

Optimization of Hydrocarbon Production in Catalytic Pyrolysis of Macaúba Epicarp and Macaúba and Baru Endocarps

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Table S1. Compounds obtained during non-catalytic pyrolysis – Macaúba epicarp (EPM), Macaúba endocarp (ENM) and Barú endocarp (ENB).

Category	Name	Formula	EPM	EPM	EPM	ENM	ENM	ENM	ENB	ENB	ENB
			550°C	650°C	750°C	550°C	650°C	750°C	550°C	650°C	750°C
Acid	3-Heptenoic acid	C7H12O2			0,46						
Acid	6-Heptenoic acid	C7H12O2							0,34		
Acid	7-Octenoic acid	C8H14O2			0,44						
Acid	8-Nonenoic acid	C9H16O2			0,43						
Acid	9-Hexadecenoic acid	C16H30O2		2,18							
Acid	Acetic acid	C2H4O2	8,98	7,67	6,29	13,19	11,46	12,04	11,86	17,34	13,20
Acid	Acetic acid, (acetyloxy)-	C6H6O4		1,58		1,86	1,49	1,86			2,52
Acid	Acetic acid, oxo-	C2H2O3							14,46		
Acid	Carbamic acid, monoammonium salt	CH6N2O2			20,93			17,68	15,68		
Acid	DL-Threonine, N-glycyl-	C6H12N2O4							1,82	2,41	
Acid	Dodecanoic acid	C12H24O2			0,73	0,45	0,66				
Acid	Formic acid	CH2O2							0,33		
Acid	Heptanoic acid	C7H14O2			0,31						
Acid	Hexanoic acid	C16H12O2				0,94					
Acid	Hydroxydehydrostevic acid	C20H30O3			0,49						
Acid	Linoelaidic acid	C18H32O2			5,74						
Acid	L-Lactic acid	C3H6O3							0,26		
Acid	n-Hexadecanoic acid	C16H32O2	3,29	8,88	8,05	5,03	3,11	2,71			
Acid	Nonanoic acid	C9H18O2	0,52								
Acid	Octadecanoic acid	C18H36O2		3,98	1,38						
Acid	Octanoic acid	C8H16O2	0,25	0,32			0,75	0,55	0,21		
Acid	Oleic Acid	C18H34O2	11,41	11,26	10,12	13,47	6,50	8,75			
Acid	Oxalic acid	C2H2O4		16,49					16,58		

Acid	Propanoic acid, anhydride	C6H10O3	0,30						
Alcohol	(-)Spathulenol	C15H24O					2,09		
Alcohol	(E)-3-Methyl-5-((1R,4aR,8aR)-5,5,8a-trimethyl-2-methylenedecahydronaphthalen-1-yl)pent-2-en-1-ol	C20H34O				0,62			
Alcohol	(E)-4-(3-Hydroxyprop-1-en-1-yl)-2-methoxyphenol	C10H12O3	1,59	1,07	1,59			0,43	
Alcohol	1,3-Benzenedimethanol	C8H10O2				0,32			
Alcohol	1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-	C16H14O3					0,91		
Alcohol	1-Dodecanol	C12H26O					0,47		
Alcohol	1-Dodecanol, 3,7,11-trimethyl-1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-[1ar-(1a.alpha.,4a.alpha.,7.beta.,7a.beta.,7b.alpha.)]-	C15H24O					0,87	1,08	1,20
Alcohol	2,6-Dimethyl-octa-2,6-dien-1-ol	C10H18O						0,28	
Alcohol	26,27-Dinorergosta-5,23-dien-3-ol, (3.beta.)-	C26H42O		1,16					
Alcohol	2-Propen-1-ol	C3H6O					0,22		
Alcohol	3-Buten-1-ol, 2-methyl-	C5H10O	0,30						
Alcohol	4-Heptyn-2-ol	C7H12O					0,35		
Alcohol	4-Methyl-5-hexen-2-ol	C7H14O					0,44		
Alcohol	4-Penten-1-ol	C5H10O			0,41				
Alcohol	9,19-Cyclolanostan-3-ol, 24-methylene-, (3.beta.)-	C31H52O				1,19	1,26		
Alcohol	Benzeneethanol, 3-hydroxy-	C8H10O2	0,84		0,77				
Alcohol	Cholesta-5,22-dien-3-ol, (3.beta.)-	C27H44O	0,51		0,51				
Alcohol	cis-1,2-Cyclohexanediol	C6H12O2					0,45		
Alcohol	cis-11,12-Epoxytetradecen-1-ol	C16H30O3				0,31			
Alcohol	cis-9-Tetradecen-1-ol	C14H28O					0,47		
Alcohol	Cyclododeca-5,9-dien-1-ol, 2-methyl-, (Z,Z)-	C13H22O				1,42			
Alcohol	Cyclohexaneethanol	C8H16O				0,49			
Alcohol	Cyclopropyl carbinol	C4H8O	1,17	0,57	1,84	0,56	0,36	0,60	0,54
Alcohol	E-7-Tetradecenol	C14H28O			0,44		0,52		

Amine/Amide	Aziridine, 1,2-diisopropyl-3-methyl-, trans-	C9H19N													1,21
Amine/Amide	Aziridine, 2-methyl-3-(1-methylethyl)-1-(2-propenyl)-, trans-	C9H17N													1,79
Amine/Amide	Benzenamine, N,N-diethyl-4-methyl-	C11H17N													0,28
Amine/Amide	Benzenemethanamine, 3,4-dimethyl-	C9H13N													0,60
Amine/Amide	Cyclooctyldene-(2-phenylaziridin-1-yl)amine	C16H22N2													1,48
Amine/Amide	Dimethylamine	C2H7N	13,77	7,55	12,36	13,77	15,34								15,09
Amine/Amide	Formamide	CH3NO	8,28		7,38										
Amine/Amide	N-tert-Butylethylamine	C6H15N						0,35	0,27	0,21	0,20	0,28	0,21		
Amine/Amide	Propylamine, 3-(furan-2-yl)-1-methyl-	C8H13NO						0,38							
Amine/Amide	Pyrrole	C4H5N	0,63												
Amine/Amide	Valeramide, 5-chloro-N-methyl-	C6H12ClNO													0,70
Ester	(Z)-Non-3-en-1-yl propyl carbonate	C10H18O3													0,61
Ester	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	C16H22O4							0,26						5,15
Ester	1,2-Cyclopentanedione, 3-methyl-	C6H8O2	1,01	0,67	0,55	0,52	0,48	0,44	0,64						
Ester	1,3,5-Cycloheptatriene, 1-methoxy-	C8H10O								1,42					
Ester	1,3-Di-O-acetyl-alpha.-beta.-d-ribopyranose	C9H14O7													0,61
Ester	1,3-Dioxolane, 4-ethyl-	C5H10O2													0,39
Ester	1-Propene, 1-(1-methylethoxy)-, (Z)-	C6H12O								3,07					
Ester	2(5H)-Furanone	C4H4O2	0,51												
Ester	2-(tert-Butyl)-4-methoxyphenyl acetate	C13H18O3							1,10			0,33			
Ester	2,3-Dihydroxypropyl elaidate	C21H40O4							0,69						
Ester	2,4-Hexadienedioic acid, 3,4-diethyl-, dimethyl ester, (E,Z)-	C12H18O4								0,41		0,65	0,56		
Ester	2-Butenedioic acid (Z)-, dibutyl ester	C12H20O4											0,54		
Ester	2-Ethylbutyl acrylate	C9H16O2								0,18					
Ester	2-Ethylhexyl salicylate	C15H22O3											0,73		
Ester	2-Furancarboxylic acid, 1-cyclopentylethyl ester	C12H16O3										0,40			
Ester	3-Trifluoroacetoxytridecane	C15H27F3O2							0,69						
Ester	4-Heptafluorobutyryloxyhexadecane	C20H33F7O2											0,45		

Ester	8-Octadecenoic acid, methyl ester	C19H36O2	0,40	0,44	0,13	0,19				
Ester	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	C21H40O4			1,90					
Ester	9-Octadecenoic acid (Z)-, methyl ester	C19H36O2	0,36	0,52	0,72	0,29				
Ester	9-Octadecenoic acid, methyl ester, (E)-	C19H36O2		0,45						
Ester	Acetic acid, 5-hydroxy-4-nitrotetrahydropyran-3-yl ester	C7H11NO6					0,84			
Ester	Acetic acid, methyl ester	C2H4O2	1,71	1,09	1,10	1,17	1,07	1,19	2,73	4,68
Ester	Benzene, 1-(dodecyloxy)-2-nitro-	C18H29NO3			0,44					
Ester	Benzene, 1,2,3-trimethoxy-5-methyl-	C10H14O3	0,42	0,24		0,45	0,42		0,64	0,59
Ester	Bromoacetic acid, 10-undecenyl ester	C13H23BrO2				0,80				
Ester	Carbonic acid, ethyl tetradecyl ester	C17H34O3					0,49			
Ester	Decanoic acid, 2-propenyl ester	C13H24O2			0,63					
Ester	Decyl oleate	C28H54O2			1,73					
Ester	Dibutyl adipate	C14H26O4					0,71			
Ester	Diethyl Phthalate	C12H14O4						1,75		
Ester	Dodecane, 1-(methoxymethoxy)-	C14H30O2			0,45					
Ester	Hexadecanoic acid, methyl ester	C17H34O2	0,16	0,26	0,40	0,16				
Ester	Hexadecanoic acid, n.-octyl ester	C24H48O2			1,78					
Ester	Hexane, 1-(ethenyloxy)-	C8H16O				3,02				
Ester	Hexanedioic acid, bis(2-methylpropyl) ester	C14H26O4					0,49			
Ester	Homosalate	C16H22O3					0,60			
Ester	l-(+)-Ascorbic acid 2,6-dihexadecanoate	C38H68O8						0,22		
Ester	Methyl methacrylate	C5H8O2						0,49		
Ester	Methyl nitrite	CH3NO2					1,45		3,16	
Ester	Octadecanoic acid, 2-propenyl ester	C21H40O2					0,35			
Ester	Oxirane, tetradecyl-	C16H32O					0,28			
Ester	p-(Heptyloxy)phenyl 4'-(2-methylbutyl)-4-biphenylcarboxylate	C31H38O3			1,57				2,34	
Ester	Pentafluoropropionic acid, undecyl ester	C14H23F5O2	0,32							
Ester	Pregnan-20-one, 3-(acetoxy)-, (3. β .,5. β .)-	C23H36O3						0,62		

