

The NTP High Throughput Screening (HTS) Initiative

The NTP Roadmap for the 21st Century includes a major initiative to develop HTS assays to:

- identify mechanisms of action for further investigation
- develop predictive models for biological response
- prioritize substances for further toxicological evaluation

In support of this initiative, on December 14 and 15, 2005 in Arlington, VA, the NTP sponsored an HTS Assay Workshop to obtain input on HTS technology and the approach the NTP should take to implement these assays in its testing program¹. In addition, at this Workshop, members of the NIH Molecular Libraries Initiative (MLI), a part of the NIH Roadmap for Medical Research, presented information about their program.

In July 2005, the NTP became a formal participant in the MLI. The MLI is focusing on the use of high-technology screening methods to identify small molecules that can be optimized as chemical probes to study the functions of genes, cells, and biochemical pathways. The NTP, through its association with the MLI, has the opportunity to generate information that links data on the biological activity of substances generated from biochemical and cell-based HTS assays with toxicity endpoints identified in the NTP's toxicology testing program. To achieve this goal, in August 2005, the NTP began a formal collaboration with the NIH Chemical Genomics Center (NCGC) to test substances of interest to the NTP across a spectrum of HTS assays. The NCGC is one of 10 HTS centers around the country that comprise the NIH Molecular Libraries Screening Center Network (MLSCN).

Late in 2005, the NTP supplied six cell-based assays to the NCGC. These assays included two for cytotoxicity (CellTiter-Glo which measures ATP levels, Cytotox-One which measures LDH release), three for specific caspase enzyme activity associated with apoptosis (Caspase 3/7, Caspase 8, and Caspase 9), and one for activity associated with a cell membrane g-glycoprotein pump that is responsible for drug resistance (pgp-Glo Assay). These assays were selected largely because:

- it appeared that they could easily be optimized for use in the 1536-well robotics assay format used by the NCGC,
- the endpoints could be of interest from a toxicological viewpoint, and
- it was thought that the data generated by these tests could be used to establish the bioinformatic procedures needed to appropriately mine the extraordinary large sets of chemical, biological, and toxicological data that would result from HTS testing.

By January 2006, the NTP had provided a total of 1408 test substances to the NCGC (Appendix 1). Based on the plate design used by the NCGC, 1408 represents the number of chemicals that are tested per 1536-well plate. These substances were selected because all have been evaluated in one or more NTP toxicological tests or were reference substances identified by the Interagency Coordinating Committee on the Validation of Alternative Methods (ICCVAM) for the development and validation of alternative *in vitro* test methods in specific regulatory testing areas (e.g., acute toxicity, dermal corrosion, endocrine activity). Selection was based also on

¹ Information on the program and copies of the presentations can be obtained at <http://ntp.niehs.nih.gov/index.cfm?objectid=E13C3474-F1F6-975E-7CA9B6918AE38EF4>

availability, volatility, potential risk (e.g., dioxin), and solubility in DMSO (at 10 mM). The list includes 55 duplicate compounds to evaluate assay reliability. The list of test substances sent to the NCGC includes nearly every chemical class for small molecules imaginable. Molecular weights ranged from approximately 100 to 400. Functionally, the list includes solvents, fire retardants, preservatives, flavoring agents, plasticizers, therapeutic agents, inorganic and organic pollutants, drinking water disinfection byproducts, pesticides and natural products. Recently, the MLSCN has decided to place the majority of the NTP 1408 in the MLSCN chemical repository in order to make them available as a specialty compound set to other members of the network.

To date, the NCGC has tested the NTP collection of 1408 chemicals, using 14-point concentration response curves (0.5 nM to 92 μ M in 5 μ L/well) in the:

- CellTiter-Glo cytotoxicity assay, in nine human and four rodent cell types. The cell types originated from various organs (although most of the cell types were immortal cell lines derived from tumors), with some matching rodent cell types to compare responses across species. The cell types used were:
 - BJ (human foreskin fibroblasts)
 - HEK293 (human embryonic kidney)
 - HepG2 (human hepatocellular carcinoma)
 - HUV-EC-C (normal human vascular endothelial cells)
 - Jurkat (Clone E6-1, human T cell leukemia)
 - MRC-5 (human lung fibroblasts)
 - SK-N-SH [human neuroblastoma)
 - SK-SY5Y (human neuroblastoma)
 - Proximal tubules (primary cells from rat kidney)
 - H-4-II-E (rat hepatoma)
 - N2a (mouse neuroblastoma)
 - NIH 3T3 (immortal mouse fibroblasts)

The concentration response data from these studies have been evaluated by the NCGC and in-house at NIEHS to identify actives. Also, the NCGC is also using real time cell electronic sensing (RT-CES) to evaluate the kinetics of cytotoxicity for selected compounds. This information allows for further classifying the cytotoxic compounds according to differences in response kinetics.

- Caspase 3,7 assay, in six human and three rodent cell types. The cell types used were:
 - BJ (human foreskin fibroblasts)
 - HEK293 (human embryonic kidney)
 - HepG2 (human hepatocellular carcinoma)
 - HUV-EC-C (normal human vascular endothelial cells)
 - Jurkat (Clone E6-1, human T cell leukemia)
 - SK-SY5Y (human neuroblastoma)
 - H-4-II-E (rat hepatoma)
 - N2a (mouse neuroblastoma)
 - NIH 3T3 (immortal mouse fibroblasts)

The concentration response data from these studies are being evaluated by the NCGC and in-house at NIEHS to identify actives.

- Cytotox-One (LDH release) assay, in one human and one rodent cell type. The cell types used were (more cell types are anticipated):
 - HEK293 (human hepatocellular carcinoma)
 - Proximal tubules (primary cells from rat kidney)

The NCGC intends also to test the NTP 1408 as part of their in-house library of about 80,000 compounds in as many as 60 other assays currently established at their facility (see Appendix 2).

To date, this has included:

- Anthrax LF BLA
- β -lactamase (AmpC)
- β -Thal mRNA splicing GPF
- Cell signaling CRE-BLA
- DNA polymerase III
- Hsp90 co-chaperone interaction
- Huntington PC12 cell toxicity
- JNK alphascreen
- I κ B α Cell sensor Dual Luc
- O-GlcNAc Transferase
- Peroxiredoxins (Tgr-Trx-Prx)
- Tau polymerization
- YjeE FP

The normalized concentration response data from these assays are (or will be) publicly available on PubChem (<http://pubchem.ncbi.nlm.nih.gov/>).

In December 2005, a collaboration was established between the NTP HTS Faculty and the EPA Chemical Prioritization Community of Practice (CPCP) to jointly evaluate HTS assays and other model systems for their use in toxicological investigations and in chemical prioritization. In February 2006, three joint NTP-EPA focus groups were established:

- Toxicity Targets and Bioactivity Assays, the purpose of which is to identify toxicity targets and bioactivity assays targets of interest relating to various toxicities, and relevant in silico, HTS, and high content screening assays
- Chemical Selection, the purpose of which is to identify and coordinate the testing of chemicals of interest to the NTP and the EPA
- Informatics, the purpose of which is to develop and/or identify appropriate tools for chemical and biological data analysis and management across multiple databases.

This collaboration has been useful in several ways:

- The EPA recently provided approximately 400 pesticide actives and ten nuclear receptor assays (Era, LXRb, FXR, AR, PPAR α , TRb, RXRa, VDR, PPAR δ , GR) to the NCGC. Among the pesticide actives are approximately 60 compounds that were included in the NTP 1408. This will provide for an assessment of assay reproducibility across time. There is also the intent to test the NTP 1408 in the nuclear receptor assays.

- The EPA has established a number of contracts to support their HTS and high-content assay initiatives². Potentially, the NTP has the ability to use these resources.

To broaden exposure to HTS concepts as they apply to toxicology testing within the NIEHS/NTP and its CPCP counterpart at the EPA, the NTP hosted the directors of the NCGC in a day-long Chemical Genomics 101 course, held at NIEHS in RTP on April 20, 2006. Approximately 100 scientists from NIEHS, EPA, and non-government organizations attended.

To increase awareness of this Initiative, three coordinated posters were presented that related to the HTS activities at the 2007 Annual Meeting of the Society of Toxicology (March 25-28).

- The National Toxicology Program (NTP) High Throughput Screening (HTS) Initiative: Current Status and Future Directions, by R. R. Tice, J. Fostel, C. S. Smith, K. L. Witt, J. H. Freedman, C. J. Portier, A. D. Dearry, and J. R. Bucher
- Chemical Compound Profiling of Cell-based Toxicity Assays Using Quantitative High-Throughput Screening, by M. Xia, K. Witt, N. Southall, M-H. Cho, A. Jadhav, R. Huang, C. Smith, J. Fostel, R. Tice, J. Inglese, and C. Austin
- The National Toxicology Program (NTP) High Throughput Screening (HTS) Initiative: Chemical Selection - Round 1, by C. Smith, J. Bucher, A. Dearry, C. Portier, R. Tice, K. Witt, and B. Collins

Also, in collaboration with the EPA, the NCGC, and Pharma, the NTP organized a symposium at the 2007 annual meeting (April 15-19) of the Society for Biomolecular Sciences entitled “Toxicity Profiling using High-Throughput and High-Content Technologies”. The purpose of this session was to discuss the challenges associated with the use of HTS and high content screening assays to identify activities of diverse chemical compounds in toxicity-relevant assays, to facilitate the development of predictive *in vitro* models for toxicity, and to help prioritize substances for further toxicological evaluation.

