

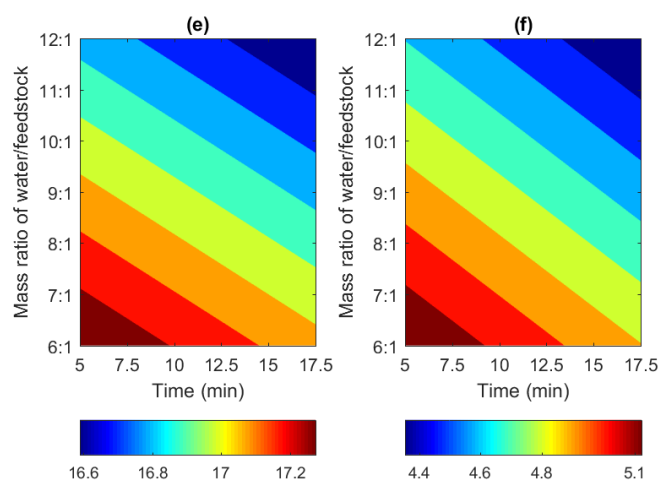
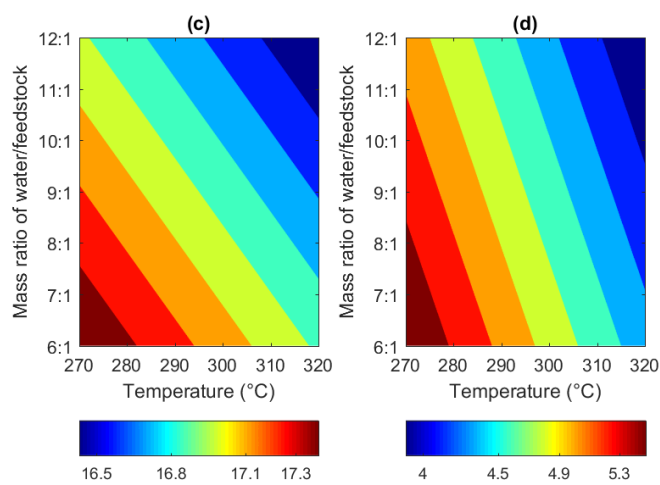
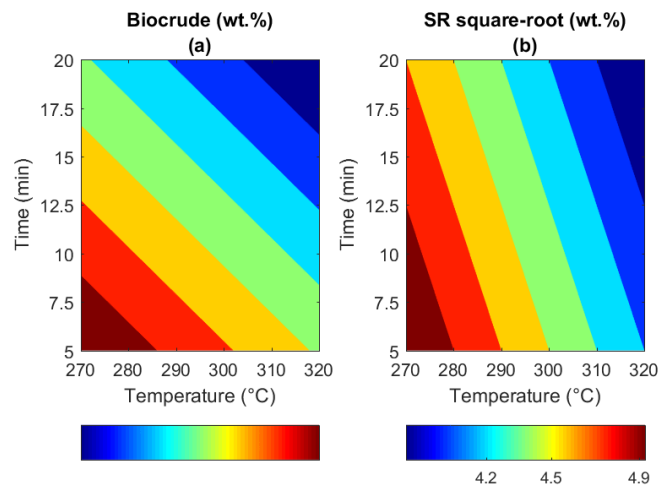
## *Supplementary Materials*

for

# **A Comparative Study on Thermochemical Valorization Routes for Spent Coffee Grounds**

**Table S1.** Raw data for microwave-assisted extraction of spent coffee grounds oil.

Standard Order	Microwave Power (W)	Solvent/Solid Ratio (mL/g)	Time (min)	SCG Oil Yield (wt.%)
1	200	4	5	6.15
2	500	4	5	5.73
3	200	8	5	8.26
4	500	8	5	7.87
5	200	4	15	3.68
6	500	4	15	5.92
7	200	8	15	8.51
8	500	8	15	8.22
9	200	6	10	6.89
10	500	6	10	6.91
11	350	4	10	6.03
12	350	8	10	7.34
13	350	6	5	7.78
14	350	6	15	7.32
15	350	6	10	7.33
16	350	6	10	7.74
17	350	6	10	7.39
18	350	6	10	7.48
19	350	6	10	7.32
20	350	6	10	7.50



**Figure S1.** Contour plots for biocrude yield (a), (c) and (e), and solid residue (SR) (b), (d) and (f) from hydrothermal liquefaction of post-extracted spent coffee grounds. Square root values of SR yield are shown in the plots.

