Supplementary Materials

Title

Investigating lignin-derived monomers and oligomers in low-molecular-weight fractions separated from depolymerized black liquor retentate by membrane filtration

Authors

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Table S1. Identified phenolic compounds in the BDM170 sample including the detected $[M-H]^-$, determined chemical formulas, classified class, obtained mass difference, obtained ^{13}C ratio, ring double bound (RDB) equivalent, retention times (RTs), obtained MS^n spectra (*: MS^n of identified fragment) [1].

[M-H]-	Chemical formula (neutral)	Classified class	Mass diff. (mDa)	^{13}C ratio	RDB	RTs (min)	MS^n	Suggested compound	Identification confidence level
121.0295	C7H6O2	Monomer	0.0	1.10	5.0	2.51		4-hydroxybenzaldehyde	1
135.0451	C8H8O2	Monomer	0.0	1.04	5.0	2.54	MS^2	4-hydroxyacetophenone	1
137.0243	C7H6O3	Monomer	-0.1	0.96	5.0	4.05	MS^2	4-hydroxybenzoic acid	1
151.0399	C8H8O3	Monomer	-0.1	1.00	5.0	1.25	MS^3	Vanillin	1
165.0554	C9H10O3	Monomer	-0.3	0.97	5.0	1.25		Acetovanillone	1
				1.00		2.23	MS^2	Homovanillin	2
167.0347	C8H8O4	Monomer	-0.3	1.03	5.0	1.62		3,4-dihydroxy-5-methoxybenzaldehyde	3
				1.04		4.08		2-(3,4-dihydroxy acetaldehyde	3
175.0761	C11H12O2	Monomer	-0.3	0.97	6.0	2.85		(5-ethylbenzo-furan-3-yl) methanol	3
181.0502	C9H10O4	Monomer	-0.4	1.06	5.0	1.63	MS^3	Syringaldehyde	1
				0.95		3.68	MS^3	3,4-dihydroxy-5-methoxy-acetophenone	2
195.0658	C10H12O4	Monomer	-0.5	1.00	5.0	1.63		Acetosyringone	1
				1.00		3.22		1-(3,4-dihydroxy-5-methoxyphenyl) propan-2-one	3
203.0709	C12H12O3	Monomer	-0.4	1.00	7.0	2.57		(7-methoxy-5-vinylbenzofuran -3-yl) methanol	3
233.0270	C12H10O3S	Dimer	-0.8	1.03		2.14			3
243.0653	C14H12O4	Dimer	-1.0	1.08	9.0	3.40			3
				0.93		3.52			3
245.0810	C14H14O4	Dimer	-0.9	0.88	8.0	5.26			3

257.0447	C14H10O5	Dimer	-0.8	1.00	10.0	3.27			3
257.0812	C15H14O4	Dimer	-0.7	0.95	9.0	2.85			3
259.0604	C14H12O5	Dimer	-0.8	0.88	9.0	3.62			3
271.0604	C15H12O5	Dimer	-0.8	1.00	10.0	3.13			3
				1.04		4.53	MS^3		3
273.0759	C15H14O5	Dimer	-0.9	1.00	9.0	3.28	MS^3		3
273.1124	C16H18O4	Dimer	-0.8	°	8.0	3.99			3
				0.92		4.19			3
287.0915	C16H16O5	Dimer	-1.0	0.92	9.0	2.94	MS^3		2
				0.94		3.13			3
299.0916	C17H16O5	Dimer	-0.9	0.86	10.0	3.50			3
301.0707	C16H14O6	Dimer	-1.0	0.96	10.0	1.26			3
				1.03		3.93	MS^3		2
				1.00		4.25	MS^3		3
301.1071	C17H18O5	Dimer	-1.0	0.99	9.0	2.99	MS^3		2
				0.92		5.48			3
301.1436	C18H22O4	Dimer	-0.9	1.00	8.0	4.87			3
303.0865	C16H16O6	Dimer	-0.9	0.90	9.0	3.69			3
313.1434	C19H22O4	Dimer	-1.1	0.98	9.0	5.18	MS^3		3
				1.00		5.75	MS^3		3
315.0862	C17H16O6	Dimer	-1.2	1.07	10.0	1.26			3
				0.89		2.78			3
				1.08		4.00	MS^3		3
				0.85		5.12			3
315.1227	C18H20O5	Dimer	-1.1	1.05	9.0	3.13	MS^3		2
317.1021	C17H18O6	Dimer	-0.9	0.85	9.0	3.60			3
323.0915	C19H16O5	Dimer	-1.0	0.91	12.0	3.86			3

329.1018	C18H18O6	Dimer	-1.2	1.00	10.0	1.26			3
				0.98		3.80	MS^2		2
				1.00		3.87	MS^2		3
				0.99		4.16	MS^2		3
				0.98		4.99			3
329.1383	C19H22O5	Dimer	-1.1	0.99	9.0	2.99			3
				1.06		6.18	MS^3		3
331.1176	C18H20O6	Dimer	-1.1	0.95	9.0	3.37			3
				1.00		4.69	MS^3		2
343.1176	C19H20O6	Dimer	-1.1	1.05	10.0	3.72			3
345.1332	C19H22O6	Dimer	-1.0	0.89	9.0	3.52			3
				1.05		6.86	MS^3		3
347.1124	C18H20O7	Dimer	-1.2	0.95	9.0	4.09			3
				1.07		5.29	MS^3		3
351.1228	C21H20O5	Dimer	-1.0	1.13	12.0	4.27			3
355.1175	C20H20O6	Dimer	-1.2	0.91	11.0	4.12			3
				0.90		4.63			3
359.1488	C20H24O6	Dimer	-1.2	1.00	9.0	4.47	MS^3		2
				0.96		4.66			3
				0.97		5.44			3
365.1018	C21H18O6	Dimer	-1.2	0.92	13.0	4.84			3
				1.00		5.48			3
373.1281	C20H22O7	Dimer	-1.2	1.09	10.0	3.66			3
				0.94		4.46			3
				0.93		5.29			3
				0.88		5.45			3
				1.00		5.50			3

379.1386	C19H24O8	Dimer	-1.2	0.94	8.0	5.22			3
399.1437	C22H24O7	Dimer	-1.2	0.92	11.0	4.05			3
419.1700	C22H28O8	Dimer	-1.1	0.88	9.0	4.77			3
				0.89		4.83			3
				0.96		5.34			3

Table S2. Identified phenolic compounds in the BDM190 sample including the detected $[M-H]^-$, determined chemical formulas, classified class, obtained mass difference, obtained ^{13}C ratio, ring double bound (RDB) equivalent, retention times (RTs), obtained MS^n spectra (*: MS^n of identified fragment).

