

## Supplemental Material

### Identification of Alverine and Benfluorex as HNF4 $\alpha$ Activators

Seung-Hee Lee, Sonalee Athavankar, Tom Cohen, Ron Piran, Alice Kiselyuk, and Fred Levine

Sanford Children's Health Research Center, Sanford-Burnham Medical Research Institute, La Jolla, California, 92037 USA.

Lee et al Supplemental Table 1

CODE	MOLENAME	cas#
01500161	CARBINOXAMINE MALEATE	3505-38-2, 486-16-8
01500111	AMIKACIN SULFATE	39831-55-5, 37517-28-5
01500169	CETYLPYRIDINIUM CHLORIDE	6004-24-6, 123-03-5
01500133	AZATHIOPRINE	446-86-6
01500143	beta-CAROTENE	7235-40-7
01500187	CHLORTHALIDONE	77-36-1
01500165	CEFOTAXIME SODIUM	64485-93-4, 63527-52-6
01500180	CHLOROTHIAZIDE	58-94-6
01500188	CHLORZOXAZONE	95-25-0
01500146	BETHANECHOL CHLORIDE	590-63-6, 674-38-4
01500102	ACETAZOLAMIDE	59-66-5
01500112	AMILORIDE HYDROCHLORIDE	17440-83-4, 2016-88-8
01500122	AMPHOTERICIN B	1397-89-3
01500134	BACITRACIN	1405-87-4
01500144	BETAMETHASONE	378-44-9
01500158	CARBACHOL	51-83-2
01500166	CEPHALOTHIN SODIUM	58-71-9, 153-61-7
01500182	CHLOROXYLENOL	88-04-0
01500189	CICLOPIROX OLAMINE	41621-49-2
01500201	CLOXACILLIN SODIUM	7081-44-9, 642-78-4
01500103	ACETOHYDROXAMIC ACID	546-88-3
01500113	POTASSIUM p-AMINOBENZOATE	
01500123	AMPICILLIN SODIUM	69-52-3, 69-53-4 [ampicillin]
01500135	BACLOFEN	1134-47-0
01500198	CLONIDINE HYDROCHLORIDE	4205-91-8, 4205-90-7
01500159	CARBAMAZEPINE	298-46-4
01500167	CEPHAPIRIN SODIUM	24356-60-3, 21593-23-7
01500181	CHLOROTRIANISENE	569-57-3
01500190	CINOXACIN	28657-80-9
01500202	CLOXYQUIN	130-16-5
01500120	AMOXICILLIN	61336-70-7, 26787-78-0
01500114	6-AMINOCAPROIC ACID	60-32-2
01500124	AMPROLIUM	121-25-5
01500137	BENSERAZIDE HYDROCHLORIDE	322-35-0
01500147	BISACODYL	603-50-9
01500160	CARBENICILLIN DISODIUM	4800-94-6, 4697-36-3
01500105	ACETYLCYSTEINE	616-91-1
01500183	CHLORPHENIRAMINE (S) MALEATE	113-92-8, 132-22-9
01500191	CLEMASTINE	15686-51-8
01500205	COLCHICINE	64-86-8
01500107	ADENOSINE	58-61-7
01500115	AMINOGLUTETHIMIDE	125-84-8
01500101	ACETAMINOPHEN	103-90-2
01500138	BENZETHONIUM CHLORIDE	121-54-0
01500148	BITHIONOL	97-18-7
01500127	ANTHRALIN	480-22-8, 1143-38-0
01500173	CHLORAMPHENICOL HEMISUCCINATE	982-57-0, 56-75-7
01500184	CHLORPROMAZINE	50-53-3
01500192	CLIDINIUM BROMIDE	3485-62-9
01500206	COLISTIMETHATE SODIUM	8068-28-8, 21362-08-3

Lee et al Supplemental Table 1

01500208	COTININE	5695-98-7, 486-56-6 [cotinine]
01500116	SODIUM p-AMINOSALICYLATE	
01500128	ANTIPYRINE	60-80-0
01500139	BENZOCAINE	94-09-7
01500152	BUSULFAN	55-98-1
01500162	CARISOPRODOL	78-44-4
01500174	CHLORAMPHENICOL	56-75-7
01500185	CHLORPROPAMIDE	94-20-2
01500193	CLINDAMYCIN HYDROCHLORIDE	21462-39-5, 58207-19-5
01500108	ALLOPURINOL	315-30-0
01500109	ALVERINE CITRATE	5560-59-8, 150-59-4 [alverine]
01500117	AMITRIPTYLINE HYDROCHLORIDE	549-18-8, 50-48-6
01500129	APOMORPHINE HYDROCHLORIDE	41372-20-7, 314-19-2
01500141	BENZTHIAZIDE	91-33-8
01500155	CAFFEINE	58-08-2, 5743-12-4
01500163	CEFADROXIL	66592-87-8, 50370-12-2
01500178	CHLOROCRESOL	59-50-7
01500186	CHLORTETRACYCLINE HYDROCHLORIDE	64-72-2
01500195	CLOFIBRIC ACID	882-09-7
01500207	CORTISONE ACETATE	50-04-4, 53-06-5 [cortisone]
01500110	AMANTADINE HYDROCHLORIDE	665-66-7, 768-94-5
01500119	AMODIAQUINE DIHYDROCHLORIDE	6398-98-7, 69-44-3
01500131	ATROPINE	51-55-8, 5908-99-6 [atropine]
01500142	BENZTROPINE	132-17-2, 86-13-5
01500156	1R-CAMPHOR	464-49-3; 76-22-2
01500164	CEFAZOLIN SODIUM	27164-46-1, 25953-19-9
01500179	CHLOROQUINE DIPHOSPHATE	54-05-7
01500157	CAPREOMYCIN SULFATE	1405-37-4, 11003-38-6
01500196	CLOMIPHENE CITRATE	50-41-9, 911-45-5
01500209	CRESOL	1319-77-3
01500210	CROMOLYN SODIUM	15826-37-6, 16110-51-3
01500224	DEFEROXAMINE MESYLATE	138-14-7, 70-51-9
01500236	DIBUCAINE HYDROCHLORIDE	61-12-1, 85-79-0 [dibucaine]
01500249	DIHYDROSTREPTOMYCIN SULFATE	5490-27-7, 128-46-1
01500262	DISULFIRAM	97-77-8
01500282	ESTRADIOL	50-28-2
01500293	ETHOPROPAZINE HYDROCHLORIDE	1094-08-2, 522-00-9
01500311	FUSIDIC ACID	6990-06-3
01500323	GUANETHIDINE SULFATE	60-02-6, 55-65-2
01500333	HOMATROPINE METHYLBROMIDE	80-49-9, 87-00-3
01500211	CYCLIZINE	82-92-8
01500225	SODIUM DEHYDROCHOLATE	
01500237	DICLOFENAC SODIUM	15307-79-6
01500251	DIMENHYDRINATE	523-87-5
01500263	DOPAMINE HYDROCHLORIDE	62-31-7, 51-61-6 [dopamine]
01500283	ESTRADIOL CYPIONATE	313-06-4
01500296	EUGENOL	97-53-0
01500312	GALLAMINE	65-29-2, 153-76-4 [gallamine]
01500324	HALAZONE	80-13-7
01500334	HYDRALAZINE HYDROCHLORIDE	304-20-1, 86-54-4
01500212	CYCLOPENTOLATE HYDROCHLORIDE	5870-29-1, 512-15-2

Lee et al Supplemental Table 1

01500226	DEMECLOCYCLINE HYDROCHLORIDE	127-33-3
01500238	DICLOXACILLIN SODIUM	13412-64-1, 343-55-5
01500255	DIOXYBENZONE	131-53-3
01500268	DYCLONINE HYDROCHLORIDE	536-43-6, 586-60-7 [dyclonine]
01500284	ESTRADIOL VALERATE	979-32-8
01500299	FLUDROCORTISONE ACETATE	514-36-3, 127-31-1
01500313	GEMFIBROZIL	25812-30-0
01500325	HALOPERIDOL	52-86-8
01500335	HYDROCHLOROTHIAZIDE	58-93-5
01500213	CYCLOPHOSPHAMIDE HYDRATE	6055-19-2, 50-18-0
01500227	DESIPRAMINE HYDROCHLORIDE	58-28-6, 50-47-5 [desipramine]
01500239	DICUMAROL	66-76-2
01500256	DIPHENHYDRAMINE HYDROCHLORIDE	147-24-0
01500269	DYPHYLLINE	479-18-5
01500285	ESTRIOL	50-27-1, 514-68-1 [as,
01500303	FLUOCINONIDE	356-12-7
01500314	GENTAMICIN SULFATE	1405-41-0, 1403-66-3
01500327	HETACILLIN POTASSIUM	5321-32-4, 3511-16-8
01500338	HYDROCORTISONE ACETATE	50-03-3
01500215	CYCLOSERINE	68-41-7
01500231	DEXAMETHASONE ACETATE	55812-90-3, 1177-87-3
01500241	DIENESTROL	84-17-3, 13029-44-2 [//E,E//]
01500258	DIPHENYLPYRALINE HYDROCHLORIDE	132-18-3 147-20-6
01500270	TRISODIUM ETHYLENEDIAMINE TETRACETATE	
01500286	ESTRONE	53-16-7
01500305	FLUOROURACIL	51-21-8
01500315	GENTIAN VIOLET	548-62-9
01500328	HEXACHLOROPHENE	70-30-4
01500341	HYDROFLUMETHIAZIDE	135-09-1
01500217	CYTARABINE	147-94-4
01500232	DEXAMETHASONE SODIUM PHOSPHATE	2392-39-4, 312-93-6
01500242	DIETHYLCARBAMAZINE CITRATE	1642-54-2, 90-89-1
01500259	DIPYRIDAMOLE	58-32-2
01500272	EMETINE	316-42-7, 483-18-1 [emetine]
01500288	ETHAMBUTOL HYDROCHLORIDE	1070-11-7, 74-55-5
01500308	FLURBIPROFEN	5104-49-4
01500316	GLUCOSAMINE HYDROCHLORIDE	3416-24-8
01500330	HEXYLRESORCINOL	136-77-6
01500343	HYDROXYPROGESTERONE CAPROATE	630-56-8, 68-96-2
01500220	DANAZOL	17230-88-5
01500233	DEXTROMETHORPHAN HYDROBROMIDE	6700-34-1, 125-69-9
01500245	DIFLUNISAL	22494-42-4
01500260	PYRITHIONE ZINC	13463-41-7
01500274	ADRENALINE BITARTRATE	
01500291	ETHINYL ESTRADIOL	57-63-6
01500309	FURAZOLIDONE	67-45-8
01500321	GUAIFENESIN	93-14-1
01500331	HISTAMINE DIHYDROCHLORIDE	51-45-6 [histamine]
01500344	HYDROXYUREA	127-07-1
01500222	DAPSONE	80-08-0
01500235	DIBENZOTHIOPHENE	132-65-0

Lee et al Supplemental Table 1

01500247	DIGOXIN	20830-75-5
01500261	DISOPYRAMIDE PHOSPHATE	3737-09-5
01500277	ERGONOVINE MALEATE	129-51-1, 60-79-7 [ergonovine]
01500292	ETHIONAMIDE	536-33-4
01500310	FUROSEMIDE	54-31-9
01500322	GUANABENZ ACETATE	23256-50-0
01500332	HOMATROPINE BROMIDE	51-56-9, 87-00-3
01500345	HYDROXYZINE PAMOATE	10246-75-0, 68-88-2
01500246	DIGITOXIN	71-63-6
01500355	ISONIAZID	54-85-3
01500365	LEVONORDEFIN	829-74-3, 18829-78-2
01500379	MEDROXYPROGESTERONE ACETATE	71-58-9, 520-85-4
01500397	METHOCARBAMOL	532-03-6
01500413	MICONAZOLE NITRATE	22832-87-7, 22916-47-8
01500428	NEOSTIGMINE BROMIDE	114-80-7, 59-99-4
01500439	NORETHYNODREL	68-23-5
01500447	ORPHENADRINE CITRATE	4682-36-4, 83-98-7
01500464	PENICILLAMINE	52-67-5
01500346	HYOSCYAMINE	101-31-5
01500356	ISOPROPAMIDE IODIDE	71-81-8, 7492-32-2
01500368	LINCOMYCIN HYDROCHLORIDE	7179-49-9, 859-18-7
01500380	MEDRYSONE	2668-66-8
01500398	METHOTREXATE	59-05-2
01500415	MINOXIDIL	38304-91-5
01500430	NIACIN	59-67-6
01500440	NORFLOXACIN	70458-96-7
01500448	OXACILLIN SODIUM	7240-38-2, 1173-88-2
01500465	BENZYL PENICILLIN POTASSIUM	69-57-8, 61-33-6 [penicillin, G]
01500347	IBUPROFEN	15687-27-1, 58560-75-1 [(+/-)]
01500357	ISOPROTERENOL HYDROCHLORIDE	51-30-9, 7683-59-2
01500372	MAFENIDE HYDROCHLORIDE	138-39-6
01500381	MEGESTROL ACETATE	595-33-5, 3562-63-8
01500400	METHOXSALEN	298-81-7
01500418	MOXALACTAM DISODIUM	8031-09-2
01500431	NIFEDIPINE	21829-25-4
01500441	NORGESTREL	6533-00-2
01500451	OXYBENZONE	131-57-7
01500473	PHENAZOPYRIDINE HYDROCHLORIDE	136-40-3, 94-78-0
01500348	IMIPRAMINE HYDROCHLORIDE	113-52-0, 50-49-7 [imipramine]
01500358	ISOSORBIDE DINITRATE	87-33-2
01500373	MAPROTILINE HYDROCHLORIDE	10347-81-6, 10262-69-8
01500383	MEPENZOLATE BROMIDE	76-90-4, 25990-43-6
01500401	METHSCOPOLAMINE BROMIDE	155-41-9
01500420	NAFCILLIN SODIUM	7177-50-6, 985-16-0
01500433	NITROFURANTOIN	67-20-9, 54-87-5
01500442	NORTRIPTYLINE	894-71-3, 72-69-5
01500453	OXYMETAZOLINE HYDROCHLORIDE	2315-02-8, 1491-59-4
01500476	PHENELZINE SULFATE	156-51-4, 51-71-8 [phenelzine]
01500349	INDAPAMIDE	26807-65-8
01500359	ISOXSUPRINE HYDROCHLORIDE	579-56-6, 395-28-8
01500374	MECAMYLAMINE HYDROCHLORIDE	826-39-1, 60-40-2

Lee et al Supplemental Table 1

01500387	MERCAPTOPYRINE	6112-76-1, 50-44-2
01500403	METHYLDOPA	41372-08-1, 555-30-6
01500422	NALOXONE HYDROCHLORIDE	357-08-4, 51481-60-8
01500434	NITROFURAZONE	59-87-0
01500443	NOSCAPINE HYDROCHLORIDE	912-60-7, 128-62-1
01500456	OXYQUINOLINE HEMISULFATE	148-24-3
01500477	PHENINDIONE	83-12-5
01500350	INDOMETHACIN	53-86-1
01500360	KANAMYCIN SULFATE	25389-94-0, 133-92-6
01500375	MECHLORETHAMINE	55-86-7, 51-75-2
01500390	METAPROTERENOL	586-06-1, 5874-97-5
01500410	METOCLOPRAMIDE HYDROCHLORIDE	54143-57-6, 7232-21-5
01500424	NAPHAZOLINE HYDROCHLORIDE	550-99-2, 835-31-4
01500435	NITROMIDE	121-81-3
01500444	NOVOBIOCIN SODIUM	1476-53-5, 303-81-1
01500457	OXYTETRACYCLINE	6153-64-6, 79-57-2
01500484	1S,2R-PHENYLPROPANOLAMINE HYDROCHLORIDE	
01500351	INDOPROFEN	31842-01-0
01500362	KETOCONAZOLE	65277-42-1
01500376	MECLIZINE HYDROCHLORIDE	31884-77-2, 1104-22-9
01500394	METHENAMINE	100-97-0
01500411	METOPROLOL TARTRATE	56392-17-7, 37350-58-6
01500425	NAPROXEN(+)	
01500436	NOREPINEPHRINE	69815-49-2, 51-40-1
01500445	NYLIDRIN HYDROCHLORIDE	1400-61-9
01500459	PAPAVERINE HYDROCHLORIDE	61-25-6, 58-74-2 [papaverine]
01500485	PHENYTOIN SODIUM	630-93-3, 57-41-0 [phenytoin]
01500353	IDOQUINOL	83-73-8
01500364	LEUCOVORIN CALCIUM	
01500377	SODIUM MECLOFENAMATE	
01500396	METHIMAZOLE	60-56-0
01500412	METRONIDAZOLE	443-48-1, 69198-10-3
01500427	NEOMYCIN SULFATE	1405-10-3, 1404-04-2
01500438	NORETHINDRONE ACETATE	51-98-9
01500446	NYSTATIN	114-90-9
01500460	PARACHLOROPHENOL	106-48-9
01500486	PHYSOSTIGMINE SALICYLATE	57-64-7, 57-47-6
01500487	PILOCARPINE NITRATE	148-72-1, 92-13-7 [pilocarpine]
01500514	PROPRANOLOL HYDROCHLORIDE (-)	318-98-9, 525-66-6
01500529	RIFAMPIN	13292-46-1
01500543	STREPTOZOSIN	18883-66-4
01500553	SULFATHIAZOLE	72-14-0
01500581	TOLBUTAMIDE	64-77-7
01500591	TRIFLUOPERAZINE HYDROCHLORIDE	440-17-5, 117-89-5
01500600	TRYPTOPHAN	73-22-3 ['L']
01500618	ACRIFLAVINIUM HYDROCHLORIDE	
01500641	PENTAMIDINE ISETHIONATE	100-33-4
01500490	PIPERAZINE	110-85-0, 144-29-6
01500516	PSEUDOEPHEDRINE HYDROCHLORIDE	345-78-8, 90-82-4
01500530	ROXARSONE	121-19-7
01500545	SULFACETAMIDE	144-80-9, 127-56-0

Lee et al Supplemental Table 1

01500556	SULINDAC	38194-50-2
01500583	TOLNAFTATE	2398-96-1
01500592	TRIHEXYPHENIDYL HYDROCHLORIDE	
01500601	TUAMINOHEPTANE SULFATE	6411-75-2, 123-82-0
01500623	BROXYQUINOLINE	521-74-4
01500642	PHENACETIN	62-44-2
01500494	PRAZIQUANTEL	55268-74-1
01500517	PYRANTEL PAMOATE	22204-24-6, 15686-83-6
01500531	SALICYL ALCOHOL	90-01-7
01500546	SULFADIAZINE	68-35-9
01500566	TETRACYCLINE HYDROCHLORIDE	64-75-5, 60-54-8 [tetracycline]
01500584	TRANLYCYPROMINE SULFATE	13492-01-8, 7081-36-9
01500593	TRIMEPRAZINE TARTRATE	4330-99-8, 41375-66-0
01500603	TYROTHRIN	1404-88-2
01500624	CARNITINE HYDROCHLORIDE	461-06-3
01500644	PHENYLMERCURIC ACETATE	62-38-4
01500500	PRIMAQUINE DIPHOSPHATE	63-45-6, 90-34-6 [primaquine]
01500520	PYRIMETHAMINE	58-14-0
01500534	SCOPOLAMINE HYDROBROMIDE	6533-68-2, 114-49-8
01500547	SULFAMERAZINE	127-79-7
01500568	THEOPHYLLINE	5967-84-0, 58-55-9
01500585	TRACETIN	102-76-1
01500594	TRIMETHOBENZAMIDE HYDROCHLORIDE	554-92-7, 138-56-7
01500605	URSODIOL	128-13-2
01500632	HEXESTROL	5635-50-7
01500645	PREGNENOLONE	145-13-1, 4598-67-8
01500505	PROCHLORPERAZINE EDISYLATE	1257-78-9, 84-02-6
01500522	QUINACRINE HYDROCHLORIDE	6151-30-0, 69-05-6
01500536	SISOMICIN SULFATE	53179-09-2, 32385-11-8
01500548	SULFAMETHAZINE	57-68-1
01500570	THIABENDAZOLE	148-79-8
01500587	TRIAMCINOLONE ACETONIDE	76-25-5
01500595	TRIMETHOPRIM	738-70-5
01500607	VANCOMYCIN HYDROCHLORIDE	1404-93-9, 1404-90-6
01500633	HEXETIDINE	141-94-6
01500648	AZELAIC ACID	123-99-9
01500509	PROMAZINE HYDROCHLORIDE	53-60-1, 58-40-2 [promazine]
01500523	QUINIDINE GLUCONATE	7054-25-3, 6591-63-5
01500538	SPECTINOMYCIN HYDROCHLORIDE	22189-32-8, 21736-83-4
01500550	SULFAMETHOXAZOLE	723-46-6
01500572	THIMEROSAL	54-64-8
01500588	TRIAMCINOLONE DIACETATE	67-78-7
01500596	TRIOXSALEN	3902-71-4
01500609	VIDARABINE	24356-66-9, 5536-17-4
01500634	IPRONIAZID SULFATE	54-92-2, 305-33-9 [as
01500649	THEOBROMINE	83-67-0
01500510	PROMETHAZINE HYDROCHLORIDE	58-33-3, 60-87-7
01500524	QUININE SULFATE	6119-70-6, 804-63-7
01500539	SPIRONOLACTONE	52-01-7
01500551	SULFAPYRIDINE	144-83-2
01500573	THIOGUANINE	154-42-7, 5580-03-0

