Supplementary Information

Structural changes in milled wood lignin (MWL) of Chinese quince (*Chaenomeles sinensis*) fruit subjected to subcritical water treatment

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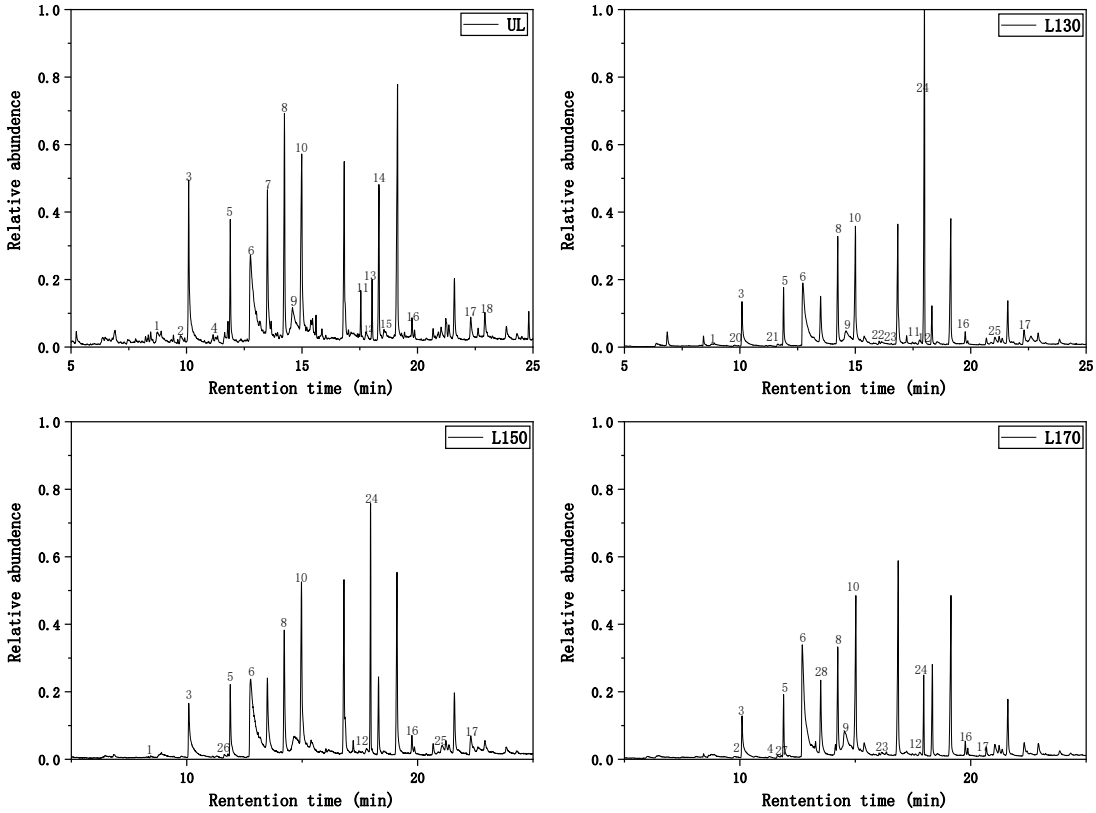

Figure S1. Py-GC/MS chromatograms of UL, L130, L150, and L170 fractions.

