

Operator: mw
 Date/time: 2016-06-05/11:53:25am
 Title/Comment: Pair Comparison w/ Residual Signals 1

lis-File: C:\massmap\web_site\reports\pepmap\lis_etc\MAB_Demo_in_silico_plus_extra1.lis

Data Sets

X: R=Reference, C=Data set to be compared

```
# X Path
1 R C:\massmap\web_site\reports\pepmap\final_evaluations\MAB_Demo1_t2_t1.mmp
2 C C:\massmap\web_site\reports\pepmap\final_evaluations\MAB_Demo2_t2_t1.mmp
```

Statistics of Relative Mass Deviations

# Data Set	Number m/z>400 amu	Mean [ppm]	StDev [ppm]
1	755	-5.16	2.35
2	638	-5.09	2.37

Intensity Sums Including Overlap Corrections if Available

# Data Set	All Signals [a.u.]	Reference Signals [a.u.]
1	1.49E+11	n.a.
2	1.46E+11	n.a.

Reference Signal Relative Retention Times

Lacking, no calculation of relative retention times

Ion Current Chromatograms to be Printed and Ion Current Chromatograms Available

BPK: Base peak chromatogram, ori: original data set, diff: difference data set, -- : lacking

# Data Set	BIC-t1/ori	BIC-t1/diff	BIC/ori	BIC/diff	BPK/ori	BPK/diff
1	n.a.	n.a.	OK	OK	OK	OK
2	n.a.	n.a.	OK	OK	OK	OK

Ion Current Chromatograms of Data Sets, Peak Lists to be Printed and Available

No printout of peak lists

Comparison Report pepmap, Comparison of Pair of Data Sets

(MAB_Demo1_t2_t1 vs. MAB_Demo2_t2_t1, MAB_Demo_in_silico_plus_extra1)

Limit for highlighted rel. intensity differences [%]: 20
 Minmum relative intensity of compared signals [%]: 0
 Mean +/- StDev of retention time differences [min]: 0.006 +/- 0.034

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
1	HC01	20.63	4.509	20.65	5.083	0.02	12.7
		21.51	0.010	21.55	0.005	0.04	-49.9
2	HC02	44.53	0.340	44.55	0.329	0.02	-3.1
3	HC03	3.45	0.025	3.46	0.027	0.01	6.9
4	HC03_pyE	3.42	0.010	3.43	0.011	0.01	2.5
5	HC05	32.07	0.036	32.08	0.041	0.01	15.1
		32.38	0.004			n.a.	n.a.
		33.12	2.714	33.12	2.954	0.00	8.8
		34.67	0.020			n.a.	n.a.
6	HC07	16.92	0.437	16.88	0.462	-0.04	5.6
7	HC08	3.20	0.012	3.21	0.013	0.01	7.5
8	HC09	26.51	0.008	26.55	0.007	0.04	-8.5
		27.45	1.655	27.49	1.811	0.04	9.4
9	HC09_ox	22.07	0.014	22.12	0.014	0.05	-0.1
10	HC09_deamid	28.81	0.090	28.79	0.092	-0.02	2.2
		29.78	0.435	29.78	0.451	0.00	3.6
11	HC10	19.80	1.246	19.78	1.356	-0.02	8.8
12	HC10_ox	16.50	0.019	16.52	0.020	0.02	6.9
13	HC12	29.94	2.077	29.94	2.247	0.00	8.2
14	HC12_ox	26.03	0.016	26.02	0.016	-0.01	-2.5
15	HC12_deamid			30.92	0.068	n.a.	n.a.
16	HC13	38.38	2.139	38.37	2.248	-0.01	5.1
17	HC13_ox	34.23	0.070	34.21	0.069	-0.02	-2.0
18	HC13_deamid	38.05	0.373	38.03	0.402	-0.02	7.7
		39.66	0.242	39.64	0.271	-0.02	12.0
19	HC13_ox_deamid	35.19	0.006	35.17	0.005	-0.02	-4.0
20	HC14	48.34	0.004			n.a.	n.a.
21	HC15	3.42	0.010	3.43	0.010	0.01	2.0
22	HC17	3.45	0.166	3.46	0.149	0.01	-10.1
23	HC18	38.20	1.643	38.34	2.548	0.14	55.0

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		Rt/min	RI/%	Rt/min	RI/%		
23	HC18	38.66	3.531	38.61	2.713	-0.05	-23.2
				38.93	3.039	n.a.	n.a.
		39.43	2.795	39.42	1.058	-0.01	-62.1
				39.82	1.734	n.a.	n.a.
		39.83	0.032			n.a.	n.a.
				40.28	0.004	n.a.	n.a.
24	HC19	29.34	3.046	29.38	2.876	0.04	-5.6
25	HC20	23.83	2.617	23.84	2.404	0.01	-8.2
26	HC21	35.65	0.004	35.63	0.004	-0.02	2.9
		41.70	3.925	41.73	4.065	0.03	3.6
				42.45	0.069	n.a.	n.a.
		53.02	0.011	53.10	0.012	0.08	15.4
27	HC22	20.03	0.003	20.06	0.003	0.03	3.4
28	HC22_A2G0	18.53	0.034	18.51	0.028	-0.02	-17.0
29	HC22_A2G0-GlcNAc	18.65	0.025	18.63	0.023	-0.02	-5.8
30	HC22_A2G1	27.40	0.003	27.44	0.004	0.04	17.8
31	HC22_A2G1-GlcNAc	18.59	0.012	18.57	0.011	-0.02	-9.1
32	HC22_A2G2S1	18.90	0.024	18.89	0.023	-0.01	-7.7
33	HC22_A2FG0	18.21	0.427	18.19	0.410	-0.02	-4.0
34	HC22_A2FG0-GlcNAc	18.37	0.020	18.39	0.016	0.02	-17.5
35	HC22_A2FG1	18.05	0.263	18.02	0.249	-0.03	-5.1
36	HC22_A2FG1-GlcNAc	18.31	0.007	18.28	0.006	-0.03	-15.5
37	HC22_A2FG2	17.94	0.031	17.91	0.031	-0.03	-1.7
38	HC22_Man5	18.43	0.025	18.45	0.019	0.02	-21.9
39	HC23	32.15	3.802	32.20	4.071	0.05	7.1
40	HC23_ox	26.56	0.159	26.59	0.162	0.03	1.6
41	HC23_deamid	32.30	2.030			n.a.	n.a.
		32.87	0.465	32.92	0.483	0.05	4.0
		33.33	0.857	33.37	0.929	0.04	8.5
42	HC23_ox_deamid	26.97	0.015	27.00	0.015	0.03	-2.2
		27.45	0.019	27.49	0.021	0.04	11.3
43	HC24	3.42	0.055	3.43	0.052	0.01	-5.1
44	HC26	22.82	2.510	22.79	2.431	-0.03	-3.1

