Supplemental information

for:

Using membrane-water partition coefficients in a critical membrane burden approach to aid the identification of neutral and ionizable chemicals that induce acute toxicity below narcosis levels

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SI section S1

Using IAM-HPLC for ionizable chemicals: accounting for confounding electrostatic attraction/repulsion

IAM-HPLC has become a commonly applied method for these research fields - the combined keywords "immobilized artificial membrane" results in 330 hits on the peer-reviewed literature and citation database Scopus (June 2019). Liposomal partition coefficients (K_{lipw}, or membrane-water partition coefficients K_{MW}) may be considered of higher relevance for extrapolation to actual cells than HPLC retention times, as they represent fluid phospholipid bilayers whereas IAM-HPLC applies immobilized phospholipid monolayers. However, liposomal partition assays are more cumbersome and costly than chromatographic studies and often lack the level of intra- and inter-laboratory consistency of IAM-HPLC data.

Recent studies have focused on deriving K_{IAM} values for ionogenic chemicals that under physiological pH are largely ionized, such as cationic and anionic surfactants.[1-6] The way phospholipids are coated to silica particles does present confounding pH-dependent surface charges on the column particles that influence the retention behavior of ionized chemicals. The silica particles contain acidic silanol groups, to which first aminopropyl anchors are bound. Phospholipids are covalently bound to propylamine anchors. As a result of the normal process of column particle manufacturing, a substantial fraction of both basic aminopropyl silica and acidic free silanol groups will reside on the IAM surface, even after end-capping.[7-11] At low pH, silanol groups are protonated and neutral, while protonated propylamine groups result in a positively charge on the sorbent's surface. At higher pH, the silanol acids dissociate and counter balance the positive charge, until at a certain pH more acidic groups than protonated propylamines result in a negative surface charge. The surface charge prevailing in an eluent buffer of a certain pH will result in confounding attraction of oppositely charged chemicals, and confounding repulsion of similarly charged chemicals. This causes an additional factor on retention time for ionic chemicals which is not related to interaction with the phospholipid coating itself. Moreover, the confounding attraction/repulsion is influenced by the ionic strength of the eluent, i.e., higher effects at lower ionic strength. These confounding electrostatic effects can be circumvented experimentally, e.g. by measuring at the eluent pH where the IAM surface is net neutral (pH 5.5-6 in Figure S1 where the ionic strength of the eluent has negligible influence on retention), and therefore the confounding attraction/repulsion for ionic chemicals is negligible and retention is only influenced by sorption to phospholipid. Since the confounding attraction/repulsion is equal for all monovalent organic ions, a (set of) reference chemical(s) can be used to adjust the confounding effect at a certain

aqueous eluent composition (pH + ionic strength) using empirical Boltzmann factors (magnitude of the green arrows in Figure S1).[3, 6]

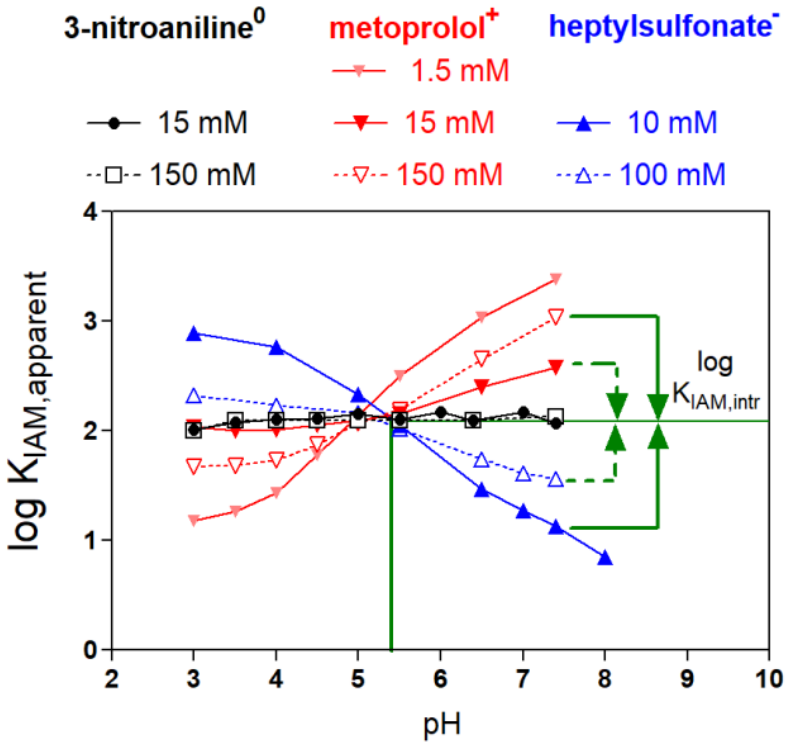


Figure S1. Apparent IAM-HPLC partition coefficients ($K_{IAM,apparent}$) as a function of aqueous eluent pH and ionic strength

