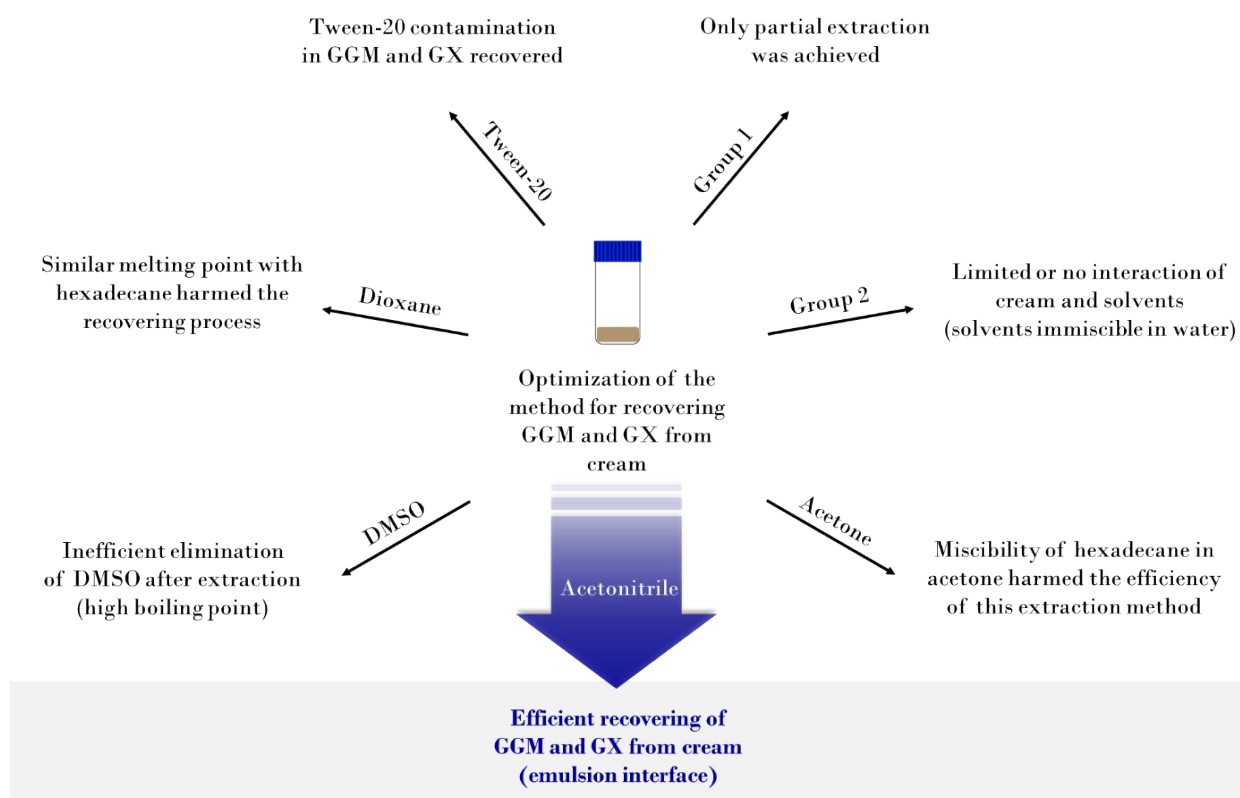


SUPPLEMENTARY INFORMATION

Active role of lignin in anchoring wood-based stabilizers to the emulsion interface

Danila M. de Carvalho, Maarit H. Lahtinen, Mamata Bhattarai, Martin Lawoko and Kirsi S. Mikkonen



Group 1: methanol, ethanol, propanol, and water.

Group 2: chloroform, heptane, hexane, isooctane, and toluene.

Figure S1 Summary of the attributes that qualified the acetonitrile as the most suitable solvent for wood-based stabilizers (*i.e.*, GGM and GX) recovering from cream.

