

Determination of the Chemical Compositions of Condensate-like Oils with Different API Gravities by Using the Distillation, Precipitation, Fractionation Mass Spectrometry (DPF MS) Method

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Table S1. List of model compounds and their purities.

Model compounds	
Chemical	Percent mass purity
n-hexylamine	99%
Diethyl disulfide	99%
Ethyl benzoate	≥ 99%
Butyl sulfone	99%
3-ethylcarbazole	97%
1,3-diphenylisobenzofuran	97%
2-methylthiophene	98%
Cholestane	≥ 97%
Nonylcyclohexane	95%
Decylcyclohexane	95%
Heptadecylbenzene	95%
p-xylene	≥ 99%
1,3,5-isopropylbenzene	95%
Hexaethylbenzene	95%
1,3,5-triethylbenzene	≥ 97%
Indane	95%

Table S2. Mass calibration for A) LQIT/orbitrap MS by using Pierce LTQ ESI positive ion calibration solution as the calibration agent on regular basis. B) GC×GC/TOF MS by using perfluorotributylamine (PFTBA) as the calibration agent on the day the analyses were performed.

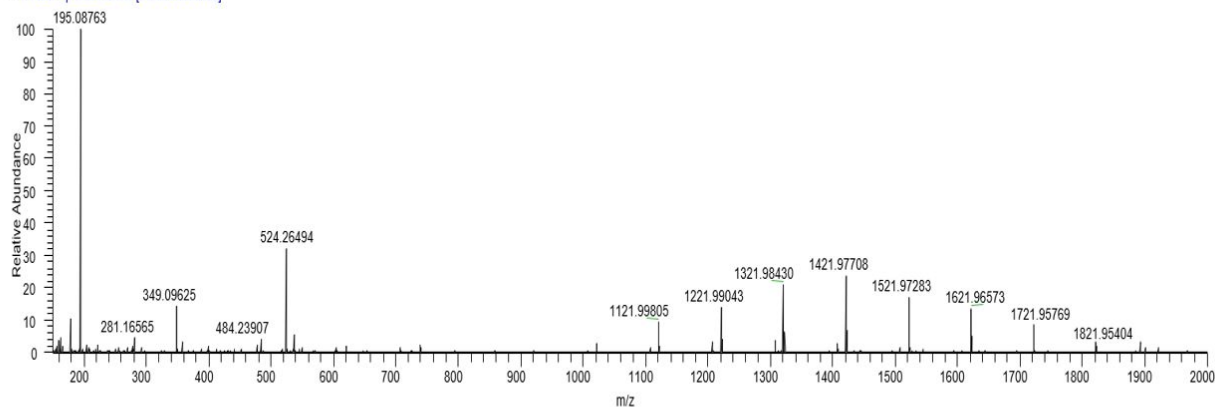
A) LQIT/orbitrap MS Mass Calibration Table		
Expected <i>m/z</i>	Observed <i>m/z</i>	Error in measured <i>m/z</i> (ppm)
195.08762	195.08763	0.05126
524.26496	524.26494	-0.03815
1121.99702	1121.99805	0.91801
1221.99064	1221.99043	-0.17185
1321.98425	1321.98430	0.03782
1421.97786	1421.97708	-0.54853
1521.97148	1521.97283	0.88701
1621.96509	1621.96573	0.39458
1721.95870	1721.95769	-0.58654
1821.95231	1821.95404	0.94953

B) GC×GC/TOF MS Mass Calibration Table		
Expected <i>m/z</i>	Observed <i>m/z</i>	Error in measured <i>m/z</i> (ppm)
68.99	68.99	- 0.05
118.99	118.99	0.25
130.99	130.99	- 0.17

218.99	218.99	- 0.36
263.99	263.99	0.24
413.98	413.98	0.36
501.97	501.97	0.01

A

(+ESI_Calibrate_HR #1 RT: 0.02 AV: 1 NL: 2.44E6
T: FTMS + p ESI Full ms [150.00-2000.00])



B

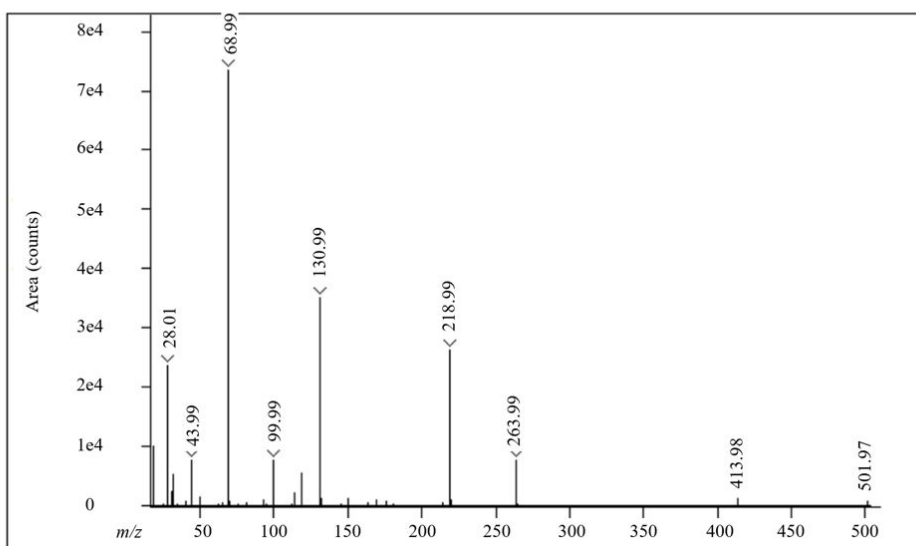


Figure S1. A) LQIT/orbitrap FTMS mass spectrum of the Pierce LTQ ESI positive ion calibration solution. B) GC×GC/TOF MS mass spectrum of the calibration agent perfluorotributylamine (PFTBA).

Table S3. Gravimetric weight percentages of the five different compound classes obtained using the DPF method for five condensate-like oil samples. Each experiment was performed twice. The averaged results, their standard deviations (SD) and 95% confidence intervals were determined based on these two trials. API gravities are shown in parenthesis.

Chemical Classes	Gravimetric weight percent (wt %)									
	5 (43.00 °API)					4 (42.40 °API)				
	Trial 1	Trial 2	SD	Average	95% Confidence interval	Trial 1	Trial 2	SD	Average	95% Confidence interval

Volatile Hydrocarbons	0.76	0.76	0.00	0.76	-	1.31	1.31	0.00	1.31	-
Heteroaromatic Compounds	0.41	0.49	0.06	0.45	0.37-0.53	0.59	0.63	0.02	0.61	0.58-0.64
Polar Compounds	0.16	0.19	0.02	0.18	0.15-0.21	1.39	0.75	0.32	1.06	0.62-1.5
Saturated Hydrocarbons	81.08	81.00	0.06	81.04	80.96-81.12	78.44	77.69	0.38	78.06	77.53-78.59
Alkyl Aromatic Hydrocarbons	7.03	6.68	0.25	6.86	6.51-7.21	6.05	7.17	0.56	6.61	5.83-7.39
Loss	10.55	10.87	0.23	10.71	10.39-11.03	12.22	12.44	0.11	12.33	12.18-12.48
Total	100.00	100.00	0.00	100.00	-	100.00	100.00	0.00	100.00	-

Table S3 continued

Chemical Classes	Gravimetric weight percent (wt %)									
	3 (41.62 °API)					2 (41.61 °API)				
	Trial 1	Trial 2	SD	Average	95% Confidence interval	Trial 1	Trial 2	SD	Average	95% Confidence interval
Volatile Hydrocarbons	1.64	1.64	0.00	1.64	-	1.45	1.45	0.00	1.45	-
Heteroaromatic Compounds	1.02	1.00	0.01	1.01	1.00-1.02	0.91	1.09	0.10	1.00	0.86-1.14
Polar Compounds	0.28	0.22	0.04	0.25	0.19-0.31	0.81	0.91	0.05	0.86	0.79-0.93
Saturated Hydrocarbons	76.10	75.74	0.25	75.92	75.57-76.27	76.55	76.16	0.20	76.36	76.08-76.64
Alkyl Aromatic Hydrocarbons	13.21	10.93	1.61	12.07	9.84-14.30	8.10	8.64	0.27	8.37	8.00-8.74
Loss	7.76	10.47	1.92	9.11	6.45-11.77	12.19	11.75	0.22	11.97	11.67-12.27
Total	100.00	100.00	0.00	100.00	-	100.00	100.00	0.00	100.00	-

Table S3 continued

Chemical Classes	Gravimetric weight percent (wt %)				
	1 (37.50 °API)				
Trial 1	Trial 2	SD	Average	95% Confidence interval	
Volatile Hydrocarbons	2.07	2.07	0.00	2.07	-
Heteroaromatic Compounds	3.27	3.11	0.11	3.19	3.04-3.34
Polar Compounds	1.68	1.49	0.13	1.59	1.41-1.77
Saturated Hydrocarbons	67.81	71.89	2.88	69.85	65.86-73.84
Alkyl Aromatic Hydrocarbons	10.81	9.83	0.69	10.32	9.36-11.28
Loss	14.35	11.61	1.94	12.98	10.29-15.67
Total	100.00	100.00	0.00	100.00	-

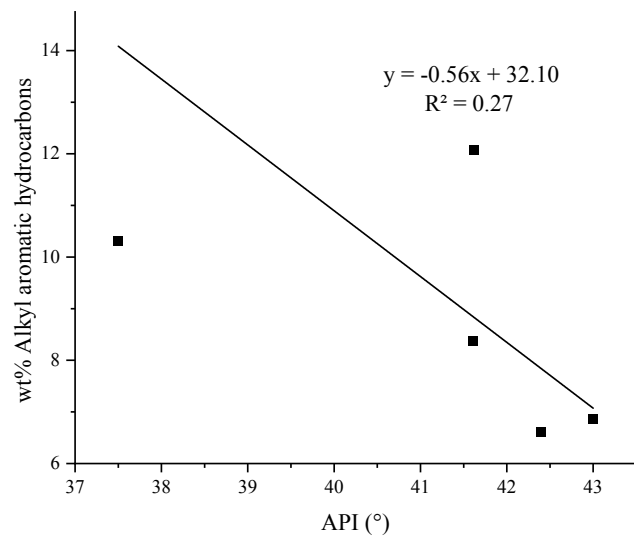


Figure S2. The average weight percent of compounds in the alkyl aromatic hydrocarbon class as a function of API gravity for five different condensate-like oils.

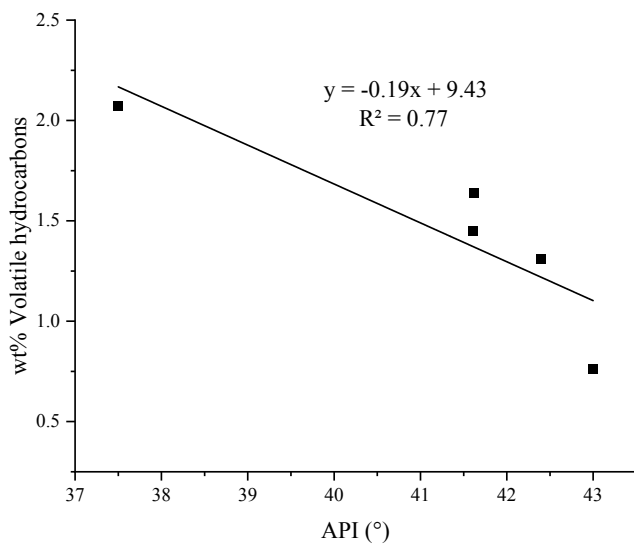


Figure S3. The average weight percent of compounds in the volatile hydrocarbon class as a function of API gravity for five different condensate-like oils.

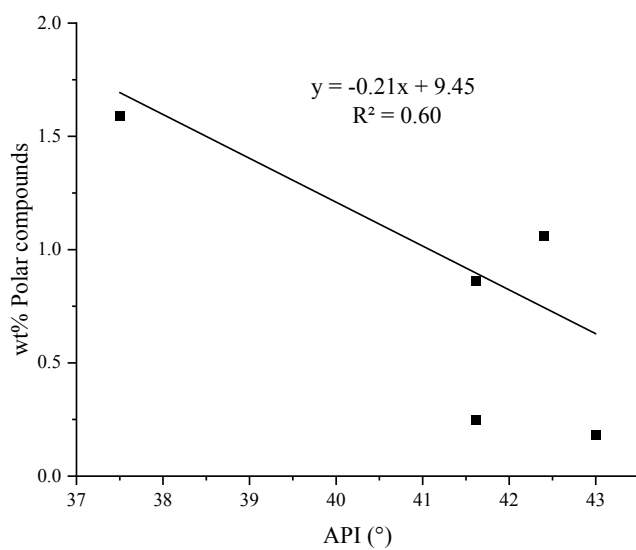


Figure S4. The average weight percent of polar compounds as a function of API gravity for five different condensate-like oils.

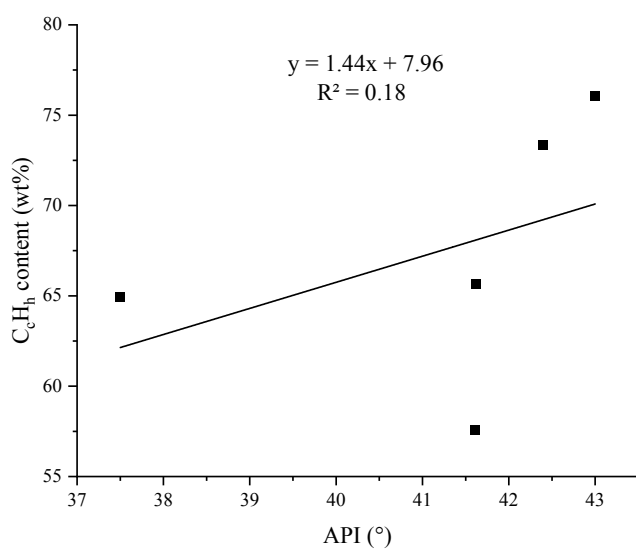


Figure S5. The average weight percent of compounds with the elemental composition C_cH_h as a function of API gravity for five different condensate-like oils.

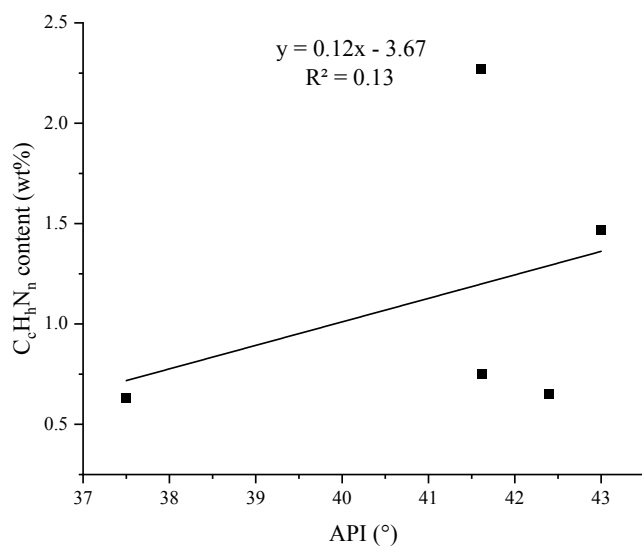


Figure S6. The average weight percent of compounds with the elemental composition $C_cH_hN_n$ as a function of API gravity for five different condensate-like oils.

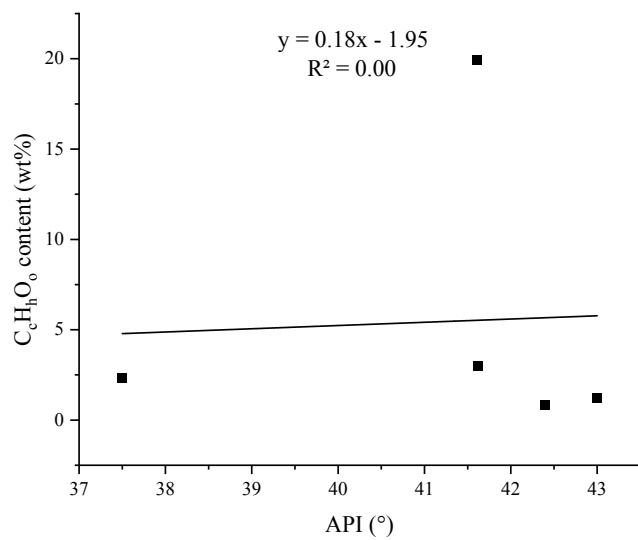


Figure S7. The average weight percent of compounds with the elemental composition $C_cH_hO_o$ as a function of API gravity for five different condensate-like oils.

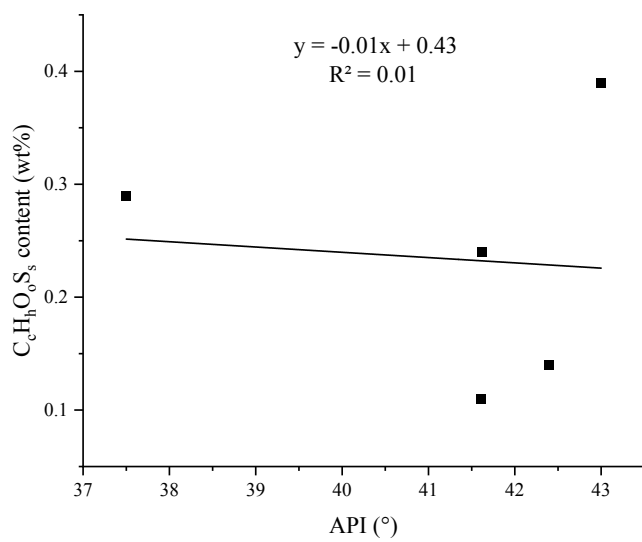


Figure S8. The average weight percent of compounds with the elemental composition $C_cH_hO_oS_s$ as a function of API gravity for five different condensate-like oils.

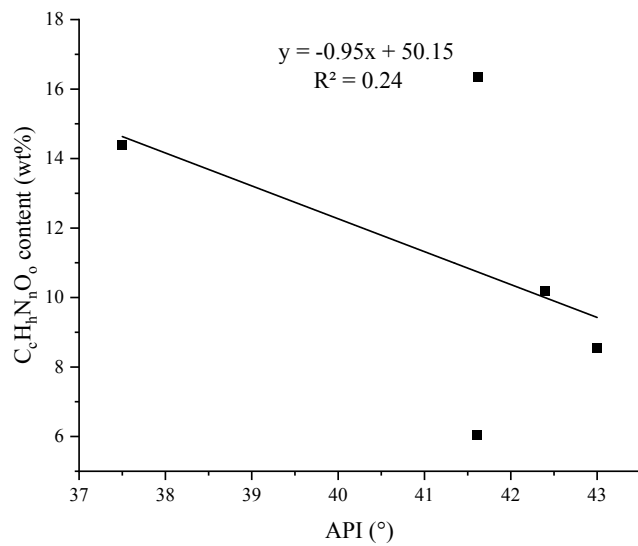


Figure S9. The average weight percent of compounds with the elemental composition $C_cH_hN_nO_o$ as a function of API gravity for five different condensate-like oils.

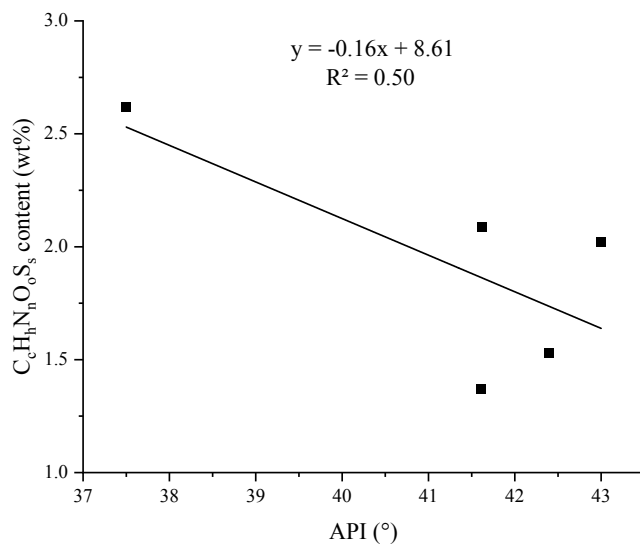


Figure S10. The average weight percent of compounds with the elemental composition $C_cH_hN_nO_oS_s$ as a function of API gravity for five different condensate-like oils.

Table S4. The elemental composition types for the compounds in the different classes for five different condensate-like oils. All data reported are averages of two trials. The total content of compounds of a specific chemical composition type in the condensate-like oil is the sum of the values measured in the five compound classes.

Condensate-like Oil Sample	Semi-quantitative average wt %							Standard Deviation of the Total Content of Compounds with a Specific Elemental Composition Type	95% Confidence interval
	Elemental Composition Type	Volatile Hydrocarbons	Heavy Saturated Hydrocarbons	Heteroaromatic Compounds	Alkyl Aromatic Hydrocarbons	Polar Compounds	Total in the Condensate-like Oil		
1	C_cH_h	1.40	53.10	0.00	10.30	0.10	65.00	1.30	63.2-66.8
2		1.20	52.10	0.60	3.50	0.10	57.60	0.10	57.46-57.74
3		1.20	58.80	0.70	4.80	0.10	65.70	0.00	-
4		1.00	69.20	0.50	2.60	0.10	73.40	0.80	66.21-80.59
5		0.60	73.70	0.40	1.30	0.10	76.10	0.40	75.55-76.65
1	$C_cH_hS_s$	0.02	0.03	0.00	0.80	0.00	0.91	0.30	0.49-1.33
2		0.06	0.00	0.01	0.20	0.00	0.30	0.10	0.16-0.44
3		0.03	0.03	0.02	0.30	0.00	0.40	0.20	0.12-0.68
4		0.09	0.00	0.00	0.20	0.00	0.30	0.10	0.16-0.44
5		0.01	0.00	0.01	0.15	0.00	0.20	0.10	0.06-0.34
1	$C_cH_hN_n$	0.03	0.49	0.02	0.00	0.10	0.60	0.10	0.46-0.74
2		0.00	1.87	0.00	0.20	0.20	2.30	0.00	-
3		0.02	0.25	0.01	0.20	0.30	0.80	0.10	0.66-0.94

4		0.02	0.40	0.00	0.20	0.10	0.70	0.20	0.42-0.98
5		0.02	1.09	0.00	0.30	0.10	1.50	0.40	0.95-2.05
1	C _c H _h O _o	0.20	1.10	0.70	0.30	0.10	2.30	0.10	2.16-2.44
2		0.00	19.20	0.00	0.60	0.10	19.90	0.10	19.76-20.04
3		0.10	2.10	0.10	0.70	0.10	3.00	0.40	2.45-3.55
4		0.10	0.30	0.10	0.30	0.00	0.80	0.10	0.66-0.94
5		0.00	0.50	0.00	0.60	0.00	1.20	0.20	0.92-1.48
1	C _c H _h O _o S _s	0.03	0.04	0.12	0.08	0.03	0.29	0.10	0.15-0.43
2		0.00	0.02	0.02	0.08	0.00	0.11	0.00	-
3		0.08	0.04	0.01	0.07	0.04	0.24	0.10	0.10-0.38
4		0.03	0.01	0.00	0.08	0.01	0.14	0.00	-
5		0.00	0.07	0.01	0.29	0.01	0.39	0.10	0.25-0.53
1	C _c H _h N _n O _o	0.20	12.10	0.20	1.20	0.70	14.40	1.40	12.46-16.34
2		0.10	3.00	0.20	2.30	0.40	6.00	0.20	5.72-6.28
3		0.10	13.20	0.20	2.60	0.30	16.30	0.90	15.05-17.8
4		0.10	7.00	0.10	2.40	0.60	10.20	1.20	8.54-11.86
5		0.10	5.50	0.10	2.70	0.20	8.60	0.20	8.32-8.88
1	C _c H _h N _n O _o S _s	0.10	0.80	0.70	0.90	0.10	2.60	0.10	2.46-2.74
2		0.00	0.00	0.10	1.10	0.10	1.40	0.00	-
3		0.10	0.70	0.10	1.20	0.10	2.10	0.20	1.82-2.38
4		0.10	0.60	0.00	0.80	0.10	1.50	0.10	1.36-1.64
5		0.00	0.30	0.10	1.60	0.00	2.00	0.40	1.45-2.55

Table S5. The total wt% of nitrogen (N), sulfur (S) and oxygen (O) containing compounds recovered from all fractions of the condensate like oils.

	Approximate (consolidated) wt% of compounds with heteroatom content									
	5 (43.00 °API)					4 (42.40 °API)				
	Trial 1	Trial 2	SD	Average	95% Confidence interval	Trial 1	Trial 2	SD	Average	95% Confidence interval
Total N content	12.4	12.5	0.07	12.5	12.4-12.6	14.1	14.0	0.1	14.1	14.0-14.2
Total S content	3.9	3.9	0.0	3.9	-	3.8	3.9	0.1	3.9	3.8-4.0
Total O content	13.1	13.0	0.07	13.1	13.0-13.2	15.3	14.1	0.8	14.7	13.9-15.5

Table S5 continued

	Approximate (consolidated) wt% of compounds with heteroatom content									
	3 (41.62 °API)					2 (41.61 °API)				
	Trial 1	Trial 2	SD	Average	95% Confidence interval	Trial 1	Trial 2	SD	Average	95% Confidence interval
Total N content	19.3	18.2	0.8	18.8	17.7-19.9	10.3	10.2	0.1	10.3	21.4-23.5
Total S content	4.0	4.6	0.4	4.3	3.7-4.9	1.8	3.7	1.3	2.8	10.1-10.3
Total O content	19.9	20.0	0.1	19.9	19.8-20.0	29.1	27.8	0.9	28.5	27.2-29.7

Table S5 continued

Approximate (consolidated) wt% of compounds with heteroatom content					
1 (37.50 °API)					
	Trial 1	Trial 2	SD	Average	95% Confidence interval
Total N content	20.5	18.1	1.7	19.3	16.9-21.7
Total S content	5.4	6.3	0.6	5.9	5.0-6.8
Total O content	24.2	20.1	2.9	22.2	18.2-26.2

Table S6. Elemental composition types of the compounds in the volatile saturated hydrocarbon class derived from five different condensate-like oils and the relative abundances of the ionized compounds based on mass spectrometry.

Elemental Compositions	Relative Ion Abundances (%)				
	5 (43.00 °API)	4 (42.4 °API)	3 (41.62 °API)	2 (41.61°API)	1 (37.50 °API)
C _c H _h	72.74	76.25	77.52	79.23	66.08
C _c H _h S _s	0.96	6.68	2.14	3.73	0.91
C _c H _h N _n	1.88	1.41	1.19	0.27	1.34
C _c H _h O _o	4.31	5.14	7.79	2.4	8.4
C _c H _h O _o S _s	0.41	2.16	4.00	0.21	1.32
C _c H _h N _n O _o	9.96	3.32	4.27	6.32	9.44
C _c H _h N _n O _o S _s	0.45	5.04	3.09	2.58	6.09
Others	9.30	0.00	0.00	5.26	6.42
Total	100.00	100.00	100.00	100.00	100.00

Table S7. Elemental composition types of the compounds in the heavy saturated hydrocarbons class derived from five different condensate-like oils and the relative abundances of the ionized compounds based on mass spectrometry.

Elemental Compositions	Relative Ion Abundances (%)				
	5 (43.00 °API)	4 (42.4 °API)	3 (41.62 °API)	2 (41.61°API)	1 (37.50 °API)
C _c H _h	90.69	88.57	77.65	68.23	77.07
C _c H _h S _s	0.00	0.00	0.04	0.00	0.04
C _c H _h N _n	1.30	0.52	0.33	2.45	0.71
C _c H _h O _o	0.60	0.44	2.74	25.17	1.62
C _c H _h O _o S _s	0.08	0.02	0.05	0.02	0.06
C _c H _h N _n O _o	6.71	8.93	17.39	3.95	17.53
C _c H _h N _n O _o S _s	0.29	0.78	0.94	0.02	0.83
Others	0.32	0.74	0.87	0.16	2.14
Total	100.00	100.00	100.00	100.00	100.00

Table S8. Elemental composition types of the compounds in the alkyl aromatic hydrocarbons class derived from five different condensate-like oils and the relative abundances of the ionized compounds based on mass spectrometry.

Elemental Compositions	Relative Ion Abundances (%)				
	5 (43.00 °API)	4 (42.4 °API)	3 (41.62 °API)	2 (41.61°API)	1 (37.50 °API)
C _c H _h	63.22	75.38	60.46	44.48	32.32
C _c H _h S _s	1.03	0.81	1.40	1.00	0.02
C _c H _h N _n	0.50	0.50	1.01	1.5	29.8
C _c H _h O _o	3.10	8.80	6.54	1.27	3.41
C _c H _h O _o S _s	2.38	0.57	1.24	2.00	3.28
C _c H _h N _n O _o	11.76	9.90	19.70	31.82	13.81
C _c H _h N _n O _o S _s	13.27	2.91	9.14	11.12	10.96
Others	4.74	1.14	0.50	6.81	6.4
Total	100.00	100.00	100.00	100.00	100

Table S9. Elemental composition types of the compounds in the heteroaromatic compound class derived from five different condensate-like oils and the relative abundances of the ionized compounds based on mass spectrometry.

Elemental Compositions	Relative Ion Abundances (%)				
	5 (43.00 °API)	4 (42.4 °API)	3 (41.62 °API)	2 (41.61°API)	1 (37.50 °API)
C _c H _h	17.56	39.72	46.14	41.77	74.29
C _c H _h S _s	2.12	2.90	3.03	2.20	6.06
C _c H _h N _n	2.07	2.45	2.17	2.26	0.33
C _c H _h O _o	8.75	5.18	6.29	6.89	2.22
C _c H _h O _o S _s	4.04	1.22	0.68	0.90	0.59
C _c H _h N _n O _o	37.51	36.52	24.74	27.90	8.59
C _c H _h N _n O _o S _s	22.01	11.94	1.15	1.12	6.38
Others	5.93	0.06	15.80	16.97	1.55
Total	100.00	100.00	100.00	100.00	100.00

Table S10. Elemental composition types of the compounds in polar compounds class derived from five different condensate-like oils and the relative abundances of the ionized compounds based on mass spectrometry.

Elemental Compositions	Relative Ion Abundances (%)				
	5 (43.00 °API)	4 (42.4 °API)	3 (41.62 °API)	2 (41.61°API)	1 (37.50 °API)
C _c H _h	16.40	10.68	17.18	15.11	7.73
C _c H _h S _s	0.88	3.36	0.75	1.61	1.15
C _c H _h N _n	9.17	5.12	31.17	22.08	2.90
C _c H _h O _o	7.06	2.95	6.26	6.31	3.47
C _c H _h O _o S _s	2.22	1.02	4.48	0.00	1.47
C _c H _h N _n O _o	44.40	49.09	37.01	43.80	41.88

$C_cH_hN_nO_oS_s$	6.95	4.12	0.08	0.08	2.84
Others	12.92	23.66	3.08	11.01	38.54
Total	100.00	100.00	100.00	100.00	100.00

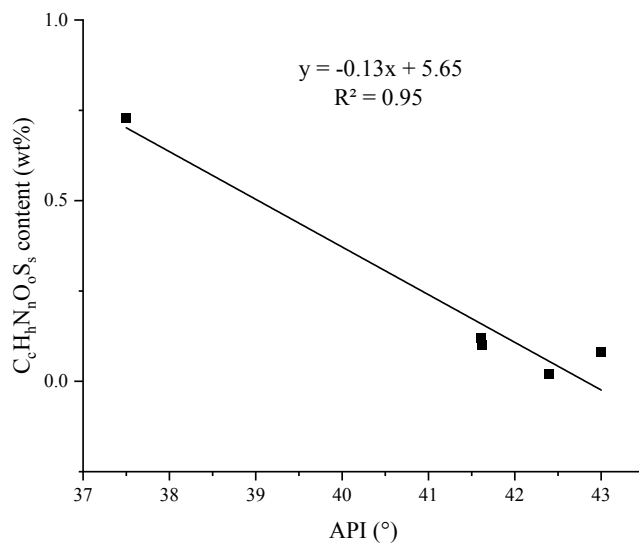


Figure S11. The average weight percent of compounds with the elemental composition type $C_cH_hN_nO_oS_s$ in each heteroaromatic compound class as a function of API gravity for five different condensate-like oils. As the API gravity increases, the approximate average content of compounds with the elemental composition type $C_cH_hN_nO_oS_s$ in the heteroaromatic compound class decreases.

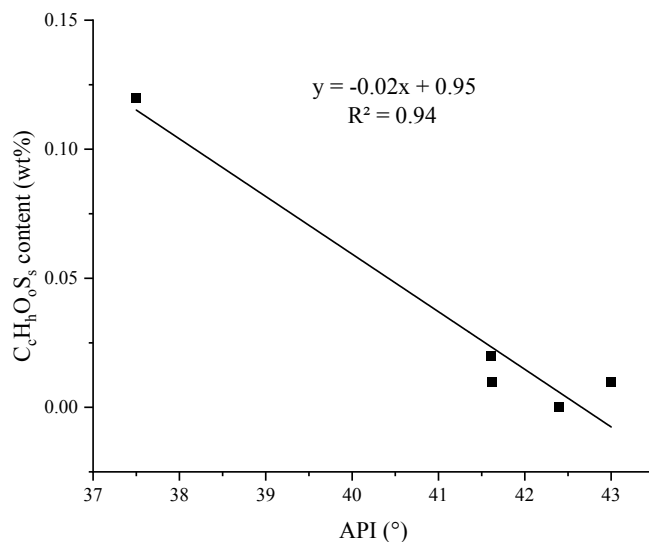


Figure S12. The average weight percent of compounds with the elemental composition type $C_cH_hO_oS_s$ in each heteroaromatic compound class as a function of API gravity for five different condensate-like oils: as the API gravity increases, the approximate average amount of compounds with the elemental composition type $C_cH_hO_oS_s$ in the heteroaromatic compound class decreases.

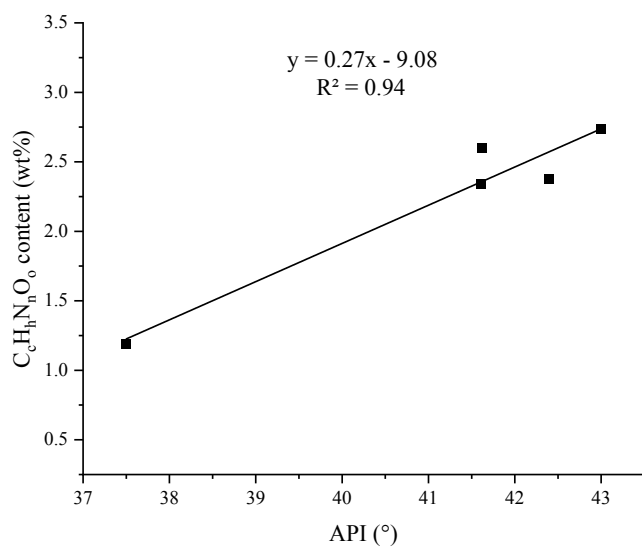


Figure S13. The average weight percent of compounds with the elemental composition type $C_cH_hN_nO_o$ in each alkyl aromatic compound class as a function of API gravity for five different condensate-like oils.

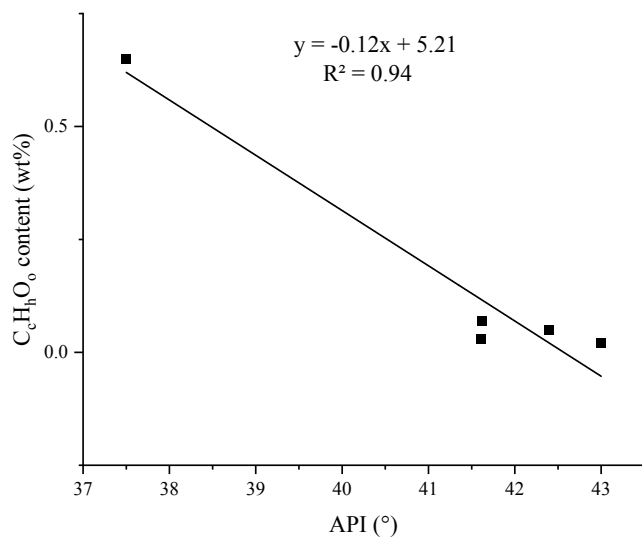


Figure S14. The average weight percent of compounds with the elemental composition type $C_cH_hO_o$ in each heteroaromatic compound class as a function of API gravity for five different condensate-like oils.

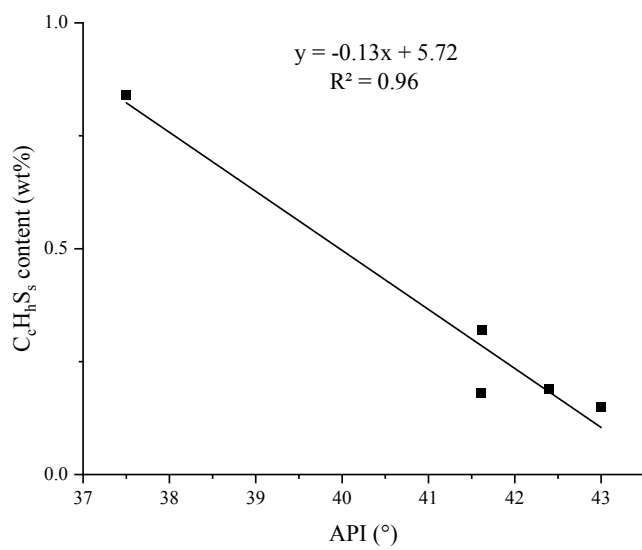


Figure S15. The average weight percent of compounds with the elemental composition type $C_cH_hS_s$ in each alkyl aromatic hydrocarbon class as a function of API gravity of five different condensate-like oils.

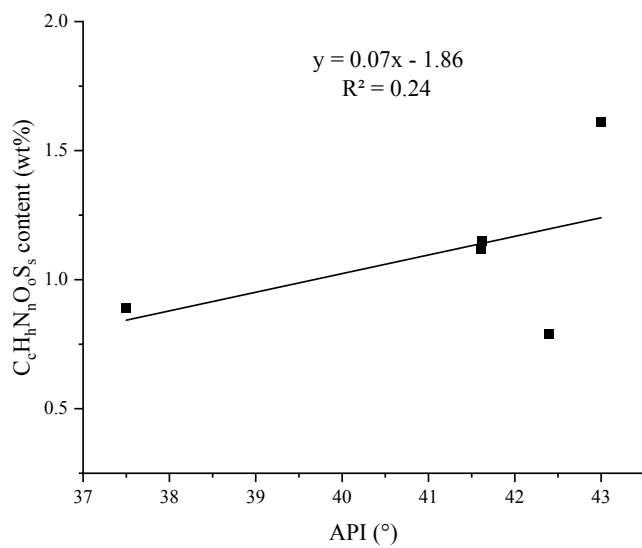


Figure S16. The average weight percent of compounds with the elemental composition type $C_cH_hN_nO_oS_s$ in each alkyl aromatic compound class as a function of API gravity of five different condensate-like oils.

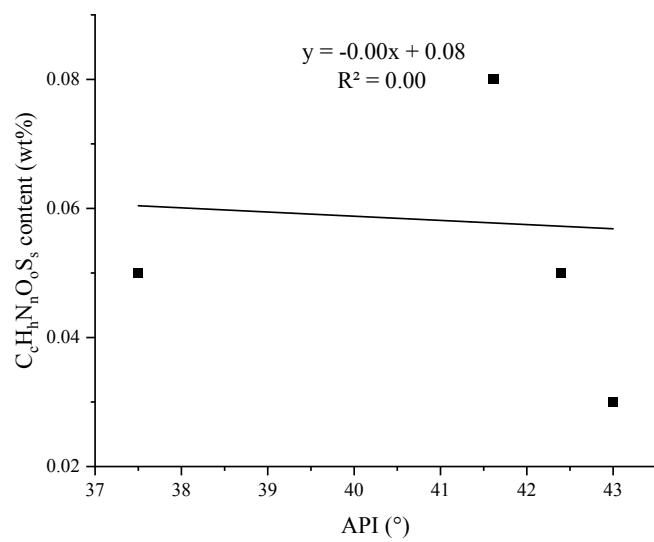


Figure S17. The average weight percent of compounds with the elemental composition type $C_cH_hN_nO_oS_s$ in each polar compound class as a function of API gravity of five different condensate-like oils.

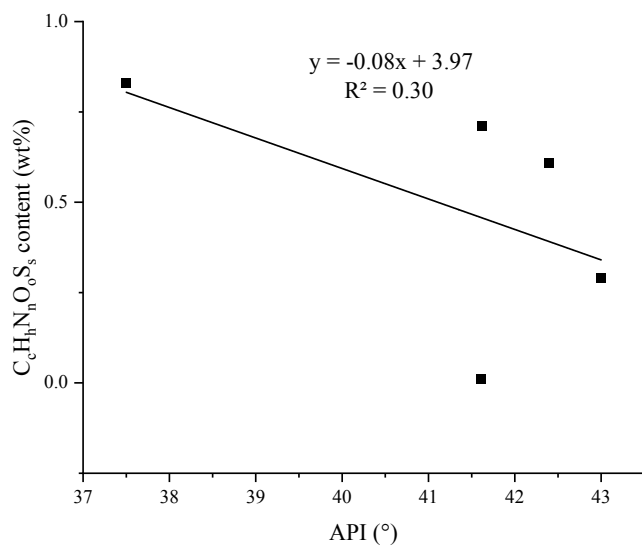


Figure S18. The average weight percent of compounds with the elemental composition type $C_cH_hN_nO_oS_s$ in each heavy saturated hydrocarbon class as a function of API gravity of five different condensate-like oils.

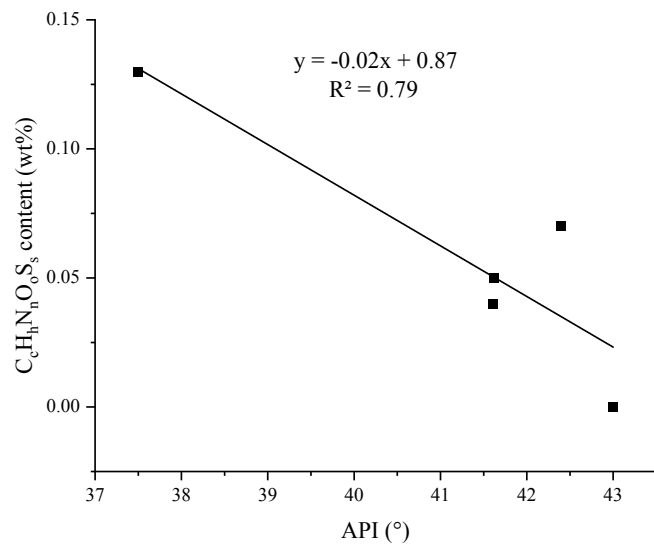


Figure S19. The average weight percent of compounds with the elemental composition type $C_cH_hN_nO_oS_s$ in each volatile hydrocarbon class as a function of API gravity of five different condensate-like oils.

