**Appendix 1:** Library of py-GC/MS products used to identify live, root, and soil samples for *Cibotium*, *Dicranopteris*, *Diplazium*, *Cheiridendron* and *Metrosideros*. All spectra were identified from primary ions based on literature (Buurman et al. 2007; Chefetz et al. 2000; Chefetz et al. 2002; Chiavari et al. 1992; Faix et al. 1987; Gallois et al. 2007; Gleixner et al. 2002; Gonzalez-Perez et al. 2007; Steinbeiss et al. 2006) and external standards.

<table>
<thead>
<tr>
<th>Lignin</th>
<th>mass</th>
<th>Major ions</th>
<th></th>
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</tr>
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<tbody>
<tr>
<td>Guaiacyl</td>
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<td></td>
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</tr>
<tr>
<td>2-methoxyphenol (Guaiacol)</td>
<td>124</td>
<td>124,109</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Phenol, 2-methoxy-4-methyl- (Methylguaiacol)</td>
<td>138</td>
<td>138,123</td>
<td></td>
<td></td>
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<tr>
<td>Phenol, 2-methoxy-4-propyl- (4-Propylguaiacol)</td>
<td>166</td>
<td>166,137</td>
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<tr>
<td>Phenol, 2-methoxy-4-vinyl- (Vinylguaiacol)</td>
<td>150</td>
<td>150,135</td>
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<tr>
<td>Phenol, 2-methoxy-4-ethyl- (Ethylguaiacol)</td>
<td>124</td>
<td>124,124</td>
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<tr>
<td>Ethaneone, 1-(4-hydroxy-3-methoxyphenyl)- (4-acetylguaiacol)</td>
<td>152</td>
<td>152,152</td>
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<tr>
<td>2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (Guaiaclacetone)</td>
<td>164</td>
<td>164,77</td>
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<tr>
<td>Phenol, 2-methoxy-4-(1-propenyl)-, (Z)- (cis-Isoeugenol)</td>
<td>164</td>
<td>164,77</td>
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<tr>
<td>Phenol, 2-methoxy-4-(1-propenyl)-, (E)- (trans-Isoeugenol)</td>
<td>164</td>
<td>164,77</td>
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<td>4-(2-propenyl)-guaiacol</td>
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<td>164,77</td>
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<td>Benzaaldehyde, 4-hydroxy-3-methoxy- (Vanillin or 4-formylguaiacol)</td>
<td>152</td>
<td>152,151</td>
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<tr>
<td>Benzoic acid, 4-hydroxy-3-methoxy (Vanillic acid)</td>
<td>168</td>
<td>168,168</td>
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<tr>
<td>Benzeneacetaldehyde, 4-hydroxy-3-methoxy- (Homovanillin)</td>
<td>166</td>
<td>166,166</td>
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<tr>
<td>Benzeneacetic acid, 4-hydroxy-3-methoxy- (Homovanillic acid)</td>
<td>182</td>
<td>182,182</td>
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<tr>
<td>4-Vinylphenol</td>
<td>120</td>
<td>120,91</td>
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</table>

**Phenol, 2-methyl**
- 1,2-Benzenediethyl (Pyrocatechol) 108 107,122
- 1,2-Benzenediethyl, 4-methyl- (Homocatechol) 110 64,110
- Benzoic acid, 3-methoxy-, methyl ester 166 135,166
- Benzoic acid, methyl ester 136 105,136
- Ethylphenol 122 107,122
- Phenol, 3,4-dimethoxy- 154 139,154

