

Operator: mw  
 Date/time: 2016-06-05/1:53:32pm  
 Title/Comment:

lis-File: C:\massmap\web\_site\reports\pepmap\lis\_etc\MAB\_Demo\_in\_silico\_plus\_extral.lis

**Data Sets**

X: G=Member of group, C=Activated for comparison, - =Evaluation insufficient

#	X	Path
1	C	C:\massmap\web_site\reports\pepmap\final_evaluations\MAB_Demo1_t2_t1.mmp
2	G	C:\massmap\web_site\reports\pepmap\final_evaluations\MAB_Demo2_t2_t1.mmp
3	G	C:\massmap\web_site\reports\pepmap\final_evaluations\MAB_Demo3_t2_t1.mmp
4	G	C:\massmap\web_site\reports\pepmap\final_evaluations\MAB_Demo4_t2_t1.mmp
5	G	C:\massmap\web_site\reports\pepmap\final_evaluations\MAB_Demo5_t2_t1.mmp
6	G	C:\massmap\web_site\reports\pepmap\final_evaluations\MAB_Demo6_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
3		717	-4.98	2.41
4		698	-5.08	2.62
5		641	-4.78	2.51
6		681	-4.57	2.44

**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.
3		1.35E+11	n.a.
4		1.26E+11	n.a.
5		1.36E+11	n.a.
6		1.30E+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
3		n.a.	n.a.	OK	OK	OK	OK
4		n.a.	n.a.	OK	OK	OK	OK
5		n.a.	n.a.	OK	OK	OK	OK
6		n.a.	n.a.	OK	OK	OK	OK

Comparison Report pepmap, Group of Data Sets (Part 1)  
(MAB\_Demo\_in\_silico\_plus\_extral)

Mean of standard deviations of retention time differences [min]: 0.020  
StDev of standard deviations of retention time differences [min]: 0.018

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
1	HC01	20.66	0.01	4.542	0.441	20.65	5.083	20.64	4.514	20.68	4.549
		21.56	0.01	0.007	0.003	21.55	0.005	21.56	0.010	21.57	0.011
		22.80	n.a.	0.002	n.a.						
2	HC02	44.56	0.01	0.326	0.010	44.55	0.329	44.54	0.334	44.58	0.335
3	HC03	3.35	n.a.	0.013	n.a.						
		3.46	0.01	0.028	0.001	3.46	0.027	3.45	0.029	3.47	0.027
4	HC03_pyE	3.42	0.02	0.011	0.000	3.43	0.011	3.41	0.012	3.43	0.011
5	HC05	32.06	0.02	0.041	0.002	32.08	0.041	32.05	0.039	32.09	0.039
		32.40	0.00	0.005	0.000			32.40	0.005	32.39	0.005
		33.13	0.01	2.908	0.110	33.12	2.954	33.14	2.774	33.13	3.033
		34.74	n.a.	0.013	n.a.						
6	HC07	16.90	0.01	0.435	0.069	16.88	0.462	16.89	0.512	16.91	0.494
7	HC08	3.21	0.02	0.015	0.001	3.21	0.013	3.24	0.016	3.20	0.016
8	HC09	26.56	0.02	0.007	0.000	26.55	0.007	26.57	0.008	26.57	0.007
		27.48	0.02	1.760	0.085	27.49	1.811	27.47	1.903	27.49	1.697
9	HC09_ox	22.10	0.01	0.014	0.001	22.12	0.014	22.09	0.016	22.10	0.013
10	HC09_deamid	28.80	0.02	0.098	0.007	28.79	0.092	28.82	0.106	28.82	0.107
		29.79	0.01	0.466	0.026	29.78	0.451	29.81	0.491	29.78	0.502
11	HC10	19.80	0.02	1.245	0.087	19.78	1.356	19.80	1.324	19.83	1.222
12	HC10_ox	16.52	0.01	0.022	0.001	16.52	0.020	16.53	0.021	16.51	0.024
13	HC12	29.86	n.a.	0.500	n.a.						
		29.95	0.02	2.297	0.118	29.94	2.247	29.97	2.453	29.94	2.403
14	HC12_ox	26.04	0.01	0.018	0.002	26.02	0.016	26.04	0.018	26.04	0.020
15	HC12_deamid	30.92	0.03	0.081	0.009	30.92	0.068	30.98	0.080	30.89	0.089
16	HC13	38.41	0.04	2.319	0.088	38.37	2.248	38.41	2.332	38.44	2.453
17	HC13_ox	34.20	0.01	0.075	0.005	34.21	0.069	34.20	0.083	34.19	0.077
18	HC13_deamid	38.05	0.03	0.419	0.025	38.03	0.402	38.08	0.451	38.06	0.414
		39.67	0.02	0.281	0.010	39.64	0.271	39.67	0.283	39.69	0.291
19	HC13_ox_deamid	35.16	0.03	0.006	0.000	35.17	0.005	35.17	0.006	35.17	0.006
20	HC14	48.39	n.a.	0.004	n.a.					48.39	0.004
21	HC15	3.42	0.01	0.010	0.001	3.43	0.010	3.41	0.011	3.43	0.010
22	HC17	3.46	0.01	0.159	0.018	3.46	0.149	3.45	0.185	3.47	0.161
23	HC18	38.26	0.04	1.594	0.768	38.34	2.548	38.27	0.609	38.26	0.769
		38.63	<b>0.08</b>	2.201	0.521	38.61	2.713	38.73	1.486		
		38.77	n.a.	0.959	n.a.						
		38.93	0.00	5.452	2.413	38.93	3.039				
		39.30	<b>0.08</b>	2.632	1.786	39.42	1.058	39.28	1.143	39.20	2.863

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
23	HC18	39.79	n.a.	0.026	n.a.						
		39.82	0.00	1.323	0.411	39.82	1.734				
		39.95	n.a.	0.412	n.a.			39.95	0.412		
		40.26	0.02	0.005	0.001	40.28	0.004			40.24	0.007
24	HC19	29.37	0.02	3.044	0.138	29.38	2.876	29.40	3.235	29.37	3.037
25	HC20	23.83	0.01	2.611	0.208	23.84	2.404	23.82	2.998	23.83	2.643
26	HC21	35.63	n.a.	0.004	n.a.	35.63	0.004				
		35.70	0.00	0.005	0.000			35.69	0.005	35.70	0.005
		41.74	0.02	4.178	0.169	41.73	4.065	41.73	4.031	41.76	4.408
		42.45	n.a.	0.009	n.a.						
		42.46	0.02	0.085	0.011	42.45	0.069	42.45	0.084	42.48	0.086
		43.54	n.a.	0.031	n.a.						
		44.66	n.a.	0.006	n.a.						
		45.55	n.a.	0.005	n.a.						
		47.46	n.a.	0.006	n.a.						
53.10	0.01	0.013	0.000	53.10	0.012	53.09	0.013	53.11	0.013		
53.47	n.a.	0.009	n.a.								
27	HC22	20.08	0.01	0.003	0.000	20.06	0.003	20.09	0.003	20.08	0.004
28	HC22_A2G0	18.54	0.02	0.029	0.004	18.51	0.028	18.57	0.036	18.54	0.031
29	HC22_A2G0-GlcNAc	18.67	0.02	0.024	0.001	18.63	0.023	18.69	0.026	18.67	0.024
30	HC22_A2G1	27.45	0.01	0.004	0.000	27.44	0.004	27.47	0.004	27.45	0.004
31	HC22_A2G1-GlcNAc	18.61	0.02	0.011	0.001	18.57	0.011	18.63	0.013	18.60	0.012
32	HC22_A2G2S1	18.90	0.01	0.024	0.002	18.89	0.023	18.89	0.023	18.92	0.027
33	HC22_A2FG0	18.21	0.01	0.413	0.050	18.19	0.410	18.20	0.403	18.23	0.491
34	HC22_A2FG0-GlcNAc	18.40	0.02	0.017	0.002	18.39	0.016	18.40	0.018	18.42	0.019
35	HC22_A2FG1	18.02	0.02	0.264	0.023	18.02	0.249	18.02	0.285	18.00	0.297
36	HC22_A2FG1-GlcNAc	18.30	0.01	0.006	0.001	18.28	0.006	18.29	0.007	18.31	0.007
37	HC22_A2FG2	17.94	0.02	0.033	0.002	17.91	0.031	17.97	0.035	17.95	0.037
38	HC22_Man5	18.44	0.02	0.021	0.003	18.45	0.019	18.46	0.023	18.42	0.025
39	HC23	32.18	0.04	3.652	0.725	32.20	4.071	32.09	2.219	32.20	4.174
40	HC23_ox	26.60	0.01	0.165	0.006	26.59	0.162	26.61	0.177	26.62	0.163
41	HC23_deamid	32.36	n.a.	1.902	n.a.			32.36	1.902		
		32.91	0.02	0.463	0.014	32.92	0.483	32.89	0.467	32.94	0.446
		33.36	0.01	0.937	0.043	33.37	0.929	33.36	0.951	33.39	0.977
42	HC23_ox_deamid	26.99	0.02	0.015	0.001	27.00	0.015	26.98	0.017	27.00	0.016
		27.50	0.01	0.021	0.001	27.49	0.021	27.51	0.023	27.49	0.020
43	HC24	3.44	0.01	0.054	0.005	3.43	0.052	3.45	0.062	3.43	0.054
44	HC26	22.78	0.01	2.424	0.235	22.79	2.431	22.79	2.455	22.77	2.835
45	HC26_deamid	23.35	0.01	0.215	0.018	23.36	0.213	23.35	0.248	23.34	0.207

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
46	HC27	3.42	0.01	0.065	0.005	3.43	0.063	3.41	0.074	3.43	0.064
47	HC29	3.45	0.02	0.037	0.004	3.43	0.037	3.45	0.043	3.47	0.037
48	HC30	21.46 21.88	0.03 0.04	0.742 0.241	0.104 0.061	21.44 21.93	0.743 0.235	21.50	0.899	21.41 21.85	0.572 0.318
49	HC31	3.42	0.01	0.042	0.003	3.43	0.041	3.41	0.047	3.43	0.041
50	HC33	51.20	0.02	0.014	0.004	51.19	0.013	51.25	0.023	51.18	0.011
51	HC33_deamid	51.50	0.03	0.006	0.001	51.52	0.006	51.51	0.005	51.53	0.007
52	HC34	26.88	0.01	1.948	0.104	26.88	1.900	26.90	2.109	26.87	1.988
53	HC34_ox	24.34	0.01	0.058	0.007	24.33	0.051	24.36	0.070	24.34	0.057
54	HC34_deamid	27.77 28.41	0.02 0.02	0.026 0.041	0.001 0.003	27.77 28.40	0.026 0.038	27.80 28.43	0.027 0.043	27.79 28.43	0.025 0.045
55	HC35	3.48	0.01	0.183	0.021	3.50	0.171	3.48	0.216	3.47	0.184
56	HC35_deamid	3.68	n.a.	0.006	n.a.	3.68	0.006				
57	HC36	24.58	0.01	6.739	0.525	24.57	6.467	24.59	7.436	24.58	7.232
58	HC36_deamid	24.29 25.19 25.34 26.08	0.01 0.01 0.03 0.01	0.026 0.262 0.684 0.030	0.015 0.028 0.120 0.003	24.28 25.19 25.34 26.07	0.014 0.264 0.553 0.029			24.29 25.18 25.32 26.08	0.016 0.296 0.895 0.034
59	HC37	3.42	0.01	0.019	0.001	3.43	0.018	3.41	0.021	3.43	0.019
60	HC04-05	29.74 30.47	0.00 0.01	0.012 0.749	0.000 0.029	29.74 30.47	0.012 0.789	29.73 30.46	0.011 0.753	29.74 30.49	0.013 0.761
61	HC07-08_deamid	22.25	0.00	0.004	0.000			22.24	0.004		
62	HC08-09_deamid	26.34	0.01	0.011	0.000	26.35	0.011	26.33	0.011	26.33	0.011
63	HC15-16	3.44	0.01	0.027	0.002	3.43	0.027	3.45	0.030	3.43	0.027
64	HC20-21	44.16 44.58	0.01 n.a.	0.115 0.001	0.010 n.a.	44.16	0.120	44.15	0.125	44.15 44.58	0.122 0.001
65	HC25-26	22.67	0.01	0.006	0.002	22.67	0.004	22.67	0.009	22.69	0.008
66	HC25-26_deamid	23.26	0.02	0.004	0.001	23.27	0.005	23.30	0.003	23.24	0.005
67	HC30-31	20.66 21.57	0.01 0.01	4.333 0.003	0.427 0.000	20.65	4.849	20.64 21.56	4.314 0.003	20.68 21.57	4.351 0.003
68	HC32-33	48.88	0.02	0.017	0.001	48.84	0.018	48.90	0.018	48.89	0.017
69	HC32-33_deamid	49.18	0.02	0.008	0.000	49.14	0.008	49.19	0.008	49.19	0.008
70	HC34-35	31.68 31.93	0.02 0.02	0.013 0.025	0.001 0.005	31.67 31.92	0.014 0.031	31.67 31.93	0.014 0.030	31.96	0.018
71	LC01	31.80 32.32	0.02 n.a.	2.438 0.023	0.068 n.a.	31.80	2.355	31.80 32.32	2.467 0.023	31.83	2.552

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
71	LC01	32.65	n.a.	0.039	n.a.			32.65	0.039		
72	LC02	22.43	0.01	4.044	0.287	22.42	3.847	22.43	4.303	22.42	4.456
73	LC02_deamid	22.08	0.02	0.400	0.028	22.07	0.412	22.09	0.446	22.06	0.361
		22.43	n.a.	2.204	n.a.						
		22.93	0.01	0.023	0.002			22.92	0.026	22.93	0.021
		23.18	0.02	0.106	0.006	23.17	0.103	23.21	0.111	23.19	0.112
		23.46	0.01	0.165	0.006	23.47	0.160	23.45	0.175	23.45	0.159
		24.01	0.01	0.012	0.003	24.01	0.009	23.99	0.017	24.01	0.011
74	LC03	2.01	0.01	0.004	0.000						
		3.42	0.01	0.076	0.002	3.43	0.073	3.41	0.080	3.43	0.075
		3.62	n.a.	0.009	n.a.						
75	LC04	18.21	0.01	0.945	0.089	18.19	0.941	18.20	0.969	18.23	1.076
76	LC05	19.32	0.02	2.359	0.191	19.28	2.249	19.33	2.466	19.31	2.619
		19.91	0.01	0.013	0.000					19.92	0.013
		22.78	0.01	0.158	0.019	22.79	0.160	22.79	0.170	22.77	0.185
77	LC07	10.29	n.a.	0.125	n.a.						
		10.67	<b>0.06</b>	0.092	0.017	10.61	0.093	10.72	0.076	10.60	0.080
		11.05	0.04	0.076	0.013	11.02	0.069	11.06	0.060	11.01	0.096
		11.22	n.a.	0.055	n.a.						
		11.36	0.02	0.052	0.009			11.34	0.062	11.37	0.040
		11.78	<b>0.07</b>	0.134	0.024	11.65	0.172	11.83	0.110	11.79	0.126
78	LC09	48.50	0.01	0.415	0.022	48.50	0.374	48.50	0.421	48.49	0.439
79	LC09_deamid	44.69	0.02	0.030	0.003	44.71	0.026	44.70	0.032	44.69	0.034
		46.07	0.01	0.004	0.000	46.06	0.004	46.06	0.004	46.05	0.004
80	LC10	4.13	0.01	0.743	0.088	4.14	0.744	4.12	0.867	4.13	0.592
81	LC12	3.42	0.01	0.050	0.004	3.43	0.048	3.41	0.057	3.43	0.049
82	LC13	23.05	0.01	0.602	0.053	23.04	0.582	23.07	0.659	23.05	0.666
		25.75	0.00	0.009	0.000						
		26.07	0.01	0.087	0.008	26.07	0.080	26.08	0.093	26.08	0.100
		26.35	0.02	0.037	0.001	26.35	0.037	26.38	0.036	26.33	0.040
83	LC13_deamid	22.01	0.01	0.041	0.003	22.03	0.044	22.00	0.047	22.01	0.039
		23.06	n.a.	0.267	n.a.						
		23.64	0.01	0.250	0.018	23.64	0.251	23.63	0.278	23.64	0.231
		23.87	0.02	0.740	0.046	23.88	0.690	23.86	0.816	23.88	0.768
		26.64	0.01	0.036	0.001	26.63	0.034	26.66	0.037	26.62	0.036
		27.10	0.01	0.019	0.001	27.10	0.019	27.13	0.020	27.09	0.019
84	LC13_pyE	25.78	0.02	0.029	0.001	25.80	0.027	25.76	0.029	25.76	0.031
		26.07	0.01	0.357	0.026	26.07	0.326	26.08	0.366	26.08	0.400
		26.35	0.02	0.092	0.009	26.35	0.094	26.38	0.093	26.33	0.105
85	LC13_deamid_pyE	24.02	0.01	0.015	0.001	24.01	0.014	24.04	0.016	24.01	0.016
		24.46	0.01	0.005	0.000	24.47	0.004	24.45	0.005	24.48	0.005
		26.63	0.01	0.131	0.005	26.63	0.122	26.61	0.138	26.62	0.135
		27.10	0.01	0.044	0.003	27.10	0.042	27.13	0.047	27.09	0.045
86	LC14	24.58	0.02	0.008	0.001	24.57	0.007	24.59	0.007	24.54	0.007
		25.29	0.01	2.794	0.197	25.30	2.599	25.29	3.000	25.28	3.065
		25.70	n.a.	0.008	n.a.						

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
86	LC14	26.32	0.02	0.065	0.004	26.30	0.069				
		35.23	0.03	0.010	0.001	35.24	0.010	35.23	0.010	35.24	0.010
		53.06	0.03	0.020	0.003	53.10	0.016	53.09	0.019	53.03	0.022
87	LC14_ox	21.31	0.01	0.032	0.001	21.30	0.034	21.31	0.032	21.31	0.031
88	LC15	3.43	0.01	0.042	0.001	3.43	0.041	3.45	0.045	3.43	0.041
		3.62	n.a.	0.003	n.a.						
89	LC16	3.43	0.01	0.110	0.008	3.43	0.107	3.45	0.123	3.43	0.109
90	LC17	4.80	0.02	1.601	0.113	4.79	1.502	4.78	1.625	4.80	1.810
91	LC18	3.44	0.01	0.061	0.005	3.43	0.059	3.45	0.069	3.43	0.060
92	LC19	3.44	0.01	0.008	0.001	3.43	0.008	3.45	0.007	3.43	0.008
94	LC07-08	4.08	n.a.	0.000	n.a.			4.08	0.000		
95	LC08-09	46.99	0.04	4.817	0.184	47.00	4.524	46.95	4.818	46.95	5.081
		47.44	0.01	1.448	0.323			47.43	1.902	47.43	1.187
96	LC08-09_deamid	43.24	0.02	0.390	0.012	43.23	0.382	43.23	0.398	43.26	0.392
		44.65	0.01	0.090	0.003	44.65	0.089	44.64	0.092	44.63	0.095
97	LC13-14_deamid	26.07	0.02	0.006	0.001	26.07	0.006	26.08	0.006	26.04	0.007
98	LC13-14_pyE	25.28	0.01	0.040	0.004	25.27	0.040	25.29	0.042	25.28	0.047
100	R1_02	3.46	0.01	0.002	0.000	3.46	0.002	3.45	0.002		
101	R1_03	2.99	0.01	0.016	0.001	2.99	0.015	2.99	0.017	3.00	0.018
102	R1_04	29.41	0.05	0.002	0.000	29.42	0.002	29.31	0.001	29.41	0.002
		29.62	n.a.	0.001	n.a.			29.62	0.001		
103	R1_05	22.45	<b>0.06</b>	0.001	0.000			22.51	0.001	22.38	0.001
		22.71	n.a.	0.000	n.a.			22.71	0.000		
		23.06	0.01	0.002	0.000			23.07	0.002	23.05	0.002
104	R1_06	19.42	0.01	0.004	0.001	19.41	0.003			19.44	0.004
		19.51	0.00	0.003	0.000			19.50	0.003		
105	R1_07	4.06	0.01	0.111	0.015	4.06	0.110	4.05	0.138	4.05	0.103
106	R1_08	4.06	0.02	0.008	0.001						
		4.40	0.04	0.001	0.000						
107	R1_09	3.00	0.00	0.004	0.000			2.99	0.004	3.00	0.004
		3.48	0.00	0.000	0.000			3.48	0.000	3.47	0.000
108	R1_10	2.45	0.01	0.026	0.002	2.46	0.025	2.43	0.025		
		2.50	<b>0.13</b>	0.009	0.004			2.62	0.006	2.37	0.013
109	R1_11	2.33	n.a.	0.003	n.a.					2.33	0.003
		2.45	0.01	0.004	0.001					2.46	0.003
		2.67	0.02	0.007	0.002	2.68	0.008			2.67	0.007
		3.12	0.04	0.004	0.000					3.07	0.004
110	R1_12	10.32	0.02	0.005	0.000	10.34	0.005	10.31	0.005	10.33	0.006

