In-situ upgrading of Napier grass pyrolysis vapour over microporous and hierarchical mesoporous zeolites

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Table 1: Characteristics of Napier grass biomass [18]

Standard used	Property	**This study**	Strezov et al. [26]	Lee et al. [27]	Braga et al. [28]	Sousa et al. [29]	De Conto et al. [30]
			Proximate analysis (wt %)				
BS EN 14774-1	Moisture Content[a]	75.27 ± 0.21	12.40	9.43	10.04	-	10.63
BS EN 15148	Volatile Matter[b]	81.51 ± 0.26	66.90	72.58	65.00	-	72.54
BS EN 14775	Ash Content[b]	1.75 ± 0.04	2.90	9.68	6.90	-	8.26
	Fixed Carbon[c]	16.74 ± 0.05	-	-	14.66	-	19.20
BS EN 14918	HHV(MJ/kg)	18.05 ± 0.07	-	-	15.61	-	15.77
			Ultimate analysis (wt%) dry basis				
	Carbon (C)	51.61 ± 0.24	41.6	42.4	44.5	41.85	39.63
	Hydrogen (H)	6.01 ± 0.02	4.83	5.96	5.4	6.77	6.31
	Nitrogen (N)	0.99 ± 0.01	0.43	1.71	1.4	0.72	1.70
	Sulfur (S)	0.32 ± 0.01	-	0.09	-	48.64	0.20
	Oxygen (O)[c]	41.07 ± 0.02	-	45.32	31.8	-	52.16
	O/C (atomic ratio)	0.80	-	-	-	-	-
	H/C (atomic ratio)	0.12	-	-	-	-	-
NREL/TP-510-42618			Structural composition (wt %)				
	Cellulose	38.75 ± 2.30		66.59	39.14	-	30.37
	Hemicellulose	19.76 ± 1.68			19.9	-	31.31
	Lignin	26.99 ± 1.29		26.72	6.18	-	26.02
	Extractives	12.07 ± 0.32		-		-	14.86
BS EN 15290			Atomic absorption analysis of ash (mg/kg)				
	Sodium (Na)	12.85±1.05	-	-	-	-	-
	Potassium (K)	3079.51±224.80	-	-	-	-	-
	Calcium (Ca)	206.71±13.20	-	-	-	-	-
	Aluminum (Al)	64.67±4.66	-	-	-	-	-
	Iron (Fe)	38.93±4.01	-	-	-	-	-
	Silicon (Si)	206.0±25.13	-	-	-	-	-

Notes: [a] as received at harvest; [b] dry basis; [c] by difference. Values are the means (n =3) ± standard deviations

Table 2: Treatment condition and characteristics of zeolite ([a]determined by X-ray fluorescence; [b]Brunauer–Emmett–Teller method; [c]t-plot method; [d]Vmeso=Vpore -Vmicro)

Catalyst	C_{NaOH}	(Si/Al)[a]	$(S_{BET})^b$	$(S_{micro})^c$	$(S_{meso})^c$	(V_{pore})	$(V_{micro})^c$	$(V_{meso})^d$	total acidity
	(mol/L)	(mol/mol)	surface area (m^2/g)			volume (cm^3/g)			(mmol/g)
ZSM-5	0.00	20.76	385.20	356.54	28.66	0.1540	0.1383	0.0157	3.8085
0.2HZSM-5	0.20	13.79	369.43	274.66	114.76	0.2685	0.1039	0.1646	3.0036
0.3HZSM-5	0.30	12.51	374.88	240.23	134.65	0.3670	0.1114	0.2556	2.9635

Table 3: Physicochemical properties of in-situ catalytic upgraded bio-oil organic phase

