

## Supplementary Materials OF

### Development of human biotransformation QSARs and application for PBT assessment refinement

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Table S1: CAS, Name and SMILES for the human biotransformation models datasets.

ID	CAS	Name	Canonical SMILES
		2,2',4,4',5,5'-	
1	000006-01-7	Hexabromodiphenyl	BrC1cc(Br)(cc1Oc1cc(Br)c(cc1Br)Br)Br
2	000050-00-0	Formaldehyde	C=O
3	000050-06-6	Phenobarbital	CCC1(C(=O)NC(=O)NC1=O)c1ccccc1
4	000050-12-4	Mephentoin	CCC1(NC(=O)N(C1=O)C)c1ccccc1
5	000050-14-6	Ergocalciferol	OC1CCC(=C)C(=CC=C2CCC3(C2CCC3C(=C)C(C)C)C)C)C1
6	000050-18-0	Cyclophosphamide	ClCCN(P1(=O)NCCO1)CC1
7	000050-23-7	Hydrocortisone	OC(=O)C1(O)CC2C1(C)C(C)O1C1C2CCC2=CC(=O)CC1C2
8	000050-24-8	Prednisolone	OC(=O)C1(O)CC2C1(C)C(C)O1C1C2CCC2=CC(=O)CC1C2
9	000050-28-2	Estradiol	OC1ccc2c(c1)CC1C2CCC2(C1CCC2O)C
10	000050-29-3	p,p'-DDT	ClC(C1ccc(cc1)Cl)c1ccc(cc1)Cl(C)Cl
11	000050-35-1	Thalidomide	O=C1CCC(C(=O)N)N1C(=O)c2c(C1=O)cccc2
12	000050-36-2	Cocaine	COC(=O)C1C(CCN(C1CC2)C)OC(=O)c1ccccc1
13	000050-37-3	Lysergide	CCN(C(=O)C1CN(C)C2(C=C1)c1ccc3c1c(2)c[nH]3)CC
14	000050-47-5	Desipramine	NCNCCN1c2ccccc2CCc2c1cccc2
15	000050-48-6	Amitriptyline	CN(CCC=C1c2ccccc2CCc2c1cccc2)C
16	000050-49-7	Imipramine	CN(CCCN1c2ccccc2CCc2c1cccc2)C
17	000050-52-2	Thioridazine	CSc1ccc2c(c1)N(CCC1CCC1N)C1c(S2)cccc1
18	000050-53-3	Chlorpromazine	CN(CCCN1c2ccccc2Sc2c1cc(C)cc2)C
19	000050-60-2	Phentolamine	Cc1ccc(cc1)N(c1ccc(c1)O)CC1=NCCN1
20	000050-78-2	Aspirin	CC(=O)Oc1ccccc1C(=O)O
21	000051-06-9	Procainamide	CCN(CCN(C(=O)c1ccc(cc1)N)CC
22	000051-21-8	Fluorouracil	Fc1c[nH]c(=O)[nH]c1=O
23	000051-34-3	Scopolamine	OC(C1CCCC1)(=O)OC1CC2N(C(C1)C1C2O1)C
24	000051-48-9	Levothyroxine	OC(=O)C(Cc1cc(I)c(c1))Oc1cc(I)c(c1))O)N
25	000051-52-5	Propylthiouracil	CCc1cc(=O)[nH]c(=S)[nH]1
26	000051-55-8	Atropine	OC(C1CCCC1)C(=O)OC1CC2CCC(C1)N2C
27	000051-75-2	Mechlorethamine	ClCCN(CCC)C
28	000052-01-7	Spirinolactone	CC(=O)SC1CC2=CC(=O)CCC2(C2C1C1CCC3(C1(C2)C)CCC(=O)O3)C
29	000052-24-4	Thiotepa	S=P(N1CC1)(N1CC1)N1CC1
30	000052-53-9	Verapamil	COc1ccc(cc1O)CCN(CCC(C1ccc(c1)OC)OC)(C(C)C#N)C
31	000052-67-5	Penicillamine	NC(C(S)(C)C)C(=O)O
32	000052-86-8	Haloperidol	Fc1ccc(cc1)C(=O)CCN1CCC(C1)O1c1ccc(cc1)Cl
33	000053-03-2	Prednisone	OC(=O)C1(O)CC2C1(C)C(C=O)C1C2CCC2=CC(=O)CC1C2
34	000053-16-7	Estrone	OC1ccc2c(c1)CC1C2CCC2(C1CCC2=O)C
35	000053-19-0	Mitotane	ClC(C1CCCC1)C1ccc(cc1)Cl
36	000053-39-4	Oxandrolone	O=C1OC2(C1)CCC1C2CC2(C1CCC2(C)O)C)C
37	000053-86-1	Indomethacin	COc1ccc2c(c1)C(C(=O)O)(n2C(=O)c1ccc(cc1)Cl)C
38	000054-05-7	Chloroquine	CCN(CCCC(Nc1ccnc2c1ccc(c2)Cl)C)CC
39	000054-11-5	Nicotine	CN1CCC1c1ccccc1
40	000054-31-9	Furosemide	OC(=O)c1cc(c(cc1NCc1ccco1)Cl)S(=O)(=O)N
41	000054-36-4	Metyrapone	O=C(C1cccnc1)C)C1cccnc1
42	000054-71-7	Pilocarpine	CCC1(C=O)OCC1Cc1cncn1C
43	000054-85-3	Isoniazid	NNC(=O)c1ccccc1
44	000055-63-0	Nitroglycerin	O=N(O)OC(CON(=O)O)CON(=O)O
45	000055-98-1	Busulfan	CS(=O)(=O)OCC(COS(=O))=O)C
46	000056-29-1	Hexobarbital	O=C1NC(=O)C(C(=O)N1C)C1=CCCCC1
47	000056-54-2	Quinidine	C=CC1CN2CCC1CC2C(c1ccnc2c1cc(OC)cc2)O
48	000056-75-7	Chloramphenicol	OC(C1ccc(cc1)N(=O)O)NC(=O)C)Cl
49	000057-27-2	Morphine	OC1C=CC2C34C1Oc1c4c(CCN(C3)C)ccc1O
50	000057-41-0	Phenytoin	O=C1NC(=O)NC1(c1ccccc1)c1ccccc1
51	000057-42-1	Meperidine	CCOC(=O)C1(CCN(C1)C)c1ccccc1
52	000057-53-4	Meproamate	CCCC(COC(=O)N)(COC(=O)N)C
53	000057-63-6	Ethinyl	HC#CC1(O)CCC2C1(C)CCC1C2CCc2c1cccc(c2)O
54	000057-66-9	Progbenecid	CCCN(S(=O))=O)c1ccc(cc1)C(=O)O)CCC
55	000057-74-9	Chlordane	ClC1CC2(C1C)C1(C2(C)C)C(=C1C)Cl(C)Cl)Cl
56	000057-83-0	Pregesterone	O=C1CCC2(C(=C1)CCC1C2CCC2(C1CCC2C(=O)C)C
57	000057-92-1	Streptomycin	OC1OC(C2C(OC3C(O)C(O)C(C3NC(=N)N)OC(=N)N)OC(C2(O)C=O)C)C(C1O)O)NC
58	000057-96-5	Sulfipyrazone	O=C1N(C2CCCC2)N(C(=O)C1CCS(=O)c1ccccc1)c1ccccc1
59	000058-00-4	R-APomorphine	CN1CCc2c3C1c1ccc(c1c1c3ccc2)O)O
60	000058-08-2	Caffeine	Cn1cnc2c1c(=O)n(C)C(=O)n2C
61	000058-14-0	Pyrimethamine	CCc1nc(N)nc(c1c1ccc(cc1)Cl)N
62	000058-22-0	Testosterone	O=C1CC2(C(=C1)CCC1C2CCC2(C1CCC2O)C)C

ID	CAS	Name	Canonical SMILES
63	000058-25-3	Chlordiazepoxide	CN=C1CN(O)C(=c2c(=N1)ccc(c2)Cl)c1ccccc1
64	000058-32-2	Dipyridamole	OCCN(c1nc(N2CCCC2)c2c(n1)(nc(n2)N(CCO)CCO)N1CCCC1)CCO
65	000058-38-8	Prochlorperazine	CN1CCN(C1)CCCN1c2ccccc2Sc2c1cc(C)cc2
66	000058-39-9	Perphenazine	OCCN1CCN(C1)CCCN1c2ccccc2Sc2c1cc(C)cc2
67	000058-40-2	Promazine	CN(CCCN1c2ccccc2Sc2c1cccc2)C
68	000058-54-8	Ethacrynic	CCC(=C)C(=O)c1ccc(c(c1)Cl)OCC(=O)O
69	000058-55-9	Theophylline	Cn1c(=O)n(C)c2c(c1=O)[nH]cn2
70	000058-73-1	Diphenhydramine	CN(CCO(c1ccccc1)c1ccccc1)C
71	000058-74-2	Papaverine	OC1ccc(cc1OC)C1nccc2c1cc(O)C(c2)OC
72	000058-89-9	HCHs	ClC1(C)C(Cl)C(C1)Cl)Cl
73	000058-93-5	Hydrochlorothiazide	Clc1cc2NCNS(=O)(=O)c2cc1S(=O)(=O)N
74	000059-42-7	Phenylephrine	CNC(C1ccc(c1)O)O
75	000059-46-1	Procaine	CCN(CCO(C(=O)c1ccc(cc1)N)CC
76	000059-66-5	Acetazolamide	CC(=O)Nc1nnc(s1)S(=O)(=O)N
77	000059-87-0	Nitrofurazone	NC(=O)NN=Cc1ccc(o1)N(=O)=O
78	000059-92-7	Levodopa	OC(=O)C(Cc1ccc(c(c1)O)N
79	000059-96-1	Phenoxybenzamine	ClCCN(C(CO1ccccc1)C)C1ccccc1
80	000060-32-2	Aminocaproic	NCCCCC(=O)O
81	000060-56-0	Methimazole	Cn1c[nH]c1=S
82	000060-57-1	Dieldrin	ClC1=C(C)C2(C1(C)Cl)C1C2CC1C1C2O1)(Cl)Cl)Cl
83	000060-80-0	Antipyrine	O=C1ccc(n1c1ccccc1)C)C
84	000060-87-7	Promethazine	CN(CCN1c2ccccc2Sc2c1cccc2)C)C
85	000060-99-1	Methotrimeprazine	COc1ccc2c(c1)N(C(CN(C)C)C)Clc1c(S2)cccc1
86	000061-32-5	Meticillin	COc1ccc(c1C(=O)N)C1C(=O)N2C1SC(C2C(=O)O)(C)C)OC
87	000061-33-6	Penicillin	O=C(Cc1ccccc1)N(C1(=O)N2C1SC(C2C(=O)O)(C)C
88	000061-68-7	Mefenamic	OC(=O)c1ccccc1Nc1ccc(c1)C)C
89	000062-44-2	Phenacetin	CCOC1ccc(cc1)NC(=O)C
90	000063-12-7	Benzquinamide	CCN(C(=O)C1CN2CCc3c(C2CC1OC(=O)C)cc(c(c3)OC)OC)CC
91	000063-98-9	Phenacemide	O=C(C1ccccc1)NC(=O)N
92	000064-77-7	Tolbutamide	CCCCN(C(=O)NS(=O)(=O)C1ccc(cc1)C
93	000064-86-8	Colchicine	COc1c(OC)cc2c(c1OC)c1ccc(cc(=O)cc1C(C2)NC(=O)C)OC
94	000066-79-5	Oxacillin	OC(=O)C1N2C(=O)C(C2SC1(C)C)NC(=O)c1c(C)onc1c1ccccc1
95	000067-20-9	Nitrofurantoin	O=C1NC(=O)N(C1)N=Cc1ccc(o1)N(=O)=O
96	000067-45-8	Furazolidone	O=C1OCCN1N=Cc1ccc(o1)N(=O)=O
97	000067-66-3	chloroform	ClC(Cl)Cl
98	000067-73-2	Fluocinolone	OC(C(=O)C12OC(OC1CC1C2)C)C(C)O)C2(C1CC(C1=CC(=O)C)C)C)C
99	000067-97-0	Cholecalciferol	CC(CCCC(C1CCC2C1(C)CCCC2=CC=C1CC(O)CCC1=C)C)C
100	000068-22-4	Norethindrone	HC#CC1(O)CCC2C1(C)CCC1C2CCC2=CC(=O)O)CCC12
101	000068-35-9	Sulfadiazine	Nc1ccc(cc1)S(=O)(=O)Nc1ncccc1
102	000068-88-2	Hydroxyzine	OCCOCCN1CCN(C1)C(c1ccc(cc1)Cl)c1ccccc1
103	000069-53-4	Ampicillin	NC(c1ccccc1)C(=O)NC1C(=O)N2C1SC(C2C(=O)O)(C)C
104	000069-65-8	Mannitol	OC(C(C(C(C)O)O)O)O
105	000070-51-9	Deferoxamine	NCCCCCN(C(=O)CCC(=O)NCCCCCN(C(=O)O)O)O
106	000071-43-2	Benzene	c1ccccc1
107	000071-63-6	Digitoxin	O=C1OCC(=C1)C1CCC2(C1)C)CCC1C2CC2C1(C)CCC(C2)OC1CC(O)C(C1O1)OC1CC(O)C(C1O1)C)O
108	000072-55-9	p,p'-DDE	Cl(C(=C1ccc(cc1)Cl)c1ccc(cc1)Cl)Cl
109	000072-69-5	Nortriptyline	NCNCC=C1c2ccccc2CCc2c1cccc2
110	000073-31-4	Melatonin	COc1ccc2c(c1)c(CCN(C=O)C)[nH]2
111	000073-48-3	Bendroflumethiazide	O=S1(=O)NC(Cc2ccccc2)Nc2c1cc(c2(C)F)F)S(=O)(=O)N
112	000074-55-5	Ethambutol	CCC(NCCN(C)CO)CCO
113	000075-01-4	VINYL	C=C
114	000075-69-4	TRICHLOROFLUOROMETHANE	FC(Cl)Cl)Cl
115	000075-71-8	Dichlorodifluoromethane	FC(Cl)Cl)F
116	000076-25-5	Triamcinolone	OC(C(=O)C12OC(OC1CC1C2)C)C(C)O)C2(C1CCC1=CC(=O)C=CC21C)F)C)C
117	000076-41-5	Oxymorphone	O=C1CCC2(C34C1Oe1c4c(CCN(C3)C)ccc1O)O
118	000076-42-6	Oxycodone	COc1ccc2c3c1OC1C43CCN(C(C2)C4)O)CC1=O)C
119	000076-43-7	Fluoxymesterone	O=C1CC2(C(=C1)CCC1C2(F)C)OC2(C1CCC2(C)O)C)C
120	000076-57-3	Codeine	COc1ccc2c3c1OC1C43CCN(C(C2)C4C=CC1O)C
121	000076-74-4	Pentobarbital	CCCC(C1(C)C(=O)NC(=O)NC1=O)C
122	000076-75-5	Thiopental	CCCC(C1(C)C(=O)NC(=S)NC1=O)C
123	000076-99-3	Methadone	CC(C(=O)C1ccccc1)(c1ccccc1)CC(N(C)C)C
124	000077-07-6	Levorphanol	OC1ccc2c(c1)C13CCC3C(C2)N(C1)C
125	000077-10-1	Phencyclidine	C1CC(C(C1)N1CCCC1)c1ccccc1
126	000077-21-4	Glutethimide	CCC1(CCC(=O)NC1=O)c1ccccc1



ID	CAS	Name	Canonical SMILES
255	000396-01-0	Triamterene	<chem>Nc1nc(N)c2c(n1)nc(c2)c1cccc1N</chem>
256	000437-38-7	Fentanyl	<chem>CCC(=O)N(c1cccc1)C1CCN(CC1)CC1CCCC1</chem>
257	000439-14-5	Diazepam	<chem>C1c1ccc2c(c1)C(=NCC(=O)N2)c1cccc1</chem>
258	000443-48-1	Metronidazole	<chem>OCCn1c(C)ncn1N(=O)=O</chem>
259	000446-86-6	Azathioprine	<chem>Cn1cnc(c1Sc1ncnc2c1[nH]n2)N(=O)=O</chem>
260	000452-35-7	Ethoxzolamide	<chem>CCOc1ccc2c(c1)sc(n2)S(=O)(=O)N</chem>
261	000461-78-9	Chlorphentermine	<chem>CC(Ccc1ccc(cc1)Cl)N(C)</chem>
262	000469-21-6	Doxylamine	<chem>CN(CCOc1c1cccc1)(c1cccc1)C</chem>
263	000469-62-5	Propoxyphene	<chem>CCC(=O)OC(c1cccc1)(C(CN(C)C)C)C1cccc1</chem>
264	000469-79-4	Ketobemidone	<chem>CCC(=O)C1(CCN(C)C)C1cccc(c1)O</chem>
265	000477-47-4	Podofilox	<chem>COc1cc(ccc1OC)C1C2C(=O)OCC2C(c2c1cc1OCoc1c2)O</chem>
266	000479-18-5	Dyphylline	<chem>OCC(Cn1cnc2c1c(=O)n(C)c(=O)n2)CO</chem>
267	000486-12-4	Triprolidine	<chem>Cc1ccc(cc1)C(=CCN1CCCC1)c1ccccn1</chem>
268	000486-16-8	Carbinoxamine	<chem>CN(CCOC(c1ccccn1)c1ccc(cc1)Cl)C</chem>
269	000486-56-6	Cotinine	<chem>O=C1CCC(N1C)c1cccnc1</chem>
270	000492-39-7	Cathine	<chem>OC1c1cccc1C(N)C</chem>
271	000514-65-8	Biperiden	<chem>OC(C1CC2C1C=C2)(c1cccc1)CCN1CCCC1</chem>
272	000520-85-4	Medroxyprogesterone	<chem>O=C1CC2(C(=C1)C(C)CC1C2CC2(C1CC2)O)(C(=O)C)C</chem>
273	000525-66-6	Propranolol	<chem>OC(COc1ccc2c1ccc2)CNC(C)C</chem>
274	000529-38-4	Cocaethylene	<chem>CCOC(=O)C1C(CCN(C1CC2)C)OC(=O)c1cccc1</chem>
275	000532-03-6	Methocarbamol	<chem>COc1cccc1OCC(COC(=O)N)O</chem>
276	000532-77-4	Hexylcaine	<chem>CC(OC(=O)c1cccc1)CNC1CCCC1</chem>
277	000533-45-9	Chlormethiazole	<chem>Cc1ncsc1CCCl</chem>
278	000536-33-4	Ethionamide	<chem>CCc1nccc(c1)C(=S)N</chem>
279	000537-46-2	Methamphetamine	<chem>CNC(Cc1cccc1)C</chem>
280	000546-88-3	Acetohydroxamic	<chem>CC(=O)NO</chem>
281	000548-04-9	Hypericin	<chem>Oc1cc(C)c2c3c1c(=O)c1c(O)c(cc4c1c3c1c3c2c(C)cc(c3C(=O)c2c1c4c(O)cc2O)O)O</chem>
282	000548-73-2	Droperidol	<chem>Fc1ccc(cc1)C(=O)CCN1CCC(=CC1)n1c(=O)[nH]c2c1cccc2</chem>
283	000552-94-3	Salsalate	<chem>Oc1cccc1C(=O)Oc1cccc1C(=O)O</chem>
284	000554-57-4	Methazolamide	<chem>CC(=O)N=c1sc(nn1C)S(=O)(=O)N</chem>
285	000555-30-6	Methyldopa	<chem>OC(=O)C(Cc1ccc(cc1)O)N(C)O</chem>
286	000561-27-3	Heroin	<chem>CC(=O)OC1C=C2C34C1Oc1c4c(CCN(C)C)ccc1OC(=O)C</chem>
287	000569-65-3	Meclizine	<chem>C1c1ccc(cc1)C(c1cccc1)N1CCN(CC1)C1cccc(c1)C</chem>
288	000586-06-1	Orciprenaline	<chem>OC(c1cc(O)cc(c1)O)CNC(C)C</chem>
289	000586-60-7	Dyclonine	<chem>CCCCOc1ccc(cc1)C(=O)CCN1CCCC1</chem>
290	000599-79-1	Sulfasalazine	<chem>OC(=O)C1=CC(=NNc2ccc(cc2)S(=O)(=O)Nc2cccnc2)C=CC1=O</chem>
291	000604-75-1	Oxazepam	<chem>O=C1Nc2ccc(cc2C(=NC1O)c1cccc1)Cl</chem>
292	000616-91-1	Acetylcysteine	<chem>SCC(C(=O)O)NC(=O)C</chem>
293	000634-03-7	Phendimetrazine	<chem>CC1N(C)CCOC1c1cccc1</chem>
294	000637-07-0	Clofibrate	<chem>CCOC(=O)C(Oc1ccc(cc1)Cl)(C)C</chem>
295	000644-62-2	Meclofenamic	<chem>OC(=O)c1cccc1Nc1c(Cl)ccc(c1Cl)C</chem>
296	000645-05-6	Altretamine	<chem>CN(C1nc(ncn1)N(C)C)N(C)C</chem>
297	000645-43-2	Guanethidine	<chem>NC(=NCCN1CCCCC1)N</chem>
298	000657-24-9	Metformin	<chem>CN(C(=N)N=C(N)N)C</chem>
299	000671-16-9	Procarbazine	<chem>CNNc1ccc(cc1)C(=O)NC(C)C</chem>
300	000672-87-7	Metyrosine	<chem>Oc1ccc(cc1)CC(C(=O)O)N(C)</chem>
301	000709-55-7	Etilefrine	<chem>CCNCC(c1ccc(c1)O)O</chem>
302	000721-50-6	Prilocaine	<chem>CCNC(C(=O)Nc1cccc1)C</chem>
303	000723-46-6	Sulfamethoxazole	<chem>Nc1ccc(cc1)S(=O)(=O)Nc1nc(c1)C</chem>
304	000738-70-5	Trimethoprim	<chem>COc1cc(Cc2cnc(nc2N)N)cc1OC)OC</chem>
305	000739-71-9	Trimipramine	<chem>CN(CC(CN1c2cccc2CC2c1cccc2)C)C</chem>
306	000745-65-3	Alprostadil	<chem>CCCCC(C=CC1C(O)CC(=O)C1CCCCC(=O)O)O</chem>
307	000768-94-5	Amantadine	<chem>NC12CC3C(C2)CC(C1)C3</chem>
308	000797-63-7	Levonorgestrel	<chem>C#CC1(O)CCC2C1(C)CC1C2CCC2=CC(=O)CCCC12</chem>
309	000846-48-0	Boldenone	<chem>O=C1C=C2(C(=C1)CC1C2CCC2(C1CCC2O)C)C</chem>
310	000846-49-1	Lorazepam	<chem>C1c1ccc2c(c1)C(=NCC(=O)N2)O)c1cccc1Cl</chem>
311	000846-50-4	Temazepam	<chem>C1c1ccc2c(c1)C(=NCC(=O)N2)O)c1cccc1</chem>
312	000848-75-9	Lormetazepam	<chem>C1c1ccc2c(c1)C(=NCC(=O)N2)O)c1cccc1Cl</chem>
313	000911-45-5	Clomifene	<chem>CCN(CCOc1ccc(cc1)C(=C(c1cccc1)Cl)c1cccc1)CC</chem>
314	000915-30-0	Diphenoxylate	<chem>CCOC(=O)C1(CCN(C)C)CCC(c1cccc1)(c1cccc1)C#N)c1cccc1</chem>
315	000968-81-0	Acetohexamide	<chem>O=C(N(S(=O)(=O)c1ccc(cc1)C(=O)N)C1CCCC1</chem>
316	000972-02-1	Diphenidol	<chem>OC(c1cccc1)(c1cccc1)CCN1CCCC1</chem>
317	001088-11-5	Desmethyldiazepam	<chem>O=C1CN=C(c2c(N1)ccc(c2)Cl)c1cccc1</chem>
318	001094-08-2	Ethopropazine	<chem>CCN(C(CN1c2cccc2Sc2c1cccc2)C)CC</chem>

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319	001134-47-0	Baclofen	<chem>NC(C1ccc(c1)Cl)CC(=O)O</chem>
320	001156-19-0	Tolazamide	<chem>O=C(N(S(=O)(=O)c1ccc(cc1)C)NN1CCCCC1</chem>
321	001163-19-5	Decabromodiphenyl	<chem>BrC1(Oc2c(Br)c(Br)c(c2Br)Br)c(Br)c(c1Br)Br</chem>
322	001197-18-8	Tranexamic	<chem>NCC1CCC(C1)C(=O)O</chem>
323	001435-55-8	Dihydroquinidine	<chem>CCC1CN2CCC1CC2C(c1ccnc2c1cc(OC)cc2)O</chem>
324	001477-40-3	Levomethadyl	<chem>CCC(C(c1cccc1)(c1cccc1)CC(N(C)C)OC(=O)C</chem>
325	001622-61-3	Clonazepam	<chem>O=C1CN=C(c2c(N1)ccc(c2)N(=O)=O)c1cccc1Cl</chem>
326	001622-62-4	Flunitrazepam	<chem>CN1C(=O)CN=C(c2c1ccc(c2)N(=O)=O)c1cccc1F</chem>
327	001665-48-1	Metaxalone	<chem>O=C1NCC(O1)COc1cc(C)cc(c1)C</chem>
328	001668-19-5	Doxepin	<chem>CN(CCC=C1c2cccc2OC2c1cccc2)C</chem>
329	001695-77-8	Spectinomycin	<chem>CNC1C(O)C2OC3OC(C)CC(=O)C3OC2C(C1O)NC)O</chem>
330	001744-22-5	Riluzole	<chem>Nc1nc2c(s1)cc(cc2)OC(F)F</chem>
331	001746-01-6	2,3,7,8-tetrachlorodibenzo-p-dioxin	<chem>Clc1cc2O3cc(Cl)c(cc3O2c2c1)Cl</chem>
332	001763-23-1	Perfluorooctanesulfonic	<chem>FC(C(C(C(C(S(=O)(=O)O)(F)F)(F)F)(F)F)(F)F)(F)F)F</chem>
333	001808-12-4	Bromodiphenhydramine	<chem>CN(CCOc1ccc(cc1)Br)c1cccc1C</chem>
334	001812-30-2	Bromazepam	<chem>O=C1CN=C(c2c(N1)ccc(c2)Br)c1cccc1</chem>
335	001912-24-9	Atrazine	<chem>CCNc1nc(NC(C)C)n(c1)Cl</chem>
336	001949-45-7	Metrizoate	<chem>CC(=O)CNC1c(I)c(NC(=O)C)c(c1)C(=O)O</chem>
337	001951-25-3	Amiodarone	<chem>CCCC1oc2c(c1C(=O)c1cc(I)c(c1)O)CCN(C)CC)cccc2</chem>
338	001972-08-3	Marinol	<chem>CCCCc1cc(O)c2c(c1)O(C1C2C=C(C)CC1)C</chem>
339	002016-88-8	Amiloride	<chem>NC(=N(C(=O)c1nc(Cl)cc(n1)N)N</chem>
340	002030-63-9	Clofazimine	<chem>Clc1ccc(cc1)Nc1cc2nc3cccc3n(c2c1=NC)C1ccc(cc1)Cl</chem>
341	002050-67-1	3,3'-dichlorobiphenyl	<chem>Clc1ccc(cc1)c1cccc(c1)Cl</chem>
342	002050-68-2	4,4'-dichlorobiphenyl	<chem>Clc1ccc(cc1)c1ccc(cc1)Cl</chem>
343	002051-24-3	Decachlorobiphenyl	<chem>Clc1c(c2c(Cl)c(Cl)c(c2Cl)Cl)c(Cl)c(Cl)c(c1Cl)Cl</chem>
344	002051-60-7	2-chlorobiphenyl	<chem>Clc1cccc1c1cccc1</chem>
345	002051-61-8	3-chlorobiphenyl	<chem>Clc1cccc(c1)c1cccc1</chem>
346	002051-62-9	4-chlorobiphenyl	<chem>Clc1ccc(cc1)c1cccc1</chem>
347	002062-78-4	Pimozide	<chem>Fc1ccc(cc1)C1c1ccc(cc1F)CCCN1CCC(C)N1c(=O)[nH]c2c1cccc2</chem>
348	002062-84-2	Benperidol	<chem>Fc1ccc(cc1)C(=O)CCN1CCC(C)N1c(=O)[nH]c2c1cccc2</chem>
349	002078-54-8	Propofol	<chem>CC(c1ccc(c1O)C(C)C)O</chem>
350	002098-66-0	Cyproterone	<chem>O=C1C=C2C(=CC3C(C2)C2(C)C)CC1(C3CCC1(O)C(=O)C)Cl</chem>
351	002176-90-6	Iothalamic	<chem>CNC(=O)c1cc(I)cc(NC(=O)C)c(c1)Cl(O)O</chem>
352	002321-07-5	Fluorescein	<chem>Oc1ccc2c(c1)Oc1c(C32OC(=O)c2c3ccc2)ccc(c1)O</chem>
353	002323-36-6	Selegiline	<chem>CC(N(C#C)O)Cc1cccc1</chem>
354	002353-33-5	Decitabine	<chem>OCC1OC(C)O1n1cnc(nc1=O)N</chem>
355	002437-79-8	2,4,2',4'-tetrachlorobiphenyl	<chem>Clc1ccc(cc1)Cl)c1ccc(cc1)Cl</chem>
356	002709-56-0	Flupenthixol	<chem>OCCN1CN(C)CCC=C1c2cccc2Sc2c1cc(cc2)C(F)F</chem>
357	002894-67-9	Delorazepam	<chem>O=C1CN=C(c2c(N1)ccc(c2)Cl)c1cccc1Cl</chem>
358	002955-38-6	Prazepam	<chem>Clc1ccc2c(c1)C(=NCC(=O)N2)C1CC1)c1cccc1</chem>
359	002974-90-5	3,4'-Dichlorobiphenyl	<chem>Clc1ccc(cc1)c1ccc(c1)Cl</chem>
360	002998-57-4	Estramustine	<chem>C1CCN(C(=O)Oc1ccc2c(c1)CCC1C2CCC2(C1CC2OP(=O)(O)O)O)CC1</chem>
361	003056-17-5	Stavudine	<chem>Cc1cn(C2OC(C=C2)CO)c(=O)[nH]c1=O</chem>
362	003094-09-5	Doxifluridine	<chem>CC1OC(C1O)N1c(F)c(=O)[nH]c1=O</chem>
363	003116-76-5	Dicloxacillin	<chem>OC(=O)C1N2C(=O)C(C2S1(C)C)NC(=O)c1c(C)onc1c1c(Cl)cccc1Cl</chem>
364	003194-55-6	HBCDs	<chem>BrC1CC(Br)C(Br)CC(C)(CC1Br)Br</chem>
365	003239-44-9	Dexfenfluramine	<chem>CCNC(Cc1cccc(c1)C(F)F)C</chem>
366	003268-87-9	Octachlorodibenzo-p-dioxin	<chem>Clc1c2O3c3c(Oc2c(c1c1)Cl)c(Cl)c(Cl)c(c3Cl)Cl</chem>
367	003385-03-3	Flunisolid	<chem>OCC(=O)C12OC(O)C1CC1C2(C)CC(O)C2C1CC(C1=CC(=O)C=CC21C)F(C)C</chem>
368	003424-98-4	Telbivudine	<chem>OCC1OC(C)O1n1cc(Cl)c(=O)[nH]c1=O</chem>
369	003440-28-6	Betamipron	<chem>O=C(c1cccc1)NCCC(=O)O</chem>
370	003562-63-8	Megestrol	<chem>O=C1CC2(C(=C1)C(=CC1C2CCC2(C1CCC2)O)(C(=O)C)C)C</chem>
371	003575-80-2	Melperone	<chem>C1CCN(C)CCC(=O)c1ccc(cc1)F</chem>
372	003579-62-2	Denaverine	<chem>CCC(COC(c1cccc1)(c1cccc1)C(=O)O)CCN(C)CC</chem>
373	003737-09-5	Disopyramide	<chem>CC(N(C)C)CCC(c1cccc1)(c1cccc1)C(=O)N(C)</chem>
374	003778-73-2	Isofamidine	<chem>C1CCN1P(=O)OCCCN1CC1</chem>
375	003930-20-9	Sotalol	<chem>CC(NCC(c1ccc(cc1)NS(=O)(=O)O)O)C</chem>
376	004093-35-0	Bromopride	<chem>CCN(CCN(C(=O)c1cc(Br)cc1OC)N)CC</chem>
377	004291-63-8	Cladribine	<chem>OCC1OC(C)O1n1cnc2c1nc(Cl)nc2N</chem>
378	004342-03-4	Dacarbazine	<chem>CN(NN=C1N=CN=C1C(=O)N)C</chem>
379	004394-00-7	Niflumic	<chem>OC(=O)c1cccnc1Nc1ccc(c1)C(F)F</chem>
380	004419-39-0	Beclomethasone	<chem>CCC(=O)OC1(C)CC2C1(C)CC(O)C1(C2CC2=CC(=O)C=CC2)Cl(C(=O)CO)C(=O)CC</chem>
381	004428-95-9	Foscarnet	<chem>OC(=O)P(=O)(O)O</chem>



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508	032598-11-1	2,5,3',4'-tetrachlorobiphenyl	ClC1ccc(c1)c1ccc(c1)c1Cl
509	032598-12-2	2,4,4',6'-Tetrachlorobiphenyl	ClC1ccc(cc1)c1c(Cl)cc(cc1Cl)Cl
510	032598-13-3	3,4,3',4'-tetrachlorobiphenyl	ClC1ccc(cc1Cl)c1ccc(c1)Cl
511	032598-14-4	pentachlorobiphenyl	ClC1ccc(cc1Cl)c1ccc(c1Cl)Cl
512	032690-93-0	2,4,5,4'-Tetrachlorobiphenyl	ClC1ccc(cc1)c1cc(Cl)(cc1Cl)Cl
		3,4,5,3',4',5'-	
513	032774-16-6	hexachlorobiphenyl	ClC1cc(cc1Cl)Clc1cc(Cl)(c1Cl)Cl
514	032795-44-1	Acecaïnide	CCN(CCN(C=O)c1ccc(cc1)N(C)=O)C)CC
515	032887-01-7	Amdinocillin	OC(=O)C1N2C(=O)C(C2SC1(C)C)N=C1CCCCC1
516	033005-95-7	Tiaprofenic	OC(=O)C(c1ccc(s1)Cl(=O)c1ccccc1)C
517	033025-41-1	2,3,4,4'-tetrachlorobiphenyl	ClC1ccc(cc1)c1ccc(c1Cl)Cl
		2,3,4,6,2',3',4',6'-	
518	033091-17-7	octachlorobiphenyl	ClC1cc(Cl)c(c1c1c(Cl)cc(c1Cl)Cl)Cl
519	033125-97-2	Etomidate	CCOC(=O)c1cncn1C1c1ccccc1
520	033284-50-3	2,4-Dichlorobiphenyl	ClC1ccc(c1Cl)Clc1ccccc1
521	033284-54-7	2,3,5,6-Tetrachlorobiphenyl	ClC1cc(Cl)c(c1Cl)Clc1ccccc1Cl
522	033342-05-1	Gliquidone	OC1ccc2c(c1)C(=O)N(C(=O)C2(C)C)CCc1ccc(cc1)S(=O)(=O)N(C=O)N1CCCCC1
523	033419-42-0	Etoposide	COc1cc(cc1O)OC1C2C(=O)OC2C(C2c1cc1OCOC1c2)OC1OC2COC(OC2C(C1O)O)C
524	033570-04-6	Bilobalide	O=C1OC2C3(C1)C(=O)OC1C3(C2)O(C)C(C)C(C)O(C=O)O1
525	033671-46-4	Clofiazepam	CCc1sc2c(c1)C(=NC(C=O)N2C)c1ccccc1
526	033817-20-8	Pivampicillin	O=C(c1c1ccccc1)N1NC1C(=O)N2C1SC(C2C(=O)OCOC(=O)C(C)C(C)C)C
527	034444-01-4	Cefamandole	OC(C(=O)NC1C(=O)N2C1SCC(=C2C(=O)O)CSc1nnn1C)c1ccccc1
528	034580-14-8	Ketotifen	CN1CCC(=C2c3ccc3CC(=O)c3c2cc3)CC1
529	034597-40-5	Fenoprofen	OC(=O)C(c1c1ccccc1)Oc1ccccc1
530	034661-75-1	Urapidil	COc1ccc1N1CCN(C1)CCNc1ccc(=O)n(c1=O)n1C
531	034787-01-4	Ticarcillin	O=C(C(C1csc1)C(=O)N)N1C(=O)N2C1SC(C2C(=O)O)(C)C
532	034834-67-8	Hydroxycotinine	O=C1C(O)CC(N1C)c1ccccc1
533	034841-39-9	Bupropion	ClC1ccc(c1)C(=O)N(C)C(C)C
534	034883-39-1	2,5-Dichlorobiphenyl	ClC1ccc(c1)c1c1ccccc1Cl
535	034883-41-5	3,5-dichlorobiphenyl	ClC1cc(Cl)cc(c1)Clc1ccccc1
536	034883-43-7	2,4'-dichlorobiphenyl	ClC1ccc(cc1)c1ccccc1Cl
		2,4,5,2',4',5'-	
537	035065-27-1	hexachlorobiphenyl	Clc1cc(Cl)c(cc1c1cc(Cl)c(cc1Cl)Cl)Cl
538	035065-28-2	hexachlorobiphenyl	Clc1cc(Cl)c(cc1c1ccc(c1Cl)Cl)Cl
		2,3,4,5,2',4',5'-	
539	035065-29-3	heptachlorobiphenyl	Clc1cc(Cl)c(cc1c1cc(Cl)c(c1Cl)Cl)Cl
		2,3,4,5,2',3',4'-	
540	035065-30-6	heptachlorobiphenyl	Clc1c(Cl)ccc(c1Cl)c1cc(Cl)c(c1Cl)Cl
541	035189-28-7	Norgestimate	ON=C1CCC2C(=C1)CCC1C2CC2(C1CC2(C#C)OC(=O)C)CC
542	035607-66-0	Cefoxitin	COC1(NC(=O)Cc2cc2)C(=O)N2C1SCC(=C2C(=O)O)COC(=O)N
543	035693-92-6	2,4,6-trichlorobiphenyl	ClC1cc(Cl)c(c1Cl)Clc1ccccc1
544	035693-99-3	2,5,2',5'-tetrachlorobiphenyl	ClC1ccc(cc1c1cc(Cl)ccc1Cl)Cl
		2,3,4,5,2',4'-	
545	035694-06-5	hexachlorobiphenyl	ClC1ccc(c1Cl)Clc1cc(Cl)c(c1Cl)Cl
546	035795-16-5	Trimazosin	COc1c(OC)c(O)cc2c1nc(nc2N)N1CCN(C1)C(=O)OCC(O)C
		1,2,3,4,6,7,8-	
547	035822-46-9	heptachlorodibenzo-p-dioxin	Clc1c(Cl)cc2c(c1Cl)Oc1c2c(Cl)c(Cl)c(c1Cl)Cl
548	036505-84-7	Buspirone	O=C1CC2(CCC2)CC(=O)N1CCCC1CCN(C1)C1cccc1
549	036507-48-9	Penbutolol	OC(CO)c1ccc1C1CCC1)CN(C)C
550	036559-22-5	2,2',3,4'-Tetrachlorobiphenyl	ClC1ccc(c1Cl)c1ccc(c1Cl)Cl
551	036735-22-5	Quazepam	ClC1ccc2c(c1)C(=NCC(=S)N2CC(F)F)F1ccccc1F
552	036791-04-5	Ribavirin	OCC1OC(C(C1O))n1cnc(n1)C(=O)N
553	037091-66-0	Azlocillin	O=C(Cc1ccc1)NC(=O)N1CCN(C1=O)N2C1SC(C2C(=O)O)(C)C
554	037115-32-5	Adinazolam	CN(Cc1nnc2n1c1ccc(cc1C=NC2)c1ccccc1)Cl
555	037148-27-9	Clenbuterol	OC(c1cc(Cl)c(c1Cl)N)CNC(C)C
556	037300-21-3	Pentosan	OC1COC(C(C1OS(=O)(=O)O)OS(=O)(=O)O)OC1COC(C(C1OS(=O)(=O)O)OS(=O)(=O)O)
557	037517-30-9	Acebutolol	CCCC(=O)Nc1ccc(c1)C(=O)OCC(CN(C)C)O
558	037680-65-2	2,5,2'-trichlorobiphenyl	ClC1ccc(c1)c1c1ccccc1Cl
559	037680-66-3	2,4,2'-trichlorobiphenyl	ClC1ccc(c1Cl)Clc1ccccc1
560	037680-68-5	3,5,2'-trichlorobiphenyl	ClC1cc(Cl)cc(c1)Clc1ccccc1
561	037680-69-6	3,4,3'-trichlorobiphenyl	ClC1ccc(c1)c1ccc(c1Cl)Cl

