

## SUPPORTING INFORMATION

### **Survey of Human Oxidoreductases and Cytochrome P450 Enzymes Involved in the Metabolism of Xenobiotic and Natural Chemicals**

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#### **Notes regarding databases**

1. The first row in the Excel formats is the title (not counted).
2. Racemates and enantioneric compounds, (*S*)- and (*R*), optical isomers (+)-, (-)-, etc. are counted as a single compound (entity), as we are not examining the differences when the same reaction is going on.
3. Some groups of chemicals, undergoing the same reaction(s), are listed as a single compound (entity); e.g. fatty acids (long chains or short chains), lipids, derivatives of a particular chemical(s), e.g. *N,N*-dialkylnitrosamines (bulky, long, and short chains).
4. Compounds originating from physiological/natural compounds but used as drugs (i.e. testosterone and other steroids) are included under physiological compounds.
5. Drugs/compound metabolites participating in further metabolism are counted as separate compounds.

## List of all compounds

(-)Camphor

(-)Deprenyl, (R)-(-)-Selegiline

(-)Fenchone

(-)OSU6162

(-)Rhazinilam

(-)Verbenone

(+)-Carvone

(+)-Fenchone

(+)-S-145

(+)-S-145, bisnor-

(+)-S-145, tetranor-

(+,-)-Flavanone

(2-Naphthyl)hydrazine

(4-Bromophenyl)-1,3-oxathiolane

(S)- and (R)-Nordeprenyl tetrahydropyridylcarbamate

(Z)-N-Ac-FFVC

[13C4,15N]-Midazolam

[18F]-FCWAY

1-(1-Propynyl)pyrene
1-(2-Pyrimidinyl)-piperazine
1-(3-Trifluoromethylphenyl)piperazine, TFMPP
1-(4-Methoxyphenyl)piperazine, MeOPP
1,1,1-Trichloroethane
1,1,2,2-Tetrafluoro-1-(2,2,2-trifluoroethoxy)ethane
1,1,2-Trichloroethane
1,1-Dichloroethylene, Vinylidene chloride
1,2,3,4,5-Pentachlorobenzene
1,2,3,5-Tetrachlorobenzene
1,2,4-Trichlorobenzene
1,2,4-Trimethylbenzene
1,2-Dibromoethane, Ethylene dibromide
1,2-Dichlorobenzene
1,2-Dichloroethane, Ethylene dichloride
1,2-Dichloropropane, Propylene dichloride
1,3-Butadiene
1,3-Dinitropyrene
1,4-Cineole
1,4-Dichlorobenzene

1,4-Dimethylbenzo[c]phenanthrene
1,6-Dinitropyrene
1,8-Cineole, Eucalyptol
1,8-Dinitropyrene
10-Acetyldocetaxel
10-Deacetylpaclitaxel
10-Hydroxycamptothecin
11,9-Epoxymethano-PGH2, U-46619
11-Deoxycorticosterone, Cortexone
11-Deoxycortisol
11-Hydroxystearate
12,13-DiOME
12-Ethoxy-fagaronine
12-Hydroxyeicosatetraenoic acid, 12-HETE
12-Hydroxyoleate
12-Hydroxystearate
13(S)-Prostaglandin H2, PGH2
13,14-Dihydroretinoic acid
15-Hydroperoxyeicosatetraenoic acid, 15-HPETE
15-Hydroxyeicosatetraenoic acid, 15-HETE

15-keto-Prostaglandin H2
17-Allylamino-17-demethoxygeldanamycin, 17-AAG
17alpha-Methyltestosterone
18-Hydroxycorticosterone
18-Methoxycoronaridine
19-Bromoandrost-1,4,6-triene-3,17-dione 10c
19-Bromoandrost-1,4-diene-3,17-dione 8c
19-Bromoandrost-4,6-diene-3,17-dione 9c
19-Bromoandrost-4-ene-3,17-dione 7c
19-Chloroandrost-1,4,6-triene-3,17-dione 10b
19-Chloroandrost-1,4-diene-3,17-dione 8b
19-Chloroandrost-4,6-diene-3,17-dione 9b
19-Chloroandrost-4-ene-3,17-dione 7b
19-Hydroxy-4beta,5beta-epoxy-androstane-3,17-dione
19-Hydroxy-6alpha-methylandrost-4-ene-3,17-dione 13
19-Hydroxy-6beta-methylandrost-4-ene-3,17-dione 12
19-Hydroxy-6-oxoandrostenedione
19-Iodoandrost-1,4,6-triene-3,17-dione 10d
19-Iodoandrost-1,4-ene-3,17-dione 8d
19-Iodoandrost-4,6-ene-3,17-dione 9d

19-Iodoandrost-4-ene-3,17-dione 7d
19-nor-Androst-4-ene-3,17-dione, Norandrostenedione
19-Oxo-4beta,5beta-epoxy-androstane-3,17-dione
19-Oxo-6alpha-methylandrost-4-ene-3,17-dione 15
19-Oxo-6beta-methylandrost-4-ene-3,17-dione 14
19-Oxo-androst-4-ene-3,17-dione
1-Acenaphthenol
1-Allyl-4-methylpyrol-1,2,3,6-tetrahydropyridine
1alpha,24(R)-dihydroxyvitamin D3
1alpha,24-Dihydroxyvitamin D2
1alpha,25-Dihydroxy-19-nor-vitamin D3
1alpha,25-Dihydroxy-20epi-vitamin D3
1alpha,25-Dihydroxy-3-epi-vitamin D3
1alpha,25-Dihydroxyvitamin D2
1alpha,25-Dihydroxyvitamin D3, Calcitriol
1alpha-Hydroxydihydrotachysterol3
1alpha-Hydroxyvitamin D2
1alpha-Hydroxyvitamin D3, Alfacalcidiol
1-Amino-4-phenyl-1,2,3,6-tetrahydropyridine, APTP
1-Aminobenzotriazole, 1-ABT

1-Aminopyrene
1-Azabenz[a]pyrene, 10-azaB[a]P
1beta,25-Dihydroxy-3-epi-vitamin D3
1beta,25-Dihydroxy-vitamin D3
1-Chlorohexane
1-Cyano-3-(3,4-xylyl)guanidine
1-Cyanomethyl-4-methylpyrol-1,2,3,6-tetrahydropyridine
1-Cylopropyl-4-aryl-2-1,2,3,6-tetrahydropyridines
1-Ethylpyrene
1-Ethynylpyrene
1-Isopropyl-4-methylpyrol-2-1,2,3,6-tetrahydropyridine
1-Methyl-4-aryl-2-1,2,3,6-tetrahydropyridines
1-Methyl-4-methylpyrol-1,2,3,6-tetrahydropyridine
1-Methyl-4-phenyl-1,2,3,6-tetrahydropyridine, MPTP
1-Methylhistamine, N-tele-methylhistamine
1-Methyl-N-4-aryloxy-1,2,3,6-tetrahydropyridine
1-Methylpyrene
1-Monochlorodibenzo-p-dioxin, 1-MCDD
1-Naphthol
1-Nitropyrene

1-Phenylazo-2-hydroxynaphthal, Sudan I

1-Propargyl-4-methylpyrol-1,2,3,6-tetrahydropyridine

1-Propargyl-4-phenyl-1,2,3,6-tetrahydropyridine

2-(4-Amino-3-methylphenyl)-5,6-difluorobenzothiazole

2-(4-Amino-3-methylphenyl)-5-fluorobenzothiazole, 5F-203

2-(4-Amino-3-methylphenyl)-6-fluorobenzothiazole, 6F-203

2-(4-Amino-3-methylphenyl)benzothiazole, DF 203, NSC 674495

2-(4-Amino-3-methylphenyl)benzothiazole, DF 203, NSC 674495

2,2',4',5,5'-Pentachlorobiphenyl, PCB 101

2,2,4,6,6-d5-Testosterone

2,2,6,6-Tetramethylpiperidine I

2,2,6,6-Tetramethylpiperidine II

2,2,6,6-Tetramethylpiperidine III

2,2-Dichloro-1,1,1-trifluoroethane, HCFC-123

2,3,4,5,6-Pentachlorophenol

2,3,7-Trichlorodibenzo-p-dioxin, 2,3,7-triCDD

2,3-Diaminopyridine derivs.