Ester	Propanoic acid, 2-oxo-, methyl ester	C4H6O3	1,13	0,87	0,70	1,02	1,35	1,03	2,07	2,28	2,09
Furan	5-Hydroxymethylfurfural	C6H6O3							1,27	1,41	0,52
Furan	Benzofuran, 2,3-dihydro-	C8H8O					0,26				0,57
Furan	Benzofuran, 2-methyl-	C9H8O					0,30				
Furan	Furan	C4H4O	0,17	0,18	0,26	0,17	0,22	0,35	0,20	0,43	0,74
Furan	Furan, 2,3-dihydro-	C4H6O				0,07	0,05				0,51
Furan	Furan, 2-ethyl-	C6H8O									0,55
Furan	Furan, 2-methyl-	C5H6O				0,28	0,30	0,45	0,38	0,51	0,86
HC	.alpha.-Calacorene	C15H20									0,23
HC	1,1'-Bicyclopentyl	C10H16O					1,71				
HC	1,3,5-Hexatriene, (Z)-	C6H8					0,09	0,32			0,42
HC	1,3-Butadiene	C4H6			3,83	0,54			1,77		
HC	1,3-Cyclopentadiene	C5H6			0,55	0,23	0,16	0,66			0,50
HC	1,3-Cyclopentadiene, 1-methyl-	C6H8						0,32			
HC	1,3-Cyclopentadiene, 5-(1-methylethylidene)-	C8H10									0,48
HC	1,3-Nonadiene, (E)-	C9H16					1,70				
HC	1,3-Pentadiene	C5H8	0,24	0,39	0,83	0,42	0,32	1,16			1,00
HC	1,4-Hexadiene, (Z)-	C6H10									0,16
HC	1,4-Undecadiene, (E)-	C11H20			0,37		1,49	0,43			
HC	1,7-Hexadecadiene	C16H30			0,47			0,41			
HC	1,7-Octadiyne	C8H10			1,01		0,55				
HC	1,9-Decadiene	C10H18		0,34							
HC	1-Butene	C4H8		2,84	2,79		0,54	1,92	0,67	0,89	1,59
HC	1-Butene, 2,3-dimethyl-	C6H12							0,24		
HC	1-Decene	C10H20		0,20	0,65		2,18	0,66			
HC	1-Dodecene	C12H24			0,45			0,50			
HC	1-Heptadecene	C17H34						0,28			
HC	1-Heptene	C7H14		0,93	1,75	0,54	0,24	1,37			

HC	1-Hexene	C6H12			3,73
HC	1-Nonene	C9H18	0,52	2,71	0,41
HC	1-Octene	C8H16	0,43	0,92	0,59
HC	1-Pentadecene	C15H30		0,54	0,46
HC	1-Pentene, 4-methyl-	C6H12		3,84	
HC	1-Tridecene	C13H26	0,29	0,61	1,21
HC	1-Undecene	C11H22	0,20	0,7	3,10
HC	2,4-Dimethyl-1-heptene	C9H18			0,13
HC	2,4-Dodecadiene, (E,Z)-	C12H22			0,60
HC	2-Butene, (Z)-	C4H8		0,75	2,32
HC	2-Decene, (Z)-	C10H20			0,28
HC	2-Hexyne	C6H10			0,55
HC	2-Methyltetracosane	C25H52	0,28	0,28	
HC	2-Pentene, 2-methyl-	C6H12			0,08
HC	3-Heptadecene, (Z)-	C17H34	0,26		
HC	3-Hexadecene, (Z)-	C16H32			0,44
HC	3-Hexyne	C6H10		0,42	
HC	3-Tetradecene, (Z)-	C14H28		0,53	0,27
HC	4,4-Dimethyl-1,1a,3a,4,5,6-hexahydrocyclopropa[c]pentalene	C11H16			0,46
HC	4-Methylenecyclopentene	C6H8		0,57	
HC	5-Decyne	C10H18			1,64
HC	6-Dodecyne	C12H22	0,23	0,40	1,23
HC	6-Tridecane	C13H24		0,45	
HC	Androst-2,16-diene	C19H28			0,19
HC	Benzene	C6H6	0,96	0,18	0,42
HC	Benzene, 1,3-dimethyl-	C8H10			1,10
HC	Benzene, propyl-	C9H12		0,91	
HC	Bicyclo[2.1.0]pentane	C5H8		0,37	0,19

HC	Cyclobutene	C4H6	2,90	0,18	1,28	0,39	1,05
HC	Cyclohexene, 1-butyl-	C10H18		2,70			
HC	Cyclopropane	C3H6		1,60	5,05	1,61	4,58
HC	Cyclopropane, 1,2-dimethyl-, cis-	C5H10		0,09	0,19		
HC	Cyclopropane, 1-butyl-1-methyl-2-propyl-	C11H22	0,80	0,82	0,47		
HC	Cyclopropane, ethylidene-	C5H8				0,39	
HC	Cyclopropane, methylmethylen-	C5H8	0,30		0,26		
HC	Cyclopropane, nonyl-	C12H24		0,40		0,66	
HC	Cycloundecene(E)	C11H20			0,56		
HC	d-Norandrostane (5.alpha.,14.alpha.)	C18H30			0,46		
HC	Dodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-	C25H48			0,61		
HC	Hexadecane	C16H34				0,18	
HC	Hexatriacontane	C36H74	1,96				
HC	Indene	C9H8		0,78			
HC	Mesitylene	C9H12		0,46			
HC	Naphthalene, 1,5-dimethyl-	C12H12			0,40		
HC	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	C15H18				0,17	
HC	Naphthalene, 2,6-dimethyl-	C12H12			0,67	0,60	0,51
HC	Phenanthrene, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,8,10,10a-dodecahydro-4a,7-dimethyl-1-methylene-, [4aS-(4a.alpha.,4a.beta.,7.beta.,1	C20H32				0,25	
HC	Propene	C3H6	10,48		3,89		
HC	p-Xylene	C8H10		0,48			
HC	Squalene	C30H50			0,92		
HC	Styrene	C8H8				0,41	
HC	Supraene	C30H50	1,18				
HC	Toluene	C7H8	0,99	1,40	0,55	0,65	1,32
HC	trans-3,5-Dimethylcyclohexene	C8H14			0,83		
HC	Vinylcyclopentane	C7H12			0,64		

Ketone	1,2-Cyclopentanedione	C5H6O2	0,7					1,92	1,74
Ketone	1,4-Dioxaspiro[2.4]heptan-5-one	C5H6O3							0,47
Ketone	1-Decen-3-one	C10H18O		0,37					
Ketone	1-Hydroxy-2-butanone	C4H8O2	0,46	0,29		0,39	0,54	0,42	
Ketone	1-Octen-3-one	C8H14O					0,63		
Ketone	2,3-Butanedione	C4H6O2	0,82	0,89	0,72	0,96	1,07	1,33	0,63
Ketone	2,3-Pentanedione	C4H6O2	0,54	0,50		0,56	0,59	0,72	0,70
Ketone	2,4(3H,5H)-Furandione, 3-methyl-	C5H6O3							
Ketone	2,5-Furandione, dihydro-3-methylene-	C5H4O3				0,22	0,24		
Ketone	2-Butanone	C4H8O	0,41	0,36	0,43	0,33	0,65	0,41	0,62
Ketone	2-Cyclopenten-1-one	C5H6O	0,47	0,42	0,51	0,33	0,29	0,41	0,27
Ketone	2-Cyclopenten-1-one, 2-hydroxy-	C5H6O2						0,93	
Ketone	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	C6H8O2						0,35	
Ketone	2-Cyclopenten-1-one, 2-methyl-	C6H8O	0,41	0,27					
Ketone	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-	C7H10O2	0,26						
Ketone	2-Cyclopenten-1-one, 3-methyl-	C6H8O	0,33			0,29			
Ketone	2-Decanone	C10H20O					0,73		
Ketone	2-Hexanone oxime	C6H13NO						0,51	
Ketone	2-Nonanone	C9H18O					1,24		
Ketone	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	C10H12O3	0,49	0,45		0,39		0,32	0,22
Ketone	2-Propanone, 1-(acetoxy)-	C5H8O3	0,38	0,38		0,30	1,16	0,34	0,34
Ketone	2-Propanone, 1-hydroxy-	C3H6O2	4,05	2,92	2,78	3,75	3,34	2,67	3,33
Ketone	3',5'-Dimethoxyacetophenone	C10H12O3	1,43	0,97		1,71	1,63	0,37	2,30
Ketone	3-Buten-2-one, 3-methyl-	C5H8O				0,06	0,10		0,21
Ketone	3-Octanone, 2-methyl-	C9H18O					0,43		
Ketone	3-Pantanone	C5H10O	0,15			0,25	0,24		
Ketone	4(1H)-Pyrimidinone, 6-methyl-	C5H6N2O	0,38					0,41	0,36
Ketone	4-Methyl-2-oxopentanenitrile	C6H9NO						0,32	

Ketone	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	C13H22O							0,65
Ketone	6-(1-Hydroxymethylvinyl)-4,8a-dimethyl-3,5,6,7,8,8a-hexahydro-1H-naphthalen-2-one	C15H22O2							0,29
Ketone	6-Oxa-bicyclo[3.1.0]hexan-3-one	C5H6O2	1,39		1,10	1,34		1,01	1,11
Ketone	9-Heptadecanone	C17H34O		0,45					
Ketone	Acetone	C3H6O	0,50	0,69	1,10	0,60	0,80	0,95	0,52
Ketone	Cyclopentadecanone, 2-hydroxy-	C15H28O2	0,73		0,73				
Ketone	Ethanone, 1-(1-methyl-2-cyclopenten-1-yl)-	C8H12O							0,16
Ketone	Ethanone, 1-(methylenecyclopropyl)-	C6H8O			0,09	0,11			
Ketone	Ethanone, 1-(methylenecyclopropyl)-	C6H8O							0,3
Ketone	Methyl vinyl ketone	C4H6O		0,32					0,65
Others	.beta.-D-Glucopyranose, 1,6-anhydro-	C6H10O5	0,61	0,60	1,24		0,81	0,53	6,46
Others	.beta.-d-Ribopyranoside, methyl, 3-acetate	C8H14O6							0,49
Others	3-Benzylxy-1-nitrobutane	C11H15NO3				2,03			
Others	3-Isopropoxy-1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane	C18H52O7Si7							0,19
Others	7-Bromo-4,5-diazaspiro[2.4]hept-4-ene	C5H7BrN2		0,75		0,54	0,45	0,51	
Others	Acetonitrile	C2H3N			0,36				
Others	Aromadendran ('2')	C15H24O2							0,21
Others	Chloromethane	CH3Cl	2,01		1,17				
Others	Cyacetamide	C3H5N3O			3,98		3,20		
Others	D-Allose	C6H12O6							7,36
Others	Glycyl-dl-serine	C5H10N2O4	0,40						7,01
Others	Methyl isocyanide	C2H3N			0,45				
Others	N-Propionylimidazole	C6H8N2O				1,66			
Others	Silane, dimethyl(1-phenylpropoxy)pentyloxy-	C16H28O2Si							1,60
Phenol	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	C11H14O3	0,92	0,65		1,31	1,06	0,26	0,93
Phenol	1,4-Benzenediol, 2-methoxy-	C7H8O3							0,22

