Source	Compound name	CAS #	logP	ion	pKa1	pKa2
EPA/Hamner	2,4-D	94-75-7	630.96	mpa	2.73	NA
EPA/Hamner	Acetochlor	34256-82-1	13803.84	neu	NA	NA
EPA/Hamner	Acifluorfen	50594-66-6	35481.34	mpa	2.03	NA
EPA/Hamner	Alachlor	15972-60-8	3890.45	neu	NA	NA
EPA/Hamner	Ametryn	834-12-8	398.11	mpb	5.74	NA
EPA/Hamner	Bensulide	741-58-2	2818.38	mpb	10.18	NA
EPA/Hamner	Bentazone	25057-89-0	5.75	mpb	8.02	NA
EPA/Hamner	Bisphenol-A	80-05-7	10964.78	dpa	9.78	10.39
EPA/Hamner	Boscalid	188425-85-6	83176.38	mpa	10.70	NA
EPA/Hamner	Carbaryl	63-25-2	288.40	mpa	14.77	NA
EPA/Hamner	Chloridazon	1698-60-8	12.88	neu	NA	NA
EPA/Hamner	Chlorpropham	101-21-3	7943.28	mpa	5.22	NA
EPA/Hamner	Cyclanilide	113136-77-9	263.03	dpa	3.56	12.61
EPA/Hamner	Cyproconazole	94361-06-5	707.95	zwi	2.26 (base)	13.34 (acid)
EPA/Hamner	Cyprodinil	121552-61-2	1621.81	zwi	3.63 (base)	13.63 (acid)
EPA/Hamner	Diazoxon	962-58-3	2398.83	mpb	3.80	NA
EPA/Hamner	Dichlobenil	1194-65-6	1096.48	neu	NA	NA
EPA/Hamner	Diethylhexyl phthalate (DEHP)	117-81-7	107151930.52	neu	NA	NA
EPA/Hamner	Dimethanimid	87674-68-8	831.76	neu	NA	NA
EPA/Hamner	Diphenylamine	122-39-4	2570.40	mpb	0.78	NA
EPA/Hamner	Dithiopyr	97886-45-8	588843.66	neu	NA	NA
EPA/Hamner	Diuron	330-54-1	338.84	mpa	13.18	NA
EPA/Hamner	Ethofumesate	26225-79-6	218.78	neu	NA	NA
EPA/Hamner	Ethoprop	13194-48-4	1659.59	neu	NA	NA
EPA/Hamner	Etoxazole	153233-91-1	416869.38	mpb	0.74	NA
EPA/Hamner	Fenarimol	60168-88-9	8317.64	zwi	1.04 (base)	12.13 (acid)
EPA/Hamner	Fenbuconazole	114369-43-6	22387.21	mpb	2.27	NA
EPA/Hamner	Fludioxonil	131341-86-1	3715.35	mpa	14.66	NA
EPA/Hamner	Flufenacet	142459-58-3	1659.59	mpa	12.58	NA
EPA/Hamner	Flusilazole	85509-19-9	47863.01	mpb	2.32	NA
EPA/Hamner	Formetanate hydrochloride	23422-53-9	12.02	zwi	8.89 (base)	14.77 (acid)
EPA/Hamner	Halosulfuron-methyl	100784-20-1	28.18	zwi	1.69 (base)	5.03 (acid)
EPA/Hamner	Hexaconazole	79983-71-4	5128.61	zwi	2.26 (base)	13.35 (acid)
EPA/Hamner	Imazalil	35554-44-0	5754.40	mpb	6.77	NA
EPA/Hamner	Imidacloprid	138261-41-3	12.59	zwi	5.28 (base)	9.39 (acid)
EPA/Hamner	Isazofos	42509-80-8	3019.95	neu	NA	NA
EPA/Hamner	Isoxaflutole	141112-29-0	138.04	neu	NA	NA
EPA/Hamner	Lindane	58-89-9	22387.21	neu	NA	NA
EPA/Hamner	MCPA	94-74-6	562.34	mpa	3.07	NA
EPA/Hamner	Novaluron	116714-46-6	1737800.83	dpa	6.30	13.89
EPA/Hamner	Oxadiazon	19666-30-9	204173.79	neu	NA	NA
EPA/Hamner	Perfluorooctane sulfonic acid	1763-23-1	269153.48	mpa	-3.32	NA
EPA/Hamner	Perfluorooctanoic acid	335-67-1	128824.96	mpa	-4.20	NA
EPA/Hamner	Permethrin	52645-53-1	501187.23	neu	NA	NA
EPA/Hamner	Propamocarb hydrochloride	25606-41-1	5.89	mpa	9.30	NA
EPA/Hamner	Propyzamide	23950-58-5	1513.56	mpa	14.21	NA
EPA/Hamner	Pryrithiobac-sodium	123343-16-8	7762.47	zwi	0.53 (base)	2.21 (acid)
EPA/Hamner	Pyrimethanil	53112-28-0	269.15	zwi	3.96 (base)	13.67 (acid)
EPA/Hamner	Resmethrin	10453-86-8	117489.76	neu	NA	NA
EPA/Hamner	Rimsulfuron	122931-48-0	6.76	zwi	1.69 (base)	4.95 (acid)
EPA/Hamner	S-Bioallethrin	28434-00-6	11481.54	neu	NA	NA
EPA/Hamner	Simazine	122-34-9	60.26	mpb	3.23	NA
EPA/Hamner	Tetraconazole	112281-77-3	7244.36	mpb	2.28	NA
EPA/Hamner	Thidiazuron	51707-55-2	74.13	mpa	8.93	NA
EPA/Hamner	Triadimefon	43121-43-3	9332.54	mpb	1.93	NA
EPA/Hamner	Triclosan	3380-34-5	95499.26	mpa	7.68	NA

