Experiment: Dodecane Low NO, $(NH_4)_2SO_4$, dry

Mean M_w (g mol^{-1}) 429.01

M_w	P_{vap} (atm)	C_A/C_{IS}	Compound Class	SMILES String
100.16	1.35E-02	1.01E-06	ketone	CCCC(=O)CC
106.17	1.14E-02	2.43E-06	alcohol	CCCC(C)O
120.19	3.73E-03	8.34E-06	alcohol	CCCCC(C)O
126.20	3.73E-03	1.13E-05	dihydrofuran	CCCC1CC=C(C)O1
128.22	3.71E-03	1.70E-05	ketone	CCCCCC(=O)CC
130.23	1.45E-03	2.64E-05	alcohol	CCCCCC(O)CC
132.20	3.99E-04	3.25E-05	ketone	CCCCCC(C)=O
134.22	4.42E-03	3.91E-06	alcohol	CCCCCC(C)O
136.19	7.66E-04	4.36E-05	furan	CC\C=C\C1=CC=C(C)O1
138.21	1.22E-03	3.42E-05	furan	CCCCC1=CC=C(C)O1
140.23	1.21E-03	6.44E-05	aldehyde	CCCCC\C=C\CC=O
142.24	4.73E-04	2.03E-04	ketone	CCCCCCCC(C)=O
144.21	1.31E-04	3.32E-04	alcohol	CCCCCCCC(C)O
148.25	3.99E-04	3.10E-05	alcohol	CCCCCCC(C)O
150.18	3.21E-05	6.13E-04	furan	CC1=CC=C(C\C=C\C=O)O1
152.24	1.01E-04	2.42E-04	ketone	CCCC\C=C\C=C\C(C)=O
154.25	1.01E-04	5.90E-04	ketone	CCCCCC\C=C\C(C)=O
156.27	1.55E-04	6.45E-04	ketone	CCCCCCCCC(C)=O
158.29	4.27E-05	1.07E-03	alcohol	CCCCCCCCC(C)O
160.26	4.73E-04	3.82E-05	ketone	CCCCCCCC(C)=O
162.27	1.31E-04	3.51E-04	alcohol	CCCCCCCC(C)O
166.26	3.32E-05	4.37E-04	aldehyde	CCCCCC\C=C\C=C\C=O
168.28	3.32E-05	1.54E-03	aldehyde	CCCCCCCC\C=C\C=O
170.30	5.06E-05	1.17E-03	aldehyde	CCCCCCCCCCC=O
172.27	2.72E-06	1.53E-02	hydroxycarbonyl	CCCCCCCC(O)CC=O
176.26	2.68E-05	5.00E-04	furan	CC\C=C\C=C\C1=CC=C(CC)O1
178.28	2.68E-05	1.42E-03	furan	CCCC\C=C\C1=CC=C(CC)O1
180.29	2.68E-05	3.74E-03	furan	CCCCCCC1=CC=C(CC)O1
164.20	4.08E-06	6.60E-02	dihydrofuran	CCC1=CCC(O1)C(=O)CCC=N
182.31	4.24E-05	6.86E-04	dihydrofuran	CCCCCCC1CC=C(CC)O1
183.25	9.93E-07	1.03E+00	dihydrofuran	CCC1=CCC(O1)C(O)CCC=N
184.32	1.65E-05	7.62E-03	ketone	CCCCCCCCC(=O)CCC
186.21	2.77E-06	2.19E-02	furan	C=CC1=CC=C(O1)C1=CC=C(O1)C=C
190.24	2.77E-06	5.83E-03	furan	CCC1=CC=C(CC2=CC=C(C)O2)O1
192.26	1.98E-06	5.88E-03	furan	CCC\C=C\C(=O)C1=CC=C(CC)O1
193.25	6.26E-07	1.03E-01	furan	CC1=CC=C(O1)C(=O)CCCCC=N
194.27	3.01E-06	5.32E-03	furan	CCCCCC(=O)C1=CC=C(CC)O1
195.26	6.26E-07	6.65E-01	furan	CC1=CC=C(O1)C(=O)CCCCC=N
196.29	1.71E-06	2.85E-02	furan	CCCCC(=O)CC1=CC=C(CC)O1
180.25	1.33E-06	5.27E-01	furan	CC1=CCC(O1)C(=O)CCCCC=N
198.31	2.75E-06	3.25E-02	ketone	CCCCCCCC(=O)CC(=O)CC
199.29	4.35E-08	1.21E+01	imine	CCCCC(O)CC(=O)CCCC=N
200.32	2.91E-07	1.93E-01	hydroxycarbonyl	CCCCCC(O)CC(=O)CCCC
208.26	6.96E-07	1.18E-01	furan	CCCC(=O)CC(=O)C1=CC=C(CC)O1
210.27	1.48E-06	3.11E-02	dihydrofuran	CCCC(=O)CC(=O)C1CC=C(CC)O1
211.26	2.99E-08	5.24E+00	dihydrofuran	CC1CC=C(O1)C(=O)CC(O)CCC=N
212.29	3.79E-07	6.22E-02	ketone	CCCCCC(=O)CC(=O)CC(=O)CC
196.29	7.27E-06	3.73E-02	furan	CCCCCCC(=O)C1CC=C(C)O1
214.31	4.84E-08	7.20E-01	hydroxycarbonyl	CCCCCC(O)CC(=O)CC(=O)CC
216.32	2.06E-09	5.40E+01	hydroxycarbonyl	CCCCCC(O)CC(=O)CC(O)CC
218.34	1.97E-10	1.61E+02	alcohol	CCCCCC(O)CC(O)CC(O)CC
224.26	2.24E-07	4.81E-02	dihydrofuran	CCC(=O)CC(=O)CC(=O)C1CC=C(C)O1
226.27	1.60E-08	7.31E-01	ketone	CCC(=O)CC(=O)CCCC(=O)CC(C)=O
228.29	2.11E-09	2.18E+01	hydroxycarbonyl	CCC(=O)CC(=O)CCCC(O)CC(C)=O
230.30	1.01E-10	5.26E+02	hydroxycarbonyl	CCC(=O)CC(O)CCCC(O)CC(C)=O
242.32	1.98E-07	6.34E-02	ester	C\C=C\C=C\C=C\C(=O)O\C=C\C=C\C=C\C=C
244.29	4.72E-12	2.32E+03	hydroxycarbonyl	CCC(=O)CC(O)CC(=O)CC(O)CC(C)=O
230.31	6.05E-07	2.16E-02	ester	CC\C=C\C=C\C=C\C(=O)O\C=C\C=C\C=C
282.47	2.11E-08	1.69E+00	ester	CCCCCCCCCOC(=O)\C=C\CCCCCC

286.41	4.60E-10	2.47E+01	acid anhydride	CCCCCCCC(=O)OC(=O)CCCC(O)CCC
382.63	1.07E-11	9.98E+02	ether	CCCCCCCC(=O)C(CCC)OC(CCCC)C(=O)CCCCCC
394.60	1.76E-12	5.92E+03	ether	CCCCCCCC(=O)C(CCC)OC(CCCC)C(=O)CC1CC=C(C)O1
396.61	1.91E-12	6.04E+03	ether	CCCCCCCC(=O)C(CCC)OC(CCCC)C(=O)CC(=O)CCCC
398.63	1.89E-13	1.12E+05	ether	CCCCCCCC(=O)C(CCC)OC(CCCC)C(=O)CC(O)CCCC
400.64	9.06E-15	3.07E+06	ether	CCCCCCCC(=O)C(CCC)OC(CCCC)C(O)CC(O)CCCC
410.60	5.30E-14	6.86E+05	ether	CCCCCCC(O)CC(=O)C(CC)OC(CC)C(=O)CCCC1=CCC(C)O1
412.61	3.36E-14	5.35E+05	ether	CCCCCCCCC(=O)C(CC)OC(CCC)C(=O)CC(=O)CC(O)CCC
414.63	1.85E-15	1.42E+07	ether	CCCCCCCCC(O)C(CC)OC(CCC)C(=O)CC(=O)CC(O)CCC
398.63	2.54E-13	9.93E+04	ether	CCCCCCCCC(O)C(CC)OC(CCC)C(=O)CC(=O)CCCCC
416.64	1.03E-16	3.73E+08	ether	CCCCCCCCC(O)C(CC)OC(CCC)C(=O)CC(O)C(O)CCCC
426.59	8.14E-15	3.73E+08	peroxyhemiacetal	CCCCCCC(=O)CC(=O)C(CC)OC(CCC)C(=O)CC(O)C(=O)CCCC
412.61	3.02E-13	3.97E+04	ether	CCCCCCCCC(O)(CCC)OOC(CCC1CC=C(CC)O1)C(=O)CC
430.63	1.50E-17	2.74E+09	peroxyhemiacetal	CCCCCCC(O)CC(=O)C(CC)OC(CCC)C(=O)CC(O)C(O)CCCC
414.63	2.19E-13	3.73E+08	peroxyhemiacetal	CCCCCCCC(O)(CCCC)OOC(CCC)C(=O)CC(=O)CCCCC
426.59	6.15E-14	2.65E+05	peroxyhemiacetal	CCCCCC(=O)CC(=O)C(CCC)OOC(O)(CCCC)CC1CC=C(CC)O1
428.61	5.68E-14	2.73E+05	peroxyhemiacetal	CCCCCC(=O)CC(=O)C(CCC)OOC(O)(CCCC)CC1CCC(CC)O1
442.59	2.71E-15	7.92E+06	peroxyhemiacetal	CCCCCC(=O)CC(=O)C(CCC)OOC(O)(CCC(C)=O)CC1CCC(CC)O1
444.61	4.86E-16	2.54E+07	peroxyhemiacetal	CCCCCC(=O)CC(=O)C(CCC)OOC(O)(CCC(C)O)CC1CCC(CC)O1

