

SUPPLEMENTAL INFORMATION FILES

A Class of Tricyclic Compounds Blocking Malaria Oocyst Development and Transmission

Richard T. Eastman,^{1,a} Sittiporn Pattaradilokrat,^{1,a} Dipak K. Raj,^{1,b} Saurabh Dixit,² Bingbing Deng,¹ Kazutoyo Miura,¹ Jing Yuan,¹ Takeshi Q. Tanaka,¹ Ronald L. Johnson,^{3,c} Hongying Jiang,¹ Ruili Huang,³ Kim Williamson,¹ Lynn E. Lambert,² Carole Long,¹ Christopher P. Austin,³ Yimin Wu,² and Xin-zhuan Su^{1,*}

¹ Laboratory of Malaria and Vector Research, National Institute of Allergy and Infectious Diseases, National Institutes of Health, Bethesda, Maryland 20892-8132, USA; ² Laboratory of Malaria Immunology and Vaccinology, National Institute of Allergy and Infectious Diseases, National Institutes of Health, Bethesda, Maryland 20892-8132, USA; and ³ NIH Chemical Genomics Center, National Human Genome Research Institute, National Institutes of Health, Bethesda, Maryland 20892-8132, USA

Running title: Discovery of drugs for blocking malaria transmission.

^a These authors contributed equally.

^b Present address: Center for International Health Research, Rhode Island Hospital, Providence, Rhode Island 02903, USA;

^c Present address: Division of Cancer Biology, National Cancer Institute, National Institutes of Health, Bethesda, Maryland 20892-8132, USA.

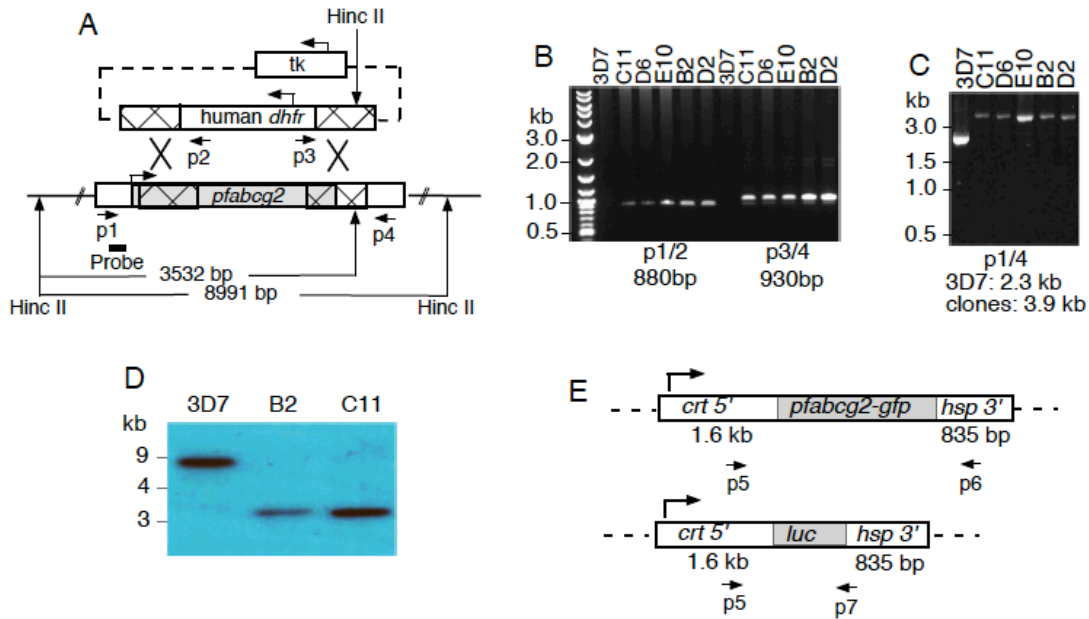


Fig. S1 Disruption of the gene encoding *Plasmodium falciparum* ABC transporter G2 (*pfabcg2*).

(A) diagram showing the pHTK plasmid contract containing the genes encoding human dihydrofolate reductase (*dhfr*) and herpes simplex virus thymidine kinase (*tk*) and the two DNA segments (hatched bars) flanking the *pfabcg2* genes. Positions of PCR primers (arrows) and a DNA probes used in Southern blot are also shown; **(B)** and **(C)** agarose gels showing PCR products amplified from 3D7 and five clones with *pfabcg2* disrupted. Primer pairs used to produce the products are shown under the gel images; **(D)** Southern blot showing a ~9-kb band from 3D7 and ~3.5-kb band from the two *pfabcg2* disrupted clones, as predicted from known restriction sites shown in (A); **(E)** Two constructs containing the genes encoding either PfABCG2 or Luciferase. *Crt 5'* is *P. falciparum* chloroquine-resistance transporter (*crt*) 5' untranslated region, and *hsp 3'* is the 3' untranslated region of the gene encoding *P. falciparum* heat shock protein 90.

Table S1 Primers used in plasmid construction and verification of construct integration into the homologous locus in the parasite genome.

Primer name	Primer sequence*
<i>Primers used to generate pfabcg2 null construct</i>	
Pf14_0244DI Fwd	<u>ggactag</u> tggttcatatatgcacac
Pf14_0244DI Rev	ga <u>agatc</u> tggaacttttatccagcttacc
Pf14_0244DII Fwd	<u>ccatcg</u> atacacttgactacttggtg
Pf14_0244DII Rev	cat <u>gccat</u> gggtcatgtgcctaccta
<i>Primers used to verify integration of pfabcg2 null construct</i>	
P1 (Pf14_0244 5' UTR)	ggtttattatatatgaggctc
P2 (<i>hrp</i> 2 3'UTR Fwd)	cataaagtacaacattaatatagc
P3 (Cam promoter Rev)	ttaacaaagaagaagctcagag
P4 (Pf14_0244 3' UTR)	caatgtaaaatggtaataatagc
Pf14_0244 promoter Fwd 2	ccccactgtataacccttatgggga
Pf14_0244 Promoter Rev	tacc <u>ctagg</u> tatggtgtaggtaggcacatgaaatacc
<i>Primers used to generate and verify rescue constructs</i>	
Pf14_0244 Fwd	tacc <u>ctagg</u> tatggttgaagggtggattcc
Pf14_0244 Rev	tac <u>ggatc</u> ctttcatttttaaggcttgggacc
Pf14_0244 Promoter Fwd	tac <u>gggccc</u> acttaaaataaaaagtacatacaggtg
Pf14_0244 Promoter Rev	tacc <u>ctagg</u> tatggtgtaggtaggcacatgaaatacc
P5 (1600crt promoter Fwd)	cgtaataataaatacacgcagtc
P6 (<i>hsp</i> 86 3' UTR Rev)	tgtagacccattgtgagtac
P7 (luciferase 3' Rev)	gagtttctactgcatacgacg

* Restriction sites are denoted with an underline

Table S2. Responses of three *Plasmodium falciparum* parasites (3D7, B2, and C11) to 2,816 drugs approved for human and animal use.

Sample ID	Name	B2 DCP	C11 DCP	Delta	Delta IC ₅₀	IC ₅₀		IC ₅₀		Activity	Activity	Activity	Efficacy	Efficacy	Efficacy
				IC ₅₀ B2	C11	3D7	IC ₅₀ B2	C11	3D7	B2	C11	3D7	B2	C11	
NCGC00167562-01	BUQUINOLATE	Sens	Sens	0.55	0.80	-6.3	-6.9	-7.1	A	A	A	-92	-92	-98	
NCGC00163221-01	AMBENONIUM	Sens	Sens	0.85	0.75	-5.5	-6.3	-6.2	A	A	A	-70	-59	-71	
NCGC00161419-02	TRIMETREXATE GLUCURONATE	Resist	Resist	-3.45	-3.45	-8.4	-4.9	-4.9	A	A	A	-98	-134	-115	
NCGC00016256-08	Pyrimethamine	Resist	Resist	-2.83		-7.4	-4.5		A	N	N	-97		-10	
NCGC00025060-04	methotrexate	Resist	Resist	-2.25	-2.20	-7.2	-4.9	-5.0	A	I	I	-95	-58	-56	
NCGC00160517-01	DIAVERIDINUM	Resist	Resist	-0.78	-0.78	-5.3	-4.5	-4.5	A	N	N	-92			
NCGC00167968-01	VALNEMULIN HYDROCHLORIDE	Resist	Resist	-0.55	-0.60	-5.7	-5.1	-5.1	A	I	I	-77	-49	-48	
NCGC00167486-01	PEMETREXED	Resist	Resist	-0.55	-0.55	-5.5	-4.9	-4.9	A	A	A	-93	-79	-80	
NCGC00015580-08	KETOTIFEN	Resist	Resist			-5.2			A	N	N	-91	-14	-16	
NCGC00167523-01	ORMETOPRIM	Resist	Resist		-0.68	-5.2		-4.5	A	N	N	-82		5	
NCGC00016055-05	Trimethoprim	Resist	Resist		-0.93	-5.5		-4.5	A	N	N	-100		11	
NCGC00016016-10	Triamterene	Resist	Resist			-5.8			A	N	N	-63	-4	-1	
NCGC00168751-01	BORTEZOMIB	Sens		0.65	0.40	-5.6	-6.2	-6.0	A	A	A	-101	-102	-103	
NCGC00181022-01	BORTEZOMIB	Sens		0.70	0.45	-5.7	-6.4	-6.1	A	A	A	-101	-99	-99	
NCGC00181051-01	STRYCHNINE SULFATE	Sens		0.50	0.40	-5.3	-5.8	-5.7	I	A	A	-55	-46	-59	
NCGC00016611-01	Bufexamac		Sens	0.25	0.55	-6.0	-6.3	-6.6	A	A	A	-94	-97	-94	
NCGC00167982-01	PIRARUBICIN		Sens	0.30	0.55	-4.9	-5.2	-5.5	A	A	A	-126	-103	-93	
NCGC00167438-01	TROSPIMUM CHLORIDE		Sens	0.35	0.75	-5.3	-5.7	-6.1	A	A	A	-95	-72	-62	
NCGC00016951-01	Clebopride maleate		Sens	0.00	0.65	-4.5	-4.5	-5.2	N	N	I			-41	
NCGC00160523-01	LANATOSIDE A		Sens		0.73	-4.5		-5.3	N	N	I		-25	-31	
NCGC00095264-01	CHLOROXYNE			-0.45	-0.25	-5.2	-4.7	-4.9	A	I	A	-104	-119	-119	
NCGC00163470-03	TACROLIMUS			-0.40	-0.05	-5.8	-5.4	-5.7	A	A	A	-98	-96	-91	
NCGC00093644-01	Amsacrine hydrochloride			-0.35	0.00	-5.8	-5.4	-5.8	A	A	A	-96	-98	-101	
NCGC00167969-01	RUBITECAN			-0.25	0.05	-5.3	-5.0	-5.3	A	A	A	-76	-83	-80	
NCGC00168786-01	DESERPIDINE			-0.25	-0.20	-6.5	-6.3	-6.3	A	A	A	-101	-98	-96	
NCGC00094422-01	SB 206553 hydrochloride			-0.20	0.10	-4.9	-4.7	-5.0	A	I	A	-90	-92	-81	
NCGC00160464-01	Rolicyclidine			-0.20	-0.05	-4.9	-4.7	-4.9	A	I	A	-101	-105	-114	
NCGC00015424-04	FLUSPIRILENE			-0.20	-0.05	-5.4	-5.2	-5.3	A	A	A	-105	-102	-97	
NCGC00094813-01	ACRIFLAVINIUM HYDROCHLORIDE			-0.20		-6.7	-6.5		A	A	N	-95	-97	-96	
NCGC00181122-01	LAURYL ISOQUINOLINIUM BROMIDE			-0.20		-6.0	-5.8		A	A	N	-98	-105	-98	
NCGC00015693-02	Mitoxantrone dihydrochloride			-0.20	0.05	-5.4	-5.2	-5.4	A	A	A	-107	-118	-106	
NCGC00024643-03	IFENPRODIL			-0.20	0.05	-5.3	-5.1	-5.3	A	A	A	-67	-74	-81	
NCGC00022001-05	Podofilox			-0.20	0.00	-5.0	-4.8	-5.0	A	A	A	-113	-143	-114	
NCGC00091250-04	Reserpine			-0.20	-0.20	-5.0	-4.8	-4.8	A	A	A	-111	-125	-133	
NCGC00025349-02	R(-)-APOMORPHINE			-0.15	0.00	-4.9	-4.8	-4.9	A	I	A	-116	-127	-111	
NCGC00166120-01	Mecetronium ethylsulfate			-0.15	0.05	-5.3	-5.2	-5.4	A	A	A	-95	-118	-108	
NCGC00095189-01	TOPOTECAN HYDROCHLORIDE			-0.15	-0.05	-5.4	-5.2	-5.3	A	A	A	-71	-77	-85	
NCGC00094476-03	R(+)-TERGURIDE			-0.15	0.15	-5.6	-5.5	-5.8	A	I	A	-42	-50	-57	
NCGC00160650-01	ACRINOL			-0.15	0.30	-5.6	-5.5	-5.9	A	A	A	-102	-108	-94	
NCGC0016961-01	Atovaquone			-0.15	-0.05	-8.9	-8.8	-8.9	A	A	A	-95	-97	-95	
NCGC00095070-01	HOMIDIUM BROMIDE			-0.15	-0.15	-6.9	-6.7	-6.7	A	A	A	-104	-99	-103	
NCGC00017042-01	Pyrvinium pamoate			-0.15	-0.35	-6.2	-6.1	-5.9	A	A	A	-106	-99	-99	
NCGC00094574-06	FIPRONIL			-0.15	-0.10	-5.5	-5.3	-5.4	A	A	A	-95	-97	-94	
NCGC00168085-01	SUBEROYLANILIDE HYDROXAMIC ACID			-0.15	-0.05	-6.3	-6.1	-6.2	A	A	A	-104	-101	-110	
NCGC00016913-08	ASTEMIZOLE			-0.15	-0.15	-6.0	-5.8	-5.8	A	A	A	-102	-101	-103	
NCGC00181330-01	NITROVIN			-0.10	0.15	-5.1	-5.0	-5.2	A	A	A	-109	-115	-97	
NCGC00016770-01	Miconazole			-0.10	0.10	-5.2	-5.1	-5.3	A	A	A	-111	-125	-116	
NCGC00159344-02	CARUBICINUM			-0.10	0.10	-5.1	-5.0	-5.2	A	A	A	-111	-117	-97	
NCGC00018268-03	itraconazole			-0.10	0.05	-5.3	-5.2	-5.4	A	A	A	-96	-104	-101	
NCGC00181017-01	PIMOBENDAN			-0.10	-0.15	-4.9	-4.8	-4.7	A	A	A	-82	-79	-93	
NCGC00095170-01	OXICONAZOLE NITRATE			-0.10	-0.05	-5.4	-5.3	-5.3	A	A	A	-99	-103	-104	
NCGC00181140-01	CARBOQUONE			-0.10	0.05	-6.1	-6.0	-6.1	A	A	A	-102	-101	-100	
NCGC00167550-01	NARASIN			-0.10	0.00	-7.3	-7.2	-7.3	A	A	A	-99	-90	-89	
NCGC00016602-01	Benperidol			-0.10	0.20	-5.4	-5.3	-5.6	A	A	A	-110	-108	-103	
NCGC00017148-01	Verteporfin			-0.10	0.15	-5.2	-5.1	-5.3	A	A	A	-100	-107	-98	
NCGC00164514-01	AMBAZONUM			-0.10	0.15	-5.2	-5.1	-5.3	A	A	A	-120	-78	-66	
NCGC00018258-03	Econazole nitrate			-0.10	0.05	-5.3	-5.2	-5.3	A	A	A	-101	-102	-98	
NCGC00166405-01	BENZALKONIUM CHLORIDE			-0.10	0.05	-5.3	-5.2	-5.3	A	A	A	-97	-129	-102	
NCGC00160648-01	Salinazid			-0.10	0.00	-4.9	-4.8	-4.9	A	A	A	-85	-109	-96	

NCGC00181023-01	NOLATREXED	-0.10	-0.10	-5.0	-4.9	-4.9	A	A	A	-89	-94	-115
NCGC00095162-01	TYLOSIN TARTRATE	-0.10	0.15	-5.7	-5.6	-5.9	A	I	A	-36	-49	-52
NCGC00159326-02	Lincomycin hydrochloride	-0.10	-0.05	-6.0	-5.9	-6.0	A	A	A	-38	-44	-59
NCGC00016336-01	Syrosingopine	-0.10	0.00	-5.8	-5.7	-5.8	A	A	A	-96	-100	-97
NCGC00167516-01	DESLORELIN ACETATE	-0.10	0.00	-5.4	-5.3	-5.4	A	A	A	-98	-102	-99
NCGC00167493-01	MANIDIPINE HYDROCHLORIDE	-0.10	-0.05	-5.4	-5.3	-5.4	A	A	A	-100	-94	-89
NCGC00094777-01	RIFAMPIN	-0.10	0.05	-5.7	-5.6	-5.8	A	A	A	-97	-106	-96
NCGC00091563-01	Tetramethylthiuram disulfide	-0.10	0.00	-5.7	-5.6	-5.7	A	A	A	-89	-97	-94
NCGC00021305-05	SIROLIMUS	-0.10	-0.05	-5.5	-5.4	-5.4	A	A	A	-102	-104	-103
NCGC00095098-01	TENIPOSIDE	-0.10	-0.05	-6.0	-5.9	-5.9	A	A	A	-96	-93	-86
NCGC00167512-01	EVEROLIMUS	-0.10	-0.05	-5.5	-5.4	-5.4	A	A	A	-101	-99	-98
NCGC00164493-01	Dipyrrithione	-0.10	-0.15	-6.2	-6.1	-6.1	A	A	A	-97	-108	-99
NCGC00091585-03	Octocrylene	-0.05	-0.05	-4.8	-4.8	-4.8	A	I	I	-112	-117	-111
NCGC00017112-01	Ciclopirox ethanolamine	-0.05	0.10	-5.2	-5.1	-5.3	A	I	A	-119	-113	-111
NCGC00091195-04	Hexachlorophene	-0.05	0.00	-4.8	-4.8	-4.8	A	I	A	-120	-115	-113
NCGC00016247-01	Cantharidin	-0.05	0.10	-5.4	-5.4	-5.5	A	A	A	-89	-92	-96
NCGC00161399-01	LOE 908 hydrochloride	-0.05	0.05	-5.3	-5.3	-5.4	A	A	A	-99	-102	-101
NCGC00166399-01	Imidocarbe	-0.05	-0.25	-5.1	-5.0	-4.8	A	A	A	-106	-99	-118
NCGC00181026-01	ROBENIDINE HYDROCHLORIDE	-0.05	0.00	-5.6	-5.5	-5.6	A	A	A	-98	-96	-97
NCGC00094424-01	Trequinsin hydrochloride	-0.05	-0.05	-5.8	-5.8	-5.8	A	A	A	-102	-95	-100
NCGC00159392-02	CHLOROBUTANOL	-0.05	0.30	-4.9	-4.8	-5.2	A	A	A	-132	-126	-104
NCGC00016486-01	(d,l)-Tetrahydroberberine	-0.05	0.20	-5.6	-5.5	-5.8	A	A	A	-82	-76	-79
NCGC00017114-01	Cefsulodin sodium salt	-0.05	0.20	-5.3	-5.3	-5.5	A	A	A	-113	-113	-105
NCGC00095150-01	TELMISARTAN	-0.05	0.10	-5.3	-5.2	-5.4	A	A	A	-87	-75	-76
NCGC00167582-01	CETALKONIUM CHLORIDE	-0.05	0.10	-4.9	-4.8	-5.0	A	A	A	-121	-109	-89
NCGC00164615-01	Prulifloxacin	-0.05	0.05	-5.4	-5.3	-5.4	A	A	A	-99	-99	-102
NCGC00164603-01	Ebastine	-0.05	0.00	-5.0	-5.0	-5.0	A	A	A	-110	-116	-110
NCGC00181142-02	PARA-CHLOROMERCURIPHENOL	-0.05	-0.05	-5.2	-5.2	-5.2	A	A	A	-89	-86	-95
NCGC00167435-01	NILVADIPINE	-0.05	-0.10	-4.9	-4.9	-4.8	A	A	A	-98	-105	-110
NCGC00167430-01	TIOCONAZOLE	-0.05	0.00	-5.4	-5.3	-5.4	A	A	A	-98	-99	-103
NCGC00016554-01	Nifuroxazide	-0.05		-5.6	-5.6		A	A	I	-90	-92	-90
NCGC00095016-01	CLOFOCTOL	-0.05	0.00	-5.4	-5.3	-5.4	A	A	A	-100	-95	-91
NCGC00095258-01	MITOMYCIN C	-0.05	0.20	-6.2	-6.2	-6.4	A	A	A	-98	-97	-92
NCGC00163233-01	IVERMECTIN	-0.05	0.15	-5.5	-5.5	-5.7	A	A	A	-98	-96	-96
NCGC00167495-01	METHYL VIOLET	-0.05	0.10	-6.2	-6.1	-6.3	A	A	A	-99	-100	-98
NCGC00167963-01	DIPHENOXYLATE HYDROCHLORIDE	-0.05	0.05	-5.5	-5.4	-5.5	A	A	A	-99	-103	-101
NCGC00015735-07	Niclosamide	-0.05	0.00	-6.0	-6.0	-6.0	A	A	A	-99	-98	-101
NCGC00091935-01	Ergotamine D-tartrate	-0.05	0.00	-6.0	-5.9	-6.0	A	A	A	-99	-98	-98
NCGC00095101-01	TANNIC ACID	-0.05	0.00	-5.5	-5.5	-5.5	A	A	A	-104	-106	-102
NCGC00164367-01	Paclitaxel	-0.05	0.00	-6.7	-6.6	-6.7	A	A	A	-75	-76	-79
NCGC00181043-01	CLOBETASONE BUTYRATE	-0.05	0.00	-5.5	-5.4	-5.5	A	A	A	-96	-99	-99
NCGC00181146-01	SIROLIMUS	-0.05	0.00	-5.4	-5.4	-5.4	A	A	A	-101	-93	-97
NCGC00091933-01	Zinc pyrithione	-0.05	-0.05	-6.4	-6.3	-6.3	A	A	A	-97	-103	-100
NCGC00094893-01	PUROMYCIN HYDROCHLORIDE	-0.05	-0.05	-6.3	-6.2	-6.2	A	A	A	-100	-102	-98
NCGC00091112-02	Chlorure de methylosanilinum	-0.05		-6.2	-6.2		A	A	N	-101	-98	-101
NCGC00160442-01	Metochalcone	0.00	0.40	-4.8	-4.8	-5.2	A	I	A	-120	-103	-96
NCGC00091023-01	Cetylpyridinium bromide	0.00	0.25	-5.2	-5.2	-5.4	A	A	A	-98	-100	-79
NCGC00095172-01	SECURININE	0.00	0.20	-4.9	-4.9	-5.1	A	A	A	-121	-116	-101
NCGC00016786-01	Mycophenolic acid	0.00	0.10	-5.6	-5.6	-5.7	A	A	A	-95	-97	-93
NCGC00159459-02	MYCOPHENOLATE MOFETIL	0.00	0.10	-5.2	-5.2	-5.3	A	A	A	-103	-95	-96
NCGC00167436-01	AZELNIDIPINE	0.00	0.10	-5.0	-5.0	-5.1	A	A	A	-110	-106	-105
NCGC00181158-01	MERCUFENOL CHLORIDE	0.00	0.10	-5.4	-5.4	-5.5	A	A	A	-104	-99	-103
NCGC00017400-05	DIHYDROERGOTAMINE	0.00	0.05	-5.1	-5.1	-5.2	A	A	A	-102	-100	-104
NCGC00091455-01	Celecoxib	0.00	0.00	-4.8	-4.8	-4.8	A	A	A	-88	-87	-93
NCGC00164571-01	Dutasteride	0.00	0.00	-5.3	-5.3	-5.3	A	A	A	-87	-85	-92
NCGC00168257-01	DRONABINOL	0.00	0.00	-5.3	-5.3	-5.3	A	A	A	-99	-99	-103
NCGC00181154-01	NITARSONE	0.00	0.00	-5.3	-5.3	-5.3	A	A	A	-96	-96	-100
NCGC00024964-02	Fulvestrant	0.00	-0.05	-4.9	-4.9	-4.8	A	A	A	-116	-113	-121
NCGC00092329-02	Eliprodil	0.00	-0.05	-5.3	-5.3	-5.3	A	A	A	-79	-87	-88
NCGC00159460-02	INDINAVIR SULFATE	0.00	-0.10	-4.9	-4.9	-4.8	A	A	A	-92	-75	-98
NCGC00164576-02	LOPINAVIR	0.00	-0.05	-5.4	-5.4	-5.3	A	A	A	-103	-106	-103
NCGC00181009-01	TIMEPIDIUM BROMIDE	0.00	0.30	-5.4	-5.4	-5.7	A	A	A	-94	-91	-81
NCGC00093556-01	Amperozide hydrochloride	0.00	0.20	-5.3	-5.3	-5.5	A	A	A	-95	-90	-93
NCGC00091826-01	N-Isopropyl-N'-phenyl-p-phenylenediamine	0.00	0.05	-5.3	-5.3	-5.4	A	A	A	-93	-95	-95

NCGC00159519-02	Tolterodina	0.00	0.05	-5.3	-5.3	-5.4	A	A	A	-99	-102	-100
NCGC00160675-01	Carminomycin	0.00	0.05	-5.3	-5.3	-5.4	A	A	A	-101	-109	-99
NCGC00163163-01	DIHYDROERGOCRISTINE	0.00	0.05	-5.3	-5.3	-5.4	A	A	A	-98	-98	-95
NCGC00167984-01	TIQUIZIUM BROMIDE	0.00	0.05	-5.3	-5.3	-5.4	A	A	A	-93	-91	-91
NCGC00167971-01	TIOTROPIUM BROMIDE MONOHYDRATE	0.00	-0.05	-5.8	-5.8	-5.7	A	A	A	-44	-46	-61
NCGC00024246-05	Daunorubicinum	0.00	0.05	-5.4	-5.4	-5.4	A	A	A	-99	-100	-100
NCGC00159499-02	QUINIDINE GLUCONATE	0.00	0.45	-6.8	-6.8	-7.3	A	A	A	-95	-98	-98
NCGC00181150-01	BRYOSTATIN-1	0.00	0.30	-5.4	-5.4	-5.7	A	A	A	-95	-98	-91
NCGC00181131-01	EPOTHILONE B	0.00	0.15	-8.8	-8.8	-9.0	A	A	A	-72	-77	-80
NCGC00095235-01	ARTENIMOL	0.00	0.15	-8.6	-8.6	-8.7	A	A	A	-98	-93	-96
NCGC00163424-01	17-Allylamino-geldanamycin	0.00	0.10	-5.8	-5.8	-5.9	A	A	A	-95	-95	-101
NCGC00167492-01	LERCANIDIPINE HYDROCHLORIDE	0.00	0.10	-5.7	-5.7	-5.8	A	A	A	-96	-96	-97
NCGC00094104-01	MG 624	0.00	0.05	-5.8	-5.8	-5.8	A	A	A	-88	-96	-97
NCGC00095128-01	ORLISTAT	0.00	0.05	-5.8	-5.8	-5.8	A	A	A	-89	-91	-87
NCGC00160207-01	Artemisinin	0.00	0.05	-8.2	-8.2	-8.2	A	A	A	-98	-95	-99
NCGC00017089-01	Monensin sodium salt	0.00	0.05	-7.6	-7.6	-7.7	A	A	A	-100	-97	-98
NCGC00091050-02	PHENYLMERCURIC ACETATE	0.00	0.05	-5.4	-5.4	-5.4	A	A	A	-97	-94	-96
NCGC00095285-01	VINBLASTINE SULFATE	0.00	0.05	-5.5	-5.5	-5.5	A	A	A	-73	-79	-83
NCGC00164591-01	Artemetero	0.00	0.05	-7.8	-7.8	-7.9	A	A	A	-103	-106	-105
NCGC00163135-01	NIGULDIPINE	0.00	0.00	-5.4	-5.4	-5.4	A	A	A	-99	-96	-101
NCGC00167484-01	CICLESONIDE	0.00	0.00	-6.0	-6.0	-6.0	A	A	A	-102	-100	-86
NCGC00167513-01	VANDETANIB	0.00	0.00	-5.7	-5.7	-5.7	A	A	A	-96	-97	-98
NCGC00166015-01	C.I. Basic Violet 14, free base	0.00	-0.05	-5.8	-5.8	-5.8	A	A	A	-93	-89	-78
NCGC00164738-01		0.00	-0.10	-5.8	-5.8	-5.7	A	A	A	-97	-97	-103
NCGC00013067-01	cinchonine	0.00		-6.8	-6.8		A	A	N	-98	-80	-102
NCGC00163507-01	OCTYLONIUM BROMIDE	0.05	0.10	-4.8	-4.9	-4.9	A	I	I	-101	-80	-93
NCGC00164283-01	Cetyltrimethylammonium bromide	0.05	0.25	-4.9	-5.0	-5.2	A	A	A	-91	-91	-84
NCGC00167576-01	APRINDINE HYDROCHLORIDE	0.05	0.10	-5.2	-5.3	-5.3	A	A	A	-104	-103	-100
NCGC00167798-01	OXALIPLATIN	0.05	0.10	-5.2	-5.3	-5.3	A	A	A	-88	-93	-93
NCGC00095256-01	QUININE ETHYL CARBONATE	0.05	0.10	-5.4	-5.4	-5.5	A	A	A	-95	-93	-103
NCGC00160378-01	PRANOLII CHLORIDUM	0.05	0.10	-5.2	-5.2	-5.3	A	A	A	-85	-79	-84
NCGC00166113-01	DIPHENYLCYCLOPROPENONE	0.05	0.10	-4.8	-4.9	-4.9	A	A	A	-119	-120	-105
NCGC00018292-04	DISTAMYCIN A	0.05	0.05	-4.9	-5.0	-5.0	A	A	A	-111	-110	-110
NCGC00073294-02	QUINOCIDUM	0.05	-0.25	-5.4	-5.5	-5.2	A	A	A	-102	-101	-123
NCGC00164548-01	Danofloxacin mesylate	0.05	0.05	-5.7	-5.8	-5.8	A	A	A	-44	-54	-56
NCGC00013217-01	2,3-DIMERCAPTOBUTANEDIOIC ACID, ARSENIC(3+) SALT	0.05	0.25	-5.4	-5.5	-5.7	A	A	A	-107	-111	-104
NCGC00164639-01	Arsenic trioxide	0.05	0.25	-5.4	-5.5	-5.7	A	A	A	-105	-108	-97
NCGC00016372-01	Roxarsone	0.05	0.20	-5.7	-5.7	-5.9	A	A	A	-91	-97	-93
NCGC00093685-01	Bestatin hydrochloride	0.05	0.30	-5.8	-5.9	-6.1	A	A	A	-85	-98	-94
NCGC00016526-02	Berberine chloride	0.05	0.20	-6.6	-6.6	-6.8	A	A	A	-95	-94	-90
NCGC00165966-02	VINORELBINE TARTRATE	0.05	0.15	-5.6	-5.7	-5.8	A	A	A	-105	-105	-102
NCGC00167586-01	PIROCTONE OLAMINE	0.05	0.10	-5.5	-5.5	-5.6	A	A	A	-102	-103	-102
NCGC00168772-01	LESTAUTINIB	0.05	0.10	-6.2	-6.3	-6.3	A	A	A	-100	-101	-102
NCGC00160275-02	HELIOMYCINUM	0.05	0.10	-5.6	-5.6	-5.7	A	A	A	-96	-90	-92
NCGC00181319-01	PLICAMYCIN	0.05	0.10	-7.3	-7.4	-7.4	A	A	A	-97	-79	-96
NCGC00094791-01	THIMEROSAL	0.05	0.05	-5.7	-5.8	-5.8	A	A	A	-96	-96	-101
NCGC00095029-01	LASALOCID SODIUM	0.05	0.05	-6.1	-6.2	-6.2	A	A	A	-96	-97	-98
NCGC00095055-01	SALINOMYCIN, SODIUM	0.05	0.05	-6.4	-6.4	-6.4	A	A	A	-99	-89	-89
NCGC00160369-01	Phanquone	0.05	0.05	-5.8	-5.9	-5.9	A	A	A	-104	-104	-98
NCGC00166066-01	DIDECYL DIMETHYL AMMONIUM CHLORIDE	0.05	0.05	-5.4	-5.4	-5.4	A	A	A	-97	-96	-100
NCGC00181306-01	DOCETAXEL	0.05	0.05	-7.7	-7.7	-7.7	A	A	A	-78	-73	-78
NCGC00015608-04	LOPERAMIDE	0.05	0.10	-4.8	-4.8	-4.9	A	A	A	-121	-118	-116
NCGC00024584-03	BROMOCRIPTINE	0.05	-0.10	-5.0	-5.1	-4.9	A	A	A	-107	-106	-126
NCGC00164600-01	ARTEMISININUM	0.05	0.05	-8.5	-8.6	-8.6	A	A	A	-99	-104	-102
NCGC00064532-02	TROVAFLOXACIN MESYLATE	0.10	0.25	-4.8	-4.9	-5.1	A	I	A	-109	-79	-89
NCGC00159451-02	TINORIDINE HYDROCHLORIDE	0.10	0.30	-5.2	-5.3	-5.5	A	A	A	-104	-108	-101
NCGC00161826-01	PHENYLMERCURIC BORATE	0.10	0.30	-5.2	-5.3	-5.5	A	A	A	-97	-100	-87
NCGC00163450-02	ILOMASTATUM	0.10	0.20	-5.1	-5.2	-5.3	A	A	A	-84	-98	-110
NCGC00159424-02	TETRAMETHYLTHIURAM MONOSULFIDE	0.10	0.05	-5.2	-5.3	-5.2	A	A	A	-101	-101	-105
NCGC00160546-01	Haloxon	0.10	0.05	-4.8	-4.9	-4.9	A	A	A	-97	-84	-97
NCGC00016283-01	Diphemanil methylsulfate	0.10	0.00	-5.2	-5.3	-5.2	A	A	A	-88	-83	-107
NCGC00095154-01	TELITHROMYCIN	0.10	0.30	-6.2	-6.3	-6.5	A	A	A	-35	-41	-49
NCGC00021394-03	ANISOTROPINE METHYLBROMIDE	0.10	0.20	-5.2	-5.3	-5.4	A	A	A	-93	-87	-89
NCGC00166121-01	TETRADONI BROMIDUM	0.10	0.05	-5.3	-5.4	-5.4	A	A	A	-97	-102	-98