Lee et al Supplemental Table 1

01500589	TRIAMTERENE	396-01-0
01500598	TRIPROLIDINE HYDROCHLORIDE	6138-79-0, 550-70-9
01500614	XYLOMETAZOLINE HYDROCHLORIDE	1218-35-5, 526-36-3
01500637	MERBROMIN	129-16-8
01500656	AJMALINE	4360-17-7
01500511	PROPANTHELINE BROMIDE	50-34-0, 298-50-0
01500527	RESORCINOL	108-46-3
01500541	STREPTOMYCIN SULFATE	3810-74-0, 57-92-1
01500552	SULFASALAZINE	599-79-1
01500578	TIMOLOL MALEATE	26921-17-5, 91524-16-2
01500590	TRICHLORMETHIAZIDE	133-67-5
01500599	TROPICAMIDE	1508-75-4
01500615	ZOMEPIRAC SODIUM	64092-49-5, 64092-48-4
01500639	OCTOPAMINE HYDROCHLORIDE	104-14-3
01500657	HYDROQUINIDINE	
01500668	KETOTIFEN FUMARATE	34580-14-8, 34580-13-7
01500674	MYCOPHENOLIC ACID	24280-93-1
01500688	KYNURENIC ACID	
01500750	NEOHESPERIDIN DIHYDROCHALCONE	
01500764	KINETIN	525-79-1
01500804	ALTHIAZIDE	5588-16-9
01500872	PALMATINE CHLORIDE	10605-02-4
01501004	DROPROPIZINE	17692-31-8
01501019	BERBAMINE HYDROCHLORIDE	478-61-5 (berbamine)
01501111	PROTOPORPHYRIN IX	
01500663	YOHIMBINE HYDROCHLORIDE	
01500675	OLEANDOMYCIN PHOSPHATE	
01500689	LIDOCAINE HYDROCHLORIDE	6108-05-0, 73-78-9
01500752	QUERCITRIN	522-12-3
01500765	NARINGIN	10236-47-2
01500811	BERBERINE CHLORIDE	633-65-8, 2086-83-1
01500873	PIPERINE	94-62-2
01501005	ETODOLAC	41340-25-4
01501026	FENDILINE HYDROCHLORIDE	
01501115	NALBUPHINE HYDROCHLORIDE	23277-43-2, 20594-83-6
01500669	BENFLUOREX HYDROCHLORIDE	23602-78-0
01500676	OUABAIN	11018-89-6, 630-60-4
01500695	ACETYL TYROSINE ETHYL ESTER	
01500753	ESERINE	57-47-6
01500767	BUTAMBEN	94-25-7
01500828	CANRENOIC ACID, POTASSIUM SALT	2181-04-6, 4138-96-9
01500901	AESCULIN	531-75-9
01501007	FENOTEROL HYDROBROMIDE	13392-18-2
01501104	METHACYCLINE HYDROCHLORIDE	3963-95-9, 914-00-1
01501116	MEBHYDROLIN NAPHTHALENESULFONATE	524-81-2
01500646	SULFANILAMIDE	63-74-1
01500679	AMINOPTERIN	54-62-6, 58602-66-7
01500699	ACETYLTRYPTOPHANAMIDE	
01500754	XANTHURENIC ACID	
01500771	CEFACLOR	70356-03-5, 53994-73-3
01500865	HARMALOL HYDROCHLORIDE	6028-07-5



Lee et al Supplemental Table 1

01500938	PROTOVERATRINE B	124-97-0
01501008	FENBUFEN	36330-85-5
01501105	PUROMYCIN HYDROCHLORIDE	58-58-2, 53-79-2 [puromycin]
01501117	MEBEVERINE HYDROCHLORIDE	2753-45-9, 3625-06-7
01500651	STRYCHNINE	57-24-9
01500680	ARECOLINE HYDROBROMIDE	300-08-3, 63-75-2 [arecoline]
01500704	N-ACETYLPROLINE	
01500758	LOBELINE HYDROCHLORIDE	90-69-7
01500772	IODIPAMIDE	606-17-7, 2618-26-0
01500864	HARMALINE	304-21-2
01500989	1 $\alpha$ -GLYCYRRHETINIC ACID	
01501009	1R,9S-HYDRASTINE	
01501107	PICROTOXININ	17617-45-7
01501118	MECLOCYCLINE SULFOSALICYLATE	73816-42-9, 2013-58-3
01500672	QUERCETIN	117-39-5
01500682	CAPTOPRIL	62571-86-2
01500707	CITROPTEN	
01500760	HECOGENIN	
01500774	THYROXINE	51-48-9
01500867	HARMINE	442-51-3
01500992	FLUMEQUINE	42835-25-6
01501010	FENOFIBRATE	49562-28-9
01501108	MEFEXAMIDE	1227-61-8
01501119	PROGLUMIDE	6620-60-6
01500606	VALPROATE SODIUM	1069-66-5, 99-66-1 [valproic
01500684	CIMETIDINE	51481-61-9
01500709	CHRYSIN	480-40-0
01500763	CALCEIN	
01500802	ALLOXAN	2244-11-3
01500869	MIMOSINE	
01500994	FLUFENAZINE HYDROCHLORIDE	
01501011	FENOPROFEN	31879-05-7
01501109	PROBUCOL	23288-49-5
01501120	MINAPRINE HYDROCHLORIDE	25953-17-7, 25905-77-5
01500673	MOLSIDOMINE	25717-80-0
01500685	CLOZAPINE	5786-21-0
01500746	NARINGENIN	480-41-1
01500761	GUANIDINE CARBONATE	
01500801	ALLANTOIN	97-59-6
01500871	NORHARMAN	244-63-3
01501003	FAMOTIDINE	76824-35-6
01501016	FENBENDAZOLE	43210-67-9
01501110	MEBENDAZOLE	31431-39-7
01501121	MEMANTINE HYDROCHLORIDE	19982-08-2
01501125	3-AMINOPROPANESULPHONIC ACID	
01501137	NEFOPAM	23327-57-3, 13669-70-0
01501157	SUXIBUZONE	27470-51-5
01501183	ESTRADIOL METHYL ETHER	1035-77-4
01501203	RETINOL	68-26-8
01502012	FOSFOSAL	6064-83-1
01502033	CEFUROXIME SODIUM	56238-63-2

Lee et al Supplemental Table 1

01502046	BEZAFIBRATE	41859-67-0
01502085	CYCLOCREATINE	
01502116	1,2-DIMETHYLHYDRAZINE HYDROCHLORIDE	
01501126	5-AMINOPENTANOIC ACID HYDROCHLORIDE	
01501138	PIRENZEPINE HYDROCHLORIDE	29868-97-1, 28797-61-7
01501161	SUPROFEN	40828-46-4
01501184	ESTRADIOL ACETATE	
01501204	LAPACHOL	84-79-7
01502014	MESNA	19767-45-4, 3375-50-6 [2-
01502034	METAMPICILLIN SODIUM	6489-97-0
01502047	LIOTHYRONINE SODIUM	55-06-1, 6893-02-3
01502095	alpha-CYANO-3-HYDROXYCINNAMIC ACID	
01502117	ATRACTYLOSIDE POTASSIUM	
01501127	ATENOLOL	29122-68-7
01501139	PRAMOXINE HYDROCHLORIDE	637-58-1, 140-65-8
01501170	ACETAMINOSALOL	118-57-0
01501189	5-FLUORO-5'-DEOXYURIDINE	
01501215	KETOPROFEN	22071-15-4
01502016	TRETINON	302-79-4
01502037	LOMEFLOXACIN HYDROCHLORIDE	98079-52-8, 98079-51-7
01502050	CEPHALORIDINE	50-59-9
01502101	PERILLIC ACID (-)	7694-45-3
01502126	GUVACINE HYDROCHLORIDE	
01501129	CARBETAPENTANE CITRATE	23142-01-0, 77-23-6
01501140	MEPHENESIN	59-47-2
01501173	ACETANILIDE	103-84-4
01501191	ESTRIOL BENZYL ETHER	
01501217	LISINOPRIL	83915-83-7, 76547-98-3
01502018	BRETYLIUM TOSYLATE	61-75-6, 59-41-6 [bretylum]
01502039	FOSFOMYCIN	26472-47-9, 23112-90-5(acid)
01502057	5-CHLOROINDOLE-2-CARBOXYLIC ACID	
01502102	QUINOLINIC ACID	
01502127	TINIDAZOLE	19387-91-8
01501130	AMINOPYRIDINE	
01501143	SULFAPHENAZOLE	526-08-9
01501174	TODRALAZINE HYDROCHLORIDE	14679-73-3
01501192	ESTRADIOL-3-SULFATE, SODIUM SALT	
01502001	ACETYL-L-LEUCINE	99-15-0
01502019	FOSCARNET SODIUM	63585-09-1
01502041	CEFAMANDOLE NAFATE	42540-40-9, 34444-01-4
01502059	7-CHLOROKYNURENIC ACID	
01502103	ANTHRAQUINONE	
01502128	CYCLOLEUCINE	
01501132	NEROL	
01501151	RANITIDINE	66357-35-5
01501178	ESTRIOL METHYL ETHER	1474-53-9
01501198	TOLFENAMIC ACID	13710-19-5
01502004	BUMETANIDE	28395-03-1
01502020	FOLIC ACID	59-30-3
01502043	PRALIDOXIME MESYLATE	154-97-2
01502074	4-NAPHTHALIMIDOBUTYRIC ACID	

Lee et al Supplemental Table 1

01502106	CARBOPLATIN	41575-94-4
01502130	AMINOCYCLOPROPANECARBOXYLIC ACID	
01501133	NICERGOLINE	27848-84-6
01501153	SULOCTIDIL	54063-56-8
01501179	ESTRADIOL PROPIONATE	113-38-2
01501199	ZAPRINAST	37762-06-4
01502005	CARBENOXOLONE SODIUM	7421-40-1, 5697-56-3
01502026	TRANEXAMIC ACID	1197-18-8
01502044	OFLOXACIN	82419-36-1
01502082	INDOLE-2-CARBOXYLIC ACID	1477-50-5
01502111	5-AZACYTIDINE	
01502153	5-NITRO-2-PHENYLPROPYLAMINO BENZOIC ACID [NPPB]	
01501134	PIMOZIDE	2062-78-4
01501154	RONIDAZOLE	7681-76-7
01501181	ESTRONE ACETATE	
01501202	GALANTHAMINE HYDROBROMIDE	357-70-0, 1953-04-4
01502006	CARPROFEN	53716-49-7
01502031	CEFOXITIN SODIUM	66309-69-1, 61622-34-2
01502045	PIROMIDIC ACID	19562-30-2
01502083	N- (9-FLUORENYLMETHOXYCARBONYL)-L-LEUCINE	35661-60-0
01502113	AZASERINE	115-02-6
01502173	N-FORMYLMETHIONYL-LEUCYLPHENYLALANINE	
01502175	N-FORMYLMETHIONYLPHENYLALANINE	
01502198	ANISINDIONE	117-37-3
01502214	LYSYLPHENYLALANYLTYSOSINE	
01502236	ABRINE (L)	
01502258	MONENSIN SODIUM (monensin A is shown)	22373-78-0, 17090-79-8
01503045	ACEXAMIC ACID	57-08-9
01503080	AMBROXOL HYDROCHLORIDE	23828-92-4, 18683-91-5
01503127	DEQUALINIUM CHLORIDE	522-51-0, 6707-58-0
01503240	PYRIDOSTIGMINE BROMIDE	101-26-8, 155-97-5
01503234	BETA-PROPIOLACTONE	
01502177	METHIONYL-LEUCYLPHENYLALANINE ACETATE	
01502202	CYCLOSPORINE	59865-13-3
01502215	S-METHYL-L-THIOCTRULLINE ACETATE	156719-41-4
01502237	HARMOL HYDROCHLORIDE	40580-83-4
01502259	MORIN	480-16-0
01503059	FLOXURIDINE	50-91-9
01503092	GLUCONOLACTONE	90-80-2
01503134	MENTHOL(-)	1490-04-6
01503242	ISOXICAM	34552-84-6
01503228	PAROMOMYCIN SULFATE	1263-89-4, 7542-37-2
01502178	LEUCINE ENKEPHALIN	
01502203	TROLEANDOMYCIN	2751-09-9
01502216	S-(1,2-DICARBOXYETHYL)GLUTATHIONE	1115-52-2
01502239	EBURNAMONINE	
01503006	BENZYL ISOTHIOCYANATE	
01503065	ALTRETAMINE	645-05-6
01503094	THIOXOLONE	
01503136	THIAMPHENICOL	15318-45-3
01503243	LABETALOL HYDROCHLORIDE	32780-64-6, 36894-69-6

Lee et al Supplemental Table 1

01503245	LEVAMISOLE HYDROCHLORIDE	16595-80-5, 14769-73-4
01502186	LYSYL-TYROSYL-LYSINE ACETATE	
01502207	L-LEUCYL-L-ALANINE	7298-84-2
01502217	N-HISTIDYL-2-AMINONAPHTHALENE (betaNA)	7424-15-9
01502243	RHAPONTIN	155-58-8
01503009	BIOTIN	58-85-5
01503069	AMINOHIPPURIC ACID	61-78-9, 94-16-6
01503102	BACAMPICILLIN HYDROCHLORIDE	37661-08-8, 50972-17-3
01503142	TENOXICAM	59804-37-4
01503230	NIFENAZONE	2139-47-1
01503254	6alpha-METHYLPREDNISOLONE ACETATE	
01502193	N-ACETYLASPARTYLGLUTAMIC ACID	3106-85-2
01502208	Tfa-VAL-TYR-VAL-OH	64577-63-5
01502219	1-BENZYLOXYCARBONYLAMINOPHENETHYL	26049-94-5
01502245	ELLAGIC ACID	
01503036	DINITOLMIDE	
01503070	MEFLOQUINE	53230-10-7
01503106	BEPRIDIL HYDROCHLORIDE	74764-40-2
01503200	CETRIMONIUM BROMIDE	57-09-0, 6899-10-1
01503237	HALCINONIDE	3093-35-4
01503273	HYDROCORTISONE BUTYRATE	13609-67-1
01502194	Ng-METHYL-L-ARGININE ACETATE	
01502209	PHENETHYL CAFFEATE (CAPE)	104594-70-9
01502221	PHENYLALANYLTYROSINE	17355-18-9
01502248	GLUTATHIONE	70-18-8
01503038	NICOTINYL TARTRATE	100-55-0
01503073	ADIPHENINE HYDROCHLORIDE	50-42-0, 64-95-9 [adiphenine]
01503110	CARMUSTINE	154-93-8
01503202	CHLOROXINE	773-76-2
01503239	HYCANTHONE	3105-97-3
01503278	MITOXANTHRONE HYDROCHLORIDE	70476-82-3, 65271-80-9
01502195	PIRACETAM	7491-74-9
01502210	VALYLTRYPTOPHAN	24587-37-9
01502223	RESVERATROL	
01502252	MONOCROTALINE	
01503041	AMINOHYDROXYBUTYRIC ACID	
01503074	ALEXIDINE HYDROCHLORIDE	22573-93-9, 22782-69-0
01503111	CEFTRIAZONE SODIUM	73384-59-5 [ceftriazone],
01503206	CLOFOCTOL	37693-01-9
01503231	NIMESULIDE	51803-78-2
01503304	URETHANE	
01502197	PIPERIDOLATE HYDROCHLORIDE	129-77-1, 82-98-4
01502212	GLYCYLLEUCYLPHENYLALANINE	
01502232	CAMPTOTHECIN	7689-03-4
01502255	SALICIN	138-52-3
01503042	ARTEMISININ	63968-64-9
01503076	QUINAPRIL HYDROCHLORIDE	82586-55-8, 85441-61-8
01503121	TRAZODONE HYDROCHLORIDE	25332-39-2, 19794-93-5
01503244	LASALOCID SODIUM	25999-31-9
01503250	MEPHENTERMINE SULFATE	1212-72-2, 6190-60-9
01503324	THIOTEPA	52-24-4

Lee et al Supplemental Table 1

01503341	CHLOROACETOXYQUINOLINE	
01503600	NIMODIPINE	66085-59-4
01503631	3,5-DINITROCATÉCHOL (OR-486)	
01503676	ESTRONE HEMISUCCINATE	
01503902	SODIUM beta-NICOTINAMIDE ADENINE DINUCLEOTIDE	
01503935	PROPAFENONE HYDROCHLORIDE	34183-22-7, 54063-53-5
01503994	CONVALLATOXIN	508-75-8
01504070	PHYSCION	521-61-9
01504145	GLICLAZIDE	21187-98-4
01504181	PRISTIMERIN	1258-84-0
01503403	EXALAMIDE	53370-90-4
01503602	SALINOMYCIN, SODIUM	53003-10-4
01503633	N- (3-TRIFLUOROMETHYLPHENYL)PIPERAZINE	
01503679	AZITHROMYCIN	83905-01-5, 117772-70-0
01503908	PACLITAXEL	33069-62-4
01503936	PERICIAZINE	2622-26-6
01504002	BAICALEIN	491-67-8
01504078	SENNOSIDE A	
01504135	TRIMEDLURE	
01504185	TETRANDRINE	518-34-3
01503412	ETANIDAZOLE	22668-01-5
01503603	ACYCLOVIR	59277-89-3
01503635	3-METHYL-1-PHENYL-2-PYRAZOLIN-5-ONE (MCI-186)	
01503802	AZADIRACHTIN	11141-17-6
01503914	BUTACAINE	149-15-5, 149-16-6 [butacaine]
01503940	SPERMIDINE TRIHYDROCHLORIDE	
01504019	GOSSYPOL	303-45-7
01504098	PHENOTHRIN	26002-80-2
01504150	MELOXICAM	71125-38-7
01504200	ISOLIQUIRITIGENIN	961-29-5
01503416	MIZORIBINE	50924-49-7
01503609	NITRENDIPINE	84845-75-0
01503637	METHIOTHEPIN MALEATE	
01503815	CEVADINE	62-59-9
01503922	TRYPTAMINE	
01503977	LOVASTATIN	75330-75-5
01504021	LUPININE	
01504099	SILDENAFIL	139755-83-2
01504151	NIMUSTINE	42471-28-3
01504205	DELTALINE	
01503419	NAFRONYL OXALATE	3200-06-4, 31329-57-4
01503614	CIPROFLOXACIN	85721-33-1
01503639	RAUWOLSCINE HYDROCHLORIDE	
01503710	CLOPIDOGREL SULFATE	113665-84-2
01503923	IOPANIC ACID	96-83-3
01503970	METHOXYAMINE HYDROCHLORIDE	
01504025	SALSOLINE	
01504101	TETRACHLOROISOPHTHALONITRILE	
01504154	PINOCEMBRIN	36052-37-6
01504206	BOVINOCIDIN (3-nitropropionic acid)	
01503422	SEMUSTINE	13909-09-6

Lee et al Supplemental Table 1

01503620	SAFROLE	94-59-7
01503641	1-PHENYLBIGUANIDE HYDROCHLORIDE	
01503712	LORATADINE	79794-75-5
01503926	LANSOPRAZOLE	103577-45-3
01503982	AGMATINE SULFATE	2482-00-0
01504027	CYTISINE	
01504104	DIHYDROJASMONIC ACID	98674-52-3
01504171	VENLAFAXINE	99300-78-4, 93413-69-5
01504210	ATOVAQUONE	95233-18-4
01503423	SPIRAMYCIN	8025-81-8
01503626	OXOTREMORINE SESQUIFUMARATE	
01503662	VERATRIDINE	71-62-5
01503720	SELAMECTIN	165108-07-6
01503932	OXYPHENCYCLIMINE HYDROCHLORIDE	125-52-0, 125-53-1
01503973	2-THIOURACIL	
01504060	EMODIC ACID	
01504105	TANNIC ACID	1401-55-4
01504174	BUPROPION	31677-93-7, 34911-55-2
01504211	CHLORGUANIDE HYDROCHLORIDE	
01503500	RESORCINOL MONOACETATE	102-29-4
01503627	N-AMINOHEXYL-5-CHLORO-1-NAPHTHALENESULFONAMIDE	
01503678	CELECOXIB	
01503722	ATORVASTATIN CALCIUM	134523-03-8, 134523-00-5
01503933	PENTOLINIUM TARTRATE	52-62-0, 144-44-5
01503991	CLEBOPRIDE MALEATE	55905-53-8
01504081	BETULINIC ACID	472-15-1
01504116	FORMESTANE	566-48-3
01504178	TETRAHYDROPALMATINE	3520-14-7
01504212	CHLORANIL	118-75-2
01504213	N-ACETYLASPARTIC ACID	
01504232	2,3-DIHYDROXY-6,7-DICHLOROQUINOXALINE	
01504260	LEVOFLOXACIN	138199-71-0
01504303	MOXIFLOXACIN HYDROCHLORIDE	
01505204	ALMOTRIPTAN	154323-57-6
01505213	ROSUVASTATIN	
01505245	TROXERUTIN	7085-55-4
01505255	HUPERZINE A	102518-79-6
01505271	CROTAMITON	483-63-6
01505299	AMITRAZ	33089-61-1
01504215	N,N-HEXAMETHYLENEAMILORIDE	
01504235	ROFECOXIB	
01504261	CANDESARTAN CILEXTIL	139481-59-7
01504401	PIOGLITAZONE HYDROCHLORIDE	111025-46-8 (pioglitazone)
01505205	OLMESARTAN MEDOXOMIL	
01505215	TEGASEROD MALEATE	
01505247	GINKGOLIC ACID	22910-60-7
01505256	SILYBIN	22888-70-6
01505272	BENZANTHRONE	82-05-3
01505300	PURPURIN	81-54-9
01504216	ZOXAZOLAMINE	61-80-3
01504237	HYDROQUINONE	123-31-9