Experiment: Dodecane High NO, $(NH_4)_2SO_4$, dry

Mean M_w ($g\ mol^{-1}$) 495.33

M_w	P_{vap} (atm)	C_A/C_{IS}	Compound Class	SMILES String
112.17	1.13E-02	5.14E-05	dihydrofuran	CCC1CC=C(C)O1
114.19	4.42E-03	6.36E-05	ketone	CCCC(=O)CCC
122.17	2.34E-03	9.59E-05	furan	C\C=C\C1=CC=C(C)O1
124.18	2.34E-03	1.51E-04	furan	CCCC1=CC=C(C)O1
126.20	3.71E-03	1.17E-04	dihydrofuran	CCCC1CC=C(C)O1
128.22	4.42E-03	7.95E-05	ketone	CCCCC(=O)CCC
130.23	3.99E-04	2.55E-04	alcohol	CCCCCCC(C)O
132.20	1.55E-05	1.37E-02	alcohol	CCCCC(O)C(C)O
134.18	5.42E-07	5.47E-01	alcohol	CCC(O)C(O)C(C)O
136.15	3.77E-09	9.64E+01	alcohol	CC(O)C(O)C(O)CO
138.21	7.66E-04	7.52E-04	furan	CCCCC1=CC=C(C)O1
139.20	2.37E-04	9.53E-04	dihydrofuran	CC1=CCC(CCC=N)O1
140.23	1.21E-03	7.55E-04	dihydrofuran	CCCCC1CC=C(C)O1
141.21	7.07E-05	3.34E-03	ketone	CC(=O)CCCCCC=N
142.20	7.07E-05	5.17E-03	ketone	CC(=O)CCCCCC=O
144.21	7.40E-06	1.14E-02	hydroxycarbonyl	CC(=O)CCCCCCO
146.23	6.80E-07	9.53E-02	alcohol	CC(O)CCCCCCO
148.16	3.46E-08	3.75E+00	hydroxycarbonyl	CC(O)C(O)C(O)CC=O
150.13	3.46E-08	1.08E+01	hydroxycarbonyl	OCC(O)C(O)C(O)C=O
151.17	6.09E-05	1.52E-03	furan	CC1=CC=C(O1)C(=O)CC=N
152.24	2.51E-04	2.10E-03	furan	CCCCC1=CC=C(CC)O1
153.18	1.30E-04	1.33E-03	dihydrofuran	CC1=CCC(O1)C(=O)CC=N
154.25	3.97E-04	1.90E-03	dihydrofuran	CCCCC1CC=C(CC)O1
155.20	9.29E-06	2.59E-02	dihydrofuran	CC1=CCC(O1)C(O)CC=N
156.27	1.55E-04	1.80E-03	ketone	CCCCCCCC(=O)CC
158.24	8.33E-06	9.93E-03	hydroxycarbonyl	CCC(O)CCCCCC=O
160.21	1.80E-07	1.28E+00	hydroxycarbonyl	CC(O)CCCC(O)CC=O
162.14	8.20E-08	6.69E+00	hydroxycarbonyl	CC(O)C(=O)C(O)C(O)C=O
163.22	1.60E-05	5.72E-03	furan	CC1=CC=C(C\C=C\CC=N)O1
164.25	8.19E-05	5.41E-03	furan	CCC\C=C\CC1=CC=C(C)O1
165.24	1.60E-05	6.05E-03	furan	CC1=CC=C(CCCCC=N)O1
166.26	8.19E-05	5.57E-03	furan	CCCCCCC1=CC=C(C)O1
167.25	2.53E-05	5.27E-03	dihydrofuran	CC1=CCC(CCCCC=N)O1
168.28	1.30E-04	5.40E-03	dihydrofuran	CCCCCCC1CC=C(C)O1
169.18	4.24E-06	2.73E-02	ketone	CC(=O)CC(=O)CC(=O)CC=N
170.25	7.56E-06	3.52E-02	ketone	CC(=O)CCCCCCCC=O
174.24	5.90E-08	1.04E+00	hydroxycarbonyl	CCC(O)CCC(O)CCC=O
176.26	2.68E-05	6.97E-03	furan	CCCC1=CC=C(O1)\C=C\C=C\C
178.28	2.68E-05	1.70E-02	furan	CCC\C=C\C1=CC=C(CCC)O1
179.22	1.60E-05	6.95E-03	furan	CC1=CC=C(C\C=C\CC=N)O1
180.29	2.68E-05	4.99E-02	furan	CCCCCCC1=CC=C(CC)O1
181.24	8.81E-07	2.23E-01	imine	CCCC(=O)CC(=O)C\C=C\C=N
182.31	4.24E-05	5.81E-02	dihydrofuran	CCCCCCC1CC=C(CC)O1
183.21	2.35E-08	1.43E+01	furan	CC(O)C1=CC=C(O1)C(O)CC=N
184.28	8.40E-06	3.39E-02	ketone	CCCCCCCC(=O)CC(C)=O
190.24	1.12E-06	1.47E-01	furan	C\C=C\C=C\C(=O)CC1=CC=C(C)O1
192.26	1.12E-06	7.29E-01	furan	CCC\C=C\C(=O)CC1=CC=C(C)O1
193.25	6.26E-07	3.16E-01	furan	CC1=CC=C(O1)C(=O)CCCCC=N
194.27	1.71E-06	1.02E+00	furan	CCCCCC(=O)CC1=CC=C(C)O1
196.29	2.71E-06	1.01E+00	dihydrofuran	CCCCCC(=O)CC1CC=C(C)O1
197.28	3.66E-07	1.44E+00	imine	CC(=O)CC(=O)CCCCCCC=N
198.31	8.08E-07	2.04E+00	ketone	CCCCCC(=O)CCCCC(C)=O
200.32	2.91E-07	5.92E-01	hydroxycarbonyl	CCCCCC(=O)CCCCC(C)O
206.24	6.25E-07	2.57E-01	furan	CCC(=O)C(=O)\C=C\C1=CC=C(CC)O1
207.27	8.41E-07	8.17E-02	furan	CCC(=N)C(=O)CCC1=CC=C(CC)O1
208.26	8.41E-07	8.90E-01	furan	CCC(=O)C(=O)CCC1=CC=C(CC)O1
209.29	8.41E-07	2.60E-01	imine	CCC(=N)C(=O)CCC1CC=C(CC)O1
210.27	1.33E-06	1.42E+00	dihydrofuran	CCC(=O)C(=O)CCC1CC=C(CC)O1

212.29	8.16E-08	9.80E+00	dihydrofuran	CCC(=O)CC(O)CC1CC=C(CC)O1
214.31	4.84E-08	7.85E+00	hydroxycarbonyl	CCCCCC(O)CC(=O)CC(=O)CC
224.26	8.56E-09	2.57E+01	furan	CC(O)CC(=O)CC(=O)CC1=CC=C(C)O1
225.29	4.60E-10	1.93E+02	furan	CC(O)CC(O)CC(=N)CC1=CC=C(C)O1
226.27	4.85E-08	1.22E+01	ketone	CCCC(=O)CC(=O)CC(=O)CC(=O)CC
227.30	7.28E-10	3.10E+02	imine	CC(O)CC(O)CC(=N)CC1CC=C(C)O1
228.29	7.28E-10	3.66E+02	dihydrofuran	CC(O)CC(O)CC(=O)CC1CC=C(C)O1
229.28	2.21E-10	4.58E+02	imine	CCCC(=O)CC(=O)CC(O)CC(O)C=N
230.30	1.01E-10	2.36E+03	hydroxycarbonyl	CC(O)CC(O)CC(=O)CCCCC(C)=O
231.29	8.39E-12	1.10E+04	imine	CCCC(=O)CC(O)CC(O)CC(O)C=N
240.26	5.93E-09	1.12E+01	ketone	CCC(=O)CC(=O)CC(=O)CC(=O)CC(C)=O
225.29	4.85E-08	5.96E+00	imine	CCCC(=O)CC(=O)CC(=O)CC(=N)CC
242.27	8.54E-10	3.32E+02	hydroxycarbonyl	CCC(O)CC(=O)CC(=O)CC(=O)CC(C)=O
243.30	4.73E-11	4.79E+04	imine	CCC(=N)CC(=O)CC(=O)CC(O)CC(C)O
244.29	4.73E-11	8.23E+03	hydroxycarbonyl	CCC(=O)CC(=O)CC(=O)CC(O)CC(C)O
245.32	1.12E-07	5.78E+00	nitrate	CCCCCCC(=O)CC(CCC)O[N+]([O-])=O
246.35	1.00E-07	1.23E+00	ether	CCC1=CC=C(CCOC\C=C\C=C\C=C\C)O1
255.27	1.16E-08	1.22E+01	nitrate	CCC(CC(=O)CC1=CC=C(CC)O1)O[N+]([O-])=O
256.30	1.42E-09	4.61E+01	acid anhydride	CCCC(=O)CCC(=O)OC(=O)CCC(=O)CC
257.29	5.48E-09	1.28E+02	nitrate	CCC(CC(O)CC1=CC=C(CC)O1)O[N+]([O-])=O
258.27	1.08E-11	1.31E+04	hydroxycarbonyl	CC(O)C(O)CC(=O)CC(=O)CC(=O)CC(C)=O
259.30	8.67E-09	8.41E+01	nitrate	CCC(CC(O)CC1=CCC(CC)O1)O[N+]([O-])=O
260.29	5.29E-13	2.07E+05	hydroxycarbonyl	CC(O)C(O)CC(O)CC(=O)CC(=O)CC(C)=O
261.32	1.97E-09	1.15E+02	nitrate	CCCCCC(O)CC(=O)CC(CC)O[N+]([O-])=O
263.33	2.19E-10	6.77E+02	nitrate	CCCCCC(O)CC(O)CC(CC)O[N+]([O-])=O
234.34	2.07E-12	9.64E+10	alcohol	CCCCCC(O)CC(O)CC(O)C(C)O
271.27	4.55E-10	1.28E+02	nitrate	CCC1=CC=C(CC(=O)CC(O[N+]([O-])=O)C(C)O)O1
273.29	6.53E-11	3.50E+03	nitrate	CCC1=CC=C(CC(O)CC(O[N+]([O-])=O)C(C)O)O1
274.31	5.72E-10	1.29E+02	acid anhydride	CCCC(O)CCC(=O)OC(=O)CCC(=O)CC
275.30	1.38E-10	1.73E+03	nitrate	CCC1CC=C(CC(CC(O)C(C)O)O[N+]([O-])=O)O1
289.28	8.51E-11	7.28E+02	nitrate	CCC1CC=C(CC(O[N+]([O-])=O)C(O)C(=O)C(C)O)O1
290.31	4.52E-14	1.29E+06	acid anhydride	CC(O)CC(=O)CCC(=O)OC(=O)CCC(O)C(C)O
291.30	1.30E-12	6.08E+04	nitrate	CC(O)C(O)CC(CC1CC=C(O1)C(C)O)O[N+]([O-])=O
292.33	1.11E-14	7.59E+06	acid anhydride	CCC(O)CCC(=O)OC(=O)CCC(O)C(O)C(C)O
304.30	2.58E-13	4.44E+05	acid anhydride	CCC(O)C(=O)CC(=O)OC(=O)CCC(O)C(=O)C(C)O
306.40	3.58E-10	2.08E+02	ester	CCCCC1=CC=C(CCC(=O)OCC2CC=C(CC)O2)O1
308.42	5.66E-10	1.35E+02	ester	CCCCC1CC=C(CCC(=O)OCC2CC=C(CC)O2)O1
325.41	3.51E-10	2.02E+02	nitrate	CC\C=C\CC(C\C=C\OCCC1CC=C(CC)O1)O[N+]([O-])=O
439.59	5.75E-14	1.01E+06	nitrate ether	CCCCCC(OC(CCC1=CCC(CC)O1)C(CC)O[N+]([O-])=O)C1CC=C(CC)O1
457.61	8.80E-16	1.20E+08	ether	CCCCCC(=O)CCC(OC(C(O)CCCC)C1CC=C(CC)O1)C(CC)O[N+]([O-])=O
459.62	1.54E-16	6.06E+08	ether	CCCCCC(=O)CCC(OC(CCCC(=O)CC)C(O)CCCC)C(CC)O[N+]([O-])=O
471.59	2.07E-17	3.62E+09	ether	CCC(O)CC(O)C(OC(CCC1=CCC(CC)O1)C(CC)O[N+]([O-])=O)C1=CCC(CC)O1
473.61	8.07E-18	8.78E+09	ether	CCC(O)CC(O)C(CCCC(=O)CC)OC(CCC1=CCC(CC)O1)C(CC)O[N+]([O-])=O
414.63	1.65E-16	4.50E+08	ether	CCCCCC(=O)CCC(CCC)OC(CCCC(=O)CC)C(O)CC(O)CC
490.64	9.29E-16	1.04E+08	nitrate ether	CCCCCCC(CCC(CC)O[N+]([O-])=O)OC(CCC(=O)CCCCC)C(CC)O[N+]([O-])=O
504.62	4.54E-17	1.91E+09	nitrate ether	CCCCCC(=O)CCC(OC(CCCC(=O)CC)CCC(CC)O[N+]([O-])=O)C(CC)O[N+]([O-])=O
506.64	1.64E-17	4.75E+09	nitrate ether	CCCCCC(=O)CCC(OC(CCCC(O)CC)CCC(CC)O[N+]([O-])=O)C(CC)O[N+]([O-])=O
518.60	7.67E-18	1.16E+10	nitrate ether	CCCCCC(=O)CCC(OC(CCCC(=O)CC)CCC(CC)O[N+]([O-])=O)C(O[N+]([O-])=O)C(C)=O