NCGC00164554-03	MUPIROCIN	0.10	0.15	-6.9	-7.0	-7.0	A	A	A	-44	-53	-63
NCGC00181127-01	VINROSIDINE SULFATE	0.10	0.20	-5.7	-5.8	-5.9	A	A	A	-91	-76	-85
NCGC00015819-06	PROPAFENONE	0.10	0.10	-5.7	-5.8	-5.8	A	A	A	-96	-96	-99
NCGC00018301-02	SULOCTIDIL	0.10	0.05	-5.8	-5.9	-5.9	A	A	A	-95	-96	-98
NCGC00091881-01	Toxaphene	0.10	0.05	-5.4	-5.5	-5.5	A	A	A	-100	-104	-106
NCGC00168784-01	GEMCITABINE HYDROCHLORIDE	0.10	0.30	-5.5	-5.6	-5.8	A	A	A	-115	-106	-111
NCGC00016622-02	HYCANTHONE	0.10	0.25	-5.0	-5.1	-5.2	A	A	A	-92	-96	-93
NCGC00016854-03	VINPOCETINE	0.10	0.25	-5.0	-5.1	-5.3	A	A	A	-107	-99	-98
NCGC00015747-03	NICARDIPINE	0.10	0.20	-5.0	-5.1	-5.2	A	A	A	-106	-100	-94
NCGC00181116-01	CARBOMYCIN	0.10	0.20	-5.0	-5.1	-5.2	A	A	A	-110	-98	-119
NCGC00015385-12	DIPYRIDAMOLE	0.10	0.15	-5.0	-5.1	-5.1	A	A	A	-99	-99	-95
NCGC00168750-01	OXALIPLATIN	0.10	0.10	-5.2	-5.3	-5.3	A	A	A	-90	-102	-97
NCGC00181100-01	ORMELOXIFENUM	0.10	0.15	-5.2	-5.3	-5.4	A	A	A	-104	-97	-102
NCGC00025155-01	Homoharringtonine	0.10	0.15	-7.8	-7.9	-7.9	A	A	A	-98	-96	-97
NCGC00159483-02	HYDROXYCHLOROQUINE SULFATE	0.10	0.10	-6.2	-6.3	-6.3	A	A	A	-101	-102	-97
NCGC00016046-02	Tyrphostin 25	0.15	0.20	-4.8	-5.0	-5.0	A	A	A	-123	-103	-100
NCGC00016747-03	DILAZEP	0.15	0.20	-4.8	-5.0	-5.0	A	A	A	-87	-87	-78
NCGC00181121-01	CARPHENAZINE MALEATE	0.15	0.20	-4.8	-5.0	-5.0	A	A	A	-123	-109	-110
NCGC00025302-01	Altanserin hydrochloride	0.15	0.15	-4.9	-5.0	-5.0	A	A	A	-114	-92	-99
NCGC00160567-01	Acetomenaphthone	0.15	0.05	-4.9	-5.0	-4.9	A	A	A	-114	-100	-112
NCGC00015256-01	Chloroquine diphosphate	0.15	0.00	-7.1	-7.2	-7.1	A	A	A	-100	-103	-103
NCGC00095182-01	GEMIFLOXACIN MESYLATE	0.15	0.30	-5.0	-5.2	-5.3	A	A	A	-96	-91	-95
NCGC00093976-03	IDARUBICIN HYDROCHLORIDE	0.15	0.25	-4.9	-5.1	-5.2	A	A	A	-127	-101	-84
NCGC00094089-01	Mibefradil dihydrochloride	0.15	0.10	-5.2	-5.4	-5.3	A	A	A	-102	-105	-99
NCGC00095165-01	CARMOFUR	0.15	0.20	-5.2	-5.3	-5.4	A	A	A	-86	-90	-88
NCGC00181085-01	MYRISTYL-GAMMA-PICOLINIUM CHLORIDE	0.15	0.20	-5.8	-5.9	-6.0	A	A	A	-89	-92	-94
NCGC00017063-01	Amodiaquin dihydrochloride dihydrate	0.15	0.15	-7.4	-7.5	-7.5	A	A	A	-97	-99	-100
NCGC00160524-01	AMINOQUINOLUM	0.15	0.10	-5.7	-5.8	-5.8	A	A	A	-99	-100	-103
NCGC00181132-01	HALOFUGINONE LACTATE	0.15	0.05	-5.5	-5.6	-5.5	A	A	A	-96	-99	-98
NCGC00181139-01	DEXTROAMPHETAMINE SACCHARATE	0.15	0.05	-6.2	-6.4	-6.3	A	A	A	-100	-96	-96
NCGC00015251-02	Clotrimazole	0.15	0.00	-5.9	-6.0	-5.9	A	A	A	-98	-97	-97
NCGC00016890-01	Cyclosporin A	0.20	0.25	-4.8	-5.0	-5.1	A	A	A	-130	-114	-113
NCGC00091010-01	Domiphen bromide	0.20	0.20	-5.1	-5.3	-5.3	A	A	A	-109	-103	-97
NCGC00164034-01	Triclocarban	0.20	0.20	-5.0	-5.2	-5.2	A	A	A	-112	-99	-101
NCGC00167481-01	ACLARUBICIN HYDROCHLORIDE	0.20	0.35	-6.4	-6.6	-6.8	A	A	A	-105	-104	-100
NCGC00017142-01	Clofilium tosylate	0.20	0.30	-6.1	-6.3	-6.4	A	A	A	-102	-101	-95
NCGC00163237-01	DECAMETHONIUM	0.20	0.30	-5.9	-6.1	-6.2	A	A	A	-84	-91	-87
NCGC00181147-01	PLICAMYCIN	0.20	0.25	-7.0	-7.2	-7.3	A	A	A	-102	-95	-98
NCGC00016752-01	Clindamycin hydrochloride	0.20		-6.7	-6.9		A	A	N	-46	-43	-26
NCGC00013130-03	AMINOQUINURIDUM	0.25	0.20	-4.9	-5.1	-5.1	A	A	A	-104	-84	-89
NCGC00163543-01	DOXORUBICIN	0.25	0.20	-4.8	-5.1	-5.0	A	A	A	-135	-117	-125
NCGC00013058-01	Malachite Green Oxalate	0.25	0.15	-5.0	-5.2	-5.1	A	A	A	-100	-105	-99
NCGC00017057-01	Quinacrine dihydrochloride dihydrate	0.25	0.20	-6.9	-7.1	-7.1	A	A	A	-99	-100	-103
NCGC00163697-01	CHROMOMYCIN A3	0.25	0.05	-6.9	-7.2	-7.0	A	A	A	-95	-98	-95
NCGC00163699-01	FUMAGILLIN	0.30	0.25	-7.7	-8.0	-8.0	A	A	A	-51	-54	-60
NCGC00016284-01	Primaquine diphosphate	0.30	0.20	-5.9	-6.2	-6.1	A	A	A	-102	-96	-96
NCGC00181356-01	OXAPIUM IODIDE	0.30	0.40	-5.4	-5.7	-5.8	A	A	A	-97	-92	-93
NCGC00166281-01	QUININE ASCORBATE	0.30	0.35	-6.3	-6.6	-6.7	A	A	A	-98	-96	-97
NCGC00024379-04	EMETINE	0.30	0.30	-6.6	-6.9	-6.9	A	A	A	-97	-97	-96
NCGC00181104-01	DITHIAZANINE IODIDE	0.30	0.30	-5.5	-5.8	-5.8	A	A	A	-98	-66	-97
NCGC00160391-01	Auranofin	0.35	0.30	-5.4	-5.8	-5.7	A	A	A	-93	-95	-93
NCGC00016373-03	Benzethonium chloride	0.40	0.35	-5.4	-5.8	-5.7	A	A	A	-100	-97	-93
NCGC00181159-01	ECTEINASCIDIN 743	0.40	0.45	-8.9	-9.3	-9.3	A	A	A	-102	-102	-100
NCGC00093889-03	PHYSOSTIGMINE	0.45	0.45	-5.3	-5.8	-5.8	A	A	A	-95	-90	-87
NCGC00013216-01	Dimercaprol	0.45	0.20	-5.6	-6.1	-5.8	A	A	A	-94	-98	-97
NCGC00015339-02	Dequalinium dichloride			-6.6			A	N	N	-103	-116	-117
NCGC00016600-01	Clofazimine		-0.05	-5.9		-5.9	A	N	I	-33	-20	-31
NCGC00166247-01	Quinaldine blue			-6.2			A	N	N	-100	-102	-101
NCGC00166288-01	ALAZANINI TRICLOFENAS			-6.7			A	N	N	-100	-107	-101
NCGC00091387-01	Ethidium bromide			-7.1			A	N	N	-105	-104	-103
NCGC00094996-01	ALEXIDINE HYDROCHLORIDE			-5.7			A	N	N	-96	-100	-98
NCGC00161831-02	Mefloquine hydrochloride			-6.9			A	N	N	-94	-95	-96
NCGC00094807-01	TYROTHRICIN			-9.4			A	N	N	-102	-119	-105
NCGC00161622-02	Actinomycin D _A			-8.3			A	N	N	-99	-106	-101

NCGC00167496-01	METHYLENE BLUE				-7.6	A	N	N	-96	-92	-93
NCGC00016833-01	Halofantrine hydrochloride				-8.0	A	N	N	-96	-91	-93
NCGC00095992-01	GRAMICIDIN				-9.3	A	N	N	-100	-105	-104
NCGC00181109-01	DECOQUINATE	0.05			-8.5	A	N	A	-95	-93	-95
NCGC00016246-03	Chlorhexidine				-5.7	A	N	N	-96	-103	-101
NCGC00017022-05	Pentamidine isethionate				-6.0	A	N	N	-103	-103	-102
NCGC00163700-01	VINCRIStINE				-6.1	A	N	N	-68	-72	-78
NCGC00016250-01	Demecarium bromide				-6.4	A	N	N	-96	-94	-97
NCGC00094849-01	CALCEIN					A	A	A	210	310	333
NCGC00159347-02	Fluorescein sodium					A	A	A	236	291	308
NCGC00167490-01	LUMEFANTRINE			-2.93	-7.5	A	N	N	-97	-97	
NCGC00159455-02	Gefitinib	-0.45	-0.45		-6.1	I	I	A	-36	-59	-67
NCGC00090753-01	Azithromycin	-0.25	-0.05		-5.1	I	I	A	-57	-70	-88
NCGC00093759-01	CNS-1102	-0.20	-0.10		-4.9	I	I	I	-45	-43	-56
NCGC00093664-01	(?)-Butaclamol hydrochloride	-0.20	-0.15		-4.9	I	I	I	-71	-62	-80
NCGC00016725-01	Josamycin	-0.20	0.10		-5.5	I	I	I	-41	-54	-63
NCGC00016714-01	Thiamphenicol	-0.15	0.00		-5.3	I	I	I	-32	-38	-47
NCGC00164543-01	Lomerizine	-0.15	-0.10		-4.9	I	I	I	-104	-110	-110
NCGC00094736-01	NITROMIDE	-0.15	-0.15		-4.9	I	I	I	-39	-37	-46
NCGC00159325-02	Desloratadine	-0.15	-0.15		-4.9	I	I	I	-89	-98	-100
NCGC00159417-02	Triclosan	-0.15	-0.15		-4.9	I	I	I	-80	-85	-97
NCGC00163168-01	MESULERGINE	-0.15	-0.15		-4.9	I	I	I	-47	-44	-63
NCGC00164559-01	DULOxETINE HYDROCHLORIDE	-0.15	-0.15		-4.9	I	I	I	-87	-86	-96
NCGC00068236-02	GATIFLOXACIN	-0.15	-0.20		-4.9	I	I	I	-42	-39	-50
NCGC00017366-04	PERGOLIDE METHANESULFONATE	-0.15	-0.20		-4.9	I	I	I	-68	-66	-76
NCGC00016922-01	Florfenicol	-0.15	-0.10		-5.4	I	I	I	-39	-57	-58
NCGC00164563-01	ENTECAVIR	-0.15	0.05		-5.0	I	A	A	-58	-89	-79
NCGC00016862-01	Budesonide	-0.10	0.00		-4.9	I	I	I	-48	-63	-69
NCGC00018102-06	FLUNARIZINE	-0.10	0.00		-4.8	I	I	I	-105	-120	-113
NCGC00091032-03	Cyproterone acetate	-0.10	0.00		-4.8	I	I	I	-57	-60	-73
NCGC00095303-02	Cloxyquin	-0.10	0.00		-4.8	I	I	I	-50	-71	-62
NCGC00160365-01	CYSTEINE HYDROCHLORIDE	-0.10	-0.05		-4.8	I	I	I	-93	-60	-107
NCGC00016507-01	Thonzonium bromide	-0.10	-0.10		-5.2	I	I	I	-68	-92	-93
NCGC00024928-06	Tamoxifen citrate	-0.10	-0.10		-4.8	I	I	I	-65	-81	-88
NCGC00163169-01	PIZOTIFEN	-0.10	-0.10		-4.8	I	I	I	-51	-54	-60
NCGC00163179-01	U-69593	-0.10	-0.10		-4.8	I	I	I	-79	-90	-96
NCGC00167538-01	CLORPRENAlINE HYDROCHLORIDE	-0.10	-0.10		-4.9	I	I	I	-74	-94	-84
NCGC00015096-07	AMIODARONE	-0.10	-0.15		-4.9	I	I	I	-103	-116	-110
NCGC00164545-01	Lacidipine	-0.10	0.05		-4.9	I	A	I	-105	-131	-107
NCGC00159333-02	SPARFLOXACIN	-0.10	0.20		-4.8	I	I	I	-82	-56	-44
NCGC00016260-05	Ethacrynic acid	-0.10	0.00		-4.8	I	I	A	-85	-98	-98
NCGC00164486-01	Ciclovalona	-0.10	-0.05		-4.8	I	I	A	-111	-97	-103
NCGC00091469-01	Saquinavir Mesylate	-0.10			-4.8	I	I	N	-67	-36	-31
NCGC00015054-06	TACRINE	-0.10	-0.05		-4.9	I	I	I	-38	-102	-98
NCGC00167542-01	TIAMULIN	-0.10	0.15		-5.0	I	I	A	-63	-62	-66
NCGC00161422-01	BIBX 1382 dihydrochloride	-0.10	0.00		-4.9	I	A	A	-97	-120	-111
NCGC00091146-02	Fenotiazina	-0.05	0.10		-4.8	I	I	I	-55	-65	-63
NCGC00094220-02	PROADIFEN HYDROCHLORIDE	-0.05	0.05		-4.8	I	I	I	-106	-127	-108
NCGC00166245-01	PROFLAVINE HEMISULFATE	-0.05	0.05		-4.8	I	I	I	-102	-113	-99
NCGC00015846-10	Phenylbutazone	-0.05	0.00		-4.8	I	I	I	-99	-97	-98
NCGC00017291-05	RIBOFLAVIN	-0.05	0.00		-4.8	I	I	I	-37	-54	-52
NCGC00095304-02	Furazolidone	-0.05	0.00		-4.8	I	I	I	-100	-107	-98
NCGC00160678-01	Fenoverina	-0.05	0.00		-4.8	I	I	I	-61	-62	-77
NCGC00015300-05	GBR-12909	-0.05	-0.05		-4.8	I	I	I	-112	-105	-120
NCGC00181034-01	LIARozOLE	-0.05	-0.05		-4.8	I	I	I	-111	-117	-131
NCGC00164631-01	Sunitinib malate	-0.05	-0.10		-4.8	I	I	I	-103	-114	-110
NCGC00167500-01	ETRETINATE	-0.05	-0.10		-4.8	I	I	I	-89	-84	-101
NCGC00094486-01	SKF 95282 dimaleate	-0.05	0.20		-4.8	I	I	I	-59	-60	-61
NCGC00159321-02	CLOPIDOGREL BISULFATE	-0.05	0.10		-4.8	I	I	I	-66	-55	-68
NCGC00093619-02	Opipramol dihydrochloride	-0.05	0.10		-4.8	I	I	A	-102	-121	-116
NCGC00015998-04	Thiothixene Hydrochloride	-0.05	0.05		-4.8	I	I	A	-105	-128	-116
NCGC00164610-01	TRICLABENDAZOLUM	-0.05	0.10		-4.8	I	I	I	-82	-94	-94
NCGC00181168-01	TRIFLUOMEPRAZINE MALEATE	-0.05	0.10		-4.7	I	I	I	-43	-36	-47
NCGC00018204-09	VINPOCETINE	-0.05	0.05		-4.8	I	I	I	-38	-52	-55

NCGC00024378-05	LOBELINE	-0.05	0.05	-4.8	-4.7	-4.8				-61	-45	-66
NCGC00093935-01	Flupirtine maleate	-0.05	0.05	-4.8	-4.7	-4.8				-118	-110	-104
NCGC00094306-02	PROPANTHELINE BROMIDE	-0.05	0.05	-4.8	-4.7	-4.8				-83	-78	-83
NCGC00159388-02	PENTAERYTHRITOL TETRANITRATE	-0.05	0.05	-4.8	-4.7	-4.8				-84	-88	-89
NCGC00015053-05	AA-861	-0.05	0.00	-4.8	-4.7	-4.8				-81	-84	-85
NCGC00015264-08	CLOMIPRAMINE	-0.05	0.00	-4.8	-4.7	-4.8				-59	-46	-73
NCGC00094446-03	LEVAMISOLE HYDROCHLORIDE	-0.05	0.00	-4.8	-4.7	-4.8				-109	-114	-110
NCGC00160566-01	Broquinolol	-0.05	0.00	-4.8	-4.7	-4.8				-121	-106	-112
NCGC00160664-01	Nitroxoline	-0.05	0.00	-4.8	-4.7	-4.8				-119	-110	-108
NCGC00181312-01	BIPERIDEN HYDROCHLORIDE	-0.05	0.00	-4.8	-4.7	-4.8				-75	-71	-78
NCGC00013495-01	Benztropine	-0.05	-0.05	-4.8	-4.7	-4.7				-56	-50	-79
NCGC00014482-01	Bristaline	-0.05	-0.05	-4.8	-4.7	-4.7				-108	-89	-118
NCGC00014648-01	benzylhydrochlorothiazide	-0.05	-0.05	-4.8	-4.7	-4.7				-70	-72	-78
NCGC00016290-01	Demeclocycline hydrochloride	-0.05	-0.05	-4.8	-4.7	-4.7				-42	-50	-61
NCGC00016821-01	Etoposide	-0.05	-0.05	-4.8	-4.7	-4.7				-78	-76	-83
NCGC00017159-05	Curcumin	-0.05	-0.05	-4.8	-4.7	-4.7				-96	-78	-87
NCGC00018098-04	IODOQUINOL	-0.05	-0.05	-4.8	-4.7	-4.7				-85	-80	-84
NCGC00024777-02	SNC 80	-0.05	-0.05	-4.8	-4.7	-4.7				-121	-99	-103
NCGC00024809-02	PRONETHALOL	-0.05	-0.05	-4.9	-4.8	-4.8				-104	-107	-106
NCGC00025167-01	Formoterol hemifumarate	-0.05	-0.05	-4.8	-4.7	-4.7				-88	-79	-95
NCGC00094434-01	Na-p-Tosyl-L-lysine chloromethyl ketone hydrochloride	-0.05	-0.05	-4.8	-4.7	-4.7				-66	-64	-69
NCGC00160383-01	Lenperone	-0.05	-0.05	-4.9	-4.9	-4.9				-44	-65	-78
NCGC00164578-01	ETORICOXIB	-0.05	-0.05	-4.8	-4.7	-4.7				-57	-48	-78
NCGC00160607-01	N-METHYL-3-PIPERIDYL BENZILATE	-0.05	0.00	-4.9	-4.9	-4.9				-47	-54	-64
NCGC00013051-05	t-Butylhydroquinone	-0.05	-0.05	-4.9	-4.9	-4.9			A	-94	-107	-112
NCGC00016959-01	Ciprofloxacin hydrochloride	-0.05	0.05	-5.3	-5.3	-5.4			A	-55	-70	-70
NCGC00016576-01	Thiostrepton	-0.05	0.30	-5.2	-5.2	-5.5		A	A	-69	-86	-65
NCGC00163158-01	S(-)-LISURIDE	0.00	0.20	-4.7	-4.7	-4.9				-44	-38	-47
NCGC00160568-01	HALETAZOLUM	0.00	0.15	-4.7	-4.7	-4.9				-78	-68	-79
NCGC00166397-02	LOFEPRAMINE HYDROCHLORIDE	0.00	0.15	-4.7	-4.7	-4.9				-86	-77	-76
NCGC00017136-01	Doxazosin mesylate	0.00	0.10	-4.7	-4.7	-4.8				-102	-89	-93
NCGC00024595-03	CARBETAPENTANE	0.00	0.10	-4.7	-4.7	-4.8				-114	-120	-117
NCGC00024885-01	Olvanil	0.00	0.10	-4.7	-4.7	-4.8				-57	-70	-80
NCGC00095071-01	AMCINONIDE	0.00	0.10	-4.7	-4.7	-4.8				-73	-58	-74
NCGC00095196-01	TILORONE	0.00	0.10	-4.7	-4.7	-4.8				-111	-111	-113
NCGC00095280-01	ENOXAPARIN SODIUM (1% wt/vol in 10%aqueous DMSO)	0.00	0.10	-4.7	-4.7	-4.8				-71	-60	-87
NCGC00162247-02	LEVALLORPHAN	0.00	0.10	-4.7	-4.7	-4.8				-115	-118	-115
NCGC00165907-02	TRIPARANOLUM	0.00	0.10	-4.7	-4.7	-4.8				-103	-81	-90
NCGC00181134-01	HALOPROGIN	0.00	0.10	-4.7	-4.7	-4.8				-45	-41	-46
NCGC00015964-09	SPIPERONE	0.00	0.05	-4.8	-4.8	-4.8				-62	-50	-66
NCGC00090774-01	Nitazoxanide	0.00	0.05	-4.8	-4.8	-4.8				-95	-94	-83
NCGC00160527-01	MOSAPRIDE CITRATE	0.00	0.05	-4.8	-4.8	-4.8				-63	-82	-98
NCGC00016059-05	THIORIDAZINE	0.00	0.05	-4.7	-4.7	-4.8				-80	-81	-93
NCGC00016824-01	Clocortolone pivalate	0.00	0.05	-4.8	-4.8	-4.9				-80	-83	-86
NCGC00025216-01	Roxindole hydrochloride	0.00	0.05	-4.7	-4.7	-4.8				-47	-64	-73
NCGC00091268-01	Oxytetracycline HCl	0.00	0.05	-4.7	-4.7	-4.8				-49	-59	-67
NCGC00159490-02	OXYTETRACYCLINE	0.00	0.05	-4.7	-4.7	-4.8				-58	-61	-76
NCGC00159551-01	DEVAZEPIDUM	0.00	0.05	-4.7	-4.7	-4.8				-83	-72	-74
NCGC00166153-01	Climbazole	0.00	0.05	-4.7	-4.7	-4.8				-103	-92	-103
NCGC00181020-01	ZEAXANTHIN	0.00	0.05	-4.7	-4.7	-4.8				-61	-39	-62
NCGC00181300-01	RIBOFLAVIN BUTYRATE	0.00	0.05	-4.7	-4.7	-4.8				-66	-63	-63
NCGC00013034-01	Depoestradiol	0.00	0.00	-4.7	-4.7	-4.7				-87	-49	-82
NCGC00014485-01	Etymemazine hydrochloride	0.00	0.00	-4.7	-4.7	-4.7				-73	-69	-74
NCGC00015246-02	Cinnarizine	0.00	0.00	-5.1	-5.1	-5.1				-38	-36	-42
NCGC00015412-06	Ebselen	0.00	0.00	-4.7	-4.7	-4.7				-114	-118	-117
NCGC00015444-04	FENOLDOPAM	0.00	0.00	-4.7	-4.7	-4.7				-67	-73	-100
NCGC00015846-11	PHENYLBUTAZONE	0.00	0.00	-4.7	-4.7	-4.7				-105	-105	-110
NCGC00016291-01	Tetracycline hydrochloride	0.00	0.00	-5.1	-5.1	-5.1				-41	-53	-69
NCGC00016423-03	Gossypol	0.00	0.00	-4.7	-4.7	-4.7				-95	-89	-91
NCGC00016695-01	Vitamin K2	0.00	0.00	-4.8	-4.8	-4.8				-93	-87	-86
NCGC00016748-01	Parthenolide	0.00	0.00	-4.7	-4.7	-4.7				-44	-47	-47
NCGC00017071-01	Isoetharine mesylate salt	0.00	0.00	-4.7	-4.7	-4.7				-57	-56	-66
NCGC00017343-07	Retinol	0.00	0.00	-4.7	-4.7	-4.7				-77	-70	-77
NCGC00022680-04	CHLORMADINONE ACETATE	0.00	0.00	-4.7	-4.7	-4.7				-64	-73	-77

NCGC00023722-05	Floxuridine	0.00	0.00	-4.7	-4.7	-4.7				-69	-83	-89
NCGC00024778-01	Bifemelane	0.00	0.00	-4.7	-4.7	-4.7				-42	-41	-48
NCGC00025187-01	Rimcazole dihydrochloride	0.00	0.00	-4.8	-4.8	-4.8				-83	-96	-93
NCGC00090686-04	Nitrofurazone	0.00	0.00	-4.7	-4.7	-4.7				-83	-87	-87
NCGC00090752-03	Retinoic acid p-hydroxyanilide	0.00	0.00	-4.7	-4.7	-4.7				-103	-102	-109
NCGC00090757-02	Melphalan	0.00	0.00	-4.7	-4.7	-4.7				-41	-79	-73
NCGC00090782-03	Nelfinavir Mesylate	0.00	0.00	-4.7	-4.7	-4.7				-105	-92	-94
NCGC00094556-01	AVERMECTIN B1	0.00	0.00	-4.7	-4.7	-4.7				-108	-108	-108
NCGC00095842-01	RIFAXIMIN	0.00	0.00	-4.8	-4.8	-4.8				-110	-109	-113
NCGC00095843-01	TOMATINE	0.00	0.00	-4.7	-4.7	-4.7				-102	-117	-95
NCGC00159318-03	CHLORDIAZEPOXIDE	0.00	0.00	-4.7	-4.7	-4.7				-88	-91	-90
NCGC00159423-02	Phytonadione	0.00	0.00	-4.7	-4.7	-4.7				-71	-42	-70
NCGC00160448-01	Tibrofam	0.00	0.00	-4.7	-4.7	-4.7				-115	-115	-117
NCGC00163155-01	BOPINDOLOL	0.00	0.00	-4.7	-4.7	-4.7				-110	-103	-108
NCGC00164139-02	OCTRIZOLUM	0.00	0.00	-4.7	-4.7	-4.7				-94	-93	-101
NCGC00164537-01	Droxidopa	0.00	0.00	-4.7	-4.7	-4.7				-109	-109	-106
NCGC00164618-01	RALTITREXED	0.00	0.00	-4.7	-4.7	-4.7				-39	-43	-52
NCGC00164624-01	ADEFOVIR DIPIVOXIL	0.00	0.00	-4.7	-4.7	-4.7				-104	-104	-108
NCGC00166134-01	ESTRADIOL CYPIONATE	0.00	0.00	-4.7	-4.7	-4.7				-74	-46	-77
NCGC00181002-01	CINACALCET HYDROCHLORIDE	0.00	0.00	-4.7	-4.7	-4.7				-117	-114	-120
NCGC00181014-01	ALFACALCIDOL	0.00	0.00	-4.7	-4.7	-4.7				-64	-70	-66
NCGC00181019-01	TESTOSTERONE ISOCAPROATE	0.00	0.00	-4.7	-4.7	-4.7				-95	-97	-106
NCGC00181103-01	PROPIVERINE HYDROCHLORIDE	0.00	0.00	-4.7	-4.7	-4.7				-46	-55	-66
NCGC00181120-01	ACETOPHENAZINE MALEATE	0.00	0.00	-4.7	-4.7	-4.7				-87	-89	-99
NCGC00181351-01	Benzamide, N-[[[4-(acetylamino)phenyl]amino]thioxomethyl]-4-(1,1-dime	0.00	0.00	-4.7	-4.7	-4.7				-89	-91	-101
NCGC00159510-02	Aripiprazole	0.00	-0.05	-4.8	-4.8	-4.7				-104	-106	-100
NCGC00090762-01	Rifabutin	0.00	-0.05	-4.8	-4.8	-4.8				-100	-86	-109
NCGC00094484-01	Trifluoperidol hydrochloride	0.00	-0.05	-4.8	-4.8	-4.8				-83	-73	-87
NCGC00162150-01	Cilnidipine	0.00	-0.05	-4.8	-4.8	-4.8				-60	-59	-82
NCGC00167489-01	SARPOGRELATE HYDROCHLORIDE	0.00	0.00	-4.8	-4.8	-4.8		A		-103	-112	-104
NCGC00016931-01	Isradipine	0.00	0.25	-5.1	-5.1	-5.4				-42	-43	-53
NCGC00016693-01	Doxycycline hydrochloride	0.00	0.10	-5.2	-5.2	-5.3				-52	-55	-60
NCGC00015195-03	3-alpha-[(4-CHLOROPHENYL)PHENYLMETHOXY]TROPANE	0.00	0.15	-4.8	-4.8	-5.0			A	-89	-81	-93
NCGC00013683-01	Chlorprothixene	0.00	0.10	-4.7	-4.7	-4.8			A	-72	-55	-76
NCGC00016966-01	Sertaconazole nitrate	0.00	0.10	-5.1	-5.1	-5.2			A	-103	-103	-108
NCGC00181048-01	DOLASETRON MESYLATE	0.00	0.10	-4.8	-4.8	-4.9			A	-73	-72	-88
NCGC00091950-01	9-Aminoacridine HCl H2O	0.00	0.05	-4.8	-4.8	-4.9			A	-111	-109	-120
NCGC00016950-01	Mometasone furate	0.00	0.00	-5.2	-5.2	-5.2			A	-109	-108	-114
NCGC00094976-01	GLUTATHIONE	0.00	0.00	-4.7	-4.7	-4.7			A	-104	-105	-114
NCGC00159456-02	IMATINIB MESYLATE	0.00	0.00	-4.8	-4.8	-4.8			A	-108	-110	-122
NCGC00016800-01	Isoconazole	0.00	-0.05	-5.2	-5.2	-5.2			A	-97	-100	-119
NCGC00015436-07	FLUPHENAZINE	0.00	0.20	-4.8	-4.8	-5.0		A	A	-101	-117	-103
NCGC00167567-01	NITROBLUE TETRAZOLIUM CHLORIDE	0.00	0.10	-4.8	-4.8	-4.9		A	A	-99	-113	-106
NCGC00162179-02	cis-(Z)-FLUPENTHIXOL	0.00	0.00	-4.8	-4.8	-4.8		A	A	-103	-100	-112
NCGC00091532-02	Clorophene	0.05	0.15	-4.7	-4.8	-4.9				-100	-62	-93
NCGC00161326-04	CALCIFEDIOL	0.05	0.15	-4.7	-4.8	-4.9				-109	-89	-103
NCGC00164620-01	Nadifloxacin	0.05	0.10	-4.7	-4.8	-4.8				-62	-63	-72
NCGC00167569-01	MEFENOREX	0.05	0.10	-4.7	-4.8	-4.8				-114	-109	-107
NCGC00181091-01	BUNAMIDINE HYDROCHLORIDE	0.05	0.10	-4.7	-4.8	-4.8				-114	-116	-113
NCGC00025179-05	MifepristoneA	0.05	0.05	-4.7	-4.8	-4.8				-114	-126	-123
NCGC00093366-03	Arsanilic acid	0.05	0.05	-4.7	-4.8	-4.8				-45	-59	-81
NCGC00159318-02	CHLORDIAZEPOXIDE	0.05	0.05	-4.7	-4.8	-4.8				-93	-94	-91
NCGC00164575-01	TULATHROMYCIN	0.05	0.05	-4.7	-4.8	-4.8				-55	-80	-93
NCGC00168748-01	ROTIGOTINE	0.05	0.05	-4.7	-4.8	-4.8				-100	-105	-104
NCGC00015469-05	GUANFACINE	0.05	0.00	-4.8	-4.9	-4.8				-46	-43	-66
NCGC00024762-02	N,N-DIETHYL-2-[4-(PHENYLMETHYL)PHENOXY]ETHANAMINE	0.05	0.00	-4.7	-4.8	-4.7				-111	-112	-121
NCGC00095025-01	PERHEXILINE MALEATE	0.05	0.00	-4.9	-4.9	-4.9				-110	-102	-105
NCGC00160676-01	APROFENUM	0.05	0.00	-4.9	-4.9	-4.9				-33	-44	-61
NCGC00163224-01	BUTYLSCOPOLAMMONIUM	0.05	0.00	-4.7	-4.8	-4.7				-43	-53	-59
NCGC00166104-01	THIOCTIC ACID AMIDE	0.05	0.00	-4.7	-4.8	-4.7				-90	-77	-85
NCGC00167424-01	TIPEPIDINE HIBENZATE	0.05	0.00	-4.7	-4.8	-4.7				-53	-57	-69
NCGC00091182-01	TEROXIRONUM	0.05	-0.05	-4.9	-4.9	-4.8				-61	-65	-81
NCGC00016504-01	Droperidol	0.05	-0.05	-4.8	-4.9	-4.8				-48	-64	-76
NCGC00094806-01	TUAMINOHEPTANE SULFATE	0.05	-0.05	-4.8	-4.9	-4.8				-62	-81	-90