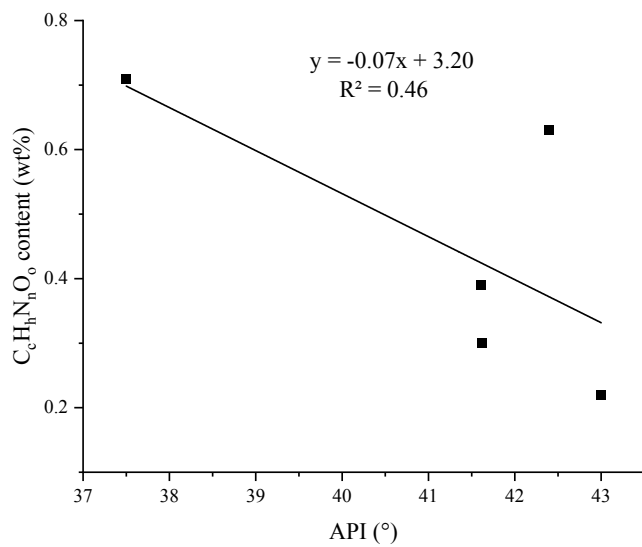


Figure S20. The average weight percent of compounds with the elemental composition type $C_cH_hN_nO_o$ in each polar compound class as a function of API gravity of five different condensate-like oils.

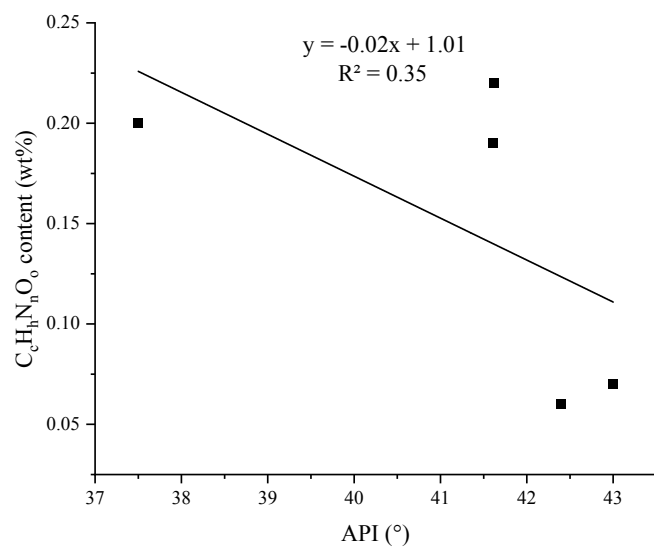


Figure S21. The average weight percent of compounds with the elemental composition type $C_cH_hN_nO_o$ in each heteroaromatic compound class as a function of API gravity of five different condensate-like oils.

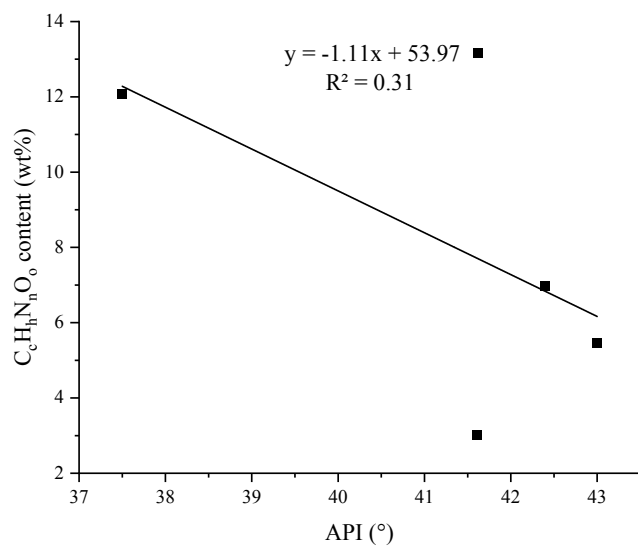


Figure S22. The average weight percent of compounds with the elemental composition type $C_cH_hN_nO_o$ in each saturated hydrocarbon class as a function of API gravity of five different condensate-like oils.

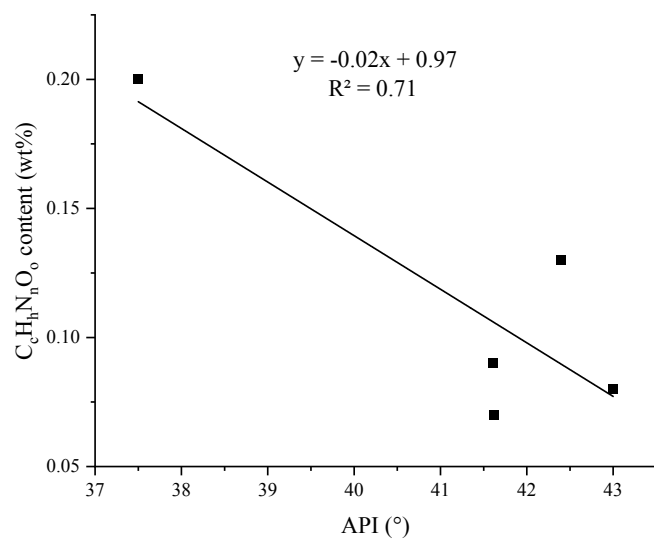


Figure S23. The average weight percent of compounds with the elemental composition type $C_cH_hN_nO_o$ in each volatile hydrocarbon class as a function of API gravity of five different condensate-like oils.

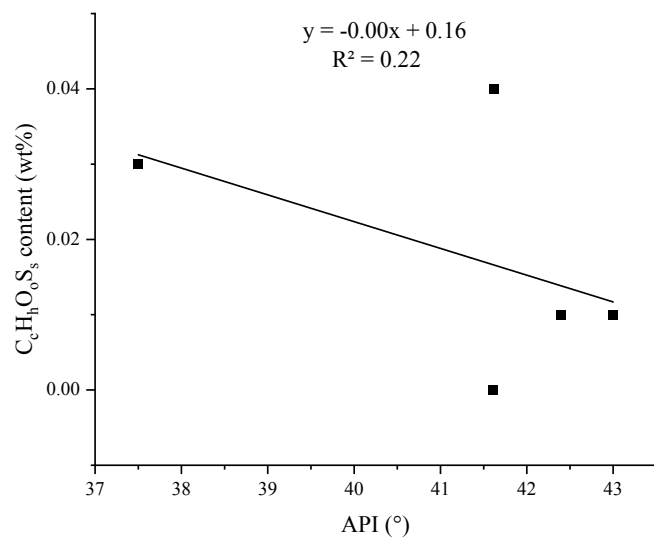


Figure 1S24. The average weight percent of compounds with the elemental composition type $C_cH_hO_oS_s$ in each polar compound class as a function of API gravity of five different condensate-like oils.

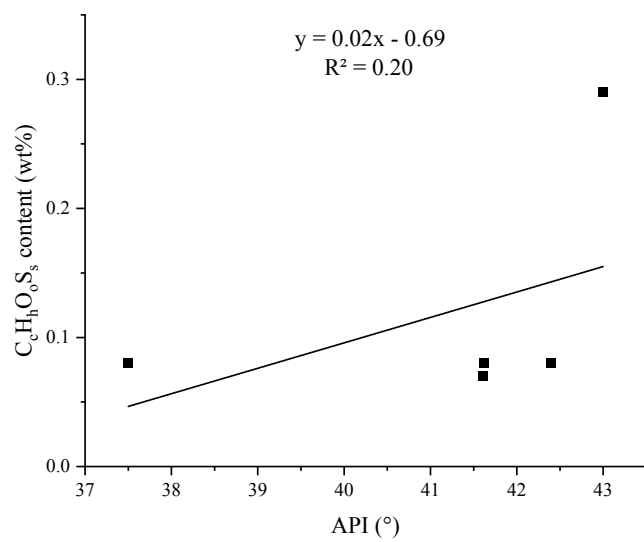


Figure 2S25. The average weight percent of compounds with the elemental composition type C_cH_hO_oS_s in each alkyl aromatic hydrocarbon class as a function of API gravity of five different condensate-like oils.

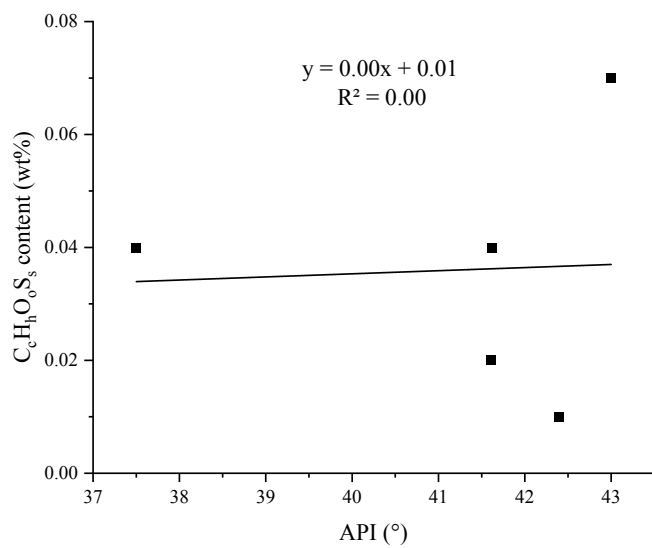


Figure S26. The average weight percent of compounds with the elemental composition type C_cH_hO_oS_s in each heavy saturated hydrocarbon class as a function of API gravity of five different condensate-like oils.

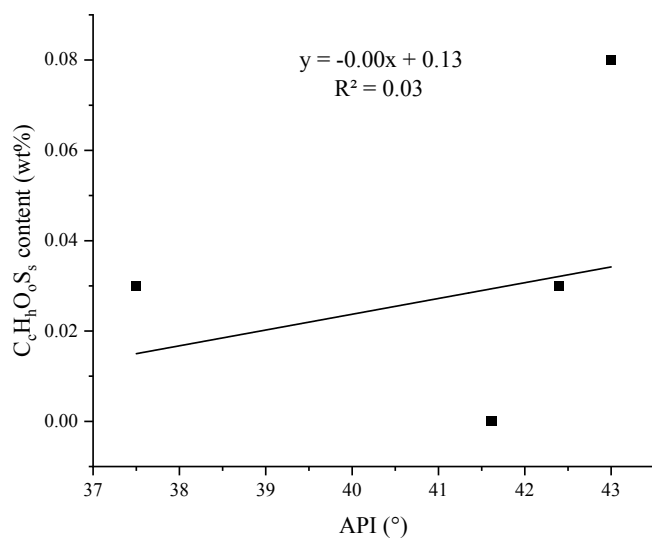


Figure S27. The average weight percent of compounds with the elemental composition type $C_cH_hO_oS_s$ in each volatile hydrocarbon class as a function of API gravity of five different condensate-like oils.

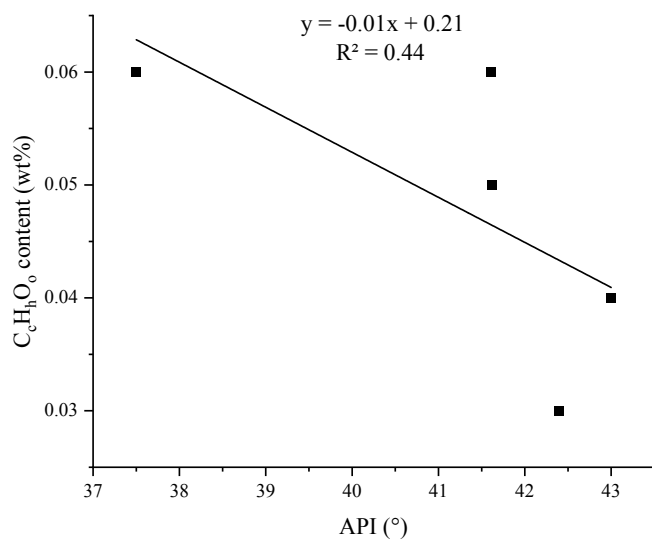


Figure S28. The average weight percent of compounds with the elemental composition type $C_cH_hO_o$ in each polar compound class as a function of API gravity of five different condensate-like oils.

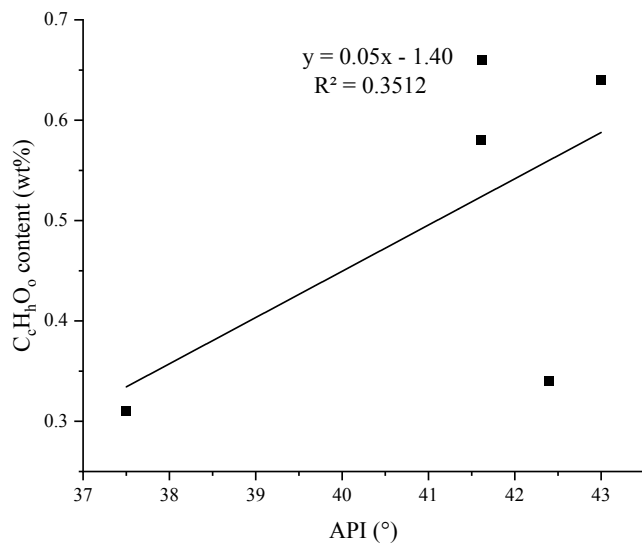


Figure S29. The average weight percent of compounds with the elemental composition type C_cH_hO_o in each alkyl aromatic hydrocarbon class as a function of API gravity of five different condensate-like oils.

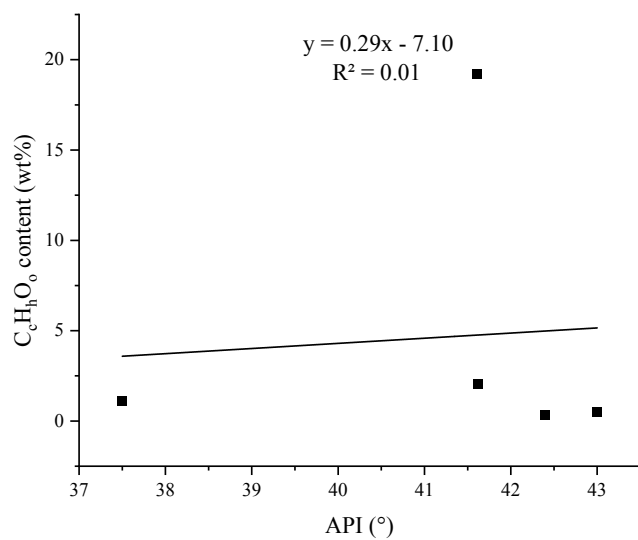


Figure S30. The average weight percent of compounds with the elemental composition type C_cH_hO_o in each heavy saturated hydrocarbon class as a function of API gravity of five different condensate-like oils.

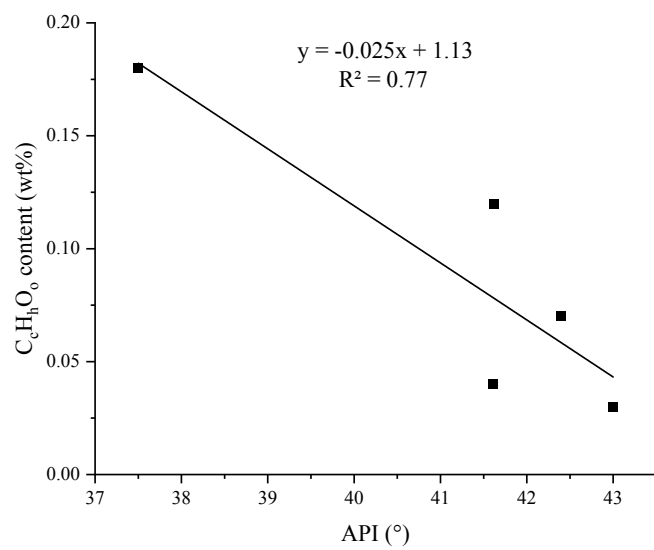


Figure S31. The average weight percent of compounds with the elemental composition type C_cH_hO_o in each volatile hydrocarbon class as a function of API gravity of five different condensate-like oils.

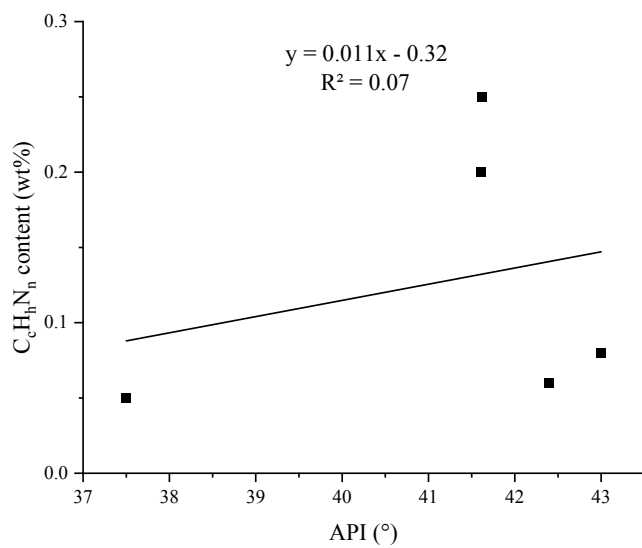


Figure S32. The average weight percent of compounds with the elemental composition type C_cH_hN_n in each polar compound class as a function of API gravity of five different condensate-like oils.

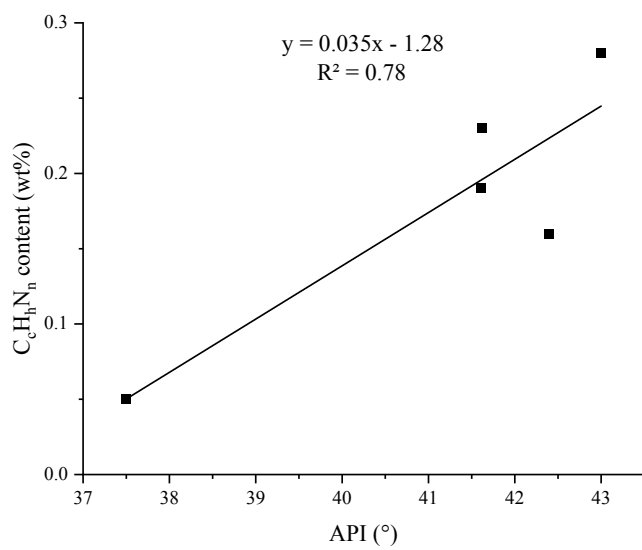


Figure S33. The average weight percent of compounds with the elemental composition type $C_cH_hN_n$ in each alkyl aromatic hydrocarbon class as a function of API gravity of five different condensate-like oils.

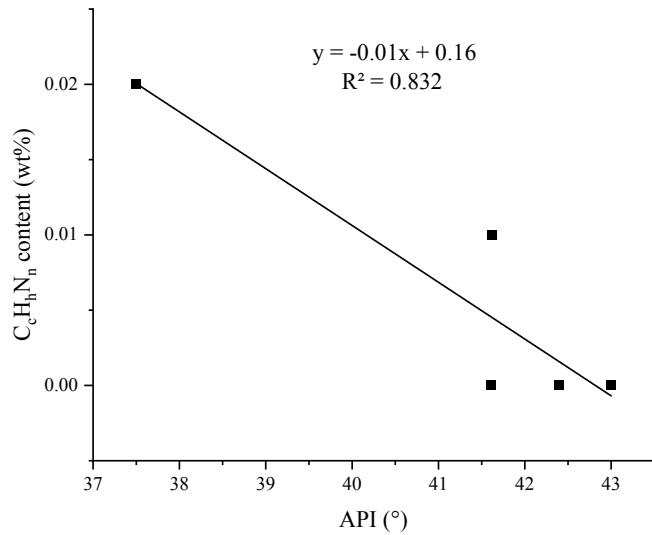


Figure S34. The average weight percent of compounds with the elemental composition type $C_cH_hN_n$ in each heteroaromatic compound class as a function of API gravity of five different condensate-like oils.

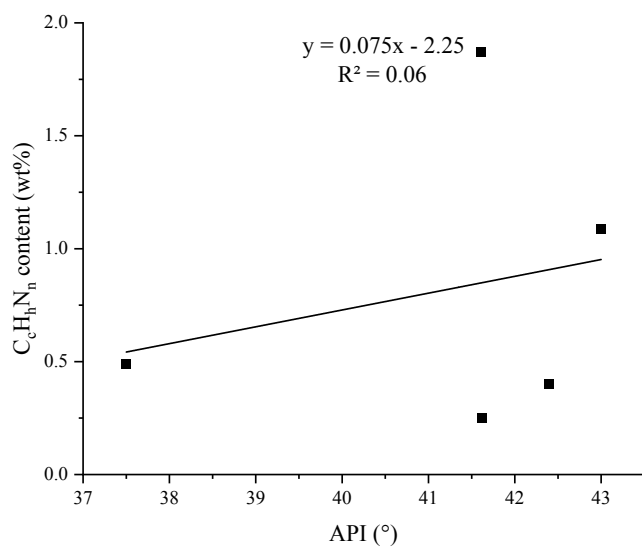


Figure S35. The average weight percent of compounds with the elemental composition type $C_cH_hN_n$ in each heavy saturated hydrocarbon class as a function of API gravity of five different condensate-like oils.

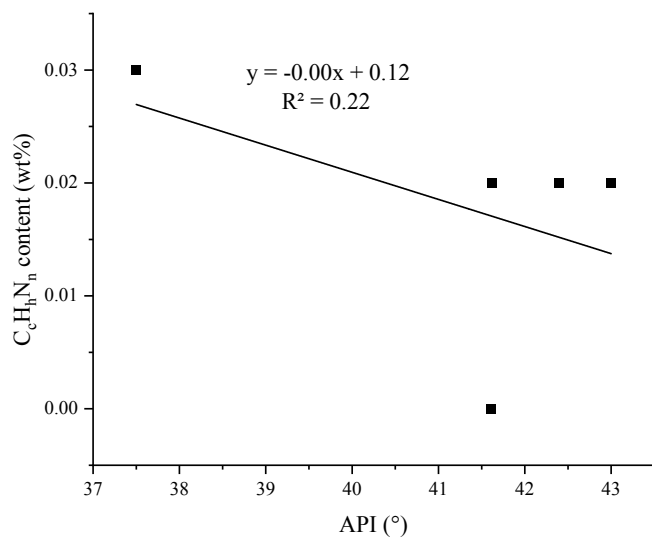


Figure S36. The average weight percent of compounds with the elemental composition type $C_cH_hN_n$ in each volatile hydrocarbon class as a function of API gravity of five different condensate-like oils.

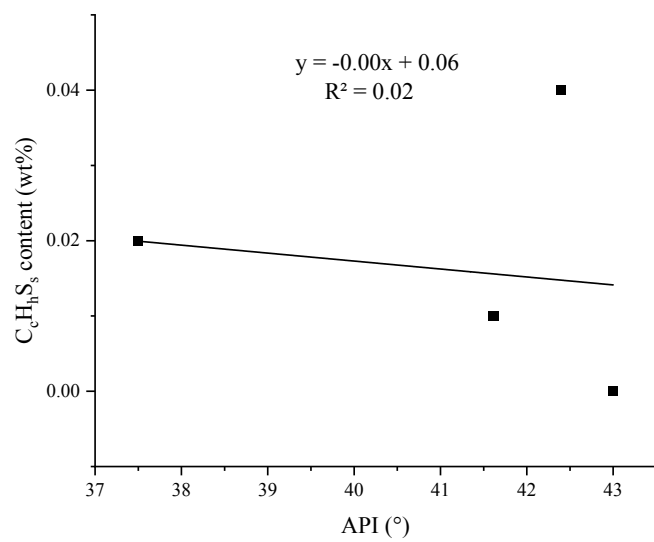


Figure S37. The average weight percent of compounds with the elemental composition type $C_cH_hS_s$ in each polar compound class as a function of API gravity of five different condensate-like oils.

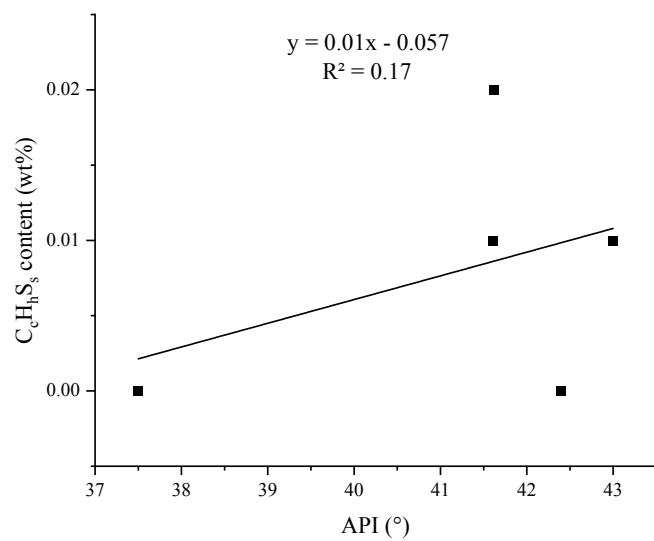


Figure S38. The average weight percent of compounds with the elemental composition type $C_cH_hS_s$ in each heteroaromatic compound class as a function of API gravity of five different condensate-like oils.

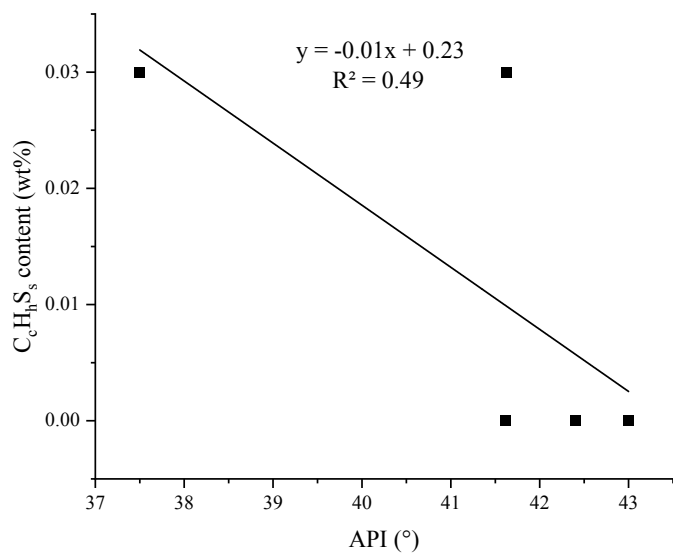


Figure S39. The average weight percent of compounds with the elemental composition type C_cH_hS_s in each heavy saturated hydrocarbon class as a function of API gravity of five different condensate-like oils.

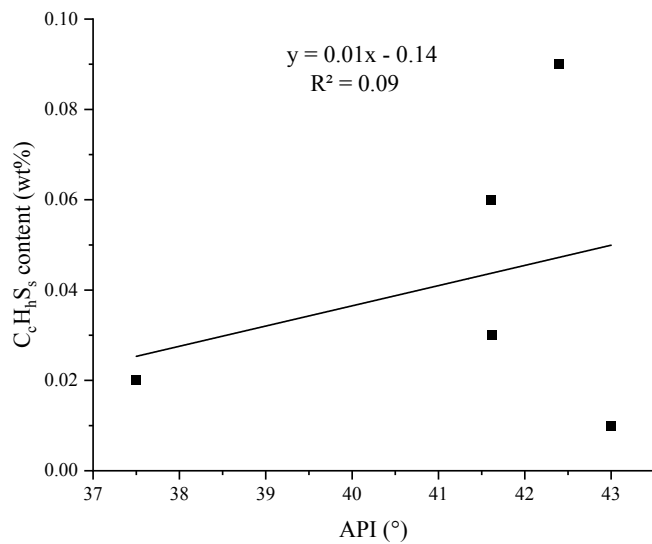


Figure S40. The average weight percent of compounds with the elemental composition type C_cH_hS_s in each volatile hydrocarbon class as a function of API gravity of five different condensate-like oils.

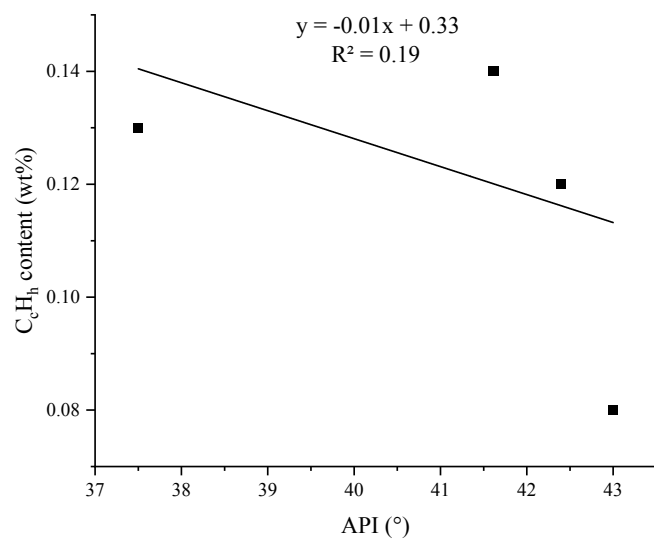


Figure S41. The average weight percent of compounds with the elemental composition type C_cH_h in each polar compound class as a function of API gravity of five different condensate-like oils.

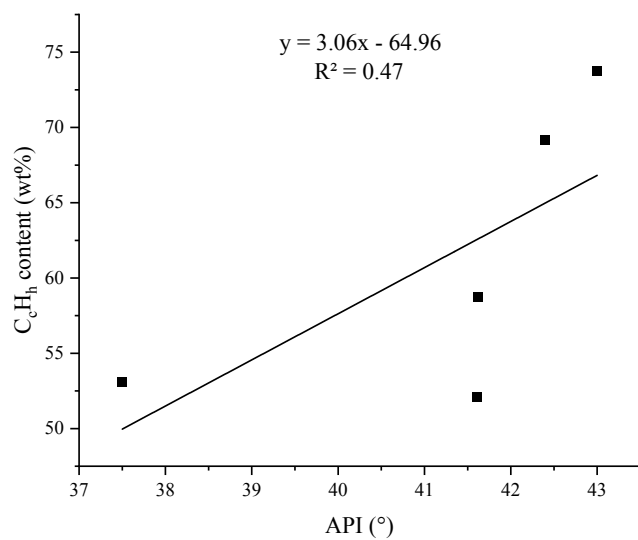


Figure S42. The average weight percent of compounds with the elemental composition type C_cH_h in each heavy saturated hydrocarbon class as a function of API gravity of five different condensate-like oils.

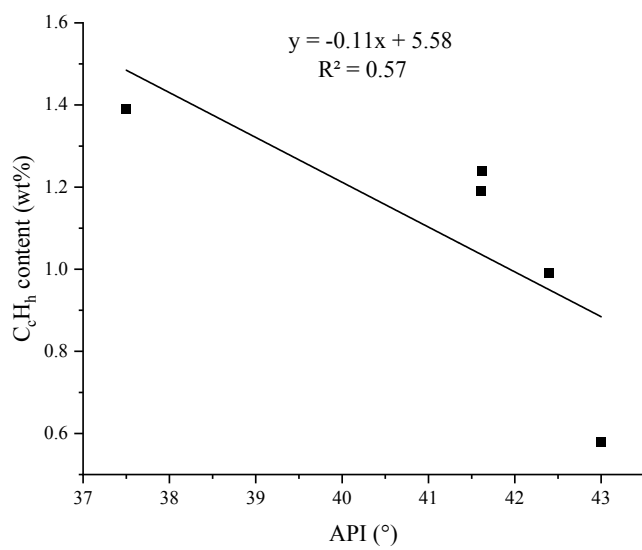


Figure S43. The average weight percent of compounds with the elemental composition type C_cH_h in each volatile hydrocarbon class as a function of API gravity of five different condensate-like oils.

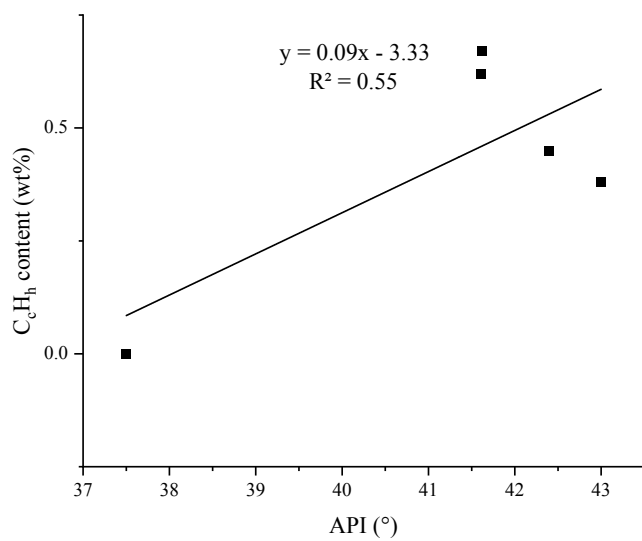


Figure S44. The average weight percent of compounds with the elemental composition type C_cH_h in heteroaromatic compound class as a function of API gravity of five different condensate-like oils.

Table S11. The average molecular weights of compounds in the different compound classes and their standard deviations (SD; based on two measurements) for five different condensate-like oils. The average molecular weights were determined based on the molecular weights determined for compounds in each individual compound class and the gravimetric weight percentage of each class.

Chemical Classes	Average molecular weight (Da)									
	5 (43.00 °API)					4 (42.40 °API)				
	Trial 1	Trial 2	SD	Average	95% Confidence interval	Trial 1	Trial 2	SD	Average	95% Confidence interval
Volatile Hydrocarbons	229.3	231.6	1.6	230.5	228.3-232.7	225.5	223.1	1.7	224.3	221.9-226.7
Heteroaromatic Compounds	339.5	336.5	2.1	338.0	335.1-340.91	332.6	330.7	1.3	331.7	329.9-333.5
Polar Compounds	216.2	216.8	0.4	216.5	215.9-217.1	286.3	285.4	0.6	285.8	285.0-286.6
Heavy Saturated Hydrocarbons	269.8	278.5	6.2	274.2	265.6-282.8	320.2	325.8	4.0	323.0	317.5-328.5
Alkyl Aromatic Hydrocarbons	410.8	422.0	7.9	416.4	405.5-427.4	388.4	386.5	1.3	387.5	385.7-389.3
Overall Average Molecular Weight of Condensate-like Oil	280.6	289.4	6.2	285.0	276.4-293.6	323.6	328.4	3.4	326.0	321.3-330.7

Table S11 continued

Chemical Classes	Average molecular weight (Da)									
	3 (41.62 °API)					2 (41.61 °API)				
	Trial 1	Trial 2	SD	Average	95% Confidence interval	Trial 1	Trial 2	SD	Average	95% Confidence interval
Volatile Hydrocarbons	228.5	228.9	0.3	228.7	228.3-229.1	225.2	227.9	1.9	226.6	224.0-229.2
Heteroaromatic Compounds	453.5	461.0	5.3	457.2	449.9-464.5	475.5	472.0	2.5	473.8	470.3-477.3
Polar Compounds	240.1	236.8	2.3	238.4	235.2-241.6	397.8	391.0	4.8	394.4	387.7-401.1
Heavy Saturated Hydrocarbons	312.6	313.1	0.3	312.9	312.5-313.3	234.7	236.3	1.1	235.5	234.0-237.0
Alkyl Aromatic Hydrocarbons	379.1	363.0	11.4	371.0	355.2-386.8	387.4	383.0	3.1	385.2	380.9-389.5
Overall Average Molecular Weight of the Condensate-like Oil	321.4	319.7	1.2	320.6	318.9-322.3	253.5	254.3	0.6	253.9	253.1-254.7

Table S11 continued

Chemical Classes	Average molecular weight (Da)				
	1 (37.50 °API)				
	Trial 1	Trial 2	SD	Average	95% Confidence interval
Volatile Hydrocarbons	231.3	234.2	2.1	232.8	229.9-235.7
Heteroaromatic Compounds	450.8	455.0	3.0	452.9	448.7-457.1
Polar Compounds	398.6	399.5	0.7	399.1	398.1-400.1
Heavy Saturated Hydrocarbons	307.3	308.0	0.5	307.6	306.9-308.3
Alkyl Aromatic Hydrocarbons	304.8	307.9	2.2	306.3	303.3-309.3
Overall Average Molecular Weight of the Condensate-like Oil	311.8	313.3	1.1	312.6	311.1-314.1

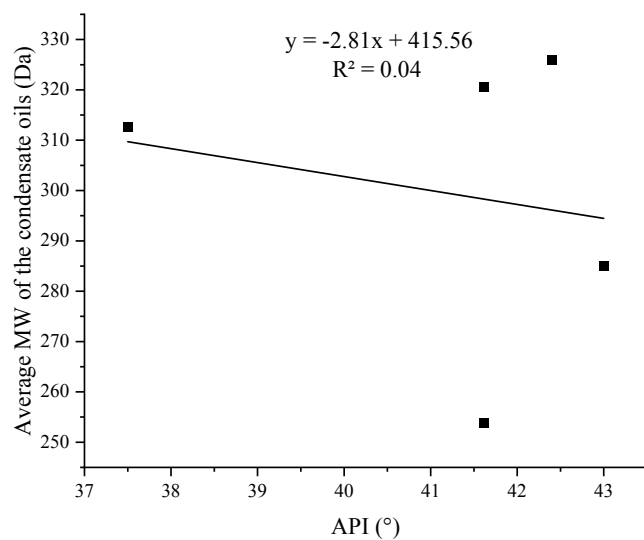


Figure S45. The overall average molecular weight of the condensate-like oil samples as a function of API gravity.

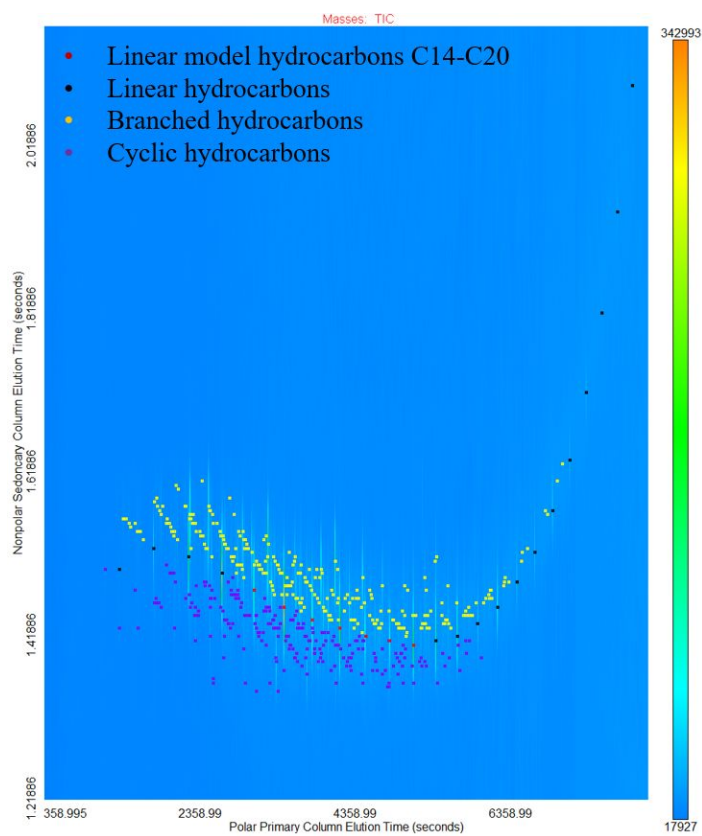


Figure S46. GCxGC/TOF chromatogram for the heavy saturated hydrocarbon fraction of oil 5.

Table S12. The RDBE values of compounds in the different compound classes of five different condensate-like oils. The average RDBE values of each individual compound class were determined based on the RDBE value of the ions and their abundances.

