Additional files

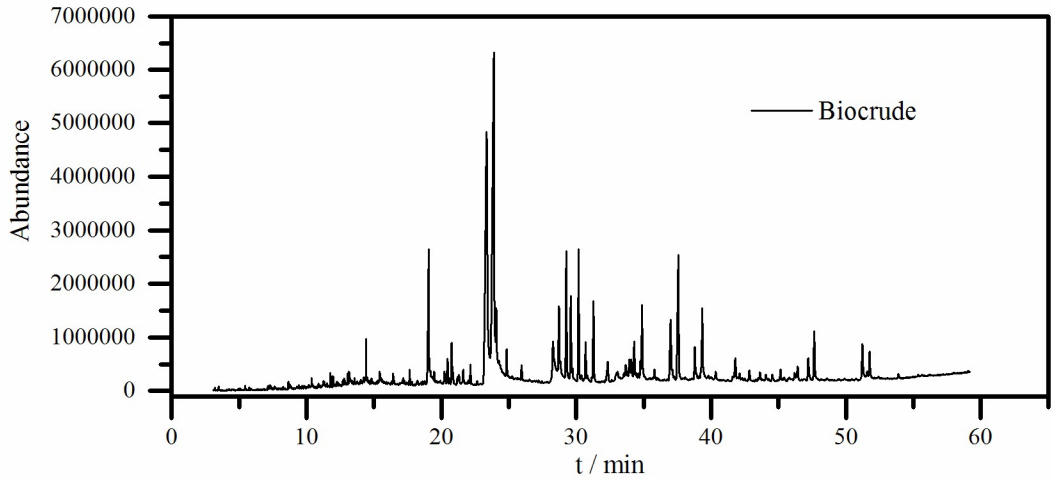

Fig. 1 Total ion chromatogram of HTL obtained biocrude

The main peaks of ion chromatogram for biocrude appeared between 10 min to 55 min. The highest two peaks were *cis-9*-Hexadecenoic acid and *n*-Hexadecenoic acid.

Table 1 The composition of biocrude.

No.	R.T. (min)	Compounds	Formation	Area
1	3.487	Toluene	C7H8	0.07%
2	5.444	Bicyclo[4.2.0]octa-1,3,5-triene	C8H8	0.08%
3	7.138	2-Octanone	C8H16O	0.07%
4	7.315	Pyrazine, 2-ethyl-6-methyl-	C7H10N2	0.07%
5	7.613	2-(1-Pyrrolidinyl)ethyl 4-propoxysalicylate	C16H23NO4	0.08%
6	8.654	Phenol, 4-methyl-	C7H8O	0.18%
7	9.415	1H-Pyrrole, 2,3,4,5-tetramethyl-	C8H13N	0.04%
8	9.827	Benzene, 1-ethyl-2,3-dimethyl-	C10H14	0.06%
9	10.239	Nicotinyl Alcohol	C6H7NO	0.05%
10	10.394	1H-Pyrrole, 3-ethyl-2,4,5-trimethyl-	C11H14O3	0.12%
11	11.246	Phenol, 3-(ethylamino)-4-methyl-	C9H13NO	0.08%
12	11.304	Phenol, 3-(ethylamino)-4-methyl-	C9H13NO	0.06%
13	11.773	1-Tridecene	C13H26	0.23%
14	11.967	Indole	C8H7N	0.26%
15	12.711	o-Methoxy-.alpha.-phenethylamine	C9H13NO	0.06%
16	12.78	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	C13H16	0.21%
17	13.06	N-[2-Hydroxyethyl]succinimide	C6H9NO3	0.18%
18	14.022	N-(1-Adamantyl)acetamide	C12H19NO	0.10%
19	14.233	N-(1-Adamantyl)acetamide	C12H19NO	0.07%
20	14.29	Phenol, 3-(ethylamino)-4-methyl-	C9H13NO	0.05%
21	14.416	7-Hexadecene, (Z)-	C16H32	0.42%
22	14.508	Pentadecane	C15H32	0.07%
23	14.817	Phenol, 4-amino-2-isopropyl-5-methyl-	C10H15NO	0.08%
24	15.429	Dodecanoic acid	C12H24O2	0.19%
25	17.157	1,7-Trimethylene-2,3-dimethylindole	C13H15N	0.09%
26	17.254	8-Heptadecene	C17H34	0.07%
27	17.644	Heptadecane	C17H36	0.28%
28	17.798	Diethyl-.alpha.-naphthylamine	C14H17N	0.16%

