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

1 Supplementary material

1.1 Hydrothermal conversion of blackcurrant pomace

1.1.1 Identification of reaction products in the aqueous phase

Table S10: Summary of GC-MS identifications for the composition of the aqueous phase produced by hydrothermal conversion of blackcurrant pomace (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
31.4	3-Pyridinol	C_3H_6O	12.0
28.5	Nitrogenous heterocycle	C_5H_5NO	7.2
4.8	Acetone		6.4
26.3	Phenol	C_6H_6O	5.5
20.7	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	5.3
23.8	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	3.9
29.1	Hetrocycle azote		3.7
31.9	3-Pyridinol, 6-methyl-	C_6H_7NO	2.7
4.2	Methyl Alcohol	CH_4O	2.3
35.9	Hydroquinone	$C_6H_6O_2$	2.2
25.4	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	2.1
15.8	Cyclopentanone	C_5H_8O	2.0
15.2	Propanoic acid	$C_3H_6O_2$	2.0
24.0	Butyrolactone	$C_4H_6O_2$	1.9
36.7	1,4-Benzenediol, 2-methyl-	$C_7H_8O_2$	1.7
19.2	2-Propenoic acid, 2-methyl-	$C_4H_6O_2$	1.7
17.5	Propanoic acid, 2-methyl-	$C_4H_8O_2$	1.5
26.8	Phenol, 2-methoxy-	$C_7H_8O_2$	1.3
19.5	Pyrazine, 2,5-dimethyl-	$C_6H_8N_2$	1.3
16.1	Pyrazine, methyl-	$C_5H_6N_2$	1.2
20.8	Butanoic acid, 2-methyl-	$C_5H_{10}O_2$	1.2
32.2	Dipropylamine, N-(3-butenyl)-	$C_{10}H_{21}N$	1.1
20.6	Butanoic acid, 3-methyl-	$C_5H_{10}O_2$	1.1
17.6	Cyclopentanone, 2-methyl-	$C_6H_{10}O$	0.9
34.1	2-Cyclohexen-1-one, 6-methyl-3(1-methylethyl)-	$C_{10}H_{16}O$	0.9
28.8	2-Pyrrolidinone	C_4H_7NO	0.9
23.6	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	0.8
24.2	2-Cyclopenten-1-one, 3,4-dimethyl-	$C_7H_{10}O$	0.8
12.9	Pyridine	C_5H_5N	0.8
34.4	Oxalic acid, monomorpholide, hexyl ester	$C_{12}H_{21}NO_4$	0.7
18.8	Butanoic acid	$C_4H_8O_2$	0.7
4.1	Methanethiol	CH_4S	0.7
21.2	Ethanone, 1-(2-furanyl)-	$C_6H_6O_2$	0.7

29.4	2,5-Pyrrolidinedione, 1-ethyl-	$C_6H_9NO_2$	0.7
31.1	1,3,5-Triazin-2(1H)-one, 4-amino-6-(ethylamino)-	$C_5H_9N_5O$	0.7
29.0	Phosphonic acid, methyl-, bis(trimethylsilyl) ester	$C_7H_{21}O_3PSi_2$	0.7
18.6	2-Cyclopenten-1-one	C_5H_6O	0.6
27.2	Ethanone, 1-(2-methyl-1-cyclopenten-1-yl)-	$C_8H_{12}O$	0.6
28.7	2,5-Pyrrolidinedione, 1-methyl-	$C_5H_7NO_2$	0.6
30.6	3,4-Methylpropylsuccinimide	$C_8H_{13}NO_2$	0.6
18.2	Cyclopentanone, 3-methyl-	$C_6H_{10}O$	0.6
50.6	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-	$C_{11}H_{18}N_2O_2$	0.6
31.2	1,2,4-Triazine-3,5(2H,4H)-dione	$C_3H_3N_3O_2$	0.6
50.4	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-	$C_{11}H_{18}N_2O_2$	0.6
27.0	2-Cyclopenten-1-one, 3-ethyl-	$C_7H_{10}O$	0.6
46.3	3,6-Diisopropylpiperazin-2,5-dione	$C_{10}H_{18}N_2O_2$	0.5
34.3	2,5-Pyrrolidinedione, 3-ethyl-1,3-dimethyl-	$C_8H_{13}NO_2$	0.5
23.8	Pentanoic acid, 3-methyl-	$C_6H_{12}O_2$	0.5
30.4	2-Acetonylcyclopentanone	$C_8H_{12}O_2$	0.5
34.7	N-[2-Hydroxyethyl]succinimide	$C_6H_9NO_3$	0.5

1.1.2 Identification of reaction products in the bio-oils

Table S11: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of blackcurrant pomace (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
50.9	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}0_2$	27.2
44.8	n-Hexadecanoic acid	$C_{16}H_{32}0_2$	4.6
60.1	9-Octadecenamide, 12-hydroxy-, [R-(Z)]-	$C_{18}H_{35}NO_2$	4.2
59.8	9-Octadecenamide, (Z)-	$C_{18}H_{35}NO$	3.1
26.3	Phenol	C_6H_6O	2.9
53.5	Hexadecanamide	$C_{16}H_{33}NO$	1.9
62.5	1-Heptatriacotanol	$C_{37}H_{76}O$	1.6
30.5	Phenol, 4-ethyl-	$C_8H_{10}O$	1.6
20.7	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	1.3
28.4	Phenol, 4-methyl-	C_7H_8O	1.2
31.4	3-Pyridinol	C_5H_5NO	1.1
29.0	Phosphonic acid, methyl-, bis(trimethylsilyl) ester	$C_7H_{21}O_3PSi_2$	1.1
31.3	Phenol, 4-ethyl-2-methoxy-	$C_9H_{12}O_2$	1.1
26.8	Phenol, 2-methoxy-	$C_7H_8O_2$	1.0
25.4	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	1.0
63.8	1-Heptatriacotanol	$C_{37}H_{76}O$	0.9
34.3	Acetamide, 2,2,2-trifluoro-N-pentyl-	$C_7H_{12}F_3NO$	0.9
28.5	2-Amino-5,6-dihydro-4,4,6-trimethyl-4H-1,3-oxazine	$C_7H_{14}N_2O$	0.9
34.4	Cyclo-(glycyl-l-leucyl)	$C_8H_{14}N_2O_2$	0.9
46.0	9,12-Octadecadienoic acid, methyl ester	$C_{19}H_{34}O_2$	0.9
45.8	9-Octadecenoic acid (Z)-, methyl ester	$C_{19}H_{36}O_2$	0.9

42.6	Pyrimidine-2,4,6(1H,3H,5H)-trione, 1-(2-phenylethyl)-	$C_{20}H_{20}N_2O_3$	0.8
23.8	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	0.8
50.2	2,5-Piperazinedione, 3,6-bis(2-methylpropyl)-	$C_{12}H_{22}N_2O_2$	0.8
47.7	3,6-Diisopropylpiperazin-2,5-dione	$C_{10}H_{18}N_2O_2$	0.7
29.1	2-Pyrrolidinone, 1-[4-(1-pyrrolidinyl)-2-butynyl]-	$C_{12}H_{18}N_2O$	0.7
11.6	Toluene	C_7H_8	0.6
29.6	Phenol, 2,3-dimethyl-	$C_8H_{10}O$	0.6
32.2	Phenol, 2,4,6-trimethyl-	$C_9H_{12}O$	0.6
28.0	2-Ethylidenecyclohexanone	$C_8H_{12}O$	0.6
28.8	1H-Pyrrole, 2-ethyl-3,4,5-trimethyl-	$C_9H_{15}N$	0.6
33.2	Phenol, 2-methoxy-4-propyl-	$C_{10}H_{14}O_2$	0.6
41.8	Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	0.5
23.6	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	0.5
37.7	1H-Indole, 2,3-dimethyl-	$C_{10}H_{11}N$	0.5
60.4	C18 Amide C_{18}	-	0.5
27.0	1H-Pyrrole, 3-ethyl-2,4-dimethyl-	$C_8H_{13}N$	0.5
24.2	2-Cyclopenten-1-one, 3,4-dimethyl-	$C_7H_{10}O$	0.5
47.5	Nà-Acetyl-l-arginine	$C_8H_{16}N_4O_3$	0.5
30.4	1H-Pyrrole, 2-ethyl-3,4,5-trimethyl-	$C_9H_{15}N$	0.5
67.7	Cyclo-(l-leucyl-l-phenylalanyl)	$C_{15}H_{20}N_2O_2$	0.5
33.9	Indole	C_8H_7N	0.5
37.2	Ethaneperoxoic acid, 1-cyano-1-(2-methylphenyl)ethyl ester	$C_{12}H_{13}NO_3$	0.5
16.2	Ethylbenzene	C_8H_{10}	0.5
4.8	Acetone	C_3H_6O	0.4
39.3	Benzene, (1-methyldecyl)-	$C_{17}H_{28}$	0.4
53.6	Dodecanal, O-methyloxime	$C_{13}H_{27}NO$	0.4
15.8	Cyclopentanone	C_5H_8O	0.4
32.7	1-Tridecanol	$C_{13}H_{28}O$	0.4
40.3	1,2-Dihydro-3-(2-hydroxyethyl)-2-oxoquinoline	$C_{11}H_{11}NO_2$	0.4

