

Supplementary material

Table S1

Comparison of the depolymerization products yields.

Catalyst	Reaction condition	Substrate	Product yield	References
NaOH	300 °C, 80 min	Organosolv lignin from olive tree	Oil: 18.5wt-%, Char: 32.5wt-%, Gas: 1.0wt-%.	Erdocia et al. ¹
Ca(OH) ₂	280 °C, 15 min	Sawdust	Oil: 9.3 wt-%, Gas: 11.9 wt-%, Char: 35.6wt-%.	Karagöz et al. ²
Ethanol Toluene	300 °C, 240 min	Straw lignin	Oil: 7.5wt-% Oil: 2.3wt-%	Murnieks et al. ³
Water	130 °C, 60 min	Kraft lignin	Oil: 10.6wt-%, Gas: 5.7wt-%, Char: 80.1wt-%.	Zhou ⁴
Ru/C, H ₂ 63%ZnCl	200 °C, 240 min	Pine wood lignin	Oil: 54.0 wt-%, Char: 38.3 wt-%, Gas: 4.6 wt-%.	Wang et al. ⁵

Table S2

Chemical composition in the bio-oil determined using GCMS. Reaction conditions:

BLAS 150 mL, T= 300 °C, t=30 min.

No.	RT	Library/ID	Area %
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1	8.95	Acetic acid	0.31%
2	18.36	2-(Vinyl-2-ethoxy)-ethanol	0.24%
3	8.14	2-Methyl-2-furan	0.68%
4	9.62	3,4-Dimethyl-2-furan	0.32%
5	9.72	2,3,4-Trimethyl-2-furan	0.18%
6	10.13	3-Methyl-2-furan	0.54%
7	10.33	2,3-Dimethyl-2-furan	0.61%
8	10.45	3,4,4-Trimethyl-2-furan	0.22%
9	13.82	2-Hydroxy-3-methyl-2-furan	0.07%
10	14.85	3-Ethyl-2-hydroxy-2-furan	0.08%
11	11.52	Acetophenone	0.13%
12	11.85	1-(2-Methylphenyl)-ethanone	0.27%
13	12.25	1,2-Dimethoxy-benzene	0.81%
14	13.36	3,4-Dimethoxytoluene	0.16%
15	14.17	2-Methoxy-phenol	27.65%
16	14.34	2-Methoxy-6-methyl-phenol	0.97%
17	14.47	4-Ethyl-1,2-dimethoxy-benzene	0.17%
18	15.35	2-(2,2-Dimethylcyclopropyl)thiophene	0.22%
19	15.55	2-Methoxy-5-methylphenol	0.44%
20	15.77	2-Methoxy-4-methyl-phenol	2.17%
21	15.86	1,2,3-Trimethoxybenzene	1.44%
22	16.51	2-Methyl-phenol	0.23%
23	16.57	Phenol	0.98%
24	16.87	2,3-Dihydro-1H-Inden-1-one	0.44%
25	16.95	4-Ethyl-2-methoxy-phenol	2.81%
26	17.28	1,2,3-Trimethoxy-5-methyl-benzene	0.38%
27	17.81	4-Methyl-phenol	0.23%

28	17.94	3-Methyl-phenol	0.12%
29	18.04	3,4-Dimethoxy-phenol	1.79%
30	18.11	1,2-Dimethyl-4-(phenylmethyl)-benzene	0.16%
31	18.19	2-Methoxy-4-propyl-phenol	0.71%
32	18.57	1-Ethenyl-3-methyl-benzene	0.17%
33	19.15	2-Propenyl-benzene	0.31%
34	19.44	1-Pentenyl-benzene	0.09%
35	20.75	2,6-Dimethoxy-phenol	36.67%
36	21.99	4-Methoxy-2-methyl-1-(methylthio)benzene	3.05%
37	22.80	1,2,3-Trimethoxy-5-methyl-benzene	3.56%
38	23.30	3-Methoxy-phenol	0.31%
39	24.20	1,2-Benzenediol	8.67%
40	9.13	2-Formylhistamine	0.14%
41	11.25	Ethyl oxamate	0.15%
42	11.42	1,1-Bis(methylthio)-ethane	0.61%
43	12.19	Thiopropionamide	0.05%
44	12.91	1-(3-Thienyl)-ethanone	0.31%
45	13.90	Dimethylhydrazone-2-propanone	0.08%
46	13.94	1-(2-Thienyl)-1-propanone	0.25%
47	16.79	N,N-Dimethylethanesulfonamide	0.06%

Table S3

Pyrolytic products distribution of the char at different reaction temperatures.