29	18.204	5-Phenyl-o-anisidine	C13H13NO	0.07%
30	18.256	Cyclooctane, 1,2-dimethyl-	C10H20	0.07%
31	18.605	4-Methyl-thieno(2,3-b)quinoline	C12H9NS	0.06%
32	18.736	9(2H)-Acridinone, 1,3,4,10-tetrahydro-2-methyl-	C14H15NO	0.04%
33	19.063	Tetradecanoic acid	C14H28O2	4.80%
34	19.469	4-Tetradecene, (Z)-	C14H28	0.26%
35	20.224	2-Pentadecanol	C15H32O	0.32%
36	20.453	2-Hexadecene, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-	C20H40	0.80%
37	20.756	2-Hexadecene, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-	C20H40	1.48%
38	21.208	1,2,3-Trimethyl-2-vinyl-1,3-diaza-2-silacyclopentane	C7H16N2Si	0.27%
39	21.3	Cyclopentane, 1-methyl-2-acetyl-3-(1-methylethenyl)-	C11H18O	0.26%
40	22.004	Tetradecane	C14H30	0.06%
41	22.662	Hexadecanoic acid, methyl ester	C17H34O2	0.08%
42	23.354	cis-9-Hexadecenoic acid	C16H30O2	19.97%
43	23.892	n-Hexadecanoic acid	C16H32O2	19.24%
44	24.069	Tetradecanamide	C14H29NO	1.65%
45	24.836	N-Methyldodecanamide	C13H27NO	0.72%
46	25.946	N,N-Dimethyldodecanamide	C14H29NO	0.46%
47	28.275	6-Octadecenoic acid, (Z)-	C18H34O2	2.53%
48	28.716	9-Octadecenamide, (Z)-	C18H35NO	2.06%
49	29.265	Hexadecanamide	C16H33NO	3.98%
50	30.175	N-Methyldodecanamide	C13H27NO	3.69%
51	30.69	Non-7-enoic acid, dimethylamide	C11H21NO	0.99%
52	31.17	Octanamide, N,N-dimethyl-	C10H21NO	0.09%
53	31.273	N,N-Dimethyldecanamide	C12H25NO	2.41%
54	33.659	Formamide, N,N-diethyl-	C5H11NO	0.27%
55	33.934	9-Octadecenamide, (Z)-	C18H35NO	0.45%
56	34.071	Undecanoic acid, pyrrolidide	C15H29NO	0.55%
57	34.758	Propanamide, N,N-dibutyl-3-cyclopentyl-	C16H31NO	0.45%
58	34.878	3-[3-(5-Amino-[1,3,4]thiadiazol-2-yl)-propyl]-3H-benzooxazol-2-one	C12H12N4O2S	2.30%
59	38.792	9-Hexadecenoic acid, pyrrolidide	C23H36O2	0.96%
60	39.244	9-Octadecenamide, n-butyl-	C22H43NO	0.16%
61	39.347	n-Dodecanoylpyrrolidine	C16H31NO	2.31%
62	40.343	Piperazine, 1-methyl-4-[2-(p-tolylsulfonyl)ethyl]-	C14H22N2O2S	0.29%
63	42.826	Oxalic acid, monoamide, N-(2-phenylethyl)-, heptyl ester	C14H21NO3S	0.34%
64	43.621	9-Hexadecenoic acid, pyrrolidide	C23H36O2	0.28%
65	44.531	3-Methoxy-D-homoestra-1,3,5(10),8-tetraene-17a-one, (14.beta.)	C20H24O2	0.28%
66	45.149	17-(1,5-Dimethylhexyl)-10,13-dimethyl-4,5,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-3H-cyclopenta[a]phenanthrene	C27H46	0.32%
67	46.185	Oxirane, hexadecyl-	C18H36O	0.16%
68	46.414	Cholesta-3,5-diene	C27H44	0.43%
69	47.192	Oxalic acid, butyl 2-phenylethyl ester	C14H18O4	0.91%
70	47.644	Phthalic acid, butyl 2-phenylethyl ester	C21H32O5	1.60%
71	51.214	Cholesterol	C27H46O	1.23%
72	51.746	Vitamin E	C29H50O2	0.93%

