Liquid fuel from waste tires: Novel Refining, Advanced Characterization and Utilization in engines with ethyl levulinate as an additive

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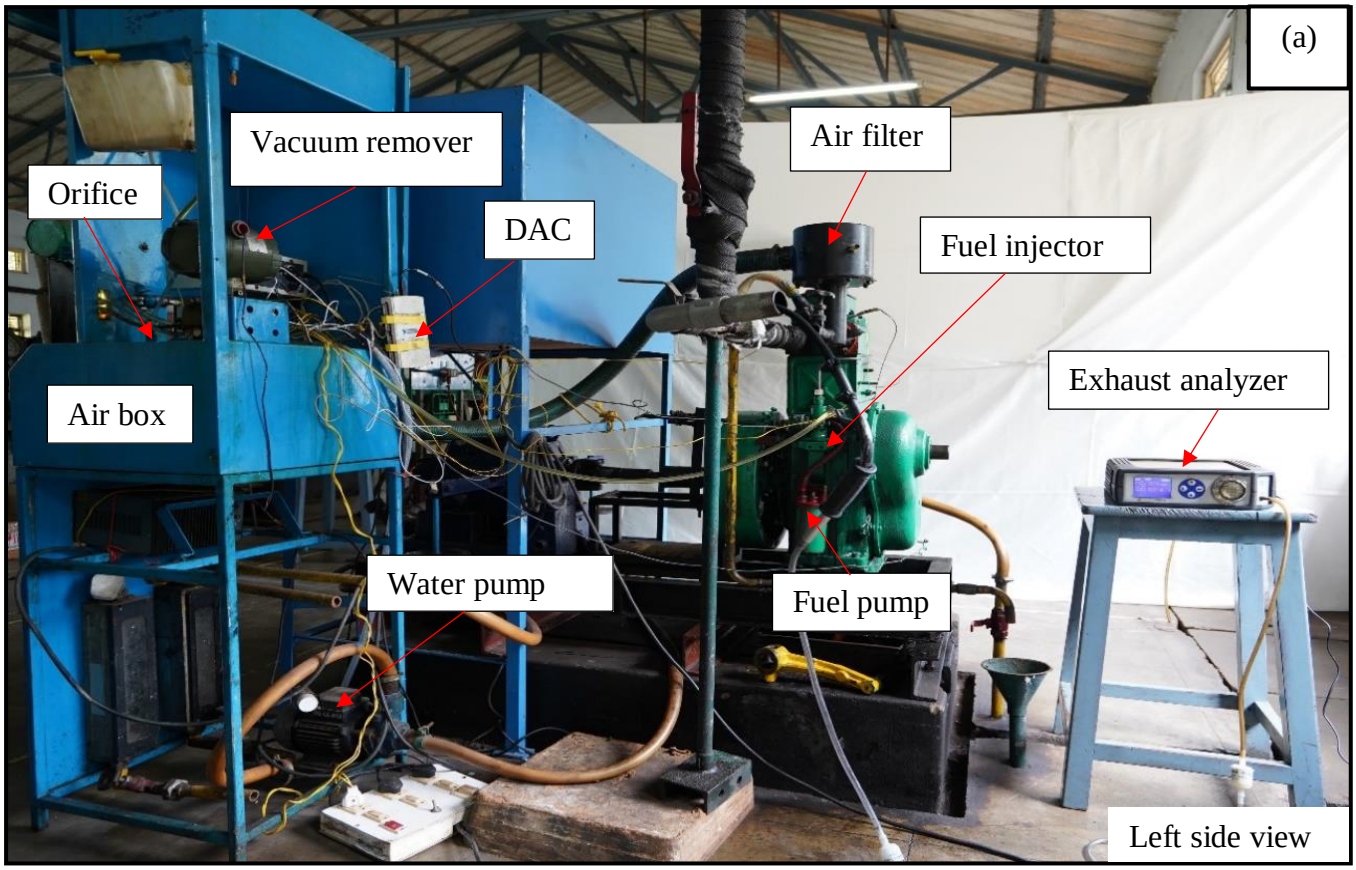
List of Figures



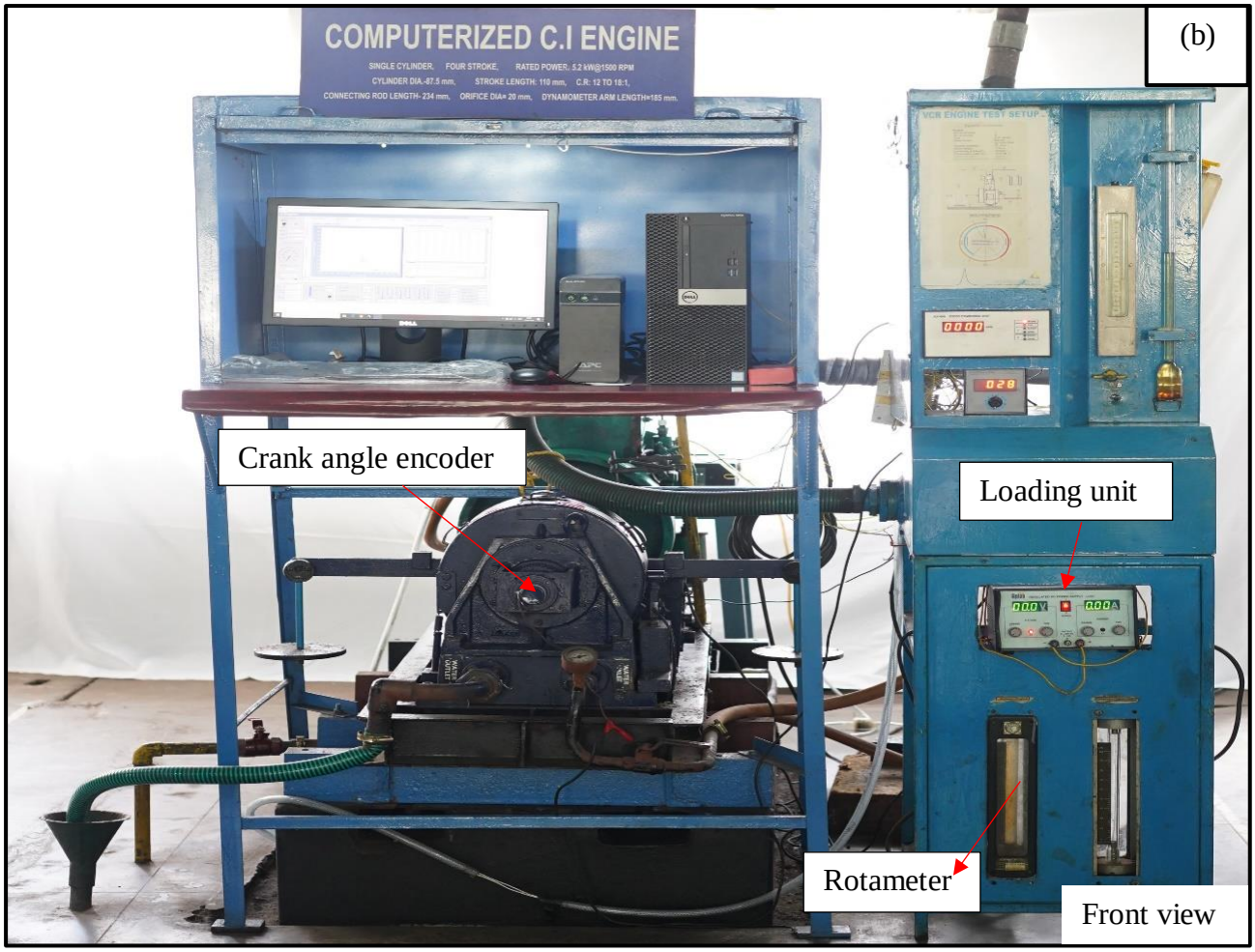


Fig. S1 (a) Left side view and (b) front view of experimental engine test facility

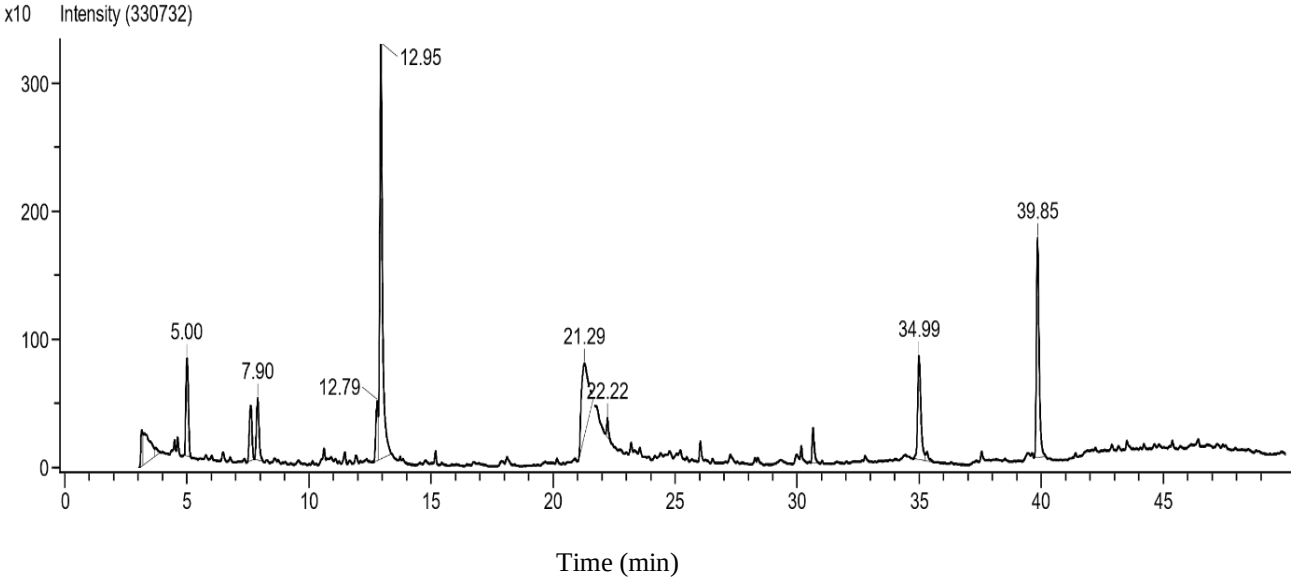


Fig. S2 Chromatogram of used silica gel washed by methanol

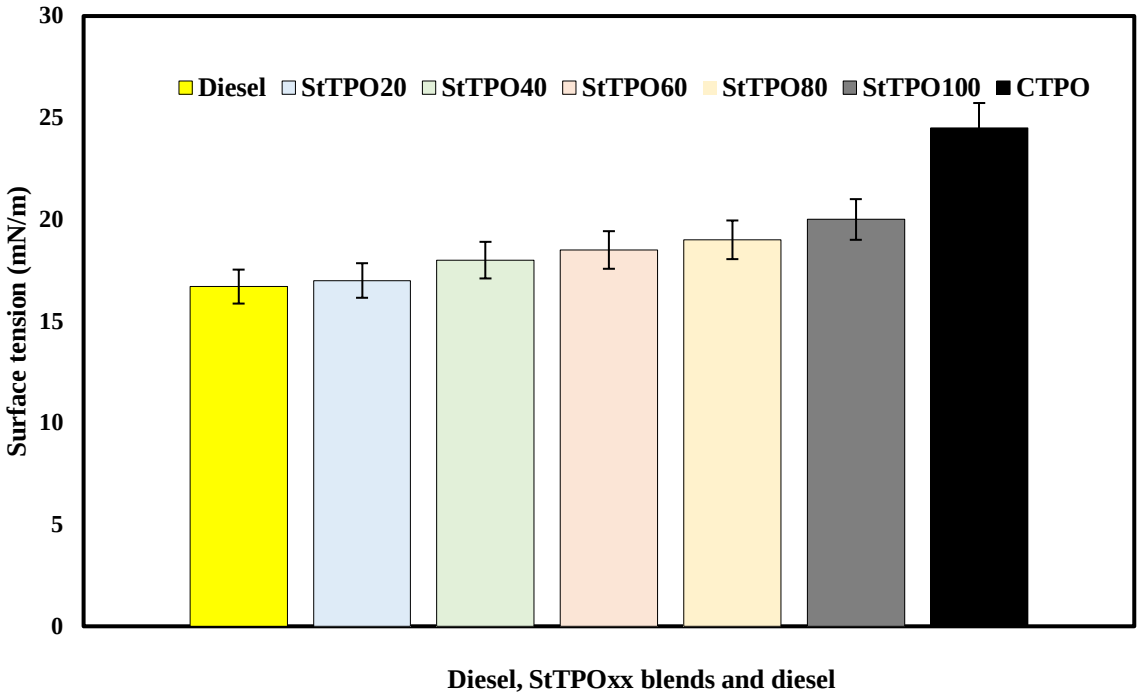


Fig. S3 Surface tension of CTPO, StTPOxx, and diesel

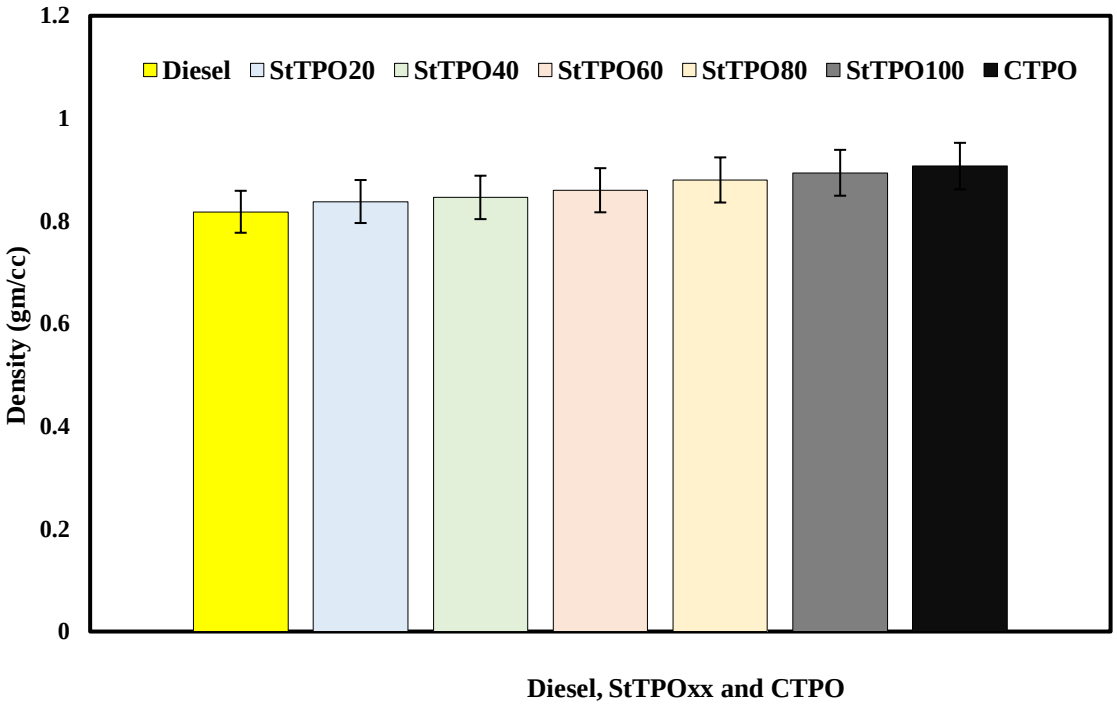


Fig. S4 Density of CTPO, StTPOxx, and diesel

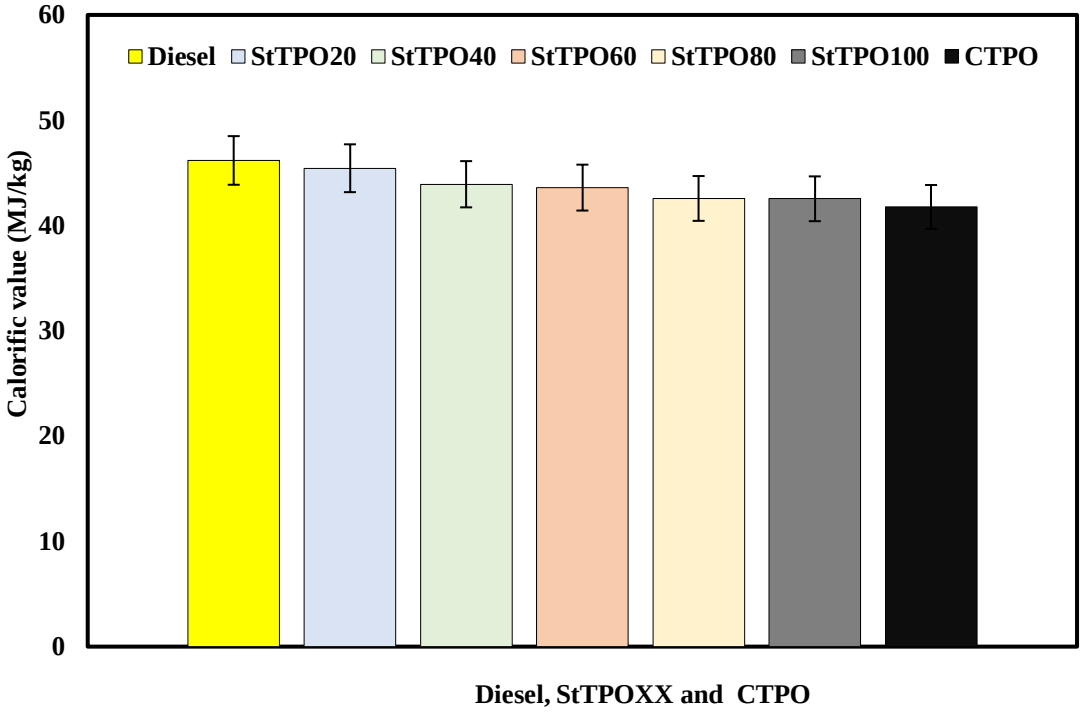


Fig. S5 Calorific value of diesel, StTPOxx, and CTPO

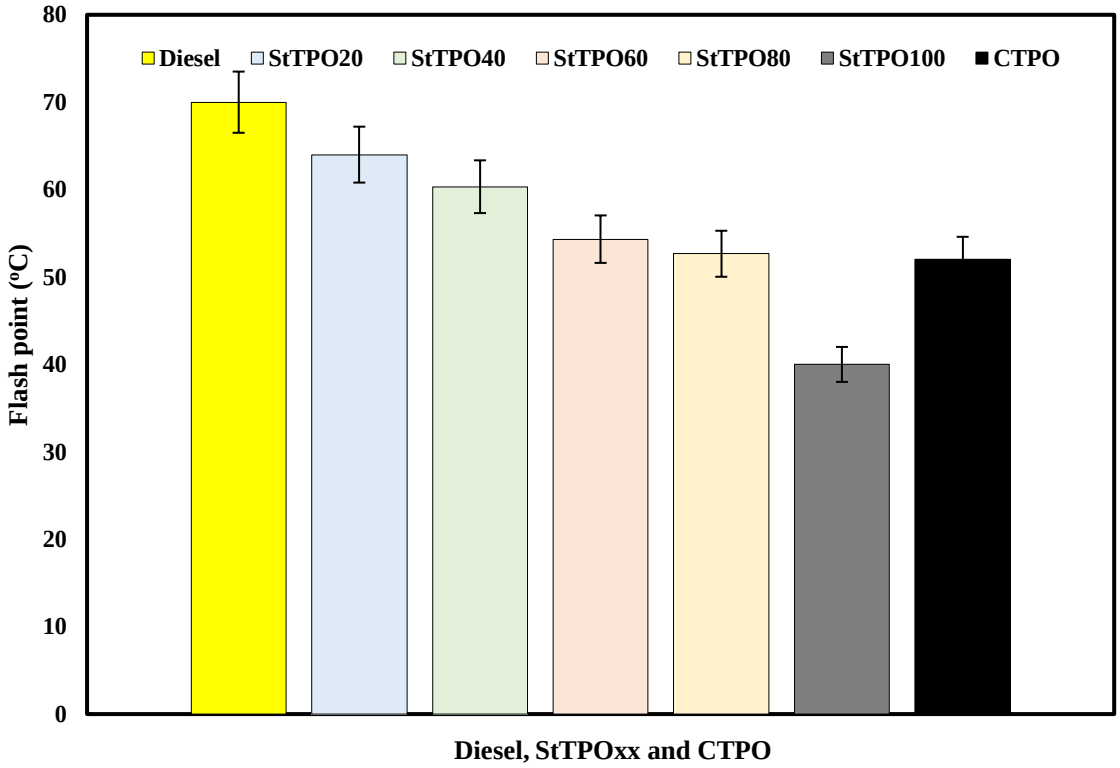


Fig. S6 Flashpoint of diesel, StTPOxx, and CTPO

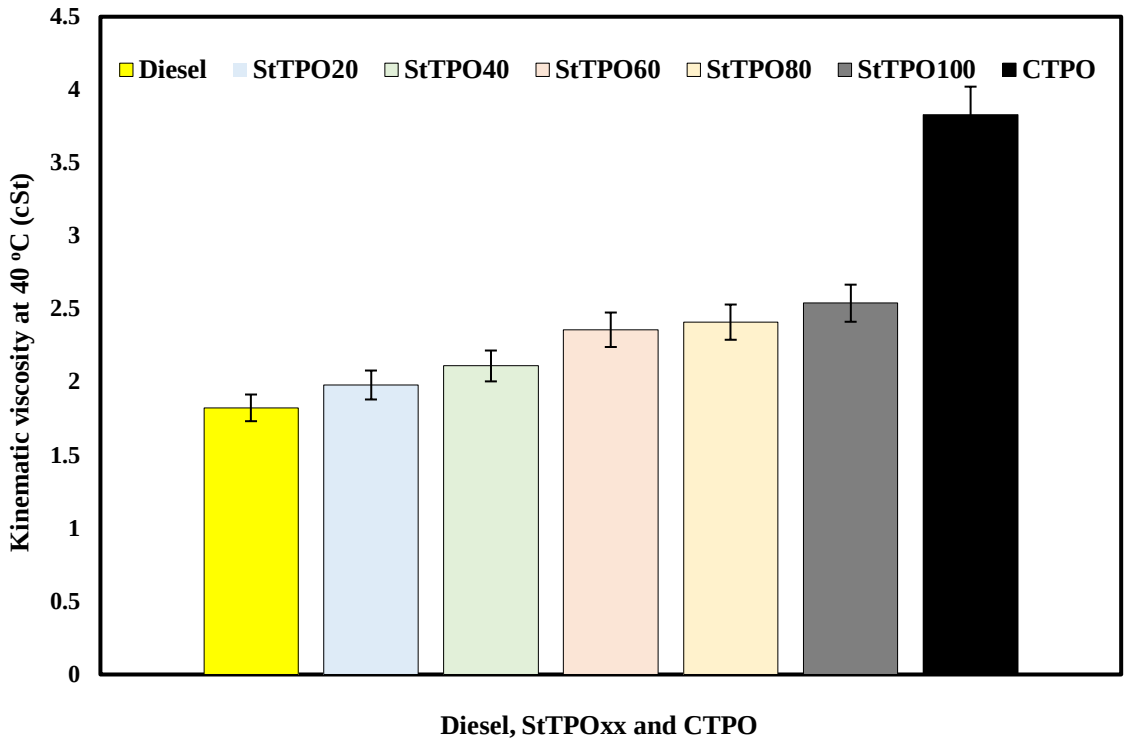


Fig. S7 Kinematic viscosity of diesel, StTPOxx, and CTPO

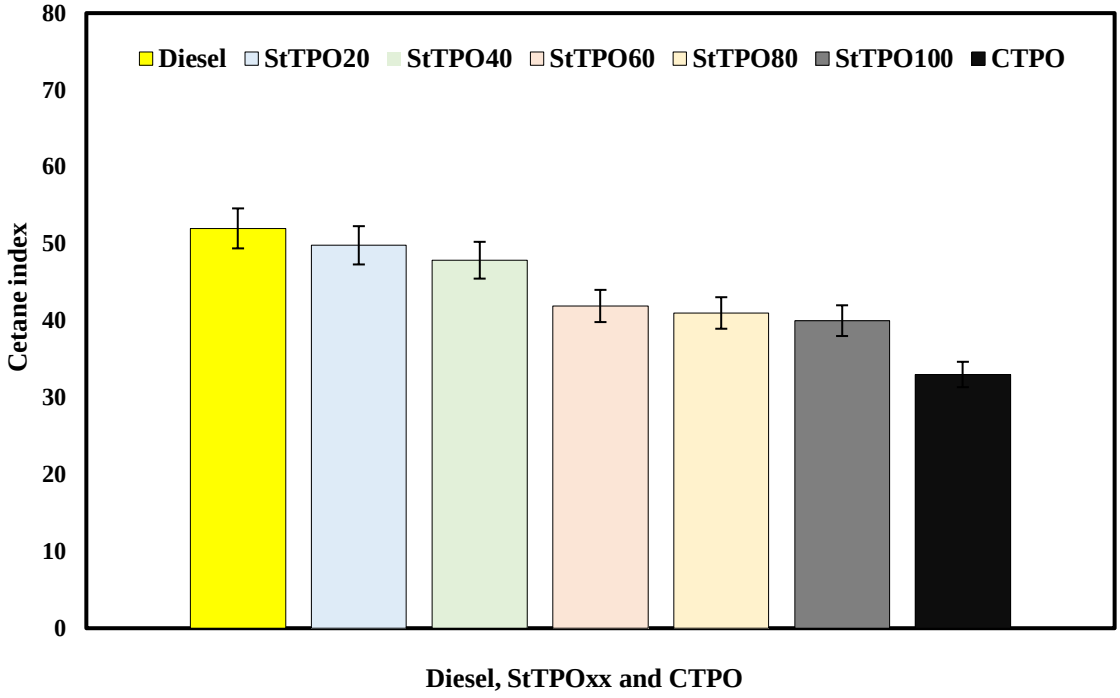


Fig. S8 Variation of cetane index of diesel, StTPOxx, and CTPO

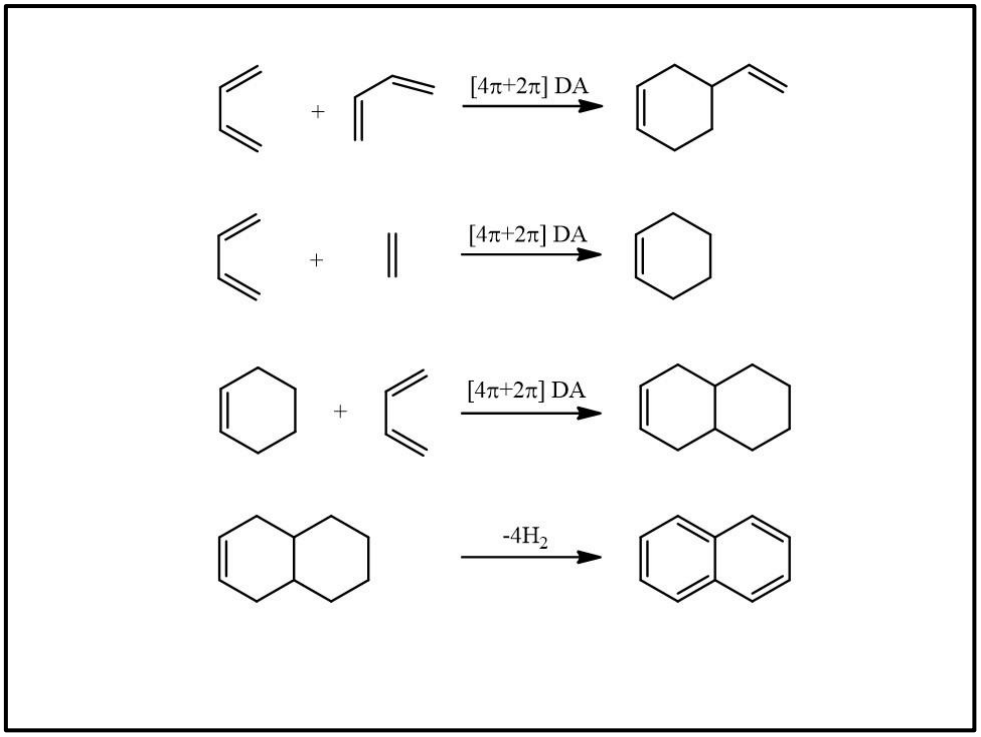
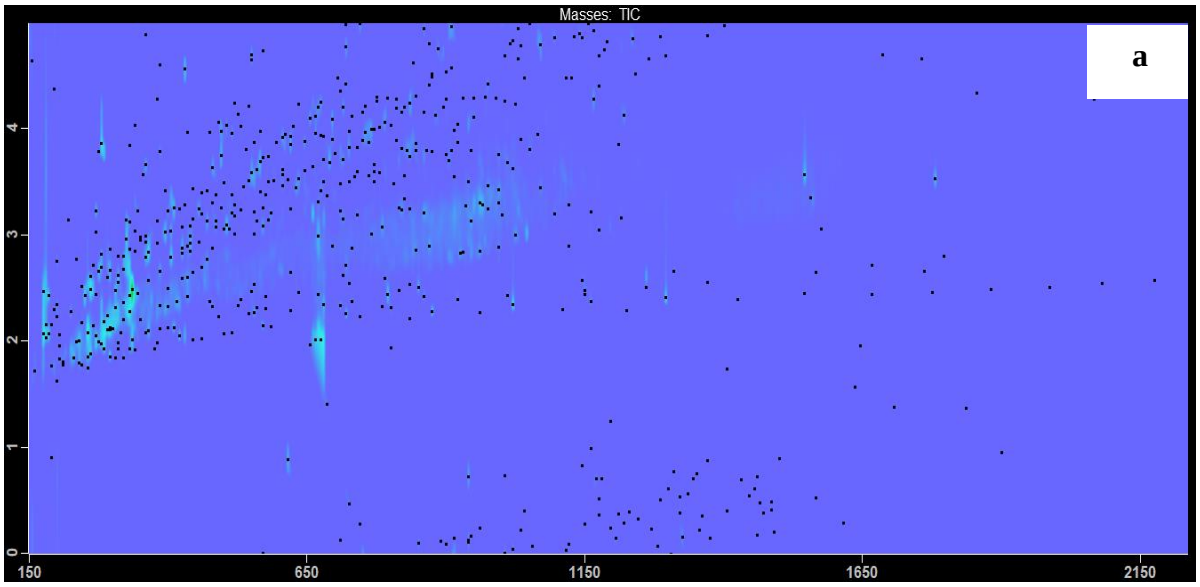