NO	Library/ID	RT	Reaction temperature/°C				
		/min	260	280	300	320	340
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1	Acetone	1.94	8.7			
2	Acetic acid	2.02	7.6			
3	Benzene	2.17	1.0	12.7	19.9	
4	Toluene	3.73	2.5	11.7	87.3	80.1
5	2,4-Dimethyl-1-heptene	4.79	0.3			
6	p-Xylene	5.36	0.5	7.1		
7	Phenol	7.61	2.0	2.9	25.3	
8	2-Hydroxy-benzaldehyde	9.21	1.3	0.8		
9	2-Methylphenol	9.36	2.2	1.7	10.0	
10	4-Methylphenol	9.84	1.6	2.1	13.1	
11	2-Methoxyphenol	10.27	15.1	12.9	24.3	
12	3-Hydroxy-4-methyl benzaldehyde	11.36	1.0	0.5		
13	2,4-Dimethylphenol	11.60	1.5	1.1	8.5	
14	2,3-Dimethylphenol	12.08		0.2		
15	2-Methoxy-3-methylphenol,	12.41	2.1	1.4		
16	2-Methoxy-5-methylphenol	12.59		0.4		
17	2-Methoxy-4-methylphenol	12.74	6.5	5.4		
18	3-Methoxyphenol	13.45		0.3		
19	3,4-Dimethoxytoluene	13.75	1.1	0.8		
20	3-Methyl-1,2-benzenediol	14.24	1.4	1.2		
21	3-Methoxy-1,2-benzenediol	14.33	7.2	5.2		
22	4-Ethyl-2-methoxy-phenol	14.74		2.1		
23	2,3-Dihydro-1H-inden-1-one	14.83		0.2		
24	4-Methyl-1,2-benzenediol	14.88		0.4		
25	2-Hydroxy-3-methoxybenzalde	15.39	1.3	0.4		
26	1,2,3-Trimeoxybenzene	15.46		0.6		
27	2-Methoxy-4-vinylphenol	15.53	2.0	1.5		

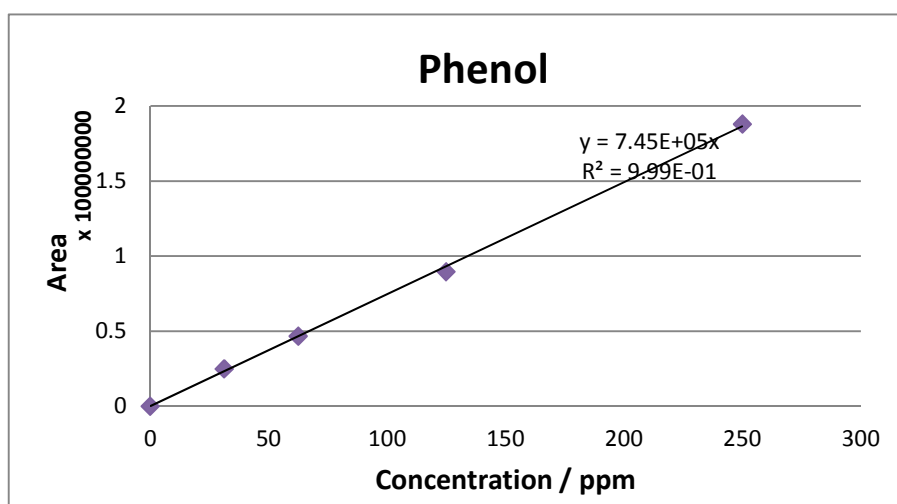
28	2,6-Dimethoxyphenol	16.34	30.8	23.0
29	3,4-Dimethoxyphenol	16.55	1.9	1.0
30	2-Methoxy-4-propylphenol	16.70		0.4
31	1,2,3-Trimeoxy-5-methylbenzene	17.43	1.1	0.9
32	4-Hydroxy-3-methoxyacetophenone	18.37	6.4	3.7
33	2-Methoxy-4-(1-propenyl)-phenol	18.46	1.4	0.6
34	4-Hydroxy-3-methoxyacetophenone	19.23	1.2	0.9
35	1,2,3-Trimethoxy-5-methylbenzene	20.00	3.4	2.0
36	4-Methyl-2,5-dimethoxybenzaldehyde	20.78	3.6	1.9
37	4-Hydroxy-3,5-dimethoxy-benzaldehyde	22.61	0.9	0.6
38	3-Methoxy-2-naphthalenol	22.74		0.4
39	4-Hydroxy-3,5-dimethoxyacetophenone	23.95	2.0	1.2
40	2,3-Dimethoxy-naphthalene	24.72	0.6	0.5
41	2-Ethyl-9,10-anthracenedione	29.82	0.6	0.4

