

"TEST SET INDEX"; "SMILES"; "NAME"; "MW"; "LogS (mols/L)"; "REFERENCE"; "GROUP"
1; "[nH0]1c2ccccc2cc2ccccc12"; "Acridine"; 179.23; -3.67; 25; "TEST"
2; "O=C(N)C=C"; "Acrylamide"; 71.09; 0.96; 25; "TEST"
3; "O=C1NC(=O)[C@H](N1)NC(=O)N"; "Allantoin"; 158.14; -1.6; 25; "TEST"
4; "O=C1NC(=O)C(=O)C(=O)N1"; "Alloxan"; 142.07; -1.25; 24; "TEST"
5; "N(C)(C)CCC=C1c2ccccc2CCc2ccccc21"; "Amitriptyline"; 277.44; -4.46; 25; "TEST"
6; "O=C1NC(=O)C(CC)(CCC(C)C)C(=O)N1"; "Amobarbital"; 226.31; -2.57; 25; "TEST"
7; "S1[C@H](N(C(=O)[C@H](NC(=O)[C@H](N)c2ccc(O)cc2)2)[C@@H](C(=O)O)C1(C)C)2"; "Amoxicillin"; 365.4; -2.09; 24; "TEST"
8; "ClC(Cl)C(=O)N[C@@H](CO)[C@@H](O)c1ccc([N](=O)[O-])cc1"; "Amphicol"; 323.13; -2.006; 24; "TEST"
9; "N=1CCNC=1CN(Cc1ccccc1)c1ccccc1"; "Antazoline"; 265.39; -2.6; 25; "TEST"
10; "O=C1NC(=O)C(CC=C)(C(=O)N1)C(C)C"; "Aprobarbital"; 210.26; -1.71; 25; "TEST"
11; "O(C)c1[nH0]c([nH0]c([nH0]1)NC(C)C)NCC"; "Atratone"; 211.31; -2.084; 26; "TEST"
12; "O=C(O)C(=C)c1ccccc1"; "Atropic acid"; 148.17; -2.06; 25; "TEST"
13; "Clc1[nH0][nH0]c(SCC(=O)N(CC)CC)c1"; "Azintamide"; 259.79; -1.716; 26; "TEST"
14; "[P]([O-])(OC)(OC)O/C(/C)=C/C(=O)NC"; "Azodrin"; 223.19; 0.651; 26; "TEST"
15; "S(N(C)C(=O)Oc1ccccc2CC(Oc21)(C)C)N(CCC(=O)OCC)C(C)C"; "Benfuracarb"; 410.59; -4.71; 26; "TEST"
16; "Ic1ccccc1C(=O)Nc1ccccc1"; "Benodanil"; 323.14; -4.21; 25; "TEST"
17; "[S]1([O-])([O-])Nc2ccccc2C(=O)N1C(C)C"; "Bentazon"; 240.31; -2.68; 25; "TEST"
18; "O=C(N)c1ccccc1"; "Benzamide"; 121.15; -0.96; 25; "TEST"
19; "[S]([O-])([O-])(N)c1ccccc1"; "Benzenesulfonamide"; 157.19; -1.56; 24; "TEST"
20; "Nc1ccc(cc1)c1ccc(N)cc1"; "Benzidine"; 184.26; -2.7; 25; "TEST"
21; "c1ccc2c(c1)Cc1cc3ccccc3cc12"; "Benzo(b)fluorene"; 216.29; -8.04; 25; "TEST"
22; "c1ccc2c(c1)c1cccc3ccc4cccc2c4c31"; "Benzo(e)pyrene"; 252.32; -7.8; 25; "TEST"
23; "c1cc2ccc3ccc4ccc5cccc6c(c1)c2c3c4c56"; "Benzo(ghi)perylene"; 276.34; -9.03; 25; "TEST"
24; "c1ccc2cc3c(cc2c1)c1cccc2cccc3c12"; "Benzo(k)fluoranthene"; 252.32; -8.49; 25; "TEST"
25; "O=C(O)c1ccccc1"; "Benzoic acid"; 122.13; -1.55; 25; "TEST"
26; "O=C(c1ccccc1)c1ccccc1"; "Benzophenone"; 182.23; -3.12; 25; "TEST"
27; "[nH0]1[nH0]c2ccccc2[nH]1"; "Benzotriazole"; 119.14; -0.78; 25; "TEST"
28; "o1c[nH0]c2ccccc12"; "Benzoxazole"; 119.13; -1.16; 25; "TEST"
29; "O=C(O)C[C@@H](N)C"; "Beta-Aminobutyric acid"; 103.14; 1.08; 25; "TEST"
30; "[nH0]1c(ccc2ccccc12)c1[nH0]c2ccccc2cc1"; "Biquinoline"; 256.32; -5.4; 25; "TEST"
31; "Brclccc(cc1)C(O)(c1ccc(Br)cc1)C(=O)OC(C)C"; "Bromopropylate"; 428.13; -4.93; 25; "TEST"
32; "O=C1NC(=O)C(CC)(C(=O)N1)[C@H](C)CC"; "Butabarbital"; 212.28; -2.39; 26; "TEST"
33; "BrC(=C)CC1(C(=O)NC(=O)NC1=O)[C@H](C)CC"; "Butallylonal"; 303.18; -2.647; 26; "TEST"
34; "O=C(OCCCC)c1ccc(O)cc1"; "Butyl-p-hydroxybenzoate"; 194.25; -2.72; 25; "TEST"
35; "O=C1N(C)c2[nH0]c[nH0](C)c2C(=O)N1C"; "Caffeine"; 194.22; -0.97; 25; "TEST"
36; "O=C(Oc1ccccc2ccccc12)NC"; "Carbaryl"; 201.24; -3.28; 25; "TEST"
37; "O=C(Oc1ccccc2CC(Oc21)(C)C)NC"; "Carbofuran"; 221.28; -2.8; 26; "TEST"
38; "Clc1ccc(SCS[P]([S-])(OCC)OCC)c1"; "Carbophenthion"; 342.9; -5.736; 26; "TEST"
39; "S1CCOC(C)=C1C(=O)Nc1ccccc1"; "Carboxin"; 235.33; -3.14; 25; "TEST"
40; "ClC(Cl)C1[C@@H](O[C@H](O[C@H]([C@H](O)[C@@H](O1)2)[C@H](O)CO)2)1"; "Chloralose"; 309.54; -1.84; 25; "TEST"
41; "Clc1cc(N)c(Cl)c(c1)C(=O)O"; "Chloramben"; 206.03; -2.47; 24; "TEST"
42; "Clc1cc(N)c(Cl)c(c1)C(=O)OC"; "Chloramben methyl ester"; 220.06; -3.26; 25; "TEST"
43; "ClC(Cl)C(=O)N[C@@H](CO)[C@@H](O)c1ccc([N](=O)[O-])cc1"; "Chloramphenicol"; 323.15; -2.11; 25; "TEST"
44; "ClC1=C(Cl)[C@](Cl)([C@H](CC=C[C@H]2([C@@](Cl)1(C1(Cl)Cl)))2)1"; "Chlordene"; 338.86; -5.64; 25; "TEST"
45; "Clc1ccc(N=CN(C)C)c(C)c1"; "Chlordimenform"; 196.7; -2.86; 25; "TEST"
46; "Clc1ccc(Cl)c(CC(=O)O)c1Cl"; "Chlorfenac"; 239.48; -3.08; 25; "TEST"