ID	CAS	Name	Canonical SMILES
		2,4,5,2',5'-	
562	037680-73-2	pentachlorobiphenyl	Clc1ccc(c1)c1cc(Cl)c(cc1Cl)Cl
563	038103-61-6	Tolamolol	OC(CO)c1ccc1C)CNCOC1ccc(cc1)C(=O)N
564	038194-50-2	Sulindac	OC(=O)CC1=C(C)C(=C2ccc(cc2)S(=O)C)c2c1cc(F)cc2
		2,2',3,5',6-	
565	038379-99-6	Pentachlorobiphenyl	Clc1ccc(c1)c1c1c(Cl)ccc(c1Cl)Cl
		2,4,5,2',4'-	
566	038380-01-7	pentachlorobiphenyl	Clc1ccc(c1Cl)c1cc(Cl)c(cc1Cl)Cl
		2,2',3,4,5'-	
567	038380-02-8	Pentachlorobiphenyl	Clc1ccc(c1)c1ccc(c1Cl)Cl
		2,3,6,3',4'-	
568	038380-03-9	pentachlorobiphenyl	Clc1ccc(cc1Cl)c1c(Cl)ccc(c1Cl)Cl
		2,2',3,4',5,6-	
569	038380-04-0	Hexachlorobiphenyl	Clc1cc(Cl)c(cc1c1c(Cl)ccc(c1Cl)Cl)Cl
		2,2',3,3',4,6'-	
570	038380-05-1	Hexachlorobiphenyl	Clc1ccc(c1Cl)Clc1c(Cl)ccc(c1Cl)Cl
		2,3,4,2',3',4'-	
571	038380-07-3	hexachlorobiphenyl	Clc1c(ccc1Cl)Clc1ccc(c1Cl)Cl
		2,3,4,5,3',4'-	
572	038380-08-4	hexachlorobiphenyl	Clc1ccc(cc1Cl)c1cc(Cl)c(c1Cl)Cl
573	038396-39-3	Bupivacaine	CCCCN1CCCCC1C(=O)Nc1c(Cl)ccccc1
		2,3,6,2',3',6'-	
574	038411-22-2	hexachlorobiphenyl	Clc1ccc(c1c1c1Cl)ccc(c1Cl)Cl
		2,2',3,3',4,5,6'-	
575	038411-25-5	Heptachlorobiphenyl	Clc1c(Cl)cc(c1Cl)Clc1c(Cl)ccc(c1Cl)Cl
576	038444-73-4	2,2',6-Trichlorobiphenyl	Clc1ccc(c1c1ccccc1Cl)Cl
577	038444-76-7	2,3',6-Trichlorobiphenyl	Clc1ccc(c1)c1c1ccc1Cl
578	038444-77-8	2,4',6-Trichlorobiphenyl	Clc1ccc(c1c1ccc(cc1)Cl)Cl
579	038444-78-9	2,2',3-Trichlorobiphenyl	Clc1ccc(c1c1ccc(c1Cl)Cl)Cl
580	038444-81-4	2,5,3'-trichlorobiphenyl	Clc1ccc(c1)c1c1ccc(c1Cl)Cl
581	038444-85-8	2,3,4'-trichlorobiphenyl	Clc1ccc(cc1)c1ccc(c1Cl)Cl
582	038444-86-9	2,3',4'-Trichlorobiphenyl	Clc1ccc(cc1Cl)c1ccccc1
583	038444-87-0	3,5,3'-trichlorobiphenyl	Clc1ccc(c1)c1cc(Cl)cc(c1Cl)Cl
584	038444-88-1	3,5,4'-trichlorobiphenyl	Clc1ccc(c1)c1cc(Cl)cc(c1Cl)Cl
585	038444-90-5	3,4,4'-trichlorobiphenyl	Clc1ccc(cc1)c1ccc(c1Cl)Cl
586	038444-93-8	2,3,2',3'-tetrachlorobiphenyl	Clc1c(Cl)ccc1c1ccc(c1Cl)Cl
587	038677-94-0	Nortilidine	CCOC(=O)C1(CCC=CC1NC)c1ccccc1
588	038821-53-3	Cephadrine	O=C(C(C1=C(C=C1)N)NC1C(=O)N2C1SCC(=C2C(=O)O)C
589	039001-02-0	Octachlorodibenzofuran	Clc1c(Cl)c(Cl)c2c(c1Cl)oc1c2c(Cl)c(c1Cl)Cl
		1,2,3,4,7,8-	
590	039227-28-6	hexachlorodibenzo-p-dioxin	Clc1cc2Oc3c(Oc2cc1Cl)c(Cl)c(c3Cl)Cl
		2,4,6,2',4'-	
591	039485-83-1	pentachlorobiphenyl	Clc1ccc(c1Cl)Clc1c(Cl)c(cc1Cl)Cl
592	039562-70-4	Nitrendipine	CCOC(=O)C1=C(C)NC(=C(C1c1ccccc1)N(=O)O)C(=O)OC
		2,3,4,5,3',4',5'-	
593	039635-31-9	heptachlorobiphenyl	Clc1cc(cc1Cl)Clc1cc(Cl)c(c1Cl)Cl
594	039715-02-1	Endralazine	NNc1nnc2c(c1)CN(C2)C(=O)c1ccccc1
		2,3,4,6,2',3',5'-	
595	040186-70-7	heptachlorobiphenyl	Clc1cc(Cl)c(c1)c1c1c(Cl)cc(c1Cl)Cl
		2,3,4,6,2',3',5',6'-	
596	040186-71-8	octachlorobiphenyl	Clc1cc(Cl)c(c1Cl)Clc1c(Cl)c(Cl)cc(c1Cl)Cl
		2,3,4,5,6,2',3',4',5'-	
597	040186-72-9	nonachlorobiphenyl	Clc1cc(Cl)c(c1Cl)Clc1c(Cl)c(Cl)c(c1Cl)Cl
		1,2,3,7,8-pentachlorodibenzo-	
598	040321-76-4	p-dioxin	Clc1cc2Oc3c(Oc2cc1Cl)cc(c3Cl)Cl
599	040828-46-4	Suprofen	OC(=O)C(c1ccc(cc1)C(=O)c1ccccc1)C
600	041318-75-6	2,4,4'-Tribromodiphenyl	BrC1ccc(c1)Oc1ccc(cc1Br)Br
601	041340-25-4	Etodolac	CCC1(OCCc2c1[nH]c1c2cccc1CC)CC(=O)O
		2,3,4,5,6,4'-	
602	041411-63-6	hexachlorobiphenyl	Clc1ccc(cc1)c1c(Cl)c(Cl)c(c1Cl)Cl
		2,3,4,5,6,3',4'-	
603	041411-64-7	heptachlorobiphenyl	Clc1cc(ccc1Cl)c1c(Cl)c(Cl)c(c1Cl)Cl
604	041464-39-5	2,3,2',5'-tetrachlorobiphenyl	Clc1ccc(c1)c1ccc(c1Cl)Cl
605	041464-40-8	2,2',4,5'-Tetrachlorobiphenyl	Clc1ccc(c1Cl)c1cc(Cl)ccc1

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606	041464-41-9	2,5,2',6'-tetrachlorobiphenyl	Cl1ccc(c1)c1c(Cl)ccc1Cl
607	041464-43-1	2,3,3',4'-tetrachlorobiphenyl	Clc1cc(c1)c1ccc(c1Cl)Cl
608	041464-46-4	2,3',4',6'-Tetrachlorobiphenyl	Clc1cc(c1c1Cl)c(Cl)ccc1Cl
609	041464-47-5	2,3,2',6'-tetrachlorobiphenyl	Clc1c(Cl)ccc1c1c(Cl)ccc1Cl
610	041464-51-1	Pentachlorobiphenyl	Clc1cc(Cl)c(cc1c1ccc(c1Cl)Cl)Cl
611	041708-72-9	Tocainide	CC(C(=O)Nc1c(Cl)ccc1C)N
612	041744-40-5	Sulbenicillin	O=C(S(=O)(=O)O)c1ccc1NC1C(=O)N2C1SC(C2C(=O)O)(C)C
613	041859-67-0	Bezafibrate	Clc1ccc(cc1)C(=O)NCC1ccc(cc1)OC(C(=O)O)(C)C
614	041952-52-7	Cefcanel	O=C(C1c1ccc1O)NC1C(=O)N2C1SC(=C2C(=O)O)CSc1nnc1(C)S
615	042200-33-9	Nadolol	OC(COc1ccc2c1c(Cl)C(C2)O)CNC(C)C
616	042228-92-2	Acivicin	NC(C(=O)O)C1CC(=NO)1Cl
617	042399-41-7	Diltiazem	COc1ccc(cc1)C1Sc2cccc2N(C(=O)C1OC(=O)C)CCN(C)C
618	042408-82-2	Butorphanol	Oc1ccc2c(c1)C13CCCC3(C(2)N)(CC1)CC1CCC1O
619	042740-50-1	octachlorobiphenyl	Clc1cc(Cl)c(c1c1cc(Cl)c(c1Cl)Cl)Cl
620	043200-80-2	Zopiclone	CN1CCN(C1)C(=O)OC1c2nccc2C(=O)N1c1ccc(en1)Cl
621	046817-91-8	Viloxazine	CCOC1c1ccc1OC1COC1
622	047141-42-4	Levobunolol	OC(COc1ccc2c1CCCC2=O)CNC(C)C
623	049562-28-9	Fenofibrate	CC(OC(=O)C(Oc1ccc(cc1)C(=O)c1ccc(cc1)Cl)(C)C)C
624	050370-12-2	Cefadroxil	O=C(C1c1ccc(cc1)O)N1NC1C(=O)N2C1SC(=C2C(=O)O)C
625	050679-08-8	Terfenadine	OC1c1ccc(cc1)C(C)C)CCN1CCC(C1)C1c1ccc1(c1ccc1)O
626	051022-71-0	Nabilone	CCCCCCC1c1cc(O)c2c(c1)OC(C1C2CC(=O)CC1)(C)C(C)C
627	051207-31-9	tetrachlorodibenzofuran	Clc1cc2c(cc1Cl)oc1c2cc(Cl)c(c1)Cl
628	051264-14-3	Amsacrine	COc1ccc(cc1)Nc1c2ccc2nc2c1ccc2)NS(=O)(=O)C
629	051333-22-3	Budesonide	CCCC1OC2C(O1)(C(=O)CO)C1(C2)C2CCC3=CC(=O)C=CC3(C2C1)O)C
630	051384-51-1	Metoprolol	COCCc1ccc(cc1)OCC(CNC(C)C)O
631	051481-65-3	Mefloquine	O=C(C1c1ccc1NC(=O)N1CCN(C1=O)S(=O)(=O)C)NC1C(=O)N2C1SC(C2C(=O)O)(C)C
632	051627-14-6	Cefatrizine	O=C(C1c1ccc(cc1)O)N1NC1C(=O)N2C1SC(=C2C(=O)O)CSc1c[nH]jnn1
633	051639-49-7	Chlorophenylpiperazine,	Clc1ccc(c1)N1CCNCC1
634	051908-16-8	hexachlorobiphenyl	Clc1cc(Cl)c(c1c1c(Cl)c(cc1Cl)Cl)Cl
635	051931-66-9	Tilidine	CCOC(=O)C1(CCG=CC1N(C)C)C1cccc1
636	052128-35-5	Trimetrexate	COc1cc(NC2c2cc3c(c2C)F(N)nc(n3)N)cc1C1OC
637	052468-60-7	Flunarizine	Fc1ccc(cc1)C1c1ccc(cc1)F)N1CCN(C1)CC=Cc1ccc1
638	052485-79-7	Buprenorphine	COc1c2ccc3(Cc1C(C)C(C)C)O)C14C2Oc2c4c(CC3N)CC1CC1)ccc2O
639	052663-58-8	2,3,4',6'-Tetrachlorobiphenyl	Clc1ccc(cc1)c1c(Cl)ccc(c1Cl)Cl
640	052663-60-2	Pentachlorobiphenyl	Clc1c(Cl)ccc1c1c(Cl)ccc(c1Cl)Cl
641	052663-61-3	Pentachlorobiphenyl	Clc1ccc(c1)c1cc(Cl)cc(c1Cl)Cl
642	052663-62-4	pentachlorobiphenyl	Clc1ccc(c1c1Cl)Clc1ccc(c1Cl)Cl
643	052663-63-5	hexachlorobiphenyl	Clc1ccc(c1c1c1c(Cl)c(Cl)cc(c1Cl)Cl)Cl
644	052663-64-6	heptachlorobiphenyl	Clc1c(Cl)cc(c1c1c(Cl)ccc(c1Cl)Cl)Cl
645	052663-65-7	heptachlorobiphenyl	Clc1cc(Cl)c(c1c1Cl)Clc1c(Cl)ccc(c1Cl)Cl
646	052663-66-8	hexachlorobiphenyl	Clc1cc(Cl)c(c1c1c1ccc(c1Cl)Cl)Cl
647	052663-68-0	heptachlorobiphenyl	Clc1cc(Cl)c(cc1c1c1c(Cl)c(Cl)cc(c1Cl)Cl)Cl
648	052663-69-1	heptachlorobiphenyl	Clc1cc(Cl)c(cc1c1c1c(Cl)cc(c1Cl)Cl)Cl
649	052663-70-4	heptachlorobiphenyl	Clc1ccc(c1c1Cl)Clc1c(Cl)c(Cl)cc(c1Cl)Cl
650	052663-71-5	heptachlorobiphenyl	Clc1c(Cl)cc(c1c1Cl)c1ccc(c1c1Cl)Cl
651	052663-72-6	hexachlorobiphenyl	Clc1cc(Cl)c(cc1c1cc(Cl)c(c1Cl)Cl)Cl
652	052663-73-7	octachlorobiphenyl	Clc1c(Cl)c(Cl)c(c1c1Cl)Clc1c(Cl)ccc(c1Cl)Cl

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653	052663-74-8	2,3,4,5,2',3',5'-heptachlorobiphenyl	Clc1cc(Cl)c(c1c1c1c(Cl)c(c1Cl)Cl)Cl
654	052663-75-9	2,3,4,5,2',3',5',6'-octachlorobiphenyl	Clc1c(Cl)cc(c1c1Cl)Clc1c(Cl)c(Cl)cc(c1Cl)Cl
655	052663-76-0	2,3,4,5,6,2',4',5'-octachlorobiphenyl	Clc1cc(Cl)c(cc1c1c1c(Cl)c(Cl)c(c1Cl)Cl)Cl
656	052663-78-2	2,3,4,5,6,2',3',4'-octachlorobiphenyl	Clc1ccc(c1c1Cl)Clc1c(Cl)c(Cl)c(c1Cl)Cl
657	052663-79-3	2,3,4,5,6,2',3',4',6'-nonachlorobiphenyl	Clc1c(Cl)cc(c1c1Cl)c1c(Cl)c(Cl)c(c1Cl)Cl)Cl
658	052704-70-8	2,2',3',3',5,6-Hexachlorobiphenyl	Clc1ccc(c1Cl)c1c(Cl)c(Cl)cc(c1Cl)Cl
659	052712-04-6	2,3,4,5,2',5'-hexachlorobiphenyl	Clc1ccc(c1c1c1c(Cl)c(Cl)c(c1Cl)Cl)Cl
660	052712-05-7	2,3,4,5,6,2',5'-heptachlorobiphenyl	Clc1ccc(c1c1c1c(Cl)c(Cl)c(c1Cl)Cl)Cl
661	052744-13-5	2,3,5,2',3',6'-hexachlorobiphenyl	Clc1cc(Cl)c(c1c1c1c(Cl)ccc(c1Cl)Cl)Cl
662	053179-11-6	Loperamide	Clc1ccc(cc1)C1(O)CCN(C1)CCC(C(=O)N)C)C1cccc1c1cccc1
663	053230-10-7	Mefloquine	OC(c1cc(nc2c1ccc2C(F)(F)F)C(F)F)C1CCCCN1
664	053267-01-9	Cibenzoline	c1ccc(cc1)C1(Cc1c1=NCN1)c1cccc1
665	053583-79-2	Amisulpride	CCN1CCCC1CNC(=O)c1cc(c1c1OC)N)S(=O)(=O)CC
666	053648-55-8	Dezocine	Oc1ccc2c(c1)C1(C)CCCCC2(C)C1N
667	053772-83-1	Zuclopenthixol	OCCN1CCN(C1)CCC=C1c2ccc2Sc2c1cc(Cl)cc2
668	053910-25-1	Pentostatin	OC1OC(C1O)n1cnc2c1N=CC2O
669	053994-73-3	Cefaclor	NC1c1ccc1C(=O)N1C(=O)N2C1SC(=C2C(=O)O)Cl
670	054024-22-5	Desogestrel	CC12C(C=C)C3C(C1CC2)O(=C)CC1=CCCCC31
671	054048-10-1	Etonogestrel	CHCC1(O)CCC2C1(C)CC(=C)C1C2CCC2=C(C=O)CCC12
672	054063-53-5	Propafenone	CCNCC(CO)c1ccc1C(=O)CCc1ccc1O
673	054143-55-4	Flecainide	O=C(c1cc(OCC(F)F)ccc1OCC(F)F)NCC1CCCCN1
674	054340-58-8	Meptazinol	CC1(CCCN(C1)C)c1ccc(c1)O
675	054340-62-4	Bufuralol	CCc1ccc2c1oc(c2)C(CN(C)C)C
676	054350-48-0	Etretinate	CCOC(=O)C=C(C=C)C=C(C1c1cc(c1c1C)OC)C
677	054739-18-3	Fluvoxamine	NCCON=C(c1ccc(c1)C(F)F)C(C)C
678	054910-89-3	Fluoxetine	CNCCC1c1ccc1O)c1ccc(cc1)C(F)F
679	054965-21-8	Albendazole	CCSc1ccc2c(c1)[nH]c(n2)NC(=O)O
680	055079-83-9	Acitretin	COc1cc(Cl)c(c1c1C)C=C(C=C)C(=O)O)C
681	055096-26-9	Nalmefene	C=C1CCC2(C34C1Oc1c4c(C2N)(C3)CC2CC2)ccc1O
682	055142-85-3	Ticlopidine	Clc1cccc1CN1CC2c(Cl)ccs2
683	055215-18-4	2,3,4,5,2',3'-hexachlorobiphenyl	Clc1ccc(c1Cl)c1cc(Cl)c(c1Cl)Cl
684	055268-74-1	Praziquantel	O=C(N1CC(=O)N2C1C1c1ccc1CC2)C1CCCC1
685	055268-75-2	Cefuroxime	CON=C(C(=O)N)C1C(=O)N2C1SC(=C2C(=O)O)COC(=O)N1ccc1O
686	055673-89-7	1,2,3,4,7,8,9-heptachlorodibenzofuran	Clc1cc2oc3c(c2c1Cl)Cl)c(Cl)c(c3Cl)Cl
687	055712-37-3	2,4,3'-trichlorobiphenyl	Clc1ccc(c1Cl)c1ccc(c1Cl)Cl
688	055720-44-0	2,3,5-trichlorobiphenyl	Clc1cc(Cl)c(c1c1c1)ccc1Cl
689	055837-25-7	Bufomedil	COc1cc(O)C)cc(c1C(=O)CCN1CCCC1)OC
690	055837-27-9	Piretanide	OC(=O)c1cc(N2CCC2)c(c1)S(=O)(=O)N1c1ccc1
691	055954-61-5	Pseudohypericin	OC1cc(O)c2c3c1c1c(Cl)cc(c4c1c1c3c3c(C2=O)C)cc(c3c2c1c(C4=O)C)O)O
692	055981-09-4	Nitazoxanide	CC(=O)Oc1ccc1C(=O)Nc1ncc(s1)N(=O)=O
693	055985-32-5	Nicardipine	CO(C=O)C1=C(C)NC(=C1C1c1ccc(c1)N(=O)O)CCN(Cc1ccc1)C
694	056030-54-7	Sufentanil	OCC1(CCN(C1)CCc1ccc1)N(c1ccc1)C(=O)CC
695	056180-94-0	Acarbose	OC1OC(CO)C(CO)C(CO)O)C(C1OC1OC(C1O)N)C1C(=O)CO(C(C1O)O)O
696	056211-40-6	Toraseamide	CCN(C(=O)N)S(=O)(=O)c1ccc1Nc1ccc(c1)C
697	056290-94-9	Medroxalol	CC(NCC1c1ccc(c1)C(=O)N)O)CC1c1ccc2c1)OCC2
698	056558-16-8	2,4,6,2',6'-pentachlorobiphenyl	Clc1cc(Cl)c(c1Cl)c1c(Cl)ccc1Cl
699	056558-17-9	2,4,6,3',4'-pentachlorobiphenyl	Clc1cc(Cl)c(c1Cl)c1ccc(c1Cl)Cl
700	056775-88-3	Zimelidine	CN(Cc(=O)c1ccc1)c1ccc(cc1)Br
701	056796-20-3	Cefmetazole	N#CCSCC(=O)N1(O)C(C(=O)N2C1SC(=C2C(=O)O)C)Sc1nnnn1C
702	056995-20-1	Flupirtine	CCOC(=O)Nc1ccc(nc1N)Nc1ccc(cc1)F

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703	057117-31-4	2,3,4,7,8-pentachlorodibenzofuran	Clc1cc2c(cc1Cl)oc1c2cc(Cl)c(c1Cl)Cl
704	057117-41-6	1,2,3,7,8-pentachlorodibenzofuran	Clc1cc2c(cc1Cl)oc1c2c(Cl)c(c1Cl)Cl
705	057117-44-9	1,2,3,6,7,8-hexachlorodibenzofuran	Clc1cc2c(c(c1Cl)Cl)oc1c2c(Cl)c(c(c1Cl)Cl)Cl
706	057460-41-0	Talinolol	OC(CNC(C)C)COc1ccc(cc1)NC(=O)NCCC1
707	057465-28-8	pentachlorobiphenyl	Clc1ccc(cc1Cl)c1cc(Cl)c(c1Cl)Cl
708	057574-09-1	Amineptine	OC(=O)CCCCNC1c2ccccc2Cc2c1cccc2
709	057653-85-7	hexachlorodibenzo-p-dioxin	Clc1c(Cl)cc2c(c1Cl)Oc1c(OC)c(Cl)c(c1Cl)Cl
710	057801-81-7	Brotizolam	Brc1cc2c(s1)n1c(CN=C2c2cccc2Cl)nn1C
711	057808-66-9	Domperidone	Clc1ccc2c(c1)nH(c(=O)n2C1CCN(CC1)CCN1c(=O)[nH]c1ccc2
712	058581-89-8	Azelastine	CN1CCCC(C1)n1nc(Cc2ccc(cc2)Cl)c2c(c1=O)cccc2
713	058957-92-9	Idarubicin	OC1C(N)CC(OC1C)OC1CC(O)(Cc2c1c(O)c1c(O)c2O)(c1=O)cccc2C(=O)C
714	059080-40-9	hexabromobiphenyl	Brc1cc(Br)c(cc1c1cc(Br)c(cc1Br)Br)Br
715	059122-46-2	Misoprostol	CCCC(C)C=CC1C(O)C=C(=O)C1CCCCC(=O)OC(O)C
716	059170-23-9	Bevantolol	COc1ccc(CNCC(C)COc2ccc(c2)Cl)O)cccc1OC
717	059291-64-4	2,3,4,2',4',6'-hexachlorobiphenyl	Clc1cc(Cl)c(c1Cl)Clc1ccc(c1Cl)Cl
718	059291-65-5	hexachlorobiphenyl	Clc1cc(Cl)c(c1Cl)Clc1cc(Cl)c(c1Cl)Cl
719	059467-70-8	Midazolam	Clc1ccc2c(c1)C(=N)Cn1n2c(C)nc1c1cccc1F
720	059729-31-6	Lorcainide	CC(N1CCC(C1)N)c1ccc(cc1)Cl(C)C(=O)C1cccc1C
721	059729-33-8	Citalopram	N#Cc1ccc2c(c1)COC2(CCCN(C)C)c1ccc(cc1)F
722	059933-66-3	Perfluorobutanesulfonic	FC(C(C(S(=O)(=O)O)(F)F)(F)F)F
723	060084-10-8	Tiazofurin	OCC1OC(C1O)O)c1ccc(n1)C(=O)N
724	060142-96-3	Gabapentin	NCC1(CCCCC1)CC(=O)O
725	060145-20-2	Pentachlorobiphenyl	Clc1cc(Cl)c(c1Cl)c1ccc(c1Cl)Cl
726	060145-21-3	2,4,6,2',5'-pentachlorobiphenyl	Clc1ccc(c1)c1c(Cl)cc(cc1Cl)Cl
727	060145-22-4	hexachlorobiphenyl	Clc1cc(Cl)c(c1Cl)Clc1cc(Cl)c(c1Cl)Cl
728	060166-93-0	Iopamidol	OCC(NC(=O)c1c(l)c(C(=O)NC(O)CO)c(c1)N)C(=O)(O)C)CO
729	060282-87-3	Gestodene	C#CC1(O)C=CC2C1(CC)CCC1C2CC2=CC(=O)CCC12
730	060348-60-9	Pentabromodiphenyl	Brc1ccc(c1Br)Oc1cc(Br)c(cc1Br)Br
731	060628-96-8	Bifonazole	c1ccc(cc1)c1ccc(cc1)C(n1ccnc1)c1cccc1
732	060643-86-9	Vigabatrin	NC(C=O)CCC(=O)O
733	060719-84-8	Amrinone	O=c1[nH]cc(cc1N)c1ccnc1
734	060851-34-5	2,3,4,6,7,8-hexachlorodibenzofuran	Clc1cc2c(c(c1Cl)Cl)oc1c2cc(Cl)c(c1Cl)Cl
735	060925-61-3	Ceforanide	NCc1cccc1CC(=O)NC1C(=O)N2C1S(=O)C(=O)CSc1nnnn1CC(=O)O
736	061270-58-4	Cefonicid	O=C(c1cccc1O)NC1C(=O)N2C1S(=O)C(=O)CSc1nnnn1CS(=O)(=O)O
737	061477-96-1	Piperacillin	CCN1CCN(C(=O)C1=O)C(=O)NC(C(=O)NC1C(=O)N2C1S(=O)C(=O)O)(C)C1cccc1
738	061622-34-2	Cefotiam	CN(Cn1nnnc1S(=O)C(=O)N)C2C(=O)N2C1S(=O)C(=O)NC(=O)C1csc(n1)N)C
739	061869-08-7	Paroxetine	Fc1ccc(cc1)C1CCNCC1COc1ccc2c(c1)OCO2
740	062571-86-2	Captopril	SCC(C(=O)N1CCCC1C(=O)O)C
741	062613-82-5	Oxiracetam	NC(=O)CN1CC(C1=O)O
742	062666-20-0	Progabide	NC(=O)CCCN(C(=O)C1C(=O)C)C=CC1=O)c1ccc(cc1)Cl
743	062796-65-0	2,4,6,2'-tetraclorobiphenyl	Clc1cc(Cl)c(c1Cl)Clc1cccc1Cl
744	062893-19-0	Cefoperazone	CCN1CCN1C(=O)C1=O)C(=O)NC(C1ccc(c1O)C(=O)N)C1C(=O)N2C1S(=O)C(=O)O)CSc1nnnn1C
745	063527-52-6	Cefotaxime	CON=C(c1csc(n1)N)C(=O)NC1C(=O)N2C1S(=O)C(=O)COC(=O)C
746	063590-64-6	Terazosin	OC1cc2nc(nc2cc1OC)N1CCN(CC1)C(=O)C1CCCC1
747	063612-50-0	Nilutamide	O=C1NC(C(=O)N1c1ccc(c1Cl)C(F)F)N(=O)(=O)C)C
748	063659-18-7	Betaxolol	OC(CO)c1ccc(cc1)CCOCC1C(C1)CNC(C)C
749	063675-72-9	Nisoldipine	COC(=O)C1=C(C)NC(C(=O)C1c1ccc1N(=O)O)C(=O)OCC(C)C(C)C
750	064221-86-9	Imipenem	CC(C1C2CC(=O)N2C1=O)C(=O)O)SCCN=C(N)O
751	064706-54-3	Bepiridil	CC(COCC(N1CCCC1)CN(c1cccc1)Cc1cccc1)C
752	064952-97-2	Moxalactam	COC1(NC(=O)C)c2ccc(cc2)C(=O)O)C(=O)N2C1OCC(=O)C(=O)CSc1nnnn1C
753	065052-63-3	Cefetamet	CON=C(c1csc(n1)N)C(=O)NC1C2S(=O)C(=O)N2C1=O)C(=O)O)C

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754	065085-01-0	Cefmenoxime	CON=C(C(=O)NC1C(=O)N2C1S(=O)C(=O)CSc1nnnn1C)c1csc(n1)N
755	065271-80-9	Mitoxantrone	OCCNCCNc1ccc(c2c1C(=O)c1c(C2=O)c(O)ccc1O)NCCNCO
756	065277-42-1	Ketoconazole	Clc1ccc(c(c1Cl)Cl)OC(C1)OC1ccc(cc1)N1CCN(CC1)C(=O)C)Cn1ccnc1
757	065472-88-0	Naftifine	CN(Cc1cccc2c1cccc2)CC=Cc1cccc1
758	065510-44-3	3,4,5,2',4'-pentachlorobiphenyl	Clc1ccc(c(c1Cl)c1cc(Cl)c(c1Cl)Cl)Cl
759	065510-45-4	Pentachlorobiphenyl	Clc1ccc(c(c1Cl)c1ccc(c1Cl)Cl)Cl
760	066085-59-4	Nimodipine	COCCOC(=O)C1=C(C)NC(=O)C1c1cccc(c1)N(=O)O)C(=O)OC(C)C(C)C
761	066104-22-1	Pergolide	CCCN1C(C)C(C)CC2C1C(c1c[nH]c3c1c2ccc3
762	066357-35-5	Ranitidine	CNC(=O)C(=O)NCCSCc1ccc(o1)N(C)C
763	066722-44-9	Bisoprolol	OC(CO)c1ccc(cc1)COC(C)C(C)CNC(C)C
764	066778-36-7	Encainide	COc1ccc(cc1)C(=O)Nc1cccc1C(CN1CCCC1)C
765	067227-57-0	Fenoldopam	OC1ccc(cc1)C1CNCCc2c1cc(O)c(c2Cl)O
766	067392-87-4	Drosiprenone	O=C1CCC2(C=C1)C1CC1C1C2CC2(C1C1CC1C1CCC(=O)O)C)C
767	067562-39-4	heptachlorodibenzofuran	Clc1cc2c(c(c1Cl)Cl)oc1c2c(Cl)c(c1Cl)Cl
768	067195-31-5	Terconazole	Clc1ccc(c(c1Cl)Cl)OC(O1)COc1ccc(cc1)N1CCN(CC1)C(C)C)Cn1ccnc1
769	068194-04-7	2,4,2',6'-tetrachlorobiphenyl	Clc1ccc(c(c1Cl)Cl)c1c(Cl)cccc1Cl
770	068194-05-8	2,3,6,2',4'-pentachlorobiphenyl	Clc1ccc(c(c1Cl)c1c(Cl)ccc(c1Cl)Cl)Cl
771	068194-08-1	2,3,6,2',4',6'-hexachlorobiphenyl	Clc1cc(Cl)c(c1Cl)Clc1c(Cl)ccc(c1Cl)Cl
772	068194-09-2	2,3,5,6,2',6'-hexachlorobiphenyl	Clc1cccc(c1c1c(Cl)c(Cl)cc(c1Cl)Cl)Cl
773	068194-13-8	2,3,5,6,2',4'-hexachlorobiphenyl	Clc1ccc(c(c1Cl)c1c(Cl)c(Cl)cc(c1Cl)Cl)Cl
774	068194-14-9	2,3,4,6,2',3'-hexachlorobiphenyl	Clc1ccc(c(c1)c1c(Cl)cc(c1Cl)Cl)Cl
775	068194-16-1	2,3,4,5,6,2',3',5'-heptachlorobiphenyl	Clc1cccc(c1Cl)c1c(Cl)c(Cl)c(c1Cl)Cl)Cl
776	068194-17-2	2,3,4,5,6,2',3',5'-octachlorobiphenyl	Clc1cc(Cl)c(c1Cl)c1c1c(Cl)c(Cl)c(c1Cl)Cl)Cl)Cl
777	068252-19-7	Pirmenol	CC1CCCC(N1CCCC1ccccn1)c1cccc1O)C
778	068291-97-4	Zonisamide	NS(=O)(=O)Cc1noc2c1ccc2
779	068302-57-8	Amleraxox	CC(c1ccc2c(c1)c(=O)c1(o2)nc(c1)C(=O)O)N)C
780	068359-37-5	Cyfluthrin	N#CC(c1ccc(c1)O)c1cccc1F)OC(=O)C1C(C)C=C(c1Cl)Cl
781	068373-14-8	Sulbactam	OC(=O)C1N2C(=O)CC2S(=O)(=O)C1(C)C
782	068401-81-0	Ceftizoxime	CON=C(c1csc(n1)N)C(=O)NC1C2S(=O)C(=O)N2C1=O)C(=O)O
783	068693-11-8	Modafinil	NC(=O)CS(=O)C(c1cccc1)c1cccc1
784	068844-77-9	Astemizole	COc1ccc(cc1)CCN1CC(C)C1)Nc1nc2c(n1Cc1ccc(cc1)F)ccc2
785	069049-73-6	Nedocromil	CCc1c2oc(cc(=O)c2cc2n1n(C)C)c(c2=O)C(=O)O)C
786	069739-16-8	Cefodizime	CON=C(c1csc(n1)N)C(=O)NC1C(=O)N2C1S(=O)C(=O)CSc1nc(c1)CC(=O)O)C
787	069756-53-2	Halofantrine	CCCCN(CCC(c1ccc2c(Cl)cc2c2c1ccc(c2)C(F)F)Cl)O)CCCC
788	069782-90-7	2,3,4,3',4',5'-hexachlorobiphenyl	Clc1c(Cl)ccc(c1Cl)c1cc(Cl)c(c1Cl)Cl)Cl
789	070362-45-7	2,3,6,2'-tetrachlorobiphenyl	Clc1cccc1c1c(Cl)ccc(c1Cl)Cl
790	070362-50-4	3,4,5,4'-tetrachlorobiphenyl	Clc1ccc(cc1)c1cc(Cl)c(c1Cl)Cl
791	070424-67-8	2,3,5,3'-tetrachlorobiphenyl	Clc1cccc(c1)c1cc(Cl)cc(c1Cl)Cl
792	070424-68-9	2,3,3',4',5'-pentachlorobiphenyl	Clc1cc(Cl)c(c1Cl)c1ccc(c1Cl)Cl)Cl
793	070424-70-3	3,4,5,2',5'-pentachlorobiphenyl	Clc1ccc(c(c1)c1cc(Cl)c(c1Cl)Cl)Cl
794	070458-92-3	Pefloxacin	CN1cc(C(=O)O)c(=O)c2c1cc(N1CCN(CC1)C)c(c2)F
795	070458-96-7	Norflloxacin	CC1cc(C(=O)O)c(=O)c2c1cc(N1CCN(CC1)C)c2)F
796	070648-26-9	1,2,3,4,7,8-hexachlorodibenzofuran	Clc1cc2c(cc1Cl)oc1c2c(Cl)c(c1Cl)Cl)Cl
797	070797-11-4	Cefpiramide	OC1ccc(cc1)C(C(=O)N)C1C(=O)N2C1S(=O)C(=O)CSc1nnnn1NC(=O)c1[nH]c(cc1=O)C
798	071195-58-9	Alifentanil	OCC1(CCN(CC1)C)Cn1nnn1C(=O)CC)N(c1cccc1)C(=O)CC
799	071320-77-9	Moclobemide	O=C(c1ccc(cc1)Cl)NCCN1CCOCC1
800	071620-89-8	Reboxetine	CCOc1cccc1OC(c1cccc1)C1OCCN1
801	072432-10-1	Aniracetam	COc1ccc(cc1)C(=O)N1CCCC1=O
802	072509-76-3	Felodipine	CCOC(=O)C1=C(C)NC(=O)C1c1cccc(c1Cl)Cl)C(=O)O)C
803	072599-27-0	Miglustat	CCCCN1CC(O)C(C1C(O)O)O



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804	072956-09-3	Carvedilol	<chem>COc1ccc1OCCNC(C)(CO)c1ccc2c1c1ccc1[nH]2)O</chem>
805	073334-07-3	lopropride	<chem>COCC(=O)Nc1c(l)(c(=O)NCC(CO)O)c(c1)C(=O)N(C(CO)O)C</chem>
806	073384-59-5	Ceftriaxone	<chem>CON=C(c1csc(n1)N)(C=O)N(C1C(=O)N2C1S(C)=C2C(=O)O)CSc1nc(=O)c(=O)[nH]n1C</chem>
807	073575-52-7	2,4,3',5'-tetrachlorobiphenyl	<chem>Clc1ccc(c1)Cl)c1cc(C)cc(c1)Cl</chem>
808	073575-53-8	2,4,5,3'-tetrachlorobiphenyl	<chem>Clc1ccc(c1)c1cc(C)cc(c1)Cl</chem>
809	073575-54-9	pentachlorobiphenyl	<chem>Clc1ccc(c1c1c(C)cccc1Cl)Cl</chem>
810	073575-55-0	pentachlorobiphenyl	<chem>Clc1cc(C)lc(c1)c1c(C)cccc1Cl</chem>
811	073575-57-2	pentachlorobiphenyl	<chem>Clc1c(C)ccc(c1Cl)c1c(C)cccc1Cl</chem>
812	073963-72-1	Cilostazol	<chem>O=C1CC2c(N1)ccc(c2)OCCc1nmm1C1CCCC1</chem>
813	074011-58-8	Enoxacin	<chem>CCn1cc(C(=O)O)c(=O)c2c1nc(N1CCNC1)c(c2)F</chem>
814	074050-98-9	Ketanserin	<chem>Fc1ccc(cc1)C(=O)C1CCN(C1)CCn1c(=O)[nH]c2c1=O)cccc2</chem>
815	074103-06-3	Ketorolac	<chem>OC(=O)C1CCn2c1ccc2(C=O)c1ccc1</chem>
816	074150-27-9	Pimobendan	<chem>COc1ccc(cc1)c1nc2c([nH]1)cc(cc2)C1=NNC(=O)CC1C</chem>
817	074191-85-8	Doxazosin	<chem>COc1ccc2nc(nc2cc1OC)N1CCN(C1)C(=O)C1COc2(O)1)ccc2</chem>
818	074338-24-2	2,3,4,3'-tetrachlorobiphenyl	<chem>Clc1ccc(c1)c1ccc(c1)Cl)Cl</chem>
819	074472-34-7	2,3,5,4'-tetrachlorobiphenyl	<chem>Clc1ccc(cc1)c1cc(C)cc(c1)Cl</chem>
820	074472-37-0	pentachlorobiphenyl	<chem>Clc1ccc(cc1)c1cc(C)lc(c1)Cl)Cl</chem>
821	074472-42-7	hexachlorobiphenyl	<chem>Clc1ccc(cc1Cl)c1c(Cl)cc(c1)Cl)Cl</chem>
822	074472-44-9	hexachlorobiphenyl	<chem>Clc1cc(ccc1Cl)c1c(Cl)c(Cl)cc(c1)Cl</chem>
823	074472-50-7	heptachlorobiphenyl	<chem>Clc1cc(Cl)c(c1c1cc(Cl)c(c1)Cl)Cl)Cl</chem>
824	074472-51-8	octachlorobiphenyl	<chem>Clc1cc(Cl)cc(c1)c1c(Cl)c(Cl)c(c1)Cl)Cl</chem>
825	074472-52-9	octachlorobiphenyl	<chem>Clc1cc(Cl)c(c1)Cl)c1c(Cl)c(Cl)c(c1)Cl)Cl</chem>
826	074738-24-2	Recainam	<chem>CC(NCCNC(=O)Nc1C)c1ccc1C</chem>
827	074863-84-6	Argatroban	<chem>NC(=NCCC(C(=O)N1CCC(C(C1=O)O)C)NS(=O))=O)c1ccc2c1NCC(C2)C)N</chem>
828	075225-51-3	Lovastatin	<chem>CCC(C(=O)O)C1C(C)C=C2C1C(CCC(C(C(=O)O)O)O)C(C=C2)C</chem>
829	075330-75-5	Lovastatin	<chem>CCC(C(=O)O)C1C(C)C=C2C1C(CCC(C(C(=O)O)O)O)C(C=C2)C</chem>
830	075607-67-9	Fludarabine	<chem>OC1C(O)C(OC1nc2c1nc(F)nc2N)COP(=O)O</chem>
831	075695-93-1	Isradipine	<chem>COC(=O)C1=C(C)N(C=C1C1ccc2c1non2)C(=O)OC(C)C</chem>
832	075696-02-5	Cinolazepam	<chem>N#CCCN1C(=O)C(O)N=C(c2c1ccc(c2)Cl)c1ccc1F</chem>
833	075706-12-6	Leflunomide	<chem>O=C(c1cnoc1C)Nc1ccc(cc1)C(F)F</chem>
834	075803-36-0	Ethinylestradiol-17-Sulfate	<chem>C#CC1(CCC2C1)CCC1C2CC2c1ccc(c2)O)OS(=O)(=O)</chem>
835	075847-73-3	Enalapril	<chem>CCOC(=O)C(NC(C(=O)N1CCC1C(=O)O)C)CCc1ccc1</chem>
836	076420-72-9	Enalaprilat	<chem>OC(=O)C(NC(C(=O)N1CCC1C(=O)O)C)CCc1ccc1</chem>
837	076470-66-1	Loracarbef	<chem>NC(c1ccc1C(=O)N)C1C2CCC(=C(N2C1=O)C(=O)O)Cl</chem>
838	076547-98-3	Lisinopril	<chem>NCCCCC(C(=O)N1CCC1C(=O)O)N(C(=O)O)CCc1ccc1</chem>
839	076824-35-6	Famotidine	<chem>NC(=Nc1ccc(n1)CSCCC(=NS(=O)=O)N)N</chem>
840	076842-07-4	pentachlorobiphenyl	<chem>Clc1c(Cl)cccc1c1cc(C)lc(c1)Cl</chem>
841	077337-76-9	Acamprosate	<chem>CC(=O)NCCCS(=O)(=O)O</chem>
842	077671-31-9	Enoximone	<chem>CSc1ccc(cc1)C(=O)c1[nH]c(=O)[nH]c1C</chem>
843	078415-72-2	Milrinone	<chem>N#CC1cc(c2cnc2)c([nH]1)=O)C</chem>
844	078755-81-4	Flumazenil	<chem>CCOC(=O)c1nnc2c1CN(C)C(=O)c1c2ccc(c1)F</chem>
845	078919-13-8	Iloprost	<chem>CC#CCC(C(C=C1C1)CC2C1CC(=CCCC(=O)OCC(=O)CCCC1C2)O)C</chem>
846	079350-37-1	Cefixime	<chem>Nc1nc(cs1)C(=NOCC(=O)O)C(=O)N1C2S(C)=C(N2C1=O)C(=O)O)C=C</chem>
847	079617-96-2	Sertraline	<chem>CNC1CC(C)c2c1ccc2c1ccc(c1)Cl</chem>
848	079660-72-3	Floxacin	<chem>FCn1cc(C(=O)O)c(=O)c2c1c(F)c(N1CCN(C1)C)c(c2)F</chem>
849	079794-75-5	Loratadine	<chem>CCOC(=O)N1CCC(=C2c3ccc(cc3CCc2nccc3)Cl)CC1</chem>
850	079902-63-9	Simvastatin	<chem>CCC(C(=O)O)C1C(C)C=C2C1C(CCC1C(C(=O)O)O)C(C=C2)C)C</chem>
851	079944-58-4	Idazoxan	<chem>C1CN=C(N1)C1COc2(O)1)ccc2</chem>
852	080125-14-0	Remoxipride	<chem>CCN1CCCC1CNC(=O)Ic(O)ccc(c1O)C)Br</chem>
853	080474-14-2	Fluticasone	<chem>FCSc(=O)C1(OC(=O)CC)C(C)CC2C1(C)CC(O)C1(C2CC(C2=C(C(=O)CC=12)C)F</chem>
854	080755-51-7	Bunazosin	<chem>CCCC(=O)N1CCCN(C1)c1nc(N)c2c1n1cc(c2)OC</chem>
855	081093-37-0	Pravastatin	<chem>CCC(C(=O)O)C1C(C)C=C2C1C(CCC(C(C(=O)O)O)O)C(C=C2)C)C</chem>
856	081147-92-4	Esmolol	<chem>COC(=O)CCc1ccc(cc1)OCC(CN(C)C)O</chem>
857	081403-80-7	Alfuzosin	<chem>COc1ccc2nc(nc2cc1OC)N(C)CCNC(=O)C1CCCO1)C</chem>