² see www.epa.gov/oamhpod1/adm_placement/prhq0614395/toxcastsummary.doc

Appendix 1. NTP 1408 Compounds Provided to the NCGC for HTS

Substance	CASRN	Substance	CASRN
Acetaldehyde	75-07-0	Benzidine	92-87-5
Acetaminophen (4-hydroxyacetanilide)	103-90-2	Benzofuran	271-89-6
Acetohexamide	968-81-0	Benzoic acid	65-85-0
Acetonitrile	75-05-8	Benzoil	119-53-9
1-Acetyl-2-phenyl hydrazide	114-83-0	p-Quinone	106-51-4
Acrolein	107-02-8	2,2'-Dithiobis-benzothiazole	120-78-5
Acrylamide	79-06-1	1,2,3-Benzotriazole	95-14-7
Acrylonitrile	107-13-1	Benzotrichloride	98-07-7
Actinomycin D	50-76-0	Benzyl acetate	140-11-4
Adipamide	628-94-4	Benzyl alcohol	100-51-6
Aldicarb	116-06-3	Benzyl chloride	100-44-7
Aldrin	309-00-2	o-Benzyl-p-chlorophenol	120-32-1
Allyl alcohol	107-18-6	Biphenyl	92-52-4
Allyl chloride	107-05-1	Bis(2-chloroethyl)ether	111-44-4
Allyl glycidyl ether	106-92-3	Bisphenol A	80-05-7
Allyl isothiocyanate	57-06-7	HC blue 2	33229-34-4
3-Amino-4-ethoxyacetanilide	17026-81-2	Boric acid	10043-35-3
1-Amino-2-methylanthraquinone	82-28-0	Bromodichloromethane	75-27-4
2-Amino-4-nitrophenol	99-57-0	Bromoethane (ethyl bromide)	74-96-4
2-Amino-5-nitrophenol	121-88-0	2-Bromo-1-ethanol	540-51-2
4-Amino-2-nitrophenol	119-34-6	Butyl benzyl phthalate	85-68-7
2-Amino-5-nitrothiazole	121-66-4	n-Butyl chloride	109-69-3
2-Aminoanthraquinone	117-79-3	n-Butyl-p-hydroxybenzoate	94-26-8
o-Aminoazotoluene	97-56-3	Butylated hydroxytoluene	128-37-0
4-Biphenylamine	92-67-1	t-Butylhydroquinone	1948-33-0
Ampicillin trihydrate	7177-48-2	beta-Butyrolactone	3068-88-0
Anethole	104-46-1	Cadmium chloride	10108-64-2
Anilazine	101-05-3	Caffeine	58-08-2
Aniline	62-53-3	Capsaicin	404-86-4
p-Anisidine hydrochloride	20265-97-8	Captan	133-06-2
o-Anthranilic acid	118-92-3	Semicarbazide hydrochloride	563-41-7
L-Ascorbic acid	50-81-7	Carbarson	121-59-5
Aspartame	22839-47-0	Carbaryl	63-25-2
Acetylsalicylic acid	50-78-2	Carbazole	86-74-8
Atrazine	1912-24-9	Carbon tetrachloride	56-23-5
Auramine	2465-27-2	D-Carvone	2244-16-8
5-Azacytidine	320-67-2	Catechol	120-80-9
6-Azacytidine	3131-60-0	Chloramben	133-90-4
Azathioprine	446-86-6	Chlorambucil	305-03-3
Sodium azide	26628-22-8	Chloramphenicol	56-75-7
Azinphosmethyl	86-50-0	Chloranil	118-75-2
Azobenzene	103-33-3	Chlorendic acid	115-28-6
3'-Azido-3'-deoxythymidine (AIDS)	30516-87-1	3-Chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone(MX)	77439-76-0
Benzaldehyde	100-52-7	2-Chloronitrobenzene	88-73-3
Benzene	71-43-2	4-Chloronitrobenzene	100-00-5

Substance	CASRN	Substance	CASRN
4-Chloro-o-phenylenediamine	95-83-0	1,2-Dichlorobenzene (o-dichlorobenzene)	95-50-1
2-Chloro-p-phenylenediamine sulfate	61702-44-1	3,3'-Dichlorobenzidine dihydrochloride	612-83-9
3-Chloro-p-toluidine	95-74-9	trans-1,4-Dichloro-2-butene	110-57-6
5-Chloro-o-toluidine	95-79-4	1,1-Dichloroethane	75-34-3
2-Chloroacetophenone (CN)	532-27-4	1,2-Dichloroethane	107-06-2
4-(Chloroacetyl)acetanilide	140-49-8	2,4-Dichlorophenol	120-83-2
p-Chloroaniline	106-47-8	2,4-Dichlorophenoxyacetic acid	94-75-7
Chlorobenzene	108-90-7	Butyl(2,4-dichlorophenoxy) acetate	94-80-4
Chlorodibromomethane	124-48-1	1,2-Dichloropropane (propylene dichloride)	78-87-5
Chloroform	67-66-3	Dichlorvos	62-73-7
2-Chloromethylpyridine hydrochloride	6959-47-3	Dicofol	115-32-2
Monuron	150-68-5	N,N'-Dicyclohexylthiourea	1212-29-9
Chloropicrin	76-06-2	Diieldrin	60-57-1
Chlorpheniramine maleate	113-92-8	Chlorpyrifos (Dursban)	2921-88-2
Chlorpropamide	94-20-2	Diethylene glycol	111-46-6
Chromium (III) acetate	1066-30-4	Diethylstilbestrol	56-53-1
Danthron	117-10-2	N,N'-Diethylthiourea	105-55-5
Cimetidine	51481-61-9	3,4-Dihydrocoumarin	119-84-6
1,2,3-Propanetricarboxylic acid, 2-hydroxy-	77-92-9	Dimethoxane	828-00-2
Cobalt sulfate heptahydrate	10026-24-1	2,4-Dimethoxyaniline hydrochloride	54150-69-5
Coumarin	91-64-5	3,3'-Dimethoxybenzidine-4,4'-diisocyanate	91-93-0
m-Cresidine	102-50-1	4-Dimethylaminoazobenzene	60-11-7
p-Cresidine	120-71-8	4-Dimethylaminoantipyrine	58-15-1
Cupferron	135-20-6	N,N-Dimethylaniline	121-69-7
beta-Cyclodextrin	7585-39-9	7,12-Dimethylbenzanthracene	57-97-6
Cyclohexanone	108-94-1	Dimethylcarbamoyl chloride	79-44-7
Cyproterone acetate	427-51-0	Dimethylformamide	68-12-2
Dacarbazine	3/4/42	Dimethylvinyl chloride (DMVC)	513-37-1
Daminozide	1596-84-5	2,4-Dinitrophenol	51-28-5
4,4'-Sulfonyldianiline (Dapsone)	80-08-0	2,6-Dinitrotoluene	606-20-2
o,p'-DDD	53-19-0	N,N'-Diphenyl-p-phenylenediamine	74-31-7
Tetrachlorodiphenylethane	72-54-8	5,5-Diphenylhydantoin (phenytoin)	57-41-0
p,p'-Dichlorodiphenyl dichloroethylene	72-55-9	2,5-Dithiobiurea	142-46-1
Dichlorodiphenyltrichloroethane (DDT)	50-29-3	Endosulfan	115-29-7
Dexamethazone	50-02-2	Epichlorhydrin	106-89-8
Diallyl phthalate	131-17-9	1,2-Epoxybutane	106-88-7
2,4-Diaminotoluene (2,4-toluene diamine)	95-80-7	17beta-Estradiol	50-28-2
Diazinon	333-41-5	Estragole	140-67-0
Dibenz(a,h)anthracene	53-70-3	Ethinyl estradiol	57-63-6
1,2-Dibromo-3-chloropropane	96-12-8	Ethionamide	536-33-4
1,2-Dibromoethane	106-93-4	2-Eethoxybenzamide	938-73-8
Dibromomannitol	488-41-5	Ethoxyquin	91-53-2
Dichloran	99-30-9	Ethanol	64-17-5
2,6-Dichloro-p-phenylenediamine	609-20-1	Ethyl bromoacetate	105-36-2
Dichloroacetic acid	79-43-6	Di(p-ethylphenyl)dichloroethane	72-56-0

Substance	CASRN	Substance	CASRN
Ethyl-3-methyl-3-phenylglycidate	77-83-8	Lovastatin	75330-75-5
N-Ethyl-n-nitrosourea	759-73-9	Malaoxon	1634-78-2
Ethylbenzene	100-41-4	Malathion	121-75-5
Ethylene glycol	107-21-1	Maleic hydrazide	123-33-1
Ethylene thiourea (ETU)	96-45-7	Melphalan	148-82-3
4-Vinyl-1-cyclohexene diepoxide	106-87-6	2-Mercaptobenzothiazole	149-30-4
2-Ethylhexanol	104-76-7	Mercuric chloride	7487-94-7
Di(2-ethylhexyl)adipate	103-23-1	Methyl mercuric chloride	115-09-3
Di(2-ethylhexyl) phthalate	117-81-7	Methoxychlor	72-43-5
1,8-Cineol	470-82-6	Hydroquinone monomethyl ether	150-76-5
Eugenol	97-53-0	8-Methoxypsoralen	298-81-7
Formulated fenaminosulf	140-56-7	Methyl-t-butyl ether	1634-04-4
Fenthion	55-38-9	Methyl methacrylate	80-62-6
Fluometuron	2164-17-2	Methyl methanesulfonate	66-27-3
5-Fluorouracil	51-21-8	1-Methyl-3-nitro-1-nitroso-guanidine	70-25-7
Furan	110-00-9	2-Methyl-1-nitroanthraquinone	129-15-7
Furfural	98-01-1	Methyl parathion	298-00-0
Furosemide	54-31-9	4,4'-Methylenebis(2-chloroaniline)	101-14-4
Gallic acid	149-91-7	Methylene chloride	75-09-2
Gemfibrozil	25812-30-0	4,4'-Methylenebis(N,N-dimethyl)benzenamine	101-61-1
Hexamethyl-p-rosaniline chloride	548-62-9	1-Methylnaphthalene	90-12-0
Gibberellic acid	77-06-5	2-Methylnaphthalene	91-57-6
Glycerol	56-81-5	Methylphenidate hydrochloride	298-59-9
Glycidol	556-52-5	6-Methylquinoline	91-62-3
Griseofulvin	126-07-8	8-Methylquinoline	611-32-5
Hematoxylin	517-28-2	6-Methyl-2-thiouracil	56-04-2
Heptachlor	76-44-8	Metronidazole	443-48-1
Heptylamine	111-68-2	Monochloroacetic acid	79-11-8
Hexachloro-1,3-butadiene	87-68-3	Myleran	55-98-1
Hexachlorocyclopentadiene	77-47-4	Nalidixic acid	389-08-2
Hexachloroethane	67-72-1	Naphthalene	91-20-3
Hexachlorophene	70-30-4	1-Naphthalene acetic acid	86-87-3
Hexanamide	628-02-4	1,5-Naphthalenediamine	2243-62-1
Propofol	2078-54-8	N-(1-Naphthyl)ethylenediamine dihydrochloride	1465-25-4
Hydrazobenzene	122-66-7	1-Naphthylamine	134-32-7
Hydrochlorothiazide	58-93-5	2-Naphthylamine	91-59-8
Hydroquinone	123-31-9	Nicotine	54-11-5
8-Hydroxyquinoline	148-24-3	Nitrilotriacetic acid (NTA)	139-13-9
Indomethacin	53-86-1	Sodium nitrite	7632-00-0
Iodoform	75-47-8	5-Nitro-o-anisidine	99-59-2
Isobutyl nitrite	542-56-3	Nitrofurazone	59-87-0
Isoniazid	54-85-3	2-Nitro-p-phenylenediamine	5307-14-2
Isoprene	78-79-5	4-Nitro-o-phenylenediamine	99-56-9
Isopropanol	67-63-0	5-Nitro-o-toluidine	99-55-8
Isosafrole (TGMX)	120-58-1	5-Nitroacenaphthene	602-87-9
Kaempferol	520-18-3	p-Nitroaniline	100-01-6
Chlordecone (kepone)	143-50-0	o-Nitroanisole	91-23-6
Lithocholic acid	434-13-9		