**Syringyl**
- Phenol, 2,6-dimethoxy- (Syringol) 154 154,139
- Phenol, 4-methyl-2,6-dimethoxy- (Methylsyringol) 168 153,168
- Phenol, 2,6-dimethoxy- (Syringol, 4-vinyl) 180 165,180
- Phenol, 4-ethyl-2,6-dimethoxy- (Ethylsyringol) 196 182,167
- Ethaneone, 1-(4-hydroxy-3,5-dimethoxyphenyl)- (Acetosyringone) 196 181,196
- 2-Propanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)- (4(propan2-one)syringol) 194 167,210
- Phenol, 2,6-dimethoxy-4-(2-propenyl)- (Methoxyeugenol) 182 91,194
- Benzaaldehyde, 4-hydroxy-3,5-dimethoxy- (Syringaldehyde) 182 181,182
- Benzoic acid, 4-hydroxy-3,5-dimethoxy (Syringic acid) 198 183,198

**Lipid**

**Alkanes**
- n-Hexane (n-C6:0) 86 57,71
- n-Heptane (n-C7:0) 100 57,71
n-Octane (n-C8:0) *
114  57,71
n-Nonane (n-C9:0) *
128  57,71
n-Decane (n-C10:0) *
142  57,71
n-Undecane (n-C11:0) *
156  57,71
n-Dodecane (n-C12:0) *
170  57,71
n-Tridecane (n-C13:0) *
184  57,71
n-Tetradecane (n-C14:0) *
198  57,71
n-Pentadecane (n-C15:0) *
212  57,71
n-Hexadecane (n-C16:0) *
226  57,71
n-Heptadecane (n-C17:0) *
240  57,71
n-Octadecane (n-C18:0) *
254  57,71
n-Nonadecane (n-C19:0) *
268  57,71
n-Eicosane (n-C20:0) *
282  57,71
n-Heneicosane (n-C21:0) *
296  57,71
n-Docosane (n-C22:0) *
310  57,71
n-Tricosane (n-C23:0) *
324  57,71
n-Tetracosane (n-C24:0) *
338  57,71
n-Pentacosane (n-C25:0) *
352  57,71
n-Hexacosane (n-C26:0) *
366  57,71
n-Heptacosane (n-C27:0) *
381  57,71
n-Octacosane (n-C28:0) *
394  57,71
n-Nonacosane (n-C29:0) *
408  57,71
n-Triacontane (n-C30:0) *
422  57,71
n-Hen triacontane (n-C31:0)
437  57,71
n-Dotriacontane (n-C32:0) *
450  57,71
n-Tritiacontane (n-C33:0)
464  57,71
n-Tetratriacontane (n-C34:0) *
562  57,71

Alkenes
n-Hexene (n-6:1)
84   55,69
n-Heptene (n-C7:1)
98   55,69
n-Octene (n-C8:1)
112  55,69
n-Nonene (n-C9:1)
126  55,69
n-Decene (n-C10:1)
140  55,69
n-Undecene (n-C11:1)
154  55,69
n-Dodecene (n-C12:1)
168  55,69
n-Tridecene (n-C13:1w5)
182  55,69
n-Tetradecene (n-C14:1)
196  55,69
n-Pentadecene (n-C15:1)
210  55,69
n-Hexadecene (n-C16:1)
224  55,69
n-Heptadecene (n-C17:1)
238  55,69
n-Octadecene, (E)- (n-18:1)
252  55,69
n-Nonadecene (n-C19:1w9)
264  55,69
n-Eicosene (n-C20:1w9)
280  55,69
n-Heneicosene (n-C21:1w10)
294  55,69
n-Docosene (n-C22:1w1)
308  55,69
n-Tricosene (n-C23:1w1)
322  55,69

Other lipids
1-nonyne
124  67,95
3-Eicosyne (C20:3) (tentative)
278  67,95
9-Eicosyne (tentative)
278  67,95
3,7,11,15-Tetramethyl-2-hexadecen-1-ol
296  81,82