Fig. S9 Mechanism of polyaromatic formation tire pyrolysis



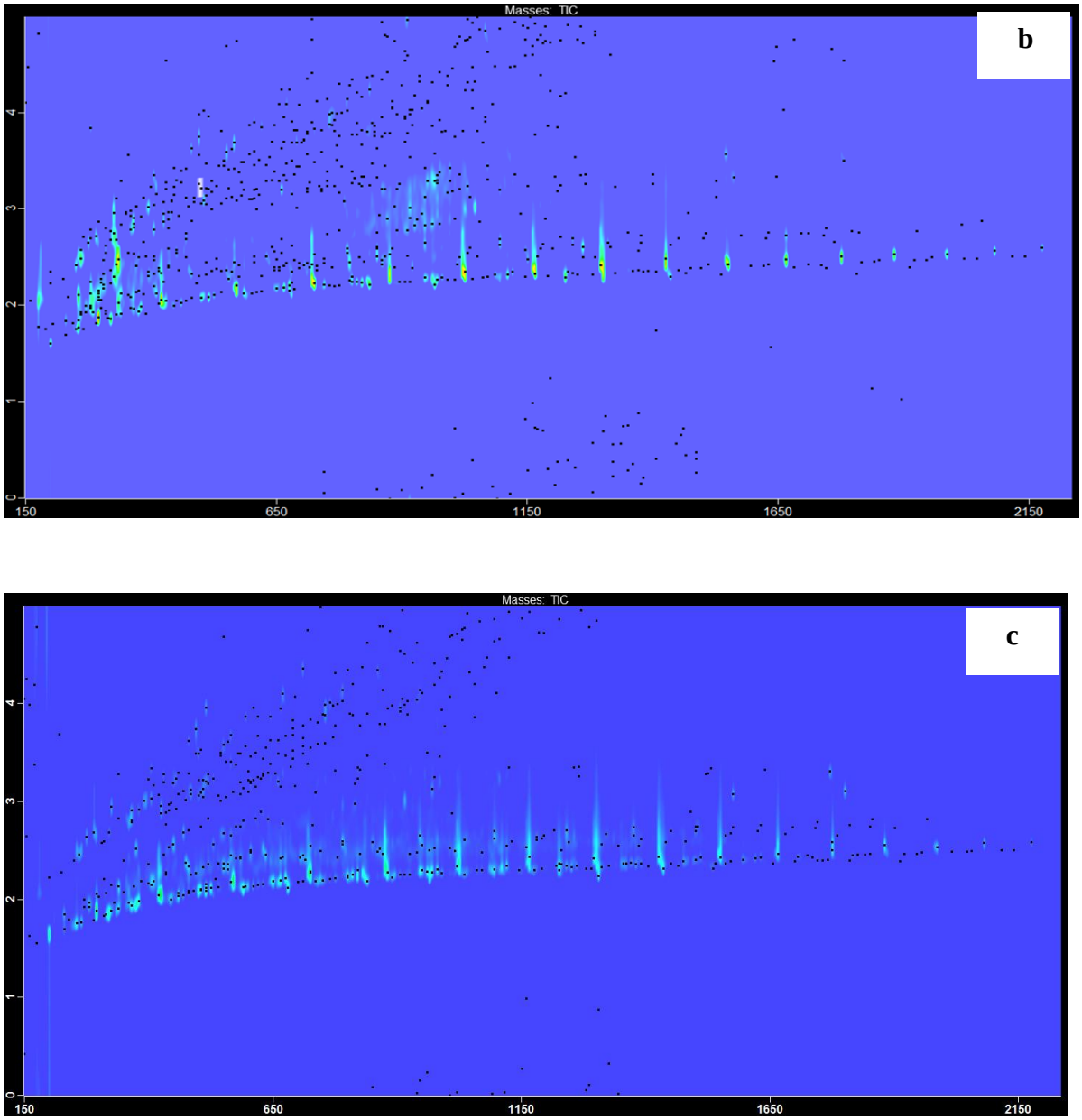


Fig. S10 Contour plot obtained from GC×GC TOF-MS (apolar×polar column combination) during the analysis of (a) CTPO, (b) StTPO, and (c) diesel

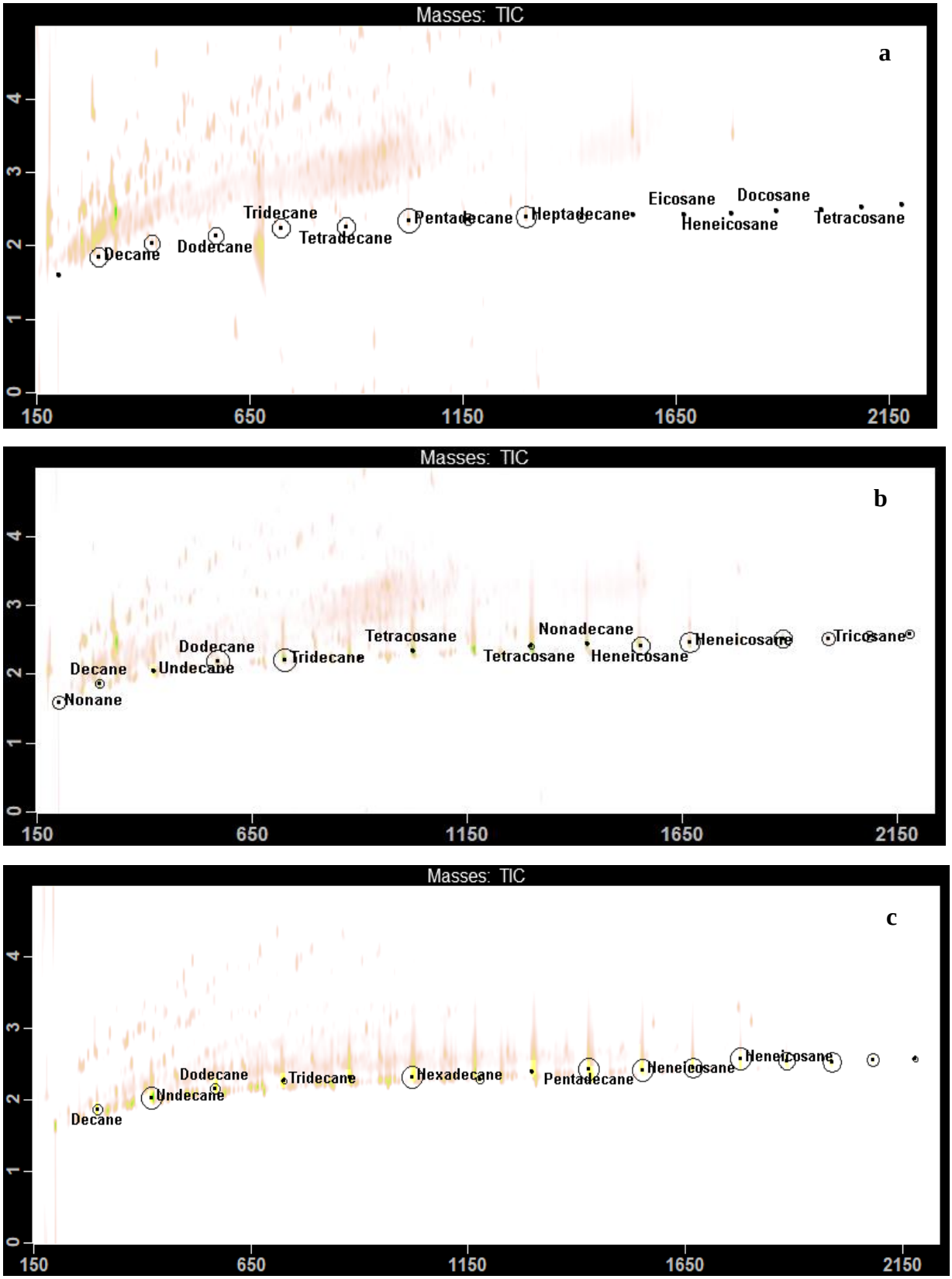
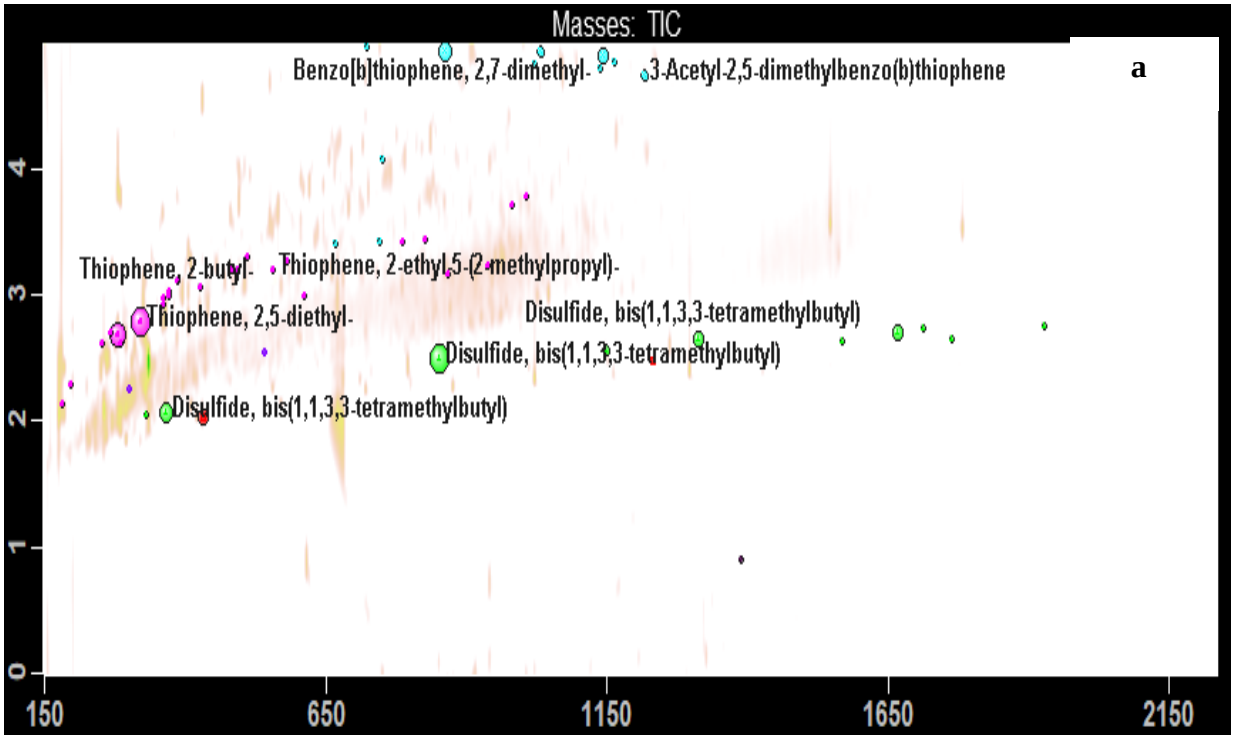
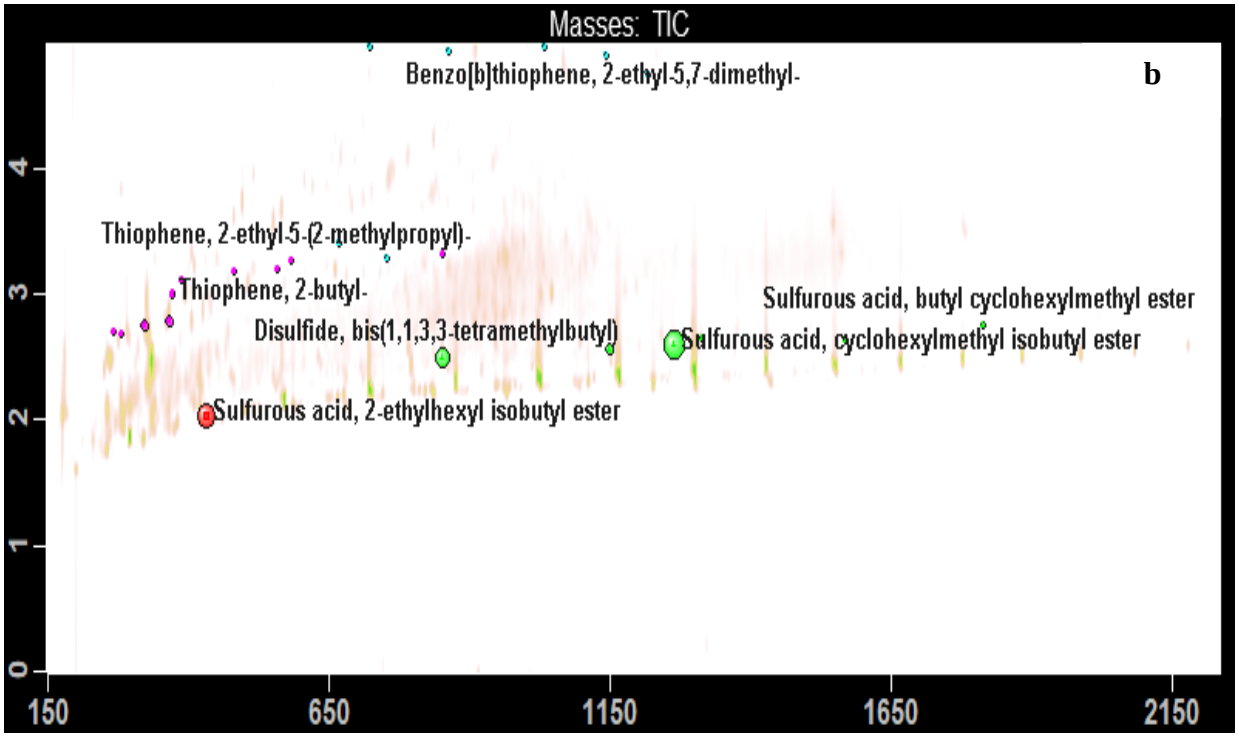


Fig. S11 Chromatogram of saturates (n-alkanes) in (a) CTPO, (b) StTPO and (c) diesel


Masses: TIC
Benzo[b]thiophene, 2,7-dimethyl-
3-Acetyl-2,5-dimethylbenzo(b)thiophene
a
Thiophene, 2-butyl-
Thiophene, 2-ethyl-5-(2-methylpropyl)-
Thiophene, 2,5-diethyl-
Disulfide, bis(1,1,3,3-tetramethylbutyl)
Disulfide, bis(1,1,3,3-tetramethylbutyl)
Disulfide, bis(1,1,3,3-tetramethylbutyl)
0
1
2
3
4
150
650
1150
1650
2150


Masses: TIC
Benzo[b]thiophene, 2-ethyl-5,7-dimethyl-
b
Thiophene, 2-ethyl-5-(2-methylpropyl)-
Thiophene, 2-butyl-
Disulfide, bis(1,1,3,3-tetramethylbutyl)
Sulfurous acid, butyl cyclohexylmethyl ester
Sulfurous acid, cyclohexylmethyl isobutyl ester
Sulfurous acid, 2-ethylhexyl isobutyl ester
0
1
2
3
4
150
650
1150
1650
2150

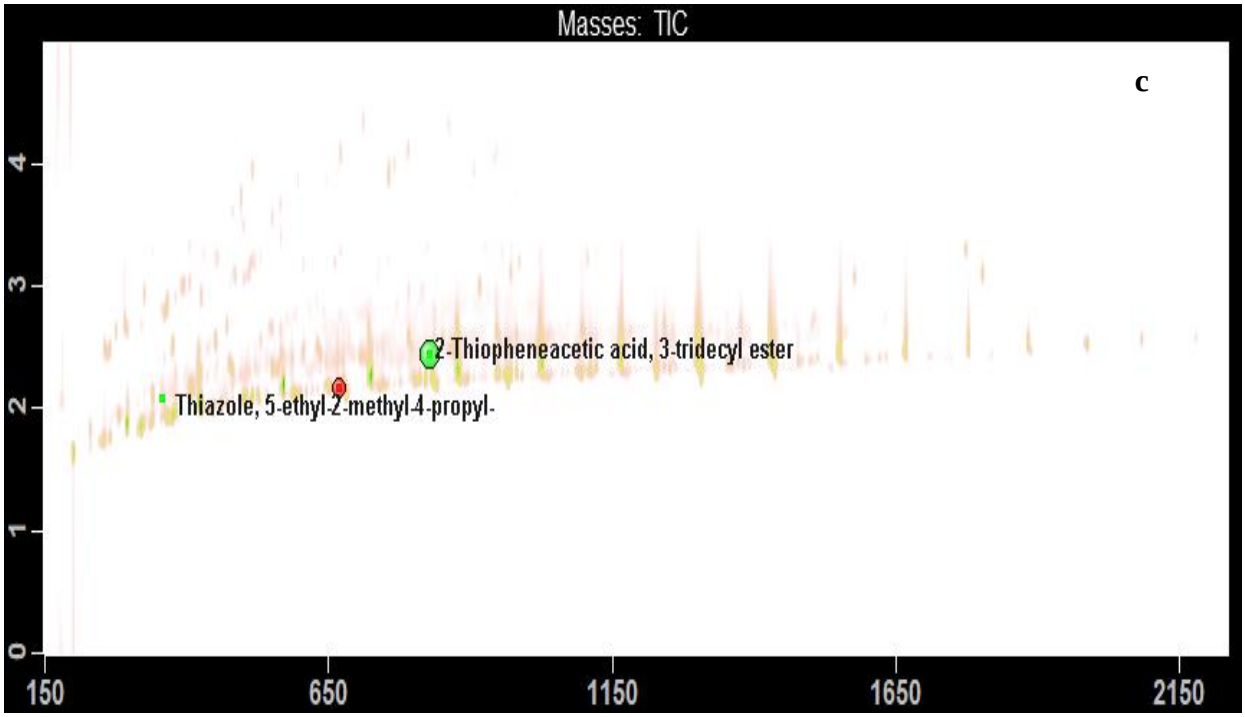


Fig. S12 Contour plot of sulfur compounds in CTPO, StTPO, and diesel detected by GC×GC TOF-MS