Phenol	2-Methoxy-4-vinylphenol	C9H10O2			2,90	1,42		2,08	2,22	0,24	
Phenol	3,5-Dimethoxy-4-hydroxytoluene	C9H12O3	0,95	0,45	0,77	0,63		1,79	1,37		
Phenol	4-((1E)-3-Hydroxy-1-propenyl)-2-methoxyphenol	C10H12O3				0,16			0,31		
Phenol	4-(1-Hydroxyallyl)-2-methoxyphenol	C10H12O3							0,22		
Phenol	4-Hydroxy-3-methylacetophenone	C9H10O2	4,37	3,26	1,31	4,15	1,15			0,60	
Phenol	5-tert-Butylpyrogallol	C10H14O3				0,59					
Phenol	Apocynin	C10H10O3	0,33	0,31		0,28		0,26	0,39		
Phenol	Creosol	C8H10O2	2,59	1,30	0,27	3,87	0,54	1,40	1,13	0,32	
Phenol	Desaspidinol	C11H14O4	0,28	0,21		0,38			0,60		
Phenol	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	C10H12O4				0,18		0,40	0,49		
Phenol	Eugenol	C10H12O2				0,30					
Phenol	Mequinol	C7H8O2						1,52			
Phenol	p-Cresol	C7H8O		0,61	0,73	0,16		0,36		0,28	
Phenol	Phenol	C6H6O	1,63	1,67	2,40	5,36	12,34	11,95	0,62	0,41	0,54
Phenol	Phenol, 2,4-dimethyl-	C8H10O	0,30	0,38	0,53	0,31		0,62			
Phenol	Phenol, 2,6-dimethoxy-	C8H10O3	2,08	1,07		2,16	2,37	0,32	2,18	1,92	0,26
Phenol	Phenol, 2,6-dimethoxy-4-(2-propenyl)-	C11H14O3	0,36	0,31		0,42	0,51		0,52	0,63	
Phenol	Phenol, 2-methoxy-	C8H10O3	4,86	2,93	0,90	3,28	1,91	0,40	1,92	1,37	
Phenol	Phenol, 2-methoxy-3-(2-propenyl)-	C10H12O2				1,82			0,22	0,38	
Phenol	Phenol, 2-methoxy-4-(1-propenyl)-, (Z)-	C10H12O2	0,57	0,46					0,21	1,56	
Phenol	Phenol, 2-methoxy-4-propyl-	C10H14O2	0,24			0,27					
Phenol	Phenol, 2-methyl-	C8H10O3	0,52	0,60	0,84	0,50	0,22	0,50	0,33	0,29	
Phenol	Phenol, 3-methyl-	C7H8O	0,63	0,86	1,14			0,63	0,49		0,54
Phenol	Phenol, 4-ethyl-2-methoxy-	C9H12O2	1,06	0,54		0,57	0,26		0,33	0,36	
Phenol	Resorcinol	C6H6O2							0,66	0,94	1,06
Phenol	trans-Isoeugenol	C10H12O2	2,61	1,99	0,50	2,43	0,75		1,18	1,20	0,26

Table S2. Compounds obtained during catalytic pyrolysis – Catalyst CaO

16

Category	Name	Formula	550-15	550-85	750-15	750-85	508-50	791-50	650-100	650-50	650-0
			CaO	CaO	CaO						
Acid	Acetic acid	C2H4O2	8,43	0,52	6,26		4,28	2,82	6,93	8,25	12,7
Acid	Acetic acid, (acetyloxy)-	C6H6O4			0,41						2,0
Acid	Carbamic acid, monoammonium salt	CH6N2O2		7,88	14,15		12,89			5,46	20,9
Acid	cis-10-Heptadecenoic acid	C17H32O2								8,09	
Acid	n-Hexadecanoic acid	C16H32O2		7,18		1,54		2,16	0,55	9,37	7,64
Acid	Nonanoic acid	C9H18O2								0,54	
Acid	Octadecanoic acid	C18H36O2									0,85
Acid	Oleic Acid	C18H34O2					0,80				6,87
Acid	Propanoic acid, anhydride	C6H10O3									0,3
Alcohol	1-Dodecanol	C12H26O			0,43						
Alcohol	1-Methylcyclopropanemethanol	C5H10O					0,55				
Alcohol	1-Nonanol	C9H20O	0,77								
Alcohol	2-Nonen-1-ol	C9H18O					1,33				
Alcohol	2-Propen-1-ol	C3H6O						0,24			
Alcohol	3-Buten-1-ol, 2-methyl-	C5H10O							1,86		
Alcohol	3-Nonen-1-ol, (Z)-	C9H18O			0,52						
Alcohol	4-Heptyn-2-ol	C7H12O			0,66						
Alcohol	4-Penten-1-ol	C5H10O					1,91		1,02		
Alcohol	9-Tetradecen-1-ol, (E)-	C14H28O								0,72	
Alcohol	Benzeneethanol, 3-hydroxy-	C8H10O2	0,61								
Alcohol	cis-11,12-Epoxytetradecen-1-ol	C16H30O3					6,18				
Alcohol	Methyl Alcohol	CH4O	6,30	7,27			4,29				3,3
Alcohol	Tetrahydro-4H-pyran-4-ol	C5H10O2	0,43								
Alcohol	Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate	C16H28O3		7,02		2,26				2,44	
Aldehyde	(E)-Hexadec-2-enal	C16H30O		0,66							

Aldehyde	2-Propenal	C3H4O		1,26					1,29	0,6	
Aldehyde	Acetaldehyde	C2H4O	2,75	3,11	4,07	3,49	1,61	4,18	1,17	1,31	1,5
Aldehyde	Acetaldehyde, hydroxy-	C6H10O3	1,19							0,71	6,1
Aldehyde	Coniferyl aldehyde	C10H10O3									0,9
Aldehyde	Formaldehyde	CH2O									1,8
Aldehyde	Furfural	C5H4O2		0,52					1,93	1,87	1,1
Aldehyde	Glycolaldehyde dimer	C4H8O									5,20
Aldehyde	Methyl glyoxal	C3H4O2									2,5
Aldehyde	Nonanal	C9H18O		0,56						0,64	0,5
Aldehyde	Octanal	C8H16O	0,51	0,73							
Aldehyde	Pentanal, 2,4-dimethyl-	C7H14O		0,39							
Aldehyde	Propanal	C3H6O	0,65								
Aldehyde	Propanal, 2-methyl-	C4H8O					0,19				
Aldehyde	Succindialdehyde	C4H6O2	0,79								1,1
Aldehyde	Vanillin	C8H8O3							0,51	0,7	
Amine/Amide	Ethylamine	C2H7N							2,53		
Amine/Amide	p-Toluidine, N-methyl-N-nitroso-	C8H10N2O		0,3							
Ester	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	C16H22O4									0,3
Ester	1,2-Cyclopentanedione, 3-methyl-	C6H8O2							1,37		0,4
Ester	2-(tert-Butyl)-4-methoxyphenyl acetate	C13H18O3									1,1
Ester	2,3-Dihydroxypropyl elaidate	C21H40O4									0,7
Ester	5-Isopropyl-2-methylphenyl 3-methylbutanoate	C15H22O2				2,68					
Ester	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	C21H40O4									1,9
Ester	9-Octadecenoic acid (Z)-, methyl ester	C19H36O2				0,45					0,4
Ester	9-Octadecenoic acid, methyl ester, (E)-	C19H36O2	1,41	2,93	0,71	0,63	4,51	0,27	1,82	1,14	
Ester	Acetic acid ethenyl ester	C4H6O2						0,57			
Ester	Acetic acid, 2-ethylbutyl ester	C8H16O2	4,94								
Ester	Acetic acid, methyl ester	C2H4O2	6,46				3,35				

Ester	Benzene, 1-(dodecyloxy)-2-nitro-	C18H29NO3									0,4	
Ester	Benzene, 1,2,3-trimethoxy-5-methyl-	C10H14O3	0,53									
Ester	Cyclodecanol, acetate	C12H22O2						0,60				
Ester	Decanoic acid, 2-propenyl ester	C13H24O2									0,6	
Ester	Decyl oleate	C28H54O2									1,7	
Ester	Dodecane, 1-(methoxymethoxy)-	C14H30O2									0,4	
Ester	Hexadecanoic acid, methyl ester	C17H34O2	1,28	1,52	0,63	0,65	2,34	0,49	0,89	0,99		
Ester	Hexadecanoic acid, n.-octyl ester	C24H48O2									1,8	
Ester	Pentadecafluorooctanoic acid, tridecyl ester	C21H27F15O2						0,80				
Ester	Propanoic acid, 2-oxo-, methyl ester	C4H6O3	0,92		0,41					1,02	0,9	
Ester	Trifluoroacetic acid,n-tridecyl ester	C15H27F3O2						0,41				
Furan	3-Furaldehyde	C5H4O2	1,15	0,69				1,01				
Furan	Furan	C4H4O	0,46	0,53	0,37				0,32	0,72		
Furan	Furan, 2-methyl-	C5H6O								0,71	0,48	0,3
HC	1,2-Dipentylcyclopropene	C13H24									0,90	
HC	1,3,3-Trimethylcyclopropene	C6H10						0,46				
HC	1,3,5,7-Cyclooctatetraene	C8H8			0,31							
HC	1,3,5-Hexatriene, (Z)-	C6H8			0,57	0,91				0,6		
HC	1,3-Butadiene	C4H6									0,5	
HC	1,3-Cyclopentadiene	C5H6			1,29	4,31			4,34		0,2	
HC	1,3-Cyclopentadiene, 1-methyl-	C6H8			0,31				1,26			
HC	1,3-Cyclopentadiene, 5-(1-methylethylidene)-	C8H10				0,70			0,90	0,96		
HC	1,3-Pentadiene, (E)-	C5H8			1,2	3,35			1,23		0,53	0,3
HC	1,3-Pentadiene, 3-methyl-, (E)-	C6H10				0,69						
HC	1,7-Hexadecadiene	C16H30			0,4	0,42				0,95		
HC	1-Butyne	C4H6			4,29	3,86			8,67			
HC	1-Decene	C10H20	0,86	0,91	0,97	0,57	1,03	0,87	0,71			
HC	1-Heptadecene	C17H34						0,45				

