Supplementary Material

Composition of the isopropanol soluble portion and fast pyrolysis products distribution of the insoluble part from Pakistan lignite

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Table S1
Alkanes detected in the SP

Peak	RT (min)	Compound name	RC (%)
40	9.86	Dodecane	0.27
55	11.34	Tridecane	0.60
70	12.71	Tetradecane	0.55
80	13.51	Pentadecane, 7-methyl-	0.60
85	13.99	Pentadecane	0.60
108	15.76	Hexadecane, 2,6,10,14-tetramethyl-	0.37
114	16.33	Hexadecane	0.36
115	16.40	Pentadecane, 2,6,10,14-tetramethyl-	0.48
120	16.80	Cyclohexane, 2-butyl-1,1,3-trimethyl-	0.68
127	17.42	Decane, 3-methyl-	0.42
138	18.45	Pentadecane, 8-hexyl-	0.47
146	19.43	Heptadecane	0.17
153	20.37	Heptadecane, 2,6,10,15-tetramethyl-	0.27
160	21.28	Pentadecane, 8-heptyl-	0.21
167	22.14	Heptadecane, 8-methyl-	0.31
171	22.97	Heptadecane, 9-octyl-	0.53
177	23.78	Nonadecane, 9-methyl-	0.52

184	24.55	Nonadecane	0.66
190	25.29	Eicosane	0.83
195	26.01	Heneicosane	1.06
202	26.70	Docosane	0.93
208	27.38	Tetracosane	0.42

Table S2
Alkenes detected in the SP

Peak	RT (min)	Compound name	RC (%)
57	11.55	Ethyl-tetramethyl-cyclopentadiene	0.05
62	11.89	1,3-Cyclohexadiene, 1,2,3,4,5,6-hexamethyl-	0.26
72	12.82	1,3-Cyclohexadiene, 1,2,3,4,5,6-hexamethyl-	0.39
118	16.68	1-Heptene, 2-isohexyl-6-methyl-	0.62
120	16.80	Cyclohexane, 2-butyl-1,1,3-trimethyl-	0.68

Table S3
Arenes detected in the SP

Peak	RT (min)	Compound name	RC (%)
14	5.97	Benzene, 1,2,3-trimethyl-	0.15
33	8.99	1H-Indene, 2,3-dihydro-5-methyl-	0.10
34	9.17	1H-Indene, 2,3-dihydro-4-methyl-	0.34
41	9.92	1H-Indene, 2,3-dihydro-1,1-dimethyl-	0.14
53	11.20	2,2-Dimethylindene, 2,3-dihydro-	0.13
61	11.83	Benzene, 1-(1-methylethenyl)-3-(1-methylethyl)-	0.40
74	12.95	Naphthalene, 1,6-dimethyl-	0.23
75	13.04	Benzene, hexamethyl-	0.23
79	13.47	Benzene, 1,2,4-trimethyl-5-(1-methylethyl)-	0.16
81	13.60	Benzene, 1,4-bis(1-methylethyl)-	0.16
83	13.73	Benzene, 1-(1,1-dimethylethyl)-3,5-dimethyl-	0.43
92	14.39	1,1,4,5,6-pentamethyl-2,3-dihydro-1H-indene	1.10
93	14.54	Naphthalene, 2,3,6-trimethyl-	0.22
95	14.69	Benzene, 1,2-diethyl-3,4-dimethyl-	0.18
96	14.74	Benzene, 1,3,5-triethyl-	0.22
98	14.85	Benzene, 1-(1,1-dimethylethyl)-3-ethyl-5-methyl-	0.22
99	14.92	Naphthalene, 1,6,7-trimethyl-	0.97
103	15.25	Naphthalene, 2,3,6-trimethyl-	0.39
105	15.60	Benzene, 1,2,4,5-tetraethyl-	0.38
113	16.24	Benzene, 1-ethyl-3,5-diisopropyl-	0.39
116	16.51	Naphthalene, 3-(1,1-dimethylethyl)-1,2-dihydro-	0.48
117	16.62	2,2'-Dimethylbiphenyl	0.30
119	16.74	1,1'-Biphenyl, 2,3'-dimethyl-	0.16
121	16.86	1-(4-Tolyl)-1-cyclohexene	0.20
122	16.93	2,2'-Dimethylbiphenyl	0.41

