

Manganelli et al.:

Integrated Strategy for Mutagenicity Prediction Applied to Food Contact Chemicals

Supplementary Data

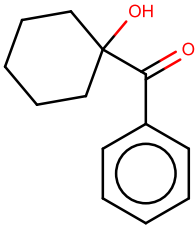
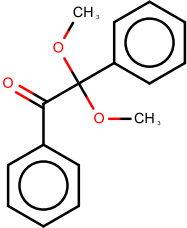
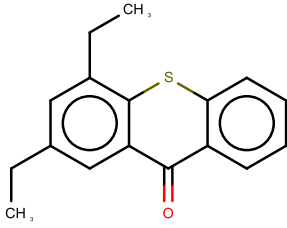
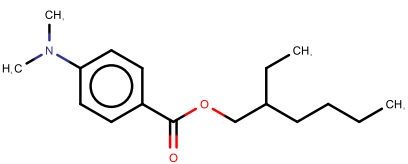
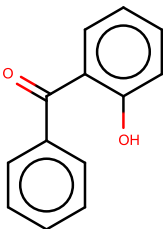
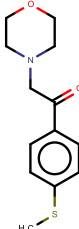
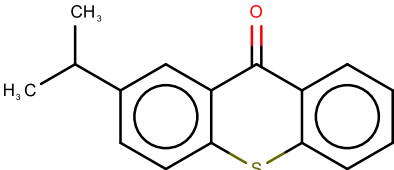
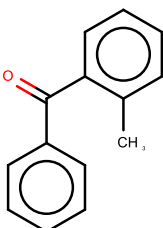
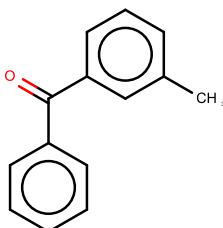
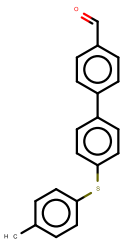
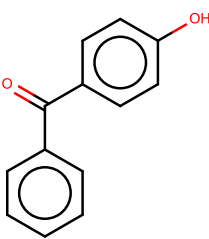
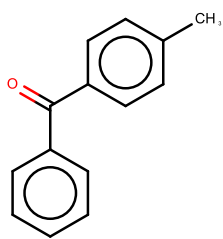
Tab. S1: List of 183 chemicals with names and structures, and the related SMILES

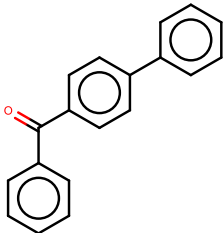
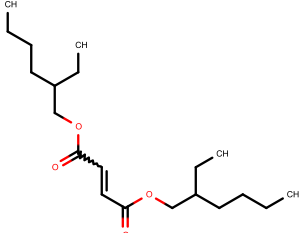
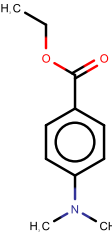
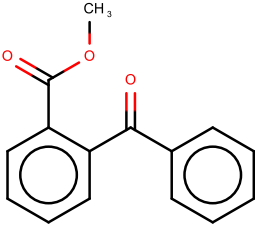
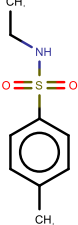
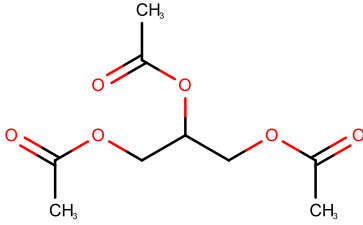
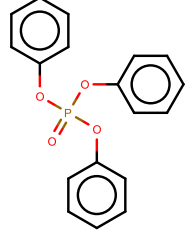
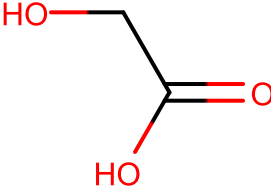
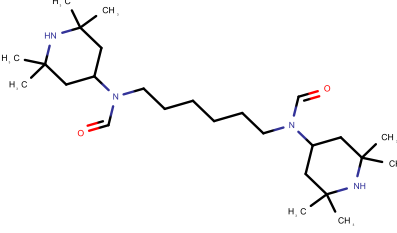
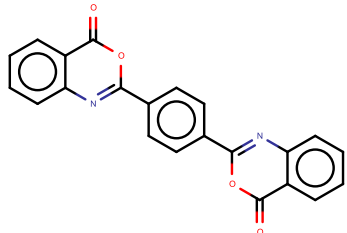
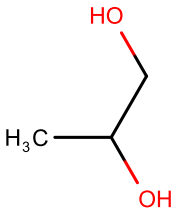
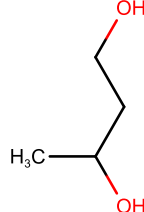
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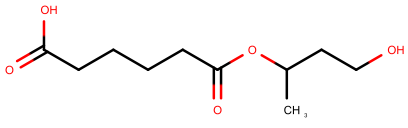
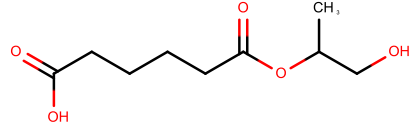
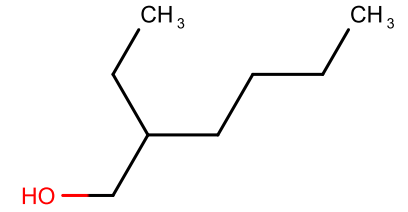
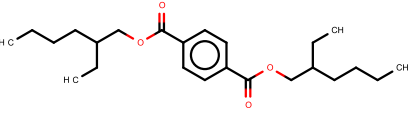
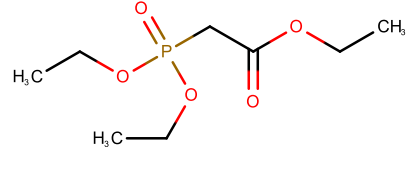
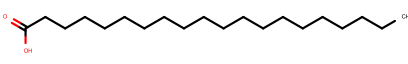
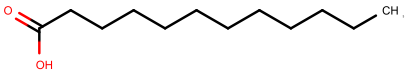
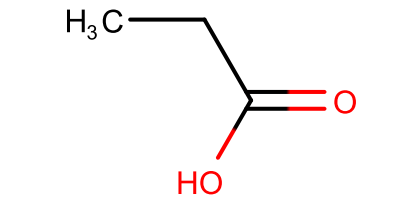
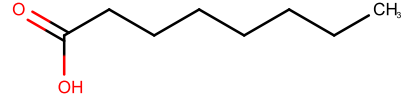
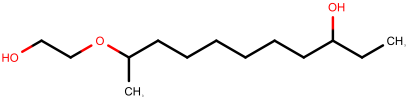
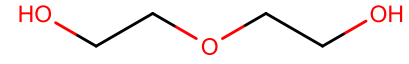
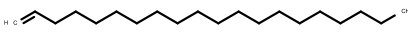


