

## Supporting Information

**Table 1.** Assay performance as measured by plate QC statistics and positive control behavior for all 13 caspase-3/7 assays.

Cell Type (Passage)	S/B	CV	Z'	Control	Concentration	EC50 ( $\mu$ M)	R2	Hill Coefficient
Mesangial cell (P18)	16.4 $\pm$ 0.6	21 $\pm$ 24	0.84 $\pm$ 0.03	Staurosporine	10 (20; 1:3)	0.2 $\pm$ 0.04	0.96 $\pm$ 0.02	1.6 $\pm$ 0.5
NIH 3T3 (P7)	8.6 $\pm$ 0.7	23 $\pm$ 26	0.81 $\pm$ 0.03	Staurosporine	3 (46; 1:3)	0.4 $\pm$ 0.2	0.89 $\pm$ 0.02	1.3 $\pm$ 0.3
SK-N-SH (P6)	11.9 $\pm$ 0.5	25 $\pm$ 23	0.87 $\pm$ 0.02	Staurosporine	10 (20; 1:3)	0.7 $\pm$ 0.2	1 $\pm$ 0.001	1.1 $\pm$ 0.1
N2a (P9)	5.5 $\pm$ 0.2	12 $\pm$ 7	0.86 $\pm$ 0.05	Staurosporine	10 (20; 1:3)	0.9 $\pm$ 0.2	1 $\pm$ 0.001	1.1 $\pm$ 0.1
BJ (P8)	9.9 $\pm$ 0.3	16 $\pm$ 13	0.87 $\pm$ 0.02	Staurosporine	10 (20; 1:3)	1.2 $\pm$ 0.4	0.99 $\pm$ 0.01	1.1 $\pm$ 0.2
SH-SY5Y (P13)	7.9 $\pm$ 0.8	20 $\pm$ 14	0.80 $\pm$ 0.04	Staurosporine	10 (20; 1:3)	1.8 $\pm$ 0.5	0.99 $\pm$ 0.003	1.2 $\pm$ 0.1
MRC-5 (P10)	9.4 $\pm$ 0.7	18 $\pm$ 12	0.82 $\pm$ 0.05	Staurosporine	10 (20; 1:3)	2.8 $\pm$ 0.3	0.99 $\pm$ 0.004	2.4 $\pm$ 0.5
Rat kidney proximal tubule (N/A)	2.0 $\pm$ 0.1	19 $\pm$ 4	-0.04 $\pm$ 0.15	Staurosporine	10 (20; 1:3)	11.4 $\pm$ 1.3	0.91 $\pm$ 0.03	1.8 $\pm$ 0.6
Jurkat (P10)	7.2 $\pm$ 0.5	26 $\pm$ 27	0.86 $\pm$ 0.03	Tamoxifen	100 (100; 1:1.5)	54 $\pm$ 10	0.91 $\pm$ 0.03	3.5 $\pm$ 0.6
HUV-EC-C (P9)	8.6 $\pm$ 0.7	28 $\pm$ 8	0.52 $\pm$ 0.11	Tamoxifen	100 (100; 1:1.5)	66 $\pm$ 11	0.95 $\pm$ 0.03	2.8 $\pm$ 0.5
H-4-II-E (P11)	14.1 $\pm$ 0.6	32 $\pm$ 42	0.46 $\pm$ 0.26	Tamoxifen	100 (100; 1:1.5)	68 $\pm$ 15	0.96 $\pm$ 0.04	3.8 $\pm$ 1.1
HEK 293 (P19)	8.7 $\pm$ 1.0	19 $\pm$ 25	0.46 $\pm$ 0.15	Tamoxifen	100 (100; 1:1.5)	76 $\pm$ 10	0.94 $\pm$ 0.03	3.0 $\pm$ 0.8
HepG2 (P15)	16.9 $\pm$ 1.1	26 $\pm$ 36	0.81 $\pm$ 0.05	Tamoxifen	100 (100; 1:1.5)	79 $\pm$ 10	0.94 $\pm$ 0.01	3.2 $\pm$ 0.7

**Table 2.** MeSH pharmacological action terms for 541 compounds in the NIEHS collection.

PubChem SID	Name	Pharmacological Action Terms
7851619	3'-Azido-3'-deoxythymidine (AZT)	Anti-HIV Agents; Antimetabolites; Antimicrobials and chemotherapeutics; Enzymes and inhibitors; HIV-PROTEASE-INHIBITORS; PEPTIDE-HYDROLASE-INHIBITORS; Reverse Transcriptase Inhibitors; REVERSE-TRANSCRIPTASE-INHIBITORS; THYMIDINE-KINASE-INHIBITORS; VIRUCIDES;
7854266	3TC (lamavudine)	Anti-HIV Agents; Antimicrobials and chemotherapeutics; Enzymes and inhibitors; Reverse Transcriptase Inhibitors; REVERSE-TRANSCRIPTASE-INHIBITORS; VIRUCIDES;
7851739	Carbaryl	ANTICHOLINESTERASES; Cholinesterase Inhibitors; Drugs acting on the nervous system; Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076304	d-Camphor	ANALEPTICS; ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; ANTIPIRETICS; Drugs acting on the respiratory system;
7852247	Isoniazid	Anesthetics and drugs relieving fever, inflammation and pain; Antimicrobials and chemotherapeutics; ANTIPIRETICS; Antitubercular Agents; TUBERCULOSTATICS;
7851905	1,2-Dibromo-3-chloropropane	Antinematodal Agents; Insecticides;
11076629	Resveratrol	ANTIARTERIOSCLEROTICS; Anticarcinogenic Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimutagenic Agents; Antineoplastic Agents, Phytogenic; Antioxidants; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Enzyme Inhibitors; HEPATOTROPICS; Platelet Aggregation Inhibitors;
7852436	Nitrofurazone	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; Anti-Infective Agents, Urinary; ANTIPIRETICS; Trypanocidal Agents;
7854030	2',3'-Dideoxyinosine (ddI)	Activity terms, miscellaneous; Anesthetics, Local; Anti-Allergic Agents; Anti-Bacterial Agents; ANTIBIOTICS; Antiemetics; ANTIEMETICS; ANTIHISTAMINES-H1; Anti-HIV Agents; Antimetabolites; Antimicrobials and chemotherapeutics; Antiparkinson Agents; Antipruritics; Antitussive Agents; Convulsants; Drugs acting on the gastrointestinal system; Enzyme Inhibitors; Enzymes and inhibitors; GABA Modulators; Histamine H1 Antagonists; HIV-PROTEASE-INHIBITORS; Hypnotics and Sedatives; PEPTIDE-HYDROLASE-INHIBITORS; Psychotropic agents; Reverse Transcriptase Inhibitors; SEDATIVES; VIRUCIDES;
7854823	2-Hydroxy-4-methoxybenzophenone	Drugs acting on the skin; RADIOPROTECTIVES; Sunscreening Agents;
7854852	Dimethyl phthalate	Fixatives; Insect Repellents;
7852422	Nicotine	Central Nervous System Stimulants; Drugs acting on the nervous system; Ganglionic Stimulants; GANGLION-STIMULANTS; Nicotinic Agonists; PARASYMPATHOMIMETICS;
7852707	Pyrazinamide	Anesthetics and drugs relieving fever, inflammation and pain; Antimicrobials and chemotherapeutics; ANTIPIRETICS; Antitubercular Agents; TUBERCULOSTATICS;
7852337	Methyl methanesulfonate	Antineoplastic Agents, Alkylating; Mutagens;
11076655	Sulfamethoxazole	Anesthetics and drugs relieving fever, inflammation and pain;

		Anti-Infective Agents; ANTIPYRETICS;
7851724	Caffeine	Activity terms, miscellaneous; ANALEPTICS; Analgesics, Non-Narcotic; Anticonvulsants; ANTICONVULSANTS; Antimutagenic Agents; Central Nervous System Stimulants; DIURETICS; Drugs acting on the nervous system; Drugs acting on the respiratory system; Phosphodiesterase Inhibitors; PSYCHOSTIMULANTS; PSYCHOTONICS; Psychotropic agents;
11076403	Indole-3-carbinol	Anticarcinogenic Agents;
7852144	Gemfibrozil	ANTIARTERIOSCLEROTICS; Antilipemic Agents; Drugs acting on the blood and cardiovascular system;
11076678	Tetrahydroaminoacridine Monohydrate	Activity terms, miscellaneous; ANTIDOTES; Cholinesterase Inhibitors; Drugs acting on the nervous system; NEUROMUSC.BLOCKERS; Nootropic Agents; Parasympathomimetics;
7854751	2',3'-Dideoxycytidine (ddC)	Anticancer drugs and carcinogens; Anti-HIV Agents; Antimetabolites; Antimetabolites, Antineoplastic; Antimicrobials and chemotherapeutics; Antiviral Agents; CYTOSTATICS; Enzymes and inhibitors; HIV-PROTEASE-INHIBITORS; Immunosuppressive Agents; PEPTIDE-HYDROLASE-INHIBITORS; Reverse Transcriptase Inhibitors; VIRUCIDES;
11076252	Carbendazim	Activity terms, miscellaneous; Adrenergic alpha-Antagonists; Adrenergic Uptake Inhibitors; ANALGESICS; Analgesics, Non-Narcotic; Anesthetics and drugs relieving fever, inflammation and pain; Anthelmintics; ANTHELMINTICS; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Anticoagulants; ANTIDEPRESSANTS; Antidepressive Agents; Antidepressive Agents, Tricyclic; ANTIDIABETICS; ANTIEMETICS; Antifungal Agents; ANTIHISTAMINES-H1; ANTIHISTAMINES-H2; Antihypertensive Agents; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimalarials; Antimanic Agents; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiparkinson Agents; Antipruritics; ANTIPYRETICS; ANTISEROTONINS; Antithyroid Agents; Biocompatible Materials; Buffers; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; Cardiovascular Agents; Cathartics; Chelating Agents; CHELATORS; Coloring Agents; CYCLOOXYGENASE-1-INHIBITORS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; DIAGNOSTICS; Diuretics; Dopamine Agonists; DOPAMINERGICS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Drugs acting on the nervous system; Drugs acting on the skin; Enzyme Inhibitors; Enzymes and inhibitors; Estradiol Antagonists; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Expectorants; Fertility Agents, Female; Fixatives; Folic Acid Antagonists; Food Additives; FUNGICIDES; Fungicides, Industrial; Gastrointestinal Agents; Gout Suppressants; Histamine Agonists; Histamine H1 Antagonists; Hormones and antagonists; HYPOTENSIVES; IMMUNOSTIMULANTS; IMMUNOSUPPRESSIVES; Indicators and Reagents; Keratolytic Agents; KERATOLYTICS; Lipotropic Agents; Mutagens; Neuromuscular Depolarizing Agents; Nootropic Agents; PARASYMPATHOMIMETICS; PENETRATION-ENHANCERS; Progestins;

		<p>PROGESTOGENS; PROSTAGLANDIN-ANTAGONISTS; PROTOZOACIDES; PSYCHOSEDATIVES; PSYCHOSTIMULANTS; Psychotropic agents; Radiation-Protective Agents; Radiopharmaceuticals; Selective Estrogen Receptor Modulators; Serotonin Agonists; SYMPATHOLYTICS-ALPHA; THROMBOXANE-ANTAGONISTS; Tocolytic Agents; TRANQUILIZERS; Vasodilator Agents; Vitamins and antagonists; VITAMINS;</p>
7853336	Diethylamine	<p>Activity terms, miscellaneous; Adrenergic alpha-Antagonists; Adrenergic Uptake Inhibitors; ANALGESICS; Analgesics, Non-Narcotic; Anesthetics and drugs relieving fever, inflammation and pain; Anthelmintics; ANTHELMINTICS; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Anticoagulants; ANTIDEPRESSANTS; Antidepressive Agents; Antidepressive Agents, Tricyclic; ANTIDIABETICS; ANTIEMETICS; Antifungal Agents; ANTIHISTAMINES-H1; ANTIHISTAMINES-H2; Antihypertensive Agents; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimalarials; Antimanic Agents; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiparkinson Agents; Antipruritics; ANTIPYRETICS; ANTISEROTONINS; Antithyroid Agents; Biocompatible Materials; Buffers; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; Cardiovascular Agents; Cathartics; Chelating Agents; CHELATORS; Coloring Agents; CYCLOOXYGENASE-1-INHIBITORS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; DIAGNOSTICS; Diuretics; Dopamine Agonists; DOPAMINERGICS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Drugs acting on the nervous system; Drugs acting on the skin; Enzyme Inhibitors; Enzymes and inhibitors; Estradiol Antagonists; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Expectorants; Fertility Agents, Female; Fixatives; Folic Acid Antagonists; Food Additives; FUNGICIDES; Fungicides, Industrial; Gastrointestinal Agents; Gout Suppressants; Histamine Agonists; Histamine H1 Antagonists; Hormones and antagonists; HYPOTENSIVES; IMMUNOSTIMULANTS; IMMUNOSUPPRESSIVES; Indicators and Reagents; Keratolytic Agents; KERATOLYTICS; Lipotropic Agents; Mutagens; Neuromuscular Depolarizing Agents; Nootropic Agents; PARASYMPATHOMIMETICS; PENETRATION-ENHANCERS; Progestins; PROGESTOGENS; PROSTAGLANDIN-ANTAGONISTS; PROTOZOACIDES; PSYCHOSEDATIVES; PSYCHOSTIMULANTS; Psychotropic agents; Radiation-Protective Agents; Radiopharmaceuticals; Selective Estrogen Receptor Modulators; Serotonin Agonists; SYMPATHOLYTICS-ALPHA; THROMBOXANE-ANTAGONISTS; Tocolytic Agents; TRANQUILIZERS; Vasodilator Agents; Vitamins and antagonists; VITAMINS;</p>
11076004	2,6-Toluenediamine	Carcinogens; Mutagens;
7851934	2,4-Dichlorophenoxyacetic acid (2,4-D)	Herbicides; HERBICIDES; Pesticides and plant hormones;
11076648	Sodium xylenesulfonate	Anticoagulants; Anti-Inflammatory Agents, Non-Steroidal; Antimicrobials and chemotherapeutics; Drugs acting on the blood and cardiovascular system; Enzyme Inhibitors;

		HEPARINOIDS; VIRUCIDES;
7851894	2,4-Diaminotoluene	Carcinogens; Mutagens;
7851863	Dapsone	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; ANTILEPROTICS; Antimalarials; Antimicrobials and chemotherapeutics; ANTIPYRETICS; Folic Acid Antagonists; Leprostatic Agents;
11076416	Isopropyl methanesulfonate	Alkylating Agents;
7854583	Ribavirin	Anti-HIV Agents; Antimetabolites; Antimicrobials and chemotherapeutics; Antiviral Agents; Enzymes and inhibitors; HIV-PROTEASE-INHIBITORS; PEPTIDE-HYDROLASE-INHIBITORS; Reverse Transcriptase Inhibitors; REVERSE-TRANSCRIPTASE-INHIBITORS; VIRUCIDES;
11076445	Melatonin	Adjuvants, Immunologic; Anticonvulsants; Antioxidants; Free Radical Scavengers;
7851768	3-Chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone, (MX)	Carcinogens; Mutagens;
11076352	dl-Camphor	ANALEPTICS; ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; ANTIPYRETICS; Drugs acting on the respiratory system;
7853387	Ethylene glycol monophenyl ether	Anesthetics; ANTICONVULSANTS; Anti-Infective Agents, Local; Drugs acting on the nervous system; PSYCHOSEDATIVES; Psychotropic agents; TRANQUILIZERS;
11076196	Ammonium nitrate	Explosive Agents; Fertilizers;
11076460	Methyl isothiocyanate	Disinfectants; Herbicides;
7851519	Acrylamide	ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain;
7852433	Sodium nitrite	Food Preservatives; Indicators and Reagents;
7852158	Glycidol	Carcinogens;
11076617	Propylene glycol	Solvents; Vehicles;
11076207	Benzene	Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076301	D4T (2',3'-Didehydro-3'-deoxythymidine)	Anti-HIV Agents; Antimetabolites; Antimicrobials and chemotherapeutics; Antiviral Agents; Enzymes and inhibitors; HIV-PROTEASE-INHIBITORS; PEPTIDE-HYDROLASE-INHIBITORS; Reverse Transcriptase Inhibitors; REVERSE-TRANSCRIPTASE-INHIBITORS; VIRUCIDES;
7851686	Boric acid	Insecticides;
11076450	Methoxyacetic acid	Immunosuppressive Agents;
7851957	Diethylstilbestrol [DES]	Antineoplastic Agents, Hormonal; Carcinogens; ESTROGENS; Estrogens, Non-Steroidal; Hormones and antagonists;
11076649	Sodium zomepirac	ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; ANTIHISTAMINES-H2; Anti-Inflammatory Agents, Non-Steroidal; Drugs acting on the gastrointestinal system;
11076132	4-Hydroxyphenyl retinamide	Anticancer drugs and carcinogens; Anticarcinogenic Agents; Antineoplastic Agents; CYTOSTATICS; VITAMINS; Vitamins and antagonists;
11076202	Azithromycin	Anti-Bacterial Agents; ANTIBIOTICS; Antimicrobials and chemotherapeutics;
11076170	Acetochlor	Herbicides;
11076612	Potassium dichromate	Caustics; Coloring Agents;
7852732	all-trans-Retinyl acetate	Adjuvants, Immunologic; ANGIOGENESIS-INHIBITORS; Anticancer drugs and carcinogens; Anticarcinogenic Agents;

