH-1(2)_TTHA-6</b>				
-4	---	1	C(18)H(26)Fe(2)N(4)O(14)	634.113
<b>Fe+2(2)_TTHA-6</b>				
-2	---	2	C(18)H(24)Fe(2)N(4)O(12)	600.099
<b>Fe+3</b> Iron(III) ion; Ferric ion				
3	20074-52-6	2512	Fe(1)	55.8452
<b>Fe+3_[14]N4:Acet*4-4</b>				
-1	---	2	C(18)H(28)Fe(1)N(4)O(8)	484.288
<b>Fe+3_[18]N3O3:Acet*3-3</b>				
0	---	2	C(18)H(30)Fe(1)N(3)O(9)	488.296
<b>Fe+3_BAMTPH-3</b>				
0	---	1	C(18)H(21)Fe(1)N(6)O(9)	521.245
<b>Fe+3_EDOHPhen*2Me*2DPI-4</b>				
-1	---	1	C(18)H(22)Fe(1)N(2)O(6)P(2)	480.176
<b>Fe+3_EHPG-4</b>				
-1	---	2	C(18)H(16)Fe(1)N(2)O(6)	412.180

<b>Fe+3_H+1_[14]N4:Acet*4-4</b>				
0	---	1	C(18)H(29)Fe(1)N(4)O(8)	485.295
<b>Fe+3_H+1_[18]N3O3:Acet*3-3</b>				
1	---	1	C(18)H(31)Fe(1)N(3)O(9)	489.304
<b>Fe+3_H+1_HPEDDA-4</b>				
0	---	1	C(18)H(17)Fe(1)N(2)O(6)	413.188
<b>Fe+3_H+1_mEHPPG-4</b>				
0	---	1	C(18)H(17)Fe(1)N(2)O(6)	413.188
<b>Fe+3_H+1_TTHA-6</b>				
-2	---	2	C(18)H(25)Fe(1)N(4)O(12)	545.261
<b>Fe+3_H+1(2)_TTHA-6</b>				
-1	---	1	C(18)H(26)Fe(1)N(4)O(12)	546.269
<b>Fe+3_HPEDDA-4</b>				
-1	---	2	C(18)H(16)Fe(1)N(2)O(6)	412.180
<b>Fe+3_mEHPPG-4</b>				
-1	---	3	C(18)H(16)Fe(1)N(2)O(6)	412.180
<b>Fe+3_OH-1_EHPPG-4</b>				
-2	---	1	C(18)H(17)Fe(1)N(2)O(7)	429.187
<b>Fe+3_OH-1_mEHPPG-4</b>				
-2	---	1	C(18)H(17)Fe(1)N(2)O(7)	429.187
<b>Fe+3_OH-1_TTHA-6</b>				
-4	---	2	C(18)H(25)Fe(1)N(4)O(13)	561.261
<b>Fe+3_OH-1(2)_TTHA-6</b>				
-5	---	1	C(18)H(26)Fe(1)N(4)O(14)	578.268

<b>Fe+3_TTHA-6</b>				
-3	---	4	C (18) H (24) Fe (1) N (4) O (12)	544.253
<b>Fe+3 (2)_OH-1_TTHA-6</b>				
-1	---	2	C (18) H (25) Fe (2) N (4) O (13)	617.106
<b>Fe+3 (2)_OH-1 (2)_TTHA-6</b>				
-2	---	3	C (18) H (26) Fe (2) N (4) O (14)	634.113
<b>Fe+3 (2)_Sulfox-2 (2)_TTHA-6</b>				
-4	---	1	C (36) H (34) Fe (2) N (6) O (20) S (2)	1046.51
<b>Fe+3 (2)_Tiron-4 (2)_TTHA-6</b>				
-8	---	1	C (30) H (28) Fe (2) N (4) O (28) S (4)	1132.49
<b>Fe+3 (2)_TTHA-6</b>				
0	---	7	C (18) H (24) Fe (2) N (4) O (12)	600.099
<b>Fumaric-2</b> Fumarate ion; trans-Butenedioate ion				
-2	142-42-7	70	C (4) H (2) O (4)	114.058
<b>Ga+3</b> Gallium(III) ion				
3	22537-33-3	472	Ga (1)	69.7230
<b>Ga+3_[14]N4:Acet*4-4</b>				
-1	---	2	C (18) H (28) Ga (1) N (4) O (8)	498.165
<b>Ga+3_[18]N3O3:Acet*3-3</b>				
0	---	1	C (18) H (30) Ga (1) N (3) O (9)	502.174
<b>Ga+3_EHPG-4</b>				
-1	---	2	C (18) H (16) Ga (1) N (2) O (6)	426.058
<b>Ga+3_H+1_[14]N4:Acet*4-4</b>				
0	---	1	C (18) H (29) Ga (1) N (4) O (8)	499.173

<b>Ga+3_H+1_EHPG-4</b>				
0	---	1	C (18) H (17) Ga (1) N (2) O (6)	427.066
<b>Ga+3_H+1_HPEDDA-4</b>				
0	---	1	C (18) H (17) Ga (1) N (2) O (6)	427.066
<b>Ga+3_H+1_mEHPG-4</b>				
0	---	1	C (18) H (17) Ga (1) N (2) O (6)	427.066
<b>Ga+3_H+1_TTHA-6</b>				
-2	---	2	C (18) H (25) Ga (1) N (4) O (12)	559.139
<b>Ga+3_H+1 (2)_TTHA-6</b>				
-1	---	2	C (18) H (26) Ga (1) N (4) O (12)	560.147
<b>Ga+3_H+1 (3)_TTHA-6</b>				
0	---	1	C (18) H (27) Ga (1) N (4) O (12)	561.155
<b>Ga+3_HPEDDA-4</b>				
-1	---	2	C (18) H (16) Ga (1) N (2) O (6)	426.058
<b>Ga+3_mEHPG-4</b>				
-1	---	2	C (18) H (16) Ga (1) N (2) O (6)	426.058
<b>Ga+3_OH-1_TTHA-6</b>				
-4	---	1	C (18) H (25) Ga (1) N (4) O (13)	575.139
<b>Ga+3_TTHA-6</b>				
-3	---	4	C (18) H (24) Ga (1) N (4) O (12)	558.131
<b>Ga+3 (2)_OH-1_TTHA-6</b>				
-1	---	1	C (18) H (25) Ga (2) N (4) O (13)	644.862
<b>Ga+3 (2)_OH-1 (2)_TTHA-6</b>				
-2	---	1	C (18) H (26) Ga (2) N (4) O (14)	661.869

<b>Ga+3 (2) _TTHA-6</b>				
0	---	4	C (18) H (24) Ga (2) N (4) O (12)	627.854
<b>Gd+3</b> Gadolinium(III) ion				
3	22541-19-1	790	Gd (1)	157.253
<b>Gd+3 _[14]N4:Acet*4-4</b>				
-1	---	2	C (18) H (28) Gd (1) N (4) O (8)	585.695
<b>Gd+3 _[18]dieneN6dipyo</b>				
3	---	1	C (18) H (26) Gd (1) N (6)	483.698
<b>Gd+3 _[18]N2O4:EtCOO*2-2</b>				
1	---	1	C (18) H (32) Gd (1) N (2) O (8)	561.714
<b>Gd+3 _[18]N3O3:Acet*3-3</b>				
0	---	1	C (18) H (30) Gd (1) N (3) O (9)	589.704
<b>Gd+3 _[2.2.2]crypt</b>				
3	---	1	C (18) H (36) Gd (1) N (2) O (6)	533.747
<b>Gd+3 _BEATA-4</b>				
-1	---	1	C (18) H (21) Gd (1) N (3) O (8)	564.633
<b>Gd+3 _H+1 _[14]N4:Acet*4-4</b>				
0	---	1	C (18) H (29) Gd (1) N (4) O (8)	586.703
<b>Gd+3 _H+1 _HPEDDA-4</b>				
0	---	2	C (18) H (17) Gd (1) N (2) O (6)	514.596
<b>Gd+3 _H+1 _TTHA-6</b>				
-2	---	2	C (18) H (25) Gd (1) N (4) O (12)	646.669
<b>Gd+3 _H+1 (2) _HPEDDA-4</b>				
1	---	1	C (18) H (18) Gd (1) N (2) O (6)	515.604



<b>Gd+3_H+1(2)_TTHA-6</b>				
-1	---	1	C(18)H(26)Gd(1)N(4)O(12)	647.677
<b>Gd+3_HPEDDA-4</b>				
-1	---	2	C(18)H(16)Gd(1)N(2)O(6)	513.588
<b>Gd+3_TTHA-6</b>				
-3	---	2	C(18)H(24)Gd(1)N(4)O(12)	645.661
<b>Glutaric-2</b> Glutarate ion; Pentanedioate ion				
-2	18667-05-5	121	C(5)H(6)O(4)	130.100
<b>Gly-1</b> Glycinate ion; Aminoacetate ion				
-1	---	1356	C(2)H(4)N(1)O(2)	74.0593
<b>GlyProDPheGly-1</b>				
-1	---	4	C(18)H(23)N(4)O(5)	375.404
<b>GlyProGlyPhe-1</b>				
-1	---	4	C(18)H(23)N(4)O(5)	375.404
<b>GlyProPheGly-1</b>				
-1	---	6	C(18)H(23)N(4)O(5)	375.404
<b>H+1</b> Hydrogen ion; Proton				
1	12408-02-5	31679	H(1)	1.00794
<b>H+1_[14]N2O2:DiBenz</b>				
1	---	2	C(18)H(23)N(2)O(2)	299.393
<b>H+1_[14]N4:2OHEt*4</b>				
1	---	2	C(18)H(41)N(4)O(4)	377.548
<b>H+1_[14]N4:Acet*4-4</b>				

-3	---	11	C(18)H(29)N(4)O(8)	429.450
<b>H+1_[18]dieneN6dipyo</b>				
1	---	2	C(18)H(27)N(6)	327.453
<b>H+1_[18]N2O4:DiIsoPr</b>				
1	---	2	C(18)H(39)N(2)O(4)	347.519
<b>H+1_[18]N2O4:DiMalon-4</b>				
-3	---	2	C(18)H(27)N(2)O(12)	463.419
<b>H+1_[18]N2O4:EtCOO*2-2</b>				
-1	---	2	C(18)H(33)N(2)O(8)	405.469
<b>H+1_[18]N2O4:Meox*2</b>				
1	---	2	C(18)H(39)N(2)O(6)	379.518
<b>H+1_[18]N3O3:Acet*3-3</b>				
-2	---	2	C(18)H(31)N(3)O(9)	433.459
<b>H+1_[2.2.2]crypt</b>				
1	---	2	C(18)H(37)N(2)O(6)	377.502
<b>H+1_[2.2.2]crypt_NH3</b>				
1	---	1	C(18)H(40)N(3)O(6)	394.532
<b>H+1_[24]N6</b>				
1	---	2	C(18)H(43)N(6)	343.580
<b>H+1_[27]N6O3</b>				
1	---	2	C(18)H(43)N(6)O(3)	391.578
<b>H+1_[27]N9</b>				
1	---	4	C(18)H(46)N(9)	388.624
<b>H+1_1238910HexMe47Phenanth</b>				
1	---	1	C(18)H(21)N(2)	265.378

<b>H+1_246Tri2Pyrid135Triazine</b>				
1	---	2	C(18)H(13)N(6)	313.341
<b>H+1_262Dpa</b>				
1	---	2	C(18)H(27)N(4)	299.439
<b>H+1_BAMTPH-3</b>				
-2	---	3	C(18)H(22)N(6)O(9)	466.408
<b>H+1_BEATA-4</b>				
-3	---	2	C(18)H(22)N(3)O(8)	408.388
<b>H+1_Codeine</b>				
1	---	1	C(18)H(22)N(1)O(3)	300.378
<b>H+1_EDOHPhen*2Me*2DPI-4</b>				
-3	---	3	C(18)H(23)N(2)O(6)P(2)	425.338
<b>H+1_EDPhen*2Me*2DPI-2</b>				
-1	---	2	C(18)H(25)N(2)O(4)P(2)	395.356
<b>H+1_EHPG-4</b>				
-3	---	2	C(18)H(17)N(2)O(6)	357.343
<b>H+1_Enalaprilat-2</b>				
-1	---	2	C(18)H(23)N(2)O(5)	347.391
<b>H+1_GlyProDPheGly-1</b>				
0	---	1	C(18)H(24)N(4)O(5)	376.412
<b>H+1_GlyProGlyPhe-1</b>				
0	---	1	C(18)H(24)N(4)O(5)	376.412
<b>H+1_GlyProPheGly-1</b>				
0	---	1	C(18)H(24)N(4)O(5)	376.412