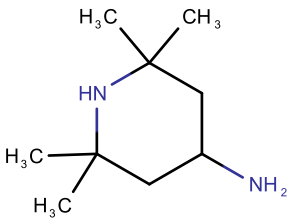
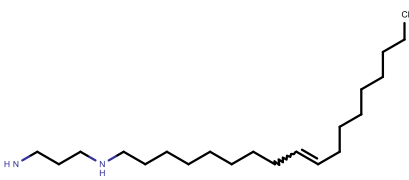
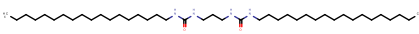
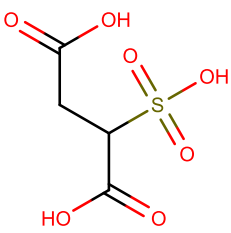
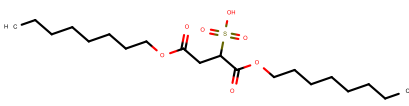
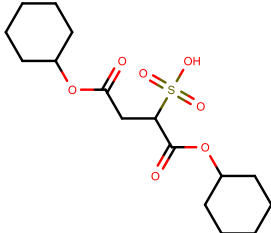
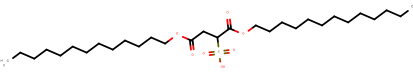
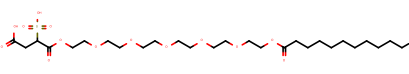
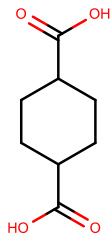
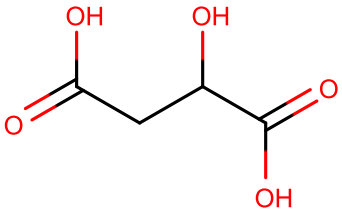
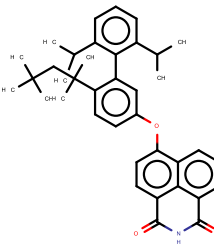
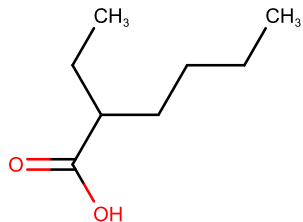
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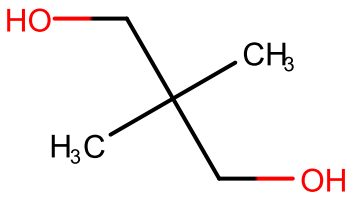
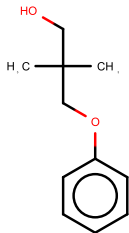
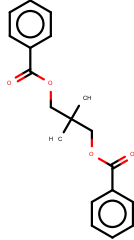
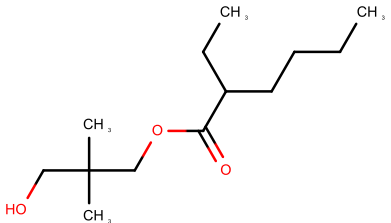
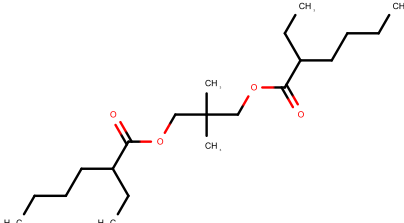
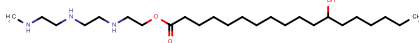
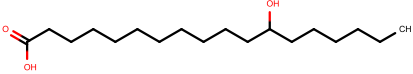
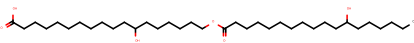
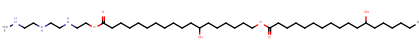
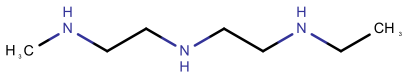
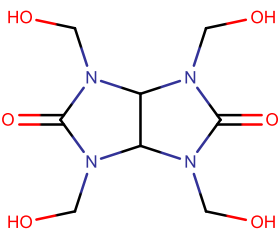
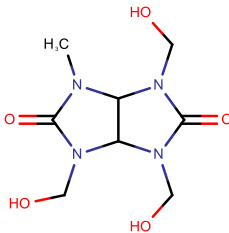
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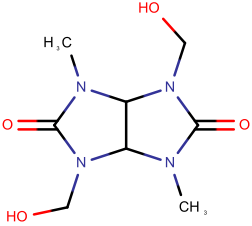
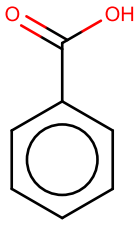
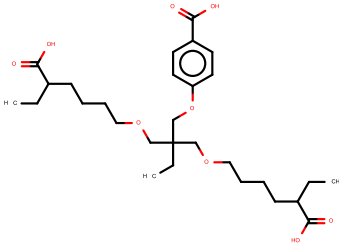
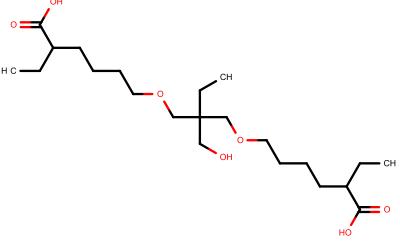
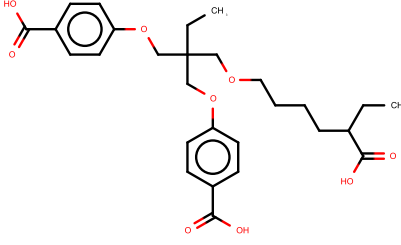
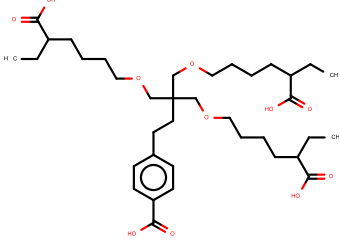
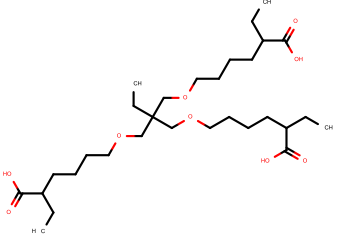
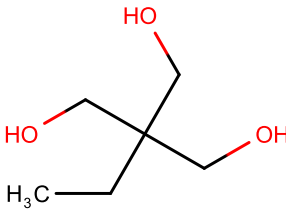
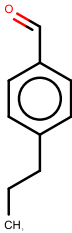
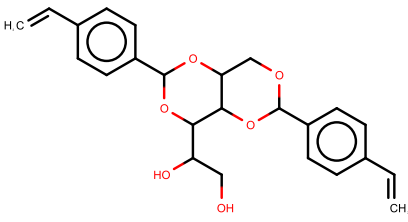
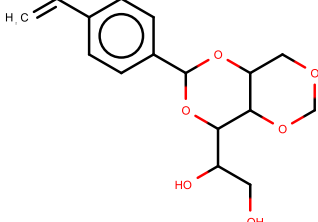
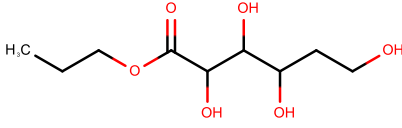
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4 	5 	6 
Id: 4 Name: 2-ethylhexyl 4-(dimethylamino)benzoate (EH DAB)	Id: 5 Name: 2-benzoylphenol	Id: 7 Name: 1-[4-(methylsulfanyl)phenyl]-2-(morpholin-4-yl)ethan-1-one
7 	8 	9 
Id: 6a Name: 2-(propan-2-yl)-9H-thioxanthen-9-one (ITX, 2-Isopropylthioxanthone)	Id: 8 Name: (2-methylphenyl) (phenyl)methanone	Id: 9 Name: (3-methylphenyl) (phenyl)methanone
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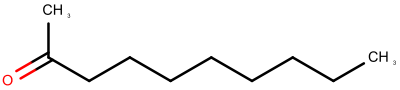
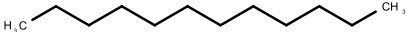
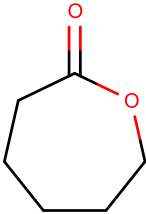
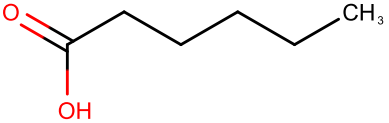
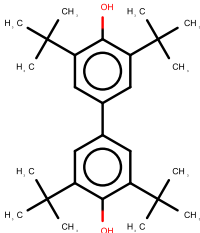
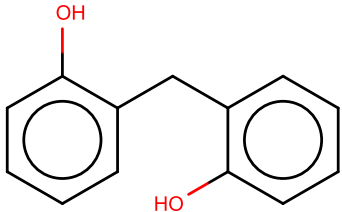
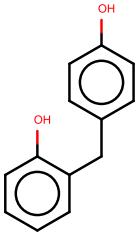
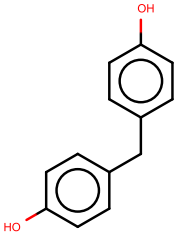
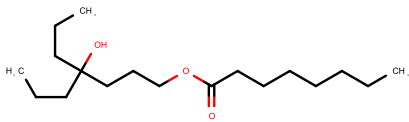
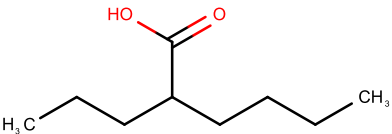
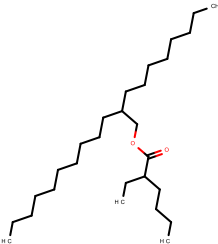
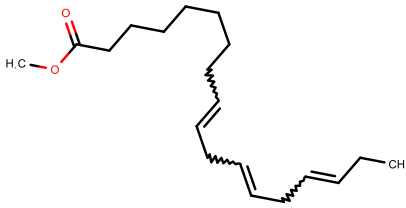
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16 	17 	18 
Id: 17 Name: methyl 2-benzoylbenzoate	Id: 18 Name: N-ethyl-4-methylbenzenesulfonamide	Id: 19 Name: 1,3-bis(acetyloxy)propan-2-yl acetate (triacetin)
19 	20 	21 
Id: 20 Name: triphenyl phosphate	Id: 21 Name: 2-hydroxyacetic acid	Id: 22 Name: N-(2,2,6,6-tetramethylpiperidin-4-yl)-N-{6-[N-(2,2,6,6-tetramethylpiperidin-4-yl)formamido]thylpiperidin-4-yl}formamide
22 	23 	24 
Id: 23 Name: 2-[4-(4-oxo-4H-3,1-benzoxazin-2-yl)phenyl]-4H-3,1-benzoxazin-4-one	Id: 24 Name: propane-1,2-diol	Id: 25 Name: butane-1,3-diol

