

# Organic Compounds in Produced Waters from Shale Gas Wells

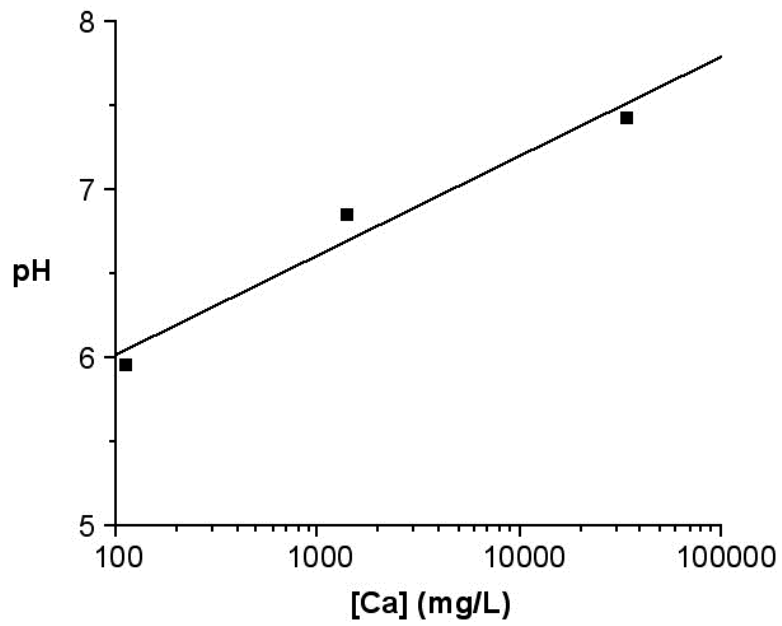
*Samuel J. Maguire-Boyle<sup>†</sup> and Andrew R. Barron<sup>†‡\$\*</sup>*

<sup>†</sup>Department of Chemistry, Rice University, Houston, Texas 77005, USA

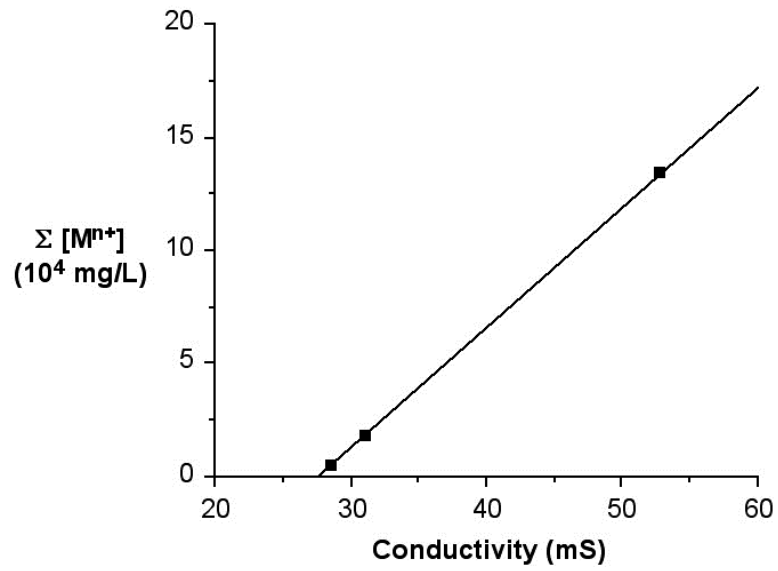
<sup>‡</sup>Department of Materials Science and Nanoengineering, Rice University, Houston, Texas  
77005, USA

<sup>§</sup>College of Engineering, Swansea University, Singleton Park, Swansea, SA2 8PP, Wales,  
UK

**Electronic Supplementary Information**



**Figure S1.** Plot of pH of produced water as a function of the calcium concentration ( $R^2 = 0.964$ ).



**Figure S2.** Plot of total cation content as a function of produced water conductivity ( $R^2 = 1.00$ ).

**Table S1.** List of wavelengths of analyzed elemental ions for ICP-OES.

Element	Wavelength (nm) <sup>a</sup>
Na	330.237
K	766.49, 404.721
Li	670.784, 610.362, 460.286, 413.256
Cs	455.531, 459.32
Rb	780.023, 420.185
Mg	285.213, 279.077, 280.271, 279.553
Ca	317.933, 315.887, 393.366, 396.847, 422.673
Sr	407.771, 460.733, 232.235
Ba	233.527, 455.403, 493.408, 230.425, 413.065
Sc	361.383, 424.683, 357.634
Y	371.029, 324.227, 360.073
La	408.672, 379.478, 407.735, 384.902
Ti	334.94, 336.121, 337.279, 334.903, 368.519
V	290.88, 310.23, 309.31, 292.402, 311.071, 270.093
Cr	267.716, 205.56, 283.563, 284.325, 357.869, 206.158, 257.717
Mn	257.61, 259.372, 260.568, 294.92, 293.305, 279.482, 403.075
Fe	239.562, 259.939, 234.349, 234.83, 238.863, 273.955
Ni	231.604, 221.648, 232.003, 341.476, 227.022
Cu	327.393, 324.752, 224.752, 213.597, 222.778, 221.459
Zn	206.2, 213.857, 202.548, 330.258
Cd	228.802, 214.44, 226.502, 361.051
Hg	253.652, 194.168, 404.656, 435.835, 302.15, 184.886, 546.074
B	249.677, 249.772, 208.889, 182.528, 208.957, 182.578
Si	251.611, 212.412, 288.158, 252.851, 221.667
Sn	189.927, 235.485, 283.998, 242.17

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P	213.617, 214.914, 178.221, 178.221, 177.434
As	188.979, 193.696, 197.197, 228.812
Sb	206.836, 217.582, 231.146, 252.851, 204.957, 203.977
Bi	223.061, 190.171, 306.766, 206.17
S	181.975, 180.669, 182.563, 189.965

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<sup>a</sup> Where more than one wavelength is given they are listed in the order they are ranked (most to least confident).

**Table S2.** List of identified molecules with GC-MS from Marcellus (PA) neutral aliquot extracted with chloroform.

Peak	R.T. (min)	A[tot] (%)	Library/compound ID	Q (%)	CAS #	M <sub>w</sub>	Molecular formula
1	1.32	30.21	2-Propanone	83	0000067-64-1	58.08	C <sub>3</sub> H <sub>6</sub> O
2	1.5	21.73	Trichloromethane	83	0000067-66-3	119.38	CHCl <sub>3</sub>
3	1.85	0.98	Methylcyclohexane	97	0000108-87-2	98.19	C <sub>7</sub> H <sub>14</sub>
4	2.09	0.7	4-Methylheptane	72	0000589-53-7	114.23	C <sub>8</sub> H <sub>18</sub>
5	2.15	0.73	Methylbenzene	70	0000108-88-3	92.14	C <sub>7</sub> H <sub>8</sub>
6	2.2	0.65	1,3-Dimethylcyclohexane	97	0000638-04-0	112.21	C <sub>8</sub> H <sub>16</sub>
7	2.28	0.12	1,1-Dimethylcyclohexane	95	0000590-66-9	112.21	C <sub>8</sub> H <sub>16</sub>
8	2.37	1.05	Octane	64	0000111-65-9	114.23	C <sub>8</sub> H <sub>18</sub>
9	2.44	0.14	1,3-Dimethylcyclohexane	97	0000638-04-0	112.21	C <sub>8</sub> H <sub>16</sub>
10	2.58	0.17	2,4-Dimethylheptane	95	0002213-23-2	128.26	C <sub>9</sub> H <sub>20</sub>
11	2.65	0.3	2,6-Dimethylheptane,	91	0001072-05-5	128.26	C <sub>9</sub> H <sub>20</sub>
12	2.73	0.89	Ethylcyclohexane	89	0001678-91-7	112.21	C <sub>8</sub> H <sub>16</sub>
13	2.93	0.23	1,2,4-Trimethylcyclohexane	97	0002234-75-5	126.24	C <sub>9</sub> H <sub>18</sub>
14	3.08	0.99	2-Methyloctane	90	0003221-61-2	128.26	C <sub>9</sub> H <sub>20</sub>
15	3.17	0.6	3-Methyloctane	91	0002216-33-3	128.26	C <sub>9</sub> H <sub>20</sub>
16	3.22	1	1,3-Dimethylbenzene	97	0000108-38-3	106.17	C <sub>8</sub> H <sub>10</sub>

17	3.34	0.12	1,1,3,5-Tetramethylcyclohexane	90	0004306-65-4	140.27	C <sub>10</sub> H <sub>20</sub>
18	3.4	0.36	1-Ethyl-4-methylcyclohexane	96	0003728-56-1	126.24	C <sub>9</sub> H <sub>18</sub>
19	3.55	1.97	Nonane	97	0000111-84-2	128.26	C <sub>9</sub> H <sub>20</sub>
20	3.62	0.18	1-Chloro-5-(chloromethoxy)-pentane	43	0145912-11-4	171.06	C <sub>6</sub> H <sub>12</sub> C <sub>12</sub> O
21	3.7	0.07	1-Ethyl-4-methyl-cyclohexane	87	0003728-56-1	126.24	C <sub>9</sub> H <sub>18</sub>
22	3.79	0.14	2,4-Dimethylhexane	72	0000589-43-5	114.23	C <sub>8</sub> H <sub>18</sub>
23	3.85	0.08	3-Hexyne	49	0000928-49-4	82.14	C <sub>6</sub> H <sub>10</sub>
24	3.91	0.26	3,5-Dimethyloctane	87	0015869-93-9	142.28	C <sub>10</sub> H <sub>22</sub>
25	4.03	0.79	2,6-Dimethyloctane	97	0002051-30-1	142.28	C <sub>10</sub> H <sub>22</sub>
26	4.12	0.24	2,6-Dimethyloctane	70	0002051-30-1	142.28	C <sub>10</sub> H <sub>22</sub>
27	4.25	0.07	1,2-Dimethylcycloheptene	52	0020053-89-8	124.22	C <sub>9</sub> H <sub>16</sub>
28	4.31	0.04	3,3,5,5-Tetramethylcyclopentane	43	0038667-10-6	124.22	C <sub>9</sub> H <sub>16</sub>
29	4.37	0.22	4-Ethyloctane	95	0015869-86-0	142.28	C <sub>10</sub> H <sub>22</sub>
30	4.46	0.63	4-Methylnonane	93	0017301-94-9	142.28	C <sub>10</sub> H <sub>22</sub>
31	4.5	0.88	2-Methylnonane	81	0000871-83-0	142.28	C <sub>10</sub> H <sub>22</sub>
32	4.62	1.01	1,2,3-Trimethylbenzene	95	0000526-73-8	120.19	C <sub>9</sub> H <sub>12</sub>
33	4.84	0.34	1-Methyl-2-propylcyclohexane	81	0004291-79-6	140.27	C <sub>10</sub> H <sub>20</sub>
34	5.08	3.32	Decane	96	0000124-18-5	142.28	C <sub>10</sub> H <sub>22</sub>
35	5.15	0.05	1,2-Dimethyl-3-(1-methylethyl)-cyclopentane	47	0000489-20-3	140.27	C <sub>10</sub> H <sub>20</sub>

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36	5.29	0.27	3,7-Dimethylundecane	59	0017301-29-0	184.36	C <sub>13</sub> H <sub>28</sub>
37	5.43	0.66	4-Methyldecane	93	0002847-72-5	156.31	C <sub>11</sub> H <sub>24</sub>
38	5.5	0.34	2-Methyldecane	70	0006975-98-0	156.31	C <sub>11</sub> H <sub>24</sub>
39	5.58	0.42	Butylcyclohexane	94	0001678-93-9	140.27	C <sub>10</sub> H <sub>20</sub>
40	5.68	0.19	3-Methyldecane	87	0013151-34-3	156.31	C <sub>11</sub> H <sub>24</sub>
41	5.97	0.59	5-Methyldecane	93	0013151-35-4	156.31	C <sub>11</sub> H <sub>24</sub>
42	6.03	0.25	4-Methyldecane	91	0002847-72-5	156.31	C <sub>11</sub> H <sub>24</sub>
43	6.08	0.63	2-Methyldecane	97	0006975-98-0	156.31	C <sub>11</sub> H <sub>24</sub>
44	6.18	0.36	3-Methyldecane	95	0013151-34-3	156.31	C <sub>11</sub> H <sub>24</sub>
45	6.38	0.23	1,2,4,5-Tetramethylbenzene	42	0000095-93-2	134.22	C <sub>10</sub> H <sub>14</sub>
46	6.49	0.12	4-Ethyl-1,2-dimethylbenzene	95	0000934-80-5	134.22	C <sub>10</sub> H <sub>14</sub>
47	6.59	0.09	1,1,3-Trimethylcyclopentane	49	0004516-69-2	112.21	C <sub>8</sub> H <sub>16</sub>
48	6.65	3.19	Undecane	96	0001120-21-4	156.31	C <sub>11</sub> H <sub>24</sub>
49	6.73	0.09	(1-Methylbutyl)-benzene	46	0002719-52-0	148.24	C <sub>11</sub> H <sub>16</sub>
50	6.79	0.16	Decahydro-2-methylnaphthalene	98	0002958-76-1	152.28	C <sub>11</sub> H <sub>20</sub>
51	6.9	0.38	Dodecane	90	0000112-40-3	170.33	C <sub>12</sub> H <sub>26</sub>
52	7	0.13	1,2,4,5-Tetramethylbenzene	93	0000095-93-2	134.22	C <sub>10</sub> H <sub>14</sub>
53	7.05	0.2	2-Methylundecane	74	0007045-71-8	170.33	C <sub>12</sub> H <sub>26</sub>
54	7.17	0.19	Pentylcyclohexane	95	0004292-92-6	154.29	C <sub>11</sub> H <sub>22</sub>

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55	7.25	0.05	Tritetracontane	38	0007098-21-7	605.16	C <sub>43</sub> H <sub>88</sub>
56	7.32	0.07	5-Methyldecane	83	0017302-36-2	156.31	C <sub>11</sub> H <sub>24</sub>
57	7.4	0.18	1-Methyl-4-(1-methylpropyl)-benzene	55	0001595-16-0	148.24	C <sub>11</sub> H <sub>16</sub>
58	7.47	0.34	2,6-Dimethyldecane	76	0013150-81-7	170.33	C <sub>12</sub> H <sub>26</sub>
59	7.53	0.16	4-Methylundecane	90	0002980-69-0	170.33	C <sub>12</sub> H <sub>26</sub>
60	7.61	0.51	2-Methylundecane	90	0007045-71-8	170.33	C <sub>12</sub> H <sub>26</sub>
61	7.7	0.24	5-Methyldecane	64	0017302-36-2	156.31	C <sub>11</sub> H <sub>24</sub>
62	7.78	0.1	(1 $\alpha$ , 3 $\beta$ , 4 $\alpha$ , 5 $\alpha$ , 7 $\beta$ )-1,4-Dimethyl-tricyclo[3.1.1.1]decane	86	0024145-89-9	164.29	C <sub>12</sub> H <sub>20</sub>
63	7.85	0.1	(1 $\alpha$ , 3 $\beta$ , 4 $\beta$ , 5 $\alpha$ , 7 $\beta$ )- 1,4-Dimethyl-tricyclo[3.1.1.1]decane	94	0024145-88-8	164.29	C <sub>12</sub> H <sub>20</sub>
64	7.93	0.12	1-Methyl-2-pentylcyclohexane	70	0054411-01-7	168.32	C <sub>12</sub> H <sub>24</sub>
65	8	0.1	1-Methylene-1H-indene	93	0002471-84-3	128.17	C <sub>10</sub> H <sub>8</sub>
66	8.14	2.76	Dodecane	96	0000112-40-3	170.33	C <sub>12</sub> H <sub>26</sub>
67	8.25	0.12	(1 $\alpha$ , 3 $\beta$ , 4 $\alpha$ , 5 $\alpha$ , 7 $\beta$ )-1,4-dimethyl-tricyclo[3.1.1.1]decane	60	0024145-89-9	164.29	C <sub>12</sub> H <sub>20</sub>
68	8.34	0.55	2,6-Dimethylundecane	94	0017301-23-4	184.36	C <sub>13</sub> H <sub>28</sub>
69	8.38	0.11	1,1'-Oxybisdecane	58	0002456-28-2	298.55	C <sub>20</sub> H <sub>42</sub> O
70	8.44	0.14	1-Chlorohexadecane	43	0004860-03-1	260.89	C <sub>16</sub> H <sub>33</sub> Cl