47;"Clc1ccc2c3ccccc3[C@@](O)(c2c1)C(=O)O";"Chlorflurecol-methyl";260.68;-4.18;25;"TEST"
48;"Clc1cccc(NC(=O)OC(C)C)c1";"Chloropham";213.68;-3.38;25;"TEST"
49;"Clc1ccc(Oc2ccc(NC(=O)N(C)C)cc2)cc1";"Chloroxuron";290.77;-4.89;25;"TEST"
50;"Clc1[nH0]c(O[P]([S-])(OCC)OCC)c(Cl)cc1Cl";"Chlorpyriphos";350.6;-5.49;25;"TEST"
51;"c1ccc2c(c1)ccc1c3ccccc3ccc21";"Chrysene";228.3;-8.06;25;"TEST"
52;"O=C([nH0]1c2ccc(OC)cc2c(CC(=O)O)c1)/C=Cc1ccccc1";"Cinmetacin";349.41;-5.54;25;"TEST"
53;"O=C(O)CC(O)(CC(=O)O)C(=O)O";"Citric acid";192.14;0.51;25;"TEST"
54;"Clc1cccc1CN1OCC(C)(C)Cl=O";"Clomazone";239.72;-2.338;26;"TEST"
55;"O=C(O[C@H](C[C@@H](N(C)[C@@H](CC1)[C@@H](C(=O)OC)2)1)2)c1ccccc1";"Cocaine";303.39;-2.23;25;"TEST"
56;"O=C1C=C2CC[C@H]([C@@H](CC[C@@](O)(C(=O)COC(=O)C)[C@](C)(CC(=O)[C@@H]3([C@](C)(CC1)2))1)1)3";"Cortisone acetate";402.53;-4;25;"TEST"
57;"Clc1ccc(cc1)[C@H](CC(=O)C)C=1C(=O)Oc2ccccc2C=1O";"Coumachlor";342.79;-5.839;26;"TEST"
58;"O=C1Oc2ccccc2C=C1";"Coumarin";146.15;-1.89;25;"TEST"
59;"O=C1NC(=O)C(CC)(C(=O)N1)C1=CCCC1";"Cyclobarbital";236.3;-2.17;25;"TEST"
60;"O=C1NC(=O)C2(CCC2)C(=O)N1";"Cyclobutyl-5-spirobarbituric acid";168.17;-1.655;26;"TEST"
61;"O=C1NC(=O)CC(Cl)C[C@H](O)[C@@H](C[C@H](C)C[C@@H](C)C1=O)1";"Cycloheximide";281.39;-1.13;25;"TEST"
62;"Cl/C(=C[C@H]([C@@H](C(=O)O[C@@H](C#N)c1cccc(Oc2ccccc2)c1)C1(C)C)1)/C(F)(F)F";"Cyhalothrin";449.88;-8.176;26;"TEST"
63;"ClC(Cl)=C[C@H]([C@@H](C(=O)O[C@@H](C#N)c1cccc(Oc2ccccc2)c1)C1(C)C)1";"Cypermethrin";416.32;-8.017;26;"TEST"
64;"OC1C(O)C(O)C(O)C1O";"D-Inositol";180.18;0.35;25;"TEST"
65;"O[C@@H](Cc1ccccc1)c1ccccc1";"DL-1,2-Diphenylethanol";198.26;-2.52;24;"TEST"
66;"Clc1cccc(O[C@H](C)C(=O)O)c1";"DL-2-(2-Chlorophenoxy)propionic acid";200.63;-2.22;25;"TEST"
67;"O=[N]([O-])c1cc([N](=O)[O-])c(O)c(C)c1";"DNOC";198.15;-1.456;26;"TEST"
68;"S=C1SCN(C)CN1C";"Dazomet";162.31;-2.13;25;"TEST"
69;"ClC1=C[C@H]([C@@H](CC[C@](OC(=O)C)(C(=O)C)[C@](C)(CC[C@H]2([C@](C)(C=CC(=O)C=C11)1)1)2)";"Delmadinone acetate";402.95;-4.95;25;"TEST"
70;"O=C1C=C2CC[C@H]([C@@H](CC[C@H](C(=O)COC(=O)C)[C@](C)(CC[C@@H]3([C@](C)(CC1)2))1)1)3";"Deoxycorticosterone acetate";372.55;-4.63;25;"TEST"
71;"F[C@]([C@H](O)C[C@](C)([C@H](C[C@@H](C)[C@@](O)(C(=O)COC(=O)C)1)[C@H](CCC2=C(C(=O)C=C[C@@](C)2)3)1)32";"Dexamethasone-17-acetate";434.55;-4.9;25;"TEST"
72;"O1c2ccccc2Oc2ccccc12";"Dibenzo-p-dioxine";184.2;-5.31;25;"TEST"
73;"Clc1cc([N](=O)[O-])ccc1O[P]([S-])(OC)OC";"Dicaphton";297.67;-4.31;25;"TEST"
74;"Clc1ccc(cc1)C(O)(c1ccc(Cl)cc1)C(Cl)(Cl)Cl";"Dicofol";370.48;-5.666;26;"TEST"
75;"Clc1ccc(NC(=O)NC(=O)c2c(F)cccc2F)cc1";"Diifluron";310.7;-6.02;25;"TEST"
76;"O=C(OCCCCC)c1ccccc1C(=O)OCCCCC";"Dihexyl phthalate";334.5;-6.144;26;"TEST"
77;"Clc1cc(NC(=O)N(C)C)ccc1N1N=C(OC1=O)C(C)(C)C";"Dimefuron";338.83;-4.328;26;"TEST"
78;"Ocl[nH0]c([nH0]c(C)c1CCCC)N(C)C";"Dimethirimol";209.33;-2.24;25;"TEST"
79;"O=[N]([O-])c1cc([N](=O)[O-])c(O)c(c1)[C@H](C)CC";"Dinoseb";240.24;-3.38;25;"TEST"
80;"O[C@@H](CC[C@@](C)(C(=CC[C@H]([C@@H](C[C@@H](O[C@](OC[C@@H](C)CC1)1([C@@H](C)[C@@H]1([C@](C)(CC[C@@H]23)4))1)4)2)C1)3)1";"Diosgenin";414.69;-7.32;25;"TEST"
81;"O=C(O)c1ccccc1c1ccccc1C(=O)O";"Diphenic acid";242.24;-2.28;25;"TEST"
82;"S=C(SSC(=S)N(CC)CC)N(CC)CC";"Disulfiram";296.6;-4.86;25;"TEST"
83;"Clc1ccc(NC(=O)N(C)C)cc1Cl";"Diuron";233.11;-3.8;25;"TEST"
84;"O=C(O)C[C@H](N)C(=O)O";"Dl-aspartic acid";133.1;-1.215;24;"TEST"
85;"O=C(O)CC[C@H](N)C(=O)O";"Dl-glutamic acid";147.13;-0.807;24;"TEST"
86;"O=C(O)[C@@H](N)CC(C)C";"Dl-leucine";131.18;-1.11;24;"TEST"