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		Rt/min	RI/%	Rt/min	RI/%		
45	HC26_deamid	23.33	0.242	23.36	0.213	0.03	-12.1
46	HC27	3.42	0.065	3.43	0.063	0.01	-3.1
47	HC29	3.45	0.036	3.43	0.037	-0.02	1.3
48	HC30	21.46	0.962	21.44 21.93	0.743 0.235	-0.02 n.a.	-22.7 n.a.
49	HC31	3.42	0.040	3.43	0.041	0.01	0.3
50	HC33	51.18	0.023	51.19	0.013	0.01	-42.8
51	HC33_deamid	51.45	0.007	51.52	0.006	0.07	-15.5
52	HC34	26.84	1.851	26.88	1.900	0.04	2.6
53	HC34_ox	24.31	0.060	24.33	0.051	0.02	-16.0
54	HC34_deamid	27.73 28.37	0.025 0.038	27.77 28.40	0.026 0.038	0.04 0.03	5.7 -0.2
55	HC35	3.49	0.201	3.50	0.171	0.01	-14.8
56	HC35_deamid			3.68	0.006	n.a.	n.a.
57	HC36	24.58	6.622	24.57	6.467	-0.01	-2.4
58	HC36_deamid	24.26 25.17 25.32 26.08	0.053 0.265 0.582 0.024	24.28 25.19 25.34 26.07	0.014 0.264 0.553 0.029	0.02 0.02 0.02 -0.01	-72.6 -0.3 -4.9 20.7
59	HC37	3.42	0.020	3.43	0.018	0.01	-6.8
60	HC04-05	29.71 30.45	0.011 0.685	29.74 30.47	0.012 0.789	0.03 0.02	11.6 15.1
61	HC07-08_deamid	22.22	0.004			n.a.	n.a.
62	HC08-09_deamid	26.32	0.011	26.35	0.011	0.03	0.2
63	HC15-16	3.42	0.026	3.43	0.027	0.01	3.6
64	HC20-21	44.12	0.118	44.16	0.120	0.04	1.9
65	HC25-26	22.66	0.007	22.67	0.004	0.01	-48.9
66	HC25-26_deamid	23.24 23.79	0.009 0.000	23.27	0.005	0.03 n.a.	-44.6 n.a.
67	HC30-31	20.63 21.51	4.330 0.003	20.65	4.849	0.02 n.a.	12.0 n.a.
68	HC32-33	48.84	0.020	48.84	0.018	0.00	-11.1

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		Rt/min	RI/%	Rt/min	RI/%		
69	HC32-33_deamid	49.14	0.008	49.14	0.008	0.00	-3.7
70	HC34-35	31.69 31.90	0.014 0.026	31.67 31.92	0.014 0.031	-0.02 0.02	1.6 19.9
71	LC01	31.78 32.68	2.266 0.035	31.80	2.355	0.02 n.a.	3.9 n.a.
72	LC02	22.41	4.169	22.42	3.847	0.01	-7.7
73	LC02_deamid	22.07 22.90 22.94 23.19 23.42 24.00	0.398 0.013 0.010 0.110 0.187 0.010	22.07 22.07 23.17 23.47 24.01	0.412 0.412 0.103 0.160 0.009	0.00 n.a. n.a. -0.02 0.05 0.01	3.6 n.a. n.a. -6.1 -14.7 -7.5
74	LC03	2.02 3.45	0.003 0.076	3.43	0.073	n.a. -0.02	n.a. -3.8
75	LC04	18.17	1.030	18.19	0.941	0.02	-8.6
76	LC05	19.29 22.82	2.423 0.168	19.28 22.79	2.249 0.160	-0.01 -0.03	-7.2 -4.5
77	LC07	10.56 10.77 11.05 11.25 11.81	0.045 0.059 0.040 0.038 0.142	10.61 10.61 11.02 11.65	0.093 0.093 0.069 0.172	0.05 n.a. -0.03 n.a. -0.16	105.4 n.a. 73.5 n.a. 21.6
78	LC09	48.50	0.367	48.50	0.374	0.00	1.9
79	LC09_deamid	44.68 46.09	0.026 0.004	44.71 46.06	0.026 0.004	0.03 -0.03	-1.6 -7.1
80	LC10	4.13	0.804	4.14	0.744	0.01	-7.4
81	LC12	3.42	0.048	3.43	0.048	0.01	0.1
82	LC13	23.01 25.76 26.08 26.32	0.638 0.010 0.081 0.041	23.04 23.04 26.07 26.35	0.582 0.582 0.080 0.037	0.03 n.a. -0.01 0.03	-8.8 n.a. -1.9 -8.0
83	LC13_deamid	21.99 23.60 23.87 26.60 27.06	0.043 0.264 0.746 0.034 0.019	22.03 23.64 23.88 26.63 27.10	0.044 0.251 0.690 0.034 0.019	0.04 0.04 0.01 0.03 0.04	1.1 -5.1 -7.5 1.3 -0.0
84	LC13_pyE	25.76 26.03 26.32	0.030 0.334 0.084	25.80 26.07 26.35	0.027 0.326 0.094	0.04 0.04 0.03	-10.4 -2.3 11.9

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		Rt/min	RI/%	Rt/min	RI/%		
85	LC13_deamid_pyE	24.00	0.015	24.01	0.014	0.01	-7.6
		24.44	0.004	24.47	0.004	0.03	0.5
		26.60	0.120	26.63	0.122	0.03	1.6
		27.11	0.041	27.10	0.042	-0.01	1.4
86	LC14	24.54	0.005	24.57	0.007	0.03	39.9
		25.28	2.627	25.30	2.599	0.02	-1.1
		26.32	0.064	26.30	0.069	-0.02	6.9
		35.26	0.009	35.24	0.010	-0.02	5.7
		52.73	0.010			n.a.	n.a.
				53.10	0.016	n.a.	n.a.
		53.58	0.006		n.a.	n.a.	
87	LC14_ox	21.32	0.037	21.30	0.034	-0.02	-6.5
88	LC15	3.42	0.041	3.43	0.041	0.01	-0.7
89	LC16	3.42	0.109	3.43	0.107	0.01	-2.2
90	LC17	4.82	1.739	4.79	1.502	-0.03	-13.7
91	LC18	3.45	0.061	3.43	0.059	-0.02	-3.3
92	LC19	3.42	0.007	3.43	0.008	0.01	12.5
93	LC03-04	33.08	0.001			n.a.	n.a.
94	LC07-08	4.09	0.000			n.a.	n.a.
95	LC08-09	46.97	4.369	47.00	4.524	0.03	3.6
		47.44	1.318			n.a.	n.a.
96	LC08-09_deamid	43.24	0.358	43.23	0.382	-0.01	6.6
		44.53	0.082	44.65	0.089	0.12	8.7
97	LC13-14_deamid	26.03	0.007	26.07	0.006	0.04	-12.5
98	LC13-14_pyE	25.25	0.040	25.27	0.040	0.02	1.1
99	R1_01	59.39	0.003			n.a.	n.a.
100	R1_02	3.45	0.002	3.46	0.002	0.01	-17.9
101	R1_03	2.99	0.017	2.99	0.015	0.00	-11.0
102	R1_04	29.22	0.001			n.a.	n.a.
		29.34	0.000			n.a.	n.a.
		29.56	0.001	29.42	0.002	-0.14	80.4
103	R1_05	22.38	0.001			n.a.	n.a.
		23.05	0.002			n.a.	n.a.
104	R1_06	19.42	0.003	19.41	0.003	-0.01	-10.7
105	R1_07	4.06	0.104	4.06	0.110	0.00	5.8