HC	1-Heptene	C7H14	4,37	3,72	4,36	2,16	4,34	2,64	2,20	0,5
HC	1-Hexene	C6H12		4,95	5,60		5,63			
HC	1-Nonene	C9H18	0,92	0,92	1,05		1,02	0,81	0,66	
HC	1-Octene	C8H16	1,5	1,46	1,72	0,80	1,66	2,23	1,00	
HC	1-Pentadecene	C15H30	1,33	0,68			0,94			
HC	1-Tetradecene	C14H28	0,98	0,56	0,99	1,03	1,25		1,17	0,97
HC	1-Tridecene	C13H26			0,83	0,93	0,92	0,35	1,10	
HC	1-Undecene	C11H22	0,66	0,74	0,92	0,93		1,00	0,72	0,60
HC	2,4-Hexadiene, 2,3-dimethyl-	C8H14		0,51						
HC	2-Butene	C4H8				0,87		3,26	3,42	0,7
HC	2-Hexene	C6H12			1,09					
HC	2-Hexyne	C6H10			0,56					
HC	2-Methyl-1-butene	C5H10			0,81	1,50		0,50		
HC	2-Pentene, (Z)-	C5H10						0,73		
HC	3-Heptadecene, (Z)-	C17H34						0,79		
HC	3-Hexyne	C6H10			0,58			0,70		
HC	4-Methylenecyclopentene	C6H8			0,83	0,93		1,57		
HC	5-Decyne	C10H18						0,58		
HC	5-Undecyne	C11H20							0,51	
HC	6-Dodecyne	C12H22	0,51		0,41	0,51		0,76	0,54	
HC	Benzene	C6H6			1,14	1,33		2,72		
HC	Benzene, 1,3-dimethyl-	C8H10			0,77					
HC	Cetene	C16H32	0,91	1,04		0,67			0,57	0,45
HC	Cyclobutane	C4H8			4,35	5,07		6,84		
HC	Cycloheptane	C7H14						0,87		
HC	Cyclopentene, 4-methyl-	C6H10					0,50			
HC	Cyclopropane	C3H6			8,21			13,14		1,6
HC	Cyclopropane, 1-hexyl-2-propyl-, cis-	C12H24	0,5							

HC	Cyclopropane, nonyl-	C12H24	0,65							
HC	Cyclopropane, nonyl-	C12H24		0,61		0,64	0,59	0,50	0,56	0,42
HC	Dodecane	C12H26	1,02	0,79						
HC	Ethylbenzene	C8H10			0,31			0,56		
HC	Heptane, 2,4-dimethyl-	C9H20		0,83	0,74	1,04		0,80		0,55
HC	Hexatriacontane	C36H74								2,0
HC	Nonane	C9H20		0,69	0,37	0,56		0,35		
HC	Octane	C8H18				0,43				
HC	o-Xylene	C8H10						0,22		
HC	Pentadecane	C15H32						0,18		
HC	Propene	C3H6		1,64		7,35			2,35	3,17
HC	Styrene	C8H8						0,65		
HC	Tetradecane	C14H30	0,67							
HC	Toluene	C7H8			1,7	1,73		2,92	1,06	
HC	Tridecane	C13H28	0,77	0,7		0,45	0,79	0,20		
HC	Undecane	C11H24	0,46	0,54						
HC	Undecane, 4,7-dimethyl-	C13H28				0,84				
Ketone	1,2-Cyclopentanedione	C5H6O2							0,67	
Ketone	1-Hydroxy-2-butanone	C4H8O2								0,4
Ketone	2,3-Butanedione	C4H6O2	0,81	1,17	1,42		1,03		1,19	1,42
Ketone	2,3-Pentanedione	C4H6O2								0,5
Ketone	2-Butanone	C4H8O	0,45	1,88	1,14	2,52	1,31	1,31	1,82	1,35
Ketone	2-Cyclopenten-1-one	C5H6O	0,50	0,71	0,4	0,42	0,85	0,26		
Ketone	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	C6H8O2	0,68							0,95
Ketone	2-Cyclopenten-1-one, 2-methyl-	C6H8O	0,85	0,98		0,51	0,82		1,12	0,68
Ketone	2-Decanone	C10H20O	1,74	2,07	1,05	1,57	2,41	0,98	1,60	0,70
Ketone	2-Heptadecanone	C17H34O	7,76				6,62		3,00	
Ketone	2-Heptanone	C7H14O		0,68	0,34	0,66		0,36	0,54	

Ketone	2-Hexanone	C6H12O		0,45		0,24		
Ketone	2-Hexanone, 4-methyl-	C7H14O					6,16	
Ketone	2-Nonadecanone	C19H38O	0,64	1,19		1,38		
Ketone	2-Nonanone	C9H18O	0,93	1,53	0,61	1,31	2,24	0,55
Ketone	2-Octanone	C8H16O	0,45	0,89	0,36	0,66	0,76	0,36
Ketone	2-Pentadecanone	C15H30O		7,06	1,62	3,10	1,59	2,27
Ketone	2-Pentanone	C5H10O			0,96		0,76	
Ketone	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	C10H12O3	0,64					0,5
Ketone	2-Propanone, 1-(acetoxy)-	C5H8O3	0,50			0,42		0,64
Ketone	2-Propanone, 1-hydroxy-	C3H6O2	2,23	1,03	2,06	0,47	1,58	2,21
Ketone	2-Undecanone	C11H22O		0,8		0,41		0,55
Ketone	3',5'-Dimethoxyacetophenone	C10H12O3		0,47		0,41		
Ketone	9-Octadecanone	C18H36O						0,45
Ketone	Acetone	C3H6O	2,54	5,6	3	6,36	3,99	3,18
Ketone	Cyclopentadecanone	C15H28O		0,64	0,97			3,13
Ketone	Cyclopentanone	C5H8O		0,51		0,41		
Ketone	Cyclopentanone, 2-methyl-	C6H10O	0,50	0,6		0,44		
Ketone	Ethanone, 1-cyclododecyl-	C14H26O	3,73			0,58		
Ketone	Methyl vinyl ketone	C4H6O			0,99		0,79	
Ketone	Octadecan-4-one	C18H36O	0,45	0,6		0,49		
Others	.beta.-D-Glucopyranose, 1,6-anhydro-	C6H10O5	0,88					
Others	2,3,5-Trimethylanizole	C10H14O					1,19	
Others	Ammonium acetate	C2H7NO2			0,49			
Others	Butane, 1-chloro-	C4H9Cl		2,64				
Others	Cyacetamide	C3H5N3O			6,69	7,46	6,75	3,98
Others	D-Allose	C6H12O6						0,59
Others	Ethylene oxide	C2H4O						3,18
Others	Hexane, 1-fluoro-	C6H13F						3,16

Others	Isobutylene epoxide	C4H8O							0,81
Others	Methallyl cyanide	C7H7N			0,48				
Phenol	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	C11H14O3	1,13	0,5		0,60			0,8
Phenol	2-Methoxy-4-vinylphenol	C9H10O2							4,1
Phenol	3-(tert-Butyl)-4-methoxyphenyl acetate	C13H18O3	0,96						
Phenol	3,5-Dimethoxy-4-hydroxytoluene	C9H12O3	1,27			0,49			0,5
Phenol	4-Hydroxy-3-methylacetophenone	C9H10O2	3,97	2,55					1,83
Phenol	Apocynin	C10H10O3							0,2
Phenol	Catechol	C6H6O2					0,71		
Phenol	Creosol	C8H10O2	3,27	1,19		1,63		0,72	1,1
Phenol	p-Cresol	C7H8O				0,44			0,47
Phenol	Phenol	C6H6O	1,00	0,91	1,17	1,22	1,23	1,42	1,39
Phenol	Phenol, 2,4-dimethyl-	C8H10O				0,42		0,97	0,42
Phenol	Phenol, 2,6-dimethoxy-	C8H10O3	1,78	0,66		0,87		0,43	1,3
Phenol	Phenol, 2,6-dimethoxy-4-(2-propenyl)-	C11H14O3							0,2
Phenol	Phenol, 2-methoxy-	C8H10O3	4,50	2,54		2,88		1,05	1,74
Phenol	Phenol, 2-methoxy-3-(2-propenyl)-	C10H12O2	0,65			0,63			0,8
Phenol	Phenol, 2-methoxy-4-propyl-	C10H14O2							0,3
Phenol	Phenol, 2-methyl-	C8H10O3	0,57		0,58	0,66	0,49	0,46	1,32
Phenol	Phenol, 3-methyl-	C7H8O				0,61	0,52		0,59
Phenol	Phenol, 4-ethyl-2-methoxy-	C9H12O2	1,30	0,55		1,11			0,4
Phenol	trans-Isoeugenol	C10H12O2	2,95	2,09		2,26		1,09	2,6

17

18

19

20

21

22

Table S3. Compounds obtained during catalytic pyrolysis – Catalyst Phosphatic mining waste (PO)

23

Category	Name	Formula	550-15	550-85	750-15	750-85	508-50	791-50	650-100	650-50
			PO	PO						
Acid	6-Octadecenoic acid, (Z)-	C18H34O2			2,98					
Acid	Acetic acid	C2H4O2	14,32	7,70	8,16	5,57	9,23		4,77	2,82
Acid	Acetic acid, (acetoxy)-	C6H6O4				0,58		0,55		0,50
Acid	Carbamic acid, monoammonium salt	CH6N2O2		22,80			18,49		39,99	14,41
Acid	Heptanoic acid	C7H14O2	0,59	0,50			0,56			
Acid	Hexanoic acid	C16H12O2		0,53			0,35			
Acid	Methylphosphonic acid, 2TMS derivative	C7H21O3PSi2			0,24			0,56		
Acid	n-Hexadecanoic acid	C16H32O2	6,75	5,47	8,81	6,26		1,77	1,24	6,14
Acid	Nonanoic acid	C9H18O2	0,46	0,34			0,44			
Acid	Octanoic acid	C8H16O2	2,05	0,69	0,68	0,50	0,72			0,51
Acid	Oleic Acid	C18H34O2	3,94	2,89		1,79				2,17
Alcohol	(6Z)-Nonen-1-ol	C9H18O							0,27	
Alcohol	1-Hexadecanol	C16H34O		0,30						
Alcohol	1-Nonanol	C9H20O								0,35
Alcohol	1-Tetradecanol	C14H30O							0,35	0,45
Alcohol	1-Undecanol	C11H24O							0,19	
Alcohol	2-Furanmethanol	C5H6O					0,41			
Alcohol	3-Buten-1-ol	C4H8O				5,79				
Alcohol	3-Buten-1-ol, 2-methyl-	C5H10O								1,31
Alcohol	4-Penten-1-ol	C5H10O				0,56				
Alcohol	Benzeneethanol, 3-hydroxy-	C8H10O2					0,43			
Alcohol	cis-11,12-Epoxytetradecen-1-ol	C16H30O3								0,73
Alcohol	cis-9-Tetradecen-1-ol	C14H28O			0,57					
Alcohol	Cyclopropyl carbinol	C4H8O		0,36			1,01			
Alcohol	Methyl Alcohol	CH4O	5,42	4,12			1,81			1,27

