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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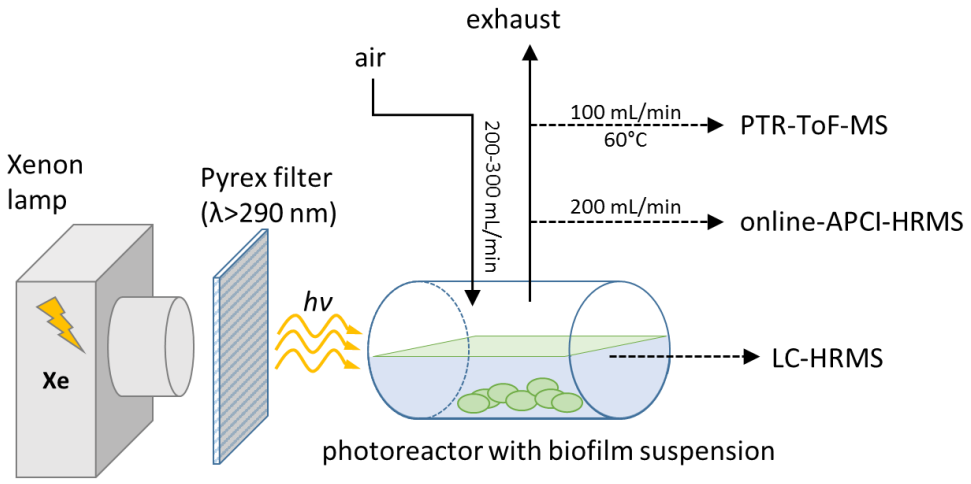

Fig. S-1: Schematic of the experimental setup. A Xenon lamp was used to irradiate the biofilm-containing photoreactor. To mimic solar irradiation at the Earth's surface, a Pyrex filter was used to cut wavelength below 290 nm. Purified air was pushed through the reactor at flow rates of 200–300 mL min^{-1}. 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^{-1} from the major flow through a heated inlet (60 °C). Liquid phase samples were taken before and after irradiation and analyzed by UHPLC-HRMS.

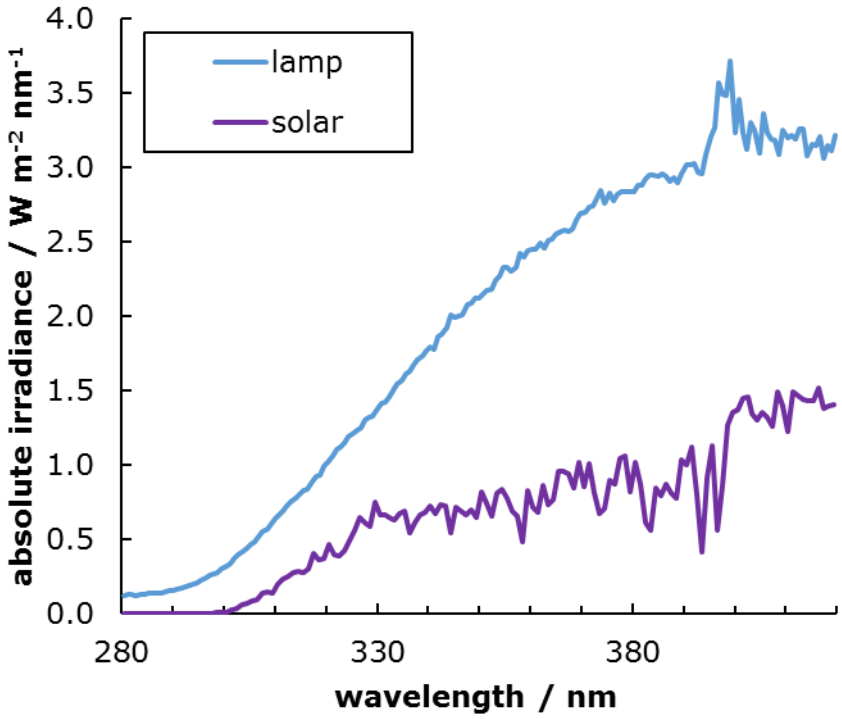

Fig. S-2: Absolute irradiance as function of wavelength for the actinic solar spectrum (calculated using the Tropospheric Ultraviolet and Visible (TUV) Radiation Model version 5.2; http://cprm.acom.ucar.edu/Models/TUV/Interactive_TUV) and the xenon lamp with Pyrex filter used for irradiation of the biofilm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

biofilm sample type	biofilm origin	laboratory growth phase (from – to)		dry biomass (g L^{-1})
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 mW·cm^{-2} in the wavelength range of 280–420 nm. Ambient VOC fluxes are calculated for a mean solar flux of 9.2 mW·cm–2 in the same wavelength range.

m/z **([M+H]$^+$)**			**biofilm (day 6)**			**biofilm (day 5)**			**dead**			**ground water**		
APCI-HRMS	**PTR-TOF-MS**	**assigned formula**	**mixing ratio / ppb**	**production / 10^7 molec. mW^{-1} s^{-1}**	**flux (ambient) / 10^7 molec. cm^{-2} s^{-1}**	**mixing ratio / ppb**	**production / 10^7 molec. mW^{-1} s^{-1}**	**flux (ambient) / 10^7 molec. cm^{-2} s^{-1}**	**mixing ratio / ppb**	**production / 10^7 molec. mW^{-1} s^{-1}**	**flux (ambient) / 10^7 molec. cm^{-2} s^{-1}**	**mixing ratio / ppb**	**production / 10^7 molec. mW^{-1} s^{-1}**	**flux (ambient) / 10^7 molec. cm^{-2} s^{-1}**
	31.019	CH_2O (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_4O (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_3H_4	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_2H_3N (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_2H_2O (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_3H_6	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_2H_3O	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_2H_4O (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_2H_6O (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_4S	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_6O_2	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_3H_5N	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_3H_4O	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_4H_8	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_3H_7N	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_3H_6O (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_3H_9N	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	$C_2H_4O_2$	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	$C_2H_6O_2$	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_5H_4	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_5H_6	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_4H_5N	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_5H_8 (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_4H_7N	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_4H_6O	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_5H_{10}	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_3H_5NO	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	$C_3H_4O_2$	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_4H_8O	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	$C_3H_8O_2$	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_6H_6	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_6H_8	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_5H_6O	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_6H_{10}	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_4H_5NO	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_5H_9N	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_5H_8O	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	$C_4H_6O_2$	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	$C_5H_{10}O$	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_7H_8	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_7H_{10}	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_6H_8O	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_7H_{12}	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	$C_6H_{10}O$	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	$C_5H_8O_2$	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	$C_6H_{12}O$	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_7H_6O	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_8H_{10}	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_6H_5NO	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_8H_{12}	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	$C_7H_{10}O$	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_8H_{14}	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	$C_7H_{12}O$	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	$C_7H_{14}O$	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_8H_8O	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	$C_5H_{12}O_3$	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_9H_{14}	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	$C_8H_{12}O$	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	$C_8H_{14}O$	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	$C_8H_{16}O$	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	$C_9H_{10}O$	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	$C_9H_{12}O$	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	$C_9H_{14}O$	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	$C_8H_{12}O_2$	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	$C_9H_{16}O$	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	$C_9H_{18}O$	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	$C_{10}H_{14}O$	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	$C_{10}H_{16}O$	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]$^+$)			cellular fraction			capsular fraction			colloidal fraction		
APCI-HRMS	PTR-TOF-MS	assigned formula	mixing ratio / ppb	production / 10^7 molec. mW^{-1} s^{-1}	flux (ambient) / 10^7 molec. cm^{-2} s^{-1}	mixing ratio / ppb	production / 10^7 molec. mW^{-1} s^{-1}	flux (ambient) / 10^7 molec. cm^{-2} s^{-1}	mixing ratio / ppb	production / 10^7 molec. mW^{-1} s^{-1}	flux (ambient) / 10^7 molec. cm^{-2} s^{-1}
	31.019	CH_2O (formaldehyde)	0.191	5.653	51.855	0.101	2.985	27.383	0.038	1.128	10.344
	33.034	CH_4O (methanol)	3.114	92.201	845.774	4.114	121.804	1117.325	0.201	5.950	54.577
	41.038	C_3H_4	1.973	58.422	535.914	1.493	44.204	405.489	0.391	11.575	106.175
	42.034	C_2H_3N (acetonitrile)	0.930	27.539	252.621	11.648	344.882	3163.642	1.834	54.291	498.021
	43.017	C_2H_2O (ketene)	1.230	36.419	334.080	0.664	19.653	180.278	0.368	10.910	100.078
	43.054	C_3H_6	0.557	16.490	151.266	0.341	10.110	92.737	0.102	3.035	27.837
	44.022	C_2H_3O	0.041	1.224	11.227	0.021	0.614	5.631	0.022	0.647	5.939
	45.032	C_2H_4O (acetaldehyde)	4.411	130.623	1198.218	3.420	101.268	928.947	2.064	61.101	560.487
	47.048	C_2H_6O (ethanol)	0.303	8.986	82.429	0.192	5.681	52.114	0.025	0.747	6.850
	49.010	CH_4S	0.059	1.748	16.033	0.031	0.905	8.301	0.011	0.339	3.111
51.0611	51.043	CH_6O_2	0.206	6.092	55.886	0.287	8.486	77.847	0.026	0.763	6.996
*56.0496	56.054	C_3H_5N	0.129	3.816	35.006	0.075	2.210	20.277	0.025	0.752	6.898
57.0336	57.032	C_3H_4O	5.850	173.226	1589.020	2.007	59.434	545.200	0.593	17.573	161.198
57.0700	57.067	C_4H_8	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_3H_7N	0.060	1.784	16.367	0.030	0.883	8.103	0.007	0.212	1.945
59.0492	59.047	C_3H_6O (acetone)	9.727	288.008	2641.932	6.858	203.068	1862.765	6.521	193.085	1771.192
60.0808	60.079	C_3H_9N	0.071	2.103	19.291	-	-	-	-	-	-
61.0284	61.026	$C_2H_4O_2$	0.186	5.507	50.513	0.217	6.437	59.043	0.165	4.896	44.914
63.0441	63.041	$C_2H_6O_2$	0.075	2.225	20.408	0.066	1.946	17.850	0.040	1.173	10.759
65.0385	65.021	C_5H_4	0.018	0.526	4.822	0.018	0.520	4.774	0.026	0.765	7.016
67.0542	67.051	C_5H_6	0.825	24.416	223.968	0.310	9.188	84.284	0.104	3.070	28.158

68.0495	68.048	C_4H_5N	0.107	3.155	28.937	0.031	0.922	8.457	0.012	0.347	3.184
69.0698	69.067	C_5H_8 (isoprene)	3.439	101.829	934.087	3.191	94.485	866.726	0.574	16.992	155.870
70.0651	70.061	C_4H_7N	3.531	104.544	958.990	0.971	28.742	263.651	0.343	10.159	93.187
71.0491	71.045	C_4H_6O	2.734	80.963	742.687	0.341	10.100	92.647	0.105	3.108	28.507
71.0855	71.077	C_5H_{10}	0.252	7.456	68.398	0.094	2.797	25.656	0.019	0.572	5.248
72.0443	72.046	C_3H_5NO	0.155	4.603	42.228	0.027	0.792	7.269	0.009	0.279	2.558
73.0284	73.024	$C_3H_4O_2$	0.023	0.687	6.305	0.013	0.398	3.655	0.016	0.481	4.413
73.0648	73.061	C_4H_8O	0.650	19.254	176.621	0.686	20.315	186.350	0.185	5.477	50.239
77.0597	77.055	$C_3H_8O_2$	0.075	2.207	20.244	0.046	1.351	12.391	0.024	0.697	6.392
79.0542	79.050	C_6H_6	0.078	2.303	21.129	0.057	1.702	15.609	0.021	0.630	5.778
81.0698	81.065	C_6H_8	0.670	19.853	182.113	0.362	10.705	98.199	0.115	3.397	31.161
83.0491	83.044	C_5H_6O	0.096	2.855	26.190	0.030	0.878	8.051	0.013	0.380	3.484
83.0855	83.080	C_6H_{10}	1.745	51.669	473.966	0.560	16.575	152.043	0.144	4.254	39.027
84.0444	84.049	C_4H_5NO	0.055	1.614	14.809	0.026	0.767	7.039	0.013	0.395	3.626
84.0807	84.082	C_5H_9N	0.153	4.521	41.467	0.046	1.353	12.408	0.015	0.445	4.078
85.0647	85.059	C_5H_8O	5.547	164.253	1506.709	3.153	93.360	856.403	1.229	36.380	333.715
87.0440	87.039	$C_4H_6O_2$	0.073	2.172	19.924	0.032	0.937	8.595	0.021	0.632	5.793
87.0804	87.075	$C_5H_{10}O$	0.679	20.118	184.547	0.905	26.810	245.934	0.200	5.907	54.190
93.0698	93.063	C_7H_8	0.102	3.019	27.696	0.037	1.100	10.089	0.010	0.290	2.660
95.0855	95.079	C_7H_{10}	0.720	21.312	195.495	0.118	3.509	32.184	0.027	0.789	7.239
97.0648	97.059	C_6H_8O	0.070	2.081	19.086	0.034	1.005	9.223	0.036	1.052	9.654
97.1011	97.094	C_7H_{12}	0.562	16.654	152.769	0.108	3.190	29.258	0.041	1.223	11.216
99.0804	99.074	$C_6H_{10}O$	0.474	14.048	128.865	0.207	6.135	56.281	0.072	2.129	19.530
101.0597	101.052	$C_5H_8O_2$	0.102	3.016	27.665	0.072	2.123	19.479	0.032	0.944	8.664
101.0960	101.088	$C_6H_{12}O$	0.289	8.571	78.627	0.111	3.275	30.043	0.048	1.413	12.959
107.0491	107.042	C_7H_6O	0.352	10.431	95.682	0.417	12.353	113.315	0.100	2.952	27.075
107.0855	107.077	C_8H_{10}	0.184	5.458	50.067	0.125	3.696	33.904	0.030	0.889	8.155
108.0443	108.043	C_6H_5NO	0.027	0.810	7.435	0.033	0.986	9.044	0.007	0.221	2.028
109.1011	109.093	C_8H_{12}	1.390	41.158	377.546	0.224	6.628	60.799	0.030	0.895	8.211
111.0804	111.072	$C_7H_{10}O$	1.233	36.509	334.902	0.417	12.334	113.137	0.091	2.688	24.660

111.1168	111.104	C_8H_{14}	0.355	10.523	96.530	0.085	2.504	22.967	0.027	0.792	7.262
113.0960	113.088	$C_7H_{12}O$	0.776	22.986	210.857	0.125	3.691	33.862	0.024	0.722	6.627
115.1117	115.102	$C_7H_{14}O$	0.133	3.947	36.202	0.021	0.614	5.634	0.012	0.349	3.201
121.0647	121.056	C_8H_8O	0.084	2.484	22.783	0.070	2.075	19.035	0.028	0.825	7.565
121.0858	121.085	$C_5H_{12}O_3$	0.025	0.747	6.854	0.015	0.451	4.137	0.007	0.201	1.843
123.1167	123.106	C_9H_{14}	0.081	2.389	21.913	0.018	0.541	4.961	0.005	0.158	1.448
125.0960	125.087	$C_8H_{12}O$	0.779	23.053	211.465	0.398	11.773	107.999	0.097	2.865	26.277
127.1116	127.101	$C_8H_{14}O$	1.423	42.144	386.596	0.270	7.991	73.303	0.028	0.825	7.572
129.1273	129.116	$C_8H_{16}O$	0.093	2.748	25.206	0.022	0.666	6.110	0.013	0.398	3.654
135.0803	135.075	$C_9H_{10}O$	0.017	0.489	4.484	0.025	0.726	6.659	0.014	0.407	3.735
137.0960	137.084	$C_9H_{12}O$	0.115	3.412	31.298	0.049	1.451	13.311	0.009	0.263	2.417
139.1116	139.108	$C_9H_{14}O$	0.049	1.439	13.200	0.010	0.287	2.634	0.001	0.024	0.222
141.0909	141.079	$C_8H_{12}O_2$	0.028	0.836	7.666	0.013	0.378	3.471	0.005	0.156	1.432
141.1273	141.112	$C_9H_{16}O$	0.062	1.827	16.756	0.012	0.350	3.210	0.004	0.121	1.110
143.1429	143.128	$C_9H_{18}O$	0.060	1.767	16.209	0.012	0.368	3.371	0.008	0.243	2.231
151.1116	151.099	$C_{10}H_{14}O$	0.047	1.385	12.701	0.015	0.454	4.164	0.002	0.065	0.599
153.1273	153.114	$C_{10}H_{16}O$	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).

