

Electronic supplementary Information to the Faraday Discussions article:

## **Interfacial photochemistry of biogenic surfactants: a major source of abiotic volatile organic compounds?**

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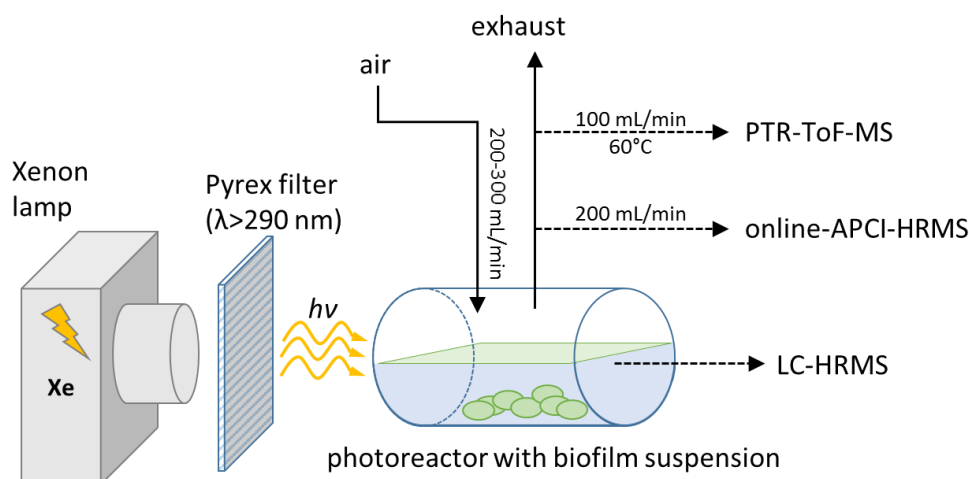


Fig. S-1: Schematic of the experimental setup. A Xenon lamp was used to irradiate the biofilm-containing photoreactor. To mimic solar irradiation at the Earth's surface, a Pyrex filter was used to cut wavelength below 290 nm. Purified air was pushed through the reactor at flow rates of 200–300 mL min<sup>-1</sup>. A combination of online-APCI-HRMS and PTR-ToF-MS was used to identify and quantify the produced VOCs. For identification experiments, the entire flow from the cell was sampled by the online-APCI-HRMS. For quantitation of VOCs, the PTR-ToF-MS was sampling 100 mL min<sup>-1</sup> from the major flow through a heated inlet (60 °C). Liquid phase samples were taken before and after irradiation and analyzed by UHPLC-HRMS.

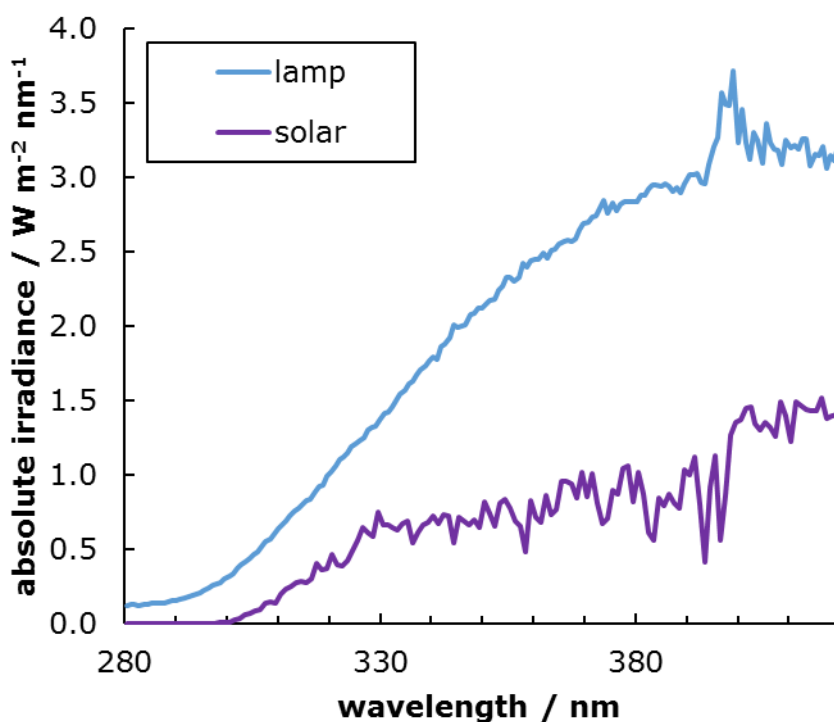


Fig. S-2: Absolute irradiance as function of wavelength for the actinic solar spectrum (calculated using the Tropospheric Ultraviolet and Visible (TUV) Radiation Model version 5.2; [http://cprm.acom.ucar.edu/Models/TUV/Interactive\\_TUV](http://cprm.acom.ucar.edu/Models/TUV/Interactive_TUV)) and the xenon lamp with Pyrex filter used for irradiation of the biofilm samples.

**Table S-1:** Information on biofilm sample type, origin, growth period, and biomass concentration. All biofilm sampling locations are situated in the further surroundings of Lyon (France).

<b>biofilm sample type</b>	<b>biofilm origin</b>	<b>laboratory growth phase (from – to)</b>		<b>dry biomass (g L<sup>-1</sup>)</b>
dead (autoclaved)	Lake Annecy	07/04/16	13/05/16	13.9
alive (measured 5 and 6 days after sampling)	Lake Annecy	07/04/16	13/05/16	23.7
colloidal fraction	River Morcille	10/10/16	10/11/16	15.8
capsular fraction	River Morcille	10/10/16	14/11/16	28.1
cellular fraction	River Morcille	10/10/16	14/11/16	28.1

**Table S-2:** Identified VOCs, corresponding production rates, and calculated fluxes under ambient conditions for all biofilm samples. Ions with  $m/z < 50$  could not be detected by online-APCI-HRMS due to  $m/z$  range limitations of the Orbitrap mass spectrometer. Production values are calculated from mixing ratios obtained by PTR-ToF-MS for an average lamp output of ca.  $26 \text{ mW}\cdot\text{cm}^{-2}$  in the wavelength range of 280–420 nm. Ambient VOC fluxes are calculated for a mean solar flux of  $9.2 \text{ mW}\cdot\text{cm}^{-2}$  in the same wavelength range.

$m/z$ ([M+H] <sup>+</sup> )	PTR-TOF-MS	assigned formula	biofilm (day 6)			biofilm (day 5)			dead			ground water		
			mixing ratio / ppb	production / $10^7$ molec. $\text{mW}^{-1}\text{s}^{-1}$	flux (ambient) / $10^7$ molec. $\text{cm}^{-2}\text{s}^{-1}$	mixing ratio / ppb	production / $10^7$ molec. $\text{mW}^{-1}\text{s}^{-1}$	flux (ambient) / $10^7$ molec. $\text{cm}^{-2}\text{s}^{-1}$	mixing ratio / ppb	production / $10^7$ molec. $\text{mW}^{-1}\text{s}^{-1}$	flux (ambient) / $10^7$ molec. $\text{cm}^{-2}\text{s}^{-1}$	mixing ratio / ppb	production / $10^7$ molec. $\text{mW}^{-1}\text{s}^{-1}$	flux (ambient) / $10^7$ molec. $\text{cm}^{-2}\text{s}^{-1}$
	31.019	CH <sub>2</sub> O (formaldehyde)	0.036	0.704	6.456	0.016	0.322	2.953	0.123	2.421	22.209	0.010	0.197	1.804
	33.034	CH <sub>4</sub> O (methanol)	0.830	16.375	150.206	0.600	11.842	108.630	5.812	114.732	1052.454	0.021	0.410	3.763
	41.038	C <sub>3</sub> H <sub>4</sub>	0.140	2.761	25.325	0.119	2.355	21.602	0.509	10.057	92.258	0.016	0.317	2.906
	42.034	C <sub>2</sub> H <sub>3</sub> N (acetonitrile)	9.167	180.953	1659.905	0.000	0.000	0.000	4.807	94.883	870.375	0.410	8.101	74.314
	43.017	C <sub>2</sub> H <sub>2</sub> O (ketene)	0.096	1.904	17.462	0.067	1.319	12.098	0.289	5.708	52.360	0.008	0.167	1.531
	43.054	C <sub>3</sub> H <sub>6</sub>	0.334	6.593	60.483	0.222	4.388	40.254	1.342	26.492	243.011	0.014	0.272	2.494
	44.022	C <sub>2</sub> H <sub>3</sub> O	0.007	0.136	1.246	0.006	0.113	1.039	0.017	0.330	3.028	0.004	0.078	0.716
	45.032	C <sub>2</sub> H <sub>4</sub> O (acetaldehyde)	1.324	26.127	239.667	0.713	14.082	129.174	4.463	88.093	808.090	0.048	0.953	8.738
	47.048	C <sub>2</sub> H <sub>6</sub> O (ethanol)	3.023	59.672	547.375	0.703	13.872	127.250	12.368	244.145	2239.567	0.010	0.198	1.821
	49.010	CH <sub>4</sub> S	0.012	0.235	2.158	0.015	0.291	2.666	0.016	0.309	2.839	0.001	0.021	0.196
51.0611	51.043	CH <sub>6</sub> O <sub>2</sub>	0.096	1.895	17.387	0.050	0.988	9.064	0.841	16.603	152.299	0.000	0.008	0.070
56.0496	56.054	C <sub>3</sub> H <sub>5</sub> N	0.011	0.226	2.071	0.010	0.203	1.866	0.036	0.717	6.576	0.003	0.068	0.623
57.0336	57.032	C <sub>3</sub> H <sub>4</sub> O	0.271	5.355	49.121	0.188	3.710	34.031	2.375	46.885	430.086	0.005	0.098	0.903
57.0700	57.067	C <sub>4</sub> H <sub>8</sub>	0.206	4.058	37.227	0.135	2.659	24.393	1.084	21.400	196.302	0.017	0.342	3.141
58.0369	58.036		0.015	0.289	2.654	0.009	0.184	1.685	0.095	1.867	17.127	0.001	0.012	0.111
58.0652	58.065	C <sub>3</sub> H <sub>7</sub> N	0.004	0.084	0.773	0.004	0.081	0.739	0.155	3.068	28.143	0.000	0.000	0.000
59.0492	59.047	C <sub>3</sub> H <sub>6</sub> O (acetone)	3.921	77.391	709.918	3.747	73.975	678.578	6.668	131.622	1207.385	0.129	2.540	23.295
60.0808	60.079	C <sub>3</sub> H <sub>9</sub> N	0.009	0.187	1.712	0.007	0.133	1.223	0.674	13.298	121.989	0.003	0.061	0.556
61.0284	61.026	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	0.057	1.134	10.400	0.023	0.450	4.130	0.092	1.820	16.697	0.007	0.131	1.200
63.0441	63.041	C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	0.045	0.884	8.105	0.018	0.349	3.201	0.182	3.597	32.994	0.003	0.052	0.476

65.0385	65.021	C <sub>5</sub> H <sub>4</sub>	0.000	0.000	0.000	0.002	0.044	0.404	-0.053	-1.037	-9.515	0.001	0.019	0.171
67.0542	67.051	C <sub>5</sub> H <sub>6</sub>	0.015	0.291	2.673	0.012	0.229	2.101	0.169	3.331	30.558	0.000	0.004	0.037
68.0495	68.048	C <sub>4</sub> H <sub>5</sub> N	0.012	0.247	2.262	0.008	0.163	1.496	0.015	0.288	2.638	0.001	0.020	0.180
69.0698	69.067	C <sub>5</sub> H <sub>8</sub> (isoprene)	0.243	4.788	43.918	0.188	3.710	34.035	1.033	20.394	187.075	0.007	0.146	1.336
70.0651	70.061	C <sub>4</sub> H <sub>7</sub> N	0.086	1.700	15.595	0.070	1.375	12.615	0.108	2.124	19.487	0.000	0.001	0.006
71.0491	71.045	C <sub>4</sub> H <sub>6</sub> O	0.121	2.397	21.985	0.084	1.655	15.184	3.075	60.705	556.859	0.004	0.086	0.793
71.0855	71.077	C <sub>5</sub> H <sub>10</sub>	0.053	1.041	9.546	0.051	1.000	9.170	0.321	6.328	58.051	0.000	0.000	0.000
72.0443	72.046	C <sub>3</sub> H <sub>5</sub> NO	0.010	0.206	1.892	0.006	0.122	1.118	0.162	3.191	29.273	0.002	0.033	0.305
73.0284	73.024	C <sub>3</sub> H <sub>4</sub> O <sub>2</sub>	0.006	0.125	1.148	0.000	0.000	0.000	0.006	0.116	1.060	0.007	0.140	1.288
73.0648	73.061	C <sub>4</sub> H <sub>8</sub> O	0.235	4.630	42.470	0.203	4.016	36.840	0.416	8.216	75.365	0.003	0.054	0.500
77.0597	77.055	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	0.023	0.445	4.083	0.011	0.216	1.979	0.104	2.057	18.870	0.001	0.020	0.188
79.0542	79.050	C <sub>6</sub> H <sub>6</sub>	0.005	0.092	0.847	0.004	0.078	0.720	0.025	0.490	4.494	0.002	0.042	0.386
81.0698	81.065	C <sub>6</sub> H <sub>8</sub>	0.018	0.355	3.256	0.010	0.205	1.877	0.157	3.108	28.509	0.000	0.003	0.025
83.0491	83.044	C <sub>5</sub> H <sub>6</sub> O	0.008	0.150	1.378	0.005	0.093	0.857	0.091	1.799	16.505	0.000	0.000	0.000
83.0855	83.080	C <sub>6</sub> H <sub>10</sub>	0.117	2.317	21.256	0.086	1.693	15.533	0.840	16.576	152.050	0.003	0.058	0.536
84.0444	84.049	C <sub>4</sub> H <sub>5</sub> NO	0.000	0.000	0.000	0.001	0.020	0.186	0.015	0.293	2.687	0.002	0.044	0.399
84.0807	84.082	C <sub>5</sub> H <sub>9</sub> N	0.014	0.271	2.490	0.010	0.199	1.824	0.076	1.508	13.829	0.001	0.018	0.162
85.0647	85.059	C <sub>5</sub> H <sub>8</sub> O	0.080	1.575	14.444	0.055	1.087	9.969	1.005	19.841	182.005	0.003	0.053	0.483
87.0440	87.039	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	0.030	0.593	5.439	0.019	0.373	3.423	0.038	0.751	6.888	0.001	0.012	0.114
87.0804	87.075	C <sub>5</sub> H <sub>10</sub> O	0.074	1.460	13.388	0.067	1.323	12.138	0.214	4.221	38.722	0.002	0.033	0.306
93.0698	93.063	C <sub>7</sub> H <sub>8</sub>	0.006	0.116	1.067	0.003	0.050	0.462	0.044	0.863	7.921	0.002	0.030	0.273
95.0855	95.079	C <sub>7</sub> H <sub>10</sub>	0.027	0.532	4.884	0.018	0.354	3.250	0.328	6.472	59.372	0.001	0.014	0.130
97.0648	97.059	C <sub>6</sub> H <sub>8</sub> O	0.005	0.092	0.844	0.005	0.091	0.838	0.130	2.570	23.574	0.000	0.008	0.074
97.1011	97.094	C <sub>7</sub> H <sub>12</sub>	0.052	1.023	9.382	0.035	0.701	6.426	0.334	6.584	60.399	0.003	0.050	0.462
99.0804	99.074	C <sub>6</sub> H <sub>10</sub> O	0.020	0.405	3.712	0.014	0.273	2.500	0.264	5.209	47.781	0.001	0.018	0.165
101.0597	101.052	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	0.023	0.461	4.231	0.018	0.347	3.181	0.038	0.750	6.881	0.000	0.000	0.000
101.0960	101.088	C <sub>6</sub> H <sub>12</sub> O	0.029	0.564	5.175	0.021	0.418	3.838	0.170	3.364	30.863	0.002	0.042	0.387
107.0491	107.042	C <sub>7</sub> H <sub>6</sub> O	0.026	0.514	4.718	0.019	0.382	3.505	0.136	2.692	24.693	0.006	0.119	1.096
107.0855	107.077	C <sub>8</sub> H <sub>10</sub>	0.008	0.149	1.367	0.007	0.134	1.233	0.053	1.050	9.635	0.002	0.030	0.275
108.0443	108.043	C <sub>6</sub> H <sub>5</sub> NO	0.002	0.045	0.417	0.000	0.000	0.000	0.009	0.180	1.652	0.001	0.019	0.172

109.1011	109.093	C <sub>8</sub> H <sub>12</sub>	0.028	0.546	5.007	0.020	0.397	3.644	0.442	8.716	79.951	0.000	0.005	0.047
111.0804	111.072	C <sub>7</sub> H <sub>10</sub> O	0.023	0.445	4.080	0.011	0.226	2.076	0.860	16.978	155.743	0.001	0.016	0.149
111.1168	111.104	C <sub>8</sub> H <sub>14</sub>	0.051	1.010	9.262	0.027	0.534	4.903	0.330	6.519	59.803	0.001	0.028	0.256
113.0960	113.088	C <sub>7</sub> H <sub>12</sub> O	0.040	0.796	7.304	0.024	0.480	4.403	0.719	14.201	130.270	0.000	0.000	0.000
115.1117	115.102	C <sub>7</sub> H <sub>14</sub> O	0.010	0.191	1.748	0.008	0.162	1.490	0.087	1.713	15.718	0.002	0.038	0.349
121.0647	121.056	C <sub>8</sub> H <sub>8</sub> O	0.022	0.431	3.957	0.018	0.363	3.334	0.027	0.525	4.818	0.001	0.021	0.196
121.0858	121.085	C <sub>5</sub> H <sub>12</sub> O <sub>3</sub>	0.008	0.154	1.413	0.005	0.100	0.915	0.018	0.358	3.285	0.000	0.001	0.006
123.1167	123.106	C <sub>9</sub> H <sub>14</sub>	0.016	0.311	2.849	0.013	0.264	2.424	0.067	1.329	12.193	0.001	0.018	0.168
125.0960	125.087	C <sub>8</sub> H <sub>12</sub> O	0.011	0.218	2.004	0.010	0.197	1.810	0.158	3.111	28.536	0.001	0.017	0.152
127.1116	127.101	C <sub>8</sub> H <sub>14</sub> O	0.060	1.178	10.805	0.041	0.812	7.451	0.809	15.972	146.513	0.001	0.018	0.168
129.1273	129.116	C <sub>8</sub> H <sub>16</sub> O	0.028	0.545	5.003	0.016	0.323	2.964	0.088	1.745	16.008	0.001	0.022	0.199
135.0803	135.075	C <sub>9</sub> H <sub>10</sub> O	0.003	0.067	0.611	0.001	0.012	0.115	0.007	0.140	1.281	0.000	0.008	0.070
137.0960	137.084	C <sub>9</sub> H <sub>12</sub> O	0.001	0.017	0.152	0.002	0.039	0.362	0.008	0.161	1.480	0.000	0.001	0.012
139.1116	139.108	C <sub>9</sub> H <sub>14</sub> O	0.017	0.332	3.047	0.015	0.301	2.757	0.070	1.374	12.602	0.000	0.008	0.072
141.0909	141.079	C <sub>8</sub> H <sub>12</sub> O <sub>2</sub>	0.003	0.067	0.614	0.001	0.029	0.263	-0.001	-0.029	-0.266	0.000	0.002	0.020
141.1273	141.112	C <sub>9</sub> H <sub>16</sub> O	0.018	0.359	3.293	0.020	0.401	3.674	0.098	1.927	17.674	0.000	0.000	0.000
143.1429	143.128	C <sub>9</sub> H <sub>18</sub> O	0.020	0.398	3.650	0.014	0.275	2.527	0.067	1.317	12.082	0.001	0.017	0.159
151.1116	151.099	C <sub>10</sub> H <sub>14</sub> O	0.004	0.070	0.643	0.003	0.051	0.467	0.019	0.378	3.464	0.000	0.000	0.000
153.1273	153.114	C <sub>10</sub> H <sub>16</sub> O	0.014	0.281	2.573	0.013	0.258	2.368	0.051	1.002	9.188	0.000	0.003	0.030

Table S-2: (continued)