		Antioxidants; Vitamins; VITAMINS; Vitamins and antagonists;
7852276	Lovastatin	ANTIARTERIOSCLEROTICS; Anticholesteremic Agents; Antineoplastic Agents; Drugs acting on the blood and cardiovascular system; HMG-COA-REDUCTASE-INHIBITORS; Hydroxymethylglutaryl-CoA Reductase Inhibitors;
7852736	Rifampicin	Antibiotics, Antitubercular; ANTIBIOTICS; ANTILEPROTICS; Antimicrobials and chemotherapeutics; COLLAGENASE-INHIBITORS; Enzyme Inhibitors; Enzymes and inhibitors; Leprostatic Agents; MATRIX-METALLOPROTEINASE-INHIBITORS; PEPTIDE-HYDROLASE-INHIBITORS; TUBERCULOSTATICS;
7852296	Melphalan	Anticancer drugs and carcinogens; Antineoplastic Agents, Alkylating; CYTOSTATICS; Myeloablative Agonists;
7853657	Alachlor	Herbicides;
11076275	cis-Dichlorodiamine platinum	Anticancer drugs and carcinogens; Antineoplastic Agents; Cross-Linking Reagents; CYTOSTATICS; Enzymes and inhibitors; PROTEIN-KINASE-C-INHIBITORS; Radiation-Sensitizing Agents; TELOMERASE-INHIBITORS;
11076451	Methoxychlor [95%]	Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076631	Rifabutin	Anti-Bacterial Agents; Antibiotics, Antitubercular; ANTIBIOTICS; Antimicrobials and chemotherapeutics;
11076046	2-Ethylhexyl-p-dimethyl-aminobenzoate	Drugs acting on the skin; RADIOPROTECTIVES; Sunscreening Agents;
7852677	Prednisone	Anti-Inflammatory Agents; Antineoplastic Agents, Hormonal; CORTICOSTEROIDS; Glucocorticoids; Hormones and antagonists;
7852750	Scopolamine hydrobromide trihydrate	Adjuvants, Anesthesia; Drugs acting on the nervous system; Muscarinic Antagonists; Mydriatics; MYDRIATICS; PARASYMPATHOLYTICS; Psychotropic agents; SEDATIVES;
11076186	alpha-Cyclodextrin	Hormones and antagonists; PROSTAGLANDINS;
7853238	Di-n-butyl phthalate	Plasticizers;
11076152	5-Bromo-2'-deoxyuridine (BRDU)	Anticancer drugs and carcinogens; Antimetabolites; Antimetabolites, Antineoplastic; Antimicrobials and chemotherapeutics; Antiviral Agents; CYTOSTATICS; Radiation-Sensitizing Agents; VIRUCIDES;
11076288	Curcumin	ANTIHISTAMINES-H2; Anti-Inflammatory Agents, Non-Steroidal; Antineoplastic Agents; Coloring Agents; Drugs acting on the gastrointestinal system; Enzyme Inhibitors; Enzymes and inhibitors; PHOSPHOLIPASE-INHIBITORS;
7852793	Tamoxifen, citrate salt	ANGIOGENESIS-INHIBITORS; Anticancer drugs and carcinogens; Antineoplastic Agents, Hormonal; Bone Density Conservation Agents; Enzymes and inhibitors; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Hormones and antagonists; PROTEIN-KINASE-C-INHIBITORS; Selective Estrogen Receptor Modulators;
7851850	beta-Cyclodextrin	Carcinogens; Food Additives;
11076522	Nitazoxanide	ANTHELMINTICS; Antimicrobials and chemotherapeutics; Antiparasitic Agents;
11076466	Methylene blue trihydrate	Activity terms, miscellaneous; Anesthetics and drugs relieving fever, inflammation and pain; ANTIDOTES; Anti-Infective Agents, Urinary; ANTIPYRETICS; Enzyme Inhibitors; Enzymes and inhibitors; GUANYLATE-CYCLASE-INHIBITORS;
11076176	Adriamycin, hydrochloride	ANTIBIOTICS; Antibiotics, Antineoplastic; Anticancer drugs and carcinogens; Antimicrobials and chemotherapeutics;

		CYTOSTATICS; DNA-INTERCALATORS; P-GLYCOPROTEIN-INHIBITORS; TOPOISOMERASE-II-INHIBITORS; TOPOISOMERASE-INHIBITORS;
11076586	Pentamidine isethionate	Antifungal Agents; Antimicrobials and chemotherapeutics; Antiprotozoal Agents; PROTOZOACIDES; Trypanocidal Agents;
7851697	Butyl benzyl phthalate	Teratogens;
11076507	Nelfinavir mesylate	Antimicrobials and chemotherapeutics; Enzymes and inhibitors; HIV Protease Inhibitors; HIV-PROTEASE-INHIBITORS; PEPTIDE-HYDROLASE-INHIBITORS; VIRUCIDES;
11076513	Nevirapine	Anti-HIV Agents; Antimicrobials and chemotherapeutics; Enzymes and inhibitors; Reverse Transcriptase Inhibitors; REVERSE-TRANSCRIPTASE-INHIBITORS; VIRUCIDES;
7851604	Atrazine	Adrenergic Agents; Adrenergic beta-Agonists; Adrenergic Uptake Inhibitors; ANORECTICS; ANTI-ASTHMATICS; BRONCHODILATORS; Central Nervous System Stimulants; Dopamine Agents; Dopamine Uptake Inhibitors; Drugs acting on the nervous system; Drugs acting on the respiratory system; Herbicides; HERBICIDES; Pesticides and plant hormones; PSYCHOSTIMULANTS; PSYCHOTONICS; Psychotropic agents; SYMPATHOMIMETICS-ALPHA; Sympathomimetics; SYMPATHOMIMETICS-BETA;
7853376	Benzophenone	Photosensitizing Agents;
11076669	tert-Butylhydroquinone	Antioxidants; Enzyme Inhibitors;
11075967	2',3'-Dideoxyadenosine (ddA)	Antimetabolites; Antiviral Agents;
7854544	Primaclone	Anticonvulsants; ANTICONVULSANTS; Drugs acting on the nervous system;
7852074	Ethoxyquin	Activity terms, miscellaneous; ANTIOXIDANTS; HERBICIDES; Pesticides and plant hormones;
7852405	Naphthalene	ACARICIDES; Carcinogens; Explosive Agents; Pesticides and plant hormones; Tocolytic Agents; Vasodilator Agents;
7851798	Chloroform	Anesthetics and drugs relieving fever, inflammation and pain; GEN-ANESTHETICS; Solvents;
7851531	Aldicarb	ACARICIDES; ANTHELMINTICS; Antimicrobials and chemotherapeutics; Cholinesterase Inhibitors; Insecticides; INSECTICIDES; Pesticides and plant hormones;
7851523	Actinomycin D	Anti-Bacterial Agents; Antibiotics, Antineoplastic; Nucleic Acid Synthesis Inhibitors; Protein Synthesis Inhibitors;
7853864	Carbamazepine	Analgesics, Non-Narcotic; Anticonvulsants; ANTICONVULSANTS; Antimanic Agents; ANTIMANICS; Drugs acting on the nervous system; Psychotropic agents;
7854036	Digoxin	Anti-Arrhythmia Agents; CARBONIC-ANHYDRASE-INHIBITORS; CARDIOGLYCOSIDES; Cardiotonic Agents; Drugs acting on the blood and cardiovascular system; Enzyme Inhibitors; Enzymes and inhibitors; NA-K-ATPASE-INHIBITORS;
11076615	Progesterone	Activity terms, miscellaneous; Adrenergic alpha-Antagonists; Adrenergic Uptake Inhibitors; Analgesics, Non-Narcotic; ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; Anthelmintics; ANTHELMINTICS; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Anticoagulants; ANTIDEPRESSANTS; Antidepressive Agents; Antidepressive Agents, Tricyclic; ANTIDIABETICS; ANTIEMETICS; Antifungal Agents; ANTIHISTAMINES-H1; ANTIHISTAMINES-H2; Antihypertensive Agents; Anti-Infective

		Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimalarials; Antimanic Agents; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiparkinson Agents; Antipruritics; ANTIPYRETICS; ANTISEROTONINS; Antithyroid Agents; Biocompatible Materials; Buffers; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; Cardiovascular Agents; Cathartics; Chelating Agents; CHELATORS; Coloring Agents; CYCLOOXYGENASE-1-INHIBITORS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; DIAGNOSTICS; Diuretics; Dopamine Agonists; DOPAMINERGICS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Drugs acting on the nervous system; Drugs acting on the skin; Enzyme Inhibitors; Enzymes and inhibitors; Estradiol Antagonists; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Expectorants; Fertility Agents, Female; Fixatives; Folic Acid Antagonists; Food Additives; Fungicides, Industrial; FUNGICIDES; Gastrointestinal Agents; Gout Suppressants; Histamine Agonists; Histamine H1 Antagonists; Hormones and antagonists; HYPOTENSIVES; IMMUNOSTIMULANTS; IMMUNOSUPPRESSIVES; Indicators and Reagents; Keratolytic Agents; KERATOLYTICS; Lipotropic Agents; Mutagens; Neuromuscular Depolarizing Agents; Nootropic Agents; PARASYMPATHOMIMETICS; PENETRATION-ENHANCERS; Progestins; PROGESTOGENS; PROSTAGLANDIN-ANTAGONISTS; PROTOZOACIDES; PSYCHOSEDATIVES; PSYCHOSTIMULANTS; Psychotropic agents; Radiation-Protective Agents; Radiopharmaceuticals; Selective Estrogen Receptor Modulators; Serotonin Agonists; SYMPATHOLYTICS-ALPHA; THROMBOXANE-ANTAGONISTS; Tocolytic Agents; TRANQUILIZERS; Vasodilator Agents; Vitamins and antagonists; VITAMINS;
7852689	beta-Propiolactone	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS; Disinfectants;
7854754	Zearalanol	ANABOLICS; Estrogens, Non-Steroidal; ESTROGENS; GONADOTROPIN-ANTAGONISTS; Hormones and antagonists;
7853750	Amphotericin B	Amebicides; Anesthetics and drugs relieving fever, inflammation and pain; Anti-Bacterial Agents; Antibiotics, Antifungal; Antifungal Agents; Antiprotozoal Agents; LOCAL-ANESTHETICS;
11076712	Zearalenone	ANABOLICS; Estrogens, Non-Steroidal; ESTROGENS; Hormones and antagonists;
7851581	Anilazine (Dyrene)	Antimicrobials and chemotherapeutics; FUNGICIDES;
7853307	p-Chlorophenol	Anti-Infective Agents, Local;
7854762	Daidzein (4',7-Dihydroxyisoflavone)	Phytoestrogens;
11076573	p-Aminophenol	Mutagens;
7852834	2,2'-Thiobis(4,6-dichlorophenol)	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; Antiplatyhelminthic Agents; ANTIPYRETICS;
11075925	13-cis-Retinal (Vitamin A aldehyde)	ANGIOGENESIS-INHIBITORS; Anticancer drugs and carcinogens; Enzymes and inhibitors; ORNITHINE-DECARBOXYLASE-INHIBITORS; VITAMINS; Vitamins and



		antagonists;
7851922	1,2-Dichlorobenzene	Insecticides;
11076281	Creosote, wood	ANTIAGGREGANTS; Disinfectants; Drugs acting on the blood and cardiovascular system; Expectorants;
7852085	N-Ethyl-N-nitrosourea	Alkylating Agents; Anticancer drugs and carcinogens; CYTOSTATICS;
11076258	Casanthranol (Cascara sagrada extract)	Drugs acting on the gastrointestinal system; LAXATIVES;
7851611	Azathioprine	Anticancer drugs and carcinogens; Antimetabolites, Antineoplastic; Antimetabolites; Antirheumatic Agents; CYTOSTATICS; Immunosuppressive Agents; IMMUNOSUPPRESSIVES;
11076303	Dazomet	ANTHELMINTICS; Antimicrobials and chemotherapeutics; FUNGICIDES; HERBICIDES; Pesticides and plant hormones;
7851608	5-Azacytidine	Antimetabolites, Antineoplastic; Enzyme Inhibitors;
11076576	Parathion	ANTICHOLINESTERASES; Cholinesterase Inhibitors; Drugs acting on the nervous system; Insecticides; INSECTICIDES; Pesticides and plant hormones;
7851733	Capsaicin	Analgesics, Non-Narcotic; Anesthetics and drugs relieving fever, inflammation and pain; RUBEFACIENTS;
11076205	Basic orange 2 (C.I. 11270)	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS;
11076067	2-Pivalyl-1,3-indandione	INSECTICIDES; Pesticides and plant hormones;
7851507	1-Acetyl-2-phenylhydrazine	Activity terms, miscellaneous; Adrenergic alpha-Antagonists; Adrenergic Uptake Inhibitors; ANALGESICS; Analgesics, Non-Narcotic; Anesthetics and drugs relieving fever, inflammation and pain; Anthelmintics; ANTHELMINTICS; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Anticoagulants; ANTIDEPRESSANTS; Antidepressive Agents; Antidepressive Agents, Tricyclic; ANTIDIABETICS; ANTIEMETICS; Antifungal Agents; ANTIHISTAMINES-H1; ANTIHISTAMINES-H2; Antihypertensive Agents; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimalarials; Antimanic Agents; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiparkinson Agents; Antipruritics; ANTIPYRETICS; ANTISEROTONINS; Antithyroid Agents; Biocompatible Materials; Buffers; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; Cardiovascular Agents; Cathartics; Chelating Agents; CHELATORS; Coloring Agents; CYCLOOXYGENASE-1-INHIBITORS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; DIAGNOSTICS; Diuretics; Dopamine Agonists; DOPAMINERGICS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Drugs acting on the nervous system; Drugs acting on the skin; Enzyme Inhibitors; Enzymes and inhibitors; Estradiol Antagonists; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Expectorants; Fertility Agents, Female; Fixatives; Folic Acid Antagonists; Food Additives; FUNGICIDES; Fungicides, Industrial; Gastrointestinal Agents; Gout Suppressants; Histamine Agonists; Histamine H1 Antagonists; Hormones and antagonists; HYPOTENSIVES; IMMUNOSTIMULANTS; IMMUNOSUPPRESSIVES; Indicators and Reagents; Keratolytic Agents; KERATOLYTICS; Lipotropic Agents; Mutagens; Neuromuscular Depolarizing Agents;