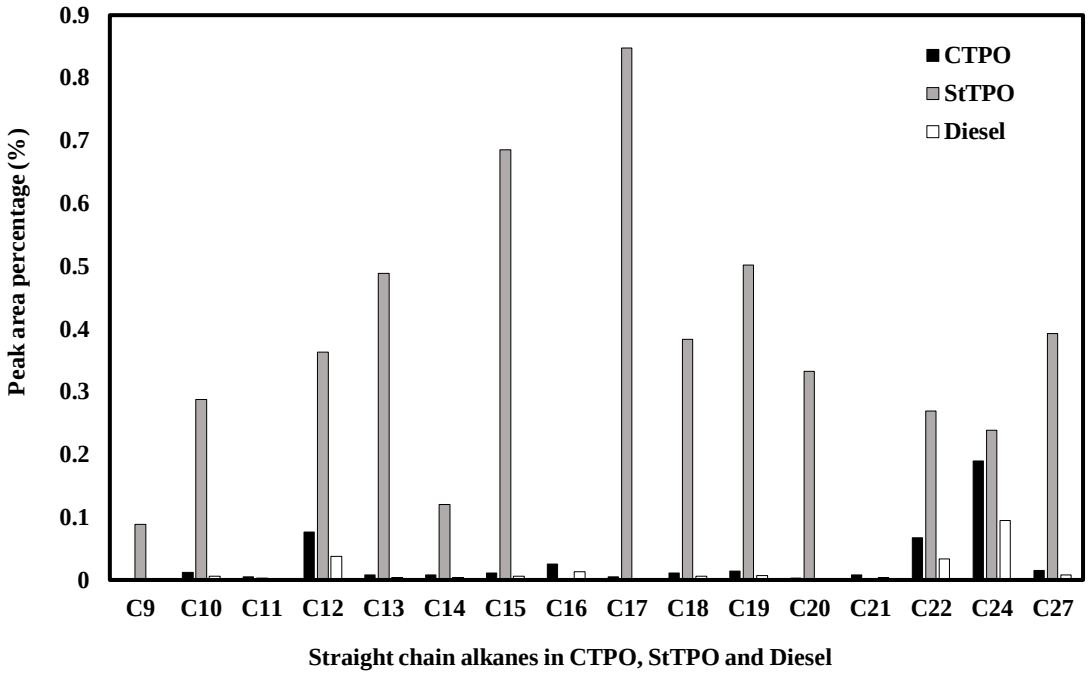


Fig. S13 Peak area percentage of carbon atoms in CTPO, StTPO and diesel

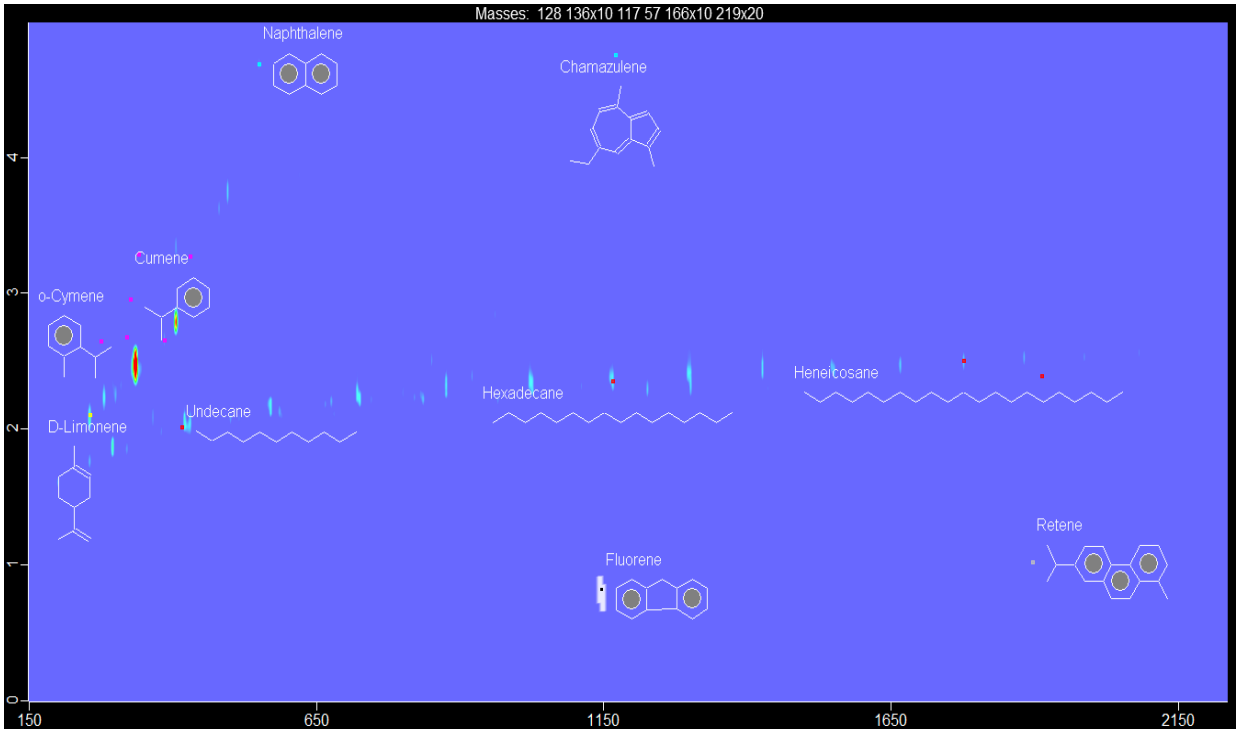


Fig. S14 Value-added compounds in StTPO

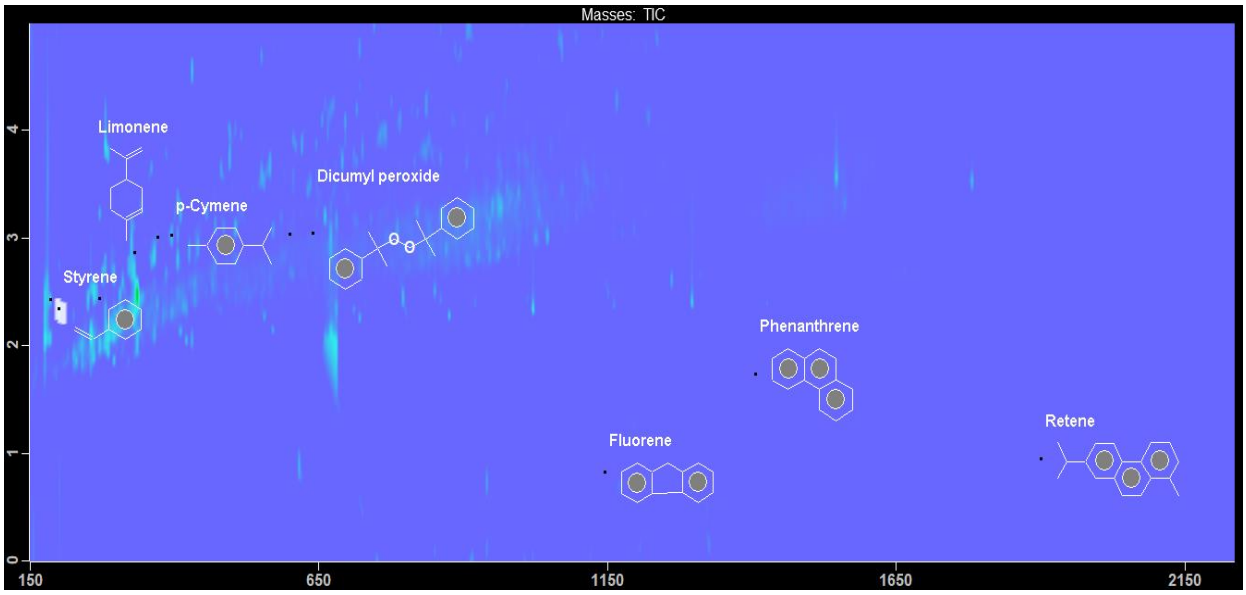


Fig. S15 Selective benzene derivatives (ring type structures) identified in CTPO

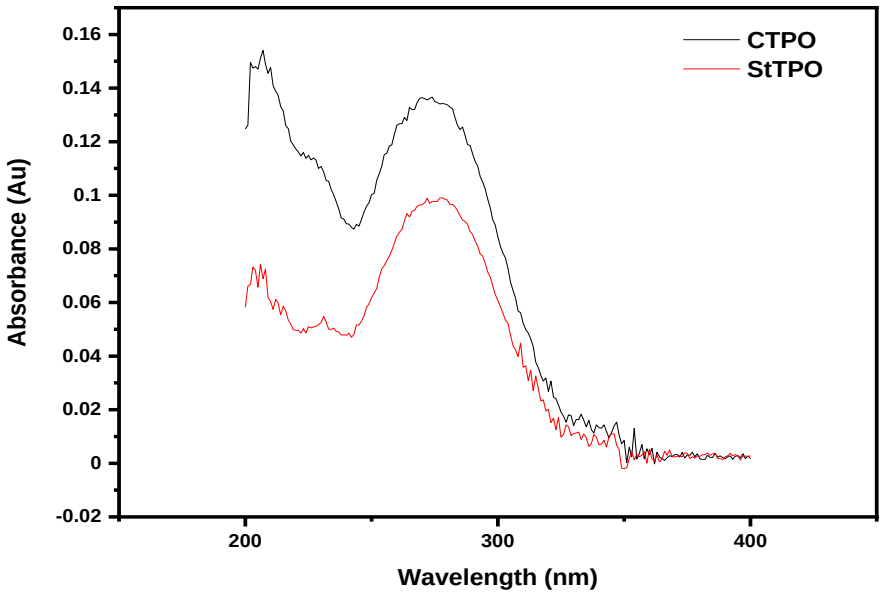


Fig. S16 UV-visible spectra of crude and upgraded tire pyrolysis oil

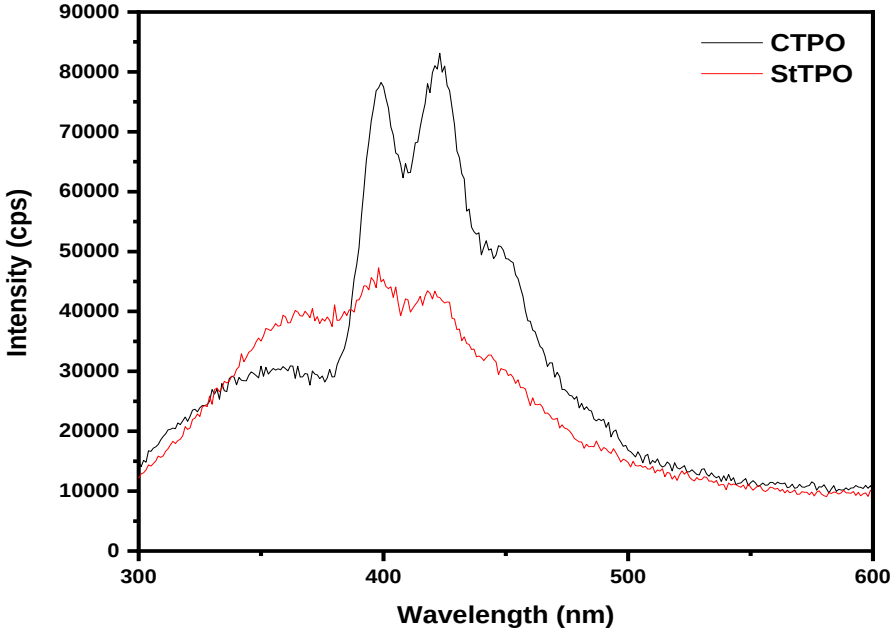


Fig. S17 Fluorescence of crude and upgraded tire pyrolysis oil

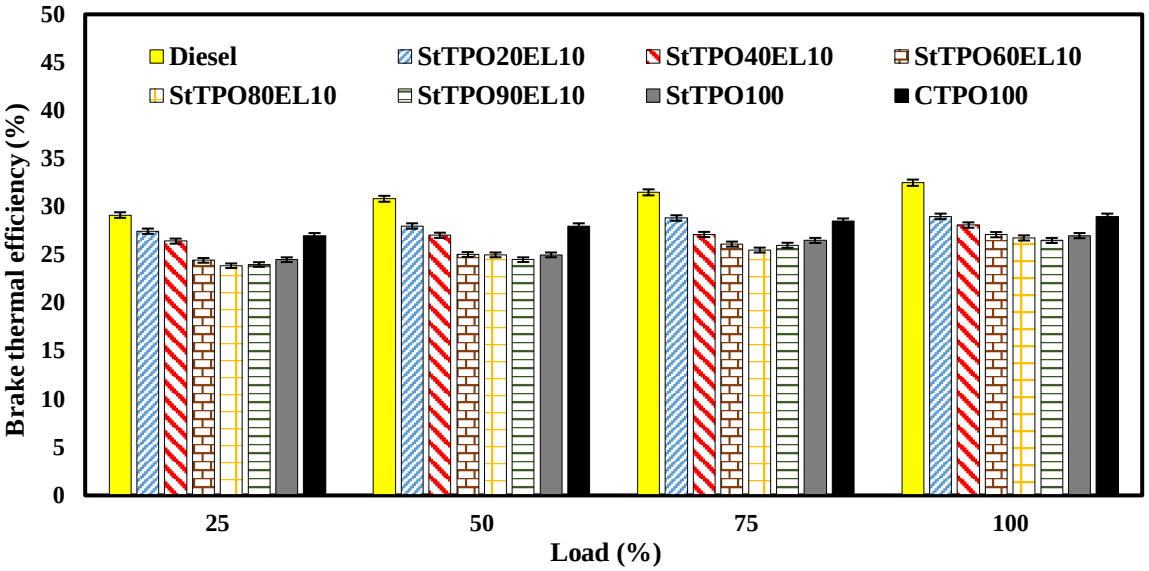


Fig. S18 Variation of brake thermal efficiency with load

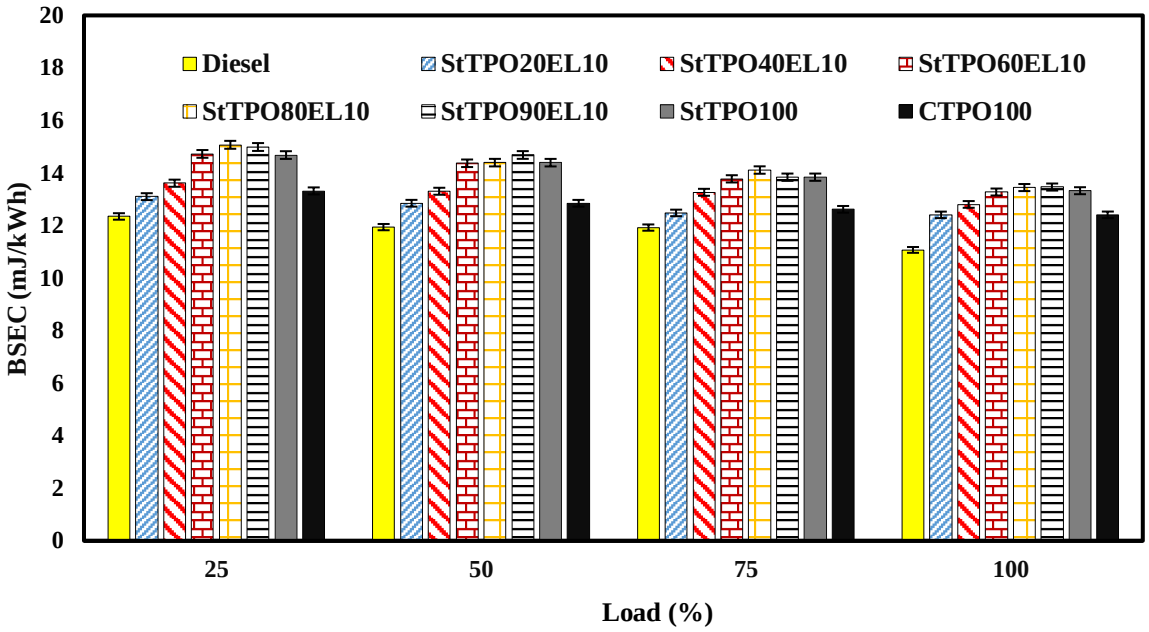


Fig. S19 Variation of brake energy fuel consumption with load

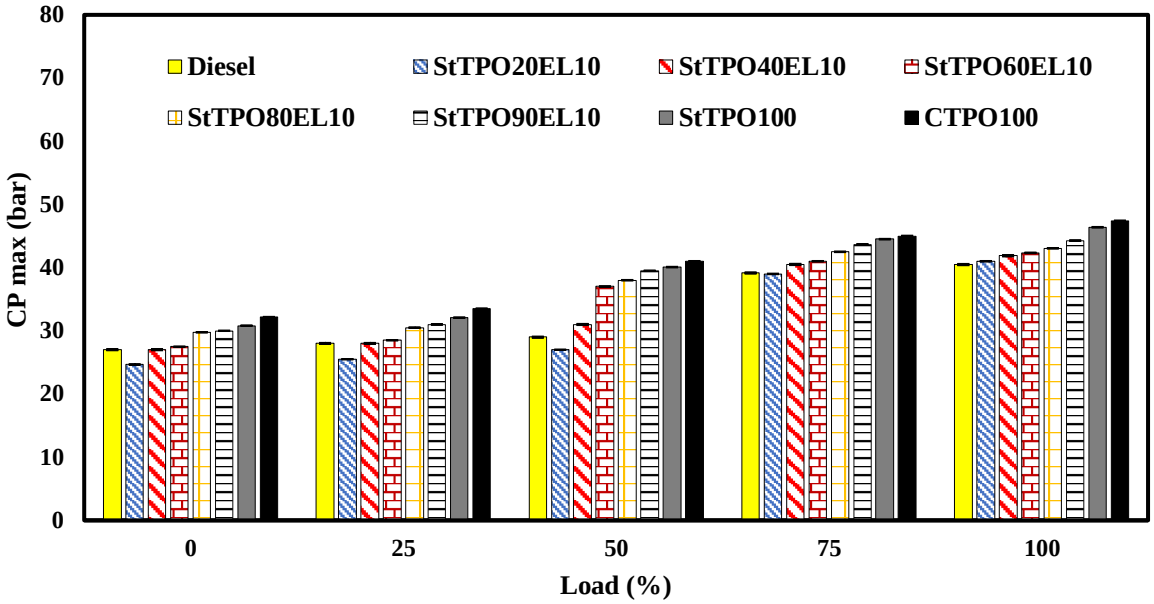


Fig. S20 Variation of maximum cylinder pressure with load

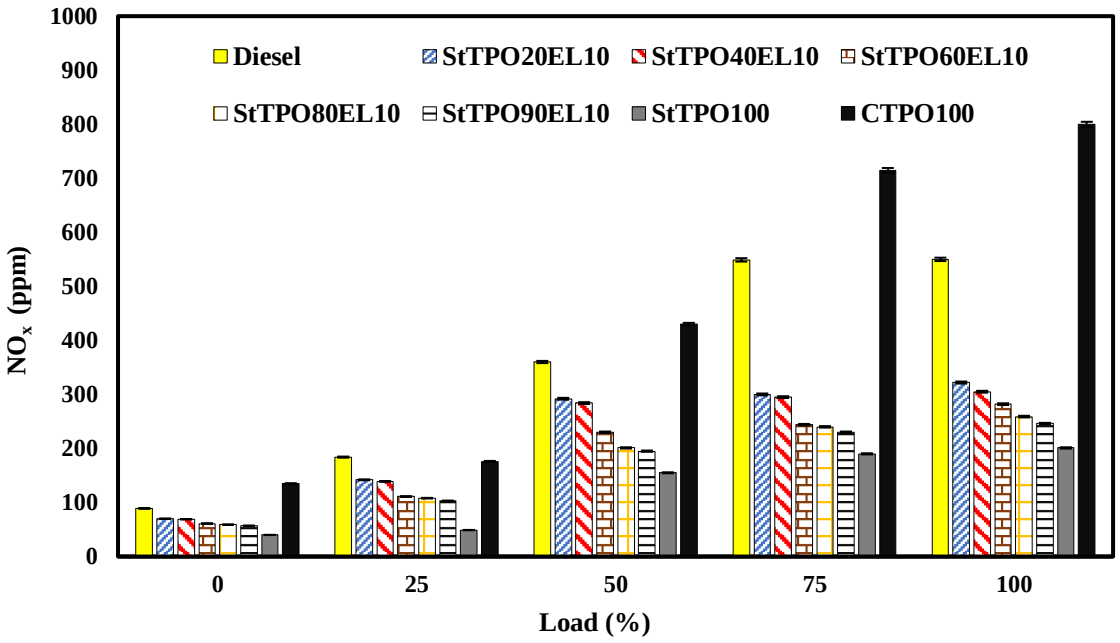


Fig. S21 Variation of nitrous oxide emission with load

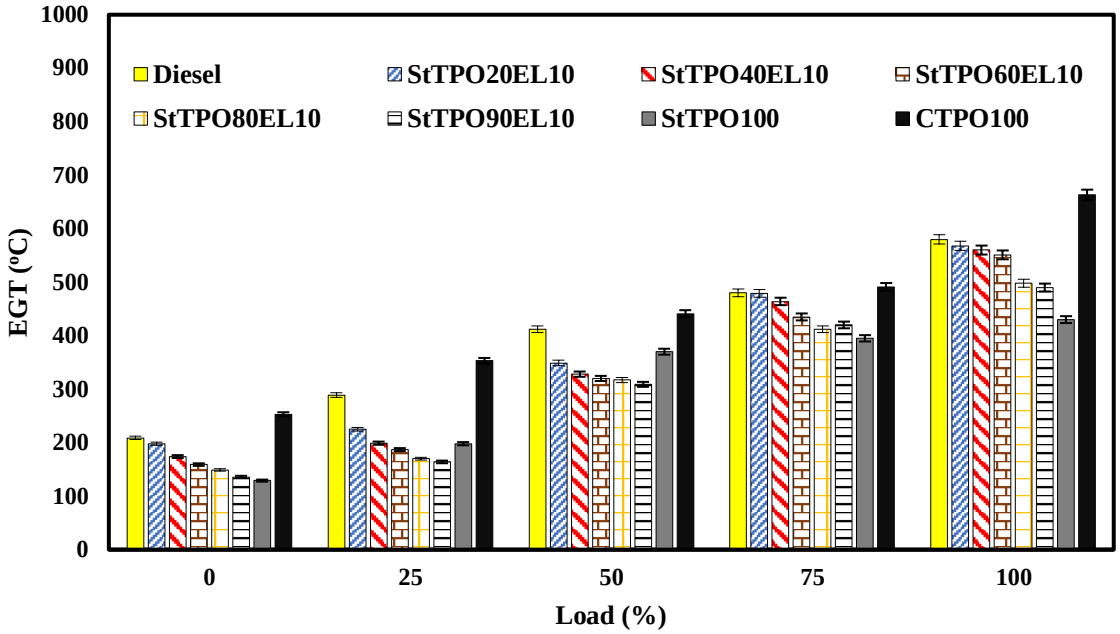


Fig. S22 Variation of exhaust gas temperature with load

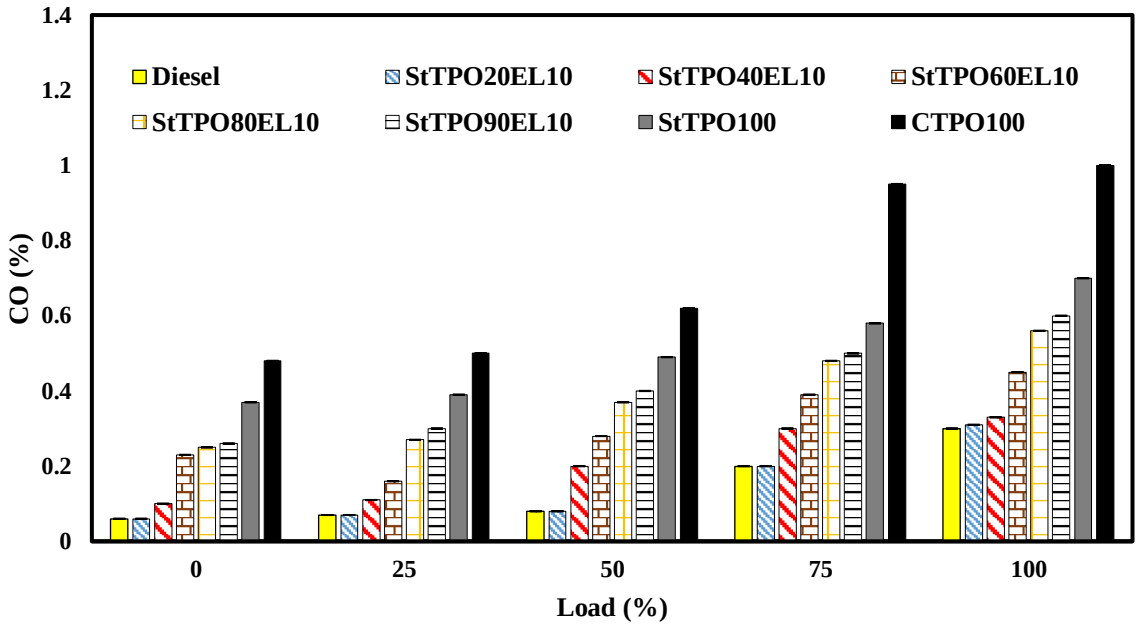


Fig. S23 Variation of carbon monoxide with load

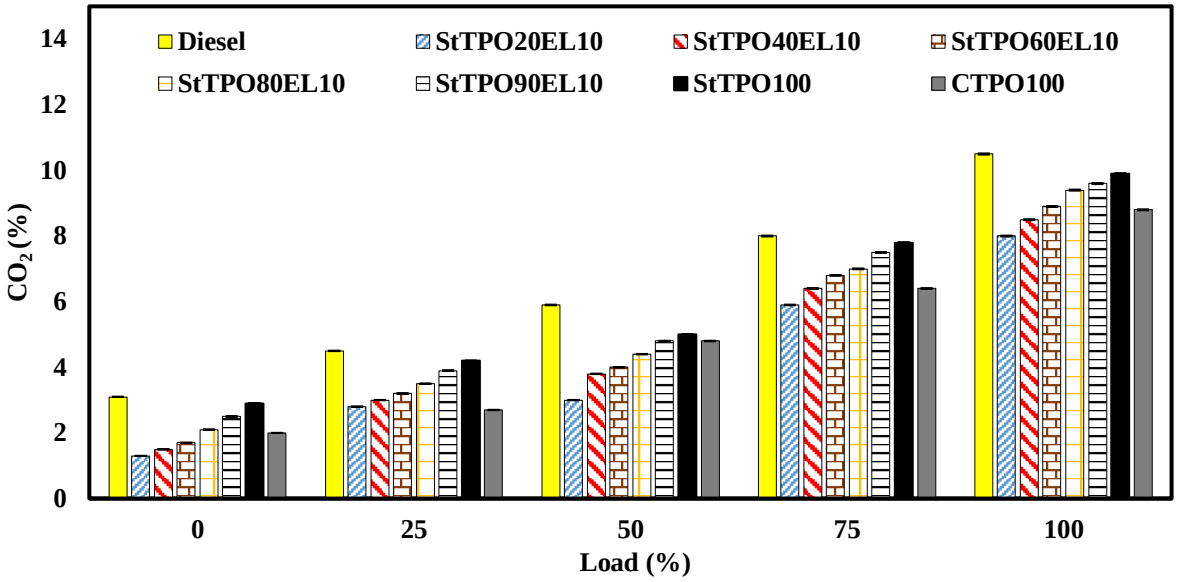


Fig. S24 Variation of carbon dioxide with load

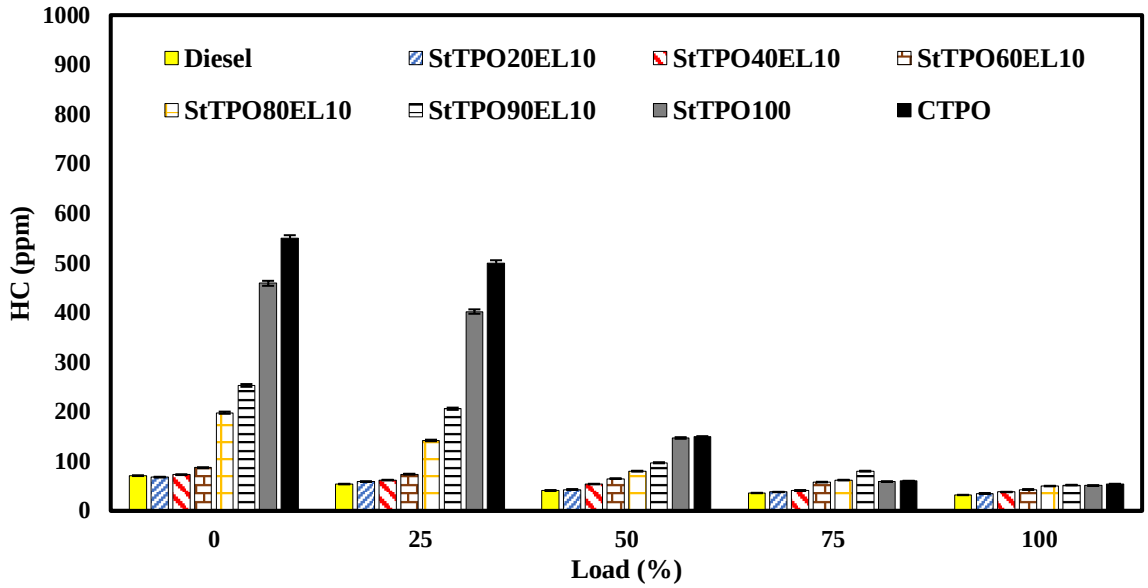


Fig. S25 Variation of hydrocarbon emission with load

List of Tables

Table S1 Specifications of single cylinder diesel engine

Model	Kirloskar TV1
Ignition type	Compression ignition
No. of cylinder	1
No. of strokes	4
Fuel	Diesel
Rated power	3.5 kW
Speed	1500 rpm
Cylinder diameter	87.5 mm
Stroke length	110 mm
Connecting rod length	234 mm
Orifice diameter	20 mm
Dynamometer arm length	185 mm
Displacement volume	661.45 cc
Fuel pipe diameter	12.40 mm
Pulse per revolution	360^{o}
Compression ratio	17.5:1
Fuel ignition timing	23^{o} before TDC
Fuel injection pressure	180 bar
Cooling	water cooled
Lubricant	20W40

Table S2 Specifications of AVL digas 444 exhaust gas analyzer

Parameters	**Measurement range**	**Resolution**
CO	0-10% vol.	0.01% vol.
HC	0-2000 ppm vol.	10 ppm
CO_2	0-20% vol.	0.1% vol.
NO	0-5000 ppm vol.	1 ppm

Table S3 Hedonic scale for odour measurements

Rating Scale	Explanation
1	Like extremely
2	Like very much
3	Like moderately
4	Like slightly
5	Neither like nor dislike
6	Dislike slightly
7	Dislike moderately
8	Dislike very much
9	Dislike extremely

Table S4 Rating scale and description of spot test

Rating	Description
1	Homogeneous spot with no inner ring
2	The faint or poor inner ring
3	Well defined inner ring, slightly darker than the background
4	Well defined inner ring, darker than the background
5	Very dark solid at the center, darker than the background

Table S5 List of compounds identified in CTPO

Compounds	R.T. (s)	Area %
Nonane	200 , 1.630	0.02782
Cyclopropane, 1,2-dimethyl-3-pentyl-	240 , 1.800	0.13264
Heptane, 3-ethyl-2-methyl-	245 , 1.780	0.08344
Nonane, 4-methyl-	255 , 1.750	0.03653
Decane	295 , 1.860	0.09988
3-Heptene, 2,2,4,6,6-pentamethyl-	305 , 1.850	0.07182
Butane, 2,2-dimethyl-	310 , 1.930	0.04046
Nonane, 2,6-dimethyl-	320 , 1.850	0.09323
2,2,4,4-Tetramethyloctane	330 , 1.930	0.35574
Nonane, 3,7-dimethyl-	340 , 1.920	0.04546
Decane, 2-methyl-	375 , 1.930	0.02382
Decane, 3-methyl-	380 , 1.990	0.02564

Undecane	420 , 2.050	0.14564
Disulfide, bis(1,1,3,3-tetramethylbutyl)	430 , 2.050	0.08334
Undecane	445 , 2.020	0.09249
Decane, 3,7-dimethyl-	460 , 2.030	0.06057
Hexane, 4-ethyl-2-methyl-	500 , 2.070	0.12607
Undecane, 2-methyl-	515 , 2.080	0.01493
Dodecane	570 , 2.150	0.24492
Undecane, 2,6-dimethyl-	585 , 2.140	0.15547
Caprolactam	665 , 2.020	0.96069
Hexadecane	665 , 2.190	0.01242
4-Heptanone, 5,5-diethyl-2,2,3,3-tetramethyl-	680 , 2.240	0.02432
Tridecane	720 , 2.260	0.34356
Decane, 3,7-dimethyl-	745 , 2.230	0.03573
Dodecane, 2,6,10-trimethyl-	835 , 2.220	0.03921
Tetradecane	875 , 2.280	0.19226
Tridecane, 4-methyl-	960 , 2.270	0.03355
Pentadecane	1020 , 2.350	0.23128
Heptadecane, 2,6,10,14-tetramethyl-	1110 , 2.300	0.0188
Heptane, 3-bromo-	1150 , 2.440	0.02279
Heptadecane	1160 , 2.380	0.10021
Decane, 2,6,8-trimethyl-	1225 , 2.290	0.0426
Disulfide, bis(1,1,3,3-tetramethylbutyl)	1230 , 2.500	0.04166
2,2,4,4-Tetramethyloctane	1260 , 2.510	0.03263
Heptadecane	1295 , 2.410	0.27011
Eicosane	1425 , 2.400	0.08673
Heptadecane, 2-methyl-	1545 , 2.450	0.02901
Heptadecane, 2-methyl-	1665 , 2.440	0.03865
Heptadecane, 2-methyl-	1775 , 2.460	0.03578
Heptadecane, 2-methyl-	1880 , 2.490	0.03166
Octadecane, 2-methyl-	1985 , 2.510	0.06646
Heptacosane	2080 , 2.550	0.06687
Heptacosane	2175 , 2.580	0.07424
1-Hexene, 3,5-dimethyl-	310 , 1.990	0.08963
Sulfurous acid, di(cyclohexylmethyl) ester	330 , 2.060	0.06576
2-Pentene, 2,4,4-trimethyl-	335 , 2.020	0.68649
Pentane, 3-methyl-	355 , 2.020	0.04153
1-Undecene	355 , 2.060	0.03122
1-Heptene, 3-methyl-	360 , 2.080	0.06855
Disulfide, bis(1,1,3,3-tetramethylbutyl)	365 , 2.090	0.52101
1-Hexene, 3,5-dimethyl-	365 , 2.100	0.3185
1-Heptene, 3-methyl-	385 , 2.120	0.10034
Cyclopropane, 1-heptyl-2-methyl-	400 , 2.130	0.05639

Cyclohexane, 1-ethyl-1-methyl-	405 , 2.200	0.05817
Cyclopropane, 1-heptyl-2-methyl-	410 , 2.130	0.11173
Cyclopentane, butyl-	480 , 2.330	0.07724
3-Undecene, 4-methyl-	490 , 2.230	0.05413
4-Nonene, 2,3,3-trimethyl-, (Z)-	505 , 2.300	0.0807
(S)-(+)-6-Methyl-1-octanol	525 , 2.340	0.02227
1-Octene, 2-methyl-	545 , 2.260	0.02355
1-Dodecene	555 , 2.270	0.10321
Cyclooctane, 1,4-dimethyl-, cis-	560 , 2.320	0.02768
Cyclopentane, 1,1'-ethylidenebis-	560 , 2.350	0.0171
4-Dodecene	575 , 2.310	0.01711
1,1'-Bicyclooctyl	610 , 2.370	0.01577
Cyclopropane, 1-hexyl-2-methyl-	620 , 2.290	0.0603
Cyclooctane, (1-methylpropyl)-	665 , 2.400	0.01537
Cyclohexane, 1-isopropyl-1-methyl-	670 , 2.440	0.02255
2-Pentene, 3,4,4-trimethyl-	680 , 2.350	0.30688
3-Tetradecene, (Z)-	710 , 2.340	0.07406
Cyclooctane, 1,4-dimethyl-, trans-	730 , 2.380	0.03492
Heptane, 1-iodo-	730 , 2.410	0.15408
3-Heptene, 2,2,4,6,6-pentamethyl-	745 , 2.310	0.04171
1-Hexene, 5,5-dimethyl-	785 , 2.330	0.06417
2-Pentene, 2,4,4-trimethyl-	795 , 2.440	0.5383
2,2,4,4-Tetramethyloctane	800 , 2.320	0.27253
Oxalic acid, butyl cyclohexylmethyl ester	815 , 2.480	0.01905
Cyclohexane, 1-methyl-4-(1-methylethyl)-, cis-	835 , 2.540	0.03041
Disulfide, bis(1,1,3,3-tetramethylbutyl)	850 , 2.510	0.42475
1-Dodecene	860 , 2.420	0.09095
Cyclohexane, (2,2-dimethylcyclopentyl)-	870 , 2.470	0.01725
Disulfide, bis(1,1,3,3-tetramethylbutyl)	920 , 2.400	0.37245
1-Tridecene	1010 , 2.430	0.06503
Sulfurous acid, cyclohexylmethyl isobutyl ester	1145 , 2.580	0.33151
1-Hexanol, 2,2-dimethyl-	1200 , 2.590	0.03562
Cyclopropane, 3-chloro-1,1,2,2-tetramethyl-	1260 , 2.610	0.47655
Disulfide, bis(1,1,3,3-tetramethylbutyl)	1310 , 2.660	0.23845
Meclofenoxate	1365 , 2.710	0.02741
Sulfurous acid, cyclohexylmethyl isobutyl ester	1565 , 2.650	0.143
1-Hexene, 2,4,4-triethyl-	1610 , 2.700	0.01568
Disulfide, bis(1,1,3,3-tetramethylbutyl)	1660 , 2.760	0.06469
Sulfurous acid, cyclohexylmethyl isobutyl ester	1665 , 2.720	0.24267
Disulfide, bis(1,1,3,3-tetramethylbutyl)	1710 , 2.750	0.01533
Disulfide, bis(1,1,3,3-tetramethylbutyl)	1760 , 2.660	0.06531
Pyrene	1795 , 2.800	0.04778

Sulfurous acid, cyclohexylmethyl hexyl ester	1925 , 2.770	0.07654
Formic acid, 2,4,4-trimethylpentyl ester	2015 , 2.840	0.09249
Cyclohexane, 1,3-dimethyl-2-methylene-, cis-	175 , 2.220	0.03846
Thiophene, 2-ethyl-	180 , 2.160	0.01999
Hexanenitrile	185 , 2.430	0.29753
Thiophene, 2,3-dimethyl-	195 , 2.300	0.01048
Ethylbenzene	200 , 2.230	0.04496
Styrene	200 , 2.350	0.11334
Benzene, (1-methylethyl)-	225 , 2.280	0.23357
Cyclopentanone, 2-ethyl-	235 , 2.770	0.02813
Benzene, 2-propenyl-	245 , 2.520	0.04206
Benzene, propyl-	250 , 2.430	0.22124
Thiophene, 2-ethyltetrahydro-	250 , 2.630	0.0257
Hexanoic acid, 6-bromo-	255 , 2.560	0.01932
Benzene, 1-ethyl-4-methyl-	260 , 2.490	1.78484
Thiophene, 2-(1-methylethyl)-	260 , 2.610	0.03326
Thiophene, 2-(1-methylethyl)-	265 , 2.720	0.12286
Hexanoic acid	270 , 2.440	0.07464
Heptanonitrile	270 , 3.030	0.03659
Benzene, 1-ethyl-4-methyl-	275 , 2.660	0.16262
4-(Aminomethyl)pyridine	280 , 2.380	0.04671
Thiophene, 2,3,4-trimethyl-	280 , 2.700	0.06555
à-Methylstyrene	280 , 2.820	0.14604
trans-2-Ethyl-3-methylthiophane	285 , 2.640	0.02522
1,5-Heptadiene, 2,3,6-trimethyl-	290 , 2.600	0.11158
Mesitylene	295 , 2.670	0.29952
Benzene, 2-propenyl-	295 , 2.870	0.15452
1,3-Cyclopentadiene, 1,2,5,5-tetramethyl-	305 , 2.480	0.24602
1-Nonen-4-yne	310 , 2.560	0.06714
Benzene, (1-methylpropyl)-	310 , 2.620	0.33605
(E)-1-Phenyl-1-butene	310 , 2.800	0.03763
o-Cymene	320 , 2.680	0.77235
Thiophene, 2,5-diethyl-	320 , 2.800	0.0805
Benzene, 1,2,3-trimethyl-	325 , 2.960	0.65686
o-Cymene	325 , 3.140	0.10408
Cyclohexanone, 3-butyl-	330 , 2.520	0.01108
o-Cymene	330 , 2.680	0.02747
Limonene	330 , 2.870	0.06997
Benzene, 2-propenyl-	330 , 3.120	0.15439
Limonene	335 , 2.490	0.24533
o-Cymene	340 , 2.850	0.05229
Benzene, 1-ethyl-2-methyl-	340 , 3.040	0.01527

