[VTIMPKAcDIQLAR+3H]3+

Fragmentation Diagram for: VTIMPKDIQLAR



Detailed Data

n	classification	line
1	usable	y6 (1+) @ 715.44 & b6 (2+) @ 356.66
2	internal_acid	y5 (1+) @ 600.46 & bi5-7 (1+) @ 383.1
3	usable	y2 (1+) @ 245.82 & b10 (2+) @ 591.38
4	internal_acid	bi5-9 (1+) @ 624.4 & y3 (1+) @ 359.18
5	usable	y4 (1+) @ 487.22 & a8(2+) @ 456.75
6	usable	y9 (2+) @ 557.42 & [b3-NH3] (1+) @ 296.01
7	non_complementary	y6 (2+) @ 359.14 & b9 (2+) @ 534.76
8	usable	y10 (2+) @ 614.08 & b2 (1+) @ 200.71
9	usable	[y4-NH3] (2+) @ 234.85 & b8 (1+) @ 940.45
10	usable	y5 (1+) @ 600.38 & b7 (2+) @ 414.18
11	non_complementary	y4 (1+) @ 487.33 & b7 (1+) @ 827.44
12	usable	y5 (2+) @ 300.5 & b7 (1+) @ 827.42
13	usable	y2 (1+) @ 245.82 & [b10-NH3] (2+) @ 582.35
14	usable	y10 (2+) @ 614.08 & a2 (1+) @ 172.63
15	usable	y6 (1+) @ 715.45 & c5 (1+) 559.34
16	non_complementary	y2 (1+) @ 245.79 & b9 (1+) @ 1068.42
17	usable	y7 (2+) @ 443.34 & b5 (1+) @ 542.33
18	usable	y4 (2+) @ 243.98 & b8 (1+) @ 940.41
19	usable	y1 (1+) @ 174.58 & b11 (2+) @ 626.99

21			
y6 (1+) @ 715.54 & [b6-NH3] (2+) @ 347.56 y6 (1+) @ 715.54 & [b6-NH3] (2+) @ 347.56 y8 (2+) @ 491.82 & a4 (1+) @ 417.1 sable y8 (2+) @ 359.14 & [b5-NH3] (1+) @ 525.62 usable y8 (2+) # 19.82 & a4 (1+) @ 417.1 y6 (2+) @ 359.14 & [b5-NH3] (1+) @ 525.62 usable y8 (2+) # 19.96 & [b4 - CH3SH - CO] (1+) 369.04 y8 (2+) # 19.96 & [b4 - CH3SH - CO] (1+) 369.04 y8 (2+) # 19.96 & [b4 - CH3SH - CO] (1+) 369.04 y8 (2+) # 19.96 & [b4 - CH3SH - CO] (1+) 369.04 y8 (2+) # 19.96 & [b4 - CH3SH - CO] (1+) 369.04 y8 (2+) # 19.96 & [b4 - CH3SH - CO] (1+) 369.04 y8 (1+) # 19.96 & [b4 - CH3SH - CO] (1+) 369.04 y8 (1+) # 19.96 & [b4 - CH3SH - CO] (1+) 369.04 y8 (1+) # 19.96 & [b4 - CH3SH - CO] (1+) 369.04 y8 (1+) # 19.96 & [b4 - CH3SH - CO] (1+) # 19.04 y8 (1+) # 19.04 & 19.04 y8 (1+) # 19.04 y8	20	usable	y8 (2+) @ 491.76 & b4 (1+) @ 444.98
23 non_complementary	21	usable	[y6-NH3] (1+) @ 698.39 & b6 (2+) @ 356.64
24 usable y8 (2+) @ 491.82 & a4 (1+) @ 417.1 25 non_complementary y6 (2+) @ 359.14 & [b5-NH3] (1+) @ 525.62 26 usable y8 (2+)491.96 & [b4 - CH3SH - CO] (1+) 369.04 27 usable [y8-NH3] (2+) @ 482.8 & b4 (1+) @ 445.14 28 internal_acid y6 (1+) @ 715.66 & bi5-6 @ 267.85 29 internal_acid [bi4-7 - HCOOH] (1+) @ 468.13 & 445.09 30 internal_acid [bi4-7 - HCOOH] (1+) @ 468.13 & 445.09 31 usable y5(1+) @ 600.3 & [b7-NH3] (2+) @ 405.11 32 internal_acid bi5-10 (1+) @ 737.3 & y2 (1+) 245.92 33 usable [y10-NH3] (2+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 600.44 & a5 (1+) @ 514.24 36 usable y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07 37 usable y8(2+) @ 491.95 & [b4-NH3] (1+) @ 487.01 38 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 487.14 40 usable [y5-NH3](2+) @ 245.81 & [b9-NH3] (1+) @ 1051.61 41 unclear b(22	usable	y6 (1+) @ 715.54 & [b6-NH3] (2+) @ 347.56
25 non_complementary y6 (2+) @ 359.14 & [b5-NH3] (1+) @ 525.62 26 usable y8 (2+)491.96 & [b4 - CH3SH - CO] (1+) 369.04 27 usable [y8-NH3] (2+) @ 482.8 & b4 (1+) @ 445.14 28 internal_acid y6 (1+) @ 715.66 & bi5-6 @ 267.85 29 internal_acid y4 (1+) @ 487.09 & [bi4-7 - HCOOH] (1+) @ 468.13 & 445.09 30 internal_acid [bi4-7 - HCOOH] (1+) @ 468.13 & 445.09 31 usable y5(1+) @ 600.3 & [b7-NH3] (2+) @ 405.11 32 internal_acid bi5-10 (1+) @ 737.3 & y2 (1+) 245.92 33 usable [y10-NH3] (2+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 604.41 & b4 (1+) 444.93 35 usable y5(1+) @ 600.44 & a5 (1+) @ 514.24 36 usable y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07 37 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 487.01 38 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 487.14 40 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 487.14 41 unclear b8(1+) @ 940.89 & ??? @ 195.81 42 usable y5(2+)	23	non_complementary	b6 (1+) @ 712.43 & [y2 – H2O] (1+) 228.63