87;"O=C(N)Nc1ccc(OCC)cc1";"Dulcin";180.23;-2.17;25;"TEST"
88;"Cc1cc(C)c(C)cc1C";"Durene";134.22;-4.587;24;"TEST"
89;"O=C1N(C)c2[nH0]c[nH0](C[C@@H](O)CO)c2C(=O)N1C";"Dyphylline";254.28;-
0.17;25;"TEST"
90;"O=C(O)[C@H]([C@H](N(C)[C@@H](C[C@@H](O)1)CC2)2)1";"Ecgonine";185.25;-
0.02;25;"TEST"
91;"S1[C@H](C[C@@H](CC[C@@H]([C@H](CC[C@@H](O)[C@](C)(CC[C@@H]2([C@@](C)(C[C@@H]
11)3)4)4)2)3)1";"Epitiostanol";306.56;-5.41;25;"TEST"
92;"O=C1C[C@H](O)c2cc(O)cc(O)c21)c1ccc(O)c(O)c1";"Eriodictyol";288.27;-
3.62;25;"TEST"
93;"O=C1CC[C@H]([C@H](CCc2cc(O)ccc2[C@H](CC[C@](C)11)2)2)1";"Estrone";270.37;-
3.96;24;"TEST"
94;"O=C1C=C2CC[C@H]([C@@H](CC[C@@](O)(C#C)[C@](C)(CC[C@@H]3([C@](C)(CC1)2))1)1)3
";"Ethisterone";312.49;-5.66;25;"TEST"
95;"s1c2cc(OCC)ccc2[nH0]c1[S]([O-])([O-])N";"Ethoxazolamide";258.35;-
3.81;25;"TEST"
96;"O=C1Oc2cccc2C(O)=C1C(C=1C(=O)Oc2cccc2C=1O)C(=O)OCC";"Ethyl
biscoumacetate";408.38;-3.66;25;"TEST"
97;"O=C(OCC)c1ccc(O)cc1";"Ethyl-p-hydroxybenzoate";166.19;-2.35;25;"TEST"
98;"O=C(OCC)c1[nH0](c[nH0]c1)[C@@H](C)c1cccc1";"Etomidate";244.32;-
4.735;26;"TEST"
99;"O=C1OC[C@H]([C@H]1([C@@H](c1cc(OC)c(O)c(OC)c1)c1cc2OCoc2cc1[C@H](O[C@@H](O[C
@H](CO[C@@H](O[C@H]1([C@@H](O)[C@H](O)2))C)1)2)1))1";"Etoposide";588.61;-
3.571;26;"TEST"
100;"s1cc([nH0]c1N=C(N)N)CSCCC(N)=N[S]([O-])([O-])N";"Famotidine";337.45;-
2.49;24;"TEST"
101;"S(CCCCOc1cccc1)C(=O)N(C)C";"Fenothiocarb";253.4;-3.927;26;"TEST"
102;"F[C@]([C@H](O)C[C@](C)([C@H](CC[C@@](O)(C(=O)CO)1)[C@H](CCC2=CC(=O)CC[C@@](
C)2)3)1)32";"Fludrocortisone";380.5;-3.43;25;"TEST"
103;"Clc1cccc(F)c1CN(CC)c1c([N](=O)[O-])cc(ccl1[N](=O)[O-
)C(F)(F)F";"Flumetralin";421.76;-6.78;26;"TEST"
104;"Fc1cc(ccc1c1cccc1)[C@H](C)C(=O)O";"Flurbiprofen";244.28;-4.49;25;"TEST"
105;"Fc1ccc(cc1)c1c2cccc2[nH0](c1/C=C/[C@@H](O)C[C@H](O)CC(=O)O)C(C)C";"Fluvast
atin";411.47;-3.83;24;"TEST"
106;"O=CNc1cccc1";"Formanilide";121.15;-0.68;25;"TEST"
107;"OC[C@@](O)(OC[C@H](O)[C@H](O)[C@H](O)1)1";"Fructose";180.18;0.64;25;"TEST"
108;"Clc1cc(NC2occc2)c(cc1[S]([O-])([O-])N)C(=O)O";"Furosemide";330.77;-
3.66;25;"TEST"
109;"ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl";"Gamma-hexachlorocyclohexane";290.82;-
4.59;25;"TEST"
110;"O=C1O[C@@](C=C[C@@H](O)[C@](C)1([C@H]([C@H](C(=O)O)[C@](CC(=C)[C@](O)(CC[C@
H]12)C3)32)2))12";"Gibberellic acid";346.41;-1.84;25;"TEST"
111;"Clc1c2O[C@@](C(OC)=CC(=O)C[C@@H](C)3)(C(=O)c2c(OC)cc1OC)3";"Griseofulvin";3
52.79;-4.61;25;"TEST"
112;"O=C1C=C2C[C@](O)(COc3c(ccc(O)c3O)C3=C2C=C1O)3";"Hematein";300.28;-
2.7;25;"TEST"
113;"ClC(Cl)=C(Cl)C(Cl)=C(Cl)Cl";"Hexachloro-1,3-butadiene";260.74;-
4.92;26;"TEST"
114;"ClC(Cl)(Cl)C(Cl)(Cl)Cl";"Hexachloroethane";236.72;-3.67;25;"TEST"
115;"Oc1ccc(cc1)[C@@H](CC)[C@@H](CC)c1ccc(O)cc1";"Hexestrol";270.4;-
4.43;25;"TEST"
116;"O=C(OCCCCC)c1ccc(N)cc1";"Hexyl-4-aminobenzoate";221.33;-3.95;25;"TEST"
117;"O=C1NCC(=O)N1";"Hydantoin";100.09;-0.4;25;"TEST"
118;"O=C1C=C2CC[C@H]([C@@H](CC[C@@](O)(C(=O)CO)[C@](C)(C[C@@H](O)[C@@H]3([C@](C)
(CC1)2))1)1)3";"Hydrocortisone";362.51;-2.97;25;"TEST"
119;"O=C1CC[C@H]([C@@H](CC[C@H](C[C@H](O)CC[C@](C)2([C@H]([C@@H](O)C[C@@](C)11)3
)2)3)1";"Hydroxyisoandrosterone";306.49;-3.59;25;"TEST"