Catalyst	(wt%)	(g)	Biomass (g)	Bio-oil organic phase elemental analysis (%) C	H	N	S	O	DOD	HHV (MJ/kg)	PH
Raw	0.0	0.00	200.00	50.89	6.02	0.88	0.23	41.98	0.00	26.77	2.65
ZSM-5	0.5	1.00	200.00	58.92	6.42	0.85	0.44	33.37	20.51	27.11	2.99
	1.0	2.00	200.00	62.11	6.55	0.95	0.56	29.83	28.94	29.10	2.97
	2.0	4.00	200.00	64.40	6.76	0.53	0.53	27.78	33.83	30.07	2.88
	3.0	6.00	200.00	65.12	6.79	0.97	0.64	26.48	36.92	31.51	2.95
0.2HZSM-5	0.5	1.00	200.00	61.72	6.11	0.78	0.26	31.13	25.85	29.97	2.9
	1.0	2.00	200.00	63.01	6.23	0.81	0.34	29.61	29.47	33.18	2.70
	2.0	4.00	200.00	63.87	6.56	0.91	0.41	28.25	32.71	36.56	2.60
	3.0	6.00	200.00	66.09	6.22	0.87	0.39	26.43	37.04	37.34	2.60
0.3HZSM-5	0.5	1.00	200.00	61.95	6.21	0.81	0.28	30.75	26.75	28.88	2.60
	1.0	2.00	200.00	62.98	6.31	0.88	0.29	29.54	29.63	35.18	2.90
	2.0	4.00	200.00	64.51	6.33	0.96	0.24	27.96	33.40	35.89	3.00
	3.0	6.00	200.00	66.77	6.24	0.79	0.25	25.95	38.18	38.71	3.50

Table 4: Group of organic compound in the deoxygenated bio-oil over ZSM-5, 0.2HZSM-5 and 0.3HZSM-5

Composition (%)	ZSM-5 CBR (wt %)			
	0.00	1.00	2.00	3.00
HC	4.67	16.30	22.88	28.89
ARHC	2.53	15.19	11.17	15.69
MARHC	2.18	3.41	17.48	9.93
PHOL	28.15	18.71	33.10	29.55
MPHOL	37.87	14.51	11.30	9.13
AAK	16.88	5.94	1.77	0.69
MEST	4.68	6.33	1.23	0.00
OVAC	3.05	19.62	1.07	6.12
	0.2HZSM-5 CBR (wt %)			
	0.00	1.00	2.00	3.00
HC	4.67	15.46	14.62	12.18
ARHC	2.53	2.60	8.31	14.16
MARHC	2.18	1.20	5.99	0
PHOL	28.15	57.95	54.50	61.41
MPHOL	37.87	4.92	0	0
AAK	16.88	2.18	2.90	5.75
MEST	4.68	4.60	4.13	5.45
OVAC	3.05	11.08	9.56	1.05
	0.3HZSM-5 CBR (wt %)			
	0.00	1.00	2.00	3.00
HC	4.67	9.25	11.55	7.19
ARHC	2.53	8.98	6.31	24.72
MARHC	2.18	9.21	3.09	4.30
PHOL	28.15	61.01	58.14	45.03
MPHOL	37.87	3.83	4.64	0.00
AAK	16.88	0.00	4.31	2.84
MEST	4.68	4.40	0.00	5.84
OVAC	3.05	3.33	11.96	10.08

(HC) hydrocarbons, (ARHC) aromatic hydrocarbons, (MARHC) methoxy aromatics, (PHOL) phenol, (MPHOL) methoxy phenol, (AAK) acids, aldehydes and ketones, (MEST) methyl ester and (OVAC) other value added chemical.

