Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Depolymerization of alkaline lignin over mesopores $KF/\gamma\text{-}Al_2O_3$

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1. GC/MS analysis of liquid products from lignin depolymerization with no catalyst

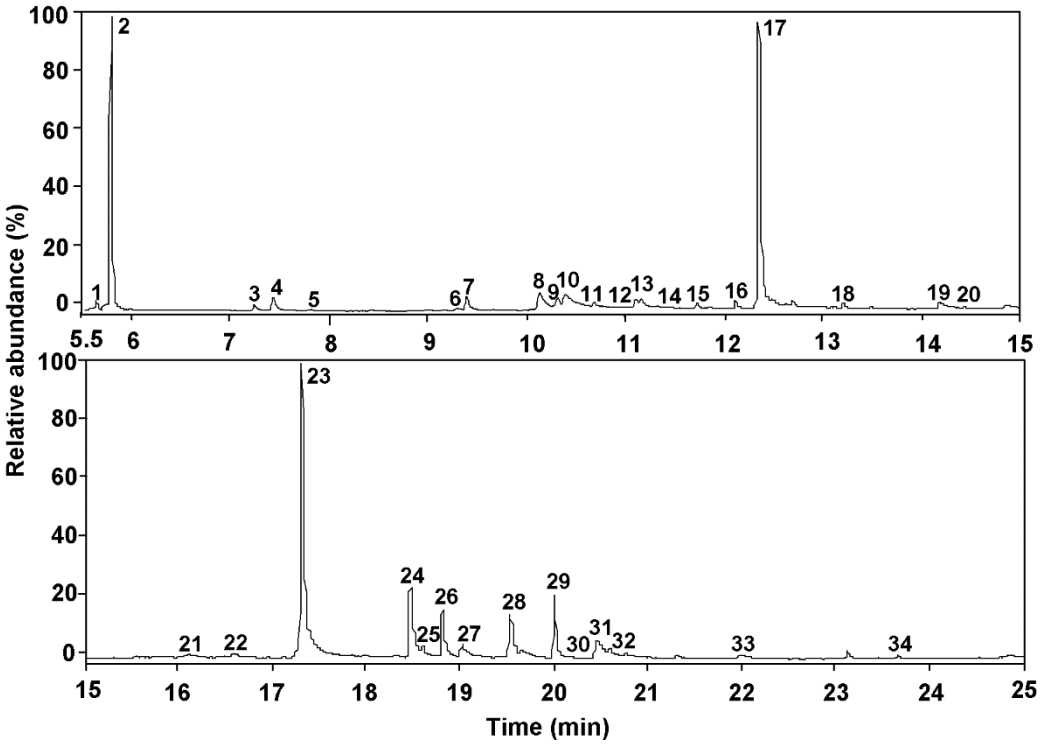

Fig. S1. TIC of liquid product from lignin depolymerization with no catalyst at 190 ℃.

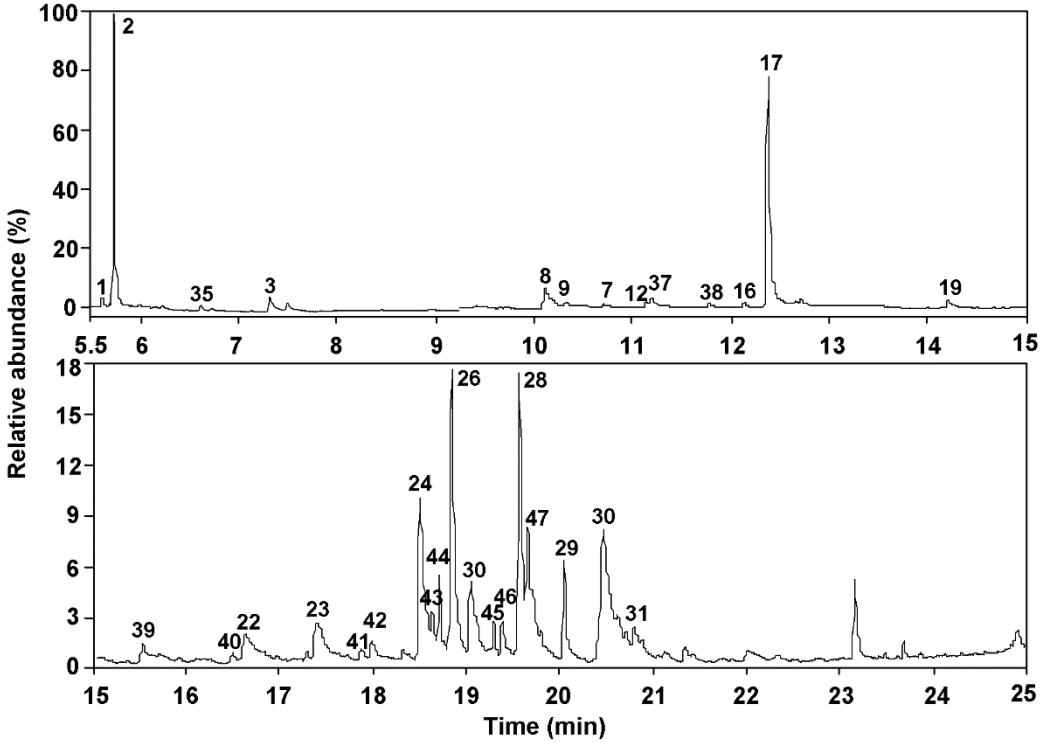

Fig. S2. TIC of liquid product from lignin depolymerization with no catalyst at 210 ℃.