Chemical Classes	Average RDBE values									
	5 (43.00 °API)					4 (42.40 °API)				
	Trial 1	Trial 2	SD	Average	95% Confidence interval	Trial 1	Trial 2	SD	Average	95% Confidence interval
Volatile Hydrocarbons	1.9	1.5	0.3	1.7	1.3-2.1	2.1	2.1	-	2.1	-
Heteroaromatic Compounds	8.8	8.8	0.0	8.8	-	10.2	9.2	0.7	9.7	8.7-10.7
Polar Compounds	2.8	2.4	0.3	2.6	2.2-3.0	6.0	5.9	0.1	5.9	5.8-6.0
Heavy Saturated Hydrocarbons	1.9	1.9	0.0	1.9	-	2.1	2.0	0.1	2.0	1.9-2.1
Alkyl Aromatic Hydrocarbons	7.2	7.4	0.1	7.3	7.2-7.4	6.4	5.4	0.7	5.9	6.9-4.9
Overall Average RDBE Values of the Condensate-like Oil	2.4	2.4	0.0	2.4	-	2.5	2.4	0.1	2.4	2.3-2.5

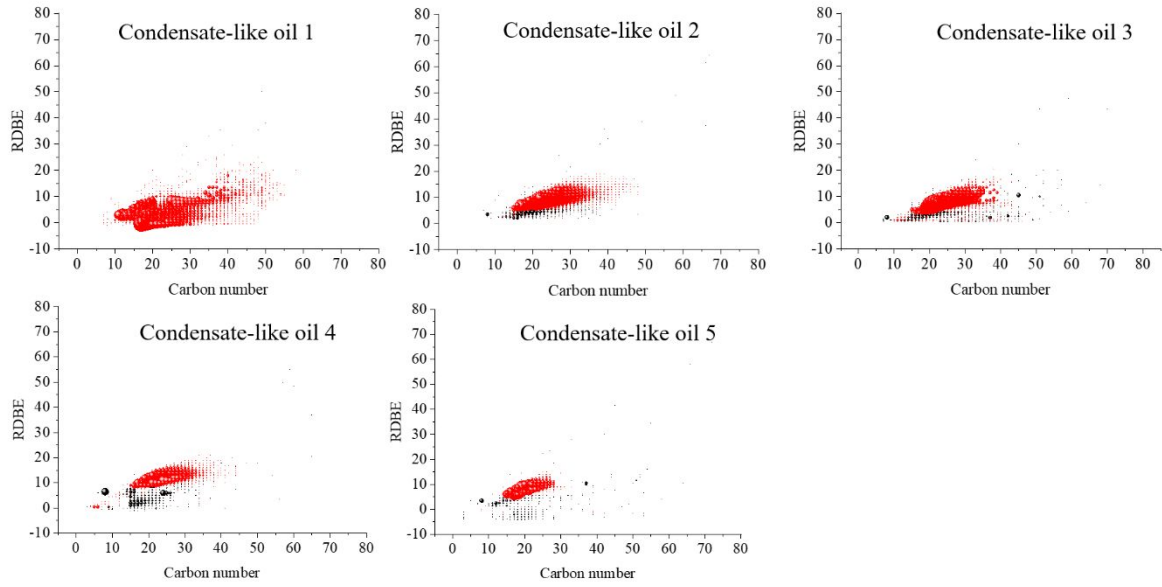
Table S12 continued

Chemical Classes	Average RDBE values									
	3 (41.62 °API)					2 (41.61 °API)				
	Trial 1	Trial 2	SD	Average	95% Confidence interval	Trial 1	Trial 2	SD	Average	95% Confidence interval
Volatile Hydrocarbons	2.5	2.5	0.1	2.5	2.4-2.6	2.6	2.1	0.3	2.4	2.0-2.8
Heteroaromatic Compounds	9.0	9.2	0.1	9.1	9.0-9.2	10.0	9.7	0.2	9.9	9.6-10.2
Polar Compounds	3.3	3.3	0.0	3.3	-	4.0	3.7	0.2	3.9	3.6-4.2
Heavy Saturated Hydrocarbons	2.8	2.8	0.0	2.8	-	1.6	1.6	0.0	1.6	-
Alkyl Aromatic Hydrocarbons	5.0	5.3	0.2	5.2	4.9-5.5	5.5	5.8	0.2	5.6	5.3-5.9
Overall Average RDBE Values of the Condensate-like Oil	3.1	3.2	0.0	3.1	-	2.1	2.1	0.0	2.1	-

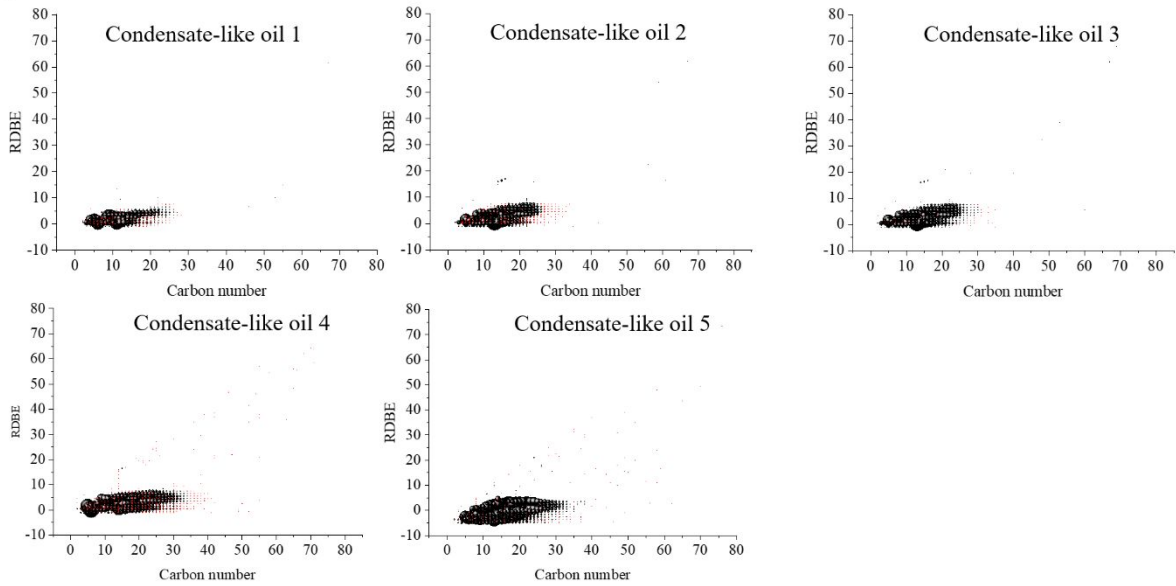
Table S12 continued

Chemical Classes	Average RDBE values				
	1 (37.50 °API)				
	Trial 1	Trial 2	SD	Average	95% Confidence interval
Volatile Hydrocarbons	3.3	2.5	0.6	2.9	2.1-3.7
Heteroaromatic Compounds	6.6	6.8	0.1	6.7	6.6-6.8
Polar Compounds	2.3	2.2	0.1	2.2	2.1-2.3
Heavy Saturated Hydrocarbons	2.8	2.8	0.0	2.8	-
Alkyl Aromatic Hydrocarbons	4.6	4.6	0.1	4.6	4.5-4.7
Overall Average RDBE Values of the Condensate-like Oil	3.3	3.3	0.0	3.3	-

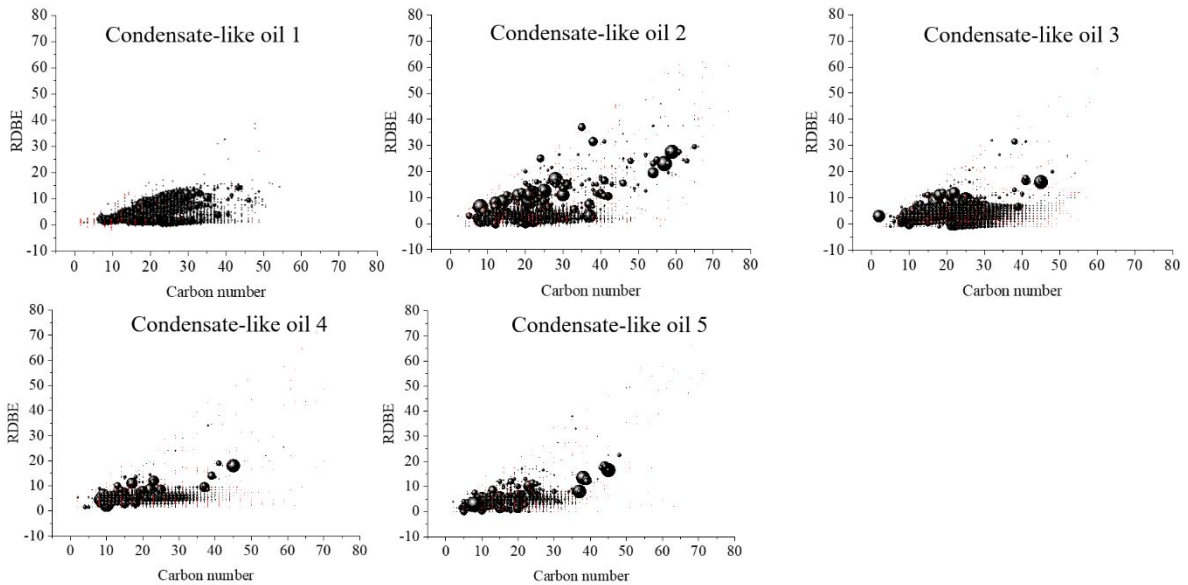
A



B



C



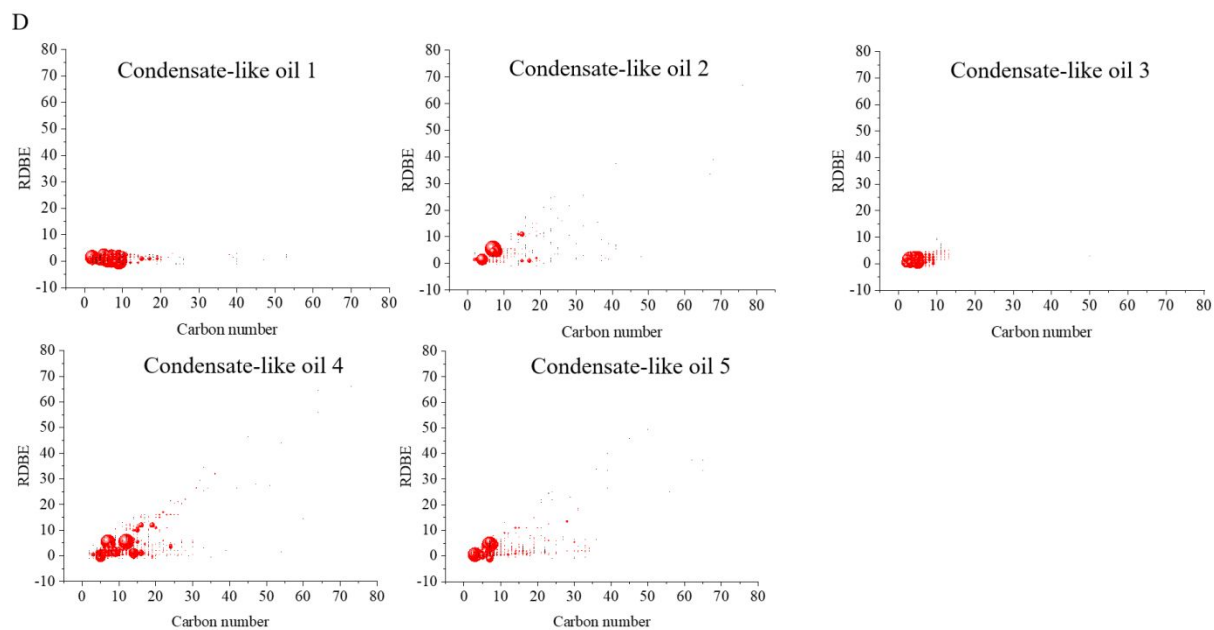


Figure S47. Color-mapped bubble plots of ring and double bond equivalent values (RDBE) versus carbon number for ionized compounds derived from the four nonvolatile condensate-like oil fractions that were separated and characterized by using the DPF-MS method. A) Heteroaromatic compound fraction. B) Saturated and cyclic hydrocarbon fraction. C) Alkyl aromatic hydrocarbon fraction. D) Polar compound fraction. Bubble size indicates the relative abundance of the ions. The black bubbles represent ions containing only C and H. Red bubbles represent ions containing heteroatoms (N, O and/or S) along with C and H.

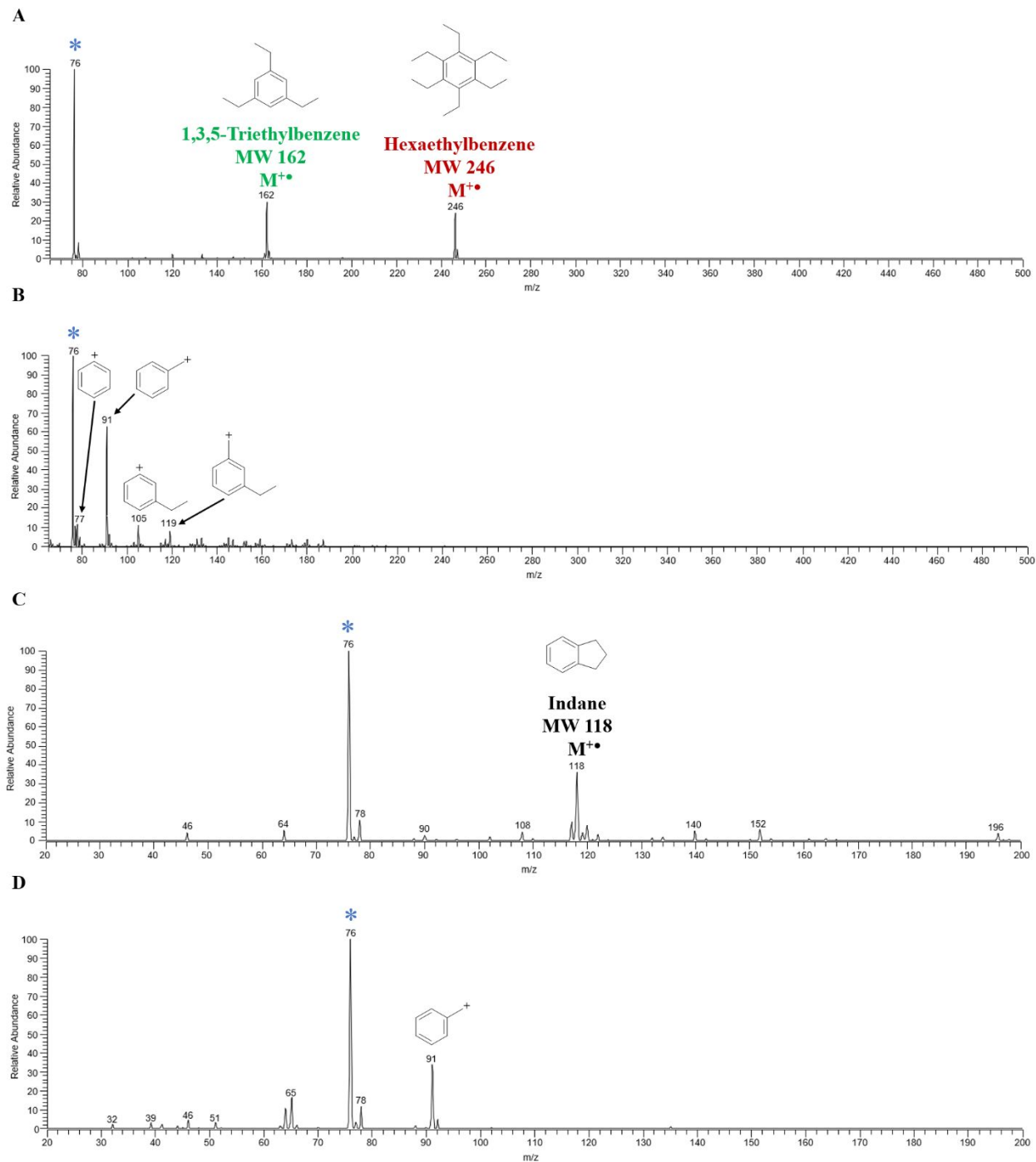


Figure S48. A) (+) APCI/N₂/CS₂ low resolution mass spectrum of an equimolar (1 mM) mixture of two alkylaromatic hydrocarbon model compounds. B) ISCAD mass spectrum of the mixture of the two ionized alkylaromatic model compounds, illustrating the ability to use ISCAD to cleave off most of the alkyl substituents on the aromatic cores. C) (+) APCI/N₂/CS₂ low resolution mass spectrum of 1 mM solution of indane. D) ISCAD mass spectrum of the ions shown in part C, including indane molecular ions. Peaks at *m/z* 76 designated with a blue asterisk (*) are due to the molecular ion of CS₂.

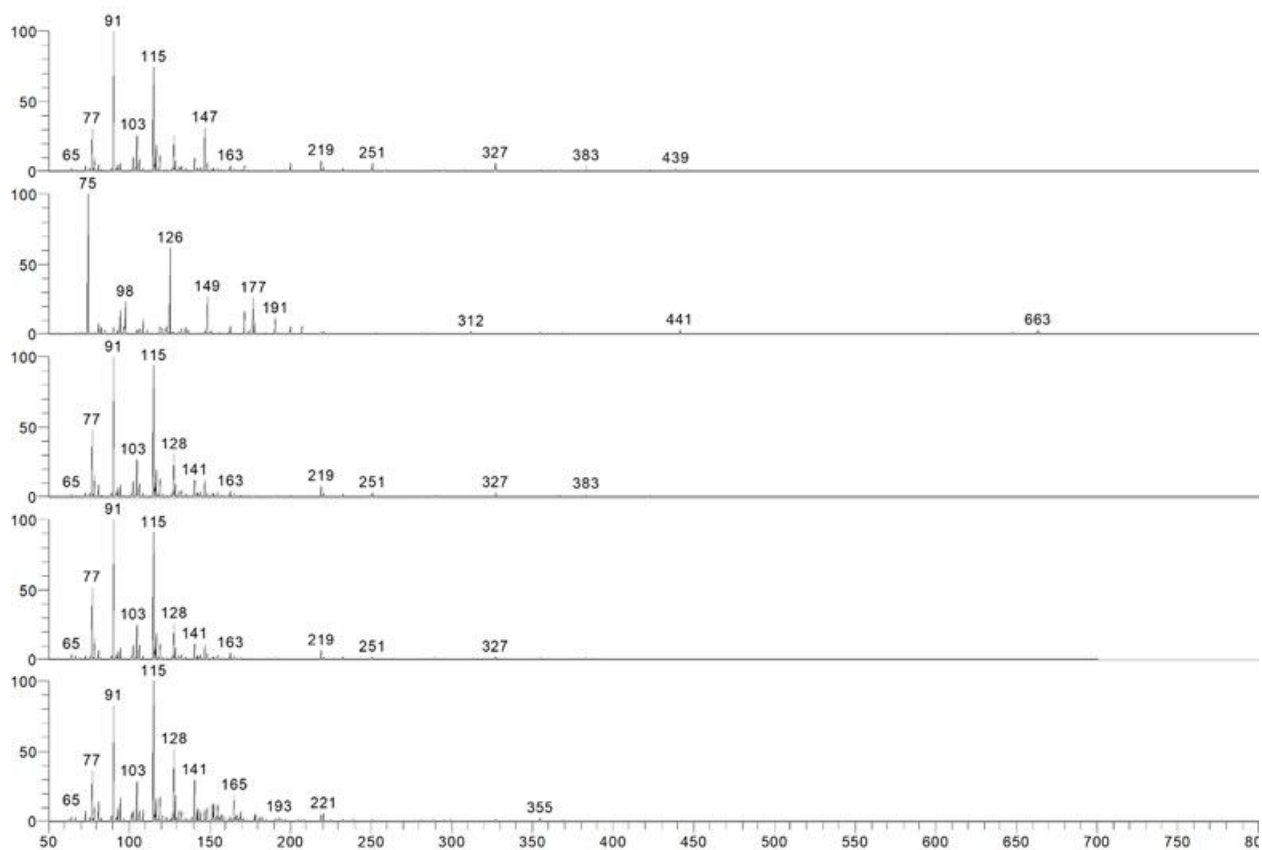


Figure 3S49. (+) APCI/CS₂ mass spectra after ISCAD for the ionized compounds in the alkyl aromatic hydrocarbon classes of the five condensate-like oils from top to bottom in this order: 4, 5, 3, 2, and 1.

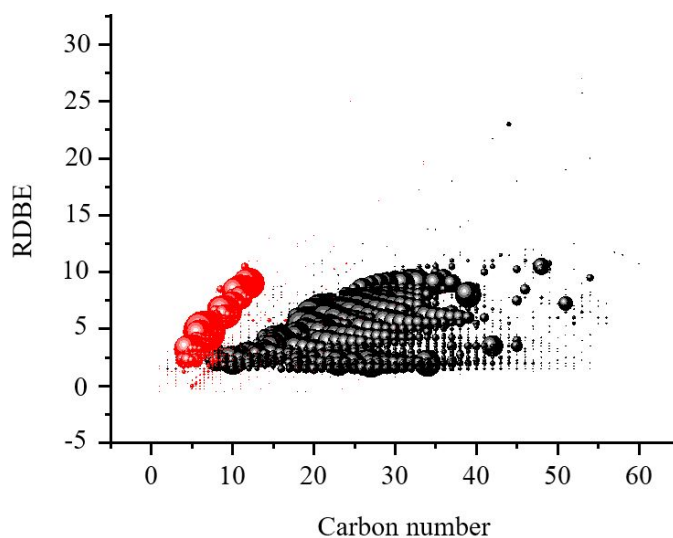


Figure S504. Ring and double bond equivalent (RDBE) versus carbon number plot for APCI mass spectrum (black) and ISCAD spectrum (red) of the alkyl aromatic hydrocarbon fraction of condensate-like oil 1.

Table S13. The MW of the aromatic cores and the total number of carbons in the alkyl side chains of the alkyl aromatic hydrocarbons with averages and standard deviations from two experiments for the five condensate-like oils. API gravities are shown in parenthesis

	The average MW of the aromatic cores and the average total number of carbons in the alkyl side chains of the alkyl aromatic hydrocarbons									
	5 (43.00 °API)					4 (42.40 °API)				
	Trial 1	Trial 2	SD	Average	95% Confidence interval	Trial 1	Trial 2	SD	Average	95% Confidence interval
MW of the Aromatic Cores (Da)	125.9	125.8	0.1	125.8	125.7-125.9	127.1	127.6	0.4	127.4	126.8-128.0
Total Number of Carbons in the Alkyl Side Chains	22.2	21.4	0.6	21.8	21.0-22.6	19.7	19.5	0.1	19.6	19.5-19.7

Table S13 continued

	The average MW of the aromatic cores and the average total number of carbons in the alkyl side chains of the alkyl aromatic hydrocarbons									
	3 (41.62 °API)					2 (41.61 °API)				
	Trial 1	Trial 2	SD	Average	95% Confidence interval	Trial 1	Trial 2	SD	Average	95% Confidence interval
MW of the Aromatic Cores (Da)	126.1	126.2	0.0	126.2	-	112.6	113.2	0.4	112.9	112.3-113.5
Total Number of Carbons in the Alkyl Side Chains	19.1	17.9	0.8	18.5	17.4-19.6	20.6	20.3	0.3	20.4	20.0-20.8

Table S13 continued

	The average MW of the aromatic cores and the average total number of carbons in the alkyl side chains of the alkyl aromatic hydrocarbons					
	1 (37.50 °API)					
	Trial 1	Trial 2	SD	Average	95% Confidence interval	
MW of the Aromatic Cores (Da)	123.8	124.4	0.4	124.1	123.5-124.7	
Total Number of Carbons in the Alkyl Side Chains	13.9	14.1	0.1	14.0	13.9-14.1	

Table S14. Data obtained for compounds in the distillate fraction of condensate-like oil 2 by using GCxGC/(+EI) TOF MS. Data provided are based on ChromaTOF software prediction of the molecular ion *m/z* value and the identification of the compound by using the EI mass spectral library match using a match factor threshold of 800. Formulas with a question mark “?” might not have been accurately identified. The ratio of the peak area of each of these questionable compounds relative to all peak areas of the detected compounds is provided in the table below.

Name	Formula	Retention Times (s) on the Primary and Secondary Columns	Molecular Ion <i>m/z</i>	Chromatographic Peak Area	Ratio (Peak area/sum of all peak areas)
3-Methylheptane	C ₈ H ₁₈	406.002, 2.412	114.1403	403434	
4-Methylpropiolactam	C ₄ H ₇ NO	418.005, 2.389	85.0522	9956	
3,3-Dipropylcyclobutanone	C ₁₀ H ₁₈ O ?	424.007, 2.314	154.1352	121454	
4-Octen-3-one	C ₈ H ₁₄ O	430.009, 2.389	126.1039	14514	
Octane	C ₈ H ₁₈	442.012, 2.607	114.1403	1293932	
cis-1,3-Dimethylcyclohexane	C ₈ H ₁₆	454.016, 2.391	112.1247	4353762	

2,2,3,3-Tetramethylcyclobutane	C ₈ H ₁₄ O	454.016, 2.616	126.1039	27788	
2,2,4-Trimethylhexane	C ₉ H ₂₀	460.017, 2.798	128.156	435562	
2,4-Dimethylheptane	C ₉ H ₂₀	466.019, 2.823	128.156	176761	
1,1-Dimethylcyclohexane	C ₈ H ₁₆	478.022, 2.427	112.1247	705398	
2,6-Dimethylheptane	C ₉ H ₂₀	478.022, 2.885	128.156	574057	
2-Octyl ethynyl ether	C ₁₀ H ₁₈ O	484.024, 2.520	154.1352	76398	
1,2-Dimethylcyclohexane	C ₈ H ₁₆	496.028, 2.510	112.1247	1051584	
3,5-Dimethylheptane	C ₉ H ₂₀	496.028, 2.931	128.156	2397681	
1,4-Dimethylcyclohexane	C ₈ H ₁₆	514.033, 2.546	112.1247	1076015	
1,3,5-Triamine pentane	C ₅ H ₁₅ N ₃	526.036, 2.844	117.126	3200	
3-Ethyl-2,4-dimethylpentane	C ₉ H ₂₀	526.036, 3.007	128.156	52768	
1,3,5-Trimethyl-, (1à,3à,5à)cyclohexane	C ₉ H ₁₈	538.04, 2.782	126.1403	750720	
Tuberolactone	C ₁₀ H ₁₄ O ₂	538.04, 2.903	166.0988	8658	
1,1,3-Trimethylcyclohexane	C ₉ H ₁₈	556.045, 2.829	126.1403	1489200	
2,3,3,6,6,7-Hexamethyl-1,4,7-octatriene	C ₁₄ H ₂₄	556.045, 2.875	192.1873	38408	
1-Bicyclo[2.2.2]octanol	C ₈ H ₁₄ O ?	574.05, 2.925	126.1039	7147	6.40E-5
3-Methyloctane	C ₉ H ₂₀	580.052, 3.209	128.156	3164154	
Ethylcyclohexane	C ₈ H ₁₆	586.053, 2.700	112.1247	1128224	
1,2,4-Trimethyl-cyclohexane	C ₉ H ₁₈	592.055, 2.921	126.1403	1193093	
2,2,5-trimethylhexane	C ₉ H ₂₀	592.055, 3.403	128.156	20793	
Toluene	C ₇ H ₈	598.057, 2.067	92.0621	209836	
2-Oxepanone	C ₆ H ₁₀ O ₂	616.062, 3.007	114.0675	9329	
(Z)-3-(Hydroxymethyl)-7-methylocta-2,6-dien-1-yl acetate	C ₁₂ H ₂₀ O ₃ ?	616.062, 3.025	212.1407	9522	8.60E-5
3,3-Dimethylheptane	C ₉ H ₂₀	628.065, 3.517	128.156	73612	
O-(tert-Butoxycarbonyl)-N-isopropylidene oxime	C ₈ H ₁₅ NO ₃	646.071, 3.447	173.1046	13770	
1,1,3,5-Tetramethylcyclohexane	C ₁₀ H ₂₀	652.072, 3.222	140.156	197139	
Nonane	C ₉ H ₂₀	658.074, 3.405	128.156	2970311	
1,2,3-Trimethyl-, (1à,2à,3à)-cyclohexane	C ₉ H ₁₈	670.078, 3.055	126.1403	469884	
Methylcycloheptane	C ₈ H ₁₆	676.079, 2.781	112.1247	8641	

2,4-Dimethylhexane	C ₈ H ₁₈	676.079, 3.667	114.1403	912814
3,5-Dimethyloctane	C ₁₀ H ₂₂	700.086, 3.718	142.1716	1901320
1-Ethyl-4-methylcyclohexane	C ₉ H ₁₈	706.088, 3.101	126.1403	2103969
1,1,3,5-Tetramethylcyclohexane	C ₁₀ H ₂₀	718.091, 3.338	140.156	273592
2,6-Dimethyloctane	C ₁₀ H ₂₂	730.095, 3.770	142.1716	1638518
(E)-1,3-Hexadiene	C ₆ H ₁₀	748.1, 2.760	82.0777	86271
3-Methylnonane	C ₁₀ H ₂₂	760.103, 3.785	142.1716	825709
1-Ethyl-2-methylcyclohexane	C ₉ H ₁₈	778.109, 3.178	126.1403	941838
Heptanal	C ₇ H ₁₄ O	790.112, 3.792	114.1039	109601
3,3,6-Trimethyl-1,2-dioxane	C ₇ H ₁₃ O ₂	802.115, 3.608	129.091	8287
1-Ethyl-1-methylcyclohexane	C ₉ H ₁₈	808.117, 3.153	126.1403	193199
5-Methylundecane	C ₁₂ H ₂₆	814.119, 3.862	170.2029	1393101
(1-Methylethyl)cyclohexane	C ₉ H ₁₈	832.124, 3.204	126.1403	168744
4-Methylnonane	C ₁₀ H ₂₂	832.124, 3.929	142.1716	2992154
3-Nonyne	C ₉ H ₁₆	838.126, 2.978	124.1247	147187
1-Ethyl-2,4-dimethylcyclohexane	C ₁₀ H ₂₀	838.126, 3.502	140.156	555003
(R)-3-(Tert-butylsulfinyl)butanoic acid	C ₈ H ₁₆ O ₃ S	838.126, 4.209	192.0815	129278
Decane	C ₁₀ H ₂₂	844.127, 4.173	142.1716	79269
3-Methyldodecane	C ₁₃ H ₂₈	850.129, 4.225	184.2186	57459
Propylcyclohexane	C ₉ H ₁₈	856.131, 3.292	126.1403	759545
Octahydro-cis-1H-indene	C ₉ H ₁₆	874.136, 3.106	124.1247	144668
1-Ethyl-4-methyl-trans-cyclohexane	C ₉ H ₁₈	874.136, 3.225	126.1403	100699
1-Ethyl-2-propylcyclohexane	C ₁₁ H ₂₂	874.136, 3.533	154.1716	203834
1-Methyl-2-methylene-3-(1-methylethyl)-cis-cyclopentane	C ₁₀ H ₁₈	880.138, 3.375	138.1403	96215
Ethylbenzene	C ₈ H ₁₀	886.14, 2.378	106.0777	68545
Cyclobutylidenacetaldehyde	C ₆ H ₈ O	898.143, 3.383	96.057	32889
1-Ethyl-1,3-dimethyl-trans-cyclohexane	C ₁₀ H ₂₀	898.143, 3.516	140.156	168787
1,3-Dimethylbenzene,	C ₈ H ₁₀	904.145, 2.417	106.0777	820707
4-Methylundecane	C ₁₂ H ₂₆	916.148, 4.251	170.2029	77287

3,3-Dimethyl-2-oxetanone	C ₅ H ₈ O ₂	946.157, 3.456	100.0519	10373	
Dimethyl ester-2-butynedioic acid	C ₆ H ₆ O ₄	946.157, 3.543	142.0261	27280	
Undecane	C ₁₁ H ₂₄	952.158, 4.297	156.1873	188480	
1-(2-Furanyl)-4-methyl-1-penten-3-ol	C ₁₀ H ₁₄ O ₂ ?	964.162, 3.579	166.0988	26015	2.34E-4
Ethyl 2-cyanohepta-4,5-dienoate	C ₉ H ₁₁ NO ₂ ?	970.164, 4.140	165.0784	14041	1.26E-4
1-Isopropyl-4-methylcyclohexane	C ₁₀ H ₂₀	982.167, 3.595	140.156	414672	
Dodecane	C ₁₂ H ₂₆	988.169, 4.341	170.2029	650880	
1-Butyl-2-methylenecyclopentane	C ₁₀ H ₁₈	994.171, 3.154	138.1403	29059	
1-Hexyne	C ₆ H ₁₀	1012.18, 3.472	82.0777	31352	
1-Ethylcyclohexene	C ₈ H ₁₄	1018.18, 3.456	110.109	106299	
1-Methyl-3-(1-methylethyl)-cyclohexane	C ₁₀ H ₂₀	1018.18, 3.672	140.156	506003	
2,6-Dimethylnonane	C ₁₁ H ₂₄	1024.18, 4.356	156.1873	1352944	
(E)-4-Hexen-1-ol	C ₆ H ₁₂ O	1048.19, 3.093	100.0883	10630	
Undec-3-en-5-yn-2-ol	C ₁₁ H ₁₈ O ?	1048.19, 3.335	166.1352	39074	3.52E-5
Pinane-10-diol	C ₁₀ H ₁₈ O ₂	1054.19, 3.911	170.1301	29783	
6-Ethyl-2-methyloctane	C ₁₁ H ₂₄	1054.19, 4.335	156.1873	645744	
2-Ethylcyclohexyl 2-thiopheneacetate	C ₁₄ H ₂₀ O ₂ S ?	1072.19, 3.646	252.1179	394899	3.55E-3
2,6,11-Trimethyldodecane	C ₁₅ H ₃₂	1078.19, 4.371	212.2499	613681	
1-Ethyl-4-methyl-cis-cyclohexane	C ₉ H ₁₈	1096.2, 3.636	126.1403	266918	
4-Phenylpent-1-ene	C ₁₁ H ₁₄	1102.2, 2.577	146.109	23369	
3,7-Dimethylnonane	C ₁₁ H ₂₄	1102.2, 4.356	156.1873	619490	
Methyl octadeca-13,14-dienoate	C ₁₉ H ₃₄ O ₂ ?	1114.2, 3.481	294.2553	16052	1.44E-4
3-Ethoxy-1-propyne	C ₅ H ₈ O	1126.21, 3.925	84.057	53546	
1-(Dodecycloxy)-4-methoxybutan-2-one	C ₁₇ H ₃₄ O ₃ ?	1126.21, 4.314	286.2502	20112	1.81E-4
1-Cyclooctyl-1-propanone	C ₁₁ H ₂₀ O	1132.21, 3.949	168.1509	184729	
2-Methylundecane	C ₁₂ H ₂₆	1132.21, 4.712	170.2029	44258	
Pentadecane	C ₁₅ H ₃₂	1150.22, 4.407	212.2499	506831	
(E)-Dec-5-en-2-ol	C ₁₀ H ₂₀ O ?	1168.22, 3.773	156.1509	19617	1.76E-4
5-Methyldecane	C ₁₁ H ₂₄	1174.22, 4.423	156.1873	1473756	

3,6-Dimethyl-2-benzo[b]furanone	C ₁₀ H ₁₆ O ₂	1180.22, 3.354	168.1145	21300	
Dibutyl ethanedioate	C ₁₀ H ₁₈ O ₄	1180.22, 4.728	202.12	33721	
5-Cyclohexylidene--1-penten-3-ol	C ₁₁ H ₁₈ O ?	1186.23, 3.810	166.1352	9778	8.80E-5
2-(Aminomethyl)-cis-cyclopropanecarboxylic acid	C ₅ H ₉ NO ₂	1186.23, 3.985	115.0628	18101	
4-Methyldecane	C ₁₁ H ₂₄	1186.23, 4.433	156.1873	451862	
4',4'-Dimethylspiro[1,3-dioxolane-2,3'-cholestan-7'-one]	C ₃₁ H ₅₂ O ₃ ?	1192.23, 4.504	472.3911	4604	4.14E-5
2-methyldecane	C ₁₁ H ₂₄	1198.23, 4.449	156.1873	1266319	
Azetidine	C ₃ H ₇ N	1210.23, 3.866	57.0573	19609	
N-Benzyl-N-[(3E)-3,5-hexadien-1-yl]amine	C ₁₃ H ₁₉ N	1216.23, 2.657	189.1512	30286	
3-Phenoxytetracyclo[3.2.0.0.2,7.0 4,6]heptane	C ₁₃ H ₁₂ O	1222.24, 2.641	184.0883	16637	
(1-Methylpropyl)cyclohexane	C ₁₀ H ₂₀	1222.24, 3.634	140.156	73715	
5-Butylnonane	C ₁₃ H ₂₈	1222.24, 4.392	184.2186	109565	
Butylcyclohexane	C ₁₀ H ₂₀	1234.24, 3.693	140.156	726115	
3-Methyldecane	C ₁₁ H ₂₄	1234.24, 4.423	156.1873	1009186	
2,6-Dimethyl-1-octanol	C ₁₀ H ₂₂ O ?	1258.25, 3.972	158.1665	108369	9.75E-4
1-Ethyl-2-methylbenzene	C ₉ H ₁₂	1264.25, 2.638	120.0934	331698	
1-Methylpropylcyclooctane	C ₁₂ H ₂₄	1276.25, 3.965	168.1873	397961	
Mesitylene	C ₉ H ₁₂	1288.25, 2.659	120.0934	1026177	
1-Methyl-1-nitrocyclohexane	C ₇ H ₁₃ NO ₂	1300.26, 3.970	143.0941	25607	
1,17-Octadecadiene	C ₁₈ H ₃₄	1312.26, 4.299	250.2655	48794	
2,6,10-Trimethyltridecane	C ₁₆ H ₃₄	1312.26, 4.703	226.2655	86134	
4,6-Dimethyldecane-1-ol	C ₁₂ H ₂₆ O ?	1318.26, 3.944	186.1978	179400	1.61E-3
Tricosane	C ₂₃ H ₄₈	1330.27, 4.667	324.3751	152005	
Octadecane	C ₁₈ H ₃₈	1342.27, 4.687	254.2968	249831	
1-Ethyl-4-methylbenzene	C ₉ H ₁₂	1372.28, 2.608	120.0934	60924	
1-Methyl-3-propyl cyclohexane	C ₁₀ H ₂₀	1384.28, 3.907	140.156	185975	
Tridecane	C ₁₃ H ₂₈	1390.28, 4.706	184.2186	1411236	
2-Methylpropyl)benzene	C ₁₀ H ₁₄	1402.29, 2.836	134.109	23964	

m-Menthane	C ₁₀ H ₂₀	1414.29, 4.011	140.156	333766	
Tetradecane	C ₁₄ H ₃₀	1420.29, 4.680	198.2342	425685	
O-(1-Phenylethyl)acetaldoxime	C ₁₀ H ₁₃ NO ?	1432.3, 2.806	163.0992	24251	2.18E-4
3,7-Dimethyldecane	C ₁₂ H ₂₆	1444.3, 4.649	170.2029	522190	
Decahydronaphthalene	C ₁₀ H ₁₈	1468.31, 3.343	138.1403	254209	
Heptadecane	C ₁₇ H ₃₆	1468.31, 4.685	240.2812	382716	
Methyl(1-methylethyl) benzene	C ₁₀ H ₁₄	1492.31, 2.777	134.109	105588	
N-(But-2-enoyl)prop-2-enamide	C ₇ H ₁₁ NO	1498.32, 4.205	125.0835	31150	
4-Methyloctane	C ₉ H ₂₀	1498.32, 4.588	128.156	76087	
1-Isopropyl-1-methylcyclohexane	C ₁₀ H ₂₀	1516.32, 3.911	140.156	64801	
2-(1-Phenylethyl)phenol	C ₁₄ H ₁₄ O ?	1534.33, 4.942	198.1039	24740	2.22E-4
Diocetyl disulfide	C ₁₆ H ₃₄ S ₂	1540.33, 4.889	290.2096	13230	
4-Ethyldecane	C ₁₂ H ₂₆	1546.33, 4.639	170.2029	210017	
2-Butoxyethanol	C ₆ H ₁₄ O ₂	1552.33, 4.936	118.0988	75003	
6-Methylundecane	C ₁₂ H ₂₆	1564.33, 4.634	170.2029	861108	
1,1,3-Trimethyl-3-(2-methyl-2-propenyl)cyclopentane	C ₁₂ H ₂₂	1570.34, 4.222	166.1716	188177	
4-Ethyloctane	C ₁₀ H ₂₂	1570.34, 4.618	142.1716	928014	
1,2,3-Trimethylbenzene	C ₉ H ₁₂	1588.34, 2.613	120.0934	130610	
2,2-Dimethylpropane	C ₅ H ₁₂	1606.35, 4.953	72.0934	186871	
Diphenylhexane	C ₁₈ H ₂₀	1642.36, 2.799	236.156	16949	
3-Methylundecane	C ₁₂ H ₂₆	1642.36, 4.587	170.2029	1041652	
1-Hydroxymethyl-1,3-dimethyl cyclopentane	C ₈ H ₁₆ O	1660.36, 4.200	128.1196	132418	
2-Ethyl-1,4-dimethylbenzene	C ₁₀ H ₁₄	1672.37, 2.757	134.109	416535	
sec-Butylcyclooctane	C ₁₂ H ₂₄	1684.37, 4.091	168.1873	44417	
N-(1-Adamantyl)oxy-N,N-dibutylamine	C ₁₈ H ₃₃ NO ?	1714.38, 3.300	279.2557	35520	3.19E-4
1-Methyldecahydronaphthalene	C ₁₁ H ₂₀	1756.39, 3.483	152.156	104574	
1-(1-Cyclopentenyl)-1-hydroxy-5,5-dimethyl-6-hepten-3-one	C ₁₄ H ₂₂ O ₂ ?	1768.39, 4.359	222.1614	27139	2.44E-4
Dibutyl sulfite	C ₈ H ₁₈ O ₃ S	1780.4, 4.788	194.0971	251745	
2,4-Dimethyl-1,3-hexanediol	C ₈ H ₁₈ O ₂ ?	1786.4, 4.021	146.1301	34424	3.09E-4

2,6-Dimethylundecane	C ₁₃ H ₂₈	1786.4, 4.793	184.2186	3261178	
1-Butyl-2-hexylcyclopropane	C ₁₃ H ₂₆	1798.4, 3.999	182.2029	16049	
(2"E)-2'-Methyl-2'-(1",4"-trimethylpent-2"-enyloxy)propyl cyclopropanecarboxylate	C ₁₆ H ₂₈ O ₃ ?	1804.4, 4.405	268.2033	46401	4.17E-4
2,3,3-Trimethyl-(Z)- 4-nonene	C ₁₂ H ₂₄	1810.4, 4.142	168.1873	147898	
Tetraethylbutanedinitrile	C ₁₂ H ₂₀ N ₂	1834.41, 4.163	192.1621	14224	
1-Methyl-2-pentylcyclohexane	C ₁₂ H ₂₄	1840.41, 4.109	168.1873	224220	
Heptacosane	C ₂₇ H ₅₆	1846.42, 5.020	380.4377	31661	
1,1'-(1,2-Dimethyl-1,2-ethanediyl)bis-cyclohexane	C ₁₆ H ₃₀	1852.42, 4.063	222.2342	214903	
Ethyl 5,7,9-trimethyltridec-3-enethioate	C ₁₈ H ₃₄ OS ?	1864.42, 4.359	298.2325	66209	5.95E-4
2,3-Dimethylundecane	C ₁₃ H ₂₈	1864.42, 4.716	184.2186	294724	
1-(2,4-Dimethylphenyl)-4-methyl-1-pentanone	C ₁₄ H ₂₀ O ?	1882.43, 2.863	204.1509	8096	7.28-5
1-Methyl-2-(tricyclo[4.1.0.0(2,7)]hept-1-yl)benzene	C ₁₄ H ₁₆	1882.43, 2.918	184.1247	17101	
2,9-Dimethyldecane	C ₁₂ H ₂₆	1882.43, 4.735	170.2029	136149	
3,4-Dimethylcumene	C ₁₁ H ₁₆	1888.43, 2.854	148.1247	63166	
2-Cyclohexyldecane	C ₁₆ H ₃₂	1900.43, 4.025	224.2499	110054	
4-Methyldodecane	C ₁₃ H ₂₈	1900.43, 4.659	184.2186	90938	
S-Butyl cyclohexanecarbothioate	C ₁₁ H ₂₀ OS	1912.43, 4.261	200.1229	25938	
1,2-Diethyl-cis-cyclohexane	C ₁₀ H ₂₀	1930.44, 4.312	140.156	62526	
Hexadecane	C ₁₆ H ₃₄	1936.44, 4.958	226.2655	387334	
(2-Methylpropyl)cyclohexane	C ₁₀ H ₂₀	1942.44, 3.975	140.156	149251	
3,3-Dimethylcyclohex-1-en-1-ylbut-2-enoate	C ₁₂ H ₁₈ O ₂ ?	1942.44, 4.217	194.1301	26303	2.36E-4
2-Methylcyclopentylacetophenone	C ₁₄ H ₁₈ O	1948.44, 2.681	202.1352	20636	
4-Ethylundecane	C ₁₃ H ₂₈	1954.45, 4.659	184.2186	204820	
1,2,3,4-Tetramethylbenzene	C ₁₀ H ₁₄	1960.45, 2.751	134.109	139505	
3-Cyclohexyl-(2S-trans)-oxiranemethanol	C ₉ H ₁₆ O ₂	1960.45, 3.662	156.1145	12543	
2,6,10,14-Tetramethylhexadecane,	C ₂₀ H ₄₂	1960.45, 4.932	282.3281	47954	
4-Methylchroman	C ₁₀ H ₁₂ O	1966.45, 2.852	148.0883	13187	
4-Propyl-2,8-dioxabicyclo[3.3.0]octan-3-one	C ₉ H ₁₄ O ₃	1972.45, 4.245	170.0937	22513	