Polysaccharides
α-D-Glucopyranoside, phenyl 2,3,4,6-tetra-O-methyl-
1,2-Cyclohexanedi one
112  55,112
1,2-Cyclopentanedi one
98   55,98
1,2-Cyclopentanedi one, 3-methyl-
2(3H)-Benzofuranone, 3-methyl-
148  91,120
2(3H)-Furanone, 5-methyl-
98   55,98
2(5H)-Furanone
84   55,84
2(5H)-Furanone, 5-methyl-
98   55,98
2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one
144  43,101
2,5-Dimethyl-4-hydroxy-3(2H)-furanone
128  43,57
2,5-Furfandione, 3-methyl-
112  39,68
2-Acetyl furan
110  95,110
2-Acetyl-5-methyl furan
124  109,124
2-Butanone
72   43,72
2-Cyclohexen-1-one, 3-methyl-  
2-Cyclopenten-1-one, 2,3-dimethyl-  
2-Cyclopenten-1-one, 2-hydroxy-3-methyl-  
2-Cyclopenten-1-one, 2-methyl-  
2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-  
2-Cyclopenten-1-one, 3-methyl-  
2-Cyclopentene-1,4-dione  
2-Furancarboxaldehyde, 5-(hydroxymethyl)-  
2-Furanmethanol  
2,5-Furandione, 3-methyl-  
2H-Pyran-2-one  
3-Acetimidofuran  
3-Furaldehyde  
4-hydroxy-5,6-dihydro-2H-pyranone  
4H-Pyran-4-one, 3-hydroxy-2-methyl- (Maltol)  
4H-Pyran-4-one, 3,5-dihydroxy-2-methyl- (5-hydroxy Maltol)  
5-Ethyl-2-furaldehyde  
Acetic acid  
Acetic acid, methyl ester  
Acetic anhydride  
Benzo[b]furan, 2-methyl-  
Benzo[b]furan, 2,3-dihydro-  
Benzo[b]furan, 2,4-dimethyl-  
Butanal, 2-methyl-  
Butanal, 3-methyl-  
Cycloheptanone  
Cyclohexanone  
Cyclopent-2-ene-1-one, 2,3,4-trimethyl-  
Cyclopentanone  
Cyclopropanecarboxaldehyde, methylene-  
Furan, 2-(methoxymethyl)-  
Furan, 2,3,5-trimethyl-  
Furan, 2,4-dimethyl-  
Furan, 2,5-dimethyl-  
Furan, 2-ethyl-  
Furan, 2-ethyl-5-methyl-  
Furan, 2-propyl-  
Furan, 2-methyl-  
Furan, 3-methyl-  
Furan, 2-propyl  
Furfural (2-Furaldehyde)  
Furfural, 5-methyl-  
Levogluconan  
Levogluconosenone  
Methyl 2-furoate  
Pentanal  
Vinylfuran  
Ethane, 1-(3-hydroxy-2-furanyl)- (Isomaltol)  

N-bearing
1,2-Benzenediold, mono(methyl carbamate)  
1,7-Dimethyl-1,8-naphthyridin-4-one-3-carboxyhydrizide  
1H-Pyrazole, 4,5-dihydro-1,5-dimethyl-  
1H-Pyrrole, 2,5-dimethyl-  
1H-Pyrrole, 2-ethyl-4-methyl-  
1H-Pyrrole, 3-methyl-  
1H-Pyrrole-2-carboxaldehyde  
1H-Pyrrole-2-carboxaldehyde, 1-methyl-  
1H-Tetrazole, 1-methyl-  
1-Propanol, 2-(dimethylamino)-2-methyl-  
2-(N-Methyl-N-ethylamino)phenol  
2,3,4-Trimethylpyrrole  
2,4(1H,3H)-Pyridinedione, 1,3,5-trimethyl-  
2-Pyridinemethanol, acetate (ester)  
2-Pyridinamine  
2,5-Piperazinedione, 3-ethyl-6-(2-
methylpropyl)-
2-Pyrazoline, 4-ethyl-1-methyl-
2-Pyrindinecarbonitrile