Lee et al Supplemental Table 1

01504263	ROSIGLITAZONE	122320-73-4
01504410	PICROPODOPHYLLOTOXIN	477-47-4
01505207	CEFTIBUTEN	97519-39-6
01505222	DERACOXIB	169590-41-4
01505248	CANRENONE	976-71-6
01505257	ICARIIN	489-32-7
01505281	ZOLMITRIPTAN	
01505302	GENETICIN	108321-42-2, 49863-47-
01504218	ACRISORCIN	7527-91-5
01504243	OXCARBAZEPINE	28721-07-5
01504268	LOSARTAN	124750-99-8, 114798-26-4
01504910	DIHYDROJASMONIC ACID, METHYL ESTER	24851-98-7
01505208	CEFDINIR	91832-40-5
01505230	CILOSTAZOL	73963-72-1
01505249	APRAMYCIN	37321-09-8
01505262	SERTRALINE HYDROCHLORIDE	79559-97-0; 79617-96-2(base)
01505293	DIALLYL SULFIDE	592-88-1
01505304	SECNIDAZOLE	3366-95-8
01504221	PHENYLBUTYRATE SODIUM	90-27-7 (phenylbutyric acid)
01504244	BETAMIPRON	3440-28-6
01504272	GATIFLOXACIN	160738-57-8
01505200	BENZAEPRILOL HYDROCHLORIDE	86541-74-4
01505209	VALSARTAN SODIUM	137862-53-4 (valsartan)
01505234	AVOCADYNE	34524-38-4
01505250	MADECASSIC ACID	18449-41-7
01505263	ALFLUZOCIN	
01505294	CARBADOX	6804-07-5
01505305	PEFLOXACINE MESYLATE	149676-40-4
01504228	CRUSTECDYSONE	5289-74-7
01504257	CARVEDILOL TARTRATE	72956-09-3 (carvedilol)
01504273	MIGLITOL	72432-03-2
01505201	FAMCICLOVIR	104227-87-4
01505210	SIBUTRAMINE HYDROCHLORIDE	84485-00-7; 106650-56-0
01505235	AVOCADYNONE ACETATE	24607-10-1
01505251	IMIDACLOPRID	13826-41-3
01505264	TRANDOLAPRIL	87679-37-6
01505296	OXFENDAZOLE	53716-50-0
01505306	ASPARTAME	22839-47-0
01504229	METAXALONE	1665-48-1
01504258	NATEGLINIDE	105816-04-4
01504300	ORLISTAT	96829-58-2
01505202	AMLODIPINE BESYLATE	111470-99-6
01505211	TORSEMIDE	56211-40-6
01505241	SPARTEINE HYDROIODIDE	
01505252	PALMATINE	3486-67-7
01505265	TELITHROMYCIN	
01505297	PERILLYL ALCOHOL	536-59-4, 18457-55-1
01505307	TRIADIMEFON	43121-43-3
01504231	CLARITHROMYCIN	81103-11-9
01504259	IRBESARTAN	138402-11-6
01504302	VALDECOXIB	181695-72-7

Lee et al Supplemental Table 1

01505203	EZETIMIBE	
01505212	PERINDOPRIL ERBUMINE	107133-36-8; 82834-16-0
01505244	CITICOLINE	987-78-0
01505253	SINOMENINE	115-53-7
01505267	OXAPROZIN	21256-18-8
01505298	3-ISOBUTYL-1-METHYLXANTHINE (IBMX)	28822-58-4
01505308	CHLOROPHYLLIDE Cu COMPLEX Na SALT	15611-43-5
01505309	BIFONAZOLE	60628-96-8
01505320	INDOLE-3-CARBINOL	700-06-1
01505331	3,3'-DIINDOLYLMETHANE	1968-05-4
01505342	7-NITROINDAZOLE	2942-42-9
01505803	PRAVASTATIN SODIUM	
01505276	CAPSANTHIN	465-42-9
02300094	ASTEMIZOLE	68844-77-9
02300229	GLYBURIDE	10238-21-8
00300038	JUGLONE	481-39-0
00300610	ACETOSYRINGONE	
01505311	DIBENZOYLMETHANE	120-46-7
01505321	RIFAXIMIN	80621-81-4
01505332	AZAPERONE	1649-18-9
01505347	RIBOFLAVIN	83-88-5
01505810	PEONIFLORIN	23180-57-6
01800067	COLCHICEINE	477-27-0
02300147	N-ACETYLNEURAMIC ACID	
02300259	NICOTINE DITARTRATE	
00300047	ANISODAMINE	
00201580	POMIFERIN	
01505312	TYLOSIN TARTRATE	1405-54-5, 1401-69-0(base)
01505322	CEPHARANTHINE	481-49-2
01505333	TRANILAST	53902-12-8
01505345	CURCUMIN	458-37-7
01505815	N-CHLOROETHYL-N-ETHYL-2'-METHYLBENZYLAMINE	
01800166	KOJIC ACID	
02300309	VESAMICOL HYDROCHLORIDE	120447-62-3
02300329	1-METHYLXANTHINE	
00300146	VULPINIC ACID	
00201664	CELASTROL	34157-83-0
01505314	SARAFLOXACIN HYDROCHLORIDE	91296-87-6
01505323	CARBIMAZOLE	22232-54-8
01505334	SECURININE	5610-40-2
01505348	RILUZOLE	1744-22-5
01505816	PREGABALIN	148553-50-8
02300204	ISOBUTYLMETHYLXANTHINE	
02300296	MEXAMINE	608-07-1
02300345	NIPECOTIC ACID	
00300147	USNIC ACID	125-46-2
00201138	DEGUELIN(-)	522-17-8
01505315	6-AMINONICOTINAMIDE	329-89-5
01505327	CHLORMADINONE ACETATE	
01505336	VALERYL SALYCILATE	64206-54-8
01505360	CEFDITORIN PIVOXIL	117467-28-4



Lee et al Supplemental Table 1

01600716	2,6-DI-t-BUTYL-4-METHYLPHENOL	128-37-0
02300192	DESMETHYLDIHYDROCAPSAICIN	
02300100	HYDROXYTACRINE MALEATE	
02300347	PENTETRAZOLE	
00300547	PHLORIDZIN	60-81-1
00201606	RUTILANTINONE	21288-61-9
01505316	PROTHIONAMIDE	14222-60-7
01505328	4'-DEMETHYLEPIPODOPHYLLOTOXIN	
01505337	ELAIDYLPHOSPHOCHOLINE	
01505361	MODAFINIL	68693-11-8
01600654	CHAULMOSULFONE	473-32-5
02300228	KAINIC ACID	487-79-6
02300104	9-AMINO-1,2,3,4-TETRAHYDROACRIDINE HYDROCHLORIDE	
02300348	1- (2-METHOXYPHENYL)PIERAZINE HYDROCHLORIDE	
00300548	SPARTEINE SULFATE	6160-12-9, 299-39-8
00200013	ROTENONE	83-79-4
01505317	CARMOFUR	61422-45-5
01505329	MILTEFOSINE	58066-85-6
01505339	L-PHENYLALANINOL	3182-95-4
01505801	TOPIRAMATE	
01600300	CREATININE	60-27-5
02300332	PODOFILOX	518-28-5
02300137	N-HYDROXYMETHYLNICOTINAMIDE	3569-99-1
00300024	HYDROCORTISONE	50-23-7
00300534	ISORESERPINE	
00200007	GAMBOGIC ACID	2752-65-0
01505319	CLOPIDOL	2971-90-6
01505330	OXICONAZOLE NITRATE	64211-46-7
01505340	AZELASTINE HYDROCHLORIDE	58581-89-8
01505802	GEMIFLOXACIN MESYLATE	
01601021	PAEONOL	552-41-0
02300219	EDROPHONIUM CHLORIDE	116-38-1, 312-48-1
02300205	LEVODOPA	59-92-7
00300013	PIMPINELLIN	131-12-4
00300546	BERGAPTEN	484-20-8
00200022	AKLAVINE HYDROCHLORIDE	60504-57-6 (aklavine)
01500564	TETRACAINE HYDROCHLORIDE	136-47-0, 94-24-6 [tetracaine]
01500408	METHYLTHIOURACIL	56-04-2
01500549	SULFAMETHIZOLE	144-82-1
01500762	ROSOLIC ACID	
01501135	NICARDIPINE HYDROCHLORIDE	54527-84-3, 55985-32-5
01501172	AZOBENZENE	103-33-3
01500567	TETRAHYDROZOLINE HYDROCHLORIDE	522-48-5, 84-22-0
01500455	OXYPHENBUTAZONE	7081-38-1, 129-20-4
01500554	SULFINPYRAZONE	57-96-5
01500665	ACEBUTOLOL HYDROCHLORIDE	34381-68-5, 37517-30-9
01500993	FLUNARIZINE HYDROCHLORIDE	30484-77-6, 52468-60-7
01501148	SULCONAZOLE NITRATE	61318-91-0, 61318-90-9
01501175	FLURANDRENOLIDE	1524-88-5
01501214	ENALAPRIL MALEATE	76095-16-4, 75847-73-3
01500575	THIORIDAZINE HYDROCHLORIDE	130-61-0, 50-52-2

Lee et al Supplemental Table 1

01500515	PROPYLTHIOURACIL	51-52-5
01500555	SULFISOXAZOLE	127-69-5
01500690	MELATONIN	
01500995	FLUTAMIDE	13311-84-7
01501149	RITODRINE HYDROCHLORIDE	23239-51-2, 26652-09-5
01501180	ESTRADIOL DIACETATE	34334-88-6
01502040	CEFMETAZOLE SODIUM	56796-39-5
01500576	THIOTHIXENE	5591-45-7, 3313-26-6 [//Z//]
01500518	PYRAZINAMIDE	98-96-4
01500621	AMINOPHENAZONE	83-07-8, 747-30-8
01500702	ACETYLTRYPTOPHAN	
01500779	SUPROFEN METHYL ESTER	
01500996	GLAFENINE	3820-67-5
01501150	SULPIRIDE	15676-16-1
01501185	ECONAZOLE NITRATE	68797-31-9, 27220-47-9
01502042	CEFOPERAZONE SODIUM	62893-20-3, 62893-19-0
01500580	TOLAZOLINE HYDROCHLORIDE	59-97-2, 59-98-3 [tolazoline]
01500521	PYRVINIUM PAMOATE	3546-41-6
01500647	VINCAMINE	
01500703	ACETYLGLUTAMIC ACID	
01500810	AMINACRINE	90-45-9, 134-50-9 [aminacrine]
01501000	ETHAVERINE HYDROCHLORIDE	985-13-7, 486-47-5
01501152	SPIPERONE	
01501187	FLUNISOLIDE	
01502035	NARASIN	55134-13-9
01500582	TOLMETIN SODIUM	64490-92-2, 26171-23-3
01500532	SALICYLAMIDE	65-45-2
01500678	gamma-AMINOBUTYRIC ACID	56-12-2
01500715	ACETYLGLUCOSAMINE	
01501002	DROPERIDOL	548-73-2
01501155	SULFAMETER	651-06-9
01501188	EBSELEN	60940-34-3
01502060	SNAP (S-NITROSO-N-ACETYLPENICILLAMINE)	
01500586	TRIAMCINOLONE	124-94-7
01500544	SULFABENZAMIDE	127-71-9
01500759	QUINALIZARIN	
01500813	BUDESONIDE	51333-22-3 [11(gr b), 16(gr a)]
01501015	FLUFENAMIC ACID	530-78-9
01501156	SULFAMETHOXYPYRIDAZINE	80-35-3
01501195	FUREGRELATE SODIUM	87463-91-0, 85666-24-6
01502070	6,7-DICHLORO-3-HYDROXY-2-QUINOXALINECARBOXYLIC	
01500294	CINEOLE	
01500266	DOXYCYCLINE HYDROCHLORIDE	17086-28-1, 564-25-0
01500655	ACONITINE	302-27-2
01500861	CORALYNE CHLORIDE	38989-38-7
01503904	PATULIN	149-29-1
01501171	SACCHARIN	81-07-2
01501200	XYLAZINE	23076-35-9, 7361-61-7
01502089	ACETYLCARNITINE	
01502092	5-FLUOROINDOLE-2-CARBOXYLIC ACID	399-76-8
01502213	TARGININE HYDROCHLORIDE	156706-47-7, 17035-90-

Lee et al Supplemental Table 1

01503086	TIAPRIDE HYDROCHLORIDE	51012-32-9
01503205	CITIOLONE	1195-16-0
01503252	METHAZOLAMIDE	554-57-4
01503297	HEXAMETHONIUM BROMIDE	55-97-0, 60-26-4
01503822	RAMIFENAZONE	3615-24-5
01503934	PERPHENAZINE	58-39-9
01504088	ETHYLNOREPINEPHRINE HYDROCHLORIDE	3198-07-0, 536-24-3
01502094	ROSMARINIC ACID	537-15-5
01502244	AMYGDALIN	29883-15-6
01503101	AZLOCILLIN SODIUM	37091-66-0
01503207	CYCLOBENZAPRINE HYDROCHLORIDE	6202-23-9, 303-53-7
01503253	METHYLBENZETHONIUM CHLORIDE	1320-44-1, 25155-18-4
01503298	DIPYRONE	5907-38-0, 68-89-3
01503647	2- (2,6-DIMETHOXYPHENOXYETHYL)AMINOMETHYL-1,4-	
01503913	NIGERICIN SODIUM	28380-24-7
01503941	THIOCTIC ACID	62-46-4
01504094	TENIPOSIDE	29767-20-2
01502107	CISPLATIN	15663-27-1
01503104	BENDROFUMETHIAZIDE	73-48-3
01503215	ENOXACIN	74011-58-8
01503257	MIDODRINE HYDROCHLORIDE	3092-17-9, 42794-76-3
01503650	NABUMETONE	42924-53-8
01503918	CLOBETASOL PROPIONATE	25122-46-7, 25122-41-2
01503947	CACODYLIC ACID	75-60-5
01504144	DIRITHROMYCIN	62013-04-1
01502109	ZIDOVUDINE [AZT]	30516-87-1
01503014	AKLOMIDE	3011-89-0
01503107	BROMHEXINE HYDROCHLORIDE	611-75-6, 3572-43-8
01503221	ETHISTERONE	434-03-7
01503260	NADOLOL	42200-33-9
01503391	D-PHENYLALANINE	673-06-3
01503675	ANDROSTERONE SODIUM SULFATE	
01503920	CLOPERASTINE HYDROCHLORIDE	3703-76-2
01503954	TULOButEROL	41570-61-0
01504148	MEPIVACAINE HYDROCHLORIDE	1722-62-9, 96-88-8
01502155	N (g)-NITRO-L-ARGININE	2149-70-4
01503043	BUCLADESINE	362-74-3
01503108	BROMOPRIDE	4093-35-0
01503222	FIPEXIDE HYDROCHLORIDE	34161-24-5
01503262	NALTREXONE HYDROCHLORIDE	16676-29-2, 16590-41-3
01503604	RETINYL PALMITATE	
01503801	NAPROXOL	26159-36-4
01503921	CYPROTERONE	2098-66-0
01503978	HYDROXYCHLOROQUINE SULFATE	747-36-4, 118-42-3
01504152	NILUTAMIDE	63612-50-0
01502162	p-CHLOROPHENYLALANINE	7424-00-2(dl); 14173-39-8(l)
01503077	PRIDINOL METHANESULFONATE	511-45-5
01503115	VINPOCETINE	42971-09-5
01503227	PERHEXILINE MALEATE	6724-53-4, 6621-47-2
01503267	NOMIFENSIN MALEATE	32795-47-4, 24526-64-5
01503610	BENZALKONIUM CHLORIDE	8001-54-5

Lee et al Supplemental Table 1

01503816	AMCINONIDE	51022-69-6
01503925	KETOROLAC TROMETHAMINE	74103-07-4, 74103-06-3
01503985	BROMPHENIRAMINE MALEATE	980-71-2, 86-22-6
01502182	d[-Arg-2]KYOTORPHAN ACETATE	
01503083	AMIPRILOSE	56824-20-5, 60414-06-4
01503117	TRIMIPRAMINE MALEATE	521-78-8, 739-71-9
01503229	METHAPYRILENE HYDROCHLORIDE	135-23-9, 91-80-5
01504153	NORCANTHARIDIN	
01503270	PRILOCAINE HYDROCHLORIDE	1786-81-8, 721-50-6
01503611	PENTOXIFYLLINE	6493-05-6
01503818	BUPIVACAINE HYDROCHLORIDE	14252-80-3, 2180-92-9
01503927	LEFUNAMIDE	
01502196	ETHOSUXIMIDE	77-67-8
01503085	PYRITHYLDIONE	77-04-3
01503204	CINNARAZINE	298-57-7
01503251	METARAMINOL BITARTRATE	
01503276	ROXITHROMYCIN	80214-83-1
01503628	PRONETALOL HYDROCHLORIDE	54-80-8
01503821	CYSTAMINE DIHYDROCHLORIDE	56-17-7
01503931	MORANTEL CITRATE	26155-31-7, 20574-50-9
01504190	AVOBENZONE	70356-09-1
01502112	CYCLOHEXIMIDE	66-81-9
02300325	METOLAZONE	17560-51-9
02300061	CLOMIPRAMINE HYDROCHLORIDE	17321-77-6, 303-49-1
01504209	DIPLOSALSALATE	
01502002	ACIVICIN	42228-92-2
01501176	ERYTHROMYCIN ESTOLATE	134-36-1, 114-07-8
02300253	1R,2S-PHENYLPROPYLAMINE	
02300062	CHLORMEZANONE	80-77-3
01504223	FENBUTYRAMIDE	
01503906	ANISOMYCIN	
01501144	SULFADIMETHOXINE	122-11-2
02300214	DILTIAZEM HYDROCHLORIDE	33286-22-5, 42399-41-7
02300063	1,3-DIPROPYL-8-CYCLOPENTYLXANTHINE [DPCPX]	
01504173	FLUOXETINE	54910-89-3
01504225	2-MERCAPTOBENZOTHAZOLE	149-30-4
01500519	PYRILAMINE MALEATE	59-33-6, 91-84-9 [pyrilamine]
01501146	SULFAGUANIDINE	57-67-0
02300170	PARAXANTHINE	
02300078	ETHYL 1-BENZYL-3-HYDROXY- 2-OXO[5H]PYRROLE-4-	
01504226	MERCAPTAMINE HYDROCHLORIDE	60-23-1
02300242	LOXAPINE SUCCINATE	27833-64-3, 1977-10-2
01502028	CEPHALEXIN	23325-78-2, 15686-71-2
02300206	DIAZOXIDE	364-98-7
00300565	METERGOLINE	17692-51-2
01504182	3-METHYLXANTHINE	
01504739	beta-PELTATIN	518-29-6
02300241	LOPERAMIDE HYDROCHLORIDE	34552-83-5, 53179-11-6
02300193	8-CYCLOPENTYLTHEOPHYLLINE	
02300161	AMOXEPINE	14028-44-5
01504184	AMINOLEVULINIC ACID HYDROCHLORIDE	

Lee et al Supplemental Table 1

01504800	CHRYSANTHEMIC ACID	10453-89-1
00100032	GEDUNIN	2753-30-2
01501103	MEFENAMIC ACID	61-68-7
02300307	VERAPAMIL HYDROCHLORIDE	152-11-4, 52-53-9 [verapamil]
02300165	AMIODARONE HYDROCHLORIDE	1951-25-3
01601020	DEET	
01504187	TELENZEPINE HYDROCHLORIDE	80880-90-6
01505270	PROPRANOLOL HYDROCHLORIDE (+/-)	3506-09-0
01501201	TOLAZAMIDE	1156-19-0
01501142	SULFACHLORPYRIDAZINE	80-32-0
02300176	PHENOXYBENZAMINE HYDROCHLORIDE	63-92-3, 59-96-1
01503804	COLFORSIN	66575-29-9
01500391	METHACHOLINE CHLORIDE	62-51-1, 55-92-5
01500483	PHENYLEPHRINE HYDROCHLORIDE	61-76-7, 59-42-7
01500501	PRIMIDONE	125-33-7
01500104	ACETYLCHOLINE	60-31-1, 51-84-3
01500273	EPHEDRINE (1R,2S) HYDROCHLORIDE	50-98-6 [((-)-)ephedrine,
01500395	METHICILLIN SODIUM	7246-14-2, 132-92-3
01500488	PINDOLOL	
01500502	PROBENECID	57-66-9
00310028	QUASSIN	76-78-8
01502084	PROADIFEN HYDROCHLORIDE	78997-40-7
01500276	ERGOCALCIFEROL	50-14-6
01500399	METHOXAMINE HYDROCHLORIDE	61-16-5, 390-28-3
01500489	PIPERACILLIN SODIUM	59703-84-3, 66258-76-2
01500503	PROCAINAMIDE HYDROCHLORIDE	614-39-1, 51-06-9
01500130	ASPIRIN	50-78-2
01500300	FLUMETHAZONE PIVALATE	2002-29-1, 2135-17-3
01500404	METHYLERGONOVINE MALEATE	57432-61-8, 7054-07-1
01500491	PIROXICAM	36322-90-4
01500507	PROCYCLIDINE HYDROCHLORIDE	1508-76-5, 77-37-2
00210186	CITRININ	518-75-2
00310040	alpha-TOCHOPHERYL ACETATE	
01500168	CEPHRADINE	38821-53-3 [anhydrous],
01500304	FLUOROMETHOLONE	426-13-1
01500406	METHYLPREDNISOLONE	83-43-2
01500450	OXIDOPAMINE HYDROCHLORIDE	1199-18-4
01500508	PROGESTERONE	57-83-0
01500244	DIETHYLSTILBESTROL	56-53-1
01500339	HYDROCORTISONE HEMISUCCINATE	83784-20-7, 2203-97-6
01500496	PREDNISOLONE	50-24-8 [anhydrous], 52438-85-
00200846	APIGENIN	520-36-5
01501021	FENSPIRIDE HYDROCHLORIDE	5053-08-7, 5053-06-5
01500253	DIMETHADIONE	695-53-4
01500354	IPRATROPIUM BROMIDE	66985-17-9, 22254-24-6
01500467	PENICILLIN V POTASSIUM	132-98-9, 87-08-1 [penicillin,
01500497	PREDNISOLONE ACETATE	52-21-1
01500557	TAMOXIFEN CITRATE	54965-24-1, 10540-29-1
00310300	VERATRINE SULFATE	62-59-9
01500264	DOXEPIN HYDROCHLORIDE	1229-29-4, 1668-19-5
01500363	LACTULOSE	4618-18-2

