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Nm	PubChem SID	Test Substance CASRN	STRUCTURE_SMILES	Test Substance Chemical Name	BJ	Jurkat	Hek93	HepG2	MRC5	SK-N-SH	All tests
1	7851494	75070	CC=O	Acetaldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
2	7851498	103902	C1(=CC=C(C=C1)O)NC(C)=O	Acetaminophen (4-hydroxyacetanilide)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
3	7851499	968810	O=S(=O)(C1=CC=C(C=C1)C(=O)C)NC(=O)NC2CCCCC2	Acetohexamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
4	7851501	75058	CC#N	Acetonitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
5	7851507	114830	C1(NNC(C)=O)=CC=CC=C1	1-Acetyl-2-phenyl hydrazide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
6	7851515	107028	C=CC=O	Acrolein	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
7	7851521	107131	C=CC#N	Acrylonitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
8	7851523	50760	C12C(OC3=C(N=1)C(=CC=C3C)C(N[C@@H]4C(N[C@@H](C(N5[C@H](CCC5)C(N(CC(N([C@H](C(O[C@H]4C)C(=O)C(C)C)C(=O)C)=O)O)C(C)C)=O)=O)N)=O)C	Actinomycin D	Active	Active	Active	Inactive	Inactive	Inactive	Active
9	7851524	628944	NC(=O)CCCCC(=O)N	Adipamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
10	7851531	116063	CC(C=NOC(=O)NC)(SC)C	Aldicarb	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
11	7851532	309002	C1C(C(Cl)(Cl)C43Cl)(C(Cl)=C4Cl)C1C3C2=CC1C2	Aldrin	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
12	7851536	107186	C=CCO	Allyl alcohol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
13	7851537	107051	C=CCCI	Allyl chloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
14	7851538	106923	C=CCOCC1CO1	Allyl glycidyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
15	7851539	57067	C=CCN=C=S	Allyl isothiocyanate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
16	7851545	17026812	NC1=C(C=CC(=C1)NC(=O)C)OCC	3-Amino-4-ethoxyacetanilide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
17	7851549	82280	O=C1C2=C(C(=CC=C2C(=O)C3=C1C=CC=C3)C)N	1-Amino-2-methylanthraquinone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
18	7851554	99570	O=[N+](C1=CC(=C(C=C1)O)N)[O-]	2-Amino-4-nitrophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
19	7851555	121880	O=[N+](C1=CC(=C(C=C1)N)O)[O-]	2-Amino-5-nitrophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
20	7851556	119346	OC1=C(C=C(C=C1)N)[N+]=(O)[O-]	4-Amino-2-nitrophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
21	7851558	121664	O=[N+](C1=CN=C(S1)N)[O-]	2-Amino-5-nitrothiazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
22	7851560	117793	O=C1C2=CC(=CC=C2C(=O)C3=C1C=CC=C3)N	2-Aminoanthraquinone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
23	7851561	97563	CC1=C(C=CC=C1)N=NC2=CC(=C(C=C2)N)C	o-Aminoazotoluene	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
24	7851563	92671	NC1=CC=C(C=C1)C2=CC=CC=C2N12[C@@H]([C@@H](C1=O)(NC([C@H](C3=CC=CC=C3)N)=O)[H])(SC( Ampicillin trihydrate	4-Biphenylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
25	7851575	7177482	[C@@H]2C(O)=O)(C)C)[H]		Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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26	7851578	104461	CC=CC1=CC=C(C=C1)OC C1C=NC(=NC(=N1)NC2=CC=CC=C2Cl)Cl	Anethole	Inactive							
27	7851581	101053	NC1=CC=CC=C1	Anilazine	Inactive							
28	7851582	62533	C1(=CC=C(N)C=C1)OC	Aniline	Inactive							
29	7851585	20265978	NC1=C(C=CC=C1)C(=O)O	p-Anisidine hydrochloride	Inactive							
30	7851586	118923	OC=1[C@H](OC(=O)C=1O)[C@@H](O)CO	o-Anthranilic acid	Inactive							
31	7851598	50817	O=C([C@H](CC1=CC=CC=C1)NC(=O)[C@H](CC(=O)O)N)OC	L-Ascorbic acid	Inactive							
32	7851599	22839470	C1C=NC(=NC(=N1)NC(C)C)NCC N=C(C2=CC=C(N(C)C)C=C2)C1=C C=C(N(C)C)C=C1	Aspartame	Inactive							
33	7851604	1912249	NC1=NC(=O)N(C=N1)[C@@H]2O[C@H](CO)[C@H](O)[C@H]2O	Atrazine	Inactive							
34	7851606	2465272	NC1=NC(=O)N(C=N1)[C@@H]2O[C@H](CO)[C@H](O)[C@H]2O	Auramine	Inconclusive	Inconclusive	Inconclusive	Active	Inconclusive	Inconclusive	Inconclusive	Active
35	7851608	320672	O[C@H]([C@@H]2O)[C@@H](O)[C@@H]2CO)N(N=CC(N)=N1)C1=O	5-Azacytidine	Inactive	Active	Active	Inactive	Inconclusive	Active	Active	Active
36	7851609	3131600	O[C@H]([C@@H]2O)[C@@H](O)[C@@H]2CO)N(N=CC(N)=N1)C1=O	6-Azacytidine	Inactive							
37	7851611	446866	[O-] ][N+](C(N=C3)=C(SC1=NC=NC2=C 1NC=N2)N3C)=O	Azathioprine	Inactive	Active	Active	Inconclusive	Inactive	Active	Active	Active
38	7851614	86500	O=C1C2=C(C=CC=C2)N=NN1CSP(=S)(OC)OC	Azinphosmethyl	Inactive	Inactive	Inactive	Inactive	Inconclusive	Inconclusive	Inconclusive	Inconclusive
39	7851615	103333	C1(N=NC2=CC=CC=C2)=CC=CC=C1	Azobenzene	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Active
40	7851619	30516871	CC1=CN(C(=O)NC1=O)[C@H]2C[C@H](N=[N+]#[N-])[C@@H](CO)O2	3'-Azido-3'-deoxythymidine (AIDS)	Inactive							
41	7851626	100527	O=CC1=CC=CC=C1 NC1=CC=C(C2=CC=C(N)C=C2)C=C1	Benzaldehyde	Inactive							
42	7851629	92875	C1=COC2=C1C=CC=C2	Benzidine	Inactive							
43	7851633	271896	OC(=O)C1=CC=CC=C1	Benzofuran	Inactive							
44	7851635	65850	C1=CC=CC(=C1)C(C(C2=CC=CC=C2)=O)O	Benzoic acid	Inactive							
45	7851636	119539	O=C1C=CC(=O)C=C1	Benzoin	Inactive							
46	7851637	106514	N1=C(SSC2=NC3=C(C=CC=C3)S2) SC4=C1C=CC=C4	p-Quinone	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Active
47	7851638	120785	1,2,3-Benzotriazole	2,2'-Dithiobis-benzothiazole	Inactive							
48	7851639	95147	NC1=CC=C(C=CC=C2)N=N1	1,2,3-Benzotriazole	Inactive							
49	7851643	140114	CC(=O)OCC1=CC=CC=C1	Benzyl acetate	Inactive							
50	7851644	100516	OCC1=CC=CC=C1	Benzyl alcohol	Inactive							
51	7851645	100447	C1CC1=CC=CC=C1	Benzyl chloride	Inactive							
52	7851646	120321	OC1=C(C=C(C=C1)Cl)CC2=CC=CC=C2	o-Benzyl-p-chlorophenol	Inactive							
53	7851653	92524	C1=C(C=CC=C1)C2=CC=CC=C2	Biphenyl	Inactive							
54	7851660	111444	C1CCOCC1	Bis(2-chloroethyl)ether	Inactive							
55	7851685	33229344	C1(=C(C=CC(=C1)N(CC)CO)CC)NC CO)[N+](O-)=O	HC blue 2	Inconclusive	Inconclusive	Inconclusive	Inconclusive	Inactive	Inconclusive	Inconclusive	Inconclusive

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56	7851690	75274	C1C(Cl)Br	Bromodichloromethane	Inactive							
57	7851691	74964	CCBr	Bromoethane (ethyl bromide)	Inactive							
58	7851692	540512	OCCBr	2-Bromo-1-ethanol	Inactive							
59	7851697	85687	C1=(C(C=CC=C1)C(OCCCC)=O)C(OCC2=CC=CC=C2)=O	Butyl benzyl phthalate	Inactive							
60	7851698	109693	CCCCCCl	n-Butyl chloride	Inactive							
61	7851701	94268	C(C1=CC=C(C=C1)O)(=O)OCCCC	n-Butyl-p-hydroxybenzoate	Inactive							
62	7851708	128370	OC1=C(C=C(C=C1C(C)(C)C)C)C(C)	Butylated hydroxytoluene	Inactive							
63	7851712	1948330	CC(C)(C)c1cc(O)ccc1O	t-Butylhydroquinone	Inactive							
64	7851715	3068880	CC1CC(=O)O1	beta-Butyrolactone	Inactive							
65	7851724	58082	O=C1C2=C(N=CN2C)N(C(=O)N1C)C	Caffeine	Inactive							
66	7851733	404864	OC1=C(C=C(C=C1)CNC(=O)CCCCC=C(C(C)C)OC	Capsaicin	Inactive							
67	7851736	563417	C(NN)(N)=O	Semicarbazide hydrochloride	Inactive							
68	7851739	63252	O=C(OC1=C2C(=CC=C1)C=CC=C2)NC	Carbaryl	Inactive							
69	7851740	86748	C12C3=C(C=CC=C3)NC1=CC=CC=2	Carbazole	Inactive							
70	7851748	2244168	O=C1C[C@H](CC=C1C)C(C)=C	D-Carvone	Inactive							
71	7851749	120809	OC1=C(C=CC=C1)O	Catechol	Inactive	Active	Active	Inactive	Inactive	Inactive	Active	Inactive
72	7851754	133904	C1C1=C(C=C1C(=O)O)Cl)N	Chloramben	Inactive							
73	7851755	305033	C1CCN(C1=CC=C(C=C1)CCCC(=O)O)CCCI	Chlorambucil	Inconclusive	Active	Active	Inactive	Inconclusive	Inconclusive	Active	Inactive
74	7851757	56757	O=C(C(Cl)Cl)N[C@H](CO)[C@@H](C1=CC=C([N+](O-))=O)C=C1)O	Chloramphenicol	Inactive							
75	7851758	118752	O=C1C(=C(C(=O)C(=C1Cl)Cl)Cl)Cl	Chloranil	Active	Active	Inconclusive	Inconclusive	Inconclusive	Active	Active	Active
76	7851760	115286	C1C2(Cl)C1(Cl)C(Cl)=C(Cl)C2(Cl)C(C1C(O)=O)C(O)=O	Chlorendic acid	Inactive							
77	7851768	77439760	O=C1OC(O)C(C(Cl)Cl)=C1Cl	3-Chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone(MX)	Active	Active	Inconclusive	Inconclusive	Inconclusive	Active	Active	Active
78	7851772	88733	C1C1=C(C=CC=C1)[N+](=O)[O-]	2-Chloronitrobenzene	Inactive							
79	7851773	100005	O=[N+](C1=CC=C(C=C1)Cl)[O-]	4-Chloronitrobenzene	Inactive							
80	7851775	95830	NC1=C(C=CC=C1)Cl)N	4-Chloro-o-phenylenediamine	Inactive	Active	Inactive	Inconclusive	Inactive	Inactive	Inactive	Active
81	7851776	61702441	Nc1cc(Cl)c(N)cc1	2-Chloro-p-phenylenediamine sulfate	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive	Inconclusive	Inconclusive
82	7851778	95749	C1C1=C(C=CC=C1)N	3-Chloro-p-toluidine	Inactive							
83	7851779	95794	NC1=CC=C(C=C1)Cl	5-Chloro-o-toluidine	Inactive							
84	7851785	532274	O=C(C1=CC=CC=C1)CCI	2-Chloroacetophenone (CN)	Active	Active	Active	Inconclusive	Inconclusive	Active	Active	Active
85	7851786	140498	C1CC(=O)C1=CC=C(NC(=O)C)C=C1	4-(Chloroacetyl)acetanilide	Active	Active	Active	Active	Inconclusive	Active	Active	Active
86	7851787	106478	NC1=CC=C(C=C1)Cl	p-Chloroaniline	Inactive							
87	7851790	108907	C1C1=CC=CC=C1	Chlorobenzene	Inactive							
88	7851792	124481	C1C(Br)Br	Chlorodibromomethane	Inactive							

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89	7851798	67663	C1C(Cl)Cl	Chloroform	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
90	7851800	6959473	C1(C=CC=CN=1)CCI	2-Chloromethylpyridine hydrochloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
91	7851803	150685	O=C(N(C)C)NC1=CC=C(C=C1)Cl	Monuron	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
92	7851807	76062	C1([N+](=O)[O-])(Cl)Cl	Chloropicrin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
93	7851814	94202	O=S(=O)(C1=CC=C(C=C1)Cl)NC(=O)NCCC	Chlorpropamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
94	7851820	117102	O=C1C2=C(C=CC=C2O)C(=O)C3=CC=CC(=C13)O	Danthron	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
95	7851821	51481619	C1(CSCCNC(NC)=NC#N)=C(C)NC=N1	Cimetidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
96	7851824	77929	OC(CC(=O)O)(CC(=O)O)C(=O)O	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Active
97	7851840	91645	O=C1OC2=C(C=CC=C2)C=C1	Coumarin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
98	7851841	102501	COCC1=CC(=C(C=C1)N)C	m-Cresidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
99	7851842	120718	NC1=CC(=CC=C1OC)C	p-Cresidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
100	7851844	135206	C1(N(N=O)O)=CC=CC=C1	Cupferron	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
101	7851850	7585399	O[C@H]8[C@@H](O)[C@@H]1O[C@H](CO)[C@H]8O[C@H]7O[C@H](CO)[C@H](O)[C@H]6O[C@H](CO)[C@H](O)[C@H]5O[C@H](CO)[C@H](O)[C@H]4O[C@H](CO)[C@H](O)[C@H]3O[C@H](CO)[C@H](O)[C@H]2O[C@H](CO)[C@H](O)[C@H](O1)[C@H](O)[C@H]2O)[C@H](O)[C@H]3O[C@H](O)[C@H]4O)[C@H](O)[C@H]5O)[C@H](O)[C@H](O)[C@H]6O)[C@H](O)[C@H]7O	beta-Cyclodextrin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
102	7851851	108941	O=C1CCCCC1	Cyclohexanone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
103	7851858	427510	O=C1[C@H]3[C@H](C3)[C@@@](C)[C@H]4([H])[C@@@](C)[C@H]5([H])[C@](C)[C@]5(CC5)(C(C)=O)OC(C)=O)(C)CC4([H])C=C2Cl)(C)C2=C1	Cyproterone acetate	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inconclusive	Inconclusive	Inconclusive
104	7851861	4342034	O=C(N)C1=C(N=CN1)N=NN(C)C	Dacarbazine	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
105	7851862	1596845	O=C(CCC(=O)O)NN(C)C	Daminozide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
106	7851863	80080	O=S(=O)(C1=CC=C(C=C1)N)C2=C C=C(C=C2)N	4,4'-Sulfonyldianiline (Dapsone)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
107	7851864	53190	C1C(C(1=C(C=CC=C1)Cl)C2=CC=C(C=C2)Cl)Cl	o,p'-DDD	Inconclusive	Inconclusive	Inconclusive	Inactive	Inconclusive	Inconclusive	Inconclusive	Inconclusive
108	7851865	72548	C1C(C(1=CC=C(C=C1)Cl)C2=CC=C(C=C2)Cl)Cl	Tetrachlorodiphenylethane	Active	Inconclusive	Active	Inactive	Active	Active	Active	Active
109	7851867	50293	C1C(C(1=CC=C(C=C1)Cl)C2=CC=C(C=C2)Cl)Cl	Dichlorodiphenyltrichloroethane (DDT)	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
110	7851876	50022	OCC(=O)[C@H]4(O)[C@H](C)C[C@H]1[C@H]4(C)C[C@H](O)[C@H]2(F)[C@H]3(C)C=CC(=O)C=C3CC[C@H]12	Dexamethazone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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111	7851884	131179	O=C(C1=CC(C=CC=C1)C(=O)OCC=C)OCC=C	Diallyl phthalate	Inactive							
112	7851894	95807	NC1=C(C=CC(=C1)N)C	2,4-Diaminotoluene (2,4-toluene diamine)	Inactive							
113	7851899	333415	S=P(OC1=NC(=NC(=C1)C)C(C)C)(OCC)OCC	Diazinon	Inactive							
114	7851901	53703	C1=C2C=CC3=CC=CC=C3C2=CC4=CC=C5C(=C14)C=CC=C5	Dibenz(a,h)anthracene	Inactive							
115	7851905	96128	BrC(CCl)CBr	1,2-Dibromo-3-chloropropane	Inactive							
116	7851907	106934	BrCCBr	1,2-Dibromoethane	Inactive							
117	7851908	488415	O[C@H]([C@H](O)CBr)[C@H](O)[C@H](O)CBr	Dibromomannitol	Inactive							
118	7851918	99309	O=[N+](C1=CC(=C(C(=C1)Cl)N)Cl)[O-]	Dichloran	Inactive							
119	7851919	609201	NC1=C(C=C(C=C1Cl)N)Cl	2,6-Dichloro-p-phenylenediamine	Inactive							
120	7851920	79436	OC(=O)C(Cl)Cl	Dichloroacetic acid	Inactive							
121	7851922	95501	C1C=CC(=C1)Cl	1,2-Dichlorobenzene (o-dichlorobenzene)	Inactive							
122	7851925	612839	C1C=CC(C2=CC(Cl)=C(N)C=C2)=CC=C1N	3,3'-Dichlorobenzidine dihydrochloride	Inconclusive	Active	Inactive	Inactive	Inconclusive	Active	Active	Active
123	7851926	110576	C1CCC=CC1	trans-1,4-Dichloro-2-butene	Inactive							
124	7851929	75343	CC(Cl)Cl	1,1-Dichloroethane	Inactive							
125	7851930	107062	C1CCCC1	1,2-Dichloroethane	Inactive							
126	7851931	120832	C1C=CC(=C1)ClO	2,4-Dichlorophenol	Inactive							
127	7851934	94757	C1C=CC(=C1)OCC(=O)O	2,4-Dichlorophenoxyacetic acid	Inactive							
128	7851935	94804	C1C=CC(=C1)OCC(=O)OC CCC	Butyl(2,4-dichlorophenoxy) acetate	Inactive							
129	7851940	78875	CC(Cl)CCI	1,2-Dichloropropane (propylene dichloride)	Inactive							
130	7851941	62737	O=P(OC=C(Cl)Cl)(OC)OC	Dichlorvos	Inactive							
131	7851942	115322	OC(C1=CC=C(C=C1)Cl)(C2=CC=C(C=C2)Cl)C(Cl)(Cl)Cl	Dicofol	Inactive	Inconclusive	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
132	7851943	1212299	S=C(NC1CCCCC1)NC1CCCCC1 C1C2=C(Cl)C3(Cl)C1C4CC(C1C2(Cl)C3(Cl)Cl)C5OC45	N,N'-Dicyclohexylthiourea	Inconclusive	Inactive	Inconclusive	Inactive	Inactive	Inconclusive	Inconclusive	Inconclusive
133	7851945	60571		Dieldrin	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
134	7851950	2921882	S=P(OC1=NC(=C(C=C1)Cl)Cl)(OCC)OCC	Chlorpyrifos (Dursban)	Inactive							
135	7851954	111466	OCCOCCO	Diethylene glycol	Inactive							
136	7851957	56531	OC2=CC=C(C=C2)C(CC)=C(CC)C1=CC=C(O)C=C1	Diethylstilbestrol	Inactive	Active	Inconclusive	Inactive	Inactive	Inactive	Inactive	Active
137	7851958	105555	S=(NCC)NCC	N,N'-Diethylthiourea	Inactive							
138	7851966	119846	O=C1OC2=C(C=CC=C2)CC1	3,4-Dihydrocoumarin	Inactive							
139	7851972	828002	CC1CC(OC(O1)C)OC(=O)C	Dimethoxane	Inactive							
140	7851975	54150695	C1(=CC(=C1)OC)OC	2,4-Dimethoxyaniline hydrochloride	Inactive							
141	7851976	91930	COCl=C(C=CC(=C1)C2=CC(=C(C=C3'3'-Dimethoxybenzidine-4,4'-C2)N=C=O)OC)N=C=O	diisocyanate	Inactive							