		Nootropic Agents; PARASYMPATHOMIMETICS; PENETRATION-ENHANCERS; Progestins; PROGESTOGENS; PROSTAGLANDIN-ANTAGONISTS; PROTOZOACIDES; PSYCHOSEDATIVES; PSYCHOSTIMULANTS; Psychotropic agents; Radiation-Protective Agents; Radiopharmaceuticals; Selective Estrogen Receptor Modulators; Serotonin Agonists; SYMPATHOLYTICS-ALPHA; THROMBOXANE-ANTAGONISTS; Tocolytic Agents; TRANQUILIZERS; Vasodilator Agents; VITAMINS; Vitamins and antagonists;
7852030	N,N'-Diphenyl-p-phenylenediamine	Antioxidants;
11076654	Sulfacetamide	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; Anti-Infective Agents, Urinary; ANTIPIRETICS;
7852865	Triamterene	Activity terms, miscellaneous; Diuretics; DIURETICS;
11076394	Halothane	Anesthetics and drugs relieving fever, inflammation and pain; Anesthetics, Inhalation; GEN.ANESTHETICS;
7851983	4-Dimethylaminoazobenzene	Carcinogens; Coloring Agents;
11076682	Thioctic acid	Antioxidants; Vitamin B Complex;
7852878	2,4,6-Trichlorophenol	Mutagens;
7852404	Nalidixic acid	Anti-Infective Agents; Enzyme Inhibitors;
11076355	Econazole nitrate	Antifungal Agents; Antimicrobials and chemotherapeutics; FUNGICIDES;
7852658	Piperonyl butoxide	Pesticide Synergists;
7851996	4-Dimethylaminoantipyrine (Aminopyrine)	ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; Anti-Inflammatory Agents, Non-Steroidal; ANTIPIRETICS; Indicators and Reagents;
7854664	6-Thioguanine (6-TG)	Anticancer drugs and carcinogens; Antimetabolites, Antineoplastic; CYTOSTATICS;
7853959	Iodochlorohydroxyquinoline	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPIRETICS;
7852208	Hydroquinone	Anesthetics and drugs relieving fever, inflammation and pain; Antioxidants; ANTIPIRETICS; Mutagens; Radiation-Protective Agents;
7852701	6-Propyl-2-thiouracil	Antimetabolites; Antithyroid Agents; ANTITHYROIDES; Hormones and antagonists;
7853373	Phenyl salicylate	Drugs acting on the skin; Plasticizers; RADIOPROTECTIVES;
11076567	p,p'-DDE (p,p'-Dichlorodiphenyldichloroethylene)	Insecticides;
11076366	Ethyl methanesulfonate	Antineoplastic Agents, Alkylating; Mutagens;
7852918	Urea	Activity terms, miscellaneous; PENETRATION-ENHANCERS;
7852140	Furosemide	Activity terms, miscellaneous; Diuretics; DIURETICS; Enzymes and inhibitors; PHOSPHOLIPASE-INHIBITORS; PROTEIN-KINASE-C-INHIBITORS; Sodium Potassium Chloride Symporter Inhibitors;
7852322	8-Methoxypsoralen	Activity terms, miscellaneous; RADIOSENSITIZERS;
7851807	Chloropicrin	Chemical Warfare Agents;
7852748	Salicylazosulfapyridine	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; ANTIPIRETICS; Antirheumatic Agents; Gastrointestinal Agents;
11076486	Myleran	Alkylating Agents; Anticancer drugs and carcinogens; Antineoplastic Agents, Alkylating; CYTOSTATICS;

		Immunosuppressive Agents; Myeloablative Agonists;
11076334	Dimenhydrinate	Activity terms, miscellaneous; Anesthetics, Local; Anti-Allergic Agents; Anti-Bacterial Agents; ANTIBIOTICS; Antiemetics; ANTIEMETICS; ANTIHISTAMINES-H1; Anti-HIV Agents; Antimetabolites; Antimicrobials and chemotherapeutics; Antiparkinson Agents; Antipruritics; Antitussive Agents; Convulsants; Drugs acting on the gastrointestinal system; Enzyme Inhibitors; Enzymes and inhibitors; GABA Modulators; Histamine H1 Antagonists; HIV-PROTEASE-INHIBITORS; Hypnotics and Sedatives; PEPTIDE-HYDROLASE-INHIBITORS; Psychotropic agents; Reverse Transcriptase Inhibitors; SEDATIVES; VIRUCIDES;
11076206	Benomyl	Anthelmintics; Antimicrobials and chemotherapeutics; FUNGICIDES; Fungicides, Industrial; Tubulin Modulators;
11076627	Pyrene	Fluorescent Dyes;
7852254	2-Propanol	Solvents;
11076566	p -n -Nonylphenol	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; ANTIPYRETICS; Disinfectants; Sclerosing Solutions;
11076289	cyanuric chloride	Cross-Linking Reagents;
11076489	N,N,N',N' - Tetramethylhexanediamine	Heparin Antagonists;
11076229	beta-Resorcylic acid	Antifungal Agents; Anti-Infective Agents; Antimetabolites, Antineoplastic; Food Preservatives;
7853280	Diethylethanolamine	Anti-Inflammatory Agents, Non-Steroidal;
11076656	sulfamic acid; midosulfonic acid	Herbicides; Indicators and Reagents;
11076151	5-Aminosalicylic acid	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Inflammatory Agents, Non-Steroidal; ANTIPYRETICS;
7852852	Toluene	Solvents;
7853227	Methyl acetate	ANALGESICS; Analgesics, Opioid; Anesthetics and drugs relieving fever, inflammation and pain; Narcotics;
7852402	Busulfan	Alkylating Agents; Anticancer drugs and carcinogens; Antineoplastic Agents, Alkylating; CYTOSTATICS; Immunosuppressive Agents; Myeloablative Agonists;
7852811	tetrachloroethylene	ANTHELMINTICS; Antimicrobials and chemotherapeutics; Carcinogens; Environmental Pollutants; Solvents;
7853354	n-Hexanol	Anesthetics; Nicotinic Antagonists;
7852155	Glycerol	Cryoprotective Agents;
7851674	Bisphenol A	Air Pollutants, Occupational; Estrogens, Non-Steroidal; Free Radical Scavengers;
7851824	Citric Acid	Activity terms, miscellaneous; Adrenergic alpha-Antagonists; Adrenergic Uptake Inhibitors; ANALGESICS; Analgesics, Non-Narcotic; Anesthetics and drugs relieving fever, inflammation and pain; Anthelmintics; ANTHELMINTICS; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Anticoagulants; ANTIDEPRESSANTS; Antidepressive Agents; Antidepressive Agents, Tricyclic; ANTIDIABETICS; ANTIEMETICS; Antifungal Agents; ANTIHISTAMINES-H1; ANTIHISTAMINES-H2; Antihypertensive Agents; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimalarials; Antimanic Agents; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiparkinson Agents; Antipruritics; ANTIPYRETICS; ANTISEROTONINS; Antithyroid Agents; Biocompatible Materials; Buffers; CALCIUM-ANTAGONISTS;

		Calcium Channel Blockers; Cardiovascular Agents; Cathartics; Chelating Agents; CHELATORS; Coloring Agents; CYCLOOXYGENASE-1-INHIBITORS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; DIAGNOSTICS; Diuretics; Dopamine Agonists; DOPAMINERGICS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Drugs acting on the nervous system; Drugs acting on the skin; Enzyme Inhibitors; Enzymes and inhibitors; Estradiol Antagonists; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Expectorants; Fertility Agents, Female; Fixatives; Folic Acid Antagonists; Food Additives; FUNGICIDES; Fungicides, Industrial; Gastrointestinal Agents; Gout Suppressants; Histamine Agonists; Histamine H1 Antagonists; Hormones and antagonists; HYPOTENSIVES; IMMUNOSTIMULANTS; IMMUNOSUPPRESSIVES; Indicators and Reagents; Keratolytic Agents; KERATOLYTICS; Lipotropic Agents; Mutagens; Neuromuscular Depolarizing Agents; Nootropic Agents; PARASYMPATHOMIMETICS; PENETRATION-ENHANCERS; Progestins; PROGESTOGENS; PROSTAGLANDIN-ANTAGONISTS; PROTOZOACIDES; PSYCHOSEDATIVES; PSYCHOSTIMULANTS; Psychotropic agents; Radiation-Protective Agents; Radiopharmaceuticals; Selective Estrogen Receptor Modulators; Serotonin Agonists; SYMPATHOLYTICS-ALPHA; THROMBOXANE-ANTAGONISTS; Tocolytic Agents; TRANQUILIZERS; Vasodilator Agents; Vitamins and antagonists; VITAMINS;
11076319	dicyclohexylamine	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS; Enzyme Inhibitors; Explosive Agents;
11076547	o-methoxyphenol	ANTIAGGREGANTS; Disinfectants; Drugs acting on the blood and cardiovascular system; Expectorants;
11076677	tetraethylenepentamine	Anion Exchange Resins; ANTIARTERIOSCLEROTICS; Antilipemic Agents; Drugs acting on the blood and cardiovascular system;
11076619	Propylparaben	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS;
7853008	maleic acid	Activity terms, miscellaneous; Adrenergic alpha-Antagonists; Adrenergic Uptake Inhibitors; ANALGESICS; Analgesics, Non-Narcotic; Anesthetics and drugs relieving fever, inflammation and pain; Anthelmintics; ANTHELMINTICS; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Anticoagulants; ANTIDEPRESSANTS; Antidepressive Agents; Antidepressive Agents, Tricyclic; ANTIDIABETICS; ANTIEMETICS; Antifungal Agents; ANTIHISTAMINES-H1; ANTIHISTAMINES-H2; Antihypertensive Agents; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimalarials; Antimanic Agents; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiparkinson Agents; Antipruritics; ANTIPYRETICS; ANTISEROTONINS; Antithyroid Agents; Biocompatible Materials; Buffers; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; Cardiovascular Agents; Cathartics; Chelating Agents; CHELATORS; Coloring Agents; CYCLOOXYGENASE-1-INHIBITORS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; DIAGNOSTICS; Diuretics;

		Dopamine Agonists; DOPAMINERGICS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Drugs acting on the nervous system; Drugs acting on the skin; Enzyme Inhibitors; Enzymes and inhibitors; Estradiol Antagonists; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Expectorants; Fertility Agents, Female; Fixatives; Folic Acid Antagonists; Food Additives; Fungicides, Industrial; FUNGICIDES; Gastrointestinal Agents; Gout Suppressants; Histamine Agonists; Histamine H1 Antagonists; Hormones and antagonists; HYPOTENSIVES; IMMUNOSTIMULANTS; IMMUNOSUPPRESSIVES; Indicators and Reagents; Keratolytic Agents; KERATOLYTICS; Lipotropic Agents; Mutagens; Neuromuscular Depolarizing Agents; Nootropic Agents; PARASYMPATHOMIMETICS; PENETRATION-ENHANCERS; Progestins; PROGESTOGENS; PROSTAGLANDIN-ANTAGONISTS; PROTOZOACIDES; PSYCHOSEDATIVES; PSYCHOSTIMULANTS; Psychotropic agents; Radiation-Protective Agents; Radiopharmaceuticals; Selective Estrogen Receptor Modulators; Serotonin Agonists; SYMPATHOLYTICS-ALPHA; THROMBOXANE-ANTAGONISTS; Tocolytic Agents; TRANQUILIZERS; Vasodilator Agents; Vitamins and antagonists; VITAMINS;
7853109	2-Methylbutyric acid	Antineoplastic Agents; Antiviral Agents; Dental Materials; Ophthalmic Solutions;
7854264	Lactic acid	Activity terms, miscellaneous; Adrenergic Agents; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; CALMODULIN-ANTAGONISTS; CARBONIC-ANHYDRASE-INHIBITORS; Drugs acting on the blood and cardiovascular system; Enzymes and inhibitors; Vasodilator Agents;
7851600	Acetylsalicylic acid	Analgesics; ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; ANTIAGGREGANTS; ANTIHISTAMINES-H2; Anti-Inflammatory Agents, Non-Steroidal; ANTIPYRETICS; CYCLOOXYGENASE-1-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Enzymes and inhibitors; Fibrinolytic Agents; Hormones and antagonists; Platelet Aggregation Inhibitors; PROSTAGLANDIN-ANTAGONISTS;
11076645	Sodium hydrogen sulfate	Cathartics;
11076401	Imidazole	Enzyme Inhibitors; Hormones and antagonists; THROMBOXANE-ANTAGONISTS;
7854764	4-Octylphenol	Estrogens, Non-Steroidal;
7853293	N,N-dimethylbenzylamine	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; ANTIPYRETICS; Detergents; Disinfectants; Preservatives, Pharmaceutical;
7851613	Sodium azide	Enzyme Inhibitors; Indicators and Reagents; Mutagens; Vasodilator Agents;
7851941	Dichlorvos (DDVP)	Anthelmintics; ANTHELMINTICS; Antimicrobials and chemotherapeutics; Cholinesterase Inhibitors; Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076374	Fluoranthene	Enzyme Inhibitors;
7853361	n-Octanol	Solvents;
11076597	phosphoric acid	Anti-Bacterial Agents; ANTIBIOTICS; Antimicrobials and

		chemotherapeutics; Cathartics; Dental Materials;
11076292	Cycloheximide	Antibiotics, Antifungal; ANTIBIOTICS; ANTICONVULSANTS; Antimicrobials and chemotherapeutics; Drugs acting on the nervous system; FUNGICIDES; GABA-ANTAGONISTS; Protein Synthesis Inhibitors;
11076420	Kepona	Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076463	Methyl testosterone	Anabolic Agents; ANDROGENS; Antineoplastic Agents, Hormonal; Hormones and antagonists;
7851757	Chloramphenicol	Anti-Bacterial Agents; ANTIBIOTICS; Antimicrobials and chemotherapeutics; Protein Synthesis Inhibitors;
11076700	Triton X-100	Activity terms, miscellaneous; Antifoaming Agents; Detergents; Excipients; Spermatocidal Agents; Surface-Active Agents; SURFACTANTS;
7854790	5a-Dihydrotestosterone	Androgens;
11076398	Hydroxyflutamide	Androgen Antagonists; ANDROGEN-ANTAGONISTS; Hormones and antagonists;
11076280	Colchicine	Activity terms, miscellaneous; Anesthetics and drugs relieving fever, inflammation and pain; Anticancer drugs and carcinogens; ANTIPYRETICS; CYTOSTATICS; Gout Suppressants; P-GLYCOPROTEIN-INHIBITORS; SELECTIN-ANTAGONISTS; Tubulin Modulators;
7854842	Phenolphthalin	Cathartics; Drugs acting on the gastrointestinal system; Indicators and Reagents; LAXATIVES;
11076614	Procymidone	Fungicides, Industrial;
7854795	Testosterone	ANABOLICS; Androgens; ANDROGENS; Hormones and antagonists;
7851876	Dexamethasone	Antiemetics; Anti-Inflammatory Agents; Antineoplastic Agents, Hormonal; CORTICOSTEROIDS; Glucocorticoids; Hormones and antagonists;
7851866	p,p' -DDE	Insecticides;
11076646	Sodium lauryl sulfate	Surface-Active Agents;
11076691	Trichloroacetic acid	Caustics;
11076260	Cetylpyridinium bromide	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; ANTIPYRETICS; Detergents; Hormone Antagonists; Hormones and antagonists; LULIBERIN-ANTAGONISTS; RELEASING-FACTOR-INHIBITORS;
7854794	Progesterone	Activity terms, miscellaneous; Adrenergic alpha-Antagonists; Adrenergic Uptake Inhibitors; Analgesics, Non-Narcotic; ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; Anthelmintics; ANTHELMINTICS; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Anticoagulants; ANTIDEPRESSANTS; Antidepressive Agents; Antidepressive Agents, Tricyclic; ANTIDIABETICS; ANTIEMETICS; Antifungal Agents; ANTIHISTAMINES-H1; ANTIHISTAMINES-H2; Antihypertensive Agents; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimalarials; Antimanic Agents; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiparkinson Agents; Antipruritics; ANTIPYRETICS; ANTISEROTONINS; Antithyroid Agents; Biocompatible Materials; Buffers; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; Cardiovascular Agents; Cathartics; Chelating Agents; CHELATORS; Coloring Agents; CYCLOOXYGENASE-1-INHIBITORS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors;

