Supplementary
Impact of milled wood lignin purifications on spruce lignocellulose

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Table S1. Compositional and carbohydrate analysis of steam exploded spruce. The amount of all components are expressed as percentage of dry matter. The amount of carbohydrates were calculated using the mass of anhydrous sugar.

Severity factor (log R_0)	Glucan (%)	Arabinan (%)	Mannan (%)	Galactan (%)	Xylan (%)	Lignin (%)	Moisture (%)
—	44.6	1.6	10	1.5	5.2	31.2	8.9
3.1	37.3	1	6.7	1.2	5	32.1	76.7
3.3	37.4	0.8	5.9	1	5.1	33.2	74.4
3.4	36.1	0.8	5.2	0.9	4	34.1	76.5
3.6	38	0.6	4.2	0.7	3.2	34.8	76
3.6	37.2	0.8	3.7	0.6	3.1	35.7	74.9
3.9	38.2	0.6	2.4	0.4	2.6	37.2	75.1
3.9	37.9	0.5	2.9	0.3	2.9	39	74.1
4.2	39.7	0.3	2.2	0.2	1.8	41.7	75.3

Table S2. List of standards used for GC-MS analysis.

Standard	Retention time (min)	$M^{+\cdot}$(m/z)
2-methoxyphenol	27.652	109.0
2-methylphenol	28.482	108.0
4-methylphenol	29.478	107.0
3-methylphenol	29.482	108.0
2-methoxy-5-methylphenol	30.482	123.0
1-(2-hydroxy-5-methylphenyl)ethanone	33.900	135.0
3-methoxy-1,2-benzenediol	36.066	140.0
2-methoxy-4-(2-propenyl)phenol	37.192	164.0
2-methoxy-4-propylphenol-	37.274	137.0
1,2,4-trimethoxybenzene	37.767	153.0
1,2-dihydroxybenzene	38.120	110.0
2,6-dimethoxyphenol	38.379	154.0
1,2,3-trimethoxy-5-methylbenzene	38.549	182.0
2-methoxy-4-(1E-propenyl)phenol	39.481	164.0
2-methoxy-4-(1Z-propenyl)phenol	42.185	164.0
3,5-dimethoxy-4-hydroxytoluene	42.705	168.0
3-methoxy-4-hydroxybenzaldehyde	43.225	152.0
3-methoxy-4-hydroxyacetophenone	46.973	151.0
1-(3,4-dimethoxyphenyl)ethanone	49.585	165.0
2,6-dimethoxy-4-(2-propenyl)phenol	50.198	194.0
1-(3-hydroxy-4-methoxyphenyl)ethanone	51.504	151.0
4-hydroxy-3,5-dimethoxybenzaldehyde	57.303	182.0
1-(4-hydroxy-3,5-dimethoxyphenyl)ethanone	60.761	181.0

Table S3. Mass spectrometry fragmentation pattern of the two possible hemicellulose indicators.

Component	RT	m/z	relative intensity	m/z	relative intensity	m/z	relative intensity
Not identified 1	23.01	114	25	86	80	55	100
Not identified 2	24.17	114	100	58	80	57	35

Table S4. Assignment of ^{13}C-^{1}H correlations in HSQC spectra of untreated spruce (MWLp), severity factor 3.1 and severity factor 4.2.

Label	δ_C/δ_H [ppm]	Assignment
C_β	53.1/3.44	C_β – H_β in phenylcoumarane substructures (C)
B_β	53.4/3.06	C_β – H_β in resinol substructures (B)
F_β	55.0/2.75	C_β – H_β in diphenylethane substructures (F)
MeO	55.3/3.74	C – H in methoxyls
A_γ	59.8/3.3-3.7	C_γ – H_γ in β-O-4’ substructures (A)
C_γ	62.5/3.7	C_γ – H_γ in phenylcoumarane substructures (C)
A_α	71.1/4.7	C_α – H_α in β-O-4’ substructures (A)
A_β	83.8/4.27	C_β – H_β in β-O-4’ substructures (A)
B_α	84.7/4.6	C_α – H_α in resinol substructures (B)
C_α	86.9/5.46	C_α – H_α in phenylcoumarane substructures (C)
G_2	110.9/6.98	C_2 – H_2 in guaiacyl units (G)
G_5	115/6.8	C_5 – H_5 in guaiacyl units (G)
G_6	119/6.8	C_6 – H_6 in guaiacyl units (G)
Gal1	91.9/4.9	C_1 – H_1 in galactose with reducing end
Glu1	92.2/4.9	C_1 – H_1 in glucose with reducing end
Man1	93.9/4.9	C_1 – H_1 in mannose with reducing end
F3	109.4/6.6	C_3 – H_3 in 5-hydroxymethylfuran (F)
F6	55.7/4.5	C_6 – H_6 in 5-hydroxymethylfuran (F)

