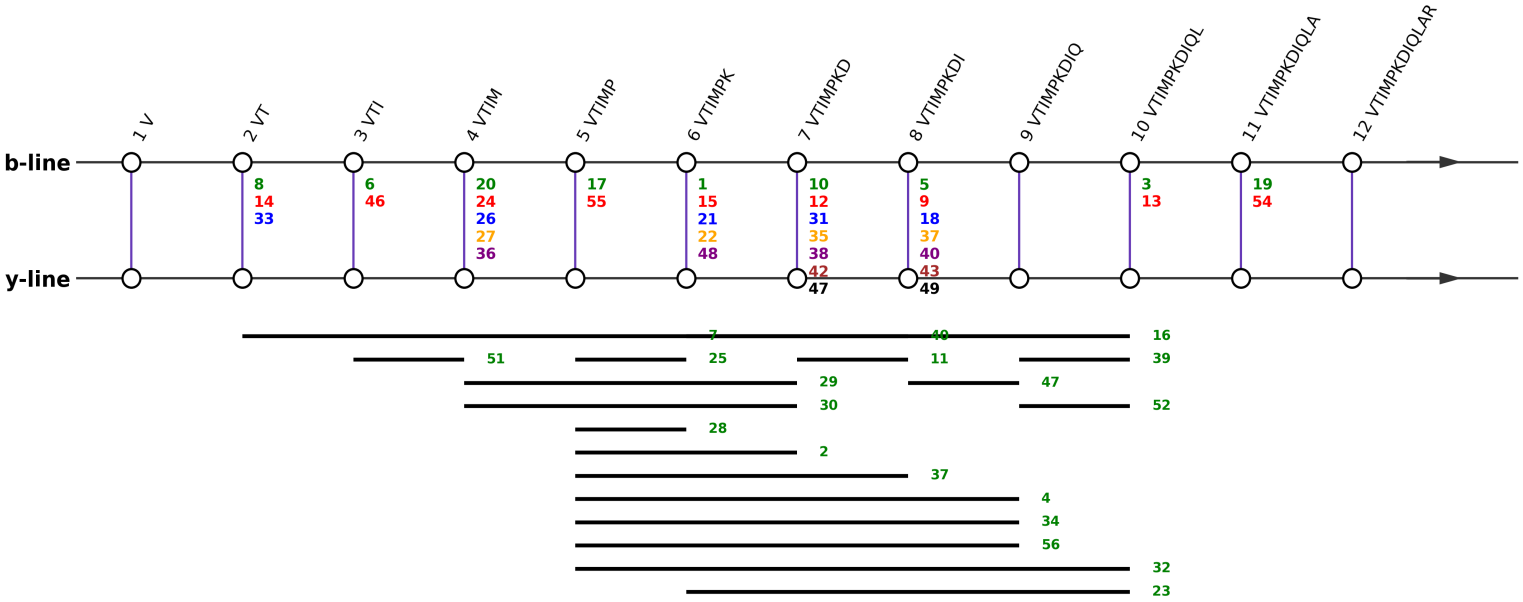
[VTIMPK(Ac)DIQLAR+3H]3+

Fragmentation Diagram for: VTIMPKDIQLAR



Detailed Data

n	classification	line	mass1	correct_mass1	mass2	correct_mass2	m1+m2	2m1+m2	m1+2m2	chosen_sum
1	usable	y6 (1+) @ 715.44 & b6 (2+) @ 356.66	715.44	715.41	356.66	356.71	1072.1	1787.54	1428.76	1428.76
2	internal_acid	y5 (1+) @ 600.46 & bi5-7 (1+) @ 383.1	600.46	600.38	383.1	383.19	983.56	1584.02	1366.66	1366.66