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
111	R1_13	3.86	0.02	0.018	0.002	3.85	0.018	3.83	0.018	3.89	0.017
112	R1_14	4.10	0.02	0.003	0.000	4.10	0.003	4.08	0.004	4.09	0.003
113	R1_15	21.51	0.00	0.003	0.000	21.50	0.003				
114	R1_16	4.82	0.01	0.001	0.000	4.83	0.001	4.82	0.001	4.80	0.001
115	R1_17	2.43	0.03	0.265	0.060	2.46	0.265	2.37	0.153	2.46	0.312
		2.53	n.a.	0.137	n.a.			2.53	0.137		
116	R1_18	3.50	0.02	0.010	0.001	3.50	0.010	3.48	0.010		
		3.77	<b>0.07</b>	0.017	0.007	3.85	0.016	3.77	0.008	3.64	0.023
		4.09	0.04	0.005	0.001			4.05	0.006		
		4.24	n.a.	0.004	n.a.						
117	R1_19	2.37	0.00	0.014	0.002	2.36	0.012	2.37	0.015		
		2.48	0.04	0.022	0.008	2.52	0.012	2.53	0.013	2.46	0.028
118	R1_20	2.69	0.02	0.007	0.002			2.71	0.009		
		2.84	0.03	0.010	0.003	2.82	0.013	2.90	0.006	2.81	0.015
119	R1_21	2.99	0.00	0.002	0.000			2.99	0.002	3.00	0.003
120	R1_22	10.30	0.01	0.135	0.006			10.31	0.140		
		10.67	<b>0.06</b>	0.096	0.017	10.61	0.096	10.72	0.079	10.60	0.083
		10.88	n.a.	0.045	n.a.					10.88	0.045
		11.10	<b>0.06</b>	0.076	0.024	11.02	0.085	11.06	0.089	11.08	0.055
		11.43	<b>0.07</b>	0.049	0.008			11.41	0.038		
		11.62	n.a.	0.047	n.a.			11.62	0.047		
		11.72	0.00	0.165	0.004	11.72	0.161			11.72	0.169
		11.94	<b>0.08</b>	0.087	0.018			12.04	0.065		
122	R1_24	3.64	0.01	0.003	0.000	3.63	0.003	3.66	0.003	3.64	0.003
123	R1_25	2.99	0.01	0.165	0.011	2.99	0.145	2.99	0.168	3.00	0.175
124	R1_26	26.07	0.01	0.000	0.000			26.08	0.000	26.08	0.000
125	R1_27	21.79	0.01	0.000	0.000	21.77	0.000	21.78	0.000	21.80	0.000
126	R1_28	4.84	0.01	0.002	0.000	4.83	0.002	4.82	0.002	4.85	0.002
127	R1_29	4.04	0.01	0.002	0.000	4.03	0.002	4.05	0.002	4.05	0.001
128	R1_30	4.05	0.02	0.043	0.005	4.03	0.043	4.05	0.051	4.05	0.040
129	R1_31	4.05	0.02	0.004	0.001	4.03	0.005	4.05	0.005		
130	R1_32	4.06	0.01	0.030	0.004	4.06	0.030	4.05	0.036	4.05	0.029
131	R1_33	23.93	0.01	0.005	0.000	23.92	0.005	23.94	0.006	23.92	0.005
132	R1_34	16.20	0.03	0.006	0.000	16.16	0.005	16.24	0.006	16.22	0.006
133	R1_35	4.04	0.01	0.008	0.001	4.03	0.008	4.05	0.009	4.05	0.008
134	R1_36	4.11	0.01	0.001	0.000	4.10	0.001				
137	R1_39	2.41	0.04	0.068	0.021	2.36	0.036	2.43	0.086	2.44	0.087
		2.53	0.00	0.039	0.003	2.52	0.036				

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
138	R1_40	15.24	0.02	0.029	0.002	15.23	0.027	15.24	0.030	15.21	0.028
139	R1_41	15.21	n.a.	0.006	n.a.					15.21	0.006
140	R1_42	4.16	0.00	0.002	0.000			4.16	0.002		
141	R1_43	15.25	0.01	0.003	0.001	15.23	0.003				
		15.25	0.01	0.003	0.000			15.24	0.003	15.26	0.003
142	R1_44	3.53	0.01	0.004	0.000	3.53	0.003	3.51	0.004	3.54	0.003
		16.90	0.01	0.440	0.072	16.88	0.469	16.89	0.520	16.91	0.501
143	R1_45	59.37	0.01	0.005	0.001	59.36	0.006				
144	R1_46	2.97	0.04	0.009	0.001	2.96	0.008	2.99	0.009	3.00	0.010
145	R1_47	25.60	0.00	0.001	0.000	25.59	0.001			25.60	0.002
		25.66	0.01	0.001	0.000			25.66	0.001		
146	R1_48	3.00	0.01	0.004	0.000	2.99	0.004	3.02	0.004	3.00	0.005
147	R1_49	4.72	0.00	0.003	0.000	4.72	0.003	4.71	0.004	4.72	0.003
		19.33	0.00	0.001	0.000	19.32	0.002				
148	R1_50	3.58	0.01	0.250	0.031	3.58	0.247	3.56	0.298	3.59	0.251
		4.12	n.a.	0.011	n.a.						
		4.24	0.02	0.017	0.001	4.22	0.018			4.26	0.017
		4.80	0.01	0.001	0.000	4.79	0.001	4.78	0.001	4.80	0.001
150	R1_52	3.00	0.01	0.026	0.003	2.99	0.025	2.99	0.029	3.00	0.029
151	R1_53	4.06	0.01	0.012	0.003	4.06	0.011	4.05	0.017	4.05	0.010
152	R1_54	59.34	0.02	0.008	0.003	59.36	0.010	59.36	0.010		
153	R1_55	3.81	0.02	0.005	0.001	3.79	0.006	3.83	0.006	3.83	0.005
154	R1_56	16.16	0.01	0.017	0.001	16.16	0.015	16.17	0.017	16.15	0.018
155	R1_57	59.31	0.01	0.011	0.004	59.30	0.014	59.30	0.014	59.33	0.007
156	R1_58	25.55	0.00	0.005	0.000	25.55	0.005	25.56	0.005	25.56	0.005
157	R1_59	4.18	0.02	0.002	0.000	4.18	0.002	4.16	0.002		
158	R1_60	4.28	0.02	0.001	0.000	4.28	0.001	4.25	0.001	4.26	0.001
159	R1_61	4.27	0.02	0.001	0.000	4.28	0.001	4.25	0.001	4.26	0.001
160	R1_62	4.28	0.02	0.018	0.001	4.28	0.017	4.25	0.018	4.26	0.017
161	R1_63	59.25	0.00	0.014	0.006			59.25	0.019	59.26	0.009
162	R1_64	21.79	0.01	0.004	0.000			21.78	0.004	21.80	0.004
163	R1_65	19.47	0.02	0.003	0.000					19.49	0.003
164	R1_66	19.20	0.02	0.005	0.001	19.17	0.005	19.21	0.005	19.20	0.006
		20.74	0.02	0.008	0.001	20.72	0.010	20.76	0.008	20.76	0.009
165	R1_67	3.71	n.a.	0.004	n.a.			3.71	0.004		



#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
166	R1_68	3.00	0.00	0.004	0.000			2.99	0.004	3.00	0.004
167	R1_69	3.81	<b>0.06</b>	0.001	0.000	3.73	0.001			3.83	0.001
169	R1_71	22.57 23.64	n.a. 0.00	0.001 0.001	n.a. 0.000					22.57 23.64	0.001 0.002
170	R1_72	19.21	0.00	0.004	0.000	19.21	0.004	19.21	0.004	19.20	0.004
171	R1_73	5.21	0.01	0.005	0.000	5.23	0.004	5.22	0.004	5.19	0.005
172	R1_74	59.21	0.02	0.016	0.006	59.20	0.015	59.21	0.024	59.21	0.011
173	R1_75	22.87	0.01	0.014	0.001	22.88	0.013	22.88	0.014	22.86	0.015
174	R1_76	22.87	0.01	0.017	0.001	22.88	0.016	22.88	0.018	22.86	0.018
175	R1_77	16.70	0.03	0.004	0.000	16.66	0.004	16.74	0.005	16.70	0.005
176	R1_78	59.25	0.00	0.006	0.000			59.25	0.006		
177	R1_79	2.75 2.78	<b>0.15</b> 0.04	0.005 0.012	0.001 0.003			2.90 2.71	0.004 0.013		2.81 0.014
178	R1_80	25.84	0.02	0.011	0.001	25.84	0.012	25.86	0.010	25.86	0.012
179	R1_81	20.18	0.01	0.010	0.001	20.17	0.009	20.19	0.010	20.19	0.011
180	R1_82	59.20 59.21	0.01 0.00	0.005 0.005	0.001 0.001					59.20 59.21	0.004 0.006
181	R1_83	22.84	0.02	0.006	0.001	22.83	0.007	22.84	0.008	22.81	0.007
182	R1_84	20.89	0.02	0.000	0.000	20.85	0.000	20.90	0.000	20.90	0.000
183	R1_85	20.87	0.02	0.001	0.000	20.85	0.001	20.85	0.001	20.90	0.001
184	R1_86	59.19	0.02	0.018	0.005	59.20	0.018	59.21	0.026	59.21	0.011
185	R1_87	4.05	0.00	0.004	0.000			4.05	0.004		
186	R1_88	17.64	0.01	0.055	0.002	17.64	0.056	17.65	0.057	17.62	0.054
187	R1_89	59.18 59.21	0.03 0.01	0.009 0.008	0.001 0.002	59.15	0.008	59.21	0.009		59.21 0.005
188	R1_90	23.50	0.00	0.003	0.000	23.51	0.003	23.50	0.003	23.50	0.003
189	R1_91	59.19	0.02	0.018	0.003	59.15	0.019	59.21	0.020	59.21	0.014
190	R1_92	20.76	n.a.	0.003	n.a.			20.76	0.003		
192	R1_94	25.86	0.01	0.006	0.000	25.89	0.006	25.86	0.006	25.86	0.007
193	R1_95	20.35	0.02	0.008	0.001	20.34	0.009	20.37	0.008	20.36	0.008
194	R1_96	19.55 28.73	0.01 0.01	0.003 0.000	0.000 0.000	19.55	0.003	19.55 28.72	0.003 0.000	19.54 28.72	0.003 0.000
195	R1_97	28.73	0.01	0.200	0.018	28.74	0.190	28.72	0.218	28.72	0.222

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
196	R1_98	19.55	0.01	0.029	0.003	19.55	0.027	19.55	0.028	19.54	0.031
		21.58	0.02	0.010	0.001	21.61	0.011	21.56	0.010	21.57	0.011
197	R1_99	19.55	0.01	0.003	0.000	19.55	0.003	19.55	0.003	19.54	0.003
198	R1_100	19.55	0.01	0.002	0.000	19.55	0.001	19.55	0.001	19.54	0.002
199	R1_101	2.44	0.04	0.271	0.055	2.43	0.282	2.37	0.181	2.44	0.334
		2.44	<b>0.09</b>	0.142	0.012			2.53	0.154		
200	R1_102	24.96	0.03	0.001	0.000	24.99	0.001	24.97	0.001	24.92	0.001
201	R1_103	19.24	0.01	0.001	0.000			19.25	0.001	19.23	0.001
202	R1_104	21.20	0.01	0.019	0.001	21.21	0.020	21.21	0.020	21.21	0.019
203	R1_105	28.71	0.02	0.000	0.000	28.70	0.000	28.72	0.000	28.72	0.000
204	R1_106	59.14	0.02	0.012	0.001	59.15	0.014	59.15	0.010	59.11	0.011
205	R1_107	29.55	0.02	0.001	0.000	29.55	0.001	29.57	0.001	29.55	0.001
206	R1_108	29.55	0.02	0.010	0.001	29.55	0.009	29.57	0.009	29.55	0.009
207	R1_109	29.55	0.02	0.001	0.000	29.55	0.001	29.57	0.001	29.55	0.001
208	R1_110	25.81	n.a.	0.003	n.a.						
209	R1_111	24.22	0.02	0.005	0.000	24.23	0.005	24.21	0.006	24.23	0.006
210	R1_112	32.89	n.a.	0.001	n.a.					32.89	0.001
211	R1_113	28.72	0.01	0.001	0.000	28.70	0.001	28.72	0.001	28.72	0.001
212	R1_114	28.73	0.01	0.001	0.000	28.74	0.000	28.72	0.001	28.72	0.001
213	R1_115	59.14	0.02	0.022	0.008	59.15	0.030	59.15	0.017	59.16	0.009
214	R1_116	19.97	0.01	0.002	0.000					19.96	0.002
		19.97	0.02	0.002	0.000	19.95	0.002	19.97	0.002		
215	R1_117	19.97	0.02	0.018	0.001	19.95	0.019	19.97	0.019	19.96	0.019
216	R1_118	3.71	n.a.	0.000	n.a.			3.71	0.000		
217	R1_119	59.14	0.02	0.016	0.003	59.15	0.021	59.15	0.012	59.16	0.013
218	R1_120	59.14	0.02	0.032	0.005	59.15	0.038	59.15	0.026	59.16	0.027
219	R1_121	28.44	n.a.	0.005	n.a.						
221	R1_123	20.72	0.01	0.010	0.001	20.72	0.011	20.71	0.010	20.72	0.011
222	R1_124	59.11	0.02	0.014	0.001	59.11	0.015	59.10	0.014	59.11	0.015
223	R1_125	16.27	0.02	0.004	0.000			16.24	0.004	16.29	0.004
224	R1_126	21.81	0.02	0.039	0.004	21.82	0.037	21.78	0.039	21.80	0.043
225	R1_127	25.94	0.02	0.016	0.003	25.94	0.014	25.96	0.016	25.96	0.020

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
226	R1_128	28.91	0.02	0.005	0.000	28.91	0.005	28.94	0.006	28.88	0.005
228	R1_130	59.11	0.02	0.019	0.003	59.11	0.021	59.10	0.015	59.11	0.017
229	R1_131	25.86	0.01	0.012	0.001	25.89	0.010	25.86	0.012	25.86	0.014
230	R1_132	21.79	0.01	0.003	0.000			21.78	0.003	21.80	0.004
231	R1_133	59.11	0.02	0.035	0.003	59.11	0.036	59.10	0.031	59.11	0.033
232	R1_134	59.07	0.03	0.015	0.002	59.11	0.014	59.05	0.018	59.05	0.018
233	R1_135	29.20	0.01	0.000	0.000	29.18	0.000	29.20	0.000	29.21	0.000
234	R1_136	29.20	0.01	0.001	0.000	29.18	0.001	29.20	0.001	29.21	0.001
235	R1_137	29.20	0.01	0.014	0.001	29.18	0.013	29.20	0.015	29.21	0.014
236	R1_138	17.29	0.01	0.006	0.000	17.29	0.005	17.30	0.006	17.27	0.007
237	R1_139	22.32	0.01	0.008	0.001	22.32	0.007	22.33	0.009	22.31	0.009
238	R1_140	36.67	0.03	0.019	0.001	36.66	0.018	36.66	0.019	36.67	0.019
239	R1_141	59.07	0.03	0.019	0.002	59.11	0.018	59.05	0.018	59.05	0.021
240	R1_142	16.96	0.02	0.001	0.000	16.93	0.001	16.99	0.001	16.96	0.001
241	R1_143	59.07	0.03	0.034	0.004	59.11	0.028	59.05	0.033	59.05	0.038
242	R1_144	18.97	0.02	0.004	0.000			18.95	0.004	18.99	0.004
243	R1_145	30.15	0.01	0.004	0.000			30.14	0.004	30.16	0.004
244	R1_146	59.05	0.00	0.011	0.002			59.05	0.009	59.05	0.011
245	R1_147	34.89	0.02	0.001	0.000	34.86	0.001	34.91	0.001	34.92	0.001
246	R1_148	32.39	0.01	0.007	0.000	32.38	0.007	32.40	0.007	32.39	0.007
247	R1_149	2.69	0.02	0.007	0.002			2.71	0.009		
		2.82	0.05	0.011	0.004	2.77	0.016	2.90	0.005	2.81	0.014
248	R1_150	2.37	n.a.	0.137	n.a.			2.37	0.137		
		2.48	0.04	0.183	0.039	2.43	0.211	2.53	0.116	2.50	0.176
249	R1_151	21.79	0.01	0.001	0.000	21.77	0.001	21.78	0.001	21.80	0.001
250	R1_152	21.79	0.01	0.040	0.005	21.77	0.037	21.78	0.041	21.80	0.044
251	R1_153	5.02	0.01	0.001	0.000			5.02	0.001	5.04	0.001
252	R1_154	21.79	0.01	0.001	0.000	21.77	0.001	21.78	0.001	21.80	0.001
253	R1_155	5.02	0.01	0.001	0.000	5.02	0.001	5.02	0.001	5.04	0.001
254	R1_156	5.02	0.01	0.001	0.000	5.02	0.001	5.02	0.001	5.04	0.001
255	R1_157	59.07	0.03	0.004	0.001	59.11	0.003	59.05	0.005	59.05	0.005
256	R1_158	28.97	0.02	0.007	0.000	28.97	0.007	29.00	0.007	28.94	0.007

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
257	R1_159	21.79	0.01	0.003	0.000			21.78	0.003	21.80	0.004
258	R1_160	59.05	0.00	0.037	0.004			59.05	0.036	59.05	0.041
		59.11	n.a.	0.023	n.a.	59.11	0.023				
259	R1_161	17.38	0.02	0.008	0.000	17.36	0.007	17.37	0.007	17.41	0.008
260	R1_162	59.00	0.01	0.014	0.005	58.99	0.006	59.00	0.017	59.01	0.019
261	R1_163	19.02	0.02	0.008	0.001	19.00	0.008	19.01	0.008	19.04	0.009
262	R1_164	59.00	0.00	0.005	0.000			59.00	0.005		
		59.01	0.00	0.004	0.001					59.01	0.005
263	R1_165	26.40	0.02	0.006	0.000	26.40	0.006	26.42	0.006	26.42	0.007
264	R1_166	29.41	0.05	0.003	0.001			29.49	0.002	29.37	0.004
265	R1_167	30.47	0.01	0.001	0.000			30.46	0.001	30.49	0.001
		59.02	0.02	0.019	0.005	59.06	0.011	59.00	0.020	59.01	0.024
266	R1_168	58.99	0.03	0.012	0.002			59.00	0.010	59.01	0.013
267	R1_169	58.99	0.02	0.015	0.004	58.99	0.009	59.00	0.018	59.01	0.018
268	R1_170	16.76	0.01	0.003	0.000			16.74	0.004	16.77	0.003
269	R1_171	58.98	0.03	0.012	0.005	58.94	0.006	59.00	0.015	59.01	0.017
270	R1_172	58.99	0.03	0.004	0.000			59.00	0.004	59.01	0.005
271	R1_173	21.07	0.03	0.008	0.001	21.03	0.009	21.09	0.009	21.09	0.008
272	R1_174	30.72	0.02	0.184	0.006	30.70	0.184	30.74	0.184	30.72	0.194
273	R1_175	58.97	0.03	0.018	0.006	58.94	0.010	59.00	0.020	58.97	0.023
274	R1_176	5.23	0.02	0.004	0.000			5.22	0.004	5.26	0.004
275	R1_177	33.39	n.a.	0.002	n.a.						
		58.98	0.02	0.034	0.011	58.99	0.019	59.00	0.036	58.97	0.044
276	R1_178	58.95	0.01	0.012	0.004	58.94	0.008	58.95	0.014	58.97	0.015
277	R1_179	30.72	0.02	0.019	0.001	30.70	0.021	30.74	0.019	30.72	0.020
278	R1_180	26.10	0.02	0.014	0.001	26.11	0.013	26.08	0.014	26.08	0.015
		28.15	0.02	0.012	0.000	28.15	0.012	28.18	0.012	28.18	0.013
279	R1_181	26.88	n.a.	0.004	n.a.						
		26.89	<b>0.07</b>	0.004	0.001			26.82	0.003		
		27.18	n.a.	0.003	n.a.			27.18	0.003		
		27.67	0.03	0.002	0.000			27.69	0.002		
280	R1_182	58.95	0.01	0.009	0.004	58.94	0.005	58.95	0.009	58.97	0.013
281	R1_183	30.73	0.01	0.006	0.000			30.74	0.005	30.72	0.006
282	R1_184	58.95	n.a.	0.004	n.a.						
283	R1_185	21.41	0.01	0.001	0.000	21.39	0.001	21.40	0.001	21.41	0.001

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
284	R1_186	24.38	0.02	0.002	0.000			24.36	0.003		
		27.09	n.a.	0.009	n.a.					27.09	0.009
		27.33	0.04	0.008	0.001	27.32	0.007	27.38	0.009		
		27.96	n.a.	0.009	n.a.	27.96	0.009				
		28.16	0.02	0.008	0.001			28.18	0.008		
		28.31	n.a.	0.007	n.a.					28.31	0.007
285	R1_187	2.41	0.04	0.076	0.035	2.36	0.061	2.43	0.145	2.37	0.054
		2.54	0.03	0.053	0.022	2.52	0.059			2.50	0.086
286	R1_188	58.94	0.03	0.030	0.009	58.89	0.019	58.95	0.032	58.97	0.040
287	R1_189	2.36	0.01	0.066	0.013			2.37	0.084	2.37	0.058
		2.49	0.03	0.099	0.018	2.43	0.128	2.53	0.071	2.50	0.092
288	R1_190	21.74	0.01	0.004	0.000			21.73	0.004	21.75	0.005
289	R1_191	58.94	0.01	0.011	0.002	58.94	0.008	58.95	0.011	58.92	0.013
290	R1_192	22.79	n.a.	0.020	n.a.			22.79	0.020		
291	R1_193	19.88	0.01	0.001	0.000	19.86	0.001	19.88	0.001	19.87	0.001
292	R1_194	19.88	0.01	0.011	0.001	19.86	0.012	19.88	0.012	19.87	0.011
293	R1_195	19.88	0.01	0.001	0.000	19.86	0.001	19.88	0.001	19.87	0.001
294	R1_196	21.45	n.a.	0.002	n.a.			21.45	0.002		
295	R1_197	25.10	0.02	0.005	0.000	25.12	0.005	25.10	0.005	25.10	0.005
296	R1_198	58.92	0.02	0.016	0.004	58.89	0.010	58.95	0.014	58.92	0.019
298	R1_200	58.91	n.a.	0.009	n.a.						
299	R1_201	58.92	0.02	0.007	0.002	58.89	0.006	58.95	0.007	58.92	0.010
300	R1_202	24.89	0.01	0.023	0.002	24.90	0.024	24.88	0.024	24.88	0.023
301	R1_203	36.26	0.02	0.001	0.000	36.24	0.001				
302	R1_204	36.24	0.03	0.019	0.001	36.24	0.018	36.24	0.020	36.25	0.022
303	R1_205	27.45	n.a.	0.001	n.a.						
		33.88	n.a.	0.003	n.a.						
		33.95	0.01	0.004	0.000			33.96	0.004	33.94	0.004
304	R1_206	19.29	<b>0.08</b>	0.017	0.008					19.36	0.024
		19.32	0.05	0.022	0.007	19.32	0.028	19.33	0.029	19.23	0.010
		22.60	<b>0.17</b>	0.004	0.001					22.77	0.006
		26.51	0.02	0.008	0.000	26.50	0.008	26.53	0.009	26.53	0.008
305	R1_207	28.80	0.02	0.002	0.000	28.79	0.002	28.82	0.002	28.82	0.002
306	R1_208	18.22	0.02	0.002	0.000	18.19	0.002	18.20	0.002		
		29.50	0.01	0.001	0.000	29.51	0.001				
		29.80	0.02	0.005	0.000			29.81	0.005	29.78	0.005
307	R1_209	28.80	0.02	0.002	0.000	28.79	0.002	28.82	0.003	28.82	0.003
308	R1_210	58.90	0.03	0.017	0.006	58.89	0.013	58.95	0.015	58.87	0.027

