

Supplementary Materials

Analysis of Distribution of Organic Compounds and Drugs between Biological Tissues in the Framework of Solute Partitioning in Aqueous Two-Phase Systems

Luisa A. Ferreira ¹, Vladimir N. Uversky ^{2,*}, Boris Y. Zaslavsky ^{1,*}

- ¹ Analiza, Inc., 3615 Superior Ave., Cleveland, OH 44114, USA; E-Mails: Luisa.ferreira@cleveland-diagnostics.com (L.A.F.); Boris.Zaslavsky@Cleveland-Diagnostics.com (B.Y.Z.)
- ² Department of Molecular Medicine and Byrd Alzheimer's Research Institute, Morsani College of Medicine, University of South Florida, Tampa, FL 33612, USA; E-Mail: vuversky@health.usf.edu
- * Authors to whom correspondence should be addressed; V.N.U. E-Mail: vuversky@health.usf.edu; Tel.: +1-813-973-5816; Fax: +1-813-974-7357; B.Y.Z. E-Mail: Boris.Zaslavsky@Cleveland-Diagnostics.com; Tel.: +1- 216-432-9050 (ext. 111); Fax: +1-216-432-9050.

Table S1. *In vitro* air-tissue and blood-tissue distributions of various compounds analyzed in this study.¹

Compound	log K (air-tissue)						log K (blood-tissue)				
	Air-Adipose	Air-Brain	Air-Liver	Air-Lung	Air-Muscle	Air-Blood	Blood-Adipose	Blood-Brain	Blood-Liver	Blood-Lung	Blood-Muscle
neon		-1.81	-	-		-2.01		0.2			
nitrous oxide	0.04	-0.31	-0.38	-0.37	-0.43	-0.34	0.38	0.03	-0.04	-0.03	-0.09
ethylbenzene	3.22		1.78		1.41	1.47	1.75		0.31		-0.06
styrene	3.52		2.14		1.67	1.67	1.85		0.47		0
radon	0.68	-0.51	-0.51	-	-0.81	-0.39	1.07	-0.12	-0.12		-0.42
m-methylstyrene	4.08		2.51		2.26	2.28	1.8		0.23		-0.02
propylbenzene						1.67					
p-xylene	3.28		1.95		1.58	1.61	1.67		0.34		-0.03
1,2-dibromoethane	3.09		2.08		1.66	2.08	1.01		0		-0.42
propyl bromide	2.37		0.91		0.62	0.97	1.4		-0.06		-0.35
butane			-	-		-0.53					
1,3-butadiene	1.35	-0.08	0.17	-0.32	-0.06	0.09	1.26	-0.17	0.08	-0.41	-0.15
1-bromo-2-chloroethane	2.98		1.63		1.40	1.60	1.38		0.03		-0.2
allyl chloride	2.00				1.04	1.24	0.76				-0.2
1,2-dichloroethane	2.54		1.55		1.37	1.39	1.15		0.16		-0.02
2-methylpentane	1.94	0.58	0.65	-0.10	0.46	-0.39	2.33	0.97	1.04	0.29	0.85
2-pentanone	2.57		2.27		2.00	2.14	0.43		0.13		-0.14
1-methoxy-2-propanol						4.09					
1-nitropropane	2.70		2.18		1.46	2.31	0.39		-0.13		-0.85
4-methyl-2-pentanone	2.72		2.19		1.81	1.96	0.76		0.23		-0.15
isopropyl acetate	2.48	1.95	2.17		1.85	1.55	0.93	0.4	0.62		0.3
m-xylene	3.29		1.96		1.62	1.59	1.7		0.37		0.03
1,3,5-trimethylbenzene						1.64					
bromobenzene						1.72					
methylcyclohexane	2.65	1.66	1.09			0.70	1.95	0.96	0.39		
toluene	2.92	1.41	1.64	1.32	1.49	1.14	1.78	0.27	0.5	0.18	0.35
chlorobenzene	3.11		1.94		1.53	1.63	1.48		0.31		-0.1
2-isopropoxyethanol						4.16					
propyl acetate	2.71	2.00	2.36		1.93	1.88	0.83	0.12	0.48		0.05
pentane	1.60	0.34	0.32	-0.3	-0.15	-0.29	1.89	0.63	0.61	-0.01	0.14