Lee et al Supplemental Table 1

00200046	GRISEOFULVIN	126-07-8
01500499	PREDNISONE	53-03-2
01500558	TERBUTALINE HEMISULFATE	23031-32-5, 23031-25-6
01500478	PHENIRAMINE MALEATE	132-20-7, 86-21-5
01500525	RACEPHEDRINE HYDROCHLORIDE	134-71-4, 90-81-3
00300029	DESOXYCORTICOSTERONE ACETATE	56-47-3
01500126	ANTAZOLINE PHOSPHATE	154-68-7, 91-75-8 [antazoline]
01500267	DOXYLAMINE SUCCINATE	562-10-7, 469-21-6
01501113	PERUVOSIDE	1182-67-2
01503223	PARAROSANILINE PAMOATE	7232-51-1, 569-61-9
01502254	MENADIONE	58-27-5
01503017	AMINOTHIAZOLE	96-50-4
01500756	NALIDIXIC ACID	389-08-2, 3374-05-8
01503648	GABOXADOL HYDROCHLORIDE	64603-91-4
01500230	DEXAMETHASONE	50-02-2
01500200	CLOTRIMAZOLE	23593-75-1
01504079	TOMATINE	86273-92-9
01503051	RETINYL ACETATE	
01500295	EUCATROPINE HYDROCHLORIDE	536-93-6, 100-91-4
02300270	PINACIDIL	85371-64-8, 60560-33-0
01504136	ALAPROCLATE	60719-82-6

Lee et al Supplemental Table 1

plate	position	FORMULA	MolWt	BIOACTIVITY
206001	A02	C20H23ClN2O5	406.8697	antihistaminic
206001	A03	C22H47N5O21S2	781.7688	antibacterial
206001	A04	C21H38ClN	339.9967	antiinfective (topical)
206001	A05	C9H7N7O2S	277.2658	immunosuppressant, antineoplastic, antirheumatic
206001	A06	C40H56	536.8923	provitamin A
206001	A07	C14H11ClN2O4S	338.7718	diuretic, antihypertensive
206001	A08	C16H16N5NaO7S	477.453	antibacterial
206001	A09	C7H6ClN3O4S2	295.7246	diuretic, antihypertensive
206001	A10	C7H4ClNO2	169.5684	muscle relaxant (skeletal)
206001	A11	C7H17ClN2O2	196.6787	cholinergic
206001	B02	C4H6N4O3S2	222.2454	carbonic anhydrase inhibitor, diuretic, antiglaucoma
206001	B03	C6H9Cl2N7O	266.0909	Na <sup>+</sup> channel inhibitor, diuretic
206001	B04	C47H73NO17	924.1024	antifungal
206001	B05	C66H103N17O16	1422.725	antibacterial
206001	B06	C22H29FO5	392.4718	glucocorticoid, antiinflammatory
206001	B07	C6H15ClN2O2	182.6517	cholinergic, miotic
206001	B08	C16H15N2NaO6S	418.4256	antibacterial
206001	B09	C8H9ClO	156.6133	antibacterial, topical and urinary antiseptic
206001	B10	C14H24N2O3	268.359	antifungal
206001	B11	C19H17ClN3NaO	457.8712	antibacterial
206001	C02	C2H5NO2	75.06765	urease inhibitor, antiurolithic, antibacterial
206001	C03	C7H6KNO2	175.2334	ultraviolet screen
206001	C04	C16H18N3NaO4S	371.3934	antibacterial
206001	C05	C10H12ClNO2	213.6656	muscle relaxant (skeletal)
206001	C06	C9H10Cl3N3	266.5592	antihypertensive
206001	C07	C15H12N2O	236.2757	analgesic, anticonvulsant
206001	C08	C17H16N3NaO6S	445.4514	antibacterial
206001	C09	C23H21ClO3	380.875	estrogen
206001	C10	C12H10N2O5	262.2239	antibacterial
206001	C11	C9H6ClNO	179.6073	antibacterial, antifungal
206001	D02	C16H19N3O5S	365.4109	antibacterial
206001	D03	C6H13NO2	131.176	hemostatic
206001	D04	C14H20Cl2N4	315.2483	coccidiostat
206001	D05	C10H16ClN3O5	293.7091	decarboxylase inhibitor
206001	D06	C22H19NO4	361.401	cathartic
206001	D07	C17H16N2Na2O6	422.3705	antibacterial
206001	D08	C5H9NO3S	163.1964	mucoytic
206001	D09	C20H23ClN2O4	390.8703	antihistaminic
206001	D10	C25H30ClNO5	459.9746	antihistaminic
206001	D11	C22H25NO6	399.4477	antimitotic, antigout agent
206001	E02	C10H13N5O4	267.2462	antiarrhythmic, cardiac depressant
206001	E03	C13H16N2O2	232.2847	aromatase inhibitor, antineoplastic, testosterone
206001	E04	C8H9NO2	151.1664	analgesic, antipyretic
206001	E05	C27H42ClNO2	448.0943	antiinfective (topical)
206001	E06	C12H4Cl4Na2O2	400.0201	anthelmintic, antiseptic
206001	E07	C14H10O3	226.234	antipsoriatic
206001	E08	C15H16Cl2N2O8	423.2094	antibacterial, antirickettsial, inhibits protein synthesis
206001	E09	C17H19ClN2S	318.8714	antiemetic, antipsychotic
206001	E10	C22H26BrNO3	432.3614	anticholinergic
206001	E11	C57H103N16Na5	1735.816	antibacterial

Lee et al Supplemental Table 1

206001	F02	C10H12N2O	176.2199	antidepressant
206001	F03	C7H7NO3	153.1387	antibacterial, tuberculostatic
206001	F04	C11H12N2O	188.2311	analgesic
206001	F05	C9H11NO2	165.1935	anesthetic (topical)
206001	F06	C6H14O6S2	246.3029	antineoplastic, alkylating agent
206001	F07	C12H24N2O4	260.3361	muscle relaxant (skeletal)
206001	F08	C11H12Cl2N2O5	323.1347	antibacterial, antirickettsial, inhibits protein synthesis
206001	F09	C10H13ClN2O3S	276.7437	antidiabetic
206001	F10	C18H34Cl2N2O5	461.4521	antibacterial, inhibits protein synthesis
206001	F11	C5H4N4O	136.1138	antihyperuricemia, antigout, antiurolithic
206001	G02	C27H37NO6	471.599	anticholinergic
206001	G03	C20H24ClN	313.874	antidepressant
206001	G04	C17H18ClNO2	303.7915	emetic
206001	G05	C15H14ClN3O4S	431.9415	diuretic, antihypertensive
206001	G06	C8H10N4O2	194.1945	CNS stimulant
206001	G07	C16H17N3O5S	363.395	antibacterial
206001	G08	C7H7ClO	142.5862	antiinfectant
206001	G09	C22H24Cl2N2O8	515.3512	antibacterial, antiamebic, Ca chelator, hepatotoxic;
206001	G10	C10H11ClO3	214.6504	antihyperlipoproteinemic
206001	G11	C23H30O6	402.492	glucocorticoid
206001	H02	C10H18ClN	187.7147	antiviral, antiparkinsonian; treatment of drug-induced
206001	H03	C20H24Cl3N3O	428.7928	antimalarial
206001	H04	C17H25NO7S	387.4553	anticholinergic, mydriatic
206001	H05	C21H27NO5S	405.517	anticholinergic
206001	H06	C10H16O	152.2384	analgesic, antiinfective, antipruritic
206001	H07	C14H13N8NaO4S	476.4927	antibacterial
206001	H08	C18H32ClN3O8P	515.8716	antimalarial, antiamebic, antirheumatic, intercalating
206001	H09	C25H46N14O12S	766.796	antibacterial, tuberculostatic
206001	H10	C32H36ClNO8	598.0986	gonad stimulating principle
206001	H11	C7H8O	108.1412	antiinfectant
206002	A02	C23H14Na2O11	512.341	antiasthmatic, antiallergy
206002	A03	C26H52N6O11S	656.8019	chelating agent (Fe & Al)
206002	A04	C20H30ClN3O2	379.934	anesthetic (local)
206002	A05	C21H43N7O16S	681.6782	antibacterial, tuberculostatic
206002	A06	C10H20N2S4	296.5403	alcohol antagonist
206002	A07	C18H24O2	272.3908	estrogen
206002	A08	C19H25ClN2S	348.9415	antiparkinsonian, anticholinergic
206002	A09	C31H48O6	516.7246	antibacterial
206002	A10	C10H24N4O4S	296.3912	antihypertensive, mitotic agent
206002	A11	C17H24BrNO3	370.2897	anticholinergic (ophthalmic)
206002	B02	C18H22N2	266.3894	H1 antihistamine
206002	B03	C24H33NaO5	424.5174	choleric
206002	B04	C14H10Cl2NNaO	318.1371	antiinflammatory
206002	B05	C24H28ClN5O3	469.9755	antiemetic
206002	B06	C8H12ClNO2	189.6433	cardiotonic, antihypotensive
206002	B07	C26H36O3	396.575	estrogen
206002	B08	C10H12O2	164.2059	analgesic (topical), antiseptic, antifungal
206002	B09	C30H60I3N3O3	891.5442	muscle relaxant (skeletal)
206002	B10	C7H5Cl2NO4S	270.0922	antiinfectant
206002	B11	C8H9ClN4	196.6407	antihypertensive
206002	C02	C17H26ClNO3	327.8547	mydriatic



Lee et al Supplemental Table 1

206002	C03	C21H22Cl2N2O8	501.3241	antibacterial
206002	C04	C19H16Cl2N3Na	492.3163	antibacterial
206002	C05	C14H12O4	244.2493	ultraviolet screen
206002	C06	C18H28ClNO2	325.8824	anesthetic (topical)
206002	C07	C23H32O3	356.5097	estrogen
206002	C08	C23H31FO6	422.4983	mineralocorticoid
206002	C09	C15H22O3	250.3408	antihyperlipoproteinemic
206002	C10	C21H23ClFNO2	375.8744	antidyskinetic, antipsychotic
206002	C11	C7H8ClN3O4S2	297.7405	diuretic
206002	D02	C7H17Cl2N2O3P	279.1049	antineoplastic, alkylating agent
206002	D03	C18H23ClN2	302.8504	antidepressant
206002	D04	C19H12O6	336.3039	anticoagulant
206002	D05	C17H22ClNO	291.824	antihistaminic
206002	D06	C10H14N4O4	254.2475	bronchodilator
206002	D07	C18H24O3	288.3902	estrogen
206002	D08	C26H32F2O7	494.5375	antiinflammatory, glucocorticoid
206002	D09	C21H45N5O11S	575.6837	antibacterial
206002	D10	C19H22KN3O4S	427.5709	antibacterial
206002	D11	C23H32O6	404.5079	glucocorticoid, antiinflammatory
206002	E02	C3H6N2O2	102.0935	antibacterial (tuberculostatic)
206002	E03	C24H31FO6	434.5095	glucocorticoid, antiinflammatory
206002	E04	C18H18O2	266.343	estrogen
206002	E05	C19H24ClNO	317.8622	antihistaminic
206002	E06	C10H16N2Na3O8	361.217	chelating agent, antioxidant
206002	E07	C18H22O2	270.3748	estrogen
206002	E08	C4H3FN2O2	130.0791	antineoplastic, pyrimidine antimetabolite
206002	E09	C25H30ClN3	407.991	antibacterial, anthelmintic
206002	E10	C13H6Cl6O2	406.9096	antiinfective (topical)
206002	E11	C8H8F3N3O4S2	331.2939	antihypertensive, diuretic
206002	F02	C9H13N3O5	243.2211	antineoplastic, antiviral, antimetabolite
206002	F03	C22H28FNa2O8P	516.4155	glucocorticoid, antiinflammatory
206002	F04	C16H29N3O8	391.4248	anthelmintic
206002	F05	C24H40N8O4	504.6376	coronary vasodilator
206002	F06	C29H42Cl2N2O4	553.5751	inhibits RNA, DNA and protein synthesis
206002	F07	C10H26Cl2N2O2	277.2369	antibacterial (tuberculostatic)
206002	F08	C15H13FO2	244.2681	antiinflammatory, analgesic
206002	F09	C6H14ClNO5	215.6352	antiarthritic
206002	F10	C12H18O2	194.2761	anthelmintic, topical antiseptic
206002	F11	C27H40O4	428.6175	progestogen
206002	G02	C22H27NO2	337.466	anterior pituitary suppressant
206002	G03	C18H26BrNO	352.318	antitussive
206002	G04	C13H8F2O3	250.2037	analgesic, antiinflammatory
206002	G05	C10H10N2O2S2Z	319.7014	antibacterial, antifungal, antiseborrheic
206002	G06	C13H19NO9	333.2977	adrenergic agonist, bronchodilator, antiglaucoma
206002	G07	C20H24O2	296.4131	estrogen, plus progestogen as oral contraceptive
206002	G08	C8H7N3O5	225.1621	antibacterial
206002	G09	C10H14O4	198.2207	expectorant
206002	G10	C5H11Cl2N3	184.0695	H receptor agonist, induces edema in mammalian
206002	G11	CH4N2O2	76.05523	antineoplastic, inhibits ribonucleoside diphosphate
206002	H02	C12H12N2O2S	248.3056	antibacterial, leprostatic, dermatitis herpetiformis
206002	H03	C12H8S	184.2616	keratolytic

Lee et al Supplemental Table 1

206002	H04	C41H64O14	780.9588	cardiac stimulant
206002	H05	C21H32N3O5P	437.4801	antiarrhythmic
206002	H06	C23H27N3O6	441.4881	oxytocic, 5HT antagonist
206002	H07	C8H10N2S	166.2463	antibacterial, tuberculostatic
206002	H08	C12H11Cl2N2O5S	330.7489	diuretic, antihypertensive
206002	H09	C10H12Cl2N4O2	291.1387	antihypertensive
206002	H10	C16H22BrNO3	356.2626	anticholinergic (ophthalmic)
206002	H11	C44H43ClN2O8	763.2949	anxiolytic, antihistaminic
206003	A02	C41H64O13	764.9594	inotropic, cardiotonic
206003	A03	C6H7N3O	137.1422	antibacterial, tuberculostatic
206003	A04	C9H13NO3	183.2089	vasoconstrictor
206003	A05	C24H34O4	386.5362	contraceptive
206003	A06	C11H15NO5	241.2459	muscle relaxant (skeletal)
206003	A07	C18H15Cl4N3O4	479.15	antifungal (topical)
206003	A08	C12H19BrN2O2	303.2014	cholinergic
206003	A09	C20H26O2	298.429	progestogen, in combination with estrogen as oral
206003	A10	C24H31NO8	461.5166	muscle relaxant (skeletal), antihistaminic
206003	A11	C5H11NO2S	149.2129	chelating agent (Cu), antirheumatic
206003	B02	C17H23NO3	289.3778	anticholinergic, analgesic
206003	B03	C23H33IN2O	480.4367	anticholinergic
206003	B04	C18H35ClN2O6S	443.0065	antibacterial
206003	B05	C22H32O3	344.4985	glucocorticoid
206003	B06	C20H22N8O5	454.4489	antineoplastic, antirheumatic, folic acid antagonist
206003	B07	C9H15N5O	209.2528	antihypertensive, antialopecia agent
206003	B08	C6H5NO2	123.1123	antihyperlipidemic, vitamin (enzyme cofactor)
206003	B09	C16H18FN3O3	319.3386	antibacterial
206003	B10	C19H18N3NaO5S	423.4262	antibacterial
206003	B11	C16H17KN2O4S	372.4909	antibacterial
206003	C02	C13H18O2	206.2872	antiinflammatory
206003	C03	C11H18ClNO3	247.724	bronchodilator
206003	C04	C7H11ClN2O2S	222.6949	antibacterial
206003	C05	C24H32O4	384.5202	progestogen, antineoplastic
206003	C06	C12H8O4	216.1952	antipsoriatic, pigmentation agent
206003	C07	C20H18N6Na2O9	564.4449	antibacterial
206003	C08	C17H18N2O6	346.3428	antianginal, antihypertensive
206003	C09	C21H28O2	312.4561	progestogen
206003	C10	C14H12O3	228.2499	ultraviolet screen
206003	C11	C11H12ClN5	249.7048	analgesic
206003	D02	C19H25ClN2	316.8775	antidepressant
206003	D03	C6H8N2O8	236.1393	antianginal
206003	D04	C20H24ClN	313.874	antidepressant
206003	D05	C21H26BrNO3	420.3503	anticholinergic
206003	D06	C18H24BrNO4	398.3003	anticholinergic
206003	D07	C21H21N2NaO5S	436.4657	antibacterial
206003	D08	C8H6N4O5	238.1608	antibacterial
206003	D09	C19H21N	263.3859	antidepressant
206003	D10	C16H25ClN2O	296.8435	adrenergic agonist, nasal decongestant
206003	D11	C8H14N2O4S	234.2758	antidepressant
206003	E02	C16H16ClN3O3S	365.8412	diuretic, antihypertensive
206003	E03	C18H24ClNO3	337.8499	vasodilator
206003	E04	C11H22ClN	203.7577	antihypertensive

Lee et al Supplemental Table 1

206003	E05	C5H4N4S	152.1784	antineoplastic, purine antimetabolite
206003	E06	C10H13NO4	211.2194	antihypertensive
206003	E07	C19H22CINO4	363.8445	narcotic antagonist
206003	E08	C6H6N4O4	198.1391	antiinfective (topical)
206003	E09	C22H24CINO7	449.8921	antitussive
206003	E10	C9H9NO5S	243.2398	antiinfectant
206003	E11	C15H10O2	222.2458	anticoagulant
206003	F02	C19H16CINO4	357.7967	antiinflammatory, antipyretic, analgesic
206003	F03	C18H38N4O15S	582.5854	antibacterial
206003	F04	C5H11CI2N	156.0561	antineoplastic, alkylating agent
206003	F05	C11H17NO3	211.263	bronchodilator
206003	F06	C14H23CI2N3O2	336.2643	antiemetic
206003	F07	C14H15CIN2	246.7421	adrenergic agonist, nasal decongestant
206003	F08	C7H5N3O5	211.135	antibacterial, coccidiostat
206003	F09	C31H35N2NaO11	634.6212	antibacterial
206003	F10	C22H25CIN2O9	496.9056	antibacterial
206003	F11	C9H14CINO	187.671	decongestant, anorexic
206003	G02	C17H15NO3	281.314	analgesic, antiinflammatory
206003	G03	C26H28CI2N4O4	531.4435	antifungal
206003	G04	C25H29CI3N2	463.8823	antiemetic
206003	G05	C6H12N4	140.1893	antibacterial (urinary)
206003	G06	C19H31NO9	417.4602	antihypertensive, antianginal
206003	G07	C14H14O3	230.2659	antiinflammatory, analgesic, antipyretic
206003	G08	C8H11NO3	169.1818	adrenergic agonist, antihypotensive
206003	G09	C19H26CINO2	335.8776	vasodilator (peripheral)
206003	G10	C20H22CINO4	375.8556	muscle relaxant (smooth), cerebral vasodilator
206003	G11	C15H11N2NaO2	274.2569	anticonvulsant, antiepileptic
206003	H02	C9H5I2NO	396.9551	antiamebic
206003	H03	C20H21CaN7O7	511.5131	antianemic, antidote to folic acid antagonists
206003	H04	C14H10CI2NNaO	318.1371	antiinflammatory, antipyretic
206003	H05	C4H6N2S	114.1698	antihyperthyroid
206003	H06	C6H9N3O3	171.1569	antiprotozoal
206003	H07	C23H48N6O17S	712.733	antibacterial
206003	H08	C22H28O3	340.4667	Oral contraceptive (in combination with estrogen)
206003	H09	C47H75NO17	926.1183	antifungal, binds to membrane sterols
206003	H10	C6H5CIO	128.5592	topical antibacterial (topical)
206003	H11	C22H27N3O5	413.4776	cholinergic, anticholinesterase, mitotic
206004	A02	C11H17N3O5	271.2752	antiglaucoma agent, miotic
206004	A03	C16H22CINO2	295.8122	antihypertensive, antianginal, antiarrhythmic
206004	A04	C43H58N4O12	822.9613	antibacterial (tuberculostatic)
206004	A05	C8H15N3O7	265.2247	antineoplastic, alkylating agent
206004	A06	C9H9N3O2S2	255.319	antibacterial
206004	A07	C12H18N2O3S	270.3529	antidiabetic
206004	A08	C21H26CI2F3N3S	480.4267	antipsychotic
206004	A09	C11H12N2O2	204.2305	antidepressant, nutrient; LD50(rat) 1634 mg/kg ip
206004	A10	C14H14CIN3	259.7408	antiinfective, intercalating agent
206004	A11	C23H36N4O10S2	592.6922	antiprotozoal, inhibits nucleic acid & protein synthesis
206004	B02	C4H10N2	86.1377	anthelmintic
206004	B03	C10H16CINO	201.6981	decongestant
206004	B04	C6H6AsNO6	263.0394	antibacterial
206004	B05	C8H10N2O3S	214.2445	antibacterial

