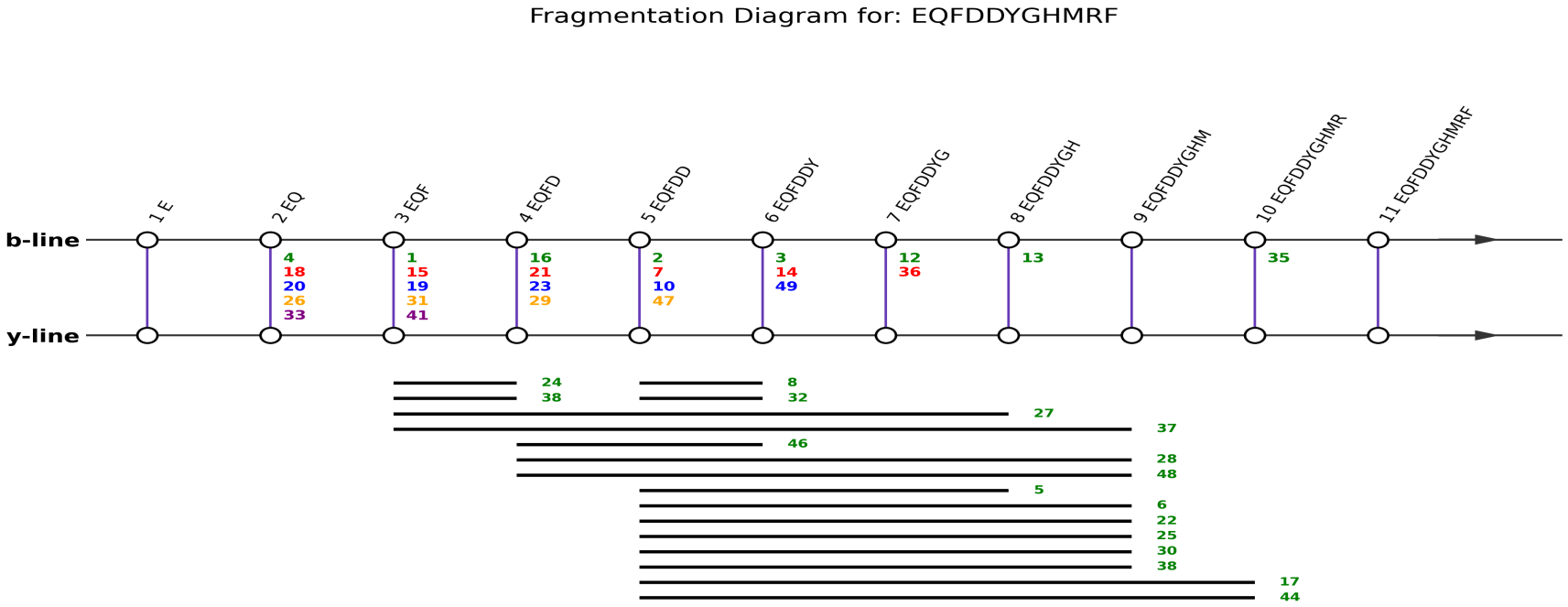
output


Fragmentation Diagram for: EQFDDYGHMRF
b-line
y-line
1 E
2 EQ
3 EQF
4 EQFD
5 EQFDD
6 EQFDDY
7 EQFDDYG
8 EQFDDYGH
9 EQFDDYGHM
10 EQFDDYGHMR
11 EQFDDYGHMRF
4
18
20
26
33
1
15
19
31
41
16
21
23
29
2
7
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47
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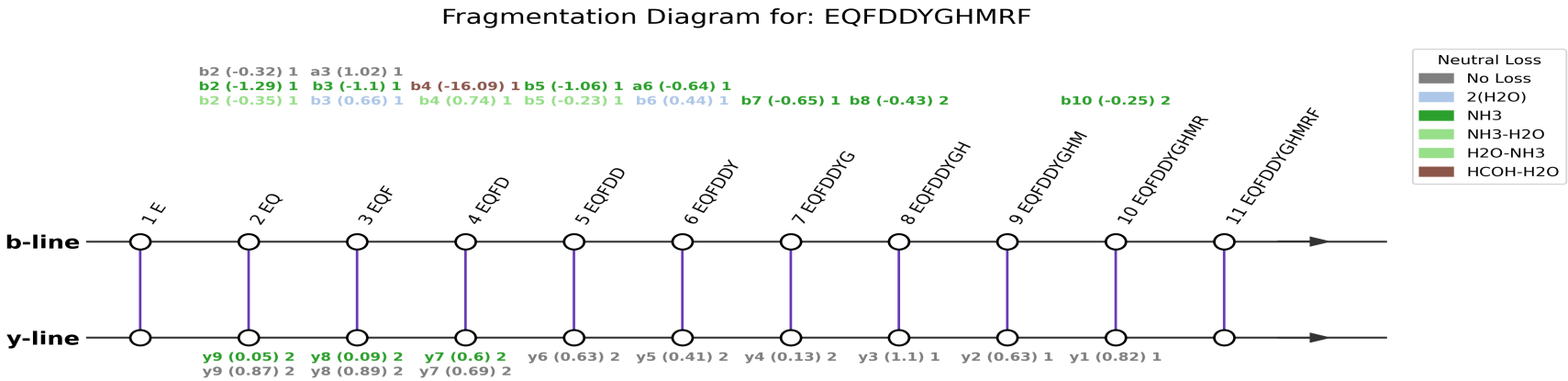
44



