Electronic Supplementary Material (ESI) for Green Chemistry.

Evaluating lignin valorization via pyrolysis and vapor-phase hydrodeoxygenation for production of aromatics and alkenes

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2.1. Lignin samples

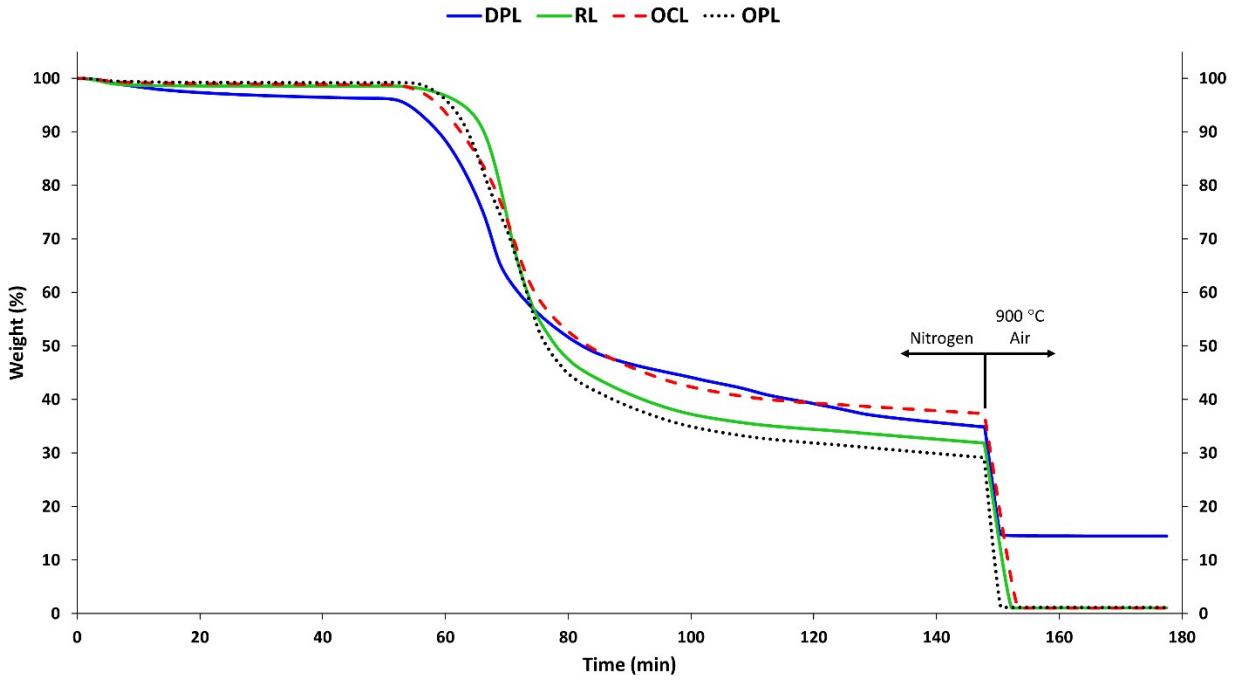

Figure S1. TGA results of DPL, RL, OCL, and OPL

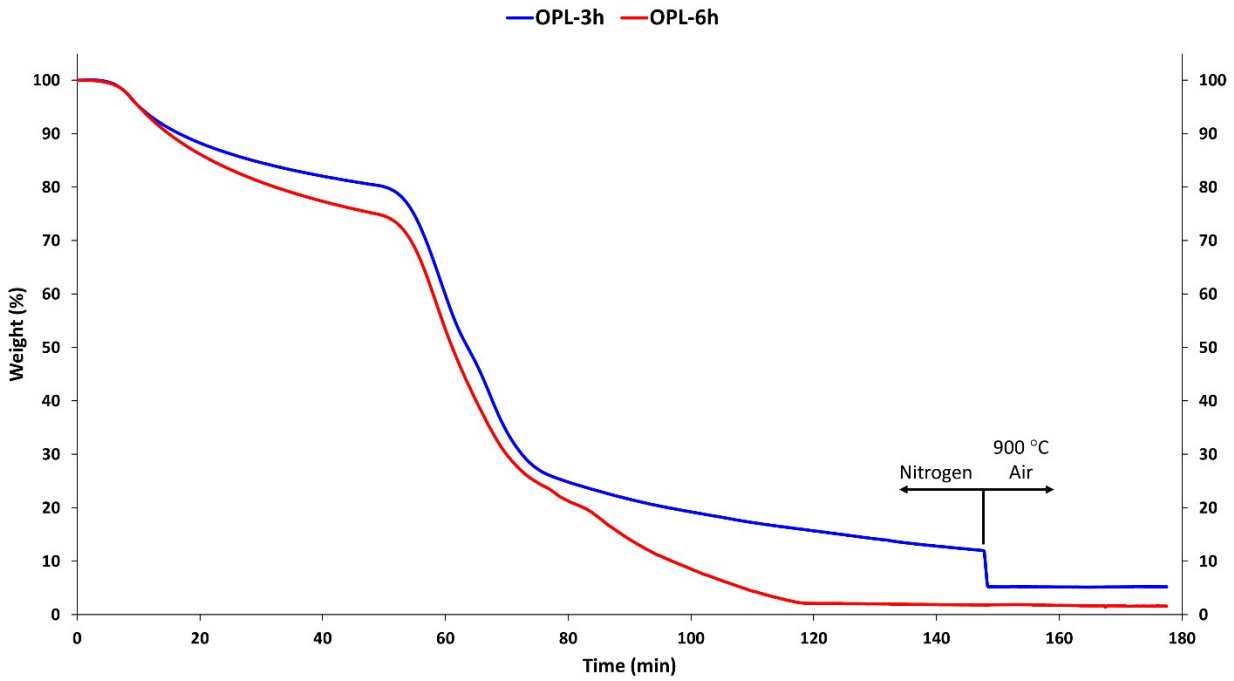

Figure S2. TGA results of OPL-3h and OPL-6h

2.2. Pyrolysis and HDO reactions

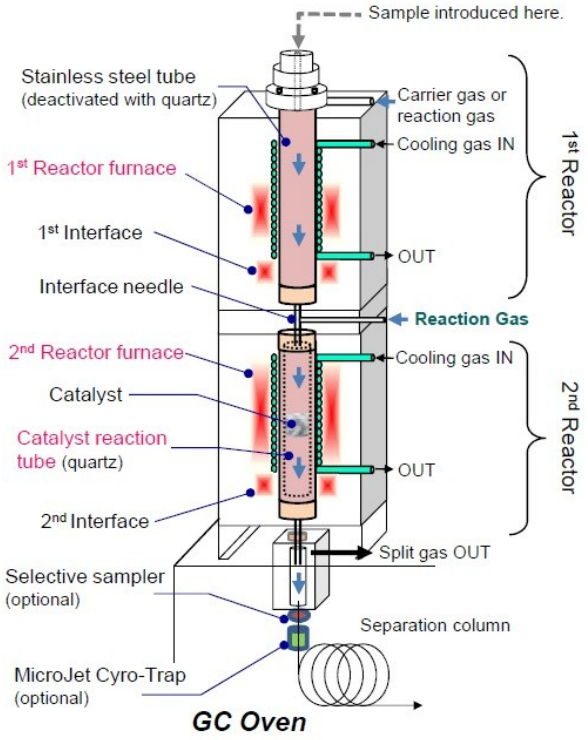

Figure S3. Schematic view of the single-shot tandem micro-pyrolyzer/reactor (RX-3050TR)

2.3. Product identification and quantification

Chemicals were purchased from different vendors (Airgas, Sigma-Aldrich, Alfa Aesar, and Acros Organics) and used as received. The chemicals used are included in Table S1. In addition, ultra-high purity H_2 and He, and ultra-zero Air were purchased from Airgas and used for these experiments.

Table S1. List of calibrated compounds for quantification using TCD and FID

Compound			Category	Detector
5% CO	5% CO_2	2% Methane	CO CO_2 Methane	TCD
2% Ethane 2% Propane	1% iso-Butane 2% n-Butane	2% n-Pentane	Alkanes	TCD
2% Ethylene 2% Propylene	4% 1-Butene 2% *cis*-2-Butene	1% *trans*-2-Butene 1% 1-Pentene	Alkenes	TCD
n-Hexane	Cyclohexane	Methylcyclohexane	Alkanes	TCD/FID
1-Hexene Cyclohexene	2-Methyl-1-pentene	1-Methylcyclopentene	Alkenes	TCD/FID
Benzene Toluene Ethylbenzene o-Xylene	m-Xylene p-Xylene Mesitylene	n-Propylbenzene 1,4-Diethylbenzene Pentamethylbenzene	MAR	FID
Naphthalene 1-Methylnaphthalene	Indane	Indene	DAR	FID
Fluorene	Anthracene		PAH	FID
Acetic acid Propionic acid Methanol Acetone Propanal Hydroxyacetone Furan 2-Methylfuran	2,5-Dimethylfuran Furfural Furfuryl alcohol 5-Hydroxymethylfurfural 2-Butanone 2-Hexanone Cyclopentanone	2-Cyclopenten-1-one 2,3-Butanedione gamma-Valerolactone Methyl formate Methyl pyruvate Methyl lactate Levoglucosan	Non-phenolics	FID
Phenol o-Cresol m-Cresol p-Cresol 4-Ethylphenol 4-Propylphenol 2,5-Dimethylphenol Catechol 4-Vinylphenol 2-Allylphenol 2-secbutylphenol Vanillin Eugenol	Anisole 4-Methylanisole 4-Ethylanisole 3,4-Dimethoxytoluene 1,2,4-Trimethoxybenzene Guaiacol Creosol 4-Ethylguaiacol 4-Vinylguaiacol 4-Propylguaiacol Isoeugenol (cis/trans) 2,3-Dihydrobenzofuran Butylated Hydroxytoluene	Syringol 4-Allylsyringol Syringaldehyde Acetosyringone Acetophenone 3',5'-Dimethoxyacetophenone 4'-Hydroxy-3'-methoxyacetophenone Benzaldehyde 4-Propylbenzaldehyde 4-Hydroxybenzaldehyde 2-Methoxybenzaldehyde 2,6-Dimethoxybenzaldehyde	Phenolics	FID
Pyrrole 2,5-Dimethylpyrrole	Caprolactam	N-hydroxy succinimide	Nitrogen compounds	FID

2.4. Techno-economic analysis

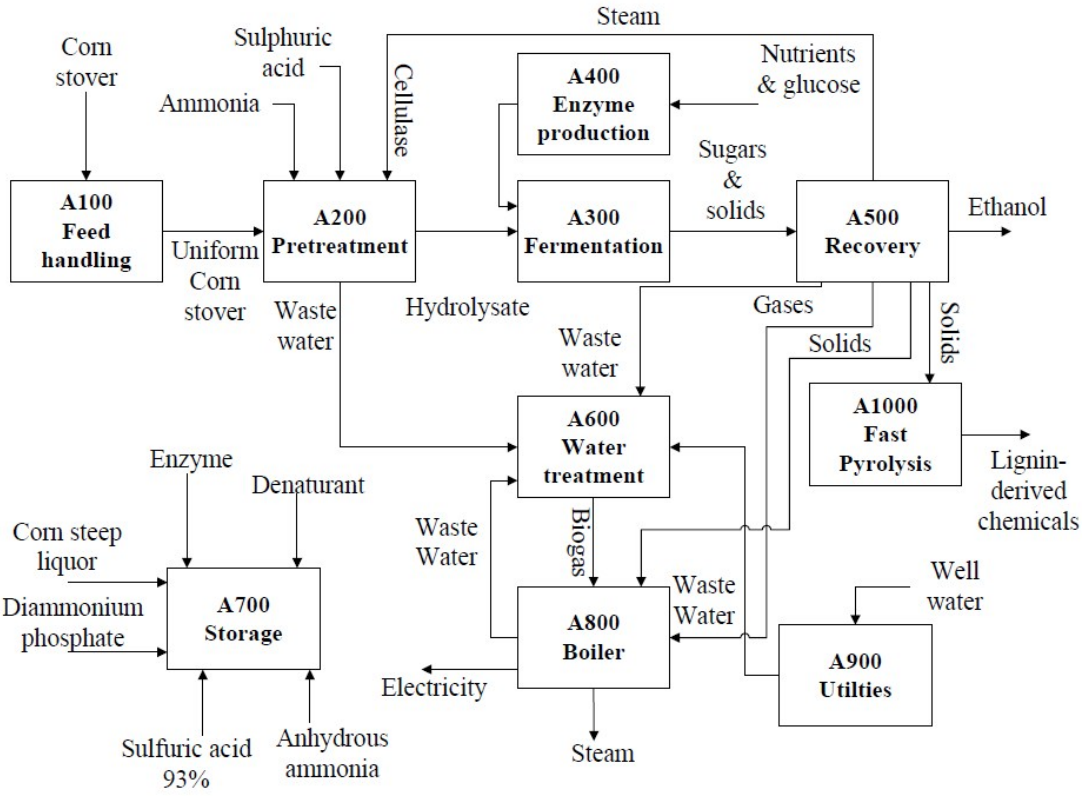

Figure S4. Corn stover fermentation to ethanol and lignin pyrolysis and vapor-phase upgrading to lignin-derived chemicals.