1) Project / Set preferences		
m/z value format	5 decimals	
Retention time value format	2 decimals	
Intensity format	1 decimal with exponent	
2) Raw data methods / Peak detection / Mass detection		
Mass detector	exact mass	
	Noise level	10^4
MS level	1	
3) Raw data methods / Peak detection / FTMS shoulder peaks filter		
Mass resolution	140000	
Peak model function	gaussian	
4) Raw data methods / Peak detection / Chromatogram builder		
Min time span	0.1	
Min height	$5 \cdot 10^4$	
m/z tolerance	0.0001 m/z or 2 ppm	
5) Smoothing		
Filter width	7	
6) Peak list methods / Peak detection / Chromatogram deconvolution		
Peak resolver	Local minimum search	
	Chromatographic threshold	85%
	Search minimum in RT range	0.1
	Minimum relative height	5%
	Minimum absolute height	$5 \cdot 10^4$
	Min ratio of peak top/edge	1.6
	Peak duration range (min)	0.1 - 10
7) Peak list methods / Isotopes / Isotopic peaks grouper		
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	
8) Adduct search		
retention time tolerance	0.2 min	
adducts	[M+acetonitrile+H]	41.0266
	[M-H+CH2O2]	46.0055
	[M-H+CHO2Na]	67.9869
m/z tolerance	0.0001 m/z or 2 ppm	
max relative adduct peak height	100%	
9) Complex search		
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%	
10) Join aligner		
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	10^3	
minimum score	70%	
11) Gap filling		
intensity tolerance	10%	
m/z tolerance	0.0001 m/z or 2 ppm	
retention time tolerance	0.2 min	
RT correction	no	
12) Formula prediction		
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	10^3	
minimum score	70%	
13) Duplicate peak filter		
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	$C_2H_4O_2$	8.85E+05	1.33E+07	8.55E+06	2.67E+06	4.83E+06	2.10E+04
69.03467	C_4H_6O	1.95E+05	3.08E+05	8.36E+04	1.03E+05	3.27E+03	1.12E+03
71.01389	$C_3H_4O_2$	1.12E+06	9.88E+06	1.08E+07	2.17E+06	2.51E+05	2.45E+04
73.02949	$C_3H_6O_2$	2.37E+06	9.52E+05	3.20E+06	2.00E+05	4.80E+04	2.17E+03
74.02483	$C_2H_5NO_2$	1.92E+06	3.30E+06	2.23E+06	1.45E+06	1.36E+05	0.00E+00
78.98600	CH_4O_2S	0.00E+00	8.88E+03	2.19E+03	4.44E+04	6.63E+05	1.09E+03
83.05032	C_5H_8O	2.49E+05	3.26E+05	7.32E+04	5.88E+04	0.00E+00	2.16E+03
84.00915	$C_3H_3NO_2$	0.00E+00	2.74E+06	5.83E+06	0.00E+00	2.34E+06	7.10E+05
85.02955	$C_4H_6O_2$	2.40E+06	2.17E+06	1.44E+06	3.93E+05	4.70E+04	0.00E+00

85.06597	$C_5H_{10}O$	9.36E+04	3.95E+04	1.67E+05	2.64E+03	1.38E+06	8.79E+02
87.00882	$C_3H_4O_3$	3.67E+06	5.43E+06	2.55E+06	5.82E+05	5.96E+05	5.65E+04
89.02451	$C_3H_6O_3$	4.55E+07	4.37E+07	4.57E+07	1.40E+07	2.76E+08	1.01E+06
91.05539	C_7H_8	1.57E+06	7.11E+05	1.20E+06	8.22E+04	3.47E+06	0.00E+00
94.98090	CH_4O_3S	1.21E+05	5.52E+05	3.85E+05	2.30E+05	1.39E+06	3.34E+04
99.00873	$C_4H_4O_3$	1.06E+06	7.68E+05	1.22E+06	7.51E+04	2.57E+06	3.84E+04
101.02446	$C_4H_6O_3$	9.39E+06	7.32E+06	2.37E+07	2.30E+06	8.83E+05	8.04E+04
101.06088	$C_5H_{10}O_2$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.39E+05	0.00E+00
102.03097	$C_2H_5N_3O_2$	8.21E+03	3.50E+03	9.10E+04	1.03E+04	6.60E+05	6.01E+02
102.05610	$C_4H_9NO_2$	2.68E+03	3.62E+03	3.32E+04	0.00E+00	9.96E+05	0.00E+00
103.00376	$C_3H_4O_4$	1.79E+07	1.57E+07	4.99E+06	1.85E+06	2.46E+07	3.05E+04
103.04013	$C_4H_8O_3$	6.44E+07	5.44E+07	2.80E+07	1.94E+07	7.02E+05	6.47E+04
104.03544	$C_3H_7NO_3$	2.18E+07	3.17E+07	2.75E+07	1.67E+07	3.49E+05	5.40E+04
107.03506	$C_3H_8O_4$	2.33E+05	2.50E+05	1.02E+05	5.28E+04	0.00E+00	0.00E+00
107.05035	C_7H_8O	1.46E+03	5.30E+03	2.04E+03	1.29E+03	3.90E+05	0.00E+00
111.00883	$C_5H_4O_3$	1.88E+07	7.65E+06	3.01E+07	6.39E+05	4.38E+03	9.41E+03
111.02007	$C_4H_4N_2O_2$	3.53E+07	1.85E+07	1.81E+07	3.74E+06	1.36E+07	9.74E+04
111.04520	$C_6H_8O_2$	7.69E+05	2.68E+05	6.08E+05	8.37E+04	1.50E+04	1.49E+03
111.08167	$C_7H_{12}O$	1.54E+03	5.79E+05	0.00E+00	1.85E+05	0.00E+00	0.00E+00
112.01533	$C_3H_3N_3O_2$	4.93E+04	9.98E+03	7.32E+04	1.56E+04	4.32E+05	0.00E+00
112.04051	$C_5H_7NO_2$	0.00E+00	2.10E+05	8.09E+04	1.12E+04	8.69E+05	0.00E+00
113.02450	$C_5H_6O_3$	1.66E+07	1.48E+07	1.96E+07	6.26E+06	3.79E+05	1.11E+05
113.06091	$C_6H_{10}O_2$	3.45E+04	1.16E+05	0.00E+00	1.01E+04	1.09E+06	3.37E+03
114.03096	$C_3H_5N_3O_2$	1.29E+05	2.65E+04	2.84E+05	5.98E+04	1.99E+06	0.00E+00
115.00371	$C_4H_4O_4$	2.09E+07	1.25E+07	2.22E+07	5.56E+06	2.57E+03	1.45E+05
115.04012	$C_5H_8O_3$	1.25E+07	5.95E+06	1.61E+07	1.20E+06	3.90E+07	4.73E+04
116.07175	$C_5H_{11}NO_2$	2.41E+04	2.36E+04	2.73E+04	3.87E+04	9.56E+05	0.00E+00
117.01937	$C_4H_6O_4$	2.73E+07	1.36E+07	5.65E+07	7.76E+06	1.62E+04	3.56E+05
117.05572	$C_5H_{10}O_3$	3.36E+06	2.56E+07	2.06E+06	8.24E+05	8.89E+05	4.90E+04
118.00478	C_5HN_3O	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.99E+04
118.05106	$C_4H_9NO_3$	7.30E+06	1.67E+07	3.74E+06	4.50E+06	5.87E+05	2.88E+04
119.03501	$C_4H_8O_4$	1.72E+07	1.59E+07	1.63E+07	4.32E+06	1.55E+06	4.72E+04
119.05028	C_8H_8O	1.74E+05	1.95E+05	7.80E+04	2.06E+04	1.50E+03	0.00E+00
120.01248	$C_3H_7NO_2S$	1.66E+05	7.92E+04	1.09E+05	2.70E+04	0.00E+00	0.00E+00
121.02956	$C_7H_6O_2$	7.69E+06	4.84E+06	1.23E+07	1.76E+06	5.60E+06	2.75E+05

121.10236	C_9H_{14}	2.38E+05	4.72E+05	6.56E+04	1.04E+05	1.27E+04	0.00E+00
122.02469	$C_6H_5NO_2$	1.81E+05	3.85E+04	2.71E+05	1.13E+05	0.00E+00	9.34E+03
122.02479	$C_6H_5NO_2$	1.32E+05	1.55E+04	7.39E+05	2.62E+04	0.00E+00	4.19E+03
122.97568	$C_2H_4O_4S$	9.79E+04	1.23E+05	1.97E+06	0.00E+00	1.21E+05	3.59E+04
123.08163	$C_8H_{12}O$	5.43E+05	1.02E+06	2.08E+05	2.45E+05	1.00E+04	0.00E+00
125.03568	$C_5H_6N_2O_2$	9.32E+05	5.05E+05	3.43E+05	1.17E+05	2.35E+06	1.91E+04
126.01973	$C_5H_5NO_3$	2.29E+05	0.00E+00	1.52E+06	3.85E+05	8.28E+05	3.93E+03
126.05611	$C_6H_9NO_2$	1.48E+05	7.43E+03	0.00E+00	9.81E+03	1.82E+04	0.00E+00
127.02625	$C_3H_4N_4O_2$	0.00E+00	0.00E+00	1.29E+03	0.00E+00	4.00E+04	0.00E+00
127.04018	$C_6H_8O_3$	2.20E+05	4.26E+05	1.37E+05	1.83E+05	3.97E+04	4.76E+03
127.07645	$C_7H_{12}O_2$	9.06E+04	2.45E+06	3.51E+05	8.39E+03	5.10E+05	3.43E+04
128.03537	$C_5H_7NO_3$	3.50E+08	2.03E+08	1.52E+08	9.71E+07	5.54E+08	2.24E+05
128.07177	$C_6H_{11}NO_2$	5.68E+05	2.56E+05	1.76E+05	2.32E+04	3.41E+05	0.00E+00
128.08305	$C_5H_{11}N_3O$	0.00E+00	2.27E+04	3.78E+04	3.39E+04	3.62E+05	0.00E+00
129.01937	$C_5H_6O_4$	3.22E+07	1.36E+07	1.60E+07	1.02E+06	9.25E+05	1.48E+05
129.05580	$C_6H_{10}O_3$	1.28E+07	2.69E+07	7.53E+07	5.81E+06	3.94E+08	9.56E+04
129.97579	C_7HNS	0.00E+00	1.86E+06	3.55E+05	1.01E+06	2.05E+06	2.78E+05
130.05097	$C_5H_9NO_3$	1.58E+05	4.00E+06	3.45E+06	9.06E+05	1.08E+07	5.26E+03
130.08734	$C_6H_{13}NO_2$	1.55E+06	2.40E+06	3.51E+05	7.83E+04	4.71E+05	5.81E+02
131.00989	$C_3H_4N_2O_4$	2.63E+04	6.43E+04	7.40E+05	2.01E+05	2.70E+06	0.00E+00
131.03500	$C_5H_8O_4$	4.55E+06	4.81E+06	2.84E+06	4.37E+05	8.55E+06	4.81E+04
131.04627	$C_4H_8N_2O_3$	1.04E+06	7.76E+06	3.77E+05	1.24E+06	1.67E+05	0.00E+00
131.07138	$C_6H_{12}O_3$	1.32E+06	1.14E+06	9.24E+05	1.53E+05	1.67E+06	8.59E+04
131.08262	$C_5H_{12}N_2O_2$	3.40E+06	4.58E+06	4.73E+06	3.56E+06	3.35E+06	1.28E+04
132.03028	$C_4H_7NO_4$	1.79E+08	2.24E+08	1.52E+08	4.80E+07	1.81E+06	3.51E+05
132.04151	$C_3H_7N_3O_3$	6.87E+05	6.19E+05	1.84E+06	2.23E+05	9.14E+05	0.00E+00
133.01429	$C_4H_6O_5$	2.05E+08	1.72E+08	2.17E+08	6.44E+07	1.24E+06	4.36E+05
134.04730	$C_5H_5N_5$	0.00E+00	4.80E+06	2.42E+03	1.66E+06	0.00E+00	5.01E+04
135.03127	$C_5H_4N_4O$	4.04E+07	3.73E+07	2.33E+07	1.74E+07	0.00E+00	1.60E+04
137.03567	$C_6H_6N_2O_2$	2.60E+05	6.39E+04	2.90E+05	4.18E+05	3.20E+06	8.01E+04
137.09727	$C_9H_{14}O$	8.42E+04	2.83E+05	7.26E+03	6.93E+03	4.68E+03	0.00E+00
139.07649	$C_8H_{12}O_2$	2.47E+05	7.49E+05	3.62E+05	1.16E+05	1.80E+06	1.65E+03
140.01022	$C_4H_3N_3O_3$	0.00E+00	0.00E+00	3.66E+04	1.28E+04	1.06E+06	0.00E+00
141.05585	$C_7H_{10}O_3$	5.06E+03	3.55E+05	0.00E+00	2.33E+04	2.92E+03	1.11E+03
141.09217	$C_8H_{14}O_2$	1.49E+03	2.77E+04	0.00E+00	0.00E+00	3.81E+05	0.00E+00

142.05093	$C_6H_9NO_3$	6.11E+05	2.80E+05	2.96E+05	3.24E+04	0.00E+00	2.25E+03
142.08736	$C_7H_{13}NO_2$	1.56E+06	8.83E+05	2.43E+05	7.83E+04	9.89E+05	0.00E+00
142.98084	$C_5H_4O_3S$	2.92E+05	1.14E+05	2.17E+05	1.72E+06	7.52E+06	1.96E+04
143.03497	$C_6H_8O_4$	1.23E+07	1.13E+07	1.03E+07	2.26E+06	6.69E+04	2.35E+03
143.07140	$C_7H_{12}O_3$	2.15E+06	4.42E+06	9.58E+05	8.25E+05	1.22E+06	9.06E+03
144.04550	C_9H_7NO	6.50E+06	4.07E+06	1.23E+07	1.51E+06	5.88E+06	1.77E+04
144.06668	$C_6H_{11}NO_3$	1.26E+04	5.29E+04	9.00E+03	1.97E+04	1.77E+03	0.00E+00
144.07787	$C_5H_{11}N_3O_2$	2.53E+05	1.46E+06	7.47E+05	1.76E+06	6.99E+06	4.97E+03
145.01428	$C_5H_6O_5$	1.27E+06	1.61E+05	8.05E+06	8.88E+04	1.81E+03	0.00E+00
145.03669	$C_3H_6N_4O_3$	8.24E+04	3.26E+04	1.45E+06	1.50E+05	3.96E+06	0.00E+00
145.05066	$C_6H_{10}O_4$	0.00E+00	3.48E+06	0.00E+00	0.00E+00	0.00E+00	7.86E+04
145.08705	$C_7H_{14}O_3$	0.00E+00	1.86E+06	0.00E+00	0.00E+00	0.00E+00	5.04E+05
147.01219	$C_5H_8O_3S$	8.25E+05	6.23E+05	9.94E+05	5.15E+04	2.56E+06	0.00E+00
147.02992	$C_5H_8O_5$	5.71E+06	1.12E+06	4.08E+06	2.06E+05	1.86E+06	4.09E+03
147.06625	$C_6H_{12}O_4$	1.66E+05	1.21E+05	5.73E+05	5.25E+04	5.02E+06	1.07E+04
147.08149	$C_{10}H_{12}O$	1.49E+05	5.55E+04	3.59E+05	6.54E+03	0.00E+00	0.00E+00
148.04384	$C_5H_{11}NO_2S$	1.76E+06	1.32E+06	5.42E+05	5.69E+05	6.77E+04	0.00E+00
149.02443	$C_8H_6O_3$	2.66E+04	5.84E+04	2.35E+05	0.00E+00	7.32E+05	1.20E+04
149.09720	$C_{10}H_{14}O$	1.46E+06	2.47E+06	2.30E+05	3.41E+05	0.00E+00	0.00E+00
150.04219	$C_5H_5N_5O$	0.00E+00	1.45E+06	0.00E+00	1.24E+06	0.00E+00	0.00E+00
151.02615	$C_5H_4N_4O_2$	2.45E+08	2.73E+08	8.26E+07	1.15E+08	2.30E+07	1.55E+03
151.04007	$C_8H_8O_3$	7.84E+04	2.78E+05	6.16E+05	5.75E+04	1.97E+06	8.31E+03
152.03533	$C_7H_7NO_3$	9.68E+03	2.84E+03	2.55E+03	4.98E+03	3.81E+04	1.15E+03
153.03051	$C_6H_6N_2O_3$	7.44E+04	2.19E+05	3.00E+04	1.17E+04	0.00E+00	0.00E+00
153.05582	$C_8H_{10}O_3$	5.44E+05	8.21E+05	2.10E+05	2.03E+05	2.38E+04	0.00E+00
153.09216	$C_9H_{14}O_2$	7.16E+05	1.84E+05	1.51E+06	2.46E+05	1.12E+06	1.17E+03
154.01799	$C_3H_9NO_4S$	5.89E+06	5.21E+06	1.07E+07	3.83E+06	1.39E+06	1.39E+04
154.06228	$C_6H_9N_3O_2$	4.41E+06	7.48E+06	7.03E+06	2.75E+06	5.05E+06	0.00E+00
155.00204	$C_3H_8O_5S$	1.85E+07	7.91E+06	3.86E+07	2.93E+06	2.42E+06	0.00E+00
155.02113	$C_4H_4N_4O_3$	0.00E+00	8.86E+04	9.86E+04	1.24E+05	0.00E+00	1.62E+04
155.10787	$C_9H_{16}O_2$	0.00E+00	1.32E+04	0.00E+00	0.00E+00	9.03E+05	0.00E+00
157.01185	$C_{10}H_6S$	1.04E+06	1.56E+06	2.26E+06	1.53E+06	3.69E+07	5.66E+05
157.03675	$C_4H_6N_4O_3$	3.62E+06	1.86E+06	6.23E+06	1.44E+06	3.10E+07	0.00E+00
157.05065	$C_7H_{10}O_4$	4.95E+05	6.31E+05	1.29E+05	6.98E+04	6.80E+05	2.62E+04
157.08700	$C_8H_{14}O_3$	3.12E+06	2.27E+06	3.77E+06	7.80E+05	1.32E+06	1.63E+04