Detailed Data - Table 1

Unnamed: 0	b2	b3	b4	b5	b6	b7	b8	b10
2(H2O)	nan	b3-2(H2O) (0.66) (1 , 2)	nan	nan	b6-2(H2O) (0.44) (1 , 2)	nan	nan	nan
H2O-NH3	b2-H2O-NH3 (-0.35) (1 , 2)	nan	b4-H2O-NH3 (0.74) (1 , 1)	b5-H2O-NH3 (-0.23) (1 , 2)	nan	nan	nan	nan
NH3	b2-NH3 (-1.29) (1 , 2)	b3-NH3 (-1.1) (1 , 2)	nan	b5-NH3 (-1.06) (1 , 2)	a6-NH3 (-0.64) (1 , 2)	b7-NH3 (-0.65) (1 , 2)	b8-NH3 (-0.43) (2 , 1)	b10-NH3 (-0.25) (2 , 1)
HCOH-H2O	nan	nan	b4-HCOH-H2O (-16.09) (1 , 1)	nan	nan	nan	nan	nan
No Loss	b2 (-0.32) (1 , 2)	a3 (1.02) (1 , 1)	nan	nan	nan	nan	nan	nan

Detailed Data - Table 2

Unnamed: 0	y1	y2	y3	y4	y5	y6	y7	y8	y9
NH3	nan	nan	nan	nan	nan	nan	y7-NH3 (0.6) (2 , 1)	y8-NH3 (0.09) (2 , 1)	y9-NH3 (0.05) (2 , 1)
No Loss	y1 (0.82) (1 , 2)	y2 (0.63) (1 , 1)	y3 (1.1) (1 , 1)	y4 (0.13) (2 , 1)	y5 (0.41) (2 , 1)	y6 (0.63) (2 , 1)	y7 (0.69) (2 , 1)	y8 (0.89) (2 , 1)	y9 (0.87) (2 , 1)