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		Rt/min	RI/%	Rt/min	RI/%		
106	R1_08	4.06	0.009			n.a.	n.a.
107	R1_09	2.99	0.004			n.a.	n.a.
		3.45	0.000			n.a.	n.a.
108	R1_10	2.36	0.009	2.46	0.025	0.10	181.6
109	R1_11	2.41	0.004			n.a.	n.a.
		2.62	0.005	2.68	0.008	0.06	69.1
110	R1_12	10.37	0.005	10.34	0.005	-0.03	9.6
111	R1_13	3.84	0.016	3.85	0.018	0.01	13.8
112	R1_14	4.09	0.003	4.10	0.003	0.01	4.6
113	R1_15			21.50	0.003	n.a.	n.a.
114	R1_16	4.82	0.001	4.83	0.001	0.01	-8.9
115	R1_17	2.33	0.074			n.a.	n.a.
		2.47	0.212	2.46	0.265	-0.01	25.0
116	R1_18	3.57	0.019	3.50	0.010	-0.07	-47.6
		3.90	0.006	3.85	0.016	-0.05	162.6
		4.16	0.006			n.a.	n.a.
117	R1_19	2.36	0.012	2.36	0.012	0.00	-0.4
		2.50	0.014	2.52	0.012	0.02	-13.3
118	R1_20	2.71	0.008			n.a.	n.a.
		2.90	0.004	2.82	0.013	-0.08	197.9
119	R1_21	2.99	0.002			n.a.	n.a.
120	R1_22	10.30	0.095			n.a.	n.a.
		10.56	0.047	10.61	0.096	0.05	105.4
		10.77	0.061			n.a.	n.a.
		11.05	0.042	11.02	0.085	-0.03	105.8
		11.25	0.040			n.a.	n.a.
		11.46	0.038			n.a.	n.a.
		11.88	0.105	11.72	0.161	-0.16	53.6
121	R1_23	3.62	0.000			n.a.	n.a.
122	R1_24	3.62	0.004	3.63	0.003	0.01	-17.3
123	R1_25	2.99	0.163	2.99	0.145	0.00	-11.5
124	R1_26	26.03	0.000			n.a.	n.a.
125	R1_27	21.77	0.000	21.77	0.000	0.00	3.0
126	R1_28	4.86	0.002	4.83	0.002	-0.03	-17.1

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		Rt/min	RI/%	Rt/min	RI/%		
127	R1_29	4.06	0.002	4.03	0.002	-0.03	-2.0
128	R1_30	4.06	0.040	4.03	0.043	-0.03	6.6
129	R1_31	4.06	0.004	4.03	0.005	-0.03	9.9
130	R1_32	4.06	0.028	4.06	0.030	0.00	7.8
131	R1_33	23.91	0.005	23.92	0.005	0.01	3.2
132	R1_34	16.21	0.005	16.16	0.005	-0.05	-0.7
133	R1_35	4.06	0.007	4.03	0.008	-0.03	3.3
134	R1_36	4.13	0.001	4.10	0.001	-0.03	29.2
137	R1_39			2.36	0.036	n.a.	n.a.
		2.45	0.078	2.52	0.036	0.07	-53.3
138	R1_40	15.23	0.033	15.23	0.027	0.00	-18.5
140	R1_42	4.16	0.002			n.a.	n.a.
141	R1_43	15.28	0.003	15.23	0.003	-0.05	-25.6
142	R1_44	3.53	0.004	3.53	0.003	0.00	-26.9
		16.92	0.445	16.88	0.469	-0.04	5.5
143	R1_45	59.39	0.004	59.36	0.006	-0.03	65.5
144	R1_46	2.95	0.007	2.96	0.008	0.01	10.2
145	R1_47	25.56	0.001	25.59	0.001	0.03	2.6
146	R1_48	2.99	0.004	2.99	0.004	0.00	-6.1
147	R1_49	4.74	0.003	4.72	0.003	-0.02	-1.8
				19.32	0.002	n.a.	n.a.
148	R1_50	3.62	0.271	3.58	0.247	-0.04	-8.9
				4.22	0.018	n.a.	n.a.
		4.82	0.001	4.79	0.001	-0.03	-6.3
150	R1_52	2.99	0.026	2.99	0.025	0.00	-6.8
151	R1_53	4.06	0.011	4.06	0.011	0.00	8.0
152	R1_54	59.33	0.007	59.36	0.010	0.03	41.8
153	R1_55	3.78	0.005	3.79	0.006	0.01	12.9
154	R1_56	16.14	0.015	16.16	0.015	0.02	0.6
155	R1_57	59.29	0.012	59.30	0.014	0.01	11.0