1-chlorobutane						0.63					
2-methoxyethanol						4.52					
divinyl ether	1.60	0.54	0.48		0.34	0.41	1.19	0.13	0.07		-0.07
ethyl formate						1.65					
furan	1.81		0.77			0.82	0.99		-0.05		
isobutyl acetate	3.05	2.14	2.42		2.04	1.69	1.36	0.45	0.73		0.35
2-heptanone	3.66		2.63		2.33	2.33	1.33		0.3		0
hexane	2.12	0.89	0.69	0.00	0.58	0.21	1.91	0.68	0.48	-0.21	0.37
2-ethoxyethanol						4.34					
cyclohexane	2.44		1.05	0.43	0.52	0.17	2.27		0.88	0.26	0.35
1-hexanol						3.21					
octane	2.72	1.37	1.41		0.93	0.55	2.17	0.82	0.86		0.38
1-octene	2.89	1.81	1.35			1.07	1.82	0.74	0.28		
2-butoxyethanol						3.90					
nonane	2.92	1.69				1.17	1.75	0.52			
undecane						1.31					
dodecane						1.39					
propene	0.76	-0.27	-0.28	-0.24	-0.27	-0.21	0.97	-0.06	-0.07	-0.03	-0.06
dimethyl ether						1.16					
1,1,2,4,4-pentafluorobutane						0.87					
3-methyl-1-butanol	3.18	2.79	2.97		2.90	2.75	0.43	0.04	0.22		0.15
butyl acetate	3.18	2.22	2.45		2.20	1.94	1.24	0.28	0.51		0.26
1,4-dioxane						3.27					
isopentyl acetate	3.44	2.34	2.55		2.32	1.79	1.65	0.55	0.76		0.53
1-nonene	3.24	2.04	1.71			1.18	2.06	0.86	0.53		
decane	3.05		2.09			1.17	1.88		0.92		
chlorodibromomethane	3.28		2.10		1.75	1.88	1.4		0.22		-0.13
teflurane	1.30	0.05	0.01		0.34	-0.22	1.52	0.27	0.23		0.56
2-chloro-1,3-butadiene				1.12		0.77				0.35	
tetrachloroethylene	3.21		1.85	1.86	1.30	1.19	2.02		0.66	0.67	0.11
hydrogen					-1.76	-1.77					0.01
enflurane	1.97	0.49	0.62	0.56	0.64	0.35	1.62	0.14	0.27	0.21	0.29
ethyl acetate	2.18	1.90	2.03		1.84	1.90	0.28	0	0.13		-0.06
heptane	2.51	0.94	0.96	0.40	0.85	0.50	2.01	0.44	0.46	-0.1	0.35

halothane	2.27	0.71	0.86	0.46	0.74	0.57	1.7	0.14	0.29	-0.11	0.17
cis-1,2-dichloroethene	2.36		1.18		0.78	1.16	1.2		0.02		-0.38
trans-1,2-dichloroethene	2.17		0.95		0.55	0.88	1.29		0.07		-0.33
methyl tert-butyl ether	1.97	1.54	1.35		1.57	1.18	0.79	0.36	0.17		0.39
1,1-dichloro-1-fluoroethane	1.56		0.52		0.02	0.32	1.24		0.2		-0.3
1,2,4-trimethylcyclohexane	3.19	1.89	1.54			0.87	2.32	1.02	0.67		
sulfur hexafluoride		-1.78		-2.14	-1.85	-2.17		0.39		0.03	0.32
isoflurane	1.92	0.39	0.56	0.20	0.31	0.20	1.72	0.19	0.36	0	0.11
tricyclo[5.2.1.0 _{2,6}]decane	4.01		2.74			1.76	2.25		0.98		
1-chloro-1,2,2,2-tetrafluoroethane						0.18					
sevoflurane	1.62	0.10	0.43	0.11	0.22	-0.20	1.82	0.3	0.63	0.31	0.42
cyclopentane						0.24					
cycloheptane						0.72					
allylbenzene						1.71					
2,2-dichloro-1,1,1-trifluoroethane	1.80		0.67		0.39	0.61	1.19		0.06		-0.22
t-butylcyclohexane	3.17	1.77	1.68			1.16	2.01	0.61	0.52		
2-methyloctane	2.56	1.50	1.17			0.52	2.04	0.98	0.65		
2-methylnonane	2.84					0.76	2.08				
fluoroethane						0.09					
1-chloro-2,2-difluoroethene	1.30	0.04	0.04	0.00	0.00	0.06	1.24	-0.02	-0.02	-0.06	-0.06
1,1,2,2-tetrafluoroethane						-0.12					
pentafluorobenzene						0.51					
1,2-difluorobenzene						0.96					
1,2,4-trifluorobenzene						0.76					
1,3,5-trifluorobenzene						0.49					
1,1,1,2,2,3,3,4,4-nonafluorobutane						-1.52					
1,1,2,2,3,3,4,4-octafluorobutane						-0.36					
hexafluorobenzene						0.39					
fluoroxene	1.53	0.29	0.33		0.35	0.15	1.38	0.14	0.18	--	0.2
2-fluoropropane						0.06					