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
309	R1_211	28.79	0.02	0.001	0.000	28.79	0.001	28.82	0.002	28.77	0.002
310	R1_212	42.53	0.03	0.020	0.001	42.51	0.018	42.51	0.020	42.54	0.022
311	R1_213	31.33	0.02	0.003	0.000			31.30	0.002	31.34	0.002
312	R1_214	20.21	0.02	0.008	0.001	20.22	0.008	20.19	0.009	20.19	0.009
313	R1_215	58.89	0.00	0.007	0.000	58.89	0.007	58.89	0.007		
		58.89	0.02	0.009	0.004					58.87	0.014
314	R1_216	58.89	0.01	0.011	0.004	58.89	0.009	58.89	0.009	58.87	0.019
315	R1_217	58.89	0.01	0.004	0.001	58.89	0.003	58.89	0.002	58.87	0.006
316	R1_218	25.01	0.02	0.014	0.001	24.99	0.015	25.01	0.015	25.01	0.015
		30.00	0.04	0.006	0.000	30.06	0.005	30.04	0.006	29.98	0.006
317	R1_219	19.81	n.a.	0.003	n.a.						
		20.61	0.01	0.005	0.000	20.59	0.005	20.61	0.005	20.61	0.005
318	R1_220	20.61	0.01	0.059	0.006	20.59	0.066	20.61	0.060	20.61	0.059
319	R1_221	16.00	0.02	0.002	0.000	16.02	0.002	15.96	0.002	16.00	0.002
320	R1_222	15.91	0.02	0.004	0.000			15.88	0.004	15.93	0.004
321	R1_223	58.88	0.01	0.007	0.002	58.89	0.005	58.89	0.005	58.87	0.010
322	R1_224	29.33	0.01	0.002	0.000	29.33	0.002	29.31	0.003	29.33	0.002
323	R1_225	4.07	0.01	0.006	0.002	4.06	0.006	4.08	0.009	4.05	0.004
324	R1_226	58.88	0.01	0.007	0.003	58.89	0.006	58.89	0.006	58.87	0.013
325	R1_227	36.44	0.01	0.259	0.022	36.44	0.248	36.45	0.258	36.45	0.302
326	R1_228	36.42	0.01	0.017	0.001						
327	R1_229	14.19	0.03	0.045	0.003	14.23	0.041	14.16	0.045	14.20	0.049
328	R1_230	36.44	0.01	0.131	0.006	36.44	0.124	36.45	0.134	36.45	0.141
329	R1_231	27.41	0.00	0.001	0.000	27.40	0.000				
330	R1_232	36.44	0.01	0.090	0.007	36.44	0.087	36.45	0.093	36.45	0.102
331	R1_233	58.87	0.01	0.006	0.003	58.89	0.004			58.87	0.011
332	R1_234	25.47	0.01	0.012	0.002	25.46	0.009	25.47	0.013	25.47	0.014
333	R1_235	19.00	0.01	0.005	0.002			19.01	0.004	18.99	0.008
334	R1_236	58.88	0.01	0.005	0.002	58.89	0.004	58.89	0.004	58.87	0.009
		59.11	n.a.	0.001	n.a.					59.11	0.001
335	R1_237	36.44	0.01	0.013	0.002	36.44	0.014	36.45	0.013	36.45	0.016
336	R1_238	31.57	0.01	0.008	0.002	31.58	0.004	31.58	0.009	31.55	0.009
337	R1_239	36.41	0.05	0.004	0.001					36.45	0.004

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
338	R1_240	36.45	0.02	0.005	0.001	36.44	0.005	36.45	0.005	36.45	0.006
339	R1_241	36.47	0.02	0.003	0.000			36.49	0.003	36.45	0.003
340	R1_242	28.57	0.02	0.004	0.000			28.61	0.004	28.55	0.004
341	R1_243	34.87	0.01	0.003	0.000	34.86	0.003				
		34.92	0.00	0.004	0.000			34.91	0.003	34.92	0.004
342	R1_244	42.64	0.01	0.005	0.000	42.64	0.005	42.64	0.005	42.66	0.006
343	R1_245	42.63	0.01	0.007	0.000	42.64	0.006	42.64	0.006	42.60	0.007
344	R1_246	24.41	0.02	0.004	0.000			24.40	0.004	24.44	0.003
345	R1_247	42.64	0.01	0.004	0.000	42.64	0.004	42.64	0.004	42.66	0.004
346	R1_248	22.18	0.02	0.006	0.002	22.17	0.005	22.19	0.011	22.21	0.005
347	R1_249	36.84	0.02	0.020	0.001	36.83	0.021	36.84	0.021	36.85	0.020
348	R1_250	24.98	0.01	0.004	0.000	24.99	0.004	24.97	0.004	24.97	0.004
349	R1_251	36.84	0.02	0.010	0.000	36.83	0.010	36.84	0.010	36.85	0.010
350	R1_252	24.16	0.02	0.030	0.002	24.17	0.028	24.15	0.034	24.17	0.031
351	R1_253	31.63	0.02	0.004	0.000	31.63	0.004	31.63	0.004	31.65	0.004
352	R1_254	34.89	0.02	0.012	0.001	34.86	0.011	34.91	0.012	34.92	0.013
353	R1_255	23.05	0.01	0.009	0.001	23.04	0.009	23.07	0.010	23.05	0.010
354	R1_256	34.08	n.a.	0.001	n.a.			34.08	0.001		
355	R1_257	23.04	0.01	0.013	0.001	23.04	0.014	23.03	0.015	23.05	0.014
356	R1_258	22.56	0.02	0.002	0.000	22.59	0.002	22.56	0.002	22.57	0.002
358	R1_260	24.15	n.a.	0.004	n.a.			24.15	0.004		
359	R1_261	28.45	0.02	0.013	0.001	28.46	0.011	28.49	0.013	28.43	0.014
360	R1_262	20.17	0.02	0.009	0.001	20.17	0.010	20.14	0.010	20.19	0.011
		22.00	n.a.	0.004	n.a.			22.00	0.004		
		23.65	n.a.	0.022	n.a.						
		23.89	0.01	0.044	0.000					23.88	0.044
		28.45	0.02	0.011	0.001	28.46	0.011	28.49	0.011	28.43	0.013
361	R1_263	23.05	0.01	0.036	0.003	23.04	0.036	23.07	0.040	23.05	0.040
362	R1_264	2.40	0.00	0.058	0.012						
363	R1_265	2.37	n.a.	0.038	n.a.					2.37	0.038
		2.54	0.03	0.034	0.013	2.52	0.034	2.56	0.028	2.50	0.059
364	R1_266	36.52	0.02	0.007	0.000	36.49	0.007	36.55	0.007	36.50	0.007
365	R1_267	27.90	0.02	0.007	0.000	27.90	0.007	27.92	0.007	27.92	0.007
366	R1_268	39.00	0.04	0.004	0.000	38.98	0.004	39.02	0.004	39.02	0.004

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
367	R1_269	38.99	0.04	0.008	0.000	38.98	0.008	38.97	0.008	39.02	0.008
368	R1_270	36.80	0.03	0.005	0.000	36.78	0.005	36.79	0.005	36.85	0.005
369	R1_271	36.45	0.03	0.002	0.000	36.44	0.001	36.49	0.002	36.45	0.002
370	R1_272	31.54	0.03	0.004	0.000	31.51	0.004	31.51	0.004	31.55	0.004
371	R1_273	40.28	0.01	0.003	0.000	40.28	0.003				
		40.34	0.01	0.004	0.000			40.32	0.003	40.34	0.004
372	R1_274	25.08	0.01	0.159	0.008	25.08	0.155	25.10	0.166	25.06	0.171
373	R1_275	30.27	0.05	0.017	0.006	30.21	0.011			30.32	0.023
		30.40	0.01	0.024	0.007	30.40	0.012	30.39	0.030		
		30.66	0.01	0.008	0.000	30.65	0.008			30.67	0.007
374	R1_276	25.08	0.01	0.081	0.005	25.08	0.084	25.10	0.086	25.06	0.086
375	R1_277	27.84	0.03	0.013	0.000	27.83	0.014	27.86	0.014	27.86	0.014
376	R1_278	20.67	0.01	0.037	0.002	20.65	0.041	20.68	0.037	20.68	0.036
		29.96	0.02	0.019	0.000			29.97	0.020		
		30.47	n.a.	0.002	n.a.	30.47	0.002				
		30.59	n.a.	0.002	n.a.	30.59	0.002				
		30.91	0.04	0.001	0.000	30.86	0.002	30.92	0.001	30.95	0.001
377	R1_279	25.07	0.01	0.062	0.005	25.08	0.065	25.06	0.065	25.06	0.067
378	R1_280	25.72	0.02	0.003	0.000			25.71	0.003	25.71	0.003
		26.13	0.01	0.003	0.000					26.12	0.004
379	R1_281	21.48	n.a.	0.003	n.a.						
		24.97	0.03	0.003	0.001	24.99	0.002	24.97	0.004	24.92	0.003
380	R1_282	25.03	0.01	0.002	0.000	25.04	0.002	25.01	0.001	25.01	0.002
381	R1_283	32.10	0.01	0.002	0.000			32.09	0.002		
		32.32	n.a.	0.002	n.a.			32.32	0.002		
		33.79	0.03	0.095	0.002	33.77	0.093	33.83	0.096	33.81	0.096
382	R1_284	20.67	<b>0.07</b>	0.006	0.003	20.59	0.005	20.58	0.003	20.76	0.007
		20.68	0.05	0.006	0.002	20.72	0.009	20.71	0.006	20.61	0.004
383	R1_285	28.50	0.01	0.005	0.000			28.49	0.005	28.49	0.006
		30.76	0.02	0.024	0.001	30.75	0.025	30.74	0.024	30.78	0.026
384	R1_286	30.76	0.02	0.006	0.000	30.75	0.006	30.74	0.006	30.78	0.007
385	R1_287	47.57	0.02	0.003	0.000	47.54	0.004	47.58	0.003	47.58	0.004
386	R1_288	40.30	0.04	0.030	0.001	40.28	0.028	40.32	0.029	40.29	0.032
		47.58	n.a.	0.003	n.a.					47.58	0.003
387	R1_289	24.89	0.02	0.004	0.000	24.86	0.004	24.88	0.004	24.92	0.005
		25.04	n.a.	0.004	n.a.						
388	R1_290	24.84	0.01	0.005	0.001	24.86	0.005	24.84	0.005	24.83	0.005
389	R1_291	47.51	n.a.	0.003	n.a.						
		47.59	0.00	0.003	0.000	47.59	0.003	47.58	0.003	47.58	0.003



#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
390	R1_292	40.31	0.04	0.049	0.002	40.28	0.048	40.32	0.047	40.34	0.051
		41.74	0.02	0.006	0.000					41.76	0.006
391	R1_293	40.28	0.02	0.024	0.001	40.28	0.025	40.27	0.023	40.29	0.025
392	R1_294	25.04	0.02	0.087	0.006	25.04	0.091	25.06	0.094	25.01	0.092
393	R1_295	24.51	0.01	0.004	0.000	24.50	0.004	24.52	0.004	24.51	0.004
394	R1_296	40.28	0.02	0.008	0.002	40.28	0.007	40.27	0.007	40.29	0.007
395	R1_297	40.30	0.03	0.004	0.000	40.28	0.004	40.32	0.004	40.34	0.004
396	R1_298	25.96	n.a.	0.003	n.a.					25.96	0.003
397	R1_299	32.84	0.01	0.013	0.000	32.83	0.012	32.85	0.013	32.84	0.013
398	R1_300	20.58	0.01	0.007	0.001	20.56	0.008	20.58	0.006	20.58	0.007
399	R1_301	2.36	n.a.	0.023	n.a.	2.36	0.023				
		2.44	0.03	0.042	0.009	2.49	0.036	2.40	0.052	2.44	0.030
		2.55	0.01	0.022	0.004			2.56	0.019	2.56	0.021
400	R1_302	19.91	0.01	0.006	0.001	19.90	0.005	19.93	0.006	19.92	0.006
401	R1_303	38.00	0.02	0.004	0.000	38.00	0.003	38.00	0.004	37.98	0.004
402	R1_304	27.21	0.01	0.009	0.000	27.21	0.009	27.24	0.009	27.20	0.008
403	R1_305	23.75	0.01	0.002	0.000	23.76	0.001	23.75	0.002	23.76	0.002
404	R1_306	23.74	0.01	0.048	0.005	23.73	0.044	23.75	0.056	23.72	0.052
405	R1_307	23.75	0.01	0.001	0.000	23.76	0.001	23.75	0.002	23.76	0.002
406	R1_308	36.08	0.03	0.015	0.000	36.05	0.015	36.11	0.015	36.12	0.016
407	R1_309	37.38	0.02	0.013	0.002	37.37	0.012	37.37	0.013	37.40	0.014
408	R1_310	26.77	0.01	0.001	0.000	26.76	0.001	26.79	0.001	26.76	0.001
409	R1_311	26.77	0.01	0.021	0.006	26.76	0.018	26.79	0.018	26.76	0.017
410	R1_312	19.92	0.01	0.030	0.003	19.90	0.032	19.93	0.031	19.92	0.032
411	R1_313	28.08	0.03	0.008	0.001	28.09	0.009	28.12	0.005	28.05	0.009
412	R1_314	22.31	0.01	0.008	0.001	22.32	0.007	22.29	0.009	22.31	0.009
413	R1_315	27.63	0.01	0.001	0.000	27.62	0.001	27.64	0.002	27.63	0.002
414	R1_316	27.63	0.01	0.002	0.000	27.62	0.002	27.64	0.003	27.63	0.002
415	R1_317	27.63	0.01	0.027	0.001	27.62	0.028	27.64	0.029	27.63	0.026
416	R1_318	27.63	0.01	0.002	0.000	27.62	0.002	27.64	0.002	27.63	0.002
417	R1_319	27.64	0.01	0.002	0.000			27.64	0.002	27.63	0.002
418	R1_320	16.17	0.02	0.006	0.000	16.16	0.006	16.17	0.006	16.15	0.007

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
419	R1_321	35.01	0.02	0.056	0.004	34.99	0.052	35.04	0.055	35.04	0.062
420	R1_322	34.99	0.00	0.002	0.000	34.99	0.002	35.04	0.002	35.04	0.002
		35.03	0.01	0.002	0.000	35.91	0.010	35.90	0.010	35.91	0.010
		35.90	0.03	0.010	0.000						
421	R1_323	35.01	0.02	0.010	0.002	34.99	0.010	35.04	0.011	35.04	0.012
422	R1_324	31.62	0.01	0.005	0.000	31.63	0.005	31.63	0.006	31.61	0.006
424	R1_326	33.28	0.02	0.018	0.001	33.28	0.017	33.27	0.017	33.30	0.019
425	R1_327	2.53	0.03	0.036	0.012			2.50	0.049	2.56	0.024
426	R1_328	41.59	0.02	0.079	0.004	41.58	0.075	41.58	0.079	41.61	0.084
427	R1_329	25.10	n.a.	0.010	n.a.			25.10	0.010		
		33.11	0.01	0.169	0.006	33.12	0.174	33.10	0.161	33.13	0.175
		33.41	<b>0.16</b>	0.016	0.008					33.57	0.008
428	R1_330	28.45	0.03	0.001	0.000			28.49	0.001	28.43	0.001
429	R1_331	34.08	0.00	0.005	0.002			34.08	0.008	34.07	0.004
430	R1_332	31.16	0.01	0.008	0.001	31.17	0.008	31.17	0.008	31.14	0.009
431	R1_333	38.59	0.02	0.006	0.000	38.58	0.006	38.61	0.006	38.60	0.006
432	R1_334	33.89	n.a.	0.003	n.a.			33.89	0.003		
433	R1_335	20.90	0.01	0.006	0.000	20.90	0.006	20.90	0.006	20.90	0.006
434	R1_336	38.71	0.02	0.124	0.004	38.69	0.117	38.73	0.130	38.72	0.125
435	R1_337	31.62	0.01	0.005	0.000	31.63	0.004	31.63	0.005	31.61	0.005
436	R1_338	38.71	0.02	0.007	0.000	38.69	0.007	38.73	0.007	38.72	0.007
437	R1_339	27.46	0.01	0.004	0.000	27.44	0.004	27.47	0.004		
		29.95	0.02	2.293	0.117	29.94	2.242	29.97	2.446	29.94	2.400
		30.92	0.05	0.071	0.027	30.92	0.036	30.98	0.042	30.89	0.098
		32.09	0.01	0.006	0.001	32.08	0.006				
438	R1_340	42.39	0.00	0.003	0.000			42.39	0.003		
		42.70	n.a.	0.001	n.a.	42.70	0.001				
439	R1_341	41.58	0.01	0.081	0.046	41.58	0.159			41.58	0.050
		41.75	0.01	0.068	0.059					41.76	0.127
		42.26	<b>0.08</b>	0.004	0.000	42.33	0.004				
		42.40	<b>0.12</b>	0.181	0.026	42.45	0.145	42.27	0.217	42.60	0.163
440	R1_342	41.56	0.02	0.007	0.000	41.55	0.007	41.55	0.007	41.58	0.007
		41.76	0.00	0.002	0.000					41.76	0.002
		42.05	<b>0.07</b>	0.012	0.004			41.98	0.008	42.12	0.016
		42.32	0.01	0.027	0.002	42.33	0.025				
		42.54	0.03	0.021	0.001			42.51	0.022		
		42.73	n.a.	0.014	n.a.					42.73	0.014
441	R1_343	29.99	0.03	0.003	0.000	29.98	0.003	30.04	0.003	29.98	0.003
442	R1_344	25.00	0.01	0.006	0.000	24.99	0.006	25.01	0.006	25.01	0.007

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
443	R1_345	25.04	0.02	0.090	0.006	25.04	0.091	25.06	0.094	25.01	0.098
444	R1_346	18.11	0.01	0.004	0.000	18.10	0.004	18.11	0.004	18.10	0.004
445	R1_347	18.14	0.01	0.004	0.000	18.14	0.004	18.15	0.004	18.14	0.005
446	R1_348	25.04	0.02	0.010	0.001	25.04	0.011	25.06	0.011	25.01	0.011
447	R1_349	18.12	0.02	0.004	0.000	18.10	0.004	18.11	0.004	18.14	0.004
		19.80	0.02	0.007	0.001	19.78	0.008	19.80	0.008	19.83	0.006
448	R1_350	18.10	0.02	0.004	0.000	18.10	0.004	18.11	0.004	18.10	0.004
449	R1_351	25.01	n.a.	0.004	n.a.			25.01	0.004		
450	R1_352	24.92	0.01	0.019	0.002	24.90	0.019	24.92	0.021	24.92	0.021
		36.44	0.01	0.007	0.000	36.44	0.007	36.45	0.007	36.45	0.008
451	R1_353	36.43	0.02	0.028	0.001	36.39	0.027	36.45	0.031	36.45	0.028
452	R1_354	24.93	0.01	0.003	0.000	24.95	0.003	24.92	0.003	24.92	0.003
		36.44	0.01	0.010	0.002	36.44	0.009	36.45	0.010	36.45	0.014
453	R1_355	40.18	0.03	0.008	0.001	40.18	0.007	40.16	0.008	40.24	0.008
454	R1_356	19.00	0.01	0.057	0.006	19.00	0.056	19.01	0.058	18.99	0.067
455	R1_357	19.09	0.02	0.015	0.004	19.06	0.013	19.13	0.019	19.10	0.020
456	R1_358	24.59	n.a.	0.017	n.a.						
		25.40	0.02	0.014	0.005	25.38	0.014	25.40	0.018	25.40	0.016
		28.08	0.03	0.020	0.001	28.09	0.020	28.12	0.020	28.05	0.021
		41.63	0.01	0.026	0.006	41.62	0.030	41.62	0.019		
		41.83	0.03	0.049	0.011			41.81	0.049	41.80	0.067
457	R1_359	19.00	0.01	0.010	0.002	19.00	0.010	19.01	0.010	18.99	0.014
458	R1_360	19.00	0.01	0.005	0.000			19.01	0.005	18.99	0.006
459	R1_361	32.80	0.01	0.171	0.005	32.78	0.170	32.80	0.174	32.80	0.180
460	R1_362	32.79	0.02	0.022	0.001	32.78	0.024	32.80	0.023	32.80	0.022
462	R1_364	32.79	0.02	0.004	0.000	32.78	0.004	32.80	0.004	32.80	0.004
463	R1_365	25.61	0.02	0.068	0.005	25.59	0.063	25.61	0.070	25.60	0.078
		38.24	0.02	0.051	0.005	38.23	0.051	38.23	0.055	38.26	0.059
		38.36	<b>0.09</b>	0.006	0.001	38.45	0.006				
		38.47	0.02	0.006	0.002			38.45	0.008	38.49	0.004
		38.60	0.04	0.044	0.023	38.61	0.012	38.65	0.048	38.57	0.037
		38.73	0.04	0.046	0.021			38.76	0.043	38.76	0.073
		38.86	0.02	0.007	0.001					38.84	0.006
		39.11	0.03	0.058	0.020	39.12	0.085			39.11	0.068
		39.40	0.05	0.115	0.048			39.36	0.172		
		39.59	0.03	0.029	0.006					39.61	0.023
		39.92	n.a.	0.035	n.a.					39.92	0.035
464	R1_366	22.92	n.a.	0.001	n.a.	22.92	0.001				
		23.46	0.01	0.002	0.000	23.47	0.002	23.45	0.002		
		23.74	0.01	0.004	0.002	23.73	0.003	23.75	0.008	23.72	0.004
		24.01	n.a.	0.001	n.a.					24.01	0.001