For the neutral chemical 3-nitroaniline (black symbols, data from ref[3]), a largely protonated chemical metoprolol (pKa 9.5, red symbols, data from ref[3]) and the fully anionic chemical heptylsulfonate (blue symbols, data from ref[2]). These three reference compounds have nearly similar *intrinsic* IAM-HPLC partition coefficients ($K_{IAM,intr.}$), but at for example pH 7.4 can differ in their $K_{IAM,apparent}$) by more than 2 orders of magnitude. Lines connect consecutive pH. $K_{IAM,intr.}$ is determined directly for these ionized chemicals as the partition ratio at the eluent pH at which ionic strength has no effect on retention, i.e., where the IAM particles' surface charge is net neutral, which in these IAM-HPLC columns was determined to be pH5 - 5.5. It should be noted that this may be column/batch specific and needs to be pre-determined with reference chemicals. Alternatively, $K_{IAM,intr.}$ can be derived indirectly from measurements at for example to commonly used pH 7.4, and then accounting for the appropriate Boltzmann correction factor for the eluent composition (pH and ionic strength), indicated by green arrows.

SI section S2

Additional considerations for selecting chemicals from EPA's FHM database

In the EPA-FHM data set, different groups of narcotic effects have been distinguished:

- NARCOSIS_I
- NARCOSIS_II
- a combination of 'Narcosis I & II',
- Narcosis III ('NARCO_ESTER'),
- narcotic acrylates ('NARC_ACRYLATE').

FHM chemicals with a specific modes of action (MoA) are grouped as:

- uncoupler of oxidative phosphorylation ('UNCOUPLER'),
- inhibitor of acetylcholinesterase ('ACHE'),
- Respiratory blocker/inhibitor ('BLOCK'),
- chemicals with electrophile/proelectrophile reactivity ('REACTIVE'),
- chemicals acting as central nervous system seizure/stimulant ('NEUROTOX').

The MoA for a bin of 42 chemicals is termed 'MIXED', for 36 chemicals no toxicity was observed in 96h at highest tested level ('EMPTY').

Most of the chemicals in the FHM data set were assigned an ID number in an earlier evaluation of the classification of this set of chemicals, as listed in Column 3 to facilitate future cross-comparison.[12] As indicated in that study and a follow-up evaluation,[13] the MoA assignments by EPA sometimes differ from the Verhaar classification rules applied in Toxtree 1.6 and 2.5, even for narcotic chemicals, as indicated in Columns 4-6 of Table S1.

The *Verhaar*-classification divides chemicals by structural feature in relation to known toxicity of analogs:

- Class 1 for (narcosis or baseline toxicity)
- Class 2 (less inert compounds)
- Class 3 (unspecific reactivity)
- Class 4 (compounds and groups of compounds acting by a specific mechanism)
- Class 5 (Not possible to classify according to these rules)

Class 2 would be expected to relate to Narcosis_II, or 'polar narcosis' used for example in the comparison of the lethal body burdens based on Kow and K_{MLW} by Vaes et al.[14]. Expert judgement of classification was used as a post-filter to assign chemicals from unknown class 5 (Not possible to classify according to these rules) to any of the other Toxtree classes.

To select as many 'data-poor' narcotic compounds (i.e., no prior measured K_{MLW} available), a first screen of the FHM database was made using reported liposomal K_{MW} values listed in a 2011 review,[15] and IAM-HPLC based K_{MW} values using the Unilever SEAC database.[16] For the total of 276 narcotic I and II compounds in the FHM dataset (240 Narcosis_I and 36 Narcosis_II, each with 4 levels of confidence), liposomal K_{MLW} values were available for 31 compounds (11%). IAM-HPLC based K_{MLW}

values were available for 31 compounds, but with 9 overlapping compounds, these experimental data cover 53 compounds (19%).

Literature reported experimental pp-LFER descriptors (L, A, B, S) are derived from the UFZ database for 132 of the FHM narcotic compounds (48%). These ppLFER calculations are expected to provide K_{MLW} estimates with an SD of 0.3 log units.[15] The ppLFER values overlapped with 50 of the 53 experimental K_{MLW} values. The set of 50 narcotic compounds for IAM-HPLC measurements were selected to be entirely outside the pp-LFER and IAM-HPLC set (Figure 1), and only relate to FHM narcotic compounds with level 1 or 2 confidence. Of this set of 50, one was a largely protonated base (4-(2-hydroxyethyl) morpholine), one a largely dissociated acid (3-hydroxy-2-nitropyridine).

A substantial number of chemicals in the FHM set are ionizable compounds. Forty-nine of the FHM chemicals are strong bases that are largely ionized at neutral pH (pKa>8) or quaternary ammonium cations. Most of these bases are classified MoA as "UNSURE_AMINES". Nineteen of the FHM chemicals are acids that have a pKa <6, and thus toxicity may at least partially depend on chemical speciation and properties of the anionic species. Nine of these acids are classified MoA as "UNSURE", and only two as narcotics.

