

## **Hydrothermal liquefaction vs. fast/flash pyrolysis for biomass-to-biofuel conversion: New insights and comparative review of liquid biofuel yield, composition, and properties**

Farid Alizad Oghyanus<sup>1</sup>, Cigdem Eskicioglu<sup>1,2,3,\*</sup>

<sup>1</sup>UBC Bioreactor Technology Group, School of Engineering, University of British Columbia, Okanagan Campus, 3333 University Way, Kelowna, BC V1V 1V7, Canada.

<sup>2</sup>ICREA – Catalan Institution for Research and Advanced Studies, Pg. Lluís Companys 23, Barcelona, Spain.

<sup>3</sup>*Current address:* GEMMA – Group of Environmental Engineering and Microbiology, Department of Civil and Environmental Engineering, Universitat Politècnica de Catalunya – Barcelona Tech., c/Jordi Girona 1-3, Building D1, E-08034 Barcelona, Spain.

\* Corresponding author

E-mail addresses: [cigdem.eskicioglu@ubc.ca](mailto:cigdem.eskicioglu@ubc.ca). Tel.: +1 250 807 8544

**Table S1** Organic compounds in pyrolysis oil and bio-crude oil used for preparing Figure 8.

**Alcohols**

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2-Furanmethanol  
2,3-Propanediol  
2-Methyl-1-butanol  
3-Pyridinol  
3-hexanol  
Cholest-5-en-3-ol (3.beta)-  
Octaethylene glycol monododecyl ether  
Octaethylene glycol  
1,2-propanediol  
2,4-Dimethyl-2-oxazoline-4-methanol  
2-Furylmethanol  
Glycol  
Tetrahydrofurfuryl alcohol  
Glycerol  
1,3-diphenyl-1-butene-1-ol  
1,4-Cyclohexanediol, trans  
2-Hexadecen-1-ol,3,7,11,15-tetramethyl  
Terpineol  
6-epi-shyobunol  
(1.alpha.,2.beta.,5.alpha.)-(./-)-5-Methyl-2-(1-  
Dihydrocholesterol  
Stigmastenol  
3,7,11,15-Tetramethyl-2-hexadecen-1-ol  
Isophytol  
26-Norcoprostan-16,22-epoxy-3.alpha.,25-diol 3-O-acetyl-

## Acids

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3-Methyl-pentanoic acid  
Tetradecanoic acid  
Hexadecanoic acid  
Palmitic acid  
Pentanoic acid  
Acetic acid  
2-Butenoic acid, 2-methyl-, (E)-  
Oleic Acid  
Octanoic acid  
Capric acid  
Lauric acid  
Myristic acid  
Hexanoic acid  
Butanoic acid  
Propionic acid  
Palmitinic acid  
Pentadecanoic acid  
Lactic acid  
Benzoic acid, 3-hydroxy-  
Benzoic acid, 4-hydroxy-  
Dodecanoic acid  
Benzeneacetic acid, 3-hydroxy-  
Palmitelaidic acid  
11-cis-Octadecenoic acid  
Octadecanoic acid  
Eicosanoic acid  
Gamolenic acid  
9,12-Octadecadieoic acid  
Pentadecanoic acid  
Palmitic acid  
Palmitoleic acid  
Sulfurous acid, 2-propyl tetradecyl ester

## Phenols

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4-Methylphenol

2-Methylphenol (also known as o-Cresol)

4-Ethylphenol

2-Ethylphenol

2-Methoxyphenol (also known as Guaiacol)

Phenol

p-Cresol

3,5-Dimethylphenol

Benzene-1,2-diol (also known as Catechol)

2,4-Dimethylphenol

Phenol, 2-methoxy-4-methyl-

Phenol, 4-ethyl-2-methoxy-

Phenol, 2,6-dimethoxy-

Phenol, 2-methoxy-4-propyl-

2,6-Dimethylphenol

3,5-Dihydroxytoluene

Benzene-1,2,3-triol

4-(1-Hydroxy-ethylene)-2-methoxyphenol

4-[(1E)-3-Hydroxyprop-1-en-1-yl]phenol

2-Methylphenol (o-Cresol)