158.04594	$C_6H_9NO_4$	1.19E+06	5.33E+06	1.61E+06	1.99E+06	3.67E+06	0.00E+00
159.02998	$C_6H_8O_5$	2.40E+05	7.23E+05	1.23E+05	2.42E+04	2.79E+05	5.06E+03
159.10273	$C_8H_{16}O_3$	4.43E+05	8.67E+05	2.37E+05	0.00E+00	6.07E+05	1.10E+05
160.04047	$C_9H_7NO_2$	4.51E+03	1.17E+04	8.75E+03	0.00E+00	2.91E+05	0.00E+00
160.06159	$C_6H_{11}NO_4$	1.26E+04	6.63E+04	2.96E+05	7.02E+04	1.32E+06	0.00E+00
161.04561	$C_6H_{10}O_5$	5.83E+07	4.72E+07	5.52E+07	1.40E+07	1.73E+07	1.76E+05
163.02624	$C_6H_4N_4O_2$	9.31E+05	4.81E+05	6.97E+05	1.44E+05	0.00E+00	0.00E+00
163.04015	$C_9H_8O_3$	1.08E+07	5.30E+06	7.61E+06	1.70E+06	1.58E+07	9.21E+04
163.06131	$C_6H_{12}O_5$	1.28E+05	6.80E+05	0.00E+00	1.29E+05	1.04E+06	4.76E+04
163.11298	$C_{11}H_{16}O$	9.42E+03	2.13E+06	0.00E+00	6.36E+05	0.00E+00	0.00E+00
164.03532	$C_8H_7NO_3$	6.96E+05	1.21E+06	8.29E+05	3.83E+05	1.05E+06	3.66E+04
164.03872	$C_5H_{11}NO_3S$	1.03E+06	1.56E+06	3.03E+05	2.85E+05	6.85E+06	0.00E+00
164.07172	$C_9H_{11}NO_2$	9.10E+06	9.67E+06	5.19E+06	2.58E+06	7.49E+06	8.99E+02
165.09212	$C_{10}H_{14}O_2$	6.19E+05	4.52E+06	5.28E+05	2.04E+05	1.41E+06	0.00E+00
166.03712	$C_5H_5N_5O_2$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.75E+05	0.00E+00
166.99620	$C_{11}H_4S$	1.12E+05	1.89E+04	2.71E+06	9.51E+03	0.00E+00	0.00E+00
167.01331	$C_3H_8N_2O_4S$	2.21E+05	0.00E+00	3.82E+06	6.81E+04	3.81E+03	1.69E+03
167.02111	$C_5H_4N_4O_3$	1.04E+06	9.22E+04	6.54E+05	5.26E+04	3.45E+07	1.27E+03
167.03504	$C_8H_8O_4$	0.00E+00	0.00E+00	1.74E+04	0.00E+00	2.53E+05	3.56E+03
167.07143	$C_9H_{12}O_3$	2.70E+06	3.65E+06	1.18E+06	1.20E+06	2.84E+04	0.00E+00
167.10780	$C_{10}H_{16}O_2$	5.05E+05	2.50E+06	2.74E+05	6.35E+04	0.00E+00	0.00E+00
167.99728	$C_3H_7NO_5S$	2.14E+07	1.04E+07	3.37E+07	7.37E+06	1.94E+06	4.81E+04
168.98128	$C_3H_6O_6S$	5.56E+06	1.83E+06	1.45E+07	1.24E+06	3.70E+06	3.89E+03
169.08714	$C_9H_{14}O_3$	2.39E+05	6.17E+05	1.31E+05	1.28E+05	1.47E+05	1.07E+04
171.02756	$C_{11}H_8S$	3.98E+07	3.59E+07	1.91E+07	1.41E+07	9.73E+03	1.87E+03
171.06638	$C_8H_{12}O_4$	0.00E+00	1.97E+06	0.00E+00	0.00E+00	0.00E+00	7.14E+05
171.10273	$C_9H_{16}O_3$	2.18E+06	9.59E+06	8.44E+05	1.66E+06	7.34E+05	3.51E+04
172.04044	$C_{10}H_7NO_2$	6.10E+05	2.69E+05	1.02E+06	3.57E+05	0.00E+00	5.82E+03
172.06163	$C_7H_{11}NO_4$	8.32E+05	4.47E+05	3.12E+05	6.69E+04	4.20E+06	9.96E+02
173.00915	$C_6H_6O_6$	3.60E+06	1.62E+06	5.50E+06	2.35E+04	1.28E+04	0.00E+00
173.04558	$C_7H_{10}O_5$	9.70E+05	6.98E+05	3.31E+05	1.51E+05	4.71E+05	3.94E+03
173.08197	$C_8H_{14}O_4$	1.36E+06	2.91E+06	1.86E+05	2.34E+05	7.63E+05	1.58E+03
173.09325	$C_7H_{14}N_2O_3$	8.48E+04	6.37E+05	2.74E+03	1.32E+04	6.64E+04	0.00E+00
173.11836	$C_9H_{18}O_3$	3.44E+05	2.44E+05	8.02E+04	5.01E+04	5.25E+05	1.13E+03
174.00208	C_9H_5NOS	1.04E+05	5.88E+04	7.88E+04	8.80E+04	2.14E+07	1.04E+03

174.04082	$C_6H_9NO_5$	6.49E+05	5.49E+04	1.37E+06	5.16E+04	5.11E+04	0.00E+00
174.05612	$C_{10}H_9NO_2$	1.49E+04	6.06E+04	4.12E+04	4.64E+04	3.98E+06	0.00E+00
174.08846	$C_6H_{13}N_3O_3$	1.33E+06	1.84E+06	3.09E+05	3.61E+04	9.88E+06	0.00E+00
175.04736	$C_4H_8N_4O_4$	1.32E+06	1.11E+06	2.25E+06	1.17E+05	8.37E+05	0.00E+00
175.06125	$C_7H_{12}O_5$	1.86E+07	8.21E+06	1.53E+07	5.45E+06	2.63E+06	1.36E+04
175.07256	$C_6H_{12}N_2O_4$	3.27E+05	2.23E+06	0.00E+00	6.05E+04	2.36E+05	0.00E+00
177.07695	$C_7H_{14}O_5$	8.81E+04	2.25E+05	5.39E+05	6.48E+05	1.36E+05	0.00E+00
178.03719	$C_6H_5N_5O_2$	3.92E+03	8.04E+03	7.26E+04	7.30E+03	0.00E+00	0.00E+00
179.02102	$C_6H_4N_4O_3$	2.14E+05	3.30E+05	4.04E+05	3.18E+04	0.00E+00	0.00E+00
179.03497	$C_9H_8O_4$	1.71E+06	1.22E+06	7.50E+05	4.06E+05	4.35E+06	6.85E+04
179.05611	$C_6H_{12}O_6$	9.80E+07	9.09E+07	9.31E+07	2.41E+07	1.27E+06	5.82E+04
179.07147	$C_{10}H_{12}O_3$	2.82E+05	4.00E+05	2.33E+05	1.30E+05	9.75E+03	0.00E+00
179.10785	$C_{11}H_{16}O_2$	2.70E+04	1.36E+05	4.61E+04	0.00E+00	3.80E+05	2.54E+03
180.03368	$C_5H_{11}NO_4S$	3.97E+05	7.59E+05	5.68E+05	2.23E+06	4.50E+05	4.85E+04
180.06667	$C_9H_{11}NO_3$	3.28E+06	6.93E+06	1.52E+05	1.19E+06	3.61E+06	0.00E+00
181.08713	$C_{10}H_{14}O_3$	9.95E+05	1.25E+06	4.81E+05	2.32E+05	3.39E+05	0.00E+00
182.99113	$C_{11}H_4OS$	1.60E+06	7.33E+05	1.33E+06	1.56E+05	0.00E+00	0.00E+00
183.01603	$C_5H_4N_4O_4$	0.00E+00	3.47E+04	3.20E+05	3.06E+05	4.60E+06	0.00E+00
183.02755	$C_{12}H_8S$	1.94E+06	8.70E+05	2.92E+06	7.31E+04	5.43E+06	0.00E+00
183.06637	$C_9H_{12}O_4$	2.44E+05	4.23E+05	1.97E+05	1.29E+05	9.14E+05	1.92E+03
183.10272	$C_{10}H_{16}O_3$	1.09E+07	6.26E+06	1.02E+07	2.44E+06	1.45E+05	4.74E+03
185.00669	$C_{11}H_6OS$	1.30E+06	1.15E+05	3.41E+06	7.54E+04	1.81E+03	0.00E+00
185.02769	$C_8H_{10}O_3S$	0.00E+00	3.09E+05	1.77E+06	1.63E+05	0.00E+00	3.62E+04
185.04320	$C_{12}H_{10}S$	1.39E+06	9.70E+05	7.51E+05	4.37E+05	2.03E+06	1.32E+03
185.08202	$C_9H_{14}O_4$	2.68E+06	2.83E+06	1.35E+06	8.13E+05	3.44E+06	1.45E+05
185.11842	$C_{10}H_{18}O_3$	5.12E+03	1.10E+04	5.97E+03	1.69E+03	6.88E+05	0.00E+00
186.03850	$C_{11}H_9NS$	2.05E+05	8.24E+05	2.58E+04	2.80E+05	6.13E+04	0.00E+00
186.05212	$C_6H_9N_3O_4$	2.08E+05	2.09E+05	3.70E+05	1.02E+05	1.79E+06	0.00E+00
186.07727	$C_8H_{13}NO_4$	2.05E+06	1.19E+06	2.06E+05	8.26E+04	1.24E+03	0.00E+00
187.06126	$C_8H_{12}O_5$	1.57E+06	1.37E+06	1.07E+06	3.85E+05	3.65E+06	1.11E+04
187.10893	$C_8H_{16}N_2O_3$	2.21E+06	5.60E+06	1.61E+05	5.03E+05	2.57E+04	0.00E+00
187.13407	$C_{10}H_{20}O_3$	0.00E+00	0.00E+00	3.25E+04	0.00E+00	7.70E+06	9.82E+03
188.01769	$C_{10}H_7NOS$	2.39E+06	3.95E+06	3.27E+05	1.24E+06	1.22E+03	0.00E+00
188.05640	$C_7H_{11}NO_5$	1.50E+05	1.28E+04	2.86E+05	2.35E+04	7.50E+05	0.00E+00
189.07699	$C_8H_{14}O_5$	8.53E+05	5.66E+05	5.14E+05	1.51E+05	1.37E+06	9.41E+03

189.11338	$C_9H_{18}O_4$	1.94E+05	1.80E+06	2.65E+04	1.42E+05	3.98E+04	1.35E+03
190.03585	$C_6H_9NO_6$	6.59E+06	1.70E+06	0.00E+00	0.00E+00	1.04E+05	0.00E+00
190.03701	$C_7H_5N_5O_2$	1.09E+05	4.28E+03	1.24E+06	7.16E+04	0.00E+00	0.00E+00
190.05099	$C_{10}H_9NO_3$	1.38E+05	1.22E+05	2.52E+05	2.55E+04	2.82E+05	9.43E+02
191.01982	$C_6H_8O_7$	4.80E+08	2.05E+08	6.68E+08	3.44E+07	1.90E+06	1.17E+03
191.07143	$C_{11}H_{12}O_3$	6.70E+05	2.97E+05	9.59E+05	4.53E+04	0.00E+00	0.00E+00
193.07182	$C_7H_{14}O_6$	3.33E+06	1.44E+06	4.14E+06	2.72E+06	0.00E+00	1.66E+04
193.08701	$C_{11}H_{14}O_3$	4.40E+06	6.47E+06	1.40E+06	1.58E+06	6.25E+05	0.00E+00
193.12346	$C_{12}H_{18}O_2$	7.43E+05	5.73E+06	3.98E+05	1.05E+05	9.80E+05	0.00E+00
195.10264	$C_{11}H_{16}O_3$	3.31E+06	3.00E+06	1.61E+06	7.28E+05	3.39E+04	0.00E+00
195.13913	$C_{12}H_{20}O_2$	9.56E+05	5.34E+06	6.90E+05	2.26E+05	0.00E+00	0.00E+00
196.01090	$C_5H_3N_5O_4$	5.56E+04	3.06E+04	8.07E+04	9.67E+04	0.00E+00	2.40E+03
196.02279	$C_{12}H_7NS$	6.11E+07	3.59E+07	2.64E+07	2.34E+07	8.15E+07	2.68E+04
196.04770	$C_6H_7N_5O_3$	0.00E+00	0.00E+00	4.32E+04	5.39E+03	3.38E+03	0.00E+00
197.04322	$C_{13}H_{10}S$	1.66E+07	9.19E+06	2.11E+07	2.32E+06	3.54E+07	2.51E+04
197.08196	$C_{10}H_{14}O_4$	1.18E+06	8.03E+05	1.64E+06	3.29E+05	1.23E+06	1.22E+03
197.11839	$C_{11}H_{18}O_3$	7.25E+05	5.10E+05	7.07E+05	2.12E+05	6.83E+03	1.11E+03
198.03852	$C_{12}H_9NS$	0.00E+00	1.60E+05	1.12E+04	1.24E+04	1.40E+06	0.00E+00
199.01105	$C_5H_4N_4O_5$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.16E+06	0.00E+00
199.02255	$C_{12}H_8OS$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.50E+05	1.19E+03
199.07250	$C_8H_{12}N_2O_4$	6.81E+05	3.91E+05	2.18E+05	7.18E+04	1.33E+06	0.00E+00
199.13408	$C_{11}H_{20}O_3$	3.76E+05	4.97E+05	2.35E+05	1.06E+05	1.17E+04	0.00E+00
200.01779	$C_{11}H_7NOS$	1.37E+06	2.33E+06	1.01E+06	9.17E+05	2.00E+06	3.16E+03
200.05662	$C_8H_{11}NO_5$	0.00E+00	1.72E+04	1.01E+04	0.00E+00	1.63E+05	0.00E+00
200.09296	$C_9H_{15}NO_4$	1.34E+03	4.27E+03	9.73E+02	0.00E+00	1.85E+05	0.00E+00
201.00185	$C_{11}H_6O_2S$	4.85E+04	3.93E+04	5.50E+04	5.23E+05	5.08E+03	1.87E+03
201.03819	$C_{12}H_{10}OS$	9.17E+03	0.00E+00	7.70E+03	5.16E+03	2.30E+07	0.00E+00
201.07697	$C_9H_{14}O_5$	9.90E+05	4.42E+05	3.04E+05	1.14E+05	4.55E+05	1.06E+04
201.11340	$C_{10}H_{18}O_4$	1.61E+06	8.81E+06	1.66E+05	2.70E+06	1.05E+06	3.62E+03
201.12460	$C_9H_{18}N_2O_3$	1.96E+06	4.73E+06	2.77E+05	2.28E+05	2.41E+03	0.00E+00
201.16506	$C_{15}H_{22}$	6.42E+04	3.01E+05	1.13E+04	1.37E+04	7.81E+04	0.00E+00
202.03349	$C_{11}H_9NOS$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.90E+05	0.00E+00
202.07218	$C_8H_{13}NO_5$	1.75E+06	7.36E+05	1.08E+06	9.73E+04	5.72E+05	0.00E+00
202.08357	$C_7H_{13}N_3O_4$	8.01E+04	7.54E+05	0.00E+00	1.19E+04	0.00E+00	0.00E+00
203.08266	$C_{11}H_{12}N_2O_2$	2.18E+06	3.32E+06	6.92E+05	6.34E+05	0.00E+00	7.05E+02

