

Supplementary information for:

PM10 organic aerosol fingerprints by using Liquid Chromatography Orbitrap Mass Spectrometry: Urban vs Suburban in an Eastern Mediterranean medium-sized coastal city

Evangelos Stergiou^{1,2}, Anastasia Chrysovalantou Chatziioannou^{1,3}, Spiros A. Pergantis¹, Maria Kanakidou^{1,2,4}

¹ECPL, Department of Chemistry, University of Crete, Voutes Campus, Heraklion, Greece,
stergiouvaggelis98@gmail.com, spergantis@uoc.gr, mariak@uoc.gr

²CSTACC, ICE-HT, FORTH, Patras, Greece

³International Agency for Research on Cancer (IARC/WHO), Nutrition and Metabolism Branch, Lyon, France,
chatziioannou@iarc.who.int

⁴LAMOS, Institute of Environmental Physics, University of Bremen, Bremen, Germany

*Correspondence: stergiouvaggelis98@gmail.com; mariak@uoc.gr

Table S1. The processing wizard parameters of Mzmine

Local minimum feature resolver	
Minimum absolute height	5.0E4
Min ratio of peak top/edge	1.80
Peak duration range (min/mobility)	0.00 - 3.01
Minimum scans (data points)	4
Smoothing algorithm	Savitzky Golay
¹³ C isotope filter	
m/z tolerance (intra-sample)	0.0015 m/z or 3.0 ppm
Retention time tolerance	0.08 minutes
Join aligner	
m/z tolerance (sample-to-sample)	0.0015 m/z or 5.0 ppm
Retention time tolerance	0.40 minutes

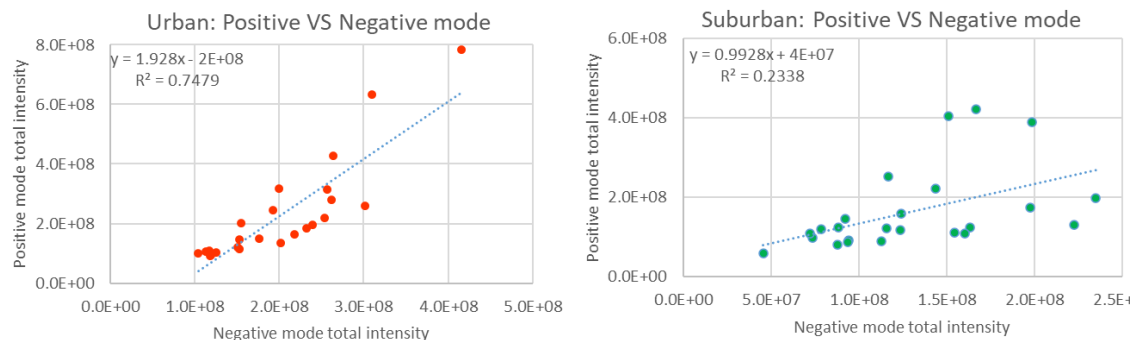


Figure S1. Scatter plots for the comparison of the polarity modes between urban and suburban stations in Heraklion, Crete, Greece

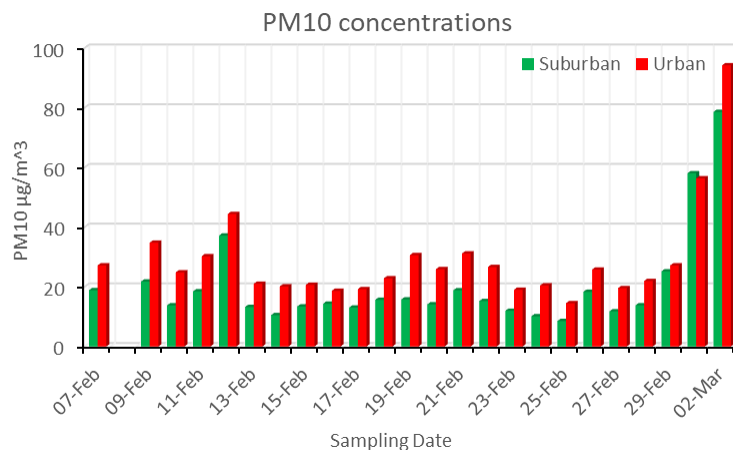


Figure S2. Daily average PM10 mass concentrations for the study period, for the 2 stations in Heraklion, Crete, Greece

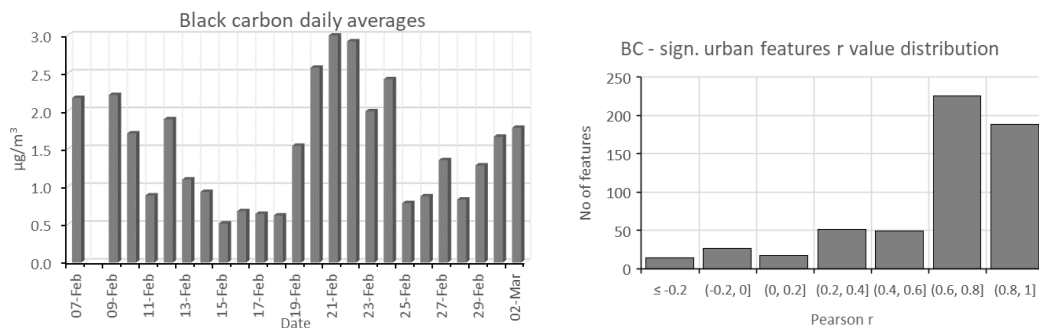


Figure S3. Daily average urban BC concentrations in Heraklion for the study period (left). Pearson r correlation values histogram for BC-significant positive mode urban features (right).

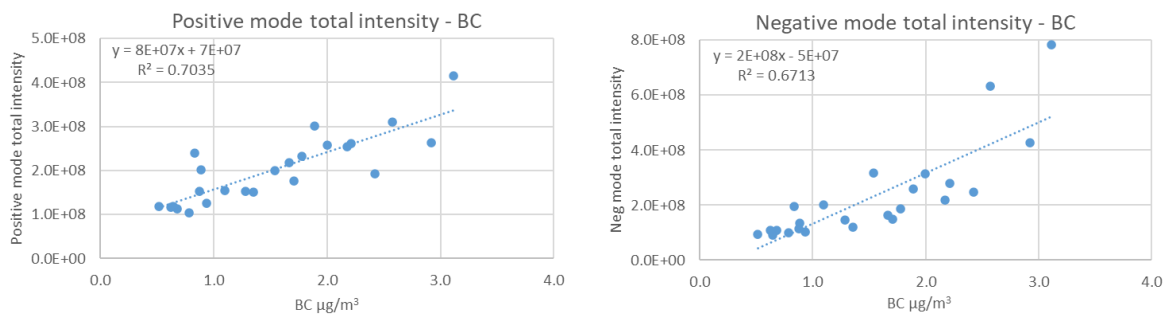


Figure S4. Correlation of BC with urban total intensity of Positive (left) and Negative mode (right)