Lee et al Supplemental Table 1

206004	B06	C20H17FO3S	356.4191	antiinflammatory
206004	B07	C19H17NOS	307.4174	antifungal
206004	B08	C20H32CINO	337.9371	anticholinergic, antiparkinsonian
206004	B09	C7H19NO4S	213.2978	adrenergic agonist
206004	B10	C9H5Br2NO	302.9543	antiinfectant, disinfectant
206004	B11	C10H13NO2	179.2206	analgesic, antipyretic
206004	C02	C19H24N2O2	312.4153	anthelmintic
206004	C03	C34H30N2O6S	594.692	anthelmintic
206004	C04	C7H8O2	124.1406	anesthetic (local), antiinflammatory
206004	C05	C10H10N4O2S	250.2808	antibacterial
206004	C06	C22H25CIN2O8	480.9062	antibacterial, antiamebic, antirickettsial
206004	C07	C9H13NO4S	231.2723	antidepressant
206004	C08	C22H28N2O6S	448.5423	antipruritic
206004	C09	C66H85N11O15	1272.478	topical antibacterial (topical)
206004	C10	C7H16CINO3	197.6635	antihyperlipoproteinemic, gastric and
206004	C11	C8H8HgO2	336.7418	antifungal
206004	D02	C15H27N3O9P2	455.3447	antimalarial
206004	D03	C12H13CIN4	248.7172	antimalarial
206004	D04	C17H22BrNO4	384.2732	anticholinergic, treatment of motion sickness
206004	D05	C11H12N4O2S	264.3079	antibacterial
206004	D06	C7H8N4O2	180.1674	bronchodilator
206004	D07	C9H14O6	218.2083	antifungal (topical)
206004	D08	C21H29CIN2O5	424.9287	antiemetic
206004	D09	C24H40O4	392.584	anticholelithogenic; LD50(rat) 890 mg/kg ip
206004	D10	C18H22O2	270.3748	estrogen, antineoplastic (hormonal)
206004	D11	C21H32O2	316.488	glucocorticoid, antiinflammatory
206004	E02	C22H30CIN3O6S	564.1459	antiemetic, antipsychotic, treatment of vertigo
206004	E03	C23H32Cl3N3O	472.89	anthelmintic, antimalarial, intercalating agent
206004	E04	C19H39N5O11S	545.6136	antibacterial, binds to ribosomes
206004	E05	C12H14N4O2S	278.335	antibacterial
206004	E06	C10H7N3S	201.2514	anthelmintic
206004	E07	C24H31FO6	434.5095	antiinflammatory
206004	E08	C14H18N4O3	290.3246	antibacterial
206004	E09	C67H77Cl3N8O24	1484.759	antibacterial
206004	E10	C21H45N3	339.6129	antifungal
206004	E11	C9H16O4	188.2255	antiacne, antiproliferative agent
206004	F02	C17H21CIN2S	320.8873	antipsychotic
206004	F03	C26H36N2O9	520.5848	antiarrhythmic, antimalarial
206004	F04	C14H26Cl2N2O7	405.2785	antibacterial
206004	F05	C10H11N3O3S	253.2815	antibacterial, antipneumocystis
206004	F06	C9H9HgNaO2S	404.8147	antiinfective, preservative
206004	F07	C25H31FO8	478.5194	antiinflammatory
206004	F08	C14H12O3	228.2499	melanizing agent, antipsoriatic
206004	F09	C10H13N5O4	267.2462	antiviral
206004	F10	C9H15N3O5S	277.301	monoamine oxidase inhibitor, antidepressant
206004	F11	C7H8N4O2	180.1674	diuretic, bronchodilator, cardiotonic
206004	G02	C17H21CIN2S	320.8873	antihistaminic
206004	G03	C20H26N2O6S	422.504	antimalarial, skeletal muscle relaxant
206004	G04	C24H32O4S	416.5842	diuretic
206004	G05	C11H11N3O2S	249.2932	antibacterial
206004	G06	C5H5N5S	167.1931	antineoplastic, purine antimetabolite

Lee et al Supplemental Table 1

206004	G07	C12H11N7	253.2684	diuretic
206004	G08	C19H23ClN2	314.8616	antihistaminic
206004	G09	C16H25ClN2	280.8441	adrenergic agonist, nasal decongestant
206004	G10	C20H8Br2HgNa2	750.6608	antibacterial
206004	G11	C20H26N2O2	326.4424	antiarrhythmic (Class Ia): inhibits glucose uptake by
206004	H02	C23H30BrNO3	448.4045	anticholinergic
206004	H03	C6H6O2	110.1135	keratolytic, antiseborheic
206004	H04	C21H41N7O16S	679.6622	antibacterial (tuberculostatic)
206004	H05	C18H14N4O5S	398.4001	anticolitis and Crohn's disease
206004	H06	C17H28N4O7S	432.4993	betaadrenergic blocker
206004	H07	C8H8Cl3N3O4S2	380.6577	diuretic, antihypertensive
206004	H08	C17H20N2O2	284.3612	anticholinergic (ophthalmic)
206004	H09	C15H14ClNO3	291.7367	analgesic, antiinflammatory
206004	H10	C8H12ClNO2	189.6433	adrenergic agonist
206004	H11	C20H26N2O2	326.4424	antiarrhythmic, antimalarial
206005	A02	C23H23NO5S	425.5075	antiasthmatic
206005	A03	C17H20O6	320.3454	antineoplastic
206005	A04	C10H7NO3	189.1722	nutrient in vitamin B deficiency diseases
206005	A05	C28H36O15	612.5901	sweetener
206005	A06	C10H9N5O	215.2161	auxin, plant growth regulator, plant cell division
206005	A07	C11H14ClN3O4S	383.8969	diuretic
206005	A08	C21H22ClNO4	387.8668	antibacterial, uterine contractant
206005	A09	C13H20N2O2	236.3166	antitussive
206005	A10	C37H42Cl2N2O6	681.6631	antihypertensive, skeletal muscle relaxant
206005	A11	C34H34N4O4	562.6745	hepatoprotectant
206005	B02	C21H27ClN2O3	390.9139	alpha adrenergic blocker, mydriatic, antidepressant
206005	B03	C35H64NO16P	785.8712	antibacterial
206005	B04	C14H23ClN2O	270.8052	anesthetic (local), antiarrhythmic
206005	B05	C21H20O11	448.387	antihemorrhagic
206005	B06	C27H32O14	580.5477	antihaemorrhagic, antiinflammatory
206005	B07	C20H18ClNO4	371.8238	antiarrhythmic, alpha2 agonist, cholinesterase,
206005	B08	C17H19NO3	285.3459	analeptic, antibacterial
206005	B09	C17H21NO3	287.3618	antiinflammatory
206005	B10	C23H26ClN	351.9234	coronary vasodilator
206005	B11	C21H28ClNO4	393.9146	analgesic, narcotic antagonist
206005	C02	C19H21ClF3NO2	387.8329	antihyperlipoproteinemic
206005	C03	C29H44O12	584.6668	antiarrhythmic, cardiotoxic, hypertensive, Na/K
206005	C04	C13H17NO4	251.2847	chymotrypsin substrate
206005	C05	C15H21N3O2	275.3535	anticholinesterase, mitotic, antiglaucoma, cognition
206005	C06	C11H15NO2	193.2477	anesthetic (local)
206005	C07	C22H29KO4	396.576	aldosterone antagonist, diuretic
206005	C08	C15H16O9	340.2894	antiinflammatory
206005	C09	C17H22BrNO4	384.2732	betaadrenergic agonist
206005	C10	C22H23ClN2O8	478.8902	antibacterial
206005	C11	C29H28N2O6S2	564.6843	H1 antihistamine
206005	D02	C6H8N2O2S	172.2069	antibacterial
206005	D03	C19H20N8O5	440.4219	antineoplastic, antirheumatic, folic acid antagonist
206005	D04	C13H15N3O2	245.2834	antidepressant, nutrient
206005	D05	C10H7NO4	205.1716	caspase activator, guanylyl cyclase stimulant
206005	D06	C15H14ClN3O4S	367.8135	antibacterial
206005	D07	C12H13ClN2O	236.7032	anthelmintic, narcotic agent

Lee et al Supplemental Table 1

206005	D08	C41H63NO15	809.957	antihypertensive, emetic; LD50(mouse) 0.21 mg/kg
206005	D09	C16H14O3	254.2882	antiinflammatory
206005	D10	C22H31Cl2N7O5	544.4423	antineoplastic, antiprotozoal
206005	D11	C25H36ClNO5	466.0224	muscle relaxant (smooth)
206005	E02	C21H22N2O2	334.4217	central stimulant
206005	E03	C8H14BrNO2	236.1103	anthelmintic (Cestodes), hypotensive, cathartic
206005	E04	C7H11NO3	157.1706	antirheumatic
206005	E05	C22H28ClNO2	373.927	antiasthmatic, respiratory stimulant
206005	E06	C12H11I3N2O4	627.9457	radioopaque agent
206005	E07	C13H14N2O	214.2693	CNS stimulant, antiparkinsonian agent
206005	E08	C30H46O4	470.6987	antiinflammatory
206005	E09	C21H21NO6	383.4046	uterine hemostatic, antiseptic
206005	E10	C15H16O6	292.2912	convulsant, GABA receptor antagonist, ichthyotoxin
206005	E11	C29H27ClN2O14	695.0605	antibacterial
206005	F02	C15H10O7	302.2428	capillary protectant, antioxidant. antineoplastic, anti-
206005	F03	C9H15NO3S	217.2888	antihypertensive
206005	F04	C11H10O4	206.2	photosensitizing agent
206005	F05	C27H42O4	430.6334	antiinflammatory
206005	F06	C15H11I4NO4	776.8768	antihypercholesterimic, thyromimetic
206005	F07	C13H12N2O	212.2534	antiparkinsonian, CNS stimulant
206005	F08	C14H12FNO3	261.255	antibacterial
206005	F09	C20H21ClO4	360.841	antihyperlipidemic
206005	F10	C15H25ClN2O3	316.8311	stimulant (central)
206005	F11	C18H26N2O4	334.4189	anticholinergic
206005	G02	C8H15NaO2	166.1974	anticonvulsant
206005	G03	C10H16N6S	252.3432	antiulcerative
206005	G04	C15H10O4	254.2446	diuretic
206005	G05	C30H26N2O13	622.5473	chelating agent (Ca, Mg)
206005	G06	C4H2N2O4	142.0715	specific cytotoxin (pancreatic islet betacell)
206005	G07	C8H10N2O4	198.1799	depilatory agent
206005	G08	C22H28Cl2F3N3	510.4532	H1 antihistamine
206005	G09	C15H14O3	242.277	antiinflammatory
206005	G10	C31H48O2S2	516.855	antihyperlipidemic
206005	G11	C17H24Cl2N4O	371.313	psychotropic
206005	H02	C9H14N4O4	242.2363	antianginal
206005	H03	C18H19ClN4	326.8319	antipsychotic
206005	H04	C15H12O5	272.2599	antiulcer, gibberellin antagonist
206005	H05	C2H7N3O3	121.0964	striated muscle stimulant
206005	H06	C4H6N4O3	158.1174	wound healing agent
206005	H07	C11H8N2	168.1998	plant growth inhibitor; mutagen
206005	H08	C8H15N7O2S3	337.4465	H2 antihistamine
206005	H09	C15H13N3O2S	299.3538	anthelmintic
206005	H10	C16H13N3O3	295.3003	anthelmintic
206005	H11	C12H22ClN	215.7688	muscle relaxant (skeletal)
206006	A02	C3H9NO3S	139.1741	antibacterial
206006	A03	C17H19NO	253.3471	analgesic
206006	A04	C24H26N2O6	438.4846	analgesic, antipyretic, antiinflammatory
206006	A05	C19H26O2	286.4179	estrogen
206006	A06	C20H30O	286.4615	vitamin A
206006	A07	C7H7O6P	218.104	analgesic, antiinflammatory
206006	A08	C16H15N4NaO8S	446.3738	antibacterial

Lee et al Supplemental Table 1

206006	A09	C19H20ClNO4	361.8286	antihyperlipidemic
206006	A10	C5H9N3O2	143.1464	regulator of creatine biosynthesis
206006	A11	C2H9ClN2	96.56043	antineoplastic
206006	B02	C5H12ClNO2	153.6099	GABA <sub>B</sub> antagonist
206006	B03	C19H23Cl2N5O2	424.3335	antiulcerative
206006	B04	C14H12O3S	260.3139	antiinflammatory
206006	B05	C20H26O3	314.4284	estrogen
206006	B06	C15H14O3	242.277	antineoplastic, antifungal
206006	B07	C2H5NaO3S2	164.1782	mucolytic
206006	B08	C17H18N3NaO4S	383.4045	antibacterial
206006	B09	C15H11I3NNaO4	672.9622	thyroid hormone
206006	B10	C10H7NO3	189.1722	inhibit mitochondrial pyruvate transport
206006	B11	C30H44K2O16S2	803.0076	oxidative phosphorylation inhibitor
206006	C02	C14H22N2O3	266.343	beta adrenergic blocker
206006	C03	C17H28ClNO3	329.8706	anesthetic (topical)
206006	C04	C15H13NO4	271.2752	analgesic, antipyretic
206006	C05	C9H11FN2O5	246.1968	antineoplastic, pyrimidine antimetabolite
206006	C06	C16H14O3	254.2882	antiinflammatory
206006	C07	C20H28O2	300.445	keratolytic
206006	C08	C17H20ClF2N3O	387.8171	antibacterial
206006	C09	C19H17N3O4S2	415.493	antibacterial
206006	C10	C10H14O2	166.2219	inhibits posttranslational cys isoprenylation, blocks G-
206006	C11	C6H10ClNO2	163.6051	muscarinic agonist
206006	D02	C26H39NO10	525.6014	antitussive
206006	D03	C10H14O3	182.2213	muscle relaxant (skeletal)
206006	D04	C8H9NO	135.167	analgesic, antipyretic
206006	D05	C25H30O3	378.5161	estrogen
206006	D06	C21H31N3O5	405.4983	ACE inhibitor
206006	D07	C18H24BrNO3S	414.3649	inhibitor of norepinephrine release
206006	D08	C3H5CaO4P	176.1247	antibacterial
206006	D09	C9H6ClNO2	195.6067	NMDA receptor antagonist (gly)
206006	D10	C7H5NO4	167.1222	differentiates between cerebral and forebrain NMDA
206006	D11	C8H13N3O4S	247.2745	antiprotozoal
206006	E02	C5H6N2	94.11697	Kchannel blocker
206006	E03	C15H14N4O2S	314.3684	antibacterial
206006	E04	C11H13ClN4O2	268.7049	antihypertensive, peripheral vasodilator
206006	E05	C18H23NaO5S	374.4348	estrogen
206006	E06	C8H15NO3	173.2137	antivertigo
206006	E07	CNa3O5P	191.9514	antiviral
206006	E08	C19H17N6NaO6S	512.5017	antibacterial
206006	E09	C10H6ClNO3	223.6172	NMDA receptor antagonist (gly)
206006	E10	C14H8O2	208.2187	irritant
206006	E11	C6H11NO2	129.1601	NMDA receptor antagonist (gly)
206006	F02	C10H18O	154.2544	weak estrogen receptor blocker
206006	F03	C13H22N4O3S	314.4093	H2 antihistamine
206006	F04	C19H26O3	302.4173	estrogen
206006	F05	C14H12ClNO2	261.7102	antiinflammatory, analgesia
206006	F06	C17H20N2O5S	364.4234	diuretic
206006	F07	C19H19N7O6	441.4066	hematopoietic vitamin
206006	F08	C8H12N2O4S	232.2598	cholinesterase reactivator
206006	F09	C16H13NO4	283.2863	aldose reductase inhibitor

Lee et al Supplemental Table 1

206006	F10	C6H12N2O4Pt	371.2635	antineoplastic, convulsant
206006	F11	C4H7NO2	101.1059	NMDA partial agonist (gly)
206006	G02	C24H26BrN3O3	484.3971	vasodilator
206006	G03	C20H35NOS	337.5721	peripheral vasodilator
206006	G04	C21H28O3	328.4555	estrogen
206006	G05	C13H13N5O2	271.2809	cGMP phosphodiesterase inhibitor
206006	G06	C34H48Na2O7	614.7371	antiinflammatory, antisecretory, antiulcer
206006	G07	C8H15NO2	157.2143	hemostatic
206006	G08	C18H20FN3O4	361.3762	antibacterial
206006	G09	C9H7NO2	161.1616	NMDA receptor antagonist (gly)
206006	G10	C8H12N4O5	244.2086	antineoplastic, pyrimidine antimetabolite
206006	G11	C16H16N2O4	300.3169	chloride channel blocker
206006	H02	C28H29F2N3O	461.5596	antipsychotic
206006	H03	C6H8N4O4	200.1551	antiprotozoal
206006	H04	C20H24O3	312.4125	estrogen
206006	H05	C17H22BrNO3	368.2738	anticholinesterase, analgesic, antiAlzheimer
206006	H06	C15H12ClNO2	273.7214	antiinflammatory, analgesic
206006	H07	C16H16N3NaO7S	449.4396	antibacterial
206006	H08	C14H16N4O3	288.3086	antibacterial
206006	H09	C21H23NO4	353.4218	antiinflammatory
206006	H10	C5H7N3O4	173.1292	antineoplastic, amino acid antagonist
206006	H11	C21H31N3O5S	437.5623	chemotactic peptide
206007	A02	C15H20N2O4S	324.4017	chemotactic peptide
206007	A03	C16H12O3	252.2722	anticoagulant
206007	A04	C24H32N4O5	456.5464	TAN inhibitor
206007	A05	C12H14N2O2	218.2576	insecticide
206007	A06	C37H63NaO10	690.8985	antibacterial
206007	A07	C8H15NO3	173.2137	wound healing agent
206007	A08	C13H19Br2ClN2O	414.5702	expectorant
206007	A09	C30H40Cl2N4	527.5861	antiinfectant
206007	A10	C9H13BrN2O2	261.1202	cholinergic
206007	A11	C3H4O2	72.06413	antiinfective
206007	B02	C22H35N3O6S	469.6048	chemotactic peptide
206007	B03	C62H111N11O12	1202.642	immunosuppressant
206007	B04	C7H15N3O2S	205.2805	nitric oxide synthase inhibitor
206007	B05	C12H11ClN2O	234.6873	MAO inhibitor
206007	B06	C15H10O7	302.2428	P450 and ATPase inhibitor
206007	B07	C9H11FN2O5	246.1968	antineoplastic, antimetabolite
206007	B08	C6H10O6	178.143	chelating agent
206007	B09	C10H20O	156.2703	analgesic (topical), antipruritic agent
206007	B10	C14H13N3O5S	335.3408	antiinflammatory
206007	B11	C23H47N5O18S	713.7177	antibacterial, antiamebic
206007	C02	C28H37N5O7	555.6364	opioid neuromodulator
206007	C03	C41H67NO15	813.9888	antibacterial
206007	C04	C15H23N3O10S	437.4287	antiinflammatory, antiallergy, mast cell degranulation
206007	C05	C19H22N2O	294.4	cerebrotonic, muscle stimulant
206007	C06	C8H7NS	149.2157	antineoplastic, antibacterial, antifungal
206007	C07	C9H18N6	210.284	antineoplastic
206007	C08	C7H4O3S	168.1721	antiseborrheic
206007	C09	C12H15Cl2NO5S	356.2271	antibacterial
206007	C10	C19H25ClN2O3	364.8757	adrenergic blocker



Lee et al Supplemental Table 1

206007	C11	C11H13CIN2S	240.7567	immunomodulator
206007	D02	C23H39N5O7	497.5966	Induces nicks at apurinic and apyrimidinic sites in
206007	D03	C9H18N2O3	202.2554	ubiquitin blocker, neurite growth inhibitor
206007	D04	C16H16N4O	280.3321	beta-glucosidase inhibitor
206007	D05	C21H24O9	420.42	antifungal, antioxidant
206007	D06	C10H16N2O3S	244.3146	vitamin B complex
206007	D07	C9H10N2O3	194.1917	renal function diagnosis
206007	D08	C21H28CIN3O7S	501.9902	antibacterial
206007	D09	C13H11N3O4S2	337.3783	antiinflammatory
206007	D10	C17H16N4O2	308.3427	analgesic, antiinflammatory
206007	D11	C24H32O6	416.519	glucocorticoid
206007	E02	C11H16N2O8	304.2588	neurotransmitter, mgluR3 receptors
206007	E03	C21H28F3N3O6	475.469	elastase (human) inhibitor
206007	E04	C18H18CINO3	331.8021	peptidase inhibitor, esterase inhibitor
206007	E05	C14H6O8	302.1991	hemostatic, antineoplastic, antimutagenic
206007	E06	C8H7N3O5	225.1621	antiprotozoal
206007	E07	C17H16F6N2O	378.3203	antimalarial
206007	E08	C24H35CIN2O	403.0124	antiarrhythmic
206007	E09	C19H42BrN	364.4573	antiinfectant
206007	E10	C24H32CIFO5	454.971	glucocorticoid, antiinflammatory
206007	E11	C25H36O6	432.5621	glucocorticoid, antiinflammatory
206007	F02	C9H20N4O4	248.2842	NO synthesis inhibitor
206007	F03	C17H16O4	284.3147	antineoplastic, antiinflammatory, immunomodulator,
206007	F04	C18H20N2O4	328.3711	TAN inhibitor
206007	F05	C10H17N3O6S	307.3275	antioxidant
206007	F06	C10H13NO7	259.2176	vasodilator
206007	F07	C20H26CINO2	347.8887	muscle relaxant (smooth)
206007	F08	C5H9Cl2N3O2	214.0524	antineoplastic, alkylating agent
206007	F09	C9H5Cl2NO	214.0523	chelating agent
206007	F10	C20H24N2O2S	356.4905	anthelmintic, hepatotoxic
206007	F11	C22H30Cl2N4O6	517.4136	antineoplastic
206007	G02	C6H10N2O2	142.1588	antinauseant
206007	G03	C16H21N3O3	303.3641	ACE inhibitor
206007	G04	C14H12O3	228.2499	antifungal, antibacterial
206007	G05	C16H23NO6	325.3648	antineoplastic, insect sterilant
206007	G06	C4H9NO3	119.1212	antiepileptic
206007	G07	C26H58Cl2N10	581.7252	antibacterial
206007	G08	C18H16N8Na2O7	598.5492	antibacterial
206007	G09	C21H26Cl2O	365.3468	antibacterial
206007	G10	C13H12N2O5S	308.315	antiinflammatory
206007	G11	C3H7NO2	89.09474	antineoplastic, cytotoxic
206007	H02	C21H26CINO2	359.8999	antispasmodic
206007	H03	C17H25N3O4	335.4065	immunostimulant
206007	H04	C20H16N2O4	348.3615	antineoplastic
206007	H05	C13H18O7	286.2842	analgesic, antipyretic
206007	H06	C15H22O5	282.3396	antimalarial
206007	H07	C25H31CIN2O5	474.9892	antihypertensive, ACE inhibitor
206007	H08	C19H23Cl2N5O	408.3341	antidepressant
206007	H09	C34H53NaO8	612.7865	antibacterial
206007	H10	C11H19NO4S	261.3424	vasoconstrictor
206007	H11	C6H12N3PS	189.2204	antineoplastic, alkylating agent