120; "O=C1CC[C@H]([C@@H](CC[C@H](C[C@H](O)C[C@H](O)[C@](C)2([C@@H](CC[C@@](C)11)3)2)3)1"; "Hydroxyoandrosterone"; 306.45; -3.59; 24; "TEST"
121; "[nH]1cccc2cccc12"; "Indole"; 117.16; -1.52; 25; "TEST"
122; "O=C(O)Cc1c[nH]c2cccc21"; "Indole-3-acetic acid"; 175.2; -2.07; 25; "TEST"
123; "O=C1NCCN1C(=O)NCC(C)C"; "Isocarbamid"; 185.26; -2.15; 25; "TEST"
124; "Oc1[nH]c2[nH]c[nH]c2c(N)[nH]1"; "Isoguanine"; 151.15; -3.401; 26; "TEST"
125; "O=C(NN)c1cc[nH]ccl1"; "Isoniazid"; 137.16; 0.01; 25; "TEST"
126; "O=[N]([O-])c1cc(cc([N](=O)[O-])c1N(CCC)CCC)C(C)C"; "Isopropalin"; 309.41; -6.49; 26; "TEST"
127; "O=C(Nc1ccc(cc1)C(C)C)N(C)C"; "Isoproturon"; 206.32; -3.54; 25; "TEST"
128; "O=C(Oc1cccc(NC(=O)N(C)C)c1)NC(C)C"; "Karbutilate"; 279.38; -2.93; 25; "TEST"
129; "O=C(c1cccc1)c1cccc(c1)[C@H](C)C(=O)O"; "Ketoprofen"; 254.3; -3.7; 25; "TEST"
130; "O=C1C=C(Oc2c(OC)c3occc3c(OC)c12)C"; "Khellin"; 260.26; -2.4; 25; "TEST"
131; "O=C(O)[C@H](N)Cc1[nH]c[nH]c1"; "L histidine"; 155.16; -0.573; 24; "TEST"
132; "O[C@@H](OC[C@@H](O)[C@@H](O)[C@H](O)1)1"; "L-Arabinose"; 150.15; 0.39; 25; "TEST"
133; "O=C(O)[C@H](N)Cc1ccc(O)c(O)c1"; "Levodopa"; 197.21; -1.6; 25; "TEST"
134; "[S-][P](SCC(=O)N(C)C(=O)OCC)(OCC)OCC"; "Mecarbam"; 329.42; -2.518; 26; "TEST"
135; "O=C(O)c1cccc1Nc1cccc(C)c1C"; "Mefenamic acid"; 241.31; -3.78; 25; "TEST"
136; "O=C1C=C(C)C(=O)c2cccc12"; "Menadione"; 172.19; -3.03; 25; "TEST"
137; "O[C@@H](C[C@H](C)CC[C@@H]1(C(C)C)1)1"; "Menthol"; 156.3; -2.53; 25; "TEST"
138; "O=C1N(C(=Nc2cccc12)C)c1cccc1C"; "Methaqualone"; 250.32; -2.925; 26; "TEST"
139; "O=C1NC(=O)C(CC)(CC)C(=O)N1C"; "Metharbital"; 198.25; -2.23; 25; "TEST"
140; "S1C([S]([O-])([O-])N)=NN(C)C1=NC(=O)C"; "Methazolamide"; 236.31; -1.83; 25; "TEST"
141; "O=C(OC[C@@H](O)COc1cccc1OC)N"; "Methocarbamol"; 241.27; -0.985; 26; "TEST"
142; "O=C1Oc2c(C=C1)cc1ccoc1c2OC"; "Methoxsalen"; 216.2; -3.66; 25; "TEST"
143; "O=C(O)[C@@H](C)CCCCCCCC"; "Methyl laurate"; 214.34; -4.69; 24; "TEST"
144; "O=C(OC)c1c[nH]c1ccc1"; "Methyl nicotinate"; 137.15; -0.46; 25; "TEST"
145; "O=C(OC)c1ccc(OC)cc1"; "Methyl-4-methoxybenzoate"; 166.19; -2.41; 25; "TEST"
146; "O=C(NC(C)C)c1cccc1N(C)c1cccc1"; "Methyldymron"; 268.39; -3.35; 26; "TEST"
147; "S1c2cccc2N(C)c2cc(ccc12)CC(=O)O"; "Metiazinic acid"; 271.36; -3.94; 25; "TEST"
148; "O[C@H](COc1ccc(cc1)CCOC)CNC(C)C"; "Metoprolol"; 267.36; -1.43; 24; "TEST"
149; "O=[N]([O-])c1[nH]c(ccc1)C([nH]c1)C"; "Metronidazole"; 171.18; -1.26; 25; "TEST"
150; "ClC12C3(C1)C4(C1)C5(C1)C(C1)(C1(C1)C4(C1)C1)C2(C1)C(C1)(C1)C35C1"; "Mirex"; 545.5; -6.8; 26; "TEST"
151; "Clc1ccc(NC(=O)N(C)C)cc1"; "Monuron"; 198.67; -2.89; 25; "TEST"
152; "O=C1C(O)=C(Oc2cc(O)cc(O)c21)c1ccc(O)cc1O"; "Morin"; 302.25; -3.08; 25; "TEST"
153; "OCCCCCCCCCCCC"; "Myristyl alcohol"; 214.44; -6.05; 25; "TEST"
154; "O=C(OCCNCCCC)c1ccc(N)cc1"; "Naepaine"; 250.38; -3.27; 25; "TEST"
155; "O=C1c2ccc([nH]c2N(C=C1C(=O)O)CC)C"; "Nalidixic acid"; 232.26; -3.37; 25; "TEST"
156; "c1ccc2cc3cc4cccc4cc3cc2c1"; "Naphthacene"; 228.3; -8.6; 25; "TEST"
157; "c1ccc2cccc2c1"; "Naphthalene"; 128.18; -3.6; 25; "TEST"
158; "O=C(CO)[C@@H](O)[C@@H](O)[C@@H](O)CO"; "Nevulose"; 180.16; 0.64; 24; "TEST"
159; "O=C(N)c1c[nH]c1ccc1"; "Nicotinamide"; 122.14; 0.61; 25; "TEST"
160; "O=[N]([O-])c1ccc2N(C)C(=O)CN=C(c2c1)c1cccc1"; "Nimetazepam"; 295.32; -3.8; 25; "TEST"
161; "Clc1c[nH]c(ccc1)C(C1)(C1)C1"; "Nitrapyrin"; 230.9; -3.76; 25; "TEST"
162; "Clc1ccc(Oc2ccc([N](=O)[O-])cc2)c(C1)c1"; "Nitrofen"; 284.1; -5.46; 25; "TEST"
163; "O=C(N[C@@H](C[C@H](C[C@H]([C@@H](CCC[C@H]12)2)2)1)2)N(C)C"; "Norea"; 222.37; -3.171; 26; "TEST"
164; "O=C1C=C2CC[C@H]([C@@H](CC[C@](OC(=O)C)(C#C)[C@](C)(CC[C@H]([C@H](CC1)2)1)2)2)1"; "Norethindrone acetate"; 340.5; -4.8; 26; "TEST"
165; "Clc1ccc(cc1)[C@@H](c1cccc1Cl)C(C1)(C1)C1"; "O,p'-DDT"; 354.48; -6.62; 25; "TEST"
166; "O=C(OCCCCCCC)c1ccc(N)cc1"; "Octyl-4-aminobenzoate"; 249.39; -5.4; 25; "TEST"