$m/z$ ([M+H] <sup>+</sup> )		assigned formula	cellular fraction			capsular fraction			colloidal fraction		
APCI-HRMS	PTR-TOF-MS		mixing ratio / ppb	production / 10 <sup>7</sup> molec. mW <sup>-1</sup> s <sup>-1</sup>	flux (ambient) / 10 <sup>7</sup> molec. cm <sup>-2</sup> s <sup>-1</sup>	mixing ratio / ppb	production / 10 <sup>7</sup> molec. mW <sup>-1</sup> s <sup>-1</sup>	flux (ambient) / 10 <sup>7</sup> molec. cm <sup>-2</sup> s <sup>-1</sup>	mixing ratio / ppb	production / 10 <sup>7</sup> molec. mW <sup>-1</sup> s <sup>-1</sup>	flux (ambient) / 10 <sup>7</sup> molec. cm <sup>-2</sup> s <sup>-1</sup>
	31.019	CH <sub>2</sub> O (formaldehyde)	0.191	5.653	51.855	0.101	2.985	27.383	0.038	1.128	10.344
	33.034	CH <sub>4</sub> O (methanol)	3.114	92.201	845.774	4.114	121.804	1117.325	0.201	5.950	54.577
	41.038	C <sub>3</sub> H <sub>4</sub>	1.973	58.422	535.914	1.493	44.204	405.489	0.391	11.575	106.175
	42.034	C <sub>2</sub> H <sub>3</sub> N (acetonitrile)	0.930	27.539	252.621	11.648	344.882	3163.642	1.834	54.291	498.021
	43.017	C <sub>2</sub> H <sub>2</sub> O (ketene)	1.230	36.419	334.080	0.664	19.653	180.278	0.368	10.910	100.078
	43.054	C <sub>3</sub> H <sub>6</sub>	0.557	16.490	151.266	0.341	10.110	92.737	0.102	3.035	27.837
	44.022	C <sub>2</sub> H <sub>3</sub> O	0.041	1.224	11.227	0.021	0.614	5.631	0.022	0.647	5.939
	45.032	C <sub>2</sub> H <sub>4</sub> O (acetaldehyde)	4.411	130.623	1198.218	3.420	101.268	928.947	2.064	61.101	560.487
	47.048	C <sub>2</sub> H <sub>6</sub> O (ethanol)	0.303	8.986	82.429	0.192	5.681	52.114	0.025	0.747	6.850
	49.010	CH <sub>4</sub> S	0.059	1.748	16.033	0.031	0.905	8.301	0.011	0.339	3.111
51.0611	51.043	CH <sub>6</sub> O <sub>2</sub>	0.206	6.092	55.886	0.287	8.486	77.847	0.026	0.763	6.996
*56.0496	56.054	C <sub>3</sub> H <sub>5</sub> N	0.129	3.816	35.006	0.075	2.210	20.277	0.025	0.752	6.898
57.0336	57.032	C <sub>3</sub> H <sub>4</sub> O	5.850	173.226	1589.020	2.007	59.434	545.200	0.593	17.573	161.198
57.0700	57.067	C <sub>4</sub> H <sub>8</sub>	1.037	30.694	281.562	0.733	21.691	198.979	0.402	11.895	109.118
58.0369	58.036		0.257	7.598	69.698	0.098	2.907	26.664	0.034	0.997	9.148
58.0652	58.065	C <sub>3</sub> H <sub>7</sub> N	0.060	1.784	16.367	0.030	0.883	8.103	0.007	0.212	1.945
59.0492	59.047	C <sub>3</sub> H <sub>6</sub> O (acetone)	9.727	288.008	2641.932	6.858	203.068	1862.765	6.521	193.085	1771.192
60.0808	60.079	C <sub>3</sub> H <sub>9</sub> N	0.071	2.103	19.291	-	-	-	-	-	-
61.0284	61.026	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	0.186	5.507	50.513	0.217	6.437	59.043	0.165	4.896	44.914
63.0441	63.041	C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	0.075	2.225	20.408	0.066	1.946	17.850	0.040	1.173	10.759
65.0385	65.021	C <sub>5</sub> H <sub>4</sub>	0.018	0.526	4.822	0.018	0.520	4.774	0.026	0.765	7.016
67.0542	67.051	C <sub>5</sub> H <sub>6</sub>	0.825	24.416	223.968	0.310	9.188	84.284	0.104	3.070	28.158

68.0495	68.048	C <sub>4</sub> H <sub>5</sub> N	0.107	3.155	28.937	0.031	0.922	8.457	0.012	0.347	3.184
69.0698	69.067	C <sub>5</sub> H <sub>8</sub> (isoprene)	3.439	101.829	934.087	3.191	94.485	866.726	0.574	16.992	155.870
70.0651	70.061	C <sub>4</sub> H <sub>7</sub> N	3.531	104.544	958.990	0.971	28.742	263.651	0.343	10.159	93.187
71.0491	71.045	C <sub>4</sub> H <sub>6</sub> O	2.734	80.963	742.687	0.341	10.100	92.647	0.105	3.108	28.507
71.0855	71.077	C <sub>5</sub> H <sub>10</sub>	0.252	7.456	68.398	0.094	2.797	25.656	0.019	0.572	5.248
72.0443	72.046	C <sub>3</sub> H <sub>5</sub> NO	0.155	4.603	42.228	0.027	0.792	7.269	0.009	0.279	2.558
73.0284	73.024	C <sub>3</sub> H <sub>4</sub> O <sub>2</sub>	0.023	0.687	6.305	0.013	0.398	3.655	0.016	0.481	4.413
73.0648	73.061	C <sub>4</sub> H <sub>8</sub> O	0.650	19.254	176.621	0.686	20.315	186.350	0.185	5.477	50.239
77.0597	77.055	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	0.075	2.207	20.244	0.046	1.351	12.391	0.024	0.697	6.392
79.0542	79.050	C <sub>6</sub> H <sub>6</sub>	0.078	2.303	21.129	0.057	1.702	15.609	0.021	0.630	5.778
81.0698	81.065	C <sub>6</sub> H <sub>8</sub>	0.670	19.853	182.113	0.362	10.705	98.199	0.115	3.397	31.161
83.0491	83.044	C <sub>5</sub> H <sub>6</sub> O	0.096	2.855	26.190	0.030	0.878	8.051	0.013	0.380	3.484
83.0855	83.080	C <sub>6</sub> H <sub>10</sub>	1.745	51.669	473.966	0.560	16.575	152.043	0.144	4.254	39.027
84.0444	84.049	C <sub>4</sub> H <sub>5</sub> NO	0.055	1.614	14.809	0.026	0.767	7.039	0.013	0.395	3.626
84.0807	84.082	C <sub>5</sub> H <sub>9</sub> N	0.153	4.521	41.467	0.046	1.353	12.408	0.015	0.445	4.078
85.0647	85.059	C <sub>5</sub> H <sub>8</sub> O	5.547	164.253	1506.709	3.153	93.360	856.403	1.229	36.380	333.715
87.0440	87.039	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	0.073	2.172	19.924	0.032	0.937	8.595	0.021	0.632	5.793
87.0804	87.075	C <sub>5</sub> H <sub>10</sub> O	0.679	20.118	184.547	0.905	26.810	245.934	0.200	5.907	54.190
93.0698	93.063	C <sub>7</sub> H <sub>8</sub>	0.102	3.019	27.696	0.037	1.100	10.089	0.010	0.290	2.660
95.0855	95.079	C <sub>7</sub> H <sub>10</sub>	0.720	21.312	195.495	0.118	3.509	32.184	0.027	0.789	7.239
97.0648	97.059	C <sub>6</sub> H <sub>8</sub> O	0.070	2.081	19.086	0.034	1.005	9.223	0.036	1.052	9.654
97.1011	97.094	C <sub>7</sub> H <sub>12</sub>	0.562	16.654	152.769	0.108	3.190	29.258	0.041	1.223	11.216
99.0804	99.074	C <sub>6</sub> H <sub>10</sub> O	0.474	14.048	128.865	0.207	6.135	56.281	0.072	2.129	19.530
101.0597	101.052	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	0.102	3.016	27.665	0.072	2.123	19.479	0.032	0.944	8.664
101.0960	101.088	C <sub>6</sub> H <sub>12</sub> O	0.289	8.571	78.627	0.111	3.275	30.043	0.048	1.413	12.959
107.0491	107.042	C <sub>7</sub> H <sub>6</sub> O	0.352	10.431	95.682	0.417	12.353	113.315	0.100	2.952	27.075
107.0855	107.077	C <sub>8</sub> H <sub>10</sub>	0.184	5.458	50.067	0.125	3.696	33.904	0.030	0.889	8.155
108.0443	108.043	C <sub>6</sub> H <sub>5</sub> NO	0.027	0.810	7.435	0.033	0.986	9.044	0.007	0.221	2.028
109.1011	109.093	C <sub>8</sub> H <sub>12</sub>	1.390	41.158	377.546	0.224	6.628	60.799	0.030	0.895	8.211
111.0804	111.072	C <sub>7</sub> H <sub>10</sub> O	1.233	36.509	334.902	0.417	12.334	113.137	0.091	2.688	24.660



111.1168	111.104	C <sub>8</sub> H <sub>14</sub>	0.355	10.523	96.530	0.085	2.504	22.967	0.027	0.792	7.262
113.0960	113.088	C <sub>7</sub> H <sub>12</sub> O	0.776	22.986	210.857	0.125	3.691	33.862	0.024	0.722	6.627
115.1117	115.102	C <sub>7</sub> H <sub>14</sub> O	0.133	3.947	36.202	0.021	0.614	5.634	0.012	0.349	3.201
121.0647	121.056	C <sub>8</sub> H <sub>8</sub> O	0.084	2.484	22.783	0.070	2.075	19.035	0.028	0.825	7.565
121.0858	121.085	C <sub>5</sub> H <sub>12</sub> O <sub>3</sub>	0.025	0.747	6.854	0.015	0.451	4.137	0.007	0.201	1.843
123.1167	123.106	C <sub>9</sub> H <sub>14</sub>	0.081	2.389	21.913	0.018	0.541	4.961	0.005	0.158	1.448
125.0960	125.087	C <sub>8</sub> H <sub>12</sub> O	0.779	23.053	211.465	0.398	11.773	107.999	0.097	2.865	26.277
127.1116	127.101	C <sub>8</sub> H <sub>14</sub> O	1.423	42.144	386.596	0.270	7.991	73.303	0.028	0.825	7.572
129.1273	129.116	C <sub>8</sub> H <sub>16</sub> O	0.093	2.748	25.206	0.022	0.666	6.110	0.013	0.398	3.654
135.0803	135.075	C <sub>9</sub> H <sub>10</sub> O	0.017	0.489	4.484	0.025	0.726	6.659	0.014	0.407	3.735
137.0960	137.084	C <sub>9</sub> H <sub>12</sub> O	0.115	3.412	31.298	0.049	1.451	13.311	0.009	0.263	2.417
139.1116	139.108	C <sub>9</sub> H <sub>14</sub> O	0.049	1.439	13.200	0.010	0.287	2.634	0.001	0.024	0.222
141.0909	141.079	C <sub>8</sub> H <sub>12</sub> O <sub>2</sub>	0.028	0.836	7.666	0.013	0.378	3.471	0.005	0.156	1.432
141.1273	141.112	C <sub>9</sub> H <sub>16</sub> O	0.062	1.827	16.756	0.012	0.350	3.210	0.004	0.121	1.110
143.1429	143.128	C <sub>9</sub> H <sub>18</sub> O	0.060	1.767	16.209	0.012	0.368	3.371	0.008	0.243	2.231
151.1116	151.099	C <sub>10</sub> H <sub>14</sub> O	0.047	1.385	12.701	0.015	0.454	4.164	0.002	0.065	0.599
153.1273	153.114	C <sub>10</sub> H <sub>16</sub> O	0.095	2.814	25.812	0.015	0.440	4.040	0.003	0.092	0.848

**Table S-3:** Parameter settings used for processing the LC-MS raw data from negative mode measurements using the MZmine 2.21 software package (<http://mzmine.github.io>).

<b>1) Project / Set preferences</b>		
m/z value format	5 decimals	
Retention time value format	2 decimals	
Intensity format	1 decimal with exponent	
<b>2) Raw data methods / Peak detection / Mass detection</b>		
Mass detector	exact mass	
	Noise level	10 <sup>4</sup>
MS level	1	
<b>3) Raw data methods / Peak detection / FTMS shoulder peaks filter</b>		
Mass resolution	140000	
Peak model function	gaussian	
<b>4) Raw data methods / Peak detection / Chromatogram builder</b>		
Min time span	0.1	
Min height	5·10 <sup>4</sup>	
m/z tolerance	0.0001 m/z or 2 ppm	
<b>5) Smoothing</b>		
Filter width	7	
<b>6) Peak list methods / Peak detection / Chromatogram deconvolution</b>		
Peak resolver	Local minimum search	
	Chromatographic threshold	85%
	Search minimum in RT range	0.1
	Minimum relative height	5%
	Minimum absolute height	5·10 <sup>4</sup>
	Min ratio of peak top/edge	1.6
	Peak duration range (min)	0.1 - 10
<b>7) Peak list methods / Isotopes / Isotopic peaks grouper</b>		
m/z tolerance	0.0005 m/z or 5 ppm	
Retention time tolerance	0.2 (absolute)	
Monotonic shape	No	
Maximum charge	1	
Representative isotope	Most intense	
<b>8) Adduct search</b>		
retention time tolerance	0.2 min	
adducts	[M+acetonitrile+H]	41.0266
	[M-H+CH <sub>2</sub> O <sub>2</sub> ]	46.0055
	[M-H+CHO <sub>2</sub> Na]	67.9869
m/z tolerance	0.0001 m/z or 2 ppm	
max relative adduct peak height	100%	
<b>9) Complex search</b>		
ionization method	[M-H]-	
retention time tolerance	0.2 min	
m/z tolerance	0.0001 m/z or 2 ppm	
max relative complex peak height	100%	
<b>10) Join aligner</b>		
m/z tolerance	0.0001 m/z or 2 ppm	
weight for m/z	10	
retention time tolerance	0.2 min	

weight for RT	10	
compare isotope pattern	yes	
isotope m/z tolerance	0.0005 m/z or 5 ppm	
min absolute intensity	10 <sup>3</sup>	
minimum score	70%	
<b>11) Gap filling</b>		
intensity tolerance	10%	
m/z tolerance	0.0001 m/z or 2 ppm	
retention time tolerance	0.2 min	
RT correction	no	
<b>12) Formula prediction</b>		
ionization method	[M-H]-	
m/z tolerance	0.0001 m/z or 2 ppm	
elements	C	1 - 50
	H	0 - 100
	O	0 - 40
	N	0 - 5
	S	0 - 2
element count heuristics	H/C ratios	yes
	NOPS/C ratios	yes
	multiple element counts	yes
RDBE restrictions	RDBE range	0 - 25
	must be an integer	yes
isotope pattern filter	yes	
isotope m/z tolerance	0.0005 m/z or 5 ppm	
min absolute intensity	10 <sup>3</sup>	
minimum score	70%	
<b>13) Duplicate peak filter</b>		
m/z tolerance	0.0001 m/z or 2 ppm	
retention time tolerance	0.2 min	
require same identification	yes	

**Table S-4:** Signals, peak areas, and assigned formulas obtained from (-)-HESI-UHPLC-HRMS data for different biofilm sample types and ground water. All samples were analyzed in triplicates and the data were processed using the non-target screening approach of the MZmine 2.21 software package (see Table S-3). Subsequently, peak areas were averaged, and background subtracted.

m/z for [M-H]-	assigned formula	Capsular fraction	Cellular fraction	Colloidal fraction	Cellular & Capsular	Cellular (after sonication)	Ground water
59.01388	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	8.85E+05	1.33E+07	8.55E+06	2.67E+06	4.83E+06	2.10E+04
69.03467	C <sub>4</sub> H <sub>6</sub> O	1.95E+05	3.08E+05	8.36E+04	1.03E+05	3.27E+03	1.12E+03
71.01389	C <sub>3</sub> H <sub>4</sub> O <sub>2</sub>	1.12E+06	9.88E+06	1.08E+07	2.17E+06	2.51E+05	2.45E+04
73.02949	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	2.37E+06	9.52E+05	3.20E+06	2.00E+05	4.80E+04	2.17E+03
74.02483	C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	1.92E+06	3.30E+06	2.23E+06	1.45E+06	1.36E+05	0.00E+00
78.98600	CH <sub>4</sub> O <sub>2</sub> S	0.00E+00	8.88E+03	2.19E+03	4.44E+04	6.63E+05	1.09E+03
83.05032	C <sub>5</sub> H <sub>8</sub> O	2.49E+05	3.26E+05	7.32E+04	5.88E+04	0.00E+00	2.16E+03
84.00915	C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub>	0.00E+00	2.74E+06	5.83E+06	0.00E+00	2.34E+06	7.10E+05
85.02955	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	2.40E+06	2.17E+06	1.44E+06	3.93E+05	4.70E+04	0.00E+00

85.06597	C <sub>5</sub> H <sub>10</sub> O	9.36E+04	3.95E+04	1.67E+05	2.64E+03	1.38E+06	8.79E+02
87.00882	C <sub>3</sub> H <sub>4</sub> O <sub>3</sub>	3.67E+06	5.43E+06	2.55E+06	5.82E+05	5.96E+05	5.65E+04
89.02451	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	4.55E+07	4.37E+07	4.57E+07	1.40E+07	2.76E+08	1.01E+06
91.05539	C <sub>7</sub> H <sub>8</sub>	1.57E+06	7.11E+05	1.20E+06	8.22E+04	3.47E+06	0.00E+00
94.98090	CH <sub>4</sub> O <sub>3</sub> S	1.21E+05	5.52E+05	3.85E+05	2.30E+05	1.39E+06	3.34E+04
99.00873	C <sub>4</sub> H <sub>4</sub> O <sub>3</sub>	1.06E+06	7.68E+05	1.22E+06	7.51E+04	2.57E+06	3.84E+04
101.02446	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	9.39E+06	7.32E+06	2.37E+07	2.30E+06	8.83E+05	8.04E+04
101.06088	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.39E+05	0.00E+00
102.03097	C <sub>2</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	8.21E+03	3.50E+03	9.10E+04	1.03E+04	6.60E+05	6.01E+02
102.05610	C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>	2.68E+03	3.62E+03	3.32E+04	0.00E+00	9.96E+05	0.00E+00
103.00376	C <sub>3</sub> H <sub>4</sub> O <sub>4</sub>	1.79E+07	1.57E+07	4.99E+06	1.85E+06	2.46E+07	3.05E+04
103.04013	C <sub>4</sub> H <sub>8</sub> O <sub>3</sub>	6.44E+07	5.44E+07	2.80E+07	1.94E+07	7.02E+05	6.47E+04
104.03544	C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>	2.18E+07	3.17E+07	2.75E+07	1.67E+07	3.49E+05	5.40E+04
107.03506	C <sub>3</sub> H <sub>8</sub> O <sub>4</sub>	2.33E+05	2.50E+05	1.02E+05	5.28E+04	0.00E+00	0.00E+00
107.05035	C <sub>7</sub> H <sub>8</sub> O	1.46E+03	5.30E+03	2.04E+03	1.29E+03	3.90E+05	0.00E+00
111.00883	C <sub>5</sub> H <sub>4</sub> O <sub>3</sub>	1.88E+07	7.65E+06	3.01E+07	6.39E+05	4.38E+03	9.41E+03
111.02007	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	3.53E+07	1.85E+07	1.81E+07	3.74E+06	1.36E+07	9.74E+04
111.04520	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	7.69E+05	2.68E+05	6.08E+05	8.37E+04	1.50E+04	1.49E+03
111.08167	C <sub>7</sub> H <sub>12</sub> O	1.54E+03	5.79E+05	0.00E+00	1.85E+05	0.00E+00	0.00E+00
112.01533	C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O <sub>2</sub>	4.93E+04	9.98E+03	7.32E+04	1.56E+04	4.32E+05	0.00E+00
112.04051	C <sub>5</sub> H <sub>7</sub> NO <sub>2</sub>	0.00E+00	2.10E+05	8.09E+04	1.12E+04	8.69E+05	0.00E+00
113.02450	C <sub>5</sub> H <sub>6</sub> O <sub>3</sub>	1.66E+07	1.48E+07	1.96E+07	6.26E+06	3.79E+05	1.11E+05
113.06091	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	3.45E+04	1.16E+05	0.00E+00	1.01E+04	1.09E+06	3.37E+03
114.03096	C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	1.29E+05	2.65E+04	2.84E+05	5.98E+04	1.99E+06	0.00E+00
115.00371	C <sub>4</sub> H <sub>4</sub> O <sub>4</sub>	2.09E+07	1.25E+07	2.22E+07	5.56E+06	2.57E+03	1.45E+05
115.04012	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>	1.25E+07	5.95E+06	1.61E+07	1.20E+06	3.90E+07	4.73E+04
116.07175	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	2.41E+04	2.36E+04	2.73E+04	3.87E+04	9.56E+05	0.00E+00
117.01937	C <sub>4</sub> H <sub>6</sub> O <sub>4</sub>	2.73E+07	1.36E+07	5.65E+07	7.76E+06	1.62E+04	3.56E+05
117.05572	C <sub>5</sub> H <sub>10</sub> O <sub>3</sub>	3.36E+06	2.56E+07	2.06E+06	8.24E+05	8.89E+05	4.90E+04
118.00478	C <sub>5</sub> HN <sub>3</sub> O	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.99E+04
118.05106	C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub>	7.30E+06	1.67E+07	3.74E+06	4.50E+06	5.87E+05	2.88E+04
119.03501	C <sub>4</sub> H <sub>8</sub> O <sub>4</sub>	1.72E+07	1.59E+07	1.63E+07	4.32E+06	1.55E+06	4.72E+04
119.05028	C <sub>8</sub> H <sub>8</sub> O	1.74E+05	1.95E+05	7.80E+04	2.06E+04	1.50E+03	0.00E+00
120.01248	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S	1.66E+05	7.92E+04	1.09E+05	2.70E+04	0.00E+00	0.00E+00
121.02956	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	7.69E+06	4.84E+06	1.23E+07	1.76E+06	5.60E+06	2.75E+05

