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

Hydrotreating of bio-crude obtained from hydrothermal liquefaction of biopulp: Effect of aqueous phase recirculation on the hydrotreated oil

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Table S1. Ultimate, proximate, and biochemical properties of the biomass.

Analysis	Value
Ultimate analysis (wt. %)	
C	51.7 ± 0.4
H	7.5 ± 0.1
N	3.3 ± 0.1
O*	27.8 ± 0.6
HHV (MJ/kg) [a]	23.2 ± 0.02
Proximate analysis (wt. %)	
Moisture	78.5 ± 0.9
Ash[b]	9.7 ± 0.4
Volatile matter [a]	71.9 ± 1.8
Fixed carbon [a]	18.4 ± 0.8
Biochemical analysis (wt. %)	
Crude fats	19.2 ± 2.1
Crude proteins	20.6 ± 0.6
Carbohydrate and extractives [c]	50.5 ± 2.7

[a] DAF basis [b] Dry basis [*]Calculated by difference

Table S2. The chemicals utilized to quantify the N-species in the bio-crude and upgraded oil samples.

Substance	Quantifier	Qualifier	Calibration curve	R^2
2-Piperidone	113	56	y = 16904,4247 · x	0.9463
Quinoline	99	43	y = 127674,4240 · x	0.9596
Indole	117	89	y = 130280,3948 · x	0.9525
Quinoline, 2-methyl	143	128	y = 159483,2547 · x	0.9599
Indole, 2-methyl	130	131	y = 167490,8118 · x	0.9529
Quinoline, 2,6-dimethyl	157	146	y = 176516,6541 · x	0.9663
Indole, 2,3-dimethyl	144	130	y = 118984,6070 · x	0.9679
Hexadecanamide	59	72	y = 43705,2335 · x - 15858,5964	0.9926
Hexadecanamide, N-methyl	73	86	Hexadecanamide as calibration reference	
Hexadecanamide, N-ethyl	87	100	Hexadecanamide as calibration reference	
Octadecanamide	59	72	y = 37350,2247 · x - 10180,5311	0.9962
Octadecanamide, N-methyl	73	86	Octadecanamide as calibration reference	
Octadecanamide, N-ethyl	87	100	Octadecanamide as calibration reference	

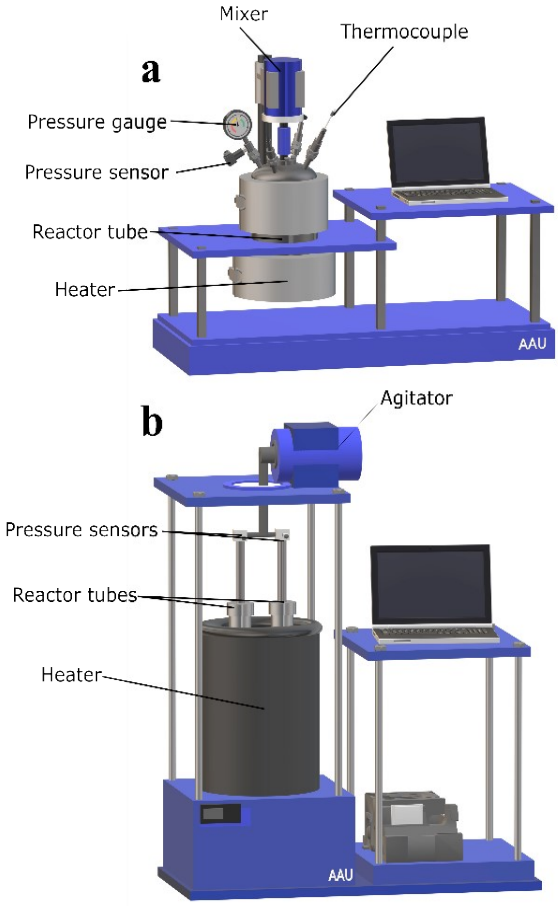

Figure S1. Schematic view of a) HTL and b) HT setups.