EPA/Hamner	Triflumizole	68694-11-1	3801.89	dpb	3.52	6.31
EPA/Hamner	Triticonazole	131983-72-7	2238.72	zwi	2.26 (base)	13.33 (acid)
EPA/Hamner	Zoxamide	156052-68-5	43651.58	neu	NA	NA
TNO	Acrylamide	79-06-1	0.21	neu	NA	NA
TNO	Chlorpyrifos	2921-88-2	50118.72336	neu	NA	NA
TNO	Warfarin	81-81-2	3235.94	mpa	5.00	NA
TNO	Phenytoin	57-41-0	141.25	dpa	6.46	14.71
TNO	Valproic acid	99-66-1	524.81	mpa	4.56	NA
TNO	Diazepam	53320-84-6	630.96	mpb	2.92	NA
TNO	Cyclosporin A	59865-13-3	831.76	neu	NA	NA
TNO	Methoxyacetic acid	625-45-6	0.32	mpa	3.57	NA
Ito/Riley	Alprazolam	28981-97-7	234.42	dpa	1.42	8.19
Ito/Riley	Bosentan	147536-97-8	87096.36	mpb	5.80	NA
Ito/Riley	Caffeine	58-08-2	0.28	neu	NA	NA
Ito/Riley	Diclofenac	64118-84-9	9120.11	dpa	3.76	8.61
Ito/Riley	Diltiazem	42399-41-7	537.03	zwi	8.18 (base)	12.86 (acid)
Ito/Riley	Hexobarbitone	56-29-1	17.78	mpa	8.41	NA
Ito/Riley	Ibuprofen	15687-27-1	6918.31	mpa	4.85	NA
Ito/Riley	Imipramine	50-49-7	19054.61	mpb	9.20	NA
Ito/Riley	Metoprolol	37350-58-6	57.54	zwi	9.67 (base)	14.09 (acid)
Ito/Riley	Midazolam	59467-70-8	2137.96	dpb	5.67	7.42
Ito/Riley	Nicardipine	55985-32-5	3630.78	dpb	5.42	8.18
Ito/Riley	Nilvadipine	75530-68-6	173.78	neu	NA	NA
Ito/Riley	Ondansetron	99614-02-5	223.87	mpb	7.34	NA
Ito/Riley	Phenacetin	62-44-2	25.70	neu	NA	NA
Ito/Riley	Tolbutamide	64-77-7	199.53	mpa	4.33	NA
ECVAM	Antipyrine	60-80-0	2.40	mpb	0.37	NA
ECVAM	2,5-Hexanedione	110-13-4	0.54	neu	NA	NA
ECVAM	Acetylsalicylic acid	50-78-2	15.49	mpa	3.41	NA
ECVAM	Acrylamide	79-06-1	0.21	zwi	0.83	16.70
ECVAM	Benz(a)anthracene	56-55-3	575439.94	neu	NA	NA
ECVAM	Benzene	71-43-2	134.90	neu	NA	NA
ECVAM	Bisphenol A	80-05-7	2089.30	dpa	9.78	10.39
ECVAM	Carbendazim	10605-21-7	33.11	zwi	4.28 (acid)	9.70 (base)
ECVAM	Chlorpyrifos	2921-88-2	91201.08	neu	NA	NA
ECVAM	Deltamethrin	52918-63-5	1584893.19	mpa	10.62	NA
ECVAM	Diethylene glycol	111-46-6	0.07	dpa	14.82	15.42
ECVAM	Diquat	2764-72-9	46.77	neu	NA	NA
ECVAM	Domoic acid	14277-97-5	0.85	ppa & zwi	1.68 (acid)	4.22 (acid) & 4.86 (acid) & 11.59 (base)
ECVAM	Endosulfan	115-29-7	6760.83	neu	NA	NA
ECVAM	Flutamide	13311-84-7	2238.72	mpa	13.17	NA
ECVAM	Genistein	446-72-0	208.93	ppa	6.61	8.79 & 9.46
ECVAM	Glycidamide	5694-00-8	0.06	mpa	15.25	NA
ECVAM	Gossypol	303-45-7	446683.59	ppa	7.80	8.29 & 8.74 & 9.32 & 11.77 & 12.37
ECVAM	Hexachlorobenzene	118-74-1	537031.80	neu	NA	NA
ECVAM	Hexachlorophene	70-30-4	34673685.05	dpa	5.15	8.79
ECVAM	Ketoconazole	65277-42-1	22387.21	dpb	3.69	6.75
ECVAM	Lead acetate	6080-56-4	1.86	NA	NA	NA
ECVAM	Lindane	58-89-9	5248.07	neu	NA	NA
ECVAM	Nicotine	54-11-5	14.79	dpb	2.70	8.86
ECVAM	Ochratoxin A	303-47-9	54954.09	dpa	3.17	7.95