2-Pyrindinemethanol, acetate (ester) 151 108,109
3-Methylpyridazine 94 65,94
3-Phenylpyridine 155 154,155
3-Pyridinecarbonitrile 104 77,104
3-Pyridinol 95 95,96
4(1H)-Pyridinone, 2,3-dihydro-1-methyl-
4-Amino-2(1H)-pyridinone 110 82,110
4-Methyl-2-oxopentanenitrile 111 41,43
4-Pyrindinecarboxaldehyde 107 51,107
4(1H)-Pyridinone, 2,3-dihydro-1-methyl-
5,10-Diethoxy-2,3,7,8-tetrahydro-1H,6H-di-
pyrrolo[1,2-a;1’,2’-d]pyrazine 250 166,194
5H-1-Pyridine 117 90,117
Acetamide, N-hydroxy 75 43,75
Acetonitrile, (dimethylamino)-
Alpha-amino-gamma-butyrolactone 101 43,101
Ammonium acetate 77 43,45
Aniline 93 66,93
Crotorny isothiocyanate 127 39,69
Ethanone, 1-(1H-pyrrol-2-yl)-
Ethanone, 1-(1-methyl-1H-pyrrol-2-yl)-
Formamide, N,N-dimethyl-
Hexadecanenitrile 237 43,57
Hexanedinitrile
Hydrogen azide 43 15,43
N-Butyl-tert-butylamine 129 58,114
Nicotinyl Alcohol
N-Isopropyl-4-piperidine
p-Aminotoluene 107 106,107
Piperidine-2,5-dione 113 84,113
Piperidine, 2,6-dimethyl- (Nanfin) 113 84,113

Piperidine-2,5-dione 113 84,113
Propane, 2-nitro-
Propanenitrile 55 54,28
Pyrazole[5,1-c][1,2,4]benzotriazin-8-ol 186 103,186
Pyridine 3-methyl 93 66,93
Pyridine 3-methyl 93 66,93
Pyridine, 2-ethyl 107 106,107
Pyridine, 3-methoxy-
Pyridine, 4-methoxy-
Pyrimidine 109 79,109
Pyrimidine 80 53,80
Pyrimidine, 2-methyl-
Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-
(2-methylpropyl)-
1H-Pyrrole, 2-ethyl- 95 80,95
1H-Pyrrole, 1-methyl-
1H-Pyrrole, 2-methyl-
3-Methylindole 131 130,131
4-Pyridinamine
Benzepropanenitrile 131 91,131
Benzonitrile 103 76,103
Benzyl nitrile 117 90,117
Ethylbenzene 106 91,106
Indole 117 90,117
Pyridine 79 79,52
Pyridine 2-methyl 93 66,93
Pyridine, 3,5-dimethyl-
Pyrrole 107 106,107
Styrene 67 67,39