126	17.27	Benzene, nonyl-	0.30
132	17.79	Benzene, 1-methyl-2-[(4-methylphenyl)methyl]-	0.20
135	18.09	s-Indacene, 1,2,3,5,6,7-hexahydro-4,8-dimethyl-	0.24
137	18.35	Benzene, undecyl-	0.38
139	18.61	1,1'-Biphenyl, 3-(1-methylethyl)-	0.12
140	18.71	Phenanthrene, 9-butyl-1,2,3,4,5,6,7,8-octahydro-	0.15
143	18.95	Anthracene, 1-methyl-	0.20
145	19.38	Benzene, tridecyl-	0.13
150	20.12	Naphthalene, 1,2-dihydro-4-phenyl-	0.20
156	20.99	Naphthalene, 1-phenyl-	0.06
158	21.16	Phenanthrene, 2,3,5-trimethyl-	0.03
163	21.91	11H-Benzo[b]fluorene	0.06
164	21.96	Pyrene, 1-methyl-	0.03
165	22.02	Naphthalene, 1-(phenylmethyl)-	0.08
166	22.10	9-Phenyl-5H-benzocycloheptene	0.10
168	22.36	Benzene, 1,1'-(1,3,5-hexatriene-1,6-diyl)bis-	0.07
174	23.27	o-Terphenyl	0.14
192	25.47	Naphthacene, 5-(1-naphthalenyl)-	0.24
209	27.43	A'-Neogammacer-22(29)-ene	0.46
213	28.16	Anthracene, 9-(3-butenyl)-	1.04

Table S4

OCOCs detected in the SP

Peak	RT (min)	Compound name	RC (%)
4	2.29	2-Pentanol, 2-methyl-	0.17
5	2.36	Methyl Isobutyl Ketone	0.40
6	2.48	4-Penten-2-one, 4-methyl-	0.06
7	2.53	2-Hexanol	0.31
8	2.91	2-Hexanone	0.04
9	2.96	3-Buten-2-one, 3-methyl-	0.03
10	3.02	3-Penten-2-one, 4-methyl-	0.98
11	3.66	Butanoic acid, 1-methylethyl ester	0.02
12	4.56	Butanoic acid, 3-methyl-, 1-methylethyl ester	0.03
13	5.41	Pentanoic acid, 1-methylethyl ester	0.03
15	6.37	2-Hexanone, 4-methyl-	0.03
16	6.48	Phenol	1.08
22	7.29	Cyclohexanone, 3,3,5-trimethyl-	0.06
24	7.76	Phenol, 2-methyl-	0.53
26	8.11	p-Cresol	0.73
27	8.24	Phenol, 3-methyl-	0.57
30	8.51	p-Cresol	0.36
31	8.76	Acetic acid, 4-methylphenyl ester	0.14

32	8.85	Heptanoic acid, propyl ester	0.03
35	9.29	Phenol, 3,4-dimethyl-	0.35
36	9.36	Phenol, 2,5-dimethyl-	0.21
37	9.63	Phenol, 3-ethyl-	0.76
39	9.76	Phenol, 3,5-dimethyl-	0.44
42	10.06	Phenol, 3-(1-methylethyl)-	0.58
43	10.19	Phenol, 4-ethyl-	0.14
45	10.41	Phenol, 2-propyl-	0.04
46	10.49	Phenol, 3-ethyl-5-methyl-	0.49
48	10.64	Phenol, 2-ethyl-5-methyl-	0.35
49	10.71	Phenol, 2-ethyl-4-methyl-	0.22
50	11.02	Phenol, 3-(1-methylethyl)-	0.37
51	11.06	3,4-Dimethylbenzyl alcohol	0.14
52	11.14	Phenol, 2,3,5-trimethyl-	0.18
54	11.27	3-Methyl-4-isopropylphenol	0.32
56	11.43	Phenol, 2-methyl-5-(1-methylethyl)-	0.26
58	11.63	Phenol, 2,3,6-trimethyl-	0.19
59	11.67	Thymol	0.16
60	11.74	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	0.47
64	12.09	1-Penten-3-one, 1-phenyl-	0.08
65	12.15	1H-Inden-5-ol, 2,3-dihydro-	0.37
68	12.39	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-	0.38
69	12.59	Benzene, 1-butyl-4-methoxy-	0.30
71	12.77	Ethanone, 1-(4-ethylphenyl)-	0.46
73	12.90	Benzene, 1-(1,1-dimethylethyl)-4-ethoxy-	0.32
77	13.28	2-Propanone, 1-(3,5,5-trimethyl-2-cyclohexen-1-ylidene)-, (E)-	0.65
78	13.41	5-Formyl-2,2-dimethyl-1,3-benzodioxole	0.42
90	14.24	4-Hydroxy-2,4,5-trimethyl-2,5-cyclohexadien-1-one	0.36
91	14.32	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl-	0.29
94	14.63	Benzofuran, 2,3-dihydro-2,2,4,6-tetramethyl-	0.59
100	15.02	2,3,5,6-Tetramethylacetophenone	0.23
101	15.10	Pentamethylbenzaldehyde	0.27
102	15.19	Benzofuran, 2,3-dihydro-2,2,5,6-tetramethyl-	0.63
104	15.36	3-Hydroxy-4-methoxybenzoic acid	0.42
106	15.65	Phenol, 2-(1,1-dimethyl-2-propenyl)-3,6-dimethyl-	0.24
107	15.71	1-Naphthalenol, 2-methyl-	0.27
125	17.19	1-Naphthol, 6,7-dimethyl-	0.40
129	17.61	2-Propenoic acid, 3-(4-methoxyphenyl)-, (E)-	0.17
130	17.66	1-Naphthalenecarboxaldehyde, 4-methoxy-	0.18
133	17.91	Ethanone, 1-(2-hydroxy-1-naphthalenyl)-	0.32
136	18.17	1-Naphthalenecarboxaldehyde, 2-methoxy-	0.21