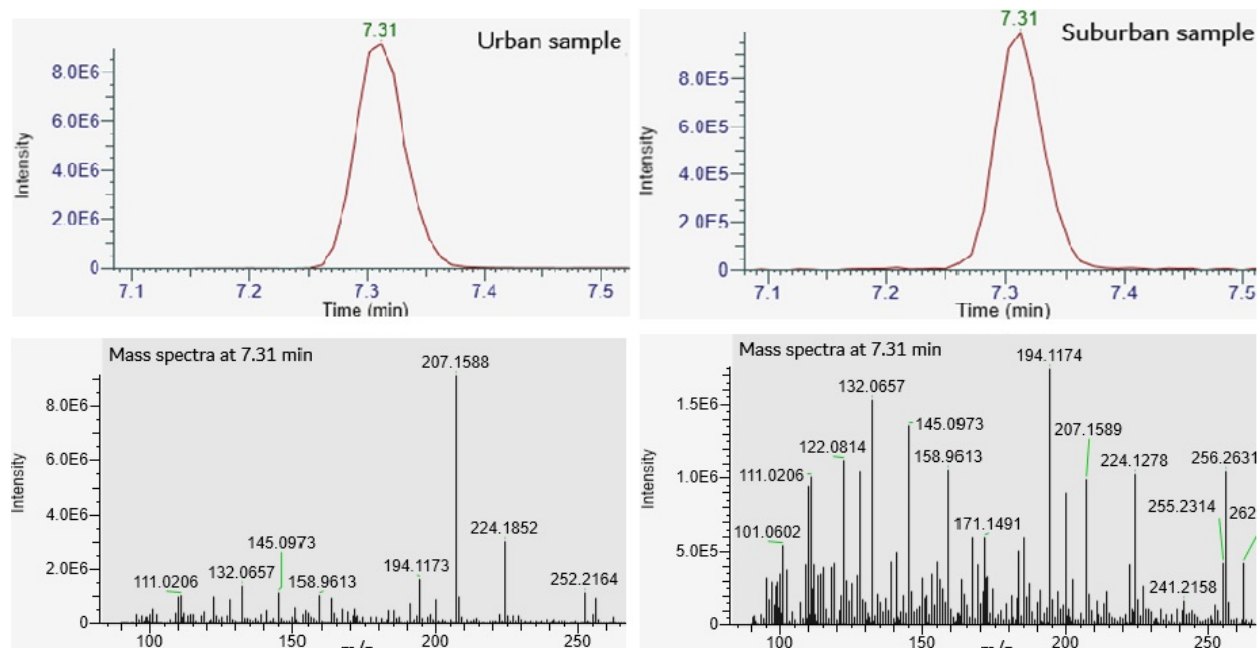


Figure S5. Chromatographic peak of a significant urban feature (207.1589 m/z and RT 7.32 min) as an example. Lower panels show the corresponding Full MS mass spectra at 7.31 min.

Table S2. The calculated elemental composition for each significant combustion-related urban feature in positive ion mode.

m/z	RT	[M+H] ⁺	RDBe	ppm.error	Avg.Peak.Area	logCo	BC pear. r
102.1281	2.17	C6 H16 N	-0.5	4.12	4.12E+05	6.60	0.77
102.1281	3.79	C6 H16 N	-0.5	4.12	1.65E+05	6.60	0.80
109.0288	5.89	C6 H5 O2	4.5	3.71	4.77E+04	6.49	0.75
116.1437	5.55	C7 H18 N	-0.5	2.66	1.50E+04	6.19	0.86
132.0809	0.96	C9 H10 N	5.5	1.12	5.13E+04	5.38	0.82
133.0650	8.52	C9 H9 O	5.5	1.60	1.78E+04	5.87	0.86
133.0762	2.32	C8 H9 N2	5.5	1.26	3.64E+04	4.82	0.85
133.0861	7.31	C6 H13 O3	0.5	1.57	1.29E+04	5.61	0.62
147.0442	6.10	C9 H7 O2	6.5	0.85	1.08E+04	5.36	0.91
147.0805	13.16	C10 H11 O	5.5	0.31	9.60E+03	5.43	0.87
149.0597	13.09	C9 H9 O2	5.5	0.18	1.46E+04	5.36	0.84
149.1074	0.96	C9 H13 N2	4.5	0.33	1.58E+04	4.42	0.65
154.0499	4.14	C7 H8 O3 N	4.5	0.09	1.19E+04	3.18	0.74
154.1591	5.33	C10 H20 N	1.5	0.32	2.41E+04	4.97	0.84
157.0496	8.82	C7 H9 O4	3.5	0.29	2.30E+04	4.36	0.91
157.0760	4.39	C10 H9 N2	7.5	-0.04	3.24E+04	4.01	0.77
157.0760	3.53	C10 H9 N2	7.5	-0.01	4.43E+04	4.01	0.78
158.0888*	0.75				1.30E+04		0.66
158.1904	6.96	C10 H24 N	-0.5	0.38	5.39E+03	4.97	0.65
160.1121	5.39	C11 H14 N	5.5	-0.04	2.50E+04	4.56	0.82
161.1073	1.04	C10 H13 N2	5.5	-0.21	3.88E+04	4.01	0.77
162.0913	5.22	C10 H12 O N	5.5	-0.26	7.03E+04	3.44	0.90
163.1196	0.95				2.40E+04		0.81
163.1229	0.95	C10 H15 N2	4.5	-0.27	4.21E+06	4.01	0.80
163.1265	0.95	C7 H19 N2 S	-0.5	0.85	2.04E+04		0.77
164.1192	1.02				2.27E+04		0.82

