Supplementary Materials: Composition of Lignin-to-Liquid Solvolysis Oils from Lignin Extracted in a Semi-Continuous Organosolv Process

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Table S1. Extended overview of reaction conditions, input material and product output from LtL-solvolysis. High (+) and low (-) values, together with intermediate centre points (0), for the variables V1 (FA loading) and V2 (reaction temperature) are included in the table.

In/Out	Experiment	WO.1.1	WO.1.2	WO.2.1	WO.2.2	WO.3.1	WO.3.2
	V1 V2	--	+-	00-1	00-2	-+	++
In	Lignin (g)	0.51	0.51	0.50	0.50	0.51	0.51
	Formic Acid (g)	0.61	1.22	0.93	0.93	0.62	1.22
	V1 Formic Acid (mL)	0.50	1.00	0.76	0.76	0.51	1.00
	V2 Temperature (°C)	320	320	340	340	360	360
	Water (g)	4.00	4.05	4.02	4.02	4.05	4.03
	Total mass input (g)	5.12	5.78	5.45	5.45	5.18	5.76
	Lignin percentage of mass input (%)	9.9	8.8	9.2	9.2	9.8	8.8
Out	Gas (g)	0.60	1.10	0.90	0.90	0.60	1.20
	LtL-oil (g)	0.40	0.48	0.45	0.45	0.35	0.45
	Solids (g)	0.12	0.05	0.04	0.04	0.10	0.03
	Aqueous-phase (g)	3.89	4.01	3.91	3.90	4.02	3.89
	Total mass output (g)	5.00	5.70	5.30	5.29	5.07	5.57
Results	Gas (% of FA input)	98.4	90.2	96.8	96.8	96.8	98.4
	Aqueous-phase (% of solvent input)	97.3	99.1	97.4	97.1	99.3	96.6
	Solids (% of lignin input)	22.7	9.7	7.5	7.0	19.1	5.7
	LtL-oil yield (% of lignin input)	77.9	94.2	89.3	89.4	69.2	88.7
	Mass recovery (%)	97.7	97.6	97.2	96.9	97.9	96.8

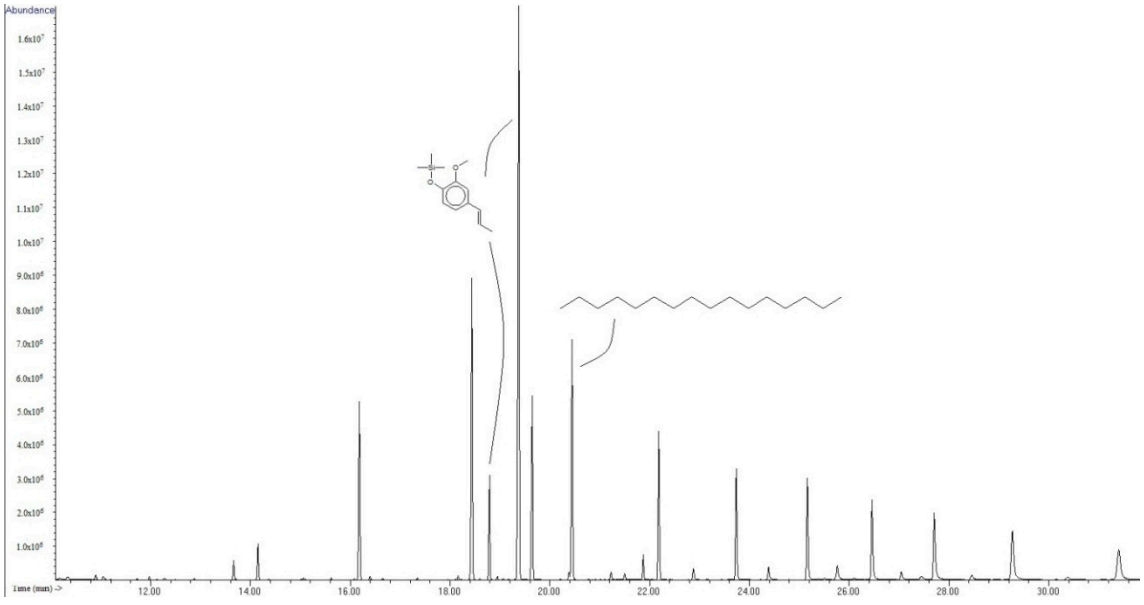

Figure S1. GC-MS chromatogram of a silylated sample of isoeugenol (mix of *cis* and *trans*) together with hexadecane which has reacted with the septum in the vial cap. All the unmarked peaks represent various silicon oxides.