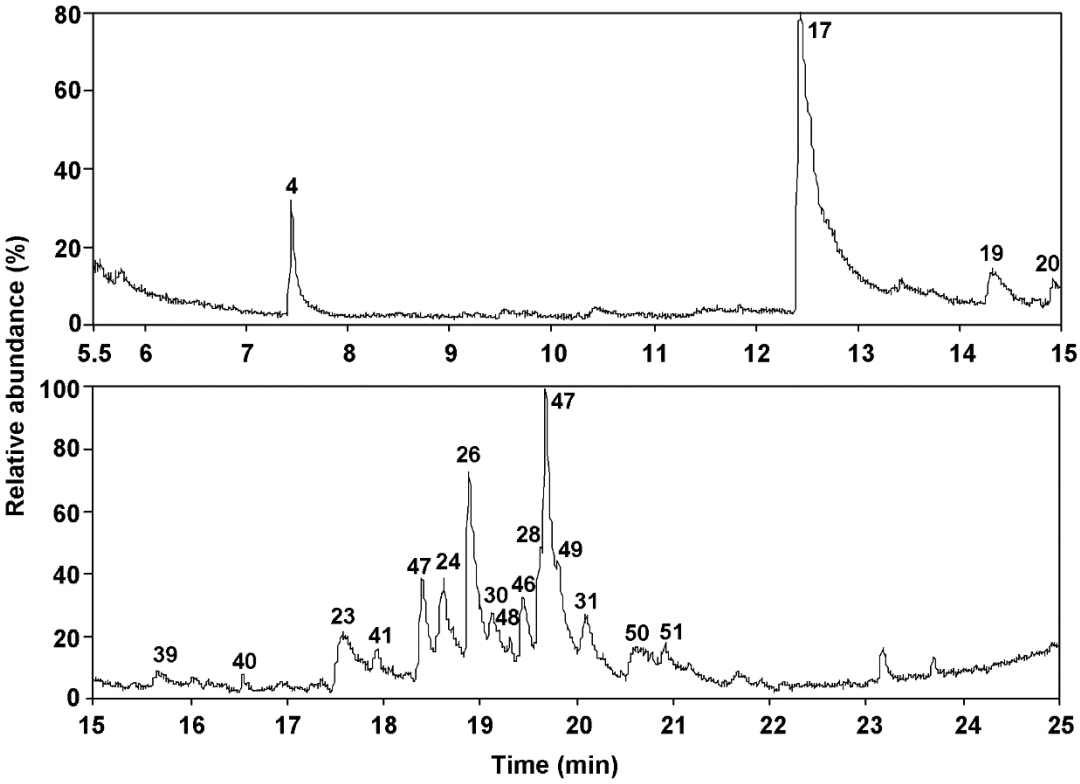

Fig. S3. TIC of liquid product from lignin depolymerization with no catalyst at 230 ℃.

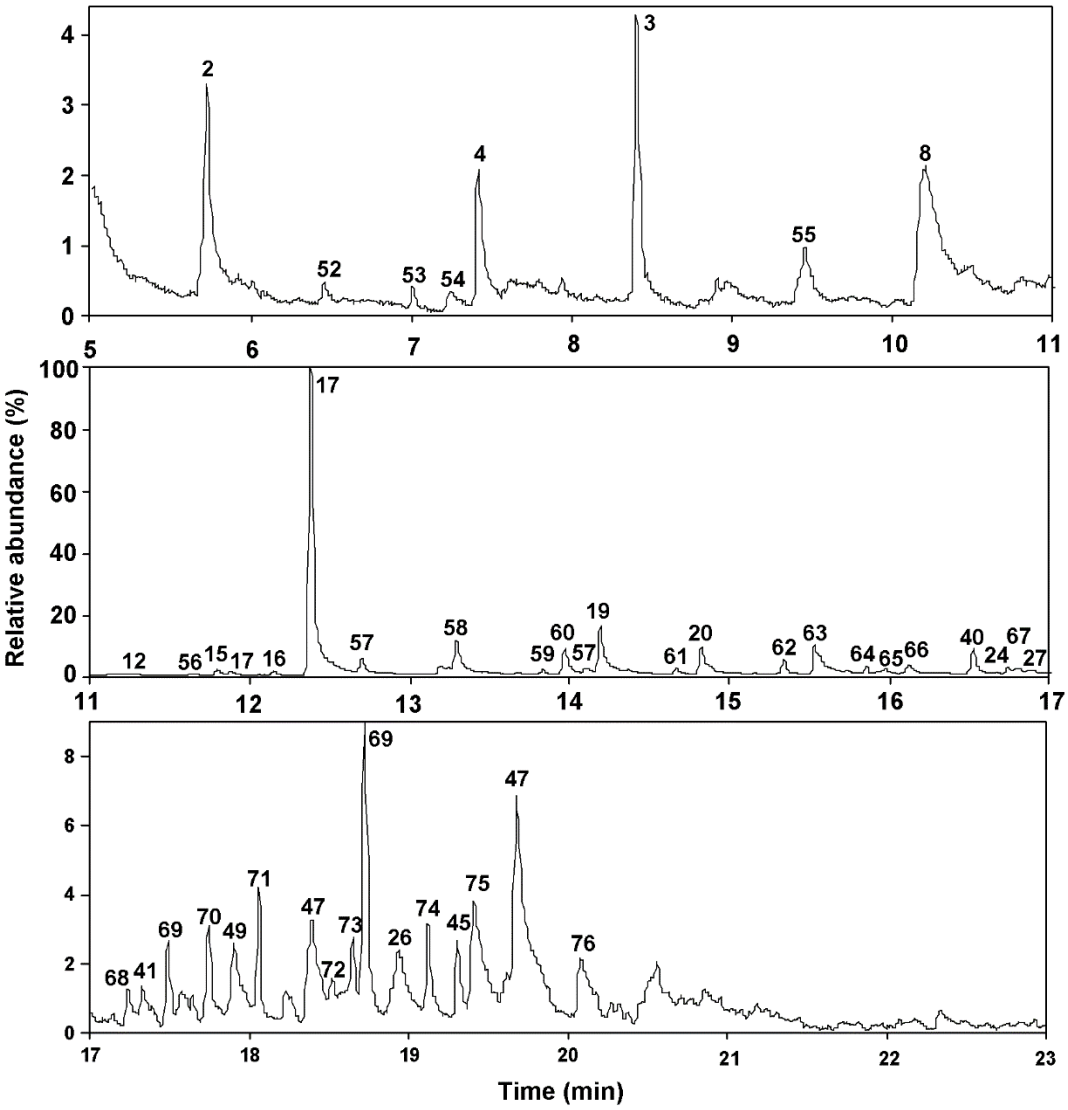

Fig. S4. TIC of liquid product from lignin depolymerization with no catalyst at 250 ℃.