142	18.84	5H-Dibenzo[a,d]cyclohepten-5-ol, 10,11-dihydro-	0.23
149	20.02	7H-Furo(3,2-g)(1)benzopyran-7-one, 4-(2,3-epoxy-3-methylbutoxy)-, (S)-(-)-	0.21
151	20.20	2(3H)-Phenanthrenone, 4,4a,9,10-tetrahydro-4a-methyl-	0.17
162	21.50	4,9(11)-Androstadiene-3,17-dione	0.02
178	23.82	Phenol, 3-pentadecyl-	0.26
186	24.73	Docosanoic acid	0.23
211	27.84	.beta.-Tocopherol	0.47
212	27.96	.gamma.-Tocopherol	0.80
214	28.26	4,7-Methanoindan, 3a,4,7,7a-tetrahydro-1,2-epoxy-4,5,6,7,8,8-hexachloro-	0.22
223	31.55	Triacontanoic acid	0.39

Table S5
NCOCs detected in the SP

Peak	RT (min)	Compound name	RC (%)
3	1.85	Hydrazine, ethyl-	0.16
21	7.21	m-Aminophenylacetylene	0.09
23	7.47	Fampridine	0.05
110	15.98	N,N-Diethyl-3-nitroaniline	0.38
111	16.07	1H-Pyrazole, 3-methyl-1-phenyl-	0.32
112	16.12	Benzenacetamide, N-allyl-	0.37
123	17.02	4-Pyrimidinamine, 2-chloro-N-cyclopropyl-5-fluoro-	0.20
124	17.08	2H-Isoindole, 4,5,6,7-tetramethyl-	0.24
128	17.53	1,2-Dimethyl-3-formylindole	0.20
134	17.97	2-Benzothiazolamine, 4-chloro-	0.22
144	19.19	Tetrahydrozoline	0.40
148	19.68	Lumiflavine	0.15
152	20.32	2,5-Dimethyl-4-(3-amino-4-methylphenyl)pyridine	0.04
155	20.89	9-Acridinamine, 1,2,3,4-tetrahydro-2-methyl-	0.05
159	21.23	2,5-Diaminobenzophenone	0.02
161	21.44	2-Buten-1-ol, 2-methyl-4-(1H-purin-6-ylamino)-, (E)-	0.05
169	22.49	Azepino[4,5-b]indole, 1,2,3,4,5,6-hexahydro-5-phenyl-	0.17
170	22.77	1-Phenyl-3-(3-nitrophenyl)-2-pyrazoline	0.07
172	23.08	Quinoline, 8-methyl-2-(2-methylphenyl)-	0.13
175	23.41	Benzo[a]phenazine, 7-oxide	0.17
176	23.48	4-(2-Chloroethylthio)-N,N-diethyl-6-methylthio-1,3,5-triazin-2-amine	0.14
185	24.70	6-Methoxy-1-methyl-2-phenyl-4(1H)-	0.15

		quinolinone (eduline)	
189	25.20	5-Quinolinesulfonamide, N-ethyl-8-methoxy-N-phenyl-	0.30
193	25.68	Pyrazine, 2-methyl-5-(2-propenyl)-	0.36
196	26.14	Benzoic acid, pentachloro-	0.26
207	27.16	Isonipecotic acid, N-(4-fluoro-2-trifluoromethylbenzoyl)-, isohexyl ester	0.62
216	28.48	7H-Dinaphtho[2,3-b:2',3'-h]carbazole	0.39
222	30.38	Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-	0.07

Table S6
Alcohols detected in the OCOCs

Peak	Compound name	RC (%)
4	2-Pentanol, 2-methyl-	0.17
7	2-Hexanol	0.31
51	3,4-Dimethylbenzyl alcohol	0.14
65	1H-Inden-5-ol, 2,3-dihydro-	0.39
91	3,7-Benzofurandiol, 2,3-dihydro-2,2-dimethyl-	0.29
125	1-Naphthol, 6,7-dimethyl-	0.4
142	5H-Dibenzo[a,d]cyclohepten-5-ol, 10,11-dihydro-	0.23
214	4,7-Methanoindan, 3a,4,7,7a-tetrahydro-1,2-epoxy-4,5,6,7,8,8-hexachloro-	0.22