203.09256	$C_9H_{16}O_5$	2.43E+05	8.60E+05	1.58E+05	6.27E+04	2.02E+06	8.05E+03
205.07181	$C_8H_{14}O_6$	1.37E+05	1.99E+05	3.78E+04	5.12E+04	3.97E+05	0.00E+00
206.01295	$C_6H_9NO_5S$	2.81E+05	4.74E+05	1.08E+05	0.00E+00	1.41E+06	0.00E+00
206.03189	$C_7H_5N_5O_3$	1.21E+05	1.39E+03	8.39E+05	8.00E+04	0.00E+00	0.00E+00
207.01222	$C_{10}H_8O_3S$	1.69E+06	1.32E+06	1.99E+06	3.31E+06	0.00E+00	2.87E+03
207.08753	$C_8H_{16}O_6$	0.00E+00	1.96E+06	0.00E+00	0.00E+00	0.00E+00	1.39E+05
209.06678	$C_7H_{14}O_7$	1.76E+05	6.25E+04	1.10E+05	4.27E+03	6.65E+05	0.00E+00
209.08202	$C_{11}H_{14}O_4$	3.13E+05	2.25E+05	1.97E+05	6.64E+04	2.90E+05	0.00E+00
209.11837	$C_{12}H_{18}O_3$	1.62E+06	1.39E+06	1.94E+06	6.33E+05	1.94E+04	0.00E+00
211.09773	$C_{11}H_{16}O_4$	8.39E+04	1.02E+06	9.42E+04	0.00E+00	4.51E+06	1.17E+04
211.13411	$C_{12}H_{20}O_3$	7.67E+03	2.84E+04	5.15E+03	7.67E+03	7.38E+05	0.00E+00
212.00582	$C_5H_3N_5O_5$	7.65E+03	1.04E+04	3.19E+04	2.38E+05	0.00E+00	0.00E+00
212.01785	$C_{12}H_7NOS$	3.03E+03	0.00E+00	9.63E+03	1.93E+04	2.52E+03	0.00E+00
213.01226	$C_3H_{10}N_4O_3S_2$	8.68E+05	2.67E+05	1.84E+05	1.78E+06	6.82E+06	5.36E+04
213.01302	$C_{11}H_6N_2OS$	2.75E+06	2.60E+06	1.48E+06	1.42E+06	1.68E+07	0.00E+00
213.01542	$C_7H_6N_2O_6$	0.00E+00	1.03E+06	0.00E+00	8.62E+05	0.00E+00	1.84E+05
213.02427	$C_{10}H_6N_4S$	3.63E+03	1.16E+03	6.44E+04	1.80E+04	2.52E+05	0.00E+00
213.03821	$C_{13}H_{10}OS$	0.00E+00	0.00E+00	3.57E+03	3.73E+03	4.79E+05	1.76E+03
213.07703	$C_{10}H_{14}O_5$	2.19E+05	3.85E+05	1.21E+05	3.91E+04	5.31E+04	1.28E+04
213.11336	$C_{11}H_{18}O_4$	1.78E+06	2.85E+06	6.79E+05	5.13E+05	3.96E+06	1.06E+04
213.12459	$C_{10}H_{18}N_2O_3$	1.24E+06	1.50E+06	7.02E+04	1.72E+05	1.28E+03	0.00E+00
213.14978	$C_{12}H_{22}O_3$	7.06E+03	3.92E+04	9.62E+03	1.18E+04	9.36E+06	0.00E+00
213.96395	$C_7H_5NO_3S_2$	4.56E+05	5.97E+05	6.78E+05	2.18E+05	5.86E+05	2.10E+04
214.01018	$C_6H_5N_3O_6$	3.09E+04	4.34E+04	5.50E+04	3.85E+05	9.80E+05	1.51E+04
214.03335	$C_{12}H_9NOS$	7.99E+05	6.05E+05	1.37E+06	9.60E+04	6.24E+06	0.00E+00
214.99967	$C_{12}H_8S_2$	2.23E+05	1.09E+05	5.74E+05	1.49E+04	1.09E+06	0.00E+00
215.05372	$C_{13}H_{12}OS$	5.92E+03	0.00E+00	1.02E+03	0.00E+00	1.09E+06	0.00E+00
215.06741	$C_8H_{12}N_2O_5$	5.05E+05	6.87E+05	2.73E+04	0.00E+00	1.24E+06	0.00E+00
215.09250	$C_{10}H_{16}O_5$	1.98E+06	1.62E+06	6.96E+05	3.08E+05	2.30E+06	9.25E+03
215.12896	$C_{11}H_{20}O_4$	3.90E+03	4.49E+03	1.40E+03	1.27E+03	8.04E+05	0.00E+00
215.14016	$C_{10}H_{20}N_2O_3$	1.57E+06	1.46E+06	2.84E+03	4.64E+04	0.00E+00	0.00E+00
215.14413	$C_{15}H_{20}O$	3.78E+03	3.07E+05	1.89E+03	3.99E+03	0.00E+00	0.00E+00
215.16531	$C_{12}H_{24}O_3$	0.00E+00	7.29E+04	3.05E+04	0.00E+00	9.72E+05	3.23E+03
216.03123	$C_{12}H_3N_5$	8.51E+05	6.80E+05	2.09E+05	1.26E+05	1.26E+04	0.00E+00
216.04909	$C_{12}H_{11}NOS$	0.00E+00	3.00E+03	0.00E+00	0.00E+00	7.06E+05	0.00E+00

217.02987	$C_{15}H_6O_2$	4.20E+07	3.23E+07	4.83E+07	1.25E+07	1.45E+05	3.45E+04
217.07184	$C_9H_{14}O_6$	1.36E+05	1.49E+06	1.21E+05	1.29E+05	9.06E+05	4.90E+04
217.08291	$C_8H_{14}N_2O_5$	1.70E+06	5.82E+05	5.54E+05	4.25E+05	8.85E+05	3.51E+03
217.10817	$C_{10}H_{18}O_5$	3.37E+06	2.17E+06	1.80E+06	6.55E+05	3.55E+06	1.38E+04
217.11943	$C_9H_{18}N_2O_4$	8.48E+05	2.67E+06	9.71E+04	1.62E+05	5.62E+03	0.00E+00
217.15989	$C_{15}H_{22}O$	7.32E+04	3.29E+06	0.00E+00	1.06E+06	0.00E+00	0.00E+00
218.06824	$C_9H_9N_5O_2$	2.32E+04	2.89E+04	5.73E+05	1.40E+04	7.99E+02	0.00E+00
218.10339	$C_9H_{17}NO_5$	9.52E+05	3.60E+05	1.67E+06	1.77E+05	3.20E+06	0.00E+00
219.05240	$C_9H_8N_4O_3$	1.01E+07	7.08E+06	8.62E+06	9.83E+05	0.00E+00	7.70E+02
219.07752	$C_{11}H_{12}N_2O_3$	8.13E+05	1.95E+05	1.05E+05	6.56E+04	5.27E+05	0.00E+00
219.10266	$C_{13}H_{16}O_3$	3.14E+05	2.54E+05	4.82E+05	4.12E+04	2.72E+04	0.00E+00
219.13911	$C_{14}H_{20}O_2$	1.43E+06	1.57E+06	5.53E+05	5.31E+05	6.71E+05	0.00E+00
219.17559	$C_{15}H_{24}O$	1.73E+03	6.17E+05	0.00E+00	2.30E+05	1.75E+03	0.00E+00
221.06669	$C_8H_{14}O_7$	8.03E+06	5.59E+06	6.49E+06	3.01E+06	3.78E+04	2.85E+04
221.08205	$C_{12}H_{14}O_4$	4.20E+04	2.61E+05	2.35E+04	4.51E+04	0.00E+00	9.49E+03
221.11842	$C_{13}H_{18}O_3$	1.25E+06	3.28E+06	2.73E+05	6.84E+05	4.75E+04	1.21E+03
222.00214	$C_{13}H_5NOS$	0.00E+00	0.00E+00	1.30E+03	1.01E+03	2.49E+05	0.00E+00
222.07731	$C_{11}H_{13}NO_4$	2.30E+03	2.69E+03	0.00E+00	0.00E+00	3.01E+05	0.00E+00
223.09767	$C_{12}H_{16}O_4$	5.79E+04	0.00E+00	1.27E+05	0.00E+00	3.29E+05	2.42E+04
223.13406	$C_{13}H_{20}O_3$	1.04E+07	1.11E+07	7.50E+06	3.22E+06	3.64E+03	4.05E+03
225.07440	$C_{15}H_{14}S$	2.87E+05	1.15E+05	4.94E+05	4.27E+04	1.24E+05	9.53E+02
225.07691	$C_{11}H_{14}O_5$	9.07E+05	2.84E+05	6.94E+05	1.35E+05	4.92E+03	0.00E+00
225.08823	$C_{10}H_{14}N_2O_4$	0.00E+00	1.11E+03	1.09E+03	0.00E+00	6.62E+05	0.00E+00
225.11337	$C_{12}H_{18}O_4$	5.49E+05	1.99E+06	2.77E+05	1.84E+05	1.48E+06	2.42E+03
225.14972	$C_{13}H_{22}O_3$	3.36E+06	1.88E+06	1.02E+06	6.76E+05	6.96E+04	0.00E+00
226.00279	$C_5H_9NO_7S$	1.28E+07	3.90E+06	3.82E+07	4.26E+06	0.00E+00	3.10E+04
227.06735	$C_9H_{12}N_2O_5$	3.24E+07	2.70E+07	1.55E+07	9.32E+06	0.00E+00	0.00E+00
227.09264	$C_{11}H_{16}O_5$	6.60E+05	1.11E+06	4.77E+05	1.74E+05	6.04E+05	3.52E+04
227.10385	$C_{10}H_{16}N_2O_4$	2.32E+06	1.58E+06	8.17E+05	2.71E+05	4.25E+06	2.30E+03
227.12901	$C_{12}H_{20}O_4$	2.66E+06	3.72E+06	1.64E+06	1.30E+06	2.36E+06	6.31E+03
227.14028	$C_{11}H_{20}N_2O_3$	2.23E+06	4.30E+06	1.60E+05	6.81E+05	0.00E+00	0.00E+00
227.99874	$C_9H_3N_5OS$	0.00E+00	0.00E+00	7.20E+03	4.22E+03	0.00E+00	0.00E+00
228.05152	$C_9H_{11}NO_6$	9.87E+02	0.00E+00	0.00E+00	0.00E+00	3.57E+05	0.00E+00
229.03311	$C_{13}H_{10}O_2S$	1.64E+04	2.43E+04	8.45E+04	7.55E+04	4.11E+05	0.00E+00
229.03887	$C_6H_{14}O_7S$	0.00E+00	2.49E+05	0.00E+00	0.00E+00	0.00E+00	1.60E+04

229.06942	$C_{14}H_{14}OS$	1.32E+06	5.86E+05	6.41E+04	6.39E+04	0.00E+00	0.00E+00
229.07186	$C_{10}H_{14}O_6$	4.91E+05	2.03E+05	8.33E+04	1.72E+04	4.12E+04	0.00E+00
229.08310	$C_9H_{14}N_2O_5$	2.57E+05	3.07E+05	6.35E+04	4.72E+04	1.28E+06	0.00E+00
229.10826	$C_{11}H_{18}O_5$	6.88E+05	1.01E+06	1.11E+05	2.95E+05	3.23E+05	2.38E+03
229.14464	$C_{12}H_{22}O_4$	4.26E+05	6.47E+05	1.51E+05	2.90E+05	1.09E+06	1.37E+03
229.15592	$C_{11}H_{22}N_2O_3$	2.22E+06	3.45E+06	8.23E+04	1.30E+05	1.34E+03	0.00E+00
231.02744	$C_{16}H_8S$	2.23E+06	6.47E+05	1.68E+06	1.16E+05	2.86E+06	1.93E+04
231.13511	$C_{10}H_{20}N_2O_4$	5.81E+05	1.00E+06	3.95E+04	3.16E+04	2.77E+03	0.00E+00
231.13918	$C_{15}H_{20}O_2$	1.85E+05	1.96E+06	3.12E+04	1.21E+05	0.00E+00	0.00E+00
232.09415	$C_8H_{15}N_3O_5$	5.09E+04	1.18E+06	0.00E+00	8.81E+03	3.59E+03	0.00E+00
232.99801	$C_5H_6N_4O_5S$	3.11E+06	3.33E+06	7.29E+05	2.14E+06	0.00E+00	3.62E+03
233.00667	$C_{15}H_6OS$	5.63E+04	5.84E+04	1.17E+05	1.95E+04	0.00E+00	0.00E+00
233.07802	$C_8H_{14}N_2O_6$	2.82E+06	3.76E+06	2.68E+05	2.13E+05	1.44E+06	0.00E+00
233.15481	$C_{15}H_{22}O_2$	0.00E+00	8.39E+04	0.00E+00	0.00E+00	0.00E+00	5.34E+03
235.00866	$C_{12}H_4N_4S$	1.16E+04	1.61E+03	4.63E+03	3.28E+03	2.16E+06	0.00E+00
235.05899	$C_{16}H_{12}S$	3.52E+05	4.93E+05	1.09E+05	1.67E+05	0.00E+00	0.00E+00
235.09774	$C_{13}H_{16}O_4$	1.25E+05	2.98E+05	2.81E+04	3.24E+04	3.14E+03	0.00E+00
236.00388	$C_{11}H_3N_5S$	4.26E+05	2.13E+06	1.27E+05	8.83E+05	1.62E+05	6.25E+02
236.05657	$C_{11}H_{11}NO_5$	1.17E+04	0.00E+00	8.35E+03	1.63E+03	3.09E+05	0.00E+00
237.08834	$C_{11}H_{14}N_2O_4$	1.85E+04	2.77E+05	3.33E+03	2.82E+04	0.00E+00	0.00E+00
237.11338	$C_{13}H_{18}O_4$	1.64E+06	1.62E+06	7.44E+05	6.34E+05	4.76E+05	0.00E+00
237.11674	$C_{10}H_{22}O_4S$	1.98E+05	6.91E+04	7.24E+05	2.29E+05	0.00E+00	0.00E+00
237.14978	$C_{14}H_{22}O_3$	1.75E+04	1.37E+05	7.13E+03	8.88E+03	9.12E+05	0.00E+00
239.12905	$C_{13}H_{20}O_4$	0.00E+00	4.24E+06	0.00E+00	0.00E+00	0.00E+00	1.03E+06
239.16552	$C_{14}H_{24}O_3$	5.49E+03	2.23E+05	1.13E+03	5.51E+04	8.20E+04	0.00E+00
240.04906	$C_{14}H_{11}NOS$	3.78E+05	1.85E+05	9.16E+04	1.71E+04	2.48E+03	0.00E+00
240.06037	$C_{13}H_{11}N_3S$	1.25E+04	3.02E+04	5.04E+04	9.02E+03	3.12E+05	0.00E+00
241.08315	$C_{10}H_{14}N_2O_5$	2.56E+07	2.83E+07	1.79E+07	1.08E+07	1.17E+06	4.92E+04
241.10589	$C_{16}H_{18}S$	6.57E+05	6.88E+05	3.36E+05	0.00E+00	3.24E+05	3.20E+04
241.10835	$C_{12}H_{18}O_5$	1.19E+06	1.40E+06	4.78E+05	4.46E+05	8.76E+05	1.06E+04
241.11958	$C_{11}H_{18}N_2O_4$	3.86E+06	2.36E+06	1.29E+06	2.98E+05	2.15E+06	1.96E+03
241.14481	$C_{13}H_{22}O_4$	3.88E+05	2.58E+05	2.64E+05	1.47E+05	8.78E+04	0.00E+00
241.18114	$C_{14}H_{26}O_3$	4.61E+03	1.44E+04	3.04E+03	1.52E+03	1.43E+06	0.00E+00
242.07609	$C_{13}H_{13}N_3S$	0.00E+00	3.65E+04	0.00E+00	0.00E+00	8.62E+05	0.00E+00
242.07855	$C_9H_{13}N_3O_5$	1.30E+03	4.88E+05	1.21E+03	2.69E+05	1.51E+03	0.00E+00