Substance	CASRN	Substance	CASRN
4-Nitroanthranilic acid	619-17-0	Pyrimethamine	58-14-0
Nitrobenzene	98-95-3	p-Benzoquinone dioxime	105-11-3
6-Nitrobenzimidazole	94-52-0	C.I. Acid red 114	6459-94-5
p-Nitrobenzoic acid	62-23-7	Reserpine	50-55-5
1-Nitrobutane	627-05-4	Resorcinol	108-46-3
Nitroethane	79-24-3	Retinol acetate	127-47-9
Nitrofurantoin	67-20-9	Rifampicin	13292-46-1
Nitromethane	75-52-5	C.I. Basic red 9 monohydrochloride	569-61-9
1-Nitronaphthalene	86-57-7	Safrole	94-59-7
1-Nitropropane	108-03-2	Salicylazosulfapyridine	599-79-1
2-Nitropropane	79-46-9	Scopolamine hydrobromide trihydrate	6533-68-2
N-Nitrosodiethanolamine	1116-54-7	Sesamol	533-31-3
N-Nitrosodiethylamine	55-18-5	Sodium chlorite (water disinfection byproducts)	7758-19-2
N-Nitrosodimethylamine	62-75-9	Sodium hypochlorite	7681-52-9
N-Nitrosodiphenylamine	86-30-6	Sorbic acid	110-44-1
p-Nitrosodiphenylamine	156-10-5	Styrene	100-42-5
N-Nitrosopiperidine	100-75-4	Styrene oxide	96-09-3
Corn oil	8001-30-7	Succinic anhydride	108-30-5
Safflower oil	8001-23-8	Sulfallate	95-06-7
4,4'-Oxydianiline	101-80-4	Sulfamethazine	57-68-1
Oxytetracycline hydrochloride	2058-46-0	Sulfisoxazole	127-69-5
Parathion	56-38-2	Chlorotrianisene	569-57-3
Pentachloronitrobenzene	82-68-8	Tamoxifen citrate	54965-24-1
Pentachlorophenol, purified	87-86-5	L-Taurine	107-35-7
Phenacetin	62-44-2	1,1,2,2-Tetrachloroethane	79-34-5
Phenazopyridine hydrochloride	136-40-3	Tetrachloroethylene	127-18-4
Phenformin hydrochloride	834-28-6	Tetrachlorvinphos	961-11-5
Phenol	108-95-2	Tetrahydrofuran	109-99-9
Phenolphthalein	77-09-8	Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8
Phenothiazine	92-84-2	Tetramethylthiourea disulfide	137-26-8
Phenoxybenzamine hydrochloride	63-92-3	Tetranitromethane	509-14-8
1-Phenyl-3-methyl-5-pyrazolone	89-25-8	Theophylline	58-55-9
N-Phenyl-2-naphthylamine	135-88-6	Thiabendazole	148-79-8
1-Phenyl-2-thiourea	103-85-5	4,4-Thiobis(6-tert-butyl-m-cresol)	96-69-5
Phenylbutazone	50-33-9	2,2'-Thiobis(4,6-dichlorophenol)	97-18-7
m-Phenylenediamine	108-45-2	4,4'-Thiodianiline	139-65-1
Phenyl glycidyl ether	122-60-1	Thiosemicarbazide	79-19-6
Phenylmercuric acetate	62-38-4	Thiourea	62-56-6
o-Phenylphenol	90-43-7	Titanocene dichloride	1271-19-8
Phthalic anhydride	85-44-9	Tolbutamide	64-77-7
Piperonyl butoxide	51-03-6	Toluene	108-88-3
Prednisone	53-03-2	o-Toluidine hydrochloride	636-21-5
Probenecid	57-66-9	Toxaphene	8001-35-2
Propiolactone	57-57-8	Triamterene	396-01-0
Propranolol.HCl	318-98-9	Tribromomethane	75-25-2
1,2-Propylene glycol	57-55-6	Tricaprylin	538-23-8
6-Propyl-2-thiouracil	51-52-5		
Pyrazinamide	98-96-4		

Substance	CASRN	Substance	CASRN
Trichloroacetic acid	76-03-9	Tetradecanoic acid	544-63-8
2,4,6-Trichloroaniline	634-93-5	Trichloroacetonitrile	545-06-2
1,1,2-Trichloroethane	79-00-5	Benzamide	55-21-0
Trichloroethylene	79-01-6	2,3,4,6-Tetrachlorophenol	58-90-2
Trichlorofluoromethane	75-69-4	4-Chloro-m-cresol	59-50-7
2,4,6-Trichlorophenol	88-06-2	2-Hydroxybenzamide	65-45-2
1,2,3-Trichloropropane	96-18-4	Methanol	67-56-1
Tricresyl phosphate	1330-78-5	n-Butanol	71-36-3
2,4,5-Trimethylaniline	137-17-7	1-Pentanol	71-41-0
Tris(2-chloroethyl) phosphate	115-96-8	1,1,1-Trichloroethane	71-55-6
Tris(2-ethylhexyl)phosphate	78-42-2	Tributoxyethyl phosphate	78-51-3
Urea	57-13-6	Isobutyl alcohol	78-83-1
Vinyl acetate	108-05-4	Propylenediamine	78-90-0
4-Vinylcyclohexene	100-40-3	2-Butanol	78-92-2
Vinylidene chloride	75-35-4	Methyl acetate	79-20-9
Xylenes (mixed)	1330-20-7	p-tert-Pentylphenol	80-46-6
HC Yellow 4	52551-67-4	p-Menthane-1,8-diamine	80-52-4
Zearalenone	17924-92-4	Riboflavin	83-88-5
Ziram	137-30-4	Diethyl phthalate	84-66-2
Zineb	12122-67-7	Dibutyl phthalate	84-74-2
Acetone	67-64-1	o-Nitrophenol	88-75-5
Phthalic acid	88-99-3	Quinoline	91-22-5
Benzonitrile	100-47-0	N,N-Diethyl aniline	91-66-7
Phenylacetonitrile	140-29-4	o-Xylene	95-47-6
Bromoacetic acid	79-08-3	o-Cresol	95-48-7
Bromoacetonitrile	590-17-0	o-Chloroaniline	95-51-2
Bromochloromethane	74-97-5	3,4-Dichloroaniline	95-76-1
Butyraldehyde	123-72-8	2,3-Dibromo-1-propanol	96-13-9
Methyl ethyl ketone	78-93-3	Methyl ethyl ketoxime	96-29-7
Maleic acid	110-16-7	2,4-Dinitroaniline	97-02-9
Fumaric acid	110-17-8	2,2'-Methylene-bis (4-chlorophenol)	97-23-4
o-Chlorophenol	95-57-8	Cumene	98-82-8
Decanoic acid	334-48-5	m-Nitrotoluene	99-08-1
Dichloroacetonitrile	3018-12-0	N,N-Dimethyl-p-toluidine	99-97-8
2,3-Butanedione	431-03-8	(Diethylamino)ethanol	100-37-8
Lauric acid	143-07-7	N-Methyl aniline	100-61-8
n-Heptanal	111-71-7	Cyclohexanone oxime	100-64-1
n-Heptanoic acid	111-14-8	Diphenyl oxide	101-84-8
Adipic acid	124-04-9	2-(Dibutylamino)ethanol	102-81-8
m-Toluic acid	99-04-7	2-Nitro-1,1'-biphenyl	86-00-0
p-Toluic acid	99-94-5	2-Nitrodiphenylamine	119-75-5
Butanoic acid, 2-methyl-	116-53-0	2-Nitroethanol	625-48-9
Isobutyraldehyde	78-84-2	2-Octyl-3-isothiazolone	26530-20-1
Dibromonitromethane (water disinfection byproducts)	598-91-4	2-Pentenenitrile	13284-42-9
Stearic acid	57-11-4	2-Pivalyl-1,3-indandione	83-26-1
Octanoic acid	124-07-2	Phenol, 2-(1,1-dimethylethyl)-	88-18-6
n-Pentanal	110-62-3	2-Vinylpyridine	100-69-6
Propionaldehyde	123-38-6	3-((Ethylhexyl)oxy)propylamine	5397-31-9