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858	081409-90-7	Cabergoline	<chem>C=CCN1CC(CCC2C1Cc1[nH]c3c1c2ccc3)C(=O)N(C(=O)N)CCN(C)C</chem>
859	081447-80-5	Diprafenone	<chem>CCC(NC(C)Coc1ccc1C(=O)CC1cccc1)O)C</chem>
860	081732-65-2	Bambuterol	<chem>O=C(N(C)O)c1ccc(cc1)OC(=O)N(C)C(C)C(NC(C)C)O</chem>
861	081801-12-9	Xamoterol	<chem>OC(CO)c1ccc(cc1)O)CNCCN(C(=O)N1CCC1</chem>
862	081846-19-7	Tremostinil	<chem>CCCCC(CCC1C(O)CC2C1Cc1cccc(c1C2)O)CC(=O)O)O</chem>
863	081965-43-7	SarCNU	<chem>CC(C(=O)N)NC(=O)N(N=O)CC1</chem>
864	082009-34-5	Cilastatin	<chem>OC(=O)C(CSCCCCC=C(C(=O)O)NC(=O)C1CC1(C)C)N</chem>
865	082619-04-3	Cefpodoxime	<chem>CON=C(c1csc(n1)N)(C=O)N1C2S(C)=C(N2C1=O)C(=O)O)COC</chem>
866	082626-48-0	Zolpidem	<chem>Cc1ccc(cc1)c1nc2n(c1CC(=O)N(C)C)cc(c2)O</chem>
867	082768-85-2	Quinaprilat	<chem>CCOC(=O)C(NC(C(=O)N1C2c2cccc2C1C(=O)O)C)CCc1ccc1</chem>
868	083015-26-3	Atomoxetine	<chem>GNCCC(c1ccc1)O)c1ccc1C</chem>
869	083366-66-9	Nefazodone	<chem>CC1nn(c(=O)N1CCO)c1ccc1)CCN1CCN(C1)c1ccc(c1)Cl</chem>
870	083647-97-6	Spirapril	<chem>CCOC(=O)C(NC(C(=O)N1CC2(C1C(=O)O)S(C2)C)CCc1ccc1</chem>
871	083799-24-0	Fexofenadine	<chem>OC(=O)C(c1ccc(cc1)C(CCN1CCC(C1)C(c1ccc1)1)ccc1)O)O)C(C</chem>
872	083881-51-0	Cetirizine	<chem>OC(=O)COCCN1CCN(C1)c1ccc(cc1)Cl)c1ccc1</chem>
873	084057-84-1	Lamotrigine	<chem>Nc1nnc(c1)N1c1ccc(c1)Cl</chem>
874	084057-95-4	Ropivacaine	<chem>CCCN1CCCC1C(=O)Nc1c(C)cccc1C</chem>
875	084371-65-3	Mifepristone	<chem>C#CC1(O)CC2C1(C)CC(c1ccc(cc1)N(C)C)C1=C3CCC(=O)C=C3CC21</chem>
876	084449-90-1	Raloxifene	<chem>Oc1ccc2c(c1)sc(c2)C(=O)c1ccc(cc1)OCCN1CCCC1)c1ccc(cc1)O</chem>
877	084625-61-6	Itraconazole	<chem>CCC(n1ncn(c1=O)c1ccc(cc1)N1CCN(C1)c1ccc(cc1)OCC1COC(O1)(Cn1cncn1)c1ccc(cc1)Cl)Cl</chem>
878	085405-59-0	Hydroxydihydroquinidine,	<chem>JCC1(O)CN2CCC1CC2(c1cnc2c1cc(OC)c2)O</chem>
879	085441-61-8	Quinapril	<chem>CCOC(=O)C(NC(C(=O)N1C2c2cccc2C1C(=O)O)C)CCc1ccc1</chem>
880	085622-93-0	Temozolomide	<chem>NC(=O)C1ncn2c1nnc(c2=O)C</chem>
881	085650-52-8	Mirtazapine	<chem>CN1CN2C(C1)c1ccc1C1c2nccc1</chem>
882	085721-33-1	Ciprofloxacin	<chem>Fc1cc2c(cc1N1CCN1)nc(cc2=O)C(=O)O)C1CC1</chem>
883	086386-73-4	Fluconazole	<chem>Fc1ccc(cc1)F(C)C(N1cncn1)(Cn1cncn1)O</chem>
884	086541-75-5	Benazepril	<chem>CCOC(=O)C(NC1CC2c2(N(C1=O)CC(=O)O)ccc2)CCc1ccc1</chem>
885	087333-19-5	Ramipril	<chem>CCOC(=O)C(NC(C(=O)N1C2CCC2C1C(=O)O)C)CCc1ccc1</chem>
886	087638-04-8	Carumonam	<chem>NC(=O)OCC1C(NC(=O)C(=NOCC(=O)O)c2ccc(n2)N)(C(=O)N1S(=O)(=O)O</chem>
887	087679-37-6	Trandolapril	<chem>CCOC(=O)C(NC(C(=O)N1C2CCCC2C1C(=O)O)C)CCc1ccc1</chem>
888	087726-17-8	Panipenem	<chem>CC1(C(=O)N2C1CC(=C2C(=O)O)S1C1CN(C1)C(=N)O)O</chem>
889	087810-56-8	Fostriecin	<chem>OC=CC=CC=CC(C(C=C1CC=CC(=O)O)1)O)COP(=O)(O)O)O</chem>
890	088150-42-9	Amlodipine	<chem>NCCOC1=C(C(=O)O)C(C)C(=O)N1C)C(=O)O)c1ccc1Cl</chem>
891	088669-09-9	Trospectomycin	<chem>CCCCC1O2O3C(O)C(NC)C(C1C3OC2(C(=O)O)O)NCO</chem>
892	089194-77-4	Bisaramil	<chem>CCN1CC2CN(C(C1)C2O)C(=O)c1ccc(cc1)Cl</chem>
893	089365-50-4	Salmeterol	<chem>OC1ccc(cc1)O)C(CNCCCCOCCOCCc1ccc1)O</chem>
894	089565-68-4	Tropisetron	<chem>CN1C2CCC1C(C2)O)C(=O)c1[nH]c2c1ccc2</chem>
895	089778-26-7	Toremifene	<chem>ClCCC(=C(c1ccc1)c1ccc(cc1)O)CCN(C)C1ccc1</chem>
896	090357-06-5	Bicalutamide	<chem>N#CC1ccc(cc1(F)F)N(C(=O)O)C(S(=O)(=O)c1ccc(cc1)F)O)C</chem>
897	090402-40-7	Abanoquil	<chem>COc1ccc2CCN(Cc2cc1OC)c1ccc(N)c2c1)cc(c2)OC)OC</chem>
898	091161-71-6	Terbinafine	<chem>CN(Cc1ccc2c1ccc2)CC=C#CC(C)C</chem>
899	091374-21-9	Ropinirole	<chem>CCN(C)CC(C)ccc2c1CC(=O)N2</chem>
900	091421-43-9	Aminocamptothecin,	<chem>CCC1(O)C(=O)OCC2c1cc1c3nc4cccc(c4c3Cn1c2=O)N</chem>
901	091714-94-2	Bromfenac	<chem>OC(=O)C1ccc(c1N)C(=O)c1ccc(cc1)Br</chem>
902	091832-40-5	Cefdinir	<chem>ON=C(c1csc(n1)N)C(=O)N1C(=O)N2C1S(C)=C2C(=O)O)C=C</chem>
903	092623-85-3	Milnacipran	<chem>NCC1CC1(c1ccc1)C(=O)N(C)CC</chem>
904	092665-29-7	Cefprozil	<chem>CC=C1=C(C(=O)O)N2C(SC1)C(C2=O)NC(=O)C(c1ccc(cc1)O)N</chem>
905	093390-81-9	Fosphenytoin	<chem>O=C1N(COP(=O)(O)O)C(=O)N(C1c1ccc1)1ccc1</chem>
906	093413-69-5	Venlafaxine	<chem>CCc1ccc(cc1)C(C1(O)CCCC1)CN(C)C</chem>
907	093479-97-1	Glimepiride	<chem>COC1=C(C)N(C1=O)C(=O)NCCc1ccc(cc1)S(=O)(=O)N(C(=O)N1CCC(C1)C</chem>
908	093957-54-1	Fluvastatin	<chem>OC(=O)CC(C(C=Cc1c2ccc(cc2)F)c2c1n(C)C)ccc2)O)O</chem>
909	094079-80-8	Cicaprost	<chem>CCCHCC(C)C(C#CC1C(O)CC2C1CC(=CCOCC(=O)O)C2)O</chem>
910	095153-31-4	Perindoprilat	<chem>CCCC(C(=O)O)N(C(=O)N1C2CCCC2CC1C(=O)O)C</chem>
911	095399-71-6	Fosinoprilat	<chem>OC(=O)C1CC(N1(=O)CP(=O)(CCCc1ccc1)O)C1CCCC1</chem>
912	Sch34343	Sch34343	<chem>CC(C1C2S(C=C(N2C1=O)C(=O)O)S(CO)C(=O)N)O</chem>
913	096036-03-2	Meropenem	<chem>CC(C1C(=O)N2C1C(C)C=C2C(=O)O)S1C1CC(N1)C(=O)N(C)C)O</chem>
914	096829-58-2	Olistat	<chem>CCCCCCCCCC(C(C1OC(=O)C1CCCCO)OC(=O)C(C)C)CNC=O</chem>
915	097240-79-4	Topiramate	<chem>NS(=O)(=O)CC12OC3C(C2O)C(O1)C)OC(O3)C)C</chem>
916	097322-87-7	Troglitazone	<chem>O=C1NC(=O)C(S1)C1ccc(cc1)OCC1(C)CC2c(O1)C)C(c2C)O)C</chem>
917	097682-44-5	Irinotecan	<chem>CCC1(O)C(=O)OCC2c1cc1c3nc4cccc(c4c3Cn1c2=O)CC)OC(=O)N1CCCC(C1)N1CCCC1</chem>
918	098048-97-6	Fosinopril	<chem>CCC(=O)OC(C)COP(=O)(C)C(=O)N1C(C)C(C1=O)O)C1CCCC1)CCCC1ccc1</chem>
919	098079-51-7	Lomefloxacin	<chem>CN1ccc(C(=O)O)c(=O)c2c1c(F)c(N1CCN(C1)C)c(c2)F</chem>
920	098319-26-7	Finasteride	<chem>O=C1=C(C2(N1)CC1C2CCC2)C1CCC2(C(=O)N(C)C)C)C</chem>
921	099011-02-6	Imiquimod	<chem>CC(Cn1cnc2c1ccc1nc2)N</chem>

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922	099614-02-5	Ondansetron	O=C1C(CCC2c1c1cccc1n2C)Cn1ccc1C
923	100643-71-8	Desloratadine	Clc1ccc2c(e1)CCc1c(C2=C2CCNCC2)ncccc1
924	100986-85-4	Levofloxacin	CN1CCN(CC1)c1c(F)c2c3c1OCC(n3cc(e2=O)C(=O)O)C
925	101526-83-4	Semaltidie	CCN(CCN(C=O)c1ccc(cc1)NS(=O)=O)C)CC
926	101828-21-1	Butenafine	CN(Cc1cccc2c1cccc2)Cc1ccc(cc1)C(C)C
927	102767-28-2	Levetiracetam	CCC(N1CCCC1=O)C(=O)N
928	103577-45-3	Lansoprazole	O=S(c1nc2c([nH]1)cccc2)Cc1nccc(c1C)OCC(F)F
929	103628-46-2	Sumatriptan	CNS(=O)(=O)C1ccc2c(c1)C(CCN(C)C)c[nH]2
930	103775-10-6	Moexipril	CCOC(=O)C(NC(C=O)N)N1C2c2cc(OC)c(c2CC1C(=O)O)C)C)CCc1cccc1
931	104227-87-4	Famciclovir	CC(=O)OCC(CCN1cnc2c1nc(N)nc2)CO(C=O)C
932	104632-26-0	Prampixole	CCNC1CCc2c(C1)sc[n]2N
933	105102-22-5	Mometasone	C1C(=O)C1(O)C(C)CC2C1(C)C(O)C1(C2CCC2=CC(=O)C=CC12)C1
934	105816-04-4	Nateginidie	CC(C1CCC(CC1)C(=O)N)C(=O)C1ccc1c
935	105956-97-6	Cinafloxacin	NC1CCN(C1)c1c(F)cc2c(e1C1)n(cc(e2=O)C(=O)O)C1CC1
936	106133-20-4	Tamsulosin	CCOC1cccc1OCCN(Cc1ccc(c(c1)S(=O)=O)N)O)C
937	106266-06-2	Risperidone	Fc1ccc2c(e1)onc2C1CCN(C1)CCc1c(C)nc2n(c1=O)CCCC2
938	106516-24-9	Sirtindole	Clc1ccc2c(e1)c(en2c1ccc(cc1)F)C1CCN(CCN1CCNC1=O
939	106650-56-0	Sibutramine	CC(C(C1(CCC1)c1ccc(cc1)N)C)C)C
940	106941-25-7	Adefovir	Nc1nnc2c1nnc2CCOP(=O)O
941	107133-36-8	Perindopril	CCCC(C(=O)O)CCN(C(=O)N)C2CCCC2CC1C(=O)O)C
942	107233-08-9	Cevimeline	CC1SCC2(O1)CN1CCC2C1
943	107724-20-9	Eplerenone	CO(C=O)C1CC2=CC(=O)CCC2(C23C1C1CCC4(C1)C(C)C3O2)CCC(=O)O)4C
944	107753-78-6	Zafirlukast	COc1ccc(ccc1C)en(c2c1ccc(cc2)N)C(=O)O)C1CCCC1C(=O)NS(=O)=O)C1cccc1C
945	107868-30-4	Exemestane	O=C1C=CC2(C=C1)C(=O)C1C2CCC2(C1CCC2=O)C
946	108319-06-8	Temafloxacin	CC1NCCN(C1)c1ccc2n(cc(c1=O)c2cc1F)C(=O)O)c1ccc1F
947	109889-09-0	Garnisetrone	CN1C2CCC1CC(C)CC(NC(=O)c1nnc2c1ccc2)C
948	110871-86-8	Sparifloxacin	C1N(C)C(C)N(C1)c1c(F)c(N)C2c(c1F)n(cc(c2=O)C(=O)O)C1CC1
949	111025-46-8	Progiltazone	Cc1ccc(cc1)CCOC1ccc(cc1)CC15C(=O)NC1=O
950	111406-87-2	Zileuton	ON(C1c1cc2c(s1)cccc2)C(=O)N
951	111974-69-7	Quetiapine	OCOCOCN1CCN(CC1)C1=Nc2cccc2Sc2c1cccc2
952	112809-51-5	Letrozole	N#CC1ccc(cc1)C(n1cncn1)c1ccc(cc1)C#N
953	112811-59-3	Garifloxacin	COc1c(N2CCN(C2)O)C(F)c2c1n(cc(c2=O)C(=O)O)C1CC1
954	112953-11-4	Hydroxystaurosporine,	CNC1C2O(C1C(O)C)N1c3cccc3c3c1n2c2cccc2c1c1c3(C(NC1=O)O
955	113665-84-2	Clodiprogrel	CO(C=O)C1c1cccc1C)N1CC2c(C1)ccc2
956	113806-05-6	Olopatadine	CN(CCC=C1c2cc(ccc2O)C2c1cccc2)CC(=O)O)C
957	113852-37-2	Cidofovir	OCC(Cn1ccc(nc1=O)N)OCP(=O)(O)O
958	114899-77-3	Trabectedin	COc1ccc2c(c1)O)CCN(C1C2C2c3c(OC(=O)C)C)4c(e3C)COC1(O)N1C2C2N(C(C1O)C1c2c(O)c(c1c1)C)OC)C)OC)4
959	115103-54-3	Tiagabine	OC(=O)C1CCN(C1)CCC=C(c1sc1cc1)C1ccc1C
960	115256-11-6	Dofetilidie	CN(CCC1ccc(cc1)NS(=O)=O)C)CCOC1ccc(cc1)NS(=O)=O)C
961	115956-12-2	Dolasetron	O=C1CN2C3CC1CC2CC(C3)OC(=O)c1[nH]2c1cccc2
962	116644-53-2	Mibefradil	COCC(=O)O)C1(CCN(CCCc2nc3c([nH]2)cccc3)C)CC2c(C1C(C)C)ccc(c2)F
963	117467-28-4	Cefiditron	CON=C(c1csc(n1)N)C(=O)N)C1C(=O)N2C1S(C=C2C(=O)O)C(O)C(C)C)C=Cc1scnc1C
964	117976-89-3	Rabeprazole	COCCOC1cnc(c1C)CS(=O)c1nc2c([nH]1)cccc2
965	118292-40-3	Tazarotene	CCOC(=O)c1ccc(nc1)C#Cc1ccc2c(c1)C(C)C)CCS2
966	118457-14-0	Nebivolol	OC(C1CCc2c(O1)ccc(c2)F)CNCC(C1CCc2c(O1)ccc(c2)F)O
967	119169-78-7	Epristeridie	OC(=O)C1=CC2=CCC3C(C2CC1)C)CCC1(C3CCC1C(=O)N)C(C)C)C
968	119817-90-2	Dexlorglumidie	CCCCCN(C(=O)C(NC(=O)c1ccc(c1)C)C)CC(C=O)O)CCCC
969	119914-60-2	Grepafloxacin	CC1NCCN(C1)c1ccc2c(c1F)C(=O)c(en2C1CC1)C(=O)O
970	120014-06-4	Domepizil	COc1ccc2c(c1)O)C(C(=O)C)C1CCN(C1)Cc1ccc1C
971	120054-86-6	Donepigulidipine	CCCN1C(=C(C(=O)O)N2CCC(C2)(c2cccc2)c2cccc2)C(C=C1C)C(=O)O)C1cccc1N(=O)=O)C
972	120443-16-5	Verlucast	OC(=O)C)C)C1ccc(c1)C=Cc1ccc2c(n1)cc(c2)C)S)CCCC(=O)N)C
973	120511-73-1	Anastrozole	N#CC1c1cc(cc1)C(C#N)C(C)Cn1nnc1(C)C
974	120924-80-3	Genaconazole	Fc1ccc(c1)F)C(C(=O)O)C(C)C)C1(Cn1cncn1)O
975	121032-29-9	Nelarabine	OCC1OC(C(C1O)O)n1cnc2c1nc(N)nc2O
976	121679-13-8	Naratriptan	CNS(=O)(=O)CCc1ccc2c(e1)c([nH]2)c1CCN(C1)C
977	122320-73-8	Rosiglitazone	O=C1NC(=O)C(S1)C1ccc(cc1)OCCN(c1cccc1)C
978	122647-31-4	Ibutilidie	CCCCCCN(CCC(C1c1ccc(cc1)NS(=O)=O)C)O)CC
979	123318-82-1	Clofarabine	OCC1OC(C(C1O)F)n1cnc2c1nc(C1)nc2N
980	123441-03-2	Rivastigmine	CCN(C(=O)O)c1ccc(c1)C(N)C)C)C
981	123948-87-8	Topotecan	CCC1(O)C(=O)O)C2c1ccc1c3nc4ccc(c1c4cc3Cn1c2=O)CN(C)C)O
982	124937-51-5	Tolterodine	Cc1ccc(c1)C1c1cccc1)CCN(C(C)C)C(C)O
983	125974-72-3	Intoplicine	CN(CCCN1nccc(c2c1c1([nH]2)ccc2c1ccc(c2)O)C
984	127779-20-8	Saquinavir	NC(=O)CC(C(=O)N)C(C)C(CN1CC2CCCC2CC1C(=O)N)C(C)C)O)C1cccc1N(=O)c1ccc2c(n1)cccc2
985	128470-16-6	Arbutamine	Oc1ccc(cc1)CCCCNCC(c1ccc(c1)O)O

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986	129453-61-8	Fulvestrant	O=S(CCCC(C(F)F)F)F)CCCCCCCCC1Cc2cc(O)ccc2C2C1C1CCC(C1(C2)C)O
987	129618-40-2	Nevirapine	Cc1cnc2c1[nH]c(e1O)c1c(n2C2C2)ncccc1
988	129722-12-9	Aripiprazole	O=C1CC2c(N1)ccc(cc2)OCCCN1CCN(CC1)c1cccc(c1)C)Cl
989	130209-82-4	Latanoprost	OC(Cc1cccc1)CCC(C1O)C(C)C1CC=CCCC(C)O)C(C)O
990	130929-57-6	Entacapone	CCN(C(=O)C=Cc1cc(O)c(c1)N(=O)=O)O)C#N)CC
991	131918-61-1	Paricalcitol	OC1CC(O)CC(=CC=C2CCCC3(C2CC3C(C=C)C(C)C)C)C1
992	132539-61-1	Olanzapine	CN1CCN(CC1)C1=c2cc(sc2=Nc2C(N1)cccc2
993	132875-61-7	Remifentaniil	CO(C=O)C1(CCN(C1)CCC(=O)O)CN(c1cccc1)C(=O)CC
994	133040-61-4	Eprosartan	CCCC1ncc(n1C1ccc(cc1)C(=O)O)C=C(C(=O)O)C1cccc1
995	133099-04-4	Darifenacin	NC(=O)C(c1cccc1)c1cccc1C1CCN(C1)CCc1ccc2c1)C)CCO2
996	133163-28-7	Midodrine	COc1ccc(cc1)C(CN(=O)O)C
997	134234-12-1	Traxoprodil	Oc1ccc(cc1)C(C)N1CCC(C)C1)O)c1cccc1)C)O
998	134308-13-7	Tolcapone	Cc1ccc(cc1)C(=O)c1cc(O)c(c1)N(=O)=O)O
999	134523-00-5	Atorvastatin	OC(C(C(=O)O)O)CCn1c(C)C)C)C(c1c1cccc(cc1)F)c1cccc1)C(=O)Nc1cccc1
1000	134678-17-4	Lamivudine	Nc1ccn(c=O)n1C1CSC(O)1O
1001	135062-02-1	Repaglinidie	CC1ccc(ccc1C(=O)O)CC(=O)N(Cc1cccc1N1CCCC1)CC(C)C
1002	135729-61-2	Palonosetron	O=C1N(C2C2c1cccc3CCC2)C1CN2C2CC1CC2
1003	136434-34-9	Duloxetine	CNCCC(c1cccc1)O)c1ccc2c1ccc2
1004	136470-78-5	Abacavir	OCC1C=CC(C1)n1nc2c1nc(N)nc2N1CC1
1005	136790-76-6	Lubiprostone	CCCC(C1(O)CCC2(O1)CC(=O)C2CCCCC(=O)O)F)F
1006	136817-59-9	Delavirdine	CC(Nc1cccc1N1CCN(CC1)C(=O)c1cc2c([nH]1)ccc(c2)NS(=O)=O)C)C
1007	137234-62-9	Voriconazole	Fc1ccc(c1)F)C(C1nncn1F)C(C)N1cncn1O
1008	137862-53-4	Pravastatin	CCCC(=O)N(C)C(C(=O)O)C(C)C)C1ccc(cc1)c1cccc1c1n[nH]n1
1009	139110-80-8	Zanamivir	OC(C(C1OC=CC1N(C=O)O)N=C(N)N)C(=O)O)O
1010	139264-17-8	Zolmitriptan	CN(C(Cc1[nH]c2c1ccc(C1COC(=O)N1)c2)C
1011	139481-59-7	Candesartan	CCOC1nc2c(n1C1ccc(cc1)c1cccc1n[nH]n1)(ccc2)C(=O)O
1012	139755-83-2	Sildenafil	CC1nnc1c2c1[nH]c(nc2=O)c1ccc(cc1O)C(S(=O)=O)N1CCN(CC1)C)C
1013	141505-33-1	Levosimendan	N#CC(=NNc1ccc(cc1)C1=NNC(=O)CC1)C#N
1014	142340-99-6	Adefovir	O=C(C(C)C)OCOP(=O)(OCOC(=O)C(C)C)COCCn1cnc2c1ncc2N
1015	142373-60-2	Tirofiban	CCCCS(=O)=O)N(C(=O)O)C1ccc(cc1)O)CCCC1CCN(C1
1016	142387-99-3	Ranolazine	COc1cccc1OCC(C1CCN(C1)C)C(=O)Nc1c1C)cccc1C)O
1017	143322-58-1	Eletriptan	CN1CCCC1C1c1[nH]c2c1ccc(cc2)CCS(=O)=O)O)c1cccc1
1018	143443-90-7	Ifetroban	CCCCNC(=O)c1ccc(n1)C1C2CCC(C1C1cccc1CC(=O)O)O2
1019	143491-57-0	Emitricabine	Nc1nc(=O)n(cc1F)C1CSC(O)1O
1020	144034-80-0	Rizatriptan	CN(Cc1[nH]c2c1ccc(cc2)Cn1cncn1)C
1021	144412-49-7	Lamifiban	OC(=O)COC1CCN(CC1)C(=O)C(NC(=O)c1ccc(cc1)C(=N)N)C1ccc(cc1)O
1022	145987-75-4	Paliperidone	Fc1ccc2c(c1)onc2C1CCN(CC1)CCc1c(C)nc2n(c1=O)CCCC2O
1023	144701-48-4	Telmisartan	CCc1nc2c(n1Cc1ccc(cc1)c1cccc1C(=O)O)cc(c2)C1nc2c(n1)cccc2
1024	144980-29-0	Repinotan	O=C1c2cccc2S(=O)=O)N1CCCCNCC1CCc2c(O1)cccc2
1025	145108-58-3	Dexmedetomidine	Cc1cccc(c1C)C1cnc(nH)1C
1026	145158-71-0	Tegaserod	CCCCNC(=N)N=Cc1c[nH]c2c1ccc(O)cc2
1027	145599-86-6	Cerivastatin	COCC1c(c2ccc(cc2)F)C=C(C)C(C(=O)O)O)C(nc1C(C)C)C)C
1028	145918-75-8	Troxacetabine	Nc1cnc(c=O)n1C1COC(O)1O
1029	146426-40-6	Flavopiridol	CN1CCC(C1)O)c1c(O)cc(c2c1oc(cc2=O)c1cccc1C)O
1030	146939-27-7	Ziprasidonie	O=C1Nc2c(C1)cc(c2)C)CCN1CCN(CC1)c1nsc2c1cccc2
1031	147059-72-1	Trovafoxacin	NC1C2C1CN(C2)c1nc2c(cc1F)C(=O)c(en2c1ccc(cc1)F)C(=O)O
1032	147127-20-6	Tenofovir	CC(Cn1cnc2c1nnc2N)O)CP(=O)(O)O
1033	147536-97-8	Bosentan	OCOC1nc(nc1O)c1cccc1O)NS(=O)=O)c1ccc(cc1)C(C)C)C1ncccc1
1034	148553-50-8	Pregabalin	NC(C(=O)O)C(C)C
1035	148717-90-2	Squalamine	NCCCCNCCN1CCC2(C1)C(C)C(C1C2CCC2(C1CCC2(C)C)C)O(S(=O)=O)O)C)O)C
1036	149647-78-9	Vorinostat	ONC(=O)CCCCC(=O)Nc1cccc1
1037	149908-53-2	Azimilidie	CN1CCN(CC1)CCCCN1C(=O)CN(C1=O)N=Cc1ccc(O)1cccc1
1038	150378-17-9	Indinavir	OC(CN1CCN(CC1C(=O)N)C(C)C)C)C1c1cccc1)C(C(=O)N)C1(C)O)C2c1cccc2)Cc1cccc1
1039	151096-09-2	Moxifloxacin	COc1c(N2CC3C(C2)CCN3)c(F)cc2c1nc(cc2=O)C(=O)C1CC1
1040	151276-95-8	KRN-5500	CCCCCCCCC=Cc(=O)NCC(=O)N)C1C(C)O)Nc1nnc2c1[nH]n2)C(C)O
1041	151319-34-5	Zaleplon	CCN(c1cccc(c1)c1cnc2n1ncc2#N)C(=O)C
1042	152459-95-5	Imatinib	CN1CCN(C1)C1ccc(cc1)C(=O)Nc1ccc(cc1)N1c1cccc1)C
1043	153259-65-5	Gilomilast	N#CC1(CCC(C1)C(=O)O)c1ccc(cc1)O)CCCC1OC
1044	153559-49-0	Bexarotene	Cc1cc2c(cc1C(=O)c1ccc(cc1)C(=O)O)C(C)C)CCC2(C)C
1045	153832-46-3	Ertapenem	O=C(C1NCC(C1)S)C1=C(C(=O)O)N2C1(C)C(C2=O)C(O)C)Nc1cccc1C(=O)O
1046	154323-57-6	Almotriptan	CN(Cc1c[nH]c2c1ccc(cc2)CS(=O)=O)N1CCCC1C
1047	154361-50-9	Capecitabine	CCCCOC(=O)Nc1nc(=O)n(cc1F)C1OC(C1)O)C
1048	154397-77-0	Napsagatran	O=C(C)C(=O)N(C1CC1)CC(=O)NS(=O)=O)c1ccc2c(c1)cccc2NCC1CCN(C1)C(=N)N
1049	154598-52-4	Efavirenz	FC(C1(C#CC2CC2)OC(=O)Nc2c1cc(C1)cc2)F)F

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1050	155206-00-1	Bimatoprost	<chem>CN(C=O)CCCC=CC1C(O)CC(C1C=CC(C1cccc1)O)</chem>
1051	155213-67-5	Ritonavir	<chem>O=C(NC(C)CC(Cc1cccc1)NC(=O)C(C)C)NC(=O)N(C1cscn1)(C(C)C)O)C1cccc1)OCc1cncs1</chem>
1052	156053-89-3	Alvimopan	<chem>OC(=O)NC(C=O)C(Cc1cccc1)CN1CCC(C(C)C)C(C)c1cccc(c1)O</chem>
1053	156090-18-5	Topixantrone	<chem>OCNCn1nc2c31ccc(c3c(=O)c12enc1)NCCN(C)C</chem>
1054	157283-68-6	Travoprost	<chem>CC(OC(=O)CCCC=CCC1C(O)CC(C1C=CC(CO)c1cccc(c1)C(F)(F)O)O)C</chem>
1055	158681-13-1	Rimonabant	<chem>C1c1ccc(cc1)c1c(C)cn1c1ccc(cc1C)C(=O)NN1CCCCC1</chem>
1056	158747-02-5	Frovatriptan	<chem>CNC1Cc2c(Cc1)[nH]c1c2cc(cc1)C(=O)N</chem>
1057	158966-92-8	Montelukast	<chem>OC(=O)C1(C)C(Cc2cccc(c2)C=Cc2ccc3c(n)cc(cc3)C)CCc2cccc2C(O)(C)CC1</chem>
1058	159776-70-2	Melagatran	<chem>OC(=O)CNC(C(=O)N1CCC1C(=O)NCc1cccc(c1)C(=N)N)C1CCCCC1</chem>
1059	159989-64-7	Nelfinavir	<chem>OC(C(NC(=O)c1cccc(c1C)O)CSc1cccc1)CN1CC2CCCC2CC1C(=O)NC(C)(C)C</chem>
1060	161814-49-9	Amprenavir	<chem>CC(CN(S(=O)=O)c1ccc(cc1)N)CC(C(Cc1cccc1)NC(=O)OC1CCOC1)O)C</chem>
1061	162011-90-7	Rofecoxib	<chem>O=C1OCC(=C1c1cccc1)c1ccc(cc1)S(=O)(=O)C</chem>
1062	163222-33-1	Ezetimibe	<chem>Oc1cccc(c1)C1C(CCC(c2ccc(cc2)F)O)C(=O)N1c1ccc(cc1)F</chem>
1063	164656-23-9	Dutasteride	<chem>O=C1C=CC2(C(N)1)CCC1C2CCC2(C1CCC2C(=O)Nc1ccc(ccc1C(F)(F)F)C(F)(F)F)C)C</chem>
1064	165800-03-3	Linezolid	<chem>CC(=O)NCC1OC(=O)N(C1)c1ccc(c(c1)F)N1CCCCC1</chem>
1065	167221-71-8	Clevidipine	<chem>CCCC(=O)OCC(=O)C1=C(C)NC(=C(C1c1cccc(c1)C)C)C(=O)OC)C</chem>
1066	169590-42-5	Celecoxib	<chem>Cc1ccc(cc1)c1ccc(cc1)nc1ccc(cc1)S(=O)(=O)N(C)C(F)F</chem>
1067	171228-49-2	Posaconazole	<chem>CC(C1n1cn(c1=O)c1ccc(cc1)N1CCN(C1)c1cccc(c1)OC1COC(C1)(Cn1cncn1)c1ccc(cc1F)C(O)C</chem>
1068	171596-29-5	Tadalafil	<chem>O=C1N(C)CC(=O)N2C1c1c1c2c2ccc3c(c2)OC(O3)[nH]c21cccc2</chem>
1069	173334-57-1	Aliskiren	<chem>COCCCC1cc(c1c1O)CC(C(C)C)C(C(C)C(=O)NCC(C(=O)N)(C)C(C)O)N</chem>
1070	175463-14-6	Gemifloxacin	<chem>NCC1CN(C1=NOC)C1nc2c(cc1F)c(=O)nc2c1CC1C(=O)O</chem>
1071	176644-21-6	Eniporida	<chem>NC(=N(C=O)c1ccc(cc1)N1cccc1)S(=O)(=O)C)N</chem>
1072	179324-69-7	Bortezomib	<chem>CC(C(B(O)N)C(=O)C(NC(=O)c1cncnc1)C1cccc1)C</chem>
1073	180384-57-0	Tezosentan	<chem>OCOC1nc(nc1O)c1cccc1OC)NS(=O)(=O)c1ccc(cc1)C(C)C)C1ccnc(c1)1nn[nH]n1</chem>
1074	181695-72-7	Valdecoxib	<chem>Cc1onc(c1c1ccc(cc1)S(=O)(=O)N)c1cccc1</chem>
1075	183321-74-6	Erlotinib	<chem>COCCOC1cc2c(ncnc2c1OCCOC)Nc1cccc(c1)C#C</chem>
1076	184475-35-2	Gefitinib	<chem>COc1cc2nnc(c2cc1OCCCN1CCOCC1)Nc1ccc(c(c1)Cl)F</chem>
1077	187227-45-8	Oseltamivir	<chem>CCOC(=O)C1=CC(C(C1)N)NC(=O)C)OC(CC)CC</chem>
1078	187523-35-9	Maxipost	<chem>COc1ccc(cc1C(F)C(=O)Nc2c1ccc(cc2)C(F)(F)F)Cl</chem>
		2,2',4,4',6-	
1079	189084-64-8	Pentabromodiphenyl	<chem>BrC1cc(Br)c(c(c1)Br)Oc1cc(Br)cc(c1)Br</chem>
1080	191732-72-6	Lenalidomide	<chem>O=C1CCC(C(=O)N)N1Cc2c(C1=O)cccc2N</chem>
1081	192939-46-1	Ximelagatran	<chem>CCOC(=O)CNC(C(=O)N1CCC1C(=O)NCc1cccc(c1)C(=N)N)C1CCCCC1</chem>
1082	194798-83-9	Fosfluconazole	<chem>Fc1ccc(c(c1)F)OP(=O)(O)O)(Cn1cncn1)Cn1cncn1</chem>
1083	196597-26-9	Ramelteon	<chem>CCC(=O)NCCC1CCc2c1c1CCOC1cc2</chem>
1084	198904-31-3	Atazanavir	<chem>CO(C=O)NC(C(C)C)C(=O)NN(Cc1ccc(cc1)c1cccc1)CC(C(Cc1cccc1)NC(=O)C(C)C)NC(=O)OC)O</chem>
1085	202409-33-4	Etoricoxib	<chem>C1c1cnc(c1)c1ccc(cc1)S(=O)(=O)C)c1ccc(nc1)C</chem>
1086	204697-65-4	Olcegepant	<chem>NCCCC(C(=O)N1CCN(C1)c1ccncc1)NC(=O)C(NC(=O)N1CCCC(C1)N1Cc2cccc2NC1=O)Cc1cc(Br)c(c(c1)Br)O</chem>
		2,2',4,4',5,6'-	
1087	207122-15-4	Hexabromodiphenyl	<chem>BrC1cc(Br)c(c(c1)Br)Oc1cc(Br)cc(c1)Br</chem>
		2,2',3,4,4',5',6-	
1088	207122-16-5	heptabromodiphenyl	<chem>BrC1cc(Br)c(cc1O)c1c(Br)cc(c(c1)Br)Br</chem>
1089	210101-16-9	Conivaptan	<chem>Cc1[nH]c2c(n1)c1cccc1N(CC2)C(=O)c1ccc(cc1)NC(=O)c1cccc1c1cccc1</chem>
1090	210245-80-0	Zonampanel	<chem>OC(=O)Cn1c2cc(n3cnc3)c(cc2[nH]c(=O)c1=O)N(=O)=O</chem>
1091	219989-84-1	Ixabepilone	<chem>O=C1N(C)CC2O(C)CCC(C(C)C(=O)C(C1)O)(C)C)O)C)C(=Cc1csc(n1)C)C</chem>
1092	220991-20-8	Lumiracoxib	<chem>OC(=O)Cc1ccc(C)ccc1Nc1c1F)cccc1Cl</chem>
1093	222400-20-6	Tomopenem	<chem>O=C(N1CCN(C1)C(=O)C1CC(CN1C)S1=C(C(=O)O)N2C(C1C)C(C2=O)C(O)CN=C(N)N</chem>
1094	224785-90-4	Vardenafil	<chem>CCOC1ccc(cc1c1nc(=O)c2n([nH]1)c(CCC)nc2C)S(=O)(=O)N1CCN(C1)CC</chem>
1095	226256-56-0	Cinacalcet	<chem>CC(c1cccc2c1cccc2)NCCc1cccc(c1)C(F)F</chem>
1096	249296-44-4	Varenicline	<chem>N1CC2CC(C1)c1c2cc2c(c1)ncn2</chem>
1097	251565-85-2	Tesaglitazar	<chem>CCOC(C(=O)O)Cc1ccc(cc1)OCCc1ccc(cc1)O5(=O)=O)C</chem>
1098	276680-63-8	Exatecan	<chem>CCC1(O)C(=O)OCc2c1ccc1c3nc4cc(F)c(c5c4c(c3Cn1c2=O)C(N)CC5)C</chem>
1099	284461-73-0	Sorafenib	<chem>CNC(=O)c1ncccc(c1)Oc1ccc(cc1)NC(=O)Nc1ccc(c(c1)C(F)(F)F)Cl</chem>
1100	287714-41-4	Rosuvastatin	<chem>OC(C(C(C(=O)O)O)C=Cc1c(nc1c1ccc(cc1)F)N(S(=O)(=O)C)C(C)C</chem>
1101	302962-49-8	Dasatinib	<chem>OCNC1CCN(C1)c1ccc(cc1)C)Nc1ncc(s1)C(=O)Nc1c(c)cccc1Cl</chem>
1102	376348-65-1	Maraviroc	<chem>O=C(C1CCC(C1)(F)F)NC(c1cccc1)CN1C2CCC1CC(C2)n1c(C)nn1C(C)C</chem>
1103	486460-32-6	Sitagliptin	<chem>NC(Cc1cc(F)cc1F)CC(=O)N1Cn2c(C1)nn2C(F)F</chem>
1104	557795-19-4	Sunitinib	<chem>CN(CCN(C=O)c1c(C)[nH]c(c1)C)C=C1C(=O)Nc2c1cc(F)cc2)CC</chem>
1105	608137-32-2	Lisdexamfetamine	<chem>NCCCC(C(=O)N)NC(C1cccc1)C)N</chem>

Table S2: Model predictions, residuals and hat values calculated for human biotransformation datasets

(Training set chemicals are in bold, prediction set chemicals are underlined; chemicals in *italic* have not experimental data)

