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	Nama	Canonical CMILEC
ID	CAS	Name	Canonical SMILES
	000000 04 7	2,2',4,4',5,5'-	D. 4. (D. V. 40.4 (D. V. 40.10.10.10.10.10.10.10.10.10.10.10.10.10
1	000006-01-7 000050-00-0	Hexabromodiphenyl	Brc1cc(Br)c(cc1Oc1cc(Br)c(cc1Br)Br)Br
2	000050-00-0	Formaldehyde Phenobarbital	C=O CCC1{C(=O)NC(=O)NC1=O)c1ccccc1
4	000050-12-4	Mephenytoin	CCC1(NC(=0)N(C1=0)C)c1ccccc1
5	000050-12-4	Ergocalciferol	OC1CCC(=C)C(=CC2CCCC3(C2CCC3C(C=CC(C(C)C)C)C)C1
6	000050-18-0	Cyclophosphamide	CICCN(P1(=0)NCCCO1)CCCI
7	000050-23-7	Hydrocortisone	OCC(=0)C1(0)CCC2C1(C)CC(0)C1C2CCC2=CC(=0)CCC12C
8	000050-24-8	Prednisolone	OCC(=0)C1(0)CCC2C1(C)CC(0)C1C2CCC2=CC(=0)C=CC12C
9	000050-28-2	Estradiol	Oc1cc2c(c1)CCC1C2CC2(C1CCC2O)C
10	000050-29-3	p,p'-DDT	ClC(C(e1ecc(cc1)Cl)c1ccc(cc1)Cl)(Cl)Cl
11	000050-35-1	Thalidomide	O=C1CCC(C(=O)N1)N1C(=O)c2c(C1=O)cccc2
12	000050-36-2	Cocaine	COC(=0)C1C(CC2N(C1CC2)C)OC(=0)c1ccccc1
13	000050-37-3	Lysergide	CCN(C(=O)C1CN(C)C2C(=C1)c1cccc3c1c(C2)c[nH]3)CC
14	000050-47-5	Desipramine	CNCCCN1c2cccc2CCc2c1cccc2
15	000050-48-6	Amitriptyline	CN(CCC=C1c2ccccc2CCc2c1cccc2)C
16	000050-49-7	Imipramine	CN(CCCN1c2cccc2CCc2c1cccc2)C
17	000050-52-2	Thioridazine	CSc1ccc2c(c1)N(CCC1CCCCN1C)c1c(S2)cccc1
18	000050-53-3	Chlorpromazine	CN(CCCN1c2cccc2Sc2c1cc(Cl)cc2)C
19	000050-60-2	Phentolamine	Cc1ccc(cc1)N(c1cccc(c1)O)CC1=NCCN1
20	000050-78-2	Aspirin	CC(=0)Oc1ccccc1C(=0)O
21	000051-06-9	Procainamide	CCN(CCNC(=0)c1ccc(cc1)N)CC
22	000051-21-8	Fluorouracil	Fc1c[nH]c(=0)[nH]c1=0
23	000051-34-3	Scopolamine	OCC(c1cccc1)C(=0)OC1CC2N(C(C1)C1C2O1)C
24 25	000051-48-9 000051-52-5	Levothyroxine	OC(=0)C(Cc1cc(I)c(c(c1)I)Oc1cc(I)c(c(c1)I)O)N
25	000051-52-5	Propylthiouracil Atropine	CCCc1cc(=0)[nH]c(=S)[nH]1 OCC(c1ccccc1)C(=0)OC1CC2CCC(C1)N2C
27	000051-35-8	Mechlorethamine	CICCN(CCCI)C
28	000051-73-2	Spironolactone	CC(=0)SC1CC2=CC(=0)CCC2(C2C1C1CCC3(C1(CC2)C)CCC(=0)O3)C
29	000052-24-4	Thiotepa	S=P(N1CC1)(N1CC1)N1CC1
30	000052-53-9	Verapamil	COc1ccc(cc10C)CCN(CCCC(c1ccc(c(c1)OC)OC)(C(C)C)C#N)C
31	000052-67-5	Penicillamine	NC(C(S)(C)C)C(=0)O
32	000052-86-8	Haloperidol	Fc1ccc(cc1)C(=O)CCCN1CCC(CC1)(O)c1ccc(cc1)Cl
33	000053-03-2	Prednisone	OCC(=0)C1(0)CCC2C1(C)CC(=0)C1C2CCC2=CC(=0)C=CC12C
34	000053-16-7	Estrone	Oc1ccc2c(c1)CCC1C2CCC2(C1CCC2=O)C
35	000053-19-0	Mitotane	CIC(C(c1ccccc1Cl)c1ccc(cc1)Cl)Cl
36	000053-39-4	Oxandrolone	O=C1OCC2(C(C1)CCC1C2CCC2(C1CCC2(C)O)C)C
37	000053-86-1	Indomethacin	COc1ccc2c(c1)c(CC(=0)0)c(n2C(=0)c1ccc(cc1)Cl)C
38	000054-05-7	Chloroquine	CCN(CCCC(Nc1ccnc2c1ccc(c2)Cl)C)CC
39	000054-11-5	Nicotine	CN1CCCC1c1cccnc1
40	000054-31-9	Furosemide	OC(=0)c1cc(c(cc1NCc1ccco1)Cl)S(=0)(=0)N
41	000054-36-4	Metyrapone	O=C(C(c1cccnc1)(C)C)c1cccnc1
42	000054-71-7	Pilocarpine	CCC1C(=0)OCC1Cc1cncn1C
43 44	000054-85-3 000055-63-0	Isoniazid Nitroglycerin	NNC(=0)c1ccncc1
44	000055-98-1	Busulfan	0=N(=0)OC(CON(=0)=0)CON(=0)=0 CS(=0)(=0)OCCCCOS(=0)(=0)C
46	000055-98-1	Hexobarbital	0=C1NC(=0)C(C(=0)N1C)(C)C1=CCCCC1
47	000056-54-2	Quinidine	C=CC1CN2CCC1CC2C(c1ccnc2c1cc(OC)cc2)O
48	000056-75-7	Chloramphenicol	OCC(C(c1ccc(cc1)N(=0)=0)0)NC(=0)C(Cl)Cl
49	000057-27-2	Morphine	OC1C=CC2C34C10c1c4c(CC2N(CC3)C)ccc10
50	000057-41-0	Phenytoin	O=C1NC(=O)NC1(c1ccccc1)c1ccccc1
51	000057-42-1	Meperidine	CCOC(=0)C1(CCN(CC1)C)c1ccccc1
52	000057-53-4	Meprobamate	CCCC(COC(=O)N)(COC(=O)N)C
53	000057-63-6	Ethinyl	C#CC1(O)CCC2C1(C)CCC1C2CCc2c1ccc(c2)O
54	000057-66-9	Probenecid	CCCN(S(=O)(=O)c1ccc(cc1)C(=O)O)CCC
55	000057-74-9	Chlordane	CIC1CC2C(C1CI)C1(C(C2(CI)C(=C1CI)CI)(CI)CI)CI
56	000057-83-0	Progesterone	O=C1CCC2(C(=C1)CCC1C2CCC2(C1CCC2C(=O)C)C)C
57	000057-92-1	Streptomycin	OCC1OC(OC2C(OC3C(0)C(0)C(C(C3NC(=N)N)O)NC(=N)N)OC(C2(O)C=O)C)C(C(C1O)O)NC
58	000057-96-5	Sulfinpyrazone	O=C1N(c2cccc2)N(C(=O)C1CCS(=O)c1ccccc1)c1ccccc1
59	000058-00-4	R-Apomorphine	CN1CCc2c3C1Cc1ccc(c(c1c3ccc2)O)O
60	000058-08-2	Caffeine	Cn1cnc2c1c(=0)n(C)c(=0)n2C
61	000058-14-0	Pyrimethamine	CCc1nc(N)nc(c1c1ccc(cc1)Cl)N
62	000058-22-0	Testosterone	O=C1CCC2(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(N2CCCCC2)c2c(n1)c(nc(n2)N(CCO)CCO)N1CCCCC1)CCO
65	000058-38-8	Prochlorperazine	CN1CCN(CC1)CCCN1c2ccccc2Sc2c1cc(Cl)cc2
66	000058-39-9	Perphenazine	OCCN1CCN(CC1)CCCN1c2ccccc2Sc2c1cc(Cl)cc2
67	000058-40-2	Promazine	CN(CCCN1c2ccccc2Sc2c1cccc2)C
68	000058-54-8	Ethacrynic	CCC(=C)C(=O)c1ccc(c(c1Cl)Cl)OCC(=O)O
69	000058-55-9	Theophylline	Cn1c(=O)n(C)c2c(c1=O)[nH]cn2
70	000058-73-1	Diphenhydramine	CN(CCOC(clecccc1)clccccc1)C
71	000058-74-2	Papaverine	COc1ccc(cc1OC)Cc1nccc2c1cc(OC)c(c2)OC
72	000058-89-9	HCHs	ClC1C(Cl)C(Cl)C(C(C1Cl)Cl)Cl
73	000058-93-5	Hydrochlorothiazide	Clc1cc2NCNS(=O)(=O)c2cc1S(=O)(=O)N
74	000059-42-7	Phenylephrine	CNCC(c1cccc(c1)0)0
75	000059-46-1	Procaine	CCN(CCOC(=0)clccc(cc1)N)CC
76	000059-66-5	Acetazolamide	CC(=0)Nc1nnc(s1)S(=0)(=0)N
77	000059-87-0	Nitrofurazone	NC(=0)NN=Cc1ccc(o1)N(=0)=0
78	000059-92-7	Levodopa	OC(=0)C(Cc1ccc(c(c1)0)O)N
79	000059-96-1	Phenoxybenzamine	CICCN(C(COc1ccccc1)C)Cc1ccccc1
80	000060-32-2	Aminocaproic	NCCCCC(=0)0
81	000060-56-0	Methimazole	Cn1cc(nH)c1=S
82	000060-50-0	Dieldrin	CIC1=C(CI)C2(C(C1(CI)C1C2C2CC1C1C2O1)(CI)CI)CI
83	000060-37-1	Antipyrine	O=c1cc(n(n1c1ccccc1)C)C
83 84	000060-80-0		
		Promethazine	CN(C(CN1c2cccc2Sc2c1cccc2)C)C
85	000060-99-1	Methotrimeprazine	COc1ccc2c(c1)N(CC(CN(C)C)C)c1c(S2)cccc1
86	000061-32-5	Meticillin	COc1cccc(c1C(=0)NC1C(=0)N2C1SC(C2C(=0)0)(C)C)OC
87	000061-33-6	Penicillin	O=C(Cc1ccccc1)NC1C(=O)N2C1SC(C2C(=O)O)(C)C
88	000061-68-7	Mefenamic	OC(=0)c1ccccc1Nc1cccc(c1C)C
89	000062-44-2	Phenacetin	CCOc1ccc(cc1)NC(=O)C
90	000063-12-7	Benzquinamide	CCN(C(=0)C1CN2CCc3c(C2CC1OC(=0)C)cc(c(c3)OC)OC)CC
91	000063-98-9	Phenacemide	O=C(Cc1ccccc1)NC(=O)N
92	000064-77-7	Tolbutamide	CCCCNC(=0)NS(=0)(=0)c1ccc(cc1)C
93	000064-86-8	Colchicine	COc1c(OC)cc2c(c1OC)c1ccc(c(=0)cc1C(CC2)NC(=0)C)OC
94	000066-79-5	Oxacillin	OC(=0)C1N2C(=0)C(C2SC1(C)C)NC(=0)c1c(C)onc1c1ccccc1
95	000067-20-9	Nitrofurantoin	O=C1NC(=0)N(C1)N=Cc1ccc(o1)N(=0)=O
96	000067-45-8	Furazolidone	O=C1OCCN1N=Cc1ccc(o1)N(=O)=O
97	000067-66-3	chloroform	CIC(CI)CI
98	000067-73-2	Fluocinolone	OCC(=0)C12OC(OC1CC1C2(C)CC(O)C2(C1CC(C1=CC(=0)C=CC21C)F)F)(C)C
99	000067-97-0	Cholecalciferol	CC(CCCC(C1CCC2C1(C)CCCC2=CC=C1CC(O)CCC1=C)C)C
100	000068-22-4	Norethindrone	C#CC1(O)CCC2C1(C)CCC1C2CCC2=CC(=O)CCC12
101	000068-35-9	Sulfadiazine	Nc1ccc(cc1)S(=O)(=O)Nc1ncccn1
102	000068-88-2	Hydroxyzine	OCCOCCN1CCN(CC1)C(c1ccc(cc1)Cl)c1ccccc1
103	000069-53-4	Ampicillin	NC(c1cccc1)C(=0)NC1C(=0)N2C1SC(C2C(=0)O)(C)C
104	000069-65-8	Mannitol	OCC(C(C(C(CO)O)O)O)O
105	000070-51-9	Deferoxamine	NCCCCCN(C(=0)CCC(=0)NCCCCCN(C(=0)CCC(=0)NCCCCCN(C(=0)C)O)O)O
106	000071-43-2	Benzene	clccccc1
107	000071-63-6	Digitoxin	O=C1OCC(=C1)C1CCC2(C1(c)CCC1C2CCC2C1(c)CCC(C2)OC1CC(O)C(C(O1)C)OC1CC(O)C(C(O1)C)OC1CC(O)C(C(O1)C)OC1CC(O)C(C(O1)C)OC1CC(O)C(C(O1)C)OC1CC(O)C(C(O1)C)OC1CC(O)C(C(O1)C)OC1CC(O)C(C(O1)C)OC1CC(O1)C(O1)
108	000072-55-9	p,p'-DDE	CIC(=C(c1ccc(cc1)CI)c1ccc(cc1)CI)CI
109	000072-69-5	Nortriptyline	CNCCC=C1c2cccc2CCc2c1cccc2
110	000073-31-4	Melatonin	COc1ccc2c(c1)c(CCNC(=0)C)c[nH]2
111	000073-48-3	Bendroflumethiazide	O=S1(=O)NC(Cc2cccc2)Nc2c1cc(c(c2)C(F)(F)F)S(=O)(=O)N
112	000074-55-5	Ethambutol	CCC(NCCNC(CO)CC)CO
113	000075-01-4	VINYL	CIC=C
114	000075-69-4	TRICHLOROFLUOROMETHANE	FC(CI)(CI)CI
115	000075-71-8	Dichlorodifluoromethane	FC(CI)(CI)F
116	000075-71-8	Triamcinolone	OCC(=0)C12OC(OC1CC1C2(C)CC(0)C2(C1CCC1=CC(=0)C=CC21C)F)(C)C
117	000076-23-3	Oxymorphone	
			0=C1CCC2(C34C10c1c4c(CC2N(CC3)C)ccc10)0
118	000076-42-6	Oxycodone	COc1ccc2c3c10C1C43CCN(C(C2)C4(0)CCC1=0)C
119	000076-43-7	Fluoxymesterone	0=C1CCC2(C(=C1)CCC1C2(F)C(0)CC2(C1CCC2(C)O)C)C
120	000076-57-3	Codeine	COc1ccc2c3c1OC1C43CCN(C(C2)C4C=CC1O)C
121	000076-74-4	Pentobarbital	CCCC(C1(CC)C(=0)NC(=0)NC1=0)C
122	000076-75-5	Thiopental	CCCC(C1(CC)C(=0)NC(=S)NC1=0)C
123	000076-99-3	Methadone	CCC(=0)C(c1ccccc1)(c1ccccc1)CC(N(C)C)C
124	000077-07-6	Levorphanol	Oc1ccc2c(c1)C13CCCCC3C(C2)N(CC1)C
125	000077-10-1	Phencyclidine	C1CCC(CC1)(N1CCCCC1)c1ccccc1
126	000077-21-4	Glutethimide	CCC1(CCC(=0)NC1=0)c1ccccc1

ID	CAS	Name	Canonical SMILES	ID	CAS	Name	Canonical SMILES
127	000077-26-9	Butalbital	C=CCC1(CC(C)C)C(=0)NC(=0)NC1=0	191	000121-14-2	2,4-Dinitrotoluene	O=N(=O)c1ccc(c(c1)N(=O)=O)C
128	000077-28-1	Butethal	CCCCC1(CC)C(=0)NC(=0)NC1=0	192	000121-75-5	Malathion	CCOC(=0)CC(C(=0)OCC)SP(=S)(OC)OC
129	000077-36-1	Chlorthalidone	O=C1NC(c2c1cccc2)(O)c1ccc(c(c1)S(=O)(=O)N)Cl	193	000122-09-8	Phentermine	CC(Cc1ccccc1)(N)C
130	000077-37-2	Procyclidine	OC(c1cccc1)(C1CCCCC1)CCN1CCCC1	194	000123-91-1		O1CCOCC1
131	000077-41-8	Methsuximide	CN1C(=0)CC(C1=0)(C)c1ccccc1	195	000123-99-9	Azelaic	OC(=0)CCCCCCC(=0)O
132	000077-67-8	Ethosuximide	CC1(CC)CC(=0)NC1=0	196	000124-94-7	Triamcinolone	OCC(=0)C1(0)C(0)CC2C1(C)CC(0)C1(C2CCC2=CC(=0)C=CC12C)F
133	000078-44-4	Carisoprodol	CCCC(COC(=0)N)(COC(=0)NC(C)C)C	197	000125-29-1	Hydrocodone	COc1ccc2c3c1OC1C43CCN(C(C2)C4CCC1=O)C
134	000078-93-3	Methylethylketone	CCC(=0)C	198	000125-33-7	Primidone	CCC1(C(=O)NCNC1=O)c1ccccc1
135	000079-01-6	Trichloroethylene	CIC=C(CI)CI	199	000125-64-4	Methyprylon	CCC1(CC)C(=0)NCC(C1=0)C
136	000079-43-6	Dichloroacetic	CIC(C(=0)0)CI	200	000125-71-3		COc1ccc2c(c1)C13CCCCC3C(C2)N(CC1)C
137	000079-94-7	3,3'5,5'-Tetrabromobisphenol	CC(c1cc(Br)c(c(c1)Br)O)(c1cc(Br)c(c(c1)Br)O)C	201	000125-84-8	Aminoglutethimide	CCC1(CCC(=O)NC1=O)c1ccc(cc1)N
138	000080-05-7	Bisphenol	CC(c1ccc(cc1)O)(c1ccc(cc1)O)C	202	000126-07-8	Griseofulvin	COC1=CC(=0)CC(C210c1c(C2=0)c(OC)cc(c1Cl)OC)C
139	0-80-08000	Dapsone	Nc1ccc(cc1)S(=0)(=0)c1ccc(cc1)N	203	000126-52-3	Ethinamate	C#CC1(CCCC1)OC(=O)N
140	000083-43-2	Methylprednisolone	OCC(=0)C1(0)CCC2C1(C)CC(0)C1C2CC(C2=CC(=0)C=CC12C)C	204	000127-07-1	Hydroxyurea	NC(=O)NO
141	000083-89-6	Quinacrine	CCN(CCCC(Nc1c2cc(OC)ccc2nc2c1ccc(c2)Cl)C)CC	205	000127-31-1	Fludrocortisone	OCC(=0)C1(0)CCC2C1(C)CC(0)C1(C2CCC2=CC(=0)CCC12C)F
142	000083-98-7	Orphenadrine	CN(CCOC(c1ccccc1C)c1ccccc1)C	206	000127-69-5	Sulfisoxazole	Nc1ccc(cc1)S(=O)(=O)Nc1onc(c1C)C
143	000085-68-7	Butyl	CCCCOC(=0)c1ccccc1C(=0)OCc1ccccc1	207	000128-20-1	Eltanolone	OC1CCC2(C(C1)CCC1C2CCC2(C1CCC2C(=O)C)C)C
144	000086-35-1	Ethotoin	CCN1C(=0)NC(C1=0)c1ccccc1	208	000132-21-8	Dexbrompheniramine	CN(CCC(c1ccccn1)c1ccc(cc1)Br)C
145	000086-42-0	Amodiaquine	CCN(Cc1cc(ccc10)Nc1ccnc2c1ccc(c2)Cl)CC	209	000132-22-9	Chlorpheniramine	CN(CCC(c1ccccn1)c1ccc(cc1)Cl)C
146	000086-50-0	Methylazinphos	COP(=S)(SCn1nnc2c(c1=O)cccc2)OC	210	000134-49-6	Phenmetrazine	CC1NCCOC1c1ccccc1
147	000086-54-4	Hydralazine	NNc1nncc2c1cccc2	211	000135-09-1	Hydroflumethiazide	FC(c1cc2NCNS(=O)(=O)c2cc1S(=O)(=O)N)(F)F
148	000087-08-1	Penicillin	O=C(NC1C(=O)N2C1SC(C2C(=O)O)(C)C)COc1ccccc1	212	000137-58-6	Lidocaine	CCN(CC(=O)Nc1c(C)cccc1C)CC
149	000087-33-2	Isosorbide	O=N(=0)OC1COC2C1OCC2ON(=0)=O	213	000138-56-7	Trimethobenzamide	COc1cc(cc(c1OC)OC)C(=O)NCc1ccc(cc1)OCCN(C)C
150	000087-61-6	1,2,3-Trichlorobenzene	Clc1c(Cl)cccc1Cl	214	000144-11-6		OC(c1ccccc1)(C1CCCCC1)CCN1CCCCC1
151	000087-86-5	Pentachlorophenol	Clc1c(O)c(Cl)c(cc1Cl)Cl)Cl	215	000144-75-2		OS(=O)CNc1ccc(cc1)S(=O)(=O)c1ccc(cc1)NCS(=O)O
152	000089-57-6	Mesalazine	Nc1ccc(c(c1)C(=0)0)O	216	000144-80-9	Sulfacetamide	CC(=O)NS(=O)(=O)c1ccc(cc1)N
153	000090-34-6	Primaquine	NCCCC(Nc1cc(OC)cc2c1nccc2)C	217	000144-82-1		Nc1ccc(cc1)S(=O)(=O)Nc1nnc(s1)C
154	000090-82-4	Pseudoephedrine	CNC(C(c1ccccc1)O)C	218	000144-83-2	Sulfapyridine	Nc1ccc(cc1)S(=O)(=O)Nc1ccccn1
155	000090-89-1	Diethylcarbamazine	CCN(C(=0)N1CCN(CC1)C)CC	219	000146-22-5		O=C1CN=C(c2c(N1)ccc(c2)N(=O)=O)c1ccccc1
156	000091-80-5	Thionylan	CN(CCN(c1ccccn1)Cc1cccs1)C	220	000146-48-5	Yohimbine	COC(=O)C1C(O)CCC2C1CC1N(C2)CCc2c1[nH]c1c2cccc1
157	000092-52-4	Biphenyl	c1ccc(cc1)c1ccccc1	221	000147-52-4	Nafcillin	CCOc1ccc2c(c1C(=0)NC1C(=0)N3C1SC(C3C(=0)0)(C)C)cccc2
158	000093-14-1	Guaifenesin	OCC(COc1ccccc1OC)O	222	000147-55-7	Phenethicillin	CC(C(=O)NC1C(=O)N2C1SC(C2C(=O)O)(C)C)Oc1ccccc1
159	000094-20-2	Chlorpropamide	CCCNC(=0)NS(=0)(=0)c1ccc(cc1)Cl	223	000147-94-4	Cytarabine	OCC1OC(C(C1O)O)n1ccc(nc1=O)N
160	000094-75-7	2,4-D	OC(=0)COc1ccc(cc1Cl)Cl	224	000148-79-8	Thiabendazole	c1scc(n1)c1nc2c([nH]1)cccc2
161	000095-47-6	ortho-xylene	Cc1ccccc1C	225	000148-82-3	Melphalan	CICCN(c1ccc(cc1)CC(C(=0)O)N)CCCI
162	000096-88-8	Mepivacaine	CN1CCCCC1C(=O)Nc1c(C)cccc1C	226	000151-83-7	Methohexital	CCC#CC(C1(CC=C)C(=O)NC(=O)N(C1=O)C)C
163	000098-95-3	Nitrobenzene	O=N(=O)c1ccccc1	227	000152-02-3		C=CCN1CCC23C(C1Cc1c3cc(cc1)O)CCCC2
164	000098-96-4	Pyrazinamide	NC(=0)c1cnccn1	228	000152-62-5	Dydrogesterone	O=C1CCC2(C(=C1)C=CC1C2CCC2(C1CCC2C(=O)C)C)C
165	000099-66-1	Valproic	cccc(c(=0)0)ccc	229	000153-61-7	Cefalotin	CC(=0)OCC1=C(C(=0)O)N2C(SC1)C(C2=0)NC(=0)Cc1cccs1
166	000100-00-5	1-CHLORO-4-NITROBENZENE	Clc1ccc(cc1)N(=O)=O	230	000154-93-8	Carmustine	CICCNC(=O)N(CCCI)N=O
167	000100-01-6	4-NITROANILINE	Nc1ccc(cc1)N(=O)=O	231	000155-09-9	Tranylcypromine	NC1CC1c1ccccc1
168	000100-33-4	Pentamidine	NC(=N)c1ccc(cc1)OCCCCOc1ccc(cc1)C(=N)N	232	000156-08-1	Benzphetamine	CN(C(Cc1ccccc1)C)Cc1ccccc1
169	000100-92-5	Mephentermine	CNC(Cc1ccccc1)(C)C	233	000156-60-5	Ethene,	CIC=CCI
170	000101-84-8	Diphenylether	c1ccc(cc1)Oc1ccccc1	234	000298-46-4		NC(=O)N1c2cccc2C=Cc2c1cccc2
171	000103-90-2	Acetaminophen	CC(=0)Nc1ccc(cc1)O	235	000298-81-7	Methoxsalen	COc1c2oc(=O)ccc2cc2c1occ2
172	000104-29-0	Chlorphenesin	OCC(COc1ccc(cc1)Cl)O	236	000300-62-9	Amphetamine	CC(Cc1ccccc1)N
173	000104-31-4	Benzonatate	COCCOCCOCCOCCOCCOCCOCCCCC(=0)c1ccc(cc1)NCCCC	237	000302-41-0	Piritramide	N#CC(c1ccccc1)(c1ccccc1)CCN1CCC(CC1)(N1CCCCC1)C(=O)N
174	000106-42-3	para-xylene	Cc1ccc(cc1)C	238	000303-49-1	Clomipramine	CN(CCCN1c2ccccc2CCc2c1cc(CI)cc2)C
175	000106-60-5	Aminolevulinic	NCC(=0)CCC(=0)O	239	000303-53-7	Cyclobenzaprine	CN(CCC=C1c2ccccc2C=Cc2c1cccc2)C
176	000108-38-3	meta-xylene	Cc1cccc(c1)C	240	000303-70-8	Hydroxyimipramine,	CN(CCCN1c2cccc2CCc2c1ccc(c2)O)C
177	000108-95-2	Phenol	Ocicccc1	241	000304-55-2	Succimer	SC(C(C(=0)0)S)C(=0)0
178	000113-00-8	Guanidine	NC(=N)N	242	000305-03-3	Chlorambucil	CICCN(c1ccc(cc1)CCCC(=O)O)CCCI
179	000113-15-5	Ergotamine	O=C(C1CN(C)C2C(=C1)c1cccc3c1c(C2)c[nH]3)NC1(C)OC2(N(C1=O)C(Cc1ccccc1)C(=O)N1C2CCC1)O	243	000307-24-4	Perfluorohexanoic	OC(=O)C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)
180	000113-18-8	Ethchlorvynol	CCC(C#C)(C=CCI)O	244	000309-29-5	Doxapram	CCN1CC(C(C1=O)(c1ccccc1)c1ccccc1)CCN1CCOCC1
181	000113-42-8	Methylergonovine	CCC(NC(=0)C1CN(C)C2C(=C1)c1cccc3c1c(C2)c[nH]3)CO	245	000320-67-2	Azacitidine	OCC1OC(C(C1O)O)n1cnc(nc1=O)N
182	000113-45-1	Methylphenidate	COC(=0)C(c1ccccc1)C1CCCCN1	246	000321-64-2		Nc1c2CCCc2nc2c1cccc2
183	000113-59-7	Chlorprothixene	CN(CCC=C1c2cccc2Sc2c1cc(Cl)cc2)C	247	000335-67-1	Perfluorooctanoate	OC(=O)C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F
184	000115-38-8	Methylphenobarbital	CCC1(C(=0)NC(=0)N(C1=0)C)c1ccccc1	248	000339-44-6	Glycodiazine	COCCOc1cnc(nc1)NS(=0)(=0)c1ccccc1
185	000115-67-3	Paramethadione	CCC1(C)OC(=0)N(C1=0)C	249	000355-46-4	Perfluorohexanesulfonic	FC(C(C(C(C(C(S(=O)(=O)O)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)
186	000117-39-5	Quercetin	Oc1cc(O)c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O	250	000357-70-0	Galantamine	COc1ccc2c3c1OC1C3(CCN(C2)C)C=CC(C1)O
187	000117-81-7	Di(2-ethylhexyl)phthalate	CCCCC(COC(=0)c1ccccc1C(=0)OCC(CCCC)CC)CC	251	000359-83-1	Pentazocine	CC(=CCN1CCC2(C(C1Cc1c2cc(cc1)O)C)C)C
188	000117-96-4	Diatrizoic	CC(=0)Nc1c(I)c(NC(=0)C)c(c(c1I)C(=0)O)I	252	000364-62-5	Metoclopramide	CCN(CCNC(=O)c1cc(Cl)c(cc1OC)N)CC
189	000118-42-3	Hydroxychloroquine	OCCN(CCCC(Nc1ccnc2c1ccc(c2)Cl)C)CC	253	000364-98-7	Diazoxide	Clc1ccc2c(c1)S(=0)(=0)N=C(N2)C
190	000118-74-1	Hexachlorobenzene	Clc1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl	254	000389-08-2	Nalidixic	CCn1cc(C(=0)0)c(=0)c2c1nc(C)cc2

ID	CAS	Name	Canonical SMILES	ID	CAS	Name	Canonical SMILES
255	000396-01-0	Triamterene	Nc1nc(N)c2c(n1)nc(c(n2)c1ccccc1)N	319	001134-47-0	Baclofen	NCC(c1ccc(cc1)Cl)CC(=0)O
256	000437-38-7	Fentanyl	CCC(=O)N(c1ccccc1)C1CCN(CC1)CCc1ccccc1	320	001156-19-0	Tolazamide	O=C(NS(=O)(=O)c1ccc(cc1)C)NN1CCCCCC1
257	000439-14-5	Diazepam	Clc1ccc2c(c1)C(=NCC(=0)N2C)c1cccc1	321	001163-19-5	Decabromodiphenyl	Brc1c(Oc2c(Br)c(Br)c(c(c2Br)Br)Br)c(Br)c(c(c1Br)Br)Br
258	000443-48-1	Metronidazole	OCCn1c(C)ncc1N(=O)=O	322	001197-18-8	Tranexamic	NCC1CCC(CC1)C(=O)O
259	000446-86-6	Azathioprine	Cn1cnc(c1Sc1ncnc2c1[nH]cn2)N(=O)=O	323	001435-55-8	Dihydroquinidine	CCC1CN2CCC1CC2C(c1ccnc2c1cc(OC)cc2)O
260	000452-35-7	Ethoxzolamide	CCOc1ccc2c(c1)sc(n2)S(=O)(=O)N	324	001477-40-3	Levomethadyl	CCC(C(c1ccccc1)(c1ccccc1)CC(N(C)C)C)OC(=O)C
261	000461-78-9	Chlorphentermine	CC(Cc1ccc(cc1)Cl)(N)C	325	001622-61-3	Clonazepam	O=C1CN=C(c2c(N1)ccc(c2)N(=O)=O)c1ccccc1Cl
262	000469-21-6	Doxylamine	CN(CCOC(c1ccccn1)(c1ccccc1)C)C	326	001622-62-4	Flunitrazepam	CN1C(=O)CN=C(c2c1ccc(c2)N(=O)=O)c1ccccc1F
263	000469-62-5	Propoxyphene	CCC(=O)OC(c1ccccc1)(C(CN(C)C)C)Cc1ccccc1	327	001665-48-1	Metaxalone	O=C1NCC(O1)COc1cc(C)cc(c1)C
264	000469-79-4	Ketobemidone	CCC(=O)C1(CCN(CC1)C)c1cccc(c1)O	328	001668-19-5	Doxepin	CN(CCC=C1c2cccc2OCc2c1cccc2)C
265	000477-47-4	Podofilox	COc1cc(cc(c10C)OC)C1C2C(=0)OCC2C(c2c1cc10COc1c2)O	329	001695-77-8	Spectinomycin	CNC1C(O)C2OC3OC(C)CC(=O)C3(OC2C(C1O)NC)O
266	000479-18-5	Dyphylline	OCC(Cn1cnc2c1c(=0)n(C)c(=0)n2C)O	330	001744-22-5	Riluzole	Nc1nc2c(s1)cc(cc2)OC(F)(F)F
267	000486-12-4	Triprolidine	Cc1ccc(cc1)C(=CCN1CCCC1)c1ccccn1			2,3,7,8-tetrachlorodibenzo-p-	
268	000486-16-8	Carbinoxamine	CN(CCOC(c1ccccn1)c1ccc(cc1)Cl)C	331	001746-01-6	dioxin	Clc1cc2Oc3cc(Cl)c(cc3Oc2cc1Cl)Cl
269	000486-56-6	Cotinine	O=C1CCC(N1C)c1cccnc1	332	001763-23-1	Perfluorooctanesulfonic	FC(C(C(C(C(S(=O)(=O)O)(F)F)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)
270	000492-39-7	Cathine	OC(c1cccc1)C(N)C	333	001808-12-4	Bromodiphenhydramine	CN(CCOC(c1ccc(cc1)Br)c1ccccc1)C
271	000514-65-8	Biperiden	OC(C1CC2CC1C=C2)(c1ccccc1)CCN1CCCCC1	334	001812-30-2	Bromazepam	O=C1CN=C(c2c(N1)ccc(c2)Br)c1ccccn1
272	000520-85-4	Medroxyprogesterone	O=C1CCC2(C(=C1)C(C)CC1C2CCC2(C1CCC2(O)C(=O)C)C)C	335	001912-24-9	Atrazine	CCNc1nc(NC(C)C)nc(n1)Cl
273	000525-66-6	Propranolol	OC(COc1cccc2c1cccc2)CNC(C)C	336	001949-45-7	Metrizoate	CC(=O)CNc1c(I)c(NC(=O)C)c(c(c1I)C(=O)O)I
274	000529-38-4	Cocaethylene	CCOC(=0)C1C(CC2N(C1CC2)C)OC(=0)c1ccccc1	337	001951-25-3	Amiodarone	CCCCc1oc2c(c1C(=0)c1cc(I)c(c(c1)I)OCCN(CC)CC)cccc2
275	000532-03-6	Methocarbamol	COc1ccccc1OCC(COC(=0)N)O	338	001972-08-3	Marinol	CCCCCc1cc(O)c2c(c1)OC(C1C2C=C(C)CC1)(C)C
276	000532-77-4	Hexylcaine	CC(OC(=O)c1ccccc1)CNC1CCCCC1	339	002016-88-8	Amiloride	NC(=NC(=O)c1nc(Cl)c(nc1N)N)N
277	000533-45-9	Chlormethiazole	Cc1ncsc1CCCI	340	002030-63-9	Clofazimine	Clc1ccc(cc1)Nc1cc2nc3ccccc3n(c2cc1=NC(C)C)c1ccc(cc1)Cl
278	000536-33-4	Ethionamide	CCc1nccc(c1)C(=S)N	341	002050-67-1	3,3'-dichlorobiphenyl	Clc1cccc(c1)c1cccc(c1)Cl
279	000537-46-2	Methamphetamine	CNC(Cc1ccccc1)C	342	002050-68-2	4,4'-dichlorobiphenyl	Clc1ccc(cc1)c1ccc(cc1)Cl
280	000546-88-3	Acetohydroxamic	CC(=O)NO	343	002051-24-3	Decachlorobiphenyl	Clc1c(c2c(Cl)c(Cl)c(c(c2Cl)Cl)Cl)c(c(c1Cl)Cl)Cl
281	000548-04-9	Hypericin	Oc1cc(C)c2c3c1C(=O)c1c(O)cc(c4c1c3c1c3c2c(C)cc(c3C(=O)c2c1c4c(O)cc2O)O)O	344	002051-60-7	2-chlorobiphenyl	Clc1ccccc1c1ccccc1
282	000548-73-2	Droperidol	Fc1ccc(cc1)C(=0)CCCN1CCC(=CC1)n1c(=0)[nH]c2c1cccc2	345	002051-61-8	3-chlorobiphenyl	Clc1cccc(c1)c1ccccc1
283	000552-94-3	Salsalate	Oc1cccc1C(=0)Oc1cccc1C(=0)O	346	002051-62-9	4-chlorobiphenyl	Clc1ccc(cc1)c1ccccc1
284	000554-57-4	Methazolamide	CC(=O)N=c1sc(nn1C)S(=O)(=O)N	347	002062-78-4	Pimozide	Fc1ccc(cc1)C(c1ccc(cc1)F)CCCN1CCC(CC1)n1c(=O)[nH]c2c1cccc2
285	000555-30-6	Methyldopa	OC(=0)C(Cc1ccc(c(c1)O)O)(N)C	348	002062-84-2	Benperidol	Fc1ccc(cc1)C(=0)CCCN1CCC(CC1)n1c(=0)[nH]c2c1cccc2
286	000561-27-3	Heroin	CC(=0)OC1C=CC2C34C1Oc1c4c(CC2N(CC3)C)ccc1OC(=0)C	349	002078-54-8	Propofol	CC(c1cccc(c10)C(C)C)C
287	000569-65-3	Meclizine	Clc1ccc(cc1)C(c1ccccc1)N1CCN(CC1)Cc1cccc(c1)C	350	002098-66-0	Cyproterone	O=C1C=C2C(=CC3C(C2(C2C1C2)C)CCC1(C3CCC1(O)C(=O)C)C)Cl
288	000586-06-1	Orciprenaline	OC(c1cc(O)cc(c1)O)CNC(C)C	351	002276-90-6	Iothalamic	CNC(=O)c1c(I)c(NC(=O)C)c(c(c1I)C(=O)O)I
289	000586-60-7	Dyclonine	CCCCOc1ccc(cc1)C(=0)CCN1CCCCC1	352	002321-07-5	Fluorescein	Oc1ccc2c(c1)Oc1c(C32OC(=O)c2c3cccc2)ccc(c1)O
290	000599-79-1	Sulfasalazine	OC(=0)C1=CC(=NNc2ccc(cc2)S(=0)(=0)Nc2ccccn2)C=CC1=O	353	002323-36-6	Selegiline	CC(N(CC#C)C)Cc1ccccc1
291	000604-75-1	Oxazepam	O=C1Nc2ccc(cc2C(=NC1O)c1ccccc1)Cl	354	002353-33-5	Decitabine	OCC1OC(CC1O)n1cnc(nc1=O)N
292	000616-91-1	Acetylcysteine	SCC(C(=O)O)NC(=O)C	355	002437-79-8	2,4,2',4'-tetrachlorobiphenyl	Clc1ccc(c(c1)Cl)c1ccc(cc1Cl)Cl
293	000634-03-7	Phendimetrazine	CC1N(C)CCOC1c1ccccc1	356	002709-56-0	Flupenthixol	OCCN1CCN(CC1)CCC=C1c2ccccc2Sc2c1cc(cc2)C(F)(F)F
294	000637-07-0	Clofibrate	CCOC(=0)C(Oc1ccc(cc1)Cl)(C)C	357	002894-67-9	Delorazepam	O=C1CN=C(c2c(N1)ccc(c2)Cl)c1ccccc1Cl
295	000644-62-2	Meclofenamic	OC(=0)c1ccccc1Nc1c(Cl)ccc(c1Cl)C	358	002955-38-6	Prazepam	Clc1ccc2c(c1)C(=NCC(=O)N2CC1CC1)c1ccccc1
296	000645-05-6	Altretamine	CN(c1nc(nc(n1)N(C)C)N(C)C)C	359	002974-90-5	3,4'-Dichlorobiphenyl	Clc1ccc(cc1)c1cccc(c1)Cl
297	000645-43-2	Guanethidine	NC(=NCCN1CCCCCC1)N	360	002998-57-4	Estramustine	CICCN(C(=O)Oc1ccc2c(c1)CCC1C2CCC2(C1CCC2OP(=O)(O)O)C)CCCI
298	000657-24-9	Metformin	CN(C(=N)N=C(N)N)C	361	003056-17-5	Stavudine	Cc1cn(C2OC(C=C2)CO)c(=O)[nH]c1=O
299	000671-16-9	Procarbazine	CNNCc1ccc(cc1)C(=0)NC(C)C	362	003094-09-5	Doxifluridine	CC1OC(C(C1O)O)n1cc(F)c(=O)[nH]c1=O
300	000672-87-7	Metyrosine	Oc1ccc(cc1)CC(C(=O)O)(N)C	363	003116-76-5	Dicloxacillin	OC(=O)C1N2C(=O)C(C2SC1(C)C)NC(=O)c1c(C)onc1c1c(CI)cccc1CI
301	000709-55-7	Etilefrine	CCNCC(c1ccc(c1)0)0	364	003194-55-6	HBCDs	BrC1CCC(Br)C(Br)CCC(C(CCC1Br)Br)Br
302	000721-50-6	Prilocaine	CCCNC(C(=0)Nc1ccccc1C)C	365	003239-44-9	Dexfenfluramine	CCNC(Cc1cccc(c1)C(F)(F)F)C
303	000723-46-6	Sulfamethoxazole	Nc1ccc(cc1)S(=0)(=0)Nc1noc(c1)C	366	003268-87-9	Octachlorodibenzo-p-dioxin	Clc1c2Oc3c(Oc2c(c(c1Cl)Cl)Cl)c(Cl)c(c(c3Cl)Cl)Cl
304	000738-70-5	Trimethoprim	COc1cc(Cc2cnc(nc2N)N)cc(c1OC)OC	367	003385-03-3	Flunisolide	OCC(=0)C12OC(OC1CC1C2(C)CC(0)C2C1CC(C1=CC(=0)C=CC21C)F)(C)C
305	000739-71-9	Trimipramine	CN(CC(CN1c2cccc2CCc2c1cccc2)C)C	368	003424-98-4	Telbivudine	OCC1OC(CC1O)n1cc(C)c(=O)[nH]c1=O
306	000745-65-3	Alprostadil	CCCCCC(C=CC1C(0)CC(=0)C1CCCCCC(=0)O)O	369	003440-28-6	Betamipron	O=C(c1ccccc1)NCCC(=O)O
307	000768-94-5	Amantadine	NC12CC3CC(C2)CC(C1)C3	370	003562-63-8	Megestrol	O=C1CCC2(C(=C1)C(=CC1C2CCC2(C1CCC2(O)C(=O)C)C)C)C
308	000797-63-7	Levonorgestrel	C#CC1(O)CCC2C1(CC)CCC1C2CCC2=CC(=O)CCC12	371	003575-80-2	Melperone	CC1CCN(CC1)CCCC(=O)c1ccc(cc1)F
309	000846-48-0	Boldenone	O=C1C=CC2(C(=C1)CCC1C2CCC2(C1CCC2O)C)C	372	003579-62-2	Denaverine	CCC(COC(c1ccccc1)(c1ccccc1)C(=O)OCCN(C)C)CC
310	000846-49-1	Lorazepam	Clc1ccc2c(c1)C(=NC(C(=0)N2)O)c1ccccc1Cl	373	003737-09-5	Disopyramide	CC(N(C(C)C)CCC(c1ccccn1)(c1ccccc1)C(=O)N)C
311	000846-50-4	Temazepam	Clc1ccc2c(c1)C(=NC(C(=O)N2C)O)c1ccccc1	374	003778-73-2	Ifosfamide	CICCNP1(=0)OCCCN1CCCI
312	000848-75-9	Lormetazepam	Clc1ccc2c(c1)C(=NC(C(=0)N2C)O)c1ccccc1Cl	375	003930-20-9	Sotalol	CC(NCC(c1ccc(cc1)NS(=0)(=0)C)O)C
313	000911-45-5	Clomifene	CCN(CCOc1ccc(cc1)C(=C(c1ccccc1)Cl)c1cccccc1)CC	376	004093-35-0	Bromopride	CCN(CCNC(=O)c1cc(Br)c(cc1OC)N)CC
314	000915-30-0	Diphenoxylate	CCOC(=0)C1(CCN(CC1)CCC(c1ccccc1)(c1ccccc1)C#N)c1ccccc1	377	004291-63-8	Cladribine	OCC1OC(CC1O)n1cnc2c1nc(Cl)nc2N
315	000968-81-0	Acetohexamide	O=C(NS(=O)(=O)c1ccc(cc1)C(=O)C)NC1CCCCC1	378	004342-03-4	Dacarbazine	CN(NN=C1N=CN=C1C(=O)N)C
316	000972-02-1	Diphenidol	OC(c1ccccc1)(c1ccccc1)CCCN1CCCCC1	379	004394-00-7	Niflumic	OC(=O)c1cccnc1Nc1cccc(c1)C(F)(F)F
317	001088-11-5	Desmethyldiazepam	O=C1CN=C(c2c(N1)ccc(c2)CI)c1ccccc1	380	004419-39-0	Beclomethasone	CCC(=O)OC1(C(C)CC2C1(C)CC(O)C1(C2CCC2=CC(=O)C=CC12C)CI)C(=O)COC(=O)CC
318	001094-08-2	Ethopropazine	CCN(C(CN1c2cccc2Sc2c1cccc2)C)CC	381	004428-95-9	Foscarnet	OC(=O)P(=O)(O)O
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ID	CAS	Name	Canonical SMILES	ID	CAS	Name	Canonical SMILES
382 383	004618-18-2 004697-36-3	Lactulose Carbenicillin	OCC10C(C(C10C10C(C0)C(C(C10)0)0)0)(0)C0 O=C(C(c1ccccc1)C(=0)0)NC1C(=0)N2C1SC(C2C(=0)0)(C)C	446	019387-91-8	Tinidazole 1,2,3,7,8,9-	CCS(=0)(=0)CCn1c(C)ncc1N(=0)=0
383	004891-15-0	Estramustine	CICCN(C(=0)Oc1ccc2c(c1)CCC1C2CCC2(C1CCC2O)C)CCCI	447	019408-74-3	hexachlorodibenzo-p-dioxin	Clc1c(Cl)cc2c(c1Cl)Oc1c(O2)cc(c(c1Cl)Cl)Cl
385	005051-62-7	Guanabenz	NC(=NN=Cc1c(Cl)cccc1Cl)N	448	019794-93-5	Trazodone	Clc1cccc(c1)N1CCN(CC1)CCCn1nc2n(c1=0)cccc2
386	005053-06-5	Fenspiride	O=C1NCC2(O1)CCN(CC2)CCc1ccccc1	449	019982-08-2	Memantine	CC12CC3CC(C1)(C)CC(C2)(C3)N
387	005104-49-4	Flurbiprofen	OC(=0)C(c1ccc(c(c1)F)c1ccccc1)C	450	020537-88-6	Amifostine	NCCCNCCSP(=0)(0)0
388	005250-39-5	Flucloxacillin	O=C1C(NC(=O)c2c(C)onc2c2c(F)cccc2C1)C2N1C(C(=O)O)C(S2)(C)C	451	020594-83-6	Nalbuphine	OC1CCC2(C34C1Oc1c4c(CC2N(CC3)CC2CCC2)ccc1O)O
389	005436-43-1	2,2',4,4'-Tetrabromodiphenyl	Brc1ccc(c(c1)Br)Oc1ccc(cc1Br)Br	452	020830-75-5	Digoxin	O=C1OCC(=C1)C1CCC2(C1(C)C(O)CC1C2CCC2C1(C)CC(C2)OC1CC(O)C(C(O1)C)OC1CC(O1)C(O1)
390	005534-09-8	Beclomethasone	OCC(=0)C1(0)C(C)CC2C1(C)CC(O)C1(C2CCC2=CC(=0)C=CC12C)CI	453	020830-81-3	Daunorubicin	COc1cccc2c1C(=0)c1c(C2=0)c(O)c2c(c1O)C(OC1CC(N)C(C(O1)C)O)CC(C2)(O)C(=0)C
391	005534-95-2	Pentagastrin	CSCCC(C(=0)NC(C(=0)NC(C(=0)N)Cc1ccccc1)CC(=0)O)NC(=0)C(Cc1c[nH]c2c1cccc2)NC(=0)CCNC(=0)OCC(C)CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	454	021187-98-4	Gliclazide	O=C(NS(=O)(=O)c1ccc(cc1)C)NN1CC2C(C1)CCC2
392	005588-33-0	Mesoridazine	CN1CCCC1CCN1c2ccccc2Sc2c1cc(cc2)S(=O)C	455	021256-18-8	Oxaprozin	OC(=O)CCc1nc(c(o1)c1ccccc1)c1ccccc1
393	005591-45-7	Thiothixene	CN1CCN(CC1)CCC=C1c2ccccc2Sc2c1cc(cc2)S(=O)(=O)N(C)C	456	021593-23-7	Cephapirin	O=C(NC1C(=0)N2C1SCC(=C2C(=0)O)COC(=0)C)CSc1ccncc1
394	005633-20-5	Oxybutynin	CCN(CC#CCOC(=O)C(c1ccccc1)(C1CCCCC1)O)CC	457	021679-14-1	Fludarabine	OCC1OC(C(C1O)O)n1cnc2c1nc(F)nc2N
395	005786-21-0	Clozapine	CN1CCN(CC1)C1=c2cccc2=Nc2c(N1)cc(Cl)cc2	458	021738-42-1	Oxamniquine	OCc1cc2CCC(Nc2cc1N(=0)=0)CNC(C)C
396	006190-39-2	Dihydroergotamine	CN1CC(CC2C1Cc1c[nH]c3c1c2ccc3)C(=0)NC1(C)OC2(N(C1=0)C(Cc1ccccc1)C(=0)N1C2CCC1)O	459	021829-25-4	Nifedipine	COC(=0)C1=C(C)NC(=C(C1c1ccccc1N(=0)=0)C(=0)OC)C
397	006452-71-7	Oxprenolol	C=CCOc1cccc10CC(CNC(C)C)0	460	022071-15-4	Ketoprofen	OC(=0)C(c1cccc(c1)C(=0)c1ccccc1)C
398 399	006493-05-6 006621-47-2	Pentoxifylline Perhexiline	CC(=0)CCCCn1c(=0)c2n(C)cnc2n(c1=0)C C1CCC(NC1)CC(C1CCCCC1)C1CCCCC1	461 462	022195-34-2 022204-53-1	Guanadrel Naproxen	NC(=NCC1COC2(O1)CCCCC2)N COc1ccc2c(c1)ccc(c2)C(C(=O)O)C
				462		- P	
400 401	006740-88-1 006893-02-3	Ketamine Liothyronine	CNC1(CCCCC1=0)c1ccccc1Cl OC(=0)C(Cc1cc(l)c(c(c1)l)Oc1ccc(c(c1)l)O)N	463 464	022232-71-9 022316-47-8	Mazindol Clobazam	Clc1ccc(cc1)C1(O)c2ccccc2C2=NCCN12 Clc1ccc2c(c1)N(C(=0)CC(=0)N2C)c1ccccc1
401	006990-06-3	Fusidic	CC(=0)CC1CC2(C(C1=C(C(=0)0)CCC=C(C)C)CC(C1C2(C)CCC2C1(C)CCC(C2C)0)0)C	464	022316-47-8	Diflunisal	Fc1ccc(c(c1)F)c1ccc(c(c1)C(=0)O)O
402	007012-37-5	2,4,4'-trichlorobiphenyl	Clc1ccc(cc1)c1ccc(cc1Cl)Cl	466	023031-25-6	Terbutaline	OC(c1cc(0)cc(c1)0)CNC(C)(C)C
404	007203-91-0		CN(N=Nc1cc(cc1)C(=0)O)C	467	023155-02-4	Fosfomycin	CC10C1P(=0)(0)0
405	007261-97-4	Dantrolene	O=C1CN(C(=O)N1)N=Cc1ccc(o1)c1ccc(cc1)N(=O)=O	468	023214-92-8	Doxorubicin	OCC(=0)C1(0)CC(OC2CC(N)C(C(O2)C)O)c2c(C1)c(O)c1c(c2O)C(=0)c2c(C1=0)cccc2OC
406	007481-89-2	Zalcitabine	Nc1ccn(c(=O)n1)C1CCC(O1)CO	469	023288-49-5	Probucol	CC(Sc1cc(c(c(c1)C(C)(C)C)O)C(C)(C)C)(Sc1cc(c(c1)C(C)(C)C)O)C(C)(C)C)C)C
407	007683-59-2	Isoproterenol	CC(NCC(c1ccc(c(c1)O)O)O)C	470	023593-75-1	Clotrimazole	Clc1cccc1C(n1cncc1)(c1ccccc1)c1ccccc1
408	010206-21-0	Cefacetrile	CC(=O)OCC1=C(N2C(SC1)C(C2=O)NC(=O)CC#N)C(=O)O	471	023887-31-2	Clorazepate	OC(=0)C1N=C(c2cccc2)c2c(NC1=0)ccc(c2)Cl
409	010238-21-8	Glibenclamide	COc1ccc(cc1C(=0)NCCc1ccc(cc1)S(=0)(=0)NC(=0)NC1CCCCC1)Cl	472	024219-97-4	Mianserin	CN1CCN2C(C1)c1ccccc1Cc1c2cccc1
410	010262-69-8	Maprotiline	CNCCCC12CCC(c3c1cccc3)c1c2cccc1	473	024526-64-5	Nomifensine	CN1CC(c2cccc2)c2c(C1)c(N)ccc2
411	010540-29-1	Tamoxifen	CCC(=C(c1ccccc1)c1ccc(cc1)OCCN(C)C)c1ccccc1	474	024560-70-1	Ethinylestradiol-3-Sulfate	C#CC1(O)CCC2C1(C)CCC1C2CCc2c1ccc(c2)OS(=O)(=O)O
412	012650-69-0	Mupirocin	OC(=0)CCCCCCCC(=0)C=C(CC10CC(C(C10)0)CC10C1C(C(0)C)C)C	475	025451-15-4	Felbamate	NC(=0)OCC(c1cccc1)COC(=0)N
413	013010-47-4	Lomustine	CICCN(C(=O)NC1CCCCC1)N=O	476	025569-80-6	2,3'-Dichlorobiphenyl	Clc1cccc(c1)c1ccccc1Cl
414	013029-08-8	2,2'-dichlorobiphenyl	Clc1ccccc1Cl	477	025614-03-3	Bromocriptine	CC(CC1C(=0)N2CCCC2C2(N1C(=0)C(O2)(NC(=0)C1CN(C)C2C(=C1)c1ccc3c1c(C2)c([nH]3)Br)C(C)C)O)C
415		Fenoterol	CC(Cc1ccc(cc1)O)NCC(c1cc(O)cc(c1)O)O	478	025812-30-0		Cc1ccc(c(c1)OCCCC(C(=0)O)(C)C)C
416 417	013392-28-4	Rimantadine Pindolol	CC(C12CC3CC(C2)CC(C1)C3)N	479 480	025953-19-9	Cefazolin Tolmetin	0=C(NC1C(=0)N2C1SCC(=C2C(=0)0)CSc1nnc(s1)C)Cn1cnnn1
417	013523-86-9 013539-59-8		OC(COc1cccc2c1cc[nH]2)CNC(C)C CCCC1C(=0)n2n(C1=0)c1cc(C)ccc1nc2N(C)C	481	026171-23-3 026652-09-5	Ritodrine	OC(=0)Cc1ccc(n1C)C(=0)c1ccc(cc1)C Oc1ccc(cc1)CCNC(C(c1ccc(cc1)0)O)C
418	013647-35-3	Azapropazone Trilostane	N#CC1=C(0)C2C3(C(C1)(C)C1CCC4(C(C1CC3)CCC40)C)O2	482	026787-78-0	Amoxicillin	0=C(C(c1ccc(cc1)O)N)NC1C(=O)N2C1SC(C2C(=O)O)(C)C
420	013655-52-2	Alprenolol	C=CCc1cccc10CC(CNC(C)C)O	483	026807-65-8	Indapamide	Cc1Cc2c(N1NC[=0]c1cc(c[c1)S[=0)[=0]N)Clcccc2
421	013669-70-0	Nefopam	CN1CCOC(c2c(C1)cccc2)c1cccc1	484	026839-75-8	Timolol	OC(COc1nsnc1N1CCOCC1)CNC(c)(C)C
422	014028-44-5	Amoxapine	Clc1ccc2c(c1)C(=Nc1c(O2)cccc1)N1CCNCC1	485	026844-12-2	Indoramin	O=C(c1cccc1)NC1CCN(CC1)CCc1cc2c([nH]1)cccc2
423	014769-73-4	Levamisole	C1CN2C(=NC(C2)c2cccc2)S1	486	027203-92-5	Tramadol	COcleccc(c1)C1(O)CCCCC1CN(C)C
424	015291-75-5	Ginkgolide	O=C1OC2C(C1C)(O)C13C4(C2)C(OC3=O)CC(C24C(O1)OC(=O)C2O)C(C)(C)(C)C	487	028395-03-1	Bumetanide	CCCCNc1cc(cc(c1Oc1ccccc1)S(=O)(=O)N)C(=O)O
425	015291-77-7	Ginkgolide	O=C1OC2C(C1C)(O)C13C4(C2O)C(OC3=O)CC(C24C(O1)OC(=O)C2O)C(C)(C)C	488	028523-86-6	Sevoflurane	FCOC(C(F)(F)F)C(F)(F)F
426	015307-86-5	Diclofenac	OC(=O)Cc1ccccc1Nc1c(Cl)cccc1Cl	489	028657-80-9	Cinoxacin	CCn1nc(C(=0)0)c(=0)c2c1cc10C0c1c2
427	015676-16-1	Sulpiride	CCN1CCC1CNC(=0)c1cc(ccc1OC)S(=0)(=0)N	490	028721-07-5	Oxcarbazepine	O=C1Cc2cccc2N(c2c1cccc2)C(=O)N
428	015686-71-2	Cephalexin	NC(c1ccccc1)C(=0)NC1C(=0)N2C1SCC(=C2C(=0)O)C	491	028860-95-9	Carbidopa	NNC(C(=0)0)(Cc1ccc(c(c1)0)0)C
429	015687-27-1	Ibuprofen	CC(Cc1ccc(cc1)C(C(=0)O)C)C	492	028911-01-5	Triazolam	Clc1ccc2c(c1)C(=NCc1n2c(C)nn1)c1ccccc1Cl
430	015722-48-2	Olsalazine	OC(=0)C1=CC(=NNc2ccc(c(c2)C(=0)0)0)C=CC1=0	493	028981-97-7	Alprazolam	Clc1ccc2c(c1)C(=NCc1n2c(C)nn1)c1ccccc1
431	015793-40-5	Terodiline	CC(NC(C)(C)C)CC(c1ccccc1)c1ccccc1	494	029094-61-9	Glipizide	Cc1ncc(nc1)C(=0)NCCc1ccc(cc1)S(=0)(=0)NC1CCCCC1
432	015862-07-4	2,4,5-trichlorobiphenyl	Clc1cc(Cl)c(cc1c1cccc1)Cl	495	029110-47-2	Guanfacine	O=C(Cc1c(Cl)ccc1Cl)N=C(N)N
433 434	015968-05-5 016051-77-7	2,6,2',6'-tetrachlorobiphenyl Isosorbide	Clc1cccc(c1c1c(Cl)cccc1Cl)Cl O=N(=O)OC1COC2C1OCC2O	496 497	029122-68-7 029218-27-7	Atenolol Toloxatone	OC(COc1ccc(cc1)CC(=0)N)CNC(C)C OCC1OC(=0)N(C1)c1cccc(c1)C
434	016051-77-7	Isosorbide Isosorbide-2-Mononitrate	0=N(=0)0C1C0C2C10CC20 0=N(=0)0C1C0C2C10CC20	497	029218-27-7	Teniposide	COc1cc(cc(c10)OC)C1C2C(=0)OCC2C(c2c1cc1OCOc1c2)OC1OC2COC(OC2C(C10)O)c1cccs1
435	016106-20-0	Cromoglicate	OC(COc1cccc2c1occ2c0 OC(COc1cccc2c(c2)C(=0)O)COc1ccc2c(c1)c(=0)cc(o2)C(=0)O	498	029767-20-2	Estazolam	Clc1ccc2c(c1)C(=NCc1n2cnn1)c1ccccc1
436	016590-41-3	Naltrexone	0=C1CCC2(C34C10c1c4c(CC2N(CC3)CC2CC2)ccc10)0	500	030516-87-1	Zidovudine	OCC10C(CC1N=N#N)n1cc(C)c(=0)[nH]c1=0
437	016606-02-3	2,5,4'-trichlorobiphenyl	Clc1ccc(cc1)c1cc(Cl)ccc1Cl	501	031036-80-3	Lofexidine	CC(C1=NCCN1)Oc1c(Cl)cccc1Cl
439	017230-88-5	Danazol	C#CC1(0)CCC2C1(C)CCC1C2CCC2=Cc3c(CC12C)cno3	502	031431-39-7	Mebendazole	COC(=0)Nc1nc2c([nH]1)cc(cc2)C(=0)c1ccccc1
440	017560-51-9	Metolazone	CC1Nc2cc(Cl)c(cc2C(=0)N1c1ccccc1C)S(=0)(=0)N	552	-51.51.55 /	2,4,5,3',4'-	
441	017617-23-1	Flurazepam	CCN(CCN1C(=0)(CN=C(c2c1cc(c2)(c))(c1ccccc1F)CC	503	031508-00-6	pentachlorobiphenyl	Clc1cc(Cl)c(cc1c1ccc(c(c1)Cl)Cl)Cl
442	018323-44-9	Clindamycin	CCCC1CN(C(C1)C(=0)NC(C10C(SC)C(C(C10)0)O)C(CI)C)C	504	031828-71-4	Mexiletine	CC(COc1c(C)cccc1C)N
443	018559-94-9	Salbutamol	OCc1cc(ccc10)C(CNC(C)(C)C)O	505	031883-05-3	Moricizine	CCOC(=O)Nc1ccc2c(c1)N(C(=O)CCN1CCOCC1)c1c(S2)cccc1
444	018883-66-4	Streptozocin	OCC1OC(0)C(C(C10)0)NC(=0)N(N=0)C	506	032222-06-3	Calcitriol	OC1CC(O)C(=C)C(=CC=C2CCCC3(C2CCC3C(CCCC(O)(C)C)C)C1
445	019216-56-9	Prazosin	COc1cc2nc(nc(c2cc1OC)N)N1CCN(CC1)C(=0)c1ccco1	507	032598-10-0	2,4,3',4'-tetrachlorobiphenyl	Clc1ccc(c(c1)Cl)c1ccc(c(c1)Cl)Cl