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142	7851983	60117	CN(C1=CC=C(C=C1)N=NC2=CC=C C=C2)C	4-Dimethylaminoazobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
143	7851996	58151	O=C1N(C2=CC=CC=C2)N(C(=C1N( C)C)C)	4-Dimethylaminoantipyrine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
144	7851999	121697	CN(C1=CC=CC=C1)C CC1=C2C=CC=CC2=C(C3=CC=C4 C(=C13)C=CC=C4)C	N,N-Dimethylaniline 7,12-Dimethylbenzanthracene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
145	7852002	57976	O=C(N(C)C)Cl CC(C)=CCl	Dimethylcarbamoyl chloride Dimethylvinyl chloride (DMVC)	Active	Active	Active	Inactive	Active	Active	Active	Active
146	7852004	79447	OC1=C(C=C(C=C1)[N+](=O)[O-]) [N+] (=O)[O-]	2,4-Dinitrophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
147	7852012	513371	CC1=C(C=CC=C1[N+](=O)[O-]) [N+] (=O)[O-]	2,6-Dinitrotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
148	7852015	51285	CC1=C(C=CC=C1[N+](=O)[O-]) [N+] (=O)[O-]	N,N'-Diphenyl-p-phenylenediamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
149	7852020	606202	N(C1=CC=C(C=C1)NC2=CC=CC=C 2)C3=CC=CC=C3	5,5-Diphenylhydantoin (phenytoin)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
150	7852030	74317	O=C1C(C2=CC=CC=C2)(C3=CC=C C=C3)NC(=O)N1	2,5-Dithiobiurea	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
151	7852033	57410	CIC2=C(Cl)C3(Cl)C1COS(=O)OCC1 C2(Cl)C3(Cl)Cl	Endosulfan	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
152	7852037	142461	NC(=S)NNC(=S)N	Epichlorhydrin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
153	7852052	115297	CICC1CO1	1,2-Epoxybutane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
154	7852058	106898	Oc3cc4CC[C@H]1[C@H](CC[C@ ]2(C)[C@H](O)CC[C@H]12)c4c	17beta-Estradiol	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
155	7852061	106887	c3	Estragole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
156	7852065	50282	[H]C@]14[C@H]([C@]3([H])CC[C@ ]2(C)[C@H](O)CC[C@H]12)c4c	17beta-Estradiol	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive	Active	Inactive
157	7852067	140670	C=CCC1=CC=C(C=C1)OC [H]C@]14[C@H]([C@]3([H])CC[C@ ]2(C)[C@H](O)CC[C@H]12)c4c	Ethionamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
158	7852068	57636	CC2=CC(O)=CC=C12	Ethynodiolide	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive	Inactive	Inconclusive
159	7852069	536334	NC(=S)C1=CC=(NC=C1)CC	Ethionamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
160	7852073	938738	NC(=O)C1=C(C=CC=C1)OCC	2-Eethoxybenzamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
161	7852074	91532	CC1=CC(NC2=C1C=C(C=C2)OCC)( C)C	Ethoxyquin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
162	7852076	64175	CCO	Ethanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
163	7852079	105362	O=C(OCC)CBr	Ethyl bromoacetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
164	7852081	72560	C1C(C1=CC=C(C=C1)CC)C2=CC =C(C=C2)CC)Cl	Di(p-ethylphenyl)dichloroethane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
165	7852083	77838	CC1(C2=CC=CC=C2)C(O1)C(=O)O CC	Ethyl-3-methyl-3-phenylglycidate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
166	7852085	759739	NC(=O)N(CC)N=O	N-Ethyl-n-nitrosourea	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
167	7852088	100414	CCC1=CC=CC=C1	Ethylbenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
168	7852089	107211	C(CO)O	Ethylene glycol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
169	7852093	96457	S=C1NCCN1	Ethylene thiourea (ETU)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
170	7852096	106876	O1C2C1CCC(C2)C1CO1	4-Vinyl-1-cyclohexene diepoxide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
171	7852097	104767	CCC(CCCCC)CO	2-Ethylhexanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
172	7852098	103231	CCC(COC(=O)CCCCC(=O)OCC(CC) CC)CCCC	Di(2-ethylhexyl)adipate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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173	7852099	117817	O=C(C1=CC=C1)C(=O)OCC(CCCC)OC(O)CCCC	Di(2-ethylhexyl) phthalate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
174	7852108	470826	CC2(C)OC1(C)CCCC2CC1	1,8-Cineol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
175	7852109	97530	OC1=C(C=C(C=C1)CC=C)OC	Eugenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
176	7852111	140567	CN(C)c1ccc(N=NS(O)(=O)=O)cc1	Formulated fenaminosulf	Inactive	Inactive	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
177	7852112	55389	S=P(OC1=CC(=C(C=C1)SC)C)(OC)OC	Fenthion	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
178	7852120	2164172	O=C(NC1=CC=CC(=C1)C(F)(F)F)N(C)C	Fluometuron	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
179	7852126	51218	O=C1C(=CNC(=O)N1)F	5-Fluorouracil	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
180	7852138	110009	C1=CO=C1	Furan	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
181	7852139	98011	O=CC1=CC=CO1	Furfural	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
182	7852140	54319	NS(C1=C(Cl)C=C(NCC2=CC=CO2)C(C(O)=O)=C1)(=O)=O	Furosemide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
183	7852142	149917	OC(=O)C1=CC(=C(C(=C1)O)O)O	Gallic acid	Inactive	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
184	7852144	25812300	CC1=C(C=C(C=C1)OC)CCCC(C(=O)O)(C)C	Gemfibrozil	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
185	7852145	548629	C[N+](C)=C1C=CC(C=C1)=C(c2ccc(cc2)N(C)C)c3ccc(cc3)N(C)C	Hexamethyl-p-rosaniline chloride	Active	Active	Active	Active	Active	Active	Active	Active
186	7852148	77065	OC(=O)[C@H]3[C@H]51C[C@H]([O])[CC[C@H]1C@@H]24C=C[C@H]([O])[C@@H](C(C(=O)O)O)[C@@H]34)C(=C)C5	Gibberellic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
187	7852158	556525	OCC1CO1	Glycidol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
188	7852166	126078	O=C2C1=C(OC)C=C(OC)C(Cl)=C1O[C@H]32C(OC)=CC(C[C@H]3(C)C)H]=O	Griseofulvin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
189	7852170	517282	OC1=C(O)C=C4C(C[C@H](COC2=CC3=CC(O)=C2O)([C@@H]3[H])O)=C1	Hematoxylin C1	Inconclusive	Active	Inconclusive	Inactive	Inactive	Inconclusive	Active	
190	7852171	76448	C1C1C=CC2C1C3(Cl)C(Cl)=C(Cl)C2(Cl)C3(Cl)Cl	Heptachlor	Inconclusive	Inconclusive	Inconclusive	Inactive	Inactive	Inconclusive	Inconclusive	
191	7852173	111682	CCCCCCCN	Heptylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
192	7852175	87683	C1C(Cl)=C(Cl)C(Cl)=C(Cl)Cl	Hexachloro-1,3-butadiene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
193	7852180	77474	C1C1(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl	Hexachlorocyclopentadiene	Inactive	Active	Inactive	Active	Inactive	Inactive	Active	
194	7852181	67721	C1C(C(Cl)(Cl)Cl)(Cl)Cl	Hexachloroethane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
195	7852182	70304	OC1=C(C=C(C(=C1CC2=C(C(=CC(=C2Cl)Cl)Cl)O)Cl)Cl)Cl	Hexachlorophene	Inactive	Inconclusive	Inconclusive	Active	Inactive	Inconclusive	Active	
196	7852188	628024	NC(=O)CCCCC	Hexanamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
197	7852191	2078548	C1(C(C)C)=CC=CC(C(C)C)=C1O	Propofol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
198	7852202	122667	N(C1=CC=CC=C1)NC2=CC=CC=C2	Hydrazobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
199	7852205	58935	O=S1(=O)C2=C(C=C(C(=C2)S(=O)(=O)N)Cl)NCN1	Hydrochlorothiazide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
200	7852208	123319	OC1=CC=C(C=C1)O	Hydroquinone	Inactive	Active	Inconclusive	Inactive	Inactive	Inconclusive	Active	
201	7852232	53861	CC1=C(C2=C(C=CC(=C2)OC)N1C(=O)C3=CC=C(C=C3)Cl)CC(=O)O	Indomethacin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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231	7852379	91623	CC1=CC2=CC=CN=C2C=C1	6-Methylquinoline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
232	7852380	611325	CC1=CC=CC2=CC=CN=C12	8-Methylquinoline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
233	7852382	56042	CC1=CC(=O)NC(=S)N1	6-Methyl-2-thiouracil	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
234	7852384	443481	N1(C(=CN=C1C)[N+](=O)[O-])CCO	Metronidazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
235	7852393	79118	OC(=O)CCI	Monochloroacetic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
236	7852404	389082	O=C1C2=C(N=C(C=C2)C)N(C=C1C(=O)O)CC	Nalidixic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
237	7852405	91203	C1=C2C(=CC=C1)C=CC=C2	Naphthalene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
238	7852407	86873	OC(=O)CC1=C2C(=CC=C1)C=CC=C2	1-Naphthalene acetic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
239	7852408	2243621	NC1=C2C(=CC=C1)C(=CC=C2)N	1,5-Naphthalenediamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
240	7852409	1465254	C12C(=CC=CC=1NCCN)C=CC=C2	N-(1-Naphthyl)ethylenediamine dihydrochloride	Inactive	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
241	7852412	134327	NC1=CC=CC2=C1C=CC=C2	1-Naphthylamine	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Active
242	7852413	91598	NC1=CC2=C(C=CC=C2)C=C1	2-Naphthylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
243	7852422	54115	CN(CCC2)[C@@H]2[C@]1=CN=CC=C1	Nicotine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
244	7852431	139139	OC(=O)CN(CC(=O)O)CC(=O)O	Nitrilotriacetic acid (NTA)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
245	7852435	99592	O=[N+](C1=CC(=C(C=C1)OC)N)[O-]	5-Nitro-o-anisidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
246	7852436	59870	O=[N+](C1=CC=C(O1)C=NNC(=O)N)[O-]	Nitrofurazone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
247	7852449	5307142	NC1=C(C=C(C=C1)N)[N+](=O)[O-]	2-Nitro-p-phenylenediamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
248	7852450	99569	O=[N+](C1=CC(=C(C=C1)N)N)[O-]	4-Nitro-o-phenylenediamine	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
249	7852451	99558	O=[N+](C1=CC(=C(C=C1)C)N)[O-]	5-Nitro-o-toluidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
250	7852452	602879	O=[N+](C1=CC=C2C3=C1C=CC=C3CC2)[O-]	5-Nitroacenaphthene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
251	7852453	100016	O=[N+](C1=CC=C(C=C1)N)[O-]	p-Nitroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
252	7852454	91236	COC1=C(C=CC=C1)[N+](=O)[O-]	o-Nitroanisole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
253	7852455	619170	O=[N+](C1=CC(=C(C=C1)C(=O)O)N)[O-]	4-Nitroanthranilic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
254	7852456	98953	O=[N+](C1=CC=CC=C1)[O-]	Nitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
255	7852457	94520	O=[N+](C1=CC2=C(C=C1)NC=N2)[O-]	6-Nitrobenzimidazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
256	7852458	62237	OC(=O)C1=CC=C(C=C1)[N+](=O)[O-]	p-Nitrobenzoic acid	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
257	7852459	627054	[O-][N+](=O)CCCC	1-Nitrobutane	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
258	7852461	79243	O=[N+](CC)[O-]	Nitroethane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
259	7852464	67209	O=C1N(CC(=O)N1)N=CC2=CC=C(O2)[N+](=O)[O-]	Nitrofuranoin	Inactive	Active	Inconclusive	Inconclusive	Inactive	Inactive	Active
260	7852469	75525	[O-][N+](C)=O	Nitromethane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
261	7852470	86577	O=[N+](C1=C2C(=CC=C1)C=CC=C2)[O-]	1-Nitronaphthalene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
262	7852472	108032	O=[N+](CCC)[O-]	1-Nitropropane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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263	7852473	79469	CC([N+](=O)[O-])C	2-Nitropropane	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
264	7852519	1116547	O=NN(CCO)CCO	N-Nitrosodiethanolamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
265	7852520	55185	CCN(CC)N=O	N-Nitrosodiethylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
266	7852521	62759	CN(N=O)C	N-Nitrosodimethylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
267	7852522	86306	O>NN(C1=CC=CC=C1)C2=CC=CC=C2	N-Nitrosodiphenylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
268	7852523	156105	N(C1C=CC(=CC=1)N=O)C2=CC=C2	p-Nitrosodiphenylamine	Inconclusive	Active	Active	Inactive	Inconclusive	Active	Active	
269	7852552	100754	O>NN1CCCCC1	N-Nitrosopiperidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
270	7852586	101804	NC1=CC=C(C=C1)OC2=CC=C(C=C2)N	4,4'-Oxydianiline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
271	7852589	2058460	O=C1[C@](C(O)=C2[C@@@]3([H])[C@@@](O)(C)C4=C(C(O)=CC=C4)C2=O)(O)[C@](C[C@H]3O)([H])[C@H](N(C)C)C(O)=C1C(N)=O	Oxytetracycline hydrochloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
272	7852597	82688	C1C=C(C(=C1Cl)Cl)Cl)[N+](=O)[O-]	Pentachloronitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
273	7852598	87865	OC1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl	Pentachlorophenol, purified	Inactive	Active	Inconclusive	Inactive	Inactive	Inactive	Inactive	Active
274	7852608	62442	CC(=O)NC1=CC=C(C=C1)OCC	Phenacetin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
275	7852610	136403	NC1=CC=C(N=NC2=CC=CC=C2)C(N)=N1	Phenazopyridine hydrochloride	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
276	7852613	834286	C1(CCNC(NC(N)=N)=N)=CC=CC=C1	Phenformin hydrochloride	Inconclusive	Inactive	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
277	7852616	108952	OC1=CC=CC=C1	Phenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
278	7852617	77098	O=C1OC(C2=C1C=CC=C2)(C3=CC=C(C=C3)O)C4=CC=C(C=C4)O	Phenolphthalein	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
279	7852618	92842	N1C2=C(C=CC=C2)SC3=CC=CC=C13	Phenothiazine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
280	7852619	63923	C1CCN(C(COC2=CC=CC=C2)C)CC1=CC=CC=C1	Phenoxybenzamine hydrochloride	Inactive	Inconclusive	Inconclusive	Active	Inactive	Inconclusive	Active	
281	7852622	89258	O=C1N(C2=CC=CC=C2)N=C(C1)C	1-Phenyl-3-methyl-5-pyrazolone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
282	7852623	135886	C1=C2C(=CC=C1NC3=CC=CC=C3)C=CC=C2	N-Phenyl-2-naphthylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
283	7852628	50339	O=C1N(C2=CC=CC=C2)N(C3=CC=CC=C3)C(=O)C1CCCC	Phenylbutazone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
284	7852629	108452	NC1=CC(=CC=C1)N	m-Phenylenediamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
285	7852637	122601	O(C1=CC=CC=C1)CC2CO2	Phenyl glycidyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
286	7852643	90437	OC1=C(C=CC=C1)C2=CC=CC=C2	o-Phenylphenol	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
287	7852651	85449	O=C1C2=C(C=CC=C2)C(=O)O1	Phthalic anhydride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
288	7852658	51036	CCCC1=CC2=C(C=C1COCCOCCO)CCCCOCO2	Piperonyl butoxide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
289	7852677	53032	OCC(=O)[C@@@]3(O)CC[C@H]2[C@@H]4CCC1=CC(=C(C=C1)C(=O)O)[C@H]4C(=O)C[C@H]23C	Prednisone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
290	7852680	57669	O=S(=O)(C1=CC=C(C=C1)C(=O)O)N(CCC)CCC	Probenecid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
291	7852689	57578	O=C1CCO1	Propiolactone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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292	7852690	318989	OC(COC1=CC=CC2=C1C=CC=C2) CNC(C)C	Propranolol.HCl	Inactive							
293	7852701	51525	O=C1C=C(NC(=S)N1)CCC	6-Propyl-2-thiouracil	Inactive							
294	7852707	98964	NC(=O)C1=NC=CN=C1	Pyrazinamide	Inactive							
295	7852709	58140	NC1=C(C(=NC(=N1)N)CC)C2=CC=C(C=C2)Cl	Pyrimethamine	Inactive	Active	Active	Active	Inactive	Active	Active	Active
296	7852714	105113	ON=C1C=CC(=NO)C=C1 CC1=CC(C4=CC(C)=C(N=NC5=CC=C(OS(=O)(C6=CC=C(C)C=C6)=O) =C5)C=C4)=CC=C1N=NC2=C(O)C=CC3=CC(S(=O)(O)=O)=CC(S(=O)(O)=O)=C23	p-Benzoquinone dioxime	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Active
297	7852716	6459945	C.I. Acid red 114		Inconclusive	Inconclusive	Inconclusive	Inconclusive	Inactive	Inconclusive	Inconclusive	Inconclusive
298	7852729	50555	COc1cc(cc(OC)c1OC)C(=O)O[C@H]4C[C@H]5CN6CCC3=C(Nc2cc(OC)ccc23)[C@H]6C[C@H]5[C@H](C(=O)OC)[C@H]4OC	Reserpine	Inconclusive	Active	Inconclusive	Inconclusive	Inconclusive	Active	Active	Active
299	7852730	108463	OC1=CC(=CC=C1)O	Resorcinol	Inactive							
300	7852732	127479	CC1(C(=C(CCC1)C)=CC(=CC=CC(=CCOC(=O)C)C)C)	Retinol acetate	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Active
301	7852736	13292461	O=C1C(C2=C(C(O)=C3C)C(O)=C(NC(C)=CC=C[C@@H]5C)=O)C(C=NN4CCN(C)CC4)=C2O)=C3O[C@H](C)OC[C@H](C)[C@H](C)[C@H](O)OC[C@H](C)[C@H](C)O	Rifampicin	Inactive							
302	7852739	569619	C(C1=CC=C(C=C1)N)(C2=CC=C(C=C2)N)=C3C=CC(C=C3)=N	C.I. Basic red 9 monohydrochloride	Inconclusive	Active	Active	Active	Inconclusive	Inconclusive	Active	Active
303	7852746	94597	C=CCC1=CC=C2C(=C1)OCO2	Safrole	Inactive							
304	7852748	599791	C3=CC=CC(NS(=O)(=O)C2=CC=C(N=NC1=CC=C(O)C(C(O)=O)=C1)C=C2)=N3	Salicylazosulfapyridine	Inactive							
305	7852759	533313	OC1=CC2=C(C=C1)OCO2	Sesamol	Inactive							
306	7852769	110441	OC(=O)C=CC=CC	Sorbic acid	Inactive							
307	7852776	100425	C=CC1=CC=CC=C1	Styrene	Inactive							
308	7852778	96093	C1C(C2=CC=CC=C2)O1	Styrene oxide	Inactive							
309	7852779	108305	O=C1OC(=O)CC1	Succinic anhydride	Inactive							
310	7852781	95067	S=C(N(CC)CC)SCC(=C)Cl	Sulfallate	Inactive							
311	7852782	57681	O=S(=O)(C1=CC=C(C=C1)N)NC2=NC(=C(C=N2)C)C	Sulfamethazine	Inactive							
312	7852784	127695	C2=C(N)C=CC(S(=O)(=O)NC1ON=C(C)C=C2)	Sulfisoxazole	Inactive							
313	7852791	569573	C1C(=C(C1=CC=C(C=C1)OC)C2=C(C=C2)OC)C3=CC=C(C=C3)O	Chlorotriianisene	Inactive							
314	7852796	107357	NCCS(O)(=O)=O	L-Taurine	Inactive							
315	7852810	79345	C1C(Cl)ClCl	1,1,2,2-Tetrachloroethane	Inactive							