6-Methyldodecane	C ₁₃ H ₂₈	1972.45, 4.649	184.2186	1643386	
Hexadecanoic acid	C ₁₆ H ₃₂ O ₂ ?	1972.45, 4.926	256.2397	67741	6.09
3-Ethyl-6-ethylidene-3-methyl-1,4-cyclohexadiene	C ₁₁ H ₁₆	1984.45, 2.874	148.1247	23147	
1-Ethyl-3,5-dimethyl- benzene	C ₁₀ H ₁₄	1996.46, 2.721	134.109	224148	
1-(2-Ethylphenyl)ethan-1-one	C ₁₀ H ₁₂ O	1996.46, 2.835	148.0883	18451	
2,3,7-Trimethyloctane	C ₁₁ H ₂₄	2002.46, 4.947	156.1873	1696737	
2-Methyldodecane	C ₁₃ H ₂₈	2014.46, 4.663	184.2186	909384	
2-Methylazetidide	C ₄ H ₉ N	2014.46, 4.932	71.073	54396	
1-Methyl-4-(1-methylpropyl)benzene	C ₁₁ H ₁₆	2020.47, 2.865	148.1247	214683	
Pentylidenecyclohexane	C ₁₁ H ₂₀	2026.47, 3.340	152.156	23411	
1-Ethyl-4-(1-methylethyl)benzene	C ₁₁ H ₁₆	2038.47, 2.816	148.1247	63926	
Neopentyl 2-oxobutanoate	C ₉ H ₁₆ O ₃	2038.47, 4.572	172.1094	108730	
2-Methylpyrrolizidine	C ₈ H ₁₃ N	2050.47, 4.188	125.1199	25877	
Germacrene	C ₁₅ H ₃₀	2056.48, 4.248	210.2342	233261	
1-Methyladamantane	C ₁₁ H ₁₈	2074.48, 3.109	150.1403	18584	
Hexylcyclohexane	C ₁₂ H ₂₄	2086.48, 3.924	168.1873	771719	
2-Methyl-4-hexyn-3-ol	C ₇ H ₁₂ O	2086.48, 4.180	112.0883	107032	
Tetrahydromethyl-2-furanpropanoic acid	C ₈ H ₁₄ O ₃ ?	2104.49, 4.781	158.0937	32452	2.92E-4
10-Acetoxydecanal	C ₁₂ H ₂₂ O ₃ ?	2110.49, 4.202	214.1563	223112	2.00E-3
Bis(2-cyclohexyl-1-methylethyl 1,2-dioxidediazene	C ₁₈ H ₃₄ N ₂ O ₂ ?	2122.49, 4.469	310.2615	55201	4.96E-4
(1,1-Dimethylpropyl)benzene	C ₁₁ H ₁₆	2128.5, 2.849	148.1247	73575	
2-(3,5-Dimethyl-1-adamantyl)-1,2-dicyanoethane	C ₁₆ H ₂₂ N ₂	2128.5, 3.563	242.1778	12520	
1'-Cyclobutan]-2'-one, 1,4,4-trimethylspiro[bicyclo[3.2.0]hept-6-ene-2	C ₁₃ H ₁₈ O	2134.5, 2.847	190.1352	23570	
3-Methyl-, [R-(E)]-4-hexenal	C ₇ H ₁₂ O	2134.5, 4.115	112.0883	84744	
<i>trans</i> -1-Methyl-2-nonyl-cyclohexane	C ₁₆ H ₃₂	2152.5, 4.092	224.2499	77812	
<i>cis,trans</i> -2-Ethylbicyclo[4.4.0]decane	C ₁₂ H ₂₂	2158.5, 3.569	166.1716	145306	
1-Methyl-2-(2'-methylprop-2'-enyl)cyclododecan-1-ol	C ₁₇ H ₃₂ O?	2164.51, 4.390	252.2448	20329	1.82E-4
1,4-Dimethyl-2-(2-methylpropyl)benzene	C ₁₂ H ₁₈	2170.51, 2.978	162.1403	87696	
1-Ethyl-2,3-dimethylbenzene	C ₁₀ H ₁₄	2176.51, 2.664	134.109	37821	

2-(4'-Methylphenyl)-propanal	C ₁₀ H ₁₂ O	2182.51, 2.813	148.0883	112253	
Benzyl 4-methylphenyl ketone	C ₁₅ H ₁₄ O ?	2188.51, 2.963	210.1039	12242	1.10
2-Methyl-2-dicyanomethyladamantane	C ₁₄ H ₁₈ N ₂	2194.51, 3.277	214.1465	31277	
3,4-Trimethylbenzeneacetaldehyde	C ₁₁ H ₁₄ O	2200.52, 2.932	162.1039	58723	
(Z)-6-Undecen-3-ol	C ₁₁ H ₂₂ O	2200.52, 3.494	170.1665	11941	
Ethyl N-cyano-N-pentylcarbamate	C ₉ H ₁₆ N ₂ O ₂ ?	2206.52, 4.051	184.1206	27111	2.43E-4
(2Z,4E)-5-(2'-Furyl)-3-methylpenta-2,4-dienal	C ₁₀ H ₁₀ O ₂	2212.52, 2.898	162.0675	11393	
1-Octadecanol	C ₁₈ H ₃₈ O ?	2218.52, 4.040	270.2917	22434	2.01E-4
1-Phenyl-(Z)-2-Butene	C ₁₀ H ₁₂	2230.53, 2.546	132.0934	17652	
1-(1-Methyl-1-phenylethyl)-4-phenyl-1,2,4-triazolidine-3,5-dione	C ₁₇ H ₁₇ N ₃ O ₂	2236.53, 2.986	295.1315	24655	
2-Nitrocyclotridecanone	C ₁₃ H ₂₃ NO ₃	2236.53, 4.164	241.1672	10269	
(E)-1,1,2,2-Tetramethyl-3-oxahepta-4,6-dienyl acrylate	C ₁₃ H ₂₀ O ₃	2236.53, 4.354	224.1407	26956	
3-Oxo-1,3-dihydro-1-isobenzofuranyl phenylacetate	C ₁₆ H ₁₂ O ₄	2242.53, 2.976	268.073	16185	
2,2,7-Trimethyl-6-octene-3-one	C ₁₁ H ₂₀ O	2254.53, 4.335	168.1509	59683	
3,3,4,4-Tetraethylhexane	C ₁₄ H ₃₀	2254.53, 4.704	198.2342	33497	
2,6-Nonanedione	C ₉ H ₁₆ O ₂	2254.53, 4.935	156.1145	19777	
4a-Methyl-5,6,7,8-tetrahydro-2(4aH)naphthalenone	C ₁₁ H ₁₄ O	2260.53, 2.982	162.1039	11813	
6,9-Dimethyltetradecane	C ₁₆ H ₃₄	2260.53, 4.663	226.2655	199591	
Decahydro-1,1,6-trimethyl Naphthalene	C ₁₃ H ₂₄	2266.54, 3.702	180.1873	18598	
(E)-5-Heptenenitrile	C ₇ H ₁₁ N	2272.54, 3.713	109.0886	11814	
1-(2',3'-Dihydro-1'-methyl-1H-inden-3'-yl)-3-hydroxy-3-methylbutan-1-one	C ₁₅ H ₂₀ O ₂ ?	2284.54, 2.715	232.1458	8436	7.59E-5
1,2-bis[p-Methylbenzoyloxy-(p-tolyl)]ethane	C ₃₂ H ₂₈ O ₄	2290.54, 2.769	476.1982	11987	1.07E-4
2,2-Dimethyl-4-(methylethyl)-2H-imidazole	C ₈ H ₁₄ N ₂	2296.54, 4.270	138.1151	30186	
p-Methylphenyl 2-(o-methylphenyl)-2-propyl sulfone	C ₁₇ H ₂₀ O ₂ S ?	2302.55, 2.927	288.1179	16842	1.51E-4
(5S,7S,9S,E)-S-Ethyl 5,7,9-trimethyltridec-3-enethioate	C ₁₈ H ₃₄ OS	2302.55, 4.275	298.2325	25611	
6-Methyl-1,2,3,4-tetrahydronaphthalene-1-methanol	C ₁₂ H ₁₆ O ?	2320.55, 2.810	176.1196	19259	1.73
3-(2-Propenyl)-5-hexen-2-one	C ₉ H ₁₄ O	2326.55, 4.378	138.1039	3408	
1,2,3,4-Tetrahydronaphthalene	C ₁₀ H ₁₂	2332.55, 2.472	132.0934	36077	

Methyl (E)-4,5-epoxyhex-2-enoate	C ₇ H ₁₀ O ₃	2332.55, 4.238	142.0624	18965	
(1RS,7RS)-1,4,7,10-Tetramethyl-2,8-dioxatricyclo[7.3.0.0(3,7)]dodeca-3,9-diene	C ₁₄ H ₂₀ O ₂	2338.56, 4.304	220.1458	21552	
(1,1-Dimethylbutyl)benzene	C ₁₂ H ₁₈	2344.56, 2.919	162.1403	42347	
3,3-Dimethylhexane	C ₈ H ₁₈	2350.56, 4.634	114.1403	133244	
(2E)-1-O-Acetyl-3,7-dimethyl-2-octen-1-ol 6,7-epoxide	C ₁₂ H ₂₀ O ₃ ?	2356.56, 4.597	212.1407	21636	1.94E-4
1-Methyl-3-(2-methylpropyl)cyclopentane	C ₁₀ H ₂₀	2362.56, 4.001	140.156	82724	
6-Methyltridecane	C ₁₄ H ₃₀	2368.56, 4.602	198.2342	1184032	
Methyl p-(isopropyl)benzyl sulfoxide	C ₁₁ H ₁₆ OS	2374.57, 2.870	196.0916	32948	
(E)-4-Methyl-6-(2',5',6',6'-tetramethylcyclohex-1'-enyl)hex-3-en-1-ol	C ₁₇ H ₃₀ O ?	2374.57, 3.687	250.2291	32560	2.93E-4
2,5,9-Trimethyldecane	C ₁₃ H ₂₈	2374.57, 4.860	184.2186	93286	
5-Methyltridecane	C ₁₄ H ₃₀	2380.57, 4.593	198.2342	493646	
3-Butenal	C ₄ H ₆ O	2380.57, 4.855	70.0413	18130	
2,2-Dimethylindan	C ₁₁ H ₁₄	2386.57, 2.637	146.109	20036	
2,6-Dimethyl-4-heptanone	C ₉ H ₁₈ O	2386.57, 4.830	142.1352	35844	
4-Methyltridecane	C ₁₄ H ₃₀	2398.57, 4.608	198.2342	497242	
3-Cyclohexyl-, 3-cyclohexyldecane	C ₁₆ H ₃₂	2410.58, 3.885	224.2499	17539	
1,2,4-Trimethyl-3-nitro-, (2-endo,3-exo,4-exo)-(+)-bicyclo[3.3.1]nonan-9-one	C ₁₂ H ₁₉ NO ₃ ?	2422.58, 3.671	225.1359	34141	3.07E-4
(-)-8-Phenylmenthyl 2-phenyl-3-ethenylcyclopropane-1-carboxylate	C ₂₈ H ₃₄ O ₂	2428.58, 3.039	402.2553	4370	
2,7,10-Trimethyldecane	C ₁₅ H ₃₂	2434.58, 4.809	212.2499	1737835	
2,6,10,14-Tetramethylheptadecane	C ₂₁ H ₄₄	2452.59, 4.567	296.3438	949943	
4-[1'-Phenylethenyloxymethyl]pyridine	C ₁₄ H ₁₃ NO ?	2482.6, 2.922	211.0992	6674	6.00E-5
3-Octyl-1,3-dihydro-1-isobenzofuranone	C ₁₆ H ₂₂ O ₂	2482.6, 3.027	246.1614	17182	
2-Hydroxy-2-mesityl-2-phenylacetaldehyde	C ₁₀ H ₁₁ O	2494.6, 2.973	147.0804	10756	
1,2,3,4-Tetrahydro-2-methylnaphthalene	C ₁₁ H ₁₄	2500.6, 2.588	146.109	32086	
1-Ethyl-4-(1-methylpropyl)benzene	C ₁₂ H ₁₈	2500.6, 2.900	162.1403	25151	
4-Butyl-2-methylpyrrole-3-carbonitrile	C ₁₀ H ₁₄ N ₂	2530.61, 2.904	162.1151	25813	
(1S)-4-(1,3-Dithian-2-yl)-3-methoxy-2-butanone	C ₉ H ₁₆ O ₂ S ₂	2542.61, 2.982	220.0586	9551	

1,1'-Bicyclohexyl	C ₁₂ H ₂₂	2548.62, 3.382	166.1716	30699	
1-Methylcyclohexyl 1-phenyl-2-propenyl ketone	C ₁₇ H ₂₂ O ?	2578.63, 4.100	242.1665	15246	1.37E-4
1-(N-Methoxycarbonyl-2-pyrrolidinyl)thymine	C ₁₁ H ₁₅ N ₃ O ₄ ?	2584.63, 2.272	253.1057	12216	1.09E-4
3-Acetylpropylbenzene	C ₁₁ H ₁₄ O ?	2596.63, 2.845	162.1039	44232	3.98E-4
4-Methyl-benzaldehyde	C ₈ H ₈ O	2614.64, 2.979	120.057	9310	
5-Ethyl-5-methyl-2-oxepanone	C ₉ H ₁₆ O ₂ ?	2614.64, 4.333	156.1145	38250	3.44E-4
Ethenyl cyclohexanoate	C ₉ H ₁₄ O ₂ ?	2644.64, 4.231	154.0988	42195	3.79E-4
2,6,8-Trimethyldecane	C ₁₃ H ₂₈	2644.64, 4.646	184.2186	214263	
Hexacosane	C ₂₆ H ₅₄	2662.65, 4.840	366.422	182684	
(cis)-1-Butyl-2-undecylcyclopropane	C ₁₈ H ₃₆	2668.65, 4.249	252.2812	63694	
2,6-Dimethylheptadecane	C ₁₉ H ₄₀	2680.65, 4.598	268.3125	326491	
Bis(cyclopentylmethyl) ether	C ₁₂ H ₂₂ O	2698.66, 4.086	182.1665	28595	
4-Phenyl-6-thioxo-6,7-dihydro-8H-pyrimido[1,6-a]pyrimidin-8-one	C ₁₃ H ₉ N ₃ OS ?	2704.66, 3.807	255.0461	12939	1.16E-4
2,3-Dihydro-1,4,7-trimethyl-1H-indene	C ₁₂ H ₁₆	2716.66, 2.727	160.1247	17481	
N-Phenyl-N'-[6-(4(5)-imidazolyl)hexyl]thiourea oxalate	C ₁₆ H ₂₂ N ₄ S ?	2722.67, 3.749	302.156	19103	1.71E-4
4-Hexyl-4-methyl-5-methylene-1,3-dioxolan-2-one	C ₁₁ H ₁₈ O ₃	2722.67, 4.220	198.125	17780	
2,3-Dihydro-6-methyl-1H-inden-5-ol	C ₁₀ H ₁₂ O	2728.67, 2.675	148.0883	10573	
(3,5-cis)-3-Pentyl-5-methyl-1,2-oxathiolane-(2,3-trans)-2-oxide	C ₉ H ₁₈ O ₂ S	2728.67, 4.289	190.1022	39723	
1,2,3,4-Tetrahydro-5-methylnaphthalene	C ₁₁ H ₁₄	2746.67, 2.530	146.109	79699	
5,5-Dimethylpentacyclo[5.4.2.0(4,11).0(6,8).0(7,11)]tridec-9-en-1-ol	C ₁₅ H ₂₀ O ?	2752.68, 2.931	216.1509	17872	1.60E-4
2,3-Dihydro-1,5,7-trimethyl-1H-indene	C ₁₂ H ₁₆	2764.68, 2.701	160.1247	44331	
2-Isobutyl-3-methylcyclopentan-1-one	C ₁₀ H ₁₈ O	2764.68, 3.984	154.1352	22919	
5-Methyl-tetradecane	C ₁₅ H ₃₂	2764.68, 4.536	212.2499	493618	
2,2',3',5'-Tetrahydro-2,3'-bifuran	C ₈ H ₁₀ O ₂	2776.68, 4.144	138.0675	29795	
4-Methyltetradecane	C ₁₅ H ₃₂	2782.68, 4.546	212.2499	458412	
Nonadecane	C ₁₉ H ₄₀	2788.69, 4.717	268.3125	139772	
2-Phenyl-3-(p-tolyl)butane	C ₁₇ H ₂₀	2794.69, 2.915	224.156	8821	

3-Methyltridecane	C ₁₄ H ₃₀	2800.69, 4.541	198.2342	886113	
3-Methyltetradecane	C ₁₅ H ₃₂	2836.7, 4.500	212.2499	803038	
Isopropoxy-3-methylbenzyl	C ₁₁ H ₁₆ O	2848.7, 2.944	164.1196	13067	
(E,Z)-7,9-Dodecadien-1-ol	C ₁₂ H ₂₂ O ?	2848.7, 3.617	182.1665	7397	6.65E-5
2,5-Dimethylpyrrole-3-carbonitrile	C ₇ H ₈ N ₂	2878.71, 2.909	120.0682	12613	
3,3,12,12-Tetramethyl-1,2-diaza-1,5,9-cyclododecatriene	C ₁₄ H ₂₄ N ₂	2878.71, 3.705	220.1934	5881	
2-Pent-1-enyltetrahydrofuran	C ₉ H ₁₆ O	2878.71, 4.153	140.1196	50301	
1,2,3,4-Tetrahydro-1,4-dimethylnaphthalene	C ₁₂ H ₁₆	2890.71, 2.656	160.1247	19558	
1-Phenyl-1-undecyn-5-ol	C ₁₇ H ₂₄ O ?	2890.71, 2.757	244.1822	10032	9.02E-5
(1R,2R)-1,2-Dihydroxy-3-cyclohexene	C ₆ H ₁₀ O ₂	2896.72, 4.110	114.0675	41245	
1,2,3,4-Tetrahydro-2,7-dimethylnaphthalene	C ₁₂ H ₁₆	2902.72, 2.639	160.1247	52774	
(2S, 2R)-2-Isobutyl-3-methylcyclopentan-1-one	C ₁₀ H ₁₈ O	2902.72, 4.158	154.1352	45784	
1,2,3,4-Tetrahydro-6-methylnaphthalene	C ₁₁ H ₁₄	2908.72, 2.458	146.109	35115	
Octylcyclohexane	C ₁₄ H ₂₈	2908.72, 3.893	196.2186	802198	
(1E)-1-Hexenylbenzene	C ₁₂ H ₁₆	2914.72, 2.650	160.1247	16909	
1-Ethyl-1,4-dimethyl-trans-cyclohexane	C ₁₀ H ₂₀	2926.73, 4.115	140.156	179387	
1,2,3,4-Tetrahydro-1,1-dimethylnaphthalene	C ₁₂ H ₁₆	2938.73, 2.605	160.1247	19119	
1,12-Octadecandiol	C ₁₈ H ₃₈ O ₂ ?	2938.73, 3.598	286.2866	31470	2.83E-4
(2R,3S)-cis-2,3-Epoxytridecan-1-ol	C ₁₃ H ₂₆ O ₂ ?	2938.73, 4.088	214.1927	29820	2.68E-4
(+)- <i>trans</i> -2-(2,5-Octadiynyl)-3-undecyloxirane	C ₂₁ H ₃₄ O	2950.73, 4.017	302.2604	76817	
3-Methyl-1-hexen-5-one	C ₇ H ₁₂ O	2974.74, 4.052	112.0883	34677	
2-(<i>trans</i> -2-Methyl-2-butenoxy)cycloheptene	C ₁₂ H ₂₀ O	2980.74, 4.056	180.1509	23752	
Octyl Allyl Ether	C ₁₁ H ₂₂ O	2980.74, 4.545	170.1665	32222	
3',3',5'-Trimethylcyclohexyl (cis)-(3-thienylglyoxyl)carboxylate	C ₁₅ H ₂₀ O ₃ S ?	2986.74, 4.002	280.1128	23912	2.15E-4
3-Ethyl-octane	C ₁₀ H ₂₂	2992.74, 4.599	142.1716	85567	
o-(4-Ethylbenzoyl)-o'-(3-methylbenzoyl)-1,3-benzenediol	C ₂₃ H ₂₀ O ₄ ?	3004.75, 2.868	360.1356	17787	1.60E-4
1-Methylnaphthalene	C ₁₁ H ₁₀	3022.75, 2.319	142.0777	63818	
1-Isocyanobutane	C ₅ H ₉ N	3028.75, 4.099	83.073	21097	

(R)-5-(1-Decenyl)-2-oxotetrahydrofuran	C ₁₄ H ₂₄ O ₂	3058.76, 4.009	224.1771	19883	
2-Isononenal	C ₉ H ₁₆ O	3058.76, 4.175	140.1196	17807	
(6R,12R)-6,12-Dimethylpentadec-1-ene	C ₁₇ H ₃₄	3070.77, 3.712	238.2655	12897	
(3R,4S,5R,7R)-3,5,7-Trimethyl-1-nonen-4-ol	C ₁₂ H ₂₄ O ?	3112.78, 4.169	184.1822	43711	3.93E-4
2,4-Dimethyl-3-pentanone	C ₇ H ₁₄ O	3124.78, 4.696	114.1039	76365	
1,1'-Bicyclooctyl	C ₁₆ H ₃₀	3136.79, 4.146	222.2342	48000	
4-Methylpentadecane	C ₁₆ H ₃₄	3148.79, 4.474	226.2655	405045	
1-Methyl-3-(phenylsulfonyl)pyrrolidine	C ₁₁ H ₁₅ NO ₂ S ?	3166.79, 3.904	225.0818	29920	2.69E-4
2-Methylnonadecane	C ₂₀ H ₄₂	3166.79, 4.464	282.3281	762289	
2,6-dimethyloctadecane	C ₂₀ H ₄₂	3202.8, 4.423	282.3281	679061	
4,5- <i>trans</i> -4-(2-Methylpropyl)-5-ethenyl-1,3-dioxolan-2-one	C ₉ H ₁₄ O ₃	3220.81, 4.165	170.0937	14474	
1,2-Dibutyl- <i>cis</i> -cyclopropane	C ₁₁ H ₂₂	3232.81, 4.115	154.1716	35746	
<i>trans</i> -1,2-Dibutyl-cyclopropane	C ₁₁ H ₂₂	3250.82, 4.094	154.1716	57260	
1,2,3,4-Tetrahydro-5,6-dimethylnaphthalene	C ₁₂ H ₁₆	3268.82, 2.526	160.1247	76855	
Heptyl propyl oxalate	C ₁₂ H ₂₂ O ₄ ?	3268.82, 4.549	230.1513	91456	8.23E-4
1-Cyclohexyl-3-methylbenzene	C ₁₃ H ₁₈	3286.83, 2.658	174.1403	24025	
n-Nonylcyclohexane	C ₁₅ H ₃₀	3286.83, 3.862	210.2342	711824	
2-Ethyl-2,4,5-trimethyl-2,5-dihydro-1H-imidazole	C ₈ H ₁₆ N ₂	3286.83, 4.068	140.1308	16133	
(Tetrahydro-2-furanyl)methyl butanoate	C ₉ H ₁₆ O ₃ ?	3322.84, 4.485	172.1094	146973	1.32E-3
3-Ethylcosane	C ₂₂ H ₄₆	3334.84, 4.692	310.3594	219953	
1,2-Epoxy-3-tetradecanol	C ₁₄ H ₂₈ O ₂	3370.85, 4.001	228.2084	198247	
1,7-Dimethylnaphthalene	C ₁₂ H ₁₂	3418.87, 2.386	156.0934	95308	
2-Cyclohexyloxirane	C ₈ H ₁₄ O	3418.87, 4.067	126.1039	1549	
2-Methyloct-3-enal	C ₉ H ₁₆ O	3418.87, 4.161	140.1196	13069	
2,6,10-Trimethylpentadecane	C ₁₈ H ₃₈	3418.87, 4.670	254.2968	2218430	
3-Acetoxy-1H-pyrrole	C ₆ H ₇ NO ₂	3436.87, 4.123	125.0471	40434	
[3-(Ethylthio)-1-methyl-1-butenyl]benzene	C ₁₃ H ₁₈ S	3442.87, 2.470	206.1124	5737	
2,7-Dimethylundecane	C ₁₃ H ₂₈	3478.88, 4.382	184.2186	426023	
2,5-Dimethylheptane	C ₉ H ₂₀	3490.89, 4.607	128.156	67846	

4-Methylhexadecane	C ₁₇ H ₃₆	3496.89, 4.418	240.2812	337368	
4-(2-Tetrahydropyranyl)oxybutanal	C ₉ H ₁₆ O ₃	3496.89, 4.807	172.1094	66789	
1,8-Dimethylnaphthalene	C ₁₂ H ₁₂	3502.89, 2.350	156.0934	35917	
Neopentyl 2,2-dimethylbutanoate	C ₁₁ H ₂₂ O ₂ ?	3502.89, 4.377	186.1614	47433	4.26E-4
2-Methyleicosane	C ₂₁ H ₄₄	3508.89, 4.428	296.3438	601850	
3,7-Dimethyl-1H-Indene-5-carboxaldehyde	C ₁₂ H ₁₂ O	3514.89, 2.488	172.0883	10762	
3-Butene-1,2-diol	C ₄ H ₈ O ₂	3514.89, 4.789	88.0519	46406	
2'-Methylspiro[cyclopropane-1,1'-ind-2'-ene]	C ₁₂ H ₁₂	3520.9, 2.335	156.0934	86239	
3-(2-Methylphenyl)cyclohexene	C ₁₃ H ₁₆	3520.9, 2.477	172.1247	14387	
1,4-bis(Isopropylamino) anthraquinone	C ₂₀ H ₂₀ N ₂ O ₂	3550.9, 4.047	320.1519	17798	
3-Methylhexadecane	C ₁₇ H ₃₆	3550.9, 4.356	240.2812	515320	
1-Methyl-2,3-dihydro-4-pyridone	C ₆ H ₉ NO	3556.91, 3.830	111.0679	16804	
1-Ethyl-naphthalene	C ₁₂ H ₁₂	3598.92, 2.331	156.0934	12993	
Tetradecylcyclooctane	C ₂₂ H ₄₄	3604.92, 4.118	308.3438	143286	
2,2-Dimethylbutane	C ₆ H ₁₄	3664.94, 4.487	86.109	151737	
Cyclopentadec-5-ene	C ₁₅ H ₂₈	3700.95, 3.946	208.2186	37902	
(trans)-1-Butyl-2-undecylcyclopropane	C ₁₈ H ₃₆	3718.95, 3.973	252.2812	247026	
6-Hydroxy-3-hexanone	C ₆ H ₁₂ O ₂	3754.96, 4.566	116.0832	59749	
2-(1-Methylethyl)naphthalene	C ₁₃ H ₁₄	3766.97, 2.420	170.109	14213	
7-Phenyltetracyclo [4.1.0.0.2,4.0.3,5]heptane	C ₁₃ H ₁₂	3772.97, 2.282	168.0934	19338	
3-Methyl-1-[(1H)-1,2,4-triazol-1-yl]butan-2-one	C ₇ H ₁₁ N ₃ O	3772.97, 3.887	153.0897	30038	
1-Methyl-4-(1-methylethyl)-trans-cyclohexane	C ₁₀ H ₂₀	3790.97, 3.965	140.156	137464	
3,4-Dimethyl-4H-1,2,4-triazole	C ₄ H ₇ N ₃	3796.97, 4.018	97.0634	50502	
4-Methylheptadecane	C ₁₈ H ₃₈	3826.98, 4.346	254.2968	337989	
2,3-Epoxytridecan-1-ol	C ₁₃ H ₂₆ O ₂ ?	3832.99, 3.896	214.1927	27297	2.45E-4
1,2,2,3,3,4,4,5-Octamethyl-6-oxabicyclo[3.1.0]hexane	C ₁₃ H ₂₄ O	3838.99, 4.053	196.1822	5768	
8-Heptylpentadecane	C ₂₂ H ₄₆	3838.99, 4.402	310.3594	514166	
2-Isocyano-2-methylpropane	C ₅ H ₉ N	3844.99, 3.892	83.073	47767	
5-Methylhept-2-yn-4-ol	C ₈ H ₁₄ O ?	3844.99, 3.948	126.1039	71078	6.39E-4

4,6,8-Trimethylazulene	C ₁₃ H ₁₄	3869, 2.386	170.109	42518	
Methyl 3-(p-nitrophenyl)bicyclo[1.1.1]pentane-1-carboxylate	C ₁₃ H ₁₃ NO ₄ ?	3875, 2.490	247.0839	18964	1.70E-4
4-tert-Butylhex-1-ene	C ₁₀ H ₂₀	3875, 4.320	140.156	157992	
1,6,7-Trimethylnaphthalene	C ₁₃ H ₁₄	3881, 2.406	170.109	54128	
1-(3-Methyl-2-butenyl)-2-hexylcyclopropane	C ₁₄ H ₂₆	3887, 3.837	194.2029	14376	
Methyl (1S,2R,3S,4R)-3-[(4S)-4-(2,2-dimethyl-1,3-dioxolo)]bicyclo[2.2.1]-5-hepten-2-ylcarboxylate	C ₁₄ H ₂₀ O ₄ ?	3929.01, 3.980	252.1356	10737	9.66E-5
1,6,7-Trimethylnaphthalene	C ₁₃ H ₁₄	3965.02, 2.393	170.109	54631	
7-Oxatridecane	C ₁₂ H ₂₆ O	3989.03, 4.422	186.1978	45463	
(Z)-2,2,3,5,5-Pentamethyl-3-hexene	C ₁₁ H ₂₂	4055.05, 3.921	154.1716	61954	
n-Decyl prop-2-ynoate	C ₁₃ H ₂₂ O ₂ ?	4061.05, 3.971	210.1614	48716	4.38E-4
n-Cetyl thiocyanate	C ₁₇ H ₃₃ NS?	4067.05, 4.340	283.2328	95651	8.60E-4
3,4'-Dimethyl-1,1'-biphenyl	C ₁₄ H ₁₄	4121.07, 2.311	182.109	22041	
3,3'-Dimethylbiphenyl	C ₁₄ H ₁₄	4163.08, 2.313	182.109	18660	
(4E)-2,7-Dimethyl-4-octene-3,6-dione	C ₁₀ H ₁₆ O ₂	4181.09, 4.249	168.1145	42423	
2-Methyloctadecane	C ₁₉ H ₄₀	4193.09, 4.279	268.3125	410169	
2-(1,3-Dioxolan-2-yl)-1-(2-furyl)ethene	C ₉ H ₁₀ O ₃	4211.09, 4.396	166.0624	99070	
2,4,4-Trimethylhexane	C ₉ H ₂₀	4235.1, 4.383	128.156	56630	
7-Methylbicyclo[3.2.1]octan-1-ol	C ₉ H ₁₆ O	4265.11, 3.931	140.1196	25243	
2,6-Dimethylcyclohexane-1-(cis)-carbaldehyde	C ₉ H ₁₆ O	4265.11, 4.101	140.1196	32116	
2-Cyanocyclohexanol	C ₇ H ₁₁ NO	4331.13, 4.316	125.0835	59362	
Bicyclo[4.3.1]deca-1-ol	C ₁₀ H ₁₈ O?	4343.13, 3.858	154.1352	11229	1.01E-4
Cyclohexylmethyl octadecyl sulfuric acid ester	C ₂₅ H ₅₀ O ₃ S?	4415.15, 3.903	430.3475	283235	2.54E-3
2,4-Dimethyl-1-methylethyl ester, (S)-pentanoic acid	C ₁₀ H ₂₀ O ₂ ?	4415.15, 4.442	172.1458	46722	4.20E-4
Hexyl octyl ester sulfuric acid	C ₁₄ H ₃₀ O ₃ S?	4421.15, 4.299	278.191	124949	1.12E-3
2,5,9-Trimethyldecane	C ₁₃ H ₂₈	4427.16, 4.585	184.2186	61920	
4-Methylhexanoic acid	C ₇ H ₁₄ O ₂ ?	4439.16, 4.585	130.0988	51375	4.62E-4
Eicosane	C ₂₀ H ₄₂	4451.16, 4.583	282.3281	129887	
3,8-Dimethylundecane	C ₁₃ H ₂₈	4493.17, 4.248	184.2186	308602	

1-Propanoyl-2-butanylethylene	C ₉ H ₁₄ O ₂	4505.18, 4.030	154.0988	41660	
3-(1,1-Dimethylethoxy)-1-propene	C ₇ H ₁₄ O	4517.18, 4.336	114.1039	77327	
2-Methoxy-1,4-pentadiene	C ₆ H ₁₀ O	4529.18, 4.323	98.0726	15074	
1-Deuteriocyclohexene	C ₆ H ₉ D	4601.21, 3.796	83.084	24572	
Tetrahydroacetate-2-furanmethanol	C ₇ H ₁₂ O ₃	4637.22, 4.277	144.0781	42654	
2-(2,2-Dimethylpropylidene)-1,3-cyclohexanedione	C ₁₁ H ₁₆ O ₂ ?	4649.22, 2.241	180.1145	17266	1.55E-4
3-Hydroxy-2,7,7-trimethyl-1,8-nonadien-5-one	C ₁₂ H ₂₀ O ₂ ?	4661.22, 3.908	196.1458	40285	3.62E-4
[[2-(2-Propenyloxy)-1-propenyl]sulfonyl]-(E)-benzene	C ₁₂ H ₁₄ O ₃ S ?	4667.22, 3.931	238.0658	76846	6.91E-4
10-Methyleicosane	C ₂₁ H ₄₄	4673.23, 4.263	296.3438	545922	
3-Ethyl-3-methylhexane	C ₉ H ₂₀	4697.23, 4.237	128.156	142061	
Heneicosane	C ₂₁ H ₄₄	4739.25, 4.269	296.3438	577749	
2-Methoxy-1-(1H-1,2,3-triazol-4-yl)ethylamine	C ₅ H ₁₀ N ₄ O	4775.26, 3.822	142.0849	55364	
2,6,10,15-Tetramethylheptadecane	C ₂₁ H ₄₄	4775.26, 4.238	296.3438	304181	
(E)-Deca-1,6-dien-3-one	C ₁₀ H ₁₆ O	4823.27, 4.333	152.1196	45544	
2-Ethyl-6-oxabicyclo[3.1.0]hexan-2-ol	C ₇ H ₁₂ O ₂	4913.3, 4.253	128.0832	22538	
Undecylcyclohexane	C ₁₇ H ₃₄	4925.3, 3.744	238.2655	251720	
5-Methyl-6-carbomethoxy-2-oxabicyclo[3.1.0]hexane	C ₉ H ₁₄ O ₃ ?	4949.31, 3.934	170.0937	45322	4.07E-4
2,4,9,11-Tetramethyldodeca-5,7-diyne-4,9-diol	C ₁₆ H ₂₆ O ₂ ?	4961.31, 4.246	250.1927	89912	8.09E-4
9-Hydroxyinalool	C ₁₀ H ₁₈ O ₂ ?	5003.32, 4.243	170.1301	95522	8.59E-4
Tert-butyl (2E)-penta-2,4-dienylcarbamate	C ₁₀ H ₁₇ NO ₂ ?	5009.32, 4.460	183.1254	55333	4.97E-4
11-Decyldocosane	C ₃₂ H ₆₆	5015.32, 4.258	450.5159	347597	
3-Amino-5-nitro-1H-indazole	C ₇ H ₆ N ₄ O ₂	5027.33, 2.132	178.0485	10655	
2,2,4,5-Tetramethylhex-5-en-3-one	C ₁₀ H ₁₄ O	5063.34, 4.288	150.1039	33317	
2,2,4-Trimethyl-2H-imidazole	C ₆ H ₁₀ N ₂	5075.34, 3.968	110.0838	38105	
2-Methylidihydrothiophene	C ₅ H ₈ S	5093.35, 4.302	100.0341	30150	
(E)-6-Tosyl-4-nonene	C ₁₆ H ₂₄ O ₂ S ?	5153.36, 4.047	280.1492	15290	1.37E-4
1-Hexadecene	C ₁₆ H ₃₂	5171.37, 3.801	224.2499	23230	
Eicosylcyclohexane	C ₂₆ H ₅₂	5201.38, 3.754	364.4064	193321	
1-Oxa-spiro[5.2]octane-2-carbaldehyde	C ₈ H ₁₂ O ₂	5219.38, 3.881	140.0832	47417	

2,2,3,4,5,5-Hexamethyl-(meso)hexane	C ₁₂ H ₂₆	5249.39, 4.235	170.2029	103187	
n-Octyl ethynyl ether	C ₁₀ H ₁₈ O	5267.4, 4.223	154.1352	112975	
1-Ethyl-1H-1,2,4-triazole	C ₄ H ₇ N ₃	5273.4, 3.868	97.0634	80146	
Octacosane	C ₂₈ H ₅₈	5279.4, 4.217	394.4533	286398	
3-tert-Butyl-1,2-dimethoxy-5-methylbenzene	C ₁₃ H ₂₀ O ₂ ?	5291.4, 2.356	208.1458	10237	9.21E-5
1a,9b-dihydro-cyclopropa[1]phenanthrene	C ₁₅ H ₁₂	5327.41, 2.201	192.0934	14816	
2,3,4,5-Tetrahydro-6-hexylpyridine	C ₁₁ H ₂₁ N	5339.42, 3.827	167.1669	107650	
7-Phenylindene	C ₁₅ H ₁₂	5357.42, 2.189	192.0934	15851	
3-Methyl-5-methylenon-2-en-4-ol	C ₁₁ H ₂₀ O ?	5375.43, 4.277	168.1509	17946	1.61E-4
2,2-Dimethyl-3,4-undecanedione	C ₁₃ H ₂₄ O ₂ ?	5381.43, 4.285	212.1771	61853	5.56E-4
3-Ethoxyacrylonitrile	C ₅ H ₇ NO	5435.44, 3.792	97.0522	35367	
Tritriacontane	C ₃₃ H ₆₈	5459.45, 4.233	464.5316	238170	
2-(2-Oxopropyl)-cyclopentanone	C ₈ H ₁₂ O ₂	5477.46, 3.891	140.0832	38692	
Bicyclo[3.2.1]octan-1-ol	C ₈ H ₁₄ O	5495.46, 3.876	126.1039	24579	
1-Hydroxy-2-methyl-bicyclo[3.3.1]nonan-3-one	C ₁₀ H ₁₆ O ₂ ?	5603.49, 3.811	168.1145	84771	7.62E-4
2-Ethylanthracene	C ₁₆ H ₁₄	5717.53, 2.242	206.109	12128	
4,6-Dimethylundecane	C ₁₃ H ₂₈	5729.53, 4.222	184.2186	105181	
Docosane	C ₂₂ H ₄₆	5801.55, 4.185	310.3594	76783	
1,4-Bis(cyclohex-1-enyl)buta-1,3-diyne	C ₁₆ H ₁₈	5867.57, 4.264	210.1403	42155	
3,5-Diethylhex-5-ene-3-ol	C ₁₀ H ₂₀ O ?	5945.59, 4.211	156.1509	53279	4.79E-4
6-Hexyl-4-oxa-5-azaspiro[2.4]hept-5-ene	C ₁₁ H ₁₉ NO	5975.6, 3.756	181.1461	72198	
2,3-Octanedione	C ₈ H ₁₄ O ₂	5993.61, 4.225	142.0988	50333	
4-(1,1-Dimethylethyl)-2-methyl-2-nitro-trans-cyclohexanone	C ₁₁ H ₁₉ NO ₃ ?	6203.67, 4.268	213.1359	28764	2.58E-4
(3R)-3-Phenyl-2,3-dihydro-1H-indol-1-one	C ₁₄ H ₁₁ NO ?	6245.68, 1.099	209.0835	25254	2.27E-4
2-Methylhexadecane	C ₁₇ H ₃₆	6377.72, 4.284	240.2812	244918	
2-Naphthalenesulfonic acid	C ₁₀ H ₈ O ₃ S ?	6545.76, 1.097	208.0189	403842	3.63E-3
cis-exo-7-Oxabicyclo[2.2.1]hept-5-ene-2,3-diol	C ₆ H ₈ O ₃ ?	6731.82, 4.360	128.0468	21755	1.95E-4
5-Carbamoyltetrazole	C ₂ H ₃ N ₅ O	6887.86, 4.643	113.0332	7173	

Tetratetracontane	C ₄₄ H ₉₀	6941.88, 4.397	618.7037	483099	
(S)-2-Ethylheptanol	C ₉ H ₂₀ O ?	7049.91, 4.590	144.1509	58667	5.28E-4
Benzene	C ₆ H ₆	7446.02, 1.090	78.0464	64600	
Diethyl 1,4-dihydro-2,6-dimethyl-4-(3-pyridazinyl)--3,5-pyridinedicarboxylate	C ₁₇ H ₂₁ N ₃ O ₄ ?	7650.08, 1.728	331.1527	10001	9.00E-5
Pentatriacontane	C ₃₅ H ₇₂	7854.14, 5.422	492.5629	178296	
2-(1,1-Dimethylprop-2-en-1-yl)-1,3-dioxolane	C ₈ H ₁₄ O ₂	7902.15, 1.163	142.0988	34057	
(E)-Non-3-en-8-yn-2-one	C ₉ H ₁₂ O	7926.16, 1.379	136.0883	7366	
Ethyl (E)-4-Benzoyl-4-(imidazolidin-2-ylidene)but-2-enoate	C ₁₆ H ₁₈ N ₂ O ₃ ?	7968.17, 1.260	286.1312	19868	1.78E-4
(R)-3-(4-Methoxyphenyl)butanoic Acid	C ₁₁ H ₁₄ O ₃ ?	7986.18, 1.384	194.0937	15139	1.36E-4
tert-Butyl(3-Isopentyltetrahydrofuran-2-ylidene)acetate	C ₁₅ H ₂₆ O ₃ ?	7998.18, 0.745	254.1876	14007	1.26E-4
(1R,2R)-2,3-Dibenzoyloxy-1-[2-(1,3-dioxolan-2-yl)]ethylpropyl methanesulfanate	C ₂₃ H ₃₀ O ₇ S ?	7998.18, 1.173	450.1707	37050	3.334E-4
2-(3,3-Dimethyl-1-butenyl)-(E)-1-cyclohexene-1-carboxaldehyde	C ₁₃ H ₂₀ O ?	7998.18, 1.493	192.1509	6727	6.05E-5
4-Ethoxycarbonyl-2,2,5-trimethyl-3-(n-decyl)-2H-pyrrole 1-oxide	C ₂₀ H ₃₃ NO ₃ ?	8082.2, 1.461	337.2611	4285	3.85E-5
(S)-(E)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C ₂₀ H ₂₈ O ₃ ?	8088.21, 1.111	316.2033	76200	6.85E-4
Octanoic acid	C ₈ H ₁₆ O ₂ ?	8130.22, 1.441	144.1145	4599	4.13E-5
2-Methoxy-4-(methoxycarbonyl)phenyl benzoate	C ₁₆ H ₁₄ O ₅ ?	8136.22, 1.360	286.0836	7711	6.93E-5
Methyl 5-(4-methoxyphenyl)-2,2,4,4-tetramethyl-3,5-dioxopentanoate	C ₁₇ H ₂₂ O ₅ ?	8166.23, 1.377	306.1462	14504	1.30E-4
5-(Pyridine-4-yl)-1,3,4-oxadiazole-2-(3H)-thione	C ₇ H ₅ N ₃ OS	8208.24, 1.205	179.0148	32849	
(3S)-3-Phenyl-2,3-dihydro-1H-isoindol-1-one	C ₁₄ H ₁₁ NO ?	8214.24, 1.183	209.0835	7174	6.45E-5

Table S15. Data obtained for the distillate fraction of 1 condensate-like oil by using GCxGC/(+EI) TOF MS. Data provided are based on ChromaTOF software prediction of the molecular ion *m/z* value and the identification of the compound by using the EI mass spectral library match using a match factor threshold of 800. Formulas with a question mark “?” might not have been accurately identified. The ratio of the peak area of each of these questionable compounds relative to all peak areas of the detected compounds is provided in the table below

Name	Formula	Retention Times (s) on the Primary and Secondary Columns	Molecular Ion <i>m/z</i>	Chromatographic Peak Area	Ratio (Peak area/total sum of peak areas)
3-Methylheptane	C ₈ H ₁₈	406.002, 2.407	114.1403	228664	

