Prediction of FID response factor of pyrolysis bio-oil components by effective carbon number model

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SUPPLEMENTARY INFORMATION

The chemicals in this study are purchased from Sigma Aldrich: Acetic acid 99.5%, propionic acid 99.5%, butyric acid 99%, isobutyric acid 99%, phenol 99%, anisole 99.7%, m-cresol 98%, 2,6-dimethoxyphenol 99%, acetol 90%, furfural 99% and 3,4-dihydropyran 97%, 2,5-dimethoxy toluene 99%, 2-ethyl phenol 99%, 3,4,5-trimethoxytoluene 97%, 2-allyl-6-methylphenol 98%, Eugenol 99%, 4-ethoxy phenol 99%, 1-indanone 99%, 2-ethoxyphenol 98%, 4-ethylphenol 99%, 3,4-dimethoxy toluene 96%, 3,5-dimethoxy toluene 98%, 4-ethylguaiacol 98%, 2-allyl phenol 98%, 2-methoxy-4-propylphenol 99%, 3-isopropylphenol 97%, 3-methylanisole 99%, 2-methoxy-4-methylphenol 99%, 2-methylanisole 99%, 4-methylanisole 99%, guaiacol 98%, p-cresol solid 99%, 2,3,5-trimethyl phenol 99% solid, 2,4-dimethylphenol 99%, guaiacol 98%, 2'-hydroxy-4'-methylacetophenone 97%, m-tolyl acetate 97%.

Reported values of RRFs from Meier et al., Dietz et al. and Katritzky et al. are used as the database for our model [1-3]. These data are reported in Table S1 below.

No.	Chemical names	Chemical family	$RRF_{i/heptane}$ Dietz et al.	$RRF_{i/heptane}$ Katritzky et al.	RRF_{Meier} Meier et al.
1	phenylacetic acid	Acid		0.63	
2	formic acid	Acid	0.01		
3	acetic acid	Acid	0.24		4.87
4	propionic acid	Acid	0.4		
5	butyric acid	Acid	0.48		
6	hexanoic acid	Acid	0.63		
7	heptanoic acid	Acid	0.61		
8	octanoic acid	Acid	0.65		
9	cyclohexanecarboxylic acid	Acid		0.6	
10	acetol	Alcohol			6.6

11	Hydroxy acetaldehyde	Alcohol			7.9
12	benzyl alcohol	Alcohol		0.86	
13	isopropanol	Alcohol	0.53		
14	sec-butanol	Alcohol	0.63		
15	methylisobutylcarbinol	Alcohol	0.74		
16	isobutanol	Alcohol	0.68		
17	methanol	Alcohol	0.23		
18	ethanol	Alcohol	0.46		
19	propanol	Alcohol	0.6		
20	m-butanol	Alcohol	0.66		
21	amyl alcohol	Alcohol	0.71		
22	hexyl alcohol	Alcohol	0.74		
23	1-octanol	Alcohol	0.85	0.77	
24	1-decanol	Alcohol	0.84	0.7	
25	1,3-propanediol	Alcohol		0.45	
26	1,4-butanediol	Alcohol		0.47	
27	tert-butanol	Alcohol	0.74		
28	benzaldehyde	Carbonyl		0.81	
29	acetophenone	Carbonyl		0.81	
30	propiophenone	Carbonyl		0.84	
31	cyclohexyl phenyl ketone	Carbonyl		0.75	
32	acetone	Carbonyl	0.49		
33	methylethylketone	Carbonyl	0.61		
34	cyclopentanone	Carbonyl		0.72	
35	cyclohexanone	Carbonyl	0.72	0.76	
36	cycloheptanone	Carbonyl		0.78	
37	ethylamylketone	Carbonyl	0.8		
38	diisobutylketone	Carbonyl	0.72		
39	methylisobutylketone	Carbonyl	0.71		
40	2,4-dimethyl-3-pentanone	Carbonyl		0.78	
41	ethylbutylketone	Carbonyl	0.71		
42	butyraldehyde	Carbonyl	0.62		
43	heptanoic aldehyde	Carbonyl	0.77		
44	octaldehyde	Carbonyl	0.78		
45	capric aldehyde	Carbonyl	0.8		
46	methyl acetate	Ester	0.2		
47	ehtyl acetate	Ester	0.38		

48	isopropylacetate	Ester	0.49		
49	isobutylacetate	Ester	0.54		
50	isoamylacetate	Ester	0.62		
51	methylamylacetate	Ester	0.63		
52	ethyl-(2)-ethylhexanoate	Ester	0.72		
53	n-butylacetate	Ester	0.55		
54	sec-butylacetate	Ester	0.52		
55	hexylcaproate	Ester	0.78		
56	1-decene	Hydrocarbons	1.01	0.94	
57	Acetylene	Hydrocarbons	1.07		
58	ethylene	Hydrocarbons	1.02		
59	cyclopentane	Hydrocarbons	1.04		
60	cyclohexane	Hydrocarbons	1.01	1.04	
61	hexene-1	Hydrocarbons	0.99		
62	1,1-dimethylcyclopentane	Hydrocarbons	1.03		
63	2-methylhexane	Hydrocarbons	1.02		
64	2,4-dimethylpentane	Hydrocarbons	1.02		
65	cycloheptane	Hydrocarbons	1.01		
66	1-octene	Hydrocarbons	1.03	1	
67	ethylcyclohexane	Hydrocarbons	1.01		
68	isopropylcyclopentane	Hydrocarbons	0.98		
69	n-propylcyclopentane	Hydrocarbons	0.97		
70	methane	Hydrocarbons	0.97		
71	ethane	Hydrocarbons	0.97		
72	propane	Hydrocarbons	0.98		
73	butane	Hydrocarbons	1.09		
74	pentane	Hydrocarbons	1.04		
75	hexane	Hydrocarbons	1.03		
76	heptane	Hydrocarbons	1	1	
77	octane	Hydrocarbons	0.97		
78	nonane	Hydrocarbons	0.98		
79	3,3-dimethylheptane	Hydrocarbons	1		
80	isopropylcyclohexane	Hydrocarbons	0.98		
81	1,2,4-trimethylbenzene	Aromatic HC	0.97		
82	1,3,5-trimethylbenzene	Aromatic HC	0.98		
83	m-xylene	Aromatic HC	1.04		
84	benzene	Aromatic HC	1.12	1.09	