165.0770	3.20	C7 H9 O N4	5.5	-0.29	1.21E+04	1.19	0.84
165.0770	2.37	C7 H9 O N4	5.5	-0.27	5.77E+04	1.19	0.83
165.0770	1.72	C7 H9 O N4	5.5	-0.23	4.85E+04	1.19	0.81
165.1022	5.57	C9 H13 O N2	4.5	-0.22	1.96E+04	2.69	0.79
168.1019	5.85	C9 H14 O2 N	3.5	-0.27	1.78E+04	3.14	0.74
168.1383	8.07	C10 H18 O N	2.5	0.01	2.86E+04	3.44	0.88
168.1383	8.17	C10 H18 O N	2.5	0.06	1.46E+04	3.44	0.89
168.1383	8.29	C10 H18 O N	2.5	0.06	1.46E+04	3.44	0.85
169.0495	7.18	C8 H9 O4	4.5	0.04	5.20E+04	4.10	0.84
170.0923	0.81	C7 H12 O2 N3	3.5	-0.53	7.70E+03	1.64	0.72
171.0916	5.42	C11 H11 N2	7.5	-0.32	3.58E+04	3.60	0.84
175.0600	3.25	C7 H11 O5	2.5	-0.74	4.43E+04	3.28	0.80
176.1069	5.69	C11 H14 O N	5.5	-0.55	3.62E+04	3.07	0.88
177.0908	13.15	C11 H13 O2	5.5	-0.89	4.97E+05	4.55	0.86
177.1021	1.12	C10 H13 O N2	5.5	-0.84	1.02E+05	2.32	0.80
178.0861	5.90	C10 H12 O2 N	5.5	-0.65	2.11E+04	2.78	0.84
179.1177	1.12	C10 H15 O N2	4.5	-0.93	9.74E+04	2.32	0.75
179.1277	5.44	C8 H19 O4	-0.5	-0.65	6.10E+04	4.10	0.62
180.1382	6.50	C11 H18 O N	3.5	-0.50	9.25E+03	3.07	0.80
180.1382	8.54	C11 H18 O N	3.5	-0.33	1.81E+04	3.07	0.84
183.0651	8.06	C9 H11 O4	4.5	-0.46	1.40E+05	3.81	0.81
183.0651	6.89	C9 H11 O4	4.5	-0.29	7.88E+05	3.81	0.80
184.0603	6.10	C8 H10 O4 N	4.5	-0.46	3.03E+04	2.12	0.73
185.0443	5.90	C8 H9 O5	4.5	-0.61	7.65E+04	3.08	0.77
186.0871	1.01	C7 H12 O3 N3	3.5	-1.09	1.66E+04	0.95	0.64
186.0912	5.57	C12 H12 O N	7.5	-0.78	1.18E+05	2.70	0.77
186.1276	7.57	C13 H16 N	6.5	-0.58	2.32E+04	3.75	0.89
186.1276	7.26	C13 H16 N	6.5	-0.52	1.45E+04	3.75	0.86
186.2215	7.91	C12 H28 N	-0.5	-0.43	1.86E+04	4.16	0.71
187.0752	7.68	C12 H11 O2	7.5	-0.59	5.95E+03	4.14	0.87
188.1433	6.44	C13 H18 N	5.5	-0.63	3.45E+04	3.75	0.90
191.1541	6.16	C12 H19 N2	4.5	-0.74	3.25E+04	3.20	0.85
192.1018	6.91	C11 H14 O2 N	5.5	-0.51	3.75E+04	2.42	0.83
192.1746	7.27	C13 H22 N	3.5	-0.53	9.40E+04	3.75	0.79
193.0494	6.99	C10 H9 O4	6.5	-0.45	3.47E+05	3.50	0.81
194.0811	5.99	C10 H12 O3 N	5.5	-0.59	1.11E+04	2.11	0.77
195.0803	10.96	C14 H11 O	9.5	-0.80	8.79E+03	3.68	0.83
196.1542	5.38				1.00E+04		0.63
196.2058	6.36	C13 H26 N	1.5	-0.73	8.95E+03	3.75	0.64
197.0807	8.07	C10 H13 O4	4.5	-0.73	9.20E+04	3.50	0.80
197.0807	7.04	C10 H13 O4	4.5	-0.69	3.98E+05	3.50	0.74
197.0807	9.01	C10 H13 O4	4.5	-0.68	4.76E+04	3.50	0.74
197.0959	10.89	C14 H13 O	8.5	-0.85	9.54E+03	3.68	0.82
198.0758	6.27	C9 H12 O4 N	4.5	-1.39	6.15E+03	1.77	0.78
198.0760	6.88	C9 H12 O4 N	4.5	-0.66	3.38E+04	1.77	0.73
198.0760	6.79	C9 H12 O4 N	4.5	-0.62	2.12E+04	1.77	0.83
198.1850	11.11	C12 H24 O N	1.5	-0.97	1.36E+05	2.70	0.89
199.0600	6.75	C9 H11 O5	4.5	-0.54	1.03E+05	2.85	0.75
199.0600	7.40	C9 H11 O5	4.5	-0.48	2.58E+04	2.85	0.82
199.0600	7.28	C9 H11 O5	4.5	-0.48	1.39E+04	2.85	0.78
199.0752	10.37	C13 H11 O2	8.5	-0.84	1.31E+04	3.72	0.80
200.2371	8.60	C13 H30 N	-0.5	-0.92	2.09E+05	3.75	0.75
201.0756	7.19	C9 H13 O5	3.5	-0.57	1.56E+05	2.85	0.84
201.0908	10.61	C13 H13 O2	7.5	-0.88	2.70E+04	3.72	0.86
201.0909	8.65	C13 H13 O2	7.5	-0.74	3.21E+04	3.72	0.86
202.0861	5.41	C12 H12 O2 N	7.5	-1.01	3.11E+04	2.05	0.83