Lee et al Supplemental Table 1

206008	A02	C11H8ClNO2	221.6449	antifungal
206008	A03	C21H26N2O7	418.4506	vasodilator
206008	A04	C6H4N2O6	200.1086	catechol O-methyltransferase inhibitor
206008	A05	C22H26O5	370.4495	estrogen
206008	A06	C21H27N7NaO17	765.3972	cofactor in aryl & steroidal hydroxylation
206008	A07	C21H28ClNO3	377.9152	antiarrhythmic
206008	A08	C29H42O10	550.6521	cardiotonic
206008	A09	C16H12O5	284.271	antibacterial, cathartic
206008	A10	C15H21N3O3S	323.4169	antidiabetic
206008	A11	C30H40O4	464.6509	antineoplastic, antiinflammatory
206008	B02	C13H19NO2	221.3019	antifungal
206008	B03	C42H69NaO11	773.0014	antibacterial
206008	B04	C11H14ClF3N2	266.6958	5HT agonist
206008	B05	C38H72N2O12	749.0037	antibacterial
206008	B06	C47H51NO14	853.9288	antineoplastic
206008	B07	C21H23N3OS	365.501	antipsychotic
206008	B08	C15H10O5	270.244	antiviral (HIV)
206008	B09	C42H38O20	862.7592	cathartic
206008	B10	C12H21ClO2	232.753	arthropod pheromone
206008	B11	C38H42N2O6	622.7682	analgesic, antineoplastic, antihypertensive,
206008	C02	C7H10N4O4	214.1822	antineoplastic, hypoxic cell radiosensitizer
206008	C03	C8H11N5O3	225.2086	antiviral
206008	C04	C10H10N2O	174.204	antioxidant, lipoxygenase inhibitor
206008	C05	C35H44O16	720.7313	antifeedant, insecticide
206008	C06	C18H30N2O2	306.452	anesthetic (local)
206008	C07	C7H22Cl3N3	254.6325	ornithine decarboxylase inhibitor
206008	C08	C30H30O8	518.5688	antispermatogenic, antineoplastic, antiHIV
206008	C09	C23H26O3	350.4619	ectoparasiticide
206008	C10	C14H13N3O4S2	351.4054	antiinflammatory
206008	C11	C15H12O4	256.2605	aldose reductase inhibitor, antineoplastic,
206008	D02	C9H13N3O6	259.2205	immunosuppressant
206008	D03	C18H20N2O6	360.3699	antihypertensive
206008	D04	C24H28N2O4S2	472.6298	5HT1&2 receptor antagonist
206008	D05	C32H49NO9	591.7486	antihypertensive
206008	D06	C10H12N2	160.2205	psychotropic
206008	D07	C24H36O5	404.5515	antihyperlipidemic, HMGCoA reductase inhibitor
206008	D08	C10H19NO	169.269	antifeedant, antiinflammatory, oxytoxic
206008	D09	C22H30N6O4S	474.5862	impotency therapy
206008	D10	C9H13ClN6O2	272.696	antineoplastic
206008	D11	C24H37NO7	451.565	antiarrhythmic
206008	E02	C26H35NO7	473.5714	vasodilator
206008	E03	C17H18FN3O3	331.3497	antibacterial, fungicide
206008	E04	C21H27ClN2O3	390.9139	alpha2 adrenergic antagonist
206008	E05	C16H18ClNO6S2	419.906	platelet aggregation inhibitor
206008	E06	C11H12I3NO2	570.937	radioopaque agent
206008	E07	CH6ClNO	83.51807	hydroxymethyltransferase inhibitor
206008	E08	C11H15NO2	193.2477	antihypertensive, antihistamine
206008	E09	C8Cl4N2	265.9146	antifungal
206008	E10	C15H12O4	256.2605	antiinflammatory
206008	E11	C3H5NO4	119.0776	antineoplastic
206008	F02	C10H18ClN3O2	247.7269	antineoplastic

Lee et al Supplemental Table 1

206008	F03	C10H10O2	162.19	anesthetic (topical) and antiseptic, pediculicide
206008	F04	C8H12CIN5	213.6713	5HT3 receptor agonist
206008	F05	C22H23CIN2O2	382.8938	H1 antihistamine
206008	F06	C16H14F3N3O2S	369.3681	antiulcerative
206008	F07	C5H16N4O4S	228.2717	NMDA blocker, alpha-2 adrenergic agonist; NO
206008	F08	C11H14N2O	190.247	antiinflammatory, respiratory stimulant
206008	F09	C12H20O3	212.2914	plant growth regulator
206008	F10	C17H27NO2	277.4102	antidepressant
206008	F11	C22H19CIO3	366.8479	antipneumocystic, antimalarial
206008	G02	C43H74N2O14	843.0742	antibacterial
206008	G03	C16H22N2O5	322.3641	muscarinic agonist
206008	G04	C37H53NO12	703.8345	antihypertensive
206008	G05	C43H63NO11	769.9817	antiparasitic, antimite
206008	G06	C20H29CIN2O3	380.9187	anticholinergic
206008	G07	C4H4N2OS	128.1533	thyroid depressant
206008	G08	C15H8O7	300.2268	cathartic, purgative
206008	G09	C76H52O46	1701.234	nonspecific enzyme/receptor blocker
206008	G10	C13H19CI2NO	276.2085	antidepressant
206008	G11	C11H17CI2N5	290.1976	antimalarial
206008	H02	C8H8O3	152.1512	antiseborrheic, antipruritic
206008	H03	C16H22CI2N2O2	377.3359	calmodulin antagonist, PDE and kinase inhibitor
206008	H04	C17H14F3N3O2S	381.3792	antiarthritic, cyclooxygenase2 inhibitor
206008	H05	C33H33CaFNO5	582.7131	antihyperlipidemic, HMGCoA reductase inhibitor
206008	H06	C23H42N2O12	538.5974	antihypertensive, ganglionic blocker
206008	H07	C24H28CIN3O6	489.9603	antiemetic, antispasmodic
206008	H08	C29H46O3	442.6882	antineoplastic
206008	H09	C20H28O2	300.445	antineoplastic, aromatase inhibitor
206008	H10	C21H25NO4	355.4377	analgesic, hypnotic, papaverine-like
206008	H11	C6CI4O2	245.8777	antipsoriatic
206009	A02	C6H9NO5	175.1423	analeptic, neurostimulant
206009	A03	C8H4CI2N2O2	231.0393	NMDA receptor antagonist (gly)
206009	A04	C18H20FN3O4	361.3762	antibacterial
206009	A05	C23H29CIFN3O4	465.9567	antibacterial
206009	A06	C17H25N3O2S	335.4717	5HT 1B/2D receptor agonist
206009	A07	C22H28FN3O6S	481.5474	antihyperlipidemic
206009	A08	C33H42O19	742.6913	vasoprotectant
206009	A09	C15H18N2O	242.3235	anticholinesterase, cognition enhancer
206009	A10	C13H17NO	203.2865	antipruritic, scabicide
206009	A11	C19H23N3	293.4153	pesticide, carcinogen
206009	B02	C12H18CIN7O	311.7766	Na/H+ antiporter inhibitor, diuretic
206009	B03	C17H14O4S	314.3627	COX2 inhibitor, antiinflammatory, antiarthritic
206009	B04	C33H34N6O6	610.6755	angiotensin 1 receptor antagonist
206009	B05	C19H21CIN2O3S	392.9078	antidiabetic
206009	B06	C29H30N6O6	558.5991	Angiotensin II inhibitor prodrug, antihypertensive
206009	B07	C20H27N5O5	417.4687	5HT4 receptor agonist, peristaltic stimulant
206009	B08	C22H34O3	346.5145	cytotoxic, apoptosis inducer, antitubercular
206009	B09	C25H22O10	482.4481	hepatoprotective agent, antioxidant
206009	B10	C17H10O	230.2687	hepatotoxic, P450 suppressant
206009	B11	C14H8O5	256.2169	xanthin oxidase inhibitor, irritant
206009	C02	C7H5CIN2O	168.5837	muscle relaxant, antirrhematic
206009	C03	C6H6O2	110.1135	antioxidant

Lee et al Supplemental Table 1

206009	C04	C18H19N3O3S	357.4344	antidiabetic
206009	C05	C22H22O8	414.4158	antineoplastic; 10% cytotoxicity of podophyllotoxin
206009	C06	C15H14N4O6S2	410.43	antibacterial
206009	C07	C17H14F3N3O3S	397.3786	antiinflammatory, antiarthritic, COX-2 inhibitor
206009	C08	C22H28O3	340.4667	aldosterone antagonist; antifibrogenic
206009	C09	C33H40O15	676.6778	hepatoprotective
206009	C10	C16H21N3O2	287.3647	antimigraine, 5HT[1B/1D] agonist
206009	C11	C20H44N4O18S2	692.7177	antibacterial
206009	D02	C25H28N2O2	388.5141	antifungal
206009	D03	C15H12N2O2	252.2751	antipsychotic
206009	D04	C22H23ClN6O	422.9212	antihypertensive, AT1 angiotensin II antagonist
206009	D05	C13H22O3	226.3185	plant growth regulator
206009	D06	C14H13N5O5S2	395.4182	antibacterial
206009	D07	C20H27N5O2	369.4705	phosphodiesterase inhibitor
206009	D08	C21H41N5O11	539.5878	antibacterial; LD50(iv) 280mg/kg(mouse)
206009	D09	C17H18Cl3N	342.6987	antidepressant, 5HT uptake inhibitor
206009	D10	C6H10S	114.2106	antibacterial, antifungal, antineoplastic,
206009	D11	C7H11N3O3	185.184	antiameobic, antitrichomonas
206009	E02	C10H11NaO2	186.1878	antihyperlipidemic
206009	E03	C10H11NO3	193.2041	sweetener
206009	E04	C19H22FN3O4	375.4033	antibacterial
206009	E05	C24H29ClN2O5	460.9621	ACE inhibitor, antihypertensive
206009	E06	C24H28N5NaO3	457.5123	Angiotensin II inhibitor, antihypertensive
206009	E07	C17H32O3	284.4428	antibacterial, antifungal
206009	E08	C30H48O6	504.7135	wound healing
206009	E09	C19H27N5O4	389.4581	alpha(1)-adrenergic blocker
206009	E10	C11H10N4O4	262.2268	antibacterial
206009	E11	C18H24FN3O6S	429.4709	antibacterial, antiproliferative
206009	F02	C27H44O7	480.6475	insect molting hormone
206009	F03	C28H32N2O10	556.5746	betaadrenergic blocker
206009	F04	C8H17NO5	207.2284	alpha-glucosidase inhibitor, antidiabetic
206009	F05	C14H19N5O4	321.3386	antiviral
206009	F06	C17H27Cl2N	316.3174	anorexic, antidepressant, uptake inhibitor (5HT,
206009	F07	C19H32O4	324.4645	antibacterial, antifungal
206009	F08	C10H11ClN4O2	254.6778	nicotinyl AChR agonist; antiparasitic
206009	F09	C24H34N2O5	430.549	antihypertensive, ACE inhibitor
206009	F10	C15H13N3O3S	315.3532	anthelmintic
206009	F11	C14H18N2O5	294.31	sweetener
206009	G02	C12H15NO3	221.2583	muscle relaxant (skeletal)
206009	G03	C19H27NO3	317.4319	antidiabetic
206009	G04	C29H53NO5	495.7495	reversible lipase inhibitor, antiobesity
206009	G05	C26H31ClN2O8S	567.0626	Ca channel blocker
206009	G06	C16H20N4O3S	348.4268	diuretic, inhibits Na/K/2Cl carrier system
206009	G07	C15H27IN2	362.3002	oxytocic
206009	G08	C21H22NO5	368.4132	uterine contractant, antibacterial, antiarrhythmic,
206009	G09	C44H65N5O10	824.0362	antibacterial
206009	G10	C10H16O	152.2384	antineoplastic, apoptosis inducer; skin irritant,
206009	G11	C14H16ClN3O2	293.7555	antifungal, P450 inhibitor
206009	H02	C38H69NO13	747.9725	antibacterial
206009	H03	C25H28N6O	428.5415	angiotensin 2 receptor antagonist
206009	H04	C16H14N2O3S	314.3656	antiinflammatory, COX-2 inhibitor

Lee et al Supplemental Table 1

206009	H05	C24H21F2NO3	409.4367	sterol absorption inhibitor
206009	H06	C23H43N3O5	441.6163	antihypertensive, ACE inhibitor
206009	H07	C14H26N4O11P2	488.3311	cognition enhancer, phosphocholine
206009	H08	C19H23NO4	329.3995	weak abortifacient, immunosuppressant, analgesic,
206009	H09	C18H15NO3	293.3252	antiinflammatory
206009	H10	C10H14N4O2	222.2487	phosphodiesterase inhibitor
206009	H11	C34H28CuN4Na2	682.1517	antineoplastic
206010	A02	C22H18N2	310.4022	antifungal, calmodulin antagonist
206010	A03	C9H9NO	147.1782	antineoplastic
206010	A04	C17H14N2	246.3145	apoptosis inducer
206010	A05	C7H5N3O2	163.1368	NO synthetase inhibitor
206010	A06	C23H35NaO7	446.521	antihyperlipidemic, HMGCoA reductase inhibitor
206010	A07	C40H56O3	584.8905	antineoplastic
206010	A08	C28H31FN4O	458.5839	H1 antihistamine (nonsedating)
206010	A09	C23H28CIN3O5S	494.0137	antihyperglycemic
206010	A10	C10H6O3	174.1575	antineoplastic, antifungal
206010	A11	C10H12O4	196.2047	insect attractant, plant hormone
206010	B02	C15H12O2	224.2617	antineoplastic
206010	B03	C43H51N3O11	785.8994	antibacterial, RNA synthesis inhibitor
206010	B04	C19H22FN3O	327.4051	tranquilizer, neuroleptic, alpha adrenergic blocker
206010	B05	C17H20N4O6	376.3722	Vitamin B2; Vitamin cofactor; LD50(rat) 560 mg/kg ip
206010	B06	C23H30O11	482.489	antiinflammatory, antispasmodic, antihypertensive,
206010	B07	C21H23NO6	385.4206	antimitotic
206010	B08	C11H19NO9	309.2754	immunomodulator, adjuvant
206010	B09	C18H26N2O12	462.4141	nicotinyl acetylcholine receptor agonist,
206010	B10	C17H23NO4	305.3772	anticholinergic, antispasmodic
206010	B11	C25H24O6	420.4664	antioxidant
206010	C02	C46H77NO17	916.1231	antibacterial
206010	C03	C37H38N2O6	606.7252	antineoplastic, hepatoprotectant, radioprotective
206010	C04	C18H17NO5	327.3399	antiallergic, mast cell degranulation inhibitor,
206010	C05	C21H20O6	368.39	antiedemic, antiinflammatory, bile stimulant;
206010	C06	C12H19Cl2N	248.1979	inhibits dopamine & norepinephrine accumulation in
206010	C07	C6H6O4	142.1123	chelator, antibacterial, skin whitening agent
206010	C08	C17H26CINO	295.8559	acetylcholine transport blocker (vesicular)
206010	C09	C6H6N4O2	166.1403	diuretic, adenosine antagonist
206010	C10	C19H14O5	322.3204	antiinflammatory, antimicrobial
206010	C11	C29H38O4	450.6238	antineoplastic, antiinflammatory, NO synthesis
206010	D02	C20H18CIF2N3O	421.8346	antibacterial
206010	D03	C7H10N2O2S	186.234	antithyroid
206010	D04	C13H15NO2	217.27	GABAA receptor blocker, CNS stimulant
206010	D05	C8H5F3N2OS	234.2011	anticonvulsant, glutamate release inhibitor
206010	D06	C8H17NO2	159.2302	anticonvulsant
206010	D07	C10H14N4O2	222.2487	phosphodiesterase inhibitor
206010	D08	C11H15CIN2O	226.708	5HT agonist
206010	D09	C6H11NO2	129.1601	GABA uptake inhibitor
206010	D10	C18H16O7	344.324	antibacterial
206010	D11	C23H22O6	394.4282	antineoplastic, antiviral, insecticide
206010	E02	C6H7N3O	137.1422	antineoplastic, apoptosis inducer
206010	E03	C23H29ClO4	404.9382	progesterin, antiandrogen
206010	E04	C12H14O4	222.243	COX-1 inhibitor
206010	E05	C25H28N6O7S3	620.7299	antibacterial

Lee et al Supplemental Table 1

206010	E06	C15H24O	220.3579	antioxidant
206010	E07	C17H27NO3	293.4096	analgesic (topical), depletes Substance P
206010	E08	C17H18N2O5	330.3434	cholinesterase inhibitor, antiparkinsonian
206010	E09	C6H10N4	138.1734	analeptic, circulation stimulant
206010	E10	C21H24O10	436.4194	induces experimental glucosuria, antifeedant
206010	E11	C22H20O9	428.3993	coccidiostat
206010	F02	C9H12N2S	180.2734	antibacterial
206010	F03	C21H20O8	400.3888	antineoplastic
206010	F04	C23H48NO4P	433.6171	antineoplastic
206010	F05	C15H15NO2S	273.3563	analeptic
206010	F06	C48H76N2O4S	777.2159	antilepreitic
206010	F07	C10H15NO4	213.2354	glutamate receptor agonist, anthelmintic
206010	F08	C13H15CIN2	234.7309	anticholinesterase, K channel blocker
206010	F09	C11H17CIN2O	228.7239	5HT1 receptor agonist
206010	F10	C15H28N2O4S	332.4654	oxytocic
206010	F11	C23H22O6	394.4282	acaricide, ectoparasiticide, antineoplastic,
206010	G02	C11H16FN3O3	257.2669	antineoplastic
206010	G03	C21H46NO4P	407.5789	antineoplastic
206010	G04	C9H13NO	151.2101	antiulcer
206010	G05	C12H21NO8S	339.3671	anticonvulsant, antimigraine, GABA-A agonist,
206010	G06	C4H7N3O	113.1199	metabolic enhancer
206010	G07	C22H22O8	414.4158	antineoplastic, inhibits microtubule assembly, and
206010	G08	C7H8N2O2	152.154	cholagogue
206010	G09	C21H30O5	362.4703	glucocorticoid, antiinflammatory
206010	G10	C33H40N2O9	608.6948	antihypertensive
206010	G11	C38H44O8	628.7696	antiinflammatory, cytotoxic, inhibits HeLa cells in
206010	H02	C7H7Cl2NO	192.0459	antiplatelet
206010	H03	C18H14Cl4N4O4	492.1487	antifungal
206010	H04	C22H25Cl2N3O	418.3701	H1 antihistamine (nonsedating); leucotriene
206010	H05	C19H24FN5O7S	485.4948	antibacterial
206010	H06	C9H10O3	166.1783	antibacterial
206010	H07	C10H16CINO	201.6981	acetylcholinesterase inhibitor
206010	H08	C9H11NO4	197.1923	antiparkinsonian
206010	H09	C13H10O5	246.2217	GABA receptor antagonist, phototoxin
206010	H10	C12H8O4	216.1952	antipsoriatic, antiinflammatory
206010	H11	C30H36CINO10	606.0751	antibacterial, antineoplastic
206011	A02	C15H25CIN2O2	300.8317	anesthetic (local)
206011	A03	C5H6N2OS	142.1804	antithyroid agent
206011	A04	C9H10N4O2S2	270.3337	antibacterial
206011	A05	C19H14O3	290.3216	diagnostic aid
206011	A06	C26H30CIN3O6	515.9985	vasodilator
206011	A07	C12H10N2	182.2269	acaricide
206011	A08	C13H17CIN2	236.7468	adrenergic agonist, nasal decongestant
206011	A09	C19H20N2O3	324.3829	antiinflammatory
206011	A10	C23H20N2O3S	404.4915	uricosuric
206011	A11	C18H29CIN2O4	372.8958	antihypertensive, antianginal, antiarrhythmic
206011	B02	C26H28Cl2F2N2	477.4293	vasodilator
206011	B03	C18H16Cl3N3O3	460.7695	antifungal
206011	B04	C24H33FO6	436.5254	antiinflammatory
206011	B05	C24H32N2O9	492.5306	ACE inhibitor, antihypertensive
206011	B06	C21H27CIN2S2	407.0437	antipsychotic