ECVAM	Paraben	120-47-8	91.20	mpa	8.50	NA
ECVAM	Parathion	56-38-2	6760.83	neu	NA	NA
ECVAM	Pentachlorophenol (=2,4-D)	87-86-5	131825.67	mpa	4.98	NA
ECVAM	Phenanthrene	85-01-8	28840.32	neu	NA	NA
ECVAM	Potassium cyanide	151-50-8	1.02	mpb	9.50	NA
ECVAM	Pyrene	129-00-0	75857.76	neu	NA	NA
ECVAM	Toluene	108-88-3	537.03	neu	NA	NA
ECVAM	Trimethadione	127-48-0	1.58	neu	NA	NA
ECVAM	Trimethyltin	1066-45-1	43.65	neu	NA	NA

fup	Rbp	MW	VP	fvol	CLint,h		Papp
	Uchimura (2010) Biopharm		http://www.ncbi.nlm.nih.gov /pccompound				\\tsn.tno.nl\Data\Projects\031\
		g/mol	133.3224 mmHg / Pa		*L/h/xx*	*hep /1E6 cells; mic /mg prot*	*cm/s*
0.040	2.11	221.04	1.10E-05	0			2.32E-05
0.160	0.87	269.77	4.53E-06	0			6.36E-04
0.005	0.64	361.66	2.00E-06	1			5.36E-06
0.133	0.85	269.77	3.05E-03	1			5.54E-04
0.005	0.64	227.33	3.65E-04	1			2.97E-04
0.006	0.65	397.51	1.07E-04	1			2.14E-04
0.020	0.71	240.28	9.20E-06	0			7.71E-05
0.068	0.79	228.29	5.20E-05	1			9.08E-05
0.032	0.74	343.21	7.20E-07	0			2.85E-04
0.692	0.85	201.23	1.81E-04	1			2.94E-04
0.427	0.92	221.65	6.00E-05	1			9.19E-05
0.005	0.64	213.67	2.40E-02	1			2.12E-04
0.984	0.61	274.11	1.21E-06	0			1.79E-05
0.109	0.84	291.78	4.48E-07	1			2.49E-04
0.005	0.64	225.30	4.91E-04	1			5.19E-04
0.327	0.92	288.29	NA	0			3.93E-04
0.062	0.79	172.01	8.80E-02	1			2.48E-04
		390.57	1.89E-05	1			9.99E-05
0.232	0.90	275.80	NA	0			6.20E-04
0.005	0.64	169.23	8.93E-02	1			7.83E-04
0.005	0.64	401.41	NA	0			3.40E-04
0.161	0.87	233.10	9.20E-06	0			2.52E-04
0.131	0.85	286.35	6.53E-04	1			1.68E-04
0.093	0.82	242.33	5.07E-02	1			4.36E-04
0.005	0.64	359.42	2.19E-06	0			7.95E-04
0.037	0.75	331.20	NA	0			1.70E-04
0.005	0.64	336.83	NA	0			1.33E-04
0.005	0.64	248.19	NA	0			1.24E-04
0.137	0.86	363.33	9.00E-05	1			1.40E-04
0.029	0.73	315.40	NA	0			3.79E-04
0.885	0.73	257.70	0.00E+00	0			1.53E-04
0.009	0.67	434.81	NA	0			9.44E-06
0.041	0.76	314.22	NA	0			2.63E-04
0.030	0.73	297.19	1.60E-04	1			4.73E-04
0.656	0.87	255.67	4.00E-10	0			3.45E-05
0.065	0.79	313.74	1.16E-02	1			5.59E-04
0.017	0.70	359.32	1.00E-08	0			5.02E-05
0.005	0.64	290.83	5.60E-03	1			9.91E-04
0.590	1.30	200.62	7.87E-04	1			2.74E-05
0.005	0.64	492.71	NA	0			8.56E-05
0.005	0.64	345.23	1.53E-05	1			2.88E-04
0.005	0.64	500.13	2.67E-01	1			1.51E-05
0.005	0.64	414.07	2.00E+01	1			2.94E-05
0.005	0.64	391.30	2.91E-06	1			4.76E-04
0.843	0.76	224.77	NA	0			3.43E-05
0.068	0.79	256.13	NA	0			4.96E-04
0.027	0.73	348.74	NA	0			3.20E-05
0.017	0.70	199.26	2.20E-03	1			4.82E-04
0.005	0.64	338.45	1.51E-06	0			5.63E-04
0.628	0.88	431.44	NA	0			8.36E-06
0.237	0.90	302.42	1.60E-02	1			1.29E-04
0.284	0.91	201.66	2.93E-06	1			2.27E-04
0.025	0.72	372.15	1.80E-04	1			3.30E-04
0.028	0.73	220.25	3.07E-09	0			3.46E-05
0.114	0.84	293.76	2.00E-06	0			1.84E-04
0.005	0.64	289.55	1.37E-08	0			4.74E-04

