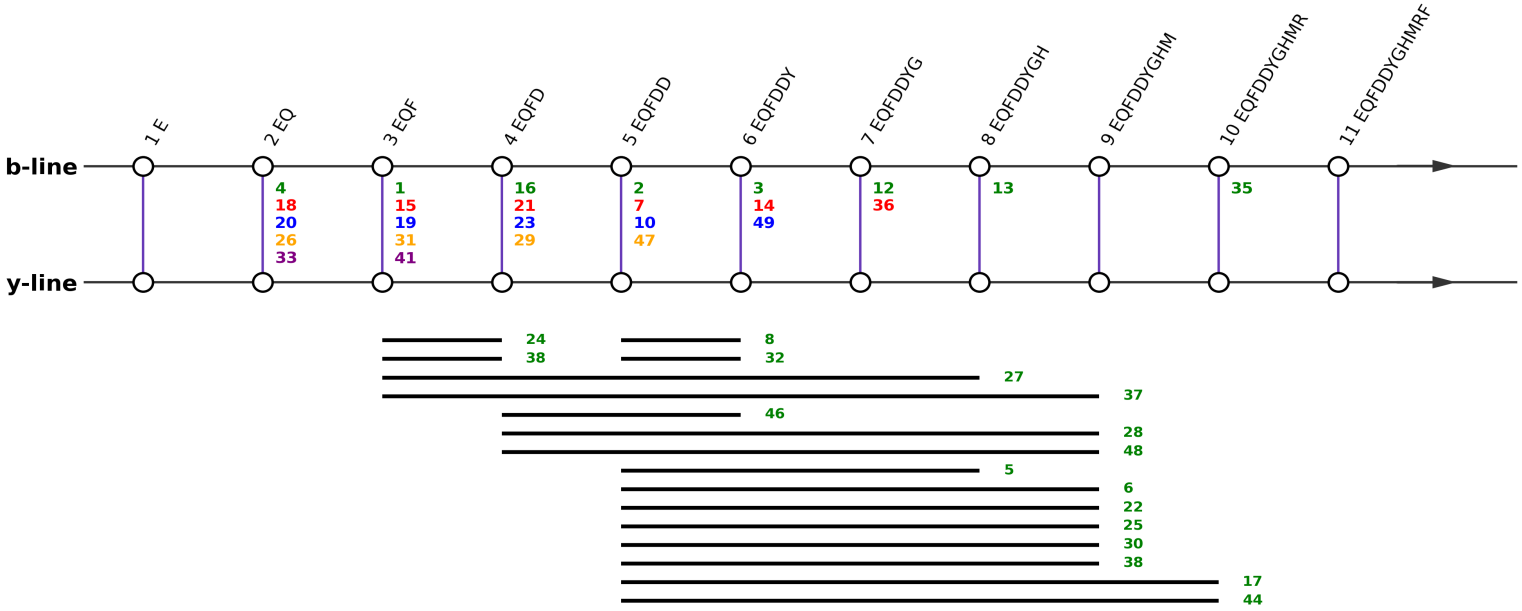
[EQFDDY(p)GHMRF(NH2) +3H]3+

Fragmentation Diagram for: EQFDDYGHMRF



Detailed Data

n	classification	line	mass1	correct_mass1	mass2	correct_mass2	m1+m2	2m1+m2	m1+2m2	chosen_sum
1	usable	y8(2+) @ 560.4 & [b3-NH3] (1+) @ 387.05	560.4	559.7	387.05	388.15	947.45	1507.85	1334.5	1507.85
2	usable	y6(2+) @ 445.29 & [b5-NH3] (1+) @ 617.14	445.29	444.68	617.14	618.2	1062.43	1507.72	1679.57	1507.72

