

Operator: mw
Date/time: 2016-06-05/11:13:04am
Title/Comment: Single-Report simple

Data set: C:\massmap\web_site\reports\pepmap\final_evaluations\MAB_Demo1_t2_t1.mmp
Memo:

lis-File: C:\massmap\web_site\reports\pepmap\lis_etc\MAB_Demo_2_mod_cleaned.lis

Statistics of Relative Mass Deviations

Number m/z>400 amu: 231
Mean [ppm]: -4.97
Standard deviation [ppm]: 2.19

Sum of Intensities

Sum all signals [a.u.]: 1.30E+11
Sum reference signals [a.u.]: no reference signals selected

No Printout of Details of Identified Signals

Date	Date	Date	Date
.....
Name1	Name2	Name3	Name4
Responsibility1	Responsibility2	Responsibility3	Responsibility4

(MAB_Demo1_t2_t1, MAB_Demo_2_mod_cleaned)

Identified molecules, part 1 (order corresponding to res_summary-file)

S=U: user assessment only, S=A: including fully autom. assessment, S=N: partially w/o assessment;

#	S	Name of Molecule	Retention Time [min]	RRT	mi-Mass [amu]	Deviation [ppm]	Corr. Intensity [amu]	Abundance [%] (All Signals)
1	A	HC01	20.63	-	1796.9632	-1.44	-	6.7461E+09
2	A	HC01	21.51	-	1796.9632	2.55	-	1.5687E+07
3	A	HC02	44.53	-	2323.9918	2.55	-	5.0834E+08
4	A	HC03	3.45	-	601.3071	1.46	-	3.8089E+07
5	A	HC03_pyE	3.42	-	584.2806	2.34	-	1.5374E+07
6	A	HC05	32.07	-	2350.1005	0.50	-	5.3491E+07
7	A	HC05	32.38	-	2350.1005	0.13	-	6.2998E+06
8	A	HC05	33.12	-	2350.1005	1.39	-	4.0612E+09
9	A	HC05	34.67	-	2350.1005	3.62	-	2.9525E+07
10	A	HC07	16.92	-	622.3439	-2.02	-	6.5421E+08
11	A	HC08	3.20	-	446.2125	-3.72	-	1.8611E+07
12	A	HC09	26.51	-	1309.6700	-0.59	-	1.133E+07
13	A	HC09	27.45	-	1309.6700	-2.95	-	2.4756E+09
14	A	HC09_ox	22.07	-	1325.6649	-0.21	-	2.0286E+07
15	A	HC09_deamid	28.81	-	1310.6540	-0.31	-	1.3536E+08
16	A	HC09_deamid	29.78	-	1310.6540	-0.53	-	6.5109E+08
17	A	HC10	19.80	-	1366.5170	-2.98	-	1.8646E+09
18	U	HC10_ox	16.50	-	1382.5119	-2.38	-	2.8344E+07
19	A	HC12	29.94	-	2690.1595	1.22	-	3.1076E+09
20	A	HC12_ox	26.03	-	2706.1544	1.37	-	2.4058E+07
22	A	HC13	38.38	-	2860.4351	1.15	-	3.2007E+09
23	A	HC13_ox	34.23	-	2876.4300	0.22	-	1.0492E+08
24	A	HC13_deamid	38.05	-	2861.4191	1.32	-	5.5825E+08
25	A	HC13_deamid	39.66	-	2861.4191	1.94	-	3.6165E+08
26	A	HC13_ox_deamid	35.19	-	2877.4140	1.42	-	8.2688E+06
27	A	HC14	48.34	-	6556.1221	0.95	-	5.6303E+06
28	A	HC15	3.42	-	360.2009	-1.34	-	1.4916E+07
29	A	HC17	3.45	-	483.3169	-1.04	-	2.4796E+08