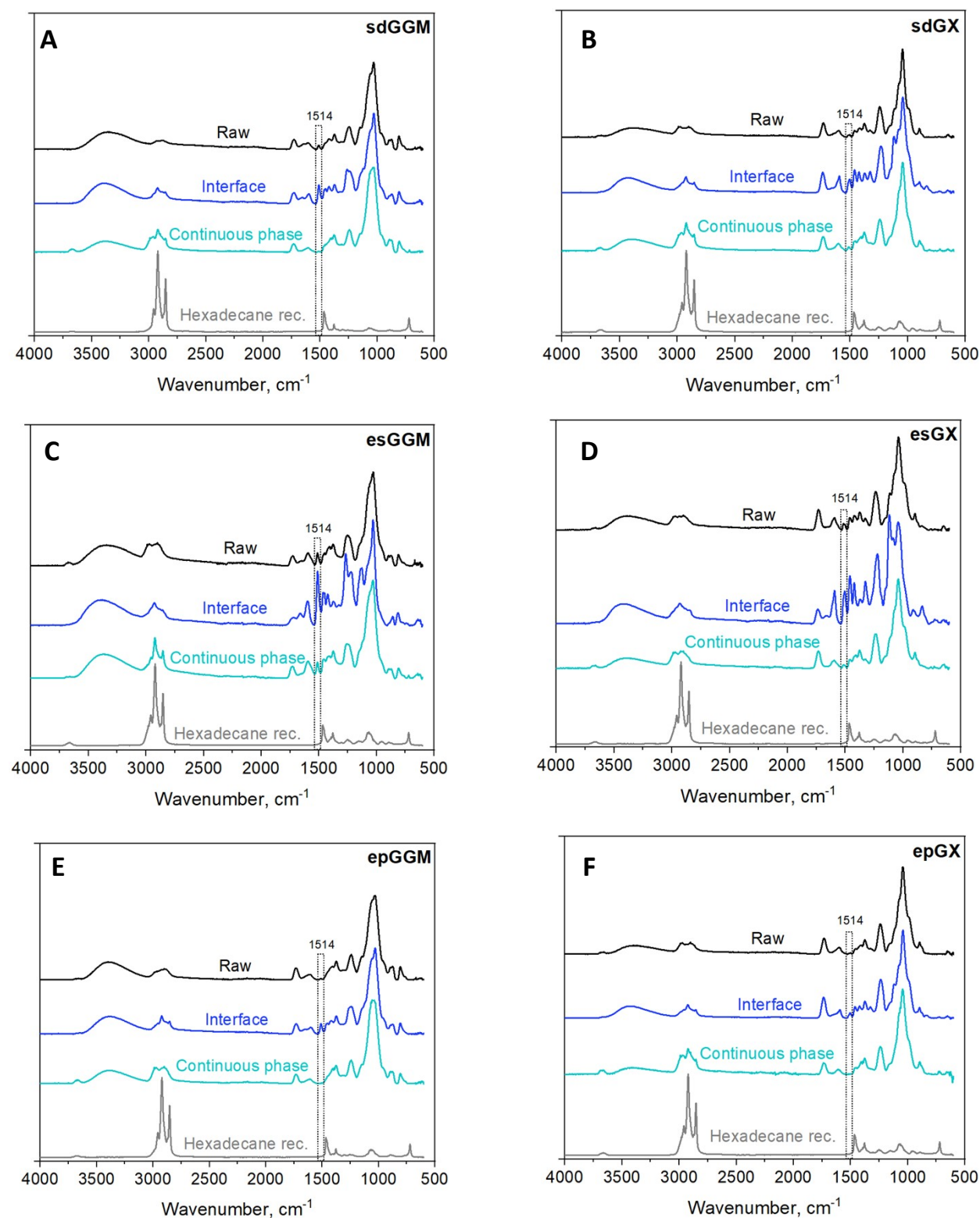


Figure S2 FTIR spectra of raw GGM and GX samples, fractions recovered from interface and continuous phase of emulsion prepared using sdGGM (A), sdGX (B), esGGM (C), esGX (D), epGGM (E), and epGX (F) as stabilizers, and hexadecane recovered from emulsions. Assignment for the relevant bands observed in FTIR spectra are presented in Table S1.

Table S1 Assignment for the relevant bands observed in FTIR spectra.

Absorption band (cm ⁻¹)	Band assignments ^a
3750-3000	O-H stretching vibration of hydrogen-bonded
2907	Aliphatic C-H stretching
1734	C=O stretching vibration carbonyl groups
1706	Free acetic acid (absent in the spectra)
1665	C=O stretching in conjugation to the aromatic ring
1602	Water absorption
1514	Aromatic skeletal vibration of lignin rings
1426	Asymmetric aliphatic C-H deformation of methoxyl
1377	Symmetric aliphatic C-H bending of methoxyl in acetyl groups
1241	C-O stretching
1042	C-O and C-C stretching or C-OH bending
896	β-glycosidic linkage between sugar units

^aBand assignments were assessed according to the literature.¹⁻⁸ Dashed box indicates the assignment of the band identified in Figure S2.

Table S2 Assignment for the lignin units and relevant lignin substructures, lignin side and end groups, and lignin-carbohydrates bonds cross-signals in sdGGM, esGGM, epGGM, sdGX, esGX, and epGX samples recovered from interface and continuous phase of emulsions. The cross-signals used in this study for qualitative identification are highlighted in bold and variation in the signals among samples are in the range of ± 0.1 ppm and ± 1.0 ppm for ^1H and ^{13}C dimensions, respectively.