[M-H]-	Chemical formula (neutral)	Classified class	Mass diff. (mDa)	^{13}C ratio	RDB	RTs (min)	MS^n	Suggested compound	Identification confidence level
109.0296	C6H6O2	Monomer	0.1	0.96	4.0	0.56		Catechol	3
121.0295	C7H6O2	Monomer	0.0	1.00	5.0	2.52		4-hydroxybenzaldehyde	1
135.0450	C8H8O2	Monomer	0.0	1.08	5.0	2.55		4-hydroxyacetophenone	1
137.0243	C7H6O3	Monomer	-0.1	0.86	5.0	1.24			3
				1.00		4.02			3
151.0399	C8H8O3	Monomer	-0.1	1.00	5.0	1.25	MS^3	Vanillin	1
				0.97		3.62			3
161.0605	C10H10O2	Monomer	-0.3	0.89	6.0	2.83	MS^2		2
				0.91		2.90			3
				0.94		2.95			3
				1.08		3.08			3
165.0555	C9H10O3	Monomer	-0.2	1.03	5.0	1.25		Acetovanillone	1
				1.09		2.24	MS^3		2
167.0346	C8H8O4	Monomer	-0.4	0.92	5.0	1.24			3
				1.00		1.63			3
175.0761	C11H12O2	Monomer	-0.3	0.91	6.0	2.69			3
				0.89		2.80			3
				1.08		2.86			3
177.0554	C10H10O3	Monomer	-0.3	0.92	6.0	3.55			3
				0.92		3.65			3
179.0709	C10H12O3	Monomer	-0.4	0.93	5.0	1.20			3
	C10H12O3			0.92		2.19			3

	C10H12O3			0.91		2.81			3
	C10H12O3			0.85		3.74			3
181.0503	C9H10O4	Monomer	-0.3	1.00	5.0	1.63	MS^3	Syringaldehyde	1
183.0295	C8H8O5	Monomer	-0.4	0.95	5.0	1.24			3
191.0709	C11H12O3	Monomer	-0.4	0.89	6.0	1.61			3
				0.92		1.77			3
				0.96		3.62			3
195.0658	C10H12O4	Monomer	-0.5	1.01	5.0	1.63		Acetosyringone	1
				1.02		2.93			3
				0.85		3.21			3
213.0551	C13H10O3	Monomer	-0.6	0.97	9.0	3.63			3
				0.86		3.56			3
241.0499	C14H10O4	Dimer	-0.7	0.92	10.0	3.30			3
				1.00		4.70			3
243.0654	C14H12O4	Dimer	-0.9	1.09	9.0	3.40			3
				1.00		3.52			3
245.0810	C14H14O4	Dimer	-0.7	0.86	8.0	0.56			3
				0.97		2.53			3
255.0656	C15H12O4	Dimer	-0.7	0.85	10.0	3.05			3
257.0812	C15H14O4	Dimer	-0.7	0.95	9.0	2.87			3
				0.85		3.28			3
				0.87		3.34			3
				0.90		3.62			3
				0.85		3.80			3
				0.90		4.10			3
259.0604	C14H12O5	Dimer	-0.8	0.95	9.0	3.50			3
				1.04		3.62			3

259.0969	C15H16O4	Dimer	-0.7	0.86	8.0	0.59			3
				0.96		2.18			3
				0.86		4.67			3
271.0604	C15H12O5	Dimer	-0.8	0.89	10.0	4.54			3
271.0967	C16H16O4	Dimer	-0.9	0.88	9.0	3.74			3
				0.90		4.04			3
273.0759	C15H14O5	Dimer	-0.9	1.00	9.0	3.28	MS^3		3
				0.97		3.58	MS^3		3
				1.00		4.25			3
273.1123	C16H18O4	Dimer	-0.9	0.87	8.0	0.59			3
				0.89		2.06			3
				0.93		4.19			3
275.0915	C15H16O5	Dimer	-1.0	0.89	8.0	3.78			3
				0.85		5.29			3
285.0760	C16H14O5	Dimer	-0.8	0.96	10.0	4.22			3
285.1124	C17H18O4	Dimer	-0.8	0.86	9.0	4.03			3
287.0915	C16H16O5	Dimer	-1.0	0.88	9.0	2.95			3
				1.00		3.15			3
287.1280	C17H20O4	Dimer	-0.9	0.90	8.0	4.15			3
289.0708	C15H14O6	Dimer	-0.9	0.99	9.0	3.66			3
299.0916	C17H16O5	Dimer	-0.9	1.00	10.0	4.06			3
301.0707	C16H14O6	Dimer	-1.0	1.00	10.0	1.25			3
				1.00		3.94	MS^3		2
				0.96		4.04			3
				1.01		4.26	MS^3		3
301.1071	C17H18O5	Dimer	-1.0	1.01	9.0	3.02			3
				0.97		3.08			3