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316	7852812	961115	C1C=CC(Cl)=C(C(OP(=O)(OC)OC)=CCl)C=C1Cl	Tetrachlorvinphos	Inactive	Active	Inconclusive	Inactive	Inactive	Active	Active	Active
317	7852820	109999	C1CCCC1	Tetrahydrofuran	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
318	7852824	137268	S=C(N(C)C)SSC(=S)N(C)C	Tetramethylthiouram disulfide	Inconclusive	Active	Active	Active	Active	Active	Active	Active
319	7852826	509148	O=[N+](C([N+]([O-])([O-])[N+](=O)[O-])[N+](=O)[O-])	Tetranitromethane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
320	7852828	58559	O=C2C=1N=CNC=1N(C)C(=O)N2C	Theophylline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
321	7852829	148798	N1C(=NC2=C1C=CC=C2)C3=CSC=N3	Thiabendazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
322	7852833	96695	CC(C1=CC(=C(C=C1O)C)SC2=CC(=C(C=C2O)C(C)(C)C)C)OC1=C(C=C(C=C1SC2=C(C(=CC(=C2Cl)Cl)O)Cl)Cl	4,4-Thiobis(6-tert-butyl-m-cresol)	Active	Active	Active	Active	Active	Active	Active	Active
323	7852834	97187	C1=CC=C(C=C1)SC2=CC=C(C=C2)N	2,2'-Thiobis(4,6-dichlorophenol)	Inactive	Active	Active	Active	Inconclusive	Inconclusive	Active	Active
324	7852836	139651	4,4'-Thiodianiline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
325	7852838	79196	NC(=S)NN	Thiosemicarbazide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
326	7852840	62566	NC(=S)N	Thiourea	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
327	7852851	64777	O=S(=O)(C1=CC=C(C=C1)C)NC(=O)NCCCC	Tolbutamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
328	7852856	636215	NC1=CC=CC(C)=C1	o-Toluidine hydrochloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
329	7852860	8001352	C1C2(Cl)C1(Cl)C(=C)C(CCl)(CCl)C2(Cl)C(Cl)C1Cl	Toxaphene	Inconclusive	Active	Active	Inactive	Inactive	Active	Active	Active
330	7852865	396010	NC1=C2C(=NC(=N1)N)N=C(C(=N2)C3=CC=CC=C3)N	Triamterene	Inconclusive	Inconclusive	Active	Inconclusive	Inconclusive	Active	Active	Active
331	7852866	75252	BrC(Br)Br	Tribromomethane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
332	7852867	538238	O=C(OC(COC(=O)CCCCCCCC)COC(=O)CCCCCCCC)CCCCCCCC	Tricaprylin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
333	7852871	634935	NC1=C(C=C(C=C1Cl)Cl)Cl	2,4,6-Trichloroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
334	7852872	79005	C1C(Cl)Cl	1,1,2-Trichloroethane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
335	7852875	79016	C1C(=CCl)Cl	Trichloroethylene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
336	7852876	75694	FC(Cl)(Cl)Cl	Trichlorofluoromethane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
337	7852878	88062	OC1=C(C=C(C=C1Cl)Cl)Cl	2,4,6-Trichlorophenol	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
338	7852882	96184	C1CC(Cl)CCl	1,2,3-Trichloropropane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
339	7852883	1330785	O=P(OC2=CC=C(C)C=C2)(OC3=C C=C(C)C=C3)OC1=CC=C(C)C=C1	Tricresyl phosphate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
340	7852890	137177	CC1=CC(=C(C=C1C)N)C	2,4,5-Trimethylaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
341	7852903	115968	O=P(OCCC1)OCCCC1OCCCI	Tris(2-chloroethyl) phosphate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
342	7852906	78422	O=P(OCC(CCCCC)CC)(OCC(CCCCC)CC)OCC(CCCCC)CC	Tris(2-ethylhexyl)phosphate	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
343	7852918	57136	C(N)(N)=O	Urea	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
344	7852923	108054	CC(=O)OC=C	Vinyl acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
345	7852929	100403	C=CC1CCC=CC1	4-Vinylcyclohexene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
346	7852930	75354	C=C(Cl)Cl	Vinylidene chloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
347	7852939	1330207	CC1=C(C)C=CC=C1	Xylenes (mixed)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
348	7852950	52551674	OCCNC1=C(OCCO)C=C([N+]([O-])O)C=C1	HC Yellow 4	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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349	7852952	17924924	OC1=CC(=CC2=C1C(=O)O[C@H](CCCC(=O)CCCC=C2)C)O	Zearalenone	Inactive	Inconclusive	Active	Inactive	Inactive	Inconclusive	Active
350	7852974	67641	CC(=O)C	Acetone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
351	7852976	88993	OC(C1=CC=CC=C1C(O)=O)=O	Phthalic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
352	7852982	100470	N#CC1=CC=CC=C1	Benzonitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
353	7852983	140294	N#CCC1=CC=CC=C1	Phenylacetonitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
354	7852986	79083	O=C(O)CBr	Bromoacetic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
355	7852987	590170	BrCC#N	Bromoacetonitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
356	7852994	74975	CICBr	Bromochloromethane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
357	7853004	123728	CCCC=O	Butyraldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
358	7853007	78933	CCC(=O)C	Methyl ethyl ketone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
359	7853008	110167	O=C(O)C=CC(O)=O	Maleic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
360	7853009	110178	OC(C=CC(O)=O)=O	Fumaric acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
361	7853034	95578	OC1=CC=CC=C1Cl	o-Chlorophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
362	7853044	334485	CCCCCCCCCC(O)=O	Decanoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
363	7853052	3018120	N#CC(Cl)Cl	Dichloroacetonitrile	Inactive	Active	Inactive	Inconclusive	Inactive	Inactive	Active
364	7853071	431038	CC(C(C)=O)=O	2,3-Butanedione	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
365	7853085	111717	O=CCCCCC	n-Heptanal	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
366	7853088	111148	O=C(O)CCCCCC	n-Heptanoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
367	7853093	124049	OC(CCCCCC(O)=O)=O	Adipic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
368	7853105	99047	O=C(C1=CC(C)=CC=C1)O	m-Toluic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
369	7853106	99945	CC1=CC=C(C(O)=O)C=C1	p-Toluic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
370	7853109	116530	CC(CC)C(O)=O	Butanoic acid, 2-methyl-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
371	7853123	78842	CC(C)C=O	Isobutyraldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
372	7853125	598914	BrC(Br)[N+](=O)[O-]	Dibromonitromethane (water disinfection byproducts)	Inconclusive	Active	Inactive	Inconclusive	Inconclusive	Inconclusive	Active
373	7853130	57114	CCCCCCCCCCCCCCCC(O)=O	Stearic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
374	7853141	110623	CCCC=O	n-Pentanal	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
375	7853146	123386	CCC=O	Propionaldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
376	7853154	544638	O=C(O)CCCCCCCCCCCC	Tetradecanoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
377	7853160	545062	CIC(Cl)(Cl)C#N	Trichloroacetonitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
378	7853194	55210	C1=CC=CC=C1C(=O)N	Benzamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
379	7853198	58902	OC1=C(Cl)C(Cl)=C(Cl)C=C1Cl	2,3,4,6-Tetrachlorophenol	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Active
380	7853199	59507	OC1=CC(C)=C(Cl)C=C1	4-Chloro-m-cresol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
381	7853204	65452	C1(O)=CC=CC=C1C(=O)N	2-Hydroxybenzamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
382	7853207	67561	CO	Methanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
383	7853212	71410	CCCCO	1-Pentanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
384	7853213	71556	CC(Cl)(Cl)Cl	1,1,1-Trichloroethane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
385	7853222	78513	CCCCOCCOP(=O)(OCCOCCCC)OCCOCCCC	Tributoxyethyl phosphate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
386	7853223	78831	OCC(C)C	Isobutyl alcohol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
387	7853224	78900	NCC(N)C	Propylenediamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
388	7853225	78922	CC(O)CC	2-Butanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
389	7853227	79209	CC(=O)OC	Methyl acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
390	7853230	80466	C(C1C=CC(=CC=1)O)(CC)(C)C	p-tert-Pentylphenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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391	7853231	80524	C1CC(CCC1(N)C)C(C)(N)C O=C2C1=NC3=C(C=C(C)C(C)=C3) N(C[C@H](O)[C@H](O)[C@H](O)C O)C1=NC(N2)=O	p-Menthane-1,8-diamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
392	7853235	83885	N1=CC=CC2=C1C=CC=C2 OC1=C([N+]([O-])=O)C=CC=C1	Riboflavin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
393	7853238	84742	C1=CC=C(C(=O)OCCCC)C(=C1)C(=O)OCCCC	Dibutyl phthalate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
394	7853243	88755	OC1=C([N+]([O-])=O)C=CC=C1	o-Nitrophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
395	7853248	91225	N1=CC=CC2=C1C=CC=C2	Quinoline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
396	7853250	91667	CCN(CC)C1=CC=CC=C1	N,N-Diethyl aniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
397	7853257	95476	CC1=C(C)C=CC=C1	o-Xylene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
398	7853258	95487	OC1=C(C)C=CC=C1	o-Cresol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
399	7853259	95512	NC1=C(Cl)C=CC=C1	o-Chloroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
400	7853262	95761	NC1=CC(Cl)=C(Cl)C=C1	3,4-Dichloroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
401	7853264	96139	BrCC(Br)CO	2,3-Dibromo-1-propanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
402	7853267	96297	CCC(C)=NO	Methyl ethyl ketoxime	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
403	7853269	97029	NC1=C([N+]([O-])=O)C=C([N+]([O-])=O)C=C1	2,4-Dinitroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
404	7853270	97234	OC1=CC=C(Cl)C=C1CC2=CC(Cl)=CC=C2O	2,2'-Methylene-bis (4-chlorophenol)	Inconclusive	Inconclusive	Active	Active	Inconclusive	Inconclusive	Active	Active
405	7853272	98828	C1=CC=CC=C1C(C)C	Cumene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
406	7853275	99081	CC1=CC([N+]([O-])=O)C=CC=C1	m-Nitrotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
407	7853276	99978	CN(C)C1=CC=C(C)C=C1	N,N-Dimethyl-p-toluidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
408	7853280	100378	CCN(CCO)CC	(Diethylamino)ethanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
409	7853282	100618	C1=CC=C(NC)C=C1	N-Methyl aniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
410	7853283	100641	ON=C1CCCCC1	Cyclohexanone oxime	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
411	7853287	101848	C1=CC=CC=C1OC2=CC=CC=C2	Diphenyl oxide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
412	7853293	103833	CN(C)CC1=CC=CC=C1	N,N-dimethylbenzylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
413	7853297	104881	CIC1=CC=C(C=O)C=C1	4-Chlorobenzaldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
414	7853301	105679	OC1=C(C)C=C(C)C=C1	2,4-Dimethylphenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
415	7853304	106401	NC1=CC=C(Br)C=C1	p-Bromoaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
416	7853305	106423	CC1=CC=C(C)C=C1	p-Xylene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
417	7853307	106489	OC1=CC=C(Cl)C=C1	p-Chlorophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
418	7853309	106638	C=CC(=O)OCC(C)C	Isobutyl acrylate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
419	7853310	106945	BrCCC	1-Bromopropane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
420	7853313	107120	CCC#N	Propionitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
421	7853314	107153	NCCN	Ethylenediamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
422	7853315	107197	C(O)C#C	Propargyl alcohol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
423	7853320	108101	CC(=O)CC(C)C	Methyl isobutyl ketone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
424	7853323	108930	C1CCCCC1O	Cyclohexanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
425	7853324	108996	N1=CC(C)=CC=C1	beta-Picoline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
426	7853336	109897	CCNCC	Diethylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
427	7853348	110861	N1=CC=CC=C1	Pyridine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
428	7853349	110883	C1OCOCO1	S-Trioxane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
429	7853351	111159	CC(=O)OCCOCC	Ethylene glycol monoethyl ether acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
430	7853353	111262	CCCCCCN	Hexylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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431	7853354	111273	CCCCCCO	1-hexanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
432	7853355	111422	OCCNCCO	Diethanolamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
433	7853357	111693	N#CCCCCC#N	Adiponitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
434	7853360	111864	CCCCCCCCN	1-octanamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
435	7853361	111875	CCCCCCCO	1-octanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
436	7853372	117840	CCCCCCCCC(=O)C1=CC=CC=C1C(=O)OC	Diethyl phthalate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
437	7853373	118558	C1=CC=CC(O)=C1C(=O)OC2=CC=CC=C2	Phenyl salicylate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
438	7853375	118796	OC1=C(Br)C=C(Br)C=C1Br	2,4,6-Tribromophenol	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
439	7853376	119619	C1=CC=CC=C1C(=O)C2=CC=CC=C2	Benzophenone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
440	7853379	120821	C1C=C(Cl)C=C(Cl)C=C1	1,2,4-Trichlorobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
441	7853380	121142	CC1=C(C=C(C=C1)[N+](=O)[O-])[N+](=O)[O-]	2,4-Dinitrotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
442	7853381	121324	O=CC1=CC(OCC)=C(O)C=C1	Ethylvanillin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
443	7853382	121335	C1(C=O)=CC(OC)=C(O)C=C1	Vanillin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
444	7853383	121733	C1C=CC([N+](=O)[O-])=CC=C1	m-Chloronitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
445	7853386	122394	C1=CC=CC=C1NC2=CC=CC=C2	N-Phenylbenzenamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
446	7853387	122996	C1=CC=CC=C1OC	Ethylene glycol monophenyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
447	7853392	123864	CC(=O)OCCCC	n-Butyl acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
448	7853394	126738	CCCCOP(=O)(OCCCC)OCCCC	Tributyl phosphate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
449	7853396	127004	OC(C)CCI	1-Chloro-2-propanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
450	7853401	134623	CCN(CC)C(=O)C1=CC=CC(C)=C1	N,N-Diethyl-m-toluamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
451	7853406	141435	OCCN	Ethanolamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
452	7853407	141786	CC(=O)OCC	Ethyl acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
453	7853410	142289	CICCCCI	1,3-Dichloropropane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
454	7853418	150787	COCC1=CC=C(OC)C=C1	Hydroquinone dimethyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
455	7853421	298044	CCOP(OCC)(=S)SCCS	Disulfoton	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
456	7853448	525826	C1=CC=CC=C1C2=CC(=O)C3=CC=CC=C3O2	flavone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
457	7853450	529191	C1(C#N)=CC=CC=C1C	o-Tolunitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
458	7853451	529204	C1(C=O)=C(C)C=CC=C1	o-Tolualdehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
459	7853452	534521	OC1=C(C)C=C([N+]([O-])=O)C=C1[N+](O-)=O	4,6-Dinitro-o-cresol	Inactive	Inconclusive	Inconclusive	Inconclusive	Inactive	Inconclusive	Inconclusive
460	7853455	541731	C1C=CC(Cl)=CC=C1	1,3-Dichlorobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
461	7853476	608719	OC1=C(Br)C(Br)=C(Br)C(Br)=C1Br	Pentabromophenol	Inactive	Active	Inconclusive	Inactive	Inactive	Inactive	Active
462	7853483	619807	C1=CC([N+]([O-])=O)=CC=C1C(=O)N	p-Nitrobenzamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
463	7853486	621421	OC1=CC(NC(=O)C)=CC=C1	N-Acetyl-m-aminophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
464	7853490	625865	O1C(C)=CC=C1C	2,5-Dimethylfuran	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
465	7853503	693981	CC1=NC=CN1	2-Methylimidazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
466	7853518	818611	C=CC(=O)OCCO	2-propenoic acid, 2-hydroxyethyl ester	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inconclusive	Inconclusive
467	7853525	874420	O=CC1=C(Cl)C=C(Cl)C=C1	2,4-Dichlorobenzaldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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486	7854036	20830755	O=C1OCC(=C1)[C@H]2CC[C@@]8 (O)[C@]2(C)[C@H](O)C[C@H]3[C @H]8CC[C@@H]4C[C@H](CC[C@ ]34C)O[C@H]7O[C@H](C)[C@@ H](O[C@H]6C[C@H](O)[C@H](O[C @H]5C[C@H](O)[C@H](O)[C@@H] (C)O5)[C@@H](C)O6)[C@@H](O)C 7	Digoxin	Active	Active	Active	Active	Inactive	Active	Active
487	7854264	50215	C(O)(=O)C(C)O	Lactic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
488	7854266	134678174	[C@@H]1(O[C@H](CS1)N2C(N=C( C=C2)N)=O)CO	Lamivudine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
489	7854325	57534	NC(=O)OCC(C)(CCC)COC(N)=O	Meprobamate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
490	7854544	125337	C2(=O)C(C1=CC=CC=C1)(CC)C(=O)NCN2	Primidone (primaclone)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
491	7854570	91849	C2(OC)=CC=C(CN(CCN(C)C)C1=N C=CC=C1)C=C2	Pyrilamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
492	7854576	56542	[H][C@](C[C@@H](O)C1=C(C=C(OC )=C4)C4=NC=C1)(C[C@@H]2CC 3)N3C[C@@H]2C=C	Quinidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
493	7854582	68268	C1CCC(C)=C(C=CC(C)=CC=CC(C =CC)C1(C)C	All-trans retinol	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
494	7854583	36791045	n2[C@H]1[C@@H](C[C@H](O)[C@ H](O1)CO)O)nc(C(=O)N)nc2	Ribavirin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
495	7854634	144821	N(S(=O)(=O)C1=CC=C(N)C=C1)C2 =NN=C(C)S2	Sulfamethizole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
496	7854640	63741	O=S(N)(=O)c1ccc(N)cc1	Sulfanilamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
497	7854664	154427	SC1C(N=CN2)C2=NC(N)=N1	6-Thioguanine (6-TG)	Active	Active	Active	Active	Inactive	Active	Active
498	7854709	112243	NCCNCCNCCN	Triethylenetetramine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
499	7854718	738705	C2(OC)=C(OC)C=C(CC1=C(N)N=C( N)N=C1)C=C2OC	Trimethoprim	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
500	7854737	99661	C(=O)(O)C(CCC)CCC	Valproic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
501	7854751	7481892	N1(C(N=C(C=C1)N)=O)[C@@H]2O[ C@@H](CC2)CO	2',3'-Dideoxycytidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
502	7854754	26538443	Oc1cc(O)cc2CCCCC[C@@H](O)C CC[C@H](C)OC(=O)c12	Zearalanol	Inactive	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
503	7854760	446720	O=C(C(C(C=C3)=CC=C3O)=CO2)C 1=C2C=C(O)C=C1O	Genistein	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive	Inconclusive
504	7854762	486668	O=C1C(C3=CC=C(O)C=C3)=COC2 =C1C=CC(O)=C2	4',7-Dihydroxyisoflavone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
505	7854764	1806264	OC1=CC=C(CCCCCCCC)C=C1	Phenol, 4-octyl-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
506	7854781	789026	C1C=CC=C(C=1C(C(Cl)(Cl)Cl)C2=C C=C(C=C2)Cl)Cl	o,p'-DDT	Inactive	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
507	7854790	521186	O=C3C[C@H]4CC[C@@H]2[C@ H](CC[C@]1(C)[C@@H](O)CC[C@ H]12)[C@@]4(C)CC3	5alpha dihydrotestosterone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
508	7854795	58220	[C@]12([C@]([C@@]3(CCC4[C@ @]([C@@]([CC13[H])CCC(=O)C=4 C][H])(CC[C@H]2O)[H])C	beta testosterone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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509	7854806	68047063	OC3=CC=C(C=C3)C(CC)=C(C1=C C=CC=C1)C(C=C2)=CC=C2OCCN(C C)C	4-hydroxy-tamoxifen	Active	Active	Active	Active	Active	Active	Active
510	7854810	520365	C12C(C=C(OC=1C=C(C=C2O)O)C3 C=CC(=CC=3)O)=O	Apigenin	Inactive	Inconclusive	Inconclusive	Inactive	Inconclusive	Inconclusive	Inconclusive
511	7854823	131577	C1(C=O)C2C=CC=CC=2)C(CC(=C CC=1)OC)O	2-Hydroxy-4-methoxybenzophenone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
512	7854829	97541	OC1=CC=C(C=CC)C=C1OC	Isoeugenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
513	7854830	575439	C12=C(C=C(C=C1)C)C=CC=C2C	1,6-Dimethylnaphthalene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
514	7854832	94257	C(C1C=CC(=CC=1)N)(=O)OCCCC	n-Butyl-p-aminobenzoate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
515	7854834	101779	C1(N)C=CC(=CC=1)CC2=CC=C(C=CC2)N	Methylenedianiline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
516	7854840	126001	C(CCC(=O)O)(C1C=CC(=CC=1)O)( C2=CC=C(C=C2)O)C	Diphenolic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
517	7854842	81903	C1(=C(C(=O)O)C=CC=C1)C(C2=C C=C(C=C2)O)C3=CC=C(C=C3)O	phenolphthalin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
518	7854852	131113	C1(=C(C(=O)OC)C=CC=C1)C(=O)O C	Dimethyl phthalate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
519	7854866	50226	[C@]12([C@]([C@@]3[CCC4[C@] @]([C@@]([C@H](C1O)3[H])(CCC (=O)C=4)C)[H])(CC[C@H]2C(=O)C O)[H])C	corticosterone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
520	7854869	90006	C1(=C(CC)C=CC=C1)O	o-Ethyl phenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
521	7854892	1570645	C1(=C(C=CC(=C1)Cl)O)C	4-Chloro-o-cresol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
522	7854902	84695	C1(=C(C(OCC(C)C)=O)C=CC=C1)C (OCC(C)C)=O	Diisobutyl phthalate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
523	7854911	599644	C(C1=CC=C(C=C1)O)(C2C=CC=C C=2)(C)C	Phenol, 4-(1-methyl-1-phenylethyl)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
524	11075878	67634008	O=C(OCC=C)COCCC(C)C	(3-Methylbutoxy)acetic acid, 2-propenyl ester	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
525	11075879	821067	BrCC=CCBr	(E)-1,4-Dibromo-2-butene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
526	11075880	3322938	BrCC(Br)C(CCC(Br)C1Br)C1	1,2-Dibromo-4-(1,2-dibromoethyl)cyclohexane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
527	11075881	7779308	CCC(=O)C=C[CH]1C(=CCCC1(C)C)	1-(2,6,6-Trimethyl-2-cyclohexene-1-yl)-1-penten-3-one	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
528	11075882	119391	c1ccc2C=NNC(=O)c2c1	1(2H)-Phthalazinone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
529	11075883	630160	BrC(Br)(Br)CBr	1,1,1,2-Tetrabromoethane	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Active
530	11075884	79276	C(Br)(Br)C(Br)Br	1,1,2,2-Tetrabromoethane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
531	11075885	563586	CIC(Cl)=CC	1,1-Dichloropropene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
532	11075886	103504	O(Cc(cccc1)c1)Cc(cccc2)c2	1,1-Oxybis methylene, bis benzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
533	11075887	1703588	O=C(O)C(C(C(=O)O)CC(=O)O)CC(=O)O	1,2,3,4-Butanetetracarboxylic acid (8Cl) (9Cl)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
534	11075888	634662	Clc1c(Cl)ccc(Cl)c1Cl	1,2,3,4-Tetrachlorobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
535	11075889	91214	N(CCc(c1ccc2)c2)C1	1,2,3,4-Tetrahydro isoquinoline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
536	11075890	634902	Clc1c(Cl)cc(Cl)cc1Cl	1,2,3,5-Tetrachlorobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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537	11075891	87616	Clc1c(Cl)cccc1Cl	1,2,3-Trichlorobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
538	11075892	95943	Clc1cc(Cl)c(Cl)cc1Cl	1,2,4,5-Tetrachlorobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
539	11075893	41253218	C1=NC=N[N-]1	1,2,4-Triazole, sodium salt	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
540	11075894	622208	C(CSC1=CC=CC=C1)SC2=CC=CC=C2	1,1'-(1,2-Ethanediylbis(thio))bis-benzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
541	11075895	5493458	O=C(OCC(O1)C1)C(C(C(=O)OCC(O2)C2)CCC3)C3	1,2-Cyclohexanedicarboxylic acid, bis(oxyaryl methyl) ester	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inconclusive	Inconclusive	Inconclusive
542	11075896	147477	CC2(C)NC1=C(C(C)=C2)C=CC=C1	1,2-Dihydro-2,2,4-trimethylquinoline (monomer)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
543	11075897	26780961	CC2(C)NC1=C(C(C)=C2)C=CC=C1	1,2-Dihydro-2,2,4-trimethylquinoline (polymer)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
544	11075898	83410	CC1=CC=CC(=C1C)[N+](O-)=O	1,2-Dimethyl-3-nitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
545	11075899	99514	CC1=CC=C(C=C1C)[N+](O-)=O	1,2-Dimethyl-4-nitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
546	11075900	930223	C(=C)C1CO1	1,2-Epoxy-3-butene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
547	11075901	2404446	CCCCCCCC[CH]1CO1	1,2-Epoxydecane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
548	11075902	7320378	O(C1CCCCCCCCCCCCCCC)C1	1,2-Epoxyhexadecane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
549	11075903	3234284	O(C1)C1CCCCCCCCCCCC	1,2-Epoxytetradecane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
550	11075904	108703	c(cc1Cl)Cl)(c1)Cl	1,3,5-Trichlorobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
551	11075905	926578	CICC=C(Cl)C	1,3-Dichloro-2-butene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
552	11075906	96231	OC(CCl)CCl	1,3-Dichloro-2-propanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
553	11075907	542756	CIC=CCCI	1-Propene, 1,3-dichloro-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
554	11075908	538750	N(=C=NC1CCCCC1)C2CCCCC2	Dicyclohexylcarbodiimide	Inactive	Inconclusive	Inconclusive	Active	Inactive	Inactive	Inactive	Active
555	11075909	65558692	N=C1C2=C(C=C3C(C=CC=C3)=C2)C(N1)=N	1,3-Diiminobenz (f)-isoindoline	Active	Active	Inconclusive	Active	Inconclusive	Active	Active	Active
556	11075910	81209	[N+](O)(O-)c1c(C)cccc1C	1,3-Dimethyl-2-nitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
557	11075911	89872	CC1=CC(=C(C=C1)[N+](O-)=O)C	1,3-Dimethyl-4-nitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
558	11075912	99127	CC1=CC(=CC(=C1C)[N+](O-)=O)	1,3-Dimethyl-5-nitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
559	11075913	108098	NC(CC(C)C)C	1,3-Dimethylbutylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
560	11075914	606371	[N+](O)(O-)c1cc(cc2cccc12)[N+](O)(O-)	1,3-Dinitronaphthalene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
561	11075915	102067	N=C(Nc(cccc1c1)Nc(cccc2)c2	1,3-Diphenylguanidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
562	11075916	503300	C1COC1	1,3-Propylene oxide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
563	11075917	481403	OC1=CC=C(O)C2=C1C=CC=C2O	1,4,5-Trihydroxynaphthalene	Inactive	Active	Inconclusive	Inactive	Inactive	Inconclusive	Active	
564	11075918	110634	OCCCCO	1,4-Butanediol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
565	11075919	2425798	C(OCCCCOCC1CO1)C2CO2	1,4-Butanediol diglycidyl ether	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
566	11075920	89587	[O-][N+](c1cc(C)ccc1C)=O	1,4-Dimethyl-2-nitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
567	11075921	605710	[O-][N+](O)c2cccc1c2cccc1[N+](O-)=O	1,5-Dinitronaphthalene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
568	11075922	124094	C(CCN)CCCN	1,6-Hexanediamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
569	11075923	13048334	O=C(OCCCCCCOC(=O)C=C)C=C	1,6-Hexamethylene diacrylate	Inconclusive	Active	Inconclusive	Inactive	Inactive	Inactive	Active	Active
570	11075924	81550	OC1=CC=C(C2=C1C(=O)C3=C(C2=O)C(=CC=C3O)[N+](O-)=O)[N+](O-)=O	1,8-Dihydroxy-4,5-dinitroanthraquinone	Active	Active	Active	Active	Active	Active	Active	Active