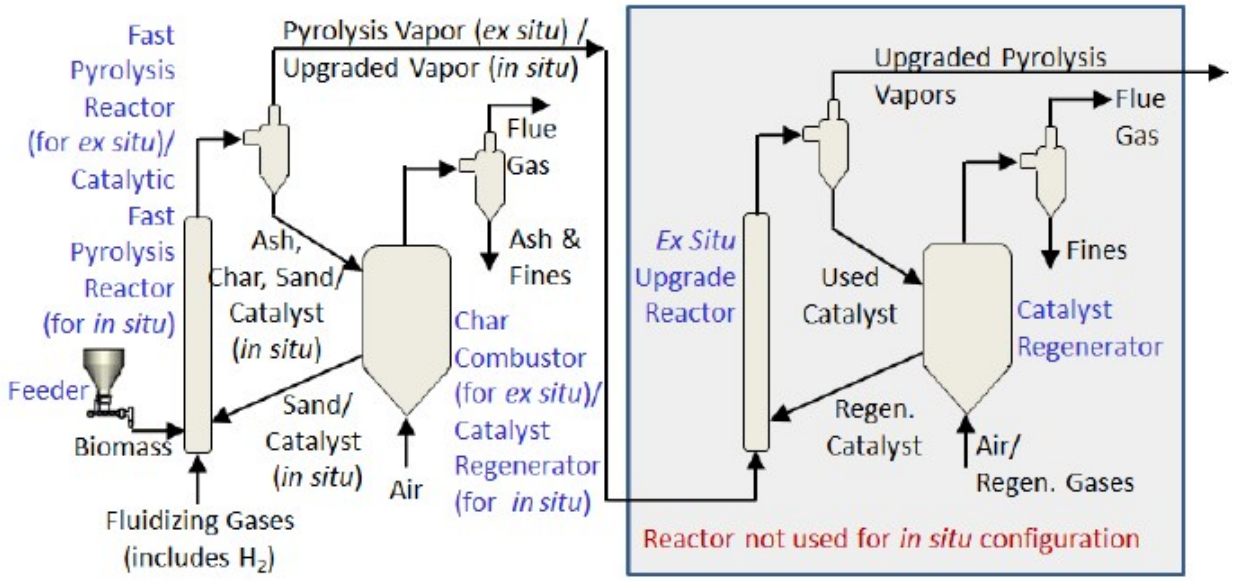

Figure S5. Simplified process model of the lignin pyrolysis and catalytic vapor upgrading (including a catalytic regeneration cycle)[1]

List S1. Other assumptions/limitations on the TEA model

- "n-th" plant economics: The economics reported is based on the assumption that this is a mature technology, whereby several plants of the same technology has been built and is operating commercially. In other words, this is not assumed to be a pioneer plant. Specific financial assumptions were used for n-th plants. These assumptions were described in Table 2 of the manuscript.
- Capital cost is assumed to have a +/- 20% uncertainty to measure the robustness of the calculations, as observed in the sensitivity analysis.
- The configurations of the pretreatment is unknown. Hence, the reduction in cost shown by the calculated minimum fuel selling price shows how much pretreatment should cost to be economically comparable to other established processes
- Performed sensitivity on other major operating parameters to test the variability of the estimated minimum selling price.

3.1. Lignin pyrolysis and HDO

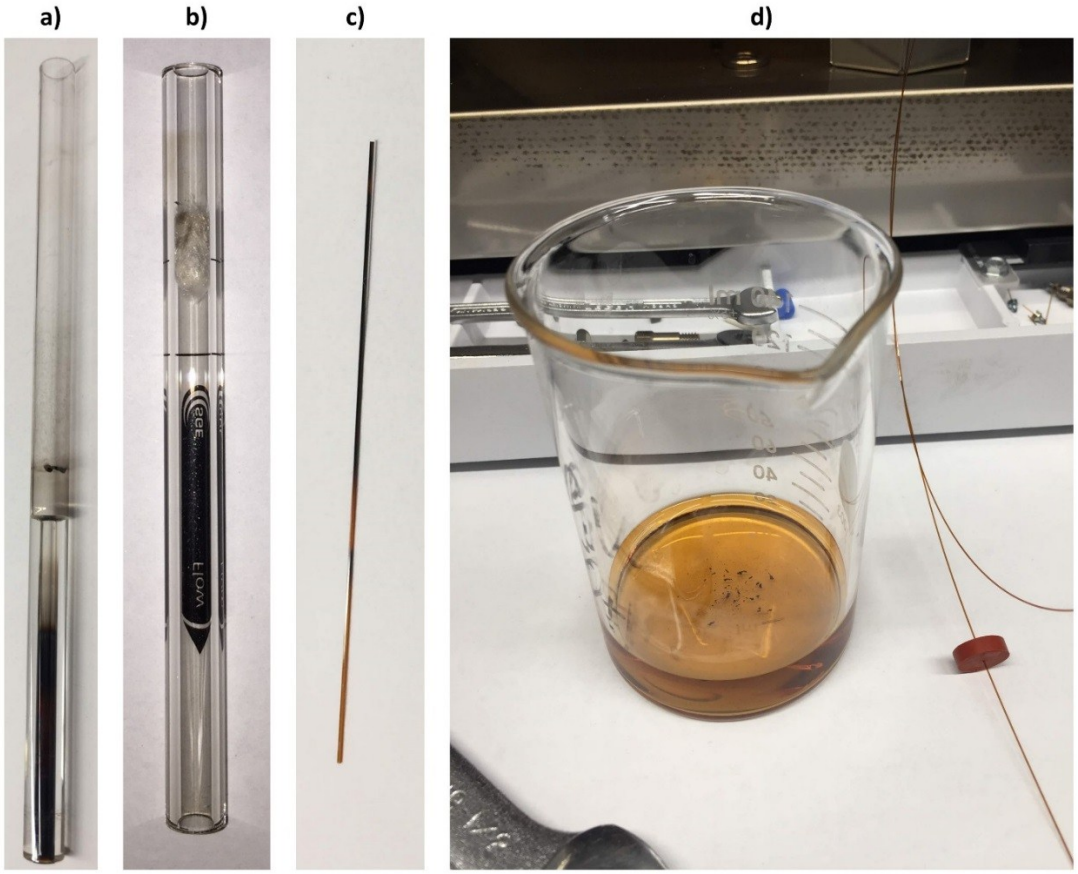

Figure S6. a) Pyrolysis tube after ~60 lignin shots, accumulating to ~30 mg lignin pyrolyzed at 500 °C, b) GC inlet liner after ~60 lignin shots, c) the first 5 cm of the guard column inside the GC, and d) waste produced from cleaning the GC inlet using ethanol/acetone solvents

Table S2. Detailed product yields from pyrolysis and HDO (5 mg MoO_3) of DPL

Peak No.	Compound	Category	Pyrolysis Yield (C%)	HDO Yield (C%)
	CO	$CO/CO_2/CH_4$	1.1973	4.3396
	CO_2		2.0421	2.3943
	Methane		-	3.1806
	Ethane	Alkanes	-	0.8026
	Propane		0.0815	2.4750
	Butanes		0.0236	2.5955
	Pentanes		-	2.0459
	Hexanes		-	1.0919
	Ethylene	Alkenes	0.0202	0.5454
	Propylene		-	1.7638
	Butenes		0.1554	1.1990
	Pentenens		-	0.3065
	Hexenes		-	0.4970
	Sum of Alkenes		*0.176*	*4.312*
1	**Benzene**	MAR	0.1111	**3.9314**
2	**Toluene**		0.1984	**4.5612**
3	**Ethylbenzene**		-	**3.8160**
4	m-Xylene		0.1910	1.1741
5	**o,p-Xylene**		-	**0.5453**
6	Styrene		trace	-
7	(1-methylethyl)-benzene		-	0.0613
8	**n-Propylbenzene**		-	**0.7534**
9	1-Ethyl-2-methylbenzene		-	0.4170
10	1-Ethyl-3-methylbenzene		-	0.2310
11	1,2,4-Trimethylbenzene		-	0.0451
12	1-Ethyl-4-methylbenzene		-	0.1754
13	**Mesitylene**		-	**0.2610**
14	1,2,3-Trimethylbenzene		-	0.0558
15	1,3-Diethylbenzne		-	0.1100
16	Propenylbenzene		-	0.2289
17	1,4-Diethylbenzne		-	0.1038
18	1,2-Diethylbenzne		-	0.0106
19	1-Methyl-4-propylbenzene		-	0.0313
20	1-Ethyl-3,5-dimethylbenzene		-	0.0184
21	1-Ethyl-2,4-dimethylbenzene		-	0.0377
22	1-Phenyl-1-butene		-	0.0299
23	1,2,3,4-Tetramethylbenzene		-	0.0145
24	1-methyl-4-(1-methylpropyl)benzene		-	0.0526
25	2,4-Dimethylstyrene		-	0.0450
26	Indene	DAR	-	0.0195
27	**Naphthalene**		0.0816	**0.0823**
28	1-Methylnaphthalene		0.0262	0.0600
29	2-Methylnaphthalene		0.0475	-
30	Fluorene	PAH	0.0309	-
31	Anthracene		0.0209	-
	Sum of Aromatics		*0.708*	*16.884*
32	Acetonitrile	N-containing	0.2667	-
33	Pyridine		0.0420	-
34	Pyrrole		0.1283	-

35	2-Methylpyrrole		0.0423	-
36	Acetamide		0.0149	-
37	N-Methylsuccinimide		0.2345	-
38	Lactamide		0.0587	-
39	3-(2-furyl)-1-methylpropylamine		0.0929	-
40	Succinimide		0.0641	-
41	Indolizine		0.0839	-
42	5-(ethoxymethyl)-2-Pyrrolidinone		0.0472	-
43	Chloromethane	Non-phenolics	0.2562	-
44	**Methanol**		**0.6342**	-
45	Ethanol		0.0685	-
46	Propanal		0.0960	-
47	Acetone		0.1395	-
48	Methyl acetate		0.0390	-
49	Isobutyraldehyde		0.0234	-
50	2-Methylfuran		0.1209	-
51	**2,3-Butanedione**		**0.2888**	-
52	Isovaleraldehyde		0.0194	-
53	2,5-Dimethylfuran		0.0216	-
54	3-Pentanone		0.0356	-
55	Acetic acid		0.4314	-
56	2,3-Pentanedione		0.0206	-
57	**Hydroxyacetone**		**0.4942**	-
58	Methyl lactate		0.1774	-
59	**Propionic acid**		**0.9668**	-
60	Methyl pyruvate		0.1801	-
61	2-Cyclopentenone		0.0606	-
62	Furfuryl alcohol		0.0245	-
63	Acetol acetate		0.0195	-
64	2-Methyl-2-cyclopentenone		0.0434	-
65	2-Hydroxy-2-cyclopenten-1-one		0.1190	-
66	1-Methyl-1-cyclopenten-3-one		0.0450	-
67	Butyrolactone		0.0997	-
68	2-Hydroxy-3-methyl cyclopenten-1-one		0.0950	-
69	3-Methyl-2(5H)-furanone		0.0489	-
70	Furfural		trace	-
71	4-Methylanisole	Phenolics	0.0557	-
72	**Phenol**		**0.9048**	-
73	**Guaiacol**		**0.6047**	-
74	**o-Cresol**		**0.1744**	-
75	**m,p-Cresol**		**0.2684**	-
76	Creosol		0.1520	-
77	2,5-Dimethylphenol		0.0697	-
78	3,4-Dimethoxytoluene		0.0203	-
79	**4-Ethylphenol**		**0.2963**	-
80	**4-Ethylguaiacol**		**0.1798**	-
81	4-Ethyl-2-methylphenol		0.0188	-
82	**4-Vinylphenol**		**3.1640**	-
83	**4-Vinylguaiacol**		**1.9944**	-
84	Eugenol		0.0238	-
85	4-Propylguaiacol		0.0415	-
86	**Syringol**		**0.5501**	-
87	cis-Isoeugenol		0.0229	-

