

稠油样品检测报告

1 项目信息

项目名称：稠油样品组分的测定

样品名称：稠油

2 实验部分

2.1 主要设备与试剂

东西分析 GC×GC-TOF MS 3300 型全二维气质联用仪

分析天平、冰箱、25mL 具塞玻璃试管、移液枪。

试剂：CS₂ 溶剂

2.2 样品处理

准确称取 1g 稠油样品，放入 25mL 具塞玻璃试管中，准确加入 5mL CS₂ 并密封试管，置于涡旋混合器上涡旋 2min，混匀后取 0.5ul 上 GC×GC-TOF MS 分析。

2.4 分析条件

色谱条件：

第一维色谱柱 DB-5 (30m×0.25mm×0.25um) 石英毛细管柱 第二维色谱柱 DB-17HT (3m×0.25mm×0.25um) 石英毛细管柱；

恒流模式，柱流量 1 mL/min，不分流进样，分流阀打开时间 45s，进样量：0.35μL，进样口：300℃，吹扫流量：2mL/min。调制周期 12s。

第一维柱温：60℃保持 3min，然后以 1℃/min 速率升至 200℃保持 5min，再以 10℃/min 升至 310℃保持 10min。第二维柱温：60℃保持 3min，然后以 1℃/min 速率升至 200℃保持 5min，再以 10℃/min 升至 310℃保持 10min。调制器热喷温度恒定 330℃。

质谱条件： EI 源，离子源温度：260℃，接口温度：280℃，电离电压：70V，检测电压：-1800，扫描范围：40~650u，溶剂延迟：4min。

3 实验结果

3.1 稠油样品谱图

稠油样品用 CS₂ 溶解后直接进全二维气质仪，经过条件优化试验得知，样品在 90℃ 到 200℃ 之间基质非常复杂，选择非常慢的升温程序，样品基本得到完全分离，得到的总离子流图见图 1 和图 2。

