Hamner Institutes for Health Sciences
Thomas Lab

Fub and Clearance Values derived for ToxCast Phase I Chemical Subset

Experimentally derived Fub values were entered into SimCyp for Css determinaiton when possible.
Default Fub value = 0.5% assigned for those chemicals for which exp. Fub = 0. For metabolic clearance, the values derived experimentally prior to linear regression analysis are provided in G-H. The values listed in the SimCyp Metab columns (L-M) were adjusted: in cases where the slope of the regression line was not significantly different from 0, the metabolic clearance was set t

Chemical Information					Experimentally derived Values		
					Metabolism		
STRUCTURE_NAME	ToxCast CAS	CAS Checksum	Hamner CAS	CAS Checksum	MW_EPS	1 uM	p-value	10 uM
d-cis,trans- Allethrin	584-79-2		584-79-2		302.42	2.58803	0.20366	17.69994
Emamectin	155569-91-8		155569-91-8		1008.3	-5.79218	0.19783	-19.21593
Picloram	1918-02-1		1918-02-1		241.46	3.10872	0.02374	2.94171
6-Desisopropylatrazine	1007-28-9		1007-28-9		173.61	-0.43106	0.53873	-1.87439
Halosulfuron-methyl	100784-20-1		100784-20-1		434.81	-5.99535	0.00468	-11.22180
Anilazine	101-05-3		101-05-3		275.53	22.49708	0.0000003	4.97080
Cloprop	101-10-0		101-10-0		200.62	-0.94432	0.54403	-10.75126
Chlorpropham	101-21-3		101-21-3		213.67	43.82635	0.11559	27.54385
Imazapic	104098-48-8		104098-48-8		275.31	-1.03782	0.33109	-5.74797
Mesotrione	104206-82-8		104206-82-8		339.32	0.35417	0.79448	-2.84398
Resmethrin	10453-86-8		10453-86-8		338.45	98.95624	0.09958	38.34818
Dimethomorph	110488-70-5		110488-70-5		387.87	0	0.00000003	5.96998
Tetraconazole	112281-77-3		112281-77-3		372.15	-13.24050	0.06412	-14.12674
Cyclanilide	113136-77-9		113136-77-9		274.11	0.33640	0.52197	0.53360
Cycloate	1134-23-2		1134-23-2		215.36	34.48205	0.00004	0
Imazamox	114311-32-9		114311-32-9		305.34	-2.54276	0.00701	0.24588
Fenbuconazole	114369-43-6		114369-43-6		336.83	11.19187	0.0000001	2.45266
Endosulfan	115-29-7		115-29-7		406.92	4.98386	0.11416	-1.18797
Dicofol	115-32-2		115-32-2		370.49	4.92063	0.00071	2.95115

Aldicarb	116-06-3	116-06-3	190.26	0.74564	0.32907	0.36361
Novaluron	116714-46-6	116714-46-6	492.71	2.87291	0.01426	6.71380
Spiroxamine	118134-30-8	118134-30-8	297.49	3.35269	0.01080	-13.20044
Tebufenpyrad	119168-77-3	119168-77-3	333.86	15.93560	0.000007	10.72608
Dichlobenil	1194-65-6	1194-65-6	172.01	7.03613	0.16622	18.71788
Fipronil	120068-37-3	120068-37-3	437.15	1.36739	0.27788	2.89341
Clorophene	120-32-1	120-32-1	218.68	5.00103	0.01558	12.93874
Dichlorprop	120-36-5	120-36-5	235.07	2.23001	0.08224	-0.02799
Malathion	121-75-5	121-75-5	330.35	87.48043	0.02109	74.74267
Fenitrothion	122-14-5	122-14-5	277.23	10.02248	0.00001	10.57927
Simazine	122-34-9	122-34-9	201.66	6.32606	0.00047	-4.35822
Rimsulfuron	122931-48-0	122931-48-0	431.44	-1.65455	0.06066	-2.38427
Phenoxyethanol	122-99-6	122-99-6	138.17	17.89438	0.21932	19.01129
Quinoxyfen	124495-18-7	124495-18-7	308.14	-1.71395	0.48598	-1.31212
dimethyl phthalate	131-11-3	131-11-3	194.19	22.25930	0.20394	45.86597
Mono-n-butyl Phthalate (MBP)	131-70-4	131-70-4	222.24	0.73586	0.16568	0.49979
Triticonazole	131983-72-7	131983-72-7	317.82	6.11750	0.00003	1.03714
Propazine	139-40-2	139-40-2	229.71	14.60422	.0000000000	0.95285
Oxasulfuron	144651-06-9	144651-06-9	406.42	3.10693	0.00531	-1.11684
THIABENDAZOLE	148-79-8	148-79-8	201.25	-4.23333	0.00221	5.83879
Napropamide	15299-99-7	15299-99-7	271.36	15.14933	0.00352	13.37802
Thiamethoxam	153719-23-4	153719-23-4	291.71	0.61150	0.57674	0.46331
Trifluralin	1582-09-8	1582-09-8	335.29	8.98446	0.08625	13.96545
Prometon	1610-18-0	1610-18-0	225.3	14.10641	)0000000000	3.05081
Methoxyfenozide	161050-58-4	161050-58-4	368.48	16.19787	0.000000008	-5.72450
Chloridazon	1698-60-8	1698-60-8	221.65	1.87139	0.10437	3.87519
Foramsulfuron	173159-57-4	173159-57-4	452.44	-2.70491	0.04835	-4.04410
Indoxacarb	173584-44-6	173584-44-6	527.84	31.36103	0.000001	3.78031
Perfluorooctane sulfonic acid	1763-23-1	1763-23-1	500.13	-7.35938	0.01746	-9.89388
Benomyl	17804-35-2	17804-35-2	290.32	56.68588	0.00108	72.28520
Benfluralin	1861-40-1	1861-40-1	335.29	17.33694	0.000007	12.63822