71	8.52	0.1	Hexatriacontane	43	0000630-06-8	506.97	C <sub>36</sub> H <sub>74</sub>
72	8.68	0.19	Hexylcyclohexane	89	0004292-75-5	168.32	C <sub>12</sub> H <sub>24</sub>
73	8.9	0.37	2,4-Dimethylundecane	81	0017312-80-0	184.35	C <sub>13</sub> H <sub>28</sub>
74	8.97	0.14	2,3-Dimethylundecane	47	0017312-77-5	184.35	C <sub>13</sub> H <sub>28</sub>
75	9.03	0.31	2-Methyldodecane	86	0001560-97-0	180.33	C <sub>13</sub> H <sub>28</sub>
76	9.14	0.89	4,6-Dimethyldodecane	74	0061141-72-8	198.39	C <sub>14</sub> H <sub>30</sub>
77	9.23	0.18	2,6,11-Trimethyldodecane	72	0031295-56-4	212.41	C <sub>15</sub> H <sub>32</sub>
78	9.53	2.44	Tridecane	98	0000629-50-5	184.36	C <sub>13</sub> H <sub>28</sub>
79	9.68	0.15	1-Iodo-2-methylundecane	72	0073105-67-6	296.23	C <sub>12</sub> H <sub>25</sub> I
80	9.76	0.18	2,5-Dimethyldodecane	91	0056292-65-0	198.39	C <sub>14</sub> H <sub>30</sub>
81	9.87	0.1	Cyclohexylbenzene	64	0000827-52-1	160.26	C <sub>12</sub> H <sub>16</sub>
82	10.11	0.15	Heptylcyclohexane	58	0005617-41-4	182.35	C <sub>13</sub> H <sub>26</sub>
83	10.18	0.2	6-Methyltridecane	83	0013287-21-3	198.39	C <sub>14</sub> H <sub>30</sub>
84	10.29	0.11	4-Methyltridecane	80	0026730-12-1	198.39	C <sub>14</sub> H <sub>30</sub>
85	10.35	0.23	2-Methyltridecane	91	0001560-96-9	198.39	C <sub>14</sub> H <sub>30</sub>
86	10.44	0.13	4-Methyltetradecane	72	0025117-24-2	212.41	C <sub>15</sub> H <sub>32</sub>
87	10.52	0.36	2,6,10-Trimethyldodecane	91	0003891-98-3	212.41	C <sub>15</sub> H <sub>32</sub>
88	10.82	1.54	Tetradecane	98	0000629-59-4	198.39	C <sub>14</sub> H <sub>30</sub>
89	10.96	0.08	3,9-Dimethylundecane	53	0017301-31-4	184.36	C <sub>13</sub> H <sub>28</sub>

90	11.17	0.09	$\alpha$ -(2-Methylpropylidene)-benzeneacetaldehyde	11	0026643-91-4	174.24	C <sub>12</sub> H <sub>14</sub> O
91	11.43	0.2	Undecane	80	0001120-21-4	156.31	C <sub>11</sub> H <sub>24</sub>
92	11.59	0.45	7-Methylpentadecane	91	0006165-40-8	226.44	C <sub>16</sub> H <sub>34</sub>
93	11.68	0.08	Pentatriacontane	74	0000630-07-9	492.95	C <sub>35</sub> H <sub>72</sub>
94	12.05	1.09	Pentadecane	96	0000629-62-9	212.41	C <sub>15</sub> H <sub>32</sub>
95	12.23	0.07	3,7,11-Trimethyl-1,3,6,10-dodecatetraene	64	0000502-61-4	204.35	C <sub>15</sub> H <sub>24</sub>
96	12.67	0.08	1-Tridecene	53	0002437-56-1	182.5	C <sub>13</sub> H <sub>26</sub>
97	12.78	0.1	2-Methylpentadecane	90	0001560-93-6	226.44	C <sub>16</sub> H <sub>34</sub>
98	13.2	0.6	Hexadecane	98	0000544-76-3	226.44	C <sub>16</sub> H <sub>34</sub>
99	13.73	0.12	5-Methyldecane	87	0017302-36-2	156.31	C <sub>11</sub> H <sub>24</sub>
100	14.29	0.36	Heptadecane	97	0000629-78-7	240.47	C <sub>27</sub> H <sub>36</sub>
101	14.35	0.18	2,6,10,14-Tetramethylpentadecane	91	0001921-70-6	268.52	C <sub>19</sub> H <sub>40</sub>
102	15.34	0.22	Octadecane	98	0000593-45-3	254.49	C <sub>18</sub> H <sub>38</sub>
103	16.32	0.13	Nonadecane	99	0000629-92-5	268.52	C <sub>19</sub> H <sub>40</sub>
104	17.27	0.08	Eicosane	97	0000112-95-8	282.55	C <sub>20</sub> H <sub>42</sub>
105	18.17	0.07	Heneicosane	99	0000629-94-7	296.57	C <sub>21</sub> H <sub>44</sub>
106	19.03	0.04	Docosane	96	0000629-97-0	310.6	C <sub>22</sub> H <sub>46</sub>
107	20.76	2.31	1,6-Dioctyloatehexanedioic acid	99	0000123-79-5	370.57	C <sub>22</sub> H <sub>42</sub> O <sub>4</sub>

**Table S3.** List of identified molecules with GC-MS from Marcellus (PA) acid aliquot extracted with chloroform.

Peak	R.T. (min)	A[Tot] (%)	Library/ID	Q (%)	CAS #	M <sub>w</sub>	Molecular Formula
1	1.26	0.21	2-Hydroxyacetic acid	9	0000079-14-1	76.05	C <sub>2</sub> H <sub>4</sub> O <sub>3</sub>
2	1.30	0.61	Hydrazine	9	0000302-01-2	32.05	N <sub>2</sub> H <sub>4</sub>
3	1.32	1.14	2-Chloroethanol	9	0000107-07-3	80.51	C <sub>2</sub> H <sub>5</sub> ClO
4	1.33	0.41	2-Methyl-1-butene	91	0000563-46-2	70.13	C <sub>5</sub> H <sub>10</sub>
5	1.36	0.02	1,1-Dimethylcyclopropane	90	0001630-94-0	70.13	C <sub>5</sub> H <sub>10</sub>
6	1.37	0.19	2-Methyl-2-butene	90	0000513-35-9	70.13	C <sub>5</sub> H <sub>10</sub>
7	1.38	0.47	2-Methylpentane	94	0000107-83-5	86.18	C <sub>6</sub> H <sub>14</sub>
8	1.44	0.36	Hexane	91	0000110-54-3	86.18	C <sub>6</sub> H <sub>14</sub>
9	1.49	0.42	Trichloromethane	83	0000067-66-3	119.38	CHCl <sub>3</sub>
10	1.62	11.31	Trichloromethane	91	0000067-66-3	119.38	CHCl <sub>3</sub>
11	1.68	0.19	1,3-Dimethylcyclopentane	95	0002453-00-1	98.19	C <sub>7</sub> H <sub>14</sub>
12	1.71	0.82	Heptane	87	0000142-82-5	100.2	C <sub>7</sub> H <sub>16</sub>
13	1.85	0.86	Methylcyclohexane	97	0000108-87-2	98.19	C <sub>7</sub> H <sub>14</sub>
14	1.90	0.05	Ethylcyclopentane	76	0001640-89-7	98.19	C <sub>7</sub> H <sub>14</sub>
15	1.93	0.11	1,2,4-Trimethylcyclopentane	93	0002815-58-9	112.21	C <sub>8</sub> H <sub>16</sub>
16	1.97	0.19	1,2,3-Trimethylcyclopentane	90	0002815-57-8	112.21	C <sub>8</sub> H <sub>16</sub>

17	2.01	0.07	3-Methyl-1-heptene	87	0004810-09-7	112.21	C <sub>8</sub> H <sub>16</sub>
18	2.08	0.49	2-Methylheptane	96	0000592-27-8	114.23	C <sub>8</sub> H <sub>18</sub>
19	2.15	0.64	Methylbenzene	93	0000108-88-3	92.14	C <sub>7</sub> H <sub>8</sub>
20	2.20	0.41	1,3-Dimethylcyclohexane	94	0000591-21-9	112.21	C <sub>8</sub> H <sub>16</sub>
21	2.30	0.27	1-Ethyl-2-methylcyclopentane	97	0003726-46-3	112.21	C <sub>8</sub> H <sub>16</sub>
22	2.35	0.46	Octane	87	0000111-65-9	114.23	C <sub>8</sub> H <sub>18</sub>
23	2.56	0.03	2,4-Dimethylheptane	64	0002213-23-2	128.26	C <sub>9</sub> H <sub>20</sub>
24	2.64	0.16	2,6-Dimethylheptane	87	0001072-05-5	128.26	C <sub>9</sub> H <sub>20</sub>
25	2.67	0.56	1,2-Dimethylcyclohexane	97	0002207-01-4	112.21	C <sub>8</sub> H <sub>16</sub>
26	2.73	0.91	Ethylcyclohexane	93	0001678-91-7	112.21	C <sub>8</sub> H <sub>16</sub>
27	2.74	0.19	1,1,3-Trimethylcyclohexane	93	0003073-66-3	126.24	C <sub>9</sub> H <sub>18</sub>
28	2.80	0.25	1-Ethyl-2-methylcyclohexane	64	0003728-54-9	126.24	C <sub>10</sub> H <sub>20</sub>
29	2.88	0.22	Methylenecyclohexane	87	0001192-18-3	96.17	C <sub>7</sub> H <sub>12</sub>
30	2.91	0.28	1,2,4-Trimethylcyclohexane	96	0007667-60-9	126.24	C <sub>9</sub> H <sub>18</sub>
31	2.94	0.38	1,3,5-Trimethylcyclohexane	94	0001839-63-0	126.24	C <sub>9</sub> H <sub>18</sub>
32	2.96	0.18	2,3-Dimethylheptane	76	0003074-71-3	128.26	C <sub>9</sub> H <sub>20</sub>
33	2.99	0.24	3-Ethylhexane	72	0000619-99-8	114.23	C <sub>8</sub> H <sub>18</sub>
34	3.00	0.01	2-Octene	46	0000111-67-1	112.21	C <sub>8</sub> H <sub>16</sub>
35	3.06	0.48	2,4-Dimethylheptane	58	0002213-23-2	128.26	C <sub>9</sub> H <sub>20</sub>

36	3.09	0.16	Ethylbenzene	95	0000100-41-4	106.17	C <sub>8</sub> H <sub>10</sub>
37	3.15	0.96	3-Methyloctane	62	0002216-33-3	128.26	C <sub>9</sub> H <sub>20</sub>
38	3.26	0.26	1,2,4-Trimethylcyclohexane	94	0007667-60-9	126.24	C <sub>9</sub> H <sub>18</sub>
39	3.34	0.07	β-Methylcyclopentanepropanol	58	0264258-62-0	142.24	C <sub>9</sub> H <sub>18</sub> O
40	3.36	0.48	1-Ethyl-4-methylcyclohexane	97	0003728-56-1	126.24	C <sub>9</sub> H <sub>18</sub>
41	3.42	0.09	1-Ethyl-3-methylcyclohexane	97	0003728-55-0	126.24	C <sub>9</sub> H <sub>18</sub>
42	3.47	0.44	1-Ethyl-3-methylcyclohexane	94	0003728-55-0	126.24	C <sub>9</sub> H <sub>18</sub>
43	3.53	0.50	Nonane	91	0000111-84-2	128.26	C <sub>9</sub> H <sub>20</sub>
44	3.59	0.32	1,1,3,5-Tetramethylcyclohexane	68	0004306-65-4	140.27	C <sub>10</sub> H <sub>20</sub>
45	3.64	0.08	1-Ethyl-4-methylcyclohexane	97	0003728-56-1	126.24	C <sub>9</sub> H <sub>18</sub>
46	3.70	0.19	1-Ethyl-2-methylcyclohexane	95	0003728-54-9	126.24	C <sub>10</sub> H <sub>20</sub>
47	3.83	0.38	Cyclohexanepropanol	64	0001124-63-5	142.24	C <sub>9</sub> H <sub>18</sub> O
48	3.97	0.33	Propylcyclohexane	96	0001678-92-8	126.24	C <sub>9</sub> H <sub>18</sub>
49	4.02	0.36	2,6-Dimethyloctane	96	0002051-30-1	142.28	C <sub>10</sub> H <sub>22</sub>
50	4.07	0.17	3-Methylnonane	93	0005911-04-6	142.28	C <sub>10</sub> H <sub>22</sub>
51	4.09	0.30	3-Methyl-3-hexene	41	0042154-69-8	98.19	C <sub>7</sub> H <sub>14</sub>
52	4.14	0.29	3-Ethyl-2-methylheptane	53	0014676-29-0	142.28	C <sub>10</sub> H <sub>22</sub>
53	4.17	0.19	( <i>E</i> )-3-Heptene	46	0014686-14-7	98.19	C <sub>7</sub> H <sub>14</sub>
54	4.27	0.11	4-Ethyl-2,3-dimethyl-2-hexene	49	0959028-24-1	140.27	C <sub>10</sub> H <sub>20</sub>

55	4.35	0.31	( <i>E</i> )-5-Decene	64	0007433-56-9	140.27	C <sub>10</sub> H <sub>20</sub>
56	4.40	0.19	( <i>E</i> )-5-Decene	62	0007433-56-9	140.27	C <sub>10</sub> H <sub>20</sub>
57	4.42	0.08	Propylbenzene	70	0000103-65-1	120.19	C <sub>9</sub> H <sub>12</sub>
58	4.44	0.41	4-Methylnonane	93	0017301-94-9	142.28	C <sub>10</sub> H <sub>22</sub>
59	4.49	0.17	1-Nonene	59	0000124-18-5	126.24	C <sub>9</sub> H <sub>18</sub>
60	4.53	0.31	1-Ethyl-3-methylbenzene	93	0000620-14-4	120.19	C <sub>9</sub> H <sub>12</sub>
61	4.59	0.44	3-Methylnonane	93	0005911-04-6	142.28	C <sub>10</sub> H <sub>22</sub>
62	4.62	0.41	1,2,4-Trimethylbenzene	93	0000095-63-6	120.19	C <sub>9</sub> H <sub>12</sub>
63	4.82	0.39	4-Propylcyclohexanone	46	0040649-36-3	140.22	C <sub>9</sub> H <sub>16</sub> O
64	4.98	0.19	4-Propyl-3-heptene	43	0004485-13-6	140.27	C <sub>10</sub> H <sub>20</sub>
65	5.06	1.21	1-Nonene	97	0000124-18-5	126.24	C <sub>9</sub> H <sub>18</sub>
66	5.23	0.59	(2-Methylpropyl)-benzene	50	0000538-93-2	134.22	C <sub>10</sub> H <sub>14</sub>
67	5.41	0.39	4-Methyldecane	93	0002847-72-5	156.31	C <sub>11</sub> H <sub>24</sub>
68	5.47	0.32	1-Ethyl-3-methylbenzene	70	0000620-14-4	120.19	C <sub>9</sub> H <sub>12</sub>
69	5.62	0.32	Propylcyclopentane	94	0002040-96-2	112.21	C <sub>8</sub> H <sub>16</sub>
70	5.71	0.27	2-Ethyl-1,1,3-trimethylcyclohexane	93	0442662-72-8	154.29	C <sub>11</sub> H <sub>22</sub>
71	5.77	0.17	( <i>R</i> )-3,7-dimethyl-6-octenal	86	0002385-77-5	154.25	C <sub>10</sub> H <sub>18</sub> O
72	5.87	0.30	Tridecyloate-2,2,3,3,4,4,4-heptafluorobutanoic acid	64	0959088-59-6	396.38	C <sub>17</sub> H <sub>27</sub> F <sub>7</sub> O <sub>2</sub>

73	5.90	0.33	17-Pentatriacontene	64	0006971-40-0	490.93	C <sub>35</sub> H <sub>70</sub>
74	5.93	0.53	1-Methyl-3-propylbenzene	93	0001074-43-7	134.22	C <sub>10</sub> H <sub>14</sub>
75	5.96	0.11	5-Methyldecane	93	0475575-94-1	156.31	C <sub>11</sub> H <sub>24</sub>
76	6.00	0.13	4-Methyldecane	90	0002847-72-5	156.31	C <sub>11</sub> H <sub>24</sub>
77	6.06	0.24	2-Methyldecane	93	0006975-98-0	156.31	C <sub>11</sub> H <sub>24</sub>
78	6.17	0.15	3-Methyldecane	97	0013151-34-3	156.31	C <sub>11</sub> H <sub>24</sub>
79	6.56	0.08	1-Ethyl-2,4-dimethylbenzene	60	0000874-41-9	134.22	C <sub>10</sub> H <sub>14</sub>
80	6.62	0.96	Undecane	97	0001120-21-4	156.31	C <sub>11</sub> H <sub>24</sub>
81	6.77	0.26	Decahydro-2-methylnaphthalene	96	0002958-76-1	152.28	C <sub>11</sub> H <sub>20</sub>
82	6.80	0.17	Decahydro-2-methylnaphthalene	95	0002958-76-1	152.28	C <sub>11</sub> H <sub>20</sub>
83	6.82	0.22	1-Methyl-4-(1-methylpropyl)-benzene	55	0001595-16-0	148.24	C <sub>11</sub> H <sub>16</sub>
84	6.99	0.13	1,2,4,5-Tetramethylbenzene	95	0000095-93-2	134.22	C <sub>10</sub> H <sub>14</sub>
85	7.03	0.31	3,7-Dimethyldecane	50	0017312-54-8	170.33	C <sub>12</sub> H <sub>26</sub>
86	7.24	0.30	4-Methylundecane	46	0002980-69-0	170.33	C <sub>12</sub> H <sub>26</sub>
87	7.44	0.11	6-Methylundecane	64	0017302-33-9	170.33	C <sub>12</sub> H <sub>26</sub>
88	7.47	0.37	1,2,4,5-Tetramethylbenzene	93	0000095-93-2	134.22	C <sub>10</sub> H <sub>14</sub>
89	7.50	0.14	1-Ethyl-2,3-dimethylbenzene	92	0000933-98-2	134.22	C <sub>10</sub> H <sub>14</sub>
90	7.52	0.14	4-Methylundecane	83	0002980-69-0	170.33	C <sub>12</sub> H <sub>26</sub>
91	7.58	0.51	4-Methylundecane	90	0007045-71-8	170.33	C <sub>12</sub> H <sub>26</sub>