1,1,3,4-Tetramethyl-cis-cyclopentane	C ₉ H ₁₈	406.002, 2.438	126.1403	115682	
1,1,2-Trimethylcyclopentane	C ₈ H ₁₆	424.007, 2.309	112.1247	266856	
Cyclopentane	C ₅ H ₁₀	436.01, 2.386	70.0777	90859	
1,3-Dimethyl-cis-cyclohexane	C ₈ H ₁₆	454.016, 2.391	112.1247	2497862	
4-Methyl-1-heptanol	C ₈ H ₁₈ O	454.016, 2.618	130.1352	127008	
5-Methyldodecane	C ₁₃ H ₂₈	460.017, 2.787	184.2186	134169	
2,4-Dimethylheptane	C ₉ H ₂₀	466.019, 2.839	128.156	92074	
1-Ethyl-2-methylcyclopentane	C ₈ H ₁₆	472.021, 2.469	112.1247	183216	
1,1-Dimethylcyclohexane	C ₈ H ₁₆	478.022, 2.433	112.1247	371592	
2,6-Dimethylheptane	C ₉ H ₂₀	478.022, 2.875	128.156	688531	
Methyl Propargyl Ether	C ₄ H ₆ O	490.026, 2.671	70.0413	40531	
1,2-Dimethyl-trans-cyclohexane	C ₈ H ₁₆	496.028, 2.501	112.1247	1044446	
Dihydro-2H-pyran-2,6(3H)-dione	C ₅ H ₆ O ₃	496.028, 2.692	114.0311	44648	
2,5-Dimethylheptane	C ₉ H ₂₀	496.028, 2.926	128.156	660487	
(2S,1'S)-(-)-2-(1-Hydroxy-6-methylheptyl)-2,5-dihydrofuran	C ₁₂ H ₂₂ O ₂ ?	502.029, 2.690	198.1614	39612	4.81E-4
1,4-Dimethylcyclohexane	C ₈ H ₁₆	514.033, 2.541	112.1247	582815	
(S)-(-)-Pipelic acid	C ₆ H ₁₁ NO ₂	514.033, 2.812	129.0784	13027	
3-Ethyl-2-methylhexane	C ₉ H ₂₀	526.036, 3.010	128.156	38067	
1,3,5-Trimethylcyclohexane	C ₉ H ₁₈	538.04, 2.793	126.1403	307540	
2,3-Dimethylheptane	C ₉ H ₂₀	550.043, 3.088	128.156	192047	
1,1,3-Trimethylcyclohexane	C ₉ H ₁₈	556.045, 2.818	126.1403	2260261	
6-Methylundecane	C ₁₂ H ₂₆	580.052, 3.204	170.2029	1606124	
Ethylcyclohexane	C ₈ H ₁₆	586.053, 2.700	112.1247	995042	
1,2,4-Trimethylcyclohexane	C ₉ H ₁₈	592.055, 2.916	126.1403	1013505	
4,5-Dimethyl-trans-1-azabicyclo[3.2.0]heptane-3,7-dione	C ₈ H ₁₁ NO ₂	592.055, 3.244	153.0784	65190	
Toluene	C ₇ H ₈	598.057, 2.062	92.0621	150890	
1,2,3-Trimethylcyclohexane	C ₉ H ₁₈	616.062, 2.957	126.1403	11390	
1-Ethyl-3-methylcyclopentane	C ₈ H ₁₆	646.071, 3.043	112.1247	30743	
3-Butyl-3,5-dimethylcyclohexanone	C ₁₂ H ₂₂ O ?	652.072, 3.214	182.1665	172392	2.09E-3

2,4-Bis(methylethyl)-2-methyl-2,5-dihydro-1H-imidazole	C ₁₀ H ₂₀ N ₂ ?	664.076, 3.178	168.1621	17236	2.09E-4	
1,2,3-Trimethylcyclohexane	C ₉ H ₁₈	670.078, 3.029	126.1403	610234		
2,4-Dimethylhexane	C ₈ H ₁₈	682.081, 3.636	114.1403	326024		
1-Ethyl-4-methylcyclohexane	C ₉ H ₁₈	706.088, 3.106	126.1403	1458057		
N-(But-2-enoyl)prop-2-enamide	C ₇ H ₁₁ NO	706.088, 3.355	125.0835	27673		
Nonane	C ₉ H ₂₀	706.088, 3.682	128.156	599857		
1,2-Diethyl-3-methylcyclohexane	C ₁₁ H ₂₂	718.091, 3.333	154.1716	293576		
Dodec-3-yn-1-ol	C ₁₂ H ₂₂ O ?	736.096, 3.470	182.1665	26464	3.21E-4	
2,6-Dimethyloctane	C ₁₀ H ₂₂	736.096, 3.739	142.1716	1467384		
6-Methylheptan-1-ol	C ₈ H ₁₈ O	748.1, 3.477	130.1352	86756		
Octahydropentalene	C ₈ H ₁₄	754.102, 2.746	110.109	180515		
3-Ethyl-2-methylheptane	C ₁₀ H ₂₂	772.107, 3.759	142.1716	1125217		
3-Propylcyclohexene	C ₉ H ₁₆	778.109, 2.988	124.1247	268884		
1-Ethyl-2-methyl-cis-cyclohexane	C ₉ H ₁₈	778.109, 3.172	126.1403	851447		
1-Ethyl-1H-1,2,4-triazole	C ₄ H ₇ N ₃	784.11, 3.525	97.0634	177174		
1-(Dodecycloxy)-4-methoxybutan-2-one	C ₁₇ H ₃₄ O ₃ ?	784.11, 3.730	286.2502	38996		4.73E-4
cis-3,4-Epoxy-1-cyclohexanol	C ₆ H ₁₀ O ₂ ?	790.112, 3.775	114.0675	42625		5.17E-4
1-Ethyl-1-methylcyclohexane	C ₉ H ₁₈	808.117, 3.143	126.1403	125110		
1-Methyl-bicyclo[3.2.0]heptan-6-one	C ₈ H ₁₂ O	814.119, 2.726	124.0883	20546		
2,5,6-Trimethyldecane	C ₁₃ H ₂₈	814.119, 3.842	184.2186	797364		
5-Acetyl-3-methyl-4,5-dihydroisoxazole	C ₆ H ₉ NO ₂	826.122, 3.818	127.0628	110312		
4-Methylnonane	C ₁₀ H ₂₂	832.124, 3.909	142.1716	1515744		
1-Ethyl-cis-1,3-dimethyl-cyclohexane	C ₁₀ H ₂₀	838.126, 3.507	140.156	396622		
2,2,4-Trimethyl-2H-imidazole	C ₆ H ₁₀ N ₂	844.127, 3.967	110.0838	13757		
Methyl pentanoate	C ₆ H ₁₂ O ₂ ?	844.127, 4.170	116.0832	48095	5.84E-4	
Propylcyclohexane	C ₉ H ₁₈	856.131, 3.284	126.1403	585906		
3-Methylnonane	C ₁₀ H ₂₂	868.134, 3.945	142.1716	568746		
Octahydro-cis-1H-indene	C ₉ H ₁₆	874.136, 3.091	124.1247	437469		
(1R,2S)-1-Methylcyclohexene oxide	C ₇ H ₁₂ O	874.136, 3.222	112.0883	86213		

2,3,3-Trimethyl-(Z)- 4-nonene	C ₁₂ H ₂₄	874.136, 3.525	168.1873	129157	
Ethylbenzene	C ₈ H ₁₀	886.14, 2.372	106.0777	56713	
4,6-Dimethyldecane-1-ol	C ₁₂ H ₂₆ O ?	898.143, 3.513	186.1978	191681	2.32E-3
p-Xylene	C ₈ H ₁₀	904.145, 2.417	106.0777	580482	
3-Cyclohexyl-(2S-trans)-oxiranemethanol	C ₉ H ₁₆ O ₂ ?	904.145, 3.359	156.1145	31656	3.84E-4
1-Ethyl-1,3-dimethyl-trans-cyclohexane	C ₁₀ H ₂₀	922.15, 3.574	140.156	803911	
2,6,10,14-Tetramethylhexadecane	C ₂₀ H ₄₂	934.153, 4.231	282.3281	83769	
1,1,2,3-Tetramethylcyclohexane	C ₁₀ H ₂₀	940.155, 3.466	140.156	780984	
4-Methyleneheptane	C ₈ H ₁₆	940.155, 4.037	112.1247	47788	
Octadecane	C ₁₈ H ₃₈	952.158, 4.262	254.2968	24027	
(2"E)-2'-Methyl-2'-(1",4",4"-trimethylpent-2"-enyloxy)propyl cyclopropanecarboxylate	C ₁₆ H ₂₈ O ₃	958.16, 3.503	268.2033	75733	
Tetrahydro-3,3'-bifuran	C ₈ H ₁₀ O ₂ ?	958.16, 4.016	138.0675	31790	3.86E-4
1-(1-Propynyl)cyclopropanol	C ₆ H ₈ O ?	964.162, 3.417	96.057	47951	5.82E-4
Decane	C ₁₀ H ₂₂	976.165, 4.063	142.1716	2505247	
1-Isopropyl-4-methylcyclohexane	C ₁₀ H ₂₀	988.169, 3.596	140.156	407611	
2,4-Bis(dimethylethyl)-2-methyl-2,5-dihydro-1H-imidazole	C ₁₂ H ₂₄ N ₂	988.169, 3.814	196.1934	25961	
Undecane	C ₁₁ H ₂₄	994.171, 4.300	156.1873	170967	
3-Methoxymethylhept-1-yn-3-ol	C ₉ H ₁₆ O ₂	1006.17, 3.577	156.1145	32143	
1-(1-Methylcyclohexyl)-ethanone	C ₉ H ₁₆ O	1006.17, 3.662	140.1196	808183	
6-Methyl-2-hepten-4-one	C ₈ H ₁₄ O	1012.18, 3.595	126.1039	396396	
1,2-Dimethylbenzene	C ₈ H ₁₀	1024.18, 2.427	106.0777	312208	
2-Methyl-2-(1-methyl-1-propenyl)cyclobutanone	C ₉ H ₁₄ O	1024.18, 3.050	138.1039	10111	
2,6-Dimethylnonane	C ₁₁ H ₂₄	1024.18, 4.351	156.1873	1441833	
2-Methyl-4-hexyn-3-ol	C ₇ H ₁₂ O	1030.18, 3.997	112.0883	26630	
4-Acetoxy-2,5-divinyltetrahydrofuran-3-yl but-3-enoate	C ₁₄ H ₁₈ O ₅ ?	1042.18, 3.991	266.1149	13219	1.60E-4
1-Pentadecanol	C ₁₅ H ₃₂ O ?	1048.19, 3.927	228.2448	18138	2.20E-4
4,8-Dimethyl-3,4-epoxy-7-nonen-2-ol	C ₁₁ H ₂₀ O ₂ ?	1054.19, 3.937	184.1458	10142	1.23E-4
cis-9-Oxabicyclo[6.1.0]non-2-ene	C ₈ H ₁₂ O	1066.19, 3.408	124.0883	11250	

Ethylpropylcyclopentane	C ₁₀ H ₂₀	1072.19, 3.662	140.156	333873	
3-Methyldodecane	C ₁₃ H ₂₈	1078.19, 4.350	184.2186	128090	
2,3,3-Trimethylcyclobutanone	C ₇ H ₁₂ O	1084.2, 4.061	112.0883	25470	
Decan-1-ol	C ₁₀ H ₂₂ O ?	1090.2, 4.029	158.1665	67430	8.19E-4
2,2-Dimethyl-3-(3-oxobutyl)-, methyl (1R-cis)-cyclopropanecarboxylate	C ₁₁ H ₁₈ O ₃ ?	1096.2, 3.795	198.125	47221	5.73E-4
(1-Methylethyl)benzene	C ₉ H ₁₂	1102.2, 2.580	120.0934	17659	
2-But-1-enyltetrahydrofuran	C ₈ H ₁₄ O	1102.2, 4.036	126.1039	26437	
3,7-Dimethylnonane	C ₁₁ H ₂₄	1102.2, 4.346	156.1873	474077	
2,5-Dimethylhex-4-enoic acid	C ₈ H ₁₄ O ₂ ?	1108.2, 3.949	142.0988	13313	1.61E-4
3-Methyl-1-hexen-5-one	C ₇ H ₁₂ O	1120.21, 4.096	112.0883	82107	
2,2-Dimethylheptanenitrile	C ₉ H ₁₇ N	1132.21, 3.926	139.1356	83236	
N-(1-Methylpropylidene)- 2-butanamine	C ₈ H ₁₇ N	1132.21, 4.061	127.1356	26293	
Methyl nonanoate	C ₁₀ H ₂₀ O ₂ ?	1132.21, 4.105	172.1458	26486	3.21E-4
(+)-cis-3-Hydroxymethyl-2,2-dimethyl-1-cyclobutaneacetic acid	C ₉ H ₁₆ O ₃ ?	1138.21, 3.904	172.1094	55047	6.68E-4
1,1-Dimethyl-2-oxopropyl-N,N-pentamethylenecarbamate	C ₁₁ H ₁₉ NO ₃ ?	1138.21, 4.094	213.1359	8844	1.07E-4
3-Decyn-1-ol	C ₁₀ H ₁₈ O ?	1156.22, 4.123	154.1352	56324	6.84E-4
1,3,5-Triazine-2,4-diamine	C ₃ H ₅ N ₃	1162.22, 3.535	111.0539	24088	
(S)-Undec-1-en-4-ol	C ₁₁ H ₂₂ O ?	1162.22, 3.591	170.1665	49397	6.00E-4
1,1-Dimethyl-3-methylene-cyclopentane	C ₈ H ₁₄	1168.22, 3.782	110.109	62665	
trans-1-Formyl-2-(1-methylethenyl)cyclopropane	C ₇ H ₁₀ O	1174.22, 3.782	110.0726	97221	
5-Methyldecane	C ₁₁ H ₂₄	1174.22, 4.402	156.1873	482015	
4-Methyl-5-propylnonane	C ₁₃ H ₂₈	1192.23, 4.392	184.2186	314314	
Dioctylsulfide	C ₁₆ H ₃₄ S ₂	1192.23, 4.718	290.2096	25577	
2-Methyldecane	C ₁₁ H ₂₄	1198.23, 4.433	156.1873	381298	
Phenylacetaldehyde	C ₈ H ₈ O	1222.24, 2.634	120.057	45787	
(1-Methylpropyl)cyclohexane	C ₁₀ H ₂₀	1222.24, 3.629	140.156	39982	
Octacosane	C ₂₈ H ₅₈	1222.24, 4.378	394.4533	64166	
Butylcyclohexane	C ₁₀ H ₂₀	1234.24, 3.687	140.156	473311	

3-Methyldecane	C ₁₁ H ₂₄	1234.24, 4.413	156.1873	331679	
cis-1,2-Diethylcyclohexane	C ₁₀ H ₂₀	1240.24, 3.955	140.156	395307	
1-Ethyl-2-methylbenzene	C ₉ H ₁₂	1264.25, 2.633	120.0934	256545	
7-Methyl-(Z)-5-undecene	C ₁₂ H ₂₄	1264.25, 3.855	168.1873	109336	
Ethylcyclooctane	C ₁₀ H ₂₀	1276.25, 3.965	140.156	330810	
1,2,3-Trimethylbenzene	C ₉ H ₁₂	1288.25, 2.654	120.0934	607085	
3-Ethoxy-1-propyne	C ₅ H ₈ O	1294.26, 3.875	84.057	34761	
1,1,2-Trimethylcyclohexane	C ₉ H ₁₈	1300.26, 4.015	126.1403	45501	
S,S-Dioxide-2-methylthiolane	C ₃ H ₁₀ O ₂ S ?	1300.26, 4.343	134.0396	12954	1.57E-4
(Z/E)-2,2,4,5-Tetramethyl-3-heptene	C ₁₁ H ₂₂	1312.26, 4.283	154.1716	29598	
3,3-Dimethylcyclohex-1-en-1-yl but-2-enoate	C ₁₂ H ₁₈ O ₂ ?	1324.27, 3.885	194.1301	56305	6.83E-4
2-hydroxylactone cyclohexaneacetic acid	C ₈ H ₁₀ O ₂ ?	1324.27, 4.101	138.0675	21075	2.56E-4
4-Hydroxy- D-isovaline	C ₅ H ₁₁ NO ₃	1324.27, 4.651	133.0733	28167	
3,3-Dimethylpentane	C ₇ H ₁₆	1330.27, 4.636	100.1247	33786	
Pentadecane	C ₁₅ H ₃₂	1336.27, 4.620	212.2499	27105	
3',3',5'-Trimethylcyclohexyl (cis)-(3-thienylglyoxyl)carboxylate	C ₁₅ H ₂₀ O ₃ S ?	1348.27, 3.907	280.1128	78381	9.52E-4
Cyclohexanone	C ₆ H ₁₀ O	1348.27, 4.387	98.0726	15783	
Dodecane	C ₁₂ H ₂₆	1366.28, 4.407	170.2029	3424632	
1-Ethyl-4-methylbenzene	C ₉ H ₁₂	1372.28, 2.602	120.0934	47914	
1,1-Dimethyl-2-propyl-cyclohexane	C ₁₁ H ₂₂	1372.28, 3.795	154.1716	468898	
2,3,4,5-Tetrahydro-6-propyl-pyridine	C ₈ H ₁₃ N	1384.28, 3.902	125.1199	49669	
1-Hexyl-3-methyl-cyclopentane	C ₁₂ H ₂₄	1390.28, 4.049	168.1873	143076	
Tridecane	C ₁₃ H ₂₈	1390.28, 4.695	184.2186	642683	
(4RS,5S)-5-Methylhept-2-yn-4-ol	C ₈ H ₁₄ O	1396.29, 3.897	126.1039	86182	
1-Ethyl-4-methyl-trans-cyclohexane	C ₉ H ₁₈	1402.29, 3.975	126.1403	485500	
1-Hydroxymethyl-1,3-dimethylcyclopentane	C ₈ H ₁₆ O	1414.29, 4.003	128.1196	214240	
2,6,10-trimethyltridecane	C ₁₆ H ₃₄	1420.29, 4.673	226.2655	146084	
3,7-Dimethyldecane	C ₁₂ H ₂₆	1444.3, 4.654	170.2029	470598	

(3R,3aR,6R,7aR)-Perhydro-3,6-dimethyl-2-benzo[b]furanone	C ₁₀ H ₁₆ O ₂ ?	1450.3, 3.770	168.1145	12119	1.47E-4
(Z)-6-Undecen-3-ol	C ₁₁ H ₂₂ O ?	1456.3, 3.727	170.1665	17928	2.17E-4
2,4-Dimethyl-1,3-hexanediol	C ₈ H ₁₈ O ₂ ?	1456.3, 4.284	146.1301	32396	3.93E-4
Decahydro-trans-naphthalene	C ₁₀ H ₁₈	1468.31, 3.338	138.1403	287771	
Methyl(1-methylethyl)benzene	C ₁₀ H ₁₄	1492.31, 2.767	134.109	77324	
1-Isopropyl-1-methyl-cyclohexane	C ₁₀ H ₂₀	1492.31, 3.899	140.156	39596	
1-Methoxy-2-butyne	C ₅ H ₈ O	1492.31, 4.266	84.057	17356	
(1R,3S)-7,7-Dimethyl-2-oxabicyclo[4.1.1.]octan-3-one	C ₉ H ₁₄ O ₂ ?	1504.32, 3.862	154.0988	60484	7.34E-4
5-Hydroxymethyl-2-tetrahydrofuraldehyde-3-one	C ₆ H ₈ O ₄	1510.32, 4.584	144.0417	41458	
2-(1-Phenylethyl)phenol	C ₁₄ H ₁₄ O	1528.32, 4.594	198.1039	113696	
1,1-Dimethoxyprop-2-yne	C ₅ H ₈ O ₂	1552.33, 4.124	100.0519	45060	
6-Methylundecane	C ₁₂ H ₂₆	1564.33, 4.629	170.2029	880101	
Methylcycloheptane	C ₈ H ₁₆	1576.34, 4.315	112.1247	56919	
2,2,5-Trimethyl-, (S)-6-hepten-1-ol	C ₁₀ H ₂₀ O ?	1582.34, 4.153	156.1509	42516	5.16E-4
2-Acetylmethylnorbornane	C ₁₀ H ₁₆ O	1588.34, 3.561	152.1196	9884	
5-Ethyl-5-methyl-2-oxepanone	C ₉ H ₁₆ O ₂	1588.34, 4.139	156.1145	37345	
5-Butylnonane	C ₁₃ H ₂₈	1588.34, 4.623	184.2186	254682	
4,7-Dimethylhexahydrocyclopentapyran-3-one	C ₁₀ H ₁₆ O ₂	1606.35, 3.982	168.1145	21639	
Tetradecane	C ₁₄ H ₃₀	1612.35, 4.906	198.2342	77183	
Aminoacetonitrile	C ₂ H ₄ N ₂	1618.35, 4.265	56.0369	15303	
1-Methyl-2-propylbenzene	C ₁₀ H ₁₄	1624.35, 2.793	134.109	156612	
3,6-Dimethylhexahydro-1-benzofuran-2(3H)-one	C ₁₀ H ₁₆ O ₂	1624.35, 3.564	168.1145	81045	
2,6,10-Trimethyltridecane	C ₁₆ H ₃₄	1630.35, 4.550	226.2655	52368	
(2S)-2-(2-Tetrahydropyran-2-yl)propanal	C ₈ H ₁₄ O ₃	1630.35, 4.834	158.0937	11561	
3-Methylene-15-methoxypentadecanol	C ₁₈ H ₃₆ O ₃ ?	1636.35, 3.912	300.2659	11582	1.40E-4
Butylbenzene	C ₁₀ H ₁₄	1642.36, 2.805	134.109	14147	
3-Methylundecane	C ₁₂ H ₂₆	1642.36, 4.593	170.2029	376205	
2-Ethylbutyronitrile	C ₆ H ₁₁ N	1648.36, 3.901	97.0886	20942	

Pentylcyclohexane	C ₁₁ H ₂₂	1654.36, 3.888	154.1716	403617	
1-(2-Hydroxyethoxy)tridecane	C ₁₅ H ₃₂ O ₂ ?	1654.36, 4.856	244.2397	10083	1.22E-4
Decahydro-2-methyl-naphthalene	C ₁₁ H ₂₀	1660.36, 3.543	152.156	357694	
(cis)-1-Butyl-2-hexylcyclopropane	C ₁₃ H ₂₆	1666.36, 4.140	182.2029	51292	
4-Ethyl-1,2-dimethylbenzene	C ₁₀ H ₁₄	1672.37, 2.757	134.109	280936	
10-Acetoxydecenal	C ₁₂ H ₂₂ O ₃ ?	1690.37, 4.161	214.1563	309050	3.75E-3
(1R,5S,6S)-5-Methyl-6-carbethoxy-2-oxabicyclo[3.1.0]hexane	C ₉ H ₁₄ O ₃ ?	1702.37, 4.089	170.0937	19545	2.37E-4
(1-Methylpropyl)benzene	C ₁₀ H ₁₄	1714.38, 2.772	134.109	47405	
(Z)-3-(Hydroxymethyl)-7-methylocta-2,6-dien-1-yl acetate	C ₁₂ H ₂₀ O ₃ ?	1720.38, 4.002	212.1407	82626	1.00E-3
E-2-Methyl-3-(phenylsulfonyl)undec-4-ene	C ₁₈ H ₂₈ O ₂ S ?	1720.38, 4.417	308.1805	28713	3.48E-4
3,3,6-Trimethyl-1,2-dioxane	C ₇ H ₁₃ O ₂	1726.38, 4.545	129.091	29348	
1,17-Octadecadiene	C ₁₈ H ₃₄	1738.38, 4.126	250.2655	29165	
2,4,9,11-Tetramethyldodeca-5,7-diene-4,9-diol	C ₁₆ H ₂₆ O ₂ ?	1744.39, 4.783	250.1927	26964	3.27E-4
1-Methyldecahydronaphthalene	C ₁₁ H ₂₀	1756.39, 3.487	152.156	320803	
1-Ethyl-2,4-dimethylbenzene	C ₁₀ H ₁₄	1768.39, 2.751	134.109	52985	
1-Methyl-2-(1-methylethyl)-benzene	C ₁₀ H ₁₄	1780.4, 2.746	134.109	134573	
1-(Hydroxycarbonyl)cyclohexane	C ₇ H ₁₂ O ₂	1786.4, 4.003	128.0832	34268	
2,6-Dimethylundecane	C ₁₃ H ₂₈	1786.4, 4.809	184.2186	2724625	
4-Methylphenyl acetone	C ₁₀ H ₁₂ O	1792.4, 2.952	148.0883	66356	
anti-2-Propylbicyclo[3.1.0]hexane-1,2,8-triene	C ₉ H ₁₆	1804.4, 3.856	124.1247	23267	
2-(4'-Methylphenyl)propanal	C ₁₀ H ₁₂ O ?	1822.41, 2.903	148.0883	57290	6.95E-4
1-Methyl-2-(tricyclo[4.1.0.0(2,7)]hept-1-yl)benzene	C ₁₄ H ₁₆	1822.41, 2.951	184.1247	20060	
1-Methyl-2-pentylcyclohexane	C ₁₂ H ₂₄	1822.41, 4.104	168.1873	308628	
3-Hydroxy-2,2-dimethyl-1-phenyl-1-butanone	C ₁₂ H ₁₆ O ₂ ?	1828.41, 2.935	192.1145	16484	2.00E-4
(3,5-cis)-3-Pentyl-5-methyl-1,2-oxathiolane-(2,3-trans)-2-oxide	C ₉ H ₁₈ O ₂ S ?	1834.41, 4.039	190.1022	46389	5.63E-4
1,2,3,6,7,7a-Hexahydro-1-(2-hydroxy-1-methylethyl)-, 7,3a-(epoxymethano)inden-9-one	C ₁₃ H ₁₈ O ₃ ?	1852.42, 2.924	222.125	23993	2.91E-4
2-Ethyl-dodecane	C ₁₃ H ₂₈ ?	1864.42, 4.721	184.2186	73201	

Nopyldiformamide	C ₁₃ H ₁₉ NO ₂ ?	1882.43, 2.900	221.141	13601	1.65E-4
3,4-Dimethylcumene	C ₁₁ H ₁₆	1888.43, 2.853	148.1247	40741	
3-Ethynyl-2,2-dimethyloxirane	C ₆ H ₈ O	1906.43, 3.391	96.057	10776	
(Z/E)-4-Ethyl-2,2-dimethyl-3-octene	C ₁₂ H ₂₄	1906.43, 3.978	168.1873	41350	
9-(E-2-Propylcyclopropyl)nonan-1-ol	C ₁₅ H ₃₀ O ?	1906.43, 4.159	226.2291	11201	1.36E-4
Ethyl 2,2,4-Trimethyl-5-phenyl-4-pentenoate	C ₁₆ H ₂₂ O ₂ ?	1918.44, 2.741	246.1614	20510	2.49E-4
Hentriacontane	C ₃₁ H ₆₄	1924.44, 4.664	436.5003	102151	
Decahydro-1,6-dimethylnaphthalene	C ₁₂ H ₂₂	1936.44, 3.682	166.1716	310887	
(2-Methylpropyl)cyclohexane	C ₁₀ H ₂₀	1942.44, 3.990	140.156	78749	
3,7,7-Trimethyl-[1S-(1à,2à,6à)]-bicyclo[4.1.0]hept-3-ene-2-thiol	C ₁₀ H ₁₆ S	1948.44, 2.675	168.0967	18248	
2,2-Dimethylanhydrosulfide propanethioic acid	C ₁₀ H ₁₈ O ₂ S ?	1948.44, 4.690	202.1022	18339	2.22E-4
2-[1-(E)-Hexenyl]tetrahydrofuran	C ₁₀ H ₁₈ O ?	1954.45, 4.322	154.1352	23786	2.88E-4
n-Cetyl thiocyanate	C ₁₇ H ₃₃ NS	1954.45, 4.649	283.2328	60263	
1,2,3,4-Tetramethylbenzene	C ₁₀ H ₁₄	1960.45, 2.751	134.109	202047	
5-Hydroxy-1,2,3,4-tetrahydronaphthalen-1-one	C ₁₀ H ₁₂ O ₂ ?	1960.45, 3.675	164.0832	29364	3.56E-4
Ethyl N-cyano-N-pentylcarbamate	C ₉ H ₁₆ N ₂ O ₂ ?	1960.45, 4.315	184.1206	42765	5.19E-4
1-Hexadecene	C ₁₆ H ₃₂	1972.45, 4.264	224.2499	8418	
6-Methyldodecane	C ₁₃ H ₂₈	1972.45, 4.654	184.2186	591451	
3-Ethyl-6-ethylidene-3-methyl-1,4-cyclohexadiene	C ₁₁ H ₁₆	1984.45, 2.873	148.1247	17584	
1,2,3,5-Tetramethylcyclohexane	C ₁₀ H ₂₀	1984.45, 4.181	140.156	227806	
N-Methyl-2-(pyrrolidin-2'-ylideneamino)propionamide	C ₈ H ₁₅ N ₃ O ?	1984.45, 4.283	169.121	33211	4.03E-4
2,4,6-Trimethylnonan-1-ol	C ₁₂ H ₂₆ O ?	1990.46, 4.197	186.1978	37458	4.55E-4
1,2,3,5-Tetramethyl benzene	C ₁₀ H ₁₄	1996.46, 2.715	134.109	367655	
2,2,4-Trimethyl-4-pentenoic acid	C ₈ H ₁₄ O ₂ ?	1996.46, 4.348	142.0988	53960	6.55E-4
4-Methyldodecane	C ₁₃ H ₂₈	2002.46, 4.639	184.2186	182346	
2,3,7-Trimethyloctane	C ₁₁ H ₂₄	2002.46, 4.968	156.1873	1910277	
1-sec-Butyl-4-methylbenzene	C ₁₁ H ₁₆	2020.47, 2.859	148.1247	105595	
Decahydro-1,5-dimethylnaphthalene	C ₁₂ H ₂₂	2044.47, 3.595	166.1716	51022	
Hexacosane	C ₂₆ H ₅₄	2044.47, 4.870	366.422	101393	

3-Methyl-1-undecen-4-ol	C ₁₂ H ₂₄ O ?	2050.47, 4.061	184.1822	12315	1.49E-4
Cyclohexyl 4-cyanobutanoate	C ₁₁ H ₁₇ NO ₂ ?	2056.48, 3.407	195.1254	10149	1.23E-4
Hexylcyclohexane	C ₁₂ H ₂₄	2086.48, 3.929	168.1873	366193	
3-(2'-Methyl-2'-propenyl)cyclopentan-1-one	C ₉ H ₁₄ O	2092.49, 3.899	138.1039	23002	
1-Butyl-2,4,6-trimethylcyclohexane	C ₁₃ H ₂₆	2104.49, 4.078	182.2029	126291	
1-(1,2-Dimethylcyclopentyl)-trans-2-propyn-1-one	C ₁₀ H ₁₄ O ?	2104.49, 4.161	150.1039	38360	4.65E-4
(1S,8R)-1-Methylhexahydro-1H-pyrrolizine [pseudoheliotridane]	C ₈ H ₁₅ N	2110.49, 4.035	125.1199	11858	
Butyl cyclobutyl oxaloate	C ₁₀ H ₁₆ O ₄ ?	2116.49, 4.105	200.1043	24111	2.92E-4
1,4-Dimethyl-cis-cyclooctane	C ₁₀ H ₂₀	2122.49, 4.058	140.156	211355	
[[2-(2-Propenyloxy)-1-propenyl]sulfonyl]-(E)-benzene	C ₁₂ H ₁₄ O ₃ S ?	2134.5, 4.113	238.0658	27814	3.37E-4
2,2-Dimethyl-1-cycloheptane-3-buten-1-ol	C ₁₂ H ₂₂ O ?	2140.5, 3.871	182.1665	27801	3.37E-4
N-Allyl-2-(methylthio)allylamine	C ₇ H ₁₃ NS	2146.5, 4.180	143.0763	11940	
cis,trans-2-Ethylbicyclo[4.4.0]decane	C ₁₂ H ₂₂	2158.5, 3.564	166.1716	158582	
Bicyclo[3.2.2]nona-6,8-dien-3-one, 6,8-dimethyl-	C ₁₁ H ₁₄ O	2170.51, 2.988	162.1039	42486	
1-(2-Ethylphenyl)ethan-1-one	C ₁₀ H ₁₂ O	2176.51, 2.762	148.0883	7291	
1,4-Dimethylcyclooctane	C ₁₀ H ₂₀	2176.51, 4.317	140.156	77392	
3,3,4-Trimethylbenzeneacetaldehyde	C ₁₁ H ₁₄ O	2200.52, 2.937	162.1039	27283	
trans-2-Ethylbicyclo[4.4.0]decane	C ₁₂ H ₂₂	2224.52, 3.511	166.1716	83470	
Cyclotetradecane	C ₁₄ H ₂₈	2224.52, 4.181	196.2186	197594	
1-Methyl-2,3-dihydroindene	C ₁₀ H ₁₂	2230.53, 2.549	132.0934	34520	
Neopentyl 2,2-dimethylpropanoate	C ₁₀ H ₂₀ O ₂ ?	2260.53, 4.697	172.1458	74573	9.05E-4
5-Hexyl-3,3-dimethylcyclopentene	C ₁₃ H ₂₄	2266.54, 3.708	180.1873	117100	
trans-1-Methyl-2-nonylcyclohexane	C ₁₆ H ₃₂	2266.54, 4.123	224.2499	121820	
Isopropyl O-(isobutoxycarbonyl)-2,3,4-trideoxy-4-methyl-D-erythrohex-2-enopyranoside	C ₁₅ H ₂₆ O ₅ ?	2272.54, 3.737	286.1775	14008	1.70E-4
1-Ethyl-4-(1-methylethyl)benzene	C ₁₁ H ₁₆	2308.55, 2.771	148.1247	41320	
2,2-Dimethylindan	C ₁₁ H ₁₄	2320.55, 2.684	146.109	28063	
2,3-Dihydro-1,5,7-trimethyl-1H-indene	C ₁₂ H ₁₆	2320.55, 2.800	160.1247	44858	
1,2,3,4-Tetrahydronaphthalene	C ₁₀ H ₁₂	2332.55, 2.479	132.0934	31092	

2,3-Dihydro-1,6-dimethyl-1H-indene	C ₁₁ H ₁₄	2332.55, 2.664	146.109	63294	
Tetraethylbutanedinitrile	C ₁₂ H ₂₀ N ₂	2332.55, 3.977	192.1621	32388	
Cyclobutyl m-toluate	C ₁₂ H ₁₄ O ₂ ?	2344.56, 2.923	190.0988	26335	3.19E-4
3-Methyl-(E)- 4-nonen-1-ol	C ₁₀ H ₂₀ O ?	2350.56, 3.632	156.1509	16079	1.18E-4
(E)-7-Methyl-5-octenoic acid	C ₉ H ₁₆ O ₂ ?	2350.56, 4.353	156.1145	32223	3.91E-4
1-Octadecanol	C ₁₈ H ₃₈ O	2362.56, 3.998	270.2917	49192	
6-Methyl tridecane	C ₁₄ H ₃₀	2368.56, 4.603	198.2342	381879	
(E)-2-Phenyl-2-pentene	C ₁₁ H ₁₄	2374.57, 2.640	146.109	16766	
2,4-Diethyl-1-methylcyclohexane	C ₁₁ H ₂₂	2374.57, 4.119	154.1716	374027	
1,3-Dimethyl-5-(1-methylethyl)- benzene	C ₁₁ H ₁₆	2380.57, 2.726	148.1247	70146	
2,3-Dihydro-1,1,4-trimethyl-1H-indene	C ₁₂ H ₁₆	2380.57, 2.775	160.1247	55692	
(R,Z)-12-Hydroxy-9-octadecenoic acid	C ₁₈ H ₃₄ O ₃ ?	2380.57, 3.750	298.2502	24648	2.99E-4
Decyl hexyl ester sulfurous acid	C ₁₆ H ₃₄ O ₃ S	2380.57, 4.598	306.2223	141494	
2,3-Dihydro-1,1-dimethyl-1H-indene	C ₁₁ H ₁₄	2386.57, 2.642	146.109	39127	
Pentyl undecyl sulfite	C ₁₆ H ₃₄ O ₃ S ?	2398.57, 4.593	306.2223	203498	2.47E-3
Vinyl neopentanoate	C ₈ H ₁₄ O ₂ ?	2404.58, 4.856	142.0988	92620	1.12E-3
(1R*,5R*-5-Methyl-1-hydroxybicyclo[3.3.1]octane-3-one	C ₁₀ H ₁₆ O ₂ ?	2416.58, 4.188	168.1145	10467	1.27E-4
2-Methyltridecane	C ₁₄ H ₃₀	2416.58, 4.608	198.2342	402203	
3-Acetyl-3-methylcyclohexanone	C ₉ H ₁₄ O ₂ ?	2422.58, 4.204	154.0988	17832	2.16E-4
Cyclohexadecane	C ₁₆ H ₃₂	2434.58, 4.191	224.2499	52464	
Heptadecane	C ₁₇ H ₃₆	2434.58, 4.783	240.2812	1575180	
Nonadecane	C ₁₉ H ₄₀	2440.59, 4.509	268.3125	38686	
2,9-Dimethyldecane	C ₁₂ H ₂₆	2458.59, 4.531	170.2029	359191	
Methyl (1,4-dihydro-4-oxo-1-hydroxynaphthalen-1-yl)-acetate	C ₁₃ H ₁₂ O ₄ ?	2464.59, 2.911	232.073	10382	1.26E-4
3-Acetoxyfuro[3,2-b]pyridine	C ₉ H ₇ NO ₃ ?	2464.59, 3.180	177.042	10443	1.26E-4
S-Butyl cyclohexanecarbothioate	C ₁₁ H ₂₀ OS ?	2470.59, 4.237	200.1229	34524	4.19E-4
2-(2',2'-Dimethyl-1',3'-dioxan-4'-yl)-ethanol	C ₈ H ₁₆ O ₃ ?	2476.6, 2.783	160.1094	13747	1.66E-4
Bicyclo[3.2.2]nona-6,8-dien-3-one, 1,5-dimethyl-	C ₁₁ H ₁₄ O ?	2500.6, 2.903	162.1039	21035	2.55E-4

3-Phenylcyclobutanol	C ₁₀ H ₁₂ O ?	2506.6, 2.581	148.0883	8214	9.87E-5
Heptylcyclohexane	C ₁₃ H ₂₆	2506.6, 3.909	182.2029	355250	
Propynoic acid amide	C ₃ H ₃ NO	2506.6, 3.950	69.0209	9344	
1,2,3,4-Tetrahydro-1,8-dimethylnaphthalene	C ₁₂ H ₁₆	2524.61, 2.738	160.1247	18546	
5,5-Dimethylfuran-2(5H)-one	C ₆ H ₈ O ₂	2548.62, 4.074	112.0519	19640	
(E)-9-Tricosene	C ₂₃ H ₄₆	2566.62, 4.040	322.3594	38886	
5,5-Dimethyl-2(5H)-furanone	C ₆ H ₈ O ₂	2566.62, 4.094	112.0519	17754	
Azulene	C ₁₀ H ₈	2584.63, 2.269	128.0621	26643	
1,4-Dimethyl-2-(2-methylpropyl)benzene	C ₁₂ H ₁₈	2596.63, 2.841	162.1403	37716	
(R)-4-Ethynyl-3,5,5-trimethylcyclohex-3-enyl acetate	C ₁₃ H ₁₈ O ₂ ?	2632.64, 2.604	206.1301	14212	1.72E-4
2,3,4,5-Tetrahydropyridine	C ₅ H ₉ N	2644.64, 4.146	83.073	62311	
1-[(2'-Methylamino-1'-naphthyl)methyl]-2-naphthol	C ₂₂ H ₁₇ NO ?	2674.65, 2.874	311.1305	12239	1.48E-4
(2S,6R)-2,6-Dimethyl-1-octanol	C ₁₀ H ₂₂ O ?	2674.65, 4.034	158.1665	64799	7.87E-4
Tricosane	C ₂₃ H ₄₈	2680.65, 4.576	324.3751	87128	
2,3-Dihydro-1,3-dimethyl-1H-indene	C ₁₁ H ₁₄	2698.66, 2.592	146.109	50864	
3-Oxo-1,3-dihydro-1-isobenzofuranyl phenylacetate	C ₁₆ H ₁₂ O ₄ ?	2716.66, 2.767	268.073	22995	2.79E-4
9,10,11-Trioxabicyclo[6.2.1]undecane	C ₈ H ₁₄ O ₃	2722.67, 4.290	158.0937	18792	
2,2,5,5-tetramethyl-3,4-bis(methylene)cyclopent-1-yl p-toluenesulfonate	C ₁₈ H ₂₄ O ₃ S ?	2728.67, 2.661	320.1441	12921	1.56E-4
2-Methyl-1-pyrroline	C ₅ H ₉ N	2734.67, 3.999	83.073	38615	
1,2,3,4-Tetrahydro-5-methylnaphthalene	C ₁₁ H ₁₄	2746.67, 2.530	146.109	72507	
4,4-Diethyl-2,5-octadiyne	C ₁₂ H ₁₈	2752.68, 2.932	162.1403	14205	
Cyclopentanodec-5-ene	C ₁₅ H ₂₈	2752.68, 4.209	208.2186	78730	
2,6,10,14-Tetramethylheptadecane	C ₂₁ H ₄₄	2752.68, 4.773	296.3438	1683818	
Cyclooctylhydroperoxide	C ₁₂ H ₂₄ O ₂ ?	2758.68, 4.144	200.1771	20846	2.53E-4
spiro[4,5-Dihydro-3-methylisoxazole-5,1'-cyclopropane]	C ₆ H ₉ NO ?	2764.68, 4.241	111.0679	18899	2.29E-4
5-Methyltetradecane	C ₁₅ H ₃₂	2764.68, 4.515	212.2499	164941	
4-Methyl- Tridecane	C ₁₄ H ₃₀	2782.68, 4.521	198.2342	166757	
1-Phenyl-1-undecyn-5-ol	C ₁₇ H ₂₄ O ?	2788.69, 2.817	244.1822	8786	1.06E-4