26 usable y8 (2+)491.96 & [b4 - CH3SH - CO] (1+) 369.04 27 usable [y8-NH3] (2+) @ 482.8 & b4 (1+) @ 445.14 28 internal_acid y6 (1+) @ 715.66 & bi5-6 @ 267.85 29 internal_acid y4 (1+) @ 487.09 & [bi4-7 - HCOOH] (1+) @ 468 30 internal_acid [bi4-7 - HCOOH] (1+) @ 468.13 & 445.09 31 usable y5(1+) @ 600.3 & [b7-NH3] (2+) @ 405.11 32 internal_acid bi5-10 (1+) @ 737.3 & y2 (1+) 245.92 33 usable [y10-NH3] (2+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 600.44 & a5 (1+) @ 514.24 36 usable y5(1+) @ 600.44 & a5 (1+) @ 514.24 36 usable y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07 37 usable y8(2+) @ 491.95 & [b4-NH3] (1+) @ 487.01 38 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56 39 non_complementary y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61 40 usable bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14 41 unclear b8(1+) @ 940.89 & ??? @ 195.81 42 usable y5(2+) @ 300.61	24	usable	y8 (2+) @ 491.82 & a4 (1+) @ 417.1
27	25	non_complementary	y6 (2+) @ 359.14 & [b5-NH3] (1+) @ 525.62
28 internal_acid y6 (1+) @ 715.66 & bi5-6 @ 267.85 29 internal_acid y4 (1+) @ 487.09 & [bi4-7 – HCOOH] (1+) @ 468 30 internal_acid [bi4-7 – HCOOH] (1+) @ 468.13 & 445.09 31 usable y5(1+) @ 600.3 & [b7-NH3] (2+) @ 405.11 32 internal_acid bi5-10 (1+) @ 737.3 & y2 (1+) 245.92 33 usable [y10-NH3] (2+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 604.93 & b2(1+) @ 200.68 35 usable y5(1+) @ 600.44 & a5 (1+) @ 514.24 36 usable y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07 37 usable bi (5-8) (1+) @ 496.41 & y4 (1+) @ 487.01 38 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56 39 non_complementary y2(1+) @ 245.81 & [b9-NH3] (1+) @ 487.14 40 usable <	26	usable	y8 (2+)491.96 & [b4 - CH3SH - CO] (1+) 369.04
29 internal_acid y4 (1+) @ 487.09 & [bi4-7 - HCOOH] (1+) @ 468 30 internal_acid [bi4-7 - HCOOH] (1+) @ 468.13 & 445.09 31 usable y5(1+) @ 600.3 & [b7-NH3] (2+) @ 405.11 32 internal_acid bi5-10 (1+) @ 737.3 & y2 (1+) 245.92 33 usable [y10-NH3] (2+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 624.41 & b4 (1+) 444.93 35 usable y5(1+) @ 600.44 & a5 (1+) @ 514.24 36 usable y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07 37 usable bi (5-8) (1+) @ 496.41 & y4 (1+) @ 487.01 38 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56 39 non_complementary y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61 40 usable bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14 41 unclear b8(1+) @ 940.89 & ??? @ 195.81 42 usable y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82 43 usable y4(2+) @ 243.81 & [b8-NH3] (1+) @ 809.82 44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.1 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3] (1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	27	usable	[y8-NH3] (2+) @ 482.8 & b4 (1+) @ 445.14
30 internal_acid [bi4-7 - HCOOH] (1+) @ 468.13 & 445.09 31 usable y5(1+) @ 600.3 & [b7-NH3] (2+) @ 405.11 32 internal_acid bi5-10 (1+) @ 737.3 & y2 (1+) 245.92 33 usable [y10-NH3] (2+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 624.41 & b4 (1+) 444.93 35 usable y5(1+) @ 600.44 & a5 (1+) @ 514.24 36 usable y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07 37 usable bi (5-8) (1+) @ 496.41 & y4 (1+) @ 487.01 38 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56 39 non_complementary y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61 40 usable bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14 41 unclear b8(1+) @ 940.89 & ??? @ 195.81 42 usable y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82 43 usable y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17 44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.1 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	28	internal_acid	y6 (1+) @ 715.66 & bi5-6 @ 267.85
31	29	internal_acid	y4 (1+) @ 487.09 & [bi4-7 – HCOOH] (1+) @ 468.09