Aldehyde	2-Propenal	C3H4O	0,47	0,49	1,36	1,57		1,28		
Aldehyde	4-Methyl-2,5-dimethoxybenzaldehyde	C10H12O3	1,27							
Aldehyde	Acetaldehyde	C2H4O	1,12	2,17	3,12	2,04	1,19	2,93	1,66	1,65
Aldehyde	Acetaldehyde, hydroxy-	C6H10O3	3,11	0,96	1,61	0,66	1,45	0,62	4,89	0,55
Aldehyde	Furfural	C5H4O2	0,92	0,63		0,49	1,01			
Aldehyde	Methyl glyoxal	C3H4O2	4,12	4,24			1,76			
Aldehyde	Nonanal	C9H18O	0,55	0,47	0,24		0,63		0,46	
Aldehyde	Octanal	C8H16O					0,40			
Aldehyde	Succindialdehyde	C4H6O2	0,77	0,32	0,17		0,59		0,17	
Aldehyde	Vanillin	C8H8O3	0,81				0,34			
Amine/Amide	2,3-Diazabicyclo[2.2.1]-hept-2-ene	C5H8N2			0,88					
Amine/Amide	N-[4-(4-Chlorophenyl)isothiazol-5-yl]-1-methylpiperidin-2-imine	C15H16ClN3S			0,50					
Amine/Amide	Pyrrole	C4H5N					0,49			
Ester	[1,1'-Bicyclohexyl]-4-carboxylic acid, 4'-pentyl-, 4-fluorophenyl ester	C24H35FO2		1,10						
Ester	1,2-Cyclopentanedione, 3-methyl-	C6H8O2	0,93	0,49			1,25			
Ester	1,4-Dioxin, 2,3-dihydro-	C4H6O2	0,25							
Ester	1-Adamantanecarboxylic acid, 5-tetradecyl ester	C25H44O2					1,75			
Ester	2-Furancarboxylic acid, 2-tetrahydrofurylmethyl ester	C10H12O4					0,29			
Ester	5-Isopropyl-2-methylphenyl 3-methylbutanoate	C15H22O2		2,73						
Ester	6,9-Octadecadienoic acid, methyl ester	C19H34O2		0,70						
Ester	8-Octadecenoic acid, methyl ester	C19H36O2			0,22					
Ester	9,11-Octadecadienoic acid, methyl ester, (E,E)-	C19H34O2					0,38			
Ester	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	C21H40O4					1,19			
Ester	9-Octadecenoic acid (Z)-, methyl ester	C19H36O2	2,75							
Ester	9-Octadecenoic acid, 1,2,3-propanetriyl ester, (E,E,E)-	C57H104O6					0,21			
Ester	9-Octadecenoic acid, methyl ester, (E)-	C19H36O2	2,63	2,74		0,92			1,85	1,72
Ester	Acetic acid, methyl ester	C2H4O2	1,23	0,65	0,88		0,99		1,14	
Ester	Acetic acid, trifluoro-, undecyl ester	C13H23F3O2	0,58							

HC	1-Decene	C10H20		1,14	1,09			0,89	
HC	1-Dodecene	C12H24			0,62			0,55	
HC	1-Heptadecene	C17H34		0,30					
HC	1-Heptene	C7H14	1,26	3,84	4,02	3,85	2,66	4,53	
HC	1-Hexene	C6H12		6,47	5,96	6,79			
HC	1-Nonene	C9H18		1,03	1,05	1,05	0,67	1,12	
HC	1-Octene	C8H16		1,57	2,08	1,87	1,05	2,95	
HC	1-Pentadecene	C15H30				0,99		0,34	
HC	1-Pentene	C5H10		5,67		6,13			
HC	1-Tridecene	C13H26		0,89	1,28	0,96	0,41	1,00	
HC	1-Undecene	C11H22		0,69		0,92	0,56	0,81	
HC	2,4-Dimethyl-1-heptene	C9H18				0,22			
HC	2-Nonene	C9H18			0,37				
HC	3-Heptadecene, (Z)-	C17H34		0,54			0,50		
HC	3-Hexadecene, (Z)-	C16H32	0,25	0,31	1,20	1,26	1,11	0,70	1,11
HC	3-Octadecene, (E)-	C18H36				0,62		1,09	
HC	3-Tetradecene, (Z)-	C14H28		1,10	1,10				
HC	4-Methylenecyclopentene	C6H8			1,08				
HC	6-Dodecyne	C12H22					0,40		
HC	7-Pentadecyne	C15H28	0,39						
HC	8-Heptadecene	C17H34		0,52	0,26	0,70		0,54	
HC	9-Octadecene, (E)-	C18H36	0,74						
HC	Benzene	C6H6		1,34	1,97	2,05	0,78		
HC	Benzene, 1,3-dimethyl-	C8H10		0,77	1,22				
HC	Bicyclo[3.1.0]hexane	C6H10				0,30			
HC	Cyclobutane, 1-ethyl-3-methylene-	C7H12		0,28		0,39			
HC	Cyclobutene	C4H6		3,71	4,69	4,50	2,74		
HC	Cyclododecene, (Z)-	C12H22			0,47	0,47	0,29	0,37	

HC	Cyclopentane, 1,3-bis(methylene)-	C7H10			0,89			
HC	Cyclopentene, 1-methyl-	C6H10			0,39			
HC	Cyclopropane, 1,2-dimethyl-, trans-	C5H10		0,44		0,56		
HC	Cyclopropane, 1-heptyl-2-methyl-	C11H22	0,31			1,17	0,55	
HC	Cycloundecene(E)	C11H20		0,58		0,41		
HC	Decane	C10H22					0,37	
HC	Dodecane	C12H26					0,27	
HC	Dodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-	C25H48		0,73				
HC	Ethylbenzene	C8H10		0,33	0,45		0,51	
HC	Heptane, 2,4-dimethyl-	C9H20		0,27	0,54		0,33	
HC	Hexadecane	C16H34					0,50	
HC	Hexane, 2-methyl-	C7H16					4,62	4,55
HC	Nonane	C9H20					0,35	0,60
HC	Nonane, 3,7-dimethyl-	C11H24					0,32	
HC	Octane	C8H18	1,08			0,53		0,73
HC	Pentadecane	C15H32			0,75			1,28
HC	Propene	C3H6		12,71	14,95		15,42	
HC	Styrene	C8H8			0,50			
HC	Tetradecane	C14H30		0,56			0,52	0,81
HC	Toluene	C7H8		2,01	2,95	0,58	2,51	1,84
HC	Tridecane	C13H28						0,58
HC	Undecane	C11H24						0,38
HC	Undecane, 3-methylene-	C12H24		0,38			0,38	
HC	Undecane, 5-methyl-	C12H26						0,35
HC	Vinylcyclopentane	C7H12			0,56			
Ketone	1,2-Cyclopentanedi one	C5H6O2					1,11	
Ketone	1-Hydroxy-2-butanone	C4H8O2					0,30	
Ketone	2,3-Butanedione	C4H6O2	1,05	0,58	1,01	1,11	0,77	0,82
							0,95	0,25

Ketone	2,3-Pentanedione	C4H6O2	0,32					
Ketone	2-Butanone	C4H8O		0,45		0,34	0,55	0,38
Ketone	2-Cyclopenten-1-one	C5H6O	0,41			0,31		
Ketone	2-Cyclopenten-1-one, 2-methyl-	C6H8O				0,30		
Ketone	2-Decanone	C10H20O	0,31	0,52		0,45		0,52
Ketone	2-Heptadecanone	C17H34O						0,88
Ketone	2-Nonadecanone	C19H38O	0,19	0,69		0,52		0,97
Ketone	2-Nonanone	C9H18O		0,32				
Ketone	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	C10H12O3	0,59	0,31		0,52		
Ketone	2-Propanone, 1-(acetoxy)-	C5H8O3				0,40		
Ketone	2-Propanone, 1-hydroxy-	C3H6O2	3,20	1,44	2,47	1,49	2,72	1,51
Ketone	3',5'-Dimethoxyacetophenone	C10H12O3		0,62		0,82		
Ketone	6-Oxa-bicyclo[3.1.0]hexan-3-one	C5H6O2		0,35				
Ketone	9-Heptadecanone	C17H34O	1,00	0,82	0,28		0,47	0,30
Ketone	Acetone	C3H6O	0,83	0,52	1,14	0,96	0,34	1,32
Ketone	Cycloheptanone	C7H12O		0,99		0,46	0,36	0,66
Ketone	Cyclohexanone	C6H10O	0,65	1,06		0,46	0,42	0,63
Ketone	Cyclopentadecanone	C15H28O						0,37
Ketone	Ethanone, 1-cyclododecyl-	C14H26O		0,82				
Others	Acetonitrile	C2H3N					0,79	0,36
Others	Ammonium acetate	C2H7NO2					6,52	
Others	Butane, 1-(ethenylthio)-	C6H12S	0,45					
Others	Chloromethane	CH3Cl	1,03	5,97				
Others	Methyl isocyanide	C2H3N				0,70		
Others	Pentadec-7-ene, 7-bromomethyl-	C16H31Br						0,81
Phenol	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	C11H14O3	1,18	0,58		0,29		0,29
Phenol	3,5-Dimethoxy-4-hydroxytoluene	C9H12O3	0,91	0,48		0,65		
Phenol	4-Hydroxy-2-methylacetophenone	C9H10O2	5,30			3,44		0,58

Phenol	5-tert-Butylpyrogallol	C10H14O3	0,36								
Phenol	Apocynin	C10H10O3	0,28								
Phenol	Creosol	C8H10O2	2,26	1,43				1,75			0,27
Phenol	Eugenol	C10H12O2	0,63								
Phenol	p-Cresol	C7H8O		0,62		0,59					
Phenol	Phenol	C6H6O	2,00	1,73	1,66	2,26	1,18	1,90	1,40	2,15	
Phenol	Phenol, 2,6-dimethoxy-	C8H10O3	1,91	0,95			1,37				
Phenol	Phenol, 2,6-dimethoxy-4-(2-propenyl)-	C11H14O3	0,40								
Phenol	Phenol, 2-methoxy-	C8H10O3	4,86	2,83			3,30		1,32	0,88	
Phenol	Phenol, 2-methoxy-4-(1-propenyl)-	C10H12O2	0,44				0,35		0,93	0,55	
Phenol	Phenol, 2-methoxy-4-propyl-	C10H14O2	0,23								
Phenol	Phenol, 2-methyl-	C8H10O3		0,52		0,73	0,35			0,79	
Phenol	Phenol, 3-methyl-	C7H8O		0,82		0,86	0,41			1,40	
Phenol	Phenol, 4-ethyl-2-methoxy-	C9H12O2	0,94	0,49			0,78				
Phenol	trans-Isoeugenol	C10H12O2	2,81	1,48			1,73				