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		Rt/min	RI/%	Rt/min	RI/%		
156	R1_58	25.51	0.005	25.55	0.005	0.04	-7.1
157	R1_59			4.18	0.002	n.a.	n.a.
158	R1_60	4.25	0.001	4.28	0.001	0.03	-4.5
159	R1_61	4.25	0.001	4.28	0.001	0.03	-9.2
160	R1_62	4.25	0.018	4.28	0.017	0.03	-5.3
161	R1_63	59.29	0.015			n.a.	n.a.
162	R1_64	21.77	0.004			n.a.	n.a.
163	R1_65	19.42	0.004			n.a.	n.a.
164	R1_66	19.18 20.74	0.006 0.008	19.17 20.72	0.005 0.010	-0.01 -0.02	-14.9 26.3
165	R1_67	3.72	0.003			n.a.	n.a.
166	R1_68	2.99	0.003			n.a.	n.a.
167	R1_69	3.72	0.001	3.73	0.001	0.01	21.8
169	R1_71	23.60	0.002	23.64	0.001	0.04	-13.1
170	R1_72	19.18	0.004	19.21	0.004	0.03	-6.8
171	R1_73	5.19	0.005	5.23	0.004	0.04	-10.9
172	R1_74	59.23	0.014	59.20	0.015	-0.03	1.1
173	R1_75	22.86	0.014	22.88	0.013	0.02	-5.2
174	R1_76	22.86	0.017	22.88	0.016	0.02	-1.0
175	R1_77	16.71	0.004	16.66	0.004	-0.05	-9.6
176	R1_78	59.23	0.005			n.a.	n.a.
177	R1_79	2.76	0.011	2.77	0.014	0.01	27.0
178	R1_80	25.80	0.012	25.84	0.012	0.04	0.1
179	R1_81	20.14	0.009	20.17	0.009	0.03	7.5
180	R1_82	59.18	0.006	59.20	0.006	0.02	-2.7
181	R1_83	22.86	0.008	22.83	0.007	-0.03	-14.9
182	R1_84	20.88	0.000	20.85	0.000	-0.03	10.8
183	R1_85	20.88	0.001	20.85	0.001	-0.03	12.7

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
184	R1_86	59.18	0.014	59.20	0.018	0.02	23.5
185	R1_87	4.06	0.003			n.a.	n.a.
186	R1_88	17.62	0.055	17.64	0.056	0.02	1.9
187	R1_89	59.18	0.008	59.15	0.008	-0.03	6.8
188	R1_90	23.47	0.004	23.51	0.003	0.04	-13.1
189	R1_91	59.18	0.018	59.15	0.019	-0.03	1.9
190	R1_92	20.74	0.003			n.a.	n.a.
192	R1_94	25.85	0.006	25.89	0.006	0.04	-0.6
193	R1_95	20.30	0.007	20.34	0.009	0.04	18.6
194	R1_96	19.57	0.003	19.55	0.003	-0.02	-1.5
		28.71	0.000			n.a.	n.a.
195	R1_97	28.71	0.184	28.74	0.190	0.03	3.5
196	R1_98	19.57	0.031	19.55	0.027	-0.02	-13.2
		21.56	0.011	21.61	0.011	0.05	-2.6
197	R1_99	19.57	0.003	19.55	0.003	-0.02	-0.8
198	R1_100	19.57	0.001	19.55	0.001	-0.02	1.5
199	R1_101	2.36	0.111			n.a.	n.a.
		2.50	0.197	2.43	0.282	-0.07	43.5
200	R1_102	24.88	0.001	24.99	0.001	0.11	-20.6
201	R1_103	19.22	0.001			n.a.	n.a.
202	R1_104	21.18	0.021	21.21	0.020	0.03	-7.3
203	R1_105	28.71	0.000	28.70	0.000	-0.01	-18.9
204	R1_106	59.13	0.017	59.15	0.014	0.02	-14.2
205	R1_107	29.51	0.001	29.55	0.001	0.04	-3.8
206	R1_108	29.51	0.009	29.55	0.009	0.04	-4.7
207	R1_109	29.51	0.001	29.55	0.001	0.04	-3.7
208	R1_110	25.80	0.004			n.a.	n.a.
209	R1_111	24.22	0.007	24.23	0.005	0.01	-29.4
210	R1_112	32.87	0.001			n.a.	n.a.

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
211	R1_113	28.71	0.001	28.70	0.001	-0.01	-0.2
212	R1_114	28.71	0.000	28.74	0.000	0.03	-0.2
213	R1_115	59.13	0.028	59.15	0.030	0.02	6.6
214	R1_116	19.97	0.002	19.95	0.002	-0.02	-4.0
215	R1_117	19.97	0.018	19.95	0.019	-0.02	4.4
216	R1_118	3.72	0.000			n.a.	n.a.
217	R1_119	59.13	0.018	59.15	0.021	0.02	12.5
218	R1_120	59.13	0.038	59.15	0.038	0.02	0.3
221	R1_123	20.71	0.010	20.72	0.011	0.01	11.8
222	R1_124	59.08	0.021	59.11	0.015	0.03	-26.1
223	R1_125	16.28	0.004			n.a.	n.a.
224	R1_126	21.77	0.037	21.82	0.037	0.05	-1.7
225	R1_127	25.90	0.018	25.94	0.014	0.04	-25.3
226	R1_128	28.87	0.005	28.91	0.005	0.04	3.5
227	R1_129	24.74	0.003			n.a.	n.a.
228	R1_130	59.08	0.023	59.11	0.021	0.03	-8.0
229	R1_131	25.85	0.014	25.89	0.010	0.04	-27.3
230	R1_132	21.77	0.003			n.a.	n.a.
231	R1_133	59.08	0.042	59.11	0.036	0.03	-14.5
232	R1_134	59.08	0.023	59.11	0.014	0.03	-39.7
233	R1_135	29.19	0.000	29.18	0.000	-0.01	-2.6
234	R1_136	29.19	0.001	29.18	0.001	-0.01	-6.1
235	R1_137	29.19	0.014	29.18	0.013	-0.01	-12.0
236	R1_138	17.27	0.005	17.29	0.005	0.02	2.3
237	R1_139	22.31	0.009	22.32	0.007	0.01	-15.9
238	R1_140	36.62	0.018	36.66	0.018	0.04	2.3
239	R1_141	59.08	0.026	59.11	0.018	0.03	-31.2
240	R1_142	16.96	0.001	16.93	0.001	-0.03	0.4

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
241	R1_143	59.08	0.043	59.11	0.028	0.03	-34.4
242	R1_144	18.96	0.004			n.a.	n.a.
243	R1_145	30.17	0.003			n.a.	n.a.
244	R1_146	59.08	0.012			n.a.	n.a.
245	R1_147	34.88	0.001	34.86	0.001	-0.02	-1.6
246	R1_148	32.38	0.006	32.38	0.007	0.00	8.9
247	R1_149	2.71 2.90	0.007 0.003	2.77	0.016	0.06 n.a.	124.2 n.a.
248	R1_150	2.41 2.53	0.067 0.103	2.43	0.211	0.02 n.a.	215.4 n.a.
249	R1_151	21.77	0.001	21.77	0.001	0.00	2.0
250	R1_152	21.77	0.039	21.77	0.037	0.00	-6.0
251	R1_153	5.06	0.001			n.a.	n.a.
252	R1_154	21.77	0.001	21.77	0.001	0.00	7.1
253	R1_155	5.06	0.001	5.02	0.001	-0.04	-26.8
254	R1_156	5.00	0.001	5.02	0.001	0.02	-20.0
255	R1_157	59.03	0.006	59.11	0.003	0.08	-54.6
256	R1_158	28.93	0.006	28.97	0.007	0.04	5.9
257	R1_159	21.77	0.003			n.a.	n.a.
258	R1_160	59.08	0.042	59.11	0.023	0.03	-46.5
259	R1_161	17.41	0.006	17.36	0.007	-0.05	3.4
260	R1_162	58.99	0.022	58.99	0.006	0.00	-71.6
261	R1_163	19.02	0.008	19.00	0.008	-0.02	-4.8
262	R1_164	58.99	0.006			n.a.	n.a.
263	R1_165	26.36	0.006	26.40	0.006	0.04	-0.1
264	R1_166	29.34	0.004			n.a.	n.a.
265	R1_167	30.45 58.99	0.000 0.025			n.a. 0.07	n.a. -57.4
266	R1_168	58.99	0.011			n.a.	n.a.