121.10236	C <sub>9</sub> H <sub>14</sub>	2.38E+05	4.72E+05	6.56E+04	1.04E+05	1.27E+04	0.00E+00
122.02469	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	1.81E+05	3.85E+04	2.71E+05	1.13E+05	0.00E+00	9.34E+03
122.02479	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	1.32E+05	1.55E+04	7.39E+05	2.62E+04	0.00E+00	4.19E+03
122.97568	C <sub>2</sub> H <sub>4</sub> O <sub>4</sub> S	9.79E+04	1.23E+05	1.97E+06	0.00E+00	1.21E+05	3.59E+04
123.08163	C <sub>8</sub> H <sub>12</sub> O	5.43E+05	1.02E+06	2.08E+05	2.45E+05	1.00E+04	0.00E+00
125.03568	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	9.32E+05	5.05E+05	3.43E+05	1.17E+05	2.35E+06	1.91E+04
126.01973	C <sub>5</sub> H <sub>5</sub> NO <sub>3</sub>	2.29E+05	0.00E+00	1.52E+06	3.85E+05	8.28E+05	3.93E+03
126.05611	C <sub>6</sub> H <sub>9</sub> NO <sub>2</sub>	1.48E+05	7.43E+03	0.00E+00	9.81E+03	1.82E+04	0.00E+00
127.02625	C <sub>3</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	0.00E+00	0.00E+00	1.29E+03	0.00E+00	4.00E+04	0.00E+00
127.04018	C <sub>6</sub> H <sub>8</sub> O <sub>3</sub>	2.20E+05	4.26E+05	1.37E+05	1.83E+05	3.97E+04	4.76E+03
127.07645	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	9.06E+04	2.45E+06	3.51E+05	8.39E+03	5.10E+05	3.43E+04
128.03537	C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub>	3.50E+08	2.03E+08	1.52E+08	9.71E+07	5.54E+08	2.24E+05
128.07177	C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub>	5.68E+05	2.56E+05	1.76E+05	2.32E+04	3.41E+05	0.00E+00
128.08305	C <sub>5</sub> H <sub>11</sub> N <sub>3</sub> O	0.00E+00	2.27E+04	3.78E+04	3.39E+04	3.62E+05	0.00E+00
129.01937	C <sub>5</sub> H <sub>6</sub> O <sub>4</sub>	3.22E+07	1.36E+07	1.60E+07	1.02E+06	9.25E+05	1.48E+05
129.05580	C <sub>6</sub> H <sub>10</sub> O <sub>3</sub>	1.28E+07	2.69E+07	7.53E+07	5.81E+06	3.94E+08	9.56E+04
129.97579	C <sub>7</sub> HNS	0.00E+00	1.86E+06	3.55E+05	1.01E+06	2.05E+06	2.78E+05
130.05097	C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub>	1.58E+05	4.00E+06	3.45E+06	9.06E+05	1.08E+07	5.26E+03
130.08734	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>	1.55E+06	2.40E+06	3.51E+05	7.83E+04	4.71E+05	5.81E+02
131.00989	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O <sub>4</sub>	2.63E+04	6.43E+04	7.40E+05	2.01E+05	2.70E+06	0.00E+00
131.03500	C <sub>5</sub> H <sub>8</sub> O <sub>4</sub>	4.55E+06	4.81E+06	2.84E+06	4.37E+05	8.55E+06	4.81E+04
131.04627	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	1.04E+06	7.76E+06	3.77E+05	1.24E+06	1.67E+05	0.00E+00
131.07138	C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>	1.32E+06	1.14E+06	9.24E+05	1.53E+05	1.67E+06	8.59E+04
131.08262	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	3.40E+06	4.58E+06	4.73E+06	3.56E+06	3.35E+06	1.28E+04
132.03028	C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub>	1.79E+08	2.24E+08	1.52E+08	4.80E+07	1.81E+06	3.51E+05
132.04151	C <sub>3</sub> H <sub>7</sub> N <sub>3</sub> O <sub>3</sub>	6.87E+05	6.19E+05	1.84E+06	2.23E+05	9.14E+05	0.00E+00
133.01429	C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>	2.05E+08	1.72E+08	2.17E+08	6.44E+07	1.24E+06	4.36E+05
134.04730	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub>	0.00E+00	4.80E+06	2.42E+03	1.66E+06	0.00E+00	5.01E+04
135.03127	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O	4.04E+07	3.73E+07	2.33E+07	1.74E+07	0.00E+00	1.60E+04
137.03567	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	2.60E+05	6.39E+04	2.90E+05	4.18E+05	3.20E+06	8.01E+04
137.09727	C <sub>9</sub> H <sub>14</sub> O	8.42E+04	2.83E+05	7.26E+03	6.93E+03	4.68E+03	0.00E+00
139.07649	C <sub>8</sub> H <sub>12</sub> O <sub>2</sub>	2.47E+05	7.49E+05	3.62E+05	1.16E+05	1.80E+06	1.65E+03
140.01022	C <sub>4</sub> H <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	0.00E+00	0.00E+00	3.66E+04	1.28E+04	1.06E+06	0.00E+00
141.05585	C <sub>7</sub> H <sub>10</sub> O <sub>3</sub>	5.06E+03	3.55E+05	0.00E+00	2.33E+04	2.92E+03	1.11E+03
141.09217	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub>	1.49E+03	2.77E+04	0.00E+00	0.00E+00	3.81E+05	0.00E+00

142.05093	C <sub>6</sub> H <sub>9</sub> NO <sub>3</sub>	6.11E+05	2.80E+05	2.96E+05	3.24E+04	0.00E+00	2.25E+03
142.08736	C <sub>7</sub> H <sub>13</sub> NO <sub>2</sub>	1.56E+06	8.83E+05	2.43E+05	7.83E+04	9.89E+05	0.00E+00
142.98084	C <sub>5</sub> H <sub>4</sub> O <sub>3</sub> S	2.92E+05	1.14E+05	2.17E+05	1.72E+06	7.52E+06	1.96E+04
143.03497	C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>	1.23E+07	1.13E+07	1.03E+07	2.26E+06	6.69E+04	2.35E+03
143.07140	C <sub>7</sub> H <sub>12</sub> O <sub>3</sub>	2.15E+06	4.42E+06	9.58E+05	8.25E+05	1.22E+06	9.06E+03
144.04550	C <sub>9</sub> H <sub>7</sub> NO	6.50E+06	4.07E+06	1.23E+07	1.51E+06	5.88E+06	1.77E+04
144.06668	C <sub>6</sub> H <sub>11</sub> NO <sub>3</sub>	1.26E+04	5.29E+04	9.00E+03	1.97E+04	1.77E+03	0.00E+00
144.07787	C <sub>5</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub>	2.53E+05	1.46E+06	7.47E+05	1.76E+06	6.99E+06	4.97E+03
145.01428	C <sub>5</sub> H <sub>6</sub> O <sub>5</sub>	1.27E+06	1.61E+05	8.05E+06	8.88E+04	1.81E+03	0.00E+00
145.03669	C <sub>3</sub> H <sub>6</sub> N <sub>4</sub> O <sub>3</sub>	8.24E+04	3.26E+04	1.45E+06	1.50E+05	3.96E+06	0.00E+00
145.05066	C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>	0.00E+00	3.48E+06	0.00E+00	0.00E+00	0.00E+00	7.86E+04
145.08705	C <sub>7</sub> H <sub>14</sub> O <sub>3</sub>	0.00E+00	1.86E+06	0.00E+00	0.00E+00	0.00E+00	5.04E+05
147.01219	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> S	8.25E+05	6.23E+05	9.94E+05	5.15E+04	2.56E+06	0.00E+00
147.02992	C <sub>5</sub> H <sub>8</sub> O <sub>5</sub>	5.71E+06	1.12E+06	4.08E+06	2.06E+05	1.86E+06	4.09E+03
147.06625	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub>	1.66E+05	1.21E+05	5.73E+05	5.25E+04	5.02E+06	1.07E+04
147.08149	C <sub>10</sub> H <sub>12</sub> O	1.49E+05	5.55E+04	3.59E+05	6.54E+03	0.00E+00	0.00E+00
148.04384	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> S	1.76E+06	1.32E+06	5.42E+05	5.69E+05	6.77E+04	0.00E+00
149.02443	C <sub>8</sub> H <sub>6</sub> O <sub>3</sub>	2.66E+04	5.84E+04	2.35E+05	0.00E+00	7.32E+05	1.20E+04
149.09720	C <sub>10</sub> H <sub>14</sub> O	1.46E+06	2.47E+06	2.30E+05	3.41E+05	0.00E+00	0.00E+00
150.04219	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O	0.00E+00	1.45E+06	0.00E+00	1.24E+06	0.00E+00	0.00E+00
151.02615	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	2.45E+08	2.73E+08	8.26E+07	1.15E+08	2.30E+07	1.55E+03
151.04007	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	7.84E+04	2.78E+05	6.16E+05	5.75E+04	1.97E+06	8.31E+03
152.03533	C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub>	9.68E+03	2.84E+03	2.55E+03	4.98E+03	3.81E+04	1.15E+03
153.03051	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>	7.44E+04	2.19E+05	3.00E+04	1.17E+04	0.00E+00	0.00E+00
153.05582	C <sub>8</sub> H <sub>10</sub> O <sub>3</sub>	5.44E+05	8.21E+05	2.10E+05	2.03E+05	2.38E+04	0.00E+00
153.09216	C <sub>9</sub> H <sub>14</sub> O <sub>2</sub>	7.16E+05	1.84E+05	1.51E+06	2.46E+05	1.12E+06	1.17E+03
154.01799	C <sub>3</sub> H <sub>9</sub> NO <sub>4</sub> S	5.89E+06	5.21E+06	1.07E+07	3.83E+06	1.39E+06	1.39E+04
154.06228	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	4.41E+06	7.48E+06	7.03E+06	2.75E+06	5.05E+06	0.00E+00
155.00204	C <sub>3</sub> H <sub>8</sub> O <sub>5</sub> S	1.85E+07	7.91E+06	3.86E+07	2.93E+06	2.42E+06	0.00E+00
155.02113	C <sub>4</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>	0.00E+00	8.86E+04	9.86E+04	1.24E+05	0.00E+00	1.62E+04
155.10787	C <sub>9</sub> H <sub>16</sub> O <sub>2</sub>	0.00E+00	1.32E+04	0.00E+00	0.00E+00	9.03E+05	0.00E+00
157.01185	C <sub>10</sub> H <sub>6</sub> S	1.04E+06	1.56E+06	2.26E+06	1.53E+06	3.69E+07	5.66E+05
157.03675	C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>3</sub>	3.62E+06	1.86E+06	6.23E+06	1.44E+06	3.10E+07	0.00E+00
157.05065	C <sub>7</sub> H <sub>10</sub> O <sub>4</sub>	4.95E+05	6.31E+05	1.29E+05	6.98E+04	6.80E+05	2.62E+04
157.08700	C <sub>8</sub> H <sub>14</sub> O <sub>3</sub>	3.12E+06	2.27E+06	3.77E+06	7.80E+05	1.32E+06	1.63E+04

158.04594	C <sub>6</sub> H <sub>9</sub> NO <sub>4</sub>	1.19E+06	5.33E+06	1.61E+06	1.99E+06	3.67E+06	0.00E+00
159.02998	C <sub>6</sub> H <sub>8</sub> O <sub>5</sub>	2.40E+05	7.23E+05	1.23E+05	2.42E+04	2.79E+05	5.06E+03
159.10273	C <sub>8</sub> H <sub>16</sub> O <sub>3</sub>	4.43E+05	8.67E+05	2.37E+05	0.00E+00	6.07E+05	1.10E+05
160.04047	C <sub>9</sub> H <sub>7</sub> NO <sub>2</sub>	4.51E+03	1.17E+04	8.75E+03	0.00E+00	2.91E+05	0.00E+00
160.06159	C <sub>6</sub> H <sub>11</sub> NO <sub>4</sub>	1.26E+04	6.63E+04	2.96E+05	7.02E+04	1.32E+06	0.00E+00
161.04561	C <sub>6</sub> H <sub>10</sub> O <sub>5</sub>	5.83E+07	4.72E+07	5.52E+07	1.40E+07	1.73E+07	1.76E+05
163.02624	C <sub>6</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	9.31E+05	4.81E+05	6.97E+05	1.44E+05	0.00E+00	0.00E+00
163.04015	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub>	1.08E+07	5.30E+06	7.61E+06	1.70E+06	1.58E+07	9.21E+04
163.06131	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>	1.28E+05	6.80E+05	0.00E+00	1.29E+05	1.04E+06	4.76E+04
163.11298	C <sub>11</sub> H <sub>16</sub> O	9.42E+03	2.13E+06	0.00E+00	6.36E+05	0.00E+00	0.00E+00
164.03532	C <sub>8</sub> H <sub>7</sub> NO <sub>3</sub>	6.96E+05	1.21E+06	8.29E+05	3.83E+05	1.05E+06	3.66E+04
164.03872	C <sub>5</sub> H <sub>11</sub> NO <sub>3</sub> S	1.03E+06	1.56E+06	3.03E+05	2.85E+05	6.85E+06	0.00E+00
164.07172	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	9.10E+06	9.67E+06	5.19E+06	2.58E+06	7.49E+06	8.99E+02
165.09212	C <sub>10</sub> H <sub>14</sub> O <sub>2</sub>	6.19E+05	4.52E+06	5.28E+05	2.04E+05	1.41E+06	0.00E+00
166.03712	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O <sub>2</sub>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.75E+05	0.00E+00
166.99620	C <sub>11</sub> H <sub>4</sub> S	1.12E+05	1.89E+04	2.71E+06	9.51E+03	0.00E+00	0.00E+00
167.01331	C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub> S	2.21E+05	0.00E+00	3.82E+06	6.81E+04	3.81E+03	1.69E+03
167.02111	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>	1.04E+06	9.22E+04	6.54E+05	5.26E+04	3.45E+07	1.27E+03
167.03504	C <sub>8</sub> H <sub>8</sub> O <sub>4</sub>	0.00E+00	0.00E+00	1.74E+04	0.00E+00	2.53E+05	3.56E+03
167.07143	C <sub>9</sub> H <sub>12</sub> O <sub>3</sub>	2.70E+06	3.65E+06	1.18E+06	1.20E+06	2.84E+04	0.00E+00
167.10780	C <sub>10</sub> H <sub>16</sub> O <sub>2</sub>	5.05E+05	2.50E+06	2.74E+05	6.35E+04	0.00E+00	0.00E+00
167.99728	C <sub>3</sub> H <sub>7</sub> NO <sub>5</sub> S	2.14E+07	1.04E+07	3.37E+07	7.37E+06	1.94E+06	4.81E+04
168.98128	C <sub>3</sub> H <sub>6</sub> O <sub>6</sub> S	5.56E+06	1.83E+06	1.45E+07	1.24E+06	3.70E+06	3.89E+03
169.08714	C <sub>9</sub> H <sub>14</sub> O <sub>3</sub>	2.39E+05	6.17E+05	1.31E+05	1.28E+05	1.47E+05	1.07E+04
171.02756	C <sub>11</sub> H <sub>8</sub> S	3.98E+07	3.59E+07	1.91E+07	1.41E+07	9.73E+03	1.87E+03
171.06638	C <sub>8</sub> H <sub>12</sub> O <sub>4</sub>	0.00E+00	1.97E+06	0.00E+00	0.00E+00	0.00E+00	7.14E+05
171.10273	C <sub>9</sub> H <sub>16</sub> O <sub>3</sub>	2.18E+06	9.59E+06	8.44E+05	1.66E+06	7.34E+05	3.51E+04
172.04044	C <sub>10</sub> H <sub>7</sub> NO <sub>2</sub>	6.10E+05	2.69E+05	1.02E+06	3.57E+05	0.00E+00	5.82E+03
172.06163	C <sub>7</sub> H <sub>11</sub> NO <sub>4</sub>	8.32E+05	4.47E+05	3.12E+05	6.69E+04	4.20E+06	9.96E+02
173.00915	C <sub>6</sub> H <sub>6</sub> O <sub>6</sub>	3.60E+06	1.62E+06	5.50E+06	2.35E+04	1.28E+04	0.00E+00
173.04558	C <sub>7</sub> H <sub>10</sub> O <sub>5</sub>	9.70E+05	6.98E+05	3.31E+05	1.51E+05	4.71E+05	3.94E+03
173.08197	C <sub>8</sub> H <sub>14</sub> O <sub>4</sub>	1.36E+06	2.91E+06	1.86E+05	2.34E+05	7.63E+05	1.58E+03
173.09325	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	8.48E+04	6.37E+05	2.74E+03	1.32E+04	6.64E+04	0.00E+00
173.11836	C <sub>9</sub> H <sub>18</sub> O <sub>3</sub>	3.44E+05	2.44E+05	8.02E+04	5.01E+04	5.25E+05	1.13E+03
174.00208	C <sub>9</sub> H <sub>5</sub> NOS	1.04E+05	5.88E+04	7.88E+04	8.80E+04	2.14E+07	1.04E+03