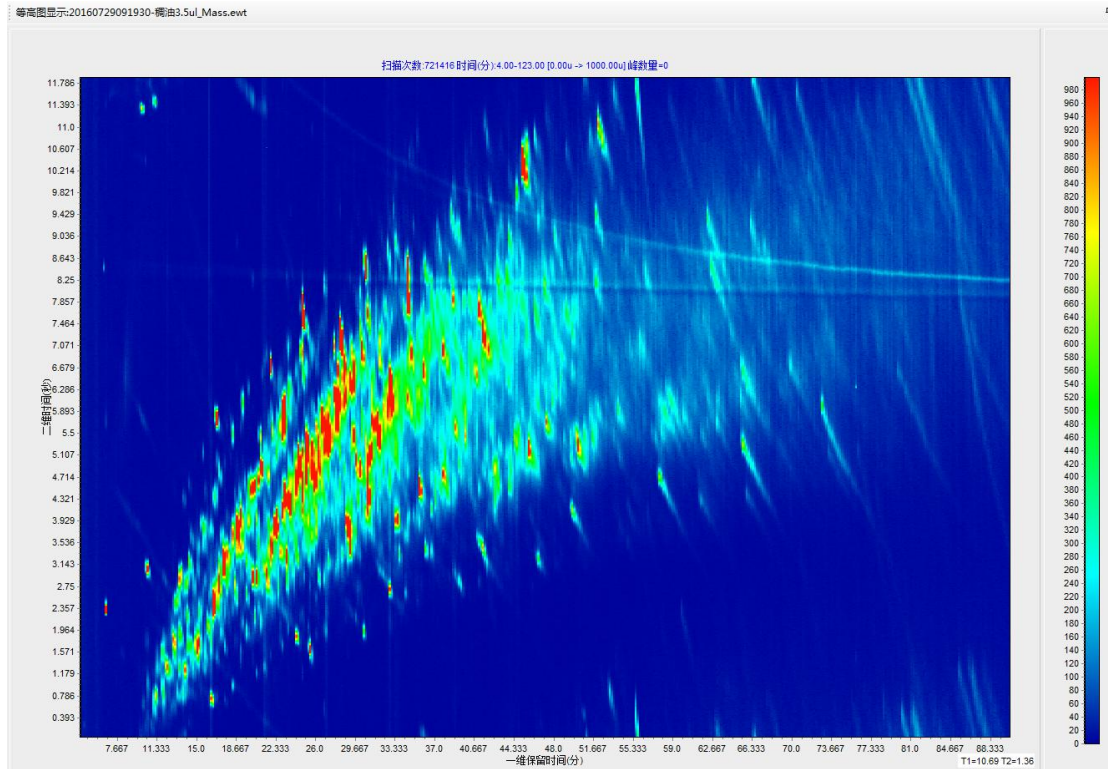


图 1 用 CS₂ 溶解的稠油样品二维显示总离子流图

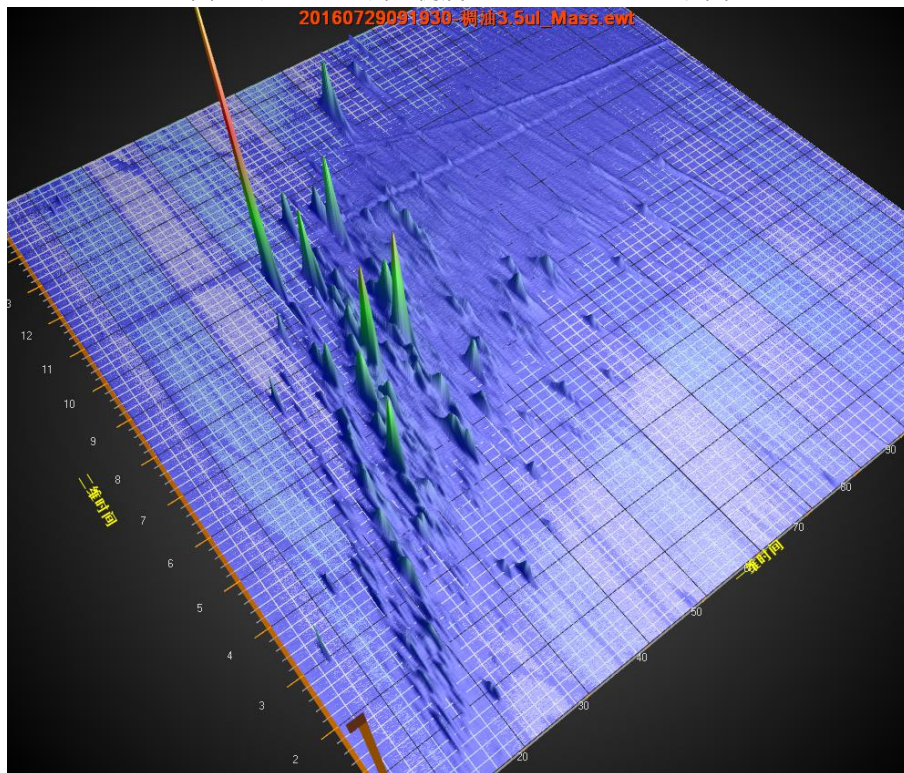


图 2 用 CS₂ 溶解的稠油样品三维显示总离子流图

通过谱库自动检索，得到定性报告，附表 1 列出了一部分化合物。检测到稠油样品的组分基本都是小分子量烷烃、环烷烃、烯烃，芳香烃非常少。当柱温高于 200℃时，只能检测到正构烷烃，正构烷烃最高分子量只能达到 C₂₈。

4 结果讨论

由于稠油样品基质复杂，一般溶剂很难溶解此样品。本次实验选择了 CS₂ 溶解稠油样品。程序升温过程中在 90℃到 200℃之间，样品组分非常多，很难分离。采用加长二维柱以及降低升温速度，样品也没有达到完全分离，附表中的定性化合物也只能作为参考，不一定准确。当柱温高于 200℃时，检测到的组分只有正构烷烃，最高只能达到 C₂₈。

本实验难点：1、稠油大多是高分子化合物，很难汽化；2、没有找到合适的溶剂溶解；3、没有明确需要分析的目标化合物，所以没有合适的样品前处理；4、样品基质复杂，对仪器污染较为严重。5、由于样品的污染柱头或样品溶剂不合适，造成峰拖尾。