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508	032598-11-1	2,5,3',4'-tetrachlorobiphenyl	Clc1ccc(c(c1)c1ccc(c(c1)Cl)Cl)Cl
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(c(c1)Cl)Cl
		2,3,4,3',4'-	
511	032598-14-4	pentachlorobiphenyl	Clc1ccc(cc1Cl)c1ccc(c(c1Cl)Cl)Cl
512	032690-93-0	2,4,5,4'-tetrachlorobiphenyl	Clc1ccc(cc1)c1cc(Cl)c(cc1Cl)Cl
		3,4,5,3',4',5'-	
513	032774-16-6	hexachlorobiphenyl	Clc1cc(cc(c1Cl)Cl)c1cc(Cl)c(c(c1)Cl)Cl
514	032795-44-1	Acecainide	CCN(CCNC(=0)c1ccc(cc1)NC(=0)C)CC
515	032887-01-7	Amdinocillin	OC(=0)C1N2C(=0)C(C2SC1(C)C)N=CN1CCCCCC1
516	033005-95-7	Tiaprofenic	OC(=0)C(c1ccc(s1)C(=0)c1ccccc1)C
517	033025-41-1	2,3,4,4'-tetrachlorobiphenyl	Clc1ccc(cc1)c1ccc(c(c1Cl)Cl)Cl
		2,3,4,6,2',3',4',6'-	
518	033091-17-7	octachlorobiphenyl	Clc1cc(Cl)c(c(c1c1c(Cl)cc(c(c1Cl)Cl)Cl)Cl)Cl
519	033125-97-2	Etomidate	CCOC(=O)c1cncn1C(c1ccccc1)C
520	033284-50-3	2,4-Dichlorobiphenyl	Clc1ccc(c(c1)Cl)c1ccccc1
521	033284-54-7	2,3,5,6-Tetrachlorobiphenyl	Clc1cc(Cl)c(c(c1Cl)c1ccccc1)Cl
	033342-05-1	Gliquidone	COc1ccc2c(c1)C(=0)N(C(=0)C2(C)C)CCc1ccc(cc1)S(=0)(=0)NC(=0)NC1CCCCC1
523	033419-42-0	Etoposide	COc1cc(cc(c10)OC)C1C2C(=0)OCC2C(c2c1cc10COc1c2)OC10C2COC(OC2C(C10)O)C
524	033570-04-6	Bilobalide	O=C1OC2C3(C1)C(=O)OC1C3(C(C2)(O)C(C)(C)C(O)C(=O)O1
525	033671-46-4	Clotiazepam	CCc1sc2c(c1)C(=NCC(=O)N2C)c1ccccc1Cl
526	033817-20-8	Pivampicillin	O=C(C(c1ccccc1)N)NC1C(=O)N2C1SC(C2C(=O)OCOC(=O)C(C)(C)C)(C)C
527	034444-01-4	Cefamandole	OC(C(=0)NC1C(=0)N2C1SCC(=C2C(=0)0)CSc1nnnn1C)c1ccccc1
528	034580-14-8	Ketotifen	CN1CCC(=C2c3ccccc3CC(=0)c3c2ccs3)CC1
529	034597-40-5	Fenoprofen	OC(=0)C(c1cccc(c1)Oc1ccccc1)C
530	034661-75-1	Urapidil	COc1cccc1N1CCN(CC1)CCCNc1cc(=0)n(c(=0)n1C)C
531	034787-01-4	Ticarcillin	O=C(C(c1cscc1)C(=0)O)NC1C(=0)N2C1SC(C2C(=0)O)(C)C
532	034834-67-8	Hydroxycotinine,	O=C1C(O)CC(N1C)c1cccnc1
533	034841-39-9	Bupropion	Clc1cccc(c1)C(=O)C(NC(C)(C)C)C
534	034883-39-1	2,5-Dichlorobiphenyl	Clc1ccc(c(c1)c1ccccc1)Cl
535	034883-41-5	3,5-dichlorobiphenyl	Clc1cc(Cl)cc(c1)c1ccccc1
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
		2,3,4,2',4',5'-	
538	035065-28-2	hexachlorobiphenyl	Clc1cc(Cl)c(cc1c1ccc(c(c1Cl)Cl)Cl)Cl
		2,3,4,5,2',4',5'-	
539	035065-29-3	heptachlorobiphenyl	Clc1cc(Cl)c(cc1c1cc(Cl)c(c(c1Cl)Cl)Cl)Cl
		2,3,4,5,2',3',4'-	
540	035065-30-6	heptachlorobiphenyl	Clc1c(Cl)ccc(c1Cl)c1cc(Cl)c(c(c1Cl)Cl)Cl
541	035189-28-7	Norgestimate	ON=C1CCC2C(=C1)CCC1C2CCC2(C1CCC2(C#C)OC(=O)C)CC
542	035607-66-0	Cefoxitin	COC1(NC(=0)Cc2cccs2)C(=0)N2C1SCC(=C2C(=0)0)COC(=0)N
543	035693-92-6	2,4,6-trichlorobiphenyl	Clc1cc(Cl)c(c(c1)Cl)c1ccccc1
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(c(c1)Cl)c1cc(Cl)c(c(c1Cl)Cl)Cl
546	035795-16-5	Trimazosin	COc1c(OC)c(OC)cc2c1nc(nc2N)N1CCN(CC1)C(=O)OCC(O)(C)C
		1,2,3,4,6,7,8-	
547	035822-46-9	heptachlorodibenzo-p-dioxin	Clc1c(Cl)cc2c(c1Cl)Oc1c(O2)c(Cl)c(c(c1Cl)Cl)Cl
548	036505-84-7	Buspirone	O=C1CC2(CCCC2)CC(=O)N1CCCCN1CCN(CC1)c1ncccn1
549	036507-48-9	Penbutolol	OC(COc1ccccc1C1CCCC1)CNC(C)(C)C
550	036559-22-5	2,2',3,4'-Tetrachlorobiphenyl	Clc1ccc(c(c1)Cl)c1cccc(c1Cl)Cl
551	036735-22-5	Quazepam	Clc1ccc2c(c1)C(=NCC(=S)N2CC(F)(F)F)c1ccccc1F
552	036791-04-5	Ribavirin	OCC10C(C(C10)O)n1cnc(n1)C(=O)N
553	037091-66-0	Azlocillin	O=C(C(c1ccccc1)NC(=O)N1CCNC1=O)NC1C(=O)N2C1SC(C2C(=O)O)(C)C
554	037115-32-5	Adinazolam	CN(Cc1nnc2n1c1ccc(cc1C(=NC2)c1ccccc1)Cl)C
555	037148-27-9	Clenbuterol	OC(c1cc(Cl)c(c(c1)Cl)N)CNC(C)(C)C
556	037300-21-3	Pentosan	OC1COC(C(C1OS(=0)(=0)O)OS(=0)(=0)O)OC1COC(C(C1OS(=0)(=0)O)OS(=0)(=0)O)O
557	037517-30-9	Acebutolol	CCCC(=0)Nc1ccc(c(c1)C(=0)C)OCC(CNC(C)C)O
558	037680-65-2	2,5,2'-trichlorobiphenyl	Clc1ccc(c(c1)c1ccccc1Cl)Cl
559	037680-66-3	2,4,2'-trichlorobiphenyl	Clc1ccc(c(c1)Cl)c1ccccc1Cl
560	037680-68-5	3,5,2'-trichlorobiphenyl	Clc1cc(Cl)cc(c1)c1ccccc1Cl
561	037680-69-6	3,4,3'-trichlorobiphenyl	Clc1cccc(c1)c1ccc(c(c1)Cl)Cl

ID	CAS	Name	Canonical SMILES
		2,4,5,2',5'-	
562	037680-73-2	pentachlorobiphenyl	Clc1ccc(c(c1)c1cc(Cl)c(cc1Cl)Cl)Cl
563	038103-61-6	Tolamolol	OC(COc1ccccc1C)CNCCOc1ccc(cc1)C(=0)N
564	038194-50-2	Sulindac	OC(=O)CC1=C(C)C(=Cc2ccc(cc2)S(=O)C)c2c1cc(F)cc2
		2,2',3,5',6-	
565	038379-99-6	Pentachlorobiphenyl	Clc1ccc(c(c1)c1c(Cl)ccc(c1Cl)Cl)Cl
		2,4,5,2',4'-	
566	038380-01-7	pentachlorobiphenyl	Clc1ccc(c(c1)Cl)c1cc(Cl)c(cc1Cl)Cl
		2,2',3,4,5'-	
567	038380-02-8	Pentachlorobiphenyl	Clc1ccc(c(c1)c1ccc(c(c1Cl)Cl)Cl)Cl
560	020200 02 0	2,3,6,3',4'-	
568	038380-03-9	pentachlorobiphenyl	Clc1cc(ccc1Cl)c1c(Cl)ccc(c1Cl)Cl
569	038380-04-0	2,2',3,4',5',6-	Cl-1(Cl)-(1-1-(Cl)(-1Cl)Cl)Cl
509	038380-04-0	Hexachlorobiphenyl 2,2',3,3',4,6'-	Clc1cc(Cl)c(cc1c1c(Cl)ccc(c1Cl)Cl)Cl
570	038380-05-1	Hexachlorobiphenyl	Clc1ccc(c(c1Cl)Cl)c1c(Cl)ccc(c1Cl)Cl
370	030300-03-1	2,3,4,2',3',4'-	
571	038380-07-3	hexachlorobiphenyl	Clc1c(ccc(c1Cl)Cl)c1ccc(c(c1Cl)Cl)Cl
3/1	038380-07-3	2,3,4,5,3',4'-	
572	038380-08-4	hexachlorobiphenyl	Clc1ccc(cc1Cl)c1cc(Cl)c(c(c1Cl)Cl)Cl
573	038396-39-3	Bupivacaine	CCCCN1CCCCC1C(=0)Nc1c(C)cccc1C
373	030330 33 3	2,3,6,2',3',6'-	0000110000010 0)11010(0)00010
574	038411-22-2	hexachlorobiphenyl	Clc1ccc(c(c1c1c(Cl)ccc(c1Cl)Cl)Cl)Cl
		2,2',3,3',4,5,6'-	and the state of the basis
575	038411-25-5	Heptachlorobiphenyl	Clc1c(Cl)cc(c(c1Cl)Cl)c1c(Cl)ccc(c1Cl)Cl
576	038444-73-4	2,2',6-trichlorobiphenyl	Clc1cccc(c1c1ccccc1Cl)Cl
577	038444-76-7	2,3',6-Trichlorobiphenyl	Clc1cccc(c1)c1c(Cl)cccc1Cl
578	038444-77-8	2,4',6-Trichlorobiphenyl	Clc1cccc(c1c1ccc(cc1)Cl)Cl
579	038444-78-9	2,2',3-Trichlorobiphenyl	Clc1ccccc1c1cccc(c1Cl)Cl
580	038444-81-4	2,5,3'-trichlorobiphenyl	Clc1ccc(c(c1)c1cccc(c1)Cl)Cl
581	038444-85-8	2,3,4'-trichlorobiphenyl	Clc1ccc(cc1)c1cccc(c1Cl)Cl
582	038444-86-9	2,3',4'-Trichlorobiphenyl	Clc1cc(ccc1Cl)c1ccccc1Cl
583	038444-87-0	3,5,3'-trichlorobiphenyl	Clc1cccc(c1)c1cc(Cl)cc(c1)Cl
584	038444-88-1	3,5,4'-trichlorobiphenyl	Clc1ccc(cc1)c1cc(Cl)cc(c1)Cl
585	038444-90-5	3,4,4'-trichlorobiphenyl	Clc1ccc(cc1)c1ccc(c(c1)Cl)Cl
586	038444-93-8	2,3,2',3'-tetrachlorobiphenyl	Clc1c(Cl)cccc1c1cccc(c1Cl)Cl
587	038677-94-0	Nortilidine	CCOC(=0)C1(CCC=CC1NC)c1ccccc1
588	038821-53-3	Cephradine	O=C(C(C1=CCC=CC1)N)NC1C(=O)N2C1SCC(=C2C(=O)O)C
589	039001-02-0	Octachlorodibenzofuran	Clc1c(Cl)c(Cl)c2c(c1Cl)oc1c2c(Cl)c(c(c1Cl)Cl)Cl
500	020227.20.6	1,2,3,4,7,8-	CL 4 - 20 - 2 - (0 - 2 - 4 Cl) - (0 l) - (- 1 - 2 Cl) Cl) Cl
590	039227-28-6	hexachlorodibenzo-p-dioxin	Clc1cc2Oc3c(Oc2cc1Cl)c(Cl)c(c(c3Cl)Cl)Cl
F01	020405 02 4	2,4,6,2',4'-	Cl=1===(=(=1)Cl>=1=(=1Cl)Cl
591 592	039485-83-1 039562-70-4	pentachlorobiphenyl	Clc1ccc(c(c1)Cl)c1c(Cl)cc(cc1Cl)Cl
392	059502-70-4	Nitrendipine 2,3,4,5,3',4',5'-	CCOC(=O)C1=C(C)NC(=C(C1c1cccc(c1)N(=O)=O)C(=O)OC)C
593	039635-31-9	heptachlorobiphenyl	Clc1cc(cc(c1Cl)Cl)c1cc(Cl)c(c(c1Cl)Cl)Cl
594	039715-02-1	Endralazine	NNc1nnc2c(c1)CN(CC2)C(=0)c1ccccc1
55.	0007,10 02 1	2,3,4,6,2',3',5'-	11102111022002701 070200002
595	040186-70-7	heptachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1c(Cl)cc(c(c1Cl)Cl)Cl)Cl
		2,3,4,6,2',3',5',6'-	
596	040186-71-8	octachlorobiphenyl	Clc1cc(Cl)c(c(c1Cl)Cl)c1c(Cl)c(Cl)cc(c1Cl)Cl
		2,3,4,5,6,2',3',4',5'-	
597	040186-72-9	nonachlorobiphenyl	Clc1cc(c(c(c1Cl)Cl)Cl)c1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl
		1,2,3,7,8-pentachlorodibenzo-	
598	040321-76-4	p-dioxin	Clc1cc2Oc3c(Oc2cc1Cl)cc(c(c3Cl)Cl)Cl
599	040828-46-4	Suprofen	OC(=0)C(c1ccc(cc1)C(=0)c1cccs1)C
600	041318-75-6	2,4,4'-Tribromodiphenyl	Brc1ccc(cc1)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(c(c1Cl)Cl)Cl
		2,3,4,5,6,3',4'-	
603	041411-64-7	heptachlorobiphenyl	Clc1cc(ccc1Cl)c1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl
604	041464-39-5	2,3,2',5'-tetrachlorobiphenyl	Clc1ccc(c(c1)c1cccc(c1Cl)Cl)Cl
605	041464-40-8	2,2',4,5'-Tetrachlorobiphenyl	Clc1ccc(c(c1)Cl)c1cc(Cl)ccc1Cl

ID	CAS	Name	Canonical SMILES	ID	CAS	Name	Canonical SMILES
606	041464-41-9	2,5,2',6'-tetrachlorobiphenyl	Clc1ccc(c(c1)c1c(Cl)cccc1Cl)Cl			2,3,4,5,2',3',5'-	
607	041464-43-1	2,3,3',4'-tetrachlorobiphenyl	Clc1cc(ccc1Cl)c1cccc(c1Cl)Cl	653	052663-74-8	heptachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1cc(Cl)c(c(c1Cl)Cl)Cl)Cl
608	041464-46-4	2,3',4',6-Tetrachlorobiphenyl	Clc1cc(ccc1Cl)c1c(Cl)cccc1Cl			2,3,4,5,2',3',5',6'-	
609	041464-47-5	2,3,2',6'-tetrachlorobiphenyl	Clc1c(Cl)cccc1c1c(Cl)cccc1Cl	654	052663-75-9	octachlorobiphenyl	Clc1c(Cl)cc(c(c1Cl)Cl)c1c(Cl)cc(c1Cl)Cl
		2,2',3,4',5'-				2,3,4,5,6,2',4',5'-	
610	041464-51-1	Pentachlorobiphenyl	Clc1cc(Cl)c(cc1c1cccc(c1Cl)Cl)Cl	655	052663-76-0	octachlorobiphenyl	Clc1cc(Cl)c(cc1c1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl)Cl
611	041708-72-9	Tocainide	CC(C(=0)Nc1c(C)cccc1C)N			2,3,4,5,6,2',3',4'-	
612	041744-40-5	Sulbenicillin	O=C(C(S(=O)(=O)O)c1ccccc1)NC1C(=O)N2C1SC(C2C(=O)O)(C)C	656	052663-78-2	octachlorobiphenyl	Clc1ccc(c(c1Cl)Cl)c1c(Cl)c(c(c(c1Cl)Cl)Cl
613	041859-67-0	Bezafibrate	Clc1ccc(cc1)C(=0)NCCc1ccc(cc1)OC(C(=0)O)(C)C			2,3,4,5,6,2',3',4',6'-	
614	041952-52-7	Cefcanel	O=C(C(c1ccccc1)O)NC1C(=O)N2C1SCC(=C2C(=O)O)CSc1nnc(s1)C	657	052663-79-3	nonachlorobiphenyl	Clc1c(Cl)cc(c(c1Cl)c1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl)Cl
615	042200-33-9	Nadolol	OC(COc1cccc2c1CC(O)C(C2)O)CNC(C)(C)C			2,2',3,3',5,6-	
616	042228-92-2	Acivicin	NC(C(=0)0)C1CC(=N01)Cl	658	052704-70-8	Hexachlorobiphenyl	Clc1cccc(c1Cl)c1c(Cl)cc(c1Cl)Cl
617	042399-41-7	Diltiazem	COc1ccc(cc1)C1Sc2ccccc2N(C(=0)C1OC(=0)C)CCN(C)C			2,3,4,5,2',5'-	
618	042408-82-2	Butorphanol	Oc1ccc2c(c1)C13CCCCC3(C(C2)N(CC1)CC1CC1)O	659	052712-04-6	hexachlorobiphenyl	Clc1ccc(c(c1)c1cc(Cl)c(c(c1Cl)Cl)Cl)Cl
		2,3,4,5,2',3',4',6'-				2,3,4,5,6,2',5'-	
619	042740-50-1	octachlorobiphenyl	Clc1cc(Cl)c(c(c1c1cc(Cl)c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	660	052712-05-7	heptachlorobiphenyl	Clc1ccc(c(c1)c1c(Cl)c(c(c1Cl)Cl)Cl)Cl
620	043200-80-2	Zopiclone	CN1CCN(CC1)C(=0)OC1c2nccnc2C(=0)N1c1ccc(cn1)Cl			2,3,5,2',3',6'-	
621	046817-91-8	Viloxazine	CCOc1ccccc1OCC1COCCN1	661	052744-13-5	hexachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1c(Cl)ccc(c1Cl)Cl)Cl
622	047141-42-4	Levobunolol	OC(COc1cccc2c1CCCC2=O)CNC(C)(C)C	662	053179-11-6	Loperamide	Clc1ccc(cc1)C1(O)CCN(CC1)CCC(C(=O)N(C)C)(c1ccccc1)c1ccccc1
623	049562-28-9	Fenofibrate	CC(OC(=O)C(Oc1ccc(cc1)C(=O)c1ccc(cc1)Cl)(C)C)C	663	053230-10-7	Mefloquine	OC(c1cc(nc2c1cccc2C(F)(F)F)C(F)(F)F)C1CCCCN1
624	050370-12-2	Cefadroxil	O=C(C(c1ccc(cc1)O)N)NC1C(=O)N2C1SCC(=C2C(=O)O)C	664	053267-01-9	Cibenzoline	clccc(cc1)C1(CC1C1=NCCN1)clccccc1
625	050679-08-8	Terfenadine	OC(c1ccc(cc1)C(C)(C)C)CCCN1CCC(CC1)C(c1ccccc1)(c1ccccc1)O	665	053583-79-2		CCN1CCCC1CNC(=0)c1cc(c(cc10C)N)S(=0)(=0)CC
	051022-71-0		CCCCCC(c1cc(0)c2c(c1)OC(C1C2CC(=0)CC1)(C)C)C	666	053648-55-8	Dezocine	Oc1ccc2c(c1)C1(C)CCCCC(C2)C1N
		2.3.7.8-	The second secon	667	053772-83-1	Zuclopenthixol	OCCN1CCN(CC1)CCC=C1c2cccc2Sc2c1cc(Cl)cc2
627	051207-31-9	tetrachlorodibenzofuran	Clc1cc2c(cc1Cl)oc1c2cc(Cl)c(c1)Cl	668	053910-25-1	Pentostatin	OCC1OC(CC10)n1cnc2c1NC=NCC20
628	051264-14-3	Amsacrine	COc1cc(ccc1Nc1c2cccc2nc2c1cccc2)NS(=O)(=O)C	669	053994-73-3	Cefaclor	NC(c1ccccc1)C(=0)NC1C(=0)N2C1SCC(=C2C(=0)O)Cl
629	051333-22-3	Budesonide	CCCC1OC2C(01)(C(=0)C0)C1(C(C2)C2CCC3=CC(=0)C=CC3(C2C(C1)O)C)C	670	054024-22-5	Desogestrel	CCC12CC(=C)C3C(C1CCC2(O)C#C)CCC1=CCCCC31
630	051384-51-1	Metoprolol	COCCelecc(ce1)OCC(CNC(c)C)O	671	054048-10-1	Etonogestrel	C#CC1(O)CCC2C1(CC)CC(=C)C1C2CCC2=CC(=O)CCC12
	051481-65-3		O=C(C(c1ccccc1)NC(=0)N1CCN(C1=0)S(=0)(=0)C)NC1C(=0)N2C1SC(C2C(=0)0)(C)C	672	054063-53-5	Propafenone	CCCNCC(COc1ccccc1C(=O)CCc1ccccc1)O
632	051627-14-6	Cefatrizine	O=C(C(c1ccc(cc1)O)N)NC1C(=O)N2C1SCC(=C2C(=O)O)CSc1c[nH]nn1	673	054143-55-4	Flecainide	O=C(c1cc(OCC(F)(F)F)ccc1OCC(F)(F)F)NCC1CCCCN1
	051639-49-7	Chlorophenylpiperazine,	Clc1cccc(c1)N1CCNCC1	674	054340-58-8	Meptazinol	CCC1(CCCCN(C1)C)c1cccc(c1)O
033	031033 43 7	2,3,5,2',4',5'-	dittettimetet	675	054340-62-4	Bufuralol	CCc1cccc2c1oc(c2)C(CNC(C)(C)C)O
634	051908-16-8		Clc1cc(Cl)c(c(c1)c1cc(Cl)c(cc1Cl)Cl)Cl	676	054350-48-0	Etretinate	CCOC(=0)C=C(C=CC=C(C=Cc1c(C)cc(c(c1C)C)OC)C
635	051931-66-9	Tilidine	CCOC(=0)C1(CCC=CC1N(C)C)c1ccccc1	677	054739-18-3	Fluvoxamine	NCCON=C(c1ccc(cc1)C(F)(F)F)CCCCOC
636	052128-35-5	Trimetrexate	COc1cc(NCc2ccc3c(c2C)c(N)nc(n3)N)cc(c1OC)OC	678	054910-89-3	Fluoxetine	CNCCC(c1ccccc1)Oc1ccc(cc1)C(F)(F)F
637	052468-60-7	Flunarizine	Fc1ccc(cc1)C(c1ccc(cc1)F)N1CCN(CC1)CC=Cc1ccccc1	679	054965-21-8	Albendazole	CCCSc1ccc2c(c1)[nH]c(n2)NC(=0)OC
638	052485-79-7	Buprenorphine	COC12CCC3(CC1C(C)(C)C)(0)C)C14C2Oc2c4c(CC3N(CC1)CC1CC1)ccc2O	680	055079-83-9	Acitretin	COc1cc(C)c(c(c1C)C)C=CC(=CC(=C(=O)O)C)C
639	052663-58-8		Clc1ccc(cc1)c1c(Cl)ccc(c1Cl)Cl	681	055096-26-9	Nalmefene	C=C1CCC2(C34C1Oc1c4c(CC2N(CC3)CC2CC2)ccc1O)O
039	032003-38-8	2,2',3,3',6-	detector/etaletale	682	055142-85-3	Ticlopidine	Clc1cccc1CN1CCc2c(C1)ccs2
640	052662-60-2	Pentachlorobiphenyl	Clc1c(Cl)cccc1c1c(Cl)ccc(c1Cl)Cl	002	033142-03-3	2,3,4,5,2',3'-	defluction feetze(ef).cs2
040	032003-00-2	2,2',3,5,5'-	Citiqui percitifici (citiqui percitifici)	683	055215-18-4	hexachlorobiphenyl	Clc1cccc(c1Cl)c1cc(Cl)c(c(c1Cl)Cl)Cl
641	052662 61 2	Pentachlorobiphenyl	Clc1ccc(c(c1)c1cc(Cl)cc(c1Cl)Cl)Cl	684	055268-74-1	Praziquantel	O=C(N1CC(=0)N2C(C1)c1cccc1CC2)C1CCCCC1
041	032003-01-3	2,3,4,2',3'-	Citation (Citation Citation) Citation (Citation Citation	685	055268-74-1	Cefuroxime	CON=C(C(=0)NC1C(=0)N2C1SCC(=C2C(=0)O)COC(=0)N)c1ccco1
642	052663-62-4	pentachlorobiphenyl	Clc1ccc(c(c1Cl)Cl)c1cccc(c1Cl)Cl	003	033206-73-2	1,2,3,4,7,8,9-	CON-C(C(-O)NCIC(-O)NZCI3CC(-CZC(-O)O)COC(-O)NZCIZCCI
042	032003-02-4		Chitach (Chiche) Chitach (Chiche)	coc	055672.00.7	heptachlorodibenzofuran	Cl-1 2 2 -l - 2 -l - 2 (C) -l C C C C C C C C C C C C C
643	052663-63-5	2,3,5,6,2',5'- hexachlorobiphenyl	Clad and (ad) ad a (Cl) a (Cl) a (Cl) a (Cl) Cl) Cl	686 687	055673-89-7 055712-37-3		Clc1cc2oc3c(c2c(c1Cl)Cl)c(Cl)c(c(c3Cl)Cl)Cl
643	052003-03-5	2,3,5,6,2',3',6'-	Clc1ccc(c(c1)c1c(Cl)cc(c1Cl)Cl)Cl	688	055712-37-3	2,4,3 -trichlorobiphenyl	Clc1ccc(c(c1)Cl)c1ccccc(c1)Cl Clc1cc(Cl)c(c(c1)c1ccccc1)Cl
644	052663-64-6			689			
644	052663-64-6	- P	Clc1c(Cl)cc(c(c1c1c(Cl)ccc(c1Cl)Cl)Cl)Cl		055837-25-7		COc1cc(C)cc(c1C(=0)CCCN1CCCC1)OC
645	052662 65 7	2,3,4,6,2',3',6'-		690	055837-27-9	Piretanide	OC(=0)c1cc(N2CCC2)c(c(c1)S(=0)(=0)N)Oc1ccccc1
645	052663-65-7	heptachlorobiphenyl	Clc1cc(Cl)c(c(c1Cl)Cl)c1c(Cl)ccc(c1Cl)Cl	691	055954-61-5	Pseudohypericin	OCc1cc(O)c2c3c1c1c(C)cc(c4c1c1c3c3c(C2=O)c(O)cc(c3c2c1c(C4=O)c(O)cc2O)O)O
		2,3,4,,2',3',5'-		692	055981-09-4	Nitazoxanide	CC(=0)Oc1ccccc1C(=0)Nc1ncc(s1)N(=0)=0
646	052663-66-8	hexachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1ccc(c(c1Cl)Cl)Cl)Cl	693	055985-32-5	Nicardipine	COC(=0)C1=C(C)NC(=C(C1c1cccc(c1)N(=0)=0)C(=0)OCCN(Cc1ccccc1)C)C
	050000 00 0	2,3,5,6,2',4',5'-		694	056030-54-7	Sufentanil	COCC1(CCN(CC1)CCc1cccs1)N(c1ccccc1)C(=0)CC
647	052663-68-0	heptachlorobiphenyl	Clc1cc(Cl)c(cc1c1c(Cl)cc(c1Cl)Cl)Cl	695	056180-94-0	Acarbose	OCC10C(OC2C(CO)OC(C(C2O)O)O)C(C(C1OC1OC(C)C(C(C1O)O)NC1C=C(CO)C(C(C1O)O)O)O)O
		2,3,4,6,2',4',5'-		696	056211-40-6	Torasemide	CC(NC(=0)NS(=0)(=0)c1cnccc1Nc1cccc(c1)C)C
648	052663-69-1	heptachlorobiphenyl	Clc1cc(Cl)c(cc1c1c(Cl)cc(c(c1Cl)Cl)Cl)Cl	697	056290-94-9	Medroxalol	CC(NCC(c1ccc(c(c1)C(=0)N)O)O)CCc1ccc2c(c1)OCO2
		2,3,5,6,2',3',4'-				2,4,6,2',6'-	
649	052663-70-4		Cle1ccc(c(c1Cl)Cl)c1c(Cl)c(Cl)c(c1Cl)Cl	698	056558-16-8	pentachlorobiphenyl	Clc1cc(Cl)c(c(c1)Cl)c1c(Cl)cccc1Cl
		2,3,4,6,2',3',4'-				2,4,6,3',4'-	
650	052663-71-5	heptachlorobiphenyl	Clc1c(Cl)cc(c(c1Cl)c1ccc(c(c1Cl)Cl)Cl)Cl	699	056558-17-9	pentachlorobiphenyl	Clc1cc(Cl)c(c(c1)Cl)c1ccc(c(c1)Cl)Cl
		2,4,5,3',4',5'-		700	056775-88-3	Zimelidine	CN(CC=C(c1cccnc1)c1ccc(cc1)Br)C
651	052663-72-6	hexachlorobiphenyl	Clc1cc(Cl)c(cc1c1cc(Cl)c(c(c1)Cl)Cl)Cl	701	056796-20-4	Cefmetazole	N#CCSCC(=0)NC1(OC)C(=0)N2C1SCC(=C2C(=0)0)CSc1nnnn1C
		2,3,4,5,6,2',3',6'-		702	056995-20-1	Flupirtine	CCOC(=0)Nc1ccc(nc1N)NCc1ccc(cc1)F
652	052663-73-7	octachlorobiphenyl	Cle1c(Cl)c(Cl)c(c(c1Cl)Cl)c1c(Cl)ccc(c1Cl)Cl				

ID	CAS	Name	Canonical SMILES	ID	CAS	Name	Canonical SMILES
		2,3,4,7,8-		754	065085-01-0	Cefmenoxime	CON=C(C(=O)NC1C(=O)N2C1SCC(=C2C(=O)O)CSc1nnnn1C)c1csc(n1)N
703	057117-31-4	pentachlorodibenzofuran	Clc1cc2c(cc1Cl)oc1c2cc(Cl)c(c1Cl)Cl	755	065271-80-9	Mitoxantrone	OCCNCCNc1ccc(c2c1C(=0)c1c(C2=0)c(0)ccc10)NCCNCCO
		1,2,3,7,8-		756	065277-42-1	Ketoconazole	Clc1ccc(c(c1)Cl)C1(OCC(O1)COc1ccc(cc1)N1CCN(CC1)C(=0)C)Cn1cncc1
704	057117-41-6	pentachlorodibenzofuran	Clc1cc2c(cc1Cl)oc1c2c(Cl)c(c(c1)Cl)Cl	757	065472-88-0	Naftifine	CN(Cc1cccc2c1cccc2)CC=Cc1ccccc1
		1,2,3,6,7,8-	The second secon			3,4,5,2',4'-	
705	057117-44-9	hexachlorodibenzofuran	Clc1cc2c(c(c1Cl)Cl)oc1c2c(Cl)c(c(c1)Cl)Cl	758	065510-44-3	pentachlorobiphenyl	Clc1ccc(c(c1)Cl)c1cc(Cl)c(c(c1)Cl)Cl
				/30	003310-44-3		
706	057460-41-0	Talinolol	OC(CNC(C)(C)C)COc1ccc(cc1)NC(=0)NC1CCCCC1			2,2',3,4,4'-	
		3,4,5,3',4'-		759	065510-45-4	Pentachlorobiphenyl	Clc1ccc(c(c1)Cl)c1ccc(c(c1Cl)Cl)Cl
707	057465-28-8	pentachlorobiphenyl	Clc1ccc(cc1Cl)c1cc(Cl)c(c(c1)Cl)Cl	760	066085-59-4	Nimodipine	COCCOC(=O)C1=C(C)NC(=C(C1c1ccccc(c1)N(=O)=O)C(=O)OC(C)C)C
708	057574-09-1	Amineptine	OC(=0)CCCCCNC1c2cccc2CCc2c1cccc2	761	066104-22-1	Pergolide	CCCN1CC(CSC)CC2C1Cc1c[nH]c3c1c2ccc3
		1,2,3,6,7,8-		762	066357-35-5	Ranitidine	CNC(=CN(=O)=O)NCCSCc1ccc(o1)CN(C)C
709	057653-85-7	hexachlorodibenzo-p-dioxin	Clc1c(Cl)cc2c(c1Cl)Oc1c(O2)c(Cl)c(c(c1)Cl)Cl	763	066722-44-9	Bisoprolol	OC(COc1ccc(cc1)COCCOC(C)C)CNC(C)C
710	057801-81-7	Brotizolam	Brc1cc2c(s1)n1c(CN=C2c2cccc2Cl)nnc1C	764	066778-36-7	Encainide	COc1ccc(cc1)C(=O)Nc1ccccc1C(CN1CCCCC1)C
711	057808-66-9	Domperidone	Clc1ccc2c(c1)[nH]c(=0)n2C1CCN(CC1)CCCn1c(=0)[nH]c2c1cccc2	765	067227-57-0	Fenoldopam	Oc1ccc(cc1)C1CNCCc2c1cc(O)c(c2Cl)O
712	058581-89-8	Azelastine	CN1CCCC(CC1)n1nc(Cc2ccc(cc2)Cl)c2c(c1=0)cccc2	766	067392-87-4	Drospirenone	0=C1CCC2(C(=C1)C1CC1C1C2CCC2(C1C1CC1C12CCC(=0)O1)C)C
				766	06/392-8/-4		0=010002(0(=01)0100101020002(0101001012000(=0)01)0)0
713	058957-92-9	Idarubicin	OC1C(N)CC(OC1C)OC1CC(O)(Cc2c1c(O)c1c(c2O)C(=O)c2c(C1=O)cccc2)C(=O)C			1,2,3,4,6,7,8-	
		2,2',4,4',5,5'-		767	067562-39-4	heptachlorodibenzofuran	Clc1cc2c(c(c1Cl)Cl)oc1c2c(Cl)c(c(c1Cl)Cl)Cl
714	059080-40-9	hexabromobiphenyl	Brc1cc(Br)c(cc1c1cc(Br)c(cc1Br)Br)Br	768	067915-31-5	Terconazole	Clc1ccc(c(c1)Cl)C1(OCC(O1)COc1ccc(cc1)N1CCN(CC1)C(C)C)Cn1cncn1
715	059122-46-2	Misoprostol	CCCCC(CC=CC1C(O)CC(=0)C1CCCCCCC(=0)OC)(O)C	769	068194-04-7	2,4,2',6'-tetrachlorobiphenyl	Clc1ccc(c(c1)Cl)c1c(Cl)cccc1Cl
716	059170-23-9	Bevantolol	COc1cc(CCNCC(COc2ccc(c2)C)O)ccc1OC			2,3,6,2',4'-	
		2,3,4,,2',4',6'-		770	068194-05-8	pentachlorobiphenyl	Clc1ccc(c(c1)Cl)c1c(Cl)ccc(c1Cl)Cl
717	059291-64-4	hexachlorobiphenyl	Clc1cc(Cl)c(c(c1)Cl)c1ccc(c(c1Cl)Cl)Cl	,,,	00015 1 05 0	2,3,6,2',4',6'-	
/1/	033231-04-4	2,4,6,3',4',5'-		771	068194-08-1	hexachlorobiphenyl	Clc1cc(Cl)c(c(c1)Cl)c1c(Cl)ccc(c1Cl)Cl
			21 - (20 / (20) / (20	//1	000194-00-1		
718	059291-65-5	hexachlorobiphenyl	Clc1cc(Cl)c(c(c1)Cl)c1cc(Cl)c(c(c1)Cl)Cl			2,3,5,6,2',6'-	
719	059467-70-8	Midazolam	Clc1ccc2c(c1)C(=NCc1n2c(C)nc1)c1ccccc1F	772	068194-09-2	hexachlorobiphenyl	Clc1cccc(c1c1c(Cl)cc(c1Cl)Cl)Cl
720	059729-31-6	Lorcainide	CC(N1CCC(CC1)N(c1ccc(cc1)Cl)C(=0)Cc1ccccc1)C			2,3,5,6,2',4'-	
721	059729-33-8	Citalopram	N#Cc1ccc2c(c1)COC2(CCCN(C)C)c1ccc(cc1)F	773	068194-13-8	hexachlorobiphenyl	Clc1ccc(c(c1)Cl)c1c(Cl)cc(c1)Cl)Cl
722	059933-66-3	Perfluorobutanesulfonic	FC(C(C(S(=O)(=O)O)(F)F)(F)F)F			2,3,4,6,2',5'-	
723	060084-10-8	Tiazofurin	OCC1OC(C(C1O)O)c1scc(n1)C(=O)N	774	068194-14-9	hexachlorobiphenyl	Clc1ccc(c(c1)c1c(Cl)cc(c(c1Cl)Cl)Cl)Cl
724	060142-96-3	Gabapentin	NCC1(CCCC1)CC(=O)O			2,3,4,5,6,2',3'-	
,	000112 30 3	2,2',3,3',5-	11001(000001)00(10)0	775	068194-16-1	heptachlorobiphenyl	Clc1cccc(c1Cl)c1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl
725	000145 20 2		(1-11(1)-11-1)-11-1(1(1)(1)(1)	//3	008134-10-1		Ciclest (Circles) Cicles (Cicles) Cicles (Cicles) Circles (Circles) Circles (Circles
725	060145-20-2	Pentachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1cccc(c1Cl)Cl)Cl			2,3,4,5,6,2',3',5'-	
		2,4,6,2',5'-		776	068194-17-2		Clc1cc(Cl)c(c(c1)c1c(Cl)c(c(c1Cl)Cl)Cl)Cl
726	060145-21-3	pentachlorobiphenyl	Clc1ccc(c(c1)c1c(Cl)cc(cc1Cl)Cl)Cl	777	068252-19-7	Pirmenol	CC1CCCC(N1CCCC(c1ccccn1)(c1ccccc1)O)C
		2,4,5,2',4',6'-		778	068291-97-4	Zonisamide	NS(=O)(=O)Cc1noc2c1cccc2
727	060145-22-4	hexachlorobiphenyl	Clc1cc(Cl)c(c(c1)Cl)c1cc(Cl)c(cc1Cl)Cl	779	068302-57-8	Amlexanox	CC(c1ccc2c(c1)c(=0)c1c(o2)nc(c(c1)C(=0)O)N)C
728	060166-93-0	Iopamidol	OCC(NC(=0)c1c(I)c(C(=0)NC(C0)C0)c(c(c1I)NC(=0)C(0)C)I)CO	780	068359-37-5	Cyfluthrin	N#CC(c1ccc(c(c1)Oc1ccccc1)F)OC(=O)C1C(C1(C)C)C=C(CI)CI
729	060282-87-3	Gestodene	C#CC1(O)C=CC2C1(CC)CCC1C2CCC2=CC(=O)CCC12	781	068373-14-8	Sulbactam	OC(=0)C1N2C(=0)CC2S(=0)(=0)C1(C)C
, 25	000202 07 5	2,2',4,4',5-	C//	782	068401-81-0	Ceftizoxime	CON=C(c1csc(n1)N)C(=0)NC1C2SCC=C(N2C1=0)C(=0)O
730	060348-60-9	Pentabromodiphenyl	Brc1ccc(c(c1)Br)Oc1cc(Br)c(cc1Br)Br	783	068693-11-8	Modafinil	NC(=0)CS(=0)C(c1ccccc1)c1ccccc1
				784		Astemizole	
731	060628-96-8	Bifonazole	c1ccc(cc1)c1ccc(cc1)C(n1ccnc1)c1ccccc1		068844-77-9		COc1ccc(cc1)CCN1CCC(CC1)Nc1nc2c(n1Cc1ccc(cc1)F)cccc2
732	060643-86-9	Vigabatrin	NC(C=C)CCC(=0)O	785	069049-73-6	Nedocromil	CCCc1c2oc(cc(=0)c2cc2c1n(CC)c(cc2=0)C(=0)0)C(=0)0
733	060719-84-8	Amrinone	O=c1[nH]cc(cc1N)c1ccncc1	786	069739-16-8	Cefodizime	CON=C(c1csc(n1)N)C(=O)NC1C(=O)N2C1SCC(=C2C(=O)O)CSc1nc(c(s1)CC(=O)O)C
		2,3,4,6,7,8-		787	069756-53-2	Halofantrine	CCCCN(CCC(c1cc2c(Cl)cc(cc2c2c1ccc(c2)C(F)(F)F)Cl)O)CCCC
734	060851-34-5	hexachlorodibenzofuran	Clc1cc2c(c(c1Cl)Cl)oc1c2cc(Cl)c(c1Cl)Cl			2,3,4,3',4',5'-	
735	060925-61-3	Ceforanide	NCc1ccccc1CC(=O)NC1C(=O)N2C1SCC(=C2C(=O)O)CSc1nnnn1CC(=O)O	788	069782-90-7	hexachlorobiphenyl	Clc1c(Cl)ccc(c1Cl)c1cc(Cl)c(c(c1)Cl)Cl
736	061270-58-4	Cefonicid	O=C(C(c1cccc1)O)NC1C(=O)N2C1SCC(=C2C(=O)O)CSc1nnnn1CS(=O)(=O)O	789	070362-45-7	2,3,6,2'-tetrachlorobiphenyl	Clc1ccccc1c1c(Cl)ccc(c1Cl)Cl
737	061477-96-1	Piperacillin	CCN1CCN(C(=0)C1=0)C(=0)NC(C(=0)NC1C(=0)N2C1SC(C2C(=0)0)(C)C)c1ccccc1	790	070362-50-4	3,4,5,4'-tetrachlorobiphenyl	Clc1ccc(cc1)c1cc(Cl)c(c(c1)Cl)Cl
738	061622-34-2	Cefotiam	CN(CCn1nnnc1SCC1=C(C(=0)0)N2C(SC1)C(C2=0)NC(=0)Cc1csc(n1)N)C	791	070424-67-8	2,3,5,3'-tetrachlorobiphenyl	Clc1ccc(c1)c1cc(Cl)cc(c1Cl)Cl
739				791	070424-07-6		
	061869-08-7	Paroxetine	Fc1ccc(cc1)C1CCNCC1COc1ccc2c(c1)OCO2			2,3,3',4',5-	
740	062571-86-2	Captopril	SCC(C(=0)N1CCCC1C(=0)0)C	792	070424-68-9	Pentachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1ccc(c(c1)Cl)Cl)Cl
741	062613-82-5	Oxiracetam	NC(=0)CN1CC(CC1=0)O			3,4,5,2',5'-	
742	062666-20-0	Progabide	NC(=0)CCCNC(=C1C=C(F)C=CC1=0)c1ccc(cc1)Cl	793	070424-70-3	pentachlorobiphenyl	Clc1ccc(c(c1)c1cc(Cl)c(c(c1)Cl)Cl)Cl
743	062796-65-0	2,4,6,2'-tetrachlorobiphenyl	Clc1cc(Cl)c(c(c1)Cl)c1ccccc1Cl	794	070458-92-3	Pefloxacin	CCn1cc(C(=O)O)c(=O)c2c1cc(N1CCN(CC1)C)c(c2)F
744	062893-19-0	Cefoperazone	CCN1CCN(C(=0)C1=0)C(=0)NC(c1ccc(cc1)0)C(=0)NC1C(=0)N2C1SCC(=C2C(=0)0)CSc1nnnn1C	795	070458-96-7	Norfloxacin	CCn1cc(C(=0)0)c(=0)c2c1cc(N1CCNCC1)c(c2)F
745	063527-52-6	Cefotaxime	CON=C(c1csc(n1)N)C(=0)NC1C(=0)N2C1SCC(=C2C(=0)0)COC(=0)C			1,2,3,4,7,8-	
746	063590-64-7	Terazosin	COc1cc2nc(nc(c2cc1OC)N)N1CCN(CC1)C(=0)C1CCCO1	796	070648-26-9	hexachlorodibenzofuran	Clc1cc2c(cc1Cl)oc1c2c(Cl)c(c(c1Cl)Cl)Cl
746		Nilutamide	O=C1NC(C(=0)N1c1ccc(c(c1)C(F)(F)F)N(=0)=0)(C)C	790	070048-20-9	Cefpiramide	
	063612-50-0						Oc1ccc(cc1)C(C(=0)NC1C(=0)N2C1SCC(=C2C(=0)0)CSc1nnnn1C)NC(=0)c1c[nH]c(cc1=0)C
748	063659-18-7	Betaxolol	OC(COc1ccc(cc1)CCOCC1CC1)CNC(C)C	798	071195-58-9	Alfentanil	COCC1(CCN(CC1)CCn1nnn(c1=0)CC)N(c1ccccc1)C(=0)CC
749	063675-72-9	Nisoldipine	COC(=0)C1=C(C)NC(=C(C1c1ccccc1N(=0)=0)C(=0)OCC(C)C)C	799	071320-77-9	Moclobemide	O=C(c1ccc(cc1)Cl)NCCN1CCOCC1
750	064221-86-9	Imipenem	CC(C1C2CC(=C(N2C1=0)C(=0)O)SCCN=CN)O	800	071620-89-8	Reboxetine	CCOc1ccccc1OC(c1ccccc1)C1OCCNC1
751	064706-54-3	Bepridil	CC(COCC(N1CCCC1)CN(c1ccccc1)Cc1ccccc1)C	801	072432-10-1	Aniracetam	COc1ccc(cc1)C(=0)N1CCCC1=0
752	064952-97-2	Moxalactam	COC1(NC(=0)C(c2ccc(cc2)0)C(=0)0)C(=0)N2C1OCC(=C2C(=0)0)CSc1nnnn1C	802	072509-76-3	Felodipine	CCOC(=0)C1=C(C)NC(=C(C1c1cccc(c1Cl)Cl)C(=0)OC)C
753	065052-63-3	Cefetamet	CON=C(c1csc(n1)N)C(=0)NC1C2SCC(=C(N2C1=0)C(=O)O)C	803	072599-27-0	Miglustat	CCCCN1CC(O)C(C(C1CO)O)O
						=	