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Table S4. Compounds obtained during catalytic pyrolysis – Catalyst Niobium Oxide (Nb₂O₅)

37

Category	Name	Formula	550-15	550-85	750-15	750-85	508-50	791-50	650-100	650-50	650-0
			Nb	Nb	Nb						
Acid	2-Propenoic acid	C ₃ H ₄ O ₂							0,38		
Acid	3-Heptenoic acid	C ₇ H ₁₂ O ₂				0,70					
Acid	5-Hexenoic acid	C ₆ H ₁₀ O ₂				0,50					
Acid	7-Octenoic acid	C ₈ H ₁₄ O ₂				0,44					
Acid	8-Nonenoic acid	C ₉ H ₁₆ O ₂				0,30					
Acid	Acetic acid	C ₂ H ₄ O ₂	15,12	17,35	18,29	22,53	14,89	15,37	22,13	17,46	12,7
Acid	Acetic acid, (acetoxy)-	C ₆ H ₆ O ₄	2,02	1,75	2,64				1,10		2,0
Acid	Acetic anhydride	C ₄ H ₆ O ₃							0,86		
Acid	Carbamic acid, monoammonium salt	CH ₆ N ₂ O ₂	16,04						7,24		20,9
Acid	cis-10-Heptadecenoic acid	C ₁₇ H ₃₂ O ₂						15,03			
Acid	Hexanoic acid	C ₆ H ₁₂ O ₂	0,5	0,71		0,60	0,76		0,79	0,74	
Acid	n-Hexadecanoic acid	C ₁₆ H ₃₂ O ₂	7,94	7,78	4,98	2,48	12,66	0,66	4,92	10,45	2,5
Acid	Nonanoic acid	C ₉ H ₁₈ O ₂	0,27	0,40			0,45		0,47	0,39	
Acid	Octadecanoic acid	C ₁₈ H ₃₆ O ₂	1,56								
Acid	Octanoic acid	C ₈ H ₁₆ O ₂	1,06	1,14					0,70	0,95	
Acid	Oleanitrile	C ₁₈ H ₃₃ N							0,49		
Acid	Oleic Acid	C ₁₈ H ₃₄ O ₂	6,77	11,82	1,36	0,53			2,99	10,94	
Acid	Propanoic acid	C ₃ H ₆ O ₂	0,3	0,41		0,54		0,46	0,53		
Acid	Propanoic acid, anhydride	C ₆ H ₁₀ O ₃									0,3
Alcohol	1,6-Heptadien-4-ol	C ₇ H ₁₂ O					0,31				
Alcohol	2-Propen-1-ol	C ₃ H ₆ O			0,34				0,28		
Alcohol	4-Penten-1-ol	C ₅ H ₁₀ O				0,44					
Alcohol	Cyclopropyl carbinol	C ₄ H ₈ O					1,04				
Alcohol	Methyl Alcohol	CH ₄ O	2,99	4,08		5,35	1,67		5,55	3,80	3,3
Aldehyde	2-Butenal	C ₄ H ₆ O			0,34	0,81					

Aldehyde	2-Propenal	C3H4O	0,54	1,01	2,09	1,58	0,69	1,28	1,88	1,18	0,6
Aldehyde	4-Methyl-2,5-dimethoxybenzaldehyde	C10H12O3									0,50
Aldehyde	Acetaldehyde	C2H4O	1,25	2,17	3,39	3,73	1,70	2,20	3,37	2,55	1,5
Aldehyde	Acetaldehyde, hydroxy-	C6H10O3	2,19	1,55	1,32	0,65	0,68		0,46	1,43	6,1
Aldehyde	Benzaldehyde, 3-hydroxy-4-methoxy-	C8H8O3							0,71		
Aldehyde	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	C9H10O4	0,27					0,24			
Aldehyde	Butanal	C4H8O								0,47	
Aldehyde	Coniferyl aldehyde	C10H10O3									0,9
Aldehyde	Formaldehyde	CH2O	0,52								1,8
Aldehyde	Furfural	C5H4O2	1,64	2,46	2,31			2,52			1,1
Aldehyde	Hexanal	C6H12O	0,18	0,29			0,34			0,38	
Aldehyde	Methyl glyoxal	C3H4O2	1,79								2,5
Aldehyde	Nonanal	C9H18O	0,26	0,73					0,55	0,68	0,5
Aldehyde	Octanal	C8H16O	0,33	0,53					0,64	0,61	
Aldehyde	Propanal	C3H6O			0,40		1,30				
Aldehyde	Succindialdehyde	C4H6O2	0,68	0,61							1,1
Aldehyde	Vanillin	C8H8O3	0,59	0,45					0,51	0,65	0,7
Amine/Amide	2,4-Diaminopyrimidine	C4H6N4				0,31					
Amine/Amide	3,5-Dimethylpyrazole	C5H8N2						1,58			
Amine/Amide	Aziridine, 1,2-diisopropyl-3-methyl-, trans-	C9H19N			0,79						
Amine/Amide	Aziridine, 2-(1,1-dimethylethyl)-3-methyl-, trans-	C7H15N				1,59					
Amine/Amide	N-tert-Butylethylamine	C6H15N	0,23				0,31				
Amine/Amide	Pyrrolidine, N-(3-methyl-3-butenyl)-	C9H17N				0,28					
Ester	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	C16H22O4									0,3
Ester	1,2-Cyclopentanedione, 3-methyl-	C6H8O2	0,75	0,95	0,44	0,47	1,35		0,94	0,75	0,4
Ester	2-(tert-Butyl)-4-methoxyphenyl acetate	C13H18O3									1,1
Ester	2,3-Dihydroxypropyl elaidate	C21H40O4									0,7
Ester	8-Octadecenoic acid, methyl ester	C19H36O2	0,32		0,83						

Ester	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	C19H34O2	0,33		0,24			
Ester	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	C21H40O4					1,9	
Ester	9-Octadecenoic acid (Z)-, methyl ester	C19H36O2					0,4	
Ester	9-Octadecenoic acid, methyl ester, (E)-	C19H36O2	1,59	3,87		2,21	3,36	2,25
Ester	Acetic acid ethenyl ester	C4H6O2		1,07				
Ester	Acetic acid, methyl ester	C2H4O2		2,15		2,08	3,38	1,75
Ester	Benzene, 1-(dodecyloxy)-2-nitro-	C18H29NO3					0,4	
Ester	Benzene, 1,2,3-trimethoxy-5-methyl-	C10H14O3	0,3		0,42			
Ester	cis-Cyclohexane-1,4-dimethanol, diacetate	C12H20O4				0,32		
Ester	Decanoic acid, 2-propenyl ester	C13H24O2					0,6	
Ester	Decyl oleate	C28H54O2					1,7	
Ester	Dodecane, 1-(methoxymethoxy)-	C14H30O2					0,4	
Ester	Ethyl Oleate	C20H38O2	0,17	0,30				
Ester	Hexadecanoic acid, methyl ester	C17H34O2	0,76	1,95	0,61	1,27	2,22	1,37
Ester	Hexadecanoic acid, n.-octyl ester	C24H48O2					1,8	
Ester	Methyl nitrite	CH3NO2		1,64	1,07			
Ester	Octadecanoic acid, 2-propenyl ester	C21H40O2	0,51	0,67			0,69	
Ester	Oxetane, 3-(1-methylethyl)-	C6H12O		1,03				
Ester	Propanoic acid, 2-oxo-, methyl ester	C4H6O3	1,03	0,98	1,28	0,94	0,77	0,78
Ester	Resorcinol monoacetate	C8H8O3				0,58		
Furan	2(5H)-Furanone	C4H4O2			0,46			
Furan	3-Furaldehyde	C5H4O2			2,06		1,97	1,70
Furan	Benzofuran, 2,3-dihydro-	C8H8O		0,77	0,55	0,61		
Furan	Furan	C4H4O	0,26	0,93	2,03	0,99	1,55	0,91
Furan	Furan, 2,5-dimethyl-	C6H8O			0,50			
Furan	Furan, 2-ethyl-	C6H8O			0,43	0,26		
Furan	Furan, 2-methyl-	C5H6O	0,32	0,72	1,02	1,34	1,08	1,22
HC	1,3,5-Hexatriene, (Z)-	C6H8		0,60	0,76		0,75	0,3

HC	1,3-Butadiene	C4H6	3,25	2,20	4,70		0,5	
HC	1,3-Cyclopentadiene	C5H6	1,51	1,12	2,98	0,39	0,2	
HC	1,3-Cyclopentadiene, 1-methyl-	C6H8	0,38		1,18			
HC	1,3-Cyclopentadiene, 5-(1-methylethylidene)-	C8H10		0,62				
HC	1,3-Pentadiene, (E)-	C5H8	0,70		0,91		0,3	
HC	1,3-Pentadiene, (Z)-	C5H8		0,89		0,74		
HC	1,4-Pentadiene	C5H8	1,52					
HC	1-Buten-3-yne	C4H4			0,28			
HC	1-Butyne	C4H6				0,71	0,90	
HC	1-Decene	C10H20	0,80	0,49	0,48		0,36	
HC	1-Heptadecene	C17H34	0,37					
HC	1-Heptene	C7H14	2,43	1,63	1,66	1,23	1,34	0,5
HC	1-Hexene	C6H12	3,57	3,99	3,01			
HC	1-Nonene	C9H18	0,72	0,45	0,46		0,42	
HC	1-Octene	C8H16	0,90	0,71	0,76		0,51	
HC	1-Pentadecene	C15H30			0,32		0,42	
HC	1-Pentene, 4-methyl-	C6H12					2,89	
HC	1-Tetradecene	C14H28	0,55	0,75		0,47		
HC	1-Tridecene	C13H26		0,62	0,27			
HC	1-Undecene	C11H22	0,79	0,58	0,48		0,35	
HC	2-Butene, (Z)-	C4H8	3,62		4,24		0,7	
HC	2-Hexene, (E)-	C6H12			0,31			
HC	2-Methyl-1-butene	C5H10			0,58			
HC	2-Pentene, (Z)-	C5H10	0,45		0,59			
HC	4-Methylenecyclopentene	C6H8	1,01		1,36			
HC	Benzene	C6H6	1,05	1,31	3,28	0,62		
HC	Benzene, 1,2,3-trimethyl-	C9H12				0,51		
HC	Benzene, 1,3-dimethyl-	C8H10			0,30	1,34		