Cresol (refers to o-Cresol, p-Cresol, and m-Cresol)

3-Methoxycatechol

4-Ethylguaiacol

4-Methylcatechol

2,6-Dimethoxyphenol (also known as Syringol)

2-Methylcatechol

Phenol, 2,4-bis(1,1-dimethylethyl)-

## Ketones

|                                                |                                           |
|------------------------------------------------|-------------------------------------------|
| 3-Methyl-2-cyclopenten-1-one                   | 7-methylene-bicyclo[3.3.0]octan-2-one     |
| 2-Cyclopenten-1-one,2-methyl-                  | Bicyclo[3.3.0]octan-2-one, 7-benzylidene- |
| 3-Hydroxy-2-butanone                           | 1-Propanone, 1,3-diphenyl                 |
| Cyclopentanone                                 | 2-Heptadecanone                           |
| 2,3-Butanedione                                | acetovanillone                            |
| 1-Acetyloxy-2-Propanone                        | Cyclopentanone                            |
| 2-Methyl furyl ketone                          | 1,2,3-Trimethylpiperidin-4-one            |
| 3-Methyl-2-cyclopenten-1-one                   | Cyclopentanone                            |
| 1,4-Butanedione                                | Cyclohexanone                             |
| 2-Hydroxy-2-cyclopenten-1-one                  | 3,4-Dimethyl-2-cyclopenten-1-one          |
| 2-Hydroxy-3-methyl-2-cyclopenten-1-one         | 2,3,4-Trimethyl-2-cyclopenten-1-one       |
| 2,3-Dimethyl-2-cyclopenten-1-one               | 2-Pentadecanone                           |
| 3,5-Dimethyl-2-cyclopenten-1-one               | 1,2 cyclopentanedione                     |
| 3-Ethyl-2-hydroxy-2-cyclopenten-1-one          | 2-Methyl-2-cyclopenten-1-one              |
| 2-Cyclopenten-1-one, 2-methyl-                 | 2,3-Dimethyl-2-cyclopenten-1-one          |
| 1,2-Cyclopentanedione, 3-methyl-               | Methyl ionone                             |
| 2-Cyclopenten-1-one                            | 2-Methyl-cyclopentanone                   |
| 2-Cyclopenten-1-one, 2,3-dimethyl-             | 2-Cyclopenten-1-one, 3-ethyl-             |
| 2-cyclopentanone                               | 2-Pentanone, 4-hydroxy-4-methyl-          |
| 3,5-dimethylcyclopentenolone                   | 3,6-Heptanedione                          |
| 2-Cyclopenten-1-one                            | 3-Penten-2-one, 4-methyl-                 |
| 1,2-Cyclopentanedione, 3-methyl                | 7-Ethyl-4,6-heptadecandione               |
| 2-Cyclopenten-1-one, 3-methyl                  | 4-Piperidinone, 2,2,6,6-tetramethyl       |
| 2-Cyclopenten-1-one, 2,3-dimethyl              | 4,6-Octadiyn-3-one, 2-methyl              |
| 2-Cyclopenten-1-one, 3-ethyl-2-hydroxy         | 2-Cyclopenten-1-one, 2-methyl             |
| Cyclopentanone                                 |                                           |
| 2-hydroxy-3-methyl-2-cyclopenten-1-one         |                                           |
| 2,3-Dimethyl —2-Cyclopenten-1-one              |                                           |
| 2-methyl-2-cyclopenten-1-one                   |                                           |
| 3-ethyl-2-cyclopenten-1-one                    |                                           |
| 2-Furyl methyl ketone                          |                                           |
| 2-Cyclopenten-1-one, 2-methyl                  |                                           |
| Ethanone, 1-(2-furanyl)-                       |                                           |
| 2,5-Hexanedione                                |                                           |
| 2-Pentanone, 4-hydroxy-4-                      |                                           |
| 2-Cyclopenten-1-one, 2-hydroxy-                |                                           |
| 2-Cyclopenten-1-one, 3,5,5-trimethy            |                                           |
| 2-Cyclopenten-1-one, 2,3-                      |                                           |
| 2-Cyclopenten-1-one, 2,3-dimethyl              |                                           |
| 2-Cyclopenten-1-one, 2,3,4-trimethyl-          |                                           |
| Bicyclo[4.3.0]nonan-7-one, 1-(2-methoxyvinyl)- |                                           |

