Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary material

Hydrothermal Co-liquefaction of Biomasses – Quantitative Analysis of Bio-crude and Aqueous Phase Composition

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Table S1 – Elemental distribution in bio-crude from HTL of model compounds. Carbohydrate (cellulose:hemicellulose 3:1), protein (soya protein), lipid (unrefined rapeseed oil)

	C [%]	H [%]	N [%]	S [%]	O [%]
Carbohydrate	78.49	7.38	0.10	0.17	13.87
Protein	76.11	9.28	5.75	0.89	7.97
Carbohydrate:Lipid	77.11	11.04	0.09	0.09	11.68
Protein:Lipid	70.34	10.93	2.67	0.27	15.79
Carbohydrate:Protein	77.30	8.82	5.63	0.49	7.76
Carbohydrate:Protein:Lipid	75.59	10.53	2.76	0.19	10.93

Figure S2 – Normalized peak areas of monoglycerides

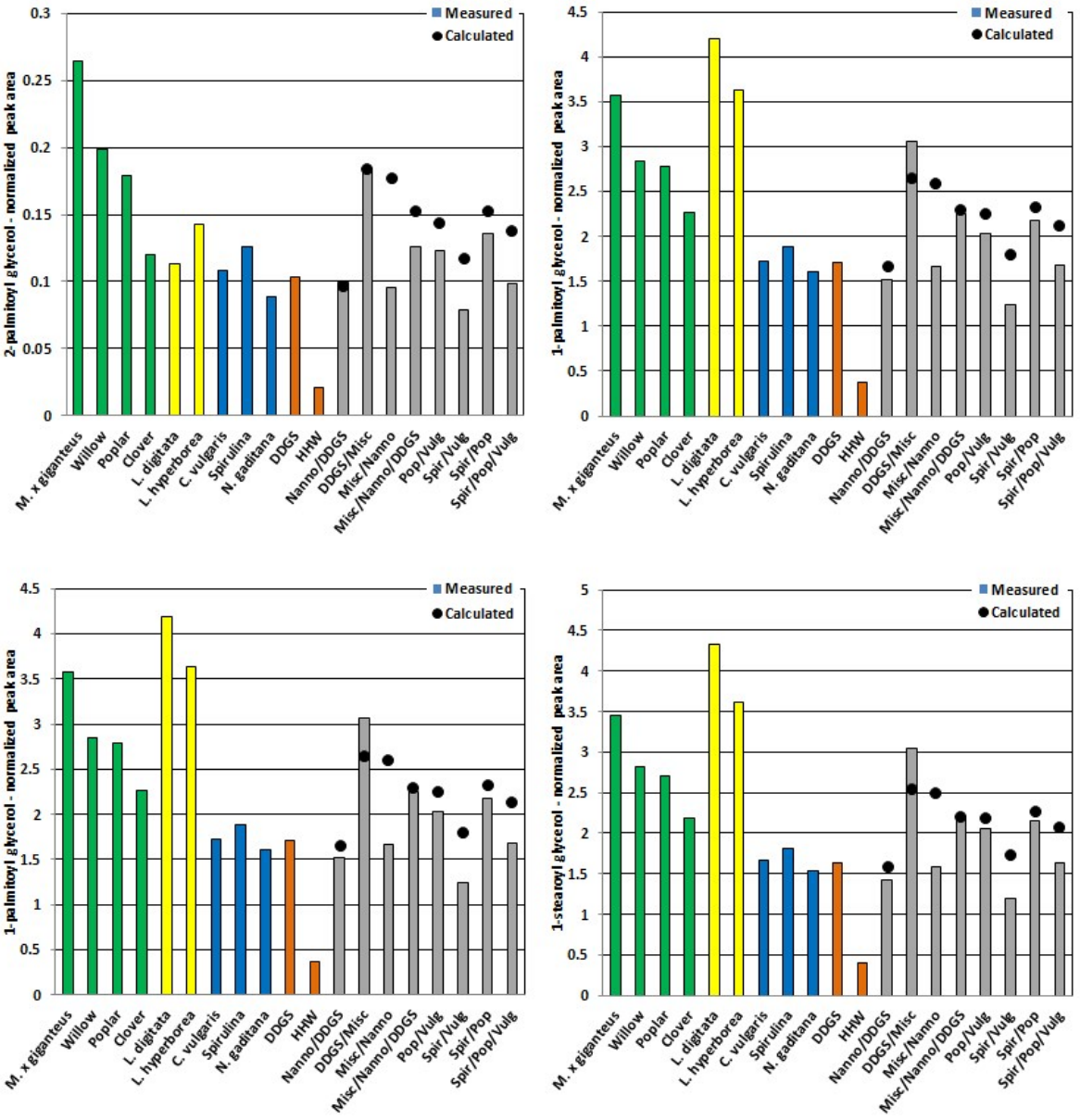

Table S3 – Compounds quantitated in the aqueous phase

Small organic acids	***Fatty acids***
acetic acid	tetradecanoic acid
isobutyric acid	palmitoleic acid
methacrylic acid	palmitic acid
butyric acid	linoleic acid
crotonic acid	oleic acid
isovaleric acid	stearic acid
pent-4-enoic acid	***Oxygenated aromatics***
pent-3-enoic acid	benzoic acid
valeric acid	phenol
tigllic acid	phenyl acetic acid
3-methylbut-2-enoic acid	m-cresol
3-methylpentanoic acid	p-cresol
4-methylpentanoic acid	hydrocinnamic acid
5-hexenoic acid	***Cyclic oxygenates***
3-methylpent-2-enoic acid	cyclopentanone
3-methylpent-3-enoic acid	2-methylcyclopent-2-enone
2-methylpent-2-enoic acid	butyrolactone
levulinic acid	3-methylcyclopent-2-enone
4-oxohexanoic acid	2,3-dimethylcyclopent-2-enone
4-methylpent-3-enoic acid	δ-valerolactone
5-oxohexanoic acid	3,4-dimethylcyclopentenone
octanoic acid	(?,?)-dimethylcyclopentenone
dodecanoic acid	4,4-dimethylcyclopentenone
oxalic acid	3-ethylcyclopent-2-enone
malonic acid	***Nitrogenates***
succinic acid	pyrazine
methylsuccinic acid	methylpyrazine
glutaric acid	2,5-dimethylpyrazine
ethylsuccinic acid	ethylpyrazine
adipic acid	2,3-dimethylpyrazine
2-oxoglutaric acid	2,3,5-trimethylpyrazine
propantricarboxylic acid	2-pyrrolidone
	3-hydroxypyridine, monoacetate
	3-hydroxypyridine

Figure S4 – Measured and calculated concentrations of small organic acids, fatty acids, oxygenated aromatics, and cyclic oxygenates quantitated in aqueous phase from HTL of mixtures of biomass.