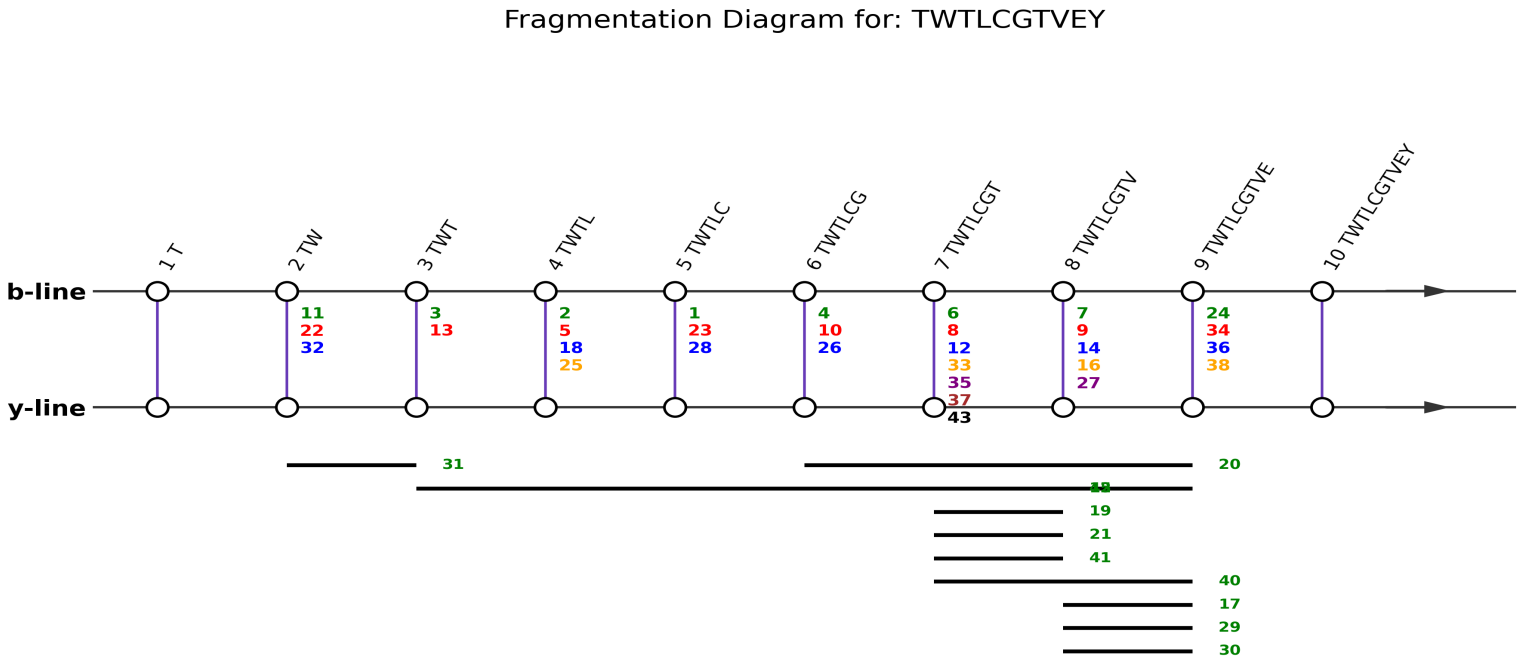
[TWT(p)LCGTVEY+2H]2+



Detailed Data

n	classification	line	mass1	correct_mass1	mass2	correct_mass2	m1+m2	2m1+m2	m1+2m2	chosen_sum
1	usable	y5 (1+) @ 568.12 & b5 (1+) @ 685.12	568.12	568.26	685.12	685.24	1253.24	1821.36	1938.36	1253.24
2	usable	y6 (1+) @ 671.16 & b4 (1+) @ 582.03	671.16	671.27	582.03	582.23	1253.19	1924.35	1835.22	1253.19

3	usable	y7 (1+) @ 784.38 & b3 (1+) @ 469.1	784.38	784.35	469.1	469.15	1253.48	2037.86	1722.58	1253.48
4	usable	y4 (1+) @ 511.14 & b6 (1+) @ 742.16	511.14	511.24	742.16	742.26	1253.3	1764.44	1995.46	1253.3
5	usable	y6 (1+) @ 671.17 & [b4-H3PO4] (1+) @ 484.11	671.17	671.27	484.11	484.26	1155.28	1826.45	1639.39	1155.28
6	usable	y3 (1+) @ 410.06 & b7 (1+) @ 843.07	410.06	410.19	843.07	843.31	1253.13	1663.19	2096.2	1253.13
7	usable	[y2-NH3] (1+) @ 292.81 & b8 (1+) @ 942.06	292.81	294.1	942.06	942.38	1234.87	1527.68	2176.93	1234.87
8	usable	y3 (1+) @ 410.14 & [b7-H3PO4] (1+) @ 745.45	410.14	410.19	745.45	745.33	1155.59	1565.73	1901.04	1155.59
9	usable	[y2-H2O] (1+) @ 292.99 & [b8-NH3] (1+) @ 924.66	292.99	293.11	924.66	925.35	1217.65	1510.64	2142.31	1217.65
10	usable	y4 (1+) @ 511.35 & [b6-H3PO4] (1+) @ 644.83	511.35	511.24	644.83	644.29	1156.18	1667.53	1801.01	1156.18
11	usable	[y8-NH3] (1+) @ 949.32 & b2 (1+) @ 287.66	949.32	948.34	287.66	288.13	1236.98	2186.3	1524.64	1236.98
12	usable	y3 (1+) @ 410.08 & [b7-NH3] (1+) @ 825.18	410.08	410.19	825.18	826.28	1235.26	1645.34	2060.44	1235.26
13	usable	[y7-NH3] (1+) @ 766.69 & b3 (1+) @ 469.17	766.69	767.33	469.17	469.15	1235.86	2002.55	1705.03	1235.86
14	usable	y2 (1+) @ 310.82 & b8 (1+) @ 941.96	310.82	311.12	941.96	942.38	1252.78	1563.6	2194.74	1252.78
15	non_complementary	b9 (1+) @ 942.37 & [y2 – HCOOH – H2O] (1+) @ 246.94	942.37	1071.42	246.94	247.11	1189.31	2131.68	1436.25	1189.31