Table 5: Composition of non-condensable gas (nitrogen free basis) collected at 3.0 wt% CBR

Catalyst Type	CBR (wt %)	Gas Composition (vol %) N_2-free basis			
		CH_4	H_2	CO	CO_2
Raw	0.0	3.36	25.32	13.60	14.04
ZSM-5	3.0	2.34	10.36	22.14	27.95
0.2HZSM-5	3.0	3.26	8.31	33.97	30.32
0.3HZSM-5	3.0	3.01	7.94	37.67	28.07

Supplementary materials

Supplementary Table 1: GC-MS analysis of organic phase bio-oil obtained from non-catalytic pyrolysis

RT (min)	Compound	Formula	Area%
	Organic Phase		
3.85	1,3-DIMETHYL-1-CYCLOHEXENE	C_8H_{14}	4.67
4.03	1H-IMIDAZOLE-2-METHANOL	$C_4H_6ON_2$	3.05
5.13	PHENOL	C_6H_6O	8.43
5.76	PHENOL, 2-METHYL-	C_7H_8O	4.06
5.93	PHENOL, 3-METHYL-	C_7H_8O	4.96
6.06	PHENOL, 2-METHOXY-	$C_7H_8O_2$	7.65
6.51	PHENOL, 2,4-DIMETHYL-	$C_8H_{10}O$	2.50
6.64	PHENOL, 3-ETHYL-	$C_8H_{10}O$	8.20
6.86	CREOSOL	$C_8H_{10}O_2$	3.68
7.03	BENZALDEHYDE, 4-METHYL-	C_8H_8O	13.41
7.47	PHENOL, 4-ETHYL-2-METHOXY-	$C_9H_{12}O_2$	5.39
7.73	2-METHOXY-4-VINYLPHENOL	$C_9H_{10}O_2$	6.74
7.96	PHENOL, 2,6-DIMETHOXY-	$C_8H_{10}O_3$	8.85
8.57	1,2,3-TRIMETHOXYBENZENE	$C_9H_{12}O_3$	2.18
8.63	PHENOL, 2-METHOXY-4-(1-PROPENYL)-, (Z)-	$C_{10}H_{12}O_2$	2.44
9.05	4-ETHYLBIPHENYL	$C_{14}H_{14}$	2.53
9.30	4-METHYL-2,5-DIMETHOXYBENZALDEHYDE	$C_{10}H_{12}O_3$	1.74
10.08	PHENOL, 2,6-DIMETHOXY-4-(2-PROPENYL)-	$C_{11}H_{14}O_3$	3.12
10.43	DESASPIDINOL	$C_{11}H_{14}O_4$	1.73
19.06	1,4-BENZENEDICARBOXYLIC ACID, BIS(2-ETHYLHEXYL) ESTER	$C_{24}H_{38}O_4$	4.68

Supplementary Table 2: Compounds detected in the upgraded organic phase oil over ZSM-5

	In-situ upgraded samples with ZSM-5		GC-MS peak area (%)		
RT (min)	Compound	Formula	1.0 wt%	3.0 wt%	2.0 wt%
3.02	2,5-CYCLOOCTADIEN-1-OL	C8H12O	5.48	0.00	0.00
3.02	1-HEXEN-3-YNE, 2-METHYL-	C7H10	0.00	0.00	0.00
3.02	2,3-DIMETHYL-CYCLOHEXA-1,3-DIENE	C8H12	0.00	0.00	0.00
3.02	1-TRIDECENE	C13H26	0.00	7.26	0.00
3.75	2-BUTYNE, 1,4-DICHLORO-	C4H4Cl2	3.05	0.00	1.62
3.79	BICYCLO[2.2.1]HEPT-5-ENE-2,2-DIMETHANOL	C9H14O2	0.00	3.72	0.00
3.86	TRICYCLO[3.2.1.0(2,4)]OCTANE, 3-METHYLENE-	C9H12	2.56	0.00	0.00
4.14	OCTADECANOIC ACID, PHENYL ESTER	C24H40O2	4.07	0.00	0.00
4.19	BICYCLO[2.2.2]OCT-5-EN-2-ONE, 7-SYN-HYDROXY-	C8H10O2	0.00	0.00	0.00
4.54	1,7,7-TRIMETHYLBICYCLO[2.2.1]HEPTAN-2-OL	C10H18O	4.19	0.00	0.00
4.57	5,6-DIBROMO-5-METHYL-HEX-1-ENE	C7H12Br2	0.00	0.00	0.00
4.57	1,1'-BICYCLOHEPTYL	C14H26	0.00	5.12	5.08
4.67	CYCLOBUTANECARBOXYLIC ACID, UNDEC-10-ENYL ESTER	C16H28O2	0.00	0.00	0.00
4.77	CYCLOPENTANE, 1,2-DIMETHYL-3-(1-METHYLETHYL)-	C10H20	0.00	4.59	3.77
4.84	3-UNDECENE, 6-METHYL-, (E)-	C12H24	8.82	0.00	0.00
5.17	TETRADECANE, 1-CHLORO-	C14H29Cl	3.04	0.00	0.00
5.33	2-HYDROXYMETHYL-2-METHYLCYCLOPENTANOL	C7H14O2	0.00	0.00	0.00
5.85	1,1-DIMETHYL-1-SILACYCLO-2,4-HEXADIENE	C7H12Si	1.88	0.00	0.00
5.92	BICYCLO[3.2.0]HEPT-2-ENE, 4-ETHOXY-, EXO-	C9H14O	0.00	0.00	0.00
6.00	4A-METHYL-1,2,4A,5,8,8A-HEXAHYDRO-NAPHTHALENE	C11H16	15.19	0.00	0.00
6.02	BENZENE, (OCTYLOXY)-	C14H22O	0.00	8.29	9.00
6.24	PIVALIC ACID, 2-TETRAHYDROFURYLMETHYL ESTER	C10H18O3	1.88	0.00	0.00