1.2 Hydrothermal conversion of glucose and xylose

1.2.1 GC-MS Chromatograms

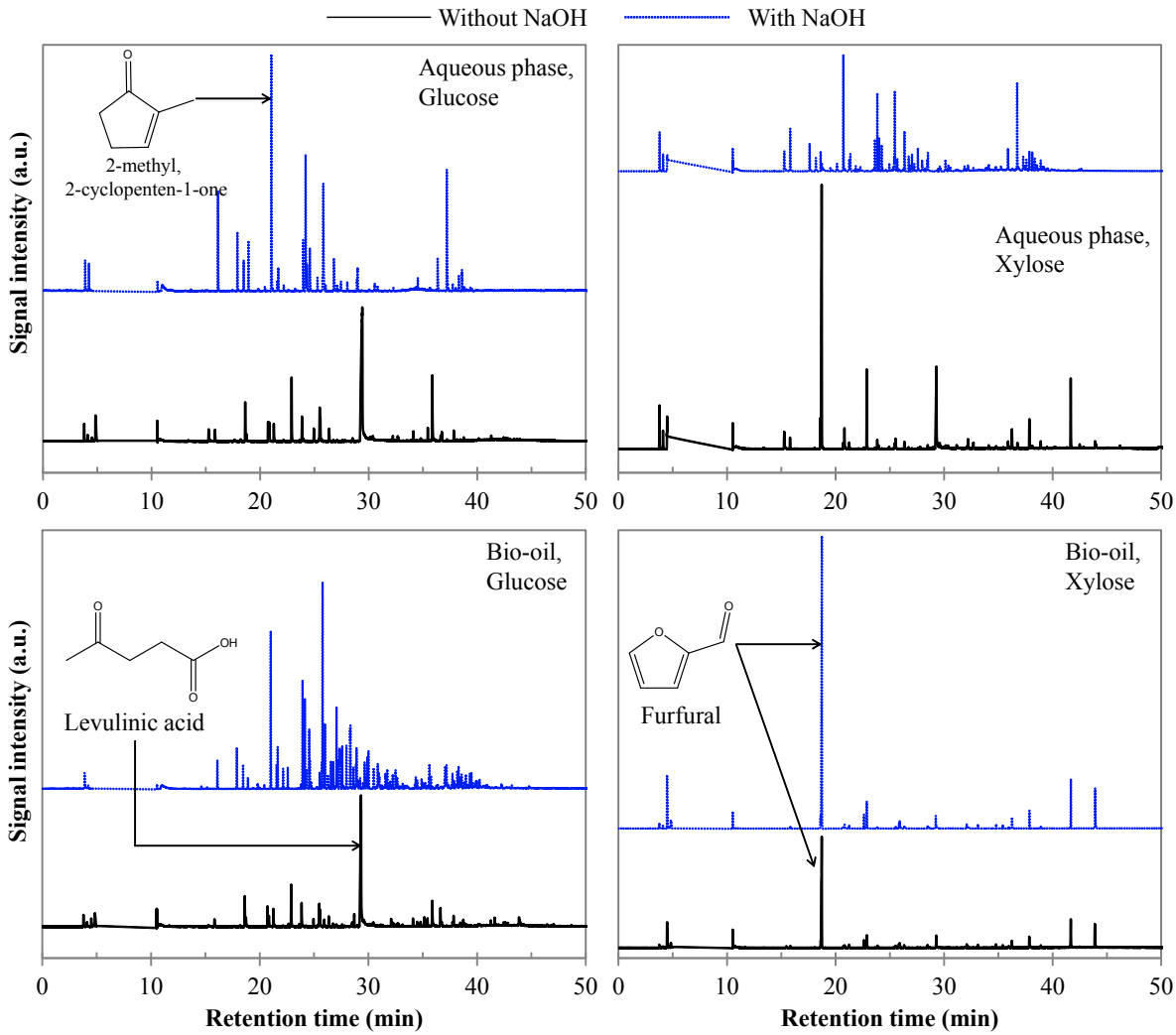


Figure S31: Chromatograms of GC-MS analysis of the aqueous phases and bio-oils from hydrothermal conversion of glucose and xylose (300 °C, 60 min)

1.2.2 Identification of the reaction products in aqueous phases

Table S12: Summary of GC-MS identifications for the composition of the aqueous phase produced by hydrothermal conversion of glucose in absence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
29.4	Pentanoic acid, 4-oxo-	$C_5H_8O_3$	47.9
35.9	Hydroquinone	$C_6H_6O_2$	6.9
22.9	2,5-Hexanedione	$C_6H_{10}O_2$	5.8
4.8	Acetone	C_3H_6O	4.4
18.6	2-Cyclopenten-1-one	C_5H_6O	3.8
25.5	1,2-Cyclopentanedione, 3-methyl-	$C_6H_8O_2$	3.8
23.9	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	2.6
25.5	3,6-Heptanedione	$C_7H_{12}O_2$	2.3
21.3	Ethanone, 1-(2-furanyl)-	$C_6H_6O_2$	2.1
15.3	Propanoic acid	$C_3H_6O_2$	1.9
20.8	2-Butanone	C_4H_8O	1.9
20.7	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	1.8
26.3	Phenol	C_6H_6O	1.6
15.8	Cyclopentanone	C_5H_8O	1.3
24.9	Furan, tetrahydro-2,5-dimethyl-, trans-	$C_6H_{12}O$	1.3
37.8	Ethanone, 1-(3-hydroxyphenyl)-	$C_8H_8O_2$	1.0
35.4	2,5-Dimethyl-2-(2-tetrahydrofuryl)tetrahydrofuran	$C_{10}H_{18}O$	1.0
18.7	Furfural	$C_5H_4O_2$	1.0
36.7	1,4-Benzenediol, 2-methyl-	$C_7H_8O_2$	0.9
34.1	2-Hexenoic acid, 3,4,4-trimethyl-5-oxo-, (Z)-	$C_9H_{14}O_3$	0.9
4.1	Acetaldehyde	C_2H_4O	0.9
41.3	1,6-Pentalenedione, hexahydro-6a-(2-propynyl)-, cis-	$C_{11}H_{12}O_2$	0.4
36.6	2-Methyl-5-hydroxybenzofuran	$C_9H_8O_2$	0.4
30.4	2H-Pyran, 3,4-dihydro-6-methyl-	$C_6H_{10}O$	0.4

Table S13: Summary of GC-MS identifications for the composition of the aqueous phase produced by hydrothermal conversion of glucose in presence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
21.0	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	17.4
24.2	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	11.4
25.8	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	11.1
37.2	3,5-Dihydroxytoluene	$C_7H_8O_2$	10.5
16.1	Cyclopentanone	C_5H_8O	7.8
17.9	2-Cyclopenten-1-one, 2-hydroxy-	$C_5H_6O_2$	4.0
26.8	Phenol	C_6H_6O	3.7
18.9	2-Cyclopenten-1-one	C_5H_6O	3.6
24.6	4,4-Dimethyl-2-cyclopenten-1-one	$C_7H_{10}O$	3.2
36.4	Hydroquinone	$C_6H_6O_2$	3.0
24.0	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	2.8
29.0	Phenol, 4-methyl-	C_7H_8O	2.8
11.0	acide acetique	CH_3COOH	2.1
24.3	Butyrolactone	$C_4H_6O_2$	2.1
38.6	1,3-Benzenediol, 4-ethyl-	$C_8H_{10}O_2$	2.1
18.5	Cyclopentanone, 3-methyl-	$C_6H_{10}O$	1.7
4.2	Acetaldehyde	C_2H_4O	1.7
21.7	Cyclopentene, 1-(1-methylethyl)-	C_8H_{14}	1.4
25.3	Furan, tetrahydro-2,5-dimethyl-, trans-	$C_6H_{12}O$	1.3
38.3	Acetophenone, 4'-hydroxy-	$C_8H_8O_2$	0.9
27.4	Furan, 2-propyl-	$C_7H_{10}O$	0.9

Table S14: Summary of GC-MS identifications for the composition of the aqueous phase produced by hydrothermal conversion of xylose in absence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
18.7	Furfural	$C_5H_4O_2$	36.0
29.3	Pentanoic acid, 4-oxo-	$C_5H_8O_3$	16.0
22.9	2,5-Hexanedione	$C_6H_{10}O_2$	7.2
41.7	1,6(2H,7H)-Naphthalenedione, 3,4,8,8a-tetrahydro-8a-methyl-	$C_{11}H_{14}O_2$	7.0
18.6	2-Cyclopenten-1-one	C_5H_6O	3.2
37.9	Ethanone, 1-(3-hydroxyphenyl)-	$C_8H_8O_2$	3.1
15.3	Propanoic acid	$C_3H_6O_2$	2.5
20.8	2-Butanone	C_4H_8O	2.2
36.3	Benzaldehyde, 3-hydroxy-	$C_7H_6O_2$	2.1
43.9	2H-1-Benzopyran-2-one, 3,5,7-trihydroxy-	$C_9H_6O_5$	1.7
4.1	Acetaldehyde	C_2H_4O	1.6
15.8	Cyclopentanone	C_5H_8O	1.3
25.5	3,6-Heptanedione	$C_7H_{12}O_2$	1.2
29.6	Succinic anhydride	$C_4H_4O_3$	1.0
23.8	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	0.9
10.5	Acide acetique	CH_3COOH	0.9
26.3	Phenol	C_6H_6O	0.9
21.2	Ethanone, 1-(2-furanyl)-	$C_6H_6O_2$	0.8
35.9	Hydroquinone	$C_6H_6O_2$	0.8
32.2	2-Cyclohexen-1-one, 4-(1-methylethyl)-	$C_9H_{14}O$	0.8
25.5	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	0.8
36.7	1,4-Benzenediol, 2-methyl-	$C_7H_8O_2$	0.7
32.7	1-Pentanone, 1-(2-furanyl)-	$C_9H_{12}O_2$	0.7
38.9	Benzene, hexyl-	$C_{12}H_{18}$	0.6
20.7	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	0.6