NCGC00095078-01	CLOBETASOL PROPIONATE	0.05	-0.05	-4.8	-4.9	-4.8				-110	-94	-117
NCGC00013226-01	Fluoperazine	0.05	-0.10	-4.8	-4.9	-4.7				-74	-55	-77
NCGC00167498-01	THIAMPHENICOL AMINOACETATE HYDROCHLORIDE	0.05	0.05	-4.8	-4.9	-4.9				-48	-43	-69
NCGC00094620-01	CHLORAMPHENICOL	0.05	-0.05	-4.9	-5.0	-4.9				-33	-45	-64
NCGC00015904-02	RIBAVIRIN	0.05	0.15	-4.8	-4.9	-5.0				-39	-66	-69
NCGC00163616-01	ROSAMICIN	0.05	0.15	-5.4	-5.4	-5.5				-49	-39	-61
NCGC00016812-01	Butoconazole nitrate	0.05	0.15	-5.1	-5.1	-5.2			A	-108	-112	-110
NCGC00015500-10	HALOPERIDOL	0.05	0.05	-4.8	-4.9	-4.9			A	-83	-71	-93
NCGC00017006-01	Tridihexethyl chloride	0.05	0.00	-5.2	-5.2	-5.2			A	-64	-74	-90
NCGC00167451-01	HALOBETASOL PROPIONATE	0.05	0.00	-4.8	-4.9	-4.8			A	-103	-101	-126
NCGC00017134-01	Meclocycline sulfosalicylate	0.05	0.20	-5.2	-5.2	-5.4			A	-58	-53	-71
NCGC00164633-01	Nisoldipine	0.05	-0.05	-4.8	-4.9	-4.8		A	A	-106	-120	-130
NCGC00095125-01	LOSARTAN	0.05		-4.7	-4.8			A	N	-73	-96	-96
NCGC00015714-09	NIMODIPINE	0.05	0.15	-4.8	-4.8	-4.9				-47	-56	-57
NCGC00016777-01	Probucol	0.05	0.15	-5.1	-5.2	-5.3				-77	-59	-74
NCGC00016841-01	Penbutolol sulfate	0.05	0.15	-5.1	-5.2	-5.3				-98	-91	-92
NCGC00018271-03	HOMOCHLORCYCLIZINE	0.05	0.10	-4.8	-4.8	-4.9				-68	-66	-76
NCGC00160544-01	6-METHYL-16-METHYLENE-3,20-DIOXOPREGNA-4,6-DIEN-17-ALPH	0.05	0.10	-4.8	-4.8	-4.9				-86	-75	-79
NCGC00164572-01	RIMONABANT	0.05	0.05	-4.8	-4.8	-4.8				-115	-114	-120
NCGC00164507-01	NIFUROXIME	0.05	0.00	-4.8	-4.8	-4.8				-41	-45	-52
NCGC00167551-01	CETOMACROGOL EMULSIFYING WAX	0.05	0.00	-4.8	-4.8	-4.8				-87	-79	-107
NCGC00164601-01	Liranaftate	0.05	-0.05	-4.8	-4.8	-4.7				-94	-69	-90
NCGC00013315-01	Buclodin	0.05	-0.05	-4.8	-4.8	-4.7		A		-106	-112	-105
NCGC00015442-02	5-Fluorouracil	0.05	0.20	-4.8	-4.8	-5.0			A	-93	-98	-95
NCGC00164574-01	Erlotinib	0.05	0.15	-4.8	-4.8	-4.9			A	-87	-84	-87
NCGC00014483-01	Pamelor	0.10	0.00	-4.8	-4.9	-4.8				-58	-42	-48
NCGC00160561-01	ACIDUM BROMEBRICUM	0.10	-0.10	-4.8	-4.9	-4.7				-91	-71	-96
NCGC00160486-01	CHLORACYZINUM	0.10	0.25	-4.9	-5.0	-5.2				-44	-45	-61
NCGC00095194-01	CEPHARANTHINE	0.10	0.20	-4.7	-4.8	-4.9				-121	-109	-101
NCGC00016787-01	Rescinnamin	0.10	0.15	-5.1	-5.2	-5.2				-50	-67	-56
NCGC00181143-01	FLUOROSALAN	0.10	0.15	-4.7	-4.8	-4.9				-95	-82	-82
NCGC00015802-08	PIMOZIDE	0.10	0.10	-4.8	-4.9	-4.9				-120	-90	-89
NCGC00015838-03	PROPIOMAZINE HYDROCHLORIDE	0.10	0.10	-4.7	-4.8	-4.8				-37	-37	-56
NCGC00016943-01	Fluticasone propionate	0.10	0.10	-5.1	-5.2	-5.2				-56	-55	-73
NCGC00016984-01	Alclometasone dipropionate	0.10	0.10	-5.1	-5.2	-5.2				-97	-49	-101
NCGC00160599-01	PARATHIAZINUM	0.10	0.05	-4.8	-4.9	-4.8				-104	-91	-92
NCGC00181088-01	MELITRACEN HYDROCHLORIDE	0.10	0.05	-4.8	-4.9	-4.8				-53	-50	-69
NCGC00016798-06	(S)-TIMOLOL	0.10	0.05	-4.7	-4.8	-4.8				-111	-107	-112
NCGC00095192-01	TEGASEROD	0.10	0.05	-4.7	-4.8	-4.8				-112	-121	-121
NCGC00159471-02	Benzatropina	0.10	0.05	-4.7	-4.8	-4.8				-44	-56	-65
NCGC00160483-01	Ftormetazine	0.10	0.05	-4.7	-4.8	-4.8				-38	-43	-50
NCGC00016511-02	Chlorotrianisene	0.10	0.00	-4.7	-4.8	-4.7				-112	-94	-118
NCGC00016645-01	Methacycline hydrochloride	0.10	0.00	-5.1	-5.2	-5.1				-47	-51	-64
NCGC00094205-01	(?)-Octoclotheptin maleate	0.10	0.00	-4.7	-4.8	-4.7				-43	-43	-52
NCGC00094372-03	Salmeterol	0.10	0.00	-4.7	-4.8	-4.7				-95	-93	-94
NCGC00095193-01	CHLOROPHYLLIDE Cu COMPLEX Na SALT	0.10	0.00	-4.7	-4.8	-4.7				-79	-67	-75
NCGC00160538-01	OCTAVERINUM	0.10	0.00	-4.7	-4.8	-4.7				-47	-45	-72
NCGC00094897-01	PIMETHIXENE MALEATE	0.10	-0.05	-4.8	-4.9	-4.7				-123	-98	-104
NCGC00181304-01	IMEXON	0.15	0.00	-4.8	-5.0	-4.8				-47	-41	-58
NCGC00025347-01	Medetomidine hydrochloride	0.15	-0.05	-4.9	-5.0	-4.8				-32	-37	-60
NCGC00091925-01	Cobalt sulfate heptahydrate	0.15	0.15	-4.9	-5.0	-5.0		A	A	-66	-79	-82
NCGC00015686-05	METHOXY VERAPAMIL	0.15	0.15	-4.8	-4.9	-4.9				-48	-41	-37
NCGC00015437-10	Fenofibrate	0.15	0.10	-4.7	-4.9	-4.8				-44	-53	-66
NCGC00167522-01	HEXOPRENALINE SULFATE	0.15	0.10	-4.7	-4.9	-4.8				-68	-74	-82
NCGC00015428-08	FLUOXETINE	0.15	0.05	-4.8	-4.9	-4.8				-52	-35	-66
NCGC00017100-01	Yohimbic acid monohydrate	0.15	0.05	-5.1	-5.3	-5.2				-51	-43	-71
NCGC00016710-01	Clemastine fumarate	0.15	0.05	-4.7	-4.8	-4.7				-39	-47	-46
NCGC00159375-02	P-PHENYLENEDIAMINE	0.15	0.05	-4.7	-4.9	-4.8				-105	-100	-114
NCGC00016202-02	Sodium nitroprusside dihydrate	0.15	0.00	-4.7	-4.9	-4.7				-70	-66	-102
NCGC00016563-01	Meclozine dihydrochloride	0.15	0.00	-5.1	-5.2	-5.1				-92	-91	-96
NCGC00024846-03	GUANABENZ	0.15	0.00	-4.8	-4.9	-4.8				-62	-50	-72
NCGC00094891-01	FENDILINE HYDROCHLORIDE	0.15	0.00	-4.7	-4.9	-4.7				-88	-96	-102
NCGC00164565-01	Zaprasidone	0.15	0.00	-4.7	-4.9	-4.7				-77	-66	-88
NCGC00181010-01	MABUTEROL HYDROCHLORIDE	0.15	0.00	-4.7	-4.9	-4.7				-97	-85	-99

NCGC00015851-02	Protriptyline hydrochloride	0.15	-0.05	-5.1	-5.3	-5.1				-45	-36	-49
NCGC00015713-07	NITRENDIPINE	0.15	0.15	-4.7	-4.9	-4.9				-39	-38	-49
NCGC000095163-01	SARAFLOXACIN HYDROCHLORIDE	0.15	0.15	-4.8	-4.9	-4.9				-46	-58	-67
NCGC00017257-09	METERGOLINE PHENYLMETHYL ESTER	0.15	0.30	-4.9	-5.1	-5.2				-61	-49	-58
NCGC00016898-01	Sulconazole nitrate	0.15	0.15	-5.1	-5.2	-5.2			A	-112	-102	-112
NCGC00163778-02	Imazail sulphate	0.15	0.10	-4.8	-4.9	-4.9		A	A	-125	-111	-126
NCGC000096003-01	TILMICOSIN	0.20	0.25	-4.8	-5.0	-5.1				-49	-50	-51
NCGC00016621-01	Halcinonide	0.20	0.20	-5.1	-5.3	-5.3				-98	-89	-92
NCGC000091505-01	Nitrofurantoin	0.20	0.05	-4.7	-4.9	-4.8				-100	-86	-106
NCGC00167509-01	PIPETHANATE ETHOBROMIDE	0.20	0.05	-4.7	-4.9	-4.8				-44	-43	-73
NCGC00015708-04	MAPROTILINE	0.20	0.00	-4.7	-4.9	-4.7				-45	-33	-43
NCGC00167467-01	VECURONIUM BROMIDE	0.20	0.10	-4.9	-5.1	-5.0				-46	-51	-69
NCGC00167585-01	IPIDACRINE HYDROCHLORIDE HYDRATE	0.20	0.30	-4.7	-4.9	-5.0			A	-116	-100	-109
NCGC000095166-01	CLOPIDOL	0.20	0.25	-4.8	-5.0	-5.0			A	-61	-46	-75
NCGC00016692-01	Bromperidol	0.20	0.15	-5.1	-5.3	-5.2			A	-63	-51	-72
NCGC00018254-03	BIFONAZOLE	0.20	0.20	-4.7	-4.9	-4.9		A	A	-116	-116	-114
NCGC00164567-01	PEROSPIRONE HYDROCHLORIDE HYDRATE	0.25	-0.05	-4.8	-5.1	-4.8				-63	-34	-56
NCGC00165810-01	INDORAMIN HYDROCHLORIDE	0.25	-0.05	-4.8	-5.0	-4.7			A	-64	-68	-71
NCGC00167433-01	ROCURONIUM BROMIDE	0.25	0.30	-5.0	-5.3	-5.3			A	-61	-59	-65
NCGC00159466-02	alprazolam	0.35	-0.10	-4.9	-5.2	-4.8		A		-105	-77	-93
NCGC00015089-08	AMILORIDE	0.35	0.00	-4.8	-5.2	-4.8		A	A	-105	-70	-119
NCGC00160398-01	NAFAMOSTAT MESILATE	0.35	0.35	-4.8	-5.1	-5.1			A	-60	-48	-64
NCGC00167821-01	CABERGOLINE	0.20	-4.7	-4.7	-4.9	-4.9		N		-41	-24	-34
NCGC00163150-01	CLENBUTEROL	0.20	-4.7	-4.7	-4.9	-4.9		N		-37	-27	-46
NCGC00163157-01	MESORIDAZINE	0.15	-4.8	-4.8	-4.9	-4.9		N		-37	-38	-40
NCGC00166250-01	ANAZOLENUM NATRICUM	0.15	-4.7	-4.7	-4.9	-4.9		N		-43	-36	-58
NCGC00016495-01	Hexylcaine hydrochloride	0.10	-5.1	-5.1	-5.2	-5.2		N		-92	-14	-97
NCGC00015872-05	QUIPAZINE	0.10	-4.7	-4.7	-4.8	-4.8		N		-78	19	-91
NCGC00160601-01	Anilamate	0.05	-4.7	-4.7	-4.8	-4.8		N		-46	-30	-65
NCGC000090704-01	Indium trichloride	0.00	-4.7	-4.7	-4.7	-4.7		N		-77	-24	-94
NCGC000095117-01	CLARITHROMYCIN	0.00	-4.8	-4.8	-4.8	-4.8		N		-105	-8	-58
NCGC00013015-01	GLUCONIC ACID, BARIUM SALT	0.00	-4.7	-4.7	-4.7	-4.7		N		-78	-29	-99
NCGC00015273-11	CHLORPROMAZINE	0.00	-4.7	-4.7	-4.7	-4.7		N		-49	-27	-43
NCGC00015619-09	LORATADINE	0.00	-4.7	-4.7	-4.7	-4.7		N		-47	-31	-36
NCGC00016909-01	Glafenine hydrochloride	0.00	-5.1	-5.1	-5.1	-5.1		N		-42	-26	-35
NCGC00024665-03	METHIOTHEPIN	0.00	-4.7	-4.7	-4.7	-4.7		N		-40	-32	-57
NCGC000092362-01	ECOPIPAMUM	0.00	-4.7	-4.7	-4.7	-4.7		N		-44	-33	-55
NCGC000092386-03	Sertraline hydrochloride (Zoloft)	0.00	-4.7	-4.7	-4.7	-4.7		N		-48	-25	-36
NCGC000094400-01	R(-)-SCH-12679 maleate	0.00	-4.7	-4.7	-4.7	-4.7		N		-35	-32	-47
NCGC000095005-01	BROMHEXINE HYDROCHLORIDE	0.00	-4.7	-4.7	-4.7	-4.7		N		-44	-34	-50
NCGC000095289-01	EXEMESTANE	0.00	-4.7	-4.7	-4.7	-4.7		N		-41	-19	-44
NCGC00024740-02	ANPIRTOLINE	-0.05	-4.8	-4.8	-4.7	-4.7		N		-125	-6	-71
NCGC000091865-01	Benzyl alcohol	-0.05	-4.8	-4.8	-4.7	-4.7		N		-65	-8	-103
NCGC00164547-01	Zafirlukast	-0.05	-4.8	-4.8	-4.7	-4.7		N		-47	-28	-36
NCGC00165953-02	(E)-2-[2-Fluoro-2-(quinuclidin-3-ylidene)ethoxy]-9H-carbazole monohydr	-0.10	-4.8	-4.8	-4.7	-4.7		N		-63	-32	-60
NCGC00017040-01	Thiopropazine dimesylate	-0.15	-5.2	-5.2	-5.1	-5.1		N		-48	-26	-86
NCGC00167536-01	TOSUFLOXACIN TOSILATE	0.10	-5.2	-5.2	-5.3	-5.3		N		-38	-32	-41
NCGC00181101-01	ISOTHIPENDYL HYDROCHLORIDE	-0.10	-5.1	-5.1	-5.0	-5.0		N		-37	-33	-49
NCGC00014670-01	Floxacinil Na salt		-4.9	-4.9					N	-108	-117	-46
NCGC000091512-04	CINNAMALDEHYDE				-4.5			N	N	-86		-94
NCGC00167476-01	CALCIUM HOPANTENATE							N	N	-76	-42	-55
NCGC00015822-09	MEPYRAMINE	-0.28	-4.8	-4.8	-4.5	-4.5		N	N	-61	-93	
NCGC00021146-06	KETANSERIN		-4.9	-4.9				N	N	-42	-18	-27
NCGC00164582-01	Feprazone		-4.8	-4.8				N	N	-46	-28	-34
NCGC00167449-01	DESOGESTREL		-4.7	-4.7				N	N	-37	-27	-24
NCGC00018130-04	Fenazopiridina		-4.8	-4.8				N	N	-39	-3	-4
NCGC00025273-01	Nemonapride							N	N	-70	-6	-8
NCGC00160476-01	FLUACIZINUM				-4.5			N	N	-64	-15	
NCGC00160539-01	Adefovir		-5.7	-5.7				N	N	-43	21	9
NCGC00167979-01	METENOLONE ENANTHATE		-4.7	-4.7				N	N	-118	-6	-5
NCGC00021274-03	ESTRADIOL BENZOATE		-4.8	-4.8				N	N	-43	-20	-31
NCGC000095066-01	SELAMECTIN		-4.7	-4.7				N	N	-46	-16	-21
NCGC000095086-01	PERICIAZINE		-4.7	-4.7				N	N	-48	-20	-31
NCGC000095136-01	OLMESARTAN MEDOXOMIL		-4.7	-4.7				N	N	-35	3	-38

NCGC00160462-01	Guanoxano			-5.3		I	N	N	-50	-29	-31
NCGC00013235-01	Estradiol phosphate	0.00		-4.5	-4.5	N	N	N			7
NCGC00013723-01	AMINOXYSCOPOLAMINE HYDROBROMIDE	0.00		-4.5	-4.5	N	N	N			5
NCGC00014313-01	Capicillin	0.00		-4.5	-4.5	N	N	N			-1
NCGC00015042-03	N-ARACHIDONYLGLYCINE	0.00		-4.5	-4.5	N	N	N			6
NCGC00015268-05	CLONIDINE	0.00		-4.5	-4.5	N	N	N			-7
NCGC00015400-02	Enoximone	0.00		-4.5	-4.5	N	N	N			0
NCGC00015416-02	Ethylene glycol-bis(2-aminoethylether)-N,N,N',N'-tetraacetic acid	0.00		-4.5	-4.5	N	N	N			3
NCGC00015441-04	Fusaric acid	0.00		-4.5	-4.5	N	N	N			-7
NCGC00015594-02	Ioxoprofen	0.00		-4.5	-4.5	N	N	N			5
NCGC00015605-06	Lamotrigine	0.00		-4.5	-4.5	N	N	N			2
NCGC00015615-02	Lansoprazole	0.00		-4.5	-4.5	N	N	N			3
NCGC00015643-07	METOCLOPRAMIDE	0.00		-4.5	-4.5	N	N	N			8
NCGC00015647-05	Nocodazole	0.00		-4.5	-4.5	N	N	N			7
NCGC00015919-04	SOTALOL	0.00		-4.5	-4.5	N	N	N			-1
NCGC00016009-10	TOLAZAMIDE	0.00		-4.5	-4.5	N	N	N			6
NCGC00016230-01	Homatropine hydrobromide (R,S)	0.00		-4.5	-4.5	N	N	N			9
NCGC00016304-01	Norethynodrel	0.00		-4.5	-4.5	N	N	N			-2
NCGC00016305-01	Sulfadiazine	0.00		-4.5	-4.5	N	N	N			7
NCGC00016313-01	Quinethazone	0.00		-4.5	-4.5	N	N	N			-3
NCGC00016329-01	Phenindione	0.00		-4.5	-4.5	N	N	N			7
NCGC00016344-03	Mesalamine	0.00		-4.5	-4.5	N	N	N			0
NCGC00016347-01	Benzthiazide	0.00		-4.5	-4.5	N	N	N			-1
NCGC00016393-01	Dioxybenzone	0.00		-4.5	-4.5	N	N	N			3
NCGC00016404-01	Hexetidine	0.00		-4.5	-4.5	N	N	N			-15
NCGC00016496-01	Etilefrine hydrochloride	0.00		-4.5	-4.5	N	N	N			3
NCGC00016508-01	Methazolamide	0.00		-4.5	-4.5	N	N	N			13
NCGC00016512-01	Isoxsuprine hydrochloride	0.00		-4.5	-4.5	N	N	N			-4
NCGC00016552-01	Cephalosporanic acid, 7-amino	0.00		-4.5	-4.5	N	N	N			5
NCGC00016754-01	Spectinomycin dihydrochloride	0.00		-4.5	-4.5	N	N	N			-2
NCGC00016757-01	Ketoprofen	0.00		-4.5	-4.5	N	N	N			-1
NCGC00016764-01	Benfotiamine	0.00		-4.5	-4.5	N	N	N			4
NCGC00016765-01	Diflunisal	0.00		-4.5	-4.5	N	N	N			-5
NCGC00016792-01	Kanamycin A sulfate	0.00		-4.5	-4.5	N	N	N			1
NCGC00016806-01	Mebendazole	0.00		-4.5	-4.5	N	N	N			7
NCGC00016853-01	Nabumetone	0.00		-4.5	-4.5	N	N	N			-4
NCGC00016858-01	Cefadroxil	0.00		-4.5	-4.5	N	N	N			3
NCGC00016869-01	Sisomicin sulfate	0.00		-4.5	-4.5	N	N	N			4
NCGC00016937-01	Ozagrel hydrochloride	0.00		-4.5	-4.5	N	N	N			-1
NCGC00016938-01	Cefixime	0.00		-4.5	-4.5	N	N	N			8
NCGC00016940-01	Simvastatin	0.00		-4.5	-4.5	N	N	N			1
NCGC00016942-01	Roxithromycin	0.00		-4.5	-4.5	N	N	N			-1
NCGC00016960-03	Glimepiride	0.00		-4.5	-4.5	N	N	N			1
NCGC00016982-01	Nafronyl oxalate	0.00		-4.5	-4.5	N	N	N			-1
NCGC00016985-01	Disopyramide	0.00		-4.5	-4.5	N	N	N			0
NCGC00017020-01	Amprolium hydrochloride	0.00		-4.5	-4.5	N	N	N			8
NCGC00017046-01	Ticarcillin sodium	0.00		-4.5	-4.5	N	N	N			6
NCGC00017055-01	Folinic acid calcium salt	0.00		-4.5	-4.5	N	N	N			3
NCGC00017059-01	Mebhydroline 1,5-naphtalenedisulfonate	0.00		-4.5	-4.5	N	N	N			4
NCGC00017070-01	Nafcillin sodium salt monohydrate	0.00		-4.5	-4.5	N	N	N			3
NCGC00017113-01	Flunixin meglumine	0.00		-4.5	-4.5	N	N	N			-1
NCGC00017120-01	Cefmetazole sodium salt	0.00		-4.5	-4.5	N	N	N			2
NCGC00017130-01	Moxalactam disodium salt	0.00		-4.5	-4.5	N	N	N			2
NCGC00017137-01	Ceftazidime pentahydrate	0.00		-4.5	-4.5	N	N	N			-9
NCGC00017260-05	RAUWOLSCINE	0.00		-4.5	-4.5	N	N	N			-3
NCGC00018242-04	Sulfacetamide	0.00		-4.5	-4.5	N	N	N			2
NCGC00021569-04	Enalapril	0.00		-4.5	-4.5	N	N	N			1
NCGC00024703-02	TROPANYL 3,5-DIMETHYLBENZOATE	0.00		-4.5	-4.5	N	N	N			5
NCGC00025236-01	Remacemide hydrochloride	0.00		-4.5	-4.5	N	N	N			9
NCGC00025346-02	Mirtazapine	0.00		-4.5	-4.5	N	N	N			-7
NCGC00074022-02	PYRIDINOL CARBAMATE	0.00		-4.5	-4.5	N	N	N			3
NCGC00077304-01	FLUANISONUM	0.00		-4.5	-4.5	N	N	N			-11
NCGC00090682-01	alpha-Pinene	0.00		-4.5	-4.5	N	N	N			5
NCGC00090698-02	1,3-Diphenylguanidine	0.00		-4.5	-4.5	N	N	N			0

NCGC00090729-01	Acesulfame K	0.00	-4.5	-4.5	N	N	N	11
NCGC00090851-04	Azacitidine	0.00	-4.5	-4.5	N	N	N	7
NCGC00091013-01	5alpha-Androstan-17beta-ol-3-one	0.00	-4.5	-4.5	N	N	N	3
NCGC00091034-02	Captan	0.00	-4.5	-4.5	N	N	N	5
NCGC00091059-01	n-Butyl chloride	0.00	-4.5	-4.5	N	N	N	7
NCGC00091175-01	o-Anthranilic acid	0.00	-4.5	-4.5	N	N	N	-1
NCGC00091352-02	ENDRIN	0.00	-4.5	-4.5	N	N	N	-10
NCGC00091398-02	Nitrobenzene	0.00	-4.5	-4.5	N	N	N	6
NCGC00091493-01	Anethole	0.00	-4.5	-4.5	N	N	N	-2
NCGC00091544-04	POLYESTRADIOL PHOSPHATE	0.00	-4.5	-4.5	N	N	N	4
NCGC00091737-01	Sorbic acid	0.00	-4.5	-4.5	N	N	N	0
NCGC00091792-01	1,2-Epoxy-3-chloropropane (Epichlorohydrin)	0.00	-4.5	-4.5	N	N	N	5
NCGC00092300-01	CINALUKASTUM	0.00	-4.5	-4.5	N	N	N	-12
NCGC00092361-05	DINOPROSTONE	0.00	-4.5	-4.5	N	N	N	2
NCGC00093534-02	ACECAINIDE HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	6
NCGC00094157-01	CR 2249	0.00	-4.5	-4.5	N	N	N	9
NCGC00094546-04	LINDANE	0.00	-4.5	-4.5	N	N	N	14
NCGC00094707-01	LACTULOSE	0.00	-4.5	-4.5	N	N	N	-3
NCGC00094799-01	TRIAMCINOLONE	0.00	-4.5	-4.5	N	N	N	5
NCGC00094882-01	DROFENINE HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	-8
NCGC00095054-01	RESORCINOL MONOACETATE	0.00	-4.5	-4.5	N	N	N	-1
NCGC00095147-01	TROXERUTIN	0.00	-4.5	-4.5	N	N	N	-1
NCGC00095160-01	ASPARTAME	0.00	-4.5	-4.5	N	N	N	8
NCGC00095183-01	PRAVASTATIN SODIUM	0.00	-4.5	-4.5	N	N	N	5
NCGC00095233-01	HYDROXYAMPHETAMINE HYDROBROMIDE	0.00	-4.5	-4.5	N	N	N	4
NCGC00095239-01	1,3,5-TRIMETHOXYBENZENE	0.00	-4.5	-4.5	N	N	N	10
NCGC00095254-04	TOCOPHEROL ACETATE	0.00	-4.5	-4.5	N	N	N	0
NCGC00095935-01	CORTISONE	0.00	-4.5	-4.5	N	N	N	2
NCGC00096059-01	TRIMEBUTINE MALEATE	0.00	-4.5	-4.5	N	N	N	1
NCGC00159323-02	Oxazepam	0.00	-4.5	-4.5	N	N	N	3
NCGC00159337-02	EFAVIRENZ	0.00	-4.5	-4.5	N	N	N	0
NCGC00159364-02	CI DIRECT RED 28	0.00	-4.5	-4.5	N	N	N	-2
NCGC00159414-02	Terpinol	0.00	-4.5	-4.5	N	N	N	4
NCGC00159438-02	SELENOMETHIONINE, SE-75	0.00	-4.5	-4.5	N	N	N	-1
NCGC00159479-02	METHYL NICOTINATE	0.00	-4.5	-4.5	N	N	N	-3
NCGC00159480-02	Cetamina	0.00	-4.5	-4.5	N	N	N	6
NCGC00160264-01	6,7-DIMETHOXYQUINAZOLINE-2,4(1H,3H)-DIONE	0.00	-4.5	-4.5	N	N	N	7
NCGC00160350-01	LINOTROBANUM	0.00	-4.5	-4.5	N	N	N	8
NCGC00160394-01	MEPHENYTOIN	0.00	-4.5	-4.5	N	N	N	9
NCGC00160405-01	Acide risedronique	0.00	-4.5	-4.5	N	N	N	9
NCGC00160440-01	Lonazolac	0.00	-4.5	-4.5	N	N	N	-9
NCGC00160475-01	Norletimol	0.00	-4.5	-4.5	N	N	N	3
NCGC00160496-01	Amanozine	0.00	-4.5	-4.5	N	N	N	-1
NCGC00160528-01	NUCLOMEDONUM	0.00	-4.5	-4.5	N	N	N	4
NCGC00160543-01	Pregnandiol	0.00	-4.5	-4.5	N	N	N	-4
NCGC00160606-01	Sulbentina	0.00	-4.5	-4.5	N	N	N	-4
NCGC00160608-01	ROLICYPRINUM	0.00	-4.5	-4.5	N	N	N	5
NCGC00160644-01	PICOLINE, ALPHA	0.00	-4.5	-4.5	N	N	N	8
NCGC00160647-01	CYPROMID	0.00	-4.5	-4.5	N	N	N	10
NCGC00160658-01	Adafenoxate	0.00	-4.5	-4.5	N	N	N	8
NCGC00161344-03	EICOSAPENTAENOIC ACID	0.00	-4.5	-4.5	N	N	N	2
NCGC00162274-02	NALTREXONE	0.00	-4.5	-4.5	N	N	N	3
NCGC00163127-02	ACITRETIN	0.00	-4.5	-4.5	N	N	N	1
NCGC00163160-01	B-HT 920	0.00	-4.5	-4.5	N	N	N	5
NCGC00163242-01	(+)-TUBOCURARINE	0.00	-4.5	-4.5	N	N	N	4
NCGC00163256-01	TIOTIDINE	0.00	-4.5	-4.5	N	N	N	16
NCGC00163798-03	TRIETHYLENE GLYCOL	0.00	-4.5	-4.5	N	N	N	9
NCGC00164140-03		0.00	-4.5	-4.5	N	N	N	-5
NCGC00164265-01	Olaquinoxã	0.00	-4.5	-4.5	N	N	N	2
NCGC00164333-01	Sorbitan monostearate	0.00	-4.5	-4.5	N	N	N	2
NCGC00164447-01	Ciprofibrate	0.00	-4.5	-4.5	N	N	N	3
NCGC00164465-01	Imiprothrin	0.00	-4.5	-4.5	N	N	N	10
NCGC00164498-01	TOLPENTAMIDUM	0.00	-4.5	-4.5	N	N	N	2
NCGC00164532-01	Parapropamol	0.00	-4.5	-4.5	N	N	N	3

NCGC00164541-01	SULFACARBAMIDUM	0.00	-4.5	-4.5	N	N	N	-6
NCGC00164560-01	ABACAVIR SULFATE	0.00	-4.5	-4.5	N	N	N	-3
NCGC00164577-01	nimetazepam	0.00	-4.5	-4.5	N	N	N	-8
NCGC00164588-01	malotilate	0.00	-4.5	-4.5	N	N	N	5
NCGC00165997-01	Bismuth subcarbonate	0.00	-4.5	-4.5	N	N	N	9
NCGC00166021-01	SODIUM HEXAFLUOROSILICATE	0.00	-4.5	-4.5	N	N	N	-3
NCGC00166077-01	Bitoscanate	0.00	-4.5	-4.5	N	N	N	2
NCGC00166097-01	Cinnamyl alcohol	0.00	-4.5	-4.5	N	N	N	9
NCGC00166206-01	PHTHARAL	0.00	-4.5	-4.5	N	N	N	-1
NCGC00166259-01	Etocrylene	0.00	-4.5	-4.5	N	N	N	5
NCGC00166295-01	Lactitol	0.00	-4.5	-4.5	N	N	N	7
NCGC00166305-01	PERACETIC ACID	0.00	-4.5	-4.5	N	N	N	1
NCGC00166321-01	FOSFRUCTOSUM	0.00	-4.5	-4.5	N	N	N	3
NCGC00166329-01	sn-Glycerol 3-phosphate bis(cyclohexylammonium) salt	0.00	-4.5	-4.5	N	N	N	2
NCGC00167447-01	PROSULTIAMINE	0.00	-4.5	-4.5	N	N	N	-8
NCGC00167459-01	DOXAPRAM HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	-4
NCGC00167480-01	N-HYDROXYMETHYLSUCCINIMIDE	0.00	-4.5	-4.5	N	N	N	5
NCGC00167507-01	LAPATINIB TOSILATE HYDRATE	0.00	-4.5	-4.5	N	N	N	5
NCGC00167558-01	FLEROXACIN	0.00	-4.5	-4.5	N	N	N	-3
NCGC00167564-01	PAMABROM	0.00	-4.5	-4.5	N	N	N	1
NCGC00167575-01	ANAGRELIDE HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	-3
NCGC00167578-01	MITIGLINIDE CALCIUM HYDRATE	0.00	-4.5	-4.5	N	N	N	4
NCGC00167580-01	COENZYME A	0.00	-4.5	-4.5	N	N	N	2
NCGC00167754-01	TALNIFLUMATUM	0.00	-4.5	-4.5	N	N	N	4
NCGC00168773-01	DARUNAVIR ETHANOLATE	0.00	-4.5	-4.5	N	N	N	-2
NCGC00181033-01	TALTIRELIN HYDRATE	0.00	-4.5	-4.5	N	N	N	11
NCGC00181045-01	PYRIDOXAMINE PHOSPHATE	0.00	-4.5	-4.5	N	N	N	-3
NCGC00181090-01	P-HYDROXYEPHEDRINE HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	4
NCGC00181167-01	ISONIAZID SODIUM METHANESULFONATE	0.00	-4.5	-4.5	N	N	N	-7
NCGC00181311-01	ADEMETIONINE	0.00	-4.5	-4.5	N	N	N	1
NCGC00181337-01	DICHLOROBENZYL ALCOHOL	0.00	-4.5	-4.5	N	N	N	-1
NCGC00181340-01	AZOSEMIDE	0.00	-4.5	-4.5	N	N	N	-2
NCGC00181352-01	ASPOXCILLIN	0.00	-4.5	-4.5	N	N	N	7
NCGC00015073-02	Amifostine	0.00	-4.5	-4.5	N	N	N	10
NCGC00015590-03	Linopirdine dihydrochloride	0.00	-4.5	-4.5	N	N	N	-12
NCGC00015716-05	NYLIDRIN	0.00	-4.5	-4.5	N	N	N	-12
NCGC00016160-02	Loxapine succinate	0.00	-4.5	-4.5	N	N	N	0
NCGC00016564-01	Metformin hydrochloride	0.00	-4.5	-4.5	N	N	N	5
NCGC00016598-01	Tranlycypromine hydrochloride	0.00	-4.5	-4.5	N	N	N	14
NCGC00016605-01	Nifenazone	0.00	-4.5	-4.5	N	N	N	11
NCGC00016956-01	loversol	0.00	-4.5	-4.5	N	N	N	11
NCGC00016998-01	Cefotiam hydrochloride	0.00	-4.5	-4.5	N	N	N	-15
NCGC00021151-02	Xanthinol niacinate	0.00	-4.5	-4.5	N	N	N	13
NCGC00024359-04	PENICILLAMINE	0.00	-4.5	-4.5	N	N	N	10
NCGC00091012-01	Triton X-100	0.00	-4.5	-4.5	N	N	N	-12
NCGC00091501-01	Resorcinol	0.00	-4.5	-4.5	N	N	N	-1
NCGC00093350-02	Amikacin sulfate	0.00	-4.5	-4.5	N	N	N	-7
NCGC00094614-03	Chloroxylenol	0.00	-4.5	-4.5	N	N	N	-23
NCGC00094630-01	COLISTIMETHATE SODIUM	0.00	-4.5	-4.5	N	N	N	-11
NCGC00094763-01	POLYMYXIN B SULFATE	0.00	-4.5	-4.5	N	N	N	10
NCGC00095003-01	TIOXOLONE	0.00	-4.5	-4.5	N	N	N	8
NCGC00159339-02	Streptomycin sulfate	0.00	-4.5	-4.5	N	N	N	-27
NCGC00159351-02	CHOLESTEROL	0.00	-4.5	-4.5	N	N	N	8
NCGC00159357-02	Mephobarbital	0.00	-4.5	-4.5	N	N	N	-20
NCGC00160374-01	TRIMETHIDINII METHOSULFAS	0.00	-4.5	-4.5	N	N	N	0
NCGC00160453-01	Morinamida	0.00	-4.5	-4.5	N	N	N	8
NCGC00160456-01	IODOHIPPURATE SODIUM, I-123	0.00	-4.5	-4.5	N	N	N	-8
NCGC00160503-01	Tritiozina	0.00	-4.5	-4.5	N	N	N	11
NCGC00160542-01	Lifibrate	0.00	-4.5	-4.5	N	N	N	13
NCGC00160623-01	Octinoxate	0.00	-4.5	-4.5	N	N	N	8
NCGC00164553-01	Clofarabine	0.00	-4.5	-4.5	N	N	N	-8
NCGC00167543-01	CEFTIOFUR CRYSTALLINE FREE ACID	0.00	-4.5	-4.5	N	N	N	-16
NCGC00167577-01	SIVELESTAT SODIUM HYDRATE	0.00	-4.5	-4.5	N	N	N	4
NCGC00167737-01	LAZABEMIDE HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	6