301.1435	C18H22O4	Dimer	-1.0	0.93	8.0	4.87			3
303.0864	C16H16O6	Dimer	-1.0	0.93	9.0	3.69	MS^3		3
315.0863	C17H16O6	Dimer	-1.1	1.06	10.0	1.25			3
				1.00		2.78			3
				0.93		3.77			3
				1.00		4.00	MS^3		3
315.1227	C18H20O5	Dimer	-1.1	0.94	9.0	2.86			3
				0.97		2.93			3
				1.00		3.14			3
				0.93		3.44			3
317.1021	C17H18O6	Dimer	-0.9	1.00	9.0	3.59			3
				0.95		4.88			3
325.1071	C19H18O5	Dimer	-1.0	0.93	11.0	4.03			3
329.1018	C18H18O6	Dimer	-1.1	1.00	10.0	1.25			3
				1.01		3.80	MS^3		2
				0.96		3.87	MS^3		3
329.1382	C19H22O5	Dimer	-1.1	0.94	9.0	2.99			3
				1.04		6.17			3
331.1176	C18H20O6	Dimer	-1.1	0.96	9.0	3.39			3
				1.00		3.50			3
				0.87		4.43			3
				0.97		4.50			3
				0.92		4.59			3
				0.96		4.69	MS^3		2
335.1125	C17H20O7	Dimer	-1.1	1.07	8.0	4.98			3
				1.05		5.03			3
				0.87		5.22			3

				1.15		5.26			3
339.1227	C20H20O5	Dimer	-1.1	0.90	11.0	3.78			3
343.1175	C19H20O6	Dimer	-1.2	0.91	10.0	2.77			3
				1.00		3.72			3
				1.01		4.84			3
				1.00		4.89			3
345.0968	C18H18O7	Dimer	-1.2	1.00	10.0	3.78			3
345.1332	C19H22O6	Dimer	-1.1	1.00	9.0	3.52			3
				1.07		4.62	MS^3		2
347.1124	C18H20O7	Dimer	-1.2	0.91	9.0	4.02			3
				1.07		4.10	MS^3		2
				1.05		5.30			3
351.1225	C21H20O5	Dimer	-1.3	0.95	12.0	4.26			3
355.1175	C20H20O6	Dimer	-1.2	0.91	11.0	4.10			3
				0.90		4.63			3
359.1125	C19H20O7	Dimer	-1.1	0.87	10.0	6.89			3
359.1488	C20H24O6	Dimer	-1.2	0.93	9.0	4.47			3
365.1019	C21H18O6	Dimer	-1.1	1.00	13.0	4.84			3
				0.92		5.48			3
373.1283	C20H22O7	Dimer	-1.0	1.00	10.0	5.49			3
375.1437	C20H24O7	Dimer	-1.2	1.00	9.0	3.37			3
				0.95		3.63			3
				1.00		4.66			3
				1.00		4.69			3
377.1230	C19H22O8	Dimer	-1.2	1.01	9.0	4.16			3
383.1488	C22H24O6	Dimer	-1.2	0.89	11.0	4.66			3
403.1386	C21H24O8	Dimer	-1.2	0.95	10.0	3.93			3

				0.93	10.0	4.22			3
419.1702	C22H28O8	Dimer	-0.9	0.92	9.0	4.62			3
				1.00		4.84			3
				0.98		5.33			3
429.1543	C23H26O8	Dimer	-1.2	0.88	11.0	4.79			3

Table S3. Identified phenolic compounds in the BDM210 sample including the detected $[M-H]^-$, determined chemical formulas, classified class, obtained mass difference, obtained ^{13}C ratio, ring double bound (RDB) equivalent, retention times (RTs), obtained MS^n spectra (*: MS^n of identified fragment).

[M-H]-	Chemical formula (neutral)	Classified class	Mass diff. (mDa)	^{13}C ratio	RDB	RTs (min)	MS^n	Suggested compound	Identification confidence level
121.0295	C7H6O2	Monomer	0.0	1.15	5.0	2.52		4-hydroxybenzaldehyde	1
135.0451	C8H8O2	Monomer	0.0	1.13	5.0	2.12			3
				1.09		2.44			3
				1.00		2.55		4-hydroxyacetophenone	1
137.0243	C7H6O3	Monomer	-0.1	0.88	5.0	1.25			3
				0.86		1.56			3
				0.88		1.63			3
				0.98		4.01		4-hydroxybenzoic acid	1
145.0294	C9H6O2	Monomer	-0.1	0.87	7.0	2.83			3
147.0450	C9H8O2	Monomer	-0.1	1.00	6.0	3.02			3
149.0606	C9H10O2	Monomer	-0.2	0.93	5.0	1.91			3
				0.91		2.49	MS^2		2
151.0398	C8H8O3	Monomer	-0.2	1.00	5.0	1.26	MS^3	Vanillin	1
161.0605	C10H10O2	Monomer	-0.3	1.00	6.0	2.69			3
				1.03		2.83	MS^2		2
				1.03		2.90			3
				1.09		2.94			3
				1.00		3.06			3
165.0554	C9H10O3	Monomer	-0.3	1.07	5.0	1.25		Acetovanillone	1
				1.03		2.24	MS^3		2
175.0761	C11H12O2	Monomer	-0.3	1.07	6.0	2.60			3
				0.94		2.69			3

				1.00		2.81			3
				1.05		2.85	MS^2		2
				0.85		2.96			3
				1.15		3.03			3
177.0554	C10H10O3	Monomer	-0.3	0.98	6.0	1.78		Coniferyl aldehyde	1
				0.96		2.74			3
				0.97		3.55			3
				1.10		3.66	MS^2		2
179.0347	C9H8O4	Monomer	-0.3	1.02	6.0	3.45			3
179.0710	C10H12O3	Monomer	-0.3	1.06	5.0	1.20			3
				0.93		2.18			3
				0.90		2.81			3
				0.88		3.03		Coniferyl alcohol	1
				0.88		3.45			3
				0.86		4.01			3
181.0501	C9H10O4	Monomer	-0.5	0.91	5.0	1.25			3
				1.00		1.63	MS^3	Syringaldehyde	1
183.0294	C8H8O5	Monomer	-0.5	1.02	5.0	1.25			3
185.0603	C12H10O2	Monomer	-0.5	1.15	8.0	1.56			3
				1.08		2.69	MS^2		2
				1.07		3.86			3
187.0396	C11H8O3	Monomer	-0.4	1.00	8.0	3.41			3
187.0760	C12H12O2	Monomer	-0.4	0.94	7.0	3.19			3
				0.92		3.23			3
191.0709	C11H12O3	Monomer	-0.4	0.93	6.0	3.38			3
				1.05		3.51			3
				1.02		3.61	MS^3		2