88	4-Allylphenol		0.0376	-
89	**trans-Isoeugenol**		**0.1714**	-
90	1,2,4-Trimethoxybenzene		0.1025	-
91	5-tert-Butylpyrogallol		0.0439	-
92	4'-hydroxy-3'-methoxyacetophenone		0.0392	-
93	**3',5'-Dimethoxyacetophenone**		**0.2745**	-
94	**4-Allylsyringol**		**0.3990**	-
95	2'-Hydroxyacetophenone		0.0355	-
96	Methyl 4-hydroxyhydrocinnamate		0.0228	-
97	3',5'-Dimethoxy-4'-hydroxyacetophenone		0.0794	-
98	Desaspidinol		0.0387	-
99	4-Ethylanisole		trace	-
100	4-Hydroxy-3-methoxyphenyl acetone		trace	-
	Pyrolytic Char	Char	58.291	58.291
	Total carbon yield		**77.949**	**98.401**

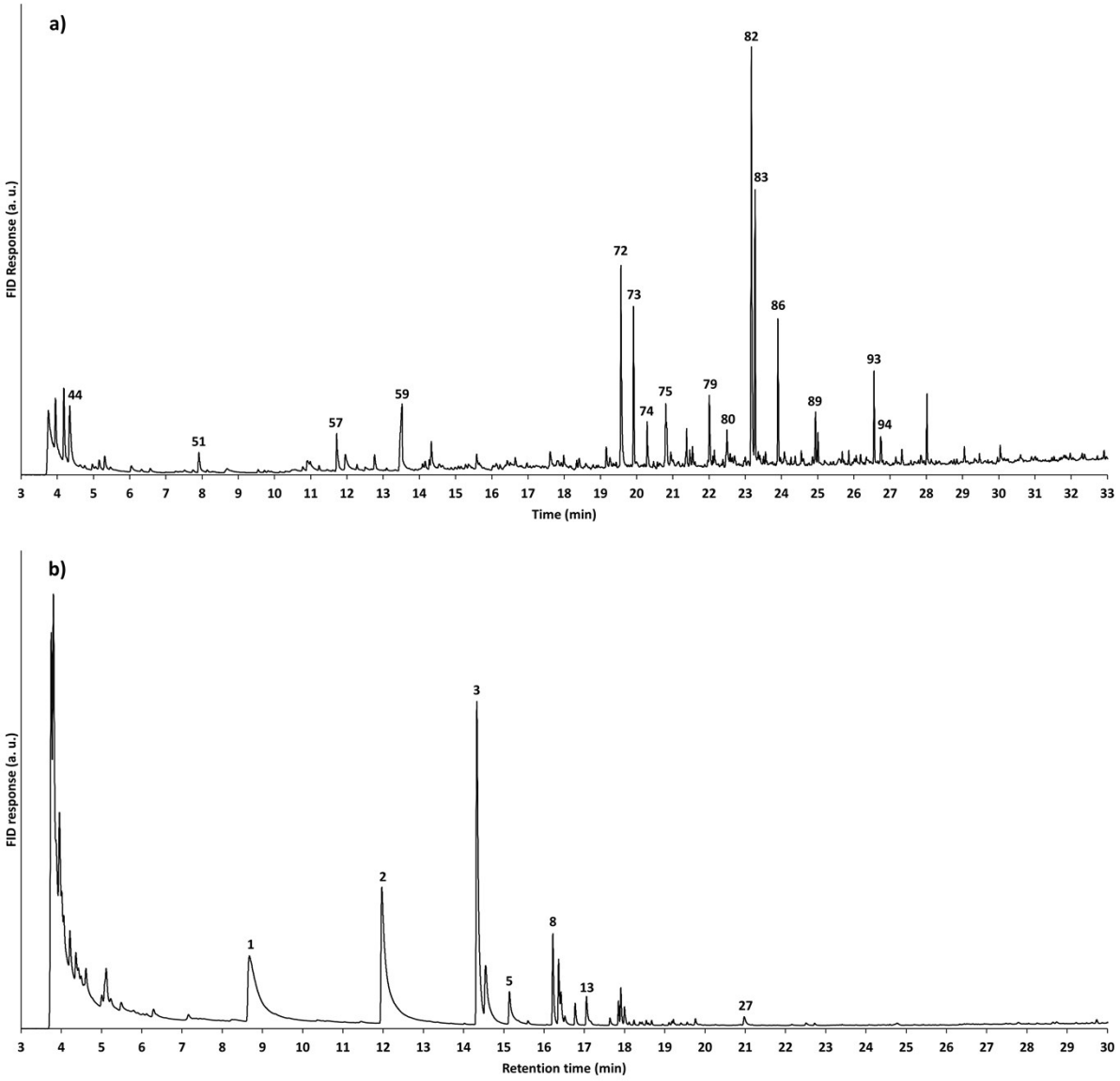

Figure S7. FID chromatograms of a) DPL pyrolysis and b) DPL pyrolysis-HDO

Table S3. Detailed product yields from pyrolysis and HDO (5 mg MoO_3) of RL

Peak No.	Compound	Category	Pyrolysis Yield (C%)	HDO Yield (C%)
	CO	$CO/CO_2/CH_4$	2.5100	5.8368
	CO_2		0.7098	0.9459
	Methane		-	5.9814
	Ethane	Alkanes	-	0.7841
	Propane		0.0423	1.9523
	Butanes		0.0199	1.8185
	Pentanes		-	1.8052
	Hexanes		-	1.4296
	Ethylene	Alkenes	0.0283	0.1821
	Propylene		0.0714	0.5627
	Butenes		0.0787	0.4640
	Pentenes		-	0.1011
	Hexenes		-	0.0699
	Sum of Alkenes		*0.178*	*1.380*
1	**Benzene**	MAR	0.1439	**5.3671**
2	**Toluene**		0.2950	**7.4864**
3	**Ethylbenzene**		-	**1.4374**
4	**m-Xylene**		0.1687	**2.1558**
5	**o,p-Xylene**		-	**0.9850**
6	**n-Propylbenzene**		-	**0.3924**
7	1-Ethyl-2-methylbenzene		-	0.2571
8	1-Ethyl-3-methylbenzene		-	0.1393
9	1,2,4-Trimethylbenzene		-	0.1516
10	1-Ethyl-4-methylbenzene		-	0.0710
11	**Mesitylene**		-	**0.3987**
12	1,2,3-Trimethylbenzene		-	0.0584
13	**2-Propenylbenzene**		0.0104	**0.1114**
14	1-Methyl-3-propylbenzene		-	0.0253
15	1-Methyl-4-propylbenzene		-	0.0042
16	1-Ethyl-3,5-dimethylbenzene		-	0.0047
17	1-Ethyl-2,4-dimethylbenzene		-	0.0057
18	1-Ethyl-2,3-dimethylbenzene		-	0.0074
19	1,2,4,5-Tetramethylbenzene		-	0.0140
20	1,2,3,4-Tetramethylbenzene		-	0.0299
21	4-Methylindan		-	0.0038
22	2,4-Dimethylstyrene		-	0.0120
23	Naphthalene	DAR	0.0797	0.0177
24	1-Methylnaphthalene		0.0349	-
25	2-Methylnaphthalene		0.0333	-
26	Biphenyl		0.0278	-
27	4-Methylbiphenyl		0.0251	-
28	Fluorene	PAH	0.0262	-
29	Anthracene		0.0288	-
	Sum of Aromatics		*0.874*	*19.136*
30	**Methanol**	Non-phenolics	**1.2834**	-
31	2-Propenal		0.1130	-
32	Acetone		0.1453	-
33	Acetic anhydride		0.1444	-
34	2-Methylfuran		0.1225	-

35	Methyl vinyl ketone		0.0195	-
36	2,3-Butanedione		0.1246	-
37	Glycolaldehyde		0.2673	-
38	2,5-Dimethylfuran		0.0342	-
39	3-Pentanone		0.0190	-
40	Acetic acid		0.1994	-
41	2,3-Pentanedione		0.0091	-
42	Hydroxyacetone		0.1964	-
43	Methyl formate		0.0320	-
44	Cyclopentanone		0.0301	-
45	2-Cyclopenten-1-one		0.0573	-
46	Furfural		0.0227	-
47	2-Hydroxy-2-cyclopenten-1-one		0.0884	-
48	5-Methylfurfural		0.0302	-
49	1-Methyl-1-cyclopenten-3-one		0.0242	-
50	Butyrolactone		0.0403	-
51	2-Hydroxy-3-methyl cyclopenten-1-one		0.1042	-
52	**Levoglucosan**		**7.3748**	-
53	4-Methylanisole	Phenolics	0.0280	-
54	**Phenol**		**0.3320**	-
55	**Guaiacol**		**0.4211**	-
56	o-Cresol		0.1228	-
57	m,p-Cresol		0.1569	-
58	5-Methylguaiacol		0.2106	-
59	**Creosol**		**0.6281**	-
60	2,5-Dimethylphenol		0.0876	-
61	3,4-Dimethoxytoluene		0.0088	-
62	4-Ethylphenol		0.1072	-
63	2,5-Dimethoxytoluene		0.0526	-
64	4-Ethylguaiacol		0.1075	-
65	4-Ethyl-2-methylphenol		0.0853	-
66	2-Propylphenol		0.0171	-
67	4-Vinylphenol		0.0368	-
68	**4-Vinylguaiacol**		**0.7804**	-
69	Eugenol		0.0387	-
70	4-Propylguaiacol		0.0232	-
71	**Syringol**		**0.9106**	-
72	cis-Isoeugenol		0.0405	-
73	3-Methoxy-5-methylphenol		0.0699	-
74	2,4-Dimethoxyphenol		0.1118	-
75	trans-Isoeugenol		0.1807	-
76	**1,2,4-Trimethoxybenzene**		**1.0579**	-
77	Vanillin		0.1702	-
78	5-tert-Butylpyrogallol		0.1875	-
79	4'-hydroxy-3'-methoxyacetophenone		0.0529	-
80	**3',5'-Dimethoxyacetophenone**		**0.3122**	-
81	**4-Allylsyringol**		**0.7694**	-
82	**Syringaldehyde**		**0.3564**	-
83	3',5'-Dimethoxy-4'-hydroxyacetophenone		0.1280	-
84	Desaspidinol		0.1652	-
85	m/z = 181, 210		0.0770	-
86	4-Hydroxy-3-methoxyphenyl acetone		trace	-

