

**Correlation between hydrogen yield and product distribution in algae
conversion through isopropanol/water system**

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Table S1. Elemental analysis and HHV of bio-oil by different isopropanol/water ratio

Ratio of i-PrOH ^a to water	C/wt%	H/wt%	N/wt%	O/wt%	HHV/ MJ·Kg ⁻¹
10: 0	69.15	9.28	7.68	13.89	33.32
9: 1	69.20	9.38	7.41	14.01	33.50
8: 2	67.82	9.30	7.00	15.88	32.70
7: 3	69.12	9.36	6.86	14.66	33.43
6: 4	69.69	8.98	6.87	14.46	33.11
5: 5	68.99	9.01	6.24	15.75	32.81
4: 6	71.12	9.42	5.65	13.81	34.50
3: 7	69.27	9.52	5.48	15.73	33.75
2: 8	68.41	9.77	5.36	16.46	33.72
1: 9	65.75	9.71	6.28	18.25	32.32
0: 10	67.62	9.74	6.72	15.92	33.29

a: isopropanol

Table S2. 30 main compounds in isopropanol bio-oil

Retention time in GC(min)	Area%	Compound
11.10	Cyclopentanol, 2-chloro-, trans-	2.15
15.51	2,5-Pyrrolidinedione, 1-methyl-	4.28
16.00	p-Cresol	6.96
16.43	Phenylethyl Alcohol	1.85

16.61	4-Methylcyclohexylamine	0.99
17.15	2,5-Pyrrolidinedione, 1-ethyl-	1.15
18.97	Phenol, 4-ethyl-	1.59
19.14	Cholestan-22(26)-epoxy-3.beta.-ol acetate	1.25
19.30	.alpha.-Methyl-.alpha.-propylsuccinimide	1.29
19.70	2H-Azepin-2-one, hexahydro-1-methyl-	1.01
20.75	2,5-Pyrrolidinedione, 1-ethyl-	1.11
21.42	Caprolactam	1.40
22.86	Indole	2.52
25.59	2,5-Pyrrolidinedione, 1-butyl-	2.63
25.83	1H-Indole, 3-methyl-	2.11
34.98	Heptadecane	3.09
37.30	2-Tetradecene, (E)-	1.19
38.48	2-Hexadecene, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-	6.93
38.92	4-Fluoroveratrole	1.01
41.48	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-	3.33
42.13	n-Hexadecanoic acid	22.17
43.16	Isopropyl palmitate	3.12
46.05	Octadec-9-enoic acid	5.70
46.44	Octadecanoic acid	1.82
46.73	Hexadecanamide	2.39
47.44	N-Methyldodecanamide	1.95
48.33	Octanamide, N,N-dimethyl-	1.07
51.17	Glutaric acid, 3-methylbutyl propyl ester	1.07
53.24	3,6,9,12-Tetraoxatetradecane-1,14-diylbis(2-methylbutanoate)	1.44

54.61	Octadecanoic acid, DMOX derivative	0.95
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Table S3. 30 main compounds in bio-oil in water system

Retention time in GC(min)	Area%	Compound
3.68	2- Bromopropionic acid, heptyl ester	1.67
15.53	3,4-Methylpropylsuccinimide	5.76
15.91	p-Cresol	4.07
16.03	1-Ethyl-2-pyrrolidinone	3.54
16.61	Phenylethyl Alcohol	3.38
17.16	2,5-Pyrrolidinedione, 1-ethyl-	2.20
18.98	Phenol, 4-ethyl-	2.24
19.24	Nanofin	1.26
20.88	2-Pyrrolidinone, 1-butyl-	1.19
22.00	Nimorazole	1.21
22.90	Indole	1.38
24.48	Piperidine, 1-methyl-	2.89
25.59	Benzoxazole, 2-[2-(4-morpholy)ethyl]thio-	2.33
25.84	1H-Indole, 3-methyl-	2.44
28.60	Benzeneethanol, 4-hydroxy-	1.29
28.80	Benzenamine, N-(1-methyl-2-propynyl)-	1.31
34.97	Heptadecane	3.18
36.18	2-Sec-Butylcyclohexanone	1.14
38.18	1-Pentadecene	1.26
38.46	2-Hexadecene, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-	7.83

41.45	2-Hydroxy-3,5,5-trimethyl-cyclohex-2-enone	1.74
42.05	n-Hexadecanoic acid	17.48
43.15	Isopropyl palmitate	1.75
46.04	Oleic Acid	7.33
46.41	Octadecanoic acid	2.41
46.72	Hexadecanamide	1.06
47.43	N-Methyldodecanamide	1.73
48.32	Octanamide, N,N-dimethyl-	1.72
51.17	Octadecanamide, N-butyl-	1.20
53.24	3-(3,4-Dimethyl-6-Phenylcyclohex-3-enyl)prop-2-enoic acid	1.22

Table S4. Elemental analysis and HHV of bio-oil by different isopropanol/water ratio with formic acid