Table S15: Summary of GC-MS identifications for the composition of the aqueous phase produced by hydrothermal conversion of xylose in presence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
20.7	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	9.8
36.7	1,4-Benzenediol, 2-methyl-	$C_7H_8O_2$	8.3
25.4	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	6.7
23.8	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	6.7
15.8	Cyclopentanone	C_5H_8O	4.3
26.3	Phenol	C_6H_6O	4.1
24.0	Butyrolactone	$C_4H_6O_2$	3.2
15.3	Propanoic acid	$C_3H_6O_2$	3.0
17.6	Cyclopentanone, 2-methyl-	$C_6H_{10}O$	2.6
24.2	2-Cyclopenten-1-one, 3,4-dimethyl-	$C_7H_{10}O$	2.5
35.9	Hydroquinone	$C_6H_6O_2$	2.3
27.6	Phenol, 2-methyl-	C_7H_8O	2.3
23.6	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	2.2
18.6	2-Cyclopenten-1-one	C_5H_6O	1.9
27.0	2-Cyclopenten-1-one, 3-ethyl-	$C_7H_{10}O$	1.8
38.1	1,3-Benzenediol, 4-ethyl-	$C_8H_{10}O_2$	1.8
37.9	Ethanone, 1-(3-hydroxyphenyl)-	$C_8H_8O_2$	1.7
28.5	Phenol, 4-methyl-	C_7H_8O	1.7
37.3	1,4-Benzenediol, 2,5-dimethyl-	$C_8H_{10}O_2$	1.3
21.4	2-Cyclopenten-1-one, 3,4-dimethyl-	$C_7H_{10}O$	1.3
28.0	2-Ethylidenecyclohexanone	$C_8H_{12}O$	1.2
18.2	Cyclopentanone, 3-methyl-	$C_6H_{10}O$	1.2
26.7	2-Cyclopenten-1-one, 2,3,4-trimethyl-	$C_8H_{12}O$	1.1
38.3	1,4-Benzenediol, 2,5-dimethyl-	$C_8H_{10}O_2$	1.1
25.4	2-Cyclopenten-1-one, 3,4-dimethyl-	$C_7H_{10}O$	1.1
30.1	Ethanone, 1-cyclohexyl-	$C_8H_{14}O$	1.0
37.6	2,5-Dimethylhydroquinone	$C_8H_{10}O_2$	1.0
21.3	Ethanone, 1-(2-furanyl)-	$C_6H_6O_2$	1.0
25.7	1-Butanone, 1-(2-furanyl)-	$C_8H_{10}O_2$	1.0
28.4	p-cresol	C_7H_8O	0.9
18.7	Furfural	$C_5H_4O_2$	0.9
38.5	Phenol, 4-ethyl-2-methoxy-	$C_9H_{12}O_2$	0.7
24.9	2(3H)-Furanone, dihydro-5-methyl-	$C_5H_8O_2$	0.7
20.1	Cyclohexanone	$C_6H_{10}O$	0.7
38.9	Phenol, 4-ethyl-2-methoxy-	$C_9H_{12}O_2$	0.6
27.2	5-Ethyl-2-furaldehyde	$C_7H_8O_2$	0.6
32.2	3-Hydroxy-2-methylbenzaldehyde	$C_8H_8O_2$	0.6
39.2	Ethanone, 1-(3-hydroxyphenyl)-	$C_8H_8O_2$	0.6
29.6	Phenol, 3,4-dimethyl-	$C_8H_{10}O$	0.5
34.1	2-Cyclohexen-1-one, 6-methyl-3-(1-methylethyl)-	$C_{10}H_{16}O$	0.5
26.9	Furan, 2,4-dimethyl-	C_6H_8O	0.5
21.9	2-Cyclopenten-1-one, 3,4-dimethyl-	$C_7H_{10}O$	0.5
30.4	2H-Pyran, 3,4-dihydro-6-methyl-	$C_6H_{10}O$	0.4
27.0	2-Cyclopenten-1-one, 2,3,4-trimethyl-	$C_8H_{12}O$	0.4
39.0	4-Hydroxy-2-methylacetophenone	$C_9H_{10}O_2$	0.4
22.3	3-Ethylcyclopentanone	$C_7H_{12}O$	0.4

37.4	4-Hydroxy-3-methylacetophenone	$C_9H_{10}O_2$	0.4
35.2	1-(1-Ethyl-2,3-dimethyl-cyclopent-2-enyl)-ethanone	$C_{11}H_{18}O$	0.4
19.5	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	0.4
31.9	1-Propanone, 1-cyclohexyl-	$C_9H_{16}O$	0.4

1.2.3 Identification of the reaction products in bio-oils

Table S16: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of glucose in absence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
29.3	Pentanoic acid, 4-oxo-	$C_5H_8O_3$	37.8
22.9	2,5-Hexanedione	$C_6H_{10}O_2$	5.6
4.8	Acetone	C_3H_6O	5.5
35.9	Hydroquinone	$C_6H_6O_2$	4.6
18.6	2-Cyclopenten-1-one	C_5H_6O	4.2
25.5	1,2-Cyclopentanedione, 3-methyl-	$C_6H_8O_2$	4.2
23.9	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	3.3
21.3	Ethanone, 1-(2-furanyl)-	$C_6H_6O_2$	2.9
43.9	2H-1-Benzopyran-2-one, 3,5,7-trihydroxy-	$C_9H_6O_5$	2.5
20.7	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	2.5
25.5	3,6-Heptanedione	$C_7H_{12}O_2$	2.3
36.6	2-Methyl-5-hydroxybenzofuran	$C_9H_8O_2$	2.0
18.7	Furfural	$C_5H_4O_2$	1.8
37.8	Ethanone, 1-(3-hydroxyphenyl)-	$C_8H_8O_2$	1.7
26.3	Phenol	C_6H_6O	1.6
20.8	2-Butanone	C_4H_8O	1.4
28.7	Benzofuran, 4,7-dimethyl-	$C_{10}H_{10}O$	1.4
15.8	Cyclopentanone	C_5H_8O	1.1
35.4	2,5-Dimethyl-2-(2-tetrahydrofuryl)tetrahydrofuran	$C_{10}H_{18}O$	1.1
24.9	2(3H)-Furanone, dihydro-5-methyl-	$C_5H_8O_2$	1.1
4.5	Furan	C_4H_4O	1.0
34.1	2-Hexenoic acid, 3,4,4-trimethyl-5-oxo-, (Z)-	$C_9H_{14}O_3$	1.0
35.1	7-Methylindan-1-one	$C_{10}H_{10}O$	0.9
38.7	Furan, 2-(2-furanylmethyl)-5-methyl-	$C_{10}H_{10}O_2$	0.8
32.1	1H-Inden-1-one, 2,3-dihydro-	C_9H_8O	0.8

Table S17: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of glucose in presence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
25.8	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	8.5
21.0	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	6.7
28.3	2-Cyclopenten-1-one, 2,3,4,5-tetramethyl-	$C_9H_{14}O$	5.1
23.9	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	4.2
24.2	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	4.1
27.1	2-Cyclopenten-1-one, 3,4,5-trimethyl-	$C_8H_{12}O$	3.4
26.0	2-Cyclopenten-1-one, 2,3,4-trimethyl-	$C_8H_{12}O$	2.6
27.4	2-Cyclopenten-1-one, 3-ethyl-	$C_7H_{10}O$	2.6
28.9	Phenol, 4-methyl-	C_7H_8O	2.4
30.0	Phenol, 3,4-dimethyl-	$C_8H_{10}O$	2.4
24.6	2-Cyclopenten-1-one, 3,4-dimethyl-	$C_7H_{10}O$	2.2
28.0	Phenol, 4-methyl-	C_7H_8O	2.0
17.9	Cyclopentanone, 2-methyl-	$C_6H_{10}O$	1.8
27.6	5-Ethyl-2-furaldehyde	$C_7H_8O_2$	1.7
21.7	2-Cyclopenten-1-one, 3,4-dimethyl-	$C_7H_{10}O$	1.6
27.3	trans,cis-1,8-Dimethylspiro[4.5]decane	$C_{12}H_{22}$	1.6
37.1	2-Methyl-5-hydroxybenzofuran	$C_9H_8O_2$	1.6
29.6	Cyclohexanone, 2-(2-propenyl)-	$C_9H_{14}O$	1.5
37.2	3,5-Dihydroxytoluene	$C_7H_8O_2$	1.5
30.9	Phenol, 2-ethyl-	$C_8H_{10}O$	1.4
26.8	Phenol	C_6H_6O	1.4
16.1	Cyclopentanone	C_5H_8O	1.3
27.2	Furan, 2,4-dimethyl-	C_6H_8O	1.3
11.0	acide acetique	CH_3COOH	1.3
29.9	1-Butanone, 1-(2-furanyl)-	$C_8H_{10}O_2$	1.2
30.9	Phenol, 3-ethyl-	$C_8H_{10}O$	1.2
31.6	Phenol, 3,4-dimethyl-	$C_8H_{10}O$	1.2
30.5	4-Hexen-2-one, 3,4-dimethyl-	$C_8H_{14}O$	1.2
35.6	Non identifié (composé aromatique)		1.1
24.6	3-Furaldehyde	$C_5H_4O_2$	1.1
28.9	Phenol, 4-methyl-	C_7H_8O	1.0
25.7	4,4-Dimethyl-2-cyclopenten-1-one	$C_7H_{10}O$	1.0
18.5	Cyclopentanone, 3-methyl-	$C_6H_{10}O$	0.9
26.5	2-Ethylidenecyclohexanone	$C_8H_{12}O$	0.9
28.6	Furan, 2,4-dimethyl-	C_6H_8O	0.9
38.2	1,4-Benzenedicarboxaldehyde, 2,5-dimethyl-	$C_{10}H_{10}O_2$	0.9
31.7	Cyclopenta[c]pyran-1,3-dione, 4,4a,5,6-tetrahydro-4,7-dimethyl-	$C_{10}H_{12}O_3$	0.9
38.3	Ethanone, 1-(3-hydroxyphenyl)-	$C_8H_8O_2$	0.8
22.6	3-Ethylcyclopentanone	$C_7H_{12}O$	0.8
39.0	Methyl 3-phenyl-but-2-enoate	$C_{11}H_{12}O_2$	0.8
21.6	Non identifié		0.8
24.3	2-Cyclopenten-1-one, 3,4,5-trimethyl-	$C_8H_{12}O$	0.8
32.5	1H-Inden-1-one, 2,3-dihydro-	C_9H_8O	0.7
29.8	Phenol, 4-ethyl-	$C_8H_{10}O$	0.7
39.3	Phenol, 4-ethyl-2-methoxy-	$C_9H_{12}O_2$	0.7