ID	CAS	Name	Canonical SMILES	ID	CAS	Name	Canonical SMILES
804	072956-09-3	Carvedilol	COc1ccccc1OCCNCC(COc1cccc2c1c1ccccc1[nH]2)O	858	081409-90-7	Cabergoline	C=CCN1CC(CC2C1Cc1c[nH]c3c1c2ccc3)C(=O)N(C(=O)NCC)CCCN(C)C
805	073334-07-3	Iopromide	COCC(=0)Nc1c(I)c(C(=0)NCC(CO)O)c(c(c1I)C(=0)N(CC(CO)O)C)I	859	081447-80-5	Diprafenone	CCC(NCC(COc1ccccc1C(=O)CCc1ccccc1)O)(C)C
806	073384-59-5	Ceftriaxone	CON=C(c1csc(n1)N)C(=0)NC1C(=0)N2C1SCC(=C2C(=0)O)CSc1nc(=0)[nH]n1C	860	081732-65-2	Bambuterol	O=C(N(C)C)Oc1cc(cc(c1)OC(=O)N(C)C)C(CNC(C)(C)C)O
807	073575-52-7	2,4,3',5'-tetrachlorobiphenyl	Clc1ccc(c(c1)Cl)c1cc(Cl)cc(c1)Cl	861	081801-12-9	Xamoterol	OC(COc1ccc(cc1)O)CNCCNC(=O)N1CCOCC1
808	073575-53-8	2,4,5,3'-tetrachlorobiphenyl	Clc1cccc(c1)c1cc(Cl)c(cc1Cl)Cl	862	081846-19-7	Treprostinil	CCCCCC(CCC1C(0)CC2C1Cc1cccc(c1C2)OCC(=0)0)0
		2,3,6,2',6'-		863	081965-43-7	SarCNU	CC(C(=O)N)NC(=O)N(N=O)CCCI
809	073575-54-9	pentachlorobiphenyl	Clc1ccc(c(c1c1c(Cl)cccc1Cl)Cl)Cl	864	082009-34-5	Cilastatin	OC(=0)C(CSCCCCC=C(C(=0)O)NC(=0)C1CC1(C)C)N
		2,3,5,2',6'-		865	082619-04-3	Cefpodoxime	CON=C(c1csc(n1)N)C(=0)NC1C2SCC(=C(N2C1=0)C(=0)O)COC
810	073575-55-0	pentachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1c(Cl)cccc1Cl)Cl	866	082626-48-0	Zolpidem	Cc1ccc(cc1)c1nc2n(c1CC(=0)N(C)C)cc(cc2)C
		2,3,4,2',6'-		867	082768-85-2	Quinaprilat	CCOC(=O)C(NC(C(=O)N1Cc2ccccc2CC1C(=O)O)C)CCc1ccccc1
811	073575-57-2	pentachlorobiphenyl	Clc1c(Cl)ccc(c1Cl)c1c(Cl)cccc1Cl	868	083015-26-3	Atomoxetine	CNCCC(c1ccccc1)Oc1ccccc1C
812	073963-72-1	Cilostazol	O=C1CCc2c(N1)ccc(c2)OCCCCc1nnnn1C1CCCCC1	869	083366-66-9	Nefazodone	CCc1nn(c(=0)n1CCOc1ccccc1)CCCN1CCN(CC1)c1cccc(c1)Cl
813	074011-58-8	Enoxacin	CCn1cc(C(=0)0)c(=0)c2c1nc(N1CCNCC1)c(c2)F	870	083647-97-6	Spirapril	CCOC(=O)C(NC(C(=O)N1CC2(CC1C(=O)O)SCCS2)C)CCc1ccccc1
814	074050-98-9	Ketanserin	Fc1ccc(cc1)C(=0)C1CCN(CC1)CCn1c(=0)[nH]c2c(c1=0)cccc2	871	083799-24-0	Fexofenadine	OC(=0)C(c1ccc(cc1)C(CCCN1CCC(CC1)C(c1ccccc1)(c1ccccc1)O)O)(C)C
815	074103-06-3	Ketorolac	OC(=0)C1CCn2c1ccc2C(=0)c1ccccc1	872	083881-51-0	Cetirizine	OC(=0)COCCN1CCN(CC1)C(c1ccc(cc1)Cl)c1ccccc1
816	074150-27-9	Pimobendan	COc1ccc(cc1)c1nc2c([nH]1)cc(cc2)C1=NNC(=0)CC1C	873	084057-84-1	Lamotrigine	Nc1nnc(c(n1)N)c1cccc(c1Cl)Cl
817	074191-85-8	Doxazosin	COc1cc2nc(nc(c2cc1OC)N)N1CCN(CC1)C(=0)C1COc2c(O1)cccc2	874	084057-95-4	Ropivacaine	CCCN1CCCC1C(=0)Nc1c(C)cccc1C
818	074338-24-2	2,3,4,3'-tetrachlorobiphenyl	Clc1cccc(c1)c1ccc(c(c1Cl)Cl)Cl	875	084371-65-3	Mifepristone	CC#CC1(O)CCC2C1(C)CC(c1ccc(cc1)N(C)C)C1=C3CCC(=O)C=C3CCC21
819	074472-34-7	2,3,5,4'-tetrachlorobiphenyl	Clc1ccc(cc1)c1cc(Cl)cc(c1Cl)Cl	876	084449-90-1	Raloxifene	Oc1ccc2c(c1)sc(c2C(=O)c1ccc(cc1)OCCN1CCCCC1)c1ccc(cc1)O
		2,3,4,5,4'-		877	084625-61-6	Itraconazole	CCC(n1ncn(c1=0)c1ccc(cc1)N1CCN(CC1)c1ccc(cc1)OCC1COC(O1)(Cn1cncn1)c1ccc(cc1Cl)Cl)C
820	074472-37-0	pentachlorobiphenyl	Clc1ccc(cc1)c1cc(Cl)c(c(c1Cl)Cl)Cl	878	085405-59-0	Hydroxydihydroquinidine,	CCC1(O)CN2CCC1CC2C(c1ccnc2c1cc(OC)cc2)O
		2,3,4,6,3',4'-		879	085441-61-8	Quinapril	CCOC(=O)C(NC(C(=O)N1Cc2ccccc2CC1C(=O)O)C)CCc1ccccc1
821	074472-42-7	hexachlorobiphenyl	Clc1ccc(cc1Cl)c1c(Cl)cc(c(c1Cl)Cl)Cl	880	085622-93-1	Temozolomide	NC(=0)c1ncn2c1nnn(c2=0)C
		2,3,5,6,2',4'-		881	085650-52-8	Mirtazapine	CN1CCN2C(C1)c1ccccc1Cc1c2nccc1
822	074472-44-9	hexachlorobiphenyl	Clc1cc(ccc1Cl)c1c(Cl)c(Cl)cc(c1Cl)Cl	882	085721-33-1	Ciprofloxacin	Fc1cc2c(cc1N1CCNCC1)n(cc(c2=0)C(=0)0)C1CC1
		2,3,4,6,3',4',5'-		883	086386-73-4	Fluconazole	Fc1ccc(c(c1)F)C(Cn1cncn1)(Cn1cncn1)O
823	074472-50-7	heptachlorobiphenyl	Clc1cc(Cl)c(c(c1c1cc(Cl)c(c(c1)Cl)Cl)Cl)Cl	884	086541-75-5	Benazepril	CCOC(=O)C(NC1CCc2c(N(C1=O)CC(=O)O)cccc2)CCc1ccccc1
		2,3,4,5,6,3',4',5'-		885	087333-19-5	Ramipril	CCOC(=O)C(NC(C(=O)N1C2CCC2CC1C(=O)O)C)CCc1ccccc1
824	074472-51-8	octachlorobiphenyl	Clc1cc(Cl)cc(c1)c1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl	886	087638-04-8	Carumonam	NC(=0)OCC1C(NC(=0)C(=NOCC(=0)O)c2csc(n2)N)C(=0)N1S(=0)(=0)O
		2,3,4,5,6,2',4',6'-		887	087679-37-6	Trandolapril	CCOC(=O)C(NC(C(=O)N1C2CCCC2CC1C(=O)O)C)CCc1ccccc1
825	074472-52-9	octachlorobiphenyl	Clc1cc(Cl)c(c(c1)Cl)c1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl	888	087726-17-8	Panipenem	CC(C1C(=O)N2C1CC(=C2C(=O)O)SC1CCN(C1)C(=N)C)O
826	074738-24-2	Recainam	CC(NCCCNC(=O)Nc1c(C)cccc1C)C	889	087810-56-8	Fostriecin	OCC=CC=CC(CC(C(C=CC1CC=CC(=0)01)(0)C)OP(=0)(0)0)0
827	074863-84-6	Argatroban	NC(=NCCCC(C(=0)N1CCC(CC1C(=0)O)C)NS(=0)(=0)c1cccc2c1NCC(C2)C)N	890	088150-42-9	Amlodipine	NCCOCC1 = C(C(=0)OCC)C(C(=C(N1)C)C(=0)OC)c1ccccc1CI
828	075225-51-3	Lovastatin	CCC(C(=0)OC1CC(C)C=C2C1C(CCC(CC(CC(=0)O)O)O)C(C=C2)C)C	891	088669-04-9	Trospectomycin	CCCCC1OC2OC3C(O)C(NC)C(C(C3OC2(C(=0)C1)O)NC)O
829	075330-75-5	Lovastatin	CCC(C(=O)OC1CC(C)C=C2C1C(CCC1CC(O)CC(=O)O1)C(C=C2)C)C	892	089194-77-4	Bisaramil	CCN1CC2CN(CC(C1)C2OC(=0)c1ccc(cc1)Cl)C
830	075607-67-9	Fludarabine	OC1C(O)C(OC1n1cnc2c1nc(F)nc2N)COP(=0)(O)O	893	089365-50-4	Salmeterol	OCc1cc(ccc10)C(CNCCCCCOCCCc1ccccc1)O
831	075695-93-1	Isradipine	COC(=O)C1=C(C)NC(=C(C1c1cccc2c1non2)C(=O)OC(C)C)C	894	089565-68-4	Tropisetron	CN1C2CCC1CC(C2)OC(=0)c1c[nH]c2c1cccc2
832	075696-02-5	Cinolazepam	N#CCCN1C(=0)C(0)N=C(c2c1ccc(c2)Cl)c1ccccc1F	895	089778-26-7	Toremifene	CICCC(=C(c1ccccc1)c1ccc(cc1)OCCN(C)C)c1ccccc1
833	075706-12-6	Leflunomide	O=C(c1cnoc1C)Nc1ccc(cc1)C(F)(F)F	896	090357-06-5	Bicalutamide	N#Cc1ccc(cc1C(F)(F)F)NC(=0)C(CS(=0)(=0)c1ccc(cc1)F)(0)C
834	075803-36-0	Ethinylestradiol-17-Sulfate	C#CC1(CCC2C1(C)CCC1C2CCc2c1ccc(c2)O)OS(=O)(=O)O	897	090402-40-7	Abanoquil	COc1cc2CCN(Cc2cc1OC)c1cc(N)c2c(n1)cc(c(c2)OC)OC
835	075847-73-3	Enalapril	CCOC(=O)C(NC(C(=O)N1CCCC1C(=O)O)C)CCc1ccccc1	898	091161-71-6	Terbinafine	CN(Cc1cccc2c1cccc2)CC=CC#CC(C)(C)C
836	076420-72-9	Enalaprilat	OC(=O)C(NC(C(=O)N1CCCC1C(=O)O)C)CCc1ccccc1	899	091374-21-9	Ropinirole	CCCN(CCC)CCc1cccc2c1CC(=O)N2
837	076470-66-1	Loracarbef	NC(c1cccc1)C(=0)NC1C2CCC(=C(N2C1=0)C(=0)0)Cl	900	091421-43-1	Aminocamptothecin,	CCC1(0)C(=0)OCc2c1cc1c3nc4cccc(c4cc3Cn1c2=0)N
	076547-98-3	Lisinopril	NCCCC(C(=0)N1CCCC1C(=0)0)NC(C(=0)0)CCc1ccccc1	901	091714-94-2	Bromfenac	OC(=O)Cc1cccc(c1N)C(=O)c1ccc(cc1)Br
839	076824-35-6	Famotidine	NC(=Nc1scc(n1)CSCCC(=NS(=O)(=O)N)N)N	902	091832-40-5	Cefdinir	ON=C(c1csc(n1)N)C(=O)NC1C(=O)N2C1SCC(=C2C(=O)O)C=C
		3,4,5,2',3'-		903	092623-85-3	Milnacipran	NCC1CC1(c1ccccc1)C(=O)N(CC)CC
840	076842-07-4	pentachlorobiphenyl	Clc1c(Cl)cccc1c1cc(Cl)c(c(c1)Cl)Cl	904	092665-29-7	Cefprozil	CC=CC1=C(C(=0)O)N2C(SC1)C(C2=O)NC(=0)C(c1ccc(cc1)O)N
841	077337-76-9	Acamprosate	CC(=O)NCCCS(=O)(=O)O	905	093390-81-9	Fosphenytoin	O=C1N(COP(=0)(O)O)C(=O)NC1(c1ccccc1)c1ccccc1
842	077671-31-9	Enoximone	CSc1ccc(cc1)C(=0)c1[nH]c(=0)[nH]c1C	906	093413-69-5	Venlafaxine	COc1ccc(cc1)C(C1(O)CCCCC1)CN(C)C
843	078415-72-2	Milrinone	N#Cc1cc(c2ccncc2)c([nH]c1=0)C	907	093479-97-1	Glimepiride	CCC1=C(C)CN(C1=0)C(=0)NCCc1ccc(cc1)S(=0)(=0)NC(=0)NC1CCC(CC1)C
	078755-81-4	Flumazenil	CCOC(=0)clncn2c1CN(C)C(=0)c1c2ccc(c1)F	908	093957-54-1	Fluvastatin	OC(=0)CC(CC(C=Cc1c(c2ccc(cc2)F)c2c(n1C(C)C)cccc2)0)0
-	078919-13-8	lloprost	CC#CCC(C(C=CC1C(O)CC2C1CC(=C)OCC(=O)oCc(=O)c1ccccc1)C2)O)C	909	094079-80-8	Cicaprost	CCC#CCC(C(C#CC1C(0)CC2C1CC(=COCC(=O)O)C2)O)C
	079350-37-1	Cefixime	Nc1nc(cs1)C(=NOCC(=0)O)C(=0)Nc1C2SCC(=C(N2C1=0)C(=0)O)C=C	910	095153-31-4	Perindoprilat	CCCC(C(=0)0)NC(C(=0)N1C2CCCC2CC1C(=0)0)C
847	079617-96-2	Sertraline	CNC1CCC(c2c1cccc2)c1ccc(c(c1)Cl)Cl	911	095399-71-6	Fosinoprilat	OC(=0)C1CC(CN1C(=0)CP(=0)(CCCCc1ccccc1)0)C1CCCC1
848	079660-72-3	Fleroxacin	FCCn1cc((=0)0)c(=0)c2c1(F)c(N1CCN(CC1)C)c(c2)F	912	095415-91-1	Sch34343	CC(C1C2SC(=C(N2C1=0)C(=0)O)SCCOC(=0)N)O
849	079794-75-5	Loratadine	CCOC(=0)N1CCC(=C2c3ccc(cc3CCc3c2nccc3)Cl)CC1	913	096036-03-2	Meropenem	CC(C1C(=0)N2C1C(C)C(=C2C(=0)O)SC1CCC(N1)C(=0)N(C)C)O
850	079902-63-9	Simvastatin	CCC(C(=0)0C1CC(C)C=C2C1C(CCC1CC(0)CC(=0)01)C(C=C2)C)(C)C	914	096829-58-2	Orlistat	CCCCCCCCCC(CC1OC(=0)C1CCCCC)OC(=0)C(CC(C)C)NC=0
	079944-58-4	Idazoxan	C1CN=C(N1)C1COc2c(O1)cccc2	915	097240-79-4	Topiramate	NS(=0)(=0)0CC120CC3C(C20C(01)(C)C)0C(03)(C)C
852	080125-14-0	Remoxipride	CCN1CCCC1CNC(=0)c1c(OC)ccc(c1OC)Br	916	097322-87-7	Troglitazone	0=C1NC(=0)C(S1)Cc1ccc(cc1)OCC1(C)CCc2c(O1)c(C)c(c(c2C)O)C
853	080474-14-2	Fluticasone	FCSC(=0)C1(OC(=0)CC)C(C)CC2C1(C)CC(O)C1(C2CC(C2=CC(=0)C=CC12C)F)F	917	097682-44-5	Irinotecan	CCC1(O)C(=O)OCc2c1cc1c3nc4ccc(cc4c(c3Cn1c2=O)CC)OC(=O)N1CCC(CC1)N1CCCCC1
854	080755-51-7	Bunazosin	CCCC(=0)N1CCCN(CC1)c1nc(N)c2c(n1)cc(c(c2)OC)OC	918	098048-97-6	Fosinopril	CCC(=0)OC(C(C)C)OP(=0)(CC(=0)N1CC(CC1C(=0)O)C1CCCCC1)CCCC1cccc1
855	081093-37-0	Pravastatin	CCC(C(=0)0C1CC(0)C=C2C1C(CCC(CC(CC(=0)0)0)O)C(C=C2)C)C	919	098079-51-7	Lomefloxacin	CCn1cc(C(=0)0)c(=0)c2c1c(F)c(N1CCNC(C1)C)c(c2)F
856	081093-37-0	Esmolol	COC(=0)CCc1ccc(cc1)OCC(CNC(C)C)O	920	098319-26-7	Finasteride	0=C1C=CC2(C(N1)CCC1C2CCC2(C1CCC2C(=0)NC(C)(C)C)C
857	081403-80-7	Alfuzosin	COc1cc2nc(nc(c2cc1OC)N)N(CCCNC(=0)C1CCCO1)C	921	099011-02-6	Imiguimod	CC(Cn1cnc2c1c1ccccc1nc2N)C
037	201403-00-7	4203111		321	333011-02-0	quiiiou	00(01120102202100002110211)0

ID	CAS	Name	Canonical SMILES	ID	CAS	Name	Canonical SMILES
922	099614-02-5	Ondansetron	O=C1C(CCc2cicicccccin2C)CniccnciC	986	129453-61-8	Fulvestrant	O=S(CCCC(C(F)(F)F)(F)F)CCCCCCCCCCCCCCCCCCC
923	100643-71-8	Desloratadine	Clc1ccc2c(c1)CCc1c(C2=C2CCNCC2)nccc1	987	129618-40-2	Nevirapine	Cc1ccnc2c1[nH]c(=0)c1c(n2C2CC2)nccc1
924	100986-85-4	Levofloxacin	CN1CCN(CC1)c1c(F)cc2c3c10CC(n3cc(c2=0)C(=0)0)C 988 129722-12-9 Aripiprazole 0=C1CCc2c(N1)cc(cc2)OCCCCN1CCN(CC1)c1cccc(c1Cl)Cl				
925	101526-83-4	Sematilide			OC(CCc1ccccc1)CCC1C(O)CC(C1CC=CCCCC(=O)OC(C)C)O		
926	101828-21-1	Butenafine	CN(Cc1cccc2c1cccc2)Cc1ccc(cc1)C(C)(C)C 990 130929-57-6 Entacapone			CCN(C(=O)C(=Cc1cc(O)c(c(c1)N(=O)=O)O)C#N)CC	
927	102767-28-2	Levetiracetam	CCC(N1CCCC1=0)C(=0)N	991	131918-61-1	Paricalcitol	OC1CC(O)CC(=CC=C2CCCC3(C2CCC3C(C=CC(C(O)(C)C)C)C)C)C1
928	103577-45-3	Lansoprazole	O=S(c1nc2c([nH]1)cccc2)Cc1nccc(c1C)OCC(F)(F)F	992	132539-06-1	Olanzapine	CN1CCN(CC1)C1=c2cc(sc2=Nc2c(N1)cccc2)C
929	103628-46-2	Sumatriptan	CNS(=0)(=0)Cc1ccc2c(c1)c(CCN(C)C)c[nH]2	993	132875-61-7	Remifentanil	COC(=0)C1(CCN(CC1)CCC(=0)OC)N(c1ccccc1)C(=0)CC
930	103775-10-6	Moexipril	CCOC(=0)C(NC(C(=0)N1Cc2cc(OC)c(cc2CC1C(=0)0)OC)C)Cc1ccccc1	994	133040-01-4	Eprosartan	CCCCc1ncc(n1Cc1ccc(cc1)C(=0)0)C=C(C(=0)0)Cc1cccs1
931 932	104227-87-4 104632-26-0	Famciclovir Pramipexole	CC(=0)OCC(CCn1cnc2c1nc(N)nc2)COC(=0)C CCCNC1CCc2c(C1)sc(n2)N	995 996	133099-04-4 133163-28-7	Darifenacin Midodrine	NC(=0)C(c1ccccc1)(c1ccccc1)C1CCN(C1)CCc1ccc2c(c1)CCO2 COc1ccc(cc1C(CNC(=0)CN)O)OC
933	105102-22-5	Mometasone	CICC(=0)C1(0)C(C)CC2C1(C)CC(0)C1(C2CCC2=CC(=0)C=CC12C)CI	997	134234-12-1	Traxoprodil	Oc1ccc(cc1)C(C(N1CCC(CC1)(O)c1ccccc1)C)O
934	105816-04-4	Nateglinide	CC(C1CCC(CC1)C(=0)NC(C(=0)O)Cc1ccccc1)C	998	134308-13-7	Tolcapone	Cc1ccc(cc1)C(=0)c1cc(0)c(c(c1)N(=0)=0)0
935	105956-97-6	Clinafloxacin	NC1CCN(C1)c1c(F)cc2c(c1C1)n(cc(c2=0)C(=0)0)C1CC1	999	134523-00-5	Atorvastatin	OC(CC(CC(=0)O)O)CCn1c(C(C)C)c(c(c1c1ccc(cc1)F)c1ccccc1)C(=0)Nc1ccccc1
936	106133-20-4	Tamsulosin	CCOclecccc1OCCNC(Cclccc(c(c1)S(=O)(=O)N)OC)C	1000	134678-17-4	Lamivudine	Nc1ccn(c(=0)n1)C1CSC(01)CO
937	106266-06-2	Risperidone	Fc1ccc2c(c1)onc2C1CCN(CC1)CCc1c(C)nc2n(c1=0)CCCC2	1001	135062-02-1	Repaglinide	CCOc1cc(ccc1C(=0)O)CC(=0)NC(c1ccccc1N1CCCCC1)CC(C)C
938	106516-24-9	Sertindole	Clc1ccc2c(c1)c(cn2c1ccc(cc1)F)C1CCN(CC1)CCN1CCNC1=O	1002	135729-61-2	Palonosetron	O=C1N(CC2c3c1cccc3CCC2)C1CN2CCC1CC2
939	106650-56-0	Sibutramine	CC(CC(C1(cCC1)c1ccc(cc1)Cl)N(C)C)C	1003	136434-34-9	Duloxetine	CNCCC(c1cccs1)Oc1cccc2c1cccc2
940	106941-25-7	Adefovir	Nc1ncnc2c1ncn2CCOCP(=0)(0)0	1004	136470-78-5	Abacavir	OCC1C=CC(C1)n1cnc2c1nc(N)nc2NC1CC1
941	107133-36-8	Perindopril	CCCC(C(=0)OCC)NC(C(=0)N1C2CCCC2CC1C(=0)O)C	1005	136790-76-6	Lubiprostone	CCCCC(C1(O)CCC2C(O1)CC(=O)C2CCCCCC(=O)O)(F)F
942	107233-08-9	Cevimeline	CC1SCC2(O1)CN1CCC2CC1	1006	136817-59-9	Delavirdine	CC(Nc1cccnc1N1CCN(CC1)C(=0)c1cc2c([nH]1)ccc(c2)NS(=0)(=0)C)C
943	107724-20-9	Eplerenone	COC(=0)C1CC2=CC(=0)CCC2(C23C1C1CCC4(C1(C)CC3O2)CCC(=0)O4)C	1007	137234-62-9	Voriconazole	Fc1ccc(c(c1)F)C(C(c1ncncc1F)C)(Cn1cncn1)O
944	107753-78-6	Zafirlukast	COc1cc(ccc1Cc1cn(c2c1cc(cc2)NC(=0)OC1CCCC1)C)C(=0)NS(=0)(=0)c1ccccc1C	1008	137862-53-4	Pravastatin	CCCCC(=O)N(C(C(=O)O)C(C)C)Cc1ccc(cc1)c1ccccc1c1n[nH]nn1
945	107868-30-4	Exemestane	O=C1C=CC2(C(=C1)C(=C)CC1C2CCC2(C1CCC2=O)C)C	1009	139110-80-8	Zanamivir	OCC(C(10C(=CC(C1NC(=O)C)N=C(N)N)C(=O)O)O
946	108319-06-8	Temafloxacin	CC1NCCN(C1)c1cc2n(cc(c(=0)c2cc1F)C(=0)0)c1ccc(cc1F)F	1010	139264-17-8	Zolmitriptan	CN(CCc1c[nH]c2c1cc(CC1COC(=0)N1)cc2)C
947	109889-09-0	Granisetron	CN1C2CCC1CC(C2)NC(=0)c1nn(c2c1cccc2)C	1011	139481-59-7	Candesartan	CCOc1nc2c(n1Cc1ccc(cc1)c1cccc1c1n[nH]nn1)c(ccc2)C(=0)O
948 949	110871-86-8 111025-46-8	Sparfloxacin Pioglitazone	CC1NC(C)CN(C1)c1c(F)c(N)c2c(c1F)n(cc(c2=0)C(=0)0)C1CC1 CCc1ccc(nc1)CC0c1ccc(cc1)CC1SC(=0)NC1=0	1012 1013	139755-83-2 141505-33-1	Sildenafil Levosimendan	CCCc1nn(c2c1[nH]c(nc2=0)c1cc(ccc10CC)S(=0)(=0)N1CCN(CC1)C)C N#CC(=NNc1ccc(cc1)C1=NNC(=0)CC1C)C#N
949	111025-46-8	Zileuton	ON(C(c1cc2c(s1)ccc2)C)C(=O)N	1013	141505-33-1	Adefovir	O=C(C(C)(C)C)COCOP(=0)(CCC(=0)C(C)(C)C)COCCn1cnc2c1ncnc2N
950	111974-69-7	Quetiapine	OCCOCCN1CCN(CC1)C1=Nc2ccccc2Sc2c1cccc2	1014	142373-60-2	Tirofiban	CCCCS(=0)(=0)NC(C(=0)0)Cc1ccc(cc1)OCCCCC1CCNCC1
952	112809-51-5	Letrozole	N#Cc1ccc(cc1)C(n1cncn1)c1ccc(cc1)C#N	1015	142373-00-2	Ranolazine	COc1cccc1OCC(CN1CCN(CC1)CC(=0)Nc1c(C)cccc1C)O
953	112811-59-3	Gatifloxacin	COc1c(N2CCNC(C2)C)c(F)cc2c1n(cc(c2=0)C(=0)0)C1CC1	1017	143322-58-1	Eletriptan	CN1CCCC1Cc1c[nH]c2c1cc(cc2)CCS(=0)(=0)c1ccccc1
954	112953-11-4	Hydroxystaurosporine,	CNC1CC2OC(C10C)(C)n1c3cccc3c3c1c1n2c2cccc2c1c1c3C(NC1=0)0	1018	143443-90-7	Ifetroban	CCCCCNC(=0)c1coc(n1)C1C2CCC(C1Cc1ccccc1CCC(=0)0)02
955	113665-84-2	Clopidogrel	COC[=0)C[c1ccccc1Cl)N1CCc2c(C1)ccs2	1019	143491-57-0	Emtricitabine	Nc1nc(=O)n(cc1F)C1CSC(O1)CO
956	113806-05-6	Olopatadine	CN(CCC=C1c2cc(ccc2OCc2c1cccc2)CC(=O)O)C	1020	144034-80-0	Rizatriptan	CN(CCc1c[nH]c2c1cc(cc2)Cn1cncn1)C
957	113852-37-2	Cidofovir	OCC(Cn1ccc(nc1=0)N)OCP(=0)(0)O	1021	144412-49-7	Lamifiban	OC(=0)COC1CCN(CC1)C(=0)C(NC(=0)c1ccc(cc1)C(=N)N)Cc1ccc(cc1)O
958	114899-77-3	Trabectedin	COc1cc2c(cc10)CCNC12CSC2c3c(OC(=0)C)c(C)c4c(c3C(COC1=0)N1C2C2N(C(C10)Cc1c2c(0)c(c(c1)C)OC)COC4	1022	144598-75-4	Paliperidone	Fc1ccc2c(c1)onc2C1CCN(CC1)CCc1c(C)nc2n(c1=0)CCCC2O
959	115103-54-3	Tiagabine	OC(=0)C1CCCN(C1)CCC=C(c1sccc1C)c1sccc1C	1023	144701-48-4	Telmisartan	CCCc1nc2c(n1Cc1ccc(cc1)c1ccccc1C(=0)0)cc(cc2C)c1nc2c(n1C)cccc2
960	115256-11-6	Dofetilide	CN(CCc1ccc(cc1)NS(=0)(=0)C)CCOc1ccc(cc1)NS(=0)(=0)C	1024	144980-29-0	Repinotan	O=C1c2cccc2S(=O)(=O)N1CCCCNCC1CCc2c(O1)cccc2
961	115956-12-2	Dolasetron	O=C1CN2C3CC1CC2CC(C3)OC(=O)c1c[nH]c2c1cccc2	1025	145108-58-3	Dexmedetomidine	Cc1cccc(c1C)C(c1cnc[nH]1)C
962	116644-53-2	Mibefradil	COCC(=0)OC1(CCN(CCCc2nc3c([nH]2)cccc3)C)CCc2c(C1C(C)C)ccc(c2)F	1026	145158-71-0	Tegaserod	CCCCCNC(=N)NN=Cc1c[nH]c2c1cc(OC)cc2
963	117467-28-4	Cefditoren	CON=C(c1csc(n1)N)C(=0)NC1C(=0)N2C1SCC(=C2C(=0)OCOC(=0)C(C)(C)C)C=Cc1scnc1C	1027	145599-86-6	Cerivastatin	COCc1c(c2ccc(cc2)F)c(C=CC(CC(CC(=O)O)O)O)c(nc1C(C)C)C(C)C
964	117976-89-3	Rabeprazole	COCCCOc1ccnc(c1C)CS(=O)c1nc2c([nH]1)cccc2	1028	145918-75-8	Troxacitabine	Nc1ccn(c(=0)n1)C1COC(01)CO
965	118292-40-3	Tazarotene	CCOC(=0)c1ccc(nc1)C#Cc1ccc2c(c1)C(C)(C)CCS2	1029	146426-40-6	Flavopiridol	CN1CCC(C(C1)0)c1c(0)cc(c2c1oc(cc2=0)c1ccccc1Cl)0
966 967	118457-14-0 119169-78-7	Nebivolol Epristeride	OC(C1CCc2c(O1)ccc(c2)F)CNCC(C1CCc2c(O1)ccc(c2)F)O OC(=0)C1=CC2=CCC3C(C2(CC1)C)CCC1(C3CCC1C(=0)NC(C)(C)C)C	1030 1031	146939-27-7 147059-72-1	Ziprasidone Trovafloxacin	O=C1Nc2c(C1)cc(c(c2)Cl)CCN1CCN(CC1)c1nsc2c1ccc2 NC1C2C1CN(C2)c1nc2c(cc1F)c(=0)c(cn2c1ccc(cc1F)F)C(=0)O
967	119169-78-7	Dexloxiglumide	CCCCCN(C(=0)C(NC(=0)c1ccc(c(c1)Cl)Cl)CCC(=0)0)CCCOC	1031	147059-72-1	Tenofovir	CC(Cn1cnc2c1ncnc2N)OCP(=0)(0)O
969	119914-60-2	Grepafloxacin	CC1NCCN(C1)c1cc2c(c(c1F)C)c(=0)c(cn2C1CC1)C(=0)O	1032	147536-97-8	Bosentan	OCCOc1nc(nc(c10c1ccccc10C)NS(=0)(=0)c1ccc(cc1)C(C)(C)C1ncccn1
970	120014-06-4	Donepezil	COc1cc2c(cc1OC)CC(C2=0)CC1CCN(CC1)Cc1cccc1	1033	148553-50-8	Pregabalin	NCC(CC(=0)O)CC(C)C
971	120054-86-6	Dexniguldipine	CCCN1C(=C(C(=0)ON2CCC(CC2)(c2ccccc2)c2ccccc2)C(C(=C1C)C(=0)OC)c1cccc(c1)N(=0)=0)C	1035	148717-90-2	Squalamine	NCCCCNCCCNC1CCC2(C(C1)CC(C1C2CCC2(C1CCC2C(CCC(C(C)C)OS(=O)(=O)O)C)C)O)C
972	120443-16-5	Verlukast	OC(=O)CCSC(c1cccc(c1)C=Cc1ccc2c(n1)cc(cc2)Cl)SCCC(=O)N(C)C	1036	149647-78-9	Vorinostat	ONC(=0)CCCCCC(=0)Nc1ccccc1
	120511-73-1	Anastrozole	N#CC(c1cc(cc(c1)C(C#N)(C)C)Cn1ncnc1)(C)C	1037	149908-53-2	Azimilide	CN1CCN(CC1)CCCCN1C(=O)CN(C1=O)N=Cc1ccc(o1)c1ccccc1
974	120924-80-3	Genaconazole	Fc1ccc(c(c1)F)C(C(S(=O)(=O)C)C)(Cn1cncn1)O	1038	150378-17-9	Indinavir	OC(CN1CCN(CC1C(=O)NC(C)(C)C)Cc1cccnc1)CC(C(=O)NC1C(O)Cc2c1cccc2)Cc1ccccc1
975	121032-29-9	Nelarabine	OCC1OC(C(C10)O)n1cnc2c1nc(N)nc2OC	1039	151096-09-2	Moxifloxacin	COc1c(N2CC3C(C2)CCCN3)c(F)cc2c1n(cc(c2=O)C(=O)O)C1CC1
976	121679-13-8	Naratriptan	CNS(=O)(=O)CCc1ccc2c(c1)c(c[nH]2)C1CCN(CC1)C	1040	151276-95-8	KRN-5500	CCCCCCCCCCCCCCC(=O)NCC(=O)NC1C(OC(C(C1O)O)Nc1ncnc2c1[nH]cn2)C(CO)O
977	122320-73-4	Rosiglitazone	O=C1NC(=0)C(S1)Cc1ccc(cc1)OCCN(c1ccccn1)C	1041	151319-34-5	Zaleplon	CCN(c1cccc(c1)c1ccnc2n1ncc2C#N)C(=O)C
978	122647-31-8	Ibutilide	CCCCCCCN(CCCC(c1ccc(cc1)NS(=0)(=0)C)O)CC	1042	152459-95-5	Imatinib	CN1CCN(CC1)Cc1ccc(cc1)C(=O)Nc1ccc(c(c1)Nc1nccc(n1)c1cccnc1)C
979	123318-82-1	Clofarabine	OCC1OC(C(C10)F)n1cnc2c1nc(Cl)nc2N	1043	153259-65-5	Cilomilast	N#CC1(CCC(CC1)C(=0)0)c1ccc(c(c1)OC1CCCC1)OC
980	123441-03-2	Rivastigmine	CCN(C(=O)Oc1cccc(c1)C(N(C)C)C)C	1044	153559-49-0	Bexarotene	Cc1cc2c(cc1C(=C)c1ccc(cc1)C(=O)O)C(C)(C)CCC2(C)C
	123948-87-8	Topotecan	CCC1(O)C(=O)OCc2c1cc1c3nc4ccc(c(c4cc3Cn1c2=O)CN(C)C)O	1045	153832-46-3	Ertapenem	O=C(C1NCC(C1)SC1=C(C(=0)O)N2C(C1C)C(C2=O)C(O)C)Nc1cccc(c1)C(=O)O
982	124937-51-5	Tolterodine	Cc1ccc(c(c1)C(c1ccccc1)CCN(C(C)C)C(C)C)O	1046	154323-57-6	Almotriptan	CN(CCc1c[nH]c2c1cc(cc2)CS(=0)(=0)N1CCCC1)C
983	125974-72-3	Intoplicine	CN(CCCNc1ncc(c2c1c1c([nH]2)ccc2c1ccc(c2)0)C)C	1047	154361-50-9	Capecitabine	CCCCCOC(=0)Nc1nc(=0)n(cc1F)C1OC(C(C10)0)C
984 985	127779-20-8 128470-16-6	Saquinavir Arbutamine	$NC(=0)CC(C(=0)NC(C(CN1CC2CCCC2CC1C(=0)NC(C)(C)C)O)Cc1ccccc1)NC(=0)c1ccc2c(n1)cccc2\\ Oc1ccc(cc1)CCCCNCC(c1ccc(c(c1)O)O)O$	1048 1049	154397-77-0 154598-52-4	Napsagatran Efavirenz	O=C(CC(C(=0)N(C1CC1)CC(=0)O)NS(=0)(=0)c1ccc2c(c1)ccc2)NCC1CCCN(C1)C(=N)N FC(C1(C#CC2CC2)OC(=0)Nc2c1cc(C1)cc2)(F)F
985	1284/0-10-6	Aibutamine	0.16.64(1.61).0.000	1049	134598-52-4	Eldvireliz	FC(C1(C#CC2CC2)OC(=O)NC2C1CC(CI)CC2)(F)F

ID	CAS	Name	Canonical SMILES
1050	155206-00-1	Bimatoprost	CCNC(=0)CCCC=CCC1C(0)CC(C1C=CC(CCc1ccccc1)O)O
1051	155213-67-5	Ritonavir	O=C(NC(C(CC1ccccc1)NC(=0)C(C(C)C)NC(=0)N(Cc1csc(n1)C(C)C)O)OCc1ccccc1)OCc1cncs1
1052	156053-89-3	Alvimopan	OC(=0)CNC(=0)C(Cc1ccccc1)CN1CCC(C(C1)C)(C)c1cccc(c1)O
1053	156090-18-5	Topixantrone	OCCNCCn1nc2c3c1ccc(c3c(=0)c1c2cncc1)NCCN(C)C
1054	157283-68-6	Travoprost	CC(OC(=0)CCCC=CCC1C(0)CC(C1C=CC(C0c1cccc(c1)C(F)(F)F)O)O)C
1055	158681-13-1	Rimonabant	Clc1ccc(cc1)c1c(C)c(nn1c1ccc(cc1Cl)Cl)C(=0)NN1CCCCC1
1056	158747-02-5	Frovatriptan	CNC1Cc2c(CC1)[nH]c1c2cc(cc1)C(=0)N
1057	158966-92-8	Montelukast	OC(=0)CC1(CSC(c2cccc(c2)C=Cc2ccc3c(n2)cc(cc3)Cl)CCc2ccccc2C(0)(C)C)CC1
1058	159776-70-2	Melagatran	OC(=0)CNC(C(=0)N1CCC1C(=0)NCc1ccc(cc1)C(=N)N)C1CCCCC1
1059	159989-64-7	Nelfinavir	OC(C(NC(=0)c1cccc(c1C)O)CSc1ccccc1)CN1CC2CCCC2CC1C(=0)NC(C)(C)C
1060	161814-49-9	Amprenavir	CC(CN(S(=0)(=0)c1ccc(cc1)N)CC(C(cc1ccccc1)NC(=0)OC1CCOC1)O)C
1061	162011-90-7	Rofecoxib	O=C1OCC(=C1c1ccccc1)c1ccc(cc1)S(=O)(=O)C
1062	163222-33-1	Ezetimibe	Oc1ccc(cc1)C1C(CCC(c2ccc(cc2)F)O)C(=O)N1c1ccc(cc1)F
1063	164656-23-9	Dutasteride	O=C1C=CC2(C(N1)CCC1C2CCC2(C1CCC2C(=O)Nc1cc(ccc1C(F)(F)F)C(F)(F)F)C)C
1064	165800-03-3	Linezolid	CC(=0)NCC1OC(=0)N(C1)c1ccc(c(c1)F)N1CCOCC1
1065	167221-71-8	Clevidipine	CCCC(=0)OCOC(=0)C1=C(C)NC(=C(C1c1cccc(c1Cl)Cl)C(=0)OC)C
1066	169590-42-5	Celecoxib	Cc1ccc(cc1)c1cc(nn1c1ccc(cc1)S(=0)(=0)N)C(F)(F)F
1067	171228-49-2	Posaconazole	CCC(n1ncn(c1=0)c1ccc(cc1)N1CCN(CC1)c1ccc(cc1)OCC1COC(C1)(Cn1cncn1)c1ccc(cc1F)F)C(O)C
1068	171596-29-5	Tadalafil	O=C1N(C)CC(=0)N2C1Cc1c(C2c2cc3c(c2)OCO3)[nH]c2c1cccc2
1069	173334-57-1	Aliskiren	$\begin{array}{ll} \text{COCCCOc1cc(ccc10C)CC(C(C)C)CC(C(C=0)NCC(C(=0)N)(C)C)C(C)C)O)N} \end{array}$
1070	175463-14-6	Gemifloxacin	NCC1CN(CC1=NOC)c1nc2c(cc1F)c(=0)c(cn2C1CC1)C(=0)0
1070	176644-21-6	Eniporide	NC(=NC(=0)c1cc(c(cc1C)n1cccc1)S(=0)(=0)C)N
1071	179324-69-7	Bortezomib	CC(CC(B(O)O)NC(=O)C(NC(=O)c1cnccn1)Cc1ccccc1)C
1072	180384-57-0	Tezosentan	OCCOc1nc(nc(c10c1ccccc10C)NS(=0)(=0)c1ccc(cn1)C(C)C)c1ccnc(c1)c1nn[nH]n1
1073	181695-72-7	Valdecoxib	Cc1onc(c1c1ccc(cc1)S(=0)(=0)N)c1ccccc1
1075	183321-74-6	Erlotinib	COCCOc1cc2c(ncnc2cc1OCCOC)Nc1cccc(c1)C#C
1076	184475-35-2	Gefitinib	COc1cc2ncnc(c2cc1OCCCN1CCOCC1)Nc1ccc(c(c1)Cl)F
1077	187227-45-8	Oseltamivir	CCOC(=0)C1=CC(C(C(C1)N)NC(=0)C)OC(CC)CC
1078	187523-35-9	Maxipost	COc1ccc(cc1C1(F)C(=O)Nc2c1ccc(c2)C(F)(F)F)Cl
1070	10/323 33 3	2,2',4,4',6-	
1079	189084-64-8	Pentabromodiphenyl	Brc1cc(Br)c(c(c1)Br)Oc1cc(Br)cc(c1)Br
1080	191732-72-6	Lenalidomide	O=C1CCC(C(=0)N1)N1Cc2c(C1=0)cccc2N
1081	192939-46-1	Ximelagatran	CCOC(=0)CNC(C(=0)N1CCC1C(=0)NCc1ccc(cc1)C(=N0)N)C1CCCCC1
1082	194798-83-9	Fosfluconazole	Fc1ccc(c(c1)F)C(OP(=0)(O)O)(Cn1cncn1)Cn1cncn1
1083	196597-26-9	Ramelteon	CCC(=0)NCCC1Cc2c1c1CCOc1cc2
1084	198904-31-3	Atazanavir	COC(=0)NC(C(C)(C)C)C(=0)NN(Cc1ccc(cc1)c1ccccn1)CC(C(Cc1ccccc1)NC(=0)C(C(C)(C)C)NC(=0)OC)O
1085	202409-33-4	Etoricoxib	Clc1cnc(c(c1)c1ccc(cc1)S(=0)(=0)C)c1ccc(nc1)C
1086	204697-65-4	Olcegepant	NCCCCC(C(=O)N1CCN(CC1)c1ccncc1)NC(=O)C(NC(=O)N1CCC(CC1)N1Cc2ccccc2NC1=O)Cc1cc(Br)c(c(c1)Br)O
1000	201037 03 1	2,2',4,4',5,6'-	
1087	207122-15-4	Hexabromodiphenyl	Brc1cc(Br)c(c(c1)Br)Oc1cc(Br)c(cc1Br)Br
/		2,2',3,4,4',5',6-	
1088	207122-16-5	heptabromodiphenyl	Brc1cc(Br)c(cc1Oc1c(Br)cc(c(c1Br)Br)Br)Br
1089	210101-16-9	Conivaptan	Cc1[nH]c2c(n1)c1ccccc1N(CC2)C(=0)c1ccc(cc1)NC(=0)c1ccccc1c1ccccc1
1090	210245-80-0	Zonampanel	OC(=0)Cn1c2cc(n3cncc3)c(cc2[nH]c(=0)c1=0)N(=0)=0
1091	219989-84-1	Ixabepilone	O=C1NC(CC2OC2(C)CCCC(C(C(=0)C(C(C1)O)(C)C)O)C)C(=Cc1csc(n1)C)C
1092	220991-20-8	Lumiracoxib	OC(=0)Cc1cc(C)ccc1Nc1c(F)cccc1Cl
1093	222400-20-6	Tomopenem	O=C(NC1CCN(C1)C(=0)C1CC(CN1C)SC1=C(C(=0)O)N2C(C1C)C(C2=O)C(O)C)CN=C(N)N
1094	224785-90-4	Vardenafil	CCOc1ccc(cc1c1nc(=0)c2n([nH]1)c(CCC)nc2C)S(=0)(=0)N1CCN(CC1)CC
1095	226256-56-0	Cinacalcet	CC(c1cccc2c1ccc2)NCCCc1cccc(c1)C(F)(F)F
1096	249296-44-4	Varenicline	N1CC2CC(C1)c1c2cc2c(c1)nccn2
1097	251565-85-2	Tesaglitazar	CCOC(C(=0)O)Cc1ccc(cc1)OCCc1ccc(cc1)OS(=0)(=0)C
1098	276680-63-8	Exatecan	CCC1(O)C(=O)OCc2c1cc1c3nc4cc(F)c(c5c4c(c3Cn1c2=O)C(N)CC5)C
1099	284461-73-0	Sorafenib	CNC(=0)c1nccc(c1)Oc1ccc(cc1)NC(=0)Nc1ccc(c(c1)C(F)(F)F)Cl
1100	287714-41-4	Rosuvastatin	OC(CC(CC)O)O)C=Cc1c(nc(nc1c1ccc(cc1)F)N(S(=O)(=O)C)C)C(C)C
1101	302962-49-8	Dasatinib	OCCN1CCN(CC1)c1cc(nc(n1)C)Nc1ncc(s1)C(=0)Nc1c(C)cccc1Cl
1102	376348-65-1	Maraviroc	O=C(C1CCC(CC1)(F)F)NC(c1ccccc1)CCN1C2CCC1CC(C2)n1c(C)nnc1C(C)C
1103	486460-32-6	Sitagliptin	NC(Cc1cc(F)c(cc1F)F)CC(=0)N1CCn2c(C1)nnc2C(F)(F)F
1104	557795-19-4	Sunitinib	CCN(CCNC(=0)c1c(C)[nH]c(c1C)C=C1C(=0)Nc2c1cc(F)cc2)CC
1105	608137-32-2	Lisdexamfetamine	NCCCCC(C(=O)NC(Cc1ccccc1)C)N
1103		LIGGERATHICUMINIC	necessary oppositions

Table S2: Model predictions, residuals and hat values calculated for human biotransformation datasets (Training set chemicals are in bold, prediction set chemicals are underlighted; chemicals in Italic have not experimental data)

1	(h*=0.0489) (h) (h*=0.0535) Fred. (ii) (h*=0.0533) (h)	l. Res	HAT i/i	Pred.		
2			(h*=0.0578)	(h)	Res	HAT i/i (h*=0.0574
1	-2.00 0.0706 3.57 -1.23 0.1305 3.21 -1.59 0.0776 3.80	-1.00	0.1161	3.83	-0.96	0.0976
1	1.19	1 0.27				0.4169
1	<u>-1.51</u> <u>0.0066</u> 0.59 -1.52 0.0104 0.52 -1.60 0.0083 <u>0.53</u>	-1.59		0.56		0.0105
To To To To To To To To	-0.32 0.0079 0.64 -0.25 0.0168 0.61 -0.27 0.008 0.39	-0.53				0.011
7		-0.42		1.28	-0.25	0.033
1				1.30		0.017
9						0.0089
10						0.0213
11						0.0142
12 0.78 0.96 0.96 0.75 0.92 0.0006 0.75 0.00114 0.89 0.45 0.00055 0.77 0.89 0.0008 0.30 0.31 0.11						0.0144
13						0.0073
15	<u>0.32</u> <u>0.0084</u> 1.06 0.60 0.0114 0.89 0.43 0.0078 0.72			0.80	0.31	0.0067
16						0.0079
17	0.14	-0.06				0.0099
18						0.0085
19						0.0182
20						0.0099
12						0.0162
23						0.0123
24	<u>0.77</u> <u>0.0224</u> 0.16 0.74 0.0157 0.91 1.49 0.0266 0.46				1.25	0.0398
15						0.0091
28						0.1775
1.06						0.0071
1.05						0.0082 0.0775
29						0.0175
107 0.62 0.015 0.022 0.79 0.53 0.0126 1.07 0.61 0.0504 0.97 0.51 0.0178 0.54 0.08						0.0599
31 0.25 0.25 0.25 0.25 0.27 0.15 0.025 0.12 0.00 0.0138 -0.24 0.0107 1.19 -0.35 33 0.78 0.31 0.009 0.66 0.12 0.0146 0.88 0.42 0.0082 0.75 0.28 0.027 0.0097 0.78 0.56 0.03 35 2.88 0.45 0.0107 0.55 0.03 0.0008 1.26 0.03 0.0009 0.72 0.0097 7.78 0.61 36 0.33 0.04 0.0107 0.95 0.01 0.008 1.26 0.0114 0.55 0.072 0.008 1.26 0.0114 1.56 0.012 1.00 0.0009 0.74 0.33 0.00 0.99 0.0163 0.011 0.0163 0.011 0.0009 0.012 0.0012 0.0012 0.012 0.0012 1.0009 0.014 0.0009 0.014 0.015 0.011 0.0009 0.012 0.0009						0.0111
125		6 -0.48	0.0395	-0.28	-0.39	0.0233
34	-0.29 0.0199 1.09 -0.46 0.0153 1.21 -0.34 0.0076 1.31	-0.24	0.0107	1.19	-0.35	0.0062
18						0.0105
37						0.0221
37						0.0138
134		0.03		1.06		0.0184
19						0.0117
40						0.0094
41 0.692 0.41 0.0088 1.07 0.72 0.0085 0.75 0.66 0.0057 0.88 0.56 0.0126 0.73 0.42 42 0.60 0.72 0.0038 0.64 0.17 0.018 0.07 0.012 0.03 0.66 0.007 0.018 0.55 0.0084 0.65 0.72 43 0.20 0.020 0.0154 0.28 0.17 0.018 0.037 0.24 0.018 0.17 0.0377 0.28 0.011 1.34 0.028 0.01 1.34 0.028 0.00 0.0377 0.28 0.01 0.0115 0.57 0.02 0.00 0.01 0.013 0.00375 0.42 0.02 0.00 0.01 0.01 0.01 0.003 0.00						0.0099
43 0.20 0.20 0.0154 0.28 0.17 0.0168 0.18 0.07 0.0121 0.36 0.22 0.0104 0.66 0.33 45 0.60 0.07 0.0059 0.33 0.24 0.0267 0.28 0.228 0.0235 0.70 0.13 0.0375 0.42 0.12 0.014 46 0.54 0.059 0.033 0.24 0.0267 0.28 0.023 0.02 0.02 0.02 0.03 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.03 0.008 0.00 0.01 0.01 0.01 0.03 0.00 0.01 0.00 0.01 0.00 0.01 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.01 0.00 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.41 0.0088 1.07 0.77 0.0085 0.76 0.46 0.0057 0.88	0.56		0.73	0.42	0.0067
44	0.72	0.55	0.0084	0.65	0.70	0.0087
45 0.60 0.77 0.0099 0.33 0.24 0.0267 0.29 0.28 0.0215 0.02 0.13 0.0375 0.42 0.15 46 0.54 0.015 0.05 0.014 0.015 0.012 0.012 0.015 0.02 0.012 0.015 0.07 0.01 0.011 0.01 0.011 0.015 0.02 0.012 0.015 0.02 0.011 0.083 0.07 0.18 48 0.79 0.059 0.29 0.006 0.85 0.50 0.011 0.27 0.28 0.011 0.008 0.88 0.01 0.008 0.88 0.01 0.009 0.012 0.009						0.0097
46 0.54 -0.15 0.0066 0.51 -0.19 0.0088 0.70 0.01 0.0115 0.57 -0.12 0.015 0.008 1.11 0.02 0.0044 0.87 -0.02 0.0069 1.00 0.01 1.008 1.07 0.01 48 0.79 0.13 0.0086 0.55 0.0112 0.72 0.014 0.89 0.18 0.014 1.00 0.22 0.014 0.64 0.29 50 0.012 0.006 0.55 0.0112 0.72 0.034 0.64 0.29 51 0.70 0.19 0.0089 0.88 0.04 0.0052 0.62 0.011 0.0052 0.62 0.011 0.0052 0.62 0.001 0.011 0.0052 0.62 0.001 0.0052 0.02 0.0055 0.03 0.0059 0.02 0.0059 0.02 0.0059 0.02 0.03 0.007 0.02 0.03 0.007 0.011 0.00 0.0059 0						0.0325
47 0.87 0.05 0.0048 1.11 0.22 0.0044 0.87 -0.02 0.0099 1.00 0.11 0.0083 1.07 0.18 48 0.79 0.13 0.0056 0.77 0.06 0.014 0.89 0.18 0.014 0.62 0.27 0.011 0.08 0.18 0.04 0.29 0.015 0.88 0.17 0.48 0.014 0.08 0.03 0.69 0.09 0.00 0.07 0.18 0.00		0.13			-0.15	0.0258
48 0.79 0.13 0.0086 0.57 0.06 0.0144 0.89 0.18 0.014 0.09 0.06 0.81 0.014 0.60 0.21 0.02 0.014 0.42 0.05 0.0112 0.73 0.014 0.62 0.27 0.014 0.64 0.27 0.014 0.64 0.27 0.014 0.64 0.27 0.014 0.64 0.027 0.014 0.64 0.028 0.08 0.88 0.018 0.088 0.028 0.02 0.027 0.023 0.00 0.025 0.22 0.00 0.00 0.00 0.00 0.00 0.00 0.014 0.02 0.00 0.02 0.00 0.00 0.02 0.00 0.00 0.02 0.00 0.00 0.02 0.00 <th< td=""><td></td><td></td><td></td><td></td><td></td><td>0.0144</td></th<>						0.0144
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52 0.45 0.69 0.0075 0.22 0.0279 0.21 0.025 0.23 0.049 0.27 53 0.93 0.06 0.065 1.14 0.15 0.0096 1.36 0.0165 0.78 0.011 0.0115 0.78 0.011 0.011 0.012 0.98 0.01 0.012 0.52 0.52 0.52 0.52 0.52 0.55 0.023 0.08 0.22 0.06 0.08 0.02 0.06 0.08 0.22 0.06 0.08 0.02 0.06 0.08 0.08 0.03 0.033 0.03 0.08 0.03 0.06 0.08 0.06 <td></td> <td></td> <td></td> <td></td> <td></td> <td>0.0069</td>						0.0069
54 0.48 -0.34 -0.0103 0.54 0.29 0.0083 0.54 0.29 0.0083 0.54 0.29 0.0083 0.24 0.022 0.013 0.25 0.58 0.38 0.220 5.27 0.02 0.56 0.03 0.23 0.38 0.23 0.06 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.69 0.68 0.023 0.06 0.69 0.69 0.68 0.023 0.06 0.69 0.68 0.023 0.06 0.69 0.68 0.023 0.06 0.69 0.68 0.00 0.00 0.00 0.06 0.69 0.00 </td <td><u>-0.69</u> <u>0.0075</u> 0.22 0.0277 0.21 0.025 0.23</td> <td>3</td> <td></td> <td>0.27</td> <td></td> <td>0.0294</td>	<u>-0.69</u> <u>0.0075</u> 0.22 0.0277 0.21 0.025 0.23	3		0.27		0.0294
55 4,13 0,81 0,2204 5,27 1,94 0,158 4,79 1,46 0,138 3,35 0,03 0,2375 3,44 0,12 57 0,02 -0,65 0,011 1,00 -0,669 0,013 1,06 -0,601 0,03 0,068 0,023 0,068 0,023 0,061 0,08 0,012 0,068 0,023 0,001 0,001 0,065 0,013 0,06 0,016 0,97 0,045 0,014 0,08 0,012 0,008 0,012 1,15 0,010 0,008 0,012 0,008 0,012 0,008 0,012 0,008 0,012 0,008 0,012 0,008 0,012 0,008 0,008 0,008 0,008 0,009 0,008 0,007 0,008 0,009 0,008 0,009 0,009 1,13 0,0005 1,18 0,027 0,012 0,007 0,002 1,12 0,014 0,007 0,014 0,007 0,014 0,009 1,13 0,00						0.0193
56 0.99 0.66 0.0161 1.00 0.66 0.013 1.06 0.60 0.0181 0.96 0.68 0.023 0.06 0.69 77 -0.02 -0.65 0.0667 0.22 0.0088 0.33 0.0316 0.08 0.023 0.65 0.66 0.25 58 0.21 -0.08 0.0121 1.03 -0.39 0.005 0.02 0.0106 0.97 -0.04 0.014 0.88 0.92 60 0.29 -0.40 0.0114 0.44 -0.25 0.0181 0.52 -0.18 0.0226 0.04 0.05 0.04 0.026 0.03 0.02 0.04 0.014 0.65 0.08 0.019 0.012 0.02 0.012 0.02 0.02 0.00 0.019 0.012 0.02 0.012 0.02 0.02 1.08 0.02 0.02 1.09 0.016 0.02 0.012 0.02 0.02 0.03 0.02 0.011 0.02				0.25		0.0149
57 Q.02 Q.65 Q.0667 O.22 O.698 O.33 O.0316 O.80 O.063 O.85 58 Q.71 O.08 O.0121 1.03 -0.098 O.0166 0.97 -0.045 O.0138 0.02 -55 59 O.62 O.79 0.0067 1.00 1.16 0.0075 0.99 1.15 0.0124 0.056 0.22 0.018 0.56 0.72 0.018 0.56 0.22 0.018 0.56 0.22 0.018 0.57 -0.13 0.00 0.02 0.00 0.018 0.52 0.018 0.52 0.018 0.57 -0.13 0.00 1.00 0.044 0.0076 1.02 0.013 0.85 0.03 0.03 1.03 0.044 0.0013 0.85 0.98 0.013 0.03 1.11 0.007 0.066 0.018 0.02 0.058 0.014 0.0014 0.014 0.0014 0.014 0.014 0.014 0.0059 1.11 0						0.2526
58 0.71 .008 0.0121 .103 .039 .0058 .042 .100 .0106 .97 .0.45 .0.0143 .0.89 .0.52 90 0.62 .079 .0.067 .100 .116 .0.0075 .0.99 .115 .0.0124 .0.56 .0.008 .0.77 .0.014 .0.56 .0.008 .0.77 .0.012 .0.014 .0.56 .0.008 .0.75 .0.0128 .0.28 .0.97 .0.062 .0.74 .0.012 .0.008 .0.75 .0.0128 .0.28 .0.97 .0.012 .0.008 .0.97 .0.012 .0.00 .0.008 .0.97 .0.012 .0.007 .0.004 .1.12 .0.005 .1.48 .0.25 .0.014 .0.005 .1.88 .0.013 .0.008 .0.001 .0.008 .0.01 .0.008 .0.001 .0.009 .0.01 .0.009 .0.01 .0.008 .0.01 .0.008 .0.008 .0.01 .0.008 .0.01 .0.008 .0.01 .0.008					-0.69	0.0205 0.6372
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65 150 0.54 0.0271 1.48 0.53 0.0244 1.46 0.51 0.0399 1.54 0.99 0.0114 1.46 0.50 66 0.49 -0.04 -0.022 1.33 0.026 0.006 1.20 0.14 0.0061 1.16 0.52 0.015 1.16 0.00 67 1.29 0.39 0.0205 1.31 0.42 0.015 1.03 0.13 0.0074 1.16 0.56 0.0179 1.13 0.25 68 0.81 0.088 0.0163 0.06 0.05 0.0128 1.14 0.092 0.0078 0.85 0.0124 0.06 0.012 0.014 0.016 0.02 0.014 0.018 0.52 0.32 0.011 0.01 0.05 0.012 0.01 0.01 0.05 0.011 0.02 0.012 0.02 0.012 0.01 0.05 0.032 0.01 0.01 0.02 0.012 0.01 0.01 0.01	-0.07 0.0149 1.12 0.19 0.0146 1.36 0.44 0.0059 1.11					0.008
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	<u>-0.50</u> <u>0.0102</u> 0.70 0.0092 1.00 0.0085 1.35	5	0.0286	1.22	_	0.0094
76 0.50 0.61 0.0136 0.46 2.266 0.0099 0.50 2.62 0.0079 1.08 2.03 0.0275 1.03 2.09 77 0.45 0.25 0.012 0.46 0.025 0.013 0.0275 1.08 2.09 2.00 0.0032 0.15 0.0033 0.34 0.22 0.0135 0.26 0.14 0.0151 0.32 0.20 0.012 0.47 0.005 0.0032 0.0032 0.0032 0.0032 0.0032 0.0033 0.34 0.22 0.0135 0.26 0.14 0.0151 0.32 0.20 0.015 0.015 0.0032						0.0125
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80 <u>0.12</u> <u>-0.57</u> <u>0.0179</u> -0.15 0.0391 -0.15 0.0394 -0.52 0.0429 -0.26						0.0129
					-0.17	0.012
81 0.28 -0.10 0.0274 0.24 -0.44 0.0211 0.56 -0.11 0.0152 0.09 -0.60 0.0248 0.31 -0.38	-0.15 0.0394 -0.52 -0.10 0.0274 0.24 -0.44 0.0211 0.56 -0.11 0.0152 0.09		0.0429	0.31	-0.38	0.0269