174.04082	C <sub>6</sub> H <sub>9</sub> NO <sub>5</sub>	6.49E+05	5.49E+04	1.37E+06	5.16E+04	5.11E+04	0.00E+00
174.05612	C <sub>10</sub> H <sub>9</sub> NO <sub>2</sub>	1.49E+04	6.06E+04	4.12E+04	4.64E+04	3.98E+06	0.00E+00
174.08846	C <sub>6</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub>	1.33E+06	1.84E+06	3.09E+05	3.61E+04	9.88E+06	0.00E+00
175.04736	C <sub>4</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>	1.32E+06	1.11E+06	2.25E+06	1.17E+05	8.37E+05	0.00E+00
175.06125	C <sub>7</sub> H <sub>12</sub> O <sub>5</sub>	1.86E+07	8.21E+06	1.53E+07	5.45E+06	2.63E+06	1.36E+04
175.07256	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>	3.27E+05	2.23E+06	0.00E+00	6.05E+04	2.36E+05	0.00E+00
177.07695	C <sub>7</sub> H <sub>14</sub> O <sub>5</sub>	8.81E+04	2.25E+05	5.39E+05	6.48E+05	1.36E+05	0.00E+00
178.03719	C <sub>6</sub> H <sub>5</sub> N <sub>5</sub> O <sub>2</sub>	3.92E+03	8.04E+03	7.26E+04	7.30E+03	0.00E+00	0.00E+00
179.02102	C <sub>6</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>	2.14E+05	3.30E+05	4.04E+05	3.18E+04	0.00E+00	0.00E+00
179.03497	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	1.71E+06	1.22E+06	7.50E+05	4.06E+05	4.35E+06	6.85E+04
179.05611	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	9.80E+07	9.09E+07	9.31E+07	2.41E+07	1.27E+06	5.82E+04
179.07147	C <sub>10</sub> H <sub>12</sub> O <sub>3</sub>	2.82E+05	4.00E+05	2.33E+05	1.30E+05	9.75E+03	0.00E+00
179.10785	C <sub>11</sub> H <sub>16</sub> O <sub>2</sub>	2.70E+04	1.36E+05	4.61E+04	0.00E+00	3.80E+05	2.54E+03
180.03368	C <sub>5</sub> H <sub>11</sub> NO <sub>4</sub> S	3.97E+05	7.59E+05	5.68E+05	2.23E+06	4.50E+05	4.85E+04
180.06667	C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>	3.28E+06	6.93E+06	1.52E+05	1.19E+06	3.61E+06	0.00E+00
181.08713	C <sub>10</sub> H <sub>14</sub> O <sub>3</sub>	9.95E+05	1.25E+06	4.81E+05	2.32E+05	3.39E+05	0.00E+00
182.99113	C <sub>11</sub> H <sub>4</sub> OS	1.60E+06	7.33E+05	1.33E+06	1.56E+05	0.00E+00	0.00E+00
183.01603	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>4</sub>	0.00E+00	3.47E+04	3.20E+05	3.06E+05	4.60E+06	0.00E+00
183.02755	C <sub>12</sub> H <sub>8</sub> S	1.94E+06	8.70E+05	2.92E+06	7.31E+04	5.43E+06	0.00E+00
183.06637	C <sub>9</sub> H <sub>12</sub> O <sub>4</sub>	2.44E+05	4.23E+05	1.97E+05	1.29E+05	9.14E+05	1.92E+03
183.10272	C <sub>10</sub> H <sub>16</sub> O <sub>3</sub>	1.09E+07	6.26E+06	1.02E+07	2.44E+06	1.45E+05	4.74E+03
185.00669	C <sub>11</sub> H <sub>6</sub> OS	1.30E+06	1.15E+05	3.41E+06	7.54E+04	1.81E+03	0.00E+00
185.02769	C <sub>8</sub> H <sub>10</sub> O <sub>3</sub> S	0.00E+00	3.09E+05	1.77E+06	1.63E+05	0.00E+00	3.62E+04
185.04320	C <sub>12</sub> H <sub>10</sub> S	1.39E+06	9.70E+05	7.51E+05	4.37E+05	2.03E+06	1.32E+03
185.08202	C <sub>9</sub> H <sub>14</sub> O <sub>4</sub>	2.68E+06	2.83E+06	1.35E+06	8.13E+05	3.44E+06	1.45E+05
185.11842	C <sub>10</sub> H <sub>18</sub> O <sub>3</sub>	5.12E+03	1.10E+04	5.97E+03	1.69E+03	6.88E+05	0.00E+00
186.03850	C <sub>11</sub> H <sub>9</sub> NS	2.05E+05	8.24E+05	2.58E+04	2.80E+05	6.13E+04	0.00E+00
186.05212	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>	2.08E+05	2.09E+05	3.70E+05	1.02E+05	1.79E+06	0.00E+00
186.07727	C <sub>8</sub> H <sub>13</sub> NO <sub>4</sub>	2.05E+06	1.19E+06	2.06E+05	8.26E+04	1.24E+03	0.00E+00
187.06126	C <sub>8</sub> H <sub>12</sub> O <sub>5</sub>	1.57E+06	1.37E+06	1.07E+06	3.85E+05	3.65E+06	1.11E+04
187.10893	C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	2.21E+06	5.60E+06	1.61E+05	5.03E+05	2.57E+04	0.00E+00
187.13407	C <sub>10</sub> H <sub>20</sub> O <sub>3</sub>	0.00E+00	0.00E+00	3.25E+04	0.00E+00	7.70E+06	9.82E+03
188.01769	C <sub>10</sub> H <sub>7</sub> NOS	2.39E+06	3.95E+06	3.27E+05	1.24E+06	1.22E+03	0.00E+00
188.05640	C <sub>7</sub> H <sub>11</sub> NO <sub>5</sub>	1.50E+05	1.28E+04	2.86E+05	2.35E+04	7.50E+05	0.00E+00
189.07699	C <sub>8</sub> H <sub>14</sub> O <sub>5</sub>	8.53E+05	5.66E+05	5.14E+05	1.51E+05	1.37E+06	9.41E+03



189.11338	C <sub>9</sub> H <sub>18</sub> O <sub>4</sub>	1.94E+05	1.80E+06	2.65E+04	1.42E+05	3.98E+04	1.35E+03
190.03585	C <sub>6</sub> H <sub>9</sub> NO <sub>6</sub>	6.59E+06	1.70E+06	0.00E+00	0.00E+00	1.04E+05	0.00E+00
190.03701	C <sub>7</sub> H <sub>5</sub> N <sub>5</sub> O <sub>2</sub>	1.09E+05	4.28E+03	1.24E+06	7.16E+04	0.00E+00	0.00E+00
190.05099	C <sub>10</sub> H <sub>9</sub> NO <sub>3</sub>	1.38E+05	1.22E+05	2.52E+05	2.55E+04	2.82E+05	9.43E+02
191.01982	C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>	4.80E+08	2.05E+08	6.68E+08	3.44E+07	1.90E+06	1.17E+03
191.07143	C <sub>11</sub> H <sub>12</sub> O <sub>3</sub>	6.70E+05	2.97E+05	9.59E+05	4.53E+04	0.00E+00	0.00E+00
193.07182	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub>	3.33E+06	1.44E+06	4.14E+06	2.72E+06	0.00E+00	1.66E+04
193.08701	C <sub>11</sub> H <sub>14</sub> O <sub>3</sub>	4.40E+06	6.47E+06	1.40E+06	1.58E+06	6.25E+05	0.00E+00
193.12346	C <sub>12</sub> H <sub>18</sub> O <sub>2</sub>	7.43E+05	5.73E+06	3.98E+05	1.05E+05	9.80E+05	0.00E+00
195.10264	C <sub>11</sub> H <sub>16</sub> O <sub>3</sub>	3.31E+06	3.00E+06	1.61E+06	7.28E+05	3.39E+04	0.00E+00
195.13913	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	9.56E+05	5.34E+06	6.90E+05	2.26E+05	0.00E+00	0.00E+00
196.01090	C <sub>5</sub> H <sub>3</sub> N <sub>5</sub> O <sub>4</sub>	5.56E+04	3.06E+04	8.07E+04	9.67E+04	0.00E+00	2.40E+03
196.02279	C <sub>12</sub> H <sub>7</sub> NS	6.11E+07	3.59E+07	2.64E+07	2.34E+07	8.15E+07	2.68E+04
196.04770	C <sub>6</sub> H <sub>7</sub> N <sub>5</sub> O <sub>3</sub>	0.00E+00	0.00E+00	4.32E+04	5.39E+03	3.38E+03	0.00E+00
197.04322	C <sub>13</sub> H <sub>10</sub> S	1.66E+07	9.19E+06	2.11E+07	2.32E+06	3.54E+07	2.51E+04
197.08196	C <sub>10</sub> H <sub>14</sub> O <sub>4</sub>	1.18E+06	8.03E+05	1.64E+06	3.29E+05	1.23E+06	1.22E+03
197.11839	C <sub>11</sub> H <sub>18</sub> O <sub>3</sub>	7.25E+05	5.10E+05	7.07E+05	2.12E+05	6.83E+03	1.11E+03
198.03852	C <sub>12</sub> H <sub>9</sub> NS	0.00E+00	1.60E+05	1.12E+04	1.24E+04	1.40E+06	0.00E+00
199.01105	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>5</sub>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.16E+06	0.00E+00
199.02255	C <sub>12</sub> H <sub>8</sub> OS	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.50E+05	1.19E+03
199.07250	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>	6.81E+05	3.91E+05	2.18E+05	7.18E+04	1.33E+06	0.00E+00
199.13408	C <sub>11</sub> H <sub>20</sub> O <sub>3</sub>	3.76E+05	4.97E+05	2.35E+05	1.06E+05	1.17E+04	0.00E+00
200.01779	C <sub>11</sub> H <sub>7</sub> NOS	1.37E+06	2.33E+06	1.01E+06	9.17E+05	2.00E+06	3.16E+03
200.05662	C <sub>8</sub> H <sub>11</sub> NO <sub>5</sub>	0.00E+00	1.72E+04	1.01E+04	0.00E+00	1.63E+05	0.00E+00
200.09296	C <sub>9</sub> H <sub>15</sub> NO <sub>4</sub>	1.34E+03	4.27E+03	9.73E+02	0.00E+00	1.85E+05	0.00E+00
201.00185	C <sub>11</sub> H <sub>6</sub> O <sub>2</sub> S	4.85E+04	3.93E+04	5.50E+04	5.23E+05	5.08E+03	1.87E+03
201.03819	C <sub>12</sub> H <sub>10</sub> OS	9.17E+03	0.00E+00	7.70E+03	5.16E+03	2.30E+07	0.00E+00
201.07697	C <sub>9</sub> H <sub>14</sub> O <sub>5</sub>	9.90E+05	4.42E+05	3.04E+05	1.14E+05	4.55E+05	1.06E+04
201.11340	C <sub>10</sub> H <sub>18</sub> O <sub>4</sub>	1.61E+06	8.81E+06	1.66E+05	2.70E+06	1.05E+06	3.62E+03
201.12460	C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	1.96E+06	4.73E+06	2.77E+05	2.28E+05	2.41E+03	0.00E+00
201.16506	C <sub>15</sub> H <sub>22</sub>	6.42E+04	3.01E+05	1.13E+04	1.37E+04	7.81E+04	0.00E+00
202.03349	C <sub>11</sub> H <sub>9</sub> NOS	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.90E+05	0.00E+00
202.07218	C <sub>8</sub> H <sub>13</sub> NO <sub>5</sub>	1.75E+06	7.36E+05	1.08E+06	9.73E+04	5.72E+05	0.00E+00
202.08357	C <sub>7</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub>	8.01E+04	7.54E+05	0.00E+00	1.19E+04	0.00E+00	0.00E+00
203.08266	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	2.18E+06	3.32E+06	6.92E+05	6.34E+05	0.00E+00	7.05E+02

203.09256	C <sub>9</sub> H <sub>16</sub> O <sub>5</sub>	2.43E+05	8.60E+05	1.58E+05	6.27E+04	2.02E+06	8.05E+03
205.07181	C <sub>8</sub> H <sub>14</sub> O <sub>6</sub>	1.37E+05	1.99E+05	3.78E+04	5.12E+04	3.97E+05	0.00E+00
206.01295	C <sub>6</sub> H <sub>9</sub> NO <sub>5</sub> S	2.81E+05	4.74E+05	1.08E+05	0.00E+00	1.41E+06	0.00E+00
206.03189	C <sub>7</sub> H <sub>5</sub> N <sub>5</sub> O <sub>3</sub>	1.21E+05	1.39E+03	8.39E+05	8.00E+04	0.00E+00	0.00E+00
207.01222	C <sub>10</sub> H <sub>8</sub> O <sub>3</sub> S	1.69E+06	1.32E+06	1.99E+06	3.31E+06	0.00E+00	2.87E+03
207.08753	C <sub>8</sub> H <sub>16</sub> O <sub>6</sub>	0.00E+00	1.96E+06	0.00E+00	0.00E+00	0.00E+00	1.39E+05
209.06678	C <sub>7</sub> H <sub>14</sub> O <sub>7</sub>	1.76E+05	6.25E+04	1.10E+05	4.27E+03	6.65E+05	0.00E+00
209.08202	C <sub>11</sub> H <sub>14</sub> O <sub>4</sub>	3.13E+05	2.25E+05	1.97E+05	6.64E+04	2.90E+05	0.00E+00
209.11837	C <sub>12</sub> H <sub>18</sub> O <sub>3</sub>	1.62E+06	1.39E+06	1.94E+06	6.33E+05	1.94E+04	0.00E+00
211.09773	C <sub>11</sub> H <sub>16</sub> O <sub>4</sub>	8.39E+04	1.02E+06	9.42E+04	0.00E+00	4.51E+06	1.17E+04
211.13411	C <sub>12</sub> H <sub>20</sub> O <sub>3</sub>	7.67E+03	2.84E+04	5.15E+03	7.67E+03	7.38E+05	0.00E+00
212.00582	C <sub>5</sub> H <sub>3</sub> N <sub>5</sub> O <sub>5</sub>	7.65E+03	1.04E+04	3.19E+04	2.38E+05	0.00E+00	0.00E+00
212.01785	C <sub>12</sub> H <sub>7</sub> NOS	3.03E+03	0.00E+00	9.63E+03	1.93E+04	2.52E+03	0.00E+00
213.01226	C <sub>3</sub> H <sub>10</sub> N <sub>4</sub> O <sub>3</sub> S <sub>2</sub>	8.68E+05	2.67E+05	1.84E+05	1.78E+06	6.82E+06	5.36E+04
213.01302	C <sub>11</sub> H <sub>6</sub> N <sub>2</sub> OS	2.75E+06	2.60E+06	1.48E+06	1.42E+06	1.68E+07	0.00E+00
213.01542	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>6</sub>	0.00E+00	1.03E+06	0.00E+00	8.62E+05	0.00E+00	1.84E+05
213.02427	C <sub>10</sub> H <sub>6</sub> N <sub>4</sub> S	3.63E+03	1.16E+03	6.44E+04	1.80E+04	2.52E+05	0.00E+00
213.03821	C <sub>13</sub> H <sub>10</sub> OS	0.00E+00	0.00E+00	3.57E+03	3.73E+03	4.79E+05	1.76E+03
213.07703	C <sub>10</sub> H <sub>14</sub> O <sub>5</sub>	2.19E+05	3.85E+05	1.21E+05	3.91E+04	5.31E+04	1.28E+04
213.11336	C <sub>11</sub> H <sub>18</sub> O <sub>4</sub>	1.78E+06	2.85E+06	6.79E+05	5.13E+05	3.96E+06	1.06E+04
213.12459	C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	1.24E+06	1.50E+06	7.02E+04	1.72E+05	1.28E+03	0.00E+00
213.14978	C <sub>12</sub> H <sub>22</sub> O <sub>3</sub>	7.06E+03	3.92E+04	9.62E+03	1.18E+04	9.36E+06	0.00E+00
213.96395	C <sub>7</sub> H <sub>5</sub> NO <sub>3</sub> S <sub>2</sub>	4.56E+05	5.97E+05	6.78E+05	2.18E+05	5.86E+05	2.10E+04
214.01018	C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub>	3.09E+04	4.34E+04	5.50E+04	3.85E+05	9.80E+05	1.51E+04
214.03335	C <sub>12</sub> H <sub>9</sub> NOS	7.99E+05	6.05E+05	1.37E+06	9.60E+04	6.24E+06	0.00E+00
214.99967	C <sub>12</sub> H <sub>8</sub> S <sub>2</sub>	2.23E+05	1.09E+05	5.74E+05	1.49E+04	1.09E+06	0.00E+00
215.05372	C <sub>13</sub> H <sub>12</sub> OS	5.92E+03	0.00E+00	1.02E+03	0.00E+00	1.09E+06	0.00E+00
215.06741	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub>	5.05E+05	6.87E+05	2.73E+04	0.00E+00	1.24E+06	0.00E+00
215.09250	C <sub>10</sub> H <sub>16</sub> O <sub>5</sub>	1.98E+06	1.62E+06	6.96E+05	3.08E+05	2.30E+06	9.25E+03
215.12896	C <sub>11</sub> H <sub>20</sub> O <sub>4</sub>	3.90E+03	4.49E+03	1.40E+03	1.27E+03	8.04E+05	0.00E+00
215.14016	C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>	1.57E+06	1.46E+06	2.84E+03	4.64E+04	0.00E+00	0.00E+00
215.14413	C <sub>15</sub> H <sub>20</sub> O	3.78E+03	3.07E+05	1.89E+03	3.99E+03	0.00E+00	0.00E+00
215.16531	C <sub>12</sub> H <sub>24</sub> O <sub>3</sub>	0.00E+00	7.29E+04	3.05E+04	0.00E+00	9.72E+05	3.23E+03
216.03123	C <sub>12</sub> H <sub>3</sub> N <sub>5</sub>	8.51E+05	6.80E+05	2.09E+05	1.26E+05	1.26E+04	0.00E+00
216.04909	C <sub>12</sub> H <sub>11</sub> NOS	0.00E+00	3.00E+03	0.00E+00	0.00E+00	7.06E+05	0.00E+00

217.02987	C <sub>15</sub> H <sub>6</sub> O <sub>2</sub>	4.20E+07	3.23E+07	4.83E+07	1.25E+07	1.45E+05	3.45E+04
217.07184	C <sub>9</sub> H <sub>14</sub> O <sub>6</sub>	1.36E+05	1.49E+06	1.21E+05	1.29E+05	9.06E+05	4.90E+04
217.08291	C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> O <sub>5</sub>	1.70E+06	5.82E+05	5.54E+05	4.25E+05	8.85E+05	3.51E+03
217.10817	C <sub>10</sub> H <sub>18</sub> O <sub>5</sub>	3.37E+06	2.17E+06	1.80E+06	6.55E+05	3.55E+06	1.38E+04
217.11943	C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	8.48E+05	2.67E+06	9.71E+04	1.62E+05	5.62E+03	0.00E+00
217.15989	C <sub>15</sub> H <sub>22</sub> O	7.32E+04	3.29E+06	0.00E+00	1.06E+06	0.00E+00	0.00E+00
218.06824	C <sub>9</sub> H <sub>9</sub> N <sub>5</sub> O <sub>2</sub>	2.32E+04	2.89E+04	5.73E+05	1.40E+04	7.99E+02	0.00E+00
218.10339	C <sub>9</sub> H <sub>17</sub> NO <sub>5</sub>	9.52E+05	3.60E+05	1.67E+06	1.77E+05	3.20E+06	0.00E+00
219.05240	C <sub>9</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub>	1.01E+07	7.08E+06	8.62E+06	9.83E+05	0.00E+00	7.70E+02
219.07752	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	8.13E+05	1.95E+05	1.05E+05	6.56E+04	5.27E+05	0.00E+00
219.10266	C <sub>13</sub> H <sub>16</sub> O <sub>3</sub>	3.14E+05	2.54E+05	4.82E+05	4.12E+04	2.72E+04	0.00E+00
219.13911	C <sub>14</sub> H <sub>20</sub> O <sub>2</sub>	1.43E+06	1.57E+06	5.53E+05	5.31E+05	6.71E+05	0.00E+00
219.17559	C <sub>15</sub> H <sub>24</sub> O	1.73E+03	6.17E+05	0.00E+00	2.30E+05	1.75E+03	0.00E+00
221.06669	C <sub>8</sub> H <sub>14</sub> O <sub>7</sub>	8.03E+06	5.59E+06	6.49E+06	3.01E+06	3.78E+04	2.85E+04
221.08205	C <sub>12</sub> H <sub>14</sub> O <sub>4</sub>	4.20E+04	2.61E+05	2.35E+04	4.51E+04	0.00E+00	9.49E+03
221.11842	C <sub>13</sub> H <sub>18</sub> O <sub>3</sub>	1.25E+06	3.28E+06	2.73E+05	6.84E+05	4.75E+04	1.21E+03
222.00214	C <sub>13</sub> H <sub>5</sub> NOS	0.00E+00	0.00E+00	1.30E+03	1.01E+03	2.49E+05	0.00E+00
222.07731	C <sub>11</sub> H <sub>13</sub> NO <sub>4</sub>	2.30E+03	2.69E+03	0.00E+00	0.00E+00	3.01E+05	0.00E+00
223.09767	C <sub>12</sub> H <sub>16</sub> O <sub>4</sub>	5.79E+04	0.00E+00	1.27E+05	0.00E+00	3.29E+05	2.42E+04
223.13406	C <sub>13</sub> H <sub>20</sub> O <sub>3</sub>	1.04E+07	1.11E+07	7.50E+06	3.22E+06	3.64E+03	4.05E+03
225.07440	C <sub>15</sub> H <sub>14</sub> S	2.87E+05	1.15E+05	4.94E+05	4.27E+04	1.24E+05	9.53E+02
225.07691	C <sub>11</sub> H <sub>14</sub> O <sub>5</sub>	9.07E+05	2.84E+05	6.94E+05	1.35E+05	4.92E+03	0.00E+00
225.08823	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>	0.00E+00	1.11E+03	1.09E+03	0.00E+00	6.62E+05	0.00E+00
225.11337	C <sub>12</sub> H <sub>18</sub> O <sub>4</sub>	5.49E+05	1.99E+06	2.77E+05	1.84E+05	1.48E+06	2.42E+03
225.14972	C <sub>13</sub> H <sub>22</sub> O <sub>3</sub>	3.36E+06	1.88E+06	1.02E+06	6.76E+05	6.96E+04	0.00E+00
226.00279	C <sub>5</sub> H <sub>9</sub> NO <sub>7</sub> S	1.28E+07	3.90E+06	3.82E+07	4.26E+06	0.00E+00	3.10E+04
227.06735	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub>	3.24E+07	2.70E+07	1.55E+07	9.32E+06	0.00E+00	0.00E+00
227.09264	C <sub>11</sub> H <sub>16</sub> O <sub>5</sub>	6.60E+05	1.11E+06	4.77E+05	1.74E+05	6.04E+05	3.52E+04
227.10385	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>	2.32E+06	1.58E+06	8.17E+05	2.71E+05	4.25E+06	2.30E+03
227.12901	C <sub>12</sub> H <sub>20</sub> O <sub>4</sub>	2.66E+06	3.72E+06	1.64E+06	1.30E+06	2.36E+06	6.31E+03
227.14028	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>	2.23E+06	4.30E+06	1.60E+05	6.81E+05	0.00E+00	0.00E+00
227.99874	C <sub>9</sub> H <sub>3</sub> N <sub>5</sub> OS	0.00E+00	0.00E+00	7.20E+03	4.22E+03	0.00E+00	0.00E+00
228.05152	C <sub>9</sub> H <sub>11</sub> NO <sub>6</sub>	9.87E+02	0.00E+00	0.00E+00	0.00E+00	3.57E+05	0.00E+00
229.03311	C <sub>13</sub> H <sub>10</sub> O <sub>2</sub> S	1.64E+04	2.43E+04	8.45E+04	7.55E+04	4.11E+05	0.00E+00
229.03887	C <sub>6</sub> H <sub>14</sub> O <sub>7</sub> S	0.00E+00	2.49E+05	0.00E+00	0.00E+00	0.00E+00	1.60E+04

