

SUPPLEMENTARY MATERIALS

IECR

Selective Producing 4-vinyl Phenol by Fast Pyrolysis of Herbaceous Biomass

Yan-Chao Qu,^a Zhi Wang^a Qiang Lu^{*b}, Ying Zhang^{*a}

^aAnhui Province Key Laboratory of Biomass Clean Energy, University of Science and Technology of China, Hefei 230026, P. R. China

^bNational Engineering Laboratory for Biomass Power Generation Equipment, North China Electric Power University, Beijing, China.

* To whom correspondence should be addressed. Fax: 86-551-6360-6689; Tel: 86-551-6360-3463; E-mail: zhzying@ustc.edu.cn (Ying Zhang), qianglu@mail.ustc.edu.cn (Qiang Lu)

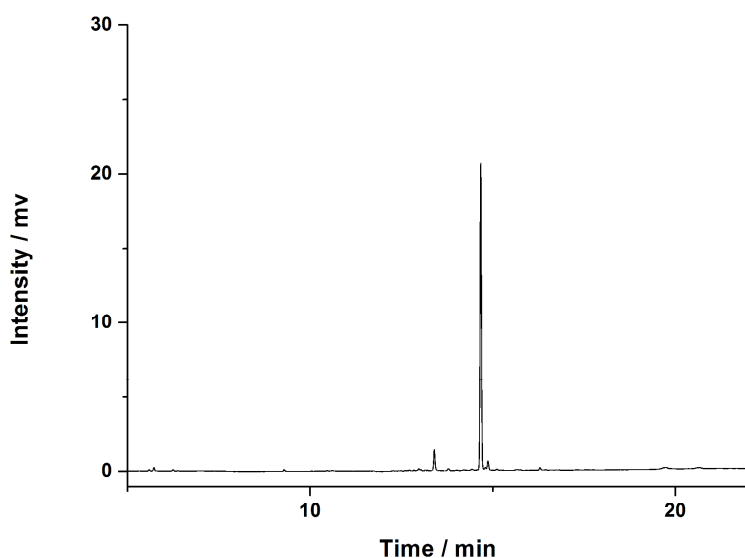
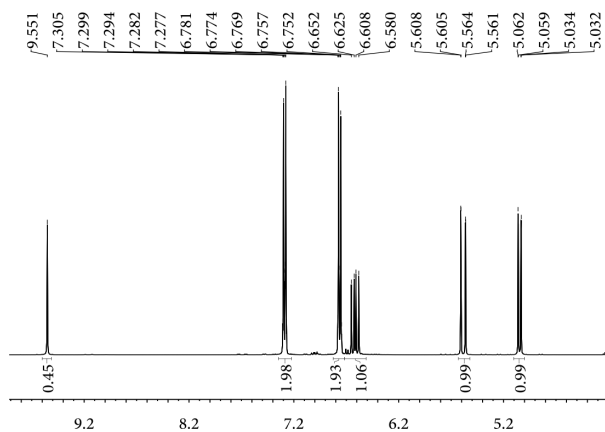


Figure S1. GC spectrum of 4-vinyl phenol isolated from pyolysis oil.