Structural units ^a	δ_{C} (ppm)	δ_{H} (ppm)	Assignments	Identified in ^b
Syringyl ($\text{S}_{2,6}$)	103.9	6.68	C_2/H_2 and C_6/H_6 in S-units	1, 3, 7, 8, 9, 10, 11, 12
Guaiacyl (G_2)	110.9	6.94	C_2/H_2 in G-units	1, 2, 3, 4, 5, 7, 8, 9, 10, 11
Guaiacyl (G_5)	115.0	6.83	C_5/H_5 in G-units	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11
Guaiacyl (G_6)	118.7	6.76	C_6/H_6 in G-units	1, 2, 3, 4, 5, 7, 8, 9, 10, 11
p-hydroxyphenyl ($\text{H}_{2,6}$)	127.5	7.21	C_2/H_2 and C_6/H_6 in H-units	1, 3, 4
β -aryl ether (β -O-4)	71.4	4.71	β -O-4 signal in α	1, 2, 3, 4, 5, 7, 8, 9, 10, 11, 12
β -aryl ether (β -O-4)	85.5	4.16	β -O-4 signal in β in S units	1, 3, 7, 8, 9, 10, 11
β -aryl ether (β -O-4)	83.4	4.28	β -O-4 signal in β in G units	1, 2, 3, 4, 5, 7, 8, 9, 10, 11
β -aryl ether (β -O-4)	59.5	3.70/3.44	β -O-4 signal in γ	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Phenylcoumaran (β -5)	87.2	5.43	β -5 signal in α	1, 2, 3, 4, 5, 7, 9, 10
Phenylcoumaran (β -5)	52.8	3.46	β -5 signal in β	1, 3, 4, 5, 7, 8, 9, 10, 11
Phenylcoumaran (β -5)	62.4	3.72	β -5 signal in γ	1, 2, 3, 4, 5, 7, 8, 9, 10, 11, 12
Dibenzodioxocin (5-5/ β -O-4)	82.9	4.81	5-5/ β -O-4 signal in α	1, 3, 9, 10
Dibenzodioxocin (5-5/ β -O-4)	86.2	3.91	5-5/ β -O-4 signal in β	1, 3, 9
Resinol (β - β)	85.1	4.61	β - β signal in α	1, 3, 4, 5, 7, 8, 9, 10, 11
Resinol (β - β)	53.6	3.04	β - β signal in β	1, 3, 4, 5, 7, 8, 9, 10, 11
Resinol (β - β)	71.2	4.14/3.83	β - β signal in γ	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11
SECO $_{\alpha}$ (β - β)	33.6	2.53/2.48	Secoisolariciresinol in α	1, 2, 3, 4, 5, 6, 7, 8, 9
SECO $_{\beta}$ (β - β)	42.3	1.84	Secoisolariciresinol in β	1, 3, 4, 5
Spirodienone (β -1)	81.2	5.00	β -1 signal in α	1, 9
Spirodienone (β -1)	59.8	2.75	β -1 signal in β	1
Spirodienone (β -1)	79.4	4.11	β -1 signal in β'	-
Methoxy group	55.4	3.73	C/H in -OMe in G- and S-units	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Cinnamyl alcohol	128.7	6.42	Cinnamyl alcohol signal in α	1, 2, 3, 4, 5, 10
Cinnamyl alcohol	127.5	6.21	Cinnamyl alcohol signal in β	1, 2, 3, 4, 5, 10
Cinnamyl alcohol	62.8	3.90	Cinnamyl alcohol signal in γ	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
OSC (G_2)	112.0	7.31	C_2/H_2 in ($\text{C}=\text{O}$) $_{\alpha}$ in G-units	1, 3, 4, 5, 9
OSC (G_6)	123.0	7.64/7.56	C_6/H_6 in ($\text{C}=\text{O}$) $_{\alpha}$ in G-units	1, 3, 9
OSC ($\text{S}_{2,6}$)	106.4	7.20/7.06	$\text{C}_{2,6}/\text{H}_{2,6}$ in ($\text{C}=\text{O}$) $_{\alpha}$ in S-units	7, 9, 10
OSC $_{\alpha}$	154.0	7.61	Cinnamyl aldehyde in α	1, 3, 4, 5, 7, 9
OSC $_{\beta}$	126.1	6.77	Cinnamyl aldehyde in β	1, 3, 4, 5, 9
DCA $_{\alpha}$	31.4	2.52	Dehydroconiferyl alcohol in α	1, 2, 3, 4, 5, 7, 9
DCA $_{\beta}$	34.4	1.67	Dehydroconiferyl alcohol in β	1, 2, 3, 4, 5, 7, 9
DCA $_{\gamma}$	60.0	3.42	Dehydroconiferyl alcohol in γ	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
PG	102.8/99.8	5.18/4.75	Phenylglycoside units	1, 2, 4, 6, 7, 8, 10
BE (BE_1)	80.2	4.50	Benzylether in C-3 and C-2	1, 3
BE (BE_2)	82.3	5.20	Benzylether in C-6 and C-5	7, 9
BEst	74.3	5.96	Benzyl ester (α -ester)	-
GE	64.0/62.0	4.50/4.00	γ -ester units	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12

^aSecoisolariciresinol (SECO β - β); Oxidized side chain (OSC); Dehydroconiferyl alcohol (DCA); PG: phenylglycoside; BE: benzylether, in which BE_1 refers to linkage at C-6 in glucose, mannose, and galactose or C-5 in arabinose and BE_2 refers to linkage at C-2 or C-3 in glucose, mannose, galactose, xylose, and arabinose; BEst: benzyl ester; and GE: γ -ester. Contours assignments were assessed according to the literature.⁹⁻¹⁵

^bThe numbers refer to the following samples: 1: sdGGM interface; 2: sdGGM continuous phase; 3: esGGM interface; 4: esGGM continuous phase; 5: epGGM interface; 6: epGGM continuous phase; 7: sdGX interface; 8: sdGX continuous phase; 9: esGX interface; 10: esGX continuous phase; 11: epGX interface; and 12: epGX continuous phase.