		CYCLOOXYGENASE-INHIBITORS; DIAGNOSTICS; Diuretics; Dopamine Agonists; DOPAMINERGICS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Drugs acting on the nervous system; Drugs acting on the skin; Enzyme Inhibitors; Enzymes and inhibitors; Estradiol Antagonists; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Expectorants; Fertility Agents, Female; Fixatives; Folic Acid Antagonists; Food Additives; Fungicides, Industrial; FUNGICIDES; Gastrointestinal Agents; Gout Suppressants; Histamine Agonists; Histamine H1 Antagonists; Hormones and antagonists; HYPOTENSIVES; IMMUNOSTIMULANTS; IMMUNOSUPPRESSIVES; Indicators and Reagents; Keratolytic Agents; KERATOLYTICS; Lipotropic Agents; Mutagens; Neuromuscular Depolarizing Agents; Nootropic Agents; PARASYMPATHOMIMETICS; PENETRATION-ENHANCERS; Progestins; PROGESTOGENS; PROSTAGLANDIN-ANTAGONISTS; PROTOZOACIDES; PSYCHOSEDATIVES; PSYCHOSTIMULANTS; Psychotropic agents; Radiation-Protective Agents; Radiopharmaceuticals; Selective Estrogen Receptor Modulators; Serotonin Agonists; SYMPATHOLYTICS-ALPHA; THROMBOXANE-ANTAGONISTS; Tocolytic Agents; TRANQUILIZERS; Vasodilator Agents; Vitamins and antagonists; VITAMINS;
7852870	Trichloroacetic acid	Caustics;
11076262	Chlorhexidine	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents; Anti-Infective Agents, Local; ANTIPYRETICS; Dentifrices; Dermatologic Agents; Disinfectants; Mouthwashes;
11076195	Amitriptyline HCl	Activity terms, miscellaneous; Adrenergic alpha-Antagonists; Adrenergic Uptake Inhibitors; ANALGESICS; Analgesics, Non-Narcotic; Anesthetics and drugs relieving fever, inflammation and pain; Anthelmintics; ANTHELMINTICS; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Anticoagulants; ANTIDEPRESSANTS; Antidepressive Agents; Antidepressive Agents, Tricyclic; ANTIDIABETICS; ANTIEMETICS; Antifungal Agents; ANTIHISTAMINES-H1; ANTIHISTAMINES-H2; Antihypertensive Agents; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimalarials; Antimanic Agents; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiparkinson Agents; Antipruritics; ANTIPYRETICS; ANTISEROTONINS; Antithyroid Agents; Biocompatible Materials; Buffers; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; Cardiovascular Agents; Cathartics; Chelating Agents; CHELATORS; Coloring Agents; CYCLOOXYGENASE-1-INHIBITORS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; DIAGNOSTICS; Diuretics; Dopamine Agonists; DOPAMINERGICS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Drugs acting on the nervous system; Drugs acting on the skin; Enzyme Inhibitors; Enzymes and inhibitors; Estradiol Antagonists; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Expectorants; Fertility Agents, Female; Fixatives; Folic Acid Antagonists; Food Additives; FUNGICIDES; Fungicides, Industrial; Gastrointestinal Agents;

		Gout Suppressants; Histamine Agonists; Histamine H1 Antagonists; Hormones and antagonists; HYPOTENSIVES; IMMUNOSTIMULANTS; IMMUNOSUPPRESSIVES; Indicators and Reagents; Keratolytic Agents; KERATOLYTICS; Lipotropic Agents; Mutagens; Neuromuscular Depolarizing Agents; Nootropic Agents; PARASYMPATHOMIMETICS; PENETRATION-ENHANCERS; Progestins; PROGESTOGENS; PROSTAGLANDIN-ANTAGONISTS; PROTOZOACIDES; PSYCHOSEDATIVES; PSYCHOSTIMULANTS; Psychotropic agents; Radiation-Protective Agents; Radiopharmaceuticals; Selective Estrogen Receptor Modulators; Serotonin Agonists; SYMPATHOLYTICS-ALPHA; THROMBOXANE-ANTAGONISTS; Tocolytic Agents; TRANQUILIZERS; Vasodilator Agents; VITAMINS; Vitamins and antagonists;
7852768	Sodium hypochlorite	Disinfectants; Oxidants;
7854806	4-Hydroxytamoxifen	Estrogen Antagonists;
7852690	Propranolol HCl	Adrenergic beta-Antagonists; Anti-Anxiety Agents; Anti-Arrhythmia Agents; ANTIARRHYTHMICS; Antihypertensive Agents; Drugs acting on the blood and cardiovascular system; Drugs acting on the nervous system; HYPOTENSIVES; SYMPATHOLYTICS-BETA; Vasodilator Agents;
11076707	Verapamil HCl	Anti-Arrhythmia Agents; Anticancer drugs and carcinogens; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; CARBONIC-ANHYDRASE-INHIBITORS; CYTOSTATICS; Drugs acting on the blood and cardiovascular system; Enzymes and inhibitors; P-GLYCOPROTEIN-INHIBITORS; PROTEIN-KINASE-C-INHIBITORS; Vasodilator Agents;
7854866	Corticosterone	Anti-Inflammatory Agents; CORTICOSTEROIDS; Hormones and antagonists;
7852592	Parathion	ANTICHOLINESTERASES; Cholinesterase Inhibitors; Drugs acting on the nervous system; Insecticides; INSECTICIDES; Pesticides and plant hormones;
7852952	Zearalenone	ANABOLICS; Estrogens, Non-Steroidal; ESTROGENS; Hormones and antagonists;
7854325	Meprobamate	Anti-Anxiety Agents; Anticonvulsants; Hypnotics and Sedatives; Muscle Relaxants, Central; PSYCHOSEDATIVES; Psychotropic agents; TRANQUILIZERS;
7851858	Cyproterone acetate	Androgen Antagonists; Antineoplastic Agents; Contraceptive Agents, Male;
7852148	Gibberellic acid	Plant Growth Regulators;
11076251	Captan 90-concentrate (solid)	Anesthetics and drugs relieving fever, inflammation and pain; Antimicrobials and chemotherapeutics; ANTIPYRETICS; FUNGICIDES; Fungicides, Industrial;
7854781	o,p' -DDT	Estrogens, Non-Steroidal;
7852260	Kaempferol	Enzymes and inhibitors; PEPTIDE-HYDROLASE-INHIBITORS;
11076377	Fluoxymestrone	Anabolic Agents; ANDROGENS; Antineoplastic Agents, Hormonal; Hormones and antagonists;
11076307	Deoxycholic acid sodium salt	Detergents;
11076124	4-Androstenedione	ANDROGENS; Hormones and antagonists;
11076362	Ethyl acrylate (inhibited)	Carcinogens; Mutagens;
7853927	Chlorothiazide	Activity terms, miscellaneous; Antihypertensive Agents; CARBONIC-ANHYDRASE-INHIBITORS; Diuretics; DIURETICS; Drugs acting on the blood and cardiovascular



		system; Enzymes and inhibitors; HYPOTENSIVES; Sodium Chloride Symporter Inhibitors;
11076364	Ethyl cyanoacrylate	Hemostatics;
7852519	N-Nitrosodiethanolamine	Carcinogens;
11076429	Linoleic acid	Abortifacient Agents, Nonsteroidal; Anti-Inflammatory Agents, Non-Steroidal; Antilipemic Agents; Dermatologic Agents; Hormones and antagonists; PROSTAGLANDINS;
7852642	Phenyl mercuric acetate	Fungicides, Industrial;
11076713	Zinc pyrithione	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS; Keratolytic Agents;
7854634	Sulfamethizole	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents; ANTIPYRETICS;
11076571	p-Amino benzoic acid	Anticonvulsants; Vitamin B Complex; Vitamins and antagonists; VITAMINS;
11076293	Cycloheximide	Antibiotics, Antifungal; ANTIBIOTICS; ANTICONVULSANTS; Antimicrobials and chemotherapeutics; Drugs acting on the nervous system; FUNGICIDES; GABA-ANTAGONISTS; Protein Synthesis Inhibitors;
7851637	p-Quinone	Drugs acting on the blood and cardiovascular system; Indicators and Reagents; NITRIC-OXIDE-SYNTASE-INHIBITORS;
11076637	Silibinin	Antioxidants; Drugs acting on the gastrointestinal system; HEPATOTROPICS; Protective Agents;
7854718	Trimethoprim	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents; Anti-Infective Agents, Urinary; Antimalarials; ANTIPYRETICS; FOLATE-ANTAGONISTS; Folic Acid Antagonists; Vitamins and antagonists;
11076421	L-5-Hydroxytryptophan	ANTICONVULSANTS; ANTIDEPRESSANTS; Antidepressive Agents, Second-Generation; Drugs acting on the nervous system; Parasympatholytics; PSYCHOSTIMULANTS; Psychotropic agents; Serotonin Antagonists; Vasodilator Agents;
11076406	Isoamyl nitrite	Vasodilator Agents;
11076332	Diisopropyl amine	Drugs acting on the blood and cardiovascular system; VASODILATORS;
7851867	p,p'-DDT (Dichlorodiphenyltrichloroethane)	CORTICOSTEROID-ANTAGONISTS; Hormones and antagonists; INSECTICIDES; Pesticides and plant hormones;
11076710	Vitamin D3	ANGIOGENESIS-INHIBITORS; Anticancer drugs and carcinogens; Bone Density Conservation Agents; Vitamins and antagonists; VITAMINS-D; Vitamins;
7851899	Diazinon	ANTICHOLINESTERASES; Cholinesterase Inhibitors; Drugs acting on the nervous system; Insecticides; INSECTICIDES; Pesticides and plant hormones;
7852069	Ethionamide	Anesthetics and drugs relieving fever, inflammation and pain; ANTILEPTOTICS; Antimicrobials and chemotherapeutics; ANTIPYRETICS; Antitubercular Agents; Leprostatic Agents; TUBERCULOSTATICS;
11076074	3,3',5,5'-Tetramethylbenzidine	Chromogenic Compounds;
11076688	trans-Retinal (Vitamin A aldehyde)	ANGIOGENESIS-INHIBITORS; Anticancer drugs and carcinogens; Enzymes and inhibitors; ORNITHINE-DECARBOXYLASE-INHIBITORS; Vitamins and antagonists; VITAMINS;
7852111	Formulated fenaminosulf	Fungicides, Industrial;
11076459	Methyl isocyanate	Antisickling Agents;

7851942	Dicofol	ACARICIDES; Insecticides; INSECTICIDES; Pesticides and plant hormones;
7852336	Methyl methacrylate	Antimutagenic Agents; Vasodilator Agents;
7852412	1-Naphthylamine	Adrenergic Agents; Adrenergic Uptake Inhibitors; ANORECTICS; Carcinogens; Central Nervous System Stimulants; Dopamine Agents; Dopamine Uptake Inhibitors; PSYCHOSTIMULANTS; PSYCHOTONICS; Psychotropic agents; Sympathomimetics;
7852384	Metronidazole (Flagyl)	Activity terms, miscellaneous; Anesthetics and drugs relieving fever, inflammation and pain; ANTIALCOHOLICS; Anti-Infective Agents; Antimicrobials and chemotherapeutics; Antiprotozoal Agents; ANTIPYRETICS; PROTOZOACIDES; Radiation-Sensitizing Agents; RADIOSENSITIZERS;
7851575	Ampicillin trihydrate	Anti-Bacterial Agents; ANTIBIOTICS; Antimicrobials and chemotherapeutics;
11076165	Abscisic acid	Plant Growth Regulators;
7851908	Dibromomannitol	Anticancer drugs and carcinogens; Antineoplastic Agents, Alkylating; CYTOSTATICS;
7852347	Methyl parathion	ANTICHOLINESTERASES; Cholinesterase Inhibitors; Drugs acting on the nervous system; Insecticides; INSECTICIDES; Pesticides and plant hormones;
7854760	Genistein (4',5,7-Trihydroxyisoflavone)	Anticancer drugs and carcinogens; Anticarcinogenic Agents; Antineoplastic Agents; Enzyme Inhibitors; Growth Inhibitors; TYROSINE-KINASE-INHIBITORS;
7851599	Aspartame	Sweetening Agents;
11076461	Methyl salicylate	Anesthetics and drugs relieving fever, inflammation and pain; ANTIHISTAMINES-H2; ANTIPYRETICS; Drugs acting on the gastrointestinal system; Fixatives;
11076387	Glutaraldehyde (Glutaric dialdehyde)	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPERSPIRANTS; ANTIPYRETICS; Cross-Linking Reagents; Disinfectants; Drugs acting on the skin; Fixatives;
7852145	Hexamethyl-p-rosaniline chloride (Gentian violet)	Anesthetics and drugs relieving fever, inflammation and pain; ANTHELMINTICS; Anti-Infective Agents, Local; Antimicrobials and chemotherapeutics; ANTIPYRETICS;
11076358	Ergotamine tartrate	Activity terms, miscellaneous; Adrenergic alpha-Agonists; Analgesics, Non-Narcotic; ANTISEROTONINS; Drugs acting on the blood and cardiovascular system; Drugs acting on the nervous system; HEMOSTATICS; UTEROTONICS; Vasoconstrictor Agents;
7851755	Chlorambucil	Anticancer drugs and carcinogens; Antineoplastic Agents, Alkylating; CYTOSTATICS;
11076518	Ninhydrin	Indicators and Reagents; Radiation-Sensitizing Agents;
11076530	n-Pentane	Anesthetics and drugs relieving fever, inflammation and pain; GEN.ANESTHETICS;
11076544	Oleic acid	Drugs acting on the blood and cardiovascular system; Sclerosing Solutions; VASOTROPICS;
7852166	Griseofulvin	Antibiotics, Antifungal; ANTIBIOTICS; Antimicrobials and chemotherapeutics; FUNGICIDES;
7852382	6-Methyl-2-thiouracil	Antithyroid Agents; ANTITHYROIDES; Hormones and antagonists;
11076484	Musk ambrette	Mutagens;
7852413	2-Naphthylamine	Carcinogens;
11076388	Glycerol	Cryoprotective Agents;
11076657	Sulfathiazole	Anesthetics and drugs relieving fever, inflammation and pain;

		ANTIPYRETICS;
7853724	Allopurinol (4-Hydroxypyrazolo[3,4-d]pyrimidine)	Anesthetics and drugs relieving fever, inflammation and pain; ANTIGOUTS; Antimetabolites; ANTIPYRETICS; Enzyme Inhibitors; Enzymes and inhibitors; Free Radical Scavengers; Gout Suppressants; XANTHINE-OXIDASE-INHIBITORS;
7852431	Nitrilotriacetic acid (NTA)	Chelating Agents;
7851701	n-Butyl-p-hydroxybenzoate	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS;
7852598	Pentachlorophenol	Antimicrobials and chemotherapeutics; Environmental Pollutants; Enzyme Inhibitors; FUNGICIDES; Herbicides; Insecticides; Pesticides; Poisons; Uncoupling Agents;
7854640	Sulfanilamide	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Bacterial Agents; ANTIPYRETICS;
7852618	Phenothiazine	Activity terms, miscellaneous; ANTHELMINTICS; Antimicrobials and chemotherapeutics; ANTIOXIDANTS; Antiprotozoal Agents;
7854737	Valproic acid	Anticonvulsants; ANTICONVULSANTS; Antimanic Agents; ANTIMANICS; Drugs acting on the nervous system; Enzyme Inhibitors; GABA Agents; Psychotropic agents;
7854832	n-Butyl-p-aminobenzoate	Anesthetics, Local; Anticancer drugs and carcinogens; Cholinergic Agents; CYTOSTATICS; Drugs acting on the nervous system; Indicators and Reagents; PARASYMPATHOMIMETICS; Uncoupling Agents; Vasodilator Agents;
11076123	4-Androstene-3,17-dione	ANDROGENS; Hormones and antagonists;
7852851	Tolbutamide	ANTIDIABETICS; Hormones and antagonists; Hypoglycemic Agents;
7852782	Sulfamethazine	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents; ANTIPYRETICS;
7854834	4,4'-Methylenedianiline	Carcinogens;
11076025	2-Aminothiazole	ANTITHYROIDS; Hormones and antagonists;
11076644	Sodium dodecyl sulfate	Surface-Active Agents;
7852784	Sulfisoxazole	Anti-Infective Agents;
7853207	Methanol	Solvents;
7852284	Maleic hydrazide	Herbicides; Plant Growth Regulators;
7852170	Hematoxylin (C.I. 75290)	Antimicrobials and chemotherapeutics; Coloring Agents; VIRUCIDES;
7851586	o-Anthranilic acid	Anticonvulsants; Vitamin B Complex; Vitamins and antagonists; VITAMINS;
7852974	Acetone	Solvents;
11076173	Acetylsalicylic acid	Analgesics; ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; ANTIAGGREGANTS; ANTIHISTAMINES-H2; Anti-Inflammatory Agents, Non-Steroidal; ANTIPYRETICS; CYCLOOXYGENASE-1-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Enzymes and inhibitors; Fibrinolytic Agents; Hormones and antagonists; Platelet Aggregation Inhibitors; PROSTAGLANDIN-ANTAGONISTS;
7851561	o-Aminoazotoluene	Coloring Agents;
11076697	Tris(2,3-epoxypropyl)isocyanurate	Anticancer drugs and carcinogens; Antineoplastic Agents; CYTOSTATICS;