_		LogH	ILT		LogH	L _{R1}		LogHL	0		LogH	Las		LogHL ₈₄	
ID	Pred. (h)	Res	HAT _{i/i} (h*=0.0489)	Pred. (h)	Res	HAT _{i/i} (h*=0.0535)	Pred. (h)	Res	HAT _{i/i} (h*=0.0533)	Pred. (h)	Res	HAT _{i/i} (h*=0.0578)	Pred. (h)	Res	HAT _{i/i} (h*=0.0574)
82	3.77	-0.18	0.0531	3.71	-0.28	0.0939	3.59	-0.40	0.0767	3.56	-0.43	0.0626	3.86	-0.13	0.1049
83	0.62	-0.46	0.0111	0.80	-0.29	0.007	0.65	-0.44	0.0092	0.61	-0.48	0.01	0.67	-0.43	0.0113
84 85	1.35 1.31	0.26 -0.17	0.0207 0.0121	1.24	0.15	0.013	1.20	0.11	0.0152	1.28	0.19	0.0187	1.29	0.20	0.0156
85 86	0.52	0.72	0.0121	1.26 0.79	-0.22 0.54	0.0113 0.009	1.28 0.55	-0.20 0.30	0.0168 0.0062	1.24 0.67	-0.25 0.42	0.0167 0.0105	1.21 0.48	-0.27 0.24	0.0108
87	0.65	0.80	0.0068	0.73	0.41	0.0126	0.58	0.17	0.007	0.68	0.27	0.0103	0.60	0.19	0.0094
88	0.70	0.40	0.0128	0.76	0.45	0.0072	0.75	0.45	0.0035	0.42	0.11	0.0133	0.66	0.35	0.0116
89	0.63	0.67	0.0078	0.58	0.61	0.0105	0.47	0.51	0.0067	0.43	0.46	0.0099	0.42	0.45	0.0086
90	0.78	0.67	0.0068	0.70	0.57	0.007	0.70	0.57	0.0118	0.70	0.53	0.0122	0.55	0.38	0.0073
91	0.61	-0.76	0.0086	0.33		0.0248	0.29		0.0106	0.37		0.0317	0.67		0.007
92 93	0.72	-0.13	0.0053 0.0054	0.56	-0.29	0.0152 0.0116	0.58	-0.26	0.0094	0.67	-0.18	0.024 0.0098	0.72 0.63	-0.13	0.0111
93 94	0.71 0.51	-1.05 0.66	0.0054	0.59	0.84	0.0116	0.65	0.58	0.0079	0.76	0.62	0.0098	0.58	0.50	0.0068
95	0.62	0.63	0.009	0.49	0.23	0.0072	0.58	0.32	0.0102	0.99	0.73	0.0136	0.94	0.68	0.0038
96	0.60	1.38	0.0094	0.45	1.22	0.0111	0.52	1.29	0.0105	0.83	1.60	0.0125	0.86	1.62	0.0081
97	1.63	1.45	0.0517	0.65	0.44	0.104	0.50	0.29	0.3797	0.56	0.34	0.0947	-0.28	-0.50	0.426
98	1.32	1.14	0.0315	0.81	0.63	0.0145	1.13	0.94	0.037	1.12	0.95	0.0388	0.57	0.40	0.0514
99	1.16	-1.66	0.0164	1.03	-1.80	0.0132	1.43	-1.40	0.0431	1.04	-1.79	0.0174	1.19	-1.64	0.0303
100	0.87	0.03	0.0073	0.98	0.14	0.0084	1.23	0.38	0.0154	0.84	-0.02	0.0089	1.04	0.19	0.0189
101 102	0.67 0.86	-0.18 -0.49	0.0084	0.79 1.12	-0.48 -0.26	0.0133 0.0202	0.85 1.03	-0.42	0.009 0.0109	1.11	-0.15	0.0297	1.20	-0.06	0.0094
102	0.86	0.35	0.025 0.0071	0.78	0.39	0.0202	0.60	-0.35 0.22	0.0109	0.76	0.29	0.0237 0.0105	0.85	-0.53 0.15	0.0129 0.0107
103	0.02	-0.20	0.0071	0.03	-0.43	0.0252	-0.07	-0.53	0.0391	0.15	-0.31	0.0333	-0.32	-0.78	0.0692
105	0.11	-0.66	0.0141	-0.17	-,	0.0401	-0.15		0.0529	-0.02		0.0329	-0.16	23	0.0531
106	0.47	-0.91	0.0338	0.27		0.0692	0.61		0.0175	-0.05		0.0876	0.41		0.0285
107	1.10	-1.16	0.0667	0.26		0.0702	1.05		0.0301	0.91		0.0135	0.23		0.0826
108	2.99	-1.89	0.0095	2.66	-2.28	0.0153	2.73	-2.20	0.0072	2.75	-2.17	0.0176	2.86	-2.05	0.0073
109	1.17	-0.30	0.0182	1.10	-0.38	0.0131	0.79	-0.69	0.0067	0.90	-0.59	0.017	0.97	-0.52	0.0096
110 111	0.79 1.56	0.94	0.0067 0.0233	0.78	0.92	0.0042	0.44 1.22	0.58	0.0061 0.0148	0.67 1.64	0.82	0.0091	0.69 1.56	0.84	0.0066 0.0159
112	0.46	-0.03	0.0233	0.45	-0.61	0.0189	0.29	-0.77	0.0148	0.17	-0.89	0.0354	0.15	-0.91	0.0139
113	0.53	1.53	0.034	-0.30	0.66	0.2076	-0.35	0.62	0.4219	0.37	1.33	0.0835	-0.53	0.43	0.4389
114	0.94	0.76	0.0331	0.27		0.0661	-0.05		0.4267	0.63		0.1164	-0.41		0.4706
115	0.69	0.52	0.026	-0.37		0.0643	-0.43		0.4716	0.49		0.1397	-0.53		0.5101
116	1.04	0.66	0.0297	0.85	0.47	0.0136	1.01	0.63	0.0305	0.99	0.59	0.0308	0.57	0.17	0.0189
117	0.57	0.45	0.0064	0.79	0.64	0.0129	0.63	0.48	0.0133	0.60	0.45	0.0153	0.50	0.34	0.0132
118	0.71	-0.03	0.0063	0.88	0.06	0.0132	0.71	-0.12	0.0101	0.96	0.13	0.0144	0.76	-0.07	0.0099
119 120	0.98	0.02	0.0186 0.0061	0.99	0.01	0.0089	1.13 0.80	0.15	0.0283 0.0111	1.18 0.83	0.21	0.0292 0.0103	0.96	-0.01 0.14	0.0148
120	0.74	-0.85	0.0061	0.50	-0.90	0.0119 0.0115	0.80	0.14 -0.96	0.0111	0.83	-0.97	0.0103	0.79	-1.00	0.009
122	0.60	0.30	0.0057	0.71	0.41	0.0097	0.59	0.28	0.0068	0.66	0.36	0.0207	0.62	0.32	0.0101
123	0.86	-0.63	0.0111	1.09	-0.52	0.014	0.80	-0.81	0.0213	0.86	-0.75	0.0219	0.58	-1.03	0.0076
124	0.68	-0.45	0.0114	1.11	-0.02	0.0115	1.05	-0.08	0.0158	0.55	-0.65	0.0109	0.75	-0.46	0.0172
125	1.12	-0.08	0.0197	1.16	-0.12	0.0186	0.66	-0.62	0.0085	0.83	-0.45	0.0221	0.87	-0.41	0.0092
126	0.56	-0.48	0.0077	0.59	-0.50	0.0084	0.51	-0.57	0.0085	0.46	-0.63	0.014	0.51	-0.57	0.011
127	0.56	-0.98	0.0062	0.43	-1.26	0.0088	0.49	-1.20	0.0095	0.48	-1.30	0.0209	0.51	-1.27	0.0098
128 129	0.47	-1.10	0.0067	0.44	-1.33	0.0115	0.43	-1.34	0.0086	0.37	-1.40	0.021	0.41	-1.37	0.0109
130	0.84	-0.72 -0.24	0.0063 0.0082	0.92 1.08	-1.09 0.01	0.0104 0.0072	1.17 0.75	-0.84 -0.32	0.0069 0.0127	1.37 0.92	-0.64 -0.42	0.0149 0.0107	1.34 0.98	-0.67 -0.36	0.0059
131	0.64	0.34	0.0079	0.72	0.36	0.0058	0.70	0.35	0.0101	0.63	0.28	0.0139	0.65	0.30	0.0129
132	0.15	-1.58	0.0176	0.28		0.0139	0.42		0.0161	0.04		0.037	0.09		0.0293
133	0.68	-0.22	0.005	0.35	-0.57	0.0247	0.30	-0.61	0.0272	0.37	-0.54	0.0471	0.38	-0.53	0.0299
134	0.14	0.06	0.0203	-0.33	-0.51	0.0737	0.16	-0.02	0.0149	-0.24	-0.41	0.0438	-0.06	-0.23	0.0262
135	1.46	-0.14	0.0429	1.35		0.0802	0.53		0.4026	1.27		0.0807	0.10		0.4297
136	0.15	0.34	0.0343	-0.10	0.07 -0.47	0.0445 0.0181	1.12 2.33	1.29 -0.01	0.0184	-0.18	-0.08	0.0577	0.36 2.27	0.46 -0.06	0.0414
137	1.52 0.78	-0.80 0.48	0.0208	1.87 0.82	0.52				0.0277	2.23	-0.10	0.0526			
138 139	0.78	-0.72	0.0131 0.006	0.82	-0.43	0.0059 0.005	0.99 0.84	0.69 -0.55	0.0105 0.0087	0.76 1.22	0.46 -0.16	0.017 0.0195	0.68 1.06	0.38 -0.32	0.0128 0.0088
140	0.83	0.47	0.0114	0.80	0.41	0.0088	0.88	0.50	0.0148	0.78	0.40	0.0203	0.60	0.22	0.0087
141	1.42	-0.66	0.0196	1.23	-0.86	0.0171	1.50	-0.59	0.02	1.35	-0.90	0.0116	1.28	-0.98	0.0096
142	1.13	-0.09	0.0105	1.14	-0.07	0.0162	0.96	-0.26	0.0121	1.10	-0.15	0.0219	0.94	-0.30	0.0128
143	0.79	1.40	0.0112	0.70	1.30	0.0084	0.45	1.05	0.0119	0.66	1.26	0.0148	0.72	1.32	0.0114
144	0.65	-0.13	0.0107	0.51	-0.40	0.0138	0.48	-0.44	0.0084	0.50	-0.43	0.0204	0.77	-0.16	0.0092
145 146	1.01 0.86	0.20 -0.62	0.0182 0.0166	1.16 1.15	0.37 -0.34	0.0148 0.0062	1.33 0.76	0.54 -0.73	0.0053 0.0073	1.09	0.10 -0.17	0.0061 0.0156	1.11	0.12 -0.21	0.0062 0.0113
145	0.86	0.54	0.0166	0.76	0.72	0.0125	0.71	0.67	0.0073	0.73	0.69	0.0156	0.83	0.79	0.0113
147	0.52	0.63	0.0177	0.70	0.65	0.0125	0.71	0.45	0.0069	0.65	0.60	0.0106	0.49	0.79	0.0151
149	0.20	-0.03	0.0142	0.41	0.17	0.0343	0.30	0.05	0.0131	0.50	0.25	0.0149	0.20	-0.05	0.0274
150	1.42	-0.26	0.0401	1.26	-0.43	0.0316	1.93	0.24	0.0243	1.45	-0.23	0.0635	1.36	-0.33	0.0502
151	1.43	-0.05	0.0651	2.32	0.85	0.0351	2.67	1.19	0.0358	1.63	0.14	0.0979	1.66	0.16	0.0731
152	0.03	0.24	0.0135	0.22	0.43	0.0138	0.48	0.69	0.0135	0.02	0.17	0.0198	0.25	0.39	0.0204
153	0.98	0.13	0.0112	0.95	0.10	0.0064	0.90	0.04	0.014	0.98		0.0181	1.02		0.0179
154 155	0.48	-0.62 -0.34	0.0099	0.59	-0.76 -0.47	0.0103	0.55 0.60	-0.79 -0.51	0.0087	0.43	-0.66	0.0128	0.53	-0.54	0.0108
155 156	1.13	-0.34 0.92	0.0103	1.21	1.01	0.0093	0.60	0.64	0.0091	1.00	-0.66 0.76	0.0142	0.43	-0.54 0.76	0.0103
157	1.08	0.92	0.0231	0.93	0.65	0.0117	0.62	0.34	0.0078	0.88	0.60	0.0145	0.87	0.76	0.0119
158	0.44	0.44	0.0108	0.41	0.41	0.0143	0.29	0.29	0.0132	0.27	0.26	0.0186	0.27	0.26	0.0157
159	0.88	-0.79	0.0142	0.60	-1.16	0.0224	0.91	-0.85	0.009	1.07	-0.69	0.0228	1.17	-0.59	0.0093
160	1.00	-0.52	0.0203	1.07	-0.46	0.0139	1.30	-0.24	0.0061	0.92	_	0.0168	1.00		0.0181
161	0.58	-1.00	0.0322	0.43	-1.28	0.0224	0.84	-0.87	0.0228	0.50	-1.19	0.0343	0.52	-1.17	0.0354
162	0.91	0.61	0.0106	0.86	0.56	0.0072	0.92	0.61	0.0075	0.84	0.52	0.0084	1.02	0.69	0.0078
163 164	0.02	-1.76	0.0204	0.32	-1.73	0.0433	0.25	-1.80	0.0197	0.17	-1.90	0.0604 0.0147	0.05	-2.02	0.0305
164	0.16	<u>-0.82</u> -0.83	0.0159 0.0156	-0.01	-1.09	0.0178 0.024	0.39 -0.01	-1.10	0.0134	-0.45	-1.54	0.0147	-0.28	-1.36	0.014
103	0.24	-0.03	0.0130	-0.01	-1.03	0.024	-0.01	-1.10	0.0241	-0.43	-1.34	0.0323	-0.20	-1.30	0.0300

		LogH	ILT		LogH	L _{R1}		LogHLe	2		LogH	Les		LogHL ₈₄	
ID	Pred.	Res	HAT _{i/i} (h*=0.0489)	Pred. (h)	Res	HAT _{i/i} (h*=0.0535)	Pred. (h)	Res	HAT _{i/i} (h*=0.0533)	Pred. (h)	Res	HAT _{i/i} (h*=0.0578)	Pred. (h)	Res	HAT i/i
166	0.16	-2.18	0.0253	0.51	-2.10	0.0318	0.63	-1.98	0.0217	0.53	-2.07	0.05/8	0.33	-2.28	(h*=0.0574) 0.0371
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
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		0.024
169 170	1.11 1.07	-0.13 -0.85	0.0186 0.0139	0.82 0.70	-0.45 -1.23	0.0128 0.0099	0.92 0.64	-0.35 -1.29	0.0209 0.0071	1.14 0.77	-1.15	0.0346 0.027	0.98 1.01	-0.91	0.0303 0.0069
171	0.34	-0.06	0.0132	0.41	0.00	0.0137	0.53	0.12	0.0053	0.06	-0.36	0.0112	0.25	-0.16	0.0118
172	0.69	0.13	0.021	0.57	-0.01	0.0226	0.82	0.25	0.0122	0.74	0.15	0.0151	0.79	0.20	0.0143
173	0.31	-0.43	0.0185	0.13	-0.61	0.0844	-0.19	-0.93	0.059	0.28	-0.46	0.0617	0.16	-0.58	0.0623
174 175	0.89	-0.59 0.10	0.0252 0.0174	0.45 -0.26	-1.14 -0.29	0.0243 0.0399	0.94 -0.01	-0.65 -0.03	0.025 0.0248	0.93 -0.37	-0.68 -0.41	0.0301 0.0289	0.93 -0.25	-0.68 -0.28	0.0302 0.0304
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	0.0374
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	0.0323
178	0.07	-0.81	0.026	-0.34		0.1065	1.16		0.056	0.13		0.1225	1.03		0.0778
179 180	0.83	0.51 -1.59	0.0137 0.0278	0.74	0.43	0.0162 0.0241	0.80 0.82	0.49	0.0131 0.0144	0.83	0.51	0.0098 0.0406	0.73	0.41	0.0129
181	0.19	0.03	0.0278	0.94	0.40	0.0077	0.79	0.25	0.0032	0.40	-0.13	0.0075	0.55	0.02	0.0064
182	0.55	-0.13	0.0126	0.62	-0.07	0.0054	0.38	-0.30	0.0063	0.38	-0.30	0.0154	0.60	-0.09	0.0072
183	1.56	0.56	0.0273	1.39	0.40	0.026	1.54	0.54	0.0074	1.67	0.67	0.0164	1.59	0.59	0.0096
184	0.50	-1.03	0.007	0.64	-1.03	0.0096	0.63	-1.04	0.0082	0.52		0.0153	0.57		0.0111
185 186	0.40	-0.85 0.74	0.0098 0.0058	0.21	-1.39 0.89	0.0188 0.0196	0.41	-1.19 1.18	0.0154 0.0128	0.25	-1.34 1.16	0.029 0.0201	0.46	1.14	0.0178
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
188	0.85	0.60	0.0103	1.71	1.41	0.0757	0.99	0.69	0.0206	1.06	0.56	0.0358	1.25	0.75	0.0272
189	0.86	-2.07	0.021	1.04	-2.03	0.0152	1.22	-1.85	0.0151	0.78		0.0159	0.82		0.0163
190 191	2.70 0.29	-1.55 -0.01	0.0946 0.01	3.66 0.49	-0.74 0.17	0.0773 0.0497	3.28 0.24	-1.11 -0.08	0.0604	2.52	-1.88 0.45	0.1399 0.0606	2.27	-2.12 0.10	0.1127
191	0.29	-0.69	0.0097	0.49	-0.96	0.0497	-0.04	-1.26	0.0148	0.75	-0.59	0.03	0.40	-0.95	0.0346
193	0.87	-0.50	0.0113	0.65	-0.80	0.0154	1.02	-0.43	0.0312	1.06		0.0553	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
195 196	0.28 0.82	0.41	0.0141 0.0158	-0.14 0.75	-0.02 0.56	0.0319 0.0117	-0.18 0.87	-0.07 0.68	0.0458 0.0267	-0.40 0.99	-0.37 0.79	0.0414 0.028	-0.23 0.50	-0.19 0.31	0.0462 0.0307
196	0.82	0.41	0.0158	0.75	0.64	0.0117	0.87	0.88	0.0104	0.83	0.79	0.028	0.78	0.43	0.0307
198	0.45	-0.66	0.0084	0.67	0.04	0.0075	0.52	0.33	0.0081	0.43	0.40	0.0112	0.52	0.43	0.0108
199	0.38	-0.67	0.0105	0.36		0.0096	0.34		0.013	0.36		0.0224	0.31		0.0149
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
201	0.60	-0.49 -0.28	0.0056	0.66 0.77	-0.44	0.0085 0.024	0.63 0.92	-0.29	0.006 0.0061	0.71	0.14	0.015 0.0199	0.70	-0.13	0.0077
202	0.44	0.09	0.0084	0.77	-0.44	0.024	0.51	0.14	0.0052	0.15	-0.21	0.0155	0.48	0.11	0.0075
204	-0.35	-0.88	0.0338	-0.44	-1.17	0.0674	0.48	-0.25	0.0208	-0.85	-1.58	0.0476	-0.16	-0.89	0.0406
205	0.87	0.32	0.0157	0.74	0.18	0.0109	0.89	0.33	0.0235	0.93	0.37	0.0271	0.62	0.07	0.0138
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
207 208	0.86 1.35	0.19 -0.04	0.0121 0.0145	1.07 1.28	0.39 -0.12	0.0081 0.0156	1.10 1.15	0.42 -0.26	0.0146 0.008	0.81 1.34	0.13	0.0152 0.0165	0.98 1.29	0.30	0.0272
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
210	0.80	-0.57	0.0131	0.76	-0.77	0.0107	0.89	-0.64	0.0104	0.76		0.0169	1.01		0.0133
211	1.17	0.46	0.025	0.75	-0.34	0.0105	1.27	0.17	0.0141	1.39	0.45	0.0561	1.37	0.43	0.0191
212 213	0.86	0.66 -0.09	0.0079 0.0056	0.85	0.64 -0.12	0.0101 0.014	0.78 0.65	0.56 -0.27	0.0107 0.0117	0.67	0.46	0.0145 0.0111	0.64	0.43	0.009
214	0.84	0.24	0.0084	1.09	0.49	0.0073	0.79	0.19	0.0117	0.92	0.32	0.0115	1.01	0.41	0.0086
215	0.39	-0.35	0.012	0.82		0.0138	0.64		0.0124	0.83		0.0119	0.69		0.0133
216	0.51	-0.48	0.0061	0.52		0.0078	0.56		0.0055	0.84		0.022	0.74		0.0062
217 218	0.62	-0.12 -0.29	0.0095 0.0073	0.98	-0.08	0.0126 0.0101	0.90 0.79	-0.16	0.0078 0.008	1.21		0.0293 0.0231	1.16 1.15		0.008 0.0082
210	0.62	-0.29	0.0073	0.74	-0.68	0.0042	0.79	-0.91	0.012	0.78	-0.64	0.0231	0.80	-0.62	0.0104
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
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
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
223 224	0.18 1.22	0.96 1.14	0.0074 0.0236	0.52 0.95	1.29 0.88	0.0095 0.0124	0.56 0.90	1.33 0.82	0.0213 0.0103	0.47 1.25	1.23 1.18	0.0132 0.0429	0.34 1.59	1.10 1.52	0.0358
225	1.04	1.04	0.0259	1.27	1.21	0.0124	1.05	0.99	0.0105	0.82	0.76	0.0429	0.87	0.81	0.0233
226	0.60	0.40	0.0061	0.44	0.23	0.0105	0.72	0.51	0.01	0.53	0.32	0.0168	0.59	0.38	0.0084
227	0.77	0.77	0.0103	1.13	1.13	0.0094	1.05	1.05	0.0122	0.63	0.62	0.0082	0.79	0.78	0.0129
228 229	1.02	0.24	0.0108	1.00 0.41	0.22	0.0135	1.06	0.29	0.0177	1.01 0.56	0.24	0.025 0.012	0.97	0.20	0.0177
229	0.40	0.42 1.41	0.012 0.0203	0.41	1.39	0.028 0.0244	0.38 0.81	1.24	0.0083 0.0542	0.56	1.07	0.012	0.52	1.32	0.0112
231	0.66	-0.13	0.0141	0.70	-0.13	0.0114	0.88	0.04	0.0242	0.85	-0.28	0.035	1.04	-0.09	0.0288
232	1.32	-0.05	0.0211	1.19	-0.18	0.025	1.10	-0.27	0.0154	1.20	-0.20	0.0267	0.99	-0.40	0.0131
233	0.96	1.49	0.0379	0.01	0.53	0.1515	-0.03	0.49	0.4019	0.81	1.32	0.089	-0.32	0.20	0.423
234 235	0.53 0.52	-1.12 0.22	0.0103 0.0088	0.70 0.59	- 0.99 0.28	0.0273 0.0081	0.55 0.45	-1.14 0.14	0.01 0.0107	0.31	-1.39 0.25	0.043 0.0155	0.76 0.54	-0.95 0.24	0.0092 0.0121
235	0.52	-0.11	0.0088	0.59	-0.40	0.0081	0.45	0.14	0.0107	0.55	U.23	0.0155	1.04	0.24	0.0121
237	0.85	-0.06	0.0057	1.25	0.34	0.009	0.51	-0.40	0.0093	0.81	-0.10	0.008	0.76	-0.15	0.0062
238	1.57	0.16	0.0254	1.38	-0.04	0.0227	1.46	0.05	0.0053	1.44	0.03	0.0135	1.44	0.03	0.0064
239 240	1.40	0.14	0.0215	1.31	0.06	0.0253	1.06	-0.19	0.0086	1.22	-0.03	0.0293	1.11	-0.14	0.0108
240 241	0.84 -0.28	-0.16 -1.96	0.0106 0.0211	1.15 -0.41	0.13	0.0072	1.00 -0.13	-0.01	0.0062	0.64 -0.32	-0.38	0.0115	0.76 -0.22	-0.25	0.008
241	1.16	1.12	0.0211	1.26	1.21	0.0239	1.04	1.00	0.0145	0.69	0.64	0.0264	0.80	0.75	0.0161
243	3.22	0.54	0.1929	0.95	-1.83	0.0159	3.57	0.79	0.158	2.33		0.5196	3.08	0.31	0.1741
244	0.79	0.18	0.0112	1.22	0.60	0.0097	0.71	0.09	0.0067	0.80	0.19	0.0125	0.74	0.14	0.0063
245	0.13	0.57	0.009	0.51	0.91	0.0102	0.60	1.00	0.0231	0.45	0.85	0.0156	0.35	0.75	0.0388
246 247	0.79 4.50	0.27 -0.18	0.0114	0.87 1.17	0.34	0.0121	0.92 4.47	0.38 -0.21	0.0168 0.2458	0.79 3.11	0.26	0.0255	1.14 4.00	0.61 -0.68	0.02 0.2734
247	0.77	0.17	0.0088	0.73	-0.24	0.0193	0.59	-0.38	0.0076	1.09		0.009	1.03	-0.00	0.0097
249	3.93	-0.87	0.2645	1.02		0.0196	4.04	-0.76	0.1966	2.98		0.6743	3.74	-1.07	0.2127

		Logi	IL _T		LogH	L ₈₁		LogHL	32		LogH	L ₈₃		LogHL ₈₄	
ID	Pred.	Res	HAT _{i/i}	Pred.	Res	HAT i/i	Pred. (h)	Res	HAT i/i	Pred.	Res	HAT i/i	Pred.	Res	HAT i/i
250	(h) 0.77	0.05	(h*=0.0489) 0.009	(h) 0.93	0.07	(h*=0.0535) 0.0088	0.88	0.01	(h*=0.0533) 0.0108	(h) 0.78	-0.09	(h*=0.0578) 0.0122	(h) 0.71	-0.15	(h*=0.0574) 0.0101
251	0.92	0.53	0.0149	1.04	0.58	0.01	1.39	0.93	0.0222	0.84	0.38	0.0152	0.88	0.42	0.014
252	0.77	-0.09	0.0116	0.88	-0.07	0.0097	0.95	-0.01	0.0103	1.03	0.08	0.0142	0.91	-0.04	0.0119
253 254	0.74	-0.94 0.03	0.012 0.0117	1.06	0.41	0.0127	1.47	0.20	0.0091	1.33 0.15	-0.34	0.0224 0.0138	1.27 0.24	-0.25	0.0107 0.0154
255	0.74	0.10	0.0117	0.67 0.92	0.41	0.0055 0.0259	0.65 1.18	0.38	0.0057 0.0307	1.29	0.64	0.0772	1.53	0.88	0.0134
256	0.75	0.28	0.0104	0.96	0.40	0.0063	0.59	0.03	0.0091	0.55	-0.01	0.0129	0.62	0.06	0.0076
257	0.98	-0.64	0.019	1.02	-0.60	0.0139	1.13	-0.49	0.0084	1.18	-0.44	0.0099	1.29	-0.33	0.0096
258 259	0.01 0.45	-0.84 -0.25	0.0143 0.0171	0.29	-0.67	0.0116	0.09	-0.87	0.012 0.0095	-0.21 0.83	-1.17	0.0189 0.0164	-0.11 0.90	-1.07	0.017 0.0087
260	0.58	-0.02	0.0077	0.77	0.15	0.0071	0.79	0.17	0.0063	1.08	0.47	0.0141	0.90	0.29	0.0072
261	1.18	-0.42	0.0195	1.09	-0.53	0.0254	1.90	0.27	0.0334	1.68		0.0629	1.67		0.0436
262	1.17	0.17	0.0097	1.12	0.12	0.0111	0.92	-0.09	0.0118	1.15	-0.07	0.0154	0.94	-0.28	0.0114
263 264	0.99	-0.27 0.20	0.0092 0.0109	0.92	-0.34 0.43	0.0041	0.86	-0.40 0.32	0.0225 0.0051	0.75	-0.54 -0.03	0.0081 0.0128	0.64	-0.64 -0.13	0.0087
265	0.57	0.13	0.0033	0.65	0.20	0.0223	0.64	0.19	0.0088	0.73	0.28	0.0052	0.56	0.11	0.0103
266	0.29	0.06	0.0064	0.64	0.18	0.0081	0.54	0.09	0.0109	0.17	-0.31	0.009	0.42	-0.06	0.011
267 268	1.33 1.27	0.63	0.0148 0.0169	1.16 1.18	0.45	0.014 0.0202	0.85 1.23	0.15	0.004 0.0049	1.11 1.36	0.40	0.0153 0.0115	1.11 1.28	0.40 -0.05	0.007 0.0076
269	0.53	-0.70	0.0169	0.64	0.00	0.0202	0.57	0.04	0.0049	0.46	0.03	0.0119	0.67	-0.05	0.0076
270	0.34	-0.38	0.0102	0.46	-0.43	0.0118	0.59	-0.29	0.015	0.36		0.0189	0.56		0.0171
271	0.95	-0.43	0.0082	1.14	-0.24	0.0088	0.82	-0.55	0.012	1.06	-0.34	0.0105	1.17	-0.23	0.0121
272 273	0.98	-0.34 0.13	0.0137 0.0071	0.93	-0.40 0.34	0.0088	1.22 0.70	-0.11 0.12	0.0218	0.99 0.54	-0.33 -0.04	0.0236 0.012	0.95 0.60	-0.37 0.02	0.014 0.0104
274	0.78	0.60	0.0071	0.74	0.56	0.0035	0.51	0.34	0.0052	0.74	0.54	0.012	0.76	0.55	0.0071
275	0.35	0.27	0.0075	0.40	0.26	0.0139	0.20	0.07	0.0133	0.16	0.03	0.0123	0.19	0.06	0.0126
276	0.68	1.46	0.0092	0.72	1.50	0.0067	0.51	1.29	0.0069	0.51	1.29	0.0121	0.67	1.45	0.0089
277 278	0.41	- 0.25 0.32	0.0432 0.0135	0.61	-0.05 0.12	0.0371 0.0151	0.64	-0.02 0.25	0.0138 0.0166	0.41	-0.24 0.50	0.029 0.0307	0.35 1.01	-0.30 0.58	0.0288
279	1.01	-0.07	0.0183	0.68	-0.41	0.0183	0.83	-0.26	0.0184	0.87	0.50	0.0229	0.90	0.50	0.0213
280	-0.24	-1.11	0.0335	-0.32		0.0698	0.29		0.0164	-0.79		0.0493	-0.35		0.0368
281 282	0.49 1.05	-1.13 0.70	0.007 0.0082	0.98	-0.65 0.45	0.0346 0.0114	0.93	-0.70 0.39	0.0118 0.0109	0.93	-0.69 0.53	0.0104 0.0139	0.98	-0.64 0.60	0.0137 0.0093
282	0.65	0.70	0.0082	0.57	0.45	0.0114	0.75 0.63	0.63	0.0109	0.63	0.53	0.0139	0.76	0.66	0.0147
284	0.37	-0.77	0.0103	0.46		0.0059	0.56		0.0071	0.89		0.0258	0.77		0.007
285	0.35	-0.42	0.0088	0.47	-0.70	0.01	0.68	-0.49	0.0076	0.45	-0.72	0.0203	0.48	-0.68	0.0127
286 287	0.95 1.59	0.55 0.81	0.0066 0.0275	0.67 1.44	0.25 0.66	0.0166 0.0242	0.68 1.43	0.26 0.66	0.0071 0.0056	0.82	0.35	0.008 0.0142	0.77 1.38	0.30	0.0075
288	0.62	-0.16	0.0054	0.62	0.00	0.0073	0.58	0.00	0.0106	0.58	0.70	0.0154	0.59	0.01	0.0038
289	0.83	0.95	0.0111	0.86	0.98	0.0135	0.42	0.54	0.0108	0.73	0.86	0.0215	0.66	0.79	0.0106
290 291	0.56	-0.32 -0.14	0.0117 0.0158	0.83	-0.72	0.009 0.0131	0.76 0.82	-0.68	0.0085 0.0215	0.74	0.70	0.0184	0.75	0.55	0.0141
291	-0.08	-0.14	0.0158	-0.20	-0.72	0.0131	-0.35	-0.68	0.0215	0.81 -0.45	-0.70	0.0156 0.0287	0.95 -0.38	-0.55	0.0107
293	0.91	-0.42	0.0119	0.91	-0.55	0.015	1.00	-0.46	0.0103	0.95	-0.73	0.0168	1.04	-0.64	0.0124
294	0.91	-0.39	0.017	0.81	-0.49	0.0186	1.09	-0.21	0.0062	1.01	-0.30	0.0146	0.89	-0.41	0.0088
295 296	1.23 1.17	0.75 0.30	0.0186 0.0145	1.19 0.61	0.70 -0.26	0.0108 0.0245	1.49 0.70	1.01 -0.18	0.0035 0.0165	1.21 0.80	0.72 -0.09	0.0137 0.0331	1.48 1.25	0.98	0.0115 0.0206
297	0.78	-0.78	0.0154	0.58	-0.20	0.0182	0.82	-0.10	0.02	0.70	-0.03	0.0471	1.16	0.30	0.0274
298	0.34	0.10	0.0155	0.11		0.0451	0.63		0.0315	0.46		0.0874	0.93		0.0439
299	0.63	1.41	0.0072	0.80	1.57	0.009	0.45	1.21	0.0106	0.62	1.37	0.0142	0.54	1.30	0.0108
300 301	0.36 0.52	-0.19 0.18	0.01 0.0083	0.53 0.57	0.08	0.0101 0.0094	0.67 0.49	0.00	0.0064 0.0096	0.33 0.36	-0.13	0.0172 0.015	0.40 0.45	-0.03	0.0117 0.0133
302	0.67	0.41	0.009	0.59	0.34	0.0118	0.49	0.24	0.0083	0.45	0.19	0.0154	0.56	0.30	0.0105
303	0.63	-0.36	0.0059	0.87	-0.19	0.0058	0.86	-0.19	0.0065	1.17	0.12	0.0202	1.02	-0.03	0.0074
304 305	0.79 1.44	- 0.20 0.07	0.0144 0.0219	0.82 1.29	-0.41 -0.07	0.0048 0.0162	0.89 1.28	-0.35 -0.08	0.0111 0.0175	1.03 1.17	-0.20 -0.21	0.0208 0.0206	0.93 1.19	-0.30 -0.19	0.0168
305	0.45	1.36	0.0219	0.16	1.06	0.0162	0.08	0.98	0.0175	0.05	0.94	0.0206	-0.03	0.86	0.0123
307	0.50	-0.70	0.0231	0.81		0.0172	1.13		0.0441	0.64		0.0527	0.99		0.0554
308	0.88	-0.09 -1.65	0.0073	0.98 1.05	0.00 -1.55	0.0088	1.17 1.02	0.19 -1.57	0.0138	0.81	-0.15 -1.75	0.0076	1.00	0.04 -1.66	0.0168
309 310	0.88 1.07	-1.65 -0.16	0.0092 0.012	1.05	-1.55 -0.05	0.0075 0.0095	1.02	-1.57 -0.04	0.0128 0.0218	1.23	-1.75 -0.01	0.0127 0.0147	0.95 1.37	-1.66 0.13	0.0157 0.0105
311	0.76	-0.16	0.012	0.84	-0.36	0.0127	0.90	-0.30	0.0218	0.89	-0.31	0.0147	1.01	-0.19	0.0103
312	1.14	0.45	0.0126	1.25	0.56	0.0089	1.29	0.60	0.0211	1.30	0.61	0.0095	1.43	0.74	0.01
313 314	1.46 0.92	-0.70 -0.19	0.0146 0.0079	1.20 1.19	-0.96 0.08	0.0157 0.0076	1.20 0.55	-0.97 -0.56	0.0081	1.42 0.79	-0.74 -0.33	0.0129 0.0102	1.32 0.65	-0.84 -0.46	0.0097 0.0078
314	0.92	0.70	0.0079	0.58	0.08	0.0076	0.55	0.54	0.007	0.79	0.76	0.0102	0.65	0.75	0.0078
316	0.84	0.24	0.0077	1.13	0.52	0.0073	0.69	0.08	0.0098	0.90	0.18	0.0118	0.90	0.18	0.0076
317	0.92	-0.75	0.0175	0.96	-0.72	0.0139	1.04	-0.64	0.01	1.09	-0.59	0.0139	1.25	-0.42	0.0095
318 319	1.41 0.57	1.23 0.39	0.0211 0.0231	1.26 0.64	1.08 0.25	0.0125 0.0208	1.27 0.93	1.09 0.55	0.021 0.0071	1.28 0.47	1.10 0.08	0.0214 0.0138	1.27 0.65	1.09 0.26	0.0185 0.0126
319	0.76	-0.09	0.0052	0.54	-0.07	0.0208	0.93	-0.06	0.0071	0.47	0.00	0.0138	0.65	0.20	0.0126
321	4.21	1.75	0.2663	3.89	1.44	0.1959	5.06	2.61	0.2333	6.07	3.61	0.3982	6.42	3.96	0.3472
322 323	0.23	-0.13 0.10	0.0124	0.27	-0.41	0.0129	0.49	-0.20	0.0081	-0.01	-0.72	0.0115	0.35	-0.35	0.014
323 324	0.85 0.97	0.10 -0.29	0.0047	1.15 0.93	0.40 -0.32	0.0073	0.86 0.78	0.11 -0.48	0.0059 0.0307	0.95	0.02 -0.58	0.0074 0.0092	1.06 0.56	0.13 -0.72	0.0085
325	0.78	-0.80	0.0123	0.82	-0.76	0.0093	0.89	-0.69	0.0112	1.14	-0.44	0.0119	1.16	-0.42	0.0102
326	0.86	-0.54	0.0118	0.82	-0.63	0.0064	0.84	-0.62	0.01	1.06	-0.39	0.0136	1.06	-0.39	0.0116
327 328	0.84 1.17	-0.12 -0.01	0.0052 0.0109	0.66 1.14	-0.33 -0.04	0.0095 0.0139	0.71 1.00	-0.28 -0.18	0.0041	0.70 1.05	-0.28 -0.13	0.0134 0.0173	0.80 1.06	-0.18 -0.12	0.0062 0.0082
328 329	0.40	0.14	0.0109	0.50	0.07	0.0139	0.56	0.13	0.0063	0.79	0.29	0.0173	0.31	-0.12	0.0082
330	1.27	0.19	0.0209	0.84	-0.24	0.0292	1.20	0.11	0.0136	1.04	-0.05	0.0671	1.25	0.16	0.0194
331	2.93	-1.91	0.0086	3.00 1.23	-1.86	0.0148	3.33 4.98	-1.53 0.36	0.014	3.21	-1.65	0.0112 1.085	3.19	-1.67 -0.04	0.0092
332 333	5.17 1.26	0.54	0.4551 0.011	1.23	0.87	0.0216 0.0152	4.98 1.14	0.36 0.73	0.3017 0.0079	3.67 1.35	0.94	1.085 0.019	4.58 1.25	-0.04 0.84	0.3367 0.0115
555	1.20	0.00	0.011	4.4.	0.07	0.0131	4.4.4	5.75	0.0073	4.33	0.34	0.013	****	0.04	0.0113

		LogH	IL _T		LogHI	L ₈₁		LogHLe	12		LogH	L _{B3}		LogHL ₈₄	
ID	Pred. (h)	Res	HAT _{i/i} (h*=0.0489)	Pred. (h)	Res	HAT _{i/i} (h*=0.0535)	Pred. (h)	Res	HAT _{i/i} (h*=0.0533)	Pred. (h)	Res	HAT _{i/i} (h*=0.0578)	Pred. (h)	Res	HAT _{i/i} (h*=0.0574
334	0.88	-0.44	0.0091	1.11	-0.51	0.0076	0.92	-0.71	0.0112	1.10	-0.52	0.0161	1.28	-0.34	0.0116
335 336	1.12	-0.36	0.016	0.51 1.26	-0.98 -0.05	0.0476 0.0287	1.19 1.07	-0.31 -0.24	0.0131 0.0182	0.89	-0.61	0.0598 0.0373	1.37	-0.13	0.0145 0.027
337	0.98 1.37	0.87 -1.55	0.013 0.0184	1.30	-1.62	0.0183	1.42	-1.50	0.0172	1.24 1.69	-0.07 -1.23	0.0373	1.42 1.64	0.11 -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	0.45	0.0161	1.26	0.20	0.0137	1.24		0.0396	1.50		0.0187
340 341	1.93 2.03	-0.45 1.29	0.0175 0.0177	1.92 1.53	-0.46 0.79	0.0174 0.013	2.09 1.64	0.90	0.0069 0.0065	1.86 1.95	-0.53 1.21	0.0091 0.0098	1.95 2.03	-0.43 1.29	0.0061 0.0063
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	0.0738	7.08	1.60	0.0737	6.65	1.17	0.0596	6.30	0.82	0.0725	6.46	0.98	0.0627
344 345	1.24 1.40	-0.07 0.78	0.0247 0.0252	0.84	0.47	0.0186 0.0186	1.03 1.12	-0.27 0.51	0.0079	1.13	-0.18 0.69	0.0168 0.0135	1.22	-0.09 0.78	0.0081
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
348 349	1.02 0.59	0.26	0.008 0.0101	0.96 0.58	0.20	0.0052 0.0092	0.78 0.83	0.02	0.0124 0.0112	0.83	0.06 -0.07	0.0137 0.0124	0.94	0.17 0.16	0.0097 0.0121
350	1.15	-0.71	0.0217	1.05	-0.83	0.0214	1.46	-0.41	0.0112	1.34	-0.52	0.0174	1.37	-0.50	0.0121
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
352 353	0.65 1.10	0.45	0.0074 0.0127	0.91	0.70 0.80	0.0121 0.0229	0.78 0.95	0.57	0.0118 0.0124	0.80	0.60	0.019 0.023	0.79	0.59	0.0147
354	0.21	0.45	0.0127	0.55	0.78	0.0093	0.66	0.90	0.0124	0.38	0.61	0.023	0.48	0.70	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 1.32	0.06	0.0184	1.16	-0.31 -0.94	0.008	1.22	-0.24	0.014	0.96	-0.51	0.0376	1.15	-0.32	0.0192
357 358	0.95	-0.98 -1.12	0.0136 0.0193	1.40 1.10	-0.98	0.0099 0.0154	1.43 1.16	- 0.91 -0.92	0.0104 0.0164	1.52 1.08	-0.82 -1.01	0.0127 0.0131	1.67 1.20	-0.67 -0.88	0.0098
359	2.05	0.66	0.0177	1.84	0.46	0.0159	2.05	0.66	0.0077	2.01	0.62	0.0093	2.04	0.65	0.0063
360	1.32	0.02	0.0194	1.51	0.20	0.0235	1.53	0.22	0.0045	1.18	-0.12	0.0101	1.48	0.18	0.0131
361 362	0.44	0.29	0.0091	0.21	-0.19 0.76	0.0149	0.61	0.22	0.0087 0.0233	0.30	-0.09 0.84	0.0121 0.0124	0.50	0.11	0.0128
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	-0.43	0.0702	2.84	-0.41	0.1336	3.76	0.50	0.144
365 366	1.64 5.11	0.49	0.0216 0.0427	0.77 5.22	-0.38 0.27	0.0117 0.0411	1.13 5.51	-0.02 0.57	0.0175 0.0342	1.09 5.40	0.46	0.0384 0.0378	1.24 5.57	0.63	0.0193 0.0372
367	1.09	0.84	0.0241	0.80	0.55	0.0132	0.96	0.70	0.0262	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		0.011	0.39		0.0096	0.44		0.015
369 370	1.00	0.61 -0.53	0.0154	0.32	0.53 -0.66	0.0128	0.31	0.52 -0.33	0.0129	- 0.07 1.03	0.08 -0.50	0.0227	0.24	0.39 -0.61	0.0181
371	1.05	0.46	0.0134	0.97	0.37	0.0114	1.00	0.40	0.0211	0.96	0.36	0.0192	0.90	0.31	0.0115
372	0.94	-0.59	0.0096	0.98	-0.55	0.0067	0.87	-0.66	0.0273	0.83	-0.70	0.014	0.70	-0.83	0.0134
373 374	0.89	0.05	0.0065	1.10 1.26	-0.09 0.11	0.0077 0.0317	0.91 1.38	-0.29 0.23	0.0134 0.0133	0.90 1.06	-0.29 - 0.09	0.0096 0.035	0.89 1.36	-0.30 0.22	0.0088
374	1.01 0.71	0.19 -0.09	0.0261 0.0046	0.70	-0.93	0.0066	0.51	-1.11	0.0133	0.72	-0.99	0.035	0.61	-1.02	0.0158
376	0.75	0.29	0.0062	0.86	0.34	0.0073	0.82	0.30	0.0105	0.99	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
378 379	0.49 1.41	-0.30 1.01	0.0104 0.021	0.75 0.79	0.40	0.0084 0.008	0.63 1.30	0.91	0.0134 0.0125	0.74 0.89	0.47	0.009 0.0389	0.98 1.25	0.83	0.0139 0.0189
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	0.0565
382 383	0.22	-0.05 0.44	0.0164 0.0078	0.19	-0.33	0.0594 0.0155	0.36 0.43	-0.16	0.034 0.0159	0.76	0.22	0.0203 0.0103	-0.20 0.40	-0.74	0.2096 0.016
384	1.18	0.80	0.0274	1.17	0.79	0.0484	1.52	1.14	0.004	1.00	0.33	0.0275	1.33	0.66	0.0124
385	1.52	0.74	0.0173	1.30	0.48	0.0195	1.93	1.10	0.0179	1.93	1.05	0.0454	2.33	1.45	0.0263
386 387	0.93	-0.22 0.15	0.0061 0.0181	0.86 0.79	- 0.39 0.08	0.009 0.008	0.61 0.82	-0.64 0.11	0.0099 0.0069	0.69	-0.52	0.0154 0.0144	0.91 0.74	-0.30	0.0079 0.0123
388	0.82	0.68	0.0131	1.01	0.41	0.0113	1.13	0.53	0.01	1.12	0.52	0.0156	1.06	0.45	0.0123
389	1.93	-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
390 391	1.09 0.22	1.39	0.0321 0.0396	0.50 - 0.27	0.80 0.51	0.0252 0.0764	1.15 0.09	1.45 0.87	0.027 0.0272	1.22 0.26	1.52 1.02	0.0235 0.012	0.90 - 0.11	1.20 0.65	0.0074 0.0363
391	0.22	-0.61	0.0396	1.41	-0.14	0.0764	1.23	-0.32	0.0272	1.29	1.02	0.012	1.25	0.00	0.0363
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
394 395	0.70 1.40	-0.16 0.40	0.006 0.0183	0.65 1.34	-0.21 0.34	0.0059 0.0178	0.67 1.49	-0.19 0.49	0.0051 0.0064	0.55 1.44	-0.31 0.44	0.0082 0.0071	0.62 1.57	-0.24 0.57	0.0046
395 396	1.40 0.82	0.40 -0.13	0.0183 0.0138	1.34 0.85	0.34 -0.11	0.0178 0.0114	1.49 0.80	0.49 -0.16	0.0064	0.81	0.44 -0.15	0.0071	1.57 0.76	0.57 -0.20	0.0084 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
399 400	1.07 0.66	-0.91 0.22	0.0162 0.019	1.08 0.80	-0.90 0.34	0.0128 0.0144	1.02 0.89	-0.97 0.43	0.0288 0.0091	0.95	-1.02 0.38	0.0353 0.0133	1.45 0.84	-0.53 0.38	0.0451
400	2.11	0.22	0.019	1.55	-0.24	0.0241	1.43	-0.35	0.0191	2.62	0.30	0.0133	2.88	J.36	0.0122
402	1.06	0.32	0.0258	0.40	-0.34	0.033	1.19	0.45	0.0425	0.72	-0.02	0.0144	0.58	-0.16	0.0046
403 404	2.61 0.44	-1.11 0.04	0.0126	2.49 0.66	0.26	0.0113	2.57 0.70	-1.15 0.30	0.0072	2.65	-1.08	0.0085	2.61	-1.11	0.0066
404 405	0.44	-0.29	0.0134	0.66	-0.36	0.0083	0.70	-0.42	0.0067	0.21	-0.49 -0.36	0.0134 0.0139	0.43	-0.27 -0.46	0.0152
406	0.30	0.22	0.0087	0.56	0.33	0.0091	0.65	0.42	0.0078	0.27	0.01	0.0129	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
408 409	0.25	0.17 0.58	0.0114 0.0165	0.24	0.02	0.031 0.0191	0.25	0.03	0.0089	1.21	0.12	0.0124	0.33 1.14	0.10	0.0104
410	1.21	-0.49	0.0174	1.35	-0.35	0.0157	0.89	-0.82	0.0114	0.99	_	0.013	0.94	_	0.009
411	1.27	-0.89	0.0114	1.15	-1.01	0.0129	0.96	-1.20	0.0146	1.10	-1.07	0.0172	0.93	-1.24	0.0109
412 413	0.48	0.78	0.0068	0.17	0.47	0.0246	0.20	0.50	0.0164	0.22	0.47	0.016	-0.08	0.17	0.0234
413 414	0.67 1.62	0.47	0.0213 0.0174	0.52 1.30	0.32 -0.17	0.0218 0.0133	0.63 1.46	0.43 -0.02	0.0284	0.44 1.50	0.25	0.0333 0.0146	0.82 1.57	0.63	0.0221
415	0.70	0.76	0.0048	0.74	0.79	0.0067	0.64	0.70	0.0107	0.74	0.71	0.0141	0.59	0.56	0.0121
416	0.81	-0.63	0.0161	0.85	-0.59	0.0177	0.97	-0.47	0.033	1.00	`	0.0478	1.28	_	0.0532
417	0.57	0.23	0.0063	0.91	0.26	0.0056	0.67	0.02	0.0094	0.49	-0.16	0.0122	0.57	-0.08	0.0113

19							
Pet Pet	$LogHL_T$ $LogHL_{61}$ $LogHL_{62}$ $LogHL_{63}$	LogHL _T	!		LogHL ₈₄		_
1.37 0.31	Pred. Por HAT (/i Pred. Por HAT (/i Pred /h) Por HAT (/i Pred. Por HAT (/i	Por HAT i/i Pri		ID	HAT i/i		,
1-22 11 0.027	<u>0.79 -0.44 0.0078</u> 0.88 0.0066 0.75 0.0106 0.68 0.0087	-0.44 <u>0.0078</u> 0.	418 <u>0.79</u>	418	-0.34 0.0116	1.28	_
0.54 0.58 0.58 0.58 0.51 1.12 0.18 0.017 1.12 0.18 0.11 0.12 0.18 0.017 0.10	0.87 -0.03 0.0075 1.01 0.10 0.011 1.02 0.11 0.0121 0.90 -0.01 0.017 0.64 0.24 0.0073 0.69 0.28 0.0084 0.58 0.16 0.0169 0.48 0.07 0.0181						
1.50							
1.55							
1.15							
6.66 0.58 0.587							
1.22 0.079	1.21 1.06 0.0193 1.12 0.97 0.0117 1.35 1.20 0.0057 1.09 0.94 0.0169 0.74 -0.10 0.0062 0.82 0.0061 0.78 0.0076 1.07 0.0091	1.06 <u>0.0193</u> <u>1.</u> -0.10 0.0062 0.					
151 000 00077	0.37	0.62 0.01 0.	428 0.37	428	-0.09 0.0081	1.22	
1.5							
0.12 0.00000 0.00000 0.00000 0.00000 0.00000							
1.72 0.50 0.0144 0.50 0.0156 0.43 0.15 0.1	2.42 0.43 0.0111 2.15 0.16 0.0099 2.32 0.33 0.0055 2.47 0.48 0.0078						
1.25 0.25					0.16 0.0121	0.66	
0.79 0.99 0.0147							
0.00	0.51 0.40 0.008 0.41 0.29 0.06 0.33 0.21 0.0129 <u>0.58</u> <u>0.28</u> <u>0.0183</u>					0.79	
3.06 -0.40 -0.0077							
1.67	<u>1.04</u> <u>-0.34</u> <u>0.0101</u> <u>1.20</u> <u>-0.18</u> <u>0.0095</u> <u>1.44</u> <u>0.06</u> <u>0.0235</u> <u>1.13</u> <u>-0.26</u> <u>0.0149</u>	-0.34 0.0101 1.	439 1.04	439	-0.40 0.0077	3.08	
1.00							
1.68 0.053 0.0563 0.0563 0.0563 0.057 0.							
1.	0.72 0.34 0.0052 0.74 -0.09 0.0058 0.66 -0.17 0.0104 0.70 -0.13 0.0201	0.34 0.0052 0.	443 0.72	443	0.65 0.0063	2.04	
0.8 B 0.72 OBS 0.037 OBS 0.048 OBS 0.43 OBS 0.043 OBS 0.04	0.07 0.85 0.0102 0.30 1.07 0.0202 0.19 0.95 0.0229 0.26 1.03 0.0113						
1.76							
1.24						1.23	
5.57							
1.0 1.0							
	0.76 0.19 0.0064 <u>1.10</u> <u>0.51</u> <u>0.0136</u> <u>0.70</u> <u>0.12</u> <u>0.0112</u> <u>0.82</u> <u>0.23</u> <u>0.0106</u>				0.26 0.0232	0.52	
192 193 194 195							
1.00	0.82 -0.22 0.0052 0.95 -0.12 0.0059 0.98 -0.09 0.015 0.99 0.0111	-0.22 0.0052 0.	454 0.82	454	-0.61 0.0106	0.92	
0.39 0.008 457 0.40 0.64 0.0104 0.73 0.0071 0.62 0.021 0.69 0.0144 0.13 1.36 0.22 0.0078 459 0.48 0.22 0.0072 0.32 0.015 0.061 0.0061 0.061 0.0061 0.023 0.014 0.013 0.22 0.021 0.005 0.0119 0.23 0.016 0.023 0.024 0.005 0.0119 0.23 0.010 0.005 0.019 0.025 0.010 0.005 0.019 0.025 0.010 0.005 0.019 0.025 0.017 0.017 0.013 0.012 0.00 0.05 0.019 0.017 0.017 0.017 0.017 0.017 0.017 0.017 0.017 0.018 0.018 0.018 0.018 0.018 0.018 0.018 0.018 0.018 0.018 0.018 0.018 0.018 0.012 0.011 1.10 0.019 0.025 0.011 0.008 0.014					0.31 0.0115	0.90	
1.5							
1.13 0.25 0.125 0.155 0.65 0.75 0.125 0.155 0.15 0.155 0.15 0.155 0.	<u>0.46</u> <u>0.22</u> <u>0.0069</u> 0.85 0.61 0.0061 0.66 0.42 0.0078 0.32 -0.14 0.0156	0.22 0.0069 0.	458 <u>0.46</u>	458	0.22 0.0158	1.36	
1.13	0.48 0.20 0.0072 0.32 0.05 0.0119 0.23 -0.05 0.0103 0.52 0.24 0.0094	0.20 0.0072 0.					
1.5							
0.41 0.0072 464 0.94 0.31 0.0161 0.94 0.35 0.0161 0.94 0.35 0.0112 1.10 0.19 0.0096 1.08 0.50 0.010 0.75 -1.21 0.0565 465 0.94 -0.06 0.035 0.02 0.024 0.0096 0.04 0.096 0.02 0.0096 0.02 0.0096 0.01 0.07 0.08 0.02 0.0064 0.99 0.94 0.011 0.07 -0.88 0.020 0.04 0.0064 0.99 0.94 0.011 0.07 -0.88 0.020 0.021 0.04 0.007 0.0173 0.87 0.020 0.012 0.94 0.097 0.0173 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.0173 0.01 0.01 0.01 0.01 0.01 0.0173 0.01 0.01 0.00 0.01 0.00 0.01 0.00 0.01 0.00 0.01 0	<u>0.62</u> <u>-0.55</u> <u>0.0119</u> 0.60 -0.58 0.0039 0.53 -0.65 0.0044 0.36 0.0084						
0.25 1.12 0.9685 465 0.94 0.06 0.0135 0.72 0.05 1.02 0.02 0.0095 0.72 0.0095 0.72 0.0095 0.72 0.0095 0.72 0.0095 0.02 0.0095 0.72 0.0095 0.02 0.0095 0.72 0.0095 0.02 0.0095 0.02 0.0095 0.02 0.0045 0.002 0.0045 0.002 0.0045 0.002 0.0045 0.002 0.0045 0.002 0.0049 0.0119 0.04 0.003 0.012 0.0047 0.004 0.0047 0.004 0.0049 0.012 0.004 0.0049 0.012 0.004 <							
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$							
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	<u>0.78 -0.40 0.0067 0.74 -0.89 0.0064 0.69 -0.94 0.011</u> 0.77 -0.86 0.0222						
1.25							
1.06			469 3.29	469	1.45 0.0263	2.33	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$							
$\begin{array}{cccccccccccccccccccccccccccccccccccc$							
0.11	0.96 0.14 0.0097 1.13 -0.05 0.0099 1.17 -0.01 0.0189 1.10 -0.08 0.0223	0.14 0.0097 1.	473 0.96		-1.63 0.0355	2.56	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$							
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1.79 0.00 0.0164 1.42 -0.37 0.0124 1.55 -0.24 0.0073 <u>1.69</u> - <u>0.10</u> <u>0.0112</u>	0.00 0.0164 1.	476 1.79	476	0.0083	1.25	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	0.94 -0.04 0.0225 0.69 -0.29 0.0168 1.10 0.13 0.0187 <u>0.99</u> <u>0.01</u> <u>0.0105</u>	-0.04 0.0225 0.	477 0.94	477	<u>-0.06</u> <u>0.0066</u>	1.12	
0.76 -0.20 0.105 -0.20 0.105 -0.20 0.0105 0.88 -0.12 0.0126 0.79 0.09 0.0033 0.73 0.03 0.004 0.41 0.01 0.61 0.09 0.0224 481 0.21 0.00 0.0087 0.76 0.34 0.0556 0.64 0.222 0.008 0.76 0.34 0.0056 0.64 0.22 0.009 0.076 0.34 0.0533 0.99 0.18 0.0092 0.74 0.33 0.013 0.99 0.18 0.0092 0.74 0.33 0.013 0.99 0.18 0.0092 0.74 0.33 0.013 0.99 0.18 0.0092 0.74 0.33 0.013 0.99 0.18 0.0092 0.74 0.33 0.01 0.00 0.0092 0.0092 0.076 0.13 0.14 0.0092 0.078 0.14 0.0093 0.0092 0.078 0.0092 0.0092 0.0092 0.0092 0.0092 0.01 0.009							
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	0.58 -0.12 0.0126 0.79 0.09 0.0033 0.73 0.03 0.004 0.41 0.0117	-0.12 0.0126 0.	480 0.58	480	-0.20 0.0105	0.76	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$							
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0.58 -0.16 0.0046 486 0.79 0.03 0.0063 0.96 0.13 0.0072 1.02 0.19 0.0166 0.92 0.09 0.012 2.61 -1.11 0.0066 487 0.48 0.41 0.0078 0.64 0.38 0.0091 0.60 0.34 0.0062 0.50 0.24 0.009	0.48 0.14 0.005 <u>0.89</u> <u>0.47</u> <u>0.0056</u> <u>0.75</u> <u>0.33</u> <u>0.0106</u> 0.64 0.22 0.0106	0.14 0.005 0.	484 0.48	484	0.38 0.0122	0.84	
2.61 -1.11 0.0066 487 0.48 0.41 0.0078 0.64 0.38 0.0091 0.60 0.34 0.0062 0.50 0.24 0.009	0.84 0.20 0.0069 1.11 0.47 0.0063 0.62 -0.02 0.0123 0.74 0.10 0.0118	0.20 0.0069 1.					
	<u>2.08</u> <u>0.80</u> <u>0.0928</u> 0.60 0.0131 1.27 0.2126 1.42 0.2433	<u>0.80</u> <u>0.0928</u> 0.	488 2.08	488	<u>-0.27</u> <u>0.0152</u>	0.43	
<u>0.33</u> <u>0.10</u> <u>0.0104</u> 492 <u>1.73</u> <u>1.30</u> <u>0.0114</u> <u>1.82</u> <u>1.38</u> <u>0.0137</u> <u>1.77</u> <u>1.33</u> <u>0.0051</u> <u>1.71</u> <u>1.27</u> <u>0.009</u>	<u>1.73</u> <u>1.30</u> <u>0.0114</u> <u>1.82</u> <u>1.38</u> <u>0.0137</u> <u>1.77</u> <u>1.33</u> <u>0.0051</u> <u>1.71</u> <u>1.27</u> <u>0.0097</u>	1.30 0.0114 1.	492 <u>1.73</u>	492	0.10 0.0104	0.33	
<u>-0.08</u> <u>0.17</u> <u>0.0234</u> 496 0.51 -0.28 0.0049 <u>0.63</u> <u>0.0077</u> <u>0.43</u> <u>0.0109</u> 0.36 0.01	0.51 -0.28 0.0049 0.63 0.0077 0.43 0.0109 0.36 0.01	-0.28 0.0049 O.	496 0.51	496	0.17 0.0234	-0.08	
						0.82	
1.28 0.0532 500 0.28 0.17 0.008 0.58 0.36 0.0041 0.56 0.34 0.0103 0.31 0.09 0.009	0.28 0.17 0.008 0.58 0.36 0.0041 0.56 0.34 0.0103 0.31 0.09 0.0092	0.17 0.008 0.	500 0.28	500	0.0532	1.28	
0.57 -0.08 0.0113 501 1.59 0.55 0.011 1.20 0.16 0.0114 1.65 0.61 0.0039 1.79 0.56 0.006	1.59 0.55 0.011 1.20 0.16 0.0114 1.65 0.61 0.0039 1.79 0.56 0.0066	0.55 0.011 1.	501 1.59	501	-0.08 0.0113	0.57	