Ellison *et al*.[13] re-evaluated the MoA appointment in the FHM set, according to existing MoA classification tools such as the Verhaar Toxtree 1.6 and 2.5 Scheme, and suggested an additional post filter prediction. Instead of the 616 chemicals, however, Ellison *et al*. evaluated 408 FHM chemicals, leaving out all FHM groups of Narcotic_esters (21), Narcotic I&II (13), Narcotic_acrylates (5), Mixed MoA (42), Unsure (38), and 36 compounds labeled EMPTY, as well as all cationic amines except the neurotoxicants amphetamine, strychnine and nicotine, and a few others.

The supplementary file [SuppInfo2-chemical data.xlsx] lists the chemicals from EPA FHM database classified as Narcosis_I and Narcosis_II Class 1-4. An overview is provided in Table S1 below. The classification according to Verhaar schemes according to Ellison *et al*.[13] is listed to demonstrate that the distinction between Narcosis_I and Narcosis_II is not necessarily equal.

Table S1A. Selection of FHM chemicals with a Narcosis MoA for IAM-HPLC measurements, based on absence of K_{MLW} info and ppLFER descriptors, and class 1-2 confidence.

Colour code: Ellison et al. 2015 evaluation of binning FHM narcotics (as listed in Enoch et al. 2008) via the Verhaar Scheme according to different filters:

Class 1 (narcosis or baseline toxicity)

Class 2 (less inert compounds)

Class 3 (unspecific reactivity)

Class 4 (compounds and groups of compounds acting by a specific mechanism)

Class 5 (Not possible to classify according to these rules)

FHM chemicals with a Narcosis MoA	US EPA-FHM MoA Class	ID in Enoch et al. 2008 REF [12]	Tox Tree 1.5 Ellison et al. 2015 REF [13]	Tox Tree 2.6 Ellison et al. 2015 REF [13]	Extra post filter Ellison et al. 2015 REF [13]	Log LC_{50} mM US EPA FHM	logP exper. Via EPI Suite	log K_{IAM} this study	Log K_{IAM} other study REF [16]	Log K_{MLW} Lipo-some 25°C REF [15]	CMB in mmol/kg based on average experi-mental LogK_{MLW}	ppLFER descriptors REF [17]						Log K_{MW} ppLFER REF [15]	Log K_{dmpc} COSMOMIC incl. -0.32 Offset as used in REF[18] This study
Narcosis I - Used in current study for IAM-HPLC measurements (sorted by increasing toxicity): no existing K_{MLW}, no ppLFER												**L**	**E**	**S**	**A**	**B**	**Vx**		
2-hydroxyethyl ether	I_2	185	5	5	5	2.85		-0.46			246								-0.42
Triethylene glycol	I_2	187	5	5	5	2.60	-1.75	0.01			408								-0.32
2-methyl-2,4-pentanediol	I_2	183	5	1	1	1.96		0.75			506								0.82
Urethane	I_2	171	5	4	4	1.77	-0.15	0.40			148								0.0
3-methyl-1-pentyn-3-ol	I_2	105	3	3	3	1.09		1.19			194								1.56
n-phenyldiethanolamine	I_2	188	5	5	5	0.61		1.84			283								1.52
3-methyl-3-pentanol	I_2	176	5	1	1	0.82		1.43			177								1.86
2-methyl-3,3,4,4-tetrafluoro-2-butanol	I_2	127	3	3	3	0.56		1.53			123								1.9
2,6-dichlorobenzamide	I_2	117	3	5	5	0.39	0.77	1.51			79								1.02
2,4,5-trimethyloxazole	I_2	208	5	5	5	0.61		1.78			241								1.6
cis-3-hexen-1-ol	I_2	47	1	5	5	0.58		1.58			146								1.63
2-phenoxyethanol	I_2	189	5	1	1	0.40	1.16	1.70			125								1.55
Diethyl benzylphosphonate	I_2	198	5	5	5	0.17	0.89	2.41			374								2.0
trans-3-hexen-1-ol	I_2	48	1	5	5	0.43		1.62	1.23		72								1.72
1-ethynyl-cyclohexanol	I_2	123	3	1	1	0.04	1.63	1.80			267								1.9
2',3',4'-trimethoxy-acetophenone	I_2	116	3	3	3	0.27		2.39			72								1.94
3,4-dimethyl-1-pentyn-3-ol	I_2	51	1	1	1	0.06		1.59			67								2.24
2-(bromomethyl)-tetrahydro-2h-pyran	I_2	202	5	5	5	0.01		1.77			58								1.16
2-amino-4-chloro-6-methylpyrimidine	I_2	203	5	5	5	0.02	1.65	1.76			94								2.1
2-dimethylaminopyridine	I_2	110	3	3	3	-0.11		1.96			110								2.49