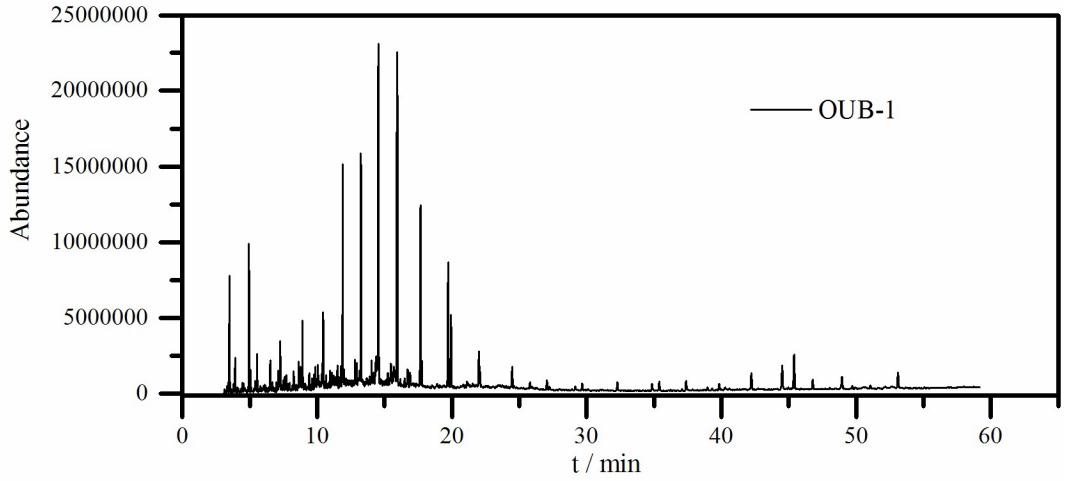

Fig. 2 Total ion chromatogram of OUB-1

The main peaks of ion chromatogram for OUB-1 appeared between 3 min to 20 min. There are still existed some small peaks after 20min. The highest two peaks were Pentadecane and Hexadecane.

Table 2 The composition of OUB-1 (obtained at Stage-1 upgrading under the optimized condition).