3	usable	y2 (1+) @ 245.82 & b10 (2+) @ 591.38	245.82	246.16	591.38	591.33	837.2	1083.02	1428.58	1428.58
4	internal_acid	bi5-9 (1+) @ 624.4 & y3 (1+) @ 359.18	624.4	624.34	359.18	359.24	983.58	1607.98	1342.76	1342.76
5	usable	y4 (1+) @ 487.22 & a8(2+) @ 456.75	487.22	487.3	456.75	456.76	943.97	1431.19	1400.72	1431.19
6	usable	y9 (2+) @ 557.42 & [b3-NH3] (1+) @ 296.01	557.42	557.31	296.01	297.18	853.43	1410.85	1149.44	1410.85
7	non_complementary	y6 (2+) @ 359.14 & b9 (2+) @ 534.76	359.14	358.21	534.76	534.79	893.9	1253.04	1428.66	1428.66
8	usable	y10 (2+) @ 614.08 & b2 (1+) @ 200.71	614.08	613.85	200.71	201.12	814.79	1428.87	1015.5	1428.87
9	usable	[y4-NH3] (2+) @ 234.85 & b8 (1+) @ 940.45	234.85	235.64	940.45	940.52	1175.3	1410.15	2115.75	1410.15
10	usable	y5 (1+) @ 600.38 & b7 (2+) @ 414.18	600.38	600.38	414.18	414.22	1014.56	1614.94	1428.74	1428.74
11	non_complementary	y4 (1+) @ 487.33 & b7 (1+) @ 827.44	487.33	487.3	827.44	827.43	1314.77	1802.1	2142.21	1314.77
12	usable	y5 (2+) @ 300.5 & b7 (1+) @ 827.42	300.5	300.69	827.42	827.43	1127.92	1428.42	1955.34	1428.42
13	usable	y2 (1+) @ 245.82 & [b10-NH3] (2+) @ 582.35	245.82	246.16	582.35	582.82	828.17	1073.99	1410.52	1410.52
14	usable	y10 (2+) @ 614.08 & a2 (1+) @ 172.63	614.08	613.85	172.63	173.11	786.71	1400.79	959.34	1400.79
15	usable	y6 (1+) @ 715.45 & c5 (1+) @ 559.34	715.45	715.41	559.34	nan	1274.79	1990.24	1834.13	1274.79
16	non_complementary	y2 (1+) @ 245.79 & b9 (1+) @ 1068.42	245.79	246.16	1068.42	1068.58	1314.21	1560.0	2382.63	1314.21
17	usable	y7 (2+) @ 443.34 & b5 (1+) @ 542.33	443.34	443.26	542.33	542.3	985.67	1429.01	1528.0	1429.01
18	usable	y4 (2+) @ 243.98 & b8 (1+) @ 940.41	243.98	244.15	940.41	940.52	1184.39	1428.37	2124.8	1428.37
19	usable	y1 (1+) @ 174.58 & b11 (2+) @ 626.99	174.58	175.12	626.99	626.85	801.57	976.15	1428.56	1428.56
20	usable	y8 (2+) @ 491.76 & b4 (1+) @ 444.98	491.76	491.79	444.98	445.25	936.74	1428.5	1381.72	1428.5
21	usable	[y6-NH3] (1+) @ 698.39 & b6 (2+) @ 356.64	698.39	698.38	356.64	356.71	1055.03	1753.42	1411.67	1411.67
22	usable	y6 (1+) @ 715.54 & [b6-NH3] (2+) @ 347.56	715.54	715.41	347.56	348.19	1063.1	1778.64	1410.66	1410.66
23	non_complementary	b6 (1+) @ 712.43 & [y2 – H2O] (1+) @ 228.63	712.43	712.41	228.63	228.15	941.06	1653.49	1169.69	1653.49
24	usable	y8 (2+) @ 491.82 & a4 (1+) @ 417.1	491.82	491.79	417.1	417.24	908.92	1400.74	1326.02	1400.74
25	non_complementary	y6 (2+) @ 359.14 & [b5-NH3] (1+) @ 525.62	359.14	358.21	525.62	525.27	884.76	1243.9	1410.38	1410.38
26	usable	y8 (2+) @ 491.96 & [b4 - CH3SH - CO] (1+) @ 369.04	491.96	491.79	369.04	369.25	861.0	1352.96	1230.04	1352.96
27	usable	[y8-NH3] (2+) @ 482.8 & b4 (1+) @ 445.14	482.8	483.27	445.14	445.25	927.94	1410.74	1373.08	1410.74
28	internal_acid	y6 (1+) @ 715.66 & bi5-6 @ 267.85	715.66	715.41	267.85	268.17	983.51	1699.17	1251.36	1251.36
29	internal_acid	y4 (1+) @ 487.09 & [bi4-7 – HCOOH] (1+) @ 468.09	487.09	487.3	468.09	468.23	955.18	1442.27	1423.27	1423.27
30	internal_acid	[bi4-7 – HCOOH] (1+) @ 468.13 & ??? @ 445.09	468.13	468.23	445.09	nan	913.22	1381.35	1358.31	1381.35