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
464	R1_366	24.48	0.01	0.011	0.003	24.47	0.012	24.49	0.014	24.48	0.012
465	R1_367	39.53	0.03	0.002	0.000	39.51	0.002	39.54	0.002	39.56	0.003
466	R1_368	19.01	0.00	0.007	0.000	19.00	0.007	19.01	0.007	19.04	0.011
467	R1_369	37.88	0.02	0.004	0.001			37.86	0.003		
468	R1_370	28.08	0.03	0.004	0.000	28.09	0.004	28.12	0.004	28.05	0.004
469	R1_371	41.48	n.a.	0.004	n.a.						
470	R1_372	26.42	0.02	0.142	0.007			26.42	0.147	26.42	0.149
471	R1_373	41.49	0.01	0.004	0.000			41.49	0.004		
472	R1_374	26.41	0.02	0.029	0.014	26.40	0.025	26.42	0.024	26.42	0.057
473	R1_375	40.32	0.03	0.022	0.001	40.28	0.021	40.32	0.022	40.34	0.023
474	R1_376	26.43	0.01	0.007	0.004			26.42	0.013	26.42	0.004
475	R1_377	40.32	0.02	0.004	0.000			40.32	0.004	40.34	0.003
476	R1_378	18.13	0.02	0.005	0.001	18.10	0.005	18.15	0.005	18.14	0.005
477	R1_379	27.19	0.02	0.004	0.000	27.21	0.004	27.18	0.005	27.20	0.004
478	R1_380	27.19	0.02	0.009	0.001	27.21	0.010	27.18	0.010	27.20	0.009
479	R1_381	27.20	0.01	0.003	0.000	27.21	0.004	27.18	0.003	27.20	0.003
480	R1_382	45.08	0.01	0.009	0.000	45.08	0.009	45.07	0.009	45.06	0.009
481	R1_383	45.07	0.03	0.035	0.002	45.08	0.036	45.01	0.036	45.06	0.037
482	R1_384	45.08	0.01	0.014	0.001	45.08	0.015	45.07	0.014	45.06	0.014
483	R1_385	25.82	0.02	0.017	0.001	25.84	0.017	25.81	0.018	25.81	0.018
484	R1_386	45.19	0.03	0.006	0.000	45.20	0.006	45.14	0.006	45.19	0.006
485	R1_387	29.83	0.02	0.016	0.001	29.85	0.016	29.85	0.018	29.81	0.017
486	R1_388	36.45	0.00	0.005	0.000	36.44	0.004	36.45	0.004	36.45	0.005
487	R1_389	44.40	0.03	0.135	0.010	44.38	0.131	44.37	0.134	44.42	0.151
488	R1_390	44.42	0.01	0.105	0.006	44.42	0.097	44.41	0.103	44.42	0.117
489	R1_391	44.40	0.03	0.044	0.004	44.38	0.039	44.37	0.040	44.42	0.050
490	R1_392	44.37	0.02	0.294	0.131	44.38	0.206	44.33	0.214	44.38	0.260
491	R1_393	44.38	0.01	0.423	0.022	44.38	0.410	44.37	0.419	44.38	0.465
492	R1_394	44.38	0.01	0.039	0.015	44.38	0.027	44.37	0.030	44.38	0.037
493	R1_395	44.30	n.a.	0.054	n.a.	44.30	0.054				
		44.38	0.01	0.172	0.046	44.38	0.189	44.37	0.196	44.38	0.210

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #2		Data Set #3		Data Set #4	
		Mean	StDev	Mean	StDev	Rt/min	RI/%	Rt/min	RI/%	Rt/min	RI/%
494	R1_396	44.37	0.02	0.128	0.006	44.34	0.126	44.37	0.126	44.38	0.140
495	R1_397	44.37	0.02	0.034	0.002	44.38	0.035	44.33	0.035	44.38	0.038
496	R1_398	44.34 44.42	0.03 n.a.	0.013 0.009	0.004 n.a.	44.30 44.42	0.008 0.009	44.33	0.017	44.38	0.018
497	R1_399	42.83 43.06 43.14 43.31	0.04 n.a. <b>0.06</b> 0.00	0.004 0.003 0.004 0.004	0.000 n.a. 0.001 0.000	42.89	0.004	43.07 43.31	0.003 0.004	42.79 43.31	0.004 0.004
498	R1_400	47.14	0.02	0.028	0.004	47.16	0.022	47.11	0.030	47.15	0.032
499	R1_401	47.12	0.02	0.092	0.005	47.11	0.087	47.11	0.096	47.11	0.100

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
1	HC01	20.66	4.803	20.67	3.760
		21.54	0.004	21.57	0.005
				22.80	0.002
2	HC02	44.56	0.307	44.56	0.327
3	HC03			3.35	0.013
		3.46	0.028		
4	HC03_pyE	3.39	0.012	3.43	0.011
5	HC05	32.06	0.041	32.04	0.043
		32.40	0.005		
		33.14	2.780	33.13	3.002
		34.74	0.013		
6	HC07	16.90	0.364	16.92	0.342
7	HC08	3.19	0.016	3.21	0.017
8	HC09	26.54	0.007	26.59	0.007
		27.45	1.714	27.50	1.676
9	HC09_ox	22.10	0.015	22.11	0.014
10	HC09_deamid	28.78	0.096	28.79	0.091
		29.78	0.434	29.80	0.453
11	HC10	19.80	1.111	19.81	1.210
12	HC10_ox	16.53	0.022	16.50	0.023
13	HC12	29.86	0.500		
		29.98	2.125	29.92	2.258
14	HC12_ox	26.05	0.017	26.05	0.017
15	HC12_deamid	30.91	0.075	30.89	0.093
16	HC13	38.46	2.202	38.35	2.361
17	HC13_ox	34.22	0.072	34.20	0.076
18	HC13_deamid	38.08	0.386	38.01	0.445
		39.70	0.267	39.65	0.291
19	HC13_ox_deamid	35.20	0.006	35.11	0.006
20	HC14				
21	HC15	3.42	0.011	3.39	0.009
22	HC17	3.46	0.168	3.47	0.130
23	HC18	38.24	2.126	38.21	1.918
		38.54	2.403		
		38.77	0.959		
				38.93	7.865
		39.29	5.463		
		39.79	0.026		
		39.82	0.911		

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
23	HC18				
24	HC19	29.37	2.912	29.35	3.160
25	HC20	23.84	2.505	23.84	2.507
26	HC21				
		41.76	4.028	41.71	4.360
		42.45	0.009		
				42.44	0.100
				43.54	0.031
				44.66	0.006
				45.55	0.005
				47.46	0.006
				53.47	0.009
27	HC22	20.10	0.003		
28	HC22_A2G0	18.56	0.026	18.54	0.026
29	HC22_A2G0-GlcNAc	18.69	0.023	18.66	0.025
30	HC22_A2G1	27.45	0.004	27.46	0.003
31	HC22_A2G1-GlcNAc	18.63	0.009	18.60	0.011
32	HC22_A2G2S1	18.89	0.024	18.92	0.022
33	HC22_A2FG0	18.22	0.424	18.21	0.335
34	HC22_A2FG0-GlcNAc	18.38	0.016	18.42	0.015
35	HC22_A2FG1	18.05	0.255	18.02	0.236
36	HC22_A2FG1-GlcNAc	18.32	0.007	18.30	0.005
37	HC22_A2FG2	17.94	0.032	17.91	0.033
38	HC22_Man5	18.44	0.018	18.42	0.019
39	HC23	32.20	3.955	32.19	3.843
40	HC23_ox	26.58	0.157	26.59	0.166
41	HC23_deamid				
		32.90	0.448	32.89	0.469
		33.35	0.857	33.35	0.970
42	HC23_ox_deamid	26.96	0.014	27.00	0.014
		27.49	0.020	27.50	0.019
43	HC24	3.46	0.056	3.43	0.047
44	HC26	22.77	2.246	22.80	2.152
45	HC26_deamid	23.36	0.192	23.35	0.217
46	HC27	3.42	0.067	3.43	0.057

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
47	HC29	3.46	0.039	3.43	0.032
48	HC30	21.48	0.760	21.46 21.85	0.735 0.168
49	HC31	3.42	0.044	3.43	0.038
50	HC33	51.20	0.011	51.19	0.011
51	HC33_deamid	51.47	0.006	51.46	0.006
52	HC34	26.87	1.793	26.88	1.952
53	HC34_ox	24.35	0.054	24.34	0.061
54	HC34_deamid	27.74 28.38	0.025 0.039	27.74 28.39	0.027 0.040
55	HC35	3.49	0.192	3.47	0.152
56	HC35_deamid				
57	HC36	24.59	6.003	24.59	6.559
58	HC36_deamid	24.30	0.047	25.20 25.31 26.09	0.227 0.617 0.025
59	HC37	3.42	0.019	3.43	0.018
60	HC04-05	29.74 30.46	0.012 0.701	29.73 30.47	0.012 0.740
61	HC07-08_deamid	22.25	0.004		
62	HC08-09_deamid	26.34	0.010	26.34	0.010
63	HC15-16	3.46	0.028	3.43	0.023
64	HC20-21	44.17	0.100	44.16	0.107
65	HC25-26	22.65	0.007	22.68	0.004
66	HC25-26_deamid			23.24	0.005
67	HC30-31	20.66	4.582	20.67	3.568
68	HC32-33	48.90	0.016	48.88	0.016
69	HC32-33_deamid	49.21	0.007	49.19	0.007
70	HC34-35	31.71 31.93	0.012 0.022	31.91	0.024
71	LC01	31.80	2.393	31.78	2.425



#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
72	LC02	22.44	3.914	22.43	3.700
73	LC02_deamid	22.10	0.392	22.06	0.387
				22.43	2.204
		22.94	0.021		
		23.15	0.106	23.19	0.096
		23.47	0.165	23.44	0.164
				24.01	0.010
74	LC03	2.00	0.004	2.01	0.004
		3.42	0.076	3.43	0.074
		3.62	0.009		
75	LC04	18.22	0.944	18.21	0.797
76	LC05	19.33	2.399	19.33	2.061
				19.90	0.013
		22.77	0.146	22.80	0.130
77	LC07			10.29	0.125
		10.73	0.119		
				11.10	0.078
		11.22	0.055		
				11.38	0.054
		11.78	0.149	11.87	0.112
78	LC09	48.51	0.420	48.48	0.421
79	LC09_deamid	44.71	0.031	44.66	0.030
		46.07	0.004	46.09	0.004
80	LC10	4.12	0.772	4.12	0.740
81	LC12	3.42	0.052	3.43	0.044
82	LC13	23.06	0.579	23.05	0.525
		25.75	0.009	25.75	0.009
		26.05	0.083	26.09	0.081
		26.34	0.037	26.34	0.036
83	LC13_deamid	22.01	0.038	22.02	0.039
		23.06	0.267		
		23.65	0.231	23.64	0.258
		23.84	0.713	23.88	0.710
		26.63	0.035	26.64	0.036
		27.10	0.018	27.10	0.017
84	LC13_pyE			25.81	0.028
		26.05	0.358	26.09	0.335
		26.34	0.079	26.34	0.087
85	LC13_deamid_pyE				
		24.45	0.004	24.45	0.005
		26.63	0.126	26.64	0.132
		27.10	0.043	27.10	0.040
86	LC14	24.59	0.009	24.59	0.009
		25.27	2.650	25.31	2.656
				25.70	0.008
				26.34	0.061
		35.27	0.009	35.18	0.011

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
86	LC14	53.05	0.020	53.04	0.025
87	LC14_ox	21.33	0.030	21.31	0.033
88	LC15	3.42 3.62	0.043 0.003	3.43	0.042
89	LC16	3.42	0.113	3.43	0.097
90	LC17	4.82	1.511	4.83	1.558
91	LC18	3.46	0.063	3.43	0.053
92	LC19	3.46	0.008	3.43	0.011
94	LC07-08				
95	LC08-09	46.98 47.45	4.748 1.254	47.07	4.912
96	LC08-09_deamid	43.28 44.66	0.371 0.088	43.22 44.66	0.407 0.086
97	LC13-14_deamid	26.05	0.007	26.09	0.005
98	LC13-14_pyE	25.27	0.037	25.27	0.036
100	R1_02				
101	R1_03	2.98	0.015	2.99	0.017
102	R1_04	29.41	0.002	29.48	0.001
103	R1_05	23.06	0.002		
104	R1_06	19.41	0.004	19.51	0.003
105	R1_07	4.08	0.095	4.05	0.109
106	R1_08	4.08 4.36	0.008 0.001	4.05 4.44	0.009 0.001
107	R1_09				
108	R1_10	2.45	0.028		
109	R1_11	2.64	0.004	2.43 2.67 3.16	0.004 0.008 0.003
110	R1_12	10.33	0.005	10.29	0.006
111	R1_13	3.86	0.015	3.87	0.020

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
112	R1_14	4.12	0.003	4.12	0.003
113	R1_15			21.51	0.002
114	R1_16	4.82	0.001	4.83	0.001
115	R1_17	2.45	0.276	2.43	0.320
116	R1_18	3.53 3.80 4.12 4.24	0.011 0.011 0.004 0.004	3.50 3.81	0.008 0.027
117	R1_19	2.45	0.027	2.43	0.031
118	R1_20	2.84	0.009	2.67 2.85	0.005 0.010
119	R1_21			2.99	0.002
120	R1_22	10.73 11.15 11.36 11.85	0.124 0.043 0.057 0.108	10.29 11.17 11.52 11.94	0.129 0.109 0.052 0.087
122	R1_24	3.62	0.003		
123	R1_25	2.98	0.167	2.99	0.170
124	R1_26	26.05	0.000		
125	R1_27	21.78	0.000	21.80	0.000
126	R1_28	4.86	0.002	4.83	0.002
127	R1_29	4.04	0.002	4.05	0.001
128	R1_30	4.08	0.036	4.05	0.046
129	R1_31	4.08	0.004		
130	R1_32	4.08	0.025	4.05	0.030
131	R1_33	23.93	0.005	23.92	0.005
132	R1_34	16.18	0.006	16.21	0.006
133	R1_35	4.04	0.007	4.05	0.008
134	R1_36	4.12	0.001		
137	R1_39	2.45	0.082	2.38 2.53	0.051 0.042
138	R1_40	15.24	0.029	15.26	0.033

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
139	R1_41				
140	R1_42			4.16	0.002
141	R1_43			15.26	0.004
142	R1_44	3.53 16.90	0.004 0.369	3.55 16.92	0.004 0.341
143	R1_45			59.37	0.004
144	R1_46	2.98	0.010	2.90	0.011
145	R1_47	25.60	0.001	25.65	0.001
146	R1_48	3.02	0.004	2.99	0.004
147	R1_49			19.33	0.001
148	R1_50	3.57 4.82	0.253 0.001	3.59 4.12 4.24	0.202 0.011 0.017
150	R1_52	3.02	0.022	2.99	0.023
151	R1_53	4.08	0.009	4.05	0.011
152	R1_54	59.31	0.004		
153	R1_55	3.80	0.004	3.81	0.005
154	R1_56	16.18	0.017	16.14	0.017
155	R1_57	59.31	0.006	59.31	0.015
156	R1_58	25.55	0.005	25.55	0.004
157	R1_59	4.20	0.002	4.16	0.002
158	R1_60	4.30	0.001	4.30	0.000
159	R1_61	4.30	0.001	4.24	0.001
160	R1_62	4.30	0.021	4.30	0.017
161	R1_63	59.25	0.007	59.25	0.020
162	R1_64			21.80	0.004
163	R1_65	19.45	0.003	19.46	0.003
164	R1_66	19.21 20.73	0.005 0.009	19.21 20.71	0.004 0.007
165	R1_67				
166	R1_68				

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
167	R1_69			3.87	0.001
169	R1_71			23.64	0.002
170	R1_72	19.21	0.004	19.21	0.003
171	R1_73	5.20	0.005	5.21	0.005
172	R1_74	59.19	0.008	59.25	0.021
173	R1_75	22.86	0.013	22.88	0.013
174	R1_76	22.86	0.017	22.88	0.016
175	R1_77	16.68	0.004	16.71	0.004
176	R1_78			59.25	0.006
177	R1_79	2.60 2.84	0.007 0.006	2.76	0.016
178	R1_80	25.81	0.009	25.85	0.012
179	R1_81	20.15	0.010	20.18	0.008
180	R1_82	59.19	0.004	59.20	0.006
181	R1_83	22.86	0.006	22.84	0.006
182	R1_84	20.91	0.001	20.89	0.000
183	R1_85	20.86	0.001	20.89	0.001
184	R1_86	59.15	0.013	59.20	0.020
185	R1_87			4.05	0.003
186	R1_88	17.62	0.054	17.65	0.053
187	R1_89			59.20	0.010
188	R1_90	23.51	0.003	23.50	0.003
189	R1_91	59.19	0.015	59.20	0.023
190	R1_92				
192	R1_94	25.86	0.006	25.85	0.006
193	R1_95	20.32	0.007	20.35	0.008
194	R1_96	19.55 28.73	0.003 0.000	19.57 28.74	0.003 0.000
195	R1_97	28.73	0.193	28.74	0.176
196	R1_98	19.55 21.60	0.025 0.008	19.57 21.57	0.032 0.010

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
197	R1_99	19.55	0.003	19.57	0.003
198	R1_100	19.55	0.001	19.57	0.002
199	R1_101	2.45	0.316	2.50 2.35	0.242 0.130
200	R1_102	24.98	0.001	24.94	0.001
201	R1_103	19.25	0.001		
202	R1_104	21.18	0.020	21.21	0.018
203	R1_105	28.68	0.000	28.74	0.000
204	R1_106	59.15	0.012	59.15	0.013
205	R1_107	29.54	0.001	29.52	0.001
206	R1_108	29.54	0.012	29.52	0.009
207	R1_109	29.54	0.001	29.52	0.001
208	R1_110			25.81	0.003
209	R1_111	24.18	0.006	24.24	0.005
210	R1_112				
211	R1_113	28.73	0.001	28.74	0.001
212	R1_114	28.73	0.001	28.74	0.000
213	R1_115	59.15	0.027	59.10	0.028
214	R1_116	19.98	0.001	20.00	0.002
215	R1_117	19.98	0.016	20.00	0.016
216	R1_118				
217	R1_119	59.15	0.018	59.10	0.019
218	R1_120	59.15	0.035	59.10	0.037
219	R1_121	28.44	0.005		
221	R1_123	20.73	0.011	20.71	0.009
222	R1_124	59.15	0.013	59.10	0.014
223	R1_125	16.25	0.004	16.28	0.004
224	R1_126	21.83	0.034	21.80	0.043
225	R1_127	25.91	0.012	25.95	0.017
226	R1_128	28.90	0.005	28.91	0.005
228	R1_130	59.15	0.019	59.10	0.021

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
229	R1_131	25.86	0.011	25.85	0.013
230	R1_132			21.80	0.004
231	R1_133	59.15	0.035	59.10	0.039
232	R1_134	59.11	0.013	59.05	0.014
233	R1_135	29.21	0.000	29.18	0.000
234	R1_136	29.21	0.001	29.18	0.001
235	R1_137	29.21	0.013	29.18	0.013
236	R1_138	17.27	0.006	17.30	0.007
237	R1_139	22.30	0.009	22.32	0.007
238	R1_140	36.71	0.019	36.63	0.018
239	R1_141	59.11	0.018	59.05	0.022
240	R1_142				
241	R1_143	59.11	0.032	59.05	0.039
242	R1_144				
243	R1_145			30.14	0.004
244	R1_146	59.05	0.011	59.05	0.013
245	R1_147	34.88	0.001	34.86	0.001
246	R1_148	32.40	0.007	32.39	0.006
247	R1_149			2.67	0.004
		2.79	0.013	2.85	0.008
248	R1_150				
		2.45	0.233	2.50	0.182
249	R1_151	21.78	0.001	21.80	0.001
250	R1_152	21.78	0.034	21.80	0.046
251	R1_153	5.01	0.001	5.02	0.001
252	R1_154	21.78	0.001	21.80	0.001
253	R1_155	5.01	0.001		
254	R1_156	5.01	0.001	5.02	0.001
255	R1_157			59.05	0.004
256	R1_158	28.96	0.007	28.98	0.007
257	R1_159			21.80	0.003
258	R1_160	59.05	0.030	59.05	0.041

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
258	R1_160				
259	R1_161	17.41	0.008	17.37	0.008
260	R1_162	59.01	0.012	59.00	0.018
261	R1_163	19.01	0.007	19.04	0.006
262	R1_164	59.01	0.003	59.00	0.005
263	R1_165	26.38	0.006	26.39	0.006
264	R1_166	29.37	0.004	29.39	0.004
265	R1_167	30.46 59.01	0.001 0.016	30.47 59.00	0.001 0.025
266	R1_168			58.95	0.013
267	R1_169			58.95	0.017
268	R1_170				
269	R1_171	59.01	0.006	58.95	0.016
270	R1_172			58.95	0.004
271	R1_173	21.04	0.006	21.08	0.007
272	R1_174	30.74	0.181	30.71	0.177
273	R1_175	59.01	0.013	58.95	0.026
274	R1_176			5.21	0.004
275	R1_177	59.01	0.024	33.39 58.95	0.002 0.045
276	R1_178	58.95	0.007	58.95	0.015
277	R1_179	30.74	0.019	30.71	0.017
278	R1_180	26.09 28.12	0.014 0.012	26.13 28.13	0.013 0.012
279	R1_181	26.96	0.005	26.88 27.64	0.004 0.002
280	R1_182	58.95	0.004	58.95	0.012
281	R1_183				
282	R1_184			58.95	0.004
283	R1_185	21.43	0.001	21.40	0.001
284	R1_186			24.39	0.002