<b>H+1_HBEDPO-6</b>				
-5	---	2	C(18)H(21)N(2)O(8)P(2)	455.321
<b>H+1_HPEDDA-4</b>				
-3	---	12	C(18)H(17)N(2)O(6)	357.343
<b>H+1_mEHPG-4</b>				
-3	---	2	C(18)H(17)N(2)O(6)	357.343
<b>H+1_MoO3_TTHA-6</b>				
-5	---	1	C(18)H(25)Mo(1)N(4)O(15)	633.376
<b>H+1_MoO3(2)_TTHA-6</b>				
-5	---	1	C(18)H(25)Mo(2)N(4)O(18)	777.337
<b>H+1_NH3</b> Ammonium ion				
1	14798-03-9	108	H(4)N(1)	18.0385
<b>H+1_Oleic-1</b> Oleic acid; Octadec-9-enoic acid; 9-Octadecenoic acid				
0	112-80-1	1	C(18)H(34)O(2)	282.467
<b>H+1_PhePhe-1</b> Di-L-phenylalanine; L-Phenylalananyl-L-phenylalanine				
0	2577-40-4	1	C(18)H(20)N(2)O(3)	312.368
<b>H+1_PheProGlyGly-1</b>				
0	---	1	C(18)H(24)N(4)O(5)	376.412
<b>H+1_PheTyr-2</b>				
-1	---	2	C(18)H(19)N(2)O(4)	327.360
<b>H+1_Stearic-1</b> Stearic acid; Octadecanoic acid; Emersol 132; Promulsin; Proviscol wax				
0	57-11-4	1	C(18)H(36)O(2)	284.483
<b>H+1_Tl+1_TTHA-6</b>				

-4	---	1	C(18)H(25)N(4)O(12)Tl(1)	693.799
<b>H+1_Tri2PicAm</b>				
1	---	2	C(18)H(19)N(4)	291.376
<b>H+1_Trigalacturonic-3</b>				
-2	---	1	C(18)H(24)O(19)	544.377
<b>H+1_TTHA-6</b>				
-5	---	9	C(18)H(25)N(4)O(12)	489.416
<b>H+1_TyrPhe-2</b>				
-1	---	2	C(18)H(19)N(2)O(4)	327.360
<b>H+1_TyrTyr-3</b>				
-2	---	2	C(18)H(18)N(2)O(5)	342.351
<b>H+1_VO2+1_TTHA-6</b>				
-4	---	2	C(18)H(25)N(4)O(14)V(1)	572.357
<b>H+1(2)_[14]N2O2:DiBenz</b>				
2	---	2	C(18)H(24)N(2)O(2)	300.401
<b>H+1(2)_[14]N4:2OHEt*4</b>				
2	---	2	C(18)H(42)N(4)O(4)	378.556
<b>H+1(2)_[14]N4:Acet*4-4</b>				
-2	---	7	C(18)H(30)N(4)O(8)	430.458
<b>H+1(2)_[18]dieneN6dipyo</b>				
2	---	2	C(18)H(28)N(6)	328.461
<b>H+1(2)_[18]N2O4:DiIsoPr</b>				
2	---	1	C(18)H(40)N(2)O(4)	348.527
<b>H+1(2)_[18]N2O4:DiMalon-4</b>				
-2	---	2	C(18)H(28)N(2)O(12)	464.427

<b>H+1 (2) _[18]N2O4:EtCOO*2-2</b>				
0	---	2	C (18)H (34)N (2)O (8)	406.477
<b>H+1 (2) _[18]N2O4:Meox*2</b>				
2	---	2	C (18)H (40)N (2)O (6)	380.525
<b>H+1 (2) _[18]N3O3:Acet*3-3</b>				
-1	---	2	C (18)H (32)N (3)O (9)	434.467
<b>H+1 (2) _[2.2.2]crypt</b>				
2	---	2	C (18)H (38)N (2)O (6)	378.510
<b>H+1 (2) _[24]N6</b>				
2	---	2	C (18)H (44)N (6)	344.588
<b>H+1 (2) _[27]N6O3</b>				
2	---	2	C (18)H (44)N (6)O (3)	392.586
<b>H+1 (2) _[27]N9</b>				
2	---	3	C (18)H (47)N (9)	389.632
<b>H+1 (2) _246Tri2Pyrid135Triazine</b>				
2	---	3	C (18)H (14)N (6)	314.349
<b>H+1 (2) _262Dpa</b>				
2	---	2	C (18)H (28)N (4)	300.447
<b>H+1 (2) _4LICAMS-6</b>				
-4	---	1	C (18)H (16)N (2)O (12)S (2)	516.451
<b>H+1 (2) _BAMTPH-3</b>				
-1	---	2	C (18)H (23)N (6)O (9)	467.415
<b>H+1 (2) _BEATA-4</b>				
-2	---	2	C (18)H (23)N (3)O (8)	409.396

<b>H+1 (2) _EDOHPhen*2Me*2DPI-4</b>				
-2	---	2	C (18) H (24) N (2) O (6) P (2)	426.346
<b>H+1 (2) _EDPhen*2Me*2DPI-2</b> Ethylenebis(imino(phenyl)methylene(methyl)phosphinic acid)				
0	---	1	C (18) H (26) N (2) O (4) P (2)	396.363
<b>H+1 (2) _EHPG-4</b>				
-2	---	3	C (18) H (18) N (2) O (6)	358.351
<b>H+1 (2) _Enalaprilat-2</b> Enalaprilat; S-(1-Carboxy-3-phenylpropyl)-L-alanyl-L-proline; Enalaprilic acid; 1-(N-1-Carboxy-3-phenylpropyl)-L-alanyl-L-proline; MK 422				
0	76420-72-9	3	C (18) H (24) N (2) O (5)	348.399
<b>H+1 (2) _HBEDPO-6</b>				
-4	---	7	C (18) H (22) N (2) O (8) P (2)	456.329
<b>H+1 (2) _HPEDDA-4</b>				
-2	---	12	C (18) H (18) N (2) O (6)	358.351
<b>H+1 (2) _mEHPG-4</b>				
-2	---	2	C (18) H (18) N (2) O (6)	358.351
<b>H+1 (2) _MoO3 _TTHA-6</b>				
-4	---	1	C (18) H (26) Mo (1) N (4) O (15)	634.384
<b>H+1 (2) _MoO3 (2) _TTHA-6</b>				
-4	---	1	C (18) H (26) Mo (2) N (4) O (18)	778.344
<b>H+1 (2) _PhePhe-1</b>				
1	---	1	C (18) H (21) N (2) O (3)	313.376
<b>H+1 (2) _PheTyr-2</b>				
0	---	3	C (18) H (20) N (2) O (4)	328.368
<b>H+1 (2) _Tri2PicAm</b>				

2	---	2	C(18)H(20)N(4)	292.384
<b>H+1(2)_Trigalacturonic-3</b>				
-1	---	1	C(18)H(25)O(19)	545.385
<b>H+1(2)_TTHA-6</b>				
-4	---	11	C(18)H(26)N(4)O(12)	490.424
<b>H+1(2)_TyrPhe-2</b>				
0	17355-11-2	3	C(18)H(20)N(2)O(4)	328.368
<b>H+1(2)_TyrTyr-3</b>				
-1	---	3	C(18)H(19)N(2)O(5)	343.359
<b>H+1(2)_VO2+1_TTHA-6</b>				
-3	---	2	C(18)H(26)N(4)O(14)V(1)	573.365
<b>H+1(3)_[14]N4:2OHEt*4</b>				
3	---	2	C(18)H(43)N(4)O(4)	379.564
<b>H+1(3)_[14]N4:Acet*4-4</b>				
-1	---	3	C(18)H(31)N(4)O(8)	431.466
<b>H+1(3)_[18]dieneN6dipyo</b>				
3	---	2	C(18)H(29)N(6)	329.468
<b>H+1(3)_[18]N2O4:DiMalon-4</b>				
-1	---	1	C(18)H(29)N(2)O(12)	465.434
<b>H+1(3)_[18]N2O4:EtCOO*2-2</b>				
1	---	1	C(18)H(35)N(2)O(8)	407.485
<b>H+1(3)_[18]N3O3:Acet*3-3</b>				
1,7,13-Trioxa-4,10,16-triazacyclooctadecane-N,N',N''-triacetic acid				
0	---	2	C(18)H(33)N(3)O(9)	435.475
<b>H+1(3)_[24]N6</b>				



3	---	2	C(18)H(45)N(6)	345.596
<b>H+1 (3) _[27]N6O3</b>				
3	---	2	C(18)H(45)N(6)O(3)	393.594
<b>H+1 (3) _[27]N9</b>				
3	---	3	C(18)H(48)N(9)	390.639
<b>H+1 (3) _262Dpa</b>				
3	---	2	C(18)H(29)N(4)	301.455
<b>H+1 (3) _4LICAMS-6</b>				
-3	---	2	C(18)H(17)N(2)O(12)S(2)	517.459
<b>H+1 (3) _BAMTPH-3</b> N,N',N''-Tris[2-(N-hydroxycarbamoyl)ethyl]-1,3,5-benzenetricarboxamide				
0	---	1	C(18)H(24)N(6)O(9)	468.423
<b>H+1 (3) _BEATA-4</b>				
-1	---	2	C(18)H(24)N(3)O(8)	410.404
<b>H+1 (3) _EDOHPHEN*2Me*2DPI-4</b>				
-1	---	2	C(18)H(25)N(2)O(6)P(2)	427.354
<b>H+1 (3) _EHPG-4</b>				
-1	---	3	C(18)H(19)N(2)O(6)	359.359
<b>H+1 (3) _Enalaprilat-2</b>				
1	---	2	C(18)H(25)N(2)O(5)	349.407
<b>H+1 (3) _HBEDPO-6</b>				
-3	---	2	C(18)H(23)N(2)O(8)P(2)	457.337
<b>H+1 (3) _HPEDDA-4</b>				
-1	---	2	C(18)H(19)N(2)O(6)	359.359
<b>H+1 (3) _mEHPG-4</b>				

-1	---	2	C(18)H(19)N(2)O(6)	359.359
<b>H+1(3)_MoO3_TTHA-6</b>				
-3	---	1	C(18)H(27)Mo(1)N(4)O(15)	635.392
<b>H+1(3)_PheTyr-2</b>				
1	---	2	C(18)H(21)N(2)O(4)	329.376
<b>H+1(3)_Tri2PicAm</b>				
3	---	1	C(18)H(21)N(4)	293.392
<b>H+1(3)_Trigalacturonic-3</b> Trigalacturonic acid; a-D-GalA-[1-4]-a-D-GalA-[1-4]-D-GalA				
0	6037-45-2	1	C(18)H(26)O(19)	546.393
<b>H+1(3)_TTHA-6</b>				
-3	---	5	C(18)H(27)N(4)O(12)	491.432
<b>H+1(3)_TyrPhe-2</b>				
1	---	2	C(18)H(21)N(2)O(4)	329.376
<b>H+1(3)_TyrTyr-3</b>				
0	1050-28-8	3	C(18)H(20)N(2)O(5)	344.367
<b>H+1(3)_VO2+1_TTHA-6</b>				
-2	---	1	C(18)H(27)N(4)O(14)V(1)	574.373
<b>H+1(4)_[14]N4:2OHEt*4</b>				
4	---	1	C(18)H(44)N(4)O(4)	380.572
<b>H+1(4)_[14]N4:Acet*4-4</b>				
0	---	3	C(18)H(32)N(4)O(8)	432.474
<b>H+1(4)_[18]dieneN6dipyo</b>				
4	---	1	C(18)H(30)N(6)	330.476
<b>H+1(4)_[18]N3O3:Acet*3-3</b>				