1-fluoropropane						0.02					
cyanoethylene oxide	3.11		2.66			3.22	-0.11		-0.56		
fluorobenzene						1.06					
1,2,3-trimethylbenzene						1.82					
1,4-difluorobenzene						0.87					
1-chloropropane	2.07		0.71		0.32	0.59	1.48		0.12		-0.27
2,2,4-trimethylpentane	2.47		1.03		0.52	0.23	2.24		0.8		0.29
1,3-dichlorobenzene						2.30					
1-chloropentane						0.87					
carbon tetrachloride	2.56		1.15		0.66	0.62	1.94		0.53		0.04
3-methylpentan-2-one						2.23					
2,3,4-trimethylpentane	2.65		1.27		0.64	0.57	2.08		0.7		0.07
desflurane						-0.37					
1,2-dimethylcyclohexane	3.24	1.98	1.74			0.91	2.33	1.07	0.83		
2-methylcyclohexanone						2.87					
3-methylhexane	2.44	1.01	1.04		1.04	0.11	2.33	0.9	0.93		0.93
2-hexanone						2.10					
2-methylheptane	2.30	1.35	0.75			0.49	1.81	0.86	0.26		
vinyl bromide	1.69		0.52		0.35	0.49	1.2		0.03		-0.14
fluorochloromethane	1.19		0.54		0.39	0.71	0.48		-0.17		-0.32
diethyl ether	1.74	1.10	0.94	1.14	0.87	1.11	0.63	-0.01	-0.17	0.03	-0.24
p-methylstyrene	4.05		2.51		2.26	2.37	1.68		0.14		-0.11
pentyl acetate	3.57	2.38	2.64		2.36	1.98	1.59	0.4	0.66		0.38
carbon monoxide				-1.69		-1.67				-0.02	
1,1,1,2-tetrachloroethane	3.33		1.95		1.60	1.55	1.78		0.4		0.05
ethyl tert-butyl ether	2.13	1.29	1.52		1.35	1.07	1.06	0.22	0.45		0.28
ethanol	2.34	3.15		3.07	3.08	3.27	-0.93	-0.12		-0.2	-0.19
methanol	2.33			3.24		3.41	-1.08			-0.17	
2-propanol	2.35	2.91	2.99	2.77	2.87	3.02	-0.67	-0.11	-0.03	-0.25	-0.15
propanone	1.91	2.19	2.38	2.20	2.21	2.36	-0.45	-0.17	0.02	-0.16	-0.15
chloroform	2.38	1.30	1.28	1.12	1.12	1.15	1.23	0.15	0.13	-0.03	-0.03
hexachloroethane	3.52		2.57		1.88	1.76	1.76		0.81		0.12
halopropane	2.35					0.75	1.6				
1,1,2,2,3-pentafluoropropane						-0.48					

1-propanol	2.54	2.98	3.11	2.91	2.95	3.06	-0.52	-0.08	0.05	-0.15	-0.11
1-butanol	2.95	3.06	3.10		2.95	3.08	-0.13	-0.02	0.02		-0.13
1-pentanol	3.41	3.03	3.24		2.91	2.83	0.58	0.2	0.41		0.08
benzene	2.64	1.25	1.26	1.08	1.11	1.05	1.59	0.2	0.21	0.03	0.06
1,1,1-trichloroethane	2.41	0.92	1.07	0.67	0.67	0.63	1.78	0.29	0.44	0.04	0.04
krypton	-0.48	-1.38	-1.14		-1.38	-1.22	0.74	-0.16	0.08		-0.16
argon		-1.49			-1.64	-1.52		0.03			-0.12
helium				-1.98	-1.93	-2.00				0.02	0.07
xenon	0.26	-0.70	-1.00		-1.00	-0.85	1.11	0.15	-0.15		-0.15
methane		-1.39			-1.41	-1.42		0.03			0.01
ethane				-1.28		-1.02				-0.26	
Ethene	0.20	-0.23	-0.30	-0.25	-0.20	-0.53	0.73	0.3	0.23	0.28	0.33
acetylene				-0.06	0.03	-0.06				0	0.09
methyl chloride	1.13		0.54		-0.01	0.31	0.82		0.23		-0.32
dibromomethane	2.90		1.83		1.61	1.87	1.03		-0.04		-0.26
bromochloromethane	2.51		1.47		1.05	1.21	1.3		0.26		-0.16
chloroethane	1.59		0.56		0.51	0.49	1.1		0.07		0.02
vinyl chloride	1.30		0.20		0.32	0.17	1.13		0.03		0.15
iodoethane						0.83					
dichloromethane	2.01	0.78	1.01	0.76	0.79	1.12	0.89	-0.34	-0.11	-0.36	-0.33
difluoromethane	0.16		0.44		0.16	0.20	-0.04		0.24		-0.04
carbon disulfide		0.90	0.78			0.30		0.6	0.48		
cyclopropane	0.99	-0.10	-0.19	-0.51	-0.31	-0.21	1.2	0.11	0.02	-0.3	-0.1
ethylene oxide	1.64	1.81	1.73	1.79	1.75	1.80	-0.16	0.01	-0.07	-0.01	-0.05
tribromomethane						2.15					
isopropyl bromide	2.20		0.64		0.61	0.64	1.56		0		-0.03
bromodichloromethane	2.72		1.49			1.49	1.23		0		--
2-chloropropane	1.84		0.50		0.31	0.32	1.52		0.18		-0.01
1,1-dichloroethane	2.21		1.03		0.71	0.88	1.33		0.15		-0.17
1,1-dichloroethylene	1.84		0.65		0.31	0.70	1.14		-0.05		-0.39
1,1-difluoroethane						0.42					
1,1-difluoroethene	-0.10		-0.10		-0.54	-0.74	0.64		0.64		0.2
propylene oxide						1.80					
2-methyl-2-propanol	2.20	2.79	2.69		2.80	2.68	-0.48	0.11	0.01		0.12
fluorotrichloromethane						-0.06					