Experiment: Cyclododecane Low NO, $(NH_4)_2SO_4$, dry

Mean M_w ($g\ mol^{-1}$) 384.52

M_w	P_{vap} (atm)	C_A/C_{IS}	Compound Class	SMILES String
110.16	7.17E-03	1.97E-05	furan	CCC1=CC=C(C)O1
116.16	2.38E-04	1.11E-04	hydroxycarbonyl	CCC(O)CCC=O
118.13	3.32E-05	1.82E-03	hydroxycarbonyl	CC(O)C(O)C(C)=O
120.10	2.60E-07	5.20E-01	hydroxycarbonyl	OCC(O)C(O)C=O
122.17	2.34E-03	3.09E-05	furan	C\C=C\C1=CC=C(C)O1
124.18	2.34E-03	1.98E-05	furan	CCCC1=CC=C(C)O1
126.16	7.24E-04	2.50E-05	dihydrofuran	CC1=CCC(CC=O)O1
128.17	2.16E-04	1.29E-04	ketone	CC(=O)CCCCC=O
129.16	2.38E-04	1.77E-04	hydroxycarbonyl	CCCC(O)CC=O
130.19	7.79E-05	5.15E-04	hydroxycarbonyl	CCCCC(O)CC=O
132.16	1.69E-06	1.24E-01	hydroxycarbonyl	CC(O)CC(O)CC=O
133.19	8.32E-04	3.96E-05	imine	CCCCC(O)C=N
134.13	3.85E-07	6.52E-01	hydroxycarbonyl	CC(O)C(O)C(O)C=O
118.18	3.14E-04	8.90E-05	hydroperoxide	CCCCCCOO
136.10	8.14E-11	1.70E+03	carboxylic acid	OCC(O)C(O)C(O)=O
120.10	7.02E-06	2.84E-03	hydroperoxide	CC(O)C(OO)C=O
138.21	7.66E-04	7.47E-05	furan	CCCCC1=CC=C(C)O1
140.23	1.21E-03	3.74E-05	dihydrofuran	CCCCC1CC=C(C)O1
146.19	1.98E-06	5.20E-02	hydroxycarbonyl	CC(O)CCCC(O)C=O
130.19	2.72E-04	9.77E-04	hydroxycarbonyl	CCCCCC(O)C=O
149.23	1.03E-04	2.58E-04	hydroxycarbonyl	CCCCCCCOO
150.22	2.51E-04	6.86E-04	furan	CC\C=C\C1=CC=C(CC)O1
152.24	2.51E-04	6.09E-04	furan	CCCCC1=CC=C(CC)O1
153.25	3.97E-04	4.95E-05	dihydrofuran	CCCCC1CC=C(CC)O1
154.25	3.97E-04	2.49E-04	dihydrofuran	CCCCC1CC=C(CC)O1
156.23	3.66E-05	1.31E-03	dihydrofuran	CCC(O)CC1CC=C(C)O1
156.27	1.55E-04	2.52E-04	ketone	CCCCCC(=O)CCCC
158.24	8.33E-06	7.30E-03	hydroxycarbonyl	CCCCC(=O)CC(O)CC
160.21	3.23E-07	5.33E-01	hydroxycarbonyl	CCCCC(O)C(O)CC=O
160.24	2.55E-05	2.54E-02	imine	CCCCCC(O)CC=N
161.22	2.55E-05	3.93E-03	hydroxycarbonyl	CCCCCC(O)CC=O
162.25	5.32E-05	1.52E-02	hydroperoxide	CCCCCC(CC)OO
163.22	1.60E-05	7.43E-03	furan	CCC1=CC=C(O1)\C=C\CC=N
164.25	8.19E-05	2.46E-03	furan	CCC\C=C\C1=CC=C(CC)O1
166.26	1.30E-04	7.00E-04	dihydrofuran	CCCCCC1CC=C(CC)O1
168.28	1.30E-04	6.48E-04	dihydrofuran	CCCCCC1CC=C(CC)O1
170.30	5.06E-05	7.98E-04	aldehyde	CCCCCCCCCCC=O
173.26	5.90E-08	3.93E-01	alcohol	CCCCC(O)CC(O)CC=N
174.20	8.82E-09	8.50E+00	hydroxycarbonyl	OC(CCC=O)CC(O)CC=O
176.17	5.53E-10	3.01E+02	hydroxycarbonyl	OC(CC=O)C(O)C(O)CC=O
177.20	4.48E-10	6.04E+01	imine	CCC(O)C(O)C(O)C(O)C=N
178.28	2.68E-05	2.28E-02	furan	CCCC\C=C\C1=CC=C(CC)O1
179.26	5.23E-06	1.83E-02	furan	CCCCC1=CC=C(CCC=N)O1
180.29	2.68E-05	6.15E-02	furan	CCCCCCC1=CC=C(CC)O1
181.28	8.27E-06	3.27E-02	dihydrofuran	CCC1=CCC(CCCCC=N)O1
182.31	4.24E-05	6.33E-03	dihydrofuran	CCCCCCC1CC=C(CC)O1
184.32	1.65E-05	8.95E-03	ketone	CCCCCCC(=O)CCCCC
186.30	8.90E-07	4.34E-02	hydroxycarbonyl	CCCCCC(O)CCCCC=O
190.24	1.31E-09	5.40E+01	hydroxycarbonyl	CC(O)CCCC(O)CC(O)C=O
192.26	1.12E-06	2.44E-01	furan	CCCC(=O)\C=C\C1=CC=C(CC)O1
193.29	3.01E-06	1.38E-02	furan	CCCCC1=CC=C(O1)C(=N)CCC
194.27	1.71E-06	3.86E-01	furan	CCCC(=O)CCC1=CC=C(CC)O1
195.26	5.23E-06	1.79E-02	furan	CCC1=CC=C(CCCCC=N)O1
196.29	2.71E-06	5.57E-01	furan	CCCC(=O)CCC1CC=C(CC)O1

197.32	8.08E-07	2.55E-01	imine	CCCCCC(=O)CCC(=N)CCC
198.31	2.75E-06	1.71E-01	ketone	CCCCCCC(=O)CC(=O)CCC
199.29	4.35E-08	3.43E+00	hydroxycarbonyl	OC(CCCCCCC=O)CCC=N
205.30	3.63E-07	5.28E-02	hydroperoxide	CCCC(CCCCCC=O)OO
206.19	4.72E-12	4.15E+03	hydroxycarbonyl	OC(CC(O)C(O)C(O)CC=O)C=O
208.26	2.84E-07	3.08E-01	furan	CCC1=CC=C(CCC(=O)CC(C)=O)O1
210.27	4.49E-07	7.11E-01	furan	CCC1=CCC(CCC(=O)CC(C)=O)O1
211.26	2.52E-09	1.97E+01	imine	CCC1=CC=C(CC(O)C(O)CC=N)O1
212.29	1.20E-07	2.45E+00	ketone	CCCCCC(=O)CCC(=O)CC(C)=O
213.28	3.98E-09	1.44E+01	imine	CCC1=CCC(CC(O)C(O)CC=N)O1
214.31	4.84E-08	4.24E+00	hydroxycarbonyl	CCCCCC(O)CCC(=O)CC(C)=O
220.27	2.60E-13	9.08E+04	hydroxycarbonyl	OCCCC(O)C(O)CC(O)CCC=O
226.27	1.76E-08	3.27E+00	dihydrofuran	CCC1=CCC(O1)C(O)CC(=O)CC(C)=O
228.29	9.90E-09	1.02E+01	hydroxycarbonyl	CCCCCC(=O)C(O)CC(=O)CC(C)=O
230.30	6.12E-10	1.01E+02	hydroxycarbonyl	CCCCCC(O)C(O)CC(=O)CC(C)=O
256.25	1.82E-10	1.54E+02	hydroxycarbonyl	CC(=O)CC(=O)CC(O)C(=O)CC(=O)CC(C)=O
234.34	7.16E-12	5.69E+03	alcohol	CCCCCCC(O)C(O)C(O)C(O)CC
282.42	8.55E-09	4.36E+00	acid anhydride	CCCCCCCC(=O)OC(=O)CCC\C=C\CCC
284.48	2.11E-08	2.53E+00	ester	CCCCCCCCCOC(=O)CCCCCCCC
344.54	2.82E-13	1.13E+05	ester	CCCCCCCCCC(=O)OCCC(O)CCCC(O)CCC
376.58	2.15E-12	5.48E+04	peroxyhemiacetal	OC1(CC\C=C/CCCCC\C=C\1)OOC1CCCCCCC\C=C/CC1
390.56	2.92E-14	3.62E+06	ether	O=CCCCCC(CCC(=O)CCC=O)OC1CC\C=C/CCCCC\C=C\1
391.60	2.15E-12	1.61E+04	peroxyhemiacetal	OC1(CC\C=C/CCCCC\C=C\1)OOC1CC\C=C/CCC\C=C/CC1

Experiment: Cyclododecane High NO, $(NH_4)_2SO_4$, dry

Mean M_w ($g\ mol^{-1}$) 458.38

M_w	P_{vap} (atm)	C_A/C_{IS}	Compound Class	SMILES String
112.17	1.13E-02	5.51E-05	dihydrofuran	CCC1CC=C(C)O1
122.17	2.34E-03	3.17E-04	furan	C\C=C\C1=CC=C(C)O1
124.18	2.34E-03	3.41E-04	furan	CCCC1=CC=C(C)O1
125.13	6.60E-04	5.68E-04	imine	C=CC(=O)C(=O)CC=N
126.20	3.71E-03	2.69E-04	dihydrofuran	CCC1CC=C(CC)O1
128.17	4.45E-04	1.67E-03	dihydrofuran	CC(O)C1=CCC(C)O1
130.19	7.79E-05	2.85E-02	hydroxycarbonyl	CCCC(=O)CC(C)O
132.16	3.02E-06	1.33E+00	hydroxycarbonyl	CC(O)C(O)CC(C)=O
133.15	3.85E-07	3.03E+00	imine	CC(O)C(O)C(O)C=N
115.15	2.38E-04	1.49E-02	hydroxycarbonyl	CC(O)CCCC=O
117.17	4.73E-05	1.52E-02	hydroxycarbonyl	CCCC(O)C(C)O
136.19	7.66E-04	1.56E-03	alcohol	CCC1=CC=C(O1)\C=C\C
137.14	5.51E-04	8.81E-04	furan	CC1=CC=C(O1)C(=O)C=N
138.21	7.66E-04	2.22E-03	furan	CCCC1=CC=C(CC)O1
139.15	1.17E-03	4.15E-04	dihydrofuran	CC1=CCC(O1)C(=O)C=N
140.09	5.67E-05	2.07E-02	ketone/aldehyde	O=CC(=O)\C=C\C(=O)C=O
142.11	8.59E-05	8.63E-03	ketone/aldehyde	O=CC(=O)CCC(=O)C=O
144.21	2.55E-05	4.23E-02	hydroxycarbonyl	CC(O)CCCCCC=O
146.14	3.64E-07	7.67E+00	hydroxycarbonyl	OC(CC=O)CC(O)C=O
147.17	6.86E-08	6.51E+00	imine	CC(O)CC(O)C(O)C=N
148.21	2.51E-04	1.36E-02	furan	CCC1=CC=C(O1)\C=C\C=C
131.15	1.69E-06	4.10E-01	hydroxycarbonyl	CC(O)CC(O)CC=O
150.22	2.51E-04	5.99E-03	furan	CC\C=C\C1=CC=C(CC)O1
151.12	7.22E-05	1.01E-02	furan	N=CC1=CC=C(O1)C(=O)C=O
152.24	2.51E-04	6.29E-03	furan	CCCCCC1=CC=C(C)O1
153.14	9.22E-06	5.35E-02	furan	OC(C=O)C1=CC=C(O1)C=N
154.21	7.74E-05	1.32E-02	furan	CCC1=CCC(CCC=O)O1
156.23	2.31E-05	5.83E-02	ketone/aldehyde	CCC(=O)CCCCCC=O
158.24	8.33E-06	5.44E-01	hydroxycarbonyl	CCC(O)CCCCCC=O
159.19	1.19E-07	7.01E+00	imine	CC(O)C(=O)CC(O)CC=N
160.21	3.23E-07	2.24E+01	hydroxycarbonyl	CCCC(O)C(O)CCC=O
161.20	6.17E-09	2.38E+02	imine	CC(O)C(O)CC(O)CC=N
162.23	8.19E-05	6.69E-02	furan	CCC1=CC=C(O1)\C=C\C=C\C
163.22	1.05E-05	9.89E-02	imine	CCC1=CC=C(C\C=C\C=N)O1
164.25	8.19E-05	4.13E-02	furan	CC\C=C\CC1=CC=C(CC)O1
165.24	1.60E-05	4.62E-02	imine	CCC1=CC=C(CCCC=N)O1
166.26	8.19E-05	2.31E-02	furan	CCCCCC1=CC=C(CC)O1
167.25	2.53E-05	3.23E-02	imine	CCC1=CCC(CCCC=N)O1
168.28	1.30E-04	8.36E-03	dihydrofuran	CCCCCC1CC=C(CC)O1
170.30	5.06E-05	1.01E-02	ketone/aldehyde	CCCCCCCCC(=O)CC
172.27	1.90E-05	4.09E-02	hemiacetal	CCCCC1CCC(O)(CC)O1
174.20	3.71E-03	7.35E-04	dihydrofuran	CCC1CC=C(CC)O1
175.23	4.00E-09	1.36E+02	imine	CCC(O)CC(O)CC(O)C=N
176.26	2.68E-05	1.98E-01	furan	CC\C=C\CC1=CC=C(O1)\C=C\C
177.25	5.23E-06	2.69E-01	imine	CCC1=CC=C(C\C=C\CC=N)O1
178.28	2.68E-05	3.94E-01	furan	CCC\C=C\CC1=CC=C(CC)O1
179.18	2.85E-06	1.63E+00	imine	CC(=O)C1=CC=C(O1)C(=O)CC=N
180.29	2.68E-05	1.39E+00	furan	CCCCCCC1=CC=C(CC)O1
181.19	5.74E-06	1.12E+00	dihydrofuran	CC(=O)C1=CCC(O1)C(=O)CC=N
182.31	4.24E-05	9.83E-02	dihydrofuran	CCCCCCC1CC=C(CC)O1
184.28	3.91E-06	4.80E-01	dihydrofuran	CCCC(O)CC1CC=C(CC)O1
188.27	1.93E-08	3.39E+01	hydroxycarbonyl	CC(O)CC(O)CCCCCC=O
190.24	6.59E-10	5.20E+03	hydroxycarbonyl	CCC(O)CCC(O)C(O)CC=O
191.23	2.71E-06	3.58E-01	nitrate	CCCC(CC(O)CC)O[N+]([O-])=O
192.26	1.12E-06	7.01E+00	furan	CCC(=O)\C=C\CC1=CC=C(CC)O1
193.29	1.71E-06	1.03E+00	imine	CCC(=N)CCCC1=CC=C(CC)O1
194.27	1.71E-06	1.38E+01	furan	CCCCC(=O)CC1=CC=C(CC)O1
195.31	2.71E-06	1.73E+00	imine	CCC(=N)CCCC1CC=C(CC)O1
196.29	2.71E-06	8.73E+00	dihydrofuran	CCCCC(=O)CC1CC=C(CC)O1
197.32	8.08E-07	4.38E+00	imine	CCC(=N)CCCCCCC(=O)CC
198.31	8.08E-07	4.63E+00	ketone/aldehyde	CCCCC(=O)CCCCC(=O)CC
200.28	4.35E-08	3.65E+01	hydroxycarbonyl	CCC(O)CCCCC(=O)CCC=O
205.25	1.38E-11	1.78E+04	imine	CCC(O)CC(O)CC(O)C(O)C=N
206.24	2.11E-07	7.72E+00	furan	CCC1=CC=C(O1)\C=C\C(=O)CC(C)=O
207.23	2.56E-08	2.94E+01	nitrate	CCC(O)C(CCC(C)O)O[N+]([O-])=O