Table S3 Assignment for the relevant carbon-hydrogen correlation signals of polysaccharides linkages in sdGGM, esGGM, epGGM, sdGX, esGX, and epGX samples recovered from interface and continuous phase of emulsions. The cross-signals used in this study for qualitative identification are highlighted in bold and variation in the signals among samples are in the range of ± 0.1 ppm and ± 1.0 ppm for ^1H and ^{13}C dimensions, respectively.

Structural units	δ_{C} (ppm)	δ_{H} (ppm)	Assignments ^a	Identified in ^b
Acetyl	20.9	2.01	-CH ₃ in acetyl	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Ara ₁	107.8	4.76	C ₁ /H ₁ in β -L-arabinopyranoside	1, 2, 3, 4, 5, 6, 8, 10
Ara ₂	83.2	3.75	C ₂ /H ₂ in β -L-arabinopyranoside	1, 2, 4, 6, 8, 9, 10
Ara ₄	85.1	4.00	C ₄ /H ₄ in β -L-arabinopyranoside	1, 2, 3, 4, 6, 9
Ara ₅	62.3	3.42/3.36	C ₅ /H ₅ in β -L-arabinopyranoside	1, 2, 3, 4, 5, 7, 8, 9, 10, 11, 12
Glc ₁	102.0	4.32	C ₁ /H ₁ in β -D-glucopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Glc ₂	74.8	2.90	C ₂ /H ₂ in β -D-glucopyranoside	1, 2, 4, 5, 6, 7, 8, 9, 10, 11, 12
Glc ₃	76.7	3.05	C ₃ /H ₃ in β -D-glucopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Glc ₄	79.9	3.38	C ₄ /H ₄ in β -D-glucopyranoside	1, 2, 4, 5, 6, 7, 8, 10, 11, 12
Glc ₅	70.2	3.18	C ₅ /H ₅ in β -D-glucopyranoside	2, 4, 5, 6, 7, 8, 9, 10, 11, 12
Glc ₆ /Man ₆	60.0	3.59	C ₆ /H ₆ in β -D-gluco-/mannopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl ₁	101.5	4.38	C ₁ /H ₁ in β -D-xylopyranoside	1, 2, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl ₂	72.7	3.03	C ₂ /H ₂ in β -D-xylopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl ₂ (r _a)	69.7	3.27	C ₂ /H ₂ in β -D-xylopyranoside of xylans reduction end	1, 2, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl ₂ -Ac	73.0	4.40	C ₂ /H ₂ in 2-O-acetyl- β -D-xylopyranoside	1, 3, 4, 5, 7, 8, 9, 10, 11, 12
Xyl ₁ (₂ Ac)	100.8	4.49	C ₁ /H ₁ in 2-O-acetyl- β -D-xylopyranoside	1, 2, 3, 4, 5, 6, 7, 8
Xyl ₃	74.5	3.28	C ₃ /H ₃ in β -D-xylopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl ₃ -Ac	74.5	4.81	C ₃ /H ₃ in 3-O-acetyl- β -D-xylopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl _{2,3} -Ac	71.6	4.51	C ₂ /H ₂ in 2,3-O-acetyl- β -D-xylopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl _{2,3} -Ac	72.9	4.90	C ₃ /H ₃ in 2,3-O-acetyl- β -D-xylopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl ₁ (_{2,3} Ac)	99.3	4.68	C ₁ /H ₁ in 2,3-O-acetyl- β -D-xylopyranoside	1, 2, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl ₄	75.7	3.51	C ₄ /H ₄ in β -D-xylopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl ₅	62.8	3.78/3.17	C ₅ /H ₅ in β -D-xylopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl ₄ (nr)	66.0	3.31	C ₄ /H ₄ in β -D-xylopyranoside of xylans non-reducing end	1, 2, 4, 5, 6, 8
Xyl ₅ (nr)	65.3	3.62/2.98	C ₅ /H ₅ in β -D-xylopyranoside of xylans non-reducing end	1, 2, 3, 4, 5, 7, 8, 9, 10, 11, 12
Xyl ₆ (nr)	103.4	4.15	C ₁ /H ₁ in β -D-xylopyranoside of xylans non-reducing end	1, 2, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl ₆ (r _a)	92.3	4.85	C ₁ /H ₁ in α -D-xylopyranoside of xylans reduction end	1, 2, 4, 5, 6, 7, 8, 9, 10, 11, 12
Xyl ₆ (r _b)	97.3	4.21	C ₁ /H ₁ in β -D-xylopyranoside of xylans reduction end	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Man ₁	100.3	4.51	C ₁ /H ₁ in β -D-mannopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 11, 12
Man ₂	74.5	2.90	C ₂ /H ₂ in β -D-mannopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Man ₂ -Ac	70.8	5.25	C ₂ /H ₂ in 2-O-acetyl- β -D-mannopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 10, 11, 12
Man ₃	76.6	3.08	C ₃ /H ₃ in β -D-mannopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Man ₃ -Ac	73.0	4.82	C ₃ /H ₃ in 3-O-acetyl- β -D-mannopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Man ₄	79.3	3.38	C ₄ /H ₄ in β -D-mannopyranoside	1, 2, 4, 5, 6, 7, 8, 10, 11, 12
Man ₅	76.6	3.63	C ₅ /H ₅ in β -D-mannopyranoside	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
Man ₆ (r _a)	93.5	4.86	C ₁ /H ₁ in α -D-mannopyranoside of mannan reduction end	1, 2, 3, 4, 5, 6, 8, 10, 12
Man ₆ (r _b)	93.6	4.59	C ₁ /H ₁ in β -D-mannopyranoside of mannan reduction end	1, 2, 4, 5, 6, 8
Gal ₁	105.0	4.26	C ₁ /H ₁ in β -D-galactopyranoside	1, 2, 4, 5, 6, 8, 10, 12
U ₁	97.4	5.10	C ₁ /H ₁ in 4-O-methyl- α -D-glucuronic acid	1, 5, 7, 8, 10, 11, 12
U ₄	81.6	3.08	C ₄ /H ₄ in 4-O-methyl- β -D-glucuronic acid	1, 2, 5, 6, 7, 8, 9, 10, 11, 12
U _{Gal A}	91.6/94.3	5.19/4.89	C ₁ /H ₁ in galacturonic acid	1, 2, 4, 5, 6, 8, 10, 12