附表 1.稠油样品（溶剂 CS₂）部分定性表（仅作参考）

1D	2D time	化合物名称	Match	分子式	分子量	CAS
7.15	10.69	Sulfur dioxide	93	O ₂ S	64	744609
9.93	8.29	Methyl 2-hydroxydecanoate	69	C ₁₁ H ₂₂ O ₃	202	712712
12.7	0.56	1-Dodecyn-4-ol	68	C ₁₂ H ₂₂ O	182	746463
12.7	1.27	1,5-Heptadiene, 2-methyl-, (Z)-	59	C ₈ H ₁₄	110	410446
11.95	14.33	3-Hexanone, 2,2-dimethyl-	78	C ₈ H ₁₆ O	128	540579
12.2	0.79	trans-8a-Methylperhydroazulen-4(1H)-one	61	C ₁₁ H ₁₈ O	166	321664
11.95	7.35	Phenol	79	C ₆ H ₆ O	94	108952
11.95	0.13	Hexanenitrile, 5-methyl-	73	C ₇ H ₁₃ N	111	194243
12.7	1.32	Norbornane, 2-isobutyl-	73	C ₁₁ H ₂₀	152	181271
12.7	2.21	1,5-Hexadiene, 3-methyl-	66	C ₇ H ₁₂	96	154133
12.7	3.87	1-Pentanol, 3-methyl-	74	C ₆ H ₁₄ O	102	589355
13.21	0.37	1-Undecyn-4-ol	72	C ₁₁ H ₂₀ O	168	221278
13.71	1.04	4-Nonene, 2,3,3-trimethyl-, (Z)-	75	C ₁₂ H ₂₄	168	638306
12.96	14.9	Isobutyl nitrite	73	C ₄ H ₉ NO ₂	103	542563
13.96	1.66	4-Ethyl-2-hexynal	64	C ₈ H ₁₂ O	124	719329
14.72	1.02	5-Undecene, 5-methyl-, (Z)-	71	C ₁₂ H ₂₄	168	570249

14.72	2.02	Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1.alpha.,3.alpha.,6.alpha.)]-	70	C10H18	138	606997
14.72	3.76	Propane, 2-methyl-2-nitro-	75	C4H9NO2	103	594707
13.71	14.44	Heptane, 2,5,5-trimethyl-	79	C10H22	142	118999
15.23	1.61	4-Octene, 2,6-dimethyl-, [S-(Z)]-	80	C10H20	140	629607
15.98	0.74	4-Nonene, 2,3,3-trimethyl-, (E)-	69	C12H24	168	638306
15.98	2.29	Bicyclo[3.1.1]heptan-3-one, 2,6,6-trimethyl-, (1.alpha.,2.beta.,5.alpha.)-	71	C10H16O	152	153588
16.24	3.17	5-Undecyne	71	C11H20	152	229472
16.49	1.07	Cyclohexanemethanol, 4-(1-methylethyl)-, trans-	68	C10H20O	156	136741
16.74	1.61	trans-8a-Methylperhydroazulen-4(1H)-one	66	C11H18O	166	321664
16.74	2.39	1,4-Heptadiene, 3,3,6-trimethyl-	65	C10H18	138	744988
16.74	3.66	Cyclopropane, 1-(1-methylethyl)-2-(2-methyl-1-methylenepropyl)-	66	C11H20	152	562591
17.24	1.07	3-Decene, 2,2-dimethyl-, (E)-	62	C12H24	168	554990
17.24	1.65	2-Decyne	59	C10H18	138	238470
17.24	2.27	Cyclohexane, 1-ethyl-1,3-dimethyl-, cis-	70	C10H20	140	622383
17.24	2.87	trans-4-tert-butylcycloheptanol	70	C11H22O	170	622153
17.24	3.3	Cyclohexene, 1-butyl-	78	C10H18	138	328253
17.24	5.45	1,5-Hexadiene, 2-methyl-	76	C7H12	96	404981
17.5	1.6	Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)-	67	C15H28	208	297884
17.75	2.13	Cyclohexanemethanol, 4-(1-methylethyl)-, trans-	71	C10H20O	156	136741
17.75	2.81	4-Octene, 2,3,6,7-tetramethyl-	75	C12H24	168	638306
17.75	3.61	Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1.alpha.,3.alpha.,6.alpha.)]-	72	C10H18	138	606997
18	4.04	3-Octyne, 2,2,7-trimethyl-	63	C11H20	152	554021
18.51	1.73	4-Nonene, 2,3,3-trimethyl-, (E)-	71	C12H24	168	638306