## Aliphatics

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|                                                   |               |
|---------------------------------------------------|---------------|
| 3,4-Dihydroxy-1-butene                            | Neophytadiene |
| Diethylacetylene                                  |               |
| Spiropentane                                      |               |
| 2-Methyl-1,3-butadiene                            |               |
| Stigmastan-3,5-diene                              |               |
| Cyclododecane                                     |               |
| Cholest-2 (4)-ene                                 |               |
| cholesta-3,5-diene                                |               |
| Udecane                                           |               |
| Dodecane                                          |               |
| Tridecane                                         |               |
| Tetradecane                                       |               |
| Pentadecane                                       |               |
| Hexadecane                                        |               |
| 8-Heptadecene                                     |               |
| Heptadecane                                       |               |
| cyclohexane                                       |               |
| 2,3,4-Trimethylhexane                             |               |
| 2,6,11-Trimethyldodecane                          |               |
| Octadecane, 5-methyl                              |               |
| n-Eicosane                                        |               |
| 2,4,8,8-Tetramethyldecahydrocyclopropa            |               |
| Octadecane,3-ethyl-5-(2-ethylbutyl)               |               |
| 1,4-Dimethyl-2-octadecyl-cyclohexane              |               |
| Octadecane                                        |               |
| Octadecane, 4-methyl                              |               |
| Tricosane                                         |               |
| Heneicosane                                       |               |
| 1,1'-(1,2-Dimethyl-1,2-ethanediyl)bis-cyclohexane |               |
| Eicosane                                          |               |
| Dodecane                                          |               |
| Tetradecane                                       |               |
| 1-Pentadecene                                     |               |
| 8-Heptadecene                                     |               |
| 2,6,6-Trimethylbicyclo[3.1.1]heptane              |               |
| 2,6,10,14-Tetramethyl-2-hexadecene                |               |
| Butane, 2,3-dimethyl-                             |               |
| Cyclopentane, 1,1,3-trimethyl                     |               |
| 5-Decene, 1-bromo                                 |               |
| Cyclopentane, (2-methylbutyl)                     |               |
| 7-Pentadecyne                                     |               |
| Decane,3,7-dimethyl-                              |               |

## Aromatics

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2,4-Dimethylfuran

Toluene

Ethylbenzene

Xylenes

Styrene

Benzene, 1,2,3-trimethyl-

Benzene, 1,2,4-trimethyl-

Benzene, 2-propenyl-

Benzene, 1-ethenyl-2-methyl-

Indane

Benzene, 1-propynyl

Benzene, 4-ethenyl-1,2-dimethyl-

1H-indene, 3-methyl-

Naphthalene, 1,2-dihydro-

Benzene, (1-methylene-2-propenyl)-

3-Methylindene

1H-indene, 1-methylene-

Naphthalene, 1,2-dihydro-3-methyl-

Naphthalene, 2-methyl-

Naphthalene, 1,4-dimethyl-

Naphthalene, 2-(1-methylethyl)-

Naphthalene, 2,3,6-trimethyl-

1H-Indene,1-hexadecyl-2,3-dihydro-

Maltol

Benzene, 1-ethyl-3-methyl-

furfural

Benzo[a]pyrene

$\beta$ -Ylangene

$\beta$ -phellandrene

$\Delta$ -cadinene

Methyl phenantharene

Ethyl benzene

Styrene

Benzedrex

Dibutyl phthalate

Benzene, 1-ethyl-2-methyl

Benzene, (1-methylethyl)