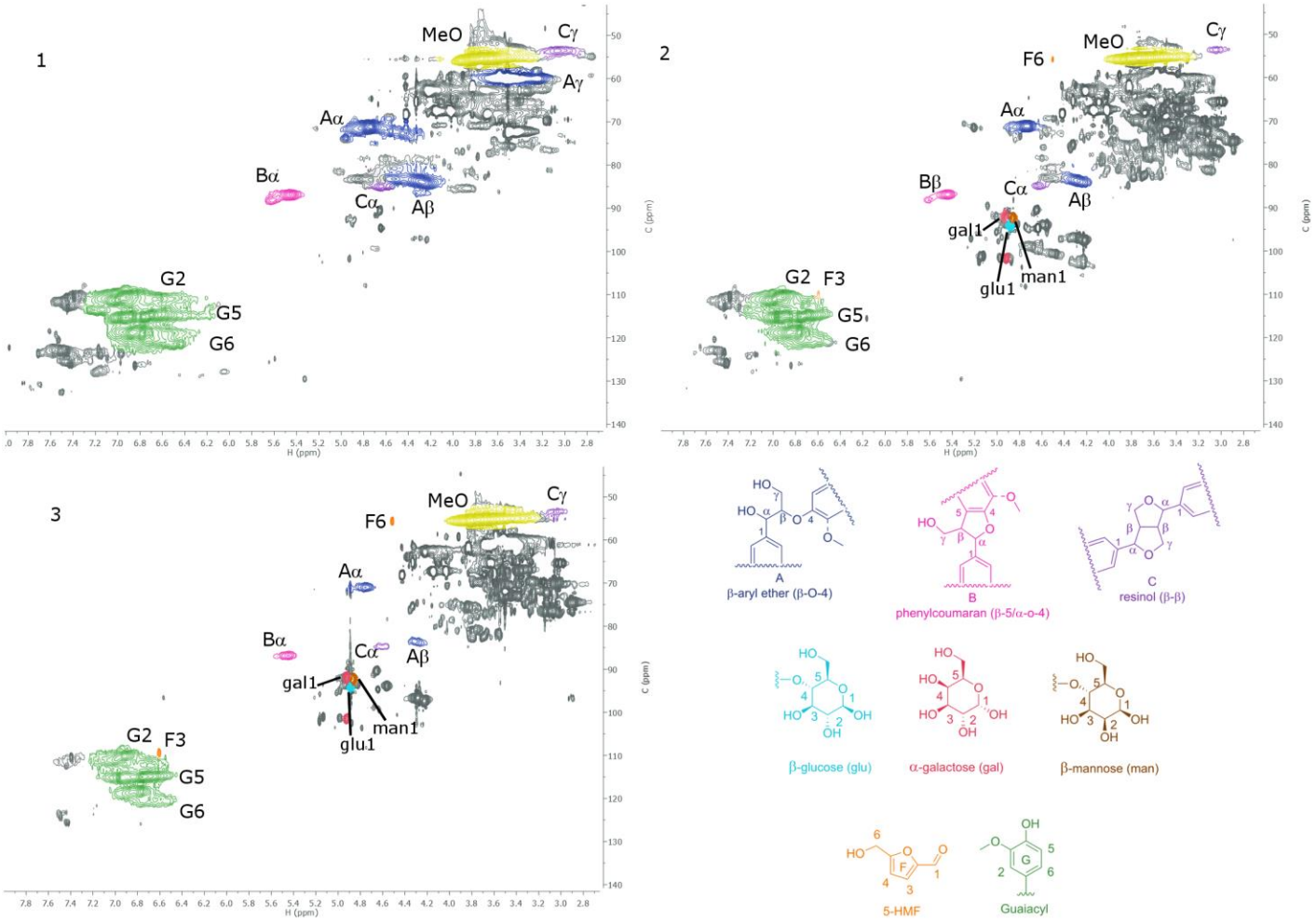

Figure S1. HSQC spectra of untreated spruce (MWLp, 1), severity factor 3.1 (2) and severity factor 4.2 (3). Focused on area 8.0 – 2.65 ^{1}H and 140.8 – 43.0 ^{13}C.