18.51	2.92	2-Propen-1-one, 1-(2,2-dimethylcyclopropyl)-	61	C8H12O	124	778469
18.25	4.6	Cyclopropane, 1-(1-methylethyl)- 2-(2-methyl-1-methylenepropyl)-	66	C11H20	152	562591
18	5.84	Oxirane, (2,2-dimethylpropyl)-	68	C7H14O	114	224529
19.01	2.11	3-Decene, 2,2-dimethyl-, (E)-	75	C12H24	168	554990
19.26	2.92	Cyclohexanemethanol, 4-(1-methylethyl)-, trans-	69	C10H20O	156	136741
19.26	3.81	1,6-Heptadiene, 3-methyl-	73	C8H14	110	508710
19.26	4.4	5,10-Pentadecadien-1-ol, (Z,Z)-	65	C15H28O	224	642755
20.02	1.64	1-Undecyn-4-ol	78	C11H20O	168	221278
20.02	1.98	1-Dodecyn-4-ol	74	C12H22O	182	746463
20.02	3.63	1,1'-Bicyclopropyl, 2,2,2',2'-tetramethyl-	69	C10H18	138	689982
20.02	4.8	Cyclohexane, butylidene-	70	C10H18	138	227203
20.02	5.7	3-Octyne, 7-methyl-	68	C9H16	124	370500
20.78	0.94	3-Hexanone, 2,2-dimethyl-	79	C8H16O	128	540579
20.27	2.6	1-Hexyl-2-nitrocyclohexane	65	C12H23NO2	213	1.18E+
20.78	3.34	2,9-Dimethyl-5-decyne	57	C12H22	166	195505
20.02	4.89	4-Decyne	69	C10H18	138	238486
21.03	3.08	3-Decene, 2,2-dimethyl-, (E)-	71	C12H24	168	554990
21.28	5.49	5,10-Pentadecadien-1-ol, (Z,Z)-	70	C15H28O	224	642755
21.53	1.91	2-Propen-1-one, 1-(2,2-dimethylcyclopropyl)-	53	C8H12O	124	778469
21.78	3.5	Naphthalene, decahydro-2,2-dimethyl-	69	C12H22	166	311248
21.28	5.47	5,10-Pentadecadien-1-ol, (Z,Z)-	64	C15H28O	224	642755
21.78	6.06	Bicyclo[2.2.1]heptane, 2-ethyl-	76	C9H16	124	214641

21.53	7.31	2-Nonen-1-ol	74	C9H18O	142	221047
22.04	2.35	Cyclohexanemethanol, 4-(1-methylethyl)-, trans-	60	C10H20O	156	136741
22.54	2.86	4-Octene, 2,3,6,7-tetramethyl-	70	C12H24	168	638306
22.54	2.07	Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)-	62	C15H28	208	297884
22.29	4.05	Thujone	75	C10H16O	152	546805
23.55	1.21	3-Hexanone, 2,2-dimethyl-	76	C8H16O	128	540579
23.8	3.44	4-Octene, 2,3,6,7-tetramethyl-	68	C12H24	168	638306
23.55	4.65	2,9-Dimethyl-5-decyne	64	C12H22	166	195505
24.05	4.86	Naphthalene, decahydro-2,2-dimethyl-	70	C12H22	166	311248
23.55	6.92	3-Nonyne	72	C9H16	124	201848
24.56	4.99	Naphthalene, decahydro-2,2-dimethyl-	68	C12H22	166	311248
24.81	7.58	Norbornane, 2-isobutyl-	74	C11H20	152	181271
25.32	2.38	1-Dodecyn-4-ol	72	C12H22O	182	746463
25.32	3.33	Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)-	68	C15H28	208	297884
25.32	3.99	4-Octene, 2,3,6,7-tetramethyl-	77	C12H24	168	638306
25.32	4.97	1,1'-Bicyclopropyl, 2,2,2',2'-tetramethyl-	67	C10H18	138	689982
25.57	4.93	Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, .alpha.,3.alpha.,6.alpha.)]-	67	C10H18	138	606997
25.57	7.95	Norbornane, 2-isobutyl-	67	C11H20	152	181271
26.07	3.7	Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)-	79	C15H28	208	297884
26.07	5.68	cis,cis- and cis,trans-1,9-dimethylspiro[4.5]decane	75	C12H22	166	0
25.57	7.97	Cyclodecene, 3-bromo-	64	C10H17Br	216	563255
26.07	10.43	1-Adamantanemethanol	66	C11H18O	166	770718
28.59	4.32	Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)-	71	C15H28	208	297884