30	A	HC18	38.20	-	2925.3309	-1.47	-	2.4584E+09
31	A	HC18	38.66	-	2925.3309	-1.41	-	5.2823E+09
32	A	HC18	39.43	-	2925.3309	-0.83	-	4.1822E+09
33	A	HC18	39.83	-	2925.3309	-1.21	-	4.8222E+07
34	A	HC19	29.34	-	1099.6489	-1.77	-	4.5569E+09
35	A	HC20	23.83	-	1119.5846	-0.97	-	3.9153E+09
36	A	HC21	35.65	-	2844.2991	1.08	-	6.3589E+06
37	A	HC21	41.70	-	2844.2991	-1.13	-	5.8718E+09
38	U	HC21	53.02	-	2844.2991	1.30	-	1.574E+07
39	A	HC22	20.03	-	1156.5149	-0.53	-	4.7344E+06
40	A	HC22_A2G0	18.53	-	2454.9912	2.11	-	5.019E+07
41	A	HC22_A2G0-GlcNAc	18.65	-	2251.9118	0.92	-	3.7197E+07
42	A	HC22_A2G1	27.40	-	2617.0441	-4.54	-	5.2058E+06
43	A	HC22_A2G1-GlcNAc	18.59	-	2413.9647	2.55	-	1.7627E+07
44	A	HC22_A2G2S1	18.90	-	3070.1925	0.58	-	3.6529E+07
45	A	HC22_A2FG0	18.21	-	2601.0492	1.58	-	6.3892E+08
46	A	HC22_A2FG0-GlcNAc	18.37	-	2397.9698	2.33	-	2.9912E+07
47	A	HC22_A2FG1	18.05	-	2763.1021	1.03	-	3.9288E+08
48	A	HC22_A2FG1-GlcNAc	18.31	-	2560.0227	1.73	-	1.1076E+07
49	A	HC22_A2FG2	17.94	-	2925.1550	0.56	-	4.6677E+07
50	A	HC22_Man5	18.43	-	2372.9382	2.59	-	3.6757E+07
51	A	HC23	32.15	-	1852.9142	-3.08	-	5.6887E+09
52	A	HC23_ox	26.56	-	1868.9091	-5.13	-	2.3832E+08
53	A	HC23_deamid	32.30	-	1853.8982	1.10	-	3.0366E+09
54	A	HC23_deamid	32.87	-	1853.8982	-0.65	-	6.9572E+08
55	A	HC23_deamid	33.33	-	1853.8982	-1.15	-	1.2816E+09
56	A	HC23_ox_deamid	26.97	-	1869.8931	0.01	-	2.2303E+07
57	A	HC23_ox_deamid	27.45	-	1869.8931	0.31	-	2.8241E+07
58	A	HC24	3.42	-	422.2165	-0.95	-	8.2434E+07
59	A	HC26	22.82	-	1242.6608	-3.60	-	3.7552E+09
60	A	HC26_deamid	23.33	-	1243.6449	-1.34	-	3.617E+08
61	A	HC27	3.42	-	447.2693	-0.72	-	9.7638E+07
62	A	HC29	3.45	-	456.2809	-1.18	-	5.4229E+07
63	A	HC30	21.46	-	1209.6758	-2.71	-	1.4392E+09
64	U	HC31	3.42	-	605.2843	0.50	-	6.0536E+07
65	A	HC33	51.18	-	3618.6323	1.25	-	3.3833E+07
66	A	HC33_deamid	51.45	-	3619.6163	3.62	-	1.0881E+07
67	A	HC34	26.84	-	1964.8826	-0.42	-	2.7692E+09
68	A	HC34_ox	24.31	-	1980.8775	0.71	-	9.0154E+07
69	A	HC34_deamid	27.73	-	1965.8666	1.46	-	3.6748E+07
70	A	HC34_deamid	28.37	-	1965.8666	1.57	-	5.6286E+07
71	A	HC35	3.49	-	600.3595	0.36	-	3.009E+08

(MAB_Demo1_t2_t1, MAB_Demo_2_mod_cleaned)

Identified molecules, part 2 (order corresponding to res_summary-file)

S=U: user assessment only, S=A: including fully autom. assessment, S=N: partially w/o assessment;