22.1	Cyclopentene, 1-(1-methylethyl)-	C_8H_{14}	0.7
39.5	4-Hydroxy-2-methylacetophenone	$C_9H_{10}O_2$	0.6
38.6	1,3-Benzenediol, 4-ethyl-	$C_8H_{10}O_2$	0.6
32.2	Cyclohexanecarboxylic acid, ethenyl ester	$C_9H_{16}O_2$	0.6
35.7	Ethanone, 1-(4-ethylphenyl)-	$C_{10}H_{12}O$	0.6

Table S18: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of xylose in absence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
18.7	Furfural	$C_5H_4O_2$	42.8
41.7	1,6(2H,7H)-Naphthalenedione, 3,4,8,8a-tetrahydro-8a-methyl-	$C_{11}H_{14}O_2$	8.3
43.9	2H-1-Benzopyran-2-one, 3,5,7-trihydroxy-	$C_9H_6O_5$	8.0
4.5	Furan	C_4H_4O	7.5
10.5	Acide acetique	CH_3COOH	5.6
29.3	Pentanoic acid, 4-oxo-	$C_5H_8O_3$	4.2
22.9	2,5-Hexanedione	$C_6H_{10}O_2$	3.0
37.8	Ethanone, 1-(3-hydroxyphenyl)-	$C_8H_8O_2$	2.8
36.2	Benzaldehyde, 3-hydroxy-	$C_7H_6O_2$	2.0
22.6	Benzofuran	C_8H_6O	1.9
25.9	Benzofuran, 2-methyl-	C_9H_8O	1.0
21.2	Ethanone, 1-(2-furanyl)-	$C_6H_6O_2$	0.9
25.8	Cinnamaldehyde, (E)-	C_9H_8O	0.8
26.3	Phenol	C_6H_6O	0.8
34.8	2,2'-Bifuran	$C_8H_6O_2$	0.8
20.8	2-Butanone	C_4H_8O	0.7
33.1	Benzofuran, 4,7-dimethyl-	$C_{10}H_{10}O$	0.7
32.1	1H-Inden-1-one, 2,3-dihydro-	C_9H_8O	0.7
28.5	Phenol, 4-methyl-	C_7H_8O	0.6
15.5	Propanoic acid	$C_3H_6O_2$	0.6
15.8	Cyclopentanone	C_5H_8O	0.6
23.9	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	0.6
25.5	3,6-Heptanedione	$C_7H_{12}O_2$	0.6
35.4	Ethanone, 1-(2-benzofuranyl)-	$C_{10}H_8O_2$	0.6
38.9	Benzene, hexyl-	$C_{12}H_{18}$	0.5

Table S19: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of xylose in presence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
18.7	Furfural	$C_5H_4O_2$	58.7
4.5	Furan	C_4H_4O	9.6
43.9	2H-1-Benzopyran-2-one, 3,5,7-trihydroxy-	$C_9H_6O_5$	6.9
41.7	1,6(2H,7H)-Naphthalenedione, 3,4,8,8a-tetrahydro-8a-methyl-	$C_{11}H_{14}O_2$	6.0
22.9	2,5-Hexanedione	$C_6H_{10}O_2$	3.7
29.2	Pentanoic acid, 4-oxo-	$C_5H_8O_3$	2.4
37.9	Ethanone, 1-(3-hydroxyphenyl)-	$C_8H_8O_2$	2.4
22.6	Benzofuran	C_8H_6O	1.7
36.2	Benzaldehyde, 4-hydroxy-	$C_7H_6O_2$	1.6
25.9	Benzofuran, 2-methyl-	C_9H_8O	1.0
10.5	Acide acetique	CH_3COOH	0.7
25.8	Benzofuran, 2-methyl-	C_9H_8O	0.7
20.8	2-Butanone	C_4H_8O	0.6
21.2	Ethanone, 1-(2-furanyl)-	$C_6H_6O_2$	0.5
34.8	2,2'-Bifuran	$C_8H_6O_2$	0.5
33.1	Non identifié		0.5
26.3	Phenol	C_6H_6O	0.5
32.1	1H-Inden-1-one, 2,3-dihydro-	C_9H_8O	0.4
35.4	Ethanone, 1-(2-benzofuranyl)-	$C_{10}H_8O_2$	0.4
28.5	Phenol, 4-methyl-	C_7H_8O	0.4
15.8	Cyclopentanone	C_5H_8O	0.3
25.5	3,6-Heptanedione	$C_7H_{12}O_2$	0.3

1.3 Hydrothermal conversion of glutamic acid

1.3.1 Chromatograms

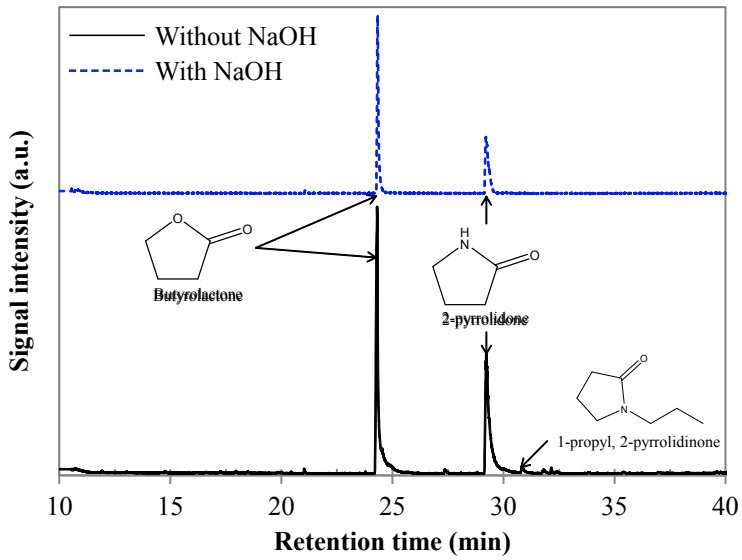


Figure S32: GC-MS chromatograms of the aqueous phase from hydrothermal conversion of glutamic acid (300 °C, 60 min)

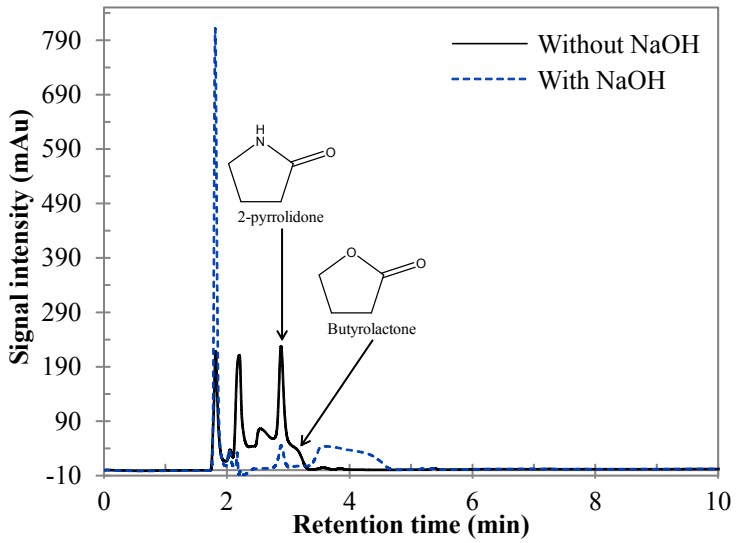


Figure S33 : HPLC-UV chromatograms of the aqueous phase from hydrothermal conversion of glutamic acid (300 °C, 60 min)

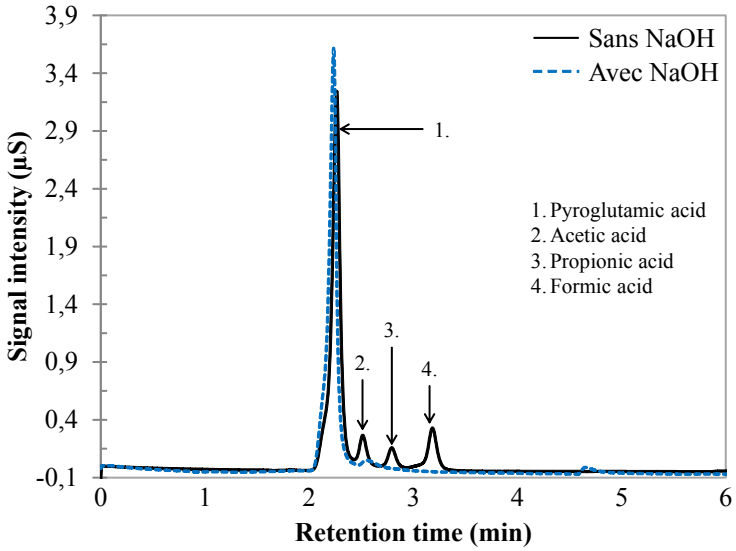


Figure S34 : HPIC Chromatograms of the aqueous phase from hydrothermal conversion of glutamic acid (300 °C, 60 min)

1.3.2 Identification of the reaction products

Table S20: Summary of GC-MS identifications for the composition of the aqueous phase produced by hydrothermal conversion of glutamic acid in absence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
24.3	Butyrolactone	$C_4H_6O_2$	53.9
29.2	2-Pyrrolidinone	C_4H_7NO	42.4
30.8	2-Pyrrolidinone, 1-propyl-	$C_7H_{13}NO$	1.2
31.8	2,5-Pyrrolidinedione, 1-propyl-	$C_7H_{11}NO_2$	0.7
4.2	Acetaldehyde	C_2H_4O	0.6
32.2	5-Hexenal	$C_6H_{10}O$	0.6
27.4	Phenol, 2-methoxy-	$C_7H_8O_2$	0.5

Table S21: Summary of GC-MS identifications for the composition of the aqueous phase produced by hydrothermal conversion of glutamic acid in presence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
24.3	Butyrolactone	$C_4H_6O_2$	54.8
29.2	2-Pyrrolidinone	C_4H_7NO	39.1
10.8	Not identified		2.7
4.2	Not identified		1.8
4.2	Not identified		1.6

