

Supporting information

Characterization and Comparison of Fast Pyrolysis Bio-oils from Pinewood, Rapeseed Cake, and Wheat Straw Using ^{13}C NMR and Comprehensive GC \times GC

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Table: Table S1

Table S1. List of identified compounds and detailed composition of the bio-oils (wt. %) obtained via a GC×GC-FID/TOF-MS analytical approach. M: molecular mass.

M [g mol ⁻¹]	Compound	Pinewood bio-oil [wt. %]	Wheat straw bio-oil [wt. %]	Rapes eed cake bio-oil [wt. %]	Refer ences
Non-aromatic compounds					
Alcohols					
58	2-propenol (allyl alcohol)	0.24			5
58	2-propen-1-ol		0.18		14
72	Cyclobutanol		0.07		
118	1,2,3-cyclopentanetriol		0.05		
184	Z-2-dodecenol		0.003		
184	Z-4-dodecenol			0.05	
184	Z-8-dodecen-1-ol			0.26	
212	3-isopropyl-4-methyl-dec-1-en-4-ol	0.03			5
244	1,15-pentadecanediol		0.02		
297	3,7,11,15-tetramethyl-2-hexadecen-1-ol		0.004		
<u>Total</u>		<u>0.27</u>	<u>0.32</u>	<u>0.30</u>	
Carboxylic acids					
60	acetic acid	4.58	3.79		5, 14
74	propionic acid	0.23	0.36		5, 14
86	3-butenic acid	0.05	0.03		
88	butyric acid	0.04	0.11	0.14	5
88	2-methyl-propanoic (isobutyric) acid	0.006			5, 14

100	2-methylcyclopropanecarboxylic acid		0.004		
104	4-hydroxybutyric acid		0.41	0.74	5
128	3-heptenoic acid		0.01		
130	heptanoic acid		0.01		
144	octanoic acid		0.02		
214	tridecanoic acid		0.01		
228	tetradecanoic acid			0.05	
240	Z-8-methyl-9-tetradecenoic acid		0.04		
256	hexadecanoic (palmitic) acid		0.05	0.07	26
284	octadecanoic (stearic) acid		0.01		
<u>Total</u>		<u>4.90</u>	<u>4.85</u>	<u>0.10</u>	
Aldehydes					
44	Acetaldehyde	0.57	0.16		5, 14
60	Glycolaldehyde (hydroxyacetaldehyde)	2.03	1.14		5, 14
90	2,3-dihydroxy-propanal (glyceraldehyde)	0.08	0.17		5, 14
100	1,5-pentanedial (glutaraldehyde)	0.15			5, 14
210	E-12-tetradecenal			0.09	
252	3-heptadecenal		0.01		
<u>Total</u>		<u>2.82</u>	<u>1.48</u>	<u>0.09</u>	
Ketones					
58	Acetone	0.24	0.15		5, 14
72	2-butanone	0.15			
74	1-hydroxy-2-propanone (acetol)	1.354	2.72		5, 14
82	2-cyclopenten-1-one	0.05	0.19		5, 14, 39
88	1-hydroxy-2-butanone		0.48		5, 14, 39

96	2-methyl-2-cyclopenten-1-one	0.05	0.10	5, 14
96	2-cyclohexen-1-one		0.01	5, 39
96	1-(2-methylidenecyclopropyl)ethanone			0.05
98	1,2-cyclopentanedione	0.05		5
98	2-hydroxy-2-cyclopenten-1-one		0.01	5, 14, 39
102	1-hydroxy-3-methyl-2-butanone		0.02	5
110	2,3-dimethyl-2-cyclopenten-1-one	0.03	0.08	5, 14
110	2-cyclohexene-1,4-dione		0.04	5
110	3-ethyl-2-cyclopenten-1-one		0.04	5
110	3,4-dimethyl-2-cyclopenten-1-one		0.02	5, 14
112	2-hydroxy-3-methyl-2-cyclopenten-1-one	0.33	0.55	5, 14, 39
112	3-methyl-1,2-cyclopentanedione		0.03	5
112	1-cyclopentyl-ethanone		0.02	
114	2,5-hexanedione		0.03	5
114	3-hydroxy-cyclohexanone		0.02	5
116	1-(acetyloxy)-2-propanone	0.05	0.12	5, 14
124	2-ethylidenecyclohexanone		0.02	
126	3-ethyl-2-hydroxy-2-cyclopenten-1-one	0.05	0.15	5, 14
130	1-(acetyloxy)-2-Butanone	0.05	0.04	5
208	6,10-dimethyl-5,9-dodecadien-2-one		0.03	
226	2-pentadecanone		0.02	
254	2-heptadecanone		0.04	
268	6,10,14-trimethyl-2-pentadecanone			
Total		<u>2.39</u>	<u>4.94</u>	<u>0.05</u>
Esters				
104	1,2-ethanediol, monoacetato	0.12	0.06	

144	2-ethylbutyl acetate	0.03		
160	1,3-propanediol, diacetate	0.06		
296	11-octadecenoic acid, methyl ester			0.72
296	trans-13-octadecenoic acid, methyl ester			0.62
Total		<u>0.21</u>	<u>0.06</u>	<u>1.34</u>

