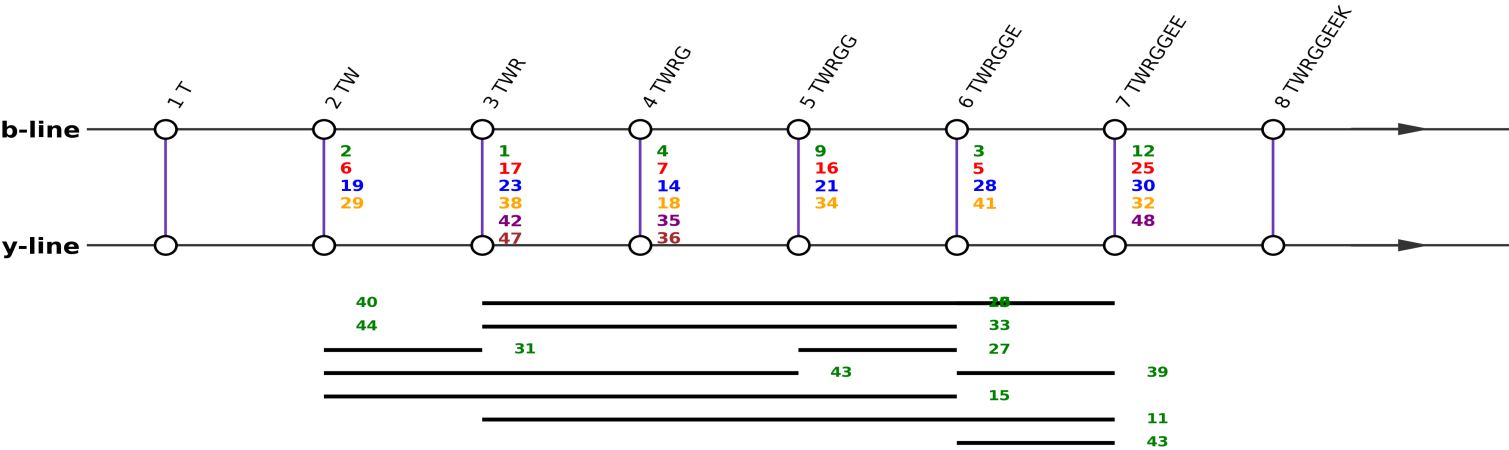


[TWR(Me2)GGEEK+3H]3+

Fragmentation Diagram for: TWRGGEEK



Detailed Data

n	classification	line	mass1	correct_mass1	mass2	correct_mass2	m1+m2	2m1+m2	m1+2m2	chosen_sum
1	usable	y5 (1+) @ 519.33 & b3 (2+) @ 236.46	519.33	519.24	236.46	236.64	755.79	1275.12	992.25	992.25
2	usable	y6 (2+) @ 352.17 & b2 (1+) @ 287.97	352.17	352.19	287.97	288.13	640.14	992.31	928.11	992.31

3	usable	y2 (1+) @ 276.0 & b6 (2+) @ 358.22	276.0	276.16	358.22	358.18	634.22	910.22	992.44	992.44
4	usable	y4 (1+) @ 462.2 & b4 (2+) @ 265.05	462.2	462.22	265.05	265.15	727.25	1189.45	992.3	992.3
5	usable	y2 (1+) @ 275.95 & [b6-NH3] (2+) @ 349.0	275.95	276.16	349.0	349.67	624.95	900.9	973.95	973.95
6	usable	y6 (2+) @ 352.25 & a2 (1+) @ 260.09	352.25	352.19	260.09	260.12	612.34	964.59	872.43	964.59
7	usable	b4 (1+) @ 529.34 & lm(W) @ 158.68	529.34	529.29	158.68	nan	688.02	1217.36	846.7	846.7
8	undefined	379.75 & 197.76	379.75	nan	197.76	nan	577.51	957.26	775.27	957.26
9	usable	[y3-NH3] (1+) @ 387.08 & [b5-NH3] (2+) @ 284.5	387.08	388.17	284.5	285.15	671.58	1058.66	956.08	956.08
10	non_complementary	[y2-NH3] (2+) @ 129.42 & b7 (2+) @ 422.56	129.42	130.07	422.56	422.7	551.98	681.4	974.54	974.54
11	internal_acid	[bi3-7 - HCOOH] (1+) @ 511.25 & lm (W) @ 158.67	511.25	511.26	158.67	nan	669.92	1181.17	828.59	828.59
12	usable	y1(1+) @ 146.68 & [b7-NH3](2+) @ 413.81	146.68	147.11	413.81	414.19	560.49	707.17	974.3	974.3
13	internal_acid	bi3-6 (1+) @ 428.14 & y2 (1+) @ 276.01	428.14	428.23	276.01	276.16	704.15	1132.29	980.16	980.16
14	usable	y4 (1+) @ 462.16 & [b4-NH3] (2+) @ 255.92	462.16	462.22	255.92	256.63	718.08	1180.24	974.0	974.0
15	internal_acid	bi2-6 (1+) @ 614.19 & y2 (1+) @ 276.05	614.19	614.3	276.05	276.16	890.24	1504.43	1166.29	890.24
16	usable	y3 (1+) @ 405.15 & [b5-NH3] (2+) @ 284.45	405.15	405.2	284.45	285.15	689.6	1094.75	974.05	974.05
17	usable	y5 (1+) @ 519.29 & [b3-NH3] (2+) @ 227.3	519.29	519.24	227.3	228.12	746.59	1265.88	973.89	973.89
18	usable	y4 (2+) @ 231.48 & [b4-NH3] (1+) @ 511.28	231.48	231.61	511.28	512.26	742.76	974.24	1254.04	974.24
19	usable	[y6 - CH3NHCH3] (1+) @ 658.39 & lm(W) 158.65	658.39	658.32	nan	nan	nan	nan	nan	nan
20	undefined	519.31 & 343.18	519.31	nan	343.18	nan	862.49	1381.8	1205.67	862.49
21	usable	[y3-NH3] (1+) @ 387.17 & b5 (2+) @ 293.58	387.17	388.17	293.58	293.66	680.75	1067.92	974.33	974.33
22	undefined	583.42 & 243.89	583.42	nan	243.89	nan	827.31	1410.73	1071.2	1071.2
23	usable	y5 (1+) @ 519.34 & [b3-H2O-NH3] (2+) @ 218.59	519.34	519.24	218.59	219.12	737.93	1257.27	956.52	956.52
24	undefined	360.8 & 257.89	360.8	nan	257.89	nan	618.69	979.49	876.58	979.49
25	usable	y1 (1+) @ 146.68 & b7 (2+) @ 422.86	146.68	147.11	422.86	422.7	569.54	716.22	992.4	992.4
26	non_complementary	[y2-NH3] (2+) @ 129.33 & [b7-NH3] (2+) @ 413.55	129.33	130.07	413.55	414.19	542.88	672.21	956.43	956.43
27	internal_acid	[b4-NH3] (1+) @ 511.38 & bi5-6 (1+) @ 186.59	511.38	512.26	186.59	187.07	697.97	1209.35	884.56	884.56
28	usable	[y2-NH3] (2+) @ 129.46 & a6(2+) @ 342.91	129.46	130.07	342.91	344.17	472.37	601.83	815.28	815.28
29	usable	y6(2+) @ 353.02 & [b2-H2O] (1+) @ 268.68	353.02	352.19	268.68	270.12	621.7	974.72	890.38	974.72
30	usable	y6 (2+) @ 352.16 & [y1-H2O] (1+) @ 117.43	352.16	352.19	117.43	129.1	469.59	821.75	587.02	821.75