difluorodichloromethane						-0.82						
carbon tetrafluoride						-1.10						
2,2-dimethylbutane	1.82	0.45	0.54	-0.22	0.00	-0.59	2.41	1.04	1.13	0.37	0.59	
tert-amyl alcohol	2.66	2.66	2.68		2.59	2.59	0.07	0.07	0.09		0	
2-chloro-1,1,1-trifluoroethane	1.43	0.26	0.31	0.34	0.22	0.14	1.29	0.12	0.17	0.2	0.08	
1,1,1,2,3,3,4,4,4-octafluorobutane						-0.59						
pentachloroethane	3.61		2.41		1.86	2.02	1.59		0.39			-0.16
1,2-dichlorotetrafluoroethane						-0.82						
methoxyflurane	2.90	1.40	1.47	1.20	1.35	1.28	1.62	0.12	0.19	-0.08	0.07	
2,3,4,5,6-pentafluorotoluene						0.73						
nitrogen	-1.27	-1.80				-1.83	0.56	0.03				
oxygen				-1.62		-1.58				-0.04		
isophorone						3.37						
2-methyl-1,3-butadiene	1.84		0.42		0.26	0.10	1.74		0.32		0.16	
2-methyl-1-propanol	2.73	2.78	2.94	2.60	2.74	2.92	-0.19	-0.14	0.02	-0.32	-0.18	
1,2-dichloropropane	2.70		1.39		1.08	1.14	1.56		0.25		-0.06	
butan-2-one	2.26	2.07	2.36	2.01	2.14	2.24	0.02	-0.17	0.12	-0.23	-0.1	
1,1,2-trichloroethane	3.16		1.86		1.36	1.67	1.49		0.19		-0.31	
trichloroethene	2.75	1.25	1.41	1.15	1.13	1.14	1.61	0.11	0.27	0.01	-0.01	
methyl acetate	2.00	1.85	1.95		1.81	1.98	0.02	-0.13	-0.03		-0.17	
2,3-dimethylbutane						0.78						
1,1,2,2-tetrachloroethane	3.58		2.29		2.00	2.13	1.45		0.16		-0.13	
2-nitropropane	2.19		1.80		1.46	2.23	-0.04		-0.43		-0.77	
1,1,1,2-tetrafluoroethane						-0.25						
2-methylnonane		1.81	1.45									
1-decene	3.36	2.17	1.98			1.21	2.15	0.96	0.77			
ethyl tert-pentyl ether						1.25						
1,2-epoxy-3-butene	2.23		1.74		1.66	1.97	0.26		-0.23		-0.31	
o-xylene	3.20	1.39	1.76	1.94	1.71	1.42	1.78	-0.03	0.34	0.52	0.29	
1,2-dichlorobenzene						2.63						
1,2,4-trimethylbenzene	3.25	1.63	2.20			1.85	1.4	-0.22	0.35			
3-methylpentane	2.01	0.64	0.69	-0.05	0.58	-0.37	2.38	1.01	1.06	0.32	0.95	

1,2,3-trichloropropane						2.01					
3-pentanone						2.21					
methylcyclopentane	2.25	0.86	0.89	0.23	0.70	-0.07	2.32	0.93	0.96	0.3	0.77
tert-butylbenzene	3.26	1.67	2.32			1.24	2.02	0.43	1.08		
4-chlorobenzotrifluoride	2.99	1.60	1.71	1.63		1.43	1.56	0.17	0.28	0.2	
isopropylbenzene						1.57					
tert-amyl methyl ether	2.52	1.39	1.50		1.38	1.22	1.3	0.17	0.28		0.16
neon		-1.81	-	-		-2.01		0.2			
nitrous oxide	0.04	-0.31	-0.38	-0.37	-0.43	-0.34	0.38	0.03	-0.04	-0.03	-0.09
ethylbenzene	3.22		1.78		1.41	1.47	1.75		0.31		-0.06
styrene	3.52		2.14		1.67	1.67	1.85		0.47		0
radon	0.68	-0.51	-0.51	-	-0.81	-0.39	1.07	-0.12	-0.12		-0.42
m-methylstyrene	4.08		2.51		2.26	2.28	1.8		0.23		-0.02
propylbenzene						1.67					
p-xylene	3.28		1.95		1.58	1.61	1.67		0.34		-0.03

Table S2. *In vivo* tissue-blood distribution of drugs in rat analyzed in this study.²