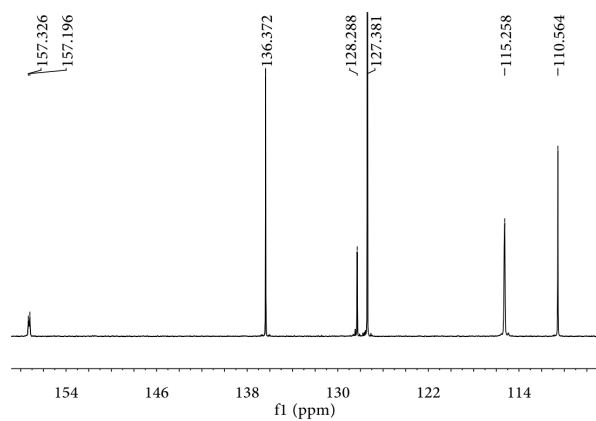


Figure S2. 400-MHz ¹H NMR and ¹³C NMR spectra of the target compound in DMSO-d₆

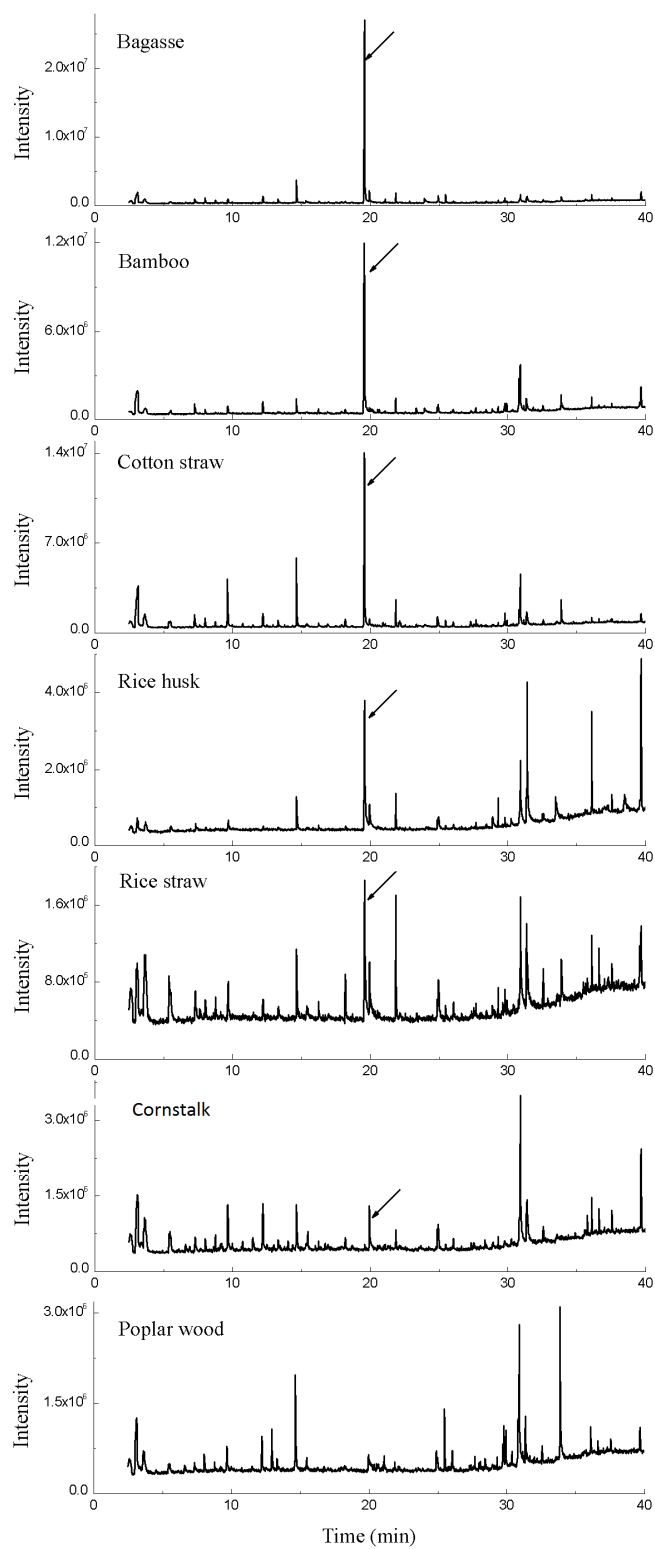


Figure S3. The ion chromatograms from fast pyrolysis of different biomass at 350 °C. The arrow points to the target compound.