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
267	R1_169	58.99	0.019	58.99	0.009	0.00	-52.9
268	R1_170	16.71	0.003			n.a.	n.a.
269	R1_171	58.99	0.019	58.94	0.006	-0.05	-69.6
270	R1_172	58.99	0.004			n.a.	n.a.
271	R1_173	21.06	0.008	21.03	0.009	-0.03	5.2
272	R1_174	30.72	0.177	30.70	0.184	-0.02	3.9
273	R1_175	58.99	0.023	58.94	0.010	-0.05	-57.0
274	R1_176	5.26	0.003			n.a.	n.a.
275	R1_177	33.37	0.002			n.a.	n.a.
		58.99	0.041	58.99	0.019	0.00	-54.5
276	R1_178	58.94	0.016	58.94	0.008	0.00	-46.4
277	R1_179	30.72	0.019	30.70	0.021	-0.02	9.7
278	R1_180	26.08	0.013	26.11	0.013	0.03	-4.1
		28.11	0.011	28.15	0.012	0.04	10.0
279	R1_181	26.80	0.003			n.a.	n.a.
280	R1_182	58.94	0.014	58.94	0.005	0.00	-63.8
281	R1_183	33.20	0.005			n.a.	n.a.
282	R1_184	58.94	0.004			n.a.	n.a.
283	R1_185	21.36	0.001	21.39	0.001	0.03	-17.9
284	R1_186	27.32	0.006	27.32	0.007	0.00	23.4
		28.05	0.009	27.96	0.009	-0.09	-0.2
285	R1_187	2.41	0.038	2.36	0.061	-0.05	61.7
		2.53	0.061	2.52	0.059	-0.01	-3.2
286	R1_188	58.94	0.036	58.89	0.019	-0.05	-47.8
287	R1_189	2.41	0.040	2.43	0.128	0.02	219.0
		2.53	0.065			n.a.	n.a.
288	R1_190	21.73	0.004			n.a.	n.a.
289	R1_191	58.94	0.013	58.94	0.008	0.00	-39.3
290	R1_192	22.82	0.020			n.a.	n.a.
291	R1_193	19.88	0.001	19.86	0.001	-0.02	3.9

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
292	R1_194	19.88	0.011	19.86	0.012	-0.02	5.2
293	R1_195	19.88	0.001	19.86	0.001	-0.02	-0.1
294	R1_196	21.41	0.002			n.a.	n.a.
295	R1_197	25.06	0.005	25.12	0.005	0.06	0.3
296	R1_198	58.94	0.017	58.89	0.010	-0.05	-39.1
297	R1_199	19.76	0.001			n.a.	n.a.
298	R1_200	58.94	0.007			n.a.	n.a.
299	R1_201	58.94	0.009	58.89	0.006	-0.05	-32.3
300	R1_202	24.88	0.024	24.90	0.024	0.02	3.3
301	R1_203	36.26	0.001	36.24	0.001	-0.02	27.3
302	R1_204	36.26	0.017	36.24	0.018	-0.02	3.4
303	R1_205	27.45	0.001			n.a.	n.a.
		33.92	0.004			n.a.	n.a.
304	R1_206	19.29	0.032	19.32	0.028	0.03	-12.0
		26.46	0.008	26.50	0.008	0.04	1.7
305	R1_207	28.81	0.002	28.79	0.002	-0.02	3.6
306	R1_208	18.21	0.002	18.19	0.002	-0.02	-3.6
		29.47	0.001	29.51	0.001	0.04	19.8
		29.78	0.003			n.a.	n.a.
307	R1_209	28.81	0.002	28.79	0.002	-0.02	6.0
308	R1_210	58.89	0.020	58.89	0.013	0.00	-31.0
309	R1_211	28.76	0.001	28.79	0.001	0.03	3.6
310	R1_212	42.53	0.018	42.51	0.018	-0.02	-2.0
311	R1_213	31.35	0.002			n.a.	n.a.
312	R1_214	20.19	0.008	20.22	0.008	0.03	1.8
313	R1_215	58.89	0.010	58.89	0.007	0.00	-21.8
314	R1_216	58.89	0.012	58.89	0.009	0.00	-26.4
315	R1_217	58.89	0.003	58.89	0.003	0.00	-14.5
316	R1_218	24.97	0.014	24.99	0.015	0.02	6.5
		30.07	0.005	30.06	0.005	-0.01	12.1

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
317	R1_219	20.60	0.004	20.59	0.005	-0.01	7.7
318	R1_220	20.60	0.062	20.59	0.066	-0.01	5.8
319	R1_221	16.00	0.002	16.02	0.002	0.02	0.1
320	R1_222	15.93	0.003			n.a.	n.a.
321	R1_223	58.89	0.006	58.89	0.005	0.00	-18.6
322	R1_224	29.30	0.002	29.33	0.002	0.03	-4.6
323	R1_225	4.06	0.007	4.06	0.006	0.00	-12.9
324	R1_226	58.89	0.007	58.89	0.006	0.00	-16.8
325	R1_227	36.46	0.238	36.44	0.248	-0.02	4.2
326	R1_228	36.41	0.020			n.a.	n.a.
327	R1_229	14.23	0.040	14.23	0.041	0.00	3.7
328	R1_230	36.46	0.119	36.44	0.124	-0.02	4.3
329	R1_231	27.45	0.001	27.40	0.000	-0.05	-41.8
330	R1_232	36.46	0.084	36.44	0.087	-0.02	4.2
		41.70	0.035			n.a.	n.a.
331	R1_233	58.89	0.004	58.89	0.004	0.00	-10.1
332	R1_234	25.47	0.012	25.46	0.009	-0.01	-23.7
333	R1_235	18.96	0.008			n.a.	n.a.
334	R1_236	58.89	0.004	58.89	0.004	0.00	-9.9
335	R1_237	36.46	0.013	36.44	0.014	-0.02	2.2
336	R1_238	31.55	0.009	31.58	0.004	0.03	-54.9
337	R1_239	36.46	0.004			n.a.	n.a.
338	R1_240	36.46	0.005	36.44	0.005	-0.02	3.1
339	R1_241	36.51	0.003			n.a.	n.a.
340	R1_242	28.55	0.004			n.a.	n.a.
341	R1_243	34.88	0.003	34.86	0.003	-0.02	0.1
342	R1_244	42.65	0.005	42.64	0.005	-0.01	-7.4
343	R1_245	42.59	0.006	42.64	0.006	0.05	-2.9

