

Supporting information

Characterization of pseudo-lignin from steam exploded birch

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It includes 12 pages with 5 figures and 1 table.

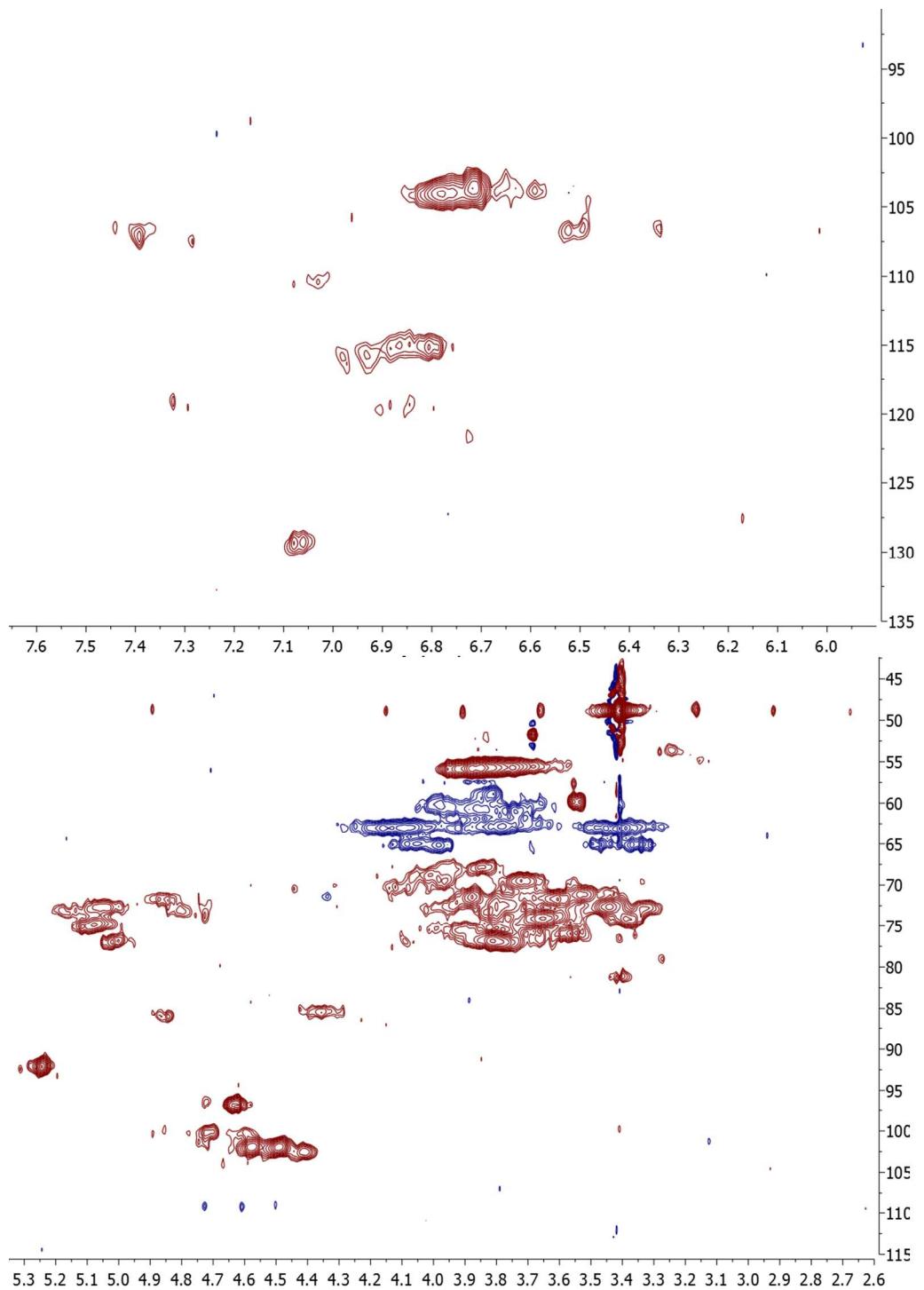


Figure S1. HSQC of SE-treated biomass of severity factor of 3.1 ($170\text{ }^{\circ}\text{C}$ – 10 min) in acetic acid-d₄. The shift values are slightly more upshift than with DMSO-d₆. The spectra are focused on aromatic region (above) and aliphatic region (below).