#	S	Name of Molecule	Retention Time [min]	RRT	mi-Mass [amu]	Deviation [ppm]	Corr. Intensity [amu]	Abundance [%] (All Signals)
73	A	HC36	24.58	-	2905.2838	-0.87	-	9.9084E+09
74	A	HC36_deamid	24.26	-	2906.2678	-0.43	-	7.9072E+07
75	A	HC36_deamid	25.17	-	2906.2678	0.59	-	3.964E+08
76	A	HC36_deamid	25.32	-	2906.2678	-0.54	-	8.7041E+08
77	A	HC36_deamid	26.08	-	2906.2678	0.03	-	3.6495E+07
78	A	HC37	3.42	-	811.4188	0.79	-	2.9509E+07
79	A	HC04-05	29.71	-	2506.2016	0.52	-	1.6336E+07
80	A	HC04-05	30.45	-	2506.2016	0.77	-	1.0254E+09
81	A	HC07-08_deamid	22.22	-	1051.5298	0.16	-	6.6159E+06
82	A	HC08-09_deamid	26.32	-	1738.8560	0.00	-	1.6463E+07
83	A	HC15-16	3.42	-	488.2958	-0.70	-	3.8392E+07
84	A	HC20-21	44.12	-	3945.8731	1.26	-	1.7646E+08
85	U	HC25-26	22.66	-	1559.7766	-0.64	-	1.064E+07
86	U	HC25-26_deamid	23.24	-	1560.7606	-0.42	-	1.2718E+07
87	U	HC25-26_deamid	23.79	-	1560.7606	0.48	-	3.7741E+05
88	A	HC30-31	20.63	-	1796.9495	5.77	-	6.4787E+09
89	U	HC30-31	21.51	-	1796.9495	9.27	-	4.7589E+06
90	A	HC32-33	48.84	-	3861.7542	-0.18	-	3.0554E+07
91	A	HC32-33_deamid	49.14	-	3862.7382	0.63	-	1.2465E+07
92	U	HC34-35	31.69	-	2547.2315	-9.76	-	2.0651E+07
93	A	HC34-35	31.90	-	2547.2315	-9.55	-	3.9104E+07
94	A	LC01	31.78	-	2503.2476	0.90	-	3.3907E+09
95	A	LC01	32.68	-	2503.2476	0.38	-	5.3066E+07
96	A	LC02	22.41	-	1802.8700	-1.23	-	6.2371E+09
97	A	LC02_deamid	22.07	-	1803.8540	0.00	-	5.9503E+08
98	U	LC02_deamid	22.94	-	1803.8540	0.32	-	1.526E+07
99	U	LC02_deamid	22.90	-	1803.8540	1.70	-	2.003E+07
100	A	LC02_deamid	23.19	-	1803.8540	0.10	-	1.6437E+08
101	A	LC02_deamid	23.42	-	1803.8540	0.20	-	2.8048E+08
102	A	LC02_deamid	24.00	-	1803.8540	-1.42	-	1.5288E+07
103	A	LC03	2.02	-	711.3300	-2.78	-	5.0594E+06
104	A	LC03	3.45	-	711.3300	-1.13	-	1.1297E+08
105	A	LC04	18.17	-	485.3577	-3.61	-	1.5411E+09
106	A	LC05	19.29	-	1264.6412	-3.29	-	3.6249E+09