1.4 Hydrothermal conversion of guaiacol

1.4.1 Chromatograms

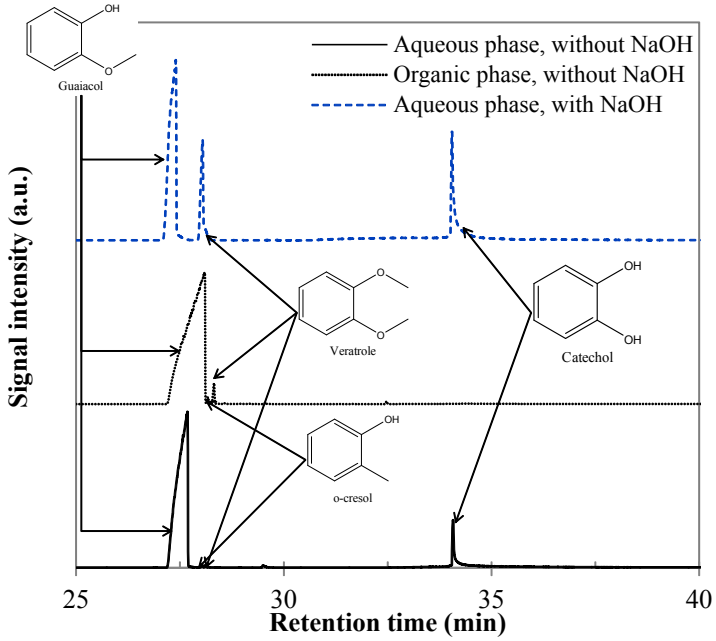


Figure S35: GC-MS chromatograms of products from hydrothermal conversion of guaiacol (300 °C, 60 min)

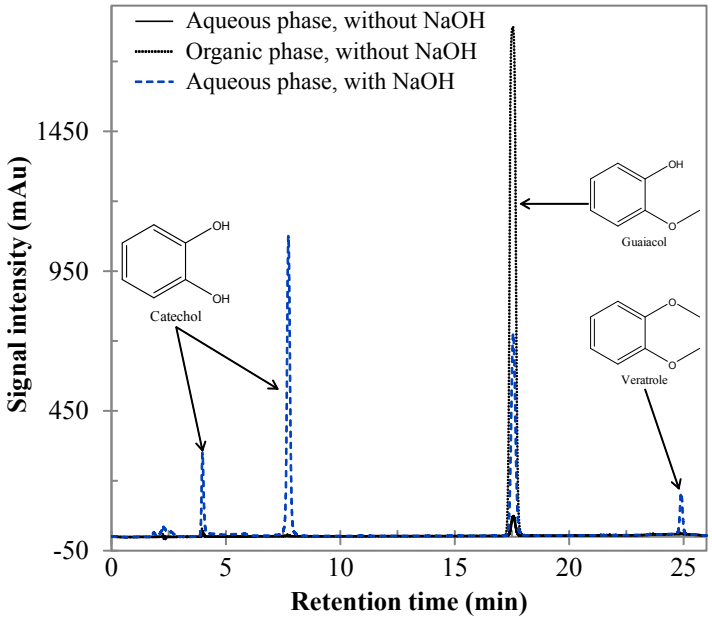


Figure S36: HPLC-UV chromatograms of the aqueous phase from hydrothermal conversion of guaiacol (300 °C, 60 min)

1.4.2 Identification of the reaction products in the aqueous phases

Table S22: Summary of GC-MS identifications for the composition of the aqueous phase produced by hydrothermal conversion of guaiacol in absence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
27.7	Phenol, 2-methoxy-	$C_7H_8O_2$	88.7
34.1	1,2-Benzenediol	$C_6H_6O_2$	9.7
4.4	Methyl Alcohol	CH_4O	0.7
29.5	Phosphonic acid, methyl-, bis(trimethylsilyl) ester	$C_7H_{21}O_3PSi_2$	0.4
28.0	Phenol, 2-methyl-	C_7H_8O	0.2
28.1	Benzene, 1,2-dimethoxy-	$C_8H_{10}O_2$	0.2

Table S23: Summary of GC-MS identifications for the composition of the aqueous phase produced by hydrothermal conversion of guaiacol in presence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
27.4	Phenol, 2-methoxy-	$C_7H_8O_2$	59.0
34.0	1,2-Benzenediol	$C_6H_6O_2$	25.5
28.0	Benzene, 1,2-dimethoxy-	$C_8H_{10}O_2$	13.4
4.3	Methyl Alcohol	CH_4O	1.8
33.8	Ethanone, 1-(2-hydroxy-4-methoxyphenyl)-	$C_9H_{10}O_3$	0.1
29.0	1,3-Benzenediol, 4-ethyl-	$C_8H_{10}O_2$	0.1
26.8	Phenol	C_6H_6O	0.0
29.6	Phenol, 4-methoxy-3-methyl-	$C_8H_{10}O_2$	0.0
29.8	2-Methoxy-5-methylphenol	$C_8H_{10}O_2$	0.0

1.4.3 Identification of the reaction products in the bio-oils

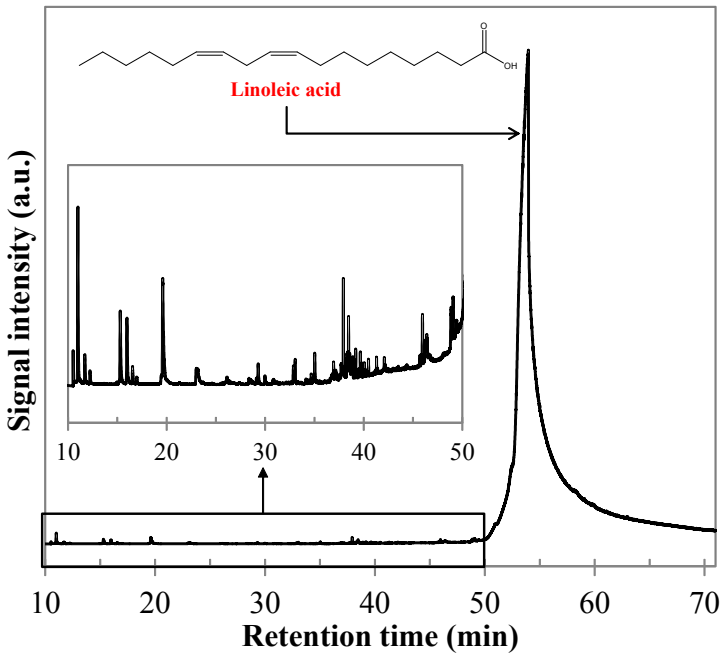
Table S24: Summary of GC-MS identifications for the composition of the organic phase produced by hydrothermal conversion of guaiacol in absence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
28.1	Phenol, 2-methoxy-	$C_7H_8O_2$	97.9
28.3	Benzene, 1,2-dimethoxy-	$C_8H_{10}O_2$	1.2
28.2	Phenol, 2-methyl-	C_7H_8O	0.4
32.5	1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3à,3aá,7á,8aà	$C_{15}H_{24}$	0.2
29.6	Phosphonic acid, methyl-, bis(trimethylsilyl) ester	$C_7H_{21}O_3PSi_2$	0.1
4.4	Methyl Alcohol	CH_4O	0.1
28.6	Phenol, 2,6-dimethyl-	$C_8H_{10}O$	0.0

28.5	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (ñ)-	$C_{10}H_{16}O$	0.0
31.8	Bicyclo[3.1.1]heptane, 6-methyl-2-methylene-6-(4-methyl-3-pentenyl)-, [1R	$C_{15}H_{24}$	0.0
29.2	Phenol, 4-methoxy-3-methyl-	$C_8H_{10}O_2$	0.0
28.9	Phenol, 4-methyl-	C_7H_8O	0.0
27.0	Phenol	C_6H_6O	0.0
29.0	Phenol, 4-methyl-	C_7H_8O	0.0
29.3	Benzofuran, 4,7-dimethyl-	$C_{10}H_{10}O$	0.0

1.5 Hydrothermal conversion of linoleic acid

1.5.1 Chromatograms



Retention time (min)	Minor compounds
11-12.2	Octene isomers
16-17	Nonene isomers
19.6	Heptanal
23.1	2-octanone
35	Phtalic anhydride
37.9	5-Nonadecen-1-ol
38.5	4-Tridecen-1-ol, acetate, (E)-
48.9	9-Hexadecen-1-ol, (Z)-
49.1	Z,Z-6,13-Octadecadien-1-ol acetate

Figure S37 : GC-MS chromatogram of the bio-oil produced by hydrothermal liquefaction of linoleic acid (300 °C, 60 min, no NaOH added)

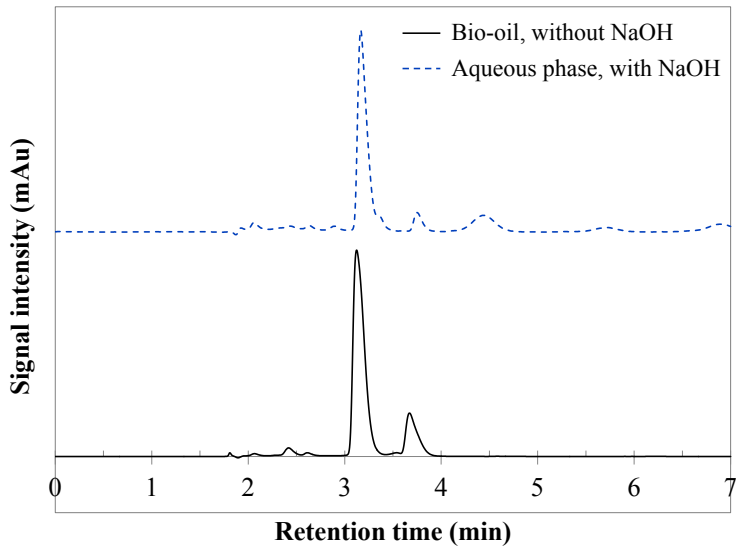


Figure S38: HPLC-UV chromatograms of the bio-oil and the aqueous phase produced by hydrothermal conversion of linoleic acid (300 °C, 60 min)