NCGC00167966-01	HYALURONATE SODIUM	0.00		-4.5	-4.5		N	N	N	8
NCGC00168759-02	PTC 124	0.00		-4.5	-4.5		N	N	N	0
NCGC00181082-01	METHYLBENACTYZIUM BROMIDE	0.00		-4.5	-4.5		N	N	N	-18
NCGC00013724-01	Proscamide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00014810-01	domperidone	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015075-04	ARECOLINE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015149-02	Bumetanide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015199-08	CHLORAMBUCIL	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015207-07	CILOSTAZOL	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015209-05	Cyclophosphamide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015380-09	DIAZOXIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015467-11	GLYBURIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015471-02	Ganciclovir	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015640-02	Metrifudil	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015649-02	Moxonidine	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015703-03	MECAMYLAMINE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015725-02	Nimesulide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015726-06	Nialamide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015836-08	PIRENZEPINE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015893-02	ROPINROLE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00015897-02	RANOLAZINE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016099-04	XAMOTEROL	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016141-02	Clodronic acid	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016241-06	Furosemide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016255-01	Sulfinpyrazone	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016285-02	Sulfanilamide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016302-01	Cyanocobalamin	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016322-08	4,4'-Sulfonyldianiline (Dapsone)	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016334-01	Hexestrol	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016362-01	Benzonate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016398-01	Trichlormethiazide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016497-05	Ethionamide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016500-01	Diperodon hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016529-01	Pramoxine hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016532-02	DIMETHADIONE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016537-01	Rolitetraacycline	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016544-01	Dehydroisoandosterone 3-acetate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016560-01	Ethambutol dihydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016586-01	Flurandrenolide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016594-01	Prilocaine hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016618-01	Dimethisoquin hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016668-02	FOSFOSAL	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016675-01	Oxprenolol hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016705-05	TOLFENAMIC ACID	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016706-01	Parbendazole	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016708-01	Selegiline hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016751-01	Gliclazide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016772-01	Terbutaline hemisulfate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016809-01	Moricizine hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016813-01	Pivmecillinam hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016817-01	Etomidate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016865-01	Carteolol hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016887-01	Meptazinol hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016897-01	Ceforanide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016973-01	Letrozole	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016977-01	Dorzolamide hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00016987-01	Ajmaline	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00017032-01	Gentamicine sulfate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00017062-01	Meclofenamic acid sodium salt monohydrate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00017093-01	Cephapirin sodium salt	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00017098-01	Indapamide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00017146-01	Canrenoic acid potassium salt	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00017337-02	Capsaicin	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	
NCGC00018113-03	SODIUM PHENYLBUTYRATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N	

NCGC00018163-06	Bithionol	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00022612-04	Cefaclorum	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00023212-07	RIBAVIRIN	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00023509-03	Lovastatin	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00024717-06	N-NITRO-ARGININE METHYL ESTER	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00024822-02	EVANS BLUE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00024870-02	REMOXIPRIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00024996-02	Colforsin	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00025070-01	CGS 19755	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00065440-02	TRIMECAINUM	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00090771-01	beta-Cyclodextrin	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00090794-01	Chloroform	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00090874-02	Piperonyl butoxide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00090961-02	n-Butyl alcohol	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00091058-04	LINOLENIC ACID	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00091099-02	MITOBRONITOL	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00091285-01	Tricaprylin	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00091338-01	p-Chloro-m-cresol	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00091345-01	Adipic acid	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00091655-02	p-tert-Pentylphenol	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00091666-01	Eucalyptol	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00091695-01	Triethylenetetramine	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00091861-01	Dacarbazine	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00091930-01	Sodium hydrogen sulfate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00091937-01	N-(1-Naphthyl)ethylenediamine 2HCl	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00092366-02	RELCOVAPTANUM	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00094159-01	Naphazoline hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00094227-01	Picrotoxin	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00094324-02	PYRIDOSTIGMINE BROMIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00094390-01	1-(2-Methoxyphenyl)piperazine hydrochloride	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00094572-01	AMITRAZ	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00094703-01	ISOSORBIDE DINITRATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00094738-01	NORETHINDRONE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00094764-01	PREDNISOLONE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00094824-01	VINCAMINE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00094894-01	MEFEXAMIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00094990-01	ACEXAMIC ACID	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00095000-01	AMIPRILOSE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00095022-01	DIOSMIN	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00095134-01	EZETIMIBE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00095179-01	ZOLPIDEM	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00095201-01	CHAULMOSULFONE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00095762-01	CREATININE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00095772-01	THIAMYLAL SODIUM	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00142391-03	Folic acid	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00142625-03	TOCOPHEROL ACETATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159317-02	HYDROCODONE BITARTRATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159329-02	Testolactone	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159332-02	Cefalotina	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159340-02	Tazobactam sodium	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159342-02	PENICILLIN G BENZATHINE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159362-02	HUPERZINE A, L-	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159372-02	SUCCINIC ACID	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159378-02	PHENYLHYDRAZINE HYDROCHLORIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159382-02	MENTHOL	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159418-02	TEGAFUR	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159426-02	CARBOCISTEINE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159429-02	Ubidecarenone	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159439-02	Lorazepam	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159463-03	PHENACAINE HYDROCHLORIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159476-02	TRIBROMSALAN	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00159502-02	N-CYCLOHEXYLBENZOTHIAZYLSULFENAMIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160198-01	6-AMINOPENICILLANIC ACID	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160445-01	Bromisovalum	0.00	0.00	-4.5	-4.5	-4.5	N	N	N

NCGC00160449-01	Fenclozic acid	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160455-01	Theofibrate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160469-01	Gamolenic acid	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160481-01	Tioxidazole	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160493-01	Fosenazida	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160562-01	Quazodine	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160580-01	Osalmid	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160591-01	HEXYL NICOTINATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160605-01	Diacetamate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160616-01	PROTIRELIN	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160625-01	Acide iophenoique	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160669-01	Pexantel	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00160673-01	Propicillin	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00161345-04	DOCOSAHEXAENOIC ACID	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00162319-02	LY-163,502	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00163245-01	GALLAMINE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00163334-03	ISOLEUCINE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00163742-03	D-LIMONENE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164091-01	Sodium dichloroisocyanurate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164400-01	Danazol	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164401-01	Betamethasone	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164431-01	Terpineol, mixture of isomers	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164512-01	GUAIACOL CARBONATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164529-01	GLYCERYL MONOSTEARATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164552-01	BROMFENAC SODIUM	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164557-01	Eprosartan mesylate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164587-01	Isepamicin	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164594-01	Loteprednol etabonate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164595-01	voglibose	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164602-01	RACTOPAMINE HYDROCHLORIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164605-01	amproxicam	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164607-01	Bentiromide	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00164623-01	OLOPATADINE HYDROCHLORIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00165973-01	THIOGLYCEROL	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00165996-01	PRAXADINUM	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00166237-01	Mepiroxol	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00166270-01	PHLOROGLUCINOL	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00166306-01	Argjpressin acetate	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00166317-01	PHOSPHAMIDON	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00166323-01	Trifluridine	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167429-01	TEMOZOLOMIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167439-01	TRENBOLONE ACETATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167454-01	PILSICAINIDE HYDROCHLORIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167462-01	ACAMPROSATE CALCIUM	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167475-01	DIETHYLPROPION HYDROCHLORIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167479-01	N,N'-1,2-ETHYLENEDIYLBIS-CYSTEINE, DIETHYL ESTER DIHYDRO	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167501-01	METHAQUALONE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167505-01	EPTIFIBATIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167526-01	CAMOSTAT MESILATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167535-01	TENOFOVIR DISOPROXIL FUMARATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167547-01	AGARICINUM	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167568-01	COLFOSCERIL PALMITATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167574-01	XALIPRODEN HYDROCHLORIDE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00167584-01	NICAMETATE CITRATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00181000-01	SUPLATAST TOSILATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00181093-01	MEGLUMINE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00181111-01	TAMIBAROTENE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00181123-01	CINEPAZIDE MALEATE	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00181148-01	METHARBITAL	0.00	0.00	-4.5	-4.5	-4.5	N	N	N
NCGC00016374-02	Carbarstone				-4.9	-4.7	N	I	I
NCGC00015277-02	Cinoxacin				-5.1	-5.1	N	I	I
NCGC00015784-07	PIRENPERONE				-4.8	-4.8	N	I	I
NCGC00015826-02	Perphenazine				-5.1	-5.1	N	I	I
NCGC00015883-05	RISPERIDONE				-4.7	-4.8	N	I	I

-21	-57	-42
-26	-34	-37
-14	-40	-39
-32	-65	-67
-19	-36	-46

NCGC00016429-05	R-(+)-PROPRANOLOL	-4.7	-4.8	N			-27	-36	-57
NCGC00017259-04	NICERGOLINE	-4.7	-4.7	N			-35	-47	-53
NCGC00018193-06	FLUVOXAMINE	-4.8	-4.9	N			-31	-50	-53
NCGC00090777-05	Methoprene	-4.7	-4.7	N			-34	-55	-71
NCGC00090879-01	6-Thioguanine (6-TG)	-4.7	-4.8	N			-18	-39	-42
NCGC00091071-01	CHLOROPHENOTHANE	-4.8	-4.7	N			-23	-52	-45
NCGC00094135-01	Minocycline hydrochloride	-4.9	-4.7	N			-28	-32	-44
NCGC00094502-01	Urapidil hydrochloride	-4.7	-4.8	N			-29	-35	-58
NCGC00094600-01	BENZTROPINE	-4.7	-4.7	N			-26	-41	-60
NCGC00094812-01	ACETARSOL	-4.8	-4.7	N			-29	-52	-42
NCGC00094991-01	PIPENZOLATE BROMIDE	-4.9	-4.8	N			-33	-39	-54
NCGC00095051-01	SEMUSTINE	-4.8	-4.7	N			-36	-61	-70
NCGC00095132-01	BENAZEPRIL HYDROCHLORIDE	-4.8	-4.7	N			-26	-70	-63
NCGC00095159-01	PEFLOXACINE MESYLATE	-4.9	-4.8	N			-27	-42	-46
NCGC00095173-01	AZELASTINE HYDROCHLORIDE	-4.7	-4.7	N			-29	-37	-46
NCGC00095597-01	ANDROGRAPHOLIDE	-4.7	-4.8	N			-35	-41	-46
NCGC00095835-01	AMLODIPINE BESYLATE	-4.7	-4.7	N			-27	-45	-50
NCGC00159428-02	Digitoxin	-4.8	-4.9	N			-33	-54	-44
NCGC00164539-01	Azaclorzina	-4.7	-4.7	N			-28	-52	-54
NCGC00166290-02	LAURETH-4	-4.8	-4.9	N			-28	-47	-55
NCGC00166308-01	DIFLOXACIN HYDROCHLORIDE	-4.8	-4.8	N			-34	-43	-46
NCGC00167457-01	GESTRINONE	-4.9	-4.9	N			-22	-39	-47
NCGC00167521-01	TENATOPRAZOLE	-4.9	-5.0	N			-23	-42	-43
NCGC00167834-01	MOEXIPRIL HYDROCHLORIDE	-4.9	-4.8	N			-25	-43	-47
NCGC00181013-01	MIZOLASTINE	-4.8	-5.0	N			-23	-39	-38
NCGC00181098-01	NELARABINE	-4.8	-4.9	N			-24	-46	-53
NCGC00181099-01	SICCANIN	-5.0	-4.9	N			-34	-43	-33
NCGC00091641-01	6-Mercaptopurine monohydrate	-5.0	-4.9	N			-27	-53	-46
NCGC00016583-01	Oxybutynin chloride	-4.7	-4.7	N	N		-12	-25	-44
NCGC00091357-01	Orotic acid	-4.7	-4.7	N	N		-8	-27	-45
NCGC00164501-01	Nihidrazona			N	N		-33	-27	-39
NCGC00164526-01	ACAMYLOPHENINE HYDROCHLORIDE	-4.9	-4.9	N	N		-20	-29	-33
NCGC00166207-01	Cridanimod	-4.8	-4.8	N	N		-17	-12	-57
NCGC00167817-01	BUCINDOLOLUM	-4.7	-4.7	N	N		-22	-28	-40
NCGC00167965-01	LUTEIN	-4.7	-4.7	N	N		-20	-27	-40
NCGC00181102-01	METOSERPATE HYDROCHLORIDE	-4.7	-4.7	N	N		-23	-29	-40
NCGC00013051-01	tert-Butylhydroquinone	-4.7	-4.7	N	N		-31	-12	-76
NCGC00015254-12	CLOZAPINE	-4.8	-4.8	N	N		-27	-39	-33
NCGC00015501-02	Hydralazine hydrochloride	-5.1	-4.8	N	N		-28	-6	-43
NCGC00015519-05	DOPAMINE	-4.7	-4.7	N	N		-17	-30	-40
NCGC00015563-07	IMIPRAMINE	-4.9	-4.9	N	N		-28	-23	-32
NCGC00015774-03	Oxatomide	-4.8	-4.8	N	N		-30	-27	-43
NCGC00016043-03	Tyrphostin 23	-4.8	-4.8	N	N		-31	-31	-43
NCGC00016066-07	URAPIDIL	-4.9	-4.9	N	N		-32	-27	-37
NCGC00016083-09	VERAPAMIL	-5.5	-4.8	N	N		-34	8	-51
NCGC00016280-02	ZOXAZOLAMINE	-4.8	-4.8	N	N		-39	-28	-45
NCGC00016525-01	Zuclopenthixol hydrochloride	-5.1	-4.8	N	N		-23	-33	-46
NCGC00016907-01	Ketoconazole	-4.7	-4.7	N	N		-25	-31	-35
NCGC00016944-01	Cisapride	-5.2	-4.8	N	N		-32	-22	-68
NCGC00016964-01	Lomefloxacin hydrochloride	-4.8	-4.8	N	N		-26	-23	-38
NCGC00074024-02	RUFLOXACINUM	-4.8	-4.8	N	N		-29	-31	-42
NCGC00091125-01	Gallic acid	-4.7	-4.7	N	N		-15	-32	-44
NCGC00092334-01	ZATEBRADINUM	-4.8	-4.8	N	N		-26	-39	-48
NCGC00094410-02	TRIFLUPROMAZINE HYDROCHLORIDE	-4.7	-4.7	N	N		-32	-29	-45
NCGC00094515-01	Zimelidine dihydrochloride	-4.9	-4.9	N	N		-22	-39	-38
NCGC00094516-01	COUMOPHOS	-4.7	-4.7	N	N		-20	-34	-47
NCGC00095907-01	NONOXYNOL-9	-4.8	-4.8	N	N		-28	-29	-46
NCGC00095978-02	Lufenuron	-4.7	-4.7	N	N		-20	-34	-35
NCGC00159518-02	RABEPRAZOLE SODIUM	-4.7	-4.7	N	N		-16	-26	-36
NCGC00159544-01	ZALDARIDUM	-4.7	-4.7	N	N		-28	-34	-45
NCGC00160410-01	CHINIOFONUM	-4.8	-4.8	N	N		-22	-27	-40
NCGC00160526-01	Befuralina	-4.9	-4.9	N	N		10	-21	-58
NCGC00160590-01	Bromindione	-4.7	-4.7	N	N		-20	-30	-41
NCGC00163132-01	DANTROLENE	-4.8	-4.8	N	N		-25	-29	-50

NCGC00163509-01	MK-571				-4.7	N	N	I	-35	-22	-36
NCGC00164611-01	GESTODENE				-4.9	N	N	I	-23	-34	-45
NCGC00166411-01	OXELADIN TANNATE				-4.7	N	N	I	-19	-27	-42
NCGC00166415-01	PALONOSETRON HYDROCHLORIDE				-4.8	N	N	I	-27	-27	-43
NCGC00167423-01	BEVONIUM METHYLSULFATE				-4.7	N	N	I	-31	-28	-41
NCGC00167508-01	DEFLAZACORT				-4.7	N	N	I	-22	-20	-38
NCGC00167525-01	TAZAROTENE				-4.7	N	N	I	-23	-31	-61
NCGC00167532-01	BALOFLOXACIN HYDRATE				-4.7	N	N	I	-25	-20	-54
NCGC00181024-01	INDOCYANINE GREEN				-4.9	N	N	I	-21	-23	-34
NCGC00181129-01	DASATINIB				-4.7	N	N	I	-32	-36	-42
NCGC00181301-01	ACETYLTRIBUTYL CITRATE				-4.7	N	N	I	-26	-29	-47
NCGC00160554-01	Bithionoloxide					N	N	N	-108	-125	-83
NCGC00015889-05	Raloxifene hydrochloride					N	N	N	-100	-89	-32
NCGC00013042-01	8-quinolinol and salicylic acid	-4.5				N	N	N		-9	-12
NCGC00159486-02	METHENAMINE HIPPURATE					N	N	N	-99	-97	-97
NCGC00164248-01	Sucralox					N	N	N	-18	-52	3
NCGC00166307-01	ERGOCALCIFEROL	-4.5				N	N	N		-100	-26
NCGC00016395-01	Diphenylpyraline hydrochloride					N	N	N	6	-28	-62
NCGC00014437-01	strychnidin-10-one		-4.9	-5.2		N	I	I	-17	-44	-43
NCGC00014496-01	Dexrazoxane		-4.8	-5.0		N	I	I	-32	-37	-45
NCGC00096122-03	Thionosine		-4.9	-4.8		N	I	I	-26	-61	-60
NCGC00163241-01	STRYCHNINE		-4.8	-5.2		N	I	I	-24	-47	-41
NCGC00094525-01	DIURON		-5.3	-5.3		N	I	I	-29	-58	-66
NCGC00094932-01	LANATOSIDE C		-5.2	-5.3		N	I	I	-10	-39	-40
NCGC00016528-01	Proguanil hydrochloride			-5.5		N	N	I	-29	-39	-63
NCGC00016687-01	Spiramycin			-5.4		N	N	I	-22	-17	-36
NCGC00016830-01	Midecamycin			-5.4		N	N	I	-32	-29	-37
NCGC00016916-01	Norfloxacin			-5.4		N	N	I	-19	-28	-36
NCGC00016106-04	Zardaverine					N	N	N	-17	-32	-77
NCGC00167465-01	CALCIPOTRIENE					N	N	N	-81	-8	-31
NCGC00159494-02	riboflavin	-4.5				N	N	N		-86	-34
NCGC00024309-05	DILTIAZEM					N	N	N	7	-62	-52
NCGC00160682-01	Isobutamben		-4.5			N	N	A	-1	-38	-8
NCGC00013037-01	isobornyl thiocyanacetate					N	N	N	0	-91	-45
NCGC00167566-01	BOLDO					N	N	N	-93	-100	-29
NCGC00160423-01	Bametano	-4.5				N	N	N		-49	-38
NCGC00167426-01	CARAMIPHEN EDISYLATE	-4.5				N	N	N		-102	-95
NCGC00027960-02	ACIDUM CAPOBENICUM		-4.9			N	N	A	-35	-22	-12
NCGC00015630-02	Metolazone		-4.5			N	N	N	4		-33
NCGC00024633-02	AMI-193					N	I	N	-96	-90	-55
NCGC00160555-01	Nifursol					N	N	N	-94	-37	-100
NCGC00013414-03	PROCODAZOLUM					N	N	N	-100	-99	-101
NCGC00167431-01	RIFAPENTINE					N	N	N	-97	-97	-97
NCGC00094384-01	R(-)-Denopamine					N	N	N	-47	-73	-75
NCGC00160641-01	Sulazepam					N	N	N	-56	-60	-61
NCGC00095996-01	ACIVICIN	-4.5				N	N	N	-102		-101
NCGC00090714-01	Sodium xylenesulfonate		-7.9			N	N	A	-2	-8	-30
NCGC00168777-01	ETONOGESTREL					N	N	N	-31	-83	-81
NCGC00017245-02	ELLAGIC ACID	-5.8	-5.8			N	A	A	-99	-96	-103
NCGC00181323-01	SQUALENE					N	N	N	-100	-97	-98
NCGC00181302-01	CYTOCHROME C					N	N	N	-72	-50	-75
NCGC00018256-02	OXYPHENONIUM BROMIDE					N	N	N	-90	-92	-94
NCGC00166289-01	HYDROXYSTILBAMIDINE ISETHIONATE	-4.5				N	N	N		-51	-64
NCGC00094851-01	IODIPAMIDE	-4.5				N	N	N		-98	-100
NCGC00016367-01	Succinylsulfathiazole	-4.5				N	N	N		-63	-56
NCGC00091456-01	2-Methylimidazole	-4.5				N	N	N		-55	-61
NCGC00016589-01	(1-[(4-Chlorophenyl)phenyl-methyl]-4-methylpiperazine)	-4.5				N	N	N		-58	-38
NCGC00159345-02	ATROPINE					N	N	N	2	-68	-56
NCGC00094935-01	ACETYL-L-LEUCINE		-6.3			N	N	A	-29	-23	-5
NCGC00160295-01	Benaxibine					N	N	N	-27	-33	-42
NCGC00165791-02	EPINASTINE HYDROCHLORIDE	-4.7				N	I	N	-78	-51	-31
NCGC00159387-02	Laureth 10s	-5.7				N	I	N	-5	-55	5
NCGC00016562-01	Ethopropazine hydrochloride	-5.1				N	I	N	-28	-36	-33
NCGC00163232-01	PANCURONIUM	-5.0				N	I	N	-8	-39	-31

NCGC00160572-01	Metazida				N	A	N	14	40	28
NCGC00166141-01	Carbinoxamine maleate				N	N	N	-34	-8	-12
NCGC00013012-01	D-XYLO-5-HEXULOSONIC ACID, CALCIUM SALT		-4.5		N	N	N	-5	12	
NCGC00013225-01	2-Oxopentanedioic acid	-4.5	-4.5		N	N	N	-1		
NCGC00013260-01	Yohimbine		-4.5		N	N	N	0		-1
NCGC00013273-01	Pyridoxamine dichlorohydrate	-4.5			N	N	N		1	1
NCGC00013289-01	pridinol		-4.5		N	N	N	-1		0
NCGC00013426-01	Cholic Acid		-4.5		N	N	N	-3		5
NCGC00013489-01	sulfaquinoxaline		-4.5		N	N	N	-1		1
NCGC00013628-01	Solvocillin				N	N	N	-2	-1	-8
NCGC00013679-02	Fenticlor				N	N	N	-10	-8	-27
NCGC00013687-01	Phosphotex				N	N	N	0	17	12
NCGC00013718-01	HOMATROPINE		-4.5		N	N	N	0		-2
NCGC00013722-01	scopolamine		-4.5		N	N	N	-2		6
NCGC00013725-01	Mintussin		-4.5		N	N	N	-9		-2
NCGC00013796-01	Atropine oxide		-4.5		N	N	N	-1		9
NCGC00013841-01	Flexeril				N	N	N	-24	-30	-33
NCGC00013895-01	benzbromarone	-4.5	-4.5		N	N	N	-2		
NCGC00014017-01	DL-Proline				N	N	N	3	7	11
NCGC00014361-03	Phosphonoacetic acid				N	N	N	-31	-25	-22
NCGC00014486-01	Adriamycin-DNA hydrochloride	-4.5	-4.5		N	N	N	-1		
NCGC00014617-01			-4.5		N	N	N	1	11	
NCGC00014633-01	Floxacillin	-4.5			N	N	N		4	9
NCGC00014711-01	Spiclomazine		-4.5		N	N	N	-1	10	
NCGC00014750-02	Ebumamonine (-)				N	N	N	-10	3	-15
NCGC00014918-01	oxaprozin				N	N	N	1	7	-1
NCGC00014993-07	Nonanedioic acid				N	N	N	-1	2	12
NCGC00015004-09	AMOXAPINE				N	N	N	-1	-12	-12
NCGC00015009-08	4-AMINOPYRIDINE				N	N	N	16	-11	1
NCGC00015036-03	AMANTIDINE				N	N	N	3	14	15
NCGC00015038-03	AMINOPTERIN	-4.5	-4.5		N	N	N	11		
NCGC00015043-07	GABA				N	N	N	-1	14	-1
NCGC00015061-02	Acyclovir		-4.5		N	N	N	1		-2
NCGC00015067-04	Acetylsalicylic acid	-4.5			N	N	N		8	-1
NCGC00015092-02	Aminocaproic acid				N	N	N	0	7	-3
NCGC00015094-02	Allopurinol				N	N	N	0	0	0
NCGC00015099-05	ALPRENOLOL				N	N	N	-7	-8	-21
NCGC00015100-02	Altretamine	-4.5			N	N	N		8	3
NCGC00015116-10	ANIRACETAM	-4.5			N	N	N		7	5
NCGC00015159-06	BETAXOLOL		-4.5		N	N	N	4		-16
NCGC00015162-04	BUSPIRONE		-4.5		N	N	N	1		-11
NCGC00015191-06	CHLORMEZANONE		-4.5	-4.5	N	N	N	0		
NCGC00015196-04	CIRAZOLINE			-4.5	N	N	N	2	1	
NCGC00015204-05	Carmustine				N	N	N	5	8	7
NCGC00015208-09	Caffeine, citrated				N	N	N	0	10	4
NCGC00015215-02	EPICATECHIN	-4.5			N	N	N		-1	-2
NCGC00015234-11	Carbamazepine		-4.5	-4.5	N	N	N	-5		
NCGC00015238-02	Chlorzoxazone			-4.5	N	N	N	-2	4	
NCGC00015240-06	CIMETIDINE			-4.5	N	N	N	2	-1	
NCGC00015242-04	Chlorothiazide			-4.5	N	N	N	2	4	
NCGC00015243-02	Clemizole hydrochloride			-4.5	N	N	N	-8	0	
NCGC00015247-04	1-(3-CHLOROPHENYL)PIPERAZINE				N	N	N	-2	6	4
NCGC00015252-08	CYPROHEPTADINE			-4.5	N	N	N	6	10	
NCGC00015255-04	p-Chlorophenylalanine	-4.5			N	N	N		4	6
NCGC00015269-03	Cilostamide				N	N	N	0	-3	2
NCGC00015278-09	Carisoprodol		-4.5		N	N	N	3	12	
NCGC00015288-06	CYCLOTHIAZIDE	-4.5			N	N	N		5	-1
NCGC00015321-04	DOBUTAMINE				N	N	N	9	26	13
NCGC00015335-07	DIPHENHYDRAMINE			-4.5	N	N	N	4	12	
NCGC00015340-02	Desipramine hydrochloride				N	N	N	-16	-11	-14
NCGC00015344-03	Doxepin hydrochloride	-4.5	-4.5		N	N	N	-1		
NCGC00015360-05	Pentetic acid				N	N	N	-10	-5	-7
NCGC00015389-08	PROPOFOL	-4.5	-4.5		N	N	N	3		
NCGC00015397-02	Ethamivan				N	N	N	7	3	3

NCGC00015397-06	Vanillic acid diethylamide				N	N	N	6	7	2
NCGC00015409-02	Edrophonium chloride			-4.5	N	N	N	-8	4	
NCGC00015410-04	EFAROXAN				N	N	N	-16	-3	-9
NCGC00015429-08	FELBAMATE		-4.5		N	N	N	1		-2
NCGC00015439-06	FLUMAZENIL		-4.5		N	N	N		5	9
NCGC00015443-06	FLECAINIDE			-4.5	N	N	N	12	13	
NCGC00015446-05	FAMOTIDINE			-4.5	N	N	N	0	3	
NCGC00015452-09	Flutamide				N	N	N	4	4	4
NCGC00015455-03	Felodipine				N	N	N	-11	-7	-20
NCGC00015466-08	Gabapentin			-4.5	N	N	N	1		
NCGC00015513-04	HISTAMINE			-4.5	N	N	N	7		
NCGC00015520-03	HYDROXYUREA		-4.5		N	N	N		7	6
NCGC00015523-02	Hydroquinone				N	N	N	-18	-13	-21
NCGC00015529-09	Ibuprofen				N	N	N	15	12	18
NCGC00015547-02	Imazodan			-4.5	N	N	N	1	4	
NCGC00015558-06	ISOPROTERENOL				N	N	N	-1	-12	-11
NCGC00015570-04	IMILOXAN		-4.5	-4.5	N	N	N	6		
NCGC00015611-10	LIDOCAINE				N	N	N	7	12	9
NCGC00015656-06	MIANSERIN				N	N	N	8	15	11
NCGC00015661-02	Molsidomine			-4.5	N	N	N	7		5
NCGC00015678-02	Moxisylyte hydrochloride		-4.5		N	N	N		7	10
NCGC00015705-04	MEMANTINE				N	N	N	8	11	-12
NCGC00015718-06	NAFTOPIDIL			-4.5	N	N	N	-11	-1	
NCGC00015724-10	NIFLUMIC ACID			-4.5	N	N	N	9	2	
NCGC00015741-06	MASOPROCOL			-4.5	N	N	N	4		17
NCGC00015748-11	NIFEDIPINE				N	N	N	-1	-6	-16
NCGC00015754-08	Nilutamide			-4.5	N	N	N	4	14	
NCGC00015755-03	NIMUSTINE		-4.5		N	N	N		7	3
NCGC00015766-08	OXYMETAZOLINE				N	N	N	-15	-6	-24
NCGC00015768-02	Oxiracetam				N	N	N	-5	-13	-12
NCGC00015786-11	PINDOLOL			-4.5	N	N	N	-2	13	
NCGC00015801-02	Pentoxifylline			-4.5	N	N	N	0	1	
NCGC00015806-03	Pirfenidone		-4.5		N	N	N		5	-5
NCGC00015810-02	Papaverine hydrochloride				N	N	N	0	-4	-8
NCGC00015817-05	PROMETHAZINE			-4.5	N	N	N	7	16	
NCGC00015823-02	Piroxicam				N	N	N	-3	-9	-7
NCGC00015824-07	3-n-PROPYLXANTHINE				N	N	N	10	28	14
NCGC00015827-06	PENTYLENETETRAZOLE		-4.5		N	N	N		4	6
NCGC00015833-09	Pyrazinamide		-4.5		N	N	N		9	0
NCGC00015834-11	PRIMIDONE		-4.5		N	N	N		8	6
NCGC00015841-02	Pargyline hydrochloride		-4.5		N	N	N		7	7
NCGC00015857-05	PIRIBEDIL				N	N	N	-4	0	2
NCGC00015861-04	PROPENTOFYLLINE				N	N	N	6	-2	2
NCGC00015864-02	Procaine hydrochloride		-4.5		N	N	N		6	4
NCGC00015876-07	RANITIDINE				N	N	N	9	8	7
NCGC00015877-06	Ritanserin				N	N	N	-22	-24	-25
NCGC00015884-09	RILMENIDINE			-4.5	N	N	N	-1	-6	
NCGC00015894-02	Resveratrol				N	N	N	-12	-18	-23
NCGC00015931-04	SR 57227A			-4.5	N	N	N	-3	2	
NCGC00015947-02	Siguazodan		-4.5		N	N	N	6		6
NCGC00015954-02	Sobuzoxane		-4.5	-4.5	N	N	N	3		
NCGC00015955-09	SALBUTAMOL			-4.5	N	N	N	4	-2	
NCGC00015959-03	Sanguinarine		-4.5		N	N	N		12	4
NCGC00015970-02	Sulindac			-4.5	N	N	N	-11		-13
NCGC00015982-05	4,5,6,7-TETRAHYDROISOXAZOLO[5,4-c]PYRIDIN-3-OL				N	N	N	-3	1	6
NCGC00015984-03	TROPISETRON				N	N	N	8	20	4
NCGC00015987-05	TELENZEPINE			-4.5	N	N	N	1	17	
NCGC00015989-09	(+/-)-Thalidomide		-4.5	-4.5	N	N	N	-3		
NCGC00015996-02	Tiaprider hydrochloride		-4.5		N	N	N	0		0
NCGC00015997-06	TAURINE				N	N	N	14	-1	7
NCGC00015999-10	TOLBUTAMIDE			-4.5	N	N	N	-2	-1	
NCGC00016000-08	Disulfiram				N	N	N	-9	-10	-17
NCGC00016023-11	Theobromine				N	N	N	7	-3	9
NCGC00016047-03	TRIM			-4.5	N	N	N	4	8	