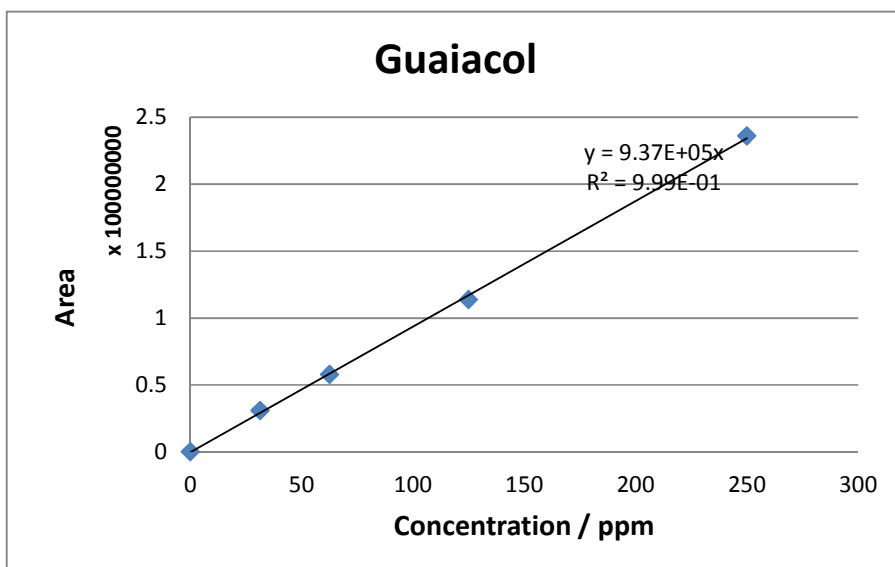
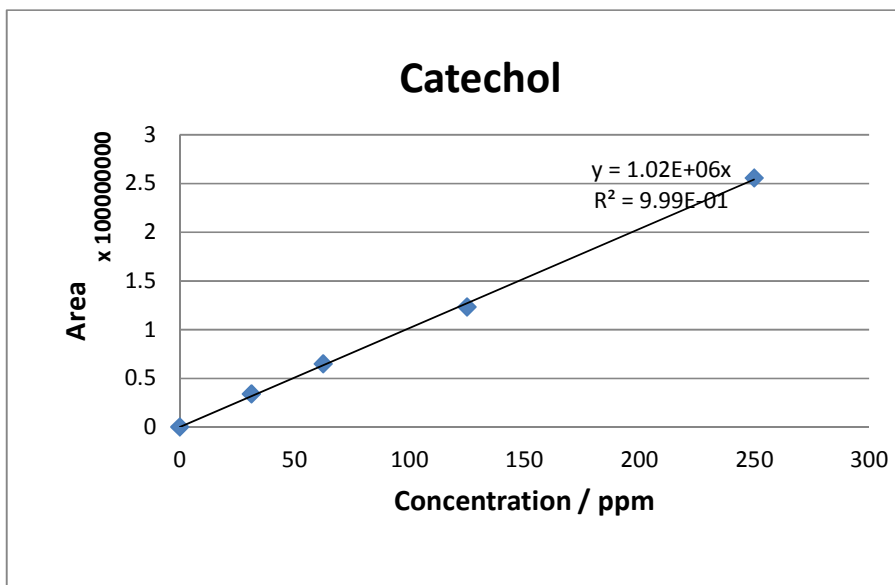
Table S4

Pyrolytic products distribution of the char at different reaction time.