(E)-6-Tosyl-4-nonene	C ₁₆ H ₂₄ O ₂ S ?	2794.69, 4.056	280.1492	104284	1.26E-3
3-Methyltridecane	C ₁₄ H ₃₀	2800.69, 4.526	198.2342	437619	
1,2,2-Trimethylindan	C ₁₂ H ₁₆	2818.69, 2.674	160.1247	44767	
endo-2,3-Di(methoxycarbonyl)-benzo[e]bicyclo[2.2.2]octane	C ₁₆ H ₁₈ O ₄	2824.7, 2.793	274.12	9665	
2-Methyl-, (E)-3-hexen-5-yn-2-ol	C ₇ H ₁₀ O ?	2836.7, 3.606	110.0726	19126	2.32E-4
2,6,10,15-Tetramethylheptadecane	C ₂₁ H ₄₄	2836.7, 4.474	296.3438	308354	
Methyl 3-methyl-2,4-hexadienoate	C ₈ H ₁₀ O ₄ ?	2842.7, 4.153	170.0574	7877	9.56E-5
4-(Phenylthio)-2,4-dimethyl-2-pentene	C ₁₃ H ₁₈ S	2848.7, 3.838	206.1124	27792	
O-(tert-Butoxycarbonyl)-N-isopropylidene oxime	C ₈ H ₁₅ NO ₃	2884.71, 4.181	173.1046	7946	
1-Heptadecanol	C ₁₇ H ₃₆ O ?	2896.72, 3.911	256.2761	94026	1.14E-3
1-Methoxybicyclo(3.2.1)octane	C ₉ H ₁₆ O	2896.72, 4.142	140.1196	18753	
Octylcyclohexane	C ₁₄ H ₂₈	2908.72, 3.873	196.2186	299890	
2,3-Dihydro-1,1,4,6-tetramethyl-1H-indene	C ₁₃ H ₁₈	2926.73, 2.730	174.1403	33243	
2,2-dimethyl-5-hexen-1-ol tosylate	C ₁₅ H ₂₃ O ₃ S ?	2926.73, 4.132	283.1362	24887	3.02E-4
1-Eicosanol	C ₂₀ H ₄₂ O ?	2944.73, 4.213	298.323	90814	1.10E-4
2,3-Dihydro-1,4,7-trimethyl-1H-indene	C ₁₂ H ₁₆	2962.74, 2.584	160.1247	11279	
1,2-Dibutyl-trans-cyclopropane	C ₁₁ H ₂₂	2974.74, 4.298	154.1716	27741	
1-Tetradecanol	C ₁₄ H ₃₀ O ?	3016.75, 4.102	214.2291	135772	1.64E-4
1-Ethylidene-1H-indene	C ₁₁ H ₁₀	3022.75, 2.319	142.0777	165945	
3-Methoxy-1-propyne	C ₄ H ₆ O	3022.75, 4.149	70.0413	61177	
1-Methyl-3-(2-methylpropyl)cyclopentane	C ₁₀ H ₂₀	3040.76, 4.047	140.156	177458	
1-Octyl-1,4-dihydronaphthalene	C ₁₈ H ₂₆	3052.76, 2.514	242.2029	12070	
Hexadecane	C ₁₆ H ₃₄	3070.77, 4.461	226.2655	85225	
7-Methylpentadecane	C ₁₆ H ₃₄	3106.78, 4.469	226.2655	505545	
3-Benzyl-4-ethyl-4-methyl-oxetan-2-one	C ₁₃ H ₁₆ O ₂ ?	3118.78, 2.534	204.1145	13478	1.63E-4
(E)-1-[2'-(3",4",4"-Trimethylpent-1"-yl)phenyl]ethanone	C ₁₆ H ₂₂ O ?	3154.79, 2.713	230.1665	17376	2.11E-4
(1S,2R)-6,6-Dimethyl-2-ethylbicyclo[3.1.1]heptan-3-one	C ₁₁ H ₁₈ O ?	3202.8, 4.068	166.1352	11060	1.34E-4
2,6,8-Trimethyldecane	C ₁₃ H ₂₈	3244.82, 4.567	184.2186	325128	

2-(1,1-Dimethylethyl)-3(2H)-pyridazinone	C ₈ H ₁₂ N ₂ O	3256.82, 4.014	152.0944	48529	
5-Acetyllongipinandioline	C ₁₇ H ₂₆ O ₄ ?	3262.82, 4.068	294.1826	28325	3.44E-4
1,2,3,4-Tetrahydro-5,7-dimethylnaphthalene	C ₁₂ H ₁₆	3274.82, 2.506	160.1247	73070	
1,2,3,4-Tetrahydro-1,1,6-trimethylnaphthalene	C ₁₃ H ₁₈	3274.82, 2.693	174.1403	21535	
1,3-Dimethyl-2-pentylidene cyclohexanecarboxaldehyde	C ₁₄ H ₂₄ O ?	3286.83, 3.754	208.1822	12501	1.51E-4
(5S,7S,9S,E)-S-Ethyl 5,7,9-trimethyltridec-3-enethioate	C ₁₈ H ₃₄ OS ?	3298.83, 4.063	298.2325	50733	6.16E-4
1-Cyano-2,6-dimethyl-1,5-heptadien-3-ol	C ₁₀ H ₁₅ NO ?	3304.83, 4.257	165.1148	11847	1.43E-4
1-Ethyl-naphthalene	C ₁₂ H ₁₂	3382.86, 2.367	156.0934	30497	
1,7-Dimethylnaphthalene	C ₁₂ H ₁₂	3418.87, 2.386	156.0934	272739	
Methyl 3-(p-nitrophenyl)bicyclo[1.1.1]pentane-1-carboxylate	C ₁₃ H ₁₃ NO ₄	3430.87, 2.536	247.0839	7990	
Tritriacontane	C ₃₃ H ₆₈	3454.88, 4.397	464.5316	429391	
3,6-Dihydro-4-phenyl-1-oxide-2H-thiopyran	C ₁₁ H ₁₂ OS	3466.88, 2.524	192.0603	9899	
(E)-3-Octen-2,5-dione	C ₈ H ₁₂ O ₂	3478.88, 3.918	140.0832	57040	
3,8-Dimethylundecane	C ₁₃ H ₂₈	3496.89, 4.377	184.2186	142538	
1,6-Dimethylnaphthalene	C ₁₂ H ₁₂	3502.89, 2.345	156.0934	122237	
1-Phenyl-2,3-diazabicyclo[2.2.1]hept-2-ene	C ₁₁ H ₁₂ N ₂	3520.9, 2.475	172.0995	21334	
2,6,11-Trimethyldodecane	C ₁₅ H ₃₂	3586.91, 4.742	212.2499	1839748	
1,2-Dimethylnaphthalene	C ₁₂ H ₁₂	3622.92, 2.305	156.0934	21643	
Undecylcyclohexane	C ₁₇ H ₃₄	3652.93, 3.811	238.2655	201593	
1,2-Epoxy-3-tetradecanol	C ₁₄ H ₂₈ O ₂ ?	3718.95, 3.971	228.2084	33183	4.03E-4
2-(1,3-Dioxolan-2-yl)-1-(2-furyl)ethane	C ₉ H ₁₀ O ₃ ?	3724.95, 4.387	166.0624	46807	5.68E-4
3,5- <i>trans</i> -3-Hydroxy-5-[(E)-1-pentenyl]-4,5-dihydro-2(3H)-furanone	C ₉ H ₁₄ O ₃ ?	3748.96, 4.015	170.0937	37678	4.57E-4
2-(1-Methylethyl)naphthalene	C ₁₃ H ₁₄	3754.96, 2.433	170.109	32394	
1,4,5-Trimethylnaphthalene	C ₁₃ H ₁₄	3766.97, 2.418	170.109	46919	
4-Methyl-1,1'-biphenyl	C ₁₃ H ₁₂	3772.97, 2.271	168.0934	26430	
Heneicosane	C ₂₁ H ₄₄	3826.98, 4.339	296.3438	136147	
5,7-Dimethyl-1,4-dihydro-1,4-methanonaphthalene	C ₁₃ H ₁₄	3844.99, 2.358	170.109	14779	
endo-7-(3-Carboxy-3-butenyl)-8-hexyl-2,9-dioxabicyclo[4,3,0]nonane	C ₂₀ H ₃₄ O ₄ ?	3850.99, 4.254	338.2452	21742	2.64E-4

4-(2-Tetrahydropyranyl)oxybutanal	C ₉ H ₁₆ O ₃ ?	3947.02, 4.410	172.1094	28861	3.50E-4
1,4,6-Trimethylnaphthalene	C ₁₃ H ₁₄	3965.02, 2.381	170.109	194557	
(2E)-1-O-Acetyl-3,7-dimethyl-2-octen-1-ol 6,7-epoxide	C ₁₂ H ₂₀ O ₃ ?	4103.06, 4.299	212.1407	36585	4.44E-4
n-Octyl ethynyl ether	C ₁₀ H ₁₈ O ?	4109.06, 4.292	154.1352	74433	9.04E-4
4-Methylundecane	C ₁₂ H ₂₆	4145.07, 4.281	170.2029	63718	
2-(Hydroxymethyl)-5-hexyltetrahydrofuran	C ₁₁ H ₂₂ O ₂ ?	4157.08, 2.431	186.1614	8459	1.02E-4
Dehydrochamazulene	C ₁₄ H ₁₄	4163.08, 2.315	182.109	16743	
(2S)-2-(1-Ethyl-1-methoxypropyl)-N-((E)-1-[(3-methyl-2-butenyl)oxy]methyl}propylidene)-1-pyrrolidinamine	C ₁₉ H ₃₆ N ₂ O ₂ ?	4175.08, 4.106	324.2771	24984	3.03E-4
Neopentyl 2-oxobutanoate	C ₉ H ₁₆ O ₃ ?	4193.09, 4.263	172.1094	151023	1.83E-3
(E)-Deca-1,6-dien-3-one	C ₁₀ H ₁₆ O ?	4211.09, 4.524	152.1196	6853	8.32E-5
2,3,3,6,6,7-Hexamethyl-1,4,7-octatriene	C ₁₄ H ₂₄	4223.1, 3.974	192.1873	23453	
((Z)-Hept-5-ene-1,3-diynyl)-benzene	C ₁₃ H ₁₀	4253.11, 2.202	166.0777	11613	
3-Ethylcosane	C ₂₂ H ₄₆	4265.11, 4.519	310.3594	65264	
Heptacosane	C ₂₇ H ₅₆	4289.12, 4.202	380.4377	2063047	
2,2-Dimethyl-3-heptanone	C ₉ H ₁₈ O ?	4307.12, 4.458	142.1352	19587	2.37E-4
3-(1,1-Dimethylethoxy)-1-propene	C ₇ H ₁₄ O	4307.12, 4.556	114.1039	16529	
1,4,5,8-Tetramethylnaphthalene	C ₁₄ H ₁₆	4367.14, 2.417	184.1247	53765	
(Dodecyloxy)methyl isonitrile	C ₁₄ H ₂₇ NO ?	4385.14, 3.937	225.2087	107405	1.30E-3
Methyl (1RS,3RS,4SR)-3,4-epoxycyclohexanecarboxylate	C ₈ H ₁₂ O ₃ ?	4475.17, 3.838	156.0781	35088	4.26E-4
Tetracosane	C ₂₄ H ₅₀	4493.17, 4.224	338.3907	121644	
Heptane	C ₇ H ₁₆	4505.18, 4.491	100.1247	43187	
2H-3,4-Dihydro-5-methylpyrrole	C ₄ H ₁₁ N	4601.21, 3.792	73.0886	26459	
5,5-Diphenylpentanoic acid	C ₁₇ H ₁₈ O ₂ ?	4613.21, 2.244	254.1301	24524	2.97E-4
2-Methylene-3-butenylamine	C ₅ H ₉ N	4625.21, 3.763	83.073	69726	
9-Methyl-9H-fluorene	C ₁₄ H ₁₂	4649.22, 2.235	180.0934	34450	
cis-Bicyclo[3.3.0]octan-1-ol	C ₈ H ₁₄ O ?	4679.23, 3.952	126.1039	34498	4.19E-4
2,3-Dimethyl-9H-fluorene	C ₁₅ H ₁₄	5087.35, 2.253	194.109	7495	
1,4-Bis(cyclohex-1-enyl)buta-1,3-diyne	C ₁₆ H ₁₈	5207.38, 4.235	210.1403	40009	

3- <i>tert</i> -Butyl-1,2-dimethoxy-5-methylbenzene	C ₁₃ H ₂₀ O ₂ ?	5255.39, 2.359	208.1458	21832	2.65E-4
1,4-Dihydro-4,4-dimethyl-1,3-diphenylisoquinoline	C ₂₃ H ₂₁ N	5273.4, 2.353	311.1669	10750	
2-Ethyl-(1 α ,2 α ,5 α)-6-oxabicyclo[3.1.0]hexan-2-ol	C ₇ H ₁₂ O ₂ ?	5279.4, 4.162	128.0832	42444	5.15E-4
9,10-Dihydro-9,10-dimethylanthracene	C ₁₆ H ₁₆	5291.4, 2.349	208.1247	17524	
6a,10b-Dihydro-6a,10b-dimethyl-trans-cyclopentaheptalene	C ₁₆ H ₁₆	5321.41, 2.329	208.1247	9000	
7-Phenylindene	C ₁₅ H ₁₂	5459.45, 2.164	192.0934	26744	
9,10-Dihydro-3,6-dimethylphenanthrene	C ₁₆ H ₁₆	5465.45, 2.331	208.1247	9621	
2,7-Dimethylphenanthrene	C ₁₆ H ₁₄	5669.51, 2.233	206.109	9378	
3,6-Dimethylphenanthrene	C ₁₆ H ₁₄	5717.53, 2.235	206.109	73731	
2-(2-Oxopropyl)-cyclopentanone	C ₈ H ₁₂ O ₂ ?	5729.53, 3.751	140.0832	29634	3.59E-4
2,2-Dimethylpentane	C ₇ H ₁₆	5801.55, 4.235	100.1247	27923	
(3R)-3-Phenyl-2,3-dihydro-1H-isoindol-1-one	C ₁₄ H ₁₁ NO ?	6563.77, 1.096	209.0835	743078	9.02E-3
<i>cis</i> - and <i>trans</i> -3,6-Dicetoxy-1-cyclohexene	C ₁₀ H ₁₄ O ₄ ?	6971.89, 1.084	198.0887	9769	1.18E-4
4-Methylhexanoic acid	C ₇ H ₁₄ O ₂ ?	7325.99, 4.679	130.0988	51542	6.26E-4
(1S,2S)-N-Amino-2-methylamino-1-phenyl-1-propanol	C ₁₁ H ₁₆ N ₂ O ?	7349.99, 1.158	192.1257	30680	3.72E-4
5,10-Dihydro-4H-cyclopenta[b]thieno[6,5-b]quinoline-4,5-dione	C ₁₄ H ₇ NO ₂ S ?	7698.09, 1.712	253.0192	101633	1.23E-3
1-(6,6-Dicyano-1,3,5-hexatrienyl)-1,3,5-cycloheptatriene	C ₁₅ H ₁₂ N ₂	7884.15, 0.648	220.0995	21032	
5-(Pyridine-4-yl)-1,3,4-oxadiazole-2-(3H)-thione	C ₇ H ₅ N ₃ OS	7902.15, 1.204	179.0148	12351	
Ethyl N-[(9-fluorenyl)methoxycarbonyl]-DL-dithioalanine	C ₂₀ H ₂₁ NO ₂ S ₂ ?	8064.2, 1.208	371.1008	11800	1.43E-4
(S)-(E)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C ₂₀ H ₂₈ O ₃ ?	8160.23, 1.111	316.2033	135274	1.64E-3
[(Methylbenzyl)oxy](methoxy)methyl	C ₁₀ H ₁₄ O ₂ ?	8196.24, 1.080	166.0988	10058	1.22E-4
3,4-Dihydro-2,4-diphenyl-7,12-methanocyclodeca[b]pyridine	C ₂₇ H ₂₁ N	8196.24, 1.285	359.1669	16551	

Table 2S16. Data obtained for the distillate fraction of condensate-like oil 5 by using GCxGC/(+EI)-TOF MS. Data provided are based on ChromaTOF software prediction of the molecular ion *m/z* value and the identification of the compound by using the EI mass spectral library match using a match factor threshold of 800. Formulas with a question mark “?” might not have been accurately identified. The ratio of the peak area of each of these questionable compounds relative to all peak areas of the detected compounds is provided in the table below

Name	Formula	Retention Times (s) on the Primary, Secondary Column	Molecular Ion <i>m/z</i>	Chromatographic Peak Area	Ratio (Peak area/total sum of peak areas)	
3-Methylheptane	C ₈ H ₁₈	406.002, 2.402	114.1403	169906		
1,1,3,4-Tetramethyl-cis-cyclopentane	C ₉ H ₁₈	412.003, 2.448	126.1403	32752		
4-Methylpropiolactam	C ₄ H ₇ NO	418.005, 2.383	85.0522	8125		
1,1,2-Trimethylcyclopentane	C ₈ H ₁₆	424.007, 2.304	112.1247	176745		
2,4-Dimethylhexane	C ₈ H ₁₈	442.012, 2.597	114.1403	512088		
1,3-Dimethyl-cis-cyclohexane	C ₈ H ₁₆	454.016, 2.386	112.1247	1909811		
4-Methyl-1-heptanol	C ₈ H ₁₈ O	454.016, 2.607	130.1352	67932		
3-Methylundecane	C ₁₂ H ₂₆	460.017, 2.793	170.2029	379081		
1,1-Dimethylcyclohexane	C ₈ H ₁₆	478.022, 2.422	112.1247	649319		
2,6-Dimethylheptane	C ₉ H ₂₀	478.022, 2.875	128.156	596482		
1,2-Dimethylcyclohexane	C ₈ H ₁₆	496.028, 2.501	112.1247	638086		
(2S,1'S)-(-)-2-(1-Hydroxy-6-methylheptyl)-2,5-dihydrofuran	C ₁₂ H ₂₂ O ₂ ?	496.028, 2.693	198.1614	83464		7.93E-4
3,5-Dimethylheptane	C ₉ H ₂₀	496.028, 2.916	128.156	1131183		
1,4-Dimethyl-cyclohexane	C ₈ H ₁₆	514.033, 2.535	112.1247	592032		
6-Methylheptan-1-ol	C ₈ H ₁₈ O	514.033, 2.777	130.1352	15811		
1,3,5-Trimethylcyclohexane	C ₉ H ₁₈	538.04, 2.777	126.1403	300219		
5-Ethyldecane	C ₁₁ H ₂₄	550.043, 3.093	156.1873	162299		
1,1,3-Trimethylno space cyclohexane	C ₉ H ₁₈	562.047, 2.808	126.1403	1490003		
4-Methyloctane	C ₉ H ₂₀	562.047, 3.131	128.156	678506		
1,7-Dial-2-heptene	C ₇ H ₁₀ O ₂	574.05, 2.664	126.0675	17119		
6-Methylundecane	C ₁₂ H ₂₆	580.052, 3.194	170.2029	1235637		
Ethylcyclohexane	C ₈ H ₁₆	586.053, 2.685	112.1247	501599		

1,2,4-trimethylcyclohexane	C ₉ H ₁₈	592.055, 2.911	126.1403	608681		
1-Nonadecanol	C ₁₉ H ₄₀ O ?	592.055, 3.117	284.3074	14317	1.36E-4	
Methylbenzene,	C ₇ H ₈	598.057, 2.057	92.0621	104019		
1,1,3,5-Tetramethylcyclohexane	C ₁₀ H ₂₀	652.072, 3.206	140.156	320680		
Nonane	C ₉ H ₂₀	658.074, 3.389	128.156	761784		
trans-1-Ethyl-4-methyl-cyclohexane	C ₉ H ₁₈	706.088, 3.096	126.1403	1040919		
3,5-Dimethyloctane	C ₁₀ H ₂₂	706.088, 3.682	142.1716	1093105		
2,6-Dimethyloctane,	C ₁₀ H ₂₂	736.096, 3.734	142.1716	1543047		
1,2-Dibutyl-cis-cyclopropane	C ₁₁ H ₂₂	742.098, 3.489	154.1716	11320		
(Z)-5-Undecen-1-ol	C ₁₁ H ₂₂ O ?	754.102, 2.740	170.1665	39230		3.72E-4
3,6-Dimethyloctane	C ₁₀ H ₂₂	760.103, 3.770	142.1716	432462		
N-1-Methyl-6-(1'-piperidinyl)hexyl-1-amine	C ₁₂ H ₂₆ N ₂	766.105, 3.804	198.2091	12810		
1-Ethyl-4-methylcyclohexane	C ₉ H ₁₈	778.109, 3.163	126.1403	582755		
Heptanal	C ₇ H ₁₄ O	790.112, 3.763	114.1039	72771		
1-Ethyl-1-methylcyclohexane	C ₉ H ₁₈	808.117, 3.137	126.1403	173691		
(+)-(S)-1-Butyl-2-methylenecyclopentane	C ₁₀ H ₁₈	814.119, 2.734	138.1403	22288		
4-Ethyloctane	C ₁₀ H ₂₂	814.119, 3.831	142.1716	799473		
trans-1,1,3,5-Tetramethylcyclohexane	C ₁₀ H ₂₀	820.121, 3.410	140.156	267160		
4-Methylnonane	C ₁₀ H ₂₂	832.124, 3.903	142.1716	1548636		
3-Nonyne	C ₉ H ₁₆	838.126, 2.978	124.1247	174285		
3,4-Di(ethyl)-3-hexene	C ₁₀ H ₂₀	838.126, 3.493	140.156	205010		
1-Azido-1-ethenylcyclopropane	C ₅ H ₇ N ₃	844.127, 3.153	109.0634	20279		
1,2-Diethyl-3-methylcyclohexane	C ₁₁ H ₂₂	850.129, 3.494	154.1716	378334		
Propylcyclohexane	C ₉ H ₁₈	856.131, 3.275	126.1403	338322		
3-Methylnonane	C ₁₀ H ₂₂	868.134, 3.924	142.1716	749919		
cis-Octahydro-1H-indene	C ₉ H ₁₆	874.136, 3.082	124.1247	119334		
2,3,3-Trimethyl-(Z)- 4-nonene	C ₁₂ H ₂₄	874.136, 3.538	168.1873	174139		
1,7,7-Trimethyl-bicyclo[2.2.1]heptane	C ₁₀ H ₁₈	886.14, 2.975	138.1403	9472		
1,2-Dimethylbenzene	C ₈ H ₁₀	904.145, 2.407	106.0777	163761		

3-Methoxy-1-propyne	C ₄ H ₆ O	910.146, 3.478	70.0413	24350	
2,6,10-Trimethyltridecane	C ₁₆ H ₃₄	916.148, 4.257	226.2655	91976	
1-Ethyl-trans-1,3-dimethylcyclohexane	C ₁₀ H ₂₀	922.15, 3.559	140.156	621883	
1,1,2,3-Tetramethylcyclohexane	C ₁₀ H ₂₀	940.155, 3.461	140.156	202761	
4-Methylundecane	C ₁₂ H ₂₆	946.157, 4.238	170.2029	54013	
Di-N-methylpentan-2,3-imine	C ₇ H ₁₄ N ₂	952.158, 3.398	126.1151	5961	
1-Ethyl-1,3-dimethyl-cis-cyclohexane	C ₁₀ H ₂₀	952.158, 3.518	140.156	266473	
3,7,7-Trimethyl-1,3,8-nonatrien-5-one	C ₁₂ H ₁₈ O ?	952.158, 3.565	178.1352	15848	1.50E-4
2,2-Dimethyl-3,5-diphenyl-1-oxide-2H-pyrrole	C ₁₈ H ₁₇ NO ?	952.158, 3.769	263.1305	15138	1.43E-4
Decane	C ₁₀ H ₂₂	976.165, 4.063	142.1716	1985109	
1-Isopropyl-4-methylcyclohexane	C ₁₀ H ₂₀	982.167, 3.574	140.156	325676	
2,4-Dimethyldecane	C ₁₂ H ₂₆	994.171, 4.294	170.2029	435063	
1-Methyl-3-propyl-cyclohexane	C ₁₀ H ₂₀	1006.17, 3.657	140.156	505881	
trans-1-Methyl-4-(1-methylethyl)cyclohexane	C ₁₀ H ₂₀	1018.18, 3.662	140.156	340150	
1,4-Dimethylbenzene	C ₈ H ₁₀	1024.18, 2.427	106.0777	73255	
2,6-Dimethylnonane	C ₁₁ H ₂₄	1024.18, 4.351	156.1873	1774353	
1,5-Diethyl-2,3-dimethyl-cyclohexane	C ₁₂ H ₂₄	1054.19, 3.885	168.1873	99866	
6-Ethyl-2-methyloctane	C ₁₁ H ₂₄	1054.19, 4.330	156.1873	503297	
1-(2-Propynyloxy)-2-butene	C ₇ H ₁₀ O	1072.19, 3.387	110.0726	42115	
Methyl benzenesulphinate	C ₁₈ H ₂₈ O ₂ S ?	1078.19, 3.859	308.1805	44289	4.20E-4
2,4-Di(dimethylethyl)-2-methyl-2,5-dihydro-1H-imidazole	C ₁₂ H ₂₄ N ₂ ?	1078.19, 3.923	196.1934	17418	1.65E-4
2,9-Dimethyldecane	C ₁₂ H ₂₆	1078.19, 4.366	170.2029	565415	
(1S,2S)-1-Amino-2-propylcyclopropanecarbonitrile	C ₇ H ₁₂ N ₂	1090.2, 3.427	124.0995	23082	
1-Methyl-4-(1-methylethyl)-cyclohexane	C ₁₀ H ₂₀	1096.2, 3.631	140.156	231973	
2-Ethyl-4-methyl-1H-imidazole	C ₆ H ₁₀ N ₂	1096.2, 3.785	110.0838	20016	
3,7-Dimethylnonane	C ₁₁ H ₂₄	1102.2, 4.335	156.1873	475618	
5,6-Epoxy-6-methyl-1,9-decadien-4-one	C ₁₁ H ₁₆ O ₂ ?	1126.21, 3.917	180.1145	64743	6.15E-4
rac-(+)-2-(tert-Butylsulfonyl)pentyl acetate	C ₁₁ H ₂₂ O ₄ S	1126.21, 4.324	250.1233	14237	
2-Methylundecane	C ₁₂ H ₂₆	1138.21, 4.690	170.2029	30465	

6-Ethyltridecane	C ₁₄ H ₃₀	1144.21, 4.377	198.2342	379146	
2-methylnonane	C ₁₀ H ₂₂	1168.22, 4.361	142.1716	105947	
2,6,6-Trimethyl bicyclo[3.1.1]heptane	C ₁₀ H ₁₈	1180.22, 3.640	138.1403	20311	
2,2-Dimethylundecane	C ₁₃ H ₂₈	1180.22, 4.709	184.2186	41243	
4-Methyldecane	C ₁₁ H ₂₄	1192.23, 4.384	156.1873	509049	
2-Methyldecane	C ₁₁ H ₂₄	1198.23, 4.433	156.1873	610534	
Butylcyclohexane	C ₁₀ H ₂₀	1234.24, 3.682	140.156	404759	
3-Methyldecane	C ₁₁ H ₂₄	1234.24, 4.413	156.1873	554663	
Ethylcyclooctane	C ₁₀ H ₂₀	1240.24, 3.929	140.156	169894	
4,9-Dimethyl-7-oxabicyclo[4.3.0]nonan-8-one	C ₁₀ H ₁₆ O ₂ ?	1246.24, 3.688	168.1145	14545	1.38E-4
2,2,5-Trimethylhexane	C ₉ H ₂₀	1258.25, 4.673	128.156	16313	
(1-Methylethyl)benzene	C ₉ H ₁₂	1264.25, 2.623	120.0934	64517	
3,3,6-Trimethyl-1,2-dioxane	C ₇ H ₁₃ O ₂	1264.25, 3.932	129.091	36607	
1-Isopropyl-2-((phenylthio)methyl)cyclopentene	C ₁₅ H ₂₀ S	1276.25, 3.615	232.128	9355	
Tetrahydro-2-furanpropanenitrile	C ₇ H ₁₁ NO	1276.25, 4.694	125.0835	21980	
Mesitylene	C ₉ H ₁₂	1288.25, 2.654	120.0934	397011	
1-Methyl-2-(2'-methylprop-2'-enyl)cyclododecan-1-ol	C ₁₇ H ₃₂ O ?	1300.26, 3.901	252.2448	26671	2.53E-4
4,4,7,7-Tetramethyl-1,9-decadiene	C ₁₄ H ₂₆	1312.26, 4.277	194.2029	105641	
2,2,5-Trimethyl-(S)-6-hepten-1-ol	C ₁₀ H ₂₀ O ?	1318.26, 3.927	156.1509	57926	5.50E-4
Cacospongin A	C ₂₀ H ₃₀ O ?	1330.27, 3.622	286.2291	21494	2.04E-4
2-Methyl-4-hexyn-3-ol	C ₇ H ₁₂ O	1330.27, 4.356	112.0883	85574	
2,2,4,5-Tetramethylhex-5-en-3-one	C ₁₀ H ₁₄ O ?	1342.27, 4.691	150.1039	62765	5.96E-4
Octacosane	C ₂₈ H ₅₈	1348.27, 4.651	394.4533	129622	
Dodecane	C ₁₂ H ₂₆	1366.28, 4.413	170.2029	4046704	
4-(1-Methylethylidene)bicyclo[3.1.0]hex-2-ene	C ₉ H ₁₂	1372.28, 2.602	120.0934	18414	
Dotriacontane	C ₃₂ H ₆₆	1372.28, 4.660	450.5159	49812	
cis-1-Ethyl-4-methylcyclohexane	C ₉ H ₁₈	1384.28, 3.902	126.1403	127255	
1,2,4,6-Tetraeneheptane	C ₇ H ₈	1402.29, 2.828	92.0621	11088	

1,2,4-Trimethylbenzene	C ₉ H ₁₂	1414.29, 2.664	120.0934	292327	
2,4,6,8-Tetramethylundecene	C ₁₅ H ₃₀	1414.29, 4.227	210.2342	137781	
3,9-Epoxy-p-menthan-9-one	C ₁₀ H ₁₆ O ₂ ?	1420.29, 3.535	168.1145	28855	2.74E-4
3,3-Dimethylhexane	C ₈ H ₁₈	1420.29, 4.675	114.1403	432137	
Bis(2-cyclohexyl-1-methylethyl)-1,2-dioxidediazene	C ₁₈ H ₃₄ N ₂ O ₂	1426.29, 3.776	310.2615	32449	3.08E-4
1-Ethyl-2-propylcyclohexane	C ₁₁ H ₂₂	1438.3, 3.945	154.1716	297536	
3,7-Dimethyldecane	C ₁₂ H ₂₆	1444.3, 4.644	170.2029	768556	
Decahydronaphthalene	C ₁₀ H ₁₈	1468.31, 3.343	138.1403	151938	
2-Methyl-4-(2-methylpropyl)cyclopentanone	C ₁₀ H ₁₈ O ?	1468.31, 3.934	154.1352	447746	4.25E-3
Tetradecane	C ₁₄ H ₃₀	1468.31, 4.644	198.2342	329958	
Isobutylbenzene	C ₁₀ H ₁₄	1492.31, 2.768	134.109	51406	
3,3-Dimethyl-1-nonyne	C ₁₁ H ₂₀	1522.32, 3.493	152.156	4336	
7-Methylpentadecane	C ₁₆ H ₃₄	1528.32, 4.594	226.2655	279199	
Octadecane	C ₁₈ H ₃₈	1540.33, 4.892	254.2968	31246	
3-Ethoxy-1-propyne	C ₅ H ₈ O	1552.33, 4.136	84.057	137533	
1,2,3-Trimethylbenzene	C ₉ H ₁₂	1588.34, 2.613	120.0934	67729	
1-Methyl-3-(1-methylethyl)-cyclopentane	C ₉ H ₁₈	1594.34, 3.817	126.1403	22942	
2,5,9-Trimethyldecane	C ₁₃ H ₂₈	1606.35, 4.922	184.2186	479568	
(E)-2,3-Epoxytetradecan-1-ol	C ₁₄ H ₂₈ O ₂ ?	1630.35, 4.184	228.2084	70100	6.66E-4
(1-Methylpropyl)benzene	C ₁₀ H ₁₄	1636.35, 2.806	134.109	23460	
Pentyl-cyclohexane	C ₁₁ H ₂₂	1654.36, 3.873	154.1716	502385	
Decahydro-2-methylnaphthalene	C ₁₁ H ₂₀	1660.36, 3.543	152.156	106838	
Ethyl 5-(1-dimethylaminoethylidene)cyclopenta-1,3-dienyl]hydroxyacetate	C ₁₃ H ₁₉ NO ₃ ?	1666.36, 4.785	237.1359	29568	2.80E-4
4-Ethyl-1,2-dimethylbenzene	C ₁₀ H ₁₄	1672.37, 2.757	134.109	223735	
1,2-di[p-Methylbenzoyloxy-(p-tolyl)]ethene	C ₃₂ H ₂₈ O ₄	1678.37, 2.744	476.1982	9764	
1,3-Dimethyladamantane	C ₁₂ H ₂₀	1690.37, 3.525	164.156	50328	
1-Isobutyl-2,5-dimethylcyclohexane	C ₁₂ H ₂₄	1690.37, 4.150	168.1873	406912	
1-Methylimidazole-5-carbaldehyde	C ₅ H ₆ N ₂ O	1696.37, 4.164	110.0475	16321	

2-(1-Phenylethyl)phenol	C ₁₄ H ₁₄ O ?	1702.37, 4.755	198.1039	25134	2.38E-4
1,17-Octadecadiene	C ₁₈ H ₃₄	1720.38, 4.061	250.2655	53775	
1-Methyldecahydronaphthalene	C ₁₁ H ₂₀	1756.39, 3.489	152.156	68107	
Diocetyl disulfide	C ₁₆ H ₃₄ S ₂	1762.39, 4.731	290.2096	33028	
1-Ethyl-2,3-dimethylbenzene	C ₁₀ H ₁₄	1768.39, 2.748	134.109	33328	
cis-1-Butyl-2-undecylcyclopropane	C ₁₈ H ₃₆	1768.39, 4.391	252.2812	57743	
Pentadecane	C ₁₅ H ₃₂	1768.39, 4.752	212.2499	161040	
Tridecane	C ₁₃ H ₂₈	1774.39, 4.536	184.2186	6196757	
2,6-Dimethylundecane	C ₁₃ H ₂₈	1786.4, 4.798	184.2186	5345893	
(1-Methylbutyl)benzene	C ₁₁ H ₁₆	1792.4, 2.942	148.1247	80220	
3-Acetyl-3-methylcyclohexanone	C ₉ H ₁₄ O ₂	1792.4, 4.316	154.0988	31137	
1-Methyl-3-propyl-cyclooctane	C ₁₂ H ₂₄	1810.4, 4.132	168.1873	69988	
1-Methyl-4-(1-methylethyl)-benzene	C ₁₀ H ₁₄	1822.41, 2.904	134.109	57972	
3-Phenyl-2-butanone	C ₁₀ H ₁₂ O	1822.41, 2.946	148.0883	46989	
1-Methyl-2-pentyl-cyclohexane	C ₁₂ H ₂₄	1822.41, 4.094	168.1873	618065	
2,6,10-Trimethyldodecane	C ₁₅ H ₃₂	1834.41, 4.731	212.2499	1301290	
(4-Methylphenyl)propanoic acid	C ₁₀ H ₁₂ O ₂ ?	1852.42, 2.905	164.0832	24368	2.31E-4
1,1'-(1,2-Dimethyl-1,2-ethanediyl)bis-cyclohexane	C ₁₆ H ₃₀	1852.42, 4.063	222.2342	180013	
Decahydro-2,2-dimethylnaphthalene	C ₁₂ H ₂₂	1858.42, 3.692	166.1716	66059	
Methylcyclohexane-methyl amine	C ₈ H ₁₇ N	1864.42, 4.288	127.1356	24547	
2,2-Dimethyl-3-butenal	C ₆ H ₁₀ O	1870.42, 4.060	98.0726	30717	
3-Phenylbutanal	C ₁₀ H ₁₂ O ?	1882.43, 2.897	148.0883	13009	1.23E-4
(S)-Undec-1-en-4-ol	C ₁₁ H ₂₂ O ?	1882.43, 4.048	170.1665	22126	2.10E-4
3,4-Dimethylcumene	C ₁₁ H ₁₆	1888.43, 2.854	148.1247	60767	
(1-Methylpropyl)-cyclohexane	C ₁₀ H ₂₀	1900.43, 4.027	140.156	182248	
5,5-Dimethylfuran-2(5H)-one	C ₆ H ₈ O ₂	1936.44, 4.338	112.0519	37964	
2,7,10-Trimethyldodecane	C ₁₅ H ₃₂	1936.44, 4.963	212.2499	326229	
(3-Methylpentyl)cyclohexane	C ₁₂ H ₂₄	1942.44, 3.975	168.1873	141843	
3-Methyldodecane	C ₁₃ H ₂₈	1948.44, 4.968	184.2186	72526	

4-Ethylundecane	C ₁₃ H ₂₈	1954.45, 4.654	184.2186	198420
1-Methyl-2-(1-methylethyl)benzene	C ₁₀ H ₁₄	1960.45, 2.751	134.109	86445
1-Ethyl-cis-1,4-dimethyl cyclohexane	C ₁₀ H ₂₀	1960.45, 4.225	140.156	146673
6-Methyldodecane	C ₁₃ H ₂₈	1972.45, 4.649	184.2186	1593030
3-Ethyl-2,3-dihydro-1-benzofuran	C ₁₀ H ₁₂ O	1984.45, 2.868	148.0883	14147
(1R,3S)-7,7-Dimethyl-2-oxabicyclo[4.1.1.]octan-3-one	C ₉ H ₁₄ O ₂	1984.45, 4.289	154.0988	125028
Tricosane	C ₂₃ H ₄₈	1990.46, 4.913	324.3751	16514
1,2,3,4-Tetramethylbenzene	C ₁₀ H ₁₄	1996.46, 2.715	134.109	139120
Germacrane	C ₁₅ H ₃₀	2002.46, 4.224	210.2342	250312
4-Methyldodecane	C ₁₃ H ₂₈	2002.46, 4.639	184.2186	497826
2,3,7-Trimethyloctane	C ₁₁ H ₂₄	2002.46, 4.953	156.1873	4067569
1,2-Diethylcyclooctane	C ₁₂ H ₂₄	2014.46, 4.257	168.1873	119716
2-Methyl-dodecane	C ₁₃ H ₂₈	2014.46, 4.665	184.2186	995367
(1,1-Dimethylpropyl)benzene	C ₁₁ H ₁₆	2020.47, 2.865	148.1247	133266
1-Pentylcyclohexene	C ₁₁ H ₂₀	2026.47, 3.342	152.156	32422
1-Ethyl-4-(1-methylethyl)-benzene	C ₁₁ H ₁₆	2038.47, 2.823	148.1247	34803
N-(But-2-enoyl)prop-2-enamide	C ₇ H ₁₁ NO	2038.47, 4.512	125.0835	48841
4-Methyltridecane	C ₁₄ H ₃₀	2038.47, 4.575	198.2342	106789
Methyl p-(isopropyl)benzyl sulfoxide	C ₁₁ H ₁₆ OS	2044.47, 2.805	196.0916	10490
1-Methyl-4-(1-methylbutyl)-cyclohexane	C ₁₂ H ₂₄	2062.48, 4.207	168.1873	286511
2-Methyladamantane	C ₁₁ H ₁₈	2074.48, 3.106	150.1403	31306
Hexylcyclohexane	C ₁₂ H ₂₄	2086.48, 3.919	168.1873	658005
Undecane	C ₁₁ H ₂₄	2092.49, 4.784	156.1873	107421
Hexyl butyl ether	C ₁₀ H ₂₂ O	2116.49, 4.808	158.1665	56223
2-(3,5-Dimethyl-1-adamantyl)-1,2-dicyanoethane	C ₁₆ H ₂₂ N ₂	2128.5, 3.554	242.1778	27424
[[2-(2-Propenyloxy)-1-propenyl]sulfonyl]-(E)-benzene	C ₁₂ H ₁₄ O ₃ S	2134.5, 4.107	238.0658	48790
8-Methyl-1-[(phenylthio)methyl]cyclooctane	C ₁₆ H ₂₂ S	2152.5, 3.582	246.1437	16563
1-Isopropyl-1-methyl-cyclohexane	C ₁₀ H ₂₀	2152.5, 4.093	140.156	125215

1-Propanoyl-2-(butanoyl)ethylene	C ₉ H ₁₄ O ₂ ?	2164.51, 4.026	154.0988	16824	1.17E-4
7,7-Dimethylbicyclo[3.2.1]octan-1-ol	C ₁₀ H ₁₈ O	2164.51, 4.109	154.1352	12387	
2,2-Dimethylheptanenitrile	C ₉ H ₁₇ N	2164.51, 4.370	139.1356	33297	
1,4-Dimethyl-2-(2-methylpropyl)benzene	C ₁₂ H ₁₈	2170.51, 2.978	162.1403	80472	
3-Methyl-1-hexen-5-one	C ₇ H ₁₂ O	2194.51, 4.467	112.0883	34875	
2,3-Dihydro-1-methyl-1H-Indene	C ₁₀ H ₁₂	2230.53, 2.545	132.0934	9772	
1-Ethyl-3-methylcyclopentane	C ₈ H ₁₆	2236.53, 4.200	112.1247	57632	
(E)-5-Methyl-7-(2',6',6'-trimethylcyclohex-1'-enyl)hept-4-en-2-one	C ₁₇ H ₂₈ O ?	2242.53, 3.741	248.2135	17947	1.70E-4
Heptadecane	C ₁₇ H ₃₆	2248.53, 4.701	240.2812	202430	
6,9-Dimethyltetradecane	C ₁₆ H ₃₄	2260.53, 4.680	226.2655	213691	
(exo)-9-Methylbicyclo[6.1.0]nonane	C ₁₀ H ₁₈	2302.55, 3.745	138.1403	9085	
1-(1,1-Dimethylethyl)-4-methylbenzene	C ₁₁ H ₁₆	2308.55, 2.766	148.1247	46560	
1-Ethyl-1,4-dimethyl-trans-cyclohexane	C ₁₀ H ₂₀	2314.55, 4.270	140.156	71787	
2,2-Dimethylindan	C ₁₁ H ₁₄	2320.55, 2.676	146.109	12796	
6-Methyl-1,2,3,4-tetrahydronaphthalene-1-methanol	C ₁₂ H ₁₆ O ?	2320.55, 2.800	176.1196	21369	1.49E-4
Hexadecane	C ₁₆ H ₃₄	2320.55, 4.634	226.2655	279836	
(Z)-5-Methylundec-4-en-6-yn-3-ol	C ₁₂ H ₂₀ O ?	2326.55, 3.770	180.1509	15695	1.75E-4
1,1'-(1,4-Butanediyl)bis-cyclohexane	C ₁₆ H ₃₀	2326.55, 4.036	222.2342	50771	
(1,1-Dimethylbutyl)benzene	C ₁₂ H ₁₈	2344.56, 2.922	162.1403	49213	
1,4-Dipropylbenzene	C ₁₂ H ₁₈	2356.56, 2.898	162.1403	32528	
1-Methyl-3-(2-methylpropyl)-cyclopentane	C ₁₀ H ₂₀	2362.56, 3.991	140.156	78948	
1-Tridecene	C ₁₃ H ₂₆	2380.57, 4.154	182.2029	102222	
5-Methyltridecane	C ₁₄ H ₃₀	2380.57, 4.593	198.2342	565349	
[[1-Methyl-3-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2-propenyl]sulfonyl]benzene	C ₁₉ H ₂₆ O ₂ S	2398.57, 3.627	318.1648	33931	
2,6,11-Trimethyldodecane	C ₁₅ H ₃₂	2404.58, 4.834	212.2499	440876	
Dicyclohexyl-acetaldehyde	C ₁₄ H ₂₆ O ₂ ?	2410.58, 3.914	226.1927	26972	2.56E-4
1,7-Dimethyl-4-(1-methylethyl)cyclodecane	C ₁₅ H ₃₀	2410.58, 4.223	210.2342	298452	
2-Methyltridecane	C ₁₄ H ₃₀	2416.58, 4.613	198.2342	1189595	