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
344	R1_246	24.41	0.003			n.a.	n.a.
345	R1_247	42.59	0.004	42.64	0.004	0.05	-0.7
346	R1_248	22.17	0.010	22.17	0.005	0.00	-51.8
347	R1_249	36.80	0.022	36.83	0.021	0.03	-6.2
348	R1_250	24.97	0.003	24.99	0.004	0.02	5.6
349	R1_251	36.80	0.011	36.83	0.010	0.03	-8.0
350	R1_252	24.15	0.032	24.17	0.028	0.02	-10.4
351	R1_253	31.65	0.004	31.63	0.004	-0.02	-9.7
352	R1_254	34.88	0.011	34.86	0.011	-0.02	-2.4
353	R1_255	23.01	0.009	23.04	0.009	0.03	1.1
354	R1_256	34.11	0.001			n.a.	n.a.
355	R1_257	23.01	0.013	23.04	0.014	0.03	3.3
		33.08	0.001			n.a.	n.a.
356	R1_258	22.57	0.002	22.59	0.002	0.02	-5.9
357	R1_259	25.80	0.002			n.a.	n.a.
		32.96	0.001			n.a.	n.a.
358	R1_260	24.10	0.003			n.a.	n.a.
359	R1_261	28.43	0.012	28.46	0.011	0.03	-3.8
360	R1_262	20.14	0.009	20.17	0.010	0.03	14.9
		21.99	0.003			n.a.	n.a.
		28.43	0.011	28.46	0.011	0.03	-1.2
361	R1_263	23.05	0.041	23.04	0.036	-0.01	-12.8
362	R1_264	2.45	0.039			n.a.	n.a.
363	R1_265	2.41	0.026			n.a.	n.a.
		2.53	0.042	2.52	0.034	-0.01	-19.3
364	R1_266	36.51	0.006	36.49	0.007	-0.02	2.7
365	R1_267	27.85	0.006	27.90	0.007	0.05	4.8
366	R1_268	38.99	0.004	38.98	0.004	-0.01	5.9
367	R1_269	38.99	0.007	38.98	0.008	-0.01	15.4
368	R1_270	36.80	0.005	36.78	0.005	-0.02	-6.5

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
369	R1_271	36.46	0.001	36.44	0.001	-0.02	-2.0
370	R1_272	31.48	0.004	31.51	0.004	0.03	-7.3
371	R1_273	40.30	0.003	40.28	0.003	-0.02	1.2
372	R1_274	25.06	0.154	25.08	0.155	0.02	0.8
373	R1_275			30.21	0.011	n.a.	n.a.
		30.33	0.019	30.40	0.012	0.07	-39.3
		30.61	0.008	30.65	0.008	0.04	-1.7
374	R1_276	25.06	0.082	25.08	0.084	0.02	1.6
375	R1_277	27.85	0.013	27.83	0.014	-0.02	9.8
376	R1_278			20.65	0.041	n.a.	n.a.
				30.47	0.002	n.a.	n.a.
		30.61	0.003	30.59	0.002	-0.02	-31.2
		30.95	0.001	30.86	0.002	-0.09	144.5
377	R1_279	25.06	0.064	25.08	0.065	0.02	2.2
378	R1_280	25.71	0.003			n.a.	n.a.
379	R1_281			24.99	0.002	n.a.	n.a.
380	R1_282	25.01	0.002	25.04	0.002	0.03	7.0
381	R1_283	32.11	0.002			n.a.	n.a.
		33.80	0.092	33.77	0.093	-0.03	0.5
382	R1_284	20.57	0.004	20.59	0.005	0.02	8.5
		20.74	0.007	20.72	0.009	-0.02	29.8
383	R1_285	28.49	0.005			n.a.	n.a.
		30.72	0.024	30.75	0.025	0.03	3.3
384	R1_286	30.72	0.006	30.75	0.006	0.03	3.4
385	R1_287	47.58	0.004	47.54	0.004	-0.04	1.6
386	R1_288	40.30	0.026	40.28	0.028	-0.02	7.4
387	R1_289	24.88	0.004	24.86	0.004	-0.02	4.0
388	R1_290	24.31	0.000			n.a.	n.a.
		24.84	0.005	24.86	0.005	0.02	13.4
389	R1_291	47.53	0.003	47.59	0.003	0.06	-6.7
390	R1_292	40.30	0.045	40.28	0.048	-0.02	7.5
391	R1_293	40.30	0.021	40.28	0.025	-0.02	18.2

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
392	R1_294	25.01	0.088	25.04	0.091	0.03	3.7
393	R1_295	24.48	0.004	24.50	0.004	0.02	1.9
394	R1_296	40.25	0.006	40.28	0.007	0.03	23.9
395	R1_297	40.30	0.004	40.28	0.004	-0.02	21.9
396	R1_298	25.95	0.003			n.a.	n.a.
397	R1_299	32.83	0.012	32.83	0.012	0.00	-1.1
398	R1_300	20.54	0.007	20.56	0.008	0.02	10.4
399	R1_301			2.36	0.023	n.a.	n.a.
		2.45	0.025	2.49	0.036	0.04	45.4
		2.55	0.017			n.a.	n.a.
400	R1_302	19.88	0.005	19.90	0.005	0.02	8.1
401	R1_303	38.01	0.004	38.00	0.003	-0.01	-7.5
402	R1_304	27.22	0.008	27.21	0.009	-0.01	3.1
403	R1_305	23.71	0.002	23.76	0.001	0.05	-18.7
404	R1_306	23.71	0.051	23.73	0.044	0.02	-14.8
405	R1_307	23.71	0.002	23.76	0.001	0.05	-16.2
406	R1_308	36.06	0.014	36.05	0.015	-0.01	5.1
407	R1_309	37.39	0.011	37.37	0.012	-0.02	4.8
408	R1_310	26.73	0.001	26.76	0.001	0.03	1.1
409	R1_311	26.73	0.016	26.76	0.018	0.03	8.4
410	R1_312	19.93	0.031	19.90	0.032	-0.03	2.4
411	R1_313	28.05	0.008	28.09	0.009	0.04	7.6
412	R1_314	22.27	0.007	22.32	0.007	0.05	-3.0
413	R1_315	27.63	0.001	27.62	0.001	-0.01	3.4
414	R1_316	27.63	0.002	27.62	0.002	-0.01	6.1
415	R1_317	27.63	0.025	27.62	0.028	-0.01	12.1
416	R1_318	27.63	0.002	27.62	0.002	-0.01	3.4
417	R1_319	27.63	0.001			n.a.	n.a.
418	R1_320	16.21	0.006	16.16	0.006	-0.05	-0.4