#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
284	R1_186	27.28	0.006		
		28.18	0.007	28.13	0.008
285	R1_187	2.45	0.065	2.46	0.056
		2.57	0.028	2.55	0.041
286	R1_188	58.95	0.019	58.95	0.039
287	R1_189			2.35	0.056
		2.48	0.100	2.50	0.105
288	R1_190			21.75	0.004
289	R1_191			58.95	0.011
290	R1_192				
291	R1_193	19.89	0.001	19.90	0.001
292	R1_194	19.89	0.010	19.90	0.011
293	R1_195	19.89	0.001	19.90	0.001
294	R1_196				
295	R1_197	25.07	0.004	25.12	0.005
296	R1_198			58.91	0.020
298	R1_200			58.91	0.009
299	R1_201	58.95	0.004	58.91	0.007
300	R1_202	24.89	0.022	24.90	0.020
301	R1_203	36.28	0.001		
302	R1_204	36.28	0.019	36.20	0.019
303	R1_205	27.45	0.001		
				33.88	0.003
304	R1_206	19.21	0.009		
		19.37	0.020	19.33	0.025
				22.43	0.003
		26.49	0.008	26.49	0.008
305	R1_207	28.78	0.002	28.79	0.002
306	R1_208	18.22	0.002	18.25	0.001
		29.50	0.001	29.48	0.001
307	R1_209	28.78	0.002	28.79	0.002
308	R1_210	58.89	0.009	58.91	0.019
309	R1_211	28.78	0.001	28.79	0.001

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
310	R1_212	42.57	0.019	42.50	0.020
311	R1_213			31.34	0.003
312	R1_214	20.20	0.008	20.23	0.007
313	R1_215				
		58.89	0.005	58.91	0.009
314	R1_216	58.89	0.006	58.91	0.012
315	R1_217			58.91	0.004
316	R1_218	24.98	0.013	25.04	0.013
		29.98	0.005	29.96	0.006
317	R1_219			19.81	0.003
		20.62	0.005	20.61	0.004
318	R1_220	20.62	0.059	20.61	0.048
319	R1_221	16.03	0.002	16.00	0.002
320	R1_222	15.89	0.004	15.92	0.004
321	R1_223			58.86	0.006
322	R1_224	29.33	0.002	29.35	0.002
323	R1_225	4.08	0.006	4.08	0.005
324	R1_226	58.89	0.004	58.86	0.008
325	R1_227	36.43	0.248	36.41	0.240
326	R1_228	36.43	0.018	36.41	0.016
327	R1_229	14.16	0.044	14.19	0.048
328	R1_230	36.43	0.128	36.41	0.126
329	R1_231			27.41	0.001
330	R1_232	36.43	0.085	36.41	0.082
331	R1_233			58.86	0.004
332	R1_234	25.47	0.009	25.50	0.013
333	R1_235	19.01	0.004		
334	R1_236			58.86	0.005
335	R1_237	36.43	0.012	36.41	0.012
336	R1_238	31.58	0.008	31.55	0.008
337	R1_239			36.36	0.003
338	R1_240	36.48	0.004	36.41	0.004

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
339	R1_241				
340	R1_242	28.56	0.004	28.57	0.004
341	R1_243	34.88	0.003	34.86	0.003
342	R1_244	42.63	0.005	42.62	0.005
343	R1_245	42.63	0.006	42.62	0.007
344	R1_246			24.39	0.003
345	R1_247	42.63	0.004	42.62	0.004
346	R1_248	22.19	0.005	22.16	0.004
347	R1_249	36.88	0.020	36.82	0.019
348	R1_250			24.99	0.003
349	R1_251	36.88	0.010	36.82	0.010
350	R1_252	24.13	0.026	24.17	0.029
351	R1_253	31.63	0.004	31.60	0.004
352	R1_254	34.88	0.012	34.86	0.012
353	R1_255	23.06	0.009	23.05	0.008
354	R1_256				
355	R1_257	23.02	0.013	23.05	0.012
356	R1_258	22.56	0.002	22.54	0.002
358	R1_260				
359	R1_261	28.44	0.012	28.45	0.012
360	R1_262	20.15	0.009	20.18	0.007
		23.65	0.022		
		23.89	0.045		
		28.44	0.011	28.45	0.011
361	R1_263	23.06	0.034	23.05	0.032
362	R1_264	2.40	0.046	2.40	0.070
363	R1_265	2.57	0.022	2.55	0.029
364	R1_266	36.53	0.007	36.51	0.007
365	R1_267	27.87	0.007	27.87	0.007
366	R1_268	39.03	0.004	38.93	0.004
367	R1_269	39.03	0.008	38.93	0.008

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
368	R1_270	36.83	0.005	36.76	0.004
369	R1_271	36.48	0.001	36.41	0.001
370	R1_272	31.58	0.004	31.55	0.004
371	R1_273	40.35	0.003	40.29	0.003
372	R1_274	25.07	0.149	25.08	0.154
373	R1_275	30.42	0.027	30.40	0.028
374	R1_276	25.07	0.075	25.08	0.076
375	R1_277	27.80	0.013	27.87	0.013
376	R1_278	20.66 29.94	0.036 0.019	30.85	0.002
377	R1_279	25.07	0.055	25.08	0.057
378	R1_280	25.70 26.13	0.003 0.003	25.75	0.003
379	R1_281	21.48 24.98	0.003 0.002		
380	R1_282	25.03	0.001	25.04	0.001
381	R1_283	32.10 33.78	0.002 0.091	33.76	0.098
382	R1_284	20.69	0.011	20.71	0.006
383	R1_285	28.50 30.74	0.005 0.025	28.51 30.77	0.005 0.023
384	R1_286	30.74	0.006	30.77	0.006
385	R1_287	47.59	0.003		
386	R1_288	40.35	0.030	40.24	0.032
387	R1_289	24.89	0.004	25.04	0.004
388	R1_290	24.84	0.004	24.85	0.004
389	R1_291	47.59	0.003	47.51	0.003
390	R1_292	40.35	0.048	40.24	0.051

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
390	R1_292			41.71	0.006
391	R1_293	40.30	0.023	40.24	0.025
392	R1_294	25.03	0.080	25.04	0.080
393	R1_295	24.51	0.004	24.52	0.003
394	R1_296	40.30	0.007	40.24	0.011
395	R1_297	40.30	0.004	40.24	0.005
396	R1_298				
397	R1_299	32.85	0.012	32.85	0.013
398	R1_300	20.59	0.007	20.57	0.006
399	R1_301	2.43	0.049	2.53	0.028
400	R1_302	19.89	0.005	19.90	0.006
401	R1_303	38.04	0.004	37.97	0.004
402	R1_304	27.21	0.008	27.21	0.008
403	R1_305	23.73	0.001	23.76	0.001
404	R1_306	23.73	0.046	23.76	0.044
405	R1_307	23.73	0.001	23.76	0.001
406	R1_308	36.08	0.016	36.06	0.016
407	R1_309	37.42	0.013	37.35	0.016
408	R1_310	26.76	0.001	26.77	0.001
409	R1_311	26.76	0.016	26.77	0.033
410	R1_312	19.93	0.025	19.94	0.029
411	R1_313	28.06	0.009	28.06	0.009
412	R1_314	22.30	0.008	22.32	0.007
413	R1_315	27.63	0.001	27.64	0.001
414	R1_316	27.63	0.002	27.64	0.002
415	R1_317	27.63	0.026	27.64	0.026
416	R1_318	27.63	0.002	27.64	0.002
417	R1_319	27.63	0.002	27.64	0.002
418	R1_320	16.18	0.006	16.21	0.006
419	R1_321	35.01	0.053	34.99	0.058

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
420	R1_322			34.99	0.002
		35.01	0.002		
		35.95	0.011	35.85	0.011
421	R1_323	35.01	0.007	34.99	0.011
422	R1_324	31.63	0.005	31.60	0.005
424	R1_326	33.31	0.018	33.25	0.019
425	R1_327				
426	R1_328	41.61	0.075	41.56	0.084
427	R1_329			33.09	0.172
		33.11	0.162		
				33.25	0.024
428	R1_330	28.44	0.001		
429	R1_331			34.08	0.004
430	R1_332	31.16	0.007	31.14	0.007
431	R1_333	38.62	0.006	38.55	0.006
432	R1_334				
433	R1_335	20.91	0.006	20.89	0.005
434	R1_336	38.73	0.122	38.67	0.125
435	R1_337	31.63	0.005	31.60	0.005
436	R1_338	38.73	0.006	38.67	0.007
437	R1_339			27.46	0.004
		29.98	2.122	29.92	2.253
		30.97	0.081	30.83	0.096
		32.10	0.007		
438	R1_340	42.38	0.004		
439	R1_341	41.58	0.046	41.56	0.070
		41.73	0.010		
				42.18	0.003
		42.38	0.178	42.31	0.201
440	R1_342	41.58	0.007	41.53	0.008
		41.76	0.002		
				42.31	0.029
		42.57	0.020		
441	R1_343	29.94	0.003	30.00	0.002
442	R1_344	24.98	0.006	24.99	0.006
443	R1_345	25.03	0.083	25.04	0.085

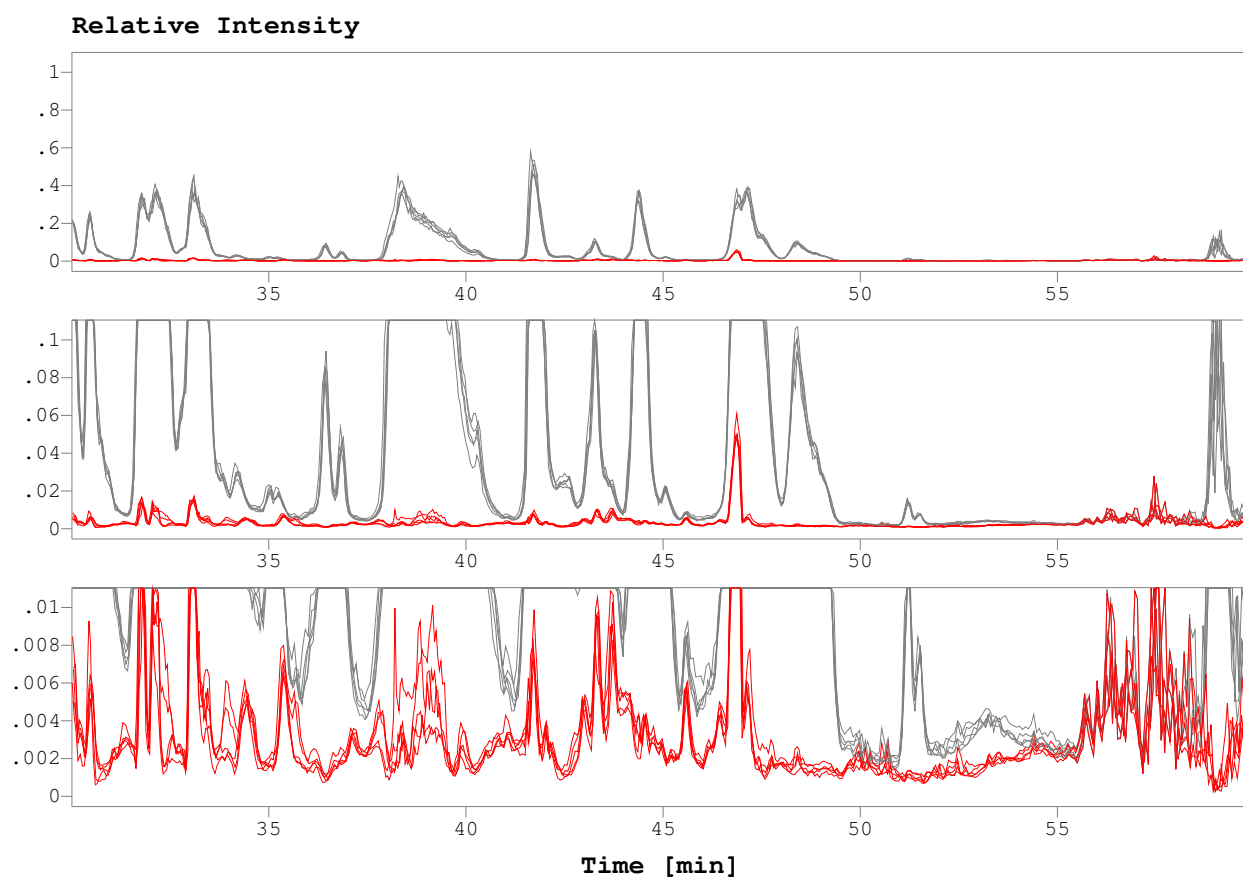
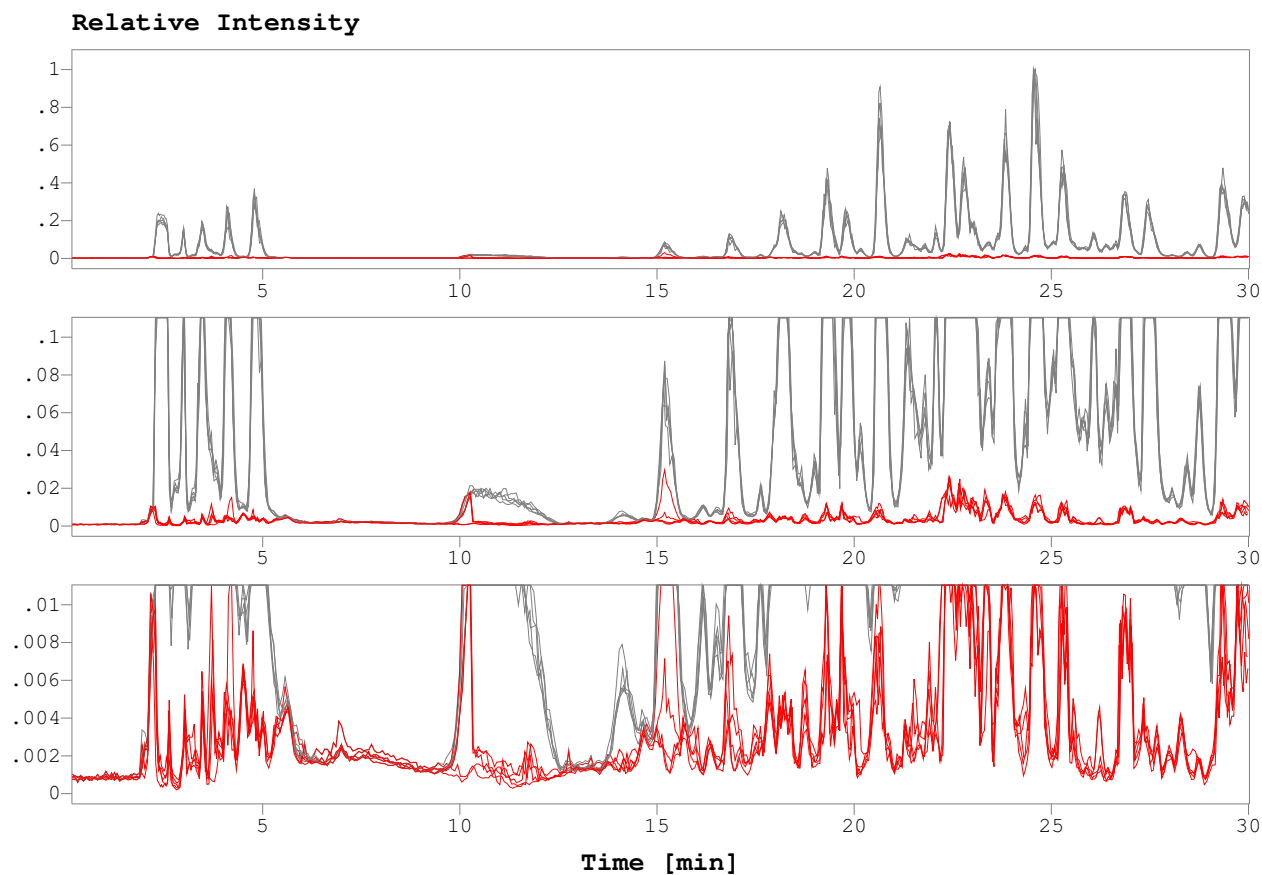
#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
444	R1_346	18.10	0.004	18.12	0.003
445	R1_347	18.14	0.004	18.12	0.004
446	R1_348	25.03	0.009	25.04	0.009
447	R1_349	18.14 19.80	0.004 0.005	18.12 19.81	0.004 0.006
448	R1_350	18.14	0.004	18.07	0.003
449	R1_351				
450	R1_352	24.94 36.43	0.018 0.007	24.94 36.41	0.016 0.007
451	R1_353	36.43	0.029	36.41	0.028
452	R1_354	24.94 36.43	0.003 0.009	36.41	0.009
453	R1_355	40.19	0.008	40.14	0.009
454	R1_356	19.01	0.057	18.98	0.048
455	R1_357	19.07	0.012	19.10	0.011
456	R1_358	25.39 28.06 41.65 41.89	0.005 0.021 0.023 0.041	24.59 25.43 28.06 41.63 41.83	0.017 0.015 0.019 0.033 0.039
457	R1_359	19.01	0.010	18.98	0.008
458	R1_360				
459	R1_361	32.81	0.165	32.80	0.167
460	R1_362	32.81	0.021	32.75	0.021
462	R1_364	32.81	0.004	32.75	0.004
463	R1_365	25.60 38.28 38.62 39.08 39.38 39.56	0.067 0.046 0.082 0.035 0.055 0.034	25.65 38.21 38.27 38.55 38.67 38.88 39.15 39.47	0.064 0.045 0.007 0.042 0.022 0.008 0.044 0.118
464	R1_366	23.47 23.73 24.48	0.002 0.004 0.005	23.44 23.76 24.48	0.002 0.003 0.011

#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
465	R1_367	39.56	0.002	39.47	0.003
466	R1_368	19.01	0.007	18.98	0.006
467	R1_369			37.89	0.005
468	R1_370	28.06	0.004	28.06	0.004
469	R1_371			41.48	0.004
470	R1_372	26.38	0.132	26.44	0.142
471	R1_373			41.48	0.004
472	R1_374	26.38	0.019	26.44	0.022
473	R1_375	40.35	0.022	40.29	0.022
474	R1_376			26.44	0.004
475	R1_377	40.35	0.004	40.29	0.004
476	R1_378	18.14	0.005	18.12	0.004
477	R1_379	27.15	0.004	27.21	0.004
478	R1_380	27.15	0.009	27.21	0.009
479	R1_381				
480	R1_382	45.09	0.008	45.10	0.009
481	R1_383	45.09	0.032	45.10	0.033
482	R1_384	45.09	0.012	45.10	0.013
483	R1_385	25.81	0.016	25.85	0.017
484	R1_386	45.21	0.007	45.23	0.006
485	R1_387	29.82	0.014	29.84	0.015
486	R1_388				
487	R1_389	44.44	0.136	44.39	0.121
488	R1_390	44.44	0.106	44.43	0.105
489	R1_391	44.44	0.046	44.39	0.043
490	R1_392	44.39	0.553	44.35	0.239
491	R1_393	44.39	0.420	44.39	0.402
492	R1_394	44.39	0.068	44.39	0.035
493	R1_395	44.39	0.082	44.39	0.184
494	R1_396	44.39	0.127	44.39	0.121

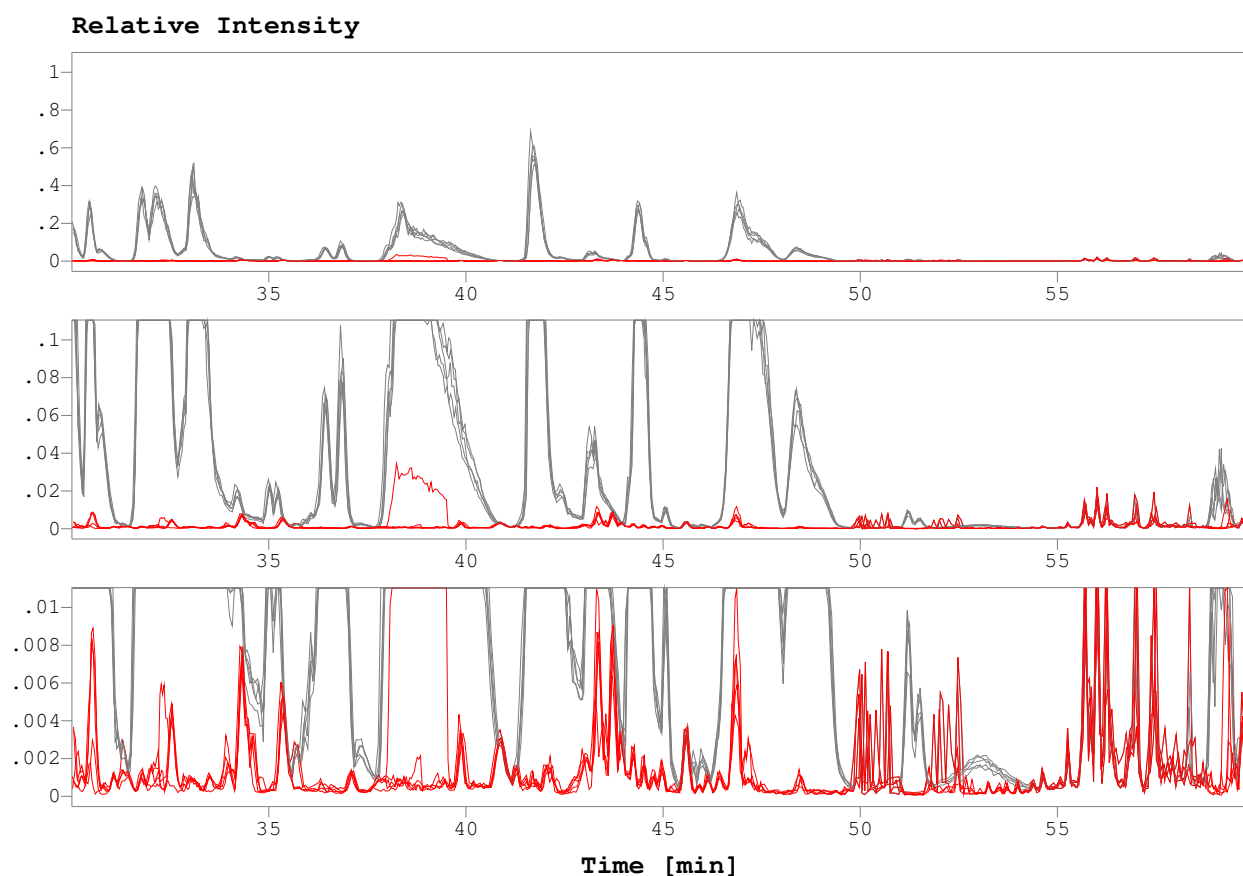
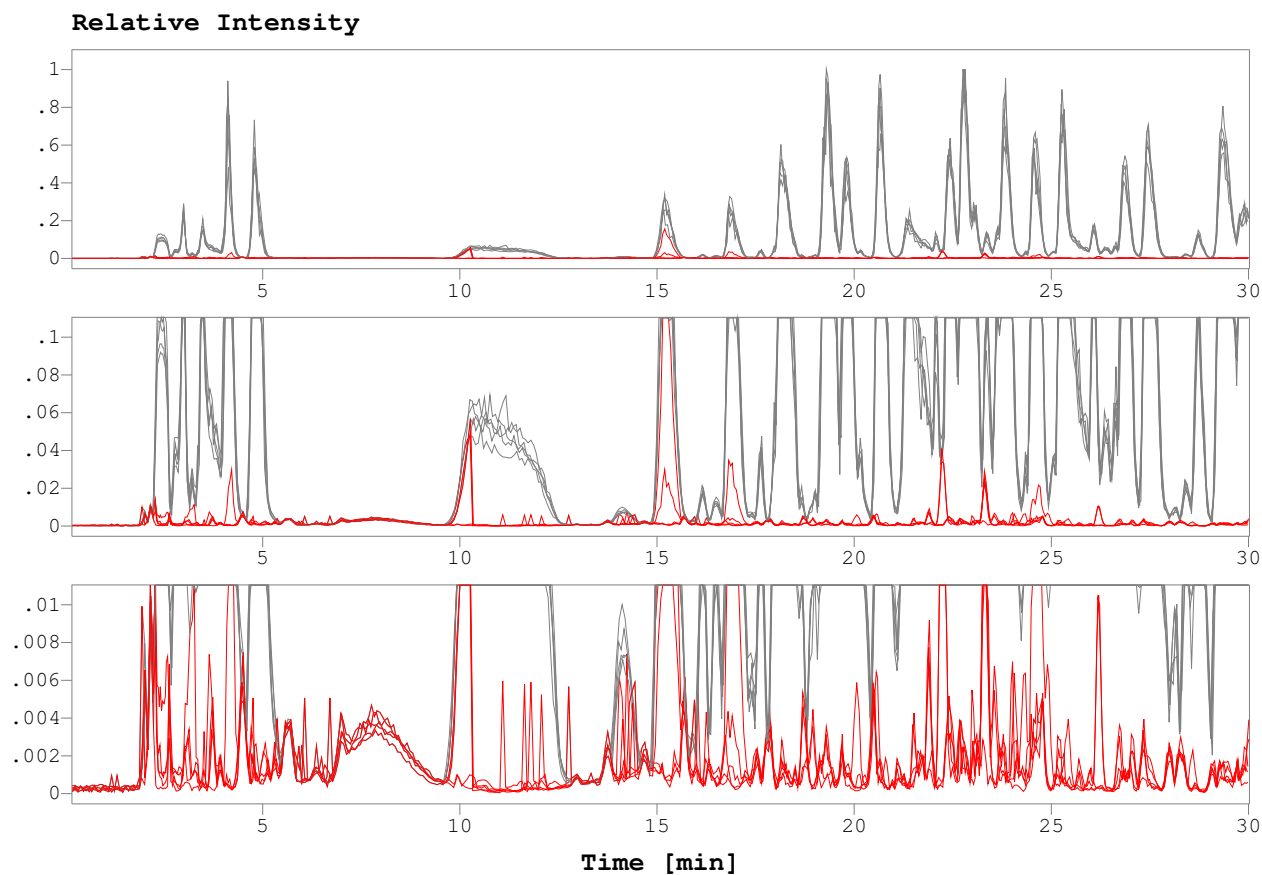