	Pyrolytic char	Char	55.191	55.191
	Total carbon yield		**77.842**	**96.261**

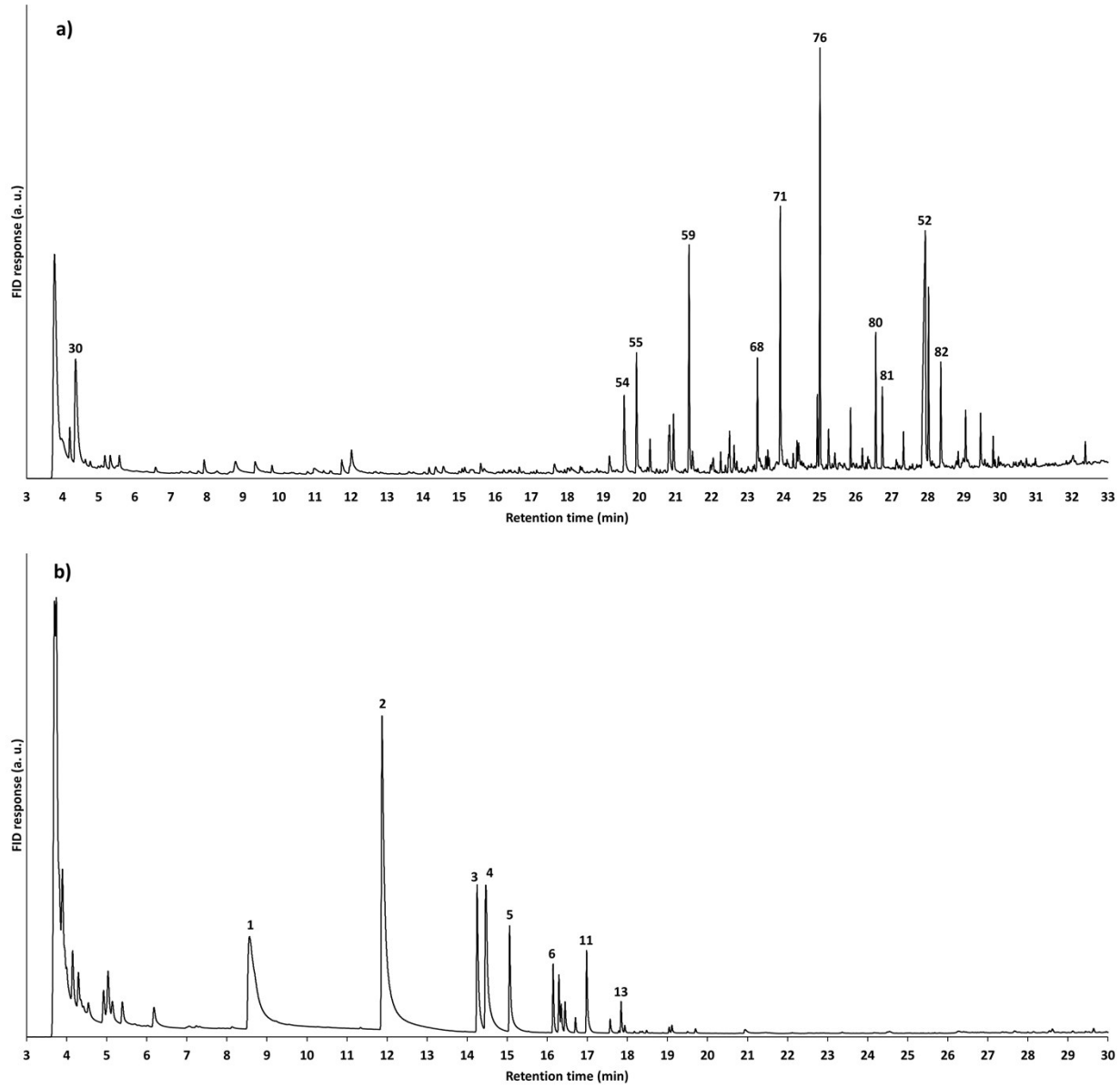

Figure S8. FID chromatograms of a) RL pyrolysis and b) RL pyrolysis-HDO

Table S4. Detailed product yields from pyrolysis and HDO (5 mg MoO_3) of OCL

Peak No.	Compound	Category	Pyrolysis Yield (C%)	HDO Yield (C%)
	CO	CO/CO2/CH4	1.5485	3.9285
	CO2		1.3740	1.4474
	Methane		-	4.8579
	Ethane	Alkanes	-	0.6867
	Propane		0.0462	0.9299
	Butanes		0.0351	1.4462
	Pentanes		-	1.4622
	Hexanes		-	0.9865
	Heptanes		-	0.1318
	Ethylene	Alkenes	0.0294	0.4577
	Propylene		0.1106	0.6364
	Butenes		0.1497	0.6232
	Pentenes		-	0.4191
	Hexenes		-	0.6596
	Sum of Alkenes		*0.290*	*2.796*
1	**Benzene**	MAR	0.0660	**5.0652**
2	**Toluene**		0.2116	**6.0191**
3	**Ethylbenzene**		-	**5.0549**
4	**m-Xylene**		0.1309	**1.4247**
5	**p-Xylene**		-	**0.8268**
6	Styrene		0.0286	-
7	(1-methylethyl)-benzene		-	0.0847
8	**Propylbenzene**		-	**0.8436**
9	1-Ethyl-2-methylbenzene		-	0.5759
10	1-Ethyl-3-methylbenzene		-	0.3091
11	1,2,4-Trimethylbenzene		-	0.0674
12	1-Ethyl-4-methylbenzene		-	0.2291
13	**Mesitylene**		-	**0.3288**
14	1,2,3-Trimethylbenzene		-	0.0797
15	1,3-Diethylbenzne		-	0.1759
16	2-Propenylbenzene		-	0.3765
17	1,4-Diethylbenzne		-	0.2031
18	1,2-Diethylbenzne		-	0.0174
19	1-Methyl-4-propylbenzene		-	0.0501
20	1-Ethyl-3,5-dimethylbenzene		-	0.0254
21	1-Ethyl-2,4-dimethylbenzene		-	0.0637
22	1-Phenyl-1-butene		-	0.0736
23	1,2,3,4-Tetramethylbenzene		-	0.0224
24	1-methyl-4-(1-methylpropyl)benzene		-	0.0757
25	2,4-Dimethylstyrene		-	0.0759
26	Indene	DAR	0.0471	0.0342
27	4-Methylindan		-	0.0258
28	**Naphthalene**		0.0570	**0.2792**
29	1-Methylnaphthalene		0.0201	0.1872
30	2-Methylnaphthalene		0.0153	-
31	Fluorene	PAH	0.0514	-
32	Anthracene		0.0274	-
	Sum of Aromatics		*0.655*	*22.595*
33	N-Methyl-ε-caprolactam	N-containing	0.0784	-

34	**Caprolactam**		**1.0614**	-
35	4-Hydroxy-3,5-dimethoxybenzohydrazide		0.0127	-
36	Chloromethane	Non-phenolics	0.0244	-
37	**Methanol**		**0.9613**	-
38	Acetone		0.1240	-
39	Methyl acetate		0.0960	-
40	2-Methylfuran		0.1892	-
41	2-Butanone		0.0361	-
42	Isovaleraldehyde		0.0191	-
43	2,5-dimethylfuran		0.0158	-
44	**Acetic acid**		**2.2122**	-
45	Cyclopentanone		0.0248	-
46	Furfural		0.0726	-
47	Anisole	Phenolics	0.0339	-
48	4-Methylanisole		0.0578	-
49	**Phenol**		**0.8663**	-
50	**Guaiacol**		**0.5457**	-
51	o-Cresol		0.1443	-
52	**m,p-Cresol**		**0.4696**	-
53	3-Methylguaiacol		0.1488	-
54	**Creosol**		**0.4969**	-
55	2,5-Dimethylphenol		0.0708	-
56	3,4-Dimethoxytoluene		0.0127	-
57	**4-Ethylphenol**		**0.5004**	-
58	5-Methoxy-2,3-dimethylphenol		0.0293	-
59	4-Ethylguaiacol		0.2462	-
60	4-Ethyl-2-methylphenol		0.0254	-
61	**4-Vinylphenol**		**4.9666**	-
62	**4-Vinylguaiacol**		**2.1047**	-
63	Eugenol		0.0255	-
64	**Syringol**		**0.5609**	-
65	4-Isopropenylphenol		0.0750	-
66	cis-Isoeugenol		0.0295	-
67	3-Methoxy-5-methylphenol		0.1038	-
68	4-Allylphenol		0.0388	-
69	trans-Isoeugenol		0.1283	-
70	**1,2,4-Trimethoxybenzene**		**0.4049**	-
71	Vanillin		0.0735	-
72	2,3,5-Trimethylhydroquinone		0.0243	-
73	1-(4-Hydroxybenzylidene)acetone		0.0175	-
74	5-tert-Butylpyrogallol		0.0921	-
75	Methyl vanillate		0.0247	-
76	4'-hydroxy-3'-methoxyacetophenone		0.0293	-
77	4-hydroxybenzaldehyde		0.0475	-
78	3',5'-Dimethoxyacetophenone		0.2101	-
79	**4-Allylsyringol**		**0.4899**	-
80	1,2-Dimethoxy-4-n-propylbenzene		0.0461	-
81	Methyl 4-hydroxyhydrocinnamate		0.0526	-
82	Syringaldehyde		0.0827	-
83	3',5'-Dimethoxy-4'-hydroxyacetophenone		0.1668	-
84	Desaspidinol		0.0975	-
85	Methyl p-coumarate		0.0459	-