Drug	Rat tissue-blood distribution of drugs <i>in vivo</i>													
	Muscle	Bone	Brain	Heart	Intestine	Skin	Lungs	Spleen	Adipose	Liver	Kidney	Stomach	Pancreas	log P
5-butyl-5-ethyl barbituric acid	-0.0706		-0.0655	0.0128	-8.77E-03	-0.1079	-0.102	-0.2366	-0.0132	0.1931	0.3784	-0.0362	-0.3188	
5-heptyl-5-ethyl barbituric acid	0.1818		0.0864	0.1492	0.1038	0.2068	0.045	0.0453	0.7959	0.4249	0.3263	0.4857	0.2068	
5-hexyl-5-ethyl barbituric acid	0.2553		0.2455	0.2279	0.2068	0.3444	0.033	0	0.8859	0.525	0.356	0.4786	0.2068	
5-methyl-5-ethyl barbituric acid	-0.1427		-0.2007	-0.1612	-0.2366	-0.0862	-0.131	-0.1938	-0.6021	0.1959	0.1038	-0.585	-0.3098	
5-nonyl-5-ethyl barbituric acid	0.0899		0.42	0.0828	0.3222	0.5775	0.554	0.4983	0.8627	0.6758	0.3139	0.5478	0.4609	
5-octyl-5-ethyl barbituric acid	0.0453		0.3444	0.1761	0.1673	0.5145	0.528	0.3032	0.7882	0.7284	0.444	0.2788	0.4116	
5-pentyl-5-ethyl barbituric acid	0.0414		-0.1612	0.0294	-0.0506	-0.1427	-0.119	-0.2441	0.2304	0.2095	0.2279	0.017	-0.1192	
5-propyl-5-ethyl barbituric acid	0.0969		-0.0223	4.32E-03	-0.0757	0.0334	0.053	-0.0809	-0.0605	0.29	0.4713	-0.2076	-0.1612	
Acebutolol	0.6513		-0.4089	0.6758	1.933	0.415	0.89		-0.0757	1.4265	1.4314			1.53
Alfentanyl	-0.2924	-1.3979	-0.6383	-0.041	0.601	-0.4685	0.111	0.1335	0.5988	0.2742	0.1903		0.2553	2.81
Alprazolam	0.3385		0.1987		0.1399	0.281			4.32E-03	0.8463	0.4249			3.02
Barbital	-0.0862		-0.1739	-0.1367	-0.2291	-0.0809	-0.071	-0.1938	-0.3468	0.3385	0.2279	-0.5528	-0.3279	1.45
Betaxolol	0.8376		0.8156	1.0531	1.2923	0.4997	1.988		0.1644	1.7796	1.4533			2.54
Biperiden	0.5224	0.8169	0.8382	0.8463	1.017	0.5809	1.753		1.7796		1.0086			3.54
Bisoprolol	0.5933	0.2923	0.0969	0.683	1.281	0.2068	1.489		-0.1249	1.2253	1.2601			2.2
Carvedilol	0.1206	0.5328		0.7853				0.8222		0.932	0.716			3.42
Cefazolin	-0.6576			-0.7212	-0.4089	-0.2007	-0.377			0.2788	0.8267			1.52
Ceftazidime	-0.7212	-0.6383		-0.6576	-0.3872	-0.4089	-0.357		-0.7959	-0.6021	0.6884			-4.55
Chlordiazepoxide	-0.2596		-0.2757	0.2718	0.1492	-0.4685			0.49	0.5416	0.2878			0.03
Cisapride			0.1461	0.238			0.988			1.1875	0.8189			2.49
Cotinine	-0.1612		-0.3468	-0.2924	-0.2218		-0.237		-1.0969	-0.1938	-4.36E-03			0.21
Decane	0.7202		1.0334						1.4216	1.0334				4.91
Deltamethrin	1.5159		0.1106		0.4116				2.4579	0.4116				5.74
Diazepam	0.3541		0.3096	0.6937	0.5911	0.7332	0.66		1.415	0.7966	0.6618			3.08
Dicloxacillin	-1.301			-1.1549			-0.921	-1.0458						2.91
Dideoxyinosine	-0.1612		-0.7696		-0.2924			-0.1739		-0.1192	0.8357		-0.1487	0.04
Digoxin	0.0828			0.2068	0.7543		0.303			1.1644	0.2967			2.37
Domperidone	0.4298		-1.0458	0.48			0.901			1.0294	1.243			4.25
Enoxacin	0.1875			0.0531		0.1584	0.083	0.238		0.5328	0.6902			-0.98
Etodolac		0.1847	-1.0458	-0.1938					-0.6198	-0.301	-0.3188			3.44