16	usable	y2 (1+) @ 310.96 & [b8-NH3] (1+) @ 924.24	310.96	311.12	924.24	925.35	1235.2	1546.16	2159.44	1235.2
17	internal_acid	b7 (1+) @ 843.12 & bi8-9 (1+) @ 228.81	843.12	843.31	228.81	229.12	1071.93	1915.05	1300.74	1300.74
18	usable	[y6-NH3] (1+) @ 653.25 & [b4-H3PO4] (1+) @ 484.86	653.25	654.24	484.86	484.26	1138.11	1791.36	1622.97	1138.11
19	non_complementary	[y2-NH3] (1+) @ 292.74 & b7 (1+) @ 844.74	292.74	294.1	844.74	843.31	1137.48	1430.22	1982.22	1137.48
20	internal_acid	b5 (1+) @ 685.65 & bi6-9 (1+) @ 387.07	685.65	685.24	387.07	387.19	1072.72	1758.37	1459.79	1072.72
21	non_complementary	y2 (1+) @ 310.67 & b7 (1+) @ 844.47	310.67	311.12	844.47	843.31	1155.14	1465.81	1999.61	1155.14
22	usable	[y8-NH3] (1+) @ 947.45 & a2 (1+) @ 259.8	947.45	948.34	259.8	260.12	1207.25	2154.7	1467.05	1207.25
23	usable	y5 (1+) @ 568.07 & [b5-H3PO4] (1+) @ 587.19	568.07	568.26	587.19	587.26	1155.26	1723.33	1742.45	1155.26
24	usable	y1 (1+) @ 181.5 & [b9-NH3] (1+) @ 1053.38	181.5	182.08	1053.38	1054.4	1234.88	1416.38	2288.26	1234.88
25	usable	[y6-NH3] (1+) @ 653.29 & b4 (1+) @ 582.18	653.29	654.24	582.18	582.23	1235.47	1888.76	1817.65	1235.47
26	usable	y4 (1+) @ 511.3 & [b6-NH3] (1+) @ 724.3	511.3	511.24	724.3	725.24	1235.6	1746.9	1959.9	1235.6
27	usable	[b8-H2O] (1+) @ 924.37 & [y2 – HCOOH – H2O] (1+) @ 246.98	924.37	924.37	246.98	247.11	1171.35	2095.72	1418.33	1171.35
28	usable	[y5-NH3] (1+) @ 550.54 & b5 (1+) @ 685.25	550.54	551.23	685.25	685.24	1235.79	1786.33	1921.04	1235.79
29	internal_acid	[b7-H2O] (1+) @ 825.19 & bi8-9 (1+) @ 228.81	825.19	825.3	228.81	229.12	1054.0	1879.19	1282.81	1282.81
30	internal_acid	[b7-H3PO4] (1+) 745.72 & bi8-9 (1+) @ 228.74	nan	nan	228.74	229.12	nan	nan	nan	nan

31	non_complementary	y7 (1+) @ 784.12 & b2 (1+) @ 287.76	784.12	784.35	287.76	288.13	1071.88	1856.0	1359.64	1359.64
32	usable	y8 (1+) @ 965.41 & b2 (1+) @ 287.94	965.41	965.37	287.94	288.13	1253.35	2218.76	1541.29	1253.35