	Pyrolytic char	Char	53.112	53.112
	Total carbon yield		**75.576**	**94.380**

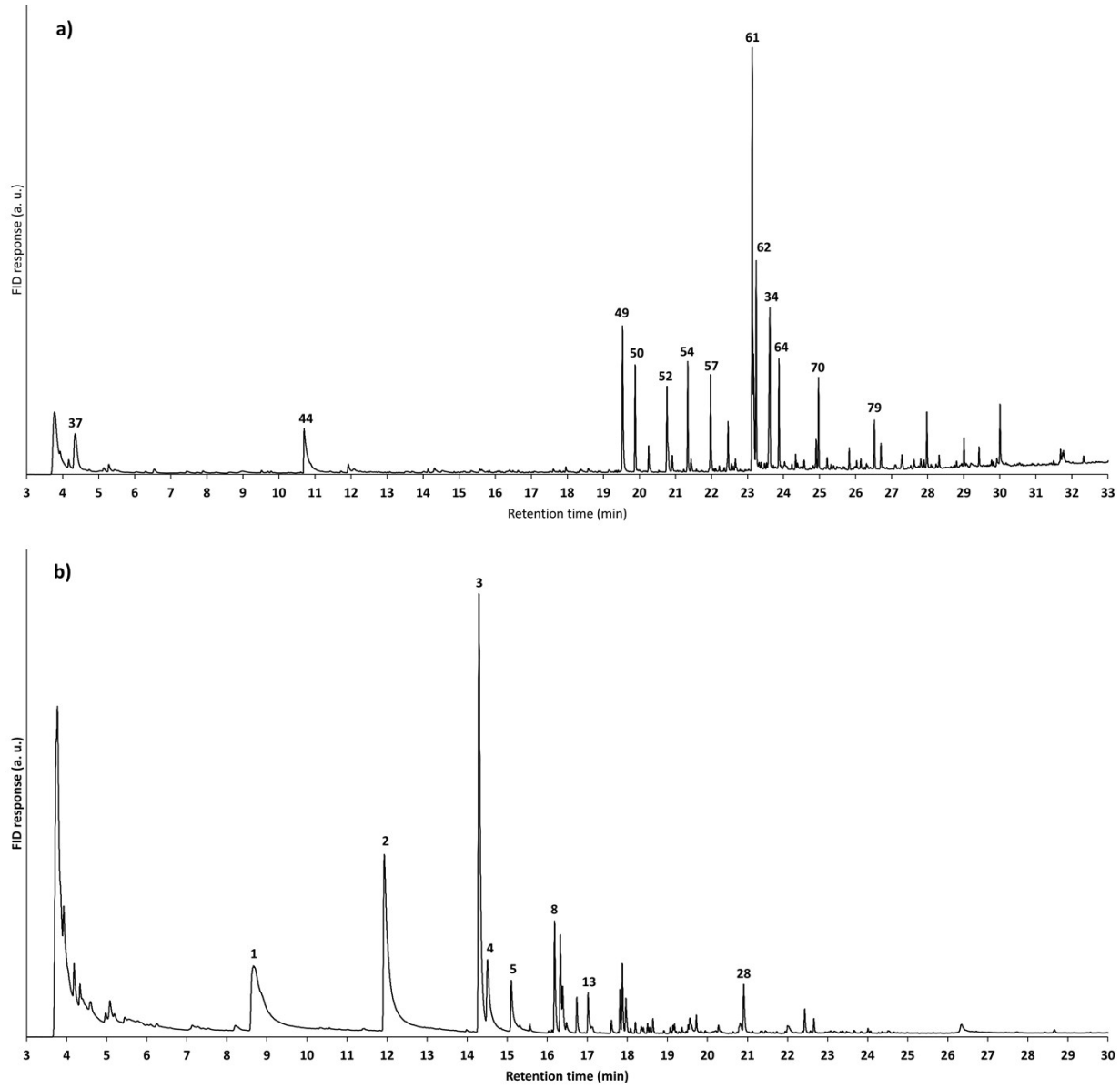

Figure S9. FID chromatograms of a) OCL pyrolysis and b) OCL pyrolysis-HDO

Table S5. Detailed product yields from pyrolysis and HDO (3 mg MoO_3) of OPL

Peak No.	Compound	Category	Pyrolysis Yield (C%)	HDO Yield (C%)
	CO	CO/CO2/CH4	2.6808	4.9838
	CO2		0.5868	0.7181
	Methane		-	8.6831
	Ethane	Alkanes	-	0.1570
	Propane		-	0.7816
	Butanes		-	1.0047
	Pentanes		-	0.5782
	Hexanes		-	0.2398
	Ethylene	Alkenes	0.0161	0.1375
	Propylene		-	0.3305
	Butenes		-	0.2088
	Sum of Alkenes		*0.016*	*0.677*
1	**Benzene**	MAR	0.1498	**8.8830**
2	**Toluene**		0.2350	**9.5975**
3	**Ethylbenzene**		-	**2.5202**
4	**m-Xylene**		0.1185	**2.3190**
5	**p-Xylene**		-	**1.0962**
6	Styrene		0.0092	-
7	(1-methylethyl)-benzene		-	0.0301
8	**Propylbenzene**		-	**1.7855**
9	1-Ethyl-2-methylbenzene		-	0.3952
10	1-Ethyl-3-methylbenzene		-	0.2104
11	1,2,4-Trimethylbenzene		-	0.1386
12	1-Ethyl-4-methylbenzene		-	0.1718
13	**Mesitylene**		-	**0.4626**
14	1,2,3-Trimethylbenzene		-	0.0969
15	**2-Propenylbenzene**			**0.7322**
16	1-Methyl-3-propylbenzene		-	0.1615
17	1-Methyl-4-propylbenzene		-	0.1076
18	1-Ethyl-3,5-dimethylbenzene		-	0.0192
19	1-Ethyl-2,4-dimethylbenzene		-	0.0234
20	2-Butenylbenzene		-	0.0166
21	1-Butenylbenzene		-	0.0422
22	1-Ethyl-2,3-dimethylbenzene		-	0.0096
23	1,2,3,4-Tetramethylbenzene		-	0.0385
24	1,2,4,5-Tetramethylbenzene		-	0.0705
25	1-Methyl-2-(2-propenyl)benzene		-	0.0915
26	2,4-Dimethylstyrene		-	0.1194
27	Indene	DAR	0.0184	0.0324
28	Naphthalene		0.1153	0.1340
29	1-Methylnaphthalene		0.0198	0.0774
30	Fluorene	PAH	0.0142	-
	Sum of Aromatics		*0.680*	*29.383*
31	4-Hydroxy-3,5-dimethoxybenzohydrazide	N-containing	0.0315	-
32	**Methanol**	Non-phenolics	**5.6584**	-
33	2-Propenal		0.0781	-
34	1,4-Dioxane		0.0193	-
35	Acetic acid		0.0976	-
36	Furfural		0.0076	-

37	Anisole	Phenolics	0.0199	-
38	4-Methylanisole		0.0220	-
39	2,3-Dimethylanisole		0.0248	-
40	**Phenol**		**1.9778**	-
41	Guaiacol		0.4362	-
42	o-Cresol		0.2311	-
43	m,p-Cresol		0.1412	-
44	3-Methylguaiacol		0.0990	-
45	**Creosol**		**0.5741**	-
46	2,5-Dimethylphenol		0.0792	-
47	3,4-Dimethoxytoluene		0.0276	-
48	3-Ethylphenol		0.0270	-
49	3,5-Dimethoxytoluene		0.0527	-
50	5-Methoxy-2,3-dimethylphenol		0.0395	-
51	4-Ethylguaiacol		0.1294	-
52	3-Propylphenol		0.0145	-
53	4-Vinylphenol		0.0416	-
54	**4-Vinylguaiacol**		**1.5069**	-
55	Eugenol		0.2598	-
56	4-Propylguaiacol		0.0284	-
57	**Syringol**		**0.7788**	-
58	cis-Isoeugenol		0.1798	-
59	3-Methoxy-5-methylphenol		0.1133	-
60	Butylated Hydroxytoluene		0.1073	-
61	4-Allylphenol		0.0250	-
62	**trans-Isoeugenol**		**0.9825**	-
63	1,2,4-Trimethoxybenzene		0.7199	-
64	**Vanillin**		**0.3421**	-
65	2,3,5-Trimethylhydroquinone		0.0244	-
66	1-(4-Hydroxybenzylidene)acetone		0.1326	-
67	5-tert-Butylpyrogallol		0.0969	-
68	4-Propylguaiacol		0.1746	-
69	Methyl vanillate		0.0234	-
70	4'-hydroxy-3'-methoxy-Acetophenone		0.1362	-
71	**3',5'-Dimethoxyacetophenone**		**0.6133**	-
72	4-Hydroxy-3-methoxyphenyl acetone		0.0336	-
73	**Methylparaben**		**0.6087**	-
74	1,2-Dimethoxy-4-n-propylbenzene		0.0389	-
75	**4-Allylsyringol**		**1.7962**	-
76	**Syringaldehyde**		**0.7231**	-
77	4-((1E)-3-Hydroxy-1-propenyl)-2-methoxyphenol		0.2697	-
78	4-Hydroxybenzoic acid		0.6845	-
79	3',5'-Dimethoxy-4'-hydroxyacetophenone		0.2476	-
80	**4-((1E)-3-Hydroxy-1-propenyl)-2-methoxyphenol**		**0.4383**	-
81	Desaspidinol		0.0972	-
82	**Coniferyl aldehyde**		**0.4569**	-
83	m/z = 181, 210		0.1414	-
84	m/z = 168, 167, 212, 224		0.0959	-
85	m/z = 210, 167		0.1134	-
86	m/z = 210, 167		0.2058	-
87	**Sinapinaldehyde**		**0.4934**	-
	Pyrolytic char	Char	51.876	51.876

Total carbon yield	78.360	99.082

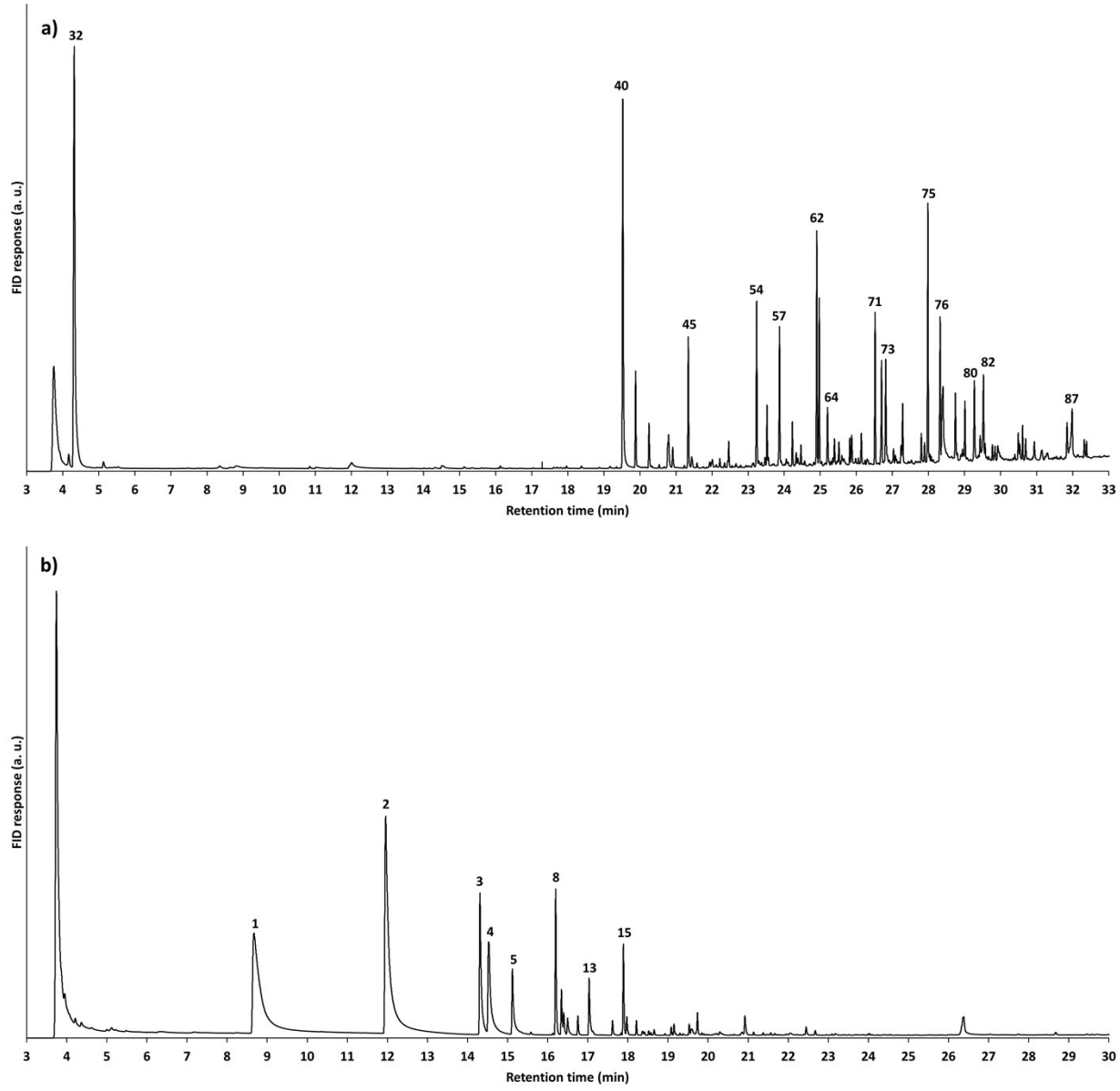

Figure S10. FID chromatograms of a) OPL pyrolysis and b) OPL pyrolysis-HDO

3.2. Pyrolysis and HDO of pretreated lignin

Table S6. Detailed product yields from pyrolysis and HDO (10 mg MoO_3) of OPL-3h

Peak No.	Compound	Category	Pyrolysis Yield (C%)	HDO Yield (C%)
	CO	CO/CO2/CH4	1.0589	2.8356
	CO2		0.2340	0.4542
	Methane		-	9.2107
	Ethane	Alkanes	-	1.0662
	Propane		0.0289	3.0321
	Butanes		0.0092	1.4663
	Pentanes		-	0.8705
	Hexanes		-	0.3776
	Ethylene	Alkenes	0.0380	0.1559
	Propylene		0.0603	0.9058
	Butenes		0.0612	0.3402
	Sum of Alkenes		*0.152*	*1.402*
1	**Benzene**	MAR	-	**10.2819**
2	**Toluene**		0.0300	**15.3170**
3	**Ethylbenzene**		0.0112	**3.9418**
4	**m-Xylene**		0.0154	**5.0654**
5	**p-Xylene**		-	**2.2501**
6	Styrene		0.0129	-
7	**Propylbenzene**		0.0058	**8.4103**
8	1-Ethyl-2-methylbenzene		-	0.8354
9	1-Ethyl-3-methylbenzene		-	0.4249
10	1,2,4-Trimethylbenzene		-	0.4371
11	1-Ethyl-4-methylbenzene		-	0.2872
12	**Mesitylene**		-	**1.2841**
13	1,2,3-Trimethylbenzene		0.0028	0.2217
14	**2-Propenylbenzene**		-	**2.4070**
15	1-Methyl-3-propylbenzene		-	0.5387
16	1-Methyl-4-propylbenzene		-	0.3874
17	1-Ethyl-3,5-dimethylbenzene		-	0.0382
18	1-Ethyl-2,4-dimethylbenzene		-	0.0569
19	2-Butenylbenzene		-	0.0201
20	1-Butenylbenzene		-	0.0497
21	1-Ethyl-2,3-dimethylbenzene		-	0.0150
22	1,2,3,4-Tetramethylbenzene		-	0.1161
23	1,2,4,5-Tetramethylbenzene		-	0.2064
24	1-Methyl-2-(2-propenyl)benzene		-	0.1831
25	**2,4-Dimethylstyrene**		-	**0.3024**
26	Indene	DAR	-	0.0691
27	Naphthalene		-	0.2468
28	1-Methylnaphthalene		0.0064	0.1310
29	5,7-Dimethyltetralin		0.0263	-
	Sum of Aromatics		*0.111*	*53.525*
30	2,2'-Dimethyl-6,6'-dinitro-diphenyl	N-containing	0.0546	-
31	4-Hydroxy-3,5-dimethoxybenzohydrazide		0.1192	-
32	**Methanol**	Non-phenolics	**1.3353**	-
33	Propanal		0.0535	-
34	Methyl acetate		0.0595	-
35	Acetic acid		0.0621	-