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603	11075957	935955	Clc1c(Cl)cc(Cl)c(Cl)c1O	2,3,5,6-Tetrachlorophenol	Inactive	Active	Inconclusive	Inactive	Inactive	Inconclusive	Active
604	11075958	933788	Oc1cc(Cl)cc(Cl)c1Cl	2,3,5-Trichlorophenol	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
605	11075959	933755	Oc(c(ccc1Cl)Cl)c1Cl	2,3,6-Trichlorophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
606	11075960	600055	O=C(C(Br)CBr)O	2,3-Dibromopropionic Acid	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
607	11075961	616239	CICC(Cl)CO	2,3-Dichloro-1-propanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
608	11075962	78886	C(=C)(Cl)CCl	2,3-Dichloropropylene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
609	11075963	50453	OC(=O)c1cccc(Cl)c1Cl	2,3-Dichlorobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
610	11075964	3209221	[N+](=O)[O-]c1cccc(Cl)c1Cl	2,3-Dichloronitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
611	11075965	576249	Clc1c(Cl)cccc1O	2,3-Dichlorophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
612	11075966	2213630	Clc1nc2cccc2nc1Cl	2,3-Dichloroquinoxaline	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
613	11075967	4097227	Nc3ncn2c3ncn2[C@H]1CC[C@@H](CO)O1	2',3'-Dideoxyadenosine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
614	11075968	526750	Cc1c(C)cccc1O	2,3-Dimethyl phenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
615	11075969	79298	C(C(C)C)(C)C	2,3-Dimethylbutane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
616	11075970	602017	[O-][N+](C1=C([N+](O-)=O)C=CC=C1)O	2,3-Dinitrotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
617	11075971	87592	NC1=CC=CC(C)=C1C	2,3-Xyldidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
618	11075972	4938721	c1c(cc(c1)OCC(OCC(C)C=O)Cl)Cl)Cl	2,4,5-T isobutyl ester	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
619	11075973	89690	[N+](=O)[O-]c1cc(Cl)c(Cl)cc1Cl	2,4,5-Trichloronitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
620	11075974	95954	OC1=C(Cl)C=C(Cl)C(Cl)=C1	2,4,5-Trichlorophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
621	11075975	63213296	c(c(OCC)c(c1)OCC)c(OCC)c1C(=O)C	2,4,5-Triethoxyacetophenone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
622	11075976	18708708	O=[N+]([O-])c1c(Cl)cc(Cl)cc1Cl	2,4,6-Trichloronitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
623	11075977	13014181	C(Cl)(Cl)Cl)c1cc(Cl)cc1Cl	2,4,a,a,a-Pentachlorotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
624	11075979	25168267	O=C(COC1=C(Cl)C=C(Cl)C=C1)OC(C(CC)CCCC	2,4-D, Isooctyl ester, 67%	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
625	11075980	25152845	O=CC=CC=CCCCCC	2,4-Decadienal	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Active
626	11075981	554007	Clc1cc(Cl)ccc1N	2,4-Dichloroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
627	11075982	50840	C(=O)O)c1ccc(Cl)cc1Cl	2,4-Dichlorobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
628	11075983	611063	[N+](=O)[O-]c1ccc(Cl)cc1Cl	2,4-Dichloronitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
629	11075984	367259	Fc1cc(F)ccc1N	2,4-Difluoroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
630	11075985	446355	FC1=CC(F)=CC=C1[N+](O-)=O	2,4-Difluoronitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
631	11075987	483841	OC1=C2C=C(C=CC2=C(C=C1[N+](O-)=O)[N+](O-)=O)S(O)(=O)=O	8-Hydroxy-5,5-dinitro-2-naphthalenesulfonic acid (8Cl)(9Cl)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
632	11075988	142836	O=CC=CC=CC	2,4-Hexadienal	Inactive	Active	Inactive	Inactive	Inactive	Inconclusive	Active
633	11075989	625694	OC(CC(O)C)C	2,4-Pentanediol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
634	11075990	584849	O=C=NC1=CC(N=C=O)=CC=C1C	2,4-Toluene diisocyanate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
635	11075991	95681	Nc(cc(c1)C)C)c1	2,4-Xyldidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
636	11075992	95829	Nc(c(cc1Cl)Cl)c1	2,5-Dichloroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
637	11075993	50793	C(=O)O)c1cc(Cl)ccc1Cl	2,5-Dichlorobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
638	11075994	583788	Oc1cc(Cl)ccc1Cl	2,5-Dichlorophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
639	11075995	95874	Oc(c(cc1C)C)c1	2,5-Dimethyl phenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
640	11075996	110032	OC(CCC(O)(C)C)C	2,5-Hexanediol, 2,5-dimethyl-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
641	11075997	95783	Nc(c(cc1C)C)c1	2,5-Xyldidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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642	11075998	83385	Clc1cccc(Cl)c1C=O	2,6-Dichlorobenzaldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
643	11075999	50306	C(=O)(O)c1c(Cl)cccc1Cl	2,6-Dichlorobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
644	11076000	4659454	CIC(C1=C(Cl)C=CC=C1Cl)=O	2,6-Dichlorobenzoyl chloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
645	11076001	87650	Oc1c(Cl)cccc1Cl	2,6-Dichlorophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
646	11076002	576261	OC1=C(C=CC=C1C)C	2,6-Dimethyl phenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
647	11076003	91087	O=C=Nc(c(c(N=C=O)cc1)C)c1	2,6-Diisocyanatotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
648	11076004	823405	NC1=CC=CC(N)=C1C	1,3-Benzenediamine, 2-methyl-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
649	11076005	87627	Nc(c(ccc1)C)c1C	2,6-Xyldine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
650	11076006	1421632	C(=O)(CCC)c1cc(O)c(O)cc1O	2',4',5'-Trihydroxybutyrophenone	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive	Inconclusive	Inconclusive
651	11076007	1122629	CC(=O)c1ccccn1	2-Acetylpyridine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
652	11076008	24295032	O=C(C)C1=NC=CS1	2-Acetylthiazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
653	11076009	98373	Nc1cc(ccc1O)S(O)(=O)=O	2-Amino-1-phenol-4-sulfonic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
654	11076010	6358072	[N+](=O)([O-])c1cc(O)c(N)cc1Cl	2-Amino-4-chloro-5-nitrophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
655	11076011	19952477	NC2=Nc1c(Cl)cccc1S2	2-Amino-4-chlorobenzothiazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
656	11076012	95852	Nc1cc(Cl)ccc1O	2-Amino-4-chlorophenol	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
657	11076013	5464799	COc1c2c(SC(N)=N2)ccc1	2-Amino-4-methoxybenzothiazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
658	11076014	1477425	Cc1c2c(SC(N)=N2)ccc1	2-Amino-4-methylbenzothiazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
659	11076015	95841	Nc1cc(C)ccc1O	2-Amino-4-methylphenol	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inconclusive	Active
660	11076016	52253697	Nc1nc(cs1)c2ccccc2	2-Amino-4-phenylthiazole HBr H2O	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
661	11076017	29676719	C1(N=C(N)SC=1)CC(O)=O	2-Amino-4-thiazoleacetic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
662	11076018	29927080	Cc1cc2nc(N)sc2cc1C	2-Amino-5,6-dimethylbenzothiazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
663	11076019	94451	CCOc1ccc2nc(N)sc2c1	2-Amino-6-ethoxybenzothiazole	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
664	11076020	6285570	[O-][N+](=O)c1ccc2nc(N)sc2c1	2-Amino-6-nitrobenzothiazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
665	11076021	613138	Nc1ccc2cc3cccc3cc2c1	2-Aminoanthracene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
666	11076022	934327	NC(N2)=Nc1c2cccc1	2-Aminobenzimidazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
667	11076023	136958	Nc1nc2ccccc2s1	2-Aminobenzothiazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
668	11076024	90415	C1(C2=C(C=CC=C2N)(=CC=CC=C1)	2-Biphenylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
669	11076025	96504	s1c(N)nc1	2-Thiazolamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
670	11076026	24370250	N(C(N)=O)C1=Nc2ccccc2N1	Benzimidazol-2-ylurea	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
671	11076027	1817738	O=[N+](c1cc(Br)c(N)c([N+]([O-])=O)c1)[O-]	2-Bromo-4,6-dinitroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
672	11076028	2052075	Brc2ccccc2c1ccccc1	2-Bromobiphenyl	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
673	11076029	75263	BrC(C)C	2-Bromopropane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
674	11076031	594718	CC(Cl)([N+]([O-])=O)C	2-Chloro-2-nitropropane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
675	11076032	1929824	CIC(Cl)(C1=NC(Cl)=CC=C1Cl)	2-Chloro-6-(trichloromethyl)pyridine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
676	11076033	89985	O=Cc(c(ccc1)Cl)c1	2-Chlorobenzaldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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677	11076034	91587	C1C=CC1=CC=CC=C1C=C2	2-Chloronaphthalene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
678	11076035	930687	O=C1CCCC=C1	2-Cyclohexen-1-one	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
679	11076036	19780111	O=C(C(CC=CCCCCCCC)C1)OC1=O	(2-Dodecetyl)succinic anhydride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
680	11076037	110805	CCOCCCO	Ethylene glycol monoethyl ether (EGMEE)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
681	11076038	94962	OCC(C(O)CCC)CC	2-Ethyl-1,3-hexanediol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
682	11076039	123057	C(CC)(C=O)CCCC	2-Ethylhexanal	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
683	11076040	149575	O=C(O)C(CCCC)CC	2-Ethylhexanoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
684	11076041	103117	O=C(OCC(CCCC)CC)C=C	2-Ethylhexyl acrylate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
685	11076042	2461156	C(OCC(CC)CCCC)C1CO1	2-Ethylhexyl glycidyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
686	11076043	6197304	c(ccc1C(-c(ccc2)cc2)=C(C#N)C(=O)OCC(CC)CCCC)cc1	2-Ethylhexyl 2-cyano-3,3-diphenylacrylate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
687	11076045	104756	NCC(CCCC)CC	2-Ethylhexylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
688	11076046	21245023	O=C(OCC(CC)CCCC)C1=CC=C(N(C)C)C=C1	2-Ethylhexyl-p-dimethylaminobenzoate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
689	11076047	393522	C(Cl)(=O)c1ccccc1F	2-Fluorobenzoyl chloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
690	11076048	594616	O=C(C(O)(C)C)O	2-Hydroxyisobutyric acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
691	11076049	17376044	ICC-c(ccc1)cc1	Iodoethyl benzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
692	11076050	583391	S=C1Nc2cccc2N1	2-Mercaptobenzimidazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
693	11076051	105306	OCC(C)CCC	1-Pentanol, 2-methyl-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
694	11076052	4403616	N#CC(C)=CC	2-Methyl-2-butenenitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
695	11076053	637923	O(C(C)(C)C)CC	2-Methyl-2-ethoxypropane (etbe)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
696	11076054	603838	[N+](=O)[O-]c1cccc(N)c1C	2-Methyl-3-nitroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
697	11076055	1975504	O=[N+]([O-])c1cccc(C(O)=O)c1C	2-Methyl-3-nitrobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
698	11076056	99525	[N+]=(O)[O-]c1ccc(N)c(C)c1	2-Methyl-4-nitroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
699	11076057	13506768	O=C(O)c1ccccc1[N+](=O)[O-]	2-Methyl-6-nitrobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
700	11076058	527855	Cc1ccccc1C(N)=O	2-Methylbenzamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
701	11076059	78820	N#CC(C)C	2-Methylpropanenitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
702	11076060	96479	CC1OCCC1	2-Methyltetrahydrofuran	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
703	11076061	102818	OCCN(CCCC)CCCC	2-(Dibutylamino)ethanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
704	11076062	86000	O=[N+]([O-])c1ccccc1c2cccc2	2-Nitro-1,1'-biphenyl	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
705	11076063	119755	O=[N+]([O-])c1ccccc1Nc2cccc2	2-Nitrodiphenylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
706	11076064	625489	OCC[N+](=O)[O-]	2-Nitroethanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
707	11076065	26530201	O=C1=CSN1CCCCCCCC	2-Octyl-3-isothiazolone	Inactive	Active	Active	Inconclusive	Active	Active	Active	Active
708	11076066	13284429	N#CC=CCC	2-Pentenenitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
709	11076067	83261	C(=O)(C1C(=O)c2cccc2C1=O)C(C)C	2-Pivalyl-1,3-indandione	Inactive	Inconclusive	Inconclusive	Inconclusive	Inactive	Active	Active	Active
710	11076068	88186	OC1=C(C(C)(C)C)C=CC=C1	Phenol, 2-(1,1-dimethylethyl)-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
711	11076069	100696	C=CC1=CC=CC=N1	2-Vinylpyridine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
712	11076070	5397319	O(CC(CCCC)CC)CCCN	3-((Ethylhexyl)oxy)propylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
713	11076071	3268493	O=CCCSC	3-(Methylthio)propanal	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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714	11076072	16323436	OC(=O)C=CC1=CC=C(C=CC(O)=O)C=C1	3,3'-(1,4-Phenylene)bis-2-propenoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
715	11076074	54827177	Nc(c(cc(c(cc(c(N)c1C)C)c1)c2)C)c2C	3,3',5,5'-Tetramethylbenzidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
716	11076075	118569	O=C(OC1CC(C)CC(C)(C)C1)c2cccc2cO	3,3,5-Trimethylcyclohexyl salicylate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
717	11076076	2373980	Nc1c(O)cc(c2cc(O)c(N)cc2)cc1	3,3'-Dihydroxybenzidine	Inactive	Active	Inconclusive	Inactive	Inactive	Inactive	Inactive	Active
718	11076077	119904	O(c(c(N)ccc1c(ccc(N)c2OC)c2)c1)C	3,3'-Dimethoxybenzidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
719	11076078	119937	NC1=C(C=C(C2=CC(C)=C(N)C=C2)C=C1)C	3,3'-Dimethylbenzidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
720	11076079	1119626	O=C(CCSSCCC(O)=O)O	3,3-Dithiodipropionic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
721	11076080	20098480	[O-][N+](=O)C1=CC(=C(Cl)C(=C1)Cl)Cl	3,4,5-Trichloronitrobenzene	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
722	11076081	609198	Oc1cc(Cl)c(Cl)c(Cl)c1	3,4,5-Trichlorophenol	Inactive	Inconclusive	Inconclusive	Active	Inactive	Inconclusive	Active	
723	11076082	13014249	C(Cl)(Cl)(Cl)c1ccc(Cl)c(Cl)c1	a,a,a,3,4-Pentachlorotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
724	11076083	496720	Nc1cc(C)ccc1N	3,4-Diaminotoluene	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Active
725	11076084	6287383	Clc1ccc(C=O)cc1Cl	3,4-Dichlorobenzaldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
726	11076085	51445	C(=O)(O)c1ccc(Cl)c(Cl)c1	3,4-Dichlorobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
727	11076086	99547	[N+](=O)[O-]c1ccc(Cl)c(Cl)c1	3,4-Dichloronitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
728	11076087	95772	Clc1cc(O)ccc1Cl	3,4-Dichlorophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
729	11076088	102363	O=C=NC1=CC(Cl)=C(Cl)C=C1	3,4-Dichlorophenyl isocyanate	Inactive	Inconclusive	Active	Inconclusive	Inconclusive	Inconclusive	Inconclusive	Active
730	11076089	95658	OC1=CC(C)=C(C)C=C1	3,4-Dimethyl phenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
731	11076090	610399	[O-][N+](C1=CC=C(C)C=C1[N+])([O-])=O	3,4-Dinitrotoluene	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
732	11076091	95647	Cc1cc(N)ccc1C	3,4-Xyldine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
733	11076092	626437	NC1=CC(Cl)=CC(Cl)=C1	3,5-Dichloroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
734	11076093	51365	OC(=O)c1cc(Cl)cc(Cl)c1	3,5-Dichlorobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
735	11076094	591355	Oc1cc(Cl)cc(Cl)c1	3,5-Dichlorophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
736	11076095	108689	Cc1cc(C)cc(O)c1	3,5-Dimethyl phenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
737	11076096	108690	Cc1cc(C)cc(N)c1	3,5-Xyldine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
738	11076097	10599709	O=C(C)C1=C(C)OC(C)=C1	3-Acetyl-2,5-dimethylfuran	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
739	11076098	98168	FC(F)(F)c(ccc1N)c1	3-Amino-a,a,a-trifluorotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
740	11076099	627189	OCCCBr	3-Bromo-1-propanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
741	11076100	1522925	C(CBr)(CBr)(CBr)CO	3-Bromo-2,2-bis(bromomethyl)propanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
742	11076101	3132998	O=CC1=CC(Br)=CC=C1	3-Bromobenzaldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
743	11076102	2113577	Brc1cccc(c1)c2cccc2	3-Bromobiphenyl	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
744	11076103	563473	CC(=C)CCI	3-Chloro-2-methylpropene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
745	11076104	87605	Nc(c(cc1Cl)C)c1	3-Chloro-o-toluidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
746	11076106	542767	N#CCCCI	3-Chloropropionitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
747	11076107	91689	N(CC)(CC)c1cccc(O)c1	3-Diethylaminophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
748	11076108	99070	N(C)(C)c1cccc(O)c1	3-Dimethylaminophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
749	11076109	120376	Oc(ccc(c1NCC)C)c1	3-Ethylamino-4-methylphenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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750	11076110	101188	Oc2cccc(Nc1ccccc1)c2	3-Hydroxy-N-phenylaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
751	11076111	5437387	O=[N+]([O-])c1c(ccc1C)C(O)=O	3-Methyl-2-nitrobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
752	11076112	3113711	O=[N+]([O-])c1ccc(cc1C)C(O)=O	3-Methyl-4-nitrobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
753	11076113	98464	C(F)(F)(F)c1cccc(c1)[N+](=O)[O-]	3-Nitro-a,a,a-trifluorotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
754	11076114	4635874	N#CCC=CC	3-Pentenenitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
755	11076115	121391	C(=O)(OCC)C1OC1c2cccc2	Ethyl 3-phenylglycidate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
756	11076116	17369594	O=C(Oc1cccc2)=CCC)c12	3-Propylenephthalide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
757	11076117	3446897	O=CC1=CC=C(SC)C=C1	4-(methylthio)benzaldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
758	11076118	1761713	NC1CCC(CC2CCC(N)CC2)CC1	4,4'-Diaminodicyclohexylmethane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
759	11076120	101688	O=C=NC1=CC=C(CC2=CC=C(N=C=O)C2)C=C1	4,4'-Diphenylmethane diisocyanate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
760	11076121	584134	NN1C=NN=C1	4-amino-1,2,4-triazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
761	11076122	6219892	Oc2ccc(Nc1cc(C)c(N)cc1)cc2	4-Amino-4'-hydroxy-3-methyl-diphenylamine	Inactive	Active	Active	Inconclusive	Inactive	Active	Active	Active
762	11076123	63058	O=C3C=C4CC[C@H]2[C@H](CC[C@]1(C)C(=O)CC[C@H]12)[C@@H]4(C)CC3	Androstenedione	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
763	11076125	92660	Brc1ccc(cc1)c2cccc2	4-Bromobiphenyl	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
764	11076126	619669	O=C(O)C1=CC=C(C=O)C=C1	Benzoic acid, 4-formyl-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
765	11076127	89634	NC1=C([N+]([O-])=O)C=C(Cl)C=C1	4-Chloro-2-nitroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
766	11076128	393759	[N+]=(O)[O-])c1cc(cc([N+]=(O)[O-])c1Cl)C(F)(F)F	4-Chloro-3,5-dinitro-a,a,a-trifluorotoluene	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Active
767	11076129	121175	O=[N+]([O-])c1cc(ccc1Cl)C(F)(F)F	4-Chloro-3-nitro-a,a,a-trifluorotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
768	11076130	98566	C(F)(F)c1ccc(Cl)cc1	p-Chloro-a,a,a-trifluorotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
769	11076131	203645	c12c3cccc2Cc4cccc(cc3)c14	Cyclopentaphenanthrene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
770	11076132	65646686	O=C(NC2=CC=C(O)C=C2)C=C(C)C=CC=C(C)C=CC1=C(C)CCCC(C)1C	4-(hydroxyphenyl)retinamide	Active	Active	Active	Active	Active	Active	Active	Active
771	11076133	97325	C(=O)(Nc1ccccc1)c2ccc(OC)c(c2)[N+]=(O)[O-]	4-Methoxy-3-nitro-N-phenylbenzamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
772	11076134	693958	CC1=CSC=N1	4-Methylthiazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
773	11076135	89623	[O-][N+](c1cc(C)ccc1N)=O	4-Methyl-2-nitroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
774	11076136	119324	[O-][N+](c1cc(N)ccc1C)=O	4-Methyl-3-nitroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
775	11076137	96980	O=[N+]([O-])c1cc(ccc1C)C(O)=O	4-Methyl-3-nitrobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
776	11076138	822366	CC1=CNC=N1	4-Methylimidazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
777	11076139	41122707	CCCCCCc1ccc(cc1)c2ccc(C#N)cc2	4-n-Hexyl-4'-cyanobiphenyl	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
778	11076140	5131588	[N+]=(O)[O-])c1ccc(N)cc1N	4-Nitro-1,3-benzenediamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
779	11076141	3682197	[O-][N+]=(O)c1ccc2c(c1)C(=O)NNC2=O	6-Nitrophthalhydrazide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
780	11076142	5466842	O=C1OC(=O)c2ccc(cc12)[N+]=(O)[O-]	4-Nitrophthalic anhydride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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781	11076143	89407	O=C1NC(=O)c2ccc([N+](=[O-])=O)cc12	4-Nitrophthalimide	Inactive	Inactive						
782	11076144	592518	N#CCCC=C	4-Pentenenitrile	Inactive	Inactive						
783	11076145	38716686	O=C(CNC(C1=CC=C(CO)O1)=O)O	5-(Hydroxymethyl) furoyl glycine	Inactive	Inactive						
784	11076146	67470	O=CC1=CC=C(CO)O1	5-(Hydroxymethyl)-2-furural	Inactive	Inactive						
785	11076147	6338416	OC(C1=CC=C(CO)O1)=O	5-(Hydroxymethyl)-2-furoic acid	Inactive	Inactive						
786	11076148	2107768	CC1=CC(=O)OC2=C1C(=CC(=C2)O)O	5,7-Dihydroxy-4-methylcoumarin	Inactive	Inactive						
787	11076149	6201872	O=S(O)(=O)c1cc(N)cc(C(O)=O)c1O	5-Amino-3-sulfosalicylic acid	Inactive	Inactive						
788	11076150	2835952	Oc(c(cc1N)C)c1	5-Amino-o-cresol	Inactive	Inactive						
789	11076151	89576	C(=O)(O)c1cc(N)ccc1O	5-Aminosalicylic acid	Inactive	Inactive						
790	11076152	59143	O=C(NC2=O)N(C=C2Br)[C@H]1[C@H]1O[C@H]1CO	5-Bromo-2'-deoxyuridine (BRDU)	Inactive	Inactive						
791	11076153	2818691	Clc1ccc2NC(C)=Nc2c1	5-Chloro-2-methyl-1H-benzimidazole	Inactive	Inactive						
792	11076154	484208	O(C)c1c2C=COc2cc3OC(=O)Cc13	5-Methoxysoralen	Inactive	Inactive						
793	11076155	578461	[N+]([O-])c1ccc(C)cc1N	5-Methyl-2-nitroaniline	Inactive	Inactive						
794	11076156	6088513	Oc4ccc3cc(SSc2ccc1cc(O)ccc1c2)cc3c4	DDD (6-hydroxy-2-naphthyl disulfide)	Active	Active	Active	Inactive	Active	Active	Active	Active
795	11076157	6112761	Sc2ncnc1NC=Nc12	6-Mercaptopurine monohydrate	Active	Active	Active	Active	Inactive	Active	Active	Active
796	11076158	1747600	NC2=Nc1c(S2)cc(OC)cc1	6-Methoxy-2-benzothiazolamine	Inactive	Inactive						
797	11076159	92488	c1c(C)cc2C=CC(=O)Oc2c1	Methyl coumarin	Inactive	Inactive						
798	11076160	91441	CC1=CC(=O)Oc2cc(ccc12)N(CC)C	7-Diethylamino-4-methylcoumarin	Inactive	Inactive						
799	11076161	612602	Cc1cc2ncccc2cc1	7-Methylquinoline	Inactive	Inactive						
800	11076162	148243	OC1=CC=CC2=CC=CN=C12	8-Hydroxyquinoline	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Active	Active
801	11076163	52417228	Nc1c3cccc3nc2cccc12	9-Aminoacridine, monohydrochloride, monohydrate	Inconclusive	Active	Inconclusive	Inconclusive	Active	Active	Active	Active
802	11076164	602608	c1cc2c([N+](=O)[O-])c3cccc3cc2cc1	9-Nitroanthracene	Inactive	Inactive						
803	11076165	14375452	OC(C(C)=C1)(C=CC(C)=CC(O)=O)C(C)(C)C1=O	Abscisic acid	Inactive	Inactive						
804	11076166	55589623	O=S([N-]C1=O)(OC(C)=C1)=O	Acesulfame potassium	Inactive	Inactive						
805	11076167	105577	CCOC(C)OCC	Acetal	Inactive	Inactive						
806	11076168	108247	O=C(OC(=O)C)C	Acetic anhydride	Inactive	Inactive						
807	11076169	102012	O=C(Nc(ccc1c1)CC(=O)C	Acetoacetanilide	Inactive	Inactive						
808	11076170	34256821	CICC(=O)N(COCC)c1c(C)cccc1CC	Acetochlor	Active	Active	Inconclusive	Inconclusive	Inconclusive	Inconclusive	Inconclusive	Active
809	11076171	110134	O=C(CCC(C)=O)C	2,5-Hexanedione	Inactive	Inactive						
810	11076172	81397673	O=C(C)O[C@H]1[C@H]2[C@H]([C@H]2C(=O)CC[C@H]2C)=O	Acetoxyvalerenic Acid C(C)C1	Inactive	Inactive						

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811	11076173	50782	OC(=O)C1=C(C=CC=C1)OC(=O)C	Acetylsalicylic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
812	11076174	79061	NC(=O)C=C	Acrylamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
813	11076175	18642449	O[C@H]1[C@H](OC3[C@@](C)(C)[C@@]4([H])[C@@](CC3)(C7)[C@]27[C@](CC4)([H])[C@@](C[C@H]6[C@@H]5[C@H](C)C[C@]8(OC(Actein O)[C@@]9(C)[C@@H]8O9)O6)(C)[C@@]5(C)CC2)OC[C@@H](O)[C@@H]1O		Inactive	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inconclusive	
814	11076176	25316409	OC[C@@](C[C@@](C[C@@H](C4=C(C(C2=C(C=CC=C23)OC)=O)=C(C(O)=C4C5)C3=O)O)[C@H](O)C[C@@H](C)[C@@H]1C)ON5O)=O	Adriamycin, hydrochloride	Active	Active	Active	Inactive	Inconclusive	Active	Active	
815	11076177	1646873	O=C(NC)ON=CC(C)(C)S(C)=O	Aldicarb sulfoxide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
816	11076178	2243767	O=C(O)c1cc(ccc1O)N=Nc2ccc(cc2)[N+](O-)=O	Alizarin Yellow R, free acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
817	11076179	591877	O=C(OCC=C)C	Allyl acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
818	11076180	7493632	O=C(OCC=C)c1cccc1N	Allyl anthranilate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
819	11076181	106956	BrCC=C	Allyl bromide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
820	11076182	7493723	CCCCCCCC(=O)OCC=C	Allyl nonanoate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
821	11076183	109579	NC(=S)NCC=C	Allyl thiourea	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
822	11076184	98873	c(ccc1)(c1)C(Cl)Cl	alpha,alpha-Dichlorotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
823	11076185	100390	BrCc(ccc1)c1	alpha-Bromotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
824	11076186	10016203	OC[C@@H]2[C@H](O)[C@H](O)[C@H](O)[C@H]4[C@H](O)[C@H](O)[C@H]7O[C@H](O)[C@H]7O[C@H]6[C@H](O)[C@H](O)[C@H](O)[C@H]6O)O5(CO)CO)[C@H](O)[C@H]4O)CO)O[C@H]1[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H]3O[C@H]5[C@H](O)[C@H]3O)CO)[C@H](CO)O1	alpha-Cyclodextrin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
825	11076187	532285	C(O)(C#N)c1ccccc1	alpha-Hydroxybenzeneacetonitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
826	11076188	328507	O=C(C(CCC(O)=O)=O)O	alpha-Ketoglutaric acid alpha	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
827	11076189	101393	C(=C(C)C=O)c1ccccc1	alpha-Methyl cinnamaldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
828	11076190	98839	C(C)(=C)c1ccccc1	alpha-Methylstyrene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
829	11076191	551064	N(=C=S)c1cccc2cccc12	alpha-Naphthyl isothiocyanate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
830	11076192	80568	CC1(C)C2C(C)=CCC1C2	alpha-Pinene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
831	11076193	546805	O=C1C[C@H]2(C[C@H]2[C@H]1C)C(C)	alpha-Thujone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
832	11076194	2016888	Clc1nc(C(=O)NC(N)=N)nc1N	Amiloride hydrochloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
833	11076195	549188	CN(C)CCCC=C1C(C=CC=C3)=C3CC2=C1C=CC=C2	Amitriptyline HCl	Inactive	Inconclusive	Inactive	Inconclusive	Inconclusive	Inconclusive	Inconclusive	Inconclusive

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834	11076199	1393631	O=C(O)C=CC(C)=CC=CC(C)=CC=CC=C(C)C=CC=C(C)C=CC(O)=O	Annatto Extract Acid Proof	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
835	11076200	1143380	O=C1c2c(O)cccc2Cc3cccc(O)c13	Anthralin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
836	11076201	20562021	[H][C@]36N(C[C@@H](C)CC6)[C@]2([H])[C@@]([C@@H]3C)([H])[C@@]([C@@]4([H])C2)(C)CC[C@]5([H])[C@@]([C@@]4([H])C7)=CC[C@@]45[H])(C)CCC7O[C@H]1[C@H](O[C@@H]8[C@H](O)[C@H](O)[C@@H](O)[C@@H](O)[C@@H](C)O8)[C@@H](O[C@@H]9[C@H](O)[C@@H](O)[C@@H](O)[C@@H](CO)O9)[C@@H](O)[C@@H](CO)O1	alpha-Solanine	Active	Active	Active	Active	Active	Active	Active	Active
837	11076202	83905015	O[C@@](C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@@](O)(C)[C@@H](CC)OC3=O)(C)[C@@](O[C@@H]2O[C@H](C)[C@H](N(C)C)[C@H]2O)[H])[C@@H](C)[C@J]([C@H]3C)([H])O[C@H]1C[C@](OC)(C)[C@@H](O)[C@H](C)O1	Azithromycin (AIDS Initiative)	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
838	11076203	123773	O=C(N=NC(=O)N)N	Azodicarbonamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
839	11076204	495487	[O-][N+](c2ccccc2)=Nc1cccc1	Azoxybenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
840	11076205	532821	NC1=CC(N)=CC=C1N=NC2=CC=C2	C.I. Basic orange 2	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
841	11076206	17804352	CCCCNC(=O)n1c2cccc2nc1NC(=O)OC	Benomyl	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Active
842	11076207	71432	C1=CC=CC=C1	Benzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
843	11076208	98113	O=S(=O)(O)c(cccc1)c1	Benzene sulfonic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
844	11076209	98099	CIS(C1=CC=CC=C1)(=O)=O	Benzenesulfonyl chloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
845	11076210	121540	CC(C)(C)CC(C)(C)c2ccc(OCCOCC[N+]C(C)Cc1cccc1)c2	Benzethonium chloride	Active	Active	Inconclusive	Active	Inconclusive	Inconclusive	Inconclusive	Active
846	11076211	51172	c12N=CNc1cccc2	Benzimidazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
847	11076212	205992	C1(C(C=CC=C5)=C5C2=CC=C3)=C2C3=C(C=CC=C4)C4=C1	Benzo(b)fluoranthene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
848	11076213	192972	C12=C3C4=C5C(C=CC=C5)=C1C=CC=C2C=CC3=CC=C4	Benzo(e)pyrene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
849	11076214	85029	c12cccc2ccc3c1ccn3	Benzo(f)-quinoline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
850	11076215	207089	C2(C4=C3C=C(C=CC=C5)C5=C4)=C1C3=CC=CC1=CC=C2	Benzo(k)fluoranthene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
851	11076216	574061	CC(=O)OC(C(=O)c1cccc1)c2cccc2	Benzoin acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
852	11076217	95169	c1cccc2ncsc2c1	Benzothiazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
853	11076218	98077	C1C(=CC=CC=C1)(Cl)Cl	Benzotrichloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
854	11076219	98088	FC(F)(F)c(cccc1)c1	Benzotrifluoride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
855	11076220	501531	O=C(Cl)OCC1=CC=CC=C1	Carbonochloridic acid, phenylmethyl ester	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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856	11076221	102169	O=C(OCc1ccccc1)Cc2ccccc2	Benzyl phenylacetate	Inactive							
857	11076222	118581	O=C(OCc(ccc1)c1)c(c(O)ccc2)c2	Benzyl salicylate	Inactive							
858	11076223	538749	C(SCc1cccc1)c2cccc2	Benzyl sulfide	Inactive							
859	11076224	2550267	O=C(CCC1=CC=CC=C1)C	benzylacetone	Inactive							
860	11076225	56939	C[N+](C)(C)Cc1ccccc1	Benzyltrimethyl ammonium chloride	Inactive							
861	11076226	633658	COc2ccc1cc3c4cc5OCOc5cc4CC[n+]3cc1c2OC	Berberine chloride	Inactive	Inconclusive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
862	11076227	106229	OCCC(C)CCC=C(C)C	Citronellol	Inactive							
863	11076228	5153673	[O-][N+](C=CC1=CC=CC=C1)=O	beta-Nitrostyrene	Inactive	Active	Inconclusive	Inconclusive	Inconclusive	Inconclusive	Inconclusive	Active
864	11076229	89861	C(=O)(O)c1ccc(O)cc1O	beta-Resorcylic acid	Inactive							
865	11076230	108601	CC(CCl)OC(C)CCl	Bis(2-chloro-1-methylethyl) ether	Inactive							
866	11076231	111911	C1CCCCOC1	Bis(2-chloroethoxy)methane	Inactive							
867	11076233	80057	OC2=CC=C(C=C2)C(C)(C)C1=CC=C(C(O)C=C1	Bisphenol A	Inactive							
868	11076234	1675543	CC(C1=CC=C(OCC2CO2)C=C1)(C3=CC=C(OCC4CO4)C=C3)C	Bisphenol A diglycidyl ether	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
869	11076235	108190	O=C(N)NC(N)=O	Imidodicarbonic diamide	Inactive							
870	11076236	6983795	COc(=O)C=CC=C(C)C=CC=C(C)C=CC=C(C)C=CC(O)=O	Bixin	Inactive							
871	11076238	123353	C(=C)(C=C)CCC=C(C)C	beta-Myrcene	Inactive							
872	11076240	108861	c(cccc1)c1Br	Bromobenzene	Inactive							
873	11076241	5589968	O=C(C(Cl)Br)O	Bromochloroacetic acid	Inactive							
874	11076242	71133147	C(C(Cl)(Cl)Br)(=O)O	Bromodichloroacetic acid	Inactive							
875	11076243	110690	N(O)=CCCC	Butanal oxime	Inactive							
876	11076244	7756969	C(=O)(OCCCC)c1ccccc1N	Butyl anthranilate	Inactive							
877	11076245	29911271	OC(C)CO(C)COCCC	Butyl Dipropasol Solvent	Inactive							
878	11076246	106310	O=C(OC(CCC)=O)CCC	Butanoic acid, anhydride	Inactive							
879	11076247	141753	CCCC(Cl)=O	Butyryl chloride	Inactive							
880	11076250	111648	O=C(CCCCCCCC)Cl	Caprylyl chloride	Inactive							
881	11076251	133062	O=C1N(C(=O)C2C1CC=CC2)SC(Cl)(Cl)Cl	Captan 90-concentrate (solid)	Active							
882	11076252	10605217	N(C(=O)OC)C1=Nc2ccccc2N1	Carbendazim	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Active
883	11076253	75150	S=C=S	Carbon disulfide	Inactive							
884	11076254	56235	C1C(Cl)(Cl)Cl	Carbon tetrachloride	Inactive							
885	11076255	78444	C(C)(CCC)(COC(N)=O)COC(=O)NC(C)C	Carisoprodol	Inactive							
886	11076256	99489	OC(C=CCC1C(=C)C)C1	Carveol	Inactive							
887	11076257	97427	O=C(OC(C=CCC1C(=C)C)C1)C	Carvyl acetate	Inactive							
888	11076260	140727	CCCCCCCCCCCCCCCC[N+]1=CC=CC=C1	Cetylpyridinium bromide	Active							
889	11076261	12789036	C1C2(C(Cl)3Cl)C(Cl)=C(Cl)C3(Cl)C1CC(Cl)C(Cl)C12	Chlordane (technical grade)	Inconclusive	Active	Active	Inactive	Inconclusive	Inconclusive	Inconclusive	Active