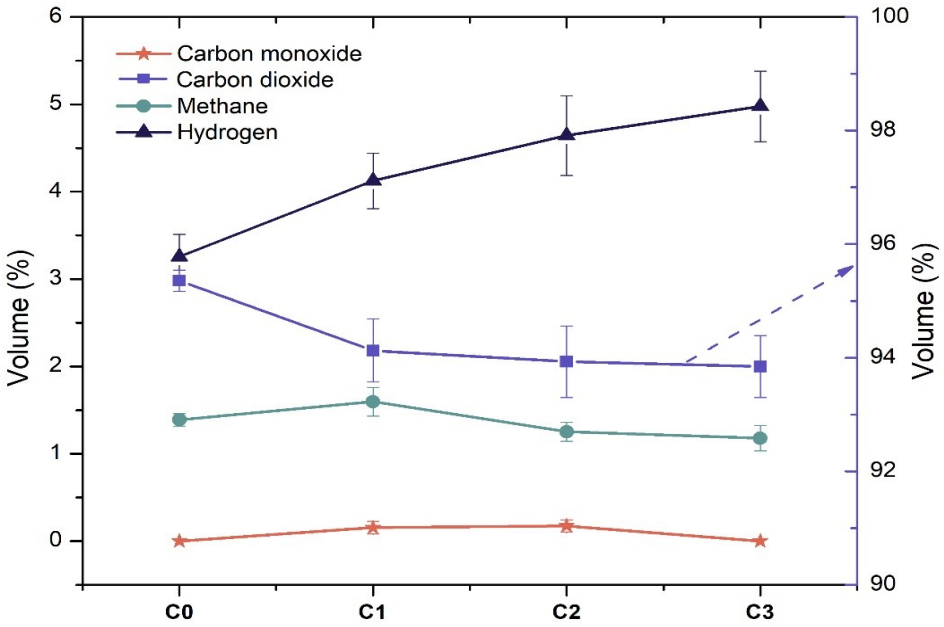

Figure S2. The gas composition of HTL experiments.

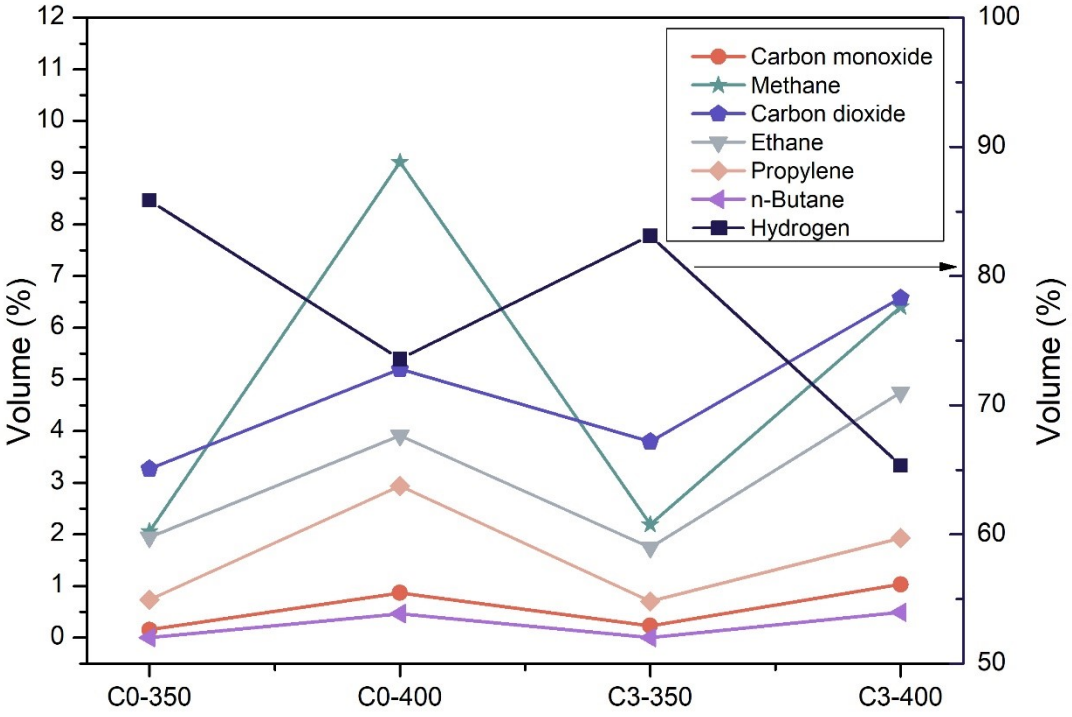

Figure S3. The gas composition of HT experiments.