No.	R.T. (min)	Compounds	Formation	Area
1	3.304	Cyclopentene, 4,4-dimethyl-	C7H12	0.25%
2	3.419	Heptane, 2-methyl-	C8H18	0.20%
3	3.487	Toluene	C7H8	2.57%
4	3.791	cis-1-Butyl-2-methylcyclopropane	C8H16	0.29%
5	3.911	Octane	C8H18	0.76%
6	4.472	Cyclohexane, ethyl-	C8H16	0.25%
7	4.941	Ethylbenzene	C8H10	3.12%
8	5.072	Benzene, 1,3-dimethyl-	C8H10	0.46%
9	5.404	1-Nonene	C9H18	0.26%
10	5.479	Benzene, 1,3-dimethyl-	C8H10	0.25%
11	5.547	Nonane	C9H20	0.70%
12	6.131	Octane, 2,6-dimethyl-	C10H22	0.19%
13	6.52	Benzene, propyl-	C9H12	0.59%
14	6.657	Benzene, 1-ethyl-3-methyl-	C9H12	0.29%
15	6.978	Benzene, 1-ethyl-2-methyl-	C9H12	0.23%
16	7.121	1-Decene	C10H20	0.55%
17	7.207	Benzene, 1,2,4-trimethyl-	C9H12	0.19%
18	7.264	Decane	C10H22	0.87%
19	7.607	1H-Pyrrole, 2,3,5-trimethyl-	C7H11N	0.28%
20	7.71	Benzene, 1,2,4-trimethyl-	C9H12	0.34%
21	7.945	Benzene, cyclopropyl-	C9H10	0.23%
22	8.168	Phenol, 2-methyl-	C7H8O	0.20%
23	8.26	Benzene, butyl-	C10H14	0.47%
24	8.3	Phenol, 2-methyl-	C7H8O	0.32%
25	8.563	Benzenamine, 3-methyl-	C7H9N	0.18%
26	8.637	Phenol, 4-methyl-	C7H8O	0.95%
27	8.775	1-Undecene	C11H22	0.51%
28	8.906	Undecane	C11H24	1.18%
29	8.963	1H-Pyrrole, 3-ethyl-2,4-dimethyl-	C8H13N	0.31%

30	9.41	1H-Pyrrole, 2,3,4,5-tetramethyl-	C8H13N	0.41%
31	9.621	Phenol, 2-ethyl-	C8H10O	0.31%
32	9.782	Phenol, 2,4-dimethyl-	C8H10O	0.58%
33	9.867	Phenylethyl Alcohol	C8H10O	0.53%
34	10.062	Phenol, 4-ethyl-	C8H10O	0.51%
35	10.325	Cyclododecane	C12H24	0.30%
36	10.388	1H-Pyrrole, 3-ethyl-2,4,5-trimethyl-	C9H15N	0.73%
37	10.451	Dodecane	C12H26	1.27%
38	10.657	Undecane, 2,6-dimethyl-	C13H28	0.23%
39	10.955	Phenol, 2,4,6-trimethyl-	C9H12O	0.56%
40	11.109	Phenol, 4-ethyl-3-methyl-	C9H12O	0.27%
41	11.389	Benzene, hexyl-	C12H18	0.19%
42	11.464	Phenol, 3,5-dimethyl-	C8H10O	0.20%
43	11.744	6-Tridecene, (Z)-	C13H26	0.19%
44	11.779	1-Tridecene	C13H26	0.40%
45	11.899	Tridecane	C13H28	4.55%
46	12.156	Thymol	C10H14O	0.24%
47	12.54	Heptylcyclohexane	C13H26	0.18%
48	12.82	Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	C13H18	0.70%
49	12.934	Dodecane, 2,6,11-trimethyl-	C15H32	0.38%
50	13.049	Acetamide, N-[1-(4-hydroxyphenyl)ethyl]-	C10H13NO2	0.20%
51	13.135	2-Tetradecene, (E)-	C14H28	0.23%
52	13.249	Tetradecane	C14H30	4.97%
53	13.438	Acetamide, N-[1-(4-hydroxyphenyl)ethyl]-	C10H13NO2	0.20%
54	14.039	Heptadecane, 2,6,10,14-tetramethyl-	C21H44	0.50%
55	14.182	Cyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis-	C22H40	0.37%
56	14.291	Cyclopentadecane	C15H30	0.18%
57	14.359	6-Tridecene	C13H26	0.41%
58	14.559	Pentadecane	C15H32	15.22%
59	15.252	Cyclohexane, 1,1'-(1,4-butanediyl)bis-	C16H30	0.35%
60	15.481	1H-Indole, 5,6,7-trimethyl-	C11H13N	0.42%
61	15.692	7-Hexadecene, (Z)-	C16H32	0.75%
62	15.778	7-Hexadecene, (Z)-	C16H32	0.40%
63	15.95	Hexadecane	C16H34	15.08%
64	16.493	5-Methyl-3-isopropylindole	C12H15N	0.27%
65	16.717	Tridecane, 5-propyl-	C16H34	0.65%
66	16.888	Cyclopentane, undecyl-	C16H32	0.74%
67	17.672	Heptadecane	C17H36	5.94%
68	17.775	Pentadecane, 2,6,10,14-tetramethyl-	C19H40	0.84%
69	19.721	Octadecane	C18H38	4.39%
70	19.938	Hexadecane, 2,6,10,14-tetramethyl-	C20H42	2.76%
71	21.128	E-15-Heptadecenal	C17H32O	0.26%
72	22.004	Nonadecane	C19H40	1.42%
73	24.47	Eicosane	C20H42	0.89%
74	25.797	Nonane, 4,5-dimethyl-	C11H24	0.26%
75	27.051	Heneicosane	C21H44	0.41%
76	27.239	Heptadecanenitrile	C17H33N	0.18%
77	29.145	Dodecanamide	C12H25NO	0.22%
78	29.665	Heptadecane	C17H36	0.31%
79	32.28	Heptadecane	C17H36	0.41%
80	34.85	Tetracosane	C24H50	0.34%