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890	11076262	55561	N=C(NC1=CC=C(Cl)C=C1)NC(NCC CCCCNC(NC(C=C2)=CC=C2Cl) Chlorhexidine =N)=N=N	Inconclusive	Active	Active	Active	Active	Active	Active	Active
891	11076264	327979	O=[C@@](O)[C@]1(O)C[C@@H](O) )[C@@H](O)C(OC(C=Cc2cc(O)c(O) cc2)=O)C1 Chlorogenic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
892	11076266	63449398	C1C(CCCC(Cl)CCC(Cl)CCC(Cl)CCC (Cl)CCCC(Cl)CCC)CCC Chlorowax 40	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
893	11076267	51990126	C1C(C(Cl)C(Cl)C(Cl)C(Cl)CC(Cl)C C Chlorowax 500C	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
894	11076268	481743	O=C1c2cccc(O)c2C(=O)c3c(O)cc(C cc13 Chrysophanic acid (1,8-dihydroxy- 3-methylanthraquinone)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
895	11076269	70831560	O=C(O[C@H](C(O)=O)[C@H](C(O)=O) OC(C=CC2=CC=C(O)C(O)=C Cichoric Acid 2)=O)C=CC1=CC(O)=C(O)C=C1	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
896	11076270	27994112	O[C@H]1[C@H](OC4[C@](C)(C)[C @@]2([H])[C@@](CC4)(C7)[C@@] 37C([C@@](CC6C5[C@H](C)CC8( OC(O)C9(C)C8O9)O6)(C)[C@]5(C) CC3)=CC2)OC[C@H](O)[C@H]1O Cimicifugoside	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
897	11076271	104552	O=CC=CC1=CC=CC=C1 Cinnamaldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
898	11076272	14371109	O=CC=CC1=CC=CC=C1 trans-Cinnamaldehyde	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
899	11076273	540590	C1C=CCI cs & trans 1,2-Dichloroethylene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
900	11076274	156592	C1C=CCI cis-1,2-Dichloroethylene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
901	11076276	645498	C1C=CC=CC=1C=CC2=CC=CC=C2 cis-Stilbene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
902	11076277	5392405	O=CC=C(CCC=C(C)C)CC Citral	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
903	11076280	64868	CC(=O)N[C@H]2Cc3cc(OC)c(OC) c(OC)c3C1=CC=C(OC)C(=O)C=C1 Colchicine 2	Inactive	Active	Inactive	Inactive	Inactive	Active	Active	Active
904	11076281	8021394	C1=CC=CC(OC)=C1O Creosote, wood	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
905	11076282	1319773	OC1=CC=C(C)C=C1 m,p-Cresol mixture	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
906	11076284	4170303	O=CC=CC Crotonaldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
907	11076285	1552427	CN(C)c1ccc(cc1)C3(OC(=O)c2cc(cc c23)N(C)C)c4ccc(cc4)N(C)C Crystal violet lactone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
908	11076287	80159	O(O)C(c(ccc1c1)(C)C Cumene hydroperoxide	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Active
909	11076288	458377	O=C(CC(C=CC2=CC=C(O)C(OC)= C2)=O)C=CC1=CC=C(O)C(OC)=C1 Curcumin	Inconclusive	Active	Active	Inactive	Active	Active	Active	Active
910	11076289	108770	C1C=NC(Cl)=NC(Cl)=N1 1,3,5-Triazine, 2,4,6-trichloro-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
911	11076290	931975	C(#N)C1(O)CCCCC1 Cyclohexanone cyanohydrin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
912	11076291	286204	O(C1CCCC2)C12 Cyclohexene oxide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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913	11076293	66819	C[C@H]1C[C@H](C)C([C@@]([C@H](O)CC(CC(N2)=O)CC2=O)([H])C1 Cycloheximide )=O	Inactive	Active	Active	Inactive	Inactive	Inactive	Inactive	Active
914	11076295	287923	C1CCCC1 Cyclopentane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
915	11076296	96413	OC1CCCC1 Cyclopentanol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
916	11076297	6055192	O=P1(N(CCCl)CCCl)OCCN1 Cyclophosphamide monohydrate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
917	11076298	1182349	OC1=CC=C(C=CC(O[C@]2([C@](O)=O)C@H)(O)[C@H](O)C@H)(O)C2=C1O Cynarin (Echinacea)(1,3-C(C=CC3=CC=C(O)C(O)=C3)=O) Dicaffeoylquinic Acid)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
918	11076299	8003223	c1ccc2nc(C3C(=O)c4ccccc4C3(=O)cccc2c1 D & C yellow no. 11	Active	Inconclusive	Active	Inconclusive	Active	Active	Active	Active
919	11076300	13473262	O=C1C(C(Cl)=C(Cl)C(Cl)=C2Cl)=C2C3(C5=C(C(Br)=C(O)C(Br)=C5)OC4 D & C red no. 27 =C3C=C(Br)C(O)=C4Br)O1	Inactive	Inactive	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
920	11076302	23541506	O=C1C(C(O)=C(C[C@]([C@](C)=O)(O)C5)C([C@H]5O[C@H]4C[C@H](N)[C@H](O)[C@H](C)O4)=C3O)=C3C(C2=C1C=CC=C2OC)=O Daunomycin HCL	Active	Active	Active	Active	Active	Active	Active	Active
921	11076303	533744	CN1CN(C)CSC1=S Dazomet	Inactive	Active	Inconclusive	Inactive	Inactive	Inactive	Inactive	Active
922	11076304	464493	O=C1[C@]2(C)CC[C@H]([C@@]([C@H](C)2C)C1 D-Camphor	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
923	11076305	91178	C12CCCCC1CCCC2 Decalin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
924	11076307	302954	O=C(O)CC[C@H](C)[C@]3([H])[C@]1(C)[C@](CC3([H])[C@]([CC4([H])[C@]([C@]2(C)[C@]4([H])[C@H](O)C2)([H])[C@H](O)C2)([H])[C@H]1O) Deoxycholic acid sodium salt	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
925	11076308	15345898	O=C1OC(C=CC2=CC=CC=C2)=CC(OC)=C1 Desmethoxyyangonin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
926	11076309	117828	O=C(OCCOC)c(ccc1)C(=O)OC(O)C1 Di(2-methoxyethyl)phthalate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
927	11076310	1187424	NC(C#N)=C(C#N)N Diaminomaleonitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
928	11076311	136356	N(=NNc(cccc1)c1)c(cccc2)c2 Diazoaminobenzene	Inactive	Inactive	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
929	11076312	262204	c12cccc1Sc3cccc3O2 Dibenzoxathiane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
930	11076313	2743386	O=[C@@](O)[C@H](OC(C1=CC=C2=CC=CC=C2)=O)[C@H](O)OC(C Dibenzoyl-L-tartaric acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
931	11076314	1623081	O=P(OCC2=CC=CC=C2)(O)OCC1=CC=CC=C1 Dibenzyl phosphate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
932	11076315	631641	BrC(Br)C(O)=O Dibromoacetic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
933	11076316	3252435	N#CC(Br)Br Dibromoacetonitrile	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
934	11076318	80433	O(OC(c(cccc1)c1)(C)C)C(c(cccc2)c2)C Dicumyl peroxide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
935	11076320	101837	N(C(CCCC1)C1)C(CCCC2)C2 Dicyclohexylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
936	11076321	77736	C(C(C=CC12)C1)C2C=C3)C3 Dicyclopentadiene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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937	11076322	3056175	CC1=CN(C(=O)NC1=O)[C@H]2C=C[C@@H](CO)O2	Dideoxydidehydrothymidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
938	11076323	105588	O=C(OCC)OCC	Diethyl carbonate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
939	11076324	78386	CCOP(=O)(CC)OCC	Diethyl ethylphosphonate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
940	11076325	84662	CCOC(=O)C1=CC=CC=C1C(=O)OCC	Diethyl phthalate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
941	11076326	4074888	O=C(OCCOCCOC(=O)C=C)C=C	Diethylene glycol diacrylate	Active	Active	Active	Inactive	Inconclusive	Active	Active	Active
942	11076327	112732	O(CCOCOCOC)CCCC	Diethylene glycol dibutyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
943	11076328	11024241	O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CO)O[C@H]1O[C@H]1[C@@H](O)[C@@H](O[C@H](CO)[C@H]1O)[C@@H]1O[C@H]2OC[C@H](O)[C@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@@H](O)[C@H](O)[C@H]3CO[C@H]8C[C@H]9C[C@H]5[C@H](CC[C@]6(C)[C@H]7[C@H](C)[C@@]4(CC[C@@H](C)CO4)O[C@H]7[C@@H](O)[C@@H]56)[C@@]9(C)C[C@H]8O	Digitonin	Active	Active	Active	Active	Active	Active	Active	Active
944	11076329	101906	C1=C(C=CC=C1OCC2CO2)OCC3CO3	Diglycidyl resorcinol ether (DGRE)	Active	Active	Active	Inconclusive	Active	Active	Active	Active
945	11076330	587633	O=C1OC(CCC2=CC=CC=C2)CC(O)C=C1	Dihydrokavain	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
946	11076331	3155575	O=C1OC(CCC(C=C3)=CC2=C3OCO2)CC(OC)=C1	Dihydromethysticin	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
947	11076332	108189	N(C(C)C)C(C)C	Diisopropylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
948	11076333	693130	C(=NC(C)C)=NC(C)C	Diisopropylcarbodiimide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
949	11076335	627930	C(CCCC(=O)OC)C(=O)OC	Dimethyl adipate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
950	11076336	1119400	COC(=O)CCCC(=O)OC	Dimethyl glutarate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
951	11076337	10563298	NCCCCN(C)C	dimethyldipropylene-triamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
952	11076338	624920	S(C)SC	Dimethyldisulfide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
953	11076339	996350	CC(C)N(C)C	dimethylisopropylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
954	11076340	28804888	C1=CC=C2C(=C1)C(=C(C=C2)C)C	Dimethylnaphthalene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
955	11076341	106650	C(=O)(OC)CCC(=O)OC	Dimethylsuccinate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
956	11076342	2050922	N(CCCCC)CCCCC	Di-n-amylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
957	11076343	131168	O=C(OCCC)C(C=CC=C1)=C1C(OC(=O)C)C	Di-n-propylphthalate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
958	11076344	131180	O=C(OCCCCCC)C(C=CC=C1)=C1C(OC(=O)C)C	Di-n-pentylphthalate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
959	11076345	102078	O=C(NC1=CC=CC=C1)NC2=CC=C2	Diphenylurea	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
960	11076347	25265718	OC(OC(O)CC)CC	Dipropylene glycol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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961	11076348	992596	OS(=O)(=O)c5cc(N=Nc1ccc(cc1C)c4ccc(N=Nc3cc(c2cccc2c3N)S(O)(=O)c(C)c4)c(N)c6cccc56)	C.I. Direct red 2	Inactive	Inconclusive	Inconclusive	Inconclusive	Inactive	Inactive	Inconclusive
962	11076349	110054	O(OC(C)(C)C(C)(C)C	Di-tert-butyl peroxide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
963	11076350	3648202	O=C(OCCCCCCCCCCC)C1=CC=C C=C1C(OCCCCCC)C=O	Diundecyl phthalate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
964	11076351	1321740	C=Cc1cccc1C=C	Divinylbenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
965	11076352	76222	O=C1C(CC2)(C)C(C)(C)C2C1	Camphor	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
966	11076353	538716	C[N+](CCOC1=CC=CC=C1)(C)CCC	Domiphen bromide	Active	Active	Active	Active	Active	Active	Active
			CCCCCCCC								
			O[C@H]1[C@H](O[C@@H]2[C@@H](O)[C@H](O)[C@@H](CO)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H]1O								
967	11076354	82854373	O=C1c2c(O)cc(C)cc2C(=O)c3cc(O)cc(O)c13	Echinacoside	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
968	11076355	24169026	Clc3ccc(C(OCc1ccc(Cl)cc1)Cn2ccn2)c(Cl)c3	Econazole nitrate	Inconclusive	Active	Inconclusive	Inconclusive	Inactive	Inconclusive	Active
969	11076356	518821	O=C1c2c(O)cc(C)cc2C(=O)c3cc(O)cc(O)c13	Emodin	Inactive	Inconclusive	Inconclusive	Inconclusive	Inactive	Active	Active
970	11076357	759944	CCCN(CCC)C(=O)SCC	S-ethyl dipropylthiocarbamate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
971	11076359	58548	C(=O)(C(=C)CC)c1ccc(OCC(=O)O)c1Cl	Ethacrynic acid	Inconclusive	Active	Inconclusive	Inconclusive	Inactive	Active	Active
972	11076360	1239458	CC[n+]3c4cc(N)ccc4c1ccc(N)cc1c3	Ethidium bromide	Inconclusive	Active	Inconclusive	Inactive	Inactive	Inactive	Active
973	11076361	627032	OCC(OCCC)=O	Ethoxyacetic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
974	11076362	140885	O=C(OCC)C=C	Ethyl acrylate (inhibited)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
975	11076363	87252	O=C(OCC)c(c(N)ccc1)c1	Ethyl anthranilate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
976	11076364	7085850	O=C(OCC)C(=C)C#N	Ethyl cyanoacrylate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
977	11076365	1191419	O=C(OCC)CCCCCCCC=CCC=CCC	Ethyl linolenate	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
978	11076366	62500	O(CC)S(C)(=O)=O	Ethyl methanesulfonate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
979	11076367	1629589	C(=O)(CC)C=C	Ethyl vinyl ketone	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
980	11076368	609143	O=C(OCC)C(C)C(C)=O	Ethyl-2-methyl acetoacetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
981	11076369	629141	O(CCOCC)CC	Ethylene glycol diethyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
982	11076370	111762	CCCCOCOC	Ethylene glycol monobutyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
983	11076371	16219753	C(C(C=CC12)C1)(=CC)C2	Ethyldenenorbornene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
984	11076372	13360639	N(CCCC)CC	N-Ethyl-n-butylamine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
985	11076374	206440	c1cccc4c1c2cccc3cccc4c23	Fluoranthene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
986	11076375	462066	Fc1ccccc1	Fluorobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
987	11076377	76437	F[C@]1([C@](CC2)([H])[C@@]([C]4([H])C[C@]([C@H]1O)[C@]([CC3](C)C2=CC3=O	Fluoxymestrone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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988	11076378	13311847	[O-] ][N+](C(C=C1)=C(C=C1NC(C(C)C)=O)C(F)(F)F)=O Flutamide (pubertal study)	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
989	11076379	75127	C(N)=O	Formamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
990	11076380	103708	O=CN(cccc1)c1	Formanilide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
991	11076381	764421	N#CC=CC#N	Fumaronitrile	Inconclusive	Active	Inconclusive	Inactive	Inactive	Active	Active
992	11076382	627634	CIC(C=CC(Cl)=O)=O	fumaryl chloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
993	11076383	623176	O=C(OCC(OC=C1)=C1)C	Furfuryl acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
994	11076385	105873	O=C(C)OCC=C(C)CCC=C(C)C	Geranyl acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
995	11076387	111308	O=CCCCC=O	Glutaraldehyde	Inactive	Active	Inactive	Inactive	Inactive	Inconclusive	Active
996	11076388	56815	OCC(O)CO	Glycerol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
997	11076389	106912	C(OC(=O)C(C)=C)C1CO1	Glycidyl methacrylate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
998	11076390	107222	O=CC=O	Glyoxal	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
999	11076391	39025246	[H][C@]1(CC2)[C@@](CC3=O)([H]) [C@](C3=CC)(C)CC[C@]([H])1[C @](CC4)(C)C2=CC4=O [H][C@]1(CC2)[C@@](CC3=O)([H]) [C@](C3=CC)(C)CC[C@]([H])1[C @](CC4)(C)C2=CC4=O S(=O)(=O)(N(Cl)Cl)c1ccc(cc1)C(=O) O	Guggulsterones E	Inactive	Active	Inconclusive	Inactive	Inactive	Inconclusive	Active
1000	11076392	39025235	[H][C@]1(CC2)[C@@](CC3=O)([H]) [C@](C3=CC)(C)CC[C@]([H])1[C @](CC4)(C)C2=CC4=O S(=O)(=O)(N(Cl)Cl)c1ccc(cc1)C(=O) O	Guggulsterones Z	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
1001	11076393	80137	Halazone	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1002	11076394	151677	FC(F)(F)C(Cl)Br	Halothane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1003	11076395	111499	N1CCCCCC1	Hexamethyleneimine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1004	11076396	101860	O=CC(CCCCCC)=CC1=CC=CC=C1	Octanal, 2-(phenylmethylene)-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1005	11076397	118081	COc2ccc1OC(=O)c1c2OC)C4N(C Cc5cc3OCOc3cc45	Hydrastine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1006	11076398	52806538	[O-] ][N+](C(C=C1)=C(C=C1NC(C(O)(C C)=O)C(F)(F)F)=O Hydroxyflutamide	Hydroxyvalerenic Acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1007	11076400	1619165	O[C@H]1[C@@]2([H])C([C@H](C=C(C)C(=O)OC(C)=O)CC[C@H]2C)=C(C)C1	1H-Imidazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1008	11076401	288324	N1=CNC=C1	Prevention 4 (indole-3-carbinol)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1009	11076403	700061	OCC1=CNC2=C1C=CC=C2	Isoamyl acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1010	11076404	123922	Isoamyl cinnamate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1011	11076405	7779659	Isoamyl nitrite	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1012	11076406	110463	Isobutyl methacrylate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1013	11076407	97869	Isocyanatocyclohexane	Ethanone, 1-(1,2,3,4,5,6,7,8-octahydro-2,3,8,8-tetramethyl-2-naphthalenyl)-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1014	11076408	3173533	O=C(C2(C)CC1=C(CC2C)CCCC(C 1)C	Isophorone diisocyanate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1015	11076409	54464572	CC(C)CCC[CH](C)CCC[CH](C)CCC [C](C)(O)C=C	Isophytol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1016	11076410	4098719									
1017	11076411	505328									

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1018	11076412	108225	O=C(C)OC(C)=C	Isopropenyl acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1019	11076413	108214	O(C(C)C)C(C)=O	Isopropyl acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1020	11076414	4016142	C(OC(C)C)C1CO1	Isopropyl glycidyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1021	11076415	75332	CC(C)S	Isopropyl mercaptan	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1022	11076416	926067	O=S(OC(C)C)(C)=O	Isopropyl methanesulfonate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1023	11076417	4861852	c(ccc1CC(=O)OC(C)C)cc1	Isopropyl phenylacetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1024	11076418	51309	Oc1ccc(cc1O)C(O)CNC(C)C	Isoproterenol hydrochloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1025	11076419	500641	O=C1C=C(OC)C[C@H](C=CC2=CC=CC=C2)O1	Kavain, DL-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1026	11076421	4350098	OC(=O)[C@@H](N)CC2=CNC1ccc(O)cc12	L-5-Hydroxytryptophan	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1027	11076422	143077	CCCCCCCCCC(O)=O	Lauric acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1028	11076423	112527	CCCCCCCCCCCI	Lauryl chloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1029	11076424	2461189	C1(CO1)COCCCCCCCCCCC	Lauryl glycidyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1030	11076428	78706	OC(C=C)(CCC=C(C)C)C	Linalool	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1031	11076429	60333	O=C(O)CCCCCCCC=CCC=CCCCC	Linoleic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1032	11076430	463401	O=C(O)CCCCCCCC=CCC=CCC=C	Linolenic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1033	11076431	521313	Oc1nnc(O)c2c(N)cccc12	Luminol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1034	11076433	118718	O1C(C)=C(O)C(=O)C=C1	Maltol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1035	11076434	121471	O=S(=O)(O)c(cccc1N)c1	3-Aminobenzenesulfonic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1036	11076435	102283	N(C(C)=O)c1cccc(N)c1	m-Aminoacetanilide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1037	11076436	591275	Oc(cccc1N)c1	3-Aminophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1038	11076437	536903	O(C)c1cccc(N)c1	m-Anisidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1039	11076438	591173	c(cccc1Br)(c1)C	m-Bromotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1040	11076439	108429	Clc1cccc(N)c1	m-Chloroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1041	11076440	535808	C(=O)(O)c1cccc(Cl)c1	m-Chlorobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1042	11076441	98157	FC(F)F)c1cccc(Cl)c1	m-Chlorobenzotrifluoride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1043	11076442	108430	Clc1cccc(O)c1	m-Chlorophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1044	11076443	99650	[O-][N+](C1=CC=CC([N+]([O-])=O)=C1)=O	m-Dinitrobenzene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1045	11076444	71589	CC(=O)[C@]2(CC[C@H]3[C@@H]4[C@H]4CC[C@]23C)OC(C)=O	Medroxyprogesteroneacetate	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1046	11076445	73314	O=C(C)NCCCC1=CNC2=C1C=C(OC)C=C2	Melatonin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1047	11076446	494906	C[CH]1CCC2=C(C1)OC=C2C	Menthofuran	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1048	11076447	79390	O=C(N)C(C)=C	Methacrylamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1049	11076448	126987	CC(=C)C#N	Methacrylonitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1050	11076449	40596698	O=C(OC(C)C)=C(C)C=CCC(C)CC	Methoprene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1051	11076450	625456	O=C(COC)O	Methoxyacetic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1052	11076451	72435	C1C(C1=CC=C(C=C1)OC)C2=CC=C(C=C2)OC(Cl)Cl	Methoxychlor [95%]	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1053	11076452	96333	C=CC(=O)OC	Methyl acrylate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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1054	11076453	134203	O=C(OC)c(c(N)ccc1)c1	Methyl anthranilate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1055	11076454	93583	C(=O)(OC)c1ccccc1	Methylbenzoate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1056	11076455	105340	O=C(CC#N)OC	Methyl cyanoacetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1057	11076456	1338234	CC(CC)(OOC(C)(CC)OO)OO	Methyl ethyl ketone peroxide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1058	11076457	534225	CC1=CC=CO1	2-Methyl furan	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1059	11076458	4553622	N#CC(CCC#N)C	Methylglutaronitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1060	11076459	624839	CN=C=O	Methyl isocyanate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1061	11076460	556616	S=C=NC	Methane, isothiocyanato-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1062	11076461	119368	O=C(OC)c(c(O)ccc1)c1	Methyl salicylate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1063	11076462	122576	O=C(C=Cc(ccc1)c1)C	Methyl styryl ketone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1064	11076463	58184	O=C2C=C3[C@@](CC2)(C)[C@]1([H])[C@](CC3)([H])[C@](CC4)([H])[C@](C)[C@@]4(C)O)(C)CC1	Methyl testosterone	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive	Inconclusive
1065	11076464	78944	O=C(C=C)C	Methyl vinyl ketone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1066	11076465	6317186	C(SC#N)SC#N	Methylene bis(thiocyanate)	Active	Active	Active	Active	Active	Active	Active	Active
1067	11076466	7220793	CN(C)c1ccc2nc3cccc3[s+]c2c1)N(C)C	Methylene blue trihydrate	Inconclusive	Active	Active	Active	Active	Active	Active	Active
1068	11076467	93152	O(C)c1cc(CC=C)ccc1OC	Methyleugenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1069	11076468	1571080	CO(C(=O)c1ccc(C=O)cc1	Methyl-p-formyl benzoate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1070	11076469	99752	O=C(OC)c(ccc(c1)C)c1	Methyl-p-toluate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1071	11076470	2365482	O=C(CS)OC	Methylthioglycolate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1072	11076471	495852	O=C1C=C(OC)C[C@H](C=CC2=CC=C3C(OCO3)=C2)O1	Methysticin	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1073	11076472	121891	O=C(c1cccc([N+])([O-])=O)c1)C	m-Nitroacetophenone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1074	11076473	99092	[N+](=O)([O-])c1cccc(N)c1	m-Nitroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1075	11076474	645090	C(N)(=O)c1cccc(c1)[N+](=O)[O-]	m-Nitrobenzamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1076	11076475	121926	C(=O)(O)c1cccc(c1)[N+](=O)[O-]	m-Nitrobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1077	11076476	121904	O=C(c1cccc([N+](=O)[O-])c1)Cl	m-Nitrobenzoyl chloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1078	11076477	619238	[N+](=O)([O-])c1cccc(CCl)c1	m-Nitrobenzyl chloride	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1079	11076478	554847	OC1=CC=CC(=C1)[N+](=O)[O-]=O	m-Nitrophenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1080	11076479	2212671	O=C(SCC)N1CCCCCCC1	Molinate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1081	11076480	4376209	CCCCC(CC)COC(=O)c1cccc1C(O)=O	Mono(2-ethylhexyl)phthalate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1082	11076482	621330	O(CC)c1cccc(N)c1	m-Phenetidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1083	11076483	620224	C(#N)c1cccc(C)c1	m-Tolunitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1084	11076484	83669	[O-][N+](=O)c1c(c([N+](=O)[O-])=O)c(OC)c(C(C)(C)C)c1)C	Musk ambrette	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1085	11076485	108383	CC1=CC(C)=CC=C1	m-Xylene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1086	11076486	55981	O(S(=O)(=O)C)CCCCOS(=O)(C)=O	Myleran	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1087	11076487	607910	O(CO1)c(cc(c2)CC=C)c1c2OC	Myristicin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1088	11076488	793248	N(c(cc(Nc(ccc1)c1)c2)c2)C(CC(C)N-(1,3-Dimethylbutyl)-N'-phenyl-p-C)C	N,N,N',N'-Tetramethylhexanediamine	Inactive	Active	Inconclusive	Inactive	Inactive	Inactive	Inactive	Active
1089	11076489	111182	CN(C)CCCCCN(C)C		Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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1090	11076490	100221	N(c(ccc(N(C)C)c1)c1)(C)C	N,N,N',N'-Tetramethyl-p-phenylenediamine	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1091	11076491	85983	O=C(N(c(ccc1)c1)CC)N(c(ccc2)c2)CC	N,N'-Diethylcarbanilide	Inactive						
1092	11076492	93050	N(c(ccc(N)c1)c1)(CC)CC	N,N-Diethyl-p-phenylenediamine	Inconclusive	Active	Inconclusive	Inactive	Inconclusive	Inconclusive	Active
1093	11076493	68122	CN(C=O)C	N,N-Dimethylformamide	Inactive						
1094	11076494	138896	CN(C)c1ccc(N=O)cc1	N,N-Dimethyl-p-nitrosoaniline	Inactive	Active	Active	Inconclusive	Active	Active	Active
1095	11076495	99989	N(c(ccc(N)c1)c1)(C)C	N,N-Dimethyl-p-phenylenediamine	Active	Active	Inconclusive	Inactive	Inconclusive	Active	Active
1096	11076496	6225065	O=C(CCCC)N(C)C	N,N-Dimethylvaleramide	Inactive						
1097	11076497	101962	N(c(ccc(NC(CC)C)c1)c1)C(CC)C	N,N'-Di-sec-butyl-p-phenyldiamine	Active						
1098	11076498	110269	O=C(NCNC(=O)C=C)C=C	N,N'-methylenebisacrylamide	Inactive						
1099	11076499	537928	N(C(C)=O)c1cccc(C)c1	N-Acetyl-m-toluidine	Inactive						
1100	11076500	120661	O=C(Nc(c(ccc1)C)c1)C	Acetyl-o-toluidine	Inactive						
1101	11076501	103899	O=C(C)Nc1ccc(C)cc1	N-Acetyl-p-toluidine	Inactive						
1102	11076502	141322	O=C(OCCCC)C=C	n-Butyl acrylate	Inactive						
1103	11076503	71363	CCCCO	n-Butyl alcohol	Inactive						
1104	11076504	2426086	C(OCCCC)C1CO1	n-Butyl glycidyl ether	Inactive						
1105	11076505	80308	S(=O)(=O)(NC1CCCCC1)c2ccc(C)c2	n-Cyclohexyl-4-methylbenzenesulfonamide	Inactive						
1106	11076506	3179473	CCCCCCOC(=O)C(C)=C	Decyl methacrylate	Inactive						
			OC1=CC=CC(C[N@@H]1C[C@H](CSC2=CC=CC=C2)[C@H](CN3[C@H](C[C@H]3C)O)[C@H]1C)[C@H](C[C@H]1C)O=C1								
1107	11076507	159989658	C@@[C@H](NC(C)(C)C)=O)C[C@H]1[C@H]([C@H]1C)Nelfinavir mesylate	Active	Active	Active	Active	Active	Active	Active	Active
			C[C@H]1[C@H]([C@H]1O[C@H]2[C@H]([C@H]([C@H]2O)O)[C@H]([C@H]1O)[C@H]([C@H]1O)O)OC3=CC(=C(C(=C4C)O)O)C(=C3)O								
1108	11076508	20702776	O[C@H]1[C@H]([C@H]1O[C@H]2[C@H]([C@H]([C@H]2O)O)[C@H]([C@H]1O)[C@H]([C@H]1O)O)OC3=CC(=C(C(=C4C)O)O)C(=C3)O	Neohesperidin dihydrochalcone	Inactive						
1109	11076509	17557232	O(C1COCC(C)(C)COCC(O2)C2)C1	Neopentyl glycol diglycidyl ether	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1110	11076510	103695	N(c(ccc1)c1)CC	N-Ethyl aniline	Inactive						
1111	11076511	80397	CCNS(=O)(C1=CC=C(C=C1)C)=O	N-Ethyl-4-methylbenzenesulfonamide	Inactive						
1112	11076512	92591	CCN(CC1=CC=CC=C1)C2=CC=CC=C2	N-Ethyl-n-phenyl benzylamine	Inactive						
1113	11076513	129618402	O=C2C1=CC=CN=C1N(C3CC3)C(N=CC=C4C)=C4N2	Nevirapine	Inactive						
1114	11076514	142096	CCCCCCOC(=O)C(C)=C	n-Hexyl methacrylate	Inactive						
1115	11076515	495181	C(=O)(NO)c1cccc1	N-Hydroxybenzamide	Inactive						
1116	11076517	21829254	COC(=O)C1=C(C)NC(=C(C1c2cccc2N=O)[O-])C(=O)OC)C	Nifedipine	Inactive	Inconclusive	Inactive	Inactive	Inconclusive	Inconclusive	Inconclusive
1117	11076518	485472	O=C(c(c(C1=O)ccc2)c2)C1(O)O	Ninhydrin	Inconclusive	Active	Inactive	Inactive	Active	Inconclusive	Active