92	8.11	2.05	Dodecane	96	0000112-40-3	170.33	C <sub>12</sub> H <sub>26</sub>
93	8.15	0.17	(1-methyl-1-buten-1-yl)-benzene	90	0053172-84-2	146.23	C <sub>11</sub> H <sub>14</sub>
94	8.26	0.19	Diocetadecyloate phosphoric acid	60	0003037-89-6	602.95	C <sub>36</sub> H <sub>75</sub> O <sub>4</sub> P
95	8.30	0.40	2,6-Dimethylundecane	97	0017301-23-4	184.36	C <sub>13</sub> H <sub>28</sub>
96	8.36	0.10	1-methyl-3-(1-methylethyl)-benzene	42	0000535-77-3	134.22	C <sub>10</sub> H <sub>14</sub>
97	8.59	0.39	1-Pentyl-2-propylcyclopentane	95	0062199-51-3	182.35	C <sub>13</sub> H <sub>26</sub>
98	8.85	0.17	2,6-Dimethylundecane	76	0017301-23-4	184.36	C <sub>13</sub> H <sub>28</sub>
99	9.00	0.19	2-Methyldodecane	87	0001560-97-0	180.33	C <sub>13</sub> H <sub>28</sub>
100	9.05	0.20	2,10-Dimethylundecane	80	0017301-27-8	184.35	C <sub>13</sub> H <sub>28</sub>
101	9.10	0.10	Tridecane	80	0000629-50-5	184.36	C <sub>13</sub> H <sub>28</sub>
102	9.12	0.23	7-Methyltridecane	87	0026730-14-3	198.39	C <sub>14</sub> H <sub>30</sub>
103	9.46	0.03	( <i>R</i> )-3,7-Dimethyl-6-octenal	50	0002385-77-5	154.25	C <sub>10</sub> H <sub>18</sub> O
104	9.50	0.51	Tridecane	98	0000629-50-5	184.36	C <sub>13</sub> H <sub>28</sub>
105	9.76	0.12	1-Methylnaphthalene	94	0000090-12-0	142.2	C <sub>11</sub> H <sub>10</sub>
106	9.80	0.24	1,4-Dihydro-1,4-methanonaphthalene	93	0004453-90-1	142.2	C <sub>11</sub> H <sub>10</sub>
107	9.91	0.37	2-(2-Buten-1-yl)-1,3,5-trimethylbenzene	47	0063435-25-6	174.28	C <sub>13</sub> H <sub>18</sub>
108	10.03	0.28	8-Methyl-3-undecene	38	0876314-66-8	168.32	C <sub>12</sub> H <sub>24</sub>
109	10.11	0.37	1,2,3,4-Tetrahydro-2,5,7-trimethylnaphthalene	59	0065001-61-8	174.28	C <sub>13</sub> H <sub>18</sub>
110	10.20	0.31	5-Methyltridecane	38	0025117-31-1	198.39	C <sub>14</sub> H <sub>30</sub>

111	10.37	0.09	4-Methyloctane	38	0002216-34-4	128.26	C <sub>9</sub> H <sub>20</sub>
112	10.50	0.17	2,6,10-Trimethyldodecane	91	0003891-98-3	212.41	C <sub>15</sub> H <sub>32</sub>
113	10.54	0.08	3,7-Dimethylnonane	87	0017302-32-8	156.31	C <sub>11</sub> H <sub>24</sub>
114	10.58	0.25	1,2,3,4-Tetrahydro-2,5,8-trimethylnaphthalene	56	0030316-17-7	174.28	C <sub>13</sub> H <sub>18</sub>
115	10.80	0.44	Tetradecane	98	0000629-59-4	198.39	C <sub>14</sub> H <sub>30</sub>
116	11.06	0.32	Diocetadecyloate phosphoric acid	52	0003037-89-6	602.95	C <sub>36</sub> H <sub>75</sub> O <sub>4</sub> P
117	11.15	0.19	1,5-Dimethylnaphthalene	97	0000571-61-9	156.22	C <sub>12</sub> H <sub>12</sub>
118	11.16	0.13	2,7-Dimethylnaphthalene	97	0000582-16-1	156.22	C <sub>12</sub> H <sub>12</sub>
119	11.17	0.43	2,3-Dimethylnaphthalene	97	0000581-40-8	156.22	C <sub>12</sub> H <sub>12</sub>
120	11.17	0.19	1,6-Dimethylnaphthalene	97	0000575-43-9	156.22	C <sub>12</sub> H <sub>12</sub>
121	11.39	0.30	2,7-Dimethylnaphthalene	97	0000582-16-1	156.22	C <sub>12</sub> H <sub>12</sub>
122	11.41	0.16	1,5-Dimethylnaphthalene	90	0000571-61-9	156.22	C <sub>12</sub> H <sub>12</sub>
123	11.42	0.57	2,6-Dimethylnaphthalene	90	0000581-42-0	156.22	C <sub>12</sub> H <sub>12</sub>
124	11.44	0.14	2,7-Dimethylnaphthalene	89	0000582-16-1	156.22	C <sub>12</sub> H <sub>12</sub>
125	11.46	0.19	2,7-Dimethylnaphthalene	81	0000582-16-1	156.22	C <sub>12</sub> H <sub>12</sub>
126	11.58	0.26	Hexacosane	87	0000630-01-3	366.71	C <sub>26</sub> H <sub>54</sub>
127	11.64	0.14	Pentacosane	87	0000629-99-2	352.68	C <sub>25</sub> H <sub>52</sub>
128	11.70	0.14	Heptacosane	87	0000593-49-7	380.73	C <sub>27</sub> H <sub>56</sub>
129	11.74	0.09	1-Hexadecene	64	0000629-73-2	224.43	C <sub>16</sub> H <sub>32</sub>

130	12.03	0.40	Pentadecane	98	0000629-62-9	212.41	C <sub>15</sub> H <sub>32</sub>
131	12.56	0.45	Tritetracontane	58	0007098-21-7	605.16	C <sub>43</sub> H <sub>88</sub>
132	12.65	0.09	Cyclopentadecane	83	0000295-48-7	210.4	C <sub>15</sub> H <sub>30</sub>
133	12.79	0.23	Tetracontane	64	0004181-95-7	563.08	C <sub>40</sub> H <sub>82</sub>
134	12.85	0.48	10-Methylnonadecane	64	0056862-62-5	282.55	C <sub>20</sub> H <sub>42</sub>
135	12.89	0.14	2,3,6-Trimethylnaphthalene	95	0000829-26-5	170.25	C <sub>13</sub> H <sub>14</sub>
136	12.96	0.16	1,6,7-Trimethylnaphthalene	95	0002245-38-7	170.25	C <sub>13</sub> H <sub>14</sub>
137	13.18	0.35	Hexadecane	98	0000544-76-3	226.44	C <sub>16</sub> H <sub>34</sub>
138	13.32	0.17	Tridecane	56	0000629-50-5	184.36	C <sub>13</sub> H <sub>28</sub>
139	13.39	0.14	1,6,7-Trimethylcyclopentane	51	0004516-69-2	112.21	C <sub>8</sub> H <sub>16</sub>
140	13.62	0.15	1,6,7-Trimethylnaphthalene	42	0003031-15-0	184.28	C <sub>14</sub> H <sub>16</sub>
141	13.73	0.23	2,6,10-Trimethylpentadecane	97	0003892-00-0	254.49	C <sub>18</sub> H <sub>38</sub>
142	13.79	0.39	Tridecane	81	0000629-50-5	184.36	C <sub>13</sub> H <sub>28</sub>
143	13.85	0.30	Dodecane	76	0000112-40-3	170.33	C <sub>12</sub> H <sub>26</sub>
144	13.91	0.40	1,1,3-Trimethylcyclopentane	35	0004516-69-2	112.21	C <sub>8</sub> H <sub>16</sub>
145	13.99	0.33	2,6,10-Trimethyl-9-undecenal	35	0000141-13-9	210.36	C <sub>14</sub> H <sub>26</sub> O
146	14.00	0.06	1-Octadecene	74	0000112-88-9	252.48	C <sub>18</sub> H <sub>36</sub>
147	14.12	0.19	(1-Pentyloctyl)-cyclohexane	30	0013151-91-2	266.51	C <sub>19</sub> H <sub>38</sub>
148	14.20	0.25	1-Butyl-2-pentylcyclopentane	89	0061142-52-7	196.37	C <sub>14</sub> H <sub>28</sub>

149	14.27	1.25	Heptadecane	96	0000629-78-7	240.47	C <sub>27</sub> H <sub>56</sub>
150	14.33	1.26	2,6,10,14-Tetramethylpentadecane	98	0001921-70-6	268.52	C <sub>19</sub> H <sub>40</sub>
151	14.39	0.43	1-Heptadecene	80	0006765-39-5	238.45	C <sub>17</sub> H <sub>34</sub>
152	14.55	1.19	1-Pentyl-2-propylcyclopentane	49	0062199-51-3	182.35	C <sub>13</sub> H <sub>26</sub>
153	14.58	0.37	1,1,3-Trimethylcyclopentane	52	0004516-69-2	112.21	C <sub>8</sub> H <sub>16</sub>
154	14.88	0.31	Tetradecane	86	0000629-59-4	198.39	C <sub>14</sub> H <sub>30</sub>
155	15.06	0.37	1-Butyl-2-pentylcyclopentane	81	0061142-52-7	196.37	C <sub>14</sub> H <sub>28</sub>
156	15.17	0.32	3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol	60	0004602-84-0	222.37	C <sub>15</sub> H <sub>26</sub> O
157	15.21	0.26	3,7-Dimethyl-7-octenal	44	0000141-26-4	154.25	C <sub>10</sub> H <sub>18</sub> O
158	15.32	1.19	Octadecane	99	0000593-45-3	254.49	C <sub>18</sub> H <sub>38</sub>
159	15.41	1.04	2,6,10,14-Tetramethylhexadecane	99	0000638-36-8	282.55	C <sub>20</sub> H <sub>42</sub>
160	15.58	0.54	5-Butyl-6-hexyloctahydro-1H-indene	66	0055044-36-5	264.49	C <sub>19</sub> H <sub>36</sub>
161	15.77	0.21	Cyclotetradecane	53	0000295-17-0	196.37	C <sub>14</sub> H <sub>28</sub>
162	15.82	0.35	2-Pentyl-2-nonanal	62	0003021-89-4	210.36	C <sub>14</sub> H <sub>26</sub> O
163	15.97	0.23	Methyl 2-butenoate	50	0018707-60-3	100.12	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>
164	16.30	1.02	Nonadecane	98	0000629-92-5	268.52	C <sub>19</sub> H <sub>40</sub>
165	16.36	0.15	17-Pentatriacontene	70	0006971-40-0	490.93	C <sub>35</sub> H <sub>70</sub>
166	16.50	0.16	2-Methylphenanthrene	87	0002531-84-2	192.26	C <sub>15</sub> H <sub>12</sub>
167	16.54	0.89	9-Methylanthracene	87	0000779-02-2	192.26	C <sub>15</sub> H <sub>12</sub>

168	16.59	0.09	1a, 9b-Dihydro-1H-cyclopropa[1]phenanthrene	86	0000949-41-7	192.26	C <sub>15</sub> H <sub>12</sub>
169	16.64	0.07	2-Methyl-4-tetradecene	70	0866760-27-2	210.45	C <sub>15</sub> H <sub>30</sub>
170	16.74	0.15	13-Tetradecen-1-ol	42	0067400-04-8	212.37	C <sub>14</sub> H <sub>28</sub> O
171	16.77	0.03	10,11-Dihydro-5H-dibenzo[a,d]cyclohepten-5-ol	42	0001210-34-0	210.27	C <sub>15</sub> H <sub>14</sub> O
172	16.79	0.13	Hexadecane	59	0000544-76-3	226.44	C <sub>16</sub> H <sub>34</sub>
173	16.94	0.17	14-Bromo-1-tetradecene	70	0074646-31-4	275.27	C <sub>14</sub> H <sub>27</sub> Br
174	17.24	0.51	Eicosane	98	0000112-95-8	282.55	C <sub>20</sub> H <sub>42</sub>
175	17.32	0.02	1,7,11-Trimethyl-4-(1-methylethyl)- cyclotetradecane	96	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>
176	17.38	0.19	1-(1,5-dimethylhexyl)-4-(4-methylpentyl)- cyclohexane	91	0056009-20-2	280.53	C <sub>20</sub> H <sub>40</sub>
177	17.67	0.47	1-acetate-13-tetradecen-1-ol	78	0056221-91-1	254.41	C <sub>16</sub> H <sub>30</sub> O <sub>2</sub>
178	17.70	0.36	3-Methylcyclopentadecanone	94	0000541-91-3	238.41	C <sub>16</sub> H <sub>30</sub> O
179	17.76	0.17	Tricyclo[8.4.1.1]hexadeca-1,3,5,7,9,11,13- heptaene	70	0055821-04-0	206.28	C <sub>16</sub> H <sub>14</sub>
180	17.89	0.49	Octadecane	95	0000593-45-3	254.49	C <sub>18</sub> H <sub>38</sub>
181	18.03	0.17	1-Octadecanethiol	83	0002885-00-9	286.56	C <sub>18</sub> H <sub>38</sub> S
182	18.11	0.40	Eicosane	97	0000112-95-8	282.55	C <sub>20</sub> H <sub>42</sub>
183	18.19	0.41	Heneicosane	97	0000629-94-7	296.57	C <sub>21</sub> H <sub>44</sub>

184	18.26	1.00	1-acetate-8-methyl-9-tetradecen-1-ol	81	0912629-93-7	268.43	C <sub>17</sub> H <sub>32</sub> O <sub>2</sub>
185	18.55	0.43	1,7,11-Trimethyl-4-(1-methylethyl)- cyclotetradecane	90	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>
186	18.59	0.38	1,2-Diethylcyclohexadecane	70	0014113-60-1	280.53	C <sub>20</sub> H <sub>40</sub>
187	18.64	0.32	1-Chlorooctadecane	78	0003386-33-2	288.94	C <sub>18</sub> H <sub>37</sub> Cl
188	19.02	0.40	Eicosane	97	0000112-95-8	282.55	C <sub>20</sub> H <sub>42</sub>
189	19.38	0.27	Docosane	97	0000629-97-0	310.6	C <sub>22</sub> H <sub>46</sub>
190	19.61	0.17	Eicosane	80	0000112-95-8	282.55	C <sub>20</sub> H <sub>42</sub>
191	19.69	0.30	Nonadecane	80	0000629-92-5	268.52	C <sub>19</sub> H <sub>40</sub>
192	19.73	0.54	2-(Acetyloxy)-1,2,3-tributyloate-1,2,3- propanetricarboxylic acid	74	0000077-90-7	402.48	C <sub>20</sub> H <sub>34</sub> O <sub>8</sub>
193	19.83	0.65	1,2,3-Tributyloate-2-hydroxy-1,2,3- propanetricarboxylic acid	53	0000077-94-1	360.44	C <sub>18</sub> H <sub>32</sub> O <sub>7</sub>
194	19.85	0.70	Tricosane	96	0000638-67-5	324.63	C <sub>23</sub> H <sub>48</sub>
195	19.96	0.46	Hexatriacontane	93	0000630-06-8	506.97	C <sub>36</sub> H <sub>74</sub>
196	19.23	1.74	9-Methylnonadecane	93	0013287-24-6	282.55	C <sub>20</sub> H <sub>42</sub>
197	20.38	0.77	1,7,11-Trimethyl-4-(1-methylethyl)- cyclotetradecane	49	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>
198	20.41	0.42	2,6,10-Trimethyl-9-undecenoic acid	49	0097993-62-9	226.35	C <sub>14</sub> H <sub>26</sub> O <sub>2</sub>