^aContours assignments were assessed according to the literature.¹⁰

^bThe numbers refer to the following samples: 1: sdGGM interface; 2: sdGGM continuous phase; 3: esGGM interface; 4: esGGM continuous phase; 5: epGGM interface; 6: epGGM continuous phase; 7: sdGX interface; 8: sdGX continuous phase; 9: esGX interface; 10: esGX continuous phase; 11: epGX interface; and 12: epGX continuous phase.

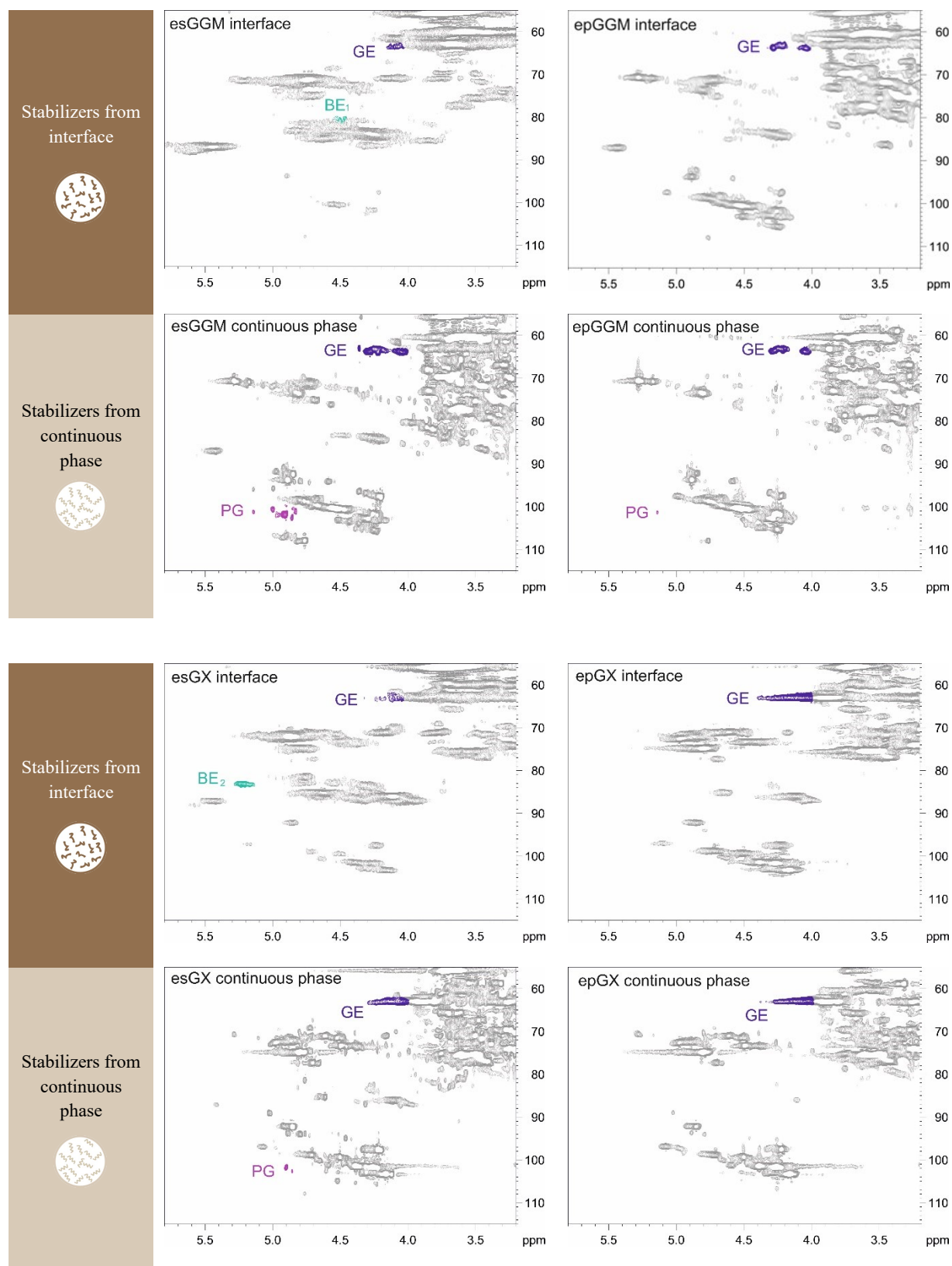


Figure S3 Distribution profile of lignin-carbohydrate structures from sdGGM, esGGM, epGGM, sdGX, esGX, and epGX distributed between interface and continuous phase of oil-in-water emulsions. Cross-signal for phenylglycoside (PG), benzylether (BE) and gamma-ester (GE) identified in samples are highlighted in the spectra.