		Activity terms, miscellaneous; Adrenergic alpha-Antagonists; Adrenergic Uptake Inhibitors; ANALGESICS; Analgesics, Non-Narcotic; Anesthetics and drugs relieving fever, inflammation and pain; Anthelmintics; ANTHELMINTICS; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Anticoagulants; ANTIDEPRESSANTS; Antidepressive Agents; Antidepressive Agents, Tricyclic; ANTIDIABETICS; ANTIEMETICS; Antifungal Agents; ANTIHISTAMINES-H1; ANTIHISTAMINES-H2; Antihypertensive Agents; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimalarials; Antimanic Agents; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiparkinson Agents; Antipruritics; ANTIPYRETICS; ANTISEROTONINS; Antithyroid Agents; Biocompatible Materials; Buffers; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; Cardiovascular Agents; Cathartics; Chelating Agents; CHELATORS; Coloring Agents; CYCLOOXYGENASE-1-INHIBITORS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; DIAGNOSTICS; Diuretics; Dopamine Agonists; DOPAMINERGICS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Drugs acting on the nervous system; Drugs acting on the skin; Enzyme Inhibitors; Enzymes and inhibitors; Estradiol Antagonists; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Expectorants; Fertility Agents, Female; Fixatives; Folic Acid Antagonists; Food Additives; FUNGICIDES; Fungicides, Industrial; Gastrointestinal Agents; Gout Suppressants; Histamine Agonists; Histamine H1 Antagonists; Hormones and antagonists; HYPOTENSIVES; IMMUNOSTIMULANTS; IMMUNOSUPPRESSIVES; Indicators and Reagents; Keratolytic Agents; KERATOLYTICS; Lipotropic Agents; Mutagens; Neuromuscular Depolarizing Agents; Nootropic Agents; PARASYMPATHOMIMETICS; PENETRATION-ENHANCERS; Progestins; PROGESTOGENS; PROSTAGLANDIN-ANTAGONISTS; PROTOZOACIDES; PSYCHOSEDATIVES; PSYCHOSTIMULANTS; Psychotropic agents; Radiation-Protective Agents; Radiopharmaceuticals; Selective Estrogen Receptor Modulators; Serotonin Agonists; SYMPATHOLYTICS-ALPHA; THROMBOXANE-ANTAGONISTS; Tocolytic Agents; TRANQUILIZERS; Vasodilator Agents; Vitamins and antagonists; VITAMINS;
7853009	Fumaric acid	
7851803	Monuron	HERBICIDES; Pesticides and plant hormones;
7852182	Hexachlorophene	Anesthetics and drugs relieving fever, inflammation and pain; ANTHELMINTICS; Antihypertensive Agents; Anti-Infective Agents, Local; Antimicrobials and chemotherapeutics; ANTIPYRETICS; Drugs acting on the blood and cardiovascular system; HYPOTENSIVES; Vasodilator Agents;
11076194	Amiloride HCl	Activity terms, miscellaneous; Diuretics; DIURETICS; Enzymes and inhibitors; PROTEIN-KINASE-C-INHIBITORS; Sodium Channel Blockers;
7852840	Thiourea	Indicators and Reagents;
11076557	o-Phenanthroline	Chelating Agents; Cholinesterase Inhibitors; Cross-Linking Reagents; Intercalating Agents; Iron Chelating Agents; Protease Inhibitors;

7852875	Trichloroethylene	ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; Anesthetics, Inhalation; GEN.ANESTHETICS; Solvents;
7851785	Chloroacetophenone	Irritants; Tear Gases;
11076596	p-Hexylresorcinol	Anesthetics and drugs relieving fever, inflammation and pain; ANTHELMINTICS; Anti-Infective Agents, Local; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiplatyhelminthic Agents; ANTIPYRETICS;
11076418	Isoproterenol HCl	Adrenergic beta-Agonists; Bronchodilator Agents; Cardiotonic Agents; Sympathomimetics;
11076317	Dichlorvos (Vapona)	Anthelmintics; ANTHELMINTICS; Antimicrobials and chemotherapeutics; Cholinesterase Inhibitors; Insecticides; INSECTICIDES; Pesticides and plant hormones;
7853401	N,N-Diethyl-m-toluamide (DEET)	Insect Repellents;
7852709	Pyrimethamine	Antimalarials; Antimicrobials and chemotherapeutics; Antiprotozoal Agents; FOLATE-ANTAGONISTS; Folic Acid Antagonists; PROTOZOACIDES; Vitamins and antagonists;
11076433	Maltol	Activity terms, miscellaneous; CHELATORS;
11076393	Halazone	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS;
7851499	Acetohexamide	ANTIDIABETICS; Hormones and antagonists; Hypoglycemic Agents;
7854576	Quinidine	Adrenergic alpha-Antagonists; Analgesics, Non-Narcotic; Anesthetics and drugs relieving fever, inflammation and pain; Anti-Arrhythmia Agents; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Antimalarials; Antimicrobials and chemotherapeutics; ANTIPYRETICS; Drugs acting on the blood and cardiovascular system; Enzyme Inhibitors; Muscarinic Antagonists; Muscle Relaxants, Central; P-GLYCOPROTEIN-INHIBITORS; PROTOZOACIDES;
7851740	Carbazole	Carcinogens;
7851606	Auramine	Anti-Infective Agents; Coloring Agents; Disinfectants;
7851638	2,2'-Dithiobisbenzothiazole	Antifungal Agents; Antimicrobials and chemotherapeutics; FUNGICIDES;
11076495	N,N-Dimethyl-p-phenylenediamine	Fluorescent Dyes;
11076444	Medroxyprogesterone acetate	Antineoplastic Agents, Hormonal; Contraceptive Agents, Female; Contraceptive Agents, Male; Contraceptives, Oral, Synthetic; Hormones and antagonists; PROGESTOGENS;
11076673	Tetrachloroethylene	ANTHELMINTICS; Antimicrobials and chemotherapeutics; Carcinogens; Environmental Pollutants; Solvents;
7852729	Reserpine	Adrenergic Uptake Inhibitors; Anticancer drugs and carcinogens; Antihypertensive Agents; Antipsychotic Agents; DOPAMINE-ANTAGONISTS; Drugs acting on the blood and cardiovascular system; Drugs acting on the nervous system; HYPOTENSIVES; NEUROLEPTICS; P-GLYCOPROTEIN-INHIBITORS; PSYCHOSEDATIVES; Psychotropic agents; TRANQUILIZERS;
11076204	Azoxybenzene	ANTIHISTAMINES-H2; Drugs acting on the gastrointestinal system;
7851758	Chloranil	Antimicrobials and chemotherapeutics; ANTIPSORIATICS; Drugs acting on the skin; FUNGICIDES; Fungicides, Industrial;
11076211	Benzimidazole	Anthelmintics;
7851749	Catechol (1,2-Benzenediol)	Anticancer drugs and carcinogens; Anticarcinogenic Agents;

		Anti-Inflammatory Agents, Non-Steroidal; Antimutagenic Agents; Antioxidants; BIOFLAVONOIDS; Drugs acting on the gastrointestinal system; HEPATOTROPICS; IMMUNOSTIMULANTS; Neuroprotective Agents; Protease Inhibitors; Radiation-Protective Agents; Vitamins and antagonists; VITAMINS;
7852589	Oxytetracycline HCl	Anti-Bacterial Agents; ANTIBIOTICS; Antimicrobials and chemotherapeutics;
7852628	Phenyl butazone	Anesthetics and drugs relieving fever, inflammation and pain; ANTIHISTAMINES-H2; Anti-Inflammatory Agents, Non-Steroidal; ANTIPYRETICS; Drugs acting on the gastrointestinal system; Hormones and antagonists; PROSTAGLANDIN-ANTAGONISTS;
7853105	m-Toluic acid	Antifungal Agents; Anti-Infective Agents; Antimetabolites, Antineoplastic; Food Preservatives;
7852271	Lithocholic acid	Detergents;
7851931	2,4-Dichlorophenol	Anthelmintics;
7851862	Succinic acid-2,2-dimethylhydrazide (Daminozide)	Herbicides; Plant Growth Regulators;
11075889	1,2,3,4-Tetrahydroisoquinoline	ANTIPSORIATICS; Drugs acting on the skin;
7852867	Tricaprylin	Excipients;
7852409	N-(1-Naphthyl)ethylenediamine 2HCl	ANTHELMINTICS; Antimicrobials and chemotherapeutics; Cholinesterase Inhibitors; Insecticides; INSECTICIDES; Pesticides and plant hormones;
7853235	Riboflavin	Photosensitizing Agents; Vitamin B Complex; Vitamins and antagonists; VITAMINS-B2;
11076233	Bisphenol A	Air Pollutants, Occupational; Estrogens, Non-Steroidal; Free Radical Scavengers;
7851582	Aniline	Carcinogens; Indicators and Reagents;
11076694	Trifluralin	Herbicides; HERBICIDES; Pesticides and plant hormones; Tubulin Modulators;
11076685	Toluene	Solvents;
7852597	Pentachloronitrobenzene	Antimicrobials and chemotherapeutics; Fungicides, Industrial; FUNGICIDES;
7852739	Basic red 9 (p-Rosaniline HCl) (C.I. 42500)	Activity terms, miscellaneous; Adrenergic alpha-Antagonists; Adrenergic Uptake Inhibitors; ANALGESICS; Analgesics, Non-Narcotic; Anesthetics and drugs relieving fever, inflammation and pain; Anthelmintics; ANTHELMINTICS; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Anticoagulants; ANTIDEPRESSANTS; Antidepressive Agents; Antidepressive Agents, Tricyclic; ANTIDIABETICS; ANTIEMETICS; Antifungal Agents; ANTIHISTAMINES-H1; ANTIHISTAMINES-H2; Antihypertensive Agents; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimalarials; Antimanic Agents; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiparkinson Agents; Antipruritics; ANTIPYRETICS; ANTISEROTONINS; Antithyroid Agents; Biocompatible Materials; Buffers; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; Cardiovascular Agents; Cathartics; Chelating Agents; CHELATORS; Coloring Agents; CYCLOOXYGENASE-1-INHIBITORS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; DIAGNOSTICS; Diuretics; Dopamine Agonists; DOPAMINERGICS; Drugs acting on the

		blood and cardiovascular system; Drugs acting on the gastrointestinal system; Drugs acting on the nervous system; Drugs acting on the skin; Enzyme Inhibitors; Enzymes and inhibitors; Estradiol Antagonists; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Expectorants; Fertility Agents, Female; Fixatives; Folic Acid Antagonists; Food Additives; FUNGICIDES; Fungicides, Industrial; Gastrointestinal Agents; Gout Suppressants; Histamine Agonists; Histamine H1 Antagonists; Hormones and antagonists; HYPOTENSIVES; IMMUNOSTIMULANTS; IMMUNOSUPPRESSIVES; Indicators and Reagents; Keratolytic Agents; KERATOLYTICS; Lipotropic Agents; Mutagens; Neuromuscular Depolarizing Agents; Nootropic Agents; PARASYMPATHOMIMETICS; PENETRATION-ENHANCERS; Progestins; PROGESTOGENS; PROSTAGLANDIN-ANTAGONISTS; PROTOZOACIDES; PSYCHOSEDATIVES; PSYCHOSTIMULANTS; Psychotropic agents; Radiation-Protective Agents; Radiopharmaceuticals; Selective Estrogen Receptor Modulators; Serotonin Agonists; SYMPATHOLYTICS-ALPHA; THROMBOXANE-ANTAGONISTS; Tocolytic Agents; TRANQUILIZERS; Vasodilator Agents; Vitamins and antagonists; VITAMINS;
7852175	Hexachloro-1,3-butadiene	Fungicides, Industrial;
7851813	Chlorpheniramine maleate	Activity terms, miscellaneous; Anti-Allergic Agents; ANTIHISTAMINES-H1; Antipruritics; Histamine H1 Antagonists;
7852866	Bromoform	Carcinogens; Psychotropic agents; SEDATIVES; Teratogens;
11076600	Picloram	Herbicides;
7853044	Decanoic acid	Antifungal Agents;
7853270	2,2'-Methylenebis-(4-chlorophenol)	Anesthetics and drugs relieving fever, inflammation and pain; ANTHELMINTICS; Anticestodal Agents; Antifungal Agents; Antimicrobials and chemotherapeutics; Antiprotozoal Agents; ANTIPYRETICS; FUNGICIDES;
7853698	Acetanilide	ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; Antihypertensive Agents; ANTIPYRETICS; Drugs acting on the blood and cardiovascular system; Herbicides; HERBICIDES; HYPOTENSIVES; Pesticides and plant hormones;
11076531	N-Phenyl-1-naphthylamine	Carcinogens; Fluorescent Dyes;
7852139	Furfural	Antimicrobials and chemotherapeutics; FUNGICIDES;
7852828	Theophylline	Activity terms, miscellaneous; ANTIASTHMATICS; Bronchodilator Agents; BRONCHODILATORS; CALCIUM-ANTAGONISTS; CARBONIC-ANHYDRASE-INHIBITORS; Cardiogenic Agents; DIURETICS; Drugs acting on the blood and cardiovascular system; Drugs acting on the respiratory system; Enzymes and inhibitors; Phosphodiesterase Inhibitors; Vasodilator Agents; VASODILATORS;
11076200	Anthralin	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPSORIATICS; ANTIPYRETICS; Dermatologic Agents; Drugs acting on the skin;
11076234	Bisphenol A diglycidyl ether	Carcinogens;
7852791	Chlorotrianisene	Antineoplastic Agents, Hormonal; ESTROGENS; Estrogens, Non-Steroidal; Hormones and antagonists;
7852610	Phenazopyridine HCl	Anesthetics and drugs relieving fever, inflammation and pain; Anesthetics, Local; ANTIPYRETICS;