31	usable	y5(1+) @ 600.3 & [b7-NH3] (2+) @ 405.11	600.3	600.38	405.11	405.71	1005.41	1605.71	1410.52	1410.52
32	internal_acid	bi5-10 (1+) @ 737.3 & y2 (1+) @ 245.92	737.3	737.42	245.92	246.16	983.22	1720.52	1229.14	1229.14
33	usable	[y10-NH3] (2+) @ 604.93 & b2(1+) @ 200.68	604.93	605.34	200.68	201.12	805.61	1410.54	1006.29	1410.54
34	internal_acid	bi5-9 (1+) @ 624.41 & b4 (1+) @ 444.93	624.41	624.34	444.93	445.25	1069.34	1693.75	1514.27	1514.27
35	usable	y5(1+) @ 600.44 & a5 (1+) @ 514.24	600.44	600.38	514.24	514.29	1114.68	1715.12	1628.92	1628.92
36	usable	y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07	491.95	491.79	427.07	428.22	919.02	1410.97	1346.09	1410.97
37	usable	bi (5-8) (1+) @ 496.41 & y4 (1+) @ 487.01	496.41	496.28	487.01	487.3	983.42	1479.83	1470.43	1470.43
38	usable	[y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56	291.64	292.18	827.56	827.43	1119.2	1410.84	1946.76	1410.84
39	non_complementary	y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61	245.81	246.16	1051.61	1051.55	1297.42	1543.23	2349.03	1543.23
40	usable	bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14	841.49	841.45	487.14	487.3	1328.63	2170.12	1815.77	1328.63
41	unclear	b8(1+) @ 940.89 & ??? @ 195.81	940.89	940.52	195.81	nan	1136.7	2077.59	1332.51	1332.51
42	usable	y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82	300.61	300.69	809.82	810.41	1110.43	1411.04	1920.25	1411.04
43	usable	y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17	243.81	244.15	922.17	923.49	1165.98	1409.79	2088.15	1409.79
44	unclear	b6(1+) @ 712.31 & ??? @ 200.73	712.31	712.41	200.73	nan	913.04	1625.35	1113.77	1625.35
45	unclear	y9 (2+) @ 557.39 & ??? @ 250.74	557.39	557.31	250.74	nan	808.13	1365.52	1058.87	1365.52
46	usable	[y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.11	548.5	548.79	296.11	297.18	844.61	1393.11	1140.72	1393.11
47	usable	b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91	827.88	827.43	241.91	242.15	1069.79	1897.67	1311.7	1311.7
48	usable	y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69	715.27	715.41	335.69	334.19	1050.96	1766.23	1386.65	1386.65
49	usable	[y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.41	234.7	235.64	922.41	923.49	1157.11	1391.81	2079.52	1391.81
50	unclear	y8 (1+) @ 983.52 & ??? @ 216.78	983.52	982.57	216.78	nan	1200.3	2183.82	1417.08	1417.08
51	non_complementary	y8(2+) @ 491.84 & b3(1+) @ 313.96	491.84	491.79	313.96	314.21	805.8	1297.64	1119.76	1297.64
52	non_complementary	[b9-2(H2O)] (1+) @ 516.81 & y2 (1+) @ 245.85	516.81	1032.55	245.85	246.16	762.66	1279.47	1008.51	1279.47
53	unclear	??? @ 755.18 & y6(2+) @ 359.22	755.18	nan	359.22	358.21	1114.4	1869.58	1473.62	1473.62
54	usable	y1 (1+) @ 174.8 & a10 (2+) @ 577.12	174.8	175.12	577.12	577.33	751.92	926.72	1329.04	1329.04
55	usable	y7 (2+) @ 443.31 & [b5-NH3] (1+) @ 524.29	443.31	443.26	524.29	525.27	967.6	1410.91	1491.89	1410.91
56	internal_acid	bi5-9 (1+) @ 624.36 & [b4- H2O] (1+) @ 427.13	624.36	624.34	427.13	427.24	1051.49	1675.85	1478.62	1478.62