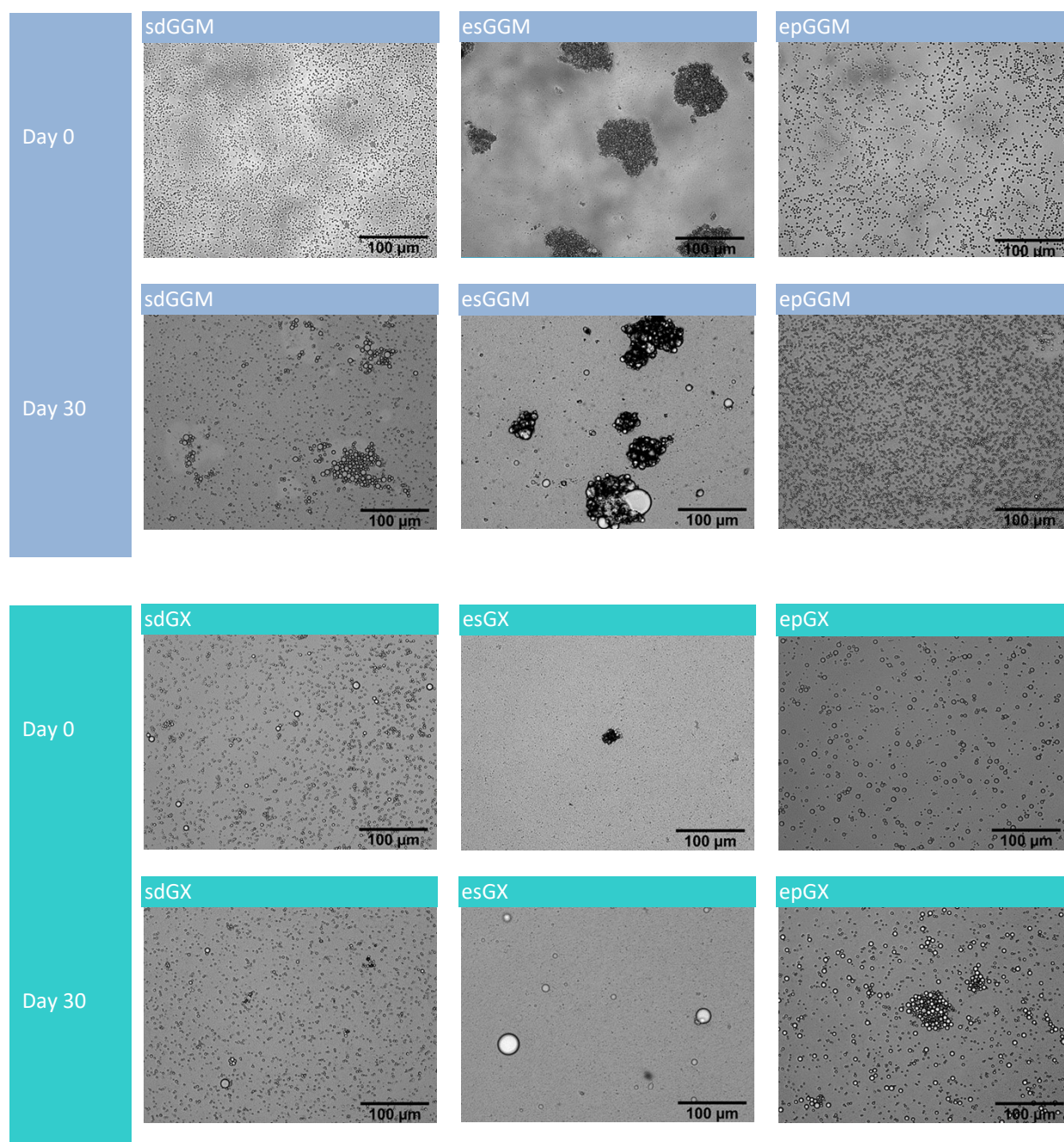


Figure S4 Droplet morphology of oil-in-water emulsions with 5% (w/w) hexadecane as oil component and stabilized by 1% (w/w) sdGGM, esGGM, epGGM, sdGX, esGX, and epGX assessed just after emulsion preparation (day 0) and after storage for 30 days.

Table S4 Mass balance and chemical characterization of glucuronoxylan (GX) samples^a.

Samples		sdGX	esGX	epGX
Mass balance based on original spruce wood (%)		20.7	6.0	13.4
Normalized chemical composition of sugars and lignin (%)	Xyl	68.9 ± 1.0	63.8 ± 0.9	73.7 ± 0.7
	GlcA	0.9 ± 0.3	0.1 ± 0.0	1.5 ± 0.4
	Man	3.8 ± 0.3	1.9 ± 0.2	3.6 ± 0.2
	Glc	2.5 ± 0.2	1.0 ± 0.4	4.0 ± 0.2
	Gal	2.2 ± 0.1	1.1 ± 0.1	3.3 ± 0.1
	Ara	0.0 ± 0.0	0.2 ± 0.1	0.0 ± 0.0
	Rha	1.4 ± 0.1	1.5 ± 0.1	1.0 ± 0.0
	Fuc	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.1
	GalA	0.4 ± 0.1	0.0 ± 0.0	0.2 ± 0.2
Lignin		19.9 ± 1.2	30.4 ± 1.3	12.7 ± 0.5
GX purity (%) ^b		69.8 ± 0.7	63.9 ± 0.9	75.2 ± 0.4
Residual GM (%) ^b		6.3 ± 0.5	2.8 ± 0.6	7.6 ± 0.3
Residual pectin (%) ^b		4.0 ± 0.2	2.9 ± 0.3	4.5 ± 0.3
Acetyl groups	Content (%) ^c	9.1	7.4	10.0
	DS _{Ac} ^d	0.46	0.40	0.48
	Distribution ^e	0.5:1.0:0.2	0.7:1.0:0.3	0.5:1.0:0.2
Molar mass	Mn (kDa)	1.2 ± 0.0	0.6 ± 0.0	1.6 ± 0.0
	Mw (kDa)	4.2 ± 0.6	1.2 ± 0.1	4.9 ± 0.1