## N-containing compounds

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|                                          |                                                                |
|------------------------------------------|----------------------------------------------------------------|
| N,N-Dimethylmethanamine                  | Dodecanamide                                                   |
| 2-Methylpyridine                         | Hexadecanamine                                                 |
| 4-Methylpyridine                         | 3-Hydroxybutylquinoline                                        |
| 3-Methylpyridine                         | 1-Heptadecanamine, N,N-dimethyl-                               |
| Pyridine                                 | N-(2-Phenylethyl)acetamide                                     |
| Hexadecanamide                           | L-Proline, N-valeryl-, heptadecyl ester                        |
| (Z)-9-Hexadecenamide                     | 2,8,9-Trioxa-5-aza-1-silabicyclo[3.3.3]undecane, 1-ethyl-      |
| Octadecanamide                           | N,N-Dimethyloctanamide                                         |
| Ethanamine                               | Cyclo(L-leucyl-L-phenylalanine)                                |
| Propanamide                              | Ergotaman-3',6',18-trione, 9,10-dihydro-12'-hydroxy-2'-methyl- |
| Pyrrole                                  | 13-Docosenamide, (Z)-                                          |
| Indole                                   | Methylphenidate                                                |
| Indolizine                               | 2-Ethoxy-4,4,5,5-tetramethyloxazoline                          |
| 1-Methylindole                           | N-Ethyl-2-isopropoxycarbonylazetidine                          |
| 2-Pyrrolidinone                          | Trimethylamine                                                 |
| 1-Methyl-2,5-pyrrolidinedione            | 1-Butylhydantoin                                               |
| (Z)-9-Octadecenamide                     | 3,6-Diisopropylpiperazine-2,5-dione                            |
| 2,5-Pyrrolidinedione                     | Diphenylamine                                                  |
| Benzyl cyanide                           | Azelaic dihydrazide                                            |
| 2-Piperidinone                           | 2-Chloro-N-(1,2-dichloroethenyl)ethanimidamide                 |
| 3-Methylindole                           | N-(1-Methylbutyl)-2-pentanamine                                |
| Pentadecanenitrile                       | 3,6-Bis(2-methylpropyl)-2,5-piperazinedione                    |
| Glycylproline                            | N-Hydroxy-N-methylmethanamine                                  |
| Tetradecanamide                          | N-Ethylmyristamide                                             |
| Heptadecanenitrile                       | N-Methylmyristamide                                            |
| N,N-Dimethyloctanamide                   | N-(3-Methylbutyl)myristamide                                   |
| Pramoxine                                | 10-Methyl-dodecanoic acid pyrrolidide                          |
| 3-Hydroxypyridine                        | N-Butyl-(Z)-9-octadecenamide                                   |
| N-Methylformamide                        | Pyrrolidine, 1-(1-oxo-9-octadecenyl)-                          |
| Oleonnitrile (octadecanenitrile)         | N-Ethyl-2-isopropoxycarbonylazetidine                          |
| Pterin-6-carboxylic acid                 | Trimethylamine                                                 |
| N-(2-Amino-2-oxoethyl)-2-tetradecynamide | Hydantoin, 1-butyl                                             |
| 4-Piperidinone, 2,2,6,6-tetramethyl      | 3,6-Diisopropylpiperazin-2,5-dione                             |
| 1-(2-Phenylethyl)piperidine              | Diphenylamine                                                  |
| N-Methyldodecanamide                     | Azelaic dihydrazide                                            |
| 1-Ethyl-2-pyrrolidinone                  | Ethanimidamide, 2-chloro-N-(1,2-dichloroethenyl)               |
| 1-Methylpyrazine                         | 2-Pentanamine, N-(1-methylbutyl)                               |
| 2,5-Dimethylpyrazine                     | 2,5-Piperazinedione, 3,6-bis(2-methylpropyl)                   |
| 2,3,4,5-Tetramethylpyrrole               | Methanamine, N-hydroxy-N-methyl-                               |
| 3-Ethyl-2,4,5-trimethylpyrrole           |                                                                |