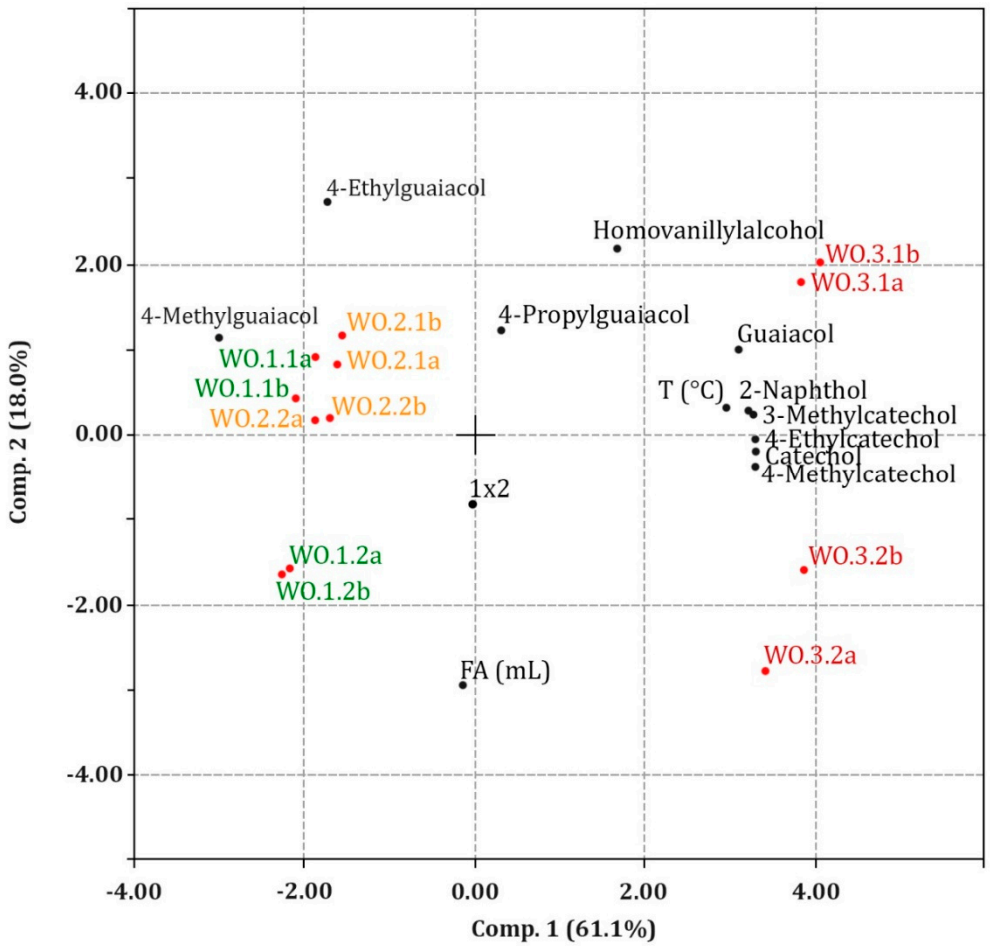

Figure S2. Biplot from principal component analysis (PCA) of data from LtL-oil quantification responses together with experimental coding. Colour coding of the experiments corresponds to the Van Krevelen plot in Figure 3 and the biplot in Figure 4 in the main text.