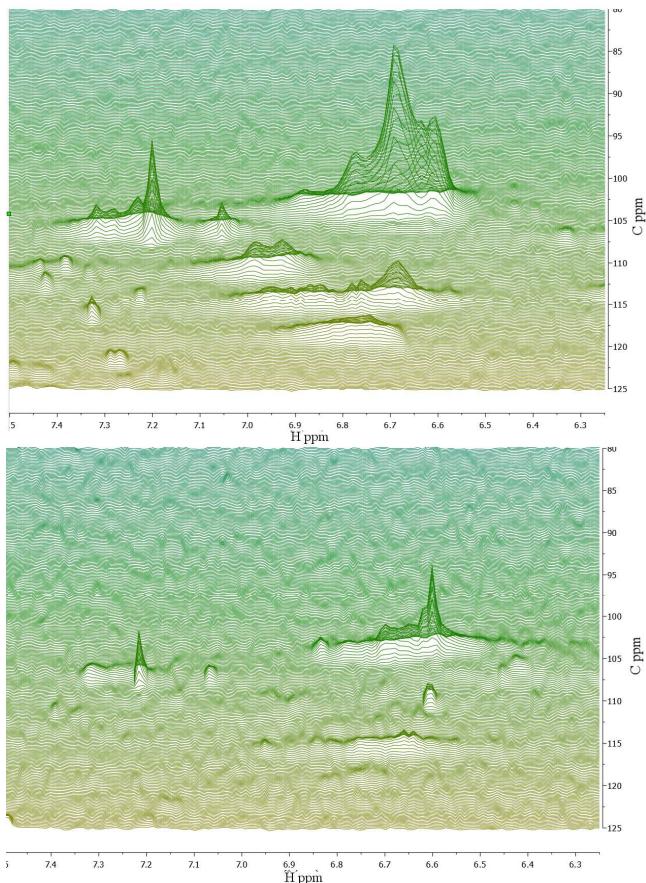


Figure S2. Topographic visualization of lignocellulosic biomass at untreated (above) and severity 4.7 (220 °C – 15 min) (below), focused on aromatic region.