2,3-Dichlorobutane

2,3-Dichlorodibenzo-p-dioxin, 2,3-DCDD

2,4,3',5'-Tetramethoxystilbene, TMS

2,4,5,2',4',5'-Hexachlorobiphenyl, PCB 153

2,4-Dichlorophenol

2,4-Dichlorophenoxyacetic acid

2,6-Dichlorobenzonitrile, Dichlobenil

2,6-Dichlorophenyl methylsulfone

2,6-Dimethylaniline

2,7-Dichlorodibenzo-p-dioxin, 2,7-DCDD

2-[2-{(2,6-Dichlorophenyl)amino}]phenyl ethanol

20(S)-; 20(R)-Hydroxycholesterol

20alpha,22(R)-Dihydroxycholesterol

20alpha-Hydroxycholesterol

20-Hydroxy-leukotriene B4, 20-hydroxy-LTB4

22(S)-; 22(R)-Hydroxycholesterol

23(S),25,26-Trihydroxyvitamin D3

24(R),25-Dihydroxyvitamin D3

24-; 24(S)-Hydroxycholesterol

24alpha-Methylcholesterol

24beta-Ethylcholesterol

24-Hydroxy-4-cholest-en-3-one

24-Ketocholesterol

24-Oxo-25-hydroxyvitamin D3

25-Hydroxy-19-nor-vitamin D3

25-Hydroxy-3-epi-vitamin D3

25-Hydroxy-4-cholest-en-3-one

25-Hydroxycholesterol

25-Hydroxyvitamin D3, Calcifediol

25-Hydroxyvitamin D3-26,23-lactol

26(R)-Hydroxy-cholesterol

26,27-Hexafluoro-1alpha,23(S),25-trihydroxyvitamin D3

26,27-Hexafluoro-1alpha,25-dihydroxyvitamin D3

26S-Hydroxy-cholesterol

27-Hydroxycholesterol

2-Acetylaminofluorene, 2-AAF

2alpha-methyl-19-ol-androst-4-ene-3,17-dione 26

2alpha-methyl-19-one-androst-4-ene-3,17-dione 28

2alpha-methyl-androst-4-ene-3,17-dione 6

2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine, PhIP

2-Amino-3,4-dimethylimidazo[4,5-f]quinoline, MeIQ

2-Amino-3-methylimidazo[4,5-f]quinoline, IQ

2-Amino-6-methyldipyrido[1,2-a3,2'-d]-imidazole, Glu-P-1

2-Amino-alpha-carboline

2-Aminoanthracene, 2-AA

2-Aminodipyrido[1,2-a3,2'-d]-imidazole, Glu-P-2

2-Aminofluorene, 2-AF

2-Aroylthiophene deriv. 1

2-Aroylthiophene deriv. 2

2-Aroylthiophene deriv. 2a

2-Aroylthiophene deriv. 2b

2-Aroylthiophene deriv. 3, TPP

2-Aroylthiophene deriv. 4

2-Aroylthiophene deriv. 5

2-Aroylthiophene deriv. 6, TPE

2-Aroylthiophene deriv. 7

2-Aroylthiophene deriv. 8

2-Aroylthiophene deriv. 9

2beta-methyl-androst-4-ene-3,17-dione 5

2C-B

2C-D

2C-E

2-Chloro-1,1-difluoroethene

2C-I
2C-T-2
2C-T-7
2-Heptenal
2-Hexenal
2-Hydroxypalmitate
2-Hydroxystearate
2-Isopropenyl-2-methyladamantane, 2-PMADA
2'-Methoxyacetophenone
2-Methoxyamphetamine
2-Methoxyphenamine
2-Methyl-1,3-benzodithiole
2-Methylene-androst-4-ene-3,17-dione 17
2-Monochlorodibenzo-p-dioxin, 2-MCDD
2-Naphthol
2-Naphthyl methyl sulfide
2-Naphthylamine, beta-NA
2-Nitroanisole
2-Nitronaphthalene
2-Nitropyrene

2-Nonanol
2-Nonenal
2n-Propylquinoline
2-Octenal
2-Pentenal
2-Phenylbenzotriazoles, 4-amino deriv.
2-Phenylethylamine, beta-Phenylethylamine
2-Phenylthiophene
3-(N-nitrosomethylamino)propionaldehyde, NMPA
3-(N-nitrosomethylamino)propionaldehyde, NMPA
3-(N-nitrosomethylamino)propionitrile, NMPN
3-(N-phenylamino)propane-1,2-diol, PAP
3,3'-Diindolylmethane
3,3-Tetramethyleneglutarimides
3',4'-Dimethoxyflavone
3,4-Dimethoxyphenyldiaziridine 1c
3,4-Methylenedioxymphetamine N-propyl, MDA N-propyl
3,4-Methylenedioxymphetamine, Love pills, MDA
3,4-Methylenedioxymethylamphetamine (R,S)-, Eve, MDE
3,4-Methylenedioxymethamphetamine, Ecstasy, MDMA; MDMA (R)-(-)-; MDMA (S)-(+)-

3,5,7-Trihydroxyflavone, Galangin
3,5-Dihydroxy-4'-methoxystilbene, Desoxyrhapontigenin
3-[(Arylthio)-ethyl]sydnone, TTMS
3-[2-(2,6-Dichlorophenyl)amino]benzyloxy]propan-1-ol
3-[2,3-Dichloro-4-(2-thenoyl)phenoxy] propan-1-ol
3-Acetylaminobenzanthrone, 3-Ac-ABA
3-Amino-1,4-dimethyl-5H-pyrido[4,3-b]indole, Trp-P-1
3-Amino-1-methyl-5H-pyrido[4,3-b]indole, Trp-P-2
3-Aminobenzanthrone, 3-ABA
3beta-Hydroxy-5-beta-pregnan-20-one
3beta-Hydroxy-5-cholestenal
3beta-Hydroxy-5-cholestenoic acid
3beta-Hydroxylanost-7-en-32-ol
3-Butene-1,2-diol
3-Butyryl-7-methoxycoumarin, BMC
3-Cyano-7-ethoxycoumarin, CEC
3-Deoxy-androst-4-ene-3,17-dione
3-Hydroxyphenethylamine
3-Isporenyl-3-methyldiamantane, 3-PMDIA
3-Methoxy-4-aminoazobenzene, 3-MeO-AAB

3-Methoxymorphinan
3-Methoxyphenethylamine
3-Methoxyphenyldiaziridine 7
3-Methyl-4-methoxyphenyldiaziridine 1e
3-Methylcholanthrene, 3MC
3-Methylindole, Skatole
3-Nitrobenzanthrone, 3-NBA
3-Nitrofluoranthene
3-N-nitrosoguvacoline, NG
3-O-methylfluorescein
4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanol, NNAL
4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone, NNK
4-(N,N-diethylaminomethyl)-7-benzyloxycoumarin
4-(N,N-diethylaminomethyl)-7-methoxycoumarin
4-(N,N-diethylaminomethyl)-7-propoxycoumarin
4-(N,N-dimethylaminomethyl)-7-ethoxycoumarin
4,4-Dimethylpiperidine-2,6-diones
4,4'-Methylene bis(2-chloroaniline), MOCA
4',5'-Dihydro-8-methoxypsoralen
4,5-Methylenephenanthrene