6.64	CYCLOHEXENE, 1,4-DIMETHYL-	C8H14	0.00	0.00	0.00
6.69	PHENOL, 4-BUTYL-	C10H14O	3.31	0.00	0.00
6.72	P-CRESOL	C7H8O	0.00	0.00	0.00
6.75	PHENOL, 2-METHYL-	C7H8O	3.06	3.25	0.00
6.93	PHENOL, 3-METHYL-	C7H8O	0.00	4.06	7.06
7.05	PHENOL, 2-METHOXY-	C7H8O2	4.21	0.00	0.00
7.08	1,3-HEPTADIENE, 2,3-DIMETHYL-	C9H16	0.00	7.23	12.41
7.10	3-HEPTYNE, 2,2-DIMETHYL-	C9H16	0.00	0.00	0.00
7.72	PHENOL, 2-ETHYL-	C8H10O	0.00	8.86	0.00
7.74	PHENOL, 3-ETHYL-	C8H10O	4.35	0.00	1.66
7.91	1-TRIMETHYLSILYLPENT-1-EN-4-YNE	C8H14Si	3.86	0.00	0.00
8.16	BENZOFURAN, 2,3-DIHYDRO-	C8H8O	0.00	0.00	0.00
8.18	1,2-BENZENEDIMETHANOL	C8H10O2	5.14	13.39	24.38
8.70	PHENOL, 4-ETHYL-2-METHOXY-	C9H12O2	5.99	0.00	0.00
8.97	CYCLOHEXENE, 2-ETHENYL-1,3,3-TRIMETHYL-	C11H18	0.00	4.69	0.00
8.99	2-METHOXY-4-VINYLPHENOL	C9H10O2	0.00	0.00	9.09
9.20	PHENOL, 2,6-DIMETHOXY-	C8H10O3	4.31	9.13	0.75
9.90	2,4-DIMETHOXYBENZYL ALCOHOL	C9H12O3	0.00	0.00	0.00
9.90	1,2,4-TRIMETHOXYBENZENE	C9H12O3	0.00	1.64	5.03
9.93	ETHANONE, 1-(2,3,4-TRIHYDROXYPHENYL)-	C8H8O4	2.04	0.00	0.00
10.44	5-TERT-BUTYLPYROGALLOL	C10H14O3	2.85	0.00	0.00
10.44	ETHYL BENZENE	C14H14	0.00	15.69	0.00
10.46	BENZENE, 1,2,3-TRIMETHOXY-5-METHYL-	C10H14O3	0.00	0.00	4.07
10.48	BENZENE, 1,1'-ETHYLIDENEBIS-	C14H14	0.00	0.00	8.40
10.52	BENZENE, [BIS(METHYLTHIO)METHYL]-	C9H12S2	0.00	0.00	2.77
10.54	PHENOL, 4-ETHYL-2-METHOXY-	C9H12O2	0.00	0.00	1.47
10.88	CYCLOOCTASILOXANE, HEXADECAMETHYL-	C16H48O8Si8	2.95	0.00	0.00
10.97	HEPTASILOXANE, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-TETRADECAMETHYL-	C14H44O6Si7	0.75	0.00	0.00