1.5.2 Identification of the reaction products

Table S25: Summary of GC-MS identifications for the composition of the organic phase produced by hydrothermal conversion of linoleic acid in absence of NaOH (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
54.0	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}O_2$	99.5
19.6	Heptanal	$C_7H_{14}O$	0.1
11.0	1-Octene	C_8H_{16}	0.1
15.3	Hexanal (impurete alino)		0.0
16.0	1-Nonene	C_9H_{18}	0.0
49.1	Z,Z-6,13-Octadecadien-1-ol acetate	$C_{20}H_{36}O_2$	0.0
37.9	11-Tetradecen-1-ol, acetate, (Z)-	$C_{16}H_{30}O_2$	0.0
46.0	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}O_2$	0.0
48.9	1,15-Hexadecadiene	$C_{16}H_{30}$	0.0
23.2	2-octanone	$C_8H_{16}O$	0.0
38.5	4-Tridecen-1-ol, acetate, (E)-	$C_{15}H_{28}O_2$	0.0
46.4	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}O_2$	0.0
11.7	1-Octene	C_8H_{16}	0.0
23.0	2-octanone	$C_8H_{16}O$	0.0
35.0	Phthalic anhydride	$C_8H_4O_3$	0.0
49.4	7-Hexadecenal, (Z)-	$C_{16}H_{30}O$	0.0
46.3	9-Octadecenoic acid (Z)-, methyl ester	$C_{19}H_{36}O_2$	0.0
16.5	1-Nonene	C_9H_{18}	0.0
29.3	2,5-Furandione, dihydro-3-methyl-	$C_5H_6O_3$	0.0
38.4	3-Heptadecen-5-yne, (Z)-	$C_{17}H_{30}$	0.0
33.0	11-Hexadecen-1-ol, (Z)-	$C_{16}H_{32}O$	0.0
39.2	3-Heptadecen-5-yne, (Z)-	$C_{17}H_{30}$	0.0
38.6	2,4-Dodecadiene, (E,Z)-	$C_{12}H_{22}$	0.0
12.2	1-Octene	C_8H_{16}	0.0
4.3	Pentane	C_5H_{12}	0.0
32.9	8-Heptadecene	$C_{17}H_{34}$	0.0
38.3	9,12-Tetradecadien-1-ol, (Z,E)-	$C_{14}H_{26}O$	0.0
39.7	Bicyclo[3.1.1]hept-2-ene-2-ethanol, 6,6-dimethyl-	$C_{11}H_{18}O$	0.0
19.5	2-Heptanone	$C_7H_{14}O$	0.0
38.9	3-Heptadecen-5-yne, (Z)-	$C_{17}H_{30}$	0.0

1.6 Hydrothermal conversion of binary mixtures

1.6.1 Glucose-Glutamic acid binary mixture: identification of products

Table S26: Summary of GC-MS identifications for the composition of the aqueous phase produced by hydrothermal conversion of a Glucose-Glutamic acid binary mixture (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
21.0	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	21.1
24.3	Butyrolactone	$C_4H_6O_2$	15.3
29.2	2-Pyrrolidinone	C_4H_7NO	13.0
32.3	3-Pyridinol, 6-methyl-	C_6H_7NO	5.4
31.8	2,5-Pyrrolidinedione, 1-propyl-	$C_7H_{11}NO_2$	4.7
17.9	Cyclopentanone, 2-methyl-	$C_6H_{10}O$	2.7
16.1	Cyclopentanone	C_5H_8O	2.6
19.8	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	2.0
25.9	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	1.6
18.5	Cyclopentanone, 3-methyl-	$C_6H_{10}O$	1.6
34.2	Pyrrolidine, 1-(1-cyclohexen-1-yl)-	$C_{10}H_{17}N$	1.5
30.9	Cyclohexanone, 2-propyl-	$C_9H_{16}O$	1.5
29.8	2,5-Pyrrolidinedione, 1-ethyl-	$C_6H_9NO_2$	1.5
21.6	Ethanone, 1-(2-furanyl)-	$C_6H_6O_2$	1.4
13.1	Pyridine	C_5H_5N	1.3
35.6	5,7-Octadien-2-one, 3-acetyl-	$C_{10}H_{14}O_2$	1.3
31.9	2,5-Pyrrolidinedione, 1-propyl-	$C_7H_{11}NO_2$	1.1
31.2	3-Pyridinol, 2-methyl-	C_6H_7NO	1.1
31.5	1,3,5-Triazin-2(1H)-one, 4-amino-6-(ethylamino)-	$C_5H_9N_5O$	1.1
36.5	4,5-Heptadien-2-one, 3,3,6-trimethyl-	$C_{10}H_{16}O$	1.1
32.5	3-Pyridinol, 6-methyl-	C_6H_7NO	1.1
29.5	2,6-Piperazinedione, 4,4'-(1-methyl-1,2-ethanediyl)bis-, (S)-	$C_{11}H_{16}N_4O_4$	1.1
14.7	3-Hexanone	$C_6H_{12}O$	1.0
34.5	2-Hexenoic acid, 3,4,4-trimethyl-5-oxo-, (Z)-	$C_9H_{14}O_3$	1.0
27.4	2-Cyclopenten-1-one, 3-(1-methylethyl)-	$C_8H_{12}O$	1.0

Table S27: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of a Glucose-Glutamic acid binary mixture (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
21.0	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	3.9
33.0	Pentadecane	$C_{15}H_{32}$	3.0
32.4	(4-Ethoxyphenyl)ethylamine	$C_{10}H_{15}NO$	2.8
31.0	Phenol, 4-methylamino, ethyl(ether)	$C_9H_{13}NO$	2.7
29.1	2-Pyrrolidinone	C_4H_7NO	2.5
33.4	4-Amino-3,5-diethylpyridine	$C_9H_{14}N_2$	2.4
29.2	4(1H)-Pyridinone, 1,2,6-trimethyl-	$C_8H_{11}NO$	2.4
32.0	Tyrosine	$C_9H_{11}NO_3$	2.1
35.8	1,2,3,4-Tetrahydroisoquinoline, 7-hydroxy-6-methoxy-1-(5-hydroxy-4-methoxy	$C_{19}H_{23}NO_4$	1.9
24.3	Butyrolactone	$C_4H_6O_2$	1.9
34.7	1,2,3,4,5,8-Hexahydroisoquinoline, 1-[3-hydroxybenzyl]-6-methoxy-	$C_{17}H_{21}NO_2$	1.8
31.2	Phenol, 4-methylamino, ethyl(ether)	$C_9H_{13}NO$	1.7
33.7	6-Propylbenzo[1,3]dioxol-5-ylamine	$C_{10}H_{13}NO_2$	1.6
32.3	(4-Ethoxyphenyl)ethylamine	$C_{10}H_{15}NO$	1.5
36.8	9-Hexadecen-1-ol, (Z)-	$C_{16}H_{32}O$	1.4
33.7	4-Amino-3,5-diethylpyridine	$C_9H_{14}N_2$	1.4
30.7	Phenol, 3-(ethylamino)-4-methyl-	$C_9H_{13}NO$	1.4
28.7	4(1H)-Pyridinone, 1,2,6-trimethyl-	$C_8H_{11}NO$	1.2
29.4	1H-Pyrrole, 2-ethyl-3,4,5-trimethyl-	$C_9H_{15}N$	1.2
40.6	dl-5-Methyltryptophan	$C_{12}H_{14}N_2O_2$	1.2
27.3	1H-Pyrrole, 3-ethyl-2,4-dimethyl-	$C_8H_{13}N$	1.2
36.0	1,2,3,4-Tetrahydroisoquinolin-6-ol, 1-benzyl-7-methoxy-	$C_{17}H_{19}NO_2$	1.1
38.1	1H-Indole, 2,5-dimethyl-	$C_{10}H_{11}N$	1.1
28.0	1H-Pyrrole, 2,3,4,5-tetramethyl-	$C_8H_{13}N$	1.0
32.1	Tyrosine	$C_9H_{11}NO_3$	1.0
34.4	1,2,3,4,5,8-Hexahydroisoquinoline, 1-[3-hydroxybenzyl]-6-methoxy-	$C_{17}H_{21}NO_2$	1.0
26.5	Bicyclo[2.2.2]octane, 2-methyl-	C_9H_{16}	1.0
31.9	Tyrosine	$C_9H_{11}NO_3$	1.0
33.2	4-Amino-3,5-diethylpyridine	$C_9H_{14}N_2$	1.0
29.9	Cyclohexanone, 2-(1-methylethylidene)-	$C_9H_{14}O$	1.0

1.6.2 Glucose – Guaiacol binary mixture: identification of products in the bio-oil

Table S28: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of a Glucose-Guaiacol binary mixture (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
27.9	Phenol, 2-methoxy-	$C_7H_8O_2$	93.3
31.3	Benzofuran, 7-methoxy-	$C_9H_8O_2$	0.7
29.9	Phenol, 2-methoxy-4-methyl-	$C_8H_{10}O_2$	0.5
59.1	Ethanone, 2-hydroxy-1,2-bis(4-methoxyphenyl)-	$C_{16}H_{16}O_4$	0.4
28.0	Phenol, 2-methyl-	C_7H_8O	0.3
33.6	Furan, 2-(2-furanylmethyl)-5-methyl-	$C_{10}H_{10}O_2$	0.3
29.1	2-Methoxy-6-methylphenol	$C_8H_{10}O_2$	0.3
32.4	1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl	$C_{15}H_{24}$	0.2
31.8	Phenol, 4-ethyl-2-methoxy-	$C_9H_{12}O_2$	0.2
44.7	7-Methoxy-3,4,8-trimethyl-chromen-2-one	$C_{13}H_{14}O_3$	0.2
19.0	2-Cyclopenten-1-one	C_5H_6O	0.2
59.4	Xanthen-9-one, 1,3,5,8-tetrahydroxy-	$C_{13}H_8O_6$	0.2
49.7	1,4-Naphthalenedione, 2-hydroxy-3-methoxy-	$C_{11}H_8O_4$	0.2
51.2	(-)-Nortrachelogenin	$C_{20}H_{22}O_7$	0.2
52.5	1,4-Naphthalenedione, 5,8-dihydroxy-2,3-dimethyl-	$C_{12}H_{10}O_4$	0.2
21.1	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	0.1
39.0	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	$C_{10}H_{12}O_3$	0.1
29.6	2-Methoxy-5-methylphenol	$C_8H_{10}O_2$	0.1
30.9	Phenol, 4-ethyl-2-methoxy-	$C_9H_{12}O_2$	0.1
61.2	p-Methoxyphenyl-methanediol diacetate	$C_{12}H_{14}O_5$	0.1
28.2	Benzene, 1,2-dimethoxy-	$C_8H_{10}O_2$	0.1
26.7	Not identified		0.1
21.7	Ethanone, 1-(2-furanyl)-	$C_6H_6O_2$	0.1
50.4	Not identified		0.1
36.4	Vanillin	$C_8H_8O_3$	0.1