4,7,10,13,16-(Z)-Docosapentaenoic acid

4,7,10,13,16,19-(Z)-Docosahexaenoic acid

4-[N-tert-Butyl)aminomethyl]-7-methoxycoumarin

480156-S

4-Aminobiphenyl

4-Androstene-3,6,17-trione

4beta,5beta-Epoxy-androstane-3,17-dione

4beta-Hydroxycholesterol

4-Biphenylaldehyde

4-Chloroindole

4-Chloromethyl-7-ethoxycoumarin

4-Chlorophenyldiaziridine 8

4-Cholesten C7alpha-hydroxy-3-one

4-Cholesten-3-one

4-Ethoxyphenyldiaziridine 1b

4-ethylDDC, DDEP

4-Hydroxyphenethylamine

4-Hydroxy-trans-2-nonenal

4-Ipomeanol

4'-Methoxy-alpha-pyrrolidinopropiophenone, MOPPP

4-Methoxyamphetamine, para-Methoxyamphetamine

4'-Methoxyflavanone

4-Methoxymethamphetamine

4-Methoxy-N-(n-butyl)amphetamine

4-Methoxy-N-ethyl-amphetamine

4-Methoxyphenethylamine

4-Methoxyphenyldiaziridine 1a

4-Methoxyphenylketone 10

4'-Methyl-alpha-pyrrolidinobutyrophenone, MPBP

4'-Methyl-alpha-pyrrolidinopropiophenone, MPPP

4-Methylaminoantipyrine

4-Methylphenol, p-Cresol

4-Methylthio-amphetamine

4-Methylthiophenyldiaziridine 1d

4-Nitroanisole

4-Nitropyrene

4-Nonylphenol

4-Nonylphenol

4-O-Bzl-indole

4-Vinyl-1-cyclohexene (S)- and (R)-

5,24-Cholestadien-3beta-ol
5,4'-Dihydroxy-3-methoxystilbene
5,4'-Dimethoxyisoflavone
5,6-Dimethylxanthenone-4-acetic acid, DMXAA
5,7,4'-Trimethoxyflavone
5,7-Dimethoxyflavone
5,9-Dimethyldibenzo[c,g]carbazole, diMeDBC
58C80
5alpha-Androstane-3,17-dione 5
5alpha-Androstane-3alpha,17beta-diol
5alpha-Androstane-3beta,17beta-diol
5alpha-Dihydroprogesterone
5alpha-Dihydrotestosterone, DHT
5-AOT
5beta-Cholestane-3alpha,7alpha,12alpha,27-tetrol
5beta-Cholestane-3alpha,7alpha,12alpha-triol
5beta-Cholestane-3alpha,7alpha-diol
5-beta-Pregnan-3-one-20alpha-hydroxy
5-Bromo-7-nitroindoline
5-Bromoindoline

5-Chloromethylfluorescein diethylether, 5-CMFDee

5-Cholesten-27-nor-3beta-ol-25-one

5-DPT

5-Hydroxyeicosatetraenoic acid, 5-HETE

5-Hydroxypsoralen

5-Methoxyindole

5-Methoxy-N,N-diisopropyltryptamine, 5-MeO-DIPT, Foxy

5-Methoxy-N,N-dimethyltryptamin, 5-MDMT

5-Methoxytryptamine

5-Methylchrysene

5-Methylindole

5-O-Bzl-indole

6,6-d2-Testosterone

6',7'-Dihydroxybergamottin, DHB

6alpha-d1-Testosterone

6alpha-Butoxyandrost-1,4-diene-3,17-dione 3c

6alpha-Butoxyandrost-4-ene-3,17-dione 1c

6alpha-Ethoxyandrost-1,4-diene-3,17-dione 3b

6alpha-Ethoxyandrost-4-ene-3,17-dione 1b

6alpha-Methoxyandrost-1,4-diene-3,17-dione 3a

6alpha-Methoxyandrost-4-ene-3,17-dione 1a

6alpha-Methylandrost-4-ene-3,17-dione

6-Aminochrysene

6beta-Butoxyandrost-1,4-diene-3,17-dione 4c

6beta-Butoxyandrost-4-ene-3,17-dione 2c

6beta-d1-Testosterone

6beta-Ethoxyandrost-1,4-diene-3,17-dione 4b

6beta-Ethoxyandrost-4-ene-3,17-dione 2b

6beta-Methoxyandrost-1,4-diene-3,17-dione 4a

6beta-Methoxyandrost-4-ene-3,17-dione 2a

6beta-Methylandrost-4-ene-3,17-dione

6-Chloromethylfluorescein diethylether, 6-CMFDee

6-Methylchrysene

6-Nitrochrysene

6-Nitroindoline

6-Nitropyrene

6-Oxoandrostenedione

7,10,13,16,19-(Z)-Docosapentaenoic acid

7,12-Dimethylbenz[a]anthracene, 7,12-DMBA

7,8-BF, 7,8-Benzoflavone, alpha-Naphthoflavone

7alpha-Hydroxy-4-cholesten-3-one
7alpha-Methyl-19-nortestosterone, Trestolone
7-Benzylxy-4-(trifluoromethyl)coumarin comp., BFBFC
7-Benzylxy-4-(trifluoromethyl)-coumarin, BFC
7-Benzylxy-4, N,N-diethylamino-methyl- coumarin, BDAC
7-Benzylxyquinoline, 7-BQ
7-Benzylxyresorufin, BzRes
7-Butoxycoumarin
7-Butoxyresorufin
7-d2-Benzylxyquinoline, 7-BQ
7-Dehydrocholesterol
7-Dimethylamino-4-trifluoromethylcoumarin, C152
7-Ethoxy-4-trifluoromethylcoumarin, 7-EFC
7-Ethoxycoumarin
7-Ethoxyresorufin, 7-ER
7H-Dibenzo[c,g]carbazole, DBC
7-Heptoxycoumarin
7-Ketocholesterol
7-Methoxy-3-cyanocoumarin, CMC
7-Methoxy-4-(aminomethyl)-coumarin, MAMC

7-Methoxy-4-(methylpyridinium)-coumarin, MMPyrC

7-Methoxy-4-methylcoumarin comp., AMMC

7-Methoxy-4-trifluoromethylcoumarin comp., MeAMFC

7-Methoxy-4-trifluoromethylcoumarin, 7-MFC

7-Methoxy-4-trifluoromethylcoumarin-3-acetic acid, FCA

7-Methoxycoumarin

7-Methoxyresorufin

7-Methylbenz(c)acridine, 7MBAC

7-Pentoxyresorufin

7-Propoxyresorufin

8-Ethylfurafylline

8-Geranyloxysoralen

8-Hydroxyeicosatetraenoate, 8-HETE

8-Hydroxysoralen

8iso-Prostaglandin H<sub>2</sub>, 8iso-PGH<sub>2</sub>

8-Prenylnaringenin

9,10-Dihydrophenanthrene

9,10-Dihydroxystearic acid, 9,10-DiSTA

9,10-DiOME

9,11-Diazo-15-deoxy-PGH<sub>2</sub>, U-51605

9,11-Epoxymethano-PGH<sub>2</sub>, U-44069

9-Anthralaldehyde

9cUAB30

9-Hydroxyeicosatetraenoate, 9-HETE

9-Methylanthracene

Abacavir

ABC 302367

Abecarnil

ABT-418

ABT-438

ABT-761

Aceclofenac

Acenocoumarol; (R)-; (S)-

Acepromazine, Acetopromazine

Acetaldehyde

Acetaminophen, Paracetamol

Acetanilide

Acetochlor

Acetylmethadol, L-alpha-, LAAM

Acetylmethadol, nor-L-alpha-, norLAAM

Acetylsalicylic acid
Acrylonitrile, vinyl cianide, cyanoethylene
Adamantan 950
Adinazolam
Adrenaline, Epinephrine
Aflatoxin B1, AFB1
Aflatoxin B1-dialdehyde
Aflatoxin G1, AFG1
AG7088
Alachlor
Albendazole
Albuterol, Salmeterol
Alfentanil
Allopregnanolone
Allylisopropylacetamide, AIA
Almotriptan
Alosetron
alpha-Dihydroergocryptine, DHEC
alpha-Thujone
alpha-Tocopherol, Vitamin E

Alpidem
Alprazolam
Alprenolol
Ambroxol
Ametryne
Amiflamine
Amino-3'-methylphenylnorharman
Aminoflavone, NSC 68628
Aminophenylharman
Aminophenylnorharman
Aminopyrine, Amidopyrine, Aminophenazole
Amiodarone
Amitriptyline
Amlodipine
Amodiaquine
Amoxapine
Amphetamine
Amprenavir
Amsulalol
Anandamide