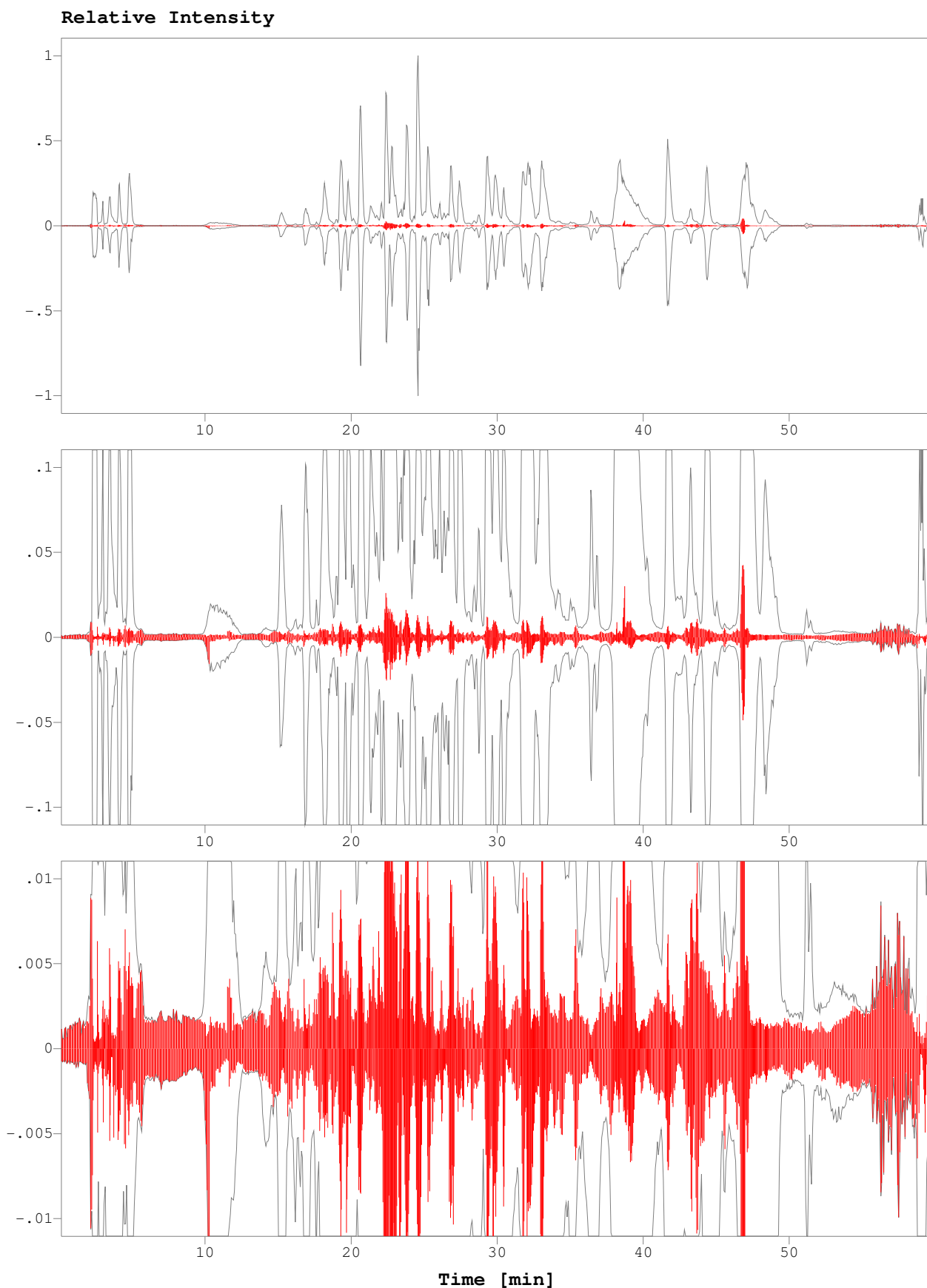
#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
419	R1_321	35.00	0.054	34.99	0.052	-0.01	-4.2
420	R1_322	35.00	0.002	34.99	0.002	-0.01	1.4
		35.92	0.010	35.91	0.010	-0.01	1.2
421	R1_323	35.00	0.011	34.99	0.010	-0.01	-8.6
422	R1_324	31.61	0.005	31.63	0.005	0.02	-0.7
423	R1_325	35.19	0.003			n.a.	n.a.
424	R1_326	33.25	0.016	33.28	0.017	0.03	3.6
425	R1_327	2.41	0.023			n.a.	n.a.
		2.53	0.033			n.a.	n.a.
426	R1_328	41.59	0.077	41.58	0.075	-0.01	-2.8
427	R1_329	25.14	0.008			n.a.	n.a.
		25.43	0.001			n.a.	n.a.
		33.12	0.161	33.12	0.174	0.00	8.0
428	R1_330	28.43	0.001			n.a.	n.a.
429	R1_331	34.11	0.004			n.a.	n.a.
430	R1_332	31.14	0.007	31.17	0.008	0.03	8.9
431	R1_333	38.58	0.005	38.58	0.006	0.00	3.9
432	R1_334	33.86	0.003			n.a.	n.a.
433	R1_335	20.88	0.007	20.90	0.006	0.02	-5.9
434	R1_336	38.69	0.108	38.69	0.117	0.00	8.2
435	R1_337	31.61	0.005	31.63	0.004	0.02	-7.2
436	R1_338	38.69	0.006	38.69	0.007	0.00	28.6
437	R1_339	27.40	0.004	27.44	0.004	0.04	8.7
		29.94	2.072	29.94	2.242	0.00	8.2
		30.95	0.043	30.92	0.036	-0.03	-16.5
		32.11	0.004	32.08	0.006	-0.03	28.8
438	R1_340	42.59	0.001	42.70	0.001	0.11	-17.3
439	R1_341	41.59	0.055	41.58	0.159	-0.01	191.9
		41.78	0.016			n.a.	n.a.
		42.00	0.055			n.a.	n.a.
		42.16	0.005			n.a.	n.a.
				42.33	0.004		n.a.
	42.59	0.108	42.45	0.145	-0.14	35.0	
440	R1_342	41.55	0.007	41.55	0.007	0.00	-4.1