202.1224	6.12	C13 H16 O N	6.5	-1.03	1.66E+05	2.34	0.89
202.1589	6.73	C14 H20 N	5.5	-0.74	2.64E+04	3.34	0.92
203.0701	8.91	C12 H11 O3	7.5	-0.76	3.31E+04	3.55	0.83
203.0701	8.57	C12 H11 O3	7.5	-0.66	3.34E+04	3.55	0.84
203.0912	5.16	C9 H15 O5	2.5	-1.10	2.78E+04	2.85	0.93
203.0912	8.82	C9 H15 O5	2.5	-0.76	3.10E+04	2.85	0.92
203.0913	6.75	C9 H15 O5	2.5	-0.67	1.08E+04	2.85	0.77
204.1017	5.44	C12 H14 O2 N	6.5	-0.99	6.16E+04	2.05	0.81
204.1018	8.30	C12 H14 O2 N	6.5	-0.66	1.03E+04	2.05	0.74
205.0492	7.69	C11 H9 O4	7.5	-1.53	1.14E+04	3.17	0.76
205.0704	1.86	C8 H13 O6	2.5	-1.39	1.15E+05	1.97	0.79
205.1698	6.86	C13 H21 N2	4.5	-0.76	2.35E+04	2.79	0.80
206.0809	4.92	C11 H12 O3 N	6.5	-1.17	3.19E+04	1.75	0.77
206.0962	5.64	C7 H16 O2 N3 S	1.5	2.12	3.81E+04	0.87	0.83
206.1173	4.84	C12 H16 O2 N	5.5	-1.16	9.29E+04	2.05	0.71
206.1173	5.09	C12 H16 O2 N	5.5	-1.07	5.56E+04	2.05	0.76
206.1901	7.77	C14 H24 N	3.5	-0.95	8.72E+04	3.34	0.92
206.1902	8.53	C14 H24 N	3.5	-0.76	4.98E+04	3.34	0.88
207.0650	7.87	C11 H11 O4	6.5	-0.80	1.18E+05	3.17	0.85
207.1589	7.32	C10 H23 O4	-0.5	-0.83	5.87E+05	3.50	0.62
207.1589	6.73	C10 H23 O4	-0.5	-0.75	8.66E+04	3.50	0.90
208.1694	7.51	C13 H22 O N	3.5	-0.87	1.05E+04	2.34	0.77
209.0807	6.75	C11 H13 O4	5.5	-0.78	9.28E+04	3.17	0.71
209.0958	11.42	C15 H13 O	9.5	-1.17	3.39E+04	3.24	0.84
209.0959	11.89	C15 H13 O	9.5	-1.07	1.65E+04	3.24	0.86
210.0911	10.10	C14 H12 O N	9.5	-1.06	1.90E+04	1.97	0.72
210.0911	5.90	C14 H12 O N	9.5	-1.00	1.21E+04	1.97	0.83
210.1275	5.95	C15 H16 N	8.5	-0.97	3.71E+04	2.94	0.83
211.0599	7.09	C10 H11 O5	5.5	-0.75	5.21E+04	2.59	0.70
211.0963	8.01	C11 H15 O4	4.5	-0.89	1.74E+05	3.17	0.73
211.1114	11.94	C15 H15 O	8.5	-1.83	1.58E+04	3.24	0.89
212.0913	7.72	C10 H14 O4 N	4.5	-1.93	2.00E+04	1.42	0.78
212.0916	6.99	C10 H14 O4 N	4.5	-0.74	6.50E+03	1.42	0.80
212.1068	6.66	C14 H14 O N	8.5	-0.93	1.18E+05	1.97	0.86
212.1180	5.93	C13 H14 N3	8.5	-1.04	4.28E+05	1.83	0.82
212.1278	5.16	C11 H18 O3 N	3.5	-1.37	5.20E+03	1.75	0.91
212.1432	6.20	C15 H18 N	7.5	-1.00	2.29E+04	2.94	0.67
213.0755	7.76	C10 H13 O5	4.5	-1.06	7.42E+04	2.59	0.75
213.0756	8.36	C10 H13 O5	4.5	-0.87	2.44E+04	2.59	0.81
213.0756	8.29	C10 H13 O5	4.5	-0.79	1.37E+04	2.59	0.77
213.0908	9.26	C14 H13 O2	8.5	-0.91	3.39E+04	3.30	0.89
214.1435	6.10	C11 H20 O3 N	2.5	-1.21	1.49E+04	1.75	0.78
214.1435	7.57	C11 H20 O3 N	4.5	-0.78	8.66E+03	1.75	0.72
214.1588	7.20	C15 H20 N	6.5	-0.89	9.52E+04	2.94	0.89
215.0911	8.06	C10 H15 O5	3.5	-1.17	2.47E+05	2.59	0.81
216.1381	6.44	C14 H18 O N	6.5	-1.07	5.66E+04	1.97	0.82
216.1592	8.67	C11 H22 O3 N	1.5	-1.05	1.07E+05	1.75	0.90
216.1745	6.60	C15 H22 N	5.5	-1.01	2.71E+04	2.94	0.69
216.1745	7.07	C15 H22 N	5.5	-1.00	2.69E+04	2.94	0.88
217.0704	6.06	C9 H13 O6	3.5	-1.15	4.64E+04	1.79	0.77
217.0857	8.63	C13 H13 O3	7.5	-1.02	1.01E+05	3.16	0.78
217.1221	9.28	C14 H17 O2	6.5	-1.12	9.70E+04	3.30	0.79
217.1618	10.27	C12 H25 O S	0.5	-1.12	4.22E+04	3.04	0.69
218.1020	7.19	C9 H16 O5 N	2.5	-1.32	2.65E+04	1.07	0.84
218.1173	5.67	C13 H16 O2 N	6.5	-1.23	7.21E+04	1.69	0.73
218.1385	7.98	C10 H20 O4 N	1.5	-0.90	1.30E+04	1.42	0.94