229.06942	C <sub>14</sub> H <sub>14</sub> OS	1.32E+06	5.86E+05	6.41E+04	6.39E+04	0.00E+00	0.00E+00
229.07186	C <sub>10</sub> H <sub>14</sub> O <sub>6</sub>	4.91E+05	2.03E+05	8.33E+04	1.72E+04	4.12E+04	0.00E+00
229.08310	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>5</sub>	2.57E+05	3.07E+05	6.35E+04	4.72E+04	1.28E+06	0.00E+00
229.10826	C <sub>11</sub> H <sub>18</sub> O <sub>5</sub>	6.88E+05	1.01E+06	1.11E+05	2.95E+05	3.23E+05	2.38E+03
229.14464	C <sub>12</sub> H <sub>22</sub> O <sub>4</sub>	4.26E+05	6.47E+05	1.51E+05	2.90E+05	1.09E+06	1.37E+03
229.15592	C <sub>11</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>	2.22E+06	3.45E+06	8.23E+04	1.30E+05	1.34E+03	0.00E+00
231.02744	C <sub>16</sub> H <sub>8</sub> S	2.23E+06	6.47E+05	1.68E+06	1.16E+05	2.86E+06	1.93E+04
231.13511	C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub>	5.81E+05	1.00E+06	3.95E+04	3.16E+04	2.77E+03	0.00E+00
231.13918	C <sub>15</sub> H <sub>20</sub> O <sub>2</sub>	1.85E+05	1.96E+06	3.12E+04	1.21E+05	0.00E+00	0.00E+00
232.09415	C <sub>8</sub> H <sub>15</sub> N <sub>3</sub> O <sub>5</sub>	5.09E+04	1.18E+06	0.00E+00	8.81E+03	3.59E+03	0.00E+00
232.99801	C <sub>5</sub> H <sub>6</sub> N <sub>4</sub> O <sub>5</sub> S	3.11E+06	3.33E+06	7.29E+05	2.14E+06	0.00E+00	3.62E+03
233.00667	C <sub>15</sub> H <sub>6</sub> OS	5.63E+04	5.84E+04	1.17E+05	1.95E+04	0.00E+00	0.00E+00
233.07802	C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> O <sub>6</sub>	2.82E+06	3.76E+06	2.68E+05	2.13E+05	1.44E+06	0.00E+00
233.15481	C <sub>15</sub> H <sub>22</sub> O <sub>2</sub>	0.00E+00	8.39E+04	0.00E+00	0.00E+00	0.00E+00	5.34E+03
235.00866	C <sub>12</sub> H <sub>4</sub> N <sub>4</sub> S	1.16E+04	1.61E+03	4.63E+03	3.28E+03	2.16E+06	0.00E+00
235.05899	C <sub>16</sub> H <sub>12</sub> S	3.52E+05	4.93E+05	1.09E+05	1.67E+05	0.00E+00	0.00E+00
235.09774	C <sub>13</sub> H <sub>16</sub> O <sub>4</sub>	1.25E+05	2.98E+05	2.81E+04	3.24E+04	3.14E+03	0.00E+00
236.00388	C <sub>11</sub> H <sub>3</sub> N <sub>5</sub> S	4.26E+05	2.13E+06	1.27E+05	8.83E+05	1.62E+05	6.25E+02
236.05657	C <sub>11</sub> H <sub>11</sub> NO <sub>5</sub>	1.17E+04	0.00E+00	8.35E+03	1.63E+03	3.09E+05	0.00E+00
237.08834	C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>	1.85E+04	2.77E+05	3.33E+03	2.82E+04	0.00E+00	0.00E+00
237.11338	C <sub>13</sub> H <sub>18</sub> O <sub>4</sub>	1.64E+06	1.62E+06	7.44E+05	6.34E+05	4.76E+05	0.00E+00
237.11674	C <sub>10</sub> H <sub>22</sub> O <sub>4</sub> S	1.98E+05	6.91E+04	7.24E+05	2.29E+05	0.00E+00	0.00E+00
237.14978	C <sub>14</sub> H <sub>22</sub> O <sub>3</sub>	1.75E+04	1.37E+05	7.13E+03	8.88E+03	9.12E+05	0.00E+00
239.12905	C <sub>13</sub> H <sub>20</sub> O <sub>4</sub>	0.00E+00	4.24E+06	0.00E+00	0.00E+00	0.00E+00	1.03E+06
239.16552	C <sub>14</sub> H <sub>24</sub> O <sub>3</sub>	5.49E+03	2.23E+05	1.13E+03	5.51E+04	8.20E+04	0.00E+00
240.04906	C <sub>14</sub> H <sub>11</sub> NOS	3.78E+05	1.85E+05	9.16E+04	1.71E+04	2.48E+03	0.00E+00
240.06037	C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> S	1.25E+04	3.02E+04	5.04E+04	9.02E+03	3.12E+05	0.00E+00
241.08315	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>5</sub>	2.56E+07	2.83E+07	1.79E+07	1.08E+07	1.17E+06	4.92E+04
241.10589	C <sub>16</sub> H <sub>18</sub> S	6.57E+05	6.88E+05	3.36E+05	0.00E+00	3.24E+05	3.20E+04
241.10835	C <sub>12</sub> H <sub>18</sub> O <sub>5</sub>	1.19E+06	1.40E+06	4.78E+05	4.46E+05	8.76E+05	1.06E+04
241.11958	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	3.86E+06	2.36E+06	1.29E+06	2.98E+05	2.15E+06	1.96E+03
241.14481	C <sub>13</sub> H <sub>22</sub> O <sub>4</sub>	3.88E+05	2.58E+05	2.64E+05	1.47E+05	8.78E+04	0.00E+00
241.18114	C <sub>14</sub> H <sub>26</sub> O <sub>3</sub>	4.61E+03	1.44E+04	3.04E+03	1.52E+03	1.43E+06	0.00E+00
242.07609	C <sub>13</sub> H <sub>13</sub> N <sub>3</sub> S	0.00E+00	3.65E+04	0.00E+00	0.00E+00	8.62E+05	0.00E+00
242.07855	C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub>	1.30E+03	4.88E+05	1.21E+03	2.69E+05	1.51E+03	0.00E+00

242.17639	C <sub>13</sub> H <sub>25</sub> NO <sub>3</sub>	0.00E+00	1.37E+06	0.00E+00	0.00E+00	0.00E+00	2.63E+05
243.01812	C <sub>6</sub> H <sub>12</sub> O <sub>8</sub> S	3.31E+07	2.85E+07	7.92E+06	3.95E+06	1.74E+07	0.00E+00
243.04870	C <sub>14</sub> H <sub>12</sub> O <sub>2</sub> S	2.76E+06	1.29E+06	2.40E+06	8.01E+05	3.76E+05	1.96E+03
243.06236	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub>	5.23E+06	4.72E+07	1.63E+07	2.52E+07	7.73E+05	2.90E+03
243.08750	C <sub>11</sub> H <sub>16</sub> O <sub>6</sub>	4.51E+05	2.72E+05	7.11E+05	6.75E+04	1.23E+04	1.22E+03
243.12393	C <sub>12</sub> H <sub>20</sub> O <sub>5</sub>	4.08E+06	3.09E+06	1.69E+06	8.76E+05	2.28E+06	2.61E+03
243.17156	C <sub>12</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>	6.17E+05	2.02E+06	4.79E+04	4.94E+04	0.00E+00	0.00E+00
243.97793	C <sub>5</sub> H <sub>3</sub> N <sub>5</sub> O <sub>5</sub> S	1.83E+04	2.21E+04	5.48E+03	3.24E+05	0.00E+00	1.47E+03
244.13044	C <sub>10</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>	4.22E+05	1.10E+06	1.99E+04	1.95E+04	0.00E+00	9.55E+02
244.99819	C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>5</sub> S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.68E+05	0.00E+00
245.02817	C <sub>13</sub> H <sub>10</sub> O <sub>3</sub> S	0.00E+00	1.34E+04	0.00E+00	1.72E+04	2.51E+05	0.00E+00
245.11433	C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub>	4.48E+06	6.11E+06	1.50E+06	5.60E+05	1.58E+05	0.00E+00
245.15481	C <sub>16</sub> H <sub>22</sub> O <sub>2</sub>	5.78E+05	9.23E+05	1.80E+05	1.14E+05	5.28E+05	0.00E+00
246.06217	C <sub>9</sub> H <sub>13</sub> NO <sub>7</sub>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.19E+05	8.20E+02
247.13415	C <sub>15</sub> H <sub>20</sub> O <sub>3</sub>	2.70E+06	1.02E+07	4.54E+04	1.98E+06	0.00E+00	0.00E+00
247.17055	C <sub>16</sub> H <sub>24</sub> O <sub>2</sub>	4.87E+04	4.80E+04	7.31E+03	2.24E+04	4.31E+05	0.00E+00
247.98478	C <sub>11</sub> H <sub>7</sub> NO <sub>2</sub> S <sub>2</sub>	4.20E+05	8.94E+04	1.01E+06	5.08E+05	1.41E+06	0.00E+00
248.05417	C <sub>16</sub> H <sub>11</sub> NS	2.53E+06	5.56E+06	1.74E+05	1.02E+06	2.87E+06	0.00E+00
249.14983	C <sub>15</sub> H <sub>22</sub> O <sub>3</sub>	4.78E+05	1.03E+06	2.22E+05	2.19E+05	3.64E+04	0.00E+00
251.05965	C <sub>9</sub> H <sub>16</sub> O <sub>6</sub> S	0.00E+00	1.88E+05	4.19E+04	0.00E+00	0.00E+00	1.35E+04
251.07871	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>4</sub>	4.45E+06	3.95E+06	4.33E+06	4.02E+06	0.00E+00	0.00E+00
251.09022	C <sub>17</sub> H <sub>16</sub> S	1.83E+06	9.10E+05	1.80E+06	3.97E+05	3.05E+03	0.00E+00
251.10403	C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>	4.60E+04	2.66E+05	4.21E+03	6.00E+03	0.00E+00	0.00E+00
251.11386	C <sub>10</sub> H <sub>20</sub> O <sub>7</sub>	0.00E+00	2.65E+06	0.00E+00	0.00E+00	0.00E+00	1.91E+05
251.12912	C <sub>14</sub> H <sub>20</sub> O <sub>4</sub>	1.07E+05	2.80E+05	0.00E+00	0.00E+00	0.00E+00	4.13E+04
252.07383	C <sub>9</sub> H <sub>11</sub> N <sub>5</sub> O <sub>4</sub>	1.77E+06	1.11E+06	4.27E+06	5.57E+05	0.00E+00	0.00E+00
253.06956	C <sub>16</sub> H <sub>14</sub> OS	2.25E+05	4.43E+05	1.17E+05	8.81E+04	3.36E+05	0.00E+00
253.10831	C <sub>13</sub> H <sub>18</sub> O <sub>5</sub>	1.55E+06	1.70E+06	6.32E+05	3.97E+05	1.12E+05	0.00E+00
253.14476	C <sub>14</sub> H <sub>22</sub> O <sub>4</sub>	1.28E+05	4.01E+05	8.99E+04	0.00E+00	0.00E+00	3.51E+04
253.18110	C <sub>15</sub> H <sub>26</sub> O <sub>3</sub>	2.19E+05	3.67E+05	8.44E+04	6.32E+04	1.06E+05	0.00E+00
254.06474	C <sub>15</sub> H <sub>13</sub> NOS	2.44E+06	3.54E+05	8.64E+04	2.85E+04	0.00E+00	0.00E+00
254.10107	C <sub>16</sub> H <sub>17</sub> NS	5.52E+06	1.01E+05	4.04E+06	3.68E+06	0.00E+00	5.22E+03
255.06253	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub>	0.00E+00	0.00E+00	3.31E+02	0.00E+00	9.87E+05	0.00E+00
255.09651	C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> S	2.79E+05	9.26E+05	1.55E+04	9.34E+04	0.00E+00	0.00E+00
255.12397	C <sub>13</sub> H <sub>20</sub> O <sub>5</sub>	2.24E+06	1.26E+06	2.33E+06	5.20E+05	1.64E+06	0.00E+00

255.16043	C <sub>14</sub> H <sub>24</sub> O <sub>4</sub>	1.48E+03	1.60E+03	0.00E+00	0.00E+00	2.54E+05	0.00E+00
255.19685	C <sub>15</sub> H <sub>28</sub> O <sub>3</sub>	0.00E+00	5.51E+03	1.48E+03	1.24E+03	6.77E+05	0.00E+00
256.09400	C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> O <sub>5</sub>	4.87E+06	1.33E+06	4.93E+06	7.25E+05	6.01E+05	3.81E+03
256.95538	C <sub>12</sub> H <sub>2</sub> O <sub>5</sub> S	1.13E+05	5.20E+05	0.00E+00	1.61E+05	1.30E+06	5.61E+04
256.99103	C <sub>13</sub> H <sub>6</sub> O <sub>4</sub> S	2.70E+04	2.04E+04	2.23E+04	2.00E+04	5.46E+04	0.00E+00
256.99639	C <sub>11</sub> H <sub>6</sub> N <sub>4</sub> S <sub>2</sub>	3.12E+03	2.69E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
257.06829	C <sub>12</sub> H <sub>10</sub> N <sub>4</sub> O <sub>3</sub>	3.61E+03	0.00E+00	0.00E+00	0.00E+00	4.72E+05	0.00E+00
257.07792	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>6</sub>	8.95E+06	3.93E+06	4.70E+06	8.76E+05	1.03E+07	1.18E+03
257.10323	C <sub>12</sub> H <sub>18</sub> O <sub>6</sub>	9.67E+05	5.15E+05	2.12E+05	9.31E+04	1.96E+05	3.12E+03
257.13961	C <sub>13</sub> H <sub>22</sub> O <sub>5</sub>	4.48E+05	3.76E+05	4.16E+05	5.53E+04	3.12E+05	1.09E+03
257.17614	C <sub>14</sub> H <sub>26</sub> O <sub>4</sub>	5.53E+03	6.23E+03	0.00E+00	1.40E+03	4.27E+05	0.00E+00
257.99026	C <sub>9</sub> HN <sub>5</sub> O <sub>5</sub>	2.70E+03	2.48E+06	1.99E+03	0.00E+00	4.13E+05	0.00E+00
257.99334	C <sub>6</sub> H <sub>5</sub> N <sub>5</sub> O <sub>5</sub> S	4.77E+06	3.46E+06	1.78E+06	2.96E+06	5.98E+06	1.93E+03
258.99200	C <sub>9</sub> H <sub>8</sub> O <sub>7</sub> S	4.06E+05	3.03E+05	6.54E+04	4.75E+04	0.00E+00	0.00E+00
259.01375	C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> O <sub>5</sub> S	8.76E+05	6.52E+05	1.12E+06	1.77E+05	3.29E+06	0.00E+00
259.13002	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> O <sub>5</sub>	7.45E+06	5.86E+06	2.31E+06	1.15E+06	1.09E+05	8.89E+02
259.13411	C <sub>16</sub> H <sub>20</sub> O <sub>3</sub>	1.36E+05	1.04E+06	1.77E+04	2.27E+04	3.03E+04	0.00E+00
259.15520	C <sub>13</sub> H <sub>24</sub> O <sub>5</sub>	2.61E+06	1.05E+06	9.37E+05	1.57E+05	5.80E+03	0.00E+00
259.19180	C <sub>14</sub> H <sub>28</sub> O <sub>4</sub>	2.82E+03	2.29E+05	0.00E+00	3.51E+03	1.35E+04	0.00E+00
259.95509	C <sub>5</sub> H <sub>3</sub> N <sub>5</sub> O <sub>4</sub> S <sub>2</sub>	7.39E+04	1.26E+05	2.54E+04	5.03E+05	0.00E+00	1.22E+04
260.04543	C <sub>7</sub> H <sub>11</sub> N <sub>5</sub> O <sub>4</sub> S	1.92E+05	2.90E+05	1.05E+05	1.13E+05	4.52E+04	0.00E+00
260.07784	C <sub>10</sub> H <sub>15</sub> NO <sub>7</sub>	3.34E+03	3.08E+03	1.21E+03	0.00E+00	2.62E+05	0.00E+00
261.07296	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>7</sub>	4.54E+06	1.17E+06	1.30E+06	7.30E+04	4.19E+06	0.00E+00
261.07455	C <sub>18</sub> H <sub>14</sub> S	4.62E+05	3.85E+05	4.29E+04	5.70E+04	0.00E+00	0.00E+00
261.12472	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	6.88E+05	1.68E+06	3.04E+04	1.78E+05	0.00E+00	0.00E+00
261.14976	C <sub>16</sub> H <sub>22</sub> O <sub>3</sub>	3.01E+06	1.26E+07	8.12E+05	3.30E+06	1.98E+05	0.00E+00
263.03865	C <sub>13</sub> H <sub>12</sub> O <sub>4</sub> S	0.00E+00	7.68E+04	0.00E+00	0.00E+00	4.17E+03	0.00E+00
263.07716	C <sub>10</sub> H <sub>16</sub> O <sub>8</sub>	1.63E+06	1.31E+06	1.30E+06	1.98E+05	1.27E+04	0.00E+00
263.12907	C <sub>15</sub> H <sub>20</sub> O <sub>4</sub>	1.72E+06	2.25E+06	5.64E+05	7.47E+05	5.05E+05	0.00E+00
263.16545	C <sub>16</sub> H <sub>24</sub> O <sub>3</sub>	6.04E+07	1.15E+08	2.58E+07	2.77E+07	1.54E+07	1.39E+03
265.03084	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O <sub>9</sub>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.10E+06	1.33E+03
265.10852	C <sub>14</sub> H <sub>18</sub> O <sub>5</sub>	5.15E+04	2.19E+05	3.97E+03	3.22E+04	3.19E+03	0.00E+00
265.11967	C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	4.70E+04	2.68E+05	4.07E+03	2.16E+04	0.00E+00	0.00E+00
265.14471	C <sub>15</sub> H <sub>22</sub> O <sub>4</sub>	1.16E+05	7.84E+05	1.74E+04	3.20E+04	1.63E+05	0.00E+00
265.14808	C <sub>12</sub> H <sub>26</sub> O <sub>4</sub> S	2.29E+05	1.02E+06	3.17E+05	7.75E+05	7.91E+05	1.11E+05