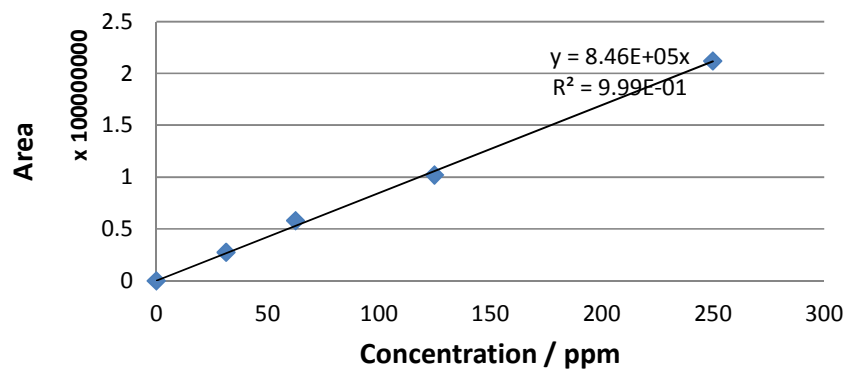
NO	Library/ID	RT /min	Reaction time/min				
			0	30	60	90	120
1	Benzene	2.17				16.0	
2	Toluene	3.73	2.2	11.7	7.9		26.6
3	p-Xylene	5.36	1.5	7.1	5.5	7.2	17.3
4	Phenol	7.61	6.6	25.3	18.1	24.2	34.9
5	2-Hydroxy-benzaldehyde	9.21	2.1				
6	2-Methylphenol	9.36	4.3	10.0	7.5	8.5	

7	4-Methylphenol	9.85	4.2	13.1	14.2	17.4	21.2
8	2-Methoxyphenol,	10.27	21.9	24.3	18.3	12.9	
9	3-Hydroxy-4-methyl benzaldehyde	11.37	0.9				
10	2,4-Dimethylphenol	11.60	3.1	8.5	6.8	8.9	
11	2-Methoxy-3-methylphenol,	12.41	2.4				
12	Naphthalene	12.62			3.5		
13	2-Methoxy-4-methylphenol	12.75	5.1		3.0		
14	3,4-Dimethoxytoluene	13.70	1.8		2.3		
15	3-Methoxy-1,2-benzenediol	14.33	2.6				
16	4-Ethyl-2-methoxy-phenol	14.74	2.7				
17	2,3-Dihydro-1H-inden-1-one	14.83			5.8	5.0	
18	2-Hydroxy-3-methoxybenzalde	15.39	1.3				
19	1,2,3-Trimeoxybenzene	15.46	1.2				
20	2,6-Dimethoxyphenol	16.34	27.6		7.2		
21	4-Hydroxy-3-methoxyacetophenone	18.37	5.0				
22	1,2,3-Trimethoxy-5-methylbenzene	20.00	1.2				
23	4-Methyl-2,5-dimethoxybenzaldehyde	20.78	2.5				