195.0446	C13H8O2	Monomer	-0.5	0.91	10.0	4.30			3
195.0657	C10H12O4	Monomer	-0.6	0.99	5.0	1.63		Acetosyringone	1
				0.93		2.87			3
				0.94		2.93			3
				1.00		3.00			3
				1.00		3.21			3
201.0552	C12H10O3	Monomer	-0.5	0.85	8.0	3.18			3
203.0709	C12H12O3	Monomer	-0.4	0.96	7.0	2.58			3
				1.00		3.41			3
213.0551	C13H10O3	Monomer	-0.6	1.05	9.0	3.63	MS^2		2
227.0343	C13H8O4	Monomer	-0.7	1.11	10.0	4.28			3
227.0706	C14H12O3	Dimer	-0.7	0.93	9.0	3.45			3
				1.00		3.55			3
229.0499	C13H10O4	Monomer	-0.7	1.00	9.0	5.46			3
231.0655	C13H12O4	Monomer	-0.8	0.89	8.0	0.58			3
				0.90		2.72			3
241.0498	C14H10O4	Dimer	-0.8	0.93	10.0	3.28			3
			-0.8	1.07	10.0	4.25			3
			-0.8	0.89	10.0	4.72			3
241.0865	C15H14O3	Dimer	-0.5	1.14	9.0	3.41			3
243.0654	C14H12O4	Dimer	-0.8	0.98	9.0	3.41			3
				1.11		3.51			3
				1.00		3.92			3
				0.87		5.29			3
243.1018	C15H16O3	Dimer	-0.8	0.90	8.0	4.14			3
				0.86		4.34			3
245.0810	C14H14O4	Dimer	-0.9	0.95	8.0	0.56			3

				0.90		2.07			3
				1.07		2.53			3
				0.92		3.03			3
				1.00		5.26			3
				0.88		6.20			3
255.0654	C15H12O4	Dimer	-0.9	0.89	10.0	3.05			3
				0.90		3.15			3
				0.86		4.14			3
				0.97		4.46			3
257.0448	C14H10O5	Dimer	-0.7	0.87	10.0	3.41			3
				1.15		4.27			3
257.0810	C15H14O4	Dimer	-0.9	0.97	9.0	2.87			3
				0.96		3.29			3
				0.92		3.34			3
				1.05		3.64			3
				0.96		3.79			3
				0.85		3.83			3
259.0603	C14H12O5	Dimer	-0.9	0.97	9.0	3.51			3
				1.07		3.57	MS^3		2
259.0966	C15H16O4	Dimer	-1.0	0.91	8.0	0.58			3
269.0812	C16H14O4	Dimer	-0.7	0.93	10.0	4.06			3
				0.98		4.60			3
271.0604	C15H12O5	Dimer	-0.8	1.00	10.0	4.37			3
				1.02		4.54			3
				0.98		5.44			3
271.0966	C16H16O4	Dimer	-1.0	1.00	9.0	2.87			3
				0.86		3.64			3

				0.92		3.73			3
				0.95		4.04			3
				1.07		4.33			3
273.0758	C15H14O5	Dimer	-1.0	0.89	9.0	2.49			3
				0.92		3.00			3
				1.02		3.29	MS^3		3
				1.00		3.47			3
				1.00		3.53			3
				1.10		3.57	MS^3		2
				0.90		4.01			3
				1.02		4.25			3
273.1124	C16H18O4	Dimer	-0.8	0.88	8.0	0.59			3
				1.03		2.40			3
275.0915	C15H16O5	Dimer	-1.0	0.93	8.0	2.84			3
				0.88		3.77			3
281.0811	C17H14O4	Dimer	-0.8	0.91	11.0	4.51			3
283.0967	C17H16O4	Dimer	-0.9	0.93	10.0	4.05			3
				0.87		4.17			3
285.0760	C16H14O5	Dimer	-0.8	0.93	10.0	4.22			3
287.0553	C15H12O6	Dimer	-0.8	1.00	10.0	4.17			3
287.0914	C16H16O5	Dimer	-1.1	0.97	9.0	2.96			3
				1.00		3.15	MS^3		3
287.1280	C17H20O4	Dimer	-0.9	0.94	8.0	0.59			3
				0.86		2.37			3
289.0708	C15H14O6	Dimer	-0.9	0.98	9.0	3.66			3
				0.94		3.73			3
				1.11		3.77			3

289.1071	C16H18O5	Dimer	-1.0	0.95	8.0	4.21	MS^3		3
299.0915	C17H16O5	Dimer	-0.9	1.00	10.0	4.06			3
301.0707	C16H14O6	Dimer	-1.0	1.06	10.0	1.28			3
				0.92		3.93	MS^3		2
				1.02		4.06			3
				1.06		4.25	MS^3		3
301.1070	C17H18O5	Dimer	-1.1	0.95	9.0	3.07			3
301.1436	C18H22O4	Dimer	-0.9	1.00	8.0	4.76			3
				0.90		4.86			3
303.0863	C16H16O6	Dimer	-1.1	0.86	9.0	3.69	MS^3		3
303.1227	C17H20O5	Dimer	-1.1	1.00	8.0	4.30			3
311.0915	C18H16O5	Dimer	-1.0	0.94	11.0	4.21			3
313.1434	C19H22O4	Dimer	-1.1	1.00	9.0	5.17			3
				1.00		5.74	MS^3		3
315.1225	C18H20O5	Dimer	-1.2	0.92	9.0	2.85			3
				0.99		2.93			3
				1.04		3.13			3
				1.03		3.45			3
317.1019	C17H18O6	Dimer	-1.1	0.92	9.0	4.49			3
				1.01		4.56			3
				0.93		4.63			3
				0.94		4.88	MS^3		2
317.1383	C18H22O5	Dimer	-1.1	1.00	8.0	3.54			3
319.1177	C17H20O6	Dimer	-1.0	0.85	8.0	5.00			3
329.1382	C19H22O5	Dimer	-1.2	1.00	9.0	2.99			3
331.1176	C18H20O6	Dimer	-1.1	1.00	9.0	3.50			3
				0.95		4.34			3