1	---	2	C(18)H(34)N(3)O(9)	436.483
<b>H+1(4)_[24]N6</b>				
4	---	2	C(18)H(46)N(6)	346.603
<b>H+1(4)_[24]N6_5ADP-3</b>				
1	---	1	C(28)H(58)N(11)O(10)P(2)	770.784
<b>H+1(4)_[24]N6_5AMP-2</b>				
2	---	1	C(28)H(58)N(11)O(7)P(1)	691.812
<b>H+1(4)_[24]N6_5ATP-4</b>				
0	---	1	C(28)H(58)N(11)O(13)P(3)	849.756
<b>H+1(4)_[24]N6_Adipic-2</b>				
2	---	1	C(24)H(54)N(6)O(4)	490.731
<b>H+1(4)_[24]N6_Fumaric-2</b>				
2	---	1	C(22)H(48)N(6)O(4)	460.661
<b>H+1(4)_[24]N6_Glutaric-2</b>				
2	---	1	C(23)H(52)N(6)O(4)	476.704
<b>H+1(4)_[24]N6_Maleic-2</b>				
2	---	1	C(22)H(48)N(6)O(4)	460.661
<b>H+1(4)_[24]N6_Malonic-2</b>				
2	---	1	C(21)H(48)N(6)O(4)	448.650
<b>H+1(4)_[24]N6_Oxalic-2</b>				
2	---	1	C(20)H(46)N(6)O(4)	434.623
<b>H+1(4)_[24]N6_Pimelic-2</b>				
2	---	1	C(25)H(56)N(6)O(4)	504.757
<b>H+1(4)_[24]N6_Succinic-2</b>				
2	---	1	C(22)H(50)N(6)O(4)	462.677

<b>H+1 (4) _[27]N6O3</b>				
4	---	2	C (18) H (46) N (6) O (3)	394.602
<b>H+1 (4) _[27]N9</b>				
4	---	5	C (18) H (49) N (9)	391.647
<b>H+1 (4) _262Dpa</b>				
4	---	1	C (18) H (30) N (4)	302.463
<b>H+1 (4) _4LICAMS-6</b>				
-2	---	1	C (18) H (18) N (2) O (12) S (2)	518.467
<b>H+1 (4) _BEATA-4</b> N,N-Bis(2-aminoethyl)aniline-N',N'',N''',N''''-tetraacetic acid				
0	87732-99-8	1	C (18) H (25) N (3) O (8)	411.412
<b>H+1 (4) _EDOHPhen*2Me*2DPI-4</b> Ethylenebis[imino(2-hydroxyphenyl)methylene(methyl)phosphinic acid				
0	---	1	C (18) H (26) N (2) O (6) P (2)	428.362
<b>H+1 (4) _EHPG-4</b> EHPG; Ethylenediaminedi(o-hydroxyphenylacetic acid); N,N'-Ethylenebis[2-(2-hydroxyphenyl)glycine]; EDDHA; rac-Ethylenediiminobis[(2-hydroxyphenyl)acetic acid]				
0	1170-02-1	2	C (18) H (20) N (2) O (6)	360.367
<b>H+1 (4) _HBEDPO-6</b>				
-2	---	2	C (18) H (24) N (2) O (8) P (2)	458.345
<b>H+1 (4) _HPEDDA-4</b>				
0	---	2	C (18) H (20) N (2) O (6)	360.367
<b>H+1 (4) _mEHPG-4</b> meso-N,N'-Ethylenebis[2-(o-hydroxyphenyl)glycine]				
0	---	1	C (18) H (20) N (2) O (6)	360.367
<b>H+1 (4) _MoO3_TTHA-6</b>				
-2	---	1	C (18) H (28) Mo (1) N (4) O (15)	636.400

<b>H+1 (4) _TTHA-6</b>				
-2	---	5	C (18)H (28)N (4)O (12)	492.440
<b>H+1 (4) _TyrTyr-3</b>				
1	---	2	C (18)H (21)N (2)O (5)	345.375
<b>H+1 (5) _[14]N4:Acet*4-4</b>				
1	---	2	C (18)H (33)N (4)O (8)	433.482
<b>H+1 (5) _[18]N3O3:Acet*3-3</b>				
2	---	1	C (18)H (35)N (3)O (9)	437.491
<b>H+1 (5) _[24]N6</b>				
5	---	2	C (18)H (47)N (6)	347.611
<b>H+1 (5) _[24]N6_5ADP-3</b>				
2	---	1	C (28)H (59)N (11)O (10)P (2)	771.792
<b>H+1 (5) _[24]N6_5AMP-2</b>				
3	---	1	C (28)H (59)N (11)O (7)P (1)	692.820
<b>H+1 (5) _[24]N6_5ATP-4</b>				
1	---	1	C (28)H (59)N (11)O (13)P (3)	850.764
<b>H+1 (5) _[24]N6_Adipic-2</b>				
3	---	1	C (24)H (55)N (6)O (4)	491.739
<b>H+1 (5) _[24]N6_Fumaric-2</b>				
3	---	1	C (22)H (49)N (6)O (4)	461.669
<b>H+1 (5) _[24]N6_Glutaric-2</b>				
3	---	1	C (23)H (53)N (6)O (4)	477.712
<b>H+1 (5) _[24]N6_Maleic-2</b>				
3	---	1	C (22)H (49)N (6)O (4)	461.669

<b>H+1 (5) _[24]N6_Malonic-2</b>				
3	---	1	C (21) H (49) N (6) O (4)	449.658
<b>H+1 (5) _[24]N6_Oxalic-2</b>				
3	---	1	C (20) H (47) N (6) O (4)	435.631
<b>H+1 (5) _[24]N6_Succinic-2</b>				
3	---	1	C (22) H (51) N (6) O (4)	463.685
<b>H+1 (5) _[27]N6O3</b>				
5	---	2	C (18) H (47) N (6) O (3)	395.610
<b>H+1 (5) _[27]N9</b>				
5	---	5	C (18) H (50) N (9)	392.655
<b>H+1 (5) _HBEDPO-6</b>				
-1	---	2	C (18) H (25) N (2) O (8) P (2)	459.353
<b>H+1 (5) _HPEDDA-4</b>				
1	---	1	C (18) H (21) N (2) O (6)	361.375
<b>H+1 (5) _TTHA-6</b>				
-1	---	5	C (18) H (29) N (4) O (12)	493.448
<b>H+1 (6) _[14]N4:Acet*4-4</b>				
2	---	1	C (18) H (34) N (4) O (8)	434.490
<b>H+1 (6) _[24]N6</b>				
6	---	1	C (18) H (48) N (6)	348.619
<b>H+1 (6) _[24]N6_135BenzTriCOO-3</b>				
3	---	1	C (27) H (51) N (6) O (6)	555.739
<b>H+1 (6) _[24]N6_5ADP-3</b>				
3	---	1	C (28) H (60) N (11) O (10) P (2)	772.800

<b>H+1(6)_[24]N6_5AMP-2</b>				
4	---	1	C(28)H(60)N(11)O(7)P(1)	693.828
<b>H+1(6)_[24]N6_5ATP-4</b>				
2	---	1	C(28)H(60)N(11)O(13)P(3)	851.772
<b>H+1(6)_[24]N6_Adipic-2</b>				
4	---	1	C(24)H(56)N(6)O(4)	492.746
<b>H+1(6)_[24]N6_Citric-3</b>				
3	---	1	C(24)H(53)N(6)O(7)	537.721
<b>H+1(6)_[24]N6_Fumaric-2</b>				
4	---	1	C(22)H(50)N(6)O(4)	462.677
<b>H+1(6)_[24]N6_Glutaric-2</b>				
4	---	1	C(23)H(54)N(6)O(4)	478.720
<b>H+1(6)_[24]N6_Maleic-2</b>				
4	---	1	C(22)H(50)N(6)O(4)	462.677
<b>H+1(6)_[24]N6_Malonic-2</b>				
4	---	1	C(21)H(50)N(6)O(4)	450.666
<b>H+1(6)_[24]N6_Oxalic-2</b>				
4	---	1	C(20)H(48)N(6)O(4)	436.639
<b>H+1(6)_[24]N6_SO4-2</b>				
4	---	1	C(18)H(48)N(6)O(4)S(1)	444.677
<b>H+1(6)_[24]N6_Squaric-2</b>				
4	---	1	C(22)H(48)N(6)O(4)	460.661
<b>H+1(6)_[24]N6_Succinic-2</b>				
4	---	1	C(22)H(52)N(6)O(4)	464.693

<b>H+1 (6) _[27]N6O3</b>				
6	---	1	C (18) H (48) N (6) O (3)	396.618
<b>H+1 (6) _[27]N6O3 _135BenzTriCOO-3</b>				
3	---	1	C (27) H (51) N (6) O (9)	603.737
<b>H+1 (6) _[27]N6O3 _5ADP-3</b>				
3	---	1	C (28) H (60) N (11) O (13) P (2)	820.798
<b>H+1 (6) _[27]N6O3 _5AMP-2</b>				
4	---	1	C (28) H (60) N (11) O (10) P (1)	741.826
<b>H+1 (6) _[27]N6O3 _5ATP-4</b>				
2	---	1	C (28) H (60) N (11) O (16) P (3)	899.771
<b>H+1 (6) _[27]N6O3 _Citric-3</b>				
3	---	1	C (24) H (53) N (6) O (10)	585.719
<b>H+1 (6) _[27]N6O3 _Fumaric-2</b>				
4	---	1	C (22) H (50) N (6) O (7)	510.675
<b>H+1 (6) _[27]N6O3 _Maleic-2</b>				
4	---	1	C (22) H (50) N (6) O (7)	510.675
<b>H+1 (6) _[27]N6O3 _Malonic-2</b>				
4	---	1	C (21) H (50) N (6) O (7)	498.664
<b>H+1 (6) _[27]N6O3 _Oxalic-2</b>				
4	---	1	C (20) H (48) N (6) O (7)	484.637
<b>H+1 (6) _[27]N6O3 _SO4-2</b>				
4	---	1	C (18) H (48) N (6) O (7) S (1)	492.675
<b>H+1 (6) _[27]N6O3 _Squaric-2</b>				
4	---	1	C (22) H (48) N (6) O (7)	508.659



<b>H+1 (6) _[27]N6O3_Succinic-2</b>				
4	---	1	C (22) H (52) N (6) O (7)	512.691
<b>H+1 (6) _[27]N6O3_Tartaric-2</b>				
4	---	1	C (22) H (52) N (6) O (9)	544.690
<b>H+1 (6) _[27]N9</b>				
6	---	5	C (18) H (51) N (9)	393.663
<b>H+1 (6) _HBEDPO-6</b>				
0	---	1	C (18) H (26) N (2) O (8) P (2)	460.361
<b>H+1 (6) _TTHA-6</b> TTHA; Triethylenetetraaminehexaethanoic acid; Triethylenetetraminehexaacetic acid; 3,6,9,12-Tetrakis(carboxymethyl)-3,6,9,12-tetraazatetradecanedioic acid				
0	869-52-3	5	C (18) H (30) N (4) O (12)	494.456
<b>H+1 (7) _[27]N9</b>				
7	---	5	C (18) H (52) N (9)	394.671
<b>H+1 (7) _TTHA-6</b>				
1	---	2	C (18) H (31) N (4) O (12)	495.464
<b>H+1 (8) _[27]N9</b>				
8	---	4	C (18) H (53) N (9)	395.679
<b>H+1 (8) _TTHA-6</b>				
2	---	1	C (18) H (32) N (4) O (12)	496.472
<b>H+1 (9) _[27]N9</b>				
9	---	1	C (18) H (54) N (9)	396.687
<b>H+1 (9) _TTHA-6</b>				
3	---	1	C (18) H (33) N (4) O (12)	497.480
<b>H2O</b> Water				