3,4-Dipropylcyclohex-3-enone	C ₁₂ H ₂₀ O ?	2428.58, 3.640	180.1509	34177	3.24E-4
Germa-crane-B	C ₁₅ H ₃₀	2434.58, 4.199	210.2342	92896	
trans-1,2-Dibutylno spacecyclopropane	C ₁₁ H ₂₂	2440.59, 4.132	154.1716	47355	
N-Butyl-N,N-di(2-pyridiylmethyl)amine	C ₁₆ H ₂₁ N ₃	2452.59, 3.363	255.173	9539	
1-Methylcyclohexyl acetate	C ₉ H ₁₆ O ₂	2452.59, 3.908	156.1145	6649	
3-Methyl-tridecane	C ₁₄ H ₃₀	2458.59, 4.531	198.2342	1001169	
3-Methyleneaminotricyclo[3.3.1.1(3,7)]decane	C ₁₁ H ₁₇ N	2464.59, 3.182	163.1356	30410	
trans-1-Ethyl-2-methyl cyclohexane	C ₉ H ₁₈	2476.6, 4.217	126.1403	78793	
2-Methyl-1-cyclooctanol	C ₉ H ₁₈ O	2536.61, 4.128	142.1352	67015	
(2S,2'S) and (2S,2'R)-N-[2'-Hydroxy-2'-(p-methylphenyl)ethyl]-2-(methoxymethyl)pyrrolidine	C ₁₅ H ₂₃ NO ₂	2584.63, 2.271	249.1723	9419	
trans-1-Butyl-2-hexylcyclopropane	C ₁₃ H ₂₆	2590.63, 4.041	182.2029	51004	
1-Hexyl-3-methylcyclopentane	C ₁₂ H ₂₄	2632.64, 4.132	168.1873	109985	
1,1-Dimethoxyprop-2-yne	C ₅ H ₈ O ₂ ?	2638.64, 4.689	100.0519	9419	1.80E-4
trans-1-Methyl-2-nonyl-cyclohexane	C ₁₆ H ₃₂	2680.65, 4.063	224.2499	283114	
1-Azabicyclo[3.1.0]hexane	C ₅ H ₉ N	2692.66, 4.024	83.073	102160	
2,4,9,11-Tetramethyldodeca-5,7-diene-4,9-diol	C ₁₆ H ₂₆ O ₂	2692.66, 4.805	250.1927	57363	
p-Methylpivalophenone	C ₁₂ H ₁₆ O	2716.66, 2.909	176.1196	9820	1.51E-4
4-(Allyloxy)-2-butyne	C ₇ H ₁₀ O	2722.67, 3.933	110.0726	13326	
trans-1-(Cyclohexylmethyl)-3-methylcyclohexane	C ₁₄ H ₂₆	2734.67, 3.988	194.2029	149668	
5-Methyl-2,2,4-triethyl-2H-imidazole	C ₁₀ H ₁₈ N ₂	2734.67, 4.232	166.1465	10057	
2,3-Dimethyl-2-butenic acid	C ₆ H ₁₀ O ₂	2740.67, 4.728	114.0675	14597	
1,2,3,4-Tetrahydro-5-methylnaphthalene	C ₁₁ H ₁₄	2746.67, 2.523	146.109	51792	
5-Propyldecane	C ₁₃ H ₂₈	2746.67, 4.544	184.2186	1150816	
2,6,10,14-Tetramethyl-heptadecane	C ₂₁ H ₄₄	2752.68, 4.762	296.3438	3149250	
5,6,6-Trimethylbicyclo[3.2.0]heptan-2-one	C ₁₀ H ₁₆ O ?	2758.68, 4.254	152.1196	27364	2.60E-4
1,2,3,4-Tetrahydro-1,8-dimethylnaphthalene	C ₁₂ H ₁₆	2764.68, 2.683	160.1247	40724	
10-Methylnonadecane	C ₂₀ H ₄₂	2764.68, 4.504	282.3281	574911	
2-Oxo-3-pentenitrile	C ₅ H ₅ NO	2782.68, 3.659	95.0366	9973	

4-Methyltetradecane	C ₁₅ H ₃₂	2782.68, 4.535	212.2499	513427	
5-Methyl-3-hexyn-2-ol	C ₇ H ₁₂ O	2824.7, 4.194	112.0883	28734	
2,6,10-trimethyltridecane	C ₁₆ H ₃₄	2824.7, 4.435	226.2655	76122	
3-Methyltetradecane	C ₁₅ H ₃₂	2836.7, 4.469	212.2499	879617	
1,2,3,4-Tetrahydro-1,4-dimethylnaphthalene	C ₁₂ H ₁₆	2902.72, 2.636	160.1247	36499	
Octylcyclohexane	C ₁₄ H ₂₈	2908.72, 3.883	196.2186	713244	
Tetradecylcyclooctane	C ₂₂ H ₄₄	2926.73, 4.071	308.3438	123702	
2-Pent-1-enyltetrahydrofuran	C ₉ H ₁₆ O	2938.73, 4.082	140.1196	41779	
Nonadecane	C ₁₉ H ₄₀	2974.74, 4.572	268.3125	512729	
Heptane	C ₇ H ₁₆	3004.75, 4.743	100.1247	24876	
4-(3-Hydroxy-3-methylbutenyl)imidazole	C ₈ H ₁₂ N ₂ O	3016.75, 2.831	152.0944	5118	
5-Phenylpent-1-en-3-yne	C ₁₁ H ₁₀	3022.75, 2.314	142.0777	83346	
2-Methyl-3-oxazoline	C ₄ H ₇ NO	3028.75, 4.536	85.0522	12051	
Eicosane	C ₂₀ H ₄₂	3034.76, 4.517	282.3281	100199	
Indan-9-ethoxy-7a,3a-(nitrilometheno)	C ₁₂ H ₁₅ NO ?	3076.77, 2.831	189.1148	10677	3.05E-4
6-Methylpentadecane	C ₁₆ H ₃₄	3112.78, 4.454	226.2655	1519679	
1-n-Butyl-1,2,3,4-tetrahydronaphthalene	C ₁₄ H ₂₀	3118.78, 2.527	188.156	9410	
1-Methyl-2-pyrazoline	C ₄ H ₈ N ₂	3118.78, 4.263	84.0682	27072	
1-Methylnaphthalene	C ₁₁ H ₁₀	3124.78, 2.278	142.0777	39716	
3-Ethylcosane	C ₂₂ H ₄₆	3124.78, 4.640	310.3594	121462	
4-Methylpentadecane	C ₁₆ H ₃₄	3148.79, 4.449	226.2655	589448	
Hexahydro-1H-pyrrolizin-1-one	C ₇ H ₁₁ NO ?	3154.79, 3.865	125.0835	19094	5.73E-4
3,3,4,4-Tetraethylhexane	C ₁₄ H ₃₀	3190.8, 4.576	198.2342	89557	
3-Methylpentadecane	C ₁₆ H ₃₄	3202.8, 4.407	226.2655	672137	
1-Octadecanol	C ₁₈ H ₃₈ O ?	3208.81, 4.072	270.2917	26911	2.55E-4
1-Buten-3,4-dicarboxylic acid	C ₆ H ₈ O ₄	3208.81, 4.587	144.0417	89180	
(E)-2-Phenyl-3-octene	C ₁₄ H ₂₀	3256.82, 2.784	188.156	12334	
1,2,3,4-Tetrahydro-5,7-dimethylnaphthalene	C ₁₂ H ₁₆	3274.82, 2.503	160.1247	46516	
1-Cyclohexyl-3-methylbenzene	C ₁₃ H ₁₈	3286.83, 2.657	174.1403	37394	

n-Nonylcyclohexane	C ₁₅ H ₃₀	3286.83, 3.842	210.2342	558527	
6-Hydroxy-3-hexanone	C ₆ H ₁₂ O ₂	3310.84, 4.541	116.0832	252832	
9-Hydroxyinalol	C ₁₀ H ₁₈ O ₂ ?	3376.85, 4.659	170.1301	24150	2.29E-4
1-Ethyl-naphthalene	C ₁₂ H ₁₂	3382.86, 2.369	156.0934	12256	
cis-Bicyclo[3.3.0]octan-1-ol	C ₈ H ₁₄ O	3388.86, 3.563	126.1039	19773	
(Z)-2-(4,4-Dimethyl-2-oxo-2-C13-dihydrofuran-3(2H)-ylidene)acetic acid	C ₈ H ₁₀ O ₄	3394.86, 4.619	170.0574	6673	
1,7-Dimethylnaphthalene	C ₁₂ H ₁₂	3418.87, 2.386	156.0934	154622	
2-Methoxymethylfuran	C ₆ H ₈ O ₂	3460.88, 4.089	112.0519	22629	
2,6,8-Trimethyldecane	C ₁₃ H ₂₈	3460.88, 4.397	184.2186	1465120	
1-(1-Cyclopentenyl)-1-hydroxy-5,5-dimethyl-6-hepten-3-one	C ₁₄ H ₂₂ O ₂ ?	3478.88, 4.144	222.1614	27327	2.59E-4
2,7-Dimethylundecane	C ₁₃ H ₂₈	3478.88, 4.392	184.2186	510633	
Hexahydro-1H-pyrrolizine	C ₇ H ₁₃ N	3490.89, 4.022	111.1043	7551	
4-Methyl-2-propyl-2,5-dihydrofuran	C ₈ H ₁₄ O	3496.89, 3.902	126.1039	37125	
4-Methylhexadecane	C ₁₇ H ₃₆	3496.89, 4.392	240.2812	394562	
1,5-Dimethylnaphthalene	C ₁₂ H ₁₂	3502.89, 2.350	156.0934	61922	
2-Methyloctadecane	C ₁₉ H ₄₀	3514.89, 4.392	268.3125	691076	
3-Hydroxy-7,7-dimethyl-1,8-nonadien-5-one	C ₁₁ H ₁₈ O ₂ ?	3526.9, 4.117	182.1301	84877	8.06E-4
3-Methylhexadecane	C ₁₇ H ₃₆	3550.9, 4.335	240.2812	509525	
1,3-Dimethylnaphthalene	C ₁₂ H ₁₂	3598.92, 2.326	156.0934	20139	
1-(2-Methoxyethenyl)cyclopropane	C ₆ H ₁₀ O	3598.92, 4.113	98.0726	15579	
Cyclopentanodec-5-ene	C ₁₅ H ₂₈	3610.92, 4.028	208.2186	108355	
1-Heptacosanol	C ₂₇ H ₅₆ O ?	3616.92, 4.007	396.4326	40443	3.84E-4
2,4,4-Trimethylhexane	C ₉ H ₂₀	3616.92, 4.675	128.156	424257	
1,8-Dimethylnaphthalene	C ₁₂ H ₁₂	3622.92, 2.289	156.0934	10031	
Undecylcyclohexane	C ₁₇ H ₃₄	3652.93, 3.816	238.2655	406360	
n-Cetyl thiocyanate	C ₁₇ H ₃₃ NS	3712.95, 4.367	283.2328	133265	
1-Oxa-spiro[5.2]octane-2-carbaldehyde	C ₈ H ₁₂ O ₂	3718.95, 4.143	140.0832	51740	
1-Heptadecanol	C ₁₇ H ₃₆ O ?	3736.96, 3.994	256.2761	70284	6.67E-4

2-Methylene-3-butenylamine	C ₅ H ₉ N	3754.96, 3.977	83.073	97531	
3-Methyltricosane	C ₂₄ H ₅₀	3754.96, 4.339	338.3907	56426	
2-Methyl-1,1'-biphenyl	C ₁₃ H ₁₂	3772.97, 2.268	168.0934	40384	
(1R*,5S*,7R*)-7-Methylbicyclo[3.2.1]octan-1-ol	C ₉ H ₁₆ O	3778.97, 4.057	140.1196	44399	
2-(1-Cyclohexyl-1-methylethyl)propanedicarbonitrile	C ₁₂ H ₁₈ N ₂	3790.97, 4.121	190.1465	25017	
2-Isobutyl-3-methylcyclopentan-1-one	C ₁₀ H ₁₈ O	3796.97, 4.034	154.1352	68369	
Phenyl ethyl benzeneethanimidate	C ₁₆ H ₁₇ NO ?	3814.98, 2.273	239.1305	15880	1.50E-4
4-Methylheptadecane	C ₁₈ H ₃₈	3826.98, 4.320	254.2968	222456	
2-Methyleicosane	C ₂₁ H ₄₄	3838.99, 4.335	296.3438	743644	
2,3,6-Trimethylnaphthalene	C ₁₃ H ₁₄	3869, 2.386	170.109	76351	
1,6,7-trimethyl-naphthalene	C ₁₃ H ₁₄	3881, 2.397	170.109	83936	
3,8-Dimethylundecane	C ₁₃ H ₂₈	3881, 4.284	184.2186	445486	
2-p-Tolyl-1H-pyrrole	C ₁₁ H ₁₁ N	3911.01, 2.649	157.0886	9668	
2,2,3,3-Tetramethylbutane	C ₈ H ₁₈	3911.01, 4.644	114.1403	85702	
2,2-Dimethylbutane	C ₆ H ₁₄	3953.02, 4.449	86.109	153113	
6-Allyltetrahydropyran-2-one	C ₈ H ₁₂ O ₂	3959.02, 4.436	140.0832	82478	
1,4,6-Trimethylnaphthalene	C ₁₃ H ₁₄	3965.02, 2.381	170.109	86101	
3,3'-Dimethyl-1,1'-biphenyl	C ₁₄ H ₁₄	4121.07, 2.305	182.109	82943	
3,4'-Dimethyl-1,1'-biphenyl	C ₁₄ H ₁₄	4163.08, 2.309	182.109	43064	
(E)-Deca-1,6-dien-3-one	C ₁₀ H ₁₆ O	4169.08, 4.579	152.1196	20175	
2,6,10,15-Tetramethylheptadecane	C ₂₁ H ₄₄	4181.09, 4.608	296.3438	917232	
Heptacosane	C ₂₇ H ₅₆	4193.09, 4.243	380.4377	344773	
trans--1-Butyl-2-undecylcyclopropane	C ₁₈ H ₃₆	4367.14, 3.933	252.2812	52121	
1-(1-Methylcyclohexyl)-ethanone	C ₉ H ₁₆ O	4415.15, 3.898	140.1196	153780	
2,4,6-Trimethyl-1,1'-biphenyl	C ₁₅ H ₁₆	4433.16, 2.340	196.1247	53978	
3,7-Dimethyldecane	C ₁₂ H ₂₆	4445.16, 4.243	170.2029	137176	
(E)-3-Octen-2,5-dione	C ₈ H ₁₂ O ₂ ?	4475.17, 3.850	140.0832	98937	2.47E-3
3,3-Dimethylheptane	C ₉ H ₂₀	4565.2, 4.416	128.156	72944	
1-Methoxybicyclo(3.2.1)octane	C ₉ H ₁₆ O	4655.22, 3.927	140.1196	66873	

2-Methylpyrrolizidine	C ₈ H ₁₅ N	4673.23, 3.948	125.1199	25486	
Pentatriacontane	C ₃₅ H ₇₂	4673.23, 4.263	492.5629	466027	
2,2,3,3-Tetramethylhexane	C ₁₀ H ₂₂	4709.24, 4.243	142.1716	70431	
2-Methyl-4-methylidenehex-5-en-3-ol	C ₈ H ₁₄ O	4889.29, 3.784	126.1039	13097	
4-Methylstilbene	C ₁₅ H ₁₄	4967.31, 2.292	194.109	10224	
anti-9-Methyl-1,6-methanofluorene	C ₁₅ H ₁₄	4985.32, 2.294	194.109	10067	
Heneicosane	C ₂₁ H ₄₄	4985.32, 4.223	296.3438	50325	
Benzo[A]azulene	C ₁₄ H ₁₀	5027.33, 2.124	178.0777	26705	
1-Hydroxy-2-methyl-bicyclo[3.3.1]nonan-3-one	C ₁₀ H ₁₆ O ₂ ?	5273.4, 3.851	168.1145	64185	6.09E-4
2,10-Dimethylundecane	C ₁₃ H ₂₈	5309.41, 4.193	184.2186	137521	
4-Methylphenanthrene	C ₁₅ H ₁₂	5327.41, 2.193	192.0934	18641	
(E)-5-Heptenenitrile	C ₇ H ₁₁ N	5339.42, 3.820	109.0886	17066	
8,9-Dihydrocyclopent[a]acenaphthylene,	C ₁₅ H ₁₂	5357.42, 2.181	192.0934	22597	
1H-1a,9b-dihydro-cyclopropa[1]phenanthrene	C ₁₅ H ₁₂	5441.45, 2.175	192.0934	8827	
Docosane	C ₂₂ H ₄₆	5459.45, 4.221	310.3594	142439	
2,2,4,6,6-Pentamethyl heptane	C ₁₂ H ₂₆	5561.48, 4.196	170.2029	77571	
2,2-Dimethylpropyl nitrite	C ₅ H ₁₁ NO ₂	6791.83, 4.402	117.0784	21843	
Tetracosane	C ₂₄ H ₅₀	6941.88, 4.392	338.3907	111796	
4-Hydroxyhex-2-en-1-al	C ₆ H ₁₀ O ₂	7139.93, 4.512	114.0675	42626	
Benzene	C ₆ H ₆	7163.94, 1.098	78.0464	11743	
2,2-Dimethyl-3-butyl-4-(2'-propenyl)-2,5-dihydrofuran	C ₁₃ H ₂₂ O ?	7788.12, 1.202	194.1665	24815	2.35E-4
2-(1,1-Dimethylprop-2-en-1-yl)-1,3-dioxolane	C ₈ H ₁₄ O ₂	7998.18, 1.162	142.0988	19952	
2-(3,3-Dimethyl-1-butenyl)-(E)-1-cyclohexene-1-carboxaldehyde	C ₁₃ H ₂₀ O	8076.2, 1.375	192.1509	8089	

Table S17. Data obtained for the distillate fraction of condensate-like oil 4 by using GCxGC/(+EI) TOF MS. Data provided are based on ChromaTOF software prediction of the molecular ion *m/z* value and the identification of the compound by using the EI mass spectral library match using a match factor threshold of 800. Formulas with a question mark “?” might not have been accurately identified. The ratio of the peak area of each of these questionable compounds relative to all peak areas of the detected compounds is provided in the table below

Name	Formula	Retention Times (s) on the Primary, Secondary Column	Molecular Ion <i>m/z</i>	Chromatographic Peak Area	Ratio (Peak area/total sum of peak areas)
3-Methylheptane	C ₈ H ₁₈	406.002, 2.407	114.1403	345175	
Isooctanol	C ₈ H ₁₈ O	430.009, 2.300	130.1352	66947	
1-Buten-1-one	C ₄ H ₆ O	436.01, 2.373	70.0413	26391	
Octane	C ₈ H ₁₈	442.012, 2.597	114.1403	805143	
cis-1,3-Dimethylcyclohexane	C ₈ H ₁₆	454.016, 2.386	112.1247	2614525	
2-Methyl-1-pentanol	C ₆ H ₁₄ O	454.016, 2.597	102.1039	18640	
2,4-Dimethylhexane	C ₈ H ₁₈	460.017, 2.793	114.1403	361560	
Di(2-ethylbutyl) ether	C ₁₂ H ₂₆ O ?	472.021, 2.826	186.1978	66954	9.11E-4
1,1-Dimethylcyclohexane	C ₈ H ₁₆	478.022, 2.422	112.1247	457605	
2,6-Dimethylheptane	C ₉ H ₂₀	478.022, 2.875	128.156	468932	
(S)-(+)-2-Acetoxyoctane	C ₁₀ H ₂₀ O ₂ ?	484.024, 2.489	172.1458	14487	1.97E-4
trans-1,2-Dimethylcyclohexane	C ₈ H ₁₆	496.028, 2.497	112.1247	647324	
3,5-Dimethylno hyphenheptane	C ₉ H ₂₀	496.028, 2.916	128.156	1310843	
trans-1,3-Dimethylcyclohexane	C ₈ H ₁₆	514.033, 2.530	112.1247	648656	
(+)-4-Vinyldecanal	C ₁₂ H ₂₂ O ?	514.033, 2.767	182.1665	8349	1.14E-4
1,3,5-Trimethylcyclohexane	C ₉ H ₁₈	538.04, 2.772	126.1403	362435	
5-Methyldecane	C ₁₁ H ₂₄	550.043, 3.107	156.1873	174985	
1,1,3-Trimethylcyclohexane	C ₉ H ₁₈	562.047, 2.803	126.1403	846536	
2,4-Dimethylheptane	C ₉ H ₂₀	562.047, 3.137	128.156	1077895	
3-Methyloctane	C ₉ H ₂₀	580.052, 3.189	128.156	1956654	
Ethylcyclohexane	C ₈ H ₁₆	586.053, 2.685	112.1247	751674	
1,2,4-Trimethylcyclohexane	C ₉ H ₁₈	592.055, 2.906	126.1403	636493	

Methylbenzene	C ₇ H ₈	598.057, 2.057	92.0621	138021	
Heptane	C ₇ H ₁₆	628.065, 3.495	100.1247	32149	
3-Butyl-3,5-dimethylcyclohexanone	C ₁₂ H ₂₂ O ?	658.074, 3.185	182.1665	121589	1.65E-4
Nonane	C ₉ H ₂₀	658.074, 3.384	128.156	1730365	
1,2,3-Trimethylcyclohexane	C ₉ H ₁₈	670.078, 3.022	126.1403	218158	
1-Hydroxy-3-penten-2-one	C ₅ H ₈ O ₂	676.079, 3.348	100.0519	8841	
2,4,6-Trimethylheptane	C ₁₀ H ₂₂	682.081, 3.636	142.1716	669735	
1-Ethyl-4-methylcyclohexane	C ₉ H ₁₈	706.088, 3.096	126.1403	1193567	
2,5-Dimethyloctane	C ₁₀ H ₂₂	706.088, 3.682	142.1716	1035019	
3,6-Dimethyloctane	C ₁₀ H ₂₂	736.096, 3.734	142.1716	979910	
trans-1-Ethyl-4-methyl cyclohexane	C ₉ H ₁₈	778.109, 3.168	126.1403	512119	
4,5-Dimethyloctane	C ₁₀ H ₂₂	790.112, 3.784	142.1716	53327	
1-Ethyl-1-methylcyclohexane	C ₉ H ₁₈	808.117, 3.131	126.1403	132873	
4-Ethylloctane	C ₁₀ H ₂₂	814.119, 3.837	142.1716	762796	
Dodecane	C ₁₂ H ₂₆	832.124, 3.898	170.2029	1896380	
Diethylcyclohexane	C ₁₀ H ₂₀	838.126, 3.487	140.156	285406	
5H-Tetrazol-5-amine	CH ₃ N ₅	844.127, 4.171	85.0383	174881	
2,3,3-Trimethyl-4-nonene	C ₁₂ H ₂₄	850.129, 3.485	168.1873	165314	
Propylcyclohexane,	C ₉ H ₁₈	856.131, 3.266	126.1403	419216	
3-Methylnonane	C ₁₀ H ₂₂	868.134, 3.919	142.1716	1061294	
cis-Octahydroindene	C ₉ H ₁₆	874.136, 3.099	124.1247	85930	
1-Methyl-2-methylene-3-(1-methylethyl)cyclopentane	C ₁₀ H ₁₈	880.138, 3.349	138.1403	45149	
Ethylbenzene	C ₈ H ₁₀	886.14, 2.369	106.0777	30331	
8-Methyl-1,7-nonadien-4-one	C ₁₀ H ₁₆ O ?	898.143, 3.482	152.1196	89535	1.21E-3
o-Xylene	C ₈ H ₁₀	904.145, 2.412	106.0777	418068	
2-Eethyl-1H-imidazole	C ₅ H ₈ N ₂	904.145, 3.344	96.0682	10520	
4-Methylundecane	C ₁₂ H ₂₆	916.148, 4.240	170.2029	27620	
trans-1-Ethyl-1,3-dimethyl cyclohexane	C ₁₀ H ₂₀	922.15, 3.559	140.156	483840	
Decane	C ₁₀ H ₂₂	976.165, 4.053	142.1716	2846145	

1-Isopropyl-4-methylcyclohexane	C ₁₀ H ₂₀	982.167, 3.579	140.156	229053	
2,4-Bis(dimethylethyl)-2-methyl-2,5-dihydro-1H-imidazole	C ₁₂ H ₂₄ N ₂	982.167, 3.837	196.1934	39775	
1-Methyl-3-propylcyclohexane	C ₁₀ H ₂₀	1006.17, 3.651	140.156	907920	
13,13-Diethoxy-(Z)-1,11-tridecadiene	C ₁₇ H ₃₂ O ₂ ?	1012.18, 3.569	268.2397	41253	5.61E-4
(E)-1-((1'S,2'S)-trans-2-(Methyl)cyclopentyl)-2-butylethylene	C ₁₂ H ₂₂	1018.18, 3.441	166.1716	26423	
1,2-Dimethylbenzene	C ₈ H ₁₀	1024.18, 2.417	106.0777	170341	
2,6,7-Trimethyldecane	C ₁₃ H ₂₈	1024.18, 4.330	184.2186	1143855	
2,7,10-Trimethyldecane	C ₁₅ H ₃₂	1078.19, 4.356	212.2499	364035	
Methyl p-methylbenzyl sulfoxide	C ₉ H ₁₂ OS	1102.2, 2.570	168.0603	11736	
Tetradecane	C ₁₄ H ₃₀	1102.2, 4.346	198.2342	327260	
1-Hydroxymethyl-1,3-dimethylcyclopentane	C ₈ H ₁₆ O	1114.2, 3.646	128.1196	28619	
1-Cyclopropyl-2-propen-1-one	C ₆ H ₈ O	1120.21, 3.600	96.057	28861	
N-Methylene-tert-butylamine	C ₅ H ₁₁ N	1120.21, 4.299	85.0886	15479	
2-Methylundecane	C ₁₂ H ₂₆	1138.21, 4.654	170.2029	16146	
6-Methylno hyphen-tridecane	C ₁₄ H ₃₀	1144.21, 4.356	198.2342	335839	
2,2-Dimethyl-4-(methylethyl)-2H-imidazole	C ₈ H ₁₄ N ₂	1162.22, 3.578	138.1151	20608	
4-Methyl-decane	C ₁₁ H ₂₄	1192.23, 4.382	156.1873	509051	
2-Methyldecane	C ₁₁ H ₂₄	1198.23, 4.423	156.1873	600613	
Undecane	C ₁₁ H ₂₄	1216.23, 4.691	156.1873	75699	
(1-Methylpropyl)cyclohexane	C ₁₀ H ₂₀	1222.24, 3.597	140.156	22323	
1-Methylaziridine	C ₃ H ₇ N	1222.24, 4.672	57.0573	69399	
6-Ethyl-2-methyloctane	C ₁₁ H ₂₄	1228.24, 4.349	156.1873	115214	
Butylcyclohexane	C ₁₀ H ₂₀	1234.24, 3.672	140.156	425014	
4,6-Dimethyldecane-1-ol	C ₁₂ H ₂₆ O ?	1234.24, 3.939	186.1978	275040	3.74E-3
3-Methyldecane	C ₁₁ H ₂₄	1234.24, 4.392	156.1873	614752	
1-Ethyl-4-methylno hyphen-benzene	C ₉ H ₁₂	1264.25, 2.628	120.0934	173809	
(2S,6R)-2,6-Dimethyl-1-octanol	C ₁₀ H ₂₂ O	1276.25, 3.956	158.1665	267793	
1,2,4-Trimethylbenzene	C ₉ H ₁₂	1288.25, 2.649	120.0934	539832	
3-Methyl-1-hexen-5-one	C ₇ H ₁₂ O	1312.26, 4.264	112.0883	15677	

Hexadecane	C ₁₆ H ₃₄	1348.27, 4.642	226.2655	136373	
Octacosane	C ₂₈ H ₅₈	1372.28, 4.647	394.4533	47236	
(4RS,5S)-5-Methylhept-2-yn-4-ol	C ₈ H ₁₄ O	1396.29, 3.910	126.1039	56414	
1-Isopropyl-1-methylno hyphen-cyclohexane	C ₁₀ H ₂₀	1420.29, 3.970	140.156	174765	
3,3-Dimethylhexane	C ₈ H ₁₈	1420.29, 4.665	114.1403	279770	
N-Methoxy-N-methylbenzamide	C ₉ H ₁₁ NO ₂	1438.3, 2.783	165.0784	10031	
3,7-Dimethyldecane	C ₁₂ H ₂₆	1450.3, 4.608	170.2029	345459	
trans-Decahydronaphthalene	C ₁₀ H ₁₈	1468.31, 3.327	138.1403	131521	
(2-Methylbutyl)cyclohexane	C ₁₁ H ₂₂	1474.31, 3.929	154.1716	282149	
Methyl(1-methylethyl)benzene	C ₁₀ H ₁₄	1492.31, 2.761	134.109	65850	
2-Methylheptadecane	C ₁₈ H ₃₈	1510.32, 4.589	254.2968	148470	
5-Ethyldecane	C ₁₂ H ₂₆	1528.32, 4.572	170.2029	227256	
3-Ethoxy-1-propyne	C ₅ H ₈ O	1552.33, 4.115	84.057	28580	
1-Ethyl-2,4-dimethylcyclohexane	C ₁₀ H ₂₀	1570.34, 4.199	140.156	112395	
2,6-Dimethylno hyphen-undecane	C ₁₃ H ₂₈	1570.34, 4.593	184.2186	1129458	
1,2,4-Trimethylbenzene	C ₉ H ₁₂	1588.34, 2.603	120.0934	82582	
1-Methyl-3-propylbenzene	C ₁₀ H ₁₄	1624.35, 2.782	134.109	114077	
4-Methyldecane	C ₁₃ H ₂₈	1630.35, 4.535	184.2186	97000	
Nonadecane	C ₁₉ H ₄₀	1636.35, 4.831	268.3125	33266	
1-(2-Methylphenyl)-3-phenyl-2-propanone	C ₁₆ H ₁₆ O ?	1642.36, 2.783	224.1196	10836	1.47E-4
3-Methylundecane	C ₁₂ H ₂₆	1642.36, 4.572	170.2029	675891	
Pentylcyclohexane	C ₁₁ H ₂₂	1654.36, 3.867	154.1716	404304	
Octadecane	C ₁₈ H ₃₈	1654.36, 4.825	254.2968	89841	
trans-2-Methyldecalin	C ₁₁ H ₂₀	1660.36, 3.538	152.156	129156	
1-Ethyl-2,4-dimethylbenzene	C ₁₀ H ₁₄	1672.37, 2.757	134.109	259121	
2-(1-Phenylethyl)phenol	C ₁₄ H ₁₄ O ?	1708.38, 4.808	198.1039	63926	8.69E-4
7,9-Dimethylhexadecane	C ₁₈ H ₃₈	1738.38, 4.773	254.2968	319480	
4-(Allyloxy)-2-butyne	C ₇ H ₁₀ O	1744.39, 4.062	110.0726	17546	
trans-4a-Methyldecahydronaphthalene	C ₁₁ H ₂₀	1756.39, 3.473	152.156	51382	

1,2-Dibutylcyclopropan	C ₁₁ H ₂₂	1768.39, 4.346	154.1716	20883	
Pentadecane	C ₁₅ H ₃₂	1768.39, 4.746	212.2499	97892	
Tridecane	C ₁₃ H ₂₈	1774.39, 4.536	184.2186	4795319	
cis-1,2-Dibutylcyclopropane	C ₁₁ H ₂₂	1786.4, 4.053	154.1716	15605	
(1-Methylbutyl)benzene	C ₁₁ H ₁₆	1792.4, 2.938	148.1247	69884	
1-Tridecyne	C ₁₃ H ₂₄	1792.4, 3.466	180.1873	8999	
o-Cymene	C ₁₀ H ₁₄	1816.41, 2.726	134.109	98098	
1-Methyl-2-pentylcyclohexane	C ₁₂ H ₂₄	1822.41, 4.094	168.1873	376000	
1-Methyl-3-(1-methylethyl)benzene	C ₁₀ H ₁₄	1828.41, 2.881	134.109	44118	
9-Octadecenoic acid	C ₁₈ H ₃₄ O ₂	1870.42, 3.968	282.2553	8959	
3-Methyl-dodecane	C ₁₃ H ₂₈	1882.43, 4.710	184.2186	98229	
3,4-Dimethylcumene	C ₁₁ H ₁₆	1888.43, 2.841	148.1247	40425	
2-Methyl-2-methyl-2-propenyl butanoate	C ₉ H ₁₆ O ₂	1900.43, 4.645	156.1145	38921	
(2S-trans)-3-Octyloxiranemethanol	C ₁₁ H ₂₂ O ₂ ?	1918.44, 4.295	186.1614	15203	2.07E-4
2-Methyl-4-hexyn-3-ol	C ₇ H ₁₂ O	1924.44, 4.217	112.0883	20883	
2,6,10,15-Tetramethylheptadecane	C ₂₁ H ₄₄	1936.44, 4.927	296.3438	314975	
1,2,4,5-Tetramethylbenzene	C ₁₀ H ₁₄	1960.45, 2.746	134.109	85776	
trans-1-Butyl-2-hexylcyclopropane	C ₁₃ H ₂₆	1960.45, 4.318	182.2029	26925	
6-Methyl-dodecane	C ₁₃ H ₂₈	1972.45, 4.639	184.2186	840710	
4-Methyl-1,6-heptadien-4-ol	C ₈ H ₁₄ O	1972.45, 4.910	126.1039	20658	
3-Ethyl-2,3-dihydro-1-benzofuran	C ₁₀ H ₁₂ O ?	1984.45, 2.864	148.0883	16876	2.30E-4
2,4-Dimethylundecane	C ₁₃ H ₂₈	1984.45, 4.608	184.2186	214732	
1,2,3,4-Tetramethylbenzene	C ₁₀ H ₁₄	1996.46, 2.710	134.109	130414	
2,3,7-Trimethyloctane	C ₁₁ H ₂₄	2008.46, 4.906	156.1873	986150	
2-Methyl-2-dicyanomethyladamantane	C ₁₄ H ₁₈ N ₂	2014.46, 3.390	214.1465	12653	
2-Methyl-dodecane	C ₁₃ H ₂₈	2014.46, 4.644	184.2186	659951	
1-Methyl-4-(1-methylpropyl)benzene	C ₁₁ H ₁₆	2020.47, 2.854	148.1247	120308	
(E)-1-Cyclohexyl-1-hexene	C ₁₂ H ₂₂	2026.47, 3.333	166.1716	12993	
Hexylcyclohexane	C ₁₂ H ₂₄	2086.48, 3.914	168.1873	464435	

1-(4-Methylphenyl)-1-propanone	C ₁₀ H ₁₂ O	2098.49, 2.853	148.0883	39592	
3-Cyclohexylcyclohexanone	C ₁₂ H ₂₀ O	2104.49, 4.165	180.1509	67775	
1-Methyl-2-(1-methylethyl)benzene	C ₁₀ H ₁₄	2128.5, 2.835	134.109	40262	
(4R,5S,8R)-5-Isopropyl-8-methyl-1-oxaspiro[3.5]nonane	C ₁₂ H ₂₂ O ?	2128.5, 4.173	182.1665	14706	2.00E-4
2,6,10,14-Tetramethylhexadecane	C ₂₀ H ₄₂	2164.51, 4.718	282.3281	281089	
(1,1-Dimethylbutyl)benzene	C ₁₂ H ₁₈	2170.51, 2.973	162.1403	54617	
4-Methyl-1-[4-(1-methylethenyl)-1-cyclohexen-1-yl]-3-penten-1-one	C ₁₅ H ₂₂ O ?	2200.52, 3.260	218.1665	23844	
Heptadecane	C ₁₇ H ₃₆	2224.52, 4.690	240.2812	740136	
1-Ethenyl-5-(1-methylethylidene)-1,3-cyclopentadiene	C ₁₀ H ₁₂	2230.53, 2.555	132.0934	10185	
1-(1,1-Dimethylethyl)-4-methylbenzene	C ₁₁ H ₁₆	2308.55, 2.768	148.1247	27447	
1-Methyl-3-(2-methylpropyl)-cyclopentane	C ₁₀ H ₂₀	2308.55, 4.024	140.156	126700	
1,2,3,4-Tetrahydronaphthalene	C ₁₀ H ₁₂	2332.55, 2.473	132.0934	18659	
1-Ethyl-4-(1-methylethyl)benzene	C ₁₁ H ₁₆	2332.55, 2.729	148.1247	18739	
1-Methyl-3-(1-methylethyl)-cyclohexane	C ₁₀ H ₂₀	2332.55, 3.995	140.156	71111	
Hexacosane	C ₂₆ H ₅₄	2350.56, 4.608	366.422	76370	
Ethyl-1,2,4-trimethylbenzene	C ₁₁ H ₁₆	2380.57, 2.718	148.1247	19923	
5-Methyltridecane	C ₁₄ H ₃₀	2380.57, 4.587	198.2342	361510	
3,3,5-Trimethylheptane	C ₁₀ H ₂₂	2380.57, 4.814	142.1716	171053	
Tetracosane	C ₂₄ H ₅₀	2392.57, 4.832	338.3907	38905	
4-Methyltridecane	C ₁₄ H ₃₀	2398.57, 4.587	198.2342	366109	
2,6,11-Trimethyldecane	C ₁₅ H ₃₂	2404.58, 4.824	212.2499	244147	
2-Methyltridecane	C ₁₄ H ₃₀	2416.58, 4.587	198.2342	664095	
1,17-Octadecadiene	C ₁₈ H ₃₄	2458.59, 4.170	250.2655	50087	
3-Methyltridecane,	C ₁₄ H ₃₀	2458.59, 4.531	198.2342	649109	
2-(1,1-Dimethylethyl)-1,2,3,4,5,6,7,8-octahydronaphthalene	C ₁₄ H ₂₄	2464.59, 3.170	192.1873	14212	
1,4-Dimethyl-2-(2-methylpropyl)benzene	C ₁₂ H ₁₈	2596.63, 2.835	162.1403	28678	
m-Menthane	C ₁₀ H ₂₀	2656.65, 4.058	140.156	322420	
(4E)-2,2,4-Trimethylhex-4-en-3-one	C ₉ H ₁₆ O	2668.65, 4.200	140.1196	19002	
trans-1-Ethyl-1,4-dimethylno space cyclohexane	C ₁₀ H ₂₀	2674.65, 4.047	140.156	105327	

1-Methyl-2-octylcyclopropane	C ₁₂ H ₂₄	2698.66, 4.059	168.1873	20192	
trans-1-methyl-2-nonylcyclohexane	C ₁₆ H ₃₂	2734.67, 3.977	224.2499	51373	
cis-bicyclo[3.3.0]octan-1-ol	C ₈ H ₁₄ O	2740.67, 3.954	126.1039	28849	
1,2,3,4-Tetrahydro-6-methylnaphthalene	C ₁₁ H ₁₄	2746.67, 2.526	146.109	50083	
2,3,4,5-Tetrahydro-6-hexylpyridine	C ₁₁ H ₂₁ N	2746.67, 3.933	167.1669	31626	
7-Methylpentadecane	C ₁₆ H ₃₄	2746.67, 4.536	226.2655	792788	
2,6,10,14-Tetramethylheptadecane	C ₂₁ H ₄₄	2752.68, 4.762	296.3438	955975	
2,3-Dihydro-1,4,7-trimethylno space indene	C ₁₂ H ₁₆	2764.68, 2.684	160.1247	26478	
(S)-Undec-1-en-4-ol	C ₁₁ H ₂₂ O ?	2764.68, 4.180	170.1665	26092	3.55E-4
5-Methyltetradecane	C ₁₅ H ₃₂	2764.68, 4.505	212.2499	309867	
Octyl pentyl ether	C ₁₃ H ₂₈ O ?	2776.68, 4.488	200.2135	29603	4.03E-4
1-Ethyl-1,3-dimethylcyclohexane	C ₁₀ H ₂₀	2782.68, 4.200	140.156	56781	
4-Methylnospace tetradecane	C ₁₅ H ₃₂	2782.68, 4.515	212.2499	315210	
cis-1-Butyl-2-undecylcyclopropane	C ₁₈ H ₃₆	2806.69, 4.160	252.2812	68202	
1-Isopropyl-8-methyl-1,2,3,4-tetrahydronaphthalene	C ₁₄ H ₂₀	2818.69, 2.659	188.156	9390	
2,6-Dimethylheptadecane	C ₁₉ H ₄₀	2836.7, 4.485	268.3125	530222	
1,2,3,4-Tetrahydro-2,7-dimethylnaphthalene	C ₁₂ H ₁₆	2902.72, 2.627	160.1247	45797	
1,2,3,4-Tetrahydro-5-methylnaphthalene	C ₁₁ H ₁₄	2908.72, 2.444	146.109	19204	
Octylcyclohexane	C ₁₄ H ₂₈	2908.72, 3.862	196.2186	532023	
2-Methylnonane	C ₁₀ H ₂₂	2920.72, 4.614	142.1716	66665	
1,3-Dimethyl-1H-Inden-1-ol	C ₁₁ H ₁₂ O ?	2938.73, 2.607	160.0883	12095	1.65E-4
(Z/E)-2,2,4,5-Tetramethyl-3-heptene	C ₁₁ H ₂₂	2944.73, 4.289	154.1716	22228	
1-Hexadecene	C ₁₆ H ₃₂	3016.75, 4.041	224.2499	48889	
1-Methylnaphthalene	C ₁₁ H ₁₀	3022.75, 2.318	142.0777	35221	
1,1'-(1,2-Dimethyl-1,2-ethanediyl)bis-cyclohexane	C ₁₆ H ₃₀	3064.76, 3.981	222.2342	113425	
3-Acetyl-3-methylcyclohexanone	C ₉ H ₁₄ O ₂ ?	3112.78, 4.190	154.0988	24500	3.33E-4
1-Cyclopentylidene-2,4-cyclopentadiene	C ₁₀ H ₁₂	3118.78, 2.526	132.0934	9242	
5-Phenylpent-1-en-3-yne	C ₁₁ H ₁₀	3124.78, 2.275	142.0777	15453	
4-Methylpentadecane,	C ₁₆ H ₃₄	3148.79, 4.438	226.2655	329068	

2-Methylnonadecane	C ₂₀ H ₄₂	3166.79, 4.449	282.3281	527385	
3-Isoxazolepropanol	C ₆ H ₉ NO ₂ ?	3178.8, 4.124	127.0628	21917	2.98E-4
4,4,7,7-Tetramethyl-1,9-decadiene	C ₁₄ H ₂₆	3190.8, 4.084	194.2029	34967	
2,6,10-Trimethyltridecane	C ₁₆ H ₃₄	3190.8, 4.383	226.2655	31109	
2,5,9-Trimethyldecane	C ₁₃ H ₂₈	3334.84, 4.681	184.2186	42626	
5-Methyl-5-hexen-2-one	C ₇ H ₁₂ O?	3352.85, 3.954	112.0883	22323	3.04E-4
1,2,3,4-Tetrahydro-2,5,7-trimethyl-naphthalene	C ₁₃ H ₁₈	3394.86, 2.627	174.1403	9005	
1,7-Dimethylnaphthalene	C ₁₂ H ₁₂	3418.87, 2.382	156.0934	66766	
(E)-2-Tetradecen-1-ol	C ₁₄ H ₂₈ O?	3424.87, 3.942	212.2135	15851	2.16E-4
Tetradecylcyclooctane	C ₂₂ H ₄₄	3430.87, 3.957	308.3438	74223	
2,2,3,3-Tetramethylhexane	C ₁₀ H ₂₂	3478.88, 4.382	142.1716	240297	
4-tert-Butylhex-1-ene	C ₁₀ H ₂₀	3490.89, 4.597	140.156	67205	
4-Methylhexadecane	C ₁₇ H ₃₆	3496.89, 4.402	240.2812	217190	
1,4-Dimethylnaphthalene	C ₁₂ H ₁₂	3502.89, 2.345	156.0934	19634	
1,5-Dimethylnaphthalene	C ₁₂ H ₁₂	3520.9, 2.325	156.0934	59882	
1-Octyl-1,4-dihydronaphthalene	C ₁₈ H ₂₆	3520.9, 2.465	242.2029	9368	
3-Methylhexadecane	C ₁₇ H ₃₆	3550.9, 4.342	240.2812	378860	
2-Methylhexadecane	C ₁₇ H ₃₆	3610.92, 4.714	240.2812	237185	
Dotriacontane	C ₃₂ H ₆₆	3634.93, 4.468	450.5159	99582	
7-Phenyltetracyclo[4.1.0.0.2,4.0.3,5]heptane	C ₁₃ H ₁₂	3772.97, 2.272	168.0934	10836	
5-Methyldodecane	C ₁₃ H ₂₈	3808.98, 4.340	184.2186	178189	
2-Methyleicosane	C ₂₁ H ₄₄	3838.99, 4.346	296.3438	377357	
1,6,7-Trimethyl-naphthalene	C ₁₃ H ₁₄	3869, 2.382	170.109	25816	
1,4,6-Trimethylnaphthalene	C ₁₃ H ₁₄	3881, 2.399	170.109	31007	
3,7-Dimethylnonane	C ₁₁ H ₂₄	3881, 4.315	156.1873	283347	
2,5-Dimethylheptane	C ₉ H ₂₀	3887, 4.636	128.156	26935	
2,6,10-Trimethyltridecane	C ₁₆ H ₃₄	3917.01, 4.652	226.2655	34758	
4,4-Dimethyloctane	C ₁₀ H ₂₂	3923.01, 4.431	142.1716	32462	
2-Pyrrolidinone	C ₄ H ₇ NO?	3923.01, 4.604	85.0522	13831	1.88E-4