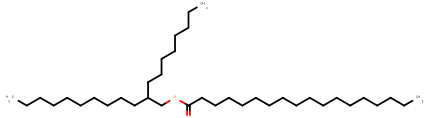
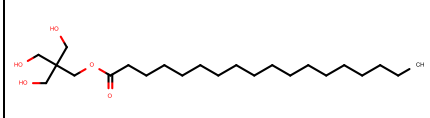
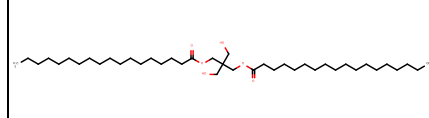
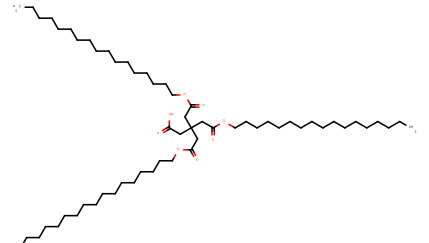
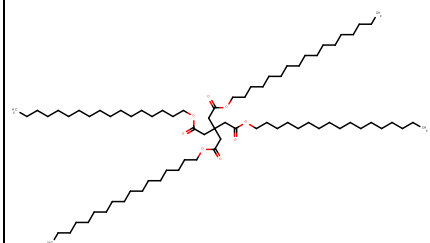
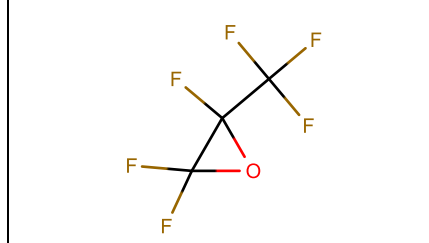
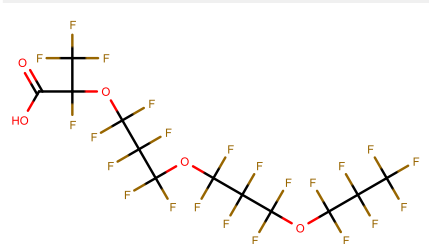
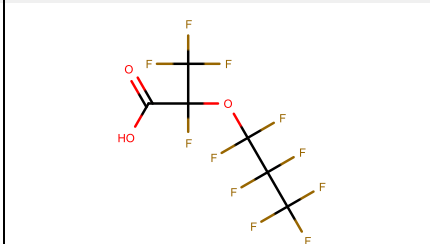
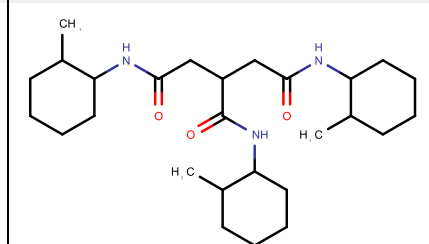
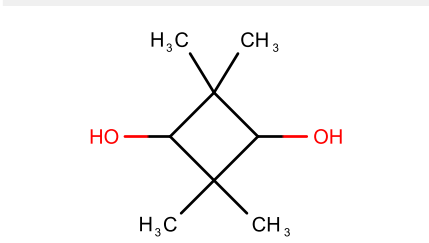
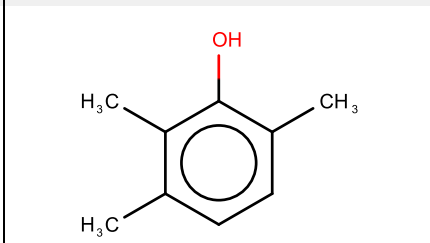
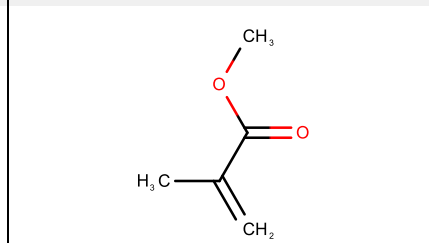
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Id: 26 Name: 6-(3-hydroxy-1-methylpropoxy)-6-oxo-hexanoic acid	Id: 27 Name: 6-(2-hydroxy-1-methylethoxy)-6-oxo-hexanoic acid	Id: 28 Name: 2-ethylhexan-1-ol
28 	29 	30 
Id: 29 Name: 1,4-bis(2-ethylhexyl) benzene-1,4-dicarboxylate	Id: 31 Name: ethyl 2-diethoxyphosphorylacetate	Id: 32 Name: icosanoic acid
31 	32 	33 
Id: 33 Name: dodecanoic acid	Id: 35 Name: propionic acid	Id: 34a Name: octanoic acid
34 	35 	36 
Id: 36 Name: (3S,10R)-10-(2-hydroxyethoxy)undecan-3-ol	Id: 37 Name: 2-(2-hydroxyethoxy)ethanol	Id: 38 Name: icos-1-ene