0	7732-18-5	5947	H(2)O(1)	18.0153
<b>HBEDPO-6</b> HBEDPO; N,N''-Bis(2-hydroxybenzyl)ethylenediamine-N,N'-bis(methylenephosphonate)				
-6	---	33	C(18)H(20)N(2)O(8)P(2)	454.313
<b>Hf+4</b> Hafnium(IV) ion				
4	22541-25-9	148	Hf(1)	178.492
<b>Hf+4_H+1(2)_TTHA-6</b>				
0	---	1	C(18)H(26)Hf(1)N(4)O(12)	668.916
<b>Hg+2</b> Mercury(II) ion; Mercuric ion				
2	14302-87-5	1203	Hg(1)	200.592
<b>Hg+2_[14]N4:2OHEt*4</b>				
2	---	1	C(18)H(40)Hg(1)N(4)O(4)	577.132
<b>Hg+2_[14]N4:Acet*4-4</b>				
-2	---	1	C(18)H(28)Hg(1)N(4)O(8)	629.034
<b>Hg+2_[2.2.2]crypt</b>				
2	---	1	C(18)H(36)Hg(1)N(2)O(6)	577.086
<b>Hg+2_Cl-1(2)</b>				
0	---	40	Cl(2)Hg(1)	271.498
<b>Hg+2_H+1_TTHA-6</b>				
-3	---	2	C(18)H(25)Hg(1)N(4)O(12)	690.008
<b>Hg+2_H+1(2)_TTHA-6</b>				
-2	---	2	C(18)H(26)Hg(1)N(4)O(12)	691.016
<b>Hg+2_H+1(3)_TTHA-6</b>				
-1	---	1	C(18)H(27)Hg(1)N(4)O(12)	692.024

<b>Hg+2_Tri2PicAm</b>				
2	---	2	C (18) H (18) Hg (1) N (4)	490.960
<b>Hg+2_Tri2PicAm_OH-1</b>				
1	---	1	C (18) H (19) Hg (1) N (4) O (1)	507.967
<b>Hg+2_Tri2PicAm (2)</b>				
2	---	1	C (36) H (36) Hg (1) N (8)	781.327
<b>Hg+2_Triphenylarsine</b>				
2	---	1	C (18) H (15) As (1) Hg (1)	506.831
<b>Hg+2_Triphenylarsine_Cl-1</b>				
1	---	2	C (18) H (15) As (1) Cl (1) Hg (1)	542.284
<b>Hg+2_Triphenylarsine (2)</b>				
2	---	2	C (36) H (30) As (2) Hg (1)	813.070
<b>Hg+2_TTHA-6</b>				
-4	---	4	C (18) H (24) Hg (1) N (4) O (12)	689.000
<b>Hg+2_TTHA-6 (2)</b>				
-10	---	2	C (36) H (48) Hg (1) N (8) O (24)	1177.41
<b>Hg+2 (2)_H+1_TTHA-6</b>				
-1	---	2	C (18) H (25) Hg (2) N (4) O (12)	890.600
<b>Hg+2 (2)_H+1 (2)_TTHA-6</b>				
0	---	1	C (18) H (26) Hg (2) N (4) O (12)	891.608
<b>Hg+2 (2)_HMTA_TTHA-6</b>				
-2	---	1	C (24) H (36) Hg (2) N (8) O (12)	1029.78
<b>Hg+2 (2)_HMTA (2)_TTHA-6</b>				
-2	---	1	C (30) H (48) Hg (2) N (12) O (12)	1169.97

<b>Hg+2 (2) _Imidazole _TTHA-6</b>				
-2	---	1	C (21) H (28) Hg (2) N (6) O (12)	957.670
<b>Hg+2 (2) _Imidazole (2) _TTHA-6</b>				
-2	---	1	C (24) H (32) Hg (2) N (8) O (12)	1025.75
<b>Hg+2 (2) _NH3 _TTHA-6</b>				
-2	---	1	C (18) H (27) Hg (2) N (5) O (12)	906.623
<b>Hg+2 (2) _NH3 (2) _TTHA-6</b>				
-2	---	1	C (18) H (30) Hg (2) N (6) O (12)	923.653
<b>Hg+2 (2) _OH-1 _TTHA-6</b>				
-3	---	2	C (18) H (25) Hg (2) N (4) O (13)	906.600
<b>Hg+2 (2) _OH-1 (2) _TTHA-6</b>				
-4	---	2	C (18) H (26) Hg (2) N (4) O (14)	923.607
<b>Hg+2 (2) _TTHA-6</b>				
-2	---	11	C (18) H (24) Hg (2) N (4) O (12)	889.592
<b>HMTA</b> Hexamethylenetetramine; Methenamine; 1,3,5,7-Tetraazatricyclo[3.3.1.1[3,7]]decane; hmta; 1,3,5,7-Tetraaza-adamantane				
0	100-97-0	6	C (6) H (12) N (4)	140.188
<b>Ho+3</b> Holmium(III) ion				
3	22541-22-6	537	Ho (1)	164.930
<b>Ho+3 _[18]N2O4:EtCOO*2-2</b>				
1	---	1	C (18) H (32) Ho (1) N (2) O (8)	569.391
<b>Ho+3 _[2.2.2]crypt</b>				
3	---	1	C (18) H (36) Ho (1) N (2) O (6)	541.424
<b>Ho+3 _BEATA-4</b>				

-1	---	1	C(18)H(21)Ho(1)N(3)O(8)	572.310
<b>Ho+3_H+1_TTHA-6</b>				
-2	---	2	C(18)H(25)Ho(1)N(4)O(12)	654.346
<b>Ho+3_H+1(2)_TTHA-6</b>				
-1	---	1	C(18)H(26)Ho(1)N(4)O(12)	655.354
<b>Ho+3_TTHA-6</b>				
-3	---	2	C(18)H(24)Ho(1)N(4)O(12)	653.338
<b>Ho+3(2)_TTHA-6</b>				
0	---	1	C(18)H(24)Ho(2)N(4)O(12)	818.268
<b>HPEDDA-4</b> N,N'-Bis(2-hydroxyphenyl)ethylenediamine-N,N'-diacetate ion; HPED ion; hedda ion				
-4	---	64	C(18)H(16)N(2)O(6)	356.335
<b>I-1</b> Iodide ion				
-1	20461-54-5	894	I(1)	126.900
<b>I+1_[2.2.2]crypt</b>				
1	---	1	C(18)H(36)I(1)N(2)O(6)	503.394
<b>I2</b> Iodine, aqueous				
0	---	20	I(2)	253.800
<b>Imidazole</b> Imidazole; 1,3-Diazole; 1H-Imidazole; im; Him				
0	288-32-4	422	C(3)H(4)N(2)	68.0782
<b>In+3</b> Indium(III) ion				
3	22537-49-1	523	In(1)	114.820
<b>In+3_[14]N4:Acet*4-4</b>				
-1	---	2	C(18)H(28)In(1)N(4)O(8)	543.262

<b>In+3_EHPG-4</b>				
-1	---	3	C(18)H(16)In(1)N(2)O(6)	471.155
<b>In+3_H+1_[14]N4:Acet*4-4</b>				
0	---	1	C(18)H(29)In(1)N(4)O(8)	544.270
<b>In+3_H+1_EHPG-4</b>				
0	---	2	C(18)H(17)In(1)N(2)O(6)	472.163
<b>In+3_H+1_HPEDDA-4</b>				
0	---	1	C(18)H(17)In(1)N(2)O(6)	472.163
<b>In+3_H+1_mEHPG-4</b>				
0	---	2	C(18)H(17)In(1)N(2)O(6)	472.163
<b>In+3_H+1_TTHA-6</b>				
-2	---	2	C(18)H(25)In(1)N(4)O(12)	604.236
<b>In+3_H+1(2)_EHPG-4</b>				
1	---	1	C(18)H(18)In(1)N(2)O(6)	473.171
<b>In+3_H+1(2)_mEHPG-4</b>				
1	---	1	C(18)H(18)In(1)N(2)O(6)	473.171
<b>In+3_H+1(2)_TTHA-6</b>				
-1	---	1	C(18)H(26)In(1)N(4)O(12)	605.244
<b>In+3_HPEDDA-4</b>				
-1	---	2	C(18)H(16)In(1)N(2)O(6)	471.155
<b>In+3_mEHPG-4</b>				
-1	---	3	C(18)H(16)In(1)N(2)O(6)	471.155
<b>In+3_OH-1_EHPG-4</b>				
-2	---	1	C(18)H(17)In(1)N(2)O(7)	488.162

<b>In+3_OH-1_mEHPG-4</b>				
-2	---	1	C(18)H(17)In(1)N(2)O(7)	488.162
<b>In+3_TTHA-6</b>				
-3	---	3	C(18)H(24)In(1)N(4)O(12)	603.228
<b>In+3(2)_OH-1_TTHA-6</b>				
-1	---	1	C(18)H(25)In(2)N(4)O(13)	735.056
<b>In+3(2)_TTHA-6</b>				
0	---	2	C(18)H(24)In(2)N(4)O(12)	718.048
<b>K+1</b> Potassium(I) ion				
1	24203-36-9	462	K(1)	39.0980
<b>K+1_[18]N2O4:Meox*2</b>				
1	---	1	C(18)H(38)K(1)N(2)O(6)	417.608
<b>K+1_[2.2.2]crypt</b>				
1	32611-95-3	1	C(18)H(36)K(1)N(2)O(6)	415.592
<b>K+1_[2.2.2]crypt:DiLactam</b>				
1	---	1	C(18)H(32)K(1)N(2)O(8)	443.559
<b>La+3</b> Lanthanum(III) ion				
3	16096-89-2	882	La(1)	138.910
<b>La+3_[14]N4:Acet*4-4</b>				
-1	---	2	C(18)H(28)La(1)N(4)O(8)	567.352
<b>La+3_[18]dieneN6dipyo</b>				
3	---	1	C(18)H(26)La(1)N(6)	465.355
<b>La+3_[18]N2O4:EtCOO*2-2</b>				
1	---	1	C(18)H(32)La(1)N(2)O(8)	543.371

<b>La+3_[2.2.2]crypt</b>				
3	---	1	C(18)H(36)La(1)N(2)O(6)	515.404
<b>La+3_BEATA-4</b>				
-1	---	1	C(18)H(21)La(1)N(3)O(8)	546.290
<b>La+3_H+1_[14]N4:Acet*4-4</b>				
0	---	1	C(18)H(29)La(1)N(4)O(8)	568.360
<b>La+3_H+1_TTHA-6</b>				
-2	---	3	C(18)H(25)La(1)N(4)O(12)	628.326
<b>La+3_H+1(2)_TTHA-6</b>				
-1	---	1	C(18)H(26)La(1)N(4)O(12)	629.334
<b>La+3_OH-1(2)_HPEDDA-4</b>				
-3	---	2	C(18)H(18)La(1)N(2)O(8)	529.260
<b>La+3_OH-1(3)_HPEDDA-4</b>				
-4	---	1	C(18)H(19)La(1)N(2)O(9)	546.267
<b>La+3_TTHA-6</b>				
-3	---	4	C(18)H(24)La(1)N(4)O(12)	627.318
<b>La+3_TTHA-6(2)</b>				
-9	---	1	C(36)H(48)La(1)N(8)O(24)	1115.73
<b>La+3(2)_Sulfox-2(2)_TTHA-6</b>				
-4	---	1	C(36)H(34)La(2)N(6)O(20)S(2)	1212.63
<b>La+3(2)_TTHA-6</b>				
0	---	3	C(18)H(24)La(2)N(4)O(12)	766.228
<b>Li+1</b> Lithium(I) ion				
1	17341-24-1	246	Li(1)	6.94100