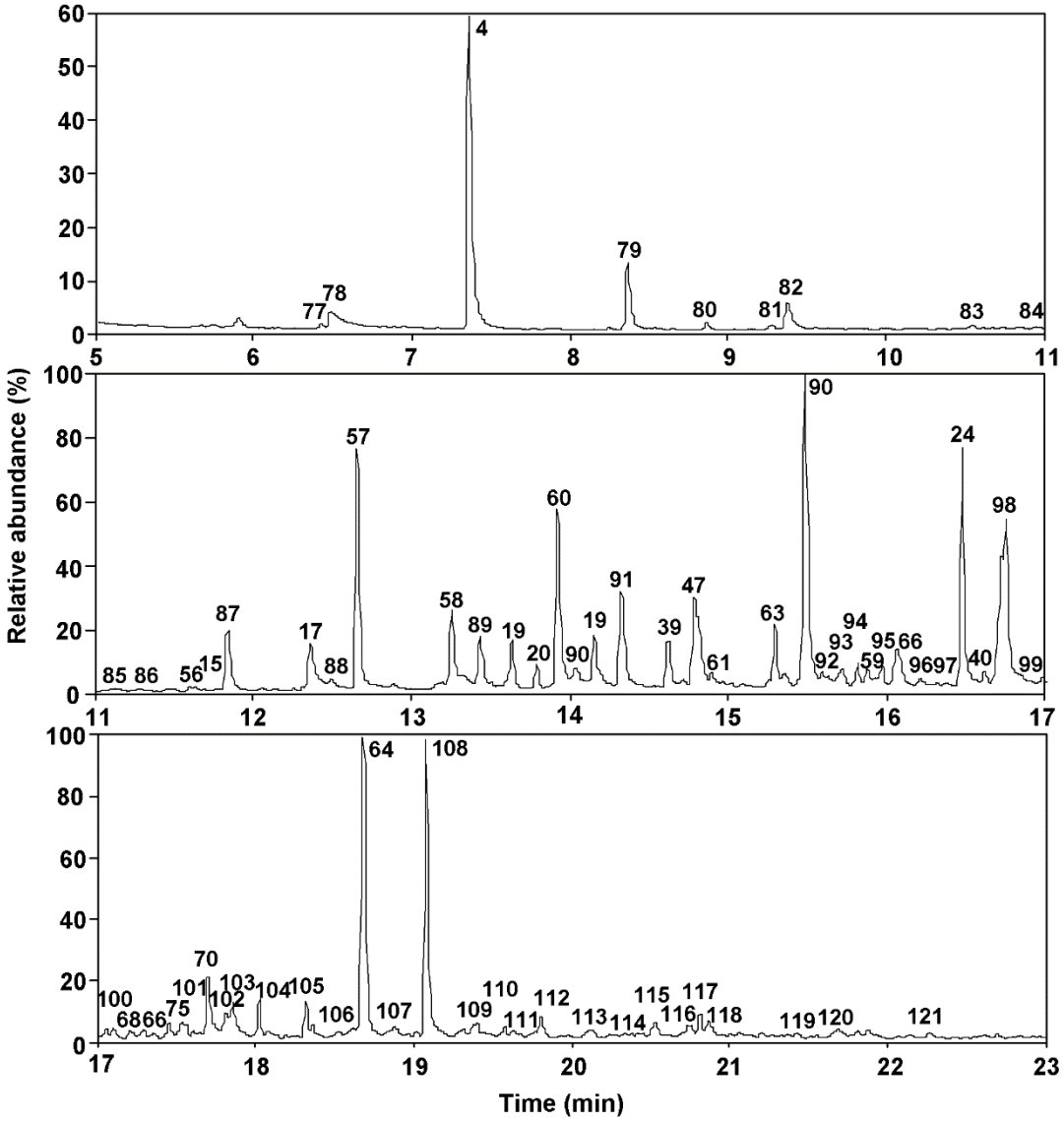

Fig. S5. TIC of liquid product from lignin depolymerization with no catalyst at 270 ℃.

Table S1

Aliphatic compounds in liquid products from lignin depolymerization at different temperatures with no catalyst.

Peak	Compound	Relative content（%）				
		190 ℃	210 ℃	230 ℃	250 ℃	270 ℃
1	methyl 2-oxopropanoate	0.36	0.63	-	-	-
2	methyl 2-hydroxypropanoate	16.14	19.94	3.80	1.31	-
3	methyl 2-hydroxybutanoate	0.27	0.69	-	1.18	-
4	4-hydroxy-4-methylpentan-2-one	0.68	-	10.80	0.81	5.79
5	4-oxopentyl formate	0.20	-	-	-	-
7	1,4-dihydroxybut-2-yl acetate	0.54	-	-	-	-
9	Methyl 4-oxovalerate	0.24	0.44	-	-	-
11	2,2-dimethylbut-1-ol	0.41	-	-	-	-
12	Dimethyl succinate	0.54	0.28	-	0.11	-
13	1,1'-oxobis (propan-2-ol)	0.30	-	-	-	-
15	Dimethyl succinate	0.56	-	-	0.58	0.04
16	1,1-dimethoxyoctane	1.85	0.63	-	0.39	-
18	1,1-dimethoxyhexane	0.99	-	-	-	-
35	3-methoxybut-2-ol	-	0.16	-	-	-
36	1-hydroxypentan-2-one	-	0.47	-	-	-
37	2-(2-(2-methoxyethoxy) ethoxy) eth-1-ol	-	0.44	-	-	-
38	Dimethyl 2-methylsuccinate	-	0.58	-	-	-
52	1-(2-methoxyethoxy) -2-methylpropan-2-ol	-	-	-	0.11	-
53	3,4,5-trihydroxyvaleraldehyde	-	-	-	0.07	-
54	2-methylpent-3-ol	-	-	-	0.10	-
77	Hex-3-ol	-	-	-	-	0.07
78	4-hydroxybutan-2-one	-	-	-	-	0.55
79	Methyl	-	-	-	-	1.40
80	Methyl	-	-	-	-	0.15
82	(E)-3-methylpent-1,3-diene	-	-	-	-	0.77
106	Pentadecane	-	-	-	-	0.10
110	Cetane	-	-	-	-	0.24

Table S2

Phenols in liquid products from lignin depolymerization at different temperatures with no catalyst.