10.98	BRALLOBARBITAL	C10H11O3N2Br	0.00	0.69	0.00
11.61	1,2-DIMETHOXY-4-(1-METHOXYETHENYL)BENZENE	C11H14O3	0.00	0.00	3.45
11.90	HEPTASILOXANE, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-TETRADECAMETHYL-OCTASILOXANE,	C14H44O6Si7	3.41	0.00	0.00
12.81	1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-HEXADECAMETHYL-SILANE, TRIMETHYL[5-METHYL-2-(1-	C16H50O7Si8	2.12	0.00	0.00
12.91	METHYLETHYL)PHENOXY]-TRISILOXANE, 1,1,1,5,5,5-HEXAMETHYL-3,3-	C13H22OSi	0.00	0.00	0.00
13.75	BIS[(TRIMETHYLSILYL)OXY]-TRISILOXANE, 1,1,1,5,5,5-HEXAMETHYL-3,3-	C12H36O4Si5	1.13	0.00	0.00
15.39	BIS[(TRIMETHYLSILYL)OXY]-	C12H36O4Si5	0.00	2.40	0.00
17.39	2-BROMO-2-CYANO-N,N-DIMETHYLACETAMIDE	C5H7ON2Br	0.00	0.00	0.00
17.52	CYCLOHEXANECARBOXYLIC ACID, 2-METHYLBUTYL ESTER	C12H22O2	0.37	0.00	0.00

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Supplementary Table 3: Compounds detected in the upgraded organic phase oil over 0.2HZSM-5

	In-situ Upgraded samples 0.2HZSM-5		GC-MS peak area (%)		
RT	Compound	formula	1.0 wt%	3.0 wt%	2.0 wt%
3.02	Z,Z-6,25-TETRATRIACTONTADIEN-2-ONE	C34H64O	0.00	5.75	0.00
3.02	3-CHLOROPROPIONIC ACID, OCTADECYL ESTER	C21H41O2Cl	0.00	0.00	4.60
3.02	4-TRIDECENE, (Z)-	C13H26	4.77	0.00	0.00
3.64	PENTANOIC ACID, 2-PROPENYL ESTER	C8H14O2	4.13	5.45	0.00
3.92	1-PENTANOL, 5-(PHENYLMETHOXY)-	C12H18O2	0.00	0.00	3.72
3.92	BENZENE, (PHENOXYMETHYL)-	C13H12O	5.99	0.00	0.00
4.70	1-PENTENE, 2,4-DIMETHYL-	C7H14	0.00	0.00	2.16