7853199	p-Chloro-m-cresol	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS; Fungicides, Industrial;
7851735	Captan	Anesthetics and drugs relieving fever, inflammation and pain; Antimicrobials and chemotherapeutics; ANTIPYRETICS; FUNGICIDES; Fungicides, Industrial;
11076259	Castor oil	Cathartics;
7852126	5-Fluorouracil	Anticancer drugs and carcinogens; Antimetabolites; Antimetabolites, Antineoplastic; CYTOSTATICS; Enzymes and inhibitors; Immunosuppressive Agents; THYMIDYLATE-SYNTHASE-INHIBITORS;
7852520	N-Nitrosodiethylamine	Alkylating Agents;
7851814	Chlorpropamide	ANTIDIABETICS; Hormones and antagonists; Hypoglycemic Agents;
7851945	Dieldrin	Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076561	Orotic acid	Drugs acting on the gastrointestinal system; HEPATOTROPICS;
7852613	Phenformin HCl	ANTIDIABETICS; Hormones and antagonists; Hypoglycemic Agents;
7851820	Danthron	Cathartics; Drugs acting on the gastrointestinal system; LAXATIVES; Mutagens;
7852622	1-Phenyl-3-methyl-5-pyrazolone	Free Radical Scavengers;
11076564	o-Toluidine	Carcinogens; Indicators and Reagents;
11076584	Pentachlorobenzene	Fungicides, Industrial; Insecticides;
7851563	4-Aminobiphenyl	Carcinogens;
7851864	o,p'-DDD	Antineoplastic Agents, Hormonal; CORTICOSTEROID-ANTAGONISTS; Hormones and antagonists; INSECTICIDES; Pesticides and plant hormones;
11075981	2,4-Dichloroaniline	Carcinogens; Indicators and Reagents;
7852608	p-Acetophenetidide	Analgesics, Non-Narcotic; ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS; Enzyme Inhibitors;
7852181	Hexachloroethane	Anthelmintics; ANTHELMINTICS; Antimicrobials and chemotherapeutics;
11076279	Colchicine	Activity terms, miscellaneous; Anesthetics and drugs relieving fever, inflammation and pain; Anticancer drugs and carcinogens; ANTIPYRETICS; CYTOSTATICS; Gout Suppressants; P-GLYCOPROTEIN-INHIBITORS; SELECTIN-ANTAGONISTS; Tubulin Modulators;
11076605	p-Nitroacetophenone	Radiation-Sensitizing Agents;
7852956	Ziram	Antimicrobials and chemotherapeutics; Fungicides, Industrial; FUNGICIDES;
7852120	Fluometuron	HERBICIDES; Pesticides and plant hormones;
7852552	N-Nitrosopiperidine	Carcinogens; Mutagens;
11076360	Ethidium bromide	Anticancer drugs and carcinogens; Antimicrobials and chemotherapeutics; DNA-INTERCALATORS; Enzyme Inhibitors; Fluorescent Dyes; Indicators and Reagents; Nicotinic Antagonists; PROTOZOACIDES; Trypanocidal Agents;
7852235	Iodoform	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS;
7852320	Hydroquinone monomethyl ether	Activity terms, miscellaneous; Anticancer drugs and carcinogens; Antineoplastic Agents; Antioxidants; ANTIOXIDANTS; Carcinogens; CYTOSTATICS;
11076091	3,4-Xylidine	Herbicides;



7853276	N,N-dimethyl-p-toluidine	Fluorescent Dyes;
11076183	Allylthiourea	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPIRETICS;
11076683	Thiophanate, methyl ester	Anthelmintics; ANTHELMINTICS; Antimicrobials and chemotherapeutics; Antinematodal Agents; Fungicides, Industrial; FUNGICIDES;
11075986	2,4-Dihydroxybenzoic acid	Antifungal Agents; Anti-Infective Agents; Antimetabolites, Antineoplastic; Food Preservatives;
7853204	2-Hydroxybenzamide	ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; ANTIPIRETICS;
7853486	N-Acetyl-m-Aminophenol	Analgesics; ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain;
7852378	Methylphenidate Hydrochloride	Adrenergic Agents; Adrenergic Uptake Inhibitors; Central Nervous System Stimulants; Dopamine Agents; Dopamine Uptake Inhibitors; PSYCHOSTIMULANTS; PSYCHOTONICS; Psychotropic agents; Sympathomimetics;
7851627	Benzene	Insecticides; INSECTICIDES; Pesticides and plant hormones;
7852096	4-Vinylcyclohexene Dioxide	Carcinogens;
11076565	Oxymetholone	Anabolic Agents; ANABOLICS; Androgens; ANDROGENS; Hormones and antagonists;
7852957	Zineb	Antimicrobials and chemotherapeutics; Fungicides, Industrial; FUNGICIDES;
11076261	Chlordane, technical grade	Insecticides; INSECTICIDES; Pesticides and plant hormones;
7852067	Estragole	ANTIAGGREGANTS; Drugs acting on the blood and cardiovascular system;
7851821	Cimetidine	ALCOHOL-DEHYDROGENASE-INHIBITORS; ANTIHISTAMINES-H2; Anti-Ulcer Agents; ANTIULCERS; Drugs acting on the gastrointestinal system; Enzyme Inhibitors; Enzymes and inhibitors; GASTRIC-SECRETION-INHIBITORS; Histamine H2 Antagonists;
11076479	Molinate	Antispermatic Agents; Herbicides; HERBICIDES; Pesticides and plant hormones;
7852109	Eugenol	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPIRETICS; LOCAL-ANESTHETICS;
11076029	2-Bromopropane	Mutagens; Solvents;
11076431	Luminol	Indicators and Reagents;
7852616	Phenol	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; ANTIPIRETICS; Disinfectants; Sclerosing Solutions;
7853909	Celecoxib	ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; ANTIHISTAMINES-H2; Anti-Inflammatory Agents, Non-Steroidal; ANTIPIRETICS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; Drugs acting on the gastrointestinal system; Enzymes and inhibitors;
7853503	2-Methylimidazole *	Activity terms, miscellaneous; ANTIARTERIOSCLEROTICS; Drugs acting on the blood and cardiovascular system; IONEXCHANGERS;
7852076	Ethanol	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; Central Nervous System Depressants; Disinfectants; Drug Carriers; GEN.ANESTHETICS; Preservatives, Pharmaceutical; Solvents; Surface-Active Agents;
7851498	Acetaminophen	ANALGESICS; Analgesics, Non-Narcotic; Anesthetics and

		drugs relieving fever, inflammation and pain; ANTIHISTAMINES-H2; ANTIPYRETICS; Drugs acting on the gastrointestinal system;
11076378	Flutamide	Androgen Antagonists; ANDROGEN-ANTAGONISTS; Antineoplastic Agents, Hormonal; Hormones and antagonists;
11076640	Sodium Chlorate	Herbicides;
11076171	Acetonylacetone	Cholinesterase Inhibitors; Cross-Linking Reagents; Neurotoxins;
11076432	Malachite Green Oxalate	Anti-Infective Agents, Local; Coloring Agents; Fungicides, Industrial;
11076634	Saquinavir Mesylate	Antimicrobials and chemotherapeutics; Enzymes and inhibitors; HIV Protease Inhibitors; HIV-PROTEASE-INHIBITORS; PEPTIDE-HYDROLASE-INHIBITORS; VIRUCIDES;
7851950	Chlorpyrifos	Cholinesterase Inhibitors; Insecticides; INSECTICIDES; Pesticides and plant hormones;
7852393	Monochloroacetic Acid *	HERBICIDES; Pesticides and plant hormones;
11076467	Methyleugenol	Anesthetics; Carcinogens; Mutagens;
7853820	Bisacodyl	Cathartics; Drugs acting on the gastrointestinal system; LAXATIVES;
7854313	Melatonin	Adjuvants, Immunologic; Anticonvulsants; Antioxidants; Free Radical Scavengers;
7851521	Acrylonitrile	Carcinogens;
7852319	Methoxychlor	Insecticides; INSECTICIDES; Pesticides and plant hormones;
7853355	Diethanolamine *	Activity terms, miscellaneous; Adrenergic alpha-Antagonists; Adrenergic Uptake Inhibitors; ANALGESICS; Analgesics, Non-Narcotic; Anesthetics and drugs relieving fever, inflammation and pain; Anthelmintics; ANTHELMINTICS; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Anticoagulants; ANTIDEPRESSANTS; Antidepressive Agents; Antidepressive Agents, Tricyclic; ANTIDIABETICS; ANTIEMETICS; Antifungal Agents; ANTIHISTAMINES-H1; ANTIHISTAMINES-H2; Antihypertensive Agents; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimalarials; Antimanic Agents; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiparkinson Agents; Antipruritics; ANTIPYRETICS; ANTISEROTONINS; Anti thyroid Agents; Biocompatible Materials; Buffers; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; Cardiovascular Agents; Cathartics; Chelating Agents; CHELATORS; Coloring Agents; CYCLOOXYGENASE-1-INHIBITORS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; DIAGNOSTICS; Diuretics; Dopamine Agonists; DOPAMINERGICS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Drugs acting on the nervous system; Drugs acting on the skin; Enzyme Inhibitors; Enzymes and inhibitors; Estradiol Antagonists; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Expectorants; Fertility Agents, Female; Fixatives; Folic Acid Antagonists; Food Additives; FUNGICIDES; Fungicides, Industrial; Gastrointestinal Agents; Gout Suppressants; Histamine Agonists; Histamine H1 Antagonists; Hormones and antagonists; HYPOTENSIVES; IMMUNOSTIMULANTS; IMMUNOSUPPRESSIVES; Indicators and Reagents; Keratolytic Agents; KERATOLYTICS; Lipotropic Agents; Mutagens; Neuromuscular Depolarizing Agents;

		Nootropic Agents; PARASYMPATHOMIMETICS; PENETRATION-ENHANCERS; Progestins; PROGESTOGENS; PROSTAGLANDIN-ANTAGONISTS; PROTOZOACIDES; PSYCHOSEDATIVES; PSYCHOSTIMULANTS; Psychotropic agents; Radiation-Protective Agents; Radiopharmaceuticals; Selective Estrogen Receptor Modulators; Serotonin Agonists; SYMPATHOLYTICS-ALPHA; THROMBOXANE-ANTAGONISTS; Tocolytic Agents; TRANQUILIZERS; Vasodilator Agents; Vitamins and antagonists; VITAMINS;
7851690	Bromodichloromethane	Carcinogens;
11075960	2,3-Dibromopropionic Acid	Antimicrobials and chemotherapeutics; FUNGICIDES;
11076621	p-tert Butylcatechol	Antioxidants;
7853421	Disulfoton	Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076300	D&C Red Dye 27	Fluorescent Dyes;
7852033	Diphenylhydantoin	Anticonvulsants; ANTICONVULSANTS; Drugs acting on the nervous system;
7851578	Anethole	ANTITUSSIVES; Drugs acting on the respiratory system; EXPECTORANTS; Flavoring Agents;
11075907	1,3-Dichloropropene	Insecticides;
7852052	Endosulfan	Insecticides; INSECTICIDES; Pesticides and plant hormones;
7852698	1,2-Propylene glycol	Solvents; Vehicles;
7852099	Di(2-Ethylhexyl phthalate)	Drugs acting on the skin; Plasticizers; RADIOPROTECTIVES;
7852730	Resorcinol	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS;
7851840	Coumarin	Anticoagulants; Antineoplastic Agents;
7851712	t-Butylhydroquinone	Antioxidants; Enzyme Inhibitors;
7852464	Nitrofurantoin	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Urinary; ANTIPYRETICS;
11076635	Scopolamine hydrobromide trihydrate	Adjuvants, Anesthesia; Drugs acting on the nervous system; Muscarinic Antagonists; Mydriatics; MYDRIATICS; PARASYMPATHOLYTICS; Psychotropic agents; SEDATIVES;
11076272	Cinnamaldehyde (trans), neat	Antimutagenic Agents; Antineoplastic Agents, Phytogenic; Flavoring Agents;
11076146	5-(Hydroxymethyl)-2-furfural ((HMF))	Activity terms, miscellaneous; UTEROTONICS;
7852171	Heptachlor	Insecticides; INSECTICIDES; Pesticides and plant hormones; Soil Pollutants;
7851598	L-Ascorbic Acid	Antioxidants; Vitamins;
7852002	7,12-Dimethylbenz(a)anthracene	Carcinogens;
11076282	Cresol (m-/p- mixture)	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; ANTIPYRETICS; Disinfectants; Sclerosing Solutions;
11076199	Annatto Extract Acid Proof	Food Coloring Agents;
11076322	Dideoxydideohydrothymidine	Anti-HIV Agents; Antimetabolites; Antimicrobials and chemotherapeutics; Antiviral Agents; Enzymes and inhibitors; HIV-PROTEASE-INHIBITORS; PEPTIDE-HYDROLASE-INHIBITORS; Reverse Transcriptase Inhibitors; REVERSE-TRANSCRIPTASE-INHIBITORS; VIRUCIDES;
11076271	Cinnamaldehyde	Antimutagenic Agents; Antineoplastic Agents, Phytogenic; Flavoring Agents;
11076255	Carisoprodol	ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; Drugs acting on the nervous system;

		Muscle Relaxants, Central; RELAXANTS;
11076210	Benzethonium chloride	Anesthetics and drugs relieving fever, inflammation and pain; Anticancer drugs and carcinogens; Anti-Infective Agents, Local; Antiprotozoal Agents; ANTIPYRETICS; CYTOSTATICS;
7851646	o-Benzyl-p-chlorophenol	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS;
7852068	Ethinyl estradiol	Estrogens; ESTROGENS; Hormones and antagonists;
7853258	o-Cresol	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; ANTIPYRETICS; Disinfectants; Sclerosing Solutions;
11076174	Acrylamide	ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain;
7852191	2,6-Diisopropylphenol	Anesthetics and drugs relieving fever, inflammation and pain; Anesthetics, Intravenous; Anticonvulsants; Antiemetics; Free Radical Scavengers; GEN.ANESTHETICS; Hypnotics and Sedatives;
11076356	Emodin (bulk)	Anticancer drugs and carcinogens; Antimicrobials and chemotherapeutics; Enzyme Inhibitors; FUNGICIDES; TYROSINE-KINASE-INHIBITORS;
7851975	2,4-Dimethoxyaniline hydrochloride	Carcinogens; Indicators and Reagents;
11076302	Daunomycin HCL	Antibiotics, Antineoplastic; ANTIBIOTICS; Anticancer drugs and carcinogens; Antimicrobials and chemotherapeutics; CYTOSTATICS; DNA-INTERCALATORS; P-GLYCOPROTEIN-INHIBITORS;
7852065	17-beta-Estradiol	Anticancer drugs and carcinogens; Antineoplastic Agents, Alkylating; Antineoplastic Agents, Hormonal; CYTOSTATICS; Estrogens; ESTROGENS; Hormones and antagonists; Radiation-Protective Agents;
7852180	Hexachlorocyclopentadiene	Teratogens;
11076647	Sodium nitrite	Food Preservatives; Indicators and Reagents;
7852617	Phenolphthalein	Cathartics; Drugs acting on the gastrointestinal system; Indicators and Reagents; LAXATIVES;
7852242	Isobutyl nitrite	Vasodilator Agents;
7853906	Cefuroxime Free Acid	Anti-Bacterial Agents; ANTIBIOTICS; Antimicrobials and chemotherapeutics;
7852824	Tetramethylthiuram disulfide	Anesthetics and drugs relieving fever, inflammation and pain; Antifungal Agents; Anti-Infective Agents, Local; Antimicrobials and chemotherapeutics; ANTIPYRETICS; Enzyme Inhibitors; Fungicides, Industrial; FUNGICIDES; Mutagens;
11076653	Succinonitrile	ANTIDEPRESSANTS; ANTIPRURITICS; Drugs acting on the skin; PSYCHOSTIMULANTS; Psychotropic agents;
11076283	Croton oil	Dermatologic Agents;
7852303	Mercuric chloride	Anti-Infective Agents, Local; Disinfectants;
11076154	5-Methoxypsoralen	Activity terms, miscellaneous; RADIOSENSITIZERS;
7853394	Tributyl phosphate	Radiation-Protective Agents;
7851736	Semicarbazide HCl	Carcinogens;
7852450	4-Nitro-o-phenylenediamine	Carcinogens; Indicators and Reagents;
7852643	o-Phenylphenol	Anti-Infective Agents; Antimicrobials and chemotherapeutics; Carcinogens; Disinfectants; Fungicides, Industrial; FUNGICIDES;
7852856	o-Toluidine HCl	Carcinogens; Indicators and Reagents;
11076689	Triacetin (1,2,3-Propanetriol	Antifungal Agents; Anti-Infective Agents, Local; Antimicrobials