265.18112	C <sub>16</sub> H <sub>26</sub> O <sub>3</sub>	3.81E+07	6.50E+07	1.55E+07	1.71E+07	2.77E+07	0.00E+00
265.95079	C <sub>8</sub> HN <sub>3</sub> O <sub>6</sub> S	1.05E+06	2.12E+06	1.99E+06	1.45E+06	2.71E+06	2.50E+05
265.99536	C <sub>11</sub> H <sub>9</sub> NO <sub>3</sub> S <sub>2</sub>	3.71E+06	1.42E+06	6.36E+06	1.78E+06	3.50E+05	1.88E+04
266.08835	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>	1.45E+06	2.46E+06	1.27E+06	2.59E+06	2.18E+04	1.65E+04
267.07235	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub>	4.99E+06	3.55E+06	6.79E+06	2.79E+06	2.65E+06	2.60E+03
267.09605	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> S	8.01E+04	1.36E+04	2.17E+05	1.08E+04	0.00E+00	0.00E+00
267.12392	C <sub>14</sub> H <sub>20</sub> O <sub>5</sub>	1.68E+05	1.34E+05	3.81E+04	1.63E+04	1.96E+05	0.00E+00
267.19675	C <sub>16</sub> H <sub>28</sub> O <sub>3</sub>	2.61E+07	5.07E+07	8.10E+06	2.63E+07	1.27E+07	9.55E+03
269.02575	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>10</sub>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.66E+05	0.00E+00
269.10322	C <sub>13</sub> H <sub>18</sub> O <sub>6</sub>	4.32E+05	1.42E+05	4.01E+05	5.30E+04	1.26E+04	0.00E+00
269.11213	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> S	3.34E+05	8.61E+05	4.39E+04	1.72E+04	0.00E+00	0.00E+00
269.21247	C <sub>16</sub> H <sub>30</sub> O <sub>3</sub>	4.67E+06	1.08E+07	2.91E+06	3.44E+06	6.47E+07	0.00E+00
270.04042	C <sub>14</sub> H <sub>9</sub> NO <sub>5</sub>	0.00E+00	0.00E+00	5.03E+04	1.56E+04	2.20E+05	0.00E+00
270.20777	C <sub>15</sub> H <sub>29</sub> NO <sub>3</sub>	0.00E+00	3.17E+05	9.16E+03	1.64E+04	6.87E+04	4.37E+03
271.00627	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub> S <sub>2</sub>	1.43E+06	1.35E+06	8.25E+05	1.53E+05	0.00E+00	0.00E+00
271.08249	C <sub>12</sub> H <sub>16</sub> O <sub>7</sub>	4.73E+06	3.32E+06	2.47E+06	7.90E+05	5.24E+03	0.00E+00
271.22816	C <sub>16</sub> H <sub>32</sub> O <sub>3</sub>	1.64E+05	4.60E+05	4.59E+04	2.94E+04	9.37E+04	4.17E+03
273.07292	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>7</sub>	4.98E+07	2.98E+07	1.93E+07	1.16E+07	4.19E+04	0.00E+00
273.13468	C <sub>13</sub> H <sub>22</sub> O <sub>6</sub>	2.52E+05	2.31E+05	6.10E+04	5.53E+04	1.84E+05	0.00E+00
273.14991	C <sub>17</sub> H <sub>22</sub> O <sub>3</sub>	6.39E+04	6.80E+05	3.74E+03	7.78E+04	0.00E+00	0.00E+00
273.18626	C <sub>18</sub> H <sub>26</sub> O <sub>2</sub>	4.59E+04	2.66E+05	6.55E+03	2.46E+04	7.68E+04	0.00E+00
273.92944	C <sub>7</sub> HNO <sub>9</sub> S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.55E+05	4.32E+04
274.07967	C <sub>8</sub> H <sub>13</sub> N <sub>5</sub> O <sub>6</sub>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.47E+05	0.00E+00
274.09343	C <sub>11</sub> H <sub>17</sub> NO <sub>7</sub>	8.14E+06	3.23E+06	2.59E+06	8.25E+05	1.70E+06	0.00E+00
274.97239	C <sub>6</sub> H <sub>4</sub> N <sub>4</sub> O <sub>7</sub> S	5.62E+05	6.02E+04	1.69E+06	9.90E+04	1.58E+03	0.00E+00
274.97616	C <sub>3</sub> H <sub>8</sub> N <sub>4</sub> O <sub>7</sub> S <sub>2</sub>	6.52E+04	3.21E+04	7.65E+05	9.86E+03	0.00E+00	0.00E+00
274.99985	C <sub>17</sub> H <sub>8</sub> S <sub>2</sub>	1.03E+05	3.35E+04	1.13E+05	2.27E+05	0.00E+00	2.33E+03
275.08848	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>7</sub>	1.08E+06	4.20E+05	3.05E+06	3.44E+05	1.64E+04	1.57E+03
275.12900	C <sub>16</sub> H <sub>20</sub> O <sub>4</sub>	2.13E+04	9.90E+05	7.28E+03	1.57E+04	1.46E+03	0.00E+00
277.03303	C <sub>17</sub> H <sub>10</sub> O <sub>2</sub> S	1.57E+07	2.16E+07	3.94E+06	8.31E+03	0.00E+00	0.00E+00
277.08649	C <sub>18</sub> H <sub>14</sub> O <sub>3</sub>	4.49E+04	1.47E+04	8.22E+04	3.00E+03	0.00E+00	0.00E+00
277.09284	C <sub>11</sub> H <sub>18</sub> O <sub>8</sub>	7.14E+05	2.22E+05	1.92E+06	1.39E+05	9.31E+03	0.00E+00
277.11960	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	1.80E+05	5.01E+05	1.07E+04	6.55E+04	3.18E+03	0.00E+00
277.14460	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	2.70E+06	1.14E+07	9.29E+05	1.31E+06	4.72E+05	2.92E+03
277.15599	C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>	7.89E+04	6.60E+05	4.54E+03	1.04E+04	0.00E+00	9.28E+02

279.05680	C <sub>19</sub> H <sub>8</sub> N <sub>2</sub> O	5.41E+05	5.32E+05	4.23E+05	1.94E+05	0.00E+00	0.00E+00
279.05991	C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> OS	1.09E+07	2.96E+06	2.01E+06	6.76E+05	2.04E+07	0.00E+00
279.09875	C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub>	6.99E+05	1.33E+06	2.00E+04	1.72E+05	1.24E+03	0.00E+00
279.12388	C <sub>15</sub> H <sub>20</sub> O <sub>5</sub>	4.00E+06	4.52E+06	1.44E+06	1.63E+06	3.11E+04	0.00E+00
279.12715	C <sub>12</sub> H <sub>24</sub> O <sub>5</sub> S	2.83E+05	1.48E+05	1.10E+06	4.05E+05	0.00E+00	0.00E+00
279.13522	C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub>	1.07E+05	5.23E+05	5.35E+03	1.14E+04	0.00E+00	0.00E+00
279.16022	C <sub>16</sub> H <sub>24</sub> O <sub>4</sub>	2.67E+07	4.10E+07	1.75E+07	1.11E+07	1.59E+07	2.39E+03
279.19674	C <sub>17</sub> H <sub>28</sub> O <sub>3</sub>	7.40E+04	7.01E+05	2.82E+03	7.48E+04	2.86E+06	0.00E+00
280.14024	C <sub>11</sub> H <sub>23</sub> NO <sub>7</sub>	9.30E+06	3.63E+06	1.05E+07	6.42E+06	0.00E+00	7.12E+04
280.98422	C <sub>13</sub> H <sub>2</sub> N <sub>2</sub> O <sub>6</sub>	3.47E+06	2.40E+06	8.63E+06	8.65E+05	7.01E+03	0.00E+00
281.08789	C <sub>11</sub> H <sub>14</sub> N <sub>4</sub> O <sub>5</sub>	4.19E+06	3.17E+06	2.53E+06	6.95E+05	1.04E+03	0.00E+00
281.10069	C <sub>18</sub> H <sub>18</sub> OS	8.31E+05	2.70E+05	1.38E+06	8.62E+03	6.52E+06	0.00E+00
281.13957	C <sub>15</sub> H <sub>22</sub> O <sub>5</sub>	2.04E+05	8.24E+04	1.61E+05	2.01E+04	2.39E+04	0.00E+00
281.14299	C <sub>12</sub> H <sub>26</sub> O <sub>5</sub> S	2.89E+05	4.83E+05	2.70E+05	1.55E+05	1.60E+03	0.00E+00
281.17593	C <sub>16</sub> H <sub>26</sub> O <sub>4</sub>	3.12E+07	4.44E+07	1.62E+07	1.22E+07	1.60E+07	3.52E+03
281.21240	C <sub>17</sub> H <sub>30</sub> O <sub>3</sub>	1.16E+04	3.41E+05	0.00E+00	5.13E+04	9.94E+05	0.00E+00
282.08455	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub>	4.01E+03	3.01E+05	1.65E+04	4.15E+05	0.00E+00	0.00E+00
283.06848	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>6</sub>	4.03E+05	1.96E+05	2.20E+06	4.37E+05	0.00E+00	0.00E+00
283.11879	C <sub>14</sub> H <sub>20</sub> O <sub>6</sub>	7.65E+05	4.75E+05	3.07E+05	1.87E+05	2.65E+04	0.00E+00
283.12764	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> S	3.83E+05	3.21E+05	0.00E+00	8.27E+03	0.00E+00	0.00E+00
283.13750	C <sub>15</sub> H <sub>24</sub> O <sub>3</sub> S	5.92E+04	3.67E+04	6.30E+04	1.17E+05	7.12E+05	6.38E+03
283.15520	C <sub>15</sub> H <sub>24</sub> O <sub>5</sub>	1.69E+06	1.95E+06	4.02E+05	4.17E+05	5.56E+05	1.25E+03
283.19159	C <sub>16</sub> H <sub>28</sub> O <sub>4</sub>	1.16E+07	2.16E+07	5.63E+06	5.90E+06	6.00E+06	2.58E+03
284.95429	C <sub>11</sub> H <sub>2</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	0.00E+00	4.41E+03	6.11E+03	7.93E+04	0.00E+00	0.00E+00
285.09821	C <sub>13</sub> H <sub>18</sub> O <sub>7</sub>	1.16E+05	3.80E+05	2.20E+04	6.74E+04	8.21E+03	0.00E+00
285.10696	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> OS	1.06E+05	3.92E+05	6.00E+03	1.06E+04	0.00E+00	0.00E+00
285.10953	C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>6</sub>	0.00E+00	1.28E+03	0.00E+00	1.10E+03	1.93E+05	0.00E+00
285.20724	C <sub>16</sub> H <sub>30</sub> O <sub>4</sub>	1.61E+07	3.55E+07	4.47E+06	1.90E+07	1.16E+07	1.39E+04
285.99639	C <sub>17</sub> H <sub>5</sub> NO <sub>2</sub> S	0.00E+00	1.33E+06	1.25E+03	0.00E+00	0.00E+00	0.00E+00
286.96992	C <sub>11</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	6.59E+03	1.61E+03	5.18E+03	5.12E+03	2.12E+06	0.00E+00
287.00111	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>7</sub> S <sub>2</sub>	4.11E+05	1.51E+06	1.09E+05	1.35E+05	1.93E+04	0.00E+00
287.07727	C <sub>12</sub> H <sub>16</sub> O <sub>8</sub>	4.91E+05	4.64E+04	1.88E+05	4.50E+03	1.51E+03	0.00E+00
287.08856	C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>7</sub>	4.58E+07	4.77E+07	3.12E+07	1.83E+07	0.00E+00	9.75E+04
287.16539	C <sub>18</sub> H <sub>24</sub> O <sub>3</sub>	4.86E+04	1.13E+06	1.51E+03	7.17E+04	2.54E+04	0.00E+00
287.22293	C <sub>16</sub> H <sub>32</sub> O <sub>4</sub>	1.22E+06	2.18E+06	6.36E+05	3.67E+05	1.39E+06	0.00E+00



288.13151	C <sub>10</sub> H <sub>19</sub> N <sub>5</sub> O <sub>5</sub>	1.38E+06	4.29E+06	4.33E+04	7.50E+05	3.21E+06	0.00E+00
288.98708	C <sub>19</sub> H <sub>2</sub> N <sub>2</sub> S	4.41E+04	0.00E+00	7.89E+05	9.26E+03	0.00E+00	0.00E+00
289.06959	C <sub>19</sub> H <sub>14</sub> O <sub>5</sub>	1.32E+05	1.45E+06	1.52E+06	1.04E+06	1.76E+04	0.00E+00
289.09258	C <sub>12</sub> H <sub>18</sub> O <sub>8</sub>	3.69E+05	3.25E+05	2.41E+05	1.63E+05	3.14E+03	0.00E+00
289.18105	C <sub>18</sub> H <sub>26</sub> O <sub>3</sub>	9.53E+05	5.21E+06	2.40E+05	1.91E+06	7.54E+05	0.00E+00
289.93649	C <sub>6</sub> HN <sub>3</sub> O <sub>9</sub> S	7.33E+04	3.86E+03	1.69E+06	5.75E+04	0.00E+00	0.00E+00
289.99205	C <sub>16</sub> H <sub>5</sub> NO <sub>3</sub> S	0.00E+00	8.31E+05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
290.06316	C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>8</sub>	9.06E+04	3.01E+05	3.34E+04	1.10E+05	0.00E+00	0.00E+00
290.08566	C <sub>15</sub> H <sub>17</sub> NO <sub>3</sub> S	4.48E+06	1.94E+06	0.00E+00	0.00E+00	4.75E+04	0.00E+00
291.08347	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>8</sub>	4.68E+09	1.71E+09	3.38E+04	3.80E+04	2.94E+08	0.00E+00
291.16370	C <sub>14</sub> H <sub>28</sub> O <sub>4</sub> S	3.86E+05	1.22E+06	7.91E+04	1.57E+06	0.00E+00	0.00E+00
291.19668	C <sub>18</sub> H <sub>28</sub> O <sub>3</sub>	1.67E+07	4.30E+07	6.09E+06	9.21E+06	7.35E+06	0.00E+00
292.02233	C <sub>12</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>	0.00E+00	0.00E+00	2.26E+04	1.40E+04	1.06E+05	0.00E+00
292.08044	C <sub>18</sub> H <sub>15</sub> NOS	1.34E+07	5.50E+06	0.00E+00	0.00E+00	5.38E+05	0.00E+00
292.10372	C <sub>11</sub> H <sub>19</sub> NO <sub>8</sub>	7.55E+06	2.76E+06	1.67E+06	2.58E+05	1.78E+04	0.00E+00
292.14035	C <sub>12</sub> H <sub>23</sub> NO <sub>7</sub>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.02E+05	0.00E+00
293.11447	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub>	3.70E+05	6.60E+05	1.43E+04	9.54E+04	0.00E+00	0.00E+00
293.13946	C <sub>16</sub> H <sub>22</sub> O <sub>5</sub>	1.98E+06	2.29E+06	4.75E+05	2.03E+05	1.61E+05	0.00E+00
293.21232	C <sub>18</sub> H <sub>30</sub> O <sub>3</sub>	2.80E+07	8.78E+07	8.54E+06	1.72E+07	2.96E+07	1.17E+03
294.02966	C <sub>10</sub> H <sub>9</sub> N <sub>5</sub> O <sub>4</sub> S	8.27E+05	1.23E+06	4.28E+05	5.10E+05	5.88E+05	8.93E+02
294.03788	C <sub>12</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>	0.00E+00	5.19E+04	5.94E+03	0.00E+00	9.10E+05	0.00E+00
294.18265	C <sub>15</sub> H <sub>25</sub> N <sub>3</sub> O <sub>3</sub>	0.00E+00	2.62E+05	1.55E+05	2.37E+05	0.00E+00	3.28E+04
295.11858	C <sub>15</sub> H <sub>20</sub> O <sub>6</sub>	1.14E+06	5.99E+05	8.77E+05	3.46E+05	2.25E+04	0.00E+00
295.13732	C <sub>16</sub> H <sub>24</sub> O <sub>3</sub> S	1.72E+04	7.69E+03	1.92E+04	6.09E+04	5.03E+05	2.52E+03
295.13980	C <sub>12</sub> H <sub>24</sub> O <sub>8</sub>	0.00E+00	2.23E+06	0.00E+00	0.00E+00	0.00E+00	1.72E+05
295.15507	C <sub>16</sub> H <sub>24</sub> O <sub>5</sub>	2.30E+05	1.25E+06	1.54E+05	0.00E+00	0.00E+00	3.01E+04
295.19141	C <sub>17</sub> H <sub>28</sub> O <sub>4</sub>	2.36E+05	5.26E+05	1.17E+04	1.64E+05	4.85E+05	8.51E+02
295.22774	C <sub>18</sub> H <sub>32</sub> O <sub>3</sub>	6.54E+06	2.77E+07	1.91E+06	6.64E+06	1.07E+07	8.98E+03
296.09992	C <sub>11</sub> H <sub>15</sub> N <sub>5</sub> O <sub>5</sub>	3.67E+05	5.24E+05	1.19E+05	8.35E+05	0.00E+00	2.57E+04
296.95410	C <sub>12</sub> H <sub>2</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	1.89E+04	2.58E+03	4.23E+04	9.31E+03	0.00E+00	0.00E+00
297.15285	C <sub>16</sub> H <sub>26</sub> O <sub>3</sub> S	5.12E+05	0.00E+00	1.72E+05	7.66E+05	2.57E+06	9.84E+04
297.17043	C <sub>16</sub> H <sub>26</sub> O <sub>5</sub>	1.40E+07	1.35E+07	1.05E+07	4.15E+06	5.90E+06	0.00E+00
297.24340	C <sub>18</sub> H <sub>34</sub> O <sub>3</sub>	6.83E+05	3.13E+06	4.88E+05	0.00E+00	1.40E+06	2.23E+05
298.15619	C <sub>17</sub> H <sub>21</sub> N <sub>3</sub> O <sub>2</sub>	6.77E+05	7.38E+05	7.00E+05	1.56E+06	1.71E+06	5.48E+04
299.14992	C <sub>15</sub> H <sub>24</sub> O <sub>6</sub>	4.03E+05	1.13E+05	1.12E+04	2.27E+04	4.98E+04	0.00E+00

299.18628	C <sub>16</sub> H <sub>28</sub> O <sub>5</sub>	1.44E+07	1.35E+07	9.72E+06	3.20E+06	4.95E+06	3.22E+03
299.20170	C <sub>20</sub> H <sub>28</sub> O <sub>2</sub>	3.53E+05	1.10E+06	2.10E+05	2.18E+05	1.26E+05	0.00E+00
300.19299	C <sub>14</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub>	9.35E+03	1.90E+05	3.03E+03	4.10E+04	0.00E+00	0.00E+00
301.10224	C <sub>24</sub> H <sub>14</sub>	1.02E+05	2.52E+05	8.55E+05	6.85E+05	6.86E+03	0.00E+00
301.12924	C <sub>14</sub> H <sub>22</sub> O <sub>7</sub>	0.00E+00	4.30E+05	0.00E+00	1.17E+03	3.12E+05	1.29E+04
301.20194	C <sub>16</sub> H <sub>30</sub> O <sub>5</sub>	5.87E+06	7.27E+06	2.34E+06	1.75E+06	5.35E+06	6.63E+02
302.03071	C <sub>14</sub> H <sub>9</sub> NO <sub>7</sub>	0.00E+00	0.00E+00	3.92E+03	3.27E+04	1.28E+04	0.00E+00
302.05055	C <sub>16</sub> H <sub>9</sub> N <sub>5</sub> S	8.82E+05	9.34E+05	1.06E+05	2.21E+04	1.34E+05	0.00E+00
302.14685	C <sub>11</sub> H <sub>21</sub> N <sub>5</sub> O <sub>5</sub>	8.58E+05	3.78E+06	1.59E+06	3.04E+06	5.59E+05	0.00E+00
303.16015	C <sub>18</sub> H <sub>24</sub> O <sub>4</sub>	1.16E+04	8.39E+05	1.71E+03	1.77E+04	7.37E+03	0.00E+00
303.21770	C <sub>16</sub> H <sub>32</sub> O <sub>5</sub>	2.06E+04	5.85E+04	1.79E+03	3.62E+03	4.17E+05	0.00E+00
304.07856	C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> O <sub>8</sub>	4.58E+05	1.04E+06	2.83E+05	2.45E+05	0.00E+00	0.00E+00
305.17578	C <sub>18</sub> H <sub>26</sub> O <sub>4</sub>	8.17E+05	1.00E+07	6.03E+05	1.06E+06	8.14E+04	0.00E+00
306.05787	C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>9</sub>	1.66E+04	7.17E+05	6.06E+04	0.00E+00	0.00E+00	0.00E+00
307.15847	C <sub>14</sub> H <sub>28</sub> O <sub>5</sub> S	2.91E+05	6.28E+05	1.64E+05	1.46E+05	1.84E+03	0.00E+00
307.19139	C <sub>18</sub> H <sub>28</sub> O <sub>4</sub>	1.90E+07	3.51E+07	7.83E+06	7.40E+06	9.28E+06	0.00E+00
308.98295	C <sub>19</sub> H <sub>2</sub> O <sub>5</sub>	1.39E+05	7.01E+05	2.83E+04	6.20E+04	3.29E+03	0.00E+00
309.13423	C <sub>16</sub> H <sub>22</sub> O <sub>6</sub>	3.20E+05	8.25E+04	1.33E+05	1.83E+04	5.67E+03	0.00E+00
309.17400	C <sub>14</sub> H <sub>30</sub> O <sub>5</sub> S	2.42E+06	7.73E+06	1.68E+06	3.94E+06	0.00E+00	1.60E+05
309.20705	C <sub>18</sub> H <sub>30</sub> O <sub>4</sub>	5.38E+07	1.01E+08	2.29E+07	2.18E+07	5.08E+07	0.00E+00
310.07930	C <sub>11</sub> H <sub>13</sub> N <sub>5</sub> O <sub>6</sub>	1.55E+05	3.17E+05	9.66E+05	3.16E+05	9.90E+05	0.00E+00
311.15001	C <sub>16</sub> H <sub>24</sub> O <sub>6</sub>	5.17E+05	1.14E+06	3.11E+05	1.00E+05	6.10E+05	0.00E+00
311.16833	C <sub>17</sub> H <sub>28</sub> O <sub>3</sub> S	3.01E+06	3.00E+05	1.83E+06	3.58E+06	3.37E+06	7.07E+05
311.18632	C <sub>17</sub> H <sub>28</sub> O <sub>5</sub>	1.42E+06	1.86E+06	4.87E+05	3.82E+05	1.32E+06	9.41E+02
311.22270	C <sub>18</sub> H <sub>32</sub> O <sub>4</sub>	1.65E+07	3.39E+07	5.50E+06	8.94E+06	1.09E+07	7.91E+03
312.09493	C <sub>11</sub> H <sub>15</sub> N <sub>5</sub> O <sub>6</sub>	5.94E+03	1.88E+06	5.44E+03	2.23E+06	0.00E+00	7.05E+04
312.17194	C <sub>18</sub> H <sub>23</sub> N <sub>3</sub> O <sub>2</sub>	4.31E+05	1.22E+06	5.64E+05	1.94E+06	1.64E+06	7.03E+04
313.06527	C <sub>24</sub> H <sub>10</sub> O	1.57E+07	1.87E+07	0.00E+00	0.00E+00	1.06E+07	0.00E+00
313.16554	C <sub>16</sub> H <sub>26</sub> O <sub>6</sub>	5.05E+06	6.51E+06	3.28E+06	1.02E+06	4.41E+06	0.00E+00
313.18094	C <sub>20</sub> H <sub>26</sub> O <sub>3</sub>	7.09E+03	9.34E+05	4.71E+03	2.47E+04	1.96E+03	0.00E+00
313.20209	C <sub>17</sub> H <sub>30</sub> O <sub>5</sub>	5.42E+03	1.07E+04	1.19E+03	0.00E+00	2.69E+05	0.00E+00
313.23841	C <sub>18</sub> H <sub>34</sub> O <sub>4</sub>	1.03E+06	2.96E+06	2.60E+05	5.21E+05	3.12E+06	2.98E+04
315.04151	C <sub>18</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub>	5.30E+05	1.22E+05	0.00E+00	0.00E+00	2.38E+05	0.00E+00
315.13504	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub>	1.50E+05	1.96E+05	6.92E+04	2.13E+04	9.32E+05	1.16E+03
315.13864	C <sub>22</sub> H <sub>20</sub> O <sub>2</sub>	1.55E+06	1.18E+05	1.69E+06	1.06E+03	0.00E+00	0.00E+00