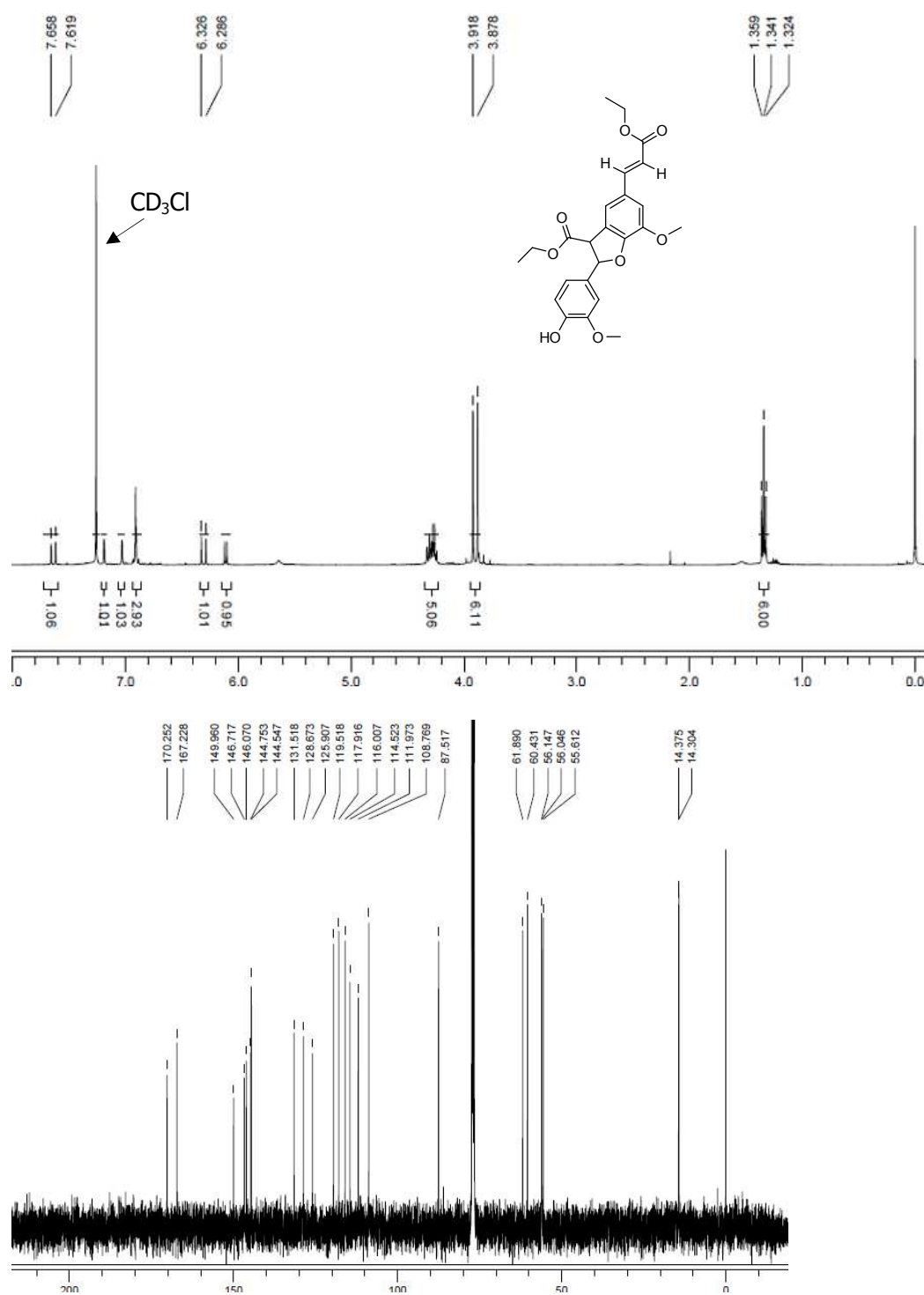


Figure S4. 400-MHz ¹H NMR and ¹³C NMR spectra of compound (c) in CD₃Cl

Table S1.

Pyrolytic products of model compound (a) at 300 °C.

Entry	RT	Compound	Area %
1	11.04	2-methoxy phenol	14.62
2	12.5	2-methoxy-4-methyl phenol	18.83
3	13.69	4-ethyl-2-methoxy phenol	2.92
4	14.39	2-methoxy-4-vinylphenol	14.40
5	16.15	2-methoxy-4(1-propenyl) phenol	4.96
6	19.92	trans-4-methoxycinnamaldehyde	15.59

Table S2.