107	A	LC05	22.82	-	1264.6412	-3.39	-	2.5095E+08
108	A	LC07	10.56	-	501.3162	-3.33	-	6.7457E+07
109	A	LC07	10.77	-	501.3162	-3.29	-	8.8255E+07
110	A	LC07	11.05	-	501.3162	-3.30	-	5.9751E+07
111	A	LC07	11.25	-	501.3162	-3.41	-	5.7542E+07
112	A	LC07	11.81	-	501.3162	-3.01	-	2.1198E+08
113	A	LC09	48.50	-	3571.7181	0.96	-	5.495E+08
114	A	LC09_deamid	44.68	-	3572.7021	1.86	-	3.9301E+07
115	A	LC09_deamid	46.09	-	3572.7021	1.91	-	5.6602E+06
116	A	LC10	4.13	-	587.3279	-2.35	-	1.2024E+09
117	A	LC12	3.42	-	675.3188	0.47	-	7.2256E+07
118	A	LC13	23.01	-	1590.7274	-0.85	-	9.5435E+08
119	A	LC13	25.76	-	1590.7274	-0.32	-	1.4955E+07
120	A	LC13	26.08	-	1590.7274	-0.31	-	1.2177E+08
121	A	LC13	26.32	-	1590.7274	-0.08	-	6.084E+07
122	A	LC13_deamid	21.99	-	1591.7114	1.19	-	6.4632E+07
123	A	LC13_deamid	23.60	-	1591.7114	0.53	-	3.9571E+08
124	A	LC13_deamid	23.87	-	1591.7114	0.29	-	1.1165E+09
125	A	LC13_deamid	26.60	-	1591.7114	0.78	-	5.0318E+07
126	A	LC13_deamid	27.06	-	1591.7114	1.10	-	2.7731E+07
127	A	LC13_pyE	25.76	-	1573.7009	-0.66	-	4.5061E+07
128	U	LC13_pyE	26.03	-	1573.7009	-0.28	-	4.9961E+08
129	A	LC13_pyE	26.32	-	1573.7009	-0.10	-	1.2596E+08
130	A	LC13_deamid_pyE	24.00	-	1574.6849	3.42	-	2.3018E+07
131	A	LC13_deamid_pyE	24.44	-	1574.6849	1.04	-	6.6262E+06
132	A	LC13_deamid_pyE	26.60	-	1574.6849	0.93	-	1.8028E+08
133	A	LC13_deamid_pyE	27.11	-	1574.6849	0.68	-	6.1865E+07
134	A	LC14	24.54	-	1533.7232	2.32	-	7.8642E+06
135	A	LC14	25.28	-	1533.7232	-0.74	-	3.9306E+09
136	A	LC14	26.32	-	1533.7232	2.00	-	9.6006E+07
137	A	LC14	35.26	-	1533.7232	-8.27	-	1.3612E+07
138	U	LC14	52.73	-	1533.7232	-0.05	-	1.5189E+07
139	U	LC14	53.58	-	1533.7232	0.39	-	9.7119E+06
140	A	LC14_ox	21.32	-	1549.7182	0.01	-	5.4844E+07
141	A	LC15	3.42	-	710.2871	0.78	-	6.1001E+07
142	A	LC16	3.42	-	1347.5514	-0.56	-	1.6317E+08

