

Table S1. Elemental composition of the lignin and oil samples. In the case of replicate experiments performed, the value presented in the table is an average of the experiments in question.

Sample name	mol % N	mol % C	mol % S	mol % H	mol % O	O/C	H/C
SW1	0.01	3.92	0.0902	5.31	2.79	0.71	1.35
SW1-kraft-320	0.06	5.92	0.0032	7.40	1.29	0.22	1.25
SW1-kraft-360	0.06	6.40	0.0026	8.11	0.88	0.14	1.27
HW1	0.02	5.00	0.0003	5.96	2.11	0.42	1.19
HW1-wetox-320	0.08	5.73	0.0010	7.20	1.43	0.25	1.26
HW1-wetox-360	0.07	6.06	0.0006	7.36	1.18	0.19	1.21
G1	0.02	5.03	0.0003	5.38	2.12	0.42	1.07
G1-wetox-320	0.08	5.74	0.0004	6.89	1.44	0.25	1.20
G1-wetox-360	0.08	6.23	0.0009	7.73	1.02	0.16	1.24
HW2	0.02	3.74	0.0004	5.08	3.11	0.83	1.36
HW2-milox-320	0.08	6.09	0.0011	7.99	1.11	0.18	1.31
HW2-milox-360	0.08	6.39	0.0011	8.40	0.86	0.14	1.31
G2	0.20	3.60	0.0012	5.88	3.01	0.84	1.63
G2-deac-320	0.23	6.10	0.0017	8.67	0.93	0.15	1.42
G2-deac-360	0.24	6.26	0.0007	9.03	0.78	0.12	1.44
G3	0.16	3.34	0.0007	5.18	3.28	0.98	1.55
G3-deac-320	0.18	6.21	0.0010	9.30	1.05	0.14	1.50
G3-deac-360	0.21	6.23	0.0007	9.06	0.82	0.13	1.45
G4	0.15	3.35	0.0011	5.63	3.25	0.97	1.68
G4-deac-320	0.21	6.15	0.0011	9.25	0.87	0.14	1.51
G4-deac-360	0.22	6.26	0.0013	9.35	0.78	0.12	1.49
G5	0.20	3.87	0.0329	5.37	2.78	0.72	1.39
G5-acid-320	0.21	6.09	0.0009	8.48	0.97	0.16	1.39
G5-acid-360	0.22	6.26	0.0016	8.91	0.80	0.13	1.42
SW2	0.06	5.12	0.0308	5.86	1.93	0.38	1.14
SW2-kraft-320	0.08	5.87	0.0009	7.06	1.34	0.23	1.20
SW2-kraft-360	0.05	6.11	0.0010	7.57	1.15	0.19	1.24
SW4	0.01	4.86	0.002	5.19	2.26	0.47	1.07
SW4-wetox-320	0.08	5.81	0.003	6.80	1.39	0.24	1.17
SW4-wetox-360	0.07	5.95	0.003	6.51	1.31	0.22	1.09

Table S2. Quantification of selected compounds (weight percent of bio-oil). The sample with the highest content of each compound is given in bold.

	SW1-kraft-320	SW1-kraft-360	HW1-wetox-320	HW1-wetox-360	G1-wetox-320	G1-wetox-360	HW2-milox-320	G2-deac-360	G2-dec-360	G3-deac-320	G4-deac-360	G5-acid-360	SW2-kraft-320	SW2-kraft-360	SW4-wetox-320	SW4-wetox-360				
Phenol	0.140	0.297	0.001	0.095	0.113	0.182	0.120	0.160	0.146	0.239	0.266	0.470	0.270	0.473	0.390	0.445	0.238	0.272	0.004	0.005
Phenylethylalcohol	NA	NA	NA	NA	NA	NA	NA	NA	0.001	0.076	0.068	0.100	0.086	0.140	0.041	NA	NA	NA	NA	NA
Syringol	NA	NA	0.880	0.755	1.077	0.100	0.054	NA	NA	NA	NA	NA	NA	NA	0.085	NA	NA	NA	NA	NA
4-methylphenol	0.078	0.326	NA	0.118	Trace	0.214	NA	0.090	0.073	0.180	0.093	0.260	0.133	0.277	0.160	0.296	0.122	0.246	NA	0.013
guaiacol	0.583	0.152	1.308	1.074	1.408	0.662	0.363	0.118	0.135	0.047	0.332	0.256	0.232	0.189	0.661	0.206	1.793	0.660	0.145	0.145
4-methylguaiacol	0.059	0.019	0.273	0.294	0.464	0.141	0.024	NA	0.014	Trace	NA	NA	NA	NA	NA	0.340	0.136	0.043	0.061	
Catechol	0.942	0.108	0.347	0.627	0.473	0.671	0.376	0.292	0.464	0.381	0.792	0.940	0.481	1.014	0.764	0.887	1.520	1.243	0.052	0.018
3-methylcatechol	0.260	0.092	0.088	0.130	0.179	0.117	0.121	0.055	0.039	0.043	NA	0.123	NA	0.140	0.077	0.094	0.099	0.155	0.018	0.030
4-ethylcatechol	0.466	0.173	0.071	0.190	0.132	0.297	0.100	0.133	0.396	0.466	0.804	1.216	0.504	0.752	0.968	1.282	0.662	0.726	trace	0.012
4-propylguaiacol	0.146	0.064	0.101	0.079	0.091	0.065	0.051	0.010	0.001	NA	NA	NA	0.017	NA	0.045	NA	0.322	0.076	0.030	0.027
3-methoxycatechol	NA	NA	0.430	0.347	0.315	0.013	0.030	NA	0.001	NA	0.053	NA	0.033	NA	0.084	NA	NA	NA	NA	NA
2-naphthol	Trace	Trace	NA	0.052	Trace	0.046	Trace	0.010	0.001	Trace	0.055	0.081	0.047	0.001	0.065	0.078	0.075	0.084	NA	NA
4-ethylphenol	0.060	0.137	Trace	0.040	Trace	0.084	Trace	0.050	0.574	0.820	0.938	1.656	1.017	1.178	1.135	1.323	0.151	0.206	NA	NA
4-ethylguaiacol	0.240	0.037	0.155	0.232	0.150	0.157	0.094	0.030	0.195	0.051	0.549	0.494	0.312	0.190	1.238	0.442	0.881	0.303	0.009	0.017
2-(4-hydroxy-phenyl)ethanol	NA	NA	0.001	NA	NA	NA	NA	NA	0.119	NA	0.186	0.211	0.143	0.348	0.105	0.132	Trace	Trace	0.012	NA

Table S3. Results from regression modelling of the individual compounds based on biomass origin, pretreatment method and temperature.

The higher the regression coefficient, the better the model explains the results.

Compounds	Regression coefficient R Biomass	Regression coefficient R Pretreatment	Regression coefficient R Temperature
Phenol	0.623	0.821	0.329
Phenylethylalcohol	0.604	0.738	0.140
Syringol	0.457	0.531	0.192
4-methylphenol	0.420	0.620	0.651
Guaiacol	0.245	0.455	0.353
4-methylguaiacol	0.251	0.556	0.209
Catechol	0.272	0.594	0.004
3-methylcatechol	0.197	0.504	0.080
4-ethylcatechol	0.592	0.800	0.150
4-propylguaiacol	0.526	0.513	0.330
3-methoxycatechol	0.556	0.488	0.227
2-naphthol	0.259	0.402	0.165
4-ethylphenol	0.751	0.929	0.150
4-ethylguaiacol	0.322	0.499	0.308
2-(4-hydroxyphenyl)ethanol	0.640	0.785	0.065