Indane	345 , 3.230	0.58647
Benzene, 3-butenyl-	350 , 2.950	0.20954
3-Phenylbut-1-ene	350 , 2.980	0.03651
Benzene, 1-methyl-3-propyl-	360 , 2.790	0.18701
Thiophene, 2-methyl-5-propyl-	360 , 2.940	0.10733
Thiophene, 2,5-diethyl-	360 , 2.990	0.05768
Thiocyanic acid, ethyl ester	360 , 3.060	0.01418
1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-	365 , 2.580	0.2037
Unknown 2	365 , 2.750	0.01276
Benzene, n-butyl-	365 , 2.840	0.2216
Benzene, (1-methylpropyl)-	370 , 2.980	0.05923
Thiophene, 2-butyl-	370 , 3.010	0.055
Thiophene, 2,5-diethyl-	370 , 3.040	0.08971
Benzene, 1-methyl-4-propyl-	380 , 2.930	0.22531
Benzene, 2-butenyl-	380 , 3.130	0.0238
Cyclohexene, 4-methyl-1-(1-methylethenyl)-	385 , 2.660	0.10953
Thiophene, 3,4-diethyl-	385 , 3.130	0.05143
p-Cymene	395 , 3.030	0.80449
Octanenitrile	395 , 3.420	0.02666
Benzene, 3-butenyl-	400 , 3.190	0.0179
(E)-1-Phenyl-1-butene	400 , 3.230	0.1434
Cyclohexene, 1-methyl-4-(1-methylethylidene)-	405 , 2.790	0.13971
Benzene, 1-ethyl-2,4-dimethyl-	405 , 3.040	0.39552
1,4-Cyclohexadiene, 3,3,6,6-tetramethyl-	410 , 2.670	0.04881
Benzene, 1-ethyl-2,4-dimethyl-	410 , 3.160	0.09817
Benzene, 1-methyl-3-(1-methylethenyl)-	410 , 3.260	0.96707
Benzene, 2-ethenyl-1,4-dimethyl-	420 , 3.250	0.02393
Benzeneethanol, 2-methyl-	425 , 2.830	0.03283
Benzene, 1-methyl-4-butyl	425 , 2.880	0.08279
Benzene, 1,4-diethyl-	425 , 2.950	0.06635
Thiophene, 2-ethyl-5-propyl-	425 , 3.080	0.09669
Benzene, 2-ethyl-1,4-dimethyl-	430 , 3.290	0.12923
Ether, p-methylbenzyl vinyl	435 , 2.900	0.10685
Thiophene, 2-methyl-5-[4-bromo-n-butyl]-	435 , 3.050	0.04181
3-Acetyl-2,5-dimethylthiophene	435 , 3.080	0.01618
2,8-Decadiyne	440 , 2.850	0.0238
Benzene, 1-methyl-4-(1-methylpropyl)-	440 , 2.930	0.10334
Benzene, 1,4-diethyl-2-methyl-	440 , 2.990	0.09393
Benzene, (1-methyl-1-butenyl)-	440 , 3.090	0.03068
Benzene, 1-methyl-3-(1-methyl-2-propenyl)-	445 , 3.150	0.05913
Benzene, 2-butenyl-	445 , 3.440	0.02519
Benzene, (3-methylbutyl)-	455 , 2.940	0.05009

Benzene, 1,2,3,4-tetramethyl-	455 , 3.250	0.523
Benzene, 2-ethenyl-1,3,5-trimethyl-	460 , 3.200	0.02952
Benzene, (2-methyl-2-propenyl)-	460 , 3.400	0.07525
Amantadine	470 , 2.800	0.08203
3,4-Dimethylcumene	470 , 3.130	0.30917
2,4-Dimethylstyrene	470 , 3.420	0.04413
2,4,6-Octatriene, 2,6-dimethyl-, (E,E)-	480 , 2.880	0.06844
Benzene, 1-methyl-4-(1-methylpropyl)-	480 , 3.110	0.04138
Thiophene, 2-ethyl-5-propyl-	480 , 3.210	0.03608
Naphthalene, 1,2,3,4-tetrahydro-1-methyl-	480 , 3.300	0.06723
1H-Indene, 2,3-dihydro-5-methyl-	480 , 3.640	0.59774
1,5-Heptadien-3-yne	480 , 3.690	0.02546
Benzene, 1-methyl-4-(1-methylpropyl)-	485 , 3.080	0.1816
3,4-Dimethylcumene	485 , 3.130	0.18628
1H-Indene, 2,3-dihydro-1,3-dimethyl-	485 , 3.380	0.01665
1-Propanone, 1-(5-methyl-2-thienyl)-	490 , 3.220	0.01398
Benzene, 4-pentenyl-	495 , 3.260	0.09412
1H-Indene, 2,3-dihydro-4-methyl-	495 , 3.750	0.62772
Benzene, 1-methyl-4-(2-methylpropyl)-	500 , 3.060	0.07356
Benzene, 2,4-diethyl-1-methyl-	500 , 3.220	0.05113
Benzene, 1,2,3,4-tetramethyl-	500 , 3.490	0.05832
Benzene, pentyl-	505 , 3.100	0.09322
Benzene, 3-pentenyl-	505 , 3.310	0.01705
Benzene, 1-methyl-4-butyl	510 , 3.060	0.10424
Benzene, (1,1-dimethylnonyl)-	510 , 3.150	0.10823
Thiophene, 2-ethyl-5-propyl-	510 , 3.310	0.05327
Benzene, 1-methyl-4-(1-methylpropyl)-	515 , 3.210	0.14782
Benzene, (2-methyl-3-butenyl)-	515 , 3.380	0.09269
Bicyclo[2.2.2]oct-5-en-2-one	520 , 3.010	0.05995
Benzene, (1-methylbutyl)-	520 , 3.180	0.19409
Benzene, 2,4-diethyl-1-methyl-	520 , 3.290	0.05691
Benzene, 1-methyl-4-(1-methylpropyl)-	530 , 3.240	0.14607
Bicyclo[4.2.0]octa-1,3,5-triene, 7-isopropyl-	535 , 3.460	0.177
Benzene, 1-ethyl-4-(1-methylethyl)-	545 , 3.460	0.04337
Benzene, 1-methyl-3-(1-methyl-2-propenyl)-	545 , 3.510	0.1438
Benzene, 1-ethyl-4-(2-methylpropyl)-	555 , 3.010	0.03556
Thiophene, 2-ethyl-5-(2-methylpropyl)-	555 , 3.220	0.04571
1,2-Benzenediol, o-(3-cyclopentylpropionyl)-o'-(2-methylbenzoyl)-	555 , 3.410	0.08795
Benzene, (1-methylpentyl)-	560 , 3.130	0.2309
endo-3-Methylenetricyclo[3.2.1.0(2,4)]oct-6-ene	560 , 3.300	0.02223
Benzene, 1-ethyl-4-(1-methylethyl)-	565 , 3.410	0.10878
Benzene, 1-ethyl-4-(2-methylpropyl)-	570 , 3.090	0.39492

Benzene, 1-(1-methylethenyl)-3-(1-methylethyl)-	570 , 3.260	0.03678
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	575 , 3.380	0.02616
Benzene, (1,3-dimethylbutyl)-	580 , 3.140	0.08998
Thiophene, 2-ethyl-5-(2-methylpropyl)-	580 , 3.280	0.06477
Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	585 , 3.210	0.13151
Benzene, 1,3-dimethyl-	595 , 3.100	0.03741
Unknown 5	595 , 3.320	0.01512
Geijerene	600 , 3.040	0.04507
Benzene, (1,3-dimethylbutyl)-	605 , 3.140	0.02353
Dimethyl sulfone	610 , 3.000	0.06313
Benzeneacetaldehyde, à,2,5-trimethyl-	620 , 3.250	0.07358
Tricyclo[7.1.0.0[1,3]]decane-2-carbaldehyde	640 , 3.030	0.25936
Dicumyl peroxide	640 , 3.050	0.04965
Cyclopropane, 1-(2-methylene-3-butenyl)-1-(1-methylenepropyl)-	670 , 3.120	0.02728
Benzene, 2-(chloromethyl)-1,3,5-trimethyl-	680 , 3.160	0.23894
Benzene, (1-methylhexyl)-	715 , 3.150	0.31094
Benzenepropanoic acid, 3-phenylpropyl ester	780 , 3.450	0.05342
1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1à,4à,4aà,10aà)-	785 , 3.080	0.15452
Thiophene, 2-ethyl-5-isopentyl-	785 , 3.430	0.01992
Cyclopropane, 1-benzyl-2-bromo-	785 , 3.760	0.04121
Naphthalene, 1,2,3,4-tetrahydro-6-propyl-	790 , 3.580	0.11538
2-Methyl-6-(p-tolyl)hept-2-en-4-ol	795 , 3.170	0.04622
Naphthalene, 1,2,3,4-tetrahydro-1-propyl-	800 , 3.670	0.04839
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	800 , 3.780	0.0299
1H-Indene, 2,3-dihydro-1,1,2,3,3-pentamethyl-	805 , 3.140	0.02927
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	805 , 3.320	0.04275
6-Phenyl-n-hexanol	805 , 3.480	0.03838
1-[(2-Thienylcarbonyl)oxy]-2,5-pyrrolidinedione	810 , 3.390	0.03524
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	810 , 3.890	0.04401
Benzene, (1-methylhexyl)-	815 , 3.260	0.02888
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	815 , 3.710	0.13349
Heptacyclo[8.4.0(2,6).0(3,8).0(5,7).0(9,13).0(12,14)]tetradecane	815 , 3.930	0.04688
Benzene, heptyl-	820 , 3.240	0.19227
Benzene, 1-methyl-4-(1-methylpropyl)-	820 , 3.340	0.09582
Benzene, (1,2-dicyclopropyl-2-phenylethyl)-	820 , 3.820	0.06833
Benzene, (1-methylhexyl)-	825 , 3.340	0.03287
Thiophene, 2-heptyl-	825 , 3.450	0.01655
8-Phenyl-1-octanol	825 , 3.560	0.03301
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	830 , 3.800	0.38579
2,3-Diazabicyclo[2.2.1]hept-2-ene, 7,7-dimethyl-5-phenyl-, (1à,4à,5á)-	830 , 3.900	0.1076

3-Isopropylidene-tricyclo[4.3.1.1(2,5)]undecan-10-one	835 , 3.160	0.20487
Benzene, 1-isopentyl-2,4,5-trimethyl-	835 , 3.250	0.06908
3-Ethyl-3-phenyl-1-pentene	835 , 3.740	0.0277
Benzene, (1-methyl-1-butenyl)-	835 , 3.830	0.03812
Benzenepropanamine	840 , 3.690	0.01583
11-Azabicyclo[4.4.1]undeca-1,3,5,7,9-pentaene	840 , 3.860	0.06304
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	840 , 3.900	0.22003
Benzene, 2-heptenyl-	845 , 3.800	0.03109
3-Ethyl-3-phenyl-1-pentene	845 , 3.860	0.10354
Thiophene, 2-ethyl-5-hexyl-	850 , 3.330	0.0337
1H-Inden-1-one, 2,3-dihydro-3,3,4,5-tetramethyl-	850 , 3.630	0.04996
2-Hexanone, 5-methyl-5-phenyl-	860 , 3.210	0.30972
Benzene, (2,4-dimethylcyclopentyl)-	860 , 3.750	0.16398
Benzene, 1-(1-formylethyl)-4-(1-buten-3-yl)-	860 , 3.940	0.03859
Thiocyanic acid, 1,1,3-trimethyl-3-phenylbutyl ester	865 , 3.180	0.05853
4a,5-Dimethyl-3-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalen-1-ol	865 , 3.220	0.23243
2,5-Dimethylbenzyl cyanide	865 , 3.460	0.03676
3-Ethyl-3-phenyl-1-pentene	865 , 3.800	0.0419
Benzene, 2-(2-butenyl)-1,3,5-trimethyl-	875 , 3.710	0.02615
Naphthalene, 1,2,3,4-tetrahydro-1-propyl-	875 , 3.790	0.09042
1H-Inden-1-one, 2,3-dihydrotetramethyl-	890 , 3.750	0.03797
2,3,4-Trifluorobenzoic acid, 3-phenylpropyl ester	895 , 3.620	0.01505
Spiro[3.6]deca-5,7-dien-1-one,5,9,9-trimethyl	900 , 3.290	0.10967
1H-Indene, 3-ethyl-1-(1-methylethyl)-	900 , 3.760	0.01587
Benzene, (2-cyclohexylethyl)-	900 , 3.820	0.02179
Benzene, 1-(1,5-dimethylhexyl)-4-methyl-	905 , 3.210	0.0181
Naphthalene, 1,2,3,4-tetrahydro-1-methyl-8-(1-methylethyl)-	905 , 3.700	0.11932
Benzene, (1,1,2-trimethylpropyl)-	910 , 3.290	0.03036
Benzene, 3-cyclohexen-1-yl-	910 , 3.750	0.0187
Naphthalene, 1,2,3,4-tetrahydro-1-methyl-8-(1-methylethyl)-	910 , 3.800	0.06254
1-Penten-3-one, 1-(4-methoxyphenyl)-4-methyl-	915 , 3.220	0.0356
Benzene, 1-methyl-4-(1,2,2-trimethylcyclopentyl)-, (R)-	915 , 3.300	0.01709
aR-Himachalene	915 , 3.550	0.02584
1-Pentene, 5-(2,2-dimethylcyclopropyl)-2-methyl-4-methylene-	920 , 3.160	0.64485
Unknown 11	920 , 3.180	0.08331
Naphthalene, 1,2,3,4-tetrahydro-1-propyl-	920 , 3.870	0.05708
Tricyclo[5.4.0.0(2,8)]undec-9-ene, 2,6,6,9-tetramethyl-, (1R,2S,7R,8R)-	925 , 3.300	0.05599
Benzenepropanoic acid, 3-phenylpropyl ester	930 , 3.500	0.01676
Thiophene, 2-ethyl-5-heptyl-	935 , 3.250	0.05809
Caryophyllene	935 , 3.280	0.06102
Benzene, 1-methyl-4-(4-methyl-4-pentenyl)-	940 , 3.500	0.07792

1(2H)-Naphthalenone, 3,4-dihydro-4,5,6-trimethyl-	945 , 3.800	0.08072
Unknown 12	950 , 3.290	0.19201
(1R,4R,4aS,8aR)-4,7-Dimethyl-1-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,8a-octahydronaphthalene	950 , 3.300	0.1864
(3-Methylphenyl) methanol, n-pentyl ether	955 , 3.280	0.0472
1,3-Cyclohexadiene, 5-(1,5-dimethyl-4-hexenyl)-2-methyl-, [S-(R*,S*)]-	960 , 3.300	0.03862
Benzene, 1-(1-buten-3-yl)-2-vinyl-	960 , 3.930	0.04989
(1R,4R,4aS,8aR)-4,7-Dimethyl-1-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,8a-octahydronaphthalene	965 , 3.290	0.07131
Benzene, 1-methyl-4-(4-methyl-4-pentenyl)-	965 , 3.580	0.097
Benzene, 1-(1-methyl-2-propenyl)-4-(2-methylpropyl)-	965 , 3.720	0.12191
Benzene, octyl-	970 , 3.340	0.07512
Benzene, octyl-	975 , 3.250	0.14087
(3-Methylphenyl) methanol, 1-methylpropyl ether	975 , 3.400	0.04467
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	975 , 3.470	0.05369
Benzene, 1-(1-buten-3-yl)-2-vinyl-	975 , 3.880	0.02138
2-n-Propylthiane	980 , 3.730	0.0205
3,9-Dodecadiyne	985 , 3.450	0.04583
Unknown 15	985 , 3.590	0.01192
Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene-	990 , 3.310	0.02598
ç-Dehydro-ar-himachalene	990 , 3.890	0.04522
1,2-Benzenediol, o-(2-chloropropionyl)-o'-(4-ethylbenzoyl)-	995 , 3.300	0.09551
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	995 , 3.430	0.03463
(+)-Cycloisolongifol-5-ol	995 , 3.720	0.01959
Biphenylene, 1,2,3,6,7,8,8a,8b-octahydro-4,5-dimethyl-	995 , 3.760	0.0355
Tyrosine	1005 , 3.290	0.09702
Cyclooctane, phenyl-	1005 , 3.750	0.10415
trans-3-Methyl-2-n-propylthiophane	1005 , 3.790	0.03026
3,6-Dihydrochamazulene	1005 , 4.260	0.03212
Neoisolongifolene, 8,9-dehydro-	1010 , 3.680	0.02657
trans-Calamenene	1010 , 3.950	0.04175
4-Methyl-2-phenyl-pent-3-en-1-ol	1010 , 4.020	0.03272
Unknown 17	1010 , 4.050	0.02488
Santolina triene	1015 , 3.350	0.13002
4-Ethylbenzoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester	1015 , 3.370	0.03725
Succinic acid, 3-chlorophenyl 3-phenylprop-2-en-1-yl ester	1015 , 3.680	0.0475
cis-Calamenene	1020 , 3.630	0.07207
Cyclopropane, 2-bromo-1-methyl-1-phenyl-	1020 , 3.810	0.05858
Benzene, (2-cyclohexylethyl)-	1020 , 3.830	0.02055
Cyclooctane, phenyl-	1020 , 3.910	0.03454
Unknown 18	1025 , 3.340	0.05362
1H-Indene, 3-ethyl-1-(1-methylethyl)-	1025 , 4.230	0.15751

Hexane, 2-phenyl-3-propyl-	1030 , 3.260	0.17595
Benzene, 1-methyl-4-(1,2,2-trimethylcyclopentyl)-, (R)-	1035 , 3.900	0.02413
1,3-Cyclohexadiene, 5,6-dimethyl-	1040 , 3.870	0.01948
Naphthalene, 3-(1,1-dimethylethyl)-1,2-dihydro-	1040 , 4.230	0.09298
Benzene, (3-cyclopentylpropyl)-	1050 , 3.810	0.07037
Benzene, 1-(1-formylethyl)-4-(1-buten-3-yl)-	1050 , 3.860	0.04298
1H-Inden-1-one, 2,3-dihydrotetramethyl-	1050 , 4.150	0.01436
Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S-cis)-	1055 , 3.820	0.05942
à-Dehydro-ar-himachalene	1055 , 3.970	0.0191
(S,Z)-2-Methyl-6-(p-tolyl)hept-2-en-1-ol	1060 , 3.350	0.14164
Cadina-1(10),6,8-triene	1060 , 3.690	0.01475
Anthracene, 1,2,3,4,4a,9,9a,10-octahydro-	1060 , 4.370	0.04618
p-Menthane, 2,3-dibromo-8-phenyl-	1065 , 3.340	0.0661
Naphthalene, 1,2,3,4-tetrahydro-1-propyl-	1065 , 3.910	0.05093
1-Naphthalenemethanol, 1,2,3,4-tetrahydro-8-methyl-	1065 , 3.950	0.04778
Benzenebutanal	1065 , 4.010	0.03088
1,2,3,1',2',3'-Hexamethyl-bicyclopentyl-2,2'-diene	1070 , 3.450	0.15606
Azulene, 1,2,3,3a,4,5,6,7-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1R-(1à,3aá,4à,7á)]-	1080 , 3.290	0.04139
à-Dehydro-ar-himachalene	1080 , 4.140	0.02052
Phenol, 2-ethyl-	1090 , 3.680	0.01906
Benzene, 1,2-bis(1-buten-3-yl)-	1100 , 4.130	0.09121
Cyclohexene, 4-[(1E)-1,5-dimethyl-1,4-hexadien-1-yl]-1-methyl-	1105 , 3.320	0.02466
Unknown 19	1105 , 3.500	0.03204
Unknown 20	1105 , 3.650	0.09904
Naphthalene, 1,2,3,4-tetrahydro-1-octyl-	1105 , 3.710	0.0552
3,6-Dihydrochamazulene	1105 , 4.420	0.01809
Benzene, 1,1'-[3-(3-cyclopentylpropyl)-1,5-pentanediyl]bis-	1110 , 3.660	0.05108
Cycloisolongifolene, 8,9-dehydro-	1110 , 3.680	0.03057
(S,Z)-2-Methyl-6-(p-tolyl)hept-2-en-1-ol	1125 , 3.510	0.14449
Pent-1-yne, 5-benzyloxy-	1125 , 3.640	0.02857
Bicyclo[4.1.0]hept-3-ene, 7,7-dimethyl-3-vinyl-	1145 , 3.550	0.16315
Benzenebutanal, ç,4-dimethyl-	1145 , 3.580	0.11449
Benzene, (1,2-dicyclopropyl-2-phenylethyl)-	1165 , 3.780	0.03765
Cadala-1(10),3,8-triene	1165 , 4.000	0.01994
Phenol, 4-(1,1,3,3-tetramethylbutyl)-	1165 , 4.280	0.44178
Benzeneacetonitrile, à-acetyl-	1170 , 4.410	0.02327
1,4,6,7-Tetramethyl1,2,3,4-tetrahydronaphthalene	1175 , 4.400	0.04916
Benzene, 1,1'-[3-(3-cyclopentylpropyl)-1,5-pentanediyl]bis-	1200 , 3.760	0.04648
4b,5,6,7,8,8a,9,10-Octahydro-1-methylphenanthrene	1200 , 4.150	0.0207
1H-Indene, 5-hexyl-2,3-dihydro-	1210 , 3.850	0.03983

Phenol, 2-methyl-4-(1,1,3,3-tetramethylbutyl)-	1220 , 4.130	0.40888
Benzene, 4-hexenyl-	1225 , 4.200	0.05251
6-tert-Butyl-2,4-dimethylphenol	1250 , 4.040	0.06557
Cyclohexanol, 5-methyl-2-(1-methyl-1-phenylethyl)-	1255 , 4.070	0.03102
Bicyclo[2.2.1]heptane, 2-(phenylmethyl)-	1260 , 3.920	0.02495
4-Isopropyl-6-methyl-1-methylene-1,2,3,4-tetrahydronaphthalene	1265 , 4.360	0.04647
2-Furancarboxylic acid, 2-phenylethyl ester	1280 , 4.110	0.05629
3-Methyl-2-propionyl-benzoic acid	1295 , 4.010	0.02022
Phenol, 2-methyl-4-(1,1,3,3-tetramethylbutyl)-	1300 , 4.350	0.05154
Benzonitrile, 2-methyl-	430 , 4.560	0.57772
Phenol, 2,6-dimethyl-	435 , 3.970	0.07219
Phenol, 2-ethyl-	475 , 3.970	0.03292
Phenol, 2,3-dimethyl-	490 , 4.060	0.20962
Cycloprop[a]indene, 1,1a,6,6a-tetrahydro-	495 , 3.980	0.21655
Benzene, 1-butynyl-	505 , 4.030	0.25034
Naphthalene, 1,2,3,4-tetrahydro-	515 , 3.960	0.22356
Naphthalene, 1,2-dihydro-	520 , 4.240	0.01845
Benzoic acid, ethyl ester	525 , 4.140	0.04748
Phenol, 4-ethyl-	530 , 4.020	0.06223
1H-Indene, 2,3-dimethyl-	540 , 3.810	0.06711
Phenol, 2-ethyl-6-methyl-	545 , 4.210	0.01887
Benzenemethanol, à,à,4-trimethyl-	550 , 4.070	0.0645
Ethanone, 1-(4-methylphenyl)-	550 , 4.650	0.05411
Naphthalene	550 , 4.700	0.48519
Benzene, (2-cyclopropylethenyl)-	555 , 3.870	0.01632
1H-Indene, 1-ethyl-2,3-dihydro-	560 , 3.620	0.20179
1H-Indene, 2,3-dihydro-1,6-dimethyl-	565 , 3.690	0.73476
Benzene, (2-cyclopropylethenyl)-	565 , 3.980	0.02451
Benzoic acid	570 , 3.730	0.01643
m-Ethylbenzonitrile	570 , 4.730	0.19604
Benzene, 1,3-dimethyl-5-(1-methylethyl)-	580 , 3.500	0.07522
Benzoic acid	580 , 3.740	0.29675
1H-Indene, 2,3-dihydro-1,1,6-trimethyl-	590 , 3.510	0.0639
Naphthalene, 1,2,3,4-tetrahydro-2-methyl-	595 , 3.870	0.03616
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	605 , 3.470	0.13754
trans-1-Phenyl-1-pentene	605 , 3.570	0.06247
Benzene, 1-methyl-2-(1-methyl-2-propenyl)-	605 , 3.620	0.10245
Benzene, cyclopentyl-	605 , 3.920	0.29746
Naphthalene, 1,2,3,4-tetrahydro-1-methyl-	610 , 3.950	0.11626
Cyclopropane, 2-bromo-1-methyl-1-phenyl-	615 , 3.520	0.03784
Benzene, 1,3-dimethyl-5-(1-methylethyl)-	620 , 3.670	0.04307
1H-Indene, 2,3-dihydro-4,7-dimethyl-	620 , 3.850	0.18626

1H-Indene, 1-ethyl-2,3-dihydro-	620 , 3.930	0.02292
p-Cumenol	625 , 4.020	0.16279
4-Ethylbenzoic acid, tridec-2-ynyl ester	630 , 3.300	0.02392
Dec-5-ene-3,7-diyne, 2,9-dimethyl-	630 , 3.400	0.01256
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-	630 , 3.450	0.31825
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-	635 , 3.530	0.2487
Benzene, (2-cyclopropylethenyl)-	635 , 4.230	0.06198
Benzene, 1-cyclopropylmethyl-4-(1-methylethyl)-	640 , 3.310	0.01485
Benzene, cyclohexyl-	645 , 3.610	0.02921
1H-Indene, 2,3-dihydro-4,7-dimethyl-	645 , 3.880	0.2512
2-Thiophenecarboxylic acid, 4-nitrophenyl ester	650 , 3.390	0.03903
1H-Indene, 1,3-dimethyl-	655 , 4.100	0.3112
Benzene, pentyl-	660 , 3.230	0.04068
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	660 , 3.650	0.24392
Thiophene, 2-hexyl-	665 , 3.420	0.03174
1H-Indene, 2,3-dihydro-1,3-dimethyl-	665 , 3.960	0.19045
1H-Indene, 1,3-dimethyl-	665 , 4.120	0.514
Benzene, (1-methylpentyl)-	670 , 3.310	0.15447
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-	670 , 3.670	0.0287
3-Chloropropionic acid, 3-phenylpropyl ester	670 , 4.100	0.05054
1H-Indene, 2,3-dimethyl-	670 , 4.200	0.23171
Benzene, 4-hexenyl-	675 , 3.420	0.08498
Benzene, 2-ethyl-1,4-dimethyl-	675 , 3.450	0.04229
1H-Indene, 2,3-dihydro-1,6-dimethyl-	675 , 3.940	0.05191
1H-Indene, 2,3-dimethyl-	675 , 4.250	0.28088
Benzene, 4-hexenyl-	680 , 3.500	0.04012
Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	680 , 3.710	0.11663
(1-Methylenepent-2-enyl)benzene	680 , 3.930	0.05213
Benzene, 1-ethyl-4-(2-methylpropyl)-	685 , 3.370	0.08241
Benzene, cyclohexyl-	690 , 3.680	0.18392
Alanine, N-methyl-N-(2-methoxyethoxycarbonyl)-, decyl ester	690 , 3.710	0.08629
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	690 , 3.760	0.18213
1,2,3-Trimethylindene	695 , 3.900	0.1221
1H-Indene, 2,3-dihydro-1,6-dimethyl-	695 , 4.090	0.39061
Unknown 8	700 , 3.340	0.0176
Naphthalene, 1,2,3,4-tetrahydro-2,5,8-trimethyl-	700 , 3.370	0.02576
Isoquinoline, 1-butyl-3,4-dihydro-	700 , 3.710	0.05917
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	700 , 3.770	0.0259
Cyclobutane, 1,3-diphenyl-, trans-	700 , 3.810	0.03874
1H-Indene, 2,3-dihydro-1,1,4,7-tetramethyl-	705 , 3.470	0.02282
1H-Indene, 2,3-dimethyl-	705 , 4.480	0.02687
Benzene, (1-methylhexyl)-	710 , 3.230	0.03194

Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	710 , 3.480	0.03382
(1,3,5-Cycloheptatrien-7-yl)propanedinitrile	710 , 3.620	0.09662
1H-Indene, 2,3-dihydro-4-propyl-	710 , 3.640	0.07394
Naphthalene, 1,2,3,4-tetrahydro-5-methyl-	710 , 4.360	0.03603
3-Pyridinecarbonitrile, 1,4-dihydro-1-methyl-	715 , 3.180	0.02993
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	715 , 3.710	0.16258
Phenol, p-tert-butyl-	715 , 4.200	0.28844
à-Bromo-p-tolunitrile	715 , 4.660	0.03467
Benzene, 1-cyclopenten-1-yl-	720 , 4.420	0.10219
Naphthalene, 1-methyl-	720 , 4.770	0.32427
3-Methylbenzothiophene	720 , 4.980	0.04377
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	725 , 3.500	0.03425
Benzene, 1-heptenyl-	725 , 3.520	0.02697
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	725 , 3.830	0.27297
Benzenebutanenitrile	725 , 3.860	0.04405
1,2,3-Trimethylindene	725 , 3.980	0.11847
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	730 , 3.590	0.0216
1,2,3-Trimethylindene	730 , 4.120	0.07586
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	735 , 3.550	0.03196
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	740 , 3.600	0.03884
Naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl-	740 , 3.830	0.10921
Benzoic acid, 4-[2-(4-tolylthio)ethoxy]-	740 , 4.120	0.01777
1H-Indene, 1,1,3-trimethyl-	740 , 4.180	0.01747
Thiophene, 2-ethyl-5-isopentyl-	745 , 3.430	0.0123
Naphthalene, 1-methyl-	745 , 4.990	0.36757
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	750 , 3.300	0.03977
1H-Indene, 2,3-dihydro-4-propyl-	750 , 3.890	0.07224
à-Cyclopropyl-2-thiophenemethanol	750 , 4.090	0.01516
(1-Methylpenta-2,4-dienyl)benzene	750 , 4.160	0.0672
1,5,6,7-Tetramethylbicyclo[3.2.0]hepta-2,6-diene	755 , 3.320	0.03471
Naphthalene, 1,2,3,4-tetrahydro-2,6-dimethyl-	755 , 3.890	0.08802
Benzene, cyclohexyl-	755 , 3.970	0.12984
(1-Methylpenta-2,4-dienyl)benzene	755 , 4.210	0.04103
Naphthalene, 1,2,3,4-tetrahydro-6-propyl-	760 , 3.560	0.03887
N-Acetylindole	760 , 3.610	0.02975
1H-Indene, 2,3-dihydro-4-propyl-	760 , 3.870	0.13356
2-Methyl-4-phenylthiolane, 1,1-dioxide	765 , 3.630	0.02574
1H-Indene, 3-ethenyl-2,3-dihydro-1,1-dimethyl-	765 , 3.820	0.03736
1,4-Methanonaphthalen-9-ol, 1,2,3,4-tetrahydro-	765 , 3.920	0.05902
Naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl-	765 , 4.000	0.65068
2-Methyl-6-propylphenol	765 , 4.240	0.01602
Hex-1-enylbenzene	770 , 3.600	0.0282

Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	770 , 3.660	0.03632
Biphenylene, 1,2,3,6,7,8,8a,8b-octahydro-, trans-	770 , 3.900	0.01325
Naphthalene, 2-ethyl-1,2,3,4-tetrahydro-	770 , 4.000	0.01953
Benzene, (1,1-dimethyl-2-butynyl)-	775 , 4.240	0.01869
Benzene, 3-cyclohexen-1-yl-	775 , 4.260	0.26512
1,4-Ethanonaphthalene, 1,2,3,4-tetrahydro-	775 , 4.300	0.12469
Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	780 , 4.010	0.05378
Benzene, 1,3-bis(1-methylethenyl)-	790 , 4.140	0.06938
Phenol, 2-(1,1-dimethylethyl)-6-methyl-	795 , 4.210	0.01967
1,2,3-Trimethylindene	795 , 4.290	0.09402
1,2,3-Trimethylindene	805 , 4.150	0.02411
Phenol, 2-(1,1-dimethylethyl)-5-methyl-	810 , 4.190	0.07648
(1-Methylpenta-1,3-dienyl)benzene	810 , 4.280	0.13061
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	820 , 4.160	0.10364
(1-Methylpenta-1,3-dienyl)benzene	825 , 4.200	0.02824
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	830 , 4.380	0.01656
1H-Indene, 1,1,3-trimethyl-	835 , 4.240	0.41837
2-Propanone, 1-(4-methoxyphenyl)-	840 , 4.120	0.0407
1,4-Methanonaphthalen-9-one, 1,2,3,4-tetrahydro-	840 , 4.620	0.01534
1,2,3-Trimethylindene	845 , 4.310	0.23043
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	860 , 4.160	0.02842
Benzo[b]thiophene, 2,7-dimethyl-	860 , 4.940	0.13998
1,2,3-Trimethylindene	870 , 4.410	0.11847
Diphenylmethane	870 , 4.800	0.01348
Benzene, (1,2,3-trimethyl-2-cyclopropen-1-yl)-	875 , 4.490	0.05173
Cyclohexene, 1-phenyl-	875 , 4.520	0.0183
1H-Indene, 2,3-dihydro-1,1,5,6-tetramethyl-	880 , 4.070	0.04898
1, 1, 5-Trimethyl-1, 2-dihydronaphthalene	880 , 4.130	0.18499
Naphthalene, 2,6-dimethyl-	885 , 4.750	0.25607
Naphthalene, 1,2-dihydro-1,1,6-trimethyl-	895 , 4.200	0.03315
1H-Indole, 2,3-dihydro-1,2,3,3-tetramethyl-	895 , 4.720	0.21216
Phenol, 2,4-bis(1-methylethyl)-	900 , 4.080	0.06724
Benzene, 3-cyclohexen-1-yl-	900 , 4.160	0.03308
1, 1, 5-Trimethyl-1, 2-dihydronaphthalene	900 , 4.280	0.05207
1,2,3-Trimethylindene	900 , 4.540	0.02808
Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, cis-	905 , 4.240	0.07251
Acenaphthylene, 1,2,2a,3,4,5-hexahydro-	910 , 4.570	0.08956
Naphthalene, 1,6-dimethyl-	910 , 4.960	0.72824
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	915 , 4.030	0.02633
3-Ethyl-3-phenyl-1-pentene	920 , 4.040	0.09468
Naphthalene, 1,2-dihydro-2,5,8-trimethyl-	925 , 4.180	0.10733
1H-Indene, 1-methyl-3-propyl-	930 , 4.290	0.07127

2,7-Ethanonaphth[2,3-b]oxirene, 1a,2,7,7a-tetrahydro-, (1aà,2à,7à,7aà)-	935 , 4.390	0.03633
Naphthalene, 1,2,3,4-tetrahydro-1,4,6-trimethyl-	940 , 4.050	0.20332
2,4-Dimethylstyrene	940 , 4.070	0.03851
1H-Indene, 1-methyl-3-propyl-	945 , 4.200	0.02928
3-Ethyl-3-phenyl-1-pentene	950 , 4.110	0.06517
Naphthalene, 1,2-dihydro-1,5,8-trimethyl-	950 , 4.290	0.02743
1H-Indene, 3-ethenyl-2,3-dihydro-1,1-dimethyl-	960 , 4.300	0.03217
2,7-Ethanonaphth[2,3-b]oxirene, 1a,2,7,7a-tetrahydro-, (1aà,2à,7à,7aà)-	970 , 4.300	0.13923
1H-Indene, 3-ethenyl-2,3-dihydro-1,1-dimethyl-	975 , 4.420	0.27238
Naphthalene, 1,2-dihydro-1,4,6-trimethyl-	990 , 4.290	0.02698
Naphthalene, 1-propyl-	1005 , 4.690	0.09681
Naphthalene, 2-(1-methylethyl)-	1015 , 4.800	0.03766
Benzo[b]thiophene, 2,5,7-trimethyl-	1020 , 4.830	0.01468
Naphthalene, 1,4,5-trimethyl-	1030 , 4.660	0.06195
Benzo[b]thiophene, 2-ethyl-7-methyl-	1030 , 4.940	0.05415
Naphthalene, 1,4,5-trimethyl-	1035 , 4.780	0.03951
Naphthalene, 1,2-dihydro-1,4,6-trimethyl-	1040 , 4.480	0.08755
1-(4-Tolyl)-1-cyclohexene	1070 , 4.640	0.01799
Naphthalene, 2,3,6-trimethyl-	1070 , 4.790	0.66608
Benzene, 3-cyclohexen-1-yl-	1085 , 4.480	0.03523
Naphthalene, 1,4,5-trimethyl-	1095 , 4.860	0.32843
Naphthalene, 1-methyl-7-(1-methylethyl)-	1115 , 4.480	0.03083
1H-Indene, 3-ethyl-1-(1-methylethyl)-	1125 , 4.480	0.08387
1,1'-Biphenyl, 2-ethyl-	1130 , 4.870	0.07085
Benzo[b]thiophene, 3,5-dimethyl-	1135 , 4.810	0.02124
Benzo[b]thiophene, 2-ethyl-5,7-dimethyl-	1140 , 4.900	0.17575
Naphthalene, 3-(1,1-dimethylethyl)-1,2-dihydro-	1145 , 4.590	0.05742
Unknown 21	1145 , 4.650	0.02323
Succinic acid, naphth-2-ylmethyl 3-fluorophenyl ester	1145 , 4.760	0.0385
4,4'-Dimethylbiphenyl	1145 , 4.860	0.02205
Naphthalene, 1-butyl-	1160 , 4.630	0.07774
Benzo[b]thiophene, 2,3-diethyl-	1160 , 4.850	0.01663
4,4'-Dimethylbiphenyl	1165 , 4.920	0.03383
Naphthalene, 1,2,3,4-tetramethyl-	1175 , 4.690	0.07774
Naphthalene, 3-(1,1-dimethylethyl)-1,2-dihydro-	1175 , 4.800	0.01663
Naphthalene, 2-methyl-1-propyl-	1185 , 4.740	0.03044
Naphthalene, 1-methyl-7-(1-methylethyl)-	1190 , 4.820	0.31276
Benzene, 1,1'-(1-methyl-1,2-ethanediyl)bis-	1195 , 4.980	0.04904
3-Acetyl-2,5-dimethylbenzo(b)thiophene	1215 , 4.750	0.11014
Naphthalene, 1-methyl-7-(1-methylethyl)-	1215 , 4.830	0.07869
Benzene, 1,1'-(1,3-propanediyl)bis-	1235 , 4.850	0.37559

Phenol, 4-(1,1-dimethylpropyl)-	1240 , 4.520	0.06931
Benzene, 1,1'-propylidenebis-	1250 , 4.780	0.01934
1H-Indole-3-carbonitrile, 2-benzenesulfonylmethyl-1-methyl-	1250 , 4.940	0.02386
1,4,5,8-Tetramethylnaphthalene	1255 , 4.900	0.02815
Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	1265 , 4.660	0.08547
Benzene, 1,1',1",1'"-(1,2-ethanediylidene)tetrakis-	1285 , 4.870	0.02156
Butane, 2,3-dimethyl-2,3-di-(2,2'-naphthyl)-	1295 , 4.690	0.03418
1,2,3,3a,8,9,9a,9b-Octahydrocyclopenta[def]phenanthrene	1315 , 4.610	0.03749
Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	1355 , 4.690	0.02699
Ethylbenzene	175 , 2.070	0.53611
Pentanoic acid	180 , 2.040	0.0351
Benzene, 1,3-dimethyl-	185 , 2.070	1.05282
1,3-Hexadiene, 3-ethyl-2-methyl-	190 , 1.770	0.12899
Cyclopropene, 1-butyl-2-ethyl-	195 , 1.780	0.03065
Ethanone, 1-(2-methyl-2-cyclopenten-1-yl)-	195 , 1.790	0.16202
1,5-Heptadiene, 3,4-dimethyl-	200 , 1.800	0.02184
Cyclohexene, 4-bromo-	205 , 1.810	0.08708
1,3-Hexadiene, 3-ethyl-2-methyl-	205 , 1.840	0.14341
1,3-Cyclopentadiene, 5-(1,1-dimethylethyl)-	205 , 1.960	0.05115
1,3-Cyclohexadiene, 5,6-dimethyl-	205 , 2.060	0.05445
Cyclohexane, 1-ethyl-4-methyl-, trans-	210 , 1.810	0.05965
Cyclopentanecarboxylic acid, 4-nitrophenyl ester	215 , 1.840	0.02037
1-Octene, 6-methyl-	215 , 1.860	0.11996
3,4-Octadiene, 7-methyl-	215 , 1.900	0.16398
trans-1-Butenylcyclopentane	225 , 1.940	0.03377
3-Cyclohexene-1-carboxaldehyde, 4-methyl-	225 , 1.990	0.06092
Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-	230 , 1.850	0.09194
cis,cis-2,7-Nonadiene	235 , 2.000	0.12357
Imidazole-2-hydrazide-1-carboxylic acid, methyl ester	240 , 1.900	0.03004
(1,3-Dimethyl-2-methylene-cyclopentyl)-methanol	240 , 2.000	0.10631
Bicyclo[2.2.1]hept-2-ene, 1,7,7-trimethyl-	240 , 2.010	0.10782
1,2,4,4-Tetramethylcyclopentene	240 , 2.040	0.02708
3,5-Heptadien-2-ol, 2,6-dimethyl-	240 , 2.110	0.02381
trans-8a-Methylperhydroazulen-4(1H)-one	245 , 1.910	0.0286
Pentalene, octahydro-2-methyl-	245 , 2.020	0.17826
2,6-Octadiyne	245 , 2.170	0.0607
Cycloheptanol, 1-methyl-2-methylene-	245 , 2.180	0.03156
4-Methyl-1,5-Heptadiene	250 , 1.910	0.02109
Cyclohexene, 1-methyl-4-(1-methylethylidene)-	255 , 2.080	0.08351
1,5-Cyclooctadiene, 3,4-dimethyl-	255 , 2.120	0.41692
1,5-Cyclooctadiene, 1-ethyl-	260 , 2.080	0.14649
ç-Terpinene	265 , 2.150	0.01782

Cyclohexene, 4-methyl-1-(1-methylethyl)-, (R)-	270 , 2.010	0.14182
1,6-Octadiene, 2,6-dimethyl-, (Z)-	270 , 2.050	0.22922
Bicyclo[2.2.1]heptane, 2,2,3-trimethyl-	275 , 2.000	0.10249
3-Carene	275 , 2.200	0.0858
Cyclooctane, 1,2-dimethyl-	280 , 1.980	0.05554
2,6-Dimethyl-2-trans-6-octadiene	280 , 2.080	0.19386
1,3-Cyclohexadiene, 1,5,5,6-tetramethyl-	280 , 2.280	0.32081
3,3-Tetramethyleneglutaric anhydride	285 , 2.050	0.17614
Cyclopentene, 1-methyl-	285 , 2.070	0.18791
Cyclohexene, 4-methyl-1-(1-methylethenyl)-	285 , 2.190	0.04233
Cyclohexane, butylidene-	290 , 2.110	0.12726
5-t-Butyl-4-methylimidazole	290 , 2.170	0.16999
2-Methyl-1-nonene-3-yne	290 , 2.240	0.03294
2,6-Dimethyl-2-trans-6-octadiene	295 , 2.110	0.05187
(5R,8R,8aS)-5-Heptyl-8-methyloctahydroindolizine	295 , 2.130	0.02852
4,6-O-Furylidene-d-glucopyranose	300 , 2.070	0.04195
3-Nonyne	300 , 2.120	0.77075
1-[3-(methylthio)propyl]-2-formylpyrrole	300 , 2.270	0.05346
1,4-Hexadiene, 3-ethyl-4,5-dimethyl-	305 , 2.180	0.23838
1,3-Heptadiene, 3-ethyl-2-methyl-	305 , 2.220	0.08013
á-Pinene	305 , 2.320	0.18428
Cyclodecane	315 , 2.080	0.02984
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1à,3à,6à)]-	320 , 2.210	0.59225
ç-Terpinene	320 , 2.370	0.17718
Cyclohexene, 1-methyl-4-(1-methylethyl)-	330 , 2.280	0.15266
Cyclohexane, 1-methyl-4-(1-methylethenyl)-, trans-	330 , 2.330	0.05338
Tricyclo[2.2.1.0(2,6)]heptane, 1,3,3-trimethyl-	330 , 2.430	0.09971
1-Pyrrolidinylacetonitrile	335 , 2.280	0.04676
Spiro[2.4]heptane, 1,5-dimethyl-6-methylene-	340 , 2.430	0.16145
Cyclohexene, 4-methyl-1-(1-methylethenyl)-	345 , 2.450	0.27487
Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-, [1S-(1à,2á,5à)]-	350 , 2.190	0.01858
3-Dodecyne	350 , 2.210	0.41257
4-Ethyl-2-hexynal	355 , 2.300	0.21204
Unknown 1	360 , 2.350	0.05044
Naphthalene, 1,2,3,4,4a,5,8,8a-octahydro-4a-methyl-, trans-	360 , 2.360	0.02593
anti-10-Methyl-endo-tricyclo[5.2.1.0(2.6)]decane	360 , 2.390	0.09805
Benzene, (1-nitroethyl)-	360 , 2.500	0.14227
1-Adamantanol	365 , 2.210	0.13821
photocitral A	365 , 2.250	0.02552
Pyridine, 4-methoxy-	365 , 2.280	0.09858
1,5-Cyclooctadiene, 1,3-dimethyl-	370 , 2.410	0.14343
4-Ethyl-2-hexynal	380 , 2.270	0.79205

1-Piperidineacetonitrile	380 , 2.320	0.02684
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1à,3à,6à)]-	385 , 2.340	0.06324
2,5-Cyclohexadien-1-one, 4-ethyl-3,4-dimethyl-	390 , 2.490	0.14009
1,3-Benzenediol, 4-propyl-	395 , 2.350	0.03305
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1à,3à,6à)]-	400 , 2.330	0.29997
2-Caren-10-al	400 , 2.500	0.01813
Benzene, (1-methoxy-4-methyl-3-pentenyl)-	405 , 2.470	0.05657
6-Butyl-1,4-cycloheptadiene	405 , 2.500	0.03269
1-Pentanone, 1-(1H-imidazol-2-yl)-	410 , 2.420	0.08223
Ethyl (Z)-hex-3-enyl carbonate	415 , 2.370	0.15407
1,6-Octadiene, 2,6-dimethyl-, (Z)-	415 , 2.380	0.55542
2,4-Dimethyl-1,5-diazabicyclo[3.1.0]hexane (cis)	420 , 2.300	0.02593
2,5-Dimethylhex-5-en-3-yn-2-ol	420 , 2.380	0.05507
p-Menth-8-ene, 3-methylene-	425 , 2.590	0.11448
Germacyclopent-3-ene, 1,1-dichloro-3,4-dimethyl-	425 , 2.640	0.0439
2-n-Heptylfuran	430 , 2.440	0.1547
3-Hexen-1-ol, formate, (Z)-	435 , 2.420	0.18579
4,4-Dimethyl-2-propenylcyclopentanone	435 , 2.500	0.26306
Cyclohexene, 2-ethenyl-1,3,3-trimethyl-	435 , 2.600	0.09598
Cyclohexene, 3-(bromomethyl)-	445 , 2.380	0.06784
1,10-Undecadiene	445 , 2.590	0.48684
Benzene, (1,2-dimethoxyethyl)-	445 , 2.620	0.02901
Cyclohexane, 4-methyl-2-methylene-1-(1-methylethylidene)-	445 , 2.650	0.25606
p-Menth-8-ene, 3-methylene-	460 , 2.700	0.08262
Unknown 3	465 , 2.480	0.05638
Bicyclo[5.1.0]octane, 8-(1-methylethylidene)-	465 , 2.540	0.08351
Cyclohexane, pentyl-	475 , 2.380	0.03659
2-n-Heptylfuran	485 , 2.430	0.2417
4-Ethyl-2-hexynal	500 , 2.430	0.15482
1,1'-Bicyclopropyl, 2,2,2',2'-tetramethyl-	515 , 2.420	0.08255
5-Trimethylsilylpent-2-en-4-yne	525 , 2.580	0.02712
Cyclohexane, 1-methyl-4-(1-methylbutyl)-	530 , 2.400	0.03256
1-Nonyne, 7-methyl-	530 , 2.460	0.41707
Unknown 4	530 , 2.500	0.05569
2-Cyano-2-O-fluorosulfatofluoropropane	540 , 2.560	0.07248
1-Undecyne	550 , 2.470	0.06747
5-Dodecyne	555 , 2.540	0.23171
4-Methylene-3a,4,5,6,7,9a-hexahydrocycloocta[1,3]dioxole-2-thione	555 , 2.720	0.05357
Bicyclo[2.2.1]heptane, 2-(1-buten-3-yl)-	560 , 2.540	0.09538
2-n-Heptylfuran	570 , 2.610	0.15285
Octanoic acid	570 , 2.750	0.01006
Cyclopentane, 1-hydroxymethyl-1,3-dimethyl-	575 , 2.420	0.0271

2-(3-methyl-2-cyclopenten-1-yl)-2-methylpropionaldehyde	585 , 2.510	0.08695
2,5-Cyclohexadiene, 1,4-diethyl-1,4-dimethyl-	585 , 2.840	0.03989
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1à,3à,6à)]-	600 , 2.690	0.10692
Unknown 6	605 , 2.890	0.05753
3-Buten-1-ol, 4-chloro-2-methyl-1-phenyl-	615 , 2.790	0.06479
3-Dodecyne	620 , 2.650	0.22036
(1à,2à,3á)-Dimethyl 1,3-dimethyl-4-cyclohexene-1,2-dicarboxylate	625 , 2.860	0.00928
Cyclododecane	635 , 2.460	0.02456
Unknown 7	635 , 2.930	0.0655
Cyclopentane, 2-ethylidene-1,1-dimethyl-	645 , 2.560	0.12061
1-Pentene, 5-(2,2-dimethylcyclopropyl)-2-methyl-4-methylene-	665 , 2.920	0.19288
1,4,9-Decatriene, (E)-	665 , 2.930	0.02835
1,3-Dicyanobenzene	670 , 2.990	0.83363
Cyclohexene, 4-(2-bromoethyl)-	680 , 2.570	0.04711
1,3-Dimethyl-5-trifluoroacetoxycyclohexane	680 , 2.620	0.11902
7-Octylidenebicyclo[4.1.0]heptane	680 , 2.920	0.15451
1H-3a,7-Methanoazulene, octahydro-1,4,9,9-tetramethyl-	695 , 2.900	0.30904
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-	700 , 2.690	0.1209
4-Tridecen-6-yne, (E)-	705 , 2.930	0.14092
Cyclohexene, 3-methyl-6-(1-methylethyl)-	710 , 2.640	0.04699
4(1H)-Pyridone	715 , 2.620	0.04444
Spiro[2.4]heptane, 1,2,4,5-tetramethyl-6-methylene-	715 , 2.980	0.09098
1-Heptadecyne	720 , 2.720	0.09982
Tricyclo[2.2.1.0(2,6)]heptane, 1,3,3-trimethyl-	720 , 2.880	0.16082
Cyclohexane, 1-bromo-4-methyl-	725 , 2.550	0.04411
Bicyclo[6.1.0]nonane, 9-(1-methylethylidene)-	730 , 2.880	0.22752
2-Pentadecen-4-yne, (Z)-	740 , 2.920	0.0884
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-	745 , 2.720	0.16104
Unknown 9	745 , 2.960	0.09095
3-Isopropylidene-tricyclo[4.3.1.1(2,5)]undecan-10-one	745 , 2.990	0.03762
Dispiro[2.1.2.1]octane, 1,1,6,6-tetramethyl-	750 , 2.800	0.11978
1,4,9-Decatriene, (E)-	750 , 2.930	0.09582
1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1à,4à,4aà,10aà)-	765 , 3.010	0.09708
1H-3a,7-Methanoazulene, octahydro-1,4,9,9-tetramethyl-	775 , 3.000	0.2465
1,7-Nonadiene, 4,8-dimethyl-	785 , 2.770	0.2168
Cyclohexane, (1-methylethyl)-	790 , 2.590	0.0357
Cyclopropane, 1-isopropenyl-1-(terahydrofuran-2,5-dion-3-yl)-	800 , 2.940	0.20329
1,E-4,Z-8-Dodecatriene	805 , 2.760	0.19442
Cyclohexanemethanol, 4-(1-methylethyl)-, trans-	815 , 2.620	0.05236
Cyclopentaneethanol, á,2,3-trimethyl-	825 , 2.760	0.09282
1,3,7-Octatriene, 2,7-dimethyl-	830 , 2.800	0.21081

Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)-	830 , 2.840	0.0538
1-Pentene, 5-(2,2-dimethylcyclopropyl)-2-methyl-4-methylene-	840 , 2.830	0.05405
1H-Cycloprop[e]azulene, decahydro-1,1,4,7-tetramethyl-, [1aR-(1aà,4á,4aá,7á,7aá,7bà)]-	845 , 2.860	0.43782
2-Cyclopentene-1-carboxylic acid, 1,2,3-trimethyl-, ethyl ester, (.+-.)-	850 , 2.750	0.06325
2H-Benzocyclohepten-2-one, 1,4a,5,6,7,8,9,9a-octahydro-4a-methyl-, trans-	850 , 2.810	0.12327
Santolina epoxide	865 , 2.730	0.24974
9,12-Tetradecadien-1-ol, (Z,E)-	865 , 2.910	0.2868
2,6,9,11-Dodecatetraenal, 2,6,10-trimethyl-, (E,E,E)-	870 , 2.900	0.02823
3,7,11,Trimethyl-8,10- dodecedienylacetate	880 , 2.860	0.14934
Lycorenan-7-one, 1-methyl-9,10-[methylenebis(oxy)]-	890 , 2.640	0.03556
1,6-Heptadiene, 2,5,5-trimethyl-	890 , 2.760	0.26229
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1à,3à,6à)]-	890 , 2.850	0.18839
Hexane, 1-(isopropylidenecyclopropyl)-	900 , 2.920	0.15507
1,2-Dipentylcyclopropene	905 , 2.790	0.01667
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1à,3à,6à)]-	910 , 2.780	0.46904
Trivinyl(chloromethyl)silane	910 , 2.860	0.14643
Bicyclo[10.1.0]tridec-1-ene	915 , 3.010	0.21235
1,5-Heptadiene, 2-methyl-, (E)-	920 , 2.960	0.12668
1,5,9-Undecatriene, 2,6,10-trimethyl-, (Z)-	925 , 2.830	0.20421
Bicyclo[6.1.0]nonane, 9-(1-methylethylidene)-	930 , 2.840	0.04951
1,5,9-Undecatriene, 2,6,10-trimethyl-, (Z)-	935 , 2.770	0.10278
1,5,9-Decatriene, 2,3,5,8-tetramethyl-	935 , 2.790	0.18903
1,6-Octadiene, 3,5-dimethyl-, trans-	945 , 2.810	0.14862
1-Cyclohexyl-1-pentyne	945 , 2.870	0.30228
Benzene, 1-(1,5-dimethylhexyl)-4-methyl-	945 , 3.130	0.43162
1,5,9-Undecatriene, 2,6,10-trimethyl-, (Z)-	960 , 2.850	0.3367
Unknown 13	960 , 3.080	0.01722
1-Cyclohexyl-1-pentyne	970 , 2.950	0.12026
Unknown 14	970 , 3.100	0.03721
2,3-Diazabicyclo[2.2.1]hept-2-ene, 4-methyl-1-(pent-4-en-1-yl)-	980 , 2.880	0.10154
1,5-Heptadiene, 2,3,6-trimethyl-	980 , 2.940	0.0349
1,4-Methanophthalazine, 1,4,4a,5,6,7,8,8a-octahydro-1,4,9,9-tetramethyl-, (1à,4à,4aà,8aà)-	990 , 3.190	0.02309
1,2-Dipentylcyclopropene	995 , 2.750	0.0203
Bicyclo[6.1.0]nonane, 9-(1-methylethylidene)-	995 , 2.890	0.02948
Caparratriene	995 , 2.910	0.02516
1,2-Di-but-2-enyl-cyclohexane	1000 , 2.980	0.08793
Unknown 16	1000 , 3.170	0.02649
(3-Methylphenyl) methanol, neopentyl ether	1000 , 3.190	0.05064
anti-10-Methyl-endo-tricyclo[5.2.1.0(2.6)]decane	1025 , 3.000	0.05494
cis-á-Farnesene	1030 , 3.230	0.02551

à-Farnesene	1035 , 3.140	0.09661
1H-Cycloprop[e]azulene, decahydro-1,1,4,7-tetramethyl-, [1aR-(1aà,4á,4aá,7á,7aá,7bà)]-	1040 , 3.060	0.20462
Aromadendran ('2')	1045 , 3.020	0.19146
Cyclopropane, 1-(5-hexenyl)-2-iodo-	1050 , 3.050	0.1021
1,2-Di-but-2-enyl-cyclohexane	1055 , 2.960	0.09645
4-Ethylbenzoic acid, tridec-2-ynyl ester	1070 , 3.220	0.04578
Bicyclo[10.1.0]tridec-1-ene	1085 , 2.940	0.0941
(3-Methylphenyl) methanol, neopentyl ether	1085 , 3.110	0.01898
Benzene, 1-(1,5-dimethylhexyl)-4-methyl-	1095 , 3.200	0.18312
1-Tridecyne	1120 , 2.900	0.08587
1-Hexene, 3-methyl-6-phenyl-4-(1-phenylethoxy)-	1160 , 3.220	0.05002
Bicyclo[10.1.0]tridec-1-ene	1175 , 3.050	0.04603
Bicyclo[6.1.0]nonane, 9-(1-methylethylidene)-	1195 , 3.080	0.06047
Benzene, (1,1-dimethylnonyl)-	1215 , 3.160	0.17036
1-methyl-1-indanol	1215 , 3.260	0.04898
1,8,11-Heptadecatriene, (Z,Z)-	1295 , 3.060	0.17096
4-Ethylbenzoic acid, tridec-2-ynyl ester	1325 , 3.230	0.02691
Bicyclo[3.3.1]nonan-9-one, 1,2,4-trimethyl-3-nitro-, (2-endo,3-exo,4-exo)-(.+-.)-	1480 , 3.010	0.19299
1,5,9-Decatriene, 2,3,5,8-tetramethyl-	1485 , 3.140	0.03095
trans-Farnesol	1495 , 3.010	0.10957
Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-	1500 , 3.280	1.55957
Geranyl nitrile	1515 , 3.030	0.03778
1,5-Heptadiene, 2,6-dimethyl-	1520 , 3.010	0.04669
(2,4,6-Trimethylcyclohexyl) methanol	1555 , 3.180	0.06568
1,3-Bis-(2-cyclopropyl,2-methylcyclopropyl)-but-2-en-1-one	1555 , 3.350	0.43712
Tridecanoic acid, methyl ester	1575 , 3.060	0.0135
Fluorene	1145 , 0.830	0.05396
1,1'-Biphenyl, 2-ethyl-	1285 , 0.510	0.03047
9H-Fluorene, 1-methyl-	1300 , 0.620	0.06539
9H-Fluorene, 2-methyl-	1310 , 0.780	0.10473
9H-Fluorene, 9,9-dimethyl-	1320 , 0.390	0.06655
3,3'-Dimethylbiphenyl	1320 , 0.500	0.02366
2,2'-Dimethylbiphenyl	1320 , 0.540	0.16031
1,4,5,8-Tetramethylnaphthalene	1325 , 0.160	0.30289
1,1'-Biphenyl, 2-ethyl-	1335 , 0.570	0.09054
Benzo[f]quinoline-2-carbonitrile, 1-benzoyl-1,2-dihydro-	1335 , 0.620	0.07852
4-(Phenylmethyl)benzeneethanamine	1335 , 1.000	0.01977
9H-Fluorene, 9,9-dimethyl-	1345 , 0.710	0.02978
4,4'-Dimethylbiphenyl	1350 , 0.760	0.05912
1,1'-Biphenyl, 4-(1-methylethyl)-	1355 , 0.230	0.15646
1,1'-Biphenyl, 4-(1-methylethyl)-	1360 , 0.360	0.02331