Detailed Data - Table 3

n	classification	line	mass1	correct_mass1	mass2	correct_mass2	chosen_sum	Cluster ID eps_1.0	Cluster ID eps_0.8	Cluster ID eps_0.6	Cluster ID eps_0.4
1	usable	y8(2+) @ 560.4 & [b3-NH3] (1+) @ 387.05	560.4	559.7	387.05	388.15	1507.85	0.0	0.0	0.0	0.0
2	usable	y6(2+) @ 445.29 & [b5-NH3] (1+) @ 617.14	445.29	444.68	617.14	618.2	1507.72	0.0	0.0	0.0	0.0
3	usable	y5(2+) @ 323.67 & [b6-NH3] (1+) @ 860.17	323.67	323.16	860.17	861.23	1507.51	0.0	0.0	0.0	0.0
4	usable	y9(2+) @ 633.88 & [b2-NH3] (1+) @ 239.74	633.88	633.24	239.74	241.08	1507.5	0.0	0.0	0.0	0.0
5	internal_acid	bi5-8 (1+) @ 1553.17 & y3 (1+) @ 452.35	1553.17	553.14	452.35	451.24	2005.52	-1.0	-1.0	-1.0	-1.0
6	internal_acid	bi5-9 (1+) @ 684.16 & y2 (1+) @ 321.1	684.16	684.18	321.1	320.2	1689.42	-1.0	-1.0	-1.0	-1.0
7	usable	y6(2+) @ 445.35 & a3(1+) @ 378.1	445.35	444.68	378.1	377.17	1268.8	-1.0	-1.0	-1.0	-1.0
8	internal_acid	y5+ @ 646.41 & bi5-6 (1+) @ 359.02	646.41	nan	359.02	359.06	1651.84	-1.0	-1.0	-1.0	-1.0
9	undefined	503.73 & 498.42	503.73	nan	498.42	nan	1505.88	-1.0	-1.0	-1.0	-1.0
10	usable	[b5-H2O-NH3] (1+) @ 599.96 & y6 (2+) @ 445.31	599.96	600.19	445.31	444.68	1490.58	1.0	1.0	1.0	1.0
11	usable	y5 (1+) 646.38 & ai5-6 (1+) @ 330.84	nan	nan	330.84	331.05	nan	nan	nan	nan	nan
12	usable	y4(1+) @ 589.39 & [a6-NH3](2+) @ 416.05	589.39	588.29	416.05	417.12	1594.83	-1.0	-1.0	-1.0	-1.0
13	usable	y3(1+) @ 452.19 & [b8-NH3](2+) @ 527.73	452.19	451.24	527.73	528.16	1507.65	0.0	0.0	0.0	0.0
14	usable	[b6-2(H2O)] (1+) @ 842.68 & y5 (2+) @ 323.57	842.68	842.24	323.57	323.16	1489.82	1.0	1.0	2.0	2.0
15	usable	y8(2+) @ 560.27 & [a3-NH3](1+) @ 358.97	560.27	559.7	358.97	360.14	1479.51	2.0	2.0	3.0	3.0
16	usable	[b4-H2O-NH3] (1+) @ 485.79 & [y7- CHONH2] (2+) @ 480.35	485.79	485.17	480.35	479.68	1451.93	-1.0	-1.0	-1.0	-1.0
17	internal_acid	bi5-10 (1+) @ 840.5 & y1 (1+) 164.73	840.5	840.29	nan	nan	nan	nan	nan	nan	nan