Androst-1,4,6-triene-3,17-dione

Androst-1,4,6-triene-3,17-diones, 6-alkyl-analogs

Androst-1,4-diene-3,17-diones, 6-ether-analogs

Androst-4,6-diene-3,17-dione

Androst-4,6-diene-3,17-diones, 6-alkyl-analogs

Androst-4-ene-17-one

Androst-4-ene-3,17-dione 16alpha-hydroxy

Androst-4-ene-3,17-dione, Androstenedione

Androst-4-ene-3,17-diones, 6alpha- and 6beta-alkyl-analogs

Androst-4-ene-3,17-diones, 6-ether-analogs

Androst-4-ene-6,17-dione

Androst-5-ene-17-one

Androst-5-ene-4,17-dione

Androst-5-ene-7,17-dione

Androstadiene-3,17-dione, 6-alkyl-analogs

Androstenedione 1beta-H3

Androstenedione 2alpha-bromo

Androstenedione 2alpha-chloro

Androstenedione 2alpha-ethoxy

Androstenedione 2alpha-fluoro

Androstenedione 2alpha-methoxy
Androstenedione 2alpha-methyl
Androstenedione, delta1,6-
Androstenedione, delta1,6-, 6-alkyl-
Androstenedione, delta6-
Androstenedione, delta6-, 6-alkyl-
Androsterone
Aniline
Anthracene
Anthracene-9-carboxaldehyde
anti Hydroxy-spirosulfonamide
Antipyrine, Phenazone
Apigenin
Aplidine
Aprepitant
Aprindine
AQ4N
Arachidonate, Arachidonic acid
Arecoline
Aripiprazole

Aristolochic acid I
Aristolochic acid II
Arteether
Artelinic acid
Artemisinin
Artesunate, Artesunic acid
Aryl-1,3-dithiolanes
Aryl-1,3-oxathiolanes
Arylamines
Astemizole
Atomoxetine, Tomoxetine, LY139603
Atorvastatin lactone
Atorvastatin, Atorvastatin acid
Atrasentan
Atrazine
AWD 131-138
Azabicyclofuranopyridine carboxamide 1
Azabicyclopypidinecarboxamide 1
Azelastine
Azelnidipine

Azimilide
Azinphos-methyl
Barnidipine
BAY 59-7939
Benidipine
Benidipine; (-)-alpha-; (+)-alpha-
Benz[a]anthracene, 1,2-Benzanthracene
Benzbromarone
Benzbromarone 16
Benzbromarone 2a
Benzene
Benzene dihydrodiol
Benzhydrol
Benzo[a]perylene
Benzo[a]pyrene, B[a]P
Benzo[b]perylene
Benzo[c]phenanthrene, B[c]P
Benzo[c]phenanthridine BP-7
Benzodioxazolylbutanamine (S,R)-, BDB
Benzophenone

Benzphetamine
Benztropine 4',4"-Cl
Benzydamine
Benzyl isothiocyanate
Benzylamine
Benzylamines para-substituted
Bepridil
Bergamottin, 5-Geranoxypsoralen, GF-I-2
Bergapten, 5-Methoxypsoralen
beta-Tocopherol
Betaxolol
Bezafibrate
Bicalutamide (S)-, (R)-
Bicifadine
Bicifadine M12
Bisoprolol (S)- and (R)-
Bisphenol A
BK8644, BayK8644
BMS-1
BMS-2

BMS-214778
BMS-3
BMS-310705
BMS-378806
BO-653
BO-653
Boldenone
Bortezomib M1
Bortezomib M2
Bortezomib, PS341
Bosentan
Brinzolamide
BRL0L075
Brofaromine
Bromocriptine
Bromodichloromethane
Bromoperidol, Bromperidol
Bromuconazole 47
Propirimine
Brotizolam

Budesonide
Buflomedil
Bufuralol; (S)-; (R)-
Bunitrolol (+)-, (-)-
Bupivacaine
Bupranolol
Buprenorphine
Bupropion
Buspirone
Busulphan
Butachlor
Butadiene monoxide, 1,2-Epoxy-3-butene
BVT.2938
BYZX
Ca. roseus
Caffeine
Canadine
Candesartan
Cannabinol
Capravirine

Capravirine S-oxide
Capsaicin
Captopril
Carbamazepine
Carbamazepine C2-hydroxy
Carbamazepine C3-hydroxy
Carbaryl
Carbofuran
Carbon tetrachloride
Carebastine
Carisoprodol
Carteolol
Carvedilol; (S)-; (R)-
Celecoxib
Celecoxib deriv. 1
Celecoxib deriv. 10
Celecoxib deriv. 11
Celecoxib deriv. 12
Celecoxib deriv. 13c
Celecoxib deriv. 2

Celecoxib deriv. 3
Celecoxib deriv. 4
Celecoxib deriv. 5
Celecoxib deriv. 6
Celecoxib deriv. 7
Celecoxib deriv. 8
Celecoxib deriv. 9
Cephalomannine
Cerivastatin lactone
Cerivastatin O-demethyl
Cerivastatin, Cerivastatin acid
Cetirizine (R,S)-; (S)-, ucb 28557; (R)-, Levocetirizine
Chenodeoxycholate, Chenodeoxycholic acid
Chlorodehydro-17alpha-methyltestosterone
Chloroform, Trichloromethane
Chloroquine
Chlorpheniramine
Chlorproguanil
Chlorpromazine
Chlorpropamide

Chlorpyrifos
Chlorsulfuron
Chlortoluron
Chlorzoxazone
Cholate, Cholic acid
Cholestanol
Cholesterol 3-fatty acid esters
Cholesterol 3-methylether
Cholesterol 3-sulfate
Cholesterol C7alpha-hydroxy
Chrysene
Cibenzoline; (S)-(-); (R)-(+)-
Ciclesonide, des
Cilnidipine
Cilostazol
Cimetidine
Cinacalcet
Cinnarizine
Ciprofibrate
cis-(Z)-Clopenthixol, Zuclopenthixol

Cisapride rac., (+)-; (-)-
Cisplatin
Citalopram, rac; (R)-; (S)-, Escitalopram
Citalopram aldehyde
CJ-036878
CJ-036878 M10
Clarithromycin
Clindamycin
Clivorine
Clobazam C4'-hydroxy
Clobazam N-desmethyl
Clofibrate
Clomethiazole, Chlormethiazole
Clomipramine
Clonazepam
Clopidogrel
Clopidogrel 2-oxo
Clotiazepam
Clozapine
CMV423

Cocaine, Cocaine (-)-, Cocaine l-
Codeine
Colchicine
Compound A
Compound A (NS5B)
Compound A int. antag.
Compound S4
Corticosterone
Cortisol, Hydrocortisone
Cotinine, (S)-Cotinine
Coumarin
CP-122,721
CP-125,611
CP-195,543
CP-199,331
CP-358,774
CP-677,623
CP-919,230
CQA 206-291
Curcumin

Cyamemazine
Cyclic phosphate prodrug 7
Cyclo Leu-Phe
Cyclo Lue-Pro
Cyclo Phe-Pro
Cyclobenzaprine
Cyclocoumarol 9(S)-, 9(R)-
Cyclohexylline
Cyclopenta[c,d]pyrene
Cyclophosphamide
Cyclosporin A, Cyclosporine, Cyclosporin, Ciclosporin
Cyclosporin G
Cyproterone acetate
D0870
Dacarbazine
Daidzein
Danazol
Dantrolene
Dapsone
Darunavir

Daunomycin, Daunorubicin
DB844
DDB
Debrisoquine
Decanoic acid, Capric acid
Decursinol angelate
Deguelin
Dehydroaripiprazole, OPC-14857
Dehydroascorbic acid
Dehydroepiandrosterone 3-sulfate, DHEA 3-sulfate
Dehydroepiandrosterone, DHEA
Dehydropranidipine
Delavirdine
delta3-Carene
Deltamethrin
delta-Tocotrienol
Denitronifedipine
Deoxycholate, Deoxycholic acid
Deoxypodophyllotoxin
Deramciclane