**N-containing compounds (Continued)**

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2-Methyl-5-hydroxypyridine

9-Octadecenamide

9-Octadecenamide, N,N-dimethyl-

Dodecanamide, N-ethyl-

Myristamide, N-(3-methylbutyl)-

10-Methyl-dodecanoic acid, pyrrolidide

9-Octadecenamide, n-butyl-

Pyrrolidine, 1-(1-oxo-9-octadecenyl)-

5,10-Diethoxy-2,3,7,8-tetrahydro-1H,6H-dipyrrolo[1,2-a:10',20'-d]pyrazine

Myristamide, N-ethyl-

Hexadecanamide

Myristamide, N-methyl-

Myristamide, N-ethyl-

## Oxygenated compounds

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|                                                            |                                                       |
|------------------------------------------------------------|-------------------------------------------------------|
| 2(5H)-Furanone                                             | Cyclobutyl tridecyl oxalate                           |
| Methyl butanedioate                                        | Ethyl octadecanoate                                   |
| 3,4-Anhydro-d-galactosan                                   | Heptadecanolide                                       |
| Propaldehyde                                               | 4,4-Dimethyl-2-(1-hydroxyheptadec-8-enyl)-2-oxazoline |
| 2-Cyclopenten-1-one                                        | Oxalic acid, butyl cyclohexylmethyl ester             |
| Ethenyl acetate                                            | Dimethyl 2-ethyl-3-methylbutenedioate                 |
| Acetaldehyde                                               | Butyl cyclohexylmethyl oxalate                        |
| Dihydro-2(3H)-furanone                                     | Methyl hexadecanoate                                  |
| 3,4-Dihydropyran                                           |                                                       |
| Methoxyethylene                                            |                                                       |
| 2-Hydroxy-3,4-dimethyl-2-cyclopenten-1-one                 |                                                       |
| Dianhydro-mannitol                                         |                                                       |
| Isosorbide                                                 |                                                       |
| 1,2-Benzenediol, 4-methyl-                                 |                                                       |
| Bis(2-methylpropyl) 1,2-benzenedicarboxylate               |                                                       |
| Methyl hexadecanoate                                       |                                                       |
| Ethyl hexadecanoate                                        |                                                       |
| Diisooctyl 1,2-benzenedicarboxylate                        |                                                       |
| Tetradecyl hexadecanoate                                   |                                                       |
| 1,4,7,10,13,16-Hexaoxacyclooctadecane                      |                                                       |
| Octaethylene glycol monododecyl ether                      |                                                       |
| 18,18'-Bi-1,4,7,10,13,16-hexaoxacyclononadecane            |                                                       |
| 1,4,7,10,13-Pentaoxacyclopentadecane                       |                                                       |
| 2-(2-[2-(2-Methoxy-ethoxy)-ethoxy]-ethoxy)-ethoxy)-ethanol |                                                       |
| Dianhydromannitol                                          |                                                       |
| Methyl palmitate                                           |                                                       |
| 2-Furancarboxaldehyde                                      |                                                       |
| 2-Furancarboxaldehyde, 5-methyl                            |                                                       |
| 4-Hydroxybenzaldehyde                                      |                                                       |
| 4-Hydroxy-3-methoxybenzaldehyde                            |                                                       |
| 4-Hydroxy-3,5-dimethoxybenzaldehyde                        |                                                       |
| Vanillin                                                   |                                                       |
| N-Decanal                                                  |                                                       |
| Lauraldehyde                                               |                                                       |
| Butyric acid, 4-pentadecyl ester                           |                                                       |
| 5,6,7,7a-Tetrahydro-4,4,7a-trimethyl-2(4H)-benzofuranone   |                                                       |
| Trans-Z-alpha-bisabolene epoxide                           |                                                       |
| Diocetyl phthalate                                         |                                                       |
| Geranyl acetate                                            |                                                       |
| Methyl palmitate                                           |                                                       |
| Methyl 2-oxo-1-pyrrolidine acetate                         |                                                       |
| Methyl tetradecanoate                                      |                                                       |
| Tridec-2-ynyl 4-cyanobenzoate                              |                                                       |
| Gamma-tocopherol                                           |                                                       |
| (+)-Gamma-tocopherol O-methyl                              |                                                       |
| Tetrahydropyran Z-10-dodecenoate                           |                                                       |