Table S7
Ketones detected in the OCOCs

Peak	Compound name	RC (%)
5	Methyl Isobutyl Ketone	0.4
6	4-Penten-2-one, 4-methyl-	0.06
8	2-Hexanone	0.04
9	3-Buten-2-one, 3-methyl-	0.03
10	3-Penten-2-one, 4-methyl-	0.98
15	2-Hexanone, 4-methyl-	0.03
22	Cyclohexanone, 3,3,5-trimethyl-	0.06
60	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	0.47
64	1-Penten-3-one, 1-phenyl-	0.08
68	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-	0.38
71	Ethanone, 1-(4-ethylphenyl)-	0.46
77	2-Propanone, 1-(3,5,5-trimethyl-2-cyclohexen-1-ylidene)-, (E)-	0.65
90	4-Hydroxy-2,4,5-trimethyl-2,5-cyclohexadien-1-one	0.36
100	2,3,5,6-Tetramethylacetophenone	0.23
133	Ethanone, 1-(2-hydroxy-1-naphthalenyl)-	0.32
149	7H-Furo(3,2-g)(1)benzopyran-7-one, 4-(2,3-epoxy-3-methylbutoxy)-, (S)-(-)-	0.21
151	2(3H)-Phenanthrenone, 4,4a,9,10-tetrahydro-4a-methyl-	0.17
162	4,9(11)-Androstadiene-3,17-dione	0.02

Table S8
Esters detected in the OCOCs

Peak	Compound name	RC (%)
11	Butanoic acid, 1-methylethyl ester	0.02
12	Butanoic acid, 3-methyl-, 1-methylethyl ester	0.03
13	Pentanoic acid, 1-methylethyl ester	0.03
31	Acetic acid, 4-methylphenyl ester	0.14
32	Heptanoic acid, propyl ester	0.03

Table S9

Phenols detected in the OCOCs

Peak	Compound name	RC (%)
16	Phenol	1.08
24	Phenol, 2-methyl-	0.53
26	p-Cresol	0.73
27	Phenol, 3-methyl-	0.57
30	p-Cresol	0.36
35	Phenol, 3,4-dimethyl-	0.35
36	Phenol, 2,5-dimethyl-	0.21
37	Phenol, 3-ethyl-	0.76
39	Phenol, 3,5-dimethyl-	0.44
42	Phenol, 3-(1-methylethyl)-	0.58
43	Phenol, 4-ethyl-	0.14
45	Phenol, 2-propyl-	0.04
46	Phenol, 3-ethyl-5-methyl-	0.49
48	Phenol, 2-ethyl-5-methyl-	0.35
49	Phenol, 2-ethyl-4-methyl-	0.22
50	Phenol, 3-(1-methylethyl)-	0.37
52	Phenol, 2,3,5-trimethyl-	0.18
54	3-Methyl-4-isopropylphenol	0.32
56	Phenol, 2-methyl-5-(1-methylethyl)-	0.26
58	Phenol, 2,3,6-trimethyl-	0.19
59	Thymol	0.16
106	Phenol, 2-(1,1-dimethyl-2-propenyl)-3,6-dimethyl-	0.24
107	1-Naphthalenol, 2-methyl-	0.27
178	Phenol, 3-pentadecyl-	0.26
211	.beta.-Tocopherol	0.47
212	.gamma.-Tocopherol	0.8

Table S10
Aldehydes detected in the OCOCs

Peak	Compound name	RC (%)
78	5-Formyl-2,2-dimethyl-1,3-benzodioxole	0.42
101	Pentamethylbenzaldehyde	0.27
136	1-Naphthalenecarboxaldehyde, 2-methoxy-	0.21

Table S11
Ethers detected in the OCOCs

Peak	Compound name	RC (%)
69	Benzene, 1-butyl-4-methoxy-	0.3
73	Benzene, 1-(1,1-dimethylethyl)-4-ethoxy-	0.32

Table S12
OTCs detected in the OCOCs

Peak	Compound name	RC (%)
94	Benzofuran, 2,3-dihydro-2,2,4,6-tetramethyl-	0.59
102	Benzofuran, 2,3-dihydro-2,2,5,6-tetramethyl-	0.63

104	3-Hydroxy-4-methoxybenzoic acid	0.42
129	2-Propenoic acid, 3-(4-methoxyphenyl)-, (E)-	0.17
186	Docosanoic acid	0.23
223	Triacontanoic acid	0.39

