Supplementary file

for

Catalytic hydrothermal liquefaction of Spent Coffee Grounds: Optimization of process parameters for production of biocrude oil through combined RSM and ANN based methodology

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Table S1: Fit summary of the designed model by comparing with different statistical parameters for biocrude yield (wt.%)

Source	Sequential p-value	Lack of Fit P-value	Adjusted R^2	Predicted R^2	Remarks
Linear	0.0003	0.0009	0.6230	0.3639	
2FI	0.0142	0.0030	0.7889	0.3582	
Quadratic	0.0003	0.0862	0.9554	0.8398	**Suggested**
Cubic	0.0553	0.3357	0.9804	–4.097	**Aliased**

Table S2: Components derived from GC-MS of biocrude derived from non-catalytic and catalytic HTL of SCGs.

Retention time (min)	Relative Area (%)	Component
Non-catalytic HTL		
30.2	45.73	n-Hexadecanoic acid
32.08	14.72	9,12-Octadecandienoic acid (Z,Z)-
32.23	14.03	Octadecandienoic acid
32.44	9.21	9-Octadecenenamide
33.97	16.28	9-Octadecenenamide, (Z)-
KOH catalyzed HTL		
30.24	37.02	n-Hexadecanoic acid
32.09	36.46	9,12-Octadecandienoic acid (Z,Z)-
32.27	7.99	Octadecandienoic acid
32.47	6.10	Octadecenenamide, (Z)-
32.68	4.32	Archidamide, N-methyl-
33.98	5.55	9-Octadecenenamide, (Z)-
35.64	2.53	Pyrrolidide of 14-methyl-pentadecanoate
Fe catalyzed HTL		

30.21	15.97	n-Hexadecanoic acid
32.24	15.06	Octadecandienoic acid
32.44	5.47	9-Octadecenenamide, (Z)-
32.67	3.93	5-Methyl-2-hexanone oxime
33.97	15.51	9-Octadecenenamide, (Z)-
32.09	41.85	9,12-Octadecandienoic acid (Z,Z)-
35.65	2.17	4,8,12-Trimethyl-tridecanoic acid, pyrrolidide