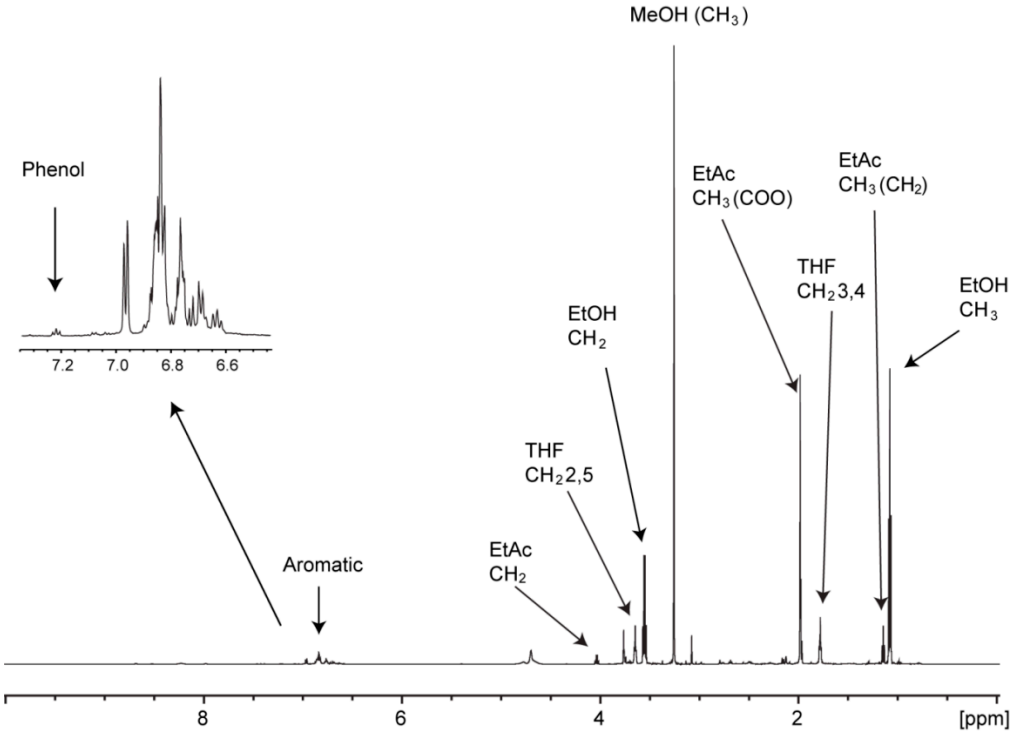

Figure S3. ^{1}H-spectra of the aqueous phase from experiment WO.2.1.

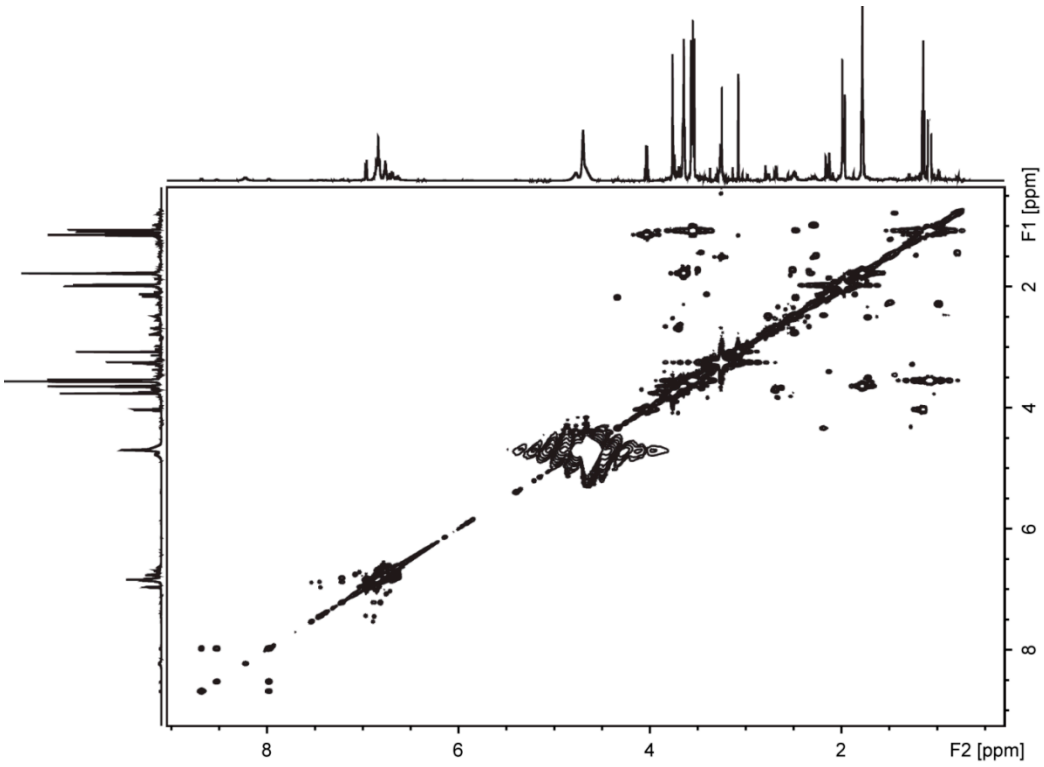

Figure S4. ^{1}H-^{1}H-COSY spectra of the aqueous phase from experiment WO.2.1.