167;"[S]([O-]) (Cc1[nH0]cc(C)c(OC)c1C)c1[nH0]c2cc(OC)ccc2[nH]1";"Omeprazole";345.42;-3.42;24;"TEST"

168;"O=Cc1ccc(OC)c(OC)c1C(=O)O";"Opianic acid";210.2;-1.92;25;"TEST"

169;"O=C1NC(=O)C=C(N1)C(=O)O";"Orotic acid";156.11;-1.93;25;"TEST"

170;"Clc1cc(Cl)c(N2N=C(OC2=O)C(C)(C)C)cc1OC(C)C";"Oxadiazon";345.25;-5.69;25;"TEST"

171;"O=C(O)C(=O)O";"Oxalic acid";90.04;0.38;25;"TEST"

172;"Clc1ccc2NC(=O)[C@H](O)N=C(c2c1)c1cccc1";"Oxazepam";286.73;-3.952;26;"TEST"

173;"O=C1N(N(c2ccc(O)cc2)C(=O)[C@H](CCCC)1)c1cccc1";"Oxyphenbutazone";324.41;-3.73;25;"TEST"

174;"Clc1ccc(cc1)C(c1ccc(Cl)cc1)C(Cl)Cl";"P,p?-DDD";320.04;-7.2;25;"TEST"

175;"Clc1ccc(cc1)C(c1ccc(Cl)cc1)=C(Cl)Cl";"P,p?-DDE";318.02;-6.9;25;"TEST"

176;"O=C(OCCN(CC)CC)c1ccc(OCC)cc1";"Parethoxycaine";265.39;-2.71;25;"TEST"

177;"S(CCC)C(=O)N(CC)CCCC";"Pebulate";203.39;-3.53;26;"TEST"

178;"SC(C)(C)[C@H](N)C(=O)O";"Pencillamine";149.24;-0.13;25;"TEST"

179;"ClC(Cl)=C[C@H]([C@H](C(=O)OCc1cccc(Oc2cccc2)c1)Cl)C1(C)C1";"Permethrin";391.31;-6.29;25;"TEST"

180;"Clc1ccc2Sc3cccc3N(CCCN3CCN(CC3)CCO)c2c1";"Perphenazine";404.02;-4.16;25;"TEST"

181;"O=C1NC(=O)C(CC=C)(C(=O)N1)c1cccc1";"Phenallymal";244.27;-2.18;25;"TEST"

182;"O=C(OC)Nc1cccc(OC(=O)Nc2cccc(C)c2)c1";"Phenmedipham";300.34;-4.805;26;"TEST"

183;"Oc1cccc1";"Phenol";94.12;0;25;"TEST"

184;"O=C(O)COc1cccc1";"Phenoxyacetic acid";152.16;-1.1;25;"TEST"

185;"O=C(Oc1cccc1)c1cccc1O";"Phenyl salicylate";214.23;-3.15;25;"TEST"

186;"O[C@H](CN)c1cccc1";"Phenylethanolamine";137.2;-0.48;25;"TEST"

187;"N#Cc1cccc1C#N";"Phthalonitrile";128.14;-2.38;25;"TEST"

188;"O=C1c2c[nH0]c([nH0]c2N(C=C1C(=O)O)CC)N1CCNCC1";"Pipedemic acid";303.36;-2.98;25;"TEST"

189;"O=Cc1ccc2OCoc2c1";"Piperonal";150.14;-1.63;25;"TEST"

190;"O=C1CC[C@H]([C@H](CC=C2C[C@H](O)CC[C@](C)2([C@H](CC[C@@](C)11)2)2)1";"Prasterone";288.47;-4.12;25;"TEST"

191;"O=C1C=C[C@@](C)(C(=C1)CC[C@H]([C@H](CC[C@@](O)(C(=O)COC(=O)C)[C@](C)(C[C@@H](O)[C@H]12)3)1)2";"Prednisolone acetate";402.53;-4.37;25;"TEST"

192;"O=C(C)[C@H](CC[C@H]([C@H](CC=C1C[C@H](O)CC[C@](C)1([C@H](CC[C@](C)12)3)3)1)2";"Pregnenolone";316.53;-4.65;25;"TEST"

193;"O=C1NCNC(=O)C1(CC)c1cccc1";"Primidone";218.28;-2.64;25;"TEST"

194;"O=C1NC(=O)C(CC)(C(=O)N1)C(C)C";"Probarbital";198.25;-2.21;25;"TEST"

195;"Clc1cc(Cl)cc(N2C(=O)[C@](C)(C[C@@](C)(C2=O)2)2)c1";"Procymidone";284.15;-4.8;26;"TEST"

196;"O(C)c1[nH0]c([nH0]c([nH0]1)NC(C)C)NC(C)C";"Prometon";225.34;-2.478;26;"TEST"

197;"Clc1ccc(NC(=O)CC)cc1Cl";"Propanil";218.09;-3;25;"TEST"