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1118	11076519	2210255	O=C(NC(C)C)C=C	N-Isopropyl acrylamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1119	11076520	768525	C1=CC=CC=C1)NC(C)C	N-Isopropylaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1120	11076521	101724	N(c1ccccc1)c2ccc(cc2)NC(C)C	N-Isopropyl-N'-phenyl-p-phenylenediamine	Inconclusive	Active	Inconclusive	Inconclusive	Inconclusive	Active	Active	Active
1121	11076522	55981094	O=C(NC2=NC=C([N+]([O-])=O)S2)C1=C(OC(C)=O)C=CC=C1	Nitazoxanide	Inconclusive	Active	Active	Inconclusive	Inconclusive	Active	Active	Active
1122	11076523	55867	N(C)(CCCI)CCCI	Nitrogen mustard hydrochloride	Inconclusive	Active	Active	Inactive	Active	Active	Active	Active
1123	11076524	100152	CNc1ccc([N+]([O-])=O)cc1	N-Methyl-4-nitroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1124	11076525	613934	C(=O)(NC)c1cccc1	N-Methylbenzamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1125	11076526	13114722	CNC(=O)N(c1ccccc1)c2cccc2	N'-methyl-N,N-diphenylurea	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1126	11076528	111842	C(CCCCCCCC)C	Nonane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1127	11076529	542405	O=C(O)C=CC(C)=CC=CC(C)=CC=CC=C(C)C=CC(C)=CC(O)=O	Norbixin (cis/trans mixture)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1128	11076530	109660	C(CCC)C	n-Pentane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1129	11076531	90302	N(c(c(c(cc1)cc2)c1)c2)c(ccc3)c3	N-Phenyl-1-naphthylamine	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1130	11076532	88211	S(=O)(=O)(O)c1cccc1N	Orthonilic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1131	11076533	95556	Oc(c(N)ccc1)c1	o-Aminophenol	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1132	11076534	90040	NC1=C(OC)C=CC=C1	o-Anisidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1133	11076535	95465	c(c(ccc1)Br)(c1)C	o-Bromotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1134	11076536	118912	C(=O)(O)c1cccc1Cl	o-Chlorobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1135	11076537	88164	FC(F)(F)c1cccc1Cl	o-Chlorobenzotrifluoride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1136	11076538	109091	n(c(cc1)Cl)c1	o-Chloropyridine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1137	11076539	2039874	C(=C)c1cccc1Cl	o-Chlorostyrene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1138	11076540	2210799	O(CC1CO1)c2cccc2C	o-Cresyl glycidyl ether	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1139	11076541	32536520	Brc1c(cc(Br)c(Br)c1Br)Oc2cc(Br)c(Br)c2Br	Octabromodiphenyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1140	11076542	124072	CCCCCC(O)=O	Octanoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1141	11076543	770058	NCC(O)C(C=C1)CC=C1O	Octopamine HCL	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1142	11076544	112801	O=C(CCCCCCCC=CCCCCCCC)O	Oleic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1143	11076545	93834	O=C(N(CCO)CCO)CCCCCCCC=CC	Oleic acid diethanolamine condensate	Inactive	Active	Inconclusive	Inactive	Inactive	Inconclusive	Active	Active
1144	11076546	500663	CCCCCc1cc(O)cc(O)c1	Olivetol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1145	11076547	90051	C1=CC=CC(OC)=C1O	o-methoxyphenol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1146	11076548	577593	C(C)(=O)c1cccc1[N+](=O)[O-]	o-Nitroacetophenone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1147	11076549	88744	[N+](=O)[O-]c1cccc1N	o-Nitroaniline	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1148	11076550	610151	C(N)(=O)c1cccc1[N+](=O)[O-]	o-Nitrobenzamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1149	11076551	552169	C(=O)(O)c1cccc1[N+](=O)[O-]	o-Nitrobenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1150	11076552	610140	O=C(c1c([N+](=O)[O-])cccc1)Cl	o-Nitrobenzoyl chloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1151	11076553	612237	C(Cl)c1cccc1[N+](=O)[O-]	o-Nitrobenzyl chloride	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1152	11076554	15121843	O=[N+](=O)[O-]c1c(ccc1)CCO	o-Nitrophenethyl alcohol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1153	11076555	610662	O=[N+](=O)[O-]c1c(ccc1)CC#N	(o-Nitrophenyl)acetonitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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1154	11076556	88722	[N+](=O)([O-])c1ccccc1C	o-Nitrotoluene	Inactive							
1155	11076557	66717	c12ncccc2ccc3c1nccc3	o-Phenanthroline	Inactive	Active	Active	Active	Inactive	Active	Active	Active
1156	11076558	94702	CCOc1ccccc1N	o-Phenetidine	Inactive							
1157	11076559	95545	Nc(c(N)ccc1)c1	o-Phenylenediamine	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1158	11076561	65861	C(=O)(O)c1cc(O)nc(O)n1	Orotic acid	Inactive							
1159	11076562	89725	C1(=C(O)C=CC=C1)C(CC)C	o-sec-Butylphenol	Inactive							
1160	11076563	118901	O=C(O)c(c(ccc1)C)c1	o-Toluic acid	Inactive							
1161	11076564	95534	Nc(c(ccc1)C)c1	o-Toluidine	Inactive							
1162	11076565	434071	O=C3C[C@H]4CC[C@H]1[C@H]2(C)[C@@](C)(O)CC[C@@H]12[C@@]4(C)CC3=CO	Oxymetholone	Inconclusive	Active	Inconclusive	Inactive	Inactive	Inconclusive	Inconclusive	Active
1163	11076566	104405	CCCCCCCCC1=CC=C(O)C=C1	p -n -Nonylphenol	Inconclusive	Inactive	Inconclusive	Inactive	Inconclusive	Inconclusive	Inconclusive	Inconclusive
1164	11076567	72559	C1C(=C(C1=CC=C(C=C1)Cl)C2=CC=C(C=C2)Cl)Cl	p,p'-DDE (p,p'-Dichlorodiphenyldichloroethylene)	Inactive							
1165	11076568	80079	S(=O)(=O)(c1ccc(Cl)cc1)c2ccc(Cl)c2	p,p'-Dichlorodiphenyl Sulfone	Inactive							
1166	11076569	556081	CC(=O)Nc1ccc(cc1)C(O)=O	p-Acetamidobenzoic acid	Inactive							
1167	11076570	121573	O=S(=O)(O)c(ccc(N)c1)c1	4-Aminobenzenesulfonic acid	Inactive							
1168	11076571	150130	O=C(O)c(ccc(N)c1)c1	p-Aminobenzoic acid	Inactive							
1169	11076572	122805	O=C(Nc(ccc(N)c1)c1)C	p-Amino acetanilide	Inactive							
1170	11076573	123308	Oc(ccc(N)c1)c1	p-Aminophenol	Active	Active	Active	Inconclusive	Active	Active	Active	Active
1171	11076574	123115	O=CC1=CC=C(OC)C=C1	p-Anisaldehyde	Inactive							
1172	11076575	104949	Nc1ccc(OC)cc1	p-Anisidine	Inactive							
1173	11076576	56382	S=P(OC1=CC=C(C=C1)[N+](=O)[O-])(OCC)OCC	Parathion	Inactive							
1174	11076577	1562943	[O-][N+](c2ccc(OC)cc2)=Nc1ccc(OC)cc1	p-Azoxyanisole	Inactive							
1175	11076578	106387	c(ccc(c1)Br)(c1)C	p-Bromotoluene	Inactive							
1176	11076579	74113	C(=O)(O)c1ccc(Cl)cc1	p-Chlorobenzoic acid	Inactive							
1177	11076580	106434	Cc1ccc(Cl)cc1	p-Chlorotoluene	Inactive							
1178	11076581	105066	C=CC1=CC=C(C=C)C=C1	p-Divinylbenzene	Inactive							
1179	11076582	60348609	BrC2=C(C=C(Br)C(Br)=C2)OC1=CC2,4,4',5-Pentabromodiphenyl ether	=C(Br)C=C1Br	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1180	11076583	32534819	BrC2=C(C=C(Br)C(Br)=C2)OC1=CC Pentabromodiphenyl oxide =C(Br)C=C1Br	(technical) (DE 71)	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1181	11076584	608935	C1C=C(Cl)C(Cl)=C(Cl)C(Cl)=C1	Pentachlorobenzene	Inactive							
1182	11076585	3524683	O=C(OCC(CO)(COC(=O)C=C)COC(=O)C=C)C=Pentaerythritol triacrylate	C=C	Inactive	Active	Active	Inactive	Active	Active	Active	Active
1183	11076587	22224926	Cc1cc(ccc1SC)OP(=O)(NC(C)C)OC	Phenamiphos	Inactive							
1184	11076588	85018	C1=CC2=C(C=C1)C3=C(C=CC=C3)C=C2	Phenanthrene	Inactive							
1185	11076589	133186	C(=O)(OCCc1ccccc1)c2ccccc2N	Phenethyl anthranilate	Inactive							

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1186	11076590	103639	BrCCC1=CC=CC=C1	phenethyl bromide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1187	11076592	13684634	O=C(NC2=CC(C)=CC=C2)OC1=CC (NC(OC)=O)=CC=C1	3-((Methoxycarbonyl)amino)phenyl N-(3-methylphenyl)carbamate (Phenmedipham)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1188	11076593	122598	O(CC(=O)O)c1ccccc1	Phenoxy acetic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1189	11076594	1074120	C(=O)(C=O)c1ccccc1	Phenylglyoxal	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1190	11076595	103855	NC(=S)NC1=CC=CC=C1	Phenylthiourea	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1191	11076596	136776	OC1=C(C=CC(=C1)O)CCCCC	4-Hexylresorcinol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1192	11076598	1498517	O=P(Cl)(Cl)OCC	Phosphorodichloridic acid, ethyl ester	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1193	11076599	10026138	CIP(Cl)(Cl)(Cl)Cl	phosphorus pentachloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1194	11076600	1918021	CIC1=C(Cl)N=C(C(O)=O)C(Cl)=C1N	Picloram	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1195	11076601	473552	CC2(C)C1CC2C(C)CC1	Pinane	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1196	11076602	120570	C(=O)c1ccc2OCOc2c1	Piperonal	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1197	11076603	326614	C(OC(C)=O)c1ccc2OCOc2c1	Piperonyl acetate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1198	11076604	589184	OCc(ccc(c1)C)c1	p-Methyl benzyl alcohol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1199	11076605	100196	C(C)(=O)c1ccc(cc1)[N+]([O-])=O	p-Nitroacetophenone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1200	11076606	122043	O=C(c1ccc([N+]([O-])=O)cc1)Cl	p-Nitrobenzoyl chloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1201	11076607	2645070	C(=O)(NCC(=O)O)c1ccc(cc1)[N+]([O-])=O	p-Nitrohippuric acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1202	11076608	100276	O=[N+]([O-])c1ccc(cc1)CCO	p-Nitrophenethyl alcohol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1203	11076609	99990	O=N(=O)c1ccc(C)cc1	p-Nitrotoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1204	11076610	2493847	CCCCCCCOc1ccc(cc1)C(O)=O	p-n-Octyloxybenzoic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1205	11076611	25703791	O=C(OCC(O)C)C(C)=C	Poly(2-hydroxypropyl methacrylate)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1206	11076613	156434	O(c(ccc(N)c1)c1)CC	p-Phenetidine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1207	11076614	32809168	O=C1C3(C)C(C3)(C)C(N1C2=CC(Cl)=CC(Cl)=C2)=O	Procymidone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1208	11076615	57830	[C@]12([C@]([C@@]3[CCC4[C@]12[C@H]3[H]](CCC(=O)C=4[C@H]4[C@H]2C(=O)C)[H])C	Progesterone	Inactive	Inconclusive	Active	Inactive	Inactive	Inconclusive	Active	
1209	11076616	1569013	OC(C)COCCC	2-Propanol, 1-propoxy-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1210	11076617	57556	CC(CO)O	Propylene glycol	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1211	11076618	57018527	OC(COC(C)(C)C)C	Propylene glycol mono-t-butyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1212	11076619	94133	C(C1=CC=C(C=C1)O)(=O)OCCC	Propylparaben	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1213	11076620	80546	O=CC(C)CC1=CC=C(C(C)(C)C)C=C1	Benzene propanal, 4-(1,1-dimethylethyl)-.alpha.-methyl-	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1214	11076621	98293	Oc(c(O)cc(c1)C(C)(C)C)c1	p-tert-Butylcatechol	Inactive	Active	Inactive	Inactive	Inactive	Active	Active	Active
1215	11076622	98511	c(ccc(c1)C)(c1)C(C)(C)C	p-tert-Butyltoluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1216	11076623	70553	O=S(C1=CC=C(C)C=C1)N=O	p-Toluenesulfonamide	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1217	11076624	104858	N#Cc(ccc(c1)C)c1	p-Tolunitrile	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1218	11076625	89827	O=C(C(=C(C)C)CCC1C)C1	Pulegone	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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1219	11076626	125315	Cc1cc(c(C)cc1O)C3(OS(=O)(=O)c2cccc23)c4cc(C)c(O)cc4C	p-Xylenol blue	Inactive							
1220	11076627	129000	C12=CC=CC4=C1C3=C(C=CC=C3C=C4)C=C2	Pyrene	Inactive							
1221	11076628	87661	Oc(c(O)ccc1)c1O	Pyrogallol	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inconclusive	Inconclusive	Inconclusive
1222	11076629	501360	OC1=CC(C=CC(C=C2)=CC=C2O)=CC(O)=C1	Resveratrol	Inactive							
1223	11076630	478433	O=C1c2c(O)cccc2C(=O)c3cc(cc(O)c13)C(=O)O	Rhein (1,8-dihydroxy-3-carboxyl anthraquinone)	Inactive	Inconclusive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive
1224	11076631	72559069	O=C(C(NC(C(C)=CC=C[C@H](C)[C@@H]([C@@H](C)[C@@H](O)[C@H](C)[C@@H](OC(C)=O)[C@H](C)[C@@H](OC(C)=O)=O)c3C2=NC5(CCN(CC(C)C)CC5)N3)C1=C2C(C([C@]6(C)O4)=O)=C4C(C)=C1O	Rifabutin	Inactive	Inconclusive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1225	11076632	2941642	O=C(SCC)Cl	S-(ethyl)chlorothioformic acid	Inactive							
1226	11076633	13889924	O=C(SCCC)Cl	S-(n-propyl)chlorothioformic acid	Inactive							
1227	11076634	149845067	O=[C@J](NC(C)(C)C)[C@H]2N(C[C@@H](O)[C@H](NC([C@H](CC(N)=O)NC(C4=NC(C=CC=C5)C5C=C4)=O)O)CC3=CC=CC=C3)C[C@H]1([H])CCCC[C@J]([H])1C2	Saquinavir mesylate (AIDS Initiative)	Inconclusive	Active	Inconclusive	Active	Inconclusive	Inconclusive	Inconclusive	Active
1228	11076635	6533682	O=C([C@H](CO)[C@]2=CC=CC=C2)O[C@H]1C[C@H](N4C)[C@@H](O3)[C@H]3[C@@H]4C1	Scopolamine hydrobromide trihydrate	Inactive							
1229	11076637	22888706	O=C1C(C(O)=CC(O)=C2)=C2O[C@H]([C@J](C=C5)=CC3=C5O[C@H](CO)[C@H](C[C@H]4=C(C(OC)=C(O)C=C4)O3)[C@H]1O	Silybin	Inactive							
1230	11076641	361091	O=C(O)CC[C@@H](C)[C@]4([H])[C@1(C)[C@](CC4)([H])[C@@](C)[C@H](O)C3)([H])[C@](C)[C@2(C)C[C@H]3([H])C[C@H](O)CC2)([H])[C@H]1O	Sodium Cholate	Inactive							
1231	11076646	151213	OS(=O)(=O)OCCCCCCCCCC	Sodium lauryl sulfate	Inactive							
1232	11076648	1300727	Cc1ccc(cc1)S(O)(=O)=O	Sodium xylenesulfonate	Inactive							
1233	11076649	64092484	O=C(C2=C(C)C=C(C(C([O-])=O)N2C)C1=CC=C(Cl)C=C1	Sodium zomepirac	Inactive							
1234	11076653	110612	N#CCCC#N	Succinonitrile	Inactive							
1235	11076654	144809	S(=O)(=O)(NC(C)=O)c1ccc(N)cc1	Sulfacetamide	Inactive							
1236	11076655	723466	Cc1cc(NS(=O)(=O)c2ccc(N)cc2)no1	Sulfamethoxazole	Inactive							
1237	11076656	5329146	O=S(N)(O)=O	sulfamic acid	Inactive							
1238	11076657	72140	S(=O)(=O)(NC1=NC=CS1)c2ccc(N)cc2	Sulfathiazole	Inactive							

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1239	11076658	94075	OC(C1=CC=C(O)C=C1)CNC	p-Syneprine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1240	11076659	994058	CO(C(C)C)CC	Tertiary amyl methyl ether (TAME)	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1241	11076660	762754	O(C(C)(C)C)C=O	t-Butyl formate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1242	11076661	7665727	O(C1COC(C)(C)C)C1	t-Butyl glycidyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1243	11076662	614459	C(=O)(OOC(C)(C)C)c1ccccc1	tert-Butyl perbenzoate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1244	11076663	3101608	O(C1COC(ccc(c2)C(C)(C)C)c2)C1	t-Butyl phenyl glycidyl ether	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1245	11076664	25103586	C(C(C(C)C(C)C)(C(C)(C)S)(C)C	tert-Dodecyl mercaptan	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1246	11076665	80443410	OC(C(C)(C)CN2N=CN=C2)CCC1	Tebuconazole	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1247	11076666	100210	=CC=C(Cl)C=C1	C(=O)(O)c1ccc(cc1)C(=O)O	Terephthalic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1248	11076668	75912	tert-Butyl Hydroperoxide (70% Solution in Water)	C(C)(C)OO	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1249	11076670	79947	Tetrabromobisphenol A	C(C)(C)c1cc(Br)c(O)c(Br)c1)c2cc(Br)c(O)c(Br)c2	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1250	11076671	21850442	BrC1=CC(C(C)(C)C2=CC(Br)=C(OC	C(Br)CBr)C(Br)=C2=CC(Br)=C1OC	Tetrabromobisphenol A-bis(2,3-dibromopropyl ether)	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Active	
1251	11076672	632791	C(Br)CBr	O=C(OC(=O)c1c(c(c(c2Br)Br)Br)Br)c12	Tetrabromophthalic anhydride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1252	11076673	127184	Tetrachloroethylene	CIC(=C(Cl)Cl)Cl	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1253	11076674	117088	Tetrachlorophthalic anhydride	O=C(OC(=O)c1c(c(c(c2Cl)Cl)Cl)Cl)c12	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1254	11076675	17831719	Tetraethylene glycol diacrylate	O=C(OCCOCCOCCOCCOC(=O)C=C	C)C=C	Inactive	Active	Active	Inactive	Inconclusive	Active	Active	
1255	11076677	112572	Tetraethylenepentamine	N(CCNCCN)CCNCCN	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1256	11076678	1684408	1,2,3,4-Tetrahydro-9-acridinamine monohydrochloride	NC1=C2C(CCCC2)=NC3=CC=CC=C31)	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive	
1257	11076679	119642	Tetralin	C12=CC=CC=C1CCCC2	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1258	11076680	14866332	tetra-N-Octylammonium bromide	CCCCCCCC[N+](CCCCCCCC)(CCCCCCCC)CCCCCCCC	Active	Active	Active	Active	Active	Active	Active	Active	
1259	11076681	102089	Thiocarbanilide	N(c(ccc1)c1)C(=S)Nc(ccc2)c2	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1260	11076682	1077287	alpha-Lipoic acid	C(CCC(=O)O)C1CCSS1	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1261	11076683	23564058	Thiophanate M	S=C(Nc1cccc1NC(=S)NC(=O)OC)NC(=O)OC	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1262	11076684	110021	Thiophene	C1=CSC=C1	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1263	11076685	108883	Toluene	CC1=CC=CC=C1	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1264	11076686	156605	trans-1,2-Dichloroethylene	C1C=CCI	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1265	11076687	3234024	2,3-Dibromo-2-butene-1,4-diol	C(Br)(CO)=C(Br)CO	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1266	11076688	116314	Retinal	C1(C=CC(=CC=CC(=CC=O)C)C)=C(CCCC1(C)C)C	Active	Active	Active	Inconclusive	Active	Active	Active	Active	
1267	11076689	102761	Triacetin	O=C(C)OCC(OC(C)=O)COC(C)=O	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1268	11076690	1025156	Triallyl isocyanurate	C(C=C)N1C(=O)N(CC=C)C(=O)N(C=C)C1=O	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	