Table S13
Attribution of infrared peak functional groups from PLC and ISP

Peak	Wavelength (cm^{-1})	Assignment	Area (%)		
			PLC	ISP	Increasing Rate
1	3600-3500	OH-π	22.01	5.64	-16.37
2	3500-3350	OH–OH	31.96	28.76	-3.2
3	3350-3260	OH–ether O	19.40	25.67	+6.27
4	3260-3170	Cyclic OH	16.99	36.69	+19.7
5	3170-3000	OH-N	9.64	3.24	-6.4
6	3000-2930	Asymmetric stretching vibration of CH_3	12.32	21.61	+9.29
7	2930-2900	Asymmetric stretching vibration of CH_2 in alkanes	43.08	38.45	-4.63
8	2900-2870	Stretching vibration of CH in alkanes	17.69	17.49	-0.2
9	2870-2800	Symmetric stretching vibration of CH_2 in alkanes	26.91	22.45	-4.46
10	1800-1700	Stretching vibration of C=O in carboxylic acids	10.26	5.82	-4.44
11	1700-1600	Stretching vibration of highly conjugated C=O	22.65	27.40	+4.75
12	1600-1480	Stretching vibration of C=C in aromatic rings	12.89	19.35	+6.46
13	1480-1400	Asymmetric deformation vibration of CH_3	15.84	26.18	+10.34
14	1400-1240	Symmetric CH_3–Ar, R	11.65	9.97	-1.68
15	1240-1160	Stretching vibration of C–OH in phenols	12.36	5.87	-6.49
16	1160-1090	Stretching vibration of C–O in esters	9.77	2.50	-7.27
17	1090-1030	Stretching vibration of C–O in alkyl ether	4.58	2.91	-1.67
18	900-860	Isolated aromatic hydrogens (1H)	2.66	21.81	+19.15
19	860-810	Two adjacent hydrogens per ring (2H)	43.76	23.58	-20.18
20	810-750	Three adjacent hydrogens per ring (3H)	29.01	32.90	+3.89
21	750-720	Four adjacent hydrogens per ring (4H)	24.57	21.71	-2.86

Table S14
Alkanes from PLC and ISP pyrolysis by Py-GC/MS

Peak	RT (min)	Compound name	RC (%)

			PLC	ISP
2	1.658	Cyclopropane		5.9
5	1.846	Butane	4.87	
29	11.707	Undecane	0.44	0.21
41	13.39	Decane	1.09	0.64
44	13.66	2,6-Dimethylundecane	0.32	0.15
54	14.446	2,6,11-Trimethyldodecane	0.21	
58	14.791	Tridecane	1.13	0.8
72	15.679	Dodecane, 2,6,11-trimethyl-	0.17	
74	15.919	Dodecane	1.13	1.15
75	15.963	Cyclooctane, methyl-	0.29	
85	16.534	Dodecane	0.53	0.22
88	16.748	Cyclopropane, 1-methyl-2-octyl-	0.14	
90	16.871	Tridecane	1.14	1.3
92	17.104	7-Tetradecyne	0.29	
93	17.105	6-Tridecane		0.16
113	18.058	Pentadecane, 2,6,10-trimethyl-	0.38	0.23
116	18.17	Tridecane, 7-cyclohexyl-	0.17	
117	18.187	Cyclohexane, (1,3-dimethylbutyl)		0.17
120	18.265	Propane, 3-cyclohexyl-1-phenyl-		0.11
124	18.416	Hexadecane	0.97	1.9
126	18.711	Cyclohexane, 2-butyl-1,1,3-trimethyl-		0.12
138	19.078	Hexadecane	0.92	2
147	19.685	Heptadecane	0.85	1.3
156	20.225	Cyclotetradecane		0.89
159	20.257	Pentadecane		1.1
161	20.563	Octacosane	0.17	
163	20.767	Cyclopentadecane	0.59	0.98
164	20.793	Hexadecane	0.82	1.3
173	21.28	Cyclotetradecane		0.94
175	21.303	Eicosane	1.61	1
179	21.417	17-Pentatriacontene		0.1
182	21.791	Eicosane, 2-methyl-	1.82	1.71
187	22.116	Hexadecane, 5-decyl		0.15
190	22.28	Dotriacontane	1.66	2.2
196	22.776	Hexatriacontane	2.9	1.83
204	23.65	Octane, 3,4,5,6-tetramethyl- $	0.36	
206	23.863	Dotriacontane		1.82
223	25.187	Tetratetracontane	1.84	1.83
225	25.992	hexatetracontane	1.31	1.44