		LogH	IL _T		LogH	L ₈₁		LogHL	2		LogH	IL ₈₃		LogHL ₈₄	
ID	Pred. (h)	Res	HAT _{i/i} (h*=0.0489)	Pred. (h)	Res	HAT _{i/i} (h*=0.0535)	Pred. (h)	Res	HAT _{i/i} (h*=0.0533)	Pred. (h)	Res	HAT _{i/i} (h*=0.0578)	Pred. (h)	Res	HAT _{i/i} (h*=0.0574)
502	0.73	0.69	0.0071	0.81	0.76	0.0135	0.63	0.58	0.0076	0.69	0.64	0.0225	0.87	0.83	0.0064
503 504	3.78 0.96	-0.87 -0.04	0.0118 0.0107	3.82 0.61	-0.96 -0.43	0.0167 0.009	3.95 0.89	-0.84 -0.15	0.0165 0.0194	3.83 1.11	- 0.94 0.07	0.013 0.0336	3.78 1.14	-1.00 0.10	0.0121 0.029
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
506	1.15	0.34	0.018	0.80	-0.01	0.009	1.29	0.48	0.04	1.02	0.21	0.017	1.02	0.21	0.0126
507	3.16	-0.05	0.0101	3.13	-0.07	0.0119	3.26	0.05	0.0106	3.20	0.00	0.0091	3.14	-0.06	0.008
508	3.14	1.07 -0.38	0.0099	2.92	0.85	0.0082	3.00	0.93	0.0073	3.15	1.07	0.009	3.13	1.06	0.0079
509 510	3.10 3.29	0.47	0.0099 0.0121	3.13 3.16	-0.36 0.33	0.0108 0.0239	3.01 3.50	-0.47 0.68	0.0074 0.0174	3.16 3.37	-0.33 0.55	0.009 0.0105	3.08 3.31	-0.40 0.49	0.0077 0.0097
511	3.76	-0.57	0.0119	3.61	-0.81	0.0236	3.94	-0.48	0.0162	3.82	-0.60	0.0123	3.77	-0.66	0.0118
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
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
514 515	0.74	- 0.06 0.57	0.0057 0.0068	0.72 0.92	- 0.78 0.87	0.0076 0.0062	0.48 0.76	-1.03 0.71	0.0154	0.52	- 0.98 0.49	0.017 0.0096	0.45	-1.05 0.60	0.0161 0.0115
516	0.53	0.23	0.011	0.72	0.42	0.0048	0.51	0.20	0.0057	0.47	-0.11	0.0122	0.50	-0.07	0.0116
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
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
519 520	0.65 1.88	-0.01 0.30	0.0106 0.0164	0.80 1.66	0.13	0.0052 0.0121	0.56 1.80	-0.11 0.22	0.0057 0.0055	0.57 1.89	-0.10 0.31	0.0097	0.64 1.86	-0.03 0.28	0.0065
521	2.70	-0.30	0.0104	2.37	-0.64	0.0121	2.51	-0.50	0.0123	2.71	-0.30	0.0142	2.62	-0.38	0.0101
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
523	0.53	-0.22	0.0086	0.31	-0.76	0.0748	0.64	-0.42	0.0208	0.81		0.0076	0.19		0.1054
524	0.50	-0.01	0.0148	0.44	-0.12 0.41	0.0235	0.31	-0.25	0.0338	0.62	0.05	0.0221	0.18	-0.39	0.0356
525 526	0.89 0.76	0.29 0.76	0.0186 0.0117	1.01 0.61	0.41	0.0147 0.014	1.10 0.57	0.50 0.56	0.0071 0.0082	1.18 0.96	0.58	0.0069	0.69	0.63	0.008
527	0.29	0.42	0.0186	0.46	-0.01	0.0204	0.35	-0.12	0.0156	0.71	0.23	0.0134	0.57	0.09	0.0111
528	0.68	-0.64	0.0091	1.05	-0.27	0.0226	0.78	-0.54	0.012	0.89		0.0252	0.85		0.0142
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
530 531	0.71	0.16	0.0054	0.86 0.75	0.31 -0.12	0.0055 0.016	0.76 0.47	0.21 -0.39	0.0074 0.0148	0.56	-0.03 -0.10	0.0089	0.62	0.03 -0.35	0.0077
532	0.33	-0.44	0.0119	0.75	-0.12	0.0058	0.47	-0.33	0.0124	0.76	-0.10	0.0099	0.43	-0.33	0.0136
533	1.18	-0.20	0.0183	0.94	-0.45	0.0136	1.05	-0.34	0.0043	1.36	-0.07	0.0179	1.27	-0.16	0.0058
534	1.79	0.21	0.0163	1.44	-0.14	0.0124	1.55	-0.03	0.0073	1.71	0.13	0.0107	1.75	0.17	0.0068
535	1.96 1.96	0.88	0.0172	1.58	0.50	0.0134	1.64	0.56	0.0065	1.92 1.93	0.84	0.0087	1.93	0.85	0.0063
536 537	4.28	0.33 -0.83	0.0171 0.0155	1.61 4.53	-0.03 -0.61	0.012 0.0194	1.80 4.40	0.16 -0.74	0.0055 0.0181	4.29	-0.85	0.0086 0.0171	1.96 4.26	0.33 -0.88	0.0058 0.0161
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
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
540	4.88	-0.48	0.0246	4.90	-0.48	0.0353	5.08	-0.30	0.0273	4.86	-0.53	0.0253	4.86	-0.53	0.024
541 542	0.69	-0.63 0.38	0.0173 0.0153	0.84 0.50	-0.49 0.53	0.0105 0.014	1.13 0.44	-0.20 0.47	0.016 0.007	0.33	-0.99 0.59	0.013 0.0113	0.56 0.52	-0.76 0.51	0.0303 0.01
543	2.28	0.40	0.0133	2.26	0.38	0.0094	2.24	0.36	0.0058	2.31	0.43	0.0015	2.22	0.34	0.0071
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
545	4.19	-1.22	0.0152	4.35	-1.05	0.0189	4.39	-1.01	0.018	4.20	-1.20	0.0158	4.14	-1.27	0.0154
546 547	0.55	0.06	0.008	0.69	0.16	0.0133	0.84	0.32	0.0053	0.60	0.06	0.0061	0.65	0.11	0.0058
547	4.52 0.71	-0.08 0.31	0.0279 0.0056	4.61 0.88	-0.12 0.49	0.0321 0.0061	4.96 0.53	0.23	0.0269 0.0125	4.82 0.56	0.09	0.0252 0.0115	4.93 0.68	0.20	0.0259
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
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
551	2.07	0.47	0.04	1.30	-0.29	0.0136	1.80	0.21	0.0276	1.93	0.34	0.062	2.10	0.52	0.0337
552 553	0.18	-1.47 0.38	0.0101 0.01	0.59	-1.23 -0.02	0.0092 0.0178	0.54	-1.28 -0.10	0.0194 0.0112	0.56	-1.26 0.01	0.0115 0.0141	0.38	-1.44 -0.10	0.0323 0.0146
554	1.42	1.09	0.0182	1.40	0.84	0.0178	1.33	0.77	0.0112	1.40	0.84	0.0062	1.50	0.94	0.0052
555	1.27	-0.31	0.0106	1.34	-0.28	0.0087	1.68	0.06	0.0126	1.67		0.0277	1.64		0.015
556	0.14	-0.54	0.0906	-0.52		0.2485	0.19		0.0523	0.78		0.0377	-0.65		0.4238
557 558	0.59	0.04	0.0047	0.56	-0.12	0.0061	0.35	-0.33	0.0128	0.37 2.08	-0.31 -0.40	0.0137	0.23	-0.45 -0.38	0.0136
558 559	2.18 2.36	-0.31 0.18	0.0121 0.0111	1.96 2.18	-0.52 0.00	0.0123 0.0086	1.97 2.23	-0.51 0.05	0.0094 0.0058	2.34	0.16	0.0122	2.10 2.32	0.14	0.0085 0.0062
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
561	2.66	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
562	3.55	0.07	0.0103	3.59	0.11	0.013	3.45	-0.04	0.0099	3.53	0.05	0.0113	3.50	0.02	0.0103
563 564	0.52	0.12 0.01	0.0043 0.0098	0.69 0.95	0.30 0.07	0.0074 0.005	0.39 1.04	-0.01 0.16	0.0087 0.0063	0.57	0.13	0.0068	0.43	-0.01	0.0092
565	3.21	0.01	0.0098	3.15	0.14	0.0225	2.94	-0.07	0.0183	3.12	0.11	0.0104	3.10	0.09	0.0137
566	3.65	-0.84	0.0106	3.80	-0.69	0.0128	3.70	-0.78	0.0115	3.67	-0.81	0.0118	3.61	-0.87	0.0107
567	3.53	0.30	0.0102	3.39	0.16	0.0099	3.44	0.21	0.0099	3.52	0.30	0.0104	3.48	0.26	0.0102
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
569 570	4.03 4.01	0.39	0.0147 0.0149	4.09 3.88	0.45	0.0185 0.0167	3.89 3.88	0.25	0.0152 0.0155	3.98 3.96	0.34	0.015 0.0152	3.95 3.93	0.32	0.0149
571	4.24	-0.32	0.0143	4.10	-0.45	0.0265	4.38	-0.17	0.0179	4.25	-0.30	0.0152	4.22	-0.34	0.0151
572	4.40	-0.97	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
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	0.75	0.25	0.007
574 575	3.61	0.68	0.0199	3.65 4.56	0.72 1.15	0.0327 0.0268	3.38 4.42	0.44 1.02	0.0278 0.0229	3.48	0.54	0.023	3.45	0.51	0.0216
575 576	4.65 2.02	1.25 0.24	0.0235 0.0139	1.87	0.09	0.0268	1.89	0.10	0.0229	4.57 1.91	1.17 0.13	0.0221 0.0161	4.58 1.92	1.17 0.14	0.0218
577	2.18	-0.07	0.0133	1.98	-0.27	0.0123	1.98	-0.28	0.0094	2.10	-0.16	0.0118	2.10	-0.15	0.0015
578	2.44	-0.27	0.0117	2.17	-0.54	0.0088	2.23	-0.48	0.0058	2.43	-0.27	0.0074	2.42	-0.28	0.0058
579	2.16	-0.54	0.0122	1.79	-0.92	0.0121	1.97	-0.73	0.0094	2.10	-0.60	0.0116	2.09	-0.61	0.0085
580 581	2.43 2.49	0.28 0.99	0.0115 0.0121	2.08	-0.06 0.71	0.0126 0.0115	2.06	-0.08 0.97	0.008	2.34 2.52	0.20 1.02	0.0093 0.0067	2.38	0.24	0.0063 0.0058
581	2.50	0.53	0.0121	2.21	0.71	0.0115	2.47	0.35	0.005	2.52	0.55	0.0067	2.49	0.59	0.0058
583	2.68	0.90	0.0133	2.23	0.45	0.0134	2.16	0.39	0.0072	2.64	0.86	0.0091	2.67	0.90	0.0073
584	2.61	0.83	0.0128	2.66	0.88	0.0155	2.74	0.96	0.0104	2.61	0.83	0.0091	2.58	0.80	0.0068
585	2.67	0.89	0.0132	2.53	0.75	0.0187	2.82	1.04	0.0122	2.73	0.95	0.008	2.68	0.90	0.007

L	LogHL ₈₄		-		_		LogH	L _T		LogHI	81		LogHL	82		LogH	L _{B3}		LogH
	Por	HAT ;/i (h*=0.0574)	74		ID	Pred. (h)	Res	HAT _{i/i} (h*=0.0489)	Pred. (h)	Res	HAT _{i/i} (h*=0.0535)	Pred. (h)	Res	HAT _{i/i} (h*=0.0533)	Pred. (h)	Res	HAT _{i/i} (h*=0.0578)	Pred. (h)	Re
	0.83	0.0064			586	2.78	-0.19	0.0098	2.28	-0.68	0.0143	2.49	-0.47	0.0121	2.74	-0.23	0.0099	2.72	-0
	-1.00	0.0121			587	0.62	-0.03	0.0094	0.66	0.01	0.0064	0.50	-0.15	0.0056	0.55	-0.09	0.0074	0.53	-0.
	0.10	0.029			588 589	0.35	0.42	0.0097	0.40	-0.83	0.0339 0.0489	0.57	-0.66	0.0075 0.0435	0.50	-0.73	0.0104	0.54	<u>-0.</u>
	0.53	0.007 0.0126			590	5.49 3.94	1.32 -0.99	0.0557 0.0169	5.76 4.04	1.55 -0.93	0.0489	5.78 4.42	1.57 -0.55	0.0211	5.65 4.24	1.44 -0.72	0.0543 0.0167	5.85 4.29	<u>1.</u> -0.
	-0.06	0.008			591	3.59	-0.19	0.0104	3.78	0.00	0.0194	3.46	-0.33	0.0099	3.63	-0.16	0.0117	3.55	-0.
	1.06	0.0079			592	0.55	-0.36	0.0064	0.33	-0.59	0.011	0.31	-0.61	0.0087	0.57	-0.34	0.0099	0.50	-0
	0.40	0.0077			593	5.13	-0.27	0.0279	5.14	-0.32	0.0416	5.34	-0.12	0.0356	5.14	-0.32	0.0317	5.16	-0
	0.49 -0.66	0.0097 0.0118			594 595	0.58 4.60	-0.17 -0.04	0.0095 0.0233	1.04 4.90	-0.03 0.26	0.0063 0.0275	0.70 4.60	-0.37 -0.04	0.0091 0.0212	0.85 4.52	-0.19 -0.12	0.0087 0.0215	0.95 4.50	<u>-0</u>
	-0.55	0.008			595 596	5.09	0.21	0.0233	5.49	0.26	0.0275	5.05	0.17	0.0212	4.52	0.06	0.0215	4.50	<u>-0.</u>
	-0.21	0.0244			597	6.12	0.45	0.0546	6.38	0.71	0.0566	6.24	0.57	0.0466	5.96	0.29	0.0523	6.06	0.
	-1.05	0.0161			598	3.44	-1.44	0.0109	3.51	-1.40	0.018	3.87	-1.03	0.0168	3.73	-1.18	0.0127	3.74	-1.
	0.60	0.0115			599	0.52	0.20	0.0111	0.79	0.44	0.0063	0.61	0.27	0.0062	0.46	0.12	0.0121	0.49	0.
	-0.07 -0.17	0.0116			600	1.75	-2.67	0.0205	2.44	-2.08	0.0586	1.96	-2.56	0.0238	2.21	-2.31	0.031	2.19	-2.
	0.17	0.0077			601 602	0.61 4.18	-0.25 -0.76	0.009 0.0157	0.78 4.18	-0.09 -0.75	0.0044 0.0273	0.71 4.39	-0.16 -0.55	0.004 0.0182	0.35 4.20	-0.74	0.0073 0.0175	0.45 4.12	-0
-0.		0.0065			603	4.89	-0.25	0.0248	4.92	-0.73	0.0275	5.09	-0.05	0.0132	4.87	-0.74	0.0258	4.86	-0
	.28	0.0061			604	2.80	-0.18	0.0095	2.49	-0.49	0.0122	2.50	-0.48	0.0119	2.74	-0.24	0.0099	2.73	<u>-0</u>
-0.	38	0.0101			605	2.92	-0.10	0.0093	3.01	-0.01	0.0115	2.92	-0.10	0.007	2.89	-0.13	0.01	2.86	-0
-0.	01	0.0062			606	2.58	0.10	0.0121	2.58	0.09	0.0186	2.41	-0.07	0.0138	2.47	-0.01	0.0159	2.46	-0
		0.1054			607 608	3.11	1.04	0.0101	2.72	0.65	0.0113	3.00	0.93	0.0071	3.15 2.99	0.05	0.0078	3.12 2.95	10
0.6		0.0356			608	2.98 2.56	0.04	0.0091 0.0121	2.69	-0.25 -0.10	0.008 0.0138	2.75 2.41	-0.19 -0.07	0.0076 0.014	2.99	0.05	0.0078 0.0157	2.95	-0
0.0		0.0147			610	3.53	-0.26	0.0102	3.38	-0.40	0.0099	3.44	-0.34	0.0099	3.52	-0.26	0.0104	3.48	-0
0.0		0.0111			611	0.64	-0.44	0.0069	0.46	-0.81	0.0145	0.47	-0.81	0.0047	0.63	-0.65	0.0166	0.79	-0
		0.0142			612	0.53	0.45	0.0101	0.59	-0.22	0.017	0.46	-0.35	0.0228	0.85	0.04	0.0136	0.47	-0
	.06	0.01 0.0077			613 614	0.82 0.33	0.52	0.0249 0.0204	0.87 0.59	0.57 0.51	0.021 0.0193	1.13 0.41	0.83	0.0058 0.0163	0.72	0.13	0.01 0.0138	0.71	0
	.35	0.0077			615	0.68	-0.29	0.0204	0.59	-0.54	0.0193	0.41	-0.63	0.0163	0.78	-0.69	0.0138	0.61	0
٠	-	0.0114			616	0.67	-0.33	0.0221	0.11	0.54	0.0203	0.51	0.03	0.0181	0.86	0.03	0.013	1.10	•
-0.16		0.0058			617	0.84	0.10	0.0072	0.72	-0.56	0.0064	0.64	-0.64	0.0121	0.90	-0.38	0.0101	0.81	-1
0.17		0.0068			618	0.86	0.18	0.0077	1.18	0.47	0.0102	0.88	0.17	0.0109	0.75	0.05	0.0086	0.84	0
		0.0063			619	5.40	0.40	0.0363	5.72	0.71	0.0381	5.55	0.54	0.0328	5.31	0.31	0.0335	5.34	9
		161			620 621	0.87 0.92	0.15	0.0165 0.0123	1.09 0.72	0.36	0.0146 0.012	1.01 0.70	0.28	0.0116 0.0078	1.22 0.80	0.49	0.0112 0.0149	1.30 0.88	2
-0.71 0.016					622	0.61	-0.16	0.0063	0.72	0.08	0.0043	0.66	-0.13	0.0043	0.49	-0.03	0.0143	0.42	0
-0.79 0.023					623	1.01	-0.29	0.02	0.96	-0.34	0.0187	1.16	-0.14	0.0054	1.09	-0.21	0.0118	0.89	-0
-0.53 0.024	0.024				624	0.36	0.31	0.0102	0.49	-0.71	0.0158	0.56	-0.63	0.0094	0.64	-0.56	0.0109	0.57	-0
<u>-0.76</u> <u>0.0303</u>					625	1.09	0.55	0.0126	1.16	0.62	0.0068	0.96	0.42	0.013	1.01	0.46	0.0096	0.83	0
0.51		0.01			626	1.03	0.73	0.0132	0.94	0.64	0.0046	1.20	0.89	0.0243	0.86	0.56	0.0117	0.75	0
0.34 -0.97		0.0071			627 628	3.23 0.97	0.30	0.0148	3.76 1.07	0.09	0.0562 0.0058	4.09 0.88	0.43	0.0515 0.0041	3.50 1.12	- 0.17 0.43	0.0146 0.0094	3.50 1.10	-1
		0.0065			629	0.97	0.30	0.0034	0.80	0.40	0.0123	0.86	0.21	0.0041	0.78	0.43	0.0149	0.52	
0.11	ď	.0058			630	0.64	0.08	0.0068	0.74	0.17	0.0118	0.50	-0.08	0.0168	0.48	-0.10	0.0184	0.37	-4
0.20		0.0259			631	0.52	0.44	0.0187	0.45	0.11	0.0213	0.53	0.18	0.0125	0.71	0.37	0.0139	0.48	9
		.0099			632	0.15	0.07	0.023	0.52	-0.26	0.0178	0.41	-0.37	0.0109	0.69	-0.08	0.0133	0.54	-1
-0.85		0.0116			633	1.16	0.49	0.0235	0.90	0.23	0.0208	1.17	0.50	0.008	1.17	0.25	0.013	1.35	
<u>-0.40</u> <u>0.52</u>		0.0075			634 635	4.19 0.70	-1.18 0.00	0.015 0.0096	4.34	-1.03 0.05	0.018 0.0068	4.15	-1.22 -0.03	0.0148 0.0091	4.17	-1.20 -0.07	0.0157 0.0088	4.14 0.57	4
-1.44		0.0323			636	0.70	-0.33	0.0056	0.76 0.95	-0.37	0.0053	0.67 0.97	-0.35	0.012	0.64 1.16	-0.07	0.0207	1.04	- 4
-0.10		0.0146			637	1.44	-1.19	0.0169	1.26	-1.37	0.0134	0.91	-1.72	0.0125	1.12	-1.52	0.0283	1.13	- 3
0.94		0.0052			638	2.68	2.17	0.09	1.75	1.24	0.0238	1.14	0.63	0.048	1.90	1.39	0.0788	1.28	(
		0.015			639	2.98	0.04	0.0093	2.83	-0.11	0.0076	2.91	-0.03	0.0068	3.00	0.06	0.0077	2.95	9
-0.45		0.4238 0.0136			640 641	3.19 3.46	-0.42 -0.15	0.0123 0.0106	2.95	-0.66 -0.33	0.0184 0.0227	2.93	- 0.67 -0.57	0.0187	3.11 3.39	-0.50 -0.22	0.0151 0.0114	3.08 3.38	<u>-0</u>
-0.45		0.0136			642	3.46	0.25	0.0106	3.27 3.18	-0.33	0.0227	3.03 3.43	0.18	0.0161 0.01	3.51	0.26	0.0114	3.38	-0
		0062			643	3.86	0.33	0.0163	3.79	0.26	0.0321	3.48	-0.05	0.0248	3.76	0.23	0.0169	3.74	ď
0.25 0.0	0.0	069			644	4.26	0.78	0.0274	4.33	0.85	0.0482	3.92	0.44	0.0367	4.10	0.61	0.0266	4.09	9
0.91 0.0069					645	4.44	0.96	0.0246	4.66	1.18	0.0306	4.34	0.86	0.0239	4.33	0.85	0.023	4.31	9
0.02 0.03					646	4.17	-0.62	0.0149	4.13	-0.66	0.0154	4.14	-0.65	0.0148	4.15	-0.64	0.0153	4.12	4
-0.01 0.0092 0.0137					647 648	4.67 4.77	-0.46 0.03	0.0229	4.89 5.09	-0.26 0.35	0.0274 0.0262	4.60 4.85	-0.55 0.11	0.021 0.0223	4.61 4.74	-0.54 0.00	0.0215 0.0225	4.60 4.72	-1
0.0137					649	4.77	-0.23	0.0232	4.67	-0.21	0.0262	4.58	-0.30	0.0214	4.57	-0.31	0.0223	4.72	-4
-0.87 0.0107	0.0107				650	4.75	-0.16	0.0235	4.88	-0.03	0.0253	4.84	-0.07	0.0225	4.71	-0.20	0.0229	4.69	3
0.26 0.0102					651	4.43	-0.59	0.0171	4.57	-0.48	0.0247	4.65	-0.41	0.0249	4.46	-0.59	0.0195	4.43	-1
0.42 0.0103					652	5.08	1.50	0.0375	5.17	1.59	0.0439	4.87	1.29	0.0348	4.90	1.32	0.0333	4.93	1
0.32 0.0149 0.45 0.0151					653 654	4.90 5.38	-0.93 - 0.92	0.0242	4.80 5.38	-1.03 -0.93	0.0243 0.0379	4.68 5.13	-1.14 -1.17	0.0213 0.0303	4.86 5.27	-0.97 -1.03	0.0246 0.0333	4.87 5.33	-()-
-0.34 0.0151					655	5.38	-0.92 -0.08	0.0356	5.38	-0.93 0.25	0.0379	5.13	-1.17 0.07	0.0303	5.32	-1.03 -0.16	0.0333 0.0336	5.33 5.34	-(-(
-1.03 0.0182					656	5.38	0.24	0.0367	5.50	0.36	0.0426	5.53	0.39	0.0325	5.27	0.13	0.0355	5.34	0
0.25 0.007	0.007				657	5.91	0.83	0.0533	6.38	1.29	0.0542	5.99	0.91	0.0422	5.72	0.63	0.0464	5.79	0
0.51 0.0216					658	3.83	0.35	0.0162	3.57	0.09	0.0268	3.47	-0.01	0.0254	3.74	0.25	0.0177	3.72	0
1.17 0.0218 0.14 0.0115					659	4.18 4.59	0.39 1.06	0.0151 0.0243	4.03	0.24	0.016 0.0276	3.98 4.43	0.20	0.015 0.0232	4.15	0.37	0.0154	4.13	0.
0.14 0.0115 -0.15 0.0085					660 661	4.59 3.85	0.55	0.0243	4.60 3.77	1.07 0.47	0.0276	4.43 3.48	0.90	0.0232	4.50 3.75	0.97	0.0228	4.48 3.74	0.
-0.15 0.0085					662	1.08	0.05	0.0162	1.24	0.47	0.0319	1.32	0.17	0.0081	1.21	0.17	0.0189	1.07	0.
-0.61 0.0085					663	2.25	-0.45	0.055	1.01	-1.70	0.0105	1.59	-1.12	0.0539	1.48		0.1234	1.68	
0.24 0.0063					664	1.20	0.33	0.0134	1.19	0.04	0.0132	0.73	-0.43	0.0121	0.98	-0.17	0.0135	1.04	-0
0.99 0.0058					665	0.70	-0.38	0.0059	0.90	-0.43	0.0073	0.81	-0.53	0.0086	1.03	_	0.0115	0.80	
0.52 0.0058					666	0.56	0.23	0.0089	0.94	0.60	0.0095	1.09	0.76	0.015	0.55	0.16	0.0129	0.80	0
0.90 0.0073 0.80 0.0068	0.0073 0.0068				667 668	0.99 0.36	-0.31 -0.40	0.0237 0.0076	1.28 0.75	-0.02	0.0206 0.0061	1.23 0.75	-0.07	0.0061 0.0147	1.08 0.57	-0.23	0.0161 0.0134	1.12 0.65	<u>-(</u>
	0.0000				669	0.36	0.60	0.0076	0.75	0.72	0.0158	0.75	0.94	0.0085	0.84	0.87	0.0134	0.87	0.

		LogH	IL _T		LogH	L ₈₁		LogHL	32		LogH	L _{B3}		LogHL ₈₄	
ID	Pred.	Res	HAT _{i/i} (h*=0.0489)	Pred. (h)	Res	HAT _{i/i} (h*=0.0535)	Pred. (h)	Res	HAT _{i/i} (h*=0.0533)	Pred. (h)	Res	HAT _{i/i} (h*=0.0578)	Pred. (h)	Res	HAT _{i/i} (h*=0.0574)
670	0.89	-0.55	0.0089	0.98	-0.46	0.018	1.43	-0.01	0.023	0.93	-0.52	0.0102	1.13	-0.32	0.0183
671	0.87	-0.53 0.25	0.0089	0.88	-0.52	0.017	1.28	-0.12	0.0184	0.83	-0.57 0.10	0.0094	0.93	-0.47 0.05	0.0131
672 673	2.46	1.38	0.0074 0.0602	0.75 0.87	0.43 -0.45	0.0069 0.0046	0.28 1.59	-0.03 0.27	0.0108 0.0459	1.67	0.10	0.0147	1.79	0.48	0.0109
674	0.67	0.44	0.0128	0.92	0.67	0.0072	1.02	0.77	0.011	0.50	0.25	0.011	0.55	0.30	0.0097
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	0.74	0.38	0.0105
676 677	1.02	-2.44 0.25	0.0075 0.0233	0.68	-2.79 -0.50	0.0037 0.0065	0.89 0.91	-2.58 - 0.29	0.0257 0.0229	0.75 1.03	-2.71 -0.23	0.0178 0.0451	0.65 1.16	-2.81 -0.10	0.0075 0.0259
678	1.72	0.25	0.0233	0.70	-0.76	0.0068	1.09	-0.59	0.0229	1.23	-0.23	0.0306	1.36	-0.10	0.0239
679	0.63	-0.37	0.0071	0.74	-0.26	0.0221	0.53	-0.47	0.0075	0.41	-0.60	0.0301	0.67	-0.34	0.0076
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	0.39	-1.31	0.0135
681 682	0.85 1.55	-0.10 -0.45	0.0077 0.0289	1.00 1.48	0.04 -0.54	0.0108 0.0262	0.88 1.50	-0.08 -0.52	0.0075 0.0079	0.85 1.73	-0.12 -0.30	0.0117 0.014	0.83 1.71	-0.14 -0.31	0.01 0.0077
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	4.11	0.32	0.0155
684	0.74	0.67	0.01	0.87	0.81	0.0069	0.69	0.63	0.0139	0.57	0.50	0.0142	0.86	0.79	0.0123
685 686	0.13 4.85	0.09	0.0171 0.0366	0.29 5.22	-1.15 0.47	0.0183 0.046	0.33 5.36	-1.11 0.62	0.0086 0.0413	0.44 5.04	-1.00 0.28	0.0092 0.0352	0.40 5.17	-1.04 0.41	0.0087
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	2.40	0.24	0.0063
688	2.32	0.29	0.0115	1.95	-0.08	0.0115	2.07	0.04	0.008	2.33	0.29	0.0092	2.28	0.24	0.0067
689	0.69	0.18	0.0078	0.75	0.12	0.0165	0.44	-0.19	0.0087	0.81	0.17	0.0194	0.51	-0.12	0.0096
690 691	0.50	0.39 -0.90	0.0072 0.0097	0.69	0.40 -0.41	0.0088 0.0427	0.57 0.87	0.28 -0.43	0.0067 0.0116	0.57	0.27 -0.39	0.0094 0.0109	0.63	0.33 -0.35	0.0092 0.0134
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	0.81	0.25	0.0077
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	0.50	-0.11	0.0091
694 695	0.68	-0.46 -0.43	0.0067	1.04 -0.55	-0.10	0.0059	0.62	-0.53	0.0083	0.70	-0.45	0.0099 0.0161	0.55 -1.45	-0.60	0.0078 1.2842
696	0.81	0.10	0.006	0.83	0.00	0.0079	0.74	-0.09	0.0372	0.94	0.11	0.0181	0.93	0.10	0.0071
697	0.56	-0.48	0.0037	0.72	-0.32	0.0085	0.51	-0.54	0.0069	0.61		0.0081	0.50		0.0072
698	3.26	1.08	0.0116	3.48	1.30	0.0232	3.12	0.93	0.0134	3.22	1.04	0.0137	3.15	0.97	0.0125
699 700	3.65 1.39	0.64 0.46	0.0107 0.0157	3.81 1.23	0.80	0.0127 0.0174	3.70 1.08	0.70 0.16	0.0115 0.0048	3.68 1.38	0.68	0.0116 0.0167	3.62 1.32	0.61	0.0107 0.0078
701	0.13	-0.05	0.0259	0.60	0.23	0.0124	0.44	0.08	0.0079	0.61	0.22	0.0103	0.53	0.13	0.0111
702	0.96	0.04	0.0091	0.71	-0.30	0.0152	0.73	-0.28	0.0075	0.85	-0.16	0.0218	1.07	0.06	0.0077
703 704	3.86 3.72	-0.84 -0.31	0.0218 0.0168	4.17 4.21	-0.63 0.12	0.051 0.0498	4.51 4.51	-0.29 0.42	0.0455 0.0454	4.14 3.97	-0.66 -0.13	0.0223 0.0167	4.19 3.99	-0.62 -0.10	0.0222 0.0168
704	4.35	-0.59	0.0274	4.67	-0.40	0.0498	4.93	-0.14	0.0419	4.59	-0.13	0.0167	4.68	-0.10	0.0168
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	0.48	-0.89	0.0084
707	3.92	-0.24	0.0139	3.86	-0.36	0.0311	4.20	-0.02	0.025	4.01	-0.21	0.0157	3.95	-0.27	0.0146
708 709	0.57 4.01	0.70 -1.38	0.0129 0.0185	0.83 4.03	0.97 -1.47	0.0053	0.44 4.41	0.59 -1.09	0.0124	<u>-0.02</u> 4.32	0.10 -1.18	0.0266	0.33 4.38	0.44 -1.12	0.0139
710	1.49	0.81	0.0257	1.56	0.89	0.0228	1.62	0.95	0.0069	1.76	1.08	0.0155	1.96	1.28	0.0099
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	1.17	0.29	0.0091
712 713	1.12	-0.22	0.0239 0.0116	1.24	-0.11	0.02 0.0307	1.33	-0.02 -0.54	0.0086 0.016	0.98	0.00 -0.26	0.0134	0.62	0.06 - 0.62	0.0091
713	0.58 3.38	-0.62 -1.37	0.1289	0.65 4.08	-0.59 -0.82	0.1647	0.70 3.82	-1.08	0.1269	4.39	-0.52	0.1585	4.52	-0.82	0.0526
715	0.63	0.94	0.0034	0.29	0.59	0.0185	0.33	0.63	0.0192	0.42	0.71	0.0157	0.21	0.51	0.0176
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 0.0153	0.44	0.15	0.0117 0.015
717 718	4.13 4.21	0.25 -0.73	0.0147 0.0152	4.31 4.56	0.43 -0.38	0.0162 0.0192	4.15 4.40	0.27 -0.53	0.0148 0.0182	4.13	-0.72	0.0153	4.07 4.16	-0.78	0.015
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	1.55	1.06	0.0124
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	1.24	0.42	0.0072
721 722	1.19 2.25	-0.32 -0.54	0.0094 0.1042	1.35 0.66	-0.22	0.0119 0.0201	0.97 1.51	-0.59 -1.29	0.0076 0.3299	1.11 1.80	-0.46	0.0209 0.3139	0.96 1.95	-0.60 -0.85	0.0089
723	0.19	-0.58	0.0115	0.58		0.0094	0.46	-1.23	0.0153	0.62		0.0105	0.41	-0.03	0.0236
724	0.19	-0.54	0.0128	0.38		0.0098	0.34		0.0091	-0.13		0.0129	0.07		0.0132
725 726	3.43	-0.35 -0.14	0.0103 0.0115	3.06	-0.72	0.0164	3.03	-0.76	0.0163	3.38	-0.40	0.0109 0.0135	3.37	-0.41	0.0106
727	3.34 4.15	-0.33	0.0113	3.70 4.52	0.22	0.021 0.0244	3.37 4.16	-0.12 -0.33	0.0102 0.0148	3.29 4.15	-0.19 -0.34	0.0159	3.23 4.09	-0.25 -0.39	0.0118 0.015
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	1.59	0.93	0.0371
729	0.88	-0.12	0.0073	0.92	-0.09	0.012	1.15	0.14	0.012	0.80	-0.20	0.007	0.97	-0.03	0.0146
730 731	2.33 1.22	-1.78 1.04	0.0446 0.0151	3.26 1.31	-0.90 1.13	0.1162 0.0102	2.70 0.80	-1.46 0.62	0.0507 0.0092	3.21 0.90	-0.95 0.73	0.0766 0.0193	3.20 0.98	-0.95 0.81	0.0618
732	0.15	-0.95	0.0169	-0.12		0.034	0.09		0.02	-0.29		0.0285	-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	0.015	0.85	0.36	0.0084
734 735	4.49 0.17	0.06 -0.31	0.0339 0.0265	4.62 0.32	0.09	0.0488	4.93 0.39	0.40	0.042 0.0098	4.76 0.53	0.24	0.035 0.0153	4.87 0.50	0.35	0.0335 0.0129
735	0.17	-0.43	0.0322	0.32		0.0321	0.39		0.0098	0.82		0.0153	0.50		0.0129
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	0.42	-0.26	0.0162
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	0.65	0.52	0.009
739 740	1.03 0.10	-0.09 -0.20	0.0113 0.0107	1.01 0.26	-0.11	0.006 0.0091	0.92	-0.19	0.0114	0.98 -0.16	-0.14	0.0136 0.0158	1.12 0.06	0.00	0.008
741	0.10	-0.78	0.0104	0.26		0.0126	0.33		0.0099	0.02		0.012	0.14		0.0123
742	1.06	0.46	0.0205	0.89	0.26	0.0125	1.08	0.46	0.0094	1.16	0.55	0.0121	1.31	0.70	0.0082
743 744	2.77 0.18	0.68 -0.07	0.0097 0.0321	2.83 0.24	0.75 -0.26	0.0115 0.0259	2.67 0.38	0.59 -0.12	0.0084	2.76 0.67	0.67	0.0106 0.0121	2.68 0.48	0.60 -0.03	0.009
744	0.14	0.06	0.0222	0.42	0.03	0.0208	0.41	0.02	0.0146	0.56	0.17	0.0089	0.48	0.09	0.0088
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	0.80	-0.21	0.0059
747 748	1.48 0.73	-0.21 -0.50	0.0186 0.0066	0.79	-1.06 -0.49	0.009 0.0094	1.38 0.45	-0.47 -0.88	0.0143	1.33 0.60	-0.65 -0.73	0.0435 0.0121	1.47 0.50	-0.51 -0.83	0.0189 0.0234
748 749	0.73	-0.50 -0.43	0.0062	0.84	-0.49	0.0094	0.45	-0.88	0.0169	0.61	-0.73	0.0121	0.50	-0.83	0.0234
750	0.24	0.26	0.0111	0.66	0.56	0.0041	0.28	0.18	0.0077	0.35	0.24	0.0112	0.37	0.26	0.0082
751	1.28	-0.29 -0.27	0.0109	1.21	-0.35	0.0135	0.93	-0.64	0.0137	1.07 0.69	-0.49 -0.67	0.0203	1.06 0.34	-0.50 -1.03	0.0155
752 753	0.20	- 0.27 -0.12	0.021 0.0183	0.26	-1.11 -0.26	0.0249 0.0082	0.26 0.60	-1.10 -0.40	0.0219 0.0075	0.69	-0.67 -0.38	0.011 0.0103	0.34	-1.03 -0.39	0.0134
/33	5.20	0.12	0.0103	U. / M	0.20	0.0002	5.00	0.40	0.0073	0.02	0.30	0.0103	0.01	3.33	0.0034

	_	_				LogH	l _v		LogHI	91		LogHL	n		LogH	Les	
	HAT _{i/i} =0.0574			ID	Pred.	Res	HAT i/i	Pred.	Res	HAT i/i	Pred. (h)	Res	HAT i/i	Pred.	Res	HAT i/i	Pred.
0.05 0183				754	(h) 0.04	0.04	(h*=0.0489) 0.0375	(h) 0.71	0.61	(h*=0.0535) 0.0097	0.50	0.40	(h*=0.0533)	(h) 0.73	0.60	(h*=0.0578) 0.0115	(h) 0.65
01				755	0.17	-1.56	0.0141	0.81	-0.95	0.0157	0.44	-1.31	0.0125	0.41	-1.34	0.0178	0.49
01 05				756 757	1.49	1.19	0.0157	1.47	1.17 -0.54	0.0118 0.0232	1.46 0.90	1.16 -0.88	0.0042 0.0056	1.56	1.25	0.007	1.46
.00				758	1.44 3.71	-0.34 -0.88	0.022 0.011	1.24 3.85	-0.54	0.0232	3.95	-0.88	0.0056	1.24 3.76	-0.52 -0.89	0.0259 0.012	1.07 3.68
0105				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	3.60
0075				760	0.63	0.52	0.0065	0.34	0.23	0.0151	0.33	0.22	0.0103	0.67	0.55	0.0122	0.50
0259				761	1.19	-0.24	0.0168	1.38	-0.05	0.0137	1.23	-0.20	0.0173	1.13	-0.33	0.0179	1.35
0176 0076				762 763	0.73 0.72	0.41 -0.28	0.0068	0.82	-0.14 -0.71	0.0108 0.0139	0.35 0.50	-0.61 -0.92	0.0181	0.69 0.55	-0.27 -0.86	0.0268 0.0215	0.56 0.41
0135				764	0.90	0.48	0.0082	1.02	0.58	0.0053	0.84	0.40	0.0092	0.85	0.41	0.0088	0.86
0.01				765	0.65	1.73	0.0077	0.81	1.90	0.0078	1.18	2.27	0.0095	0.88	1.95	0.0124	1.06
0077				766	1.05	-0.43	0.013	1.08	-0.40	0.0148	1.09	-0.39	0.0191	0.87	-0.62	0.0158	1.20
0155 0123				767 768	4.99	0.63	0.0429	5.16 1.66	0.72 0.81	0.0472 0.012	5.35 1.70	0.91 0.85	0.0412 0.0037	5.21 1.76	0.77	0.043 0.0054	5.36 1.66
0087				769	1.76 2.84	0.92	0.0184 0.0093	2.79	0.61	0.012	2.67	0.48	0.0037	2.83	0.65	0.0034	2.78
0329				770	3.39	0.38	0.0104	3.48	0.48	0.0116	3.35	0.35	0.0101	3.36	0.36	0.0114	3.32
0063				771	3.82	0.81	0.0166	4.21	1.20	0.0265	3.81	0.81	0.016	3.74	0.74	0.0177	3.69
0067				772	3.54	0.06	0.0225	3.69	0.20	0.0333	3.39	-0.09	0.028	3.41	-0.08	0.0269	3.35
.0096 .0092				773 774	3.95 3.96	0.07	0.0153 0.0155	4.24 4.12	0.36 0.64	0.0165 0.0188	4.06 3.90	0.18 0.41	0.0145 0.0154	3.91 3.90	0.03	0.0158 0.0157	3.85 3.86
0134				775	4.57	1.08	0.0155	4.12	0.89	0.0188	4.42	0.93	0.024	4.46	0.42	0.0157	4.45
0077				776	5.32	0.23	0.0361	5.41	0.33	0.0314	5.14	0.05	0.0305	5.19	0.11	0.0324	5.23
0091				777	0.86	-0.06	0.0057	1.17	0.02	0.007	1.20	0.05	0.0149	0.98	-0.16	0.0086	1.03
0078				778	0.49	-1.31	0.0074	0.69		0.0059	0.60		0.0076	0.94		0.0103	0.88
2842 0071				779 780	0.55	0.00	0.0094	0.88	0.33	0.0068	1.02	0.47	0.0076	0.54	-0.15	0.0101	0.72
0071				780 781	1.68 0.08	0.84	0.0208 0.0122	1.28 0.53	-0.12	0.0218 0.0216	1.50 0.18	0.65 -0.46	0.0164 0.0236	1.80 0.19	0.95 -0.45	0.0136 0.0247	1.66 0.06
0125				782	0.18	0.00	0.0206	0.81	-0.06	0.006	0.57	-0.30	0.0083	0.61	-0.27	0.0124	0.60
0107				783	0.51	-0.49	0.0111	0.68	-0.50	0.0047	0.29	-0.89	0.0084	0.68	-0.51	0.0084	0.68
0078				784	1.29	-0.09	0.0094	1.22	-0.16	0.0081	0.96	-0.42	0.0092	1.01	-0.36	0.0107	1.15
0111				785 786	0.46	-0.06 -0.55	0.007 0.0471	0.59 0.58	0.07 -0.11	0.0197 0.0187	0.65 0.53	0.13 -0.17	0.0042 0.0091	0.33		0.0109 0.0129	0.38 0.58
0222				787	2.08	-0.21	0.0235	1.48	-0.11	0.0101	1.83	-0.46	0.0313	1.54	-0.74	0.0608	1.67
0168				788	4.40	-0.81	0.0171	4.35	-0.93	0.0317	4.64	-0.64	0.0246	4.44	-0.84	0.0191	4.41
0265				789	2.56	0.34	0.0121	2.40	0.17	0.0139	2.41	0.18	0.014	2.49	0.26	0.0158	2.45
0084				790 791	3.22 3.05	- 0.65 0.99	0.0105 0.0094	3.20 2.64	-0.70 0.57	0.0233 0.0117	3.51 2.59	-0.39 0.53	0.0174 0.0104	3.31 3.03	-0.59 0.96	0.0095	3.21 3.02
0139				792	3.77	0.32	0.0117	3.62	0.17	0.0111	3.69	0.24	0.0104	3.80	0.34	0.0124	3.77
.019				793	3.78	1.34	0.0116	3.51	1.07	0.0099	3.53	1.09	0.0101	3.80	1.35	0.0124	3.77
.0099				794	0.78	-0.26	0.0125	1.02	-0.05	0.0071	1.05	-0.01	0.0069	0.65	-0.42	0.0203	0.70
0091				795	0.64	0.09	0.012	0.95 4.67	-0.16	0.0064	0.92 4.93	0.10	0.0062 0.042	0.52 4.59	-0.24	0.0191 0.0273	0.65 4.68
0091				796 797	4.35 0.26	-0.43 -0.39	0.0274	0.33	-0.16	0.0473	0.44	0.10	0.0134	0.79	-0.24	0.0273	0.54
1505				798	0.64	0.44	0.0062	0.87	0.66	0.0038	0.69	0.48	0.0129	0.58	0.38	0.0091	0.48
0176				799	0.86	0.68	0.0209	0.96	0.78	0.0179	0.96	0.78	0.0102	1.06	0.89	0.0103	1.07
011				800	1.02	0.02	0.0107	0.90	-0.12	0.008	0.68	-0.34	0.0047	0.93	-0.09	0.0161	0.96
.015				801 802	0.63 1.07	0.39	0.009 0.0112	0.59	0.33 -0.17	0.0044 0.0147	0.50 1.19	0.24	0.0078 0.0077	0.63 1.15	0.37 0.15	0.0089 0.0128	0.65 1.22
012				803	0.31	-0.50	0.0112	0.48	-0.17	0.0147	0.39	0.13	0.0077	0.37	0.13	0.0128	0.21
.007				804	0.61	0.23	0.0042	0.93	0.55	0.0077	0.52	0.14	0.0079	0.69	0.30	0.0138	0.58
008				805	0.96	0.54	0.018	0.62	-1.46	0.0243	1.08	-1.01	0.0245	1.54	-0.55	0.0499	1.53
139				806 807	0.11	-0.82	0.0396 0.0099	0.59	-0.61 0.10	0.0137 0.0143	0.51	-0.70 -0.01	0.0086	0.84 3.00	-0.36 -0.18	0.0116 0.0104	0.67 2.94
023				808	3.01 3.06	-0.17 0.79	0.0094	3.28 2.96	0.10	0.0143	3.17 3.01	0.73	0.0094	3.08	0.80	0.0104	3.03
0106				809	2.98	0.79	0.0166	3.05	0.87	0.0234	2.85	0.67	0.0211	2.86	0.68	0.0227	2.81
0118				810	3.14	0.13	0.0139	3.17	0.17	0.0226	2.94	-0.06	0.0184	3.04	0.04	0.0174	3.00
.015 .0371				811 812	3.37 0.64	0.37 -0.44	0.0106 0.0066	3.16 0.86	0.15 -0.21	0.0126 0.0044	3.19 0.57	0.18 -0.50	0.0124 0.0182	3.36 0.54	0.35 -0.54	0.0115 0.0163	3.30 0.75
0146				812	0.65	-0.44	0.0066	0.86	-0.21	0.0044	0.57	-0.50	0.0182	0.50	-0.34	0.0163	0.75
0618				814	1.00	-0.08	0.0072	0.85	-0.24	0.0042	0.78	-0.30	0.0105	0.88	-0.20	0.0137	0.97
0061				815	0.55	-0.16	0.0126	0.78	-0.28	0.0031	0.46	-0.60	0.0081	0.42	-0.64	0.0159	0.55
0284				816 817	0.89	0.63 -0.32	0.0048	0.96	0.70 -0.20	0.0064	0.93	0.67 -0.25	0.0067 0.0057	1.02 0.95	0.76	0.009	1.03 0.90
.0335				817	3.05	1.01	0.0063	2.76	0.73	0.0054	0.72 3.00	0.97	0.0057	3.08	-0.02 1.05	0.0072 0.0079	3.02
0129				819	3.06	-0.17	0.0096	3.07	-0.15	0.0101	3.17	-0.06	0.009	3.09	-0.14	0.0084	3.03
0127				820	3.69	-1.30	0.0109	3.66	-1.39	0.0236	3.95	-1.10	0.0163	3.76	-1.30	0.012	3.67
0162				821	4.26	-0.38	0.0155	4.34	-0.30	0.0187	4.39	-0.25	0.018	4.28	-0.35	0.0165	4.24
.009				822 823	4.24 4.91	-1.06 -0.27	0.0152 0.0244	4.12 5.12	-1.18 -0.06	0.0152 0.0288	4.14 5.10	-1.17 -0.08	0.0148	4.24	-1.06 -0.28	0.016 0.0249	4.23 4.89
0122				824	4.84	-0.38	0.0244	4.85	-0.37	0.025	4.69	-0.52	0.0216	4.78	-0.43	0.0236	4.78
0123				825	5.20	0.32	0.0362	5.73	0.85	0.0402	5.31	0.43	0.0301	5.09	0.21	0.0313	5.08
0082				826 827	0.73 0.39	0.03 0.78	0.0064 0.0133	0.71 0.54	-0.30 0.92	0.0173 0.0079	0.65 0.55	-0.36 0.93	0.0176 0.0092	0.43	-0.58 0.89	0.0246	0.63
.009 .013				827 828	0.39	0.78	0.0133	0.54	0.92	0.0079	0.55	0.93	0.0092	0.53	0.89	0.0079	0.51
0088				829	0.72	0.09	0.0091	0.41	-0.31	0.0147	0.79	0.06	0.0101	0.52	-0.20	0.0052	0.60
0059				830	0.39	-0.91	0.015	0.59		0.0212	0.82		0.0246	0.76		0.025	0.61
0189				831	0.58	0.06	0.0064	0.51	-0.01	0.0101	0.39	-0.13	0.0066	0.65	0.13	0.0078	0.62
.0234 .0084				832 833	0.84 1.62	-0.11	0.0158 0.0204	0.87 0.88	-0.14	0.0144 0.0047	0.86 1.29	-0.15	0.0275 0.0132	0.96 1.50	-0.03	0.0146	1.05 1.58
.0084				833 834	0.80	-0.90 -0.17	0.0204	0.88	-0.14	0.0047	1.29 1.18	0.22	0.0132 0.0102	0.65		0.0309	1.58 0.82
				835	0.43	-0.61	0.0068	0.29		0.0136	0.30		0.0098	0.17		0.0117	0.08
0155				836	0.39	-1.20	0.0059	0.27		0.0143	0.28		0.0087	0.22		0.0106	0.12
0155 0134 0094				837	0.47	0.47	0.011	0.60	0.48	0.0145	0.78	0.66	0.0085	0.69	0.56	0.0111	0.72

		LogH	L _T		LogH	L _{B1}		LogHL	12		LogH	L _{B3}		LogHL ₈₄	
ID	Pred.	Res	HAT i/i	Pred.	Res	HAT i/i	Pred. (h)	Res	HAT i/i	Pred.	Res	HAT i/i	Pred.	Res	HAT i/i
838	(h) 0.29	-1.33	(h*=0.0489) 0.0066	(h) 0.27		(h*=0.0535) 0.0138	0.04		(h*=0.0533)	(h) 0.19		(h*=0.0578) 0.0126	(h) 0.11		(h*=0.0574)
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
840 841	3.75 0.38	1.31 -1.05	0.0117 0.0093	3.30 0.06	0.86	0.0136 0.0236	3.53 0.11	1.09	0.0101 0.0217	3.78 0.15	1.34	0.0119 0.0272	3.75 0.16	1.31	0.0117
842	0.69	0.69	0.0078	0.86	0.86	0.0094	0.72	0.72	0.0066	0.13	0.81	0.014	0.10	0.82	0.0068
843	0.53	0.63	0.0084	0.81	0.19	0.0069	0.56	-0.05	0.0108	0.68	0.07	0.0133	0.65	0.03	0.0125
844 845	0.81	0.91	0.0097 0.0038	0.95 0.15	1.06 0.40	0.0053 0.0653	0.96 0.52	1.07 0.76	0.0072 0.0055	0.80	0.90	0.0102	0.88	0.99	0.0105
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
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
848 849	1.22 0.87	0.28 -0.05	0.0219 0.0192	1.07	-0.29	0.0088	1.32 1.08	-0.03	0.0133	0.89	-0.46 -0.17	0.0477 0.0189	1.06	-0.29 0.13	0.0236
850	0.92	0.44	0.0152	0.79	-0.15 0.06	0.0261 0.0088	0.91	0.14	0.0068 0.0156	0.75 0.61	0.14	0.0169	1.05 0.64	0.13	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
852 853	0.83	0.09	0.0087 0.0278	0.90 0.83	0.03	0.0097 0.0109	0.93 1.18	0.06	0.0112 0.0444	1.08 1.36	0.21	0.0121 0.0447	1.00 0.85	0.13	0.0089
853 854	1.47 0.64	0.69	0.0278	0.83	0.05	0.0109	0.81	0.39	0.0444	0.72	0.57	0.0447	0.80	0.07	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
856 857	0.61	1.44 -0.12	0.0054	0.55	1.37	0.0088	0.35	1.18	0.0132	0.32	1.14 -0.22	0.0124	0.25 0.71	1.06	0.0159
857 858	0.76	-1.06	0.0064	0.69	-0.02 -0.88	0.0033 0.0086	0.61 0.79	-0.11 -1.06	0.0041 0.014	0.81	-0.22	0.0122	0.71	-0.32	0.0071
859	0.72	0.54	0.0066	0.85	0.67	0.0051	0.56	0.38	0.0096	0.59	0.41	0.0071	0.40	0.22	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 -1.05	0.0181	0.48	-0.34	0.0081
861 862	0.32	-0.57 0.19	0.0054	0.53	0.16	0.0113	0.23	-1.08 -0.04	0.0131	0.26	-0.59	0.0145 0.0129	0.23	-1.07 -0.47	0.0129 0.0152
863	0.51	0.51	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
864	0.33	0.40	0.0094	0.35	0.33	0.009	0.13	0.11	0.0163	0.21	0.19	0.0209	0.14	0.12	0.0206
865 866	0.12 1.02	-0.27 0.79	0.0201 0.0078	0.60 1.08	0.05	0.0112	0.48 1.02	-0.08 0.79	0.0071	0.58	-0.20 0.64	0.0088	0.51	-0.27 0.73	0.0084
867	0.54	0.18	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
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
869 870	0.94	0.86 -1.08	0.0218 0.0065	1.02 0.55	0.92 -0.96	0.0176 0.0114	1.03 0.42	0.92 -1.10	0.0068 0.0072	0.98	0.88 -1.15	0.0096 0.0076	1.01 0.26	0.91 -1.30	0.0081
871	0.97	-0.19	0.0101	0.95	-0.21	0.0074	0.68	-0.47	0.0054	0.62	-0.76	0.0069	0.52	-0.86	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		0.0166
873 874	1.33	-0.07 0.45	0.0153	1.21 0.87	0.53	0.0219	1.93 0.86	0.51	0.0173	1.95 0.66	0.32	0.0494 0.0086	2.19 0.79	0.46	0.0233 0.0065
874 875	1.14	-0.12	0.0101	0.87	-0.36	0.0075	1.39	0.12	0.0287	1.06	-0.20	0.0094	1.07	-0.19	0.009
876	0.74	-0.70	0.0075	1.05	-0.39	0.0083	0.66	-0.78	0.0078	0.87	-0.57	0.0152	0.85	-0.59	0.0101
877	1.47	0.07	0.0242	1.58	0.18	0.016	1.58	0.18	0.0049	1.52	0.13	0.0068	1.49	0.09	0.0057
878 879	0.88	0.05	0.0039 0.006	1.09 0.39	0.26	0.0066 0.0136	0.88 0.40	0.05	0.0081 0.0091	1.05 0.30	-0.03	0.008 0.0098	0.99	-0.13	0.0072 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
881	1.09	-0.08	0.0131	1.20	0.01	0.0121	1.02	-0.18	0.0119	0.84	-0.35	0.0115	1.04	-0.15	0.0115
882 883	0.65 1.07	0.07 -0.41	0.0118 0.0099	1.02	-0.34 -0.86	0.0071 0.0069	0.87 1.02	-0.48 -1.06	0.0104 0.0097	0.53 1.14	-0.82 -0.94	0.0211 0.0211	0.68 1.14	-0.68 -0.94	0.0158
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
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
886 887	0.02 0.45	-0.19 -0.33	0.0412 0.0054	0.17	-0.26 -0.38	0.0294 0.0119	0.20 0.40	-0.23 -0.38	0.0214 0.0079	0.55 0.21	0.13 -0.64	0.018 0.0102	0.32 0.19	-0.10 -0.66	0.019 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
889	0.56	0.39	0.0107	-0.13	-0.52	0.0316	0.34	-0.05	0.0214	0.36	-0.02	0.0252	0.22	-0.16	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
891 892	1.08	-0.63 0.15	0.0046 0.0192	0.52 1.12	-0.62 0.18	0.015 0.0157	0.52 1.28	-0.62 0.33	0.0149 0.0076	0.75 1.24	0.05	0.0085 0.0089	0.24 1.31	0.12	0.0666 0.0091
893	0.50	-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
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
895 896	1.42 1.90	-0.66 -0.25	0.0215 0.0301	1.23 1.00	-0.84 -1.18	0.0264 0.0063	1.18 1.58	-0.89 -0.59	0.007 0.0162	1.39 1.64	-0.69 -0.53	0.0149 0.0572	1.26 1.54	-0.82 -0.64	0.0082
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
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
899 900	0.83	0.05 -0.16	0.008 0.0038	0.90	0.12	0.0068 0.0059	0.56 1.00	0.11	0.0092 0.0088	0.53 0.88	0.00	0.0155 0.0084	0.58 0.97	0.09	0.0097 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
902	0.14	-0.09	0.021	0.78	0.37	0.0063	0.61	0.20	0.0078	0.58	0.12	0.0133	0.53	0.07	0.012
903 904	0.62	-0.28 0.24	0.0083	0.94	0.01 0.28	0.0099 0.0153	0.53 0.51	-0.41 0.33	0.0086 0.0084	0.67 0.56	0.31	0.009 0.0089	0.55 0.49	0.24	0.0079 0.009
904	0.46	1.06	0.0096	0.68	1.26	0.0153	0.51	1.36	0.0084	0.44	1.03	0.0089	0.49	1.25	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
907 908	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 0.0112
908 909	0.93	1.09 0.66	0.0046 0.0031	0.71	0.86	0.0051	0.70 0.69	0.86	0.0126 0.0066	0.53	0.68	0.0119 0.0185	0.52	0.67	0.0112 0.0113
910	0.31	-1.15	0.0057	0.30	-1.30	0.0119	0.35	-1.26	0.0067	0.07		0.0125	0.12		0.0099
911	0.66	-0.31	0.0035	0.56	-0.41	0.0055	0.27	-0.70	0.0105	0.51	0.22	0.0066	0.50	0.24	0.0081
912 913	0.16 0.37	0.26 0.37	0.0153 0.0049	0.51 0.58	0.49	0.0097 0.008	0.20	0.18 -0.07	0.0097 0.0059	0.34	0.32 -0.14	0.0121 0.0071	0.33	0.31 -0.18	0.0094
914	0.67	0.49	0.0058	0.44	0.26	0.0061	0.13	-0.05	0.0456	0.27	0.09	0.0329	0.11	-0.07	0.043
915	0.94	-0.38	0.0189	0.67		0.0297	0.70		0.0084	1.28	-0.07	0.0452	0.94	-0.41	0.014
916 917	0.72	-0.68 -0.14	0.0097 0.0093	0.78	-0.63	0.006	0.88	-0.53	0.0063	0.67	-0.74 -0.43	0.0083 0.0067	0.57	-0.84 -0.29	0.0053
917 918	0.81	-0.14 -0.45	0.0093	0.78	-0.34 -0.79	0.0103 0.0129	1.05 0.45	-0.07 -0.65	0.0111 0.0146	0.69	-0.43 -0.69	0.0067	0.83	-0.29 -0.81	0.0069
919	0.91	0.01	0.0148	1.01		0.0072	1.27		0.0093	0.69		0.0281	0.89		0.0184
920	1.06	0.29	0.0184	1.01	0.22	0.0149	1.04	0.26	0.0169	0.86	0.08	0.0227	1.01	0.23	0.0157
921	0.98	-0.33	0.01	1.03	-0.29	0.0145	1.20	-0.12	0.0166	1.00	-0.30	0.0227	1.31	0.01	0.0183

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	L	ogHL ₈₄	
	red. (h)	Das	HAT _{i/i} h*=0.0574
Ú.).11		0.0148
	. <u>1</u> '5	0.18 1.31	0.0204
.16			0.0233
.83		0.82	0.0068
			0.0125
.56 0.81 0.005			
.46 -0.28	-0.28		0.0138
		0.53	0.0077
.06		-0.29 0.13	0.0236
	Č).17	0.0053
.20 0.			0.0102
.00 0.13 .85 0.07			0.0089
			053
.13 -0.03	-0.03		0.0152
.25 1.06 0.015			
. 71 -0.32	-0.32		0.0071
.40 0.22	0.22		0.0084
.48 -0.34	-0.34		0.0081
.23 -1.07	-1.07		0.0129
.35 <u>-0.47</u> .63 <u>0.57</u>			0.0152 0.0281
.14 0.1			0.0206
.51 -0.2	-0.2	27	0.0084
.96 0.7	0.7	3	0.0067
.20 -1.65 .99 0.26			0.0106 0.0127
			0.0027
			0.0094
	-0.86		0.0067
			.0166
.19 0.0233 1.79 0.46 0.0065			
.07 -0.19 0.009			
.85 -0.59 0.0101			
.49 0.09 0.0057			
0.0072 0.20 -0.13 0.0106			
.08 0.68 0.0184	0.68 0.0184	0.0184	
.04 -0.15 0.0115		0.0115	
.68 <u>-0.68</u> <u>0.015</u>			
			0.0078 0.0096
			0.0096
.32 -0.10			0.019
			0.0092
			0.0066 0.0229
			.0092
1.24			0.0666
			0091
.22 -0.55 0.02 .14 0.07 0.01			
.26 -0.82 0.0			
.54 -0.64 0.019	-0.64 0.019	0.019	3
.00 0.22 0.00 .17 -0.38 0.0			
			0 132 0097
.97 0.09 0.0091			
.80 0.39 0.0126			
1.53 0.07 0.012 1.55 0.0079			
.49 0.24 0.009			
.67 <u>1.25</u> <u>0.0103</u>	1.25 0.0103	0.0103	
<u>.77</u> <u>0.05</u> <u>0.00</u>	0.05 0.00	0.00	78
			009
		0.	0112 0113
1.12 0.0	0.0	0.0	1099
0.00			
			0068
0.11 -0.18 0.0			
.94 -0.41 0.0	-0.41 0.0	0.0	14
			0053
.83 -0.29 0.0069 .27 -0.81 0.0094			
.27 -0.01 0.000-	0.0184		
0.0184			
0.0184 .01 0.23 0.0157 .31 0.01 0.0183			