81	35.387	Phenol, 2,2'-methylenebis[6-(1,1-dimethylethyl)-4-methyl-	C23H32O2	0.43%
82	37.379	Heneicosane	C21H44	0.53%
83	39.833	Octadecane	C18H38	0.27%
84	42.225	Heneicosane	C21H44	0.87%
85	44.514	Coprostane	C27H48	1.47%
86	45.395	Cholestane	C27H48	1.87%
87	46.78	Tetracosane	C24H50	0.53%
88	48.943	Octadecane	C18H38	0.64%
89	53.103	Tetracosane	C24H50	0.81%

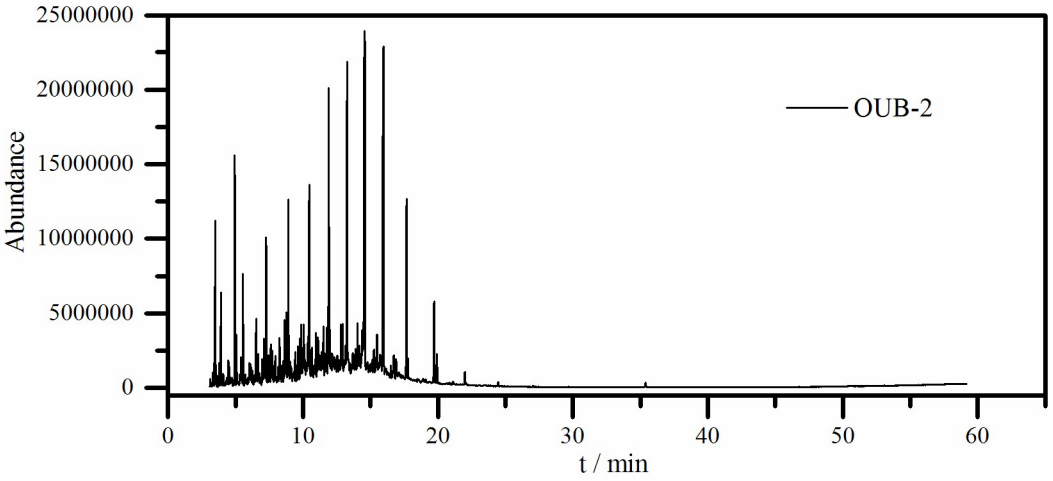

Fig. 3 Total ion chromatogram of OUB-2

The main peaks of ion chromatogram for OUB-2 appeared between 3 min to 20 min and the peaks between 3 min to 12 min accounts a higher ratio than OUB-1. The peaks after 20min were less.