242.17639	$C_{13}H_{25}NO_3$	0.00E+00	1.37E+06	0.00E+00	0.00E+00	0.00E+00	2.63E+05
243.01812	$C_6H_{12}O_8S$	3.31E+07	2.85E+07	7.92E+06	3.95E+06	1.74E+07	0.00E+00
243.04870	$C_{14}H_{12}O_2S$	2.76E+06	1.29E+06	2.40E+06	8.01E+05	3.76E+05	1.96E+03
243.06236	$C_9H_{12}N_2O_6$	5.23E+06	4.72E+07	1.63E+07	2.52E+07	7.73E+05	2.90E+03
243.08750	$C_{11}H_{16}O_6$	4.51E+05	2.72E+05	7.11E+05	6.75E+04	1.23E+04	1.22E+03
243.12393	$C_{12}H_{20}O_5$	4.08E+06	3.09E+06	1.69E+06	8.76E+05	2.28E+06	2.61E+03
243.17156	$C_{12}H_{24}N_2O_3$	6.17E+05	2.02E+06	4.79E+04	4.94E+04	0.00E+00	0.00E+00
243.97793	$C_5H_3N_5O_5S$	1.83E+04	2.21E+04	5.48E+03	3.24E+05	0.00E+00	1.47E+03
244.13044	$C_{10}H_{19}N_3O_4$	4.22E+05	1.10E+06	1.99E+04	1.95E+04	0.00E+00	9.55E+02
244.99819	$C_6H_6N_4O_5S$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.68E+05	0.00E+00
245.02817	$C_{13}H_{10}O_3S$	0.00E+00	1.34E+04	0.00E+00	1.72E+04	2.51E+05	0.00E+00
245.11433	$C_{10}H_{18}N_2O_5$	4.48E+06	6.11E+06	1.50E+06	5.60E+05	1.58E+05	0.00E+00
245.15481	$C_{16}H_{22}O_2$	5.78E+05	9.23E+05	1.80E+05	1.14E+05	5.28E+05	0.00E+00
246.06217	$C_9H_{13}NO_7$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.19E+05	8.20E+02
247.13415	$C_{15}H_{20}O_3$	2.70E+06	1.02E+07	4.54E+04	1.98E+06	0.00E+00	0.00E+00
247.17055	$C_{16}H_{24}O_2$	4.87E+04	4.80E+04	7.31E+03	2.24E+04	4.31E+05	0.00E+00
247.98478	$C_{11}H_7NO_2S_2$	4.20E+05	8.94E+04	1.01E+06	5.08E+05	1.41E+06	0.00E+00
248.05417	$C_{16}H_{11}NS$	2.53E+06	5.56E+06	1.74E+05	1.02E+06	2.87E+06	0.00E+00
249.14983	$C_{15}H_{22}O_3$	4.78E+05	1.03E+06	2.22E+05	2.19E+05	3.64E+04	0.00E+00
251.05965	$C_9H_{16}O_6S$	0.00E+00	1.88E+05	4.19E+04	0.00E+00	0.00E+00	1.35E+04
251.07871	$C_{10}H_{12}N_4O_4$	4.45E+06	3.95E+06	4.33E+06	4.02E+06	0.00E+00	0.00E+00
251.09022	$C_{17}H_{16}S$	1.83E+06	9.10E+05	1.80E+06	3.97E+05	3.05E+03	0.00E+00
251.10403	$C_{12}H_{16}N_2O_4$	4.60E+04	2.66E+05	4.21E+03	6.00E+03	0.00E+00	0.00E+00
251.11386	$C_{10}H_{20}O_7$	0.00E+00	2.65E+06	0.00E+00	0.00E+00	0.00E+00	1.91E+05
251.12912	$C_{14}H_{20}O_4$	1.07E+05	2.80E+05	0.00E+00	0.00E+00	0.00E+00	4.13E+04
252.07383	$C_9H_{11}N_5O_4$	1.77E+06	1.11E+06	4.27E+06	5.57E+05	0.00E+00	0.00E+00
253.06956	$C_{16}H_{14}OS$	2.25E+05	4.43E+05	1.17E+05	8.81E+04	3.36E+05	0.00E+00
253.10831	$C_{13}H_{18}O_5$	1.55E+06	1.70E+06	6.32E+05	3.97E+05	1.12E+05	0.00E+00
253.14476	$C_{14}H_{22}O_4$	1.28E+05	4.01E+05	8.99E+04	0.00E+00	0.00E+00	3.51E+04
253.18110	$C_{15}H_{26}O_3$	2.19E+05	3.67E+05	8.44E+04	6.32E+04	1.06E+05	0.00E+00
254.06474	$C_{15}H_{13}NOS$	2.44E+06	3.54E+05	8.64E+04	2.85E+04	0.00E+00	0.00E+00
254.10107	$C_{16}H_{17}NS$	5.52E+06	1.01E+05	4.04E+06	3.68E+06	0.00E+00	5.22E+03
255.06253	$C_{10}H_{12}N_2O_6$	0.00E+00	0.00E+00	3.31E+02	0.00E+00	9.87E+05	0.00E+00
255.09651	$C_{15}H_{16}N_2S$	2.79E+05	9.26E+05	1.55E+04	9.34E+04	0.00E+00	0.00E+00
255.12397	$C_{13}H_{20}O_5$	2.24E+06	1.26E+06	2.33E+06	5.20E+05	1.64E+06	0.00E+00

255.16043	$C_{14}H_{24}O_4$	1.48E+03	1.60E+03	0.00E+00	0.00E+00	2.54E+05	0.00E+00
255.19685	$C_{15}H_{28}O_3$	0.00E+00	5.51E+03	1.48E+03	1.24E+03	6.77E+05	0.00E+00
256.09400	$C_{10}H_{15}N_3O_5$	4.87E+06	1.33E+06	4.93E+06	7.25E+05	6.01E+05	3.81E+03
256.95538	$C_{12}H_2O_5S$	1.13E+05	5.20E+05	0.00E+00	1.61E+05	1.30E+06	5.61E+04
256.99103	$C_{13}H_6O_4S$	2.70E+04	2.04E+04	2.23E+04	2.00E+04	5.46E+04	0.00E+00
256.99639	$C_{11}H_6N_4S_2$	3.12E+03	2.69E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
257.06829	$C_{12}H_{10}N_4O_3$	3.61E+03	0.00E+00	0.00E+00	0.00E+00	4.72E+05	0.00E+00
257.07792	$C_{10}H_{14}N_2O_6$	8.95E+06	3.93E+06	4.70E+06	8.76E+05	1.03E+07	1.18E+03
257.10323	$C_{12}H_{18}O_6$	9.67E+05	5.15E+05	2.12E+05	9.31E+04	1.96E+05	3.12E+03
257.13961	$C_{13}H_{22}O_5$	4.48E+05	3.76E+05	4.16E+05	5.53E+04	3.12E+05	1.09E+03
257.17614	$C_{14}H_{26}O_4$	5.53E+03	6.23E+03	0.00E+00	1.40E+03	4.27E+05	0.00E+00
257.99026	$C_9HN_5O_5$	2.70E+03	2.48E+06	1.99E+03	0.00E+00	4.13E+05	0.00E+00
257.99334	$C_6H_5N_5O_5S$	4.77E+06	3.46E+06	1.78E+06	2.96E+06	5.98E+06	1.93E+03
258.99200	$C_9H_8O_7S$	4.06E+05	3.03E+05	6.54E+04	4.75E+04	0.00E+00	0.00E+00
259.01375	$C_7H_8N_4O_5S$	8.76E+05	6.52E+05	1.12E+06	1.77E+05	3.29E+06	0.00E+00
259.13002	$C_{11}H_{20}N_2O_5$	7.45E+06	5.86E+06	2.31E+06	1.15E+06	1.09E+05	8.89E+02
259.13411	$C_{16}H_{20}O_3$	1.36E+05	1.04E+06	1.77E+04	2.27E+04	3.03E+04	0.00E+00
259.15520	$C_{13}H_{24}O_5$	2.61E+06	1.05E+06	9.37E+05	1.57E+05	5.80E+03	0.00E+00
259.19180	$C_{14}H_{28}O_4$	2.82E+03	2.29E+05	0.00E+00	3.51E+03	1.35E+04	0.00E+00
259.95509	$C_5H_3N_5O_4S_2$	7.39E+04	1.26E+05	2.54E+04	5.03E+05	0.00E+00	1.22E+04
260.04543	$C_7H_{11}N_5O_4S$	1.92E+05	2.90E+05	1.05E+05	1.13E+05	4.52E+04	0.00E+00
260.07784	$C_{10}H_{15}NO_7$	3.34E+03	3.08E+03	1.21E+03	0.00E+00	2.62E+05	0.00E+00
261.07296	$C_9H_{14}N_2O_7$	4.54E+06	1.17E+06	1.30E+06	7.30E+04	4.19E+06	0.00E+00
261.07455	$C_{18}H_{14}S$	4.62E+05	3.85E+05	4.29E+04	5.70E+04	0.00E+00	0.00E+00
261.12472	$C_{14}H_{18}N_2O_3$	6.88E+05	1.68E+06	3.04E+04	1.78E+05	0.00E+00	0.00E+00
261.14976	$C_{16}H_{22}O_3$	3.01E+06	1.26E+07	8.12E+05	3.30E+06	1.98E+05	0.00E+00
263.03865	$C_{13}H_{12}O_4S$	0.00E+00	7.68E+04	0.00E+00	0.00E+00	4.17E+03	0.00E+00
263.07716	$C_{10}H_{16}O_8$	1.63E+06	1.31E+06	1.30E+06	1.98E+05	1.27E+04	0.00E+00
263.12907	$C_{15}H_{20}O_4$	1.72E+06	2.25E+06	5.64E+05	7.47E+05	5.05E+05	0.00E+00
263.16545	$C_{16}H_{24}O_3$	6.04E+07	1.15E+08	2.58E+07	2.77E+07	1.54E+07	1.39E+03
265.03084	$C_7H_{10}N_2O_9$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.10E+06	1.33E+03
265.10852	$C_{14}H_{18}O_5$	5.15E+04	2.19E+05	3.97E+03	3.22E+04	3.19E+03	0.00E+00
265.11967	$C_{13}H_{18}N_2O_4$	4.70E+04	2.68E+05	4.07E+03	2.16E+04	0.00E+00	0.00E+00
265.14471	$C_{15}H_{22}O_4$	1.16E+05	7.84E+05	1.74E+04	3.20E+04	1.63E+05	0.00E+00
265.14808	$C_{12}H_{26}O_4S$	2.29E+05	1.02E+06	3.17E+05	7.75E+05	7.91E+05	1.11E+05

265.18112	$C_{16}H_{26}O_3$	3.81E+07	6.50E+07	1.55E+07	1.71E+07	2.77E+07	0.00E+00
265.95079	$C_8HN_3O_6S$	1.05E+06	2.12E+06	1.99E+06	1.45E+06	2.71E+06	2.50E+05
265.99536	$C_{11}H_9NO_3S_2$	3.71E+06	1.42E+06	6.36E+06	1.78E+06	3.50E+05	1.88E+04
266.08835	$C_{10}H_{13}N_5O_4$	1.45E+06	2.46E+06	1.27E+06	2.59E+06	2.18E+04	1.65E+04
267.07235	$C_{10}H_{12}N_4O_5$	4.99E+06	3.55E+06	6.79E+06	2.79E+06	2.65E+06	2.60E+03
267.09605	$C_{16}H_{16}N_2S$	8.01E+04	1.36E+04	2.17E+05	1.08E+04	0.00E+00	0.00E+00
267.12392	$C_{14}H_{20}O_5$	1.68E+05	1.34E+05	3.81E+04	1.63E+04	1.96E+05	0.00E+00
267.19675	$C_{16}H_{28}O_3$	2.61E+07	5.07E+07	8.10E+06	2.63E+07	1.27E+07	9.55E+03
269.02575	$C_6H_{10}N_2O_{10}$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.66E+05	0.00E+00
269.10322	$C_{13}H_{18}O_6$	4.32E+05	1.42E+05	4.01E+05	5.30E+04	1.26E+04	0.00E+00
269.11213	$C_{16}H_{18}N_2S$	3.34E+05	8.61E+05	4.39E+04	1.72E+04	0.00E+00	0.00E+00
269.21247	$C_{16}H_{30}O_3$	4.67E+06	1.08E+07	2.91E+06	3.44E+06	6.47E+07	0.00E+00
270.04042	$C_{14}H_9NO_5$	0.00E+00	0.00E+00	5.03E+04	1.56E+04	2.20E+05	0.00E+00
270.20777	$C_{15}H_{29}NO_3$	0.00E+00	3.17E+05	9.16E+03	1.64E+04	6.87E+04	4.37E+03
271.00627	$C_6H_{12}N_2O_6S_2$	1.43E+06	1.35E+06	8.25E+05	1.53E+05	0.00E+00	0.00E+00
271.08249	$C_{12}H_{16}O_7$	4.73E+06	3.32E+06	2.47E+06	7.90E+05	5.24E+03	0.00E+00
271.22816	$C_{16}H_{32}O_3$	1.64E+05	4.60E+05	4.59E+04	2.94E+04	9.37E+04	4.17E+03
273.07292	$C_{10}H_{14}N_2O_7$	4.98E+07	2.98E+07	1.93E+07	1.16E+07	4.19E+04	0.00E+00
273.13468	$C_{13}H_{22}O_6$	2.52E+05	2.31E+05	6.10E+04	5.53E+04	1.84E+05	0.00E+00
273.14991	$C_{17}H_{22}O_3$	6.39E+04	6.80E+05	3.74E+03	7.78E+04	0.00E+00	0.00E+00
273.18626	$C_{18}H_{26}O_2$	4.59E+04	2.66E+05	6.55E+03	2.46E+04	7.68E+04	0.00E+00
273.92944	C_7HNO_9S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.55E+05	4.32E+04
274.07967	$C_8H_{13}N_5O_6$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.47E+05	0.00E+00
274.09343	$C_{11}H_{17}NO_7$	8.14E+06	3.23E+06	2.59E+06	8.25E+05	1.70E+06	0.00E+00
274.97239	$C_6H_4N_4O_7S$	5.62E+05	6.02E+04	1.69E+06	9.90E+04	1.58E+03	0.00E+00
274.97616	$C_3H_8N_4O_7S_2$	6.52E+04	3.21E+04	7.65E+05	9.86E+03	0.00E+00	0.00E+00
274.99985	$C_{17}H_8S_2$	1.03E+05	3.35E+04	1.13E+05	2.27E+05	0.00E+00	2.33E+03
275.08848	$C_{10}H_{16}N_2O_7$	1.08E+06	4.20E+05	3.05E+06	3.44E+05	1.64E+04	1.57E+03
275.12900	$C_{16}H_{20}O_4$	2.13E+04	9.90E+05	7.28E+03	1.57E+04	1.46E+03	0.00E+00
277.03303	$C_{17}H_{10}O_2S$	1.57E+07	2.16E+07	3.94E+06	8.31E+03	0.00E+00	0.00E+00
277.08649	$C_{18}H_{14}O_3$	4.49E+04	1.47E+04	8.22E+04	3.00E+03	0.00E+00	0.00E+00
277.09284	$C_{11}H_{18}O_8$	7.14E+05	2.22E+05	1.92E+06	1.39E+05	9.31E+03	0.00E+00
277.11960	$C_{14}H_{18}N_2O_4$	1.80E+05	5.01E+05	1.07E+04	6.55E+04	3.18E+03	0.00E+00
277.14460	$C_{16}H_{22}O_4$	2.70E+06	1.14E+07	9.29E+05	1.31E+06	4.72E+05	2.92E+03
277.15599	$C_{15}H_{22}N_2O_3$	7.89E+04	6.60E+05	4.54E+03	1.04E+04	0.00E+00	9.28E+02