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29.1	4.95	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	82	C15H28	208	297884
28.59	6.99	Bicyclo[2.2.1]heptane, 2,2,3-trimethyl-, endo-	67	C10H18	138	205364
28.34	8.5	2-Decen-1-ol	72	C10H20O	156	221048
29.6	4.28	Cyclohexane, 1,5-diethyl-2,3-dimethyl-	71	C12H24	168	746636
30.36	4.12	1-Tridecyn-4-ol	71	C13H24O	196	746463
29.86	5.18	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	75	C15H28	208	297884
29.86	7.1	7-Tetradecyne	73	C14H26	194	352161
30.11	7.54	Naphthalene, decahydro-2,2-dimethyl-	68	C12H22	166	311248
30.61	5.37	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	75	C15H28	208	297884
30.61	7.88	Cyclohexane, (2-ethyl-1-methylbutylidene)-	65	C13H24	180	748104
30.61	8.93	1,2-Cyclohexanedimethanol	71	C8H16O2	144	397129
31.62	2.4	3-Hexanone, 2,4-dimethyl-	80	C8H16O	128	186417
31.62	4.24	1-Tridecyn-4-ol	68	C13H24O	196	746463
31.62	5.82	Cyclopentene, 5-hexyl-3,3-dimethyl-	71	C13H24	180	611426
31.87	6.36	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	82	C15H28	208	297884
31.87	7.98	5,10-Pentadecadienoic acid, (Z,Z)-	63	C15H26O2	238	642756
32.38	5.22	1-Octadecyne	69	C18H34	250	629890
32.38	5.77	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	78	C15H28	208	297884
32.38	6.52	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	73	C15H28	208	297884
32.38	8.73	trans-8a-Methylperhydroazulen-4(1H)-one	66	C11H18O	166	321664
32.38	9.7	Decanal	86	C10H20O	156	112312
32.88	4.5	Cyclohexane, 1,5-diethyl-2,3-dimethyl-	67	C12H24	168	746636

32.88	5.95	3-Hexadecyne	66	C16H30	222	618866
33.13	6.67	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	76	C15H28	208	297884
32.88	8.47	3-Decyne	73	C10H18	138	238485
33.64	4.59	1-Hexyl-2-nitrocyclohexane	72	C12H23NO2	213	1.18E+
33.89	5.93	Cyclopentene, 5-hexyl-3,3-dimethyl-	72	C13H24	180	611426
34.14	7.1	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	74	C15H28	208	297884
34.4	3.74	1-Tridecyn-4-ol	69	C13H24O	196	746463
34.65	6.06	3-Tetradecyne	68	C14H26	194	602123
34.9	7.26	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	76	C15H28	208	297884
35.15	10.33	2-Decyne	63	C10H18	138	238470
35.66	6.77	7-Tetradecyne	71	C14H26	194	352161
35.66	6.08	1-Hexyl-2-nitrocyclohexane	74	C12H23NO2	213	1.18E+
36.67	7.17	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	70	C15H28	208	297884
36.67	7.71	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	75	C15H28	208	297884
36.92	8.43	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	74	C15H28	208	297884
36.41	8.91	6,10-Dimethyl-9-undecen-4-ol	64	C13H26O	198	197800
37.17	9.19	1,1-Dimethyl-4-methylenecyclohexane	72	C9H16	124	600796
37.68	8.34	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	77	C15H28	208	297884
37.68	7.71	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	68	C15H28	208	297884
37.68	6.25	Methyl 2-hydroxydecanoate	64	C11H22O3	202	712712
38.18	4.86	3-Decene, 2,2-dimethyl-, (E)-	73	C12H24	168	554990