		LogH	IL _T		LogHI	-81		LogHL	12		LogH	L _{B3}	-	LogHL ₈₄	
ID	Pred. (h)	Res	HAT _{i/i} (h*=0.0489)	Pred. (h)	Res	HAT _{i/i} (h*=0.0535)	Pred. (h)	Res	HAT _{i/i} (h*=0.0533)	Pred. (h)	Res	HAT _{i/i} (h*=0.0578)	Pred. (h)	Res	HAT _{i/i} (h*=0.0574)
1006	0.79	0.03	0.0088	0.98	0.22	0.007	0.91	0.15	0.0065	0.90	0.11	0.0083	0.91	0.12	0.0053
1007 1008	1.34	0.59 -0.51	0.0176	1.21 0.69	0.41 -0.44	0.0076 0.006	1.09 0.46	0.29 -0.66	0.0171 0.01	1.30 0.28	0.49 -0.85	0.0337 0.0106	1.23 0.34	0.42 -0.79	0.015
1008	0.46	-0.12	0.0049 0.0167	0.18	-0.44	0.006	0.12	-1.00	0.0259	0.28	-0.83	0.0106	-0.09	-1.20	0.0606
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	0.04	0.0091	0.72	-0.24	0.0041	0.45	-0.59	0.0195	0.64	-0.39	0.0093
1012 1013	0.83	0.24	0.0079 0.0081	1.10 0.96	0.51	0.0097 0.0152	1.03 0.76	0.44	0.0086 0.0105	1.14	0.55	0.0106 0.0186	0.99	0.40	0.0058
1013	0.57	0.53	0.0081	0.96	-0.51	0.0152	0.76	-0.32	0.0105	0.85 1.03	0.76	0.0186	1.02	0.73	0.0106
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 1018	0.94	0.31	0.0064 0.0075	1.24	0.62	0.0079	0.91	0.29	0.0104	0.20	0.17	0.01 0.0159	0.37	0.03	0.0058
1018	0.51	-0.83 - 0.58	0.0075	0.75	-0.59	0.0054	0.45	-0.89	0.0086	0.20		0.0159	0.37		0.013
1020	1.14	0.80	0.0101	1.27	0.78	0.0105	0.79	0.30	0.0075	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 1024	0.87	-0.43 0.58	0.0115 0.006	1.20 0.93	- 0.10 0.86	0.0129 0.0073	1.14	-0.16	0.0125 0.0098	0.52	-0.78 0.80	0.0121	0.70	0.72	0.0092
1024	0.96	0.62	0.0152	0.85	0.51	0.0122	0.61 0.93	0.53 0.59	0.0098	0.72	0.38	0.0078	0.88	0.72	0.0055
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		0.0094	0.29		0.0153	0.44		0.012
1029 1030	0.87	0.16	0.0103	1.01	0.30	0.0189	1.20	0.48	0.0082	1.21 1.21	0.29	0.0073	1.19 1.25	0.28	0.0081
1031	1.39	0.35	0.0192	1.18	0.09	0.0084	1.47	0.38	0.0152	1.13	0.05	0.0375	1.42	0.34	0.0238
1032	0.38	-0.38	0.0095	0.75	-0.91	0.0089	0.81	-0.84	0.0114	0.67	-0.98	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	0.05	0.0193	0.15	0.00	0.0215	-0.24		0.0251	-0.12	0.25	0.0305
1035 1036	0.92	-0.06 0.44	0.0252 0.0148	0.91	-0.06 0.50	0.0147 0.0123	0.99	0.02	0.0319 0.0284	0.55 -0.23	-0.44 -0.11	0.0134 0.0371	0.74 -0.04	-0.25 0.08	0.0343
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	0.0036	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 1041	0.11 0.77	0.00	0.02 0.0072	0.40 1.13	0.28 1.09	0.0107 0.0078	0.11	0.00	0.0228 0.0073	0.25	0.13	0.0136 0.0124	0.82	-0.36 0.78	0.0931
1041	0.94	-0.40	0.0072	1.26	-0.10	0.0078	0.95	-0.41	0.0073	0.83	-0.45	0.0124	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		0.0066	0.40		0.0094	0.29		0.0103
1046 1047	0.88	0.34	0.0059	1.09 0.50	0.11	0.0051 0.0142	0.75 0.51	-0.24 0.61	0.0038 0.015	1.01 0.48	0.03 0.53	0.0074 0.0104	0.89	-0.10 0.41	0.0055 0.0266
1047	0.40	0.13	0.0065 0.0185	0.30	-0.14	0.0142	0.16	-0.38	0.013	0.46	-0.11	0.0104	0.31	-0.26	0.0288
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	0.027
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 1052	0.60	0.00	0.022	0.69	0.09	0.0079	0.58	-0.02 -0.38	0.0224	0.70	0.10	0.0129	0.45	-0.15	0.0184
1052	0.74	-0.39 -1.20	0.01 0.0098	1.28	-0.44	0.0112	0.76	-0.38	0.0047	0.52		0.0089	0.40		0.011
1053	1.49	1.62	0.016	0.20	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 1058	0.25	0.64	0.0354	1.12	0.42 -0.58	0.0195	1.44	0.74 -0.76	0.011	1.06 0.24	0.36 -0.76	0.0071	0.28	0.37 -0.73	0.0098
1058	0.25	0.05	0.0087	0.88	0.25	0.0124	0.24	0.16	0.0143	0.64	0.01	0.0105	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	0.0033
1061	0.98	-0.26	0.0069	0.84		0.0034	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 1064	2.80 0.84	-0.12 0.19	0.0685	1.09 0.81	-1.83 -0.02	0.015	2.04 0.78	-0.89 -0.05	0.0514	1.85 0.79	-1.08 -0.04	0.1235 0.0101	2.08 0.89	-0.85 0.06	0.0542
1064	0.84	1.51	0.0107	0.81	1.10	0.0039	1.12	1.64	0.007	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	1.19	-0.35	0.0102	1.09	-0.46	0.0092	0.95	-0.60	0.0175	0.93	-0.61	0.0095
1068 1069	0.79	-0.45 -0.65	0.0071 0.0162	0.89	-0.39 - 0.79	0.0073 0.009	0.77	-0.51 -0.74	0.0115 0.0403	0.87	-0.41	0.0134 0.0196	0.97	-0.31	0.0141
1069	0.73	-0.30	0.0162	0.60	-0.79	0.009	0.65	-0.74	0.0403	0.73		0.0196	0.40		0.0197
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 1075	0.82	-0.16	0.0062	1.01 0.95	0.03 -0.61	0.0049 0.0091	0.89 0.78	-0.08 -0.79	0.0054 0.0079	1.21	0.23	0.012	1.15	0.17	0.0079
1075	1.13 1.11	-0.43 -0.33	0.0114 0.0116	1.10	-0.61 -0.33	0.0091	1.20	-0.79 -0.23	0.0079	0.98 1.32	-0.57 -0.12	0.0123 0.0148	0.93 1.32	-0.63 -0.13	0.0098
1077	0.62	0.37	0.0052	0.33	-1.08	0.0097	0.37	-1.04	0.0093	0.54	-0.87	0.0161	0.44	-0.97	0.0129
1078	2.01	0.44	0.0366	1.22	-0.35	0.0086	1.94	0.37	0.0245	1.96	0.40	0.0715	2.04	0.48	0.0321
1079	2.80	-1.37	0.077	4.30	0.08	0.4315	2.32	-1.89	0.0367	3.69	-0.53	0.1005	3.76	-0.46	0.0927
1080 1081	0.59	0.11	0.0083 0.0118	0.62 0.39	-0.25	0.0066 0.0112	0.57 0.30	.0.25	0.013 0.0082	0.82 0.11	-0.49	0.0114 0.0173	0.95 0.15	-0.45	0.0124 0.0164
1081	0.89	0.57	0.0118	0.83	0.21	0.0112	0.30	-0.35 0.32	0.0084	0.11	0.25	0.01/3	0.15	0.35	0.0164
1083	0.69	0.44	0.0083	0.91	0.65	0.0041	0.63	0.37	0.0139	0.43	0.19	0.0126	0.61	0.36	0.0079
1084	0.98	0.13	0.0389	0.43	-0.41	0.0116	0.76	-0.08	0.0515	0.74	-0.10	0.0124	0.39	-0.45	0.03
1085	1.25	-0.16	0.0157	1.36	-0.07	0.0134	1.42	-0.02	0.0044	1.75	0.33	0.0094	1.56	0.14	0.006
1086 1087	0.59 2.63	0.19	0.0157 0.0636	0.64 4.55	0.25	0.0084	0.72 3.06	0.33 -1.25	0.0131 0.0694	0.80 3.70	0.10	0.0183 0.1117	0.87 3.72	0.17 -0.60	0.0104
1087	2.99	-1.63 -0.88	0.0956	3.78	-0.11	0.1404	3.57	-1.25 -0.32	0.1005	4.26	-0.62 0.37	0.1117	4.35	0.46	0.1349
1089	0.83	0.00	0.007	1.17	0.33	0.012	0.75	-0.08	0.0067	0.80	-0.04	0.0179	0.90	0.07	0.0074

		LogHL ₈₄	
AT _{i/i} 0.0578)	Pred. (h)	Res	HAT _{i/i} (h*=0.0574)
.0083	0.91	0.12	0.0053
337	1.23	0.42	0.015
106	0.34	-0.79	0.0075
0156	-0.09	-1.20	0.0606
091	0.79	0.06	0.0061
195	0.64	-0.39	0.0093
106	0.99	0.40	0.0058
186	0.82	0.73	0.0106
0262	1.02	0.02	0.018
0091	0.24	-0.16	0.0155
053	0.50	-0.43	0.0045
01	1.00	0.03	0.0058
0159	0.37		0.015
0142	0.70		0.0103
009	0.88	0.39	0.0056
0111	0.40	-0.24	0.0112

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

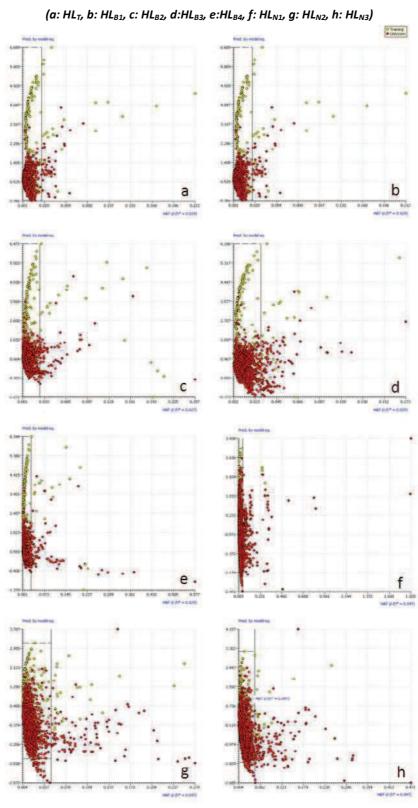


Figure S2: Iterations for the selection of the two minimum convex hulls. (a: 0 outlier, b: 1 outlier, c: 2 outliers, d:3 outliers, e: 4 outliers, f: 5 outliers, g: 6 outliers, h: 7 outliers)

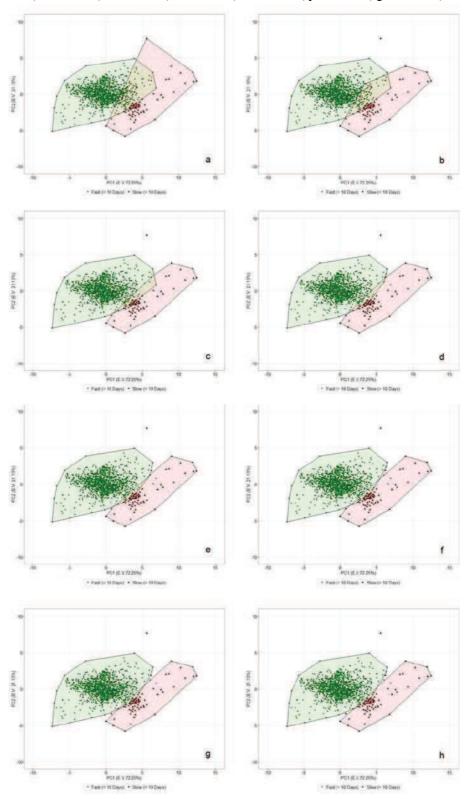


Table S3: CAS, human and fish predicted biotransformation HLs, PBT assessment and Priority level for the screened PPCPs.

(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)

			Human B	iotransforn	nation		Fish Bio	transforma	ition		F	PBT Pro	ofiler	
ID	CAS	logHL _T (h)	logHL _{B1} (h)	logHL _{B2} (h)	logHL _{B3} (h)	logHL ₈₄ (h)	logHL _{N1} (h)	logHL _{N2} (h)	logHL _{N3} (h)	PBT Index	P	В	т	Priority Level
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
52	000050-06-6	2.00	2.11	2.11	2.11	2.11	0.03	0.15	0.09	-0.60	2	1	2	Low Priority
3	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
4	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
5	000050-12-4	0.85	0.88	0.88	0.92	0.92	0.21	0.35	0.26	-0.44	2	1	2	Low Priority
6	000050-18-0	0.90	0.94	0.94	0.94	0.94	0.27	0.39	0.27	-0.67	2	1	3	Low Priority
7	000050-23-7	0.20	0.22	0.22	0.21	0.21	1.14	0.96	1.04	-2.31	2	1	2	Low Priority
8	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	0.23	0.23	0.23	0.23	0.23	1.43	1.21	1.31	-1.21	2	1	2	Low Priority
10	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
11	000050-35-1	0.67	1.04	1.04	1.05	1.05	0.00	0.15	0.07	-0.01	2	1	1	Low Priority
512 513	000050-36-2	-0.12 0.48	-0.11 0.46	-0.11 0.46	-0.11 0.49	-0.11 0.49	0.79	0.93 1.28	0.86 0.74	-0.06	2	1	2	Low Priority
514	000050-37-3 000050-44-2	0.48	0.46	0.46	0.49	0.49	1.19 0.43	1.28	0.74	0.34 0.20	2	1	2	Low Priority Low Priority
515	000050-47-5	1.34	1.35	1.35	1.35	1.35	2.14	2.06	1.83	0.70	2	1	3	Low Priority
516	000050-47-5	1.23	1.24	1.24	1.24	1.24	2.86	2.66	2.71	1.32	3	1	3	Priority (Group 2)
517	000050-49-7	1.20	1.21	1.21	1.21	1.21	2.50	2.50	2.26	1.10	2	1	3	Priority (Group 2)
18	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
19	000050-52-2	1.36	1.36	1.36	1.36	1.36	2.76	2.30	2.43	1.10	2	2	3	Priority (Group 2)
20	000050-53-3	1.04	1.05	1.05	1.05	1.05	3.00	2.53	2.80	1.64	2	2	3	High Priority
21	000050-60-2	-0.50	-0.51	-0.51	-0.49	-0.49	1.16	1.23	0.91	0.34	2	1	3	Low Priority
22	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
23	000050-78-2	-0.59	-0.58	-0.58	-0.58	-0.58	0.04	0.02	0.21	-0.35	1	1	1	Low Priority
24	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
25	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
26	000051-06-9	0.49	0.75	0.75	0.75	0.75	0.37	0.58	0.19	-1.41	2	1	2	Low Priority
27	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
28	000051-21-8	-0.60	-0.58	-0.58	-0.58	-0.58	-0.60	-0.42	-0.45	-1.20	1	1	2	Low Priority
29	000051-34-3	0.65	0.76	0.76	0.59	0.67	0.44	0.55	0.44	-0.67	2	1	3	Low Priority
30	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
31	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
32	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
33	000051-52-5	0.11	0.12	0.12	0.12	0.12	0.12	0.12	0.12	-1.83	2	1	2	Low Priority
34 35	000051-55-8	0.61	0.98	0.98	0.98	0.98 0.52	0.56 0.51	0.65	0.52	-0.67 -1.91	2	1	2	Low Priority
	000051-61-6			0.63	0.36		0.51		0.58		_	_	2	Low Priority
36 37	000051-64-9 000051-71-8	0.81 0.77	0.56 0.71	0.51	0.87	1.13 0.88	0.69	0.91 0.79	0.87	-1.04 -1.40	1	1	2	Low Priority Low Priority
37 38	000051-71-8	-0.60	-0.60	-0.60	-0.59	-0.59	1.39	1.42	1.39	-0.26	2	1	2	Low Priority
39	000051-75-2	0.75	0.77	0.72	1.21	0.93	-0.19	0.52	0.32	-0.26	2	1	1	Low Priority
40	000051-83-2	-0.78	-0.77	-0.77	-0.77	- 0.77	1.56	1.22	1.47	-0.92	2	1	2	Low Priority
41	000052-24-4	0.43	0.43	0.43	0.43	0.43	1.26	1.25	1.24	-1.37	1	1	2	Low Priority
42	000052-53-9	0.45	0.46	0.46	0.46	0.46	2.23	1.99	2.49	1.09	3	1	3	Priority (Group 2)
43	000052-67-5	0.00	0.12	0.12	0.12	0.12	-0.22	0.00	0.12	-2.61	1	1	1	Low Priority
44	000052-86-8	1.54	1.55	1.55	1.55	1.55	1.81	1.70	1.95	1.93	3	1	3	Low Priority
345	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
346	000053-16-7	1.28	1.28	1.28	1.28	1.28	1.02	0.81	0.88	-0.66	2	1	2	Low Priority
47	000053-19-0	3.33	3.33	3.33	3.33	3.33	3.03	3.03	3.03	3.57	3	2	3	High Priority
48	000053-39-4	0.95	0.95	0.95	0.95	0.95	1.14	1.18	1.22	-1.94	2	1	2	Low Priority
49	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
50	000053-86-1	0.15	0.22	0.22	0.22	0.22	1.00	0.66	0.53	2.31	2	1	2	Low Priority
51	000054-05-7	2.76	3.11	3.11	3.11	3.11	2.25	2.23	2.07	1.05	2	1	3	Priority (Group 2)
52	000054-11-5	0.30	0.38	0.38	0.38	0.38	1.41	1.62	1.16	-0.23	2	1	2	Low Priority
53	000054-31-9	0.40	0.93	0.93	0.93	0.93	0.86	0.55	0.79	0.38	2	1	2	Low Priority
54	000054-36-4	0.28	0.30	0.30	0.31	0.31	0.72	1.19	0.48	1.01	2	1	1	Low Priority
555	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
556	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
557	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
558 559	000054-85-3	0.00 0.84	0.11 1.08	0.11	0.13 0.87	0.13	-0.51 0.76	-0.17 1.14	-0.59 0.90	-1.35 -0.03	2	1	2	Low Priority
														Low Priority
60 61	000054-92-2 000055-63-0	0.78 -1.30	0.76 -1.31	0.52 -1.31	0.69 -1.30	0.85 -1.30	-0.03 1.39	0.38	-0.12 1.61	-1.00 -0.34	2	1	2	Low Priority Low Priority
62	000055-73-2	1.18	0.71	0.77	0.66	1.13	1.12	1.38	1.01	-0.34	1	1	2	Low Priority
63	000055-73-2	0.53	0.71	0.77	0.57	0.57	0.11	0.42	0.47	-0.79	2	1	1	Low Priority
64	000055-98-1	0.55	0.69	0.69	0.69	0.69	0.11	0.42	0.47	-1.31	2	1	2	Low Priority
65	000056-41-7	-0.19	-0.26	0.09	-0.51	0.03	-0.94	-0.74	-0.57	-2.57	1	1	1	Low Priority
66	000056-45-1	-0.15	-0.28	0.23	-0.31	-0.07	-0.90	-0.74	-0.52	-2.97	1	1	1	Low Priority
67	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
68	000056-54-2	0.71	0.89	0.89	0.89	0.33	1.24	1.11	0.59	0.42	2	1	2	Low Priority
69	000056-75-7	0.66	0.71	0.71	0.71	0.71	0.86	0.89	0.67	0.12	2	1	1	Low Priority
70	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
71	000056-84-8	-0.11	-0.27	-0.13	-0.27	0.04	-0.71	-0.46	-0.32	-2.76	1	1	1	Low Priority
72	000056-85-9	-0.02	-0.05	-0.01	-0.17	-0.02	-0.54	-0.29	-0.19	-3.17	1	1	1	Low Priority
73	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
74	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
75	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
576	000057-00-1	0.02	0.02	0.19	-0.15	0.13	-0.74	-0.48	-0.36	-2.77	1	1	1	Low Priority
		-	-		-	-		-						,

			Human E	Biotransforr	mation		Fish Bio	otransforma	ation		=	PBT Pr	ofiler	
ID	CAS	logHL _T (h)	logHL _{B1}	logHL _{B2}	logHL _{B3}	logHL ₈₄	logHL _{N1} (h)	logHL _{N2}	logHL _{N3}	PBT Index	Р	В	т	Priority Level
577	000057-27-2	0.30	(h) 0.35	(h) 0.35	(h) 0.35	(h) 0.35	1.59	(h) 0.86	(h) 1.17	-1.00	2	1	2	Low Priority
S78	000057-41-0	1.34	1.36	1.36	1.60	1.60	0.44	0.53	0.42	0.46	2	1	2	Low Priority
S79	000057-42-1	0.90	0.92	0.92	0.92	0.92	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	Low Priority
S81	000057-44-3	0.40	0.23	0.25	0.44	0.45	-0.33	-0.13	-0.14	-1.86	2	1	2	Low Priority
S82	000057-47-6	0.89	1.04	0.98	0.72	0.81	0.58	0.63	0.54	-0.61	2	1	2	Low Priority
S83	000057-53-4	1.15	0.32	0.26	0.29	0.35	-0.21	0.07	0.14	-2.80	2	1	1	Low Priority
S84	000057-63-6	0.99	0.99	0.99	0.99	0.99	1.57	1.35	1.41	-1.03	2	1	2	Low Priority
S85	000057-66-9	0.77	0.83	0.83	0.83	0.83	0.07	0.18	0.06	-0.24	2	1	2	Low Priority
S86	000057-67-0	0.38	0.67	0.69	0.96	0.94	-0.36	-0.15	-0.47	-2.12	2	1	2	Low Priority
S87	000057-68-1	0.78	1.02	1.06	1.13	1.10	0.07	0.53	-0.12	0.08	2	1	2	Low Priority
S88	000057-83-0	1.65	1.66	1.66	1.64	1.64	1.57	1.42	1.44	-1.13	2	1	2	Low Priority
S89	000057-85-2	0.98	0.78	0.87	0.80	0.81	1.56	1.41	1.48	-1.12	2	1	3	Low Priority
S90	000057-96-5	0.79	1.42	1.42	1.42	1.42	1.10	1.12	0.72	2.69	2	1	1	Low Priority
S91	000058-08-2	0.69	0.70	0.70	0.70	0.70	-0.03	0.42	-0.02	-0.24	1	1	2	Low Priority
S92	000058-14-0	2.15	2.23	2.23	2.25	2.25	1.54	1.60	1.37	0.31	2	1	3	Low Priority
S93	000058-15-1	0.69	0.98	0.73	0.73	0.71	0.55	0.92	0.51	-0.06	2	1	2	Low Priority
S94	000058-18-4	0.97	1.00	1.28	1.04	0.99	1.46	1.31	1.36	-1.72	2	1	2	Low Priority
S95	000058-19-5	0.88	0.97	1.05	0.91	0.99	1.19	1.20	1.20	-1.96	2	1	2	Low Priority
S96	000058-22-0	0.26	0.26	0.26	0.27	0.27	1.32	1.13	1.17	-1.71	2	1	2	Low Priority
S97	000058-25-3	0.92	0.92	0.92	0.92	0.92	1.44	1.14	1.06	1.69	2	1	1	Low Priority
S98	000058-27-5	0.52	0.63	0.48	0.65	0.58	0.75	0.68	0.65	0.20	1	1	3	Low Priority
S99	000058-38-8	0.95	0.95	0.95	0.96	0.96	3.09	2.55	2.85	1.64	3	1	3	Priority (Group 1)
S100	000058-39-9	0.97	1.06	1.06	1.06	1.06	1.84	1.35	1.75	1.19	3	1	2	Low Priority
S101	000058-40-2	0.90	0.89	0.89	0.90	0.90	2.42	2.25	2.18	1.10	2	1	3	Priority (Group 2)
S102	000058-46-8	0.86	0.87	0.85	0.85	0.77	1.35	1.17	1.36	-0.29	2	1	2	Low Priority
S103	000058-54-8	0.16	0.15	0.15	0.34	0.34	0.67	0.78	1.11	1.07	2	1	2	Low Priority
S104	000058-55-9	0.86	0.90	0.90	0.90	0.90	0.05	0.43	0.16	-0.87	1	1	2	Low Priority
S105	000058-73-1	0.97	0.98	0.98	0.98	0.98	1.89	1.99	1.83	0.97	2	1	2	Low Priority
S106	000058-74-2	0.26	0.26	0.26	0.26	0.26	2.34	1.90	2.03	2.09	2	1	2	Low Priority
S107	000058-85-5	0.31	0.61	0.47	-0.04	0.36	0.20	0.25	0.40	-2.45	1	1	1	Low Priority
S108	000058-89-9	3.07	3.27	3.27	3.30	3.30	2.98	2.98	2.98	2.28	3	1	2	Priority (Group 1)
S109	000058-93-5	1.01	0.69	0.98	1.41	1.24	0.32	0.15	0.26	-0.50	2	1	2	Low Priority
S110	000058-94-6	0.47	0.78	1.02	1.49	1.25	0.41	0.21	0.18	0.11	2	1	2	Low Priority
S111	000059-32-5	1.27	1.24	1.32	1.29	1.31	2.50	2.48	2.34	1.66	3	1	2	Priority (Group 1)
S112	000059-40-5	0.81	1.09	0.97	1.23	1.22	0.06	0.48	-0.30	1.15	2	1	2	Low Priority
S113 S114	000059-42-7 000059-43-8	0.44 0.62	0.79 0.98	0.79 1.35	0.38 1.23	0.49	0.48 1.09	0.44 1.19	0.53 0.82	-1.55 -0.45	1	1	2 1	Low Priority
	000059-43-8					1.13 - 0.88		0.49		-0.45 -1.01				Low Priority
S115 S116	000059-46-1	-0.89 -0.27	-0.89 -0.16	- 0.89 0.24	-0.88 -0.31	-0.88 -0.11	0.29 -0.20	-0.14	0.11	-1.01 -1.99	2	1	2	Low Priority Low Priority
S110 S117	000059-63-2	0.74	1.06	0.24	0.90	0.79	0.51	0.50	0.01	0.07	2	1	2	Low Priority
S117 S118	000059-66-5	1.11	3.11	3.11	3.11	3.11	-0.60	-0.23	-0.30	-1.13	2	1	2	Priority (Group 2)
S118	000059-67-6	0.07	0.16	0.35	-0.15	0.21	-0.52	-0.23	-0.50	-0.53	1	1	1	Low Priority
S120	000059-87-0	0.70	0.54	0.46	0.64	0.76	0.20	0.07	0.02	-1.10	2	1	2	Low Priority
S120	000059-92-7	0.70	0.12	0.40	0.12	0.70	0.32	0.07	0.53	-2.11	1	1	1	Low Priority
S122	000059-96-1	1.38	1.38	1.38	1.37	1.37	2.36	2.18	2.22	1.63	2	1	3	Low Priority
S122	000059-98-3	1.01	0.74	0.58	0.60	0.89	1.14	1.36	1.11	-0.42	1	1	2	Low Priority
S124	000055-58-5	0.36	0.43	0.43	-0.03	0.30	0.13	0.22	0.27	-0.71	1	1	1	Low Priority
S125	000060-18-4	0.29	0.35	0.35	0.24	0.34	0.21	0.21	0.43	-1.72	1	1	1	Low Priority
S126	000060-32-2	0.69	0.00	-0.07	-0.44	-0.14	-0.27	-0.07	0.03	-2.59	1	1	1	Low Priority
S127	000060-56-0	0.38	0.68	0.68	0.69	0.69	0.71	0.45	0.42	-1.49	1	1	1	Low Priority
S128	000060-79-7	0.54	0.80	0.83	0.42	0.52	0.84	0.90	0.40	-0.42	2	1	2	Low Priority
S129	000060-80-0	1.08	1.10	1.10	1.10	1.10	0.68	0.71	0.37	-0.02	1	1	2	Low Priority
5130	000060-87-7	1.09	1.09	1.09	1.09	1.09	2.43	2.33	2.27	1.10	2	1	3	Priority (Group 2)
S131	000060-99-1	1.48	1.48	1.48	1.48	1.48	2.27	2.03	2.09	1.01	2	1	3	Low Priority
S132	000061-00-7	0.98	1.20	0.86	0.91	0.86	1.28	1.20	1.11	1.05	2	1	3	Low Priority
S133	000061-32-5	-0.19	0.25	0.25	0.25	0.25	0.55	0.29	0.66	-0.65	2	1	2	Low Priority
5134	000061-33-6	-0.15	0.41	0.41	0.41	0.41	0.44	0.49	0.57	-0.62	2	1	2	Low Priority
S135	000061-50-7	1.10	1.05	0.89	0.98	0.91	1.61	1.88	1.37	0.17	2	1	2	Low Priority
S136	000061-51-8	1.31	1.10	0.87	1.03	1.04	1.42	1.51	1.17	0.26	2	1	2	Low Priority
S137	000061-68-7	0.30	0.31	0.31	0.31	0.31	0.74	0.87	0.61	0.31	2	1	2	Low Priority
S138	000061-72-3	0.53	0.95	1.01	1.01	0.89	1.20	0.73	0.99	1.27	2	1	2	Low Priority
S139	000061-90-5	0.14	-0.06	-0.01	-0.14	0.05	-0.32	-0.06	0.03	-2.61	1	1	1	Low Priority
S140	000062-44-2	-0.04	-0.04	-0.04	-0.03	-0.03	0.83	0.83	0.83	-0.57	2	1	2	Low Priority
S141	000062-46-4	0.41	0.60	0.52	-0.11	0.31	0.16	0.00	0.35	-1.83	1	1	1	Low Priority
S142	000063-05-8	0.93	0.92	0.98	0.95	0.87	1.40	1.23	1.19	-1.14	2	1	2	Low Priority
S143	000063-12-7	0.11	0.13	0.13	0.17	0.17	1.12	1.02	1.20	-0.11	2	1	2	Low Priority
S144	000063-68-3	0.02	0.12	0.00	-0.25	-0.07	-0.32	-0.28	-0.04	-2.60	1	1	1	Low Priority
S145	000063-74-1	0.37	0.54	0.68	0.92	0.90	-0.30	-0.13	-0.39	-1.52	2	1	2	Low Priority
S146	000063-91-2	0.28	0.32	0.24	-0.01	0.25	0.09	0.25	0.32	-1.33	1	1	1	Low Priority
S147	000063-98-9	1.37	0.44	0.33	0.36	0.67	-0.12	0.09	0.05	-1.15	1	1	2	Low Priority
S148	000064-77-7	0.85	0.85	0.85	0.85	0.85	0.22	0.36	0.30	-0.59	1	1	2	Low Priority
S149	000065-06-5	0.87	1.01	0.96	0.89	0.95	1.48	1.13	1.18	-1.71	2	1	2	Low Priority
S150	000065-23-6	0.18	0.45	0.61	0.29	0.39	0.17	0.27	-0.02	-1.54	1	1	1	Low Priority
S151	000065-45-2	0.08	0.23	0.36	0.06	0.31	-0.12	-0.15	0.04	-1.33	1	1	2	Low Priority
S152	000065-49-6	0.14	0.41	0.66	0.30	0.43	-0.08	-0.08	-0.14	-1.71	1	1	2	Low Priority
S153	000066-75-1	0.93	1.17	1.02	1.02	1.18	0.30	0.30	0.28	-0.58	2	1	2	Low Priority
S154	000066-76-2	0.64	0.69	0.92	0.77	0.86	0.89	0.59	0.87	0.90	1	1	2	Low Priority
S155	000066-79-5	-0.15	0.08	0.08	0.08	0.08	0.65	0.49	0.40	0.63	2	1	2	Low Priority
S156	000067-20-9	-0.01	0.26	0.26	0.26	0.26	0.24	0.11	-0.03	-0.16	2	1	2	Low Priority
S157	000067-45-8	-0.78	-0.76	-0.76	-0.77	-0.77	0.79	0.67	0.56	0.02	2	1	2	Low Priority
S158	000067-71-0	0.20	0.34	0.67	0.55	0.66	-0.70	-0.41	-0.27	-1.19	1	1	1	Low Priority

			Human I	Biotransforr	nation		Fish Bio	otransforma	ition		F	PBT Pro	filer	
ID	CAS	logHL _T (h)	logHL _{B1} (h)	logHL _{B2} (h)	logHL _{B3} (h)	logHL ₈₄ (h)	logHL _{N1} (h)	logHL _{N2} (h)	logHL _{N3} (h)	PBT Index	Р	В	т	Priority Level
S159	000068-22-4	0.85	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	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	-0.37	-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	1.21	2	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	0.54	1.22	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 0.71	-0.10	0.00	-2.61	1	1	1	Low Priority
S182 S183	000073-48-3 000073-49-4	0.93 0.67	0.97 0.83	0.97 1.17	1.05 1.31	1.05 1.29	0.71	1.16 0.47	0.59 0.53	2.03 -0.73	3	1	2	Low Priority Low Priority
														,
S184 S185	000074-55-5 000074-79-3	0.49 0.11	1.06 0.25	1.06 0.12	1.06 0.02	1.06 0.20	0.53 -0.38	0.73 -0.09	0.77 -0.01	-3.20 -3.95	1	1	1	Low Priority Low Priority
	000074-79-3	0.11			0.02	0.20	-0.38 -0.47		-0.01 -0.19	-3.95 -2.03	1			
S186 S187	000075-85-4	0.18	0.17 0.71	0.61 0.62	0.20	0.30	0.50	-0.19 0.74	0.69	-1.53	2	1	1 2	Low Priority Low Priority
S188	000076-22-2	0.11	0.15	0.02	0.15	0.28	1.07	0.68	0.03	-1.08	2	1	2	Low Priority
S189	000076-41-5	0.74	0.13	0.13	0.13	0.13	1.13	0.08	1.04	-0.69	3	1	1	Low Priority
S190	000076-42-0	0.74	0.98	0.83	0.83	0.83	0.91	0.73	0.46	-0.09	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
5194	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	0.13	-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	0.73	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
5223	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
5224	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
5232	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
5234	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)
5238	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 S240	000082-95-1 000083-07-8	1.59 0.55	1.46 0.78	1.72 0.72	1.66 0.71	1.50 0.84	3.61 0.06	3.39 0.24	3.81 -0.13	2.94 -0.81	3 1	3 1	3 2	High Priority Low Priority

				Human E	Biotransforr	mation		Fish Bio	otransforma	tion		Р	BT Profile	r
ity Level	ID	CAS	logHL _T (h)	logHL _{B1} (h)	logHL _{B2} (h)	logHL _{B3} (h)	logHL ₈₄ (h)	logHL _{N1} (h)	logHL _{N2} (h)	logHL _{N3} (h)	PBT Index	Р	В	Priority I
Priority	S241	000083-12-5	0.83	0.96	0.43	0.94	0.84	0.93	0.99	0.89	1.24	2		2 Low Prio
Priority	S242	000083-15-8	0.64	0.75	0.61	0.61	0.66	0.14	0.39	-0.03	-0.23	2		2 Low Price
Priority	S243	000083-66-9	0.49	0.70	0.29	0.75	0.39	1.59	1.46	1.68	0.01	2		3 Low Price
Priority	S244	000083-67-0	0.30	0.44	0.42	0.31	0.62	-0.52	-0.14	-0.58	-0.60	1		2 Low Prio
Priority	S245	000083-72-7	0.14	0.42	0.29	0.30	0.22	0.20	0.14	0.13	-0.17	1		3 Low Price
Priority	S246	000083-89-6	2.08	2.09	2.09	2.25	2.25	2.29	2.12	2.10	2.12	3		3 High Pri
Priority	S247	000083-98-7	1.22	1.22	1.22	1.25	1.25	1.96	2.05	1.91	0.97	2		2 Low Price
Priority	S248	000084-61-7	0.85	0.74	0.48	0.59	0.82	1.08	1.17	1.06	-0.07	2		3 Low Price
Priority	S249	000084-62-8	1.00	0.80	0.53	0.85	0.94	1.45	1.19	1.37	2.53	1		1 Low Price
Priority	S250	000084-66-2	0.61	0.44	0.24	0.38	0.41	0.56	0.74	0.71	-0.01	1		2 Low Price
Priority	S251	000084-69-5	0.92	0.66	0.62	0.66	0.76	0.85	1.13	1.05	-0.04	1		3 Low Pric
Priority	S252	000084-74-2	0.72	0.62	0.35	0.36	0.47	0.98	0.98	0.98	-0.04	1		3 Low Pric
Priority	S253	000084-75-3	0.68	0.69	0.30	0.25	0.35	1.12	1.25	1.15	-0.05 -0.07	1		3 Low Price ? Low Price
Priority	S254	000084-76-4	0.63	0.67	0.15 0.12	0.12	0.23	1.44	1.54	1.43	-0.07	1		
Priority Briority	S255 S256	000084-77-5 000084-96-8	0.63 1.42	0.68 1.30	1.33	0.09 1.23	1.27	1.53 2.50	1.62 2.37	1.51 2.31	1.10	2		
Priority		000085-68-7												
Priority	S257		-0.60	-0.60	-0.60	-0.60	-0.60	0.35	0.35	0.35	1.24	1		
Priority	S258	000085-69-8	0.80	0.65	0.52	0.38	0.45	1.11	1.27	1.18	-0.05			3 Low Pric
Priority	S259	000085-70-1	0.64	0.35	0.28	0.36	0.38	0.77	0.96	0.90	0.17	1		2 Low Pric
(Group 2)	S260	000085-79-0	0.81	0.99	0.64	0.55	0.61	0.69	0.84	0.28	0.39	2		3 Low Pric
Priority	S261	000086-12-4	1.34	1.26	1.05	1.18	1.20	2.41	2.24	2.07	0.88	2		3 Priority (Gr
Priority	S262	000086-13-5	1.28	1.27	0.94	1.12	1.24	2.11	2.08	1.90	0.94	2		3 Low Prio
Priority	S263	000086-14-6	1.34	1.13	1.23	1.36	1.32	2.68	2.27	2.56	0.89	2		3 Priority (Gr
Priority Priority	S264 S265	000086-21-5 000086-22-6	1.23 1.39	1.16 1.30	0.87 1.19	0.95 1.29	0.95 1.27	2.00 2.20	2.24 2.62	1.75 1.95	1.04 1.68	2		2 Low Priority (Graph Priority (Graph Priority)
Priority	S266	000086-34-0	0.61	0.53	0.47 0.91	0.52	0.63 0.92	0.52	0.66	0.60	-0.02	2		1 Low Pric
Priority	S267	000086-35-1	0.78	0.91		0.92		0.11	0.26	0.17	-0.42			2 Low Pric
riority	S268	000086-42-0	0.81	0.80	0.80	0.99	0.99	1.67	1.46	1.42	1.82	2		3 Low Pric
riority	S269 S270	000086-54-4 000087-08-1	-0.02 -0.08	0.04 0.05	0.04 0.05	0.04 0.05	0.04 0.05	0.29 0.48	0.71 0.37	0.13 0.60	-0.33 -0.62	1 2		 Low Price Low Price
riority														
riority	S271	000087-20-7	0.61	0.70	0.78	0.31	0.51	0.43 0.70	0.45	0.52	-0.61 0.67	1		3 Low Pric
riority	S272	000087-22-9	0.65	0.86	0.66	0.43	0.56		0.62	0.68		2		3 Low Pric
riority	S273	000087-33-2	0.23	0.25	0.25	0.25	0.25	1.10	0.32	1.35	-0.79			 Low Prio Low Prio
riority riority	S274	000088-29-9	0.99	0.99	0.95	1.00	0.70	1.32	1.73 0.74	1.70	-0.25	2		
	S275 S276	000089-25-8 000089-57-6	0.65 - 0.21	0.72 -0.21	0.58 -0.21	0.69 - 0.14	0.72 -0.14	0.43 -0.09	-0.08	0.26 -0.15	0.00 -1.71	1		
riority		000089-57-6												
riority	S277		0.60	0.50 0.49	0.85 0.62	0.63 0.77	0.85 0.83	0.48 0.68	0.43 0.73	0.37 0.68	-1.85 -1.30	1		2 Low Pric
riority	S278 S279	000089-81-6 000089-83-8	0.81 0.73	0.49	0.62	0.77	0.83	0.59	0.73	0.66	-0.77	1		 Low Price Low Price
Priority Priority	S279 S280	000089-83-8	-0.10	0.25	0.90	-0.18	-0.11	0.08	-0.13	0.00	-0.77	1		 Low Prio Low Prio
riority	S281	000090-05-1	0.25	0.22	0.44	0.18	0.34	0.24	-0.13	0.27	-0.74	1		2 Low Pric
Priority	S282	000090-34-6	0.25	0.85	0.85	0.80	0.93	1.35	1.42	1.05	-0.74	2		2 Low Pric
(Group 2)	5283	000090-72-2	0.97	1.03	0.95	1.00	0.83	0.91	1.22	1.21	-0.83	2		2 Low Pric
Priority	S284	000090-82-4	1.10	1.34	1.34	0.48	0.61	0.49	0.64	0.56	-1.17	1		1 Low Pric
Priority	S285	000090-84-6	0.80	0.77	0.46	0.67	0.55	0.75	0.96	0.84	-0.26	2		2 Low Pric
Priority	S286	000090-89-1	0.90	1.11	1.11	0.97	0.97	0.30	0.56	0.46	-1.55	2		1 Low Price
riority	S287	000091-16-7	0.70	0.31	0.24	0.47	0.45	1.37	1.12	1.37	-0.26	1		1 Low Price
Priority	S288	000091-33-8	0.77	1.06	1.26	1.61	1.39	0.90	0.60	0.71	1.35	2		2 Low Pric
riority	S289	000091-66-7	1.03	0.69	0.63	0.79	0.73	1.68	1.74	1.42	-0.18	2		2 Low Pric
riority	S290	000091-75-8	1.24	1.05	0.68	0.83	1.00	1.77	1.95	1.45	0.87	2		2 Low Price
riority	S291	000091-80-5	0.20	0.20	0.20	0.24	0.24	1.83	1.97	1.62	0.83	2		2 Low Price
riority	S292	000091-81-6	1.25	1.17	0.87	0.86	0.92	1.92	2.19	1.71	1.04	2		2 Low Price
riority	S293	000091-84-9	1.25	1.11	0.89	0.92	0.88	1.98	2.09	1.80	1.03	2		2 Low Pric
riority	S294	000091-87-2	1.14	0.56	0.60	0.64	0.72	2.05	1.99	1.94	-0.06	1		3 Low Pric
riority	S295	000092-62-6	1.03	1.06	1.19	1.38	1.51	0.67	0.92	0.36	0.33	2		2 Low Price
riority	S296	000093-14-1	0.00	0.01	0.01	0.01	0.01	0.63	0.41	0.72	-1.13	1		1 Low Price
riority	S297	000093-15-2	0.97	0.68	0.67	0.80	0.65	1.92	1.53	1.77	-0.05	2		2 Low Price
riority	S298	000093-16-3	0.98	0.71	0.74	0.75	0.67	2.08	1.53	1.77	-0.05	2		2 Low Price
riority	S299	000093-51-6	0.32	0.32	0.51	0.28	0.37	0.41	0.18	0.45	-0.75	1		2 Low Price
riority	S300	000094-09-7	0.57	0.55	0.53	0.55	0.66	-0.02	0.14	-0.19	-0.98	1		2 Low Price
riority	S301	000094-13-3	0.51	0.49	0.51	0.20	0.40	0.19	0.15	0.24	-0.60	1		2 Low Pric
riority	S302	000094-18-8	0.77	0.85	0.74	0.56	0.71	0.57	0.50	0.56	0.67	1		2 Low Price
riority	S303	000094-20-2	1.66	1.76	1.76	1.76	1.76	0.62	0.49	0.76	0.06	2		2 Low Price
riority	S304	000094-26-8	0.54	0.57	0.54	0.17	0.37	0.30	0.26	0.33	-0.61	1		2 Low Prio
riority	S305	000094-78-0	1.04	0.97	1.18	1.33	1.61	0.75	1.30	0.61	-0.31	2		3 Low Pric
riority	S306	000095-14-7	0.36	0.56	0.42	0.08	0.38	0.18	0.60	-0.09	0.26	1		2 Low Prio
riority	S307	000095-87-4	0.37	0.35	0.72	0.32	0.54	0.27	0.20	0.32	-0.75	1		2 Low Prio
riority	\$308	000096-17-3	0.21	-0.05	0.00	-0.09	-0.09	-0.06	-0.03	0.13	-1.41	1		2 Low Price
riority	S309	000096-88-8	0.30	0.31	0.31	0.32	0.32	0.60	0.77	0.33	-0.67	2		2 Low Prio
riority	S310	000096-91-3	-0.02	0.25	0.31	0.30	0.30	0.61	0.19	0.46	-1.11	2		1 Low Price
riority	S311	000097-18-7	2.04	2.76	2.76	2.57	2.57	2.28	1.75	2.20	2.68	3		3 High Prie
riority	S312	000097-53-0	0.52	0.58	0.73	0.40	0.43	0.86	0.45	0.71	-0.54	1	1	2 Low Pric
riority	S313	000097-86-9	0.81	0.16	0.28	0.47	0.66	0.28	0.65	0.67	-1.26	1		2 Low Price
riority	S314	000097-99-4	-0.02	0.18	0.46	-0.28	0.10	-0.45	-0.31	-0.25	-2.00	1		1 Low Price
riority	S315	000098-55-5	0.85	0.53	1.05	1.01	1.03	0.65	0.67	0.58	-1.86	2		2 Low Price
riority	S316	000098-88-4	0.12	0.17	0.43	0.23	0.36	0.40	0.65	0.56	0.48	1		2 Low Price
riority	S317	000098-92-0	0.27	0.26	0.33	0.30	0.62	-0.46	-0.14	-0.52	-0.94	2		2 Low Price
Priority	S318	000098-96-4	0.98	0.29	0.34	0.39	0.63	-0.65	-0.16	-0.66	-0.93	1		2 Low Price
Group 2)	5319	000099-43-4	0.74	0.79	0.56	0.64	0.58	0.66	0.67	0.42	-1.04	2		3 Low Price
Group 2)	5320	000099-48-9	0.71	0.33	0.83	0.76	0.89	0.62	0.63	0.57	-1.63	1		3 Low Pric
Priority	5321	000099-57-0	0.10	0.25	0.39	0.24	0.36	0.28	0.05	0.17	-1.31	1		2 Low Price
		000099-66-1	1.08	1.09	1.09	1.09	1.09	-0.13	0.02	0.06	-1.85	1	1	