Dicamba	1918-00-9	1918-00-9	221.04	0.64831	0.18721	2.20740
Nitrapyrin	1929-82-4	1929-82-4	230.91	36.83524	0.01573	12.82420
Oxadiazon	19666-30-9	19666-30-9	345.23	14.02144	0.00031	4.37452
Trifloxysulfuron-sodium	199119-58-9	199119-58-9	459.33	-0.08413	0.95043	-4.85868
Butylate	2008-41-5	2008-41-5	217.37	52.50967	0.00040	0
Mesosulfuron-methyl	208465-21-8	208465-21-8	503.5	5.45214	0.00150	3.47058
Fluometuron	2164-17-2	2164-17-2	232.21	10.05792	0.00078	2.18218
Penoxsulam	219714-96-2	219714-96-2	483.37	-1.44966	0.18243	1.55524
Phosalone	2310-17-0	2310-17-0	367.8	56.02164	0.00002	35.43663
Oxamyl	23135-22-0	23135-22-0	219.26	-1.66614	0.33082	-1.06379
Butachlor	23184-66-9	23184-66-9	311.86	100.80394	0.00218	20.16854
Propyzamide	23950-58-5	23950-58-5	256.13	5.39975	0.00099	1.42068
Etridiazole	2593-15-9	2593-15-9	247.53	126.99450	0.00286	129.63531
Norflurazon	27314-13-2	27314-13-2	303.67	11.08930	0.00002	-3.17078
Thiobencarb	28249-77-6	28249-77-6	257.78	18.27636	0.00019	0
S-Bioallethrin	28434-00-6	28434-00-6	302.42	-1.16317	0.59495	12.97801
Prodiamine	29091-21-2	29091-21-2	350.3	7.21555	0.00012	4.97262
Pirimiphos-methyl	29232-93-7	298-04-4	305.33	58.01630	0.00033	0
2,2-Bis(4-hydroxyphenyl)-1,1,1-trichl	2971-36-0	2971-36-0	317.6	136.50094	0.00004	56.86223
Disulfoton	298-04-4	298-04-4	274.39	58.01630	0.00033	0
Acephate	30560-19-1	30560-19-1	183.16	-4.43703	0.00014	-3.71532
Amitraz	33089-61-1	33089-61-1	293.42	19.30184	0.00086	0
Diazinon	333-41-5	333-41-5	304.35	52.30592	.0000000000	19.50415

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Chemical Information					Experimentally derived Values		
					Metabolism		
STRUCTURE_NAME	ToxCast CAS	CAS Checksum	Hamner CAS	CAS Checksum	MW_EPS	1 uM	p-value	10 uM
2,4-D	94-75-7		94-75-7		221.04	-1.2868	0.1365	-2.146
Acetochlor	34256-82-1		34256-82-1		269.77	59.28	< 0.0001	51.72
Acifluorfen	50594-66-6		50594-66-6		361.66	-1.983	0.2084	-5.586
Ametryn	834-12-8		834-12-8		227.33	42.06	< 0.0001	28.18
Bensulide	741-58-2		741-58-2		397.51	37.52	< 0.0001	20.56
Bentazone	25057-89-0		25057-89-0		240.28	-3.688	0.0575	0.3572
Boscalid	188425-85-6		188425-85-6		343.21	12.038	< 0.0001	8.522
Carbaryl	63-25-2		63-25-2		201.23	14.966	< 0.0001	1.2328
Chloridazon	1698-60-8		1698-60-8		221.65	-4.984	0.0292	-2.548
Cyclanilide	113136-77-9		113136-77-9		274.11	-4.918	0.0676	-7.234
Cyprodinil	121552-61-2		121552-61-2		225.3	8.81	< 0.0001	0
Diazoxon	962-58-3		962-58-3		288.29	59.02	< 0.0001	73.22
Diuron	330-54-1		330-54-1		233.1	2.742	< 0.0001	-1.031
Ethoprop	13194-48-4		13194-48-4		242.33	43.26	< 0.0001	37.34
Fenarimol	60168-88-9		60168-88-9		331.2	1.5696	0.0825	1.1058
Fludioxonil	131341-86-1		131341-86-1		248.19	37.44	< 0.0001	14.122
Flufenacet	142459-58-3		142459-58-3		363.33	40.92	< 0.0001	9.94
Formetanate hydrochloride	23422-53-9		23422-53-9		257.7	11.178	< 0.0001	8.398
Halosulfuron-methyl	100784-20-1		100784-20-1		434.81	9.948	< 0.0001	1.047
Hexaconazole	79983-71-4		79983-71-4		314.22	46.16	< 0.0001	32.88

