Supplementary Data. Wavenumbers of FT-IR spectra of untreated and steam-exploded wood.

Allocation of FT-IR bands: blue – cellulose, purple – cellulose + hemicelluloses, orange – hemicelluloses, yellow – lignin, green – cellulose + hemicelluloses + lignin

Oak

			Experimental wavenumber (cm^{-1})									
Theoretical wavenumber (cm^{-1})	**Allocation**	**References**	**Untreated**	**CSF 3.35**	**CSF 3.57**	**CSF 3.75**	**CSF 3.79**	**CSF 3.95**	**CSF 3.97**	**CSF 4.17**	**CSF 4.19**	**CSF 4.39**
1738-1709	C=O stretch in unconjugated ketones, carbonyls and in ester groups (frequently of carbohydrate origin); conjugated aldehydes and carboxylic acids absorb around and below 1700 cm^{-1}	1–4	1731	1727	1724	1724	1719	1720	1720	1718	1710	1707
1675-1655	C=O stretch; in conjugated p-substituted aryl ketones;strong electronegative substituents lower the wavenumber	2					*1655*			*1655*	*1664*	*1664*
1650-1630	OH water	1–3	1624									
1605-1593	Aromatic skeletal vibrations plus C=O stretch; S > G;G condensed > G etherified	2,3	*1594*	1596	1596	1597	1598	1601	1604	1605	1604	1604
1515-1505	Aromatic skeletal vibrations;G > S; C=C aromatic symmetrical stretching	1–4	1505	1509	1513	1514	1514	1514	1514	1514	1514	1514
1470-1455	C–H deformations; asymmetric in –CH3 and –CH2–; Asymmetric C–H bending from methoxyl group; OH plane deformation vibration	2,4	1458	1457	1458	1456	1455	1455	1453	1453	1453	1453
1430-1422	Aromatic skeletal vibrations combined with C–H in plane deformation, CH2 bending	1–4	1423	1424	1424	1425	1425	1425	1425	1426	1425	1425

1370–1365	Aliphatic C–H stretch in CH3 not in O–Me ; In-the-plane CH bending-Cellulose, hemicellulose	1–4	1368	1367	1367	1367	1363	1367	1367	1363	1362	1361
1330–1325	Phenolic OH; S ring plus G ring condensed; (i.e. G ring substituted in pos. 5) ; phenolic OH deformation of S-ring	1–4	1321	*1331*	*1331*	*1331*	*1331*	*1332*	*1333*	*1331*	*1333*	*1332*
1317–1315	CH2 rocking vibration	1–3		1319	1317	1317	1317	1317	1316	1316	1316	1316
1270–1266	G ring plus C=O stretch	1–3					*1273*	*1270*	*1270*	*1271*	*1274*	1275
1235–1225	OH plane deformation, also COOH	1–3	1233	1235	1235	1236	1235	1236	1236	*1236*	*1234*	*1236*
1230-1215	C-C, C-O, C=O stretch	2–4		*1221*	*1220*	*1221*	*1222*	*1222*	*1221*	*1221*	*1219*	*1220*
1205–1200	OH plane deformation, symetric C-O-C stretching	1,3,4			*1209*		*1210*	*1208*	*1209*	1208	1207	1207
1152-1156	C–O–C asymmetrical stretching-Cellulose, hemicellulose	1–4	1158	1157	1158	1158	1158	1158	1158	1159	1159	1159
1110–1107	Ring asymmetric valence vibration	2	1105	1108	1109	1109	1109	1108	1108	1107	1108	1108
1046-1043	C–C, C–OH secondary alcohols, C–H ring and side group vibrations-cellulose-hemicellulose	1	*1049*	*1050*	1050	*1051*	1052	1051	1052	1053	1053	1054
1035–1030	Aromatic C–H in plane deformation,G > S; plus C–O deformation in primary alcohols; plus C=Ostretch (unconj.), C-O, C=C and C-C-O stretching	2–4	1031	1030	1031	1030	1030	1030	1031	1030	1030	1030
996–985	C–O valence vibration	2,4	*989*	*988*	*986*	*986*	*986*	*987*	*986*	*987*	*986*	*986*
895	COC, CCO and CCH deformation and stretching-cellulose; glycosydic bonds-polysacharides	1	897	897	897	898	898	898	898	898	899	900
833	pectins	5	832	839	*838*	839	*835*	*838*	*838*	*839*		