2,3-Octanedione	C ₈ H ₁₄ O ₂ ?	3971.02, 4.538	142.0988	17010	2.31E-4
1,4,5-Trimethylnaphthalene	C ₁₃ H ₁₄	3977.03, 2.349	170.109	7427	
2,2,3,3-Tetramethylbutane	C ₈ H ₁₈	3989.03, 4.412	114.1403	65117	
Tricosane	C ₂₃ H ₄₈	4031.04, 4.520	324.3751	117734	
10-Methylnonadecane	C ₂₀ H ₄₂	4091.06, 4.330	282.3281	371382	
(Z)-2,2,3,5,5-pentamethyl-3-hexene	C ₁₁ H ₂₂	4145.07, 4.013	154.1716	45891	
Eicosane	C ₂₀ H ₄₂	4145.07, 4.289	282.3281	165528	
1-Methyl-4-(phenylmethyl)no hyphen benzene	C ₁₄ H ₁₄	4163.08, 2.307	182.109	9687	
2,2,4-Trimethyl-2H-imidazole	C ₆ H ₁₀ N ₂	4175.08, 3.873	110.0838	14821	
Heptacosane	C ₂₇ H ₅₆	4193.09, 4.253	380.4377	195118	
2,2,3,3,4,4,5,5-Octamethylhexane	C ₁₄ H ₃₀	4211.09, 4.356	198.2342	40228	
Undecylcyclohexane	C ₁₇ H ₃₄	4319.12, 3.749	238.2655	212672	
Allyl octyl ether	C ₁₁ H ₂₂ O ?	4349.13, 4.272	170.1665	26100	3.55E-4
(E)-9-Tricosene	C ₂₃ H ₄₆	4367.14, 3.919	322.3594	39654	
1-Hexadecanol	C ₁₆ H ₃₄ O ?	4379.14, 3.937	242.2604	30034	4.09E-4
2,6,10-Trimethylpentadecane	C ₁₈ H ₃₈	4409.15, 4.281	254.2968	112636	
Tetratetracontane	C ₄₄ H ₉₀	4673.23, 4.263	618.7037	472034	
Docosane	C ₂₂ H ₄₆	4949.31, 4.227	310.3594	371934	
2,9-Dimethyldecane	C ₁₂ H ₂₆	5015.32, 4.243	170.2029	204263	
(1-Methylethyl)cyclohexane	C ₉ H ₁₈	5471.46, 3.758	126.1403	65691	
(S)-3,5-Dimethyl-hexan-1-ol	C ₈ H ₁₈ O ?	5525.47, 4.222	130.1352	121871	1.65E-3
2,2-Dimethylpentane	C ₇ H ₁₆	5561.48, 4.193	100.1247	54317	
2-Methylene-3-butylamine	C ₅ H ₉ N	5975.6, 3.772	83.073	39535	
2,2-Dimethylbutane	C ₆ H ₁₄	6035.62, 4.200	86.109	42062	
(3R)-3-Phenyl-2,3-dihydro-1H-isoindol-1-one	C ₁₄ H ₁₁ NO ?	6155.65, 1.101	209.0835	64129	8.72E-4
Pivalic acid	C ₅ H ₁₀ O ₂ ?	6443.73, 4.263	102.0675	17759	2.42E-4

Table 3S18. Data obtained from the distillate fraction of condensate-like oil 3 by using GCxGC/(+EI)-TOF MS. Data provided are based on ChromaTOF software prediction of the molecular ion m/z value and the identification of the compound by using the EI mass spectral library match using a match factor threshold of 800. Formulas with a question mark “?” might not have been accurately identified. The ratio of the peak area of each of these questionable compounds relative to all peak areas of the detected compounds is provided in the table below

Name	Formula	Retention Times (s) on the Primary, Secondary Column	Molecular Ion m/z	Chromatographic Peak Area	Ratio (Peak area/total sum of peak areas)
3-Methylheptane	C ₈ H ₁₈	406.002, 2.407	114.1403	341309	
1,1,2-Trimethylcyclopentane	C ₈ H ₁₆	424.007, 2.310	112.1247	93151	
1,5-Octadien-3-ol	C ₈ H ₁₄ O	436.01, 2.381	126.1039	28241	
Octane	C ₈ H ₁₈	442.012, 2.602	114.1403	977057	
cis-1,3-Dimethylcyclohexane	C ₈ H ₁₆	454.016, 2.391	112.1247	2908557	
Hexane	C ₆ H ₁₄	460.017, 2.798	86.109	259659	
2,4-Dimethylheptane	C ₉ H ₂₀	466.019, 2.818	128.156	120996	
1,1-Dimethylcyclohexane	C ₈ H ₁₆	478.022, 2.427	112.1247	477175	
(E)-2-Hexenal	C ₆ H ₁₀ O	478.022, 2.671	98.0726	12733	
2,6-Dimethylheptane	C ₉ H ₂₀	478.022, 2.875	128.156	517179	
trans-1,2-Dimethylcyclohexane	C ₈ H ₁₆	496.028, 2.504	112.1247	699114	
2,5-Dimethylheptane	C ₉ H ₂₀	496.028, 2.921	128.156	1373200	
1,4-Dimethylcyclohexane	C ₈ H ₁₆	514.033, 2.541	112.1247	723005	
Piperidine	C ₅ H ₁₁ N	532.038, 3.014	85.0886	37268	
1,3,5-Trimethylnohyphencyclohexane	C ₉ H ₁₈	538.04, 2.782	126.1403	494101	
1-Bicyclo[2.2.2]octanol	C ₈ H ₁₄ O	550.043, 2.839	126.1039	27949	
5-Methyldecane	C ₁₁ H ₂₄	550.043, 3.102	156.1873	164858	
1,1,3-Trimethylcyclohexane	C ₉ H ₁₈	562.047, 2.808	126.1403	1100353	
N-(But-3'-enyl)-N-vinylformamide	C ₇ H ₁₁ NO	574.05, 2.926	125.0835	5589	
3-Methyloctane	C ₉ H ₂₀	580.052, 3.194	128.156	2025199	

Ethylcyclohexane	C ₈ H ₁₆	586.053, 2.695	112.1247	874266	
1,2,4-Trimethylcyclohexane	C ₉ H ₁₈	592.055, 2.916	126.1403	850858	
Toluene	C ₇ H ₈	598.057, 2.062	92.0621	173979	
Nonane	C ₉ H ₂₀	658.074, 3.394	128.156	2069420	
1,2,3-Trimethylcyclohexane	C ₉ H ₁₈	670.078, 3.029	126.1403	339821	
2,4,6-Trimethylheptane	C ₁₀ H ₂₂	682.081, 3.636	142.1716	589668	
1-Ethyl-4-methylcyclohexane	C ₉ H ₁₈	706.088, 3.096	126.1403	1443674	
3,5-Dimethyloctane	C ₁₀ H ₂₂	706.088, 3.677	142.1716	1195770	
cis-1,1,3,5-Tetramethylcyclohexane	C ₁₀ H ₂₀	718.091, 3.343	140.156	198005	
2,6-Dimethyloctane	C ₁₀ H ₂₂	736.096, 3.734	142.1716	1060512	
Octahydropentalene	C ₈ H ₁₄	754.102, 2.743	110.109	64666	
3,6-Dimethyloctane	C ₁₀ H ₂₂	760.103, 3.759	142.1716	592477	
cis-1-Ethyl-2-methylcyclohexane	C ₉ H ₁₈	778.109, 3.168	126.1403	672298	
3-Butyl-3,5-dimethylcyclohexanone	C ₁₂ H ₂₂ O ?	778.109, 3.441	182.1665	29229	3.70E-4
3-Hepten-2-one	C ₇ H ₁₂ O	778.109, 3.555	112.0883	10166	
2,3,3-Trimethyl-(Z)-4-nonene	C ₁₂ H ₂₄	796.114, 3.432	168.1873	67068	
1-Ethyl-1-methylcyclohexane	C ₉ H ₁₈	808.117, 3.142	126.1403	105888	
(+)-(S)-1-Butyl-2-methylenecyclopentane	C ₁₀ H ₁₈	814.119, 2.725	138.1403	18401	
4-Ethyl-octane	C ₁₀ H ₂₂	814.119, 3.847	142.1716	824269	
1,1,3,5-Tetramethyl-transcyclohexane	C ₁₀ H ₂₀	820.121, 3.409	140.156	109514	
2,4-Bis(methylethyl)-2-methyl-2,5-dihydro-1H-imidazole	C ₁₀ H ₂₀ N ₂	832.124, 3.389	168.1621	10555	
4-Methyl-nonane	C ₁₀ H ₂₂	832.124, 3.909	142.1716	1928891	
trans-1-Ethyl-1,3-dimethyl cyclohexane	C ₁₀ H ₂₀	838.126, 3.492	140.156	405342	
1-Cyano-2,6-dimethyl-1,5-heptadien-3-ol	C ₁₀ H ₁₅ NO ?	844.127, 3.552	165.1148	3422	4.33E-5
3-Methylene-1-methylcycloheptane-1,2-diol	C ₉ H ₁₆ O ₂ ?	850.129, 3.227	156.1145	24921	3.15E-4
Propylcyclohexane	C ₉ H ₁₈	856.131, 3.276	126.1403	538881	
2,4-Dimethylpentane	C ₇ H ₁₆	856.131, 4.210	100.1247	71555	
7-Methyltridecane	C ₁₄ H ₃₀	868.134, 3.939	198.2342	1031051	
cis-Octahydro-1H-indene	C ₉ H ₁₆	874.136, 3.088	124.1247	106743	

3,7,7-Trimethyl-1,3,8-nonatrien-5-one	C ₁₂ H ₁₈ O ?	874.136, 3.383	178.1352	8470	1.07E-4
(4E)-4-Ethylidenebicyclo[3.1.0]hex-2-ene	C ₈ H ₁₀	886.14, 2.371	106.0777	41103	
cis-1-Methyl-2-methylene-3-(1-methylethyl)cyclopentane	C ₁₀ H ₁₈	886.14, 3.343	138.1403	56863	
3-Cyclohexyl-(2S-trans)-oxiranemethanol	C ₉ H ₁₆ O ₂ ?	898.143, 3.365	156.1145	23926	3.03E-4
o-Xylene	C ₈ H ₁₀	904.145, 2.412	106.0777	579097	
cis-1,1,2,3-Tetramethylcyclohexane	C ₁₀ H ₂₀	940.155, 3.462	140.156	46357	
Decane	C ₁₀ H ₂₂	976.165, 4.063	142.1716	3227324	
1-Methyl-3-(1-methylethyl)-(1R-trans)cyclohexane	C ₁₀ H ₂₀	988.169, 3.576	140.156	300712	
2,4-Dimethyldecane	C ₁₂ H ₂₆	994.171, 4.305	170.2029	486717	
trans-1-Ethyl-4-methylcyclohexane	C ₉ H ₁₈	1006.17, 3.657	126.1403	1111823	
(4RS,5S)-5-Methylhept-2-yn-4-ol	C ₈ H ₁₄ O	1012.18, 3.568	126.1039	100396	
1,5-Dimethylpyrazol-4-amine	C ₅ H ₉ N ₃	1018.18, 3.552	111.0791	16582	
1,2-Dimethylbenzene	C ₈ H ₁₀	1024.18, 2.427	106.0777	236358	
2,6,7-Trimethyldecane	C ₁₃ H ₂₈	1024.18, 4.335	184.2186	1388995	
1-(Hydroxymethyl)-3-methylene-1-cyclobutanol	C ₆ H ₁₀ O ₂	1036.18, 3.603	114.0675	21648	
1-(3-Cyclopenten-1-yl)-4-methyl-4-penten-2-one	C ₁₁ H ₁₆ O ?	1054.19, 3.303	164.1196	23517	2.97E-4
6-Ethyl-2-methyloctane	C ₁₁ H ₂₄	1054.19, 4.330	156.1873	398225	
2-Ethyl-1,3-dimethylcyclohexane	C ₁₀ H ₂₀	1072.19, 3.636	140.156	266101	
2,7,10-Trimethyldodecane	C ₁₅ H ₃₂	1078.19, 4.351	212.2499	471610	
Methyl benzenesulfite	C ₁₈ H ₂₈ O ₂ S	1084.2, 3.863	308.1805	19567	
trans-1-Methyl-2-nonylcyclohexane	C ₁₆ H ₃₂	1096.2, 3.631	224.2499	223780	
(2S)-1,2-Diphenyl-2-hydroxyethanone	C ₁₄ H ₁₂ O ₂ ?	1102.2, 2.577	212.0832	12828	1.62E-4
3-Ethyl-2,7-dimethyloctane	C ₁₂ H ₂₆	1102.2, 4.325	170.2029	329967	
(1,2-Dimethylcyclopentyl)methanol	C ₈ H ₁₆ O	1114.2, 3.630	128.1196	69364	
3,3-Dimethylcyclohex-1-en-1-yl but-2-enoate	C ₁₂ H ₁₈ O ₂ ?	1138.21, 3.639	194.1301	22096	2.79E-4
Octadecane	C ₁₈ H ₃₈	1150.22, 4.351	254.2968	333249	
1-(1-Cyclopentenyl)-1-hydroxy-5,5-dimethyl-6-hepten-3-one	C ₁₄ H ₂₂ O ₂ ?	1168.22, 3.947	222.1614	80765	1.02E-3
2-Methylnonane	C ₁₀ H ₂₂	1168.22, 4.318	142.1716	79586	
4-Methyldecane	C ₁₁ H ₂₄	1192.23, 4.377	156.1873	498135	

2-Methyldecane	C ₁₁ H ₂₄	1198.23, 4.428	156.1873	636624	
Undecane	C ₁₁ H ₂₄	1216.23, 4.708	156.1873	142311	
N-Benzyl-N-[(3E)-3,5-hexadien-1-yl]amine	C ₁₃ H ₁₉ N	1222.24, 2.630	189.1512	23869	
2,6,10,14-Tetramethylhexadecane	C ₂₀ H ₄₂	1228.24, 4.352	282.3281	103975	
Butylcyclohexane	C ₁₀ H ₂₀	1234.24, 3.672	140.156	518531	
3-Methyldecane	C ₁₁ H ₂₄	1240.24, 4.366	156.1873	614389	
1-Ethyl-2-methylbenzene	C ₉ H ₁₂	1264.25, 2.623	120.0934	245105	
(1-Methylpropyl)cyclooctane	C ₁₂ H ₂₄	1276.25, 3.965	168.1873	266885	
Pentadecane	C ₁₅ H ₃₂	1282.25, 4.641	212.2499	75451	
1,2,3-Trimethylbenzene	C ₉ H ₁₂	1288.25, 2.643	120.0934	704973	
Crotonaldehyde	C ₄ H ₆ O	1288.25, 3.919	70.0413	3562	
trans-1,2-Dibutylcyclopropane	C ₁₁ H ₂₂	1300.26, 3.912	154.1716	24536	
3-Ethoxy-1-propyne	C ₅ H ₈ O	1312.26, 4.286	84.057	22680	
2-Methylundecane	C ₁₂ H ₂₆	1348.27, 4.643	170.2029	179003	
Dodecane	C ₁₂ H ₂₆	1366.28, 4.402	170.2029	4252949	
4,6-Dimethyldecane-1-ol	C ₁₂ H ₂₆ O ?	1372.28, 3.842	186.1978	41630	5.27E-4
2,2,4,5-Tetramethylhex-5-en-3-one	C ₁₀ H ₁₄ O ?	1372.28, 4.636	150.1039	50266	6.36E-4
1-Isopropyl-4-methylcyclohexane	C ₁₀ H ₂₀	1384.28, 3.915	140.156	108201	
(2-Methylpropyl)benzene	C ₁₀ H ₁₄	1402.29, 2.823	134.109	15150	
2,4,6,8-Tetramethylundecene	C ₁₅ H ₃₀	1414.29, 4.211	210.2342	53998	
1-Ethyl-2-propylcyclohexane	C ₁₁ H ₂₂	1438.3, 3.924	154.1716	309499	
3,7-Dimethyldecane	C ₁₂ H ₂₆	1450.3, 4.608	170.2029	346530	
(2S,6R)-2,6-Dimethyl-1-octanol	C ₁₀ H ₂₂ O ?	1456.3, 4.256	158.1665	25946	3.28E-4
Decahydro naphthalene	C ₁₀ H ₁₈	1468.31, 3.336	138.1403	172419	
Heptadecane	C ₁₇ H ₃₆	1468.31, 4.639	240.2812	218241	
1-Methyl-2-(1-methylethyl)benzene	C ₁₀ H ₁₄	1492.31, 2.756	134.109	78170	
1-Hydroxymethyl-1,3-dimethylcyclopentane	C ₈ H ₁₆ O	1516.32, 3.894	128.1196	46608	
6-Ethyl-2-methyl naphthendecane	C ₁₃ H ₂₈	1528.32, 4.587	184.2186	218682	
(1R,3S)-7,7-Dimethyl-2-oxabicyclo[4.1.1.]octan-3-one	C ₉ H ₁₄ O ₂	1540.33, 4.097	154.0988	12981	

Docosane	C ₂₂ H ₄₆	1546.33, 4.604	310.3594	133127	
2-But-1-enyltetrahydrofuran	C ₈ H ₁₄ O	1552.33, 4.149	126.1039	69215	
2,6-Dimethylundecane	C ₁₃ H ₂₈	1570.34, 4.582	184.2186	1126021	
2-Propyldecane-1-ol	C ₁₃ H ₂₈ O ?	1582.34, 4.834	200.2135	13463	1.70E-4
1-Ethyl-4-methylbenzene	C ₉ H ₁₂	1588.34, 2.602	120.0934	104961	
4-Methylundecane	C ₁₂ H ₂₆	1594.34, 4.577	170.2029	416818	
Octyl pentyl ether	C ₁₃ H ₂₈ O ?	1606.35, 4.870	200.2135	46864	5.93E-4
Tetradecane	C ₁₄ H ₃₀	1612.35, 4.879	198.2342	147902	
1-Methyl-3-propylbenzene	C ₁₀ H ₁₄	1624.35, 2.787	134.109	148209	
2,3-Dimethylundecane	C ₁₃ H ₂₈	1630.35, 4.524	184.2186	86873	
Methylbenzeneacetaldehyde	C ₉ H ₁₀ O	1636.35, 2.795	134.0726	58973	
3-Methylundecane	C ₁₂ H ₂₆	1642.36, 4.577	170.2029	642600	
Dibutyldisulfide	C ₈ H ₁₈ S ₂	1648.36, 4.810	178.0844	36075	
Pentylcyclohexane	C ₁₁ H ₂₂	1654.36, 3.867	154.1716	482326	
4-Hydroxy-3-methyleneoctan-2-one	C ₉ H ₁₆ O ₂ ?	1654.36, 4.116	156.1145	17649	2.23E-4
Octacosane	C ₂₈ H ₅₈	1654.36, 4.813	394.4533	69966	
Decahydro-2-methylnaphthalene	C ₁₁ H ₂₀	1660.36, 3.545	152.156	187546	
1-Isopropyl-1-methylcyclohexane	C ₁₀ H ₂₀	1660.36, 4.167	140.156	59014	
4-Ethyl-1,2-dimethylbenzene	C ₁₀ H ₁₄	1672.37, 2.746	134.109	304660	
Tricosane	C ₂₃ H ₄₈	1672.37, 4.820	324.3751	41226	
Hexyl butyl ether	C ₁₀ H ₂₂ O ?	1678.37, 4.765	158.1665	49482	6.26E-4
5-Methyl-2(3H)-benzoxazolone	C ₈ H ₇ NO ₂	1690.37, 3.525	149.0471	18450	
1,17-Octadecadiene	C ₁₈ H ₃₄	1720.38, 4.056	250.2655	31847	
2,4-Dimethyl-1,3-hexanediol	C ₈ H ₁₈ O ₂	1720.38, 4.412	146.1301	32388	
Hexacosane	C ₂₆ H ₅₄	1738.38, 4.778	366.422	314161	
1-Methyldecahydronaphthalene	C ₁₁ H ₂₀	1756.39, 3.482	152.156	91029	
3-Acetyl-3-methylcyclohexanone	C ₉ H ₁₄ O ₂ ?	1768.39, 4.388	154.0988	27720	3.51E-4
Tridecane	C ₁₃ H ₂₈	1774.39, 4.526	184.2186	5273133	
1-Methyl-3-(1-methylethyl)benzene	C ₁₀ H ₁₄	1780.4, 2.746	134.109	153443	

trans-1-Methyl-2-octylcyclopropane	C ₁₂ H ₂₄	1786.4, 3.998	168.1873	23564	
4-Methylphenyl acetone	C ₁₀ H ₁₂ O ?	1792.4, 2.940	148.0883	79794	1.01E-4
1-Methyl-3-pentylcyclohexane	C ₁₂ H ₂₄	1822.41, 4.089	168.1873	448065	
1-Methyl-4-(1-methylpropyl)benzene	C ₁₁ H ₁₆	1828.41, 2.880	148.1247	51320	
5-Hydroxy-1,2,3,4-tetrahydronaphthalen-1-one	C ₁₀ H ₁₂ O ₂ ?	1840.41, 3.767	164.0832	17659	2.23E-4
3-(Hex-1'-enyl)cyclopropane-2,2-dimethylcyclopropane-1-carbaldehyde	C ₁₂ H ₂₀ O ?	1858.42, 3.679	180.1509	63752	8.07E-4
1,4-Dicyclohexylbutane	C ₁₆ H ₃₀	1858.42, 4.032	222.2342	157119	
3-Methyldodecane	C ₁₃ H ₂₈	1882.43, 4.715	184.2186	61465	
2,4-Dimethyl-1-(1-methylethyl)benzene	C ₁₁ H ₁₆	1888.43, 2.846	148.1247	45377	
Methyl p-(isopropyl)benzyl sulfoxide	C ₁₁ H ₁₆ OS ?	1894.43, 2.836	196.0916	12872	1.63E-4
2,2-Dimethylpropyl nitrite	C ₅ H ₁₁ NO ₂	1930.44, 4.938	117.0784	28775	
(2-Methylpropyl)cyclohexane	C ₁₀ H ₂₀	1942.44, 3.967	140.156	98655	
Hentriacontane	C ₃₁ H ₆₄	1954.45, 4.639	436.5003	109177	
1,2,3,4-Tetramethylbenzene	C ₁₀ H ₁₄	1960.45, 2.746	134.109	103921	
1-Methylcyclohexyl acetate	C ₉ H ₁₆ O ₂ ?	1960.45, 4.325	156.1145	19955	2.52E-4
6-Methyldodecane	C ₁₃ H ₂₈	1972.45, 4.629	184.2186	791480	
2,4-Dimethylundecane	C ₁₃ H ₂₈	1984.45, 4.613	184.2186	228051	
Dotriacontane	C ₃₂ H ₆₆	1990.46, 4.871	450.5159	19610	
6-Hexyl-4-oxa-5-azaspiro[2.4]hept-5-ene	C ₁₁ H ₁₉ NO	2002.46, 3.883	181.1461	13384	
4-Methyldodecane	C ₁₃ H ₂₈	2002.46, 4.618	184.2186	339381	
2,3,7-Trimethyloctane	C ₁₁ H ₂₄	2008.46, 4.906	156.1873	1178836	
2-Methyldodecane	C ₁₃ H ₂₈	2014.46, 4.644	184.2186	685733	
1-(1,2-Dimethylcyclopentyl)-, trans-2-propyn-1-one	C ₁₀ H ₁₄ O ?	2032.47, 3.866	150.1039	27671	3.50E-4
1-(2-Ethylphenyl)ethan-1-one	C ₁₀ H ₁₂ O ?	2038.47, 2.809	148.0883	33101	4.19E-4
(1-Methylbutyl)benzene	C ₁₁ H ₁₆	2068.48, 2.875	148.1247	24459	
Hexylcyclohexane	C ₁₂ H ₂₄	2086.48, 3.914	168.1873	533328	
1-(4-Methylphenyl)-1-propanone	C ₁₀ H ₁₂ O ?	2098.49, 2.851	148.0883	44746	5.66E-4
cis,trans-2-Ethylbicyclo[4.4.0]decane	C ₁₂ H ₂₂	2158.5, 3.549	166.1716	90645	
(1,1-Dimethylbutyl)benzene	C ₁₂ H ₁₈	2170.51, 2.974	162.1403	62336	

Methyl(1-methylethyl)benzene	C ₁₀ H ₁₄	2176.51, 2.649	134.109	25755	
2-(4'-Methylphenyl)no hyphenpropanal	C ₁₀ H ₁₂ O ?	2182.51, 2.803	148.0883	85326	1.08E-3
6-Methylundecane	C ₁₂ H ₂₆	2194.51, 4.733	170.2029	130169	
3,4-Trimethylbenzeneacetaldehyde	C ₁₁ H ₁₄ O ?	2200.52, 2.916	162.1039	35227	4.46E-4
4-Methyl-1-[4-(1-methylethenyl)-1-cyclohexen-1-yl]-3-penten-1-one	C ₁₅ H ₂₂ O ?	2200.52, 3.253	218.1665	11023	1.39E-4
2-Methyl-2-(1-methyl-1-propenyl)no hyphen-cyclobutanone	C ₉ H ₁₄ O ?	2200.52, 3.486	138.1039	10705	1.35E-4
2-Methyl-4-hexyn-3-ol	C ₇ H ₁₂ O ?	2218.52, 4.334	112.0883	16223	2.05E-4
1-Methyl-3-propylcyclooctane	C ₁₂ H ₂₄	2224.52, 4.143	168.1873	155854	
Decahydro-1,1,6-trimethylnaphthalene	C ₁₃ H ₂₄	2266.54, 3.695	180.1873	17481	
2,2-Dimethyl-5-hexen-3-one	C ₈ H ₁₄ O	2296.54, 4.856	126.1039	30082	
Hexadecane	C ₁₆ H ₃₄	2302.55, 4.631	226.2655	148714	
1-Ehyl-4-(1-methylethyl)benzene	C ₁₁ H ₁₆	2308.55, 2.762	148.1247	36205	
(1,2-Dimethylpropyl)cyclohexane	C ₁₁ H ₂₂	2320.55, 4.052	154.1716	75779	
(E)-Deca-1,6-dien-3-one	C ₁₀ H ₁₆ O ?	2326.55, 4.865	152.1196	9930	1.25E-4
1,2,3,4-Tetrahydronaphthalene	C ₁₀ H ₁₂	2332.55, 2.464	132.0934	23183	
1-Ethyl-2-isopropenyl-benzene	C ₁₁ H ₁₄	2332.55, 2.664	146.109	21149	
cis-1-Methyl-4-(1-methylethyl)cyclohexane	C ₁₀ H ₂₀	2332.55, 4.006	140.156	101476	
6,8-Dimethylbicyclo[3.2.2]nona-6,8-dien-3-one	C ₁₁ H ₁₄ O ?	2344.56, 2.917	162.1039	40791	5.16E-4
1,10-Dicyanonohyphen-decane	C ₁₂ H ₂₀ N ₂	2362.56, 3.980	192.1621	47913	
(cis)-1-Butyl-2-undecylcyclopropane	C ₁₈ H ₃₆	2368.56, 4.225	252.2812	47597	
6-Methyltridecane	C ₁₄ H ₃₀	2368.56, 4.587	198.2342	748800	
(2S)-4-(Isopropylamino)-2-butanol	C ₇ H ₁₇ NO	2374.57, 2.645	131.1305	8496	
(E)-4-Methyl-6-(2',5',6',6'-tetramethylcyclohex-1'-enyl)hex-3-en-1-ol	C ₁₇ H ₃₀ O ?	2374.57, 3.669	250.2291	28495	3.60E-4
N-(But-2-enoyl)prop-2-enamide	C ₇ H ₁₁ NO	2374.57, 4.136	125.0835	16764	
2,6,11-Trimethyldodecane	C ₁₅ H ₃₂	2404.58, 4.856	212.2499	223726	
(Z)-5-Methylundec-4-en-6-yn-3-ol	C ₁₂ H ₂₀ O ?	2428.58, 3.667	180.1509	5147	6.52E-5
3-Methyltridecane	C ₁₄ H ₃₀	2458.59, 4.515	198.2342	628531	
N-(1-Adamantyl)oxy-N,N-dibutylamine	C ₁₈ H ₃₃ NO	2464.59, 3.185	279.2557	15333	

1-Ethyl-4-(1-methylpropyl)benzene	C ₁₂ H ₁₈	2500.6, 2.893	162.1403	21455	
trans-1-[(2-Butylcyclopropyl)methyl]benzene	C ₁₄ H ₂₀	2506.6, 2.570	188.156	10559	
Heptylcyclohexane	C ₁₃ H ₂₆	2506.6, 3.903	182.2029	601725	
trans-1-Ethyl-1,4-dimethyl cyclohexane	C ₁₀ H ₂₀	2524.61, 4.167	140.156	85062	
2,2-Dimethyl-4-(methylethyl)-2H-imidazole	C ₈ H ₁₄ N ₂	2536.61, 4.096	138.1151	40855	
2-(1-Phenylethyl)phenol	C ₁₄ H ₁₄ O ?	2536.61, 4.676	198.1039	94951	1.20E-3
3-Methyl-1-hexen-5-one	C ₇ H ₁₂ O	2620.64, 4.311	112.0883	29103	
2-Pent-1-enyltetrahydrofuran	C ₉ H ₁₆ O ?	2722.67, 3.981	140.1196	25651	3.24E-4
1-Azido-1-methylcyclohexane	C ₇ H ₁₃ N ₃	2734.67, 3.982	139.1104	92533	
1,2,3,4-Tetrahydro-5-methyl-naphthalene	C ₁₁ H ₁₄	2746.67, 2.525	146.109	62660	
(7Z,11Z)-Hexadecadienal	C ₁₆ H ₂₈ O ?	2746.67, 4.272	236.2135	37286	4.72E-4
5-Propyldecane	C ₁₃ H ₂₈	2746.67, 4.546	184.2186	693002	
2,6,10,14-Tetramethylheptadecane	C ₂₁ H ₄₄	2752.68, 4.762	296.3438	1130039	
1,2,3,4-Tetrahydro-1,8-dimethylnaphthalene	C ₁₂ H ₁₆	2764.68, 2.686	160.1247	37045	
5-Methyltetradecane	C ₁₅ H ₃₂	2764.68, 4.510	212.2499	312547	
(2S,3S)-2-Methyl-3-(2-methyl-2-propenyl)cyclopentanone	C ₁₀ H ₁₆ O ?	2776.68, 4.136	152.1196	28774	3.64E-4
4-Methyltetradecane,	C ₁₅ H ₃₂	2782.68, 4.525	212.2499	286396	
3-Methylene-5-(2-furyl)penten-5-ol	C ₁₀ H ₁₂ O ₂ ?	2806.69, 4.132	164.0832	19152	2.42E-4
Trtriacontane	C ₃₃ H ₆₈	2824.7, 4.436	464.5316	57662	
4,4,7,7-Tetramethyl-1,9-decadiene	C ₁₄ H ₂₆	2830.7, 4.108	194.2029	33496	
2,6-Dimethylheptadecane	C ₁₉ H ₄₀	2836.7, 4.474	268.3125	511742	
Isopropoxy-3-methylbenzyl	C ₁₁ H ₁₆ O ?	2848.7, 2.959	164.1196	9901	1.25E-4
Bicyclo[4.3.1]deca-1-ol	C ₁₀ H ₁₈ O ?	2896.72, 4.124	154.1352	4684	5.93E-5
2,2-Dimethylbutane	C ₆ H ₁₄	2902.72, 4.881	86.109	29381	
1,2,3,4-Tetrahydro-6-methylnaphthalene	C ₁₁ H ₁₄	2908.72, 2.456	146.109	21882	
Octylcyclohexane	C ₁₄ H ₂₈	2908.72, 3.878	196.2186	538856	
(1E)-1-Hexenylbenzene	C ₁₂ H ₁₆	2914.72, 2.633	160.1247	9885	
2,7-Dimethylindan-1-one	C ₁₁ H ₁₂ O ?	2962.74, 2.582	160.0883	14319	1.81E-4
Methyl pentanoate	C ₆ H ₁₂ O ₂	2968.74, 4.604	116.0832	67230	

5-Methyl-3-hexyn-2-ol	C ₇ H ₁₂ O	2974.74, 4.033	112.0883	13239	
Cyclopentanodec-5-ene	C ₁₅ H ₂₈	2986.74, 4.256	208.2186	17694	
1-Methylnaphthalene	C ₁₁ H ₁₀	3022.75, 2.319	142.0777	62507	
4-tert-Butyl-2-methylenebutyrolactone	C ₉ H ₁₄ O ₂ ?	3022.75, 4.227	154.0988	12283	1.55E-4
1-Methyl-2-pentylcyclohexane	C ₁₂ H ₂₄	3106.78, 3.970	168.1873	122199	
6-Methylpentadecane	C ₁₆ H ₃₄	3112.78, 4.469	226.2655	887321	
1-N-Butyl-1,2,3,4-tetrahydronaphthalene	C ₁₄ H ₂₀	3118.78, 2.526	188.156	9956	
5-Phenylpent-1-en-3-yne	C ₁₁ H ₁₀	3124.78, 2.280	142.0777	26994	
2,4,4-Trimethylhexane	C ₉ H ₂₀	3124.78, 4.668	128.156	59807	
5-Methylpentadecane	C ₁₆ H ₃₄	3130.78, 4.438	226.2655	285991	
Dioctyldisulfide	C ₁₆ H ₃₄ S ₂	3136.79, 4.623	290.2096	29323	
Eicosane	C ₂₀ H ₄₂	3142.79, 4.644	282.3281	167389	
4-Methylpentadecane	C ₁₆ H ₃₄	3148.79, 4.449	226.2655	312879	
2-Methylnonadecane	C ₂₀ H ₄₂	3166.79, 4.449	282.3281	512566	
(5S,7S,9S,E)-S-Ethyl 5,7,9-trimethyltridec-3-enethioate	C ₁₈ H ₃₄ OS	3196.8, 4.063	298.2325	14236	
2,6-Dimethyloctadecane	C ₂₀ H ₄₂	3202.8, 4.397	282.3281	394596	
2-Methyl-5-(2-methyl-3-methylenebicyclo[2.2.2]oct-5-en-2-yl)-2-penten-1-ol	C ₁₆ H ₂₄ O ?	3226.81, 2.961	232.1822	9377	1.18E-4
(1S,3R,4R)-3-(Hydroxymethyl)-2-methyl-2-azabicyclo[2.2.1]heptane	C ₈ H ₁₅ NO	3238.81, 4.064	141.1148	15482	
Germacrane-C	C ₁₅ H ₃₀	3244.82, 4.077	210.2342	52474	
1,2,3,4-Tetrahydro-5,6-dimethylnaphthalene	C ₁₂ H ₁₆	3274.82, 2.504	160.1247	59251	
1,1-Bis(2,3-epoxypropyl)ethane	C ₈ H ₁₄ O ₂	3274.82, 3.892	142.0988	16459	
Cyclohexyltoluene	C ₁₃ H ₁₈	3316.84, 2.658	174.1403	10213	
2,6,10,15-Tetramethylheptadecane	C ₂₁ H ₄₄	3334.84, 4.683	296.3438	73958	
(6R,12R)-6,12-Dimethylpentadec-1-ene	C ₁₇ H ₃₄	3364.85, 4.027	238.2655	42324	
1-Hexadecene	C ₁₆ H ₃₂	3370.85, 4.010	224.2499	58707	
2-Cyanocyclohexanol	C ₇ H ₁₁ NO	3382.86, 4.445	125.0835	142093	
1,5-Dimethylnaphthalene	C ₁₂ H ₁₂	3418.87, 2.386	156.0934	91154	
5-Methyldodecane	C ₁₃ H ₂₈	3478.88, 4.387	184.2186	254819	

4-(2-Tetrahydropyranyl)oxybutanal	C ₉ H ₁₆ O ₃ ?	3496.89, 4.776	172.1094	32032	4.05E-4
2,6-Dimethylnaphthalene	C ₁₂ H ₁₂	3502.89, 2.341	156.0934	34882	
(3R,4S,5R,7R)-3,5,7-Trimethyl-1-nonen-4-ol	C ₁₂ H ₂₄ O ?	3502.89, 4.113	184.1822	20580	2.60E-4
2'-Methyl-spiro[cyclopropane-1,1'-ind-2'-ene]	C ₁₂ H ₁₂	3520.9, 2.326	156.0934	76324	
Nonadecane	C ₁₉ H ₄₀	3520.9, 4.752	268.3125	77574	
(Z)-3-Ethyl-2,2,5,5-tetramethyl-3-hexene	C ₁₂ H ₂₄	3550.9, 4.065	168.1873	25652	
3-Methylhexadecane	C ₁₇ H ₃₆	3550.9, 4.330	240.2812	314487	
3-Hydroxy-7,7-dimethyl-1,8-nonadien-5-one	C ₁₁ H ₁₈ O ₂ ?	3574.91, 4.043	182.1301	44986	5.69E-4
1,2-Dimethylnaphthalene	C ₁₂ H ₁₂	3598.92, 2.323	156.0934	12310	
2,5-Bis(tetrahydrofuran)	C ₈ H ₁₄ O ₂ ?	3616.92, 4.668	142.0988	56289	7.13E-4
4-Methylheptadecane	C ₁₈ H ₃₈	3826.98, 4.351	254.2968	199200	
1,6,7-Trimethylnaphthalene	C ₁₃ H ₁₄	3869, 2.380	170.109	35149	
(E)-2-((E)-But-2-enylidene)hydrazinecarbothioamide	C ₅ H ₉ N ₃ S	3875, 2.476	143.0512	8889	
2,9-Dimethyldecane	C ₁₂ H ₂₆	3881, 4.296	170.2029	281719	
1,4,6-Trimethylnaphthalene	C ₁₃ H ₁₄	3887, 2.385	170.109	42239	
3-Ethyl-3-methylhexane	C ₉ H ₂₀	3887, 4.436	128.156	58412	
Octyl allyl ether	C ₁₁ H ₂₂ O ?	3911.01, 4.600	170.1665	35634	4.51E-4
1-Decene	C ₁₀ H ₂₂	3917.01, 4.424	142.1716	9111	
(E)-2-Tetradecen-1-ol	C ₁₄ H ₂₈ O ?	4055.05, 3.955	212.2135	20536	2.60E-4
10-Methylnonadecane	C ₂₀ H ₄₂	4091.06, 4.315	282.3281	400638	
2,6,8-Trimethyldecane	C ₁₃ H ₂₈	4109.06, 4.310	184.2186	250494	
5-Methyloctadecane	C ₁₉ H ₄₀	4121.07, 4.312	268.3125	90957	
3,8-Dimethylundecane	C ₁₃ H ₂₈	4145.07, 4.279	184.2186	161605	
Heptacosane	C ₂₇ H ₅₆	4157.08, 4.305	380.4377	246751	
4,4'-Dimethyl-1,1'-biphenyl	C ₁₄ H ₁₄	4163.08, 2.313	182.109	13835	
2-(Cyclohexylmethyl)tetrahydrofuran	C ₁₁ H ₂₀ O ?	4181.09, 4.593	168.1509	129608	1.64E-3
4,4-Dimethyloctane	C ₁₀ H ₂₂	4217.1, 4.518	142.1716	29694	
9-Hydroxyinalool	C ₁₀ H ₁₈ O ₂ ?	4229.1, 4.363	170.1301	116819	1.47E-3
2,3,4,5-Tetrahydro-6-hexylpyridine	C ₁₁ H ₂₁ N	4271.11, 3.740	167.1669	21019	

2,2,4-Trimethyl-2H-imidazole	C ₆ H ₁₀ N ₂	4307.12, 3.923	110.0838	13418
Undecylcyclohexane	C ₁₇ H ₃₄	4319.12, 3.754	238.2655	227962
Bicyclo[3.2.1]octan-1-ol	C ₈ H ₁₄ O	4367.14, 3.915	126.1039	79966
2,3,5-Trimethylhexane	C ₉ H ₂₀	4421.15, 4.270	128.156	72903
2,10-Dimethylundecane	C ₁₃ H ₂₈	4493.17, 4.222	184.2186	119874
2-Ethyl-1-hexene	C ₈ H ₁₈	4943.3, 4.242	114.1403	33920
9-Methyl-1,6-methanofluorene	C ₁₅ H ₁₄	4949.31, 2.300	194.109	8050
2,5,9-Trimethyldecane	C ₁₃ H ₂₈	4949.31, 4.207	184.2186	123503
2,6,10-Trimethyltridecane	C ₁₆ H ₃₄	5009.32, 4.429	226.2655	12975
1a,9b-Dihydro-1H-cyclopropa[1]phenanthrene	C ₁₅ H ₁₂	5327.41, 2.167	192.0934	10086
7-Phenylindene	C ₁₅ H ₁₂	5357.42, 2.173	192.0934	8498
2,3,3,4-Tetramethylpentane	C ₉ H ₂₀	5501.46, 4.162	128.156	19106
Methyl-2-propyl-4-2,5-dihydrofuran	C ₈ H ₁₄ O	5975.6, 3.779	126.1039	37708
(3R)-3-Phenyl-2,3-dihydro-1H-isoindol-1-one	C ₁₄ H ₁₁ NO	6203.67, 1.086	209.0835	57662
2-Isocyano-2-methylpropane	C ₅ H ₉ N	6659.8, 3.892	83.073	13399
(3S)-3-Phenyl-2,3-dihydro-1H-isoindol-1-one	C ₁₄ H ₁₁ NO	6833.85, 1.081	209.0835	331509
Benzene	C ₆ H ₆	7085.92, 1.087	78.0464	29100
Fumaronitrile	C ₄ H ₂ N ₂	7319.99, 1.093	78.0212	18870
1,3-Hexadien-5-yne	C ₆ H ₆	7349.99, 1.092	78.0464	18682
N-[(1,1-Dimethylethyl)carbonimidoyl]-5-methyl-4-isoxazolamine	C ₉ H ₁₃ N ₃ O	7938.16, 1.209	179.1053	5903