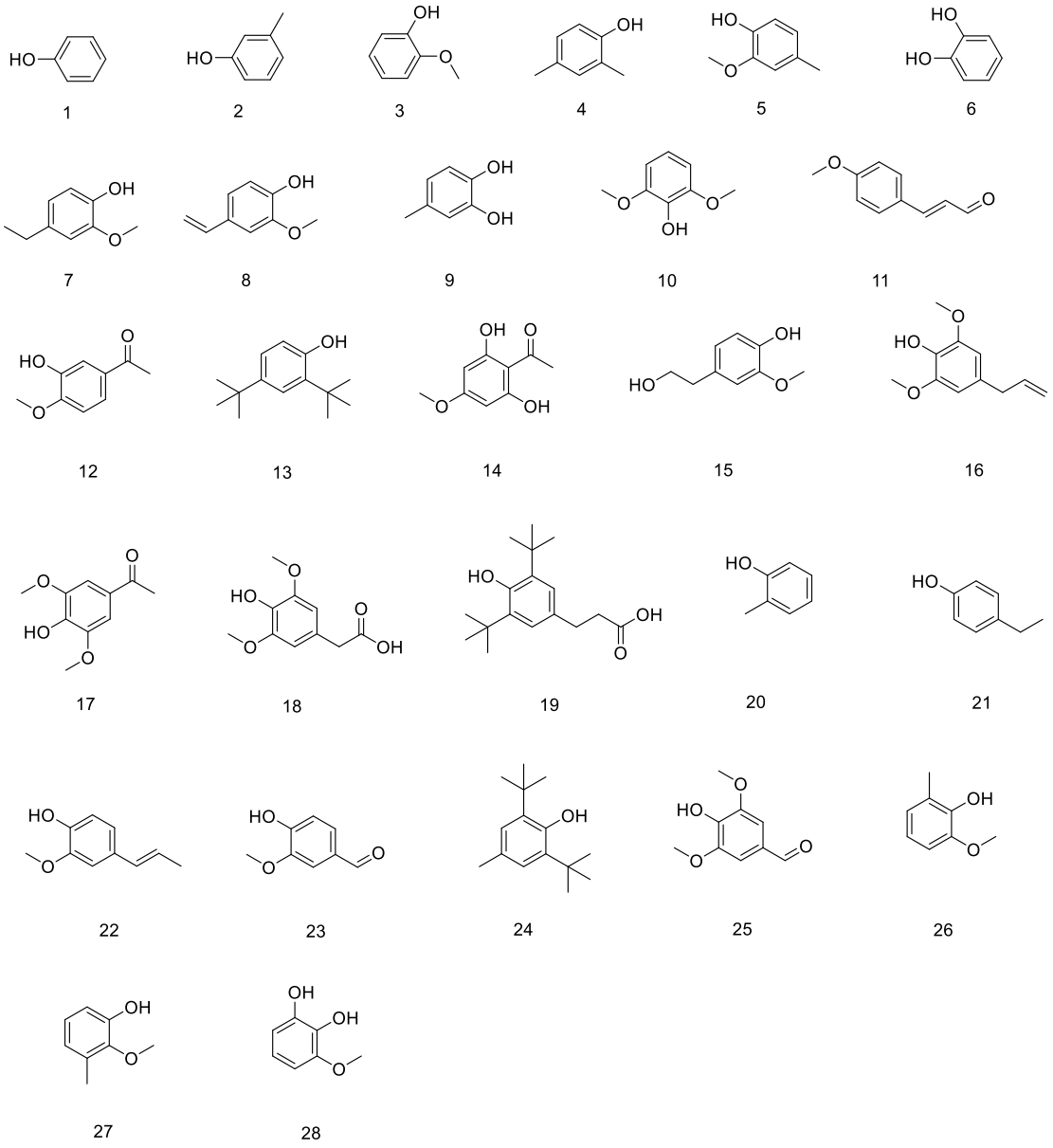

Figure S2. The structural compounds labelled in Table S1

Table S1

The identities and relative abundances of carbohydrate-derived compounds by Py-GC/MS.

NO.	Compound	Origin	UL	L130	L150	L170
1	Phenol	H	1.4	0.1	0.4	0.0
2	Phenol, 3-methyl-	H	0.5	0.0	0.0	0.2
3	Phenol, 2-methoxy-	G	12.7	7.8	11.4	7.7
4	Phenol, 2,4-dimethyl-	H	0.6	0.0	0.0	0.5
5	Creosol	G	6.1	5.7	7.1	5.5
6	Catechol	G	18.7	24.3	28.6	33.9
7	Phenol, 4-ethyl-2-methoxy-	G	9.9	0.0	0.0	0.0
8	2-Methoxy-4-vinylphenol	G	13.6	11.5	12.2	10.0
9	1,2-Benzenediol, 4-methyl-	G	3.0	2.2	0.0	4.2
10	Phenol, 2,6-dimethoxy-	S	15.1	13.8	18.3	16.5
11	trans-4-Methoxycinnamaldehyde	G	0.1	0.1	0.0	0.0
12	Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-	G	0.9	0.8	0.5	0.5
13	Phenol, 2,4-bis(1,1-dimethylethyl)-	H	2.9	0.0	0.0	0.0
14	Ethanone, 1-(2,6-dihydroxy-4-methoxyphenyl)-	G	8.5	0.0	0.0	0.0
15	Homovanillyl alcohol	G	0.4	0.0	0.0	0.0
16	Phenol, 2,6-dimethoxy-4-(2-propenyl)-	S	1.1	1.1	1.5	1.2
17	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	S	2.4	2.5	3.1	2.1
18	3,5-Dimethoxy-4-hydroxyphenylacet	S	1.9	0.0	0.0	0.0