36	1,2-Ethanediol		0.0505	-
37	R-(-)-1,2-propanediol		0.0800	-
38	2-Methyllactic acid		0.0236	-
39	2,3-Butanediol		0.0619	-
40	3-Hydroxytetrahydrofuran		0.0097	-
41	2-Methyl-2-cyclopentenone		0.0058	-
42	1,2-Butanediol		0.0324	-
43	4,4,5-Trimethyl-1,3-dioxan-5-OL		0.0171	-
44	4-(methoxymethoxy)-2-methylbutan-2-ol		0.0197	-
45	Anisole	Phenolics	0.0230	-
46	4-Methylanisole		0.0501	-
47	3,5-Dimethylanisole		0.0306	-
48	Methyl benzoate		0.0358	-
49	**Phenol**		**2.1782**	-
50	Guaiacol		0.2318	-
51	o-Cresol		0.3317	-
52	1,2-Cyclohexanediol		0.0645	-
53	2,3-Dimethylphenol		0.0480	-
54	**p-Cresol**		**0.7758**	-
55	3-Methylguaiacol		0.0663	-
56	Methyl 4-methylbenzoate		0.0631	-
57	Creosol		0.5173	-
58	2,5-Dimethylphenol		0.1061	-
59	3,4-Dimethoxytoluene		0.2066	-
60	2,3,5-Trimethylphenol		0.0358	-
61	4-Ethylphenol		0.1474	-
62	Syringol		0.0249	-
63	**4-Ethylguaiacol**		**1.1026**	-
64	3-Ethyl-5-methylphenol		0.0196	-
65	4-Ethyl-1,2-dimethoxybenzene		0.0739	-
66	2,4,5-Trimethylphenol		0.0265	-
67	1,4-Dimethoxy-2,3-dimethylbenzene		0.0104	-
68	4-Propylphenol		0.1067	-
69	4-Vinylguaiacol		0.5219	-
70	1-Sec-butyl-4-methoxybenzene		0.0154	-
71	4-Methoxy-3-(methoxymethyl)phenol		0.0591	-
72	**4-Propylguaiacol**		**4.3387**	-
73	1,2-Dimethoxy-4-n-propylbenzene		0.2436	-
74	**Methyl 4-methoxybenzoate**		**0.8792**	-
75	Formic acid, 2,6-dimethoxyphenyl ester		0.6250	-
76	2-Ethoxy-5-methoxybenzaldehyde		0.0594	-
77	3,4-Dimethoxyphenol		0.0426	-
78	1,2,3-Trimethoxy-5-methylbenzene		0.0732	-
79	Butylated Hydroxytoluene		0.0517	-
80	cis-Isoeugenol		0.1494	-
81	**1,2,4-Trimethoxybenzene**		**0.8664**	-
82	1,2-Dimethoxy-4-(1-propenyl)benzene		0.0902	-
83	Vanillin		0.0572	-
84	Dimethyl terephthalate		0.1872	-
85	m/z = 167, 196, 181, 191		0.2490	-
86	7-Methoxy-4-methylcoumarin		0.0196	-
87	m/z = 181, 210, 195		0.2261	-
88	**5-tert-Butylpyrogallol**		**0.8951**	-

89	Methyl 4-hydroxy-3-methoxybenzoate		0.0928	-
90	2'-Hydroxy-4',6'-dimethoxyacetophenone		0.0630	-
91	4-Allylphenol		0.0190	-
92	m/z = 138, 166, 151		0.0875	-
93	5-Sec-butylpyrogallol		0.1068	-
94	m/z = 137, 196, 180, 164, 149, 91, 77, 122, 45		1.4179	-
95	**m/z = 167, 196, 168, 123**		**7.7630**	-
96	Methylparaben		2.3122	-
97	1,2-Dimethoxy-4-(3-methoxypropyl)benzene		0.0863	-
98	3,4-Dimethoxyphenethyl alcohol		0.0720	-
99	Methyl 4-hydroxy-3-methylbenzoate		0.1660	-
100	3-(p-Hydroxyphenyl)-1-propanol		0.1520	-
101	Ethyl homovanillate		0.3897	-
102	4-Allylsyringol		0.4856	-
103	**Homovanillic acid**		**6.5793**	-
104	2-Ethoxy-6-(methoxymethyl)phenol		0.1413	-
105	(4-hydroxy-3-methoxyphenyl)methyl 2-oxopropanoate		0.0259	-
106	4-Hydroxy-3,5-dimethoxybenzaldehyde		0.1611	-
107	Methyl homovanillate		0.2304	-
108	3-(3,4-Dimethoxyphenyl)-1-propanol		0.2182	-
109	Methyl palmitate		0.3410	-
110	3',5'-Dimethoxy-4'-hydroxyacetophenone		0.1959	-
111	m/z = 168, 226, 167		0.8480	-
112	m/z = 167, 210		0.0893	-
113	3,5-Dimethoxy-4-hydroxyphenylacetic acid		0.1325	-
114	m/z = 167, 226, 178		0.0477	-
115	m/z = 167, 198 + 182, 226, 181, 151		0.5110	-
116	m/z = 181, 210		0.0464	-
117	Methyl 3,5-dimethoxy-4-hydroxybenzoate		0.1432	-
118	m/z = 167, 182, 210, 154		0.0822	-
119	m/z = 167, 240		0.5555	-
120	Methyl stearate		0.3282	-
121	**m/z = 167, 168, 212**		**4.0608**	-
122	m/z = 167, 168, 226		0.0892	-
123	m/z = 167, 242		0.0559	-
	Pyrolytic char	Char	17.488	17.488
	Total carbon yield		**65.098**	**91.728**