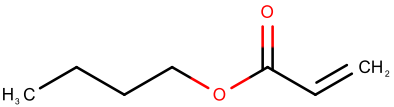
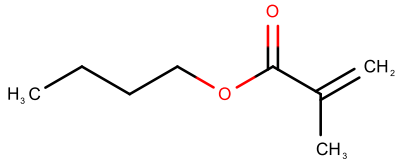
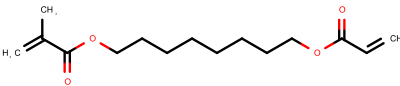
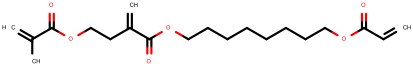
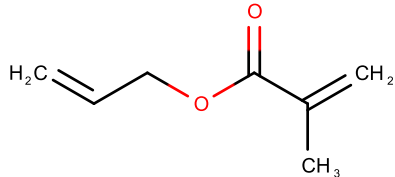
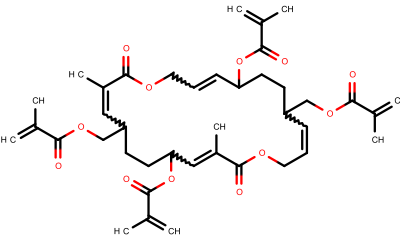
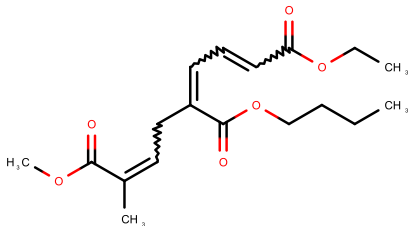
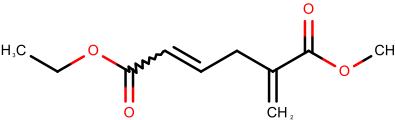
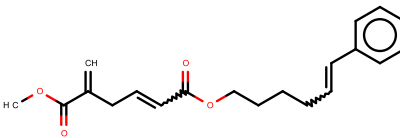
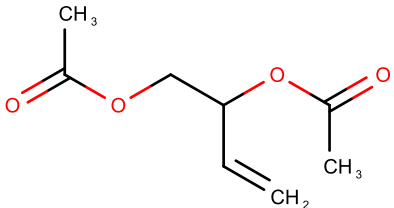
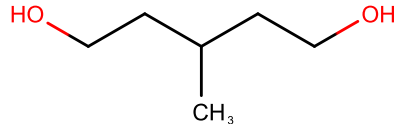
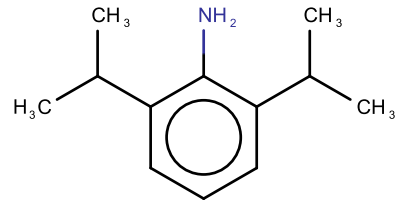
37  Id: 39 Name: 2,2,6,6-tetramethylpiperidin-4-amine	38  Id: 40 Name: N'-[(Z)-octadec-9-enyl]propane-1,3-diamine	39  Id: 41 Name: 1-octadecyl-3-[3-(octadecylcarbamoylamino)propyl]urea
40  Id: 42a Name: 2-sulfobutanedioic acid	41  Id: 43 Name: 1,4-dioctoxy-1,4-dioxo-butane-2-sulfonic acid	42  Id: 44 Name: 1,4-bis(cyclohexoxy)-1,4-dioxo-butane-2-sulfonic acid
43  Id: 45 Name: (2R)-1,4-dioxo-1,4-di(tridecoxy)butane-2-sulfonic acid	44  Id: 46 Name: 4-[2-[2-[2-[2-(2-dodecanoyloxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]-4-oxo-3-sulfo-	45  Id: 47 Name: cyclohexane-1,4-dicarboxylic acid
46  Id: 48 Name: 2-hydroxybutanedioic acid	47  Id: 49 Name: 6-[3-(2,6-diisopropylphenyl)-4-(1,1,3,3-tetramethylbutyl)phenoxy]benzo[de]isoquinoline-1,3-dione	48  Id: 50a Name: 2-ethylhexanoic acid