218.1536	5.59	C14 H20 O N	5.5	-1.34	6.94E+04	1.97	0.71
218.1900	7.71	C15 H24 N	4.5	-1.59	3.35E+04	2.94	0.84
219.1489	9.90	C13 H19 O N2	5.5	-1.21	1.40E+04	1.22	0.87
220.0965	5.21	C12 H14 O3 N	6.5	-1.38	6.75E+04	1.39	0.76
220.1117	6.19	C8 H18 O2 N3 S	1.5	1.41	2.06E+04	0.46	0.77
220.1118	10.78	C8 H18 O2 N3 S	1.5	1.70	1.50E+04	0.46	0.93
220.1119	6.91	C8 H18 O2 N3 S	1.5	2.00	1.64E+04	0.46	0.90
220.1330	8.37	C13 H18 O2 N	5.5	-0.96	2.19E+04	1.69	0.91
220.2058	8.24	C15 H26 N	3.5	-0.98	6.78E+04	2.94	0.90
221.0595	10.18	C7 H13 O4 N2 S	2.5	1.80	2.31E+04	-0.68	0.81
221.0806	8.69	C12 H13 O4	6.5	-0.92	1.00E+05	2.83	0.81
221.0958	12.64	C8 H17 O3 N2 S	1.5	1.52	9.91E+03	0.16	0.87
221.1071	6.49	C7 H17 O2 N4 S	1.5	1.94	1.48E+04	-0.19	0.88
221.1381	6.91	C10 H21 O5	0.5	-0.97	2.28E+04	2.59	0.79
223.0599	7.04	C11 H11 O5	6.5	-0.90	1.33E+04	2.30	0.77
223.1114	12.31	C16 H15 O	9.5	-1.45	1.92E+04	2.79	0.78
223.1114	11.73	C16 H15 O	9.5	-1.37	6.57E+04	2.79	0.85
223.1114	11.98	C16 H15 O	9.5	-1.32	2.41E+04	2.79	0.86
224.1067	10.90	C15 H14 O N	9.5	-1.27	2.16E+04	1.61	0.86
224.1067	10.17	C15 H14 O N	9.5	-1.19	1.19E+04	1.61	0.77
224.1854	7.32				1.93E+05		0.61
225.0755	8.03	C11 H13 O5	5.5	-0.99	1.39E+04	2.30	0.79
225.0907	12.58	C15 H13 O2	9.5	-1.50	2.19E+04	2.87	0.68
225.0907	10.89	C15 H13 O2	9.5	-1.35	5.57E+04	2.87	0.69
225.0907	10.70	C15 H13 O2	9.5	-1.35	2.45E+04	2.87	0.66
225.1271	12.59	C16 H17 O	8.5	-1.40	1.97E+04	2.79	0.90
226.1223	6.33	C15 H16 O N	8.5	-1.33	5.47E+04	1.61	0.89
226.1587	6.82	C16 H20 N	7.5	-1.23	1.20E+04	2.53	0.76
226.1588	9.20	C16 H20 N	7.5	-1.14	1.66E+04	2.53	0.86
227.0699	10.77	C14 H11 O3	9.5	-1.42	2.55E+04	2.76	0.86
227.0700	10.45	C14 H11 O3	9.5	-1.37	1.53E+04	2.76	0.81
227.0700	9.88	C14 H11 O3	9.5	-1.34	8.94E+04	2.76	0.80
227.0912	6.52	C11 H15 O5	4.5	-1.09	2.62E+04	2.30	0.81
227.0912	9.22	C11 H15 O5	4.5	-1.07	1.35E+04	2.30	0.82
227.0912	7.25	C11 H15 O5	4.5	-1.04	1.18E+04	2.30	0.75
227.0912	7.81	C11 H15 O5	4.5	-0.74	1.93E+04	2.30	0.68
227.1064	9.95	C15 H15 O2	8.5	-1.28	6.32E+04	2.87	0.73
227.1387	7.29	C11 H19 O3 N2	3.5	-1.33	9.45E+03	0.63	0.84
228.1380	6.29	C15 H18 O N	7.5	-1.45	1.13E+05	1.61	0.87
228.1743	7.70	C16 H22 N	6.5	-1.58	3.86E+04	2.53	0.87
229.1068	9.04	C11 H17 O5	3.5	-1.25	1.05E+05	2.30	0.74
230.1172	6.15	C14 H16 O2 N	7.5	-1.36	6.27E+04	1.33	0.88
230.1383	3.72	C11 H20 O4 N	2.5	-1.82	2.24E+04	1.06	0.87
231.0860	6.51	C10 H15 O6	3.5	-1.32	2.46E+04	1.58	0.86
231.0860	7.09	C10 H15 O6	3.5	-1.24	4.44E+04	1.58	0.83
231.1013	9.30	C14 H15 O3	7.5	-1.16	1.19E+05	2.76	0.74
231.1376	10.53	C15 H19 O2	6.5	-1.41	1.39E+05	2.87	0.87
232.1176	6.21	C10 H18 O5 N	2.5	-1.57	1.24E+04	0.72	0.79
232.1177	8.06	C10 H18 O5 N	2.5	-1.22	7.19E+04	0.72	0.81
232.1328	5.59	C14 H18 O2 N	6.5	-1.64	1.60E+04	1.33	0.80
232.1329	6.28	C14 H18 O2 N	6.5	-1.45	1.24E+04	1.33	0.70
232.2057	8.15	C16 H26 N	4.5	-1.12	1.68E+04	2.53	0.73
233.0806	8.98	C13 H13 O4	7.5	-1.11	5.28E+04	2.47	0.73
233.0806	8.34	C13 H13 O4	7.5	-1.05	5.96E+04	2.47	0.79
233.1104	8.58	C13 H17 N2 S	6.5	-1.26	5.55E+03		0.77
234.0970	6.71	C9 H16 O6 N	2.5	-1.05	5.65E+03	0.36	0.84

234.0972	5.87	C9 H16 O6 N	2.5	0.00	1.88E+04	0.36	0.78
234.1273	6.75	C9 H20 O2 N3 S	1.5	0.84	1.64E+04	0.05	0.89
234.1273	7.60	C9 H20 O2 N3 S	1.5	0.84	1.17E+04	0.05	0.88
234.1273	7.79	C9 H20 O2 N3 S	1.5	0.84	1.36E+04	0.05	0.80
234.1274	7.45	C9 H20 O2 N3 S	1.5	0.84	3.43E+04	0.05	0.91
234.1849	6.64	C15 H24 O N	4.5	-1.35	1.67E+04	1.61	0.72
234.2213	8.81	C16 H28 N	3.5	-1.30	9.14E+03	2.53	0.64
235.0750	12.43	C8 H15 O4 N2 S	2.5	1.17	1.39E+04	-1.14	0.82
235.0750	10.93	C8 H15 O4 N2 S	2.5	1.31	2.12E+04	-1.14	0.84
235.0750	10.79	C8 H15 O4 N2 S	2.5	1.33	2.00E+04	-1.14	0.84
235.0962	8.57	C13 H15 O4	6.5	-1.13	4.58E+04	2.47	0.77
235.0962	8.15	C13 H15 O4	6.5	-1.08	4.80E+04	2.47	0.78
235.0962	8.26	C13 H15 O4	6.5	-1.07	4.83E+04	2.47	0.74
235.1114	12.68	C9 H19 O3 N2 S	1.5	1.14	2.25E+04	-0.27	0.81
235.1436	0.63	C13 H19 O2 N2	5.5	-2.14	1.29E+04	0.58	0.85
237.0907	9.99	C8 H17 O4 N2 S	1.5	1.49	1.08E+04	-1.14	0.74
237.1119	8.35	C13 H17 O4	5.5	-0.97	5.49E+04	2.47	0.81
237.1270	12.59	C17 H17 O	9.5	-1.56	3.08E+04	2.35	0.82
238.1071	6.12	C12 H16 O4 N	5.5	-1.21	6.91E+03	0.71	0.64
238.1223	11.43	C8 H20 O3 N3 S	0.5	1.10	1.33E+04	-0.89	0.79
238.1223	10.91	C8 H20 O3 N3 S	0.5	1.38	5.60E+03	-0.89	0.81
238.1587	8.36	C17 H20 N	8.5	-1.31	1.21E+04	2.12	0.74
238.1646	6.90	C10 H24 O5 N	-0.5	-1.28	7.78E+03	0.72	0.78
239.1426	13.10	C17 H19 O	8.5	-1.87	3.19E+04	2.35	0.81
240.1742	7.69	C17 H22 N	7.5	-1.80	4.13E+04	2.12	0.84
241.0704	6.38	C11 H13 O6	5.5	-1.24	2.66E+04	1.34	0.75
241.0856	10.56	C15 H13 O3	9.5	-1.46	1.25E+05	2.36	0.87
241.1068	7.18	C12 H17 O5	4.5	-1.01	1.84E+04	2.00	0.71
242.1431	8.83	C10 H20 N5 S	3.5	-1.29	6.37E+03		0.78
243.0649	9.00	C14 H11 O4	9.5	-1.15	2.01E+04	2.10	0.80
243.0649	8.52	C14 H11 O4	9.5	-1.11	1.66E+04	2.10	0.81
243.0860	7.09	C11 H15 O6	4.5	-1.20	3.63E+04	1.34	0.72
243.1012	9.40	C15 H15 O3	8.5	-1.41	9.98E+04	2.36	0.76
245.0805	7.96	C14 H13 O4	8.5	-1.17	8.88E+03	2.10	0.80
245.1017	8.02	C11 H17 O6	3.5	-1.18	1.27E+04	1.34	0.84
245.1017	6.72	C11 H17 O6	3.5	-1.13	1.39E+04	1.34	0.73
246.1274	8.67	C10 H20 O2 N3 S	2.5	1.42	1.95E+04	-0.35	0.88
246.1333	9.01	C11 H20 O5 N	2.5	-1.39	3.36E+04	0.37	0.74
246.1333	7.25	C11 H20 O5 N	2.5	-1.29	1.88E+04	0.37	0.87
246.2213	8.48	C17 H28 N	4.5	-1.32	1.33E+04	2.12	0.85
247.0808	5.63	C10 H15 O7	3.5	-1.60	1.13E+04	0.50	0.76
247.0962	8.70	C14 H15 O4	7.5	-1.22	5.36E+04	2.10	0.76
247.1326	9.47	C15 H19 O3	6.5	-1.28	1.06E+05	2.36	0.76
247.1689	11.44	C16 H23 O2	5.5	-1.52	1.37E+04	2.44	0.82
247.1689	8.75	C16 H23 O2	5.5	-1.39	2.14E+04	2.44	0.86
247.1689	8.33	C16 H23 O2	5.5	-1.33	2.54E+04	2.44	0.80
247.1802	6.46	C15 H23 O N2	5.5	-1.37	1.62E+04	0.49	0.83
247.2263	12.52	C14 H31 O3	-0.5	-1.71	8.61E+03	2.76	0.87
248.1126	6.73	C10 H18 O6 N	2.5	-1.13	2.30E+04	0.01	0.75
248.1428	7.75	C10 H22 O2 N3 S	1.5	0.46	2.36E+04	-0.35	0.89
248.1431	9.08	C10 H22 O2 N3 S	1.5	1.34	1.61E+04	-0.35	0.79
248.1431	9.16	C10 H22 O2 N3 S	1.5	1.35	1.04E+04	-0.35	0.62
248.2006	7.14	C16 H26 O N	4.5	-1.36	1.77E+04	1.24	0.89
248.2369	10.65	C17 H30 N	3.5	-1.48	7.92E+03	2.12	0.93
248.2369	9.30	C17 H30 N	3.5	-1.44	1.58E+04	2.12	0.85
248.2370	9.05	C17 H30 N	3.5	-1.30	2.01E+04	2.12	0.89