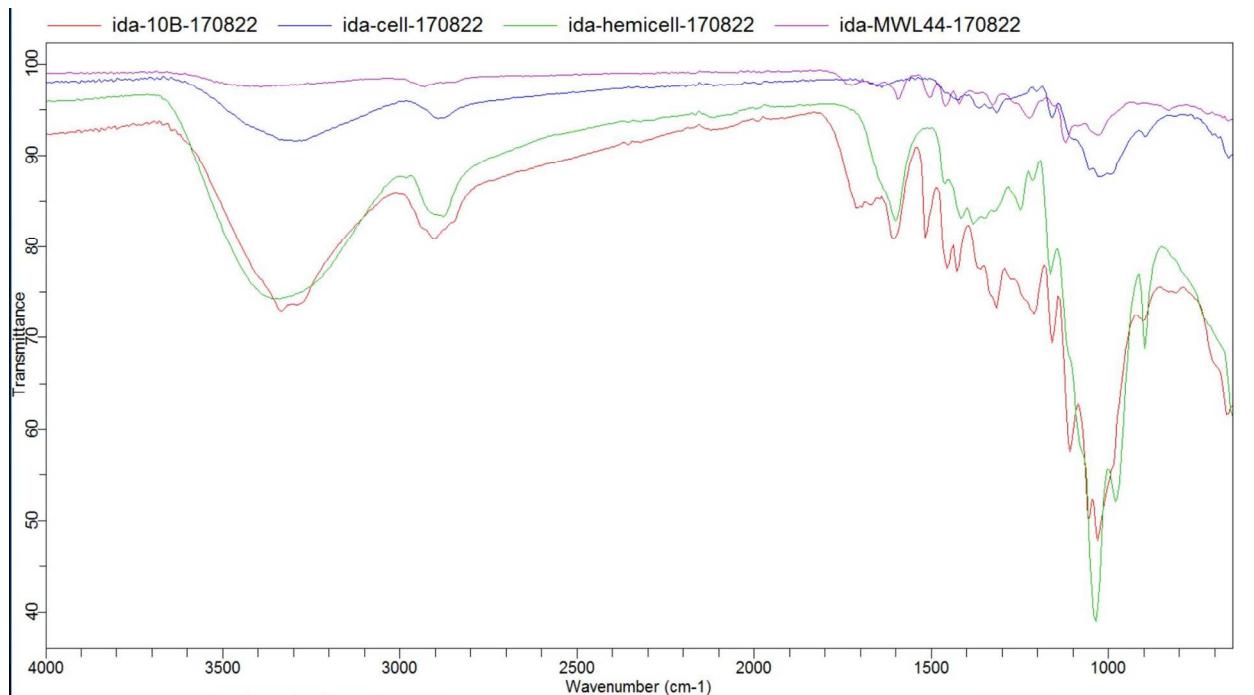


Figure S3. FTIR of milledwood lignin (red), cellulose (blue), hemicellulose (xylan, green) and se-treated biomass ($220\text{ }^{\circ}\text{C}$, 15 min, purple)

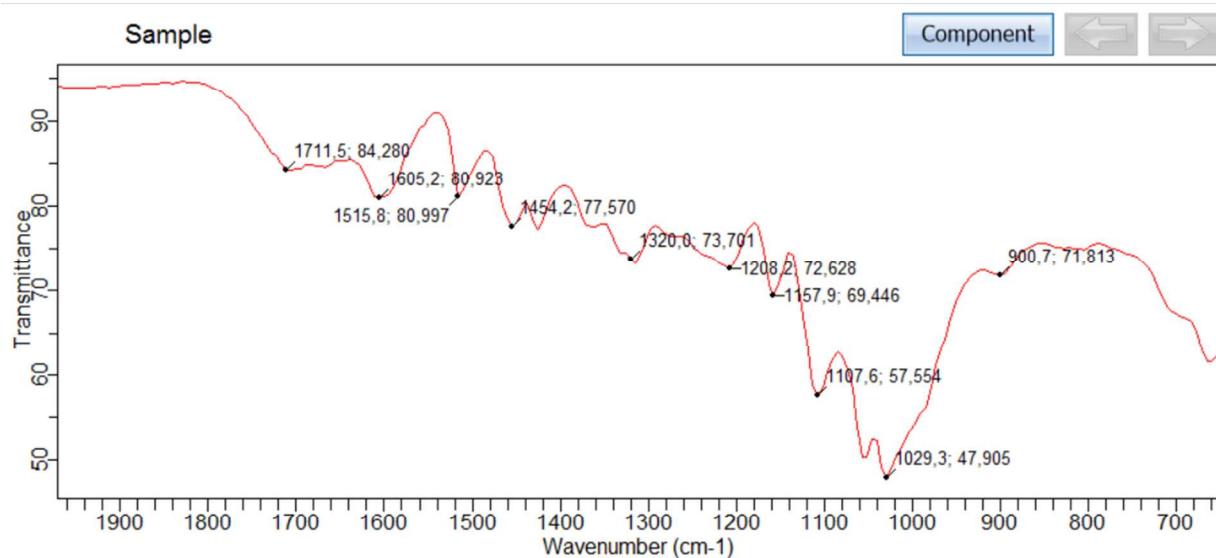
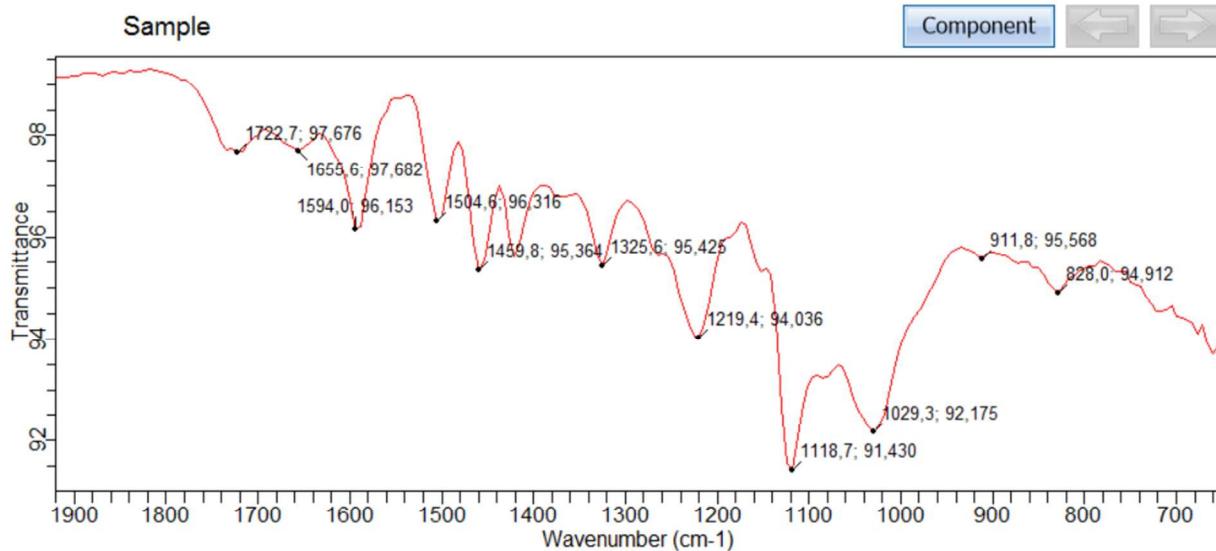