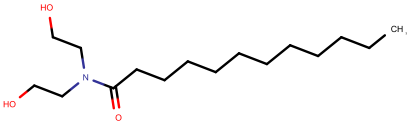
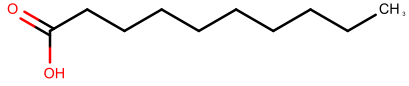
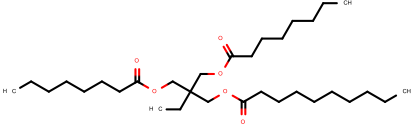
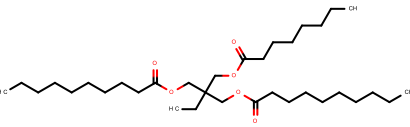
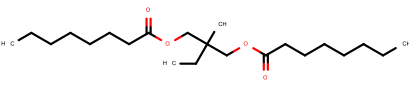
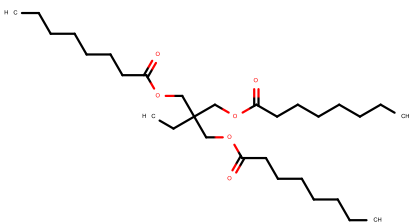
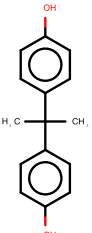
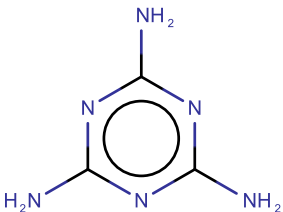
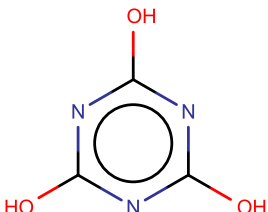
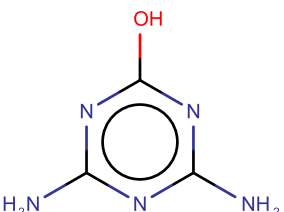
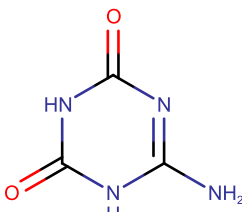
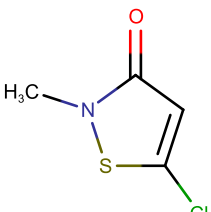
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Id: 51 Name: 2,2-dimethylpropan-1,3-diol	Id: 52 Name: 2,2-dimethyl-3-phenoxypropan-1-ol	Id: 53 Name: (3-benzoyloxy-2,2-dimethyl-propyl) benzoate
52 	53 	54 
Id: 54 Name: (3-hydroxy-2,2-dimethyl-propyl) 2-ethylhexanoate	Id: 55 Name: [3-(2-ethylhexanoyloxy)-2,2-dimethyl-propyl] 2-ethylhexanoate	Id: 56 Name: 2-[2-[2-(methylamino)ethylamino]ethyl 12-hydroxyoctadecanoate
55 	56 	57 
Id: 56a Name: 12-hydroxyoctadecanoic acid	Id: 57 Name: 12-hydroxy-18-(12-hydroxyoctadecanoyloxy)octadecanoic acid	Id: 58 Name: 2-[2-[2-(methylamino)ethylamino]ethyl 12-hydroxy-18-(12-hydroxyoctadecanoyloxy)octadecanoic acid
58 	59 	60 
Id: 59 Name: N'-[2-(ethylamino)ethyl]-N-methyl-ethane-1,2-diamine	Id: 60 Name: 1,3,4,6-tetrakis(hydroxymethyl)-3a,6a-dihydroimidazo[4,5-d]imidazole-2,5-dione	Id: 61 Name: 3,4,6-tris(hydroxymethyl)-1-methyl-3a,6a-dihydroimidazo[4,5-d]imidazole-2,5-dione

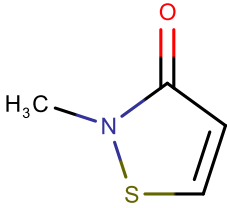
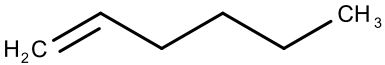
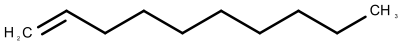
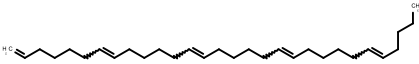
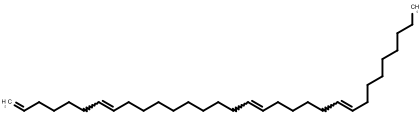
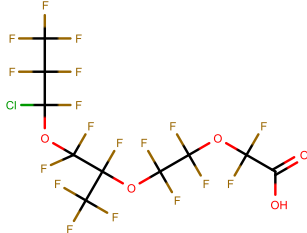
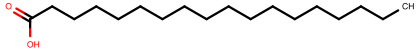
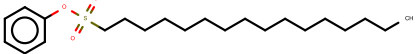
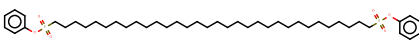
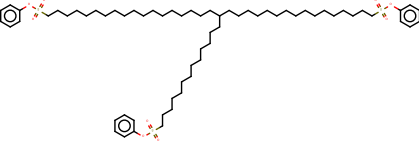
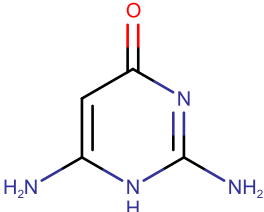
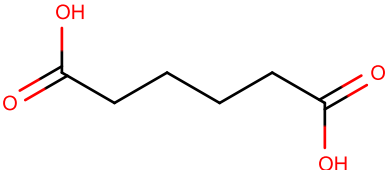
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Id: 62 Name: 3,6-bis(hydroxymethyl)-1,4-dimethyl-3a,6a-dihydroimidazo[4,5-d]imidazole-2,5-dione	Id: 64 Name: benzoic acid	Id: 65 Name: 4-[2,2-bis(5-carboxyheptoxymethyl)butoxy]benzoic acid
64 	65 	66 
Id: 66 Name: 6-[2-(5-carboxyheptoxymethyl)-2-(hydroxymethyl)butoxy]-2-ethyl-hexanoic acid	Id: 67 Name: 4-[2-(5-carboxyheptoxymethyl)-2-(4-carboxyphenoxy)methyl]butoxy]benzoic acid	Id: 68 Name: 4-[4-(5-carboxyheptoxymethyl)butyl]benzoic acid
67 	68 	69 
Id: 69 Name: 6-[2,2-bis(5-carboxyheptoxymethyl)butoxy]-2-ethyl-hexanoic acid	Id: 70 Name: 2-ethyl-2-(hydroxymethyl)propane-1,3-diol	Id: 71 Name: 4-propylbenzaldehyde
70 	71 	72 
Id: 72 Name: 1-[2,6-bis(4-vinylphenyl)-4,4a,8,8a-tetrahydro-[1,3]dioxino[5,4-d][1,3]dioxin-4-yl]ethane-	Id: 73 Name: 1-[2-(4-vinylphenyl)-4,4a,8,8a-tetrahydro-[1,3]dioxino[5,4-d][1,3]dioxin-4-yl]ethane-1,2-d	Id: 74 Name: propyl 2,3,4,6-tetrahydroxyhexanoate