NCGC00016056-02	Tomoxetine	-4.5			N	N	N		-1	1
NCGC00016058-05	MDL-72222				N	N	N	-7	-16	-15
NCGC00016064-04	Terfenadine				N	N	N	-6	2	0
NCGC00016064-06	TERFENADINE	-4.5			N	N	N	-2		-13
NCGC00016065-07	TROPICAMIDE	-4.5			N	N	N		1	4
NCGC00016087-06	VIGABATRIN	-4.5			N	N	N		7	-1
NCGC00016089-05	Nonanamide, N-[(4-hydroxy-3-methoxyphenyl)methyl]-	-4.5			N	N	N		5	8
NCGC00016101-02	Xylometazoline hydrochloride				N	N	N	-10	-13	-8
NCGC00016161-03	LORGLUMIDE SODIUM	-4.5			N	N	N	6		-1
NCGC00016193-02	PEMPIDINE TARTRATE				N	N	N	-4	6	4
NCGC00016227-01	Tiratricol, 3,3',5-triiodothyroacetic acid		-4.5		N	N	N	10	11	
NCGC00016239-01	Methantheline bromide				N	N	N	-5	-7	-9
NCGC00016240-01	Nadide	-4.5			N	N	N		6	4
NCGC00016243-01	Idoxuridine	-4.5			N	N	N		4	6
NCGC00016251-08	Probenecid		-4.5		N	N	N	6	8	
NCGC00016252-01	Sulfaguanidine	-4.5			N	N	N		-3	6
NCGC00016254-01	Testosterone propionate	-4.5	-4.5		N	N	N	-2		
NCGC00016257-04	4-Dimethylaminoantipyrine				N	N	N	11	9	12
NCGC00016267-01	Isocarboxazid	-4.5			N	N	N	3		2
NCGC00016271-01	Tolazoline hydrochloride	-4.5			N	N	N		6	2
NCGC00016273-01	Methimazole				N	N	N	0	-1	1
NCGC00016277-01	Niridazole	-4.5			N	N	N	-12		-10
NCGC00016278-07	Mefenamic acid				N	N	N	5	-4	-1
NCGC00016279-01	Aminohippuric acid		-4.5		N	N	N	-5	1	
NCGC00016281-06	Phenacetin	-4.5	-4.5		N	N	N	1		
NCGC00016282-01	Methacholine chloride		-4.5		N	N	N	0	8	
NCGC00016289-01	Chlortetracycline hydrochloride	-4.5			N	N	N	-14		-22
NCGC00016292-01	Deoxycorticosterone				N	N	N	0	-6	-4
NCGC00016296-01	Dicumarol		-4.5		N	N	N	-11	5	
NCGC00016309-02	Sulfathiazole	-4.5	-4.5		N	N	N	-5		
NCGC00016311-10	PHENTOLAMINE				N	N	N	2	-8	-9
NCGC00016314-01	Mepenzolate bromide				N	N	N	-2	3	5
NCGC00016315-02	PYRITHYLDIONE	-4.5			N	N	N		3	5
NCGC00016317-01	Chlorthalidone				N	N	N	0	0	3
NCGC00016320-01	Ethosuximide				N	N	N	2	0	-9
NCGC00016323-01	Sulfachloropyridazine				N	N	N	0	2	7
NCGC00016324-01	Sulfamethoxypyridazine		-4.5		N	N	N	3	3	
NCGC00016337-02	PTHALYLSULFATHIAZOLE	-4.5	-4.5		N	N	N	-6		-8
NCGC00016340-01	Ethotoin	-4.5			N	N	N		-1	-2
NCGC00016345-01	Hymecromone				N	N	N	2	16	3
NCGC00016346-01	Sparteine (-)	-4.5	-4.5		N	N	N	0		
NCGC00016351-01	(+,-)-Synephrine	-4.5			N	N	N		11	13
NCGC00016352-01	Benzocaine	-4.5	-4.5		N	N	N	5		
NCGC00016354-03	Butylparaben		-4.5		N	N	N	3	7	
NCGC00016357-01	Iopanoic acid	-4.5			N	N	N	7		5
NCGC00016358-01	Allantoin				N	N	N	1	8	-5
NCGC00016361-07	Acetaminophen (4-hydroxyacetanilide)		-4.5		N	N	N	6	2	
NCGC00016371-01	Dichlorphenamide	-4.5			N	N	N	2		3
NCGC00016375-01	Sulfadimethoxine		-4.5		N	N	N	6	6	
NCGC00016379-01	Glutethimide, para-amino				N	N	N	1	9	14
NCGC00016382-01	Oxethazaine		-4.5		N	N	N	-9	0	
NCGC00016383-01	Trimethadione				N	N	N	-4	-4	-2
NCGC00016384-10	Sulfisoxazole diolamine	-4.5			N	N	N		-2	-1
NCGC00016385-01	Sulfabenzamide	-4.5			N	N	N		16	5
NCGC00016387-02	Chenodiol		-4.5		N	N	N	0		9
NCGC00016388-01	Noscapine		-4.5		N	N	N	-10		-10
NCGC00016389-01	Oxyphenbutazone		-4.5	-4.5	N	N	N	1		
NCGC00016391-05	Iodochlorohydroxyquinoline	-4.5			N	N	N		-7	4
NCGC00016394-07	Oxybenzone				N	N	N	6	4	-18
NCGC00016397-01	Benzylamine hydrochloride				N	N	N	-5	-10	-6
NCGC00016403-01	Mafenide hydrochloride		-4.5		N	N	N	-3	-2	
NCGC00016407-05	Sulfamethizole		-4.5	-4.5	N	N	N	2		
NCGC00016408-01	Sulfapyridine	-4.5			N	N	N		4	-6
NCGC00016413-01	Dydrogesterone	-4.5			N	N	N		-4	-10

NCGC00016414-01	Acenocoumarol	-4.5	-4.5	N	N	N	-3		
NCGC00016416-01	Phenylpropanolamine hydrochloride			N	N	N	-3	-17	4
NCGC00016418-07	Methoxsalen			N	N	N	-3	11	7
NCGC00016421-01	Cyclizine hydrochloride			N	N	N	4	11	7
NCGC00016436-01	Fluocinonide			N	N	N	0	1	-11
NCGC00016442-01	Fluorometholone	-4.5		N	N	N	3		1
NCGC00016446-06	METRONIDAZOLE			N	N	N	1	-2	-1
NCGC00016447-01	Proscillaridin A	-4.5	-4.5	N	N	N	0		
NCGC00016448-01	Hecogenin			N	N	N	3	7	8
NCGC00016455-01	Diprophylline	-4.5		N	N	N		6	-9
NCGC00016461-01	alpha-Santonin	-4.5		N	N	N		-9	-5
NCGC00016479-06	7-(beta-HYDROXYETHYL)THEOPHYLLINE	-4.5	-4.5	N	N	N	6		
NCGC00016481-01	Hesperidin			N	N	N	-3	10	13
NCGC00016483-01	Trimipramine maleate salt	-4.5	-4.5	N	N	N	0		
NCGC00016490-06	FLUFENAMIC ACID		-4.5	N	N	N	4	6	
NCGC00016491-01	Esculin Hydrate			N	N	N	1	-1	-6
NCGC00016498-01	Dyclonine hydrochloride	-4.5	-4.5	N	N	N	-1		
NCGC00016505-01	Propoxycaine hydrochloride			N	N	N	1	-8	-11
NCGC00016509-01	Trimethobenzamide hydrochloride	-4.5		N	N	N		5	7
NCGC00016516-01	Megestrol acetate	-4.5		N	N	N		-5	-15
NCGC00016521-01	Proxiphylline			N	N	N	9	0	0
NCGC00016522-05	Bisacodyl		-4.5	N	N	N	0	4	
NCGC00016527-01	Cloпамide			N	N	N	-3	1	7
NCGC00016530-01	Sulfameter	-4.5		N	N	N	1		6
NCGC00016533-05	Sulfamethoxazole		-4.5	N	N	N	-3	2	
NCGC00016535-01	Alprostadiol	-4.5		N	N	N	1		-2
NCGC00016543-01	Phenformin hydrochloride	-4.5	-4.5	N	N	N	-19		-13
NCGC00016547-06	Clofibrilic_acid	-4.5		N	N	N		6	1
NCGC00016548-01	Chlorphensin carbamate			N	N	N	-4	5	5
NCGC00016549-01	Dosulepin hydrochloride	-4.5		N	N	N		2	-8
NCGC00016561-01	Meticrane		-4.5	N	N	N	9		2
NCGC00016569-01	Tranexamic acid	-4.5		N	N	N		6	6
NCGC00016570-01	Mephentermine hemisulfate	-4.5		N	N	N		10	5
NCGC00016575-01	Colistin sulfate		-4.5	N	N	N	6	14	
NCGC00016580-01	Vancomycin hydrochloride			N	N	N	6	9	4
NCGC00016582-01	Bacitracin	-4.5		N	N	N		5	6
NCGC00016590-01	Azaperone			N	N	N	5	11	3
NCGC00016599-01	Flucytosine	-4.5	-4.5	N	N	N	5		11
NCGC00016604-01	Flumethasone	-4.5		N	N	N		7	8
NCGC00016609-01	Epitostanol			N	N	N	2	9	17
NCGC00016610-01	Tolnaftate			N	N	N	-2	-3	3
NCGC00016612-01	Sulfadoxine		-4.5	N	N	N	2	1	
NCGC00016620-01	Midodrine hydrochloride			N	N	N	3	9	6
NCGC00016623-01	Moroxidine hydrochloride	-4.5		N	N	N	0		-2
NCGC00016627-01	Lidoflazine			N	N	N	-6	-21	-23
NCGC00016629-01	Cyclacillin			N	N	N	3	6	3
NCGC00016630-01	Clidinium bromide			N	N	N	-10	2	-11
NCGC00016636-01	Flavoxate hydrochloride	-4.5	-4.5	N	N	N	2		
NCGC00016642-01	Piperacetazine			N	N	N	-10	-10	-15
NCGC00016643-01	Trioxsalen			N	N	N	0	20	24
NCGC00016646-02	BROMOPRIDE			N	N	N	-9	-2	-13
NCGC00016649-01	Atropine-N-oxide hydrochloride			N	N	N	-5	-3	-5
NCGC00016651-03	SPAGLUMIC ACID		-4.5	N	N	N	11	13	
NCGC00016657-01	Cefalonium	-4.5		N	N	N	4		0
NCGC00016662-01	Metaproterenol sulfate, orciprenaline sulfate			N	N	N	6	8	3
NCGC00016669-01	Scopolamin-N-oxide hydrobromide		-4.5	N	N	N	0	7	
NCGC00016680-01	Oleandomycin phosphate	-4.5		N	N	N	-1		-2
NCGC00016681-01	Methotrimeprazine maleate salt	-4.5		N	N	N	-8		-15
NCGC00016685-05	RONIDAZOLE			N	N	N	4	3	16
NCGC00016686-01	Natamycin			N	N	N	6	17	11
NCGC00016688-02	TOCOPHEROL ACETATE	-4.5	-4.5	N	N	N	-1		
NCGC00016690-01	Tribenoside	-4.5	-4.5	N	N	N	-10		
NCGC00016697-01	Trimetazidine dihydrochloride		-4.5	N	N	N	1	-5	
NCGC00016701-01	Azapropazone			N	N	N	4	11	15

NCGC00016709-01	Benserazide hydrochloride							2	11	
NCGC00016711-01	Cloperastine hydrochloride							-10	-16	-21
NCGC00016712-01	Alcuronium chloride	-4.5							6	15
NCGC00016715-01	Trapidil		-4.5					-2	6	
NCGC00016720-01	Iocetamic acid		-4.5					7		4
NCGC00016721-01	Fenoterol hydrobromide		-4.5	-4.5				3		
NCGC00016723-01	Ornidazole			-4.5				4	9	
NCGC00016738-01	Streptozotocin							-1	6	4
NCGC00016741-01	Tinidazole			-4.5				0	10	
NCGC00016743-01	Piromidic acid	-4.5							-5	5
NCGC00016758-01	Guanadrel sulfate		-4.5					-2		2
NCGC00016760-01	Carbimazole			-4.5				-4	13	
NCGC00016767-02	ETANIDAZOLE		-4.5					5		4
NCGC00016773-01	Ritodrine hydrochloride							7	8	7
NCGC00016774-01	Nifurtimox							5	-9	-16
NCGC00016778-01	Nefopam hydrochloride		-4.5	-4.5				-1		
NCGC00016781-04	AMBROXOL HYDROCHLORIDE			-4.5				1	6	
NCGC00016783-01	Alfadolone acetate		-4.5	-4.5				4		
NCGC00016794-09	Gemfibrozil							6	-5	2
NCGC00016799-01	Suxibuzone							1	-1	0
NCGC00016801-01	(-) -Levobunolol hydrochloride	-4.5							-4	-5
NCGC00016804-01	Etofenamate							5	16	11
NCGC00016807-01	Bupropion hydrochloride	-4.5							3	-7
NCGC00016814-01	Tobramycin		-4.5					-2		7
NCGC00016815-01	Tiaprofenic acid		-4.5	-4.5				3		
NCGC00016819-01	Gliquidone			-4.5				7	-3	
NCGC00016827-01	Acebutolol hydrochloride	-4.5							7	10
NCGC00016829-05	ISOXICAM		-4.5					-7		-1
NCGC00016834-01	Fenbufen							5	2	1
NCGC00016836-01	Apramycin		-4.5	-4.5				2		
NCGC00016837-01	Bacampicillin hydrochloride							1	0	5
NCGC00016849-01	Etodolac			-4.5				-1	4	
NCGC00016850-01	Bezafibrate		-4.5	-4.5				3		
NCGC00016851-01	Nadolol	-4.5							1	-5
NCGC00016855-01	Fenbendazole			-4.5				-5	-2	
NCGC00016856-01	Rimexolone							-16	-12	-22
NCGC00016860-01	Butirosin disulfate salt			-4.5				5	8	
NCGC00016866-01	Pipemidic acid							1	6	2
NCGC00016871-01	Ribostamycin sulfate salt	-4.5							10	5
NCGC00016872-06	TICLOPIDINE		-4.5					-18		-3
NCGC00016876-01	Albendazole							8	-1	-5
NCGC00016878-01	Piretanide	-4.5							5	6
NCGC00016881-01	Netilmicin sulfate							8	19	0
NCGC00016886-01	Ioxaglic acid		-4.5	-4.5				-4		
NCGC00016889-01	Tenoxicam							0	-1	-2
NCGC00016892-01	Iopamidol			-4.5				1	8	
NCGC00016899-01	Rolipram							-9	-13	-17
NCGC00016902-01	Etifenin	-4.5							6	5
NCGC00016903-01	Terazosin hydrochloride	-4.5							3	5
NCGC00016908-01	Naftifine hydrochloride							-1	1	0
NCGC00016914-01	Cefotetan							-2	4	4
NCGC00016923-01	Iopromide	-4.5							8	7
NCGC00016925-06	Omeprazole							-8	-15	-1
NCGC00016926-01	Prednicarbate			-4.5				3	7	
NCGC00016928-01	Imipenem							5	10	2
NCGC00016934-01	Nizatidine	-4.5							6	6
NCGC00016939-01	Levocabastine hydrochloride			-4.5				1	-3	
NCGC00016945-01	Racecadotril			-4.5				-8	0	
NCGC00016946-01	Alfuzosin hydrochloride		-4.5	-4.5				-2		
NCGC00016947-01	Bambuterol hydrochloride	-4.5							9	1
NCGC00016948-01	Ofloxacin		-4.5					-29		5
NCGC00016949-01	Cetirizine dihydrochloride							-1	-15	-13
NCGC00016955-01	Ramipril		-4.5					6		1
NCGC00016957-01	Aceclofenac		-4.5					0		-2

NCGC00016958-01	Iodixanol	-4.5			N	N	N		9	0
NCGC00016962-01	Meropenem	-4.5			N	N	N		-4	3
NCGC00016965-01	Finasteride		-4.5		N	N	N		0	
NCGC00016979-01	Brinzolamide		-4.5		N	N	N	-10		
NCGC00017004-01	Tiletamine hydrochloride		-4.5		N	N	N	1	6	
NCGC00017005-01	Tocainide hydrochloride		-4.5		N	N	N	3	5	
NCGC00017009-01	Pentolinium bitartrate				N	N	N	2	-7	8
NCGC00017010-01	Methylatropine nitrate	-4.5			N	N	N		-1	3
NCGC00017013-01	Thiamine hydrochloride		-4.5		N	N	N	0		1
NCGC00017014-01	Prenylamine lactate				N	N	N	-6	-15	-16
NCGC00017018-01	Merbromin				N	N	N	16	28	17
NCGC00017019-01	Phenethicillin potassium salt				N	N	N	1	0	1
NCGC00017021-01	Deferoxamine mesylate	-4.5			N	N	N		7	-15
NCGC00017025-01	Bergenin monohydrate				N	N	N	-1	11	12
NCGC00017029-01	Cloxacillin sodium salt				N	N	N	0	-2	1
NCGC00017030-01	Fusidic acid sodium salt		-4.5	-4.5	N	N	N	7		
NCGC00017034-01	Diethylcarbamazine citrate	-4.5			N	N	N		8	9
NCGC00017037-01	Oxalamine citrate salt		-4.5		N	N	N	-1		-1
NCGC00017039-01	Deptropine citrate				N	N	N	-17	-6	-6
NCGC00017041-01	Ethamsylate		-4.5	-4.5	N	N	N	5		
NCGC00017043-02	Benzyl diethyl ((2,6-xylylcarbamoyl)methyl) ammonium benzoate		-4.5		N	N	N	5		-6
NCGC00017048-01	Levopropoxyphene napsylate				N	N	N	4	-1	1
NCGC00017056-01	Quercetin dihydrate				N	N	N	-4	-13	-10
NCGC00017066-01	Dextromethorphan hydrobromide monohydrate				N	N	N	0	8	2
NCGC00017073-01	Carbenoxolone disodium salt	-4.5			N	N	N		8	13
NCGC00017097-01	(R) -Naproxen sodium salt		-4.5		N	N	N	3		5
NCGC00017101-01	Cefamandole sodium salt	-4.5			N	N	N		4	7
NCGC00017104-01	Metaraminol bitartrate				N	N	N	6	7	-1
NCGC00017106-01	Azlocillin sodium salt	-4.5			N	N	N		18	11
NCGC00017108-01	Dinoprost trometamol	-4.5			N	N	N		3	9
NCGC00017115-01	Thiethylperazine malate				N	N	N	-5	-6	-10
NCGC00017116-01	Fenoprofen calcium salt dihydrate				N	N	N	2	0	6
NCGC00017117-01	Bethahistine mesylate		-4.5		N	N	N	-5		0
NCGC00017119-01	Metoprolol-(+,-) (+)-tartrate salt				N	N	N	12	6	5
NCGC00017121-01	Gabexate mesilate		-4.5		N	N	N	-10		-10
NCGC00017127-01	Atracurium besylate		-4.5		N	N	N	1		5
NCGC00017128-01	Cefotaxime sodium salt			-4.5	N	N	N	3	10	
NCGC00017129-01	Tolmetin sodium salt dihydrate				N	N	N	4	3	4
NCGC00017141-01	Lisinopril	-4.5			N	N	N		8	5
NCGC00017147-01	Cefepime hydrochloride	-4.5			N	N	N		5	8
NCGC00017244-03	ENOXOLONE		-4.5	-4.5	N	N	N	0		
NCGC00017246-02	PICROTOXIN				N	N	N	6	1	3
NCGC00017258-04	METHYLERGOMETRINE				N	N	N	3	14	16
NCGC00017280-10	TRETINOIN		-4.5	-4.5	N	N	N	0		
NCGC00017325-03	KOJIC ACID			-4.5	N	N	N	4	9	
NCGC00017333-03	Atropine		-4.5	-4.5	N	N	N	2		
NCGC00017358-05	Rotenone				N	N	N	-18	-12	-19
NCGC00018097-04	P-HYDROXYPROPIOPHENONE		-4.5	-4.5	N	N	N	-1		
NCGC00018100-04	Fasudil hydrochloride		-4.5		N	N	N	-8		-8
NCGC00018117-07	OXTRIPHYLLINE				N	N	N	1	1	16
NCGC00018140-02	MIGLUSTAT			-4.5	N	N	N	3	9	
NCGC00018143-04	ENROFLOXACIN				N	N	N	-14	-24	-19
NCGC00018164-02	AZASERINE				N	N	N	7	14	-4
NCGC00018167-03	2-Chloro-2'-deoxyadenosine	-4.5			N	N	N		-3	2
NCGC00018181-08	Nalidixic acid	-4.5			N	N	N		10	8
NCGC00018185-05	Tranilast				N	N	N	-12	-7	-13
NCGC00018200-07	Phenolphthalein				N	N	N	7	4	9
NCGC00018237-03	Trichlorfon				N	N	N	-9	-21	-10
NCGC00018241-04	BETAMIPRON			-4.5	N	N	N	2	4	
NCGC00018243-07	Sulfamethazine		-4.5	-4.5	N	N	N	1		
NCGC00018249-04	ETHOXZOLAMIDE				N	N	N	-14	-2	-5
NCGC00018251-03	METHYL AMINOLEVULINATE HYDROCHLORIDE				N	N	N	1	-30	-30
NCGC00018263-02	HYDROCORTISONE VALERATE		-4.5	-4.5	N	N	N	4		
NCGC00018274-04	DIACERIN		-4.5		N	N	N	-11		-10

NCGC00018938-03	DAZOXIBENUM				-4.5	N	N	N	12	3	
NCGC00021124-04	BUTETAMATUM					N	N	N	-1	6	10
NCGC00021141-04	PHENYLTOLOXAMINE CITRATE			-4.5		N	N	N	-18		-9
NCGC00021142-02	Cromolyn sodium					N	N	N	-2	8	-5
NCGC00021222-03	Cortexolone					N	N	N	-6	-16	-17
NCGC00021301-04	Fluocinolone acetonide					N	N	N	1	-13	-7
NCGC00021666-03	NALMEFENE HYDROCHLORIDE			-4.5		N	N	N	6		-1
NCGC00022003-03	Diflorasone diacetate			-4.5	-4.5	N	N	N	-9		
NCGC00022043-04	DESOXYCORTICOSTERONE ACETATE					N	N	N	-3	-13	-16
NCGC00022391-04	Azaribine			-4.5	-4.5	N	N	N	0		
NCGC00022472-05	Corticosterone					N	N	N	-5	-7	-9
NCGC00022715-03	6-Propyl-2-thiouracil			-4.5	-4.5	N	N	N	3		
NCGC00022848-06	HYDROCORTISONE			-4.5	-4.5	N	N	N	0		
NCGC00023100-03	5alpha-Pregnan-3alpha-ol-11,20-dione					N	N	N	7	1	2
NCGC00023193-04	Triamcinolone acetonide					N	N	N	-10	-20	-17
NCGC00023339-09	PILOCARPINE			-4.5		N	N	N	1	10	
NCGC00023648-03	Desoximetasone					N	N	N	-12	-26	-35
NCGC00023654-04	CAPTOPRIL					N	N	N	-11	-2	-1
NCGC00023673-05	ADENOSINE					N	N	N	0	10	11
NCGC00023902-06	ANDROSTENEDIONE			-4.5		N	N	N	-1	0	
NCGC00023945-05	ZIDOVUDINE			-4.5		N	N	N	4	3	
NCGC00024027-05	METHYSERGIDE			-4.5		N	N	N	3	17	
NCGC00024485-02	(E)-4-amino-2-butenic acid					N	N	N	8	20	13
NCGC00024498-02	D-ASPARTIC ACID					N	N	N	2	14	18
NCGC00024504-05	KAINIC ACID			-4.5	-4.5	N	N	N	1		
NCGC00024563-02	Y-25130					N	N	N	8	10	9
NCGC00024589-02	CIMATEROL			-4.5		N	N	N	-1		10
NCGC00024599-02	CINANSERIN			-4.5		N	N	N	9		-22
NCGC00024609-01	Flurofamide			-4.5		N	N	N	0		-2
NCGC00024714-03	trans-TRIPROLIDINE					N	N	N	-7	-12	-13
NCGC00024733-02	ACECLIDINE			-4.5		N	N	N		12	0
NCGC00024749-01	Pirlindole mesylate			-4.5	-4.5	N	N	N	-6		-2
NCGC00024810-02	PRACTOLOL				-4.5	N	N	N	5	0	
NCGC00024824-01	Statil				-4.5	N	N	N	1	3	
NCGC00024842-02	CHLORMETHIAZOLE				-4.5	N	N	N	2	9	
NCGC00024853-05	Levosulpiride					N	N	N	-2	9	3
NCGC00024915-02	SCH 50911					N	N	N	8	12	11
NCGC00024923-02	ISAMOLTANE					N	N	N	12	16	8
NCGC00024999-02	PROCATEROL			-4.5		N	N	N		-1	3
NCGC00025002-02	AF-DX 116			-4.5		N	N	N	4		2
NCGC00025004-02	GR 103691				-4.5	N	N	N	-1	4	
NCGC00025098-01	Loreclezole hydrochloride				-4.5	N	N	N	6	3	
NCGC00025125-07	Colchicine					N	N	N	4	-9	4
NCGC00025132-01	Levcromakalim					N	N	N	12	5	3
NCGC00025172-01	Linomide			-4.5		N	N	N		-1	1
NCGC00025188-04	PINACIDIL					N	N	N	-6	12	-6
NCGC00025283-01	Acifran				-4.5	N	N	N	5	13	
NCGC00025295-01	Zacopride hydrochloride			-4.5		N	N	N		0	3
NCGC00025315-01	Ipsapirone			-4.5	-4.5	N	N	N	1		
NCGC00026132-02	METANIXINUM			-4.5		N	N	N	-1		0
NCGC00027930-02	MOCLOBEMIDE			-4.5		N	N	N		-2	3
NCGC00037856-01	MEDRONIC ACID					N	N	N	5	1	-12
NCGC00042134-02	AFALANINUM				-4.5	N	N	N	-3	0	
NCGC00061506-02	NICOTREDOLUM					N	N	N	5	10	11
NCGC00063561-02	DIPHENYLIMIDAZOLE			-4.5		N	N	N	-8		-7
NCGC00065890-02	Nevirapine				-4.5	N	N	N	0	-1	
NCGC00070736-02	Imiquimod					N	N	N	-9	-2	3
NCGC00072886-02	Metralindole					N	N	N	-4	-6	-12
NCGC00073457-03	METOMIDATE HYDROCHLORIDE			-4.5	-4.5	N	N	N	-9		
NCGC00080392-01	Phosmet				-4.5	N	N	N	1		1
NCGC00090681-04	Camphor			-4.5		N	N	N		4	8
NCGC00090731-01	Ethylene glycol monophenyl ether				-4.5	N	N	N	3	9	
NCGC00090739-02	1,2-Propylene glycol				-4.5	N	N	N	3	8	
NCGC00090745-02	Boric acid					N	N	N	-1	3	1

NCGC00090749-04	Diethylstilbestrol (mixture Z,E isomers)				N	N	N	-8	0	2
NCGC00090751-01	Sodium zomepirac	-4.5			N	N	N	6		-8
NCGC00090755-02	POTASSIUM DICHROMATE				N	N	N	-12	-7	-19
NCGC00090759-01	cis-Dichlorodiamine platinum	-4.5	-4.5		N	N	N	2		
NCGC00090764-02	Padimate O	-4.5			N	N	N		9	4
NCGC00090766-01	Prednisone	-4.5			N	N	N		-12	-20
NCGC00090767-02	alpha-Cyclodextrin				N	N	N	-1	6	0
NCGC00090770-05	Broxuridina	-4.5			N	N	N		6	-3
NCGC00090781-02	Dioctyl phthalate	-4.5			N	N	N		8	7
NCGC00090791-03	2',3'-DIDEOXYADENOSINE				N	N	N	1	-3	-1
NCGC00090808-01	Amphotericin B				N	N	N	7	-1	-13
NCGC00090814-01	p-Chlorophenol			-4.5	N	N	N	-2	6	
NCGC00090820-01	p-Acetamidobenzoic acid				N	N	N	0	5	0
NCGC00090825-01	1,2-Dichlorobenzene	-4.5	-4.5		N	N	N	0		
NCGC00090827-02	o-methoxyphenol				N	N	N	0	7	3
NCGC00090868-01	Halothane				N	N	N	-1	-4	-1
NCGC00090903-01	Salicylazosulfapyridine				N	N	N	-8	8	-6
NCGC00090905-06	Busulfan	-4.5	-4.5		N	N	N	1		
NCGC00090917-01	2-Propanol	-4.5			N	N	N	1		3
NCGC00090918-04	4-Nonylphenol, branched			-4.5	N	N	N	8	9	
NCGC00090921-01	HEXADIMETHRINI BROMIDUM	-4.5			N	N	N	10		10
NCGC00090939-02	Toluene	-4.5			N	N	N	3		4
NCGC00090950-03	GLYCERIN	-4.5	-4.5		N	N	N	0		
NCGC00090957-01	caprylic acid (octanoic acid)				N	N	N	-5	9	2
NCGC00090964-02	Tetraethylenepentamine	-4.5			N	N	N		0	0
NCGC00090965-03	Propyl-4-hydroxybenzoate				N	N	N	1	11	7
NCGC00090972-01	Lactic acid				N	N	N	-1	4	-3
NCGC00090974-03	Diethyl phthalate	-4.5			N	N	N	-1		9
NCGC00090987-02	1-Naphthalene acetic acid			-4.5	N	N	N	-1	4	
NCGC00090997-02	Dichlorvos (Vapona)				N	N	N	-6	-14	-17
NCGC00091005-01	phosphoric acid	-4.5			N	N	N	6		2
NCGC00091016-02	Carbon tetrachloride	-4.5	-4.5		N	N	N	-4		
NCGC00091018-01	Testosterone	-4.5			N	N	N	-2		-5
NCGC00091021-02	Trichloroacetic acid	-4.5	-4.5		N	N	N	7		
NCGC00091027-01	Sodium hypochlorite				N	N	N	-4	8	6
NCGC00091031-01	Meprobamate	-4.5			N	N	N		1	1
NCGC00091049-04	Linoleic acid			-4.5	N	N	N	-3		-4
NCGC00091051-01	p-Amino benzoic acid	-4.5			N	N	N		8	-1
NCGC00091066-01	Isoamyl nitrite				N	N	N	0	4	6
NCGC00091070-01	Diisopropyl amine	-4.5			N	N	N		6	4
NCGC00091073-01	Diazinon				N	N	N	4	15	17
NCGC00091076-01	Acetal (Acetaldehyde diethyl acetal)			-4.5	N	N	N	0	1	
NCGC00091106-02	Methyl salicylate				N	N	N	0	0	2
NCGC00091108-01	Carbon disulfide				N	N	N	2	-1	11
NCGC00091110-01	Glutaraldehyde (Glutaric dialdehyde)	-4.5			N	N	N	3		-5
NCGC00091116-01	n-Pentane	-4.5	-4.5		N	N	N	1		
NCGC00091119-02	Oleic acid	-4.5			N	N	N	-3		4
NCGC00091120-01	Griseofulvin	-4.5	-4.5		N	N	N	1		
NCGC00091124-02	METHYLTHIOURACIL			-4.5	N	N	N	5		7
NCGC00091149-01	Valproic acid	-4.5			N	N	N		5	4
NCGC00091151-01	Phenoxy acetic acid	-4.5			N	N	N	0		0
NCGC00091162-02	AMINOTHIAZOLE				N	N	N	-9	3	-10
NCGC00091179-01	Acetone	-4.5	-4.5		N	N	N	5		
NCGC00091183-02	2,4,6-Tribromophenol	-4.5			N	N	N		-1	-2
NCGC00091196-01	2,4,5-Trichlorophenol			-4.5	N	N	N	5	-1	
NCGC00091202-01	Trichloroethylene				N	N	N	7	6	2
NCGC00091228-01	Glyoxal				N	N	N	-1	4	8
NCGC00091251-01	Azoxybenzene			-4.5	N	N	N	7	9	
NCGC00091313-01	Hexanamide	-4.5	-4.5		N	N	N	4		
NCGC00091325-05	Dichlorophen	-4.5			N	N	N		-5	2
NCGC00091326-01	Acetanilide			-4.5	N	N	N	1	19	
NCGC00091328-01	Furfural	-4.5			N	N	N		3	0
NCGC00091330-01	Anthralin			-4.5	N	N	N	-2	2	
NCGC00091341-01	Cadmium oxide				N	N	N	-1	9	2