Non-lignin aromatics
1,2,3-Benzenetriol 140 125,140
1,2-Benzenedioli, 3-methoxy-
1,3,5,7-Cyclooctatetraene 104 78,104
<table>
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<tr>
<th>Compound</th>
<th>p</th>
<th>Retention Time</th>
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<tr>
<td>1,3,5-Cycloheptatriene</td>
<td>92</td>
<td>91,92</td>
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<tr>
<td>1,3,5-Cyclooctatriene</td>
<td>92</td>
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<tr>
<td>1,4-Benzenediol, 2-methoxy</td>
<td>110</td>
<td>81,110</td>
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<tr>
<td>1,4-Dihydroxybenzene (Hydroquinone)</td>
<td>86</td>
<td>58,86</td>
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<tr>
<td>17α-Methyltestosterone</td>
<td>301</td>
<td>81,245</td>
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<tr>
<td>1H-Inden-1-one, 2,3-dihydro</td>
<td>118</td>
<td>104,132</td>
</tr>
<tr>
<td>1H-Indene, 2,3-dihydro-1,1,3-trimethyl-3-phenyl</td>
<td>236</td>
<td>143,221</td>
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<tr>
<td>1H-Indene, 5,6-dimethoxy</td>
<td>203,2</td>
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<tr>
<td>1-Naphthalenecarboxylic acid, 5-[2-(3-furanyl)ethyl]-3,4,4a,5,6,7,8,8a-octahydro-5,6,8a-trimethyl-, methyl ester, [4aS-(4aS,5a,6S,8aS)]-</td>
<td>35</td>
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<tr>
<td>2-(3,5-Dimethoxy-phenyl)-2-methyl-propionaldehyde</td>
<td>170</td>
<td>155,170</td>
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<tr>
<td>2,3,5-Trimethylnaphthalene</td>
<td>170</td>
<td>155,170</td>
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<tr>
<td>2,3,6-Trimethylnaphthalene</td>
<td>236</td>
<td>91,143</td>
</tr>
<tr>
<td>2H-1-Benzopyran-2-one</td>
<td>146</td>
<td>118,146</td>
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<tr>
<td>2-Naphthalenol, 3-methoxy</td>
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<tr>
<td>4-Hexylanisole</td>
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<td>9,10-Anthracenedione, 1,8-diethoxy-à-Calacorene</td>
<td>200</td>
<td>142,157</td>
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<td>à-Cubebene</td>
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<td>105,161</td>
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<tr>
<td>Acetophenone</td>
<td>120</td>
<td>77,105</td>
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<td>Anthracene *</td>
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<td>152,178</td>
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<tr>
<td>Asarone</td>
<td>208</td>
<td>193,208</td>
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<tr>
<td>Benzaldehyde</td>
<td>106</td>
<td>77,105</td>
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<tr>
<td>Benzene</td>
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<td>51,78</td>
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<tr>
<td>Benzene, (1,3-dimethylbutyl)-</td>
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<td>105,120</td>
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<td>Benzene, (1-methylethyl)- (Cumene)</td>
<td>134</td>
<td>119,134</td>
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<td>Benzene, 1,2,3,4-tetramethyl-</td>
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<td>119,134</td>
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<td>Benzene, 1,2,3,5-tetramethyl-</td>
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<td>Benzene, 1,2,3-dimethyl-</td>
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<td>Benzene, 1,3-bis(1,1-dimethylethyl)-</td>
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<tr>
<td>Benzene, 1,4-dimethoxy-2,3,5,6-tetramethyl-</td>
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<tr>
<td>Benzene, 1,4-dimethoxy-2-methyl-</td>
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<tr>
<td>Benzene, 1-ethyl-3-methyl-</td>
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<tr>
<td>Benzene, 2-propenyl-</td>
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<td>Benzene, 4-ethyl-1,2-dimethyl-</td>
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<tr>
<td>Benzene, butyl-</td>
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<tr>
<td>Benzene, hexyl-</td>
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<tr>
<td>Benzene, propyl-</td>
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<tr>
<td>Benzofuran</td>
<td>118</td>
<td>90,118</td>
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<tr>
<td>Benzoic acid, 4,5-dimethoxy-2-(2-phenylethenyl)-</td>
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<td>Benzoic acid, 4-hydroxy-3,5-dimethoxy-, hydrazide</td>
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<td>Beta-Pinene</td>
<td>136</td>
<td>41,93</td>
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<tr>
<td>Biphenyl</td>
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<td>ç-Selinene</td>
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<td>133,189</td>
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<td>C10H14</td>