Desglymidodrine
Desmethyladinazolam N-
Desmethylcitalopram, rac.; (R)-; (S)-
Desmethylselegiline N-, (R)-(-)-
Desmosterol
Desogestrel
Dexamethasone
Dexfenfluramine, D-(+)-fenfluramine
Dexloxioglumide
Dextromethorphan
Dextropropoxyphene, Propoxyphene
Dextrorphan
DFB
Diallyl disulfide, DADS
Diallyl sulfide, DAS
Diallyl sulfone, DASO2
Diazepam
Diazinon
Dibenz[a,h]acridine
Dibenz[a,h]anthracene

Dibenz[a,j]acridine, DBAJAC

Dibenzo[a,e]fluoranthene

Dibenzo[a,e]pyrene, DB[a,e]P

Dibenzo[a,f]fluoranthene

Dibenzo[a,h]pyrene, DB[a,h]P

Dibenzo[a,i]pyrene

Dibenzo[a,k]fluoranthene

Dibenzo[a,l]pyrene, DB[a,l]P

Dibenzo[b,k]fluoranthene

Dibenzo[e,l]pyrene, DB[e,l]P

Dibenzo[j,l]fluoranthene

Dibenzo-p-dioxin, DD

Dibenzylfluorescein, DBF

Diclofenac

Diclofenac acyl glucuronide

Diclofenac C5-hydroxy

Dicoumarol, Dicoumarin

Didesmethylcitalopram

Diethylcarbamazine

Diflomotecan, BN80915

Digitoxin
Dihydralazine
Dihydrobenzoxanthiin I
Dihydrobenzoxanthiin II
Dihydrobromoperidol (S,R)-; (S)-; (R)-
Dihydrocapsaicin
Dihydrocodeine
Dihydroequilenin, 17beta-
Dihydroergotamine
Dihydrohaloperidol (S,R)-; (S)-; (R)-
Dihydrolanosterol
Dihydropyridine comp. 10
Dihydropyridine comp. 11
Dihydropyridine comp. 13
Dihydropyridine comp. 14
Dihydropyridine comp. 15
Dihydropyridine comp. 16
Dihydropyridine comp. 17
Dihydropyridine comp. 18
Dihydropyridine comp. 19 (+)

Dihdropyridine comp. 20 (-)

Dihdropyridine comp. 21

Dihdropyridine comp. 3

Dihdropyridine comp. 8

Dihdropyridine comp. 9

Dihydrotachysterol3

Diltiazem

Dimethoate

Dimethyl benzoylphenylurea

Diphenhydramine

Diprafenone

Disopyramide, (S)-(+)-, (R)-(-)-

Disulfoton

Diuron

DL-Glyceraldehyde

DMP 543

DMP 543 despicoly

Docetaxel, Taxotere

Dolasetron

Dolasetron reduced

Domperidone
Donepezil
Dopamine
Dopamine
Dorzolamide
Doxepin E (trans-); Z (cis-)
Doxepin E (trans-) N-desmethyl
DPC 681
DPC 684
DPM777
DRF 4367
Duloxetine
DY-9760e
E2101
E7389
Ebastine
Ebastine hydroxy
Ecabapide
Efavirenz
Efavirenz C8-hydroxy

Eicosapentaenoic acid
Eicosatrienoic acid
Eletriptan
Ellipticine
Emetine
EMTPP
Emulgens, 911 and 913
Enalapril
Encainide
Endosulfan, Endosulfan alpha
Enflurane (R,S)-, (S)-, (R)-
Epiandrosterone, EPIA
Epinastine
Epitestosterone
Eplerenone
epsilon-Tocopherol
Equilenin
Ergosterol
Eriodictyol
Erlotinib

Erythromycin
Esfenvalerate
Estazolam
Estradiol 17beta-
Estradiol 17beta-D-glucuronide, E(2)17betaG
Estradiol 3-methyl ether
Estradiol C2-hydroxy
Estradiol C2-hydroxy, C3-methoxy
Estradiol C2-methoxy
Estradiol C4-hydroxy
Estragole
Estrone
Estrone 3-sulfate
Eszopiclone
ET-743, Ecteinascidin 743, Trabectedin
Ethanol
Ethinylestradiol 17alpha, Ethynodiol 17alpha-
Ethiprole
Ethofumesate
Ethosuximide

Ethoxidine
Ethyl carbamate, Urethan
Ethyl tert-butyl ether
Ethylbenzene
Ethylenethiourea
Ethylmorphine
Ethyl-p-tolyl sulfide
Etizolam
Etodolac
Etoperidone
Etoperidone p-hydroxy
Etoposide, VP-16
Etoricoxib
Eugenol
Eupatilin
Everolimus, SDZ-RAD
Ezlopitant
Ezlopitant alkene, CJ-12,458
Fadrozole, CGS 16949A
Farnesol

Fatty acid C22
Fatty acid C24, Lignoceric acid
Fatty acid C26, Cerotic acid
Fatty acids, long-chain
Fatty acids, polyunsaturated
Felbamate
Felodipine
Fenofibrate
Fenproporex
Fenretinide, 4-Hydroxyphenyl retinamide, 4-HPR
Fentanyl
Fenthion
Ferroquine, SSR97193
Finasteride
Fipronil
FK228, FR901228, Depsiptide
Flecainide
Flosequinan
Flu-1
Flucloxacillin

Flunarizine
Flunitrazepam
Fluoranthene-2,3-diol
Fluorescein diethylether, FDee
Fluoxetine rac., (R)-, (S)-
Flupentixol, Flupenthixol
Fluperlapine
Fluphenazine
Flurbiprofen; (S)-; (R)-
Flutamide
Fluticasone propionate
Fluvastatin lactone
Fluvastatin, Fluvastatin acid
Fluvoxamine
Formononetin
Formoterol
Furafylline
Furametpyr
Furan
Galanthamine

Gallopamil (S)- and (R)-

gamma-Tocopherol

Ganaxolone

Gefitinib, ZD1839

Gemfibrozil

Gemfibrozil 1-O-beta glucuronide

Genistein

Genistein 4'-methyl ether, Biochanin A

Gepirone

Gliclazide

Glimepiride

Glipizide

Glyburide, Glibenclamide

Glyceryl trinitrate, NTG

GR87442

Granisetron

GTS-21, DMXB

Guanabenz

Guanoxan

GW420867X

GW844520
H 259-31 (S)- and (R)-
Halofantrine
Haloperidol
Haloperidol pyridinium metabolite, HPP+
Haloperidol pyridinium metabolite, HPTP
Halothane
Harmine
Heptylphenyltetrahydropyridine 15
Hesperetin, Hesperitin
Hexachlorobenzene, Perchlorobenzene
Hexamethylphosphoramide
Hexane, n-
Hexobarbital; (S)-(+)-; (R)-(-)-
HM-30181
Homocapsaicin
Homodihydrocapsaicin
HP184
Hydrochloroflourocabons
Hydrocodone

Hydromorphone
Hydroxyitraconazole
Hydroxymethyl-methylformamide, HMMF
Ibogaine
Ibrolipim, NO-1886
Ibuprofen; (S)-; (R)-
Ifosfamide rac.; (R)-; (S)-
Iloperidone
Imatinib, STI571
Imazosulfuron
Imidacloprid
Imidafenacin
Imipramine
Imiquimod
Imrecoxib
Indan-1-ol; -(S)-ol; -(R)-ol
Indinavir
Indinavir N-depyridomethyl
Indiplon N-desacetyl
Indiplon, NBI-34060

Indirubin
Indisulam, E7070
Indole
Indoline
Indomethacin
Indomethacin phenethylamide, LM-4108
Indoramin
Ipriflavone
Ipriflavone M4
Irbesartan
Irinotecan, CPT-11
Isobutylamide 10
Isoflurane
Isoleukotoxin, Z12(13)-EpOME
Isoliquiritigenin, 2',4,4'-Trihydroxychalcone
Isoniazid
Isoprene
Isoquinoline
Isosorbide dinitrate, ISDN
Isoxanthohumol