<b>Li+1_[18]N2O4:Meox*2</b>				
1	---	1	C(18)H(38)Li(1)N(2)O(6)	385.451
<b>Li+1_[2.2.2]crypt</b>				
1	---	1	C(18)H(36)Li(1)N(2)O(6)	383.435
<b>Li+1_[2.2.2]crypt:DiLactam</b>				
1	---	1	C(18)H(32)Li(1)N(2)O(8)	411.402
<b>Lu+3</b> Lutetium(III) ion				
3	22541-24-8	493	Lu(1)	174.970
<b>Lu+3_[18]N2O4:DiMalon-4</b>				
-1	---	1	C(18)H(26)Lu(1)N(2)O(12)	637.381
<b>Lu+3_[18]N2O4:EtCOO*2-2</b>				
1	---	1	C(18)H(32)Lu(1)N(2)O(8)	579.431
<b>Lu+3_BEATA-4</b>				
-1	---	1	C(18)H(21)Lu(1)N(3)O(8)	582.350
<b>Lu+3_H+1_HPEDDA-4</b>				
0	---	1	C(18)H(17)Lu(1)N(2)O(6)	532.313
<b>Lu+3_H+1_TTHA-6</b>				
-2	---	1	C(18)H(25)Lu(1)N(4)O(12)	664.386
<b>Lu+3_H+1(2)_HPEDDA-4</b>				
1	---	1	C(18)H(18)Lu(1)N(2)O(6)	533.321
<b>Lu+3_HPEDDA-4</b>				
-1	---	1	C(18)H(16)Lu(1)N(2)O(6)	531.305
<b>Lu+3_TTHA-6</b>				
-3	---	2	C(18)H(24)Lu(1)N(4)O(12)	663.378

<b>Maleic-2</b> cis-Butenedioate ion; Maleate ion				
-2	142-44-9	195	C(4)H(2)O(4)	114.058
<b>Malonic-2</b> Malonate ion				
-2	156-80-9	417	C(3)H(2)O(4)	102.047
<b>mEHPG-4</b> meso-EHPG ion				
-4	---	22	C(18)H(16)N(2)O(6)	356.335
<b>Mg+2</b> Magnesium(II) ion				
2	22537-22-0	2035	Mg(1)	24.3050
<b>Mg+2_[14]N4:2OHEt*4</b>				
2	---	1	C(18)H(40)Mg(1)N(4)O(4)	400.845
<b>Mg+2_[14]N4:Acet*4-4</b>				
-2	---	1	C(18)H(28)Mg(1)N(4)O(8)	452.747
<b>Mg+2_[18]N2O4:DiMalon-4</b>				
-2	---	1	C(18)H(26)Mg(1)N(2)O(12)	486.716
<b>Mg+2_[2.2.2]crypt</b>				
2	---	1	C(18)H(36)Mg(1)N(2)O(6)	400.799
<b>Mg+2_EHPG-4</b>				
-2	---	1	C(18)H(16)Mg(1)N(2)O(6)	380.640
<b>Mg+2_H+1_[14]N4:Acet*4-4</b>				
-1	---	1	C(18)H(29)Mg(1)N(4)O(8)	453.755
<b>Mg+2_H+1_EHPG-4</b>				
-1	---	1	C(18)H(17)Mg(1)N(2)O(6)	381.648
<b>Mg+2_H+1_HBEDPO-6</b>				

-3	---	2	C (18) H (21) Mg (1) N (2) O (8) P (2)	479.626
<b>Mg+2_H+1_HPEDDA-4</b>				
-1	---	1	C (18) H (17) Mg (1) N (2) O (6)	381.648
<b>Mg+2_H+1_TTHA-6</b>				
-3	---	3	C (18) H (25) Mg (1) N (4) O (12)	513.721
<b>Mg+2_H+1 (2)_EHPG-4</b>				
0	---	1	C (18) H (18) Mg (1) N (2) O (6)	382.656
<b>Mg+2_H+1 (2)_HBEDPO-6</b>				
-2	---	2	C (18) H (22) Mg (1) N (2) O (8) P (2)	480.634
<b>Mg+2_H+1 (2)_HPEDDA-4</b>				
0	---	1	C (18) H (18) Mg (1) N (2) O (6)	382.656
<b>Mg+2_H+1 (2)_TTHA-6</b>				
-2	---	2	C (18) H (26) Mg (1) N (4) O (12)	514.729
<b>Mg+2_HBEDPO-6</b>				
-4	---	2	C (18) H (20) Mg (1) N (2) O (8) P (2)	478.618
<b>Mg+2_HPEDDA-4</b>				
-2	---	1	C (18) H (16) Mg (1) N (2) O (6)	380.640
<b>Mg+2_TTHA-6</b>				
-4	---	3	C (18) H (24) Mg (1) N (4) O (12)	512.713
<b>Mg+2 (2)_TTHA-6</b>				
-2	---	3	C (18) H (24) Mg (2) N (4) O (12)	537.018
<b>Mg+2 (3)_TTHA-6</b>				
0	---	1	C (18) H (24) Mg (3) N (4) O (12)	561.323
<b>Mn+2</b> Manganese(II) ion; Manganous ion				

2	16397-91-4	1956	Mn (1)	54.9380
<b>Mn+2_[14]N4:Acet*4-4</b>				
-2	---	1	C (18) H (28) Mn (1) N (4) O (8)	483.380
<b>Mn+2_[18]dieneN6dipyo</b>				
2	---	1	C (18) H (26) Mn (1) N (6)	381.383
<b>Mn+2_[18]N2O4:DiMalon-4</b>				
-2	---	1	C (18) H (26) Mn (1) N (2) O (12)	517.349
<b>Mn+2_H+1_HPEDDA-4</b>				
-1	---	1	C (18) H (17) Mn (1) N (2) O (6)	412.281
<b>Mn+2_H+1_TTHA-6</b>				
-3	---	2	C (18) H (25) Mn (1) N (4) O (12)	544.354
<b>Mn+2_H+1 (2)_HPEDDA-4</b>				
0	---	1	C (18) H (18) Mn (1) N (2) O (6)	413.289
<b>Mn+2_H+1 (2)_TTHA-6</b>				
-2	---	2	C (18) H (26) Mn (1) N (4) O (12)	545.362
<b>Mn+2_H+1 (3)_TTHA-6</b>				
-1	---	1	C (18) H (27) Mn (1) N (4) O (12)	546.370
<b>Mn+2_HPEDDA-4</b>				
-2	---	1	C (18) H (16) Mn (1) N (2) O (6)	411.273
<b>Mn+2_Tri2PicAm</b>				
2	---	2	C (18) H (18) Mn (1) N (4)	345.306
<b>Mn+2_Tri2PicAm_OH-1</b>				
1	---	1	C (18) H (19) Mn (1) N (4) O (1)	362.313
<b>Mn+2_TTHA-6</b>				
-4	---	3	C (18) H (24) Mn (1) N (4) O (12)	543.346

<b>Mn+2 (2) _TTHA-6</b>				
-2	---	1	C (18) H (24) Mn (2) N (4) O (12)	598.284
<b>MoO3</b>				
0	---	32	Mo (1) O (3)	143.960
<b>MoO3 (2) _TTHA-6</b>				
-6	---	1	C (18) H (24) Mo (2) N (4) O (18)	776.329
<b>MoO4-2</b> Molybdate(VI) ion				
-2	14259-85-9	281	Mo (1) O (4)	159.960
<b>MoO4-2 (2)</b>				
-4	---	3	Mo (2) O (8)	319.919
<b>Na+1</b> Sodium(I) ion				
1	17341-25-2	617	Na (1)	22.9900
<b>Na+1 _[14]N4:Acet*4-4</b>				
-3	---	1	C (18) H (28) N (4) Na (1) O (8)	451.432
<b>Na+1 _[18]N2O4:Meox*2</b>				
1	---	1	C (18) H (38) N (2) Na (1) O (6)	401.500
<b>Na+1 _[2.2.2]crypt</b>				
1	---	1	C (18) H (36) N (2) Na (1) O (6)	399.484
<b>Na+1 _[2.2.2]crypt:DiLactam</b>				
1	---	1	C (18) H (32) N (2) Na (1) O (8)	427.451
<b>Na+1 _TTHA-6</b>				
-5	---	1	C (18) H (24) N (4) Na (1) O (12)	511.398
<b>Nd+3</b> Neodymium(III) ion				

3	14913-52-1	800	Nd(1)	144.240
<b>Nd+3_[14]N4:Acet*4-4</b>				
-1	---	2	C(18)H(28)N(4)Nd(1)O(8)	572.682
<b>Nd+3_[18]N2O4:EtCOO*2-2</b>				
1	---	1	C(18)H(32)N(2)Nd(1)O(8)	548.701
<b>Nd+3_BAMTPH-3</b>				
0	---	1	C(18)H(21)N(6)Nd(1)O(9)	609.640
<b>Nd+3_BEATA-4</b>				
-1	---	1	C(18)H(21)N(3)Nd(1)O(8)	551.620
<b>Nd+3_H+1_[14]N4:Acet*4-4</b>				
0	---	1	C(18)H(29)N(4)Nd(1)O(8)	573.690
<b>Nd+3_H+1_TTHA-6</b>				
-2	---	2	C(18)H(25)N(4)Nd(1)O(12)	633.656
<b>Nd+3_H+1(2)_TTHA-6</b>				
-1	---	1	C(18)H(26)N(4)Nd(1)O(12)	634.664
<b>Nd+3_TTHA-6</b>				
-3	---	3	C(18)H(24)N(4)Nd(1)O(12)	632.648
<b>Nd+3(2)_OH-1(2)_TTHA-6</b>				
-2	---	1	C(18)H(26)N(4)Nd(2)O(14)	810.903
<b>Nd+3(2)_TTHA-6</b>				
0	---	3	C(18)H(24)N(4)Nd(2)O(12)	776.888
<b>NH3</b> Ammonia, aqueous				
0	---	1462	H(3)N(1)	17.0305
<b>Ni+2</b> Nickel(II) ion				

2	14701-22-5	5108	Ni (1)	58.6930
<b>Ni+2_[14]N2O2:DiBenz</b>				
2	---	1	C (18)H (22)N (2)Ni (1)O (2)	357.078
<b>Ni+2_[14]N4:2OHEt*4</b>				
2	---	2	C (18)H (40)N (4)Ni (1)O (4)	435.233
<b>Ni+2_[14]N4:Acet*4-4</b>				
-2	---	4	C (18)H (28)N (4)Ni (1)O (8)	487.135
<b>Ni+2_[18]N3O3:Acet*3-3</b>				
-1	---	3	C (18)H (30)N (3)Ni (1)O (9)	491.144
<b>Ni+2_[2.2.2]crypt</b>				
2	---	1	C (18)H (36)N (2)Ni (1)O (6)	435.187
<b>Ni+2_[24]N6</b>				
2	---	1	C (18)H (42)N (6)Ni (1)	401.265
<b>Ni+2_4LICAMS-6</b>				
-4	---	1	C (18)H (14)N (2)Ni (1)O (12)S (2)	573.128
<b>Ni+2_BAMTPH-3</b>				
-1	---	2	C (18)H (21)N (6)Ni (1)O (9)	524.093
<b>Ni+2_EDOHPHEN*2Me*2DPI-4</b>				
-2	---	2	C (18)H (22)N (2)Ni (1)O (6)P (2)	483.024
<b>Ni+2_EDPHEN*2Me*2DPI-2</b>				
0	---	1	C (18)H (24)N (2)Ni (1)O (4)P (2)	453.041
<b>Ni+2_EHPG-4</b>				
-2	---	2	C (18)H (16)N (2)Ni (1)O (6)	415.028
<b>Ni+2_H+1_[14]N4:2OHEt*4</b>				
3	---	2	C (18)H (41)N (4)Ni (1)O (4)	436.241

<b>Ni+2_H+1_[14]N4:Acet*4-4</b>				
-1	---	4	C(18)H(29)N(4)Ni(1)O(8)	488.143
<b>Ni+2_H+1_[18]N3O3:Acet*3-3</b>				
0	---	1	C(18)H(31)N(3)Ni(1)O(9)	492.152
<b>Ni+2_H+1_BAMTPH-3</b>				
0	---	2	C(18)H(22)N(6)Ni(1)O(9)	525.101
<b>Ni+2_H+1_EDOHPhen*2Me*2DPI-4</b>				
-1	---	2	C(18)H(23)N(2)Ni(1)O(6)P(2)	484.031
<b>Ni+2_H+1_EHPG-4</b>				
-1	---	3	C(18)H(17)N(2)Ni(1)O(6)	416.036
<b>Ni+2_H+1_HBEDPO-6</b>				
-3	---	2	C(18)H(21)N(2)Ni(1)O(8)P(2)	514.014
<b>Ni+2_H+1_HPEDDA-4</b>				
-1	---	3	C(18)H(17)N(2)Ni(1)O(6)	416.036
<b>Ni+2_H+1_mEHPG-4</b>				
-1	---	2	C(18)H(17)N(2)Ni(1)O(6)	416.036
<b>Ni+2_H+1_TTHA-6</b>				
-3	---	2	C(18)H(25)N(4)Ni(1)O(12)	548.109
<b>Ni+2_H+1(-1)_ [14]N4:2OHEt*4</b>				
1	---	1	C(18)H(39)N(4)Ni(1)O(4)	434.225
<b>Ni+2_H+1(-2)_ [14]N4:2OHEt*4</b>				
0	---	1	C(18)H(38)N(4)Ni(1)O(4)	433.217
<b>Ni+2_H+1(2)_ [14]N4:2OHEt*4</b>				
4	---	1	C(18)H(42)N(4)Ni(1)O(4)	437.249