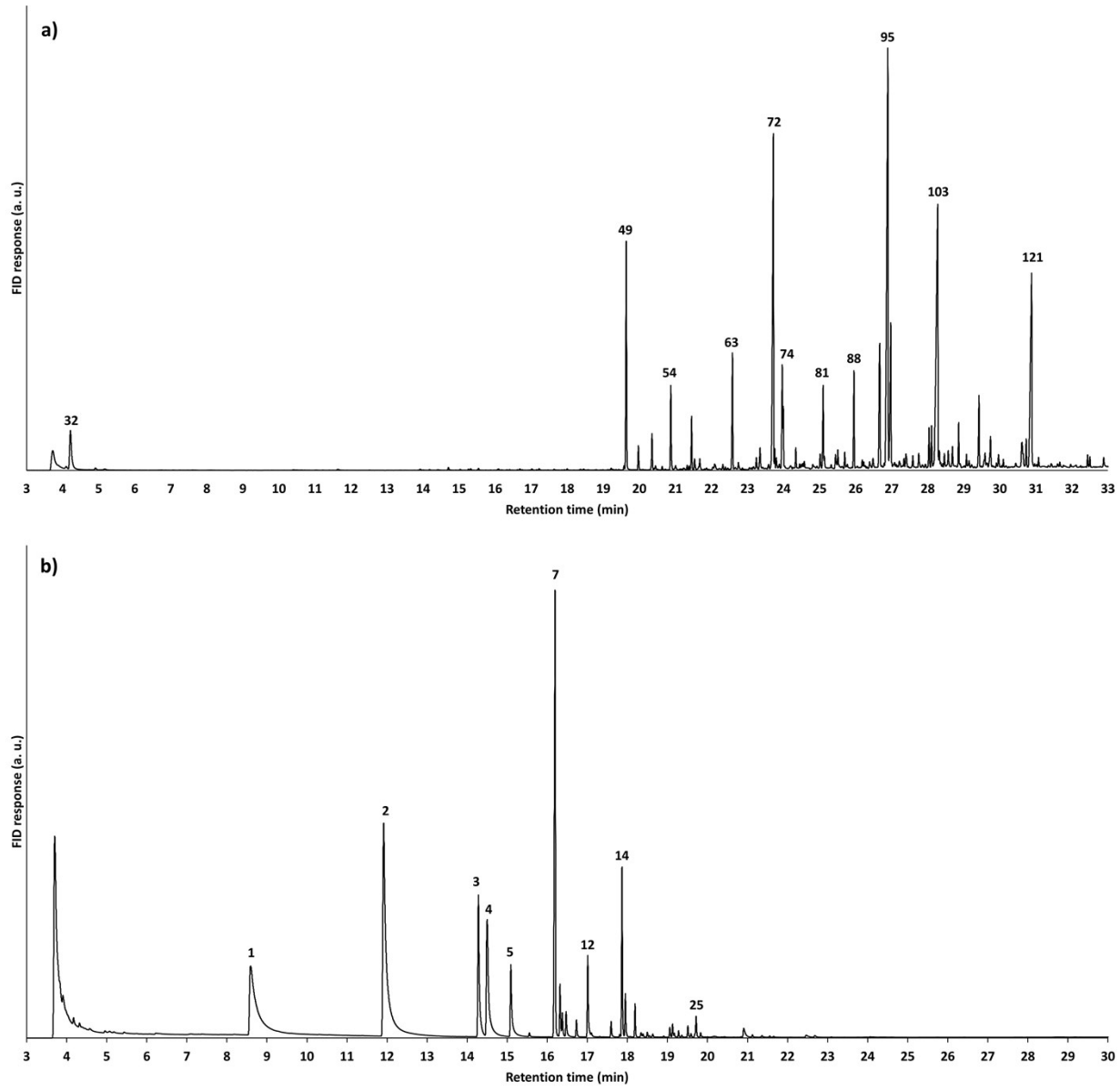

Figure S11. FID chromatograms of a) OPL-3h pyrolysis and b) OPL-3h pyrolysis-HDO

Table S7. Detailed product yields from pyrolysis and HDO (10 mg MoO_3) of OPL-6h

Peak No.	Compound	Category	Pyrolysis Yield (C%)	HDO Yield (C%)
	CO	CO/CO2/CH4	0.7898	2.2961
	CO2		0.3046	0.4168
	Methane		-	9.6513
	Ethane	Alkanes	-	1.5141
	Propane		0.0551	2.7706
	Butanes		0.0158	1.8790
	Pentanes		-	1.0974
	Hexanes		-	0.6133
	Ethylene	Alkenes	0.0469	0.2167
	Propylene		0.1177	0.8984
	Butenes		0.0707	0.5281
	Pentenes		-	0.1330
	Hexenes		-	0.2565
	Sum of Alkenes		*0.235*	*2.033*
1	**Benzene**	MAR	0.0521	**7.5887**
2	**Toluene**		0.0907	**14.0654**
3	**Ethylbenzene**		0.0623	**3.3604**
4	**m-Xylene**		0.0762	**7.3172**
5	**p-Xylene**		-	**2.8696**
6	Styrene		0.0206	-
7	**n-Propylbenzene**		0.0172	**7.0629**
8	1-Ethyl-2-methylbenzene		-	1.2676
9	1-Ethyl-3-methylbenzene		0.0151	0.6282
10	1,2,4-Trimethylbenzene		-	0.7630
11	1-Ethyl-4-methylbenzene		-	0.4268
12	**Mesitylene**		0.0965	**2.4133**
13	1,2,3-Trimethylbenzene		-	0.4438
14	**2-Propenylbenzene**		-	**2.4848**
15	1-Methyl-3-propylbenzene		-	0.7028
16	1-Methyl-4-propylbenzene		-	0.5613
17	1-Ethyl-3,5-dimethylbenzene		-	0.0933
18	1-Ethyl-2,4-dimethylbenzene		-	0.1520
19	2-Butenylbenzene		-	0.0397
20	1-Butenylbenzene		-	0.1043
21	1-Ethyl-2,3-dimethylbenzene		-	0.0433
22	1,2,3,4-Tetramethylbenzene		-	0.2281
23	1,2,4,5-Tetramethylbenzene		-	0.4083
24	1-Methyl-2-(2-propenyl)benzene		-	0.3527
25	**2,4-Dimethylstyrene**		-	**0.5349**
26	Hexamethylbenzene		0.1550	-
27	Indene	DAR	-	0.1522
28	**Naphthalene**		-	**0.5243**
29	**1-Methylnaphthalene**		0.0434	**0.5199**
30	5,7-Dimethyltetralin		0.0684	-
	Sum of Aromatics		*0.697*	*55.109*
31	**Methanol**	Non-phenolics	**0.6966**	-
32	Propanal		0.0440	-
33	Methyl acetate		0.0624	-
34	Methyl propionate		0.0257	-

35	1,2-Ethanediol		0.1603	-
36	1,2-Propanediol		0.0871	-
37	Ethyl 2-hydroxybutyrate		0.0899	-
38	2,3-Butanediol		0.1697	-
39	Cyclopentanemethanol		0.0177	-
40	2-Methyl-2-cyclopentenone		0.0081	-
41	1,2-Butanediol		0.0603	-
42	Dimethyl succinate		0.0297	-
43	trans-(2-Ethylcyclopentyl)methanol		0.0881	-
44	Acetic Acid		trace	-
45	3-Hydroxytetrahydrofuran		trace	-
46	3-Methyl-5-hexen-3-ol		trace	-
47	3-Methylcyclohexanol	Phenolics	0.0168	-
48	Cyclohexanol		0.0472	-
49	2-Methylcyclohexanol		0.0197	-
50	Cyclohexanemethanol		0.0112	-
51	3-Methylanisole		0.0250	-
52	2,4-Dimethylcyclohexanol		0.0198	-
53	4-Methylanisole		0.0265	-
54	2,5-Dimethylcyclohexanol		0.0054	-
55	4-Methylcyclohexanol		0.0614	-
56	3,5-Dimethylanisole		0.0446	-
57	**Methyl Benzoate**		**1.7665**	-
58	cis-p-mentha-1(7),8-dien-2-ol		0.0062	-
59	Phenol		0.2459	-
60	2-Isopropyl-5-methylcyclohexan-1-ol		0.0172	-
61	**Guaiacol**		**0.9212**	-
62	o-Cresol		0.0573	-
63	1,2-Cyclohexanediol		0.1329	-
64	2-Propylcyclohexanol		0.0689	-
65	4-Isopropylcyclohexanol		0.0729	-
66	2,3-Dimethylphenol		0.2707	-
67	2-Cyclohexyl-1-propanol		0.1571	-
68	**p-Cresol**		**1.1205**	-
69	3-Methylguaiacol		0.2759	-
70	1-Methyl-1,2-cyclohexanediol		0.0831	-
71	Levomenthol		0.0829	-
72	5-Methylguaiacol		0.0467	-
73	Methyl 4-methylbenzoate		0.1885	-
74	Creosol		0.3504	-
75	2,5-Dimethylphenol		0.4332	-
76	4-Isopropyl-1-methyl-1,2-cyclohexanediol		0.3682	-
77	1-Methoxy-4-(methoxymethyl)benzene		0.1135	-
78	2,3,5-Trimethylphenol		0.0874	-
79	4,4-Dimethyl-cyclohex-2-en-1-ol		0.1226	-
80	4-Ethylphenol		0.2099	-
81	3,3,5-Trimethylcyclohexanol		0.0872	-
82	1,4-Dimethoxy-2-methylbenzene		0.1236	-
83	Syringol		0.0662	-
84	2,3-Dimethylphenol		0.0816	-
85	**4-Ethylguaiacol**		**0.9830**	-
86	3-Ethyl-5-methylphenol		0.0729	-
87	4-Ethyl-1,2-dimethoxybenzene		0.3227	-

88	2,4,5-Trimethylphenol		0.0775	-
89	1,4-Dimethoxy-2,3-dimethylbenzene		0.0448	-
90	4-Propylphenol		0.3919	-
91	4-Vinylguaiacol		0.2592	-
92	2-Cyclohexyl-3-isopropyl-4-penten-2-ol		0.1128	-
93	**4-Propylguaiacol**		**4.0216**	-
94	1,2-Dimethoxy-4-n-propylbenzene		1.0169	-
95	2-(3-Hydroxy-propyl)-cyclohexanol		0.3884	-
96	**Methyl 4-methoxybenzoate**		**1.0051**	-
97	Formic acid, 2,6-dimethoxyphenyl ester		0.7919	-
98	2-Ethoxy-5-methoxybenzaldehyde		0.1593	-
99	1-Methoxy-4,4a,5,6,7,8-hexahydro-3H-naphthalen-2-one		0.1691	-
100	2,3-Dihydro-1H-inden-5-ol		0.0524	-
101	1,2,3-Trimethoxy-5-methylbenzene		0.0735	-
102	4-Isopropyl-1-methyl-1,2-cyclohexanediol		0.1517	-
103	4-sec-Butylanisole		0.0750	-
104	3',5'-Dimethoxy-4'-hydroxyacetophenone		0.1902	-
105	3-(3,5-dimethoxyphenyl)propanal		0.1869	-
106	4-Methoxy-3-(methoxymethyl)phenol		0.3488	-
107	3-Methoxy-2,5,6-trimethylphenol		0.0428	-
108	**Dimethyl terephthalate**		**0.9509**	-
109	m/z = 167, 196, 181, 191		0.3902	-
110	m/z = 181, 210, 195		0.4329	-
111	5-tert-Butylpyrogallol		0.3400	-
112	m/z = 137, 196, 138, 164		1.1063	-
113	Methyl 3,5-dimethoxyphenylacetate		0.0534	-
114	**m/z = 167, 196, 168**		**2.8457**	-
115	Methylparaben		0.8606	-
116	1,2-Dimethoxy-4-(3-methoxypropyl)benzene		0.1871	-
117	Coniferyl alcohol		0.2369	-
118	p-Hydroxyphenyl-3-propanol		0.2267	-
119	Ethyl homovanillate		0.2696	-
120	4-Allylsyringol		0.7363	-
121	**Homovanillic acid**		**2.3829**	-
122	2-Ethoxy-6-(methoxymethyl)phenol		0.2276	-
123	Methyl homovanillate		0.1463	-
124	3-(3,4-Dimethoxyphenyl)-1-propanol		0.8455	-
125	m/z = 168, 226, 167		0.2471	-
126	m/z = 182, 226, 181, 151		0.3348	-
127	Ethyl diphenylacetate		0.3220	-
128	**3,5-Dimethoxy-4-hydroxyphenylacetic acid**		**0.5395**	-
129	Anisole		trace	-
130	3,5-Dimethylcyclohexanol		trace	-
131	4-sec-Butylphenol		trace	-
132	2-(3-Hydroxy-propyl)-cyclohexanol		trace	-
133	Methyl 4-methoxy-3-methylbenzoate		trace	-
134	Vanillin		trace	-
135	Methyl 3-(3,4-dimethoxyphenyl)propanoate		trace	-
136	(3,4-Dimethoxyphenyl)-methoxymethanol		trace	-
	Pyrolytic char	Char	18.427	18.427
	Total carbon yield		**54.521**	**95.807**