31	internal_acid	bi2-3 (1+) @ 370.7 & ??? @ 197.72	370.7	371.22	197.72	nan	568.42	939.12	766.14	939.12
32	usable	[b7+H2O] (2+) @ 431.82 & y1-H2O (1+) 128.45	431.82	431.71	nan	nan	nan	nan	nan	nan
33	internal_acid	bi3-6 (1+) @ 428.11 & b2 (1+) @ 287.75	428.11	428.23	287.75	288.13	715.86	1143.97	1003.61	1003.61
34	usable	y3 (1+) @ 405.0 & b5 (2+) @ 293.55	405.0	405.2	293.55	293.66	698.55	1103.55	992.1	992.1
35	usable	y4 (1+) @ 462.22 & [a4-NH3] (2+) @ 242.05	462.22	462.22	242.05	242.63	704.27	1166.49	946.32	946.32
36	usable	y4 (2+) @ 230.81 & [a4-NH3] (1+) @ 485.42	230.81	231.61	485.42	484.25	716.23	947.04	1201.65	947.04
37	unclear	y7-H2O (2+) 436.23 & ??? @ 118.35	nan	nan	118.35	nan	nan	nan	nan	nan
38	usable	y5 (1+) @ 519.35 & [b3 - CH3NHCH3 - H2O] (2+) @ 205.31	519.35	519.24	205.31	205.1	724.66	1244.01	929.97	929.97
39	non_complementary	y1 (1+) @ 147.54 & b6 (1+) @ 715.4	147.54	147.11	715.4	715.35	862.94	1010.48	1578.34	1010.48
40	internal_acid	[y6 - CH3-NH-CH3] (1+) @ 658.42 & bi2-2 (1+) @ 186.66	658.42	658.32	186.66	187.09	845.08	1503.5	1031.74	1031.74
41	usable	[b6 - H3C-N=CH2 - NH3] (1+) @ 654.37 & y2 (1+) @ y2 (1+) 275.92	654.37	655.28	nan	nan	nan	nan	nan	nan
42	usable	y5 (1+) @ 519.11 & a2 (2+) @ 129.47	519.11	519.24	129.47	130.57	648.58	1167.69	778.05	1167.69
43	usable	bi 2-5 (1+) @ 485.29 & [bi 6-7 - HCOOH] (1+) @ 212.85	485.29	485.26	212.85	213.09	698.14	1183.43	910.99	910.99
44	internal_acid	y6 (2+) @ 352.4 & bi2-2 (1+) @ 186.67	352.4	352.19	186.67	187.09	539.07	891.47	725.74	891.47
45	unclear	y5 (1+) @ 519.0 & ??? @ 177.74	519.0	519.24	177.74	nan	696.74	1215.74	874.48	874.48
46	undefined	697.71 & 101.31	697.71	nan	101.31	nan	799.02	1496.73	900.33	900.33
47	usable	y5 (2+) @ 259.95 & b3 (1+) @ 472.14	259.95	260.12	472.14	472.27	732.09	992.04	1204.23	992.04
48	usable	y1 (1+) @ 146.75 & a5 (1+) @ 557.2	146.75	147.11	557.2	558.3	703.95	850.7	1261.15	850.7
49	undefined	404.6 & 146.46	404.6	nan	146.46	nan	551.06	955.66	697.52	955.66
50	undefined	352.05 & 131.78	352.05	nan	131.78	nan	483.83	835.88	615.61	835.88