Heterocyclic compounds

Furans

84	2(5H)-furanone (γ -crotonolacton)	0.37			5, 39
84	2(3H)-furanone	0.11			5
88	tetrahydro-2-furanol			0.46	
96	2-furaldehyde (furfural)	0.24	0.14		5, 14, 39
96	3-furaldehyde	0.01	0.02		5, 14
98	4-methyl-2(5H)-furanone	0.14	0.08		5, 14
98	3-methyl-2(5H)-furanone	0.11	0.07		5, 14
98	5-methyl-2(5H)-furanone	0.09	0.01		5, 14, 39
102	4-hydroxydihydro-2(3H)-furanone	0.14			5
110	5-methyl-2-furaldehyde	0.05	0.22		5
110	1-(2-furanyl)-ethanone (2-acetyl-furan)	0.05	0.06		5, 14
112	2,5-dihydro-3,5-dimethyl-2-furanone	0.04	0.04		5, 14
112	3-methyl-2,5-furandione		0.02		
116	5-(hydroxymethyl)dihydrofuran-2(3H)-one		0.07		
126	5-hydroxymethylfurfural	0.22			5
168	5-acetoxymethyl-2-furaldehyde	0.06			
Total		<u>1.62</u>	<u>0.72</u>	<u>0.46</u>	

Pyrans

96	4H-pyran-4-one	0.05		5
112	3,4-dihydro-6-methyl-2H-pyran-2-one	0.06		
126	3-hydroxy-2-methyl-4H-pyran-4-one (maltol)	0.13	0.07	5, 14
Total		<u>0.24</u>	<u>0.07</u>	

Other heterocyclic compounds

122	2,7-dimethyl-oxepine		0.03	
144	4-methyl-2-(1-methylpropyl)-1,3-Dioxolane	0.08		
212	dodecyl-oxirane		0.01	
Total		<u>0.08</u>	<u>0.04</u>	

Carbohydrates

144	1,4:3,6-dianhydro- α -d-glucopyranose	0.22	0.17	5, 14
144	2,3-anhydro-d-mannosan		0.24	5
162	Levoglucosan	5.58	0.66	5, 14, 39
180	D-allose	1.25	0.17	
342	Sucrose		0.03	
Total		<u>7.05</u>	<u>1.27</u>	

Non-aromatic hydrocarbons

96	1-methyl-cyclohexene		0.03	14
98	1,1-diethylcyclopropane		0.003	
98	1-heptene		0.09	
110	Z-cyclooctene		0.20	

110	1,6-octadiene	0.02
112	1-octene	0.07
114	Octane	0.02
124	(1-methylethylidene)-cyclohexane	0.02
124	(E)-1,3-nonadiene	0.05
124	1-butylcyclopentene	0.05
124	1,8-nonadiene	0.03
126	1-nonene	0.08
128	Nonane	0.02
136	D-limonene	0.01
138	(Z)-cyclodecene	0.08
138	1-butyl-cyclohexene	0.06
140	1-methyl-2-(3-methylpentyl)- cyclopropane	0.10
150	6-butyl-1,4-cycloheptadiene	0.06
152	(4E)-1,4-undecadiene	0.20
154	methyl cyclodecane	0.003
154	1-undecene	0.14
154	(E)-4-undecene	0.06
166	(E,Z)-2,4-dodecadiene	0.16
166	1-heptyl-cyclopentene	0.09
166	(5E,7E)-dodeca-5,7-diene	0.07
168	(Z)-3-dodecene	0.17
180	1-octyl-cyclopentene	0.06
180	Z-1,6-tridecadiene	0.02
182	Z-6-tridecene	0.08
194	1,13-tetradecadiene	0.08
194	E-1,9-tetradecadiene	0.05
196	1-octyl-cyclohexane	0.05

196	2-isohexyl-6-methyl-1-heptene	0.01	
196	1-tetradecene		0.13
210	1-(1-methylethyl)-2-nonyl-cyclopropane		0.07
212	2,6,10-trimethyl-dodecane		0.07
222	1,15-hexadecadiene		0.34
222	3-undecyl-cyclopentene		0.12
224	(Z)-7-hexadecene		0.09
236	1-heptadecyne		0.06
236	6,9-heptadecadiene		0.03
240	3-methyl-hexadecane		0.03
252	(E)-9-octadecene		0.39
267	cis-2-methyl-7-octadecene		0.83
269	3-methyl-octadecane		0.12
Total		0.05	4.41

Non-aromatic nitrogen-containign compounds

250	5,10-Diethoxy-2,3,7,8-tetrahydro-1H,6H-dipyrrolo[1,2-a:1',2'-d]pyrazine		0.086
263	Oleonitrile		0.312
281	(Z)-9-octadecenamide		1.341
Total			1.739