199	20.42	0.56	Tetracosane	92	0000646-31-1	338.65	C <sub>24</sub> H <sub>50</sub>
200	20.53	0.31	1,7,11-Trimethyl-4-(1-methylethyl)- cyclotetradecane	91	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>
201	20.58	0.20	1,7,11-Trimethyl-4-(1-methylethyl)- cyclotetradecane	93	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>
202	20.64	0.59	Tetracosane	98	0000646-31-1	338.65	C <sub>24</sub> H <sub>50</sub>
203	20.79	0.88	Nonadecane	95	0000629-92-5	268.52	C <sub>19</sub> H <sub>40</sub>
204	20.99	0.19	1,2-Diethylcyclohexadecane	78	0014113-60-1	280.53	C <sub>20</sub> H <sub>40</sub>
205	21.08	1.95	1,7,11-Trimethyl-4-(1-methylethyl)- cyclotetradecane	93	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>
206	21.18	0.08	1,7,11-trimethyl-4-(1-methylethyl)- cyclotetradecane,	89	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>
207	21.27	1.53	1,7,11-trimethyl-4-(1-methylethyl)- cyclotetradecane	91	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>
208	21.33	0.24	2-Tetradecyloxirane	83	0007320-37-8	240.42	C <sub>16</sub> H <sub>32</sub> O
209	21.41	0.62	Tricosane	97	0000638-67-5	324.63	C <sub>23</sub> H <sub>48</sub>
210	21.53	0.97	1,7,11-Trimethyl-4-(1-methylethyl)- cyclotetradecane	83	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>
211	21.77	0.86	Tetracosane	93	0000646-31-1	338.65	C <sub>24</sub> H <sub>50</sub>

212	21.92	0.68	1,2-bis(2-Ethylhexyl)oate-1,2-benzenedicarboxylic acid	90	0000117-81-7	390.56	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>
213	22.14	0.53	Hexacosane	99	0000630-01-3	366.71	C <sub>26</sub> H <sub>54</sub>
214	22.43	0.75	Tricosane	97	0000638-67-5	324.63	C <sub>23</sub> H <sub>48</sub>
215	22.55	0.32	(-)-1',4-Dihydroxy-7'-methoxy-2,3'-dimethyl-[1,2'-binaphthalene]-5,5',8,8'-tetrone	90	0119736-96-8	404.37	C <sub>23</sub> H <sub>16</sub> O <sub>7</sub>
216	22.56	0.27	2'-Dodecyl-1,1':3',1''-tercyclopentane	90	0055282-68-3	374.69	C <sub>27</sub> H <sub>50</sub>
217	22.57	0.21	Pentacosane	86	0000629-99-2	352.68	C <sub>25</sub> H <sub>52</sub>
218	22.60	0.16	1-Octadecene	84	0000112-88-9	252.48	C <sub>18</sub> H <sub>36</sub>
219	22.62	0.10	(-)-1',4-Dihydroxy-7'-methoxy-2,3'-dimethyl-[1,2'-Binaphthalene]-5,5',8,8'-tetrone	98	0119736-96-8	404.37	C <sub>23</sub> H <sub>16</sub> O <sub>7</sub>
220	22.65	0.10	Pentacosane	93	0000629-99-2	352.68	C <sub>25</sub> H <sub>52</sub>
221	22.76	0.02	Hexacosane	93	0000630-01-3	366.71	C <sub>26</sub> H <sub>54</sub>
222	22.85	0.19	Heptacosane	99	0000593-49-7	380.73	C <sub>27</sub> H <sub>56</sub>
223	23.17	0.24	(-)-1',4-Dihydroxy-7'-methoxy-2,3'-dimethyl-[1,2'-Binaphthalene]-5,5',8,8'-Tetrone	97	0119736-96-8	404.37	C <sub>23</sub> H <sub>16</sub> O <sub>7</sub>
224	23.27	0.37	1,3-bis(2-ethylhexyl)oate-1,3-benzenedicarboxylic acid	27	0000137-89-3	390.56	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>
225	23.29	0.01	1,2-Dioctyloate-1,2-benzenedicarboxylic acid	27	0000117-84-0	390.56	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>



226	23.32	0.23	1,2-Diisodecyloate-1,2-benzenedicarboxylic acid	27	0026761-40-0	446.74	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
227	23.35	0.30	9-Hexacosene	40	0071502-22-2	364.69	C <sub>26</sub> H <sub>52</sub>
228	23.39	0.22	9-Tricosene	40	0027519-02-4	322.61	C <sub>23</sub> H <sub>46</sub>
229	23.53	0.16	Pentacosane	98	0000629-99-2	352.68	C <sub>25</sub> H <sub>52</sub>
230	23.52	0.19	Hexacosane	98	0000630-01-3	366.71	C <sub>26</sub> H <sub>54</sub>
231	23.60	0.11	Tetracosane	98	0000646-31-1	338.65	C <sub>24</sub> H <sub>50</sub>
232	23.68	0.13	Hexacosane	74	0000630-01-3	366.71	C <sub>26</sub> H <sub>54</sub>
233	23.74	0.07	Hexacosane	92	0000630-01-3	366.71	C <sub>26</sub> H <sub>54</sub>
234	24.02	0.07	Heptacosane	91	0000593-49-7	380.73	C <sub>27</sub> H <sub>56</sub>
235	24.06	0.14	1-Butyl-2-(8-methylnonyl)-oate-1,2-benzenedicarboxylic acid	95	0000089-18-9	362.5	C <sub>22</sub> H <sub>34</sub> O <sub>4</sub>
236	24.20	0.04	Octacosane	92	0000630-02-4	394.76	C <sub>28</sub> H <sub>58</sub>
237	24.22	0.12	1,2-Didecyloate-1,2-benzenedicarboxylic acid	83	0000084-77-5	446.66	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
238	24.25	0.05	1,2-Diisodecyloate-1,2-benzenedicarboxylic acid	83	0026761-40-0	446.74	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
239	24.27	0.03	1,2-Didecyloate-1,2-benzenedicarboxylic acid	91	0000084-77-5	446.66	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
240	24.30	0.04	1,2-bis(8-Methylnonyl)oate-1,2-benzenedicarboxylic acid	90	0000089-16-7	446.66	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>

241	24.36	0.09	1,2-Diisodecyloate-1,2-benzenedicarboxylic acid	91	0026761-40-0	446.74	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
242	24.40	0.03	1,2-Didecyloate-1,2-benzenedicarboxylic acid	90	0000084-77-5	446.66	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
243	24.45	0.20	1,2-bis(8-Methylnonyl)ate-1,2-benzenedicarboxylic acid	98	0000089-16-7	446.66	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
244	24.54	0.17	1,2-Didecyloate-1,2-benzenedicarboxylic acid	91	0000084-77-5	446.66	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
245	24.61	0.24	1,2-bis(8-Methylnonyl)-ate-1,2-benzenedicarboxylic acid	90	0000089-16-7	446.66	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
246	24.62	0.23	1-Butyl-2-(8-methylnonyl)-ate-1,2-benzenedicarboxylic acid	93	0000089-18-9	362.5	C <sub>22</sub> H <sub>34</sub> O <sub>4</sub>
247	24.70	0.14	1,2-Didecyloate-1,2-benzenedicarboxylic acid	91	0000084-77-5	446.66	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
248	24.98	0.24	1,2-bis(8-Methylnonyl)ate-1,2-benzenedicarboxylic acid	93	0000089-16-7	446.66	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
249	25.08	0.37	1,2-Didecyloate-1,2-benzenedicarboxylic acid	91	0000084-77-5	446.66	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
250	25.11	0.24	1,2-Didecyloate-1,2-benzenedicarboxylic acid	72	0000084-77-5	446.66	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
251	25.17	0.32	1-Butyl-2-(8-methylnonyl)ate-1,2-benzenedicarboxylic acid	95	0000089-18-9	362.5	C <sub>22</sub> H <sub>34</sub> O <sub>4</sub>
252	25.29	0.40	1,2-Diisodecyloate-1,2-benzenedicarboxylic acid	59	0026761-40-0	446.74	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>

253	25.31	0.11	1-Butyl-2-(8-methylnonyl)oate-1,2-benzenedicarboxylic acid	59	0000089-18-9	362.5	C <sub>22</sub> H <sub>34</sub> O <sub>4</sub>
254	25.35	0.24	1-Butyl-2-(8-methylnonyl)oate-1,2-benzenedicarboxylic acid	93	0000089-18-9	362.5	C <sub>22</sub> H <sub>34</sub> O <sub>4</sub>
255	25.86	0.27	Hexacosane	62	0000630-01-3	366.71	C <sub>26</sub> H <sub>54</sub>
256	25.92	0.32	Cyclotriacontane	87	0000297-35-8	420.8	C <sub>30</sub> H <sub>60</sub>
257	25.97	0.53	(-)-1',4-Dihydroxy-7'-methoxy-2,3'-dimethyl-[1,2'-Binaphthalene]-5,5',8,8'-tetrone	93	0119736-96-8	404.37	C <sub>23</sub> H <sub>16</sub> O <sub>7</sub>
258	27.95	0.42	1,54-Dibromotetrapentacontane	83	0852228-22-9	917.24	C <sub>54</sub> H <sub>108</sub> Br <sub>2</sub>
259	29.12	0.16	1,54-Dibromotetrapentacontane	64	0852228-22-9	917.24	C <sub>54</sub> H <sub>108</sub> Br <sub>2</sub>
260	30.51	0.43	1-Bromo-11-iodoundecane	41	0139123-69-6	361.1	C <sub>11</sub> H <sub>22</sub> BrI

**Table S4.** List of identified molecules with GC-MS from Eagle Ford neutral aliquot extracted with chloroform.

Pk	R.T. (min)	A[Tot] (%)	Compound name	Qual. (%)	CAS #	Mw	Molecular Formula
1	1.26	2.37	Ammonia	2	0007664-41-7	17.03	NH <sub>3</sub>
2	1.33	2.12	2-Methyl-1-butene	91	0000563-46-2	70.13	C <sub>5</sub> H <sub>10</sub>
3	1.48	25.84	Trichloromethane	83	0000067-66-3	119.38	CHCl <sub>3</sub>
4	9.13	0.5	Hydrochloric Acid	5	0007647-01-0	36	HCl
5	9.50	1.48	Hydrochloric Acid	9	0007647-01-0	36	HCl
6	10.50	1.12	1-(Pentyloxy)-hexane	43	0032357-83-8	172.31	C <sub>11</sub> H <sub>24</sub> O
7	10.81	0.8	Pentacosane	86	0000629-99-2	352.68	C <sub>25</sub> H <sub>52</sub>
8	10.81	1.36	Tricosane	76	0000638-67-5	324.63	C <sub>23</sub> H <sub>48</sub>
9	10.83	0.22	triacontane	74	0000638-68-6	422.81	C <sub>30</sub> H <sub>62</sub>
10	10.84	2.08	Pentacosane	82	0000629-99-2	352.68	C <sub>25</sub> H <sub>52</sub>
11	10.85	1.96	Octacosane	93	0000630-02-4	394.76	C <sub>28</sub> H <sub>58</sub>
12	10.86	2.58	Dotriacontane	90	0000544-85-4	450.87	C <sub>32</sub> H <sub>66</sub>
13	10.96	1.48	Pentatriacontane	48	0000630-07-9	492.95	C <sub>35</sub> H <sub>72</sub>
14	10.23	0.84	Tetradecane	73	0000629-59-4	198.39	C <sub>14</sub> H <sub>30</sub>
15	11.41	2.48	1-Methyl-7-oxabicyclo[4.1.0]heptane	43	0001713-33-3	112.17	C <sub>7</sub> H <sub>12</sub> O
16	11.57	1.5	11-(1-Ethylpropyl)-heneicosane	80	0055282-11-6	366.71	C <sub>26</sub> H <sub>54</sub>

17	11.60	1.48	Triacontane	85	0000638-68-6	422.81	C <sub>30</sub> H <sub>62</sub>
18	11.63	2.88	Nonacosane	32	0000630-03-5	408.79	C <sub>29</sub> H <sub>60</sub>
19	11.67	1.36	1-Fluorododecane	35	0000334-68-9	188.33	C <sub>12</sub> H <sub>25</sub> F
20	11.97	2.32	2-Butyl-1-octanol	12	0003913-02-8	186.33	C <sub>12</sub> H <sub>26</sub> O
21	12.02	3.28	Pentadecane	95	0000629-62-9	212.41	C <sub>15</sub> H <sub>32</sub>
22	12.58	3.52	2,2,2-Trifluorotetradecyl ester acetic acid	37	0006222-02-2	310.4	C <sub>16</sub> H <sub>29</sub> F <sub>3</sub> O <sub>2</sub>
23	12.67	0.96	2,2,3,3,4,4,4-Heptafluoroundecyl ester butanoic acid	90	0959103-74-3	368.33	C <sub>15</sub> H <sub>23</sub> F <sub>7</sub> O <sub>2</sub>
24	12.35	3.76	17-Pentatriacontene	94	0006971-40-0	490.93	C <sub>35</sub> H <sub>70</sub>
25	12.70	0.68	Pentacosane	43	0000629-99-2	352.68	C <sub>25</sub> H <sub>52</sub>
26	12.72	0.86	Tricosane	65	0000638-67-5	324.63	C <sub>23</sub> H <sub>48</sub>
27	12.74	1.04	Eicosane	49	0000112-95-8	282.55	C <sub>20</sub> H <sub>42</sub>
28	12.76	0.66	Dotriacontane	50	0000544-85-4	450.87	C <sub>32</sub> H <sub>66</sub>
29	12.84	1.06	1-Fluorododecane	12	0000334-68-9	188.33	C <sub>12</sub> H <sub>25</sub> F
30	13.19	1.72	Pentacosane	43	0000629-99-2	352.68	C <sub>25</sub> H <sub>52</sub>
31	13.21	1.54	Tricosane	90	0000638-67-5	324.63	C <sub>23</sub> H <sub>48</sub>
32	13.13	0.42	Eicosane	65	0000112-95-8	282.55	C <sub>20</sub> H <sub>42</sub>
33	13.26	0.53	1-Dotriacontanol	23	0006624-79-9	466.87	C <sub>32</sub> H <sub>66</sub> O
34	13.72	0.94	Tritetracontane	64	0007098-21-7	605.16	C <sub>43</sub> H <sub>88</sub>

35	13.81	0.6	10-Pentadecen-1-ol	42	0129396-62-9	226.4	C <sub>15</sub> H <sub>30</sub> O
36	13.87	3.84	1-(3-Methyl-2-furanyl)-2-propanone	14	0087773-62-4	138.16	C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>
37	14.28	0.31	Heptadecane	95	0000629-78-7	240.47	C <sub>27</sub> H <sub>56</sub>
38	14.32	0.74	2,6,10-Trimethyldodecane	90	0003891-98-3	212.41	C <sub>15</sub> H <sub>32</sub>
39	14.73	0.51	2-Ethyl-1-decanol	10	0021078-65-9	186.33	C <sub>12</sub> H <sub>26</sub> O
40	14.82	1.73	Dotriacontane	47	0000544-85-4	450.87	C <sub>32</sub> H <sub>66</sub>
41	14.90	0.75	Triacontane	44	0000638-68-6	422.81	C <sub>30</sub> H <sub>62</sub>
42	14.98	1.21	10-Pentadecen-1-ol	45	0129396-62-9	226.4	C <sub>15</sub> H <sub>30</sub> O
43	15.31	0.62	Tetratetracontane	90	0007098-22-8	619.19	C <sub>44</sub> H <sub>90</sub>
44	15.32	2.28	Tritetracontane	80	0007098-21-7	605.16	C <sub>43</sub> H <sub>88</sub>
45	15.37	0.54	Triacontane	81	0000638-68-6	422.81	C <sub>30</sub> H <sub>62</sub>
46	13.38	0.76	Hexatriacontane	63	0000630-06-8	506.97	C <sub>36</sub> H <sub>74</sub>
47	15.40	1.12	Hexatriacontane	53	0000630-06-8	506.97	C <sub>36</sub> H <sub>74</sub>
48	16.31	0.61	Hexatriacontane	72	0000630-06-8	506.97	C <sub>36</sub> H <sub>74</sub>
49	17.25	0.59	Tetratetracontane	90	0007098-22-8	619.19	C <sub>44</sub> H <sub>90</sub>
50	17.30	0.22	Triacontane	69	0000638-68-6	422.81	C <sub>30</sub> H <sub>62</sub>
51	17.40	0.27	Dotriacontane	99	0000544-85-4	450.87	C <sub>32</sub> H <sub>66</sub>
52	17.50	1.02	Hexatriacontane	73	0000630-06-8	506.97	C <sub>36</sub> H <sub>74</sub>
53	17.60	4.1	Nonacosane	32	0000630-03-5	408.79	C <sub>29</sub> H <sub>60</sub>

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54	18.14	0.30	2,2,3,3-Tetramethylhexane	50	0013475-81-5	142.28	C <sub>10</sub> H <sub>22</sub>
55	18.20	0.14	Hexadecane	38	0000544-76-3	226.44	C <sub>16</sub> H <sub>34</sub>

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**Table S5.** List of identified molecules with GC-MS from Eagle Ford (TX) acid aliquot extracted with chloroform.