				0.89		4.41			3
				0.93		4.59			3
				0.91		4.69	MS^3		3
337.1071	C20H18O5	Dimer	-1.0	1.00	12.0	5.00			3
339.1227	C20H20O5	Dimer	-1.1	0.92	11.0	3.79			3
345.1331	C19H22O6	Dimer	-1.2	0.89	9.0	4.28			3
				0.95		4.46			3
				0.97		4.56			3
				0.96		4.60	MS^3		2
				1.00		6.86			3
355.1175	C20H20O6	Dimer	-1.2	0.93	11.0	4.63			3
357.1332	C20H22O6	Dimer	-1.1	0.91	10.0	1.20			3
				0.97		3.58			3
				0.97		4.60			3
				0.86		6.20			3
359.1491	C20H24O6	Dimer	-0.9	0.89	9.0	4.19			3
				0.91		5.45			3
365.1019	C21H18O6	Dimer	-1.1	0.97	13.0	5.48			3
373.1281	C20H22O7	Dimer	-1.2	0.92	10.0	5.45			3
				0.91		5.49			3
375.1437	C20H24O7	Dimer	-1.2	0.93	9.0	3.37			3
				1.08		4.66			3
				0.94		5.48			3
				1.00		5.57			3
387.1437	C21H24O7	Dimer	1.1	1.03	14.0	5.14			3
397.1281	C22H22O7	Dimer	-1.2	0.89	12.0	5.24			3
405.1543	C21H26O8	Dimer	-1.2	0.86	9.0	4.78			3

				0.89		5.07			3
511.1963	C28H32O9	Trimer	-1.0	0.96	13.0	6.11			

Table S4. Identified phenolic compounds in the 2BDM190 sample including the detected $[M-H]^-$, determined chemical formulas, classified class, obtained mass difference, obtained ^{13}C ratio, ring double bound (RDB) equivalent, retention times (RTs), obtained MS^n spectra (*: MS^n of identified fragment).

[M-H]-	Chemical formula (neutral)	Classified class	Mass diff. (mDa)	^{13}C ratio	RDB	RTs (min)	MS^n	Suggested compound	Identification confidence level
121.0296	C7H6O2	Monomer	0.1	1.03	5.0	2.50		4-hydroxybenzaldehyde	1
137.0245	C7H6O3	Monomer	0.1	0.96	5.0	4.02		4-hydroxybenzoic acid	1
151.0400	C8H8O3	Monomer	0.0	1.00	5.0	1.26	MS^3	Vanillin	1
177.0556	C10H10O3	Monomer	-0.1	1.07	6.0	3.55		(E)-3,4-dihydroxy-benzylideneacetone	3
				0.89		3.66			3
191.0712	C11H12O3	Monomer	-0.1	0.86	6.0	3.44			3
				0.96		3.61			3
195.0660	C10H12O4	Monomer	-0.3	0.88	5.0	1.64		Acetosyringone	1
				0.88		3.23		1-(3,4-dihydroxy-5-methoxyphenyl) propan-2-one	3
227.0710	C14H12O3	Dimer	-0.3	1.06	9.0	3.55			3
243.0657	C14H12O4	Dimer	-0.6	0.93	9.0	3.41			3
				1.07		3.90			3
245.0813	C14H14O4	Dimer	-0.6	1.07	8.0	2.54			3
				0.95		4.04			3
255.0657	C15H12O4	Dimer	-0.6	0.88	10.0	4.43			3
257.0813	C15H14O4	Dimer	-0.6	1.00	9.0	2.86			3
				0.89		3.27			3
				0.86		3.34			3
				1.05		3.61			3
				0.93		3.82			3

259.0608	C14H12O5	Dimer	-0.4	1.03	9.0	3.61	MS^3		2
271.0970	C16H16O4	Dimer	-0.6	0.97	9.0	2.88			3
				1.06		3.63			3
				0.85		3.92			3
				0.85		4.04			3
273.0762	C15H14O5	Dimer	-0.6	0.93	9.0	2.52			3
				1.07		3.27	MS^3		3
				1.02		3.58	MS^3		3
				1.03		4.25			3
273.1127	C16H18O4	Dimer	-0.5	0.85	8.0	2.41			3
287.0918	C16H16O5	Dimer	-0.7	1.00	9.0	3.14			3
289.1078	C16H18O5	Dimer	-0.3	0.86	8.0	4.13			3
				0.97		4.21			3
297.0763	C17H14O5	Dimer	-0.5	1.00	11.0	4.24	MS^3		3
297.1491	C19H22O3	Dimer	-0.5	1.00	9.0	4.66			3
299.0920	C17H16O5	Dimer	-0.5	0.92	10.0	3.73			3
301.0711	C16H14O6	Dimer	-0.6	1.00	10.0	3.93	MS^3		2
301.1075	C17H18O5	Dimer	-0.6	0.93	9.0	2.86			3
				1.06		3.08			3
				0.87		3.29			3
303.0868	C16H16O6	Dimer	-0.6	0.87	9.0	2.71	MS^3		3
311.0919	C18H16O5	Dimer	-0.6	0.95	11.0	4.21			3
313.1438	C19H22O4	Dimer	-0.7	1.00	9.0	5.18			3
				1.10		5.75	MS^3		3
315.0867	C17H16O6	Dimer	-0.7	0.85	10.0	1.26			3
				0.87		3.57			3
				0.88		3.76			3