1.6.3 Glucose - Linoleic acid binary mixture: identification of products

Table S29: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of a Glucose-Linoleic acid binary mixture (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
53.1	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}O_2$	74.5
52.6	Oleic Acid	$C_{18}H_{34}O_2$	21.5
19.7	Heptanal	$C_7H_{14}O$	0.1
19.1	2-Cyclopenten-1-one	C_5H_6O	0.1
60.1	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}O_2$	0.1
11.5	1-Octene	C_8H_{16}	0.1
16.2	1-Nonene	C_9H_{18}	0.1
21.1	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	0.1
15.6	Hexanal	$C_6H_{12}O$	0.1
11.4	Octane	$C_{10}H_{18}$	0.1
37.1	3-Hexadecene, (Z)-	$C_{16}H_{32}$	0.1
61.3	9-Octadecenamide, (Z)-	$C_{18}H_{35}NO$	0.1
38.7	2,4-Dodecadiene, (E,Z)-	$C_{12}H_{22}$	0.1
23.3	2,5-Hexanedione	$C_6H_{10}O_2$	0.1
39.9	Benzene, (1-methyldecyl)-	$C_{17}H_{28}$	0.1
24.3	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	0.1
12.2	3-Octene, (E)-	C_8H_{16}	0.1
26.6	Benzene, pentyl-	$C_{11}H_{16}$	0.1
23.7	Benzene, butyl-	$C_{10}H_{14}$	0.1
23.0	2-Octanone	$C_8H_{16}O$	0.1
21.7	Ethanone, 1-(2-furanyl)-	$C_6H_6O_2$	0.1
39.2	Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	$C_{12}H_{18}$	0.1
16.3	Cyclopentanone	C_5H_8O	0.1
9.1	Furan, 2,5-dimethyl-	C_6H_8O	0.1
26.0	2-Hexanone, 5-methyl-	$C_7H_{14}O$	0.1
16.8	trans--4-Nonene	C_9H_{18}	0.1
29.2	Benzofuran, 4,7-dimethyl-	$C_{10}H_{10}O$	0.1
23.2	Octanal	$C_8H_{16}O$	0.0
19.6	2-Heptanone	$C_7H_{14}O$	0.0
37.2	1-Undecanol	$C_{11}H_{24}O$	0.0

1.6.4 Glutamic acid – Guaiacol binary mixture: identification of products in the bio-oil

Table S30: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of a Glutamic acid-Guaiacol binary mixture (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
28.0.	Phenol, 2-methoxy-	$C_7H_8O_2$	96.3
34.0	1,2-Benzenediol	$C_6H_6O_2$	1.5
29.3	2-Pyrrolidinone	C_4H_7NO	0.5
28.1	Phenol, 2-methyl-	C_7H_8O	0.4
33.0	Phenol, 2-methoxy-6-(2-propenyl)-	$C_{10}H_{12}O_2$	0.2
32.4	1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3à,3aá,7á	$C_{15}H_{24}$	0.2
35.8	Phenol, 2-methoxy-4-(1-propenyl)-	$C_{10}H_{12}O_2$	0.2
37.0	L-Proline, 5-oxo-, methyl ester	$C_6H_9NO_3$	0.1
24.4	Butyrolactone	$C_4H_6O_2$	0.1
4.4	Methyl Alcohol	CH_4O	0.1
28.2	Benzene, 1,2-dimethoxy-	$C_8H_{10}O_2$	0.1
32.8	Benzoic acid amide, 4-hydroxy-3-methoxy-	$C_8H_9NO_3$	0.1
35.9	Phenol, 2-methoxy-4-(1-propenyl)-	$C_{10}H_{12}O_2$	0.1
33.1	Phenol, 2-methoxy-4-(1-propenyl)-	$C_{10}H_{12}O_2$	0.1
28.5	Phenol, 2,6-dimethyl-	$C_8H_{10}O$	0.1

1.6.5 Glutamic acid-Linoleic acid binary mixture: identification of products in the bio-oil

Table S31: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of a Glutamic acid-Linoleic acid binary mixture (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
53.5	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}O_2$	93.4
38.5	Z-4-Tridecen-1-yl acetate	$C_{15}H_{28}O_2$	0.7
58.3	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}O_2$	0.7
38.0	E,Z-2,13-Octadecadien-1-ol	$C_{18}H_{34}O$	0.5
59.9	6-Octadecenoic acid, (Z)-	$C_{18}H_{34}O_2$	0.5
38.4	5-Heptadecene, 1-bromo-	$C_{17}H_{33}Br$	0.4
51.0	Phenol, 4-dodecyl-	$C_{18}H_{30}O$	0.4
38.3	4-Tridecen-1-ol, acetate, (E)-	$C_{15}H_{28}O_2$	0.4
38.2	E,Z-2,13-Octadecadien-1-ol	$C_{18}H_{34}O$	0.3
38.4	6,9-Heptadecadiene	$C_{17}H_{32}$	0.3
38.1	5-Heptadecene, 1-bromo-	$C_{17}H_{33}Br$	0.3
38.6	Z-4-Tridecen-1-yl acetate	$C_{15}H_{28}O_2$	0.3
37.0	E-2-Octadecadecen-1-ol	$C_{18}H_{36}O$	0.2

38.5	5-Heptadecene, 1-bromo-	$C_{17}H_{33}Br$	0.2
29.2	2-Pyrrolidinone	C_4H_7NO	0.2
61.1	9-Octadecenamide, (Z)-	$C_{18}H_{35}NO$	0.2
37.9	5-Heptadecene, 1-bromo-	$C_{17}H_{33}Br$	0.1
38.7	4-Tridecen-1-ol, acetate, (E)-	$C_{15}H_{28}O_2$	0.1
38.0	E,Z-2,13-Octadecadien-1-ol	$C_{18}H_{34}O$	0.1
37.1	Oleyl Alcohol	$C_{18}H_{36}O$	0.1

1.6.6 Guaiacol-Linoleic acid binary mixture: identification of products in the bio-oil

Table S32: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of a Guaiacol-Linoleic acid binary mixture (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
27.6	Phenol, 2-methoxy-	$C_7H_8O_2$	81.7
56.1	1,14-Tetradecanediol	$C_{14}H_{30}O_2$	17.1
28.0	Phenol, 2-methyl-	C_7H_8O	0.2
46.8	9,12-Octadecadienoic acid, methyl ester, (E,E)-	$C_{19}H_{34}O_2$	0.2
46.6	9-Hexadecenoic acid, methyl ester, (Z)-	$C_{17}H_{32}O_2$	0.2
11.5	1-Heptanol	$C_7H_{16}O$	0.1
19.7	Heptanal	$C_7H_{14}O$	0.1
10.9	Acetic acid	$C_2H_4O_2$	0.1
32.4	1,3-Cyclohexadiene, 5-(1,5-dimethyl-4-hexenyl)-2-methyl-, [S-(R*,S*)]-	$C_{15}H_{24}$	0.1
16.2	1-Nonene	C_9H_{18}	0.0

1.7 Hydrothermal conversion of a Glucose-Glutamic acid-Linoleic acid ternary mixture

Table S33: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of a Glucose-Glutamic acid-Linoleic acid ternary mixture (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
55.2	E-2-Octadecadecen-1-ol	$C_{18}H_{36}O$	73.9
61.1	9-Octadecenamide, (Z)-	$C_{18}H_{35}NO$	5.9
61.4	9,12-Octadecadienoic acid, methyl ester, (E,E)-	$C_{19}H_{34}O_2$	3.4
29.2	2-Pyrrolidinone	C_4H_7NO	1.8
21.1	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	1.4
54.5	Dodecanamide	$C_{12}H_{25}NO$	1.0
28.0	Benzene, 1,2-dimethoxy-	$C_8H_{10}O_2$	0.7
24.4	Butyrolactone	$C_4H_6O_2$	0.6
22.6	1,3,8-p-Menthatriene	$C_{10}H_{14}$	0.5
61.7	(R)-(-)-14-Methyl-8-hexadecyn-1-ol	$C_{17}H_{32}O$	0.5

27.2	Phenol, 2-methoxy-	$C_7H_8O_2$	0.5
11.5	1-Octene	C_8H_{16}	0.5
4.3	Hydroxyurea	$CH_4N_2O_2$	0.4
21.8	Cyclohexene, 3-methyl-6-(1-methylethylidene)-	$C_{10}H_{16}$	0.3
32.4	1,3-Cyclohexadiene, 5-(1,5-dimethyl-4-hexenyl)-2-methyl-, [S-(R*,S*)]-	$C_{15}H_{24}$	0.3
16.2	1-Nonene	C_9H_{18}	0.3
30.0	Bicyclo[2.2.1]heptane, 1,7,7-trimethyl-	$C_{10}H_{18}$	0.3
17.1	p-Xylene	C_8H_{10}	0.2
39.8	Benzene, (1-methyldecyl)-	$C_{17}H_{28}$	0.2
27.4	2-Cyclopenten-1-one, 2,3,4-trimethyl-	$C_8H_{12}O$	0.2
22.1	Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)-	$C_{10}H_{16}$	0.2
18.1	Cyclopentanone, 2-methyl-	$C_6H_{10}O$	0.2
23.0	2-Heptanone	$C_7H_{14}O$	0.2
32.4	2(1H)-Pyridinone, 5-methyl-	C_6H_7NO	0.2
14.9	3-Hexanone	$C_6H_{12}O$	0.2