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
440	R1_342	42.00	0.009	42.33	0.025	n.a.	n.a.
		42.53	0.014			n.a.	n.a.
		43.24	0.004			n.a.	n.a.
						n.a.	n.a.
441	R1_343	29.94	0.002	29.98	0.003	0.04	2.0
442	R1_344	24.97	0.006	24.99	0.006	0.02	-4.5
443	R1_345	25.01	0.089	25.04	0.091	0.03	2.4
444	R1_346	18.09	0.005	18.10	0.004	0.01	-19.9
445	R1_347	18.13	0.004	18.14	0.004	0.01	-1.3
446	R1_348	25.01	0.011	25.04	0.011	0.03	-5.7
447	R1_349	18.13	0.004	18.10	0.004	-0.03	0.0
		19.80	0.007	19.78	0.008	-0.02	12.8
448	R1_350	18.09	0.005	18.10	0.004	0.01	-21.7
449	R1_351	25.01	0.004			n.a.	n.a.
450	R1_352	24.93	0.019	24.90	0.019	-0.03	-0.2
		36.41	0.101	36.44	0.007	0.03	-93.3
451	R1_353	36.41	0.025	36.39	0.027	-0.02	5.9
452	R1_354	24.93	0.003	24.95	0.003	0.02	14.0
		36.46	0.009	36.44	0.009	-0.02	2.9
453	R1_355	40.14	0.007	40.18	0.007	0.04	7.7
454	R1_356	18.96	0.062	19.00	0.056	0.04	-9.3
455	R1_357	19.08	0.019	19.06	0.013	-0.02	-32.9
456	R1_358	25.36	0.012	25.38	0.014	0.02	11.5
		28.05	0.019	28.09	0.020	0.04	7.6
		41.63	0.023	41.62	0.030	-0.01	27.4
		41.74	0.017			n.a.	n.a.
	41.86	0.029			n.a.	n.a.	
457	R1_359	19.02	0.013	19.00	0.010	-0.02	-24.6
458	R1_360	19.02	0.005			n.a.	n.a.
459	R1_361	32.78	0.169	32.78	0.170	0.00	0.5
460	R1_362	32.78	0.023	32.78	0.024	0.00	1.7
461	R1_363	32.78	0.007			n.a.	n.a.
462	R1_364	32.78	0.004	32.78	0.004	0.00	-7.7

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
463	R1_365	25.61	0.065	25.59	0.063	-0.02	-2.3
		38.24	0.044	38.23	0.051	-0.01	17.7
				38.45	0.006	n.a.	n.a.
				38.61	0.012	n.a.	n.a.
		38.82	0.071			n.a.	n.a.
		39.12	0.085			n.a.	n.a.
		39.57	0.043			n.a.	n.a.
		39.97	0.037			n.a.	n.a.
464	R1_366			22.92	0.001	n.a.	n.a.
		23.42	0.003	23.47	0.002	0.05	-24.0
		23.71	0.008	23.73	0.003	0.02	-54.6
		24.44	0.011	24.47	0.012	0.03	7.4
465	R1_367	39.48	0.002	39.51	0.002	0.03	-0.9
466	R1_368	19.02	0.007	19.00	0.007	-0.02	1.5
467	R1_369	37.87	0.004			n.a.	n.a.
468	R1_370	28.05	0.004	28.09	0.004	0.04	3.8
469	R1_371	41.46	0.003			n.a.	n.a.
470	R1_372	26.41	0.144			n.a.	n.a.
471	R1_373	41.52	0.004			n.a.	n.a.
472	R1_374	26.41	0.076	26.40	0.025	-0.01	-67.8
473	R1_375	40.30	0.020	40.28	0.021	-0.02	1.7
474	R1_376	26.41	0.013			n.a.	n.a.
475	R1_377	40.30	0.003			n.a.	n.a.
476	R1_378	18.13	0.006	18.10	0.005	-0.03	-16.7
477	R1_379	27.16	0.004	27.21	0.004	0.05	11.1
478	R1_380	27.16	0.009	27.21	0.010	0.05	7.5
479	R1_381	27.16	0.003	27.21	0.004	0.05	19.2
480	R1_382	45.04	0.008	45.08	0.009	0.04	9.9
481	R1_383	45.04	0.032	45.08	0.036	0.04	13.7
482	R1_384	45.04	0.013	45.08	0.015	0.04	18.0
483	R1_385	25.80	0.017	25.84	0.017	0.04	1.9
484	R1_386	45.17	0.005	45.20	0.006	0.03	14.8
485	R1_387	29.82	0.015	29.85	0.016	0.03	4.7

#	Molecule	Rt: Ret. Time, RI: Rel. Intens. Reference Data Set (R)		Rt: Ret. Time, RI: Rel. Intens. Data Set Compared (C)		Difference Rt (C-R) [min]	Rel. Difference RI (C-R)/C [%]
		Rt/min	RI/%	Rt/min	RI/%		
486	R1_388	36.41	0.004	36.44	0.004	0.03	9.4
487	R1_389	44.40	0.117	44.38	0.131	-0.02	12.6
488	R1_390	44.40	0.097	44.42	0.097	0.02	-0.1
489	R1_391	44.40	0.037	44.38	0.039	-0.02	7.3
490	R1_392	44.36	0.494	44.38	0.206	0.02	-58.3
491	R1_393	44.36	0.381	44.38	0.410	0.02	7.5
492	R1_394	44.36	0.030	44.38	0.027	0.02	-10.0
493	R1_395	44.36	0.064	44.30	0.054	n.a.	n.a.
				44.38	0.189	0.02	195.7
494	R1_396	44.36	0.113	44.34	0.126	-0.02	12.3
495	R1_397	44.36	0.027	44.38	0.035	0.02	32.1
496	R1_398	44.36	0.015	44.30	0.008	n.a.	n.a.
				44.42	0.009	0.06	-37.4
497	R1_399	42.84	0.004	42.89	0.004	0.05	2.7
498	R1_400	47.08	0.032	47.16	0.022	0.08	-32.0
499	R1_401	47.08	0.091	47.11	0.087	0.03	-4.6

Grey: Ion current chromatograms of original data sets
Red: Ion current chromatograms of difference data sets
Normal: Ion current chromatogram of reference data set
Mirrored: Ion current chromatogram of data set compared



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