Substance	CASRN	Substance	CASRN
3-(Methylthio)propanal	3268-49-3	Ethanolamine	141-43-5
3,3'-(1,4-Phenylene)bis-2-propenoic acid	16323-43-6	Ethyl acetate	141-78-6
Tetrabromobisphenol A	79-94-7	1,3-Dichloropropane	142-28-9
3,3',5,5'-Tetramethylbenzidine	54827-17-7	Hydroquinone dimethyl ether	150-78-7
3,3,5-Trimethylcyclohexyl salicylate	118-56-9	Disulfoton	298-04-4
3,3'-Dihydroxybenzidine	2373-98-0	flavone	525-82-6
3,3'-Dimethoxybenzidine	119-90-4	o-Tolunitrile	529-19-1
3,3'-Dimethylbenzidine	119-93-7	o-Tolualdehyde	529-20-4
N,N-dimethylbenzylamine	103-83-3	4,6-Dinitro-o-cresol	534-52-1
4-Chlorobenzaldehyde	104-88-1	1,3-Dichlorobenzene	541-73-1
2,4-Dimethylphenol	105-67-9	Pentabromophenol	608-71-9
p-Bromoaniline	106-40-1	p-Nitrobenzamide	619-80-7
p-Xylene	106-42-3	N-Acetyl-m-aminophenol	621-42-1
p-Chlorophenol	106-48-9	2,5-Dimethylfuran	625-86-5
Isobutyl acrylate	106-63-8	2-Methylimidazole	693-98-1
1-Bromopropane	106-94-5	2-propenoic acid, 2-hydroxyethyl ester	818-61-1
Propionitrile	107-12-0	2,4-Dichlorobenzaldehyde	874-42-0
Ethylenediamine	107-15-3	1,9-decadiene	1647-16-1
Propargyl alcohol	107-19-7	2,4,5-Trimethoxybenzaldehyde	4460-86-0
Methyl isobutyl ketone	108-10-1	2,3,4,5-Tetrachlorophenol	4901-51-3
Cyclohexanol	108-93-0	Dimethylaminopropyl chloride, hydrochloride	4/5/07
beta-Picoline	108-99-6	O,O-diethyl S-(((1,1-dimethylethyl)thio)methyl)phosphorodithioate	13071-79-9
Diethylamine	109-89-7	2',3',4'-Trichloroacetophenone	13608-87-2
Pyridine	110-86-1	Alachlor	15972-60-8
S-Trioxane	110-88-3	Acetanilide	103-84-4
Ethylene glycol monoethyl ether acetate	111-15-9	4-Hydroxypyrazolo[3,4-d]pyrimidine	315-30-0
Hexylamine	111-26-2	Amphotericin B	1397-89-3
1-hexanol	111-27-3	Bisacodyl	603-50-9
Diethanolamine	111-42-2	Carbamazepine	298-46-4
Adiponitrile	111-69-3	Cefuroxime	55268-75-2
1-octanamine	111-86-4	Celecoxib	169590-42-5
1-octanol	111-87-5	Chlorothiazide	58-94-6
Dioctyl phthalate	117-84-0	Carminic acid	1260-17-9
Phenyl salicylate	118-55-8	Iodochlorohydroxyquinoline	130-26-7
2,4,6-Tribromophenol	118-79-6	2',3'-Dideoxyinosine (AIDS Initiative)	69655-05-6
Benzophenone	119-61-9	Digoxin	20830-75-5
1,2,4-Trichlorobenzene	120-82-1	o-Methoxyphenol	90-05-1
2,4-Dinitrotoluene	121-14-2	Lactic acid	50-21-5
Ethylvanillin	121-32-4	Lamivudine	134678-17-4
Vanillin	121-33-5	Melatonin	73-31-4
m-Chloronitrobenzene	121-73-3	Meprobamate	57-53-4
N-Phenylbenzenamine	122-39-4	Primidone (primaclone)	125-33-7
Ethylene glycol monophenyl ether	122-99-6	Propyl-4-hydroxybenzoate	94-13-3
n-Butyl acetate	123-86-4	Pyrilamine	91-84-9
Tributyl phosphate	126-73-8		
1-Chloro-2-propanol	127-00-4		
N,N-Diethyl-m-toluamide	134-62-3		

Substance	CASRN	Substance	CASRN
Quinidine	56-54-2	1,2,3,4-Tetrahydro isoquinoline	91-21-4
All-trans retinol	68-26-8	1,2,3,5-Tetrachlorobenzene	634-90-2
Ribavirin	36791-04-5	1,2,3-Trichlorobenzene	87-61-6
Sulfamethizole	144-82-1	1,2,4,5-Tetrachlorobenzene	95-94-3
Sulfanilamide	63-74-1	1,2,4-Triazole, sodium salt	41253-21-8
6-Thioguanine (6-TG)	154-42-7	1,1'-(1,2-Ethanediybis(thio))bis-benzene	622-20-8
Triethylenetetramine	112-24-3	1,2-Cyclohexanedicarboxylic acid, bis(oxiranylmethyl) ester	5493-45-8
Trimethoprim	738-70-5	1,2-Dihydro-2,2,4-trimethylquinoline (monomer)	147-47-7
Valproic acid	99-66-1	1,2-Dihydro-2,2,4-trimethylquinoline (polymer)	26780-96-1
2',3'-Dideoxycytidine	7481-89-2	1,2-Dimethyl-3-nitrobenzene	83-41-0
Zearalanol	26538-44-3	1,2-Dimethyl-4-nitrobenzene	99-51-4
Genistein	446-72-0	1,2-Epoxy-3-butene	930-22-3
4',7-Dihydroxyisoflavone	486-66-8	1,2-Epoxydecane	2404-44-6
Phenol, 4-octyl-	1806-26-4	1,2-Epoxyhexadecane	7320-37-8
o-sec-Butylphenol	89-72-5	1,2-Epoxytetradecane	3234-28-4
o,p'-DDT	789-02-6	1,3,5-Trichlorobenzene	108-70-3
5alpha dihydrotestosterone	521-18-6	1,3-Dichloro-2-butene	926-57-8
Progesterone	57-83-0	1,3-Dichloro-2-propanol	96-23-1
beta testosterone	58-22-0	1-Propene, 1,3-dichloro-	542-75-6
4-hydroxy-tamoxifen	68047-06-3	Dicyclohexylcarbodiimide	538-75-0
Apigenin	520-36-5	1,3-Diiminobenz (f)-isoindoline	65558-69-2
2-Hydroxy-4-methoxybenzophenone	131-57-7	1,3-Dimethyl-2-nitrobenzene	81-20-9
Isoeugenol	97-54-1	1,3-Dimethyl-4-nitrobenzene	89-87-2
1,6-Dimethylnaphthalene	575-43-9	1,3-Dimethyl-5-nitrobenzene	99-12-7
n-Butyl-p-aminobenzoate	94-25-7	1,3-Dimethylbutylamine	108-09-8
Methylenedianiline	101-77-9	1,3-Dinitronaphthalene	606-37-1
Diphenolic acid	126-00-1	1,3-Diphenylguanidine	102-06-7
phenolphthalin	81-90-3	1,3-Propylene oxide	503-30-0
Dimethyl phthalate	131-11-3	1,4,5-Trihydroxynaphthalene	481-40-3
corticosterone	50-22-6	1,4-Butanediol	110-63-4
o-Ethyl phenol	90-00-6	1,4-Butanediol diglycidyl ether	2425-79-8
4-Chloro-o-cresol	1570-64-5	1,4-Dimethyl-2-nitrobenzene	89-58-7
Diisobutyl phthalate	84-69-5	1,5-Dinitronaphthalene	605-71-0
Phenol, 4-(1-methyl-1-phenylethyl)-(3-Methylbutoxy)acetic acid, 2-propenyl ester	599-64-4	1,6-Hexanediamine	124-09-4
(E)-1,4-Dibromo-2-butene	67634-00-8	1,6-Hexamethylene diacrylate	13048-33-4
1,2-Dibromo-4-(1,2-dibromoethyl)cyclohexane	821-06-7	1,8-Dihydroxy-4,5-dinitroanthraquinone	81-55-0
1-(2,6,6-Trimethyl-2-cyclohexene-1-yl)-1-penten-3-one	3322-93-8	13-cis-Retinal	472-86-6
1(2H)-Phthalazinone	7779-30-8	1-Chloro-1-nitropropane	600-25-9
1,1,1,2-Tetrabromoethane	119-39-1	1-Chloro-2-bromoethane	107-04-0
1,1,2,2-Tetrabromoethane	630-16-0	1-Chloronaphthalene	90-13-1
1,1-Dichloropropene	79-27-6	1-Fluoro-2,4-dinitrobenzene	70-34-8
1,1-Oxybis methylene, bis benzene	563-58-6	1-n-Hexene	592-41-6
1,2,3,4-Butanetetracarboxylic acid (8CI) (9CI)	103-50-4	1-Iodo-3-nitrobenzene	645-00-1
1,2,3,4-Tetrachlorobenzene	1703-58-8	1-Methyl pyrene	2381-21-7
	634-66-2	1-Nitro-2-methylnaphthalene	881-03-8