	triacetate)	and chemotherapeutics; Drugs acting on the blood and cardiovascular system; FUNGICIDES; HYPOTENSIVES;
7852073	2-Ethoxybenzamide (Ethenzamide)	ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain;
11076666	Terephthalic acid	Free Radical Scavengers;
11076594	Phenyl glyoxal	Enzyme Inhibitors; Indicators and Reagents;
11076021	2-Aminoanthracene	Carcinogens; Mutagens;
7852759	Sesamol	Activity terms, miscellaneous; Antioxidants; ANTIOXIDANTS; Drugs acting on the skin; RADIOPROTECTIVES;
11076706	Vat blue 1 (Indigo) (C.I. 73000)	Coloring Agents;
7852846	Titanocene dichloride	Antineoplastic Agents;
7852112	Fenthion (Baytex)	ANTICHOLINESTERASES; Cholinesterase Inhibitors; Drugs acting on the nervous system; Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076157	6-Mercaptopurine monohydrate	Anticancer drugs and carcinogens; Antimetabolites; Antimetabolites, Antineoplastic; CYTOSTATICS; Immunosuppressive Agents; Nucleic Acid Synthesis Inhibitors;
7852299	2-Mercaptobenzothiazole	Antifungal Agents; Antimicrobials and chemotherapeutics; FUNGICIDES;
7853382	Vanillin	Anticonvulsants; Antimutagenic Agents; Antioxidants;
7851555	2-Amino-5-nitrophenol	Anesthetics and drugs relieving fever, inflammation and pain; Anti-Infective Agents, Local; ANTIPYRETICS; Disinfectants; Sclerosing Solutions;
7853349	1,3,5-Trioxane	Anti-Infective Agents, Local; Disinfectants; Fixatives;
7853305	p-Xylene	Solvents;
7853257	o-Xylene	Solvents;
7852108	1,8-Cineol (Eucalyptol)	Activity terms, miscellaneous; Anesthetics and drugs relieving fever, inflammation and pain; ANTHELMINTICS; Anti-Infective Agents; Antimicrobials and chemotherapeutics; ANTIPYRETICS; ANTITUSSIVES; Drugs acting on the respiratory system; EXPECTORANTS; PENETRATION-ENHANCERS; Solvents;
7852778	Styrene oxide	Carcinogens; Mutagens;
11076320	Dicyclohexylamine	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS; Enzyme Inhibitors; Explosive Agents;
11076428	Linalool	Insecticides;
11075906	1,3-Dichloro-2-propanol	Cross-Linking Reagents; Mutagens;
11075900	1,2-Epoxy-3-butene	Mutagens;
7854709	Triethylenetetramine	Activity terms, miscellaneous; Chelating Agents; CHELATORS; Indicators and Reagents;
11076235	Biuret (Carbamylurea; Imidodicarbonic diamide)	Indicators and Reagents;
7852369	1-Methylnaphthalene	ACARICIDES; Carcinogens; Explosive Agents; Pesticides and plant hormones; Tocolytic Agents; Vasodilator Agents;
11076517	Nifedipine	CALCIUM-ANTAGONISTS; Calcium Channel Blockers; CARBONIC-ANHYDRASE-INHIBITORS; Drugs acting on the blood and cardiovascular system; Enzymes and inhibitors; Tocolytic Agents; Vasodilator Agents;
7853942	Carminic acid	Activity terms, miscellaneous; Coloring Agents; DYE; Food Coloring Agents; Hemostatics;
7852470	1-Nitronaphthalene	ACARICIDES; Carcinogens; Explosive Agents; Pesticides and plant hormones; Tocolytic Agents; Vasodilator Agents;
11075987	2,4-Dinitro-1-naphtho-7-sulfonic	Coloring Agents;

	acid	
7852325	t-Butyl methyl ether	Air Pollutants; Carcinogens;
7852205	Hydrochlorothiazide	Activity terms, miscellaneous; Antihypertensive Agents; CARBONIC-ANHYDRASE-INHIBITORS; Diuretics; DIURETICS; Drugs acting on the blood and cardiovascular system; Enzymes and inhibitors; HYPOTENSIVES; Sodium Chloride Symporter Inhibitors;
7854190	o-Methoxyphenol	ANTIAGGREGANTS; Disinfectants; Drugs acting on the blood and cardiovascular system; Expectorants;
7852769	Sorbic acid	Food Preservatives;
7854559	Propyl-4-hydroxybenzoate (Propyl paraben)	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS;
11076359	Ethacrynic acid	Diuretics; Enzyme Inhibitors;
7852232	Indomethacin	Activity terms, miscellaneous; Adrenergic alpha-Antagonists; Adrenergic Uptake Inhibitors; ANALGESICS; Analgesics, Non-Narcotic; Anesthetics and drugs relieving fever, inflammation and pain; Anthelmintics; ANTHELMINTICS; ANTIARRHYTHMICS; Anticancer drugs and carcinogens; Anticoagulants; ANTIDEPRESSANTS; Antidepressive Agents; Antidepressive Agents, Tricyclic; ANTIDIABETICS; ANTIEMETICS; Antifungal Agents; ANTIHISTAMINES-H1; ANTIHISTAMINES-H2; Antihypertensive Agents; Anti-Infective Agents; Anti-Inflammatory Agents, Non-Steroidal; Antimalarials; Antimanic Agents; Antimicrobials and chemotherapeutics; Antinematodal Agents; Antiparkinson Agents; Antipruritics; ANTIPYRETICS; ANTISEROTONINS; Antithyroid Agents; Biocompatible Materials; Buffers; CALCIUM-ANTAGONISTS; Calcium Channel Blockers; Cardiovascular Agents; Cathartics; Chelating Agents; CHELATORS; Coloring Agents; CYCLOOXYGENASE-1-INHIBITORS; CYCLOOXYGENASE-2-INHIBITORS; Cyclooxygenase Inhibitors; CYCLOOXYGENASE-INHIBITORS; DIAGNOSTICS; Diuretics; Dopamine Agonists; DOPAMINERGICS; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system; Drugs acting on the nervous system; Drugs acting on the skin; Enzyme Inhibitors; Enzymes and inhibitors; Estradiol Antagonists; Estrogen Antagonists; ESTROGEN-ANTAGONISTS; Expectorants; Fertility Agents, Female; Fixatives; Folic Acid Antagonists; Food Additives; FUNGICIDES; Fungicides, Industrial; Gastrointestinal Agents; Gout Suppressants; Histamine Agonists; Histamine H1 Antagonists; Hormones and antagonists; HYPOTENSIVES; IMMUNOSTIMULANTS; IMMUNOSUPPRESSIVES; Indicators and Reagents; Keratolytic Agents; KERATOLYTICS; Lipotropic Agents; Mutagens; Neuromuscular Depolarizing Agents; Nootropic Agents; PARASYMPATHOMIMETICS; PENETRATION-ENHANCERS; Progestins; PROGESTOGENS; PROSTAGLANDIN-ANTAGONISTS; PROTOZOACIDES; PSYCHOSEDATIVES; PSYCHOSTIMULANTS; Psychotropic agents; Radiation-Protective Agents; Radiopharmaceuticals; Selective Estrogen Receptor Modulators; Serotonin Agonists; SYMPATHOLYTICS-ALPHA; THROMBOXANE-ANTAGONISTS; Tocolytic Agents; TRANQUILIZERS; Vasodilator Agents; Vitamins and antagonists; VITAMINS;

11076297	Cyclophosphamide monohydrate	Anticancer drugs and carcinogens; Antineoplastic Agents, Alkylating; Antirheumatic Agents; CYTOSTATICS; Immunosuppressive Agents; IMMUNOSUPPRESSIVES; Mutagens; Myeloablative Agonists;
7851539	Allyl isothiocyanate	Food Preservatives;
11076679	Tetralin	INSECTICIDES; Pesticides and plant hormones;
11076287	Cumene hydroperoxide	Oxidants;
7851865	Rhothane (TDE)	Insecticides;
7853380	2,4-Dinitrotoluene	Carcinogens;
11075956	2,3,5,6-Tetrachloronitrobenzene	Antimicrobials and chemotherapeutics; FUNGICIDES;
7851708	Butylated hydroxytoluene (BHT)	Antioxidants;
7853646	Counter 15G (O,O-Diethyl-S-(((1,1-dimethylethyl)thio)methyl)	INSECTICIDES; Pesticides and plant hormones;
7852939	Xylene, mixed isomers	Solvents;
7853452	4,6-Dinitro-o-cresol	Herbicides; Pesticides; Uncoupling Agents;
11076295	Cyclopentane	Anesthetics and drugs relieving fever, inflammation and pain; GEN.ANESTHETICS;
7852522	N-Nitrosodiphenylamine	Carcinogens;
7852015	2,4-Dinitrophenol	Coloring Agents; Uncoupling Agents;
7852829	Thiabendazole	ANTHELMINTICS; Antimicrobials and chemotherapeutics; Antinematodal Agents; FUNGICIDES; PROTOZOACIDES;
7852826	Tetranitromethane	Chemical Warfare Agents; Drugs acting on the blood and cardiovascular system; Explosive Agents; Indicators and Reagents; Oxidants; VASODILATORS;
7854582	trans-Retinol acid (Vitamin A)	Adjuvants, Immunologic; ANGIOGENESIS-INHIBITORS; Anticancer drugs and carcinogens; Anticarcinogenic Agents; Antioxidants; Vitamins and antagonists; Vitamins; VITAMINS;
7852680	Probenecid	Activity terms, miscellaneous; Adjuvants, Pharmaceutic; Anesthetics and drugs relieving fever, inflammation and pain; ANTIGOUTS; Uricosuric Agents; URICOSURICS;
11076528	n-Nonane	Activity terms, miscellaneous; PENETRATION-ENHANCERS;
7852058	1,2-Epoxy-3-chloropropane (Epichlorohydrin)	Activity terms, miscellaneous; ANTIARTERIOSCLEROTICS; Drugs acting on the blood and cardiovascular system; IONEXCHANGERS;
7852262	Chlordecone (Kepone)	Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076071	3-(Methylthio)propanal	Prostaglandin Antagonists;
11075929	1-Fluoro-2,4-dinitrobenzene	Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076265	Chlorotrimethyl silane	Indicators and Reagents;
11076268	Chrysophanic acid (1,8-Dihydroxy-3-methylantraquinone)	Mutagens;
11076328	Digitonin	CARBONIC-ANHYDRASE-INHIBITORS; CARDIOGLYCOSIDES; Drugs acting on the blood and cardiovascular system; Enzymes and inhibitors; Indicators and Reagents;
11076521	N-Isopropyl-N'-phenyl-p-phenylenediamine	Antioxidants;
11076523	Nitrogen mustard HCl	Alkylating Agents; Antineoplastic Agents, Alkylating; Chemical Warfare Agents; Irritants;
7851653	Biphenyl	Fungicides, Industrial;
11076203	Azodicarbonamide	Anti-HIV Agents; Immunosuppressive Agents;
11076163	9-Aminoacridine HCl H2O	Anesthetics and drugs relieving fever, inflammation and pain; ANTHELMINTICS; Anti-Infective Agents, Local; Antimicrobials

		and chemotherapeutics; ANTIPYRETICS; Fluorescent Dyes; FUNGICIDES; Indicators and Reagents; Mutagens;
7851901	Dibenz(a,h)anthracene	Carcinogens;
11075978	2,4-D Dimethylamine salt (DMA-4)	Herbicides; HERBICIDES; Pesticides and plant hormones;
7852619	Phenoxybenzamine HCl	Adrenergic alpha-Antagonists; Antihypertensive Agents; Drugs acting on the blood and cardiovascular system; Drugs acting on the nervous system; HYPOTENSIVES; SYMPATHOLYTICS-ALPHA; Vasodilator Agents; VASODILATORS;
7852093	Ethylene thiourea	ANTITHYROIDS; Hormones and antagonists;
7851861	Dacarbazine	Anticancer drugs and carcinogens; Antineoplastic Agents, Alkylating; CYTOSTATICS;
7851644	Benzyl alcohol	ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; Anesthetics, Local;
11076591	Pheniramine maleate	Activity terms, miscellaneous; Anti-Allergic Agents; ANTIHISTAMINES-H1; Antipruritics; Histamine H1 Antagonists;
11076065	2-Octyl-3-isothiazolone	Anesthetics and drugs relieving fever, inflammation and pain; ANTIPYRETICS;
11075952	2,2'-Thiobis(4-chlorophenol)	Antimicrobials and chemotherapeutics; FUNGICIDES;
7852860	Toxaphene	Insecticides; INSECTICIDES; Pesticides and plant hormones;
7851748	D-Carvone	ANTIFLATULENTS; Antineoplastic Agents, Phytogetic; Drugs acting on the gastrointestinal system;
7851614	Azinphosmethyl (Gusathion)	Cholinesterase Inhibitors; Insecticides; INSECTICIDES; Pesticides and plant hormones;
7852838	Thiosemicarbazide	Convulsants; Drugs acting on the nervous system; Enzyme Inhibitors; GABA-ANTAGONISTS;
7851635	Benzoic acid	Antifungal Agents; Anti-Infective Agents; Antimetabolites, Antineoplastic; Food Preservatives;
7851532	Aldrin	Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076075	3,3,5-Trimethylcyclohexylsalicylate (Homosalate)	Drugs acting on the skin; RADIOPROTECTIVES;
7851738	Carbarsone	Antimicrobials and chemotherapeutics; PROTOZOACIDES;
7852282	Malaoxon	ANTICHOLINESTERASES; Drugs acting on the nervous system; Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076630	Rhein (1,8-Dihydroxy-3-carboxylantraquinone)	ANALGESICS; Anesthetics and drugs relieving fever, inflammation and pain; ANTIHISTAMINES-H2; Antimicrobials and chemotherapeutics; COLLAGENASE-INHIBITORS; Drugs acting on the gastrointestinal system; Enzyme Inhibitors; Enzymes and inhibitors; FUNGICIDES; MATRIX-METALLOPROTEINASE-INHIBITORS; PEPTIDE-HYDROLASE-INHIBITORS;
11076226	Berberine chloride	Activity terms, miscellaneous; ANTIDIARRHEICS; Drugs acting on the gastrointestinal system; TONICS;
7854570	Pyrilamine	Activity terms, miscellaneous; Anti-Allergic Agents; ANTIHISTAMINES-H1; Histamine H1 Antagonists;
7852283	Malathion	ACARICIDES; ANTICHOLINESTERASES; Cholinesterase Inhibitors; Drugs acting on the nervous system; Insecticides; INSECTICIDES; Pesticides and plant hormones;
11076419	Kavain, DL-	Anti-Anxiety Agents; Anticonvulsants;
11076298	Cynarin (Echinacea)(1,3-Dicaffeoylquinic Acid)	ANTIARTERIOSCLEROTICS; CHOLAGOGUES; Drugs acting on the blood and cardiovascular system; Drugs acting on the gastrointestinal system;



11076702	Tyramine HCL	Activity terms, miscellaneous; Adrenergic Uptake Inhibitors; Detergents; Drugs acting on the blood and cardiovascular system; Drugs acting on the nervous system; MYDRIATICS; Surface-Active Agents; SURFACTANTS; SYMPATHOMIMETICS-ALPHA; SYMPATHOMIMETICS-BETA; Sympathomimetics; VASOCONSTRICTORS;
11076658	Synephrine	Adrenergic alpha-Agonists; CARBONIC-ANHYDRASE-INHIBITORS; Drugs acting on the blood and cardiovascular system; Drugs acting on the nervous system; Enzymes and inhibitors; HYPERTENSIVES; Nasal Decongestants; SYMPATHOMIMETICS-ALPHA; Sympathomimetics; Vasoconstrictor Agents; VASOCONSTRICTORS;
11076543	Octopamine HCL	Adrenergic alpha-Agonists; ANALEPTICS; ANTIBIOTICS; Antimicrobials and chemotherapeutics; Drugs acting on the blood and cardiovascular system; Drugs acting on the nervous system; Drugs acting on the respiratory system; HYPERTENSIVES; SYMPATHOMIMETICS-ALPHA; Vasoconstrictor Agents;

**Table 3.** Cluster membership for the set of 293 compounds clustered against 26 assays, caspase activation and cell viability in 13 cell types.

