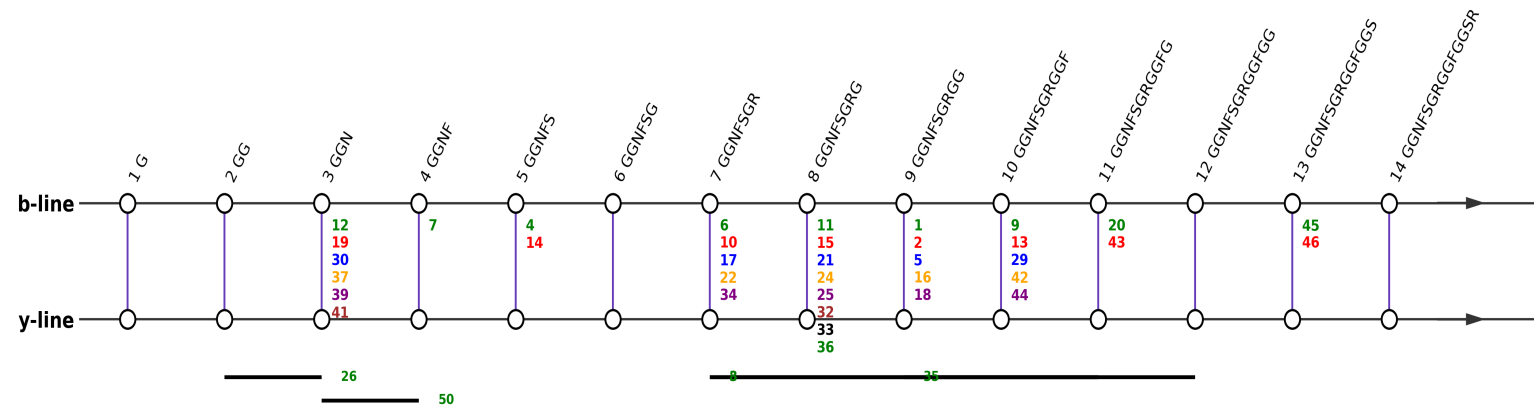


[GGNFSGRMGGFGGSR+3H]³⁺

Fragmentation Diagram for: GGNFSGRGGFGGSR



Detailed Data

n	classification	line	mass1	correct_mass1	mass2	correct_mass2	m1+m2	2m1+m2	m1+2m2	chosen_sum
1	usable	y5 (1+) @ 523.33 & [b9 - NH3] (2+) @ 394.0	523.33	523.26	394.0	394.18	917.33	1440.66	1311.33	1311.33
2	usable	y5 (1+) @ 523.33 & b9 (2+) @ 402.67	523.33	523.26	402.67	402.69	926.0	1449.33	1328.67	1328.67

3	non_complementary	y7 (2+) @ 319.0 & [b11 - NH3] (2+) @ 496.0	319.0	319.16	496.0	496.22	815.0	1134.0	1311.0	1311.0
4	usable	y9 (2+) @ 432.67 & b5 (1+) @ 463.0	432.67	432.73	463.0	463.19	895.67	1328.34	1358.67	1328.34
5	usable	y5 (2+) @ 262.0 & b9 (1+) @ 804.33	262.0	262.13	804.33	804.37	1066.33	1328.33	1870.66	1328.33
6	usable	y7 (1+) @ 637.33 & [b7 - NH3] (2+) @ 337.0	637.33	637.31	337.0	337.16	974.33	1611.66	1311.33	1311.33
7	usable	y10 (2+) @ 476.33 & a4 (1+) @ 348.0	476.33	476.24	348.0	348.15	824.33	1300.66	1172.33	1300.66
8	non_complementary	y7 (2+) @ 319.0 & b11 (2+) @ 504.67	319.0	319.16	504.67	504.74	823.67	1142.67	1328.34	1328.34
9	usable	y4 (1+) @ 376.0 & [b10 - NH3] (2+) @ 467.67	376.0	376.19	467.67	467.71	843.67	1219.67	1311.34	1311.34
10	usable	y7 (1+) @ 637.33 & b7 (2+) @ 345.67	637.33	637.31	345.67	345.67	983.0	1620.33	1328.67	1328.67
11	usable	y6 (1+) @ 580.33 & [b8 - NH3] (2+) @ 365.33	580.33	580.28	365.33	365.67	945.66	1525.99	1310.99	1310.99
12	usable	y11 (2+) @ 550.0 & [b3 - H2O] (1+) @ 210.67	550.0	549.78	210.67	211.08	760.67	1310.67	971.34	1310.67
13	usable	y4 (1+) @ 375.67 & b10 (2+) @ 476.33	375.67	376.19	476.33	476.23	852.0	1227.67	1328.33	1328.33
14	usable	y9 (2+) @ 432.67 & [b5 - NH3] (1+) @ 446.0	432.67	432.73	446.0	446.17	878.67	1311.34	1324.67	1324.67
15	usable	y6 (1+) @ 580.33 & b8 (2+) @ 374.0	580.33	580.28	374.0	374.18	954.33	1534.66	1328.33	1328.33
16	usable	y5 (1+) @ 523.33 & [b9 - H2O - NH3] (2+) @ 385.0	523.33	523.26	385.0	385.17	908.33	1431.66	1293.33	1293.33
17	usable	y7 (1+) @ 637.33 & [b7 - H2O - NH3] (2+) @ 328.0	637.33	637.31	328.0	328.15	965.33	1602.66	1293.33	1293.33
18	usable	y5 (2+) @ 262.0 & [b9 - NH3] (1+) @ 787.33	262.0	262.13	787.33	787.35	1049.33	1311.33	1836.66	1311.33
19	usable	y11 (2+) @ 550.0 & b3 (1+) @ 228.67	550.0	549.78	228.67	229.09	778.67	1328.67	1007.34	1328.67
20	usable	[b11 - H2O - NH3] (2+) @ 487.33 & y3 (1+) @ 319.0	487.33	487.22	319.0	319.17	806.33	1293.66	1125.33	1293.66
21	usable	y6 (2+) @ 290.33 & b8 (1+) @ 747.33	290.33	290.65	747.33	747.35	1037.66	1327.99	1784.99	1327.99
22	usable	y7 (2+) @ 319.0 & b7(1+) @ 690.33	319.0	319.16	690.33	690.33	1009.33	1328.33	1699.66	1328.33
23	ambiguous	[y10 - NH3 - H2O] (2+) @ 458.67 & b4/y4 (1+) @ 376.0	458.67	458.72	376.0	376.16	834.67	1293.34	1210.67	1293.34
24	usable	y6 (1+) @ 580.33 & [b8 - H2O - NH3] (2+) @ 356.67	580.33	580.28	356.67	356.66	937.0	1517.33	1293.67	1293.67
25	usable	y6 (2+) @ 290.33 & [b8-NH3] (1+) @ 730.33	290.33	290.65	730.33	730.33	1020.66	1310.99	1750.99	1310.99
26	internal_acid	[y11 + G] (2+) @ 578.33 & bi2-3 (1+) @ 171.67	578.33	578.29	171.67	172.07	750.0	1328.33	921.67	1328.33
27	unclear	y9 (2+) @ 432.67 & ??? @ 383.0	432.67	432.73	383.0	nan	815.67	1248.34	1198.67	1248.34
28	unclear	??? @ 595.33 & [b8 - NH3] (2+) @ 366.0	595.33	nan	366.0	365.67	961.33	1556.66	1327.33	1327.33
29	usable	[y4-NH3] (1+) @ 358.67 & b10 (2+) @ 476.33	358.67	359.17	476.33	476.23	835.0	1193.67	1311.33	1311.33
30	usable	[y11 - G] (2+) @ 521.67 & [b3 + G] (1+) @ 285.67	521.67	521.26	285.67	286.11	807.34	1329.01	1093.01	1329.01