208.26	2.84E-07	3.02E+01	furan	CCC(=O)CC(=O)CC1=CC=C(CC)O1
209.25	1.46E-07	1.43E+01	imine	CCCC1=CC=C(O1)C(O)C(=O)CC=N
210.27	4.49E-07	4.04E+01	dihydrofuran	CCC(=O)CC(=O)CC1CC=C(CC)O1
211.26	2.31E-07	1.42E+01	imine	CCCC1=CCC(O1)C(O)C(=O)CC=N
212.29	8.16E-08	2.18E+02	dihydrofuran	CCC(=O)CC(O)CC1CC=C(CC)O1
213.28	5.32E-09	5.70E+02	imine	CCCC1=CCC(O1)C(O)C(O)CC=N
214.31	1.42E-08	1.46E+02	hydroxycarbonyl	CCC(=O)CCCCC(O)CC(=O)CC
222.24	1.11E-07	7.27E+00	furan	CCC1=CC=C(O1)C(=O)CC(=O)CC(C)=O
223.27	6.06E-07	6.69E-01	imine	CCCCC1=CCC(O1)C(=O)C(=O)CC=N
224.26	6.18E-09	6.11E+02	furan	CCC1=CC=C(O1)C(=O)CC(O)CC(C)=O
225.29	4.60E-10	2.87E+03	imine	CCC1=CC=C(CC(O)CC(O)CC=N)O1
226.27	1.32E-08	8.33E+02	dihydrofuran	CCC1=CCC(O1)C(=O)CC(O)CC(C)=O
227.26	5.55E-07	4.49E+00	nitrate	CCC(CCCC1=CC=C(C)O1)O[N+]([O-])=O
228.29	2.11E-09	5.96E+03	hydroxycarbonyl	CCCC(=O)CC(O)CC(=O)CC(=O)CC
229.23	6.66E-08	5.74E+01	nitrate	CCC1=CC=C(CC(O[N+]([O-])=O)C(C)O)O1
230.30	1.01E-10	1.29E+04	hydroxycarbonyl	CCCC(=O)CC(O)CC(=O)CC(O)CC
238.28	1.96E-15	2.09E+08	alcohol	CC(O)CC(O)CC(O)C(O)C(O)C(C)O
239.22	3.93E-10	1.35E+03	nitrate	CCC(O)C(O)C(O)CC(C)O[N+]([O-])=O
240.26	5.84E-10	2.00E+03	furan	CCC1=CC=C(O1)C(O)CC(=O)C(O)C(C)=O
241.29	1.82E-07	2.00E+01	nitrate	CCC(CCCC1=CC=C(CC)O1)O[N+]([O-])=O
242.27	7.71E-12	2.69E+05	furan	CC(O)C(O)CC(=O)CC1=CC=C(O1)C(C)O
243.30	2.87E-07	1.14E+01	nitrate	CCCCC(CC1CC=C(CC)O1)O[N+]([O-])=O
244.29	1.22E-11	1.01E+05	dihydrofuran	CC(O)C(O)CC(=O)CC1CC=C(O1)C(C)O
293.32	1.56E-13	1.19E+07	nitrate	CCCC(O)C(O[N+]([O-])=O)C(O)CC(O)CC(=O)CC
255.27	1.16E-08	7.49E+01	nitrate	CCC(=O)CC(CC1=CC=C(CC)O1)O[N+]([O-])=O
257.29	1.83E-08	8.62E+01	nitrate	CCC(=O)CC(CC1CC=C(CC)O1)O[N+]([O-])=O
259.30	1.97E-09	8.41E+02	nitrate	CCC(=O)CCCCC(CC(=O)CC)O[N+]([O-])=O
261.32	1.97E-09	1.31E+03	nitrate	CCC(O)CCCCC(CC(=O)CC)O[N+]([O-])=O
266.29	7.99E-17	3.21E+09	hydroxycarbonyl	CC(O)C(O)C(O)CC(O)CC(O)CC(O)C=O
271.27	2.20E-09	2.74E+02	nitrate	CCC(=O)CC(CC1CC=C(O1)C(C)=O)O[N+]([O-])=O
273.29	9.74E-10	1.57E+03	nitrate	CCC(O)CC(CC1CC=C(O1)C(C)=O)O[N+]([O-])=O
275.30	9.70E-10	4.72E+02	nitrate	CCC(O)CC(CCCCC(=O)C(C)=O)O[N+]([O-])=O
287.27	1.57E-09	1.76E+02	nitrate	CCCC(=O)C(O[N+]([O-])=O)C(=O)CC(=O)CC(=O)CC
289.28	5.88E-11	9.18E+03	nitrate	CCCC(=O)C(O[N+]([O-])=O)C(=O)CC(O)CC(=O)CC
290.32	1.19E-08	5.73E+01	nitrate	CCCCC(O[N+]([O-])=O)\C=C\CC(CCC)O[N+]([O-])=O
306.36	1.05E-15	4.55E+08	ester	CCC(O)CC(O)CC(=O)OC(C)CC(O)C(O)CC=O
370.53	4.17E-14	4.88E+06	ester	CCCCCCC(=O)CCCC(=O)OC(C)CC(=O)CC(O)CCCC
372.55	3.39E-12	1.04E+05	ether	CCCCCCC(OC(CCC)\C=C\CC1=CC=C(C)O1)C1=CC=C(C)O1
374.57	3.39E-12	1.61E+05	ether	CCCCCCC(OC(CCC)CCCC1=CC=C(C)O1)C1=CC=C(C)O1
376.58	5.36E-12	1.08E+05	ether	CCCCCCC(OC(CCC)CCCC1=CC=C(C)O1)C1CC=C(C)O1
378.55	4.45E-12	2.36E+05	ether	CCCCC(=O)C(OC(CCC)CCCC1CC=C(C)O1)C1CC=C(C)O1
386.53	5.80E-13	7.92E+05	ether	CCCCCC(=O)C(OC(CCC)\C=C\CC1=CC=C(C)O1)C1=CC=C(C)O1
388.55	5.80E-13	1.40E+06	ether	CCCCCC(=O)C(OC(CCC)CCCC1=CC=C(C)O1)C1=CC=C(C)O1
390.56	9.19E-13	8.88E+05	ether	CCCCCC(=O)C(OC(CCC)CCCC1CC=C(C)O1)C1=CC=C(C)O1
392.58	9.19E-13	3.14E+06	ether	CCCCCC(=O)C(OC(CCC)CCCC1CC=C(C)O1)C1=CC=C(C)O1
402.53	1.15E-13	3.51E+06	ether	CCCCCC(=O)C(OC(CCC)C(=O)CCC1=CC=C(C)O1)C1=CC=C(C)O1
404.55	1.82E-13	4.35E+06	ether	CCCCCC(=O)C(OC(CCC)C(=O)CCC1=CC=C(C)O1)C1CC=C(C)O1
406.56	2.88E-13	3.72E+06	ether	CCCCCC(=O)C(OC(CCC)C(=O)CCC1CC=C(C)O1)C1CC=C(C)O1
408.58	5.70E-14	9.90E+06	ether	CCCCCC(=O)C(OC(CCC)C(O)CCC1CC=C(C)O1)C1CC=C(C)O1
420.55	1.66E-15	3.23E+08	ether	CCCC(OC(CCC(=O)CC(C)O)C1CC=C(C)O1)C(=O)CCC1=CC=C(C)O1
422.56	2.63E-15	1.46E+09	ether	CCCC(OC(CCC(=O)CC(C)O)C1CC=C(C)O1)C(=O)CCC1CC=C(C)O1
437.58	3.63E-14	1.27E+07	nitrate ether	CCCC(CCCC1=CC=C(C)O1)OC(CCCCC(C)O[N+]([O-])=O)C1CC=C(C)O1
439.59	5.75E-14	3.19E+07	nitrate ether	CCCC(CCCC1CC=C(C)O1)OC(CCCCC(C)O[N+]([O-])=O)C1CC=C(C)O1
453.58	9.85E-15	5.07E+07	nitrate ether	CCCC(CCCC1CC=C(C)O1)OC(C1CC=C(C)O1)C(=O)CCCC(C)O[N+]([O-])=O
455.59	2.26E-15	2.55E+08	nitrate ether	CCCC(CCCC1CC=C(C)O1)OC(C(O)CCCC(C)O[N+]([O-])=O)C1CC=C(C)O1
471.59	2.77E-17	6.05E+10	nitrate ether	CCCC(OC(C(O)CCCC(C)O[N+]([O-])=O)C1CC=C(C)O1)C(O)CCC1CC=C(C)O1
488.62	2.38E-15	1.33E+08	nitrate ether	CCCCCCCC(O[N+]([O-])=O)C(CCC)OC(CCCCC(C)O[N+]([O-])=O)C1CC=C(C)O1