NCGC00091351-02	m-Dinitrobenzene				N	N	N	4	3	11
NCGC00091367-01	Danthron			-4.5	-4.5	N	N	N	-5	-11
NCGC00091389-01	Iodoform					N	N	N		3
NCGC00091390-02	MEQUINOL					N	N	N	2	-20
NCGC00091396-02	Benzoin					N	N	N	-9	-6
NCGC00091400-01	Allylthiourea					N	N	N	3	8
NCGC00091414-02	SALICYLAMIDE					N	N	N	-5	
NCGC00091430-01	Oxymetholone					N	N	N		2
NCGC00091441-01	a-Solanine					N	N	N	1	6
NCGC00091444-02	Dichloroacetic acid					N	N	N	2	
NCGC00091449-05	Eugenol					N	N	N	1	18
NCGC00091470-02	Isoeugenol					N	N	N	-12	-1
NCGC00091502-01	Coumarin					N	N	N	-1	10
NCGC00091507-01	Pyrogallol					N	N	N	-18	-16
NCGC00091533-04	ETHINYL ESTRADIOL					N	N	N	0	8
NCGC00091560-01	Cefuroxime Free Acid					N	N	N	-1	-4
NCGC00091575-01	2-ETHYL-1,3-HEXANEDIOL					N	N	N	0	-10
NCGC00091596-02	Stearic acid					N	N	N	-7	-1
NCGC00091612-04	Triacetin					N	N	N		8
NCGC00091616-01	2-Ethoxybenzamide (Ethenzamide)					N	N	N	1	3
NCGC00091635-01	Fenthion (Baytex)					N	N	N	0	3
NCGC00091660-01	FORMALDEHYDE SOLUTION					N	N	N		6
NCGC00091708-04	COCHINEAL					N	N	N	-2	-6
NCGC00091743-01	Allyl isothiocyanate					N	N	N		-1
NCGC00091810-01	1-Fluoro-2,4-dinitrobenzene					N	N	N		-6
NCGC00091835-01	Nitrogen mustard HCl					N	N	N		5
NCGC00091888-01	Homosalate					N	N	N	1	
NCGC00091902-05	MALATHION					N	N	N	8	10
NCGC00091908-01	1,3-Dicaffeoylquinic Acid					N	N	N	-9	
NCGC00091922-02	Sodium Dichromate Dihydrate					N	N	N	-1	2
NCGC00091923-02	Scopolamine hydrobromide trihydrate					N	N	N	-1	7
NCGC00091940-01	Phenformin HCl					N	N	N	-30	-31
NCGC00091942-01	Methylphenidate hydrochloride					N	N	N	-1	
NCGC00091952-01	Pheniramine maleate					N	N	N	1	9
NCGC00092278-02	MIDAFOTELUM					N	N	N	5	7
NCGC00092299-01	MIFOBATUM					N	N	N	3	9
NCGC00092314-01	TRICIRIBINUM					N	N	N	6	12
NCGC00092328-01	CARMOXIROLUM					N	N	N	-9	-8
NCGC00093347-02	MESTRANOL					N	N	N		0
NCGC00093354-03	Niacinamide					N	N	N	-7	3
NCGC00093356-03	ZALCITABINE					N	N	N	5	8
NCGC00093552-01	p-Aminoclonidine hydrochloride					N	N	N	-3	
NCGC00093569-01	3-Aminopropionitrile fumarate					N	N	N	-6	
NCGC00093636-03	R-(+)-ATENOLOL					N	N	N	-1	6
NCGC00093656-01	(E)-5-(2-Bromovinyl)-2'-deoxyuridine					N	N	N	2	10
NCGC00093658-01	B-HT 933 dihydrochloride					N	N	N	3	
NCGC00093668-01	Benazoline oxalate					N	N	N	-9	-16
NCGC00093739-04	(-)-COTININE					N	N	N		13
NCGC00093802-04	Prasterona					N	N	N	-1	
NCGC00093811-01	Dehydroisoandrosterone 3-sulfate sodium					N	N	N	-10	
NCGC00093850-01	DL-alpha-Difluoromethylornithine hydrochloride					N	N	N	11	16
NCGC00093851-01	ET-18-OCH3					N	N	N	6	8
NCGC00093857-01	Etazolate hydrochloride					N	N	N	-6	-24
NCGC00093867-01	DL-erythro-Dihydrosphingosine					N	N	N	5	8
NCGC00093890-01	S-(-)-Eticlopride hydrochloride					N	N	N	-11	
NCGC00093898-02	FENSPIRIDE HYDROCHLORIDE					N	N	N	7	3
NCGC00093926-03	Doxifluridine					N	N	N		7
NCGC00093949-03	Hidroxiprogesterona					N	N	N	4	6
NCGC00093950-01	L-Histidine hydrochloride					N	N	N	10	13
NCGC00093969-01	lpratropium bromide					N	N	N	10	5
NCGC00094011-01	m-Iodobenzylguanidine hemisulfate					N	N	N	-34	
NCGC00094042-01	Indatraline hydrochloride					N	N	N	-19	-15
NCGC00094048-01	lofetamine hydrochloride					N	N	N	-8	4
NCGC00094063-01	CR 2945					N	N	N	-6	-10

NCGC00094071-01	4-Methylpyrazole hydrochloride	-4.5			N	N	N	1		7
NCGC00094088-01	Clorgyline hydrochloride	-4.5	-4.5		N	N	N	7		
NCGC00094090-01	Cysteamine hydrochloride				N	N	N	6	6	5
NCGC00094108-02	METHOXAMINE HYDROCHLORIDE				N	N	N	2	8	13
NCGC00094121-01	Mexiletene hydrochloride	-4.5			N	N	N		7	-1
NCGC00094136-01	(-)-MK-801 hydrogen maleate		-4.5	-4.5	N	N	N	-6		
NCGC00094140-01	NCS-356				N	N	N	7	6	12
NCGC00094179-02	METHAPYRILENE HYDROCHLORIDE				N	N	N	-17	-14	-10
NCGC00094197-01	Methylcarbarylcholine chloride				N	N	N	-3	9	12
NCGC00094199-02	NOMIFENSINE MALEATE				N	N	N	2	6	1
NCGC00094255-01	Bisoprolol hemifumarate salt				N	N	N	8	9	-5
NCGC00094285-01	R(+)-3PPP hydrochloride	-4.5	-4.5		N	N	N	-3		
NCGC00094337-02	DEXSOTALOLUM			-4.5	N	N	N	-4	8	
NCGC00094357-01	Succinylcholine chloride				N	N	N	13	20	17
NCGC00094381-03	SEMAXANIBUM				N	N	N	4	14	17
NCGC00094393-02	TRIHEXYPHENIDYL HYDROCHLORIDE	-4.5	-4.5		N	N	N	-3		
NCGC00094509-01	3-Tropanylindole-3-carboxylate methiodide				N	N	N	-7	-8	-11
NCGC00094524-01	SIMAZINE			-4.5	N	N	N	1	1	
NCGC00094561-01	PHENOTHRIN			-4.5	N	N	N	12	14	
NCGC00094570-01	IMIDACLOPRID	-4.5			N	N	N	1		4
NCGC00094576-01	ACETOHYDROXAMIC ACID				N	N	N	-1	15	18
NCGC00094607-01	CARBENICILLIN DISODIUM			-4.5	N	N	N	7	11	
NCGC00094655-01	DIHYDROSTREPTOMYCIN SULFATE	-4.5			N	N	N		5	-4
NCGC00094665-01	EPHEDRINE (1R,2S) HYDROCHLORIDE			-4.5	N	N	N	2	3	
NCGC00094670-01	ERYTHROMYCIN	-4.5			N	N	N		-3	9
NCGC00094673-01	ESTRADIOL VALERATE				N	N	N	12	8	9
NCGC00094679-01	EUCATROPINE HYDROCHLORIDE				N	N	N	4	3	4
NCGC00094688-01	GLUCOSAMINE HYDROCHLORIDE	-4.5			N	N	N	3		3
NCGC00094692-01	HETACILLIN POTASSIUM				N	N	N	4	7	11
NCGC00094700-01	INDOPROFEN				N	N	N	2	2	-8
NCGC00094713-01	MEDROXYPROGESTERONE ACETATE				N	N	N	0	-9	-2
NCGC00094720-01	METHICILLIN SODIUM	-4.5			N	N	N	7		1
NCGC00094745-01	ORPHENADRINE CITRATE	-4.5	-4.5		N	N	N	5		
NCGC00094747-01	OXIDOPAMINE HYDROCHLORIDE	-4.5			N	N	N		-5	-1
NCGC00094754-01	PHENACEMIDE				N	N	N	6	8	8
NCGC00094765-01	PREDNISOLONE ACETATE				N	N	N	1	-4	-1
NCGC00094815-01	BROXYQUINOLINE				N	N	N	4	-21	-12
NCGC00094816-01	CARNITINE HYDROCHLORIDE	-4.5			N	N	N		9	6
NCGC00094817-01	FLOPROPIONE			-4.5	N	N	N	0	5	
NCGC00094820-01	IPRONIAZID SULFATE				N	N	N	11	2	16
NCGC00094832-01	BENFLUOREX HYDROCHLORIDE				N	N	N	8	8	18
NCGC00094843-01	ACETYLGLUCOSAMINE	-4.5			N	N	N	5	4	
NCGC00094855-01	ALTHIAZIDE				N	N	N	0	13	9
NCGC00094861-01	BRUCINE				N	N	N	-11	-5	-26
NCGC00094908-01	MEPHENESIN				N	N	N	7	9	7
NCGC00094918-03	Saccharin				N	N	N	1	-1	-1
NCGC00094925-01	ESTRADIOL ACETATE			-4.5	N	N	N	2	-1	
NCGC00094929-01	TOLPERISONE HYDROCHLORIDE	-4.5			N	N	N		-5	-17
NCGC00094937-01	CARPROFEN			-4.5	N	N	N	1	7	
NCGC00094941-01	FOSCARNET SODIUM	-4.5			N	N	N		2	3
NCGC00094948-01	METAMPICILLIN SODIUM			-4.5	N	N	N	8	8	
NCGC00094949-01	FOSFOMYCIN	-4.5			N	N	N	-5		11
NCGC00094956-01	CEPHALORIDINE	-4.5	-4.5		N	N	N	2		
NCGC00094960-03	Antraquinone	-4.5			N	N	N	-11		-23
NCGC00094969-01	ANISINDIONE			-4.5	N	N	N	1	11	
NCGC00094981-03	Benzyl benzoate	-4.5			N	N	N	-7		-2
NCGC00094985-01	DINITOLMIDE			-4.5	N	N	N	-1		4
NCGC00094987-01	AMINOHYDROXYBUTYRIC ACID	-4.5			N	N	N		4	6
NCGC00094989-01	CHROMOCARB				N	N	N	-8	-2	-7
NCGC00094997-01	QUINAPRIL HYDROCHLORIDE	-4.5			N	N	N		10	4
NCGC00095002-01	GLUCONOLACTONE				N	N	N	-1	7	-1
NCGC00095010-01	THONZYLAMINE HYDROCHLORIDE				N	N	N	-1	16	13
NCGC00095019-01	EDOXUDINE				N	N	N	5	11	11
NCGC00095023-01	ETHISTERONE				N	N	N	10	16	7

NCGC00095042-04	Thiotepa				N	N	N	12	20	9
NCGC00095048-01	PIPOBROMAN				N	N	N	-14	0	-14
NCGC00095049-01	EXALAMIDE	-4.5			N	N	N	-12		-7
NCGC00095053-01	MEPARTRICIN	-4.5	-4.5		N	N	N	6		
NCGC00095068-01	NAPROXOL		-4.5		N	N	N	8	3	
NCGC00095073-01	RAMIFENAZONE				N	N	N	7	-2	7
NCGC00095074-01	THIODIGLYCOL				N	N	N	7	16	10
NCGC00095080-01	CYPROTERONE	-4.5			N	N	N	4		9
NCGC00095084-01	OXYPHENCYCLIMINE HYDROCHLORIDE				N	N	N	-19	-16	-30
NCGC00095088-01	2-THIOURACIL	-4.5			N	N	N	2		10
NCGC00095095-01	SENNOSIDE A				N	N	N	-17	-13	-15
NCGC00095105-01	ACETRIAZOIC ACID	-4.5			N	N	N	6		3
NCGC00095108-01	MEPIVACAINE HYDROCHLORIDE	-4.5			N	N	N	1		-2
NCGC00095109-01	VENLAFAXINE	-4.5			N	N	N		7	1
NCGC00095112-01	AVOBENZONE		-4.5		N	N	N	0	10	
NCGC00095116-01	METAXALONE	-4.5	-4.5		N	N	N	3		
NCGC00095118-01	ROFECOXIB	-4.5			N	N	N		6	5
NCGC00095121-01	NATEGLINIDE				N	N	N	1	2	-1
NCGC00095122-01	IRBESARTAN	-4.5			N	N	N	1		-9
NCGC00095127-01	MIGLITOL				N	N	N	3	9	8
NCGC00095129-01	VALDECOXIB				N	N	N	-9	0	-14
NCGC00095131-01	PIOGLITAZONE HYDROCHLORIDE	-4.5			N	N	N	6		0
NCGC00095133-01	FAMCICLOVIR	-4.5			N	N	N		-2	-1
NCGC00095135-01	ALMOTRIPTAN				N	N	N	1	0	-5
NCGC00095137-01	CEFTIBUTEN		-4.5		N	N	N	-6	6	
NCGC00095139-01	VALSARTAN	-4.5			N	N	N		5	-5
NCGC00095143-01	ROSUVASTATIN				N	N	N	1	3	3
NCGC00095153-01	TRANDOLAPRIL	-4.5			N	N	N		0	-2
NCGC00095155-01	ZOLMITRIPTAN				N	N	N	0	6	-1
NCGC00095156-01	CARBADOX				N	N	N	8	12	5
NCGC00095158-01	SECNIDAZOLE				N	N	N	-3	9	-2
NCGC00095164-01	PROTHIONAMIDE	-4.5	-4.5		N	N	N	1		5
NCGC00095169-01	MILTEFOSINE	-4.5			N	N	N		-3	1
NCGC00095176-03	MODAFINIL				N	N	N	-1	2	9
NCGC00095186-01	PREGABALIN				N	N	N	-1	9	-2
NCGC00095187-01	RAMELTEON		-4.5		N	N	N	0	2	
NCGC00095188-01	PANTOPRAZOLE	-4.5			N	N	N		11	-11
NCGC00095190-01	IRINOTECAN HYDROCHLORIDE	-4.5	-4.5		N	N	N	-7		
NCGC00095252-01	BISABOLOL				N	N	N	9	8	4
NCGC00095276-01	DIBEKACIN				N	N	N	-3	2	4
NCGC00095290-01	DIALLYL TRISULFIDE	-4.5			N	N	N	1		6
NCGC00095312-01	DERACOXIB		-4.5		N	N	N	3	-1	
NCGC00095316-01	DIPYROCETYL	-4.5			N	N	N		12	9
NCGC00095321-04	GOLDEN SEAL				N	N	N	-26	-17	-19
NCGC00095537-01	ARABITOL(D)	-4.5			N	N	N		4	4
NCGC00095606-01	MENTHONE		-4.5		N	N	N	8	10	
NCGC00095622-01	HYPOXANTHINE	-4.5			N	N	N	-8		0
NCGC00095661-01	CELLOBIOSE (D[+])				N	N	N	4	3	2
NCGC00095714-01	LIMONIN	-4.5			N	N	N	3		3
NCGC00095716-01	beta-SITOSTEROL	-4.5			N	N	N	3		15
NCGC00095748-01	BATYL ALCOHOL	-4.5			N	N	N		12	5
NCGC00095775-01	TRIPLENNAMINE CITRATE	-4.5	-4.5		N	N	N	2		
NCGC00095777-01	DEHYDROCHOLIC ACID				N	N	N	0	-1	-1
NCGC00095778-01	GLYCYRRHIZIC ACID		-4.5		N	N	N	10		7
NCGC00095787-01	INOSINE	-4.5			N	N	N		5	7
NCGC00095792-01	HYDROXYTOLUIC ACID		-4.5		N	N	N	4	-6	
NCGC00095832-01	HYGROMYCIN B	-4.5			N	N	N		8	4
NCGC00095836-02	SODIUM GUAIAZULENE SULFONATE	-4.5	-4.5		N	N	N	0		
NCGC00095837-01	NEROLIDOL	-4.5	-4.5		N	N	N	7		
NCGC00095838-01	SUMATRIPTAN		-4.5		N	N	N	2	-8	
NCGC00095844-01	CONESSINE	-4.5	-4.5		N	N	N	-2		
NCGC00095872-01	IPRIFLAVONE	-4.5			N	N	N	1		-18
NCGC00095896-01	CANTHAXANTHIN (euglenanone)	-4.5			N	N	N		15	0
NCGC00095899-01	RIZATRIPTAN				N	N	N	8	-6	-1

NCGC00159430-02	Hexobarbital				-4.5	N	N	N	1	1	
NCGC00159431-02	METHIONINE					N	N	N	0	12	5
NCGC00159433-02	Pamidronate disodium				-4.5	N	N	N	0		
NCGC00159434-02	BENACTYZINUM				-4.5	N	N	N		13	9
NCGC00159435-02	Amiloxate					N	N	N	3	2	
NCGC00159437-02	CLOBUTINOL HYDROCHLORIDE				-4.5	N	N	N	-3	-3	
NCGC00159440-02	Temazepam				-4.5	N	N	N		-1	-5
NCGC00159441-02	DESLANOSIDE					N	N	N	5	-8	-21
NCGC00159442-02	Galactose					N	N	N	-1		7
NCGC00159446-02	Carbutamide				-4.5	N	N	N	4		
NCGC00159448-02	DIETHANOLAMINE METHOXYCINNAMATE					N	N	N	1	-1	
NCGC00159449-02	Thiphenamil hydrochloride					N	N	N	3	0	
NCGC00159450-02	PARETHOXYCAINE HYDROCHLORIDE					N	N	N	1	8	3
NCGC00159452-02	Sorbinil				-4.5	N	N	N		9	-5
NCGC00159453-02	Zileuton					N	N	N	2	12	17
NCGC00159454-02	Ticrynafen				-4.5	N	N	N		14	8
NCGC00159454-03	ACIDUM TIENILICUM					N	N	N	1	4	5
NCGC00159458-03					-4.5	N	N	N	1		0
NCGC00159461-02	Amprenavir					N	N	N	-3	-15	-24
NCGC00159467-02	Allocoaine					N	N	N	-2	7	
NCGC00159470-02	VALINE				-4.5	N	N	N	3		1
NCGC00159472-02	Pasiniiazid				-4.5	N	N	N	2		6
NCGC00159473-02	DEXFENFLURAMINE				-4.5	N	N	N		-1	5
NCGC00159474-02	FLUPREDNISOLONE				-4.5	N	N	N		-4	3
NCGC00159475-02	Glisoxepide					N	N	N	-2		-19
NCGC00159480-03	ESKETAMINUM				-4.5	N	N	N	1		
NCGC00159481-02	Sofalcone					N	N	N	-4	-3	-15
NCGC00159482-02	Levobupivacaine hydrochloride					N	N	N	6	5	
NCGC00159485-02	EDETATE CALCIUM DISODIUM				-4.5	N	N	N	0		
NCGC00159491-02	Rimantadine hydrochloride				-4.5	N	N	N	-1		
NCGC00159493-02	PHENOBARBITAL				-4.5	N	N	N		12	7
NCGC00159495-02	Albutoin					N	N	N	10	15	2
NCGC00159496-02	Sildenafil citrate					N	N	N	-5	-12	-15
NCGC00159497-02	Allylestrenol					N	N	N	0	9	9
NCGC00159498-02	Metipranolol				-4.5	N	N	N	2		3
NCGC00159503-02	Methylprednisolone acetate					N	N	N	-2	-2	-5
NCGC00159504-02	THYMOL IODIDE					N	N	N	-14	-27	-39
NCGC00159505-02	PROPYLENE GLYCOL STEARATE SE					N	N	N	6	-2	-4
NCGC00159506-02	CYCLANDELATE				-4.5	N	N	N		10	-3
NCGC00159508-02	Rose Bengal sodium					N	N	N	0	-6	-5
NCGC00159511-02	Butenafina				-4.5	N	N	N		14	6
NCGC00159513-02	LORACARBEF					N	N	N	3	7	
NCGC00159515-02	Eszopiclone				-4.5	N	N	N		2	9
NCGC00159516-02	Meloxicam					N	N	N	-9	-8	-14
NCGC00159517-02	Nefazodone hydrochloride				-4.5	N	N	N	-7		-12
NCGC00159522-02	Cefalexina				-4.5	N	N	N	8		
NCGC00159524-01	THIOPENTAL SODIUM				-4.5	N	N	N		-1	7
NCGC00159533-01	ELTOPRAZINUM					N	N	N	3	1	
NCGC00160128-02	PEPSTATINUM				-4.5	N	N	N		8	8
NCGC00160162-02	HORDENINE					N	N	N	-4		-1
NCGC00160351-01	Isbogrel				-4.5	N	N	N	3		3
NCGC00160352-01	TENIDAPUM					N	N	N	5	12	-5
NCGC00160353-01	Nafenopin				-4.5	N	N	N	-2		-1
NCGC00160358-01	Difitalone					N	N	N	4	11	12
NCGC00160361-01	Vanitolidia				-4.5	N	N	N	5		8
NCGC00160362-01	Salacetamida					N	N	N	6	-4	1
NCGC00160363-01	BUMECAINUM				-4.5	N	N	N	-7		-13
NCGC00160364-01	Benzylsulfamide				-4.5	N	N	N	7		
NCGC00160370-01	Crotoniazida					N	N	N	1	7	3
NCGC00160373-01	Dinaline				-4.5	N	N	N		15	18
NCGC00160375-01	Maleilsulfatiazol					N	N	N	4	7	
NCGC00160376-01	METOCINI I IODIDUM					N	N	N	10	13	6
NCGC00160377-01	TOSIFENUM					N	N	N	6	7	-1
NCGC00160384-01	CLONIXINUM				-4.5	N	N	N	13	3	

NCGC00160386-01	Fluprostenol sodium	-4.5			N	N	N		-1	4
NCGC00160388-01	Fluperlapine	-4.5	-4.5		N	N	N	2		-7
NCGC00160393-01	Sapropterin	-4.5	-4.5		N	N	N	-2		
NCGC00160395-01	Dibenzepina				N	N	N	-9	-11	-6
NCGC00160397-01	IRSOGLADINE MALEATE	-4.5			N	N	N	0		4
NCGC00160399-01	FENTIAZAC	-4.5	-4.5		N	N	N	-1		
NCGC00160400-01	TETRIDAMINUM				N	N	N	3	-3	6
NCGC00160402-01	PHENIODOLUM NATRICUM			-4.5	N	N	N	-4	-1	
NCGC00160407-01	Lomoxicam				N	N	N	-14	-17	-21
NCGC00160408-01	Benziodarone	-4.5			N	N	N	3		1
NCGC00160409-01	Formetorex		-4.5		N	N	N	7	12	
NCGC00160414-01	Benzobarbital		-4.5		N	N	N	1	11	
NCGC00160415-01	Guaiactamine				N	N	N	-4	-7	-1
NCGC00160417-02	S-HYDROPRENE				N	N	N	0	12	0
NCGC00160418-01	PINCAINIDUM	-4.5			N	N	N		0	7
NCGC00160421-01	Tetrabenazine		-4.5		N	N	N	-1	0	
NCGC00160422-01	Chlorphentermine hydrochloride				N	N	N	-11	-14	-12
NCGC00160424-01	CLOBENZOREX				N	N	N	2	9	8
NCGC00160430-01	DIMETAMFETAMINUM			-4.5	N	N	N	7	1	
NCGC00160435-01	Riodipine				N	N	N	5	3	-15
NCGC00160439-01	PYRROCAINUM	-4.5			N	N	N	6		2
NCGC00160444-01	Clofenamide	-4.5			N	N	N	-3		-5
NCGC00160446-01	Cinflumide	-4.5	-4.5		N	N	N	5		
NCGC00160447-01	Demoxepam				N	N	N	11	1	2
NCGC00160450-01	Actarit	-4.5			N	N	N		-1	-10
NCGC00160451-01	Ibufenac		-4.5		N	N	N	0		5
NCGC00160452-01	Clopirac				N	N	N	-13	-10	-16
NCGC00160454-01	FELBINAC ETHYL				N	N	N	-17	-13	-7
NCGC00160457-01	Pivagabine			-4.5	N	N	N	4	11	
NCGC00160458-01	Lozilurea				N	N	N	0	11	7
NCGC00160459-01	Xilobam				N	N	N	9	8	6
NCGC00160467-01	TENOCYCLIDINUM				N	N	N	6	16	7
NCGC00160468-01	Tripalmitin	-4.5			N	N	N		3	2
NCGC00160471-01	SAFFRON	-4.5			N	N	N		0	-3
NCGC00160474-01	Benzetimidum				N	N	N	6	6	5
NCGC00160480-01	Pecazina				N	N	N	-16	-13	-24
NCGC00160484-01	ETAFENONE HYDROCHLORIDE				N	N	N	-16	-17	-23
NCGC00160485-01	DIMAZOLE DIHYDROCHLORIDE	-4.5	-4.5		N	N	N	-5		
NCGC00160487-01	1-PIPERIDINOCYCLOHEXANECARBONITRILE		-4.5		N	N	N	1	10	
NCGC00160489-01	Opiniazida		-4.5		N	N	N	5	14	
NCGC00160491-01	Azabuperona	-4.5			N	N	N	3		-1
NCGC00160492-01	Quifenadine				N	N	N	-21	-17	-21
NCGC00160501-01	Pimeclone			-4.5	N	N	N	2	7	
NCGC00160508-01	ISOSORBIDE				N	N	N	6	14	4
NCGC00160510-01	Etocarlida	-4.5			N	N	N	0		-2
NCGC00160513-01	TESTOSTERONE DECANOATE			-4.5	N	N	N	1	7	
NCGC00160514-01	Idebenone			-4.5	N	N	N	-3	-22	
NCGC00160516-01	Pidotimod	-4.5			N	N	N		9	-1
NCGC00160518-01	Orbifloxacin		-4.5		N	N	N	-1		-1
NCGC00160519-01	ACIPIMOX	-4.5	-4.5		N	N	N	12		
NCGC00160521-01	ERYTHROMYCIN		-4.5		N	N	N	-10		-20
NCGC00160525-01	Zaleplon	-4.5			N	N	N		-1	-1
NCGC00160529-01	Tizanidina	-4.5			N	N	N		17	3
NCGC00160530-01	Toremifene citrate			-4.5	N	N	N	-7	-12	
NCGC00160535-01	Fluindiona				N	N	N	1	0	3
NCGC00160536-01	Colestolone			-4.5	N	N	N	6	9	
NCGC00160540-01	Ethiazide				N	N	N	-1	15	6
NCGC00160541-01	Romazarit				N	N	N	5	7	-2
NCGC00160545-01	Benmoxin			-4.5	N	N	N	11	7	
NCGC00160547-01	FOMOCAINUM	-4.5			N	N	N		9	0
NCGC00160548-01	Ethoxazene hydrochloride				N	N	N	-8	0	1
NCGC00160552-01	INULIN (HYDROXYMETHYL, C-14)		-4.5		N	N	N	3		6
NCGC00160553-01	Diphenadione	-4.5			N	N	N	3		5
NCGC00160557-01	Clorindione				N	N	N	-1	-2	-1

NCGC00160558-01	Diamfenetida	-4.5		N	N	N	9		0
NCGC00160563-01	Carbocloral	-4.5	-4.5	N	N	N	7		
NCGC00160564-01	Difenano			N	N	N	7		4
NCGC00160569-01	Dibemethine			N	N	N	4	12	0
NCGC00160570-01	Butonate			N	N	N	0	-3	3
NCGC00160579-01	Mexenone			N	N	N	10	6	5
NCGC00160581-01	3,3,5-TRIMETHYLCYCLOHEXANOL			N	N	N	-5	8	8
NCGC00160589-01	Chlorindanol			N	N	N	1	3	6
NCGC00160592-01	Lorbamate			N	N	N	6	5	5
NCGC00160593-01	ALPHA-BENZYLIMINO-ALPHA-METHYL-O-CRESOLÃ,		-4.5	N	N	N	-4	9	
NCGC00160595-01	Clazolam			N	N	N	-6	-3	-5
NCGC00160597-01	Neocinchophen			N	N	N	23	26	30
NCGC00160598-01	Penthrichloral			N	N	N	6	15	10
NCGC00160602-01	Tenilidona			N	N	N	12	10	6
NCGC00160603-02	STYRYLPYRIDINIUM CHLORIDE		-4.5	N	N	N	5	6	
NCGC00160611-01	Povidone-iodine	-4.5		N	N	N	0		-1
NCGC00160613-01	PYRROLIDONE CARBOXYLIC ACID	-4.5	-4.5	N	N	N	-1		
NCGC00160615-01	SUCRALFATE		-4.5	N	N	N	-2	13	
NCGC00160617-01	COCARBOXYLASE			N	N	N	-4	-2	-7
NCGC00160622-01	DELTA-TOCOPHEROL, D-	-4.5		N	N	N	-2		3
NCGC00160624-01	Ethopabate	-4.5	-4.5	N	N	N	0		
NCGC00160628-01	Rutin	-4.5	-4.5	N	N	N	3		
NCGC00160631-01	FAMPHUR	-4.5		N	N	N	-17		-13
NCGC00160640-01	Bretazenil			N	N	N	-14	-12	-8
NCGC00160642-01	Veraliprida	-4.5		N	N	N	-6		5
NCGC00160643-01	PIPEROXANUM	-4.5	-4.5	N	N	N	4		
NCGC00160645-01	Butamirate citrate			N	N	N	3	-5	-7
NCGC00160646-01	Pipofezine			N	N	N	9	3	-1
NCGC00160649-01	Glycyclamide	-4.5		N	N	N		-2	12
NCGC00160651-01	SULFASUCCINAMIDUM	-4.5	-4.5	N	N	N	-2		6
NCGC00160653-01	Glisobuzol	-4.5	-4.5	N	N	N	1		
NCGC00160654-01	Ethylparaben			N	N	N	-1	11	12
NCGC00160655-01	Tenonitrozol	-4.5		N	N	N		3	-9
NCGC00160656-01	Verazide	-4.5	-4.5	N	N	N	9		
NCGC00160660-01	Dazmegrel			N	N	N	6	-8	-5
NCGC00160662-01	AMBRISENTAN			N	N	N	0	0	7
NCGC00160663-01	Flazalone			N	N	N	8	9	-2
NCGC00160668-01	Sulfabenz	-4.5	-4.5	N	N	N	4		
NCGC00160670-01	Mecarbinat	-4.5	-4.5	N	N	N	0		
NCGC00160679-01	Dinsed	-4.5		N	N	N	-10		-20
NCGC00160681-01	Risocaine			N	N	N	4	8	13
NCGC00160683-01	Ftaxilida			N	N	N	5	3	6
NCGC00161327-04	CALCITRIOL		-4.5	N	N	N	-8	1	
NCGC00161405-01	Indorenate hydrochloride			N	N	N	-1	14	13
NCGC00162100-02	Dexbrompheniramine maleate salt			N	N	N	-8	-6	-15
NCGC00162175-01	Alinidine	-4.5		N	N	N	-5		-4
NCGC00162267-02	NALOXONE		-4.5	N	N	N	4	7	
NCGC00162445-02	Misoprostol			N	N	N	8	4	-1
NCGC00163125-02	Pregnenolona	-4.5		N	N	N	5		5
NCGC00163146-01	ACONITINE			N	N	N	0	-2	-3
NCGC00163165-01	ERGONOVINE			N	N	N	-11	-12	-6
NCGC00163177-01	NALOXONE METHIODIDE		-4.5	N	N	N	8	11	
NCGC00163182-01	(-)-NORCODEINE	-4.5		N	N	N	4		-1
NCGC00163217-01	CARBAMYL-beta-METHYLCHOLINE			N	N	N	1	10	7
NCGC00163219-01	CARBAMYLCHOLINE			N	N	N	9	5	6
NCGC00163239-01	HEXAMETHONIUM			N	N	N	0	13	11
NCGC00163287-01	5-alpha-PREGNAN-3-alpha-OL-20-ONE	-4.5		N	N	N	-3		2
NCGC00163298-01	Lisofylline			N	N	N	1	3	11
NCGC00163309-01	ADENOSINE TRIPHOSPHATE	-4.5		N	N	N		11	13
NCGC00163319-01	ADENOSINE-5'-MONOPHOSPHATE (AMP)	-4.5		N	N	N	-2		7
NCGC00163335-01	D-LEUCINE			N	N	N	4	10	10
NCGC00163349-01	(-)-3,4-DIHYDROXYNOREPHEDRINE	-4.5		N	N	N		-1	-6
NCGC00163360-01	(+)-NICOTINE			N	N	N	0	-1	6
NCGC00163481-02	TRIDOLGOSIRUM	-4.5		N	N	N	0	9	