Ratio of i-PrOH ^a to water	C/wt%	H/wt%	N/wt%	O/wt%	HHV/MJ·Kg ⁻¹
10: 0	72.75	10.00	5.92	11.33	36.21
9: 1	69.28	9.50	7.45	13.77	33.73
8: 2	69.09	9.03	6.27	15.61	32.89
7: 3	68.92	9.01	6.36	15.71	32.77
6: 4	68.11	8.99	8.02	14.88	32.36
5: 5	64.73	9.55	7.56	18.15	31.58
4: 6	67.69	9.22	6.87	16.22	32.51
3: 7	69.51	8.99	6.72	14.78	33.04
2: 8	65.86	9.56	7.59	16.99	32.14

1: 9	67.54	9.87	7.02	15.57	33.45
0: 10	66.21	9.77	7.17	16.85	32.65

a: isopropanol

Table S5. 30 main compounds in bio-oil in isopropanol system with formic acid

Retention time in GC(min)	Area%	Compound
14.16	2-Nonanone	4.94
15.62	p-Cresol	1.72
16.44	3-Heptene, 2,2,3,5,6-pentamethyl-	2.19
17.32	1,7-Dimethyl-4-(1-methylethyl)cyclodecane	3.94
17.49	Cyclohexane, 1,4-dimethyl-2-(2-methylpropyl)-, (1.alpha.,2.beta.,4.alpha.)-	2.22
17.62	1-Undecene, 8-methyl-	1.67
17.90	1,3-Dimethyl-(3,7-dimethyloctyl)cyclohexane	4.60
18.18	Cyclohexane, 1,4-dimethyl-2-(2-methylpropyl)-, (1.alpha.,2.beta.,4.alpha.)-	1.60
20.34	2,5-Pyrrolidinedione, 1-propyl-	1.64
20.74	Decane, 2-methyl-	1.45
21.02	Dodecane, 4,6-dimethyl-	3.51
22.72	Dodecane, 2,6,11-trimethyl-	2.24
24.72	3-Eicosene, (E)-	1.64
25.26	Cyclododecane	2.78
25.44	Trifluoroacetic acid, pentadecyl ester	2.79

25.62	4,4-Dimethyl-cyclohex-2-en-1-ol	2.73
25.93	Disparlure	2.70
26.05	Cyclohexane, (1,2-dimethylbutyl)-	1.94
26.36	Cyclooctane, tetradecyl-	7.84
26.53	4,4,7-Trimethyl-oct-5-enal	2.03
26.82	N-(2-Fluorophenyl)-2-sulfanylacetamide	3.10
27.22	Cyclohexane, 1,4-dimethyl-2-octadecyl-	1.91
30.59	3-Ethyl-3-methylheptane	1.74
31.24	5,6,6-Trimethyl-5-(3-oxobut-1-enyl)-1-oxaspiro[2.5]octan-4-one	1.74
33.30	1,3-Dimethyl-5-n-decylcyclohexane	3.41
34.98	Heptadecane	2.11
37.30	Cyclotetradecane	1.82
38.46	2-Hexadecene, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-	2.68
41.96	n-Hexadecanoic acid	5.71
43.16	i-Propyl 14-methyl-pentadecanoate	2.42

Table S6. 30 main compounds in bio-oil in water system with formic acid

Retention time in GC(min)	Area%	Compound
3.61	1-Heptene	1.03
15.12	o-Acetyl-N,o'-carbonyl-tetrahydro-solasodine	0.81
15.56	.alpha.-Methyl-.alpha.-propylsuccinimide	5.18
16.06	p-Cresol	9.02
16.52	Phenylethyl Alcohol	4.05

17.19	2,5-Pyrrolidinedione, 1-ethyl-	2.87
19.13	Phenol, 4-ethyl-	2.34
19.26	Piperidine, 3-methyl-	1.45
20.89	2-Pyrrolidinone, 1-butyl-	0.95
22.02	Nimorazole	1.54
22.91	Indole	1.54
24.50	2-Pyrrolidinone, 1-butyl-	1.94
25.61	Benzoxazole, 2-[2-(4-morpholyl)ethyl]thio-	2.72
25.85	1H-Indole, 6-methyl-	2.44
28.60	Benzeneethanol, 3-hydroxy-	1.09
28.80	Benzonitrile, 2,4,6-trimethyl-	0.99
34.97	Heptadecane	2.59
36.19	(1-Ethyl-2-pyrrolidinyl)methanol	1.48
36.48	1-Phenethyl-pyrrolidin-2,4-dione	1.52
38.80	2-Hexadecene, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-	8.43
41.02	5,10-Diethoxy-2,3,7,8-tetrahydro-1H,6H-dipyrrolo[1,2-a:1',2'-d]pyrazine	0.88
41.46	((5R,8R,8S)-5-Propyloctahydroindolizin-8-yl)methanol	2.30
42.10	n-Hexadecanoic acid	18.93
42.44	Butalbital	1.16
43.14	i-Propyl 14-methyl-pentadecanoate	0.82
46.04	9-Octadecenoic acid, (E)-	6.11
46.44	Octadecanoic acid	3.10
46.74	Hexadecanamide	1.18
47.44	N-Methyldodecanamide	1.44
48.32	Undecanone, 2-methyl oxime	1.33