3	usable	y5(2+) @ 323.67 & [b6-NH3] (1+) @ 860.17	323.67	323.16	860.17	861.23	1183.84	1507.51	2044.01	1507.51
4	usable	y9(2+) @ 633.88 & [b2-NH3] (1+) @ 239.74	633.88	633.24	239.74	241.08	873.62	1507.5	1113.36	1507.5
5	internal_acid	bi5-8 (1+) @ 1553.17 & y3 (1+) @ 452.35	1553.17	553.14	452.35	451.24	2005.52	3558.69	2457.87	2005.52
6	internal_acid	bi5-9 (1+) @ 684.16 & y2 (1+) @ 321.1	684.16	684.18	321.1	320.2	1005.26	1689.42	1326.36	1689.42
7	usable	y6(2+) @ 445.35 & a3(1+) @ 378.1	445.35	444.68	378.1	377.17	823.45	1268.8	1201.55	1268.8
8	internal_acid	y5+ @ 646.41 & bi5-6 (1+) @ 359.02	646.41	nan	359.02	359.06	1005.43	1651.84	1364.45	1651.84
9	undefined	503.73 & 498.42	503.73	nan	498.42	nan	1002.15	1505.88	1500.57	1505.88
10	usable	[b5-H2O-NH3] (1+) @ 599.96 & y6 (2+) @ 445.31	599.96	600.19	445.31	444.68	1045.27	1645.23	1490.58	1490.58
11	usable	y5 (1+) 646.38 & ai5-6 (1+) @ 330.84	nan	nan	330.84	331.05	nan	nan	nan	nan
12	usable	y4(1+) @ 589.39 & [a6-NH3](2+) @ 416.05	589.39	588.29	416.05	417.12	1005.44	1594.83	1421.49	1594.83
13	usable	y3(1+) @ 452.19 & [b8-NH3](2+) @ 527.73	452.19	451.24	527.73	528.16	979.92	1432.11	1507.65	1507.65
14	usable	[b6-2(H2O)] (1+) @ 842.68 & y5 (2+) @ 323.57	842.68	842.24	323.57	323.16	1166.25	2008.93	1489.82	1489.82
15	usable	y8(2+) @ 560.27 & [a3-NH3](1+) @ 358.97	560.27	559.7	358.97	360.14	919.24	1479.51	1278.21	1479.51
16	usable	[b4-H2O-NH3] (1+) @ 485.79 & [y7- CHONH2] (2+) @ 480.35	485.79	485.17	480.35	479.68	966.14	1451.93	1446.49	1451.93
17	internal_acid	bi5-10 (1+) @ 840.5 & y1 (1+) 164.73	840.5	840.29	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	845.55	1479.39	1057.26	1479.39
19	usable	[y8-NH3](2+) @ 551.2 & [b3-NH3](1+) @ 387.05	551.2	551.19	387.05	388.15	938.25	1489.45	1325.3	1489.45
20	usable	y9(2+) @ 634.16 & b2(1+) @ 257.79	634.16	633.24	257.79	258.11	891.95	1526.11	1149.74	1526.11
21	usable	[y7-NH3] (2+) @ 494.13 & [b4-HCOH – H2O] (1+) @ 456.16	494.13	493.68	456.16	472.18	950.29	1444.42	1406.45	1444.42
22	internal_acid	bi5-9 (1+) @ 656.39 & y2 (1+) @ 321.11	656.39	684.18	321.11	320.2	977.5	1633.89	1298.61	1633.89
23	usable	y7 (2+) @ 502.88 & [b4-HCOH – H2O] (1+) @ 455.94	502.88	502.19	455.94	472.18	958.82	1461.7	1414.76	1461.7
24	internal_acid	[y7 – NH3] 2+ @ 494.11 & bi3-4 @ 262.78	494.11	nan	262.78	263.1	756.89	1251.0	1019.67	1251.0
25	internal_acid	[bi5-9 – CH3CH2SCH3] (1+) @ 608.2 & y2 (1+) @ 320.89	608.2	608.15	320.89	320.2	929.09	1537.29	1249.98	1537.29
26	usable	[y9-NH3] (2+) @ 624.77 & [b2-NH3] (1+) @ 239.79	624.77	624.72	239.79	241.08	864.56	1489.33	1104.35	1489.33
27	internal_acid	bi3-8 (1+) @ 815.6 & y3 (1+) @ 452.34	815.6	815.24	452.34	451.24	1267.94	2083.54	1720.28	1720.28
28	non_complementary	[b4-HCOH – H2O] (1+) @ 456.12 & y2 (1+) @ 321.07	456.12	472.18	321.07	320.2	777.19	1233.31	1098.26	1233.31
29	usable	[y7 – NH3] (2+) @ 494.28 & [b4 - H2O – NH3] (1+) @ 484.76	494.28	493.68	484.76	485.17	979.04	1473.32	1463.8	1473.32
30	internal_acid	[bi5-9] (1+) @ 683.79 & [b4 - HCOH – H2O] (1+) @ 456.23	683.79	684.18	456.23	472.18	1140.02	1823.81	1596.25	1596.25