1,1'-Biphenyl, 2-ethyl-	1370 , 0.880	0.04452
1,1'-Biphenyl, 4-(1-methylethyl)-	1375 , 0.150	0.02049
1,1'-Biphenyl, 4-(1-methylethyl)-	1380 , 0.220	0.05414
Propan-1-one, 3-(benzothiazol-2-yl)-1-phenyl-	1385 , 0.920	0.04515
1,1'-Biphenyl, 4-(1-methylethyl)-	1405 , 0.410	0.04449
Phenanthrene	1405 , 1.740	0.06219
5H-Dibenzo[a,c]cyclohepten-5-ol	1425 , 0.630	0.0265
1,1-Diphenylcyclopropane	1430 , 0.700	0.06152
9H-Fluorene, 9,9-dimethyl-	1445 , 0.550	0.03728
p-Ethyldiphenylmethane	1450 , 0.410	0.02953
1,1'-Biphenyl, 4-(1-methylethyl)-	1450 , 0.580	0.03096
9H-Fluorene, 9,9-dimethyl-	1455 , 0.620	0.05268
Anthracene, 9,10-dihydro-9,10-dimethyl-	1460 , 0.180	0.03024
9H-Fluorene, 2,3-dimethyl-	1460 , 0.730	0.0808
Benzamide, N-hexyl-	1465 , 0.480	0.11277
Anthracene, 9,10-dihydro-9,10-dimethyl-	1470 , 0.390	0.05018
1,1-di-o-Tolylethylene	1485 , 0.420	0.05922
1,1'-biphenyl, 2,4,6-trimethyl-	1485 , 0.490	0.10569
Naphthalene, 1,2,3-trimethyl-4-propenyl-, (E)-	1490 , 0.210	0.09392
9H-Fluorene, 9,9-dimethyl-	1500 , 0.900	0.04619
Naphthalene, 1,2,3-trimethyl-4-propenyl-, (E)-	1505 , 0.240	0.04814
Anthracene, 9-(3-bromopropyl)-9,10-dihydro-	1565 , 0.530	0.0622
1-Pentene, 1,5-diphenyl-	1585 , 0.450	0.06231
m-Toluic acid, 4-nitrophenyl ester	1615 , 0.290	0.02144
Naphthalene, 2-phenyl-	1635 , 1.570	0.04825
Phenanthrene, 2,5-dimethyl-	1705 , 1.380	0.03111
Phenanthrene, 2,3,5-trimethyl-	1835 , 1.160	0.03623
m-Terphenyl	1835 , 1.370	0.02191
Retene	1900 , 0.960	0.05035

Table S6 List of Compounds identified in StTPO

Compounds	**R.T. (s)**	**Peak area (%)**
Heptane, 2,6-dimethyl-	150 , 4.100	0.164861329
1-Ethyl-5-methylcyclopentene	155 , 4.470	0.151204774
Cyclohexane, ethyl-	160 , 2.050	0.306841639
Bicyclo[3.1.0]hexane, 1,5-dimethyl-	175 , 1.780	0.219595356
Octane, 3-methyl-	175 , 4.820	0.173051817
1,3-Hexadiene, 3-ethyl-2-methyl-	190 , 1.760	0.129584272
Nonane	200 , 1.610	0.081024832
Benzene, 1,3-dimethyl-	200 , 2.230	0.030513582
Styrene	200 , 2.350	0.072507406

Benzene, (1-methylethyl)-	225 , 2.280	0.240430281
Octane, 2,6-dimethyl-	230 , 1.700	0.073381895
Spiro[4.4]non-1-ene	235 , 2.090	0.119231363
Cyclopropane, 1,2-dimethyl-3-pentyl-, (1à,2à,3à)-	245 , 1.820	0.185638276
Nonane, 5-methyl-	250 , 1.760	0.111630475
Benzene, propyl-	250 , 2.420	0.189960524
Nonane, 2-methyl-	255 , 1.770	0.763363576
D-Limonene	255 , 2.110	0.513070701
4-Octene, 2,6-dimethyl-, [S-(Z)]-	260 , 1.930	0.037157552
Benzene, 1-ethyl-2-methyl-	260 , 2.490	0.919955137
Nonane, 3-methyl-	265 , 1.760	0.117627608
Thiophene, 2-(1-methylethyl)-	265 , 2.710	0.061569899
Cyclohexane, 2-ethyl-1,3-dimethyl-	270 , 1.930	0.04576815
Spiro[2.5]octane	270 , 2.000	0.422665624
Benzene, 1-ethyl-4-methyl-	275 , 2.650	0.681951235
Cyclooctane, 1,2-dimethyl-	280 , 2.000	0.51810647
1,3-Cyclohexadiene, 1,3,5,5-tetramethyl-	280 , 2.250	0.258795853
Thiophene, 2,3,4-trimethyl-	280 , 2.700	0.053977347
à-Methylstyrene	280 , 2.790	0.082053991
Benzonitrile	280 , 3.840	0.592128904
1-Decene	285 , 1.930	0.316759618
Dinocap	290 , 2.550	0.09185657
Benzene, 1,2,3-trimethyl-	290 , 2.720	0.04296871
Decane	295 , 1.880	0.059643837
2,6-Octadiene, 2,6-dimethyl-	295 , 2.130	0.250713541
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-	295 , 2.160	0.418106833
Benzene, 2-propenyl-	295 , 2.870	0.097661615
trans-4-Decene	300 , 1.980	0.078774425
m-Menthane, (1S,3S)-(+)-	300 , 2.060	0.116758861
Cyclohexene, 4-methyl-1-(1-methylethenyl)-	300 , 2.280	0.165581333
1,3-Heptadiene, 3-ethyl-2-methyl-	305 , 2.180	0.350763192
1,3-Heptadiene, 3-ethyl-2-methyl-	305 , 2.220	0.047971693
ç-Terpinene	305 , 2.330	0.165332564
3,3-Dimethyl-6-methylenecyclohexene	305 , 2.470	0.231621112
(1H)-3a,4,5,6,7,7a-Hexahydroindene	310 , 2.550	0.032852716
Benzene, (1-methylpropyl)-	310 , 2.620	0.31734329
3-Phenylbut-1-ene	310 , 2.800	0.025484296
Nonane, 2,6-dimethyl-	320 , 1.860	0.723128363
Cyclohexene, 1,5,5-trimethyl-3-methylene-	320 , 2.370	0.089630799
o-Cymene	320 , 2.680	0.26030662
Thiophene, 2,5-diethyl-	320 , 2.770	0.175843106
Cyclohexene, 1-methyl-4-(1-methylethyl)-	325 , 2.300	0.115868071

Benzene, 1-methyl-3-(1-methylethyl)-	325 , 2.750	0.156176822
Benzene, (1-methylethyl)-	325 , 2.960	0.755755279
2,2,4,4-Tetramethyloctane	330 , 1.910	0.431091915
Benzene, 1-ethyl-2,4-dimethyl-	330 , 2.680	0.314236362
Benzene, 2-propenyl-	330 , 3.110	0.085633637
Cyclohexane, 1,3-dimethyl-, cis-	335 , 2.030	1.018205055
D-Limonene	335 , 2.480	1.598671633
Nonane, 3,7-dimethyl-	340 , 1.920	0.719370337
Cyclodecane	340 , 2.130	0.222778415
o-Cymene	340 , 2.840	0.068717891
Indane	340 , 3.290	0.504180029
Benzene, 3-butenyl-	350 , 2.950	0.105534983
Benzene, 1-methyl-2-(2-propenyl)-	350 , 2.970	0.02612465
Cyclohexene, 1,5,5-trimethyl-3-methylene-	355 , 2.550	0.162175993
1-Propyne, 3-phenyl-	355 , 3.560	0.081957299
Decane, 5-methyl-	360 , 1.980	0.042972785
Benzene, 1-methyl-3-propyl-	360 , 2.790	0.199627326
Thiophene, 2-methyl-5-propyl-	360 , 2.930	0.058547623
Thiophene, 2,5-diethyl-	360 , 2.980	0.035731621
2,2'-Bifuran, octahydro-	365 , 1.970	0.197202984
Thiophene, 2-(4-methylbenzylsulfonyl)-	365 , 2.810	0.402430301
Benzene, (2-methylpropyl)-	365 , 2.850	0.316725535
Thiophene, 2,5-diethyl-	370 , 3.030	0.045399349
Decane, 2-methyl-	375 , 1.940	1.29963927
Cyclohexane, 1-ethyl-2-propyl-	375 , 2.160	0.077808245
Spiro[4.5]decane	375 , 2.500	0.04584354
Decane, 3-methyl-	380 , 1.990	0.268552493
Benzene, 1-methyl-4-propyl-	380 , 2.920	0.419518685
2-Decene, 3-methyl-, (Z)-	385 , 2.120	0.080689188
Cyclohexene, 4-methyl-1-(1-methylethenyl)-	385 , 2.660	0.106004365
Thiophene, 2,5-diethyl-	385 , 3.120	0.03008032
Heptane, 2,5-dimethyl-	390 , 1.920	0.052115561
Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-, [1R-(1à,2á,5à)]-	395 , 2.310	0.355264561
Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-, [1R-(1à,2à,5à)]-	395 , 2.350	0.040803696
Benzene, 1-methyl-3-(1-methylethyl)-	395 , 3.020	1.030081328
(E)-1-Phenyl-1-butene	400 , 3.230	0.150519964
Cyclohexane, 1-isopropyl-1-methyl-	405 , 2.200	0.306873129
Cyclohexene, 1-methyl-4-(1-methylethylidene)-	405 , 2.790	0.167835815
Benzene, 4-ethyl-1,2-dimethyl-	405 , 3.040	0.489993334
(E)-1-Phenyl-1-butene	405 , 3.350	0.786585611
1-Undecene	410 , 2.130	0.418395983
o-Cymene	410 , 3.160	0.108628389

Octane, 6-ethyl-2-methyl-	415 , 2.020	0.03610283
3-Undecyne	415 , 2.390	0.434484659
Undecane	420 , 2.060	0.049426335
Cyclopentane, (2-methylpropyl)-	425 , 2.250	0.10850669
Benzene, 1-methyl-4-(2-methylpropyl)-	425 , 2.870	0.424169168
Benzene, 1,3-diethyl-5-methyl-	425 , 2.950	0.212912302
1-Propanone, 1-(5-methyl-2-thienyl)-	425 , 3.070	0.062107819
Sulfurous acid, 2-ethylhexyl isobutyl ester	430 , 2.050	0.933646702
Benzene, 1-methyl-3-(1-methylethyl)-	430 , 3.280	0.196079355
Benzonitrile, 2-methyl-	430 , 4.540	0.139452979
3-Hexen-1-ol, formate, (Z)-	435 , 2.410	0.140827229
p-Menth-8-ene, 3-methylene-	435 , 2.590	0.089226063
Cyclohexene, 3-methyl-6-(1-methylethylidene)-	435 , 2.800	0.015031176
1-Ethanone, 1-[3-methoxy-4-[(4-methylphenyl)methoxy]phenyl]-	435 , 2.890	0.115088236
Benzene, 1-methyl-4-(1-methylpropyl)-	435 , 2.970	0.12726644
Benzene, 1,3-dimethyl-5-(1-methylethyl)-	440 , 2.970	0.119159492
Cyclopropane, 2-bromo-1-methyl-1-phenyl-	440 , 3.090	0.060108959
2,6-Dimethyldecane	445 , 2.000	0.625796279
Benzene, 1-methyl-3-(1-methyl-2-propenyl)-	445 , 3.150	0.044865691
Benzene, 1,2,3,4-tetramethyl-	445 , 3.230	0.061676224
Benzene, 1-methyl-2-(2-propenyl)-	445 , 3.430	0.016353191
Undecane, 4,7-dimethyl-	450 , 2.050	0.06689982
cis-Decalin, 2-syn-methyl-	450 , 2.550	0.04692049
Naphthalene, decahydro-2-methyl-	450 , 2.580	0.17093589
Benzene, 1,2,3,4-tetramethyl-	450 , 3.300	0.593019879
Benzene, pentyl-	455 , 2.930	0.061497102
Decane, 3,7-dimethyl-	460 , 2.030	0.293479791
(E)-1-Phenyl-1-butene	460 , 3.400	0.040045163
Undecane, 3-methyl-	470 , 2.050	0.13142846
Naphthalene, decahydro-2-methyl-	470 , 2.690	0.041817296
3,4-Dimethylcumene	470 , 3.120	0.285629207
2,4-Dimethylstyrene	470 , 3.420	0.026608295
Benzene, 1-methyl-4-(1-methylpropyl)-	475 , 3.030	0.113008615
Decane, 2,6,8-trimethyl-	480 , 2.080	0.05621312
Cyclopentane, hexyl-	480 , 2.330	0.103575393
2,4,6-Octatriene, 2,6-dimethyl-, (E,E)-	480 , 2.880	0.043928963
1H-Indene, 2,3-dihydro-5-methyl-	480 , 3.630	0.495583138
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	485 , 3.070	0.372549293
4-Undecene, 5-methyl-, (Z)-	490 , 2.230	0.046900856
Benzene, 4-pentenyl-	495 , 3.260	0.038425293
Benzene, 1,2,3,4-tetramethyl-	495 , 3.560	0.281577586
1H-Indene, 2,3-dihydro-4-methyl-	495 , 3.750	0.663035704

Cycloprop[a]indene, 1,1a,6,6a-tetrahydro-	495 , 3.980	0.142583061
Octane, 4-ethyl-	500 , 2.080	0.933008386
Benzene, 1-methyl-4-(2-methylpropyl)-	500 , 3.060	0.119830224
Benzene, pentyl-	505 , 3.090	0.288941375
1H-Indene, 1-methyl-	505 , 4.020	0.09277144
1-Hexene, 3-methyl-6-phenyl-4-(1-phenylethoxy)-	510 , 3.050	0.087883117
Benzene, (1,1-dimethylpropyl)-	510 , 3.140	0.277818264
Benzene, 2,4-dimethyl-1-(1-methylethyl)-	510 , 3.220	0.071038872
Benzene, 1-methyl-2-(1-methyl-2-propenyl)-	510 , 3.470	0.034763404
Undecane, 2-methyl-	515 , 2.090	0.392299859
Benzene, 1-methyl-4-(1-methylpropyl)-	515 , 3.210	0.266032201
Naphthalene, 1,2,3,4-tetrahydro-	515 , 3.960	0.284625239
(3-Methylphenyl) methanol, 1-methylpropyl ether	520 , 3.180	0.260188997
Undecane, 3-methyl-	525 , 2.110	0.14740896
Benzene, 1-methyl-4-(1-methylpropyl)-	530 , 3.240	0.232456702
Benzene, 2-ethenyl-1,3,5-trimethyl-	535 , 3.450	0.115651162
Decane, 2,3,7-trimethyl-	540 , 2.140	0.076898005
4-Dodecene, (E)-	540 , 2.360	0.067865259
Benzeneacetaldehyde, à,2,5-trimethyl-	540 , 3.060	0.049544884
1H-Indene, 2,3-dimethyl-	540 , 3.810	0.040989301
Benzene, pentamethyl-	545 , 3.450	0.05921428
2,2-Dimethylindene, 2,3-dihydro-	545 , 3.500	0.141458506
Cyclohexane, 1-methyl-3-pentyl-	550 , 2.370	0.15710188
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	550 , 3.110	0.15731527
1H-Indene, 2,3-dihydro-1,6-dimethyl-	550 , 3.590	0.889712923
Naphthalene	550 , 4.690	0.297960229
1-Dodecene	555 , 2.280	0.296596166
Thiophene, 2-ethyl-5-(2-methylpropyl)-	555 , 3.220	0.028598263
1,3-Benzenediol, o-(2-methylbenzoyl)-o'-(3-cyclopentylpropionyl)-	555 , 3.410	0.07643418
Benzene, (1-methylpentyl)-	560 , 3.130	0.157356206
trans-1-Phenyl-1-pentene	560 , 3.620	0.198175277
Benzene, pentamethyl-	565 , 3.420	0.050911725
1H-Indene, 2,3-dihydro-1,6-dimethyl-	565 , 3.690	0.718488809
Dodecane	570 , 2.210	0.183738887
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	570 , 3.090	0.41054188
m-Ethylbenzonitrile	570 , 4.740	0.030877937
Cyclopropane, 1-ethyl-2-heptyl-	575 , 2.300	0.094633226
Benzene, 1-(1-methylethenyl)-3-(1-methylethyl)-	575 , 3.380	0.025972943
Benzene, (1,3-dimethylbutyl)-	580 , 3.140	0.089170122
Thiophene, 2-ethyl-5-(2-methylpropyl)-	580 , 3.280	0.042819782
Benzene, 1-ethyl-2,4,5-trimethyl-	580 , 3.490	0.102767218
Undecane, 2,6-dimethyl-	585 , 2.130	1.186754577

Benzene, 1,2,4-triethyl-	585 , 3.200	0.116765159
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	585 , 3.490	0.075128281
Benzene, 1-ethyl-4-(1-methylethyl)-	595 , 3.570	0.039800469
Naphthalene, 1,2,3,4-tetrahydro-2-methyl-	595 , 3.870	0.127809731
Tetradecane	600 , 2.130	0.095135766
Benzene, (2-methylpentyl)-	600 , 3.100	0.030943325
Cyclohexane, 2-butyl-1,1,3-trimethyl-	605 , 2.450	0.363676404
Cyclohexane, 1-methyl-3-pentyl-	605 , 2.510	0.057375463
1H-Indene, 2,3-dihydro-1,4,7-trimethyl-	605 , 3.460	0.129264187
Benzene, cyclopentyl-	605 , 3.900	0.249676232
Dodecane, 2-methyl-	610 , 2.140	0.075708433
Naphthalene, 1-ethyl-1,2,3,4-tetrahydro-	615 , 3.510	0.030045866
Dodecane, 3-methyl-	620 , 2.150	0.035902592
1-Decene	620 , 2.310	0.047166481
Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	620 , 3.240	0.073408939
Benzene, (1-ethyl-1-propenyl)-	620 , 3.850	0.183403984
Cyclohexane, hexyl-	630 , 2.510	0.26377846
Naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl-	630 , 3.460	0.384584311
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-	635 , 3.540	0.178801292
Cyclopentane, 2-ethylidene-1,1-dimethyl-	640 , 2.610	0.084652267
Cyclooctane, phenyl-	640 , 3.700	0.003969007
Cyclopentane, 1-ethyl-3-methyl-, trans-	645 , 2.370	0.090532518
1H-Indene, 2,3-dihydro-4,7-dimethyl-	645 , 3.870	0.242109612
Undecane, 2,4-dimethyl-	650 , 2.180	0.279446285
Cyclohexane, 1-ethyl-1,3-dimethyl-, trans-	650 , 2.480	0.037933867
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	655 , 3.290	0.069947288
1H-Indene, 1,3-dimethyl-	655 , 4.090	0.199307982
Benzene, hexyl-	660 , 3.200	0.273639201
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	660 , 3.630	0.145608116
1H-Indene, 1,3-dimethyl-	660 , 4.240	0.347200774
Dodecane, 2-methyl-	665 , 2.190	0.169188022
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	665 , 3.350	0.041276598
Benzene, 1-(1-methylethenyl)-3-(1-methylethyl)-	665 , 3.700	0.071590498
1H-Indene, 2,3-dihydro-4,7-dimethyl-	665 , 3.950	0.192338186
Cyclohexane, 1-isopropyl-1-methyl-	670 , 2.440	0.060846561
Benzene, (1-methylpentyl)-	670 , 3.300	0.113924967
Benzene, 4-hexenyl-	670 , 3.470	0.06290877
Naphthalene, 1,2,3,4-tetrahydro-5-methyl-	670 , 4.090	0.234950691
Tridecane, 7-methyl-	675 , 2.160	0.021043128
Tridecane, 4-methyl-	675 , 2.210	0.204091278
1H-Indene, 2,3-dimethyl-	675 , 4.240	0.312672432
1-Pentanol, 2,2,4-trimethyl-	680 , 2.240	0.04142034

2-Pentene, 2,4,4-trimethyl-	680 , 2.350	0.387147207
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1à,3à,6à)]-	680 , 2.620	0.195616271
Benzene, 4-hexenyl-	680 , 3.500	0.038472157
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	680 , 3.690	0.117854705
(1-Methylpenta-1,3-dienyl)benzene	680 , 3.910	0.034688199
Decane, 2,6,8-trimethyl-	685 , 2.170	0.036618521
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	685 , 3.360	0.089425745
Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	685 , 3.820	0.215864745
Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	690 , 3.440	0.102914108
Benzene, (3-methylcyclopentyl)-	690 , 3.690	0.153703764
Benzene, pentamethyl-	690 , 3.820	0.01597661
Cyclohexane, 1-ethyl-1,4-dimethyl-, cis-	695 , 2.390	0.028739782
Cyclotridecane	695 , 2.440	0.043407529
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	695 , 3.440	0.077251061
1H-Indene, 2,3-dihydro-4,7-dimethyl-	695 , 4.080	0.349952423
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-	700 , 3.690	0.091453501
Cyclotridecane	705 , 2.420	0.226559225
Propanedinitrile, (2,3-dihydro-1-methyl-1H-inden-1-yl)-	705 , 3.710	0.099786989
3-Penten-2-one, 5-phenyl-	705 , 3.720	0.066943165
Cyclopentane, 1-hydroxymethyl-1,3-dimethyl-	710 , 2.440	0.09141701
Benzene, (1-methylhexyl)-	710 , 3.180	0.095561804
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	710 , 3.780	0.413003268
Succinic acid, 2-chloro-6-fluorophenyl 3-phenylprop-2-en-1-yl ester	710 , 3.800	0.058343866
Naphthalene, 1,2,3,4-tetrahydro-5-methyl-	710 , 4.350	0.062362515
Cyclopentane, 1-hexyl-3-methyl-	715 , 2.400	0.068556367
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	720 , 3.900	0.099834965
Benzene, 1-cyclopenten-1-yl-	720 , 4.410	0.059897978
Naphthalene, 1-methyl-	720 , 4.760	0.273069607
3-Methylbenzothiophene	720 , 4.970	0.023512111
Tridecane	725 , 2.230	2.638147469
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	725 , 3.490	0.048799133
Naphthalene, 1-ethyl-1,2,3,4-tetrahydro-	725 , 3.830	0.255780615
Cyclooctane, 1,4-dimethyl-, cis-	730 , 2.370	0.126493459
1,2,3-Trimethylindene	730 , 4.120	0.086584998
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	740 , 3.590	0.077018407
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	740 , 3.820	0.114951534
Naphthalene, 1-methyl-	745 , 0.060	0.317321433
3-Methylbenzothiophene	745 , 0.280	0.041362176
Dodecane	745 , 2.220	0.457722809
4-(1,2-Dimethyl-cyclopent-2-enyl)-butan-2-one	750 , 2.740	0.091792664
(1-Methylpenta-2,4-dienyl)benzene	750 , 4.140	0.059743678
Decane	755 , 2.210	0.047606411

Naphthalene, 1,2,3,4-tetrahydro-2,7-dimethyl-	755 , 3.880	0.197920395
Benzene, cyclohexyl-	755 , 3.980	0.104488596
1,3-Dimethyl-(3,7-dimethyloctyl)cyclohexane	760 , 2.400	0.08279715
Naphthalene, 1-ethyl-1,2,3,4-tetrahydro-	760 , 3.870	0.112203033
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	760 , 4.000	0.730276354
Decane, 2,3,5,8-tetramethyl-	765 , 2.200	0.028434517
Naphthalene, 1-ethyl-1,2,3,4-tetrahydro-	765 , 3.920	0.06757685
1-(3-Methylphenyl)4-methyl-3-pentene	770 , 3.510	0.034590951
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	770 , 3.660	0.042429309
Naphthalene, 2-ethyl-1,2,3,4-tetrahydro-	770 , 3.990	0.028173152
Dodecane, 2,7,10-trimethyl-	775 , 2.210	0.0813288
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	775 , 3.760	0.080367622
Benzene, 3-cyclohexen-1-yl-	775 , 4.260	0.188811332
1,4-Ethanonaphthalene, 1,2,3,4-tetrahydro-	775 , 4.300	0.089012488
Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	780 , 4.000	0.057671096
Cyclohexane, (1-methylethyl)-	790 , 2.590	0.223444331
Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	790 , 4.020	0.140030353
Naphthalene, 1,2,3,4-tetrahydro-1,4-dimethyl-	790 , 4.140	0.147715708
Decane, 2-methyl-	795 , 2.260	0.330873886
2-Pentene, 2,4,4-trimethyl-	795 , 2.450	0.728626846
1,2,3-Trimethylindene	795 , 4.280	0.100624246
Tridecane, 5-methyl-	800 , 2.250	0.137436337
2,2,4,4-Tetramethyloctane	800 , 2.300	0.074039476
Benzene, 1-methyl-3-hexyl-	800 , 3.270	0.075144396
Naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl-	800 , 4.340	0.048008184
Tridecane, 4-methyl-	810 , 2.250	0.305979375
Propanedinitrile, (2,3-dihydro-1-methyl-1H-inden-1-yl)-	810 , 3.770	0.058314228
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	810 , 3.890	0.060946587
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	810 , 4.210	0.031376772
Benzene, (1-methylhexyl)-	815 , 3.260	0.037951464
Tridecane, 2-methyl-	820 , 2.240	0.555226975
Benzene, heptyl-	820 , 3.240	0.207135597
p-Menthane, 2,3-dibromo-8-phenyl-	820 , 3.340	0.139081029
Naphthalene, 1,2,3,4-tetrahydro-1,4-dimethyl-	820 , 4.160	0.086405136
5-Methyl-1-heptanol	825 , 2.460	0.135875741
1-Methyl-2-n-hexylbenzene	825 , 3.340	0.194965729
Naphthalene, 1,2,3,4-tetrahydro-1,6,8-trimethyl-	830 , 3.800	0.30826831
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	830 , 4.370	0.036325481
Farnesan	835 , 2.220	0.385001828
1,2,3-Trimethylindene	835 , 4.240	0.396016763
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	840 , 3.890	0.205171006
1,2,3-Trimethylindene	840 , 4.380	0.183106869

(1,4-Dimethylpent-2-enyl)benzene	845 , 3.760	0.12180241
Benzene, 2-heptenyl-	845 , 3.800	0.034752845
3-Ethyl-3-phenyl-1-pentene	845 , 3.860	0.114525125
Biphenyl	850 , 0.100	0.168329649
Disulfide, bis(1,1,3,3-tetramethylbutyl)	850 , 2.510	0.668425455
Cyclohexane, 1,1,3-trimethyl-2-(3-methylpentyl)-	850 , 2.590	0.028997072
1-Nonylcycloheptane	850 , 2.610	0.034388861
1H-Inden-1-one, 2,3-dihydro-3,3,4,5-tetramethyl-	850 , 3.630	0.061413747
1-Dodecene	860 , 2.430	0.175734374
2-Hexanone, 5-methyl-5-phenyl-	860 , 3.210	0.333693887
Benzene, 2-heptenyl-	860 , 3.750	0.133202816
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	860 , 3.950	0.143515529
Naphthalene, 1,2,3,4-tetrahydro-5,7-dimethyl-	860 , 4.340	0.045850764
Benzo[b]thiophene, 2,7-dimethyl-	860 , 4.940	0.093609809
Cyclopentane, 1-hydroxymethyl-1,3-dimethyl-	865 , 2.510	0.202239865
1-Naphthalenemethanol, 1,2,3,4-tetrahydro-8-methyl-	865 , 3.790	0.057445481
Naphthalene, 1-ethyl-	865 , 4.800	0.152753144
1,2,3-Trimethylindene	870 , 4.420	0.093777631
1,1'-Biphenyl, 2-methyl-	870 , 4.790	0.026345263
Naphthalene, 1-ethyl-	875 , 0.000	0.09998167
Tetradecane	875 , 2.330	0.038355089
Propanedinitrile, (2,3-dihydro-1-methyl-1H-inden-1-yl)-	875 , 3.790	0.095649049
Cyclopentane, 1,1'-ethylidenebis-	880 , 2.590	0.091341805
Naphthalene, 1,2-dihydro-1,5,8-trimethyl-	880 , 4.120	0.172600216
Naphthalene, 1,5-dimethyl-	885 , 4.740	0.252370459
Dodecane, 2,6,10-trimethyl-	895 , 2.250	0.38722056
Benzo[b]thiophene, 2,7-dimethyl-	900 , 0.090	0.029604269
1, 1, 5-Trimethyl-1, 2-dihydronaphthalene	900 , 4.280	0.047866295
Tetradecane, 4-methyl-	905 , 2.250	0.075566359
Naphthalene, 1,2,3,4-tetrahydro-1-methyl-8-(1-methylethyl)-	905 , 3.700	0.154507124
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	905 , 3.940	0.075414652
Benzene, 1-cyclohexyl-3-methyl-	905 , 3.960	0.04273087
Naphthalene, 1,2,3,4-tetrahydro-6,7-dimethyl-	905 , 4.540	0.027298847
1,2,3,6,7,8-Hexahydro-as-indacene	905 , 4.640	0.078857224
1H-Indene, 2,3-dihydro-1,1,2,3,3-pentamethyl-	910 , 3.790	0.062820969
Naphthalene, 1,2,3,4-tetrahydro-6,7-dimethyl-	910 , 4.590	0.042398004
Naphthalene, 2,6-dimethyl-	910 , 4.960	0.638070063
Undecane, 3,8-dimethyl-	915 , 2.250	0.128014229
1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	915 , 3.010	0.05356835
aR-Himachalene	915 , 3.540	0.037553211
Naphthalene, 1,2,3,4-tetrahydro-6-propyl-	915 , 3.980	0.052342657
Disulfide, bis(1,1,3,3-tetramethylbutyl)	920 , 2.390	0.579709526