38.43	4.39	Cyclohexane,1,1'-[1,2-bis(1,1-dimethylethyl)-1,2-ethanediyl]bis-,*,R*)-(./-.)-	68	C22H42	306	651498
38.68	5.3	1-Hexyl-2-nitrocyclohexane	75	C12H23NO2	213	1.18E+
38.94	6.88	Cyclohexane, (2-ethyl-1-methylbutylidene)-	55	C13H24	180	748104
38.43	8.1	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	71	C15H28	208	297884
38.68	8.76	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	72	C15H28	208	297884
39.69	6.09	Bicyclo[3.3.1]nonan-9-one,1,2,4-trimethyl-3-nitro-,(2-endo,3-exo,4-exo)-(./-.)-	60	C12H19NO3	225	1.3E+0
40.2	2.5	Butane, 2,2-dimethyl-	71	C6H14	86	75832
40.7	5.12	4-Nonene, 2,3,3-trimethyl-, (Z)-	76	C12H24	168	638306
40.7	5.61	1-Undecene, 9-methyl-	72	C12H24	168	746304
40.7	6.31	Bicyclo[3.3.1]nonan-9-one,1,2,4-trimethyl-3-nitro-, 2-endo,3-exo,4-exo)-(./-.)-	62	C12H19NO3	225	1.3E+0
40.7	7.34	Bicyclo[2.2.1]heptane, 2,2,3-trimethyl-, endo-	62	C10H18	138	205364
40.7	8.37	Bicyclo[2.2.1]heptane, 2,2,3-trimethyl-, endo-	66	C10H18	138	205364
40.7	9.68	cis,trans-2,9-Dimethylspiro[5.5]undecane	68	C13H24	180	955307
40.45	10.69	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	74	C15H28	208	297884
41.96	7.07	Bicyclo[3.3.1]nonan-9-one,1,2,4-trimethyl-3-nitro-, 2-endo,3-exo,4-exo)-(./-.)-	62	C12H19NO3	225	1.3E+0
42.22	8.55	1,3-Hexadiene, 3-ethyl-2-methyl-, (Z)-	65	C9H16	124	747529
42.22	8.98	Cyclohexane, (2-ethyl-1-methylbutylidene)-	68	C13H24	180	748104
42.72	6.07	1-Hexyl-2-nitrocyclohexane	81	C12H23NO2	213	1.18E+
41.96	5.32	1-Dodecyn-4-ol	67	C12H22O	182	746463
43.73	7.73	1H-Indene, 2-butyl-5-hexyloctahydro-	60	C19H36	264	550443
42.97	9.76	5,10-Pentadecadien-1-ol, (Z,Z)-	68	C15H28O	224	642755
43.22	11.03	trans-8a-Methylperhydroazulen-4(1H)-one	73	C11H18O	166	321664

43.48	3.46	Dodecane, 1-iodo-	79	C12H25I	296	429219
44.49	4.99	Cyclohexane, 1,5-diethyl-2,3-dimethyl-	74	C12H24	168	746636
44.23	6.51	1-Hexyl-2-nitrocyclohexane	72	C12H23NO2	213	1.18E+
44.49	7.53	Bicyclo[3.3.1]nonan-9-one,1,2,4-trimethyl-3-nitro- 2-endo,3-exo,4-exo)-(.+.-)-	65	C12H19NO3	225	1.3E+0
44.23	11.2	1-Dodecyne	74	C12H22	166	765037
45.75	7.7	Bicyclo[3.3.1]nonan-9-one,1,2,4-trimethyl-3-nitro- 2-endo,3-exo,4-exo)-(.+.-)-	63	C12H19NO3	225	1.3E+0
46.25	8.78	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	68	C15H28	208	297884
45.75	9.99	8-Hexadecyne	61	C16H30	222	197818
45.75	10.75	(2,4,6-Trimethylcyclohexyl) methanol	67	C10H20O	156	137025
47.26	5.77	Cyclohexane, 1,5-diethyl-2,3-dimethyl-	74	C12H24	168	746636
47.26	7.83	Bicyclo[2.2.1]heptane, 2,2,3-trimethyl-, endo-	66	C10H18	138	205364
47.76	8.3	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	76	C15H28	208	297884
47.76	9.58	Bicyclo[3.3.1]nonan-9-one,1,2,4-trimethyl-3-nitro- 2-endo,3-exo,4-exo)-(.+.-)-	64	C12H19NO3	225	1.3E+0
48.02	10.68	trans-(2-Ethylcyclopentyl)methanol	61	C8H16O	128	362580
48.02	4.33	Dodecane, 1-iodo-	74	C12H25I	296	429219
48.77	4.3	Decane, 6-ethyl-2-methyl-	71	C13H28	184	621082
48.77	5.28	1-Tridecyn-4-ol	67	C13H24O	196	746463
47.76	8.38	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	72	C15H28	208	297884
48.02	10.65	Thujone	64	C10H16O	152	546805
50.29	6.05	1-Tridecyn-4-ol	70	C13H24O	196	746463
50.29	8.85	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	57	C15H28	208	548328
51.8	7.07	1-Hexyl-2-nitrocyclohexane	71	C12H23NO2	213	1.18E+