ID	LogHL <sub>1</sub>			LogHL <sub>21</sub>			LogHL <sub>41</sub>			LogHL <sub>61</sub>			LogHL <sub>81</sub>		
	Pred. (h)	Res	HAT (h) (n <sup>*</sup> =0.0489)	Pred. (h)	Res	HAT (h) (n <sup>*</sup> =0.0535)	Pred. (h)	Res	HAT (h) (n <sup>*</sup> =0.0578)	Pred. (h)	Res	HAT (h) (n <sup>*</sup> =0.0574)	Pred. (h)	Res	HAT (h) (n <sup>*</sup> =0.0574)
1	2.72	-2.00	<u>0.0706</u>	3.57	-1.23	<u>0.1305</u>	3.21	-1.59	<u>0.0776</u>	3.80	-1.00	<u>0.1161</u>	3.83	-0.96	<u>0.0976</u>
2	0.11	1.19	<u>0.0241</u>	-1.89	-0.81	<u>0.5271</u>	-1.37	-0.28	<u>0.3947</u>	-0.81	0.27	<u>0.1388</u>	-1.49	-0.41	<u>0.4169</u>
3	0.48	-1.51	<u>0.0066</u>	0.59	-1.52	<u>0.0104</u>	0.52	-1.60	<u>0.0083</u>	0.53	-1.59	<u>0.0174</u>	0.56	-1.56	<u>0.0105</u>
4	0.52	-0.32	<u>0.0079</u>	0.64	-0.25	<u>0.0168</u>	0.61	-0.27	<u>0.008</u>	0.39	-0.53	<u>0.0205</u>	0.55	-0.37	<u>0.0111</u>
5	1.22	-0.30	<u>0.0189</u>	0.96	-0.57	<u>0.0211</u>	1.53	0.00	<u>0.0494</u>	1.11	-0.42	<u>0.0201</u>	1.28	-0.25	<u>0.033</u>
6	0.96	0.06	<u>0.0271</u>	1.14	0.20	<u>0.0332</u>	1.23	0.29	<u>0.0151</u>	1.00	0.06	<u>0.0356</u>	1.30	0.36	<u>0.017</u>
7	0.77	0.57	<u>0.0095</u>	0.74	0.52	<u>0.0092</u>	0.84	0.62	<u>0.0103</u>	0.75	0.54	<u>0.0199</u>	0.57	0.37	<u>0.0089</u>
8	0.78	0.25	<u>0.0093</u>	0.81	0.17	<u>0.028</u>	0.83	0.20	<u>0.0109</u>	0.77	0.13	<u>0.0195</u>	0.57	-0.06	<u>0.0088</u>
9	0.81	0.58	<u>0.0054</u>	1.08	0.85	<u>0.0072</u>	1.06	0.83	<u>0.0112</u>	0.70	0.47	<u>0.0093</u>	0.96	0.73	<u>0.0213</u>
10	3.68	-0.60	<u>0.0141</u>	3.45	-0.92	<u>0.0292</u>	3.36	-1.01	<u>0.019</u>	3.25	-1.11	<u>0.0259</u>	3.36	-1.01	<u>0.0142</u>
11	0.60	-0.07	<u>0.0091</u>	0.52	-0.51	<u>0.0057</u>	0.47	-0.57	<u>0.0172</u>	0.80	-0.25	<u>0.0135</u>	0.88	-0.17	<u>0.0444</u>
12	0.78	0.90	<u>0.0076</u>	0.75	0.87	<u>0.0036</u>	0.53	0.65	<u>0.0055</u>	0.77	0.89	<u>0.0085</u>	0.79	0.90	<u>0.0073</u>
13	0.79	0.32	<u>0.0084</u>	1.06	0.60	<u>0.0114</u>	0.89	0.43	<u>0.0078</u>	0.72	0.23	<u>0.0085</u>	0.80	0.31	<u>0.0067</u>
14	1.15	-0.19	<u>0.018</u>	1.14	-0.21	<u>0.011</u>	0.77	-0.58	<u>0.0049</u>	0.83	-0.52	<u>0.0154</u>	0.95	-0.41	<u>0.0079</u>
15	1.37	0.14	<u>0.0212</u>	1.31	0.07	<u>0.0272</u>	1.09	-0.21	<u>0.008</u>	1.17	-0.06	<u>0.0317</u>	1.05	-0.18	<u>0.0095</u>
16	1.34	0.14	<u>0.0207</u>	1.31	0.09	<u>0.0168</u>	1.00	-0.21	<u>0.0064</u>	1.05	-0.17	<u>0.02</u>	1.03	-0.18	<u>0.0088</u>
17	1.43	0.07	<u>0.0229</u>	1.45	0.10	<u>0.015</u>	1.43	0.07	<u>0.0202</u>	1.48	0.12	<u>0.0218</u>	1.48	0.12	<u>0.0182</u>
18	1.53	0.49	<u>0.0269</u>	1.41	0.37	<u>0.0228</u>	1.50	0.46	<u>0.0059</u>	1.58	0.53	<u>0.0124</u>	1.55	0.50	<u>0.0083</u>
19	0.82	1.32	<u>0.0093</u>	0.92	1.42	<u>0.0066</u>	0.82	1.32	<u>0.0055</u>	0.70	1.19	<u>0.0152</u>	0.82	1.32	<u>0.0099</u>
20	0.20	0.79	<u>0.0347</u>	0.21	0.78	<u>0.0103</u>	0.26	0.84	<u>0.0075</u>	-0.18	0.40	<u>0.0157</u>	-0.01	0.56	<u>0.0162</u>
21	0.69	0.20	<u>0.0075</u>	0.81	0.23	<u>0.0103</u>	0.57	-0.10	<u>0.0169</u>	0.66	-0.09	<u>0.0163</u>	0.69	-0.12	<u>0.023</u>
22	0.17	0.77	<u>0.0224</u>	0.16	0.74	<u>0.0157</u>	0.81	1.49	<u>0.0256</u>	0.46	1.05	<u>0.0546</u>	0.67	1.25	<u>0.0398</u>
23	0.61	-0.05	<u>0.0077</u>	0.91	0.15	<u>0.0048</u>	0.56	-0.21	<u>0.005</u>	0.60	0.09	<u>0.0096</u>	0.70	0.09	<u>0.0091</u>
24	2.94	0.74	<u>0.1489</u>	2.33	0.13	<u>0.0852</u>	1.80	-0.39	<u>0.0286</u>	3.65	0.196	4.05	0.1775		
25	0.60	0.49	<u>0.0085</u>	0.02	-0.09	<u>0.0215</u>	0.16	0.04	<u>0.0126</u>	0.52	0.41	<u>0.0106</u>	0.72	0.60	<u>0.0071</u>
26	0.66	0.04	<u>0.0087</u>	0.83	-0.15	<u>0.0036</u>	0.56	-0.42	<u>0.0042</u>	0.54	-0.44	<u>0.0087</u>	0.65	-0.33	<u>0.0082</u>
27	1.06	1.06	<u>0.0404</u>	0.95	1.55	<u>0.0612</u>	0.94	1.54	<u>0.0515</u>	1.00	1.60	<u>0.0794</u>	0.83	1.22	<u>0.0726</u>
28	1.05	0.83	<u>0.0139</u>	0.85	1.63	<u>0.011</u>	1.10	1.87	<u>0.0173</u>	1.02	1.79	<u>0.0175</u>			
29	0.44	0.01	<u>0.0314</u>	0.94	0.51	<u>0.0192</u>	0.58	0.14	<u>0.0396</u>	0.66	0.23	<u>0.0694</u>	0.56	0.13	<u>0.0599</u>
30	1.07	0.62	<u>0.0105</u>	0.99	0.53	<u>0.0126</u>	1.07	0.61	<u>0.0504</u>	0.97	0.51	<u>0.0178</u>	0.54	0.08	<u>0.0111</u>
31	-0.25	-0.25	<u>0.0221</u>	0.27	0.15	<u>0.0235</u>	0.12	0.00	<u>0.0138</u>	-0.36	-0.48	<u>0.0395</u>	-0.28	-0.39	<u>0.0233</u>
32	1.25	-0.29	<u>0.0199</u>	1.09	-0.46	<u>0.0153</u>	1.21	-0.34	<u>0.0107</u>	1.31	-0.24	<u>0.0107</u>	1.19	-0.35	<u>0.0062</u>
33	0.78	0.31	<u>0.0099</u>	0.66	0.19	<u>0.0146</u>	0.89	0.42	<u>0.0082</u>	0.75	0.28	<u>0.0221</u>	0.56	0.09	<u>0.0105</u>
34	0.68	0.07	<u>0.0107</u>	1.05	-0.23	<u>0.0056</u>	1.06	-0.23	<u>0.0141</u>	0.55	-0.73	<u>0.0097</u>	0.78	-0.50	<u>0.0221</u>
35	2.88	-0.45	0.01	2.80	-0.63	<u>0.0111</u>	2.75	-0.58	<u>0.0148</u>	2.57	-0.77	<u>0.0114</u>	2.73	-0.61	<u>0.0138</u>
36	0.93	-0.02	<u>0.0107</u>	0.95	-0.01	<u>0.008</u>	1.26	0.31	<u>0.0197</u>	0.93	-0.03	<u>0.0184</u>	1.06	0.11	<u>0.0184</u>
37	0.75	0.60	<u>0.0211</u>	0.89	0.68	<u>0.0157</u>	1.10	0.88	<u>0.0039</u>	0.74	0.53	<u>0.0098</u>	0.81	0.60	<u>0.0117</u>
38	1.34	-1.42	<u>0.0196</u>	1.15	-1.96	<u>0.0172</u>	1.40	-1.72	<u>0.0188</u>	1.31	-1.81	<u>0.0152</u>	1.23	-1.89	0.015
39	0.90	0.59	<u>0.0163</u>	0.91	0.53	<u>0.0215</u>	0.81	0.43	<u>0.0126</u>	0.70	0.32	<u>0.0226</u>	0.85	0.47	<u>0.0094</u>
40	0.59	0.20	<u>0.0209</u>	0.62	-0.21	<u>0.0099</u>	0.94	0.01	<u>0.0065</u>	0.97	0.03	<u>0.0099</u>	0.97	0.03	<u>0.0099</u>
41	0.69	0.41	<u>0.0088</u>	1.07	0.77	<u>0.0085</u>	0.75	0.66	<u>0.0057</u>	0.86	0.56	<u>0.0126</u>	0.73	0.42	<u>0.0067</u>
42	0.60	0.72	<u>0.0083</u>	0.64	0.71	<u>0.005</u>	0.66	0.66	<u>0.0072</u>	0.51	0.55	<u>0.0084</u>	0.65	0.70	<u>0.0087</u>
43	0.20	0.20	<u>0.0154</u>	0.28	0.17	<u>0.0168</u>	0.18	0.07	<u>0.0121</u>	0.36	0.23	<u>0.0104</u>	0.46	0.33	<u>0.0097</u>
44	0.17	1.47	<u>0.0207</u>	-0.28	1.03	<u>0.0511</u>	-0.34	0.97	<u>0.0377</u>	0.24	1.54	<u>0.0284</u>	0.17	1.47	<u>0.0253</u>
45	0.60	0.07	<u>0.0059</u>	0.33	-0.24	<u>0.0267</u>	0.29	-0.28	<u>0.0235</u>	0.70	0.13	<u>0.0375</u>	0.42	-0.10	<u>0.0258</u>
46	0.54	-0.15	<u>0.0066</u>	0.51	-0.19	<u>0.0068</u>	0.70	0.01	<u>0.0115</u>	0.57	-0.12	<u>0.0157</u>	0.69	0.00	<u>0.0144</u>
47	0.87	0.05	<u>0.0048</u>	1.11	0.22	<u>0.0064</u>	0.87	-0.01	<u>0.0069</u>	1.00	0.11	<u>0.0083</u>	1.07	0.18	<u>0.0079</u>
48	0.79	0.13	<u>0.0086</u>	0.77	0.06	<u>0.0144</u>	0.89	0.18	<u>0.0146</u>	1.00	0.29	<u>0.015</u>	0.88	0.17	<u>0.0116</u>
49	0.59	0.29	<u>0.006</u>	0.85	0.50	<u>0.0112</u>	0.73	0.38	<u>0.0141</u>	0.62	0.27	<u>0.0124</u>	0.64	0.29	<u>0.0133</u>
50	0.62	-0.72	<u>0.0071</u>	0.79	-0.57	<u>0.017</u>	0.48	-0.88	<u>0.0107</u>	0.51	-1.08	<u>0.028</u>	0.69	-0.90	<u>0.0092</u>
51	0.70	-0.19	<u>0.0089</u>	0.88	-0.04	<u>0.0052</u>	0.62	-0.30	<u>0.0059</u>	0.62	-0.30	<u>0.0059</u>	0.57	-0.35	<u>0.0069</u>
52	0.45	-0.69	<u>0.0075</u>	0.22	0.0277	0.21	0.27	0.025	0.23	0.27	0.049	0.27	0.0294		
53	0.93	-0.06	<u>0.0065</u>	1.14	0.15	<u>0.0096</u>	1.36	0.37	<u>0.0168</u>	0.78	-0.21	<u>0.0112</u>	0.98	-0.01	<u>0.0193</u>
54	0.43	-0.34	<u>0.0103</u>	0.54	-0.29	<u>0.0083</u>	0.54	-0.29	<u>0.0078</u>	0.22	-0.61	<u>0.0137</u>	0.25	-0.58	<u>0.0148</u>
55	4.13	0.81	<u>0.2204</u>	5.27	1.94	<u>0.1588</u>	4.79	1.46	<u>0.138</u>	3.35	0.03	<u>0.2375</u>	3.44	0.17	<u>0.2526</u>
56	0.99	-0.66	<u>0.011</u>	1.00	-0.66	<u>0.013</u>	1.06	-0.60	<u>0.0181</u>	0.96	-0.68	<u>0.0253</u>	0.96	-0.69	<u>0.0205</u>
57	-0.02	-0.65	<u>0.0667</u>	0.32	0.0698	0.33	0.0316	0.80	0.0163	-0.85	0.6372				
58	0.71	-0.08	<u>0.0121</u>	1.03	-0.39	<u>0.0058</u>	0.42	-1.00	<u>0.0106</u>	0.97	-0.45	<u>0.0143</u>	0.89	-0.53	<u>0.0078</u>
59	0.62	0.79	<u>0.0067</u>	1.00	1.16	<u>0.0075</u>	0.99	1.15	<u>0.0124</u>	0.56	0.72	<u>0.0114</u>	0.76	0.92	<u>0.0147</u>
60	0.29	-0.40	<u>0.0114</u>	0.44	-0.25	<u>0.0181</u>	0.52	-0.18	<u>0.0236</u>	0.14	-0.56	<u>0.0208</u>	0.57	-0.13	<u>0.0256</u>
61	0.93	-1.22	<u>0.0196</u>	0.90	-1.33	<u>0.0405</u>	1.48	-0.75	<u>0.0178</u>	1.28	-0.97	<u>0.0642</u>	1.49	-0.76	<u>0.0248</u>
62	0.86	0.60	<u>0.0093</u>	1.00	0.74	<u>0.0076</u>	1.02	0.75	<u>0.013</u>	0.85	0.58	<u>0.0137</u>	0.95	0.68	<u>0.0169</u>
63	0.85	-0.07	<u>0.0149</u>	1.12	0.19	<u>0.0146</u>	1.36	0.44	<u>0.0059</u>	1.11	0.18	<u>0.0115</u>	1.22	0.30	<u>0.008</u>
64	0.51	0.69	<u>0.0101</u>	0.92	1.11	<u>0.0079</u>	0.65	0.84	<u>0.0116</u>	0.49	0.66	<u>0.018</u>	0.79	0.97	<u>0.0109</u>
65	1.50	0.54	<u>0.0271</u>	1.48	0.53	<u>0.0244</u>	1.46	0.51	<u>0.0039</u>	1.54	0.59	<u>0.0114</u>	1.46	0.50	<u>0.0056</u>
66	0.94	-0.04	<u>0.0232</u>	1.33	0.26	<u>0.0206</u>	1.20	0.14	<u>0.0061</u>	1.01	-0.05	<u>0.0155</u>	1.06	0.00	<u>0.0108</u>
67	1.29	0.39	<u>0.0095</u>	1.31	0.43	<u>0.0127</u>	1.03	0.33	<u>0.012</u>	1.16	0.26	<u>0.0179</u>	1.13	0.23	<u>0.0208</u>
68	0.83	0.68	<u>0.0163</u>	0.60	0.45	<u>0.0128</u>	1.14	0.99	<u>0.0078</u>	0.85	0.52	<u>0.0214</u>	0.86	0.52	<u>0.0191</u>
69	0.21	-0.65	<u>0.0128</u>	0.37	-0.53	<u>0.019</u>									

ID	Pred.	Res	HAT (h)	LogHL <sub>1</sub>	Pred.	Res	HAT (h)	LogHL <sub>2</sub>	Pred.	Res	HAT (h)	LogHL <sub>3</sub>	Pred.	Res	HAT (h)	LogHL <sub>4</sub>	Pred.	Res	HAT (h)	
155	0.16	-0.18	0.0253	0.51	-1.10	0.0138	0.63	-1.98	0.0721	0.53	-2.02	0.0128	0.53	-2.28	0.0117	0.53	-2.28	0.0117	0.53	-2.28
167	0.30	0.00	0.0112	0.27	-0.05	0.015	0.34	0.02	0.0162	0.51	0.18	0.0131	0.56	0.23	0.0151	0.51	0.18	0.0131	0.56	0.23
168	0.80	-0.60	0.0126	0.84	-0.57	0.006	0.57	-0.85	0.0204	1.11	0.0223	1.01	0.0223	1.01	0.024	1.01	0.0223	1.01	0.024	1.01
169	1.11	-0.13	0.0186	0.82	-0.45	0.0128	0.92	-0.35	0.0209	1.14	0.0346	0.98	0.0346	0.98	0.0303	0.98	0.0346	0.98	0.0303	0.98
170	1.07	-0.85	0.0139	0.70	-1.23	0.0099	0.64	-1.29	0.0071	0.77	-1.15	0.0277	1.01	-0.91	0.0069	1.01	-0.91	0.0069	1.01	-0.91
171	0.34	-0.06	0.0132	0.41	0.00	0.0137	0.53	0.12	0.0053	0.06	-0.26	0.0112	0.25	-0.16	0.0118	0.25	-0.16	0.0118	0.25	-0.16
172	0.91	0.13	0.0132	0.52	-0.61	0.0216	0.82	0.25	0.0122	0.74	0.15	0.0121	0.79	0.20	0.0143	0.79	0.20	0.0143	0.79	0.20
173	0.31	-0.43	0.0085	0.13	-0.61	0.0844	-0.19	-0.93	0.059	0.28	-0.46	0.0617	0.16	-0.58	0.0623	0.16	-0.58	0.0623	0.16	-0.58
174	0.89	-0.59	0.0252	0.45	-1.14	0.0243	0.94	-0.65	0.025	0.93	-0.68	0.0301	0.93	-0.68	0.0302	0.93	-0.68	0.0302	0.93	-0.68
175	0.02	0.10	0.0174	0.26	-0.29	0.0399	-0.01	-0.03	0.0248	-0.37	-0.41	0.0289	-0.25	-0.28	0.0304	-0.25	-0.28	0.0304	-0.25	-0.28
176	0.62	-0.90	0.0324	0.46	-1.19	0.0239	0.93	-0.72	0.0247	0.54	-1.11	0.0365	0.59	-1.06	0.0373	0.59	-1.06	0.0373	0.59	-1.06
177	-0.05	-0.60	0.0279	0.08	-0.49	0.0258	0.67	-0.10	0.0189	-0.38	-0.94	0.0413	0.08	-0.48	0.0324	0.08	-0.48	0.0324	0.08	-0.48
178	0.07	-0.81	0.026	-0.34	-0.85	0.165	1.16	0.056	0.13	0.225	1.03	0.0778	1.03	0.0778	1.03	0.0778	1.03	0.0778	1.03	0.0778
179	0.83	0.51	0.0137	0.74	0.43	0.0162	0.80	0.49	0.0131	0.83	0.51	0.0098	0.73	0.41	0.0129	0.73	0.41	0.0129	0.73	0.41
180	0.19	-1.59	0.0278	0.18	-0.24	0.0241	0.82	-0.24	0.0144	0.03	0.0406	0.17	0.0267	0.17	0.0267	0.17	0.0267	0.17	0.0267	0.17
181	0.56	0.03	0.0069	0.94	0.40	0.0077	0.79	0.25	0.0032	0.40	-0.13	0.0075	0.55	0.02	0.0064	0.55	0.02	0.0064	0.55	0.02
182	0.55	-0.13	0.0126	0.62	-0.07	0.0054	0.38	-0.30	0.0154	0.38	-0.30	0.0154	0.60	-0.09	0.0072	0.60	-0.09	0.0072	0.60	-0.09
183	1.56	0.56	0.0077	1.39	0.40	0.026	1.54	0.54	0.0074	1.67	0.67	0.0164	1.59	0.59	0.0096	1.59	0.59	0.0096	1.59	0.59
184	0.50	-1.03	0.0273	0.39	-1.03	0.0096	0.63	-1.04	0.0082	0.52	-0.61	0.0153	0.57	-0.57	0.0117	0.57	-0.57	0.0117	0.57	-0.57
185	0.40	-0.85	0.0098	0.21	-1.39	0.0188	0.41	-1.19	0.0154	0.45	-1.34	0.0215	0.46	-1.14	0.0176	0.46	-1.14	0.0176	0.46	-1.14
186	0.52	0.74	0.0058	0.67	0.89	0.0196	0.97	1.18	0.0128	0.96	1.16	0.0201	0.94	1.14	0.0175	0.94	1.14	0.0175	0.94	1.14
187	0.76	0.89	0.007	0.68	0.80	0.0076	0.60	0.72	0.0387	0.41	0.54	0.0253	0.41	0.54	0.0303	0.41	0.54	0.0303	0.41	0.54
188	0.85	0.60	0.0103	1.71	1.41	0.0257	0.99	0.69	0.0206	1.06	0.56	0.0158	1.25	0.75	0.0272	1.25	0.75	0.0272	1.25	0.75
189	0.86	-2.07	0.021	1.04	-2.03	0.0152	1.22	-1.85	0.0151	0.78	-0.78	0.0159	0.82	-0.78	0.0163	0.82	-0.78	0.0163	0.82	-0.78
190	2.70	-1.55	0.0246	3.66	-0.74	0.0773	3.28	-1.11	0.0604	2.52	-1.88	0.1399	2.27	-2.12	0.1327	2.27	-2.12	0.1327	2.27	-2.12
191	0.29	-0.01	0.01	0.49	0.17	0.0497	0.25	0.45	0.0148	0.25	0.45	0.0148	0.25	0.45	0.0148	0.25	0.45	0.0148	0.25	0.45
192	0.51	0.69	0.0097	0.26	0.96	0.0135	-0.04	-1.36	0.0322	0.63	-0.59	0.021	0.27	-0.95	0.0346	0.27	-0.95	0.0346	0.27	-0.95
193	0.87	-0.50	0.0113	0.65	-0.80	0.0154	1.02	-0.43	0.0312	1.06	-0.43	0.0553	1.14	0.0453	1.14	0.0453	1.14	0.0453	1.14	0.0453
194	0.25	0.25	0.0267	0.06	-0.04	0.055	0.57	0.47	0.0174	-0.29	-0.40	0.0776	0.37	-0.26	0.0283	0.37	-0.26	0.0283	0.37	-0.26
195	0.28	0.41	0.0141	-0.14	-0.02	0.0319	-0.18	-0.07	0.0458	-0.40	-0.37	0.0414	-0.23	-0.19	0.0462	-0.23	-0.19	0.0462	-0.23	-0.19
196	0.82	0.66	0.0158	0.75	0.56	0.0117	0.87	0.68	0.0267	0.99	0.79	0.028	0.50	0.31	0.0307	0.50	0.31	0.0307	0.50	0.31
197	0.73	0.41	0.008	0.97	0.64	0.0146	0.88	0.35	0.0104	0.83	0.48	0.0128	0.78	0.43	0.0126	0.78	0.43	0.0126	0.78	0.43
198	0.45	-0.66	0.0084	0.67	-0.88	0.0075	0.52	-0.93	0.0091	0.43	-0.92	0.012	0.52	-0.92	0.0108	0.52	-0.92	0.0108	0.52	-0.92
199	0.38	-0.67	0.0105	0.65	-0.96	0.0096	0.34	-0.94	0.013	0.36	-0.94	0.0124	0.31	-0.94	0.0129	0.31	-0.94	0.0129	0.31	-0.94
200	1.16	0.50	0.0131	1.25	0.60	0.0165	1.12	0.47	0.0149	1.03	0.37	0.0171	1.03	0.38	0.0113	1.03	0.38	0.0113	1.03	0.38
201	0.60	-0.49	0.0056	0.66	-0.68	0.0085	0.63	-0.66	0.006	0.71	-0.66	0.015	0.70	-0.66	0.0077	0.70	-0.66	0.0077	0.70	-0.66
202	0.89	-0.28	0.009	0.77	-0.44	0.024	0.92	-0.29	0.0061	1.35	-0.14	0.0199	1.09	-0.13	0.0075	1.09	-0.13	0.0075	1.09	-0.13
203	0.44	0.09	0.0084	0.29	-0.08	0.0279	0.51	0.14	0.0052	0.15	-0.21	0.0351	0.48	-0.11	0.0089	0.48	-0.11	0.0089	0.48	-0.11
204	-0.35	-0.88	0.0338	-0.44	-1.47	0.0674	0.48	-0.75	0.0308	0.85	-1.58	0.0476	-0.16	-0.89	0.0466	-0.16	-0.89	0.0466	-0.16	-0.89
205	0.87	0.32	0.0157	0.74	0.18	0.0109	0.89	0.33	0.0235	0.83	0.37	0.0271	0.62	0.07	0.0138	0.62	0.07	0.0138	0.62	0.07
206	0.69	-0.18	0.0061	0.83	-0.33	0.0063	0.88	-0.29	0.006	1.21	0.04	0.0204	1.12	-0.04	0.008	1.12	-0.04	0.008	1.12	-0.04
207	0.86	0.19	0.0121	1.07	0.39	0.0081	1.10	0.42	0.0146	0.81	0.13	0.0152	0.98	0.30	0.0272	0.98	0.30	0.0272	0.98	0.30
208	1.35	-0.04	0.0145	1.28	-0.12	0.0156	1.15	-0.26	0.008	1.34	-0.26	0.0165	1.29	-0.26	0.0083	1.29	-0.26	0.0083	1.29	-0.26
209	1.40	0.06	0.0202	1.23	-0.20	0.0219	1.33	-0.09	0.0073	1.42	-0.01	0.0122	1.36	-0.06	0.0063	1.36	-0.06	0.0063	1.36	-0.06
210	0.80	-0.57	0.0131	0.76	-0.77	0.0107	0.89	-0.64	0.0104	0.76	-0.64	0.0169	0.76	-0.64	0.0139	0.76	-0.64	0.0139	0.76	-0.64
211	1.07	0.46	0.0125	0.75	0.46	0.0125	0.75	0.46	0.0125	0.75	0.46	0.0125	0.75	0.46	0.0125	0.75	0.46	0.0125	0.75	0.46
212	0.86	0.66	0.0079	0.85	0.64	0.0101	0.78	0.56	0.0107	0.67	0.46	0.0145	0.64	0.43	0.009	0.64	0.43	0.009	0.64	0.43
213	0.81	-0.09	0.0056	0.80	-0.12	0.014	0.65	-0.27	0.0117	0.62	-0.27	0.0111	0.62	-0.27	0.0102	0.62	-0.27	0.0102	0.62	-0.27
214	0.84	0.24	0.0084	1.09	0.49	0.0073	0.79	0.19	0.0127	0.92	0.32	0.0115	1.01	0.41	0.0086	1.01	0.41	0.0086	1.01	0.41
215	0.39	-0.35	0.012	0.82	-0.35	0.0138	0.64	-0.35	0.0124	0.83	-0.35	0.0119	0.69	-0.35	0.0133	0.69	-0.35	0.0133	0.69	-0.35
216	0.51	-0.48	0.0061	0.52	-0.48	0.0078	0.56	-0.48	0.0055	0.84	-0.48	0.022	0.74	-0.48	0.0062	0.74	-0.48	0.0062	0.74	-0.48
217	0.62	-0.12	0.0095	0.98	-0.08	0.0126	0.90	-0.16	0.0078	1.21	-0.16	0.0093	1.16	-0.08	0.008	1.16	-0.08	0.008	1.16	-0.08
218	0.71	-0.29	0.0073	0.81	-0.29	0.0101	0.79	-0.29	0.008	1.12	-0.29	0.0091	1.15	-0.29	0.0082	1.15	-0.29	0.0082	1.15	-0.29
219	0.62	-0.79	0.007	0.74	-0.68	0.0042	0.51	-0.91	0.012	0.78	-0.64	0.0135	0.80	-0.62	0.0104	0.80	-0.62	0.0104	0.80	-0.62
220	0.62	0.84	0.0043	0.99	1.21	0.005	0.71	0.93	0.0082	0.59	0.81	0.0054	0.80	1.02	0.0071	0.80	1.02	0.0071	0.80	1.02
221	0.60	0.76	0.0065	0.87	0.86	0.007	0.65	0.64	0.0067	0.65	0.64	0.0088	0.56	0.55	0.009	0.56	0.55	0.009	0.56	0.55
222	0.54	0.58	0.0064	0.69	0.72	0.0128	0.57	0.61	0.0063	0.61	0.53	0.0102	0.39	0.31	0.0096	0.39	0.31	0.0096	0.39	0.31
223	0.18	0.96	0.0074	0.52	1.29	0.0095	0.56	1.33	0.0213	0.47	1.23	0.0132	0.34	1.10	0.0338	0.34	1.10	0.0338	0.34	1.10
224	1.22	1.14	0.0236	0.95	0.88	0.0124	0.90	0.82	0.0103	1.25	1.18	0.0229	1.59	1.52	0.0174	1.59	1.52	0.0174	1.59	1.52
225	1.04	1.04	0.0259	1.22	1.21	0.0185	1.05	0.												

ID	LogHL <sub>1</sub>				LogHL <sub>2</sub>				LogHL <sub>3</sub>				LogHL <sub>4</sub>			
	Pred.	Res	HAT (h)	Pred. (h)	Pred.	Res	HAT (h)	Pred. (h)	Pred.	Res	HAT (h)	Pred. (h)	Pred.	Res	HAT (h)	Pred. (h)
354	0.28	-0.04	0.0191	1.21	-0.51	0.0176	0.92	-0.74	1.10	-0.52	0.0161	1.26	-0.34	0.0117		
335	1.12	-0.36	0.016	0.51	-0.98	0.0476	1.19	-0.31	0.0131	0.89	-0.61	0.0598	1.37	-0.13	0.0145	
336	0.98	0.87	0.013	1.26	-0.05	0.0287	1.07	-0.24	0.0182	1.24	-0.07	0.0373	1.42	0.11	0.027	
337	1.37	-1.55	0.0184	1.30	-1.62	0.0183	1.42	-1.50	0.0172	1.69	-1.23	0.0288	1.64	-1.28	0.0204	
338	0.99	-0.53	0.0097	0.85	-0.67	0.0075	1.18	-0.34	0.0166	0.91	-0.61	0.0101	0.94	-0.58	0.0088	
339	0.34	-0.53	0.0195	0.70	0.0167		1.26	0.0137	1.24	0.0137	1.24	0.0137	1.30	0.0396		
340	1.93	-0.45	0.0175	1.08	-0.46	0.0183	2.09	-0.29	0.0091	1.18	-0.53	0.0091	1.95	-0.43	0.0141	
341	2.03	1.29	0.0177	1.53	0.79	0.013	1.64	0.90	0.0065	1.95	1.21	0.0098	2.03	1.29	0.0067	
342	2.14	0.75	0.0193	1.90	0.52	0.0187	2.14	0.76	0.0094	2.13	0.75	0.0099	2.15	0.77	0.0069	
343	6.67	1.19	0.0238	1.08	1.60	0.0237	6.65	1.17	0.0596	6.30	0.82	0.0276	6.46	0.98	0.027	
344	1.24	-0.07	0.0247	0.84	-0.47	0.0186	1.03	-0.27	0.0079	1.13	-0.18	0.0168	1.22	-0.09	0.0081	
345	1.40	0.78	0.0252	0.94	0.33	0.0186	1.12	0.51	0.0074	1.31	0.69	0.0135	1.39	0.78	0.0077	
346	1.49	0.88	0.0267	1.13	0.51	0.0211	1.38	0.76	0.0074	1.45	0.84	0.0114	1.51	0.90	0.0072	
347	1.40	-0.06	0.0129	1.19	-0.27	0.0107	0.96	-0.49	0.0134	0.96	-0.51	0.0238	1.15	-0.31	0.0137	
348	1.02	0.26	0.008	0.96	0.20	0.0052	0.78	0.02	0.0124	0.83	0.06	0.0137	0.94	0.17	0.0097	
349	0.59	0.08	0.0101	0.58	0.08	0.0092	0.83	0.32	0.0112	0.44	-0.07	0.0124	0.66	0.16	0.0121	
350	1.15	-0.71	0.0217	1.05	-0.83	0.0214	1.46	-0.41	0.012	1.34	-0.52	0.0174	1.37	-0.50	0.0143	
351	0.77	0.65	0.01	1.76	1.59	0.0686	0.98	0.81	0.0205	1.04	0.75	0.0355	1.23	0.94	0.0268	
352	0.65	0.45	0.0074	0.91	0.70	0.0121	0.78	0.57	0.0118	0.80	0.60	0.0159	0.79	0.59	0.0147	
353	1.10	0.99	0.0127	0.92	0.80	0.0229	0.95	0.83	0.0134	0.89	0.77	0.023	0.82	0.70	0.0086	
354	0.21	0.45	0.0071	0.55	0.78	0.0093	0.66	0.90	0.0127	0.38	0.61	0.0152	0.48	0.71	0.0156	
355	3.10	-0.38	0.0098	3.10	-0.38	0.0111	3.01	-0.47	0.0073	3.13	-0.35	0.0095	3.08	-0.40	0.0077	
356	1.53	0.06	0.0184	1.16	-0.31	0.008	1.22	-0.24	0.014	0.96	-0.51	0.0376	1.15	-0.32	0.0192	
357	1.32	-0.98	0.0136	1.40	-0.94	0.0099	1.43	-0.91	0.0104	1.47	-0.82	0.0127	1.67	-0.62	0.0098	
358	0.95	-1.12	0.0193	1.10	-0.98	0.0154	1.16	-0.92	0.0164	1.08	-1.01	0.0131	1.20	-0.88	0.0099	
359	2.05	0.66	0.0177	1.41	0.46	0.0159	2.06	0.66	0.0077	2.01	0.62	0.0093	2.04	0.65	0.0063	
360	1.32	0.29	0.0242	1.53	0.20	0.0235	1.53	0.22	0.0045	1.18	0.12	0.0131	1.48	0.18	0.0131	
361	0.44	0.29	0.0091	0.21	-0.19	0.0149	0.61	0.22	0.0087	0.30	-0.09	0.0121	0.50	0.11	0.0128	
362	0.48	0.94	0.0069	0.52	0.76	0.0093	0.69	0.93	0.0233	0.60	0.84	0.0124	0.48	0.72	0.037	
363	0.92	0.97	0.015	1.33	0.99	0.0155	1.36	1.02	0.0078	1.30	0.96	0.011	1.23	0.89	0.0104	
364	1.90	-1.35	0.0316	1.07	-2.18	0.0152	2.82	-4.03	0.0702	2.84	-0.41	0.1336	3.76	0.50	0.144	
365	1.64	0.49	0.0216	0.77	-0.38	0.0117	1.13	-0.02	0.0175	1.09	0.09	0.0384	1.24	0.19	0.0199	
366	5.11	0.29	0.0047	5.22	0.27	0.0031	5.51	0.57	0.0342	5.40	0.46	0.0378	5.57	0.63	0.0372	
367	1.09	0.84	0.0241	0.80	0.55	0.0132	0.96	0.70	0.0252	0.93	0.68	0.0252	0.52	0.26	0.0232	
368	0.39	-0.79	0.0052	0.43	0.0066	0.61	0.31	0.011	0.39	0.08	0.0096	0.44	0.44	0.015		
369	0.38	0.61	0.0154	0.32	0.53	0.0128	0.31	0.52	0.0129	-0.07	0.08	0.0227	0.24	0.39	0.0181	
370	1.00	-0.53	0.0134	0.88	-0.66	0.0114	1.20	-0.33	0.0211	1.03	-0.50	0.0236	0.92	-0.61	0.0106	
371	1.05	0.46	0.0113	0.97	0.37	0.0136	1.00	0.40	0.0201	0.96	0.36	0.0192	0.90	0.31	0.0115	
372	0.94	-0.59	0.0096	0.98	-0.55	0.0087	0.87	-0.66	0.0073	0.83	-0.70	0.014	0.70	-0.83	0.0144	
373	0.89	0.05	0.0065	1.10	-0.09	0.0077	0.91	-0.29	0.0134	0.80	-0.29	0.0095	0.88	-0.30	0.0088	
374	1.01	0.19	0.0261	1.26	0.11	0.0317	1.38	0.23	0.0133	1.06	-0.09	0.0137	1.26	-0.22	0.0158	
375	0.71	-0.09	0.0046	0.70	-0.93	0.0066	0.51	-1.11	0.0063	0.72	-0.90	0.0139	0.61	-1.02	0.0078	
376	0.75	0.29	0.0062	0.86	0.34	0.0073	0.82	0.30	0.0105	0.89	0.48	0.0158	0.88	0.37	0.0125	
377	0.57	-0.64	0.0105	0.86	-0.49	0.0095	1.19	-0.15	0.0133	0.98	-0.37	0.0175	1.13	-0.22	0.0157	
378	0.49	-0.30	0.0040	0.75	-0.40	0.0049	0.63	-0.47	0.0059	0.98	-0.47	0.0059	0.98	-0.47	0.0059	
379	1.41	0.01	0.021	1.30	0.01	0.021	1.30	0.01	0.021	1.30	0.01	0.021	1.30	0.01	0.021	
380	0.97	0.53	0.0208	0.86	0.41	0.0158	1.25	0.80	0.0144	1.11	0.66	0.0253	0.86	0.41	0.0079	
381	-0.29	-0.96	0.0261	-0.14	-1.51	0.0363	0.83	-0.54	0.0383	-0.11	-1.48	0.0754	0.25	-1.12	0.0655	
382	0.22	-0.05	0.0164	0.19	-0.33	0.0594	0.36	-0.16	0.034	0.76	0.22	0.0203	-0.20	-0.74	0.2096	
383	0.48	0.44	0.0078	0.63	0.19	0.0155	0.43	0.05	0.0159	0.65	0.05	0.0103	0.40	0.16	0.016	
384	1.18	0.80	0.0274	1.17	0.79	0.0484	1.52	1.14	0.004	1.30	0.33	0.0275	1.33	0.66	0.0124	
385	1.52	0.74	0.0173	1.90	0.48	0.0195	1.93	1.10	0.0178	1.93	1.05	0.0424	2.33	1.45	0.0263	
386	0.93	-0.22	0.0061	0.86	-0.39	0.009	0.61	-0.64	0.0099	0.69	0.0154	0.91	0.054	0.0079		
387	0.86	0.15	0.0181	0.79	0.08	0.008	0.82	0.11	0.0069	0.53	-0.52	0.0144	0.74	-0.30	0.0123	
388	0.82	0.68	0.0113	1.01	0.41	0.0113	1.13	0.53	0.01	1.12	0.52	0.0156	1.06	0.45	0.0127	
389	1.99	-2.21	0.026	3.28	-0.92	0.1466	2.33	-1.86	0.0357	2.61	-1.58	0.0483	2.56	-1.63	0.0355	
390	1.09	1.39	0.0321	0.50	0.80	0.0252	1.15	1.45	0.027	1.22	1.52	0.0235	0.90	1.20	0.0074	
391	0.22	1.00	0.0396	-0.27	0.51	0.0764	0.09	0.87	0.0272	0.26	1.02	0.012	-0.11	0.65	0.0363	
392	0.95	-0.51	0.0084	1.41	-0.14	0.0145	1.23	-0.32	0.013	1.29	0.17	0.0172	1.25	0.25	0.0083	
393	1.01	-0.17	0.0069	1.30	0.13	0.0078	1.16	-0.02	0.0089	1.25	0.07	0.0113	1.12	-0.06	0.0066	
394	1.70	-0.16	0.006	1.65	-0.21	0.0059	1.67	-0.19	0.0051	0.55	-0.31	0.0082	0.62	-0.24	0.0046	
395	0.40	0.40	0.0183	0.34	0.34	0.0178	1.49	0.49	0.0064	1.44	0.44	0.0071	1.57	0.57	0.0084	
396	0.82	-0.13	0.0138	0.85	-0.11	0.0114	0.80	-0.16	0.013	0.81	-0.15	0.0094	0.76	-0.20	0.0105	
397	0.60	0.42	0.0067	0.60	0.42	0.0091	0.52	0.34	0.0183	0.45	0.14	0.0187	0.41	0.09	0.0224	
398	0.56	0.48	0.0071	0.64	0.48	0.0078	0.70	0.54	0.0082	0.40	0.24	0.0151	0.62	0.46	0.0099	
399	1.07	-0.91	0.0162	1.08	-0.99	0.0128	1.02	-0.97	0.0388	0.95	-1.02	0.0351	1.45	-0.53	0.0451	
400	0.66	0.22	0.019	0.80	0.34	0.0144	0.89	0.43	0.0091	0.84	0.38	0.0133	0.84	0.38	0.0122	
401	2.11	0.33	0.0676	1.55	-0.24	0.0241	1.43	-0.35	0.0191	2.62	0.05	0.0905	2.88	0.0821		
402	1.06	0.32	0.0258	1.40	-0.34	0.033	1.19	0.45	0.0425	0.72	-0.02	0.0144	0.58	-0.16	0.0046	
403	2.61	-1.11	0.0126	2.49	-1.24	0.0113	2.57	-1.15	0.0072	2.65	-1.08	0.0085	2.61	-1.11	0.0066	
404	0.44	0.04	0.0134	0.66	0.26	0.0083	0.70	0.30	0.0067	0.21	-0.49	0.0134	0.43	-0.27	0.0152	
405	0.71	-0.39	0.009	0.62	-0.36	0.0056	0.62	-0.42	0.0055	0.89	-0.36	0.0139	0.89	-0.46	0.0078	
406	0.30	0.22	0.0087	0.56	0.33	0.0091	0.65	0.42	0.0078	0.27	0.01	0.0126	0.53	0.27	0.0104	
407	0.60	0.99	0.0055	0.58	0.94	0.0074	0.58	0.94	0.0101	0.57	0.90	0.0159	0.60	0.93	0.0139	
408	0.25	0.17	0.0114	0.24	0.02	0.031	0.25	0.03	0.0089	0.34	0.12	0.0124	0.33	0.10	0.0104	
409	0.92	0.58	0.0165	0.												