#	Molecule	Data Set #5		Data Set #6	
		Rt/min	RI/%	Rt/min	RI/%
495	R1_397	44.39	0.033	44.39	0.031
496	R1_398	44.32	0.007	44.39	0.014
497	R1_399	42.82	0.004	43.06	0.003
		43.13	0.003	43.22	0.005
498	R1_400	47.14	0.030	47.15	0.028
499	R1_401	47.14	0.089	47.15	0.087

Grey: Ion current chromatograms of original files of group data sets  
Red: Ion current chromatograms of difference files of group data sets



Grey: Ion current chromatograms of original files of group data sets  
Red: Ion current chromatograms of difference files of group data sets



Mean of standard deviations of retention time differences [min]: 0.019  
StDev of standard deviations of retention time differences [min]: 0.017

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
1	HC01	20.66	0.01	4.542	0.441	20.63	4.509
		21.56	0.01	0.007	0.003	21.51	0.010
		22.80	n.a.	0.002	n.a.		
2	HC02	44.56	0.01	0.326	0.010	44.53	0.340
3	HC03	3.35	n.a.	0.013	n.a.		
		3.46	0.01	0.028	0.001	3.45	<b>0.025</b>
4	HC03_pyE	3.42	0.02	0.011	0.000	3.42	<b>0.010</b>
5	HC05	32.06	0.02	0.041	0.002	32.07	<b>0.036</b>
		32.40	0.00	0.005	0.000	32.38	<b>0.004</b>
		33.13	0.01	2.908	0.110	33.12	2.714
		34.74	n.a.	0.013	n.a.	34.67	<b>0.020</b>
6	HC07	16.90	0.01	0.435	0.069	16.92	0.437
7	HC08	3.21	0.02	0.015	0.001	3.20	<b>0.012</b>
8	HC09	26.56	0.02	0.007	0.000	26.51	0.008
		27.48	0.02	1.760	0.085	27.45	1.655
9	HC09_ox	22.10	0.01	0.014	0.001	22.07	0.014
10	HC09_deamid	28.80	0.02	0.098	0.007	28.81	0.090
		29.79	0.01	0.466	0.026	29.78	0.435
11	HC10	19.80	0.02	1.245	0.087	19.80	1.246
12	HC10_ox	16.52	0.01	0.022	0.001	16.50	<b>0.019</b>
13	HC12	29.86	n.a.	0.500	n.a.		
		29.95	0.02	2.297	0.118	29.94	2.077
14	HC12_ox	26.04	0.01	0.018	0.002	26.03	0.016
15	HC12_deamid	30.92	0.03	0.081	0.009		
16	HC13	38.41	0.04	2.319	0.088	38.38	<b>2.139</b>
17	HC13_ox	34.20	0.01	0.075	0.005	34.23	0.070
18	HC13_deamid	38.05	0.03	0.419	0.025	38.05	0.373
		39.67	0.02	0.281	0.010	39.66	<b>0.242</b>
19	HC13_ox_deamid	35.16	0.03	0.006	0.000	35.19	0.006
20	HC14	48.39	n.a.	0.004	n.a.	48.34	<b>0.004</b>
21	HC15	3.42	0.01	0.010	0.001	3.42	0.010
22	HC17	3.46	0.01	0.159	0.018	3.45	0.166
23	HC18	38.26	0.04	1.594	0.768	38.20	1.643
		38.63	<b>0.08</b>	2.201	0.521	38.66	<b>3.531</b>
		38.77	n.a.	0.959	n.a.		
		38.93	0.00	5.452	2.413		
		39.30	<b>0.08</b>	2.632	1.786	<b>39.43</b>	2.795

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
23	HC18	39.79	n.a.	0.026	n.a.	39.83	<b>0.032</b>
		39.82	0.00	1.323	0.411		
		39.95	n.a.	0.412	n.a.		
		40.26	0.02	0.005	0.001		
24	HC19	29.37	0.02	3.044	0.138	29.34	3.046
25	HC20	23.83	0.01	2.611	0.208	23.83	2.617
26	HC21	35.67	0.03	0.005	0.000	35.65	<b>0.004</b>
		41.74	0.02	4.178	0.169	41.70	3.925
		42.45	n.a.	0.009	n.a.		
		42.46	0.02	0.085	0.011		
		43.54	n.a.	0.031	n.a.		
		44.66	n.a.	0.006	n.a.		
		45.55	n.a.	0.005	n.a.		
		47.46	n.a.	0.006	n.a.		
		53.10	0.01	0.013	0.000	<b>53.02</b>	<b>0.011</b>
53.47	n.a.	0.009	n.a.				
27	HC22	20.08	0.01	0.003	0.000	20.03	0.003
28	HC22_A2G0	18.54	0.02	0.029	0.004	18.53	0.034
29	HC22_A2G0-GlcNAc	18.67	0.02	0.024	0.001	18.65	0.025
30	HC22_A2G1	27.45	0.01	0.004	0.000	27.40	0.003
31	HC22_A2G1-GlcNAc	18.61	0.02	0.011	0.001	18.59	0.012
32	HC22_A2G2S1	18.90	0.01	0.024	0.002	18.90	0.024
33	HC22_A2FG0	18.21	0.01	0.413	0.050	18.21	0.427
34	HC22_A2FG0-GlcNAc	18.40	0.02	0.017	0.002	18.37	0.020
35	HC22_A2FG1	18.02	0.02	0.264	0.023	18.05	0.263
36	HC22_A2FG1-GlcNAc	18.30	0.01	0.006	0.001	18.31	0.007
37	HC22_A2FG2	17.94	0.02	0.033	0.002	17.94	0.031
38	HC22_Man5	18.44	0.02	0.021	0.003	18.43	0.025
39	HC23	32.09	n.a.	2.219	n.a.		
		32.20	0.00	4.011	0.124	32.15	3.802
40	HC23_ox	26.60	0.01	0.165	0.006	26.56	0.159
41	HC23_deamid	32.36	n.a.	1.902	n.a.	32.30	<b>2.030</b>
		32.91	0.02	0.463	0.014	32.87	0.465
		33.36	0.01	0.937	0.043	33.33	0.857
42	HC23_ox_deamid	26.99	0.02	0.015	0.001	26.97	0.015
		27.50	0.01	0.021	0.001	27.45	0.019
43	HC24	3.44	0.01	0.054	0.005	3.42	0.055
44	HC26	22.78	0.01	2.424	0.235	22.82	2.510
45	HC26_deamid	23.35	0.01	0.215	0.018	23.33	0.242

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
46	HC27	3.42	0.01	0.065	0.005	3.42	0.065
47	HC29	3.45	0.02	0.037	0.004	3.45	0.036
48	HC30	21.46 21.88	0.03 0.04	0.742 0.241	0.104 0.061	21.46	<b>0.962</b>
49	HC31	3.42	0.01	0.042	0.003	3.42	0.040
50	HC33	51.20	0.02	0.014	0.004	51.18	0.023
51	HC33_deamid	51.50	0.03	0.006	0.001	51.45	<b>0.007</b>
52	HC34	26.88	0.01	1.948	0.104	26.84	1.851
53	HC34_ox	24.34	0.01	0.058	0.007	24.31	0.060
54	HC34_deamid	27.77 28.41	0.02 0.02	0.026 0.041	0.001 0.003	27.73 28.37	0.025 0.038
55	HC35	3.48	0.01	0.183	0.021	3.49	0.201
56	HC35_deamid	3.68	n.a.	0.006	n.a.		
57	HC36	24.58	0.01	6.739	0.525	24.58	6.622
58	HC36_deamid	24.29 25.19 25.34 26.08	0.01 0.01 0.03 0.01	0.026 0.262 0.684 0.030	0.015 0.028 0.120 0.003	24.26 25.17 25.32 26.08	0.053 0.265 0.582 0.024
59	HC37	3.42	0.01	0.019	0.001	3.42	0.020
60	HC04-05	29.74 30.47	0.00 0.01	0.012 0.749	0.000 0.029	29.71 30.45	<b>0.011</b> <b>0.685</b>
61	HC07-08_deamid	22.25	0.00	0.004	0.000	22.22	<b>0.004</b>
62	HC08-09_deamid	26.34	0.01	0.011	0.000	26.32	0.011
63	HC15-16	3.44	0.01	0.027	0.002	3.42	0.026
64	HC20-21	44.16 44.58	0.01 n.a.	0.115 0.001	0.010 n.a.	44.12	0.118
65	HC25-26	22.67	0.01	0.006	0.002	22.66	0.007
66	HC25-26_deamid	23.26 n.a.	0.02 n.a.	0.004 n.a.	0.001 n.a.	23.24 <b>23.79</b>	<b>0.009</b> <b>0.000</b>
67	HC30-31	20.66 21.57	0.01 0.01	4.333 0.003	0.427 0.000	20.63 21.51	4.330 <b>0.003</b>
68	HC32-33	48.88	0.02	0.017	0.001	48.84	<b>0.020</b>
69	HC32-33_deamid	49.18	0.02	0.008	0.000	49.14	0.008
70	HC34-35	31.68 31.93	0.02 0.02	0.013 0.025	0.001 0.005	31.69 31.90	0.014 0.026
71	LC01	31.80	0.02	2.438	0.068	31.78	<b>2.266</b>

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
71	LC01	32.32	n.a.	0.023	n.a.	32.68	<b>0.035</b>
		32.65	n.a.	0.039	n.a.		
72	LC02	22.43	0.01	4.044	0.287	22.41	4.169
73	LC02_deamid	22.08	0.02	0.400	0.028	22.07	0.398
		22.43	n.a.	2.204	n.a.	<b>22.90</b>	<b>0.013</b>
		n.a.	n.a.	n.a.	n.a.		
		22.93	0.01	0.023	0.002		
		23.18	0.02	0.106	0.006	23.19	0.110
23.46	0.01	0.165	0.006	23.42	<b>0.187</b>		
24.01	0.01	0.012	0.003	24.00	0.010		
74	LC03	2.01	0.01	0.004	0.000	2.02	<b>0.003</b>
		3.42	0.01	0.076	0.002	3.45	0.076
		3.62	n.a.	0.009	n.a.		
75	LC04	18.21	0.01	0.945	0.089	18.17	1.030
76	LC05	19.32	0.02	2.359	0.191	19.29	2.423
		19.91	0.01	0.013	0.000	22.82	0.168
		22.78	0.01	0.158	0.019		
77	LC07	10.29	n.a.	0.125	n.a.	<b>10.56</b>	<b>0.045</b>
		n.a.	n.a.	n.a.	n.a.		
		10.67	<b>0.06</b>	0.092	0.017	<b>10.77</b>	0.059
		11.06	0.04	0.078	0.015	11.05	<b>0.040</b>
		11.27	<b>0.14</b>	0.056	0.010	11.25	0.038
11.78	<b>0.07</b>	0.134	0.024	11.81	0.142		
78	LC09	48.50	0.01	0.415	0.022	48.50	<b>0.367</b>
79	LC09_deamid	44.69	0.02	0.030	0.003	44.68	0.026
		46.07	0.01	0.004	0.000	46.09	0.004
80	LC10	4.13	0.01	0.743	0.088	4.13	0.804
81	LC12	3.42	0.01	0.050	0.004	3.42	0.048
82	LC13	23.05	0.01	0.602	0.053	23.01	0.638
		25.75	0.00	0.009	0.000	25.76	<b>0.010</b>
		26.07	0.01	0.087	0.008	26.08	0.081
		26.35	0.02	0.037	0.001	26.32	<b>0.041</b>
83	LC13_deamid	22.01	0.01	0.041	0.003	21.99	0.043
		23.06	n.a.	0.267	n.a.	23.60	0.264
		23.64	0.01	0.250	0.018		
		23.87	0.02	0.740	0.046		
		26.64	0.01	0.036	0.001	26.60	0.034
27.10	0.01	0.019	0.001	27.06	0.019		
84	LC13_pyE	25.78	0.02	0.029	0.001	25.76	0.030
		26.07	0.01	0.357	0.026	26.03	0.334
		26.35	0.02	0.092	0.009	26.32	0.084
85	LC13_deamid_pyE	24.02	0.01	0.015	0.001	24.00	0.015
		24.46	0.01	0.005	0.000	24.44	0.004
		26.63	0.01	0.131	0.005	26.60	0.120
		27.10	0.01	0.044	0.003	27.11	0.041
86	LC14	24.57	0.02	0.007	0.000		

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
86	LC14	24.59	0.00	0.009	0.000	24.54	<b>0.005</b>
		25.29	0.01	2.794	0.197	25.28	2.627
		25.70	n.a.	0.008	n.a.		
		26.32	0.02	0.065	0.004	26.32	0.064
		35.23	0.03	0.010	0.001	35.26	0.009
		n.a.	n.a.	n.a.	n.a.	<b>52.73</b>	<b>0.010</b>
		53.06	0.03	0.020	0.003	<b>53.58</b>	<b>0.006</b>
		n.a.	n.a.	n.a.	n.a.		
87	LC14_ox	21.31	0.01	0.032	0.001	21.32	<b>0.037</b>
88	LC15	3.43	0.01	0.042	0.001	3.42	0.041
		3.62	n.a.	0.003	n.a.		
89	LC16	3.43	0.01	0.110	0.008	3.42	0.109
90	LC17	4.80	0.02	1.601	0.113	4.82	1.739
91	LC18	3.44	0.01	0.061	0.005	3.45	0.061
92	LC19	3.44	0.01	0.008	0.001	3.42	0.007
93	LC03-04	n.a.	n.a.	n.a.	n.a.	<b>33.08</b>	<b>0.001</b>
94	LC07-08	4.08	n.a.	0.000	n.a.	4.09	<b>0.000</b>
95	LC08-09	46.99	0.04	4.817	0.184	46.97	<b>4.369</b>
		47.44	0.01	1.448	0.323	47.44	1.318
96	LC08-09_deamid	43.24	0.02	0.390	0.012	43.24	<b>0.358</b>
		n.a.	n.a.	n.a.	n.a.	<b>44.53</b>	<b>0.082</b>
		44.65	0.01	0.090	0.003		
97	LC13-14_deamid	26.07	0.02	0.006	0.001	26.03	0.007
98	LC13-14_pyE	25.28	0.01	0.040	0.004	25.25	0.040
99	R1_01	n.a.	n.a.	n.a.	n.a.	<b>59.39</b>	<b>0.003</b>
100	R1_02	3.46	0.01	0.002	0.000	3.45	<b>0.002</b>
101	R1_03	2.99	0.01	0.016	0.001	2.99	0.017
102	R1_04	29.31	n.a.	0.001	n.a.	<b>29.22</b>	<b>0.001</b>
		n.a.	n.a.	n.a.	n.a.	<b>29.34</b>	<b>0.000</b>
		29.47	<b>0.08</b>	0.001	0.000	<b>29.56</b>	0.001
103	R1_05	22.45	<b>0.06</b>	0.001	0.000	22.38	<b>0.001</b>
		22.71	n.a.	0.000	n.a.		
		23.06	0.01	0.002	0.000	23.05	0.002
104	R1_06	19.42	0.01	0.004	0.001	19.42	0.003
		19.51	0.00	0.003	0.000		
105	R1_07	4.06	0.01	0.111	0.015	4.06	0.104
106	R1_08	4.06	0.02	0.008	0.001	4.06	0.009
		4.40	0.04	0.001	0.000		
107	R1_09	3.00	0.00	0.004	0.000	2.99	<b>0.004</b>
		3.48	0.00	0.000	0.000	3.45	0.000



#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
108	R1_10	2.43	0.03	0.023	0.006	2.36	<b>0.009</b>
		2.62	n.a.	0.006	n.a.		
109	R1_11	2.33	n.a.	0.003	n.a.	<b>2.41</b>	<b>0.004</b>
		2.45	0.01	0.004	0.001	<b>2.62</b>	0.005
		2.67	0.02	0.007	0.002		
		3.12	0.04	0.004	0.000		
110	R1_12	10.32	0.02	0.005	0.000	10.37	<b>0.005</b>
111	R1_13	3.86	0.02	0.018	0.002	3.84	0.016
112	R1_14	4.10	0.02	0.003	0.000	4.09	0.003
113	R1_15	21.51	0.00	0.003	0.000		
114	R1_16	4.82	0.01	0.001	0.000	4.82	0.001
115	R1_17	2.37	n.a.	0.153	n.a.	2.33	<b>0.074</b>
		2.47	0.03	0.262	0.066	2.47	0.212
116	R1_18	3.50	0.02	0.011	0.000		
		3.50	n.a.	0.008	n.a.	3.57	<b>0.019</b>
		3.77	<b>0.07</b>	0.017	0.007	<b>3.90</b>	0.006
		4.09	0.04	0.005	0.001		
		4.24	n.a.	0.004	n.a.	<b>4.16</b>	<b>0.006</b>
117	R1_19	2.37	0.00	0.014	0.002		
		2.48	0.04	0.022	0.008	<b>2.36</b>	0.012
		n.a.	n.a.	n.a.	n.a.	<b>2.50</b>	<b>0.014</b>
118	R1_20	2.69	0.02	0.007	0.002	2.71	0.008
		2.84	0.03	0.010	0.003	2.90	0.004
119	R1_21	2.99	0.00	0.002	0.000	2.99	0.002
120	R1_22	10.30	0.01	0.135	0.006	10.30	<b>0.095</b>
		10.67	<b>0.06</b>	0.096	0.017	<b>10.56</b>	<b>0.047</b>
		10.88	n.a.	0.045	n.a.	<b>10.77</b>	<b>0.061</b>
		11.10	<b>0.06</b>	0.076	0.024	11.05	0.042
		n.a.	n.a.	n.a.	n.a.	<b>11.25</b>	<b>0.040</b>
		11.43	<b>0.07</b>	0.049	0.008	11.46	0.038
		11.62	n.a.	0.047	n.a.		
		11.72	0.00	0.165	0.004		
		11.94	<b>0.08</b>	0.087	0.018	11.88	0.105
121	R1_23	n.a.	n.a.	n.a.	n.a.	<b>3.62</b>	<b>0.000</b>
122	R1_24	3.64	0.01	0.003	0.000	3.62	<b>0.004</b>
123	R1_25	2.99	0.01	0.165	0.011	2.99	0.163
124	R1_26	26.07	0.01	0.000	0.000	26.03	0.000
125	R1_27	21.79	0.01	0.000	0.000	21.77	0.000
126	R1_28	4.84	0.01	0.002	0.000	4.86	0.002
127	R1_29	4.04	0.01	0.002	0.000	4.06	0.002
128	R1_30	4.05	0.02	0.043	0.005	4.06	0.040