31	ambiguous	[b10/y10 – H2O – 2(NH3)] (2+) @ 450.0 & y4/b4 @ 376.0	450.0	450.19	376.0	376.19	826.0	1276.0	1202.0	1276.0
32	usable	[b8 – NH3] (1+) @ 730.33 & ai9-10 (1+) @ 176.67	730.33	730.33	176.67	177.09	907.0	1637.33	1083.67	1083.67
33	usable	b8 (1+) @ 747.33 & ai9-10 (1+) 176.67	747.33	747.35	nan	nan	nan	nan	nan	nan
34	usable	y7 (2+) @ 319.0 & [b7-NH3] (1+) @ 673.33	319.0	319.16	673.33	673.31	992.33	1311.33	1665.66	1311.33
35	non_complementary	y5 (2+) @ 262.0 & b12 (2+) @ 533.0	262.0	262.13	533.0	533.25	795.0	1057.0	1328.0	1328.0
36	usable	b8 (1+) @ 748.0 & ai9-10 (1+) @ 204.67	748.0	747.35	204.67	177.09	952.67	1700.67	1157.34	1157.34
37	usable	y11(2+) @ 549.67 & a3(1+) @ 201.67	549.67	549.78	201.67	201.08	751.34	1301.01	953.01	1301.01
38	undefined	549.67 & 165.33	549.67	nan	165.33	nan	715.0	1264.67	880.33	1264.67
39	usable	y11 (2+) @ 550.0 & [a3 – 2(H2O)] (1+) @ 193.33	550.0	549.78	193.33	165.06	743.33	1293.33	936.66	1293.33
40	undefined	461.67 & 389.0	461.67	nan	389.0	nan	850.67	1312.34	1239.67	1312.34
41	usable	y11 (2+) @ 550.0 & [a3-NH3] (1+) @ 183.33	550.0	549.78	183.33	184.06	733.33	1283.33	916.66	1283.33
42	usable	y4 (2+) @ 188.0 & [b10-NH3] (1+) @ 934.33	188.0	188.6	934.33	934.42	1122.33	1310.33	2056.66	1310.33
43	usable	b11 (1+) @ 504.67 & [y3 – CO2] (1+) @ 274.0	504.67	1008.46	274.0	275.18	778.67	1283.34	1052.67	1283.34
44	usable	y4 (1+) @ 376.0 & ai9-10 (1+) @ 176.67	376.0	376.19	176.67	177.09	552.67	928.67	729.34	928.67
45	usable	[b13-H2O-NH3] (2+) @ 559.33 & y1(1+) @ 175.0	559.33	559.24	175.0	175.12	734.33	1293.66	909.33	1293.66
46	usable	y1 (1+) @ 174.67 & [b13-NH3] (2+) @ 567.67	174.67	175.12	567.67	568.25	742.34	917.01	1310.01	1310.01
47	unclear	y5 (1+) @ 523.67 & ??? @ 370.33	523.67	523.26	370.33	nan	894.0	1417.67	1264.33	1264.33
48	undefined	637.0 & 314.33	637.0	nan	314.33	nan	951.33	1588.33	1265.66	1265.66
49	undefined	589.33 & 131.67	589.33	nan	131.67	nan	721.0	1310.33	852.67	1310.33
50	internal_acid	[y10-H2O] (1+) @ 540.67 & [bi3-4 – 2(NH3)] (1+) @ 228.0	540.67	933.46	228.0	228.07	768.67	1309.34	996.67	1309.34