Substance	CASRN	Substance	CASRN
1-Nitrohexane	646-14-0	DMA-4 herbicide	2008-39-1
1-Octene	111-66-0	2,4-D, Isooctyl ester, 67%	25168-26-7
1-n-Pentene	109-67-1	2,4-Decadienal	25152-84-5
2-(2-Butoxyethoxy)ethyl thiocyanate	112-56-1	2,4-Dichloroaniline	554-00-7
2-(2-Methylpropyl) thiazole	18640-74-9	2,4-Dichlorobenzoic acid	50-84-0
2-(4-Aminophenyl)-6-methyl-7-benzothiazole sulfonic acid	130-17-6	2,4-Dichloronitrobenzene	611-06-3
2-(Dimethylamino)ethyl acrylate	2439-35-2	2,4-Difluoroaniline	367-25-9
2,2',4,4',5,5'-Hexabromodiphenyl ether	68631-49-2	2,4-Difluoronitrobenzene	446-35-5
PCB 153- 2,2'-4,4',5,5'-hexachlorobiphenyl (Toxic equivalency factor (TEF) evaluation)	35065-27-1	2,4-Dihydroxybenzoic acid	89-86-1
2,2',4,4'-Tetrabromodiphenyl ether	5436-43-1	8-Hydroxy-5,5-dinitro-2-naphthalenesulfonic acid (8CI)(9CI)	483-84-1
2,2',4'-Trichloroacetophenone	4252-78-2	2,4-Hexadienal	142-83-6
2,2-Bis(bromomethyl)-1,3-propanediol	3296-90-0	2,4-Pentanediol	625-69-4
Propanediol (2,2-bis(benzoyloxy)methyl)-dibenzoate	4196-86-5	2,4-Toluene diisocyanate	584-84-9
2,2-Dichloropropane	594-20-7	2,4-Xylidine	95-68-1
2,2'-Diethylhexylamine	106-20-7	2,5-Dichloroaniline	95-82-9
2,2-Dimethyl butanoic acid	595-37-9	2,5-Dichlorobenzoic acid	50-79-3
2,2-Dimethyl-3-pentanol	3970-62-5	2,5-Dichlorophenol	583-78-8
2,2-Dimethylbutane	75-83-2	2,5-Dimethyl phenol	95-87-4
2,2'-Thiobis(4-chlorophenol)	97-24-5	2,5-Hexanediol, 2,5-dimethyl-	110-03-2
2,3,4,5-Tetrachloronitrobenzene	879-39-0	2,5-Xylidine	95-78-3
2,3,4-Trichloronitrobenzene	17700-09-3	2,6-Dichlorobenzaldehyde	83-38-5
2,3,4-Trichlorophenol	15950-66-0	2,6-Dichlorobenzoic acid	50-30-6
2,3,5,6-Tetrachloronitrobenzene	117-18-0	2,6-Dichlorobenzoyl chloride	4659-45-4
2,3,5,6-Tetrachlorophenol	935-95-5	2,6-Dichlorophenol	87-65-0
2,3,5-Trichlorophenol	933-78-8	2,6-Dimethyl phenol	576-26-1
2,3,6-Trichlorophenol	933-75-5	2,6-Diisocyanatotoluene	91-08-7
2,3-Dibromopropionic Acid	600-05-5	1,3-Benzenediamine, 2-methyl-	823-40-5
2,3-Dichloro-1-propanol	616-23-9	2,6-Xylidine	87-62-7
2,3-Dichloropropylene	78-88-6	2',4',5'-Trihydroxybutyrophenone	1421-63-2
2,3-Dichlorobenzoic acid	50-45-3	2-Acetylpyridine	1122-62-9
2,3-Dichloronitrobenzene	3209-22-1	2-Acetylthiazole	24295-03-2
2,3-Dichlorophenol	576-24-9	2-Amino-1-phenol-4-sulfonic acid	98-37-3
2,3-Dichloroquinoxaline	2213-63-0	2-Amino-4-chloro-5-nitrophenol	7/2/58
2',3'-Dideoxyadenosine	4097-22-7	2-Amino-4-chlorobenzothiazole	19952-47-7
2,3-Dimethyl phenol	526-75-0	2-Amino-4-chlorophenol	95-85-2
2,3-Dimethylbutane	79-29-8	2-Amino-4-methoxybenzothiazole	5464-79-9
2,3-Dinitrotoluene	602-01-7	2-Amino-4-methylbenzothiazole	1477-42-5
2,3-Xylidine	87-59-2	2-Amino-4-methylphenol	95-84-1
2,4,5-T isobutyl ester	4938-72-1	2-Amino-4-phenylthiazole HBr H2O	52253-69-7
2,4,5-Trichloronitrobenzene	89-69-0	2-Amino-4-thiazoleacetic acid	29676-71-9
2,4,5-Trichlorophenol	95-95-4	2-Amino-5,6-dimethylbenzothiazole	29927-08-0
2,4,5-Triethoxyacetophenone	63213-29-6	2-Amino-6-ethoxybenzothiazole	94-45-1
2,4,6-Trichloronitrobenzene	18708-70-8	2-Amino-6-nitrobenzothiazole	6285-57-0
2,4,a,a,a-Pentachlorotoluene	13014-18-1	2-Aminoanthracene	613-13-8
		2-Aminobenzimidazole	934-32-7
		2-Aminobenzothiazole	136-95-8
		2-Biphenylamine	90-41-5
		2-Thiazolamine	96-50-4

Substance	CASRN	Substance	CASRN
Benzimidazol-2-ylurea	24370-25-0	3,4-Dimethyl phenol	95-65-8
2-Bromo-4,6-dinitroaniline	1817-73-8	3,4-Dinitrotoluene	610-39-9
2-Bromobiphenyl	7/5/52	3,4-Xylidine	95-64-7
2-Bromopropane	75-26-3	3,5-Dichloroaniline	626-43-7
2-Butoxyethanol (ethylene glycol monobutyl ether)	111-76-2	3,5-Dichlorobenzoic acid	51-36-5
2-Chloro-2-nitropropane	594-71-8	3,5-Dichlorophenol	591-35-5
2-Chloro-6-(trichloromethyl)pyridine	1929-82-4	3,5-Dimethyl phenol	108-68-9
2-Chlorobenzaldehyde	89-98-5	3,5-Xylidine	108-69-0
2-Chloronaphthalene	91-58-7	3-Acetyl-2,5-dimethylfuran	10599-70-9
2-Cyclohexen-1-one	930-68-7	3-Amino-a,a,a-trifluorotoluene	98-16-8
(2-Dodecenyl)succinic anhydride	19780-11-1	3-Bromo-1-propanol	627-18-9
Ethylene glycol monoethyl ether (EGMEE)	110-80-5	3-Bromo-2,2-bis(bromomethyl)propanol	1522-92-5
2-Ethyl-1,3-hexanediol	94-96-2	3-Bromobenzaldehyde	3132-99-8
2-Ethylhexanal	123-05-7	3-Bromobiphenyl	2113-57-7
2-Ethylhexanoic acid	149-57-5	3-Chloro-2-methylpropene	563-47-3
2-Ethylhexyl acrylate	103-11-7	3-Chloro-o-toluidine	87-60-5
2-Ethylhexyl glycidyl ether	2461-15-6	3-Chloropropionitrile	542-76-7
2-Ethylhexyl 2-cyano-3,3-diphenylacrylate	6197-30-4	3-Chloropropionitrile	542-76-7
2-Ethylhexylamine	104-75-6	3-Diethylaminophenol	91-68-9
2-Ethylhexylamine	104-75-6	3-Dimethylaminophenol	99-07-0
2-Ethylhexyl-p-dimethylaminobenzoate	21245-02-3	3-Ethylamino-4-methylphenol	120-37-6
2-Fluorobenzoyl chloride	393-52-2	3-Hydroxy-N-phenylaniline	101-18-8
2-Hydroxyisobutyric acid	594-61-6	3-Methyl-2-nitrobenzoic acid	5437-38-7
Iodoethyl benzene	17376-04-4	3-Methyl-4-nitrobenzoic acid	3113-71-1
2-Mercaptobenzimidazole	583-39-1	3-Nitro-a,a,a-trifluorotoluene	98-46-4
1-Pentanol, 2-methyl-	105-30-6	3-Pentenenitrile	4635-87-4
2-Methyl-2-butenenitrile	4403-61-6	Ethyl 3-phenylglycidate	121-39-1
2-Methyl-2-ethoxypropane (etbe)	637-92-3	3-Propylidenephthalide	17369-59-4
2-Methyl-3-nitroaniline	603-83-8	4-(methylthio)benzaldehyde	3446-89-7
2-Methyl-3-nitrobenzoic acid	1975-50-4	4,4'-Diaminodicyclohexylmethane	1761-71-3
2-Methyl-4-nitroaniline	99-52-5	p,p'-Dichlorodiphenyl sulfone	80-07-9
2-Methyl-6-nitrobenzoic acid	13506-76-8	4,4'-Diphenylmethane diisocyanate	101-68-8
2-Methylbenzamide	527-85-5	4-amino-1,2,4-triazole	584-13-4
2-Methylpropanenitrile	78-82-0	4-Amino-4'-hydroxy-3-methyl-diphenylamine	6219-89-2
2-Methyltetrahydrofuran	96-47-9	Androstenedione	63-05-8
3,3-Dithiodipropionic acid	1119-62-6	4-Androstenedione	63-05-8
3,4,5-Trichloronitrobenzene	20098-48-0	4-Bromobiphenyl	92-66-0
3,4,5-Trichlorophenol	609-19-8	Benzoic acid, 4-formyl-	619-66-9
a,a,a,3,4-Pentachlorotoluene	13014-24-9	4-Chloro-2-nitroaniline	89-63-4
3,4-Diaminotoluene	496-72-0	4-Chloro-3,5-dinitro-a,a,a-trifluorotoluene	393-75-9
3,4-Dichlorobenzaldehyde	6287-38-3	4-Chloro-3-nitro-a,a,a-trifluorotoluene	121-17-5
3,4-Dichlorobenzoic acid	51-44-5	p-Chloro-a,a,a-trifluorotoluene	98-56-6
3,4-Dichloronitrobenzene	99-54-7	Cyclopentaphenanthrene	203-64-5
3,4-Dichlorophenol	95-77-2	4-(hydroxyphenyl)retinamide	65646-68-6
3,4-Dichlorophenyl isocyanate	102-36-3	4-Methoxy-3-nitro-N-phenylbenzamide	97-32-5