279.05680	$C_{19}H_8N_2O$	5.41E+05	5.32E+05	4.23E+05	1.94E+05	0.00E+00	0.00E+00
279.05991	$C_{16}H_{12}N_2OS$	1.09E+07	2.96E+06	2.01E+06	6.76E+05	2.04E+07	0.00E+00
279.09875	$C_{13}H_{16}N_2O_5$	6.99E+05	1.33E+06	2.00E+04	1.72E+05	1.24E+03	0.00E+00
279.12388	$C_{15}H_{20}O_5$	4.00E+06	4.52E+06	1.44E+06	1.63E+06	3.11E+04	0.00E+00
279.12715	$C_{12}H_{24}O_5S$	2.83E+05	1.48E+05	1.10E+06	4.05E+05	0.00E+00	0.00E+00
279.13522	$C_{14}H_{20}N_2O_4$	1.07E+05	5.23E+05	5.35E+03	1.14E+04	0.00E+00	0.00E+00
279.16022	$C_{16}H_{24}O_4$	2.67E+07	4.10E+07	1.75E+07	1.11E+07	1.59E+07	2.39E+03
279.19674	$C_{17}H_{28}O_3$	7.40E+04	7.01E+05	2.82E+03	7.48E+04	2.86E+06	0.00E+00
280.14024	$C_{11}H_{23}NO_7$	9.30E+06	3.63E+06	1.05E+07	6.42E+06	0.00E+00	7.12E+04
280.98422	$C_{13}H_2N_2O_6$	3.47E+06	2.40E+06	8.63E+06	8.65E+05	7.01E+03	0.00E+00
281.08789	$C_{11}H_{14}N_4O_5$	4.19E+06	3.17E+06	2.53E+06	6.95E+05	1.04E+03	0.00E+00
281.10069	$C_{18}H_{18}OS$	8.31E+05	2.70E+05	1.38E+06	8.62E+03	6.52E+06	0.00E+00
281.13957	$C_{15}H_{22}O_5$	2.04E+05	8.24E+04	1.61E+05	2.01E+04	2.39E+04	0.00E+00
281.14299	$C_{12}H_{26}O_5S$	2.89E+05	4.83E+05	2.70E+05	1.55E+05	1.60E+03	0.00E+00
281.17593	$C_{16}H_{26}O_4$	3.12E+07	4.44E+07	1.62E+07	1.22E+07	1.60E+07	3.52E+03
281.21240	$C_{17}H_{30}O_3$	1.16E+04	3.41E+05	0.00E+00	5.13E+04	9.94E+05	0.00E+00
282.08455	$C_{10}H_{13}N_5O_5$	4.01E+03	3.01E+05	1.65E+04	4.15E+05	0.00E+00	0.00E+00
283.06848	$C_{10}H_{12}N_4O_6$	4.03E+05	1.96E+05	2.20E+06	4.37E+05	0.00E+00	0.00E+00
283.11879	$C_{14}H_{20}O_6$	7.65E+05	4.75E+05	3.07E+05	1.87E+05	2.65E+04	0.00E+00
283.12764	$C_{17}H_{20}N_2S$	3.83E+05	3.21E+05	0.00E+00	8.27E+03	0.00E+00	0.00E+00
283.13750	$C_{15}H_{24}O_3S$	5.92E+04	3.67E+04	6.30E+04	1.17E+05	7.12E+05	6.38E+03
283.15520	$C_{15}H_{24}O_5$	1.69E+06	1.95E+06	4.02E+05	4.17E+05	5.56E+05	1.25E+03
283.19159	$C_{16}H_{28}O_4$	1.16E+07	2.16E+07	5.63E+06	5.90E+06	6.00E+06	2.58E+03
284.95429	$C_{11}H_2N_4O_2S_2$	0.00E+00	4.41E+03	6.11E+03	7.93E+04	0.00E+00	0.00E+00
285.09821	$C_{13}H_{18}O_7$	1.16E+05	3.80E+05	2.20E+04	6.74E+04	8.21E+03	0.00E+00
285.10696	$C_{16}H_{18}N_2OS$	1.06E+05	3.92E+05	6.00E+03	1.06E+04	0.00E+00	0.00E+00
285.10953	$C_{12}H_{18}N_2O_6$	0.00E+00	1.28E+03	0.00E+00	1.10E+03	1.93E+05	0.00E+00
285.20724	$C_{16}H_{30}O_4$	1.61E+07	3.55E+07	4.47E+06	1.90E+07	1.16E+07	1.39E+04
285.99639	$C_{17}H_5NO_2S$	0.00E+00	1.33E+06	1.25E+03	0.00E+00	0.00E+00	0.00E+00
286.96992	$C_{11}H_4N_4O_2S_2$	6.59E+03	1.61E+03	5.18E+03	5.12E+03	2.12E+06	0.00E+00
287.00111	$C_6H_{12}N_2O_7S_2$	4.11E+05	1.51E+06	1.09E+05	1.35E+05	1.93E+04	0.00E+00
287.07727	$C_{12}H_{16}O_8$	4.91E+05	4.64E+04	1.88E+05	4.50E+03	1.51E+03	0.00E+00
287.08856	$C_{11}H_{16}N_2O_7$	4.58E+07	4.77E+07	3.12E+07	1.83E+07	0.00E+00	9.75E+04
287.16539	$C_{18}H_{24}O_3$	4.86E+04	1.13E+06	1.51E+03	7.17E+04	2.54E+04	0.00E+00
287.22293	$C_{16}H_{32}O_4$	1.22E+06	2.18E+06	6.36E+05	3.67E+05	1.39E+06	0.00E+00

288.13151	$C_{10}H_{19}N_5O_5$	1.38E+06	4.29E+06	4.33E+04	7.50E+05	3.21E+06	0.00E+00
288.98708	$C_{19}H_2N_2S$	4.41E+04	0.00E+00	7.89E+05	9.26E+03	0.00E+00	0.00E+00
289.06959	$C_{19}H_{14}OS$	1.32E+05	1.45E+06	1.52E+06	1.04E+06	1.76E+04	0.00E+00
289.09258	$C_{12}H_{18}O_8$	3.69E+05	3.25E+05	2.41E+05	1.63E+05	3.14E+03	0.00E+00
289.18105	$C_{18}H_{26}O_3$	9.53E+05	5.21E+06	2.40E+05	1.91E+06	7.54E+05	0.00E+00
289.93649	$C_6HN_3O_9S$	7.33E+04	3.86E+03	1.69E+06	5.75E+04	0.00E+00	0.00E+00
289.99205	$C_{16}H_5NO_3S$	0.00E+00	8.31E+05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
290.06316	$C_9H_{13}N_3O_8$	9.06E+04	3.01E+05	3.34E+04	1.10E+05	0.00E+00	0.00E+00
290.08566	$C_{15}H_{17}NO_3S$	4.48E+06	1.94E+06	0.00E+00	0.00E+00	4.75E+04	0.00E+00
291.08347	$C_{10}H_{16}N_2O_8$	4.68E+09	1.71E+09	3.38E+04	3.80E+04	2.94E+08	0.00E+00
291.16370	$C_{14}H_{28}O_4S$	3.86E+05	1.22E+06	7.91E+04	1.57E+06	0.00E+00	0.00E+00
291.19668	$C_{18}H_{28}O_3$	1.67E+07	4.30E+07	6.09E+06	9.21E+06	7.35E+06	0.00E+00
292.02233	$C_{12}H_{11}N_3O_2S_2$	0.00E+00	0.00E+00	2.26E+04	1.40E+04	1.06E+05	0.00E+00
292.08044	$C_{18}H_{15}NOS$	1.34E+07	5.50E+06	0.00E+00	0.00E+00	5.38E+05	0.00E+00
292.10372	$C_{11}H_{19}NO_8$	7.55E+06	2.76E+06	1.67E+06	2.58E+05	1.78E+04	0.00E+00
292.14035	$C_{12}H_{23}NO_7$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.02E+05	0.00E+00
293.11447	$C_{14}H_{18}N_2O_5$	3.70E+05	6.60E+05	1.43E+04	9.54E+04	0.00E+00	0.00E+00
293.13946	$C_{16}H_{22}O_5$	1.98E+06	2.29E+06	4.75E+05	2.03E+05	1.61E+05	0.00E+00
293.21232	$C_{18}H_{30}O_3$	2.80E+07	8.78E+07	8.54E+06	1.72E+07	2.96E+07	1.17E+03
294.02966	$C_{10}H_9N_5O_4S$	8.27E+05	1.23E+06	4.28E+05	5.10E+05	5.88E+05	8.93E+02
294.03788	$C_{12}H_{13}N_3O_2S_2$	0.00E+00	5.19E+04	5.94E+03	0.00E+00	9.10E+05	0.00E+00
294.18265	$C_{15}H_{25}N_3O_3$	0.00E+00	2.62E+05	1.55E+05	2.37E+05	0.00E+00	3.28E+04
295.11858	$C_{15}H_{20}O_6$	1.14E+06	5.99E+05	8.77E+05	3.46E+05	2.25E+04	0.00E+00
295.13732	$C_{16}H_{24}O_3S$	1.72E+04	7.69E+03	1.92E+04	6.09E+04	5.03E+05	2.52E+03
295.13980	$C_{12}H_{24}O_8$	0.00E+00	2.23E+06	0.00E+00	0.00E+00	0.00E+00	1.72E+05
295.15507	$C_{16}H_{24}O_5$	2.30E+05	1.25E+06	1.54E+05	0.00E+00	0.00E+00	3.01E+04
295.19141	$C_{17}H_{28}O_4$	2.36E+05	5.26E+05	1.17E+04	1.64E+05	4.85E+05	8.51E+02
295.22774	$C_{18}H_{32}O_3$	6.54E+06	2.77E+07	1.91E+06	6.64E+06	1.07E+07	8.98E+03
296.09992	$C_{11}H_{15}N_5O_5$	3.67E+05	5.24E+05	1.19E+05	8.35E+05	0.00E+00	2.57E+04
296.95410	$C_{12}H_2N_4O_2S_2$	1.89E+04	2.58E+03	4.23E+04	9.31E+03	0.00E+00	0.00E+00
297.15285	$C_{16}H_{26}O_3S$	5.12E+05	0.00E+00	1.72E+05	7.66E+05	2.57E+06	9.84E+04
297.17043	$C_{16}H_{26}O_5$	1.40E+07	1.35E+07	1.05E+07	4.15E+06	5.90E+06	0.00E+00
297.24340	$C_{18}H_{34}O_3$	6.83E+05	3.13E+06	4.88E+05	0.00E+00	1.40E+06	2.23E+05
298.15619	$C_{17}H_{21}N_3O_2$	6.77E+05	7.38E+05	7.00E+05	1.56E+06	1.71E+06	5.48E+04
299.14992	$C_{15}H_{24}O_6$	4.03E+05	1.13E+05	1.12E+04	2.27E+04	4.98E+04	0.00E+00

299.18628	$C_{16}H_{28}O_5$	1.44E+07	1.35E+07	9.72E+06	3.20E+06	4.95E+06	3.22E+03
299.20170	$C_{20}H_{28}O_2$	3.53E+05	1.10E+06	2.10E+05	2.18E+05	1.26E+05	0.00E+00
300.19299	$C_{14}H_{27}N_3O_4$	9.35E+03	1.90E+05	3.03E+03	4.10E+04	0.00E+00	0.00E+00
301.10224	$C_{24}H_{14}$	1.02E+05	2.52E+05	8.55E+05	6.85E+05	6.86E+03	0.00E+00
301.12924	$C_{14}H_{22}O_7$	0.00E+00	4.30E+05	0.00E+00	1.17E+03	3.12E+05	1.29E+04
301.20194	$C_{16}H_{30}O_5$	5.87E+06	7.27E+06	2.34E+06	1.75E+06	5.35E+06	6.63E+02
302.03071	$C_{14}H_9NO_7$	0.00E+00	0.00E+00	3.92E+03	3.27E+04	1.28E+04	0.00E+00
302.05055	$C_{16}H_9N_5S$	8.82E+05	9.34E+05	1.06E+05	2.21E+04	1.34E+05	0.00E+00
302.14685	$C_{11}H_{21}N_5O_5$	8.58E+05	3.78E+06	1.59E+06	3.04E+06	5.59E+05	0.00E+00
303.16015	$C_{18}H_{24}O_4$	1.16E+04	8.39E+05	1.71E+03	1.77E+04	7.37E+03	0.00E+00
303.21770	$C_{16}H_{32}O_5$	2.06E+04	5.85E+04	1.79E+03	3.62E+03	4.17E+05	0.00E+00
304.07856	$C_{10}H_{15}N_3O_8$	4.58E+05	1.04E+06	2.83E+05	2.45E+05	0.00E+00	0.00E+00
305.17578	$C_{18}H_{26}O_4$	8.17E+05	1.00E+07	6.03E+05	1.06E+06	8.14E+04	0.00E+00
306.05787	$C_9H_{13}N_3O_9$	1.66E+04	7.17E+05	6.06E+04	0.00E+00	0.00E+00	0.00E+00
307.15847	$C_{14}H_{28}O_5S$	2.91E+05	6.28E+05	1.64E+05	1.46E+05	1.84E+03	0.00E+00
307.19139	$C_{18}H_{28}O_4$	1.90E+07	3.51E+07	7.83E+06	7.40E+06	9.28E+06	0.00E+00
308.98295	$C_{19}H_2O_5$	1.39E+05	7.01E+05	2.83E+04	6.20E+04	3.29E+03	0.00E+00
309.13423	$C_{16}H_{22}O_6$	3.20E+05	8.25E+04	1.33E+05	1.83E+04	5.67E+03	0.00E+00
309.17400	$C_{14}H_{30}O_5S$	2.42E+06	7.73E+06	1.68E+06	3.94E+06	0.00E+00	1.60E+05
309.20705	$C_{18}H_{30}O_4$	5.38E+07	1.01E+08	2.29E+07	2.18E+07	5.08E+07	0.00E+00
310.07930	$C_{11}H_{13}N_5O_6$	1.55E+05	3.17E+05	9.66E+05	3.16E+05	9.90E+05	0.00E+00
311.15001	$C_{16}H_{24}O_6$	5.17E+05	1.14E+06	3.11E+05	1.00E+05	6.10E+05	0.00E+00
311.16833	$C_{17}H_{28}O_3S$	3.01E+06	3.00E+05	1.83E+06	3.58E+06	3.37E+06	7.07E+05
311.18632	$C_{17}H_{28}O_5$	1.42E+06	1.86E+06	4.87E+05	3.82E+05	1.32E+06	9.41E+02
311.22270	$C_{18}H_{32}O_4$	1.65E+07	3.39E+07	5.50E+06	8.94E+06	1.09E+07	7.91E+03
312.09493	$C_{11}H_{15}N_5O_6$	5.94E+03	1.88E+06	5.44E+03	2.23E+06	0.00E+00	7.05E+04
312.17194	$C_{18}H_{23}N_3O_2$	4.31E+05	1.22E+06	5.64E+05	1.94E+06	1.64E+06	7.03E+04
313.06527	$C_{24}H_{10}O$	1.57E+07	1.87E+07	0.00E+00	0.00E+00	1.06E+07	0.00E+00
313.16554	$C_{16}H_{26}O_6$	5.05E+06	6.51E+06	3.28E+06	1.02E+06	4.41E+06	0.00E+00
313.18094	$C_{20}H_{26}O_3$	7.09E+03	9.34E+05	4.71E+03	2.47E+04	1.96E+03	0.00E+00
313.20209	$C_{17}H_{30}O_5$	5.42E+03	1.07E+04	1.19E+03	0.00E+00	2.69E+05	0.00E+00
313.23841	$C_{18}H_{34}O_4$	1.03E+06	2.96E+06	2.60E+05	5.21E+05	3.12E+06	2.98E+04
315.04151	$C_{18}H_8N_2O_4$	5.30E+05	1.22E+05	0.00E+00	0.00E+00	2.38E+05	0.00E+00
315.13504	$C_{17}H_{20}N_2O_4$	1.50E+05	1.96E+05	6.92E+04	2.13E+04	9.32E+05	1.16E+03
315.13864	$C_{22}H_{20}O_2$	1.55E+06	1.18E+05	1.69E+06	1.06E+03	0.00E+00	0.00E+00