249.0755	8.03	C13 H13 O5	7.5	-1.13	1.61E+04	1.67	0.77
249.0755	8.19	C13 H13 O5	7.5	-1.01	1.44E+04	1.67	0.80
249.0906	11.61	C9 H17 O4 N2 S	2.5	1.09	3.50E+04	-1.58	0.86
249.0965	5.67	C10 H17 O7	2.5	-1.59	4.72E+04	0.50	0.78
249.1119	8.77	C14 H17 O4	6.5	-1.12	4.54E+04	2.10	0.74
249.1844	11.03	C16 H25 O2	4.5	-2.11	5.25E+04	2.44	0.68
249.1845	10.57	C16 H25 O2	4.5	-1.60	1.52E+05	2.44	0.84
249.2056	9.73	C13 H29 O4	-0.5	-1.66	1.66E+05	2.47	0.92
250.0917	4.92	C9 H16 O7 N	2.5	-1.82	2.33E+04	-0.36	0.64
250.1223	6.66	C9 H20 O3 N3 S	1.5	1.27	3.36E+04	-1.32	0.88
251.0911	7.63	C13 H15 O5	6.5	-1.01	1.29E+04	1.67	0.81
251.1063	12.11	C9 H19 O4 N2 S	1.5	0.98	4.43E+04	-1.58	0.88
251.1426	13.30	C18 H19 O	9.5	-1.89	2.63E+04	1.91	0.79
252.2166	7.32				9.45E+04		0.63
254.1536	6.22	C17 H20 O N	8.5	-1.44	9.93E+03	0.87	0.81
254.1536	6.35	C17 H20 O N	8.5	-1.37	1.12E+04	0.87	0.85
255.1012	11.36	C16 H15 O3	9.5	-1.44	8.45E+04	1.95	0.80
256.1117	12.54	C11 H18 O2 N3 S	4.5	0.90	8.75E+03	-0.75	0.80
256.1692	6.44	C17 H22 O N	7.5	-1.47	1.88E+04	0.87	0.82
256.1692	7.02	C17 H22 O N	7.5	-1.41	2.00E+04	0.87	0.85
257.0805	9.91	C15 H13 O4	9.5	-1.45	6.34E+04	1.73	0.84
257.0956	13.11	C11 H17 O3 N2 S	4.5	0.71	1.27E+04	-1.10	0.85
257.0990	11.29	C16 H17 O S	8.5	-1.86	1.07E+05	1.60	0.64
257.1169	11.00	C16 H17 O3	8.5	-1.40	2.72E+04	1.95	0.78
257.1532	10.91	C17 H21 O2	7.5	-1.55	3.63E+04	2.01	0.76
258.1484	5.89	C16 H20 O2 N	7.5	-1.79	1.66E+04	0.60	0.76
259.0961	8.43	C15 H15 O4	8.5	-1.31	2.06E+04	1.73	0.88
259.0962	9.22	C15 H15 O4	8.5	-1.26	2.60E+04	1.73	0.82
259.1112	13.56	C11 H19 O3 N2 S	3.5	0.45	3.92E+04	-1.10	0.88
259.1113	12.93	C11 H19 O3 N2 S	3.5	0.71	3.29E+04	-1.10	0.87
259.1801	6.53	C16 H23 O N2	6.5	-1.37	9.33E+03	0.13	0.89
260.1125	7.09	C11 H18 O6 N	3.5	-1.31	4.16E+04	-0.33	0.74
260.1489	8.10	C12 H22 O5 N	2.5	-1.48	3.15E+04	0.02	0.85
260.2369	8.76	C18 H30 N	4.5	-1.45	9.12E+03	1.72	0.78
261.1118	10.04	C15 H17 O4	7.5	-1.37	2.69E+04	1.73	0.77
262.1281	5.96	C11 H20 O6 N	2.5	-1.57	2.53E+04	-0.33	0.68
262.1281	6.11	C11 H20 O6 N	2.5	-1.54	2.06E+04	-0.33	0.66
263.0911	8.45	C14 H15 O5	7.5	-1.21	2.91E+04	1.34	0.77
263.1275	8.55	C15 H19 O4	6.5	-1.04	5.00E+04	1.73	0.77
263.1275	8.40	C15 H19 O4	6.5	-0.98	8.63E+04	1.73	0.78
263.1275	9.16	C15 H19 O4	6.5	-0.93	5.02E+04	1.73	0.77
263.1276	8.19	C15 H19 O4	6.5	-0.77	4.50E+04	1.73	0.78
264.1074	6.03	C10 H18 O7 N	2.5	-1.43	1.85E+04	-0.70	0.71
264.1591	9.00	C15 H22 O3 N	5.5	-1.34	1.16E+04	0.30	0.77
265.1068	8.09	C14 H17 O5	6.5	-0.83	2.91E+04	1.34	0.79
266.1172	6.37	C17 H16 O2 N	10.5	-1.43	1.59E+04	0.23	0.83
266.1230	5.67	C10 H20 O7 N	1.5	-1.64	1.39E+04	-0.70	0.78
266.2322	9.72				2.05E+04		0.88
267.1225	8.21	C14 H19 O5	5.5	-0.70	2.79E+04	1.34	0.78
267.1375	11.99	C18 H19 O2	9.5	-1.60	3.32E+04	1.58	0.88
267.1375	11.20	C18 H19 O3	9.5	-1.57	2.77E+04	1.13	0.90
269.1169	9.85	C17 H17 O3	9.5	-1.34	3.04E+04	1.54	0.74
269.1643	0.78	C17 H21 O N2	8.5	-2.02	1.89E+04	-0.24	0.72
270.1122	7.94	C16 H16 O3 N	9.5	-1.09	7.79E+03	-0.06	0.76
270.1484	5.99	C17 H20 O2 N	8.5	-1.67	1.44E+04	0.23	0.74
270.1809	8.25	C13 H24 O3 N3	3.5	-1.14	9.47E+03	-1.20	0.82