ID	Pred.	Res	LogHL <sub>1</sub>	HAT <sub>1</sub> (h)	Pred.	Res	LogHL <sub>2</sub>	HAT <sub>2</sub> (h)	Pred.	Res	LogHL <sub>3</sub>	HAT <sub>3</sub> (h)	Pred.	Res	LogHL <sub>4</sub>	HAT <sub>4</sub> (h)
ID	Pred.	Res	LogHL <sub>1</sub>	HAT <sub>1</sub> (h)	Pred.	Res	LogHL <sub>2</sub>	HAT <sub>2</sub> (h)	Pred.	Res	LogHL <sub>3</sub>	HAT <sub>3</sub> (h)	Pred.	Res	LogHL <sub>4</sub>	HAT <sub>4</sub> (h)
502	0.73	0.69	0.0171	0.81	0.76	0.0135	0.63	0.58	0.0107	0.69	0.84	0.0122	0.87	0.83	0.0105	0.74
503	3.78	-0.87	0.0118	3.82	-0.96	0.0167	3.95	-0.84	0.0165	3.83	-0.94	0.013	3.78	-1.00	0.0121	3.71
504	0.96	-0.04	0.0107	0.61	-0.43	0.009	0.89	-0.15	0.0194	1.11	0.07	0.0336	1.14	1.00	0.029	1.04
505	0.70	0.40	0.0082	0.85	0.54	0.0045	0.61	0.31	0.0073	0.73	0.43	0.013	0.83	0.53	0.007	0.79
506	1.15	0.34	0.018	1.08	-0.01	0.009	1.29	0.48	0.04	1.02	0.21	0.017	1.02	1.01	0.0126	1.06
507	3.16	-0.05	0.0101	3.13	-0.07	0.0119	3.26	0.05	0.006	3.20	0.00	0.0091	3.14	-0.06	0.008	3.14
508	3.4	1.07	0.0099	3.92	0.81	0.0082	3.20	0.21	0.0072	3.15	0.37	0.0091	3.13	1.06	0.0078	3.13
509	1.10	-0.38	0.0099	3.13	-0.36	0.0108	3.01	-0.47	0.0074	3.16	-0.33	0.009	3.08	-0.40	0.0077	3.08
510	3.29	0.47	0.0121	3.16	0.33	0.0239	3.50	0.68	0.0174	3.37	0.55	0.0105	3.31	0.49	0.0097	3.31
511	3.76	-0.57	0.0119	3.61	-0.81	0.0236	3.94	-0.68	0.0162	3.82	-0.60	0.0123	3.77	-0.66	0.0118	3.77
512	3.16	-0.78	0.01	3.15	-0.79	0.0118	3.26	-0.67	0.0107	3.21	-0.72	0.009	3.15	-0.79	0.008	3.15
513	4.64	-0.23	0.0214	4.60	-0.30	0.0403	4.90	-0.01	0.0352	4.72	-0.19	0.0266	4.70	-0.21	0.0244	4.70
514	0.74	-0.06	0.0057	0.72	-0.78	0.0076	0.48	-1.03	0.0154	0.52	-0.98	0.017	0.45	-1.05	0.0161	0.45
515	0.61	0.57	0.0068	0.92	0.87	0.0062	0.76	0.71	0.008	0.64	0.49	0.0096	0.75	0.60	0.0115	0.75
516	0.53	0.23	0.011	0.72	0.42	0.0048	0.51	0.20	0.0057	0.47	-0.11	0.0222	0.50	-0.07	0.0116	0.50
517	3.14	-0.17	0.0102	2.95	-0.36	0.0171	3.25	-0.05	0.0104	3.21	-0.09	0.0084	3.13	-0.17	0.0077	3.13
518	5.27	0.48	0.0355	5.70	0.92	0.0397	5.30	0.52	0.0299	5.16	0.38	0.0313	5.18	0.39	0.0305	5.18
519	0.65	-0.01	0.006	0.80	0.13	0.0052	0.56	-0.11	0.0057	0.57	-0.10	0.0097	0.64	-0.03	0.0065	0.64
520	1.88	0.30	0.0164	1.66	0.08	0.0121	1.80	0.22	0.0055	1.89	0.31	0.0084	1.86	0.28	0.0061	1.86
521	2.70	-0.30	0.0085	2.37	-0.60	0.0164	2.51	-0.50	0.0123	2.21	-0.30	0.014	2.62	-0.38	0.0103	2.62
522	0.93	0.03	0.0136	0.83	-0.08	0.0143	0.94	0.04	0.0071	1.02	0.09	0.0132	0.91	-0.01	0.0062	0.91
523	0.53	-0.22	0.0086	0.31	-0.76	0.0078	0.64	-0.42	0.0208	0.81	-0.07	0.0076	0.19	-0.10	0.0054	0.19
524	0.50	-0.01	0.0148	0.44	-0.12	0.0235	0.31	-0.25	0.0338	0.62	0.05	0.0221	0.18	-0.39	0.0356	0.18
525	0.89	0.29	0.0186	1.01	0.41	0.0147	1.10	0.50	0.0071	1.18	0.58	0.0069	1.22	0.63	0.008	1.22
526	0.76	0.76	0.0117	0.61	0.60	0.014	0.57	0.56	0.0082	0.97	0.95	0.0173	0.69	0.68	0.0147	0.69
527	0.29	0.66	0.0106	0.46	-0.01	0.0294	0.32	-0.12	0.0156	0.71	0.23	0.0194	0.57	0.09	0.0111	0.57
528	0.68	0.64	0.0091	1.08	0.69	0.026	1.28	0.61	0.012	0.89	0.28	0.0252	0.85	0.28	0.0142	0.85
529	0.72	0.24	0.0131	0.63	0.15	0.0066	0.58	0.11	0.0044	0.37	-0.23	0.0156	0.55	-0.06	0.01	0.55
530	0.71	0.16	0.0054	0.86	0.31	0.0055	0.76	0.21	0.0074	0.56	-0.03	0.0089	0.62	0.03	0.0077	0.62
531	0.44	0.44	0.0119	0.75	-0.12	0.016	0.47	-0.39	0.0148	0.76	-0.10	0.012	0.51	-0.35	0.0156	0.51
532	0.33	-0.44	0.0047	0.59	-0.05	0.0058	0.48	-0.09	0.0124	0.29	-0.07	0.0099	0.43	-0.07	0.0114	0.43
533	1.18	-0.20	0.0183	1.01	-0.45	0.0136	1.05	-0.34	0.0094	1.36	-0.07	0.0129	1.27	-0.16	0.0058	1.27
534	2.79	0.21	0.0163	1.44	-0.14	0.0134	1.55	-0.03	0.0073	1.71	0.13	0.0107	1.75	0.17	0.0068	1.75
535	0.96	0.88	0.0172	0.58	0.50	0.0134	1.64	0.56	0.0065	1.92	0.84	0.0082	1.93	0.85	0.0063	1.93
536	1.96	0.33	0.0171	1.61	-0.03	0.012	1.80	-0.16	0.0055	1.93	-0.29	0.0086	1.96	0.33	0.0058	1.96
537	4.28	-0.83	0.0155	4.53	-0.61	0.0194	4.40	-0.74	0.0181	4.29	-0.85	0.0171	4.26	-0.88	0.0161	4.26
538	4.26	-0.67	0.0155	4.32	-0.62	0.0188	4.39	-0.56	0.0179	4.27	-0.68	0.0164	4.24	-0.71	0.016	4.24
539	4.91	-0.75	0.0245	5.12	-0.56	0.0289	5.10	-0.58	0.0272	4.89	-0.78	0.0249	4.89	-0.79	0.0239	4.89
540	4.88	-0.48	0.0246	4.86	-0.48	0.0263	5.08	-0.30	0.0273	4.86	-0.53	0.024	4.86	-0.53	0.024	4.86
541	0.69	-0.63	0.0173	0.84	-0.49	0.0105	1.13	-0.20	0.016	0.93	-0.23	0.013	0.56	-0.76	0.0303	0.56
542	0.29	0.38	0.0153	0.50	0.53	0.014	0.44	0.47	0.007	0.60	0.59	0.0113	0.52	0.51	0.01	0.52
543	2.28	0.40	0.0116	2.26	0.38	0.0094	2.24	0.36	0.0058	2.31	0.43	0.0096	2.22	0.34	0.0071	2.22
544	2.82	-0.84	0.0098	2.67	-1.04	0.0196	2.50	-1.21	0.0118	2.73	-0.99	0.0116	2.75	-0.97	0.0085	2.75
545	4.19	-1.22	0.0158	4.35	-1.05	0.0189	4.39	-1.01	0.018	4.20	-1.06	0.0158	4.14	-1.27	0.0154	4.14
546	0.55	0.06	0.0102	0.69	0.16	0.0133	0.84	0.32	0.0053	0.60	0.26	0.0061	0.65	0.11	0.0058	0.65
547	1.52	-0.08	0.0079	1.36	-0.07	0.0099	1.46	-0.06	0.0081	1.32	-0.06	0.009	1.33	-0.06	0.0077	1.33
548	0.71	0.31	0.0056	0.88	0.49	0.0061	0.53	0.13	0.0125	0.56	0.12	0.0115	0.68	0.24	0.0099	0.68
549	0.74	-0.64	0.0073	0.95	-0.42	0.005	0.76	-0.61	0.0096	0.59	-0.87	0.0108	0.61	-0.85	0.0116	0.61
550	2.90	-0.36	0.0092	2.82	-0.43	0.0077	2.91	-0.34	0.0068	2.90	-0.36	0.0084	2.85	-0.40	0.0075	2.85
551	2.07	0.47	0.04	1.30	0.29	0.0136	1.80	0.21	0.0276	1.93	0.34	0.0062	2.10	0.52	0.0336	2.10
552	1.18	-1.47	0.0101	0.59	-1.23	0.0092	0.54	-1.28	0.0194	0.56	-1.26	0.0115	0.38	-1.44	0.0123	0.38
553	0.46	0.38	0.01	0.54	-0.02	0.0178	0.46	-0.10	0.0112	0.56	0.01	0.0141	0.46	-0.10	0.0146	0.46
554	1.42	1.09	0.0182	1.40	0.84	0.0179	1.33	0.77	0.0039	1.40	0.84	0.0062	1.50	0.94	0.0092	1.50
555	1.27	-0.31	0.0106	1.34	-0.28	0.0087	1.68	0.06	0.0126	1.67	0.07	0.0127	1.64	0.015	0.011	1.64
556	0.14	-0.54	0.0066	-0.52	-0.14	0.2485	0.19	-0.53	0.0277	0.78	-0.65	0.0248	0.65	-0.42	0.0068	0.65
557	0.59	0.04	0.0047	0.56	-0.12	0.0061	0.35	-0.33	0.0128	0.37	-0.31	0.0137	0.23	-0.45	0.0136	0.23
558	2.18	-0.31	0.021	1.96	-0.52	0.0123	1.97	-0.51	0.0094	2.08	-0.40	0.0122	2.10	-0.38	0.0085	2.10
559	2.36	0.18	0.0111	2.18	0.00	0.0086	2.23	0.05	0.0058	2.44	0.16	0.008	2.32	0.14	0.0062	2.32
560	2.35	0.32	0.0114	2.11	0.08	0.0122	2.07	0.03	0.0081	2.28	0.25	0.0093	2.28	0.25	0.0069	2.28
561	0.66	0.90	0.0129	2.34	0.58	0.0112	2.57	0.81	0.007	2.69	0.93	0.0076	2.67	0.91	0.0069	2.67
562	3.55	0.07	0.0103	3.50	0.11	0.013	3.45	0.04	0.0099	3.53	0.05	0.0113	3.50	0.02	0.0103	3.50
563	0.52	0.12	0.0043	0.69	0.30	0.0074	0.39	-0.01	0.0087	0.57	0.13	0.0068	0.43	-0.01	0.0092	0.43
564	0.90	0.01	0.0098	0.95	0.07	0.005	1.04	0.16	0.0063	0.70	0.10	0.0104	0.73	0.0137	0.73	0.73
565	3.21	0.21	0.0123	3.15	0.14	0.0225	2.94	-0.07	0.0183	3.12	0.11	0.0148	3.10	0.09	0.0133	3.10
566	3.65	-0.84	0.0106	3.80	-0.69	0.0138	3.70	-0.78	0.0115	3.67	-0.81	0.0118	3.61	-0.87	0.0107	3.61
567	3.53	0.30	0.0102	3.41	0.32	0.0099	3.44	0.21	0.0099	3.52	0.30	0.0104	3.48	0.26	0.0101	3.48
568	3.61	0.45	0.0104	3.38	0.22	0.0099	3.44	0.28	0.0099	3.61	0.45	0.0104	3.58	0.42	0.0103	3.58
569	4.03	0.39	0.0147	4.09	0.45	0.0185	3.89	0.25	0.0152	3.98	0.34	0.015	3.95	0.32	0.0149	3.95
570	4.01	0.52	0.0149	3.88	0.40	0.0167	3.88	0.40	0.0155	3.96	0.48	0.0152	3.93	0.45	0.0151	3.93
571	4.24	-0.32	0.0157	4.10	-0.45	0.0265	4.38	-0.17	0.0179	4.25	-0.30	0.0166	4.22	-0.34	0.016	4.22
572	4.40	-0.37	0.0171	4.36	-1.07	0.0317	4.64	-0.80	0.0246	4.45	-0.99	0.0192	4.41	-1.03	0.0182	4.41
573	0.79	0.30	0.0103	0.86	0.35	0.0073	0.80	0.30	0.0088	0.63	0.13	0.0096	0.76	0.25	0.0071	0.

ID	LogHL <sub>1</sub>			LogHL <sub>2</sub>			LogHL <sub>3</sub>			LogHL <sub>4</sub>		
	Pred. (h)	Res	HAT (h) (#=6578)	Pred. (h)	Res	HAT (h) (#=6533)	Pred. (h)	Res	HAT (h) (#=6578)	Pred. (h)	Res	HAT (h) (#=6574)
670	0.89	-0.55	0.0089	1.28	-0.12	0.0184	0.83	-0.57	0.0094	0.93	-0.47	0.0131
671	0.87	-0.53	0.0089	0.88	-0.52	0.017	1.28	-0.12	0.0184	0.83	-0.57	0.0094
672	0.58	0.25	0.0074	0.75	-0.43	0.0069	0.28	-0.03	0.0108	0.44	0.10	0.0147
673	2.46	1.38	0.0602	0.87	-0.45	0.0046	1.59	0.27	0.0459	1.67	0.35	0.1201
674	0.67	0.44	0.0128	0.92	0.67	0.0072	1.02	0.77	0.011	0.50	0.25	0.1011
675	0.84	0.47	0.0074	0.96	0.60	0.0045	0.84	0.48	0.0109	0.82	0.46	0.0136
676	1.02	-2.44	0.0075	0.58	-2.79	0.0077	0.89	-2.58	0.0077	0.71	-2.71	0.0138
677	1.44	0.25	0.0233	0.70	-0.50	0.0065	0.91	-0.29	0.0229	1.03	-0.23	0.0451
678	1.72	0.04	0.0223	0.93	-0.76	0.0068	1.09	-0.59	0.0136	1.23	-0.30	0.0306
679	0.63	-0.37	0.0071	0.74	-0.26	0.0221	0.53	-0.47	0.0075	0.41	-0.60	0.0201
680	0.83	-0.86	0.0185	0.67	-1.01	0.004	0.94	-0.74	0.0165	0.32	-1.38	0.0171
681	0.85	-0.10	0.0077	1.00	0.04	0.0108	0.88	-0.08	0.0075	0.85	-0.12	0.0117
682	1.55	-0.45	0.0289	1.48	-0.54	0.0262	1.50	-0.52	0.0079	1.73	-0.30	0.014
683	4.15	0.36	0.0153	3.81	0.02	0.0205	3.97	0.19	0.0153	4.13	0.35	0.016
684	0.74	0.67	0.01	0.87	0.81	0.0069	0.69	0.63	0.0149	0.57	0.50	0.0123
685	0.13	0.09	0.0171	0.29	-1.15	0.0183	0.33	-1.11	0.0086	0.44	-1.00	0.0092
686	4.85	0.25	0.0366	5.22	0.47	0.046	5.36	0.62	0.0413	5.04	0.28	0.0352
687	2.44	0.28	0.0115	2.42	0.27	0.0102	2.48	0.33	0.0062	2.42	0.27	0.0083
688	2.32	0.29	0.0115	1.95	-0.08	0.0113	2.07	0.04	0.008	2.33	0.29	0.0092
689	0.92	0.18	0.0278	0.75	0.12	0.0165	0.44	-0.19	0.0075	0.81	-0.17	0.0294
690	0.50	0.39	0.0072	0.69	0.40	0.0088	0.57	0.28	0.0067	0.57	0.27	0.0094
691	0.40	-0.90	0.0097	0.89	-0.41	0.0427	0.87	-0.43	0.0116	0.92	-0.39	0.0109
692	0.58	0.04	0.0119	0.65	0.10	0.0071	0.54	-0.01	0.0095	0.89	0.33	0.0111
693	0.64	0.03	0.0067	0.49	-0.13	0.0123	0.52	-0.10	0.0143	0.72	0.10	0.0082
694	0.88	-0.46	0.0067	1.04	-0.10	0.0059	0.62	-0.53	0.0083	0.70	-0.45	0.0099
695	0.00	-0.43	0.0653	-0.55	0.43	0.037	0.39	0.39	0.037	0.61	0.45	0.037
696	0.81	-0.10	0.006	0.83	0.00	0.0079	0.74	-0.09	0.0044	0.94	0.11	0.0133
697	0.56	-0.48	0.0037	0.72	-0.32	0.0085	0.51	-0.54	0.0069	0.61	-0.08	0.01
698	3.26	1.08	0.0348	3.48	1.30	0.0232	3.12	0.93	0.0134	3.22	1.04	0.0217
699	3.65	0.64	0.0107	3.81	0.80	0.0127	3.70	0.70	0.0115	3.68	0.68	0.0116
700	1.39	0.46	0.0157	1.23	0.30	0.0174	1.08	0.16	0.0048	1.38	0.45	0.0167
701	0.13	-0.05	0.0239	0.60	0.23	0.0124	0.44	0.08	0.0079	0.61	0.22	0.0103
702	0.96	0.04	0.0091	0.71	-0.30	0.0132	0.73	-0.19	0.0075	0.85	-0.16	0.0218
703	0.86	-0.84	0.0218	4.17	-0.63	0.051	4.51	-0.29	0.0455	4.14	-0.66	0.0223
704	3.72	-0.31	0.0168	4.21	0.12	0.0498	4.51	0.42	0.0454	3.97	-0.13	0.0167
705	4.35	-0.59	0.0274	4.67	-0.40	0.0473	4.93	-0.14	0.0419	4.59	-0.47	0.0272
706	0.69	-0.35	0.0068	0.82	-0.55	0.0068	0.61	-0.76	0.0076	0.43	-0.94	0.006
707	3.07	-0.24	0.0139	3.86	-0.36	0.0311	4.20	-0.02	0.025	4.01	-0.21	0.0157
708	0.57	0.70	0.0163	0.83	0.97	0.0063	0.44	0.59	0.0144	-0.02	0.10	0.0266
709	4.01	-0.38	0.0185	4.03	-1.47	0.0243	4.41	-1.09	0.0211	4.32	-0.78	0.0137
710	1.49	0.81	0.0257	1.56	0.89	0.0228	1.62	0.95	0.0069	1.76	1.08	0.0219
711	0.91	0.04	0.0168	1.08	0.20	0.0268	1.10	0.22	0.012	0.91	0.03	0.0218
712	1.12	-0.22	0.0239	1.24	-0.11	0.02	1.33	-0.02	0.0086	1.35	0.00	0.0134
713	0.58	-0.67	0.0116	0.65	-0.59	0.0307	0.70	-0.54	0.016	0.98	-0.26	0.0086
714	3.38	-1.32	0.0189	4.08	-0.82	0.0162	3.82	-1.08	0.0269	4.39	-0.52	0.0185
715	0.63	-0.84	0.0334	0.79	-0.99	0.0185	0.63	-1.07	0.0157	0.71	-1.31	0.0137
716	0.71	0.43	0.0058	0.76	0.48	0.0098	0.58	0.30	0.0113	0.68	0.40	0.009
717	4.13	0.25	0.0147	4.31	0.43	0.0162	4.15	0.27	0.0148	4.13	0.25	0.0153
718	4.24	-0.73	0.0152	4.56	-0.38	0.0192	4.40	-0.53	0.0182	4.22	-0.72	0.0162
719	1.19	0.70	0.0259	1.40	0.91	0.016	1.45	0.96	0.0099	1.37	0.88	0.0152
720	1.09	0.28	0.0231	1.14	0.32	0.0161	1.30	0.48	0.0078	1.16	0.33	0.0069
721	1.19	-0.32	0.0094	1.25	-0.22	0.0119	0.97	-0.59	0.0076	1.11	-0.46	0.0209
722	2.25	-0.54	0.0142	0.66	-0.20	0.0201	1.51	-1.29	0.0299	1.80	-0.99	0.0195
723	0.19	-0.58	0.0115	0.58	-0.094	0.046	0.46	0.0105	0.62	0.0105	0.41	0.0236
724	0.19	-0.54	0.0128	0.34	-0.098	0.34	0.0091	-0.13	0.0129	0.07	0.0132	0.07
725	3.43	-0.35	0.0103	3.06	-0.72	0.0164	3.03	-0.76	0.0163	3.38	-0.40	0.0109
726	3.34	-0.14	0.0115	3.70	0.22	0.021	3.37	-0.12	0.0102	3.29	-0.19	0.0135
727	4.15	-0.33	0.0148	4.52	0.04	0.0244	4.16	-0.33	0.0148	4.15	-0.34	0.0159
728	0.91	0.59	0.0222	0.48	-0.15	0.0238	0.96	0.33	0.0272	1.61	0.96	0.0502
729	0.88	-0.12	0.0073	0.92	-0.09	0.012	1.15	0.14	0.012	0.80	-0.20	0.0146
730	2.33	-1.78	0.0446	3.26	-0.90	0.0162	2.70	-1.46	0.0507	3.21	-0.95	0.0766
731	1.22	1.04	0.0151	1.31	1.13	0.0102	0.80	0.62	0.0092	0.90	0.73	0.0161
732	0.15	-0.95	0.0169	-0.12	-0.04	0.034	0.09	0.02	-0.29	0.285	-0.14	0.0284
733	0.50	0.20	0.0099	0.66	0.18	0.0087	0.57	0.08	0.0094	0.73	0.24	0.0115
734	4.49	0.06	0.0339	4.62	0.09	0.0488	4.93	0.40	0.042	4.76	0.24	0.035
735	0.17	-0.31	0.0165	0.32	-0.0221	0.39	0.63	0.098	0.53	0.0153	0.50	0.0127
736	0.22	-0.43	0.0322	0.28	0.025	0.37	0.025	0.37	0.0185	0.82	0.13	0.0127
737	0.50	0.52	0.0119	0.49	-0.19	0.0172	0.49	-0.19	0.0124	0.64	-0.04	0.0109
738	0.20	0.20	0.028	0.69	0.56	0.0193	0.57	0.44	0.0068	0.68	0.55	0.0103
739	1.03	-0.09	0.0113	1.01	-0.11	0.006	0.92	-0.19	0.0114	0.98	-0.14	0.0136
740	0.10	-0.20	0.0107	0.26	-0.0991	0.18	0.18	0.0079	-0.16	0.0158	0.06	0.0122
741	0.10	-0.78	0.0104	0.35	-0.50	0.0248	0.33	-0.88	0.0099	0.02	0.12	0.014
742	0.06	0.46	0.0205	0.89	0.26	0.0125	1.08	0.46	0.0094	1.16	0.55	0.0121
743	2.77	0.68	0.0097	2.83	0.75	0.0115	2.67	0.59	0.0084	2.76	0.67	0.0106
744	0.18	-0.07	0.0321	0.24	-0.26	0.0259	0.38	-0.12	0.0146	0.67	0.17	0.0121
745	0.14	0.06	0.0222	0.42	0.03	0.0208	0.41	0.02	0.0083	0.56	0.17	0.0089
746	0.56	-0.40	0.0061	0.75	-0.26	0.0036	0.69	-0.32	0.0035	0.80	-0.21	0.0059
747	1.48	-0.21	0.0186	0.72	-1.06	0.009	1.38	-0.47	0.0143	1.33	-0.65	0.0147
748	0.73	-0.50	0.0066	0.85	-0.02	0.0094	0.45	-0.88	0.0152	0.60	-0.73	0.0121
749	0.61	-0.43	0.0062	0.38	-0.66	0.0113	0.37	-0.67	0.0101	0.61	-0.43	0.0113
750	0.24	0.26	0.0111	0.66	0.56	0.0041	0.28	0.18	0.0077	0.35	0.24	0.0127
751	1.28	-0.29	0.0109	1.21	-0.35	0.0135	0.93	-0.64	0.0137	1.07	-0.49	0.0203
752	0.20	-0.27	0.01	0.26	-1.11	0.0249	0.26	-1.10	0.0219	0.69	-0.67	0.011
753	0.20	-0.12	0.0183	0.71	-0.26	0.0082	0.60	-0.40	0.0075	0.62	-0.38	0.0103

ID	LogHL <sub>1</sub>			LogHL <sub>2</sub>			LogHL <sub>3</sub>			LogHL <sub>4</sub>		
	Pred. (h)	Res	HAT (h) (#=6578)	Pred. (h)	Res	HAT (h) (#=6533)	Pred. (h)	Res	HAT (h) (#=6578)	Pred. (h)	Res	HAT (h) (#=6574)
754	0.04	0.04	0.0175	0.71	0.61	0.0177	0.51	0.40	0.0177	0.73	0.60	0.0177
755	0.17	-1.56	0.0141	0.81	-0.95	0.0152	0.44	-1.31	0.0125	0.41	-1.34	0.0178
756	1.49	1.19	0.0157	1.47	1.17	0.0118	1.46	1.16	0.0042	1.56	1.26	0.007
757	1.44	-0.34	0.022	1.24	-0.54	0.0232	0.90	-0.88	0.0056	1.24	-0.52	0.0259
758	3.71	-0.88	0.011	3.85	-0.80	0.0165	3.95	-0.70	0.0165	3.76	-0.89	0.012
759	3.63	-0.25	0.0106	3.60	-0.28	0.0119	3.69	-0.19	0.0113	3.66	-0.22	0.0109
760	4.93	0.57	0.0065	5.21	0.23	0.0151	4.24	0.36	0.0165	4.06	0.18	0.0123
761	1.19	-0.24	0.0168	1.38	-0.05	0.0137	1.23	-0.20	0.0173	1.13	-0.21	0.0179
7												

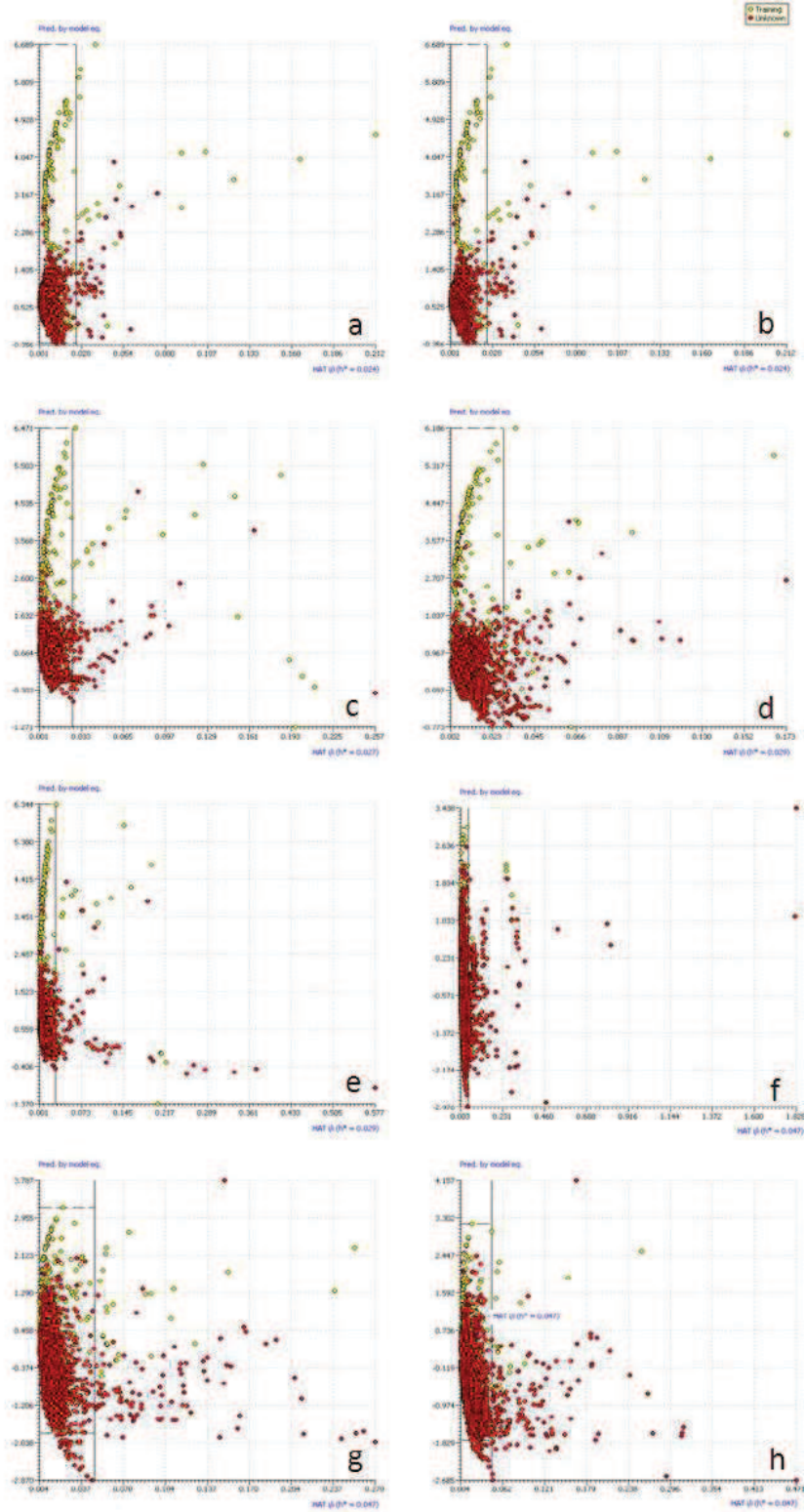


ID	LogHL <sub>1</sub>				LogHL <sub>2</sub>				LogHL <sub>3</sub>				LogHL <sub>4</sub>			
	Pred.	Res	HAT $\sigma$ (h)	HAT $\sigma$ (h)	Pred.	Res	HAT $\sigma$ (h)	HAT $\sigma$ (h)	Pred.	Res	HAT $\sigma$ (h)	HAT $\sigma$ (h)	Pred.	Res	HAT $\sigma$ (h)	HAT $\sigma$ (h)
828	1.23	-1.33	0.1185	0.1185	0.77	0.158	0.074	0.074	0.19	0.19	0.174	0.174	0.11	0.11	0.174	0.174
839	0.34	-0.10	0.0368	0.64	-0.29	0.03	0.66	-0.27	0.0175	0.95	0.03	0.0642	1.11	0.18	0.0204	0.0204
840	0.75	1.31	0.0117	3.30	0.86	0.0136	3.53	1.09	0.0101	3.78	1.34	0.0110	3.75	1.31	0.0117	0.0117
841	0.38	-1.05	0.0093	0.06	0.0236	0.11	0.0217	0.15	0.0217	0.16	0.0233	0.16	0.0233	0.16	0.0233	0.16
842	0.69	0.69	0.0078	0.86	0.86	0.0094	0.72	0.72	0.0066	0.81	0.81	0.014	0.83	0.82	0.0068	0.0068
843	0.53	0.63	0.0084	0.81	0.81	0.0069	0.56	-0.05	0.0068	0.68	0.67	0.0133	0.65	0.03	0.0125	0.0125
844	0.81	0.31	0.0097	0.96	1.06	0.0053	0.96	1.07	0.0072	0.90	0.90	0.0132	0.89	0.99	0.0099	0.0099
845	0.75	0.99	0.0038	0.15	0.40	0.0053	0.52	0.76	0.0055	0.60	0.60	0.0048	0.56	0.81	0.0054	0.0054
846	0.12	-0.39	0.0258	0.50	-0.24	0.0155	0.48	-0.26	0.0089	0.53	-0.21	0.0138	0.46	-0.28	0.0138	0.0138
847	1.83	0.41	0.0152	1.73	0.32	0.0151	2.06	0.65	0.0079	1.85	0.43	0.0074	1.95	0.53	0.0077	0.0077
848	1.22	0.28	0.0219	1.07	-0.29	0.0208	1.32	-0.03	0.0133	0.89	-0.46	0.0477	1.06	-0.29	0.0236	0.0236
849	0.87	-0.05	0.0192	0.79	-0.15	0.0261	1.08	0.14	0.0068	0.75	-0.17	0.0189	1.05	0.13	0.0209	0.0209
850	0.92	0.44	0.0158	0.53	0.06	0.0088	0.91	0.44	0.0156	0.61	0.14	0.0066	0.64	0.17	0.0053	0.0053
851	1.02	0.39	0.0132	0.77	0.12	0.0064	0.84	0.20	0.0093	0.97	0.13	0.0176	1.20	0.36	0.0102	0.0102
852	0.83	0.09	0.0087	0.90	0.03	0.0097	0.93	0.06	0.0112	1.08	0.21	0.0121	1.00	0.13	0.0089	0.0089
853	1.47	0.69	0.0278	0.83	0.05	0.0109	1.18	0.39	0.0444	1.36	0.57	0.0447	0.85	0.07	0.0611	0.0611
854	0.64	0.34	0.0053	0.78	0.47	0.0038	0.81	0.49	0.0042	0.72	0.22	0.0062	0.80	0.30	0.0053	0.0053
855	0.62	0.73	0.0064	0.15	-0.01	0.0221	0.43	0.28	0.0123	0.33	0.18	0.0129	0.13	-0.03	0.0152	0.0152
856	0.61	1.44	0.0054	0.55	1.37	0.0088	0.35	1.18	0.0132	0.32	1.14	0.0124	0.25	1.06	0.0159	0.0159
857	0.56	-0.12	0.0066	0.69	-0.02	0.0233	0.61	-0.11	0.0241	0.61	-0.22	0.0057	0.71	-0.32	0.0071	0.0071
858	0.76	-1.06	0.0072	0.97	-0.88	0.0086	0.79	-1.06	0.014	0.59	0.0212	0.71	0.0283	0.0083	0.0083	0.0083
859	0.72	0.54	0.0066	0.85	0.67	0.0051	0.56	0.38	0.0071	0.59	0.41	0.0071	0.40	0.22	0.0084	0.0084
860	0.89	0.47	0.0127	0.62	0.16	0.0128	0.51	0.05	0.0109	0.49	-0.33	0.0181	0.48	-0.34	0.0281	0.0281
861	0.32	-0.57	0.0054	0.53	-0.78	0.0113	0.23	-1.08	0.0131	0.26	-1.05	0.0145	0.23	-1.07	0.0119	0.0119
862	0.67	0.19	0.0028	0.64	0.16	0.0048	0.44	-0.10	0.0057	0.23	-0.59	0.0129	0.35	-0.47	0.0152	0.0152
863	0.51	0.81	0.0189	0.25	0.18	0.0238	0.24	0.17	0.0288	0.50	0.44	0.0396	0.63	0.57	0.0281	0.0281
864	1.33	0.40	0.0094	0.95	0.33	0.009	1.13	0.11	0.0163	1.14	0.12	0.0206	1.14	0.12	0.0206	0.0206
865	0.12	-0.27	0.0201	0.60	0.05	0.0112	0.48	-0.08	0.0071	0.58	-0.20	0.0088	0.51	-0.27	0.0084	0.0084
866	1.02	0.79	0.0078	1.08	0.84	0.0083	1.02	0.79	0.0097	0.87	0.64	0.0078	0.96	0.73	0.0067	0.0067
867	0.54	1.18	0.006	0.39	-1.47	0.0136	0.40	-1.46	0.0091	0.30	-1.55	0.0098	0.20	-1.65	0.0106	0.0106
868	1.11	0.39	0.011	0.94	0.21	0.0083	0.80	0.07	0.0087	0.97	0.25	0.0155	0.99	0.26	0.0127	0.0127
869	0.94	0.86	0.0218	1.02	0.92	0.0176	1.03	0.92	0.0068	0.98	0.88	0.0096	1.01	0.91	0.0081	0.0081
870	0.43	-1.08	0.0065	0.55	-0.98	0.0114	0.42	-1.10	0.0072	0.41	-1.16	0.0076	0.36	-1.30	0.0094	0.0094
871	0.97	-0.19	0.0101	0.95	-0.21	0.0074	0.68	-0.47	0.0054	0.62	-0.78	0.0069	0.52	-0.86	0.0067	0.0067
872	0.75	-0.16	0.0274	0.90	-0.06	0.0178	0.92	-0.04	0.0103	0.53	0.0229	0.66	0.0266	0.0133	0.0133	0.0133
873	1.33	-0.07	0.0153	1.21	-0.21	0.0219	1.93	0.51	0.0173	1.95	0.494	2.19	0.63	0.0266	0.0266	0.0266
874	0.80	0.45	0.0101	0.87	0.53	0.0075	0.86	0.51	0.008	0.66	0.32	0.0084	0.79	0.46	0.0065	0.0065
875	1.14	-0.12	0.0129	0.90	-0.36	0.0309	1.39	0.12	0.0287	1.06	-0.20	0.0094	1.07	-0.19	0.0099	0.0099
876	0.74	-0.70	0.0075	1.05	-0.39	0.0083	0.66	-0.78	0.0078	0.47	-0.77	0.0152	0.46	-0.59	0.0104	0.0104
877	1.47	0.07	0.0242	1.58	0.18	0.0216	1.58	0.18	0.0068	1.49	0.09	0.0057	1.49	0.09	0.0057	0.0057
878	0.88	0.05	0.0039	1.09	0.26	0.0066	0.88	0.05	0.0081	1.05	0.008	0.99	0.99	0.0072	0.0072	0.0072
879	0.54	0.24	0.006	0.39	0.09	0.0136	0.40	0.10	0.0091	0.30	-0.03	0.0098	0.20	-0.13	0.0106	0.0106
880	0.41	0.24	0.0118	0.72	0.33	0.0081	0.85	0.46	0.0175	0.75	0.36	0.0123	1.08	0.68	0.0184	0.0184
881	1.09	-0.08	0.0031	1.20	0.01	0.0121	1.02	-0.18	0.0119	0.84	-0.35	0.0111	1.04	-0.15	0.0118	0.0118
882	0.65	0.07	0.0118	1.02	-0.24	0.0074	0.87	-0.48	0.0104	0.53	-0.82	0.0121	0.68	-0.88	0.0158	0.0158
883	1.27	-0.41	0.0099	1.12	-0.86	0.0069	1.02	-1.04	0.0097	1.14	-0.94	0.0097	1.14	-0.94	0.0097	0.0097
884	0.46	-0.56	0.0074	0.37	-0.65	0.0144	0.38	-0.65	0.0066	0.17	-1.14	0.0143	0.22	-1.09	0.0096	0.0096
885	0.45	-0.03	0.0057	0.41	-0.07	0.0119	0.38	-0.10	0.008	0.21	-0.38	0.0102	0.17	-0.41	0.0096	0.0096
886	0.02	-0.19	0.0412	0.17	-0.26	0.0294	0.20	-0.23	0.0214	0.55	0.13	0.0118	0.32	-0.10	0.019	0.019
887	0.45	-0.33	0.0054	0.40	-0.38	0.0119	0.40	-0.38	0.0079	0.21	-0.64	0.0102	0.19	-0.66	0.0092	0.0092
888	0.46	0.47	0.005	0.72	0.62	0.0064	0.50	0.40	0.0053	0.55	0.44	0.007	0.54	0.43	0.0066	0.0066
889	0.56	0.39	0.0107	-0.13	-0.52	0.0316	0.34	-0.05	0.0244	0.36	-0.02	0.0252	0.22	-0.22	0.0229	0.0229
890	0.60	-0.93	0.0138	0.44	-1.14	0.0182	0.72	-0.86	0.008	0.85	-0.73	0.0115	0.85	-0.72	0.0092	0.0092
891	0.41	-0.63	0.0046	0.52	-0.62	0.015	0.52	-0.62	0.0149	0.75	0.0085	0.24	0.0666	0.0096	0.0096	0.0096
892	1.08	0.15	0.0192	1.12	0.18	0.0157	1.28	0.33	0.0076	1.24	0.05	0.0089	1.31	0.12	0.0091	0.0091
893	0.90	-0.24	0.0047	0.70	-0.05	0.0083	0.10	-0.65	0.0249	0.37	-0.40	0.0198	0.22	-0.55	0.024	0.024
894	0.92	0.17	0.0092	1.13	0.39	0.0054	0.82	0.08	0.008	0.96	0.10	0.0099	1.14	0.07	0.0108	0.0108
895	1.42	-0.66	0.0215	1.23	-0.84	0.0264	1.18	-0.89	0.007	1.39	-0.69	0.0149	1.26	-0.82	0.0082	0.0082
896	1.90	-0.25	0.0301	1.00	-1.18	0.0063	1.58	-0.59	0.0162	1.64	-0.53	0.0572	1.54	-0.64	0.0193	0.0193
897	1.10	0.33	0.0121	1.01	0.24	0.009	1.03	0.26	0.0081	1.15	0.37	0.0106	1.00	0.22	0.0088	0.0088
898	1.51	-0.05	0.0222	1.23	-0.33	0.0198	1.33	-0.23	0.023	1.26	-0.29	0.03	1.17	-0.38	0.0132	0.0132
899	0.83	0.05	0.008	0.90	0.12	0.0068	0.56	-0.22	0.0092	0.53	0.079	0.55	0.58	0.0097	0.0097	0.0097
900	0.69	-0.16	0.0038	0.91	0.03	0.0059	1.00	0.11	0.0088	0.88	0.00	0.0084	0.97	0.09	0.0091	0.0091
901	0.60	0.18	0.0111	0.92	0.51	0.005	0.86	0.45	0.0072	0.70	0.28	0.0122	0.80	0.39	0.0126	0.0126
902	0.14	-0.09	0.021	0.78	0.17	0.0063	0.61	0.20	0.0078	0.58	0.12	0.0133	0.53	0.07	0.012	0.012
903	0.62	-0.39	0.0083	0.94	0.01	0.0099	0.59	-0.41	0.008	0.53	-0.44	0.0084	0.44	0.27	0.0083	0.0083
904	0.32	0.24	0.0096	0.46	0.28	0.0153	0.51	0.33	0.0084	0.56	0.31	0.0089	0.49	0.24	0.009	0.009
905	0.46	1.06	0.0083	0.68	1.26	0.0267	0.78	1.36	0.0083	0.44	1.03	0.031	0.67	1.25	0.0103	0.0103
906	0.80	0.10	0.0062	0.95	0.23	0.0072	0.95	0.23	0.0106	0.92	0.20	0.0118	0.77	0.05	0.0078	0.0078
907	0.84	-0.16	0.0103	0.46	-0.54	0.0125	0.78	-0.22	0.0074	0.83	-0.17	0.0207	0.87	-0.13	0.009	0.009
908	0.93	1.09	0.0046	0.71	0.86	0.0051	0.70	0.86	0.0126	0.53	0.68	0.0119	0.52	0.67	0.0112	0.0112
909	0.70	0.66	0.0031	0.08	0.93	0.0068	0.69	0.65								