<b>Ni+2_H+1(2)_[14]N4:Acet*4-4</b>				
0	---	3	C(18)H(30)N(4)Ni(1)O(8)	489.151
<b>Ni+2_H+1(2)_BAMTPH-3</b>				
1	---	1	C(18)H(23)N(6)Ni(1)O(9)	526.108
<b>Ni+2_H+1(2)_EDOHPhen*2Me*2DPI-4</b>				
0	---	1	C(18)H(24)N(2)Ni(1)O(6)P(2)	485.039
<b>Ni+2_H+1(2)_EHPPG-4</b>				
0	---	2	C(18)H(18)N(2)Ni(1)O(6)	417.044
<b>Ni+2_H+1(2)_HBEDPO-6</b>				
-2	---	3	C(18)H(22)N(2)Ni(1)O(8)P(2)	515.022
<b>Ni+2_H+1(2)_HPEDDA-4</b>				
0	---	2	C(18)H(18)N(2)Ni(1)O(6)	417.044
<b>Ni+2_H+1(2)_mEHPPG-4</b>				
0	---	1	C(18)H(18)N(2)Ni(1)O(6)	417.044
<b>Ni+2_H+1(2)_TTHA-6</b>				
-2	---	2	C(18)H(26)N(4)Ni(1)O(12)	549.117
<b>Ni+2_H+1(3)_HBEDPO-6</b>				
-1	---	2	C(18)H(23)N(2)Ni(1)O(8)P(2)	516.030
<b>Ni+2_H+1(3)_TTHA-6</b>				
-1	---	2	C(18)H(27)N(4)Ni(1)O(12)	550.125
<b>Ni+2_H+1(4)_HBEDPO-6</b>				
0	---	1	C(18)H(24)N(2)Ni(1)O(8)P(2)	517.038
<b>Ni+2_H+1(4)_TTHA-6</b>				
0	---	1	C(18)H(28)N(4)Ni(1)O(12)	551.133

<b>Ni+2_HBEDPO-6</b>				
-4	---	2	C(18)H(20)N(2)Ni(1)O(8)P(2)	513.006
<b>Ni+2_HPEDDA-4</b>				
-2	---	2	C(18)H(16)N(2)Ni(1)O(6)	415.028
<b>Ni+2_mEHPG-4</b>				
-2	---	2	C(18)H(16)N(2)Ni(1)O(6)	415.028
<b>Ni+2_OH-1_[14]N4:Acet*4-4</b>				
-3	---	1	C(18)H(29)N(4)Ni(1)O(9)	504.143
<b>Ni+2_OH-1_[18]N3O3:Acet*3-3</b>				
-2	---	1	C(18)H(31)N(3)Ni(1)O(10)	508.151
<b>Ni+2_Tri2PicAm</b>				
2	---	2	C(18)H(18)N(4)Ni(1)	349.061
<b>Ni+2_Tri2PicAm_OH-1</b>				
1	---	1	C(18)H(19)N(4)Ni(1)O(1)	366.068
<b>Ni+2_TTHA-6</b>				
-4	---	4	C(18)H(24)N(4)Ni(1)O(12)	547.101
<b>Ni+2(2)_[14]N4:Acet*4-4</b>				
0	---	2	C(18)H(28)N(4)Ni(2)O(8)	545.828
<b>Ni+2(2)_[18]N3O3:Acet*3-3</b>				
1	---	1	C(18)H(30)N(3)Ni(2)O(9)	549.837
<b>Ni+2(2)_[27]N9</b>				
4	---	1	C(18)H(45)N(9)Ni(2)	505.002
<b>Ni+2(2)_H+1_[27]N9</b>				
5	---	1	C(18)H(46)N(9)Ni(2)	506.010

<b>Ni+2 (2) _H+1 _TTHA-6</b>				
-1	---	2	C (18) H (25) N (4) Ni (2) O (12)	606.802
<b>Ni+2 (2) _H+1 (2) _[27]N9</b>				
6	---	1	C (18) H (47) N (9) Ni (2)	507.018
<b>Ni+2 (2) _H+1 (2) _TTHA-6</b>				
0	---	1	C (18) H (26) N (4) Ni (2) O (12)	607.810
<b>Ni+2 (2) _TTHA-6</b>				
-2	---	3	C (18) H (24) N (4) Ni (2) O (12)	605.794
<b>OH-1</b> Hydroxide ion				
-1	14280-30-9	6558	H (1) O (1)	17.0073
<b>OH-1 (2) _HPEDDA-4</b>				
-6	---	2	C (18) H (18) N (2) O (8)	390.350
<b>Oleic-1</b>				
-1	---	1	C (18) H (33) O (2)	281.459
<b>Oxalic-2</b> Oxalate ion				
-2	338-70-5	1241	C (2) O (4)	88.0196
<b>Pb+2</b> Lead(II) ion				
2	14280-50-3	2437	Pb (1)	207.200
<b>Pb+2 _[14]N4:2OHEt*4</b>				
2	---	1	C (18) H (40) N (4) O (4) Pb (1)	583.740
<b>Pb+2 _[14]N4:Acet*4-4</b>				
-2	---	3	C (18) H (28) N (4) O (8) Pb (1)	635.642
<b>Pb+2 _[18]N2O4:DiIsoPr</b>				

2	---	1	C (18) H (38) N (2) O (4) Pb (1)	553.711
<b>Pb+2_[18]N2O4:DiMalon-4</b>				
-2	---	1	C (18) H (26) N (2) O (12) Pb (1)	669.611
<b>Pb+2_[18]N2O4:EtCOO*2-2</b>				
0	---	1	C (18) H (32) N (2) O (8) Pb (1)	611.661
<b>Pb+2_[18]N2O4:Meox*2</b>				
2	---	1	C (18) H (38) N (2) O (6) Pb (1)	585.710
<b>Pb+2_[2.2.2]crypt</b>				
2	---	1	C (18) H (36) N (2) O (6) Pb (1)	583.694
<b>Pb+2_[2.2.2]crypt_OH-1</b>				
1	---	1	C (18) H (37) N (2) O (7) Pb (1)	600.701
<b>Pb+2_[2.2.2]crypt_OH-1 (2)</b>				
0	---	1	C (18) H (38) N (2) O (8) Pb (1)	617.708
<b>Pb+2_[2.2.2]crypt:DiLactam</b>				
2	---	1	C (18) H (32) N (2) O (8) Pb (1)	611.661
<b>Pb+2_[27]N9</b>				
2	---	3	C (18) H (45) N (9) Pb (1)	594.816
<b>Pb+2_EHPG-4</b>				
-2	---	1	C (18) H (16) N (2) O (6) Pb (1)	563.535
<b>Pb+2_H+1_[14]N4:Acet*4-4</b>				
-1	---	3	C (18) H (29) N (4) O (8) Pb (1)	636.650
<b>Pb+2_H+1_[27]N9</b>				
3	---	4	C (18) H (46) N (9) Pb (1)	595.824
<b>Pb+2_H+1_HPEDDA-4</b>				
-1	---	3	C (18) H (17) N (2) O (6) Pb (1)	564.543

<b>Pb+2_H+1_TTHA-6</b>				
-3	---	3	C (18) H (25) N (4) O (12) Pb (1)	696.616
<b>Pb+2_H+1 (2)_[14]N4:Acet*4-4</b>				
0	---	2	C (18) H (30) N (4) O (8) Pb (1)	637.658
<b>Pb+2_H+1 (2)_[27]N9</b>				
4	---	4	C (18) H (47) N (9) Pb (1)	596.832
<b>Pb+2_H+1 (2)_HPEDDA-4</b>				
0	---	2	C (18) H (18) N (2) O (6) Pb (1)	565.551
<b>Pb+2_H+1 (2)_TTHA-6</b>				
-2	---	2	C (18) H (26) N (4) O (12) Pb (1)	697.624
<b>Pb+2_H+1 (3)_[27]N9</b>				
5	---	3	C (18) H (48) N (9) Pb (1)	597.839
<b>Pb+2_H+1 (3)_TTHA-6</b>				
-1	---	1	C (18) H (27) N (4) O (12) Pb (1)	698.632
<b>Pb+2_HPEDDA-4</b>				
-2	---	2	C (18) H (16) N (2) O (6) Pb (1)	563.535
<b>Pb+2_Tri2PicAm</b>				
2	---	2	C (18) H (18) N (4) Pb (1)	497.568
<b>Pb+2_Tri2PicAm_OH-1</b>				
1	---	1	C (18) H (19) N (4) O (1) Pb (1)	514.575
<b>Pb+2_TTHA-6</b>				
-4	---	3	C (18) H (24) N (4) O (12) Pb (1)	695.608
<b>Pb+2 (2)_[14]N4:Acet*4-4</b>				
0	---	3	C (18) H (28) N (4) O (8) Pb (2)	842.842

<b>Pb+2 (2) _[2.2.2]crypt</b>				
4	---	1	C (18) H (36) N (2) O (6) Pb (2)	790.894
<b>Pb+2 (2) _[27]N9</b>				
4	---	4	C (18) H (45) N (9) Pb (2)	802.016
<b>Pb+2 (2) _[27]N9_OH-1</b>				
3	---	3	C (18) H (46) N (9) O (1) Pb (2)	819.023
<b>Pb+2 (2) _[27]N9_OH-1 (2)</b>				
2	---	2	C (18) H (47) N (9) O (2) Pb (2)	836.030
<b>Pb+2 (2) _H+1 _[14]N4:Acet*4-4</b>				
1	---	2	C (18) H (29) N (4) O (8) Pb (2)	843.850
<b>Pb+2 (2) _H+1 _[27]N9</b>				
5	---	3	C (18) H (46) N (9) Pb (2)	803.024
<b>Pb+2 (2) _H+1 _TTHA-6</b>				
-1	---	2	C (18) H (25) N (4) O (12) Pb (2)	903.816
<b>Pb+2 (2) _H+1 (2) _TTHA-6</b>				
0	---	1	C (18) H (26) N (4) O (12) Pb (2)	904.824
<b>Pb+2 (2) _TTHA-6</b>				
-2	---	3	C (18) H (24) N (4) O (12) Pb (2)	902.808
<b>Pb (C6H5) 3+1</b> Tribenzyllead ion				
1	---	2	C (18) H (15) Pb (1)	438.517
<b>Pb (C6H5) 3+1 _I-1</b>				
0	---	1	C (18) H (15) I (1) Pb (1)	565.417
<b>Pb (C6H5) 3+1 _OH-1</b>				
0	---	1	C (18) H (16) O (1) Pb (1)	455.524