Experiment: Hexylcyclohexane Low NO, $(NH_4)_2SO_4$, dry

Mean M_w ($g\ mol^{-1}$) 310.49

M_w	P_{vap} (atm)	C_A/C_{IS}	Compound Class	SMILES String
98.15	4.28E-03	7.14E-06	ketone/aldehyde	O=C1CCCCC1
114.14	6.62E-04	3.30E-05	ketone/aldehyde	O=CCCCCC=O
116.16	2.38E-04	4.17E-05	hydroxycarbonyl	CCC(O)CCC=O
118.13	1.85E-05	9.14E-04	hydroxycarbonyl	CC(O)CC(O)C=O
120.10	4.58E-05	1.21E-03	hydroperoxide	CCC(O)C(OO)=O
122.17	1.45E-03	1.97E-05	ketone/aldehyde	O=CCC1CC=CC=C1
124.18	1.45E-03	3.53E-05	ketone/aldehyde	O=CCC1CC=CCC1
126.20	1.45E-03	5.30E-05	ketone/aldehyde	O=CCC1CCCCC1
128.17	4.68E-04	3.44E-05	hydroxycarbonyl	O=CC1(O)CCCCC1
130.19	1.25E-05	1.00E-03	alcohol	CC1(O)C(O)CCCC1
132.16	1.35E-08	3.09E+00	alcohol	OC1C(O)CC(O)CC1
134.13	3.85E-07	2.40E-01	hydroxycarbonyl	CC(O)C(O)C(O)C=O
135.12	6.51E-07	1.57E-02	imine	CC(OO)C(OO)C=N
136.10	6.51E-07	8.82E-02	hydroperoxide	CC(OO)C(OO)C=O
137.23	2.99E-04	2.67E-05	imine	N=CCCC1=CCCCC1
138.21	2.99E-04	3.00E-04	ketone/aldehyde	O=CCCC1=CCCCC1
139.11	6.44E-04	1.49E-05	imine	C=CC(C(C(C=N)=O)=O)=O
140.18	7.11E-04	5.39E-05	ketone/aldehyde	O=CC(C1CCCCC1)=O
142.20	8.90E-05	1.51E-04	hydroxycarbonyl	O=CC(O)C1CCCCC1
144.21	9.26E-06	1.05E-03	alcohol	CC(O)C1(O)CCCCC1
146.19	3.17E-08	7.98E-01	alcohol	CC1(O)C(O)CC(O)CC1
148.16	3.46E-08	2.08E+00	hydroxycarbonyl	CC(O)C(O)C(O)CC=O
149.15	3.46E-08	2.36E-01	imine	CC(O)C(OO)C(O)C=N
150.13	3.46E-08	1.05E+00	hydroperoxide	CC(O)C(OO)C(O)C=O
152.24	9.77E-05	5.16E-04	ketone/aldehyde	O=CCCCC1=CCCCC1
154.21	7.86E-05	7.47E-04	ketone/aldehyde	O=CCC(C1CCCCC1)=O
156.23	8.33E-06	1.59E-03	hydroxycarbonyl	O=CCC(O)C1CCCCC1
158.24	3.03E-06	1.15E-02	alcohol	CCC(O)C1(O)CCCCC1
159.12	3.72E-06	3.77E-02	hydroxycarbonyl	CC(O)C(C(C(O)C=O)=O)=O
161.11	2.92E-07	6.39E-02	imine	N=CC(C(O)C(OO)C=O)=O
162.14	8.20E-08	6.02E+00	hydroxycarbonyl	CC(O)C(O)C(C(O)C=O)=O
163.17	1.37E-09	4.41E+01	imine	CC(O)C(O)C(O)C(O)C=N
164.16	1.37E-09	6.21E+01	hydroxycarbonyl	CC(O)C(O)C(O)C(O)C=O
165.15	2.23E-09	5.00E+00	imine	CC(OO)C(O)C(OO)C=N
166.13	2.23E-09	1.88E+01	hydroperoxide	CC(OO)C(O)C(OO)C=O
167.27	5.06E-05	1.02E-03	ketone/aldehyde	O=CCCCCC1CCCCC1
170.21	1.02E-05	1.35E-03	hydroxycarbonyl	O=CCC(C1(O)CCCCC1)=O
174.20	1.06E-08	1.53E+00	hydroxycarbonyl	O=CC(O)C1(O)C(O)CCCC1
175.12	2.58E-07	4.59E-01	hydroperoxide	CC(O)C(C(OO)C(C=O)=O)=O
177.16	5.36E-09	3.57E+00	imine	CC(O)C(C(OO)C(O)C=N)=O
178.14	5.36E-09	7.59E+01	hydroperoxide	CC(O)C(OO)C(C(O)C=O)=O
179.17	8.66E-11	6.09E+02	imine	CC(O)C(OO)C(O)C(O)C=N
180.29	1.05E-05	9.55E-02	ketone/aldehyde	CCCC(CCC1=CCCCC1)=O
181.24	9.60E-06	1.38E-02	imine	N=CCC(C(C1CCCCC1)=O)=O
182.31	1.65E-05	7.37E-03	ketone/aldehyde	CCCC(CCC1CCCCC1)=O
183.21	1.17E-07	1.22E-01	imine	N=CC(CC(C1)(O)CCCC1=O)=O
184.28	1.53E-06	2.03E-02	hydroxycarbonyl	O=CCCCCC1(O)CCCCC1
186.25	3.53E-08	2.37E-01	hydroxycarbonyl	O=CCC(O)CC1(O)CCCCC1
190.20	2.70E-12	7.88E+03	hydroxycarbonyl	O=CCC1(O)C(O)CC(O)CC1O
191.18	2.19E-13	3.58E+04	imine	N=CC1(O)C(O)C(O)C(O)CC1O
192.17	2.19E-13	9.77E+05	hydroxycarbonyl	O=CC1(O)C(O)C(O)C(O)CC1O
193.16	4.75E-10	6.19E+01	imine	CC(OO)C(OO)C(C(O)C=N)=O
194.14	7.26E-09	1.01E+02	hydroperoxide	CC(OO)C(O)C(C(O)C=O)=O
195.17	4.77E-11	1.96E+03	imine	CC(OO)CC(OO)C(OO)C=N
196.29	8.13E-06	9.68E-02	ketone/aldehyde	CCCC(C(CC1CCCCC1)=O)=O
197.28	2.55E-07	3.77E-01	imine	N=CCC(CCC1(O)CCCCC1)=O
198.31	5.01E-07	3.81E-01	hydroxycarbonyl	CCCC(CCC1(O)CCCCC1)=O
199.29	1.16E-08	2.09E+00	imine	N=CCC(O)CCC1(O)CCCCC1
200.32	5.92E-08	3.12E-01	alcohol	CCCC(O)CCC1(O)CCCCC1
206.19	1.95E-14	6.33E+05	hydroxycarbonyl	O=CCC1(O)C(O)C(O)C(O)CC1O
207.14	1.02E-11	7.12E+02	imine	CC(OO)C(OO)C(C(C(O)=N)=O)=O
208.17	1.35E-14	4.64E+06	hydroxycarbonyl	O=CC1(O)C(O)CC(O)C(OO)C1O

209.15	3.11E-11	3.28E+02	imine	CC(OO)C(C(OO)C(OO)C=N)=O
210.14	3.11E-11	1.26E+04	hydroperoxide	CC(OO)C(C(OO)C(OO)C=O)=O
211.26	1.42E-07	3.80E-01	imine	N=CCC(C(O)C(C1CCCCC1)=O)=O
212.29	4.84E-08	5.98E+00	hydroxycarbonyl	CC(O)CC(CC(C1CCCCC1)=O)=O
195.19	4.77E-11	8.14E+02	imine	CCC(OO)C(OO)C(OO)C=N
196.31	2.75E-06	2.72E-02	ketone/aldehyde	CCCC(CC(C1CCCCC1)=O)=O
198.34	2.91E-07	3.83E-02	hydroxycarbonyl	CCCC(O)CC(C1CCCCC1)=O
224.26	3.47E-07	5.59E-02	ketone/aldehyde	CC(C(C(CC(C1CCCCC1)=O)=O)=O)=O
226.27	4.65E-08	1.66E+00	hydroxycarbonyl	CC(C(O)C(CC(C1CCCCC1)=O)=O)=O
209.21	2.89E-13	4.51E+04	imine	CC(O)C(O)C(OO)C(O)C(O)C=N
228.29	2.77E-09	3.67E+01	hydroxycarbonyl	CC(O)CC(CC(C1(O)CCCCC1)=O)=O
229.32	4.34E-11	4.21E+02	imine	CC(O)CC(CC(O)C1(O)CCCCC1)=N
230.30	8.61E-11	2.70E+02	hydroxycarbonyl	CC(O)CC(O)CC(C1(O)CCCCC1)=O
220.24	3.61E-13	9.97E+03	hydroxycarbonyl	O=CC(O)C(O)C1(OO)CCC(O)CC1
222.16	4.13E-15	1.07E+06	hydroperoxide	O=CC1(OO)C(O)C(OO)C(CC1O)=O
242.27	1.61E-09	7.69E+00	hydroperoxide	CC(CC(CC(C1(OO)CCCCC1)=O)=O)=O
226.30	5.40E-08	1.51E-01	hydroxycarbonyl	CC(CC(CC(C1(O)CCCCC1)=O)=O)=O
244.29	1.82E-11	5.33E+02	hydroperoxide	CC(CC(O)CC(C1(OO)CCCCC1)=O)=O
228.32	3.13E-09	1.45E+01	hydroperoxide	CC(CCCC(C1(OO)CCCCC1)=O)=O
246.30	8.51E-13	1.01E+04	hydroperoxide	CC(O)CC(CC(O)C1(OO)CCCCC1)=O
252.40	1.16E-08	2.80E-01	hydroxycarbonyl dimer	O=C(C(O)CC1CCCCC1)CC2CCCCC2
254.37	4.74E-10	6.96E+00	hydroxycarbonyl dimer	O=C(C(C1CCCCC1)O)CC2(O)CCCCC2
259.30	6.86E-12	6.89E+02	imine	CCC(C(CC(OO)C1(OO)CCCCC1)=O)=N
261.32	7.41E-11	8.19E+01	imine	CCC(C(CC(O)C1(OO)CCCCC1)=O)=N
263.33	1.40E-11	2.61E+02	hydroperoxide	CCCC(CC(OO)C1(OO)CCCCC1)=O
264.41	2.11E-09	2.11E+00	hydroxycarbonyl dimer	O=C(/C=C/CC1(O)CCCCC1)CC2CCCCC2
275.19	6.32E-16	5.65E+06	hydroperoxide	O=CCC(C(C1(OO)C(OO)CC(CC1O)=O)=O)=O
277.23	3.30E-15	1.01E+06	imine	N=CCC(C(C1(OO)C(OO)CC(OO)CC1)=O)=O
280.23	5.14E-17	8.13E+07	hydroperoxide	O=CCC(O)C(C1(OO)C(OO)CC(OO)CC1)=O
282.25	8.80E-19	5.79E+09	hydroperoxide	O=CCC(O)C(O)C1(OO)C(OO)CC(OO)CC1
292.24	3.40E-16	1.54E+07	hydroperoxide	O=C(CCC=O)C(C1(OO)C(OO)CC(OO)CC1)=O
294.30	6.88E-17	7.42E+07	hydroperoxide	CCC(O)C(OO)CC(C1(OO)CCC(OO)CC1)=O
296.27	2.88E-19	1.49E+10	hydroperoxide	OC(CCC=O)C(O)C1(OO)C(OO)CC(OO)CC1
304.21	6.86E-17	6.61E+07	hydroperoxide	O=C(C(CC=O)=O)C(C1(OO)C(OO)CC(CC1O)=O)=O
306.22	8.67E-18	4.68E+08	hydroperoxide	O=C(C(CC=O)=O)C(C1(OO)C(OO)CC(O)CC1O)=O
308.20	2.94E-18	1.80E+09	hydroperoxide	O=C(CC=O)C(C1(OO)C(OO)CC(OO)C(O)C1=O)=O
310.21	4.21E-20	1.62E+11	hydroperoxide	O=C(CC=O)C(C1(OO)C(OO)CC(OO)C(O)C1O)=O
312.23	1.61E-20	2.31E+11	hydroperoxide	O=C(CC=O)C(O)C1(OO)C(OO)CC(OO)C(OO)C1
318.37	2.60E-14	1.75E+05	peroxyhemiacetal	OC(OOC(C1(O)CCCCC1)=O)CC2(OO)CCCCC2
320.38	1.84E-15	1.99E+06	peroxyhemiacetal	OC(OOCC1(OO)CCCCC1)CC2(OO)CCCCC2
322.49	7.97E-12	4.25E+02	hydroxycarbonyl dimer	O=C(C(CCCC1CCCCC1)O)CCC(C2CCCCC2)=O
324.46	1.78E-13	2.56E+04	hydroxycarbonyl dimer	O=C(C(CC(O)C1CCCCC1)O)CCC(C2CCCCC2)=O
326.48	1.62E-13	2.52E+04	hydroxycarbonyl dimer	O=C(C(CC1(OO)CCCCC1)O)CCCCC2CCCCC2
334.50	1.33E-12	2.73E+03	hydroxycarbonyl dimer	O=C(/C=C/CC1(O)CCCCC1)CCCC(CC2CCCCC2)=O
336.52	2.61E-12	1.26E+03	hydroxycarbonyl dimer	O=C(C(CCCC1CCCCC1)O)CCC(CC2CCCCC2)=O
326.46	1.31E-13	2.71E+04	hydroxycarbonyl dimer	O=C(C(O)C(CC1CCCCC1)=O)CCC2(OO)CCCCC2
326.54	2.53E-12	1.85E+03	ether	OC(OCCCCCCC1(O)CCCCC1)CC2CCCCC2
350.50	1.34E-13	2.82E+04	hydroxycarbonyl dimer	O=C(C(O)CCC(C1CCCCC1)=O)CCC(CC2CCCCC2)=O
360.58	5.43E-11	8.13E+01	ether	CC(C(OC(CCC)/C=C/C1CCCCC1)C/C=C/C2CCCCC2)=O
362.60	5.43E-11	1.41E+02	ether	CC(C(OC(CCC)CCC1CCCCC1)C/C=C/C2CCCCC2)=O
366.54	1.14E-14	3.27E+05	ether	O=C(C(O)CCCCC1(O)CCCCC1)CCCC(C2CCCCC2)=O
374.57	5.47E-13	1.00E+04	ether	CCC(OC(CC)/C=C/C(C1CCCCC1)=O)/C=C/C(C2CCCCC2)=O
376.58	7.35E-13	1.06E+04	ether	CCC(OC(CC)CCC(C1CCCCC1)=O)/C=C/C(C2CCCCC2)=O
378.60	9.89E-13	9.68E+03	ether	CCC(OC(CC)CCC(C1CCCCC1)=O)CCC(C2CCCCC2)=O
380.61	6.13E-13	8.02E+03	ether	CCC(OC(CC)CCC(C1CCCCC1)=O)CCCC2(O)CCCCC2
388.55	2.06E-13	1.67E+04	ether	CCC(OC(CC)/C=C/C(C1CCCCC1)=O)C(CC(C2=CCCCC2)=O)=O
390.56	2.63E-13	3.09E+04	ether	CCC(OC(CC)CCC(C1CCCCC1)=O)C(CC(C2=CCCCC2)=O)=O
392.58	5.29E-13	2.87E+04	ether	CCC(OC(CC)CCC(C1CCCCC1)=O)C(CC(C2CCCCC2)=O)=O
394.60	9.88E-14	1.86E+05	ether	CCC(OC(CC)CCC(C1CCCCC1)=O)C(CCC2(O)CCCCC2)=O
396.61	2.28E-14	4.77E+05	ether	CCC(OC(CC)CCCC1(O)CCCCC1)C(CCC2(O)CCCCC2)=O
404.55	9.79E-14	3.30E+04	ether	CCC(OC(CC)CC(C(C1CCCCC1)=O)=O)C(CC(C2=CCCCC2)=O)=O
406.56	1.91E-13	4.73E+04	ether	CCC(OC(CC)CC(C(C1CCCCC1)=O)=O)C(CC(C2CCCCC2)=O)=O
408.58	4.34E-14	3.47E+05	ether	CCC(OC(CC)CC(C(C1CCCCC1)=O)=O)C(CCC2(O)CCCCC2)=O
410.60	6.46E-14	1.93E+05	peroxyhemiacetal	CCC(OOC(CC)(O)CC(CC1CCCCC1)=O)C(CCC2CCCCC2)=O
394.63	9.88E-14	1.18E+05	ether	CCC(OC(CC)CC(CC1(O)CCCCC1)=O)C(CCC2CCCCC2)=O
396.61	2.28E-14	3.64E+05	ether	CCC(OC(CC)CCCC1(O)CCCCC1)C(CCC2(O)CCCCC2)=O
422.56	2.83E-15	1.78E+06	ether	CC(C(OC(CC)CC(CC1(O)CCCCC1)=O)C(CC(C2CCCCC2)=O)=O)=O