Fentanyl	0.5635		0.6212	0.7275	1.0128	0.4116	1.204	1.534	1.5198	0.6532	1.1553		1.4216	3.82
Fingolimod	1.0212		1.692	1.2405			1.834	1.7931		1.6721	1.5539			4.06
Fleroxacin	0.1903			0.2945			0.22							1.12
Flunitrazepam	-0.1192	-0.0315	0.1367	-0.0223	0.601				1.7723	0.48	-0.4815			2.55
Ftorafur	-0.0458		-0.1367	-0.1612	-0.1871	-0.1427	-0.337	-0.1192	-0.5086	-0.1549	0.0899		-0.4437	0.02
Galanthamine	0.3118		0.1614							0.3856	1.1239			1.16
Glycyrrhetic acid	-0.7447		-1.1549	-0.6778			-0.5376	-0.398	-0.8861					6.03
Glycyrrhizin	-1			-1.3979			-0.5528	-1						3.13
Hexobarbital	-0.1024			0.1139	0.1523	-0.0362	0.449		0.2148	0.7752	0.179			1.25
Imipramine	0.7218		1.1038	1.1173	1.1461			1.883	1.5353	0.7987	1.4914	1.4362	1.4166	4.28
Inaperisone	0.3385		0.8156	0.5944			0.525	1.248		0.9159	1.2553	1.4886		3.57
Laniquidar	0.9513		0.5587	0.8669				1.689			1.3263	1.179		6.28
Lidocaine	0.1206		0.4065	0.3304	0.3892	0.3075	0.476	0.5763		0.9571	2.1303			0.92
Lomefloxacin	0.2253	0.2148	-0.6576	0.1523	0.2279	-0.0132	0.111	0.2553	-0.5686	0.3784	0.7024			-0.39
Lorcainide	0.3711		0.1004	0.382				1.207			-0.3279	0.6739		4.31
Lubeluzole	0.4281		0.7348					1.377			1.5611	1.1139		4.23
Matrine	0.1271		0.3139	0.1875	0.49		0.188	0.8122	-0.3372	0.7536	1.0128			1.08
Metoprolol	0.5682	0.5391	0.6464	0.6365	0.902	0.3032	1.236		-0.1805	1.4456	1.2455			1.76
Midazolam	0.1139		0.4757	0.4814	0.4829	0.4249	0.513	0.3692	0.776	1.0531	0.5079	0.4871		3.97
Miloxacin			-0.9208					-0.292	-0.4815					1.15
Molinate	0.6201								2.2504	1.1492				1.89
Nalidixic acid	-0.4559	-0.5528	-0.6778	-0.3188	-0.3188	-0.4685	-0.495	-0.4815	-1.0458	-0.2441	-0.2757			1.01
Nebivolol	0.3617		0.4639	0.5647				1.891		1.0414	0.918			3.21
Nicotine	0.2175		0.4378	0.2355	0.301	0.1072	0.243		-0.3279	0.6821	1.2504			1.16
o-Ethoxybenzamide	-0.1024		-0.0269	0	-0.2441	4.32E-03	-0.036	-0.0655	-0.1549		0.1106			1.02
Ofloxacin	0.2695	0.1875	-0.6021	0.2856			0.1106	0.167	0.3201	-0.699	0.3444	0.8414		0.65
Oxprenolol	0.6551	0.4409	0.3747	0.7218	1.2095	0.3032	1.384		-0.0809	1.1303	1.3139			2.17
Pefloxacin	0.4099		-0.7696	0.3979				0.314	0.5599		0.7543	0.6425		0.88
Penicillin	-0.9586			-0.7696	0.243			-0.553	-0.7696		-0.3468	0.828		1.08
Pentazocine	0.6149	0.5798	0.4829	0.5798	0.5119	0.5119	1.279			0.2405	0.243	1.1818		3.89
Perchloroethylene	0.2648		0.4728							2.0719	0.4099	0.3802		2.62
Phencyclidine	0.1303		0.3598	0.29				1.562		1.7396	0.8555	1.0212		4.49
Phenobarbital	-0.0862			-0.0915	0.1072	4.32E-03	-0.201		-0.6383	0.1818	-0.2147			2.14
Phenytoin	-0.0969		-0.1427	-0.0969	0.1903	0.0414	-0.125		0.2175	0.3579	0.1987			3.4
Pindolol	0.7745	0.29	0.5944	0.9652	1.243	0.3324	1.393		-0.2218	0.9455	1.49			1.69
Pipemidic acid	0.1461	0.3784	-0.8861	0				0.068	0.1875	-0.4437	0.6893	0.8965		-1.77
p-Phenylbenzoic acid	-0.8539		-1	-0.3872	-0.5686	-0.5686	-0.301	-0.7447						3.28
Procainamide	0.49			0.3909					-0.9208	0.5011	0.8028			0.95
Propranolol	0.6628	0.6739	1.238	0.9657	1.2833	0.5623	1.762		0.2989	1.29	1.1303			2.58
Prucalopride	0.4771		-0.5528	0.4502				0.843			0.7604	1.0607		0.74
Pseudocumene	0.0828		0.4031							1.7973	0.4031			3.51
Quinidine	0.4857		-0.1938	0.617	0.8579			1.486	1.2304		1.0682	1.1673		2.51
Ritanserin	0.6075		0.4698					1.508			1.3979	1.1492		5.31