0.005	0.64	345.75	NA	0			4.05E-04
0.137	0.86	317.82	NA	0			3.90E-04
0.010	0.67	336.65	8.80E-07	1			3.00E-04
		71.08	9.33E-01	1			2.70E-05
0.03	0.73	350.59	2.69E-03	0			NA
0.007	0.55	308.33	1.55E-05	1	3.30E-02	hep	2.45E-05
0.200	0.89	252.27	1.60E-08	0	2.22E-03	mic	2.67E-05
0.366	0.74	166.20	6.13E+00	1			4.80E-05
0.012	0.70	284.74	NA	0	1.88E+00	(L/h/kg) in vivo human	4.38E-05
0.062	1.28	1202.61	NA	0			8.60E-07
		90.08	4.04E+01	1			NA
0.35	0.78	308.77	NA	0	1.98E-03	hep	2.55E-05
0.02	0.71	551.61	NA	0	2.40E+00	mic	1.05E-06
1	0.80	194.19	9.73E-07	0	8.40E-05	hep	4.46E-05
0.017	0.70	312.15	8.13E-06	1	6.60E-03	hep	
0.198	0.89	414.52	NA	0	1.50E+01	mic	4.17E-05
0.62	0.88	236.27	NA	0	1.98E+01	mic	NA
0.01	0.55	206.28	6.27E-03	1	1.74E+00	mic	5.25E-05
0.107	1.10	280.41	NA	0	5.94E-02	hep	1.41E-05
1	1.00	267.36	3.73E-05	1	2.64E+00	mic	2.30E-05
0.07	0.80	325.77	NA	0	4.44E-03	hep	3.24E-05
0.084	0.71	479.53	NA	0	4.02E+02	mic	1.98E-05
0.013	0.68	385.37	NA	0	2.16E+03	mic	NA
0.25	0.83	293.36	NA	0	6.60E-03	hep	2.23E-05
1	1.01	179.22	9.23E-05	1	4.68E-03	hep	5.06E-05
0.08	0.55	270.35	NA	0	9.60E-05	hep	5.25E-05
1	0.56	188.23	NA	0	4.80E-05	hep	4.15E-05
0.90	0.69	114.14	5.73E+01	1			
0.085	0.81	180.16	3.33E-03	1			1.22E-05
0.75 (BSA)	0.82	71.08	9.33E-01	0			2.70E-05
0.01	0.67	228.29	2.53E-04	1			
0.46	0.91	78.12	1.26E+04	1			
0.05	0.77	228.29	5.20E-05	1			9.08E-05
0.26 - 0.4 (rat)	0.92	191.19	1.00E-09	0			
0.01	0.67	350.59	2.69E-03	1			
0.01	0.67	505.20	2.00E-06	0			
0.97	0.63	106.12	7.60E-01	1			
0.59	0.89	344.05	<<1.33E-05	0			
0.92	0.70	311.33	NA	0			
0.11	0.84	406.93	2.31E-05	1			
0.12	0.87	276.21					
0.01 (rat)	0.67	270.24	6.93E-10	0			
0.96	0.61	87.08	7.81E+01	1			
0.01	0.67	518.55	NA	0			
0.01	0.67	284.78	6.53E-03	1			
0.08	0.81	406.90	1.37E-08	0			
0.037 (rat)	0.75	531.43	NA	0			
0.88	0.74	325.30	NA	0			
0.02	0.71	290.83	5.60E-03	1			
0.75	0.82	162.23	5.07E-01	1			1.94E-05
0.0002	0.58	403.81	1.01E-12	0			

0.51	0.91	152.15	NA	0	
0.04	0.75	291.26	8.91E-04	1	
0.014 (mouse)	0.69	266.34	1.10E-05	0	2.32E-05
0.06	0.78	178.23	1.61E-02	1	
0.01	0.71	65.12	NA	0	
0.04	0.75	202.25	6.00E-04	1	
0.30	0.91	92.14	3.79E+03	1	
0.69	0.73	143.14	NA	0	
0.60	0.89	164.82	NA	0	