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
129	R1_31	4.05	0.02	0.004	0.001	4.06	0.004
130	R1_32	4.06	0.01	0.030	0.004	4.06	0.028
131	R1_33	23.93	0.01	0.005	0.000	23.91	0.005
132	R1_34	16.20	0.03	0.006	0.000	16.21	0.005
133	R1_35	4.04	0.01	0.008	0.001	4.06	0.007
134	R1_36	4.11	0.01	0.001	0.000	4.13	<b>0.001</b>
137	R1_39	2.41 2.53	0.04 0.00	0.068 0.039	0.021 0.003	2.45	0.078
138	R1_40	15.24	0.02	0.029	0.002	15.23	0.033
139	R1_41	15.21	n.a.	0.006	n.a.		
140	R1_42	4.16	0.00	0.002	0.000	4.16	0.002
141	R1_43	15.25 15.25	0.01 0.01	0.003 0.003	0.001 0.000	15.28	<b>0.003</b>
142	R1_44	3.53 16.90	0.01 0.01	0.004 0.440	0.000 0.072	3.53 16.92	<b>0.004</b> 0.445
143	R1_45	59.37 59.36	n.a. n.a.	0.004 0.006	n.a. n.a.	59.39	<b>0.004</b>
144	R1_46	2.97	0.04	0.009	0.001	2.95	<b>0.007</b>
145	R1_47	25.60 25.66	0.00 0.01	0.001 0.001	0.000 0.000	25.56	0.001
146	R1_48	3.00	0.01	0.004	0.000	2.99	0.004
147	R1_49	4.72 19.33	0.00 0.00	0.003 0.001	0.000 0.000	4.74	0.003
148	R1_50	3.58 4.12 4.24 4.80	0.01 n.a. 0.02 0.01	0.250 0.011 0.017 0.001	0.031 n.a. 0.001 0.000	3.62 4.82	0.271 0.001
150	R1_52	3.00	0.01	0.026	0.003	2.99	0.026
151	R1_53	4.06	0.01	0.012	0.003	4.06	0.011
152	R1_54	59.31 59.36	n.a. 0.00	0.004 0.010	n.a. 0.000	59.33	<b>0.007</b>
153	R1_55	3.81	0.02	0.005	0.001	3.78	0.005
154	R1_56	16.16	0.01	0.017	0.001	16.14	0.015
155	R1_57	59.31	0.01	0.011	0.004	59.29	0.012
156	R1_58	25.55	0.00	0.005	0.000	25.51	0.005
157	R1_59	4.18	0.02	0.002	0.000		

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
158	R1_60	4.28	0.02	0.001	0.000	4.25	0.001
159	R1_61	4.27	0.02	0.001	0.000	4.25	0.001
160	R1_62	4.28	0.02	0.018	0.001	4.25	0.018
161	R1_63	59.25	0.00	0.014	0.006	59.29	0.015
162	R1_64	21.79	0.01	0.004	0.000	21.77	0.004
163	R1_65	19.47	0.02	0.003	0.000	19.42	<b>0.004</b>
164	R1_66	19.20 20.74	0.02 0.02	0.005 0.008	0.001 0.001	19.18 20.74	0.006 0.008
165	R1_67	3.71	n.a.	0.004	n.a.	3.72	<b>0.003</b>
166	R1_68	3.00	0.00	0.004	0.000	2.99	<b>0.003</b>
167	R1_69	3.81	<b>0.06</b>	0.001	0.000	<b>3.72</b>	0.001
169	R1_71	22.57 23.64	n.a. 0.00	0.001 0.001	n.a. 0.000	23.60	<b>0.002</b>
170	R1_72	19.21	0.00	0.004	0.000	19.18	0.004
171	R1_73	5.21	0.01	0.005	0.000	5.19	0.005
172	R1_74	59.21	0.02	0.016	0.006	59.23	0.014
173	R1_75	22.87	0.01	0.014	0.001	22.86	0.014
174	R1_76	22.87	0.01	0.017	0.001	22.86	0.017
175	R1_77	16.70	0.03	0.004	0.000	16.71	0.004
176	R1_78	59.25	0.00	0.006	0.000	59.23	<b>0.005</b>
177	R1_79	2.60 2.78 2.90	n.a. 0.04 n.a.	0.007 0.012 0.004	n.a. 0.003 n.a.	2.76	0.011
178	R1_80	25.84	0.02	0.011	0.001	25.80	0.012
179	R1_81	20.18	0.01	0.010	0.001	20.14	0.009
180	R1_82	59.20 59.21	0.01 0.00	0.005 0.005	0.001 0.001	59.18	0.006
181	R1_83	22.84	0.02	0.006	0.001	22.86	0.008
182	R1_84	20.89	0.02	0.000	0.000	20.88	0.000
183	R1_85	20.87	0.02	0.001	0.000	20.88	0.001
184	R1_86	59.19	0.02	0.018	0.005	59.18	0.014
185	R1_87	4.05	0.00	0.004	0.000	4.06	<b>0.003</b>
186	R1_88	17.64	0.01	0.055	0.002	17.62	0.055

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
187	R1_89	59.18	0.03	0.009	0.001	59.18	0.008
		59.21	0.01	0.008	0.002		
188	R1_90	23.50	0.00	0.003	0.000	23.47	<b>0.004</b>
189	R1_91	59.19	0.02	0.018	0.003	59.18	0.018
190	R1_92	20.76	n.a.	0.003	n.a.	20.74	<b>0.003</b>
192	R1_94	25.86	0.01	0.006	0.000	25.85	0.006
193	R1_95	20.35	0.02	0.008	0.001	20.30	0.007
194	R1_96	19.55	0.01	0.003	0.000	19.57	0.003
		28.73	0.01	0.000	0.000	28.71	<b>0.000</b>
195	R1_97	28.73	0.01	0.200	0.018	28.71	0.184
196	R1_98	19.55	0.01	0.029	0.003	19.57	0.031
		21.58	0.02	0.010	0.001	21.56	0.011
197	R1_99	19.55	0.01	0.003	0.000	19.57	0.003
198	R1_100	19.55	0.01	0.002	0.000	19.57	0.001
199	R1_101	2.35	n.a.	0.130	n.a.	2.36	<b>0.111</b>
		2.44	0.04	0.271	0.055	2.50	0.197
		2.53	n.a.	0.154	n.a.		
200	R1_102	24.96	0.03	0.001	0.000	<b>24.88</b>	0.001
201	R1_103	19.24	0.01	0.001	0.000	19.22	0.001
202	R1_104	21.20	0.01	0.019	0.001	21.18	<b>0.021</b>
203	R1_105	28.71	0.02	0.000	0.000	28.71	<b>0.000</b>
204	R1_106	59.14	0.02	0.012	0.001	59.13	<b>0.017</b>
205	R1_107	29.55	0.02	0.001	0.000	29.51	0.001
206	R1_108	29.55	0.02	0.010	0.001	29.51	0.009
207	R1_109	29.55	0.02	0.001	0.000	29.51	0.001
208	R1_110	25.81	n.a.	0.003	n.a.	25.80	<b>0.004</b>
209	R1_111	24.22	0.02	0.005	0.000	24.22	<b>0.007</b>
210	R1_112	32.89	n.a.	0.001	n.a.	32.87	<b>0.001</b>
211	R1_113	28.72	0.01	0.001	0.000	28.71	0.001
212	R1_114	28.73	0.01	0.001	0.000	28.71	0.000
213	R1_115	59.14	0.02	0.022	0.008	59.13	0.028
214	R1_116	19.97	0.02	0.002	0.000	19.97	0.002
215	R1_117	19.97	0.02	0.018	0.001	19.97	0.018

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
216	R1_118	3.71	n.a.	0.000	n.a.	3.72	<b>0.000</b>
217	R1_119	59.14	0.02	0.016	0.003	59.13	0.018
218	R1_120	59.14	0.02	0.032	0.005	59.13	0.038
219	R1_121	28.44	n.a.	0.005	n.a.		
221	R1_123	20.72	0.01	0.010	0.001	20.71	0.010
222	R1_124	59.11	0.02	0.014	0.001	59.08	<b>0.021</b>
223	R1_125	16.27	0.02	0.004	0.000	16.28	0.004
224	R1_126	21.81	0.02	0.039	0.004	21.77	0.037
225	R1_127	25.94	0.02	0.016	0.003	25.90	0.018
226	R1_128	28.91	0.02	0.005	0.000	28.87	0.005
227	R1_129	n.a.	n.a.	n.a.	n.a.	<b>24.74</b>	<b>0.003</b>
228	R1_130	59.11	0.02	0.019	0.003	59.08	0.023
229	R1_131	25.86	0.01	0.012	0.001	25.85	0.014
230	R1_132	21.79	0.01	0.003	0.000	21.77	0.003
231	R1_133	59.11	0.02	0.035	0.003	59.08	<b>0.042</b>
232	R1_134	59.07	0.03	0.015	0.002	59.08	<b>0.023</b>
233	R1_135	29.20	0.01	0.000	0.000	29.19	0.000
234	R1_136	29.20	0.01	0.001	0.000	29.19	0.001
235	R1_137	29.20	0.01	0.014	0.001	29.19	0.014
236	R1_138	17.29	0.01	0.006	0.000	17.27	0.005
237	R1_139	22.32	0.01	0.008	0.001	22.31	0.009
238	R1_140	36.67	0.03	0.019	0.001	36.62	0.018
239	R1_141	59.07	0.03	0.019	0.002	59.08	<b>0.026</b>
240	R1_142	16.96	0.02	0.001	0.000	16.96	0.001
241	R1_143	59.07	0.03	0.034	0.004	59.08	<b>0.043</b>
242	R1_144	18.97	0.02	0.004	0.000	18.96	0.004
243	R1_145	30.15	0.01	0.004	0.000	30.17	<b>0.003</b>
244	R1_146	59.05	0.00	0.011	0.002	59.08	0.012
245	R1_147	34.89	0.02	0.001	0.000	34.88	0.001
246	R1_148	32.39	0.01	0.007	0.000	32.38	<b>0.006</b>
247	R1_149	2.72	0.04	0.010	0.005	2.71	0.007

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
247	R1_149	2.80	0.01	0.013	0.000		
		2.88	0.03	0.006	0.001	2.90	0.003
248	R1_150	2.37	n.a.	0.137	n.a.	2.41	<b>0.067</b>
		2.48	0.04	0.183	0.039	2.53	<b>0.103</b>
249	R1_151	21.79	0.01	0.001	0.000	21.77	0.001
250	R1_152	21.79	0.01	0.040	0.005	21.77	0.039
251	R1_153	5.02	0.01	0.001	0.000	5.06	0.001
252	R1_154	21.79	0.01	0.001	0.000	21.77	0.001
253	R1_155	5.02	0.01	0.001	0.000	5.06	<b>0.001</b>
254	R1_156	5.02	0.01	0.001	0.000	5.00	0.001
255	R1_157	59.07	0.03	0.004	0.001	59.03	<b>0.006</b>
256	R1_158	28.97	0.02	0.007	0.000	28.93	<b>0.006</b>
257	R1_159	21.79	0.01	0.003	0.000	21.77	0.003
258	R1_160	59.06	0.02	0.034	0.007	59.08	0.042
259	R1_161	17.38	0.02	0.008	0.000	17.41	<b>0.006</b>
260	R1_162	59.00	0.01	0.014	0.005	58.99	0.022
261	R1_163	19.02	0.02	0.008	0.001	19.02	0.008
262	R1_164	59.00	0.00	0.005	0.000		
		59.01	0.00	0.004	0.001	58.99	0.006
263	R1_165	26.40	0.02	0.006	0.000	26.36	0.006
264	R1_166	29.41	0.05	0.003	0.001	29.34	0.004
265	R1_167	30.47	0.01	0.001	0.000	30.45	<b>0.000</b>
		59.02	0.02	0.019	0.005	58.99	0.025
266	R1_168	58.99	0.03	0.012	0.002	58.99	0.011
267	R1_169	58.99	0.02	0.015	0.004	58.99	0.019
268	R1_170	16.76	0.01	0.003	0.000	16.71	0.003
269	R1_171	58.98	0.03	0.012	0.005	58.99	0.019
270	R1_172	58.99	0.03	0.004	0.000	58.99	0.004
271	R1_173	21.07	0.03	0.008	0.001	21.06	0.008
272	R1_174	30.72	0.02	0.184	0.006	30.72	0.177
273	R1_175	58.97	0.03	0.018	0.006	58.99	0.023
274	R1_176	5.23	0.02	0.004	0.000	5.26	<b>0.003</b>
275	R1_177	33.39	n.a.	0.002	n.a.	33.37	<b>0.002</b>

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
275	R1_177	58.98	0.02	0.034	0.011	58.99	0.041
276	R1_178	58.95	0.01	0.012	0.004	58.94	0.016
277	R1_179	30.72	0.02	0.019	0.001	30.72	0.019
278	R1_180	26.10	0.02	0.014	0.001	26.08	0.013
		28.15	0.02	0.012	0.000	28.11	<b>0.011</b>
279	R1_181	26.88	n.a.	0.004	n.a.	<b>26.80</b>	<b>0.003</b>
		26.89	<b>0.07</b>	0.004	0.001		
		27.18	n.a.	0.003	n.a.		
		27.67	0.03	0.002	0.000		
280	R1_182	58.95	0.01	0.009	0.004	58.94	0.014
281	R1_183	30.73	0.01	0.006	0.000		
		n.a.	n.a.	n.a.	n.a.	<b>33.20</b>	<b>0.005</b>
282	R1_184	58.95	n.a.	0.004	n.a.	58.94	<b>0.004</b>
283	R1_185	21.41	0.01	0.001	0.000	21.36	<b>0.001</b>
284	R1_186	24.38	0.02	0.002	0.000		
		27.09	n.a.	0.009	n.a.		
		27.33	0.04	0.008	0.001	27.32	0.006
		28.15	<b>0.11</b>	0.008	0.001	<b>28.05</b>	0.009
285	R1_187	2.41	0.04	0.076	0.035	2.41	0.038
		2.53	0.03	0.058	0.024	2.53	0.061
		2.55	n.a.	0.041	n.a.		
286	R1_188	58.94	0.03	0.030	0.009	58.94	0.036
287	R1_189	2.36	0.01	0.066	0.013	2.41	<b>0.040</b>
		2.49	0.03	0.099	0.018	2.53	0.065
288	R1_190	21.74	0.01	0.004	0.000	21.73	0.004
289	R1_191	58.94	0.01	0.011	0.002	58.94	0.013
290	R1_192	22.79	n.a.	0.020	n.a.	22.82	<b>0.020</b>
291	R1_193	19.88	0.01	0.001	0.000	19.88	0.001
292	R1_194	19.88	0.01	0.011	0.001	19.88	0.011
293	R1_195	19.88	0.01	0.001	0.000	19.88	0.001
294	R1_196	21.45	n.a.	0.002	n.a.	21.41	<b>0.002</b>
295	R1_197	25.10	0.02	0.005	0.000	25.06	0.005
296	R1_198	58.92	0.02	0.016	0.004	58.94	0.017
297	R1_199	n.a.	n.a.	n.a.	n.a.	<b>19.76</b>	<b>0.001</b>
298	R1_200	58.91	n.a.	0.009	n.a.	58.94	<b>0.007</b>
299	R1_201	58.92	0.02	0.007	0.002	58.94	0.009

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
300	R1_202	24.89	0.01	0.023	0.002	24.88	0.024
301	R1_203	36.26	0.02	0.001	0.000	36.26	<b>0.001</b>
302	R1_204	36.24	0.03	0.019	0.001	36.26	0.017
303	R1_205	27.45 33.93	n.a. 0.03	0.001 0.004	n.a. 0.000	27.45 33.92	<b>0.001</b> 0.004
304	R1_206	19.28 19.37 22.60 26.51	0.05 0.00 <b>0.17</b> 0.02	0.020 0.022 0.004 0.008	0.009 0.002 0.001 0.000	19.29   26.46	0.032   0.008
305	R1_207	28.80	0.02	0.002	0.000	28.81	0.002
306	R1_208	18.22 29.50 29.80	0.02 0.01 0.02	0.002 0.001 0.005	0.000 0.000 0.000	18.21 29.47 29.78	0.002 <b>0.001</b> <b>0.003</b>
307	R1_209	28.80	0.02	0.002	0.000	28.81	0.002
308	R1_210	58.90	0.03	0.017	0.006	58.89	0.020
309	R1_211	28.79	0.02	0.001	0.000	28.76	0.001
310	R1_212	42.53	0.03	0.020	0.001	42.53	0.018
311	R1_213	31.33	0.02	0.003	0.000	31.35	0.002
312	R1_214	20.21	0.02	0.008	0.001	20.19	0.008
313	R1_215	58.89 58.89	0.02 0.00	0.009 0.007	0.004 0.000	58.89	0.010
314	R1_216	58.89	0.01	0.011	0.004	58.89	0.012
315	R1_217	58.89	0.01	0.004	0.001	58.89	0.003
316	R1_218	25.01 29.99 30.06	0.02 0.03 n.a.	0.014 0.006 0.005	0.001 0.000 n.a.	24.97  30.07	0.014  <b>0.005</b>
317	R1_219	19.81 20.61	n.a. 0.01	0.003 0.005	n.a. 0.000	 20.60	 0.004
318	R1_220	20.61	0.01	0.059	0.006	20.60	0.062
319	R1_221	16.00	0.02	0.002	0.000	16.00	0.002
320	R1_222	15.91	0.02	0.004	0.000	15.93	<b>0.003</b>
321	R1_223	58.88	0.01	0.007	0.002	58.89	0.006
322	R1_224	29.33	0.01	0.002	0.000	29.30	0.002
323	R1_225	4.07 4.07	0.01 0.01	0.006 0.006	0.000 0.002	4.06	<b>0.007</b>
324	R1_226	58.88	0.01	0.007	0.003	58.89	0.007



#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
325	R1_227	36.44	0.01	0.259	0.022	36.46	0.238
326	R1_228	36.42	0.01	0.017	0.001	36.41	<b>0.020</b>
327	R1_229	14.19	0.03	0.045	0.003	14.23	<b>0.040</b>
328	R1_230	36.44	0.01	0.131	0.006	36.46	0.119
329	R1_231	27.41	0.00	0.001	0.000	27.45	0.001
330	R1_232	36.44	0.01	0.090	0.007	36.46	0.084
		n.a.	n.a.	n.a.	n.a.	<b>41.70</b>	<b>0.035</b>
331	R1_233	58.87	0.01	0.006	0.003	58.89	0.004
332	R1_234	25.47	0.01	0.012	0.002	25.47	0.012
333	R1_235	19.00	0.01	0.005	0.002	18.96	0.008
334	R1_236	58.88	0.01	0.005	0.002	58.89	0.004
		59.11	n.a.	0.001	n.a.		
335	R1_237	36.44	0.01	0.013	0.002	36.46	0.013
336	R1_238	31.57	0.01	0.008	0.002	31.55	0.009
337	R1_239	36.36	n.a.	0.003	n.a.		
		36.45	n.a.	0.004	n.a.	36.46	<b>0.004</b>
338	R1_240	36.45	0.02	0.005	0.001	36.46	0.005
339	R1_241	36.47	0.02	0.003	0.000	36.51	0.003
340	R1_242	28.57	0.02	0.004	0.000	28.55	<b>0.004</b>
341	R1_243	34.89	0.02	0.003	0.000	34.88	0.003
342	R1_244	42.64	0.01	0.005	0.000	42.65	0.005
343	R1_245	42.63	0.01	0.007	0.000	42.59	0.006
344	R1_246	24.41	0.02	0.004	0.000	24.41	0.003
345	R1_247	42.64	0.01	0.004	0.000	42.59	0.004
346	R1_248	22.18	0.02	0.006	0.002	22.17	0.010
347	R1_249	36.84	0.02	0.020	0.001	36.80	<b>0.022</b>
348	R1_250	24.98	0.01	0.004	0.000	24.97	0.003
349	R1_251	36.84	0.02	0.010	0.000	36.80	<b>0.011</b>
350	R1_252	24.16	0.02	0.030	0.002	24.15	0.032
351	R1_253	31.63	0.02	0.004	0.000	31.65	0.004
352	R1_254	34.89	0.02	0.012	0.001	34.88	0.011
353	R1_255	23.05	0.01	0.009	0.001	23.01	0.009

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
354	R1_256	34.08	n.a.	0.001	n.a.	34.11	<b>0.001</b>
355	R1_257	23.04	0.01	0.013	0.001	23.01	0.013
		n.a.	n.a.	n.a.	n.a.	<b>33.08</b>	<b>0.001</b>
356	R1_258	22.56	0.02	0.002	0.000	22.57	0.002
357	R1_259	n.a.	n.a.	n.a.	n.a.	<b>25.80</b>	<b>0.002</b>
		n.a.	n.a.	n.a.	n.a.	<b>32.96</b>	<b>0.001</b>
358	R1_260	24.15	n.a.	0.004	n.a.	24.10	<b>0.003</b>
359	R1_261	28.45	0.02	0.013	0.001	28.43	0.012
360	R1_262	20.17	0.02	0.009	0.001	20.14	0.009
		22.00	n.a.	0.004	n.a.	21.99	<b>0.003</b>
		23.65	n.a.	0.022	n.a.		
		23.89	0.01	0.044	0.000		
		28.45	0.02	0.011	0.001	28.43	0.011
361	R1_263	23.05	0.01	0.036	0.003	23.05	0.041
362	R1_264	2.40	0.00	0.058	0.012	2.45	0.039
363	R1_265	2.37	n.a.	0.038	n.a.	2.41	<b>0.026</b>
		2.54	0.03	0.034	0.013	2.53	0.042
364	R1_266	36.52	0.02	0.007	0.000	36.51	0.006
365	R1_267	27.90	0.02	0.007	0.000	27.85	<b>0.006</b>
366	R1_268	39.00	0.04	0.004	0.000	38.99	<b>0.004</b>
367	R1_269	38.99	0.04	0.008	0.000	38.99	<b>0.007</b>
368	R1_270	36.80	0.03	0.005	0.000	36.80	0.005
369	R1_271	36.45	0.03	0.002	0.000	36.46	0.001
370	R1_272	31.54	0.03	0.004	0.000	31.48	0.004
371	R1_273	40.32	0.03	0.003	0.000	40.30	0.003
372	R1_274	25.08	0.01	0.159	0.008	25.06	0.154
373	R1_275	30.21	n.a.	0.011	n.a.		
		30.32	n.a.	0.023	n.a.	30.33	<b>0.019</b>
		30.40	0.01	0.024	0.007		
		30.66	0.01	0.008	0.000	30.61	0.008
374	R1_276	25.08	0.01	0.081	0.005	25.06	0.082
375	R1_277	27.84	0.03	0.013	0.000	27.85	<b>0.013</b>
376	R1_278	20.67	0.01	0.037	0.002		
		29.96	0.02	0.019	0.000		
		30.47	n.a.	0.002	n.a.		
		30.59	n.a.	0.002	n.a.	30.61	<b>0.003</b>
		30.91	0.04	0.001	0.000	30.95	0.001
377	R1_279	25.07	0.01	0.062	0.005	25.06	0.064