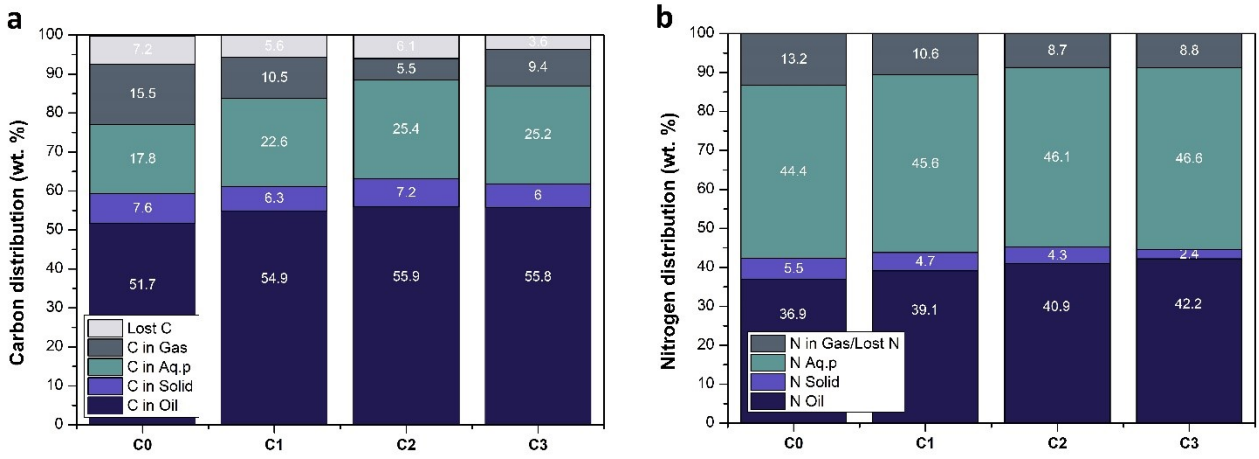

Figure S4. a) Carbon and b) Nitrogen distribution among different HTL products.

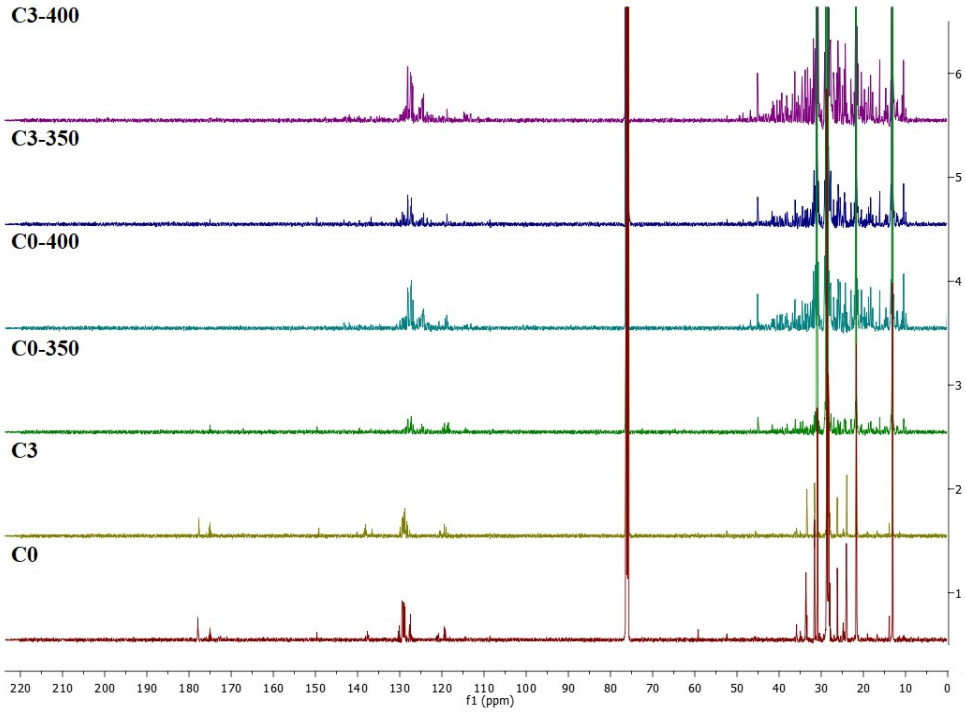

Figure S5. ^{13}C-NMR spectra of C0 and C3 bio-crudes and the corresponding hydrotreated bio-crudes.

Table S3. The absolute concentration of the N-containing class representative compounds.

Type	Compound	Concentration (ppm)					
		C0	C3	C0-350	C0-400	C3-350	C3-400
N-heterocyclic	Quinoline	6.24	6.95	0.71	2.30	1.35	4.37
	Quinoline, 2-Methyl	3.23	3.73	1.26	9.73	4.21	14.53
	Quinoline, 2,6-Dimethyl	1.57	1.91	3.17	17.35	5.25	21.45
	Indole	1.31	1.62	12.13	32.88	15.20	42.22
	Indole, 3-Methyl	14.96	17.49	15.23	55.76	21.49	54.28
	Indole, 2,3-Dimethyl	43.43	44.45	60.07	67.12	63.58	68.28
	2-Piperidone	48.94	29.19	2.44	1.34	1.19	2.60
Amide	Hexadecanamide	455.08	550.96	277.14	105.83	312.78	106.66
	Hexadecanamide, N-methyl	307.83	441.21	4.77	1.57	21.94	1.25
	Hexadecanamide, N-ethyl	1113.97	1492.84	16.70	5.60	44.36	8.70
	Octadecanamide	170.77	212.76	352.30	62.44	418.97	85.27
	Octadecanamide, N-methyl	119.76	149.73	11.54	2.15	27.81	2.63
	Octadecanamide, N-ethyl	464.59	685.74	37.71	5.55	65.42	5.30