51.55	10.01	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	72	C15H28	208	297884
51.04	10.67	Cyclohexan-1-ethanol, 1-hydroxymethyl-	67	C9H18O2	158	318728
51.3	11.84	3-Undecyne	66	C11H20	152	602123
51.8	12.5	Bicyclo[3.3.1]nonan-9-one,1,2,4-trimethyl-3-nitro-(2-endo,3-exo,4-exo)-(.+.-)-	64	C12H19NO3	225	1.3E+0
52.3	11.52	Bicyclo[2.2.1]heptane, 2,2,3-trimethyl-, endo-	68	C10H18	138	205364
52.3	3.57	Nonane, 1-iodo-	73	C9H19I	254	428242
53.06	6.88	1-Hexyl-2-nitrocyclohexane	76	C12H23NO2	213	1.18E+
52.56	8.51	photocitral B	62	C10H16O	152	604045
52.81	9.98	Cyclohexanemethanol, 4-(1-methylethyl)-, trans-	63	C10H20O	156	136741
53.82	8.3	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	68	C15H28	208	297884
53.57	9.99	Cyclohexane, 1-methyl-4-(2-hydroxyethyl)-	64	C9H18O	142	491687
54.57	8.3	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	61	C15H28	208	548328
54.83	9.77	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	64	C15H28	208	297884
55.33	9.27	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	64	C15H28	208	548328
55.33	8.47	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	60	C15H28	208	548328
56.09	8.82	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	67	C15H28	208	297884
55.33	4.36	Dodecane, 1-iodo-	82	C12H25I	296	429219
56.84	5.62	Cyclohexane, 1,2,4,5-tetraethyl-, (1.alpha.,2.alpha.,4.alpha.,5.alpha.)-	67	C14H28	196	611422
56.84	6.13	1-Tridecyn-4-ol	72	C13H24O	196	746463
57.35	10.38	Bicyclo[3.3.1]nonan-9-one,1,2,4-trimethyl-3-nitro-, 2-endo,3-exo,4-exo)-(.+.-)-	65	C12H19NO3	225	1.3E+0
55.84	13.65	Pentane, 1-chloro-5-(methylenecyclopropyl)-	56	C9H15Cl	158	0
56.34	12.31	1-Undecyne	65	C11H20	152	224398
58.36	10.55	Naphthalene,decahydro-1,6-dimethyl-4-(1-methyl ethyl)-	68	C15H28	208	297884