Figure S4. FT-IR of untreated biomass (above) and SE –treated with $\log R_0$ 4.7 (below), focused in on 700 cm^{-1} to 2000 cm^{-1} .

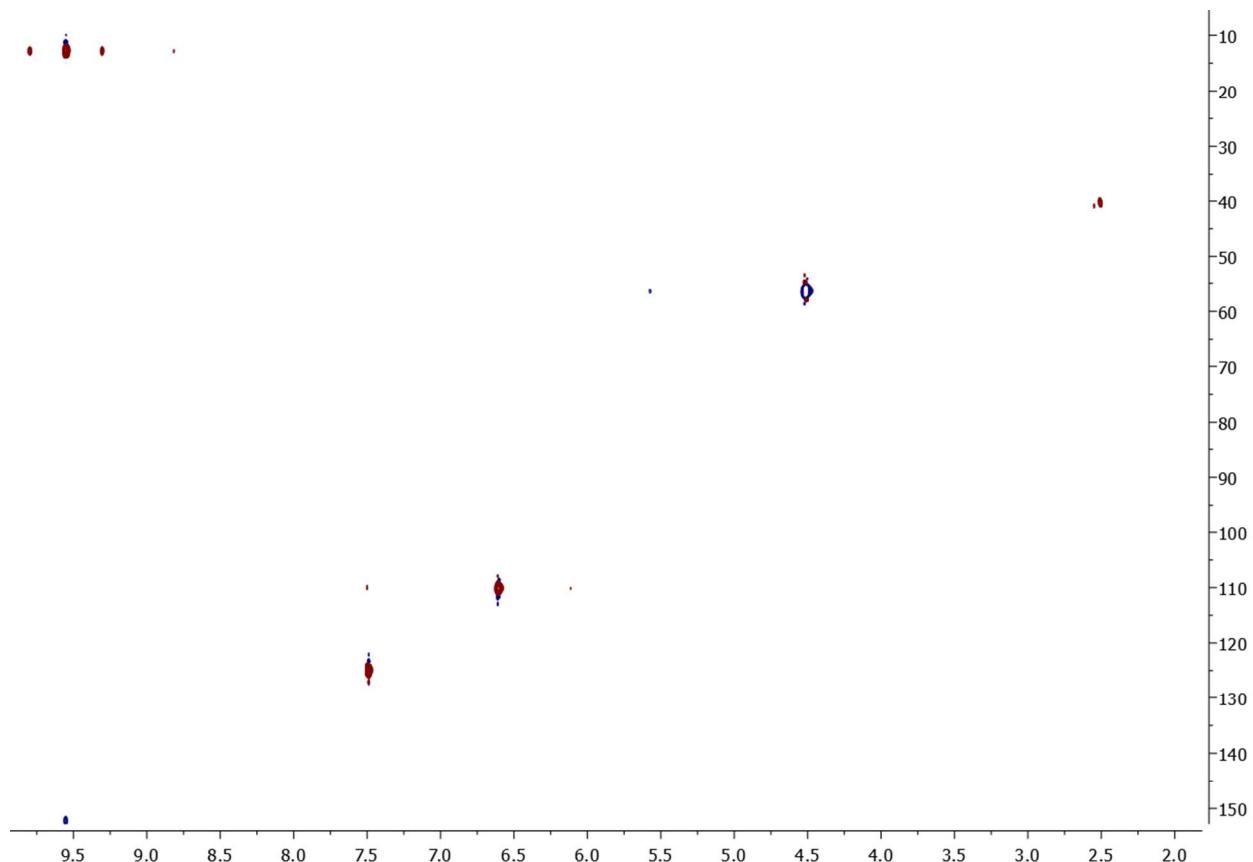
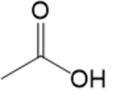
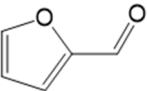
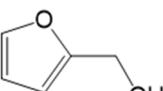
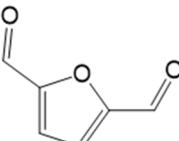
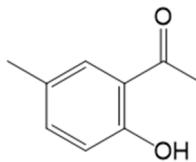
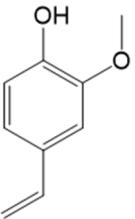