Peak	R.T. (min)	A[Tot] (%)	Compound	Q (%)	CAS #	M <sub>w</sub>	Molecular formula
1	1.27	1.185	Ammonia	3	0007664-41-7	17.03	NH <sub>3</sub>
2	1.34	1.06	4-Methyl-2-pentene	90	0004461-48-7	84.16	C <sub>6</sub> H <sub>12</sub>
3	1.4	0.25	2-Methyl-2-butene	90	0000513-35-9	70.13	C <sub>5</sub> H <sub>10</sub>
4	1.49	13.1	Trichloromethane	90	0000067-66-3	119.4	CHCl <sub>3</sub>
5	7.457	0.56	2,2,3,3-Tetramethylhexane	36	0013475-81-5	142.3	C <sub>10</sub> H <sub>22</sub>
6	7.578	0.8	1-Pentyloxyhexane	59	0032357-83-8	172.3	C <sub>11</sub> H <sub>24</sub> O
7	7.684	1.36	Pentatriacontane	72	0000630-07-9	493	C <sub>35</sub> H <sub>72</sub>
8	8.109	0.22	Dodecane	81	0000112-40-3	170.3	C <sub>12</sub> H <sub>26</sub>
9	8.866	2.08	1-(Pentyloxy)-hexane	38	0032357-83-8	172.3	C <sub>11</sub> H <sub>24</sub> O
10	8.942	1.96	11-(1-Ethylpropyl)-heneicosane	72	0055282-11-6	366.7	C <sub>26</sub> H <sub>54</sub>
11	9.003	2.58	Heneicosane	59	0000629-94-7	296.6	C <sub>21</sub> H <sub>44</sub>
12	9.01	1.48	Docosane	70	0000629-97-0	310.6	C <sub>22</sub> H <sub>46</sub>
13	9.05	0.84	Tricosane	73	0000638-67-5	324.6	C <sub>23</sub> H <sub>48</sub>
14	9.109	2.48	Nonadecane	64	0000629-92-5	268.5	C <sub>19</sub> H <sub>40</sub>
15	9.502	1.5	Tridecane	95	0000629-50-5	184.4	C <sub>13</sub> H <sub>28</sub>
16	9.6	1.48	Eicosane	58	0000112-95-8	282.6	C <sub>20</sub> H <sub>42</sub>



17	9.7	2.88	2,6-Dimethylheptane	66	0001072-05-5	128.3	C <sub>9</sub> H <sub>20</sub>
18	9.9	1.36	Tetradecane	32	0000629-59-4	198.4	C <sub>14</sub> H <sub>30</sub>
19	10.125	2.32	2,4-Dimethylundecane	3	0017312-80-0	184.4	C <sub>13</sub> H <sub>28</sub>
20	10.275	1.64	4-Methyltridecane	38	0026730-12-1	198.4	C <sub>14</sub> H <sub>30</sub>
21	10.3	1.76	Tetratetracontane	21	0007098-22-8	619.2	C <sub>44</sub> H <sub>90</sub>
22	10.31	0.48	3-Methyldodecane	47	0017312-57-1	184.4	C <sub>13</sub> H <sub>28</sub>
23	10.336	1.88	Octacosane	25	0000630-02-4	394.8	C <sub>28</sub> H <sub>58</sub>
24	10.34	0.34	Triacontane	40	0000638-68-6	422.8	C <sub>30</sub> H <sub>62</sub>
25	10.35	0.86	2-Methyltridecane	56	0001560-96-9	198.4	C <sub>14</sub> H <sub>30</sub>
26	10.36	1.04	Hexatriacontane	85	0000630-06-8	507	C <sub>36</sub> H <sub>74</sub>
27	10.37	0.66	Nonacosane	56	0000630-03-5	408.8	C <sub>29</sub> H <sub>60</sub>
28	10.38	1.06	1-Chloroheptacosane	60	0062016-79-9	415.2	C <sub>27</sub> H <sub>55</sub> Cl
29	10.39	1.72	10-Methylnonadecane	39	0056862-62-5	282.6	C <sub>20</sub> H <sub>42</sub>
30	10.4	1.54	Dotriacontane	28	0000544-85-4	450.9	C <sub>32</sub> H <sub>66</sub>
31	10.427	0.42	Dotriacontane	52	0000544-85-4	450.9	C <sub>32</sub> H <sub>66</sub>
32	10.43	0.53	Pentatriacontane	21	0000630-07-9	493	C <sub>35</sub> H <sub>72</sub>
33	10.44	0.94	Hexatriacontane	48	0000630-06-8	507	C <sub>36</sub> H <sub>74</sub>
34	10.45	0.6	Triacontane	43	0000638-68-6	422.8	C <sub>30</sub> H <sub>62</sub>
35	10.46	1.92	Tetratetracontane	22	0007098-22-8	619.2	C <sub>44</sub> H <sub>90</sub>

36	10.7	0.155	Hexatriacontane	38	0000630-06-8	507	C <sub>36</sub> H <sub>74</sub>
37	10.805	0.37	Tetradecane	95	0000629-59-4	198.4	C <sub>14</sub> H <sub>30</sub>
38	11	0.255	1-(Cyclohexylmethyl)-4-methylcyclohexane	89	0066826-95-7	194.4	C <sub>14</sub> H <sub>26</sub>
39	11.411	0.865	Cyclotetradecane	70	0000295-17-0	196.4	C <sub>14</sub> H <sub>28</sub>
40	11.457	0.75	5-Methyltetradecane	43	0025117-32-2	212.4	C <sub>15</sub> H <sub>32</sub>
41	11.578	1.21	1-Bromooctadecane	55	0000112-89-0	333.9	C <sub>18</sub> H <sub>37</sub> Br
42	11.669	0.62	1-Bromohexadecane	46	0000112-82-3	305.3	C <sub>16</sub> H <sub>33</sub> Br
43	11.7	1.14	1-Bromopentadecane	88	0000629-72-1	291.3	C <sub>15</sub> H <sub>31</sub> Br
44	11.4	0.27	1-Bromooctadecane	90	0000112-89-0	333.9	C <sub>18</sub> H <sub>37</sub> Br
45	11.881	0.38	Octahydro-4a-methyl-2(1H)-naphthalenone	83	0000938-06-7	166.3	C <sub>11</sub> H <sub>18</sub> O
46	12.033	0.56	Pentadecane	83	0000629-62-9	212.4	C <sub>15</sub> H <sub>32</sub>
47	12.123	0.305	2-Hexyl-1-decanol	38	0002425-77-6	242.4	C <sub>16</sub> H <sub>34</sub> O
48	12.578	0.59	1,5-dimethyl-7-Oxabicyclo[4.1.0]heptane	58	0162239-52-3	126.2	C <sub>8</sub> H <sub>14</sub> O
49	12.639	0.22	(2-Methylpropyl)-cyclohexane	43	0001678-98-4	140.3	C <sub>10</sub> H <sub>20</sub>
50	12.699	0.27	5-methyl-2-(1-methylethyl)-cyclohexanol	38	0001490-04-6	156.3	C <sub>10</sub> H <sub>20</sub> O
51	12.73	1.02	1,8,10-Pentadecatriene	37	1227308-82-8	206.4	C <sub>15</sub> H <sub>26</sub>
52	12.76	4.1	1,54-Dibromotetrapentacontane	41	0852228-22-9	917.2	C <sub>54</sub> H <sub>108</sub> Br <sub>2</sub>
53	13.184	0.30	Hexadecane	98	0000544-76-3	226.4	C <sub>16</sub> H <sub>34</sub>
54	13.26	0.14	(1-Butylheptyl)-undecane	46	0013151-80-9	238.5	C <sub>17</sub> H <sub>34</sub>

55	13.714	1.36	(1-Butylheptyl)-octadecane	58	0000112-89-0	333.9	C <sub>18</sub> H <sub>37</sub> Br
56	13.805	0.22	1-Methyl-3-(1-methylethyl)-cyclopentane	47	0053771-88-3	126.2	C <sub>9</sub> H <sub>18</sub>
57	13.881	1.04	17-Methylpentatriacontane	38	0056987-83-8	507	C <sub>36</sub> H <sub>74</sub>
58	13.957	0.98	1,54-Dibromotetrapentacontane	43	0852228-22-9	917.2	C <sub>54</sub> H <sub>108</sub> Br <sub>2</sub>
59	14.048	1.29	Hexadecahdropyrene	53	0002435-85-0	218.4	C <sub>16</sub> H <sub>26</sub>
60	14.275	0.74	Heptadecane	96	0000629-78-7	240.5	C <sub>27</sub> H <sub>56</sub>
61	14.235	0.42	1,54-Dibromotetrapentacontane	49	0852228-22-9	917.2	C <sub>54</sub> H <sub>108</sub> Br <sub>2</sub>
62	14.729	2.48	1,5-Dimethyl-7-oxabicyclo[4.1.0]heptane	55	0162239-52-3	126.2	C <sub>8</sub> H <sub>14</sub> O
63	14.82	1.5	1-Chlorohexadecane	38	0004860-03-1	260.9	C <sub>16</sub> H <sub>33</sub> Cl
64	14.926	1.48	(1-Propylonyl)-cyclohexane	64	0013151-84-3	252.5	C <sub>18</sub> H <sub>36</sub>
65	15.017	2.88	1,12-Dibromododecane	47	0003344-70-5	328.1	C <sub>12</sub> H <sub>24</sub> Br <sub>2</sub>
66	15.305	1.36	Tritetracontane	87	0007098-21-7	605.2	C <sub>43</sub> H <sub>88</sub>
67	15.31	2.32	Tetratetracontane	48	0007098-22-8	619.2	C <sub>44</sub> H <sub>90</sub>
68	15.32	3.28	Hexatriacontane	63	0000630-06-8	507	C <sub>36</sub> H <sub>74</sub>
69	15.33	3.52	Octadecane	21	0000593-45-3	254.5	C <sub>18</sub> H <sub>38</sub>
70	15.396	0.96	1,54-Dibromotetrapentacontane	52	0852228-22-9	917.2	C <sub>54</sub> H <sub>108</sub> Br <sub>2</sub>
71	16.305	3.76	Nonadecane	93	0000629-92-5	268.5	C <sub>19</sub> H <sub>40</sub>

**Table S6.** List of identified molecules with GC-MS from Barnett (NM) neutral aliquot extracted with chloroform.

Peak	R.T. (min)	A[Tot] (%)	Library/ID	Q (%)	CAS #	M <sub>w</sub>	Molecular formula
1	1.27	0.42	Hydroxyacetonitrile	5	0000107-16-4	57.05	C <sub>2</sub> H <sub>3</sub> NO
2	1.33	0.64	1,1-Dimethylcyclopropane	94	0001630-94-0	70.13	C <sub>5</sub> H <sub>10</sub>
3	1.46	0.98	Hexane	93	0000110-54-3	86.18	C <sub>6</sub> H <sub>14</sub>
4	1.48	4.78	Trichloromethane	83	0000067-66-3	119.38	CHCl <sub>3</sub>
5	1.62	0.94	$\alpha$ -2-Propen-1-yl-benzenemethanol	53	0000936-58-3	148.2	C <sub>10</sub> H <sub>12</sub> O
6	1.68	0.73	1,3-Dimethylcyclopentane	96	0002453-00-1	98.19	C <sub>7</sub> H <sub>14</sub>
7	1.68	0.65	<i>cis</i> -1,2-Dimethylcyclopentane	95	0001192-18-3	98.19	C <sub>7</sub> H <sub>14</sub>
8	1.68	1.47	1,3-Dimethylcyclopentane	96	0002453-00-1	98.19	C <sub>7</sub> H <sub>14</sub>
9	1.85	1.22	Methylcyclohexane	97	0000108-87-2	98.19	C <sub>7</sub> H <sub>14</sub>
10	1.92	0.37	1,2,4-Trimethylcyclopentane	90	0002815-58-9	112.21	C <sub>8</sub> H <sub>16</sub>
11	1.98	0.31	3-Methyl-1-heptene	83	0004810-09-7	112.21	C <sub>8</sub> H <sub>16</sub>
12	2.07	1.00	2-Methylheptane	96	0000592-27-8	114.23	C <sub>8</sub> H <sub>18</sub>
13	2.15	1.29	Methylbenzene	93	0000108-88-3	92.14	C <sub>7</sub> H <sub>8</sub>
14	2.19	0.74	1,3-Dimethylcyclohexane	95	0000638-04-0	112.21	C <sub>8</sub> H <sub>16</sub>
15	2.30	0.51	<i>cis</i> -1-Ethyl-2-methyl-cyclopentane	96	0000930-89-2	112.21	C <sub>8</sub> H <sub>16</sub>
16	2.36	1.73	2-Octene	70	0000111-67-1	112.21	C <sub>8</sub> H <sub>16</sub>

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17	2.63	0.12	2,6-Dimethylheptane	90	0001072-05-5	128.26	C <sub>9</sub> H <sub>20</sub>
18	2.72	2.28	Ethylcyclohexane	94	0001678-91-7	112.21	C <sub>8</sub> H <sub>16</sub>
19	2.74	1.05	1,1,3-Trimethylcyclohexane	96	0003073-66-3	126.24	C <sub>9</sub> H <sub>18</sub>
20	2.88	0.14	<i>cis</i> -1,2-Dimethylcyclopentane	87	0001192-18-3	98.19	C <sub>7</sub> H <sub>14</sub>
21	2.91	0.54	1,2,4-Trimethylcyclohexane	96	0007667-60-9	126.24	C <sub>9</sub> H <sub>18</sub>
22	3.06	0.56	2-Methyloctane	64	0003221-61-2	128.26	C <sub>9</sub> H <sub>20</sub>
23	3.10	0.37	Ethylbenzene	95	0000100-41-4	106.17	C <sub>8</sub> H <sub>10</sub>
24	3.19	1.80	1,2-Dimethylbenzene	95	0000095-47-6	106.17	C <sub>8</sub> H <sub>10</sub>
25	3.36	0.91	1-Ethyl-3-methylcyclohexane	97	0019489-10-2	126.24	C <sub>9</sub> H <sub>18</sub>
26	3.53	1.91	Nonane	87	0000111-84-2	128.26	C <sub>9</sub> H <sub>20</sub>
27	3.83	0.55	Octahydro-2-methylpentalene	55	0003868-64-2	124.22	C <sub>9</sub> H <sub>16</sub>
28	3.97	0.62	Propylcyclohexane	96	0001678-92-8	126.24	C <sub>9</sub> H <sub>18</sub>
29	4.03	0.69	1-Decene	60	0000872-05-9	140.27	C <sub>10</sub> H <sub>20</sub>
30	4.13	0.56	( <i>E</i> )-3-Heptene	45	0014686-14-7	98.19	C <sub>7</sub> H <sub>14</sub>
31	4.35	0.59	4-Decene	58	0019398-89-1	140.27	C <sub>10</sub> H <sub>20</sub>
32	4.44	0.78	4-Methylnonane	93	0017301-94-9	142.28	C <sub>10</sub> H <sub>22</sub>
33	4.53	0.60	1-Ethyl-2-methylbenzene	93	0000611-14-3	120.19	C <sub>9</sub> H <sub>12</sub>
34	4.62	0.79	1-Ethyl-2-methylbenzene	93	0000095-63-6	120.19	C <sub>9</sub> H <sub>12</sub>
35	4.71	0.17	1,2,3-Trimethylbenzene	92	0000526-73-8	120.19	C <sub>9</sub> H <sub>12</sub>