Part				Human	Biotransfori	mation		Fish Ri	otransforma	tion			PBT Pro	nfiler	
STATE	ID	CAS	logHL _T (h)	logHL _{B1}	logHL _{B2}	logHL _{B3}			logHL _{N2}	logHL _{N3}	PBT Index				Priority Level
Sign	5323	000099-76-3	0.31					-0.04			-0.57	1	1		Low Priority
Sign															Low Priority
Sign															Low Priority
Same															Low Priority
S339															Low Priority
Sample S															Low Priority
S332 00010053-6 0.28 0.28 0.22 0.41 0.01 0.36 0.07 0.07 0.07 0.71 1 1 1 10 0.09															Low Priority
\$333 000105-27 0.15 0.35 0.31 0.39 0.05 0.07 0.36 0.33 0.46 0.33 1 1 1 2 0 0.00 1.33 0.33 0.00 0.00 0.00 0.00 0.															Low Priority
\$333 000100-90-3 0.85 0.91 1.26 1.26 1.26 1.26 1.26 1.26 1.26 1.2															Low Priority
S355 000100 970 0.99 0.79 0.65 0.17 0.64 0.98 1.12 1.07 1.55 1.74 1.67 0.66 2 1 2 1.09															Low Priority
Same															Low Priority
Sign Control Sign Sign Control Sign															
\$338 000107-24 125 104 117 100 1.16 1.87 1.96 1.63 0.30 0.21 0.07 2 1 2 towyles 0.00107-24 125 1.04 1.17 1.00 1.16 1.87 1.09 1.63 0.30 0.21 1.2 towyles 0.00107-24 1.25 1.04 1.17 1.00 1.16 1.87 1.18 1.1															
Same Control Same															Low Priority
Same															Low Priority
SAH															Low Priority
SAME CONTINES CO															Low Priority
SASS 0000101-86-0 0.82															Low Priority
\$344 000103-93															Low Priority
S344 0001130-93 0.65															Low Priority
Safe															Low Priority
S347															Low Priority
\$348 000103-386 0.85 0.65 0.67 0.66 0.44 0.66 0.75 0.56 0.93 0.21 1 1 2 10w/P \$349 000103-41-3 0.97 0.87 0.56 0.61 0.83 1.43 1.12 1.17 1.29 1 1 3 10w/P \$350 000103-53-7 0.95 0.86 0.67 0.90 0.32 0.61 1.05 0.39 0.96 0.06 1 1 3 10w/P \$351 000103-54-8 0.83 0.54 0.50 0.32 0.61 1.05 0.39 0.96 0.06 1 1 3 10w/P \$352 000103-560 0.83 0.54 0.61 0.83 0.88 1.12 0.97 0.93 0.96 0.06 1 1 3 10w/P \$353 000103-59-9 0.85 0.94 0.51 0.86 0.88 0.88 1.10 0.97 0.03 1 1 3 10w/P \$353 000103-59-9 0.85 0.95 0.86 0.86 0.88 0.88 1.10 0.10 1.00 1.00 1.00 1 1 1 3 10w/P \$353 000103-59-9 0.85 0.97 0.85 0.99 0.95 0.99 0.95 0.99 0.95 0.97 0.93 1 1 3 1 0.00 P \$355 000103-59-9 0.85 0.99 0.95 0.95 0.95 0.95 0.95 0.95 0.9															Low Priority
SAMP 000103-348 0.86															Low Priority
\$359 000103-337 097 0.87 0.56 0.61 0.83 1.43 1.22 1.17 1.29 1 1 3 1.09/P \$3510 000103-348 0.85 0.86 0.54 0.50 0.32 0.61 1.05 0.89 0.56 0.06 1.1 1 3 1.09/P \$352 000103-560 0.83 0.50 0.84 0.68 0.88 0.69 0.95 1.12 0.05 0.97 0.03 1 1 3 1.09/P \$3532 000103-560 0.83 0.50 0.84 0.88 0.88 0.89 1.12 0.07 1.06 0.01 1 1 3 1.09/P \$3534 000103-567 0.87 0.50 0.44 0.61 0.38 0.68 1.19 1.07 1.06 0.01 1 1 3 1.09/P \$3535 000103-617 0.79 0.50 0.44 0.61 0.38 0.68 1.19 1.07 1.06 0.01 1 1 3 1.09/P \$3535 000103-641 0.15 0.47 0.56 1.14 1.15 1.99 1.78 1.64 0.67 1 1 2 1.09/P \$3535 000103-640 0.88 0.90 0.01 0.55 0.71 0.81 0.85 0.97 -0.21 1 1 3 1.09/P \$3536 000103-92 0.40 0.41 0.41 0.41 0.11 0.11 0.11 0.01 0.0															
Sa55 000103-54-8 0.85 0.54 0.55 0.54 0.55 0.74 1.51 1.30 1.25 1.29 1 1 3 1.09/P															Low Priority Low Priority
Sa51 000103-546 0.85 0.54 0.50 0.32 0.61 1.05 0.89 0.96 0.06 1 1 3 Low Pr Sa52 000103-560 0.83 0.50 0.48 0.28 0.59 1.12 0.95 0.97 0.03 1 1 3 Low Pr Sa53 000103-593 0.85 0.54 0.61 0.38 0.68 1.19 1.07 1.06 0.01 1 1 3 Low Pr Sa53 000103-617 0.79 0.50 0.43 0.22 0.52 1.20 1.02 1.02 1.02 0.02 1 1 3 Low Pr Sa53 000103-640 1.35 0.47 0.56 1.14 1.36 1.99 1.78 1.64 0.67 1 1 2 Low Pr Sa53 000103-942 0.40 0.41															Low Priority
SSSS 000103-59-3 0.83 0.50 0.48 0.28 0.59 1.12 0.95 0.97 0.03 1 1 3 Low Pr															Low Priority
S353 000103-59-3 0.85 0.54 0.61 0.38 0.68 1.19 1.07 1.06 0.01 1 1 3 1.09/Pr															Low Priority
SSSS 000103-61-0 35															Low Priority
\$355 000103-0-02 0.40 0.41 0.41 0.41 0.41 0.41 0.11 0.11															Low Priority
SSSF 000103-99-2															Low Priority
S357 000109-93-5 0.83 0.50 0.61 0.55 0.71 0.81 0.85 0.97 0.04 1 1 2 LowPP S358 000104-09-6 0.68 0.59 0.29 0.54 0.44 0.70 0.66 0.78 0.66 0.78 S359 000104-29-9 0.61 0.61 0.44 0.20 0.35 0.77 0.44 0.53 0.38 1 1 2 LowPP S360 000104-29-0 0.65 0.58 0.59 0.															Low Priority
SSSS 000104-09-6															Low Priority
\$359 000104-28-9 0.61 0.61 0.44 0.20 0.35 0.77 0.44 0.53 -0.38 1 1 2 Low Pr \$361 000104-93-0 0.56 0.58 0.58 0.59 0.59 1.02 0.69 1.18 0.49 1 1 1 1 Low Pr \$361 000104-93-1 0.45 0.39 0.53 -0.01 0.41 0.61 0.36 0.43 -0.49 1 1 3 Low Pr \$362 000104-93-6 1.00 0.51 0.45 0.21 0.51 0.39 0.53 0.49 0.61 -0.14 1 1 2 Low Pr \$363 000104-90-5 1.00 0.58 0.74 0.81 0.90 1.13 1.36 0.87 -0.24 2 1 2 Low Pr \$363 000104-90-5 1.00 0.58 0.74 0.81 0.90 1.13 1.36 0.87 -0.24 2 1 2 Low Pr \$365 000105-20-4 0.50 0.35 0.41 0.53 0.80 0.12 0.42 -0.01 1.63 1 1 1 Low Pr \$365 000105-20-4 0.50 0.35 0.41 0.53 0.80 0.12 0.42 0.00 0.99 1.44 1 1 2 Low Pr \$367 000105-37-3 0.41 0.27 -0.24 -0.11 0.04 -0.22 0.00 0.09 1.44 1 1 2 Low Pr \$367 000105-37-3 0.40 -0.05 0.19 0.21 0.13 0.18 0.06 0.16 1.23 1 1 1 Low Pr \$368 000105-37-3 0.40 0.05 0.19 0.21 0.13 0.18 0.06 0.16 1.23 1 1 1 Low Pr \$369 000105-67-9 0.37 0.35 0.71 0.31 0.53 0.27 0.20 0.34 0.39 1.25 1 1 2 Low Pr \$370 000105-67-9 0.37 0.35 0.71 0.31 0.53 0.27 0.20 0.33 0.74 1 1 2 Low Pr \$371 000105-90-8 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1.13 1 Low Pr \$372 000105-91-9 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 3 Low Pr \$373 000105-91-9 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 1 3 Low Pr \$374 000105-92-8 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 1 2 Low Pr \$374 000105-92-8 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 1 2 Low Pr \$373 000105-92-9 0.74 0.36 0.65 0.44 0.75 0.77 0.64 0.68 1.58 1 1 2 Low Pr \$373 000105-92-9 0.74 0.36 0.65 0.44 0.75 0.77 0.64 0.68 1.58 1 1 2 Low Pr \$373 000105-92-9 0.74 0.36 0.65 0.44 0.57 0.77 0.64 0.68 1.58 1 1 2 Low Pr \$373 000105-22-9 0.74 0.36 0.64 0.44 0.57 0.77 0.64 0.68 1.58 1 1 2 Low Pr \$373 000105-22-0 0.79 0.19 0.64 0.44 0.57 0.77 0.64 0.68 1.58 1 1 3 Low Pr \$373 000105-22-0 0.79 0.19 0.64 0.44 0.57 0.77 0.64 0.68 1.58 1 1 1 Low Pr \$383 000105-24 0.09 0.09 0.39 0.44 0.44 0.57 0.77 0.64 0.68 0.68 1.58 1 1 1 Low Pr \$383 000105-24 0.09 0.09 0.39 0.44 0.44 0.57 0.77 0.64 0.68 0.68 1.58 1 1 1 Low Pr \$383 000105-24 0.00 0.00 0.34 0.06 0.35 0.34															
SSB 000104-29-0 0.56															Low Priority
\$361 000104-874															Low Priority
SSG 000104-870 0.51															
Safa 000104-90-5 1.00 0.58 0.74 0.81 0.90 1.13 1.15 0.87 0.24 2 1 2 Low Pr Saf6 000105-20-4 0.50 0.35 0.41 0.53 0.80 0.12 0.42 -0.01 1.63 1 1 1 Low Pr Saf6 000105-37-3 0.41 -0.27 -0.24 -0.11 0.04 -0.22 0.00 0.09 -1.44 1 1 2 Low Pr Saf6 000105-37-3 0.41 -0.27 -0.24 0.01 0.04 -0.22 0.00 0.09 -1.44 1 1 2 Low Pr Saf6 000105-47-3 0.40 -0.25 -0.19 0.21 0.13 -0.18 0.06 0.16 -1.23 1 1 1 Low Pr Saf6 000105-53-3 0.62 0.24 0.06 0.30 0.17 0.09 0.34 0.39 -1.25 1 1 2 Low Pr Saf7 000105-67-9 0.37 0.35 0.71 0.31 0.53 0.27 0.20 0.33 -0.74 1 2 Low Pr Saf7 000105-97-3 0.95 0.07 0.35 0.51 0.55 1.16 1.15 1.20 -1.03 1 1 3 Low Pr Saf7 000105-91-9 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 -1.05 1 1 3 Low Pr Saf7 000105-91-9 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 -1.05 1 1 3 Low Pr Saf7 000105-91-9 0.62 0.18 0.72 0.16 0.88 0.78 0.96 0.95 -1.29 1 3 3 Low Pr Saf7 000106-25 0.66 0.38 0.66 0.04 0.87 0.95 1.08 1.03 1.51 1 2 Low Pr Saf7 000106-24 0.70 0.19 0.64 0.44 0.57 0.77 0.64 0.68 1.58 1 1 3 Low Pr Saf8 000106-25 0.06 0.09 0.09 0.04 0.44 0.57 0.77 0.64 0.68 1.58 1 1 3 Low Pr Saf8 000106-25 0.06 0.02 0.02 0.02 0.03 0.03 0.04 0.04 0.05 0.05 0.05 0.09 0.0															Low Priority
Safe 000104-93-8 1.17 0.59 0.70 1.06 1.06 1.21 1.12 1.21 1.21 1.22 1.02 1.08 1.08 1.08 1.08 1.08 1.08 1.08 1.09 1.08 1.09 1.00 1.08 1.09 1.00 1.09 1.04 1.09 1.00 1.09 1.04 1.09 1.00															Low Priority
\$365 000105-20-4 0.50 0.41 0.27 0.24 0.11 0.04 0.02 0.02 0.09 1.44 1 1 1 2 Low Pr \$366 000105-37-3 0.40 0.05 0.19 0.21 0.13 0.08 0.06 0.16 1.23 1 1 1 1 Low Pr \$367 000105-53-3 0.60 0.02 0.02 0.06 0.30 0.17 0.09 0.34 0.39 1.125 1 1 2 Low Pr \$369 000105-67-9 0.37 0.35 0.71 0.31 0.53 0.27 0.20 0.33 0.74 1 1 2 Low Pr \$379 000105-67-9 0.37 0.35 0.71 0.31 0.53 0.27 0.20 0.33 0.74 1 1 2 Low Pr \$370 000105-87-3 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 3 Low Pr \$371 000105-90-8 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 3 Low Pr \$372 000105-91-9 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 3 Low Pr \$373 000105-91-9 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 3 Low Pr \$373 000105-91-9 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 3 Low Pr \$374 000105-91-9 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 1 3 Low Pr \$375 000105-91-9 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 2 3 Low Pr \$375 000105-91-9 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 1 3 Low Pr \$375 000105-91-9 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 1.05 1 1 1 3 Low Pr \$375 000105-21-9 0.74 0.36 0.65 0.41 0.49 0.63 0.66 0.88 0.78 0.96 0.95 1.29 1 3 3 Low Pr \$375 000105-22-9 0.74 0.36 0.65 0.41 0.49 0.63 0.66 0.99 1.80 1 1 2 Low Pr \$387 000106-22-1 0.79 0.19 0.64 0.44 0.57 0.77 0.64 0.68 1.58 1 1 3 Low Pr \$387 000106-22-0 0.79 0.19 0.64 0.44 0.57 0.77 0.64 0.68 1.58 1 1 3 Low Pr \$387 000106-22-0 0.79 0.19 0.64 0.44 0.57 0.77 0.64 0.68 1.58 1 1 3 Low Pr \$380 00106-22-0 0.92 0.12 0.39 0.44 0.48 1.30 1.25 1.23 1.06 1 2 3 Low Pr \$380 00106-22-0 0.92 0.92 0.99 0.99 0.90 0.90 0.90 0.9															Low Priority
Safe 000105-37-3 0.41															Low Priority
S367 000105-45-3 0.40 -0.05 -0.19 0.21 0.13 -0.18 0.06 0.16 -1.23 1 1 1 Low Pr															Low Priority
S388 000105-53-3 0.62															Low Priority
S369 000105-67-9 0.37 0.35 0.71 0.31 0.53 0.27 0.20 0.33 -0.74 1 1 2 Low Pr															Low Priority
S370 000105-97-3 0.95 0.07 0.35 0.51 0.55 1.16 1.15 1.20 -1.03 1 1 3 Low Price 1.15 1.20 -1.05 1 1 1 1 Low Price 1.15 1.20 -1.05 1 1 1 1 Low Price 1.15 1.20 -1.05 1 1 1 Low Price 1.15 1.20 -1.05 1 1 1 1 Low Price 1.15 1.20 -1.05 1 1 1 Low Price 1.15 1.1												1			Low Priority
S371 000105-90-8 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 -1.05 1 1 3 Low Pr															Low Priority
S372 000105-91-9 0.95 0.09 0.39 0.48 0.53 1.22 1.19 1.20 -1.05 1 1 3 Low Pr															Low Priority
S373 000105-95-3 0.62 0.18 0.72 0.16 0.88 0.78 0.95 0.95 -1.29 1 3 3 1.0w Pr															Low Priority
S374 000106-02-5 0.66 0.38 0.66 0.04 0.87 0.95 1.08 1.03 -1.51 1 2 3 Low Pr															Low Priority
S375 000106-22-9 0.74 0.36 0.65 0.41 0.49 0.63 0.66 0.69 -1.80 1 1 2 Low Pr S377 000106-25-2 0.79 0.19 0.64 0.44 0.57 0.77 0.64 0.68 -1.58 1 1 3 Low Pr S377 000106-25-2 0.79 0.19 0.64 0.44 0.57 0.77 0.64 0.68 -1.58 1 1 3 Low Pr S378 000106-29-6 0.92 0.12 0.39 0.44 0.48 1.30 1.25 1.23 -1.06 1 2 3 Low Pr S379 0.0106-60-5 0.08 0.02 0.02 0.03 0.03 0.05 -0.57 -0.34 -0.28 -2.40 1 1 Low Pr S380 000106-60-5 0.51 0.17 0.17 0.18 0.15 -0.04 0.22 0.30 -1.24 1 1 1 Low Pr S381 0.00106-99 0.34 0.25 0.36 0.34 0.14 -0.20 0.29 0.29 0.29 0.89 1 2 Low Pr S381 0.00107-75-5 0.16 0.25 0.36 0.34 0.14 -0.20 0.10 0.06 -2.43 1 1 Low Pr S384 0.0108-01-0 0.04 0.05 0.25 -0.18 -0.09 -0.69 -0.47 -0.38 -1.99 1 1 Low Pr S385 0.00108-10-1 0.25 0.06 0.15 0.11 0.04 -0.05 0.25 0.32 -1.45 1 1 Low Pr S386 0.0108-10-1 0.25 0.06 0.15 0.11 0.04 -0.05 0.25 0.32 -1.45 1 1 Low Pr S387 0.00108-12-5 0.24 0.05 0.15 0.10 0.04 -0.05 0.25 0.32 -1.45 1 1 Low Pr S387 0.00108-12-5 0.24 0.09 0.34 0.06 0.13 -0.24 0.02 0.03 -2.02 1 1 Low Pr S388 0.00108-10-1 0.25 0.06 0.15 0.10 0.04 -0.05 0.25 0.32 -1.45 1 1 Low Pr S388 0.00108-39-4 0.07 0.29 0.68 -0.05 0.24 0.08 -0.01 0.14 -0.73 1 2 Low Pr S389 0.00108-39-4 0.07 0.29 0.68 -0.05 0.24 0.08 -0.01 0.14 -0.73 1 1 2 Low Pr S399 0.00108-39-5 0.06 0.06 0.05 0.05 0.05 0.04 0.05 0.05 0.05 0.05 0.05 0.05 0.05 0.05 0.05 0.05 0.05 0.07 0.09 0.06 0.05 0.					0.66		0.87	0.95	1.08			1	2		Low Priority
S376 O0106-24-1 O.79 O.19 O.64 O.44 O.57 O.77 O.64 O.68 -1.58 1 1 3 Low Price of the control of															Low Priority
S377 000106-25-2 0.79 0.19 0.64 0.44 0.57 0.77 0.64 0.68 -1,58 1 1 3 Low Pr			0.79			0.44					-1.58	1			Low Priority
S378 000106-29-6 0.92 0.12 0.39 0.44 0.48 1.30 1.25 1.23 -1.06 1 2 3 Low Pr			0.79			0.44	0.57	0.77				1			Low Priority
S379 000106-60-5 -0.08 0.02 0.02 0.03 0.03 -0.57 -0.34 -0.28 -2.40 1 1 1 Low Pr			0.92			0.44	0.48	1.30				1			Low Priority
S380 000106-65-0 0.51 0.17 0.17 0.18 0.15 -0.04 0.22 0.30 -1.24 1 1 Low Pr S381 000106-89-8 0.34 0.20 0.95 0.78 0.82 0.22 0.29 0.29 -0.89 1 1 2 Low Pr S382 000107-75-5 0.72 0.47 0.36 0.46 0.28 0.51 0.60 0.62 -1.84 2 1 2 Low Pr S384 000107-75-5 0.72 0.47 0.36 0.46 0.28 0.51 0.60 0.62 -1.84 2 1 2 Low Pr S384 000108-10-1 0.25 0.06 0.15 0.11 0.04 -0.05 0.25 0.32 -1.45 1 1 Low Pr S386 000108-10-1 0.25 0.05 -0.10 -0.04 -0.03 -0.19 0.14 0.02 0.03 -2.02 1 1			-0.08		0.02	0.03		-0.57				1	1		Low Priority
S381 000106-89-8 0.34 0.20 0.95 0.78 0.82 0.22 0.29 -0.89 1 1 2 Low Pr S382 000107-41-5 0.16 0.25 0.36 0.34 0.14 -0.20 0.10 0.06 -2.43 1 1 1 Low Pr S384 000107-75-5 0.72 0.47 0.36 0.46 0.28 0.51 0.60 0.62 -1.84 2 1 2 Low Pr S384 000108-10-1 0.04 0.05 0.25 -0.18 -0.09 -0.69 -0.47 -0.38 -1.99 1 1 1 Low Pr S385 000108-10-1 0.04 0.05 0.25 -0.18 -0.09 -0.47 -0.38 -1.99 1 1 1 Low Pr S387 000108-22-5 0.22 -0.05 -0.10 -0.04 -0.03 -0.19 0.14 0.26 -1.21 1 1 Low Pr												1			Low Priority
S382 000107-41-5 0.16 0.25 0.36 0.34 0.14 -0.20 0.10 0.06 -2.43 1 1 1 Low Pr S383 000107-75-5 0.72 0.47 0.36 0.46 0.28 0.51 0.60 0.62 -1.84 2 1 2 Low Pr S384 000108-10-1 0.25 0.06 0.15 0.11 0.04 -0.05 0.25 0.18 -0.09 -0.47 -0.38 -1.99 1 1 1 low Pr S385 000108-10-1 0.25 0.06 0.15 0.01 0.04 -0.05 0.25 0.32 -1.45 1 1 low Pr S386 000108-22-5 0.22 -0.05 -0.10 -0.04 -0.03 -0.19 0.14 0.26 -1.21 1 1 Low Pr S388 000108-39-4 0.07 0.29 0.68 -0.05 0.24 0.08 -0.01 0.14 -0.73						0.78	0.82					1	1		Low Priority
S383 000107-75-5 0.72 0.47 0.36 0.48 0.28 0.51 0.60 -1.84 2 1 2 Low Pr S384 000108-01-0 0.04 0.05 0.25 -0.18 -0.09 -0.69 -0.47 -0.38 -1.99 1 1 1 Low Pr S385 000108-10-1 0.25 0.06 0.15 0.11 0.04 -0.05 0.25 0.32 -1.45 1 1 1 Low Pr S386 000108-11-2 0.14 0.09 0.34 0.06 0.13 -0.24 0.02 0.03 -2.02 1 1 1 Low Pr S387 000108-24-7 0.16 -0.13 -0.21 -0.14 -0.16 -0.35 -0.08 0.06 -1.20 1 1 1 Low Pr S388 000108-34-9 0.07 0.29 0.68 -0.05 0.24 0.08 0.06 -1.20 1 1 1						0.34	0.14					1	1		Low Priority
S384 000108-01-0 0.04 0.05 0.25 -0.18 -0.09 -0.69 -0.47 -0.38 -1.99 1 1 1 Low Pr S385 000108-10-1 0.25 0.06 0.15 0.11 0.04 -0.05 0.25 0.32 -1.45 1 1 1 Low Pr S387 000108-22-5 0.22 -0.05 -0.10 -0.04 -0.03 -0.19 0.14 0.26 -1.21 1 1 Low Pr S388 000108-22-5 0.12 -0.14 -0.16 -0.13 -0.21 -0.14 -0.05 -1.21 1 1 Low Pr S389 000108-39-4 0.07 0.29 0.68 -0.05 0.24 0.08 -0.01 0.14 -0.73 1 1 2 Low Pr S390 000108-93-9 0.07 0.02 0.29 0.67 -0.19 0.08 -0.18 -1.11 1 1 Low Pr S39					0.36	0.46	0.28		0.60			2	1	2	Low Priority
S385 000108-10-1 0.25 0.06 0.15 0.11 0.04 -0.05 0.25 0.32 -1.45 1 1 1 Low Pr S386 000108-11-2 0.14 0.09 0.34 0.06 0.13 -0.24 0.02 0.03 -2.02 1 1 1 Low Pr S387 000108-22-5 0.22 -0.05 -0.10 -0.04 -0.03 -0.14 0.26 -1.21 1 1 1 Low Pr S388 000108-24-7 0.16 -0.13 -0.21 -0.14 -0.16 -0.35 -0.08 0.06 -1.20 1 1 1 Low Pr S389 000108-39-8 0.06 0.06 0.02 0.29 0.07 -0.16 0.15 -1.11 1 1 Low Pr S390 000108-93-8 0.76 0.08 -0.09 0.50 0.47 -0.19 0.08 0.15 -1.11 1 1 Low Pr		000108-01-0					-0.09					1	1		Low Priority
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S387 000108-22-5 0.22 -0.05 -0.10 -0.04 -0.03 -0.19 0.14 0.26 -1.21 1 1 3 Low Pr S388 000108-24-7 0.16 -0.13 -0.21 -0.14 -0.16 -0.35 -0.08 0.06 -1.20 1 1 1 Low Pr S389 000108-39-4 0.07 0.29 0.68 -0.05 0.24 0.08 -0.01 0.14 -0.73 1 1 2 Low Pr S390 000108-39-8 -0.02 0.21 0.66 0.02 0.29 0.07 -0.16 0.15 -1.11 1 1 Low Pr S391 000108-93-0 0.04 0.16 0.66 -0.18 0.36 -0.25 -0.14 -0.14 -2.03 1 1 Low Pr S393 000108-94-1 0.14 0.11 0.34 -0.08 0.27 -0.07 0.08 0.13 -1.41 1 1 Lo						0.06	0.13					1	1	1	Low Priority
S388 000108-24-7 0.16 -0.21 -0.14 -0.16 -0.35 -0.08 0.06 -1.20 1 1 1 Low Pr S389 000108-39-4 0.07 0.29 0.68 -0.05 0.24 0.08 -0.01 0.14 -0.73 1 1 2 Low Pr S390 000108-36-3 -0.02 0.21 0.66 0.02 0.29 0.07 -0.16 0.15 -1.11 1 1 Low Pr S391 000108-99-8 0.76 0.08 -0.09 0.50 0.47 -0.19 0.08 0.18 -1.23 1 1 1 Low Pr S392 000108-93-0 0.04 0.16 0.66 -0.18 0.36 -0.25 -0.14 -0.14 -2.03 1 1 Low Pr S393 000108-94-1 0.14 0.11 0.34 -0.08 0.27 -0.07 0.08 0.13 -1.46 1 1 Low Pr <t< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td>-0.03</td><td></td><td></td><td></td><td></td><td>1</td><td>1</td><td>3</td><td>Low Priority</td></t<>							-0.03					1	1	3	Low Priority
S389 000108-39-4 0.07 0.29 0.68 -0.05 0.24 0.08 -0.01 0.14 -0.73 1 1 2 Low Pr S390 000108-46-3 -0.02 0.21 0.66 0.02 0.29 0.07 -0.16 0.15 -1.11 1 1 Low Pr S391 000108-93-0 0.04 0.16 0.66 -0.18 0.36 -0.25 -0.14 -0.10 1 1 1 Low Pr S393 000108-93-0 0.04 0.16 0.66 -0.18 0.36 -0.25 -0.14 -0.14 -2.03 1 1 1 Low Pr S393 000108-95-2 0.54 0.57 0.57 0.57 0.57 -0.07 -0.08 0.13 -1.46 1 1 Low Pr S395 00010-15-6 0.05 -0.38 0.01 -0.29 -0.04 -0.85 -0.63 -0.05 -0.72 1 1 2 <t< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td>-0.16</td><td></td><td>-0.08</td><td></td><td></td><td>1</td><td>1</td><td></td><td>Low Priority</td></t<>							-0.16		-0.08			1	1		Low Priority
S390 000108-6-3 -0.02 0.21 0.66 0.02 0.29 0.07 -0.16 0.15 -1.11 1 1 1 Low Pr S391 000108-93-8 0.76 0.08 -0.09 0.50 0.47 -0.19 0.08 0.18 -1.23 1 1 1 Low Pr S392 000108-93-0 0.04 0.16 0.66 -0.18 0.36 -0.25 -0.14 -0.14 -0.14 -2.03 1 1 1 Low Pr S393 000108-91-0 0.54 0.57 0.59 0.04 -0.22 -0.05 -0.72 1 1 2 Low Pr S395 000110-15-6 0.05 -0.08 0.017				0.29		-0.05	0.24	0.08			-0.73	1	1	2	Low Priority
S391 000108-59-8 0.76 0.08 -0.09 0.50 0.47 -0.19 0.08 0.18 -1.23 1 1 Low Pr S392 000108-93-0 0.04 0.16 0.66 -0.18 0.36 -0.25 -0.14 -0.14 -2.03 1 1 1 Low Pr S393 000108-94-1 0.14 0.11 0.34 -0.08 0.27 -0.07 0.08 0.13 -1.46 1 1 1 Low Pr S394 000108-95-2 0.54 0.57 0.57 0.57 -0.57 -0.14 -0.22 -0.05 -0.72 1 1 2 Low Pr S395 000110-15-6 0.05 -0.38 0.01 -0.29 -0.04 -0.85 -0.63 -0.49 -1.97 1 1 1 Low Pr S397 000110-93-0 0.79 0.17 0.22 0.56 0.49 0.49 0.59 0.63 -1.24 1 1 <td></td> <td>Low Priority</td>															Low Priority
S392 000108-93-0 0.04 0.16 0.66 -0.18 0.36 -0.25 -0.14 -0.14 -2.03 1 1 1 Low Pr S393 000108-95-1 0.14 0.11 0.34 -0.08 0.27 -0.07 0.08 0.13 -1.46 1 1 1 Low Pr S394 000108-95-2 0.54 0.57 0.01 0.04 -0.85 -0.63 -0.49 -1.97 1 1 1 Low Pr S396 000110-46-3 0.45 -0.06 -0.22 0.56 0.49 0.49 0.59 0.63 -1.24 1															Low Priority
S393 000109-94-1 0.14 0.11 0.34 -0.08 0.27 -0.07 0.08 0.13 -1.46 1 1 1 Low Pr S394 000109-95-2 0.54 0.57 0.57 0.57 -0.74 -0.22 -0.05 -0.72 1 1 2 Low Pr S395 000110-15-6 0.05 -0.38 0.01 -0.29 -0.04 -0.85 -0.63 -0.49 -1.97 1 1 1 Low Pr S396 000110-46-3 0.45 -0.06 -0.25 -0.17 0.01 0.46 0.36 0.85 -1.39 1 1 2 Low Pr S397 000110-93-0 0.79 0.17 0.22 0.56 0.49 0.59 0.63 -1.29 1 1 2 Low Pr S398 000111-12-6 0.73 0.19 0.35 -0.02 0.46 0.46 0.65 0.70 -1.24 1 2 Low Pr															Low Priority
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S395 000110-15-6 0.05 -0.38 0.01 -0.29 -0.04 -0.85 -0.63 -0.49 -1.97 1 1 1 Low Pr S396 000110-46-3 0.45 -0.06 -0.25 -0.17 0.01 0.46 0.36 0.85 -1.39 1 1 2 Low Pr S397 000110-93-0 0.79 0.17 0.22 0.56 0.49 0.49 0.59 0.63 -1.24 1 1 2 Low Pr S398 000111-21-6 0.73 0.19 0.35 -0.02 0.46 0.46 0.65 0.70 -1.24 1 1 2 Low Pr S490 000112-05-0 0.39 0.16 -0.03 -0.51 -0.20 0.02 0.17 0.23 -1.83 1 1 2 Low Pr S401 000113-42-8 0.53 0.54 0.53 0.53 0.53 0.54 0.53 0.53 0.90 0.96															Low Priority
S396 000110-46-3 0.45 -0.06 -0.25 -0.17 0.01 0.46 0.36 0.85 -1.39 1 1 2 Low Pr S397 000110-93-0 0.79 0.17 0.22 0.56 0.49 0.49 0.59 0.63 -1.24 1 1 2 Low Pr S398 000111-12-6 0.73 0.19 0.35 -0.02 0.46 0.46 0.65 0.70 -1.24 1 1 2 Low Pr S499 000112-05-0 0.39 0.16 -0.03 -0.51 -0.20 0.02 0.17 0.23 -1.83 1 1 2 Low Pr S400 000113-42-8 0.53 0.54 0.53 0.53 0.53 0.53 0.90 0.96 0.44 -0.43 2 1 2 Low Pr S402 000113-42-8 0.68 0.68 0.68 0.68 0.68 0.64 0.75 0.65 -0.64															Low Priority
S397 000110-93-0 0.79 0.17 0.22 0.56 0.49 0.49 0.59 0.63 -1.24 1 1 2 Low Pr S398 000111-12-6 0.73 0.19 0.35 -0.02 0.46 0.46 0.65 0.70 -1.24 1 1 2 Low Pr S399 000112-05-0 0.39 0.16 -0.03 -0.51 -0.20 0.02 0.17 0.23 -1.83 1 2 Low Pr S400 000113-18-8 1.78 0.22 0.79 0.24 0.38 0.56 0.34 0.32 -0.98 2 1 3 Low Pr S401 000113-42-8 0.53 0.54 0.53 0.53 0.90 0.96 0.44 -0.43 2 1 2 Low Pr S402 000113-42-8 0.68 0.68 0.68 0.68 0.68 0.68 0.68 0.64 0.75 0.65 -0.64 1 <															Low Priority
S398 000111-12-6 0.73 0.19 0.35 -0.02 0.46 0.46 0.65 0.70 -12-4 1 1 2 Low Pr S399 000112-05-0 0.39 0.16 -0.03 -0.51 -0.20 0.02 0.17 0.23 -1.83 1 1 2 Low Pr S400 000113-18-8 1.78 0.22 0.79 0.24 0.38 0.56 0.34 0.32 -0.98 2 1 3 Low Pr S401 000113-42-8 0.53 0.54 0.53 0.53 0.90 0.96 0.44 -0.43 2 1 2 Low Pr S402 000113-45-1 0.68 0.68 0.68 0.68 0.68 0.64 0.75 0.65 -0.64 1 1 2 Low Pr S403 000113-59-7 1.00 1.00 1.00 3.35 2.70 3.26 1.86 3 2 3 High Pr <td></td> <td>Low Priority</td>															Low Priority
S399 000112-05-0 0.39 0.16 -0.03 -0.51 -0.20 0.02 0.17 0.23 -1.83 1 1 2 Low Pr S400 000113-18-8 1.78 0.22 0.79 0.24 0.38 0.56 0.34 0.32 -0.98 2 1 3 Low Pr S401 000113-42-8 0.53 0.54 0.53 0.53 0.90 0.96 0.44 -0.43 2 1 2 Low Pr S402 000113-45-1 0.68 0.68 0.68 0.68 0.69 0.64 0.75 0.65 -0.64 1 1 2 Low Pr S403 000113-59-7 1.00 1.00 1.00 1.00 3.35 2.70 3.26 1.86 3 2 3 High Pr															Low Priority
\$400 000113-18-8 1.78 0.22 0.79 0.24 0.38 0.56 0.34 0.32 -0.98 2 1 3 Low Pr \$401 000113-42-8 0.53 0.54 0.53 0.53 0.90 0.96 0.44 -0.43 2 1 2 Low Pr \$402 000113-45-1 0.68 0.68 0.68 0.68 0.68 0.69 0.64 0.75 0.65 -0.64 1 1 2 Low Pr \$403 000113-59-7 1.00 1.00 1.00 1.00 3.35 2.70 3.26 1.86 3 2 3 High Pr															Low Priority
S401 000113-42-8 0.53 0.54 0.53 0.53 0.90 0.96 0.44 -0.43 2 1 2 Low Pr S402 000113-45-1 0.68 0.68 0.68 0.68 0.60 0.64 0.75 0.65 -0.64 1 1 2 Low Pr S403 000113-59-7 1.00 1.00 1.00 1.00 3.35 2.70 3.26 1.86 3 2 3 High Pr															Low Priority
\$402 000113-45-1 0.68 0.68 0.68 0.68 0.68 0.68 0.69 0.64 0.75 0.65 -0.64 1 1 2 Low Pr \$403 000113-59-7 1.00 1.00 1.00 1.00 3.35 2.70 3.26 1.86 3 2 3 High Pr															Low Priority
S403 000113-59-7 1.00 1.00 1.00 1.00 1.00 3.35 2.70 3.26 1.86 3 2 3 High Pi															Low Priority
															High Priority
															Low Priority
				2.70	2.00	2.03						-	-	-	

			Human E	Biotransforr	mation		Fish Bio	otransforma	ition		F	BT Pro	ofiler	
ID	CAS	logHL _T (h)	logHL _{B1} (h)	logHL _{B2} (h)	logHL _{B3} (h)	logHL _{B4} (h)	logHL _{N1} (h)	logHL _{N2} (h)	logHL _{N3} (h)	PBT Index	Р	В	т	Priority Level
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	1.53	1.67	1.67	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	1.26	1.59	1.59	1.59	1.59	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	0.51	1.12	1.21	1.23	-1.05 -2.06	2	1	3	Low Priority
S410 S411	000116-02-9 000117-10-2	0.29	0.51 0.74	0.88	0.48	0.51	0.33 0.65	0.56 0.35	0.49 0.56	-2.06 0.46	2	1	2	Low Priority Low Priority
S411	000117-10-2	0.42	0.74	0.63	1.05	0.85	1.09	0.33	1.03	1.24	2	1	2	Low Priority
5413	000117-37-3	-0.12	-0.12	-0.12	-0.13	-0.13	1.82	1.82	1.82	-0.08	1	2	?	Low Priority
S414	000117-82-8	0.57	0.55	0.25	0.44	0.39	0.51	0.74	0.68	-0.03	1	1	1	Low Priority
S415	000117-83-9	0.53	0.54	0.19	0.26	0.26	0.88	1.07	0.99	-0.05	1	1	2	Low Priority
S416	000117-84-0	0.64	0.67	0.18	0.15	0.26	1.34	1.45	1.34	-0.06	1	1	?	Low Priority
S417	000117-89-5	1.63	1.34	1.45	1.35	1.41	1.73	1.94	1.56	2.73	3	1	3	Low Priority
S418	000117-96-4	0.26	0.30	0.30	0.50	0.50	0.60	0.80	0.53	0.97	3	1	2	Low Priority
S419	000117-99-7	0.55	0.77	0.57	0.44	0.57	0.57	0.47	0.48	0.66	1	1	2	Low Priority
S420	000118-23-0	1.30	1.30	1.21	1.31	1.25	2.07	2.36	2.02	1.61	2	1	3	Low Priority
S421 S422	000118-42-3 000118-56-9	2.93 0.87	3.07 0.94	3.07 1.04	0.82 0.73	0.89 0.79	1.56 0.77	1.57 0.80	1.53 0.83	0.59 -0.65	2	1 3	2	Priority (Group 2) Low Priority
5422	000118-58-1	0.87	0.94	0.74	0.75	0.79	0.77	0.53	0.59	0.67	1	1	3	Low Priority
5424	000118-60-5	0.56	0.68	0.63	0.16	0.31	0.70	0.65	0.69	-0.63	1	2	3	Low Priority
5425	000118-61-6	0.38	0.40	0.41	0.15	0.31	0.10	0.06	0.18	-0.59	1	1	2	Low Priority
S426	000119-06-2	0.61	0.71	0.06	0.03	0.15	1.79	1.84	1.74	-0.08	1	1	?	Low Priority
S427	000119-34-6	0.04	0.28	0.39	0.17	0.30	0.29	0.06	0.17	-1.31	1	1	2	Low Priority
S428	000119-36-8	0.25	0.36	0.42	0.11	0.26	-0.02	-0.06	0.09	-0.58	1	1	2	Low Priority
S429	000119-53-9	0.68	0.75	0.40	0.58	0.64	0.57	0.64	0.53	0.66	1	1	2	Low Priority
S430	000119-61-9	0.79	0.88	0.45	0.69	0.75	0.21	0.21	0.21	1.05	1	1	2	Low Priority
S431	000120-11-6	1.22	0.94	0.88	0.97	0.93	2.60	1.96	2.14	1.21	2	1	2	Priority (Group 2)
S432	000120-14-9	0.53	0.54	0.24	0.49	0.31	0.95	0.61	1.01	-0.16	2	1	2	Low Priority
S433	000120-24-1	0.94	0.74	0.70	0.75	0.73	1.79	1.23	1.43	1.26	2	1	3	Low Priority
S434 S435	000120-47-8 000120-51-4	0.40 1.00	0.44	0.48	0.16 0.72	0.29	0.08 0.91	0.04 1.02	0.15 0.95	-0.59 1.06	1	1	2	Low Priority Low Priority
S435 S436	000120-51-4	0.51	0.88	0.52	0.72	0.95	1.01	1.02	0.95	-0.60	1	1	2	Low Priority
S436	000120-72-9	0.15	0.52	0.44	-0.10	0.38	-0.29	-0.12	-0.05	-1.45	1	1	1	Low Priority
S438	000120-92-8	0.51	0.74	1.16	1.53	1.35	0.48	0.38	0.73	0.17	2	1	2	Low Priority
S439	000121-32-4	0.36	0.44	0.31	0.17	0.18	0.53	0.15	0.52	-0.54	1	1	2	Low Priority
S440	000121-33-5	0.21	0.28	0.18	0.12	0.10	0.39	0.01	0.38	-0.54	1	1	2	Low Priority
S441	000121-69-7	0.91	0.56	0.62	0.83	0.80	0.42	0.42	0.42	-0.17	2	1	2	Low Priority
S442	000121-75-5	1.20	1.22	1.22	1.22	1.22	1.67	1.67	1.67	-1.11	1	1	3	Low Priority
S443	000121-88-0	0.10	0.25	0.39	0.25	0.36	0.29	0.06	0.18	-1.31	1	1	2	Low Priority
S444	000122-03-2	0.87	0.69	0.50	0.82	0.69	0.82	0.84	0.94	-0.15	1	1	2	Low Priority
S445	000122-09-8	1.37	1.45	1.45	1.14	1.24	1.00	1.13	1.06	-1.06	2	1	2	Low Priority
S446	000122-11-2	0.72	0.73	0.77	1.13	1.09	0.20	0.34	-0.02	0.07	2	1	2	Low Priority
S447 S448	000122-16-7	0.79 0.83	0.71	0.64 0.29	1.06	0.88	0.56	0.50	0.28	0.89 0.03	2	1	2	Low Priority
S448 S449	000122-40-7 000122-48-5	0.83	0.77 0.51	0.29	0.37	0.45 0.25	1.40 0.58	1.18 0.37	1.20 0.68	-0.57	1	1	1	Low Priority Low Priority
S450	000122-48-5	0.50	0.51	0.49	0.30	0.25	1.18	1.07	1.03	0.01	1	1	2	Low Priority
S451	000122-67-8	0.89	0.85	0.44	0.47	0.65	1.59	1.37	1.32	1.28	2	1	3	Low Priority
S452	000122-91-8	0.73	0.53	0.22	0.44	0.48	0.84	0.67	0.98	-0.12	1	1	2	Low Priority
S453	000123-99-9	-0.12	-0.11	-0.11	-0.03	-0.03	-0.08	0.13	0.21	-2.00	1	1	1	Low Priority
\$454	000125-12-2	0.81	0.73	0.58	0.75	0.64	0.77	1.08	1.13	-1.49	2	1	2	Low Priority
S455	000125-13-3	0.62	0.97	0.67	0.69	0.67	1.09	0.75	0.58	1.10	2	1	3	Low Priority
S456	000125-27-9	1.00	1.14	1.20	1.34	1.27	1.58	1.55	1.28	-1.29	2	1	2	Low Priority
S457	000125-28-0	0.74	1.04	0.82	0.84	0.84	1.35	0.96	1.25	-0.84	2	1	2	Low Priority
S458	000125-29-1	0.33	0.33	0.33	0.35	0.35	1.28	0.92	1.18	-0.30	2	1	2	Low Priority
S459 S460	000125-33-7 000125-40-6	1.11 0.44	0.69 0.50	0.48 0.40	0.46 0.42	0.54 0.38	0.21 -0.12	0.31 0.12	0.24 0.08	-0.82 -1.89	2	1	2	Low Priority Low Priority
S461	000125-40-6	0.44	0.82	0.40	0.42	0.36	0.12	1.02	0.08	-0.49	2	1	2	Low Priority
S462	000125-64-4	1.04	0.33	0.27	0.44	0.36	0.13	0.31	0.25	-1.72	2	1	2	Low Priority
S463	000125-71-3	0.65	0.65	0.65	0.65	0.65	2.22	1.97	2.15	-0.29	2	1	3	Low Priority
S464	000125-84-8	1.10	0.67	0.61	0.74	0.70	0.26	0.37	-0.02	-1.22	2	1	2	Low Priority
S465	000126-07-8	1.18	1.21	1.21	1.21	1.21	1.42	0.98	1.65	0.74	2	1	2	Low Priority
S466	000126-52-3	0.35	0.36	0.36	0.36	0.36	0.04	0.18	0.24	-2.03	2	1	2	Low Priority
S467	000126-64-7	1.02	0.62	0.70	0.73	0.72	1.45	1.40	1.29	0.17	2	2	3	Low Priority
S468	000126-91-0	0.88	0.43	0.74	0.83	0.75	0.79	0.75	0.67	-1.63	2	1	3	Low Priority
S469	000127-07-1	0.53	0.73	0.73	0.73	0.73	-1.12	-1.24	-0.76	-2.94	1	1	1	Low Priority
S470	000127-17-3	-0.17	-0.19	0.35	-0.54	-0.09	-1.16	-0.98	-0.82	-1.58	1	1	1	Low Priority
S471	000127-31-1	0.54	0.56	0.56	0.56	0.56	0.73	0.66	0.27	-1.88	2	1	2	Low Priority
S472 S473	000127-48-0 000127-51-5	0.19 0.82	0.28 0.55	0.43 0.79	0.17 0.81	0.39	-0.12 1.35	0.22 1.42	0.25 1.42	-1.28 -1.08	2	1	1	Low Priority Low Priority
S473 S474	000127-51-5	0.82 0.87	1.16	0.79 1.16	0.81 1.16	1.16	0.35	0.33	0.10	-0.13	2	1	2	Low Priority
S474 S475	000127-03-3	0.81	0.90	0.79	1.15	1.07	0.33	0.36	0.10	0.31	2	1	2	Low Priority
S476	000127-71-3	0.80	0.87	0.87	0.97	0.95	0.03	0.50	-0.16	0.68	2	1	2	Low Priority
S477	000127-74-2	0.76	0.81	0.77	0.95	0.98	-0.04	0.42	-0.23	0.69	2	1	2	Low Priority
\$478	000127-79-7	0.73	0.96	0.99	1.11	1.13	-0.02	0.42	-0.22	0.09	2	1	2	Low Priority
S479	000128-13-2	0.90	0.88	1.00	0.61	0.71	1.44	1.47	1.40	-2.74	2	1	2	Low Priority
S480	000128-37-0	0.87	0.82	0.92	0.96	0.84	1.70	1.70	1.70	-0.83	2	1	3	Low Priority
S481	000128-39-2	0.93	0.79	0.93	1.02	0.94	1.10	1.50	1.51	-0.82	2	1	3	Low Priority
S482	000128-95-0	0.49	0.90	0.65	0.86	0.92	0.29	0.36	-0.02	-0.32	2	1	3	Low Priority
S483	000129-03-3	1.37	1.18	0.95	1.12	1.06	3.09	2.62	2.71	1.54	3	1	3	Priority (Group 1)
S484	000129-20-4	0.57	0.85	0.59	0.39	0.52	0.65	0.55	0.24	0.81	1	1	3	Low Priority
S485 S486	000130-26-7 000130-95-0	0.86 0.89	1.02 1.10	1.04 0.89	1.47 0.98	1.61 1.04	1.03 1.24	0.85 1.11	0.71 0.59	1.58 0.42	2	1	2	Low Priority Low Priority
3400	200130-23-0	0.05	1.10	0.03	0.50	1.04	1.24	1.11	0.33	0.42	2	-	-	LOW I HOTILY

			Human I	Biotransfori	mation		Fish Bi	otransforma	tion			PBT Pro	filer	
ID	CAS	logHL _T (h)	logHL _{B1} (h)	logHL _{B2} (h)	logHL _{B3} (h)	logHL ₈₄ (h)	logHL _{N1} (h)	logHL _{N2} (h)	logHL _{N3} (h)	PBT Index	Р	В	т	Priority Level
5487	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 S500	000133-16-4	0.81 1.41	0.93 1.80	1.02 2.06	1.08 2.28	1.03	0.87 0.80	0.76 0.68	0.71 0.69	-0.38	2	1	3	Low Priority
S500	000133-67-5 000134-09-8	0.86	0.90	0.88	0.83	2.17 1.05	0.67	0.84	0.69	0.76 -1.06	3 2	1 3	2	Low Priority Low Priority
S502	000134-09-8	1.37	1.53	1.53	0.83	1.03	1.16	1.22	1.09	-0.69	1	1	2	Low Priority
S502	000134-49-0	1.05	1.34	1.51	1.87	1.75	0.67	0.41	0.51	0.49	2	1	2	Low Priority
S504	000135-07-5	0.72	1.10	1.10	1.51	1.43	0.07	0.74	0.25	0.43	2	1	2	Low Priority
S505	000135-05-1	0.72	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	0.40	0.21	0.21	0.54	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	000130-33-0	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
5512	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
S512	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	0.82	0.83	0.55	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	0.73	0.67	0.55	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	0.95	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	0.17	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	1.40	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 000152-47-6	1.07 0.59	1.22 0.90	1.27 0.88	1.03 1.09	1.15 1.02	1.89 0.05	1.63	1.70	-0.65 0.08	3	3	3	Low Priority
S540 S541	000152-47-6	0.59	0.90	0.88	0.63	0.52	1.13	0.32 0.82	-0.17 0.75	1.27	2	1	2	Low Priority Low Priority
S541	000152-72-7	0.37	0.45	0.48	0.85	1.06	0.39	0.82	0.73	-1.85	1	1	2	Low Priority
S542 S543	000154-42-7	-0.43	-0.43	-0.43	-0.42	-0.42	0.39	0.79	0.43	-0.38	2	1	2	Low Priority
S544	000154-55-0	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	0.73	1.25	0.95	1.13	1.00	0.68	1.08	0.73	-0.04	2	1	2	Low Priority
S546	000155-41-5	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	000130-08-1	0.99	0.58	0.96	0.72	0.81	1.28	1.17	1.26	-0.89	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	1.41	1.08	1.20	0.98	0.92	0.86	0.71	1.21	2	1	3	Low Priority
	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
3302						1.00	0.21	0.48	-0.02	0.86	2		2	
S562 S563		0.60	0.97	0.97	1.03							1		
S563	000339-44-6	0.60 1.17	0.97 1.15						1.91		2	1	2	Low Priority Low Priority
		0.60 1.17 1.45	0.97 1.15 0.99	0.97 0.99 1.47	1.06 1.93	0.96 1.77	1.96 1.21	2.05		0.97 1.76		1		Low Priority Low Priority
S563 S564	000339-44-6 000341-69-5	1.17	1.15 0.99	0.99	1.06	0.96	1.96	2.05	1.91	0.97	2	1	2	Low Priority
S563 S564 S565	000339-44-6 000341-69-5 000346-18-9	1.17 1.45	1.15	0.99 1.47	1.06 1.93	0.96 1.77	1.96 1.21	2.05 1.14	1.91 1.03	0.97 1.76	2	1	2	Low Priority Low Priority

Decomposition Color				Human E	Biotransforr	nation		Fish Bio	otransforma	ition		P	BT Pro	filer	
Sept	ID	CAS	logHL _T (h)					logHL _{N1} (h)		logHL _{N3}	PBT Index	Р	В	т	Priority Level
5577 000364-67	S569	000361-37-5	0.65					0.66			0.00	2	1	2	Low Priority
000043-957	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
00371-004-00 0.30 0.30 0.73 0.43 0.86 0.33 -0.06 -0.44 0.35 0.2 1 2 0.00 Priestly 1.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	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	
0077-008-008-009-009-009-009-009-009-009-009	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
575 000389-08-2 0.56 0.37 0.37 0.49 0.49 0.13 0.27 0.23 0.21 0.2 1 1 1 10.00 Priority 1.57 000305-647 1.33 1.25 0.06 0.37 0.38 0.37 0.37 0.38 0.39 0.37 0.37 0.38 0.39 0.37 0.37 0.38 0.39 0.37 0.38 0.39 0.39 0.39 0.39 0.39 0.39 0.39 0.39	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
5575 000389-082	S574	000372-75-8	0.13	0.12	-0.01	-0.15	0.06	-0.41	-0.13	-0.04	-3.56	1	1	1	Low Priority
5977 000399647 1.33	S575	000389-08-2	0.26	0.27	0.27	0.49	0.49	0.13	0.27	-0.23	-0.21	2	1		
000427-009 0.03 1.02 0.05 0.05 0.02 0.74 1.33 0.031 1.22 0.052 0.1 2 1.00 Priently Sign 000427-057 0.052 0.057 0.052 0.057 0.052 0.057 0.052 0.057 0.052 0.057 0.052 0.057 0.052 0.057 0.052 0.052 0.057 0.052 0.057 0.052 0.057 0.052 0.0	S576	000390-28-3	0.49	0.64	0.54		0.58	0.74	0.58	0.79	-1.57	1		1	Low Priority
5979 000427-51-01 100 0.51 1.31 1.21 1.33 1.76 1.57 1.52 0.10 2 1 1 2 Low Priority 1.558 00042-52-7 0.229 0.25 0.50 0.50 0.50 0.50 0.50 0.50 0.50	S577	000390-64-7	1.33	1.25	0.96	0.97	1.01	2.73	2.64	2.61	1.97	3	2	3	High Priority
\$585 (00043-25-7)															Low Priority
SSE2 000414-071 0.91 0.90 0.91 0.11 1.33 1.66 1.22 1.92 1.53 1.39 1.75 2 2 3 Low Priority SSE3 000414-071 0.91 0.92 1.66 0.81 0.85 0.91 0.91 0.91 0.91 0.91 0.91 0.92 1.61 0.9	S579	000427-51-0	1.00	0.81	1.31	1.21	1.13	1.76	1.57	1.52	-0.10	2	1	2	Low Priority
\$383 (000149-7) \$91												_			
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5635 000519-09-5 0.60 0.80 0.60 0.43 0.55 0.37 0.46 0.38 -0.45 1 1 1 Low Priority 5636 000519-98-2 0.62 0.86 0.65 0.65 0.69 0.21 0.45 0.05 -0.44 1 1 2 Low Priority 5637 000520-33-2 0.63 0.69 0.77 0.89 0.78 1.16 0.37 1.02 -0.14 2 1 2 Low Priority 5638 000521-18-6 0.85 0.95 0.96 0.88 0.96 1.16 1.13 1.16 -1.94 2 1 2 Low Priority 5640 000522-66-7 0.87 1.14 0.87 0.93 1.03 1.08 1.11 0.59 0.21 2 1 2 Low Priority 5641 000526-66-6 0.53 0.58 0.58 0.58 0.58 0.58 0.58 0.59 0.59	S633	000514-65-8	1.38		1.38	1.40	1.40	1.77		1.18	-0.70	2	1	3	Low Priority
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5641 000525-66-6 0.53 0.58 0.58 0.58 0.58 0.58 0.97 0.99 1.02 -0.10 1 1 2 Low Priority 5642 000526-08-9 0.76 1.08 0.87 1.13 1.12 0.30 0.56 0.03 1.36 2 1 2 Low Priority 5643 000526-36-3 1.21 0.97 1.11 1.25 1.08 1.80 2.32 2.12 -0.43 2 2 3 Low Priority 5645 000532-03-6 0.58 0.69 0.59 0.49 0.51 1.07 0.94 1.14 -1.96 1 1 2 Low Priority 5645 000532-03-6 0.08 0.13 0.13 0.13 0.13 0.14 0.30 0.67 -1.33 2 1 1 Low Priority 5645 000532-77-4 -0.78 -0.78 -0.78 -0.78 0.78 0.79 0.51 -0.64		000522-66-7	0.87	1.14	0.87	0.93	1.03		1.11		0.21	2	1	2	Low Priority
5642 000526-08-9 0.76 1.08 0.87 1.13 1.12 0.30 0.56 0.03 1.36 2 1 2 Low Priority 5643 000526-36-3 1.21 0.97 1.11 1.25 1.08 1.80 2.32 2.12 -0.43 2 2 3 Low Priority 5644 000530-08-5 0.58 0.69 0.59 0.49 0.51 1.07 0.94 1.14 -1.56 1 1 2 Low Priority 5645 000532-07-6 0.08 0.13 0.13 0.13 0.13 0.44 0.30 0.67 -1.33 2 1 1 Low Priority 5645 000532-77-4 -0.78 <												_			
\$643 000526-36-3 1.21 0.97 1.11 1.25 1.08 1.80 2.32 2.12 -0.43 2 2 3 Low Priority 5644 000530-08-5 0.58 0.69 0.59 0.49 0.51 1.07 0.94 1.14 -1.96 1 1 2 Low Priority 5645 000532-03-6 0.08 0.13 0.13 0.13 0.13 0.13 0.44 0.30 0.67 -1.33 2 1 1 Low Priority 5646 000532-77-4 0.78 -0.78 -0.78 -0.78 -0.78 0.85 0.97 0.87 -0.64 1 1 3 Low Priority 5647 000536-33-4 0.40 0.42 0.42 0.42 0.42 0.76 0.95 0.51 -0.82 2 1 1 Low Priority 5648 000537-46-2 1.08 1.10 1.10 0.89 0.97 1.38 1.46 1.40 -0.60 1 1 2 Low Priority 5649 000538-65-8 0.84 0.65 0.42 0.42 0.59 1.18 1.00 0.97 0.01 1 1 2 Low Priority															
5644 000530-08-5 0.58 0.69 0.59 0.49 0.51 1.07 0.94 1.14 -1.96 1 1 2 Low Priority 5645 000532-03-6 0.08 0.13 0.13 0.13 0.44 0.30 0.67 -1.33 2 1 1 Low Priority 5646 000532-77-4 -0.78 -0.78 -0.78 -0.78 -0.78 -0.78 -0.78 -0.87 -0.78 -0.64 1 1 3 Low Priority 5647 000538-03-4 0.40 0.42 0.42 0.42 0.95 0.51 -0.82 2 1 1 Low Priority 5648 000538-65-8 0.84 0.65 0.42 0.24 0.59 1.18 1.00 0.97 0.01 1 1 2 Low Priority 5649 000538-65-8 0.84 0.65 0.42 0.24 0.59 1.18 1.00 0.97 0.01 1 1															
5645 000532-03-6 0.08 0.13 0.13 0.13 0.13 0.13 0.14 0.30 0.67 -1.33 2 1 1 Low Priority 5646 000532-77-4 -0.78 -0.78 -0.78 -0.78 -0.78 0.85 0.97 0.87 -0.64 1 1 Low Priority 5647 000536-33-4 0.42 0.42 0.42 0.76 0.95 0.51 -0.82 2 1 Low Priority 5648 000537-66-2 1.08 1.10 1.10 0.89 0.97 1.38 1.46 1.40 -0.60 1 1 2 Low Priority 5649 000538-65-8 0.84 0.65 0.42 0.24 0.59 1.18 1.00 0.97 0.01 1 1 2 Low Priority															
5646 000532-77-4 -0.78 -0.78 -0.78 -0.78 -0.78 -0.78 0.85 0.97 0.87 -0.64 1 1 3 Low Priority 5647 000536-33-4 0.40 0.42 0.42 0.42 0.42 0.59 0.51 -0.82 2 1 1 Low Priority 5648 000538-65-8 0.84 0.65 0.42 0.24 0.59 1.18 1.00 0.97 0.01 1 1 2 Low Priority 5649 000538-65-8 0.84 0.65 0.42 0.24 0.59 1.18 1.00 0.97 0.01 1 1 2 Low Priority															
5647 000536-33-4 0.40 0.42 0.42 0.42 0.95 0.51 -0.82 2 1 1 Low Priority 5648 000537-46-2 1.08 1.10 0.89 0.97 1.38 1.46 1.40 -0.60 1 1 2 Low Priority 5649 000538-65-8 0.84 0.65 0.42 0.24 0.59 1.18 1.00 0.97 0.01 1 1 2 Low Priority															
S648 000537-46-2 1.08 1.10 1.10 0.89 0.97 1.38 1.46 1.40 -0.60 1 1 2 Low Priority 5649 000538-65-8 0.84 0.65 0.42 0.24 0.59 1.18 1.00 0.97 0.01 1 1 2 Low Priority															
S649 000538-65-8 0.84 0.65 0.42 0.24 0.59 1.18 1.00 0.97 0.01 1 1 2 Low Priority															
S65U UUU541-91-3 U./5 U.62 0.96 0.37 0.91 1.17 1.25 1.15 -1.54 2 2 3 Low Priority															
	5650	UUU541-91-3	U./5	0.62	0.96	0.37	0.91	1.1/	1.25	1.15	-1.54	2	2	5	LOW Priority

			Human i	Biotransfori	mation		Fish Bio	otransforma	tion		==	PBT Pro	filer	
ID	CAS	logHL _T (h)	logHL _{B1}	logHL _{B2} (h)	logHL _{B3}	logHL _{B4} (h)	logHL _{N1} (h)	logHL _{N2} (h)	logHL _{N3} (h)	PBT Index	P	В	т	Priority Level
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	0.35	0.36	0.36	0.36	0.36	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	0.00	0.00	0.00	0.10	0.10	0.58	0.36	0.58	0.49	1	1	2	Low Priority
S657	000554-57-4	1.15	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	0.77	1.17	1.17	1.17	1.17	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	0.40	0.41	0.41	0.47	0.47	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	0.78	0.77	0.77	0.78	0.78	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 000591-81-1	0.78	0.69	0.62	0.64	0.65	0.86	0.74	0.95	-1.95	1	1	2	Low Priority
S668		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	2	1	2	Low Priority
S670	000596-51-0	1.09	1.31	1.14	1.30	1.10	1.03	1.52	1.00	-0.07	2	1	1	Low Priority
S671 S672	000599-79-1 000604-75-1	0.88 0.83	0.90 1.50	0.87 1.50	0.84 1.50	0.82 1.50	0.30 1.07	0.70 0.99	0.11 0.88	1.79 1.13	2	1	2	Low Priority Low Priority
S672 S673	000604-75-1	0.83	0.54	0.22	0.41	0.37	0.65	0.99	0.88	1.13 -0.04	1	1	2	Low Priority Low Priority
S674	000605-54-9	0.60	0.54	0.22	0.41	0.37	0.65	0.86	0.79	-0.04 0.26	1	1	2	Low Priority Low Priority
S675	000611-99-4	0.58	0.75	0.69	1.22	1.33	0.59	0.59	0.55		2	1	2	Low Priority
		0.82 0.74	-0.15	-0.33	-0.33	-0.25	-0.27	-0.08	0.37	-1.82 -2.01	1		1	
S676	000616-91-1	0.74	-0.15 0.26	-0.33 0.48	-0.33 0.11	-0.25 0.35	-0.27 0.27	-0.08 0.17	0.02	-2.01 -0.74	1	1	2	Low Priority
S677	000620-17-7		0.26	-0.01	-0.01		0.27	0.17	0.31	-0.74 -1.49	1	1	2	Low Priority
S678	000626-82-4	0.67 1.33	0.30 1.46	-0.01 1.46	-0.01 1.68	0.14	1.44	1.54	1.42	-1.49 -0.31	2	1	2	Low Priority
S679 S680	000634-03-7 000637-07-0	1.33	1.46	1.46	1.68	1.68 1.31	1.44	1.54	1.42	-0.31 0.41	2	1	2	Low Priority Low Priority
	000637-07-0	0.97	0.77		1.16	0.98		1.57	1.63	-1.67	2	2	3	Low Priority
S681	000639-99-6	0.97	0.77	1.15 0.49	0.50	0.50	1.25 1.45	1.30	1.47		2		3	Low Priority
S682		0.48	0.49	0.49	0.89	0.89	1.43	2.07		1.60	3	1	2	Low Priority
S683	000645-05-6 000646-01-5	0.04	-0.12	-0.17	-0.51	-0.23	-0.69	-0.68	1.63 -0.42	-0.25	1	1	1	
S684		-0.78	-0.12 - 0.77	-0.17 - 0.77	-0.51 - 0.76	-0.23 - 0.76	0.29		0.45	-1.80	2	1	2	Low Priority
S685	000671-16-9							0.54		-1.40		1		Low Priority
S686	000672-87-7	0.55	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	-0.17	-0.04	-0.20	-0.74	2	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	0.26	0.26	0.26	0.26	0.26	0.52	0.72	0.33	-1.02	2	1	2	Low Priority
S690	000723-46-6	0.99	1.06	1.06	1.06	1.06	0.26	0.23	-0.01	-0.12	2	1	2	Low Priority
S691	000729-99-7	0.71	0.92	1.00	1.13	1.07	0.15	0.32	-0.05	-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	3	Low Priority
S693 S694	000738-70-5 000739-71-9	0.98 1.36	1.23 1.36	1.23 1.36	1.23 1.38	1.23 1.38	1.36 2.58	1.30 2.62	1.22 2.39	-0.54 1.10	2	1 2	3	Low Priority
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	Priority (Group 2) Low Priority
S696	000743-03-3	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	1.20	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	0.97	0.99	0.99	0.97	0.97	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
5702	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
5702	000835-51-4	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	1.23	1.23	1.23	1.23	1.23	1.25	1.25	1.06	1.77	2	1	2	Low Priority
S705	000846-50-4	1.18	1.20	1.20	1.20	1.20	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	2.16	2.16	2.16	2.16	2.16	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)
5712	000915-30-0	1.11	1.11	1.11	1.11	1.11	1.55	1.63	1.44	2.48	3	3	3	Priority (Group 3)
5713	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	2	3	Low Priority
S716	000968-81-0	0.11	0.11	0.11	0.19	0.19	0.37	0.50	0.44	-0.40	2	1	2	Low Priority
S717	000972-02-1	0.60	0.61	0.61	0.72	0.72	1.42	1.43	1.19	0.40	2	1	3	Low Priority
5718	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
5720	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
5722	001003 12 7	0.83	0.99	1.34	1.21	1.26	1.30	1.33	1.27	-1.09	2	1	2	Low Priority
5723	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
		0.18	0.39	0.39	0.39	0.39	0.86	0.72	1.12	-0.69	1	1	1	Low Priority
	001134-47-0				0.48	0.56	0.53	0.43	0.44	0.66	1	1	2	Low Priority
S725	001134-47-0 001137-42-4		0.80	0.62										
S725 S726	001137-42-4	0.58	0.80 0.92	0.62 1.34										
S725 S726 S727	001137-42-4 001139-30-6	0.58 1.19	0.92	1.34	1.50	1.36	1.82	2.00	1.88	-1.39	2	1	3	Low Priority
S725 S726 S727 S728	001137-42-4 001139-30-6 001141-88-4	0.58 1.19 0.99	0.92 0.89	1.34 0.95	1.50 1.37	1.36 1.48	1.82 1.34	2.00 0.97	1.88 1.04	-1.39 -0.54	2	1	3	Low Priority Low Priority
\$725 \$726 \$727 \$728 \$729	001137-42-4 001139-30-6 001141-88-4 001143-72-2	0.58 1.19 0.99 0.45	0.92 0.89 0.65	1.34 0.95 0.74	1.50 1.37 0.67	1.36 1.48 0.71	1.82 1.34 0.76	2.00 0.97 0.32	1.88 1.04 0.66	-1.39 -0.54 -0.13	2 2 1	1 1 1	3 3 2	Low Priority Low Priority Low Priority
S725 S726 S727 S728	001137-42-4 001139-30-6 001141-88-4	0.58 1.19 0.99	0.92 0.89	1.34 0.95	1.50 1.37	1.36 1.48	1.82 1.34	2.00 0.97	1.88 1.04	-1.39 -0.54	2	1	3	Low Priority Low Priority