Peak	Compound	Relative content（%）				
		190 °	210 ℃	230 ℃	250 ℃	270 ℃
17	2-methoxyphenol	15.95	25.56	30.08	35.16	1.94
19	2-methoxy-4-methylphenol	0.73	1.20	4.01	0.18	3.29
21	2-methoxy-4-vinylphenol	0.61	-	-	-	-
22	2,6-dimethoxyphenol	0.47	1.04	-	-	-
23	3-hydroxy-4-methoxybenzaldehyde	30.44	1.49	6.09	-	-
24	1-(4-hydroxy-3-methoxyphenyl) ethan-1-one	5.74	4.25	3.80	0.28	6.60
26	4-hydroxy-3-methoxybenzoic acid methyl ester	4.01	6.84	12.93	1.27	-
27	4-(2-hydroxyethyl) -2-methoxyphenol	1.65	-	-	0.40	-
28	Methyl 2- (4-hydroxy-3-methoxyphenyl) acetate	3.49	4.23	2.29	-	-
30	2-(4-hydroxy-3-methoxyphenyl) acetic acid	2.53	7.38	1.88	-	-
31	3-(4-hydroxy-3-methoxyphenyl) propionic acid	0.22	0.35	2.54	-	-
32	3-(4-hydroxy-3-methoxyphenyl) -2-oxopropionic acid	0.30	-	-	-	-
33	1-(2,4-dihydroxyphenyl) hexan-1-one	0.82	-	-	-	-
39	4-ethyl-2-methoxyphenol	-	0.40	1.21	-	1.28
40	3-methoxy-2,4,6-trimethylphenol	-	0.09	0.66	3.14	2.36
42	(Z)-2-methoxy-4-(prop-1-en-1-yl) phenol	-	0.42	-	-	-
56	P-cresol	-	-		0.31	0.22
57	2-methoxy-5-methylphenol	-	-		1.50	6.85
60	2-methoxy-3-methylphenol	-	-		3.15	5.51
61	2,3,5-trimethylbenzene-1,4-diol	-	-	-	0.77	0.19
64	2-(tert-butyl) -4-methoxyphenol	-	-	-	0.53	7.73
67	2,5-diethylphenol	-	-	-	0.18	-
69	3-(tert-butyl) -4-methoxyphenol	-	-	-	2.34	-
70	2,3,5,6-tetramethylbenzene-1,4-diol	-	-	-	0.70	-
73	2,5-di-tert-butylphenol	-	-	-	0.25	-
88	4-methoxyphenol	-	-	-	-	0.23
90	1-(2,5-dihydroxyphenyl) ethan-1-one	-	-	-	-	9.87
91	2,4,6-trimethylphenol	-	-	-	-	2.98
93	2-isopropyl-5-methylphenol	-	-	-	-	0.56
98	2,3,4,6-tetramethylphenol	-	-	-	-	8.77
102	1-(2-hydroxy-4,5-dimethylphenyl) ethan-1-one	-	-	-	-	0.20
111	2,6-diisopropylphenol	-	-	-	-	0.10
112	2- (tert-butyl) -4,6-dimethylphenol	-	-	-	-	0.60
118	3,6-dimethyl-2- (2-methylbut-3-en-2-yl) phenol	-	-	-	-	0.39

Table S3

Non-phenolic aromatic compounds in liquid products from lignin depolymerization at different temperatures with no catalyst.

Peak	Compound	Relative content（%）				
		190 ℃	210 ℃	230 ℃	250 ℃	270 ℃
20	1,2-dimethoxy-3-methylbenzene	0.76	-	2.38	4.22	0.57
25	Dimethyl isophthalate	0.36	-	-	-	-
29	(1,1-dimethoxypropane-2-yl) benzene	4.59	1.99	-	-	-
34	Butyl isophthalate	0.28	-	-	-	-
41	3-ethoxy-4-methoxybenzaldehyde	-	0.20	0.96	0.23	-
43	Dimethyl terephthalate	-	0.55	-	-	-
44	(3,4-dimethoxyphenyl) (methoxy) methanol	-	0.80	-	-	-
45	4-(dimethoxymethyl) -1,2-dimethoxybenzene	-	0.52	-	0.54	-
46	1-(3,4-dimethoxyphenyl) ethan-1-one	-	0.65	3.67	-	-
47	3,4-dimethoxybenzaldehyde	-	1.60	9.98	1.31	4.09
49	1-ethoxy-2-methoxy-4-propylbenzene	-	-	5.45	0.87	-
50	2- (3,4-dimethoxyphenyl) -2-oxoacetaldehyde	-	-	1.77	-	-
58	1,2-dimethoxybenzene	-	-	-	3.33	0.28
59	1,2-dimethoxy-4-methylbenzene	-	-	-	0.43	0.27
62	1,5-dimethoxy-2,3-dimethylbenzene	-	-	-	1.26	-
63	1,4-dimethoxy-2-methylbenzene	-	-	-	5.12	1.27
114	2-(5-isopropyl-2-methylphenyl) ethan-1-ol	-	-	-	-	0.04
115	1-(2,3,5,6-tetramethylphenyl) ethan-1-one	-	-	-	-	0.47
116	2-(4-ethoxyphenyl) -2-methylpropanal	-	-	-	-	0.06
120	1-(4- (tert-butyl) -2,6-dimethylphenyl) ethan-1-one	-	-	-	-	0.49

Table S4

Other compounds in liquid products from lignin depolymerization at different temperatures with no catalyst.

Peak	Compound	Relative content（%）				
		190 ℃	210 ℃	230 ℃	250 ℃	270 ℃
6	Dihydrofuran-2 (3H) -one	0.09	-	-	-	-
8	Methyl furan-2-carboxylate	0.96	4.5	-	1.96	-
10	3-hydroxydihydrofuran-2 (3H) -one	0.87	-	-	-	-
14	2,2,4,5-tetramethyl-1,3-dioxolane	0.04	-	-	-	-
48	(E) methyl 2- (3,4-dimethyl-5-methylfuran-2 (5H) -subunit) acetate	-	-	0.46	-	-
51	3-isopentyl-2,4,4-trimethylcyclohex-2-en-1-one	-	-	1.39	-	-
55	2-hydroxypropionamide	-	-	-	0.52	-
81	2,3,4,5-tetramethylfuran	-	-	-	-	0.107
83	5,5-dimethylcyclohexane-1,3-dione	-	-	-	-	0.09
86	1-ethoxy-3-methoxy-5-methylcyclohexane	-	-	-	-	0.09
87	3,4,4-trimethylcyclopent-2-en-1-one	-	-	-	-	1.97
89	2,3,4,5-tetramethylcyclopent-2-en-1-one	-	-	-	-	1.34
96	1-methylnaphthalene	-	-	-	-	0.24
101	4-methoxy-6-propylbenzo [d] [1,3] dioxolene	-	-	-	-	0.07
103	1- (benzo [d] [1,3] dioxol-5-yl) propan-1-ol	-	-	-	-	0.44
107	5,5-dimethyl-1,2-dipropylcyclopentane-1,3-diene	-	-	-	-	0.20
113	5,6,7,8-tetramethyl-1,2,3,4-tetrahydronaphthalene	-	-	-	-	0.53
117	4,7-dimethoxy-2-methyl-1H-indene	-	-	-	-	0.40
121	1-(5,5-dimethylcyclopent-1-en-1-yl) -2-methoxybenzene	-	-	-	-	0.16