ID	LogHL <sub>1</sub>			LogHL <sub>1</sub>			LogHL <sub>2</sub>			LogHL <sub>3</sub>			LogHL <sub>4</sub>			LogHL <sub>4</sub>		
	Pred. (h)	Res	HAT $\nu$ (h <sup>+</sup> =0.0578)	Pred. (h)	Res	HAT $\nu$ (h <sup>+</sup> =0.0533)	Pred. (h)	Res	HAT $\nu$ (h <sup>+</sup> =0.0533)	Pred. (h)	Res	HAT $\nu$ (h <sup>+</sup> =0.0489)	Pred. (h)	Res	HAT $\nu$ (h <sup>+</sup> =0.0574)	Pred. (h)	Res	HAT $\nu$ (h <sup>+</sup> =0.0574)
1006	0.79	0.03	0.0088	1.08	0.22	0.0077	0.91	0.15	0.0082	0.91	0.12	0.0082	0.91	0.12	0.0082	0.91	0.12	0.0082
1007	1.34	0.59	0.0176	1.21	0.41	0.0076	1.09	0.29	0.0171	1.30	0.49	0.0337	1.23	0.42	0.015			
1008	0.46	-0.51	0.0049	0.69	-0.44	0.006	0.46	-0.66	0.01	0.28	-0.85	0.0106	0.34	-0.79	0.0075			
1009	0.91	-0.12	0.0167	0.18	-0.93	0.0125	0.12	-1.00	0.0259	0.28	-0.83	0.0156	-0.09	-1.20	0.00606			
1010	0.85	0.30	0.0048	0.94	0.21	0.007	0.71	-0.02	0.0053	0.66	-0.07	0.0091	0.79	0.06	0.0061			
1011	0.51	-0.44	0.0072	1.00	0.43	0.0091	0.72	-0.24	0.0041	0.45	-0.59	0.0195	0.64	-0.39	0.0093			
1012	0.31	0.24	0.0079	1.10	0.51	0.0092	1.03	0.41	0.0086	1.14	0.43	0.0096	0.99	0.40	0.0058			
1013	0.57	0.53	0.0081	0.96	0.92	0.0152	0.76	0.73	0.0105	0.85	0.76	0.0186	0.82	0.73	0.0106			
1014	0.87	0.00	0.0181	0.51	-0.51	0.0255	0.70	-0.32	0.0137	1.03	0.03	0.0262	1.02	0.02	0.018			
1015	0.51	0.30	0.0065	0.51	0.10	0.0059	0.10	-0.31	0.0161	0.28	-0.12	0.0091	0.24	-0.16	0.0155			
1016	0.71	-0.14	0.0055	0.85	-0.21	0.0052	0.75	-0.32	0.0077	0.66	-0.27	0.0053	0.50	-0.43	0.0045			
1017	0.94	0.31	0.0064	1.24	0.62	0.0079	0.91	0.29	0.0104	1.14	0.17	0.01	1.00	0.03	0.0058			
1018	0.51	-0.83	0.0075	0.75	-0.59	0.0054	0.45	-0.89	0.0086	0.20	0.0159	0.37	0.015					
1019	0.42	-0.58	0.0101	0.69	-0.074	0.80	0.80	0.0075	0.47	0.0142	0.70	0.0103						
1020	1.14	0.80	0.0147	1.27	0.78	0.0105	0.79	0.30	0.0037	0.93	0.44	0.009	0.88	0.39	0.0056			
1021	0.44	0.12	0.01	0.49	-0.06	0.0087	0.36	-0.18	0.0104	0.46	-0.17	0.0111	0.40	-0.24	0.0112			
1022	0.84	-0.52	0.0048	0.77	-0.72	0.0098	0.84	-0.65	0.008	0.71	0.0113	0.82	0.0084					
1023	0.87	-0.43	0.005	1.20	-0.10	0.0129	1.14	-0.16	0.0125	0.52	-0.78	0.0121	0.70	-0.61	0.0092			
1024	0.66	0.58	0.0106	0.93	0.86	0.0073	0.61	0.53	0.0098	0.89	0.80	0.0078	0.80	0.72	0.0055			
1025	0.26	0.62	0.0152	0.52	0.51	0.0122	0.93	0.59	0.0098	0.72	0.38	0.0155	0.88	0.54	0.0103			
1026	0.80	-0.24	0.0092	0.94	0.11	0.0066	0.62	-0.43	0.0103	0.75	-0.30	0.0166	0.84	-0.21	0.0147			
1027	0.97	0.72	0.0057	0.57	0.32	0.0059	0.74	0.48	0.0219	0.56	0.31	0.0147	0.48	0.23	0.0112			
1028	0.24	-1.68	0.0103	0.50	0.0089	0.55	0.50	0.0094	0.29	0.0153	0.44	0.012						
1029	0.87	0.16	0.0103	1.01	0.30	0.0189	1.20	0.48	0.0082	1.21	0.29	0.0073	1.19	0.28	0.0081			
1030	0.96	0.47	0.0168	1.20	0.70	0.0164	1.07	0.58	0.0081	1.21	0.72	0.0096	1.25	0.75	0.0068			
1031	1.39	0.36	0.0152	1.18	0.09	0.0084	1.47	0.38	0.0152	1.13	0.06	0.0375	1.42	0.34	0.0238			
1032	0.38	-0.38	0.0095	0.28	-0.91	0.0089	0.81	-0.84	0.0114	0.67	-0.93	0.0203	0.78	-0.87	0.0159			
1033	0.77	0.16	0.0147	0.87	0.25	0.0135	1.06	0.44	0.01	0.90	0.29	0.0118	0.88	0.28	0.0126			
1034	0.20	-0.58	0.0142	0.14	0.0193	0.15	0.15	0.0215	-0.24	0.0215	-0.12	0.0305						
1035	0.92	-0.06	0.0252	0.91	-0.06	0.0147	0.99	0.02	0.0319	0.55	-0.44	0.0134	0.74	-0.25	0.0343			
1036	0.33	0.44	0.0148	0.37	0.50	0.0123	0.06	0.18	0.0284	-0.23	-0.11	0.0371	-0.04	0.08	0.0324			
1037	0.74	-1.16	0.0055	0.91	-1.06	0.0042	0.63	-1.35	0.0075	0.75	-1.41	0.011	0.69	-1.47	0.008			
1038	0.90	0.65	0.0159	0.85	0.56	0.0056	0.73	0.43	0.0116	0.75	0.46	0.0096	0.50	0.20	0.0129			
1039	0.65	-0.26	0.0107	1.02	0.00	0.0107	0.94	-0.08	0.0074	0.54	-0.49	0.0203	0.75	-0.28	0.0171			
1040	0.11	0.00	0.02	0.40	0.28	0.0107	0.11	0.00	0.0228	0.25	0.13	0.0126	-0.24	-0.36	0.0931			
1041	0.77	0.73	0.0072	1.13	1.09	0.0078	0.74	0.70	0.0073	0.85	0.81	0.0124	0.82	0.78	0.0086			
1042	0.94	-0.40	0.007	1.26	-0.10	0.0088	0.95	-0.41	0.0061	0.91	-0.45	0.0102	0.95	-0.41	0.0062			
1043	0.75	-0.15	0.0088	0.78	-0.12	0.0036	0.62	-0.28	0.0043	0.50	-0.41	0.0103	0.56	-0.34	0.0103			
1044	1.00	0.16	0.0304	1.09	0.23	0.0106	1.37	0.52	0.0332	0.60	-0.24	0.0154	0.56	-0.28	0.0114			
1045	0.33	-0.25	0.0104	0.46	0.0121	0.44	0.44	0.0066	0.44	0.44	0.0094	0.29	0.0065	0.0103				
1046	0.88	0.34	0.0059	1.09	0.11	0.0051	0.75	-0.24	0.0038	1.01	0.03	0.0074	0.89	-0.10	0.0055			
1047	0.57	0.70	0.0065	0.50	0.60	0.0142	0.51	0.61	0.015	0.48	0.53	0.0104	0.37	0.41	0.0266			
1048	0.40	0.13	0.0185	0.39	-0.14	0.0157	0.16	-0.38	0.0183	0.46	-0.11	0.0091	0.31	-0.26	0.0089			
1049	1.72	0.04	0.0212	0.87	-0.82	0.0111	1.67	-0.02	0.0204	1.59	-0.12	0.0548	1.76	0.06	0.0227			
1050	0.59	0.71	0.0028	0.37	0.49	0.0174	0.29	0.41	0.0111	0.49	0.61	0.0084	0.35	0.47	0.013			
1051	0.60	0.00	0.022	0.69	0.00	0.0097	0.58	-0.02	0.0097	0.58	0.45	-0.15	0.0224	0.58	0.0103			
1052	0.74	-0.39	0.01	0.69	-0.44	0.0048	0.76	-0.38	0.0065	0.39	0.0089	0.40	0.011					
1053	0.45	-1.20	0.0098	1.28	0.70	0.0112	0.70	0.0047	0.52	0.0246	0.57	0.0105						
1054	1.49	1.62	0.016	2.00	0.34	0.0216	0.84	0.98	0.0211	0.92	1.05	0.0322	0.73	0.86	0.0282			
1055	1.72	-0.70	0.0146	2.17	-0.24	0.0085	2.02	-0.39	0.0098	1.98	-0.44	0.0143	2.00	-0.43	0.011			
1056	0.66	-0.72	0.0059	0.98	-0.64	0.0087	0.84	-0.78	0.0101	0.72	-0.90	0.0069	0.93	-0.68	0.0069			
1057	1.38	0.64	0.0354	1.12	0.42	0.0195	1.44	0.74	0.011	1.06	0.36	0.0071	1.07	0.37	0.0098			
1058	0.25	0.05	0.0087	0.43	-0.58	0.0124	0.24	-0.76	0.0098	0.24	-0.76	0.0105	0.28	-0.73	0.0098			
1059	0.85	0.22	0.0111	0.88	0.25	0.004	0.78	0.16	0.0143	0.64	0.01	0.0049	0.63	0.00	0.0053			
1060	0.69	-0.26	0.009	0.71	-0.24	0.0129	0.47	-0.49	0.0121	0.84	-0.11	0.0071	0.59	-0.36	0.0116			
1061	0.98	-0.26	0.0069	0.84	0.0034	0.77	0.77	0.006	1.18	0.0104	1.09	0.0079						
1062	1.29	-0.05	0.0092	0.97	-0.37	0.004	0.86	-0.48	0.0112	0.93	-0.42	0.0194	0.92	-0.43	0.0115			
1063	2.80	-0.12	0.0085	1.09	-1.81	0.015	2.04	-0.89	0.0514	1.85	-1.08	0.1235	2.08	-0.85	0.0542			
1064	0.84	0.19	0.0107	0.81	-0.02	0.0039	0.78	-0.05	0.007	0.73	-0.04	0.0101	0.89	0.06	0.0088			
1065	0.99	1.51	0.0106	0.58	1.10	0.0235	1.12	1.64	0.0107	1.08	1.60	0.0163	1.11	1.63	0.0123			
1066	1.73	0.69	0.0187	1.13	0.09	0.0066	1.49	0.45	0.0099	1.65	0.60	0.0314	1.67	0.62	0.014			
1067	1.33	-0.21	0.0178	1.10	-0.35	0.0102	1.09	-0.46	0.0092	0.95	-0.60	0.0175	0.93	-0.61	0.0095			
1068	0.79	-0.45	0.0071	0.80	-0.39	0.0073	0.77	-0.51	0.0115	0.87	-0.41	0.0134	0.97	-0.31	0.0141			
1069	0.73	-0.65	0.0162	0.60	-0.79	0.009	0.65	-0.74	0.0403	0.73	0.0196	0.40	0.40	0.0197				
1070	0.54	-0.30	0.0088	0.75	-0.06	0.0067	0.91	-0.21	0.0057	0.57	0.0155	0.71	0.0118					
1071	0.54	0.20	0.0075	0.84	0.28	0.0073	0.70	0.15	0.0037	0.88	0.35	0.0137	0.81	0.28	0.0058			
1072	0.49	-0.76	0.0051	0.60	-0.69	0.008	0.42	-0.87	0.0098	0.39	-0.88	0.0127	0.41	-0.85	0.0093			
1073	0.49	-0.09	0.0173	0.88	0.29	0.0145	0.99	0.40	0.0069	0.89	0.12	0.0129	0.89	0.12	0.0123			
1074	0.82	-0.16	0.0062	1.01	0.03	0.0049	0.89	-0.08	0.0054	1.21	0.23	0.012	1.15	0.17	0.0079			
1075	1.13	-0.43	0.0114	0.95	-0.61	0.0091	0.78	-0.79	0.0079	0.98	-0.57	0.0123	0.93	-0.63	0.0098			
1076	1.11	-0.33	0.0116	1.10	-0.33	0.009	1.20	-0.23	0.0066	1.32	-0.12	0.0						

**Figure S1: Insubria graphs for the application of the human and fish biotransformation models to the PPCP dataset.**

**(a:  $HL_T$ , b:  $HL_{B1}$ , c:  $HL_{B2}$ , d:  $HL_{B3}$ , e:  $HL_{B4}$ , f:  $HL_{N1}$ , g:  $HL_{N2}$ , h:  $HL_{N3}$ )**



**Figure S2: Iterations for the selection of the two minimum convex hulls.**  
(a: 0 outlier, b: 1 outlier, c: 2 outliers, d:3 outliers, e: 4 outliers, f: 5 outliers, g: 6 outliers, h: 7 outliers)

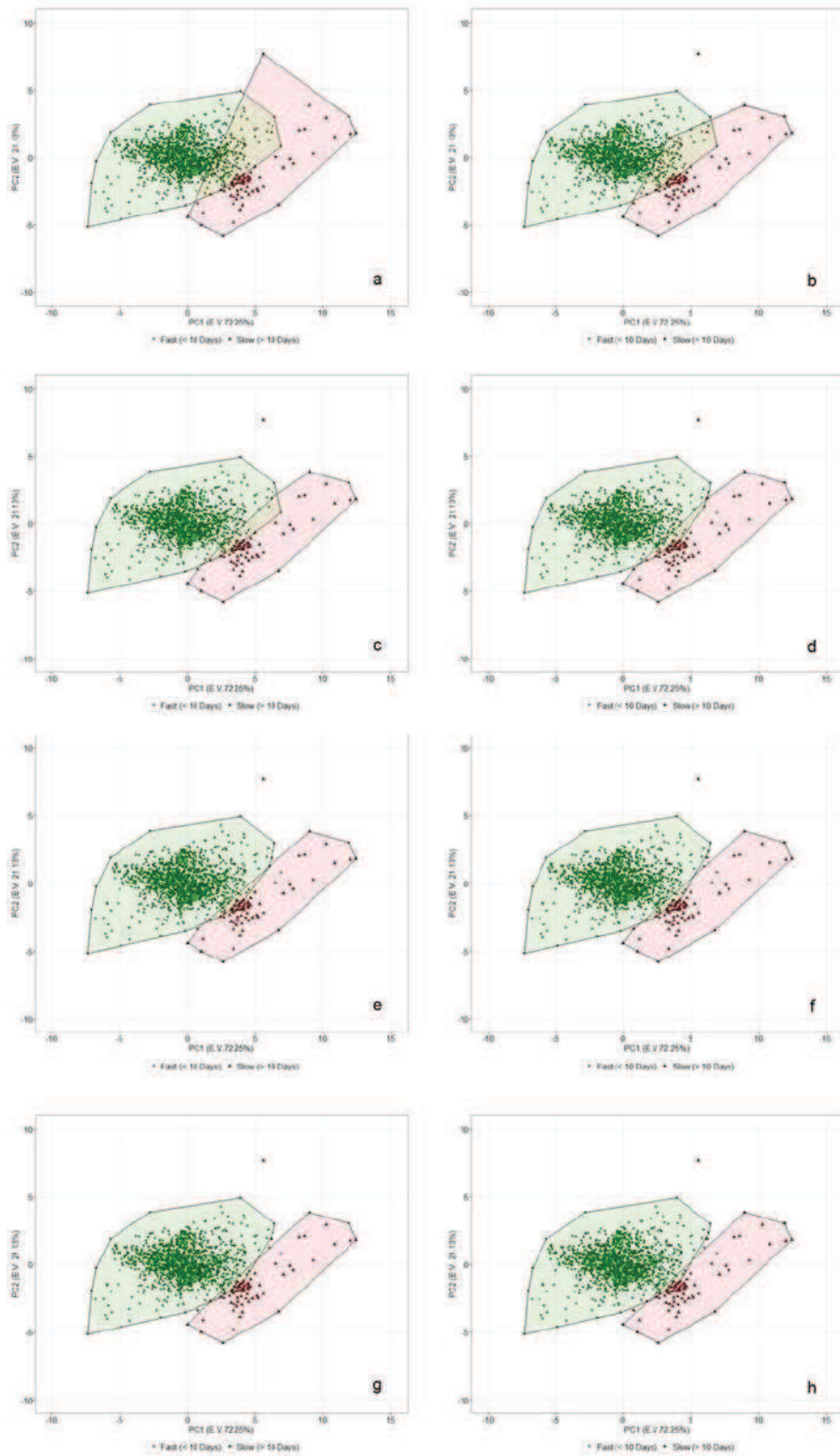


Table S3: CAS, human and fish predicted biotransformation HLs, PBT assessment and Priority level for the screened PPCPs.

(Low priority: not PBT and fast biotransformed compounds, Priority (Group 3): PBT for the PBT Profiler and slowly metabolized compounds, Priority (Group 2): not PBT but slowly biotransformed compounds, Priority (Group 1): PBT for the Insubria PBT Index and slowly metabolized compounds, High Priority: PBT by consensus and slowly metabolized compounds; experimental values are reported in bold)

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Index	PBT Profiler			Priority Level
		logHL <sub>1</sub> (h)	logHL <sub>h1</sub> (h)	logHL <sub>h2</sub> (h)	logHL <sub>h3</sub> (h)	logHL <sub>h4</sub> (h)	logHL <sub>f1</sub> (h)	logHL <sub>f2</sub> (h)	logHL <sub>f3</sub> (h)		P	B	T	
S1	000050-04-4	0.85	0.35	0.80	1.01	0.71	1.00	0.88	0.80	-1.17	3	1	2	Low Priority
S2	000050-06-6	<b>2.00</b>	<b>2.11</b>	<b>2.11</b>	<b>2.11</b>	<b>2.11</b>	0.03	0.15	0.09	-0.60	2	1	2	Low Priority
S3	000050-10-2	1.03	1.19	1.10	1.11	0.91	1.17	1.63	1.20	-0.07	2	1	1	Low Priority
S4	000050-11-3	0.38	0.26	0.28	0.36	0.42	-0.23	-0.01	-0.04	-1.50	2	1	2	Low Priority
S5	000050-12-4	<b>0.85</b>	<b>0.88</b>	<b>0.88</b>	<b>0.92</b>	<b>0.92</b>	0.21	0.35	0.26	-0.44	2	1	2	Low Priority
S6	000050-18-0	<b>0.90</b>	<b>0.94</b>	<b>0.94</b>	<b>0.94</b>	<b>0.94</b>	0.27	0.39	0.27	-0.67	2	1	3	Low Priority
S7	000050-23-7	<b>0.20</b>	<b>0.22</b>	<b>0.22</b>	<b>0.21</b>	<b>0.21</b>	1.14	0.96	1.04	-2.31	2	1	2	Low Priority
S8	000050-27-1	0.76	1.01	0.94	0.79	0.86	1.32	1.12	1.24	-1.60	2	1	2	Low Priority
S9	000050-28-2	<b>0.23</b>	<b>0.23</b>	<b>0.23</b>	<b>0.23</b>	<b>0.23</b>	1.43	1.21	1.31	-1.21	2	1	2	Low Priority
S10	000050-33-9	0.75	0.93	0.52	0.62	0.73	0.96	1.04	0.60	1.20	1	1	3	Low Priority
S11	000050-35-1	<b>0.67</b>	<b>1.04</b>	<b>1.04</b>	<b>1.05</b>	<b>1.05</b>	0.15	0.07	0.01	-0.01	2	1	1	Low Priority
S12	000050-36-2	<b>-0.12</b>	<b>-0.11</b>	<b>-0.11</b>	<b>-0.11</b>	<b>-0.11</b>	0.79	0.93	0.86	-0.06	2	1	2	Low Priority
S13	000050-37-3	<b>0.48</b>	<b>0.48</b>	<b>0.46</b>	<b>0.49</b>	<b>0.49</b>	1.19	1.28	0.74	0.34	2	1	2	Low Priority
S14	000050-44-2	0.18	0.46	0.41	0.16	0.38	0.43	1.09	0.22	0.20	1	1	2	Low Priority
S15	000050-47-5	<b>1.34</b>	<b>1.35</b>	<b>1.35</b>	<b>1.35</b>	<b>1.35</b>	2.14	2.06	1.83	0.70	1	1	3	Low Priority
S16	000050-48-6	<b>1.23</b>	<b>1.24</b>	<b>1.24</b>	<b>1.24</b>	<b>1.24</b>	2.86	2.66	2.71	1.32	3	1	3	Priority (Group 2)
S17	000050-49-7	<b>1.20</b>	<b>1.21</b>	<b>1.21</b>	<b>1.21</b>	<b>1.21</b>	2.50	2.50	2.26	1.10	2	1	3	Priority (Group 2)
S18	000050-50-0	0.91	1.11	0.89	0.79	0.94	1.54	1.30	1.44	0.63	2	2	3	Low Priority
S19	000050-52-2	<b>1.36</b>	<b>1.36</b>	<b>1.36</b>	<b>1.36</b>	<b>1.36</b>	2.76	2.30	2.43	1.70	2	2	3	Priority (Group 2)
S20	000050-53-3	<b>1.04</b>	<b>1.05</b>	<b>1.05</b>	<b>1.05</b>	<b>1.05</b>	3.00	2.53	2.80	1.64	2	2	3	High Priority
S21	000050-60-2	<b>-0.50</b>	<b>-0.51</b>	<b>-0.51</b>	<b>-0.49</b>	<b>-0.49</b>	1.16	1.23	0.91	0.34	2	1	3	Low Priority
S22	000050-65-7	1.07	1.32	1.43	1.43	1.42	1.56	1.11	1.25	1.76	2	1	3	Low Priority
S23	000050-78-2	<b>-0.59</b>	<b>-0.58</b>	<b>-0.58</b>	<b>-0.58</b>	<b>-0.58</b>	0.04	0.02	0.21	-0.35	1	1	1	Low Priority
S24	000050-81-7	-0.01	0.05	0.33	0.29	0.25	-0.54	-0.33	-0.22	-2.81	1	1	2	Low Priority
S25	000050-91-9	0.46	0.53	0.66	0.58	0.56	-0.14	0.06	-0.02	-1.65	1	1	1	Low Priority
S26	000051-06-9	<b>0.49</b>	<b>0.75</b>	<b>0.75</b>	<b>0.75</b>	<b>0.75</b>	0.37	0.58	0.19	-1.41	2	1	2	Low Priority
S27	000051-12-7	0.64	0.76	0.31	0.61	0.61	0.41	0.76	0.26	0.11	2	1	2	Low Priority
S28	000051-21-8	<b>-0.60</b>	<b>-0.58</b>	<b>-0.58</b>	<b>-0.58</b>	<b>-0.58</b>	-0.60	-0.42	-0.45	-1.20	1	1	2	Low Priority
S29	000051-34-3	<b>0.65</b>	<b>0.76</b>	<b>0.76</b>	<b>0.59</b>	<b>0.67</b>	0.44	0.55	0.44	-0.67	2	1	3	Low Priority
S30	000051-35-4	0.12	0.06	0.33	0.02	0.28	-0.45	-0.23	-0.14	-2.61	1	1	1	Low Priority
S31	000051-41-2	0.26	0.41	0.51	0.47	0.52	0.42	0.22	0.50	-2.31	1	1	1	Low Priority
S32	000051-43-4	0.41	0.52	0.54	0.47	0.51	0.60	0.39	0.65	-1.94	1	1	1	Low Priority
S33	000051-52-5	<b>0.11</b>	<b>0.12</b>	<b>0.12</b>	<b>0.12</b>	<b>0.12</b>	0.12	0.12	0.12	-1.83	2	1	2	Low Priority
S34	000051-55-8	<b>0.61</b>	<b>0.98</b>	<b>0.98</b>	<b>0.98</b>	<b>0.98</b>	0.56	0.65	0.52	-0.67	2	1	2	Low Priority
S35	000051-61-6	0.30	0.44	0.63	0.36	0.52	0.51	0.29	0.58	-1.91	1	1	2	Low Priority
S36	000051-64-9	0.81	0.56	0.91	0.87	1.13	0.84	0.91	0.87	-1.04	1	1	2	Low Priority
S37	000051-71-8	0.77	0.71	0.58	0.73	0.88	0.69	0.79	0.82	-1.40	1	1	2	Low Priority
S38	000051-75-2	<b>-0.60</b>	<b>-0.60</b>	<b>-0.60</b>	<b>-0.59</b>	<b>-0.59</b>	1.39	1.42	1.39	-0.26	2	1	2	Low Priority
S39	000051-83-2	0.75	0.77	0.72	1.21	0.93	-0.19	0.52	0.32	-1.58	2	1	1	Low Priority
S40	000052-01-7	<b>-0.78</b>	<b>-0.77</b>	<b>-0.77</b>	<b>-0.77</b>	<b>-0.77</b>	1.56	1.22	1.47	-0.92	2	1	2	Low Priority
S41	000052-24-4	<b>0.43</b>	<b>0.43</b>	<b>0.43</b>	<b>0.43</b>	<b>0.43</b>	1.26	1.25	1.24	-1.37	1	1	2	Low Priority
S42	000052-53-9	<b>0.45</b>	<b>0.46</b>	<b>0.46</b>	<b>0.46</b>	<b>0.46</b>	2.23	1.99	2.49	1.09	3	1	3	Priority (Group 2)
S43	000052-67-5	<b>0.00</b>	<b>0.12</b>	<b>0.12</b>	<b>0.12</b>	<b>0.12</b>	-0.22	0.00	0.12	-2.61	1	1	1	Low Priority
S44	000052-86-8	<b>1.54</b>	<b>1.55</b>	<b>1.55</b>	<b>1.55</b>	<b>1.55</b>	1.81	1.70	1.95	1.93	3	1	3	Low Priority
S45	000052-90-4	-0.36	-0.23	0.03	-0.51	-0.20	-0.56	-0.39	-0.22	-2.58	1	1	1	Low Priority
S46	000053-16-7	<b>1.28</b>	<b>1.28</b>	<b>1.28</b>	<b>1.28</b>	<b>1.28</b>	1.02	0.81	0.88	-0.66	2	1	2	Low Priority
S47	000053-19-0	<b>3.33</b>	<b>3.33</b>	<b>3.33</b>	<b>3.33</b>	<b>3.33</b>	<b>3.03</b>	<b>3.03</b>	<b>3.57</b>	<b>3.2</b>	<b>3</b>	<b>2</b>	<b>3</b>	High Priority
S48	000053-39-4	<b>0.95</b>	<b>0.95</b>	<b>0.95</b>	<b>0.95</b>	<b>0.95</b>	1.14	1.18	1.22	-1.94	2	1	2	Low Priority
S49	000053-43-0	0.80	0.90	0.95	0.83	0.83	1.17	0.98	0.94	-1.75	2	1	2	Low Priority
S50	000053-86-1	<b>0.15</b>	<b>0.22</b>	<b>0.22</b>	<b>0.22</b>	<b>0.22</b>	1.00	0.66	0.53	2.31	2	1	2	Low Priority
S51	000054-05-7	<b>2.76</b>	<b>3.11</b>	<b>3.11</b>	<b>3.11</b>	<b>3.11</b>	2.25	2.23	2.07	1.05	2	1	3	Priority (Group 2)
S52	000054-11-5	<b>0.30</b>	<b>0.38</b>	<b>0.38</b>	<b>0.38</b>	<b>0.38</b>	1.41	1.62	1.16	-0.23	2	1	2	Low Priority
S53	000054-31-9	<b>0.40</b>	<b>0.93</b>	<b>0.93</b>	<b>0.93</b>	<b>0.93</b>	0.86	0.55	0.79	0.38	2	1	2	Low Priority
S54	000054-36-4	<b>0.28</b>	<b>0.30</b>	<b>0.30</b>	<b>0.31</b>	<b>0.31</b>	0.72	1.19	0.48	1.01	2	1	1	Low Priority
S55	000054-42-2	0.65	0.73	0.99	0.88	0.93	0.06	0.16	0.11	-1.62	2	1	2	Low Priority
S56	000054-47-7	0.32	0.56	0.79	0.48	0.55	0.08	0.12	-0.08	-1.13	2	1	1	Low Priority
S57	000054-49-9	0.38	0.49	0.56	0.44	0.58	0.43	0.38	0.48	-1.94	1	1	2	Low Priority
S58	000054-85-3	<b>0.00</b>	<b>0.11</b>	<b>0.11</b>	<b>0.13</b>	<b>0.13</b>	-0.51	-0.17	-0.59	-1.35	2	1	2	Low Priority
S59	000054-91-1	0.84	1.08	0.95	0.87	0.96	0.76	1.14	0.90	-0.03	2	1	2	Low Priority
S60	000054-92-2	0.78	0.76	0.52	0.69	0.85	0.03	0.38	-0.12	-1.00	2	1	2	Low Priority
S61	000055-63-0	<b>-1.30</b>	<b>-1.31</b>	<b>-1.31</b>	<b>-1.30</b>	<b>-1.30</b>	1.39	0.17	1.61	-0.34	2	1	1	Low Priority
S62	000055-73-2	1.18	0.71	1.13	0.77	0.66	1.12	1.38	1.21	-0.79	1	1	1	Low Priority
S63	000055-98-1	<b>0.53</b>	<b>0.57</b>	<b>0.57</b>	<b>0.57</b>	<b>0.57</b>	0.11	0.42	0.47	-0.81	2	1	1	Low Priority
S64	000056-29-1	<b>0.69</b>	<b>0.69</b>	<b>0.69</b>	<b>0.69</b>	<b>0.69</b>	0.19	0.18	0.10	-1.31	2	1	2	Low Priority
S65	000056-41-7	-0.19	-0.26	0.29	-0.51	0.02	-0.94	-0.74	-0.57	-2.57	1	1	1	Low Priority
S66	000056-45-1	-0.26	-0.28	0.08	-0.38	-0.07	-0.90	-0.68	-0.52	-2.97	1	1	1	Low Priority
S67	000056-53-1	0.71	0.68	0.87	0.56	0.55	1.52	1.20	1.50	0.36	2	2	3	Low Priority
S68	000056-54-2	<b>0.82</b>	<b>0.89</b>	<b>0.89</b>	<b>0.89</b>	<b>0.89</b>	1.24	1.11	0.59	0.42	2	1	2	Low Priority
S69	000056-75-7	<b>0.66</b>	<b>0.71</b>	<b>0.71</b>	<b>0.71</b>	<b>0.71</b>	0.86	0.89	0.67	0.12	2	1	1	Low Priority
S70	000056-81-5	-0.11	-0.27	0.09	-0.27	-0.02	-0.86	-0.69	-0.58	-2.76	1	1	1	Low Priority
S71	000056-84-8	-0.02	-0.31	-0.13	-0.14	0.04	-0.71	-0.46	-0.32	-2.76	1	1	1	Low Priority
S72	000056-85-9	-0.01	-0.05	-0.01	-0.17	-0.02	-0.54	-0.29	-0.19	-3.17	1	1	1	Low Priority
S73	000056-86-0	0.01	-0.15	-0.02	-0.17	-0.04	-0.54	-0.29	-0.17	-2.77	1	1	1	Low Priority
S74	000056-87-1	0.09	0.08	-0.06	-0.18	0.01	-0.31	-0.10	0.00	-3.39	1	1	1	Low Priority
S75	000056-89-3	-0.04	0.20	0.02	0.09	0.06	-0.18	-0.27	0.17	-3.57	1	1	1	Low Priority
S76	000057-00-1	0.02	0.02	0.19	-0.05	0.13	-0.74	-0.48	0.36	-2.77	1	1	1	Low Priority

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Index	PBT Profiler			Priority Level
		logHL <sub>1</sub> (h)	logHL <sub>h1</sub> (h)	logHL <sub>h2</sub> (h)	logHL <sub>h3</sub> (h)	logHL <sub>h4</sub> (h)	logHL <sub>f1</sub> (h)	logHL <sub>f2</sub> (h)	logHL <sub>f3</sub> (h)		P	B	T	
S77	000057-27-2	0.30	0.35	0.35	0.35	0.35	1.59	0.86	1.17	-1.00	2	1	2	Low Priority
S78	000057-41-0	<b>1.34</b>	<b>1.36</b>	<b>1.36</b>	<b>1.60</b>	<b>1.60</b>	0.44	0.53	0.42	0.46	2	1	2	Low Priority
S79	000057-42-1	<b>0.90</b>	<b>0.92</b>	<b>0.92</b>	<b>0.92</b>	<b>0.92</b>	0.81	0.93	0.80	-0.28	2	1	2	Low Priority
S80	000057-43-2	0.59	0.53	0.54	0.55	0.53	-0.02	0.23	0.17	-1.89	2	1	2	

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	logHL <sub>4</sub> (h)	logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	PBT Index	P	B	T		
S159	000068-22-4	0.85	0.85	0.85	0.85	1.45	1.26	1.27	-1.51	2	1	2	Low Priority	
S160	000068-35-9	0.85	1.27	1.27	1.27	-0.10	0.35	-0.29	0.09	2	1	2	Low Priority	
S161	000068-41-7	-0.02	0.15	0.53	0.25	0.58	-0.60	-0.72	-2.61	1	1	2	Low Priority	
S162	000068-88-2	1.35	1.38	1.38	1.39	1.39	1.76	1.51	2.00	1	1	2	Low Priority	
S163	000069-23-8	1.37	1.24	1.28	0.95	1.09	1.28	1.49	1.10	2.34	3	1	3	Low Priority
S164	000069-53-4	0.15	0.39	0.39	0.39	0.39	0.32	0.37	0.48	-1.40	2	1	2	Low Priority
S165	000069-65-8	0.22	0.46	0.46	0.46	0.46	-0.29	-0.08	-0.02	-3.98	1	1	1	Low Priority
S166	000069-72-7	0.11	0.13	0.36	0.03	0.25	-0.11	-0.15	0.08	-0.93	1	1	2	Low Priority
S167	000070-00-8	1.07	0.58	1.11	0.99	1.01	0.40	0.83	0.58	-0.34	2	1	2	Low Priority
S168	000070-26-8	0.00	0.03	0.02	-0.22	-0.01	-0.48	-0.26	-0.15	-3.38	1	1	1	Low Priority
S169	000070-30-4	3.03	3.20	3.58	3.43	3.62	2.66	2.40	2.57	3.96	3	3	3	High Priority
S170	000070-47-3	-0.05	-0.21	-0.11	-0.16	0.04	-0.72	-0.46	-0.35	-3.16	1	1	1	Low Priority
S171	000071-00-1	0.05	0.29	0.22	-0.09	0.18	-0.41	-0.02	-0.37	-1.92	1	1	1	Low Priority
S172	000071-58-9	0.98	0.72	1.07	0.90	0.76	1.44	1.43	1.45	-0.96	2	1	2	Low Priority
S173	000072-14-0	0.73	0.88	0.80	1.22	1.21	0.04	0.17	-0.18	-0.12	2	1	2	Low Priority
S174	000072-18-4	-0.16	-0.09	0.08	-0.44	-0.13	-0.50	-0.25	-0.13	-2.60	1	1	1	Low Priority
S175	000072-19-5	-0.21	-0.14	0.07	-0.32	-0.13	-0.70	-0.49	-0.34	-2.98	1	1	1	Low Priority
S176	000072-33-3	1.00	1.18	1.35	1.06	1.09	1.64	1.42	1.49	-0.64	2	1	2	Low Priority
S177	000072-44-6	0.77	0.98	0.88	0.67	0.85	0.87	1.11	1.54	0.22	2	1	3	Low Priority
S178	000072-69-5	1.48	1.49	1.49	1.49	1.49	2.48	2.21	2.26	0.91	3	1	3	Priority (Group 2)
S179	000073-22-3	0.34	0.60	0.37	0.19	0.40	0.06	0.25	-0.04	-0.87	1	1	1	Low Priority
S180	000073-31-4	-0.15	-0.14	-0.14	-0.15	-0.15	0.65	0.78	0.54	-0.14	2	1	2	Low Priority
S181	000073-32-5	0.11	-0.07	-0.03	-0.21	0.01	-0.32	-0.10	0.00	-2.61	1	1	1	Low Priority
S182	000073-48-3	0.93	0.97	0.97	1.05	1.05	0.71	1.16	0.59	2.03	3	1	2	Low Priority
S183	000073-49-4	0.67	0.83	1.17	1.31	1.29	0.63	0.47	0.53	-0.73	2	1	2	Low Priority
S184	000074-55-5	0.49	1.06	1.06	1.06	1.06	0.53	0.73	0.77	-3.20	1	1	1	Low Priority
S185	000074-79-3	0.11	0.25	0.12	0.02	0.20	-0.38	-0.09	-0.01	-3.95	1	1	1	Low Priority
S186	000075-85-4	0.18	0.17	0.61	0.20	0.30	-0.47	-0.19	-0.19	-2.03	1	1	1	Low Priority
S187	000076-22-2	0.32	0.71	0.62	0.47	0.28	0.50	0.74	0.69	-1.53	2	1	2	Low Priority
S188	000076-41-5	0.11	0.15	0.15	0.15	0.15	1.07	0.68	0.97	-1.08	2	1	2	Low Priority
S189	000076-42-6	0.74	0.83	0.83	0.83	0.83	1.13	0.75	1.04	-0.69	3	1	1	Low Priority
S190	000076-43-7	0.96	0.98	0.98	0.97	0.97	0.91	0.89	0.46	-1.70	3	1	1	Low Priority
S191	000076-47-1	0.91	0.52	0.79	1.01	0.68	1.14	1.05	1.06	-1.76	3	1	2	Low Priority
S192	000076-57-3	0.60	0.65	0.65	0.65	0.65	1.66	0.94	1.24	-0.62	2	1	2	Low Priority
S193	000076-58-4	0.80	0.91	0.85	0.88	0.83	1.73	1.00	1.30	-0.62	2	1	2	Low Priority
S194	000076-73-3	0.53	0.52	0.44	0.45	0.40	0.21	0.26	0.19	-1.69	2	1	2	Low Priority
S195	000076-74-4	1.34	1.40	1.40	1.38	1.38	0.03	0.20	0.14	-1.89	2	1	2	Low Priority
S196	000076-75-5	0.30	0.31	0.31	0.31	0.31	0.21	0.39	0.32	-1.90	2	1	3	Low Priority
S197	000076-99-3	1.49	1.61	1.61	1.61	1.61	1.28	1.50	1.29	0.97	2	1	3	Low Priority
S198	000077-02-1	0.43	0.45	0.39	0.45	0.41	0.03	0.13	0.09	-1.67	2	1	2	Low Priority
S199	000077-07-6	1.13	1.13	1.13	1.21	1.21	1.28	1.05	1.20	-0.80	2	1	3	Low Priority
S200	000077-09-8	0.67	0.89	0.70	0.73	0.68	1.07	0.72	0.94	1.53	2	1	2	Low Priority
S201	000077-10-1	1.20	1.28	1.28	1.28	1.28	2.40	2.33	2.30	-0.21	2	1	3	Priority (Group 2)
S202	000077-19-0	0.74	0.96	0.68	0.46	0.52	1.06	1.17	0.98	-1.61	2	2	3	Low Priority
S203	000077-21-4	1.04	1.08	1.08	1.08	1.08	0.35	0.43	0.33	-0.43	2	1	2	Low Priority
S204	000077-26-9	1.54	1.69	1.69	1.78	1.78	0.13	0.22	0.16	-1.67	2	1	2	Low Priority
S205	000077-27-0	0.60	0.78	0.64	0.64	0.57	0.45	0.45	0.37	-1.69	2	1	3	Low Priority
S206	000077-28-1	1.57	1.77	1.77	1.77	1.77	-0.12	0.06	0.01	-1.88	1	1	2	Low Priority
S207	000077-36-1	1.56	2.01	2.01	2.01	2.01	0.96	1.13	0.56	2	1	2	Low Priority	
S208	000077-37-2	1.08	1.07	1.07	1.34	1.34	1.31	1.35	1.07	-0.90	2	1	3	Low Priority
S209	000077-39-4	0.87	1.10	0.82	0.89	0.99	1.31	1.35	1.08	-0.89	2	1	3	Low Priority
S210	000077-41-8	0.30	0.35	0.35	0.35	0.35	0.58	0.73	0.66	-0.04	2	1	1	Low Priority
S211	000077-53-2	0.85	1.01	1.25	1.13	1.05	1.10	1.27	1.16	-2.14	2	1	2	Low Priority
S212	000077-67-8	1.72	0.28	0.34	0.19	0.20	-0.30	-0.10	-0.11	-1.67	2	1	1	Low Priority
S213	000077-90-7	0.67	0.00	0.23	0.40	0.20	0.58	0.89	0.76	-0.95	1	1	2	Low Priority
S214	000077-93-0	0.44	0.05	0.11	0.26	0.02	0.00	0.28	0.24	-1.49	1	1	1	Low Priority
S215	000078-35-3	0.89	0.39	0.50	0.63	0.48	1.24	1.42	1.36	-1.09	2	2	3	Low Priority
S216	000078-36-4	0.95	0.38	0.46	0.61	0.46	1.25	1.30	1.25	-1.09	2	2	3	Low Priority
S217	000078-44-4	0.90	0.91	0.91	0.91	0.91	0.12	0.51	0.46	-2.47	2	1	2	Low Priority
S218	000078-59-1	0.35	0.43	0.57	0.48	0.33	0.09	0.09	0.09	-1.28	2	1	2	Low Priority
S219	000078-69-3	0.81	0.54	0.78	0.78	0.65	0.49	0.78	0.67	-2.08	2	1	2	Low Priority
S220	000078-70-6	0.88	0.43	0.74	0.83	0.75	0.79	0.75	0.67	-1.63	2	1	3	Low Priority
S221	000078-93-3	0.08	0.18	0.18	0.17	0.17	-0.52	-0.31	-0.17	-1.42	1	1	1	Low Priority
S222	000079-41-4	-0.09	-0.20	0.39	-0.62	-0.01	-0.94	-0.73	-0.57	-1.58	1	1	1	Low Priority
S223	000079-46-9	0.14	0.06	0.11	0.07	0.19	0.18	0.18	0.18	-1.40	1	1	1	Low Priority
S224	000079-69-6	0.90	0.65	0.78	0.92	0.69	1.21	1.44	1.47	-1.28	2	1	3	Low Priority
S225	000079-70-9	0.92	0.71	0.87	0.90	0.72	1.39	1.45	1.49	-1.06	2	1	3	Low Priority
S226	000079-77-6	0.93	0.65	0.68	0.89	0.71	1.29	1.24	1.27	-1.05	2	1	2	Low Priority
S227	000079-83-4	0.38	0.18	0.04	0.26	0.11	-0.18	0.13	0.11	-2.85	1	1	1	Low Priority
S228	000080-08-0	1.34	1.39	1.39	1.39	1.39	0.21	0.29	-0.11	-0.31	2	1	2	Low Priority
S229	000080-27-3	0.85	0.45	0.72	0.66	0.60	1.01	1.12	1.11	-1.29	2	1	3	Low Priority
S230	000080-35-3	0.71	0.90	0.88	1.19	1.10	0.07	0.35	-0.14	0.09	2	1	2	Low Priority
S231	000080-49-9	1.05	1.18	0.89	1.22	1.04	0.82	1.21	0.89	-0.02	2	1	1	Low Priority
S232	000080-50-2	1.13	1.15	1.05	1.16	1.01	1.16	1.61	1.24	-0.94	2	1	1	Low Priority
S233	000080-54-6	1.10	1.00	0.82	1.03	0.74	1.28	1.41	1.50	-0.17	2	1	3	Low Priority
S234	000080-77-3	0.73	0.99	1.14	1.35	1.19	1.08	0.88	1.17	0.82	2	1	2	Low Priority
S235	000081-14-1	0.47	0.85	0.41	0.72	0.39	1.50	1.66	1.69	0.19	2	1	3	Low Priority
S236	000081-81-2	0.64	0.58	0.58	0.50	0.57	0.95	0.82	0.87	1.06	2	1	2	Low Priority
S237	000082-88-2	1.36	1.11	1.00	1.11	1.10	2.61	2.51	2.56	1.32	2	1	3	Priority (Group 2)
S238	000082-92-8	1.30	1.25	0.97	1.03	1.02	2.42	2.38	2.38	1.10	2	1	2	Priority (Group 2)
S239	000082-95-1	1.59	1.46	1.72	1.66	1.50	3.61	3.39	3.81	2.94	3	3	3	High Priority
S240	000083-07-8	0.55	0.78	0.72	0.71	0.84	0.06	0.24	-0.13	-0.81	1	1	2	Low Priority

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	logHL <sub>4</sub> (h)	logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	PBT Index	P	B	T		
S241	000083-12-5	0.83	0.96	0.43	0.94	0.84	0.93	0.99	0.89	1.24	2	1	2	Low Priority
S242	000083-15-8	0.64	0.75	0.61	0.61	0.66	0.14	0.39	-0.03	-0.23	2	1	2	Low Priority
S243	000083-66-9	0.49	0.70	0.29	0.75	0.39	1.59	1.46	1.68	0.01	2	1	3	Low Priority
S244	000083-67-0	0.30	0.44	0.42	0.31	0.62	-0.52	-0.14	-0.58	-0.60	1	1	2	Low Priority
S245	000083-72-7	0.14	0.42	0.29	0.30	0.22	0.20	0.14	0.13	-0.17	1	1	3	Low Priority
S246	000083-89-6	2.08	2.09	2.09	2.25	2.25	2.29	2.12	2.10	2.12	3</			