			Human E	Biotransforr	nation		Fish Bio	otransforma	ation		-	PBT Pro	ofiler	
ID	CAS	logHL _T (h)	logHL _{B1}	logHL _{B2}	logHL _{B3}	logHL _{B4} (h)	logHL _{N1} (h)	logHL _{N2}	logHL _{N3}	PBT Index	Р	В	т	Priority Level
\$733	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	0.35	-0.15	0.08	2	1	2	Low Priority
S735	001220-94-6	0.58	0.95	0.62	0.85	0.84	0.44	0.50	0.10	0.05	2	1	2	Low Priority
S736	001222-05-5	1.39	1.17	1.41	1.65	1.44	2.11	2.55	2.54	-0.30	2	2	3	Priority (Group 2)
S737	001239-29-8	0.94	1.22	1.34	1.16	1.15	1.73	1.53	1.32	-1.08	3	1	2	Low Priority
S738	001335-66-6	0.55	0.36	0.39	0.61	0.51	0.94	0.82	0.88	-1.26	1	1	2	Low Priority
S739	001420-55-9	1.39	1.50	1.17	1.28	1.17	2.70	2.27	2.40	1.09	3	2	3	Priority (Group 2)
S740	001423-46-7	0.55	0.36	0.39	0.61	0.51	0.94	0.82	0.88	-1.26	1	1	2	Low Priority
S741	001470-79-7	0.50	0.72	0.76	0.76	0.70	0.76	0.35	0.66	-0.13	1	1	2	Low Priority
5742	001490-04-6	0.67	0.61	0.88	0.74	0.99	0.19	0.19	0.19	-2.08	1	1	2	Low Priority
S743	001491-59-4	0.72	0.88	0.92	0.83	0.75	1.11	1.53	1.40	-1.00	2	1	3	Low Priority
S744	001502-22-3	0.55	0.54	0.48	0.32	0.58	0.91	0.84	0.76	-1.32	1	1	2	Low Priority
S745	001504-55-8	0.61	0.49	0.65	0.30	0.61	0.77	0.53	0.53	-0.52	1	1	3	Low Priority
S746	001506-02-1	1.00	1.00	1.04	1.06	0.78	1.33	1.95	1.95	-0.24	2	1	3	Low Priority
S747 S748	001508-75-4	0.51	0.80	0.45	0.35 0.88	0.39	0.53	0.78 1.05	0.16	0.61	2	1	2	Low Priority
	001524-88-5	0.89		0.92		0.56	1.12		1.07	-1.97		1		Low Priority
S749	001605-89-6	0.95	0.99	1.31	1.01	0.98	1.53	1.45	1.50	-1.73	2	1	2	Low Priority
S750	001622-61-3	1.58	1.58	1.58	1.58	1.58	1.39	1.10	1.17	1.74		1	3	Low Priority
S751 S752	001622-62-4 001634-78-2	1.40	1.46 0.12	1.46 -0.02	1.45	1.45 0.28	1.09	1.23 0.34	0.79 0.34	2.04	2	1	2	Low Priority
		0.52 0.96	0.12	-0.02 0.99	0.51 0.98	0.28	0.34	0.50		-1.12	1 2	1		Low Priority
S753 S754	001665-48-1 001668-19-5	1.18	1.18	1.18	1.18	1.18	0.48 2.40	2.09	0.67 2.16	-0.57 1.19	2	1	2	Low Priority Priority (Group 2)
5755 S755	001668-19-5	0.56	0.79	0.54	0.57	0.61		0.23	-0.17	-0.22	2		2	
S755 S756	001672-58-8	0.56 1.32	0.79 1.62	0.54 1.62	0.57 1.62	0.61 1.62	0.19 0.62	1.18	-0.17 0.40	-0.22 1.53	2	1	2	Low Priority Low Priority
5756 5757	001812-30-2	1.40	1.62	1.62	1.62	1.10	1.54	1.18	1.23	3.18	3	2	3	
S757	001841-19-6	0.57	0.84	0.44	0.30	0.36	1.34	1.76	1.23	0.63	1	1	3	Priority (Group 3) Low Priority
5758 5759	001843-05-6	0.57	1.05	1.14	0.30	1.12	1.34	1.02	1.17	-2.52	2	1	2	Low Priority
S760	001852-53-5	0.89	0.68	0.37	0.99	0.60	1.34	1.03	1.02	0.13	1	1	2	Low Priority
S760 S761	001885-38-7	0.79	0.68	0.62	0.23	0.60	0.73	0.68	0.91	-1.16	2	1	3	Low Priority
S762	001948-33-0	2.91	2.92	2.92	2.92	2.92	1.71	1.56	1.42	3.09	3	2	?	High Priority
S763	001931-23-3	1.52	1.52	1.52	1.52	1.52	1.91	1.48	1.66	-0.63	3	3	3	Low Priority
S764	001977-10-2	1.26	1.24	1.40	1.40	1.51	2.51	2.17	2.17	1.83	2	1	2	Priority (Group 1)
S765	001977-10-2	1.41	1.30	1.17	1.18	1.26	2.49	2.23	2.16	1.10	2	2	3	Priority (Group 2)
5766	002022-85-7	0.15	0.21	0.84	0.37	0.80	-0.62	-0.29	-0.48	-1.60	1	1	1	Low Priority
S767	002050-08-0	0.56	0.61	0.48	0.16	0.39	0.43	0.38	0.45	-0.61	1	1	3	Low Priority
5768	002062-78-4	1.46	1.46	1.46	1.46	1.46	1.44	1.68	1.22	3.20	3	3	3	Priority (Group 3)
S769	002078-54-8	0.51	0.50	0.50	0.51	0.51	0.86	0.93	0.97	-0.80	2	1	2	Low Priority
5770	002102-59-2	0.71	0.33	0.83	0.76	0.89	0.62	0.63	0.57	-1.63	1	1	3	Low Priority
S771	002144-08-3	0.09	0.17	0.45	0.33	0.41	0.39	-0.16	0.40	-1.31	1	1	2	Low Priority
5772	002152-34-3	0.50	0.47	0.43	0.58	0.75	-0.14	0.03	-0.01	-0.77	1	1	2	Low Priority
S773	002167-85-3	0.61	0.89	0.44	0.57	0.73	0.92	0.98	0.64	0.99	2	1	3	Low Priority
S774	002173-57-1	1.21	1.03	1.11	1.01	1.10	1.61	1.61	1.61	0.78	2	1	3	Low Priority
\$775	002180-92-9	0.82	0.89	0.79	0.60	0.73	0.82	0.95	0.48	-0.69	2	1	3	Low Priority
S776	002198-61-0	0.76	0.38	0.28	0.22	0.30	0.65	0.89	0.85	-1.50	1	1	3	Low Priority
S777	002201-39-0	1.14	1.09	0.61	0.79	0.83	2.31	2.26	2.22	-0.21	2	1	3	Low Priority
S778	002207-50-3	0.81	0.65	0.84	0.74	1.08	0.66	0.91	0.67	-0.84	1	1	2	Low Priority
S779	002211-28-1	0.82	0.94	0.86	0.67	0.83	0.95	0.65	0.70	1.72	2	1	3	Low Priority
S780	002216-51-5	0.67	0.61	0.88	0.74	0.99	0.49	0.66	0.58	-2.08	1	1	2	Low Priority
S781	002244-16-8	0.89	0.37	0.66	0.90	0.90	0.71	0.75	0.73	-1.07	1	1	2	Low Priority
S782	002311-46-8	0.71	0.33	0.15	0.21	0.25	0.40	0.67	0.65	-1.49	1	1	2	Low Priority
S783	002321-07-5	0.20	0.20	0.20	0.20	0.20	1.08	0.39	0.57	2.60	2	1	2	Low Priority
S784	002349-07-7	0.68	0.35	0.18	0.13	0.26	0.54	0.77	0.76	-1.49	1	1	2	Low Priority
S785	002351-90-8	0.69	0.26	0.06	-0.02	0.22	0.88	0.74	0.75	-1.26	1	1	2	Low Priority
S786	002385-81-1	0.74	0.89	0.63	0.68	0.59	0.98	1.09	0.97	-0.31	2	1	2	Low Priority
S787	002398-96-1	1.33	1.21	1.19	1.13	1.17	2.01	1.84	1.58	2.28	2	2	3	Priority (Group 3)
S788	002409-55-4	0.52	0.52	0.70	0.53	0.55	0.73	0.88	0.96	-0.77	2	1	2	Low Priority
S789	002416-94-6	0.38	0.38	0.67	0.31	0.53	0.44	0.43	0.53	-0.76	2	1	2	Low Priority
S790	002440-22-4	0.84	1.13	1.12	0.91	1.07	0.50	0.74	0.15	1.59	2	1	2	Low Priority
S791	002447-57-6	0.56	0.84	0.82	1.09	0.96	0.19	0.32	-0.03	0.07	2	1	2	Low Priority
S792	002475-45-8	0.34	0.94	0.77	0.97	1.08	0.07	0.18	-0.20	-1.90	2	1	3	Low Priority
S793	002489-77-2	0.44	0.14	0.39	0.50	0.55	0.44	0.63	0.61	-1.70	1	1	1	Low Priority
S794	002563-07-7	0.47	0.47	0.64	0.36	0.44	0.56	0.33	0.58	-0.75	1	1	2	Low Priority
S795	002622-26-6	0.78	1.30	0.78	0.65	0.70	1.28	1.23	1.07	0.73	2	1	2	Low Priority
S796	002622-30-2	0.68	1.15	0.76	0.55	0.55	0.91	0.74	0.61	0.63	3	1	2	Low Priority
S797	002668-66-8	0.93	0.80	0.90	0.97	0.86	1.47	1.39	1.42	-1.53	2	1	2	Low Priority
S798	002709-56-0	1.46	1.47	1.47	1.47	1.47	1.62	1.63	1.53	2.56	3	1	2	Low Priority
S799	002741-06-2	1.08	0.65	0.66	0.76	1.05	1.29	1.33	0.99	-0.81	1	1	1	Low Priority
S800	002751-68-0	0.69	1.14	0.76	0.57	0.56	0.90	0.74	0.66	0.65	3	1	2	Low Priority
S801	002778-42-9	0.92	0.74	0.57	0.55	0.56	0.89	1.51	1.38	0.49	2	1	3	Low Priority
5802	002784-94-3	0.28	0.64	0.32	0.20	0.16	0.53	0.50	0.42	-1.36	2	1	1	Low Priority
S803	002801-68-5	0.92	0.72	0.77	0.96	0.89	1.35	1.14	1.41	-1.05	2	1	2	Low Priority
S804	002835-99-6	0.26	0.34	0.75	0.39	0.65	0.18	0.12	-0.01	-1.51	1	1	2	Low Priority
5805	002871-01-4	0.16	0.55	0.38	0.13	0.23	0.35	0.33	0.26	-1.73	2	1	2	Low Priority
5806	002894-67-9	2.30	2.34	2.34	2.34	2.34	1.38	1.38	1.17	2.17	2	1	3	Low Priority
S807	002898-12-6	1.24	1.23	1.31	1.44	1.47	2.56	2.37	2.24	1.86	2	1	2	Priority (Group 1)
S808 S809	002937-53-3 002955-38-6	-0.05 2.07	-0.03 2.08	0.03 2.08	0.00 2.08	0.10 2.08	-0.69	-0.60	-0.37	-2.37 1.86	1	1	1	Low Priority
		2.07 0.56					1.68	1.56	1.37		2	1	3	Low Priority
S810	002985-59-3		0.85	0.33	0.19	0.27	1.57		1.40	0.62	2	1		Low Priority
S811	002998-57-4	1.30	1.31	1.31	1.30	1.30	1.62	1.37	1.54	0.61	3	2	3	Low Priority
S812 S813	003094-09-5	-0.46 -0.06	-0.24 0.34	-0.24 0.34	-0.24 0.34	-0.24 0.34	-0.13 1.36	0.05 0.97	-0.02 1.14	-1.65 1.91	1	1	1	Low Priority
S813 S814	003116-76-5 003147-75-9	-0.06 1.05	1.29	1.31	1.08	0.34	1.36	1.71	1.14	1.91	3	1	2	Low Priority
3014	003147-73-9	1.05	1.29	1.31	1.00	0.95	1.00	1./1	1.10	1.50	2	3	3	Priority (Group 3)

			Human I	Biotransforr	nation		Fish Bi	otransforma	tion		F	PBT Pro	filer	
ID	CAS	logHL _T (h)	logHL _{B1} (h)	logHL _{B2} (h)	logHL _{B3} (h)	logHL ₈₄ (h)	logHL _{N1} (h)	logHL _{N2} (h)	logHL _{N3} (h)	PBT Index	Р	В	т	Priority Level
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	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	0.30	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
\$830	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	0.28	0.40	0.29	-0.67	2	1	3	Low Priority
S836 S837	003846-71-7 003861-72-1	1.06 0.89	1.19 0.95	1.18 0.72	1.18 0.79	1.06	2.27	2.27	2.27 1.53	1.52	2	2	3	High Priority
						0.78	1.43 1.93	1.10		-0.24				Low Priority
S838 S839	003861-76-5 003864-99-1	1.04 1.09	1.19 1.25	1.05 1.54	1.19 1.54	1.11 1.41	1.93 2.10	1.72 2.10	1.78 2.10	2.60 2.16	3	2	3	Priority (Group 3) High Priority
														0,
S840 S841	003896-11-5 003900-31-0	0.87 1.02	1.44	1.74 1.29	1.36 1.32	1.29 1.43	1.42 1.45	1.60 1.49	1.28 1.21	2.18 2.47	2	2	3	Priority (Group 3)
S841 S842	003900-31-0	0.78		0.79	0.75	0.85		0.79	1.21					Low Priority
S842 S843	003902-71-4	0.78	0.73 1.62	1.62	1.62	1.62	1.13 0.44	0.79	0.42	0.85 -1.15	2	1	2	Low Priority Low Priority
5843 5844	003930-20-9	1.18	1.62	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	0.88	0.14	0.38	0.52	0.40	0.12	0.52	2	1	2	Low Priority
S846	004065-45-6	0.55	0.40	0.23	0.14	0.21	0.55	0.40	0.12	0.52	2	1	1	Low Priority
S847	004083-64-1	0.55	0.74	0.70	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
5850	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	0.76	1.42	0.70	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	0.51	0.30	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

			Human Biotransformation					Fish Bio	PBT Profiler						
y Level	ID	CAS	logHL _T (h)	logHL _{B1}	logHL _{B2} (h)	logHL _{B3} (h)	logHL _{B4} (h)	logHL _{N1} (h)	logHL _{N2} (h)	logHL _{N3} (h)	PBT Index	Р	В	т	Priority Level
riority	5897	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
riority	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
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
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
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
Priority	S902	007540-51-4	0.74	0.36	0.65	0.41	0.49	0.63	0.66	0.69	-1.80	1	1	2	Low Priority
Priority	S903	007540-53-6	0.88	0.33	0.41	0.38	0.40	1.21	1.31	1.26	-1.29	1	1	3	Low Priority
Priority	S904	007554-65-6	0.42	0.51	0.70	0.32	0.63	-0.03	0.22	-0.25	-0.81	1	1	2	Low Priority
Priority	S905	007683-59-2	-0.39	-0.36	-0.36	-0.33	-0.33	0.86	0.73	0.95	-1.95	1	1	2	Low Priority
Priority	S906	007764-50-3	0.77	0.44	0.65	0.79	0.81	0.54	0.75	0.71	-1.29	1	1	2	Low Priority
Priority	S907	007778-83-8	0.84	0.64	0.47	0.28	0.63	1.09	0.91	0.89	0.02	1	1	2	Low Priority
Priority	S908	007779-23-9	0.96	0.45	0.51	0.56	0.43	1.40	1.42	1.33	-1.10	1	3	3	Low Priority
Priority	S909	007779-65-9	0.90	0.71	0.67	0.39	0.69	1.27	1.16	1.11	0.00	1	1	3	Low Priority
Priority	S910	007779-81-9	0.81	0.21	0.43	0.42	0.64	0.55	0.73	0.73	-1.28	1	1	2	Low Priority
Priority	S911	007779-94-4	0.78	0.55	0.52	0.61	0.42	0.82	1.17	1.10	-2.08	2	1	2	Low Priority
Priority	S912	007780-06-5	0.93	0.75	0.64	0.47	0.74	1.08	0.98	0.95	0.01	1	1	2	Low Priority
Priority	S913	007787-20-4	0.34	0.74	0.66	0.52	0.33	0.47	0.69	0.59	-1.54	2	1	2	Low Priority
Priority	S914	008000-41-7	0.83	0.67	0.93	0.96	0.95	0.46	0.64	0.56	-0.78	2	1	2	Low Priority
Priority	S915	008003-22-3	0.96	1.16	0.61	1.13	1.00	0.83	1.05	0.43	2.31	2	1	1	Low Priority
Priority	S916	010031-71-7	0.81	0.68	0.63	0.49	0.49	1.01	1.36	1.29	-0.23	2	1	3	Low Priority
Priority	S917	010031-87-5	0.64	0.14	0.10	0.17	0.20	0.32	0.57	0.65	-1.45	1	1	2	Low Priority
Priority	S918	010032-05-0	0.92	0.42	0.21	0.38	0.36	1.16	1.33	1.27	-1.56	1	1	2	Low Priority
Priority	S919	010058-43-2	0.77	0.67	0.38	0.47	0.45	0.92	0.97	1.09	-0.15	2	1	2	Low Priority
(Group 3)	S920	010233-13-3	0.72	0.43	0.03	0.04	0.12	1.05	1.26	1.20	-1.51	1	1	3	Low Priority
Priority	S921	010238-21-8	0.34	0.34	0.34	0.34	0.34	1.30	0.93	1.39	1.13	3	1	3	Low Priority
(Group 3)	S922	010262-69-8	1.71	1.70	1.70	0.97	0.94	2.41	2.27	2.35	0.69	3	1	3	Priority (Group
Priority	S923	010361-39-4	0.85	0.54	0.34	0.31	0.58	0.75	0.90	0.87	-0.21	1	1	2	Low Priority
Priority	S924	010402-33-2	0.80	0.71	0.74	0.56	0.62	1.23	0.79	0.99	0.88	2	1	3	Low Priority
riority	S925	010418-03-8	0.98	1.29	1.45	1.22	1.25	1.38	1.52	1.05	-1.08	2	1	3	Low Priority
riority	S926	010444-50-5	1.21	0.33	0.90	1.04	1.07	1.90	1.82	1.69	-1.16	2	1	3	Low Priority
riority	S927	010461-98-0	0.80	0.81	0.43	0.36	0.63	1.29	1.48	1.36	0.07	2	1	3	Low Priority
riority	S928	010486-14-3	0.93	0.55	0.56	0.49	0.56	1.25	1.47	1.38	-0.02	2	2	3	Low Priority
riority	S929	010540-29-1	2.16	2.16	2.16	2.16	2.16	2.71	2.52	2.62	2.50	2	1	3	Priority (Group
riority	S930	010580-25-3	0.86	0.35	0.41	0.34	0.36	1.28	1.38	1.32	-1.30	1	1	3	Low Priority
riority	S931	013010-47-4	0.19	0.20	0.20	0.19	0.19	0.49	0.47	0.56	-1.05	2	1	2	Low Priority
riority	S932	013020-57-0	0.60	0.78	0.59	0.46	0.59	0.54	0.45	0.46	0.66	1	1	2	Low Priority
riority	S933	013171-00-1	1.05	0.92	0.74	1.03	0.78	1.23	1.74	1.67	-0.25	2	1	3	Low Priority
riority	S934	013311-84-7	1.40	0.64	1.17	1.28	1.36	1.02	1.39	0.95	1.52	2	1	3	Low Priority
riority	S935	013392-18-2	-0.06	-0.06	-0.06	0.03	0.03	1.45	1.05	1.40	-1.07	1	1	2	Low Priority
riority	S936	013392-28-4	1.44	1.44	1.44	1.11	1.35	1.28	1.27	1.22	-2.38	2	1	2	Low Priority
riority	S937	013461-01-3	1.02	1.15	0.97	0.97	0.94	1.28	1.29	1.21	1.05	2	1	3	Low Priority
Priority	S938	013477-62-8	1.00	0.66	1.01	1.06	1.19	1.26	1.43	1.28	-1.59	1	1	2	Low Priority
Priority	S939	013523-86-9	0.34	0.65	0.65	0.65	0.65	1.13	1.14	0.80	-0.75	1	1	2	Low Priority
Priority	S940	013647-35-3	0.90	0.91	0.91	0.90	0.90	1.18	1.27	1.18	-2.09	2	1	3	Low Priority
riority	S941	013655-52-2	0.40	0.42	0.42	0.42	0.42	1.32	1.16	1.23	-0.96	2	1	2	Low Priority
Group 2)	S942	013674-05-0	0.87	0.77	0.87	0.91	0.94	1.46	1.04	1.45	-1.06	2	1	2	Low Priority
Priority	S943	013826-35-2	0.83	0.78	0.71	0.57	0.78	0.91	0.80	0.97	0.56	1	1	2	Low Priority
(Group 3)	S944	014028-44-5	0.90	0.91	0.91	0.93	0.93	2.25	1.91	1.89	1.44	2	1	2	Low Priority
riority	S945	014073-97-3	0.71	0.55	0.66	0.70	0.79	0.51	0.73	0.66	-1.52	1	1	2	Low Priority
riority	S946	014297-87-1	0.94	1.06	0.88	1.00	0.94	2.04	1.25	1.56	0.66	2	1	3	Low Priority
riority	S947	014426-25-6	1.74	1.49	1.61	1.53	1.27	2.81	2.97	2.82	2.41	3	2	3	High Priority
Priority	S948	014521-96-1	1.06	1.15	1.15	1.03	0.81	2.02	1.30	1.61	-1.08	3	1	3	Low Priority
riority	S949	014611-51-9	1.15	0.95	0.97	0.87	0.83	1.32	1.45	1.48	-0.03	2	1	2	Low Priority
riority	S950	014698-29-4	0.32	0.66	0.59	0.32	0.33	0.47	0.09	0.00	-0.22	2	1	1	Low Priority
riority	S951	014769-73-4	0.74	0.76	0.76	0.85	1.21	1.56	1.60	1.49	-0.06	1	1	2	Low Priority
riority	S952	014779-78-3	0.89	0.79	0.52	0.62	0.62	0.82	1.03	0.67	-0.24	1	1	3	Low Priority
riority	S953	014838-15-4	0.38	0.51	0.61	0.44	0.67	0.30	0.41	0.35	-1.55	1	1	1	Low Priority
riority	S954	014901-07-6	0.93	0.65	0.68	0.89	0.71	1.29	1.24	1.27	-1.05	2	1	2	Low Priority
riority	S955	015087-24-8	1.09	1.12	1.00	1.11	1.03	1.17	1.17	1.17	-0.08	2	2	3	Low Priority
Group 2)	S956	015301-48-1	0.87	1.01	0.60	0.60	0.71	1.30	1.54	0.93	2.90	3	1	1	Low Priority
riority	S957	015301-69-6	0.84	0.91	0.71	0.83	0.83	1.32	1.18	1.24	1.42	2	1	3	Low Priority
riority	S958	015307-86-5	0.15	0.15	0.15	0.15	0.15	1.50	1.40	1.43	1.62	2	1	1	Low Priority
riority	S959	015318-45-3	0.93	0.97	1.13	1.35	1.14	0.60	0.81	0.76	0.33	2	1	1	Low Priority
riority	S960	015323-35-0	1.05	1.01	0.87	1.12	0.84	1.26	1.93	1.94	-0.24	2	1	3	Low Priority
riority	S961	015356-60-2	0.67	0.61	0.88	0.74	0.99	0.49	0.66	0.58	-2.08	1	1	2	Low Priority
riority	S962	015588-95-1	0.94	0.79	0.85	1.02	0.90	1.46	1.31	1.59	-1.06	2	1	2	Low Priority
riority	S963	015676-16-1	0.85	0.87	0.81	1.04	0.90	0.42	0.44	0.48	-1.02	2	1	2	Low Priority
riority	S964	015686-71-2	-0.24	0.80	0.80	0.80	0.80	0.31	0.28	0.40	-1.19	2	1	2	Low Priority
riority	S965	015687-14-6	0.61	0.68	0.52	0.28	0.18	0.94	0.95	1.04	-1.02	2	1	3	Low Priority
riority	S966	015687-27-1	0.20	0.21	0.21	0.21	0.21	0.48	0.65	0.68	-0.57	1	1	2	Low Priority
riority	S967	016051-77-7	0.61	0.64	0.64	0.64	0.64	0.22	-0.10	0.42	-1.62	1	1	1	Low Priority
riority	S968	016397-28-7	0.86	0.87	0.49	0.37	0.52	0.95	1.20	1.16	-0.48	2	1	2	Low Priority
Group 2)	S969	016409-43-1	1.03	0.49	1.05	1.06	1.20	1.43	1.44	1.30	-1.37	1	1	3	Low Priority
riority	S970	016590-41-3	0.43	0.44	0.44	0.45	0.45	1.43	0.89	1.13	-1.10	3	1	2	Low Priority
riority	S971	016883-83-3	1.05	0.59	0.62	0.43	0.74	1.14	1.66	1.57	1.40	3	3	3	Low Priority
riority	S971	017021-26-0	0.95	0.59	1.31	1.01	0.74	1.14	1.45	1.50	-1.73	2	1	2	Low Priority
riority	S972	017021-26-0	0.98	0.99	0.76	0.68	0.56	1.46	1.45	1.76	1.04	2	1	3	Low Priority
	S974	017199-58-5	0.98	0.92	0.76	0.68	0.56	1.46	1.75	1.76	1.04	2	1	3	Low Priority
	3314	01/133-33-0							1.73	1.34			1		
	COZE	017720 00 5													
riority riority	S975	017230-88-5	1.38	1.38	1.38	1.39	1.39	1.93			-0.65	3		1	Low Priority
	S975 S976 S977	017230-88-5 017560-51-9 017617-23-1	1.38 1.30 0.36	1.38 2.00 0.37	2.00 0.37	2.00 0.37	2.00 0.37	0.96 1.63	0.75 1.69	0.72 1.41	0.88 2.45	2	1	2	Low Priority Low Priority Low Priority

			Human Biotransformation					F	PBT Pro	filer				
ID	CAS	logHL _T (h)	logHL _{B1} (h)	logHL _{B2} (h)	logHL _{B3} (h)	logHL ₈₄ (h)	logHL _{N1} (h)	logHL _{N2} (h)	logHL _{N3} (h)	PBT Index	Р	В	т	Priority Level
5979	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	0.38	0.83	0.83	0.83	0.83	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	0.30	0.32	0.32	0.32	0.32	0.46	0.43	0.11	1.10	2	1	2	Low Priority
S986 S987	019224-26-1 019356-17-3	0.78 1.19	0.66 0.91	0.39 1.40	0.65 1.05	0.61 1.08	0.95 2.17	1.09 1.98	1.04 2.00	1.27 -1.84	1 2	1 2	3	Low Priority Low Priority
S988	019387-91-8	1.11	1.21	1.21	1.21	1.21	0.57	0.75	0.45	0.00	2	1	2	Low Priority
5989	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	-0.88	-0.85	-0.85	-0.85	-0.85	-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	1.04	1.07	1.07	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	0.84	0.72	0.59	0.55	1.03	1.26	0.87	-0.26	1	2	3	Low Priority
S998 S999	021256-18-8 021500-98-1	1.74 1.03	1.74 1.05	1.74 0.74	0.28 0.94	0.59 1.01	0.89 2.30	0.93 2.07	0.73 2.19	2.24 -0.43	1 2	1	1 3	Low Priority Low Priority
S1000	021738-42-1	0.24	0.24	0.74	0.46	0.46	1.02	1.01	0.94	-0.43	2	1	2	Low Priority
S1000	021829-25-4	0.24	0.24	0.24	0.46	0.46	0.72	0.76	0.58	0.20	2	1	2	Low Priority
S1001	022004-32-6	0.26	0.78	0.82	0.28	0.86	1.56	1.39	1.66	-1.06	2	1	2	Low Priority
S1002	022071-15-4	0.32	0.48	0.48	0.48	0.48	0.50	0.57	0.43	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	1.18	1.18	1.18	0.40	0.41	0.42	0.37	0.49	0.50	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	1.06	1.05	1.05	1.33	1.37	1.48	1.36	1.35	1.27	2	1	3	Low Priority
S1008	022316-47-8	1.26	1.29	1.29	1.59	1.59	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	1.00	1.00	1.00	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	1.55	-0.98	2	1	2	Low Priority Low Priority
S1012 S1013	022839-47-0 022916-47-8	0.36 2.47	0.20 2.66	0.13 2.49	0.12 2.56	0.12 2.51	0.12 2.93	0.35 3.11	0.29 2.58	-1.37 4.62	1	1 3	1 3	High Priority
S1013 S1014	022916-47-8	0.65	0.71	0.48	0.62	0.67	0.51	0.64	0.29	0.67	2	1	2	Low Priority
S1014 S1015	023031-25-6	1.18	1.63	1.63	1.63	1.63	0.98	1.01	1.20	-1.96	1	1	2	Low Priority
S1015	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	0.28	0.23	0.38	0.26	0.18	-0.82	-0.62	-0.54	-2.22	1	1	1	Low Priority
S1018	023593-75-1	0.30	0.30	0.30	0.30	0.30	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	0.38	0.38	0.38	0.72	0.72	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	1.13 1.08	1.14	1.14 1.03	1.00 1.07	1.08	2.41	2.32	2.09 1.35	1.09	2	1	2	Priority (Group 2)
S1025 S1026	024237-00-1 024280-93-1	0.53	0.59 0.40	0.75	0.31	1.08 0.35	1.54 0.99	1.51 0.67	0.95	-1.39 -0.59	1	1	3 2	Low Priority Low Priority
S1020	024295-03-2	0.38	0.40	0.75	0.31	0.58	0.94	1.08	0.74	-0.23	1	1	2	Low Priority
S1027	024526-64-5	0.81	1.18	1.18	1.18	1.18	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	0.80	-1.32	1	1	2	Low Priority
S1031	025013-16-5	0.72	0.68	0.75	0.75	0.69	0.85	0.82	1.04	-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	0.48	0.52	0.73	0.68	1.73	1.74	1.72	-0.18	1	1	2	Low Priority
S1034	025384-17-2	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	1.33	0.43	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 S1038	025724-58-7	0.65	0.68	0.19	0.16	0.27	1.34	1.45 0.83	1.34	-0.06 -0.58	1 2	1	?	Low Priority
S1038 S1039	025812-30-0 025905-77-5	0.18 1.09	0.18 1.16	0.18 0.87	0.19 0.87	0.19 0.95	0.78 1.46	1.82	1.00	-0.58 0.84	2	1	2	Low Priority Low Priority
S1039 S1040	025966-79-4	0.71	0.98	0.87	0.87	0.95	1.46	1.22	1.17	-1.56	2	1	2	Low Priority
S1040	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	0.70	0.70	0.70	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	0.04	0.41	0.41	0.41	0.41	0.38	0.28	0.53	-1.79	2	1	2	Low Priority
S1045	026807-65-8	1.15	1.17	1.17	1.18	1.18	0.93	0.71	0.71	0.91	2	1	3	Low Priority
S1046	026839-75-8	0.34	0.42	0.42	0.42	0.42	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	0.76	0.83	0.83	0.83	0.83	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 S1053	027987-25-3 028179-44-4	1.04 0.82	0.81 1.20	0.78 1.20	0.84 1.19	0.86 1.34	1.17 0.46	1.24 0.68	1.12 0.29	-0.09 0.53	2	3 1	3 1	Low Priority Low Priority
S1055	028219-61-6	0.82	0.61	1.09	0.85	0.77	1.27	1.17	1.19	-1.61	2	2	3	Low Priority
S1054 S1055	028395-03-1	0.93	0.26	0.26	0.26	0.26	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	0.18	0.20	0.20	0.40	0.40	0.11	0.07	-0.15	-0.22	1	1	2	Low Priority
S1058	028721-07-5	0.30	0.32	0.32	0.32	0.32	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

			Human E	Biotransforr	nation	Fish Biotransformation						BT Pro	ofiler	
ID	CAS	logHL _T (h)	logHL _{B1} (h)	logHL _{B2} (h)	logHL _{B3} (h)	logHL ₈₄ (h)	logHL _{N1} (h)	logHL _{N2} (h)	logHL _{N3} (h)	PBT Index	Р	В	т	Priority Level
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	028911-01-5	0.43	0.44	0.44	0.44	0.44	2.60	2.80	2.35	3.79	2	1	3	Priority (Group 1)
S1063	028981-97-7	1.08	1.18	1.18	1.18	1.18	2.43	2.55	2.18	3.16	2	1	3	Priority (Group 1)
S1064	029110-47-2	1.18	1.48	1.48	1.48	1.48	0.73	0.71	0.90	-0.27	2	1	2	Low Priority
S1065 S1066	029122-68-7 029177-84-2	0.79 0.93	0.71 0.87	0.50 0.94	0.40 1.24	0.38 1.26	0.75 1.02	0.84 1.07	1.04 0.78	-1.74 2.28	2	1	2	Low Priority
S1066 S1067	029177-84-2	1.48	1.39	1.08	1.10	1.26	2.63	2.33	2.28	1.09	2	2	3	Low Priority Priority (Group 2)
S1067 S1068	029210-28-2	0.44	0.57	0.75	0.25	0.50	0.96	0.39	0.63	-1.48	2	1	2	Low Priority
S1069	029679-58-1	0.74	0.70	0.62	0.23	0.54	0.75	0.66	0.83	0.72	1	1	2	Low Priority
S1070	029975-16-4	1.23	1.23	1.23	1.24	1.24	2.36	2.50	2.12	3.16	2	1	3	Priority (Group 1)
S1071	030652-11-0	-0.06	0.30	0.47	-0.04	0.01	-0.01	-0.14	-0.11	-1.43	1	1	2	Low Priority
S1072	030772-79-3	0.48	0.75	0.23	0.33	0.64	0.89	0.83	0.86	-1.48	1	1	2	Low Priority
S1073	030960-39-5	0.76	0.93	0.87	0.83	0.73	1.13	1.17	1.06	-1.37	2	1	3	Low Priority
S1074	031036-80-3	1.04	1.04	1.04	1.23	1.23	1.99	1.82	1.92	0.81	2	1	2	Low Priority
S1075	031828-71-4	1.00	1.04	1.04	1.04	1.04	1.24	1.19	1.20	-1.07	2	1	2	Low Priority
S1076	031883-05-3	0.30	0.30	0.30	0.30	0.30	0.45	0.37	0.09	0.78	2	1	2	Low Priority
S1077 S1078	031906-04-4 032156-26-6	0.82 1.05	0.55 0.80	0.62 1.06	0.59 1.29	0.55 1.20	0.99 1.57	0.86 1.50	0.90 1.62	-1.64 -0.41	2	1	2	Low Priority Low Priority
S1078 S1079	032210-23-4	0.82	0.85	0.95	0.66	0.65	0.80	1.15	1.19	-1.48	2	1	3	Low Priority
S1075	032214-91-8	0.93	0.46	0.88	0.82	0.83	1.39	1.54	1.58	-1.07	2	2	3	Low Priority
S1081	032222-06-3	0.81	0.81	0.81	0.81	0.81	2.04	1.86	1.89	-2.24	2	3	3	Low Priority
S1082	032388-55-9	0.88	0.84	0.86	0.87	0.77	1.22	1.50	1.48	-1.34	2	1	3	Low Priority
S1083	032886-97-8	0.86	0.77	0.73	0.89	0.81	0.83	1.08	1.05	-0.96	2	1	3	Low Priority
S1084	032887-01-7	0.04	0.04	0.04	0.15	0.15	0.40	0.41	0.35	-1.53	2	1	2	Low Priority
S1085	033005-95-7	0.30	0.30	0.30	0.58	0.58	0.42	0.32	0.36	0.64	1	1	2	Low Priority
S1086	033125-97-2	0.66	0.66	0.66	0.66	0.66	0.71	1.03	0.54	0.84	1	1	3	Low Priority
S1087	033229-34-4	0.17	0.58	0.23	0.13	0.11	0.51	0.51	0.42	-1.76	2	1	1	Low Priority
S1088 S1089	033320-16-0 033342-05-1	0.52 0.90	-0.02 0.90	0.00 0.90	0.35 0.92	0.33 0.92	-0.42 0.73	-0.20 0.66	-0.16 0.82	-2.02 1.05	1	1	1	Low Priority
S1089 S1090	033342-05-1	0.55	0.90	1.08	0.92	0.92	0.73	0.56	0.82	1.05	2	1	2	Low Priority Low Priority
S1090	033671-46-4	0.60	0.60	0.60	0.60	0.60	1.58	1.31	1.36	1.67	2	1	3	Low Priority
S1092	033704-61-9	0.63	0.64	0.60	0.69	0.55	0.92	1.40	1.33	-1.34	2	1	2	Low Priority
S1093	034245-14-2	0.88	0.98	0.70	0.74	0.48	1.37	1.43	1.57	-0.58	2	1	2	Low Priority
S1094	034597-40-5	0.48	0.48	0.48	0.61	0.61	0.75	0.66	0.83	0.72	1	1	2	Low Priority
S1095	034902-57-3	0.68	0.45	0.73	0.04	0.89	1.37	1.17	1.14	-1.29	1	1	3	Low Priority
S1096	035189-28-7	1.32	1.33	1.33	1.32	1.32	1.57	1.21	1.44	-1.29	3	1	3	Low Priority
S1097	036104-80-0	0.89	0.82	0.94	1.02	1.18	1.30	1.34	1.17	2.06	2	1	3	Low Priority
S1098	036322-90-4	0.61	1.00	0.93	0.84	0.87	0.17	0.39	-0.07	0.88	2	1	3	Low Priority
S1099	036330-85-5	0.59	0.65 1.17	0.52	0.22 1.03	0.33	0.51	0.60 1.57	0.50	1.10	1	1	1	Low Priority
S1100 S1101	036437-37-3 036505-84-7	0.96	0.40	1.21 0.40	0.44	0.98	1.06 0.78	1.23	0.91 0.59	1.52 -0.07	3	1	2	Priority (Group 3) Low Priority
S1101 S1102	036507-48-9	1.38	1.37	1.37	1.46	1.46	1.41	1.54	1.60	-1.19	2	1	3	Low Priority
S1102	036735-22-5	1.59	1.59	1.59	1.59	1.59	2.22	2.57	1.93	4.39	3	1	2	Priority (Group 1)
S1104	036861-47-9	1.15	1.17	1.15	1.21	1.05	1.38	1.39	1.23	-0.09	2	2	3	Low Priority
S1105	036894-69-6	0.58	0.83	0.51	0.57	0.50	1.10	1.05	1.24	-0.86	2	1	2	Low Priority
S1106	037076-71-4	0.66	0.17	-0.03	0.56	0.27	0.28	0.67	0.74	-1.06	1	1	1	Low Priority
S1107	037106-97-1	0.61	0.70	0.46	0.48	0.48	0.76	0.72	0.44	1.16	2	1	2	Low Priority
S1108	037148-27-9	1.57	1.62	1.62	1.75	1.72	1.51	1.64	1.50	-0.69	2	1	2	Low Priority
S1109	037350-58-6	0.66	0.81	0.58	0.51	0.45	1.07	1.10	1.18	-1.17	2	1	2	Low Priority
S1110	037517-30-9	0.54	0.68	0.68	0.68	0.68	0.81	0.91	0.71	-1.20	2	1	2	Low Priority
S1111 S1112	037640-71-4 038194-50-2	1.46 0.89	1.38 0.89	1.11 0.89	1.05 0.72	1.00 0.71	2.70 1.04	2.67 1.03	2.39 0.89	1.09 1.90	2	1	3	Priority (Group 2) Low Priority
S1112 S1113	038304-91-5	0.38	0.65	0.68	0.72	0.71	0.12	0.25	-0.03	-1.77	2	1	2	Low Priority
S1114	038462-22-5	0.75	0.69	0.66	0.96	0.88	0.45	0.62	0.54	-1.53	2	1	2	Low Priority
S1115	039263-32-6	0.20	0.92	0.61	0.48	0.56	0.31	0.76	0.21	-0.24	2	1	2	Low Priority
S1116	039562-70-4	0.91	0.92	0.92	0.92	0.92	0.76	0.80	0.59	0.18	2	1	2	Low Priority
S1117	039860-99-6	0.71	1.21	1.12	0.72	0.74	0.78	0.65	0.51	0.82	2	1	3	Low Priority
S1118	040034-42-2	0.53	0.98	0.73	0.45	0.46	0.52	0.58	0.07	1.28	2	1	1	Low Priority
S1119	040180-04-9	0.74	0.96	1.22	1.11	1.07	0.71	0.61	1.06	1.92	2	1	2	Low Priority
S1120	040828-46-4	0.32	0.34	0.34	0.34	0.34	0.42	0.35	0.38	0.65	1	1	2	Low Priority
S1121	041078-02-8	0.43	0.41	0.38	0.35	0.66	-0.25	0.08	-0.22	-1.26	1	1	2	Low Priority
S1122 S1123	041294-56-8 041340-25-4	1.10 0.86	0.85 0.87	1.27 0.87	0.99	1.07 0.45	2.13 0.63	1.92 0.83	1.95 0.47	-1.85 -0.17	2	2	?	Low Priority Low Priority
S1123 S1124	041340-23-4	0.86	0.77	0.69	0.40	0.45	1.23	1.45	1.34	-0.17	2	2	3	Low Priority
S1124 S1125	041431-28-9	0.77	0.43	0.58	0.48	0.53	0.45	0.72	0.71	-1.82	1	1	3	Low Priority
S1126	041708-72-9	1.08	1.28	1.28	1.28	1.28	0.27	0.49	0.16	-1.39	2	1	2	Low Priority
S1127	041859-67-0	0.30	0.30	0.30	0.59	0.59	1.45	1.17	1.59	1.12	2	1	2	Low Priority
51128	042017-89-0	0.66	0.99	1.23	0.85	0.78	1.22	0.90	1.26	1.49	2	1	2	Low Priority
S1129	042200-33-9	0.96	1.38	1.38	1.38	1.38	1.13	1.28	1.39	-1.97	2	1	1	Low Priority
S1130	042399-41-7	0.75	1.29	1.29	1.29	1.29	1.06	0.84	0.73	1.16	2	1	3	Low Priority
S1131	042408-82-2	0.68	0.70	0.70	0.70	0.70	1.53	1.30	1.24	-1.31	2	1	3	Low Priority
S1132	042542-10-9	1.01	0.81	0.87	0.82	0.89	1.49	1.27	1.47	-0.67	2	1	2	Low Priority
S1133	042835-25-6	0.49	0.77	0.79	0.36	0.48	0.41	0.45	0.02	0.39	2	1	2	Low Priority
S1134 S1135	042924-53-8 043210-67-9	0.93 0.86	0.85 1.03	0.59 0.58	0.79 0.72	0.64 0.88	0.99 0.47	0.96 0.71	1.09 0.35	0.89 1.13	2	1	2	Low Priority Low Priority
S1135 S1136	043210-67-9	0.86 0.78	1.03 0.79	0.58 0.79	0.72	0.88	0.47	1.14	1.22	-1.03	2	1	3	Low Priority Low Priority
S1130 S1137	047141-42-4	1.30	1.30	1.30	1.30	1.30	1.83	1.14	2.06	1.87	2	1	3	Low Priority
S1137	050370-12-2	0.04	1.20	1.20	1.20	1.20	0.37	0.18	0.45	-1.58	2	1	1	Low Priority
S1139	050567-35-6	0.44	0.64	0.76	0.51	0.54	0.08	0.33	-0.08	-0.42	2	1	1	Low Priority
S1140	050679-08-8	0.54	0.54	0.54	0.55	0.55	1.91	2.03	1.84	1.27	3	2	3	Low Priority
S1141	051234-28-7	0.80	0.96	1.21	0.93	1.06	1.15	0.93	0.90	2.43	2	1	2	Low Priority
S1142	051264-14-3	0.67	0.67	0.67	0.69	0.69	0.59	0.70	0.32	2.67	2	1	3	Low Priority

			Human	Biotransfori	mation			==						
ID	CAS	logHL _T (h)	logHL _{B1}	logHL _{B2} (h)	logHL _{B3}	logHL _{B4} (h)	logHL _{N1} (h)	otransforma logHL _{N2} (h)	logHL _{N3} (h)	PBT Index	Р	PBT Pro B	т	Priority Level
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 S1147	051566-62-2 051781-06-7	0.97 0.62	0.46 0.85	0.41	0.55 0.51	0.55 0.48	1.07 0.87	1.26 1.07	1.22 0.92	-1.18 -1.39	1 2	1	2	Low Priority Low Priority
S1147 S1148	051803-78-2	0.84	0.85	0.69	1.02	0.48	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	1.38	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 1.08	1.03	1.03 1.33	1.04 1.02	1.04 0.80	1.88 0.66	1.61	1.77 0.69	2.48	3 2	2	3 2	Priority (Group 3)
S1156 S1157	053583-79-2 053716-49-7	0.73	1.33 1.03	1.18	0.83	0.98	0.81	0.65 0.68	0.68	-0.25 1.61	2	1	1	Low Priority 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	1.61	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 S1166	054739-18-3 054910-89-3	1.19 1.68	1.20 1.68	1.20 1.68	1.26 1.23	1.26 1.36	1.28 1.58	1.59 1.85	1.43 1.70	0.92 2.39	2	1	2	Low Priority Low Priority
S1166 S1167	054910-89-3	1.00	1.00	1.68	1.23 1.01	1.35	0.24	0.54	0.15	-0.16	2	1	3	Low Priority
S1167	054982-83-1	0.62	0.22	0.71	0.20	0.86	0.78	0.96	0.13	-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 S1176	056211-40-6	0.71 1.66	0.83 0.97	0.83 1.17	0.83 1.23	0.83 1.36	0.28 1.58	0.62 1.85	0.11 1.70	0.27 2.39	2	1	1	Low Priority
S1176 S1177	056296-78-7 056775-88-3	0.92	0.97	0.92	0.93	0.93	2.40	2.66	2.03	1.92	2	1	3 2	Low Priority Priority (Group 1)
S1177	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 S1186	058001-44-8 058817-05-3	0.08 0.80	0.14 0.79	0.21 0.42	0.06 0.44	0.12 0.44	-0.24 1.05	-0.18 1.24	-0.18 0.86	-1.84 -0.25	1	1	1 3	Low Priority Low Priority
S1180	059122-46-2	-0.30	-0.30	-0.30	-0.30	-0.30	1.03	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	0.01	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	3.54	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	1.25	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 0.72	0.43 0.42	0.18 0.34	0.10 -0.01	0.12 0.16	0.67 0.14	0.49	0.57	-1.34	1	1	1	Low Priority
S1196 S1197	060142-96-3 060628-96-8	0.72	0.42	0.34	0.17	0.16	2.50	0.30 2.58	0.35 2.20	-2.63 3.65	3	1	1 3	Low Priority 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 S1207	063250-25-9 063500-71-0	1.08 0.71	0.99 0.64	0.78 0.90	1.10 0.86	0.89 0.85	1.20 0.43	1.34 0.66	1.24 0.55	1.25 -2.08	2	1	3 1	Low Priority Low Priority
S1207 S1208	063590-71-0	0.71	1.01	1.01	1.01	0.85 1.01	0.43	0.66	-0.05	-2.08 0.01	2	1	2	Low Priority
S1208 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
S1209	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	0.54	-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 S1218	066357-35-5 066408-78-4	0.32 1.10	0.96	0.96	0.96	0.96	1.23	0.78	1.35	-0.93 -1.14	2	1	1	Low Priority
S1218 S1219	066722-44-9	1.10 1.00	0.30 1.42	0.79 1.42	0.81 1.42	0.92 1.42	1.82 1.18	1.71 1.27	1.60 1.36	-1.14	2	1	3 2	Low Priority Low Priority
S1219	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
S1220	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

		Human Biotransformation				Fish Biotransformation					P			
ID	CAS	logHL _T (h)	logHL _{B1} (h)	logHL _{B2} (h)	logHL _{B3} (h)	logHL ₈₄ (h)	logHL _{N1} (h)	logHL _{N2} (h)	logHL _{N3} (h)	PBT Index	P	В	т	Priority Level
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 S1230	068738-94-3 068738-96-5	0.66 0.79	0.93 0.71	0.59 0.69	0.70 0.80	0.46	1.15 1.30	1.12 1.11	1.20 1.18	-0.18 -1.26	2	1	3	Low Priority
S1230 S1231	068844-77-9	0.79 1.38	1.38	1.38	1.38	1.38	1.30	1.11	1.18	3.21	3	3	3	Low Priority Priority (Group 3)
51232	068991-97-9	0.64	0.71	0.67	0.66	0.47	1.23	1.10	1.17	-1.27	2	1	3	Low Priority
S1232	069655-05-6	0.43	0.76	0.80	0.49	0.76	0.05	0.51	-0.24	-0.30	1	1	2	Low Priority
S1234	069929-16-4	1.12	0.52	0.76	0.97	0.81	1.73	1.78	1.67	-1.36	1	1	3	Low Priority
S1235	070356-09-1	1.22	0.99	0.86	1.28	0.92	1.40	1.45	1.49	1.24	2	1	3	Low Priority
S1236	070374-39-9	0.71	1.18	1.35	1.41	1.38	0.69	0.44	0.49	1.31	2	1	3	Low Priority
S1237	070458-92-3	1.04	1.06	1.06	1.06	1.06	0.30	0.39	-0.15	0.33	3	1	1	Low Priority
S1238	070458-96-7	0.54	0.96	0.93	0.55	0.64	0.46	0.57	0.04	-0.06	2	1	1	Low Priority
S1239	071125-38-7	0.65	1.21	1.04	0.99	0.97	0.18	0.27	-0.05	0.66	2	1	3	Low Priority
S1240	071320-77-9	0.18 0.95	0.18	0.18 0.71	0.18	0.18 0.70	0.96 1.44	0.84 1.15	1.06	0.01	2	1	2	Low Priority
S1241 S1242	071617-10-2 071963-77-4	1.13	0.73 0.76	0.71	0.61 1.02	1.04	1.44	1.15	1.25 1.61	-1.63	2	1	1 2	Low Priority Low Priority
51242	072509-76-3	1.00	1.00	1.00	1.02	1.00	1.32	1.29	1.49	1.25	2	1	3	Low Priority
S1244	072956-09-3	0.38	0.39	0.39	0.39	0.39	1.69	1.35	1.35	1.82	2	1	2	Low Priority
S1245	073573-87-2	0.69	0.80	0.50	0.57	0.42	1.41	1.05	1.01	-0.48	2	1	2	Low Priority
S1246	073590-58-6	0.78	1.10	0.94	1.14	1.00	0.57	0.72	0.21	1.47	2	1	3	Low Priority
S1247	073963-72-1	1.08	1.08	1.08	1.08	1.08	0.75	1.15	0.63	0.47	2	1	3	Low Priority
S1248	074011-58-8	0.71	0.92	0.97	0.53	0.70	0.28	0.56	-0.09	-0.05	3	1	1	Low Priority
S1249	074191-85-8	0.97	0.97	0.97	0.97	0.97	0.65	0.39	0.21	1.28	3	1	2	Low Priority
S1250	074431-23-5	0.27	0.58	0.24	0.37	0.31	0.39	0.23	0.33	-2.46	1	1	1	Low Priority
S1251	074517-78-5	0.71	1.17	0.83	0.66	0.72	1.06	1.15	1.04	0.05	2	1	3	Low Priority
S1252 S1253	075673-16-4 075695-93-1	0.73 0.52	0.72 0.52	0.52 0.52	0.32 0.52	0.38 0.52	1.21 0.67	1.35 0.83	1.23 0.39	-0.07 0.81	1 2	2	3	Low Priority Low Priority
S1254	075706-12-6	2.53	0.92	1.34	1.53	1.56	1.05	1.37	0.84	2.37	2	1	3	Priority (Group 1)
S1255	075847-73-3	1.04	0.31	0.34	0.19	0.12	0.53	0.73	0.60	-0.65	1	1	2	Low Priority
S1256	076470-66-1	0.00	0.12	0.12	0.13	0.13	0.42	0.67	0.52	-0.54	2	1	2	Low Priority
S1257	076963-41-2	0.69	1.00	0.40	0.68	0.59	1.06	0.77	0.93	-0.93	2	1	1	Low Priority
S1258	077337-76-9	1.42	0.16	0.17	0.23	0.23	-0.36	-0.10	-0.03	-1.79	1	1	1	Low Priority
S1259	077671-31-9	0.00	0.00	0.00	0.00	0.00	0.23	0.22	0.25	-0.61	2	1	2	Low Priority
S1260	078415-72-2	-0.10	0.62	0.62	0.62	0.62	0.41	0.66	0.07	0.04	2	1	2	Low Priority
S1261	078755-81-4	-0.11	-0.11	-0.11	-0.11	-0.11	0.57	0.99	0.50	1.87	2	1	2	Low Priority
S1262	079617-96-2	1.41 0.93	1.41 1.35	1.41 1.35	1.42 1.35	1.42 1.35	2.96	2.63	2.94	1.90 1.58	2	2	3	High Priority
S1263 S1264	079660-72-3 079794-75-5	0.93	0.94	0.94	0.92	0.92	0.56 1.83	0.73 1.69	0.03 1.63	1.58	3	1 2	1	Low Priority
S1265	080012-43-7	0.89	0.97	0.92	0.74	1.15	1.38	1.48	1.10	0.44	2	1	2	Priority (Group 3) Low Priority
S1266	080125-14-0	0.74	0.87	0.87	0.87	0.87	0.98	0.95	0.94	-0.04	2	1	3	Low Priority
S1267	081098-60-4	0.97	0.99	1.22	1.29	1.18	1.71	1.31	1.42	1.10	3	1	3	Low Priority
S1268	081403-80-7	0.68	0.72	0.72	1.03	1.03	0.44	0.65	0.23	-0.34	2	1	2	Low Priority
S1269	082186-77-4	1.80	2.13	2.09	1.94	1.96	2.97	2.65	2.63	4.06	3	1	?	Priority (Group 1)
S1270	082419-36-1	0.64	1.00	1.04	0.65	0.70	0.39	0.28	-0.12	0.30	3	1	1	Low Priority
S1271	082626-48-0	0.23	0.23	0.23	0.23	0.23	0.94	1.44	0.75	2.10	2	1	3	Low Priority
S1272	082654-98-6	0.59	0.73	0.69	0.33	0.39	0.87	0.63	0.89	-0.76	1	1	2	Low Priority
S1273 S1274	082964-04-3	1.22	0.83 0.10	1.27 0.10	0.91 0.10	0.98	0.97	1.21 1.49	0.80	2.55	2	1	1	Low Priority
S1274 S1275	083366-66-9	0.08 1.51	1.52	1.52	1.56	0.10 1.56	1.68 0.70	0.53	1.44 0.69	1.84 -0.68	3	1		Low Priority
S1275	083647-97-6 083763-47-7	0.42	0.64	0.64	0.41	0.51	0.70	0.53	0.46	-1.88	2	1	2	Low Priority Low Priority
S1277	083799-24-0	1.16	1.16	1.16	1.38	1.38	1.64	1.64	1.51	1.10	2	1	1	Low Priority
S1278	083881-51-0	0.92	0.96	0.96	0.56	0.69	1.36	1.15	1.66	1.38	2	1	1	Low Priority
S1279	083915-83-7	0.31	0.29	0.11	0.20	0.17	0.44	0.65	0.48	-1.84	1	1	1	Low Priority
S1280	084041-77-0	0.18	0.57	0.27	0.08	0.14	0.47	0.47	0.37	-1.74	2	1	1	Low Priority
S1281	084057-84-1	1.40	1.42	1.42	1.99	2.22	1.36	1.65	1.26	0.96	2	1	2	Low Priority
S1282	084057-95-4	0.34	0.35	0.35	0.34	0.34	0.75	0.89	0.43	-0.68	2	1	3	Low Priority
S1283	084371-65-3	1.26	1.27	1.27	1.26	1.26	1.89	1.71	1.39	-0.04	3	2	3	Low Priority
S1284	084449-90-1	1.44	1.44 0.30	1.44	1.44	1.44	1.27	0.59	0.91	2.53	3	2	3	Priority (Group 3)
S1285 S1286	085441-61-8 085721-33-1	0.30 0.58	1.35	0.30 1.35	0.33 1.35	0.33 1.35	0.74 0.52	0.86	0.72 0.08	0.61 -0.06	2	1	2	Low Priority Low Priority
S1280	086386-73-4	1.48	2.08	2.08	2.08	2.08	0.52	1.29	0.36	2.51	3	1	2	Low Priority
S1288	086541-75-5	1.02	1.02	1.02	1.31	1.31	0.69	0.80	0.37	0.61	2	1	2	Low Priority
S1289	086803-90-9	0.65	0.97	0.56	0.58	0.78	0.96	0.91	0.97	-1.48	1	1	2	Low Priority
S1290	087333-19-5	0.48	0.48	0.48	0.58	0.58	0.65	0.80	0.64	-0.68	2	1	2	Low Priority
S1291	088150-42-9	1.53	1.58	1.58	1.58	1.58	1.00	0.88	1.12	-0.19	2	1	2	Low Priority
S1292	089365-50-4	0.74	0.75	0.75	0.77	0.77	1.57	1.48	1.58	-0.69	2	1	3	Low Priority
S1293	090357-06-5	2.15	2.17	2.17	2.18	2.18	1.18	1.86	1.02	3.46	3	1	2	Low Priority
S1294	091161-71-6	1.56	1.56	1.56	1.55	1.55	2.68	2.56	2.57	1.30	3	2	3	Priority (Group 2)
S1295	091374-21-9	0.78	0.78	0.78	0.49	0.57	0.73	0.86	0.53	-0.61	2	1	3	Low Priority
S1296	092206-54-7	0.82 0.90	1.19 0.93	1.02 0.93	0.72	0.84	1.50 0.51	1.18	1.41 0.43	0.28	2	1	3	Low Priority
S1297 S1298	092623-85-3 092952-81-3	0.90 0.28	0.93 0.48	0.93 0.34	0.68	0.58	0.51	0.63	0.43	-1.08 -1.34	2	1	2	Low Priority Low Priority
S1298 S1299	092952-81-3	0.28	1.07	0.34	0.20	0.30	0.65	0.45	-0.08	0.32	3	1	1	Low Priority Low Priority
S1300	093390-81-9	-0.60	-0.58	-0.58	-0.59	-0.59	0.06	0.47	0.08	0.32	2	1	2	Low Priority
S1301	093413-69-5	0.70	0.72	0.72	0.72	0.72	1.23	1.21	1.14	-0.87	2	1	2	Low Priority
S1302	093957-54-1	-0.15	-0.15	-0.15	-0.15	-0.15	1.09	1.07	0.63	1.78	2	1	3	Low Priority
S1303	095233-18-4	0.68	1.05	1.17	1.04	1.09	1.58	1.26	1.49	1.67	2	1	3	Low Priority
S1304	096829-58-2	0.18	0.18	0.18	0.18	0.18	1.17	1.20	1.04	-1.57	1	1	?	Low Priority
S1305	097825-25-7	0.75	0.80	0.66	0.71	0.63	1.47	1.22	1.43	-0.68	1	1	2	Low Priority
S1306	098048-97-6	1.08	1.09	1.09	1.09	1.09	0.60	0.73	0.53	-0.14	2	1	3	Low Priority

			Human	Biotransforr	nation		Fish Bio							
ID	CAS	logHL _T (h)	logHL _{B1}	logHL _{B2}	logHL _{B3}	logHL _{B4}	logHL _{N1} (h)	logHL _{N2}	logHL _{N3}	PBT Index		PBT Pro	Т	Priority Leve
1307	098079-51-7	0.90	(h) 1.01	(h) 1.29	(h) 0.74	(h) 0.89	0.64	(h) 0.85	(h) 0.15	0.54	3	1	1	Low Priority
1308	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
1309	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
310	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
311	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
312	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
1313	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
314	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
315	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
316	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
317	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
318	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
319	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
320	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
321	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
322	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
323	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
324	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
325	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
326	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
327	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
328	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
329	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
330	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
331	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
1332	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
333	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
334	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
335	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
336	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
337	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
338	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
339	129453-61-8	2.98	2.98	2.98	2.99	2.99	2.67	2.93	2.74	2.18	3	1	?	Priority (Grou
340	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 Priorit
341	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 (Grou
342	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 Priorit
1343	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
344	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
345	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
346	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 Priorit
347	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
348	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
349	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
350	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
351	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 Priorit
352	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 Priorit
353	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 Priorit
354	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 Priorit
355	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 Priorit
356	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 Priorit
357	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 Priorit
358	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 Priorit
359	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 Priorit
360	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 Priorit
361	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 Priorit
362	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 Priorit
363	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 Priorit
364	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 Priorit
365	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 Priorit
366	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 Priorit
367	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 Priorit
368	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
369	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 Priorit
370	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 Priorit
1371	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 Priorit
372	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
373	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 Priorit
374	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 Priorit
375	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