31	usable	y8 (2+) @ 560.59 & [b3 – 2(H2O)] (1+) @ 369.82	560.59	559.7	369.82	369.16	930.41	1491.0	1300.23	1491.0
32	internal_acid	y5 (1+) @ 646.41 & bi5-6 (1+) @ 312.22	646.41	645.32	312.22	359.06	958.63	1605.04	1270.85	1605.04
33	usable	y9 (2+) @ 634.11 & [b2 – H2O – NH3] (1+) @ 222.72	634.11	633.24	222.72	223.07	856.83	1490.94	1079.55	1490.94
34	unclear	b8 (2+) @ 536.55 & ??? @ 454.17	536.55	536.67	454.17	nan	990.72	1527.27	1444.89	1527.27
35	usable	y1(1+) @ 164.91 & [b10-NH3](2+) @ 671.48	164.91	164.09	671.48	671.73	836.39	1001.3	1507.87	1507.87
36	usable	y4(2+) @ 294.78 & [b7-NH3](1+) @ 917.61	294.78	294.65	917.61	918.26	1212.39	1507.17	2130.0	1507.17
37	internal_acid	bi3-9 (1+) @ 946.47 & y2 (1+) 321.09	946.47	946.28	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	946.95	1630.8	1210.05	1630.8
39	undefined	591.11 & 398.48	591.11	nan	398.48	nan	989.59	1580.7	1388.07	1580.7
40	unclear	y9 (2+) @ 634.11 & ??? @ 194.76	634.11	633.24	194.76	nan	828.87	1462.98	1023.63	1462.98
41	usable	[y8-NH3] (2+) @ 551.28 & [a3-H2O] (1+) @ 358.64	551.28	551.19	358.64	359.16	909.92	1461.2	1268.56	1461.2
42	unclear	y8(2+) @ 560.81 & ??? @ 342.47	560.81	559.7	342.47	nan	903.28	1464.09	1245.75	1464.09
43	unclear	y4(1+) @ 589.96 & ??? @ 329.12	589.96	588.29	329.12	nan	919.08	1509.04	1248.2	1509.04
44	internal_acid	bi5-10 (1+) @ 840.36 & [b4 – H2O – NH3] (1+) @ 485.91	840.36	840.29	485.91	485.17	1326.27	2166.63	1812.18	1326.27
45	undefined	518.97 & 454.06	518.97	nan	454.06	nan	973.03	1492.0	1427.09	1492.0
46	non_complementary	y5 (1+) @ 646.3 & [b4-HCOH – H2O] (1+) @ 456.09	646.3	645.32	456.09	472.18	1102.39	1748.69	1558.48	1558.48
47	usable	y6 (1+) @ 889.27 & a3 (1+) @ 378.19	889.27	888.35	378.19	377.17	1267.46	2156.73	1645.65	1645.65
48	non_complementary	[b4 – H2O – NH3] (1+) @ 484.86 & y2 (1+) @ 320.83	484.86	485.17	320.83	320.2	805.69	1290.55	1126.52	1290.55
49	usable	y5 (2+) @ 323.7 & [a6-NH3] (1+) @ 832.58	323.7	323.16	832.58	833.22	1156.28	1479.98	1988.86	1479.98
50	undefined	567.88 & 374.49	567.88	nan	374.49	nan	942.37	1510.25	1316.86	1510.25