198;"Clc1[nH0]c([nH0]c([nH0]1)NC(C)C)NC(C)C";"Propazine";229.75;-4.43;25;"TEST"

199;"Clc1ccc(c(Cl)c1)[C@@](OC[C@H](O1)CCC)1(C[nH0]1[nH0]c[nH0]c1)";"Propiconazole";342.25;-3.493;26;"TEST"

200;"O=C(Oc1cccc1OC(C)C)NC";"Propoxur";209.27;-2.05;25;"TEST"

201;"[nH0]1c[nH0]c2[nH0]cc[nH0]c2c1";"Pteridine";132.14;0.02;25;"TEST"

202;"O=C(Nc1cccc1)C=1CCCOC=1C";"Pyracarbolid";217.29;-2.56;25;"TEST"

203;"O=C(O)c1[nH0]c2cccc2cc1";"Quinolinic acid";173.1;-1.187;24;"TEST"

204;"FC(F)(F)c1cc([nH0]c2N(CC)c3[nH0]cccc3C(=O)Nc21)C";"RTI 13";322.32;-4.207;26;"TEST"

205;"Clc1ccc2NC(=O)c3ccc[nH0]c3N(CC)c2c1";"RTI 24";273.74;-5.36;26;"TEST"

206;"S=C1SCC(=O)N1";"Rhodanine";133.21;-1.77;25;"TEST"

207;"O=C(O)[C@H](N)Cc1c[nH]c2cccc21";"S-tryptophan";204.23;-1.219;24;"TEST"

208;"[S]1([O-])([O-])NC(=O)c2cccc12";"Saccharin";183.2;-1.64;25;"TEST"

209;"O=C(OC1C[C@H](N(C)[C@@H](C1)[C@H](O[C@H]12)1)2)[C@@H](CO)c1cccc1";"Scopolamine";303.39;-0.48;25;"TEST"
210;"OC[C@H](O)[C@H](O)[C@H](O)[C@H](O)CO";"Sorbitol";182.2;1.09;25;"TEST"
211;"S(C(=O)C)[C@H](CC1=CC(=O)CC[C@@](C)1([C@@H](CC[C@](C)([C@H](CC[C@@](OC(=O)C)1)1)[C@H]23)1)3)2";"Spironolactone";416.63;-4.28;25;"TEST"
212;"[S]([O-])([O-])(Nc1[nH0]ccc[nH0]1)c1ccc(N)cc1";"Sulfadiazine";250.31;-3.51;25;"TEST"
213;"[S]([O-])([O-])(Nc1[nH0]c(C)cc([nH0]1)C)c1ccc(N)cc1";"Sulfamethazine";278.37;-2.27;25;"TEST"
214;"[S]([O-])([O-])(Nc1[nH0]c([nH0]c(OC)c1)C)c1ccc(N)cc1";"Sulfamethomidine";294.37;-2.54;25;"TEST"
215;"[S]([O-])([O-])(Nc1[nH0]oc(C)c1)c1ccc(N)cc1";"Sulfamethoxazole";253.31;-2.62;25;"TEST"
216;"[S]([O-])([O-])(Nc1oc(C)c([nH0]1)C)c1ccc(N)cc1";"Sulfamoxole";267.34;-2.44;25;"TEST"
217;"[S]([O-])([O-])(NC(=O)C)c1ccc(N)cc1";"Sulfanilacetamide";214.27;-1.23;25;"TEST"
218;"[S]([O-])([O-])(N)c1ccc(N)cc1";"Sulfanilamide";172.23;-1.36;25;"TEST"
219;"[S]([O-])([O-])(Nc1[nH0]cccc1)c1ccc(N)cc1";"Sulfapyridine";249.32;-2.7;25;"TEST"
220;"[S]([O-])([O-])(Nc1[nH0]c([nH0]c(C)c1)C)c1ccc(N)cc1";"Sulfisomidine";278.37;-2.24;25;"TEST"
221;"Clc1cc(NC(=O)NC(=O)c2c(F)cccc2F)c(F)c(Cl)c1F";"Teflubenzuron";381.12;-7.28;26;"TEST"
222;"ClC=1C(=O)N(C(=O)NC=1C)C(C)(C)C";"Terbacil";216.69;-2.48;25;"TEST"
223;"[S-][P](SCSC(C)(C)C)(OCC)OCC";"Terbufos";288.48;-4.755;26;"TEST"
224;"O=C1C=C2CC[C@H]([C@@H](CC[C@H](OC(=O)C)[C@](C)(CC[C@@H]3([C@](C)(CC1)2))1)1)3";"Testosterone acetate";330.51;-5.184;26;"TEST"
225;"Clc1c(Cl)c(Cl)c(OC)c(O)c1Cl";"Tetrachloroguaiacol";261.91;-4.02;25;"TEST"
226;"O(C)CCOc1c(OC)cc(cc1OC)Cclc[nH0]c(N)[nH0]c1N";"Tetroxoprim";334.42;-2.1;25;"TEST"
227;"O=C1NC(=O)[C@@H](N2C(=O)c3cccc3C2=O)CC1";"Thalidomide";258.25;-2.676;26;"TEST"
228;"[S]([O-])([O-])(NC(=O)NN1CCCCC1)c1ccc(C)cc1";"Tolazamide";311.45;-3.68;25;"TEST"
229;"[S]([O-])([O-])(NC(=O)NC1CCCCC1)c1ccc(C)cc1";"Tolcyclamide";296.43;-4.21;25;"TEST"
230;"F[C@]([C@H](O)C[C@](C)([C@H](C[C@@H](OC(=O)C)[C@@](O)(C(=O)COC(=O)C)1)[C@H](CCC2=CC(=O)C=C[C@@](C)2)3)1)32";"Triamcinolone diacetate";478.56;-4.13;25;"TEST"
231;"Clc1cc2N[C@H](N[S]([O-])([O-])c2cc1[S]([O-])([O-])N)C(Cl)Cl";"Trichlormethiazide";380.68;-2.68;25;"TEST"
232;"Clc1[nH0]c([nH0]c([nH0]1)N(CC)CC)NCC";"Trietazine";229.75;-4.06;25;"TEST"
233;"FC(F)(F)c1cc([N](=O)[O-])c(N(CCC)CCC)c([N](=O)[O-])c1";"Trifluralin";335.32;-5.68;25;"TEST"
234;"Oclccc(cc1)CCN";"Tyramine";137.2;-1.12;25;"TEST"
235;"O=C(N)N";"Urea";60.07;0.96;25;"TEST"
236;"Clc1ccc2N(C)C(=O)CN=C(c2c1)c1cccc1";"Valium";284.75;-3.752;24;"TEST"
237;"O=C(O)C(CCC)CCC";"Valproic acid";144.21;-1.86;24;"TEST"
238;"O(C)c1ccc(cc1OC)CCN(C)CCC[C@@](C#N)(c1ccc(OC)c(OC)c1)C(C)C";"Verapamil";454.6;-4.69;24;"TEST"
239;"Clc1ccc2[nH0]3c([nH0][nH0]c3C)CN=C(c2c1)c1cccc1";"Xanax";308.77;-3.6;24;"TEST"
240;"Clc1cccc([N](=O)[O-])c1";"m-Chloronitrobenzene";157.56;-2.77;26;"TEST"
241;"O=C(Oc1cccc(C)c1)NC";"m-Tolyl methylcarbamate";165.21;-1.8;25;"TEST"
242;"O=C(O)NCCCCC";"n-Hexyl carbamate";145.2;-1.92;24;"TEST"