33	usable	[b7-2(H2O)]/[b7-NH3-H2O] (1+) @ 807.36 & y3 (1+) @ 410.11	807.36	nan	410.11	410.19	1217.47	2024.83	1627.58	1217.47
34	usable	y1(1+) @ 181.74 & [b9-H3PO4] (1+) @ 973.65	181.74	182.08	973.65	973.44	1155.39	1337.13	2129.04	1337.13
35	usable	[b7-H3PO4-H2O] (1+) @ 727.27 & y3 (1+) @ 410.25	727.27	727.32	410.25	410.19	1137.52	1864.79	1547.77	1137.52
36	usable	y1 (1+) @ 181.38 & b9 (1+) @ 1071.1	181.38	182.08	1071.1	1071.42	1252.48	1433.86	2323.58	1252.48
37	usable	b7 (1+) @ 843.61 & ai8-9 (1+) @ 200.62	843.61	843.31	200.62	201.11	1044.23	1887.84	1244.85	1244.85
38	usable	[b9-H3PO4-H2O] (1+) @ 955.76 & y1 (1+) 181.5	955.76	955.43	nan	nan	nan	nan	nan	nan
39	unclear	??? @ 867.7 & [y2 – H2O] (1+) @ 291.9	867.7	nan	291.9	293.11	1159.6	2027.3	1451.5	1159.6
40	internal_acid	b6 (1+) @ 743.52 & bi7-9 (1+) @ 329.71	743.52	742.26	329.71	330.17	1073.23	1816.75	1402.94	1402.94
41	non_complementary	y2 (1+) @ 311.27 & [b7-NH3] (1+) @ 826.46	311.27	311.12	826.46	826.28	1137.73	1449.0	1964.19	1137.73
42	internal_acid	bi3-8 (1+) @ 627.78 & y2 (1+) @ 310.79	627.78	655.25	310.79	311.12	938.57	1566.35	1249.36	1249.36
43	usable	[y3-NH3] (1+) @ 392.06 & [b7-NH3] (1+) @ 824.85	392.06	393.17	824.85	826.28	1216.91	1608.97	2041.76	1216.91
44	undefined	728.32 & 569.4	728.32	nan	569.4	nan	1297.72	2026.04	1867.12	1297.72
45	undefined	844.84 & 274.35	844.84	nan	274.35	nan	1119.19	1964.03	1393.54	1119.19
46	undefined	844.25 & 806.82	844.25	nan	806.82	nan	1651.07	2495.32	2457.89	1651.07
47	undefined	587.33 & 538.42	587.33	nan	538.42	nan	1125.75	1713.08	1664.17	1125.75
48	undefined	535.98 & 435.95	535.98	nan	435.95	nan	971.93	1507.91	1407.88	1407.88
49	undefined	939.22 & 609.33	939.22	nan	609.33	nan	1548.55	2487.77	2157.88	1548.55
50	undefined	941.73 & 274.8	941.73	nan	274.8	nan	1216.53	2158.26	1491.33	1216.53