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	logHL <sub>4</sub> (h)	logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	PBT Index	P	B	T		
S323	000099-76-3	0.31	0.45	0.55	0.15	0.28	-0.04	-0.07	0.07	-0.57	1	1	2	Low Priority
S324	000099-79-6	0.96	0.73	0.71	0.55	0.69	1.58	1.82	1.69	0.43	2	1	7	Low Priority
S325	000099-87-6	1.30	0.71	1.19	1.39	1.36	1.73	1.83	1.80	-0.18	1	1	2	Low Priority
S326	000099-96-7	0.19	0.32	0.58	0.16	0.31	-0.12	-0.15	0.07	-0.93	1	1	1	Low Priority
S327	00100-33-4	<b>1.40</b>	<b>1.42</b>	<b>1.42</b>	1.09	1.03	1.43	1.20	1.56	-0.92	2	1	2	Low Priority
S328	00100-41-4	0.88	0.41	0.50	0.65	0.72	1.38	1.40	1.36	-0.17	1	1	2	Low Priority
S329	00100-42-5	0.81	0.38	0.57	0.73	0.80	1.35	1.22	1.24	0.01	1	1	2	Low Priority
S330	00100-46-9	0.61	0.26	0.63	0.66	1.01	0.47	0.54	0.54	-1.03	1	1	2	Low Priority
S331	00100-51-6	0.28	0.22	0.41	0.01	0.36	-0.07	0.02	0.07	-0.71	1	1	1	Low Priority
S332	00100-52-7	0.16	0.33	0.09	0.05	0.07	0.36	0.33	0.46	-0.13	1	1	2	Low Priority
S333	00100-90-3	0.85	0.91	0.93	0.99	0.93	0.10	0.60	-0.06	0.67	2	1	2	Low Priority
S334	00100-92-5	<b>1.24</b>	<b>1.26</b>	<b>1.26</b>	1.18	1.07	1.55	1.74	1.67	-0.60	2	1	2	Low Priority
S335	00100-97-0	0.69	0.79	0.65	0.17	0.64	0.98	1.12	1.07	-1.49	2	1	1	Low Priority
S336	00101-20-2	1.84	1.90	2.00	1.97	2.13	1.39	1.39	1.17	2.20	2	1	3	Low Priority
S337	00101-31-5	0.67	0.85	0.58	0.53	0.63	0.56	0.65	0.52	-0.67	2	1	2	Low Priority
S338	00101-72-4	1.25	1.04	1.17	1.00	1.16	1.87	1.96	1.63	0.30	2	1	2	Low Priority
S339	00101-80-4	1.10	0.93	1.12	1.38	1.47	1.23	1.12	0.85	-0.55	2	1	2	Low Priority
S340	00101-84-8	<b>1.92</b>	<b>1.93</b>	<b>1.93</b>	<b>1.92</b>	<b>1.92</b>	<b>1.29</b>	<b>1.29</b>	<b>1.29</b>	1.00	1	1	2	Low Priority
S341	00101-85-9	0.69	0.58	0.55	0.22	0.48	1.10	0.99	0.97	-0.54	1	1	3	Low Priority
S342	00101-86-0	0.82	0.82	0.29	0.33	0.41	1.50	1.27	1.28	0.03	1	1	3	Low Priority
S343	00102-22-7	0.99	0.29	0.53	0.54	0.65	1.58	1.47	1.39	0.20	2	3	3	Low Priority
S344	00103-09-3	0.65	0.29	0.16	0.11	0.14	0.59	0.82	0.87	-1.46	1	1	2	Low Priority
S345	00103-16-2	0.90	0.85	0.79	0.69	0.86	1.06	0.77	1.06	0.55	1	1	2	Low Priority
S346	00103-26-4	0.84	0.55	0.42	0.38	0.68	0.89	0.73	0.76	0.04	1	1	2	Low Priority
S347	00103-36-6	0.85	0.63	0.47	0.34	0.64	0.99	0.82	0.82	0.03	1	1	2	Low Priority
S348	00103-38-8	0.86	0.67	0.66	0.44	0.66	0.75	0.96	0.93	-0.21	1	1	2	Low Priority
S349	00103-41-3	0.97	0.87	0.56	0.61	0.83	1.43	1.22	1.17	1.29	1	1	3	Low Priority
S350	00103-53-7	0.95	0.86	0.49	0.55	0.74	1.51	1.30	1.25	1.29	1	1	3	Low Priority
S351	00103-54-8	0.85	0.54	0.50	0.32	0.61	1.05	0.89	0.96	0.06	1	1	3	Low Priority
S352	00103-56-0	0.83	0.50	0.48	0.28	0.59	1.12	0.95	0.97	0.03	1	1	3	Low Priority
S353	00103-59-3	0.85	0.54	0.61	0.38	0.68	1.19	1.07	1.06	0.01	1	1	3	Low Priority
S354	00103-61-7	0.79	0.50	0.43	0.22	0.52	1.20	1.02	1.02	0.02	1	1	3	Low Priority
S355	00103-64-0	1.35	0.47	0.56	1.14	1.36	1.99	1.78	1.64	0.67	1	1	2	Low Priority
S356	00103-90-2	<b>0.40</b>	<b>0.41</b>	<b>0.41</b>	<b>0.41</b>	<b>0.41</b>	0.11	0.11	-0.01	-0.95	1	1	2	Low Priority
S357	00103-93-5	0.83	0.50	0.61	0.55	0.71	0.81	0.85	0.97	-0.21	1	1	2	Low Priority
S358	00104-09-6	0.68	0.59	0.29	0.54	0.44	0.70	0.66	0.78	-0.14	1	1	2	Low Priority
S359	00104-28-9	0.61	0.61	0.44	0.20	0.35	0.77	0.44	0.53	-0.38	1	1	2	Low Priority
S360	00104-29-0	<b>0.56</b>	<b>0.58</b>	<b>0.58</b>	<b>0.59</b>	<b>0.59</b>	1.02	0.69	1.18	-0.49	1	1	1	Low Priority
S361	00104-54-1	0.45	0.39	0.53	-0.01	0.41	0.61	0.36	0.43	-0.49	1	1	3	Low Priority
S362	00104-87-0	0.51	0.45	0.21	0.51	0.39	0.53	0.49	0.61	-0.14	1	1	2	Low Priority
S363	00104-90-5	1.00	0.58	0.74	0.81	0.90	1.13	1.36	0.87	-0.24	2	1	2	Low Priority
S364	00104-93-8	1.17	0.59	0.70	1.06	1.06	1.21	1.12	1.21	-0.26	1	1	2	Low Priority
S365	00105-20-4	0.50	0.35	0.41	0.53	0.80	0.12	0.42	-0.01	-1.63	1	1	1	Low Priority
S366	00105-37-3	0.41	-0.27	-0.24	-0.11	0.04	-0.22	0.00	0.09	-1.44	1	1	2	Low Priority
S367	00105-45-3	0.40	-0.05	-0.19	0.21	0.13	-0.18	0.06	0.16	-1.23	1	1	1	Low Priority
S368	00105-53-3	0.62	0.24	0.06	0.30	0.17	0.09	0.34	0.39	-1.25	1	1	2	Low Priority
S369	00105-67-9	0.37	0.35	0.71	0.31	0.53	0.27	0.20	0.33	-0.74	1	1	2	Low Priority
S370	00105-87-3	0.95	0.07	0.35	0.51	0.55	1.16	1.15	1.20	-1.03	1	1	3	Low Priority
S371	00105-90-8	0.95	0.09	0.39	0.48	0.53	1.22	1.19	1.20	-1.05	1	1	3	Low Priority
S372	00105-91-9	0.95	0.09	0.39	0.48	0.53	1.22	1.19	1.20	-1.05	1	1	3	Low Priority
S373	00105-95-3	0.62	0.18	0.72	0.16	0.88	0.78	0.96	0.95	-1.29	1	3	3	Low Priority
S374	00106-02-5	0.66	0.38	0.66	0.04	0.87	0.95	1.08	1.03	-1.51	1	2	3	Low Priority
S375	00106-22-9	0.74	0.36	0.65	0.41	0.49	0.63	0.66	0.69	-1.80	1	1	2	Low Priority
S376	00106-24-1	0.79	0.19	0.64	0.44	0.57	0.77	0.64	0.68	-1.58	1	1	3	Low Priority
S377	00106-25-2	0.79	0.19	0.64	0.44	0.57	0.77	0.64	0.68	-1.58	1	1	3	Low Priority
S378	00106-29-6	0.92	0.12	0.39	0.44	0.48	1.30	1.25	1.23	-1.06	1	2	3	Low Priority
S379	00106-60-5	<b>-0.08</b>	<b>0.02</b>	<b>0.02</b>	<b>0.03</b>	<b>0.03</b>	-0.57	-0.34	-0.28	-2.40	1	1	1	Low Priority
S380	00106-65-0	0.51	0.17	0.17	0.18	0.15	-0.04	0.22	0.30	-1.24	1	1	1	Low Priority
S381	00106-89-8	0.34	0.20	0.95	0.78	0.82	0.29	0.29	0.29	-0.89	1	1	2	Low Priority
S382	00107-41-5	0.16	0.25	0.36	0.34	0.14	-0.20	0.10	0.06	-2.43	1	1	1	Low Priority
S383	00107-75-5	0.72	0.47	0.36	0.46	0.28	0.51	0.60	0.62	-1.84	2	1	2	Low Priority
S384	00108-01-0	0.04	0.05	0.25	-0.18	-0.09	-0.69	-0.47	-0.38	-1.99	1	1	1	Low Priority
S385	00108-10-1	0.25	0.06	0.15	0.11	0.04	-0.05	0.25	0.32	-1.45	1	1	1	Low Priority
S386	00108-11-2	0.14	0.09	0.34	0.06	0.13	-0.24	0.02	0.03	-2.02	1	1	1	Low Priority
S387	00108-22-5	0.22	-0.05	-0.10	-0.04	-0.03	-0.19	0.14	0.26	-1.21	1	1	3	Low Priority
S388	00108-24-7	0.16	-0.13	-0.21	-0.14	-0.16	-0.35	-0.08	0.06	-1.20	1	1	1	Low Priority
S389	00108-39-4	0.07	0.29	0.68	-0.05	0.24	0.08	-0.01	0.14	-0.73	1	1	2	Low Priority
S390	00108-46-3	-0.02	0.21	0.66	0.02	0.29	0.07	-0.16	0.15	-1.11	1	1	1	Low Priority
S391	00108-59-8	0.76	0.08	-0.09	0.50	0.47	-0.19	0.08	0.18	-1.23	1	1	1	Low Priority
S392	00108-93-0	0.04	0.16	0.66	-0.18	0.36	-0.25	-0.14	-0.14	-2.03	1	1	1	Low Priority
S393	00108-94-1	0.14	0.11	0.34	-0.08	0.27	-0.07	0.08	0.13	-1.46	1	1	1	Low Priority
S394	00108-95-2	<b>0.54</b>	<b>0.57</b>	<b>0.57</b>	<b>0.57</b>	<b>0.57</b>	-0.14	-0.22	-0.05	-0.72	1	1	2	Low Priority
S395	00110-15-6	0.05	-0.38	0.01	-0.29	-0.04	-0.85	-0.63	-0.49	-1.97	1	1	1	Low Priority
S396	00110-46-3	0.45	-0.06	-0.25	-0.17	0.01	0.46	0.36	0.85	-1.39	1	1	2	Low Priority
S397	00110-93-0	0.79	0.17	0.22	0.56	0.49	0.49	0.59	0.63	-1.24	1	1	2	Low Priority
S398	00111-12-6	0.73	0.19	0.35	-0.02	0.46	0.46	0.65	0.70	-1.24	1	1	2	Low Priority
S399	00112-05-0	0.39	0.16	-0.03	-0.51	-0.20	0.02	0.17	0.23	-1.83	1	1	2	Low Priority
S400	00113-18-8	<b>1.78</b>	0.22	0.79	0.24	0.38	0.56	0.34	0.32	-0.98	2	1	3	Low Priority
S401	00113-42-8	<b>0.53</b>	<b>0.54</b>	<b>0.54</b>	<b>0.53</b>	<b>0.53</b>	0.90	0.96	0.44	-0.43	2	1	2	Low Priority
S402	00113-45-1	<b>0.68</b>	<b>0.68</b>	<b>0.68</b>	<b>0.68</b>	<b>0.68</b>	0.64	0.75	0.65	-0.64	1	1	2	Low Priority
S403	00113-59-7	<b>1.00</b>	<b>1.00</b>	<b>1.00</b>	<b>1.00</b>	<b>1.00</b>	3.35	3.25	3.66	1.86	3	2	3	High Priority
S404	00114-86-3	0.73	0.76	0.66	0.65	1.00	0.54	0.74	0.73	-2.21	2	1	1	Low Priority

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	logHL <sub>4</sub> (h)	logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	PBT Index	P	B	T		
S405	000115-19-5	0.17	0.21	0.84	0.08	0.42	-0.48	-0.20	-0.17	-1.79	1	1	1	Low Priority
S406	000115-38-8	<b>1.53</b>	<b>1.67</b>	<b>1.67</b>	0.57	0.58	0.09	0.21	0.13	-0.24	2	1	2	Low Priority
S407	000115-44-6	0.49	0.42	0.35	0.45	0.40	0.12	0.19	0.13	-1.68	2	1	2	Low Priority
S408	000115-67-3	<b>1.26</b>	<b>1.59</b>	<b>1.59</b>	<b>1.59</b>	<b>1.59</b>	0.00	0.30	0.30	-1.29	2	1	1	Low Priority
S409	000115-95-7	0.96	0.41	0.47	0.66									

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	logHL <sub>4</sub> (h)	logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	PBT Index	P	B		T
S487	000131-01-1	0.75	0.50	0.73	0.82	0.63	1.30	1.06	1.11	1.59	3	1	2	Low Priority
S488	000131-11-3	0.47	0.48	0.33	0.33	0.36	0.39	0.58	0.59	0.01	1	1	2	Low Priority
S489	000131-16-8	0.71	0.53	0.33	0.41	0.51	0.71	0.88	0.82	-0.03	1	1	2	Low Priority
S490	000131-17-9	0.73	0.36	0.40	0.51	0.58	1.04	0.89	0.84	0.41	1	1	3	Low Priority
S491	000131-18-0	0.74	0.65	0.32	0.34	0.46	0.99	1.14	1.05	-0.05	1	1	3	Low Priority
S492	000131-53-3	0.51	0.75	0.70	0.68	0.61	0.85	0.42	0.73	0.25	2	1	2	Low Priority
S493	000131-55-5	0.44	0.66	0.79	0.83	0.74	0.84	0.27	0.73	-0.52	1	1	2	Low Priority
S494	000131-56-6	0.53	0.75	0.68	0.60	0.63	0.67	0.41	0.58	0.26	1	1	2	Low Priority
S495	000131-57-7	0.58	0.83	0.65	0.59	0.54	0.76	0.50	0.66	0.65	2	1	2	Low Priority
S496	000131-70-4	0.47	0.53	0.43	0.05	0.27	0.09	0.24	0.17	-0.40	1	1	2	Low Priority
S497	000132-21-8	1.40	1.41	1.41	1.29	1.27	2.20	2.62	1.95	1.68	2	1	3	Priority (Group 1)
S498	000132-22-9	1.34	1.42	1.42	1.42	1.42	2.59	2.54	2.39	1.66	2	1	3	Priority (Group 1)
S499	000133-16-4	0.81	0.93	1.02	1.08	1.03	0.87	0.76	0.71	-0.38	2	1	3	Low Priority
S500	000133-67-5	1.41	1.80	2.06	2.28	2.17	0.80	0.68	0.69	0.76	3	1	2	Low Priority
S501	000134-09-8	0.86	0.90	0.88	0.83	1.05	0.67	0.84	0.42	-1.06	2	3	3	Low Priority
S502	000134-49-6	1.37	1.53	1.53	0.77	1.04	1.16	1.22	1.09	-0.69	1	1	2	Low Priority
S503	000135-07-9	1.05	1.34	1.51	1.87	1.75	0.67	0.41	0.51	0.49	2	1	2	Low Priority
S504	000135-09-1	0.72	1.10	1.10	1.51	1.43	0.22	0.74	0.25	0.77	1	1	2	Low Priority
S505	000136-44-7	0.40	0.53	0.34	0.42	0.47	-0.06	0.14	-0.18	-1.77	1	1	2	Low Priority
S506	000136-85-6	0.69	0.66	0.48	0.55	0.65	0.34	0.76	0.07	0.26	1	1	2	Low Priority
S507	000137-58-6	0.20	0.21	0.21	0.21	0.21	0.65	0.79	0.40	-0.64	2	1	2	Low Priority
S508	000138-56-7	0.90	0.92	0.92	0.85	0.62	1.22	0.80	1.26	0.62	2	1	2	Low Priority
S509	000138-59-0	0.09	0.05	0.44	0.27	0.23	-0.14	-0.11	0.00	-2.80	1	1	1	Low Priority
S510	000140-11-4	0.73	0.43	0.31	0.31	0.55	0.47	0.63	0.70	-0.16	1	1	2	Low Priority
S511	000140-27-2	0.83	0.57	0.63	0.34	0.60	1.28	1.17	1.13	0.01	1	1	3	Low Priority
S512	000140-88-5	0.41	-0.24	-0.21	-0.09	0.08	-0.04	0.01	0.12	-1.22	1	1	3	Low Priority
S513	000141-14-0	0.88	0.28	0.42	0.41	0.43	1.06	1.18	1.19	-1.27	1	2	3	Low Priority
S514	000141-78-6	0.16	-0.25	-0.22	-0.29	-0.21	-0.41	-0.18	-0.04	-1.42	1	1	2	Low Priority
S515	000141-79-7	0.25	0.07	0.23	0.10	0.15	0.12	0.26	0.34	-1.23	1	1	1	Low Priority
S516	000141-97-9	0.56	0.06	-0.07	0.31	0.20	-0.03	0.21	0.27	-1.24	1	1	1	Low Priority
S517	000142-19-8	0.65	0.20	0.02	0.01	0.15	0.70	0.73	0.72	-1.27	1	1	3	Low Priority
S518	000142-90-5	0.71	0.43	0.06	0.00	0.16	1.16	1.34	1.33	-1.28	1	1	3	Low Priority
S519	000144-11-6	0.60	0.60	0.60	0.60	0.60	1.38	1.41	1.14	-0.90	2	1	3	Low Priority
S520	000144-14-9	0.80	1.01	0.62	0.78	0.72	0.85	0.89	0.46	0.21	2	1	3	Low Priority
S521	000144-39-8	0.90	0.37	0.47	0.58	0.43	1.18	1.25	1.22	-1.07	2	1	3	Low Priority
S522	000144-80-9	1.00	0.56	0.57	0.89	0.76	-0.18	-0.02	-0.33	-0.96	2	1	2	Low Priority
S523	000144-82-1	0.74	1.06	1.06	1.21	1.12	-0.06	0.23	-0.26	-0.12	2	1	2	Low Priority
S524	000144-83-2	1.00	0.88	0.83	1.11	1.13	0.11	0.38	-0.13	0.09	2	1	2	Low Priority
S525	000146-22-5	1.41	1.42	1.42	1.42	1.42	0.83	0.53	1.10	2	1	3	Low Priority	
S526	000146-48-5	-0.22	-0.22	-0.22	-0.22	-0.22	0.85	1.01	0.58	-0.24	2	1	2	Low Priority
S527	000146-50-9	0.90	0.72	0.55	0.65	0.65	1.11	1.35	1.25	-0.05	2	3	3	Low Priority
S528	000146-54-3	1.65	1.26	1.46	1.29	1.44	1.69	1.97	1.58	2.74	3	2	3	Priority (Group 3)
S529	000147-20-6	1.22	1.13	0.87	1.09	1.11	1.99	1.99	1.81	0.93	2	1	3	Low Priority
S530	000147-52-4	-0.15	0.01	0.01	0.01	0.01	0.50	0.33	0.41	0.40	2	1	1	Low Priority
S531	000147-85-3	-0.17	0.03	0.28	-0.57	-0.08	-0.44	-0.24	-0.15	-2.22	1	1	1	Low Priority
S532	000148-79-8	0.08	0.07	0.07	0.08	0.08	1.43	1.79	1.15	1.26	1	1	3	Low Priority
S533	000148-82-3	0.00	0.06	0.06	0.06	0.06	0.84	0.93	0.77	-0.06	2	1	1	Low Priority
S534	000150-13-0	1.17	0.39	0.59	0.13	0.35	-0.21	-0.05	-0.25	-1.32	1	1	2	Low Priority
S535	000150-59-4	0.40	1.21	0.70	0.99	0.83	2.67	2.64	2.60	1.10	3	2	3	Priority (Group 2)
S536	000150-78-7	0.98	0.80	0.78	0.81	0.71	1.37	1.13	1.38	-0.25	1	1	2	Low Priority
S537	000151-83-7	0.20	0.21	0.21	0.21	0.21	0.34	0.42	0.32	-1.10	2	1	2	Low Priority
S538	000152-02-3	0.00	0.00	0.00	0.00	0.00	1.59	1.19	1.35	-0.58	2	1	3	Low Priority
S539	000152-43-2	1.07	1.22	1.27	1.03	1.15	1.89	1.63	1.70	0.65	3	3	3	Low Priority
S540	000152-47-6	0.59	0.90	0.88	1.09	1.02	0.05	0.32	-0.17	0.08	2	1	2	Low Priority
S541	000152-72-7	0.57	0.45	0.48	0.63	0.52	1.13	0.82	0.75	1.27	2	1	2	Low Priority
S542	000154-42-7	0.37	0.44	0.71	0.85	1.06	0.39	0.79	0.43	-1.85	1	1	2	Low Priority
S543	000154-93-8	-0.43	-0.43	-0.43	-0.42	-0.42	0.24	0.23	0.39	-0.38	2	1	2	Low Priority
S544	000155-09-9	0.79	0.84	0.84	1.13	1.13	0.83	0.89	0.85	-1.05	1	1	2	Low Priority
S545	000155-41-9	0.92	1.25	0.95	1.12	1.00	0.68	1.08	0.73	0.00	2	1	2	Low Priority
S546	000156-08-1	1.37	1.38	1.38	1.39	1.39	2.45	2.47	2.46	1.11	2	1	3	Priority (Group 2)
S547	000297-76-7	0.99	0.58	0.96	0.72	0.81	1.28	1.17	1.26	-0.09	2	2	3	Low Priority
S548	000298-46-4	1.65	1.69	1.69	1.71	1.71	0.82	0.54	0.22	0.49	2	1	2	Low Priority
S549	000298-50-0	1.05	0.97	0.82	0.91	0.88	1.55	1.81	1.83	0.97	2	1	2	Low Priority
S550	000298-57-7	1.39	1.27	0.78	0.97	0.97	3.27	2.84	2.89	2.61	3	2	3	High Priority
S551	000298-81-7	0.30	0.31	0.31	0.30	0.30	1.28	0.58	0.93	0.87	1	1	2	Low Priority
S552	000299-26-3	0.88	0.87	1.02	1.02	1.23	0.78	0.89	0.55	-0.58	1	1	2	Low Priority
S553	000299-42-3	0.52	0.64	0.58	0.48	0.61	0.49	0.64	0.56	-1.17	1	1	1	Low Priority
S554	000300-62-9	0.86	0.88	0.88	0.87	1.13	0.84	0.91	0.87	-1.04	1	1	2	Low Priority
S555	000303-49-1	1.41	1.41	1.41	1.41	1.41	3.08	2.78	2.88	1.64	3	2	3	High Priority
S556	000303-53-7	1.26	1.25	1.25	1.25	1.25	3.04	2.71	2.82	1.55	3	1	3	Priority (Group 1)
S557	000304-55-2	1.68	-0.36	-0.12	-0.18	-0.09	-0.32	-0.25	-0.03	-2.00	1	1	1	Low Priority
S558	000305-03-3	0.04	0.05	0.05	0.05	0.05	0.91	0.97	0.82	0.73	2	1	2	Low Priority
S559	000306-40-1	0.99	0.51	0.43	0.83	0.41	0.93	1.47	1.42	-1.30	1	1	1	Low Priority
S560	000309-29-5	0.61	0.62	0.62	0.60	0.60	1.15	1.17	0.94	0.93	2	1	3	Low Priority
S561	000316-81-4	0.91	1.61	1.08	1.20	0.98	0.92	0.86	0.71	1.21	2	1	3	Low Priority
S562	000321-64-2	0.52	0.53	0.53	0.53	0.53	0.96	1.14	0.61	0.00	2	1	2	Low Priority
S563	000339-44-6	0.60	0.97	0.97	1.03	1.00	0.21	0.48	-0.02	0.86	2	1	2	Low Priority
S564	000341-69-5	1.17	1.15	0.99	1.06	0.96	1.96	2.05	1.91	0.97	2	1	2	Low Priority
S565	000346-18-9	1.45	1.09	1.47	1.93	1.77	1.21	1.14	1.03	1.76	3	1	2	Low Priority
S566	000357-56-2	0.78	1.16	0.70	0.73	0.69	1.15	1.18	0.88	0.90	2	1	3	Low Priority
S567	000357-70-0	0.72	0.87	0.87	0.87	0.87	1.59	0.92	1.25	-0.58	2	1	3	Low Priority
S568	000359-83-1	0.40	0.46	0.46	0.46	0.46	1.60	1.38	1.53	-0.58	2	1	3	Low Priority

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	logHL <sub>4</sub> (h)	logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	PBT Index	P	B		T
S569	000361-37-5	0.65	0.97	0.91	0.48	0.56	0.63	0.24	0.00	2	1	2	Low Priority	
S570	000362-29-8	1.00	1.16	0.99	0.95	0.91	1.30	1.29	1.17	1.03	2	1	3	Low Priority
S571	000364-62-5	0.86	0.95	0.95	0.95	0.95	1.08	0.82	0.90	-0.79	2	1	2	Low Priority
S572	000364-98-7	1.68	1.14	1.46	1.39	1.24	0.52	0.48	0.35	0.45	2	1	2	Low Priority
S573	000371-40-4	0.30	0.36	0.73	0.43	0.68	-0.33	-0.06	-0.41	-0.55	2	1	2	Low Priority
S574	000372-75-8	0.13	0.12	-										



ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	logHL <sub>4</sub> (h)	logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	PBT Index	P	B	T		
S651	000546-79-2	0.59	0.75	0.80	0.88	0.73	0.49	0.68	0.57	-2.09	2	1	2	Low Priority
S652	000548-00-5	0.54	0.46	0.36	0.67	0.64	0.78	0.49	0.75	1.07	1	1	2	Low Priority
S653	000548-73-2	<b>0.35</b>	<b>0.36</b>	<b>0.36</b>	<b>0.36</b>	<b>0.36</b>	1.05	1.09	0.69	1.70	3	1	2	Low Priority
S654	000551-92-8	0.07	0.40	0.20	0.10	0.13	0.35	0.53	0.37	-0.36	2	1	2	Low Priority
S655	000552-25-0	0.89	0.92	0.76	0.65	0.60	1.27	1.44	1.03	1.02	2	1	3	Low Priority
S656	000552-94-3	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>	<b>0.10</b>	<b>0.10</b>	0.58	0.36	0.58	0.49	1	1	2	Low Priority
S657	000554-57-4	<b>1.15</b>	0.48	0.56	0.93	0.80	-0.51	-0.15	-0.21	-1.40	2	1	2	Low Priority
S658	000555-30-6	<b>0.77</b>	<b>1.17</b>	<b>1.17</b>	<b>1.17</b>	<b>1.17</b>	0.42	0.24	0.59	-2.13	1	1	1	Low Priority
S659	000555-57-7	1.14	0.88	0.79	0.82	0.87	1.07	1.15	1.18	-0.02	2	1	2	Low Priority
S660	000561-27-3	<b>0.40</b>	<b>0.41</b>	<b>0.41</b>	<b>0.47</b>	<b>0.47</b>	1.69	1.06	1.50	0.19	2	1	3	Low Priority
S661	000562-74-3	0.78	0.50	1.03	1.00	0.97	0.64	0.66	0.53	-1.88	2	1	2	Low Priority
S662	000563-80-4	0.22	-0.03	0.17	-0.01	0.15	-0.28	0.04	0.14	-1.44	1	1	1	Low Priority
S663	000569-57-3	1.43	1.10	1.33	1.48	1.33	3.01	2.54	2.94	3.12	3	3	3	High Priority
S664	000569-65-3	<b>0.78</b>	<b>0.77</b>	<b>0.77</b>	<b>0.78</b>	<b>0.78</b>	3.45	3.05	3.44	2.95	3	2	3	High Priority
S665	000575-61-1	1.00	0.95	0.69	0.81	1.01	1.16	1.09	1.05	1.28	1	1	3	Low Priority
S666	000576-26-1	0.08	0.32	0.69	0.00	0.26	0.27	0.20	0.31	-0.75	1	1	2	Low Priority
S667	000586-06-1	<b>0.78</b>	0.69	0.62	0.64	0.65	0.86	0.74	0.95	-1.95	1	1	2	Low Priority
S668	000591-81-1	0.08	-0.35	-0.08	-0.41	-0.10	-0.82	-0.63	-0.49	-2.19	1	1	1	Low Priority
S669	000595-33-5	1.00	0.65	1.06	0.93	0.73	1.61	1.44	1.45	-0.74	1	1	2	Low Priority
S670	000596-51-0	1.09	1.31	1.14	1.30	1.10	1.03	1.52	1.00	-0.77	2	1	1	Low Priority
S671	000599-79-1	<b>0.88</b>	<b>0.90</b>	<b>0.87</b>	<b>0.84</b>	<b>0.82</b>	<b>0.30</b>	<b>0.70</b>	<b>0.11</b>	<b>0.70</b>	2	1	2	Low Priority
S672	000604-75-1	<b>0.83</b>	<b>1.50</b>	<b>1.50</b>	<b>1.50</b>	<b>1.50</b>	1.07	0.99	0.88	1.13	2	1	2	Low Priority
S673	000605-54-9	0.60	0.54	0.22	0.41	0.37	0.65	0.86	0.79	-0.04	1	1	2	Low Priority
S674	000611-99-4	0.58	0.75	0.69	0.64	0.66	0.64	0.39	0.55	0.26	1	1	2	Low Priority
S675	000615-05-4	0.82	0.56	0.94	1.22	1.33	0.59	0.51	0.37	-1.82	2	1	2	Low Priority
S676	000616-91-1	<b>0.74</b>	-0.15	-0.33	-0.33	-0.25	-0.27	-0.08	0.02	-2.01	1	1	1	Low Priority
S677	000620-17-7	0.34	0.26	0.48	0.11	0.35	0.27	0.17	0.31	-0.74	1	1	2	Low Priority
S678	000626-82-4	0.67	0.30	-0.01	-0.01	0.14	0.53	0.72	0.69	-1.49	1	1	2	Low Priority
S679	000634-03-7	<b>1.33</b>	<b>1.46</b>	<b>1.46</b>	<b>1.68</b>	<b>1.68</b>	1.44	1.54	1.42	-0.31	2	1	2	Low Priority
S680	000637-07-0	<b>1.30</b>	<b>1.30</b>	<b>1.30</b>	<b>1.31</b>	<b>1.31</b>	1.41	1.20	1.63	0.41	2	1	2	Low Priority
S681	000639-99-6	0.97	0.77	1.15	1.16	0.98	1.25	1.57	1.47	-1.67	2	2	3	Low Priority
S682	000644-62-2	<b>0.48</b>	<b>0.49</b>	<b>0.49</b>	<b>0.50</b>	<b>0.50</b>	1.45	1.30	1.33	1.60	2	1	3	Low Priority
S683	000645-05-6	<b>0.87</b>	<b>0.88</b>	<b>0.88</b>	<b>0.89</b>	<b>0.89</b>	1.03	2.07	1.63	-0.25	3	1	3	Low Priority
S684	000646-01-5	0.04	-0.12	-0.17	-0.51	-0.23	-0.69	-0.68	-0.42	-1.80	1	1	1	Low Priority
S685	000671-16-9	-0.78	-0.77	-0.77	-0.76	-0.76	0.29	0.54	0.45	-1.40	2	1	2	Low Priority
S686	000672-87-7	<b>0.55</b>	0.58	0.68	0.44	0.47	0.32	0.31	0.50	-1.74	1	1	1	Low Priority
S687	000696-23-1	0.03	0.30	0.21	0.13	0.17	-0.04	-0.20	-0.74	0.20	1	1	2	Low Priority
S688	000713-95-1	0.70	0.50	0.34	0.11	0.42	0.78	0.92	0.91	-1.49	1	1	2	Low Priority
S689	000721-50-6	<b>0.26</b>	<b>0.26</b>	<b>0.26</b>	<b>0.26</b>	<b>0.26</b>	0.52	0.72	0.33	-1.02	2	1	2	Low Priority
S690	000723-46-6	<b>0.99</b>	<b>1.06</b>	<b>1.06</b>	<b>1.06</b>	<b>1.06</b>	0.26	0.23	-0.05	-0.12	2	1	2	Low Priority
S691	000729-99-7	0.71	0.92	1.00	1.13	1.07	1.15	0.32	-0.01	-0.13	2	1	2	Low Priority
S692	000734-32-7	0.81	0.88	0.91	0.80	0.90	1.33	1.17	1.11	-1.14	2	1	1	Low Priority
S693	000738-70-5	<b>0.98</b>	<b>1.23</b>	<b>1.23</b>	<b>1.23</b>	<b>1.23</b>	1.36	1.30	1.22	0.54	2	1	3	Low Priority
S694	000739-71-9	<b>1.36</b>	<b>1.36</b>	<b>1.36</b>	<b>1.38</b>	<b>1.38</b>	2.58	2.62	2.39	1.10	2	2	3	Priority (Group 2)
S695	000745-65-3	-0.90	-0.90	-0.90	-0.89	-0.89	1.12	0.95	0.84	-2.30	1	1	2	Low Priority
S696	000763-32-6	0.06	-0.12	0.27	-0.21	-0.06	-0.50	-0.32	-0.23	-1.77	1	1	1	Low Priority
S697	000768-94-5	<b>1.20</b>	0.75	1.10	0.80	1.11	1.00	1.04	0.94	-2.38	2	1	2	Low Priority
S698	000773-76-2	0.74	0.95	1.21	1.22	1.31	1.03	0.89	0.71	1.59	2	1	2	Low Priority
S699	000791-35-5	0.93	1.10	1.26	1.38	1.30	1.70	1.51	1.61	1.06	2	1	2	Low Priority
S700	000797-63-7	<b>0.97</b>	<b>0.99</b>	<b>0.99</b>	<b>0.97</b>	<b>0.97</b>	1.54	1.33	1.31	-1.52	2	1	2	Low Priority
S701	000835-11-0	0.48	0.70	0.63	0.55	0.65	0.66	0.40	0.57	0.26	1	1	2	Low Priority
S702	000835-31-4	1.16	0.98	0.69	0.81	0.99	1.28	1.49	1.26	0.65	2	1	2	Low Priority
S703	000846-46-8	0.91	0.93	0.99	0.94	0.92	1.24	1.22	1.19	-1.36	2	1	2	Low Priority
S704	000846-49-1	<b>1.23</b>	<b>1.23</b>	<b>1.23</b>	<b>1.23</b>	<b>1.23</b>	1.25	1.25	1.06	1.77	2	1	2	Low Priority
S705	000846-50-4	<b>1.18</b>	<b>1.20</b>	<b>1.20</b>	<b>1.20</b>	<b>1.20</b>	1.10	1.00	0.87	1.50	2	1	2	Low Priority
S706	000868-77-9	0.18	0.03	0.14	-0.23	-0.04	-0.54	-0.29	-0.26	-1.63	1	1	1	Low Priority
S707	000873-94-9	0.35	0.46	0.71	0.48	0.36	0.41	0.67	0.64	-1.50	2	1	2	Low Priority
S708	000882-09-7	0.60	0.89	1.24	0.77	0.79	0.86	0.59	1.10	0.07	2	1	1	Low Priority
S709	000882-33-7	1.30	1.06	0.62	1.07	1.05	2.24	1.85	2.18	1.12	1	1	2	Low Priority
S710	000911-45-5	<b>2.16</b>	<b>2.16</b>	<b>2.16</b>	<b>2.16</b>	<b>2.16</b>	2.86	2.72	2.74	3.12	3	3	3	High Priority
S711	000911-65-9	1.03	1.07	0.70	0.84	0.71	1.54	1.46	1.33	1.96	2	2	3	Priority (Group 3)
S712	000915-30-0	<b>1.11</b>	<b>1.11</b>	<b>1.11</b>	<b>1.11</b>	<b>1.11</b>	1.55	1.63	1.44	2.48	3	3	3	Priority (Group 3)
S713	000935-92-2	0.43	0.19	0.31	0.42	0.47	0.53	0.59	0.59	-0.86	1	1	3	Low Priority
S714	000965-52-6	0.51	0.79	0.70	0.67	0.60	0.81	0.44	0.38	0.50	2	1	2	Low Priority
S715	000965-90-2	0.90	1.04	1.35	1.06	1.26	1.69	1.47	1.34	-1.95	2	1	3	Low Priority
S716	000968-81-0	<b>0.11</b>	<b>0.11</b>	<b>0.11</b>	<b>0.19</b>	<b>0.19</b>	0.37	0.50	0.44	-0.40	2	1	2	Low Priority
S717	000972-02-1	<b>0.60</b>	<b>0.61</b>	<b>0.61</b>	<b>0.72</b>	<b>0.72</b>	1.42	1.43	1.19	0.40	2	1	3	Low Priority
S718	001072-67-9	0.32	0.39	0.78	0.54	0.78	0.19	0.12	-0.01	-1.23	1	1	2	Low Priority
S719	001074-95-9	0.71	0.55	0.66	0.70	0.79	0.51	0.73	0.66	-1.52	1	1	2	Low Priority
S720	001082-88-8	0.90	0.72	0.72	0.94	0.78	1.56	1.24	1.69	-1.05	2	1	2	Low Priority
S721	001085-12-7	0.50	0.60	0.39	0.00	0.21	0.59	0.53	0.59	-0.62	1	1	3	Low Priority
S722	001093-59-8	0.83	0.99	1.34	1.21	1.26	1.30	1.33	1.27	-1.09	2	1	2	Low Priority
S723	001118-27-0	0.89	0.36	0.51	0.58	0.51	1.33	1.48	1.41	-1.10	1	2	3	Low Priority
S724	001131-64-2	0.79	0.79	0.85	0.81	1.15	0.59	0.69	0.70	-1.26	2	1	2	Low Priority
S725	001134-47-0	<b>0.18</b>	<b>0.39</b>	<b>0.39</b>	<b>0.39</b>	<b>0.39</b>	0.86	0.72	1.12	-0.69	1	1	1	Low Priority
S726	001137-42-4	0.58	0.80	0.62	0.48	0.56	0.53	0.43	0.44	0.66	1	1	2	Low Priority
S727	001139-30-6	1.19	0.92	1.34	1.50	1.36	1.82	2.00	1.88	-1.39	2	1	3	Low Priority
S728	001141-88-4	0.99	0.89	0.95	1.37	1.48	1.34	0.97	1.04	-0.54	2	1	3	Low Priority
S729	001143-72-2	0.45	0.65	0.74	0.67	0.71	0.76	0.32	0.66	-0.13	1	1	2	Low Priority
S730	001156-19-0	<b>0.85</b>	<b>0.85</b>	<b>0.85</b>	0.89	0.89	0.24	0.36	0.30	-0.61	2	1	2	Low Priority
S731	001195-79-5	0.34	0.74	0.66	0.52	0.33	0.47	0.69	0.59	-1.54	2	1	2	Low Priority
S732	001197-18-8	<b>0.36</b>	<b>0.68</b>	<b>0.68</b>	<b>0.70</b>	<b>0.70</b>	0.00	0.16	0.22	-2.63	1	1	1	Low Priority

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	logHL <sub>4</sub> (h)	logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	PBT Index	P	B	T		
S733	001209-98-9	1.06	1.10	0.97	0.83	1.16	2.02	2.00	1.92	-0.63	2	1	3	Low Priority
S734	001220-83-3	0.73	0.85	0.81	1.18	1.12	0.07	0						

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level		
		logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	logHL <sub>4</sub> (h)	logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	PBT Index	P	B	T			
S815	003198-29-6	0.04	0.10	0.18	-0.10	0.09	-0.26	-0.10	-0.02	-0.73	1	1	1	Low Priority	
S816	003209-13-0	0.36	0.38	0.52	0.32	0.37	0.42	0.20	0.47	-0.74	1	1	2	Low Priority	
S817	003239-44-9	1.15	1.15	1.15	1.13	1.26	1.14	1.65	1.34	1.10	2	1	2	Low Priority	
S818	003282-30-2	0.26	0.19	0.60	0.38	0.57	0.03	0.49	0.44	-0.80	1	1	2	Low Priority	
S819	003380-34-5	1.68	2.05	2.27	2.07	2.05	1.97	1.58	1.94	2.44	2	1	3	Low Priority	
S820	003416-24-8	-0.01	0.08	-0.05	0.18	-0.14	-0.26	-0.20	-0.02	-3.77	1	1	1	Low Priority	
S821	003452-97-9	0.56	0.54	0.69	0.53	0.33	0.32	0.72	0.75	-2.01	1	1	2	Low Priority	
S822	003485-14-1	0.51	0.84	0.70	0.69	0.61	0.27	0.33	0.42	-2.71	2	1	2	Low Priority	
S823	003487-99-8	0.87	0.66	0.38	0.24	0.58	1.27	1.09	1.04	0.00	1	1	3	Low Priority	
S824	003511-16-8	0.70	0.76	0.69	0.76	0.65	0.50	0.63	0.66	-0.68	2	1	2	Low Priority	
S825	003563-58-4	1.64	1.47	1.80	2.05	1.84	0.81	1.40	1.02	-0.53	2	1	2	Low Priority	
S826	003568-94-3	0.82	0.65	0.89	0.79	1.10	0.79	1.01	1.01	0.78	-0.84	1	1	2	Low Priority
S827	003595-11-7	1.01	0.71	1.06	1.00	1.19	1.41	1.49	1.42	-1.90	1	1	2	Low Priority	
S828	003613-30-7	0.90	0.63	0.90	0.72	0.35	0.92	1.12	1.22	-1.44	2	1	2	Low Priority	
S829	003648-20-2	0.62	0.69	0.10	0.07	0.18	1.62	1.70	1.59	-0.07	1	1	?	Low Priority	
S830	003648-21-3	0.66	0.67	0.23	0.19	0.30	1.23	1.35	1.25	-0.06	1	2	3	Low Priority	
S831	003688-65-1	0.67	0.82	0.64	0.87	0.61	1.59	0.69	1.05	-0.50	2	1	2	Low Priority	
S832	003691-78-9	0.79	0.98	0.50	0.66	0.57	1.23	1.29	1.16	0.99	2	1	3	Low Priority	
S833	003736-81-0	1.16	1.01	1.30	1.47	1.40	1.33	1.21	1.09	2.34	2	1	2	Low Priority	
S834	003737-09-5	0.85	1.19	1.19	1.19	1.19	0.80	1.25	0.69	0.21	3	1	3	Low Priority	
S835	003778-73-2	0.82	1.15	1.15	1.15	1.15	0.40	0.29	-0.67	2	1	3	Low Priority		
S836	003846-71-7	1.06	1.19	1.18	1.18	1.06	2.27	2.27	1.52	2	2	3	High Priority		
S837	003861-72-1	0.89	0.95	0.72	0.79	0.78	1.43	1.10	1.23	-0.24	2	1	2	Low Priority	
S838	003861-76-5	1.04	1.19	1.05	1.19	1.11	1.93	1.72	1.78	0.6	3	2	3	Priority (Group 3)	
S839	003864-99-1	1.09	1.25	1.54	1.54	1.41	2.10	2.10	2.10	2.10	2	1	3	High Priority	
S840	003896-11-5	0.87	1.44	1.74	1.36	1.29	1.42	1.60	1.28	2.18	2	2	3	Priority (Group 3)	
S841	003900-31-0	1.02	1.03	1.29	1.32	1.43	1.45	1.49	1.21	2.47	2	1	2	Low Priority	
S842	003902-71-4	0.78	0.73	0.79	0.75	0.85	1.13	0.79	1.00	0.85	2	1	2	Low Priority	
S843	003930-20-9	0.80	1.62	1.62	1.62	1.44	0.70	0.42	-1.15	1	1	2	Low Priority		
S844	003964-81-6	1.18	1.10	0.88	0.92	0.98	2.29	2.34	1.92	1.24	2	1	3	Low Priority	
S845	004008-48-4	0.09	0.40	0.25	0.14	0.21	0.52	0.40	0.12	0.52	2	1	2	Low Priority	
S846	004065-45-6	0.55	0.70	0.76	0.88	0.71	0.55	0.30	0.53	0.68	2	1	1	Low Priority	
S847	004083-64-1	0.55	0.74	0.82	0.73	0.71	0.27	0.56	0.45	0.45	2	1	2	Low Priority	
S848	004191-73-5	0.49	0.51	0.52	0.28	0.38	0.18	0.22	0.30	-0.60	1	1	3	Low Priority	
S849	004205-90-7	1.40	1.10	1.56	1.53	1.90	1.77	1.79	1.51	0.44	2	1	2	Low Priority	
S850	004247-02-3	0.66	0.58	0.71	0.39	0.59	0.29	0.32	0.40	-0.61	1	1	2	Low Priority	
S851	004350-09-8	0.34	0.58	0.42	0.33	0.45	0.19	0.23	0.05	-1.26	1	1	1	Low Priority	
S852	004360-12-7	0.71	1.23	0.97	0.85	1.02	1.16	1.08	0.72	-1.29	2	1	2	Low Priority	
S853	004394-00-7	0.40	0.39	0.39	0.42	0.42	0.72	0.21	0.21	2.21	2	1	2	Low Priority	
S854	004407-36-7	0.45	0.39	0.53	-0.01	0.41	0.61	0.36	0.43	-0.49	1	1	3	Low Priority	
S855	004455-13-4	0.48	-0.04	-0.17	0.11	0.15	-0.04	0.00	0.21	-1.46	1	1	2	Low Priority	
S856	004697-36-3	0.04	0.62	0.46	0.66	0.42	0.22	0.29	0.39	-0.81	2	1	2	Low Priority	
S857	004707-47-5	0.28	0.47	0.54	0.30	0.36	0.38	0.23	0.51	-0.99	1	1	2	Low Priority	
S858	004721-69-1	0.65	0.78	0.89	0.65	0.85	0.98	0.96	1.01	-2.10	2	1	3	Low Priority	
S859	004764-17-4	0.90	0.77	0.94	0.95	1.07	1.24	0.98	1.23	-1.05	2	1	2	Low Priority	
S860	004969-02-2	1.43	1.38	1.19	1.21	1.30	2.76	2.44	2.68	1.10	3	2	3	Priority (Group 2)	
S861	005051-62-7	0.78	0.82	0.82	0.88	0.88	1.31	1.23	1.41	-0.12	2	1	2	Low Priority	
S862	005089-22-5	1.39	1.21	0.97	1.16	1.33	1.88	1.84	1.25	5.52	3	3	3	Priority (Group 3)	
S863	005104-49-4	0.72	0.70	0.70	1.05	1.05	0.47	0.66	0.39	1.45	2	1	2	Low Priority	
S864	005250-39-5	0.15	0.60	0.60	0.60	0.60	1.18	0.82	1.04	1.89	3	1	2	Low Priority	
S865	005307-14-2	0.22	0.35	0.38	0.53	0.66	0.11	0.07	0.02	-1.71	2	1	3	Low Priority	
S866	005320-75-2	0.87	0.78	0.58	0.58	0.76	1.42	1.20	1.13	1.28	1	1	3	Low Priority	
S867	005417-35-6	0.68	0.02	0.62	0.44	0.88	1.29	1.12	1.04	-1.36	1	1	3	Low Priority	
S868	005466-77-3	0.84	0.71	0.62	0.42	0.48	1.65	1.31	1.39	-0.02	1	2	3	Low Priority	
S869	005533-03-9	0.42	0.69	0.75	0.34	0.35	0.50	0.56	-0.75	1	1	1	Low Priority		
S870	005588-33-0	1.56	1.55	1.55	1.20	1.17	1.42	1.22	1.12	1.04	2	2	3	Low Priority	
S871	005591-45-7	1.18	1.18	1.18	1.18	1.18	1.36	1.07	1.22	1.43	3	1	3	Low Priority	
S872	005595-79-9	0.48	0.60	0.60	0.34	0.37	0.64	0.42	0.67	-0.76	1	1	2	Low Priority	
S873	005633-20-5	0.86	0.86	0.86	0.86	0.86	1.06	1.14	1.01	-0.48	2	1	2	Low Priority	
S874	005636-83-9	1.28	1.14	1.11	1.09	0.98	2.31	2.51	2.06	1.25	2	1	3	Priority (Group 2)	
S875	005638-76-6	0.96	0.67	0.51	0.52	0.78	0.88	1.11	0.60	-0.63	2	1	1	Low Priority	
S876	005638-85-7	0.18	0.36	0.58	0.21	0.50	0.28	0.07	-0.08	-0.67	1	1	2	Low Priority	
S877	005786-21-0	1.00	1.00	1.00	1.00	1.00	2.26	2.09	1.96	1.47	2	1	2	Low Priority	
S878	005988-91-0	0.83	0.50	0.18	0.51	0.35	0.85	0.92	1.02	-1.44	1	1	2	Low Priority	
S879	006091-50-5	0.81	0.49	0.62	0.77	0.83	0.68	0.73	0.68	-1.30	1	1	2	Low Priority	
S880	006197-30-4	0.77	1.01	0.66	0.46	0.57	1.41	1.61	1.33	1.42	1	3	3	Low Priority	
S881	006259-76-3	0.50	0.64	0.46	0.07	0.29	0.53	0.47	0.54	-0.62	1	2	3	Low Priority	
S882	006290-17-1	0.78	0.54	0.50	0.80	0.60	0.28	0.58	0.56	-1.50	2	1	2	Low Priority	
S883	006413-10-1	0.73	0.44	0.32	0.67	0.54	0.17	0.43	0.41	-1.49	2	1	2	Low Priority	
S884	006422-86-2	0.82	0.66	0.50	0.39	0.40	1.29	1.45	1.37	-0.06	1	2	3	Low Priority	
S885	006452-71-7	0.18	0.18	0.18	0.32	0.32	1.39	1.08	1.30	-0.96	2	1	2	Low Priority	
S886	006493-05-6	0.08	0.16	0.16	0.17	0.17	0.27	0.69	0.17	-0.06	2	1	2	Low Priority	
S887	006621-47-2	1.98	1.99	1.99	1.97	1.97	2.39	2.34	2.27	-1.93	2	3	3	Priority (Group 2)	
S888	006628-37-1	0.55	0.70	0.76	0.88	0.71	0.55	0.30	0.53	0.68	2	1	1	Low Priority	
S889	006658-48-6	0.89	0.99	0.75	0.70	0.55	1.28	1.29	1.36	-0.17	2	1	3	Low Priority	
S890	006673-35-4	0.56	0.73	0.52	0.35	0.32	0.74	0.82	0.71	-1.36	2	1	2	Low Priority	
S891	006804-07-5	0.54	0.88	0.68	0.73	0.77	0.38	0.17	-0.29	1.08	2	1	2	Low Priority	
S892	006931-54-0	0.64	0.86	0.95	0.97	0.76	1.26	1.37	1.26	-1.59	2	1	3	Low Priority	
S893	007143-69-3	1.10	0.58	0.72	0.75	0.73	1.53	1.49	1.37	0.17	2	2	3	Low Priority	
S894	007261-97-4	1.00	1.05	1.05	1.35	1.35	0.70	0.50	0.38	1.34	2	1	2	Low Priority	
S895	007370-44-7	0.71	0.55	0.19	0.01	0.31	1.16	1.28	1.27	-1.50	1	1	3	Low Priority	
S896	007370-92-5	0.70	0.51	0.29	0.08	0.39	0.88	1.02	1.01	-1.49	1	1	3	Low Priority	