Table 3 The composition of OUB-2 (Stage-2 obtained optimized upgrading biofuel)

No.	R.T. (min)	Compounds	Formation	Area
1	3.133	2-Heptyne	C7H12	0.15%
2	3.31	Cyclopentene, 4,4-dimethyl-	C7H12	0.33%
3	3.419	Heptane, 2-methyl-	C8H18	0.34%
4	3.487	Toluene	C7H8	2.36%
5	3.63	Cyclohexane, 1,2-dimethyl-, trans-	C8H16	0.21%
6	3.785	1,2-Cyclohexanedione	C6H8O2	0.67%
7	3.911	Octane	C8H18	1.40%
8	4.014	2-Octene, (Z)-	C8H16	0.15%
9	4.088	Cyclopentene, 1,2,3-trimethyl-	C8H14	0.18%
10	4.471	Cyclohexane, ethyl-	C8H16	0.45%
11	4.529	Methyl ethyl cyclopentene	C8H14	0.21%
12	4.946	Ethylbenzene	C8H10	3.52%
13	5.072	Benzene, 1,3-dimethyl-	C8H10	0.77%
14	5.324	Cyclopentane, 1-methyl-2-propyl-	C9H18	0.24%
15	5.404	1-Nonene	C9H18	0.40%
16	5.479	o-Xylene	C8H10	0.38%
17	5.553	Nonane	C9H20	1.44%
18	5.707	Cyclohexane, 1-ethyl-2-methyl-, trans-	C9H18	0.19%
19	6.022	1H-Pyrrole, 2,5-dimethyl-	C6H9N	0.41%