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36	4.80	0.30	1,3,5-Trimethylbenzene	91	0000108-67-8	120.19	C <sub>9</sub> H <sub>12</sub>
37	4.81	0.74	4-Propyl-3-heptene	55	0004485-13-6	140.27	C <sub>10</sub> H <sub>20</sub>
38	5.01	0.89	1,3,5-Trimethylbenzene	95	0000108-67-8	120.19	C <sub>9</sub> H <sub>12</sub>
39	5.05	0.23	1,2,3-Trimethylbenzene	95	0000526-73-8	120.19	C <sub>9</sub> H <sub>12</sub>
40	5.06	2.37	Decane	97	0000124-18-5	142.28	C <sub>10</sub> H <sub>22</sub>
41	5.41	0.74	4-Methyldecane	96	0002847-72-5	156.31	C <sub>11</sub> H <sub>24</sub>
42	5.47	0.61	1-Ethyl-2-methylbenzene	90	0000611-14-3	120.19	C <sub>9</sub> H <sub>12</sub>
43	5.62	0.99	Propylcyclopentane	96	0002040-96-2	112.21	C <sub>8</sub> H <sub>16</sub>
44	5.71	0.60	2-Ethyl-1,1,3-trimethylcyclohexane	95	0442662-72-8	154.29	C <sub>11</sub> H <sub>22</sub>
45	5.86	1.00	2-Methyl-1-dodecanol	64	0022663-61-2	200.36	C <sub>13</sub> H <sub>28</sub> O
46	5.92	1.08	1-Methyl-3-propylbenzene	91	0001074-43-7	134.22	C <sub>10</sub> H <sub>14</sub>
47	5.95	0.12	5-Methyltetradecane	93	0025117-32-2	212.41	C <sub>15</sub> H <sub>32</sub>
48	6.00	0.36	4-Methyldecane	64	0002847-72-5	156.31	C <sub>11</sub> H <sub>24</sub>
49	6.06	0.45	2-Methyldecane	91	0006975-98-0	156.31	C <sub>11</sub> H <sub>24</sub>
50	6.16	0.29	3-Methyldecane	95	0013151-34-3	156.31	C <sub>11</sub> H <sub>24</sub>
51	6.56	1.97	Pentylcyclohexane	38	0004292-92-6	154.29	C <sub>11</sub> H <sub>22</sub>
52	6.62	1.77	Undecane	96	0001120-21-4	156.31	C <sub>11</sub> H <sub>24</sub>
53	6.77	0.37	Decahydro-1-methyl-2-methylenenaphthalene	97	0090548-09-7	164.29	C <sub>12</sub> H <sub>20</sub>
54	6.86	0.18	Decahydro-2-methyl-naphthalene,	97	0002958-76-1	152.28	C <sub>11</sub> H <sub>20</sub>

55	6.98	0.07	1,2,4,5-Tetramethylbenzene	95	0000095-93-2	134.22	C <sub>10</sub> H <sub>14</sub>
56	7.01	0.14	1-Methyl-4-(1-methylethyl)-benzene	94	0000099-87-6	134.22	C <sub>10</sub> H <sub>14</sub>
57	7.03	0.53	4,4-Dimethyl-2-(1-methylethenyl)- cyclopentanone	50	0343270-53-1	154.25	C <sub>10</sub> H <sub>18</sub> O
58	7.47	0.69	4,4-dimethyl-2-(1-methylethenyl)-benzene	90	0000095-93-2	134.22	C <sub>10</sub> H <sub>14</sub>
59	7.51	0.08	4-Methylundecane	81	0002980-69-0	170.33	C <sub>12</sub> H <sub>26</sub>
60	7.59	0.47	Decahydro-2,3-dimethylnaphthalene	42	0001008-80-6	166.3	C <sub>12</sub> H <sub>22</sub>
61	8.12	1.89	Dodecane	95	0000112-40-3	170.33	C <sub>12</sub> H <sub>26</sub>
62	8.31	0.71	2,6-Dimethylundecane	76	0017301-23-4	184.36	C <sub>13</sub> H <sub>28</sub>
63	8.85	0.26	2,6-Dimethylundecane	81	0017301-23-4	184.36	C <sub>13</sub> H <sub>28</sub>
64	8.88	0.79	2,3-Dimethyldecane	25	0017312-44-6	170.33	C <sub>12</sub> H <sub>26</sub>
65	9.01	0.34	17-Pentatriacontene	30	0006971-40-0	490.93	C <sub>35</sub> H <sub>70</sub>
66	9.12	0.81	7-Methyltridecane	81	0026730-14-3	198.39	C <sub>14</sub> H <sub>30</sub>
67	9.51	1.99	Tridecane	96	0000629-50-5	184.36	C <sub>13</sub> H <sub>28</sub>
68	9.77	0.24	2-Methylnaphthalene	93	0000091-57-6	142.2	C <sub>11</sub> H <sub>10</sub>
69	10.10	0.07	Cyclotridecane	90	0000295-02-3	182.35	C <sub>13</sub> H <sub>26</sub>
70	10.15	0.04	1,2,3,4-Tetrahydro-1,5,7-trimethylnaphthalene	90	0021693-55-0	174.28	C <sub>13</sub> H <sub>18</sub>
71	10.16	0.22	3,5,24-Trimethyltetracontane	52	0055162-61-3	605.16	C <sub>43</sub> H <sub>88</sub>
72	10.20	0.32	Decahydro-2,3-dimethylnaphthalene	52	0001008-80-6	166.3	C <sub>12</sub> H <sub>22</sub>

73	10.50	0.30	2,6,10-Trimethyldodecane	91	0003891-98-3	212.41	C <sub>15</sub> H <sub>32</sub>
74	10.62	0.22	2,6,10,14-Tetramethylhexadecane	90	0000638-36-8	282.55	C <sub>20</sub> H <sub>42</sub>
75	10.79	0.25	Decahydro-2,3-dimethylnaphthalene	87	0001008-80-6	166.3	C <sub>12</sub> H <sub>22</sub>
76	10.80	0.44	Tetradecane	98	0000629-59-4	198.39	C <sub>14</sub> H <sub>30</sub>
77	10.85	0.09	Undecane	50	0001120-21-4	156.31	C <sub>11</sub> H <sub>24</sub>
78	11.27	0.83	1,1,3-Trimethylcyclopentane	51	0004516-69-2	112.21	C <sub>8</sub> H <sub>16</sub>
79	11.41	0.14	1,5-Dimethylnaphthalene	95	0000571-61-9	156.22	C <sub>12</sub> H <sub>12</sub>
80	11.44	0.01	1,4-Dimethylnaphthalene	94	0000571-58-4	156.22	C <sub>12</sub> H <sub>12</sub>
81	11.45	0.14	2,7-Dimethylnaphthalene	84	0000582-16-1	156.22	C <sub>12</sub> H <sub>12</sub>
82	11.57	0.44	10-Methyleicosane	91	0054833-23-7	296.57	C <sub>21</sub> H <sub>44</sub>
83	11.62	0.66	2,6,11-Trimethyldodecane	89	0031295-56-4	212.41	C <sub>15</sub> H <sub>32</sub>
84	11.68	0.34	Nonadecane	87	0000629-92-5	268.52	C <sub>19</sub> H <sub>40</sub>
85	11.78	0.42	Tritetracontane	54	0007098-21-7	605.16	C <sub>43</sub> H <sub>88</sub>
86	12.03	1.53	Pentadecane	97	0000629-62-9	212.41	C <sub>15</sub> H <sub>32</sub>
87	12.65	0.24	1-Hexacosanol	68	0000506-52-5	382.71	C <sub>26</sub> H <sub>54</sub> O
88	12.69	0.19	1,6,7-Trimethylnaphthalene	97	0002245-38-7	170.25	C <sub>13</sub> H <sub>14</sub>
89	12.70	0.59	1,4,6-Trimethylnaphthalene	97	0002131-42-2	170.25	C <sub>13</sub> H <sub>14</sub>
90	12.74	0.25	2,3,6-Trimethylnaphthalene	97	0000829-26-5	170.25	C <sub>13</sub> H <sub>14</sub>
91	12.78	0.63	3,8-Dimethyldecane	70	0017312-55-9	170.33	C <sub>12</sub> H <sub>26</sub>



92	12.89	0.36	1,4,5-Trimethylnaphthalene	96	0002131-41-1	170.25	C <sub>13</sub> H <sub>14</sub>
93	12.94	0.23	1,6,7-Trimethylnaphthalene	96	0002245-38-7	170.25	C <sub>13</sub> H <sub>14</sub>
94	13.05	0.12	2,3,6-Trimethylnaphthalene	95	0000829-26-5	170.25	C <sub>13</sub> H <sub>14</sub>
95	13.18	1.37	Hexadecane	98	0000544-76-3	226.44	C <sub>16</sub> H <sub>34</sub>
96	13.31	0.09	Tridecane	64	0000629-50-5	184.36	C <sub>13</sub> H <sub>28</sub>
97	13.59	3.19	1,2,3,4-Tetramethylnaphthalene	55	0003031-15-0	184.28	C <sub>14</sub> H <sub>16</sub>
98	13.72	0.97	2,6,10-Trimethylpentadecane	97	0003892-00-0	254.49	C <sub>18</sub> H <sub>38</sub>
99	13.91	0.09	4-Methyl-3-dodecen-1-ol	46	1372101-59-1	198.4	C <sub>13</sub> H <sub>26</sub> O
100	14.28	1.21	Heptadecane	95	0000629-78-7	240.47	C <sub>27</sub> H <sub>36</sub>
101	14.33	0.61	2,6,10,14-Tetramethylpentadecane	98	0001921-70-6	268.52	C <sub>19</sub> H <sub>40</sub>
102	14.39	0.08	Tetradecane	86	0000629-59-4	198.39	C <sub>14</sub> H <sub>30</sub>
103	14.54	0.19	1-Hentetracontanol	30	0040710-42-7	593.11	C <sub>41</sub> H <sub>84</sub> O
104	14.88	0.07	Tetradecane	84	0000629-59-4	198.39	C <sub>14</sub> H <sub>30</sub>
105	15.06	0.10	3,7-Dimethyl-7-octenal	46	0000141-26-4	154.25	C <sub>10</sub> H <sub>18</sub> O
106	15.16	0.10	1,1,3-Trimethylcyclopentane	51	0004516-69-2	112.21	C <sub>8</sub> H <sub>16</sub>
107	15.21	0.03	Tetradecane	59	0000629-59-4	198.39	C <sub>14</sub> H <sub>30</sub>
108	15.31	0.56	Octadecane	99	0000593-45-3	254.49	C <sub>18</sub> H <sub>38</sub>
109	15.40	0.48	2,6,10,14-Tetramethylhexadecane	97	0000638-36-8	282.55	C <sub>20</sub> H <sub>42</sub>
110	15.53	0.07	14-Methylhexadecanal	60	0093815-50-0	254.45	C <sub>17</sub> H <sub>34</sub> O

111	15.59	0.18	1,7,11-Trimethyl-4-(1-methylethyl)- cyclotetradecane	58	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>
112	15.65	0.34	2,6,10-Trimethylundecanoic acid	58	0001115-94-2	228.37	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>
113	15.77	0.16	Pentadecane	74	0000629-62-9	212.41	C <sub>15</sub> H <sub>32</sub>
114	15.81	0.51	2-Methyltetradecane	60	0001560-95-8	212.4	C <sub>15</sub> H <sub>32</sub>
115	16.31	0.95	Nonadecane	97	0000629-92-5	268.52	C <sub>19</sub> H <sub>40</sub>
116	16.36	0.24	1-Nonadecene	86	0018435-45-5	266.51	C <sub>19</sub> H <sub>38</sub>
117	16.50	0.10	1-Methylphenanthrene	55	0000832-69-9	192.26	C <sub>15</sub> H <sub>12</sub>
118	16.56	0.10	2-Methyltetradecane	50	0001560-95-8	212.4	C <sub>15</sub> H <sub>32</sub>
119	16.63	0.12	2-Methyltetradecane	78	0001560-95-8	212.4	C <sub>15</sub> H <sub>32</sub>
120	16.74	0.10	10,11-Dihydro-5H-dibenzo[a,d]cyclohepten-5-ol	64	0001210-34-0	210.27	C <sub>15</sub> H <sub>14</sub> O
121	16.78	2.76	2-Methyltetradecane	64	0001560-95-8	212.4	C <sub>15</sub> H <sub>32</sub>
122	16.94	0.12	4-Methyl-3-dodecen-1-ol	64	1372101-59-1	198.4	C <sub>13</sub> H <sub>26</sub> O
123	17.25	0.96	Eicosane	99	0000112-95-8	282.55	C <sub>20</sub> H <sub>42</sub>
124	17.66	0.55	1-Octadecene	80	0000112-88-9	252.48	C <sub>18</sub> H <sub>36</sub>
125	17.71	0.11	1-Hexadecene	64	0000629-73-2	224.43	C <sub>16</sub> H <sub>32</sub>
126	17.89	0.14	Octadecane	86	0000593-45-3	254.49	C <sub>18</sub> H <sub>38</sub>
127	17.98	0.10	1-Octadecanethiol	55	0002885-00-9	286.56	C <sub>18</sub> H <sub>38</sub> S
128	18.03	0.19	Octadecane	62	0000593-45-3	254.49	C <sub>18</sub> H <sub>38</sub>

129	18.15	0.73	Heneicosane	97	0000629-94-7	296.57	C <sub>21</sub> H <sub>44</sub>
130	18.25	0.37	1-Octadecanethiol	55	0002885-00-9	286.56	C <sub>18</sub> H <sub>38</sub> S
131	18.54	0.14	Hexadecane	74	0000544-76-3	226.44	C <sub>16</sub> H <sub>34</sub>
132	18.59	0.31	1-Octadecanethiol	83	0002885-00-9	286.56	C <sub>18</sub> H <sub>38</sub> S
133	18.65	0.89	Hexadecane	74	0000544-76-3	226.44	C <sub>16</sub> H <sub>34</sub>
134	19.03	0.75	Docosane	99	0000629-97-0	310.6	C <sub>22</sub> H <sub>46</sub>
135	19.39	0.18	13-Tertadecen-1-ol acetate	78	0056221-91-1	254.41	C <sub>16</sub> H <sub>30</sub> O <sub>2</sub>
136	19.44	2.44	2-Methyl-7-octadecene	83	0051050-50-1	266.51	C <sub>19</sub> H <sub>38</sub>
137	19.50	0.15	2-Tetradecyloxirane	89	0007320-37-8	240.42	C <sub>16</sub> H <sub>32</sub> O
138	19.62	0.18	Heneicosane	95	0000629-94-7	296.57	C <sub>21</sub> H <sub>44</sub>
139	19.84	0.57	Eicosane	97	0000112-95-8	282.55	C <sub>20</sub> H <sub>42</sub>
140	20.03	0.10	1-Dodecene	76	0000112-41-4	168.32	C <sub>12</sub> H <sub>24</sub>
141	20.25	0.15	1-Dodecene	87	0000112-41-4	168.32	C <sub>12</sub> H <sub>24</sub>
142	20.30	0.20	9-Tricosene	64	0027519-02-4	322.61	C <sub>23</sub> H <sub>46</sub>
143	20.34	0.11	4-Methyldocosane	64	0025117-30-0	324.63	C <sub>23</sub> H <sub>48</sub>
144	20.39	0.23	1-Pentyl-2-propylcyclopentane	88	0062199-51-3	182.35	C <sub>13</sub> H <sub>26</sub>
145	20.42	0.13	Docosane	89	0000629-97-0	310.6	C <sub>22</sub> H <sub>46</sub>
146	20.54	0.36	1,7,11-Trimethyl-4-(1-methylethyl)- cyclotetradecane	91	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>

147	20.65	0.54	Tetracosane	99	0000646-31-1	338.65	C <sub>24</sub> H <sub>50</sub>
148	21.03	1.54	2-Decyloxirane	76	0002855-19-8	184.32	C <sub>12</sub> H <sub>24</sub> O
149	21.27	0.08	Cyclotetracosane	58	0000297-03-0	336.64	C <sub>24</sub> H <sub>48</sub>
150	21.33	0.09	1,7,11-Trimethyl-4-(1-methylethyl)- cyclotetradecane	58	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>
151	21.40	0.55	Tricosane	97	0000638-67-5	324.63	C <sub>23</sub> H <sub>48</sub>
152	21.47	0.20	Tetracosane	91	0000646-31-1	338.65	C <sub>24</sub> H <sub>50</sub>
153	21.54	0.45	1,7,11-Trimethyl-4-(1-methylethyl)- cyclotetradecane	91	0001786-12-5	280.53	C <sub>20</sub> H <sub>40</sub>
154	21.66	0.04	Tricosane	83	0000638-67-5	324.63	C <sub>23</sub> H <sub>48</sub>
155	21.77	0.27	Pentacosane	83	0000629-99-2	352.68	C <sub>25</sub> H <sub>52</sub>
156	21.89	0.02	Tetracosane	70	0000646-31-1	338.65	C <sub>24</sub> H <sub>50</sub>
157	22.00	0.17	1,2-Diisooctylate-1,2-benzenedicarboxylic acid	87	0027554-26-3	390.56	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>
158	22.12	0.02	1,2-bis(2-Ethylhexyl)ate-1,2- benzenedicarboxylic acid	86	0000117-81-7	390.56	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>
159	22.18	0.13	Hexacosane	99	0000630-01-3	366.71	C <sub>26</sub> H <sub>54</sub>
160	22.28	0.03	(-)-1',4-Dihydroxy-7'-methoxy-2,3'-dimethyl- [1,2'-binaphthalene]-5,5',8,8'-tetrone	64	0119736-96-8	404.37	C <sub>23</sub> H <sub>16</sub> O <sub>7</sub>
161	22.31	0.15	Hexacosane	95	0000630-01-3	366.71	C <sub>26</sub> H <sub>54</sub>