243;"OCCN(CCO)c1cccc1";"n-Phenyldiethanolamine";181.26;-0.73;25;"TEST"
244;"O=C(O)CCCC";"n-caproic acid";116.16;-1.053;24;"TEST"
245;"Clc1cccc1[N](=O)[O-]";"o-Chloronitrobenzene";157.56;-2.55;26;"TEST"
246;"O=C(OCCCC)N";"o-butyl carbamate";117.17;-0.66;25;"TEST"
247;"Clc1cccc1C(=O)O";"o-chlorobenzoic acid";156.57;-1.89;25;"TEST"
248;"O=C(OCC)N";"o-ethyl carbamate";89.11;0.85;25;"TEST"
249;"O=C(OC)N";"o-methyl carbamate";75.08;0.97;25;"TEST"
250;"O=C(O)c1cccc1C(=O)O";"o-phthalic acid";166.14;-2.11;25;"TEST"
251;"O=C(O)c1cccc1C";"o-toluic acid";136.16;-2.06;25;"TEST"
252;"O=C(C)c1ccc(N)cc1";"p-Aminoacetophenone";135.18;-1.61;25;"TEST"
253;"O=C(O)c1ccc(N)cc1";"p-aminobenzoic acid";137.14;-1.434;24;"TEST"
254;"O=C(c1cccc1)c1ccc(cc1)[C@H](O)C(=O)O";"p-benzoyl-r-mandelic acid";256.26;-1.514;24;"TEST"
255;"Fclccc(cc1)C(=O)O";"p-fluorobenzoic acid";140.12;-2.067;24;"TEST"
256;"ClCclccc(F)cc1";"p-fluorobenzyl chloride";144.58;-2.54;25;"TEST"
257;"Clc1ccc(OCC=O)c(C)c1";"(4-Chloro-2-methylphenoxy)acet";184.62;-2.23;24;"TEST"
258;"Clc1ccc(Cl)c(Cl)c1Cl";"1,2,3,4-tetrachlorobenzene";215.88;-4.57;25;"TEST"
259;"Clc1cc(Cl)c(Cl)c(Cl)c1";"1,2,3,5-tetrachlorobenzene";215.88;-4.63;25;"TEST"
260;"c1cc2CCCC3ccc4CCc1c4c23";"1,2,3,6,7,8-hexahydropyrene";208.32;-5.96;25;"TEST"
261;"Clc1cccc(Cl)c1Cl";"1,2,3-trichlorobenzene";181.44;-4;25;"TEST"
262;"I/C=CI";"1,2-diiodoethylene";279.84;-3.22;25;"TEST"
263;"Brclcc(Br)cc(Br)c1";"1,3,5-Tribromobenzene";314.79;-5.6;26;"TEST"
264;"Clc1cc(Cl)cc(Cl)c1";"1,3,5-trichlorobenzene";181.44;-4.48;25;"TEST"
265;"O1C2(C)CCC(CC2)C1(C)C";"1,8-Cineole";154.28;-1.74;26;"TEST"
266;"Ic1cccc2cccc12";"1-Iodonaphthalene";254.07;-4.55;26;"TEST"
267;"O=C1NC=2NC(=O)NC=2C(=O)N1C";"1-Methyluric acid";182.16;-1.56;25;"TEST"
268;"OCCCCCCCCCCCCCCCC";"1-Octadecanol";270.56;-8.4;26;"TEST"
269;"Nc1cccc2[nH]c3cccc3cc12";"1-aminoacridine";194.25;-4.22;25;"TEST"
270;"Brclccc(Cl)c1";"1-bromo-4-chlorobenzene";191.45;-3.63;25;"TEST"
271;"Oc1cccc2cccc12";"1-naphthol";144.18;-2.22;25;"TEST"
272;"Nc1cccc2cccc12";"1-naphthylamine";143.2;-1.92;25;"TEST"
273;"O=NN(CC)C(=O)N";"1-nitroso-1-ethylurea";117.13;-0.96;25;"TEST"
274;"S=C(N)Nc1cccc1";"1-phenylthiourea";152.24;-1.77;25;"TEST"
275;"Clc1cc(c(Cl)c(Cl)c1Cl)c1cc(Cl)c(Cl)c(Cl)c1Cl";"2,2?,3,3?,4,4?,5,5?-PCB";429.74;-9.16;25;"TEST"
276;"Clc1ccc(c(Cl)c1Cl)c1ccc(Cl)c(Cl)c1Cl";"2,2?,3,3?,4,4?-PCB";360.86;-8.01;25;"TEST"
277;"Clc1cc(Cl)c(cc1Cl)c1ccc(Cl)c(Cl)c1Cl";"2,2?,3,4,4?,5?-PCB";360.86;-8.32;25;"TEST"
278;"Clc1cc(Cl)c(c(Cl)c1Cl)c1cccc1Cl";"2,2?,3,4,6-PCB";326.42;-7.43;25;"TEST"
279;"Clc1ccc(Cl)c(c1)c1cccc(Cl)c1Cl";"2,2?,3,5?-PCB";291.98;-6.47;25;"TEST"
280;"[nH]1cccc1c1[nH]cccc1";"2,2?-bipyridine";156.2;-1.42;25;"TEST"
281;"Clc1cc(c2cccc2)c(Cl)c(Cl)c1Cl";"2,3,4,5-PCB";291.98;-7.16;25;"TEST"
282;"Clc1cc(O)c(Cl)c(Cl)c1Cl";"2,3,4,5-Tetrachlorophenol";231.88;-3.15;26;"TEST"
283;"Oc1cccc(C)c1C";"2,3-Xylenol";122.18;-1.43;25;"TEST"
284;"Clc1ccc(c(Cl)c1)c1ccc(Cl)c(Cl)c1";"2,3?,4,4?-PCB";291.98;-7.8;25;"TEST"
285;"Clc1cc(Cl)c(O)c(Cl)c1";"2,4,6-trichlorophenol";197.44;-2.34;25;"TEST"
286;"O=[N]([O-])c1ccc(O)c([N](=O)[O-])c1";"2,4-dinitrophenol";184.11;-2.7;24;"TEST"
287;"Oc1cc(C)ccc1C";"2,5-Xylenol";122.18;-1.54;25;"TEST"
288;"Clc1cccc(Cl)c1c1cccc1";"2,6-PCB";223.1;-5.21;25;"TEST"
289;"Oc1c(C)ccc1C";"2,6-Xylenol";122.18;-1.31;25;"TEST"
290;"Nc1[nH]c(c([nH]c(C)c1)C)";"2,6-dimethyl-4-pyrimidinamine";123.18;-1.28;25;"TEST"