	DI	3.5 ± 0.4	1.9 ± 0.1	3.1 ± 0.0
Syringyl/guaiacyl ratio		6.8:1	6.1:1	11.6:1

^aIn the table: sdGX: spray-dried glucuronoxylan; esGX: ethanol-soluble glucuronoxylan; epGX: ethanol-precipitated glucuronoxylan; Xyl: xylose; GlcA: glucuronic acid; Man: mannose; Glc: glucose; Gal: galactose; Ara: arabinose; Rha: rhamnose; Fuc: fucose; GalA: galacturonic acid, DS_{Ac}: degree of acetylation of glucuronoxylan samples; Mn: number-average molar mass; Mw: weight-average molar mass; and DI: dispersity index.

^bFor the estimation of the purity of glucuronoxylan were considered the content of xylose and glucuronic acid in samples. Similarly, glucomannan content was estimated considering mannan and glucose moieties and other sugars identified, *i.e.*, galactose, arabinose, rhamnose, fucose, and galacturonic acid, were considered as residual pectin.

^cmol acetyl per 100 mol pentose.

^dDS_{Ac} was calculate considering only xylopyranosyl units, which is the sugar present in glucuronoxylan backbone and that can be naturally acetylated.

^eAcetylation distribution in xylopyranosyl units (C-2:C-3:C-2,3) obtained by semi-quantitative analysis from NMR spectra.

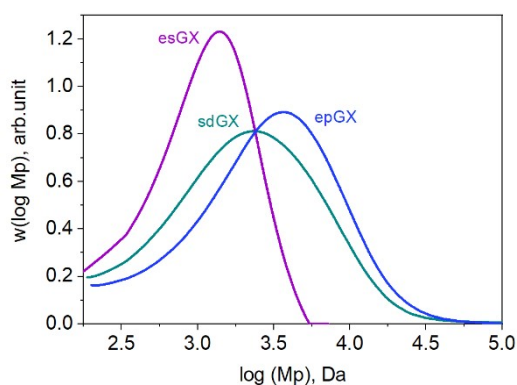
**Figure S5** Molar mass distribution of sdGX, esGX, and epGX samples.