315.18123	C <sub>16</sub> H <sub>28</sub> O <sub>6</sub>	3.02E+06	3.45E+06	2.07E+06	9.16E+05	4.26E+06	1.29E+03
315.19656	C <sub>20</sub> H <sub>28</sub> O <sub>3</sub>	8.08E+05	2.43E+06	1.12E+05	1.89E+06	6.32E+04	0.00E+00
315.21773	C <sub>17</sub> H <sub>32</sub> O <sub>5</sub>	4.64E+03	6.21E+03	0.00E+00	0.00E+00	3.17E+05	0.00E+00
315.25410	C <sub>18</sub> H <sub>36</sub> O <sub>4</sub>	3.57E+05	9.66E+05	8.63E+04	1.60E+05	3.79E+05	9.44E+03
316.15151	C <sub>13</sub> H <sub>23</sub> N <sub>3</sub> O <sub>6</sub>	3.00E+05	5.40E+05	5.07E+04	7.42E+04	0.00E+00	0.00E+00
316.18792	C <sub>14</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub>	4.67E+04	2.33E+05	8.62E+03	2.37E+04	8.99E+02	0.00E+00
317.09123	C <sub>10</sub> H <sub>22</sub> O <sub>9</sub> S	7.47E+04	8.18E+05	6.65E+04	8.81E+04	0.00E+00	2.09E+04
317.19715	C <sub>16</sub> H <sub>30</sub> O <sub>6</sub>	2.02E+03	3.77E+05	0.00E+00	8.21E+03	0.00E+00	0.00E+00
317.21217	C <sub>20</sub> H <sub>30</sub> O <sub>3</sub>	3.37E+07	1.04E+08	1.71E+07	2.66E+07	2.73E+07	1.65E+03
319.05051	C <sub>13</sub> H <sub>12</sub> N <sub>4</sub> O <sub>4</sub> S	1.63E+07	1.24E+07	1.00E+07	3.80E+06	4.32E+06	0.00E+00
319.05864	C <sub>23</sub> H <sub>12</sub> S	6.23E+06	2.72E+06	3.29E+06	1.07E+06	1.76E+06	0.00E+00
319.22793	C <sub>20</sub> H <sub>32</sub> O <sub>3</sub>	6.38E+05	5.82E+05	3.56E+05	4.69E+05	3.74E+05	0.00E+00
321.17088	C <sub>18</sub> H <sub>26</sub> O <sub>5</sub>	1.06E+05	4.56E+05	5.28E+04	2.16E+04	1.66E+04	0.00E+00
321.17409	C <sub>15</sub> H <sub>30</sub> O <sub>5</sub> S	1.08E+06	5.49E+06	1.01E+06	2.20E+05	1.28E+05	5.03E+04
323.18638	C <sub>18</sub> H <sub>28</sub> O <sub>5</sub>	8.55E+06	1.58E+07	4.22E+06	4.04E+06	3.93E+06	0.00E+00
323.22278	C <sub>19</sub> H <sub>32</sub> O <sub>4</sub>	2.46E+06	7.55E+06	5.54E+05	1.12E+06	5.56E+05	0.00E+00
324.97792	C <sub>19</sub> H <sub>2</sub> O <sub>6</sub>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.97E+04	0.00E+00
325.04145	C <sub>10</sub> H <sub>14</sub> O <sub>12</sub>	6.21E+05	1.33E+06	1.10E+05	7.36E+04	0.00E+00	0.00E+00
325.20199	C <sub>18</sub> H <sub>30</sub> O <sub>5</sub>	3.50E+07	4.52E+07	2.38E+07	1.30E+07	2.09E+07	0.00E+00
327.14503	C <sub>16</sub> H <sub>24</sub> O <sub>7</sub>	1.16E+05	1.07E+05	1.27E+05	2.87E+04	2.04E+04	0.00E+00
327.21755	C <sub>18</sub> H <sub>32</sub> O <sub>5</sub>	6.72E+07	6.06E+07	4.53E+07	1.94E+07	3.88E+07	5.37E+03
328.18800	C <sub>15</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub>	7.43E+04	2.15E+05	8.18E+03	1.72E+04	0.00E+00	0.00E+00
329.03043	C <sub>16</sub> H <sub>10</sub> O <sub>8</sub>	8.92E+05	8.91E+05	0.00E+00	0.00E+00	6.36E+05	0.00E+00
329.17591	C <sub>20</sub> H <sub>26</sub> O <sub>4</sub>	5.34E+05	2.15E+06	2.79E+05	8.40E+05	1.02E+03	0.00E+00
329.23333	C <sub>18</sub> H <sub>34</sub> O <sub>5</sub>	2.22E+07	3.09E+07	8.10E+06	7.26E+06	1.08E+07	6.05E+03
330.16722	C <sub>14</sub> H <sub>25</sub> N <sub>3</sub> O <sub>6</sub>	1.40E+05	3.99E+05	1.68E+04	2.83E+04	1.99E+03	0.00E+00
330.20357	C <sub>15</sub> H <sub>29</sub> N <sub>3</sub> O <sub>5</sub>	7.11E+04	1.81E+05	3.97E+03	6.88E+03	0.00E+00	0.00E+00
331.11478	C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>8</sub>	1.54E+05	4.37E+05	1.79E+05	2.24E+05	0.00E+00	0.00E+00
331.19154	C <sub>20</sub> H <sub>28</sub> O <sub>4</sub>	8.29E+05	6.70E+06	4.63E+05	8.12E+05	4.01E+05	0.00E+00
331.99764	C <sub>13</sub> H <sub>7</sub> N <sub>3</sub> O <sub>6</sub> S	1.50E+06	1.44E+06	4.10E+05	4.62E+05	4.20E+06	0.00E+00
333.09415	C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>9</sub>	6.50E+03	3.01E+05	6.52E+04	1.87E+05	0.00E+00	0.00E+00
333.20716	C <sub>20</sub> H <sub>30</sub> O <sub>4</sub>	2.62E+07	5.47E+07	1.07E+07	1.49E+07	4.28E+07	0.00E+00
334.21053	C <sub>14</sub> H <sub>33</sub> N <sub>5</sub> S <sub>2</sub>	1.17E+06	3.01E+06	3.37E+05	5.94E+05	8.76E+05	0.00E+00
335.04740	C <sub>8</sub> H <sub>16</sub> O <sub>14</sub>	3.38E+06	3.38E+06	0.00E+00	0.00E+00	1.00E+06	0.00E+00
335.22290	C <sub>20</sub> H <sub>32</sub> O <sub>4</sub>	1.57E+06	5.30E+06	3.62E+05	8.86E+05	8.99E+06	0.00E+00

337.23859	C <sub>20</sub> H <sub>34</sub> O <sub>4</sub>	2.35E+06	7.83E+06	7.32E+05	1.15E+06	7.28E+06	0.00E+00
339.14492	C <sub>17</sub> H <sub>24</sub> O <sub>7</sub>	5.61E+05	3.11E+05	2.60E+05	9.88E+04	1.87E+03	0.00E+00
339.16622	C <sub>14</sub> H <sub>28</sub> O <sub>9</sub>	0.00E+00	1.84E+06	0.00E+00	0.00E+00	0.00E+00	1.30E+05
339.18144	C <sub>18</sub> H <sub>28</sub> O <sub>6</sub>	1.07E+06	2.54E+06	2.66E+05	3.21E+05	8.44E+05	6.90E+03
339.20005	C <sub>19</sub> H <sub>32</sub> O <sub>3</sub> S	1.90E+05	2.44E+05	4.34E+05	3.17E+05	7.46E+05	6.88E+04
341.02963	C <sub>17</sub> H <sub>10</sub> O <sub>8</sub>	1.55E+06	3.27E+05	2.62E+06	1.61E+04	1.16E+05	0.00E+00
341.10867	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	3.29E+05	1.88E+05	8.18E+05	1.05E+05	0.00E+00	2.79E+03
341.12432	C <sub>16</sub> H <sub>22</sub> O <sub>8</sub>	8.69E+05	7.63E+05	1.59E+05	1.21E+05	8.29E+03	0.00E+00
341.16070	C <sub>17</sub> H <sub>26</sub> O <sub>7</sub>	1.22E+06	9.98E+05	1.69E+05	2.79E+05	7.71E+03	0.00E+00
341.19702	C <sub>18</sub> H <sub>30</sub> O <sub>6</sub>	6.76E+06	1.15E+07	2.97E+06	3.24E+06	4.60E+06	0.00E+00
341.23350	C <sub>19</sub> H <sub>34</sub> O <sub>5</sub>	8.35E+03	6.86E+03	6.02E+03	3.07E+03	6.45E+05	0.00E+00
341.99965	C <sub>6</sub> H <sub>9</sub> N <sub>5</sub> O <sub>10</sub> S	6.11E+05	3.92E+05	0.00E+00	0.00E+00	2.00E+06	0.00E+00
342.16715	C <sub>15</sub> H <sub>25</sub> N <sub>3</sub> O <sub>6</sub>	4.64E+05	7.26E+05	8.33E+04	1.47E+05	0.00E+00	0.00E+00
343.11308	C <sub>26</sub> H <sub>16</sub> O	1.12E+04	2.68E+04	4.14E+05	2.78E+05	0.00E+00	0.00E+00
343.21268	C <sub>18</sub> H <sub>32</sub> O <sub>6</sub>	5.89E+06	9.73E+06	4.36E+06	3.48E+06	7.81E+06	0.00E+00
343.22806	C <sub>22</sub> H <sub>32</sub> O <sub>3</sub>	4.99E+05	1.14E+06	3.14E+05	4.96E+05	2.30E+04	0.00E+00
343.99486	C <sub>17</sub> H <sub>3</sub> N <sub>3</sub> O <sub>6</sub>	4.83E+07	3.51E+07	4.73E+04	1.10E+03	4.35E+07	0.00E+00
344.18301	C <sub>15</sub> H <sub>27</sub> N <sub>3</sub> O <sub>6</sub>	8.65E+04	1.83E+05	7.38E+03	2.51E+04	4.58E+03	7.88E+02
344.21607	C <sub>20</sub> H <sub>31</sub> N <sub>3</sub> S	1.83E+04	3.87E+04	1.84E+04	6.70E+03	2.89E+05	0.00E+00
345.22850	C <sub>18</sub> H <sub>34</sub> O <sub>6</sub>	1.84E+04	1.75E+06	0.00E+00	5.88E+05	4.03E+05	0.00E+00
345.99947	C <sub>18</sub> H <sub>5</sub> NO <sub>7</sub>	1.06E+05	7.01E+04	0.00E+00	0.00E+00	1.70E+05	0.00E+00
347.18659	C <sub>20</sub> H <sub>28</sub> O <sub>5</sub>	3.59E+05	3.18E+06	1.69E+05	5.25E+05	1.58E+05	0.00E+00
348.97651	C <sub>13</sub> H <sub>6</sub> N <sub>2</sub> O <sub>8</sub> S	3.85E+05	9.00E+04	1.13E+06	6.64E+04	0.00E+00	0.00E+00
349.20215	C <sub>20</sub> H <sub>30</sub> O <sub>5</sub>	7.78E+06	1.46E+07	3.35E+06	3.59E+06	6.24E+06	0.00E+00
350.12563	C <sub>18</sub> H <sub>17</sub> N <sub>5</sub> O <sub>3</sub>	3.52E+04	1.07E+05	7.54E+04	1.08E+05	0.00E+00	2.15E+03
350.92818	C <sub>13</sub> H <sub>4</sub> O <sub>8</sub> S <sub>2</sub>	7.75E+04	7.45E+04	1.82E+05	0.00E+00	3.16E+05	2.32E+04
351.01233	C <sub>22</sub> H <sub>8</sub> O <sub>3</sub> S	6.49E+04	1.67E+05	0.00E+00	0.00E+00	1.42E+05	0.00E+00
351.21775	C <sub>20</sub> H <sub>32</sub> O <sub>5</sub>	1.64E+07	2.15E+07	8.97E+06	6.28E+06	4.95E+06	1.15E+03
351.99762	C <sub>23</sub> H <sub>3</sub> N <sub>3</sub> S	4.22E+05	6.60E+04	3.02E+04	1.64E+03	2.06E+05	0.00E+00
352.01464	C <sub>23</sub> H <sub>3</sub> N <sub>3</sub> O <sub>2</sub>	4.31E+04	4.03E+04	0.00E+00	0.00E+00	1.40E+05	0.00E+00
352.99695	C <sub>14</sub> H <sub>10</sub> O <sub>9</sub> S	3.10E+06	1.10E+06	0.00E+00	0.00E+00	3.58E+05	0.00E+00
353.01072	C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>13</sub>	4.12E+06	3.25E+06	0.00E+00	0.00E+00	4.37E+06	0.00E+00
353.14282	C <sub>18</sub> H <sub>26</sub> O <sub>5</sub> S	1.88E+05	2.47E+06	3.34E+05	5.54E+04	2.60E+04	4.53E+03
353.20049	C <sub>16</sub> H <sub>34</sub> O <sub>6</sub> S	6.23E+05	2.66E+06	4.14E+05	1.10E+06	0.00E+00	9.13E+04
353.23347	C <sub>20</sub> H <sub>34</sub> O <sub>5</sub>	3.51E+06	8.65E+06	6.83E+05	1.57E+06	3.04E+06	0.00E+00

354.99390	C <sub>13</sub> H <sub>8</sub> O <sub>12</sub>	1.40E+06	6.47E+05	4.72E+03	0.00E+00	1.34E+05	0.00E+00
355.04538	C <sub>18</sub> H <sub>12</sub> O <sub>8</sub>	2.54E+05	4.50E+03	9.19E+04	2.87E+03	0.00E+00	0.00E+00
355.13983	C <sub>17</sub> H <sub>24</sub> O <sub>8</sub>	1.14E+06	3.60E+05	9.33E+05	1.34E+05	5.49E+03	0.00E+00
355.17619	C <sub>18</sub> H <sub>28</sub> O <sub>7</sub>	1.47E+05	1.24E+05	1.28E+05	3.25E+04	1.03E+04	0.00E+00
355.24916	C <sub>20</sub> H <sub>36</sub> O <sub>5</sub>	5.73E+05	1.89E+06	1.13E+05	3.40E+05	4.62E+04	0.00E+00
356.11009	C <sub>14</sub> H <sub>19</sub> N <sub>3</sub> O <sub>8</sub>	0.00E+00	4.32E+04	0.00E+00	0.00E+00	0.00E+00	0.00E+00
357.02936	C <sub>15</sub> H <sub>10</sub> N <sub>4</sub> O <sub>5</sub> S	6.66E+05	8.24E+05	0.00E+00	0.00E+00	8.32E+05	0.00E+00
357.15556	C <sub>17</sub> H <sub>26</sub> O <sub>8</sub>	7.15E+05	4.29E+05	2.82E+05	9.61E+04	2.09E+05	0.00E+00
357.19227	C <sub>18</sub> H <sub>30</sub> O <sub>7</sub>	7.20E+03	2.29E+05	1.53E+03	3.09E+04	1.93E+04	0.00E+00
357.20742	C <sub>22</sub> H <sub>30</sub> O <sub>4</sub>	3.46E+03	1.70E+05	1.65E+03	1.44E+04	3.89E+03	0.00E+00
358.99482	C <sub>18</sub> H <sub>4</sub> N <sub>2</sub> O <sub>7</sub>	3.16E+05	2.06E+05	0.00E+00	0.00E+00	0.00E+00	9.31E+04
359.20775	C <sub>18</sub> H <sub>32</sub> O <sub>7</sub>	5.51E+04	1.22E+06	2.77E+04	6.43E+04	6.20E+05	0.00E+00
359.22297	C <sub>22</sub> H <sub>32</sub> O <sub>4</sub>	2.47E+06	2.25E+06	7.52E+05	3.92E+05	4.24E+05	5.46E+02
360.09137	C <sub>18</sub> H <sub>19</sub> NO <sub>5</sub> S	2.26E+06	1.33E+06	6.86E+05	1.98E+05	0.00E+00	0.00E+00
363.18146	C <sub>20</sub> H <sub>28</sub> O <sub>6</sub>	4.71E+05	2.34E+06	1.97E+05	1.45E+05	2.40E+05	0.00E+00
364.02611	C <sub>23</sub> H <sub>3</sub> N <sub>5</sub> O	7.52E+05	7.68E+04	5.17E+05	2.41E+04	1.51E+03	0.00E+00
364.94158	C <sub>13</sub> H <sub>2</sub> O <sub>13</sub>	5.11E+04	7.56E+03	1.77E+05	1.07E+04	0.00E+00	0.00E+00
365.19706	C <sub>20</sub> H <sub>30</sub> O <sub>6</sub>	3.47E+06	6.50E+06	8.95E+05	6.68E+05	2.11E+06	0.00E+00
367.01036	C <sub>19</sub> H <sub>4</sub> N <sub>4</sub> O <sub>5</sub>	1.96E+05	2.03E+05	0.00E+00	0.00E+00	6.67E+05	0.00E+00
367.21284	C <sub>20</sub> H <sub>32</sub> O <sub>6</sub>	1.75E+05	5.80E+05	8.38E+04	1.41E+05	1.29E+06	0.00E+00
368.00941	C <sub>15</sub> H <sub>7</sub> N <sub>5</sub> O <sub>5</sub> S	1.01E+05	4.99E+04	0.00E+00	0.00E+00	5.56E+05	0.00E+00
368.03416	C <sub>17</sub> H <sub>11</sub> N <sub>3</sub> O <sub>5</sub> S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.69E+05	0.00E+00
368.05881	C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> O <sub>12</sub>	1.63E+05	7.60E+03	1.44E+06	3.59E+04	0.00E+00	0.00E+00
369.00557	C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>14</sub>	2.40E+06	2.16E+06	1.45E+03	0.00E+00	7.27E+05	0.00E+00
369.00566	C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>14</sub>	6.29E+05	5.51E+05	0.00E+00	0.00E+00	2.28E+05	5.44E+02
369.13736	C <sub>18</sub> H <sub>26</sub> O <sub>6</sub> S	1.37E+04	9.83E+03	1.23E+04	1.54E+04	5.16E+05	0.00E+00
369.18970	C <sub>23</sub> H <sub>30</sub> O <sub>2</sub> S	8.38E+03	1.43E+04	6.86E+03	8.40E+03	3.54E+05	4.47E+02
370.95859	C <sub>19</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>	8.19E+04	1.85E+04	1.63E+05	9.19E+03	0.00E+00	0.00E+00
371.00256	C <sub>22</sub> H <sub>4</sub> N <sub>4</sub> OS	6.60E+04	4.94E+04	0.00E+00	0.00E+00	3.19E+05	0.00E+00
371.13478	C <sub>17</sub> H <sub>24</sub> O <sub>9</sub>	1.19E+06	3.27E+05	1.19E+06	5.84E+04	3.80E+03	0.00E+00
371.24411	C <sub>20</sub> H <sub>36</sub> O <sub>6</sub>	5.17E+05	8.74E+05	1.89E+05	3.42E+05	1.61E+05	0.00E+00
372.21427	C <sub>17</sub> H <sub>31</sub> N <sub>3</sub> O <sub>6</sub>	3.62E+05	3.11E+05	3.29E+05	4.87E+04	0.00E+00	0.00E+00
373.15050	C <sub>17</sub> H <sub>26</sub> O <sub>9</sub>	2.31E+06	1.67E+06	1.25E+06	4.85E+05	6.87E+04	0.00E+00
374.99273	C <sub>15</sub> H <sub>8</sub> N <sub>2</sub> O <sub>8</sub> S	6.07E+04	6.17E+04	0.00E+00	0.00E+00	2.49E+05	0.00E+00
377.19477	C <sub>25</sub> H <sub>30</sub> OS	1.63E+06	2.84E+06	8.94E+05	1.13E+06	1.01E+06	0.00E+00