Isradipine
Itopride
Itraconazole; (2R,4S,2'S)-
Ivermectin
JNJ-10287069
JPC-2056
K11777, K77
Kaempferide
Kaempferol
Karenitecin
Kavain, Kawain
Ketamine; (R)-; (S)-
Ketobemidone
Ketoconazole N-deacetyl
Ketoitraconazole
Ketone 3
KR-2
KR-31543
KR-31831
KR-32570

KR-33028, KR-1
KR-60436
Kynuramine, Diaminopropiophenone
L-754,394
L-775,606
Lanosterol
Lansoprazole rac., (R)-, (S)-
Lapachenoate
Laquinimod
Lasofoxifene
Lauric acid
Leflunomide
Lercanidipine
Leukotoxin, Z9(10)-EpOME
Leukotriene B4; 6-trans-LTB4
Levobupivacaine
Levonorgestrel
Lidocaine, Lignocaine
Lilopristone
Limonene (+)- and (-)-

Linalol
Linolate, Linoleic acid
Linolenic acid
Lipids
Lipoxin A4, LXA4
Lisofylline
Lisuride
Lithocholate, Lithocholic acid
L-methionine, Met
Lonafarnib, SCH66336
Loperamide
Loperamide N-desmethyl
Lopinavir, ABT-378
Loratadine
Lornoxicam
Losartan
Losigamone, (+-, +, -)-
Lovastatin, Lovastatin lactone
LTA
Lu 25-109

Luciferin-BE
Luciferin-CEE
Luciferin-H
Luciferin-H EGE
Luciferin-ME
Luciferin-ME-EGE
Luciferin-PFBE
Luciferin-PPXEE
Lumiracoxib
LY333531
M100907
M17055
M445526
Malathion
Maprotiline
MC12181
m-Chlorophenylpiperazine, mCPP
MDL 73005
MDPPP
Medifoxamine

Medroxyprogesterone
Mefenamic acid
Mefloquine
Melatonin
Meloxicam
Menthofuran (R)-(+)-
Meperidine, Pethidine
Mephenytoin; (S)-
Mephobarbital (R)-; (S)-
Mepyramine, Mepiramine, Pyrilamine
Mequitazine
Merck KgaA EMD 68853
Mestranol
Metamitron
Methacetin
Methadone rac., (S)-(+)- and (R)-(-)-
Methamphetamine D-, Methylamphetamine (+)-, (S)-; (-)-, (R)-
Methandrostenolone, Metandienone
Methaqualone
Methimazole

Methiocarb
Methoxalen, 8-Methoxypsoralen, Xanthotoxin
Methoxychlor
Methoxychlor catechol
Methoxychlor O-bisdesmethyl (bis-hydroxy)
Methoxychlor O-monodesmethyl (mono-hydroxy)
Methoxyflurane
Methyl tert-amyl ether
Methyl tert-butyl ether
Methylaniline, N-
Methylanisole
Methylchloride
Methylene chloride
Methyleugenol
Methyl-n-pentylnitrosamine
Methylprednisolone
Methyl-p-tolyl sulfide
Metoclopramide
Metolachlor
Metoprolol rac., (S)-, (R)-

Metronidazole
Mexazolam
Mexiletine
Mianserin (R)-, (S)-
Mibepradil
Midazolam
Mifepristone, RU38486, RU486
Milacemide
Milameline
Minaprine
Miocamycin
Mirtazapine
Mixture of aniline and norharman
MK-0457
MK-0524
MK-0767
MK-0767 M16
MK-0767 methyl mercapto M25
MKC-963
ML3603

MMDL
Moclobemide
Modafinil
Monocrotaline
Montelukast
Morphine
Morpholine-urea-Phe-Hphe-vinylsulfone, K02
Morpholinodoxorubicin, MDX
Mosapride
MPPE
MPTP 3,4-cyclopropyl
MPTP 3-pyrrolinyl
MRK-1
MTMCD
Muraglitazar
Myclobutanol
Mycophenolic acid
Myristicin
Myristicin
N-(4-ethoxyphenyl)isobutyramide

N-(4-ethoxyphenyl)propionamide

N-(4-methoxyphenyl)propionamide

N,N- Dialkylnitrosamines (short chain)

N,N',N"-Triethylene thiophosphoramide, thioTEPA

N,N-dialkylnitrosamines (bulky chains)

N,N-dialkylamphetamine

N,N-diethyldithiocarbamate, DDC

N,N-diethylformamide, DEF

N,N-diethyl-m-toluamide, DEET

N,N-dimethyl 7-methoxy-4-(aminomethyl)-coumarin, diMMAMC

N,N-dimethylaniline

N,N-dimethylformamide, DMF

N-[4-(1-methylethoxy)phenyl]acetamide

N'-4-Imidazoleethylthiourea 1

N'-4-Imidazoleethylthiourea 10

N'-4-Imidazoleethylthiourea 11

N'-4-Imidazoleethylthiourea 12

N'-4-Imidazoleethylthiourea 2

N'-4-Imidazoleethylthiourea 3

N'-4-Imidazoleethylthiourea 4

N'-4-Imidazoleethylthiourea 5

N'-4-Imidazoleethylthiourea 6

N'-4-Imidazoleethylthiourea 7

N'-4-Imidazoleethylthiourea 8

N'-4-Imidazoleethylthiourea 9

Nabumetone hydroximine

N-Ac-DFEC

N-Ac-PCBC

N-alkyltetrahydroquinoline comp. A

N-alkyltetrahydroquinoline comp. B

Naloxone

Naltrexone

Naphthalene

Naphthalene 1,2-diol

Naphtho[1,2-b]fluoranthene

Naphtho[1,2-k]fluoranthene

Naphtho[2,1-a]pyrene

Naphtho[2,3-a]pyrene

Naphtho[2,3-b]fluoranthene

Naphtho[2,3-e]pyrene
Naproxen (S,R)-, (S)-, (R)-
Naringenin
Nateglinide, AY4166
Naveglitazar
NBI-42902
N-butyl 7-methoxy-4-(aminomethyl)-coumarin, BMAMC
N-butyldamphetamine
n-Butyl-p-tolyl sulfide
NCX-4016
N-desmethyl diphenhydramine
NE-100
Nebivolol d,l
Nefazodone p-hydroxy
Nefiracetam
Nelfinavir
Nemorubicin, MMDX
Netamiftide, INN 00835
N-ethyl 7-methoxy-4-(aminomethyl)-coumarin, EMAMC
N-ethylamphetamine, Ethamphetamine

N-ethylformamide, NEF
N-ethyl-N-methylaniline
Nevirapine
N-heptyl tetrahydropyridine
N-hydroxyarginine
Nicardipine
Nicotine, (S)-(-)-Nicotine
Nifedipine
Nile Red
Niludipine
Nilvadipine
Nimodipine
Nirvanol, (S)-(+)-N-3-benzyl
Nisoldipine
Nitrendipine
Nitrophenol o-, 2-Nitrophenol
Nitrophenol p-, 4-Nitrophenol
N-methyl 7-methoxy-4-(aminomethyl)-coumarin, MMAMC
N-methyl-benzodioxazolylbutanamine (S,R)-, MBDB
N-methyldibenzo[c,g]carbazole, MeDBC

N-methylformamide, NMF
N-methyl-N-allylamphetamine
N-methyl-N-propargyl-2-phenylethylamine
N-methyl-N-propargylamphetamine
N-methyl-N-propylamphetamine
N-Methytryptoline
NNAL rac., (R)-, (S)-
N-nitrosoanabasine, NABS
N-nitrosoanatabine, NATB
N-nitrosobenzylmethylamine
N-nitroso-beta-hydroxypropylpropylamine, NHPPA
N-nitroso-beta-oxopropylpropylamine, NOPPA
N-nitrosodiamylamine, NDAA
N-nitrosodibutylamine, N,N-dibutylnitrosamine, NDBA
N-nitrosodiethylamine, N,N-diethylnitrosamine, NDEA
N-nitrosodimethylamine, N,N-dimethylnitrosamine, NDMA
N-nitrosodi-n-propylamine, N-nitrosodipropylamine, NDPA
N-nitrosoethylbutylamine, NEBA
N-nitrosomethylbutylamine, NMBA
N-nitrosomethylethylamine, NMEA