HC	Cyclobutane	C4H8		2,75		0,99	1,33
HC	Cyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyyl]bis-	C22H40				0,87	
HC	Cyclopropane	C3H6		4,99			2,96
HC	Cyclopropane, nonyl-	C12H24		0,44		0,26	
HC	Ethylbenzene	C8H10				0,59	
HC	Hexatriacontane	C36H74					2,0
HC	Indene	C9H8				0,54	
HC	Isoprene	C5H8				1,07	
HC	Naphthalene	C10H8				0,33	
HC	o-Xylene	C8H10		1,99			
HC	Propene	C3H6		6,38		8,42	
HC	Propyne	C3H4				1,11	
HC	p-Xylene	C8H10		0,68		1,14	0,76
HC	Styrene	C8H8				0,72	
HC	Toluene	C7H8		1,42	2,27	4,55	1,96
Ketone	1,2-Cyclopentanedione	C5H6O2	0,76	0,79	0,58		0,59
Ketone	1H-Inden-1-one, 2,3-dihydro-7-hydroxy-3-methyl-	C10H10O2				0,46	
Ketone	1-Hydroxy-2-butanone	C4H8O2	0,45	0,42		0,49	
Ketone	2,3-Butanedione	C4H6O2	0,89	1,17		1,37	1,93
Ketone	2,3-Pentanedione	C4H6O2	0,19				0,5
Ketone	2,4(3H,5H)-Furandione, 3-methyl-	C5H6O3				0,24	
Ketone	2-Butanone	C4H8O		0,46	0,79	1,58	0,56
Ketone	2-Cyclopenten-1-one	C5H6O				0,85	0,93
Ketone	2-Cyclopenten-1-one, 2-methyl-	C6H8O		0,39		0,58	0,38
Ketone	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	C10H12O3	0,51	0,44		0,53	
Ketone	2-Propanone, 1-(acetoxyloxy)-	C5H8O3	0,48	0,50	0,48	0,40	0,65
Ketone	2-Propanone, 1-hydroxy-	C3H6O2	3,26	2,08	3,96	1,61	3,00
Ketone	3',5'-Dimethoxyacetophenone	C10H12O3	0,92	0,90		0,85	0,54

Ketone	3-Buten-2-one, 3-methyl-	C5H8O			0,41						
Ketone	Acetone	C3H6O	0,69	1,45	1,47	2,98	1,72	2,13	2,34	1,46	0,7
Ketone	Cyclopentanone	C5H8O				0,53					
Ketone	Methyl vinyl ketone	C4H6O				1,95		1,30			
Others	.beta.-D-Glucopyranose, 1,6-anhydro-	C6H10O5					1,08				
Others	Acetonitrile	C2H3N				0,60					
Others	Cyacetacide	C3H5N3O			5,65			5,01			
Others	Heptadecanenitrile	C17H33N	0,27	0,51					0,57	0,61	
Others	Methyl isocyanide	C2H3N					0,67				
Others	Spiro[2,5-cyclohexadiene-1,7'-[2.8]dioxabicyclo[4.2.0]octane]-4,3'-dione, 5',5'-dimethyl-	C13H14O4					0,60				
Phenol	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	C11H14O3	1,02	0,92			1,09		0,46	0,53	0,8
Phenol	2-Allylphenol	C9H10O			0,36			0,37			
Phenol	2-Methoxy-4-vinylphenol	C9H10O2									4,1
Phenol	3,5-Dimethoxy-4-hydroxytoluene	C9H12O3	0,74	0,69			1,10		0,37	0,5	
Phenol	4-Hydroxy-3-methylacetophenone	C9H10O2	3,7	3,17			3,12		3,23	2,59	
Phenol	Apocynin	C10H10O3	0,31				0,41				0,2
Phenol	Creosol	C8H10O2	1,91	1,64			2,44		0,96	1,06	1,1
Phenol	Eugenol	C10H12O2		0,65							0,44
Phenol	p-Cresol	C7H8O	0,36	0,48	0,63	0,74	0,48	0,70	0,57	0,42	
Phenol	Phenol	C6H6O	1,23	2,06	2,01	2,87	1,31	2,32	2,21	1,59	1,0
Phenol	Phenol, 2-(1-methylethyl)-, methylcarbamate	C11H15NO2			0,46						
Phenol	Phenol, 2,4-dimethyl-	C8H10O		0,31	0,78	0,98	0,60	0,77			
Phenol	Phenol, 2,6-dimethoxy-	C8H10O3	1,46	1,39			1,55		0,69	0,68	1,3
Phenol	Phenol, 2,6-dimethoxy-4-(2-propenyl)-	C11H14O3	0,38	0,37			0,48				0,2
Phenol	Phenol, 2-ethyl-4-methyl-	C9H12O				0,40					
Phenol	Phenol, 2-methoxy-	C8H10O3	3,67	3,57			3,38		2,39	2,06	3,4
Phenol	Phenol, 2-methoxy-3-(2-propenyl)-	C10H12O2						0,51			0,6

Phenol	Phenol, 2-methoxy-4-(1-propenyl)-, (Z)-	C10H12O2	0,62	0,45		0,74		0,38
Phenol	Phenol, 2-methoxy-4-propyl-	C10H14O2	0,19			0,25		0,3
Phenol	Phenol, 2-methyl-	C8H10O3	0,53	0,62	0,94	1,29	0,40	1,20
Phenol	Phenol, 3-methyl-	C7H8O		1,39	1,09	1,73	0,71	1,13
Phenol	Phenol, 4-ethyl-	C8H10O					0,27	
Phenol	Phenol, 4-ethyl-2-methoxy-	C9H12O2	0,8	0,61		1,01		0,47
Phenol	trans-Isoeugenol	C10H12O2	2,84	2,60		1,67		1,86
							1,90	2,6

Table S5. Compounds obtained during catalytic pyrolysis – Catalyst Nickel supported niobium Oxide (Nb₂O₅)

59

Category	Name	Formula	550-15	550-85	750-15	750-85	508-50	791-50	650-100	650-50	650-0
			NbNi	NbNi	NbNi						
Acid	1,3-Dioxolane-4,5-dione	C3H2O4					3,55				
Acid	3-Heptenoic acid	C7H12O2							0,49		
Acid	6-Heptenoic acid	C7H12O2				0,76	0,67				
Acid	7-Octenoic acid	C8H14O2				0,41					
Acid	9-Octadecenoic acid, (E)-	C18H34O2					1,04				
Acid	Acetic acid	C2H4O2	13,94	0,52	16,16	18,98	15,60	13,83	8,94	12,60	
Acid	Acetic acid, (acetoxy)-	C6H6O4	1,96		1,50	1,96				1,16	
Acid	Acetic anhydride	C4H6O3							0,48		
Acid	Carbamic acid, monoammonium salt	CH6N2O2		7,88						26,17	
Acid	cis-10-Heptadecenoic acid	C17H32O2							3,90	8,47	
Acid	Heptanoic acid	C7H14O2	0,36								
Acid	Hexadecanenitrile	C16H31N								0,25	
Acid	Hexanoic acid	C16H12O2				0,68				0,45	0,56
Acid	n-Hexadecanoic acid	C16H32O2	10,81		5,14	3,96	7,07	1,67	5,88	6,88	
Acid	Nonanoic acid	C9H18O2	0,48				0,43			0,35	
Acid	Octanoic acid	C8H16O2	0,47		0,69	0,46	0,29			0,57	0,82
Acid	Oleic Acid	C18H34O2	11,87		2,58		9,65				
Acid	Palmitoleic acid	C16H30O2	0,39								
Acid	Propanoic acid	C3H6O2			0,51		0,66			0,32	
Alcohol	1,6-Heptadien-4-ol	C7H12O					0,36				
Alcohol	2-Furanmethanol	C5H6O					0,33				
Alcohol	2-Propen-1-ol	C3H6O						0,26			
Alcohol	4-Penten-1-ol	C5H10O				0,62					
Alcohol	9-Octadecen-1-ol, (Z)-	C18H36O							0,55		

Alcohol	Cyclopropyl carbinol	C4H8O	0,91		1,04			
Alcohol	Methyl Alcohol	CH4O	4,30	7,27		3,31	2,69	3,54
Alcohol	Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate	C16H28O3		7,02				
Aldehyde	(E)-Hexadec-2-enal	C16H30O		0,66				
Aldehyde	2-Butenal	C4H6O			0,31	0,27	0,23	
Aldehyde	2-Propenal	C3H4O			1,66	1,98	0,57	1,53
Aldehyde	Acetaldehyde	C2H4O	1,30	3,11	3,35	3,28	0,83	2,96
Aldehyde	Acetaldehyde, hydroxy-	C6H10O3	3,36		2,06	0,82	0,83	1,25
Aldehyde	Benzaldehyde, 3-hydroxy-4-methoxy-	C8H8O3				0,72		
Aldehyde	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	C9H10O4	0,24					
Aldehyde	Furfural	C5H4O2	1,81		2,19	2,12	1,45	1,50
Aldehyde	Hexanal	C6H12O						0,31
Aldehyde	Methyl glyoxal	C3H4O2	2,44					
Aldehyde	Nonanal	C9H18O	0,30		0,64	0,48	0,53	0,21
Aldehyde	Octanal	C8H16O	0,35	0,51				0,46
Aldehyde	Propanal	C3H6O	1,41	0,65	0,57	0,30	0,94	
Aldehyde	Succindialdehyde	C4H6O2						0,45
Aldehyde	Vanillin	C8H8O3	0,78					0,38
Amida	Formamide	CH3NO			6,79			
Amine/Amide	L-Alanine ethylamide, (S)-	C5H12N2O						4,60
Ester	1,2-Cyclopentanedione, 3-methyl-	C6H8O2	0,96		0,65			0,36
Ester	5-Isopropyl-2-methylphenyl pentanoate	C15H22O2						1,17
Ester	9-Octadecenoic acid, methyl ester, (E)-	C19H36O2	1,27	2,93		1,82	0,99	1,46
Ester	Acetic acid ethenyl ester	C4H6O2			1,04	1,05		
Ester	Acetic acid, 2-ethylbutyl ester	C8H16O2		4,94				3,15
Ester	Acetic acid, methyl ester	C2H4O2				2,02		
Ester	Benzene, 1,2,3-trimethoxy-5-methyl-	C10H14O3	0,48			0,44		
Ester	Hexadecanoic acid, methyl ester	C17H34O2	0,40	1,52		0,26	0,77	0,55