85	toluene	Aromatic HC	1.07	1.17	
86	ethylbenzene	Aromatic HC	1.03		
87	n-propylbenzene	Aromatic HC	1.01		
88	n-butylbenzene	Aromatic HC	0.98		
89	p-xylene	Aromatic HC	1		
90	1,2,3-trimethylbenzene	Aromatic HC	0.98		
91	isopropylbenzene	Aromatic HC	0.97		
92	o-xylene	Aromatic HC	1.02	1.04	
93	sec-butylbenzene	Aromatic HC	1		
94	tert-butylbenzene	Aromatic HC	1.02		
95	4-Hydroxy-3-methoxybenzaldehyde (vanillin)	Phenolics			1.92
96	2'-Hydroxy-4'-methylacetophenone	Phenolics			
97	butyl phenyl ether	Phenolics		0.84	
98	anisole	Phenolics		0.79	
99	2-Methoxy phenol (Guaiacol)	Phenolics			1.41
100	2-methoxy-4-Methyl phenol	Phenolics			1.49
101	4-ethyl guaiacol	Phenolics			1.26
102	4-propyl guaiacol	Phenolics			1.4
103	4-methyl syringol	Phenolics			1.84
104	1,3,5-trimethoxybenzene	Phenolics		0.46	
105	benzyl phenyl ether	Phenolics		0.84	
106	eugenol	Phenolics			1.25
107	diphenyl ether	Phenolics		0.86	
108	4-vinyl guaiacol	Phenolics			1.26
109	2-isopropoxyphenol	Phenolics		0.72	
110	homovanillin	Phenolics			1.9
111	acetoguaiacone	Phenolics			1.9
112	syringaldehyde	Phenolics			2.14
113	4-vinylsyringol	Phenolics			1.45
114	2,6-dimethoxy phenol (syringol)	Phenolics			1.44
115	4-allyl syringol	Phenolics			2
116	4-propyl syringol	Phenolics			2
117	m-cresol	Phenolics		0.77	1.06
118	p-cresol	Phenolics		0.77	1.06
119	5,6,7,8-tetrahydro-l-naphthol	Phenolics		0.82	
120	2-ethylphenol	Phenolics		0.82	
121	2-Methyl phenol (o-cresol)	Phenolics		0.82	1.05

122	Phenol	Phenolics		0.73	1.08
123	m-cresol	Phenolics		0.77	1.06
124	4-ethylphenol	Phenolics		0.78	
125	2-isopropylphenol	Phenolics		0.81	
126	4-isopropylphenol	Phenolics		0.72	
127	2,5-dimethyl phenol	Phenolics			1.08
128	2,4 -dimethyl phenol	Phenolics			1.08
129	2,5-dimethoxytetrahydrofuran (cis)	Furanics			2.5
130	2,5-dimethoxytetrahydrofuran (trans)	Furanics			2.5
131	2-furaldehyde	Furanics			2.06
132	2-furfuryl alcohol	Furanics			2.1
133	2-hydroxy-1-methyl-1-cyclopentene-3-one	Furanics			1.2
134	3-furaldehyde	Furanics			2.06
135	5-hydroxymethyl-2-furaldehyde	Furanics			3.54
136	levoglucosan	Furanics			6.85

The RRF_{Meier} values used in Meier et al.[1] is define as following

$$RRF_{Meier} = \frac{amount_{sample}}{area_{sample}} \times \frac{area_{Fluoranthene}}{amount_{Fluoranthene}}$$

RRF_{Meier} is indeed the reciprocal of $\mathrm{RRF_{sample/Fluoranthene}}$ as defined in this study.
Therefore RRF_{Meier} can be converted to mRRF with phenol as the reference using the following equation.

$$\mathrm{mRRF_{i/phenol}} = \frac{MW_i}{RRF_{Meier,i} \times RRF_{Meier,phenol} \times MW_{phenol}} \quad \text{(S1)}$$

Based on Equation S1, the $mRRF_{i/phenol}$ value is calculated from Meier et al. and compared with own experimental $mRRF_{i/phenol}$ as shown in Table S2.

Table S2. Comparison of $mRRF_{i/phenol}$ from Meier et al.[1] and this study

No.	Chemical names	$mRRF_{i/phenol}$ Meier et al.[1]	$mRRF_{i/phenol}$ From this study
1	acetic acid	0.14	0.14
2	2,4 -dimethyl phenol	1.30	1.30
3	m-cresol	1.17	1.24
4	p-cresol	1.17	1.04
5	2,6-dimethoxy phenol	1.23	1.32
6	2-Methoxy phenol (Guaiacol)	1.01	1.00
7	2-methoxy-4-Methyl phenol	1.06	1.12

8	4-ethyl guaiacol	1.39	1.34
9	eugenol	1.51	1.60
10	2-furaldehyde	0.54	0.51
11	acetol	0.13	0.16

1. D. Meier, A. Oasmaa, C. Peacocke, 1997, p. 391.
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3. A.R. Katritzky, E.S. Ignatchenko, R.A. Barcock, V.S. Lobanov, M. Karelson, Analytical Chemistry 66 (1994) 1799. 10.1021/ac00083a005