**Table S2** Chemical composition for biocrude derived from raw spent coffee grounds.

Compounds' Name	Chemical Class	Peak Area Percentage (%)
n-Hexadecanoic acid	acid	5.5
Glycodeoxycholic acid	acid	3.0
1-Dodecanol	alcohol	2.2
Ethanol, 2-(9,12-octadecadienyloxy)-, (Z,Z)-	alcohol	1.5
E,E,Z-1,3,12-Nonadecatriene-5,14-diol	alcohol	6.1
Hexadecanamide	amide	4.6
Caffeine	amine	10.0
Hexadecanoic acid, methyl ester	ester	1.3
8,11-Octadecadienoic acid, methyl ester	ester	1.2
Glycidyl palmitate	ester	4.1
Hexanedioic acid, bis(2-ethylhexyl) ester	ester	3.1
3-Hydroxypropyl palmitate, TMS derivative	ester	3.1
Heptanoic acid, dicotyl ester	ester	2.0
1,2-Propanediol, 3-(octadecyloxy)-, diacetate	ester	1.8
Propanoic acid, 3,3'-thiobis-, didodecyl ester	ester	19.1
Heptadecane, 9-hexyl-	hydrocarbon	1.6
Octadecane, 3-ethyl-5-(2-ethylbutyl)-	hydrocarbon	6.7
Spirolactone	ketone	4.9
3,6-Diisopropylpiperazin-2,5-dione	N-containing heterocycle	1.7
Cyclo-(1-leucyl-1-phenylalanyl)	N-containing heterocycle	1.6
2,5-Piperazinedione, 3,6-bis(2-methylpropyl)-	N-containing heterocycle	1.7
Phenol	phenolic	7.4
Phenol, 2,2'-methylenebis[6-(1,1-dimethylethyl)-4-ethyl- $\zeta$ -Sitosterol	phenolic	2.1
	phenolic	3.7

**Table S3** Chemical composition for biocrude derived from defatted spent coffee grounds.

Compounds' Name	Chemical Class	Peak Area Percentage (%)
n-Hexadecanoic acid	acid	7.7
Hexadecanoic acid	acid	2.4
Linoelaidic acid	acid	2.0
Octadecanoic	acid	1.5
Hexadecanamide	amide	5.2
Hexadecanoic acid, methyl ester	ester	4.7
9-Octadecenoic acid (Z)-, tetradecylester	ester	2.3
8,11-Octadecadienoic acid, methyl ester	ester	1.4
Methyl stearate	ester	1.3
Glycyl-L-histidyl-L-lysine acetate	ester	1.2
Furan, 2-pentyl-	furan	1.3
Pentacosane	hydrocarbon	3.7

Hexatriacontane	hydrocarbon	2.4
Octadecane, 3-ethyl-5-(2-ethylbutyl)-	hydrocarbon	1.2
Spironolactone	ketone	2.1
2-Cyclopenten-1-one, 2,3-dimethyl-	ketone	1.7
Caffeine	N-containing heterocycle	17.3
3,6-Diisopropylpiperazin-2,5-dione	N-containing heterocycle	3.1
2,5-Piperazinedione, 3,6-bis(2-methylpropyl)-	N-containing heterocycle	2.8
Pyrrolo[1,2-a]pyrazine-1,4-dione	N-containing heterocycle	2.5
Cyclo-(l-leucyl-l-phenylalanyl)	N-containing heterocycle	2.5
Pyrrolo[1,2-a]pyrazine-1,4-dione	N-containing heterocycle	2.3
2-Pyrrolidinone, 1-methyl-	N-containing heterocycle	2.1
3,6-Diisopropylpiperazin-2,5-dione	N-containing heterocycle	1.8
Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-	N-containing heterocycle	1.7
7-Ethyl-4,6-pentadecandione	N-containing heterocycle	1.6
2,5-Piperazinedione, 3-benzyl-6-isopropyl-	N-containing heterocycle	1.4
1,2-Cyclopentanedione, 3-methyl-	N-containing heterocycle	1.3
Phenol	phenolic	12.0
Heptatriacotanol	phenolic	2.1
Phenol, 4,4'-(1-methylethylidene)bis-	phenolic	1.7
3-Isopropoxy-1,1,1,7,7,7-hexamethyl-	phenolic	1.6