162	22.47	0.03	1-Tricosene	86	0018835-32-0	322.61	C <sub>23</sub> H <sub>46</sub>
163	22.62	0.18	(-)-1',4-Dihydroxy-7'-methoxy-2,3'-dimethyl- [1,2'-binaphthalene]-5,5',8,8'-tetrone	99	0119736-96-8	404.37	C <sub>23</sub> H <sub>16</sub> O <sub>7</sub>
164	22.74	0.18	1-Acetate-11,13-dimethyl-12-tetradecen-1-ol	58	0400037-00-5	282.46	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>
165	22.84	0.33	Heptacosane	98	0000593-49-7	380.73	C <sub>27</sub> H <sub>56</sub>
166	23.15	0.22	1-Chlorooctadecane	94	0003386-33-2	288.94	C <sub>18</sub> H <sub>37</sub> Cl
167	23.18	0.07	Hexacosane	96	0000630-01-3	366.71	C <sub>26</sub> H <sub>54</sub>
168	23.28	0.30	(Z)- 9-Methyl-4-undecene	25	0074630-56-1	168.32	C <sub>12</sub> H <sub>24</sub>
169	23.34	0.04	2,2-Dioxide-6-dodecyl-1,2-oxathiane	49	0015224-88-1	304.9	C <sub>16</sub> H <sub>32</sub> O <sub>3</sub> S
170	23.74	0.04	Hexacosane	89	0000630-01-3	366.71	C <sub>26</sub> H <sub>54</sub>
171	24.21	0.14	1-Butyl 2-(8-methylnonyl)oate-1,2- benzenedicarboxylic acid	81	0000089-18-9	362.5	C <sub>22</sub> H <sub>34</sub> O <sub>4</sub>
172	24.36	0.09	1-Butyl-2-(8-methylnonyl)oate-1,2- benzenedicarboxylic acid	93	0000089-18-9	362.5	C <sub>22</sub> H <sub>34</sub> O <sub>4</sub>
173	24.46	0.19	1,2-Didecyloate-1,2-benzenedicarboxylic acid	90	0000084-77-5	446.66	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
174	24.54	0.10	1-Butyl 2-(8-methylnonyl)oate-1,2- benzenedicarboxylic acid	98	0000089-18-9	362.5	C <sub>22</sub> H <sub>34</sub> O <sub>4</sub>
175	24.98	0.02	1-Butyl 2-(8-methylnonyl)oate-1,2- benzenedicarboxylic acid	93	0000089-18-9	362.5	C <sub>22</sub> H <sub>34</sub> O <sub>4</sub>

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176	25.30	2.31	1-Butyl-2-(8-methylnonyl)oate-1,2-benzenedicarboxylic acid	95	0000089-18-9	362.5	C <sub>22</sub> H <sub>34</sub> O <sub>4</sub>
177	25.56	0.18	1-Docosanethiol	78	0007773-83-3	342.67	C <sub>22</sub> H <sub>46</sub> S
178	26.03	0.22	(-)-1',4-Dihydroxy-7'-methoxy-2,3'-dimethyl-[1,2'-Binaphthalene]-5,5',8,8'-tetrone	97	0119736-96-8	404.37	C <sub>23</sub> H <sub>16</sub> O <sub>7</sub>
179	27.96	0.13	Nonahexacontanoic acid	74	0040710-32-5	999.83	C <sub>69</sub> H <sub>138</sub> O <sub>2</sub>
180	29.13	0.08	1,54-Dibromotetrapentacontane	76	0852228-22-9	917.24	C <sub>54</sub> H <sub>108</sub> Br <sub>2</sub>
181	30.50	0.07	<i>cis</i> -4-Ethyl-5-octyl-2,2-bis(trifluoromethyl)-1,3-dioxolane	76	0038274-72-5	350.34	C <sub>15</sub> H <sub>24</sub> F <sub>6</sub> O <sub>2</sub>

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**Table S7.** List of identified molecules with GC-MS from Barnett (NM) acid aliquot extracted with chloroform.

Peak	R.T. (min)	A[Tot] (%)	Library/ID	Q (%)	CAS #	M <sub>w</sub>	Molecular formula
1	1.26	1.27	Pentylhydroperoxide	25	0000074-80-6	104.2	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>
2	1.35	1.11	Dichloromethane	96	0000075-09-2	84.93	CH <sub>2</sub> Cl <sub>2</sub>
3	1.43	0.24	1,1-Dichloroethane	94	0000075-34-3	98.96	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>
4	1.49	0.42	1,1'-oxybis[1,1]-Dichloromethane	90	0020524-86-1	183.9	C <sub>2</sub> H <sub>2</sub> Cl <sub>4</sub> O
5	1.56	0.64	Trichloromethane	83	0000067-66-3	119.4	CHCl <sub>3</sub>
6	1.69	0.98	Trichloromethane	92	0000067-66-3	119.4	CHCl <sub>3</sub>
7	1.72	0.94	Trichloromethane	96	0000067-66-3	119.4	CHCl <sub>3</sub>
8	1.85	0.81	1H-Imidazole-2-amine	43	0007720-39-0	83.09	C <sub>3</sub> H <sub>5</sub> N <sub>3</sub>
9	1.93	0.73	2,4-Dichloro-5-oxo-2-hexenedioic acid	28	0056771-78-9	227	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>5</sub>
10	1.97	0.18	Trichloromethane	27	0000067-66-3	119.4	CHCl <sub>3</sub>
11	2.08	0.41	Trichlorodocosylsilane	42	0007325-84-0	444	C <sub>22</sub> H <sub>45</sub> Cl <sub>3</sub> Si
12	2.16	0.37	Methylbenzene	50	0000108-88-3	92.14	C <sub>7</sub> H <sub>8</sub>
13	2.20	0.27	1,4-Dimethylcyclohexane	87	0000589-90-2	112.2	C <sub>8</sub> H <sub>16</sub>
14	2.31	0.65	Hydrochloric Acid	9	0007647-01-0	36	HCl
15	2.37	0.48	O-Decylhydroxylamine	50	0029812-79-1	173.3	C <sub>10</sub> H <sub>23</sub> NO
16	2.43	1.47	Hydrochloric Acid	5	0007647-01-0	36	HCl

17	2.73	0.72	Decylcyclohexane	42	0001795-16-0	224.4	C <sub>16</sub> H <sub>32</sub>
18	2.75	1.22	1-Oxide-2-pyridinamine	53	0014150-95-9	110.1	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O
19	2.87	0.37	Hydrochloric Acid	9	0007647-01-0	36	HCl
20	2.91	0.31	2,2-Dichloro-3,6-dimethyl-1-Oxa-2-silacyclohexa-3,5-diene	83	0069586-09-0	195.1	C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> OSi
21	2.96	1.00	1-Propoxyhexane	9	0053685-78-2	144.3	C <sub>9</sub> H <sub>20</sub> O
22	3.05	1.29	4-Methyloctane	16	0002216-34-4	128.3	C <sub>9</sub> H <sub>20</sub>
23	3.10	0.74	1,2-Dimethylbenzene	59	0000095-47-6	106.2	C <sub>8</sub> H <sub>10</sub>
24	3.16	0.21	4-Propylheptane	47	0003178-29-8	142.3	C <sub>10</sub> H <sub>22</sub>
25	3.20	0.41	1,2-Dimethylbenzene	97	0000095-47-6	106.2	C <sub>8</sub> H <sub>10</sub>
26	3.26	0.51	1,2-Dimethylbenzene	95	0000095-47-6	106.2	C <sub>8</sub> H <sub>10</sub>
27	3.37	1.73	1-Ethyl-4-methylcyclohexane	81	0003728-56-1	126.2	C <sub>9</sub> H <sub>18</sub>
28	3.53	0.52	Nonane	68	0000111-84-2	128.3	C <sub>9</sub> H <sub>20</sub>
29	3.64	0.12	1-Ethyl-4-methylcyclohexane	74	0003728-56-1	126.2	C <sub>9</sub> H <sub>18</sub>
30	3.82	2.28	5-Octen-1-ol	72	0064275-73-6	128.2	C <sub>8</sub> H <sub>16</sub> O
31	3.97	0.19	Propylcyclohexane	50	0001678-92-8	126.2	C <sub>9</sub> H <sub>18</sub>
32	4.02	0.19	2,6-Dimethyloctane	92	0002051-30-1	142.3	C <sub>10</sub> H <sub>22</sub>
33	4.14	1.05	Diglycine ethyl ester	16	0000627-74-7	160.2	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
34	4.35	0.14	1,2,3,4-Tetramethylcyclohexane	46	0003726-45-2	140.3	C <sub>10</sub> H <sub>20</sub>



35	4.44	0.54	2,5,9-Trimethyldecane	50	0062108-22-9	184.36	C <sub>13</sub> H <sub>28</sub>
36	4.49	0.56	Hydrochloric Acid	47	0007647-01-0	36	HCl
37	4.53	0.37	1-Ethyl-3-methylbenzene	92	0000620-14-4	120.2	C <sub>9</sub> H <sub>12</sub>
38	4.56	1.80	1-Ethyl-2-methylbenzene	91	0000611-14-3	120.2	C <sub>9</sub> H <sub>12</sub>
39	4.59	0.91	7-Methyltridecane	83	0026730-14-3	198.4	C <sub>14</sub> H <sub>30</sub>
40	4.63	1.91	1-Propylcyclohexene	43	0002539-75-5	124.2	C <sub>9</sub> H <sub>16</sub>
41	4.78	0.55	2-Hydroxy-4-(1-methylethyl)-2-cyclopenten-1-one	42	0054639-82-6	140.2	C <sub>8</sub> H <sub>12</sub> O <sub>2</sub>
42	4.90	0.62	Hydrochloric Acid	5	0007647-01-0	36	HCl
43	5.05	0.4	Decane	95	0000124-18-5	142.3	C <sub>10</sub> H <sub>22</sub>
44	5.29	0.69	$\alpha$ -Methylbenzeneacetaldehyde	9	0000093-53-8	134.2	C <sub>9</sub> H <sub>10</sub> O
45	5.41	0.11	4-Methyldecane	64	0002847-72-5	156.3	C <sub>11</sub> H <sub>24</sub>
46	5.47	0.56	1,2,4-Trimethylbenzene	49	0000095-63-6	120.2	C <sub>9</sub> H <sub>12</sub>
47	5.51	0.59	5 (1-Methylpropylidene)-1,3-cyclopentadiene	49	0003141-02-4	120.2	C <sub>9</sub> H <sub>12</sub>
48	5.55	0.78	Decylcyclohexane	78	0001795-16-0	224.4	C <sub>16</sub> H <sub>32</sub>
49	5.63	0.60	Hydrochloric Acid	5	0007647-01-0	36	HCl
50	5.91	0.79	Decahydronaphthalene	30	0000091-17-8	138.3	C <sub>10</sub> H <sub>18</sub>
51	5.96	0.17	2,2,3,3-Tetramethylhexane	56	0013475-81-5	142.3	C <sub>10</sub> H <sub>22</sub>
52	6.00	0.30	1-Methyl-1,2-cyclohexanediol	25	0006296-84-0	130.2	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>

53	6.05	0.74	Imidazo[1,2-a]pyrimidine	50	0000274-95-3	119.1	C <sub>6</sub> H <sub>5</sub> N <sub>3</sub>
54	6.17	0.89	Octadecane	9	0000593-45-3	254.5	C <sub>18</sub> H <sub>38</sub>
55	6.27	0.23	Nonadecane	9	0000629-92-5	268.5	C <sub>19</sub> H <sub>40</sub>
56	6.62	0.34	Undecane	76	0001120-21-4	156.3	C <sub>11</sub> H <sub>24</sub>
57	6.76	2.37	<i>Trans</i> -5-Methylspiro[3,5]nonan-1-one	30	0065417-56-0	152.2	C <sub>10</sub> H <sub>16</sub> O
58	7.03	0.74	3,8-Dimethyldecane	50	0017312-55-9	170.3	C <sub>12</sub> H <sub>26</sub>
59	7.05	0.61	Hexatriacontane	50	0000630-06-8	507	C <sub>36</sub> H <sub>74</sub>
60	7.07	0.99	Dotriacontane	50	0000544-85-4	450.9	C <sub>32</sub> H <sub>66</sub>
61	7.09	0.60	Tetratetracontane	50	0007098-22-8	619.2	C <sub>44</sub> H <sub>90</sub>
62	7.11	1.00	Tritetracontane	50	0007098-21-7	605.2	C <sub>43</sub> H <sub>88</sub>
63	7.14	1.08	Pentylcyclohexane	30	0004292-92-6	154.3	C <sub>11</sub> H <sub>22</sub>
64	7.44	0.12	4-Propylheptane	64	0003178-29-8	142.3	C <sub>10</sub> H <sub>22</sub>
65	7.58	0.36	Octacosane	72	0000630-02-4	394.8	C <sub>28</sub> H <sub>58</sub>
66	7.58	0.45	Pentacosane	72	0000629-99-2	352.7	C <sub>25</sub> H <sub>52</sub>
67	7.59	0.29	Nonadecane	72	0000629-92-5	268.5	C <sub>19</sub> H <sub>40</sub>
68	7.60	1.97	Heptadecane	72	0000629-78-7	240.5	C <sub>27</sub> H <sub>36</sub>
69	7.61	1.77	Nonacosane	72	0000630-03-5	408.8	C <sub>29</sub> H <sub>60</sub>
70	7.62	0.37	Docosane	72	0000629-97-0	310.6	C <sub>22</sub> H <sub>46</sub>
71	7.63	0.18	Octadecane	72	0000593-45-3	254.5	C <sub>18</sub> H <sub>38</sub>

72	7.64	0.07	Triacontane	72	0000638-68-6	422.8	C <sub>30</sub> H <sub>62</sub>
73	7.65	0.14	Heneicosane	72	0000629-94-7	296.6	C <sub>21</sub> H <sub>44</sub>
74	7.67	0.53	Pentatriacontane	47	0000630-07-9	493	C <sub>35</sub> H <sub>72</sub>
75	7.68	0.69	Triacontane	47	0000638-68-6	422.8	C <sub>30</sub> H <sub>62</sub>
76	7.69	0.08	Tricosane	47	0000638-67-5	324.6	C <sub>23</sub> H <sub>48</sub>
77	7.70	0.47	Hexatriacontane	47	0000630-06-8	507	C <sub>36</sub> H <sub>74</sub>
78	7.71	1.89	Docosane	47	0000628-97-0	310.6	C <sub>22</sub> H <sub>46</sub>
79	7.72	0.71	Dotriacontane	47	0000544-85-4	450.9	C <sub>32</sub> H <sub>66</sub>
80	8.11	0.33	Dodecane	96	0000112-40-3	170.3	C <sub>12</sub> H <sub>26</sub>
81	8.31	0.15	2,6-Dimethylundecane	86	0017301-23-4	184.4	C <sub>13</sub> H <sub>28</sub>
82	8.94	0.26	1-Dotriacontanol	22	0006624-79-9	466.9	C <sub>32</sub> H <sub>66</sub> O
83	9.00	0.79	17-Pentatriacontene	22	0006971-40-0	490.9	C <sub>35</sub> H <sub>70</sub>
84	9.12	0.14	7-Methyltridecane	72	0026730-14-3	198.4	C <sub>14</sub> H <sub>30</sub>
85	9.20	0.34	$\alpha$ -Methyl-1H-imidazole-1-ethanol	23	0037788-55-9	126.2	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O
86	9.50	0.38	Tridecane	96	0000629-50-5	184.4	C <sub>13</sub> H <sub>28</sub>
87	9.55	0.81	1-Ethylidene-1H-indene	90	0002471-83-2	142.2	C <sub>11</sub> H <sub>10</sub>
88	9.78	1.99	1-Ethylidene-1H-Indene	83	0002471-83-2	142.2	C <sub>11</sub> H <sub>10</sub>
89	9.85	0.24	3,4,5,6-Tetrahydro-3-hydroxy-2H-cyclopentathiazol-2-imine	53	0738528-09-1	156.2	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> OS