232	26.932	Triacontane, 11,20-didecyl-	1.26

Table S15

Alkenes from PLC and ISP pyrolysis by Py-GC/MS

Peak	RT (min)	Compound name	RC (%)	
			PLC	ISP
16	7.579	1,3,5,7-Cyclooctatetraene		0.13
18	9.675	1-Decene	0.23	
23	10.417	(S)-(-)-Limonene	0.28	0.23
40	13.258	Dodecene	0.81	0.45
48	13.945	α-terpinene		0.11
55	14.69	(E)-2-tetradecene	0.9	0.62
56	14.736	(3E)-7-Methyl-3-undecene	0.24	
57	14.737	(4E)-10-Methyl-4-undecene		0.23
59	14.846	(2E)-2-Tridecene	0.54	
60	14.849	(3Z)-3-Tetradecene		0.51
62	14.982	1-Nonene	0.16	
73	15.839	1-Undecene	1.37	0.94
77	16.083	1-Dodecene	0.11	
79	16.181	(4E)-1,4-Undecadiene #	0.18	
87	16.649	(3Z)-3-Undecene-1,5-diyne		0.2
89	16.806	1-Tetradecene	1.9	0.81
107	17.635	1-Pentadecene	0.97	0.99
108	17.689	Hexadecane	1	1.12
110	17.826	1-Tetradecene		0.11
114	18.11	5-Octadecene, (E)-	0.13	
115	18.112	cis-2-Methyl-7-octadecene		0.1
118	18.237	2-Decene, (Z)-		0.1
123	18.369	Cetene	0.88	0.76
124	18.416	Hexadecane	0.97	1.9
125	18.635	1-Undecene, 5-methyl-	1.3	0.36
130	18.855	Tetradecanal	0.3	0.14
135	19.035	1-Eicosene	0.82	
136	19.037	1-Heptadecene		0.87
140	19.206	1-Tetradecene	0.11	
146	19.652	1-Heptadecene	0.65	0.93
157	20.225	1-Heptadecene	0.58	
184	21.905	1-Eicosene		0.8
220	24.82	Supraene		0.23

Table S16

Arenes from PLC and ISP pyrolysis by Py-GC/MS

Peak	RT (min)	Compound name	RC (%)	
			PLC	ISP
15	7.084	o-Xylene	0.1	
19	9.753	1,2,4-trimethylbenzene	0.43	

34	12.743	1,4,9-Decatrienyl-benzene	0.35	
50	14.22	5-Methyl-4-hexenyl-benzene	0.11	
51	14.33	Hexylbenzene	0.14	
52	14.396	1,2,3,4-tetrahydronaphthalene-1,5-diol	0.27	
64	15.083	1-Methyl-naphthalene	0.2	
65	15.108	Naphthalene		0.13
69	15.497	1,4,5,8-tetrahydronaphthalene	0.12	
78	16.126	Naphthalene, 1,2-dimethyl-	0.14	
81	16.32	Naphthalene, 1,3-dimethyl-	0.18	
86	16.647	Benzene, (2-methyl-1-butenyl)-	0.54	
103	17.536	Benzene, eicosyl-		0.16
109	17.816	3-(2-Methyl-propenyl)-1H-indene	0.27	
121	18.32	n-Heptadecylbenzene		0.2
122	18.32	Benzene, decyl-	0.28	
132	18.897	:Benzene, (4,5,5-trimethyl-1,3-cyclopentadien-1-yl)-	0.2	
177	21.382	Benzene, (3-octylundecyl)-	0.13	
203	23.49	Benzene, eicosyl-		0.1
211	24.09	Eicosane, 1-phenyl-	0.15	

Table S17

OCOCs from PLC and ISP pyrolysis by Py-GC/MS

Peak	RT (min)	Compound name	RC (%)	
			PLC	ISP
1	1.585	Carbon dioxide	23.71	3.85
3	1.76	1,3-Propanediol		2.97
7	2.117	DL-Alaninol	0.22	
8	2.373	acetic acid		1.04
9	2.561	Tetrahydrofuran		0.19
11	2.944	cyclohepta-2,4,6-trien-1-one	0.9	
12	3.724	Methyl methacrylate	0.19	
13	4.192	4-Methyl-2-pentanone		0.2
14	5.448	4-Methyl-3-penten-2-one		0.13
17	9.117	3-Methyl-2-cyclopenten-1-one	0.13	
21	10.128	Decanal	0.13	
24	10.588	2,3-dimethyl-2-cyclopenten-1-one	0.15	
25	11.137	Cresol	0.92	0.31
27	11.548	(2E)-2-Nonenal	1.4	
28	11.553	2-Decenal		0.69
30	11.766	Nonanal		0.22
31	11.767	3-Nonen-1-ol,	0.39	