58.61	11.38	Cyclohexanemethanol, 4-(1-methylethyl)-, trans-	65	C10H20O	156	136741
59.37	6.84	1-Hexyl-2-nitrocyclohexane	74	C12H23NO2	213	1.18E+
59.62	12.48	1,4-Heptadiene, 3,3,6-trimethyl-	61	C10H18	138	744988
61.13	6.56	Cyclohexane, 1,2,4,5-tetraethyl-, (1.alpha.,2.alpha.,4.alpha.,5.alpha.)-	72	C14H28	196	611422
60.38	13.11	photocitral A	65	C10H16O	152	552532
60.88	13.41	(2,4,6-Trimethylcyclohexyl) methanol	66	C10H20O	156	137025
61.89	9.81	1-Hexyl-2-nitrocyclohexane	67	C12H23NO2	213	1.18E+
61.89	13.67	photocitral A	72	C10H16O	152	552532
63.4	7.21	1,7-Dimethyl-4-(1-methylethyl)cyclodecane	72	C15H30	210	645103
63.15	10.2	Bicyclo[3.3.1]nonan-9-one,1,2,4- trimethyl-3-nitro-, 2-endo,3-exo,4-exo)-(.+.)-	64	C12H19NO3	225	1.3E+0
66.68	5.24	Dodecane, 1-iodo-	76	C12H25I	296	429219
67.44	6.73	Cyclohexane, 1,2,4,5-tetraethyl-, (1.alpha.,2.alpha.,4.alpha.,5.alpha.)-	73	C14H28	196	611422
66.68	6.34	4-Octene, 2,3,6,7-tetramethyl-	65	C12H24	168	638306
66.68	8.34	1-Hexyl-2-nitrocyclohexane	77	C12H23NO2	213	1.18E+
66.68	9.12	3-Methyl-2-(2-oxopropyl)furan	58	C8H10O2	138	877736
65.92	13.39	2,9-Dimethyl-5-decyne	59	C12H22	166	195505
68.2	6.96	1-Tridecyn-4-ol	71	C13H24O	196	746463
69.2	6.87	Methyl 2-hydroxydodecanoate	67	C13H26O3	230	510678
69.96	7.53	4-Octene, 2,3,6,7-tetramethyl-	72	C12H24	168	638306
69.71	10.31	Cyclohexanol, 4-ethyl-4-methyl-3- (1-methylethyl)-, (1.alpha.,3.beta.,4.alpha.)-	60	C12H24O	184	558695
69.71	11.86	Naphthalene, decahydro-1,6-dimethyl-4- (1-methylethyl)-	64	C15H28	208	297884
69.96	13.96	photocitral A	75	C10H16O	152	552532

72.48	7.49	1-Hexyl-2-nitrocyclohexane	70	C12H23NO2	213	1.18E+
71.98	14.73	2,5-Octadiene, 3,4,5,6-tetramethyl-	67	C12H22	166	2.48E+
75.26	9.12	1-Hexyl-2-nitrocyclohexane	77	C12H23NO2	213	1.18E+
76.01	10.65	3-Methyl-2-(2-oxopropyl)furan	67	C8H10O2	138	877736
74.75	14.91	Diphenyl sulfide	70	C12H10S	186	139662
77.78	5.98	Nonane, 1-iodo-	77	C9H19I	254	428242
71.47	1.07	Phthalic acid, isobutyl tridec-2-yn-1-yl ester	61	C25H36O4	400	0
78.54	7.4	1-Tridecyn-4-ol	68	C13H24O	196	746463
79.29	7.63	Methyl 2-hydroxydodecanoate	73	C13H26O3	230	510678
80.81	7.32	1-Hexyl-2-nitrocyclohexane	70	C12H23NO2	213	1.18E+
83.08	5.48	2,2,4-Trimethyl-3-pentanone	74	C8H16O	128	585736
85.09	7.17	1-Hexyl-2-nitrocyclohexane	64	C12H23NO2	213	1.18E+
85.09	7.73	1-Hexyl-2-nitrocyclohexane	71	C12H23NO2	213	1.18E+
84.34	10.7	Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)-	65	C15H28	208	297884
83.83	11.85	1-Hexyl-2-nitrocyclohexane	61	C12H23NO2	213	1.18E+
88.88	5.6	Dodecane, 1-iodo-	69	C12H25I	296	429219
88.37	6.68	Dodecane, 1-iodo-	77	C12H25I	296	429219
88.12	7.69	1-Tridecyn-4-ol	65	C13H24O	196	746463
88.37	8.33	1-Hexyl-2-nitrocyclohexane	70	C12H23NO2	213	1.18E+
89.38	11.68	1-Hexyl-2-nitrocyclohexane	66	C12H23NO2	213	1.18E+
89.63	14.94	trans-Chrysanthemal	65	C10H16O	152	201040
94.43	8.45	Cyclohexane, 1,5-diethyl-2,3-dimethyl-	69	C12H24	168	746636
95.18	14.61	photocitral A	69	C10H16O	152	552532

108.5	0.56	Cyclohexan-1-ethanol, 1-hydroxymethyl-	63	C9H18O2	158	318728
110.0	0.51	Cyclohexan-1-ethanol, 1-hydroxymethyl-	61	C9H18O2	158	318728
108.0	8.38	4-Octene, 2,2,3,7-tetramethyl-, [S-(E)]-	69	C12H24	168	638655
115.8	1.35	2-Dodecyne	62	C12H22	166	629492
117.6	1.38	3,5-Octadien-2-one, (E,E)-	58	C8H12O	124	300860