Lee et al Supplemental Table 1

206011	B07	C7H10N2OS	170.2346	antihyperthyroid
206011	B08	C11H13N3O3S	267.3086	antibacterial
206011	B09	C13H16N2O2	232.2847	sleep induction, modifies circadian rhythm
206011	B10	C11H11F3N2O3	276.2171	antiandrogen
206011	B11	C17H22CINO3	323.8228	muscle relaxant (smooth)
206011	C02	C22H28O4	356.4661	estrogen
206011	C03	C15H16N7NaO5S	493.5205	antibacterial
206011	C04	C23H29N3O2S2	443.6345	antipsychotic
206011	C05	C5H5N3O	123.1151	antibacterial, tuberculostatic
206011	C06	C11H13N3O	203.2458	antipyretic, analgesic
206011	C07	C13H14N2O3	246.2681	antidepressant
206011	C08	C15H14O3S	274.341	antiinflammatory
206011	C09	C19H17CIN2O4	372.8113	analgesic
206011	C10	C15H23N3O4S	341.4323	dopamine receptor antagonist, antipsychotic
206011	C11	C18H16Cl3N3O4	444.7049	antifungal
206011	D02	C25H26N9NaO8S	667.6593	antibacterial
206011	D03	C10H13CIN2	196.6815	adrenergic blocker
206011	D04	C49H43N3O6	769.9056	anthelmintic
206011	D05	C21H26N2O3	354.453	vasodilator
206011	D06	C7H11NO5	189.1694	excitatory aminoacid
206011	D07	C13H10N2	194.2381	local antiseptic
206011	D08	C24H30CINO4	431.964	antispasmodic
206011	D09	C23H26FN3O2	395.481	antipsychotic
206011	D10	C24H31FO6	434.5095	antiinflammatory
206011	D11	C43H72O11	765.0467	antibacterial, antiviral
206011	E02	C15H14NNaO3	279.2735	antiinflammatory
206011	E03	C7H7NO2	137.1393	analgesic
206011	E04	C4H9NO2	103.1218	antihypertensive
206011	E05	C8H15NO6	221.2119	antiarthritic
206011	E06	C22H22FN3O2	379.4379	neuroleptic
206011	E07	C11H12N4O3S	280.3073	antibacterial
206011	E08	C13H9NOSe	274.1828	antioxidant, lipoxigenase inhibitor, inhibits oxidation
206011	E09	C7H12N2O4S	220.2487	muscle relaxant (smooth)
206011	E10	C21H27FO6	394.4441	glucocorticoid
206011	E11	C13H12N2O3S	276.3162	antibacterial
206011	F02	C14H8O6	272.2163	antiviral, HIV-1 integrase inhibitor
206011	F03	C25H34O6	430.5461	antiinflammatory
206011	F04	C14H10F3NO2	281.2365	antiinflammatory, analgesic
206011	F05	C11H12N4O3S	280.3073	antibacterial
206011	F06	C15H10NNaO3	275.2417	thromboxane synthetase inhibitor
206011	F07	C9H4Cl2N2O3	259.0498	NMDA and kainate receptor antagonist
206011	F08	C10H18O	154.2544	anthelmintic, antiseptic, expectorant
206011	F09	C22H25CIN2O8	480.9062	antibacterial
206011	F10	C34H47NO11	645.7538	anesthetic (gastric), antipyretic, and cardiotoxin
206011	F11	C22H22CINO4	399.8779	cytostatic, intercalating agent
206011	G02	C7H6O4	154.1235	antibacterial
206011	G03	C7H5NO3S	183.1868	sweetener
206011	G04	C12H16N2S	220.3387	analgesic
206011	G05	C8H16CINO4	225.674	cholinergic
206011	G06	C9H6FNO2	179.1521	NMDA receptor antagonist (gly)
206011	G07	C7H17CIN4O2	224.6921	NO synthase inhibitor

Lee et al Supplemental Table 1

206011	G08	C15H25ClN2O4S	364.8945	neuroleptic
206011	G09	C6H9NO2S	159.2081	hepatoprotectant
206011	G10	C5H8N4O3S2	236.2725	carbonic anhydrase inhibitor
206011	G11	C12H30Br2N2	362.1943	antihypertensive, ganglionic blocker
206011	H02	C14H20ClN3O	281.788	analgesic, antipyretic, antiinflammatory
206011	H03	C21H26ClN3OS	403.9779	antipsychotic
206011	H04	C10H16ClNO3	233.6969	bronchodilator
206011	H05	C18H16O8	360.3234	antiinflammatory, antithrombotic, antiplatelet,
206011	H06	C20H27NO11	457.4383	antiinflammatory, experimental antineoplastic
206011	H07	C20H22N5NaO6S	483.482	antibacterial
206011	H08	C20H22ClN	311.858	muscle relaxant (skeletal)
206011	H09	C28H44ClNO2	462.1214	antiinfectant
206011	H10	C13H16N3NaO4S	333.344	analgesic, antipyretic
206011	H11	C19H24ClNO5	381.8598	alpha1a adrenergic blocker
206012	A02	C40H67NaO11	746.9632	antibacterial
206012	A03	C8H14O2S2	206.3276	hepatoprotectant
206012	A04	C32H32O13S	656.668	antineoplastic
206012	A05	H6Cl2N2Pt	300.0572	antineoplastic, convulsant
206012	A06	C15H14F3N3O4S	421.4197	diuretic
206012	A07	C15H17FN4O3	320.3261	antibacterial
206012	A08	C12H19ClN2O4	290.7492	antihypertensive, vasoconstrictor
206012	A09	C15H16O2	228.2936	antiinflammatory
206012	A10	C25H32ClFO5	466.9822	glucocorticoid, antiinflammatory
206012	A11	C2H7AsO2	137.9985	antieczema, dermatologic, herbicide
206012	B02	C42H78N2O14	835.095	antibacterial
206012	B03	C10H13N5O4	267.2462	RT transferase inhibitor, antiviral
206012	B04	C7H5ClN2O3	200.5825	antiprotozoal, coccidiostat
206012	B05	C14H21Br2ClN2	412.5979	expectorant
206012	B06	C21H28O2	312.4561	progestogen
206012	B07	C17H27NO4	309.409	betaadrenergic blocker
206012	B08	C9H11NO2	165.1935	antidepressant
206012	B09	C19H29NaO5S	392.4938	menstrual regulation
206012	B10	C20H25Cl2NO	366.3344	antitussive
206012	B11	C12H19Cl2NO	264.1973	bronchodilator, beta adrenergic agonist
206012	C02	C15H23Cl2NO	282.8164	anesthetic (local)
206012	C03	C6H13N5O4	219.2016	NO synthase inhibitor
206012	C04	C18H24N5O8P	469.3945	vasodilator
206012	C05	C14H22BrN3O2	344.2543	antiemetic
206012	C06	C20H22Cl2N2O4	425.3153	psychostimulant
206012	C07	C20H23NO4	341.4106	morphine antagonist
206012	C08	C36H60O2	524.8784	provitamin, antixerophthalmic
206012	C09	C14H16O2	216.2824	antiinflammatory, analgesic, antipyretic
206012	C10	C22H27ClO3	374.9117	antiandrogen
206012	C11	C18H28ClN3O5S	433.958	antimalarial, lupus suppressant
206012	D02	C12H10F3N3O4	317.2264	antiandrogen
206012	D03	C9H10ClNO2	199.6386	Irreversible inhibitor of tryptophan hydroxylase
206012	D04	C21H29NO4S	391.5336	anticholinergic
206012	D05	C22H26N2O2	350.4647	cerebral vasodilator, antimotion
206012	D06	C23H39NO4	393.5716	coronary vasodilator
206012	D07	C20H22N2O4	354.4093	antidepressant, dopamine uptake inhibitor
206012	D08	C22H40ClN	354.0238	antiinfective (topical)



Lee et al Supplemental Table 1

206012	D09	C28H35FO7	502.5854	glucocorticoid, antiinflammatory
206012	D10	C19H24N2O6	376.4129	antiinflammatory
206012	D11	C20H23BrN2O4	435.3213	H1 antihistamine
206012	E02	C17H27N5O6	397.4346	analgesic
206012	E03	C14H28CINO6	341.8354	immunomodulator, antiinflammatory
206012	E04	C24H30N2O4	410.5177	antidepressant
206012	E05	C14H20CIN3S	297.8526	H1 antihistamine
206012	E06	C8H8O4	168.1506	antineoplastic, protein phosphatase inhibitor
206012	E07	C13H21CIN2O	256.7781	anesthetic (local)
206012	E08	C13H18N4O3	278.3134	vasodilator
206012	E09	C18H29CIN2O	324.8976	anesthetic (local)
206012	E10	C12H9F3N2O2	270.2129	antineoplastic, PDGF receptor blocker
206012	E11	C7H11NO2	141.1712	anticonvulsant
206012	F02	C9H13NO2	167.2095	hypnotic, sedative
206012	F03	C26H28N2	368.5265	H1 antihistamine
206012	F04	C13H19NO8	317.2983	antihypertensive
206012	F05	C41H76N2O15	837.0673	antibacterial
206012	F06	C15H20CINO	265.7858	beta adrenergic agonist, antiarrhythmic
206012	F07	C4H14Cl2N2S2	225.2036	hepatoprotectant, radioprotectant
206012	F08	C18H24N2O7S	412.4652	anthelmintic
206012	F09	C20H22O3	310.3965	sunscreen
206012	F10	C15H23NO4	281.3549	protein synthesis inhibitor
206012	F11	C16H16CIN3O3S	365.8412	diuretic, antihypertensive
206012	G02	C19H24Cl2N2	351.3225	antidepressant
206012	G03	C16H12O6	300.2704	analgesic, antipyretic
206012	G04	C5H7CIN2O3	178.5761	antineoplastic
206012	G05	C52H97NO18S	1056.413	antibacterial
206012	G06	C9H13NO	151.2101	decongestant
206012	G07	C11H12CINO3S	273.7402	anxiolytic, muscle relaxant
206012	G08	C10H13NO	163.2212	antihyperlipidemic
206012	G09	C14H19NO4	265.3118	antiprotozoal, antifungal, protein synthesis inhibitor
206012	G10	C12H14N4O4S	310.3338	antibacterial
206012	G11	C22H27CIN2O4S	450.9885	Ca channel blocker, coronary vasodilator
206012	H02	C16H24N4O2	304.3953	A1 adenosine antagonist
206012	H03	C17H19CIF3NO	345.7953	antidepressant
206012	H04	C7H5NS2	167.2526	antifungal
206012	H05	C21H27N3O5	401.4664	antihistaminic
206012	H06	C7H10N4O2S	214.2474	antibacterial
206012	H07	C7H8N4O2	180.1674	adenosine receptor agonist
206012	H08	C14H15NO4	261.28	aldose reductase inhibitor
206012	H09	C2H8CINS	113.6098	depigmentation, radiation protectant
206012	H10	C22H24CIN3O5	445.9067	antipsychotic
206012	H11	C16H17N3O4S	347.3956	antibacterial
206013	A02	C8H7CIN2O2S	230.6742	antihypertensive, diuretic, activates K channels and
206013	A03	C25H29N3O2	403.5288	analgesic, antipyretic
206013	A04	C6H6N4O2	166.1403	phosphodiesterase inhibitor
206013	A05	C22H22O8	414.4158	antineoplastic, cytotoxic
206013	A06	C29H34Cl2N2O2	513.5125	Ca channel blocker
206013	A07	C12H16N4O2	248.2869	A1 adenosine agonist
206013	A08	C17H16CIN3O	313.7896	antidepressant, inhibits norepinephrine uptake
206013	A09	C5H10CINO3	167.5934	antineoplastic

Lee et al Supplemental Table 1

206013	A10	C10H16O2	168.2378	esters as insecticide
206013	A11	C28H34O7	482.579	antifeedant
206013	B02	C15H15NO2	241.2923	antiinflammatory, analgesic
206013	B03	C27H39CIN2O4	491.0759	adrenegic blocker, Ca channel blocker, coronary
206013	B04	C25H30CII2NO3	681.7846	adrenergic agonist, coronary vasodilator, Ca channel
206013	B05	C12H17NO	191.2754	insect repellent
206013	B06	C19H23CIN4O2S	406.9378	antiulcer, M1 muscarinic antagonist
206013	B07	C16H22CINO2	295.8122	antihypertensive, antianginal, antiarrhythmic
206013	B08	C14H21N3O3S	311.4058	antidiabetic
206013	B09	C10H9CIN4O2S	284.7258	antibacterial
206013	B10	C18H23CI2NO	340.2961	alpha adrenergic blocker
206013	B11	C22H34O7	410.5121	adenylate cyclase activator, antiglaucoma,
206013	C02	C8H18CINO2	195.6912	cholinergic, diagnostic aid
206013	C03	C9H14CINO2	203.6704	mydriatic, decongestant
206013	C04	C12H14N2O2	218.2576	anticonvulsant
206013	C05	C7H16CINO2	181.6641	antiarrhythmic, miotic, vasodilator (peripheral)
206013	C06	C10H16CINO	201.6981	bronchodilator, cardiac stimulant
206013	C07	C17H19N2NaO6S	402.4046	antibacterial
206013	C08	C14H20N2O2	248.3277	antihypertensive, antianginal, antiarrhythmic,
206013	C09	C13H19NO4S	285.3647	uricosuric
206013	C10	C22H28O6	388.4649	insecticide, antiamoebic
206013	C11	C23H32CINO2	389.97	cytochrome P450 inhibitor, Ca antagonist
206013	D02	C28H44O	396.6623	antirachitic vitamin; LD50 (rat) 56 mg/kg po
206013	D03	C11H18CINO3	247.724	alpha1 adrenoreceptor agonist, vasoconstrictor
206013	D04	C23H26N5NaO7S	539.5468	antibacterial
206013	D05	C13H22CIN3O	271.7928	antiarrhythmic
206013	D06	C9H8O4	180.1617	analgesic, antipyretic, antiinflammatory
206013	D07	C27H36F2O6	494.5812	glucocorticoid, antiinflammatory
206013	D08	C24H29N3O6	455.5152	oxytocic
206013	D09	C15H13N3O4S	331.3526	antiinflammatory
206013	D10	C19H30CINO	323.9101	anticholinergic
206013	D11	C13H14O5	250.2535	antibacterial
206013	E02	C31H52O3	472.7583	vitamin E
206013	E03	C16H19N3O4S	349.4115	antibacterial
206013	E04	C22H29FO4	376.4724	glucocorticoid, antiinflammatory
206013	E05	C22H30O5	374.4814	glucocorticoid
206013	E06	C8H12CINO3	205.6427	adrenergic agonist (ophthalmic)
206013	E07	C21H30O2	314.4721	progestogen
206013	E08	C18H20O2	268.3589	estrogen
206013	E09	C25H34O8	462.5449	glucocorticoid
206013	E10	C21H28O5	360.4543	glucocorticoid
206013	E11	C15H10O5	270.244	antispasmodic, antineoplastic, topoisomerase I
206013	F02	C15H21CIN2O2	296.7998	antiinflammatory, bronchodilator
206013	F03	C5H7NO3	129.1164	anticonvulsant
206013	F04	C20H30BrNO3	412.371	bronchodilator, antiarrhythmic
206013	F05	C16H17KN2O5S	388.4903	antibacterial
206013	F06	C23H30O6	402.492	glucocorticoid
206013	F07	C32H37NO8	563.6536	estrogen antagonist, antineoplastic
206013	F08	C32H51NO13S	689.8262	antihypertensive
206013	F09	C19H22CINO	315.8463	antidepressant
206013	F10	C12H22O11	342.3025	laxative

Lee et al Supplemental Table 1

206013	F11	C17H17ClO6	352.7744	antifungal, inhibits mitosis in metaphase
206013	G02	C21H26O5	358.4384	glucocorticoid
206013	G03	C12H21NO7S	323.3677	betaadrenergic agonist, bronchodilator
206013	G04	C20H24N2O4	356.4253	antihistaminic
206013	G05	C10H16ClNO	201.6981	bronchodilator, decongestant
206013	G06	C23H32O4	372.5091	mineralocorticoid
206013	G07	C17H22N3O4P	363.3564	antihistaminic
206013	G08	C21H28N2O5	388.4677	antihistaminic, hypnotic
206013	G09	C30H44O9	548.6798	cardiotonic
206013	G10	C42H33N3O6	675.7478	anthelmintic, antischistosomal
206013	G11	C11H8O2	172.1852	prothrombogenic agent
206013	H02	C3H4N2S	100.1427	antithyroid agent
206013	H03	C12H12N2O3	232.241	antibacterial
206013	H04	C6H9ClN2O2	176.6038	GABAa agonist, GABA <sub>c</sub> antagonist
206013	H05	C22H29FO5	392.4718	glucocorticoid
206013	H06	C22H17ClN2	344.8472	antifungal
206013	H07	C47H79NO21	994.1478	antifungal, antibacterial, antiinflammatory agent
206013	H08	C22H32O2	328.4991	vitamin precursor
206013	H09	C17H26ClNO3	327.8547	anticholinergic (ophthalmic)
206013	H10	C13H19N5	245.3299	K channel agonist, antihypertensive
206013	H11	C13H18ClNO2	255.7469	antidepressant

<b>SOURCE</b>
synthetic
semisynthetic
synthetic
synthetic
provitamin A; widespread in plants and animals
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
synthetic
Streptomyces nodosus
Bacillus licheniformis and B subtilis
semisynthetic
synthetic
semisynthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
component of Madopa (Hoffmann-LaRoche)
synthetic
semisynthetic
synthetic
synthetic
synthetic
Colchicum autumnale
widespread in living tissue
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
Bacillus colistinus

Nicotiana tabacum
synthetic
synthetic
synthetic
synthetic
synthetic
Streptomyces venezuelae
synthetic
semisynthetic; U-21251
synthetic
synthetic
synthetic
synthetic
Cofea, Theobroma, Camelia and Cola spp
semisynthetic
synthetic
Streptomyces aureofaciens
synthetic
semisynthetic
synthetic
synthetic
Atropa and Datura spp
synthetic
Cinnamomum camphora
semisynthetic
synthetic
Streptomyces capreolis
synthetic
coal tar
synthetic
Strptomyces pilosus
synthetic
Streptomyces humidus
synthetic
pregnancy urine
synthetic
Fusidium spp
synthetic
semisynthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
semisynthetic
common in plant essential oils
synthetic
synthetic
semisynthetic
synthetic

Streptomyces aureofaiens
semisynthetic
synthetic
synthetic
semisynthetic
semisynthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
synthetic
mammalian hormone
semisynthetic
Micromonospora spp
semisynthetic
semisynthetic
Streptomyces spp
semisynthetic
synthetic
synthetic
synthetic
pregnacy urine, dates and Punica granatum seeds
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
Uragoga ipecacuanha
synthetic
synthetic
polysaccharides in bacteria, fungi, higher plants,
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
Portulaca grandiflora
semisynthetic
NF-180; synthetic
synthetic
Claviceps purpurea, many plants and animals
synthetic
synthetic
synthetic

Digitalis lanata or D. orientalis Lam.,
synthetic
ergot and Convolvulaceae spp
synthetic
synthetic
synthetic
semisynthetic
synthetic
Digitalis spp
synthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
Atropa, Datura and Hyoscyamus spp
synthetic
Streptomyces lincolnensis, S espinosus, S variabilis
semisynthetic
synthetic
synthetic
widespread in the plant and fungal kingdom
synthetic
semisynthetic
Penicillium spp
synthetic
synthetic
synthetic
semisynthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic

synthetic
synthetic
synthetic
synthetic
Corydalis cava and Papaver spp
synthetic
synthetic
synthetic
Streptomyces kanamyceticus
synthetic
synthetic
synthetic
synthetic
synthetic
Streptomyces niveus and S griseus
Streptomyces rimosus
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
Papaver somniferum, Rauwolfia serpentina
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
Streptomyces fradiae
synthetic
Streptomyces noursei
synthetic
Physostigma venenosum
Pilocarpus spp
synthetic
semisynthetic; L-5103, Ba-41166/E, NSC-113926
synthetic
synthetic
synthetic
synthetic
many plants, animal protein
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic



synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
Populus sieboldii
synthetic
Streptomyces spp
synthetic
synthetic
Bacillus aneurinolyticus; mixture of gramicidins & striated muscle, liver; also in Pisum sativum
synthetic
synthetic
synthetic
Scopolia, Datura, Atropa spp
synthetic
Camelia, thea, Paullinia cupana
synthetic
synthetic
bear bile
synthetic
semisynthetic
synthetic
synthetic
Micromonospora myoensis
synthetic
synthetic
semisynthetic
synthetic
Streptomyces orientalis
synthetic
rancid fats and Lycopodium spp
synthetic
Cinchona spp
Streptomyces spectabilis
synthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
Camelia, Theobroma, Cola spp
synthetic
Cinchona spp
synthetic
synthetic
synthetic

semisynthetic
synthetic
synthetic
synthetic
Rauwolfia spp., Melodinus balansae, Tonduzia
synthetic
coal tar
Streptomyces griseus
synthetic
synthetic
synthetic
synthetic
synthetic
salivary glands of Octopus vulgaris; also Capsicum
Cinchona bark
synthetic
Penicillium brevicompactum and other Penicillium
semisynthetic
semisynthetic
yeast
synthetic
Calumba root (Jateorhiza palmata)
synthetic
Berberis spp
constituent of mamalian feces, avian pigment
Corynanthe spp
Streptomyces antibioticus
synthetic
widespread in plants
Citrus spp
Berberis and Mahonia spp
black pepper (Piper nigrum L.)
synthetic
synthetic
synthetic
synthetic
Acokanthera and Strophanthus spp
synthetic
callabar bean, Physostigma venenosum
synthetic
semisynthetic
Aesculus hippocastanum, Fraxinus spp
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
pathological metabolite of tryptophan and kynurenine
semisynthetic
Peganium harmala