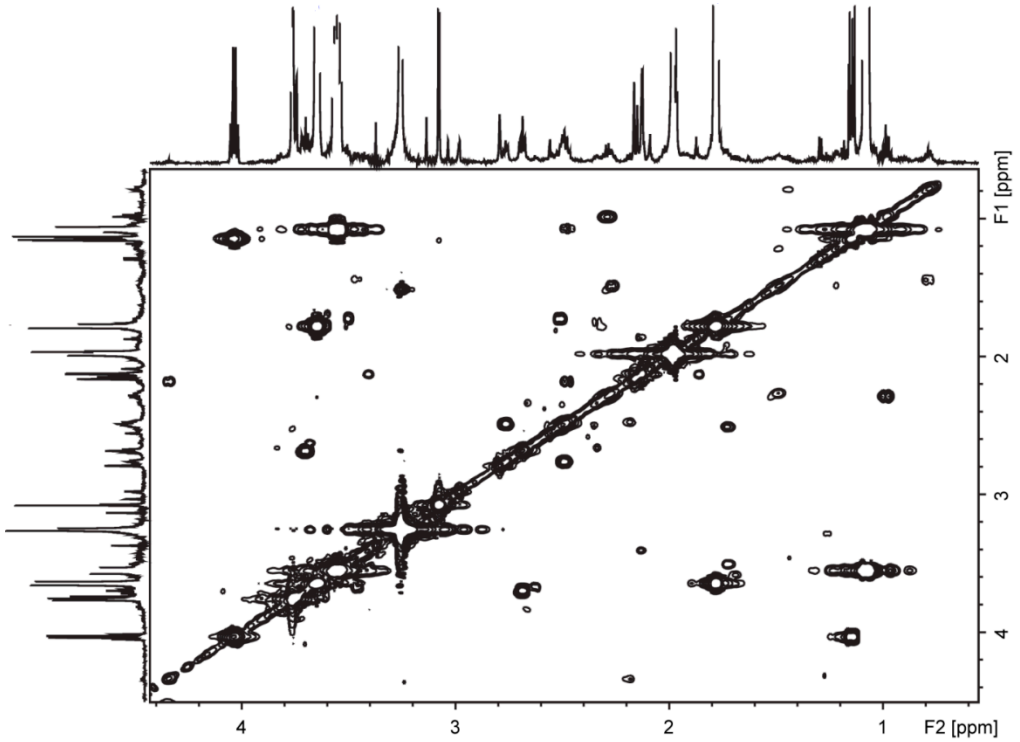

Figure S5. Enhanced ^{1}H-^{1}H-COSY spectra of the aqueous phase from experiment WO.2.1 (4.4–0.6 ppm).

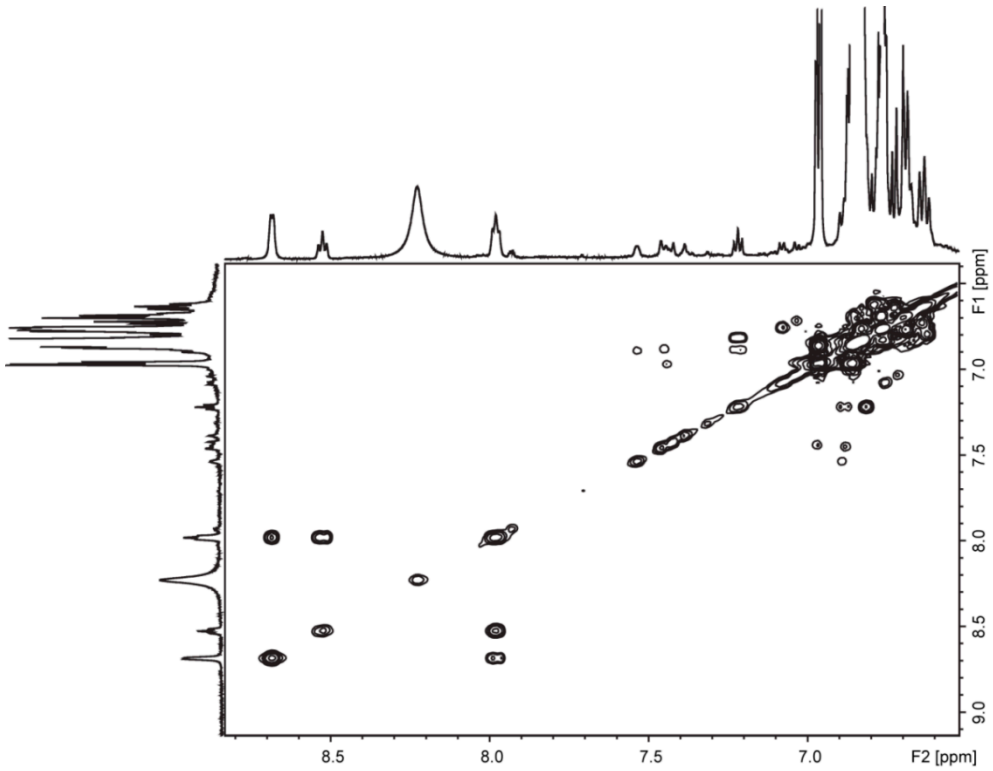

Figure S6. Enhanced ^{1}H-^{1}H-COSY spectra of the aqueous phase from experiment WO.2.1 (8.8–6.5 ppm).