Ester	Methyl nitrite	CH3NO2		1,83	1,70						
Ester	Octadecanoic acid, 2-propenyl ester	C21H40O2									0,60
Ester	Oxetane, 3-(1-methylethyl)-	C6H12O			0,81						
Ester	Propanoic acid, 2-oxo-, methyl ester	C4H6O3	0,82	1,16	0,85	0,90					0,86
Furan	2(5H)-Furanone	C4H4O2				0,44					
Furan	3-Furaldehyde	C5H4O2	0,69	1,24							1,00
Furan	4,7-Methanoisobenzofuran-1,3-dione, 3a,4,7,7a-tetrahydro-3a,7a-dimethyl-, (3a.alpha.,4.alpha.,7.alpha.,7a.alpha.)-	C11H12O3				0,30					
Furan	Benzofuran, 2,3-dihydro-	C8H8O					0,53				
Furan	Furan	C4H4O	0,53	0,59	0,90	0,33	0,76	0,65	0,67		
Furan	Furan, 2-methyl-	C5H6O			1,20	0,41	0,98	0,51	0,56		
HC	.alpha.-Methylstyrene	C9H10									1,76
HC	1,2-Dihydro-3-phenylnaphthalene	C16H14									0,32
HC	1,2-Diphenylcyclopropane	C15H14									0,40
HC	1,3,5-Hexatriene, (Z)-	C6H8		0,56	0,60						
HC	1,3-Butadiene	C4H6		3,02	3,43		4,43				
HC	1,3-Cyclopentadiene	C5H6			1,44	1,67		2,37			
HC	1,3-Cyclopentadiene, 1-methyl-	C6H8				0,33		0,81			
HC	1,3-Cyclopentadiene, 5-(1-methylethylidene)-	C8H10						0,91			
HC	1,3-Pentadiene, (E)-	C5H8				0,70		0,83			
HC	1,7-Hexadecadiene	C16H30		0,54	0,35						
HC	1,7-Octadiene	C8H14						0,14			
HC	1-Buten-3-yne	C4H4				0,22		0,27			
HC	1-Butyne	C4H6							0,59		
HC	1-Butyne, 3-methyl-	C5H8		0,74	0,75						
HC	1-Decene	C10H20	0,86	0,95	0,89		0,65		0,35		
HC	1-Heptadecene	C17H34			0,44						0,20
HC	1-Heptene	C7H14	4,37	2,79	2,70		2,10	0,90	1,41		

HC	1-Hexene	C6H12	5,28	4,56	3,48		
HC	1-Nonene	C9H18	0,92	0,84	0,83	0,60	0,40
HC	1-Octene	C8H16	1,5	1,36	1,04	0,94	0,32
HC	1-Pentadecene	C15H30	1,33	0,79	0,36	0,41	0,56
HC	1-Pentene, 4-methyl-	C6H12				1,62	
HC	1-Tetradecene	C14H28	0,56	0,84		0,19	0,42
HC	1-Tridecene	C13H26		0,71	0,59		
HC	1-Undecene	C11H22	0,74	0,97	0,91	0,67	0,34
HC	2,4-Hexadiene, 2,3-dimethyl-	C8H14	0,51				
HC	2-Butene	C4H8					1,74
HC	2-Butene, (Z)-	C4H8			3,96		
HC	2-Pentene, (E)-	C5H10		0,45	0,45	0,55	
HC	3-Hexyne	C6H10		0,90			
HC	4-Methylenecyclopentene	C6H8		0,74	1,08	1,30	
HC	5,6-Undecadiene	C11H20					0,23
HC	6-Dodecyne	C12H22	0,51	0,46	0,27		0,26
HC	Benzene	C6H6		0,96	1,32	2,16	0,61
HC	Benzene, (1-methylenepropyl)-	C10H12					0,84
HC	Benzene, (1-methylethyl)-	C9H12					0,58
HC	Benzene, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-	C16H18					0,44
HC	Benzene, 1,1'-(1,3-propanediyl)bis-	C15H16					0,29
HC	Benzene, 1,1'-(2-methyl-1-propenylidene)bis-	C16H16					0,28
HC	Benzene, 1,1'-(2-pentene-1,5-diyl)bis-	C17H18					2,48
HC	Benzene, 1,1'-(3-methyl-1-propene-1,3-diyl)bis-	C16H16					0,52
HC	Benzene, 1,3-dimethyl-	C8H10	0,76				0,50
HC	Benzene, 2-propenyl-	C9H10					0,40
HC	Benzene, propyl-	C9H12					0,69
HC	Bibenzyl	C14H14					0,44

HC	Bicyclo[2.1.0]pentane	C5H8				0,89		
HC	Cetene	C16H32	1,04					
HC	Cyclobutane	C4H8		3,85		4,31	1,22	
HC	Cyclododecene	C12H22						0,20
HC	Cyclohexene	C6H10					0,20	
HC	Cyclopentene, 3-ethyl-	C7H12	0,46					
HC	Cyclopropane	C3H6		7,22	7,72		8,58	
HC	Cyclopropane, 1-hexyl-2-propyl-, cis-	C12H24	0,5					
HC	Cyclopropane, nonyl-	C12H24	0,61	0,59	0,55	0,35		0,25
HC	Cyclopropene	C3H4					1,49	
HC	Dodecane	C12H26	0,79					
HC	Dodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-	C25H48	0,62					
HC	Ethylbenzene	C8H10			0,26	0,36	2,89	
HC	Heptane, 2,4-dimethyl-	C9H20	0,83					0,22
HC	Isoprene	C5H8		0,72	0,76			
HC	Nonane	C9H20	0,69					
HC	Propene	C3H6	1,64					
HC	Styrene	C8H8			0,35	0,42	32,32	
HC	Toluene	C7H8		1,53	1,94	2,28	3,84	0,96
HC	Tridecane	C13H28	0,7					
HC	Undecane	C11H24	0,54					
Ketone	(S)-(+)-2',3'-Dideoxyribonolactone	C5H8O3	0,31			0,32		
Ketone	1,2-Cyclopentanedione	C5H6O2	1,20			1,35		0,52
Ketone	1-Hydroxy-2-butanone	C4H8O2	0,63			0,59		
Ketone	2,3-Butanedione	C4H6O2	0,54	1,17		1,03	0,98	1,27
Ketone	2-Butanone	C4H8O	0,50	1,88	0,65	0,83	0,52	0,42
Ketone	2-Cyclopenten-1-one	C5H6O	0,71					0,42
Ketone	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	C6H8O2				1,13		

Ketone	2-Cyclopenten-1-one, 2-methyl-	C6H8O	0,29	0,98		0,37		0,29
Ketone	2-Decanone	C10H20O		2,07				
Ketone	2-Heptanone	C7H14O		0,68				
Ketone	2-Nonadecanone	C19H38O		1,19				
Ketone	2-Nonanone	C9H18O		1,53				
Ketone	2-Octanone	C8H16O		0,89				
Ketone	2-Pentadecanone	C15H30O		7,06				
Ketone	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	C10H12O3	0,65			0,61		
Ketone	2-Propanone, 1-(acetoxy)-	C5H8O3	0,56		0,46		0,72	0,37
Ketone	2-Propanone, 1-hydroxy-	C3H6O2	3,50	1,03	3,41	3,02	3,46	2,27
Ketone	2-Undecanone	C11H22O		0,8				
Ketone	3',5'-Dimethoxyacetophenone	C10H12O3	1,18	0,47			1,02	0,35
Ketone	3-Buten-2-one, 3-methyl-	C5H8O				0,21		0,21
Ketone	Acetone	C3H6O	0,45	5,6	1,54	1,65	0,70	1,79
Ketone	Cyclopentadecanone	C15H28O		0,64				
Ketone	Cyclopentanone	C5H8O		0,51				
Ketone	Cyclopentanone, 2-methyl-	C6H10O		0,6				
Ketone	Ethanone, 1-phenyl-2-(1-piperidinyl)-	C13H17NO					0,53	
Ketone	Methyl vinyl ketone	C4H6O				1,09		1,47
Ketone	Octadecan-4-one	C18H36O		0,6				
Others	4-Methyl-3,4-dihydro-[1,2,3]triazolo[4,5-d]pyrimidine-5,7-dione	C5H5N5O2					0,41	
Others	Acetonitrile	C2H3N			0,48			
Others	Butane, 1-chloro-	C4H9Cl		2,64				
Others	Cyacetamide	C3H5N3O			5,51	6,39		4,99
Others	D-Allose	C6H12O6	0,34					
Others	Heptadecanenitrile	C17H33N					0,35	
Others	Methyl isocyanide	C2H3N			0,70		0,68	
Phenol	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	C11H14O3	0,24	0,5		1,09		0,34

Phenol	1-But-3-enyl-2-methoxy-benzene	C11H14O		0,40				
Phenol	2-Allylphenol	C9H10O			0,30			
Phenol	2-Buten-1-one, 1-(4-hydroxyphenyl)-	C10H10O2	0,43					
Phenol	3,5-Dimethoxy-4-hydroxytoluene	C9H12O3	1,02		0,87			
Phenol	3-Methoxy-4-propoxyphenol	C10H14O3	0,24					
Phenol	3-Methoxy-5-methylphenol	C8H10O2	0,24					
Phenol	4-Hydroxy-3-methylacetophenone	C9H10O2	4,14	2,55		3,74		1,96
Phenol	Apocynin	C10H10O3	0,40			0,36		
Phenol	Creosol	C8H10O2	2,71	1,19		2,21	0,34	0,76
Phenol	Hydroquinone	C6H6O2	0,31					
Phenol	p-Cresol	C7H8O	0,65	0,44	0,53	0,48	0,56	0,29
Phenol	Phenol	C6H6O	1,52	0,91	1,60	1,76	1,33	1,88
Phenol	Phenol, 2,4-dimethyl-	C8H10O	0,25	0,49			0,59	0,29
Phenol	Phenol, 2,6-dimethoxy-	C8H10O3	2,03	0,66		1,87		0,56
Phenol	Phenol, 2,6-dimethoxy-4-(2-propenyl)-	C11H14O3	0,83			0,46		
Phenol	Phenol, 2-methoxy-	C8H10O3	5,03	2,54		4,36	0,95	1,73
Phenol	Phenol, 2-methoxy-4-(1-propenyl)-, (Z)-	C10H12O2				0,74		
Phenol	Phenol, 2-methoxy-4-propyl-	C10H14O2	0,33			0,27		
Phenol	Phenol, 2-methyl-	C8H10O3	0,57	0,64	0,72	0,41	0,89	0,40
Phenol	Phenol, 3-methyl-	C7H8O	0,68	0,86	0,79	0,60	0,86	0,59
Phenol	Phenol, 4-ethyl-2-methoxy-	C9H12O2	1,29	0,55		1,07		0,26
Phenol	trans-Isoeugenol	C10H12O2	3,22	2,09		3,07	0,57	1,25
Phenol'	Eugenol	C10H12O2	0,77					0,26