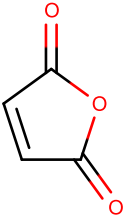
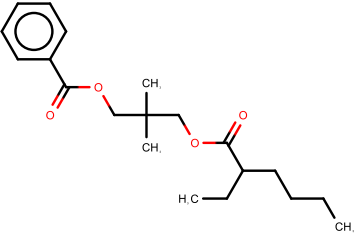
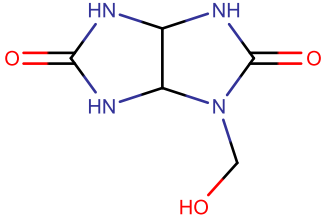
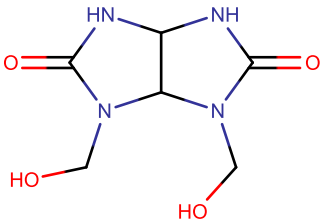
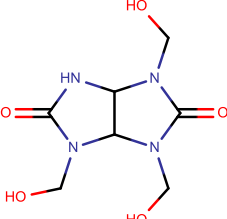
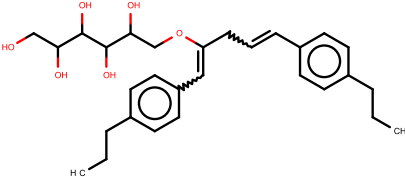
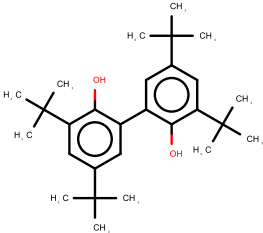
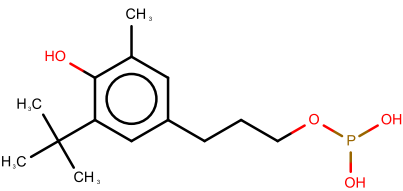
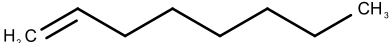
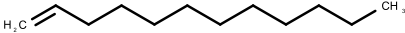
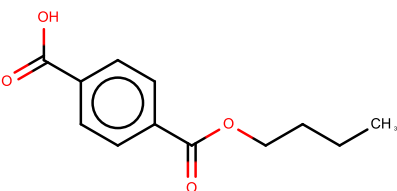
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Id: 75 Name: decan-2-one	Id: 76 Name: dodecane	Id: 77 Name: oxepan-2-one
76 	77 	78 
Id: 78 Name: hexanoic acid	Id: 79 Name: 2,6-ditert-butyl-4-(3,5-ditert-butyl-4-hydroxyphenyl)phenol	Id: 81 Name: 2-[(2-hydroxyphenyl)methyl]phenol (2,2'-biphenol F)
79 	80 	81 
Id: 82 Name: 2-[(4-hydroxyphenyl)methyl]phenol	Id: 83 Name: 4-[(4-hydroxyphenyl)methyl]phenol	Id: 84 Name: 4-hydroxy-4-propyl heptyl octanoate
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Id: 85 Name: 2-propylhexanoic acid	Id: 86 Name: 2-octyldodecyl 2-ethylhexanoate	Id: 87 Name: methyl octadeca-9,12,15-trienoate

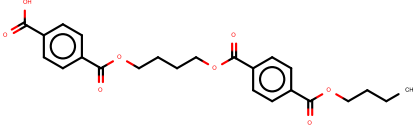
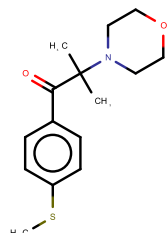
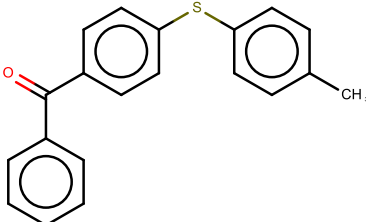
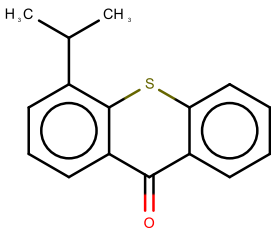
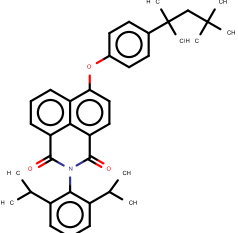
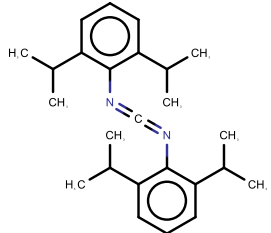
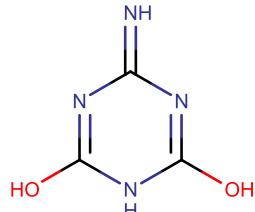
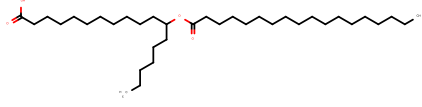
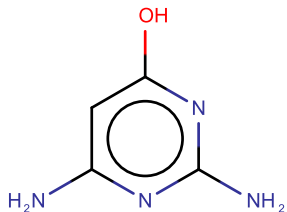
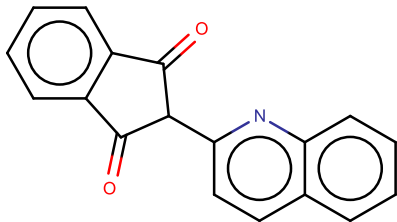
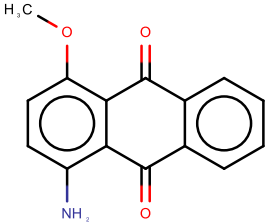
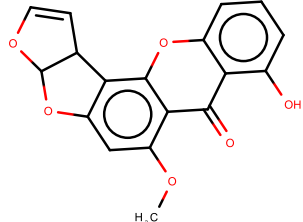
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Id: 88 Name: 2-octyldodecyl octadecanoate	Id: 89 Name: 3-hydroxy-2,2-bis(hydroxymethyl)propyl octadecanoate	Id: 90 Name: 3-hydroxy-2-(hydroxymethyl)-2-[(octadecanoyloxy)methyl]propyl octadecanoate
88 	89 	90 
Id: 91 Name: 5-(heptadecyloxy)-3,3-bis[2-(heptadecyloxy)-2-oxoethyl]-5-oxopentanoic acid	Id: 92 Name: 1,5-diheptadecyl 3,3-bis[2-(heptadecyloxy)-2-oxoethyl]pentanedioate	Id: 93 Name: 2,2,3-trifluoro-3-(trifluoromethyl)oxirane
91 	92 	93 
Id: 94 Name: 2,3,3,3-tetrafluoro-2-{1,1,2,2,3,3-hexafluoro-3-[1,1,2,2,3,3-hexafluoro-3-(heptafluoropropoxy)propanoic acid	Id: 95 Name: 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoic acid	Id: 96 Name: N,N',N''-tris(2-methylcyclohexyl)propane-1,2,3-tricarboxamide
94 	95 	96 
Id: 97 Name: 2,2,4,4-tetramethylcyclobutane-1,3-diol	Id: 98 Name: 2,3,6-trimethylphenol	Id: 99 Name: methyl 2-methylprop-2-enoate (methyl methacrylate, MMA)