424.58	1.05E-14	6.20E+05	peroxyhemiacetal	CCC(OOC(CC)(O)CC(CC1CCCCC1)=O)C(CC(C2CCCCC2)=O)=O
408.61	1.83E-14	4.97E+05	ether	CC(C(OC(CC)CC(CC1(O)CCCCC1)=O)C(CCC2CCCCC2)=O)=O
426.59	1.01E-15	6.84E+06	peroxyhemiacetal	CCC(OOC(CC)(O)CC(CC1(O)CCCCC1)=O)C(CCC2CCCCC2)=O
410.63	6.46E-14	1.51E+05	peroxyhemiacetal	CCC(OOC(CC)(O)CC(CC1CCCCC1)=O)C(CCC2CCCCC2)=O
424.61	1.05E-14	7.37E+05	peroxyhemiacetal	CCC(OOC(CC)(O)CC(CC1CCCCC1)=O)C(CC(C2CCCCC2)=O)=O
426.63	1.05E-14	7.80E+05	peroxyhemiacetal	CCC(OOC(CC)(O)CC(CC1CCCCC1)=O)C(CC(C2CCCCC2)=O)=O
440.61	7.93E-16	6.30E+06	peroxyhemiacetal	CCC(OOC(CC)(O)CC(CC1CCCCC1)=O)C(CC(C2(O)CCCCC2)=O)=O
459.62	1.76E-17	2.03E+08	peroxyhemiacetal	CCC(OOC(CC)(O)CC(CC1(O)CCCCC1)=O)CCC(C2(O)CCCCC2)=O

Experiment: Hexylcyclohexane High NO, $(NH_4)_2SO_4$, dry

Mean M_w (g mol^{-1}) 418.06

M_w	P_{vap} (atm)	C_A/C_{IS}	Compound Class	SMILES String
98.15	4.28E-03	2.18E-05	ketone/aldehyde	O=C1CCCCC1
100.16	1.35E-02	4.29E-06	ketone/aldehyde	CCCCCC=O
110.16	1.83E-03	8.07E-05	ketone/aldehyde	O=CC1=CCCCC1
116.16	2.38E-04	1.04E-04	hydroxycarbonyl	CCC(O)CCC=O
118.13	1.85E-05	2.11E-03	hydroxycarbonyl	CC(O)CC(O)C=O
102.16	2.55E-03	4.41E-06	hydroxycarbonyl	CCCC(C=O)O
122.08	2.59E-06	3.04E-02	hydroxycarbonyl	O=C(O)C(O)C=O
124.18	9.14E-04	9.00E-05	ketone/aldehyde	O=CCC1=CCCCC1
126.16	3.24E-04	2.96E-04	ketone/aldehyde	O=CC1CCCCC1=O
128.17	3.24E-04	2.94E-04	ketone/aldehyde	O=CC1CCCCC1=O
130.14	1.17E-05	3.25E-03	hydroxycarbonyl	CC(CC(O)CC=O)=O
132.16	1.69E-06	5.74E-02	hydroxycarbonyl	CC(O)CC(O)CC=O
133.15	3.85E-07	1.24E-01	imine	CC(O)C(O)C(O)C=N
134.13	3.85E-07	4.98E-01	hydroxycarbonyl	CC(O)C(O)C(O)C=O
118.16	1.85E-05	2.72E-03	hydroxycarbonyl	CC(O)CC(O)C=O
118.15	1.85E-05	7.53E-03	hydroxycarbonyl	CC(O)CC(O)C=O
120.14	3.81E-08	1.33E+00	imine	CC(O)C(O)C(O)=N
138.17	3.34E-04	5.99E-04	ketone/aldehyde	O=CC(C1=CCCCC1)=O
139.11	1.44E-05	3.82E-03	imine	O=C(C1=O)CC(CC1=O)=N
140.18	7.11E-04	1.22E-04	ketone/aldehyde	O=CC(C1CCCCC1)=O
141.13	2.84E-04	8.77E-05	imine	CC(CC(C(C=N)=O)=O)=O
142.15	1.24E-05	3.10E-03	hydroxycarbonyl	O=CC1(O)CCC(CC1)=O
144.17	1.60E-06	1.73E-02	hydroxycarbonyl	O=CC1(O)CCC(O)CC1
146.19	5.52E-07	1.61E-01	hydroxycarbonyl	CC(O)CC(O)CCC=O
147.17	1.26E-07	1.94E-01	imine	CCC(O)C(O)C(O)C=N
148.11	6.18E-09	2.91E+01	hydroxycarbonyl	OC1C(C=O)OC(O)C1O
149.15	8.82E-10	5.12E+01	imine	N=CC(O)C(O)C(O)CO
132.17	7.39E-09	1.97E+01	alcohol	OC1CC(O)CC(O)C1
133.16	3.85E-07	1.57E-01	imine	CC(O)C(O)C(O)C=N
134.10	8.83E-09	2.10E+01	hydroxycarbonyl	O=C(O)C(O)C(O)C=O
153.18	3.75E-05	1.19E-03	imine	N=CC(C1CCCCC1=O)=O
154.25	1.55E-04	9.92E-04	ketone/aldehyde	O=CCCCC1CCCCC1
155.15	5.52E-06	5.54E-03	imine	N=CC1(O)C(CCCC1=O)=O
156.18	9.24E-05	3.80E-04	hydroxycarbonyl	O=CC(C1(O)CCCCC1)=O
158.20	2.12E-06	3.72E-02	hydroxycarbonyl	O=CC(O)C1(O)CCCCC1
159.19	1.35E-08	1.98E+00	imine	N=CC1(O)C(O)CCCC1O
160.17	7.35E-09	3.60E+01	hydroxycarbonyl	O=CC1(O)CCC(O)CC1O
144.20	1.60E-06	4.55E-02	hydroxycarbonyl	O=CC1(O)CCC(O)CC1
162.14	8.20E-08	4.60E+00	hydroxycarbonyl	CC(O)C(O)C(C(O)C=O)=O
146.17	7.07E-06	1.20E-02	hydroxycarbonyl	CCC(O)C(C(O)C=O)=O
163.15	3.67E-13	5.46E+05	alcohol	OC1C(O)C(O)CC(O)C1O
147.15	2.89E-09	1.88E+01	imine	CC(C(O)C(O)C(O)=N)=O
166.26	3.20E-05	6.67E-03	ketone/aldehyde	O=CCCCCC1=CCCCC1
183.16	4.74E-08	1.35E+00	imine	N=CC(C1C(CC(O)CC1=O)=O)=O
168.24	2.57E-05	5.72E-03	ketone/aldehyde	O=CCC(CC1CCCCC1)=O
170.25	2.72E-06	1.37E-02	hydroxycarbonyl	O=CCC(O)CC1CCCCC1
171.22	1.93E-07	1.39E-01	hydroxycarbonyl	O=CCC(O)C1(O)CCCCC1
173.21	1.06E-08	2.01E+00	imine	N=CC(O)C1(O)CCCCC1O
174.20	1.06E-08	8.38E+00	hydroxycarbonyl	O=CC(O)C1(O)CCCCC1O
158.23	2.12E-06	2.82E-02	hydroxycarbonyl	O=CC(O)C1(O)CCCCC1
176.12	1.89E-09	2.33E+02	hydroxycarbonyl	CC(O)C(C(O)C(C(O)=O)=O)=O
160.20	1.35E-08	1.81E+01	hydroxycarbonyl	O=CC1(O)C(O)CCCC1O
160.10	1.26E-07	1.32E+01	hydroxycarbonyl	O=C(O)C(C(C(O)C=O)=O)=O
161.17	9.17E-05	3.05E-03	nitrate	CCC(O[N+]([O-])=O)CCC=O
180.29	1.05E-05	9.37E-02	ketone/aldehyde	CCCC(CCC1=CCCCC1)=O
181.19	7.43E-08	2.22E+00	imine	N=CCC(C1CC(CCC1=O)=O)=O