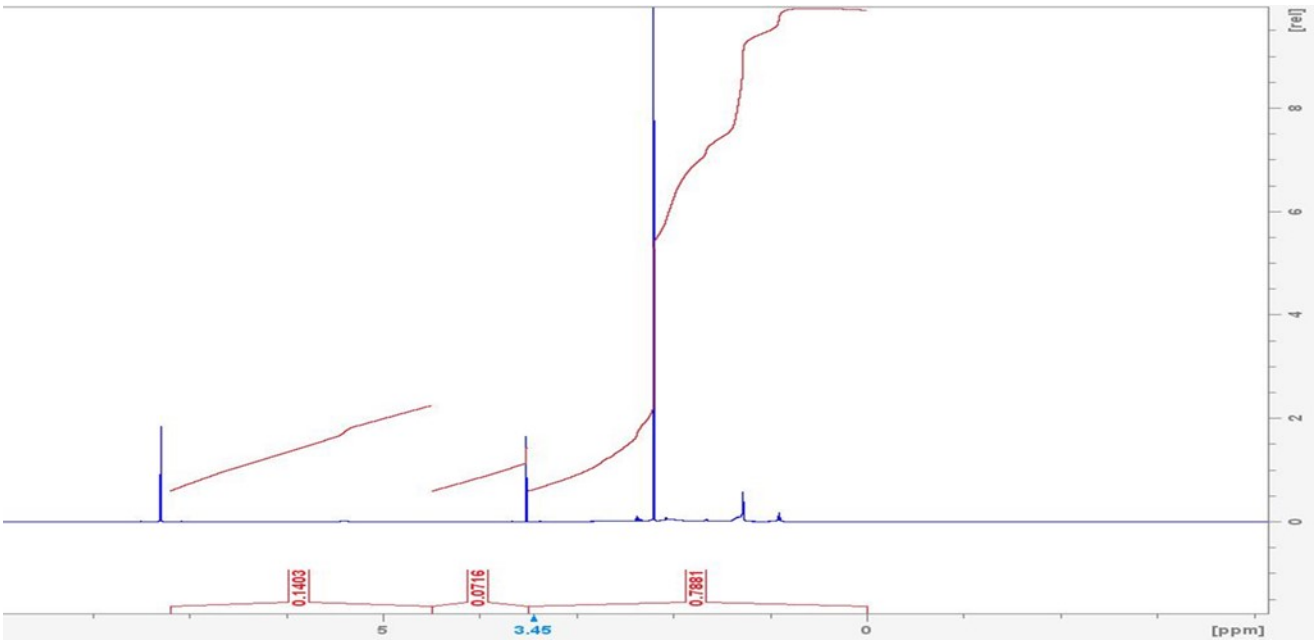

Fig. S1: (a) ^{1}H NMR of OPT-BC

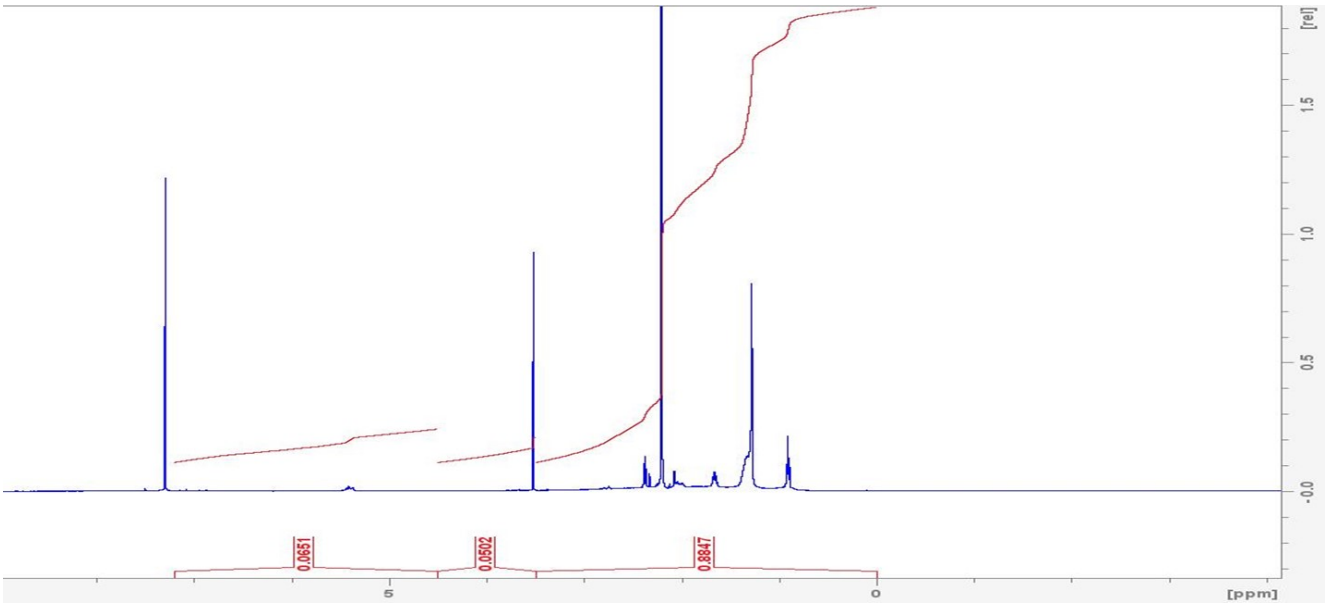

Fig. S2: (a) ^{1}H NMR of KOH-BC

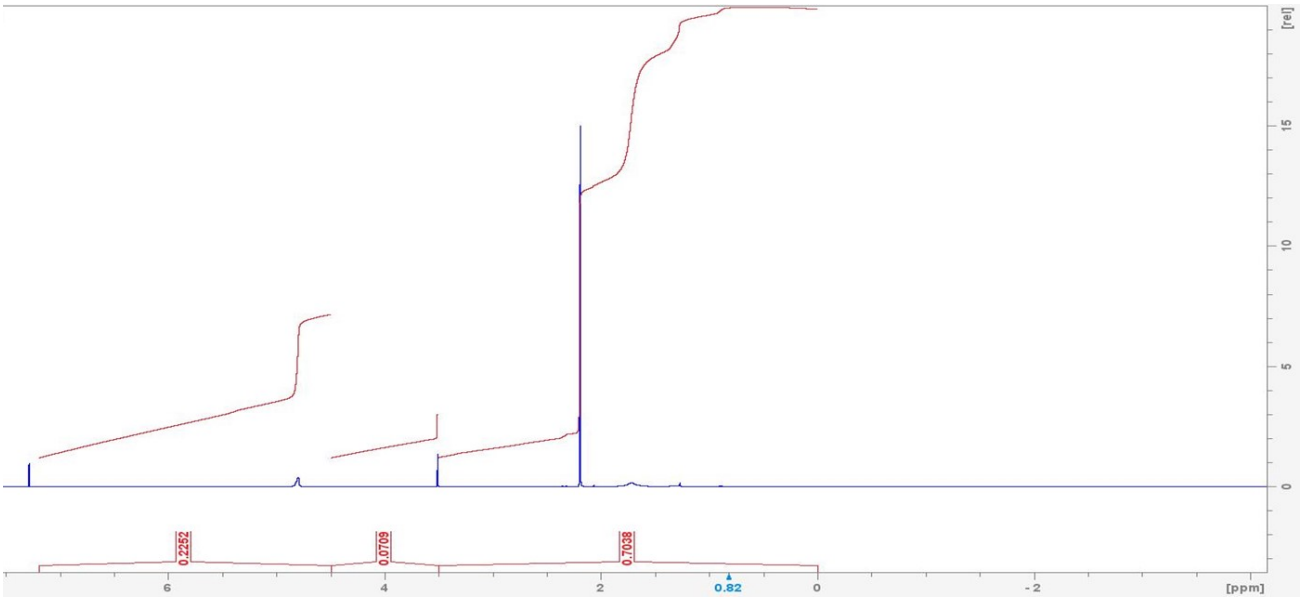

Fig. S3: (a) ^{1}H NMR of Fe-BC

Table S3: Summary of the available literature on the catalytic HTL of biomass along with their comparison with the present study on the basis of yield and compositional analysis of biocrude oil.

Catalyst	Biomass	HTL Conditions (°C, min.)	Catalytic effects on biocrude							Ref.
			Yield (% change)	C	H	O	N	S	HHV (MJ/kg)	
Pd/C	*Nannochloropsis sp.*	350, 60	20	73.4	10.8	9.01	3.88	0.52	18.5	[1]
5% Na_2CO_3	*Dunaliella tertiolecta*	360, 50	5.8	63.55	7.66	25.08	3.71	0.29	30.74	[2]
Na_2CO_3	Spirulina plantesis	350, 60	11.7	72	9.88	11.81	5.44	0.87	36.29	[3]
K_2CO_3	Barley straw	300, 30	14	67.89	7.62	23.18	0.75	0.56	27.29	[4]
KOH	Pretreated sorghum bagasse	350, 60	29	64.3	7.6	14.5	0.3	0.6	30	[5]
Fe	Wheat Straw	299.8, 39.9	1	77.1	7.1	14.4	0.8	0.3	36.1	[6]
Fe-K_2CO_3	Wheat Straw	299.8, 39.9	2.3	77.6	7.4	14.1	0.7	0.2	37	[6]
KOH	Spent Coffee Grounds	327.3, 48	4.8	78.3	9.3	10.3	1.6	0.6	37	**(Present Study)**
Fe	Spent Coffee Grounds	327.3, 48	3.1	78.8	9.4	10.7	0.9	0.4	36.6	**(Present Study)**

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