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1269	11076691	76039	CIC(C(=O)O)(Cl)Cl	Trichloroacetic acid	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1270	11076692	76028	O=C(Cl)C(Cl)(Cl)Cl	Trichloroacetyl chloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1271	11076693	78400	O=P(OCC)(OCC)OCC	Triethyl phosphate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1272	11076694	1582098	O=[N+](C1=C(C(=CC(=C1)C(F)(F)F)F)[N+](=O)[O-])N(CCC)CCC)[O-]	Trifluralin	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1273	11076695	603350	c(P(c(cccc1)c1)c(cccc2)c2)(cccc3)c3	Triphenyl phosphine	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1274	11076696	101020	O(c(cccc1)c1)P(Oc(cccc2)c2)Oc(cccc3)c3	Triphenyl phosphate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1275	11076697	2451629	C(C1CO1)N2C(=O)N(CC3CO3)C(=O)N(CC4CO4)C2=O	1,3,5-Triglycidyl isocyanurate	Active	Active	Inconclusive	Inconclusive	Active	Active	Active	Active	
1276	11076698	140089	CICCOP(OCCC)OCCCI	Tris(2-chloroethyl) phosphate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1277	11076699	3319311	O=C(OCC(CCCC)CC)c(cc(c1C(=O)OCC(CCCC)CC)C(=O)OCC(CCCC)CC)c1	Tris(2-ethylhexyl)trimellitate	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1278	11076700	9002931	OCCOC1=CC=C(C(CC(C)(C)C)(C)C)C=C1	Triton X-100	Inactive	Inactive	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inconclusive	
1279	11076701	25155231	Cc1cc(cc(C)c1)OP(=O)(Oc2cc(C)cc(C)c2)Oc3cc(C)cc(C)c3	Trixylenyl phosphate mixed isomers	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1280	11076702	60195	NCCCC1=CC=C(O)C=C1	Tyramine HCL	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1281	11076703	3569106	[H][C@@]12C([C@H](C=C(C)C(O)=O)CC[C@H]2C)=C(C)CC1	Valerenic Acid	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive	
1282	11076704	110598	N#CCCCCC	Valeronitrile valeryl chloride; pentanoyl chloride	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1283	11076705	638299	CIC(CCCC)=O	C.I Vat blue 1	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	
1284	11076706	482893	O=C1c2ccccc2NC1=C3Nc4cccc4C3=O	N#CC(CCCN(C)CCC2=CC=C(OC)C(OC)=C2)(C(C)C)C1=CC=C(OC)C(OC)=C1	C.I Vat blue 1	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1285	11076707	152114	O=C1cc(C=O)ccc1OC	Verapamil HCl	Inactive	Inconclusive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inconclusive
1286	11076708	120149	CC1=CC=CC(C=C)=C1	Veratraldehyde	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1287	11076709	25013154	C=C2C(C[C@H](O)CC2)=CC=C3[C@@]1([H])[C@@](CCC3)(C)[C@](C)CCCC(C)([H])CC1	Vinyl toluene	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
1288	11076710	67970	O=C(O2)C=C(OC)C=C2C=CC1=CC=C(OC)C=C1	Vitamin D3	Active	Active	Inconclusive	Inactive	Inconclusive	Active	Active	Active	Active
1289	11076711	500629	Yangonin		Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive

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Nm	PubChem SID	Test Substance CASRN	STRUCTURE_SMILES	TestSubstance_ChemicalName	CPDB Activity
1	7851494	75070	CC=O	Acetaldehyde	Active
2	7851498	103902	C1(CC=C(C=C1)O)NC(C)=O	Acetaminophen (4-hydroxyacetanilide)	Active
3	7851499	968810	O=S(=O)(C1=CC=C(C=C1)C(=O)C)NC(=O)NC2CCCCC2	Acetohexamide	Inactive
4	7851501	75058	CC#N	Acetonitrile	Inactive
5	7851507	114830	C1(NNC(C)=O)=CC=CC=C1	1-Acetyl-2-phenyl hydrazide	Active
6	7851515	107028	C=CC=O	Acrolein	Inactive
7	7851521	107131	C=CC#N	Acrylonitrile	Active
8	7851523	50760	C12C(OC3=C(N=1)C(=CC=C3C)C(NC4C(NC(C(N5C(CCC5)C(N(CC(N(C(C(OC4)C)=O)C(C(C)C)=O)C)=O)=O)C(C(=C2C(=NC6C(NC(C(N7C(CCC7)C(N(CC(N(C(C(OC6C)=O)C(C(C)C)=O)C)=O)=O)C(C)C)=O)=O)N)=O)C	Actinomycin D	Active
9	7851524	628944	NC(=O)CCCCC(=O)N	Adipamide	Inactive
10	7851531	116063	CC(C=NOC(=O)NC)(SC)C	Aldicarb	Inactive
11	7851532	309002	C1C(Cl)(Cl)C43Cl)(C(Cl)=C4Cl)C1C3C2C=CC1C2	Aldrin	Active
12	7851536	107186	C=CCO	Allyl alcohol	Inactive
13	7851537	107051	C=CCCI	Allyl chloride	Inactive
14	7851538	106923	C=CCOCC1CO1	Allyl glycidyl ether	Marginally Active
15	7851539	57067	C=CCN=C=S	Allyl isothiocyanate	Marginally Active
16	7851545	17026812	NC1=C(C=CC(=C1)NC(=O)C)OCC	3-Amino-4-ethoxyacetanilide	Marginally Active
17	7851549	82280	O=C1C2=C(C(=CC=C2C(=O)C3=C1C=CC=C3)C)N	1-Amino-2-methylanthraquinone	Active
18	7851554	99570	O=[N+](C1=CC(=C(C=C1)O)N)[O-]	2-Amino-4-nitrophenol	Marginally Active
19	7851555	121880	O=[N+](C1=CC(=C(C=C1)O)O)[O-]	2-Amino-5-nitrophenol	Marginally Active
20	7851556	119346	OC1=C(C=C(C=C1)N)[N+](=O)[O-]	4-Amino-2-nitrophenol	Marginally Active
21	7851558	121664	O=[N+](C1=CN=C(S1)N)[O-]	2-Amino-5-nitrothiazole	Active
22	7851560	117793	O=C1C2=CC(=CC=C2C(=O)C3=C1C=CC=C3)N	2-Aminoanthraquinone	Active
23	7851561	97563	CC1=C(C=CC=C1)N=NC2=CC(=C(C=C2)N)C	o-Aminoazotoluene	Active
24	7851563	92671	NC1=CC=C(C=C1)C2=CC=CC=C2	4-Biphenylamine	Active
25	7851575	7177482	N12C(C1=O)(NC(C(C3=CC=CC=C3)N)=O)[H])(SC(C2C(O)=O)(C)C)[H]	Ampicillin trihydrate	Inactive
26	7851578	104461	CC=CC1=CC=C(C=C1)OC	Anethole	No Conclusion
27	7851581	101053	C1C=NC(=NC(=N1)NC2=CC=CC=C2Cl)Cl	Anilazine	Inactive
28	7851582	62533	NC1=CC=CC=C1	Aniline	No Conclusion
29	7851585	20265978	C1(=CC=C(N)C=C1)OC	p-Anisidine hydrochloride	Inactive
30	7851586	118923	NC1=C(C=CC=C1)C(=O)O	o-Anthrаниlic acid	Inactive
31	7851598	50817	OC=1C(OC(=O)C=1O)C(O)CO	L-Ascorbic acid	Inactive
32	7851599	22839470	O=C(C(CC1=CC=CC=C1)NC(=O)C(CC(=O)O)N)OC	Aspartame	Inactive
33	7851604	1912249	C1C=NC(=NC(=N1)NC(C)C)NCC	Atrazine	Active
34	7851606	2465272	N=C(C2=CC=C(N(C)C)C=C2)C1=CC=C(N(C)C)C=C1	Auramine	Active
35	7851608	320672	NC1=NC(=O)N(C=N1)C2OC(CO)C(O)C2O	5-Azacytidine	Active
36	7851609	3131600	OC(C2O)C(OC2CO)N(N=CC(N)=N1)C1=O	6-Azacytidine	No Conclusion
37	7851611	446866	[O-][N+](C(N=C3)=C(SC1=NC=NC2=C1NC=N2)N3C)=O	Azathioprine	Active
38	7851614	86500	O=C1C2=C(C=CC=C2)N=NN1CSP(=S)(OC)OC	Azinphosmethyl	Inactive

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39	7851615	103333	C1(N=NC2=CC=CC=C2)=CC=CC=C1	Azobenzene	Active
40	7851619	30516871	CC1=CN(C(=O)NC1=O)C2CC(N=[N+]=[N-])C(CO)O2	3'-Azido-3'-deoxythymidine (AIDS)	Active
41	7851626	100527	O=CC1=CC=CC=C1	Benzaldehyde	Active
42	7851629	92875	NC1=CC=C(C2=CC=C(N)C=C2)C=C1	Benzidine	Active
43	7851633	271896	C1=COC2=C1C=CC=C2	Benzofuran	Active
44	7851635	65850	OC(=O)C1=CC=CC=C1	Benzoic acid	No Conclusion
45	7851636	119539	C1=CC=CC(=C1)C(C2=CC=CC=C2)=O	Benzoin	Inactive
46	7851637	106514	O=C1C=CC(=O)C=C1	p-Quinone	Active
47	7851638	120785	N1=C(SSC2=NC3=C(C=CC=C3)S2)SC4=C1C=CC=C4	2,2'-Dithiobis-benzothiazole	Inactive
48	7851639	95147	N1C2=C(C=CC=C2)N=N1	1,2,3-Benzotriazole	Inactive
49	7851643	140114	CC(=O)OCC1=CC=CC=C1	Benzyl acetate	Active
50	7851644	100516	OCC1=CC=CC=C1	Benzyl alcohol	Inactive
51	7851645	100447	CICC1=CC=CC=C1	Benzyl chloride	Active
52	7851646	120321	OC1=C(C=C(C=C1)Cl)CC2=CC=CC=C2	o-Benzyl-p-chlorophenol	Marginally Active
53	7851653	92524	C1=C(C=CC=C1)C2=CC=CC=C2	Biphenyl	Inactive
54	7851660	111444	CICCOCCCC	Bis(2-chloroethyl)ether	Marginally Active
55	7851685	33229344	C1(=C(C=CC(=C1)N(CCO)CCO)NCCO)[N+](O-)=O	HC blue 2	Inactive
56	7851690	75274	CIC(Cl)Br	Bromodichloromethane	Active
57	7851691	74964	CCBr	Bromoethane (ethyl bromide)	Active
58	7851692	540512	OCCBr	2-Bromo-1-ethanol	Active
59	7851697	85687	C1(=C(C=CC=C1)C(OCCCC)=O)C(OCC2=CC=CC=C2)=O	Butyl benzyl phthalate	Marginally Active
60	7851698	109693	CCCCCC	n-Butyl chloride	Inactive
61	7851701	94268	C(C1=CC=C(C=C1)O)(=O)OCCCC	n-Butyl-p-hydroxybenzoate	Inactive
62	7851708	128370	OC1=C(C=C(C=C1C(C(C)C)C)C(C)C)C	Butylated hydroxytoluene	Active
63	7851712	1948330	CC(C)(C)c1cc(O)ccc1O	t-Butylhydroquinone	Inactive
64	7851715	3068880	CC1CC(=O)O1	beta-Butyrolactone	Marginally Active
65	7851724	58082	O=C1C2=C(N=CN2C)N(C(=O)N1C)C	Caffeine	Inactive
66	7851733	404864	OC1=C(C=C(C=C1)CNC(=O)CCCCC=CC(C)C)OC	Capsaicin	Active
67	7851736	563417	C(NN)(N)=O	Semicarbazide hydrochloride	Active
68	7851739	63252	O=C(OC1=C2C(=CC=C1)C=CC=C2)NC	Carbaryl	Marginally Active
69	7851740	86748	C12C3=C(C=CC=C3)NC1=CC=CC=2	Carbazole	Active
70	7851748	2244168	O=C1CC(CC=C1C)C(C)=C	D-Carvone	Inactive
71	7851749	120809	OC1=C(C=CC=C1)O	Catechol	Active
72	7851754	133904	C1C1=C(C=C(C=C1)O)Cl)N	Chloramben	Marginally Active
73	7851755	305033	C1CCN(C1=CC=C(C=C1)CCCC(=O)O)CCCl	Chlorambucil	Active
74	7851757	56757	O=C(C(Cl)Cl)NC(CO)C(C1=CC=C([N+](O-)=O)C=C1)O	Chloramphenicol	No Conclusion
75	7851758	118752	O=C1C(=C(C(=O)C(=C1Cl)Cl)Cl)Cl	Chloranil	Inactive
76	7851760	115286	C1C2(Cl)C1(Cl)C(Cl)=C(Cl)C2(Cl)C(C1C(O)=O)C(O)=O	Chlorendic acid	Active
77	7851768	77439760	O=C1OC(O)C(C(Cl)Cl)=C1Cl	3-Chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone(MX)	Active
78	7851772	88733	C1C1=C(C=CC=C1)[N+](=O)[O-]	2-Chloronitrobenzene	Active
79	7851773	100005	O=[N+](C1=CC=C(C=C1)Cl)[O-]	4-Chloronitrobenzene	Active
80	7851775	95830	NC1=C(C=CC=C1)Cl)N	4-Chloro-o-phenylenediamine	Active
81	7851776	61702441	Nc1cc(Cl)c(N)cc1	2-Chloro-p-phenylenediamine sulfate	Inactive

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82	7851778	95749	C1C=C(C=CC(=C1)N)C	3-Chloro-p-toluidine	Inactive
83	7851779	95794	NC1=CC(=CC=C1C)Cl	5-Chloro-o-toluidine	Active
84	7851785	532274	O=C(C1=CC=CC=C1)CCl	2-Chloroacetophenone (CN)	Inactive
85	7851786	140498	C1CC(=O)C1=CC=C(NC(=O)C)C=C1	4-(Chloroacetyl)acetanilide	Inactive
86	7851787	106478	NC1=CC=C(C=C1)Cl	p-Chloroaniline	Inactive
87	7851790	108907	C1C=CC=CC=C1	Chlorobenzene	Marginally Active
88	7851792	124481	C1C(Br)Br	Chlorodibromomethane	Marginally Active
89	7851798	67663	C1C(Cl)Cl	Chloroform	Active
90	7851800	6959473	C1(C=CC=CN=1)CCl	2-Chloromethylpyridine hydrochloride	Inactive
91	7851803	150685	O=C(N(C)C)NC1=CC=C(C=C1)Cl	Monuron	Active
92	7851807	76062	C1C([N+](=O)[O-])(Cl)Cl	Chloropicrin	Inactive
93	7851814	94202	O=S(=O)(C1=CC=C(C=C1)Cl)NC(=O)NCCC	Chlorpropamide	Inactive
94	7851820	117102	O=C1C2=C(C=CC=C2O)C(=O)C3=CC=CC(=C13)O	Danthron	Active
95	7851821	51481619	C1(CSCCNC(NC)=NC#N)=C(C)NC=N1	Cimetidine	Inactive
96	7851824	77929	OC(CC(=O)O)(CC(=O)O)C(=O)O	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	No Conclusion
97	7851840	91645	O=C1OC2=C(C=CC=C2)C=C1	Coumarin	Active
98	7851841	102501	CO C1=CC(=C(C=C1)N)C	m-Cresidine	Active
99	7851842	120718	NC1=CC(=CC=C1OC)C	p-Cresidine	Active
100	7851844	135206	C1(N(N=O)O)=CC=CC=C1	Cupferron	Active
101	7851850	7585399	OC8C(O)C1OC(CO)C8OC7OC(CO)C(OC6OC(CO)C(OC5OC(CO)C(OC4OC(CO)C(OC3OC(CO)C(OC2OC(CO)C(O1)C(O)C2O)C(O)C3O)C(O)C4O)C(O)C5O)C(O)C6O)C(O)C7O	beta-Cyclodextrin	Inactive
102	7851851	108941	O=C1CCCC1	Cyclohexanone	Inactive
103	7851858	427510	O=C1C3C(C3)C(C4C(C5C(C(CC5)(C(C)=O)OC(C)=O)(C)CC4)C=C2Cl)(C)C2=C1	Cyproterone acetate	Active
104	7851861	4342034	O=C(N)C1=C(N=CN1)N=NN(C)C	Dacarbazine	Active
105	7851862	1596845	O=C(CCC(=O)O)NN(C)C	Daminozide	Active
106	7851863	80080	O=S(=O)(C1=CC=C(C=C1)N)C2=CC=C(C=C2)N	4,4'-Sulfonyldianiline (Dapsone)	Active
107	7851864	53190	C1C(C1=C(C=CC=C1)Cl)C2=CC=C(C=C2)Cl)Cl	o,p'-DDD	Inactive
108	7851865	72548	C1C(C1=CC=C(C=C1)Cl)C2=CC=C(C=C2)Cl)Cl	Tetrachlorodiphenylethane	Active
109	7851867	50293	C1C(C1=CC=C(C=C1)Cl)C2=CC=C(C=C2)Cl)Cl	Dichlorodiphenyltrichloroethane (DDT)	Active
110	7851876	50022	OCC(=O)C4(O)C(C)CC1C4(C)CC(O)C2(F)C3(C)C=CC(=O)C=C3CCC12	Dexamethazone	No Conclusion
111	7851884	131179	O=C(C1=C(CC=C1)C(=O)OCC=C)OCC=C	Diallyl phthalate	Inactive
112	7851894	95807	NC1=C(CC(=C1)N)C	2,4-Diaminotoluene (2,4-toluene diamine)	Active
113	7851899	333415	S=P(OC1=NC(=NC(=C1)C)C(C)C)(OCC)OCC	Diazinon	Inactive
114	7851901	53703	C1=C2C=CC3=CC=CC=C3C2=CC4=CC=C5C(=C14)C=CC=C5	Dibenz(a,h)anthracene	Marginally Active
115	7851905	96128	BrC(CCl)CBr	1,2-Dibromo-3-chloropropane	Active
116	7851907	106934	BrCCBr	1,2-Dibromoethane	Active
117	7851908	488415	OC(C(O)CBr)C(O)C(O)CBr	Dibromomannitol	Active
118	7851918	99309	O=[N+](C1=CC(=C(C=C1)Cl)N)Cl)[O-]	Dichloran	Inactive
119	7851919	609201	NC1=C(C=C(C=C1)N)Cl	2,6-Dichloro-p-phenylenediamine	Active
120	7851920	79436	OC(=O)C(Cl)Cl	Dichloroacetic acid	Active
121	7851922	95501	C1C=C(CC=C1)Cl	1,2-Dichlorobenzene (o-dichlorobenzene)	Inactive

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122	7851925	612839	C1C=CC(C2=CC(Cl)=C(N)C=C2)=CC=C1N	3,3'-Dichlorobenzidine dihydrochloride	M marginally Active
123	7851926	110576	C1CCC=CCCl	trans-1,4-Dichloro-2-butene	M marginally Active
124	7851929	75343	CC(Cl)Cl	1,1-Dichloroethane	Inactive
125	7851930	107062	C1CCCCI	1,2-Dichloroethane	Active
126	7851931	120832	C1C1=C(C=CC(=C1)Cl)O	2,4-Dichlorophenol	Inactive
127	7851934	94757	C1C1=C(C=CC(=C1)Cl)OCC(=O)O	2,4-Dichlorophenoxyacetic acid	Inactive
128	7851935	94804	C1C1=C(C=CC(=C1)Cl)OCC(=O)OCCCC	Butyl(2,4-dichlorophenoxy) acetate	Inactive
129	7851940	78875	CC(Cl)CCI	1,2-Dichloropropane (propylene dichloride)	Active
130	7851941	62737	O=P(OC=C(Cl)Cl)(OC)OC	Dichlorvos	Active
131	7851942	115322	OC(C1=CC=C(C=C1)Cl)C2=CC=C(C=C2)Cl)C(Cl)(Cl)Cl	Dicofol	M marginally Active
132	7851943	1212299	S=C(NC1CCCCC1)NC1CCCCC1	N,N'-Dicyclohexylthiourea	Inactive
133	7851945	60571	C1C2=C(Cl)C3(Cl)C1C4CC(C1C2(Cl)C3(Cl)Cl)C5OC45	Dieldrin	Active
134	7851950	2921882	S=P(OC1=NC(=C(C=C1)Cl)Cl)(OCC)OCC	Chlorpyrifos (Dursban)	Inactive
135	7851954	111466	OCCOCOC	Diethylene glycol	M marginally Active
136	7851957	56531	OC2=CC=C(C=C2)C(CC)=C(CC)C1=CC=C(O)C=C1	Diethylstilbestrol	Active
137	7851958	105555	S=C(NCC)NCC	N,N'-Diethylthiourea	Active
138	7851966	119846	O=C1OC2=C(C=CC=C2)CC1	3,4-Dihydrocoumarin	Active
139	7851972	828002	CC1CC(OC(O1)C)OC(=O)C	Dimethoxane	Active
140	7851975	54150695	C1(=CC(=CC=C1)N)OC)OC	2,4-Dimethoxyaniline hydrochloride	Inactive
141	7851976	91930	CO C1=C(C=CC(=C1)C2=CC(=C(C=C2)N=C=O)OC)N=C=O	3,3'-Dimethoxybenzidine-4,4'-diisocyanate	Active
142	7851983	60117	CN(C1=CC=C(C=C1)N=NC2=CC=CC=C2)C	4-Dimethylaminoazobenzene	M marginally Active
143	7851996	58151	O=C1N(C2=CC=CC=C2)N(C(=C1N(C)C)C)C	4-Dimethylaminoantipyrine	Inactive
144	7851999	121697	CN(C1=CC=CC=C1)C	N,N-Dimethylaniline	M marginally Active
145	7852002	57976	CC1=C2C=CC=CC2=C(C3=CC=C4C(=C13)C=CC=C4)C	7,12-Dimethylbenzanthracene	M marginally Active
146	7852004	79447	O=C(N(C)C)Cl	Dimethylcarbamoyl chloride	M marginally Active
147	7852012	513371	CC(C)=CCl	Dimethylvinyl chloride (DMVC)	Active
148	7852015	51285	OC1=C(C=C(C=C1)[N+]([O-])[O-])[N+]([O-])[O-]	2,4-Dinitrophenol	Inactive
149	7852020	606202	CC1=C(C=CC=C1[N+]([O-])[O-])[N+]([O-])[O-]	2,6-Dinitrotoluene	M marginally Active
150	7852030	74317	N(C1=CC=C(C=C1)NC2=CC=CC=C2)C3=CC=CC=C3	N,N'-Diphenyl-p-phenylenediamine	Inactive
151	7852033	57410	O=C1C(C2=CC=CC=C2)(C3=CC=CC=C3)NC(=O)N1	5,5-Diphenylhydantoin (phenytoin)	M marginally Active
152	7852037	142461	NC(=S)NNC(=S)N	2,5-Dithiobiurea	Inactive
153	7852052	115297	C1C2=C(Cl)C3(Cl)C1COS(=O)OCC1C2(Cl)C3(Cl)Cl	Endosulfan	Inactive
154	7852058	106898	C1CC1CO1	Epichlorhydrin	Active
155	7852061	106887	CCC1CO1	1,2-Epoxybutane	Active
156	7852065	50282	Oc3cc4CCC1C(CCC2(C)C(O)CCC12)c4cc3	17beta-Estradiol	No Conclusion
157	7852067	140670	C=CCC1=CC=C(C=C1)OC	Estragole	M marginally Active
158	7852068	57636	[H]C14C(C3CCC(O)(C#C)C(C)C3CC4)CCC2=CC(O)=CC=C12	Ethinyl estradiol	M marginally Active
159	7852069	536334	NC(=S)C1=CC(=NC=C1)CC	Ethionamide	M marginally Active
160	7852073	938738	NC(=O)C1=C(C=CC=C1)OCC	2-Eethoxybenzamide	M marginally Active
161	7852074	91532	CC1=CC(NC2=C1C=C(C=C2)OCC)(C)C	Ethoxyquin	Inactive
162	7852076	64175	CCO	Ethanol	Active
163	7852079	105362	O=C(OCC)CBr	Ethyl bromoacetate	No Conclusion
164	7852081	72560	C1C(C1=CC=C(C=C1)CC)C2=CC=C(C=C2)CC)Cl	Di(p-ethylphenyl)dichloroethane	Inactive