182.26	8.40E-06	3.50E-02	ketone/aldehyde	O=CCC(CCC1CCCCC1)=O
183.21	9.55E-07	5.30E-02	imine	N=CCC(C1(O)CCCCC1=O)=O
184.28	8.90E-07	8.14E-02	hydroxycarbonyl	O=CCC(O)CCC1CCCCC1
186.25	3.53E-08	6.48E-01	hydroxycarbonyl	O=CCC(O)CC1(O)CCCCC1
187.24	9.50E-10	2.30E+01	imine	N=CCC(O)C1(O)CCCCC1O
188.22	3.96E-10	7.41E+01	hydroxycarbonyl	O=CCCC1(O)C(O)CCCC1O
189.21	4.56E-11	1.11E+03	imine	OC1(C(O)C=N)C(O)CCCC1O
190.24	2.70E-12	7.27E+04	hydroxycarbonyl	O=CCC1(O)C(O)CC(O)CC1O
174.23	1.06E-08	8.97E+00	hydroxycarbonyl	O=CC(O)C1(O)CCCCC1O
192.26	9.59E-07	5.94E-01	ketone/aldehyde	C/C=C/C(CC(C1=CCCCC1)=O)=O
176.20	3.03E-11	6.18E+03	hydroxycarbonyl	O=CC1(O)C(O)CC(O)CC1O
194.27	1.29E-06	1.30E+00	ketone/aldehyde	CCCC(CC(C1=CCCCC1)=O)=O
195.22	4.69E-07	7.03E-01	imine	N=CCC(C(C1CCCCC1=O)=O)=O
196.29	2.75E-06	2.90E-01	ketone/aldehyde	CCCC(CC(C1CCCCC1)=O)=O
197.23	1.37E-06	1.06E-01	imine	N=CCC(C(C1(O)CCCCC1)=O)=O
198.31	5.01E-07	4.63E-01	hydroxycarbonyl	CCCC(CCC1(O)CCCCC1)=O
199.25	4.63E-08	1.22E+00	imine	N=CCC(C(O)C1(O)CCCCC1)=O
200.28	1.16E-08	3.87E+00	hydroxycarbonyl	O=CCCC(O)CC1(O)CCCCC1
203.24	3.70E-11	5.93E+02	imine	N=CC(O)C(O)C1(O)CCCCC1O
186.27	3.53E-08	6.17E-01	hydroxycarbonyl	O=CCC(O)CC1(O)CCCCC1
188.25	9.50E-10	6.62E+01	hydroxycarbonyl	O=CCC(O)C1(O)CCCCC1O
206.19	9.67E-14	1.29E+06	hydroxycarbonyl	O=CC(O)C1(O)C(O)CC(O)CC1O
190.23	2.45E-11	3.09E+03	hydroxycarbonyl	O=CC(O)C1(O)C(O)CC(O)CC1
208.26	1.88E-07	2.16E+00	ketone/aldehyde	CC(CC(CC(C1=CCCCC1)=O)=O)=O
209.25	5.98E-08	2.39E+00	imine	N=CCC(CC(C1CCCCC1=O)=O)=O
210.27	3.79E-07	1.84E+00	ketone/aldehyde	CC(CC(CC(C1CCCCC1)=O)=O)=O
211.26	1.65E-07	9.02E-01	imine	N=CCC(CC(C1(O)CCCCC1)=O)=O
212.29	8.32E-08	6.09E+00	hydroxycarbonyl	CC(CC(CCC1(O)CCCCC1)=O)=O
213.28	3.43E-09	2.92E+01	imine	N=CCC(CC(O)C1(O)CCCCC1)=O
214.31	6.76E-09	1.19E+01	hydroxycarbonyl	CCCC(CC(O)C1(O)CCCCC1)=O
215.29	1.33E-10	2.61E+02	imine	N=CCC(O)CC(O)C1(O)CCCCC1
220.31	4.88E-08	4.29E-01	hydroxycarbonyl dimer	O=C(C(O)C1=CCCCC1)C2=CCCCC2
221.17	4.07E-12	9.40E+03	nitrate	O=CC1(O[N+]([O-])=O)C(O)CC(O)CC1O
222.24	8.83E-13	6.71E+04	hydroxycarbonyl	O=CCCC1(O)C(O)CC(O)CC1O
205.14	1.94E-06	2.38E-02	nitrate	CC(O)C(C(C(O[N+]([O-])=O)C=O)=O)=O
224.26	1.96E-08	9.08E+00	ketone/aldehyde	CC(CC(CC(C1CCCCC1=O)=O)=O)=O
225.24	2.96E-09	3.29E+01	imine	N=CCC(CC(C1(O)CCC(CC1)=O)=O)=O
226.27	5.40E-08	7.24E+00	hydroxycarbonyl	CC(CC(CC(C1(O)CCCCC1)=O)=O)=O
227.26	9.42E-09	1.11E+01	imine	OC1(CCCCC1)C(CC(C(O)C=N)=O)=O
228.29	1.12E-09	1.75E+02	hydroxycarbonyl	CC(CC(CC(O)C1(O)CCCCC1)=O)=O
229.28	1.72E-07	4.50E-01	nitrate	O=CCCCCC1(O[N+]([O-])=O)CCCCC1
230.30	1.38E-11	2.35E+03	hydroxycarbonyl	CCCC(CCC1(O)C(O)CCCC1O)=O
214.32	6.76E-09	3.68E+00	hydroxycarbonyl	CCCC(CC(O)C1(O)CCCCC1)=O
236.36	2.84E-07	8.62E-02	ketone/aldehyde	O=C(C(C1CCCCC1)=O)CC2CCCCC2
237.26	1.11E-08	5.31E+00	imine	CC(CC(C(C(C1CCCCC1=O)=O)=O)=O)=N)=O
238.28	1.11E-08	4.33E+00	hydroxycarbonyl	OC(C(CC(CC(C)=O)=O)=O)C1=CCCCC1
239.27	4.79E-09	1.69E+01	imine	CC(CC(CC(C1(O)CCCCC1=O)=O)=O)=O)=N
240.26	4.79E-09	1.55E+01	hydroxycarbonyl	CC(CC(CC(C1(O)CCCCC1=O)=O)=O)=O)=O
241.29	3.30E-10	9.55E+02	imine	CC(C(CC(O)C(C1(O)CCCCC1)=O)=O)=O)=N
242.27	3.30E-10	4.28E+02	hydroxycarbonyl	CC(CC(CC(C1(O)CCCCC1O)=O)=O)=O)=O
243.30	3.91E-11	3.23E+03	imine	CC(C(CC(O)C(O)C1(O)CCCCC1)=O)=O)=N
244.29	3.91E-11	1.40E+03	hydroxycarbonyl	CC(C(CC(O)C(O)C1(O)CCCCC1)=O)=O)=O
245.32	1.55E-08	3.65E+00	nitrate	CCCC(O)CCC1(O[N+]([O-])=O)CCCCC1
246.30	3.09E-14	9.32E+05	hydroxycarbonyl	CCCC(CCC1(O)C(O)CC(O)CC1O)=O
248.32	2.50E-15	1.04E+07	hydroxycarbonyl	CCCC(O)CCC1(O)C(O)CC(O)CC1O
252.35	2.15E-08	1.08E+00	hydroxycarbonyl dimer	OC(C(C(C1CCCCC1)=O)=O)C2CCCCC2
236.25	3.05E-16	6.84E+07	hydroxycarbonyl	O=CC(O)C(O)C1(O)C(O)CC(O)CC1O
254.33	6.87E-11	3.52E+02	hydroxycarbonyl	O=C(C(C1(O)CCCCC1)O)C2CC(CCC2)=O
255.27	5.92E-12	1.38E+04	imine	CC(CC(CC(C1(O)CC(CCC1O)=O)=O)=O)=O)=N
256.30	2.09E-10	1.68E+02	hydroxycarbonyl	O=C(C(CC(CC(C)=O)=O)O)C1(O)CCCCC1

257.29	9.31E-09	1.39E+01	nitrate	CCC(CC(CC1(O[N+]([O-])=O)CCCCC1)=O)=O
258.31	7.54E-12	6.99E+03	hydroxycarbonyl	O=C(C(CC(CC(O)C)=O)O)C1(O)CCCCC1
259.30	9.87E-10	7.92E+01	nitrate	CCC(CC(O)CC1(O[N+]([O-])=O)CCCCC1)=O
260.33	5.96E-13	7.43E+04	hydroxycarbonyl	O=C(C(CC(O)CC(O)C)O)C1(O)CCCCC1
261.32	1.10E-10	5.28E+02	nitrate	CCC(O)CC(O)CC1(O[N+]([O-])=O)CCCCC1
262.39	2.60E-09	1.57E+01	hydroxycarbonyl dimer	OC(C(CC1=CCCCC1)=O)CCC2=CCCCC2
264.41	4.12E-09	8.20E+00	hydroxycarbonyl dimer	OC(C(CC1=CCCCC1)=O)CCC2CCCCC2
266.29	7.99E-17	6.66E+08	hydroxycarbonyl	CC(O)C(O)C(O)CC(O)CC(O)CC(O)C=O
270.24	1.57E-12	1.08E+04	hydroxycarbonyl	CC(CC(CC(C1(O)C(CC(CC1O)=O)=O)=O)=O)=O
254.27	6.10E-20	7.41E+11	alcohol	CC(O)C(O)C1(O)C(O)C(O)C(O)C(O)C(O)C1O
272.34	2.80E-13	1.24E+05	hydroxycarbonyl dimer	O=C(C(C1(O)CCC(O)CC1)O)C2(O)CCCCC2
273.29	1.07E-10	7.37E+02	nitrate	CC(CC(CCC1(O[N+]([O-])=O)CCCCC1O)=O)=O
274.36	5.75E-14	7.64E+05	ether	OC(OC1(O)CCC(O)CC1)CC2(O)CCCCC2
275.30	4.12E-12	1.25E+04	nitrate	CC(O)CC(CCC1(O[N+]([O-])=O)CCCCC1O)=O
276.37	7.44E-14	7.31E+05	ether	OC(OC(O)CCC(O)CC)CC1(O)CCCCC1
277.36	4.30E-09	6.47E+00	nitrate ether	CCCCCC(O[N+]([O-])=O)C(OCCCCCC)O
280.41	8.55E-09	3.03E+00	acid anhydride	O=C(OC(CCC1CCCCC1)=O)CC2CCCCC2
284.40	1.86E-12	9.67E+03	hydroxycarbonyl dimer	O=C(C(O)CC1(O)CCCCC1)CC2(O)CCCCC2
285.38	1.00E-08	1.31E+00	nitrate ether	O=[N+](OC1(CCCCC1)CCOCC2CCCCC2)[O-]
286.41	9.85E-13	2.09E+04	hydroxycarbonyl dimer	O=C(C(O)CC(O)CCCCC)CC1(O)CCCCC1
287.36	3.88E-08	5.97E-01	nitrate ether	O=[N+](OC1(COCC2CCCCC2)CCCCC1)[O-]
288.38	3.24E-14	1.02E+06	hydroxycarbonyl dimer	CCC(O)C(O)CC(C(O)CCC1(O)CCCCC1)=O
289.33	2.21E-11	1.58E+03	nitrate hydroxycarbonyl dimer	O=C(C(O)CC(O)CCC)C1(O[N+]([O-])=O)CCCCC1
290.36	3.19E-16	1.78E+08	nitrate hydroxycarbonyl dimer	OC1(C(O)CCCC1)COCC2(O)CCC(O)CC2O
292.37	4.17E-16	1.15E+08	ether	CCCCC(O)C(O)COCC1(O)CCC(O)CC1O
294.39	6.61E-10	8.72E+01	acid anhydride	O=C(C1CCCCC1)OC(CC(CC2CCCCC2)=O)=O
278.32	2.62E-16	2.13E+08	acid anhydride	CC(O)C(O)C(C(O)C(O)C1(O)CCCCC1O)=O
298.42	2.71E-11	6.72E+02	ester	O=C(OCCCC1(O)CCCCC1)CC2(O)CCCCC2
299.39	4.08E-13	4.77E+04	ester	O=C(OCCC1(O)CCCCC1O)CC2(O)CCCCC2
302.41	1.14E-14	3.51E+06	ether	OC(OCCC1(O)CCCCC1O)CC2(O)CCCCC2
304.30	4.97E-16	8.51E+07	acid anhydride	O=C(OC(CC(CC(O)C)=O)=O)C1(O)C(O)CCCC1O
306.40	4.74E-16	1.03E+08	ether	OC1(CCCOCC(O)C(O)C(O)CC)C(O)CCCC1
289.39	7.37E-10	3.09E+01	nitrate hydroxycarbonyl dimer	CCCCCCC(C(O)CC(O[N+]([O-])=O)CCCC)=O
308.42	2.16E-10	1.63E+02	acid anhydride	O=C(OC(CCC1CCCCC1)=O)CC(C2CCCCC2)=O
310.43	8.47E-11	3.37E+02	acid anhydride	O=C(OC(CCC1CCCCC1)=O)CCC2(O)CCCCC2
312.45	8.85E-12	2.24E+03	ester	O=C(OCCCC1(O)CCCCC1)CCC2(O)CCCCC2
314.42	1.33E-13	1.84E+05	ester	O=C(OCCC1(O)CCCCC1)CCC2(O)CCCCC2O
316.44	5.10E-15	6.51E+06	ether	OC(COCCC1(O)CCCCC1)CC2(O)CCCCC2O
318.32	3.04E-17	1.34E+09	acid anhydride	O=C(OC(C1(O)C(O)CCCC1O)=O)C2(O)C(O)CCCC2
302.43	8.59E-15	4.45E+06	ether	OC1(CCOCCC2(O)CCCCC2O)CCCCC1O
322.40	5.12E-19	7.09E+10	ether	CC(O)CC(O)CC(O)COCCC1(O)C(O)CCCC1O
324.42	5.41E-13	5.29E+04	ester	O=C(OCCC(CC1(O)CCCCC1)=O)CC2CCCCC2=O
326.43	3.98E-13	5.68E+04	ester	O=C(OCCC(CC1(O)CCCCC1)=O)CC2(O)CCCCC2
330.42	1.08E-17	2.25E+09	hydroxycarbonyl dimer	O=C(C(CC1(O)CCCCC1O)O)CCC2(O)CCCCC2O
332.35	5.28E-18	6.22E+09	acid anhydride	O=C(OC(CC1(O)C(O)CCCC1)=O)C2(O)C(O)CCCC2O
334.32	1.16E-19	2.80E+11	acid anhydride	O=C(OC(C1(O)C(O)CCCC1O)=O)C2(O)C(O)CCCC2O
335.46	2.31E-11	1.43E+03	acid anhydride	O=C(OC(CCCC1CCCCC1)=O)CC(CC2CCCCC2)=O
338.44	2.14E-12	1.58E+04	acid anhydride	O=C(OC(CCC1(O)CCCCC1)=O)CC(CC2CCCCC2)=O
340.46	2.09E-13	1.52E+05	acid anhydride	O=C(OC(CCC1(O)CCCCC1)=O)CC(O)CC2CCCCC2
342.48	1.87E-14	1.59E+06	ester	OC1(CC(O)CCOC(CCC2(O)CCCCC2)=O)CCCCC1
344.49	7.27E-16	3.90E+07	ether	OC1(CC(O)CCOCC(O)CC2(O)CCCCC2)CCCCC1
346.46	9.27E-16	3.01E+07	ether	CCC(O)C(OC(C(CC)=O)C(O)C)C(O)CC1(O)CCCCC1
348.48	1.45E-13	1.94E+05	hydroxycarbonyl dimer	O=C(C(O)CC(CC1CCCCC1)=O)CCC(CC2=CCCCC2)=O
350.50	7.55E-12	4.29E+03	acid anhydride	O=C(OC(CCCC1CCCCC1)=O)CC(CCC2CCCCC2)=O
352.47	3.93E-13	1.53E+05	acid anhydride	O=C(OC(CCC1(O)CCCCC1)=O)CCCC(C2CCCCC2)=O
354.49	1.25E-13	2.75E+05	acid anhydride	O=C(OC(CCC1(O)CCCCC1)=O)CCCCC2(O)CCCCC2
355.48	2.35E-11	9.95E+02	ester	O=C(OCCC1CCCCC1)CCCCC2(O[N+]([O-])=O)CCCCC2
356.50	6.10E-15	6.23E+06	ester	O=C(OCCC(O)CC1(O)CCCCC1)CCCC2(O)CCCCC2
358.52	1.74E-16	1.86E+08	ether	OC(OCCC(O)CC1(O)CCCCC1)CCCC2(O)CCCCC2
360.54	1.42E-12	2.31E+04	ester	O=C(OCCCCCC(CC1=CCCCC1)=O)CCCC2=CCCCC2