4.90	ETHYLBENZENE	C8H10	0.00	1.47	0.00
4.99	P-XYLENE	C8H10	2.96	0.00	2.60
5.24	P-XYLENE	C8H10	0.00	1.97	0.00
5.48	2,3,4-HEXATRIENE, 2,5-DIMETHYL-	C8H12	0.00	0.00	1.82
6.00	BENZENE, 1,2,3-TRIMETHYL-	C9H12	4.11	0.00	0.00
6.05	N-VINYLIMIDAZOLE	C5H6N2	9.56	1.05	11.08
6.26	BENZENE, 1,2,4-TRIMETHYL-	C9H12	1.23	1.14	0.00
6.66	1-METHOXY-1,3-CYCLOHEXADIENE	C7H10O	0.00	0.00	1.20
6.77	BENZENE, 2-METHYL-	C7H8O	7.19	9.57	7.24
6.95	P-CRESOL	C7H8O	7.38	8.94	7.60
7.31	PHENOL, 2,6-DIMETHYL-	C8H10O	0.00	2.70	2.13
7.36	PHENOL, 2-ETHYL-5-METHYL-	C9H12O	0.00	2.21	3.38
7.51	PHENOL, 3-ETHYL-	C8H10O	2.19	3.27	2.74
7.63	PHENOL, 2,5-DIMETHYL-	C8H10O	5.86	8.17	5.97
7.77	PHENOL, 2-ETHYL-	C8H10O	17.37	16.46	17.05
8.03	PHENOL, 3-ETHYL-5-METHYL-	C9H12O	0.00	4.36	3.85
8.04	PHENOL, 2-ETHYL-6-METHYL-	C9H12O	3.25	0.00	0.00
8.28	PHENOL, 3-(1-METHYLETHYL)-	C9H12O	3.81	4.79	4.18
8.38	PHENOL, 3-ETHYL-5-METHYL-	C9H12O	7.45	10.51	7.20
8.94	ETHYLTETRAMETHYLCYCLOPENTADIENE	C12H18	3.33	4.60	3.67
9.31	1,3-CYCLOHEXADIENE, 1,3,5,5,6,6-HEXAMETHYL-	C12H20	3.84	4.46	3.13
9.55	TETRADECANE, 1-BROMO-	C14H29Br	0.00	0.00	2.31
9.55	1-ETHYL-1(1-CYCLOBUTYLIDENETHYL)CYCLOBUTANE	C12H20	2.68	3.12	0.00
9.96	3,7-BENZOFURANDIOL, 2,3-DIHYDRO-2,2-DIMETHYL-	C10H12O3	2.90	0.00	0.00
10.25	NONADECANE, 1-BROMO-	C19H39Br	0.00	0.00	2.38

Supplementary Table 4: Compounds detected in the upgraded organic phase oil over 0.3HZSM-5

RT	In-situ Upgraded samples with 0.3HZSM-5		GC-MS peak area (%)		
	Compound	Formula	2.0wt%	1.0wt%	3.0wt%
3.02	1-HEXEN-3-ONE	C6H10O	4.31	0.00	0.00
3.02	1-HEXADECANOL, 2-METHYL-	C17H36O	0.00	3.33	0.00
3.02	CYCLODODECANOL, 1-ETHENYL-	C14H26O	0.00	0.00	4.04
3.63	ISOBUTYL NONYL CARBONATE	C14H28O3	0.00	4.40	0.00
3.63	PENTANOIC ACID, 2-PROPENYL ESTER	C8H14O2	0.00	0.00	5.84
3.64	BENZENE, 1-ETHOXY-4,4-DIMETHYL-	C9H18O	3.09	0.00	0.00
3.91	TOLUENE	C7H8	0.00	0.00	4.87
3.92	PHENOL, 2-(PHENYLMETHOXY)-	C13H12O2	4.64	0.00	0.00
3.92	PHENOL, 5-(PHENYLMETHOXY)-	C12H18O2	0.00	3.83	0.00
4.11	CYCLOHEXANOL, 1-ETHENYL-	C8H14O	0.00	0.00	2.84
4.80	BENZENE, 1-ETHOXY-4,4-DIMETHYL-	C9H18O	0.00	0.00	2.32
4.98	P-XYLENE	C8H10	2.06	4.02	3.46
5.22	BICYCLO[2.1.1]HEXAN-2-OL, 2-ETHENYL-	C8H12O	0.21	0.00	0.00
5.24	ETHYLBENZENE	C8H10	0.00	1.56	2.25
5.47	2,3,4-HEXATRIENE, 2,5-DIMETHYL-	C8H12	1.10	0.00	0.00
5.99	BENZENE, 1,2,4-TRIMETHYL-	C9H12	0.00	0.00	12.77
6.03	N-VINYLIMIDAZOLE	C5H6N2	10.69	0.00	6.03
6.04	BENZENE, (OCTYLOXY)-	C14H22O	0.00	9.21	0.00
6.25	BENZENE, 1,2,3-TRIMETHYL-	C9H12	0.00	0.00	1.37
6.65	CYCLOHEXAN-1-ETHANOL, 1-HYDROXYMETHYL-	C9H18O2	1.06	0.00	0.00
6.76	PHENOL, 2-METHYL-	C7H8O	6.45	6.86	5.63
6.95	P-CRESOL	C7H8O	7.55	7.07	5.93
7.15	BENZENE, 2-BUTENYL-	C10H12	0.00	1.17	0.00
7.30	PHENOL, 2,6-DIMETHYL-	C8H10O	1.47	1.87	0.00
7.36	PHENOL, 3-(1-METHYLETHYL)-	C9H12O	2.37	0.00	0.00