Substance	CASRN	Substance	CASRN
4-Methylthiazole	693-95-8	Allyl anthranilate	7493-63-2
4-Methyl-2-nitroaniline	89-62-3	Allyl bromide	106-95-6
4-Methyl-3-nitroaniline	119-32-4	Allyl nonanoate	7493-72-3
4-Methyl-3-nitrobenzoic acid	96-98-0	Allyl thiourea	109-57-9
4-Methylimidazole	822-36-6	alpha,alpha-Dichlorotoluene	98-87-3
4-n-Hexyl-4'-cyanobiphenyl	41122-70-7	alpha-Bromotoluene	100-39-0
4-Nitro-1,3-benzenediamine	5131-58-8	alpha-Cyclodextrin	10016-20-3
6-Nitrophthalhydrazide	3682-19-7	alpha-Hydroxybenzeneacetonitrile	532-28-5
4-Nitrophthalic anhydride	5466-84-2	alpha-Ketoglutaric acid alpha	328-50-7
4-Nitrophthalimide	89-40-7	alpha-Methyl cinnamaldehyde	101-39-3
4-Pentenitrile	592-51-8	alpha-Methylstyrene	98-83-9
5-(Hydroxymethyl) furoyl glycine	38716-68-6	alpha-Naphthyl isothiocyanate	551-06-4
5-(Hydroxymethyl)-2-furfural	67-47-0	alpha-Pinene	80-56-8
5-(Hydroxymethyl)-2-furoic acid	6338-41-6	alpha-Thujone	546-80-5
5,7-Dihydroxy-4-methylcoumarin	2107-76-8	Amiloride hydrochloride	2016-88-8
5-Amino-3-sulfosalicylic acid	6201-87-2	Amitriptyline HCl	549-18-8
5-Amino-o-cresol	2835-95-2	Nitric acid ammonium salt	6484-52-2
5-Aminosalicylic acid	89-57-6	Ammonium perchlorate	7790-98-9
5-Bromo-2'-deoxyuridine (BRDU)	59-14-3	Anise oil	8007-70-3
5-Chloro-2-methyl-1H-benzimidazole	2818-69-1	Annatto Extract Acid Proof	1393-63-1
5-Methoxypsoralen	484-20-8	Anthralin	1143-38-0
5-Methyl-2-nitroaniline	578-46-1	alpha-Solanine	20562-02-1
DDD (6-hydroxy-2-naphthyl disulfide)	6088-51-3	Azithromycin (AIDS Initiative)	83905-01-5
6-Mercaptopurine monohydrate	6112-76-1	Azodicarbonamide	123-77-3
6-Methoxy-2-benzothiazolamine	1747-60-0	Azoxybenzene	495-48-7
Methyl coumarin	92-48-8	C.I. Basic orange 2	532-82-1
7-Diethylamino-4-methylcoumarin	91-44-1	Benomyl	17804-35-2
7-Methylquinoline	612-60-2	Benzene	71-43-2
8-Hydroxyquinoline	148-24-3	Benzene sulfonic acid	98-11-3
9-Aminoacridine, monohydrochloride, monohydrate	52417-22-8	Benzenesulfonyl chloride	98-09-9
9-Nitroanthracene	602-60-8	Benzethonium chloride	121-54-0
Abscisic acid	14375-45-2	Benzimidazole	51-17-2
Acesulfame potassium	55589-62-3	Benzo(b)fluoranthene	205-99-2
Acetal	105-57-7	Benzo(e)pyrene	192-97-2
Acetic anhydride	108-24-7	Benzo(f)-quinoline	85-02-9
Acetoacetanilide	102-01-2	Benzo(k)fluoranthene	207-08-9
Acetochlor	34256-82-1	Benzoin acetate	574-06-1
2,5-Hexanedione	110-13-4	Benzothiazole	95-16-9
Acetoxyvaleric Acid	81397-67-3	Benzo-trichloride	98-07-7
Acetylsalicylic acid	50-78-2	Benzo-trifluoride	98-08-8
Acrylamide	79-06-1	Carbonochloridic acid, phenylmethyl ester	501-53-1
Actein	18642-44-9	Benzyl phenylacetate	102-16-9
Adriamycin, hydrochloride	25316-40-9	Benzyl salicylate	118-58-1
Aldicarb sulfoxide	1646-87-3	Benzyl sulfide	538-74-9
Alizarin Yellow R, free acid	2243-76-7	benzylacetone	2550-26-7
Allyl acetate	591-87-7	Benzyltrimethyl ammonium chloride	56-93-9
		Berberine chloride	633-65-8
		Citronellol	106-22-9

Substance	CASRN	Substance	CASRN
beta-Nitrostyrene	5153-67-3	cis-Dichlorodiamine platinum	15663-27-1
beta-Resorcylic acid	89-86-1	cis-Stilbene	645-49-8
Bis(2-chloro-1-methylethyl) ether	108-60-1	Citral	5392-40-5
Bis(2-chloroethoxy)methane	111-91-1	Cobaltocene	1277-43-6
Bis(cyclopentadienyl)vanadium chloride	12083-48-6	Colchicine	64-86-8
Bisphenol A	80-05-7	Colchicine	64-86-8
Bisphenol A diglycidyl ether	1675-54-3	Creosote, wood	8021-39-4
Imidodicarbonic diamide	108-19-0	m,p-Cresol mixture	1319-77-3
Bixin	6983-79-5	Croton oil	8001-28-3
Black cohosh	84776-26-1	Crotonaldehyde	4170-30-3
beta-Myrcene	123-35-3	Crystal violet lactone	1552-42-7
boron trifluoride dihydrate	13319-75-0	Litsea cubeba oil	68855-99-2
Bromobenzene	108-86-1	Cumene hydroperoxide	80-15-9
Bromochloroacetic acid	5589-96-8	Curcumin	458-37-7
Bromodichloroacetic acid	71133-14-7	1,3,5-Triazine, 2,4,6-trichloro-	108-77-0
Butanal oxime	110-69-0	Cyclohexanone cyanohydrin	931-97-5
Butyl anthranilate	7756-96-9	Cyclohexene oxide	286-20-4
Butyl Dipropasol Solvent	29911-27-1	Cycloheximide	66-81-9
Butanoic acid, anhydride	106-31-0	Cycloheximide	66-81-9
Butyryl chloride	141-75-3	Isocyanatocyclohexane	3173-53-3
Cadmium acetate, dihydrate	4/4/43	Cyclopentane	287-92-3
Cadmium oxide	1306-19-0	Cyclopentanol	96-41-3
Caprylyl chloride	111-64-8	Cyclophosphamide monohydrate	6055-19-2
Captan 90-concentrate (solid)	133-06-2	Cynarin (Echinacea)(1,3-Dicaffeoylquinic Acid)	1182-34-9
Carbendazim	10605-21-7	D & C yellow no. 11	8003-22-3
Carbon disulfide	75-15-0	D & C red no. 27	13473-26-2
Carbon tetrachloride	56-23-5	2',3'-Didehydro-3'-deoxythymidine	3056-17-5
Carisoprodol	78-44-4	Daunomycin HCL	23541-50-6
Carveol	99-48-9	Dazomet	533-74-4
Carvyl acetate	97-42-7	D-Camphor	464-49-3
Casanthrol (cascara sagrada extract)	8024-48-4	Decalin	91-17-8
Castor oil	8001-79-4	Deoxyactein, 27-(23-EPI-26-Deoxyactein)	NOCAS
Cetylpyridinium bromide	140-72-7	Deoxycholic acid sodium salt	302-95-4
Chlordane (technical grade)	12789-03-6	Desmethoxyyangonin	15345-89-8
Chlorhexidine	55-56-1	Di(2-methoxyethyl)phthalate	117-82-8
Chlorogenic acid	327-97-9	Diaminomaleonitrile	1187-42-4
Chlorogenic acid	327-97-9	Diazoaminobenzene	136-35-6
Chlorotrimethylsilane	75-77-4	Dibenzooxathiane	262-20-4
Chlorowax 40	63449-39-8	Dibenzoyl-L-tartaric acid	2743-38-6
Chlorowax 500C	51990-12-6	Dibenzyl phosphate	1623-08-1
Chrysophanic acid (1,8-dihydroxy-3-methylanthraquinone)	481-74-3	Dibromoacetic acid	631-64-1
Cichoric Acid	70831-56-0	Dibromoacetone nitrile	3252-43-5
Cimicifugoside	27994-11-2	Dichlorvos (Vapona)	62-73-7
Cinnamaldehyde	104-55-2	Dicumyl peroxide	80-43-3
trans-Cinnamaldehyde	14371-10-9	Dicyclohexylamine	101-83-7
cs & trans 1,2-Dichloroethylene	540-59-0	Dicyclohexylamine	101-83-7
cis-1,2-Dichloroethylene	156-59-2	Dicyclopentadiene	77-73-6