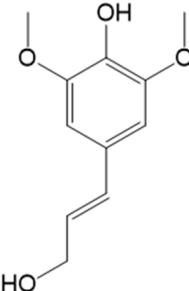
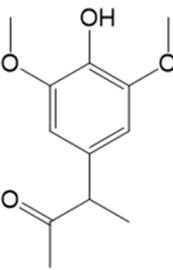
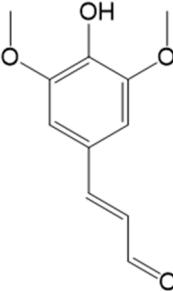
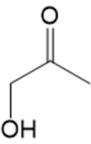
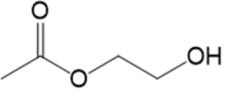
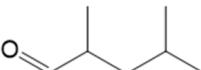
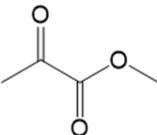
Figure S5. HSQC of 5-HMF standard in DMSO-d₆.

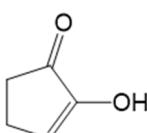
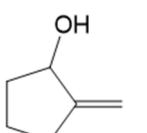
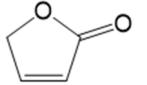
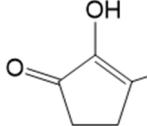
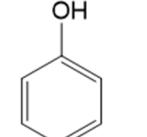
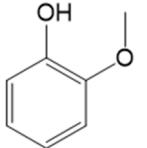
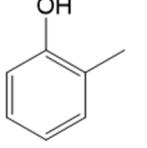
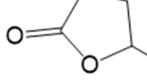
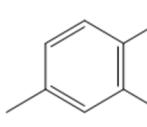
Table S1. Detected components from py-GC-MS at 350 and 600 °C.