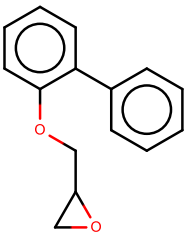
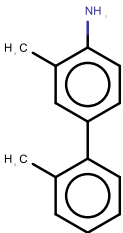
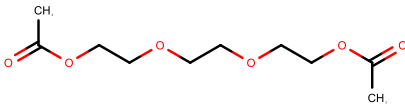
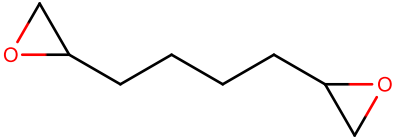
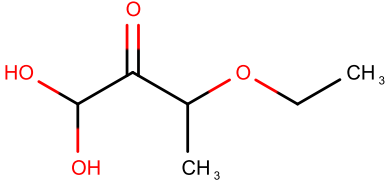
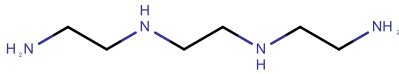
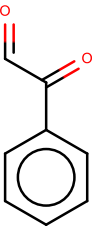
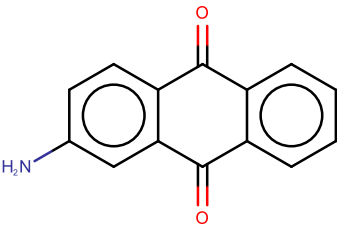
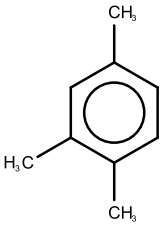
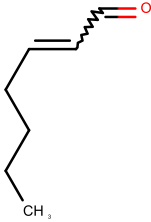
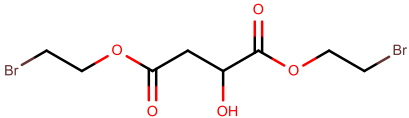
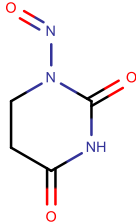
97 	98 	99 
Id: 100 Name: butyl prop-2-enoate	Id: 101 Name: butyl 2-methylprop-2-enoate	Id: 102 Name: 8-(prop-2-enoyloxy)octyl 2-methylprop-2-enoate
100 	101 	102 
Id: 103 Name: 8-(prop-2-enoyloxy)octyl 2-methylidene-4-[(2-methylprop-2-enoyl)oxy]butanoate	Id: 104 Name: prop-2-en-1-yl 2-methylprop-2-enoate	Id: 105 Name: {3,10-dimethyl-8,19-bis[(2-methylprop-2-enoyl)oxy]-16-[[2-methylprop-2-enoyl)oxy]methyl}-
103 	104 	105 
Id: 106 Name: 4-butyl 1-ethyl 7-methyl 7-methylhepta-1,3,6-triene-1,4,7-tricarboxylate	Id: 107 Name: 1-ethyl 6-methyl 5-methylidenehex-2-enedioate	Id: 108 Name: 6-methyl 1-(6-phenylhex-5-en-1-yl) 5-methylidenehex-2-enedioate
106 	107 	108 
Id: 109 Name: 1-(acetyloxy)but-3-en-2-yl acetate	Id: 110 Name: 3-methylpentane-1,5-diol	Id: 111 Name: 2,6-Diisopropylaniline

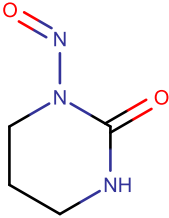
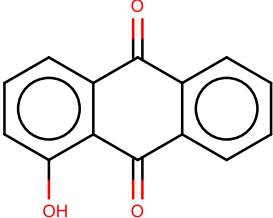
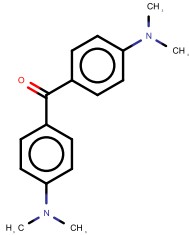
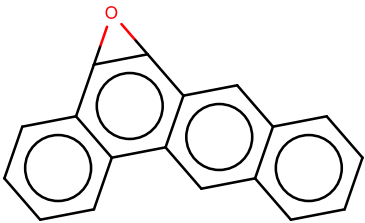
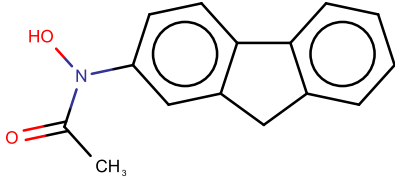
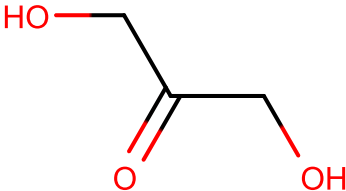
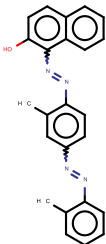
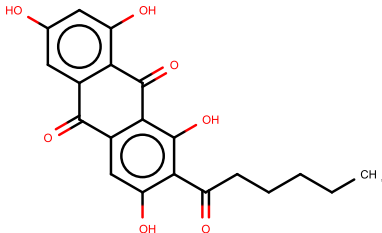
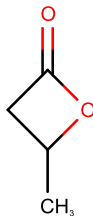
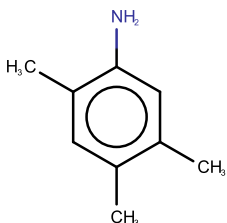
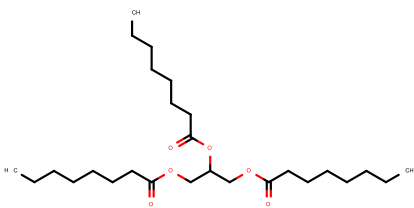
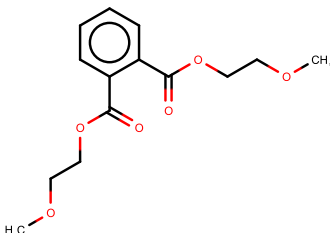
109 	110 	111 
Id: 112 Name: N,N-bis(2-hydroxyethyl)dodecanamide	Id: 113 Name: decanoic acid	Id: 114 Name: 2,2-bis[(octanoyloxy)methyl]butyl decanoate
112 	113 	114 
Id: 115a Name: 2-[(decanoyloxy)methyl]-2-[(octanoyloxy)methyl]butyl decanoate	Id: 116 Name: 2-methyl-2-[(octanoyloxy)methyl]butyl octanoate	Id: 117 Name: 2,2-bis[(octanoyloxy)methyl]butyl octanoate
115 	116 	117 
Id: 118 Name: 2,2-bis(4-hydroxyphenyl)propane	Id: 119 Name: 1,3,5-triazine-2,4,6-triamine (melamine)	Id: 120 Name: 1,3,5-triazine-2,4,6-triol
118 	119 	120 
Id: 121 Name: diamino-1,3,5-triazin-2-ol	Id: 122 Name: 6-amino-1,2,3,4-tetrahydro-1,3,5-triazine-2,4-dione	Id: 123 Name: 5-Chloro-2-methyl-2H-isothiazol-3-one (CIT)

