Thermo-Catalytic Reforming of Spent Coffee Grounds

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**Table S1.** Compounds and oxygenates detected through GC–MS analysis of produced bio-oil:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compound name | Molecular formula | SI (%) | Ret. Time (min) | Peak Area x 106 | | |
| TCR® Oil at 500°C | TCR® Oil at 600°C | TCR® Oil at 700°C |
| Ethanol | C2H5OH | 98 | 2.233 | - | - | 0.81 |
| Benzene | C6H6 | 97 | 3.629 | - | 2.1 | 1.44 |
| Toluene | C7H8 | 99 | 5.555 | 1.15 | 3.89 | 4.12 |
| Ethylbenzene | C8H10 | 98 | 7.557 | - | 1.09 | 1.13 |
| p-Xylene | C8H10 | 97 |  | - | 1.02 | - |
| Styrene | C8H8 | 96 | 8.204 | 0.81 | 3.18 | 4.51 |
| Phenol | C6H5OH | 99 | 9.833 | 0.97 | 2.21 | 2.51 |
| 1-Decene | C10H20 | 97 | 10.09 | 0.46 | - | - |
| Benzene, 1-ethenyl-2-methyl- | C9H10 | 96 | 10.23 | - | 1.09 | 0.67 |
| 1H-Indene, 1-chloro-2,3-dihydro- | C9H9Cl | 96 | 11.173 | - | 2.8 | 3.58 |
| Phenol, 2-methyl- | C7H8O | 93 | 11.192 | 0.7 | - | - |
| p-Cresol | C7H8O | 95 | 11.554 | 0.91 | 1.81 | 2.03 |
| 1-Undecene | C11H22 | 97 |  | - | 0.88 |  |
| 9,12-Octadecadienoic acid (Z,Z)- | C18H32O2 | 96 | 11.865 | 2.62 | - | - |
| 2-Methylindene | C10H10 | 95 | 12.966 | - | 1.04 | 0.81 |
| Tetracyclo[5,3,0,0<2,6>,0<3,10>]deca-4,8-diene | C10H10 | 80 | 5.555 | - | 1.34 | - |
| 1-Tridecene | C13H26 | 96 | 13.494 | 0.64 | 0.96 | - |
| Naphthalene | C10H8 | 98 | 13.622 | 2.35 | 5.59 | 10.54 |
| Isoquinoline | C9H7N | 97 | 14.436 | - | - | 0.58 |
| 1-Pentadecene | C15H30 | 96 | 15.007 | - | 0.78 | - |
| 1-Tetradecene | C14H28 | 96 | 15.007 | 1.01 | - | - |
| Indole | C8H7N | 96 | 15.183 | - | - | 1.13 |
| Naphthalene, 1-methyl- | C11H10 | 96 | 15.308 | - | 1.56 | 2.07 |
| Naphthalene, 1-methyl- | C11H10 | 97 | 15.547 | - | 1.31 | 1.71 |
| 1-Tetradecene | C14H28 | 96 | 16.425 | 0.45 | 1.31 | - |
| Biphenyl | C12H10 | 98 | 16.477 | 0.72 | - | 1.78 |
| Acenaphthylene | C12H8 | 95 | 17.518 | - | 1.05 | 2 |
| 1-Heptadecene | C17H34 | 96 | 17.759 | - | 0.84 |  |
| 1-Pentadecene | C15H30 | 96 | 17.759 | 0.52 | - | - |
| Heptadecane | C17H36 | 96 | 17.854 | - | 1.55 | - |
| Pentadecane | C15H32 | 96 | 17.855 | 1.21 | - | - |
| Fluorene | C13H10 | 94 | 19.235 | - | - | 1.16 |
| Phenanthrene | C14H10 | 97 | 21.622 | 1.1 | 1.69 | 4.32 |
| Phenanthrene | C14H10 | 96 | 21.747 | - | - | 1.06 |
| n-Hexadecanoic acid | C16H32O2 | 95 | 23.144 | 15.53 | 3.95 | - |
| Hexadecanoic acid, ethyl ester | C18H36O2 | 94 | 23.454 | 0.48 | - | - |
| Naphthalene, 2-phenyl- | C16H12 | 95 | 23.601 | - | - | 0.89 |
| Octadecanoic acid, 2-propenyl ester | [C21H40O2](https://pubchem.ncbi.nlm.nih.gov/#query=C21H40O2) | 88 | 24.276 | 1.25 | 0.96 | - |
| Pyrene | C16H10 | 96 | 24.581 | - | - | 0.71 |
| 9-Tricosene, (Z)- | C23H46 | 94 | 24.829 | 0.53 | - | - |
| Oleic Acid | C18H34O2 | 92 | 24.885 | 4.23 | - | - |
| cis-9-Hexadecenal | C16H30O | 88 | 24.933 | 3.12 | - | - |
| Octadecanoic acid | C18H36O2 | 93 | 25.09 | 3.79 | - | - |
| Pyrene | C16H10 | 94 | 25.136 | - | - | 1.03 |
| Hexadecanamide | [C16H33NO](https://pubchem.ncbi.nlm.nih.gov/#query=C16H33NO) | 76 | 25.284 | 0.67 | 1.21 | 0.71 |
| Palmitoleamide | [C16H31NO](https://pubchem.ncbi.nlm.nih.gov/#query=C16H31NO) | 92 | 26.935 | 0.75 | - | - |