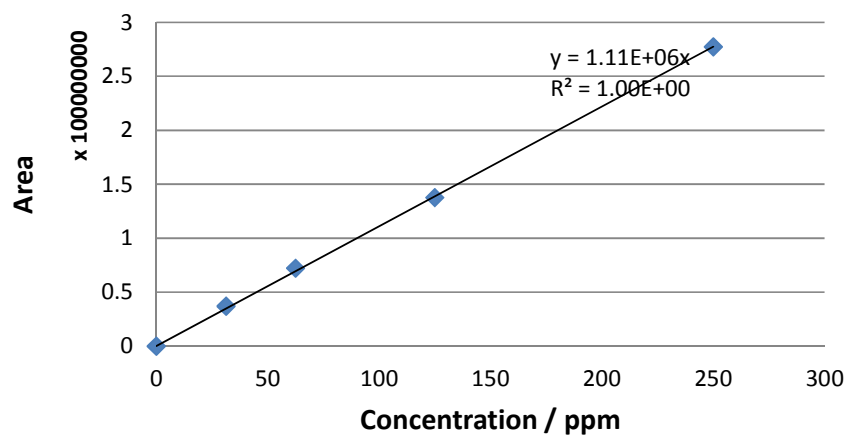




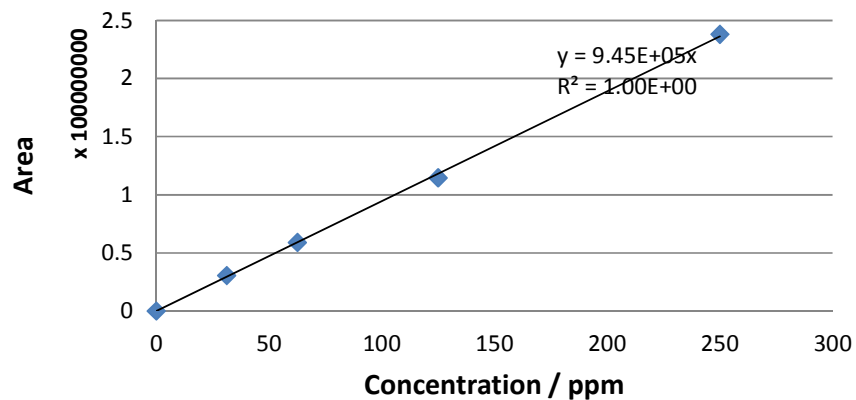
4-Hydroxyl-3-methoxyacetophenone



4-Ethylphenol



4-Methyl-2-methoxyphenol



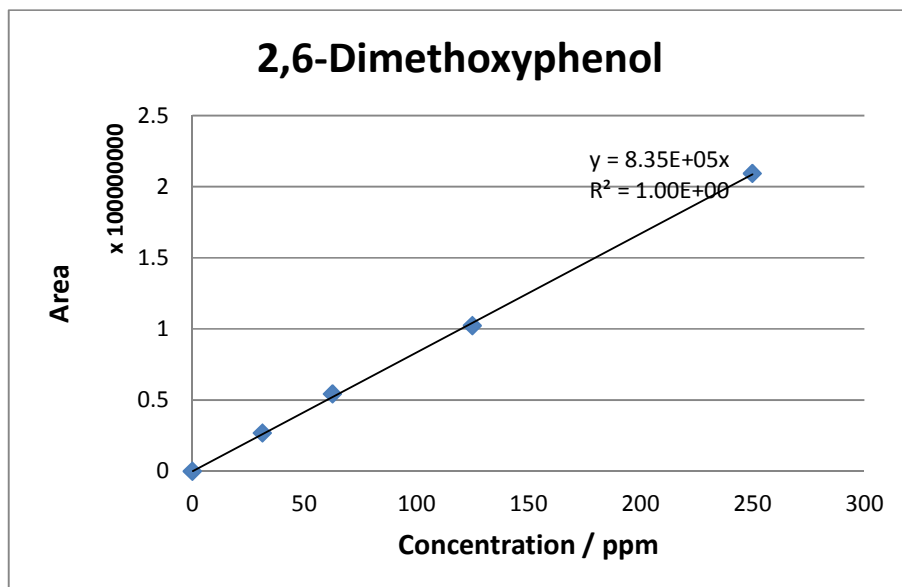


Fig. S1 The external standard curves of main monophenolics.

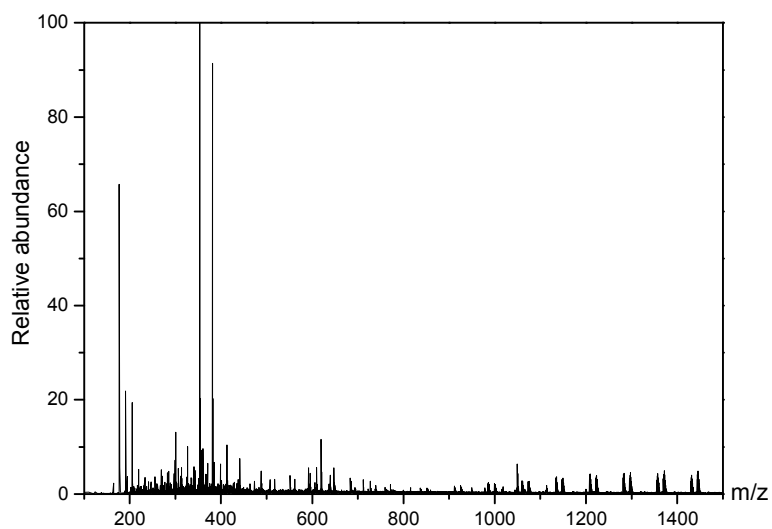


Fig. S2 ESI⁺-MS of oil product from hydrothermal conversion of BLAS. Reaction conditions: BLAS 150 mL, T= 300 °C, t =30 min.