2-phenyl-3-butyn-2-ol	I_2	192	5	1	1	-0.17	2.14	2.15			103								2.33
2,3-dihydrobenzofuran	I_2	78	2	2	2	-0.17		2.18			163	4.467	0.629	0.70	0	0.57	1.098	1.79	2.13
5-ethyl-2-methylpyridine	I_2	193	5	5	5	-0.46	1.99	2.39			186								1.46
Benzyl sulfoxide	I_2	195	5	5	5	-0.13	2.24	2.73			74								2.86
2,5-dimethylfuran	I_2	181	5	1	1	-0.39		2.00			156								2.54
benzyl-tert-butanol	I_2	178	5	5	5	-0.53		2.59			94								2.86
2-(n-ethyl-m-toluidino)ethanol	I_2	111	3	5	5	-0.61		2.50			86								1.86
A,A,A-trifluoro-o-tolunitrile	I_2	84	2	5	5	-0.77		2.54			74								2.21
A,A,A-4-tetrafluoro-*m*-toluidine	I_2	81	2	5	5	-0.78		2.64			57								2.34
A,A,A-4-tetrafluoro-*o*-toluidine	I_2	113	3	5	5	-0.85		2.54			91								1.87
4-ethoxy-2-nitroaniline	I_2	109	3	3	3	-0.87		2.81			170								1.86
4-(diethylamino)-benzaldehyde	I_2	83	2	5	5	-0.98	2.59	3.10			117								2.03
4-phenylpyridine	I_2	103	3	3	3	-1.27		3.05			118								3.75
1,1-diphenyl-2-propyn-1-ol	I_2	199	5	1	1	-1.42		3.34			167								4.13
Butyl phenyl ether	I_2	125	3	3	3	-1.56		3.64			30								2.7
4-(diethylamino)-salicylaldehyde	I_2	112	3	1	1	-1.80	3.56	3.04			125								2.18
Flavone	I_2	118	3	5	5	-2.04		3.90			149								3.24
2-amino-4'-chloro-benzophenone	I_2	102	3	5	5	-2.49	4.26	4.21			152								5.12
Di-n-butylisophthalate	I_2	128	3	3	3	-2.84		4.67			377								4.83
3-(4-tert-butylphenoxy)-benzaldehyde	I_2	129	3	3	3	-2.95		5.41			108								3.98
3-(3,4-dichlorophenoxy)-benzaldehyde	I_2	185	5	5	5	2.85		4.98			246								-0.42
narcotic FHM chemicals	**EPA-FHM MoA Class**	**ID in Enoch et al. 2008**	**Tox Tree 1.5**	**Tox Tree 2.6**	**Extra post filter**	**Log LC_{50} mM**	**logP exper. Via EPI Suite**	**log K_{IAM} this study**	**Log K_{IAM} other study**	**Log K_{MLW} Lipo-some 25°C**		**ppLFER descriptors**						**Log K_{MW} ppLFER**	**Log K_{dmpc} COSMOMIC incl. -0.32 offset**
Narcosis I - Class 1 or 2 chemicals with experimental K_{MLW} available												**L**	**E**	**S**	**A**	**B**	**Vx**		
1,1,2,2-TETRACHLOROETHANE	I_2	27	1	1	1	-0.92	2.39		2.56			3.803	0.595	0.76	0.16	0.12	0.88	2.81	2.7
1,2-DICHLOROETHANE	I_2	31	1	1	1	0.14	1.48		1.62			2.573	0.416	0.64	0.1	0.11	0.6352	1.89	
1-PROPANOL#1	I_2	20	1	1	1	1.89	0.25		0.86			2.031	0.236	0.42	0.37	0.48	0.59	0.22	0.53
2-METHYL-2-PROPANOL	I_2	175	5	1	1	1.94	0.35		1.65			1.963	0.18	0.3	0.31	0.6	0.7309	0.05	0.89
DIETHYL ETHER	I_2	17	1	1	1	1.54			1.22			2.015	0.041	0.25	0	0.45	0.7309	0.75	1.76
DICHLOROMETHANE	I_2	23	1	1	1	0.59	1.25		1.50			2.019	0.387	0.57	0.1	0.05	0.4943	1.66	1.47
NAPHTHALENE	I_1	5	1	1	1	-1.32	3.3		3.43			5.161	1.34	0.92	0	0.2	1.0854	3.43	3.17
ACETOPHENONE	I_1	96	3	5	5	0.13	1.58		2.04			4.501	0.818	1.01	0	0.48	1.0139	1.74	1.39
PROPIONITRILE	I_2	182	5	5	5	1.44	0.16		0.93			2.082	0.162	0.9	0.02	0.36	0.5451	0.22	-0.01
1-BUTANOL	I_2	21	1	1	1	1.37	0.88			0.54		2.601	0.224	0.42	0.37	0.48	0.7309	0.77	1.02
1-PENTANOL	I_1	1	1	1	1	0.73	1.51		1.61	1.08		3.106	0.219	0.42	0.37	0.48	0.8718	1.28	1.54

