

Bio-oils from vacuum ablative pyrolysis of torrefied tobacco residues

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Supplemental information

Table 1S Light oil GCMS Product list (in area %)

Retention Time (min)	Product ID	450 °C	500 °C	550 °C	600 °C	Raw 600 °C
3.85	2-Butenal					0.15
4.01	2,3-Butanedione	0.15				
4.11	2-Propanone, 1-hydroxy-	10.63	11.59	13.37	11.39	10.00
4.80	Propanoic acid	0.15	0.22		0.33	
4.86	2-Propenoic acid	1.10	1.11		0.27	
4.90	1,2-Ethanediol (Ethylene glycol)			0.81	1.21	0.48
5.36	Acetoin	0.96	1.13	1.39	1.10	1.15
5.74	Cyclobutanone, 2-methyl-	1.80	2.03	2.39	2.16	2.16
6.31	1-Butene, 2,3-dimethyl-	0.19	0.20	0.20	0.21	0.32
6.48	Pyridine	0.56	0.67	0.71	0.47	0.70
6.71	Acetonitrile, (dimethylamino)-			0.24	0.15	
6.80	2-Cyclopenten-1-one, 2-hydroxy-	0.37	0.45	0.45	0.43	0.37
7.32	1-Hydroxy-2-butanone	1.34	1.61	1.93	1.74	1.73
7.68	Pentanoic acid					0.25

8.06	2,4-Dimethyl-2-oxazoline-4-methanol	4.29	3.32	2.41	2.08	1.75
8.20	Cyclopentanone	0.73	0.67	0.95	0.72	1.02
8.45	1H-Pyrazole, 4,5-dihydro-5-methyl-	0.30	0.33	0.25	0.22	
8.51	Propanoic acid, 2-hydroxy-2-methyl-	0.18	0.22	0.27	0.21	0.22
8.68	1H-1,2,4-Triazole, 3-methyl-			1.08		0.95
9.68	2-Cyclopenten-1-one	4.63	5.54	6.00	5.32	6.66
10.02	2-Pentanone, 4-hydroxy-4-methyl-	0.28	0.20	0.14	0.22	0.22
10.10	2-Cyclopenten-1-one, 2-hydroxy-	0.25	0.22	0.26	0.19	0.38
10.40	2-Pentanone, 4-hydroxy-4-methyl-					0.17
10.49	2-Furanmethanol	2.79	2.93	2.64	2.48	2.39
10.61	2-Furanmethanol, tetrahydro-	0.26	0.36	0.38	0.37	0.39
10.77	Pyridine, 3-methyl-	0.49	0.26	0.30	0.23	0.38
10.99	2-Propanone, 1-(acetyloxy)-	2.20	2.13	1.90	1.78	1.98
11.54	4-Cyclopentene-1,3-dione	1.08	1.50	1.22	1.21	1.78
12.14	1H-1,2,4-Triazole	0.84	0.39	0.18	0.21	0.45
12.42	2-Cyclopenten-1-one, 2-methyl-	1.58	1.90	2.17	2.12	2.32
12.49	2(5H)-Furanone	0.53	0.82	0.74	0.88	0.79
12.60	Butanoic acid, 4-hydroxy-	1.98	2.00	1.96	1.87	1.52
12.80	Methyl propargyl ether	1.25	0.87	0.58	0.64	0.61
13.07	2-Cyclopenten-1-one, 2-hydroxy-	0.76	0.87	0.72	0.57	0.66
13.46	6-Methyl-1,5-diazabicyclo[3.1.0]hexane		0.16			
13.63	9-Azabicyclo(6,2,0)decan-10-one					0.16
14.49	2-Furancarboxyaldehyde	0.45	1.17	1.05	1.08	1.37
14.56	2-Cyclopenten-1-one, 3-methyl-	2.71	2.96	3.51	2.26	3.41
14.89	1-Penten-3-one, 2-methyl-	0.16	0.18	0.19	0.16	0.16
15.07	Phenol	1.15	1.39	1.26	1.26	1.50
15.39	3-Amino-s-triazole	0.92	0.71	1.07	0.94	0.89
15.59	1-(3H-Imidazol-4-yl)-ethanone	0.76	0.34	0.33	0.23	0.37
15.75	2,4-Dimethyl-2-oxazoline-4-methanol	1.12	0.92	1.41	1.16	0.86
16.10	1,1-Ethenediol, diacetate	0.50	0.97	0.41	0.41	0.86
16.66	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	2.53	2.86	2.94	3.11	2.82

17.09	2-Cyclopenten-1-one, 2,3-dimethyl-	1.06	0.92	0.70	0.76	0.88
17.21	Oxazole	0.29	0.16			0.23
17.40	1H-Tetrazol-5-amine	0.15	0.16	0.16	0.20	0.17
17.97	2-Pyrrolidinone	0.92	1.04	1.06	1.29	1.07
18.13	1H-1,2,4-Triazole	0.26				
18.34	p-Cresol	0.54	0.60	0.57	0.63	0.79
18.43	1H-Imidazole-4-methanol	0.51	0.49	0.53	0.61	0.77
18.64	3-Furancarboxylic acid, methyl ester	0.18	0.15	0.18	0.21	
18.99	3-Pyridinol	1.31	1.04	0.33	0.84	0.82
19.07	Pentanal	2.10	1.49	0.84	1.02	1.06
19.74	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-	0.74	0.77	0.68	0.68	0.66
20.65	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	0.51	0.85	0.61	0.63	0.56
20.74	Phenol, o-amino-	0.26	0.30	0.27	0.44	0.37
21.9	(S)-(+)-2',3'-Dideoxyribonolactone	0.40	0.34	0.34	0.45	0.33
22.04	Catechol	0.67	0.69	0.81	1.00	0.87
22.83	1,4:3,6-Dianhydro-alpha,-d-glucopyranose	0.46	0.35	0.30	0.53	0.33
23.02	5-Hydroxymethylfurfural	0.78	1.27	0.94	1.35	1.45
24.31	Hydroquinone	4.52	3.56	3.82	4.38	3.83
26.40	Orcinol	0.76	0.67	0.69	0.81	0.75
26.78	Nicotine Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-	12.29	14.70	14.42	14.70	14.26
-	Unknowns	19.33	15.24	14.92	18.07	16.47