Imazalil	35554-44-0	35554-44-0	297.19	46.44	< 0.0001	5.86
Imidacloprid	138261-41-3	138261-41-3	255.67	-2.14	0.0065	-3.102
Isoxaflutole	141112-29-0	141112-29-0	359.32	-3.218	0.0001	-1.5076
MCPA	94-74-6	94-74-6	200.62	-2.642	< 0.0001	-3.34
Perfluorooctane sulfonic acid	1763-23-1	1763-23-1	500.13	-7.896	0.0007	-2.562
Perfluorooctanoic acid	335-67-1	335-67-1	414.07	-3.25	0.0374	-12.386
Propamocarb hydrochloride	25606-41-1	25606-41-1	224.77	-29.08	< 0.0001	0
Pryrithiobac-sodium	123343-16-8	123343-16-8	348.74	1.9488	< 0.0001	-0.11244
Rimsulfuron	122931-48-0	122931-48-0	431.44	-5.406	0.0383	-4.96
Simazine	122-34-9	122-34-9	201.66	4.832	< 0.0001	-2.844
Tetraconazole	112281-77-3	112281-77-3	372.15	0.0519	0.8297	0.573
Thidiazuron	51707-55-2	51707-55-2	220.25	2.142	0.007	1.5264
Triflumizole	68694-11-1	68694-11-1	345.75	20.62	< 0.0001	0.9162
Zoxamide	156052-68-5	156052-68-5	336.65	41.26	< 0.0001	25.84
Alachlor	15972-60-8	15972-60-8	269.77	41.66	< 0.0001	36.48
Bisphenol-A	80-05-7	80-05-7	228.29	0	0	2.326
Chlorpropham	101-21-3	101-21-3	213.67	24.78	< 0.0001	11.49
Cyproconazole	94361-06-5	94361-06-5	291.78	2.312	< 0.0001	0
Dichlobenil	1194-65-6	1194-65-6	172.01	9.822	< 0.0001	0
Diethylhexyl phthalate (DEHP)	117-81-7	117-81-7	390.57	10.73	0.2579	1.3772
Dimethanimid	87674-68-8	87674-68-8	275.8	101.82	0.0006	47.1
Diphenylamine	122-39-4	122-39-4	169.23	38.58	< 0.0001	15.572
Dithiopyr	97886-45-8	97886-45-8	401.41	17.512	< 0.0001	15.63
Ethofumesate	26225-79-6	26225-79-6	286.35	56.4	< 0.0001	50.2
Etoxazole	153233-91-1	153233-91-1	359.42	42.28	< 0.0001	31.32
Fenbuconazole	114369-43-6	114369-43-6	336.83	3.886	0.0214	0
Flusiazole	85509-19-9	85509-19-9	315.4	5.002	< 0.0001	2.47
Isazofos	42509-80-8	42509-80-8	313.74	81.88	< 0.0001	32.8
Lindane	58-89-9	58-89-9	290.83	5.288	< 0.0001	5.758
Novaluron	116714-46-6	116714-46-6	492.71	-0.01964	0.9757	-1.4544
Oxadiazon	19666-30-9	19666-30-9	345.23	7.264	0.0006	6.812
Permethrin	52645-53-1	52645-53-1	391.3	54.7	< 0.0001	15.452
Propyzamide	23950-58-5	23950-58-5	256.13	1.7096	0.0013	1.3192

Pyrimethanil	53112-28-0	53112-28-0	199.26	11.412	< 0.0001	5.728
Resmethrin	10453-86-8	10453-86-8	338.45	96.48	< 0.0001	43.38
S-Bioallethrin	28434-00-6	28434-00-6	302.42	134.36	< 0.0001	49.62
Triclosan	3380-34-5	3380-34-5	289.55	34.66	0.0001	43.82
Triadimefon	43121-43-3	43121-43-3	293.76	11.442	< 0.0001	0
Triticonazole	131983-72-7	131983-72-7	317.82	17.984	< 0.0001	0

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