291;"Sc1[nH0]cc2[nH0]cc[nH0]c2[nH0]1";"2-Mercaptopteridine";164.19;-
2.36;24;"TEST"
292;"O=C1N=C(Oc2cccc12)clcccc1";"2-Phenyl-3,1-benzoxazin-4-one";223.24;-
4.61;25;"TEST"
293;"Nc1ccc2cc3cccc3cc2c1";"2-aminoanthracene";193.26;-5.17;25;"TEST"
294;"O=C(O)c1cccc1N";"2-aminobenzoic acid";137.15;-1.52;25;"TEST"
295;"Clc1ccc2cccc2c1";"2-chloronaphthalene";162.62;-4.14;25;"TEST"
296;"N#CN=C(N)N";"2-cyanoguanidine";84.1;-0.31;25;"TEST"
297;"[nH0]1c2cccc2[nH]c1C";"2-methylbenzimidazole";132.18;-1.96;25;"TEST"
298;"O=[N]([O-])c1cccc1NC(=O)C";"2-nitroacetanilide";180.18;-1.91;25;"TEST"
299;"Sc1[nH0]ccc(O)[nH]1";"2-thiouracil";128.17;-2.26;25;"TEST"
300;"Clc1ccc(cc1Cl)c1cccc1Cl";"2?,3,4-PCB";257.54;-6.29;25;"TEST"
301;"Clc1ccc(N)cc1Cl";"3,4-dichloroaniline";162.02;-3.24;25;"TEST"
302;"Ic1cc(cc(I)c1O)C[C@@H](N)C(=O)O";"3,5-diiodotyrosine";432.99;-
2.963;24;"TEST"
303;"Clc1cccc(OC)c1";"3-Chloroanisole";142.59;-2.78;26;"TEST"
304;"Oc1c[nH0]ccc1";"3-Hydroxypyridine";95.11;-0.46;25;"TEST"
305;"O=C1NC(c2cccc2)(c2cccc2)C(=O)N1COC(=O)CCCCC";"3-
Octanoyloxymethylphenytoin";408.54;-6.523;26;"TEST"
306;"O=C1NC(c2cccc2)(c2cccc2)C(=O)N1COC(=O)CCCC";"3-
Pentanoyloxymethylphenytoin";366.45;-4.678;26;"TEST"
307;"O=C1NC(c2cccc2)(c2cccc2)C(=O)N1COC(=O)CC";"3-
Propanoyloxymethylphenytoin";338.39;-4.907;26;"TEST"
308;"O=C(O)N(C)c1cccc(C)c1";"3-Tolyl methylcarbamate";165.19;-1.8;24;"TEST"
309;"O=C1N=CN=CC1";"4(3H)-Pyrimidone";96.1;0.59;25;"TEST"
310;"[nH0]1ccc(cc1)c1cc[nH0]cc1";"4,4'-bipyridine";156.2;-1.54;25;"TEST"
311;"Clc1cc(O)c(OC)cc1Cl";"4,5-dichloroquaiacol";193.03;-2.53;25;"TEST"
312;"Oc1cc([nH0]c2cccc12)C";"4-Hydroxy-2-methylquinoline";159.2;-1.2;25;"TEST"
313;"Sc1[nH0]c[nH0]c2[nH0]cc[nH0]c12";"4-Mercaptopteridine";164.19;-
2.77;24;"TEST"
314;"O(C)c1[nH0]cc2[nH0]cc[nH0]c2[nH0]1";"4-Methoxypteridine";162.17;-
1.11;25;"TEST"
315;"S(C)c1[nH0]c[nH0]c2[nH0]cc[nH0]c12";"4-Methylthiopteridine";178.22;-
2.36;24;"TEST"
316;"O=C(NN)Nc1cccc1";"4-Phenylsemicarbazide";151.19;-2.33;25;"TEST"
317;"O=C(O)c1ccc(N)cc1";"4-aminobenzoic acid";137.15;-0.4;25;"TEST"
318;"Clc1ccc(NC(=O)C)cc1";"4-chloroacetanilide";169.62;-2.84;25;"TEST"
319;"Clc1ccc(cc1)c1cccc1";"4-chlorobiphenyl";188.66;-5.2;25;"TEST"
320;"Clc1ccc(O)cc1";"4-chlorophenol";128.56;-0.7;25;"TEST"
321;"Fc1ccc(NC(=O)C)cc1";"4-fluoroacetanilide";153.17;-1.78;25;"TEST"
322;"O=C(Nc1ccc(OC)cc1)C";"4-methoxyacetanilide";165.21;-1.3;25;"TEST"
323;"O=[N]([O-])c1ccc(OC)cc1";"4-nitroanisole";153.15;-2.41;25;"TEST"
324;"Oc1ccc2CCCCc2c1";"5,6,7,8-Tetrahydro-2-naphthol";148.21;-1.99;24;"TEST"
325;"O=C1NC(=O)C(CC)(CC=C(C)C)C(=O)N1";"5-(3-Methyl-2-butenyl)-5-
ethylbarbital";224.29;-2.253;26;"TEST"
326;"Cc1cc2cccc2c2ccc3cccc3c12";"5-Methylchrysene";242.33;-6.59;26;"TEST"
327;"O=C1NC=C(C)C(=O)N1";"5-methyluracil";126.13;-1.52;25;"TEST"
328;"Sc1[nH0]c[nH0]c2[nH0]c[nH]c21";"6-mercaptapurine";152.18;-3.089;24;"TEST"
329;"O(C)c1[nH0]c2[nH0]c[nH0]cc2[nH0]c1";"7-Methoxypteridine";162.15;-
0.91;24;"TEST"
330;"S(C)c1[nH0]c2[nH0]c[nH0]cc2[nH0]c1";"7-Methylthiopteridine";178.22;-
1.55;24;"TEST"