1-HEXANOL	I_1	9	1	1	1	-0.02	2.03		2.11	1.72		3.61	0.21	0.42	0.37	0.48	1.0127	1.79	2.08
1-HEPTANOL	I_1	10	1	1	1	-0.53	2.62			2.38		4.115	0.211	0.42	0.37	0.48	1.1536	2.30	2.63
1-OCTANOL #2	I_1	11	1	1	1	-0.95	3			2.66		4.619	0.199	0.42	0.37	0.48	1.2945	2.81	3.18
2,4-DIMETHYL-3-PENTANOL	I_2	41	1	1	1	0.15				1.71									2.4
CYCLOHEXANOL	I_2	184	5	5	1	0.85	1.23			1.08		3.758	0.46	0.54	0.32	0.57	0.9041	1.22	1.22
2-OCTANONE	I_1	8	1	1	1	-0.55	2.37			2.42		4.257	0.108	0.68	0	0.51	1.2515	2.19	2.61
2-NONANONE	I_2	45	1	1	1	-0.97	3.14			2.83		4.735	0.119	0.68	0	0.51	1.3924	2.69	3.12
BUTYL ETHER	I_1	14	1	1	1	-0.61	3.21			2.78		3.924	0	0.25	0	0.45	1.2945	2.73	3.95
PENTYL ETHER	I_1	16	1	1	1	-1.70				3.77		4.7998	0	0.25	0	0.45	1.5763	3.67	5.27
TRICHLOROETHYLENE	I_2	26	1	1	1	-0.47	2.42			2.43		2.997	0.524	0.4	0.08	0.03	0.7146	2.80	2.86
TETRACHLOROETHYLENE #1	I_1	13	1	1	1	-1.09	3.4			3.08		3.584	0.639	0.44	0	0	0.837	3.41	3.61
1,2,4-TRICHLOROBENZENE	I_1	12	1	1	1	-1.78	4.02			4.2		5.248	0.98	0.81	0	0	1.0836	4.38	3.65
	EPA-FHM MoA Class	**ID in Enoch et al. 2008**	**Tox Tree 1.5**	**Tox Tree 2.6**	**Extra post filter**	**Log LC_{50} mM**	**logP exper. Via EPI Suite**	**log K_{IAM} this study**	**Log K_{IAM} other study**	**Log K_{MLW} Lipo-some 25°C**		**ppLFER descriptors**						**Log K_{MW} ppLFER**	**Log K_{dmpc} COSMOMIC incl. -0.32 offset**
Narcosis I - Class 3 chemicals with experimental K_{MLW} available												**L**	**E**	**S**	**A**	**B**	**Vx**		
TETRAHYDROFURAN	I_3	62	1	1	1	1.48	0.46		1.10			2.636	0.289	0.52	0	0.48	0.6223	0.53	0.75
P-XYLENE	I_3	60	1	1	1	-1.08	3.15		3.11			3.839	0.613	0.52	0	0.16	0.9982	3.10	3.38
ETHYLBENZENE #1	I_3	59	1	1	1	-0.94	3.15		3.08			3.778	0.613	0.51	0	0.15	0.9982	3.12	3.35
2-BUTANONE	I_3	54	1	1	1	1.65	0.29		0.90			2.287	0.166	0.7	0	0.51	0.6879	0.16	0.51
ACETONITRILE	I_3	211	5	5	5	1.60	-0.34		0.58			1.739	0.237	0.9	0.04	0.33	0.4042	-0.08	-0.49
PYRROLE	I_3	217	5	5	5	0.50	0.75		1.45			2.865	0.613	0.73	0.41	0.29	0.5774	1.13	1.02
NITROBENZENE	I_3	85	2	2	2	-0.01	1.85		2.32			4.557	0.871	1.11	0	0.28	0.8906	2.28	2.13
BENZOPHENONE #2	I_3	141	3	5	5	-1.11	3.18		3.34			6.852	1.447	1.5	0	0.5	1.481	3.26	2.68
BENZAMIDE	I_3	131	3	5	5	0.74	0.64		1.40				0.99	1.5	0.49	0.67	0.9728	0.77*	0.27
DIETHYL PHTHALATE	I_3	134	3	5	5	-0.84	2.42		2.91	1.77		6.73492	0.729	1.4	0	0.88	1.7106	2.14	2.57
DI-N-BUTYLORTHOPHTHALATE #1	I_3	135	3	5	5	-2.52	4.5			3.79		8.49658	0.672	1.4	0	0.88	2.2742	4.04	
CYCLOHEXANE	I_3	65	1	1	1	-1.27	3.44			3.27		2.964	0.305	0.1	0	0	0.8454	3.41	3.49
CYCLOHEXANONE #2	I_3	61	1	1	1	0.87	0.81		1.35	0.54		3.792	0.403	0.86	0	0.56	0.8611	0.92	0.76
HEXANE	I_3	64	1	1	1	-1.54	3.9		2.97	3.8		2.668	0	0	0	0	0.954	3.52	4.25
ACETONE #1	I_3	52	1	1	1	2.15	-0.24			0.02		1.696	0.179	0.7	0.04	0.51	0.547	-0.40	
2-DECANONE #1	I_3	73	1	1	1	-1.44	3.73			3.16		5.245	0.108	0.68	0	0.51	1.5333	3.20	3.67
2,3,4,5-TETRACHLOROPHENOL	I_3	235	5	5	2	-2.75	4.21			4.76		6.353	1.17	0.88	0.7	0.13	1.2647	4.67	3.81
2,3,4,6-TETRACHLOROPHENOL	I_3	209	5	4	4	-2.35	4.45			4.46		6.74	1.11				1.2647		3.76