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Source	**Compound name**	**CAS #**	**Publications RAT**
EPA/Hamner	2,4-D	94-75-7	
EPA/Hamner	Acetochlor	34256-82-1	
EPA/Hamner	Acifluorfen	50594-66-6	
EPA/Hamner	Alachlor	15972-60-8	
EPA/Hamner	Ametryn	834-12-8	
EPA/Hamner	Bensulide	741-58-2	
EPA/Hamner	Bentazone	25057-89-0	
EPA/Hamner	Bisphenol-A	80-05-7	
EPA/Hamner	Boscalid	188425-85-6	
EPA/Hamner	Carbaryl	63-25-2	
EPA/Hamner	Chloridazon	1698-60-8	
EPA/Hamner	Chlorpropham	101-21-3	
EPA/Hamner	Cyclanilide	113136-77-9	
EPA/Hamner	Cyproconazole	94361-06-5	
EPA/Hamner	Cyprodinil	121552-61-2	
EPA/Hamner	Diazoxon	962-58-3	
EPA/Hamner	Dichlobenil	1194-65-6	
EPA/Hamner	Diethylhexyl phthalate (DEHP)	117-81-7	
EPA/Hamner	Dimethanimid	87674-68-8	
EPA/Hamner	Diphenylamine	122-39-4	
EPA/Hamner	Dithiopyr	97886-45-8	
EPA/Hamner	Diuron	330-54-1	
EPA/Hamner	Ethofumesate	26225-79-6	
EPA/Hamner	Ethoprop	13194-48-4	
EPA/Hamner	Etoxazole	153233-91-1	
EPA/Hamner	Fenarimol	60168-88-9	
EPA/Hamner	Fenbuconazole	114369-43-6	
EPA/Hamner	Fludioxonil	131341-86-1	
EPA/Hamner	Flufenacet	142459-58-3	
EPA/Hamner	Flusiazole	85509-19-9	
EPA/Hamner	Formetanate hydrochloride	23422-53-9	
EPA/Hamner	Halosulfuron-methyl	100784-20-1	
EPA/Hamner	Hexaconazole	79983-71-4	
EPA/Hamner	Imazalil	35554-44-0	
EPA/Hamner	Imidacloprid	138261-41-3	
EPA/Hamner	Isazofos	42509-80-8	
EPA/Hamner	Isoxaflutole	141112-29-0	
EPA/Hamner	Lindane	58-89-9	
EPA/Hamner	MCPA	94-74-6	
EPA/Hamner	Novaluron	116714-46-6	
EPA/Hamner	Oxadiazon	19666-30-9	
EPA/Hamner	Perfluorooctane sulfonic acid	1763-23-1	
EPA/Hamner	Perfluorooctanoic acid	335-67-1	
EPA/Hamner	Permethrin	52645-53-1	
EPA/Hamner	Propamocarb hydrochloride	25606-41-1	
EPA/Hamner	Propyzamide	23950-58-5	
EPA/Hamner	Pryrithiobac-sodium	123343-16-8	
EPA/Hamner	Pyrimethanil	53112-28-0	
EPA/Hamner	Resmethrin	10453-86-8	
EPA/Hamner	Rimsulfuron	122931-48-0	
EPA/Hamner	S-Bioallethrin	28434-00-6	
EPA/Hamner	Simazine	122-34-9	
EPA/Hamner	Tetraconazole	112281-77-3	
EPA/Hamner	Thidiazuron	51707-55-2	
EPA/Hamner	Triadimefon	43121-43-3	
EPA/Hamner	Triclosan	3380-34-5	
EPA/Hamner	Triflumizole	68694-11-1	
EPA/Hamner	Triticonazole	131983-72-7	
EPA/Hamner	Zoxamide	156052-68-5	
TNO	Acrylamide	79-06-1	
TNO	Chlorpyrifos	2921-88-2	
TNO	Warfarin	81-81-2	
TNO	Phenytoin	57-41-0	Della Paschoa (1998)
TNO	Valproic acid	99-66-1	
TNO	Diazepam	53320-84-6	Musteata (2008)
TNO	Cyclosporin A	59865-13-3	
TNO	Methoxyacetic acid	625-45-6	