Veratrum album, V viride
synthetic
Streptomyces alboniger
synthetic
Strychnos nux-vomica and other Strychnos spp
betel nuts (Arica catechu)
synthetic
Lobelia spp
synthetic; L-isomer: spectrum
Peganium harmala
epimer of aglycone Glycyrrhiza glabra
Hydrastis canadensis
Anamirta cocculus, Menispermum cocculus
semisynthetic; GS-2989, NSC-78502
Solanaceae, Rhamnaceae, Passifloraceae,
synthetic
constituent of Bergamot oil
Agave and Yucca spp
thyroid gland
Peganium harmala
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
Pinus, Scutellaria, and Ulnus spp
synthetic
synthetic
Mimosa and Leucena spp
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
widely distributed in plants
synthetic
allantoic fluid; widely distributed in plants
Chrysophyllum and Nocardia spp
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
fish & liver oils, eggs, milk
synthetic
semisynthetic

synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
heartwood of Bignoniaceae
synthetic
semisynthetic
synthetic; L-isomer
synthetic
<i>Atractylis gummifera</i>
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
semisynthetic
<i>Salvia dorisiana</i>
<i>Areca catechu</i>
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
<i>Streptomyces</i> spp
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
constituent of neroli and bergamot oils
synthetic
semisynthetic
synthetic
synthetic
liver, kidney, green plants and fungi
synthetic
synthetic

synthetic
synthetic; ACPC
synthetic
synthetic
semisynthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
Galanthus, Narcissus and other Lillaceae
synthetic
semisynthetic
synthetic
synthetic; NPC-15199
Streptomyces fragilis
synthetic
synthetic
synthetic
synthetic
Abrus pectorius
Streptomyces cinnamomensis
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
Tolypocladium inflatum
synthetic
common plant alkaloid
Chlorophora tinctoria
synthetic
synthetic
Mentha piperita and other Mentha spp
synthetic
Streptomyces rimosus paramomycinus
synthetic
semisynthetic; TAO, NSC-108166
rat heart and liver
Hunteria eburnea
Tropaeolum majus, Lepidium sativum and other
synthetic
synthetic
synthetic
synthetic

synthetic
synthetic
synthetic
synthetic
Rheum spp and Eucalyptus sideroxylon
Vitamin B complex
synthetic
semisynthetic
synthetic
synthetic
semisynthetic
brain tissue
synthetic
ZPCK; synthetic
widely distributed in higher plants
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
plant and animal tissue
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
tuna muscle
Polygonum spp, Vitis vinifera
Crotalaria spp
synthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
synthetic
mamalian milk
Camptotheca acuminata
Salix spp
Artemisia annua
synthetic
synthetic
Streptomyces lasaliensis
synthetic
synthetic

synthetic
synthetic
synthetic
semisynthetic
semisynthetic
synthetic
Convallaria majalis
Xanthoria lichens, Rumex spp and various
synthetic
Celastrus and Maytenus spp
synthetic
Streptomyces albus
synthetic
semisynthetic
Taxus brevifolia
synthetic
Scutellaria baicalensis
Cassia & Rheum spp
synthetic; 5-Cl isomer present
Triclisia and Cyclea spp
synthetic
synthetic
synthetic
Melia azadirach and Azadirachta indica
synthetic
animal tissue and Coprinus comatus
Gossypium spp
synthetic
synthetic
widespread in Fabaceae
synthetic
synthetic
synthetic
Veratrum alba; contains 20% veratridine
widespread in plants
synthetic
Anabasis aphylla
synthetic
synthetic
Delphinium spp
synthetic
synthetic
Rauwolfia, Aspidosperma and Vinca spp
synthetic
synthetic
synthetic
Salsola richteri
synthetic
Pinus, Prunus, Eucalyptus spp
Aspergillus, Streptomyces spp & other
synthetic

sassafras officinale
synthetic
synthetic
synthetic
Ambrosia entemisiifolia
Thermopsis lanceolata
Jasminium spp and Vicia faba
synthetic
synthetic
Streptomyces ambofaciens
synthetic
Veratrum alba
semisynthetic
synthetic
synthetic
Penicillium cyclopium, Calopaca ferruginea
principal constituent of tree galls, esp Quercus spp;
synthetic
synthetic
synthetic
synthetic; W-7 HCl
synthetic
synthetic
synthetic
synthetic
Betula spp.
synthetic
Corydalis spp
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
derivative; rutin 7,3',4'-trihydroxyethyl ether
Lycopodium spp
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
Ginkgo biloba
Silybum marianum
synthetic
Rubia and Gallium spp
synthetic
synthetic



synthetic
Podophylum peltatum; epimer of podophyllotoxin;
semisynthetic
synthetic
synthetic
Epimedium spp
synthetic
Micromonospora spp
synthetic
synthetic
synthetic
Jasminium spp and Vicia faba
semisynthetic; CL-983, FK-482
synthetic
Streptomyces tenebrarius, Saccharomyces
synthetic
Allium spp, Wasabia japonica
synthetic
synthetic; R-757, Th-22
synthetic
synthetic; BMS-206584-01, AM-1155
synthetic
synthetic; CGP-48933
Persea spp
Centella asiatica
synthetic
synthetic
synthetic
silkworm moth Bombyx mori & the plant Achyranthes
synthetic
synthetic; BAYm-1099
synthetic
synthetic
Persia spp
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
Lupinus spp and other Leguminosae
Jateorhesa palmata, Berberis spp
semisynthetic
Ocimum gratissimum
synthetic
Streptomyces erythreus
synthetic
synthetic

synthetic
synthetic; S9490-3, McN-A2833-109
cytidine-5'-diphosphocholine
Sinomenium acutum and Stephania cepharantha
synthetic; WY-21743
synthetic
water soluble derivative of chlorophyll
synthetic
Brassica spp
synthetic
synthetic
Capsicum annum
synthetic
synthetic
leaves and nuts of Juglans spp., Carya spp and several commercial woods
Glycyrrhiza glabra
semisynthetic
synthetic
retina, whey and urine
Peonia spp
Colchicum autumnale
semisynthetic
Nicotiana tabacum
Scopolia tanguticus
Maclura pomifera
Streptomyces fradiae
Stephania spp
synthetic; MK-341
Curcuma spp
synthetic
Aspergillus spp
synthetic
major component of human urine
widespread in lichens
Celastrus scandens & Tripterygium wilfordii
synthetic
synthetic
Securinega spp and Phyllanthus discoides
synthetic
synthetic; CI-1008
synthetic
synthetic
synthetic
Usnea, Cladonia and other lichen spp
Tephrosia & Derris spp
synthetic
semisynthetic
synthetic
semisynthetic

synthetic; BHT
synthetic
synthetic
synthetic
Rosaceae spp:
Streptomyces species
synthetic
semisynthetic
synthetic
synthetic; CRL-40476, CEP-1538
synthetic
Digenia simplex
synthetic
synthetic
Lupinus spp and other Leguminosae
Derris spp
synthetic
synthetic
synthetic
synthetic
metabolite in muscle and urine; renal metabolite
Podophylotoxin Podophylum peltatum
synthetic
adrenal glands
semisynthetic
Garcinia morella, G hanburyii
synthetic
synthetic
synthetic
synthetic
Paeonia montan, Xanthorrhoea spp
synthetic
Vicia faba seedlings, Sarothamnus spp, & other
Heracleum maximum root; mp 118-119 C
widespread in Umbelliferae
Actinomyces spp
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic

synthetic
synthetic
pineal gland
synthetic
synthetic
semisynthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
SQ-13050; synthetic
semisynthetic
synthetic
synthetic
Vinca minor
synthetic
synthetic
synthetic
synthetic
semisynthetic
Streptomyces aereofaciens, and other Streptomyces
synthetic
synthetic
widely distributed in higher plants
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
eucalyptus and lavender oils
semisynthetic; GS-3065
Aconitum spp
semisynthetic
Aspergillus clavatus, Penicillium patulum
synthetic
synthetic
derivative of carnitine. striated muscle and liver
synthetic
broad-bean seeds and brain tissue

synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
Rosmarinus officinalis, Melissa officinalis,
Rosaceae spp
semisynthetic
synthetic
synthetic
synthetic
synthetic
Streptomyces hydroscopicus
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
vincamine Vinca minor
synthetic
synthetic
synthetic

synthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
semisynthetic; RU-28965, RU-965
synthetic
precursor to cysteamine
synthetic
synthetic
synthetic
synthetic
synthetic
synthetic
Streptomyces civiceus
Streptomyces erythreus
Ephedra vulgaris (MaHuang)
synthetic
synthetic
Streptomyces griseolus
synthetic
synthetic
synthetic
synthetic
synthetic; AG-63
synthetic
synthetic
synthetic
synthetic
cysteamine
synthetic
semisynthetic
synthetic
synthetic
synthetic
Podophyllum spp
synthetic
synthetic
synthetic
synthetic

esters as constituent of pyrethrum flowers
numerous Meliaceae species
synthetic
synthetic
synthetic
synthetic; N,N-diethyltoluamide
synthetic
synthetic
synthetic
synthetic
Coleus forskohlii
synthetic
synthetic
synthetic
synthetic
many Ephedra spp
semisynthetic
synthetic
synthetic
Quassia amara, Picrasma excelsa and Ailanthus
synthetic; SKF-525A
irradiation of ergosterol
synthetic
semisynthetic
synthetic
synthetic
semisynthetic
semisynthetic
synthetic
synthetic
Penicillium citrinum
derivative
semisynthetic
semisynthetic
semisynthetic
synthetic
semisynthetic
synthetic
semisynthetic
semisynthetic
parsley seed
synthetic
synthetic
synthetic
semisynthetic
semisynthetic
synthetic
Schoenocaulon officinale; shown as cevadine
synthetic
synthetic

Penicillium griseofulvum
semisynthetic
synthetic
synthetic
synthetic
semisynthetic
synthetic
synthetic
Thevetia peruviana
synthetic
Asplenium and Juglans spp.
synthetic
synthetic
synthetic; THIP hydrochloride
semisynthetic
synthetic
Solanum spp.
semisynthetic
semisynthetic
synthetic
synthetic







JACS 76:2943 (1954); Biochem Prep 12:81 (1968); J Steroid
Nature 162: 524 (1948)
Adv Carbohydr Chem 15:159 (1960); Methods Carbohydr Chem
JACS 40:1716 (1918); J Biol Chem 180:703 (1949); Arzneim-Forsch







J Chem Soc 1954: 1242; Angew Chem., 68: 13 (1956)
JACS 77: 1392, 2662 (1955); 78: 1375, 3693 (1956); 82: 3971
J Nat Prod 28: 73 (1965); Can J Chem 58: 2770 (1980)
J Indian Chem Soc 28: 225 (1951); 30: 705 (1953); Aust J Chem 9:
J Chem Soc 1950: 1534; Alkaloids 2: 406 (1952); Pharmacol Rev
JACS 61: 175 (1939); Tetrahedron 19: 773 (1963)
Coll Czech Chem Comm 35:124 (1970); J Nat Prod 40:384 (1977);
Tet Lett 1979: 1043
Ann Rev Biochem 15: 155 (1946); Helv Chim Acta 42: 1418 (1959);
J Chem Soc 1954: 3651
Naturwiss 29: 650 (1941); Phytochemistry 11: 657 (1972)
Mol Microbiol 42:553 (2001); BMC Physiology 1:7 (2001)
Biochem J 27: 727 (1933); Phytochemistry 19: 1573 (1980)

J Biol Chem 149:271 (1943); JACS 82:2242, 2252 (1960); Planta
Ber 21: 3404 (1888); Biochem J 122: 503 (1971)
Ber 63: 120 (1930)
J Nat Prod 45: 105 (1982)
JACS 57: 1111 (1935); 79: 5550 (1957); Chem Rev 67: 441 (1967)
Chem Ber 103:3674 (1970); Experientia 28:380 (1972);
Indian J Chem 13: 835 (1975)
Planta Med 63:199 (1997)
Biochem J 20: 293, 300 (1926)
Phytochemistry 7: 503 (1968)
Z Physiol Chem 244: 153 (1936)
J Chem Soc 119: 1602 (1921); 1929: 2926; Phytochemistry 1: 215
JACS 100: 6218 (1978)



Biochem Pharmacol 30: 1105 (1981)
Phytochemistry 14: 1829 (1975)
J Am Chem Soc 72: 2381 (1950); Experientia 26: 473 (1970); J Ber 51: 806, 976 (1918)
J Pharmacol Exp Ther 275: 864 (1995)
J Pharm Pharmacol 54:1521 (2002)
J Steroid Biochem 20: 945 (1984)



J Biol Chem 256: 10217 (1981)
Biochim Biophys Res Commun 189:280 (1992); Experientia 52:865
Biochem J 274:885 (1991)
PNAS 80:1116 (1983); Eur J Pharmacol 98:193 (1984); J Med
J Biol Chem 252:5931 (1977)
Biochemistry 10:3728 (1971); J Biol Chem 250:5221 (1975)
Biochem Biophys Res Comm 177: 828 (1991)
PNAS 93:9090 (1996)
Experientia 33:1348 (1977); 34:1052 (1978); Arch Int Pharmacodyn
Pharm Biol 11: 539 (1968)
Toxicol Appl Pharmacol 21: 405 (1972)
J Biol Chem 255:401 (1980); Res Commun Chem Pathol Pharmacol
Phytochemistry 13: 633 (1974); 15: 1791, 2006 (1976)
J Am Chem Soc 72: 158 (1950)
FEBS Lett 218:55 (1987)
J Am Chem Soc 88: 3888 (1966)
J Am Chem Soc 73: 5295 (1951)

Phytochemistry 13: 1805 (1974)
Helv Chim Acta 8: 140 (1925); Pharmacology 14: 1 (1976)
Metabolism 50: 688 (2001)
J Pharm Pharmacol 9: 855 (1957)
J Antibiotics 27: 814 (1954)
J Am Chem Soc 93: 2325 (1971)
Gazz Chim acta 49 (II): 47 (1919); Acta Phytochim 1: 109 (1923); Helv Chim Acta 33: 313 (1950)
Phytochemistry 14: 2524 (1975); Life Sci 68: 841 (2001)
Phytochemistry 12: 391 (1973)
J Am Chem Soc 60: 2193 (1938)
Neuropharmacol 39: 1653 (2000)
J Chem Soc 1953: 2183; Eur J Biochem 212: 87 (1992)
PNAS 77:3957 (1980); Int J Oncol 12:717 (1998)
Helv Chim Acta 11: 1062 (1928)
Carcinogenesis 21: 1879 (2000)
J Am Chem Soc 80: 497 (1958); J Org Chem 46: 3284 (1981)
Phytochemistry 12: 193 (1973); J Med Chem 33: 147 (1990)
Acta Chem Scand 5: 1, 121, 129 (1951); Chem Nat Comp 1: 111 Nature 164: 575 (1949)

J Org Chem 13: 448 (1948)
JACS 41:681 (1919); Science 263:966 (1994); Biochem J 316:247
J Chem Soc 1932: 2778; Martindale 28th Ed, 1700 (1982)
Helv Chim Acta 57: 1301 (1974); Tet Lett 3413 (1974); JACS 97:
J Am Chem Soc 91: 3401 (1969)
Helv Chim Acta 8: 126 (1925); Biochem J 34: 159 (1940)
mixed galloyl esters of penta-o-galloylglucose (m-digalloyl shown)
J Biochem 96: 1721 (1984; J Pharmac Exp Ther 251: 764 (1989)
Acta Chem Scand 19: 1661 (1965); Nature Medicine 1: 1046 (1995)
Steroids 65: 171 (2000)
Ber 56: 875 (1923); J Org Chem 33: 2785 (1968)
J Neurochem 54: 699 (1990)
Tet Lett 1960 (10): 26; Can J Chem 64: 837 (1986); Adv Med 1: 175
Toxicol Appl Pharmacol 73:411 (1984); Toxicol Lett 28:99 (1985)
Biochim Biophys Acta 944: 383 (1988)
Chem Soc Rev 8: 499 (1979); Phytochemistry 43: 1333 (1996)
Arzneim-Forsch 20: 1248 (1970); Chem Ber 108: 790, 1482 (1975);
J Biochem Toxicol. 6: 37(1991); Arch Toxicol 75: 221 (2001)
J Chem Soc 1928:229; 1929:1399; 1931:3206; Anticancer Res

JACS 73: 2909 (1951); 75: 1308 (1953); J Med Chem 32: 604
Eur J Clin Pharmacol 9: 253 (1976); Gastroenterology 124: 504 Planta Med 61: 523 (1995); J Chromatog A 963: 239 (2002)
Antimicrob Agents Chemother 6:144 (1974); J Antibiotics 28:573
Helv Chim Acta 57: 1301 (1974); Tet Lett 3413 (1974); JACS 97:
J Org Chem 41: 2087 (1976); 43: 1430 (1978); Eur J Biochem 99:
Arch Biochem Biophys 107:137 (1964); JACS 104:312 (1982); Drugs 51:621 (1996)
An Acad Brasil Cienc 42 (suplemento): 45 (1970); Tetrahedron Bull Soc Chim Fr 1967: 1890; Phytochemistry 7: 1385 (1968); 28:
J Vet Med Sci 65:1275 (2003)
J Med Chem 31:221 (1988); J Pharmacol Exp Ther 248:415 (1989)
Yakugaku Zasshi 87: 325 (1967); Arch Insect Biochem Physiol 33:
Ann Acad Brasil Cienc 42 (suplemento): 45 (1970); Tetrahedron 25: Pestic Biochem Physiol 48: 202(1994); J Pesticide Reform 21: 15
Am J Vet Res 38:465 (1977)
J Chem Soc 1949: 663
Ber 58: 2267 (1925); J Nat Prod 28: 73 (1965)
CR Hebd Seances Acad Sci 249:306 (1959); Cancer Res 57:420 Biochem J 369:71 (2003)

J Neurochem 65: 889 (1995); Neurosci Lett 273: 163 (1999)
Annalen 485: 247 (1931); J Chem Soc 1955: 3252; J
Mutat Res 308:191 (1994)
Eur J Pharmacol 313:265 (1996)
Anticancer Res 15:709 (1995); Biochem Mol Biol Int 39:1125 (1996)
Biochem Biophys Res Commun 228:153 (1996)
Eur J Pharmacol 310:115 (1996); TIPS 18:204 (1997)
Can J Chem 34: 1562 (1956)
Cancer Lett 168:125 (2001); Carcinogenesis 19:1697 (1998)
Drugs 49:467 (1995)
J Vet Pharmacol Ther 9:164 (1986); Psychopharmacol 52:107
Helv Chim Acta 35:457 (1952); Tet. Lett.,1969:3489; JACS 98:830
Tetrahedron 25:1825 (1969)
Col Czech Chem Commun 19: 805 (1954)
Naturwissenschaften 49: 281 (1962)
J Am Chem Soc 63: 1253 (1941)
Chem Ber 108:2481 (1975); Infection 5:183 (1977); Antimicrob
Biochem Pharmacol 46:1887 (1993); Antimicrob Agents Chemother
Br J Pharmacol 118:915 (1996); 122:1061 (1997); Eur J Pharmacol
Ber 51: 1347 (1918); J Pharm Pharmacol 5: 448 (1953); Cancer Res
J Med Chem 22:352 (1979)
Z Physiol Chem 24: 364 (1898); Biochem Pharmacol 30: 325 (1981)
J Am Chem Soc 72: 1824 (1950)
J Chem Soc 1963: 2884; 1972: 330; J Org Chem 30: 1729 (1965)
J Med Chem 28:1558 (1985); J Antimicrob Chemother 19:611
Clin Endocrinol 10:655 (1979)
Chem Ind 1962:1652; 1964:838, 1691; Naturwissenschaften 50:155
Neurosci Lett140:225 (1992); Anesthesiology 76:844 (1992);
Eur J Pharmacol 170: 35 (1989)
J Med Chem 30: 1 (1987)
J Neurochem 25: 797 (1975); Life Sci 19: 701 (1976)
J Chem Soc, 1953, 603; Antibiotics I (Verlag), 1967, p 611
J Am Chem Soc 56: 2415 (1934); J Org Chem 44: 2580 (1979);
Biochem Pharmacol 50:1943 (1995); Cancer Chemother Pharmacol
Cancer Metastasis Rev 6:615 (1987); Endocrin J 42:505 (1995)
Arch Biochem Biophys 317:19 (1995); OphthalmolVis Sci 39:1888







J Org Chem 40: 1804 (1975); 41: 449 (1976); Drugs of the Future
J Med Chem 38: 3415 (1995)
Drugs 61: 443 (2001)
JACS 75: 4675 (1953)
Mol Pharmacol 54: 162 (1998)
Biochem Biophys Res Comm 176: 1136 (1991); Biochem J 298: 249
Pharmacotherapy 31: 65 (1997)
Arzneimittel-Forsch 26: 1907 (1976)
J Clin Psychiatry 45: 12 (1984); Int Pharmacopsychiatry 17: 21



J Chem Soc 1945: 283
J Chem Soc 1960: 3827; 1962: 5095; 1967: 1026; 1969: 864; 1970,
Adv Drug Res 16: 309 (1987)
Gen Pharmacol 21: 17 (1990)
J Biol Chem 258:2960 (1983); J Med Chem 26:436, 486 (1983);
JACS 60:1146 (1938); 72:375 (1950); Tetrahedron 15:100 (1961);
Steroids 1959:90; Prog Chem Org Nat Prod 27:131 (1969)
J Chem Soc 1963: 3777
J Chem Soc 1963: 1477; Eur J Cancer 32A: 146 (1996); J Biol

J Chem Soc 1952: 3949
Helv Chim Acta 35:673, 730, 1073; 36:370 (1952); 45:907 (1962);
J Nat Prod 47: 901 (1984)
J Med Chem 24: 1377 (1981); 26: 895 (1983); Drugs of the Future
Chem Ber 90: 203 (1957)