	EPA-FHM MoA Class	ID in Enoch et al. 2008	Tox Tree 1.5	Tox Tree 2.6	Extra post filter	Log LC_{50} mM	logP exper. Via EPI Suite	log K_{IAM} this study	Log K_{IAM} other study	Log K_{MLW} Lipo-some 25°C		ppLFER descriptors						Log K_{MW} ppLFER	Log K_{dmpc} COSMOMIC incl. -0.32 offset
Narcosis I - Class 1 or 2 chemicals with ppLFER K_{MLW} estimates												L	E	S	A	B	Vx		
2-UNDECANONE	I_2	37	1	1	1	-2.06	4.09					5.732	0.101	0.68	0	0.51	1.6742	3.70	4.24
2-DODECANONE	I_2	50	1	1	1	-2.19							0.103	0.68	0	0.51	1.815	3.95*	4.75
2-PROPANOL #1	I_2	18	1	1	1	2.21	0.05					1.764	0.212	0.36	0.33	0.56	0.59	-0.19	0.41
2-METHYL-1-PROPANOL	I_1	2	1	1	1	1.29	0.76					2.413	0.217	0.39	0.37	0.48	0.7309	0.69	1.06
2-BUTANOL	I_2	25	1	1	1	1.69	0.61					2.338	0.217	0.36	0.33	0.56	0.7309	0.36	0.99
1-NONANOL	I_1	15	1	1	1	-1.40	3.77					5.124	0.193	0.42	0.37	0.48	1.4354	3.32	3.75
1-DECANOL	I_2	38	1	1	1	-1.82	4.57					5.628	0.191	0.42	0.37	0.48	1.5763	3.83	4.31
2-ETHYL-1-HEXANOL	I_2	29	1	1	1	-0.66						4.38011	0.209	0.39	0.37	0.48	1.2945	2.71	3.01
2-HEXANONE	I_2	40	1	1	1	0.63	1.38					3.262	0.136	0.68	0	0.51	0.9697	1.18	1.5
2-HEPTANONE	I_2	33	1	1	1	0.06	1.98					3.76	0.123	0.68	0	0.51	1.1106	1.68	2.06
1,1,1-TRICHLOROETHANE #1	I_2	22	1	1	1	-0.40	2.49					2.733	0.369	0.41	0	0.09	0.7576	2.48	2.76
1,1,2-TRICHLOROETHANE	I_1	4	1	1	1	-0.21	1.89					3.29	0.499	0.68	0.13	0.08	0.7576	2.57	2.08
PENTACHLOROETHANE	I_2	24	1	1	1	-1.43	3.22					4.267	0.648	0.66	0.17	0.06	1.0024	3.60	3.28
HEXACHLOROETHANE #1	I_2	19	1	1	1	-2.19	4.14						0.68	0.22	0	0.06	1.125	4.20*	4.09
1-BROMOPROPANE	I_2	30	1	1	1	-0.26	2.1					2.62	0.366	0.4	0	0.12	0.7063	2.22	2.46
1-BROMOBUTANE	I_2	32	1	1	1	-0.57	2.75					3.105	0.36	0.4	0	0.12	0.8472	2.72	2.99
1-BROMOHEXANE	I_2	35	1	1	1	-1.68	3.8					4.13	0.349	0.4	0	0.12	1.129	3.75	4.08
1-BROMOHEPTANE	I_2	43	1	1	1	-2.09	4.36					4.663	0.343	0.4	0	0.12	1.2699	4.28	4.63
1-BROMOOCTANE	I_2	36	1	1	1	-2.36	4.89					5	0.339	0.4	0	0.12	1.4108	4.70	5.15
1,2-DICHLOROPROPANE	I_1	3	1	1	1	0.05	1.98					2.857	0.371	0.6	0.1	0.11	0.7761	2.31	2.23
1,3-DICHLOROPROPANE #1	I_2	39	1	1	1	0.06	2					3.101	0.408	0.74	0	0.17	0.7761	2.08	2.01
1,2,3-TRICHLOROPROPANE #1	I_2	28	1	1	1	-0.35	2.27					3.582	0.547	0.65	0.03	0.31	0.8985	2.07	2.18
1,4-DICHLOROBUTANE	I_2	34	1	1	1	-0.39							0.413	0.95	0	0.17	0.917	2.30*	2.4
4-METHYL-2-PENTANONE #2	I_1	6	1	1	1	0.73	1.31					3.089	0.111	0.65	0	0.51	0.9697	1.11	
ISOPROPYL ETHER	I_1	7	1	1	1	0.89						2.53	-0.06	0.16	0	0.58	1.0127	1.06	2.58
DIPHENYLAMINE	I_2	80	2	2	2	-1.65	3.5					6.89		0.96	0.61	0.2	1.42	4.87	3.42
2,4,6-TRIMETHYLPHENOL	I_2	82	2	2	2	-1.02	2.73					5.133	0.86	0.79	0.37	0.44	1.1978	2.74	3.01
2-ETHYLPYRIDINE	I_2	77	2	2	2	0.59	1.69					3.844	0.613	0.7	0	0.59	0.9571	1.14	
2-PICOLINE	I_2	79	2	2	2	0.98	1.11					3.422	0.598	0.75	0	0.57	0.8162	0.70	1.15
1,1,1,3,3,3-HEXAFLUORO-2-PROPANOL	I_2	115	3	1	1	0.16	1.66					1.392	-0.24	0.55	0.77	0.1	0.6962	1.63	2.31
TRIBUTYL PHOSPHATE #1	I_2	190	5	5	5	-1.38	4.0					7.37	-0.1	0.9	0	1.21	2.239	2.51	4.41
N,N-DIETHYLANILINE	I_2	177	5	5	5	-0.96	3.31					5.287	0.953	0.79	0	0.41	1.3798	3.26	4.05
N,N-DIMETHYL-P-TOLUIDINE #1	I_1	164	5	5	5	-0.42	2.81					5.188	0.94	0.82	0.08	0.48	1.2389	2.66	3.6