Pyrolytic products of model compound (a) at 400 °C.

Entry	RT	Compound	Area %
1	9.87	phenol	1.70
2	11.15	2-methyl Phenol	1.39
3	11.47	3-methyl Phenol	1.23
4	12.02	2-methoxy Phenol	4.66
5	13.49	2-methoxy-4-methyl Phenol	4.21
6	13.69	1,2-benzenediol	3.16
7	14.28	4-ethyl-2-methoxy-1-methyl benzene	1.07
8	14.68	4-ethyl-2-methoxy phenol	1.71
9	14.95	2-allphenol	1.61
10	15.01	4-methyl-1,2-benzenediol	1.27
11	14.28	4-ethyl-2-methoxy-1-methyl benzene	1.07
12	15.40	2-methoxy-4-vinyl phenol	10.18
13	15.81	2-methyl-4-propyl phenol	1.01
14	15.95	6-methyl-4-indanol	0.77
15	16.32	4-ethylcatechol	1.12
16	16.64	2-methyl-6(2-propenyl)-phenol	1.10
17	17.16	2-methyl-4-(1-propenyl)-phenol	1.94
18	17.20	Vanillin	1.54
19	20.94	Trans-4-methoxycinnamaldehyde	26.41
20	21.86	1,2-benzendicarboxylicacid bis(2-methyl propyl) ester	2.76
21	22.34	2-methoxy-3-benzofurancarboxaldehyde	3.46
22	22.88	1,3-benzodioxole-5-(4-keto-butycacid)	10.43

Table S3. Pyrolytic products of model compound (a) at 500 °C.

Entry	RT	Compound	Area %
1	3.13	benzene	1.69
2	5.01	toluene	2.25
3	9.87	Phenol	2.98
4	11.15	2-methyl Phenol	1.85
5	11.47	3-methyl Phenol	2.38
6	12.02	2-methoxy Phenol	1.60
7	12.62	2,4-dimethyl Phenol	1.92
8	13.49	2-methoxy-4-methyl Phenol	1.57
9	13.69	1,2-benzenodiol	2.58
10	13.92	2-methyl Benzenne	1.41
11	13.99	1-ethyl-4-methoxy benzene	1.18
12	14.28	4-ethyl-2-methoxy-1-methyl benzene	1.27
13	14.95	2-allphenol	2.42
14	15.01	4-methyl-1,2-benzediol	3.68
15	15.40	2-methoxy-4-vinyl phenol	4.40
16	15.69	2-methyl-6(2-propenyl)-phenol	1.00
17	15.95	6-methyl-4-indanol	1.16
18	18.97	9H-xanthene	1.76
19	19.43	2-Ethoxy-1,4-dimethyl benzene	0.54
20	20.38	2-ethyl-5-propyl phenol	1.58
21	20.73	2-methyl-3-benzofurancarboxaldehyde	1.37
22	20.94	Trans-4-methoxycinnamaldehyde	23.48
23	21.45	ethyl-3-(4-hydroxy-3-methoxyphenol)-2-propenoate	1.99
24	21.80	2-methoxy-3-benzofurancarboxaldehyde	1.57
25	21.86	1,2-benzendicarboxylicacid bis(2-methyl propyl) ester	5.13
26	22.34	2-methoxy-3-benzofurancarboxaldehyde	3.45
27	22.88	1,3-benzodioxole-5-(4-keto-butycacid)	10.91

Table S4. Compounds identified by GC/MS from fast pyrolysis of bagasse and its components