2. GC/MS analysis of liquid products from lignin depolymerization over KF/γ-Al_2O_3

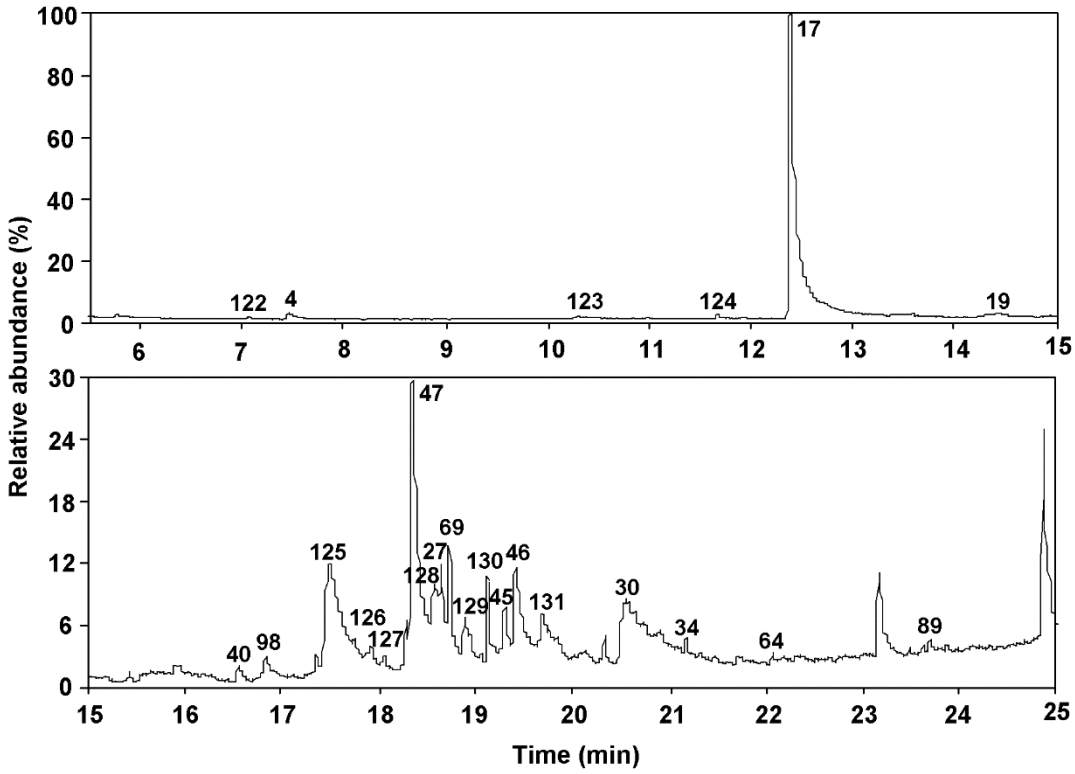

Fig. S6. TIC of liquid products from lignin depolymerization over KF/γ-Al_2O_3 at 190 ℃.

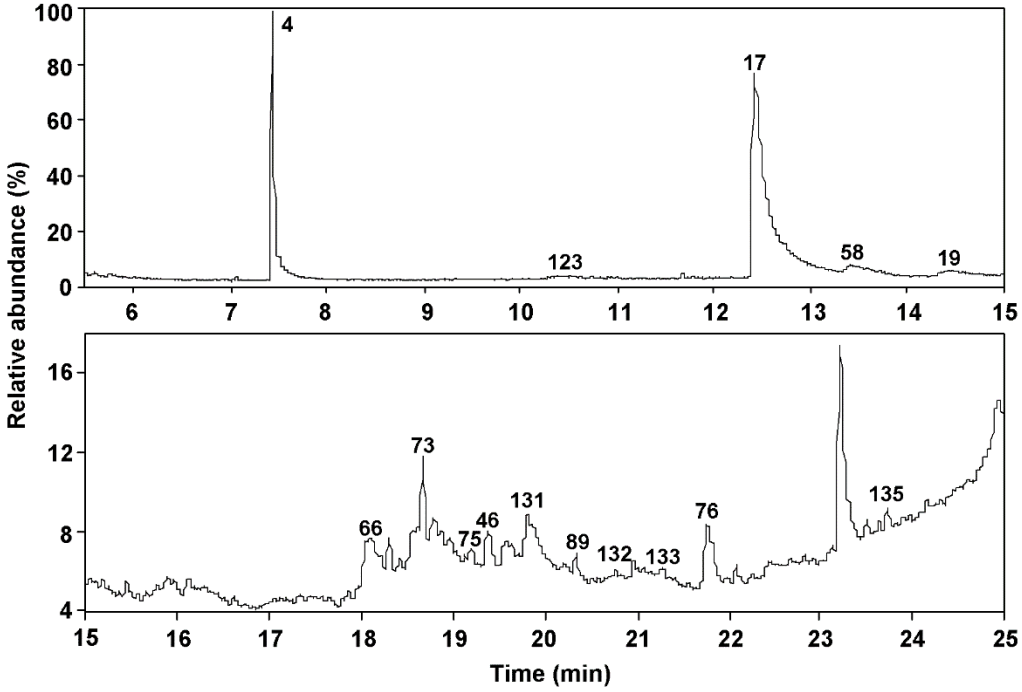

Fig. S7. TIC of liquid products from lignin depolymerization over KF/γ-Al_2O_3 at 210 ℃.