315.18123	$C_{16}H_{28}O_6$	3.02E+06	3.45E+06	2.07E+06	9.16E+05	4.26E+06	1.29E+03
315.19656	$C_{20}H_{28}O_3$	8.08E+05	2.43E+06	1.12E+05	1.89E+06	6.32E+04	0.00E+00
315.21773	$C_{17}H_{32}O_5$	4.64E+03	6.21E+03	0.00E+00	0.00E+00	3.17E+05	0.00E+00
315.25410	$C_{18}H_{36}O_4$	3.57E+05	9.66E+05	8.63E+04	1.60E+05	3.79E+05	9.44E+03
316.15151	$C_{13}H_{23}N_3O_6$	3.00E+05	5.40E+05	5.07E+04	7.42E+04	0.00E+00	0.00E+00
316.18792	$C_{14}H_{27}N_3O_5$	4.67E+04	2.33E+05	8.62E+03	2.37E+04	8.99E+02	0.00E+00
317.09123	$C_{10}H_{22}O_9S$	7.47E+04	8.18E+05	6.65E+04	8.81E+04	0.00E+00	2.09E+04
317.19715	$C_{16}H_{30}O_6$	2.02E+03	3.77E+05	0.00E+00	8.21E+03	0.00E+00	0.00E+00
317.21217	$C_{20}H_{30}O_3$	3.37E+07	1.04E+08	1.71E+07	2.66E+07	2.73E+07	1.65E+03
319.05051	$C_{13}H_{12}N_4O_4S$	1.63E+07	1.24E+07	1.00E+07	3.80E+06	4.32E+06	0.00E+00
319.05864	$C_{23}H_{12}S$	6.23E+06	2.72E+06	3.29E+06	1.07E+06	1.76E+06	0.00E+00
319.22793	$C_{20}H_{32}O_3$	6.38E+05	5.82E+05	3.56E+05	4.69E+05	3.74E+05	0.00E+00
321.17088	$C_{18}H_{26}O_5$	1.06E+05	4.56E+05	5.28E+04	2.16E+04	1.66E+04	0.00E+00
321.17409	$C_{15}H_{30}O_5S$	1.08E+06	5.49E+06	1.01E+06	2.20E+05	1.28E+05	5.03E+04
323.18638	$C_{18}H_{28}O_5$	8.55E+06	1.58E+07	4.22E+06	4.04E+06	3.93E+06	0.00E+00
323.22278	$C_{19}H_{32}O_4$	2.46E+06	7.55E+06	5.54E+05	1.12E+06	5.56E+05	0.00E+00
324.97792	$C_{19}H_2O_6$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.97E+04	0.00E+00
325.04145	$C_{10}H_{14}O_{12}$	6.21E+05	1.33E+06	1.10E+05	7.36E+04	0.00E+00	0.00E+00
325.20199	$C_{18}H_{30}O_5$	3.50E+07	4.52E+07	2.38E+07	1.30E+07	2.09E+07	0.00E+00
327.14503	$C_{16}H_{24}O_7$	1.16E+05	1.07E+05	1.27E+05	2.87E+04	2.04E+04	0.00E+00
327.21755	$C_{18}H_{32}O_5$	6.72E+07	6.06E+07	4.53E+07	1.94E+07	3.88E+07	5.37E+03
328.18800	$C_{15}H_{27}N_3O_5$	7.43E+04	2.15E+05	8.18E+03	1.72E+04	0.00E+00	0.00E+00
329.03043	$C_{16}H_{10}O_8$	8.92E+05	8.91E+05	0.00E+00	0.00E+00	6.36E+05	0.00E+00
329.17591	$C_{20}H_{26}O_4$	5.34E+05	2.15E+06	2.79E+05	8.40E+05	1.02E+03	0.00E+00
329.23333	$C_{18}H_{34}O_5$	2.22E+07	3.09E+07	8.10E+06	7.26E+06	1.08E+07	6.05E+03
330.16722	$C_{14}H_{25}N_3O_6$	1.40E+05	3.99E+05	1.68E+04	2.83E+04	1.99E+03	0.00E+00
330.20357	$C_{15}H_{29}N_3O_5$	7.11E+04	1.81E+05	3.97E+03	6.88E+03	0.00E+00	0.00E+00
331.11478	$C_{13}H_{20}N_2O_8$	1.54E+05	4.37E+05	1.79E+05	2.24E+05	0.00E+00	0.00E+00
331.19154	$C_{20}H_{28}O_4$	8.29E+05	6.70E+06	4.63E+05	8.12E+05	4.01E+05	0.00E+00
331.99764	$C_{13}H_7N_3O_6S$	1.50E+06	1.44E+06	4.10E+05	4.62E+05	4.20E+06	0.00E+00
333.09415	$C_{12}H_{18}N_2O_9$	6.50E+03	3.01E+05	6.52E+04	1.87E+05	0.00E+00	0.00E+00
333.20716	$C_{20}H_{30}O_4$	2.62E+07	5.47E+07	1.07E+07	1.49E+07	4.28E+07	0.00E+00
334.21053	$C_{14}H_{33}N_5S_2$	1.17E+06	3.01E+06	3.37E+05	5.94E+05	8.76E+05	0.00E+00
335.04740	$C_8H_{16}O_{14}$	3.38E+06	3.38E+06	0.00E+00	0.00E+00	1.00E+06	0.00E+00
335.22290	$C_{20}H_{32}O_4$	1.57E+06	5.30E+06	3.62E+05	8.86E+05	8.99E+06	0.00E+00

337.23859	$C_{20}H_{34}O_4$	2.35E+06	7.83E+06	7.32E+05	1.15E+06	7.28E+06	0.00E+00
339.14492	$C_{17}H_{24}O_7$	5.61E+05	3.11E+05	2.60E+05	9.88E+04	1.87E+03	0.00E+00
339.16622	$C_{14}H_{28}O_9$	0.00E+00	1.84E+06	0.00E+00	0.00E+00	0.00E+00	1.30E+05
339.18144	$C_{18}H_{28}O_6$	1.07E+06	2.54E+06	2.66E+05	3.21E+05	8.44E+05	6.90E+03
339.20005	$C_{19}H_{32}O_3S$	1.90E+05	2.44E+05	4.34E+05	3.17E+05	7.46E+05	6.88E+04
341.02963	$C_{17}H_{10}O_8$	1.55E+06	3.27E+05	2.62E+06	1.61E+04	1.16E+05	0.00E+00
341.10867	$C_{12}H_{22}O_{11}$	3.29E+05	1.88E+05	8.18E+05	1.05E+05	0.00E+00	2.79E+03
341.12432	$C_{16}H_{22}O_8$	8.69E+05	7.63E+05	1.59E+05	1.21E+05	8.29E+03	0.00E+00
341.16070	$C_{17}H_{26}O_7$	1.22E+06	9.98E+05	1.69E+05	2.79E+05	7.71E+03	0.00E+00
341.19702	$C_{18}H_{30}O_6$	6.76E+06	1.15E+07	2.97E+06	3.24E+06	4.60E+06	0.00E+00
341.23350	$C_{19}H_{34}O_5$	8.35E+03	6.86E+03	6.02E+03	3.07E+03	6.45E+05	0.00E+00
341.99965	$C_6H_9N_5O_{10}S$	6.11E+05	3.92E+05	0.00E+00	0.00E+00	2.00E+06	0.00E+00
342.16715	$C_{15}H_{25}N_3O_6$	4.64E+05	7.26E+05	8.33E+04	1.47E+05	0.00E+00	0.00E+00
343.11308	$C_{26}H_{16}O$	1.12E+04	2.68E+04	4.14E+05	2.78E+05	0.00E+00	0.00E+00
343.21268	$C_{18}H_{32}O_6$	5.89E+06	9.73E+06	4.36E+06	3.48E+06	7.81E+06	0.00E+00
343.22806	$C_{22}H_{32}O_3$	4.99E+05	1.14E+06	3.14E+05	4.96E+05	2.30E+04	0.00E+00
343.99486	$C_{17}H_3N_3O_6$	4.83E+07	3.51E+07	4.73E+04	1.10E+03	4.35E+07	0.00E+00
344.18301	$C_{15}H_{27}N_3O_6$	8.65E+04	1.83E+05	7.38E+03	2.51E+04	4.58E+03	7.88E+02
344.21607	$C_{20}H_{31}N_3S$	1.83E+04	3.87E+04	1.84E+04	6.70E+03	2.89E+05	0.00E+00
345.22850	$C_{18}H_{34}O_6$	1.84E+04	1.75E+06	0.00E+00	5.88E+05	4.03E+05	0.00E+00
345.99947	$C_{18}H_5NO_7$	1.06E+05	7.01E+04	0.00E+00	0.00E+00	1.70E+05	0.00E+00
347.18659	$C_{20}H_{28}O_5$	3.59E+05	3.18E+06	1.69E+05	5.25E+05	1.58E+05	0.00E+00
348.97651	$C_{13}H_6N_2O_8S$	3.85E+05	9.00E+04	1.13E+06	6.64E+04	0.00E+00	0.00E+00
349.20215	$C_{20}H_{30}O_5$	7.78E+06	1.46E+07	3.35E+06	3.59E+06	6.24E+06	0.00E+00
350.12563	$C_{18}H_{17}N_5O_3$	3.52E+04	1.07E+05	7.54E+04	1.08E+05	0.00E+00	2.15E+03
350.92818	$C_{13}H_4O_8S_2$	7.75E+04	7.45E+04	1.82E+05	0.00E+00	3.16E+05	2.32E+04
351.01233	$C_{22}H_8O_3S$	6.49E+04	1.67E+05	0.00E+00	0.00E+00	1.42E+05	0.00E+00
351.21775	$C_{20}H_{32}O_5$	1.64E+07	2.15E+07	8.97E+06	6.28E+06	4.95E+06	1.15E+03
351.99762	$C_{23}H_3N_3S$	4.22E+05	6.60E+04	3.02E+04	1.64E+03	2.06E+05	0.00E+00
352.01464	$C_{23}H_3N_3O_2$	4.31E+04	4.03E+04	0.00E+00	0.00E+00	1.40E+05	0.00E+00
352.99695	$C_{14}H_{10}O_9S$	3.10E+06	1.10E+06	0.00E+00	0.00E+00	3.58E+05	0.00E+00
353.01072	$C_9H_{10}N_2O_{13}$	4.12E+06	3.25E+06	0.00E+00	0.00E+00	4.37E+06	0.00E+00
353.14282	$C_{18}H_{26}O_5S$	1.88E+05	2.47E+06	3.34E+05	5.54E+04	2.60E+04	4.53E+03
353.20049	$C_{16}H_{34}O_6S$	6.23E+05	2.66E+06	4.14E+05	1.10E+06	0.00E+00	9.13E+04
353.23347	$C_{20}H_{34}O_5$	3.51E+06	8.65E+06	6.83E+05	1.57E+06	3.04E+06	0.00E+00

354.99390	$C_{13}H_8O_{12}$	1.40E+06	6.47E+05	4.72E+03	0.00E+00	1.34E+05	0.00E+00
355.04538	$C_{18}H_{12}O_8$	2.54E+05	4.50E+03	9.19E+04	2.87E+03	0.00E+00	0.00E+00
355.13983	$C_{17}H_{24}O_8$	1.14E+06	3.60E+05	9.33E+05	1.34E+05	5.49E+03	0.00E+00
355.17619	$C_{18}H_{28}O_7$	1.47E+05	1.24E+05	1.28E+05	3.25E+04	1.03E+04	0.00E+00
355.24916	$C_{20}H_{36}O_5$	5.73E+05	1.89E+06	1.13E+05	3.40E+05	4.62E+04	0.00E+00
356.11009	$C_{14}H_{19}N_3O_8$	0.00E+00	4.32E+04	0.00E+00	0.00E+00	0.00E+00	0.00E+00
357.02936	$C_{15}H_{10}N_4O_5S$	6.66E+05	8.24E+05	0.00E+00	0.00E+00	8.32E+05	0.00E+00
357.15556	$C_{17}H_{26}O_8$	7.15E+05	4.29E+05	2.82E+05	9.61E+04	2.09E+05	0.00E+00
357.19227	$C_{18}H_{30}O_7$	7.20E+03	2.29E+05	1.53E+03	3.09E+04	1.93E+04	0.00E+00
357.20742	$C_{22}H_{30}O_4$	3.46E+03	1.70E+05	1.65E+03	1.44E+04	3.89E+03	0.00E+00
358.99482	$C_{18}H_4N_2O_7$	3.16E+05	2.06E+05	0.00E+00	0.00E+00	0.00E+00	9.31E+04
359.20775	$C_{18}H_{32}O_7$	5.51E+04	1.22E+06	2.77E+04	6.43E+04	6.20E+05	0.00E+00
359.22297	$C_{22}H_{32}O_4$	2.47E+06	2.25E+06	7.52E+05	3.92E+05	4.24E+05	5.46E+02
360.09137	$C_{18}H_{19}NO_5S$	2.26E+06	1.33E+06	6.86E+05	1.98E+05	0.00E+00	0.00E+00
363.18146	$C_{20}H_{28}O_6$	4.71E+05	2.34E+06	1.97E+05	1.45E+05	2.40E+05	0.00E+00
364.02611	$C_{23}H_3N_5O$	7.52E+05	7.68E+04	5.17E+05	2.41E+04	1.51E+03	0.00E+00
364.94158	$C_{13}H_2O_{13}$	5.11E+04	7.56E+03	1.77E+05	1.07E+04	0.00E+00	0.00E+00
365.19706	$C_{20}H_{30}O_6$	3.47E+06	6.50E+06	8.95E+05	6.68E+05	2.11E+06	0.00E+00
367.01036	$C_{19}H_4N_4O_5$	1.96E+05	2.03E+05	0.00E+00	0.00E+00	6.67E+05	0.00E+00
367.21284	$C_{20}H_{32}O_6$	1.75E+05	5.80E+05	8.38E+04	1.41E+05	1.29E+06	0.00E+00
368.00941	$C_{15}H_7N_5O_5S$	1.01E+05	4.99E+04	0.00E+00	0.00E+00	5.56E+05	0.00E+00
368.03416	$C_{17}H_{11}N_3O_5S$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.69E+05	0.00E+00
368.05881	$C_{10}H_{15}N_3O_{12}$	1.63E+05	7.60E+03	1.44E+06	3.59E+04	0.00E+00	0.00E+00
369.00557	$C_9H_{10}N_2O_{14}$	2.40E+06	2.16E+06	1.45E+03	0.00E+00	7.27E+05	0.00E+00
369.00566	$C_9H_{10}N_2O_{14}$	6.29E+05	5.51E+05	0.00E+00	0.00E+00	2.28E+05	5.44E+02
369.13736	$C_{18}H_{26}O_6S$	1.37E+04	9.83E+03	1.23E+04	1.54E+04	5.16E+05	0.00E+00
369.18970	$C_{23}H_{30}O_2S$	8.38E+03	1.43E+04	6.86E+03	8.40E+03	3.54E+05	4.47E+02
370.95859	$C_{19}H_4N_2O_3S_2$	8.19E+04	1.85E+04	1.63E+05	9.19E+03	0.00E+00	0.00E+00
371.00256	$C_{22}H_4N_4OS$	6.60E+04	4.94E+04	0.00E+00	0.00E+00	3.19E+05	0.00E+00
371.13478	$C_{17}H_{24}O_9$	1.19E+06	3.27E+05	1.19E+06	5.84E+04	3.80E+03	0.00E+00
371.24411	$C_{20}H_{36}O_6$	5.17E+05	8.74E+05	1.89E+05	3.42E+05	1.61E+05	0.00E+00
372.21427	$C_{17}H_{31}N_3O_6$	3.62E+05	3.11E+05	3.29E+05	4.87E+04	0.00E+00	0.00E+00
373.15050	$C_{17}H_{26}O_9$	2.31E+06	1.67E+06	1.25E+06	4.85E+05	6.87E+04	0.00E+00
374.99273	$C_{15}H_8N_2O_8S$	6.07E+04	6.17E+04	0.00E+00	0.00E+00	2.49E+05	0.00E+00
377.19477	$C_{25}H_{30}OS$	1.63E+06	2.84E+06	8.94E+05	1.13E+06	1.01E+06	0.00E+00