NCGC00163597-02	LS-63800	-4.5	-4.5	N	N	N	-1		
NCGC00163674-01	RIFAMYCIN SV-NA	-4.5	-4.5	N	N	N	0		
NCGC00163745-03	CLOFENVINFOSUM			N	N	N	-7	-13	-24
NCGC00163754-02	ALANINE	-4.5		N	N	N	3		8
NCGC00163786-03	BIORESMETHRINUM	-4.5		N	N	N	3		-10
NCGC00163803-03	CYROMAZINUM	-4.5		N	N	N	-1		-1
NCGC00163910-02	TEMEFOSUM	-4.5		N	N	N		8	0
NCGC00163935-02	MAGNESIUM TRISILICATE			N	N	N	8		0
NCGC00164071-01	Tetradecanoic acid, 1-methylethyl ester	-4.5	-4.5	N	N	N	-5		-1
NCGC00164076-01	D-Gluconic acid, monosodium salt	-4.5		N	N	N		15	5
NCGC00164086-01	Disiloxane, hexamethyl-			N	N	N	7	12	6
NCGC00164127-02	TYLOXAPOL		-4.5	N	N	N	6	-1	
NCGC00164155-01	benzyl 4-hydroxybenzoate	-4.5		N	N	N		-8	1
NCGC00164173-02	OCTABENZONUM		-4.5	N	N	N	6	1	
NCGC00164237-01	3-Butenoic acid, 2-amino-4-(2-aminoethoxy)-, monohydrochloride, (S)-(E)			N	N	N	16	22	12
NCGC00164243-01	Chloramine T trihydrate		-4.5	N	N	N	1	9	
NCGC00164246-01	D-Mannitol		-4.5	N	N	N	-1	2	
NCGC00164256-01	Monocrotaline	-4.5		N	N	N		9	4
NCGC00164329-02	DECTAFLURUM	-4.5	-4.5	N	N	N	5		2
NCGC00164336-01	Levothyroxine	-4.5		N	N	N		-6	-3
NCGC00164344-01	Symclocsene	-4.5	-4.5	N	N	N	1		-3
NCGC00164358-01	Hexadecanoic acid	-4.5		N	N	N	1		-9
NCGC00164362-01	Dodecylbenzenesulfonic acid, sodium salt			N	N	N	0	-1	2
NCGC00164375-01	2-Propanol, 1-phenoxy-		-4.5	N	N	N	3	14	
NCGC00164378-01	Cyanamide		-4.5	N	N	N	2	13	
NCGC00164379-01	Amrinone			N	N	N	10	16	
NCGC00164380-02	FORMESTANUM	-4.5		N	N	N	1		-18
NCGC00164388-01	ImidazolidinyI urea			N	N	N	5	8	6
NCGC00164390-01	Milrinone		-4.5	N	N	N	-10		-2
NCGC00164429-01	Feredato sodico			N	N	N	-10	-5	-9
NCGC00164445-01	Troglitazone			N	N	N	-8	-19	-19
NCGC00164446-01	Ciglitizone			N	N	N	2	-9	-17
NCGC00164480-01	MECLORALUREA	-4.5		N	N	N		12	11
NCGC00164482-01	Molracetam	-4.5	-4.5	N	N	N	-5		
NCGC00164483-01	AMINDOCATUM			N	N	N	2	2	3
NCGC00164489-01	AMIPHENAZOLUM	-4.5		N	N	N		8	0
NCGC00164491-01	Lidofenin	-4.5	-4.5	N	N	N	-2		
NCGC00164492-01	Sulfisomidine		-4.5	N	N	N	-1	4	
NCGC00164495-01	Nicotiazone	-4.5		N	N	N	9		1
NCGC00164496-01	ALAFOSFALINUM			N	N	N	-7	6	10
NCGC00164497-01	GLYOCTAMIDUM	-4.5		N	N	N		8	1
NCGC00164499-01	TOCOPHEROL NICOTINATE			N	N	N	11	17	10
NCGC00164500-01	MONOPHOSPHOTHIAMINUM		-4.5	N	N	N	-4		0
NCGC00164502-01	Nifuraldezone			N	N	N	-7	-20	-13
NCGC00164503-01	MYRALACTUM			N	N	N	-2	-6	-17
NCGC00164506-01	Tiliquinol			N	N	N	-20	-22	-2
NCGC00164510-01	Idrocilamida			N	N	N	18	-4	6
NCGC00164513-01	CALCI BENZAMIDOSALICYLAS	-4.5		N	N	N		-1	0
NCGC00164516-01	Eprobemida			N	N	N	-3	-2	-3
NCGC00164517-01	OXACEPROLUM		-4.5	N	N	N	4	12	
NCGC00164525-01	MUROMONAB-CD3	-4.5		N	N	N		8	2
NCGC00164527-01	Lysine	-4.5		N	N	N		-1	6
NCGC00164528-01	GLYCEROL MONOLAURATE	-4.5		N	N	N		2	1
NCGC00164530-01	CINROMIDUM	-4.5		N	N	N		11	0
NCGC00164533-01	BUFORMIN HYDROCHLORIDE		-4.5	N	N	N	-1	5	
NCGC00164534-01	PHENOLSULFONIC ACID		-4.5	N	N	N	7	5	
NCGC00164535-01	Phenmetrazine Hydrochloride	-4.5	-4.5	N	N	N	7		
NCGC00164540-01	CLOFEXAMIDUM	-4.5	-4.5	N	N	N	-6		
NCGC00164544-01	LANOCONAZOLE			N	N	N	-5	-13	-8
NCGC00164546-01	Faropenem		-4.5	N	N	N	-4	12	
NCGC00164549-01	Dofetilide	-4.5		N	N	N		3	5
NCGC00164550-01	LAFUTIDINE	-4.5	-4.5	N	N	N	10		-3
NCGC00164551-01	Biapenem	-4.5		N	N	N	0		5
NCGC00164555-01	Entacapone			N	N	N	-2	-6	-14

NCGC00164556-01	FUDOSTEINE				-4.5	N	N	N	1	12			
NCGC00164558-01	PARGEVERINUM					N	N	N	9	14	10		
NCGC00164561-01	Zanamivir				-4.5	-4.5	N	N	N	-2			
NCGC00164562-01	SIMENDANUM				-4.5	-4.5	N	N	N	7			
NCGC00164564-01	EMTRICITABINE					-4.5	N	N	N	7	11		
NCGC00164566-01	Pitavastatin				-4.5	-4.5	N	N	N	0			
NCGC00164568-01	MONTELUKAST SODIUM			-4.5			N	N	N		-3	-4	
NCGC00164569-01	Capecitabine						N	N	N	4	-18	-10	
NCGC00164573-01	flurazepam						N	N	N	-10	-14	-20	
NCGC00164581-01	ESTRAMUSTINE PHOSPHATE SODIUM					-4.5	N	N	N	13	2		
NCGC00164586-01	Pitofenona					-4.5	N	N	N	2	-15		
NCGC00164589-01	Phenprobamate					-4.5	N	N	N	0			
NCGC00164590-01	Drospirenona			-4.5			N	N	N		-21	-14	
NCGC00164597-01	ROPIVACAINE HYDROCHLORIDE MONOHYDRATE						N	N	N	-1	0	6	
NCGC00164604-01	Fluvastatina					-4.5	N	N	N	-2	-5		
NCGC00164606-01	TROCIMINUM						N	N	N	7	15	9	
NCGC00164609-01	FLUCLOXACILLIN MAGNESIUM					-4.5	-4.5	N	N	N	3		
NCGC00164612-01	ISOPROPYLANTIPYRINE					-4.5	-4.5	N	N	N	9		
NCGC00164613-01	Epalrestat					-4.5	-4.5	N	N	N	2		
NCGC00164617-01	Adapalene			-4.5			N	N	N		8	6	
NCGC00164619-01	Anastrozole			-4.5			N	N	N		10	11	
NCGC00164625-02	CERIVASTATIN SODIUM						N	N	N	-14	-14	-14	
NCGC00164626-01	Tiagabine hydrochloride			-4.5			N	N	N		-3	-1	
NCGC00164628-01	Linezolid						N	N	N	-6	6	-15	
NCGC00164632-01	TIBOLONE					-4.5		N	N	N	1	-14	
NCGC00164637-01	Nifekalant						N	N	N	2	-10	-6	
NCGC00165714-02	ADRAFINILUM						N	N	N	-1	-1	0	
NCGC00165774-02	CLOPROSTENOL SODIUM					-4.5		N	N	N	2	-2	
NCGC00165787-02	DALTROBANUM					-4.5	-4.5	N	N	N	4		
NCGC00165802-02	GANAXOLONUM						N	N	N	8	2	3	
NCGC00165864-02	PIPAMPERONE HYDROCHLORIDE			-4.5			N	N	N		-12	-12	
NCGC00165883-02	RUFINAMIDE					-4.5		N	N	N	4	8	
NCGC00165912-02	TOFISOPAM						N	N	N	3	-1	4	
NCGC00165968-01	REPARIXIN						N	N	N	4	9	6	
NCGC00165970-01	Etiracetam					-4.5		N	N	N	1	-2	
NCGC00165971-01	PERFLUNAFENUM						N	N	N	3	3	14	
NCGC00165972-01	PHENYLPROPANOL						N	N	N	0	7	0	
NCGC00165976-01	HEXAMETHYLTETRACOSANE						N	N	N	0	0	9	
NCGC00165978-01	SODIUM POLYSTYRENE SULFONATE						N	N	N	6	9	5	
NCGC00165979-01	CINNAMIC ACID					-4.5	-4.5	N	N	N	1		
NCGC00165983-01	FD & C Red Dye No. 2					-4.5		N	N	N	-5		-6
NCGC00165991-01	FLUROTYLUM			-4.5				N	N	N		10	6
NCGC00165993-01	CHROMIUM PICOLINATE					-4.5		N	N	N	-1		8
NCGC00165999-01	Cyclamic acid					-4.5		N	N	N	-2		-11
NCGC00166000-01	Iohexol					-4.5		N	N	N	-1		4
NCGC00166005-01	Mecisteina						N	N	N	1	-4	0	
NCGC00166018-01	Actinoquinolum					-4.5	-4.5	N	N	N	6		
NCGC00166020-01	TRICAINE METHANESULFONATE					-4.5	-4.5	N	N	N	0		
NCGC00166022-01	METHENAMINE					-4.5		N	N	N	0		11
NCGC00166024-01	Hetaflur			-4.5				N	N	N		-1	-1
NCGC00166025-01	Methylpentynolum						N	N	N	-1	2	0	
NCGC00166035-01	Demecolcine					-4.5	-4.5	N	N	N	4		
NCGC00166041-01	Dimepranolum						N	N	N	3	8	1	
NCGC00166043-01	Flamenol					-4.5	-4.5	N	N	N	6		
NCGC00166056-01	ETHYL NICOTINATE						N	N	N	-1	1	9	
NCGC00166059-01	Aluminum subacetate					-4.5		N	N	N	0		3
NCGC00166061-01	L-CYSTEINE ETHYLESTER HYDROCHLORIDE					-4.5	-4.5	N	N	N	2		
NCGC00166070-01	Decaminol						N	N	N	-11	-28	-20	
NCGC00166071-01	ISOLEUCINE						N	N	N	2	4	5	
NCGC00166075-01	Piconol						N	N	N	3	10	12	
NCGC00166079-01	SCARLET RED						N	N	N	4	6	-1	
NCGC00166080-01	DEANOLI ACEGLUMAS			-4.5			N	N	N		0	0	
NCGC00166086-01	OCTODRINUM			-4.5			N	N	N		12	0	
NCGC00166088-01	5-Aza-2'-deoxycytidine					-4.5		N	N	N	1	8	

NCGC00167437-01	RAMOSETRON HYDROCHLORIDE		-4.5	-4.5	N	N	N	-6		
NCGC00167440-01	BOSENTAN			-4.5	-4.5	N	N	N	-1	
NCGC00167441-01	PRAMIPEXOLE DIHYDROCHLORIDE		-4.5		N	N	N		8	2
NCGC00167442-01	TAMSULOSIN HYDROCHLORIDE			-4.5	N	N	N	4	2	
NCGC00167443-01	AFLOQUALONE			-4.5	-4.5	N	N	N	5	
NCGC00167444-01	CEFPYRAMIDE SODIUM		-4.5		N	N	N		2	3
NCGC00167445-01	EPRAZINONE HYDROCHLORIDE			-4.5	N	N	N	12	3	
NCGC00167446-01	METHYCLOTHIAZIDE		-4.5		N	N	N		3	-4
NCGC00167448-01	TREPIBUTONE				N	N	N	2	-9	-5
NCGC00167450-01	TRILOSTANE				N	N	N	-12	-21	-26
NCGC00167452-01	PIRENOXINE				N	N	N	-18	-17	-25
NCGC00167453-01	CLINOFIBRATE			-4.5	-4.5	N	N	N	1	
NCGC00167455-01	ZOFENOPRIL				N	N	N	4	7	7
NCGC00167456-01	BISIBUTHIAMINE			-4.5	N	N	N	-3		-2
NCGC00167463-01	CEFMENOXIME HYDROCHLORIDE			-4.5	-4.5	N	N	N	2	
NCGC00167464-01	HYDROCORTISONE SODIUM PHOSPHATE				N	N	N	3	1	3
NCGC00167466-01	LOMUSTINE			-4.5	-4.5	N	N	N	6	
NCGC00167468-01	BENORILATE			-4.5	-4.5	N	N	N	5	13
NCGC00167469-01	MIVACURIUM CHLORIDE			-4.5	N	N	N	-6		-12
NCGC00167470-01	MEZLOCILLIN SODIUM MONOHYDRATE		-4.5		N	N	N		11	0
NCGC00167471-01	ANETHOLE TRITHIONE				N	N	N	-16	-13	-24
NCGC00167473-01	CAPREOMYCIN SULFATE				N	N	N	10	-1	2
NCGC00167474-01	CANDESARTAN CILEXETIL			-4.5	N	N	N	8	6	
NCGC00167477-01	FIDARESTAT		-4.5		N	N	N		3	-1
NCGC00167478-01	GAMMA ORYZANOL			-4.5	N	N	N	1	5	
NCGC00167491-01	LENALIDOMIDE				N	N	N	-3	7	10
NCGC00167494-01	ANDROSTENEDIONE		-4.5		N	N	N		5	0
NCGC00167497-01	ACIPIMOX				N	N	N	6	5	8
NCGC00167499-01	ROXATIDINE ACETATE HYDROCHLORIDE			-4.5	N	N	N	2		8
NCGC00167506-01	PIMECROLIMUS		-4.5		N	N	N		4	6
NCGC00167510-01	DORIPENEM HYDRATE				N	N	N	6	22	24
NCGC00167511-01	PEMOLINE			-4.5	N	N	N	1		6
NCGC00167515-01	ENOCITABINE			-4.5	N	N	N	-5		-2
NCGC00167518-01	TEMSIROLIMUS		-4.5		N	N	N		6	-5
NCGC00167519-01	RAMATROBAN			-4.5	-4.5	N	N	N	-2	-1
NCGC00167520-01	CILOMILAST		-4.5		N	N	N		2	3
NCGC00167527-01	GREPAFLOXACIN HYDROCHLORIDE				N	N	N	-2	-2	-7
NCGC00167528-01	ALOSETRON HYDROCHLORIDE			-4.5	N	N	N	1		-7
NCGC00167530-01	ARBEKACIN SULFATE			-4.5	-4.5	N	N	N	-2	
NCGC00167531-01	RIVASTIGMINE TARTRATE			-4.5	N	N	N	-5		-2
NCGC00167534-01	PAZUFLOXACIN				N	N	N	4	0	-9
NCGC00167537-01	DONEPEZIL HYDROCHLORIDE			-4.5	N	N	N	-8		-14
NCGC00167539-01	INDOLUM				N	N	N	-4	4	7
NCGC00167540-01	SKATOLUM			-4.5	N	N	N	-3		-5
NCGC00167541-01	EPIDIHYDROCHOLESTERIN			-4.5	-4.5	N	N	N	-4	
NCGC00167544-01	BISOCTRIZOLE				N	N	N	2	1	5
NCGC00167546-02	ADEMETHIONINE				N	N	N	3	7	-1
NCGC00167549-01	N-CARBAMYL-L-GLUTAMIC ACID				N	N	N	-3	10	8
NCGC00167552-01	PIPEROCAINE HYDROCHLORIDE				N	N	N	5	4	-3
NCGC00167556-01	CARUMONAM SODIUM				N	N	N	-2	-3	-2
NCGC00167559-01	5A-ANDROSTA-16-ENE-3-ONE				-4.5	N	N	N	-1	-1
NCGC00167560-01	3,4-DIAMINOPYRIDINE PHOSPHATE				-4.5	N	N	N	8	13
NCGC00167561-01	TOCOPHERYL SUCCINATE		-4.5		N	N	N		5	-6
NCGC00167563-01	MOFEZOLAC			-4.5	-4.5	N	N	N	0	
NCGC00167565-01	CARBAZOCHROME SODIUM SULFONATE				-4.5	N	N	N	8	15
NCGC00167573-01	FLAVIN ADENINE DINUCLEOTIDE			-4.5	-4.5	N	N	N	4	
NCGC00167581-01	CEFTAZIDIME SODIUM				N	N	N	4	-1	3
NCGC00167583-01	1,3-PROPANEDISULFONIC ACID, DISODIUM SALT				-4.5	N	N	N	6	5
NCGC00167588-02	GOSERELIN ACETATE				-4.5	N	N	N	5	9
NCGC00167729-01	LINTITRIPTUM				N	N	N	3	6	9
NCGC00167744-01	MELPERONUM			-4.5	-4.5	N	N	N	9	
NCGC00167808-01	FANANSERINUM				N	N	N	2	4	5
NCGC00167838-01	CILASTATIN SODIUM		-4.5		N	N	N		6	0
NCGC00167840-01	LOXORIBINUM			-4.5	N	N	N	3		-3

NCGC00167973-01	EPERISONE HYDROCHLORIDE	-4.5			N	N	N		6	0
NCGC00167980-01	PRANOPROFEN	-4.5			N	N	N		10	9
NCGC00167983-01	DESONIDE		-4.5	-4.5	N	N	N	-13		
NCGC00168249-01	CLOBAZAM			-4.5	N	N	N	9	13	
NCGC00168250-01	ESTAZOLAM		-4.5	-4.5	N	N	N	9		
NCGC00168251-01	ETHYLMORPHINE HYDROCHLORIDE				N	N	N	-13	-32	-38
NCGC00168252-01	FENTANYL		-4.5	-4.5	N	N	N	6		
NCGC00168253-01	DIAMORPHINE HYDROCHLORIDE				N	N	N	8	6	8
NCGC00168255-01	NALORPHINE HYDROCHLORIDE			-4.5	N	N	N	4	5	
NCGC00168258-01	TRIAZOLAM		-4.5	-4.5	N	N	N	-4		
NCGC00168345-01	ETRYPTAMINUM			-4.5	N	N	N	5	15	
NCGC00168346-01	FENAMOLUM				N	N	N	4	2	9
NCGC00168347-01	BETAPRODINUM		-4.5	-4.5	N	N	N	6		
NCGC00168348-01	ISBUFYLLINUM		-4.5		N	N	N	-8		1
NCGC00168349-01	IODOPHTHALEINUM NATRICUM				N	N	N	-9	-6	-2
NCGC00168746-01	METILDIGOXIN				N	N	N	-5	6	2
NCGC00168747-01	METHOXYFLURANE			-4.5	N	N	N	1	2	
NCGC00168749-01	DIFLUPREDNATE				N	N	N	-14	-16	-28
NCGC00168778-01	SOLIFENACIN SUCCINATE				N	N	N	-11	-2	-14
NCGC00168779-01	VALGANCICLOVIR HYDROCHLORIDE				N	N	N	2	12	9
NCGC00168780-01	MILNACIPRAN		-4.5		N	N	N		12	14
NCGC00168781-01	TADALAFIL		-4.5	-4.5	N	N	N	5		
NCGC00168783-01	ISOFLUOROPHATE			-4.5	N	N	N	-4		5
NCGC00168785-01	DICLAZURIL		-4.5		N	N	N		-4	-9
NCGC00168787-01	NORELGESTROMIN				N	N	N	-17	-23	-22
NCGC00169077-02	POTASSIUM RICINOLEATE		-4.5	-4.5	N	N	N	3		
NCGC00180996-01	PROPYL SALICYLATE		-4.5		N	N	N	-4		2
NCGC00181001-01	LAURIC DIETHANOLAMIDE				N	N	N	7	18	16
NCGC00181005-01	SOMATOSTATIN		-4.5		N	N	N		0	6
NCGC00181006-01	P-HYDROXYEPHEDRINE HYDROCHLORIDE		-4.5		N	N	N		-1	8
NCGC00181007-01	CEFOSELIS SULFATE			-4.5	N	N	N	3		4
NCGC00181008-01	OLSALAZINE SODIUM		-4.5	-4.5	N	N	N	0		
NCGC00181012-01	CEFOZOPRAN HYDROCHLORIDE		-4.5	-4.5	N	N	N	8		
NCGC00181016-01	BEXAROTENE				N	N	N	-12	-1	-5
NCGC00181018-01	ANECORTAVE ACETATE		-4.5		N	N	N	5		2
NCGC00181025-01	TRANSFLUTHRIN		-4.5		N	N	N		8	17
NCGC00181027-01	5-METHYLTETRAHYDROFOLATE SODIUM SALT				N	N	N	12	11	11
NCGC00181028-01	PANTETHINE			-4.5	N	N	N	6	11	
NCGC00181029-01	DIMYRISTOYL LECITHIN		-4.5		N	N	N		8	11
NCGC00181030-01	URACIL			-4.5	N	N	N	6		7
NCGC00181031-01	HYDROXYCITRONELLAL				N	N	N	2	4	-1
NCGC00181036-01	FENIPENTOL		-4.5		N	N	N		13	8
NCGC00181038-01	LACTALFATUM			-4.5	N	N	N	2	2	
NCGC00181039-01	ETHYL LINOLEATE				N	N	N	4	12	3
NCGC00181040-01	CONIINE		-4.5		N	N	N	5		1
NCGC00181041-01	METHYLCHLOROISOTHIAZOLINONE				N	N	N	4	8	3
NCGC00181042-01	MENTHYL SALICYLATE			-4.5	N	N	N	-1	-1	
NCGC00181044-01	SELENOMETHIONINE, L-		-4.5		N	N	N	5		6
NCGC00181049-01	URIC ACID				N	N	N	8	1	11
NCGC00181083-01	PIPETHANATE HYDROCHLORIDE		-4.5		N	N	N	4		5
NCGC00181084-01	LEFETAMINE HYDROCHLORIDE		-4.5	-4.5	N	N	N	1		
NCGC00181092-01	IPODATE CALCIUM			-4.5	N	N	N	5	13	
NCGC00181094-01	TYROPANOATE SODIUM		-4.5		N	N	N	5		5
NCGC00181095-01	IPRONIDAZOLE		-4.5		N	N	N	3		10
NCGC00181110-01	CAMBENDAZOLE		-4.5		N	N	N	1		-11
NCGC00181115-01	18ALPHA-GLYCYRRHETINIC ACID				N	N	N	2	5	0
NCGC00181117-01	VIRGINIAMYCIN				N	N	N	-1	-7	-11
NCGC00181130-01	ELETRIPTAN HYDROBROMIDE		-4.5		N	N	N	-15		-12
NCGC00181133-01	DESMOPRESSIN ACETATE		-4.5		N	N	N		9	-3
NCGC00181136-01	PYRROLNITRIN			-4.5	N	N	N	7	-3	
NCGC00181137-01	SULFATOLAMIDE				N	N	N	11	18	0
NCGC00181141-01	SODIUM SANTONINATE		-4.5	-4.5	N	N	N	-1		
NCGC00181149-01	PHENYLPROPANOLAMINE MALEATE				N	N	N	0	1	4
NCGC00181151-01	METOCURINE IODIDE		-4.5	-4.5	N	N	N	0		

NCGC00181152-01	NEDAPLATIN				N	N	N	-7	11	0
NCGC00181156-01	OXABOLONE CIPIONATE		-4.5		N	N	N	2	5	
NCGC00181160-01	ECABET SODIUM	-4.5			N	N	N	0		0
NCGC00181161-01	ETHYL SALICYLATE		-4.5		N	N	N	2	9	
NCGC00181164-01	ISOLEUCINE	-4.5	-4.5		N	N	N	-4		
NCGC00181165-02	DECANOHYDROXAMIC ACID				N	N	N	4	9	7
NCGC00181166-01	MESNA		-4.5		N	N	N	-1	8	
NCGC00181169-01	PENTISOMICINUM				N	N	N	1	6	6
NCGC00181170-01	BENDAMUSTINUM	-4.5			N	N	N	6		1
NCGC00181290-01	FURAZABOL				N	N	N	2	-9	-21
NCGC00181294-01	THIAMINE DISULFIDE				N	N	N	-4	10	-1
NCGC00181296-01	SERATRODAST				N	N	N	-10	-22	-27
NCGC00181297-01	MEBROFENIN	-4.5			N	N	N		-5	-26
NCGC00181305-01	MAGNESIUM SALICYLATE		-4.5	-4.5	N	N	N	7		
NCGC00181307-01	FEBANTEL				N	N	N	7	10	6
NCGC00181308-01	SORBITAN MONOPALMITATE			-4.5	N	N	N	0	-20	
NCGC00181318-01	HYDROXOCOBALAMIN ACETATE	-4.5	-4.5		N	N	N	4		
NCGC00181320-01	MERSALYL SODIUM				N	N	N	3	-6	1
NCGC00181327-01	25-Hydroxycholesterol			-4.5	N	N	N	-2	2	
NCGC00181332-01	3b-(2-Diethylaminoethoxy)androst-5-en-17-one, HCl	-4.5			N	N	N	-12		-8
NCGC00181334-01	DIBUNATE SODIUM		-4.5		N	N	N	7	3	
NCGC00181335-01	DIETHYLSTILBESTROL DIPHOSPHATE		-4.5		N	N	N	11	10	
NCGC00181336-01	FLUDARABINE PHOSPHATE		-4.5		N	N	N	1	2	
NCGC00181338-01	Triiodothyronine, reverse	-4.5	-4.5		N	N	N	-3		
NCGC00181339-01	CEFPIROME SULPHATE				N	N	N	-10	-5	-15
NCGC00181342-01	IMIDAPRIL HYDROCHLORIDE	-4.5			N	N	N	2		8
NCGC00181345-01	TEMOCAPRIL HYDROCHLORIDE	-4.5			N	N	N	-14		-11
NCGC00181346-01	CILASTATIN SODIUM				N	N	N	11	-6	3
NCGC00181347-01	ACIPIMOX	-4.5	-4.5		N	N	N	-3		
NCGC00181348-01	TEICOPLANIN				N	N	N	-1	11	-1
NCGC00181349-01	STRONTIUM RANELATE				N	N	N	8	4	6
NCGC00181353-01	NORGESTIMATE				N	N	N	-16	-21	-17
NCGC00181354-01	TOCORETINATE	-4.5			N	N	N		12	1
NTOC00000202-01			-4.5		N	N	N	7	-3	
NCGC00013103-01	GLYCINE		-4.5		N	N	N	4	4	
NCGC00013287-06	CARZENIDUM	-4.5	-4.5		N	N	N	8		
NCGC00013556-01	Detrothyronin				N	N	N	-20	-24	-32
NCGC00014044-01	Dimetacrine				N	N	N	-34	-32	-31
NCGC00014529-01	mesoridazine	-4.5			N	N	N		-14	-8
NCGC00014684-03	PIFEXOLUM	-4.5	-4.5		N	N	N	8		
NCGC00015012-02	ALAPROCLATE	-4.5	-4.5		N	N	N	6		
NCGC00015060-06	Azathioprine				N	N	N	-22	-12	-23
NCGC00015074-10	Acetazolamide			-4.5	N	N	N	2	7	
NCGC00015155-03	BEPRIDIL	-4.5	-4.5		N	N	N	-29		
NCGC00015216-11	Chlorpropamide	-4.5			N	N	N		14	6
NCGC00015226-07	Mitotane				N	N	N	-27	-23	-30
NCGC00015279-02	Meclofenoxate hydrochloride				N	N	N	15	27	17
NCGC00015426-04	FURAFYLLINE		-4.5		N	N	N	5	1	
NCGC00015506-03	HYDROXYTACRINE		-4.5		N	N	N	2	5	
NCGC00015560-06	IDAZOXAN				N	N	N	-14	-12	-25
NCGC00015609-03	Lonidamine	-4.5	-4.5		N	N	N	-6		
NCGC00015610-02	Lefunomide		-4.5		N	N	N	0	3	
NCGC00015760-06	DL-OCTOPAMINE	-4.5			N	N	N		-4	-6
NCGC00015762-06	OXOLINIC ACID				N	N	N	-20	-9	-20
NCGC00015793-03	Palmitoylethanolamide				N	N	N	10	12	8
NCGC00015821-02	Piracetam		-4.5		N	N	N	7	1	
NCGC00015829-02	Promazine hydrochloride				N	N	N	-16	-4	-20
NCGC00015830-02	Phenelzine sulfate				N	N	N	-12	-17	-31
NCGC00015882-09	RILUZOLE		-4.5		N	N	N	1	6	
NCGC00015908-05	SPIROXATRINE	-4.5	-4.5		N	N	N	-13		
NCGC00015958-03	SP 600125	-4.5	-4.5		N	N	N	-9		
NCGC00015985-03	Tracazolate hydrochloride				N	N	N	6	-16	-13
NCGC00016049-02	Tetracaine hydrochloride				N	N	N	22	28	23
NCGC00016098-07	XYLAZINE				N	N	N	-31	-12	-25

NCGC00016105-03	Zaprinast				-4.5	N	N	N	-22	-19	
NCGC00016119-02	Bretylium tosylate					N	N	N	-19	-11	-31
NCGC00016224-02	NIACINAMIDE			-4.5	-4.5	N	N	N	-8		
NCGC00016226-01	Pralidoxime chloride				-4.5	N	N	N	0	3	
NCGC00016233-01	Lynestrenol			-4.5		N	N	N		3	10
NCGC00016258-02	MENADIONE					N	N	N	-21	-29	-28
NCGC00016270-04	L-3,4-DIHYDROXYPHENYL-ALANINE				-4.5	N	N	N	8	9	
NCGC00016274-04	Phenazone				-4.5	N	N	N	11	19	
NCGC00016308-01	Isopropamide iodide			-4.5		N	N	N		-2	-23
NCGC00016338-01	Dibucaine			-4.5		N	N	N		3	-16
NCGC00016339-01	Phensuximide				-4.5	-4.5	N	N	-7		
NCGC00016353-03	BUTAMBEN					N	N	N	12	14	13
NCGC00016360-01	Monobenzene					N	N	N	-28	-27	-27
NCGC00016366-01	Azacyclonol			-4.5		N	N	N		9	0
NCGC00016431-01	Triflusal			-4.5		N	N	N		15	10
NCGC00016433-01	Isoflupredone acetate			-4.5		N	N	N		0	5
NCGC00016438-01	Procabazine hydrochloride				-4.5	-4.5	N	N	-10		
NCGC00016492-01	Methocarbamol					-4.5	N	N	-4	-3	
NCGC00016494-01	Amyleine hydrochloride				-4.5	-4.5	N	N	2		
NCGC00016513-01	Debrisoquin sulfate					-4.5	N	N	3	7	
NCGC00016534-01	Cyclopenthiiazide			-4.5		N	N	N		1	3
NCGC00016551-01	Meprylcaine hydrochloride					N	N	N	-3	6	7
NCGC00016557-01	Ethaverine hydrochloride					N	N	N	-20	-13	-30
NCGC00016572-01	Sulfamonomethoxine			-4.5		N	N	N		0	16
NCGC00016587-01	Metixene hydrochloride					N	N	N	-31	-22	-31
NCGC00016616-01	Medrysone			-4.5		N	N	N		-8	-19
NCGC00016617-01	Mebeverine hydrochloride					N	N	N	-21	-26	-32
NCGC00016638-01	Furaltadone hydrochloride					N	N	N	-30	-30	-28
NCGC00016639-01	Ifosfamide			-4.5		N	N	N		6	-1
NCGC00016653-01	(cis-) Nanophine			-4.5		N	N	N		11	12
NCGC00016654-01	Flurbiprofen					N	N	N	-27	-12	-24
NCGC00016661-01	Cyclopentolate hydrochloride					N	N	N	16	31	22
NCGC00016676-01	Proglumide				-4.5		N	N	2	5	
NCGC00016755-01	Oxamniquine			-4.5		N	N	N		-4	1
NCGC00016769-01	Famprofazone					N	N	N	-5	-10	-16
NCGC00016805-01	Metrizamide			-4.5		N	N	N		13	9
NCGC00016810-01	Labetalol hydrochloride					N	N	N	-7	-11	-16
NCGC00016823-01	Pivampicillin				-4.5		N	N	1	5	
NCGC00016831-01	Buflomedil hydrochloride			-4.5		N	N	N		0	5
NCGC00016877-01	Praziquantel			-4.5		N	N	N		10	10
NCGC00016906-01	Dipivefrin hydrochloride				-4.5		N	N	-6	-20	
NCGC00016912-01	Terconazole					N	N	N	-10	4	-20
NCGC00016924-02	SULMAZOLE				-4.5		N	N	9	9	
NCGC00016927-01	Enoxacin					N	N	N	-12	-1	-3
NCGC00016978-01	Repaglinide			-4.5		N	N	N		11	8
NCGC00017045-01	Trimeprazine tartrate					N	N	N	-8	-2	-1
NCGC00017096-01	Morantel tartrate					N	N	N	-13	-5	-12
NCGC00017135-01	Ketorolac tromethamine				-4.5		N	N	0	-7	
NCGC00018122-08	LY 171883					N	N	N	-13	-15	-20
NCGC00018211-03	FLUMEQUINE				-4.5		N	N	-8	-5	
NCGC00018221-06	CINCHOPHENUM				-4.5	-4.5	N	N	9		
NCGC00018238-04	OXIBENDAZOLE			-4.5		N	N	N		-2	-5
NCGC00024667-04	Methyldopa sesquihydrate					N	N	N	-9	-8	-9
NCGC00025303-03	S(-)-RACLOPRIDE			-4.5		N	N	N		1	5
NCGC00025325-02	VAPIPROST HYDROCHLORIDE				-4.5		N	N	-11		-14
NCGC00025335-01	Reboxetine mesylate					N	N	N	-16	-29	-21
NCGC00025357-01	Nicorandil					N	N	N	14	21	24
NCGC00026844-02	ACIDUM NIXYLICUM				-4.5	-4.5	N	N	10		
NCGC00037064-02	Zearalanol			-4.5		N	N	N		-13	-22
NCGC00063341-02	GIPARMENUM					N	N	N	9.5	16	11.5
NCGC00075916-01	ETEROBARBUM				-4.5		N	N	5	2	
NCGC00090793-02	Naphthalene					N	N	N	7	8	11
NCGC00090797-03	Digoxin			-4.5		N	N	N		-25	-19
NCGC00090892-01	Urea			-4.5		N	N	N		15	15