Table S5 Assignment for the relevant lignin substructures, lignin side and end groups and lignin-carbohydrates bonds cross-signals in sdGX, esGX, and epGX samples. The cross-signals used in this study for qualitative identification are highlighted in bold and variation in the signals among samples are in the range of ± 0.1 ppm and ± 1.0 ppm for ^1H and ^{13}C dimensions, respectively.

Structural units ^a	δ_{C} (ppm)	δ_{H} (ppm)	Assignments	Identified in
Syringyl ($\text{S}_{2,6}$)	103.9	6.68	C_2/H_2 and C_6/H_6 in S-units	sdGX, esGX, epGX
Guaiacyl (G_2)	110.9	6.94	C_2/H_2 in G-units	sdGX, esGX, epGX
Guaiacyl (G_5)	115.0	6.83	C_5/H_5 in G-units	sdGX, esGX
Guaiacyl (G_6)	118.7	6.76	C_6/H_6 in G-units	sdGX, esGX, epGX
p-hydroxyphenyl ($\text{H}_{2,6}$)	127.5	7.21	C_2/H_2 and C_6/H_6 in H-units	esGX
β -aryl ether (β -O-4)	71.4	4.71	β -O-4 signal in α	sdGX, esGX, epGX
β -aryl ether (β -O-4)	85.5	4.16	β -O-4 signal in β in S units	sdGX, esGX, epGX
β -aryl ether (β -O-4)	59.5	3.70/3.44	β -O-4 signal in γ	sdGX, esGX, epGX
Phenylcoumaran (β -5)	87.2	5.43	β -5 signal in α	sdGX, esGX, epGX
Phenylcoumaran (β -5)	52.8	3.46	β -5 signal in β	sdGX, esGX, epGX
Phenylcoumaran (β -5)	62.4	3.72	β -5 signal in γ	sdGX, esGX, epGX
Dibenzodioxocin (5-5/ β -O-4)	82.9	4.81	5-5/ β -O-4 signal in α	sdGX, esGX
Dibenzodioxocin (5-5/ β -O-4)	86.2	3.91	5-5/ β -O-4 signal in β	esGX
Resinol (β - β)	85.1	4.61	β - β signal in α	sdGX, esGX, epGX
Resinol (β - β)	53.6	3.04	β - β signal in β	sdGX, esGX, epGX
Resinol (β - β)	71.2	4.14/3.83	β - β signal in γ	sdGX, esGX, epGX
SECO $_{\alpha}$ (β - β)	33.6	2.53/2.48	Secoisolariciresinol in α	-
SECO $_{\beta}$ (β - β)	42.3	1.84	Secoisolariciresinol in β	-
Spirodienone (β -1)	81.2	5.00	β -1 signal in α	-
Spirodienone (β -1)	59.8	2.75	β -1 signal in β	-
Spirodienone (β -1)	79.4	4.11	β -1 signal in β'	-
Methoxy group	55.4	3.73	C/H in -OMe in G- and S-units	sdGX, esGX, epGX
Cinnamyl alcohol	128.7	6.42	Cinnamyl alcohol signal in α	esGX
Cinnamyl alcohol	127.5	6.21	Cinnamyl alcohol signal in β	esGX
Cinnamyl alcohol	62.8	3.90	Cinnamyl alcohol signal in γ	sdGX, esGX, epGX
OSC ($\text{S}_{2,6}$)	106.4	7.20/7.06	$\text{C}_{2,6}/\text{H}_{2,6}$ in $(\text{C}=\text{O})_{\alpha}$ in S-units	sdGX, esGX
OSC $_{\alpha}$	154.0	7.61	Cinnamyl aldehyde in α	sdGX, esGX
OSC $_{\beta}$	126.1	6.77	Cinnamyl aldehyde in β	sdGX, esGX
DCA $_{\alpha}$	31.4	2.52	Dehydroconiferyl alcohol in α	sdGX, esGX
DCA $_{\beta}$	34.4	1.67	Dehydroconiferyl alcohol in β	sdGX, esGX
DCA $_{\gamma}$	60.0	3.42	Dehydroconiferyl alcohol in γ	sdGX, esGX, epGX
PG	104.5/99.8	5.18/4.75	Phenylglycoside units	sdGX, esGX, epGX
BE (BE_1)	80.2	4.50	Benzylether in C-3 and C-2	-
BE (BE_2)	82.3	5.20	Benzylether in C-6 and C-5	sdGX, esGX
BEst	74.3	5.96	Benzyl ester (α -ester)	-
GE	64.0/62.0	4.50/4.00	γ -ester units	sdGX, esGX, epGX

^aSecoisolariciresinol (SECO β - β); Oxidized side chain (OSC); Dehydroconiferyl alcohol (DCA); PG: phenylglycoside; BE: benzylether, in which BE_1 refers to linkage at C-6 in glucose, mannose, and galactose or C-5 in arabinose and BE_2 refers to linkage at C-2 or C-3 in glucose, mannose, galactose, xylose, and arabinose; BEst: benzyl ester; and GE: γ -ester. Contours assignments were assessed according to the literature.⁹⁻¹⁵

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