Substance	CASRN	Substance	CASRN
Dideoxydidehydrothymidine	3056-17-5	Ethylene glycol monobutyl ether	111-76-2
Diethyl carbonate	105-58-8	Ethylidenenorbornene	16219-75-3
Diethyl ethylphosphonate	78-38-6	N-Ethyl-n-butylamine	13360-63-9
Diethyl phthalate	84-66-2	Ferrocene	102-54-5
Diethylene glycol diacrylate	4074-88-8	Fluoranthene	206-44-0
Diethylene glycol dibutyl ether	112-73-2	Fluorobenzene	462-06-6
Digitonin	11024-24-1	fluorosulfonic acid	7789-21-1
Diglycidyl resorcinol ether (DGRE)	101-90-6	Fluoxymestrone	76-43-7
Dihydrokavain	587-63-3	Flutamide (pubertal study)	13311-84-7
Dihydromethysticin	3155-57-5	Formamide	75-12-7
Diisopropylamine	108-18-9	Formanilide	103-70-8
Diisopropylcarbodiimide	693-13-0	Fumaronitrile	764-42-1
Dimenhydrinate	523-87-5	fumaryl chloride	627-63-4
Dimethyl adipate	627-93-0	Furfuryl acetate	623-17-6
Dimethyl glutarate	1119-40-0	1-Propanamine, 3-(triethoxysilyl)-	919-30-2
dimethyldipropylene-triamine	10563-29-8	Geranyl acetate	105-87-3
Dimethyldisulfide	624-92-0	Ginkgo biloba extract	90045-36-6
dimethylisopropylamine	996-35-0	Glutaraldehyde	111-30-8
Dimethylnaphthalene	28804-88-8	Glycerol	56-81-5
Dimethylsuccinate	106-65-0	Glycidyl methacrylate	106-91-2
Di-n-amylamine	2050-92-2	Glyoxal	107-22-2
Di-n-propylphthalate	131-16-8	Guggulsterones E	39025-24-6
Di-n-pentylphthalate	131-18-0	Guggulsterones Z	39025-23-5
Diphenylurea	102-07-8	Halazone	80-13-7
Dipropylene glycol	25265-71-8	Halothane	151-67-7
Dipropylene glycol	25265-71-8	Hexamethyleneimine	111-49-9
C.I. Direct red 2	992-59-6	Octanal, 2-(phenylmethylene)-	101-86-0
Di-tert-butyl peroxide	110-05-4	Hydrastine	118-08-1
Diundecyl phthalate	3648-20-2	Hydroxyflutamide	52806-53-8
Divinylbenzene	1321-74-0	Hydroxylamine sulfate (2:1)	10039-54-0
Camphor	76-22-2	Hydroxyvaleric Acid	1619-16-5
Domiphen bromide	538-71-6	1H-Imidazole	288-32-4
Echinacoside	82854-37-3	Indium trichloride	10025-82-8
Econazole nitrate	24169-02-6	Prevention 4 (indole-3-carbinol)	700-06-1
Emodin	518-82-1	Isoamyl acetate	123-92-2
S-ethyl dipropylthiocarbamate	759-94-4	Isoamyl cinnamate	7779-65-9
Ergotamine tartrate	379-79-3	Isoamyl nitrite	110-46-3
Ethacrynic acid	58-54-8	Isobutyl methacrylate	97-86-9
Ethidium bromide	1239-45-8	Isocyanatocyclohexane	3173-53-3
Ethoxyacetic acid	627-03-2	Ethanone, 1-(1,2,3,4,5,6,7,8- octahydro-2,3,8,8-tetramethyl-2- naphthalenyl)-	54464-57-2
Ethyl acrylate (inhibited)	140-88-5	Isophorone diisocyanate	4098-71-9
Ethyl anthranilate	87-25-2	Isophytol	505-32-8
Ethyl cyanoacrylate	7085-85-0	Isopropenyl acetate	108-22-5
Ethyl linolenate	1191-41-9	Isopropyl acetate	108-21-4
Ethyl methanesulfonate	62-50-0	Isopropyl glycidyl ether	4016-14-2
Ethyl vinyl ketone	1629-58-9	Isopropyl mercaptan	75-33-2
Ethyl-2-methyl acetoacetate	609-14-3	Isopropyl methanesulfonate	926-06-7
Ethylene glycol diethyl ether	629-14-1		

Substance	CASRN	Substance	CASRN
Isopropyl phenylacetate	4861-85-2	Methylene bis(thiocyanate)	6317-18-6
Isoproterenol hydrochloride	51-30-9	Methylene blue trihydrate	7220-79-3
Kavain, DL-	500-64-1	Methyleugenol	93-15-2
Kepona	143-50-0	Methyl-p-formyl benzoate	1571-08-0
L-5-Hydroxytryptophan	9/8/50	Methyl-p-toluate	99-75-2
Lauric acid	143-07-7	Methylthioglycolate	2365-48-2
Lauryl chloride	112-52-7	Methysticin	495-85-2
Lauryl glycidyl ether	2461-18-9	m-Nitroacetophenone	121-89-1
Lead acetate (II) trihydrate	6080-56-4	m-Nitroaniline	99-09-2
Lead acetate (II) trihydrate	6080-56-4	m-Nitrobenzamide	645-09-0
Lime oil	8008-26-2	m-Nitrobenzoic acid	121-92-6
Linalool	78-70-6	m-Nitrobenzoyl chloride	121-90-4
Linoleic acid	60-33-3	m-Nitrobenzyl chloride	619-23-8
Linolenic acid	463-40-1	m-Nitrophenol	554-84-7
Luminol	521-31-3	Molinate	2212-67-1
Malachite green oxalate	2437-29-8	Mono(2-ethylhexyl)phthalate	4376-20-9
Maltol	118-71-8	Monobutyltin trichloride	1118-46-3
3-Aminobenzenesulfonic acid	121-47-1	m-Phenetidine	621-33-0
m-Aminoacetanilide	102-28-3	m-Tolunitrile	620-22-4
3-Aminophenol	591-27-5	Musk ambrette	83-66-9
m-Anisidine	536-90-3	m-Xylene	108-38-3
m-Bromotoluene	591-17-3	Myleran	55-98-1
m-Chloroaniline	108-42-9	Myristicin	607-91-0
m-Chlorobenzoic acid	535-80-8	N-(1,3-Dimethylbutyl)-N'-phenyl-p-phenylenediamine	793-24-8
m-Chlorobenzotrifluoride	98-15-7	N,N,N',N'-	111-18-2
m-Chlorophenol	108-43-0	Tetramethylhexanediamine	
m-Dinitrobenzene	99-65-0	N,N,N',N'-Tetramethyl-p-phenylenediamine	100-22-1
Medroxyprogesteroneacetate	71-58-9	N,N'-Diethylcarbanilide	85-98-3
Melatonin	73-31-4	N,N-Diethyl-p-phenylenediamine	93-05-0
Menthofuran	494-90-6	N,N-Dimethylformamide	68-12-2
Methacrylamide	79-39-0	N,N-Dimethyl-p-nitrosoaniline	138-89-6
Methacrylonitrile	126-98-7	N,N-Dimethyl-p-phenylenediamine	99-98-9
Methoprene	40596-69-8	N,N-Dimethylvaleramide	6/5/25
Methoxyacetic acid	625-45-6	N,N'-Di-sec-butyl-p-phenyldiamine	101-96-2
Methoxychlor [95%]	72-43-5	N,N'-methylenebisacrylamide	110-26-9
Methyl acrylate	96-33-3	N-Acetyl-m-toluidine	537-92-8
Methyl anthranilate	134-20-3	Acetyl-o-toluidine	120-66-1
Methylbenzoate	93-58-3	N-Acetyl-p-toluidine	103-89-9
Methyl cyanoacetate	105-34-0	n-Butyl acrylate	141-32-2
Methyl ethyl ketone peroxide	1338-23-4	n-Butyl alcohol	71-36-3
2-Methyl furan	534-22-5	n-Butyl glycidyl ether	8/6/26
Methylglutaronitrile	4553-62-2	n-Cyclohexyl-4-methylbenzenesulfonamide	80-30-8
Methyl isocyanate	624-83-9	Decyl methacrylate	3179-47-3
Methane, isothiocyanato-	556-61-6	Nelfinavir mesylate	159989-65-8
Methyl salicylate	119-36-8	Neohesperidin dihydrochalcone	20702-77-6
Methyl styryl ketone	122-57-6	Neopentyl glycol diglycidyl ether	17557-23-2
Methyl testosterone	58-18-4		
Methyl vinyl ketone	78-94-4		

Substance	CASRN	Substance	CASRN
N-Ethyl aniline	103-69-5	o-Nitrotoluene	88-72-2
N-Ethyl-4-methylbenzenesulfonamide	80-39-7	o-Phenanthroline	66-71-7
N-Ethyl-n-phenyl benzylamine	92-59-1	o-Phenetidine	94-70-2
Nevirapine	129618-40-2	o-Phenylenediamine	95-54-5
n-Hexyl methacrylate	142-09-6	Organofunctional Silane 45-49	82985-35-1
N-Hydroxybenzamide	495-18-1	Orotic acid	65-86-1
Nickelocene	1271-28-9	o-sec-Butylphenol	89-72-5
Nifedipine	21829-25-4	o-Toluic acid	118-90-1
Ninhydrin	485-47-2	o-Toluidine	95-53-4
N-Isopropyl acrylamide	2210-25-5	Oxymetholone	434-07-1
N-Isopropylaniline	768-52-5	p -n -Nonylphenol	104-40-5
N-Isopropyl-N'-phenyl-p-phenylenediamine	101-72-4	p,p'-DDE (p,p'-Dichlorodiphenyldichloroethylene)	72-55-9
Nitazoxanide	55981-09-4	p,p'-Dichlorodiphenyl Sulfone	80-07-9
Nitrogen mustard hydrochloride	55-86-7	p-Acetamidobenzoic acid	556-08-1
N-Methyl-4-nitroaniline	100-15-2	4-Aminobenzenesulfonic acid	121-57-3
N-Methylbenzamide	613-93-4	p-Aminobenzoic acid	150-13-0
N'-methyl-N,N-diphenylurea	13114-72-2	p-Amino acetanilide	122-80-5
N-Methyl-p-aminophenol sulfate	55-55-0	p-Aminophenol	123-30-8
Nonane	111-84-2	p-Anisaldehyde	123-11-5
Norbixin (cis/trans mixture)	542-40-5	p-Anisidine	104-94-9
n-Pentane	109-66-0	Parathion	56-38-2
N-Phenyl-1-naphthylamine	90-30-2	p-Azoxyanisole	1562-94-3
Orthanilic acid	88-21-1	p-Bromotoluene	106-38-7
o-Aminophenol	95-55-6	p-Chlorobenzoic acid	74-11-3
o-Anisidine	90-04-0	p-Chlorotoluene	106-43-4
o-Bromotoluene	95-46-5	p-Divinylbenzene	105-06-6
o-Chlorobenzoic acid	118-91-2	2,2',4,4',5-Pentabromodiphenyl ether	60348-60-9
o-Chlorobenzotrifluoride	88-16-4	Pentabromodiphenyl oxide (technical) (DE 71)	32534-81-9
o-Chloropyridine	109-09-1	Pentachlorobenzene	608-93-5
o-Chlorostyrene	2039-87-4	Pentaerythritol triacrylate	3524-68-3
o-Cresyl glycidyl ether	2210-79-9	Pentamidine isethionate	140-64-7
Octabromodiphenyl ether	32536-52-0	Phenamiphos	22224-92-6
Octanoic acid	124-07-2	Phenanthrene	85-01-8
Octopamine HCL	770-05-8	Phenethyl anthranilate	133-18-6
Oleic acid	112-80-1	phenethyl bromide	103-63-9
Oleic acid diethanolamine condensate	93-83-4	Pheniramine maleate	132-20-7
Olivetol	500-66-3	3-((Methoxycarbonyl)amino)phenyl N-(3-methylphenyl)carbamate (Phenmedipham)	13684-63-4
o-methoxyphenol	90-05-1	Phenoxy acetic acid	122-59-8
o-Nitroacetophenone	577-59-3	Phenylglyoxal	1074-12-0
o-Nitroaniline	88-74-4	Phenylthiourea	103-85-5
o-Nitrobenzamide	610-15-1	4-Hexylresorcinol	136-77-6
o-Nitrobenzoic acid	552-16-9	Phosphoric acid	7664-38-2
o-Nitrobenzoyl chloride	610-14-0	Phosphorodichloridic acid, ethyl ester	1498-51-7
o-Nitrobenzyl chloride	612-23-7	phosphorus pentachloride	10026-13-8
o-Nitrophenethyl alcohol	15121-84-3		
(o-Nitrophenyl)acetonitrile	610-66-2		