				0.88		3.99			3
315.1231	C18H20O5	Dimer	-0.7	1.06	9.0	2.94	MS^3		2
				1.08		3.12	MS^3		2
				1.00		3.44			3
323.0919	C19H16O5	Dimer	-0.6	0.91	12.0	3.86			3
				0.90		4.75			3
329.1024	C18H18O6	Dimer	-0.6	1.02	10.0	3.79	MS^3		2
				1.00		4.45			3
329.1387	C19H22O5	Dimer	-0.7	0.92	9.0	6.18			3
331.0815	C17H16O7	Dimer	-0.8	0.93	10.0	3.92			3
331.1180	C18H20O6	Dimer	-0.7	1.00	9.0	4.28			3
333.0972	C17H18O7	Dimer	-0.8	0.91	9.0	3.78			3
339.1231	C20H20O5	Dimer	-0.7	0.89	11.0	3.78			3
343.1181	C19H20O6	Dimer	-0.6	0.96	10.0	2.77			3
				1.07		3.60			3
				1.00		3.72			3
				0.85		4.89			3
343.1543	C20H24O5	Dimer	-0.8	1.00	9.0	3.01			3
				0.94		3.11			3
345.0971	C18H18O7	Dimer	-0.9	0.93	10.0	3.78			3
345.1337	C19H22O6	Dimer	-0.6	1.02	9.0	4.62	MS^3		2
				0.94		6.87			3
349.1073	C21H18O5	Dimer	-0.8	1.00	13.0	3.95			3
357.1336	C20H22O6	Dimer	-0.7	0.91	10.0	2.66			3
				0.90		3.57			3
				0.96		4.22			3
361.0920	C18H18O8	Dimer	-0.9	0.96	10.0	3.90			3

361.1647	C20H26O6	Dimer	-0.9	1.06	8.0	5.06	MS^3		2
				1.00		5.31			3
365.1024	C21H18O6	Dimer	-0.6	0.92	13.0	5.48			3
373.1285	C20H22O7	Dimer	-0.8	0.99	10.0	5.45			3
				0.92		5.51			3
375.1442	C20H24O7	Dimer	-0.7	0.95	9.0	4.66			3
379.1179	C22H20O6	Dimer	-0.8	0.99	13.0	4.13			3
387.1439	C21H24O7	Dimer	-1.0	1.02	10.0	4.36			3
389.1595	C21H26O7	Dimer	-1.1	1.00	9.0	4.71			3
				0.92		5.16			3
403.1390	C21H24O8	Dimer	-0.8	1.04	10.0	3.93			3
403.1757	C22H28O7	Dimer	-0.5	1.03	9.0	4.54			3
405.1546	C21H26O8	Dimer	-0.9	0.87	9.0	4.75			3
				0.85		5.07			3
409.1283	C23H22O7	Dimer	-1.0	1.00	13.0	4.19			3
				0.94		4.84			3
423.1076	C23H20O8	Dimer	-0.9	0.99	14.0	5.12			3
433.1495	C22H26O9	Dimer	-0.6	1.04	10.0	4.36			3
				0.88		4.42			3
451.1759	C26H28O7	Trimer	-0.3	0.86	13.0	4.62			3
465.1910	C27H30O7	Trimer	-0.9	1.01	13.0	4.42			3
483.2019	C27H32O8	Trimer	-0.5	0.96	12.0	5.19			3
				0.85		5.40			3
				0.95		5.83			3
511.1965	C28H32O9	Trimer	-0.8	0.93	13.0	5.56			3
				0.90		6.12			3
				0.92		6.16			3

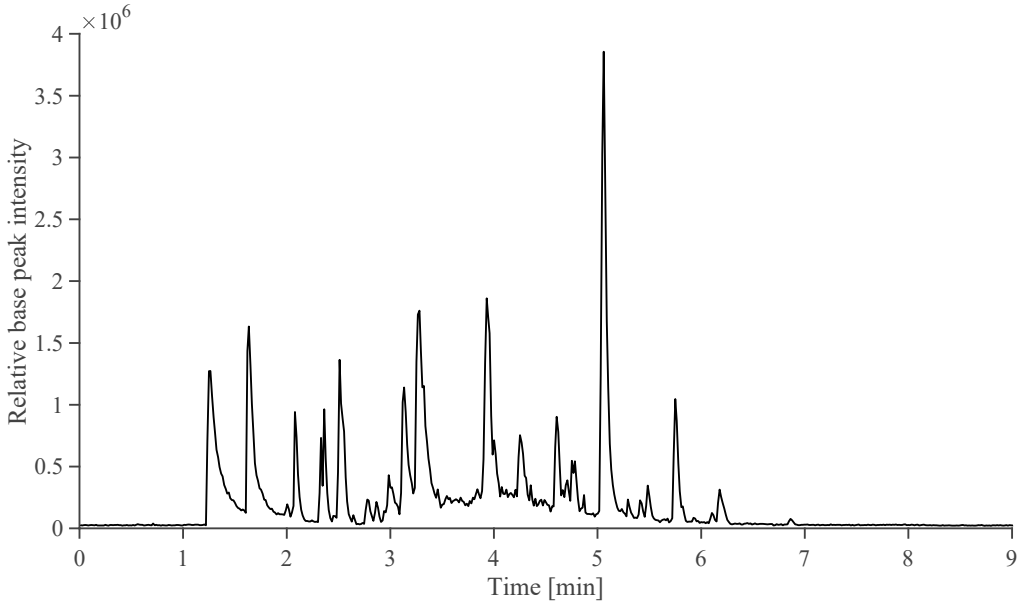

Figure S1. BPI of BDM170 (data already presented previously in Prothmann et al. 2020 [1].