Poplar

			Experimental wavenumber (cm^{-1})									
Theoretical wavenumber (cm^{-1})	**Allocation**	**References**	**Untreated**	**CSF 3.35**	**CSF 3.57**	**CSF 3.75**	**CSF 3.79**	**CSF 3.95**	**CSF 3.97**	**CSF 4.17**	**CSF 4.19**	**CSF 4.39**
1738-1709	C=O stretch in unconjugated ketones, carbonyls and in ester groups (frequently of carbohydrate origin); conjugated aldehydes and carboxylic acids absorb around and below 1700 cm^{-1}	1–4	1730	1725	1725	1719	1719	1719	1708	1707	1701	
1675-1655	C=O stretch; in conjugated p-substituted aryl ketones;strong electronegative substituents lower the wavenumber	2		*1654*	*1654*	*1654*	*1654*	*1654*	*1654*	*1654*	*1655*	
1650-1630	OH water	1–3	1637									
1605-1593	Aromatic skeletal vibrations plus C=O stretch; S > G;G condensed > G etherified	2,3	*1595*	1594	1605;1593	1605;1594	1605;1593	1605;1594	1605;1594	1605;1594	1605;1594	
1515-1505	Aromatic skeletal vibrations;G > S; C=C aromatic symmetrical stretching	1–4	1507	1512	1508	1508	1513	1513	1514	1514	1514	
1470-1455	C–H deformations; asymmetric in –CH3 and –CH2–; Asymmetric C–H bending from methoxyl group; OH plane deformation vibration	2,4	1459	1455	1459	1458	1457	1456	1455	1453	1453	
1430-1422	Aromatic skeletal vibrations combined with C–H in plane deformation, CH2 bending	1–4	1424	1424	1424	1424	1424	1425	1425	1425	1425	
1370–1365	Aliphatic C–H stretch in CH3 not in O–Me ; In-the-plane CH bending-	1–4	1370	1370	1370	1370	1370	1370	1369	1369	1369	

	Cellulose, hemicellulose											
1330–1325	Phenolic OH; S ring plus G ring condensed; (i.e. G ring substituted in pos. 5) ; phenolic OH deformation of S-ring	1–4	1331	*1331*	*1331*	*1331*	*1332*	*1331*	1331	*1331*	*1332*	
1317–1315	CH2 rocking vibration	1–3	1318	1317	1317	1317	1316	1316	1316	1316	1316	
1270–1266	G ring plus C=O stretch	1–3		*1262*	1265	1265	1263	1263	1266	1269	1272	
1235–1225	OH plane deformation, also COOH	1–3	1243	1236	1236	1236	1236	1237	1236	1235	1235	
1230-1215	C-C, C-O, C=O stretch	2–4							*1220*	*1220*	*1221*	
1205–1200	OH plane deformation, symetric C-O-C stretching	1,3,4		*1207*	*1208*	*1208*	*1208*	*1208*	1207	1209	1208	
1152-1156	C–O–C asymmetrical stretching-Cellulose, hemicellulose	1–4	1159	1159	1159	1159	1159	1159	1159	1159	1160	
1110–1107	Ring asymmetric valence vibration	2	1105	1105	1105	1104	1108	1109	1108	1108	1108	
1046-1043	C–C, C–OH secondary alcohols, C–H ring and side group vibrations-cellulose-hemicellulose	1	*1047*	1050	1050	1050	1052	1051	1053	1054	1054	
1035–1030	Aromatic C–H in plane deformation,G > S; plus C–O deformation in primary alcohols; plus C=Ostretch (unconj.), C-O, C=C and C-C-O stretching	2–4	1031	1031	1030	1031	1030	1030	1030	1030	1030	
996–985	C–O valence vibration	2,4		*986*	*986*	*986*	*986*	*986*	*986*	*986*	*986*	
895	COC, CCO and CCH deformation and stretching-cellulose; glycosydic bonds-polysacharides	1	897	897	897	897	897	898	898	898	899	
833	pectins	5		*835*	*835*	*832*	*831*	*831*	*835*	*831*	*834*	

Spruce

			Experimental wavenumber (cm^{-1})									
Theoretical wavenumber (cm^{-1})	**Allocation**	**References**	**Untreated**	**CSF 3.57**	**CSF 3.72**	**CSF 3.86**	**CSF 3.97**	**CSF 4.11**	**CSF 4.17**	**CSF 4.26**	**CSF 4.32**	**CSF 4.47**
1738-1709	C=O stretch in unconjugated ketones, carbonyls and in ester groups (frequently of carbohydrate origin); conjugated aldehydes and carboxylic acids absorb around and below 1700 cm^{-1}	[1–4]	1735	1720	1719	1719	1719	1701	1701	1701	1701	1701
1675-1655	C=O stretch; in conjugated p-substituted aryl ketones;strong electronegative substituents lower the wavenumber	[2]	1654	1654	1654	1655	1654	1654	1663	1663	1664	1664
1650-1630	OH water	[1–3]	1637									
1605-1593	Aromatic skeletal vibrations plus C=O stretch; S > G;G condensed > G etherified	[2,3]	1605	1598	1598	1598	1598	1593	1600	1601	1600	1600
1515-1505	Aromatic skeletal vibrations;G > S; C=C aromatic symmetrical stretching	[1–4]	1509	1510	1511	1511	1511	1512	1512	1512	1512	1512
1470-1455	C–H deformations; asymmetric in –CH3 and –CH2–; Asymmetric C–H bending from methoxyl group; OH plane deformation vibration	[2,4]	1451	1451	1451	1451	1451	1450	1451	1451	1451	1451
1430-1422	Aromatic skeletal vibrations combined with C–H in plane deformation, CH2 bending	[1–4]	1421	1425	1425	1426	1425	1425	1426	1427	1426	1427
1370–1365	Aliphatic C–H stretch in CH3 not in O–Me ; In-the-plane CH bending-Cellulose, hemicellulose	[1–4]	1370	1370	1370	1369	1369	1369	1368	1369	1368	1368