Ito/Riley	Alprazolam	28981-97-7	Wang (1999)
Ito/Riley	Bosentan	147536-97-8	Horiuchi (2009); Treiber (2004)
Ito/Riley	Caffeine	58-08-2	Pelissier-Alicot (2002)
Ito/Riley	Diclofenac	64118-84-9	Leon-Reyes (2009)
Ito/Riley	Diltiazem	42399-41-7	Yeung (2009); Tsui (1994)
Ito/Riley	Hexobarbitone	56-29-1	Igari (1982)
Ito/Riley	Ibuprofen	15687-27-1	Satterwhite (1991)
Ito/Riley	Imipramine	50-49-7	Szymura-Oleksiak (1983); Okiyama (1988)
Ito/Riley	Metoprolol	37350-58-6	Boralli (2005)
Ito/Riley	Midazolam	59467-70-8	Kotegawa (2002)
Ito/Riley	Nicardipine	55985-32-5	Du (2010)
Ito/Riley	Nilvadipine	75530-68-6	Tokuma (1988)
Ito/Riley	Ondansetron	99614-02-5	Yang (2008)
Ito/Riley	Phenacetin	62-44-2	Cruz (2002)
Ito/Riley	Tolbutamide	64-77-7	Wang (2010)
ECVAM	Antipyrine	60-80-0	Aanderud (1983)
ECVAM	2,5-Hexanedione	110-13-4	Misumi (1997) Neurochem Res 22(1):27-32
ECVAM	Acetylsalicylic acid	50-78-2	Fu (1991) J Pharmacokin Biopharm 19(2):157-173
ECVAM	Acrylamide	79-06-1	Doerge (2005) Toxicol Appl Pharmacol 208:199-209
ECVAM	Benz(a)anthracene	56-55-3	Modica (1983) Toxicol Lett 18:103-109
ECVAM	Benzene	71-43-2	Haddad (2000) Toxicol Appl Pharmacol 167:199-209
ECVAM	Bisphenol A	80-05-7	Yoo (2000) J Toxicol Environ Health A 61(2):131-139
ECVAM	Carbendazim	10605-21-7	Krechniak (1986) Xenobiotica 16:809-815
ECVAM	Chlorpyrifos	2921-88-2	Timchalk (2002) Toxicol Sci 66(1):34-53; Abdel-Rahman (2002) Arch Toxicol 76(8):452-9
ECVAM	Cotinine	486-56-6	Plowchalk (1992) Toxicol Appl Pharmacol 116(2):177-88
ECVAM	Deltamethrin	52918-63-5	Anadon (1996) Toxicol Appl Pharmacol 141(1):8-16
ECVAM	Diethylene glycol	111-46-6	Heilmair (1993) Arch Toxicol 67:655-666
ECVAM	Diquat	2764-72-9	Charles (1978) Toxicol 9:59-67
ECVAM	Domoic acid	14277-97-5	Suzuki (1993) Food Chem Toxicol 31(10):701-706
ECVAM	Endosulfan	115-29-7	Chan (2005) Environ Toxicol 20:533-541
ECVAM	Flutamide	13311-84-7	Zuo (2002) J Pharm Pharmaceut Sci 5(3):292-298
ECVAM	Genistein	446-72-0	Coldham (2002) Eur J Drug Metab Pharmacokin 27(4):249-258
ECVAM	Glycidamide	5694-00-8	Doerge (2005) Toxicol Appl Pharmacol 208:199-209
ECVAM	Gossypol	303-45-7	Othman (1988) Proc Soc Exp Bio Med 188:17-22
ECVAM	Hexachlorobenzene	118-74-1	Scheufler (1984) Toxicol Appl Pharmacol 75:190-197
ECVAM	Hexachlorophene	70-30-4	Klaassen (1979) Toxicol Appl Pharmacol 49(1):113-117
ECVAM	Ketoconazole	65277-42-1	Matthew (1993) Pharmaceut Res 10(3):418-422
ECVAM	Lead acetate	6080-56-4	Timchalk (2006) Toxicol 222(1):86-94
ECVAM	Lindane	58-89-9	Tusell (1987) Arch Toxicol 60:432-437
ECVAM	Nicotine	54-11-5	Plowchalk (1992) Toxicol Appl Pharmacol 116:177-188
ECVAM	Ochratoxin A	303-47-9	Hagelberg (1989) J Appl Toxicol 9(2):91-96
ECVAM	Paraben	120-47-8	Kiwada (1980) J Pharm Dyn 3:353-363
ECVAM	Parathion	56-38-2	Eigenberg (1983) Drug Metab Dispos 11(4):366-370
ECVAM	Paraoxon		Eigenberg (1983) Drug Metab Dispos 11(4):366-370
ECVAM	Pentachlorophenol	87-86-5	Reigner (1991) Xenobiotica 21(12):1547-1558; Schmieder and Henry (1988) Comp Biochem Physiol C 91(2):413-8
ECVAM	Phenanthrene	85-01-8	Kadry (1995) Toxicol Lett 78:153-163
ECVAM	Potassium cyanide	151-50-8	Sousa (2003) Arch Toxicol 77(6):330-334
ECVAM	Pyrene	129-00-0	Withey (1991) J Toxicol Environ Health 32:429-447
ECVAM	Toluene	108-88-3	Turkall (1991) Arch Environ Contam Toxicol 20(2):155-160
ECVAM	Trimethadione	127-48-0	Tanaka (1981) J Pharm Dyn 4(8):567-583

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Carbendazim
Jia 2003
rat
0.185 kg
1000 mg/kg po

Time (h)	Plasma concentration (ug/mL)
0.25	10.0413
0.5	11.6217
1	14.695
2	20.2263
4	14.1331
8	4.58575
20	0.04945

Deltamethrin
Anadon 1996
rat
0.19 kg
26 mg/kg po
1.2 mg/kg iv

Time (h)	Plasma concentration (ug/mL)	Plasma conce (ug/mL)
0.5	0.22158	0.58879
1	0.38734	0.46480
2	0.47776	0.25905
4	0.37199	0.11404
6	0.24497	0.05020
8	0.16590	0.02273
10	0.11715	0.01773
12	0.09250	0.01568
24	0.05870	0.01095
48	0.03446	0.00491

Antipyrine
Aanderud 1983
rat
0.25 kg
15 mg/kg iv

Time (h)	Plasma conce (ug/mL)
0.5	9.83278
0.75	8.62642
1	7.54053
1.5	5.32347
2.25	3.51820
3	2.34160
4	1.40657

Alprazolam
Wang 1999

rat			
0.305	1.25	7	12.5
kg	mg/kg iv	mg/kg po	mg/kg po
Time (h)	Plasma conc (ug/mL)		
0.03333	0.79120	0.00925	0.08540
0.08333	0.37231	0.06778	0.19444
0.16667	0.21870	0.10596	0.17311
0.25	0.15776	0.07708	0.13931
0.33333	0.11576	NA	NA
0.5	0.07149	0.05681	0.08760
0.75	0.03353	NA	NA
1	0.02140	0.07774	0.05498
1.5	0.01000	0.08568	0.19230
2	0.00380	0.07074	0.22128
3	NA	0.03362	0.12686
4	NA	0.01097	0.06205
6	NA	0.00200	0.00141