Cluster ID	PubChem SID	Name
0	7852412	1-Naphthylamine
0	7851615	Azobenzene
0	7851942	Dicofol
0	11076583	Pentabromodiphenyl Oxide (DE-71) Repackaged
0	11075980	2,4-Decadienal
0	11076283	Croton oil
0	7851775	4-Chloro-o-phenylenediamine
0	7853052	Dichloroacetonitrile
0	11076128	4-Chloro-3,5-dinitro-a,a,a-trifluorotoluene
0	7852180	Hexachlorocyclopentadiene
0	11076387	Glutaraldehyde (Glutaric dialdehyde)
1	11076160	7-Diethylamino-4-methylcoumarin
1	11075880	1-(1,2-Dibromoethyl)-3,4-dibromocyclohexane
1	7852126	5-Fluorouracil
1	11076637	Silibinin
1	7853909	Celecoxib
1	11076650	Solvent black 5 (C.I. 50415)
2	7851733	Capsaicin
2	7852878	2,4,6-Trichlorophenol
2	11076209	Benzenesulfonyl chloride
2	7852651	Phthalic anhydride
2	7851556	4-Amino-2-nitrophenol
2	11075966	2,3-Dichloroquinoxaline
2	11076553	o-Nitrobenzyl chloride
2	11076090	3,4-Dinitrotoluene
2	11076316	Dibromoacetonitrile
2	11076272	Cinnamaldehyde (trans), neat
2	7852823	Tetrakis(hydroxymethyl)phosphonium SO4
2	11076331	Dihydromethysticin
2	11075953	2,3,4,5-Tetrachloronitrobenzene
2	7853518	Hydroxyethyl acrylate
2	11076303	Dazomet
2	11076517	Nifedipine
2	7851749	Catechol (1,2-Benzenediol)
2	7852305	Methyl mercuric (II) chloride
3	11075941	2,2',4,4',5,5'-Hexabromodiphenyl Ether (PBDE-153)
3	7851646	o-Benzyl-p-chlorophenol
3	7852171	Heptachlor
3	11075958	2,3,5-Trichlorophenol
3	7853198	2,3,4,6-Tetrachlorophenol
3	11075943	2,2',4,4'-Tetrabromodiphenyl Ether (PBDE 47)
3	11076226	Berberine chloride

3	11076300	D&C Red Dye 27
3	11076124	4-Androstenedione
3	7852182	Hexachlorophene
3	11076260	Cetylpyridinium bromide
3	11076210	Benzethonium chloride
3	11076680	tetra-N-Octylammonium bromide
4	11075960	2,3-Dibromopropionic Acid
4	7851861	Dacarbazine
4	7852166	Griseofulvin
4	11076582	Pentabromodiphenyl Ether (PBDE 99) *
4	11076206	Benomyl
4	11076234	Bisphenol A diglycidyl ether
4	11076287	Cumene hydroperoxide
4	7851532	Aldrin
4	11076252	Carbendazim
4	7852068	Ethinyl estradiol
4	7852065	17-beta-Estradiol
5	11076707	Verapamil HCl
5	7852409	N-(1-Naphthyl)ethylenediamine 2HCl
5	11076027	2-Bromo-4,6-dinitroaniline
5	7852015	2,4-Dinitrophenol
5	11076308	Desmethoxyyangonin
5	11076678	Tetrahydroaminoacridine Monohydrate
5	11076555	o-Nitrophenyl acetonitrile
5	11076398	Hydroxyflutamide
5	7852791	Chlorotrianisene
5	11076700	Triton X-100
5	7854781	o,p' -DDT
5	7852111	Formulated fenaminosulf
5	11076248	Cadmium acetate, dihydrate
5	7851718	Cadmium II chloride
5	7852865	Triamterene
6	11076365	Ethyl linolenate
6	11076509	Neopentyl glycol diglycidyl ether
6	7851820	Danthron
6	11076669	tert-Butylhydroquinone
6	7854754	Zearalanol
6	11076587	Phenamiphos
6	11076006	2'4'5'-Trihydroxybutyrophenone
6	11076015	2-Amino-4-methylphenol
6	11076621	p-tert Butylcatechol
6	7851614	Azinphosmethyl (Gusathion)
6	11076566	p -n -Nonylphenol
6	11076507	Nelfinavir mesylate
7	7851776	2-Chloro-p-phenylenediamine SO4
7	11076628	Pyrogallol
7	11076202	Azithromycin
7	7852052	Endosulfan

7	11076012	2-Amino-4-chlorophenol
7	11076630	Rhein (1,8-Dihydroxy-3-carboxylantraquinone)
7	7852464	Nitrofurantoin
7	11075929	1-Fluoro-2,4-dinitrobenzene
7	7852208	Hydroquinone
7	11076359	Ethacrynic acid
7	7851758	Chloranil
8	11076177	Aldicarb sulfoxide
8	11076681	Thiocarbanilide
8	11076629	Resveratrol
8	7852436	Nitrofurazone
8	7852030	N,N'-Diphenyl-p-phenylenediamine
8	11076020	2-Amino-6-nitrobenzothiazole
8	7854583	Ribavirin
8	11076651	Solvent black 7 (C.I. 50415B)
8	11076378	Flutamide
8	7851943	N,N'-Dicyclohexylthiourea
8	7852613	Phenformin HCl
8	11075908	1,3-Dicyclohexylcarbodiimide
9	7852260	Kaempferol
9	7851864	o,p'-DDD
9	7853125	Dibromonitromethane
9	11076228	beta-Nitrostyrene
9	7852729	Reserpine
10	11076080	3,4,5-Trichloronitrobenzene
10	11076529	Norbixin (cis/trans mixture)
10	11076577	p-Azoxyanisole
10	11076589	Phenethyl anthranilate
10	7851983	4-Dimethylaminoazobenzene
10	11076471	Methysticin
10	11076205	Basic orange 2 (C.I. 11270)
10	11076345	Diphenylurea
10	11076018	2-Amino-5,6-dimethylbenzothiazole
10	11076477	m-Nitrobenzyl chloride
10	7851549	1-Amino-2-methylantraquinone (C.I. 60700)
10	7852610	Phenazopyridine HCl
10	7851560	2-Aminoanthraquinone
10	11076299	D & C Yellow II
10	11076360	Ethidium bromide
10	11076356	Emodin (bulk)
10	11076522	Nitazoxanide
10	7853959	Iodochlorohydroxyquinoline
11	11076334	Dimenhydrinate
11	7852690	Propranolol HCl
11	7852142	Gallic acid
11	7853448	Flavone
11	11076631	Rifabutin
11	7851867	p,p'-DDT (Dichlorodiphenyltrichloroethane)

11	7854760	Genistein (4',5,7-Trihydroxyisoflavone)
11	11075925	13-cis-Retinal (Vitamin A aldehyde)
12	7852714	p-Quinone dioxime (p-Benzoquinone dioxime)
12	11076083	3,4-Diaminotoluene
12	7852846	Titanocene dichloride
12	11076533	o-Aminophenol
12	11076275	cis-Dichlorodiamine platinum
12	7853476	Pentabromophenol
12	11076559	o-Phenylenediamine
12	11075917	1,4,5-Trihydroxynaphthalene
12	11076518	Ninhydrin
12	11076076	3,3'-Dihydroxybenzidine
12	11076358	Ergotamine tartrate
12	7852598	Pentachlorophenol
12	11075883	1,1,1,2-Tetrabromoethane
12	7852523	p-Nitrosodiphenylamine
12	11076494	N,N-Dimethyl-p-nitrosoaniline
12	11076122	4-Amino-4'-hydroxy-3-methyldiphenylamine
12	11076328	Digitonin
12	7852956	Ziram
12	11076527	N-Methyl-p-aminophenol sulfate
12	7852824	Tetramethylthiuram disulfide
12	11076065	2-Octyl-3-isothiazolone
12	11076251	Captan 90-concentrate (solid)
12	11076132	4-Hydroxyphenyl retinamide
12	7852793	Tamoxifen, citrate salt
13	7854866	Corticosterone
13	7851832	Cobalt sulfate heptahydrate
13	11076451	Methoxychlor [95%]
13	7852623	N-Phenyl-2-naphthylamine
13	7854582	trans-Retinol acid (Vitamin A)
13	7854794	Progesterone
13	7852276	Lovastatin
14	11076592	Phenmedipham (3-Methoxycarbonylamino-phenyl-N-3'-methylphenyl)
14	11076270	Cimicifugoside
14	11076311	Diazoaminobenzene
14	7852339	2-Methyl-1-nitroanthraquinone
14	11076073	3,3',5,5'-Tetrabromo bisphenol A
14	7851561	o-Aminoazotoluene
14	7852319	Methoxychlor
14	11076444	Medroxyprogesterone acetate
14	11076586	Pentamidine isethionate
14	11076175	Actein
15	7852357	4,4'-Methylene-bis-2-chloroaniline (MOCA)
15	7852736	Rifampicin
15	11076317	Dichlorvos (Vapona)
15	7852617	Phenolphthalein
15	11076488	n-(1,3-Dimethylbutyl)-n`-phenyl-p-phenylenediamine

15	11076521	N-Isopropyl-N'-phenyl-p-phenylenediamine
15	11076261	Chlordane, technical grade
15	7852619	Phenoxybenzamine HCl
15	11076163	9-Aminoacridine HCl H2O
16	11075895	1,2-Cyclohexanedicarboxylic acid, bis(oxiranylmethyl) ester
16	11075957	2,3,5,6-Tetrachlorophenol
16	11076280	Colchicine
16	11076279	Colchicine
16	7851755	Chlorambucil
16	7851523	Actinomycin D
16	11076697	Tris(2,3-epoxypropyl)isocyanurate
16	7851865	Rhothane (TDE)
16	7852296	Melphalan
16	11076329	Diglycidyl resorcinol ether
16	11076432	Malachite Green Oxalate
16	11076302	Daunomycin HCL
17	11076490	N,N,N',N'-Tetramethyl-p-phenylenediamine
17	7852732	all-trans-Retinyil acetate
17	11075988	2,4-Hexadienal
17	11076463	Methyl testosterone
17	11076615	Progesterone
17	7854810	Apigenin
17	7851925	3,3'-Dichlorobenzidine 2HCl
17	11076162	8-Hydroxyquinoline
17	7852222	8-Hydroxyquinoline
17	7852952	Zearalenone
17	11076381	Fumaronitrile
17	11075923	1,6-Hexanediol diacrylate
17	11076391	Guggulsterones E
17	11076712	Zearalenone
17	11076565	Oxymetholone
17	7851785	Chloroacetophenone
17	7851786	4'-(Chloroacetyl)acetanilide
18	7852812	Tetrachlorvinphos (Gardona)
18	7852338	N-Methyl-N'-nitro-N-nitrosoguanidine
18	11076326	Diethylene glycol diacrylate
18	7851768	3-Chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone, (MX)
18	11076675	Tetraethylene glycol diacrylate
18	7851606	Auramine
18	11076465	Methylene bis(thiocyanate)
18	11076676	Tetraethylene glycol diacrylate
18	11076523	Nitrogen mustard HCl
18	11076710	Vitamin D3
18	11075944	2,2',4'-Trichloroacetophenone
18	7851735	Captan
18	11076176	Adriamycin, hydrochloride
18	11076585	Pentaerythritol Triacrylate
18	11076634	Saquinavir Mesylate

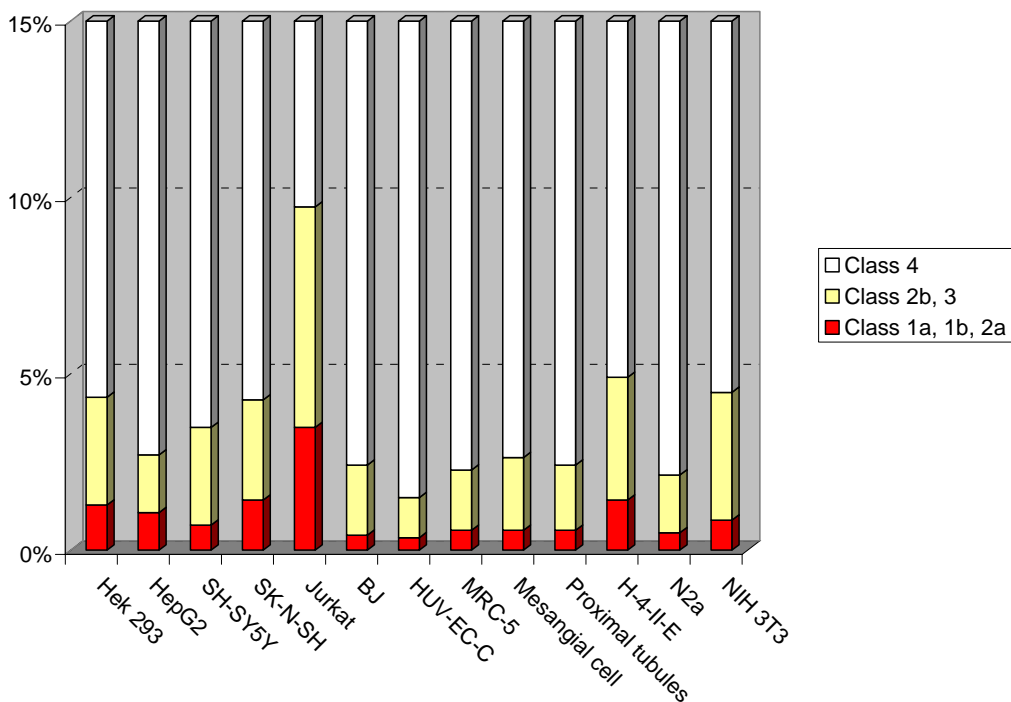
18	7852860	Toxaphene
18	11075909	1,3-Diiminobenz (f)-isoindoline
18	11076688	trans-Retinal (Vitamin A aldehyde)
19	7852002	7,12-Dimethylbenz(a)anthracene
19	11076170	Acetochlor
19	7854036	Digoxin
19	11076495	N,N-Dimethyl-p-phenylenediamine
19	11076492	N,N-Diethyl-p-phenylenediamine
19	11076156	6-Hydroxy-2-naphthyl disulfide (DDD)
19	7851608	5-Azacytidine
19	11076288	Curcumin
19	11076642	Sodium Dichromate Dihydrate
19	11076643	Sodium dichromate dihydrate (VI)
19	11076612	Potassium dichromate
20	11076353	Domiphen bromide
20	7854806	4-Hydroxytamoxifen
20	11076420	Kepone
20	7852262	Chlordecone (Kepone)
20	7852833	4,4-Thiobis(6-t-butyl-m-cresol)
21	7851957	Diethylstilbestrol [DES]
21	7853657	Alachlor
21	11076348	Direct red 2 (C.I. 23500)
21	11076392	Guggulsterones Z
21	7852170	Hematoxylin (C.I. 75290)
21	11076195	Amitriptyline HCl
21	11076293	Cycloheximide
21	11076545	Oleic acid diethanolamine condensate (1:1)
21	11076232	Bis(cyclopentadienyl)vanadium chloride
21	7852303	Mercuric chloride
21	7852642	Phenyl mercuric acetate
21	11076713	Zinc pyrithione
21	11076573	p-Aminophenol
22	11076212	Benzo(b)fluoranthene
22	7851858	Cyproterone acetate
22	11076067	2-Pivalyl-1,3-indandione
22	7852709	Pyrimethamine
22	7851611	Azathioprine
22	11076157	6-Mercaptopurine monohydrate
22	7854664	6-Thioguanine (6-TG)
22	11076292	Cycloheximide
23	7853452	4,6-Dinitro-o-cresol
23	11076081	3,4,5-Trichlorophenol
23	7851685	HC blue 2
23	11076557	o-Phenanthroline
23	7852716	Acid red 114 (C.I. 23635)
23	11076466	Methylene blue trihydrate
23	7852834	2,2'-Thiobis(4,6-dichlorophenol)
23	11076088	3,4-Dichlorophenyl isocyanate

23	11076262	Chlorhexidine
23	7852739	Basic red 9 (p-Rosaniline HCl) (C.I. 42500)
23	11076201	a-Solanine
23	7853942	Carminic acid
23	7853612	2,3,4,5-Tetrachlorophenol
23	11075952	2,2'-Thiobis(4-chlorophenol)
23	11075924	1,8-Dihydroxy-4,5-dinitroanthraquinone
23	11076497	N,N'-Di-sec-butyl-p-phenylenediamine
23	7853270	2,2'-Methylenebis-(4-chlorophenol)
23	11076355	Econazole nitrate
23	7852145	Hexamethyl-p-rostaniline chloride (Gentian violet)



**Figure 1**

(a) Activity distributions of the set of 1408 compounds in the 13 caspase activation assays



(b) Potency distributions of the set of 1408 compounds that were class 1-3 in the 13 caspase activation assays