NCGC00091057-01	Silibinin				N	N	N	-15	-15	-17
NCGC00091104-02	Aspartame				N	N	N	15	31	21
NCGC00091238-02	2-MERCAPTOBENZOTHAZOLE	-4.5			N	N	N		8	11
NCGC00091423-02	METACETAMOL		-4.5	-4.5	N	N	N	10		
NCGC00091572-01	Mercuric chloride				N	N	N	-32	-34	-36
NCGC00093372-02	D-TRYPTOPHAN			-4.5	N	N	N	10	15	
NCGC00093792-01	L-3,4-Dihydroxyphenylalanine methyl ester hydrochloride				N	N	N	-19	-14	-21
NCGC00094087-01	Mizoribine				N	N	N	7	15	9
NCGC00094091-01	NG-Monomethyl-L-arginine acetate	-4.5			N	N	N		-2	6
NCGC00094280-01	Quazinone				N	N	N	-14	-2	-1
NCGC00094363-03	D-SERINE			-4.5	N	N	N	7	0	
NCGC00094412-02	TULOButEROL				N	N	N	-17	-17	-17
NCGC00094439-01	Tetraethylammonium chloride				N	N	N	-9	2	7
NCGC00094507-01	Olprinone hydrochloride		-4.5	-4.5	N	N	N	-8		
NCGC00094779-01	SALICYL ALCOHOL	-4.5			N	N	N		10	10
NCGC00094917-01	ACETAMINOSALOL	-4.5			N	N	N		5	7
NCGC00094995-01	ADIPHENINE HYDROCHLORIDE		-4.5	-4.5	N	N	N	-9		
NCGC00095024-01	FIPEXIDE HYDROCHLORIDE				N	N	N	-17	-15	-32
NCGC00095043-01	TETROQUINONE				N	N	N	-11	-14	-18
NCGC00095111-01	AMINOLEVULINIC ACID HYDROCHLORIDE	-4.5			N	N	N		-22	-14
NCGC00095130-01	MOXIFLOXACIN HYDROCHLORIDE				N	N	N	-19	-19	-26
NCGC00095148-01	CANRENONE		-4.5		N	N	N	-11		-11
NCGC00095191-01	OSELTAMIVIR TARTRATE				N	N	N	-14	-15	-16
NCGC00095403-01	TOMATIDINE HYDROCHLORIDE				N	N	N	-11	-24	-30
NCGC00095782-01	N-METHYL (-)EPHEDRINE			-4.5	N	N	N	4	1	
NCGC00096009-01	CLAVULANATE LITHIUM			-4.5	N	N	N	0	-4	
NCGC00096040-01	BLEOMYCIN (bleomycin B2 shown)	-4.5			N	N	N		3	1
NCGC00159363-02	ETHISTERONUM			-4.5	N	N	N	8	6	
NCGC00159374-02	CHLORAL HYDRATE		-4.5	-4.5	N	N	N	1		
NCGC00159389-02	THIOACETAZONUM				N	N	N	9	7	16
NCGC00159478-02	Benzoxiquine		-4.5	-4.5	N	N	N	-16		
NCGC00159520-02	Valacyclovir hydrochloride	-4.5			N	N	N		1	10
NCGC00159553-01	FANAPANELUM		-4.5	-4.5	N	N	N	10		
NCGC00160359-01	Cefaloram		-4.5	-4.5	N	N	N	0		
NCGC00160387-01	Clothiapine				N	N	N	-21	-25	-30
NCGC00160396-01	Pravadoline maleate				N	N	N	9	8	12
NCGC00160412-01	Indocate				N	N	N	14	17	16
NCGC00160416-01	Chlormidazole				N	N	N	-15	-9	-12
NCGC00160434-01	Esaprazola			-4.5	N	N	N	1	8	
NCGC00160461-01	Quindoxin			-4.5	N	N	N	6	11	
NCGC00160479-01	Ftorpropazine	-4.5			N	N	N		-22	-21
NCGC00160498-01	Clostebol				N	N	N	-12	-8	-23
NCGC00160499-01	DICARBINUM	-4.5			N	N	N		-3	-4
NCGC00160534-01	Flurogestone acetate			-4.5	N	N	N	4	4	
NCGC00160556-01	Rafoxanide				N	N	N	-10	0	-15
NCGC00160559-01	TOLAMOLOLUM		-4.5	-4.5	N	N	N	5		
NCGC00160573-01	Menbutone	-4.5			N	N	N		9	7
NCGC00160575-01	URACIL MUSTARD			-4.5	N	N	N	8	13	
NCGC00160577-01	LAURIXAMINUM				N	N	N	-21	-8	-8
NCGC00160587-01	Dixanthogen		-4.5		N	N	N	4		7
NCGC00160653-02	GLYSOBUZOLUM	-4.5			N	N	N		1	10
NCGC00160657-01	Frentizole				N	N	N	-9	-15	-23
NCGC00160665-01	Proroxanum		-4.5	-4.5	N	N	N	6		
NCGC00160671-01	VIOMYCIN SULFATE	-4.5			N	N	N		10	8
NCGC00160674-01	Aconiazida	-4.5			N	N	N		5	5
NCGC00160677-01	Butinolina				N	N	N	-6	-11	-17
NCGC00160680-01	NOREXIMIDUM			-4.5	N	N	N	0	10	
NCGC00161328-03	SECALCIFEROL				N	N	N	-13	-15	-25
NCGC00161336-02	POTASSIUM RICINOLEATE	-4.5			N	N	N		10	9
NCGC00162222-01	Cibenzoline succinate				N	N	N	-14	-13	-26
NCGC00162275-02	NALBUPHINE	-4.5			N	N	N		11	9
NCGC00163240-01	NEOSTIGMINE				N	N	N	-18	-12	-15
NCGC00163318-01	SURAMIN				N	N	N	-18	-3	-17
NCGC00163344-01	O-PHOSPHO-L-SERINE	-4.5	-4.5		N	N	N	7		

NCGC00163355-01	INDIGO				N	N	N	-26	-21	-19
NCGC00164511-01	Menadiol				N	N	N	-18	-15	-25
NCGC00164518-01	SULFONETHYLMETHANE		-4.5	-4.5	N	N	N	8		
NCGC00164522-01	METISAZONUM				N	N	N	-20	-29	-28
NCGC00164542-01	TALINOLOLUM				N	N	N	-17	-22	-34
NCGC00164583-01	Amdinocillin		-4.5		N	N	N		-13	-18
NCGC00164592-01	ARGATROBAN			-4.5	N	N	N	1		
NCGC00164621-01	FENPIVERINII BROMIDUM				N	N	N	-14	-5	-15
NCGC00164622-01	Voriconazole			-4.5	N	N	N	2	-1	
NCGC00164636-01	TRIPTORELIN PAMOATE			-4.5	N	N	N	8	-1	
NCGC00165769-02	CLORICROMENUM			-4.5	N	N	N	0	-1	
NCGC00166026-01	Nikethamide			-4.5	N	N	N	1	7	
NCGC00166087-01	TIMONACICUM		-4.5		N	N	N		3	8
NCGC00166140-01	PYRITHIOXINE		-4.5		N	N	N		9	9
NCGC00166216-01	AMYL CINNAMAL			-4.5	N	N	N	0	11	
NCGC00166242-01	SWEET SPIRITS OF NITRE				N	N	N	-13	9	-10
NCGC00166266-02	CARMUSTINE			-4.5	N	N	N	11		
NCGC00166304-01	Captamina		-4.5		N	N	N		12	12
NCGC00167428-01	IBANDRONATE SODIUM			-4.5	N	N	N	5	6	
NCGC00167472-01	AMLEXANOX				N	N	N	-17	-25	-36
NCGC00167487-01	BICALUTAMIDE			-4.5	N	N	N		-7	-12
NCGC00167514-01	ETHYLESTRENOL			-4.5	N	N	N		11	8
NCGC00167524-01	AMOROLFINE HYDROCHLORIDE			-4.5	N	N	N	7	2	
NCGC00167533-01	VARDENAFIL HYDROCHLORIDE				N	N	N	-16	-18	-24
NCGC00167554-01	TRYPAN BLUE				N	N	N	-27	-19	-25
NCGC00167571-01	DEXAMETHASONE METASULFOBENZOATE SODIUM				N	N	N	13	8	8
NCGC00167725-01	TIANEPTINUM		-4.5	-4.5	N	N	N	4		
NCGC00168254-01	MIDAZOLAM HYDROCHLORIDE				N	N	N	2	0	-2
NCGC00168256-01	PRAZEPAM				N	N	N	-9	-25	-19
NCGC00168352-01	TETRAMETHRINUM			-4.5	N	N	N	15	10	
NCGC00168353-01	FENOBAMUM			-4.5	N	N	N	3	1	
NCGC00168774-01	RASAGILINE MESYLATE			-4.5	N	N	N	11	11	
NCGC00168775-01	DARIFENACIN HYDROBROMIDE				N	N	N	-22	-33	-32
NCGC00168776-01	DELAVIDRINE MESYLATE				N	N	N	-14	-9	-18
NCGC00180998-01	AMYLMETACRESOL			-4.5	N	N	N		4	5
NCGC00181011-01	GIMERACIL			-4.5	N	N	N	10	15	
NCGC00181021-01	BUFOGENIN			-4.5	N	N	N	9		
NCGC00181037-01	ISOFLURANE			-4.5	N	N	N	-11	3	
NCGC00181046-01	RASBURICASE				N	N	N	0	16	3
NCGC00181050-01	PENTASTARCH			-4.5	N	N	N	6		
NCGC00181081-01	FLUDROCORTISONE ACETATE			-4.5	N	N	N	9	-2	
NCGC00181096-01	CHLOPHEDIANOL HYDROCHLORIDE			-4.5	N	N	N		-6	-14
NCGC00181097-01	DIMEFLINE HYDROCHLORIDE				N	N	N	9	-1	
NCGC00181107-01	AROTINOLOL HYDROCHLORIDE				N	N	N	-14	-13	-30
NCGC00181108-01	CELIPROLOL HYDROCHLORIDE			-4.5	N	N	N	6		
NCGC00181126-01	ARFORMOTEROL TARTRATE				N	N	N	-28	-8	-22
NCGC00181135-01	PENTAMYCIN			-4.5	N	N	N	5	6	
NCGC00181153-01	TREOSULFAN			-4.5	N	N	N	-7		
NCGC00181343-01	IVABRADINE HYDROCHLORIDE				N	N	N	-21	-21	-34
NCGC00181350-01	VATALANIBUM				N	N	N	-12	-15	-17
NCGC00181355-01	CARPRONIUM CHLORIDE			-4.5	N	N	N		8	9
NCGC00013095-01	GERANIOL	0.00		-4.5	N	N	N		9	
NCGC00013109-01	Fenolipuna	0.00		-4.5	N	N	N		-1	
NCGC00013319-01	ouabain	0.00		-4.5	N	N	N		-6	
NCGC00014702-03	WY 14643	0.00		-4.5	N	N	N		2	
NCGC00015014-05	Acetohexamide	0.00		-4.5	N	N	N		-1	
NCGC00015121-08	Fenoxibenzamina	0.00		-4.5	N	N	N		6	
NCGC00015156-11	BACLOFEN	0.00		-4.5	N	N	N		6	
NCGC00015257-08	Clofibrate	0.00		-4.5	N	N	N		8	
NCGC00015462-07	GLIPIZIDE	0.00		-4.5	N	N	N		13	
NCGC00015479-09	Genistein	0.00		-4.5	N	N	N		-5	
NCGC00015508-08	HYDROCHLOROTHIAZIDE	0.00		-4.5	N	N	N		7	
NCGC00015673-08	MINOXIDIL	0.00		-4.5	N	N	N		4	
NCGC00015680-11	MELATONIN	0.00		-4.5	N	N	N		17	

NCGC00015715-04	NISOXETINE	0.00	-4.5	-4.5	N	N	N	0
NCGC00015859-07	PROCAINAMIDE	0.00	-4.5	-4.5	N	N	N	11
NCGC00015925-02	Sulfaphenazole	0.00	-4.5	-4.5	N	N	N	5
NCGC00016011-08	4-HYDROXYPHENETHYLAMINE	0.00	-4.5	-4.5	N	N	N	-3
NCGC00016032-06	alpha-Lipoic acid	0.00	-4.5	-4.5	N	N	N	5
NCGC00016035-02	Trazodone hydrochloride	0.00	-4.5	-4.5	N	N	N	1
NCGC00016069-09	UK 14,304	0.00	-4.5	-4.5	N	N	N	5
NCGC00016149-03	FUREGRELATE SODIUM	0.00	-4.5	-4.5	N	N	N	8
NCGC00016242-01	Metyrapone	0.00	-4.5	-4.5	N	N	N	0
NCGC00016268-02	NIACIN	0.00	-4.5	-4.5	N	N	N	2
NCGC00016272-01	Guanethidine sulfate	0.00	-4.5	-4.5	N	N	N	-1
NCGC00016288-01	Bemegride	0.00	-4.5	-4.5	N	N	N	0
NCGC00016306-01	D-cycloserine	0.00	-4.5	-4.5	N	N	N	0
NCGC00016312-01	Bendroflumethiazide	0.00	-4.5	-4.5	N	N	N	10
NCGC00016327-01	Khellin	0.00	-4.5	-4.5	N	N	N	1
NCGC00016330-01	Methylprednisolone, 6-alpha	0.00	-4.5	-4.5	N	N	N	-12
NCGC00016335-01	Dienestrol	0.00	-4.5	-4.5	N	N	N	4
NCGC00016348-02	Ethoxyquin	0.00	-4.5	-4.5	N	N	N	-12
NCGC00016350-01	Guaiifenesin	0.00	-4.5	-4.5	N	N	N	2
NCGC00016386-01	Sulfamerazine	0.00	-4.5	-4.5	N	N	N	10
NCGC00016390-01	Piperidolate hydrochloride	0.00	-4.5	-4.5	N	N	N	-11
NCGC00016401-01	Hydroflumethiazide	0.00	-4.5	-4.5	N	N	N	4
NCGC00016410-06	Thiabendazole	0.00	-4.5	-4.5	N	N	N	-4
NCGC00016411-01	Butacaine	0.00	-4.5	-4.5	N	N	N	1
NCGC00016462-01	Crotamiton	0.00	-4.5	-4.5	N	N	N	4
NCGC00016485-01	Tetrahydrozoline hydrochloride	0.00	-4.5	-4.5	N	N	N	0
NCGC00016519-01	Thiocolchicoside	0.00	-4.5	-4.5	N	N	N	7
NCGC00016558-01	Lymecycline	0.00	-4.5	-4.5	N	N	N	11
NCGC00016566-01	Dexamethasone acetate	0.00	-4.5	-4.5	N	N	N	4
NCGC00016585-01	Procyclidine hydrochloride	0.00	-4.5	-4.5	N	N	N	5
NCGC00016613-01	Antazoline hydrochloride	0.00	-4.5	-4.5	N	N	N	-6
NCGC00016614-01	Methyldopate hydrochloride	0.00	-4.5	-4.5	N	N	N	4
NCGC00016634-01	Acetopromazine maleate salt	0.00	-4.5	-4.5	N	N	N	-4
NCGC00016660-01	Felbinac	0.00	-4.5	-4.5	N	N	N	11
NCGC00016666-01	Hydrocotarnine hydrobromide	0.00	-4.5	-4.5	N	N	N	2
NCGC00016667-01	Benoxinate hydrochloride	0.00	-4.5	-4.5	N	N	N	8
NCGC00016717-01	Molindone hydrochloride	0.00	-4.5	-4.5	N	N	N	5
NCGC00016737-01	Epirizole	0.00	-4.5	-4.5	N	N	N	0
NCGC00016784-01	Articaine hydrochloride	0.00	-4.5	-4.5	N	N	N	3
NCGC00016845-01	Talampicillin hydrochloride	0.00	-4.5	-4.5	N	N	N	4
NCGC00016846-01	Suprofen	0.00	-4.5	-4.5	N	N	N	12
NCGC00016879-01	Torseamide	0.00	-4.5	-4.5	N	N	N	-2
NCGC00016893-01	Clorsulon	0.00	-4.5	-4.5	N	N	N	1
NCGC00016936-01	Aztreonam	0.00	-4.5	-4.5	N	N	N	10
NCGC00016954-05	(-)-QUINPIROLE	0.00	-4.5	-4.5	N	N	N	6
NCGC00016981-01	Troleandomycin	0.00	-4.5	-4.5	N	N	N	-1
NCGC00016983-01	Flunisolide	0.00	-4.5	-4.5	N	N	N	5
NCGC00016995-01	Betazole hydrochloride	0.00	-4.5	-4.5	N	N	N	-7
NCGC00017033-01	Novobiocin sodium salt	0.00	-4.5	-4.5	N	N	N	-1
NCGC00017047-01	Alverine citrate salt	0.00	-4.5	-4.5	N	N	N	3
NCGC00017049-01	Dipyron	0.00	-4.5	-4.5	N	N	N	12
NCGC00017082-02	DICLOFENAC SODIUM	0.00	-4.5	-4.5	N	N	N	3
NCGC00017256-04	GALANTHAMINE	0.00	-4.5	-4.5	N	N	N	3
NCGC00017332-05	(1S,9R)-beta-HYDRASTINE	0.00	-4.5	-4.5	N	N	N	-1
NCGC00018230-03	DROPROPIZINE	0.00	-4.5	-4.5	N	N	N	9
NCGC00021139-03	PHENYTOIN	0.00	-4.5	-4.5	N	N	N	-4
NCGC00021144-02	BUCLADESINE	0.00	-4.5	-4.5	N	N	N	1
NCGC00022304-05	N-acetylcysteine	0.00	-4.5	-4.5	N	N	N	3
NCGC00024257-04	Fenilefrina	0.00	-4.5	-4.5	N	N	N	10
NCGC00024493-02	D-ALANINE	0.00	-4.5	-4.5	N	N	N	11
NCGC00024596-05	CARBIDOPA	0.00	-4.5	-4.5	N	N	N	-1
NCGC00024613-01	Alrestatin	0.00	-4.5	-4.5	N	N	N	18
NCGC00042523-02	MORPHOLINYLMERCAPTOBENZOTHAZOLE	0.00	-4.5	-4.5	N	N	N	1
NCGC00065934-02	OXCARBAZEPINE	0.00	-4.5	-4.5	N	N	N	6

NCGC00090680-01	Carbaryl	0.00	-4.5	-4.5	N	N	N	-7
NCGC00090802-01	beta-Propiolactone	0.00	-4.5	-4.5	N	N	N	0
NCGC00090955-03	Dicyclohexylamine	0.00	-4.5	-4.5	N	N	N	8
NCGC00091020-03	Sodium dodecyl sulfate	0.00	-4.5	-4.5	N	N	N	5
NCGC00091038-01	Deoxycholic acid sodium salt	0.00	-4.5	-4.5	N	N	N	5
NCGC00091062-04	5-HYDROXY-L-TRYPTOPHAN	0.00	-4.5	-4.5	N	N	N	4
NCGC00091172-01	Methanol	0.00	-4.5	-4.5	N	N	N	8
NCGC00091208-04	4-Hexylresorcinol	0.00	-4.5	-4.5	N	N	N	8
NCGC00091219-02	DIETHYLTOLUAMIDE	0.00	-4.5	-4.5	N	N	N	6
NCGC00091225-02	HALAZONE	0.00	-4.5	-4.5	N	N	N	1
NCGC00091527-01	Ethylenediamine	0.00	-4.5	-4.5	N	N	N	9
NCGC00091766-01	Ethyl acetate	0.00	-4.5	-4.5	N	N	N	10
NCGC00091921-01	Ammonium nitrate	0.00	-4.5	-4.5	N	N	N	13
NCGC00093701-01	Citicoline sodium	0.00	-4.5	-4.5	N	N	N	1
NCGC00094144-03	Metyrosine	0.00	-4.5	-4.5	N	N	N	7
NCGC00094540-01	PARADICHLOROBENZENE	0.00	-4.5	-4.5	N	N	N	-8
NCGC00094557-01	AKLONIDE	0.00	-4.5	-4.5	N	N	N	-8
NCGC00094586-01	AMOXICILLIN	0.00	-4.5	-4.5	N	N	N	5
NCGC00094646-01	DIBENZOTHIOPHENE	0.00	-4.5	-4.5	N	N	N	6
NCGC00094811-01	ZOMEPIRAC SODIUM	0.00	-4.5	-4.5	N	N	N	1
NCGC00094856-01	ADENINE	0.00	-4.5	-4.5	N	N	N	8
NCGC00094902-01	MINAPRINE HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	1
NCGC00094952-01	CEFOPERAZONE SODIUM	0.00	-4.5	-4.5	N	N	N	4
NCGC00094983-01	BETAINE HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	12
NCGC00095015-01	CITIOLONE	0.00	-4.5	-4.5	N	N	N	5
NCGC00095021-01	HEPTAMINOL HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	1
NCGC00095037-01	HYDROCORTISONE BUTYRATE	0.00	-4.5	-4.5	N	N	N	1
NCGC00095041-01	URETHANE	0.00	-4.5	-4.5	N	N	N	5
NCGC00095045-01	SULFANITRAN	0.00	-4.5	-4.5	N	N	N	2
NCGC00095089-01	FLUCONAZOLE	0.00	-4.5	-4.5	N	N	N	14
NCGC00095124-01	ROSIGLITAZONE	0.00	-4.5	-4.5	N	N	N	0
NCGC00095140-01	SIBUTRAMINE HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	11
NCGC00095161-01	REBAMIPIDE	0.00	-4.5	-4.5	N	N	N	9
NCGC00095181-01	TOPIRAMATE	0.00	-4.5	-4.5	N	N	N	8
NCGC00095227-01	ALIZARIN	0.00	-4.5	-4.5	N	N	N	3
NCGC00095271-01	ALOIN	0.00	-4.5	-4.5	N	N	N	9
NCGC00095599-01	ARBUTIN	0.00	-4.5	-4.5	N	N	N	11
NCGC00095933-01	FENAMISAL	0.00	-4.5	-4.5	N	N	N	1
NCGC00096014-01	SALSALATE	0.00	-4.5	-4.5	N	N	N	4
NCGC00142580-03	PYRIDOXAL HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	0
NCGC00159343-02	Tramadolol	0.00	-4.5	-4.5	N	N	N	-1
NCGC00159350-02	TYROSINE	0.00	-4.5	-4.5	N	N	N	5
NCGC00159367-03	PARALDEHYDE	0.00	-4.5	-4.5	N	N	N	16
NCGC00159370-02	DOCOSANOL	0.00	-4.5	-4.5	N	N	N	4
NCGC00159377-02	4-T-BUTYLPHENOL FORMALDEHYDE RESIN	0.00	-4.5	-4.5	N	N	N	-2
NCGC00159380-02	Benzoyl peroxide	0.00	-4.5	-4.5	N	N	N	5
NCGC00159394-02	NICOFURANOSUM	0.00	-4.5	-4.5	N	N	N	4
NCGC00159395-03	Fenicarbazida	0.00	-4.5	-4.5	N	N	N	13
NCGC00159430-03	HEXOBARBITAL	0.00	-4.5	-4.5	N	N	N	1
NCGC00159449-03	TIFENAMILUM	0.00	-4.5	-4.5	N	N	N	1
NCGC00159463-02	Phenacaine hydrochloride	0.00	-4.5	-4.5	N	N	N	2
NCGC00159465-02	Cefazolin	0.00	-4.5	-4.5	N	N	N	3
NCGC00159484-02	CHLORALOSUM	0.00	-4.5	-4.5	N	N	N	9
NCGC00159495-03	ALBUTOINUM	0.00	-4.5	-4.5	N	N	N	6
NCGC00159507-02	Alclofenac	0.00	-4.5	-4.5	N	N	N	2
NCGC00159512-02	Cefdinir	0.00	-4.5	-4.5	N	N	N	1
NCGC00159514-02	Didanosine	0.00	-4.5	-4.5	N	N	N	3
NCGC00159521-02	Zoledronic acid	0.00	-4.5	-4.5	N	N	N	12
NCGC00159559-02	Eplerenone	0.00	-4.5	-4.5	N	N	N	5
NCGC00160239-01	THEBAINE	0.00	-4.5	-4.5	N	N	N	10
NCGC00160357-01	SORBITANI LAURAS	0.00	-4.5	-4.5	N	N	N	8
NCGC00160385-01	Dinoprost tromethamine	0.00	-4.5	-4.5	N	N	N	4
NCGC00160419-01	Clofenoxide	0.00	-4.5	-4.5	N	N	N	-1
NCGC00160437-01	Etebenecid	0.00	-4.5	-4.5	N	N	N	11

NCGC00160470-01	LEUCIGLUMERUM	0.00	-4.5	-4.5	N	N	N	10
NCGC00160482-01	Sulfalene	0.00	-4.5	-4.5	N	N	N	-2
NCGC00160494-01	Nicaraven	0.00	-4.5	-4.5	N	N	N	3
NCGC00160497-01	Benzoclidina	0.00	-4.5	-4.5	N	N	N	-5
NCGC00160588-02	ANOXOMER	0.00	-4.5	-4.5	N	N	N	2
NCGC00160594-02	IPROHEPTINE HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	6
NCGC00160614-01	GLUCURONAMIDE	0.00	-4.5	-4.5	N	N	N	6
NCGC00160667-01	Sulfaethidole	0.00	-4.5	-4.5	N	N	N	9
NCGC00163230-01	CHLORISONDAMINE	0.00	-4.5	-4.5	N	N	N	16
NCGC00163333-01	D-GLUTAMINE	0.00	-4.5	-4.5	N	N	N	10
NCGC00163473-01	OUABAIN	0.00	-4.5	-4.5	N	N	N	-3
NCGC00164015-01	1-Phenyl-3-methyl-5-pyrazolone	0.00	-4.5	-4.5	N	N	N	0
NCGC00164057-01	Bronopol	0.00	-4.5	-4.5	N	N	N	-1
NCGC00164128-01	Hexadecanoic acid, 1-methylethyl ester	0.00	-4.5	-4.5	N	N	N	7
NCGC00164321-01	2-Phenylphenol sodium salt tetrahydrate technical	0.00	-4.5	-4.5	N	N	N	3
NCGC00164327-02	NATRII ETASULFAS	0.00	-4.5	-4.5	N	N	N	3
NCGC00164339-02	EDETOLUM	0.00	-4.5	-4.5	N	N	N	0
NCGC00164357-01	L-Ascorbic acid	0.00	-4.5	-4.5	N	N	N	1
NCGC00164402-01	Beclomethasone	0.00	-4.5	-4.5	N	N	N	4
NCGC00164487-01	CHLORPHENOCTII AMSONAS	0.00	-4.5	-4.5	N	N	N	-2
NCGC00164494-01	Nithiamide	0.00	-4.5	-4.5	N	N	N	1
NCGC00164509-01	OXFENICINUM	0.00	-4.5	-4.5	N	N	N	-1
NCGC00164515-01	SULFONMETHANE	0.00	-4.5	-4.5	N	N	N	11
NCGC00164520-01	THREONINE	0.00	-4.5	-4.5	N	N	N	1
NCGC00164531-01	CYSTINE	0.00	-4.5	-4.5	N	N	N	1
NCGC00164584-01	Cetraxate hydrochloride	0.00	-4.5	-4.5	N	N	N	0
NCGC00164585-01	Halometasona	0.00	-4.5	-4.5	N	N	N	-1
NCGC00164629-01	Alibendol	0.00	-4.5	-4.5	N	N	N	7
NCGC00164630-01	PENCICLOVIR SODIUM	0.00	-4.5	-4.5	N	N	N	12
NCGC00164634-01	BALSALAZIDE DISODIUM	0.00	-4.5	-4.5	N	N	N	1
NCGC00164737-01	pirbuterol hydrochloride	0.00	-4.5	-4.5	N	N	N	11
NCGC00165767-02	CYCLOFENIL	0.00	-4.5	-4.5	N	N	N	0
NCGC00166095-01	BISMUTH OXIDE	0.00	-4.5	-4.5	N	N	N	11
NCGC00166100-01	CAMPHENE	0.00	-4.5	-4.5	N	N	N	4
NCGC00166103-01	Xylose	0.00	-4.5	-4.5	N	N	N	-2
NCGC00166111-01	Epiestriol	0.00	-4.5	-4.5	N	N	N	5
NCGC00166146-01	Quinestrol	0.00	-4.5	-4.5	N	N	N	0
NCGC00166149-01	NITENPYRAM	0.00	-4.5	-4.5	N	N	N	2
NCGC00166210-01	PAROMOMYCIN SULFATE	0.00	-4.5	-4.5	N	N	N	6
NCGC00166219-01	Bipenamol hydrochloride	0.00	-4.5	-4.5	N	N	N	3
NCGC00166238-01	Benznidazol	0.00	-4.5	-4.5	N	N	N	12
NCGC00166260-01	Bumetrizole	0.00	-4.5	-4.5	N	N	N	9
NCGC00166261-01	5-Hydroxy-2-adamantanone	0.00	-4.5	-4.5	N	N	N	-1
NCGC00166280-01	Bismuth Subgallate	0.00	-4.5	-4.5	N	N	N	2
NCGC00166283-01	PROTOPORPHYRIN DISODIUM	0.00	-4.5	-4.5	N	N	N	-4
NCGC00166284-01	Dikegulac	0.00	-4.5	-4.5	N	N	N	13
NCGC00167417-01	BORNEOL	0.00	-4.5	-4.5	N	N	N	0
NCGC00167425-01	DEFERIPRONE	0.00	-4.5	-4.5	N	N	N	4
NCGC00167458-01	CEFONICID SODIUM	0.00	-4.5	-4.5	N	N	N	6
NCGC00167460-01	CEFTIZOXIME SODIUM	0.00	-4.5	-4.5	N	N	N	12
NCGC00167461-01	BENDAZAC	0.00	-4.5	-4.5	N	N	N	1
NCGC00167529-01	ITOPRIDE HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	5
NCGC00167553-01	NORFENEFRINE HYDROCHLORIDE	0.00	-4.5	-4.5	N	N	N	12
NCGC00167555-01	SODIUM BUTYRATE	0.00	-4.5	-4.5	N	N	N	0
NCGC00167557-01	METHYLMETHIONINE SULFONIUM CHLORIDE	0.00	-4.5	-4.5	N	N	N	13
NCGC00167800-01	CARBOPLATIN	0.00	-4.5	-4.5	N	N	N	3
NCGC00168247-01	AMPHETAMINE ADIPATE	0.00	-4.5	-4.5	N	N	N	0
NCGC00168248-01	BENZOYLECGONINE	0.00	-4.5	-4.5	N	N	N	8
NCGC00168771-01	FOSAMPRENAVIR CALCIUM	0.00	-4.5	-4.5	N	N	N	9
NCGC00180997-01	ETHYLPHENACEMIDE	0.00	-4.5	-4.5	N	N	N	-4
NCGC00181015-01	BROPYRIMINE	0.00	-4.5	-4.5	N	N	N	10
NCGC00181053-01	MALIC ACID	0.00	-4.5	-4.5	N	N	N	10
NCGC00181118-01	SULFABROMOMETHAZINE SODIUM	0.00	-4.5	-4.5	N	N	N	6
NCGC00181155-01	PIPERAZINE-CARBON DISULFIDE COMPLEX	0.00	-4.5	-4.5	N	N	N	5

NCGC00181341-01	EMEDASTINE DIFUMARATE	0.00	-4.5	-4.5	N	N	N	9		
NCGC00095007-01	CEFTRIAXONE SODIUM TRIHYDRATE				N	N	N	-12	-21	-15
NCGC00095120-01	CARVEDILOL TARTRATE				N	N	N	-27	1	-24
NCGC00167488-01	SORAFENIB TOSYLATE				N	N	N	-6	-10	-30

Notes for Dataset 1

DCP- differential chemical phenotype is a compound showing ≥ 0.7 Log IC₅₀ (IC₅₀, 5-fold difference) between the parental 3D7 line and a *pfabcg2* knockout line (B2 or C11). IC₅₀ is half maximal inhibitory concentration in molar and log transformed. Drugs that are more active in a *pfabcg2* knockout line are indicated as sensitive (Sens) and those less active are indicated as resistant (Resist). **Pink shading**- DCP compounds in both B2 and C11 lines that are not known antifolates. **Blue shading**- DCP antifolates in both B2 and C11 lines. **Delta IC₅₀**- difference in Log IC₅₀ between 3D7 and the indicated *pfabcg2* knockout line. **IC₅₀**- Log IC₅₀ values of compounds showing dose-response curves determined as active (A) or inconclusive (I) with a curve-fit *P*-value ≤ 0.05 are shown. Values are not shown for curve-fit *P*-values > 0.05 or for inactive (N) compounds having curve-fits below threshold activity (~30%). Inactive compounds with no curve-fit were assigned a IC₅₀ of -4.5, the highest tested concentration. Compounds with IC₅₀ < -9.3 (the lowest tested concentration) or > -4.5 (the highest tested concentration) were assigned -9.3 or -4.5, respectively. **Activity**- Activity classification based on curve fit quality metrics, Active (A)- high quality dose-response curve (Class 1.1, 1.2 and 2.1), Inconclusive (I)- lower quality curve (Class 2.2 and 3) and Inactive (N) (Class 4). See reference 44. **Efficacy**- Maximum percent activity (inhibition) of a compound based on the curve fit of the dose response data. Inactive (N) compounds where no curve fit was generated have no efficacy values and are therefore left blank. Compounds are ranked first by DCP status (columns C and D, then 3D7 activity (column J), then Delta Log IC50 B2 (column E).