18	usable	y9(2+) @ 633.84 & [a2-NH3](1+) @ 211.71	633.84	633.24	211.71	213.07	1479.39	2.0	2.0	3.0	3.0
19	usable	[y8-NH3](2+) @ 551.2 & [b3-NH3](1+) @ 387.05	551.2	551.19	387.05	388.15	1489.45	1.0	1.0	2.0	2.0
20	usable	y9(2+) @ 634.16 & b2(1+) @ 257.79	634.16	633.24	257.79	258.11	1526.11	-1.0	-1.0	-1.0	-1.0
21	usable	[y7-NH3] (2+) @ 494.13 & [b4-HCOH – H2O] (1+) @ 456.16	494.13	493.68	456.16	472.18	1444.42	-1.0	-1.0	-1.0	-1.0
22	internal_acid	bi5-9 (1+) @ 656.39 & y2 (1+) @ 321.11	656.39	684.18	321.11	320.2	1633.89	-1.0	-1.0	-1.0	-1.0
23	usable	y7 (2+) @ 502.88 & [b4-HCOH – H2O] (1+) @ 455.94	502.88	502.19	455.94	472.18	1461.7	3.0	3.0	4.0	-1.0
24	internal_acid	[y7 – NH3] 2+ @ 494.11 & bi3-4 @ 262.78	494.11	nan	262.78	263.1	1251.0	-1.0	-1.0	-1.0	-1.0
25	internal_acid	[bi5-9 – CH3CH2SCH3] (1+) @ 608.2 & y2 (1+) @ 320.89	608.2	608.15	320.89	320.2	1537.29	-1.0	-1.0	-1.0	-1.0
26	usable	[y9-NH3] (2+) @ 624.77 & [b2-NH3] (1+) @ 239.79	624.77	624.72	239.79	241.08	1489.33	1.0	1.0	2.0	2.0
27	internal_acid	bi3-8 (1+) @ 815.6 & y3 (1+) @ 452.34	815.6	815.24	452.34	451.24	1720.28	-1.0	-1.0	-1.0	-1.0
28	non_complementary	[b4-HCOH – H2O] (1+) @ 456.12 & y2 (1+) @ 321.07	456.12	472.18	321.07	320.2	1233.31	-1.0	-1.0	-1.0	-1.0
29	usable	[y7 – NH3] (2+) @ 494.28 & [b4 - H2O – NH3] (1+) @ 484.76	494.28	493.68	484.76	485.17	1473.32	-1.0	-1.0	-1.0	-1.0
30	internal_acid	[bi5-9] (1+) @ 683.79 & [b4 - HCOH – H2O] (1+) @ 456.23	683.79	684.18	456.23	472.18	1596.25	-1.0	-1.0	-1.0	-1.0
31	usable	y8 (2+) @ 560.59 & [b3 – 2(H2O)] (1+) @ 369.82	560.59	559.7	369.82	369.16	1491.0	1.0	1.0	1.0	1.0
32	internal_acid	y5 (1+) @ 646.41 & bi5-6 (1+) @ 312.22	646.41	645.32	312.22	359.06	1605.04	-1.0	-1.0	-1.0	-1.0
33	usable	y9 (2+) @ 634.11 & [b2 – H2O – NH3] (1+) @ 222.72	634.11	633.24	222.72	223.07	1490.94	1.0	1.0	1.0	1.0
34	unclear	b8 (2+) @ 536.55 & ??? @ 454.17	536.55	536.67	454.17	nan	1527.27	-1.0	-1.0	-1.0	-1.0
35	usable	y1(1+) @ 164.91 & [b10-NH3](2+) @ 671.48	164.91	164.09	671.48	671.73	1507.87	0.0	0.0	0.0	0.0
36	usable	y4(2+) @ 294.78 & [b7-NH3](1+) @ 917.61	294.78	294.65	917.61	918.26	1507.17	0.0	0.0	0.0	0.0
37	internal_acid	bi3-9 (1+) @ 946.47 & y2 (1+) 321.09	946.47	946.28	nan	nan	nan	nan	nan	nan	nan
38	internal_acid	bi5-9 (1+) @ 683.85 & bi3-4 (1+) @ 263.1	683.85	684.18	263.1	263.1	1630.8	-1.0	-1.0	-1.0	-1.0
39	undefined	591.11 & 398.48	591.11	nan	398.48	nan	1580.7	-1.0	-1.0	-1.0	-1.0
40	unclear	y9 (2+) @ 634.11 & ??? @ 194.76	634.11	633.24	194.76	nan	1462.98	-1.0	-1.0	-1.0	-1.0
41	usable	[y8-NH3] (2+) @ 551.28 & [a3-H2O] (1+) @ 358.64	551.28	551.19	358.64	359.16	1461.2	3.0	3.0	4.0	-1.0
42	unclear	y8(2+) @ 560.81 & ??? @ 342.47	560.81	559.7	342.47	nan	1464.09	-1.0	-1.0	-1.0	-1.0
43	unclear	y4(1+) @ 589.96 & ??? @ 329.12	589.96	588.29	329.12	nan	1509.04	-1.0	-1.0	-1.0	-1.0
44	internal_acid	bi5-10 (1+) @ 840.36 & [b4 – H2O – NH3] (1+) @ 485.91	840.36	840.29	485.91	485.17	1326.27	-1.0	-1.0	-1.0	-1.0
45	undefined	518.97 & 454.06	518.97	nan	454.06	nan	1492.0	1.0	-1.0	-1.0	-1.0

46	non_complementary	y5 (1+) @ 646.3 & [b4-HCOH – H2O] (1+) @ 456.09	646.3	645.32	456.09	472.18	1558.48	-1.0	-1.0	-1.0	-1.0
47	usable	y6 (1+) @ 889.27 & a3 (1+) @ 378.19	889.27	888.35	378.19	377.17	1645.65	-1.0	-1.0	-1.0	-1.0
48	non_complementary	[b4 – H2O – NH3] (1+) @ 484.86 & y2 (1+) @ 320.83	484.86	485.17	320.83	320.2	1290.55	-1.0	-1.0	-1.0	-1.0
49	usable	y5 (2+) @ 323.7 & [a6-NH3] (1+) @ 832.58	323.7	323.16	832.58	833.22	1479.98	2.0	2.0	3.0	-1.0
50	undefined	567.88 & 374.49	567.88	nan	374.49	nan	1510.25	-1.0	-1.0	-1.0	-1.0