20	6.102	Cyclohexane, propyl-	C9H18	0.25%
21	6.24	1H-Pyrrole, 2,3-dimethyl-	C6H9N	0.34%
22	6.405	cis-1,4-Dimethyl-2-methylenecyclohexane	C9H16	0.15%
23	6.526	Benzene, propyl-	C9H12	0.82%
24	6.657	Benzene, 1-ethyl-2-methyl-	C9H12	0.49%
25	6.772	Octane, 2,6-dimethyl-	C10H22	0.14%
26	6.978	Benzene, 1-ethyl-2-methyl-	C9H12	0.46%
27	7.029	Cyclodecane	C10H20	0.19%
28	7.121	1-Decene	C10H20	1.03%
29	7.212	Benzene, 1,2,3-trimethyl-	C9H12	0.32%
30	7.269	Decane	C10H22	1.84%
31	7.453	1H-Pyrrole, 2-ethyl-4-methyl-	C7H11N	0.40%
32	7.504	Benzene, (1-methylpropyl)-	C10H14	0.18%
33	7.538	1H-Pyrrole, 2-ethyl-4-methyl-	C7H11N	0.19%
34	7.607	1H-Pyrrole, 2,3,5-trimethyl-	C7H11N	0.55%
35	7.647	1H-Pyrrole, 2-ethyl-4-methyl-	C7H11N	0.24%
36	7.71	Benzene, 1,2,4-trimethyl-	C9H12	0.55%
37	7.842	Cyclohexane, butyl-	C10H20	0.22%
38	7.899	Cyclopentane, pentyl-	C10H20	0.15%
39	7.945	Tetracyclo[3.3.1.0(2,8).0(4,6)]-non-2-ene	C9H10	0.58%
40	8.259	Benzene, butyl-	C10H14	0.73%
41	8.443	Benzene, 1-methyl-2-propyl-	C10H14	0.22%
42	8.551	Benzenamine, 3-methyl-	C7H9N	0.34%
43	8.637	Phenol, 4-methyl-	C7H8O	1.34%
44	8.78	Indan, 1-methyl-	C10H12	1.19%
45	8.917	Undecane	C11H24	2.27%
46	8.963	1H-Pyrrole, 3-ethyl-2,4-dimethyl-	C8H13N	0.29%
47	9.06	1H-Pyrrole, 3-ethyl-2,4-dimethyl-	C8H13N	0.29%
48	9.226	Naphthalene, decahydro-2-methyl-	C11H20	0.14%
49	9.415	5-Dimethylaminopyrimidine	C6H9N3	0.59%
50	9.507	Cyclohexane, pentyl-	C11H22	0.22%
51	9.558	Cyclopentane, hexyl-	C11H22	0.18%
52	9.621	1H-Indene, 2,3-dihydro-4-methyl-	C10H12	0.60%
53	9.696	Bicyclo[4.2.0]octa-1,3,5-triene, 7-isopropyl-	C11H14	0.19%
54	9.793	Benzene, 1-methyl-2-(2-propenyl)-	C10H12	1.17%
55	9.993	Naphthalene, 1,2,3,4-tetrahydro-	C10H12	0.19%
56	10.062	Phenol, 4-ethyl-	C8H10O	0.76%
57	10.331	1-Dodecene	C12H24	0.25%
58	10.457	Dodecane	C12H26	2.57%
59	10.525	.alpha.,.beta.,.beta.-Trimethylstyrene	C11H14	0.37%
60	10.657	Undecane, 2,6-dimethyl-	C13H28	0.38%
61	10.954	2,3-Dimethylanisole	C9H12O	1.00%
62	11.115	Phenol, 2-ethyl-5-methyl-	C9H12O	0.45%
63	11.395	Benzene, hexyl-	C12H18	0.33%
64	11.504	Sulfurous acid, 2-ethylhexyl heptadecyl ester	C25H52O3S	0.85%
65	11.778	1-Tridecene	C13H26	0.61%
66	11.847	Cyclotridecane	C13H26	0.19%
67	11.91	Tridecane	C13H28	5.41%
68	11.967	Naphthalene, 2-methyl-	C11H10	0.88%
69	12.162	2,5-Diethylphenol	C10H14O	0.23%
70	12.545	Heptylcyclohexane	C13H26	0.33%
71	12.826	Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	C13H18	0.66%
72	12.934	Dodecane, 2,6,11-trimethyl-	C15H32	0.58%
73	13.14	1-Tetradecene	C14H28	0.22%

74	13.266	Tetradecane	C14H30	6.45%
75	13.913	Cyclotetradecane	C14H28	0.29%
76	14.039	Heptadecane, 2,6,10,14-tetramethyl-	C21H44	0.67%
77	14.187	Cyclopentadecane	C15H30	0.59%
78	14.393	1H-Indole, 1-ethyl-	C10H11N	0.91%
79	14.576	Pentadecane	C15H32	14.18%
80	15.12	Pentadecane, 7-methyl-	C16H34	0.22%
81	15.252	Cyclopentane, decyl-	C15H30	0.42%
82	15.486	Ethanone, 1-(1H-indol-3-yl)-	C10H9NO	0.68%
83	15.967	Hexadecane	C16H34	14.19%
84	16.499	1H-Indole, 2,3-dihydro-1,3,3-trimethyl-2-methylene-	C12H15N	0.29%
85	16.722	Pentadecane, 2,6,10-trimethyl-	C18H38	0.60%
86	16.894	Cyclopentane, undecyl-	C16H32	0.63%
87	17.672	Heptadecane	C17H36	4.17%
88	17.775	Pentadecane, 2,6,10,14-tetramethyl-	C19H40	0.46%
89	19.709	Octadecane	C18H38	1.98%
90	19.921	Hexadecane, 2,6,10,14-tetramethyl-	C20H42	0.81%
91	21.992	Nonadecane	C19H40	0.43%
92	35.376	Phenol, 2,2'-methylenebis[6-(1,1-dimethylethyl)-4-methyl-	C23H32O2	0.16%