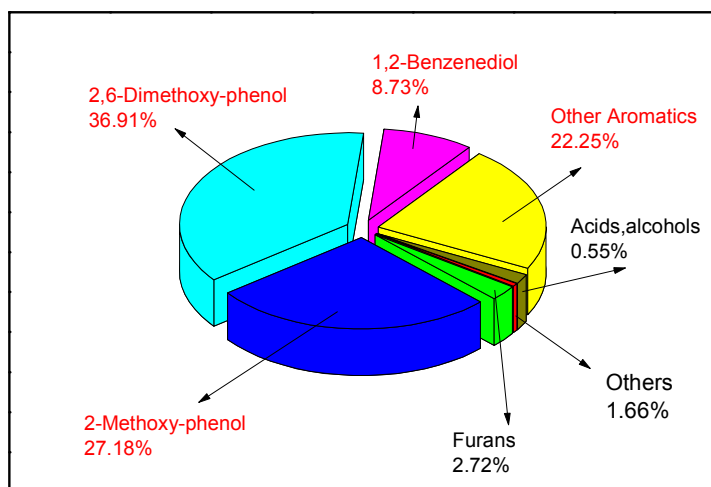


Fig. S3 Monomeric products distribution (based on peak area% by GCMS) in bio-oil compounds. Reaction conditions: BLAS 150 mL, T= 300 °C, t =30 min.

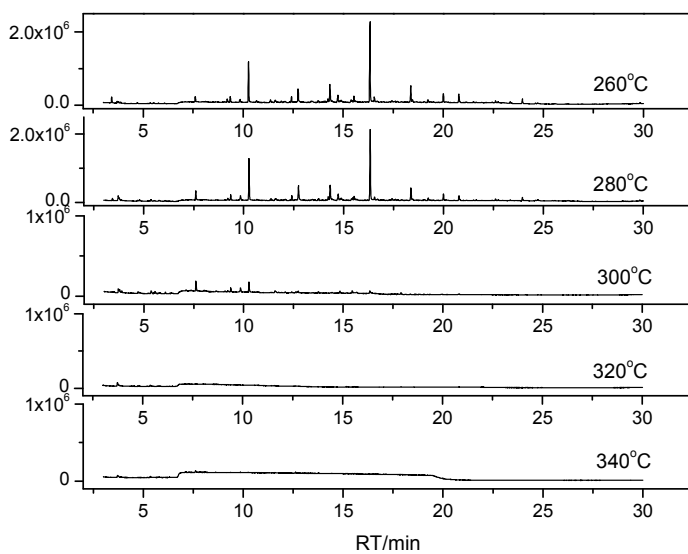


Fig. S4 The typical ion chromatograms of pyrolysis of the char from different reaction temperatures.

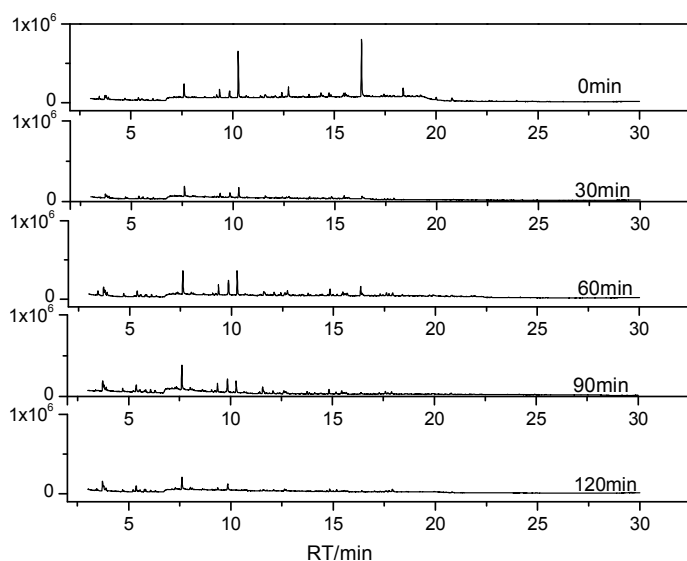


Fig. S5 The typical ion chromatograms of pyrolysis of the char from different reaction time.

References

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- (5) Wang, H.; Zhang, L.; Deng, T.; Ruan, H.; Hou, X.; Cort, J. R.; Yang, B. ZnCl_2 induced catalytic conversion of softwood lignin to aromatics and hydrocarbons. *Green Chem.* **2016**, 18, 2802-2810.