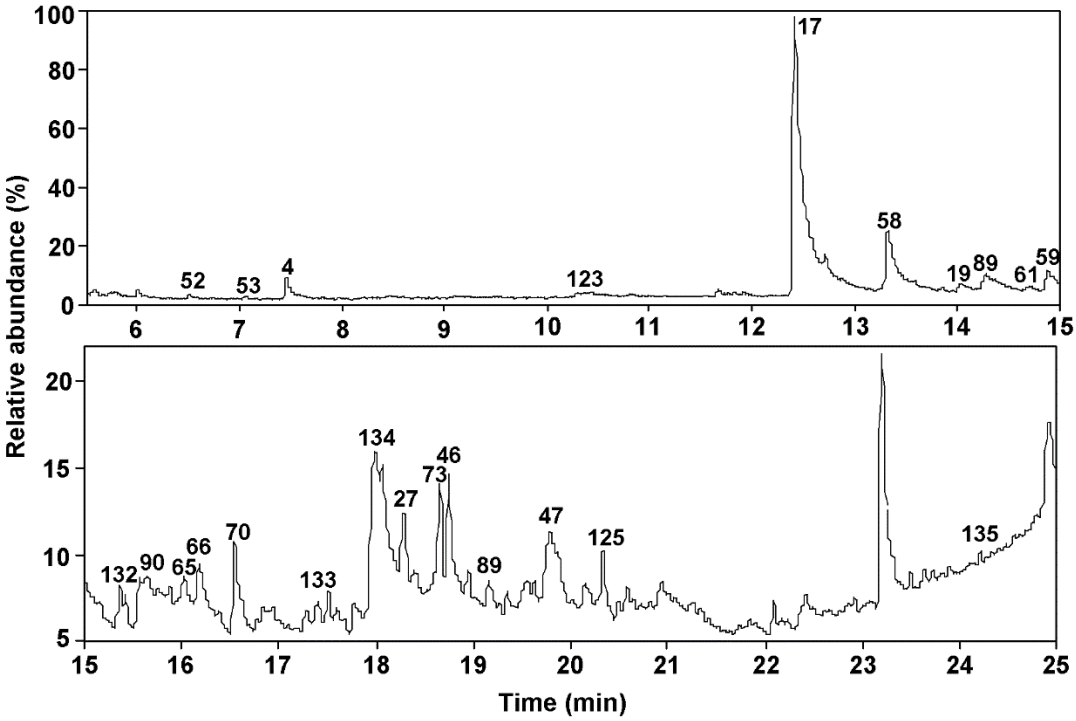

Fig. S8. TIC of liquid product from lignin depolymerization over KF/γ-Al_2O_3 at 230 ℃.

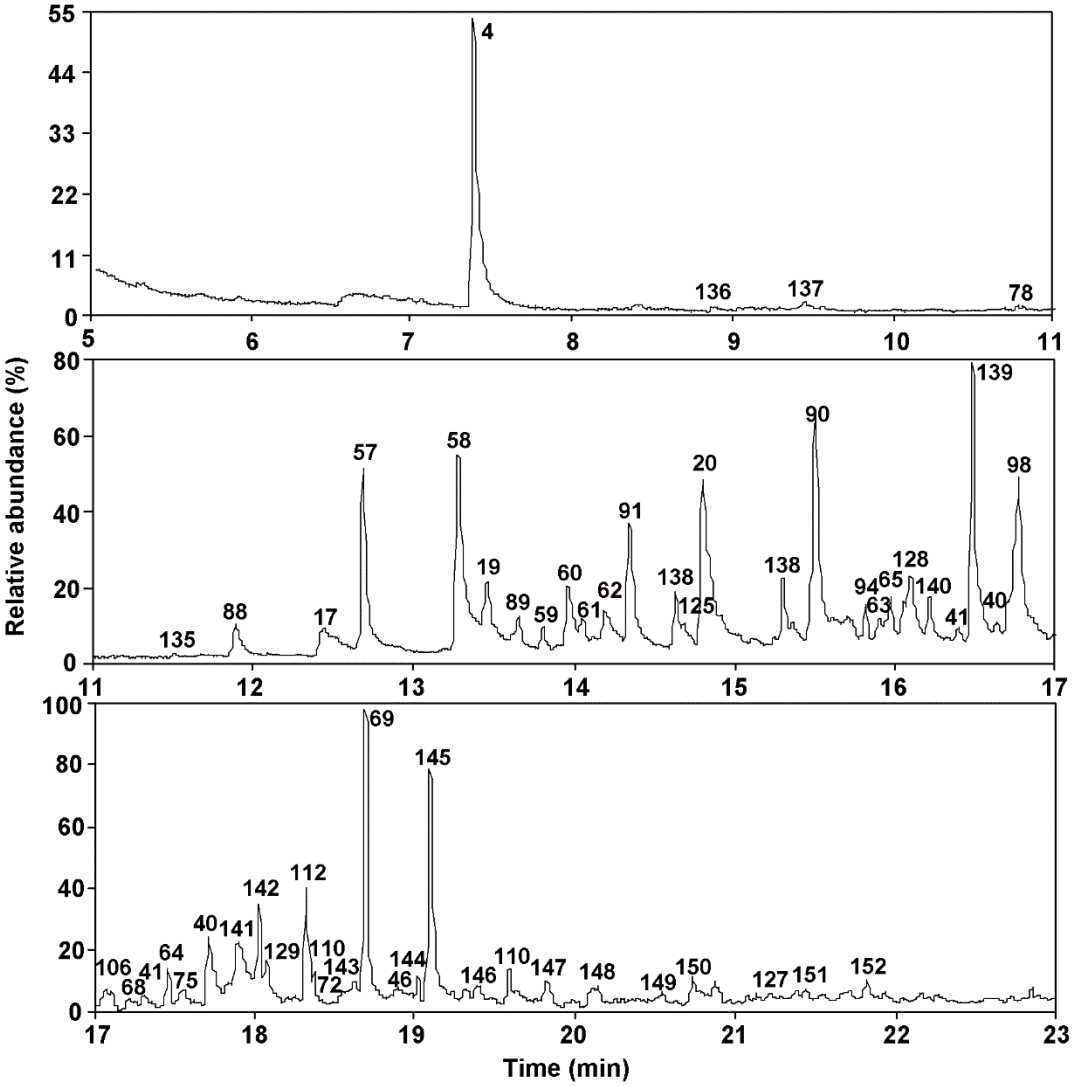

Fig. S9. TIC of liquid product from lignin depolymerization over KF/γ-Al_2O_3 at 250 ℃.