P-DIMETHOXYBENZENE	I_1	166	5	1	1	-0.07	2.04					5.044	0.806	1	0	0.5	1.1156	2.13	2.39
N,N-DIMETHYLANILINE #1	I_1	165	5	5	5	-0.19	2.31					4.701	0.957	0.84	0	0.42	1.098	2.39	3.0
CINEOLE	I_2	191	5	1	1	-0.18	2.74					4.29	0.383	0.49	0	0.76	1.3591	1.55	3.08
2-(2-ETHOXYETHOXY)ETHANOL	I_2	186	5	1	1	2.30	-0.54					4.12	0.22	0.72	0.21	1.21	1.1301	-0.95	0.46
ETHANOL	I_2	173	5	1	1	2.49	-0.31					1.485	0.246	0.42	0.37	0.48	0.4491	-0.31	0.04
METHANOL-RHODAMINE B	I_2	174	5	1	1	2.96	-0.77					0.97	0.278	0.44	0.43	0.47	0.3082	-0.81	
N-OCTYL CYANIDE #1	I_1	167	5	5	5	-1.45	3.12						0.159	0.9	0	0.36	1.391	2.99*	3.17
4'-AMINOPROPIOPHENONE	I_2	104	3	5	5	-0.01							1.17	1.39	0.32	0.65	1.1137	1.50*	1.09
PHENYL SULFOXIDE	I_2	197	5	5	5	-0.36	2.06						1.5	2.15	0	0.72	1.5464	2.31*	1.77
narcotic FHM chemicals	**EPA-FHM MoA Class**	**ID in Enoch et al. 2008**	**Tox Tree 1.5**	**Tox Tree 2.6**	**Extra post filter**	**Log LC_{50} mM**	**logP exper. Via EPI Suite**	**log K_{IAM} this study**	**Log K_{IAM} other study**	**Log K_{MLW} Lipo-some 25°C**		**ppLFER descriptors**						**Log K_{MW} ppLFER**	**Log K_{dmpc} COSMOMIC incl. -0.32 offset**
Narcosis I - Class 1 or 2 chemicals with only COSMO K_{MLW} estimates																			
TRANS-2-PHENYL-1-CYCLOHEXANOL	I_2	49	1	1	1	-0.60													2.62
1,5-DICHLOROPENTANE	I_2	42	1	1	1	-0.75													2.85
TRANS-1,2-DICHLOROCYCLOHEXANE	I_2	46	1	1	1	-0.92	3.18												3.01
2,5-DIMETHYL-2,4-HEXADIENE	I_2	44	1	1	1	-1.46	3.5												4.15
2',4'-DICHLOROACETOPHENONE	I_1	98	3	5	1	-1.21													2.54
2,6-DIMETHOXYTOLUENE	I_1	168	5	1	1	-0.88	2.87												3.39
2,2,2-TRICHLOROETHANOL	I_1	97	3	1	1	0.30	1.42												1.83
1,1,1-TRICHLORO-2-METHYL-2-PROPANOL(HYDRATE)	I_2	120	3	1	1	-0.12	2.03												2.39
2,4,6-TRIBROMOPHENOL	I_1	75	2	2	2	-1.70	4.13												3.75
2,6-DIISOPROPYLANILINE #1	I_1	76	2	2	2	-1.10	3.18												3.94
P-(TERT-BUTYL)BENZAMIDE	I_1	100	3	5	5	-0.74	2.51												1.41
M-BROMOBENZAMIDE	I_1	99	3	5	5	-0.33	1.65												1.07
3-HYDROXY-3,7,11-TRIMETHYL-1,6,10-DODECATRIENE	I_2	121	3	3	3	-2.19													5.32
P-CHLOROPHENYL-O-NITROPHENYL ETHER	I_2	101	3	5	5	-2.11													3.81
B-IONONE	I_2	107	3	3	3	-1.58	3.84												2.81
ISOPROPYL DISULFIDE	I_2	119	3	3	3	-1.26	1.52												4.31
4-BROMOPHENYL 3-PYRIDYL KETONE	I_2	124	3	5	5	-1.11													2.13
A-DECANOLACTONE	I_2	114	3	5	5	-0.98	2.72												2.55
2-METHYL-3-BUTYN-2-OL	I_2	108	3	3	3	1.59	0.28												1.08
4-HEXYLOXYANILINE #1 (NOMINAL CONC,)	I_1	169	5	5	5	-1.84	3.64												3.86
(1R,2S,5R)-(-)-MENTHOL	I_2	200	5	5	1	-0.92	3.19												3.48
3,6-DITHIAOCTANE	I_2	201	5	5	5	-0.40													3.15
4,7-DITHIADECANE	I_2	170	5	5	5	-1.38													4.19
3-HYDROXY-2-NITROPYRIDINE	I_2	207	5	5	5	0.08													1.27
2,2,5,5-TETRAMETHYLTETRAHYDROFURAN	I_2	206	5	1	1	0.12	2.06												2.79