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<tr>
<td>C15 Napthalene (20071-49-2)</td>
<td>204</td>
<td>161,189</td>
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<tr>
<td>C15 bicyclicdecane</td>
<td>204</td>
<td>79,93</td>
</tr>
<tr>
<td>C15 Napthalene (Valencene)</td>
<td>204</td>
<td>105,161</td>
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<tr>
<td>Cadinene</td>
<td>198</td>
<td>183,198</td>
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<tr>
<td>Cadina-1(10),6,8-triene</td>
<td>202</td>
<td>159,187</td>
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<tr>
<td>Calamenene (Napthalene)</td>
<td>202</td>
<td>159,160</td>
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<tr>
<td>Cyclohexanol, 4-methyl-1-(1-methylethyl)-</td>
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<td>54,67</td>
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<td>Cyclohexene</td>
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<td>Cyclopentane, bromo-</td>
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<tr>
<td>Dimethylbenzofuran</td>
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<tr>
<td>Dimethylphenol</td>
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<td>68,93</td>
</tr>
<tr>
<td>D-Limonene</td>
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<td>107,122</td>
</tr>
<tr>
<td>Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-</td>
<td>150</td>
<td>135,150</td>
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<tr>
<td>Ethanone, 1-(3-methoxyphenyl)-</td>
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<tr>
<td>Chemical</td>
<td>CAS Number</td>
<td>Description</td>
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<tr>
<td>Fluorene *</td>
<td>166 165,166</td>
<td>(E)-1,3-Butadien-1-ol</td>
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<tr>
<td>Indane</td>
<td>288 181,183</td>
<td>1,3-Benzenedicarboxylic acid, dimethyl ester</td>
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<td>Isoelemidin</td>
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<td>1-Undecanol</td>
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<td>Mequinol</td>
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<tr>
<td>Methyl naphthalene</td>
<td>142 141,142</td>
<td>2-Butanone, 3,3-dimethyl-</td>
</tr>
<tr>
<td>Monobenzone</td>
<td>200 91,200</td>
<td>2-Butenoic acid, methyl ester, (E)-</td>
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<tr>
<td>m-xylene</td>
<td>106 91,106</td>
<td>2-Heptanone</td>
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<tr>
<td>Naphthalene *</td>
<td>128 128,129</td>
<td>2-Pentanone</td>
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<tr>
<td>Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methyl)ethyl</td>
<td>204 105,119</td>
<td>2-Propenoic acid, 3-phenyl-, methyl ester, (E)-</td>
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<tr>
<td>Naphthalene, 1,2-dihydro-4-methyl-</td>
<td>144 129,144</td>
<td>2,3-Pentanedione</td>
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<td>Oxirane, ethenyl-</td>
<td>70 39,42</td>
<td>3-Buten-2-ol</td>
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<tr>
<td>Phenol, 2,4-bis(1,1-dimethyl)ethyl-</td>
<td>206 191,206</td>
<td>3-Penten-2-one, (E)-</td>
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<tr>
<td>Phenol, 2-methoxy-5-(1-propenyl)-, (E)-</td>
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<td>4-Penten-2-one</td>
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<td>Phenol, 3,4-dimethyl-</td>
<td>122 107,122</td>
<td>5-Heptadecene, 1-bromo-</td>
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<tr>
<td>Phenol, 3-methyl-</td>
<td>108 107,108</td>
<td>Acetic acid, hydroxy-, methyl ester</td>
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<td>Phenol, 4-ethyl-</td>
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<td>Amylene Hydrate</td>
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<td>Phenol, 4-methoxy-3-methyl-</td>
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<td>Benzene, penty1-</td>
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<td>Spiro[2.4]hepta 4,6 diene</td>
<td>92 91,92</td>
<td>Dimethyl 3,3'-oxydipropanoate</td>
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<tr>
<td>Trimethylphenol</td>
<td>136 121,136</td>
<td>Isobutyl nitrite</td>
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<td>Phenol</td>
<td>94 66,94</td>
<td>Methanecarbothiolic acid</td>
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<tr>
<td>Phenol, 4-methyl-</td>
<td>108 107,108</td>
<td>Phosphoric acid, (p-hydroxyphenyl)-</td>
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<tr>
<td>Toluene</td>
<td>92 91,92</td>
<td>Phosphoric acid, trimethyl ester</td>
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<tr>
<td>Phenols</td>
<td></td>
<td>Propanoic acid, 2-hydroxy-, methyl ester, (Ô)-</td>
</tr>
<tr>
<td>Unclassified</td>
<td></td>
<td>Pyruvaldehyde</td>
</tr>
<tr>
<td>*Identified by external standards. ‡ Identified from purified cellulose (Courtney's references)</td>
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Vinyl crotonate