

Upgrading of Napier grass pyrolytic oil using microporous and hierarchical mesoporous zeolites: products distribution, composition and reaction pathways

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Table S 1: Composition of the aqueous phase from thermal and catalytic cracking of Napier grass pyrolytic oil over Zeolite

Reaction condition: 400 °C, 60 min and 2.0 wt% Catalyst loading

Compound	% Peak area
Thermal Cracking	
Cyclopentanol, 1-[3-(methylthio)-2-propenyl]-	5.94
1-Cyclohexene, 1-ethynyl-	4.82
1-Cyclohexene-1-acetonitrile	4.07
Cyclohexanone, 2-ethyl-, oxime	4.78
(2-Methyl-cyclohex-2-enylidene)-acetaldehyde	4.02
5-Methyl-2-nitrobenzyl alcohol	4.27
Phenol, 2,6-dimethyl-	3.78
Tricyclo[3.3.0.0(2,8)]octane-3,7-dione, 4-methyl-4-(propan-2-on-1-yl)-	3.79
1,3-Cyclohexadiene-1-methanol, 4-(1-methylethyl)-	4.79
1,5-Bis(4-nitrophenyl)carbazine	4.15
1,3-Benzenediol, 2-methyl-	6.56
2,3-Dimethoxyphenethylamine	3.60
2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-1-methoxy-	4.38
Benzenemethanol, 3-hydroxy-5-methoxy-	7.57
2,4-Dimethoxybenzeneethanamine	7.07
Benzaldehyde, 2,3-dimethoxy-	3.50
Cyclopentaneacetaldehyde, 2-formyl-3-methyl-à-methylene-	9.29
9-Ethoxy-10-oxatricyclo[7.2.1.0(1,6)]dodecan-11-one	6.12
2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-1-methoxy-	3.77
Bicyclo[4.3.0]nonan-7-one, 1-(2-methoxyvinyl)-	3.74
ZSM-5	
1,2,3,4,5-Cyclopentanepentol	3.26
Butanoic acid, 4-hydroxy-	2.53
2(1H)-Pyridinone, 1-ethenyl-	1.77
2,4-Hexadiyne-1,6-diol	12.01
2-Cyclopenten-1-one, 3,4-dimethyl-	2.51
Benzyl alcohol	6.78
Phenol, 2-methyl-	9.08
Phenol, 4-ethyl	1.78
Phenol, 2,4-dimethyl-	4.07
Phenol, 2,6-dimethyl-	9.53
2,4-Hexadiyne-1,6-diol	11.70
Phenol, 2-ethyl-6-methyl-	1.80
1,3-Benzenediol, 2-methyl-	4.72
Resorcinol	4.38
1,3-Benzenediol, 2-methyl-	6.73
1,4-Benzenediol, 2-methyl-	5.14
1,4-Benzenediol, 2,6-dimethyl-	2.18
4-Ethylcatechol	5.27
1,3-Benzenediol, 4-propyl-	2.44
Cyclopentan-1-al, 4-isopropylidene-2-methyl-	2.32

0.2HZSM-5

D-Valine	4.15
Butane, 2-ethoxy-2-methyl-	4.46
1,4-Cyclohexanediol, cis-	3.99
Pyridine, 3-methyl-	3.38
2(3H)-Furanone, 5-ethoxydihydro-	5.03
Bicyclo[2.2.0]hexane-1-carboxaldehyde	10.19
2,4-Cyclopentadiene-1-ethanamine	8.79
1-Cyclohexene, 1-ethynyl-	6.81
2-Cyclopenten-1-one, 2,3,4-trimethyl-	4.25
Phenol, 2,3-dimethyl-	4.21
3-Caren-10-al	6.66
Phenol, 2,6-dimethyl-	6.74
3,6,10,10-Tetramethyl-1-oxa-spiro[4.5]deca-3,6-dien-2-one	3.00
Phenol, 3,4,5-trimethyl-	4.38
1,3-Benzenediol, 2-methyl-	4.74
1,4-Benzenediol, 2,5-dimethyl-	3.31
2,3-Dimethylhydroquinone	4.12
2-Cyclopenten-1-one, 4-hydroxy-3-methyl-2-(2-propenyl)-	3.98
Benzoic acid, 2,5-bis(trimethylsiloxy)-, trimethylsilyl ester	3.30
Benzoic acid, 2,5-bis(trimethylsiloxy)-, trimethylsilyl ester	4.48

0.3HZSM-5

L-Glucose, 6-deoxy-3-O-methyl-	4.81
3,4-Dihydroxy-5-methyl-dihydrofuran-2-one	4.06
Methyl 4-hydroxybutanoate	6.36
2-Cyclopenten-1-one, 2,3-dimethyl-	3.42
2,4-Heptadien-6-yn-1-ol, (E,E)-	8.23
Benzeneethanamine, 4-methoxy-	5.85
Spirohexan-4-one, 5,5-dimethyl-	5.70
Spiro[4.4]non-3-en-2-one, 4-methyl-3-(1H-tetrazol-5-yl)-1-oxa-	5.57
Benzyl alcohol, p-hydroxy-à-[(methylamino)methyl]-	4.59
Phenol, 2,6-dimethyl-	3.87
Cyclopentanone, 2-cyclopentylidene-	3.47
(2-Methyl-cyclohex-2-enylidene)-acetaldehyde	3.69
2-Cyclopenten-1-one, 4-hydroxy-3-methyl-2-(2-propenyl)-	5.10
1,3-Benzenediol, 2-methyl-	5.32
Cyclohexene, 1-(2-nitro-2-propenyl)-	4.23
2,3-Dimethylhydroquinone	3.79
1-Cyclohexene-1-ethanol, 2,6,6-trimethyl-	3.82
3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl-	3.34
Cyclohexene, 4-isopropenyl-1-methoxymethoxymethyl-	11.23
1,4-Benzenediol, 2,3,5-trimethyl-	3.58