362.51	9.80E-13	3.02E+04	ester	O=C(OCCC(CC(CC1CCCCC1)=O)=O)CCCC2=CCCCC2
364.48	7.52E-17	4.47E+08	ester	CCCCCC(OCCC(O)CC(O)COCCC(O)C(O)CC)=O
351.46	1.06E-11	2.37E+03	ester	O=C(OCC(C(CC1CCCCC1)=O)=O)CC(CC2CCCCC2)=O
366.45	2.03E-19	1.56E+11	ether	OC1(CCC(O)OCC(O)C2(O)C(O)CCCC2)C(O)CCCC1
368.51	1.39E-14	4.76E+06	ester	O=C(OCCC(CC1(O)CCCCC1)=O)CCCCC2(O)CCCCC2
370.53	2.00E-15	1.79E+07	ester	O=C(OCCC(O)CC1(O)CCCCC1)CCCCC2(O)CCCCC2
371.52	3.21E-13	7.87E+04	imine ether	O=C(CC(CCOC(C=N)CCC1=CCCCC1)=O)/C=C/C2=CCCCC2
372.50	3.56E-17	1.40E+09	ester	O=C(OCCC(O)CC1(O)CCCCC1)CC(O)CC2(O)CCCCC2
373.54	3.65E-13	7.57E+04	imine ester	O=C(OC(C(C)=N)CCC1=CCCCC1)CCCC(CC2=CCCCC2)=O
374.57	3.34E-13	1.72E+05	ether	CCC(OC(C)CCC(CC1=CCCCC1)=O)C(CC(C2CCCCC2)=O)=O
310.49	6.55E-11	5.98E+02	ether	O=C(CCOCCCCC1(O)CCCCC1)C2CCCCC2
378.55	5.11E-13	5.76E+04	ether	CCC(OC(C=O)CC(CC1CCCCC1)=O)CC(CC2CCCCC2)=O
384.51	2.05E-17	1.47E+09	hydroxycarbonyl dimer	O=C(C(O)CCCC1(O)CCCCC1)CCC(C(O)C2(O)CCCCC2)=O
386.49	2.65E-18	1.70E+10	acid anhydride	O=C(OC(CCCC1(O)CCCCC1O)=O)CCCC2(O)CCCCC2O
387.52	3.78E-15	6.96E+06	nitrate ether	OC1CCCC(CCCCOCCCCC2(O)CCCCC2)(O[N+]([O-])=O)C1
370.50	7.47E-18	8.08E+09	hydroxycarbonyl dimer	O=C(C(O)CC(CC1(O)CCCCC1)=O)CC(O)CC2(O)CCCCC2
389.54	4.76E-14	6.88E+05	imine ester	N=CC(OC(CC(CCCC1=CCCCC1)=O)=O)CCC(C2CCCCC2)=O
390.56	1.06E-13	5.25E+05	ether	CCC(OC(C(CC)=O)CC(C1CCCCC1)=O)CC(CC2=CCCCC2)=O
391.55	5.04E-14	6.01E+05	imine ether	CCC(OC(CC=N)CC(C1CCCCC1)=O)CC(C(C2CCCCC2)=O)=O
392.58	1.47E-13	3.44E+05	ether	CCC(OC(CC(CC(C)=O)=O)C1CCCCC1)CC(CC2CCCCC2)=O
394.60	1.02E-13	2.99E+05	ether	CCC(OC(CC(CC(C)=O)=O)C1CCCCC1)CCCC2(O)CCCCC2
400.52	7.76E-14	3.46E+05	ether	CC(C(OC(CC(/C=C/C)=O)C1=CCCCC1)C(C(CC2=CCCCC2)=O)=O)=O
402.53	9.55E-14	4.07E+05	ether	CC(C(OC(CC(CCC)=O)C1=CCCCC1)C(C(CC2=CCCCC2)=O)=O)=O
403.56	5.90E-14	5.34E+05	imine ether	CC(C(OC(CC(CC(C)=N)=O)C1=CCCCC1)C(CCC2CCCCC2)=O)=O
404.55	1.51E-13	3.92E+05	ether	CC(C(OC(CC(CCC)=O)C1CCCCC1)C(C(CC2=CCCCC2)=O)=O)=O
388.53	2.47E-20	1.28E+12	hydroxycarbonyl dimer	O=C(C(O)C(O)CCC1(O)CCCCC1)CC(O)C(O)C2(O)CCCCC2
406.56	2.39E-13	2.96E+05	ether	CC(C(OC(CC(CCC)=O)C1CCCCC1)C(C(CC2CCCCC2)=O)=O)=O
407.60	1.08E-12	3.67E+04	nitrate ether	CCC(OC(CCC)CCC1(O[N+]([O-])=O)CCCCC1)/C=C/CC2=CCCCC2
408.58	1.83E-14	2.12E+06	ether	CC(C(OC(CC(CCC)=O)C1CCCCC1)C(CCC2(O)CCCCC2)=O)=O
417.55	8.46E-24	3.53E+15	imine ether	CC(C(OC(C(CC)=N)CC(C1CCCCC1)=O)C(C(CC2=CCCCC2)=O)=O)=O
418.53	8.46E-24	4.29E+15	hydroxycarbonyl dimer	O=C(C(O)CC(O)CC1(O)CCCCC1O)CC(O)CC(O)C2(O)CCCCC2
419.56	4.30E-14	8.84E+05	imine ether	CC(C(OC(C(CC)=N)CC(C1CCCCC1)=O)C(C(CC2CCCCC2)=O)=O)=O
420.55	4.30E-14	1.32E+06	ether	CC(C(OC(C(CC)=O)CC(C1CCCCC1)=O)C(C(CC2CCCCC2)=O)=O)=O
421.58	1.02E-14	3.41E+06	imine ether	CC(C(OC(C(CC)=N)CC(C1CCCCC1)=O)C(C(O)CC2CCCCC2)=O)=O
422.56	1.02E-14	4.38E+06	ether	CC(C(OC(C(CC)=O)CC(C1CCCCC1)=O)C(C(O)CC2CCCCC2)=O)=O
423.59	4.85E-16	7.94E+07	imine ether	CC(O)C(OC(C(CC)=N)CC(C1CCCCC1)=O)C(C(O)CC2CCCCC2)=O
424.58	4.85E-16	6.89E+07	ether	CC(O)C(OC(C(CC)=O)CC(C1CCCCC1)=O)C(C(O)CC2CCCCC2)=O
433.55	7.70E-16	3.55E+07	imine ether	CC(C(OC(C(CC)=O)CC(C(C1)CCCC1=N)=O)C(C(CC2CCCCC2)=O)=O)=O
434.53	7.70E-16	3.34E+07	ether	CC(C(OC(C(CC)=O)CC(C(C1)CCCC1=O)=O)C(C(CC2CCCCC2)=O)=O)=O
435.56	9.83E-17	3.28E+08	imine ether	CC(O)C(OC(C(CC)=O)CC(C(C1)CCCC1=N)=O)C(C(CC2CCCCC2)=O)=O
436.55	9.83E-17	2.89E+08	ether	CC(O)C(OC(C(CC)=O)CC(C(C1)CCCC1=O)=O)C(C(CC2CCCCC2)=O)=O
437.58	1.61E-17	2.57E+09	imine ether	CC(O)C(OC(C(CC)=O)CC(O)C(C1)CCCC1=N)C(C(CC2CCCCC2)=O)=O
438.56	5.79E-16	5.92E+07	ether	CC(C(OC(C(CC)=O)CC(O)C1CCCCC1)C(C(C(O)C2CCCCC2)=O)=O)=O
439.59	2.60E-17	1.73E+09	imine ether	CC(O)C(OC(C(CC)=N)CC(O)C1CCCCC1)C(C(C(O)C2CCCCC2)=O)=O
441.61	5.26E-19	6.55E+10	imine ether	CC(O)C(OC(C(CC)=N)CC(O)C1CCCCC1)C(C(O)C(O)C2CCCCC2)=O
449.54	3.97E-15	6.40E+06	imine ether	CC(C(OC(C(CC)=N)C(C(C1CCCCC1)=O)=O)C(C(O)C(C2CCCCC2)=O)=O)=O
451.56	1.49E-16	2.19E+08	imine ether	CC(C(OC(C(CC)=N)C(CC1(O)CCCCC1)=O)C(C(O)C(C2CCCCC2)=O)=O)=O
453.58	6.04E-18	7.55E+09	imine ether	CC(O)C(OC(C(CC)=N)C(CC1(O)CCCCC1)=O)C(C(O)C(C2CCCCC2)=O)=O
455.59	2.30E-19	1.58E+11	imine ether	CC(O)C(OC(C(CC)=N)C(CC1(O)CCCCC1)=O)C(C(O)CC2(O)CCCCC2)=O
467.56	2.46E-18	1.24E+10	imine ether	CC(C(OC(C(C(C)=O)=N)C(CC1(O)CCCCC1)=O)C(C(O)CC2(O)CCCCC2)=O)=O
469.58	6.20E-17	5.32E+08	nitrate ether	CCC(OC(C(CC)=O)C(CC1(O)CCCCC1)=O)CC(CC2(O[N+]([O-])=O)CCCCC2)=O
471.59	8.33E-18	3.12E+09	nitrate ether	CCC(OC(C(CC)=O)C(CC1(O)CCCCC1)=O)CC(O)CC2(O[N+]([O-])=O)CCCCC2
486.61	6.25E-16	3.54E+07	nitrate ether	CCC(OC(C(CC)=O)CCC1(O[N+]([O-])=O)CCCCC1)CCCC2(O[N+]([O-])=O)CCCCC2
502.61	1.10E-17	1.74E+09	nitrate ether	CCC(OC(C(CC)=O)CCC1(O[N+]([O-])=O)CCCCC1)CC(O)CC2(O[N+]([O-])=O)CCCCC2