90	10.32	0.07	Dotriacontane	59	0000544-85-4	450.9	C <sub>32</sub> H <sub>66</sub>
91	10.33	0.04	Octacosane	59	0000630-02-4	394.8	C <sub>28</sub> H <sub>58</sub>
92	10.34	0.22	11-(1-Ethylpropyl)-heneicosane	59	0055282-11-6	366.7	C <sub>26</sub> H <sub>54</sub>
93	10.35	0.32	Heptacosane	59	0000593-49-7	380.7	C <sub>27</sub> H <sub>56</sub>
94	10.36	0.30	3,8-Dimethyldecane	59	0017312-55-9	170.3	C <sub>12</sub> H <sub>26</sub>
95	10.41	0.22	Hexatriacontane	59	0000630-06-8	507	C <sub>36</sub> H <sub>74</sub>
96	10.42	0.25	Triacontane	59	0000638-68-6	422.8	C <sub>30</sub> H <sub>62</sub>
97	10.43	0.44	Dotriacontane	59	0000544-85-4	450.9	C <sub>32</sub> H <sub>66</sub>
98	10.49	0.09	Tetratetracontane	59	0007098-22-8	619.2	C <sub>44</sub> H <sub>90</sub>
99	10.50	0.12	2,6,10-Trimethyldodecane	91	0003891-98-3	212.4	C <sub>15</sub> H <sub>32</sub>
100	10.81	0.33	Tetradecane	98	0000629-59-4	198.4	C <sub>14</sub> H <sub>30</sub>
101	11.22	0.83	2,7-Dimethylnaphthalene	93	0000582-16-1	156.2	C <sub>12</sub> H <sub>12</sub>
102	11.40	0.14	2-Mercaptocyclohexyl ester Acetic Acid,	22	0016849-98-2	174.3	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> S
103	11.56	0.18	2,6,10-Trimethyldodecane	86	0003891-98-3	212.4	C <sub>15</sub> H <sub>32</sub>
104	12.02	0.29	Pentadecane	97	0000629-62-9	212.4	C <sub>15</sub> H <sub>32</sub>
105	12.64	0.01	2-methyl- 2-hydroxy-2-methyl-3-buten-1-yl ester 2-Butenoic acid	53	1418543-90-4	184.2	C <sub>10</sub> H <sub>16</sub> O <sub>3</sub>
106	12.75	0.14	Dodecane	55	0000112-40-3	170.3	C <sub>12</sub> H <sub>26</sub>
107	13.17	0.28	Hexadecane	98	0000544-76-3	226.4	C <sub>16</sub> H <sub>34</sub>

108	13.71	0.15	3,6-Dimethylundecane	72	0017301-28-9	184.4	C <sub>13</sub> H <sub>28</sub>
109	13.81	0.44	(1,3-Dimethylbutyl)-cyclohexane	38	0061142-19-6	168.3	C <sub>12</sub> H <sub>24</sub>
110	13.85	0.66	Tridecanal	38	0010486-19-8	198.3	C <sub>13</sub> H <sub>26</sub> O
111	13.85	0.34	Tetradecanal	38	0000124-25-4	212.4	C <sub>14</sub> H <sub>28</sub> O
112	13.87	0.42	3,8-Dimethyldecane	53	0017312-55-9	170.3	C <sub>12</sub> H <sub>26</sub>
113	14.28	0.21	Heptadecane	95	0000629-78-7	240.5	C <sub>27</sub> H <sub>56</sub>
114	14.32	0.21	2,6,10,14-Tetramethylpentadecane	91	0001921-70-6	268.5	C <sub>19</sub> H <sub>40</sub>
115	14.33	1.53	Triacontane	78	0000638-68-6	422.8	C <sub>30</sub> H <sub>62</sub>
116	14.34	0.24	Pentatriacontane	78	0000630-07-9	493	C <sub>35</sub> H <sub>72</sub>
117	14.35	0.19	Tetratetracontane	78	0007098-22-8	619.2	C <sub>44</sub> H <sub>90</sub>
118	15.20	0.59	11-(1-Ethylpropyl)-heneicosane	78	0055282-11-6	366.7	C <sub>26</sub> H <sub>54</sub>
119	15.31	0.23	Octadecane	98	0000593-45-3	254.5	C <sub>18</sub> H <sub>38</sub>
120	15.40	0.19	2,6,10,14-Tetramethylhexadecane	91	0000638-36-8	282.6	C <sub>20</sub> H <sub>42</sub>
121	16.31	0.19	Nonadecane	95	0000629-92-5	268.5	C <sub>19</sub> H <sub>40</sub>
122	17.24	0.15	Eicosane	98	0000112-95-8	282.6	C <sub>20</sub> H <sub>42</sub>
123	18.14	0.13	Heneicosane	96	0000629-94-7	296.6	C <sub>21</sub> H <sub>44</sub>
124	19.02	0.12	Hexatriacontane	83	0000630-06-8	507	C <sub>36</sub> H <sub>74</sub>
125	19.71	0.25	1,6-Dibutylesterhexanedioic acid	45	0000105-99-7	258.4	C <sub>14</sub> H <sub>26</sub> O <sub>4</sub>
126	19.84	0.09	Pentatriacontane	90	0000630-07-9	493	C <sub>35</sub> H <sub>72</sub>

127	19.86	0.63	11-(1-Ethylpropyl)-heneicosane	90	0055282-11-6	366.7	C <sub>26</sub> H <sub>54</sub>
128	20.48	0.36	Triacontane	90	0000638-68-6	422.8	C <sub>30</sub> H <sub>62</sub>
129	20.62	0.23	Tetratetracontane	91	0007098-22-8	619.2	C <sub>44</sub> H <sub>90</sub>
130	20.65	0.12	Triacontane	91	0000638-68-6	422.8	C <sub>30</sub> H <sub>62</sub>
131	20.69	1.37	Tricosane	91	0000638-67-5	324.6	C <sub>23</sub> H <sub>48</sub>
132	20.76	0.09	Hexatriacontane	91	0000630-06-8	507	C <sub>36</sub> H <sub>74</sub>
133	20.91	3.19	Pentatriacontane	91	0000630-07-9	493	C <sub>35</sub> H <sub>72</sub>
134	21.38	0.97	Hexatriacontane	78	0000630-06-8	507	C <sub>36</sub> H <sub>74</sub>
135	21.90	0.09	1,2-diisooctylate-1,2-Benzenedicarboxylic acid	53	0027554-26-3	390.6	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>
136	22.12	1.21	1-Chloroheptacosane	91	0062016-79-9	415.2	C <sub>27</sub> H <sub>55</sub> Cl
137	22.84	0.61	1-Chloroheptacosane	72	0062016-79-9	415.2	C <sub>27</sub> H <sub>55</sub> Cl
138	23.52	0.08	Nonacosane	59	0000630-03-5	408.8	C <sub>29</sub> H <sub>60</sub>
139	23.71	0.19	Hexatriacontane	59	0000630-06-8	507	C <sub>36</sub> H <sub>74</sub>
140	23.77	0.07	1-Chloroheptacosane	59	0062016-79-9	415.2	C <sub>27</sub> H <sub>55</sub> Cl
141	23.84	0.10	1-Chlorooctadecane	59	0003386-33-2	288.9	C <sub>18</sub> H <sub>37</sub> Cl
142	24.40	0.10	Pentatriacontane	59	0000630-07-9	493	C <sub>35</sub> H <sub>72</sub>
143	24.53	0.05	1,2-bis(8-methylnonyl)-oate-1,2- benzenedicarboxylic acid	78	0000089-16-7	446.7	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>
144	24.82	0.03	1,2-diisonoyloate-1,2-benzenedicarboxylic acid	64	0028553-12-0	418	C <sub>26</sub> H <sub>42</sub> O <sub>4</sub>

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145	24.90	0.56	1,2-bis(8-methylnonyl)-oate-1,2- benzenedicarboxylic acid	78	0000089-16-7	446.7	$C_{28}H_{46}O_4$
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**Table S8.** Selected compounds (present in at least two well samples) identified in the CHCl<sub>3</sub> extraction of produced water.

Class	Formula	Compound name	Produced water source
Saturated (Aliphatic)	C <sub>5</sub> H <sub>10</sub>	2-methyl-1-butene	Marcellus, Eagle Ford
		2-methyl-2-butene	Marcellus, Eagle Ford
		1,1-dimethylcyclopropane	Marcellus, Barnett
	C <sub>6</sub> H <sub>14</sub>	hexane	Marcellus, Barnett
	C <sub>7</sub> H <sub>14</sub>	methylcyclohexane	Marcellus, Barnett
		1,3-dimethylcyclopentane	Marcellus, Barnett
		(E)-3-heptene	Marcellus, Barnett
	C <sub>8</sub> H <sub>16</sub>	2-octene	Marcellus, Barnett
		1,3-dimethylcyclohexane	Marcellus, Barnett
		ethylcyclohexane	Marcellus, Barnett
		propylcyclopentane	Marcellus, Barnett
		1,2,4-trimethylcyclopentane	Marcellus, Barnett
		1,1,3-trimethylcyclopentane	Marcellus, Barnett
		3-methyl-1-heptene	Marcellus, Barnett
	C <sub>8</sub> H <sub>18</sub>	2-methyl-heptane	Marcellus, Barnett
	C <sub>9</sub> H <sub>18</sub>	propyl-cyclohexane	Marcellus, Barnett
		1,1,3-trimethylcyclohexane	Marcellus, Barnett
		1-ethyl-4-methylcyclohexane	Marcellus, Barnett
		1,2,4-trimethylcyclohexane	Marcellus, Barnett
	C <sub>9</sub> H <sub>20</sub>	2-methyloctane	Marcellus, Barnett
nonane		Marcellus, Barnett	



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	2,6-dimethylheptane	Marcellus, Eagle Ford
C <sub>10</sub> H <sub>20</sub>	4-propyl-3-heptene	Marcellus, Barnett
C <sub>10</sub> H <sub>22</sub>	decane	Marcellus, Barnett
	2,6-dimethyloctane	Marcellus, Barnett
	2,2,3,3-tetramethylhexane	Eagle Ford, Barnett
	4-methylnonane	Marcellus, Barnett
C <sub>11</sub> H <sub>22</sub>	2-ethyl-1,1,3-trimethylcyclohexane	Marcellus, Barnett
	pentylcyclohexane	Marcellus, Barnett
C <sub>11</sub> H <sub>24</sub>	undecane	Marcellus, Barnett
	4-methyldecane	Marcellus, Barnett
	2-methyldecane	Marcellus, Barnett
	3-methyldecane	Marcellus, Barnett
C <sub>12</sub> H <sub>26</sub>	dodecane	Marcellus, Eagle Ford, Barnett
	4-methylundecane	Marcellu, Barnett
C <sub>13</sub> H <sub>26</sub>	1-pentyl-2-propylcyclopentane	Marcellus, Barnett
C <sub>13</sub> H <sub>28</sub>	tridecane	Marcellus, Eagle Ford, Barnett
	2,6-dimethylundecane	Marcellus, Barnett
	2,4-dimethyl-undecane	Marcellus, Eagle Ford
C <sub>14</sub> H <sub>28</sub>	cyclotetradecane	Marcellus, Eagle Ford
C <sub>14</sub> H <sub>30</sub>	tetradecane	Marcellus, Eagle Ford, Barnett
	2-methyl-tridecane	Marcellus, Eagle Ford
	7-methyltridecane	Marcellus, Barnett
	4-methyltridecane	Marcellus, Eagle Ford
C <sub>15</sub> H <sub>32</sub>	pentadecane	Marcellus, Eagle Ford, Barnett

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	2,6,10-trimethyldodecane	Marcellus, Eagle Ford, Barnett
	2,6,11-trimethyl-dodecane	Marcellus, Barnett
	5-Methyltetradecane	Eagle Ford, Barnett
C <sub>16</sub> H <sub>32</sub>	1-hexadecene	Marcellus, Barnett
C <sub>16</sub> H <sub>34</sub>	hexadecane	Marcellus, Eagle Ford, Barnett
C <sub>17</sub> H <sub>36</sub>	heptadecane	Marcellus, Eagle Ford, Barnett
C <sub>18</sub> H <sub>36</sub>	1-octadecene	Marcellus, Barnett
C <sub>18</sub> H <sub>38</sub>	octadecane	Marcellus, Eagle Ford, Barnett
	2,6,10-trimethylpentadecane	Marcellus, Barnett
C <sub>19</sub> H <sub>40</sub>	nonadecane	Marcellus, Eagle Ford, Barnett
	2,6,10,14-tetramethylpentadecane	Marcellus, Barnett
C <sub>20</sub> H <sub>40</sub>	1,7,11-trimethyl-4-(1-methylethyl)-cyclotetradecane	Marcellus, Barnett
C <sub>20</sub> H <sub>42</sub>	eicosane	Marcellus, Eagle Ford, Barnett
	2,6,10,14-tetramethylhexadecane (phytane)	Marcellus, Barnett
	10-methylnonadecane	Marcellus, Eagle Ford
C <sub>21</sub> H <sub>44</sub>	heneicosane	Marcellus, Eagle Ford, Barnett
C <sub>22</sub> H <sub>46</sub>	docosane	Marcellus, Eagle Ford, Barnett
C <sub>23</sub> H <sub>46</sub>	9-tricosene	Marcellus, Barnett
C <sub>23</sub> H <sub>48</sub>	tricosane	Marcellus, Eagle Ford, Barnett
C <sub>24</sub> H <sub>50</sub>	tetracosane	Marcellus, Barnett

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$C_{25}H_{52}$	pentacosane	Marcellus, Eagle Ford, Barnett
$C_{26}H_{54}$	hexacosane	Marcellus, Barnett
	11-(1-ethylpropyl)-heneicosane	Eagle Ford, Barnett
$C_{27}H_{56}$	heptacosane	Marcellus, Barnett
$C_{28}H_{58}$	octacosane	Marcellus, Eagle Ford, Barnett
$C_{29}H_{60}$	nonacosane	Eagle Ford, Barnett
$C_{30}H_{62}$	triacontane	Eagle Ford, Barnett
$C_{32}H_{66}$	dotriacontane	Eagle Ford, Barnett
$C_{35}H_{70}$	17-pentatriacontene	Marcellus, Eagle Ford, Barnett
$C_{35}H_{72}$	pentatriacontane	Marcellus, Eagle Ford, Barnett
$C_{36}H_{74}$	hexatriacontane	Marcellus, Eagle Ford, Barnett
$C_{43}H_{88}$	tritetracontane	Marcellus, Eagle Ford, Barnett
$C_{44}H_{90}$	tetratetracontane	Eagle Ford, Barnett
Aromatic		
$C_7H_8$	toluene	Marcellus, Barnett
$C_8H_{10}$	ethylbenzene	Marcellus, Barnett
$C_8H_{18}$	2-methyl-heptane	Marcellus, Barnett
$C_9H_{12}$	1,2,3-trimethylbenzene	Marcellus, Barnett
	1,2,4-trimethylbenzene	Marcellus, Barnett
	1-ethyl-3-methyl-benzene	Marcellus, Barnett
$C_{10}H_{14}$	1,2,4,5-tetramethylbenzene	Marcellus, Barnett
	1-methyl-3-propylbenzene	Marcellus, Barnett

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	C <sub>11</sub> H <sub>20</sub>	decahydro-2-methyl-naphthalene	Marcellus, Barnett
	C <sub>12</sub> H <sub>12</sub>	1,5-dimethyl-naphthalene	Marcellus, Barnett
		2,7-dimethyl-naphthalene	Marcellus, Barnett
	C <sub>13</sub> H <sub>14</sub>	1,6,7-trimethylnaphthalene	Marcellus, Barnett
		2,3,6-trimethylnaphthalene	Marcellus, Barnett
	C <sub>14</sub> H <sub>18</sub>	1,2,3,4-tetramethyl-naphthalene	Marcellus, Barnett
Resin and asphaltine			
	C <sub>10</sub> H <sub>18</sub> O	3,7-dimethyl-7-octenal	Marcellus, Barnett
	C <sub>15</sub> H <sub>14</sub> O	10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ol	Marcellus, Barnett
	C <sub>16</sub> H <sub>30</sub> O <sub>2</sub>	13-tetradecen-1-ol acetate	Marcellus, Barnett
	C <sub>16</sub> H <sub>32</sub> O	2-tetradecyloxirane	Marcellus, Barnett
	C <sub>16</sub> H <sub>33</sub> Cl	1-chloro-hexadecane	Marcellus, Eagle Ford
	C <sub>18</sub> H <sub>37</sub> Cl	1-chlorooctadecane	Marcellus, Barnett
	C <sub>18</sub> H <sub>38</sub> S	1-octadecanethiol	Marcellus, Barnett
	C <sub>22</sub> H <sub>34</sub> O <sub>4</sub>	1,2-benzenedicarboxylic acid, 1-butyl 2-(8-methylnonyl) ester	Marcellus, Barnett
	C <sub>24</sub> H <sub>18</sub> O <sub>8</sub>	1',4-Dihydroxy-7'-methoxy-2,3'-dimethyl-,(-)-[1,2'-binaphthalene]-5,5',8,8'-tetrone	Marcellus, Barnett
	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>	1,2-benzenedicarboxylic acid, 1,2-bis(2-ethylhexyl) ester	Marcellus, Barnett
	C <sub>27</sub> H <sub>55</sub> Cl	1-chloro-heptacosane	Eagle Ford, Barnett
	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>	1,2-benzenedicarboxylic acid, 1,2-didecyl ester	Marcellus, Barnett
		1,2-benzenedicarboxylic acid, 1,2-bis(8-methylnonyl) ester	Marcellus, Barnett
	C <sub>32</sub> H <sub>66</sub> O	1-dotriacontanol	Eagle Ford, Barnett

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$C_{54}H_{108}Br$  1,54-dibromo-tetrapentacontane

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Marcellus, Eagle Ford,  
Barnett

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