377.23348	C <sub>22</sub> H <sub>34</sub> O <sub>5</sub>	4.87E+05	1.04E+06	7.84E+04	2.17E+05	4.61E+05	0.00E+00
377.27313	C <sub>20</sub> H <sub>42</sub> O <sub>4</sub> S	0.00E+00	0.00E+00	0.00E+00	2.98E+05	0.00E+00	5.37E+04
379.15634	C <sub>24</sub> H <sub>20</sub> N <sub>4</sub> O	1.27E+05	8.66E+04	9.28E+04	6.22E+05	1.62E+06	3.35E+04
379.21053	C <sub>25</sub> H <sub>32</sub> OS	1.18E+05	3.53E+05	1.12E+04	3.80E+04	2.00E+05	0.00E+00
381.00575	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O <sub>14</sub>	3.22E+04	4.45E+04	7.58E+03	0.00E+00	2.05E+05	0.00E+00
381.19195	C <sub>20</sub> H <sub>30</sub> O <sub>7</sub>	6.37E+05	1.20E+06	5.67E+05	1.19E+05	1.32E+05	0.00E+00
383.19246	C <sub>16</sub> H <sub>32</sub> O <sub>10</sub>	0.00E+00	1.34E+06	0.00E+00	0.00E+00	0.00E+00	9.21E+04
383.20769	C <sub>20</sub> H <sub>32</sub> O <sub>7</sub>	2.48E+04	7.74E+04	1.32E+04	1.30E+04	5.35E+05	0.00E+00
384.15227	C <sub>15</sub> H <sub>23</sub> N <sub>5</sub> O <sub>7</sub>	3.57E+05	4.12E+04	2.20E+05	2.51E+04	8.20E+03	0.00E+00
384.93533	C <sub>9</sub> H <sub>6</sub> O <sub>15</sub> S	2.15E+06	5.72E+05	7.52E+05	3.16E+05	7.41E+05	9.40E+04
387.28651	C <sub>20</sub> H <sub>40</sub> N <sub>2</sub> O <sub>5</sub>	2.29E+05	6.39E+05	1.40E+05	2.98E+05	0.00E+00	5.21E+04
389.11877	C <sub>27</sub> H <sub>18</sub> O <sub>3</sub>	2.23E+06	1.56E+06	3.54E+06	1.16E+06	0.00E+00	1.88E+03
389.16781	C <sub>15</sub> H <sub>26</sub> N <sub>4</sub> O <sub>8</sub>	3.00E+06	2.15E+06	4.49E+06	1.80E+06	1.19E+05	0.00E+00
390.98758	C <sub>15</sub> H <sub>8</sub> N <sub>2</sub> O <sub>9</sub> S	1.06E+05	1.04E+05	3.58E+03	0.00E+00	4.05E+05	0.00E+00
391.04654	C <sub>22</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>	1.97E+06	1.29E+06	0.00E+00	0.00E+00	8.17E+04	0.00E+00
393.12334	C <sub>17</sub> H <sub>22</sub> N <sub>4</sub> O <sub>5</sub> S	8.91E+04	2.38E+05	2.84E+04	1.03E+05	1.60E+04	0.00E+00
393.18986	C <sub>25</sub> H <sub>30</sub> O <sub>2</sub> S	2.08E+05	4.74E+05	1.15E+05	1.29E+05	1.43E+05	0.00E+00
395.20563	C <sub>25</sub> H <sub>32</sub> O <sub>2</sub> S	3.87E+05	5.38E+05	1.41E+05	2.91E+04	3.87E+05	0.00E+00
396.12692	C <sub>22</sub> H <sub>23</sub> NO <sub>4</sub> S	1.28E+06	4.04E+05	1.39E+06	3.08E+05	6.40E+02	0.00E+00
397.22126	C <sub>25</sub> H <sub>34</sub> O <sub>2</sub> S	4.00E+03	7.96E+03	0.00E+00	1.36E+03	3.51E+05	0.00E+00
397.22693	C <sub>18</sub> H <sub>38</sub> O <sub>7</sub> S	0.00E+00	5.67E+05	0.00E+00	0.00E+00	0.00E+00	3.57E+04
399.98536	C <sub>19</sub> H <sub>3</sub> N <sub>3</sub> O <sub>8</sub>	3.43E+03	3.55E+03	3.25E+03	0.00E+00	5.95E+05	0.00E+00
401.19496	C <sub>27</sub> H <sub>30</sub> OS	2.09E+04	7.26E+04	3.24E+03	1.91E+05	1.43E+03	0.00E+00
401.92553	C <sub>8</sub> H <sub>5</sub> NO <sub>16</sub> S	5.87E+04	1.16E+05	2.94E+05	5.73E+04	1.00E+06	6.68E+04
405.02825	C <sub>18</sub> H <sub>14</sub> O <sub>9</sub> S	1.04E+06	2.07E+04	4.30E+06	2.24E+03	0.00E+00	0.00E+00
408.20587	C <sub>18</sub> H <sub>35</sub> NO <sub>7</sub> S	7.67E+04	0.00E+00	3.48E+05	1.00E+05	0.00E+00	0.00E+00
411.11407	C <sub>28</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	4.69E+04	4.48E+03	1.59E+05	2.33E+03	0.00E+00	0.00E+00
411.15107	C <sub>29</sub> H <sub>20</sub> N <sub>2</sub> O	5.06E+03	6.73E+02	0.00E+00	4.66E+04	0.00E+00	0.00E+00
412.14727	C <sub>16</sub> H <sub>23</sub> N <sub>5</sub> O <sub>8</sub>	2.97E+04	4.82E+04	1.39E+05	6.26E+04	0.00E+00	0.00E+00
417.07574	C <sub>19</sub> H <sub>18</sub> N <sub>2</sub> O <sub>7</sub> S	0.00E+00	0.00E+00	4.31E+03	0.00E+00	2.24E+05	0.00E+00
418.91634	C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>17</sub> S	3.65E+04	3.90E+04	4.20E+04	0.00E+00	2.49E+05	1.08E+04
421.22688	C <sub>20</sub> H <sub>38</sub> O <sub>7</sub> S	0.00E+00	1.39E+05	0.00E+00	2.48E+05	0.00E+00	2.67E+04
425.08052	C <sub>12</sub> H <sub>18</sub> N <sub>4</sub> O <sub>13</sub>	0.00E+00	0.00E+00	2.07E+06	7.09E+04	0.00E+00	0.00E+00
425.18199	C <sub>21</sub> H <sub>30</sub> O <sub>9</sub>	1.16E+04	1.98E+05	8.28E+03	1.51E+04	1.50E+03	0.00E+00
427.01037	C <sub>24</sub> H <sub>4</sub> N <sub>4</sub> O <sub>5</sub>	1.50E+05	0.00E+00	5.73E+05	0.00E+00	0.00E+00	0.00E+00

429.12531	C <sub>28</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	3.30E+04	5.32E+03	1.05E+05	3.40E+03	0.00E+00	0.00E+00
430.08469	C <sub>14</sub> H <sub>17</sub> N <sub>5</sub> O <sub>11</sub>	4.65E+04	0.00E+00	0.00E+00	0.00E+00	1.07E+06	0.00E+00
431.10450	C <sub>27</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>	2.35E+06	1.87E+06	2.46E+06	1.07E+06	0.00E+00	0.00E+00
431.18995	C <sub>24</sub> H <sub>32</sub> O <sub>5</sub> S	2.21E+03	0.00E+00	1.23E+03	2.44E+03	7.91E+03	0.00E+00
433.01509	C <sub>9</sub> H <sub>14</sub> N <sub>4</sub> O <sub>14</sub> S	0.00E+00	1.87E+04	0.00E+00	0.00E+00	4.22E+05	1.37E+03
437.00424	C <sub>15</sub> H <sub>10</sub> N <sub>4</sub> O <sub>10</sub> S	6.18E+06	3.65E+06	4.11E+06	3.69E+06	2.81E+06	0.00E+00
439.07641	C <sub>25</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub> S	3.32E+07	2.27E+07	5.26E+07	1.22E+07	3.14E+05	9.72E+04
439.18249	C <sub>18</sub> H <sub>32</sub> O <sub>12</sub>	0.00E+00	1.46E+04	0.00E+00	4.52E+04	6.28E+02	0.00E+00
440.14214	C <sub>17</sub> H <sub>23</sub> N <sub>5</sub> O <sub>9</sub>	9.50E+04	2.76E+04	2.83E+05	9.06E+04	0.00E+00	0.00E+00
440.88897	C <sub>10</sub> H <sub>2</sub> O <sub>18</sub> S	5.59E+04	8.35E+04	6.45E+04	2.10E+05	0.00E+00	1.88E+04
441.17728	C <sub>22</sub> H <sub>26</sub> N <sub>4</sub> O <sub>6</sub>	4.08E+04	2.05E+05	1.39E+04	1.69E+04	1.94E+03	0.00E+00
445.17227	C <sub>21</sub> H <sub>26</sub> N <sub>4</sub> O <sub>7</sub>	2.47E+04	2.45E+04	0.00E+00	0.00E+00	1.63E+05	0.00E+00
448.99250	C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>18</sub>	8.65E+03	1.36E+03	6.36E+04	0.00E+00	0.00E+00	0.00E+00
452.92275	C <sub>16</sub> H <sub>6</sub> O <sub>12</sub> S <sub>2</sub>	3.07E+06	6.45E+05	5.89E+05	5.72E+05	1.71E+06	3.64E+04
460.20509	C <sub>18</sub> H <sub>31</sub> N <sub>5</sub> O <sub>9</sub>	3.91E+04	1.62E+03	4.38E+03	4.53E+03	0.00E+00	0.00E+00
462.97530	C <sub>14</sub> H <sub>12</sub> N <sub>2</sub> O <sub>12</sub> S <sub>2</sub>	9.49E+04	2.60E+04	1.28E+05	1.51E+04	6.61E+04	0.00E+00
468.89694	C <sub>19</sub> H <sub>2</sub> O <sub>11</sub> S <sub>2</sub>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.07E+04
469.91311	C <sub>15</sub> H <sub>5</sub> NO <sub>13</sub> S <sub>2</sub>	2.21E+04	1.79E+04	3.02E+04	1.43E+04	1.99E+05	6.34E+03
472.16666	C <sub>30</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub>	1.99E+05	1.13E+06	1.64E+06	1.71E+04	1.22E+04	0.00E+00
477.17260	C <sub>32</sub> H <sub>22</sub> N <sub>4</sub> O	3.54E+06	1.14E+06	3.25E+06	8.53E+05	0.00E+00	0.00E+00
482.92876	C <sub>11</sub> H <sub>4</sub> N <sub>2</sub> O <sub>20</sub>	0.00E+00	0.00E+00	2.38E+05	2.59E+05	0.00E+00	7.02E+04
485.25369	C <sub>28</sub> H <sub>38</sub> O <sub>7</sub>	4.00E+06	2.46E+06	2.98E+06	3.30E+05	1.47E+06	0.00E+00
486.17769	C <sub>26</sub> H <sub>25</sub> N <sub>5</sub> O <sub>5</sub>	1.49E+05	3.90E+04	2.32E+05	2.39E+05	0.00E+00	0.00E+00
495.18268	C <sub>32</sub> H <sub>24</sub> N <sub>4</sub> O <sub>2</sub>	2.70E+07	6.55E+06	1.64E+07	3.33E+06	0.00E+00	8.60E+03
496.18686	C <sub>29</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub>	2.33E+04	6.48E+04	2.96E+03	4.49E+03	0.00E+00	0.00E+00
503.16162	C <sub>31</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub>	6.76E+06	6.45E+06	2.18E+07	1.28E+07	1.95E+05	3.69E+04
507.17265	C <sub>22</sub> H <sub>28</sub> N <sub>4</sub> O <sub>10</sub>	0.00E+00	5.63E+02	5.71E+02	9.16E+03	0.00E+00	0.00E+00
514.89363	C <sub>10</sub> H <sub>4</sub> N <sub>4</sub> O <sub>17</sub> S <sub>2</sub>	3.07E+05	1.15E+06	2.93E+05	3.80E+05	5.44E+05	1.90E+04
520.91078	C <sub>18</sub> H <sub>2</sub> O <sub>19</sub>	1.59E+05	8.32E+04	1.58E+05	6.30E+04	3.34E+05	5.12E+03
542.24773	C <sub>23</sub> H <sub>37</sub> N <sub>5</sub> O <sub>10</sub>	0.00E+00	4.62E+04	0.00E+00	0.00E+00	7.00E+05	0.00E+00
549.16775	C <sub>32</sub> H <sub>26</sub> N <sub>2</sub> O <sub>7</sub>	1.26E+05	7.97E+04	4.30E+04	0.00E+00	5.78E+04	3.71E+03
563.17242	C <sub>22</sub> H <sub>32</sub> N <sub>2</sub> O <sub>15</sub>	1.32E+06	3.27E+05	7.40E+05	3.59E+05	0.00E+00	0.00E+00
571.15098	C <sub>34</sub> H <sub>24</sub> N <sub>2</sub> O <sub>7</sub>	1.48E+03	1.64E+03	5.35E+04	1.95E+04	0.00E+00	0.00E+00
583.17570	C <sub>37</sub> H <sub>28</sub> O <sub>7</sub>	3.00E+07	7.18E+06	1.30E+03	0.00E+00	9.10E+04	0.00E+00
584.17867	C <sub>30</sub> H <sub>27</sub> N <sub>5</sub> O <sub>8</sub>	4.85E+06	7.63E+05	0.00E+00	0.00E+00	0.00E+00	0.00E+00

587.29238	C <sub>38</sub> H <sub>40</sub> N <sub>2</sub> O <sub>4</sub>	3.97E+05	5.12E+05	4.89E+03	3.06E+05	6.42E+05	0.00E+00
603.11023	C <sub>26</sub> H <sub>24</sub> N <sub>2</sub> O <sub>15</sub>	1.63E+05	1.89E+05	5.49E+04	3.38E+04	1.96E+03	0.00E+00
605.08690	C <sub>29</sub> H <sub>22</sub> N <sub>2</sub> O <sub>11</sub> S	0.00E+00	2.71E+04	3.46E+04	6.20E+04	0.00E+00	9.36E+03
605.15748	C <sub>34</sub> H <sub>26</sub> N <sub>2</sub> O <sub>9</sub>	1.40E+07	7.32E+06	0.00E+00	0.00E+00	4.66E+05	0.00E+00
617.15755	C <sub>35</sub> H <sub>26</sub> N <sub>2</sub> O <sub>9</sub>	1.29E+05	3.88E+05	2.08E+06	2.67E+06	0.00E+00	0.00E+00
617.15795	C <sub>23</sub> H <sub>30</sub> N <sub>4</sub> O <sub>16</sub>	1.73E+04	9.64E+04	8.38E+05	1.04E+06	0.00E+00	0.00E+00
646.21677	C <sub>19</sub> H <sub>41</sub> N <sub>3</sub> O <sub>21</sub>	3.25E+04	1.02E+03	2.00E+05	6.08E+03	0.00E+00	0.00E+00
656.21228	C <sub>19</sub> H <sub>39</sub> N <sub>5</sub> O <sub>20</sub>	4.68E+04	2.25E+04	2.63E+05	3.75E+05	6.28E+03	0.00E+00
664.35485	C <sub>44</sub> H <sub>47</sub> N <sub>3</sub> O <sub>3</sub>	4.39E+05	4.57E+05	3.43E+05	1.88E+05	0.00E+00	0.00E+00
665.21734	C <sub>34</sub> H <sub>38</sub> N <sub>2</sub> O <sub>10</sub> S	2.15E+06	1.84E+06	1.53E+06	2.65E+06	1.07E+05	0.00E+00
678.39137	C <sub>42</sub> H <sub>53</sub> N <sub>3</sub> O <sub>5</sub>	6.30E+04	6.24E+04	2.49E+05	6.29E+04	2.74E+05	2.61E+04
679.21702	C <sub>22</sub> H <sub>40</sub> N <sub>4</sub> O <sub>20</sub>	5.02E+04	2.83E+04	2.26E+05	1.93E+05	6.90E+04	0.00E+00
683.22911	C <sub>42</sub> H <sub>36</sub> O <sub>9</sub>	1.23E+07	7.62E+06	8.79E+06	3.37E+05	0.00E+00	0.00E+00
683.22942	C <sub>30</sub> H <sub>40</sub> N <sub>2</sub> O <sub>16</sub>	0.00E+00	0.00E+00	1.89E+06	3.14E+05	0.00E+00	0.00E+00
695.00464	C <sub>24</sub> H <sub>16</sub> N <sub>4</sub> O <sub>19</sub> S	2.92E+05	4.91E+05	1.87E+05	2.10E+05	0.00E+00	0.00E+00
711.22397	C <sub>35</sub> H <sub>40</sub> N <sub>2</sub> O <sub>12</sub> S	7.89E+05	1.95E+05	1.10E+06	1.30E+05	0.00E+00	1.75E+03
711.22466	C <sub>31</sub> H <sub>40</sub> N <sub>2</sub> O <sub>17</sub>	1.82E+06	1.57E+06	1.69E+06	1.36E+06	6.64E+03	0.00E+00
722.24279	C <sub>32</sub> H <sub>41</sub> N <sub>3</sub> O <sub>16</sub>	2.77E+05	3.10E+05	2.02E+05	9.72E+04	4.60E+04	0.00E+00
722.24340	C <sub>20</sub> H <sub>45</sub> N <sub>5</sub> O <sub>23</sub>	9.98E+04	2.23E+05	3.44E+04	1.45E+04	1.90E+05	0.00E+00
733.20638	C <sub>28</sub> H <sub>38</sub> N <sub>4</sub> O <sub>19</sub>	4.92E+03	1.20E+03	2.46E+04	4.21E+05	0.00E+00	0.00E+00
737.23999	C <sub>33</sub> H <sub>42</sub> N <sub>2</sub> O <sub>17</sub>	1.37E+04	7.92E+03	6.35E+04	3.05E+05	3.28E+04	0.00E+00
737.74171	C <sub>49</sub> H <sub>94</sub> N <sub>4</sub>	5.61E+03	5.94E+03	2.38E+04	1.60E+05	1.09E+04	0.00E+00