Bosentan
Treiber 2004

rat		
0.275	10	1
kg	mg/kg iv	mg/kg po
Time (h)	Plasma conc (ug/mL)	
0	NA	0
0.0333	1.94796	NA
0.16667	0.32312	NA
0.33333	0.21236	NA
0.5	0.16788	NA
1	0.12833	0.62151
2	0.07886	0.60778
3	0.06131	NA
4	0.03831	0.36022
6	0.01830	0.15667
8	0.01052	0.06000
24	NA	0

Caffeine
Pelissier-Alicot 2002

rat	
0.275	25
kg	mg/kg sc
Time (h)	Plasma conc (ug/mL)
0	0.00E+00
0.25	22.9916
0.5	25.2101
1	26.8739
2	24
4	18.605
8	12.3529
12	6
24	1.21008

	Diclofenac		**Diltiazem**						**Hexobarbitone**
	Leon-Reyes 2009		*Yeung 2009*			*Tsui 1994*			*Igari 1982*
	rat		rat			rat			rat
	0.19	18	0.4	5	20	0.45	20	20	0.29
	kg	mg/kg po	kg	5x mg/kg sc	mg/kg sc	kg	mg/kg iv	mg/kg po	kg
	Time (h)	Plasma conc (ug/mL)	Time (h)	Plasma conc (ug/mL)		Time (h)	Plasma conc (ug/mL)		Time (h)
0.00E+00	0	0.03093	0	0.01878		0	13.02687	NA	0.03333
25.8151	0.04167	6.40206	1	1.13844	1.76620	0.16	7.86720	1.22225	0.41667
27.9832	0.08333	7.85567	2	0.37900	1.34419	0.25	5.05057	0.48796	0.83333
25.8655	0.125	10.1	3	0.12617	0.92978	1	2.53058	0.24830	0.16667
28.5378	0.16667	8.56701	4	0.04553	0.71735	1.5	1.51088	0.18895	0.25
23.8992	0.25	8.07216	5	0.03576	NA	2	0.95633	0.27055	0.3
15.7311	0.5	5.50515	6	0.02772	0.42122	3	0.63595	0.16028	0.5
8.92437	0.75	3.83505	8	0.01398	0.25418	4	0.20169	0.05284	0.75
1.76471	1	3.34021				6	0.06926	0.01943	1
	2	2.87629				8	0.07797	NA	1.5
	4	2.90722				10	0.02246	NA	
	6	2.19588							
	8	1.45361							

	Ibuprofen				**Imipramine**				**Metoprolol**
	Satterwhite 1991		*Satterwhite 1991*		*Szymura 1983*		*Okiyama 1988*		*Boralli 2005*
	rat		rat		rat		rat		rat
60	0.4	2.5	0.4	25	0.2	10	0.25	50	0.235
mg/kg iv	kg	mg/kg iv	kg	mg/kg iv	kg	mg/kg iv	kg	mg/kg po	kg
Plasma conc (ug/mL)	Time (h)	Plasma conc (ug/mL)	Time (h)	Plasma conc (ug/mL)	Time (h)	Plasma conc (ug/mL)	Time (h)	Plasma conc (ug/mL)	Time (h)
128.63252	0.00	16.04907	0.00	163.20370	0.05789	2.34437	0.25	0.09910	0
96.93727	0.28	7.86032	0.22	90.02850	0.12871	1.62225	0.5	0.07568	0.03333
73.74130	0.73	4.70880	0.56	60.78130	0.5	0.85333	1	0.12046	0.06667
47.32502	0.94	3.77042	0.88	26.43139	1	0.71851	2	0.07387	0.1
33.68455	1.46	2.81281	1.49	16.07941	2	0.23778	4	0.05869	0.13333
28.14108	2.45	1.62006	2.41	9.74990	4	0.04626	8	0.03861	0.16667
18.91371	3.94	1.02768	3.92	8.24556			16	0.03346	0.33333
9.94163	5.86	0.73074	5.91	4.62285			24	0.02831	0.5
6.01874	7.93	0.42342	7.85	2.50657					0.66667
3.59950	10.06	0.32695	10.09	1.52542					0.83333
	11.98	0.21726	11.94	0.77364					1
	16.14	0.05377	15.69	0.16793					1.5
									2
									2.5
									3
									4

		Midazolam			**Nicardipine**		**Nilvadipine**		
		Kotegawa 2002			*Du 2010*	** orally desin*	*Tokuma 1988*		
		rat			rat		rat	m	f
20		0.36	5	15	0.2	???	0.24; 0.18	0.1	
mg/kg po		kg	mg/kg iv	mg/kg po	kg	mg/kg po	kg	mg/kg iv	
Plasma conc		Time	Plasma conc		Time	Plasma conc			
(ug/mL)		(h)	(ug/mL)		(h)	(ug/mL)			
					????				
0	0	0.08333	2.21223	0.01292	0.08333	0.66767	0.08333	0.02924	0.02735
0.21934	0.19910	0.16667	1.07604	0.07110	0.16667	2.34586	0.25	0.01183	0.01600
0.42511	0.37970	0.25	0.96401	0.13396	0.33333	4.58346	0.5	0.00716	0.00800
0.09325	NA	0.5	0.57012	0.16279	0.5	5.70226	1	0.00350	0.00443
0.07935	0.08464	1	0.25459	0.12301	1	10.9353	2	0.00219	0.00248
0.06862	0.10782	1.5	0.12535	0.11296	2	9.92481	4	0.00082	0.00067
0.05474	0.07935	2	0.06248	0.08853	4	9.52782	6	0.00039	NA
0.05300	0.05300	3	0.01610	0.03773	6	8.46316	8	NA	NA
0.03838	0.05387	4	0.001	0.01978	8	7.18195	10	NA	NA
0.02443	0.03541				10	6.44211			
0.01388	0.02443				12	5.3594			
0.00815	0.01005				24	3.46466			
0.00661	0.01220				48	0.32481			
0.00214	0.00449								
0.00145	0.00207								
NA	0.00105								