N-nitrosomethyl-n-amylamine
N-nitrosomethylphenylamine, NMPhA
N-nitrosomethylpropylamine, NMPA
N-nitrosomorpholine, NMOR
N'-nitrosonornicotine, N-nitrosonornicotine, NNN; , NNN (R)-; (S)-
N-nitrosopiperidine, NPIP
N-nitrosopyrrolidine, NPYR
n-Octylamine
Nomifensine
Nonane
Nonanoic acid
Nonivamide
Nonylphenyltetrahydropyridine 17
Noradrenaline, Norepinephrine
Norbuprenorphine
Norcocaine
Norcodeine
Nordiazepam, N-desmethyldiazepam
Nordihydroapsaicin
Norverapamil rac., (R)-, (S)-

Norfluoxetine (S)-
Norflurazon
Noroxycodone
Nortestosterone
Nortriptyline
N-propyl 7-methoxy-4-(aminomethyl)-coumarin, PMAMC
N-propylajmaline
n-Propyl-p-tolyl sulfide
NS-21
n-Vinillyldecanamide
O6-Benzyl-8-oxoguanine
O6-Benzylguanine
o-Aminoazotoluene
o-Anisidine, 2-Methoxyaniline
Ochratoxin A
Octanoate, Octanoic acid
Octopamine, p-Norsynephrine, Noroxedrine
Octylphenyltetrahydropyridine 16
Olanzapine
Oleate, Oleic acid

Olopatadine
Omeprazole (S)-, (R)-, rac.
Omeprazole sulfide
Onapristone, ZK 98.299
Ondansetron
OPIPramol
Oracin
Org 30659
Org 4060
Orphenadrine
Oxatomide
Oxazolidinedione comp. A
Oxedrine, Synephrine, p-
Oxodipine
Oxybutynin rac., (S)-, (R)-
Oxycodone
Oxymetazoline
Oxymorphone
Paclitaxel
Paclitaxel 3'-phenyl-hydroxy

Paclitaxel 6alpha-hydroxy
Pafuramide, DB289
Pafuramide, DB289-M1
Pafuramide, DB289-M3
Pafuramide, DB289-M4
Palmitate, Palmitic acid
Palmitoleic acid
Pantoprazole
para-Biphenylhydrazine
Parathion
Paraxanthine, 1,7-Dimethylxanthine
Pargyline
Paroxetine
p-Benzoylphenol
p-Benzoylphenol
p-CF <sub>3</sub> -Benzylamine
p-Chloro-m-xylenol, PCMX
Pefloxacin
Pentamidine
Pentylamino comp. 1

Pentylphenyltetrahydropyridine 14
Perazine
Perchloroethylene
Perhexiline, rac., (-)-, (+)-
Perospirone
Perphenazine
Phenacetin
Phenanthrene
Phenanthrene C9,10-quinone
Phencyclidine
Phenelzine
Phenethyl isothiocyanate
Phenformin, Phenphormine
Phenobarbital
Phenobarbital, (R)-(-)-N-3-benzyl
Phenol
Phenolic fluorescent dyes
Phenothiazine
Phenprocoumon (S)-, (R)-
Phenprocoumon 4-MeO, (S)-, (R)-

Phenyl ketone 1

Phenylacrylamide 1

Phenylbutazone

Phenyldiazene

Phenyldiaziridine 9

Phenylethyl comp. 5

Phenylethylamines para-substituted

Phenylethylamino comp. 2

Phenylethylamino comp. 4

Phenylphenol o-

Phenylthiourea

Phenytoin, C3'-hydroxy

Phenytoin, C4'-hydroxy

Phenytoin, Diphenylhydantoin

Phorate

Phosphatidylcholine, PC

Phthalimide analogues

Phytanic acid

Piceid

Pigment Yellow 74, PY74

Pilocarpine
Pimobendan
Pimozone
Pinacidil
Pinoline
Pioglitazone
Pirenzepine
Piroxicam
Pitavastatin lactone
Pitavastatin, Pitavastatin acid, NK-104
p-Nitrobenzylamine
p-Nitrophenylethylamine
PNU-171990
PPI-2458
Pradefovir
Pranidipine
Pranidipine metabolite, MOP-13031
Prasugrel 2-oxo, R-95913
Pravastatin, Pravastatin acid
Praziquantel

Prednisone
Pregnenolone
Pregnenolone C17alpha-hydroxy
Pregnenolone C21-hydroxy
Primaquine
Procainamide
Progesterone
Progesterone C20alpha-hydroxy
Proguanil, Chloroguanide
PROLI-NO
Promethazine
Prometryne
Propafenone (R,S)-, (S)-, (R)-
Propionylpromazine
Propofol
Propranolol; (2R)-(+)-; (2S)-(-)-
Propranolol (2S)- difluoro
Propranolol (2S)- monofluoro
Propranolol (2S,4R)- trifluoro; (2S)- trifluoro; (2R)- trifluoro
Propranolol deshydroxy

Propranolol i-propylmethyl
Propranolol t-butylmethyl
Propranolol trifluoro deshydroxy
Propranolol trifluoroethyl
Propyljamaline, N-
Propylphenyltetrahydropyridine 12
Prostaglandin D2, PGD2
Prostaglandin E2, PGE2, Dinoprostone
Prostaglandin F2alpha, PGF2alpha
Prostaglandin G2, PGG2
Prostaglandin H1, PGH1
Prostaglandin H2, PGH2
Prostaglandin H3, PGH3
Prunetin
PS-15
PSG26, 3,4,5-Trimethoxyphenyldiaziridine 1f
Psoralen
Pulegone (R)-(+)-
PY74-M1
Pyrantel

Pyrazoloacridine
Pyrene
Pyributicarb
Pyridine metab. 21
Pyrimethamine
Pyriminobac-methyl
Quazepam
Quazepam 2-oxo
Quetiapine, Seroquel
Quinacrine, Mepacrine
Quinidine
Quinine
Quinoline
Quinoline 6-methoxy
Quinoline 6-methoxydeuterio
Quizalofop-ethyl
R-568
R-95913
Rabeprazole thioether
Rabeprazole, LY307640, E3810

Raloxifene
Ranitidine
Ranolazine
Rasagiline, (S)-, S-PAI
Rebamipide
Reboxetine (S,S)- and (R,R)-
Rec 27.0110
Reduced haloperidol pyridinium metabolite, RHPP+
Remoxipride
Repaglinide
Repertaxin
Resiquimod
Resveratrololoside
Retinal 9-cis-, Isoretinene A
Retinal all trans-, Retinene
Retinoic acid 13-cis-, Isotretinoin
Retinoic acid 9-cis-, Panretin
Retinoic acid all trans-, ATRA, Tretinoin
Retinol all trans-, Vitamin A1
Retrorsine

Riddelliine
Rifabutin
Rifabutin, 25-O-desacetyl, LM565
Rifalazil, Benzoxazinorifamycin, KRM-1648
Riluzole
Risperidone
Ritonavir
Rizatriptan
RL3142
RO115-1954
RO3300074
Rofecoxib
Ropinirole
Ropivacaine
Roquinimex
Rosiglitazone
Rosuvastatin lactone
Rosuvastatin, Rosuvastatin acid, ZD 4522
Rotenone
Roxatidine metabolite M4

Roxatidine metabolite M5
Roxithromycin
Roxithromycin decladinosyl
Roxithromycin N-desmethyl
Roxithromycin O-dealkyl
RP 73401, Piclamilast, DCMB, PNU 249173
RPR 106541
RPR 127025
RPR 130863; (+)-; (-)-
Rupatadine
Rutecarpine, Rutaecarpine
RWJ-51204
RWJ-53050
RWJ-69528
S 16020
S-2-[4-(3-Methyl-2-thienyl)phenyl]propionic acid, S-MTPPA
Safrole
Salicylate, Salicylic acid
S-allyl-L-cysteine
Saquinavir