32 internal_acid bi5-10 (1+) @ 737.3 & y2 (1+) 245.92 33 usable [y10-NH3] (2+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 624.41 & b4 (1+) 444.93 35 usable y5(1+) @ 600.44 & a5 (1+) @ 514.24 36 usable y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07 37 usable bi (5-8) (1+) @ 496.41 & y4 (1+) @ 487.01 38 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56 39 non_complementary y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61 40 usable bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14 41 unclear b8(1+) @ 940.89 & ??? @ 195.81 42 usable y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82 43 usable y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17 44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 241.91 48 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69	30	internal_acid	[bi4-7 – HCOOH] (1+) @ 468.13 & 445.09
33 usable [y10-NH3] (2+) @ 604.93 & b2(1+) @ 200.68 34 internal_acid bi5-9 (1+) @ 624.41 & b4 (1+) 444.93 35 usable y5(1+) @ 600.44 & a5 (1+) @ 514.24 36 usable y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07 37 usable bi (5-8) (1+) @ 496.41 & y4 (1+) @ 487.01 38 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56 39 non_complementary y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61 40 usable bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14 41 unclear b8(1+) @ 940.89 & ??? @ 195.81 42 usable y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82 43 usable y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17 44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.1 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3] (1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	31	usable	y5(1+) @ 600.3 & [b7-NH3] (2+) @ 405.11
34 internal_acid bi5-9 (1+) @ 624.41 & b4 (1+) 444.93 35 usable y5(1+) @ 600.44 & a5 (1+) @ 514.24 36 usable y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07 37 usable bi (5-8) (1+) @ 496.41 & y4 (1+) @ 487.01 38 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56 39 non_complementary y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61 40 usable bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14 41 unclear b8(1+) @ 940.89 & ??? @ 195.81 42 usable y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82 43 usable y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17 44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.1 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78	32	internal_acid	bi5-10 (1+) @ 737.3 & y2 (1+) 245.92
35	33	usable	[y10-NH3] (2+) @ 604.93 & b2(1+) @ 200.68
36 usable y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07 37 usable bi (5-8) (1+) @ 496.41 & y4 (1+) @ 487.01 38 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56 39 non_complementary y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61 40 usable bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14 41 unclear b8(1+) @ 940.89 & ??? @ 195.81 42 usable y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82 43 usable y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17 44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.1 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	34	internal_acid	bi5-9 (1+) @ 624.41 & b4 (1+) 444.93
37 usable bi (5-8) (1+) @ 496.41 & y4 (1+) @ 487.01 38 usable [y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56 39 non_complementary y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61 40 usable bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14 41 unclear b8(1+) @ 940.89 & ??? @ 195.81 42 usable y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82 43 usable y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17 44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.1 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	35	usable	y5(1+) @ 600.44 & a5 (1+) @ 514.24