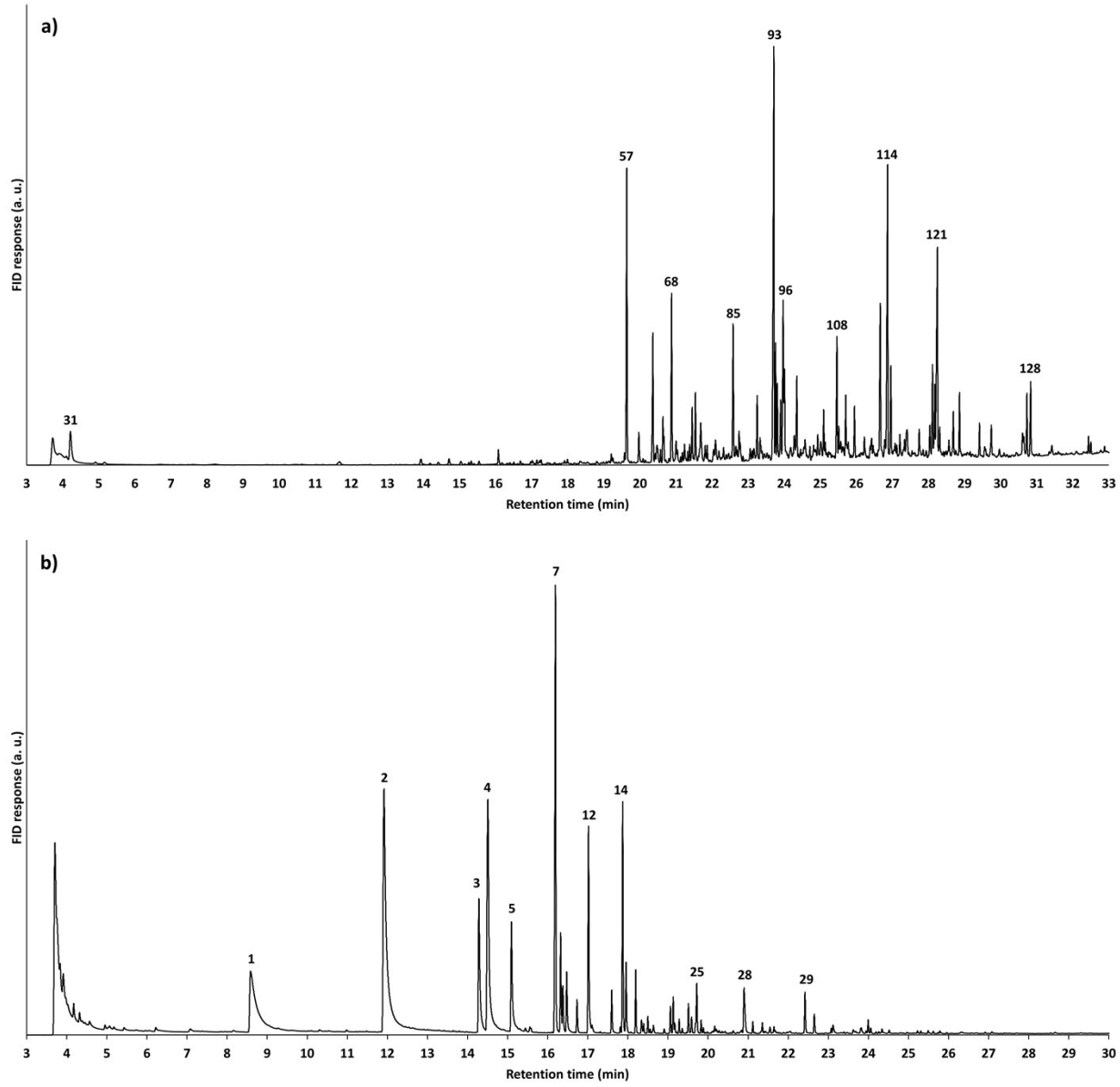

Figure S12. FID chromatograms of a) OPL-6h pyrolysis and b) OPL-6h pyrolysis-HDO

3.3. Techno-economic analysis results

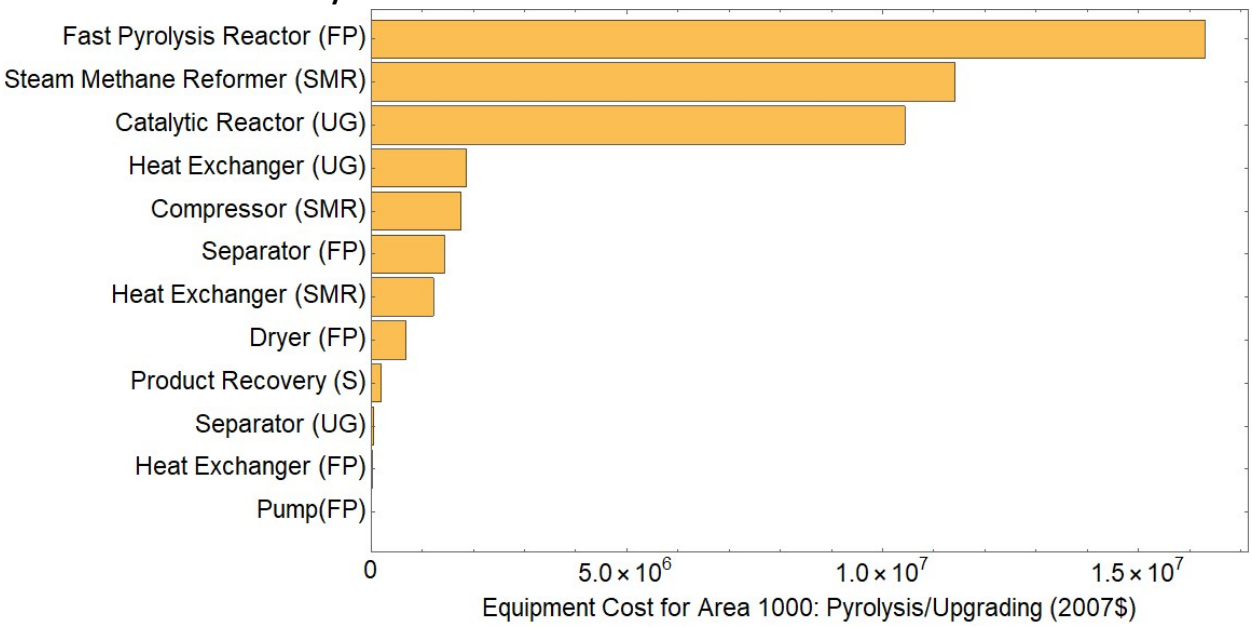

Figure S13. Breakdown of the different equipment cost for Area 1000: Pyrolysis/Upgrading (Equipment used in Fast Pyrolysis, Upgrading, Steam Methane Reforming, and Separation are labeled with FP, UG, SMR, and S, respectively.)

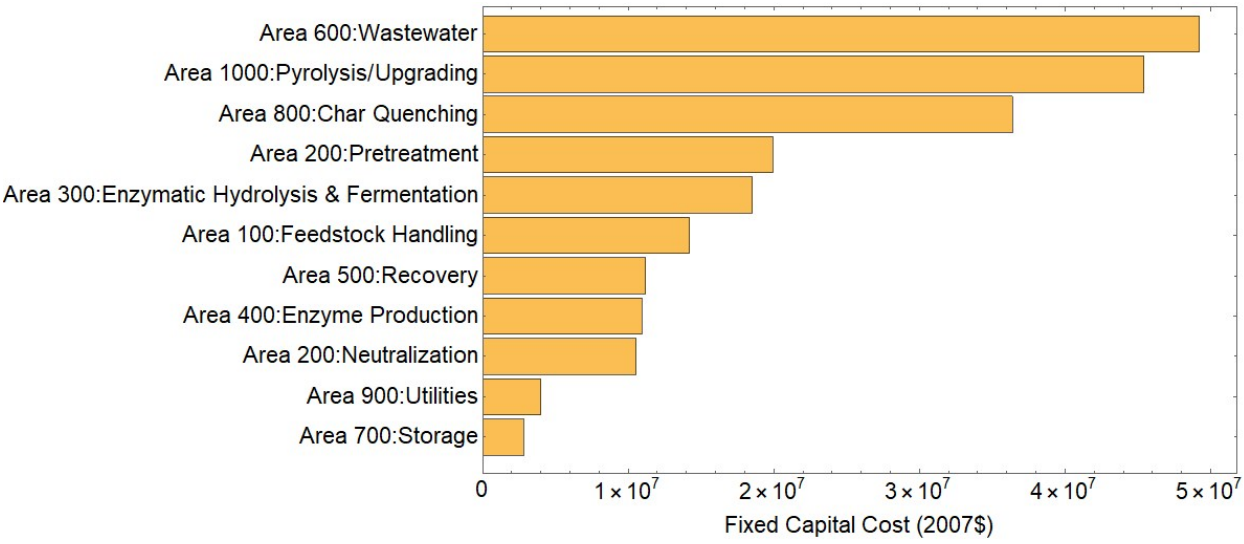

Figure S14. Capital cost breakdown for the 2000 MTPD biorefinery with incorporation of pyrolysis and hydrodeoxygenation.

Table S8. Operating cost contributions to the minimum ethanol-selling price (MESP) in $/gal for all seven scenarios.

Parameters	Power	DPL	RL	OCL	OPL	OPL-3h	OPL-6h
Feedstock	0.74	0.74	0.74	0.74	0.74	0.74	0.74
Sulfuric Acid	0.02	0.02	0.02	0.02	0.02	0.02	0.02
Natural Gas	0.00	0.02	0.02	0.02	0.02	0.01	0.01
Ammonia	0.07	0.07	0.07	0.07	0.07	0.07	0.07
Corn Steep Liquor	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Diammonium Phosphate	0.02	0.02	0.02	0.02	0.02	0.02	0.02
Sorbitol	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Glucose	0.19	0.19	0.19	0.19	0.19	0.19	0.19
Host nutrients	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Sulfur Dioxide	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Caustic (as pure)	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Boiler Chems	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FGD Lime	0.02	0.02	0.02	0.02	0.02	0.02	0.02
Cooling Tower Chems	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Makeup Water	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Disposal of Ash	0.03	0.03	0.03	0.03	0.03	0.03	0.03
CFP Catalyst	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Grid Electricity (kW)	-0.15	-0.12	-0.12	-0.12	-0.11	-0.04	-0.04
Area 100 Electricity	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01
Fixed	0.18	0.19	0.19	0.19	0.19	0.19	0.19
Aromatics + Olefins	0.00	-0.52	-0.59	-0.74	-0.87	-1.77	-1.83
Depreciation	0.33	0.42	0.42	0.42	0.42	0.42	0.42
Income Tax	0.20	0.25	0.25	0.25	0.25	0.25	0.25
Return on Investment	0.48	0.60	0.60	0.60	0.60	0.59	0.59
MESP	**2.20**	**2.02**	**1.93**	**1.79**	**1.67**	**0.82**	**0.75**
Feedstock Contribution to MESP	34%	37%	38%	41%	44%	91%	98%
MESP without Aromatics & Olefins credit	2.20	2.54	2.52	2.53	2.54	2.59	2.58

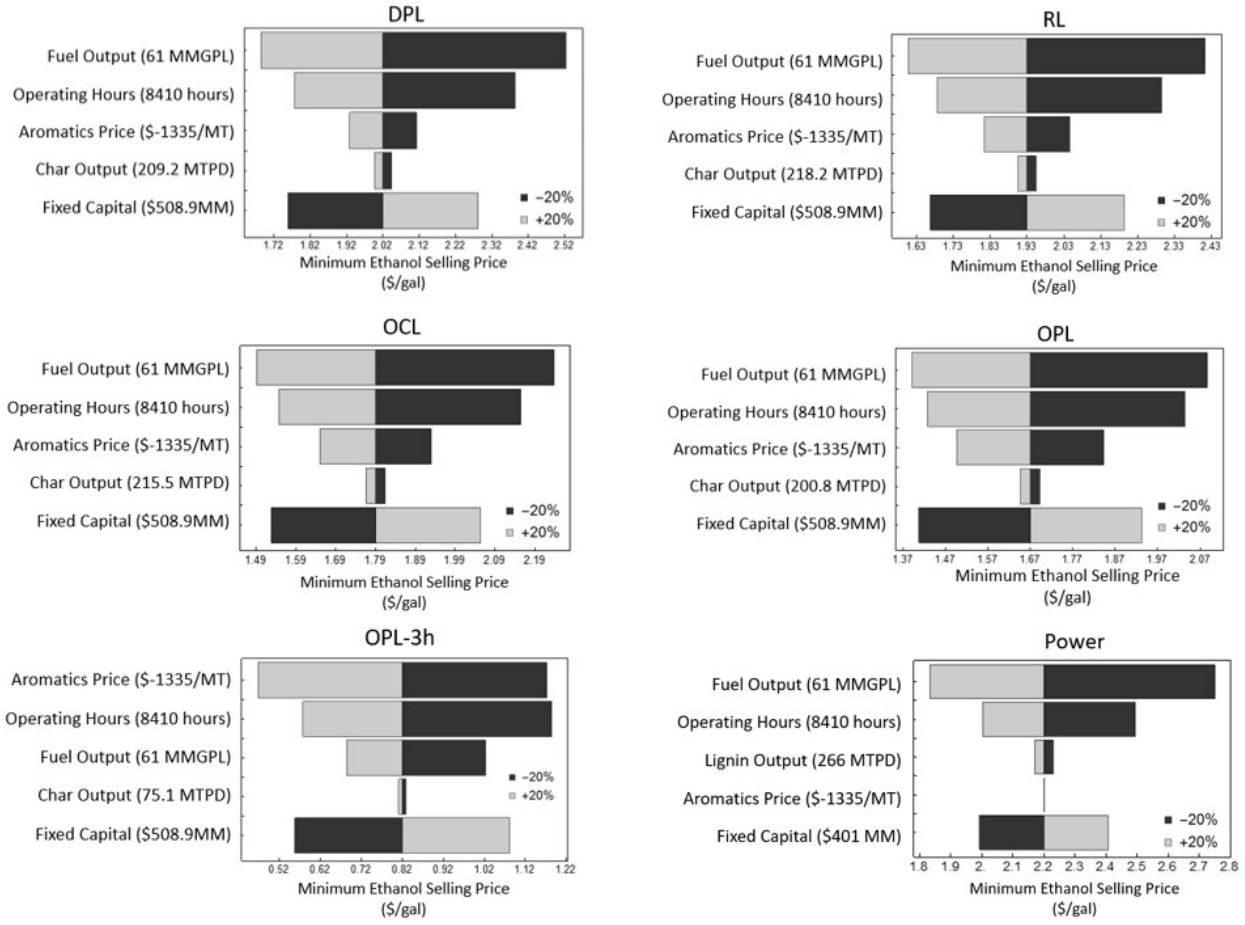

Figure S15. Sensitivity analysis for the Power, DPL, RL, OCL, OPL, and OPL-3h scenarios based on ±20% change in key model parameters.

References

1. A. Dutta, A. H. Sahir, E. Tan, D. Humbird, L. J. Snowden-Swan, P. A. Meyer, J. Ross, D. Sexton, R. Yap and J. Lukas, *Process design and economics for the conversion of lignocellulosic biomass to hydrocarbon fuels: Thermochemical research pathways with in situ and ex situ upgrading of fast pyrolysis vapors*, Pacific Northwest National Laboratory, Richland, WA (US), 2015.