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165	7852083	77838	CC1(C2=CC=CC=C2)C(O1)C(=O)OCC	Ethyl-3-methyl-3-phenylglycidate	Inactive
166	7852085	759739	NC(=O)N(CC)N=O	N-Ethyl-n-nitrosourea	Active
167	7852088	100414	CCC1=CC=CC=C1	Ethylbenzene	Active
168	7852089	107211	C(CO)O	Ethylene glycol	Inactive
169	7852093	96457	S=C1NCCN1	Ethylene thiourea (ETU)	Active
170	7852096	106876	O1C2C1CCC(C2)C1CO1	4-Vinyl-1-cyclohexene diepoxyde	No Conclusion
171	7852097	104767	CCC(CCCC)CO	2-Ethylhexanol	Marginally Active
172	7852098	103231	CCC(COC(=O)CCCCC(=O)OCC(CCCC)CC)CCCC	Di(2-ethylhexyl)adipate	Active
173	7852099	117817	O=C(C1=C(C=CC=C1)C(=O)OCC(CCCC)CC)OCC(CCCC)CC	Di(2-ethylhexyl) phthalate	Active
174	7852108	470826	CC2(C)OC1(C)CCC2CC1	1,8-Cineol	No Conclusion
175	7852109	97530	OC1=C(C=C(C=C1)CC=C)OC	Eugenol	Inactive
176	7852111	140567	CN(C)c1ccc(N=NS(O)(=O)=O)cc1	Formulated fenaminosulf	Inactive
177	7852112	55389	S=P(OC1=CC(=C(C=C1)SC)C)(OC)OC	Fenthion	Inactive
178	7852120	2164172	O=C(NC1=CC=CC(=C1)C(F)(F)F)N(C)C	Fluometuron	Inactive
179	7852126	51218	O=C1C(=CNC(=O)N1)F	5-Fluorouracil	Active
180	7852138	110009	C1=COC=C1	Furan	Active
181	7852139	98011	O=CC1=CC=CO1	Furfural	Active
182	7852140	54319	NS(C1=C(Cl)C=C(NCC2=CC=CO2)C(C(O)=O)=C1)(=O)=O	Furosemide	Marginally Active
183	7852142	149917	OC(=O)C1=CC(=C(C=C1)O)O	Gallic acid	No Conclusion
184	7852144	25812300	CC1=C(C=C(C=C1)C)OCCCC(C(=O)O)(C)C	Gemfibrozil	Marginally Active
185	7852145	548629	C[N+](C)=C1C=CC(=C1)=C(c2ccc(cc2)N(C)Cc3ccc(cc3)N(C)C	Hexamethyl-p-rosaniline chloride	Active
186	7852148	77065	OC(=O)C3C51CC(O)(CCC1C24C=CC(O)C(C)(C(=O)O2)C34)C(=C)C5	Gibberellic acid	Inactive
187	7852158	556525	OCC1CO1	Glycidol	Active
188	7852166	126078	O=C2C1=C(OC)C=C(OC)C(Cl)=C1OC32C(OC)=CC(CC(C)3[H])=O	Griseofulvin	Active
189	7852170	517282	OC1=C(O)C=C4C(CC(COC2=C3C=CC(O)=C2O)(C34[H])O)=C1	Hematoxylin	Active
190	7852171	76448	C1C=CC2C1C3(Cl)C(Cl)=C(Cl)C2(Cl)C3(Cl)Cl	Heptachlor	Active
191	7852173	111682	CCCCCCN	Heptylamine	No Conclusion
192	7852175	87683	C1C(Cl)=C(Cl)C(Cl)=C(Cl)Cl	Hexachloro-1,3-butadiene	Active
193	7852180	77474	C1C(=C(C(=C1Cl)Cl)Cl)Cl	Hexachlorocyclopentadiene	Inactive
194	7852181	67721	C1C(Cl)(Cl)Cl(Cl)Cl	Hexachloroethane	Active
195	7852182	70304	OC1=C(C=C(C=C1CC2=C(C(=CC(=C2Cl)Cl)Cl)O)Cl)Cl	Hexachlorophene	Inactive
196	7852188	628024	NC(=O)CCCCC	Hexanamide	Marginally Active
197	7852202	122667	N(C1=CC=CC=C1)NC2=CC=CC=C2	Hydrazobenzene	Active
198	7852205	58935	O=S1(=O)C2=C(C=C(C=C2)S(=O)(=O)N)Cl)NCN1	Hydrochlorothiazide	Inactive
199	7852208	123319	OC1=CC=C(C=C1)O	Hydroquinone	Active
200	7852232	53861	CC1=C(C2=C(C=CC(=C2)OC)N1C(=O)C3=CC=C(C=C3)Cl)CC(=O)O	Indomethacin	Marginally Active
201	7852235	75478	IC(I)I	Iodoform	Inactive
202	7852242	542563	CC(CON=O)C	Isobutyl nitrite	Active
203	7852247	54853	O=C(C1=CC=NC=C1)NN	Isoniazid	Active
204	7852253	78795	CC(=C)C=C	Isoprene	Active
205	7852254	67630	OC(C)C	Isopropanol	Inactive
206	7852259	120581	CC=CC1=CC2=C(C=C1)OCO2	Isosafrole (TGMX)	Inactive
207	7852260	520183	O=C1C2=C(C=C(C=C2O)O)OC(=C1O)C3=CC=C(C=C3)O	Kaempferol	Inactive

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208	7852262	143500	C1C54C(=O)C1(Cl)C2(Cl)C5(Cl)C3(Cl)C4(Cl)C1(Cl)C2(Cl)C3(Cl)Cl	Chlordecone (kepone)	Active
209	7852271	434139	O=C(O)CCC(C)C3C(CC2)(C)C(CC3)C(CC4)C2C1(C)C4CC(O)CC1	Lithocholic acid	Inactive
210	7852276	75330755	CC(CC)C(=O)OC2CC(C)=C3C=CC(C)C(CCC1CC(O)CC(=O)O1)C23	Lovastatin	Active
211	7852282	1634782	O=C(C(SP(=O)(OC)OC)CC(=O)OCC)OCC	Malaoxon	Inactive
212	7852283	121755	O=C(C(SP(=S)(OC)OC)CC(=O)OCC)OCC	Malathion	Inactive
213	7852284	123331	O=C1C=CC(=O)NN1	Maleic hydrazide	Inactive
214	7852296	148823	OC(C(CC1=CC=C(N(CCC1)CC1)C=C1)N)=O	Melphalan	Active
215	7852299	149304	SC1=NC2=C(C=CC=C2)S1	2-Mercaptobenzothiazole	Active
216	7852320	150765	COC1=CC=C(C=C1)O	Hydroquinone monomethyl ether	Active
217	7852322	298817	COC1=C2C(=CC3=C1OC=C3)C=CC(=O)O2	8-Methoxysoralen	Active
218	7852325	1634044	CC(OC)(C)C	Methyl-t-butyl ether	Active
219	7852336	80626	O=C(C(=C)C)OC	Methyl methacrylate	Inactive
220	7852337	66273	CS(=O)(=O)OC	Methyl methanesulfonate	Active
221	7852338	70257	N=C(N(N=O)C)N[N+](=O)[O-]	1-Methyl-3-nitro-1-nitroso-guanidine	Active
222	7852339	129157	O=C1C2=C(C=CC=C2C(=O)C3=C1C=CC=C3)C[N+](=O)[O-]	2-Methyl-1-nitroanthraquinone	Active
223	7852347	298000	S=P(OC1=CC=C(C=C1)[N+](=O)[O-])(OC)OC	Methyl parathion	Inactive
224	7852357	101144	C1C1=C(C=CC(=C1)CC2=CC(=C(C=C2)N)Cl)N	4,4'-Methylenebis(2-chloroaniline)	Active
225	7852360	75092	C1C1I	Methylene chloride	Active
226	7852361	101611	CN(C)C2=CC=C(C=C2)CC1=CC=C(N(C)C)C=C1	4,4'-Methylenebis(N,N-dimethyl)benzenamine	Active
227	7852369	90120	CC1=C2C(=CC=C1)C=CC=C2	1-Methylnaphthalene	Inactive
228	7852370	91576	CC2=CC1=CC=CC=C1C=C2	2-Methylnaphthalene	Inactive
229	7852378	298599	C(C1=CC=CC=C1)(C2CCCCN2)C(OC)=O	Methylphenidate hydrochloride	Active
230	7852379	91623	CC1=CC2=CC=CN=C2C=C1	6-Methylquinoline	Inactive
231	7852380	611325	CC1=CC=CC2=CC=CN=C12	8-Methylquinoline	Inactive
232	7852382	56042	CC1=CC(=O)NC(=S)N1	6-Methyl-2-thiouracil	Inactive
233	7852384	443481	N1(C(=CN=C1C)[N+](=O)[O-])CCO	Metronidazole	Active
234	7852393	79118	OC(=O)CCI	Monochloroacetic acid	Inactive
235	7852404	389082	O=C1C2=C(N=C(C=C2)C)N(C=C1C(=O)O)CC	Nalidixic acid	Active
236	7852405	91203	C1=C2C(=CC=C1)C=CC=C2	Naphthalene	M marginally Active
237	7852407	86873	OC(=O)CC1=C2C(=CC=C1)C=CC=C2	1-Naphthalene acetic acid	Inactive
238	7852408	2243621	NC1=C2C(=CC=C1)C(=CC=C2)N	1,5-Naphthalenediamine	Active
239	7852409	1465254	C12C(=CC=CC=1NCCN)C=CC=C2	N-(1-Naphthyl)ethylenediamine dihydrochloride	Inactive
240	7852412	134327	NC1=CC=CC2=C1C=CC=C2	1-Naphthylamine	M marginally Active
241	7852413	91598	NC1=CC2=C(C=CC=C2)C=C1	2-Naphthylamine	Active
242	7852422	54115	CN(CCC2)C2C1=CN=CC=C1	Nicotine	Inactive
243	7852431	139139	OC(=O)CN(CC(=O)O)CC(=O)O	Nitrilotriacetic acid (NTA)	Active
244	7852435	99592	O=[N+](C1=CC(=C(C=C1)OC)N)[O-]	5-Nitro-o-anisidine	Active
245	7852436	59870	O=[N+](C1=CC=C(O1)C=NNC(=O)N)[O-]	Nitrofurazone	Active
246	7852449	5307142	NC1=C(C=C(C=C1)N)[N+](=O)[O-]	2-Nitro-p-phenylenediamine	M marginally Active
247	7852450	99569	O=[N+](C1=CC(=C(C=C1)N)N)[O-]	4-Nitro-o-phenylenediamine	Inactive
248	7852451	99558	O=[N+](C1=CC(=C(C=C1)C)N)[O-]	5-Nitro-o-toluidine	Active
249	7852452	602879	O=[N+](C1=CC=C2C3=C1C=CC=C3CC2)[O-]	5-Nitroacenaphthene	Active
250	7852453	100016	O=[N+](C1=CC=C(C=C1)N)[O-]	p-Nitroaniline	Inactive

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251	7852454	91236	COC1=C(C=CC=C1)[N+](=O)[O-]	o-Nitroanisole	Active
252	7852455	619170	O=[N+](C1=CC(=C(C=C1)C(=O)O)N)[O-]	4-Nitroanthranilic acid	Inactive
253	7852456	98953	O=[N+](C1=CC=CC=C1)[O-]	Nitrobenzene	Active
254	7852457	94520	O=[N+](C1=CC2=C(C=C1)NC=N2)[O-]	6-Nitrobenzimidazole	Active
255	7852458	62237	OC(=O)C1=CC=C(C=C1)[N+](=O)[O-]	p-Nitrobenzoic acid	Marginally Active
256	7852459	627054	[O-][N+](=O)CCCC	1-Nitrobutane	No Conclusion
257	7852461	79243	O=[N+](CC)[O-]	Nitroethane	Inactive
258	7852464	67209	O=C1N(CC(=O)N1)N=CC2=CC=C(O2)[N+](=O)[O-]	Nitrofuranoin	Active
259	7852469	75525	[O-][N+](C)=O	Nitromethane	Active
260	7852470	86577	O=[N+](C1=C2C(=CC=C1)C=CC=C2)[O-]	1-Nitronaphthalene	Inactive
261	7852472	108032	O=[N+](CCC)[O-]	1-Nitropropane	Inactive
262	7852473	79469	CC([N+](=O)[O-])C	2-Nitropropane	Inactive
263	7852519	1116547	O>NN(CCO)CCO	N-Nitrosodiethanolamine	Active
264	7852520	55185	CCN(CC)N=O	N-Nitrosodiethylamine	Active
265	7852521	62759	CN(N=O)C	N-Nitrosodimethylamine	Active
266	7852522	86306	O>NN(C1=CC=CC=C1)C2=CC=CC=C2	N-Nitrosodiphenylamine	Active
267	7852523	156105	N(C1C=CC(=CC=1)N=O)C2=CC=CC=C2	p-Nitrosodiphenylamine	Active
268	7852552	100754	O=NN1CCCCC1	N-Nitrosopiperidine	Active
269	7852586	101804	NC1=CC=C(C=C1)OC2=CC=C(C=C2)N	4,4'-Oxydianiline	Active
270	7852589	2058460	O=C1C(C(O)=C2C3C(O)(C)C4=C(C(O)=CC=C4)C2=O)(O)C(C3O)C(N(C)C)C(O)=C1C(N)=O	Oxytetracycline hydrochloride	Inactive
271	7852597	82688	CIC1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)[N+](=O)[O-]	Pentachloronitrobenzene	M marginally Active
272	7852598	87865	OC1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl	Pentachlorophenol, purified	No Conclusion
273	7852608	62442	CC(=O)NC1=CC=C(C=C1)OCC	Phenacetin	Active
274	7852610	136403	NC1=CC=C(N=NC2=CC=CC=C2)C(N)=N1	Phenazopyridine hydrochloride	Active
275	7852613	834286	C1(CCNC(NC(N)=N)=N)=CC=CC=C1	Phenformin hydrochloride	Inactive
276	7852616	108952	OC1=CC=CC=C1	Phenol	Inactive
277	7852617	77098	O=C1OC(C2=C1C=CC=C2)(C3=CC=C(C=C3)O)C4=CC=C(C=C4)O	Phenolphthalein	Active
278	7852618	92842	N1C2=C(C=CC=C2)SC3=CC=CC=C13	Phenothiazine	Inactive
279	7852619	63923	C1CCN(C(COC2=CC=CC=C2)C)CC1=CC=CC=C1	Phenoxybenzamine hydrochloride	Active
280	7852622	89258	O=C1N(C2=CC=CC=C2)N=C(C1)C	1-Phenyl-3-methyl-5-pyrazolone	Inactive
281	7852623	135886	C1=C2C(=CC=C1NC3=CC=CC=C3)C=CC=C2	N-Phenyl-2-naphthylamine	Inactive
282	7852628	50339	O=C1N(C2=CC=CC=C2)N(C3=CC=CC=C3)C(=O)C1CCCC	Phenylbutazone	Active
283	7852629	108452	NC1=CC(=CC=C1)N	m-Phenylenediamine	Inactive
284	7852637	122601	O(C1=CC=CC=C1)CC2CO2	Phenyl glycidyl ether	Active
285	7852643	90437	OC1=C(C=CC=C1)C2=CC=CC=C2	o-Phenylphenol	M marginally Active
286	7852651	85449	O=C1C2=C(C=CC=C2)C(=O)O1	Phthalic anhydride	Inactive
287	7852658	51036	CCCC1=CC2=C(C=C1COCCOCCOCCCC)OCO2	Piperonyl butoxide	Active
288	7852677	53032	OCC(=O)C3(O)CCC2C4CCC1=CC(=O)C=CC1(C)C4C(=O)CC23C	Prednisone	Inactive
289	7852680	57669	O=S(=O)(C1=CC=C(C=C1)C(=O)O)N(CCC)CCC	Probenecid	M marginally Active
290	7852689	57578	O=C1CCO1	Propiolactone	Active
291	7852690	318989	OC(COC1=CC=CC2=C1C=CC=C2)CNC(C)C	Propranolol.HCl	Inactive
292	7852701	51525	O=C1C=C(NC(=S)N1)CCC	6-Propyl-2-thiouracil	Active

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293	7852707	98964	NC(=O)C1=NC=CN=C1	Pyrazinamide	Inactive
294	7852709	58140	NC1=C(C(=NC(=N1)N)CC)C2=CC=C(C=C2)Cl	Pyrimethamine	M marginally Active
295	7852714	105113	ON=C1C=CC(=NO)=C1	p-Benzoquinone dioxime	M marginally Active
296	7852716	6459945	CC1=CC(C4=CC(C)=C(N=NC5=CC=C(OS(=O)(C6=CC=C(C)C=C6)=O)C=C5)C=C4)=CC=C1N=NC2=C(O)C=CC3=CC(S(=O)(O)=O)=CC(S(=O)(O)=O)=C23	C.I. Acid red 114	Active
297	7852729	50555	COc1cc(cc(OC)c1OC)C(=O)OC4CC5CN6CCC3=C(Nc2cc(OC)ccc23)C6CC5C(C(=O)OC)C4OC	Reserpine	Active
298	7852730	108463	OC1=CC(=CC=C1)O	Resorcinol	Inactive
299	7852732	127479	CC1(C(=C(CCC1)C)C=CC(=CC=CC(=CCOC(=O)C)C)C)	Retinol acetate	Active
300	7852736	13292461	O=C1C(C2=C(C(O)=C3C)C(O)=C(NC(C(C)=CC=CC5C)=O)C(C=NN4CCN(C)CC4)=C2O)=C3OC(C1OC=CC(OC)C(C)C(OC(C)=O)C(C)C(O)C(C)C5O	Rifampicin	M marginally Active
301	7852739	569619	C(C1=CC=C(C=C1)N)C2=CC=C(C=C2)N=C3C=CC(C=C3)=N	C.I. Basic red 9 monohydrochloride	Active
302	7852746	94597	C=CCC1=CC=C2C(=C1)OCO2	Safrole	Active
303	7852748	599791	C3=CC=CC(NS(=O)(=O)C2=CC=C(N=NC1=CC=C(O)C(C(O)=O)=C1)C=C2)=N3	Salicylazosulfapyridine	Active
304	7852759	533313	OC1=CC2=C(C=C1)OCO2	Sesamol	Active
305	7852769	110441	OC(=O)C=CC=CC	Sorbic acid	Inactive
306	7852776	100425	C=CC1=CC=CC=C1	Styrene	M marginally Active
307	7852778	96093	C1C(C2=CC=CC=C2)O1	Styrene oxide	Active
308	7852779	108305	O=C1OC(=O)CC1	Succinic anhydride	Inactive
309	7852781	95067	S=C(N(CC)CC)SCC(=C)Cl	Sulfallate	Active
310	7852782	57681	O=S(=O)(C1=CC=C(C=C1)N)NC2=NC(=CC(=N2)C)C	Sulfamethazine	Active
311	7852784	127695	C2=C(N)C=CC(S(=O)(=O)NC1ON=C(C)C=1C)=C2	Sulfisoxazole	Inactive
312	7852791	569573	C1C(=C(C1=CC=C(C=C1)OC)C2=CC=C(C=C2)OC)C3=CC=C(C=C3)OC	Chlorotrianisene	Inactive
313	7852796	107357	NCCS(O)(=O)=O	L-Taurine	Inactive
314	7852810	79345	C1C(Cl)Cl)Cl	1,1,2,2-Tetrachloroethane	Active
315	7852812	961115	C1C(=CC(Cl)=C(C(OP(=O)(OC)OC)=CCl)C=C1Cl	Tetrachlorvinphos	M marginally Active
316	7852820	109999	C1CCCC1	Tetrahydrofuran	Active
317	7852824	137268	S=C(N(C)C)SSC(=S)N(C)C	Tetramethylthiouram disulfide	Inactive
318	7852826	509148	O=[N+](C([N+])(=O)[O-])([N+](=O)[O-])[N+](=O)[O-])[O-]	Tetranitromethane	Active
319	7852828	58559	O=C2C=1N=CNC=1N(C)C(=O)N2C	Theophylline	Inactive
320	7852829	148798	N1C(=NC2=C1C=CC=C2)C3=CSC=N3	Thiabendazole	Inactive
321	7852833	96695	CC(C1=CC(=C(C=C10)C)SC2=CC(=C(C=C2C)O)C(C)(C)C)(C)C	4,4-Thiobis(6-tert-butyl-m-cresol)	Inactive
322	7852834	97187	OC1=C(C=C(C=C1SC2=C(C=CC(=C2)Cl)Cl)O)Cl)Cl	2,2'-Thiobis(4,6-dichlorophenol)	Inactive
323	7852836	139651	C1=CC=C(C=C1)SC2=CC=C(C=C2)N	4,4'-Thiodianiline	Active
324	7852838	79196	NC(=S)NN	Thiosemicarbazide	Inactive
325	7852840	62566	NC(=S)N	Thiourea	M marginally Active
326	7852851	64777	O=S(=O)(C1=CC=C(C=C1)C)NC(=O)NCCCC	Tolbutamide	Inactive
327	7852856	636215	NC1=CC=CC(C)=C1	o-Toluidine hydrochloride	Active
328	7852860	8001352	C1C2(Cl)C1(Cl)C(=C)C(CCl)(CCl)C2(Cl)C(Cl)C1Cl	Toxaphene	Active
329	7852865	396010	NC1=C2C(=NC(=N1)N)N=C(C(=N2)C3=CC=CC=C3)N	Triamterene	Active
330	7852866	75252	BrC(Br)Br	Tribromomethane	Active
331	7852867	538238	O=C(OC(COC(=O)CCCCCCCC)CO(=O)CCCCCCCC)CCCCCCCC	Tricaprylin	M marginally Active

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332	7852871	634935	NC1=C(C=C(C=C1Cl)Cl)Cl	2,4,6-Trichloroaniline	Active
333	7852872	79005	CIC(CCl)Cl	1,1,2-Trichloroethane	Active
334	7852875	79016	CIC(=CCl)Cl	Trichloroethylene	Active
335	7852876	75694	FC(Cl)(Cl)Cl	Trichlorofluoromethane	Inactive
336	7852878	88062	OC1=C(C=C(C=C1Cl)Cl)Cl	2,4,6-Trichlorophenol	Active
337	7852882	96184	CICC(Cl)CCI	1,2,3-Trichloropropane	Active
338	7852883	1330785	O=P(OC2=CC=C(C)C=C2)(OC3=CC=C(C)C=C3)OC1=CC=C(C)C=C1	Tricresyl phosphate	Inactive
339	7852890	137177	CC1=CC(=C(C=C1C)N)C	2,4,5-Trimethylaniline	Active
340	7852903	115968	O=P(OCCC)(OCCCC)OCCCI	Tris(2-chloroethyl) phosphate	Active
341	7852906	78422	O=P(OCC(CCCC)CC)(OCC(CCCC)CC)OCC(CCCC)CC	Tris(2-ethylhexyl)phosphate	M marginally Active
342	7852918	57136	C(N)(N)=O	Urea	Inactive
343	7852923	108054	CC(=O)OC=C	Vinyl acetate	Active
344	7852929	100403	C=CC1CCC=CC1	4-Vinylcyclohexene	M marginally Active
345	7852930	75354	C=C(Cl)Cl	Vinylidene chloride	Active
346	7852939	1330207	CC1=C(C)C=CC=C1	Xylenes (mixed)	Inactive
347	7852952	17924924	OC1=CC(=CC2=C1C(=O)OC(CCCC(=O)CCCC=C2)C)O	Zearalenone	Active
348	7853213	71556	CC(Cl)(Cl)Cl	1,1,1-Trichloroethane	Inactive
349	7853380	121142	CC1=C(C=C(C=C1)[N+](=O)[O-])[N+](=O)[O-]	2,4-Dinitrotoluene	No Conclusion
350	7853396	127004	OC(C)CCI	1-Chloro-2-propanol	Inactive
351	11075907	542756	CIC=CCCI	1-Propene, 1,3-dichloro-	M marginally Active
352	11075945	3296900	OCC(CO)(CBr)CBr	2,2-Bis(bromomethyl)-1,3-propanediol	Active
353	11075979	25168267	O=C(COC1=C(Cl)C=C(Cl)C=C1)OCC(CC)CCCC	2,4-D, Isooctyl ester, 67%	Inactive
354	11076103	563473	CC(=C)CCI	3-Chloro-2-methylpropene	Active
355	11076162	148243	OC1=CC=CC2=CC=CN=C12	8-Hydroxyquinoline	Inactive
356	11076173	50782	OC(=O)C1=C(C=CC=C1)OC(=O)C	Acetylsalicylic acid	Inactive
357	11076174	79061	NC(=O)C=C	Acrylamide	Active
358	11076207	71432	C1=CC=CC=C1	Benzene	Active
359	11076218	98077	CIC(C1=CC=CC=C1)Cl	Benzotrichloride	Active
360	11076230	108601	CC(CCl)OC(C)CCI	Bis(2-chloro-1-methylethyl) ether	Active
361	11076233	80057	OC2=CC=C(C=C2)C(C)(C)C1=CC=C(O)C=C1	Bisphenol A	Inactive
362	11076251	133062	O=C1N(C(=O)C2C1CC=CC2)SC(Cl)(Cl)Cl	Captan 90-concentrate (solid)	Active
363	11076254	56235	CIC(Cl)(Cl)Cl	Carbon tetrachloride	Active
364	11076266	63449398	CIC(CCCC(Cl)CCC(Cl)CCC(Cl)CCCC(Cl)CCC)CCC	Chlorowax 40	Active
365	11076288	458377	O=C(CC(C=CC2=CC=C(O)C(OC)=C2)=O)C=CC1=CC=C(O)C(OC)=C1	Curcumin	No Conclusion
366	11076329	101906	C1=C(C=CC=C1OCC2CO2)OCC3CO3	Diglycidyl resorcinol ether (DGRE)	Active
367	11076362	140885	O=C(OCC)C=C	Ethyl acrylate (inhibited)	Active
368	11076388	56815	OCC(O)CO	Glycerol	Inactive
369	11076451	72435	CIC(C(=C=CC=C(C=C1)OC)C2=CC=C(C=C2)OC)(Cl)Cl	Methoxychlor [95%]	Inactive
370	11076486	55981	O(S(=O)(=O)C)CCCCOS(=O)(C)=O	Myleran	No Conclusion
371	11076493	68122	CN(C=O)C	N,N-Dimethylformamide	Inactive
372	11076567	72559	CIC(=C(C1=CC=C(C=C1)Cl)C2=CC=C(C=C2)Cl)Cl	p,p'-DDE (p,p'-Dichlorodiphenyldichloroethylene)	Active
373	11076576	56382	S=P(OC1=CC=C(C=C1)[N+](=O)[O-])(OCC)OCC	Parathion	Inactive
374	11076595	103855	NC(=S)NC1=CC=CC=C1	Phenylthiourea	Inactive

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375	11076596	136776	<chem>OC1=C(C=CC(=C1)O)CCCCC</chem>	4-Hexylresorcinol	Inactive
376	11076600	1918021	<chem>C1C=C(Cl)N=C(C(O)=O)C(Cl)=C1N</chem>	Picloram	Inactive
377	11076617	57556	<chem>CC(CO)O</chem>	Propylene glycol	Inactive
378	11076635	6533682	<chem>O=C(C(CO)C2=CC=CC=C2)OC1CC(N4C)C(O3)C3C4C1</chem>	Scopolamine hydrobromide trihydrate	Inactive
379	11076673	127184	<chem>C1C(=C(Cl)Cl)Cl</chem>	Tetrachloroethylene	Active
380	11076685	108883	<chem>CC1=CC=CC=C1</chem>	Toluene	Active
381	11076691	76039	<chem>C1C(C(=O)O)(Cl)Cl</chem>	Trichloroacetic acid	Active
382	11076694	1582098	<chem>O=[N+](C1=C(C(=CC(=C1)C(F)(F)F)[N+]([O-])N(CCC)CCC)[O-]</chem>	Trifluralin	Active
383	11076709	25013154	<chem>CC1=CC=CC(C=C)=C1</chem>	Vinyl toluene	Inactive