270.1809	8.17	C13 H24 O3 N3	3.5	-1.07	9.45E+03	-1.20	0.84
270.3151	10.44	C18 H40 N	-0.5	-1.61	2.67E+04	1.72	0.60
271.1145	12.00	C9 H23 O3 N2 S2	-0.5	0.06	8.57E+04	-1.58	0.64
271.1324	11.65	C9 H23 O5 N2 S	-0.5	0.84	1.21E+04	-2.85	0.79
273.0965	6.90	C12 H17 O7	4.5	-1.33	1.54E+04	0.07	0.76
273.1117	10.05	C16 H17 O4	8.5	-1.47	1.88E+04	1.35	0.81
273.1117	9.97	C16 H17 O4	8.5	-1.45	3.10E+04	1.35	0.81
274.1281	7.66	C12 H20 O6 N	3.5	-1.61	1.39E+04	-0.68	0.76
274.2008	5.95	C14 H28 O4 N	1.5	-1.62	2.21E+04	-0.01	0.78
275.0911	8.84	C15 H15 O5	8.5	-1.26	1.07E+04	0.99	0.81
275.0911	8.96	C15 H15 O5	8.5	-1.24	1.21E+04	0.99	0.79
275.1274	10.69	C16 H19 O4	7.5	-1.40	2.60E+04	1.35	0.77
275.1638	11.52	C17 H23 O3	6.5	-1.50	1.08E+04	1.54	0.75
275.2112	7.70	C17 H27 O N2	5.5	-2.17	7.72E+04	-0.24	0.76
276.1438	6.75	C12 H22 O6 N	2.5	-1.38	2.32E+04	-0.68	0.75
277.1278	8.82	C12 H21 O7	2.5	-1.37	1.20E+05	0.07	0.92
277.1433	9.24	C16 H21 O4	6.5	-0.56	3.12E+04	1.35	0.76
278.1230	6.99	C11 H20 O7 N	2.5	-1.36	6.19E+03	-1.05	0.80
278.1536	6.88	C19 H20 O N	10.5	-1.28	2.67E+04	0.14	0.80
278.1747	10.51	C16 H24 O3 N	5.5	-1.47	6.39E+03	-0.06	0.61
280.1328	6.18	C18 H18 O2 N	10.5	-1.61	3.11E+04	-0.13	0.74
281.1531	12.56	C19 H21 O2	9.5	-1.65	2.16E+04	1.15	0.69
283.1486	12.94				6.04E+03		0.82
283.1799	1.12	C10 H27 O3 N4 S	-0.5	0.29	1.11E+04	-2.79	0.73
285.1117	11.52	C17 H17 O4	9.5	-1.60	2.64E+04	0.96	0.76
285.1302	12.72	C10 H17 O4 N6	5.5	-1.46	5.99E+04	-4.15	0.68
285.1592	0.75	C9 H25 O4 N4 S	-0.5	0.23	1.72E+04	-3.69	0.74
285.1844	11.41	C19 H25 O2	7.5	-1.63	2.21E+04	1.15	0.88
286.1281	6.38	C13 H20 O6 N	4.5	-1.34	1.14E+04	-1.03	0.73
286.1645	7.07	C14 H24 O5 N	3.5	-1.25	1.30E+04	-0.69	0.82
286.1797	6.43	C18 H24 O2 N	7.5	-1.43	1.39E+04	-0.13	0.75
287.1274	10.61	C17 H19 O4	8.5	-1.51	1.28E+04	0.96	0.81
288.1438	7.09	C13 H22 O6 N	3.5	-1.30	3.86E+04	-1.03	0.73
288.1589	5.75	C17 H22 O3 N	7.5	-1.69	1.71E+04	-0.42	0.69
289.1066	9.59	C16 H17 O5	8.5	-1.39	2.35E+04	0.64	0.80
289.1067	8.87	C16 H17 O5	8.5	-1.14	1.53E+04	0.64	0.81
289.1430	11.17	C17 H21 O4	7.5	-1.43	9.74E+03	0.96	0.76
290.1536	7.26	C20 H20 O N	11.5	-1.22	1.19E+04	-0.22	0.81
291.2062	5.74	C17 H27 O2 N2	5.5	-1.65	1.47E+04	-0.88	0.78
292.2267	7.48	C18 H30 O2 N	4.5	-1.48	1.24E+04	-0.13	0.71
293.1016	9.28	C15 H17 O6	7.5	-1.08	7.53E+03	0.17	0.74
294.1485	6.62	C19 H20 O2 N	10.5	-1.30	4.95E+04	-0.50	0.73
294.1543	8.82	C12 H24 O7 N	1.5	-1.32	2.38E+04	-1.39	0.92
297.1118	9.95	C18 H17 O4	10.5	-1.23	1.73E+04	0.56	0.83
298.1070	6.13	C17 H16 O4 N	10.5	-1.39	1.23E+04	-1.09	0.67
298.1194	12.03	C9 H16 O N9 S	6.5	0.26	6.26E+03	-4.83	0.81
298.1646	8.45	C15 H24 O5 N	4.5	-1.11	9.04E+03	-1.05	0.76
299.1097	8.82	C10 H23 O4 N2 S2	0.5	1.08	3.63E+04	-3.33	0.82
299.1638	10.88	C19 H23 O3	8.5	-1.25	8.75E+03	0.71	0.81
299.1748	0.91	C18 H23 O2 N2	8.5	-2.02	1.48E+04	-1.25	0.77
300.1590	6.00	C18 H22 O3 N	8.5	-1.53	2.04E+04	-0.79	0.70
300.2165	10.71	C16 H30 O4 N	2.5	-1.47	2.01E+04	-0.73	0.76
300.2529	12.86	C17 H34 O3 N	1.5	-1.56	6.15E+03	-0.42	0.67
301.2005	10.53	C16 H29 O5	2.5	-1.37	7.00E+03	0.64	0.68
301.2157	11.57	C20 H29 O2	6.5	-1.62	8.64E+03	0.71	0.68