ID	Name	M ⁺	Retention time (min)	Structure
1	Acetic acid	60	7.99	
2	Furfural	96	19.58	
3	2-Furanmethanol	98	21.22	
4	Not identified ¹	114	23.98	
5	Not identified	114	25.21	
6	Not identified	128	27.35	
7	2,5-Furandicarboxaldehyde	124	28.35	
8	Not identified	-	29.68	
9	Furan	68	30.93	
10	Not identified	152	33.87	
11	2-Methoxy-4-vinylphenol	150	35.05	

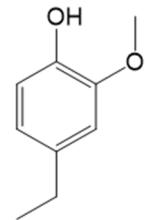
¹

12	5-Hydroxymethyl furfural	126	35.94
13	2,6-Dimethoxyphenol	154	37.14
14	Carbohydrate	180	39.72
15	4-Hydroxy-3-methoxybenzaldehyde	152	41.27
16	Not identified	--	43.4
17	1-(3,4-dimethoxyphenyl)ethanone	180	47.35
18	Carbohydrate	180	51.48
19	Not identified	166	51.79
20	4-Allyl-2,6-dimethoxyphenol	194	53.75
21	4-Hydroxy-3,5-dimethoxybenzaldehyde	182	54.79
22	Not identified	196	56.9

23	4-[(E)-3-hydroxyprop-1-enyl]-2,6-dimethoxyphenol	210	60.07	
24	3-(4-hydroxy-3,5-dimethoxyphenyl)butan-2-one	224	62.02	
25	3,5-Dimethoxy-4-hydroxycinnamaldehyde	208	70	
26	1-hydroxy-2-propanone	74	9.31	
27	1,2-Ethanediol, monoacetate	104	16.53	
28	Pentanal, 2,4-dimethyl-	114	18.48	
29	Propanoic acid, 2-oxo-, methyl ester	102	18.74	

30	2-Hydroxy-2-cyclopenten-1-one	98	23.24	
31	2-Methylene cyclopentanol	98	23.66	
32	2-Furanone	84	24.48	
33	Not identified	112	25.77	
34	2-Hydroxy-3-methyl-2-cyclopenten-1-one	112	25.89	
35	Phenol	94	26.31	
36	Phenol-2-methoxy-	124	27.14	
37	Phenol-2-methyl-	108	27.66	
38	5-Hydroxymethylidihydrofuran-2-one	116	28.9	
39	Not identified	--	29.95	
40	2-Methoxy-4-methylphenol	138	30.14	

41	Coeluting	114/152	32.38
42	Not identified	--	32.64



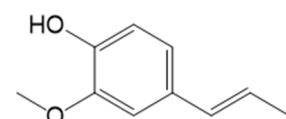
43	4-Ethyl-2-methoxyphenol	152	32.95
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44	Not identified	164	36.06
		138/	

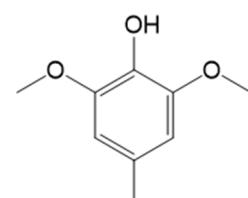
45	Coeluting	164/	38.39
		180	

46	Not identified	144	38.95
47	Carbohydrate	244	39.71

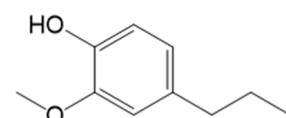
48	2-methoxy-4-(1-propenyl)phenol	164	40.66
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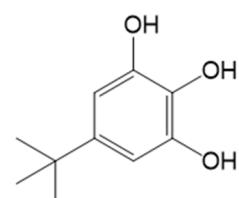
49	2,6-Dimethoxy-4-methylphenol	168	41.18
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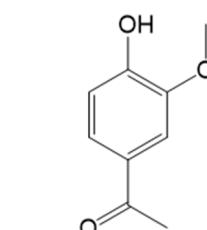
50	2-Methoxy-4-propylphenol	166	43.97
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51	5-tert-butylbenzene-1,2,3-triol	182	44.69
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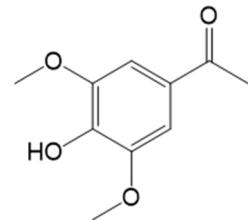
52	1-(4-Hydroxy-3-methoxyphenyl)ethanone	166	45.13
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53	Not identified	194	48.33
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54	Not identified	194	50.87
55	Carbohydrate	180	51.55

56	1-(4-Hydroxy-3,5-dimethoxyphenyl)ethanone	196	58.12
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57	1-(4-Hydroxy-3,5-dimethoxyphenyl)propan-1-one	210	61.77
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