Substance	CASRN	Substance	CASRN
Picloram	2/1/18	Sodium hydrogen sulfate	7681-38-1
Pinane	473-55-2	Sodium lauryl sulfate	151-21-3
Piperonal	120-57-0	Sodium nitrite	7632-00-0
Piperonyl acetate	326-61-4	Sodium xylenesulfonate	1300-72-7
p-Methyl benzyl alcohol	589-18-4	Sodium zomepirac	64092-48-4
p-Nitroacetophenone	100-19-6	C.I. Solvent black 5	11099-03-9
p-Nitrobenzoyl chloride	122-04-3	C.I. Solvent Black 7	2/5/05
p-Nitrohippuric acid	2645-07-0	Styrax balsam	8046-19-3
p-Nitrophenethyl alcohol	100-27-6	Succinonitrile	110-61-2
p-Nitrotoluene	99-99-0	Sulfacetamide	144-80-9
p-n-Octyloxybenzoic acid	2493-84-7	Sulfamethoxazole	723-46-6
Poly(2-hydroxypropyl methacrylate)	25703-79-1	sulfamic acid	5329-14-6
Potassium dichromate	7778-50-9	Sulfathiazole	72-14-0
p-Phenetidine	156-43-4	p-Synephrine	94-07-5
Procymidone	32809-16-8	Tertiary amyl methyl ether (TAME)	994-05-8
Progesterone	57-83-0	t-Butyl formate	762-75-4
2-Propanol, 1-propoxy-	1569-01-3	t-Butyl glycidyl ether	7665-72-7
Propylene glycol	57-55-6	tert-Butyl perbenzoate	614-45-9
Propylene glycol mono-t-butyl ether	57018-52-7	t-Butyl phenyl glycidyl ether	3101-60-8
Propylparaben	94-13-3	tert-Dodecyl mercaptan	25103-58-6
Benzenepropanal, 4-(1,1-dimethylethyl)-.alpha.-methyl-	80-54-6	Tebuconazole	80443-41-0
p-tert-Butylcatechol	98-29-3	Terephthalic acid	100-21-0
p-tert-Butyltoluene	98-51-1	tert-Butyl hydroperoxide	75-91-2
p-Toluenesulfonamide	70-55-3	tert-Butyl Hydroperoxide (70% Solution in Water)	75-91-2
p-Tolunitrile	104-85-8	tert-Butylhydroquinone	1948-33-0
Pulegone	89-82-7	Tetrabromobisphenol A	79-94-7
p-Xylenol blue	125-31-5	Tetrabromobisphenol A-bis(2,3-dibromopropyl ether)	21850-44-2
Pyrene	129-00-0	Tetrabromophthalic anhydride	632-79-1
Pyrogallol	87-66-1	Tetrachloroethylene	127-18-4
Resveratrol	501-36-0	Tetrachlorophthalic anhydride	117-08-8
Rhein (1,8-dihydroxy-3-carboxyl anthraquinone)	478-43-3	Tetraethylene glycol diacrylate	17831-71-9
Rifabutin	72559-06-9	Tetraethylene glycol diacrylate	17831-71-9
S-(ethyl)chlorothioformic acid	2941-64-2	Tetraethylenepentamine	112-57-2
S-(n-propyl)chlorothioformic acid	13889-92-4	1,2,3,4-Tetrahydro-9-acridinamine monohydrochloride	1684-40-8
Saquinavir mesylate (AIDS Initiative)	149845-06-7	Tetralin	119-64-2
Scopolamine hydrobromide trihydrate	6533-68-2	tetra-N-Octylammonium bromide	14866-33-2
Sesame oil	8008-74-0	Thiocarbanilide	102-08-9
Silybin	22888-70-6	alpha-Lipoic acid	1077-28-7
Sodium bromate	7789-38-0	Thiophanate M	23564-05-8
Sodium bromate	7789-38-0	Thiophene	110-02-1
Sodium chlorate	9/9/75	Toluene	108-88-3
Sodium Cholate	361-09-1	trans-1,2-Dichloroethylene	156-60-5
Sodium dichromate dihydrate (VI)	7789-12-0	2,3-Dibromo-2-butene-1,4-diol	2/4/34
Sodium dichromate dihydrate (VI)	7789-12-0	Retinal	116-31-4
Sodium dodecyl sulfate	151-21-3	Triacetin	102-76-1
		Triallyl isocyanurate	1025-15-6

Substance	CASRN
Trichloroacetic acid	76-03-9
Trichloroacetyl chloride	76-02-8
Triethyl phosphate	78-40-0
Trifluralin	1582-09-8
Triphenyl phosphine	603-35-0
Triphenyl phosphate	101-02-0
1,3,5-Triglycidyl isocyanurate	2451-62-9
Tris(2-chloroethyl) phosphate	140-08-9
Tris(2-ethylhexyl)trimellitate	3319-31-1
Triton X-100	9002-93-1
Trixylenyl phosphate mixed isomers	25155-23-1
Tyramine HCL	60-19-5
Valerenic Acid	10/6/69
Valeronitrile	110-59-8
valeryl chloride; pentanoyl chloride	638-29-9
C.I Vat blue 1	482-89-3
Verapamil HCl	152-11-4
Veratraldehyde	120-14-9
Vinyl toluene	25013-15-4
Vitamin D3	67-97-0
Yangonin	500-62-9
Zearalenone	17924-92-4
Zinc pyrithione	13463-41-7

Appendix 2. Other HTS Assays Available at the NCGC

Project Name	Disease application (if any)	Project Name	Disease application (if any)
Acrosome reaction GFP		Malarial PSAC	Malaria
Anthrax LF BLA	Anthrax	Multi-protein DNA Replication System	
ATR Activation	Ataxia telangiectasia (OMIM 607585)	O-Glc NAc Transferase	
b-AdrR PCA bifrucated GFP		Opsin trafficking	Retinitis pigmentosa (OMIM 180380)
b-lactamase (AmpC)		ALPHA orphan GPCR -ADHD	ADHD
b-glucoocerebrosidase FI	Gaucher disease (OMIM 230800)	Oxidoreductase HADH2	
b-Thal mRNA splicing GFP	Beta-thalassemia	Oxidoreductase DCXR	
Cell signaling AP-1-BLA		Oxidoreductase HSD17b4	
Cell signaling CRE-BLA		Oxidoreductase retSDR3	
Cell signaling HRE-BLA		Oxidoreductase SPR	
Cell signaling M1 NTR		P450 CYP1A2, Luc	
Cell signaling NFAT-BLA		P450 CYP2C9, Luc	
Cell signaling SIE-BLA		P450 CYP2C19, Luc	
Cell Translocation GR-EFC		P450 CYP2D6, Luc	
Cell Translocation GR-GFP		P450 CYP3A4, Luc	
Cell Translocation p65 HaloTag		Pantothenate Kinase	Tuberculosis
cLANA	HSV	Peroxiredoxins (Tgr-Trx-Prx)	Schistosomiasis
Cpd aggregation FRET-1 (AggFRET)		PI5K4Pbeta	Diabetes
DNA damage GFP-x gene		Progeria mRNA splicing GFP/RFP	Progeria (OMIM 176670)
DNA polymerase III		Proteosome ubiquitin-GFP	Various
Drosophila Fat cell GFP		PyruvateKinase Luc	Hemolytic anemia (OMIM 266200)
ER/GR Translocation		RAS-RAF PCA bifrucated GFP	
Fluor-DNA displacement-1		Sialic aciduria	Sialuria (OMIM 269921)
Fluorescent Profiling-1		SMA Cellular promoter act BLA	Spinal Muscular Atrophy (OMIM 253300)
GPVI Luciferase		Tau polymerization	Alzheimer, Frontotemporal dementia (OMIM 600274)
HIV Nucleocapsid FP	HIV	TF assay-cancer	Cancer
Hsp90 co-chaperone interaction		TPO Luciferase	Thrombocytopenia
Huntingtin PC12 cell toxicity	Huntington's Disease (OMIM 143100)	Ubiquitin Pathway	Various
IkBa Cell sensor Dual Luc	Rare lymphomas	YjeE FP	
JNK ALPHAScreen			
Locus Derepression			
Assay-1 GFP			
Luciferase profiling			