32	12.565	2-Ethyl-phenol	0.08	
33	12.693	2,6-dimethyl-Phenol	0.51	0.31
36	13.026		0.33	
37	13.064	2,5-dimethyl-Phenol	0.1	0.15
38	13.075	2,3-dimethyl-Phenol	0.32	
43	13.56	2-Ethyl-6-methyl-phenol		0.2
46	13.764	ethenoxybenzene	0.1	
47	13.932	2,4-Hexadiyn-1,6-diol	0.43	
49	14.089	2-ethyl-5-methyl-Phenol	0.14	
53	14.402	2,3,6-Trimethylphenol		0.09
63	15.04	4-Hydroxybenzyl alcohol	0.17	
66	15.167	p-Allylphenol	0.1	
67	15.435	2-Decyn-1-ol	0.33	
68	15.437	(E)-2-tridecen-1-al		0.14
82	16.408	2-Nonenal, (E)-	0.16	
84	16.477	2-Hexyl-1-octanol		0.16
94	17.186	Cyclopropanecarboxylic acid		0.14
95	17.187	1-Naphthalenol	0.24	
96	17.213	1,1,4,5,6-Pentamethyl-2,3-dihydro-1H-indene	0.14	
97	17.265	1-Naphthalenol	0.19	0.9
101	17.409	Hexadecanal		0.1
102	17.478	3-Methyl-5-phenylpentan-1-ol	0.27	0.25
111	18.021	1-Methyl-2-naphthol	0.25	
112	18.022	1-Hydroxy-1,2,3,4-tetrahydronaph		0.17
119	18.262	2-(2-Phenyl-cyclohexyl)-ethanol	0.3	
127	18.711	1-Nonanol, 4,8-dimethyl-	0.48	
129	18.777	2,5-Dimethyl-3-phenylfuran		0.11
131	18.897	Decanoic acid		0.18
142	19.363	Succinic acid		0.8
143	19.433	Hexadecanoic acid		0.1
144	19.53	Pentadecanal-		0.11
149	19.723	2-Heptadecanone	0.54	
152	19.804	2-Undecene, 9-methyl-, (E)-		0.14
151	19.839	Methyl 4-methyloctanoate	0.9	
153	19.963	Phenol, 2-undecyl-	0.9	
160	20.432	1-Heneicosanol	0.9	
166	20.847	2-Hexadecanone	0.45	0.35
169	20.938	Pentadecanoic acid, methyl ester		0.1
171	21.113	11-Tridecen-1-ol		0.16
176	21.363	1-Methylcyclohexyl acetate		0.9

185	22.011	2-Propenoic acid, 3-(4-methoxyphenyl)-	0.13	
189	22.193	trans-2-Pinanol	0.17	
205	23.743	4-tert-Butylcyclohexyl acetate	0.28	
208	23.97	Cyclopropaneoctanoic acid	0.9	
218	24.733	Ethanol, 2-(9-octadecenyloxy)-		0.12
219	24.734	Pentadecanal-	0.13	
221	24.83	2,6,10-Dodecatrienoic acid, 3,7,11-trimethyl-,	0.1	
222	24.91	Cyclopropaneundecanal, 2-nonyl-	0.22	
228	26.243	2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro-	0.67	
234	27.572	Ergost-25-ene-3,5,6,12-tetrol	0.31	

Table S18

NCOCs from PLC and ISP pyrolysis by Py-GC/MS

Peak	RT (min)	Compound name	RC (%)	
			PLC	ISP
6	2.079	Hydrazinecarboxylicacid,1-methylethylester		0.27
7	2.117	DL-Alaninol	0.22	
10	2.927	Carbamimidothioic acid, 1-methylethyl ester		0.14
20	9.879	Phenyl carbamate	1.98	0.29
61	14.98	Diaziridinone		0.22
66	15.167	p-Allylphenol	0.1	
70	15.597	3-methyl-2-nitrobenzyl alcohol	0.53	
134	18.986	Propane, 3-cyclohexyl-1-phenyl-	0.34	
172	21.193	Benzenamine, 4,4'-methylenebis-	0.46	0.32
188	22.188	9-Octadecenamide, (Z)-		0.28
197	22.834	9-Octadecenenitrile, (Z)-	2.68	3.45
198	22.926	Nonadecanenitrile		0.19
214	24.516	9-Octadecenamide, (Z)-		1.24
215	24.627	Octadecanamide		0.24
226	26.07	9-Octadecenamide, (Z)-		0.11

Table S19

Alcohols detected in the OCOCs from PLC and ISP

Peak	RT (min)	Compound name	RC (%)	
			PLC	ISP
3	1.76	1,3-Propanediol		2.97
7	2.117	DL-Alaninol	0.22	
31	11.767	3-Nonen-1-ol,	0.39	
47	13.932	2,4-Hexadiyn-1,6-diol	0.43	
63	15.04	4-Hydroxybenzyl alcohol	0.17	
67	15.435	2-Decyn-1-ol	0.33	
84	16.477	2-Hexyl-1-octanol		0.16
102	17.478	3-Methyl-5-phenylpentan-1-ol	0.27	0.25
119	18.262	2-(2-Phenyl-cyclohexyl)-ethanol	0.3	
127	18.711	1-Nonanol, 4,8-dimethyl-	0.48	
160	20.432	1-Heneicosanol	0.9	
171	21.113	11-Tridecen-1-ol		0.16
189	22.193	trans-2-Pinanol	0.17	
218	24.733	Ethanol, 2-(9-octadecenyloxy)-		0.12
234	27.572	Ergost-25-ene-3,5,6,12-tetrol	0.31	