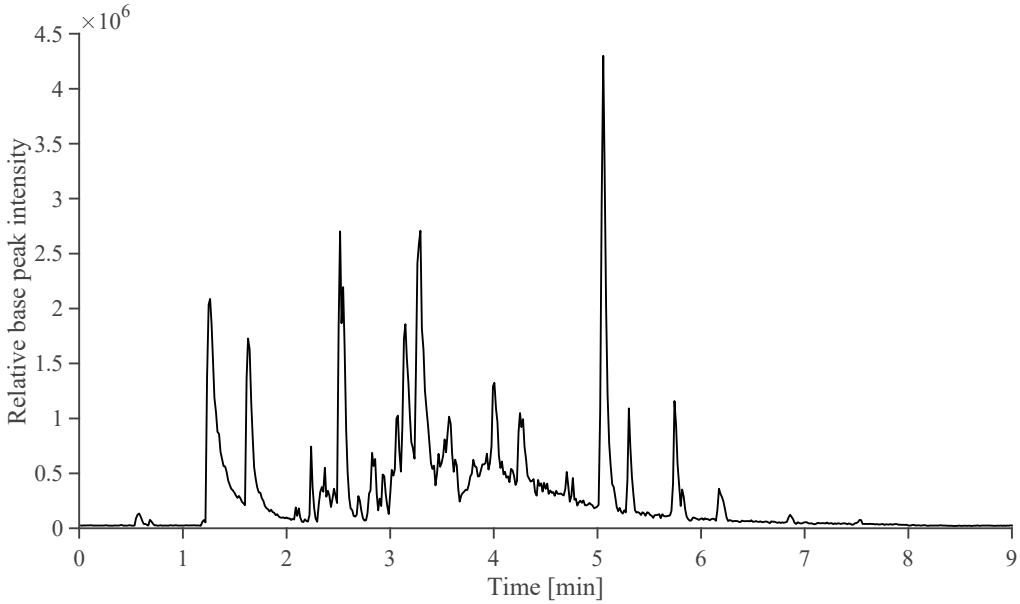

Figure S2. BPI of sample BDM210.

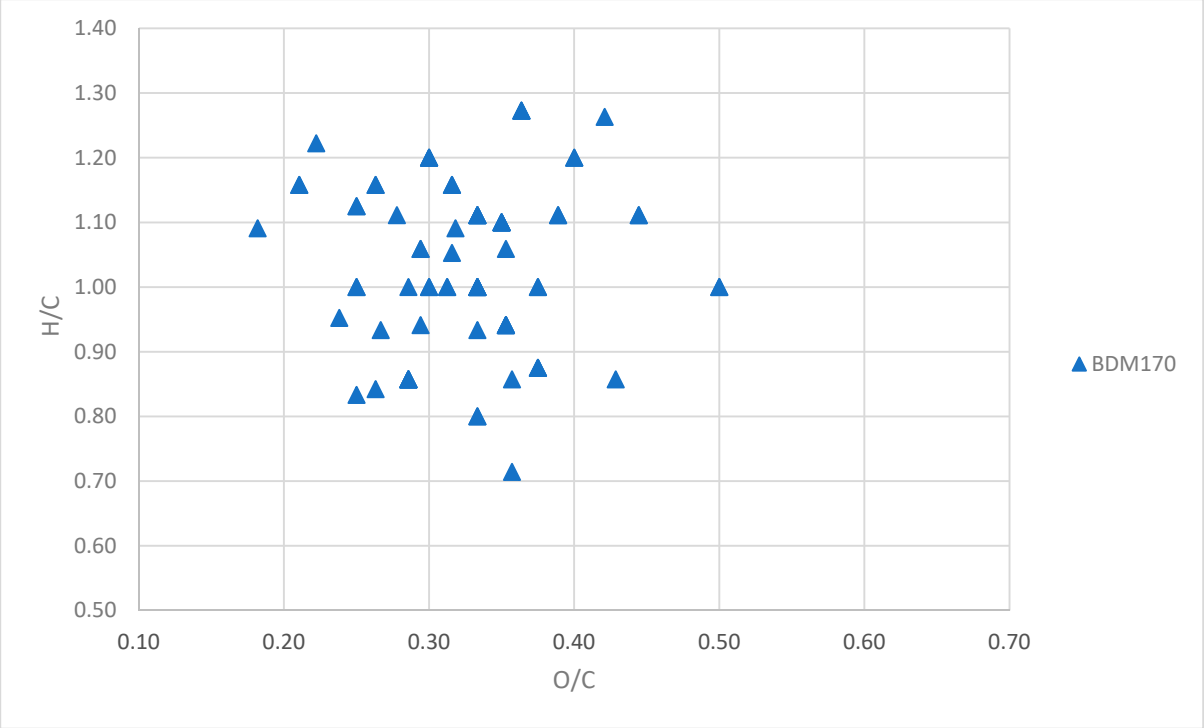

Figure S3. Van-Krevelen plot of sample BDM170.

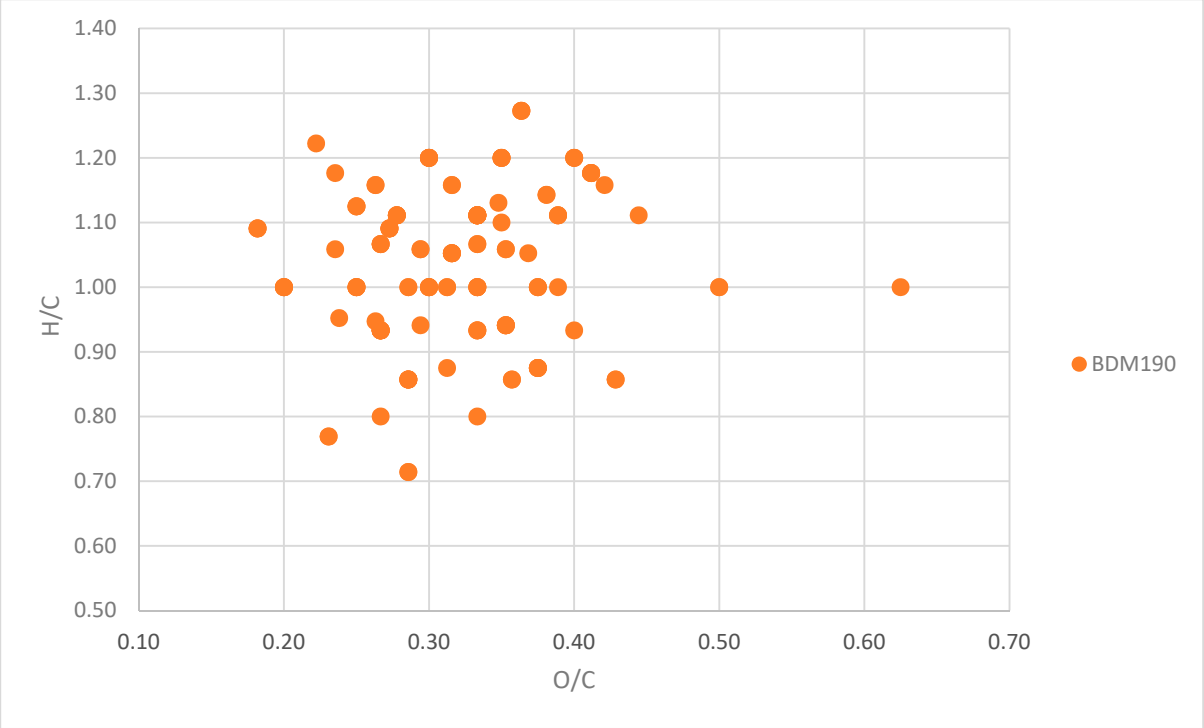

Figure S4. Van-Krevelen plot of sample BDM190.