		Ondansetron							
		Yang 2008					*Yang 2008*		
m	f	rat					rat		
10		0.26	1	4	8	20	0.26	4	8
mg/kg po		kg	mg/kg iv	mg/kg iv	mg/kg iv	mg/kg iv	kg	mg/kg po	mg/kg po
		Time (h)	Plasma conc (ug/mL)				Time (h)	Plasma conc (ug/mL)	
		0.01667	16.24651	37.11163	104.21734	174.64252	0.05	0.07004	0.1
0.03459	0.27051	0.05	0.78051	3.05000	6.28362	17.64575	0.08333	0.24356	0.24941
0.04426	0.16004	0.11667	0.42007	1.48047	3.24496	10.10369	0.16667	0.17059	0.29801
0.01465	0.07575	0.25	0.23080	0.83039	1.85806	5.55124	0.33333	0.08369	0.13778
0.01073	0.09923	0.5	0.12945	0.42883	0.95953	2.92664	0.5	0.04906	0.09203
0.00301	0.02785	0.75	0.07261	0.25590	0.59673	1.85806	0.66667	0.03962	0.07004
0.00489	0.02210	1	0.04706	0.17646	0.37886	1.25502	0.83333	0.03016	0.05793
0.00284	0.01500	1.25	0.03114	0.11203	0.24554	0.81341	1	0.02350	0.04057
0.00126	0.01217	1.5	NA	0.07567	0.17646	0.56089	1.5	NA	0.02137
		2	NA	0.03828	0.08744	0.30817	2	NA	NA
		2.5	NA	NA	0.04423	0.18390			
		3	NA	NA	0.02332	0.10104			
		4	NA	NA	NA	0.03908			

	Phenacetin		**Tolbutamide**				**Phenytoin**		
	Cruz 2002		*Wang 2010*		*Nagata 2007*		*Della Paschoa 1998*		*Kim 2008*
	rat		rat		rat		rat		rat
20	0.23	23	0.275	10	0.295	20	0.263	40	0.255
mg/kg po	kg	mg/kg iv	kg	mg/kg iv	kg	mg/kg po	kg	mg/kg iv	kg
	Time (h)	Plasma conc (ug/mL)	Time (h)	Plasma conc (ug/mL)	Time (h)	Plasma conc (ug/mL)	Time (h)	Plasma conc (ug/mL)	Time (h)
0.49059	0.04167	26.2802	0.16667	64.1638	0.25	79.1477	0.08333	54.26627	0.01667
1.11273	0.08333	24.3478	0.33333	57.0648	0.5	84.7159	0.16667	33.83997	0.83333
0.80764	0.16667	21.8357	0.66667	49.6928	1	85.9091	0.25	26.85035	0.25
0.44089	0.25	18.9372	1	43.413	2	76.3636	0.33333	23.15741	0.5
0.28758	0.5	16.1031	1.5	38.3618	4	52.8977	0.5	19.25130	0.75
0.25540	0.75	12.2383	2	33.4471	6	35.7955	0.66667	16.76370	1
0.19670	1	9.01771	3	29.3515	8	26.6477	1	14.20561	1.5
0.16462	1.5	6.63446	4	25.256	12	17.8977	1.5	11.71440	2
0.08270	2	4.31562	5	23.0717			2	8.96972	3
0.04678			6	19.5222			2.5	7.19398	4
							3	4.79394	6
							3.5	3.02173	8
							4	2.27135	10
									12

Chlorpyrifos

Timchalk 2002

rat

25 mg/kg iv	25 mg/kg po	0.24 kg	5 mg/kg po	10 mg/kg po	50 mg/kg po	100 mg/kg po
Plasma conc (ug/mL)	Plasma conc (ug/mL)	Time (h)	Plasma conc (ug/mL)			
460.69129	NA	0.08333	NA	NA	0.00056	0.00067
37.42571	NA	0.3333	NA	NA	0.00142	0.00747
21.46397	4.11735	1	0.00139	0.00505	0.05099	0.24598
15.84893	3.37473	3	0.03005	0.10925	0.32607	0.75911
12.10403	2.62183	6	0.01312	0.01866	0.07928	0.20158
8.78824	1.81608	12	0.00181	0.00176	0.01551	0.27793
4.63291	1.20153					
2.48383	0.88480					
1.49834	1.17427					
0.83083	1.12159					
NA	0.77098					
NA	0.75927					
NA	0.86472					
NA	0.49471					