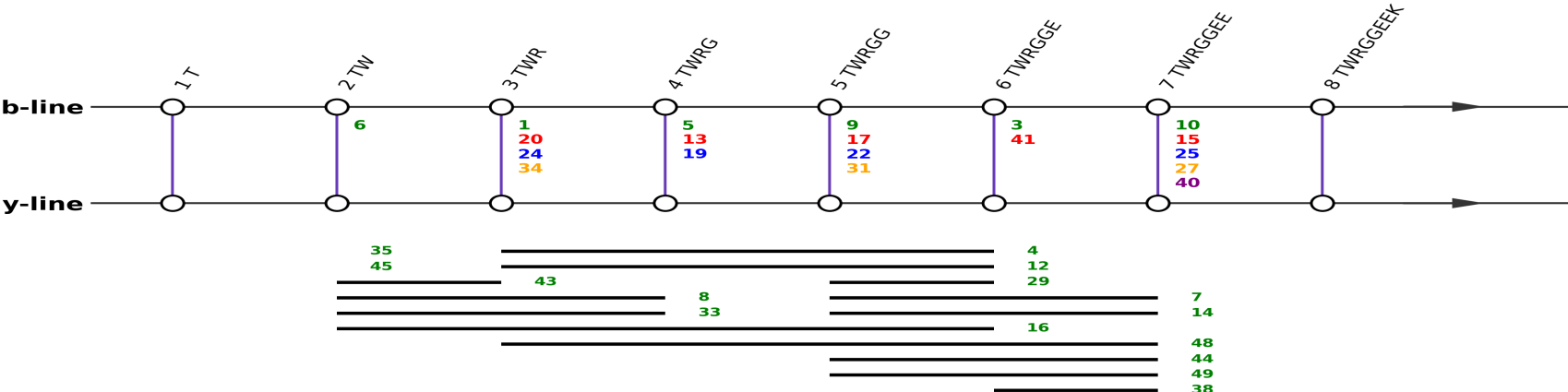
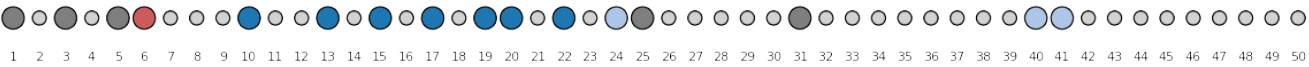


ME17_3+: [TWR(Me2)GGEEK+3H]3+

Fragmentation Diagram for: TWRGGEEK



	b1y7	b2y6	b3y5	b4y4	b5y3	b6y2	b7y1	Row_Count	Unexplained Count	Abs Average Mass Difference	Unexplained Pairs
Parent	--	--	(b3,y5) (2+ , 1+) (-0.18, 0.09) 1	(b4,y4) (2+ , 1+) (-0.1, -0.02) 5	(b5,y3) (2+ , 1+) (-0.17, -0.22) 31	(b6,y2) (2+ , 1+) (-0.16, 0.04) 3	(b7,y1) (2+ , 1+) (-0.43, 0.11) 25	5	1	0.3	-0.43(28)
(NH3)	--	--	--	--	--	--	--	0	0	0.0	
(H2O)	--	--	((H2O),y5) (2+ , 1+) (-0.24, 0.05) 20	((H2O),y4) (1+ , 2+) (-0.17, 0.17) 19	(b5,(H2O)) (2+ , 1+) (-0.17, -0.02) 22	--	((H2O),y1) (2+ , 1+) (-0.43, 0.11) 15	4	0	0.32	
(NH3)-(H2O)	--	--	--	--	--	--	--	0	0	0.0	
a	--	(a2,y6) (1+ , 2+) (-0.03, 0.06) 6	--	--	--	--	--	1	0	0.09	
2(H2O)	--	--	(2(H2O),y5) (2+ , 1+) (0.2, 0.1) 24	--	--	(2(H2O),y2) (2+ , 1+) (-0.09, 0.17) 41	(2(H2O),y1) (2+ , 1+) (-0.64, -0.07) 40	3	0	0.42	
2(NH3)	--	--	--	--	--	--	--	0	0	0.0	
Col_Count	0	1	3	2	2	2	3	13	1	0.16	nan
Ion Mass	(102.05, 889.45)	(288.13, 703.37)	(472.27, 519.24)	(529.29, 462.22)	(586.31, 405.2)	(715.35, 276.16)	(844.39, 147.11)	0	0	0.0	0



Not Highlighted (H2O) (H2O)-(NH3) (NH3) (NH3)-(H2O) 2(H2O) 2(NH3) CH3-NH2 Parent a