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
378	R1_280	25.72	0.02	0.003	0.000	25.71	0.003
		26.13	0.01	0.003	0.000		
379	R1_281	21.48	n.a.	0.003	n.a.		
		24.97	0.03	0.003	0.001		
380	R1_282	25.03	0.01	0.002	0.000	25.01	0.002
381	R1_283	32.09	n.a.	0.002	n.a.		
		32.10	n.a.	0.002	n.a.	32.11	<b>0.002</b>
		32.32	n.a.	0.002	n.a.		
		33.79	0.03	0.095	0.002	33.80	0.092
382	R1_284	20.66	<b>0.08</b>	0.005	0.001	<b>20.57</b>	0.004
		20.68	0.04	0.008	0.003	20.74	0.007
383	R1_285	28.50	0.01	0.005	0.000	28.49	0.005
		30.76	0.02	0.024	0.001	30.72	0.024
384	R1_286	30.76	0.02	0.006	0.000	30.72	0.006
385	R1_287	47.57	0.02	0.003	0.000	47.58	0.004
386	R1_288	40.30	0.04	0.030	0.001	40.30	<b>0.026</b>
		47.58	n.a.	0.003	n.a.		
387	R1_289	24.89	0.02	0.004	0.000	24.88	0.004
		25.04	n.a.	0.004	n.a.		
388	R1_290	n.a.	n.a.	n.a.	n.a.	<b>24.31</b>	<b>0.000</b>
		24.84	0.01	0.005	0.001	24.84	0.005
389	R1_291	47.57	0.03	0.003	0.000	47.53	0.003
390	R1_292	40.31	0.04	0.049	0.002	40.30	<b>0.045</b>
		41.74	0.02	0.006	0.000		
391	R1_293	40.28	0.02	0.024	0.001	40.30	<b>0.021</b>
392	R1_294	25.04	0.02	0.087	0.006	25.01	0.088
393	R1_295	24.51	0.01	0.004	0.000	24.48	0.004
394	R1_296	40.24	n.a.	0.011	n.a.	40.25	<b>0.006</b>
		40.29	0.01	0.007	0.000		
395	R1_297	40.30	0.03	0.004	0.000	40.30	0.004
396	R1_298	25.96	n.a.	0.003	n.a.	25.95	<b>0.003</b>
397	R1_299	32.84	0.01	0.013	0.000	32.83	0.012
398	R1_300	20.58	0.01	0.007	0.001	20.54	0.007
399	R1_301	2.44	0.03	0.042	0.009	<b>2.55</b>	<b>0.017</b>
		2.50	<b>0.08</b>	0.023	0.003	2.45	0.025
400	R1_302	19.91	0.01	0.006	0.001	19.88	0.005
401	R1_303	38.00	0.02	0.004	0.000	38.01	0.004

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
402	R1_304	27.21	0.01	0.009	0.000	27.22	0.008
403	R1_305	23.75	0.01	0.002	0.000	23.71	0.002
404	R1_306	23.74	0.01	0.048	0.005	23.71	0.051
405	R1_307	23.75	0.01	0.001	0.000	23.71	0.002
406	R1_308	36.08	0.03	0.015	0.000	36.06	<b>0.014</b>
407	R1_309	37.38	0.02	0.013	0.002	37.39	0.011
408	R1_310	26.77	0.01	0.001	0.000	26.73	0.001
409	R1_311	26.77	0.01	0.021	0.006	26.73	0.016
410	R1_312	19.92	0.01	0.030	0.003	19.93	0.031
411	R1_313	28.08	0.03	0.008	0.001	28.05	0.008
412	R1_314	22.31	0.01	0.008	0.001	22.27	0.007
413	R1_315	27.63	0.01	0.001	0.000	27.63	<b>0.001</b>
414	R1_316	27.63	0.01	0.002	0.000	27.63	<b>0.002</b>
415	R1_317	27.63	0.01	0.027	0.001	27.63	<b>0.025</b>
416	R1_318	27.63	0.01	0.002	0.000	27.63	<b>0.002</b>
417	R1_319	27.64	0.01	0.002	0.000	27.63	<b>0.001</b>
418	R1_320	16.17	0.02	0.006	0.000	16.21	0.006
419	R1_321	35.01	0.02	0.056	0.004	35.00	0.054
420	R1_322	35.00	0.01	0.002	0.000		
		35.02	0.03	0.002	0.000		
		35.04	n.a.	0.002	n.a.	35.00	<b>0.002</b>
		35.90	0.03	0.010	0.000	35.92	0.010
421	R1_323	35.01	0.02	0.010	0.002	35.00	0.011
422	R1_324	31.62	0.01	0.005	0.000	31.61	0.005
423	R1_325	n.a.	n.a.	n.a.	n.a.	<b>35.19</b>	<b>0.003</b>
424	R1_326	33.28	0.02	0.018	0.001	33.25	<b>0.016</b>
425	R1_327	n.a.	n.a.	n.a.	n.a.	<b>2.41</b>	<b>0.023</b>
		2.53	0.03	0.036	0.012	2.53	0.033
426	R1_328	41.59	0.02	0.079	0.004	41.59	0.077
427	R1_329	25.10	n.a.	0.010	n.a.	25.14	<b>0.008</b>
		n.a.	n.a.	n.a.	n.a.	<b>25.43</b>	<b>0.001</b>
		33.11	0.01	0.169	0.006	33.12	0.161
		33.41	<b>0.16</b>	0.016	0.008		
428	R1_330	28.45	0.03	0.001	0.000	28.43	<b>0.001</b>

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
429	R1_331	34.08	0.00	0.005	0.002	34.11	0.004
430	R1_332	31.16	0.01	0.008	0.001	31.14	0.007
431	R1_333	38.59	0.02	0.006	0.000	38.58	<b>0.005</b>
432	R1_334	33.89	n.a.	0.003	n.a.	33.86	<b>0.003</b>
433	R1_335	20.90	0.01	0.006	0.000	20.88	0.007
434	R1_336	38.71	0.02	0.124	0.004	38.69	<b>0.108</b>
435	R1_337	31.62	0.01	0.005	0.000	31.61	0.005
436	R1_338	38.71	0.02	0.007	0.000	38.69	<b>0.006</b>
437	R1_339	27.46	0.01	0.004	0.000	27.40	0.004
		29.95	0.02	2.293	0.117	29.94	2.072
		30.92	<b>0.05</b>	0.071	0.027	30.95	0.043
		32.08	n.a.	0.006	n.a.		
		32.10	n.a.	0.007	n.a.	32.11	<b>0.004</b>
438	R1_340	42.39	0.00	0.003	0.000		
		42.70	n.a.	0.001	n.a.	<b>42.59</b>	<b>0.001</b>
439	R1_341	41.58	0.01	0.081	0.046	41.59	0.055
		41.75	0.01	0.068	0.059	41.78	0.016
		n.a.	n.a.	n.a.	n.a.	<b>42.00</b>	<b>0.055</b>
		42.18	n.a.	0.003	n.a.	42.16	<b>0.005</b>
		42.33	n.a.	0.004	n.a.		
		42.35	<b>0.07</b>	0.185	0.027		
		42.60	n.a.	0.163	n.a.	42.59	<b>0.108</b>
440	R1_342	41.56	0.02	0.007	0.000	41.55	0.007
		41.76	0.00	0.002	0.000		
		41.98	n.a.	0.008	n.a.	42.00	<b>0.009</b>
		42.12	n.a.	0.016	n.a.		
		42.32	0.01	0.027	0.002		
		42.54	0.03	0.021	0.001	42.53	<b>0.014</b>
		42.73	n.a.	0.014	n.a.		
		n.a.	n.a.	n.a.	n.a.	<b>43.24</b>	<b>0.004</b>
441	R1_343	29.99	0.03	0.003	0.000	29.94	0.002
442	R1_344	25.00	0.01	0.006	0.000	24.97	0.006
443	R1_345	25.04	0.02	0.090	0.006	25.01	0.089
444	R1_346	18.10	0.00	0.004	0.000		
		18.12	n.a.	0.003	n.a.	18.09	<b>0.005</b>
445	R1_347	18.14	0.01	0.004	0.000	18.13	0.004
446	R1_348	25.04	0.02	0.010	0.001	25.01	0.011
447	R1_349	18.12	0.02	0.004	0.000	18.13	0.004
		19.80	0.02	0.007	0.001	19.80	0.007
448	R1_350	18.07	n.a.	0.003	n.a.	18.09	<b>0.005</b>
		18.11	0.02	0.004	0.000		

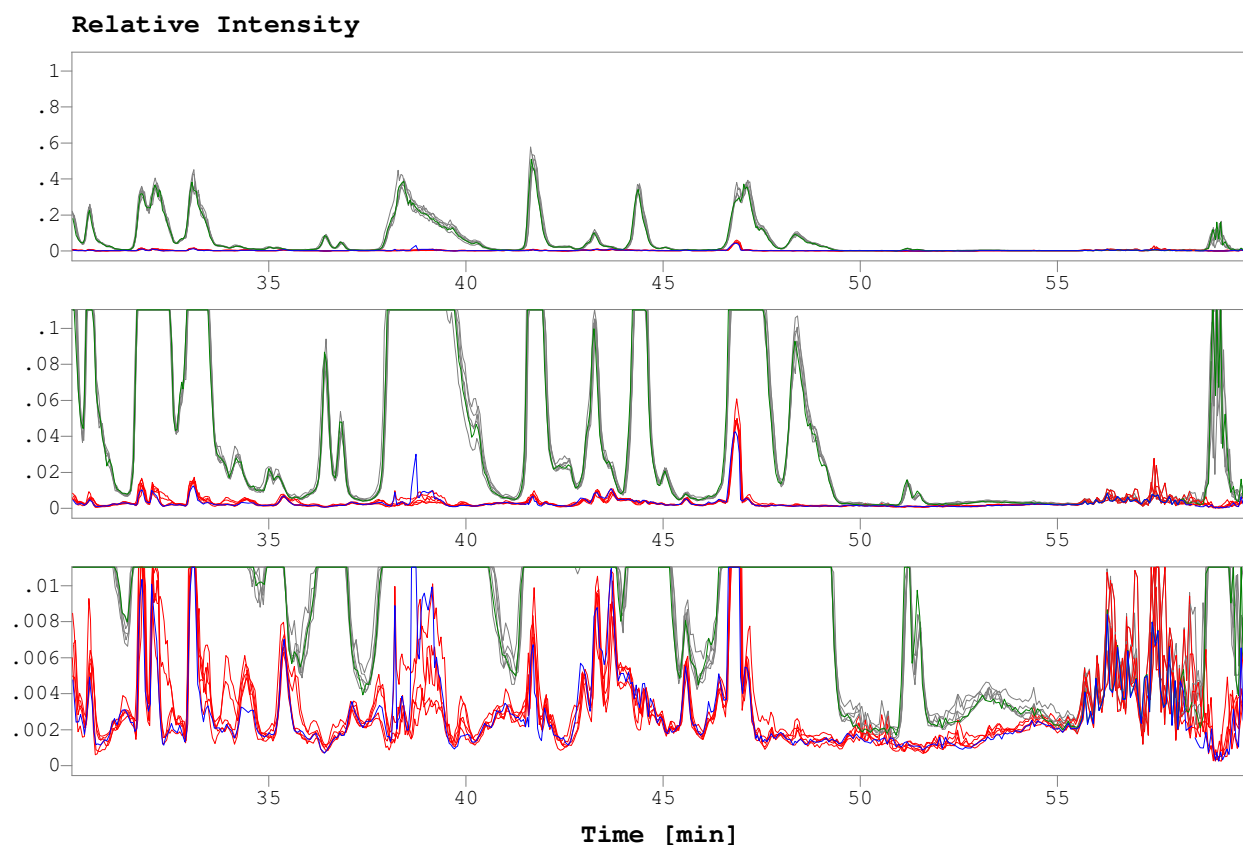
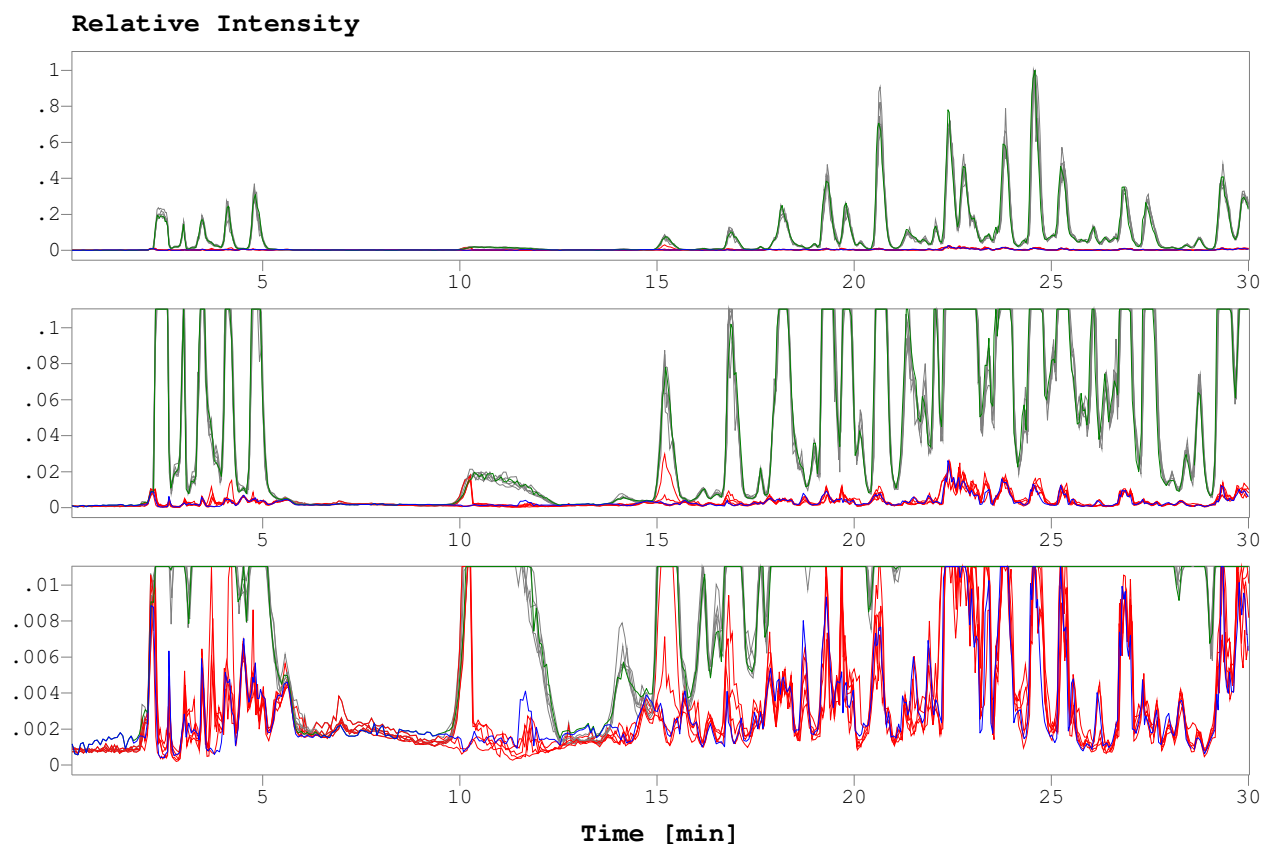
#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
449	R1_351	25.01	n.a.	0.004	n.a.	25.01	<b>0.004</b>
450	R1_352	24.92	0.01	0.019	0.002	24.93	0.019
		n.a.	n.a.	n.a.	n.a.	<b>36.41</b>	<b>0.101</b>
		36.44	0.01	0.007	0.000		
451	R1_353	36.43	0.02	0.028	0.001	36.41	<b>0.025</b>
452	R1_354	24.93	0.01	0.003	0.000	24.93	0.003
		36.44	0.01	0.010	0.002	36.46	0.009
453	R1_355	40.18	0.03	0.008	0.001	40.14	<b>0.007</b>
454	R1_356	19.00	0.01	0.057	0.006	18.96	0.062
455	R1_357	19.09	0.02	0.015	0.004	19.08	0.019
456	R1_358	24.59	n.a.	0.017	n.a.		
		25.40	0.02	0.014	0.005	25.36	0.012
		28.08	0.03	0.020	0.001	28.05	<b>0.019</b>
		41.63	0.01	0.026	0.006	41.63	0.023
		41.83	0.03	0.049	0.011	<b>41.74</b>	<b>0.017</b>
		n.a.	n.a.	n.a.	n.a.	<b>41.86</b>	<b>0.029</b>
457	R1_359	19.00	0.01	0.010	0.002	19.02	0.013
458	R1_360	19.00	0.01	0.005	0.000	19.02	0.005
459	R1_361	32.80	0.01	0.171	0.005	32.78	0.169
460	R1_362	32.79	0.02	0.022	0.001	32.78	0.023
461	R1_363	n.a.	n.a.	n.a.	n.a.	<b>32.78</b>	<b>0.007</b>
462	R1_364	32.79	0.02	0.004	0.000	32.78	0.004
463	R1_365	25.61	0.02	0.068	0.005	25.61	0.065
		38.24	0.02	0.051	0.005	38.24	0.044
		38.36	<b>0.09</b>	0.006	0.001		
		38.47	0.02	0.006	0.002		
		38.60	0.04	0.044	0.023		
		38.73	0.04	0.046	0.021	<b>38.82</b>	0.071
		38.86	0.02	0.007	0.001		
		39.11	0.03	0.058	0.020		
		39.37	0.01	0.114	0.058		
		39.55	<b>0.06</b>	0.059	0.043	39.57	0.043
		39.92	n.a.	0.035	n.a.	39.97	<b>0.037</b>
464	R1_366	22.92	n.a.	0.001	n.a.		
		23.46	0.01	0.002	0.000	23.42	<b>0.003</b>
		23.74	0.01	0.004	0.002	23.71	0.008
		24.01	n.a.	0.001	n.a.		
		24.48	0.01	0.011	0.003	24.44	0.011
465	R1_367	39.49	0.02	0.002	0.000	39.48	0.002
		39.55	0.01	0.002	0.000		
466	R1_368	19.01	0.03	0.008	0.002		
		19.01	0.00	0.007	0.000	19.02	0.007
467	R1_369	37.88	0.02	0.004	0.001	37.87	0.004

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
468	R1_370	28.08	0.03	0.004	0.000	28.05	0.004
469	R1_371	41.48	n.a.	0.004	n.a.	41.46	<b>0.003</b>
470	R1_372	26.42	0.02	0.142	0.007	26.41	0.144
471	R1_373	41.49	0.01	0.004	0.000	41.52	0.004
472	R1_374	26.41	0.02	0.029	0.014	26.41	<b>0.076</b>
473	R1_375	40.32	0.03	0.022	0.001	40.30	0.020
474	R1_376	26.43	0.01	0.007	0.004	26.41	0.013
475	R1_377	40.32	0.02	0.004	0.000	40.30	<b>0.003</b>
476	R1_378	18.13	0.02	0.005	0.001	18.13	0.006
477	R1_379	27.19	0.02	0.004	0.000	27.16	0.004
478	R1_380	27.19	0.02	0.009	0.001	27.16	0.009
479	R1_381	27.20	0.01	0.003	0.000	27.16	0.003
480	R1_382	45.08	0.01	0.009	0.000	45.04	<b>0.008</b>
481	R1_383	45.07	0.03	0.035	0.002	45.04	0.032
482	R1_384	45.08	0.01	0.014	0.001	45.04	0.013
483	R1_385	25.82	0.02	0.017	0.001	25.80	0.017
484	R1_386	45.19	0.03	0.006	0.000	45.17	<b>0.005</b>
485	R1_387	29.83	0.02	0.016	0.001	29.82	0.015
486	R1_388	36.45	0.00	0.005	0.000	36.41	0.004
487	R1_389	44.40	0.03	0.135	0.010	44.40	0.117
488	R1_390	44.42	0.01	0.105	0.006	44.40	0.097
489	R1_391	44.40	0.03	0.044	0.004	44.40	0.037
490	R1_392	44.37	0.02	0.294	0.131	44.36	0.494
491	R1_393	44.38	0.01	0.423	0.022	44.36	0.381
492	R1_394	44.38	0.01	0.039	0.015	44.36	0.030
493	R1_395	44.30	n.a.	0.054	n.a.		
		44.38	0.01	0.172	0.046	44.36	<b>0.064</b>
494	R1_396	44.37	0.02	0.128	0.006	44.36	<b>0.113</b>
495	R1_397	44.37	0.02	0.034	0.002	44.36	<b>0.027</b>
496	R1_398	44.34	0.03	0.013	0.004	44.36	0.015
		44.42	n.a.	0.009	n.a.		
497	R1_399	42.83	0.04	0.004	0.000	42.84	0.004

#	Molecule	Ret. Times (Rt) [min] Group of Data Sets		Rel. Intens. (RI) Group of Data Sets		Data Set #1	
		Mean	StDev	Mean	StDev	Rt/min	RI/%
497	R1_399	43.06	n.a.	0.003	n.a.		
		43.14	<b>0.06</b>	0.004	0.001		
		43.31	0.00	0.004	0.000		
498	R1_400	47.14	0.02	0.028	0.004	47.08	0.032
499	R1_401	47.12	0.02	0.092	0.005	47.08	0.091



Grey: Ion current chromatograms of original files of group data sets  
Red: Ion current chromatograms of difference files of group data sets  
Olive: Ion current chromatogram of original file of data set compared  
Blue: Ion current chromatogram of difference file of data set compared



Grey: Ion current chromatograms of original files of group data sets  
Red: Ion current chromatograms of difference files of group data sets  
Olive: Ion current chromatogram of original file of data set compared  
Blue: Ion current chromatogram of difference file of data set compared