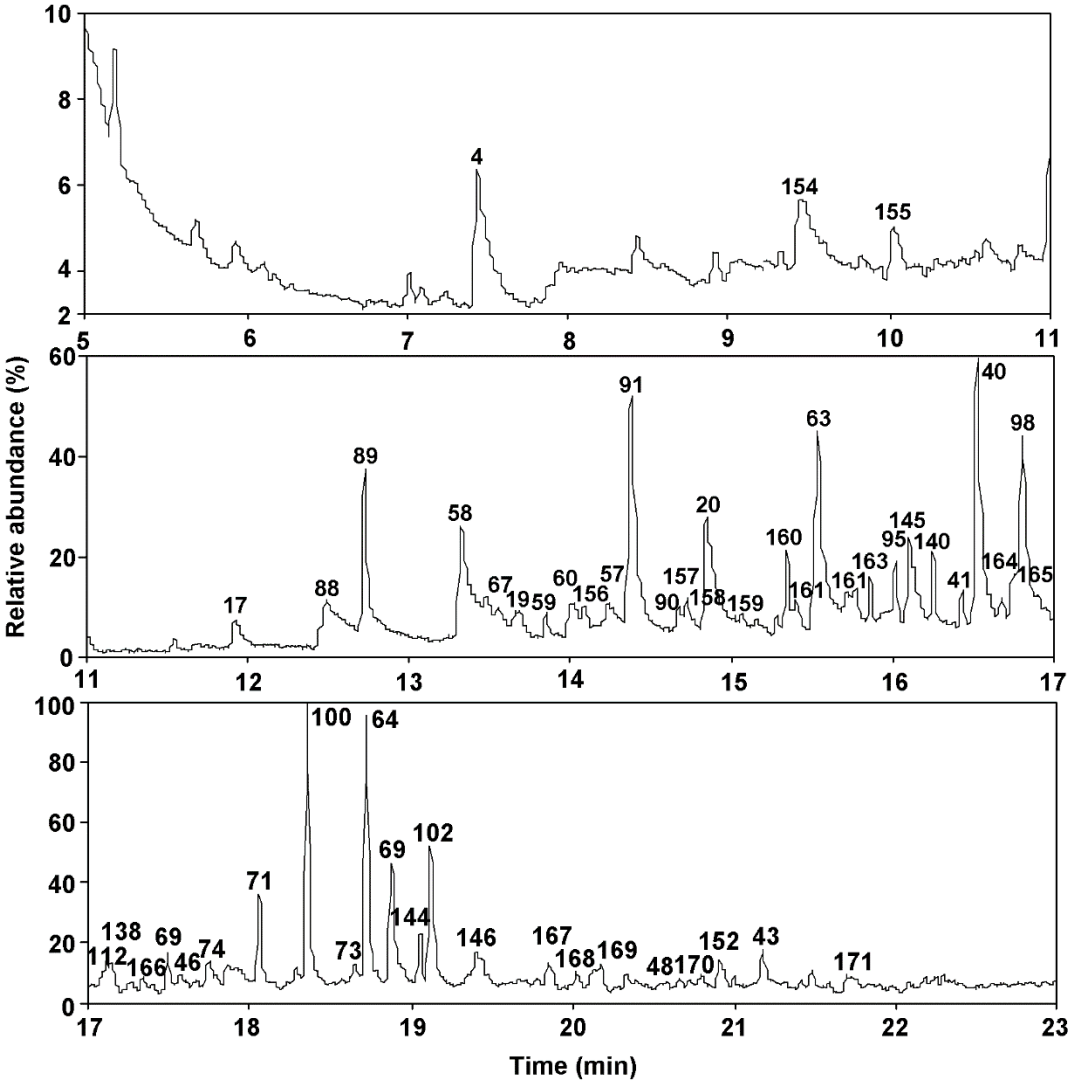

Fig. S10. TIC of liquid product from lignin depolymerization over KF/γ-Al_2O_3 at 270 ℃.

Table S5

Aliphatic compounds in liquid products from lignin depolymerization at different temperatures over KF/γ-Al_2O_3.

Peak	Compound	Relative content（%）				
		190 ℃	210 ℃	230 ℃	250 ℃	270 ℃
1	Methyl 2-oxopropionate	0.28	-	-	-	-
2	Methyl 2-hydroxypropionate	0.95	-	-	0.13	0.76
4	4-hydroxy-4-methylpentan-2-one	9.32	13.58	9.46	2.58	0.92
52	1-(2-methoxyethoxy)-2-methylpropan-2-ol	-	-	0.16	-	-
53	3,4,5-trihydroxyvaleraldehyde	-	-	0.19	0.23	-
78	4-hydroxybutan-2-one	-	-	-	0.24	
79	Methyl 2-hydroxy-3-methylbutanoate	-	-	-	-	2.18
106	Pentadecane	-	-	-	1.03	-
110	Cetane	-	-	-	0.85	-
154	2,2'-oxybis (ethyl-1-ol)	-	-	-	0.49	0.48

Table S6

Phenols in liquid products from lignin depolymerization at different temperatures over KF/γ-Al_2O_3

Peak	Compound	Relative content（%）				
		190 ℃	210 ℃	230 ℃	250 ℃	270 ℃
17	2-methoxyphenol	51.74	59.29	53.28	1.82	1.02
19	2-methoxy-4-methylphenol	1.09	4.77	1.36	1.56	0.11
27	4-(2-hydroxyethyl) -2-methoxyphenol	0.54	-	0.90	-	-
30	2- (4-hydroxy-3-methoxyphenyl) acetic acid	3.40	-	-	-	-
40	3-methoxy-2,4,6-trimethylphenol	0.41	-	-	2.98	7.66
57	2-methoxy-5-methylphenol	-	-	-	4.95	0.59
60	2-methoxy-3-methylphenol	-	-	-	1.72	0.75
61	2,3,5-trimethylbenzene-1,4-diol	-	-	0.89	0.35	-
64	2-(tert-butyl) -4-methoxyphenol	0.14	-	-	0.82	8.96
67	2,5 diethylphenol	-	-	-	0.12	0.07
69	3-(tert-butyl) -4-methoxyphenol	1.34	-	-	6.94	4.99
70	2,3,5,6-tetramethylbenzene-1,4-diol	-	-	1.56	-	-
73	2,5-di-tert-butylphenol	-	1.01	0.78	-	0.43
88	4-methoxyphenol	-	-	-	1.22	2.69
89	2-methoxy-5-methylphenol	-	3.22	-	0.64	3.71
90	1-(2,5-dihydroxyphenyl) ethan-1-one	-	-	0.89	6.83	0.38
91	2,4,6-trimethylphenol	-	-	-	3.66	6.61
98	2,3,4,6-tetramethylphenol	0.67	-	-	5.71	3.56
102	1-(2-hydroxy-4,5-dimethylphenyl) ethan-1-one	-	-	-	-	3.92
112	2-(tert-butyl) -4,6-dimethylphenol	-	-	-	1.98	0.07
123	phenol	0.36	0.64	0.72	-	-
125	4-hydroxy-3-methoxybenzaldehyde	9.20	-	-	0.13	-
126	2-hydroxy-4-methoxybenzaldehyde	0.66	-	-	-	-
127	3-hydroxy-4-methoxybenzaldehyde	0.25	-	-	0.12	-
128	5-methoxy-2,3,4-trimethylphenol	0.60	-	-	2.02	-
129	3-hydroxy-4-methoxybenzoic acid methyl ester	1.12	-	-	0.50	-
139	1-(4-hydroxy-3-methoxyphenyl) ethan-1-one	-	-	-	7.89	-
140	4,5-dimethylbenzene-1,3-diol	-	-	-	0.98	1.03
145	2-(tert-butyl) -6-methylphenol	-	-	-	7.12	2.79
149	(E) -4-methyl-2- (pent-3-en-2-yl) phenol	-	-	-	0.42	-
150	2-allyl-5-ethoxy-4-methoxyphenol	-	-	-	0.04	-
160	1-(2,6-dihydroxy-3-methylphenyl) ethan-1-one	-	-	-	-	0.99
161	1-(3,4-dihydroxyphenyl) propan-1-one	-	-	-	-	0.32
164	4-methoxy-2,3,6-trimethylphenol	-	-	-	-	0.18

Table S7

Non-phenolic aromatic compounds in liquid products from lignin depolymerization at different temperatures over KF/γ-Al_2O_3.