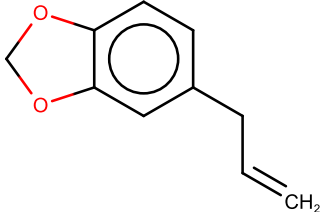
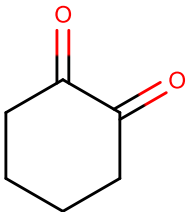
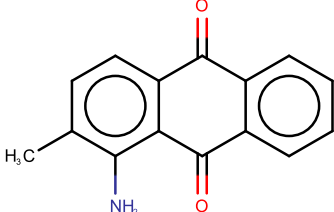
121 	122 	123 
Id: 124 Name: 2-methyl-2H-isothiazol-3-one (MIT)	Id: 125 Name: hex-1-ene	Id: 126 Name: dec-1-ene
124 	125 	126 
Id: 127 Name: triaconta-1,7,13,19,25-pentaene	Id: 128 Name: dotriaconta-1,7,17,23-tetraene	Id: 129 Name: 2-(2-([1-(1-chloro-1,2,2,3,3,3-hexafluoropropoxy)-1,1,2,3,3,3-hexafluoropropan-2-yl]oxy))-1
127 	128 	129 
Id: 130 Name: octadecanoic acid	Id: 131 Name: phenyl hexadecane-1-sulfonate	Id: 132 Name: diphenyl dotriacontane-1,32-disulfonate
130 	131 	132 
Id: 133 Name: diphenyl 17-[13-(phenoxysulfonyl)tridecyl]pentatriacontane-1,35-disulfonate	Id: 134 Name: 2,6-diamino-1,4-dihydropyrimidin-4-one	Id: 1_p Name: adipic acid

133 	134 	135 
Id: 2_p Name: maleic anhydride	Id: 3_p Name: Neopentyl glycol, diester with benzoic acid and 2-ethylhexanoic acid	Id: 4_p Name: 3-(hydroxymethyl)-3a,6a-dihydroimidazo[4,5-d]imidazole-2,5-dione
136 	137 	138 
Id: 5_p Name: 3,6-bis(hydroxymethyl)-1,4-dimethyl-3a,6a-dihydroimidazo[4,5-d]imidazole-2,5-dione	Id: 6_p Name: 3,4,6-tris(hydroxymethyl)-3a,6a-dihydroimidazo[4,5-d]imidazole-2,5-dione	Id: 7_p Name: Bis(4-propylbenzylidene)propylsorbitol
139 	140 	141 
Id: 8_p Name: 3,3',5,5'-tetrakis(tert-butyl)-2,2'-dihydroxybiphenyl	Id: 9_p Name: [3-(3-tert-butyl-4-hydroxy-5-methylphenyl)propyl]oxyphosphonous acid	Id: 10_p Name: 1-octene
142 	143 	144 
Id: 11_p Name: 1-dodecene	Id: 12_p Name: 1-tetradecene	Id: 13_p Name: 4-(butoxycarbonyl)benzoic acid

145 	146 	147 
Id: 14_p Name: 4-({4-[4-(butoxycarbonyl)benzoyloxy]butoxy}carbonyl)benzoic acid	Id: 15_p Name: 2-methyl-4-(methylthio)-2-morpholinopropiophenone	Id: 16_p Name: 4-(4-Methylphenylthio) benzophenone
148 	149 	150 
Id: 17_p Name: 4-Isopropylthioxanthone (4-ITX)	Id: 18_p Name: N-(2,6-Diisopropylphenyl)-6-[4-(1,1,3,3-tetramethylbutyl)phenoxy]-1H-benzo[de]isoquinolin-	Id: 19_p Name: bis(2,6-diisopropylphenyl)carbodiimide
151 	152 	153 
Id: 20_p Name: Ammelide (6-amino-2,4-dihydroxy-1,3,5-triazine)	Id: 21_p Name: 12-hydroxystearic acid stearate	Id: 22_p Name: 2,4-Diamino-6-hydroxypyrimidine
154 	155 	156 
Id: 1_s Name: 2-(2-quinolyl)indane-1,3-dione	Id: 2_s Name: anthraquinone, 1-amino-4-methoxy-	Id: 3_s Name: 8-hydroxy-6-methoxy-3a,12c-dihydro-7h-furo[3',2':4,5]furo[2,3-c]xanthene-7-one

157  Id: 6_s Name: 2-[(biphenyl-2-ylomethyl)oxirane]methoxy	158  Id: 7_s Name: 2',3-dimethyl-(1,1'-biphenyl)-4-amine	159  Id: 9_s Name: ethane-1,2-diylbis(oxyethane-2,1-diyl) diacetate
160  Id: 11_s Name: 1,2,7,8-diepoxyoctane	161  Id: 13_s Name: ketoxal	162  Id: 16_s Name: triethylene tetramine
163  Id: 19_s Name: oxo(phenyl)acetaldehyde	164  Id: 20_s Name: 2-amino-9,10-anthracenedione	165  Id: 21_s Name: 1,2,4-trimethylbenzene
166  Id: 22_s Name: (2E)-hept-2-enal	167  Id: 23_s Name: bis(2-bromoethyl) 2-hydroxybutanedioate	168  Id: 24_s Name: 1-nitroso-5,6-dihydrouracil

169 	170 	171 
Id: 26_s Name: 2(1h)-pyrimidinone, tetrahydro-1-nitroso-	Id: 27_s Name: 1-hydroxyanthracene-9,10-dione	Id: 28_s Name: 4,4'-bis(dimethylamino)benzophenone
172 	173 	174 
Id: 29_s Name: Benzanthracene-5,6-oxide	Id: 30_s Name: n-hydroxy-2-acetylaminofluorene	Id: 32_s Name: 1,3-dihydroxypropan-2-one
175 	176 	177 
Id: 33_s Name: 1-({2-methyl-4-[(2-methylphenyl)diazenyl]phenyl}diazenyl)naphthalen-2-ol	Id: 34_s Name: anthraquinone, 2-hexanoyl-1,3,6,8-tetrahydroxy-	Id: 35_s Name: 4-methyloxetan-2-one
178 	179 	180 
Id: 36_s Name: 2,4,5-trimethylaniline	Id: 37_s Name: propane-1,2,3-triyl trioctanoate	Id: 38_s Name: bis(2-methoxyethyl) phthalate

181	182	183
		
Id: 39_s Name: 5-(2-propenyl)-1,3-benzodioxole	Id: 40_s Name: 1,2-cyclohexanedione	Id: 42_s Name: 1-amino-2-methylanthracene-9,10-dione