Table 2S Heavy oil GCMS Product list (in area %)

Retention Time (min)	Product ID	450 °C	500 °C	550 °C	600 °C	Raw 600 °C
3.62	1,4-Cyclohexadiene	0.24	0.25	0.31		
4.01	2-Pentanone	0.15				
4.09	Benzene	1.38	1.08	1.79	2.11	
4.21	Neopentane	0.20				
4.63	Propanoic acid	0.28	0.24			
4.71	2-Pentanone	0.69	0.77	0.85		
5.28	Furan, 2,5-dimethyl	1.02	0.89	0.98		
5.35	Acetoin	0.16				
5.53	4-Methyl-2H-pyran	0.13				
6.12	Propane, 2-nitro-	0.10				
6.32	1H-Pyrrole, 1-methyl-	0.44	0.27	0.45		
6.48	1-Methylcyclohexa-2,4-diene	0.67	0.37	0.82		
6.74	Pyrrole	1.24	0.81	1.34		
7.33	Toluene	2.39	2.47	3.69	3.83	3.51
7.42	3-Buten-2-one, 3-methyl-	0.28	0.26	0.44		
7.95	3-Hexanone	0.12				
8.04	Oxazole, 4,5-dihydro-2,2,2-trimethyl-	1.35	0.95	1.36		
8.2	Cyclopentanone	0.46	0.41	0.62		
8.51	Ethanone, 1-(2-furanyl)-	0.35	0.30	0.35		
9.31	2-Acetyl-2-methyltetrahydrofuran	0.05				
10.02	2-Pentanone, 4-hydroxy-4-methyl-	0.26	0.33	0.32		
10.11	2-cyclopenten-1-one,2-hydroxy-	0.45	0.49	0.69		
10.40	R-+-3-Methylcyclopentanone	0.19	0.15			
10.47	2-Furanmethanol	1.58	1.23	1.23	1.49	
10.85	Ethylbenzene	0.64	0.66	0.91		
11.53	4-Cyclopentene-1,3-dione	0.63	0.69	0.57		
12.41	2-Cyclopenten-1-one, 2-methyl-	1.51	1.32	1.70	1.72	
12.50	2(5H)-Furanone	0.19	0.22			
12.59	Ethanone, 1-(2-furanyl)-	1.10	0.87	0.97		

13.63	2-Cyclopenten-1-one, 3,4-dimethyl-	0.36	0.30	0.37		
13.91	Phenyl-pentamethyl-disiloxane	0.21	0.25	0.37		7.30
14.48	2-Furancarboxaldehyde, 5-methyl-	1.09	1.01	1.09	1.57	
14.55	2-Cyclopenten-1-one, 3-methyl- *4-Methyl-2H-Pyran	*1.87	2.04	2.37	3.15	
15.05	Phenol	4.11	4.46	4.82	6.92	4.09
15.58	4,4-Dimethyl-2-cyclopenten-1-one	0.42	0.37	0.41		
16.65	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	1.96	1.76	1.78	2.52	
17.08	2-Cyclopenten-1-one, 2,3-dimethyl-	1.62	1.53	1.85	2.38	
17.63	o-Cresol	2.51	3.11	3.42	5.12	3.05
18.22	1-Hexanone, 5-methyl-1-phenyl-	0.25	0.21			
18.35	p-Cresol	2.52	3.50	3.96	7.75	4.58
18.82	2-Cyclopenten-1-one, 3,4,5-trimethyl- *Phenol, 2-methoxy	*2.35	1.87	2.08	2.41	
19.05	Cyclopropyl carbinol	1.41	1.24	1.03		
19.21	2-cyclohexen-1-one, 4,4-dimethyl-	1.65	1.33	1.32	1.65	
19.74	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-	1.15	0.99	1.08	1.31	
20.35	(2S,6R,7S,8E)-(+)-2,7-Epoxy-4,8-megastigmadiene	0.49	0.67	0.54		
20.73	Phenol, 3,4-dimethyl-	0.53	0.88	0.85		
20.8	Phenol, 2,4-dimethyl-	0.82	1.25	1.16	2.33	
21.27	Phenol, 4-ethyl-	0.48	0.92	1.05	1.78	
22.03	Catechol *Phenol, 2-ethoxy-	*1.34	1.48	2.20	2.77	
23.98	1,2-Benzenediol, 3-methyl-	1.69	1.25	1.27	2.58	
24.29	Hydroquinone	0.30	0.37			
24.92	2H-Inden-2-one, 1,3-dihydro-	3.45	2.54	3.08	6.35	2.20
25.23	Indole	0.53	0.64	0.62		
25.69	2-Methoxy-4-vinylphenol	0.59	0.62	0.63		
26.39	Orcinol	0.68	0.55	0.46	1.29	
26.78	Nicotine Pyridine, 3-(1-Methyl-2-pyrrolidinyl)-, (S)-	4.74	5.28	5.50	10.77	9.42
50.96	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	2.35	7.27	1.46	1.88	11.46
-	Unknowns	35.76	33.32	30.93	16.66	34.84