1.8 Hydrothermal conversion of other model mixtures

1.8.1 Identification of reaction products in the aqueous phases

Table S34: Summary of GC-MS identifications for the composition of the aqueous phase produced by hydrothermal conversion of the model mixture 1 (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
27.0	Phenol, 2-methoxy-	$C_7H_8O_2$	88.1
33.6	1,2-Benzenediol	$C_6H_6O_2$	9.6
20.7	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	0.6
4.2	Methyl Alcohol	CH_4O	0.4

Table S35: Summary of GC-MS identifications for the composition of the aqueous phase produced by hydrothermal conversion of the model mixture 2 (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
26.8	Phenol, 2-methoxy-	$C_7H_8O_2$	19.3
4.2	Methyl Alcohol	CH_4O	11.7
20.7	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	7.9
23.8	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	5.3
24.0	Butyrolactone	$C_4H_6O_2$	4.2
15.8	Cyclopentanone	C_5H_8O	3.8
4.1	Methanethiol	CH_4S	3.7

28.7	2-Pyrrolidinone	C_4H_7NO	3.2
29.2	Cyclohexane, (methylthio)-	$C_7H_{14}S$	3.1
26.3	Phenol	C_6H_6O	2.8
29.4	Phenol, 4-methoxy-3-methyl-	$C_8H_{18}O_2$	2.7
38.5	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	$C_{10}H_{12}O_3$	2.5
35.9	Hydroquinone	$C_6H_6O_2$	2.3
40.9	Benzeneacetic acid, 4-hydroxy-3-methoxy-	$C_9H_{10}O_4$	2.2
36.7	3,5-Dihydroxytoluene	$C_7H_8O_2$	2.0
16.1	Pyrazine, methyl-	$C_5H_6N_2$	1.6
25.4	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	1.6
31.3	Phenol, 4-ethyl-2-methoxy-	$C_9H_{12}O_2$	1.5
28.5	1H-Imidazole, 1-methyl-4-nitro-	$C_4H_5N_3O_2$	1.4
29.0	Phosphonic acid, methyl-, bis(trimethylsilyl) ester	$C_7H_{21}O_3PSi_2$	1.3
23.6	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	1.2
17.6	Cyclopentanone, 2-methyl-	$C_6H_{10}O$	1.1
33.5	1-(Tihenyl-2)-1-formylethylene	C_7H_6OS	1.1
24.2	2-Cyclopenten-1-one, 3,4-dimethyl-	$C_7H_{10}O$	0.8
26.2	1-Methylcyclooctene	C_9H_{16}	0.7
25.3	Dihydro-2-(3H)-thiophenone	C_4H_6OS	0.6
28.6	Phenol, 4-methoxy-3-methyl-	$C_8H_{18}O_2$	0.6
38.1	2-Methoxy-5-methylphenol	$C_8H_{10}O_2$	0.6
24.9	2(3H)-Furanone, dihydro-5-methyl-	$C_5H_8O_2$	0.6
27.0	2-Cyclopenten-1-one, 3-ethyl-	$C_7H_{10}O$	0.6

1.8.2 Identification of reaction products in the bio-oils

Table S36: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of the model mixture 1 (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
27.3	Phenol, 2-methoxy-	$C_7H_8O_2$	84.5
50.8	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}O_2$	5.4
45.8	9-Octadecenoic acid (Z)-, methyl ester	$C_{19}H_{36}O_2$	1.2
46.0	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	$C_{19}H_{34}O_2$	1.0
33.6	1,2-Benzenediol	$C_6H_6O_2$	0.9
29.4	Phenol, 2-methoxy-4-methyl-	$C_8H_{10}O_2$	0.8
60.2	Fatty acid derivative		0.7
29.0	Phosphonic acid, methyl-, bis(trimethylsilyl) ester	$C_7H_{21}O_3PSi_2$	0.7

31.3	Phenol, 4-ethyl-2-methoxy-	$C_9H_{12}O_2$	0.6
28.9	2-Pyrrolidinone	C_4H_7NO	0.6
59.8	9-Octadecenamide, (Z)-	$C_{18}H_{35}NO$	0.6
59.9	Dodecanal, O-methyloxime	$C_{13}H_{27}NO$	0.6
60.1	2-Methyl-Z,Z-3,13-octadecadienol	$C_{19}H_{36}O$	0.6
33.2	Phenol, 2-methoxy-4-propyl-	$C_{10}H_{14}O_2$	0.5
30.4	Phenol, 4-ethyl-2-methoxy-	$C_9H_{12}O_2$	0.5
28.6	2-Methoxy-6-methylphenol	$C_8H_{10}O_2$	0.5
32.0	1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3à,3aá,7á,8aà)]-	$C_{15}H_{24}$	0.4

Table S37: Summary of GC-MS identifications for the composition of the bio-oil produced by hydrothermal conversion of the model mixture 2 (300 °C, 60 min)

Retention time (min)	Identification	Chemical formula	Relative peak area (%)
50.7	9,12-Octadecadienoic acid	$C_{18}H_{32}O_2$	36.3
26.8	Phenol, 2-methoxy-	$C_7H_8O_2$	6.0
59.8	9-Octadecenamide, (Z)-	$C_{18}H_{35}NO$	3.9
45.9	9-Octadecenoic acid (Z)-, methyl ester	$C_{19}H_{36}O_2$	3.9
29.4	Phenol, 2-methoxy-4-methyl-	$C_8H_{10}O_2$	2.6
31.3	Phenol, 4-ethyl-2-methoxy-	$C_9H_{12}O_2$	2.4
45.8	9-Octadecenoic acid (Z)-, methyl ester	$C_{19}H_{36}O_2$	2.3
60.0	Not identified		1.9.
33.2	Phenol, 2-methoxy-4-propyl-	$C_{10}H_{14}O_2$	1.6
20.7	2-Cyclopenten-1-one, 2-methyl-	C_6H_8O	1.5
26.2	2-Ethylidenecyclohexanone	$C_8H_{12}O$	1.3
33.5	1-(Tihenyl-2)-1-formylethylene	C_7H_6OS	1.3
60.8	Not identified		1.2
61.3	(-)-Nortrachelogenin	$C_{20}H_{22}O_7$	1.1
46.0	9,12-Octadecadienoic acid, methyl ester	$C_{19}H_{36}O_2$	1.1
28.6	2-Methoxy-6-methylphenol	$C_8H_{10}O_2$	1.0
46.2	11,14-Eicosadienoic acid, methyl ester	$C_{21}H_{38}O_2$	1.0
28.7	2-Pyrrolidinone		1.0
39.3	Benzene, (1-methyldecyl)-	$C_{17}H_{28}$	0.9
25.4	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	0.9
23.8	2-Cyclopenten-1-one, 3-methyl-	C_6H_8O	0.9
41.8	Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	0.8
23.6	2-Cyclopenten-1-one, 2,3-dimethyl-	$C_7H_{10}O$	0.7
44.7	n-Hexadecanoic acid	$C_{16}H_{3202}$	0.7

46.0	9,12-Octadecadienoic acid, methyl ester	$C_{19}H_{36}O_2$	0.7
26.3	Phenol	C_6H_6O	0.7
27.2	Ethanone, 1-(3-thienyl)-	C_6H_6OS	0.7
29.2	Phosphonic acid, methyl-, bis(trimethylsilyl) ester	$C_7H_{21}O_3PSi_2$	0.7
4.2	Methyl Alcohol	CH_4O	0.7
20.4	Propane, 2,2-bis(methylthio)-	$C_5H_{12}S_2$	0.6
27.0	Ethanone, 1-(3-thienyl)-	C_6H_6OS	0.6
30.1	2-Acetyl-5-methylthiophene	C_7H_8OS	0.5
60.4	(R)-(-)-14-Methyl-8-hexadecyn-1-ol (derive acide gras)	$C_{17}H_{34}O$	0.5
26.1	Benzene, pentyl-	$C_{11}H_{16}$	0.5
30.9	Phenol, 4-ethyl-2-methoxy-	$C_9H_{12}O_2$	0.5
31.9	(4-Ethoxyphenyl)ethylamine	$C_{10}H_{15}NO$	0.5
53.5	Hexadecanamide	$C_{16}H_{33}NO$	0.5
40.9	Methyl-(2-hydoxy-3-ethoxy-benzyl)ether	$C_{10}H_{14}O_3$	0.4
30.4	Phenol, 4-ethyl-2-methoxy-	$C_9H_{12}O_2$	0.4
48.8	(R)-(-)-14-Methyl-8-hexadecyn-1-ol	$C_{17}H_{34}O$	0.4
29.5	2-Cyclopenten-1-one, 2,3,4,5-tetramethyl-	$C_9H_{14}O$	0.4
38.5	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	$C_{10}H_{12}O_3$	0.4
15.8	Cyclopentanone	C_5H_8O	0.4
32.7	2,5-Dimethoxyethylbenzene	$C_{10}H_{14}O_2$	0.4
23.3	Benzene, butyl-	$C_{10}H_{14}O_2$	0.4
37.9	Iridomyrmecin	$C_{10}H_{16}O_2$	0.4
60.8	Homovanillyl alcohol	$C_9H_{12}O_3$	0.3
61.3	(-)-Nortrachelogenin	$C_{20}H_{22}O_7$	0.3
52.8	2-Isopropyl-10-methylphenanthrene	$C_{18}H_{18}$	0.2
53.7	Hexanal, O-methyloxime	$C_7H_{15}NO$	0.2