Table S20

Ketones detected in the OCOCs from PLC and ISP

Peak	RT (min)	Compound name	RC (%)	
			PLC	ISP
11	2.944	cyclohepta-2,4,6-trien-1-one	0.9	
13	4.192	4-Methyl-2-pentanone		0.2
14	5.448	4-Methyl-3-penten-2-one		0.13
24	10.588	2,3-dimethyl-2-cyclopenten-1-one	0.15	
149	19.723	2-Heptadecanone	0.54	
166	20.847	2-Hexadecanone	0.45	0.35

Table S21

Esters detected in the OCOCs from PLC and ISP

Peak	RT (min)	Compound name	RC (%)	
			PLC	ISP
12	3.724	Methyl methacrylate	0.19	
151	19.839	Methyl 4-methyloctanoate	0.9	
169	20.938	Pentadecanoic acid, methyl ester		0.1
176	21.363	1-Methylcyclohexyl acetate		0.9
205	23.743	4-tert-Butylcyclohexyl acetate	0.28	

Table S22

Phenols detected in the OCOCs from PLC and ISP

Peak	RT (min)	Compound name	RC (%)

			PLC	ISP
25	11.137	Cresol	0.92	0.31
32	12.565	2-Ethyl-phenol	0.08	
33	12.693	2,6-dimethyl-Phenol	0.51	0.31
36	13.026	4-Ethyl-phenol	0.33	
37	13.064	2,5-dimethyl-Phenol	0.1	0.15
38	13.075	2,3-dimethyl-Phenol	0.32	
43	13.56	2-Ethyl-6-methyl-phenol		0.2
49	14.089	2-ethyl-5-methyl-Phenol	0.14	
53	14.402	2,3,6-Trimethyl-phenol		0.09
66	15.167	p-Allyl-phenol	0.1	
95	17.187	1-Naphthalenol	0.24	
111	18.021	1-Methyl-2-naphthol	0.25	
153	19.963	Phenol, 2-undecyl-	0.9	

Table S23

Aldehydes detected in the OCOCs from PLC and ISP

Peak	RT (min)	Compound name	RC (%)	
			PLC	ISP
21	10.128	Decanal	0.13	
27	11.548	(2E)-2-Nonenal	1.4	
28	11.553	2-Decenal		0.69
30	11.766	Nonanal		0.22
68	15.437	(E)-2-tridecen-1-al		0.14
82	16.408	2-Nonenal, (E)-	0.16	
101	17.409	Hexadecanal		0.1
144	19.53	Pentadecanal-		0.11
219	24.734	Pentadecanal-	0.13	
222	24.91	Cyclopropaneundecanal, 2-nonyl-	0.22	

Table S24

Ethers detected in the OCOCs from PLC and ISP

Peak	RT (min)	Compound name	RC (%)	
			PLC	ISP
46	13.764	ethenoxybenzene	0.1	

Table S25

OTCs detected in the OCOCs from PLC and ISP

Peak	RT (min)	Compound name	RC (%)	
			PLC	ISP
1	1.585	Carbon dioxide	23.71	3.85
8	2.373	acetic acid		1.04
9	2.561	Tetrahydrofuran		0.19
94	17.186	Cyclopropanecarboxylic acid		0.14
96	17.213	1,1,4,5,6-Pentamethyl-2,3-dihydro-1H-indene	0.14	

112	18.022	1-Hydroxy-1,2,3,4-tetrahydronaph		0.17
129	18.777	2,5-Dimethyl-3-phenylfuran		0.11
131	18.897	Decanoic acid		0.18
142	19.363	Succinic acid		0.8
143	19.433	Hexadecanoic acid		0.1
152	19.804	2-Undecene, 9-methyl-, (E)-		0.14
185	22.011	2-Propenoic acid, 3-(4-methoxyphenyl)-	0.13	
208	23.97	Cyclopropaneoctanoic acid	0.9	
221	24.83	2,6,10-Dodecatrienoic acid, 3,7,11-trimethyl-,	0.1	
228	26.243	2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro-	0.67	

Table S26

Nomenclature

Full name	Nomenclature
Relative abundance (%)	RA
Relative content (area %)	RC
Oxygen-containing organic compounds	OCOCs
Other compounds	OCs
Nitrogen-containing organic compounds	NCOCs
Moisture content	M
Ash content	A
Volatile matter content	VM
Fixed carbon content	FC
Aliphatic carbon	C_{al}
Aromatic carbon	C_{ar}