Sabeluzole			0.8055				1.54			1.6513	1.0899			4.09
Salicylic acid	-0.6021	-0.585	-1.0458	-0.4685	-0.4202	-0.3098	-0.456			-0.3768	-0.0915			1.98
Styrene	-0.0655						-0.194		1.6117	0.0719				2.71
Sufentanyl	0.3927		0.4771	0.415			0.951			-0.1739	0.2279			3.61
Tenoxicam	-1.0969	-1	-2	-0.7447	-0.699	-0.8239	-0.509	-1.1549	-1.5229	0.0607	0.017		-0.9208	1.22
Tetracycline	0.301	0.9504			0.574				0.0414	0.6721	0.6075			-3.47
Theophylline	-0.2147		-0.4437				-0.143							-0.81
Thiopental	-0.1427		-0.1308	0.0792	0.1335	0.1492	0.124	-0.2147	0.8169	0.5302	0.4133		0.0253	2.78
Timolol	0.5763	-0.0458	-0.0177	0.6866	1.2625	0.1553	1.389		-0.2366	0.8579	1.0828			1.34
Tolbutamide	-0.8239		-0.9586	-0.4815	-0.8539	-0.5528	-0.482	-0.6576	-0.8539	-0.7696	-0.7959		-0.7447	3.11
Triazolam	0.6064				0.902	0.5635			0.6064	0.3997	0.752			3.63
Valproic acid	-0.6778		-0.4685	-0.2366	-0.2147	-0.1938	-0.244		-0.699	0.3909	0.3118			2.8
Verapamil	0.6138			0.8482			1.769				1.1673			5.04
Zearalenone	-0.3665		0.0253	0.0645	1.5775		0.364	-0.0915	0.5198	0.659	-0.2596	0.1139		4.37
5-butyl-5-ethyl barbituric acid	-0.0706		-0.0655	0.0128	-8.77E-03	-0.1079	-0.102	-0.2366	-0.0132	0.1931	0.3784	-0.0362	-0.3188	
5-heptyl-5-ethyl barbituric acid	0.1818		0.0864	0.1492	0.1038	0.2068	0.045	0.0453	0.7959	0.4249	0.3263	0.4857	0.2068	
5-hexyl-5-ethyl barbituric acid	0.2553		0.2455	0.2279	0.2068	0.3444	0.033	0	0.8859	0.525	0.356	0.4786	0.2068	
5-methyl-5-ethyl barbituric acid	-0.1427		-0.2007	-0.1612	-0.2366	-0.0862	-0.131	-0.1938	-0.6021	0.1959	0.1038	-0.585	-0.3098	
5-nonyl-5-ethyl barbituric acid	0.0899		0.42	0.0828	0.3222	0.5775	0.554	0.4983	0.8627	0.6758	0.3139	0.5478	0.4609	
5-octyl-5-ethyl barbituric acid	0.0453		0.3444	0.1761	0.1673	0.5145	0.528	0.3032	0.7882	0.7284	0.444	0.2788	0.4116	
5-pentyl-5-ethyl barbituric acid	0.0414		-0.1612	0.0294	-0.0506	-0.1427	-0.119	-0.2441	0.2304	0.2095	0.2279	0.017	-0.1192	
5-propyl-5-ethyl barbituric acid	0.0969		-0.0223	4.32E-03	-0.0757	0.0334	0.053	-0.0809	-0.0605	0.29	0.4713	-0.2076	-0.1612	
Acebutolol	0.6513		-0.4089	0.6758	1.933	0.415	0.89		-0.0757	1.4265	1.4314			1.53
Alfentanyl	-0.2924	-1.3979	-0.6383	-0.041	0.601	-0.4685	0.111	0.1335	0.5988	0.2742	0.1903		0.2553	2.81
Alprazolam	0.3385		0.1987		0.1399	0.281			4.32E-03	0.8463	0.4249			3.02
Barbital	-0.0862		-0.1739	-0.1367	-0.2291	-0.0809	-0.071	-0.1938	-0.3468	0.3385	0.2279	-0.5528	-0.3279	1.45
Betaxolol	0.8376		0.8156	1.0531	1.2923	0.4997	1.988		0.1644	1.7796	1.4533			2.54
Biperiden	0.5224	0.8169	0.8382	0.8463	1.017	0.5809	1.753		1.7796		1.0086			3.54
Bisoprolol	0.5933	0.2923	0.0969	0.683	1.281	0.2068	1.489		-0.1249	1.2253	1.2601			2.2
Carvedilol	0.1206	0.5328		0.7853				0.8222		0.932	0.716			3.42
Cefazolin	-0.6576			-0.7212	-0.4089	-0.2007	-0.377			0.2788	0.8267			1.52
Ceftazidime	-0.7212	-0.6383		-0.6576	-0.3872	-0.4089	-0.357		-0.7959	-0.6021	0.6884			-4.55
Chlordiazepoxide	-0.2596		-0.2757	0.2718	0.1492	-0.4685			0.49	0.5416	0.2878			0.03
Cisapride			0.1461	0.238			0.988			1.1875	0.8189			2.49
Cotinine	-0.1612		-0.3468	-0.2924	-0.2218		-0.237		-1.0969	-0.1938	-4.36E-03			0.21