No.	RT	Compound	No.	RT	Compound
1	1.95	methanol	41	19.33	4-methyl-phenol
2	2.00	acetaldehyde	42	20.32	2-methoxy-phenol
3	2.24	furan	43	21.26	4-methyl-2(5H)-furanone
4	2.37	acetone	44	21.30	5-hydroxymethyldihydrofuran-2-one
5	2.37	2-propenal	45	22.04	2,4-dimethyl-phenol
6	3.00	2-methyl furan	46	22.79	2,4-dimethyl-phenol
7	3.27	acetic acid	47	23.33	4-ethyl-phenol
8	3.37	hydroxyacetaldehyde	48	23.74	2,3-dihydroxybenzaldehyde
9	3.52	3-pentanone	49	23.92	2-methoxy-4-methyl-phenol
10	4.68	2-butenal	50	24.29	1,2-benzenediol
11	5.25	1-hydroxy-2-propanone	51	25.29	2,3-dihydro-benzofuran
12	5.93	1,2-ethanediol	52	25.85	4-ethyl-2-methoxy-phenol
13	6.21	2,3-dihydroxy-propanal	53	26.77	3-methoxy-1,2-benzenediol
14	6.51	toluene	54	27.09	5-(hydroxymethyl)-2-furaldehyde
15	8.08	1-hydroxy-2-butanone	55	27.59	5-(hydroxymethyl)-2-furaldehyde
16	8.68	acetoxycetic acid	56	28.64	2-methoxy-4-vinylphenol
17	9.65	methyl pyruvate	57	29.18	1,3-di-O-acetyl-d-ribopyranose
18	9.97	2-methyl-pentanoic acid	58	29.34	3-methoxy-5-methylphenol
19	10.87	furfural	59	29.64	2-methoxy-4-(2-propenyl)-phenol
20	11.24	2-cyclopenten-1-one	60	29.93	5-acetoxymethyl-2-furaldehyde
21	11.81	acrylic acid methyl ester	61	30.87	2,6-dimethoxy-phenol
22	12.22	5-methyl-2(3H)-furanone	62	31.62	4-hydroxy-benzaldehyde

23	12.43	1-(acetyloxy)-2-propanone	63	33.11	2-methoxy-4-propenyl-phenol
24	12.49	4-hydroxydihydro-2(3H)-furanone	64	33.15	4-hydroxy-3-methoxy-benzaldehyde
25	13.39	2-cyclopentene-1,4-dione	65	33.55	1,2,4-trimethoxy-benzene
26	13.65	1-(2-furanyl)-ethanone	66	34.77	2-methoxy-4-propyl-phenol
27	13.99	1,3-dihydroxy-2-propanone	67	35.69	1-(4-hydroxy-3-methoxyphenyl)-2-ethanone
28	14.42	1,2-cyclopentanedione	68	36.84	1-(4-hydroxy-3-methoxyphenyl)-2-propanone
29	14.57	5-oxotetrahydro-2-furancarboxylic acid	69	37.30	levoglucosan
30	15.56	phenol	70	37.43	3,5-dimethoxyacetophenone
31	16.01	2-(5H)-furanone	71	41.33	4-allyl-2,6-dimethoxy-phenol
32	16.32	5-methyl-furfural	72	41.56	4-hydroxy-3,5-dimethoxy-benzaldehyde
33	16.57	3-methyl-2-cyclopentenone	73	43.26	1-(4-hydroxy-3,5-dimethoxyphenyl)-ethanone
34	16.81	3-methyl-2,5-furandione	74	43.41	4-hydroxy-2-methoxycinnamaldehyde
35	17.20	5-acetyldihydro-2(3H)-furanone	75	43.57	2-propenoic acid, 3-(4-hydroxyphenyl)-, methyl ester
36	17.28	2H-pyran-2-one	76	44.04	1-(2,4,6-trihydroxy-3-methylphenyl)-1-butanone
37	17.54	2H-pyran-2,6-(3H)-dione	77	44.59	hexadecanoic acid
38	18.27	2-hydroxy-3-methyl-2-cyclopenten-1-one	78	45.02	4'-phenylpropiophenone
39	18.46	2-methyl-phenol	79	47.95	3,5-dimethoxy-4-hydroxycinnamaldehyde
40	18.87	2,3-dimethyl-2-cyclopentenone			