<b>Pd+2</b> Palladium(II) ion				
2	16065-88-6	567	Pd(1)	106.420
<b>Pd+2_[18]N3O3:Acet*3-3</b>				
-1	---	3	C(18)H(30)N(3)O(9)Pd(1)	538.871
<b>Pd+2_262Dpa</b>				
2	---	1	C(18)H(26)N(4)Pd(1)	404.851
<b>Pd+2_H+1_[18]N3O3:Acet*3-3</b>				
0	---	1	C(18)H(31)N(3)O(9)Pd(1)	539.879
<b>Pd+2_OH-1_[18]N3O3:Acet*3-3</b>				
-2	---	1	C(18)H(31)N(3)O(10)Pd(1)	555.878
<b>Pd+2(2)_[18]N3O3:Acet*3-3</b>				
1	---	3	C(18)H(30)N(3)O(9)Pd(2)	645.291
<b>Pd+2(2)_H+1_[18]N3O3:Acet*3-3</b>				
2	---	1	C(18)H(31)N(3)O(9)Pd(2)	646.299
<b>Pd+2(2)_OH-1_[18]N3O3:Acet*3-3</b>				
0	---	1	C(18)H(31)N(3)O(10)Pd(2)	662.298
<b>Phe-1</b> Phenylalanate ion; L-Phenylalanate ion; beta-phenylalanate ion; alpha-aminohydrocinnamate ion; alpha-amino-beta-phenylpropionate ion; L-2-amino-3,5-phenylpropanoate ion				
-1	19701-97-4	562	C(9)H(10)N(1)O(2)	164.184
<b>Phenanth</b> 1,10-Phenanthroline; phen; Phenanthroline; Orthophenathroline (sic)				
0	66-71-7	406	C(12)H(8)N(2)	180.209
<b>PhePhe-1</b>				
-1	---	6	C(18)H(19)N(2)O(3)	311.361

<b>PheProGlyGly-1</b>				
-1	---	7	C (18) H (23) N (4) O (5)	375.404
<b>PheTyr-2</b>				
-2	---	13	C (18) H (18) N (2) O (4)	326.352
<b>Pimelic-2</b> Pimelate ion				
-2	---	22	C (7) H (10) O (4)	158.154
<b>Pr+3</b> Praseodymium(III) ion				
3	22541-14-6	722	Pr (1)	140.910
<b>Pr+3_[18]N2O4:EtCOO*2-2</b>				
1	---	1	C (18) H (32) N (2) O (8) Pr (1)	545.371
<b>Pr+3_[2.2.2]crypt</b>				
3	---	1	C (18) H (36) N (2) O (6) Pr (1)	517.404
<b>Pr+3_BEATA-4</b>				
-1	---	1	C (18) H (21) N (3) O (8) Pr (1)	548.290
<b>Pr+3_H+1_TTHA-6</b>				
-2	---	2	C (18) H (25) N (4) O (12) Pr (1)	630.326
<b>Pr+3_H+1 (2)_TTHA-6</b>				
-1	---	1	C (18) H (26) N (4) O (12) Pr (1)	631.334
<b>Pr+3_TTHA-6</b>				
-3	---	2	C (18) H (24) N (4) O (12) Pr (1)	629.318
<b>Pt+2_CN-1 (4)</b>				
-2	---	31	C (4) N (4) Pt (1)	299.151
<b>Pt+2_H+1 (4)_[27]N9_CN-1 (4)</b>				
2	---	1	C (22) H (49) N (13) Pt (1)	690.798



<b>Pt+2_H+1(5)_[27]N9_CN-1(4)</b>				
3	---	1	C(22)H(50)N(13)Pt(1)	691.806
<b>Pt+2_H+1(6)_[27]N9_CN-1(4)</b>				
4	---	1	C(22)H(51)N(13)Pt(1)	692.814
<b>Pt+2_H+1(7)_[27]N9_CN-1(4)</b>				
5	---	1	C(22)H(52)N(13)Pt(1)	693.822
<b>Pt+2_H+1(8)_[27]N9_CN-1(4)</b>				
6	---	1	C(22)H(53)N(13)Pt(1)	694.830
<b>Pu+4</b> Plutonium(IV) ion				
4	22541-44-2	378	Pu(1)	244.000
<b>Pu+4_BAMTPH-3</b>				
1	---	1	C(18)H(21)N(6)O(9)Pu(1)	709.400
<b>Rb+1</b> Rubidium(I) ion				
1	22537-38-8	125	Rb(1)	85.4680
<b>Rb+1_[18]N2O4:Meox*2</b>				
1	---	1	C(18)H(38)N(2)O(6)Rb(1)	463.978
<b>Rb+1_[2.2.2]crypt</b>				
1	---	1	C(18)H(36)N(2)O(6)Rb(1)	461.962
<b>Rb+1_[2.2.2]crypt:DiLactam</b>				
1	---	1	C(18)H(32)N(2)O(8)Rb(1)	489.929
<b>Sm+3</b> Samarium(III) ion				
3	22541-17-9	732	Sm(1)	150.362
<b>Sm+3_[14]N4:Acet*4-4</b>				

-1	---	2	C (18) H (28) N (4) O (8) Sm (1)	578.804
<b>Sm+3_[18]N2O4:EtCOO*2-2</b>				
1	---	1	C (18) H (32) N (2) O (8) Sm (1)	554.823
<b>Sm+3_[2.2.2]crypt</b>				
3	---	1	C (18) H (36) N (2) O (6) Sm (1)	526.856
<b>Sm+3_BEATA-4</b>				
-1	---	1	C (18) H (21) N (3) O (8) Sm (1)	557.742
<b>Sm+3_H+1_[14]N4:Acet*4-4</b>				
0	---	1	C (18) H (29) N (4) O (8) Sm (1)	579.812
<b>Sm+3_H+1_TTHA-6</b>				
-2	---	2	C (18) H (25) N (4) O (12) Sm (1)	639.778
<b>Sm+3_H+1 (2)_TTHA-6</b>				
-1	---	1	C (18) H (26) N (4) O (12) Sm (1)	640.786
<b>Sm+3_TTHA-6</b>				
-3	---	2	C (18) H (24) N (4) O (12) Sm (1)	638.770
<b>Sm+3 (2)_TTHA-6</b>				
0	---	1	C (18) H (24) N (4) O (12) Sm (2)	789.132
<b>Sn (C6H5) 3+1</b> Tribenzyltin ion				
1	---	1	C (18) H (15) Sn (1)	350.027
<b>Sn (C6H5) 3+1_OH-1</b>				
0	---	1	C (18) H (16) O (1) Sn (1)	367.035
<b>SO4-2</b> Sulfate ion; Sulphate ion				
-2	14808-79-8	1270	O (4) S (1)	96.0576

<b>Squaric-2</b> Squarate ion				
-2	---	27	C(4)O(4)	112.042
<b>Sr+2</b> Strontium(II) ion				
2	22537-39-9	693	Sr(1)	87.6200
<b>Sr+2_[14]N4:Acet*4-4</b>				
-2	---	2	C(18)H(28)N(4)O(8)Sr(1)	516.062
<b>Sr+2_[18]N2O4:DiMalon-4</b>				
-2	---	1	C(18)H(26)N(2)O(12)Sr(1)	550.031
<b>Sr+2_[18]N2O4:EtCOO*2-2</b>				
0	---	1	C(18)H(32)N(2)O(8)Sr(1)	492.081
<b>Sr+2_[2.2.2]crypt</b>				
2	---	1	C(18)H(36)N(2)O(6)Sr(1)	464.114
<b>Sr+2_[2.2.2]crypt:DiLactam</b>				
2	---	1	C(18)H(32)N(2)O(8)Sr(1)	492.081
<b>Sr+2_H+1_[14]N4:Acet*4-4</b>				
-1	---	2	C(18)H(29)N(4)O(8)Sr(1)	517.070
<b>Sr+2_H+1_TTHA-6</b>				
-3	---	2	C(18)H(25)N(4)O(12)Sr(1)	577.036
<b>Sr+2_H+1(2)_TTHA-6</b>				
-2	---	1	C(18)H(26)N(4)O(12)Sr(1)	578.044
<b>Sr+2_TTHA-6</b>				
-4	---	3	C(18)H(24)N(4)O(12)Sr(1)	576.028
<b>Sr+2(2)_TTHA-6</b>				
-2	---	1	C(18)H(24)N(4)O(12)Sr(2)	663.648

<b>Stearic-1</b>				
-1	---	1	C(18)H(35)O(2)	283.475
<b>Succinic-2</b> Succinate ion				
-2	56-14-4	635	C(4)H(4)O(4)	116.073
<b>Sulfox-2</b> 8-Hydroxy-5-quinoline sulphonate ion; 8-Hydroxy-5-quinoline sulfonate ion; 8-Hydroxyquinoline-5-sulfonate ion; 8-Hydroxyquinoline-5-sulphonate ion				
-2	40747-73-7	190	C(9)H(5)N(1)O(4)S(1)	223.203
<b>Tartaric-2</b> Tartrate ion				
-2	---	393	C(4)H(4)O(6)	148.072
<b>Tb+3</b> Terbium(III) ion				
3	22541-20-4	549	Tb(1)	158.930
<b>Tb+3_[18]N2O4:EtCOO*2-2</b>				
1	---	1	C(18)H(32)N(2)O(8)Tb(1)	563.391
<b>Tb+3_[2.2.2]crypt</b>				
3	---	1	C(18)H(36)N(2)O(6)Tb(1)	535.424
<b>Tb+3_BEATA-4</b>				
-1	---	1	C(18)H(21)N(3)O(8)Tb(1)	566.310
<b>Tb+3_H+1_TTHA-6</b>				
-2	---	2	C(18)H(25)N(4)O(12)Tb(1)	648.346
<b>Tb+3_H+1(2)_TTHA-6</b>				
-1	---	1	C(18)H(26)N(4)O(12)Tb(1)	649.354
<b>Tb+3_TTHA-6</b>				
-3	---	2	C(18)H(24)N(4)O(12)Tb(1)	647.338

<b>Th+4</b> Thorium(IV) ion				
4	16065-92-2	659	Th (1)	232.040
<b>Th+4_H+1_TTHA-6</b>				
-1	---	1	C (18) H (25) N (4) O (12) Th (1)	721.456
<b>Th+4_OH-1 (2)_HPEDDA-4</b>				
-2	---	2	C (18) H (18) N (2) O (8) Th (1)	622.390
<b>Th+4_OH-1 (4)_HPEDDA-4</b>				
-4	---	1	C (18) H (20) N (2) O (10) Th (1)	656.404
<b>Th+4_TTHA-6</b>				
-2	---	2	C (18) H (24) N (4) O (12) Th (1)	720.448
<b>Tiron-4</b> 4,5-Dihydroxy-1,3-benzenedisulphonate ion; 4,5-Dihydroxy-1,3-benzenedisulfonate ion; 1,2-Dihydroxybenzene-3,5-disulphonate ion; 4,5-Dihydroxybenzene-1,3-disulphonate ion; Disodium 3,5-pyrocatecholdisulfonate ion; PDS				
-4	77310-82-8	263	C (6) H (2) O (8) S (2)	266.197
<b>Tl+1</b> Thalium(I) ion; Thallium(I) ion; Thallous ion				
1	22537-56-0	254	Tl (1)	204.383
<b>Tl+1_[2.2.2]crypt</b>				
1	51156-84-4	1	C (18) H (36) N (2) O (6) Tl (1)	580.877
<b>Tl+1_TTHA-6</b>				
-5	---	2	C (18) H (24) N (4) O (12) Tl (1)	692.791
<b>Tl+3_H+1_TTHA-6</b>				
-2	---	1	C (18) H (25) N (4) O (12) Tl (1)	693.799
<b>Tl+3_TTHA-6</b>				
-3	---	1	C (18) H (24) N (4) O (12) Tl (1)	692.791

<b>Tm+3</b> Thulium(III) ion				
3	22541-23-7	441	Tm(1)	168.930
<b>Tm+3_[18]N2O4:EtCOO*2-2</b>				
1	---	1	C(18)H(32)N(2)O(8)Tm(1)	573.391
<b>Tm+3_BEATA-4</b>				
-1	---	1	C(18)H(21)N(3)O(8)Tm(1)	576.310
<b>Tm+3_H+1_TTHA-6</b>				
-2	---	2	C(18)H(25)N(4)O(12)Tm(1)	658.346
<b>Tm+3_H+1(2)_TTHA-6</b>				
-1	---	1	C(18)H(26)N(4)O(12)Tm(1)	659.354
<b>Tm+3_TTHA-6</b>				
-3	---	2	C(18)H(24)N(4)O(12)Tm(1)	657.338
<b>Tri2PicAm</b> 2,2',2''-Nitrilotrimethylenetripyridine; Nitrilotris(methylene-2-pyridine); Tri-2-picolylamine; TPA; NTPY; Tris-(2-pyridylmethyl)amine				
0	---	25	C(18)H(18)N(4)	290.368
<b>Trigalacturonic-3</b>				
-3	---	6	C(18)H(23)O(19)	543.369
<b>Triphenylarsine</b> Triphenylarsine				
0	603-32-7	11	C(18)H(15)As(1)	306.239
<b>TTHA-6</b> Triethylenetetranitrilo-hexa-acetate				
-6	---	266	C(18)H(24)N(4)O(12)	488.408
<b>TyrPhe-2</b>				
-2	---	21	C(18)H(18)N(2)O(4)	326.352