38	36	usable	y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07
39 non_complementary y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61 40 usable bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14 41 unclear b8(1+) @ 940.89 & ??? @ 195.81 42 usable y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82 43 usable y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17 44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.10 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.40 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	37	usable	bi (5-8) (1+) @ 496.41 & y4 (1+) @ 487.01
40 usable bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14 41 unclear b8(1+) @ 940.89 & ??? @ 195.81 42 usable y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82 43 usable y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17 44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.1 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	38	usable	[y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56
41 unclear b8(1+) @ 940.89 & ??? @ 195.81 42 usable y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82 43 usable y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17 44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.1 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	39	non_complementary	y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61
42 usable y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82 43 usable y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17 44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.10 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.40 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	40	usable	bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14
43 usable y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17 44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.1 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	41	unclear	b8(1+) @ 940.89 & ??? @ 195.81
44 unclear b6(1+) 712.31 & ??? @ 200.73 45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.1 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	42	usable	y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82
45 unclear y9 (2+) @ 557.39 & ??? @ 250.74 46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.1 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	43	usable	y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17
46 usable [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.1 47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	44	unclear	b6(1+) 712.31 & ??? @ 200.73
47 usable b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	45	unclear	y9 (2+) @ 557.39 & ??? @ 250.74
48 usable y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	46	usable	[y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.11
49 usable [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.4 50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	47	usable	b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91
50 unclear y8 (1+) @ 983.52 & ??? @ 216.78 51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	48	usable	y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69
51 non_complementary y8(2+) @ 491.84 & b3(1+) @ 313.96	49	usable	[y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.41
	50	unclear	y8 (1+) @ 983.52 & ??? @ 216.78
52 non_complementary [b9-2(H2O)] (1+) @ 516.81 & y2 (1+) @ 245.85	51	non_complementary	y8(2+) @ 491.84 & b3(1+) @ 313.96
	52	non_complementary	[b9-2(H2O)] (1+) @ 516.81 & y2 (1+) @ 245.85
53 unclear ??? @ 755.18 & y6(2+) @ 359.22	53	unclear	??? @ 755.18 & y6(2+) @ 359.22
54 usable y1 (1+) @ 174.8 & a10 (2+) @ 577.12	54	usable	y1 (1+) @ 174.8 & a10 (2+) @ 577.12

55	usable	y7 (2+) @ 443.31 & [b5-NH3] (1+) @ 524.29
56	internal_acid	bi5-9 (1+) @ 624.36 & [b4- H2O] (1+) @ 427.13