302.1594	7.67	C14 H24 O6 N	3.5	-1.51	1.10E+04	-1.38	0.70
302.2321	9.62	C16 H32 O4 N	1.5	-1.44	7.48E+03	-0.73	0.61
303.1223	9.86	C17 H19 O5	8.5	-1.24	2.82E+04	0.28	0.76
303.1224	9.33	C17 H19 O5	8.5	-1.07	1.04E+04	0.28	0.81
303.1224	9.01	C17 H19 O5	8.5	-1.04	9.82E+03	0.28	0.85
304.1387	5.85	C13 H22 O7 N	3.5	-1.39	2.56E+04	-1.74	0.76
304.1387	8.15	C13 H22 O7 N	3.5	-1.10	2.82E+04	-1.74	0.67
304.1540	6.43	C17 H22 O4 N	7.5	-1.23	7.61E+04	-1.09	0.70
304.1692	7.58	C21 H22 O N	11.5	-1.12	1.77E+04	-0.59	0.78
305.1381	8.65	C17 H21 O5	7.5	-0.78	7.57E+03	0.28	0.81
307.1173	9.79	C16 H19 O6	7.5	-0.96	6.25E+03	-0.15	0.75
307.1174	8.34	C16 H19 O6	7.5	-0.74	8.49E+03	-0.15	0.73
308.1336	6.90	C12 H22 O8 N	2.5	-1.26	1.60E+04	-2.10	0.75
308.1336	6.79	C12 H22 O8 N	2.5	-1.25	1.30E+04	-2.10	0.75
310.1195	10.50	C10 H16 O N9 S	7.5	0.66	1.02E+04	-5.22	0.84
311.1273	10.50	C19 H19 O4	10.5	-1.41	1.28E+05	0.16	0.80
313.0889	6.85	C10 H13 O6 N6	7.5	-0.65	9.18E+03	-5.56	0.64
313.1066	10.68	C18 H17 O5	10.5	-1.36	3.44E+04	-0.10	0.79
313.1067	10.19	C18 H17 O5	10.5	-1.05	1.04E+04	-0.10	0.83
314.1382	7.75	C18 H20 O4 N	9.5	-1.42	4.90E+03	-1.45	0.80
315.1224	9.65	C18 H19 O5	9.5	-1.09	3.09E+04	-0.10	0.81
315.1697	0.72	C18 H23 O3 N2	8.5	-1.90	6.39E+04	-1.90	0.70
317.2107	10.57	C20 H29 O3	6.5	-1.26	9.60E+03	0.29	0.79
319.1173	8.00	C17 H19 O6	8.5	-0.90	1.71E+04	-0.49	0.77
324.1438	8.34	C16 H22 O6 N	6.5	-1.05	1.44E+04	-2.09	0.72
325.1068	9.22	C19 H17 O5	11.5	-0.91	1.70E+04	-0.47	0.76
325.1430	10.99	C20 H21 O4	10.5	-1.23	5.98E+04	-0.24	0.78
327.1224	10.66	C19 H19 O5	10.5	-0.96	1.37E+04	-0.47	0.83
329.1854	1.00	C19 H25 O3 N2	8.5	-1.79	1.91E+04	-2.26	0.75
332.1700	8.13	C15 H26 O7 N	3.5	-1.06	1.33E+04	-2.43	0.69
332.3307	10.45	C23 H42 N	3.5	-1.41	6.13E+04	-0.32	0.68
333.1329	8.55	C18 H21 O6	8.5	-1.04	1.55E+04	-0.84	0.74
334.2373	6.39	C20 H32 O3 N	5.5	-1.21	1.61E+04	-1.51	0.80
339.1223	9.72	C20 H19 O5	11.5	-1.11	2.46E+04	-0.86	0.80
341.1380	10.41	C20 H21 O5	10.5	-1.14	2.11E+04	-0.86	0.78
341.1380	7.00	C20 H21 O5	10.5	-1.06	2.27E+04	-0.86	0.80
342.2424	7.45	C22 H32 O2 N	7.5	-1.11	5.43E+03	-1.59	0.71
343.1173	8.37	C19 H19 O6	10.5	-0.87	7.98E+03	-1.19	0.81
347.1121	9.98	C18 H19 O7	9.5	-1.15	8.49E+03	-1.65	0.78
354.1544	8.66	C17 H24 O7 N	6.5	-0.89	1.81E+04	-3.14	0.72
356.2426	13.17	C19 H34 O5 N	3.5	-1.45	6.43E+05	-2.48	0.86
357.2031	10.72	C18 H25 O2 N6	9.5	-0.70	7.08E+03	-5.70	0.75
358.2583	11.40	C19 H36 O5 N	2.5	-1.31	1.71E+04	-2.48	0.65
360.3620	11.20	C25 H46 N	3.5	-1.28	6.86E+03	-1.13	0.81
361.1278	9.44	C19 H21 O7	9.5	-0.92	9.14E+03	-1.98	0.77
361.1980	13.17	C17 H25 O3 N6	8.5	-0.80	5.57E+04	-5.99	0.85
364.1387	9.98	C18 H22 O7 N	8.5	-1.07	7.75E+03	-3.49	0.81
403.1386	8.15	C21 H23 O8	10.5	-0.40	9.29E+03	-3.48	0.79

*158.0888 m/z refers to the elemental composition C18H24O3N2 in the form of [M+2H]²⁺