1330–1325	Phenolic OH; S ring plus G ring condensed; (i.e. G ring substituted in pos. 5) ; phenolic OH deformation of S-ring	1–4	1334	1334	1334	1334	1334	1334	1334	1334	1334	1334
1317–1315	CH2 rocking vibration	1–3	1316	1316	1316	1316	1316	1315	1315	1315	1315	1315
1270–1266	G ring plus C=O stretch	1–3	1263	1264	1266	1267	1266	1267	1267	1269	1268	1269
1235–1225	OH plane deformation, also COOH	1–3	1233	1233	1235	1235	1235	1235	1235	1235	1234	1233
1230-1215	C-C, C-O, C=O stretch	2–4										
1205–1200	OH plane deformation, symetric C-O-C stretching	1,3,4	*1209*	1208	1209	1208	1208	1208	1207	1206	1206	1205
1152-1156	C–O–C asymmetrical stretching-Cellulose, hemicellulose	1–4	1155	1157	1158	1158	1158	1158	1158	1159	1158	1158
1110–1107	Ring asymmetric valence vibration	2	1105	1104	1104	1105	1104	1105	1105	1105	1105	1106
1046-1043	C–C, C–OH secondary alcohols, C–H ring and side group vibrations-cellulose-hemicellulose	1	1050	1053	1053	1054	1053	1054	1053	1054	1054	1054
1035–1030	Aromatic C–H in plane deformation,G > S; plus C–O deformation in primary alcohols; plus C=Ostretch (unconj.), C-O, C=C and C-C-O stretching	2–4	1024	1028	1028	1028	1028	1030	1028	1029	1029	1030
996–985	C–O valence vibration	2,4	*988*	*986*	*986*	*986*	*986*	*986*	*986*	*986*	*986*	*986*
895	COC, CCO and CCH deformation and stretching-cellulose; glycosydic bonds-polysacharides	1	897	896	896	897	897	896	897	897	897	897

References

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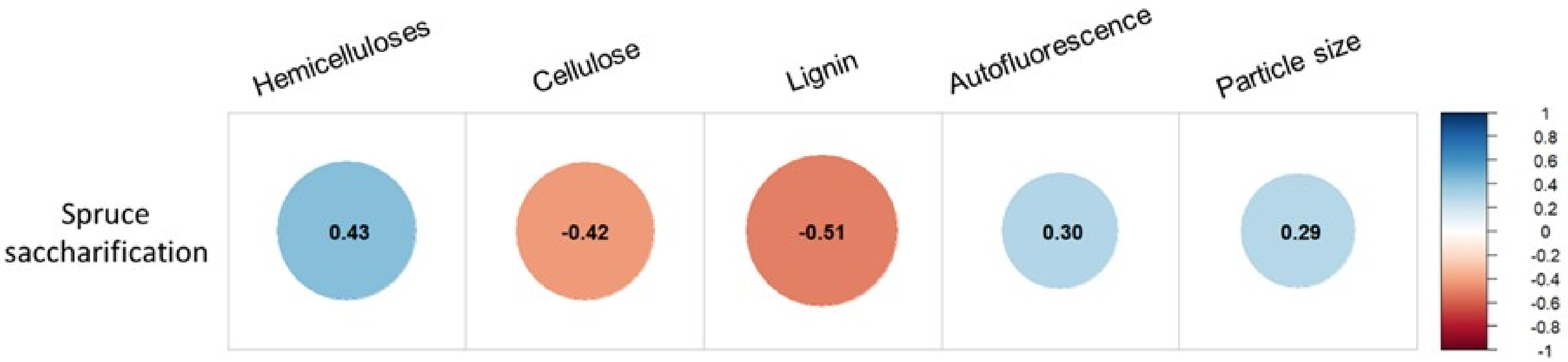
Supplementary Figure. Correlation coefficients between physicochemical features and spruce enzymatic saccharification yield.



Supplementary Figure. PCA plots of pretreated wood samples, one plot per species: oak (A) and poplar (B). "Glc_man" stands for the enzymatic saccharification yields.