Decane	0.7202		1.0334						1.4216	1.0334			4.91
Deltamethrin	1.5159		0.1106		0.4116				2.4579	0.4116			5.74
Diazepam	0.3541		0.3096	0.6937	0.5911	0.7332	0.66		1.415	0.7966	0.6618		3.08
Dicloxacillin	-1.301			-1.1549			-0.921	-1.0458					2.91
Dideoxyinosine	-0.1612		-0.7696		-0.2924			-0.1739		-0.1192	0.8357	-0.1487	0.04
Digoxin	0.0828			0.2068	0.7543		0.303			1.1644	0.2967		2.37
Domperidone	0.4298		-1.0458	0.48			0.901			1.0294	1.243		4.25
Enoxacin	0.1875			0.0531		0.1584	0.083	0.238		0.5328	0.6902		-0.98
Etodolac		0.1847	-1.0458	-0.1938					-0.6198	-0.301	-0.3188		3.44
Fentanyl	0.5635		0.6212	0.7275	1.0128	0.4116	1.204	1.534	1.5198	0.6532	1.1553	1.4216	3.82
Fingolimod	1.0212		1.692	1.2405			1.834	1.7931		1.6721	1.5539		4.06
Fleroxacin	0.1903			0.2945			0.22						1.12
Flunitrazepam	-0.1192	-0.0315	0.1367	-0.0223	0.601				1.7723	0.48	-0.4815		2.55
Ftorafur	-0.0458		-0.1367	-0.1612	-0.1871	-0.1427	-0.337	-0.1192	-0.5086	-0.1549	0.0899	-0.4437	0.02
Galanthamine	0.3118		0.1614							0.3856	1.1239		1.16
Glycyrrhetic acid	-0.7447		-1.1549	-0.6778			-0.5376	-0.398	-0.8861				6.03
Glycyrrhizin	-1			-1.3979			-0.5528	-1					3.13
Hexobarbital	-0.1024			0.1139	0.1523	-0.0362	0.449		0.2148	0.7752	0.179		1.25
Imipramine	0.7218		1.1038	1.1173	1.1461		1.883	1.5353	0.7987	1.4914	1.4362	1.4166	4.28
Inaperisone	0.3385		0.8156	0.5944		0.525	1.248		0.9159	1.2553	1.4886		3.57
Laniquidar	0.9513		0.5587	0.8669			1.689			1.3263	1.179		6.28
Lidocaine	0.1206		0.4065	0.3304	0.3892	0.3075	0.476	0.5763		0.9571	2.1303		0.92
Lomefloxacin	0.2253	0.2148	-0.6576	0.1523	0.2279	-0.0132	0.111	0.2553	-0.5686	0.3784	0.7024		-0.39
Lorcainide	0.3711		0.1004	0.382			1.207			-0.3279	0.6739		4.31
Lubeluzole	0.4281		0.7348				1.377			1.5611	1.1139		4.23
Matrine	0.1271		0.3139	0.1875	0.49		0.188	0.8122	-0.3372	0.7536	1.0128		1.08
Metoprolol	0.5682	0.5391	0.6464	0.6365	0.902	0.3032	1.236		-0.1805	1.4456	1.2455		1.76
Midazolam	0.1139		0.4757	0.4814	0.4829	0.4249	0.513	0.3692	0.776	1.0531	0.5079	0.4871	3.97
Miloxacin			-0.9208				-0.292	-0.4815					1.15
Molinate	0.6201								2.2504	1.1492			1.89
Nalidixic acid	-0.4559	-0.5528	-0.6778	-0.3188	-0.3188	-0.4685	-0.495	-0.4815	-1.0458	-0.2441	-0.2757		1.01
Nebivolol	0.3617		0.4639	0.5647			1.891			1.0414	0.918		3.21
Nicotine	0.2175		0.4378	0.2355	0.301	0.1072	0.243		-0.3279	0.6821	1.2504		1.16
o-Ethoxybenzamide	-0.1024		-0.0269	0	-0.2441	4.32E-03	-0.036	-0.0655	-0.1549		0.1106		1.02
Ofloxacin	0.2695	0.1875	-0.6021	0.2856			0.1106	0.167	0.3201	-0.699	0.3444	0.8414	0.65
Oxprenolol	0.6551	0.4409	0.3747	0.7218	1.2095	0.3032	1.384		-0.0809	1.1303	1.3139		2.17
Pefloxacin	0.4099		-0.7696	0.3979			0.314	0.5599		0.7543	0.6425		0.88
Penicillin	-0.9586			-0.7696	0.243		-0.553	-0.7696		-0.3468	0.828		1.08
Pentacocine	0.6149	0.5798	0.4829	0.5798	0.5119	0.5119	1.279		0.2405	0.243	1.1818		3.89
Perchloroethylene	0.2648		0.4728						2.0719	0.4099	0.3802		2.62
Phencyclidine	0.1303		0.3598	0.29			1.562		1.7396	0.8555	1.0212		4.49
Phenobarbital	-0.0862			-0.0915	0.1072	4.32E-03	-0.201		-0.6383	0.1818	-0.2147		2.14
Phenytoin	-0.0969		-0.1427	-0.0969	0.1903	0.0414	-0.125		0.2175	0.3579	0.1987		3.4

Pindolol	0.7745	0.29	0.5944	0.9652	1.243	0.3324	1.393		-0.2218	0.9455	1.49			1.69
Pipemidic acid	0.1461	0.3784	-0.8861	0			0.068	0.1875	-0.4437	0.6893	0.8965			-1.77
p-Phenylbenzoic acid	-0.8539		-1	-0.3872	-0.5686	-0.5686	-0.301	-0.7447						3.28
Procainamide	0.49			0.3909					-0.9208	0.5011	0.8028			0.95
Propranolol	0.6628	0.6739	1.238	0.9657	1.2833	0.5623	1.762		0.2989	1.29	1.1303			2.58
Prucalopride	0.4771		-0.5528	0.4502			0.843			0.7604	1.0607			0.74
Pseudocumene	0.0828		0.4031						1.7973	0.4031				3.51
Quinidine	0.4857		-0.1938	0.617	0.8579		1.486	1.2304		1.0682	1.1673			2.51
Ritanserin	0.6075		0.4698				1.508			1.3979	1.1492			5.31
Sabeluzole			0.8055				1.54			1.6513	1.0899			4.09
Salicylic acid	-0.6021	-0.585	-1.0458	-0.4685	-0.4202	-0.3098	-0.456			-0.3768	-0.0915			1.98
Styrene	-0.0655						-0.194		1.6117	0.0719				2.71
Sufentanyl	0.3927		0.4771	0.415			0.951			-0.1739	0.2279			3.61
Tenoxicam	-1.0969	-1	-2	-0.7447	-0.699	-0.8239	-0.509	-1.1549	-1.5229	0.0607	0.017		-0.9208	1.22
Tetracycline	0.301	0.9504			0.574				0.0414	0.6721	0.6075			-3.47
Theophylline	-0.2147		-0.4437				-0.143							-0.81
Thiopental	-0.1427		-0.1308	0.0792	0.1335	0.1492	0.124	-0.2147	0.8169	0.5302	0.4133		0.0253	2.78
Timolol	0.5763	-0.0458	-0.0177	0.6866	1.2625	0.1553	1.389		-0.2366	0.8579	1.0828			1.34
Tolbutamide	-0.8239		-0.9586	-0.4815	-0.8539	-0.5528	-0.482	-0.6576	-0.8539	-0.7696	-0.7959		-0.7447	3.11
Triazolam	0.6064				0.902	0.5635			0.6064	0.3997	0.752			3.63
Valproic acid	-0.6778		-0.4685	-0.2366	-0.2147	-0.1938	-0.244		-0.699	0.3909	0.3118			2.8
Verapamil	0.6138			0.8482			1.769				1.1673			5.04

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