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	logHL <sub>4</sub> (h)	logHL <sub>1</sub> (h)	logHL <sub>2</sub> (h)	logHL <sub>3</sub> (h)	PBT Index	P	B	T		
S897	007392-19-0	0.93	0.56	0.95	1.21	1.01	1.39	1.51	1.35	-1.39	2	1	3	Low Priority
S898	007416-34-4	0.65	0.78	0.74	0.72	0.71	0.75	1.04	0.73	-1.17	2	1	2	Low Priority
S899	007420-86-2	1.33	1.03	1.04	1.07	1.31	1.64	1.66	1.17	2.08	2	1	2	Low Priority
S900	007492-32-2	1.08	1.17	1.09	1.03	0.90	1.22	1.62	1.49	0.20	2	1	2	Low Priority
S901	007512-17-6	0.17	0.09	-0.12	0.22	-0.20	-0.13	-0.05	0.05	-3.20	1	1	1	Low Priority
S902	007540-51-4	0.74	0.36	0.65	0.41	0.49	0.63	0.66						

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>1a1</sub> (h)	logHL <sub>1a2</sub> (h)	logHL <sub>1a3</sub> (h)	logHL <sub>1a4</sub> (h)	logHL <sub>1a1</sub> (h)	logHL <sub>1a2</sub> (h)	logHL <sub>1a3</sub> (h)	PBT Index	P	B		T
S979	018323-44-9	0.32	0.39	0.39	0.39	0.39	0.64	0.65	0.76	-2.53	2	1	2	Low Priority
S980	018368-91-7	0.64	0.72	0.99	1.03	0.82	0.77	1.02	0.86	-2.15	2	1	2	Low Priority
S981	018479-58-8	0.83	0.52	0.76	0.77	0.64	0.65	0.78	0.70	-1.84	2	1	2	Low Priority
S982	018559-94-9	<b>0.38</b>	<b>0.83</b>	<b>0.83</b>	<b>0.83</b>	<b>0.83</b>	0.90	1.08	1.14	-1.97	1	1	2	Low Priority
S983	018694-40-1	1.05	0.90	0.85	0.86	0.96	1.47	1.82	1.39	1.03	2	1	2	Low Priority
S984	018871-14-2	0.63	0.53	0.37	0.29	0.42	0.71	0.89	0.91	-1.49	1	1	2	Low Priority
S985	019216-56-9	<b>0.30</b>	<b>0.32</b>	<b>0.32</b>	<b>0.32</b>	<b>0.32</b>	0.46	0.43	0.11	1.10	2	1	2	Low Priority
S986	019224-26-1	0.78	0.66	0.39	0.65	0.61	0.95	1.09	1.04	1.27	1	1	3	Low Priority
S987	019356-17-3	1.19	0.91	1.40	1.05	1.08	2.17	1.98	2.00	-1.84	2	2	?	Low Priority
S988	019387-91-8	<b>1.11</b>	<b>1.21</b>	<b>1.21</b>	<b>1.21</b>	<b>1.21</b>	0.57	0.75	0.45	0.00	2	1	2	Low Priority
S989	019395-41-6	0.40	0.60	0.40	0.05	0.40	0.61	0.73	0.71	-1.00	1	1	1	Low Priority
S990	020485-39-6	0.51	0.33	0.21	0.40	0.48	0.22	0.42	0.14	-0.41	1	1	2	Low Priority
S991	020537-88-6	<b>-0.88</b>	<b>-0.85</b>	<b>-0.85</b>	<b>-0.85</b>	<b>-0.85</b>	-0.14	-0.02	0.16	-3.40	1	1	1	Low Priority
S992	020574-50-9	1.40	1.13	1.17	1.30	1.47	2.03	1.77	1.70	-0.04	2	1	2	Low Priority
S993	020770-40-5	0.93	0.34	0.60	0.50	0.53	1.37	1.40	1.36	-1.07	1	2	3	Low Priority
S994	021145-77-7	1.00	1.00	1.04	1.06	0.78	1.33	1.95	1.95	-0.24	2	1	3	Low Priority
S995	021187-98-4	<b>1.04</b>	<b>1.07</b>	<b>1.07</b>	0.98	0.98	0.31	0.44	0.37	-0.61	2	1	2	Low Priority
S996	021245-01-2	0.94	0.86	0.80	0.76	0.74	0.82	1.10	0.74	-0.24	2	1	3	Low Priority
S997	021245-02-3	0.87	0.80	0.72	0.59	0.55	1.03	1.26	0.87	-0.26	1	2	3	Low Priority
S998	021256-18-8	<b>1.74</b>	<b>1.74</b>	<b>1.74</b>	0.28	0.59	0.89	0.93	0.73	2.4	1	1	1	Low Priority
S999	021500-98-1	1.03	1.05	0.74	0.94	1.01	2.30	2.07	2.19	-0.24	1	1	3	Low Priority
S1000	021738-42-1	<b>0.24</b>	<b>0.24</b>	<b>0.24</b>	<b>0.46</b>	<b>0.46</b>	1.02	1.01	0.94	-1.37	2	1	2	Low Priority
S1001	021829-25-4	<b>0.28</b>	<b>0.28</b>	<b>0.28</b>	<b>0.28</b>	<b>0.28</b>	0.72	0.76	0.58	0.20	2	1	2	Low Priority
S1002	022004-32-6	0.96	0.78	0.82	0.99	0.86	1.56	1.39	1.66	-1.06	2	1	2	Low Priority
S1003	022071-15-4	<b>0.32</b>	<b>0.48</b>	<b>0.48</b>	<b>0.48</b>	<b>0.48</b>	0.57	0.43	0.50	0.85	1	1	1	Low Priority
S1004	022199-08-2	0.69	0.87	0.88	1.10	1.17	-0.10	0.35	-0.29	0.09	2	1	2	Low Priority
S1005	022204-53-1	<b>1.18</b>	<b>1.18</b>	<b>1.18</b>	0.40	0.41	0.42	0.37	0.49	0.51	1	1	1	Low Priority
S1006	022232-54-8	0.65	0.43	0.42	0.46	0.70	0.46	0.33	0.35	-1.07	2	1	2	Low Priority
S1007	022232-71-9	<b>1.06</b>	<b>1.05</b>	<b>1.05</b>	1.33	1.37	1.48	1.36	1.35	1.27	2	1	3	Low Priority
S1008	022316-47-8	<b>1.26</b>	<b>1.29</b>	<b>1.29</b>	<b>1.59</b>	<b>1.59</b>	1.37	1.15	1.11	1.87	2	1	2	Low Priority
S1009	022345-47-7	1.20	0.82	1.02	1.04	0.87	2.57	2.36	2.77	1.44	3	2	3	Priority (Group 2)
S1010	022494-42-4	<b>1.00</b>	<b>1.00</b>	<b>1.00</b>	0.80	0.90	0.67	0.84	0.67	1.73	2	1	2	Low Priority
S1011	022664-55-7	0.60	0.67	0.50	0.46	0.32	1.12	1.21	1.65	-0.98	2	1	2	Low Priority
S1012	022839-47-0	0.36	0.20	0.13	0.12	0.12	0.12	0.35	0.29	-1.37	1	1	1	Low Priority
S1013	022916-47-8	2.47	2.66	2.49	2.56	2.51	2.93	3.11	2.58	4.62	3	3	3	High Priority
S1014	022994-85-0	0.65	0.71	0.48	0.62	0.67	0.51	0.64	0.29	0.67	2	1	2	Low Priority
S1015	023031-25-6	<b>1.18</b>	<b>1.63</b>	<b>1.63</b>	<b>1.63</b>	<b>1.63</b>	0.98	1.01	1.20	0.98	1	1	2	Low Priority
S1016	023092-17-3	1.64	1.07	1.59	1.62	1.75	2.04	2.33	1.90	3.81	3	1	3	Low Priority
S1017	023155-02-4	<b>0.28</b>	<b>0.33</b>	<b>0.38</b>	0.26	0.18	-0.82	-0.22	-1.1	1	1	1	1	Low Priority
S1018	023593-75-1	<b>0.30</b>	<b>0.30</b>	<b>0.30</b>	<b>0.30</b>	<b>0.30</b>	3.05	2.78	2.79	3.99	3	3	3	High Priority
S1019	023787-90-8	0.68	0.80	0.70	0.78	0.58	0.99	1.22	1.12	-1.58	2	1	2	Low Priority
S1020	023887-31-2	<b>0.38</b>	<b>0.38</b>	<b>0.38</b>	<b>0.72</b>	<b>0.72</b>	1.00	0.93	0.81	1.33	2	1	2	Low Priority
S1021	023911-56-0	0.58	0.62	0.43	0.57	0.56	0.60	0.60	0.65	0.66	2	1	2	Low Priority
S1022	023985-25-3	0.90	0.45	0.46	0.71	0.62	0.88	0.88	0.83	-1.07	1	1	2	Low Priority
S1023	024166-13-0	1.27	1.44	1.46	1.51	1.59	1.39	1.23	1.14	1.92	3	1	3	Low Priority
S1024	024219-97-4	<b>1.13</b>	<b>1.14</b>	<b>1.14</b>	1.00	1.08	2.41	2.32	2.09	1.09	2	1	2	Priority (Group 2)
S1025	024237-00-1	1.08	0.59	1.03	1.07	1.08	1.54	1.51	1.35	-1.39	1	1	3	Low Priority
S1026	024280-93-1	0.53	0.40	0.75	0.31	0.35	0.99	0.67	0.95	-0.59	1	1	2	Low Priority
S1027	024295-03-2	0.38	0.31	0.56	0.31	0.58	0.94	1.08	0.74	-0.23	1	1	2	Low Priority
S1028	024526-64-5	<b>0.81</b>	<b>1.18</b>	<b>1.18</b>	<b>1.18</b>	1.51	1.49	1.19	0.22	2	1	2	Low Priority	
S1029	024717-85-9	0.90	0.31	0.62	0.46	0.53	1.36	1.37	1.32	-1.08	1	2	3	Low Priority
S1030	024851-98-7	0.67	0.40	0.24	0.36	0.37	0.72	0.89	1.00	-1.32	1	1	2	Low Priority
S1031	025013-16-5	0.72	0.68	0.75	0.75	0.69	0.85	0.84	0.84	-0.78	2	1	2	Low Priority
S1032	025046-79-1	0.71	0.83	0.65	0.97	0.83	0.46	0.42	0.25	0.27	2	1	2	Low Priority
S1033	025340-17-4	0.91	0.83	0.52	0.73	0.68	1.73	1.74	1.72	-0.18	1	1	2	Low Priority
S1034	025384-17-4	0.87	0.75	0.75	0.67	0.64	1.26	1.22	1.18	-0.04	2	1	3	Low Priority
S1035	025451-15-4	<b>1.33</b>	<b>0.43</b>	0.21	0.26	0.55	-0.03	0.20	0.26	-1.51	2	1	1	Low Priority
S1036	025485-88-5	0.61	0.66	0.62	0.34	0.64	0.51	0.44	0.49	-0.63	1	1	3	Low Priority
S1037	025724-58-7	0.65	0.68	0.19	0.16	0.27	1.34	1.45	1.34	-0.06	1	1	?	Low Priority
S1038	025812-30-0	<b>0.18</b>	<b>0.18</b>	<b>0.18</b>	<b>0.19</b>	<b>0.19</b>	0.78	0.83	1.00	-0.58	2	1	2	Low Priority
S1039	025905-77-5	1.09	1.16	0.87	0.87	0.95	1.46	1.82	1.24	0.84	2	1	2	Low Priority
S1040	025966-79-4	0.71	0.98	0.90	0.83	0.61	1.02	1.22	1.17	-1.56	2	1	2	Low Priority
S1041	025973-55-1	1.10	1.19	1.26	1.17	1.00	1.20	1.80	1.14	1.51	2	3	3	Priority (Group 3)
S1042	026171-23-3	<b>0.70</b>	<b>0.70</b>	<b>0.70</b>	0.44	0.40	0.27	0.41	-0.04	0.63	1	1	2	Low Priority
S1043	026761-40-0	0.76	0.72	0.57	0.28	0.40	1.53	1.70	1.59	-0.07	2	1	?	Low Priority
S1044	026787-78-0	<b>0.04</b>	<b>0.41</b>	<b>0.41</b>	<b>0.41</b>	<b>0.41</b>	0.38	0.28	0.53	-1.79	2	1	2	Low Priority
S1045	026807-65-8	<b>1.15</b>	<b>1.17</b>	<b>1.17</b>	<b>1.18</b>	<b>1.18</b>	0.93	0.71	0.91	2	1	3	Low Priority	
S1046	026839-75-8	<b>0.34</b>	<b>0.42</b>	<b>0.42</b>	<b>0.42</b>	<b>0.42</b>	0.69	1.07	0.75	-1.40	2	1	2	Low Priority
S1047	026896-48-0	0.46	0.88	0.75	0.36	0.82	0.68	0.74	0.74	-2.45	2	1	2	Low Priority
S1048	027203-92-5	<b>0.76</b>	<b>0.83</b>	<b>0.83</b>	<b>0.83</b>	<b>0.83</b>	1.14	1.11	1.03	-0.88	2	1	2	Low Priority
S1049	027262-47-1	0.82	0.89	0.79	0.60	0.73	0.82	0.95	0.48	-0.69	2	1	3	Low Priority
S1050	027503-81-7	0.78	1.02	1.03	0.88	1.01	0.25	0.54	0.01	1.61	1	1	2	Low Priority
S1051	027554-26-3	0.77	0.70	0.59	0.36	0.45	1.34	1.54	1.43	-0.06	2	1	?	Low Priority
S1052	027987-25-3	1.04	0.81	0.78	0.84	0.86	1.17	1.24	1.12	-0.09	2	3	3	Low Priority
S1053	028179-44-4	0.82	1.20	1.20	1.19	1.34	0.46	0.68	0.29	0.53	2	1	1	Low Priority
S1054	028219-61-6	0.93	0.61	1.09	0.85	0.77	1.27	1.17	1.19	-1.61	2	2	3	Low Priority
S1055	028395-03-1	<b>0.08</b>	<b>0.26</b>	<b>0.26</b>	<b>0.26</b>	<b>0.26</b>	0.61	0.57	0.41	-0.09	2	1	2	Low Priority
S1056	028553-12-0	0.77	0.70	0.58	0.34	0.44	1.39	1.58	1.47	-0.07	2	1	?	Low Priority
S1057	028657-80-9	<b>0.18</b>	<b>0.20</b>	<b>0.20</b>	<b>0.40</b>	<b>0.40</b>	0.11	0.07	-0.15	-0.22	1	1	2	Low Priority
S1058	028721-07-5	<b>0.30</b>	<b>0.32</b>	<b>0.32</b>	<b>0.32</b>	<b>0.32</b>	0.34	0.40	0.02	0.46	2	1	2	Low Priority
S1059	028782-42-5	0.84	1.18	0.56	0.58	0.55	1.28	1.36	1.25	2.15	3	1	1	Low Priority
S1060	028797-61-7	0.78	1.03	0.82	0.76	0.90	0.26	0.51	-0.07	0.79	3	1	2	Low Priority

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>1a1</sub> (h)	logHL <sub>1a2</sub> (h)	logHL <sub>1a3</sub> (h)	logHL <sub>1a4</sub> (h)	logHL <sub>1a1</sub> (h)	logHL <sub>1a2</sub> (h)	logHL <sub>1a3</sub> (h)	PBT Index	P	B		T
S1061	028860-95-9	0.18	0.37	0.37	0.39	0.39	0.32	0.16	0.50	-2.53	1	1	1	Low Priority
S1062														

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>01</sub> (h)	logHL <sub>02</sub> (h)	logHL <sub>03</sub> (h)	logHL <sub>04</sub> (h)	logHL <sub>01</sub> (h)	logHL <sub>02</sub> (h)	logHL <sub>03</sub> (h)	PBT Index	P	B		T
S1143	051384-51-1	0.56	0.58	0.58	0.58	0.58	1.07	1.10	1.18	-1.17	2	1	2	Low Priority
S1144	051414-25-6	0.82	0.56	0.63	0.57	0.55	0.98	0.84	0.87	-1.65	2	1	2	Low Priority
S1145	051481-61-9	0.57	0.85	0.39	0.16	0.51	0.44	0.93	0.52	-1.26	2	1	2	Low Priority
S1146	051566-62-2	0.97	0.46	0.41	0.55	0.55	1.07	1.26	1.22	-1.18	1	1	2	Low Priority
S1147	051781-06-7	0.62	0.85	0.69	0.51	0.48	0.87	1.07	0.92	-1.39	2	1	2	Low Priority
S1148	051803-78-2	0.84	0.75	0.61	1.02	0.90	0.87	0.64	0.64	1.12	2	1	2	Low Priority
S1149	051940-44-4	0.39	0.89	0.81	0.34	0.58	0.21	0.53	-0.09	-0.62	2	1	1	Low Priority
S1150	052128-35-5	1.23	1.32	1.32	1.32	1.32	1.52	1.49	1.35	0.14	3	1	2	Low Priority
S1151	052365-63-6	0.87	0.74	0.62	0.66	0.54	0.94	1.19	1.42	-0.84	2	1	2	Low Priority
S1152	052468-60-7	2.64	2.63	2.63	2.64	2.64	2.21	2.14	1.93	3.59	3	2	3	High Priority
S1153	052485-79-7	0.51	0.51	0.51	0.51	0.51	3.41	3.38	3.64	-0.94	3	1	3	Priority (Group 2)
S1154	052645-53-1	1.39	1.58	1.56	1.60	1.56	1.94	2.00	1.77	2.51	2	1	3	Low Priority
S1155	053179-11-6	1.03	1.03	1.03	1.04	1.04	1.88	1.61	1.77	2.48	3	2	3	Priority (Group 3)
S1156	053583-79-2	1.08	1.33	1.33	1.02	0.80	0.66	0.65	0.69	-0.25	2	1	2	Low Priority
S1157	053716-49-7	0.73	1.03	1.18	0.83	0.98	0.81	0.68	0.68	1.61	2	1	1	Low Priority
S1158	053716-50-0	0.73	0.99	0.59	0.83	0.90	0.17	0.57	-0.13	1.27	2	1	2	Low Priority
S1159	053994-73-3	-0.12	-0.07	-0.07	-0.02	-0.02	0.42	0.47	0.51	-0.54	2	1	1	Low Priority
S1160	054024-22-5	1.44	1.44	1.44	1.45	1.45	1.80	1.59	1.49	-1.52	2	2	3	Low Priority
S1161	054048-10-1	1.40	1.40	1.40	1.40	1.40	1.43	1.42	-1.31	2	1	2	Low Priority	
S1162	054063-53-5	0.32	0.32	0.32	0.34	0.34	1.13	1.05	1.04	0.23	2	1	2	Low Priority
S1163	054143-55-4	1.08	1.32	1.32	1.32	1.32	2.00	2.56	1.98	2.79	3	2	3	High Priority
S1164	054464-57-2	0.90	0.76	0.94	1.01	0.72	1.13	1.47	1.41	-1.34	2	2	3	Low Priority
S1165	054739-18-3	1.19	1.20	1.20	1.26	1.26	1.59	1.43	1.28	0.92	2	1	2	Low Priority
S1166	054910-89-3	1.68	1.68	1.68	1.23	1.36	1.58	1.85	1.70	2.39	2	1	3	Low Priority
S1167	054965-21-8	1.00	1.00	1.00	1.01	1.01	0.54	0.15	-0.24	-0.16	2	1	3	Low Priority
S1168	054982-83-1	0.62	0.22	0.71	0.20	0.86	0.78	0.96	0.94	-1.29	1	1	3	Low Priority
S1169	055268-74-1	0.06	0.06	0.06	0.07	0.07	0.97	1.03	0.90	-0.09	2	1	2	Low Priority
S1170	055981-09-4	0.54	0.55	0.55	0.56	0.56	0.55	0.33	0.25	0.86	2	1	2	Low Priority
S1171	055985-32-5	0.61	0.62	0.62	0.62	0.62	0.98	0.97	0.72	1.44	2	1	2	Low Priority
S1172	056030-54-7	1.15	1.15	1.15	1.15	1.15	1.21	1.14	0.86	-0.77	2	1	3	Low Priority
S1173	056039-58-8	0.90	0.93	1.12	1.00	0.88	0.71	0.73	0.62	-0.04	2	1	1	Low Priority
S1174	056177-80-1	0.61	0.28	0.63	0.56	0.81	-0.29	0.02	-0.18	-0.83	1	1	1	Low Priority
S1175	056211-40-6	0.71	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.27	2	1	1	Low Priority
S1176	056296-78-7	1.66	0.97	1.17	1.23	1.36	1.58	1.85	1.70	2.39	2	1	3	Low Priority
S1177	056775-88-3	0.92	0.92	0.92	0.93	0.93	2.40	2.66	2.03	1.92	2	1	2	Priority (Group 1)
S1178	056932-44-6	0.17	0.55	0.40	0.17	0.23	0.40	0.38	0.34	-1.71	2	1	2	Low Priority
S1179	056995-20-1	0.93	1.01	1.01	1.01	1.01	0.38	0.86	0.36	0.13	3	1	3	Low Priority
S1180	057345-19-4	1.37	1.05	1.56	1.43	1.30	1.91	2.00	1.90	-1.65	3	2	3	Low Priority
S1181	057574-09-1	-0.12	-0.14	-0.14	-0.12	-0.12	1.49	1.51	1.70	0.35	2	1	1	Low Priority
S1182	057775-29-8	0.70	1.11	0.80	0.64	0.72	1.27	1.38	1.06	0.54	2	1	2	Low Priority
S1183	057808-66-9	0.88	0.88	0.88	0.88	0.88	1.12	0.94	0.94	1.09	2	1	1	Low Priority
S1184	057849-23-7	1.22	0.83	0.93	0.93	1.05	2.07	1.88	2.02	-0.44	2	1	3	Low Priority
S1185	058001-44-8	0.80	0.14	0.21	0.06	0.12	-0.24	-0.18	-0.18	-1.84	1	1	1	Low Priority
S1186	058817-05-3	0.80	0.79	0.42	0.44	0.44	1.05	1.24	0.86	-0.25	1	1	3	Low Priority
S1187	059122-46-2	-0.30	-0.30	-0.30	-0.30	-0.30	1.27	1.12	1.02	-1.92	2	1	3	Low Priority
S1188	059170-23-9	0.28	0.28	0.28	0.28	0.28	1.64	1.25	1.64	0.11	2	1	2	Low Priority
S1189	059259-38-0	0.59	0.47	0.38	0.31	0.48	0.39	0.65	0.61	-1.91	1	1	2	Low Priority
S1190	059338-93-1	0.61	1.05	0.79	0.75	0.71	0.40	0.59	-0.12	0.51	2	1	2	Low Priority
S1191	059467-70-8	0.49	0.49	0.49	0.49	0.49	1.57	1.73	1.29	3.04	3	1	3	Low Priority
S1192	059708-52-0	0.78	0.85	0.60	0.58	0.53	1.14	1.20	0.81	1.19	2	1	3	Low Priority
S1193	059729-33-8	1.52	1.57	1.57	1.57	1.57	1.65	1.42	1.66	3	1	2	Low Priority	
S1194	059804-37-4	0.61	1.07	0.99	0.99	0.99	0.12	0.16	-0.11	0.67	2	1	3	Low Priority
S1195	059820-43-8	0.21	0.43	0.18	0.10	0.12	0.67	0.49	0.57	-1.34	1	1	1	Low Priority
S1196	060142-96-3	0.72	0.42	0.34	-0.01	0.16	0.14	0.30	0.35	-2.63	1	1	1	Low Priority
S1197	060628-96-8	0.18	0.18	0.18	0.17	0.17	2.50	2.58	2.20	3.65	3	1	3	Priority (Group 1)
S1198	060643-86-9	1.10	-0.01	0.14	-0.17	-0.02	-0.11	-0.08	0.03	-2.38	1	1	1	Low Priority
S1199	060719-84-8	0.30	0.49	0.49	0.49	0.49	0.38	0.36	-0.06	-0.93	2	1	2	Low Priority
S1200	060770-00-5	0.45	0.59	0.62	0.29	0.35	0.24	0.21	0.32	-0.60	1	1	2	Low Priority
S1201	061869-08-7	1.11	1.11	1.11	1.11	1.11	1.28	1.15	1.34	1.06	2	1	3	Low Priority
S1202	062406-73-9	1.08	0.74	1.15	1.13	1.20	1.49	1.78	1.61	-1.63	2	1	3	Low Priority
S1203	062571-86-2	0.30	0.29	0.19	-0.09	0.12	0.11	0.26	0.19	-1.71	1	1	2	Low Priority
S1204	062666-20-0	0.60	0.62	0.62	0.61	0.61	1.35	1.28	1.44	1.34	2	1	3	Low Priority
S1205	063187-91-7	0.65	0.69	0.84	0.58	0.72	0.67	0.84	0.89	-2.05	2	1	2	Low Priority
S1206	063250-25-9	1.08	0.99	0.78	1.10	0.89	1.20	1.34	1.24	1.25	2	1	3	Low Priority
S1207	063500-71-0	0.71	0.64	0.90	0.86	0.85	0.43	0.66	0.55	-2.08	2	1	1	Low Priority
S1208	063590-64-7	0.95	1.01	1.01	1.01	1.01	0.27	0.42	-0.05	0.01	2	1	2	Low Priority
S1209	063659-18-7	1.23	1.33	1.33	1.33	1.33	1.29	1.31	1.40	-1.18	2	1	2	Low Priority
S1210	063675-72-9	1.04	1.04	1.04	1.04	1.04	0.84	0.95	0.71	0.16	2	1	2	Low Priority
S1211	065277-42-1	0.30	0.30	0.30	0.31	0.31	1.92	1.80	1.91	3.43	3	1	3	Low Priority
S1212	065405-77-8	0.50	0.53	0.54	0.11	0.34	0.85	0.47	0.55	-0.40	1	1	3	Low Priority
S1213	065405-84-7	0.81	0.73	0.69	0.78	0.53	1.46	1.43	1.55	-1.24	2	2	3	Low Priority
S1214	066085-59-4	0.11	0.11	0.11	0.11	0.11	0.78	0.91	0.66	0.16	2	1	2	Low Priority
S1215	066104-22-1	1.43	1.43	1.43	1.46	1.46	1.91	1.71	1.64	0.25	2	1	3	Low Priority
S1216	066327-54-6	1.00	0.81	0.78	0.88	0.66	1.40	1.24	1.27	-1.27	2	2	3	Low Priority
S1217	066357-35-5	0.32	0.96	0.96	0.96	0.96	1.23	0.78	1.35	-0.93	2	1	1	Low Priority
S1218	066408-78-4	1.10	0.30	0.79	0.81	0.92	1.82	1.71	1.60	-1.14	2	1	3	Low Priority
S1219	066722-44-9	1.00	1.42	1.42	1.42	1.42	1.18	1.27	1.36	-1.18	2	1	2	Low Priority
S1220	066778-36-7	0.41	0.44	0.44	0.44	0.44	1.13	1.03	0.75	0.61	2	1	3	Low Priority
S1221	067845-30-1	0.82	0.71	0.55	0.78	0.82	1.28	1.12	1.17	-1.27	2	1	3	Low Priority
S1222	068039-49-6	0.53	0.29	0.36	0.55	0.47	0.81	0.64	0.72	-1.24	1	1	2	Low Priority
S1223	068140-48-7	0.91	1.07	0.89	0.90	0.78	1.33	1.95	1.94	-0.24	2	2	3	Low Priority
S1224	068291-97-4	1.80	0.71	0.60	0.97	0.90	0.07	0.07	-0.21	0.12	2	1	2	Low Priority

ID	CAS	Human Biotransformation				Fish Biotransformation				PBT Profiler			Priority Level	
		logHL <sub>1</sub> (h)	logHL <sub>01</sub> (h)	logHL <sub>02</sub> (h)	logHL <sub>03</sub> (h)	logHL <sub>04</sub> (h)	logHL <sub>01</sub> (h)	logHL <sub>02</sub> (h)	logHL <sub>03</sub> (h)	PBT Index	P	B		T
S1225	068475-42-3	1.21	1.21	1.49	1.51	1.70	0.86	0.89	0.76	0.90	2	1	2	Low Priority
S1226	068527-74-2	0.55	0.73	0.85	0.56	0.60	0.68	0.47	0.74	-0.77	2	1	1	Low Priority
S1227	068527-76-4	0.58	0.68	0.77	0.54	0.58	0.79	0.57	0.82	-0.77	2	1	2	Low Priority
S1228	068693-11-8	1.00	1.18	1.18	1.18	1.18	0.50	0.53	0.39	0.45	2	1	2	Low Priority
S1229	068738-94-3	0.66	0.93	0.59	0.70	0.46	1.15	1.12						

ID	CAS	Human Biotransformation			Fish Biotransformation			PBT Profiler			Priority Level			
		logHL <sub>1</sub> (h)	logHL <sub>11</sub> (h)	logHL <sub>12</sub> (h)	logHL <sub>13</sub> (h)	logHL <sub>14</sub> (h)	logHL <sub>11</sub> (h)	logHL <sub>12</sub> (h)	logHL <sub>13</sub> (h)	PBT Index		P	B	T
S1307	098079-51-7	0.90	1.01	1.29	0.74	0.89	0.64	0.85	0.15	0.54	3	1	1	Low Priority
S1308	098105-99-8	0.99	1.09	1.15	0.86	1.00	0.84	1.03	0.38	1.86	3	1	1	Low Priority
S1309	098106-17-3	1.11	1.13	1.26	0.94	1.03	0.69	0.85	0.19	2.25	3	1	1	Low Priority
S1310	098319-26-7	0.78	0.78	0.78	0.78	0.78	1.41	1.36	1.27	-1.97	3	1	3	Low Priority
S1311	100418-33-5	0.30	0.61	0.42	0.13	0.19	0.53	0.48	0.39	-0.95	2	1	1	Low Priority
S1312	102187-19-9	0.97	1.18	0.93	0.88	0.84	1.19	1.23	0.70	2.53	2	2	3	Priority (Group 3)
S1313	102767-28-2	0.85	0.10	0.00	0.09	0.30	-0.23	-0.05	-0.09	-2.07	2	1	2	Low Priority
S1314	103577-45-3	0.00	0.00	0.00	0.00	0.00	1.45	2.17	1.13	3.36	3	1	3	Low Priority
S1315	103628-46-2	0.23	0.32	0.32	0.32	0.32	0.20	0.47	0.07	0.07	2	1	2	Low Priority
S1316	104333-00-8	1.07	0.56	0.86	0.89	0.95	0.91	1.25	0.84	0.54	2	1	1	Low Priority
S1317	106133-20-4	0.83	0.89	0.89	0.89	0.89	1.25	0.87	1.34	0.10	2	1	2	Low Priority
S1318	106266-06-2	0.51	0.52	0.52	0.52	0.52	1.26	1.41	0.84	1.62	3	1	2	Low Priority
S1319	107233-08-9	0.70	0.72	0.72	1.08	1.08	1.26	1.16	1.13	-1.62	2	1	2	Low Priority
S1320	107724-20-9	0.70	0.84	0.84	0.83	0.83	1.16	1.01	1.05	-0.97	3	1	3	Low Priority
S1321	108319-06-8	0.90	1.13	1.53	1.05	1.22	1.08	1.36	0.61	2.50	3	1	1	Low Priority
S1322	110871-86-8	1.30	1.37	1.37	1.37	1.37	0.62	0.98	0.12	-0.05	3	1	1	Low Priority
S1323	111025-46-8	0.70	0.69	0.69	0.71	0.71	0.90	0.81	0.66	0.89	2	1	3	Low Priority
S1324	111974-69-7	0.78	0.79	0.79	0.78	0.78	1.14	1.07	1.07	0.79	2	1	2	Low Priority
S1325	112809-51-5	1.65	1.67	1.67	1.67	1.67	1.22	1.90	1.48	2.46	2	1	2	Low Priority
S1326	113665-84-2	0.90	0.90	0.90	0.90	0.90	1.56	1.18	1.58	1.45	2	1	2	Low Priority
S1327	115103-54-3	1.00	1.01	1.01	1.01	1.01	1.27	0.82	1.20	0.48	2	1	1	Low Priority
S1328	115956-12-2	-0.89	-0.90	-0.90	-0.89	-0.89	0.88	1.11	0.60	0.35	2	1	2	Low Priority
S1329	117976-89-3	0.00	0.00	0.00	0.01	0.01	0.91	1.29	0.61	1.43	2	1	3	Low Priority
S1330	120014-06-4	1.85	1.85	1.85	1.91	1.91	1.62	1.33	1.48	0.98	2	1	3	Low Priority
S1331	120511-73-1	1.70	1.23	0.85	0.88	0.67	1.16	2.05	1.56	1.14	2	1	2	Low Priority
S1332	121251-67-0	1.35	1.10	1.47	1.57	1.45	1.72	2.00	1.91	-1.62	2	2	3	Low Priority
S1333	121251-68-1	1.35	1.10	1.47	1.57	1.45	1.72	2.00	1.91	-1.62	2	2	3	Low Priority
S1334	122021-01-6	0.74	0.72	0.52	0.40	0.41	1.11	1.11	0.89	-0.04	2	2	3	Low Priority
S1335	122320-73-4	0.59	0.59	0.59	0.59	0.59	0.72	0.67	0.52	0.89	2	1	2	Low Priority
S1336	125304-04-3	0.77	1.14	0.77	0.56	0.64	1.35	1.53	0.86	1.52	2	1	?	Low Priority
S1337	128489-04-3	0.65	0.66	0.94	0.64	0.68	0.97	0.71	0.97	-0.55	2	1	2	Low Priority
S1338	128794-94-5	0.61	0.37	0.69	0.61	0.48	1.10	0.79	1.10	-0.22	2	1	3	Low Priority
S1339	129453-61-8	2.98	2.98	2.98	2.98	2.98	2.67	2.93	2.74	2.18	3	1	?	Priority (Group 1)
S1340	129618-40-2	1.72	1.73	1.73	1.73	1.73	0.33	0.68	0.04	0.62	2	1	3	Low Priority
S1341	129722-12-9	1.88	1.87	1.87	1.88	1.88	1.88	1.51	1.73	1.96	3	2	3	Priority (Group 3)
S1342	131766-73-9	0.74	0.58	0.58	0.61	0.51	0.61	0.84	0.87	-1.49	2	1	2	Low Priority
S1343	131812-52-7	1.35	1.14	1.49	1.41	1.23	2.06	2.40	2.34	-0.32	2	2	3	Priority (Group 2)
S1344	132539-06-1	1.57	1.59	1.59	1.59	1.59	1.71	1.69	1.38	0.62	2	1	2	Low Priority
S1345	133040-01-4	0.32	0.52	0.52	0.52	0.52	0.97	0.90	0.62	1.57	2	1	3	Low Priority
S1346	134523-00-5	1.15	1.14	1.14	0.60	0.59	1.14	1.37	0.77	3.02	2	1	1	Low Priority
S1347	136236-51-6	1.12	0.94	0.88	0.73	0.98	1.40	1.42	1.48	-0.41	1	1	2	Low Priority
S1348	137862-53-4	0.98	1.13	1.13	1.13	1.13	0.45	1.10	0.28	1.94	1	1	2	Low Priority
S1349	143491-57-0	1.00	0.74	0.82	0.54	0.73	-0.14	0.16	-0.09	-1.44	1	1	1	Low Priority
S1350	144494-65-5	0.51	0.55	0.17	0.30	0.28	0.95	0.92	1.03	-1.00	1	1	2	Low Priority
S1351	145599-86-6	0.26	0.26	0.26	0.26	0.26	1.30	1.59	1.10	0.90	2	1	3	Low Priority
S1352	146939-27-7	0.49	0.50	0.50	0.50	0.50	1.13	0.91	1.07	2.18	3	1	3	Low Priority
S1353	147059-72-1	1.04	1.09	1.09	1.09	1.09	0.82	1.28	0.40	2.11	3	1	1	Low Priority
S1354	148553-50-8	0.78	0.22	0.20	-0.13	-0.01	0.02	0.27	0.34	-2.62	1	1	1	Low Priority
S1355	151319-34-5	0.04	0.04	0.04	0.04	0.04	0.69	1.44	0.53	2.35	2	1	2	Low Priority
S1356	153559-49-0	0.85	0.85	0.85	0.84	0.84	1.32	1.68	1.82	0.92	2	1	1	Low Priority
S1357	154171-77-4	1.14	1.02	1.33	1.17	1.07	1.87	2.02	1.95	-1.63	3	2	3	Low Priority
S1358	154598-52-4	1.68	1.69	1.69	1.70	1.70	1.33	1.47	1.13	2.10	3	1	2	Low Priority
S1359	158747-02-5	1.38	1.61	1.61	1.61	1.61	0.62	0.87	0.48	-0.95	2	1	2	Low Priority
S1360	162011-90-7	1.23	0.86	0.79	1.12	1.02	1.00	1.08	1.05	1.69	2	1	2	Low Priority
S1361	163222-33-1	1.34	1.34	1.34	1.34	1.34	1.51	1.62	1.13	2.78	3	1	3	Low Priority
S1362	165800-03-3	0.65	0.83	0.83	0.83	0.83	0.09	0.44	-0.13	0.12	3	1	2	Low Priority
S1363	166301-22-0	0.94	0.65	1.01	0.90	1.06	1.10	1.29	1.18	-1.58	1	1	2	Low Priority
S1364	169198-72-5	0.81	1.10	1.19	1.20	1.23	1.26	1.04	0.92	3.66	2	1	2	Low Priority
S1365	169590-42-5	1.04	1.04	1.04	1.05	1.05	0.91	1.50	0.80	3.91	2	1	3	Low Priority
S1366	171596-29-5	1.24	1.28	1.28	1.29	1.29	1.12	0.97	0.76	1.62	2	1	2	Low Priority
S1367	175463-14-6	0.85	1.12	1.12	0.60	0.71	0.45	0.66	0.00	-0.04	3	1	1	Low Priority
S1368	181695-72-7	0.98	0.97	0.97	0.98	0.98	0.89	0.76	0.65	2.03	2	1	3	Low Priority
S1369	190085-41-7	0.56	0.71	0.53	0.06	0.23	1.00	0.92	0.94	-0.65	1	1	3	Low Priority
S1370	196618-13-0	0.64	0.35	0.40	0.55	0.48	0.59	0.70	0.65	-2.29	2	1	2	Low Priority
S1371	219989-84-1	1.23	1.24	1.24	1.23	1.23	1.10	1.39	1.02	-1.29	2	1	3	Low Priority
S1372	226256-56-0	1.54	1.55	1.55	1.54	1.54	1.63	2.04	1.74	3.45	3	1	2	Low Priority
S1373	249296-44-4	1.38	1.12	0.85	0.85	1.12	1.25	1.58	0.93	0.44	2	1	1	Low Priority
S1374	302776-68-7	0.62	0.87	0.65	0.42	0.37	1.05	0.96	0.66	0.80	2	2	3	Low Priority
S1375	486460-32-6	1.08	1.76	1.76	1.76	1.76	1.17	2.33	1.35	3.85	3	1	2	Low Priority