Aromatic compounds

Aromatic hydrocarbons

92	Toluene	0.39	39
104	bicyclo[4.2.0]octa-1,3,5-triene	0.12	
106	1,3-dimethyl-benzene (m-xylene)	0.05	

106	Ethylbenzene			0.10	
148	Pentylbenzene			0.11	
<u>Total</u>				<u>0.77</u>	
Aromatic oxygenates (others)					
132	2,3-dihydro-1H-Inden-1-one	0.02			5, 14
132	1,3-dihydro-2H-Inden-1-one		0.03		
140	2-methoxyresorcinol		0.09		
146	2,3-dihydro-2-methyl-1H-Inden-1-one		0.01		
150	2,3-dimethyl-benzoic acid	0.03	0.06		
150	4-hydroxy-2-methylacetophenone	0.01			5
150	4-chromanol		0.02		
150	3,4-dimethyl-benzoic acid		0.02		
154	2,6-dimethoxy-phenol (syringol)		0.20	0.11	5
164	3-allyl-6-methoxyphenol		0.09		
166	1-(3-Hydroxy-4-methoxyphenyl)ethanone	0.21	0.10		14
168	1,2,4-trimethoxybenzene		0.06		5
180	1,2-dimethoxy-4-n-propylbenzene		0.03		14
180	1-(4-hydroxy-3-methoxyphenyl)-2-propanone		0.07		14
180	4-methyl-2,5-dimethoxybenzaldehyde			0.31	
182	2-ethoxy-6-(methoxymethyl)phenol		0.05		
210	1-(2,6-dihydroxy-4-methoxyphenyl)-1-butanone		0.02		
278	mono(2-ethylhexyl) phthalate		0.01		
<u>Total</u>		<u>0.27</u>	<u>0.86</u>	<u>0.42</u>	

Aldehydes

122	2-hydroxy-benzaldehyde	0.04			5, 14
122	3-hydroxy-benzaldehyde	0.04			5, 14
178	4-hydroxy-2-methoxycinnamaldehyde		0.07		
Total		<u>0.08</u>	<u>0.07</u>		

Phenols

94	Phenol	0.06	0.28	0.50	5, 14, 39
108	4-methyl-phenol (p-cresol)	0.04	0.20	0.54	5, 14
108	2-methyl-phenol (o-cresol)	0.03	0.22	0.12	5, 14
122	2,4-dimethyl-phenol	0.03	0.12		5, 14
122	2,3-dimethyl-phenol	0.02			5
122	3-ethyl-phenol		0.17		5, 14
122	2,5-dimethyl-phenol		0.04		5, 39
122	2-ethyl-phenol		0.04		5, 14
122	4-ethyl-phenol			0.11	5
134	4-(2-propenyl)-phenol	0.09			5, 14
136	2-ethyl-6-methyl-phenol	0.02			5, 14
136	3-ethyl-5-methyl-phenol	0.02			5, 14
136	2,4,5-trimethyl-phenol	0.01			5, 14
136	2-ethyl-5-methyl-phenol		0.04		14
Total		<u>0.30</u>	<u>1.11</u>	<u>1.27</u>	

Benzenediols

110	1,2-benzenediol (catechol)	0.22	0.22		5, 14
110	1,3-benzenediol (resorcinol)	0.15			5
110	1,4-benzenediol (hydroquinone)	0.07	0.08		5, 14
124	4-methyl-1,2-benzenediol	(4- 0.07	0.15		5, 14

	methylcatechol)			
124	3-methylcatechol	0.04		5, 14
124	2-methylhydroquinone		0.04	5
124	2-methyl-resorcinol		0.03	5
138	4-ethyl-resorcinol	0.03		5, 14
138	4,5-dimethylresorcinol	0.06		5, 14
138	4-ethylcatechol	0.04		5
138	2,5-dimethylhydroquinone	0.19		5, 14
152	4-propyl-1,3-benzenediol (4-propylresorcinol)	0.02		14
152	3,4-dihydroxyacetophenone (4-acetylpyrocatechol)		0.02	
Total		0.90	0.54	
Methoxy-, dimethoxy phenol derivatives				
124	2-methoxy-phenol (guaiacol)	0.50	0.44	5, 14, 39
138	4-methylguaiacol (creosol)	0.58		5
140	3-methoxy-1,2-benzenediol		0.07	
152	Vanillin	0.25	0.13	5, 14, 39
152	4-ethylguaiacol	0.15		5, 14, 39
164	2-methoxy-5-(1-propenyl)-phenol, (E)-		0.05	
164	4-allylguaiacol (eugenol)		0.01	5
166	4-propylguaiacol		0.02	5
180	4-(3-hydroxy-1-propenyl)-2- methoxy-phenol		0.02	
182	2-ethoxy-6-(methoxymethyl)phenol		0.05	
194	2,6-dimethoxy-4-(2-propenyl)- phenol		0.07	
350	4-methoxyphenyl nonyl succinate		0.03	

<u>Total</u>		<u>1.47</u>	<u>0.88</u>
Aromatic nitrogen-containing compounds			
117	benzyl nitrile		0.10
117	Indole		0.07
131	Benzenepropanenitrile		0.04
131	3-methylindolizine		0.16
179	3,4-dimethylphenyl methylcarbamate		0.13
<u>Total</u>			<u>0.50</u>