Naphthalene, 1,2,3,4-tetrahydro-1-propyl-	920 , 3.870	0.084022842
3-Ethyl-3-phenyl-1-pentene	920 , 4.030	0.138093547
1,5,9-Decatriene, 2,3,5,8-tetramethyl-	925 , 2.830	0.261790714
Naphthalene, 1,2-dihydro-2,5,8-trimethyl-	925 , 4.180	0.102698496
Fumaric acid, octyl 3-phenylpropyl ester	930 , 3.490	0.018992218
1H-Indene, 1-methyl-3-propyl-	935 , 4.380	0.028150368
Naphthalene, 1,2,3,4-tetrahydro-2,5,8-trimethyl-	940 , 4.040	0.192598995
Tetradecane	945 , 2.290	0.073038472
Cyclohexane, octyl-	945 , 2.650	0.287412825
1,5,9-Decatriene, 2,3,5,8-tetramethyl-	945 , 2.830	0.409090942
Benzene, 1-(1,5-dimethylhexyl)-4-methyl-	945 , 3.130	0.53417403
(1R,4R,4aS,8aR)-4,7-Dimethyl-1-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,8a-octahydronaphthalene	950 , 3.290	0.378211523
Naphthalene, 1,2-dimethyl-	960 , 0.250	0.075781601
1,5,9-Undecatriene, 2,6,10-trimethyl-, (Z)-	960 , 2.850	0.370918494
Naphthalene, 1,2-dihydro-2,5,8-trimethyl-	960 , 4.310	0.041779138
Heptadecane, 2,6,10,14-tetramethyl-	965 , 2.220	0.986058081
Tetradecane, 2-methyl-	970 , 2.270	0.454469916
Benzene, octyl-	970 , 3.300	0.196917724
1H-Indene, 3-ethenyl-2,3-dihydro-1,1-dimethyl-	975 , 4.420	0.305673739
Tetradecane, 3-methyl-	980 , 2.290	0.043940447
Decane, 3,7-dimethyl-	990 , 2.270	0.195823733
Naphthalene, 1,2-dihydro-1,4,6-trimethyl-	990 , 4.280	0.029481273
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	995 , 3.430	0.031713898
1,2,3,4-Tetrahydro-3-isopropyl-5-methylnaphthalene	995 , 3.760	0.064758331
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	1000 , 4.460	0.034995131
1,1'-Biphenyl, 4-methyl-	1005 , 0.010	0.183076305
Acenaphthene	1005 , 0.730	0.0636134
Pentadecane	1005 , 2.270	0.078048123
Naphthalene, 1-propyl-	1005 , 4.680	0.079551481
3-Hexadecene, (Z)-	1010 , 2.430	0.161762366
2,2'-Dimethylbiphenyl	1010 , 4.710	0.01809865
Cyclopentadecane	1015 , 2.500	0.241327369
Phenol, o-[(à-methylbenzyl)sulfonyl]-	1015 , 3.210	0.129286415
Naphthalene, 2-(1-methylethyl)-	1015 , 4.790	0.037819763
1,1'-Biphenyl, 4-methyl-	1020 , 0.050	0.115767489
Pentadecane	1020 , 2.360	0.048032449
Pentadecane	1025 , 2.350	1.556702074
4,6,8-Trimethylazulene	1025 , 4.750	0.043239522
Oxalic acid, di(cyclohexylmethyl) ester	1030 , 2.550	0.073317434
Benzo[b]thiophene, 2-ethyl-7-methyl-	1030 , 4.970	0.083853539
Naphthalene, 1,4,5-trimethyl-	1035 , 4.780	0.01983355
1-Isopropenylnaphthalene	1040 , 0.400	0.047956689

Heptadecane	1040 , 2.280	0.181502002
Naphthalene, 3-(1,1-dimethylethyl)-1,2-dihydro-	1040 , 4.230	0.120513552
Naphthalene, 1,2-dihydro-1,4,6-trimethyl-	1040 , 4.470	0.036160623
Naphthalene, 2-(1-methylethyl)-	1040 , 4.930	0.044201071
1,1,4,5,6-Pentamethyl-2,3-dihydro-1H-indene	1045 , 4.320	0.034729876
Benzene, (3-cyclopentylpropyl)-	1050 , 3.810	0.076695174
Bibenzyl	1050 , 4.990	0.093809491
7-Octadecyne, 2-methyl-	1055 , 2.870	0.355653367
Naphthalene, 1,4,5-trimethyl-	1055 , 4.860	0.109245033
Heptadecane	1060 , 2.290	0.064433801
Cadina-1(10),6,8-triene	1060 , 3.690	0.03011996
Naphthalene, 1,2,3,4-tetrahydro-5-methyl-1-(1-methylethyl)-	1065 , 3.950	0.07394371
Naphthalene, 1,4,5-trimethyl-	1065 , 4.850	0.608572119
Pentadecane, 3-methyl-	1070 , 2.300	0.024516078
2-Ethyl-3-methylene-indan-1-one	1070 , 4.630	0.027057302
Benzo[b]thiophene, 2,5,7-trimethyl-	1080 , 0.130	0.022373478
Decane, 5-propyl-	1085 , 2.320	0.633115797
Naphthalene, 1,4,5-trimethyl-	1090 , 0.000	0.189510035
Cyclopentane, decyl-	1095 , 2.630	0.075348709
n-Nonylcyclohexane	1095 , 2.690	0.158938289
p-Menthane, 2,3-dibromo-8-phenyl-	1095 , 3.200	0.257107631
Naphthalene, 1,4,6-trimethyl-	1095 , 4.870	0.117226206
Pentadecane, 2-methyl-	1110 , 2.320	0.613688835
Naphthalene, 1,4,5-trimethyl-	1115 , 0.050	0.152449731
Naphthalene, 1-methyl-7-(1-methylethyl)-	1115 , 4.470	0.034374412
Pentadecane, 3-methyl-	1120 , 2.350	0.15277389
Hexane, 2-phenyl-3-propyl-	1125 , 3.360	0.045030919
3,6-Dihydrochamazulene	1125 , 4.480	0.084587435
4-Ethylbiphenyl	1125 , 4.940	0.076223939
Benzo[b]thiophene, 2-ethyl-5,7-dimethyl-	1140 , 4.900	0.160701901
Fluorene	1145 , 0.830	0.043617584
Pentadecane, 2,6,10-trimethyl-	1145 , 2.300	0.138918949
Sulfurous acid, cyclohexylmethyl hexyl ester	1145 , 2.580	0.579340726
Benzene, [(tetramethylcyclopropylidene)methyl]-	1145 , 4.590	0.074403831
Naphthalene, 2-butyl-	1145 , 4.760	0.041429602
Naphthalene, 1,4,6-trimethyl-	1150 , 0.290	0.057942093
Cetene	1150 , 2.480	0.058223278
1,1'-Biphenyl, 3,4'-dimethyl-	1150 , 4.880	0.059507135
4-Ethylbiphenyl	1155 , 4.990	0.069905981
1,1'-Biphenyl, 2-methyl-	1160 , 0.990	0.037784939
1,1'-Biphenyl, 4-methyl-	1165 , 0.740	0.040216875
Heptadecane	1165 , 2.330	0.800375534

Hexadecane	1165 , 2.360	0.02024903
4,4'-Dimethylbiphenyl	1165 , 4.920	0.059024971
1,1'-Biphenyl, 4-methyl-	1170 , 0.720	0.113489112
1-Nonadecene	1170 , 2.510	0.09805746
Chamazulene	1170 , 4.760	0.070601905
Oxalic acid, di(cyclohexylmethyl) ester	1175 , 2.590	0.047591963
1,4,6,7-Tetramethyl1,2,3,4-tetrahydronaphthalene	1175 , 4.390	0.06556947
1,1'-Biphenyl, 2-methyl-	1180 , 0.710	0.047983177
Cyclohexane, 1-methyl-2-pentyl-	1180 , 2.640	0.126211162
Naphthalene, 2-methyl-1-propyl-	1185 , 4.740	0.035558428
Naphthalene, 1-methyl-7-(1-methylethyl)-	1185 , 4.890	0.163616186
1,1'-Biphenyl, 2-ethyl-	1190 , 0.310	0.075984432
Hexadecane	1190 , 2.310	0.155261767
Diphenylamine	1195 , 1.250	0.043563681
1,4,5,8-Tetramethylnaphthalene	1195 , 4.730	0.174409766
4,4'-Dimethylbiphenyl	1205 , 0.140	0.094559873
4-Ethylbiphenyl	1210 , 0.380	0.060765243
Pentadecane, 2-methyl-2-phenyl-	1210 , 3.190	0.229731355
1H-Indene, 5-hexyl-2,3-dihydro-	1210 , 3.850	0.044109195
Cyclohexane, 1-methyl-2-pentyl-	1215 , 2.710	0.054023099
Phenol, 2-methyl-4-(1,1,3,3-tetramethylbutyl)-	1215 , 4.170	0.024554792
Nor-pristane	1225 , 2.290	0.677833856
1,1'-Biphenyl, 2-ethyl-	1230 , 0.400	0.072812116
Tetradecane, 4-ethyl-	1230 , 2.350	0.116006256
Benzene, 1,1'-(1,3-propanediyl)bis-	1230 , 4.910	0.295126706
Hexadecane, 4-methyl-	1240 , 2.340	0.017829134
Cyclohexane, octyl-	1240 , 2.700	0.158949589
4-Ethylbiphenyl	1245 , 0.320	0.025869212
Nonadecane, 2-methyl-	1250 , 2.320	0.084289024
Benzene, 1,1'-propylidenebis-	1250 , 4.760	0.029316786
1,4,5,8-Tetramethylnaphthalene	1255 , 4.890	0.063581169
2,2,4,4-Tetramethyloctane	1260 , 2.500	0.061330577
Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	1260 , 4.720	0.108507061
1,4,5,8-Tetramethylnaphthalene	1280 , 0.070	0.094290543
4-Ethylbiphenyl	1280 , 0.580	0.025745105
Heptadecane	1280 , 2.320	0.068027339
3-Octadecene, (E)-	1285 , 2.500	0.063282757
Heptadecane	1295 , 2.420	0.027974396
9H-Fluorene, 3-methyl-	1300 , 0.700	0.031873569
9H-Fluorene, 2-methyl-	1305 , 0.860	0.082719537
Cyclohexane, 1-isopropyl-1-methyl-	1315 , 2.610	0.032135675
1,4,5,8-Tetramethylnaphthalene	1320 , 0.230	0.196626722

9H-Fluorene, 9,9-dimethyl-	1320 , 0.380	0.060250108
4,4'-Dimethylbiphenyl	1320 , 0.560	0.092285757
Octadecane, 2-methyl-	1325 , 2.340	0.073577873
1,1'-Biphenyl, 4-(1-methylethyl)-	1350 , 0.290	0.141646704
1,1'-Biphenyl, 4-(1-methylethyl)-	1360 , 0.360	0.02182111
Pentadecane, 2,6,10-trimethyl-	1360 , 2.360	0.248820821
Heptadecane, 4-methyl-	1370 , 2.370	0.020026564
1,1'-Biphenyl, 4-(1-methylethyl)-	1375 , 0.160	0.026507528
1-Docosene	1375 , 2.650	0.051062135
Cyclohexane, undecyl-	1375 , 2.730	0.126841143
Benzene, 1,2-dimethyl-4-(phenylmethyl)-	1380 , 0.220	0.037563585
Heptadecane, 2-methyl-	1380 , 2.350	0.062968971
Octadecane, 2-methyl-	1390 , 2.360	0.119853934
Phenanthrene	1405 , 1.740	0.037667686
Hexadecane	1405 , 2.350	0.048670766
Octadecane	1425 , 2.460	0.015554462
Heneicosane	1425 , 2.490	0.18010608
Phytan	1435 , 2.300	0.640490885
Oxalic acid, cyclohexylmethyl propyl ester	1435 , 2.630	0.099351875
9H-Fluorene, 9,9-dimethyl-	1445 , 0.570	0.041725605
Heptadecane	1450 , 2.370	0.032878834
Cyclohexane, 1-methyl-2-pentyl-	1450 , 2.700	0.10263422
9H-Fluorene, 2,3-dimethyl-	1455 , 0.660	0.074766148
9H-Fluorene, 2,3-dimethyl-	1460 , 0.730	0.03867295
Anthracene, 9,10-dihydro-9,10-dimethyl-	1465 , 0.450	0.054679939
Pentadecane, 2,6,10-trimethyl-	1465 , 2.340	0.134135284
Eicosane, 10-methyl-	1475 , 2.390	0.188599054
Heptadecane, 4-methyl-	1495 , 2.390	0.198349026
1-Eicosanol	1500 , 2.700	0.026589587
Cyclohexane, octyl-	1505 , 2.750	0.072807485
Nonadecane, 2-methyl-	1510 , 2.430	0.12882685
Heptadecane, 2,6,10,15-tetramethyl-	1535 , 2.320	0.160932147
Hexadecanenitrile	1545 , 3.570	0.042255004
Nonadecane	1550 , 2.430	0.814893242
Cyclohexane, 1-methyl-3-propyl-	1575 , 2.730	0.047481934
Nonadecane	1595 , 2.410	0.404283937
Heptadecane, 2-methyl-	1620 , 2.410	0.087395396
Cyclopentane, heneicosyl-	1625 , 2.700	0.024230818
1-Iodo-2-methylundecane	1630 , 2.430	0.146442039
Cyclohexane, octyl-	1630 , 2.760	0.043434203
4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	1640 , 4.530	0.052082033
Eicosane	1665 , 2.480	0.565287585

Hexadecane	1680 , 2.400	0.068758827
Cyclohexane, 1-methyl-2-propyl-	1695 , 2.750	0.044212
Heptadecane, 2,6-dimethyl-	1710 , 2.430	0.283020743
Nonadecane, 2-methyl-	1735 , 2.420	0.121710163
Cyclopentane, heneicosyl-	1740 , 2.730	0.018731779
Heptacosane	1745 , 2.390	0.188701303
Cyclohexane, undecyl-	1745 , 2.800	0.047178521
Disulfide, bis(1,1,3,3-tetramethylbutyl)	1760 , 2.660	0.034714687
Heneicosane	1775 , 2.510	0.497672762
Octadecanenitrile	1780 , 3.500	0.043655372
Fluoranthene	1795 , 2.770	0.027407024
Hexadecane, 2,6,10,14-tetramethyl-	1805 , 2.330	0.051432603
Sulfurous acid, butyl cyclohexylmethyl ester	1810 , 2.760	0.029052827
Nonadecane	1815 , 2.450	0.182425023
Phenanthrene, 2,3,5-trimethyl-	1835 , 1.140	0.038116508
Eicosane, 2-methyl-	1840 , 2.460	0.190533267
Nonadecane, 2-methyl-	1850 , 2.470	0.178263373
Docosane	1880 , 2.530	0.800544282
Retene	1895 , 1.030	0.042529706
Phytan	1910 , 2.400	0.060399962
Octacosane	1920 , 2.470	0.134863068
Octadecane, 2-methyl-	1945 , 2.470	0.209453058
Hexadecane, 3-methyl-	1955 , 2.500	0.10055571
Tricosane	1985 , 2.530	0.922169423
Octacosane	2020 , 2.490	0.0855099
Heptacosane	2045 , 2.490	0.152717764
Tetracosane	2080 , 2.570	0.459521245
Heptacosane	2115 , 2.510	0.114056298
Heptacosane	2140 , 2.510	0.076284881
Pentacosane	2175 , 2.600	0.394447646

Table S7 List of compounds identified in diesel

Compounds	**R.T. (s)**	**Area%**
Heptane, 2,4-dimethyl-	150 , 0.430	0.05828
Heptane, 2,6-dimethyl-	150 , 4.050	0.36885
Heptane, 2,5-dimethyl-	155 , 2.650	0.05334
Cyclopentane, propyl-	155 , 4.250	0.16588
Cyclohexane, ethyl-	160 , 1.630	0.0349
Cyclohexane, 1,1,3-trimethyl-	160 , 3.990	0.51128
Cyclohexane, 1,3,5-trimethyl-, (1à,3à,5á)-	170 , 3.380	0.02148
Hexane, 3-ethyl-	170 , 4.190	0.23781
Octane, 2-methyl-	175 , 1.560	0.0701

Octane, 3-methyl-	175 , 4.780	1.37332
Benzene, 1,3-dimethyl-	200 , 2.230	0.01718
Benzene, (1-methylethyl)-	220 , 3.690	0.03884
Benzene, (1-methylethyl)-	225 , 2.280	0.04481
Octane, 3,6-dimethyl-	230 , 1.700	0.12789
Cyclopentane, butyl-	230 , 1.850	0.17372
Cyclooctane, 1,2-dimethyl-	240 , 1.800	0.13612
Benzene, propyl-	250 , 2.400	0.21379
Nonane, 2-methyl-	255 , 1.760	0.15904
Benzene, 1-ethyl-2-methyl-	260 , 2.460	2.43994
Nonane, 3-methyl-	265 , 1.770	0.3199
Cyclopentane, 1-methyl-3-(1-methylethyl)-	270 , 1.930	0.52269
Cyclohexene, 1-ethyl-	270 , 2.000	0.15493
Benzene, 1-ethyl-2-methyl-	275 , 2.640	0.70276
Cyclodecane	280 , 1.930	0.14467
1-Methyl-4-(1-methylethyl)-cyclohexane	280 , 1.970	0.62768
Octane, 2,3,7-trimethyl-	290 , 1.790	0.02597
Benzene, 1,2,3-trimethyl-	290 , 2.690	0.09731
Decane	295 , 1.890	0.08756
Cyclohexane, 1,2-diethyl-, cis-	295 , 2.060	0.08651
Cyclohexane, 1-methyl-2-propyl-	300 , 2.030	0.15802
Benzene, (2-methylpropyl)-	305 , 2.580	0.09376
Hexane, 3,3,4,4-tetramethyl-	310 , 1.840	0.05743
Cyclohexene,3-butyl-	310 , 2.210	0.04398
Benzene, (1-methylpropyl)-	310 , 2.600	0.24852
Decane	315 , 1.850	1.3622
Cyclodecane	315 , 2.070	0.11046
Benzene, 1-methyl-3-(1-methylethyl)-	320 , 2.690	0.46264
Dodecane, 2,7,10-trimethyl-	325 , 1.890	0.37718
Cyclohexane, 1-methyl-2-propyl-	325 , 2.150	0.09419
Benzene, 1,2,3-trimethyl-	325 , 2.950	0.69259
n-Tridecan-1-ol	330 , 1.970	0.10975
Nonane, 3,7-dimethyl-	340 , 1.910	0.5353
Cyclopentane, pentyl-	340 , 2.140	0.17524
Benzene, 1-methyl-3-(1-methylethyl)-	340 , 2.830	0.04804
Indane	340 , 3.280	0.28895
Cyclohexane, 1,2-diethyl-3-methyl-	350 , 2.080	0.07886
1H-Indene, octahydro-5-methyl-	350 , 2.400	0.22033
Octane, 4-ethyl-	360 , 1.970	0.02701
Heptane, 2,5-dimethyl-	365 , 1.940	0.37869
Benzeneacetaldehyde, à-methyl-	365 , 2.790	1.29748
Benzene, (2-methylpropyl)-	365 , 2.810	0.14344

Benzene, 1-methyl-3-(1-methylethyl)-	365 , 2.910	0.5782
Cyclooctane, ethyl-	370 , 2.140	0.15493
Naphthalene, decahydro-, trans-	375 , 2.520	0.16694
Decane, 3-methyl-	380 , 1.990	0.11209
Benzene, 1-methyl-4-propyl-	380 , 2.920	0.81728
Cyclohexane, 1-ethyl-2-propyl-	385 , 2.190	0.34363
Benzene, 4-ethyl-1,2-dimethyl-	390 , 3.010	1.15961
Cyclopentane, 1,2-dibutyl-	400 , 2.170	0.10169
2,6-Dimethylbicyclo[3.2.1]octane	400 , 2.360	0.06138
(E)-1-Phenyl-1-butene	400 , 3.230	0.15306
3-Undecene, (Z)-	405 , 2.150	0.31517
Benzene, 4-ethyl-1,2-dimethyl-	405 , 3.030	0.65109
(E)-1-Phenyl-1-butene	405 , 3.340	0.37897
Cyclohexane, 1-methyl-2-pentyl-	410 , 2.190	1.4165
Benzene, 2-ethyl-1,3-dimethyl-	410 , 3.170	0.10989
Undecane	420 , 2.050	0.03421
Benzene, 1-methyl-2-(1-methyl-2-propenyl)-	420 , 3.070	0.01272
Benzene, 1-methyl-4-(2-methylpropyl)-	425 , 2.880	0.334
Benzene, 1,3-diethyl-5-methyl-	425 , 2.960	0.50927
cis-Decalin, 2-syn-methyl-	430 , 2.460	0.30033
1H-Indene, 2,3-dihydro-1,1-dimethyl-	430 , 3.200	0.04773
o-Cymene	430 , 3.280	0.3511
Cyclopentane, 1,2-dibutyl-	435 , 2.260	0.08218
Cyclohexane, 1-ethyl-4-methyl-, cis-	435 , 2.280	0.06632
Naphthalene, decahydro-, cis-	435 , 2.770	0.01811
Benzene, (1-methylbutyl)-	435 , 2.890	0.07001
Naphthalene, decahydro-2-methyl-	440 , 2.540	0.08544
Benzene, 1-methyl-4-(1-methylpropyl)-	440 , 2.910	0.219
3,4-Dimethylcumene	440 , 2.970	0.08861
Dodecane	445 , 2.000	2.38515
Benzene, 1-ethyl-4-(1-methylethyl)-	445 , 2.990	0.08666
Naphthalene, decahydro-2-methyl-	450 , 2.570	0.16112
Benzene, 1,2,3,4-tetramethyl-	450 , 3.190	0.04735
Benzene, (3-methylbutyl)-	455 , 2.930	0.10188
Benzene, 1,2,3,4-tetramethyl-	455 , 3.240	0.37176
Decane, 3,7-dimethyl-	460 , 2.040	0.31412
Heptane, 3,3-dimethyl-	460 , 2.070	0.02087
3,4-Dimethylcumene	460 , 3.080	0.02543
1H-Indene, 2,3-dihydro-1,3-dimethyl-	460 , 3.300	0.0384
Undecane, 3-methyl-	470 , 2.050	0.4275
Naphthalene, decahydro-2-methyl-	470 , 2.690	0.11996
Benzene, 2,4-diethyl-1-methyl-	470 , 3.110	0.0495

Cyclohexane, pentyl-	475 , 2.380	0.61158
Benzene, 1-methyl-4-(1-methylpropyl)-	475 , 3.020	0.2146
Decane, 3,8-dimethyl-	480 , 2.070	0.01805
Pentadecane, 7-methyl-	480 , 2.090	0.01529
Cyclopentane, hexyl-	480 , 2.340	0.35534
Naphthalene, decahydro-2-methyl-	480 , 2.710	0.03445
1H-Indene, 2,3-dihydro-1,3-dimethyl-	480 , 3.290	0.0839
1H-Indene, 2,3-dihydro-4-methyl-	480 , 3.620	0.41371
Cyclohexane, 3-ethyl-5-methyl-1-propyl-	485 , 2.260	0.3913
Benzene, 1-methyl-4-(1-methylpropyl)-	485 , 3.080	0.68876
3,4-Dimethylcumene	485 , 3.120	0.09522
Decane, 4-ethyl-	490 , 2.090	0.21263
Cyclohexane, 1-methyl-4-(1-methylbutyl)-	495 , 2.270	0.17057
Benzene, 1-methyl-4-(2-methylpropyl)-	495 , 3.490	0.05379
2,4-Dimethylstyrene	495 , 3.740	0.5568
Benzene, 1-methyl-4-(2-methylpropyl)-	500 , 3.060	0.21537
Benzene, 1,4-diethyl-2-methyl-	500 , 3.220	0.0876
Benzene, 1,2,3,4-tetramethyl-	500 , 3.490	0.21671
Undecane, 6-methyl-	505 , 2.100	1.33278
Undecane, 4-methyl-	505 , 2.110	0.40261
Naphthalene, decahydro-2-methyl-	505 , 2.750	0.02771
Benzene, pentyl-	505 , 3.090	0.23677
Benzene, 1-methyl-4-(1-methylpropyl)-	505 , 3.530	0.05406
Cyclohexane, 1,4-dimethyl-2-(2-methylpropyl)-, (1à,2á,4à)-	510 , 2.330	0.09991
Benzene, 1-methyl-4-butyl	510 , 3.050	0.24167
Benzene, 1-methyl-4-(1-methylpropyl)-	510 , 3.130	0.53499
3,4-Dimethylcumene	510 , 3.220	0.1174
Undecane, 2-methyl-	515 , 2.090	0.05483
Hexadecane	515 , 2.120	0.08928
Undecane, 3-methyl-	515 , 2.160	0.01211
Benzene, 1-methyl-4-(1-methylpropyl)-	515 , 3.210	0.44075
Naphthalene, 1,2,3,4-tetrahydro-	515 , 3.960	0.48733
Cyclohexane, 1-methyl-4-(1-methylbutyl)-	520 , 2.360	0.0676
Decalin, syn-1-methyl-, cis-	520 , 2.830	0.02425
Benzene, 1-methyl-4-butyl	520 , 3.180	0.42338
Benzene, 2,4-diethyl-1-methyl-	520 , 3.280	0.1247
Undecane, 3-methyl-	525 , 2.120	0.0534
Naphthalene, decahydro-2,6-dimethyl-	530 , 2.570	0.05631
Benzene, 1-methyl-4-(1-methylpropyl)-	530 , 3.240	0.38121
1-Octene, 3,7-dimethyl-	535 , 2.210	0.08739
Decane, 2,3,7-trimethyl-	540 , 2.130	0.15183
4-Undecene, 3-methyl-, (E)-	540 , 2.370	0.12132

Benzene, (1-ethyl-1-methylpropyl)-	540 , 3.060	0.15043
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	545 , 3.010	0.03308
Benzene, 2,4-diethyl-1-methyl-	545 , 3.470	0.0175
Benzene, 1-methyl-3-(1-methyl-2-propenyl)-	545 , 3.500	0.19112
3-Dodecene, (Z)-	550 , 2.320	0.15469
Cyclohexane, 1-methyl-3-pentyl-	550 , 2.370	0.26675
Naphthalene, decahydro-1,5-dimethyl-	550 , 2.680	0.09463
1H-Indene, 2,3-dihydro-1,6-dimethyl-	550 , 3.580	0.14486
Naphthalene	550 , 4.680	0.12726
Benzene, 1-ethyl-4-(2-methylpropyl)-	555 , 3.050	0.18891
Benzene, 1-methyl-4-(1-methylpropyl)-	555 , 3.410	0.15631
Cyclopentane, 1-hexyl-3-methyl-	560 , 2.310	0.3395
Cyclohexane, 1-methyl-2-pentyl-	560 , 2.360	0.18469
1H-Indene, 1-ethyl-2,3-dihydro-	560 , 3.610	0.08909
Dodecane	565 , 2.180	0.54731
Cyclohexane, 1-methyl-4-(1-methylbutyl)-	565 , 2.450	0.29834
1-Octadecyne	565 , 2.660	0.04341
Benzene, pentamethyl-	565 , 3.410	0.10314
1H-Indene, 2,3-dihydro-1,6-dimethyl-	565 , 3.680	0.42733
Benzene, 1-ethyl-4-(2-methylpropyl)-	570 , 3.100	0.18355
Cyclohexane, 1-methyl-4-(1-methylbutyl)-	575 , 2.420	0.00904
Naphthalene, decahydro-2,3-dimethyl-	575 , 2.750	0.03496
Naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl-	575 , 3.380	0.05698
Benzene, 1-ethyl-2,4,5-trimethyl-	580 , 3.490	0.14656
Cyclooctane, 1,2-diethyl-	585 , 2.420	0.03109
Cyclohexane, 1-methyl-3-(1-methylethyl)-	585 , 2.440	0.02696
Naphthalene, decahydro-2,6-dimethyl-	585 , 2.750	0.03095
Benzene, (1,3-dimethylbutyl)-	585 , 3.080	0.05015
Benzene, 2,4-diethyl-1-methyl-	585 , 3.200	0.04285
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	585 , 3.490	0.0955
Undecane, 2,8-dimethyl-	590 , 2.130	0.21117
Naphthalene, decahydro-2,3-dimethyl-	590 , 2.810	0.05548
Benzene, 1-ethyl-4-(2-methylpropyl)-	590 , 3.140	0.0159
Undecane	595 , 2.140	2.21638
Benzene, 2,4-dimethyl-1-(1-methylethyl)-	595 , 3.570	0.08687
Naphthalene, 1,2,3,4-tetrahydro-2-methyl-	595 , 3.870	0.34048
Benzene, hexyl-	600 , 3.100	0.02619
Benzene, 1-methyl-2-(1-ethylpropyl)-	600 , 3.220	0.09289
Benzene, 1,2,4-triethyl-	600 , 3.310	0.01977
Cyclohexane, 2-butyl-1,1,3-trimethyl-	605 , 2.480	0.38898
Cyclohexane, 2-butyl-1,1,3-trimethyl-	605 , 2.510	0.14207
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	605 , 3.190	0.07949

Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	605 , 3.210	0.25852
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	605 , 3.460	0.03743
Heptadecane, 2,6,10,14-tetramethyl-	610 , 2.140	0.34492
Benzene, (1,3-dimethylbutyl)-	610 , 3.220	0.04374
Naphthalene, 1,2,3,4-tetrahydro-1-methyl-	610 , 3.960	0.20576
trans, cis-3-Ethylbicyclo[4.4.0]decane	615 , 2.830	0.07359
Benzene, (2-methylpentyl)-	615 , 3.150	0.03992
Naphthalene, 1-ethyl-1,2,3,4-tetrahydro-	615 , 3.500	0.01448
Undecane, 2,9-dimethyl-	620 , 2.150	0.32856
Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	620 , 3.250	0.07062
Benzene, pentamethyl-	620 , 3.670	0.0231
Benzene, (1-ethyl-1-propenyl)-	620 , 3.870	0.18565
Naphthalene, decahydro-1,6-dimethyl-	625 , 2.900	0.04427
Benzene, 1,3,5-trimethyl-2-propyl-	625 , 3.240	0.07577
Dodecane, 3-methyl-	630 , 2.160	0.05998
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	630 , 3.270	0.17745
Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	630 , 3.290	0.12186
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	630 , 3.440	0.09318
Cyclododecane	635 , 2.460	0.16802
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	635 , 3.550	0.10592
Cyclododecene, (E)-	640 , 2.820	0.10248
Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	640 , 3.300	0.05843
Benzene, 1,3,5-trimethyl-2-propyl-	645 , 3.390	0.15667
Benzene, cyclohexyl-	645 , 3.630	0.02217
1H-Indene, 2,3-dihydro-4,7-dimethyl-	645 , 3.870	0.25859
Undecane, 2,4-dimethyl-	650 , 2.190	1.17077
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	655 , 3.290	0.18432
Benzene, hexyl-	660 , 3.210	0.17424
Benzene, 1,2,4-trimethyl-5-(1-methylethyl)-	660 , 3.490	0.02667
Benzene, 1-(1-methylethenyl)-3-(1-methylethyl)-	660 , 3.630	0.05224
Hexadecane	665 , 2.200	0.71144
Cyclopentane, (2-methylbutyl)-	665 , 2.420	0.22434
1,3,5-Cycloheptatriene, 2,4-diethyl-7,7-dimethyl-	665 , 3.150	0.11163
1H-Indene, 2,3-dihydro-4,7-dimethyl-	665 , 3.950	0.23195
Oxalic acid, di(cyclohexylmethyl) ester	670 , 2.440	0.2008
1,1,6,6-Tetramethylspiro[4.4]nonane	670 , 2.780	0.06214
Naphthalene, 1,2,3,4-tetrahydro-6-methyl-	670 , 4.100	0.42908
Tetradecane, 2,5-dimethyl-	675 , 2.220	0.27326
Benzeneacetaldehyde, à,2,5-trimethyl-	675 , 3.470	0.02256
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	675 , 3.670	0.03949
Octane, 2,3,7-trimethyl-	680 , 2.120	0.10166
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	685 , 3.360	0.14766

Benzene, 1,3,5-trimethyl-2-propyl-	690 , 3.440	0.22547
Benzene, 1,2,4-trimethyl-5-(1-methylethyl)-	690 , 3.520	0.02629
Benzene, cyclohexyl-	690 , 3.680	0.02491
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	690 , 3.750	0.11898
Benzene, pentamethyl-	690 , 3.830	0.03115
Benzene, 1-methyl-4-(1-methylpropyl)-	695 , 3.160	0.06639
1H-Indene, 2,3-dihydro-4,7-dimethyl-	695 , 4.070	0.1589
Undecane, 4,7-dimethyl-	700 , 2.180	0.03173
Cyclotridecane	705 , 2.430	0.38322
Dodecane, 4,6-dimethyl-	710 , 2.190	0.17023
Cyclohexane, 1-methyl-3-pentyl-	710 , 2.450	0.19911
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	710 , 3.490	0.02903
Benzene, 1,3,5-trimethyl-2-propyl-	710 , 3.570	0.09586
1H-Indene, 2,3-dihydro-4-propyl-	710 , 3.650	0.09514
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	710 , 3.780	0.31941
Naphthalene, 1,2,3,4-tetrahydro-5-methyl-	710 , 4.360	0.26056
Cyclopentane, 1-hexyl-3-methyl-	715 , 2.410	0.1644
2,4,6-Trimethylpropiophenone	720 , 3.390	0.02308
Naphthalene, 1-methyl-	720 , 4.750	0.16292
Undecane, 4,7-dimethyl-	725 , 2.280	2.12589
Tridecane	725 , 2.290	0.05601
Cyclohexane, 1-ethyl-1-methyl-	725 , 2.550	0.01371
1H-Indene, 2,3-dihydro-1,1,4,6-tetramethyl-	725 , 3.550	0.03842
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	725 , 3.840	0.1508
8-Hexadecyne	730 , 2.760	0.02044
Tetradecane	735 , 2.190	0.38304
1,1'-Bicyclohexyl	735 , 3.090	0.01196
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	740 , 3.590	0.05611
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	740 , 3.810	0.01428
1-Dodecanol, 3,7,11-trimethyl-	745 , 2.500	0.04523
1H-Indene, 1-ethylidene-	745 , 4.980	0.11046
Decane, 2,6,8-trimethyl-	750 , 2.200	0.5536
1H-Indene, 2,3-dihydro-4-propyl-	750 , 3.890	0.04367
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	755 , 3.600	0.03324
Naphthalene, 1,2,3,4-tetrahydro-2,7-dimethyl-	755 , 3.880	0.33375
Benzene, cyclohexyl-	755 , 3.990	0.07843
Decane, 2,3,5,8-tetramethyl-	765 , 2.210	0.12272
Naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl-	765 , 4.010	0.3267
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	770 , 3.660	0.02592
Naphthalene, 2-ethyl-1,2,3,4-tetrahydro-	770 , 3.980	0.05193
Tridecane, 3-methyl-	775 , 2.220	0.6091
(3-Methylphenyl) methanol, neopentyl ether	775 , 3.320	0.0363

Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	775 , 3.780	0.06852
1,4-Ethanonaphthalene, 1,2,3,4-tetrahydro-	775 , 4.310	0.05042
Cyclopentane, 1-pentyl-2-propyl-	780 , 2.430	0.16917
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	780 , 4.000	0.03382
Cyclotridecane	790 , 2.570	0.07893
Heptylcyclohexane	790 , 2.600	0.3111
Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	790 , 4.030	0.07094
Naphthalene, 1,2,3,4-tetrahydro-2,7-dimethyl-	790 , 4.140	0.27168
Undecane, 2,6-dimethyl-	800 , 2.230	0.07637
Tridecane, 5-methyl-	800 , 2.250	0.45603
Naphthalene, 1,2,3,4-tetrahydro-1,5-dimethyl-	800 , 4.340	0.16861
Benzene, 1,2,4-trimethyl-5-(1-methylethyl)-	805 , 3.900	0.01911
Tridecane, 4-methyl-	810 , 2.260	0.39974
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	810 , 3.880	0.1184
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	810 , 4.200	0.20682
1,1'-Bicyclohexyl, 2-methyl-, cis-	815 , 2.980	0.01749
Benzeneacetaldehyde, à-methyl-4-(2-methylpropyl)-	815 , 3.180	0.02455
Tetradecane, 4-methyl-	820 , 2.300	0.00978
Benzene, heptyl-	820 , 3.240	0.09347
1,3,5-Cycloheptatriene, 3,7,7-trimethyl-	820 , 3.350	0.13005
Cyclooctane, 1,4-dimethyl-, trans-	825 , 2.470	0.57452
1-Methyl-2-n-hexylbenzene	825 , 3.330	0.20885
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	825 , 3.780	0.19419
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	830 , 4.370	0.07293
Dodecane, 2,6,10-trimethyl-	840 , 2.190	1.49398
Benzene, 1,3,5-trimethyl-2-propyl-	840 , 3.470	0.09584
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	840 , 3.900	0.1596
Acenaphthylene, 1,2,2a,3,4,5-hexahydro-	840 , 4.620	0.02303
Biphenyl	850 , 0.090	0.10604
Cyclohexane, 1,1,3-trimethyl-2-(3-methylpentyl)-	850 , 2.590	0.06725
Cyclotetradecane	860 , 2.490	0.4542
Naphthalene, 1,2,3,4-tetrahydro-5,7-dimethyl-	860 , 4.340	0.10758
Cyclopentane, 1-hydroxymethyl-1,3-dimethyl-	865 , 2.520	0.06308
1-Naphthalenemethanol, 1,2,3,4-tetrahydro-8-methyl-	865 , 3.790	0.09925
Naphthalene, 1-ethyl-	865 , 4.790	0.04625
Cyclopentane, 1-hexyl-3-methyl-	870 , 2.470	0.2286
Naphthalene, 1,2,3,4-tetrahydro-2,5,8-trimethyl-	870 , 4.140	0.01756
1,1'-Biphenyl, 2-methyl-	870 , 4.790	0.04692
Benzene, 1-isopentyl-2,4,5-trimethyl-	875 , 3.390	0.02408
Naphthalene, 1,2,3,4-tetrahydro-1-propyl-	875 , 3.790	0.06339
Tetradecane	880 , 2.280	2.71423
Benzene, (cyclohexylmethyl)-	880 , 3.950	0.04263

Naphthalene, 2,7-dimethyl-	885 , 4.740	0.13067
Tetradecane	890 , 2.230	0.59772
3-Ethyl-3-phenyl-1-pentene	890 , 3.980	0.06747
Heptadecane	905 , 2.260	0.1157
Naphthalene, 1,2,3,4-tetrahydro-1,4,6-trimethyl-	905 , 3.920	0.02601
Benzene, 1-cyclohexyl-3-methyl-	905 , 3.960	0.09656
Naphthalene, 1,2,3,4-tetrahydro-5,7-dimethyl-	905 , 4.540	0.10343
3-Ethyl-3-phenyl-1-pentene	910 , 4.050	0.05295
Naphthalene, 1,3-dimethyl-	910 , 4.950	0.26838
Heptadecane	915 , 2.260	0.19532
Naphthalene, 1,2,3,4-tetrahydro-6-propyl-	915 , 3.990	0.06108
Naphthalene, 1,2,3,4-tetrahydro-5,7-dimethyl-	915 , 4.510	0.02184
Naphthalene, 1,2,3,4-tetrahydro-1-propyl-	920 , 3.890	0.03702
1-Naphthalenemethanol, 1,2,3,4-tetrahydro-8-methyl-	920 , 4.030	0.06211
Tetradecane, 3-methyl-	925 , 2.260	0.01332
1-Nonadecene	925 , 2.470	0.24198
Fluorene, 1,2,3,4,4a,9a-hexahydro-, cis-	930 , 4.420	0.03254
Naphthalene, 1,3-dimethyl-	940 , 0.030	0.04818
10-Heneicosene (c,t)	940 , 2.480	0.1171
Naphthalene, 1,2,3,4-tetrahydro-2,5,8-trimethyl-	940 , 4.040	0.13073
3,5-Dimethyl-3-phenyl-3H-pyrazole	940 , 4.620	0.02275
Naphthalene, 1,7-dimethyl-	945 , 0.160	0.01812
Cyclohexane, octyl-	945 , 2.660	0.40275
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	945 , 4.140	0.27991
Tetradecane, 5-methyl-	950 , 2.300	0.61396
Cyclotetradecane	950 , 2.560	0.13388
Naphthalene, 1,2,3,4-tetrahydro-6-propyl-	950 , 4.110	0.06981
Naphthalene, 1,2-dimethyl-	960 , 0.240	0.0287
Tetradecane, 4-methyl-	960 , 2.290	0.02724
Benzene, 1-isopentyl-2,4,5-trimethyl-	960 , 3.500	0.03467
Cyclopentane, 1-methyl-2-(4-methylpentyl)-, trans-	965 , 2.510	0.05567
Tetradecane, 2-methyl-	970 , 2.280	0.03387
Decahydro-1,1,4a,5,6-pentamethylnaphthalene	970 , 3.130	0.06573
1-Docosene	975 , 2.530	0.46233
Benzene, octyl-	975 , 3.250	0.08069
Naphthalene, 1,2,3,4-tetrahydro-2,5,8-trimethyl-	975 , 4.190	0.04741
1H-Indene, 3-ethenyl-2,3-dihydro-1,1-dimethyl-	975 , 4.410	0.03383
Tetradecane, 3-methyl-	980 , 2.310	0.03346
Benzene, 1-(2,2-dimethylpropyl)-2,4,5-trimethyl-	985 , 3.460	0.0456
Naphthalene, 1,2,3,4-tetrahydro-2,5,8-trimethyl-	985 , 4.270	0.0481
Decane, 3,7-dimethyl-	990 , 2.270	0.37871
1,4,6,7-Tetramethyl1,2,3,4-tetrahydronaphthalene	990 , 3.940	0.02928

Naphthalene, 1,2,3,4-tetrahydro-1,6,8-trimethyl-	990 , 4.330	0.03513
1,2,3,4-Tetrahydro-3-isopropyl-5-methylnaphthalene	995 , 3.770	0.09435
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	1000 , 4.460	0.06336
1,1'-Biphenyl, 4-methyl-	1005 , 0.010	0.12357
Cyclopentadecane	1005 , 2.530	0.17978
1H-Indene, 3-butyl-1-methyl-	1005 , 4.070	0.03233
Naphthalene, 1-propyl-	1005 , 4.680	0.03551
7-Pentadecyne	1010 , 2.880	0.38718
4,4'-Dimethylbiphenyl	1010 , 4.700	0.04294
Cyclopentadecane	1015 , 2.500	0.49252
1,1'-Biphenyl, 4-methyl-	1020 , 0.040	0.04488
Hexadecane	1020 , 2.340	0.07935
4,4'-Dimethylbiphenyl	1020 , 4.710	0.02153
Naphthalene, 1,4,5-trimethyl-	1030 , 4.650	0.05642
2,2'-Dimethylbiphenyl	1030 , 4.760	0.03541
Tetradecane	1035 , 2.260	0.39925
Cyclohexane, 1-methyl-2-pentyl-	1035 , 2.610	0.32633
Naphthalene, 1,4,5-trimethyl-	1035 , 4.770	0.01637
Naphthalene, 2-(1-methylethyl)-	1040 , 4.920	0.01259
1,1,4,5,6-Pentamethyl-2,3-dihydro-1H-indene	1045 , 4.320	0.04182
Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S-cis)-	1055 , 3.860	0.06679
1H-Inden-1-one, 2,3-dihydro-3,3,4,5-tetramethyl-	1055 , 4.200	0.01793
Heptadecane	1060 , 2.300	0.13284
Naphthalene, 1,4,6-trimethyl-	1065 , 4.840	0.1746
Pentadecane, 3-methyl-	1070 , 2.300	0.05141
Cyclotridecane	1070 , 2.480	0.16202
1H-Indene, 3-butyl-1-methyl-	1075 , 4.370	0.01735
1H-Indene, 3-butyl-1-methyl-	1080 , 4.470	0.03824
Naphthalene, 1,4,5-trimethyl-	1090 , 0.020	0.07864
Pentadecane, 5-methyl-	1095 , 2.310	0.69362
Cyclopentane, decyl-	1095 , 2.630	0.19178
n-Nonylcyclohexane	1095 , 2.700	0.28097
Naphthalene, 1,2,3,4-tetrahydro-1,5,7-trimethyl-	1095 , 4.640	0.03141
Naphthalene, 1,4,6-trimethyl-	1095 , 4.860	0.04132
Naphthalene, 6-butyl-1,2,3,4-tetrahydro-	1100 , 4.110	0.02854
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	1105 , 4.660	0.02427
Naphthalene, 1,4,6-trimethyl-	1115 , 0.040	0.07239
Pentadecane, 3-methyl-	1120 , 2.350	0.02444
Cyclohexane, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-	1120 , 2.550	0.26858
Hexane, 2-phenyl-3-propyl-	1125 , 3.350	0.05585
Naphthalene, 3-(1,1-dimethylethyl)-1,2-dihydro-	1125 , 4.470	0.02081
4-Ethylbiphenyl	1125 , 4.940	0.02438

1,7-Dimethyl-4-(1-methylethyl)cyclodecane	1130 , 2.600	0.05321
Heptadecane	1145 , 2.300	0.06726
Naphthalene, 1,4,5-trimethyl-	1150 , 0.280	0.03512
4,4'-Dimethylbiphenyl	1150 , 4.870	0.08167
Naphthalene, 1-(2-propenyl)-	1160 , 0.990	0.01885
Cyclopentane, 1-butyl-2-propyl-	1160 , 2.540	0.44462
Hexadecane	1165 , 2.440	0.03722
4,4'-Dimethylbiphenyl	1165 , 4.940	0.06233
Hexadecane	1175 , 2.300	0.18454
Heptacos-1-ene	1180 , 2.610	0.06833
Cyclohexane, 1-methyl-2-pentyl-	1180 , 2.640	0.41505
Naphthalene, 2-methyl-1-propyl-	1185 , 4.730	0.01834
Octadecane	1190 , 2.320	0.13637
Cyclohexane, (1-methylethyl)-	1190 , 2.630	0.02294
Cyclohexane, 1-methyl-2-pentyl-	1195 , 2.660	0.021
Naphthalene, 1,2,3,4-tetramethyl-	1195 , 4.720	0.05338
Cyclohexane, 1-methyl-2-propyl-	1215 , 2.710	0.02926
Pentadecane	1220 , 2.350	0.26219
Pentadecane, 2,6,10-trimethyl-	1225 , 2.300	0.01971
Tridecane, 5-propyl-	1225 , 2.370	0.0197
1,4,5,8-Tetramethylnaphthalene	1225 , 4.860	0.02388
Tetradecane, 4-ethyl-	1230 , 2.360	0.01649
Cyclooctane, 1,2-dimethyl-	1230 , 2.510	0.30026
Hexadecane, 4-methyl-	1240 , 2.350	0.03473
Cyclohexane, decyl-	1240 , 2.710	0.25254
1-Docosene	1245 , 2.590	0.29559
Hexadecane, 2-methyl-	1250 , 2.330	0.30259
p-Menthane, 2,3-dibromo-8-phenyl-	1255 , 3.350	0.04961
Hexadecane, 3-methyl-	1260 , 2.350	0.05864
Benzene, decyl-	1265 , 3.260	0.04412
Benzene, (1-methylnonyl)-	1265 , 3.360	0.05046
Anthracene, 1,2,3,4,5,6,7,8-octahydro-	1270 , 4.950	0.01891
1,4,5,8-Tetramethylnaphthalene	1280 , 0.060	0.02885
Heptadecane	1280 , 2.320	0.18951
1,4,5,8-Tetramethylnaphthalene	1285 , 0.110	0.01688
1,1'-biphenyl, 2,4,6-trimethyl-	1285 , 4.780	0.03023
Octadecane	1290 , 2.320	0.06284
Heptadecane	1295 , 2.420	0.0342
Benzene, 1-methyl-3-[(4-methylphenyl)methyl]-	1300 , 4.850	0.01864
9H-Fluorene, 2-methyl-	1305 , 0.880	0.03595
Heptadecane, 2,6,10,14-tetramethyl-	1305 , 2.240	0.27431
Decane, 2,6,8-trimethyl-	1310 , 2.330	0.04112

1-Docosene	1310 , 2.570	0.18915
Cyclohexane, 1-methyl-3-propyl-	1320 , 2.670	0.25994
Anthracene, 1,2,3,4,5,6,7,8-octahydro-	1325 , 0.330	0.01647
Heneicosane	1325 , 2.350	0.12241
1,1'-biphenyl, 2,4,6-trimethyl-	1345 , 0.020	0.01226
10-Heneicosene (c,t)	1345 , 2.550	0.25531
Tridecane, 5-propyl-	1355 , 2.370	1.33858
Tetradecane, 4-ethyl-	1360 , 2.370	0.18969
Heptadecane, 4-methyl-	1370 , 2.380	0.02775
Cyclopentadecane	1375 , 2.660	0.07132
Cyclohexane, undecyl-	1375 , 2.740	0.24107
Heptadecane, 2-methyl-	1380 , 2.360	0.13417
1,1'-Bicyclooctyl	1385 , 2.550	0.06528
Heptadecane, 3-methyl-	1390 , 2.370	0.14536
Cyclohexane, 1-ethyl-2-propyl-	1390 , 2.620	0.11569
Octadecane	1405 , 2.340	0.12446
Pentadecane	1425 , 2.440	0.08006
Hexadecane, 2,6,10,14-tetramethyl-	1435 , 2.320	0.01517
1-Docosene	1440 , 2.590	0.09954
Octacosane	1450 , 2.370	0.11287
Sulfurous acid, cyclohexylmethyl tetradecyl ester	1450 , 2.700	0.2348
Pentadecane, 2,6,10-trimethyl-	1465 , 2.350	0.10895
Eicosane, 10-methyl-	1475 , 2.390	0.40837
1,7-Dimethyl-4-(1-methylethyl)cyclodecane	1480 , 2.600	0.07514
8-Hexadecyne	1490 , 2.900	0.14297
Octadecane, 2-methyl-	1500 , 2.410	0.02601
Cyclopentane, decyl-	1500 , 2.700	0.05506
2-Piperidinone, N-[4-bromo-n-butyl]-	1500 , 2.750	0.03696
Cyclohexane, undecyl-	1505 , 2.750	0.14311
Nonadecane, 2-methyl-	1510 , 2.430	0.56787
p-Menthane, 2,3-dibromo-8-phenyl-	1520 , 3.280	0.08978
Benzene, dodecyl-	1525 , 3.290	0.02501
Benzene, (1-methylundecyl)-	1530 , 3.340	0.06704
Hexadecane, 2,6,10,14-tetramethyl-	1535 , 2.320	0.28254
Heptadecane	1540 , 2.370	0.00997
Heneicosane	1550 , 2.430	0.10093
Hexadecane, 2,6,10,14-tetramethyl-	1560 , 2.370	0.01848
Sulfurous acid, cyclohexylmethyl undecyl ester	1560 , 2.660	0.02358
Heptadecane	1570 , 2.390	0.20361
Oxalic acid, cyclohexylmethyl propyl ester	1570 , 2.680	0.04732
Sulfurous acid, cyclohexylmethyl hexyl ester	1575 , 2.740	0.14221
Hexadecanoic acid, methyl ester	1575 , 3.080	0.19225

Nonadecane	1595 , 2.410	0.57167
Nonadecane, 2-methyl-	1620 , 2.420	0.3128
1-Heneicosanol	1625 , 2.700	0.0516
Eicosane, 2-methyl-	1630 , 2.430	0.31121
Cyclohexane, undecyl-	1630 , 2.760	0.09978
1,3-Benzenediol, O-(4-methylbenzoyl)-O'-propoxycarbonyl-	1640 , 3.330	0.02489
Tetracosane	1655 , 2.370	0.08038
Heneicosane	1665 , 2.470	0.02231
Cyclopentane, 1-hydroxymethyl-1,3-dimethyl-	1680 , 2.670	0.15887
Cyclohexane, 1-methyl-2-pentyl-	1695 , 2.740	0.05919
Octadecane	1700 , 2.390	0.02408
Eicosane, 10-methyl-	1705 , 2.440	0.22432
Eicosane, 2-methyl-	1725 , 2.450	0.02225
Eicosane, 2-methyl-	1735 , 2.430	0.08362
1-Eicosanol	1740 , 2.730	0.03401
Heneicosane	1745 , 2.400	0.12832
Cyclohexane, undecyl-	1745 , 2.790	0.05329
Eicosane	1755 , 2.400	0.05385
Hexadecane	1765 , 2.410	0.07441
9-Octadecenoic acid (Z)-, methyl ester	1770 , 3.310	0.07329
Octadecane	1775 , 2.510	0.0175
Heneicosane	1775 , 2.590	0.05582
1-Docosene	1785 , 2.660	0.11748
Methyl stearate	1800 , 3.110	0.31442
Heptacosane	1810 , 2.400	0.06096
Cyclohexane, 1-methyl-3-propyl-	1810 , 2.760	0.03407
Eicosane, 10-methyl-	1815 , 2.450	0.19368
Pentane, 3-ethyl-2,4-dimethyl-	1825 , 2.460	0.03724
Eicosane, 2-methyl-	1840 , 2.460	0.20971
Eicosane, 2-methyl-	1850 , 2.470	0.22761
Cyclopentane, heneicosyl-	1850 , 2.750	0.01901
n-Pentadecylcyclohexane	1855 , 2.820	0.04876
Docosane	1880 , 2.560	0.4798
Oxalic acid, cyclohexylmethyl propyl ester	1900 , 2.730	0.05503
Hexadecane, 2,6,10,14-tetramethyl-	1910 , 2.390	0.04891
Heneicosane	1920 , 2.470	0.22799
Eicosane, 2-methyl-	1945 , 2.470	0.23476
Eicosane, 2-methyl-	1955 , 2.480	0.13176
Cyclohexane, undecyl-	1965 , 2.820	0.02618
Tetracosane	1985 , 2.540	0.91788
Eicosane, 10-methyl-	2015 , 2.490	0.14447
Heptacosane	2045 , 2.490	0.14941

Heptacosane	2055 , 2.500	0.1276
Tetracosane	2080 , 2.580	0.43872
Octacosane	2115 , 2.510	0.14666
Eicosane, 2-methyl-	2140 , 2.510	0.069
Heptacosane	2175 , 2.590	0.11168

Table S8 Physical properties of StTPOxxEL10 ternary fuel blends

Fuel blends	Density (g/cc)	Flashpoint (ºC)	Kinematic viscosity (cSt)	GCV (MJ/kg)	CCI
StTPO20EL10	0.8353±0.001	62±0.5	2.33±0.8	40.595±0.08	39.80±0.07
StTPO40EL10	0.8541±0.002	60±0.4	2.45±0.5	39.778±0.09	37.59±0.05
StTPO60EL10	0.8749±0.001	59±0.6	2.51±0.7	37.965±0.06	32.72±0.04
StTPO80EL10	0.8809±0.002	50±0.5	2.61±0.8	37.530±0.07	28.65±0.03
StTPO90EL10	0.8909±0.001	44±0.3	2.63±0.6	37.095±0.09	24.50±0.07
StTPO100	0.8682[#]	40[#]	2.54[#]	41.760[#]	40.00[#]
CTPO100	0.907[#]	52[#]	3.83[#]	42.980[#]	33.00[#]
Diesel	0.830[*]	50[*]	2-4[*]	43.800[*]	50[*]

[#]Mohan et al. (2019), [*]Tudu et al. (2016)

Table S9 Carbon content in ethyl levulinate, StTPO, CTPO, and diesel

Fuel/Additive	Formulae	Carbon (%)	Ref.
EL	$C_7H_{12}O_3$	58.00	[61]
StTPO	$C_{83.26}H_{11.34}N_{1.77}O_{2.93}S_{0.70}$	83.52	[15]
CTPO	$C_{85.67}H_{10.04}O_{2.02}S_{1.12}N_{1.15}$	85.67	[62]
Diesel	$C_5H_{32}O_3$	85.00	[61]

List of equations used in the present research study

1. Brake power (BP) = $\frac{2\times3.14\times N\times T\times60}{1000}$
2. Total fuel consumption (TFC) = $\frac{10\times Density\times3600}{1000\times t}$
3. Brake thermal efficiency (BTE) = $\frac{BP\times3600}{TFC\times CV}$
4. Absolute viscosity (A.V) = Kinematic viscosity × Density

5. Kinematic viscosity = $0.26 \times t - \frac{179}{t}$; if t < 100s
6. Kinematic viscosity = $0.247 \times t - \frac{50}{t}$; if t > 100s
7. Standard deviation (S.D) = $\sqrt{\frac{\sum(x-\overline{x})}{N-1}}$

Uncertainty analysis

The overall uncertainty of experiments is given by the following equation:

Overall uncertainty = square root of [(uncertainty in crank angle encoder)^2 + (uncertainty in in-cylinder pressure)^2 + (uncertainty in temperature)^2 + (uncertainty in load)^2 + (uncertainty in HC)^2 + (uncertainty in NO_x) + (uncertainty in CO)^2 + (uncertainty in CO_2)^2 + (uncertainty in time)^2) + (uncertainty in speed)^2]

Overall uncertainty = square root of [$(0.6324)^2 + (0.1111)^2 + (0.7432)^2 + (0.0096)^2 + (0.86)^2 + (0.6546)^2 + (0.084)^2 + (0.2923)^2 + (0.44)^2 + (0.2746)^2$

Thus, the overall uncertainty is given by ± 1.5793%