SCH 351125
SDZ IMM 125
SDZ NKT 343
Se-benzyl-L-selenocysteine
Seleno-l-methionine
Senecionine
Seratrodast
Serotonin, 5-Hydroxytryptamine, 5-HT
Sertindole
Sertraline
Sevoflurane
Sildenafil
Silodosin
Silybin, Silibinin
Simazine
Simvastatin acid
Simvastatin, Simvastatin lactone
Sinomenine
Sirolimus, Rapamycin
Sitagliptin

SM-12502
S-methyl-esonarimod
S-methyl-N,N-diethyldithiocarbamate, MeDDC
SNI-2011
Solifenacin
Sorafenib
Sparteine
Spirosulfonamide
SQ109
SR-144190
Stearic acid
Sterigmatocystin
Sterinodole
Stilbestrol, Diethylstilbestrol
Styrene, Vinyl benzene
SU5416
Sufentanil
Sulfadiazine
Sulfamethoxazole
Sulfamethoxazole N-hydroxy

Sulfamidine, Sulfadimidine, Sulfamethazine

Sulfaphenazole deriv. 23, DMZ

Sulfinpyrazone

Sulfinpyrazone sulfide

Sulindac sulfide

Sulprofos

Sumatriptan

Sunitinib

Suprofen

syn Hydroxy-spirosulfonamide

TA compound 1

Tacrine

Tacrolimus, FK506

Tadalafil

Tamarixetin

Tamoxifen

Tamoxifen 3-hydroxy, Droloxifene

Tamoxifen 4-hydroxy; trans-4-hydroxy (Z)

Tamoxifen N-desmethyl

Tamoxifen N-oxide

Tamsulosin
Tandospirone
Tangeretin
Tanshinone I
Targretin
Tasosartan
Taurochenodeoxycholate, Taurochenodeoxycholic acid
Tauromustine
Tazarotenic acid
Tazofelone
Tegafur
Tegaserod
Telithromycin
Temazepam
Temsirolimus
Teniposide
Tenoxicam
Tentoxin
Terbinafine
Terbutylazine

Terbutryne
Terfenadine
Terfenadine, hydroxy metabolite
Terfenadone
Terfenadone 1
Terfenadone 17
Terfenadone 2
Terfenadone 3
Terfenadone 4
Terfenadone 5
Terfenadone 6
Tergitol NP-10, Nonoxytol
Terguride
Territrem A
Territrem A
Territrem B
Territrem C
Tesmilifene, DPPE
Testosterone
Testosterone, 16alpha-hydroxy

Tetradecanoic acid, Myristic acid
Tetradecylphenyltetrahydropyridine 19
Tetrahydrocannabinol THC 11-oxo-delta8-
Tetrahydrocannabinol THC 7alpha-hydroxy-delta8-; 7beta-hydroxy-delta8-
Tetrahydrocannabinol THC delta8-
Tetrahydrocannabinol THC delta9-
Teucrin A
TG100435
Thalidomide
Thalidomide C5-hydroxy
Theobromine, 3,7-Dimethylxanthine
Theophylline, 1,3-Dimethylxanthine
Thiabendazole
Thiacetazone
Thiamylal (S)- and (R)-
Thioacetamide
Thiobenzamide
Thiocoraline
Thioridazine
Thiourea

Tiagabine
Tibolone
Tibolone 3alpha-hydroxy; 3beta-hydroxy
Ticlopidine
Tienilic acid
Timolol
Tinidazole
Tipranavir
Tiracizine
Tirilazad
Tizanidine
Tocol
Tofisopam; (R)-; (S)-
Tofisopam (R)- ; (S)-C4'-O-desmethyl, M3
Tofisopam (R)-; (S)-C7-O-desmethyl, M1
Tolbutamide
Tolcapone acetylamine
Tolcapone amine
Tolmetin
Tolperisone

Tolterodine
Toluene
Torasemide, Torsemide
TPA023
TR-14035
Tramadol, rac., cis-
trans-(+)-DB[a,l]P-(11S,12S)-diol, trans-(-)-DB[a,l]P-(11R,12R)-diol
trans-(+,-)-, -(+)-, -(-)-B[a]P-7,8-dihydrodiol
trans-(+.-)-B[a]P-4,5-dihydrodiol
trans-1,2-Dihydro-1,2-dihydroxy-6-nitrochrysene
trans-12-MBA-3,4-diol
trans-2,3-Dihydroxy-2,3-dihydrofluoranthene
trans-5,6-Dimethylchrysene-1,2-diol
trans-5-Methylchrysene-1,2-diol
trans-5-Methylchrysene-7,8-diol
trans-6-Aminochrysene-1,2-diol
trans-7,12-DMBA-3,4-diol
trans-7-MBA-3,4-diol
trans-B[b]F-9,10-diol
trans-B[c]P-3,4-diol

trans-B[g]C-11,12-diol
trans-B[j]F-4,5-diol
trans-Benz[a]anthracene-1,2-diol
trans-Benz[a]anthracene-3,4-diol
trans-Benz[a]anthracene-5,6-diol
trans-Benz[a]anthracene-8,9-diol
trans-Bromuconazole
trans-Chrysene-1,2-diol
trans-DB[a,l]P-11,12-diol
trans-Phenylpropene
trans-Resveratrol, trans-3,4',5-Trihydroxystilbene
trans-Stilbene
Traxoprodil
Trazodone
Triacetyloleandomycin, Troleandomycin, TAO
Triadimefon
Triamterene
Triazolam
Triazolo[4,3alpha]pyridine 1
Trichloroethylene, TCE

Trifluoperazine
Trifluperidol
Triflupromazine
Trimethoprim
Trimethylamine
Trimipramine N-desmethyl
Trimipramine rac, L-
tris-(2,3-Dibromopropyl)phosphate
Triton N-101
Triton X-114
Trofosfamide
Troglitazone
Tropisetron
Tryptamine
Tyramine, m-
Tyramine, p-
U-89578, reduced tirlazad meabolite
Udenafil, DA-8159
UK-343,664
Undecylphenyltetrahydropyridine 18

UO126
Uroporphyrinogen
Ursodeoxycholate, Ursodeoxycholic acid
V102862
V10332
V1113741
V11294
V11689
Vaccenic acid
Valdecoxib
Valproate, Valproic acid
Valsartan
Valspodar, PSC-833, SDZ PSC 833
Vanoxerine, GBR12909
Venlafaxine
Verapamil; (R)-; (S)-
Vesnarinone
Vicriviroc, SCH 417690
Vinblastine
Vincristine

Vindesine
Vinorelbine, Navelbine
Vinyl bromide, Bromothylene
Vinyl carbamate
Vinyl chloride, Chloroethylene
Vinylcyclohexane
Vitamin D2, Calciferol
Vitamin D3, Cholecalciferol
VividBlue, BOMCC
VividBlue, EOMCC
VividCyan, BOMFC
VividGreen, BOMF
VividRed, OOMR
Voriconazole
V-PROLI-NO
V-PYRRO NO
Warfarin; (S)-; and (R)-
Warfarin (S)-2-MeO
Warfarin (S)-4-MeO
WHI-P131, JANEX-1

Xanomeline
Xylene m-
Xylene o-
Xylene p-
Y disopyramide
YM17E
YM511
YM796
YM905
YM992
Yohimbine
Z14(15)-Epoxyeicosatrienoic acid, Z14(15)-EET
Z8(9)-Epoxyeicosatrienoic acid, Z8(9)-EET
Z9,10-Epoxyoctadecanoic acid, Z9(10)-EpSTA
Zafirlukast
Zaleplon
Zaltoprofen
Zatosetron, LY277359
ZD2249
ZD6021

Zidovudine, Azidothymidine, AZT

Zileuton N-dehydroxy, Abbott-66193

Zileuton, ABT-077

Zimosterol

Zolmitriptan

Zolpidem

Zomepirac

Zopiclone

Zotarolimus

Zotepine

Zoxazolamine