377.23348	$C_{22}H_{34}O_5$	4.87E+05	1.04E+06	7.84E+04	2.17E+05	4.61E+05	0.00E+00
377.27313	$C_{20}H_{42}O_4S$	0.00E+00	0.00E+00	0.00E+00	2.98E+05	0.00E+00	5.37E+04
379.15634	$C_{24}H_{20}N_4O$	1.27E+05	8.66E+04	9.28E+04	6.22E+05	1.62E+06	3.35E+04
379.21053	$C_{25}H_{32}OS$	1.18E+05	3.53E+05	1.12E+04	3.80E+04	2.00E+05	0.00E+00
381.00575	$C_{10}H_{10}N_2O_{14}$	3.22E+04	4.45E+04	7.58E+03	0.00E+00	2.05E+05	0.00E+00
381.19195	$C_{20}H_{30}O_7$	6.37E+05	1.20E+06	5.67E+05	1.19E+05	1.32E+05	0.00E+00
383.19246	$C_{16}H_{32}O_{10}$	0.00E+00	1.34E+06	0.00E+00	0.00E+00	0.00E+00	9.21E+04
383.20769	$C_{20}H_{32}O_7$	2.48E+04	7.74E+04	1.32E+04	1.30E+04	5.35E+05	0.00E+00
384.15227	$C_{15}H_{23}N_5O_7$	3.57E+05	4.12E+04	2.20E+05	2.51E+04	8.20E+03	0.00E+00
384.93533	$C_9H_6O_{15}S$	2.15E+06	5.72E+05	7.52E+05	3.16E+05	7.41E+05	9.40E+04
387.28651	$C_{20}H_{40}N_2O_5$	2.29E+05	6.39E+05	1.40E+05	2.98E+05	0.00E+00	5.21E+04
389.11877	$C_{27}H_{18}O_3$	2.23E+06	1.56E+06	3.54E+06	1.16E+06	0.00E+00	1.88E+03
389.16781	$C_{15}H_{26}N_4O_8$	3.00E+06	2.15E+06	4.49E+06	1.80E+06	1.19E+05	0.00E+00
390.98758	$C_{15}H_8N_2O_9S$	1.06E+05	1.04E+05	3.58E+03	0.00E+00	4.05E+05	0.00E+00
391.04654	$C_{22}H_8N_4O_4$	1.97E+06	1.29E+06	0.00E+00	0.00E+00	8.17E+04	0.00E+00
393.12334	$C_{17}H_{22}N_4O_5S$	8.91E+04	2.38E+05	2.84E+04	1.03E+05	1.60E+04	0.00E+00
393.18986	$C_{25}H_{30}O_2S$	2.08E+05	4.74E+05	1.15E+05	1.29E+05	1.43E+05	0.00E+00
395.20563	$C_{25}H_{32}O_2S$	3.87E+05	5.38E+05	1.41E+05	2.91E+04	3.87E+05	0.00E+00
396.12692	$C_{22}H_{23}NO_4S$	1.28E+06	4.04E+05	1.39E+06	3.08E+05	6.40E+02	0.00E+00
397.22126	$C_{25}H_{34}O_2S$	4.00E+03	7.96E+03	0.00E+00	1.36E+03	3.51E+05	0.00E+00
397.22693	$C_{18}H_{38}O_7S$	0.00E+00	5.67E+05	0.00E+00	0.00E+00	0.00E+00	3.57E+04
399.98536	$C_{19}H_3N_3O_8$	3.43E+03	3.55E+03	3.25E+03	0.00E+00	5.95E+05	0.00E+00
401.19496	$C_{27}H_{30}OS$	2.09E+04	7.26E+04	3.24E+03	1.91E+05	1.43E+03	0.00E+00
401.92553	$C_8H_5NO_{16}S$	5.87E+04	1.16E+05	2.94E+05	5.73E+04	1.00E+06	6.68E+04
405.02825	$C_{18}H_{14}O_9S$	1.04E+06	2.07E+04	4.30E+06	2.24E+03	0.00E+00	0.00E+00
408.20587	$C_{18}H_{35}NO_7S$	7.67E+04	0.00E+00	3.48E+05	1.00E+05	0.00E+00	0.00E+00
411.11407	$C_{28}H_{16}N_2O_2$	4.69E+04	4.48E+03	1.59E+05	2.33E+03	0.00E+00	0.00E+00
411.15107	$C_{29}H_{20}N_2O$	5.06E+03	6.73E+02	0.00E+00	4.66E+04	0.00E+00	0.00E+00
412.14727	$C_{16}H_{23}N_5O_8$	2.97E+04	4.82E+04	1.39E+05	6.26E+04	0.00E+00	0.00E+00
417.07574	$C_{19}H_{18}N_2O_7S$	0.00E+00	0.00E+00	4.31E+03	0.00E+00	2.24E+05	0.00E+00
418.91634	$C_7H_4N_2O_{17}S$	3.65E+04	3.90E+04	4.20E+04	0.00E+00	2.49E+05	1.08E+04
421.22688	$C_{20}H_{38}O_7S$	0.00E+00	1.39E+05	0.00E+00	2.48E+05	0.00E+00	2.67E+04
425.08052	$C_{12}H_{18}N_4O_{13}$	0.00E+00	0.00E+00	2.07E+06	7.09E+04	0.00E+00	0.00E+00
425.18199	$C_{21}H_{30}O_9$	1.16E+04	1.98E+05	8.28E+03	1.51E+04	1.50E+03	0.00E+00
427.01037	$C_{24}H_4N_4O_5$	1.50E+05	0.00E+00	5.73E+05	0.00E+00	0.00E+00	0.00E+00

429.12531	$C_{28}H_{18}N_2O_3$	3.30E+04	5.32E+03	1.05E+05	3.40E+03	0.00E+00	0.00E+00
430.08469	$C_{14}H_{17}N_5O_{11}$	4.65E+04	0.00E+00	0.00E+00	0.00E+00	1.07E+06	0.00E+00
431.10450	$C_{27}H_{16}N_2O_4$	2.35E+06	1.87E+06	2.46E+06	1.07E+06	0.00E+00	0.00E+00
431.18995	$C_{24}H_{32}O_5S$	2.21E+03	0.00E+00	1.23E+03	2.44E+03	7.91E+03	0.00E+00
433.01509	$C_9H_{14}N_4O_{14}S$	0.00E+00	1.87E+04	0.00E+00	0.00E+00	4.22E+05	1.37E+03
437.00424	$C_{15}H_{10}N_4O_{10}S$	6.18E+06	3.65E+06	4.11E+06	3.69E+06	2.81E+06	0.00E+00
439.07641	$C_{25}H_{16}N_2O_4S$	3.32E+07	2.27E+07	5.26E+07	1.22E+07	3.14E+05	9.72E+04
439.18249	$C_{18}H_{32}O_{12}$	0.00E+00	1.46E+04	0.00E+00	4.52E+04	6.28E+02	0.00E+00
440.14214	$C_{17}H_{23}N_5O_9$	9.50E+04	2.76E+04	2.83E+05	9.06E+04	0.00E+00	0.00E+00
440.88897	$C_{10}H_2O_{18}S$	5.59E+04	8.35E+04	6.45E+04	2.10E+05	0.00E+00	1.88E+04
441.17728	$C_{22}H_{26}N_4O_6$	4.08E+04	2.05E+05	1.39E+04	1.69E+04	1.94E+03	0.00E+00
445.17227	$C_{21}H_{26}N_4O_7$	2.47E+04	2.45E+04	0.00E+00	0.00E+00	1.63E+05	0.00E+00
448.99250	$C_8H_{10}N_4O_{18}$	8.65E+03	1.36E+03	6.36E+04	0.00E+00	0.00E+00	0.00E+00
452.92275	$C_{16}H_6O_{12}S_2$	3.07E+06	6.45E+05	5.89E+05	5.72E+05	1.71E+06	3.64E+04
460.20509	$C_{18}H_{31}N_5O_9$	3.91E+04	1.62E+03	4.38E+03	4.53E+03	0.00E+00	0.00E+00
462.97530	$C_{14}H_{12}N_2O_{12}S_2$	9.49E+04	2.60E+04	1.28E+05	1.51E+04	6.61E+04	0.00E+00
468.89694	$C_{19}H_2O_{11}S_2$	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.07E+04
469.91311	$C_{15}H_5NO_{13}S_2$	2.21E+04	1.79E+04	3.02E+04	1.43E+04	1.99E+05	6.34E+03
472.16666	$C_{30}H_{23}N_3O_3$	1.99E+05	1.13E+06	1.64E+06	1.71E+04	1.22E+04	0.00E+00
477.17260	$C_{32}H_{22}N_4O$	3.54E+06	1.14E+06	3.25E+06	8.53E+05	0.00E+00	0.00E+00
482.92876	$C_{11}H_4N_2O_{20}$	0.00E+00	0.00E+00	2.38E+05	2.59E+05	0.00E+00	7.02E+04
485.25369	$C_{28}H_{38}O_7$	4.00E+06	2.46E+06	2.98E+06	3.30E+05	1.47E+06	0.00E+00
486.17769	$C_{26}H_{25}N_5O_5$	1.49E+05	3.90E+04	2.32E+05	2.39E+05	0.00E+00	0.00E+00
495.18268	$C_{32}H_{24}N_4O_2$	2.70E+07	6.55E+06	1.64E+07	3.33E+06	0.00E+00	8.60E+03
496.18686	$C_{29}H_{27}N_3O_5$	2.33E+04	6.48E+04	2.96E+03	4.49E+03	0.00E+00	0.00E+00
503.16162	$C_{31}H_{24}N_2O_5$	6.76E+06	6.45E+06	2.18E+07	1.28E+07	1.95E+05	3.69E+04
507.17265	$C_{22}H_{28}N_4O_{10}$	0.00E+00	5.63E+02	5.71E+02	9.16E+03	0.00E+00	0.00E+00
514.89363	$C_{10}H_4N_4O_{17}S_2$	3.07E+05	1.15E+06	2.93E+05	3.80E+05	5.44E+05	1.90E+04
520.91078	$C_{18}H_2O_{19}$	1.59E+05	8.32E+04	1.58E+05	6.30E+04	3.34E+05	5.12E+03
542.24773	$C_{23}H_{37}N_5O_{10}$	0.00E+00	4.62E+04	0.00E+00	0.00E+00	7.00E+05	0.00E+00
549.16775	$C_{32}H_{26}N_2O_7$	1.26E+05	7.97E+04	4.30E+04	0.00E+00	5.78E+04	3.71E+03
563.17242	$C_{22}H_{32}N_2O_{15}$	1.32E+06	3.27E+05	7.40E+05	3.59E+05	0.00E+00	0.00E+00
571.15098	$C_{34}H_{24}N_2O_7$	1.48E+03	1.64E+03	5.35E+04	1.95E+04	0.00E+00	0.00E+00
583.17570	$C_{37}H_{28}O_7$	3.00E+07	7.18E+06	1.30E+03	0.00E+00	9.10E+04	0.00E+00
584.17867	$C_{30}H_{27}N_5O_8$	4.85E+06	7.63E+05	0.00E+00	0.00E+00	0.00E+00	0.00E+00

587.29238	$C_{38}H_{40}N_2O_4$	3.97E+05	5.12E+05	4.89E+03	3.06E+05	6.42E+05	0.00E+00
603.11023	$C_{26}H_{24}N_2O_{15}$	1.63E+05	1.89E+05	5.49E+04	3.38E+04	1.96E+03	0.00E+00
605.08690	$C_{29}H_{22}N_2O_{11}S$	0.00E+00	2.71E+04	3.46E+04	6.20E+04	0.00E+00	9.36E+03
605.15748	$C_{34}H_{26}N_2O_9$	1.40E+07	7.32E+06	0.00E+00	0.00E+00	4.66E+05	0.00E+00
617.15755	$C_{35}H_{26}N_2O_9$	1.29E+05	3.88E+05	2.08E+06	2.67E+06	0.00E+00	0.00E+00
617.15795	$C_{23}H_{30}N_4O_{16}$	1.73E+04	9.64E+04	8.38E+05	1.04E+06	0.00E+00	0.00E+00
646.21677	$C_{19}H_{41}N_3O_{21}$	3.25E+04	1.02E+03	2.00E+05	6.08E+03	0.00E+00	0.00E+00
656.21228	$C_{19}H_{39}N_5O_{20}$	4.68E+04	2.25E+04	2.63E+05	3.75E+05	6.28E+03	0.00E+00
664.35485	$C_{44}H_{47}N_3O_3$	4.39E+05	4.57E+05	3.43E+05	1.88E+05	0.00E+00	0.00E+00
665.21734	$C_{34}H_{38}N_2O_{10}S$	2.15E+06	1.84E+06	1.53E+06	2.65E+06	1.07E+05	0.00E+00
678.39137	$C_{42}H_{53}N_3O_5$	6.30E+04	6.24E+04	2.49E+05	6.29E+04	2.74E+05	2.61E+04
679.21702	$C_{22}H_{40}N_4O_{20}$	5.02E+04	2.83E+04	2.26E+05	1.93E+05	6.90E+04	0.00E+00
683.22911	$C_{42}H_{36}O_9$	1.23E+07	7.62E+06	8.79E+06	3.37E+05	0.00E+00	0.00E+00
683.22942	$C_{30}H_{40}N_2O_{16}$	0.00E+00	0.00E+00	1.89E+06	3.14E+05	0.00E+00	0.00E+00
695.00464	$C_{24}H_{16}N_4O_{19}S$	2.92E+05	4.91E+05	1.87E+05	2.10E+05	0.00E+00	0.00E+00
711.22397	$C_{35}H_{40}N_2O_{12}S$	7.89E+05	1.95E+05	1.10E+06	1.30E+05	0.00E+00	1.75E+03
711.22466	$C_{31}H_{40}N_2O_{17}$	1.82E+06	1.57E+06	1.69E+06	1.36E+06	6.64E+03	0.00E+00
722.24279	$C_{32}H_{41}N_3O_{16}$	2.77E+05	3.10E+05	2.02E+05	9.72E+04	4.60E+04	0.00E+00
722.24340	$C_{20}H_{45}N_5O_{23}$	9.98E+04	2.23E+05	3.44E+04	1.45E+04	1.90E+05	0.00E+00
733.20638	$C_{28}H_{38}N_4O_{19}$	4.92E+03	1.20E+03	2.46E+04	4.21E+05	0.00E+00	0.00E+00
737.23999	$C_{33}H_{42}N_2O_{17}$	1.37E+04	7.92E+03	6.35E+04	3.05E+05	3.28E+04	0.00E+00
737.74171	$C_{49}H_{94}N_4$	5.61E+03	5.94E+03	2.38E+04	1.60E+05	1.09E+04	0.00E+00