<b>TyrTyr-3</b>				
-3	---	23	C(18)H(17)N(2)O(5)	341.343
<b>U+4</b> Uranium(IV) ion				
4	16089-60-4	405	U(1)	238.029
<b>U+4_H+1_TTHA-6</b>				
-1	---	1	C(18)H(25)N(4)O(12)U(1)	727.445
<b>U+4_TTHA-6</b>				
-2	---	2	C(18)H(24)N(4)O(12)U(1)	726.437
<b>UO2+2</b> Uranyl ion; U(VI) cation; Uranate				
2	16637-16-4	1268	O(2)U(1)	270.028
<b>UO2+2_[2.2.2]crypt</b>				
2	---	1	C(18)H(36)N(2)O(8)U(1)	646.522
<b>UO2+2_[2.2.2]crypt(2)</b>				
2	---	1	C(36)H(72)N(4)O(14)U(1)	1023.02
<b>UO2+2_H+1_TTHA-6</b>				
-3	---	2	C(18)H(25)N(4)O(14)U(1)	759.444
<b>UO2+2_H+1(2)_TTHA-6</b>				
-2	---	2	C(18)H(26)N(4)O(14)U(1)	760.452
<b>UO2+2_H+1(3)_TTHA-6</b>				
-1	---	2	C(18)H(27)N(4)O(14)U(1)	761.460
<b>UO2+2_TTHA-6</b>				
-4	---	2	C(18)H(24)N(4)O(14)U(1)	758.436
<b>UO2+2(2)_[2.2.2]crypt</b>				
4	---	1	C(18)H(36)N(2)O(10)U(2)	916.549

<b>UO<sub>2</sub>+2 (2) _H+1 (2) _TTHA-6</b>				
0	---	1	C (18) H (26) N (4) O (16) U (2)	1030.48
<b>VO<sub>2</sub>+1 _TTHA-6</b>				
-5	---	1	C (18) H (24) N (4) O (14) V (1)	571.349
<b>Yb+3</b> Ytterbium(III) ion				
3	18923-27-8	594	Yb (1)	173.050
<b>Yb+3 _[14]N<sub>4</sub>:Acet*4-4</b>				
-1	---	2	C (18) H (28) N (4) O (8) Yb (1)	601.492
<b>Yb+3 _[18]N<sub>2</sub>O<sub>4</sub>:EtCOO*2-2</b>				
1	---	1	C (18) H (32) N (2) O (8) Yb (1)	577.511
<b>Yb+3 _[2.2.2]crypt</b>				
3	---	1	C (18) H (36) N (2) O (6) Yb (1)	549.544
<b>Yb+3 _BEATA-4</b>				
-1	---	1	C (18) H (21) N (3) O (8) Yb (1)	580.430
<b>Yb+3 _H+1 _[14]N<sub>4</sub>:Acet*4-4</b>				
0	---	1	C (18) H (29) N (4) O (8) Yb (1)	602.500
<b>Yb+3 _H+1 _TTHA-6</b>				
-2	---	2	C (18) H (25) N (4) O (12) Yb (1)	662.466
<b>Yb+3 _H+1 (2) _TTHA-6</b>				
-1	---	1	C (18) H (26) N (4) O (12) Yb (1)	663.474
<b>Yb+3 _TTHA-6</b>				
-3	---	2	C (18) H (24) N (4) O (12) Yb (1)	661.458
<b>Zn+2</b> Zinc(II) ion				
2	23713-49-7	4977	Zn (1)	65.3820



<b>Zn+2_[14]N4:2OHEt*4</b>				
2	---	1	C(18)H(40)N(4)O(4)Zn(1)	441.922
<b>Zn+2_[14]N4:Acet*4-4</b>				
-2	---	4	C(18)H(28)N(4)O(8)Zn(1)	493.824
<b>Zn+2_[18]dieneN6dipyo</b>				
2	---	1	C(18)H(26)N(6)Zn(1)	391.827
<b>Zn+2_[18]N2O4:DiMalon-4</b>				
-2	---	1	C(18)H(26)N(2)O(12)Zn(1)	527.793
<b>Zn+2_[18]N2O4:EtCOO*2-2</b>				
0	---	1	C(18)H(32)N(2)O(8)Zn(1)	469.843
<b>Zn+2_[18]N3O3:Acet*3-3</b>				
-1	---	3	C(18)H(30)N(3)O(9)Zn(1)	497.833
<b>Zn+2_[2.2.2]crypt</b>				
2	---	1	C(18)H(36)N(2)O(6)Zn(1)	441.876
<b>Zn+2_[24]N6</b>				
2	---	1	C(18)H(42)N(6)Zn(1)	407.954
<b>Zn+2_4LICAMS-6</b>				
-4	---	1	C(18)H(14)N(2)O(12)S(2)Zn(1)	579.817
<b>Zn+2_BAMTPH-3</b>				
-1	---	2	C(18)H(21)N(6)O(9)Zn(1)	530.782
<b>Zn+2_EHPG-4</b>				
-2	---	2	C(18)H(16)N(2)O(6)Zn(1)	421.717
<b>Zn+2_Enalaprilat-2</b>				
0	---	2	C(18)H(22)N(2)O(5)Zn(1)	411.765

<b>Zn+2_Enalaprilat-2(2)</b>				
-2	---	3	C(36)H(44)N(4)O(10)Zn(1)	758.148
<b>Zn+2_H+1_[14]N4:Acet*4-4</b>				
-1	---	3	C(18)H(29)N(4)O(8)Zn(1)	494.832
<b>Zn+2_H+1_[18]N3O3:Acet*3-3</b>				
0	---	2	C(18)H(31)N(3)O(9)Zn(1)	498.841
<b>Zn+2_H+1_BAMTPH-3</b>				
0	---	2	C(18)H(22)N(6)O(9)Zn(1)	531.790
<b>Zn+2_H+1_EHPG-4</b>				
-1	---	3	C(18)H(17)N(2)O(6)Zn(1)	422.725
<b>Zn+2_H+1_Enalaprilat-2(2)</b>				
-1	---	3	C(36)H(45)N(4)O(10)Zn(1)	759.156
<b>Zn+2_H+1_HBEDPO-6</b>				
-3	---	1	C(18)H(21)N(2)O(8)P(2)Zn(1)	520.703
<b>Zn+2_H+1_HPEDDA-4</b>				
-1	---	3	C(18)H(17)N(2)O(6)Zn(1)	422.725
<b>Zn+2_H+1_mEHPG-4</b>				
-1	---	2	C(18)H(17)N(2)O(6)Zn(1)	422.725
<b>Zn+2_H+1_TTHA-6</b>				
-3	---	3	C(18)H(25)N(4)O(12)Zn(1)	554.798
<b>Zn+2_H+1(2)_[18]N3O3:Acet*3-3</b>				
1	---	1	C(18)H(32)N(3)O(9)Zn(1)	499.849
<b>Zn+2_H+1(2)_BAMTPH-3</b>				
1	---	1	C(18)H(23)N(6)O(9)Zn(1)	532.797

<b>Zn+2_H+1(2)_EHPG-4</b>				
0	---	2	C(18)H(18)N(2)O(6)Zn(1)	423.733
<b>Zn+2_H+1(2)_Enalaprilat-2(2)</b>				
0	---	2	C(36)H(46)N(4)O(10)Zn(1)	760.164
<b>Zn+2_H+1(2)_HPEDDA-4</b>				
0	---	2	C(18)H(18)N(2)O(6)Zn(1)	423.733
<b>Zn+2_H+1(2)_mEHPG-4</b>				
0	---	1	C(18)H(18)N(2)O(6)Zn(1)	423.733
<b>Zn+2_H+1(2)_TTHA-6</b>				
-2	---	2	C(18)H(26)N(4)O(12)Zn(1)	555.806
<b>Zn+2_H+1(3)_TTHA-6</b>				
-1	---	1	C(18)H(27)N(4)O(12)Zn(1)	556.814
<b>Zn+2_HBEDPO-6</b>				
-4	---	1	C(18)H(20)N(2)O(8)P(2)Zn(1)	519.695
<b>Zn+2_HPEDDA-4</b>				
-2	---	2	C(18)H(16)N(2)O(6)Zn(1)	421.717
<b>Zn+2_mEHPG-4</b>				
-2	---	2	C(18)H(16)N(2)O(6)Zn(1)	421.717
<b>Zn+2_OH-1_[14]N4:Acet*4-4</b>				
-3	---	1	C(18)H(29)N(4)O(9)Zn(1)	510.832
<b>Zn+2_OH-1_[18]N3O3:Acet*3-3</b>				
-2	---	1	C(18)H(31)N(3)O(10)Zn(1)	514.840
<b>Zn+2_OH-1_Enalaprilat-2</b>				
-1	---	2	C(18)H(23)N(2)O(6)Zn(1)	428.772

<b>Zn+2_OH-1_Enalaprilat-2(2)</b>				
-3	---	2	C(36)H(45)N(4)O(11)Zn(1)	775.156
<b>Zn+2_Tri2PicAm</b>				
2	---	2	C(18)H(18)N(4)Zn(1)	355.750
<b>Zn+2_Tri2PicAm_OH-1</b>				
1	---	1	C(18)H(19)N(4)O(1)Zn(1)	372.757
<b>Zn+2_TTHA-6</b>				
-4	---	3	C(18)H(24)N(4)O(12)Zn(1)	553.790
<b>Zn+2(2)_[14]N4:Acet*4-4</b>				
0	---	2	C(18)H(28)N(4)O(8)Zn(2)	559.206
<b>Zn+2(2)_[18]N3O3:Acet*3-3</b>				
1	---	3	C(18)H(30)N(3)O(9)Zn(2)	563.215
<b>Zn+2(2)_[27]N9</b>				
4	---	2	C(18)H(45)N(9)Zn(2)	518.380
<b>Zn+2(2)_[27]N9_OH-1</b>				
3	---	3	C(18)H(46)N(9)O(1)Zn(2)	535.387
<b>Zn+2(2)_[27]N9_OH-1(2)</b>				
2	---	2	C(18)H(47)N(9)O(2)Zn(2)	552.394
<b>Zn+2(2)_H+1_[14]N4:Acet*4-4</b>				
1	---	1	C(18)H(29)N(4)O(8)Zn(2)	560.214
<b>Zn+2(2)_H+1_[18]N3O3:Acet*3-3</b>				
2	---	1	C(18)H(31)N(3)O(9)Zn(2)	564.223
<b>Zn+2(2)_H+1_[27]N9</b>				
5	---	1	C(18)H(46)N(9)Zn(2)	519.388

<b>Zn+2 (2) _H+1 _TTHA-6</b>				
-1	---	2	C (18) H (25) N (4) O (12) Zn (2)	620.180
<b>Zn+2 (2) _H+1 (2) _[27]N9</b>				
6	---	1	C (18) H (47) N (9) Zn (2)	520.396
<b>Zn+2 (2) _H+1 (2) _TTHA-6</b>				
0	---	1	C (18) H (26) N (4) O (12) Zn (2)	621.188
<b>Zn+2 (2) _OH-1 _[18]N3O3:Acet*3-3</b>				
0	---	2	C (18) H (31) N (3) O (10) Zn (2)	580.222
<b>Zn+2 (2) _OH-1 (2) _[18]N3O3:Acet*3-3</b>				
-1	---	1	C (18) H (32) N (3) O (11) Zn (2)	597.230
<b>Zn+2 (2) _TTHA-6</b>				
-2	---	3	C (18) H (24) N (4) O (12) Zn (2)	619.172
<b>Zr+4</b> Zirconium(IV) ion				
4	15543-40-5	291	Zr (1)	91.2420
<b>Zr+4 _H+1 (2) _TTHA-6</b>				
0	---	1	C (18) H (26) N (4) O (12) Zr (1)	581.666