Peak	Compound	Relative content（%）				
		190 ℃	210 ℃	230 ℃	250 ℃	270 ℃
20	1,2-dimethoxy-3-methylbenzene	-	-	-	5.95	4.39
34	Butyl isophthalate	0.28	-	-	-	-
41	3-ethoxy-4-methoxybenzaldehyde	-	-	-	0.55	0.51
43	Dimethyl terephthalate	-	-	-	-	1.06
45	4-(dimethoxymethyl) -1,2-dimethoxybenzene	0.99	-	-	-	-
46	1-(3,4-dimethoxyphenyl) ethan-1-one	3.24	1.85	1.07	0.25	0.20
47	3,4-dimethoxybenzaldehyde	9.44	0.46	1.82	-	-
58	1,2-dimethoxybenzene	-	3.27	8.97	7.66	6.28
59	1,2-dimethoxy-4-methylbenzene	-	-	2.82	0.89	0.38
63	1,4-dimethoxy-2-methylbenzene	-	-	-	1.43	6.01
65	1,2,3-trimethoxybenzene	-	-	0.15	0.74	-
66	4-ethyl-1,2-dimethoxybenzene	-	1.74	0.98	-	-
68	Isopropyl 2-methoxybenzoate	-	-	-	0.26	-
71	1-(2,4-dimethoxyphenyl) propan-2-one	-	-	-	-	2.30
72	(E)-1,2-dimethoxy-4- (prop-1-en-1-yl) benzene	-	-	-	0.44	-
74	(4- (tert-butyl) phenyl) methanol	-	-	-	0.16	0.48
75	1-(2,4-dimethoxyphenyl) ethan-1-one	-	2.90	-	1.50	-
94	3,5-dimethoxy-4-methylbenzaldehyde	-	-	-	0.54	-
95	4-isopropylbenzoic acid	-	-	-	-	1.27
100	1-(tert-butyl) -2-methoxy-3-methylbenzene	-	-	-	-	8.50
130	2-isopropyl-1-methoxy-4-methylbenzene	1.31		-	-	
131	3,4-Dimethoxybenzoic acid methyl ester	0.72	2.87	-	-	-
134	1-ethyl-2-methoxy-4- (methoxymethyl) benzene	-	-	5.24	-	-
138	1-(2-methoxyphenyl) ethan-1-ol	-	-	-	1.07	0.16
141	1,2-dimethoxy-4- (methoxymethyl) benzene	-	-	-	2.04	-
142	1,4-dimethoxy-2-((vinyloxy) methyl) benzene	-	-	-	1.52	-
143	1-(3,4-dimethoxyphenyl) butan-1-one	-	-	-	0.22	-
144	1,3-diisopropyl-2-methoxybenzene	-	-	-	0.52	1.45
146	2-(tert-butyl) -1,4-dimethoxybenzene	-	-	-	0.46	1.66
147	2,4-diisopropylphenyl acetate	-	-	-	0.81	-
148	1-(3,4-dimethoxyphenyl) propan-1-one	-	-	-	0.26	-
152	1,3,5-triisopropylbenzene	-	-	-	0.10	1.25
153	(4-(tert-butyl) phenoxy) methyl acetate	-	-	-	-	-
156	1,4dimethoxybenzene	-	-	-	-	0.31
157	2-methoxy-4- (prop-1-en-2-yl) phenyl acetate	-	-	-	-	0.29
158	2-methoxy-1,3,4-trimethylbenzene	-	-	-	-	0.07

162	2-(2-methoxyphenyl) acetaldehyde	-	-	-	-	0.25
165	1,2,3-trimethoxy-5-methylbenzene	-	-	-	-	0.13
166	3-ethoxy-4-methoxybenzaldehyde	-	-	-	-	0.36
168	phthalate-4,5-dimethyl	-	-	-	-	0.41
171	1,4-bis (pent-3-yl) benzene	-	-	-	-	0.02

Table S8

Other compounds in liquid products from lignin depolymerization at different temperatures over KF/γ-Al_2O_3.

Peak	Compound	Relative content（%）				
		190 ℃	210 ℃	230 ℃	250 ℃	270 ℃
48	(E) methyl 2- (3,4-dimethyl-5-methylfuran-2 (5H) -subunit) acetate	-	-	-	-	0.05
89	2,3,4,5-tetramethylcyclopent-2-en-1-one	0.46	1.06	1.52	-	-
132	1-(2-ethyl-5-methoxy-4-methylphenyl) propan-2-amine	-	0.76	0.36	-	-
133	2-amino-1-phenylpropan-1-ol	-	0.87	0.32	-	-
135	4-(4-methylcyclohexyl) benzene-1,2-diol	0.54	1.37	4.40	0.10	-
137	(Z)-cyclooct-4-ene-1-carbaldehyde	-	-	-	0.11	-
151	1,1'-(6-hydroxybenzofuran-2,5-diyl) bis (ethyl-1-one)	-	-	-	0.14	-
155	1,2,3,4,5-pentamethylcyclopentane-1,3-diene	-	-	-		0.32
159	1-(3,4-dihydroxyphenyl)-2- (methylamino) ethan-1-one	-	-	-	-	0.10
163	2,2-dimethyl-2,3-dihydrobenzofuran-3,7-diol	-	-	-	-	0.64
167	1-(2,3-dihydrobenzo [b] [1,4] dioxin-6-yl) ethan-1-one	-	-	-	-	0.99
169	1,1-dimethyl-2,3-dihydro-1H-indene-4-carboxylic acid ethyl ester	-	-	-	-	0.87
170	4,4-dimethyl-[1,1'-bis (cyclohexane)]-1', 3'-diene-2,6-dione	-	-	-	-	0.18
172	8,9-dimethyl-2H-furo [2,3-h] chromen-2-one	-	-	-	-	0.13
174	3-(acetoxymethyl) biphenylene-2-carboxylic acid methyl ester	-	-	-	-	0.41

-no detected