Table ME17_3+

n	classification	ion1	loss1	mass1	correct_mass1	mass_difference1	ion2	loss2	mass2	correct_mass2	mass_difference2	chosen_sum
1	usable	b3	nan	236.46	236.64	-0.18	y5	nan	519.33	519.24	0.09	992.25
2	internal_acid	b2	nan	287.97	288.13	-0.16	ai(3-6)	(NH3)-(CH3NH2)	352.17	351.14	1.03	992.31
3	usable	y2	nan	276.0	276.16	-0.16	b6	nan	358.22	358.18	0.04	992.44
4	internal_acid	y2	nan	275.96	276.16	-0.2	bi(3-6)	2(NH3)-(CH3NHCH3)	349.12	348.11	1.01	974.2
5	usable	b4	nan	265.05	265.15	-0.1	y4	nan	462.2	462.22	-0.02	992.3
6	usable	a2	nan	260.09	260.12	-0.03	y6	nan	352.25	352.19	0.06	964.59
7	internal_acid	bi(5-7)	nan	158.68	158.06	0.62	b4	nan	529.34	529.29	0.05	846.7
8	internal_acid	bi(2-4)	2(NH3)	197.76	197.09	0.67	y4	2(H2O)-(HCOOH)	379.75	380.19	-0.44	957.26
9	usable	b5	(H2O)	284.5	284.65	-0.15	y3	(H2O)	387.08	387.19	-0.11	956.08
10	usable	y1	(H2O)	129.42	129.1	0.32	b7	nan	422.56	422.7	-0.14	974.54
11	unclear	???	nan	343.97	nan	nan	???	nan	351.1	nan	nan	1039.04
12	internal_acid	y2	nan	276.01	276.16	-0.15	bi(3-6)	nan	428.14	427.22	0.92	980.16
13	usable	b4	(H2O)	256.0	256.14	-0.14	y4	nan	462.15	462.22	-0.07	974.15
14	internal_acid	bi(5-7)	nan	158.67	158.06	0.61	b4	(H2O)	511.25	511.28	-0.03	828.59
15	usable	y1	nan	146.68	147.11	-0.43	b7	(H2O)	413.81	413.7	0.11	974.3
16	internal_acid	y2	nan	276.05	276.16	-0.11	bi(2-6)	nan	614.19	613.3	0.89	890.24
17	usable	b5	(H2O)	284.45	284.65	-0.2	y3	nan	405.15	405.2	-0.05	974.05
18	internal_acid	ai(2-3)	nan	343.18	342.2	0.98	y5	nan	519.31	519.24	0.07	862.49
19	usable	y4	nan	231.44	231.61	-0.17	b4	(H2O)	511.45	511.28	0.17	974.33
20	usable	b3	(H2O)	227.39	227.63	-0.24	y5	nan	519.29	519.24	0.05	974.07
21	internal_acid	ai(2-2)	nan	158.65	158.07	0.58	y6	(CH3NHCH3)	658.39	658.32	0.07	975.69
22	usable	b5	nan	293.55	293.66	-0.11	y3	(H2O)	387.17	387.19	-0.02	974.27
23	unclear	???	nan	258.02	nan	nan	???	nan	360.25	nan	nan	978.52
24	usable	b3	2(H2O)	218.83	218.63	0.2	y5	nan	519.34	519.24	0.1	957.0
25	usable	y1	nan	146.68	147.11	-0.43	b7	nan	422.81	422.7	0.11	992.3

26	unclear	???	nan	243.89	nan	nan	???	nan	583.42	nan	nan	1071.2
27	usable	y1	(H2O)	129.36	129.1	0.26	b7	(H2O)	413.81	413.7	0.11	956.98
28	unclear	???	nan	128.46	nan	nan	???	nan	431.81	nan	nan	992.08
29	internal_acid	bi(5-6)	nan	186.59	186.06	0.53	b4	(H2O)	511.38	511.28	0.1	884.56
30	internal_acid	ai(2-5)	(H2O)-(CH3NHCH3)	197.72	197.09	0.63	y3	2(NH3)	370.81	371.14	-0.33	939.34
31	usable	b5	nan	293.49	293.66	-0.17	y3	nan	404.98	405.2	-0.22	991.96
32	unclear	???	nan	117.43	nan	nan	???	nan	352.16	nan	nan	821.75
33	non_complementary	b2	nan	287.75	288.13	-0.38	y4	2(NH3)	428.11	428.17	-0.06	1003.61
34	usable	a3	2(NH3)	205.31	205.61	-0.3	y5	nan	519.35	519.24	0.11	929.97
35	internal_acid	bi(2-2)	nan	186.66	186.08	0.58	y6	(CH3NHCH3)	658.42	658.32	0.1	1031.74
36	unclear	???	nan	275.92	nan	nan	???	nan	654.37	nan	nan	930.29
37	non_complementary	a2	(H2O)	242.05	242.11	-0.06	y4	nan	462.22	462.22	0.0	946.32
38	non_complementary	y1	nan	147.54	147.11	0.43	b6	nan	715.4	715.35	0.05	1010.48
39	rare_mode	a2	(HCOH)	230.81	230.11	0.7	y5	2(NH3)	485.42	485.19	0.23	947.04
40	usable	y1	nan	146.47	147.11	-0.64	b7	2(H2O)	404.62	404.69	-0.07	955.71
41	usable	y2	nan	276.07	276.16	-0.09	b6	2(H2O)	340.34	340.17	0.17	956.75
42	rare_mode	b3	(H2O)-(HCOH)	212.85	212.63	0.22	y5	2(NH3)	485.29	485.19	0.1	910.99
43	internal_acid	bi(2-3)	(NH3)	177.74	177.1	0.64	y5	nan	519.0	519.24	-0.24	874.48
44	internal_acid	bi(5-7)	2(NH3)-(HCOOH)	118.33	118.03	0.3	a4	2(NH3)-(HCOH)	436.7	437.21	-0.51	991.73
45	internal_acid	bi(2-2)	nan	186.67	186.08	0.59	y6	nan	352.4	352.19	0.21	891.47
46	rare_mode	b2	(HCOH)	129.47	129.57	-0.1	y5	nan	519.11	519.24	-0.13	1167.69
47	rare_mode	y1	(H2O)	129.46	129.1	0.36	b6	(CH3NH2)	342.89	342.66	0.23	815.24
48	internal_acid	y1	nan	146.75	147.11	-0.36	bi(3-7)	nan	557.2	556.26	0.94	850.7
49	internal_acid	bi(5-7)	nan	158.49	158.06	0.43	b4	2(H2O)	493.18	493.27	-0.09	1144.85
50	rare_mode	a2	nan	259.95	260.12	-0.17	y5	(NH3)-(HCOH)	472.14	472.2	-0.06	992.04