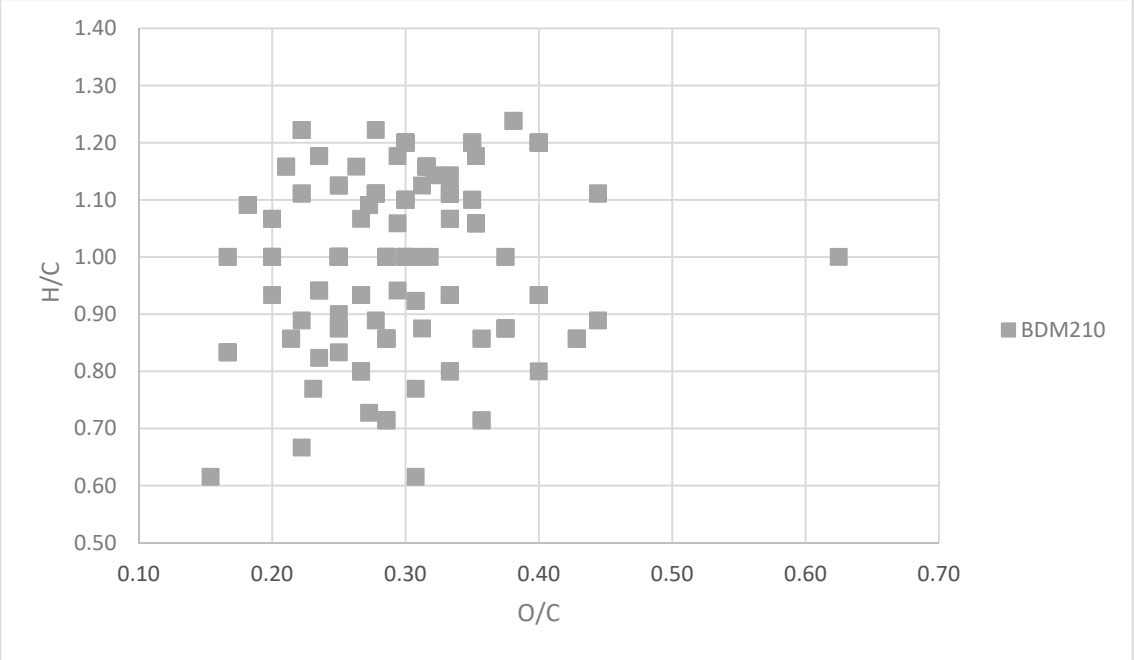

Figure S5. Van-Krevelen plot of sample BDM210.

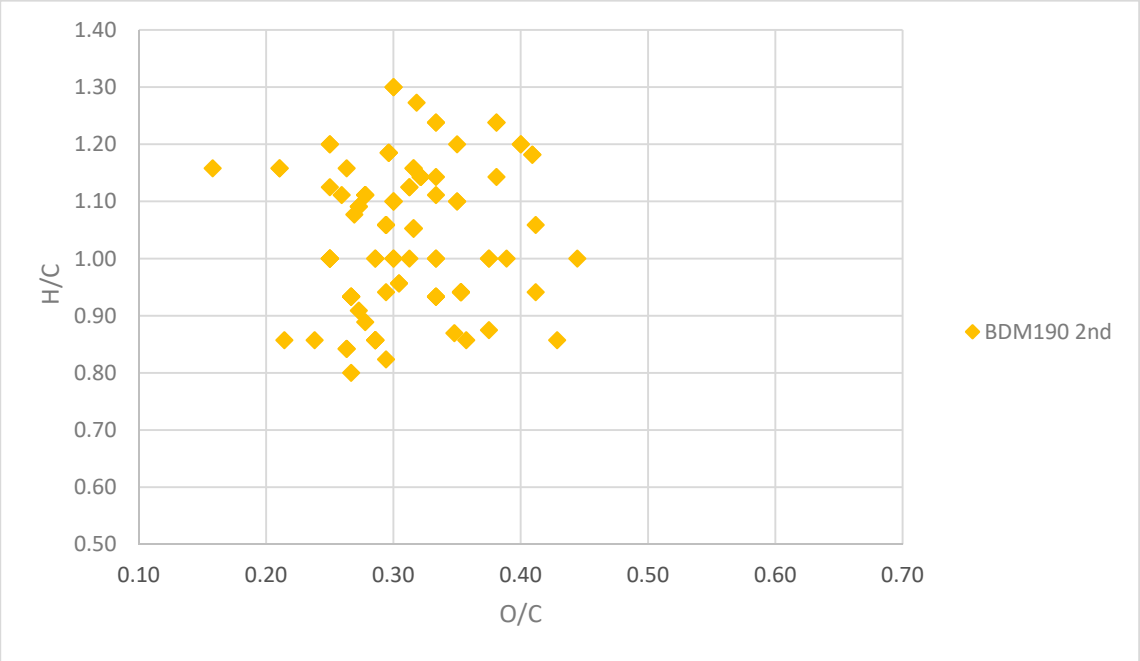

Figure S6. Van-Krevelen plot of sample 2BDM190.

Reference

[1] J. Prothmann, K. Li, C. Hulteberg, P. Spégel, M. Sandahl, C. Turner, Nontargeted Analysis Strategy for the Identification of Phenolic Compounds in Complex Technical Lignin Samples, ChemSusChem. (2020) 4605–4612. https://doi.org/10.1002/cssc.202000951.