7.36	PHENOL, 2-ETHYL-5-METHYL-	C9H12O	0.00	2.07	0.00
7.50	PHENOL, 2-ETHYL-	C8H10O	2.44	2.37	0.00
7.62	PHENOL, 2,5-DIMETHYL-	C8H10O	5.22	5.59	4.69
7.76	PHENOL, 3-ETHYL-	C8H10O	17.68	14.02	13.54
8.02	PHENOL, 2-ETHYL-4-METHYL-	C9H12O	0.00	2.69	3.42
8.03	PHENOL, 2-ETHYL-6-METHYL-	C9H12O	2.39	0.00	0.00
8.27	PHENOL, 3-(1-METHYLETHYL)-	C9H12O	3.55	3.01	3.31
8.36	PHENOL, 3-ETHYL-5-METHYL-	C9H12O	6.69	6.86	5.06
8.53	BENZENEMETHANOL, 4-ETHYL-	C9H12O	2.32	0.00	0.00
8.53	PHENOL, 2-PROPYL-	C9H12O	0.00	2.15	0.00
8.86	PHENOL, 2,4,6-TRIMETHYL-	C9H12O	0.00	1.25	0.00
8.71	PHENOL, 2-ETHYL-4,5-DIMETHYL-	C10H14O	0.00	1.29	0.00
8.81	THYMOL	C10H14O	0.00	0.91	0.00
8.92	ETHYLTETRAMETHYLCYCLOPENTADIENE	C11H18	2.75	0.00	0.00
8.94	2,5-DIETHYLPHENOL	C10H14O	0.00	2.99	3.45
9.02	1H-INDENE, 2,3-DIHYDRO-4,5,7-TRIMETHYL-	C12H16	0.00	2.22	0.00
9.02	BENZENE, 1-(1-METHYLETHENYL)-2-(1-METHYLETHYL)-	C12H16	2.50	0.00	0.00
9.29	1,3-CYCLOHEXADIENE, 1,3,5,5,6,6-HEXAMETHYL-	C12H20	2.35	2.81	2.52
9.53	1-ETHYL-1(1-CYCLOBUTYLIDENETHYL)CYCLOBUTANE	C12H20	0.00	3.53	0.00
9.54	BENZENE, 1-METHOXY-4-(1-METHYLPROPYL)-	C11H16O	0.00	0.00	1.98
9.54	TRIDECANE, 1-BROMO-	C13H27Br	2.61	0.00	0.00
9.84	BENZENE, 2-(2-BUTENYL)-1,3,5-TRIMETHYL-	C13H18	1.75	0.00	0.00
9.95	HEPTADECANE, 1-BROMO-	C17H35Br	2.75	0.00	0.00
10.24	TRIDECANE, 1-BROMO-	C13H27Br	0.00	2.05	0.00
10.25	DODECANE, 1,12-DIBROMO-	C12H24Br2	0.00	0.00	2.49
11.53	OCTADECANE, 1-CHLORO-	C18H37Cl	0.00	0.87	2.18