(MAB_Demo1_t2_t1, MAB_Demo_2_mod_cleaned)

Identified molecules, part 3 (order corresponding to res_summary-file)

S=U: user assessment only, S=A: including fully autom. assessment, S=N: partially w/o assessment;

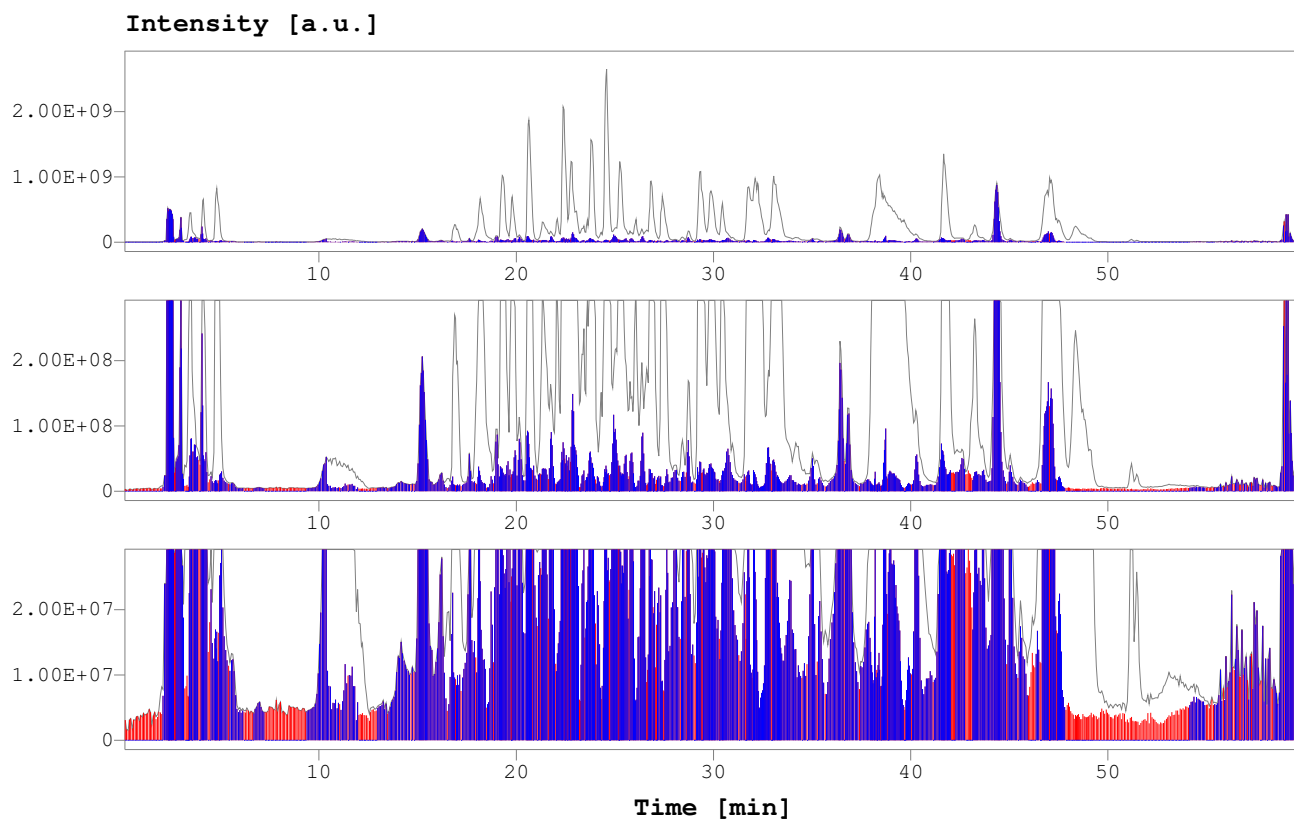
#	S	Name of Molecule	Retention Time [min]	RRT	mi-Mass [amu]	Deviation [ppm]	Corr. Intensity [amu]	Abundance [%] [a.u.] (All Signals)
143	A	LC17	4.82	-	831.4702	-2.81	-	2.6023E+09 1.992
144	A	LC18	3.45	-	522.2550	-1.18	-	9.0935E+07 0.070
145	U	LC19	3.42	-	422.1107	-2.48	-	1.0667E+07 0.008
146	U	LC03-04	33.08	-	1178.6772	2.91	-	1.6371E+06 0.001
147	U	LC07-08	4.09	-	657.4174	-1.77	-	4.8041E+05 0.000
148	A	LC08-09	46.97	-	3727.8192	1.79	-	6.5364E+09 5.002
149	A	LC08-09	47.44	-	3727.8192	1.43	-	1.9718E+09 1.509
150	A	LC08-09_deamid	43.24	-	3728.8032	1.66	-	5.3578E+08 0.410
151	A	LC08-09_deamid	44.53	-	3728.8032	2.25	-	1.2248E+08 0.094
152	A	LC13-14_deamid	26.03	-	3107.4241	0.10	-	1.0419E+07 0.008
153	A	LC13-14_pyE	25.25	-	3089.4135	5.44	-	5.928E+07 0.045

Molecules not identified, part 1 (order corresponding to res_summary-file)

No obligatory molecules defined

#	Name of Molecule	#	Name of Molecule	#	Name of Molecule
21	HC12_deamid	72	HC35_deamid		

Grey: Chromatogram of original data set
Red: Chromatogram of difference data set
Blue: Peaks of difference data set with at least .1% of maximum peak area of original data set
Time range for evaluation of peak intensities: .17 min - 59.84 min
Memo original data set: Parameter for suppression of low-intensity signals: 2
Memo difference data set: Parameter for suppression of low-intensity signals: 2



Grey: Chromatogram of original data set
Red: Chromatogram of difference data set
Blue: Peaks of difference data set with at least .1% of maximum peak area of original data set
Time range for evaluation of peak intensities: .17 min - 59.84 min
Memo original data set: Orbitrap analyzer, resolution at 1000 amu: 55000, exponent: -.5
Memo difference data set: Orbitrap analyzer, resolution at 1000 amu: 55000, exponent: -.5