	ic acid					
19	3,5-di-tert-Butyl-4-hydroxyphenylpropionic acid	H	0.0	0.0	0.0	0.0
20	Phenol, 2-methyl-	H	0.0	0.1	0.0	0.0
21	Phenol, 4-ethyl-	H	0.0	0.1	0.0	0.0
22	Phenol, 2-methoxy-4-(1-propenyl)-	G	0.0	0.3	0.0	0.0
23	Vanillin	G	0.0	0.4	0.0	0.5
24	Butylated Hydroxytoluene	H	0.0	29.0	14.8	5.4
25	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	S	0.0	1.3	1.5	1.9
26	2-Methoxy-6-methylphenol	G	0.0	0.0	0.7	0.0
27	Phenol, 2-methoxy-3-methyl-	G	0.0	0.0	0.0	0.5
28	1,2-Benzenediol, 3-methoxy-	G	0.0	0.0	0.0	9.5
	H%		5.4	29.3	15.2	6.1
	G%		73.9	53.1	60.5	72.3
	S%		20.5	18.7	24.4	21.7
	S/G		0.34	0.45	0.51	0.35

Table S2

Assignments of main lignin ^{13}C-^{1}H cross signals in the 2D HSQC spectra of the UL and L170.

Label	δ_C/δ_H	Assignment
B_β	54.3/2.99	C_β−H_β in β-β (resinol) substructures (B)
−OCH_3	56.4/3.68	C−H in methoxyls
A_γ	60.4//3.30−3.79	C_γ−H_γ in β-O-4 substructures (A)
Est	62.7/4.30	γ-ester of LCC
Ara-6	63.3/3.40	C_6−H_6 in arabinosyl units
C_γ	63.3/3.66	C_γ−H_γ in phenylcoumaran substructures (C)
B_γ	71.8/3.75−4.12	C_γ−H_γ in β-β resinol substructures (B)
A_α	72.6/4.81	C_α−H_α in β-O-4 substructures (A)
Glu-5	73.3/3.25	C_5−H_5 in glucosyl units
$A_{\beta(G/H)}$	84.3/4.23	C_β−H_β in β-O-4 linked to G/H unit (A)
B_α	85.7/4.59	C_α−H_α in β-β resinol substructures (B)
$A_{\beta(S)}$	86.7/4.06	C_β−H_β in β-O-4 linked to a S unit (A)
C_α	87.7/5.38	C_α−H_α in phenylcoumaran substructures (C)
$S_{2,6}$	104.5/6.63	$C_{2,6}$−$H_{2,6}$ in syringyl units (S)
$S'_{2,6}$	107.2/7.26	$C_{2,6}$−$H_{2,6}$ in oxidized S units (S′)
G_2	111.8/6.94	C_2−H_2 in guaiacyl units (G)
G'_2	112.0/7.52	C_2−H_2 in oxidized G units (G′)
PCA_8	114.2/6.27	C_8−H_8 in *p*-coumaric acid (PCA)
$PCA_{3,5}$	115.2/6.71	$C_{3,5}$−$H_{3,5}$ in *p*-coumaric acid (PCA)
G_5	115.6/6.65	C_5−H_5 in guaiacyl units (G)
G_6	119.6/6.75	C_6−H_6 in guaiacyl units (G)
J_β	125.6/6.82	C_β-H_β in cinnamaldehyde end groups (J)
$H_{2,6}$	129.2/7.17	$C_{2,6}$−$H_{2,6}$ in H units (H)