N,N-BIS(2,2-DIETHOXYETHYL)METHYLAMINE #1	I_2	205	5	5	5	0.38													3.64
4-METHYLOXAZOLE	I_2	196	5	5	5	1.22													0.77
4-(2-HYDROXYETHYL)MORPHOLINE	I_2	194	5	5	5	1.32													0.04
3,6-DIMETHYL-1-HEPTYN-3-OL	I_2	126	3	3	3	-0.46													
Narcosis I - Chemicals not included as unknown influence of ionization																			
TOLAZOLINE HYDROCHLORIDE	I_2	172	5	5	5	0.26													
TRIPROPARGYLAMINE	I_2	204	5	5	5	0.35	1.27												
2-(DIISOPROPYLAMINO)ETHANOL	I_2	179	5	5	5														
N,N-DIETHYLETHANOLAMINE	I_2	180	5	5	5														
1-(2-CHLOROETHYL)PYRROLIDINE,HCL	I_2	122	3	5	5														
narcotic FHM chemicals	**EPA-FHM MoA Class**	**ID in Enoch et al. 2008**	**Tox Tree 1.5**	**Tox Tree 2.6**	**Extra post filter**	**Log LC_{50} mM**	**logP exper. Via EPI Suite**	**log K_{IAM} this study**	**Log K_{IAM} other study**	**Log K_{MLW} Lipo-some 25°C**		**ppLFER descriptors**						**Log K_{MW} ppLFER**	**Log K_{dmpc} COSMOMIC incl. -0.32 offset**
Narcosis II - Class 1 or 2 chemicals used in current study for IAM-HPLC measurements																			
6-chloro-2-pyridinol	II_1	268	5	5	5	0.22	0.93	1.34											1.77
2-amino-5-bromopyridine	II_1	261	3	5	4	-0.63	0.96	1.74											1.59
4-amino-2-nitrophenol	II_2	270	5	5	5	0.01		2.12											1.29
2-chloro-4-methylaniline	II_1	251	2	2	2	-0.60		2.55											2.32
2-chloro-4-nitroaniline	II_1	250	2	2	2	-0.96	2.14	2.84											1.69
3-trifluoromethyl-4-nitrophenol	II_2	252	2	2	2	-1.36		3.28											2.86
Narcosis II - Class 1 or 2 chemicals with experimental K_{MLW} available												**L**	**E**	**S**	**A**	**B**	**Vx**		
4-CHLORO-3-METHYL PHENOL #1	II_1	240	2	2	2	-1.29	3.1			3.29		5.29	0.92	1.02	0.67	0.22	1.0384	3.22	2.62
2-CHLOROPHENOL #1	II_1	244	2	2	2	-0.97	2.15			2.79		4.178	0.853	0.88	0.32	0.31	0.8975	2.16	2.27
PYRIDINE #1	II_1	249	2	2	2	0.13	0.65		1.38			3.022	0.631	0.84	0	0.52	0.6753	0.37	0.59
ANILINE #1	II_1	241	2	2	2	0.16	0.9		1.63			3.934	0.955	0.96	0.26	0.41	0.8162	1.42	1.23
2-CHLOROANILINE #2	II_1	243	2	2	2	-1.351	1.9		2.48			4.674	1.033	0.92	0.25	0.31	0.9386	2.47	1.86
PHENOL #1	II_1	248	2	2	2	-0.51	1.46		1.96	1.97		3.766	0.805	0.89	0.6	0.3	0.7751	1.75	1.74
4-NITROPHENOL #1	II_1	245	2	2	2	-0.38	1.91		2.82	2.72		5.876	1.07	1.72	0.82	0.26	0.9493	2.56	1.94
O-CRESOL	II_2	253	2	2	2	-0.89	1.95		2.30	2.45		4.218	0.84	0.86	0.52	0.3	0.916	2.26	2.2
1-NAPHTHOL	II_1	242	2	2	2	-1.49	2.85		3.36			6.13	1.52	1.05	0.61	0.37	1.1441	3.22	2.79
Narcosis II - Class 3 chemicals with experimental K_{MLW} available												**L**	**E**	**S**	**A**	**B**	**Vx**		
2-NITROPHENOL	II_3	257	2	2	2	0.06	1.79			1.89		4.76	1.015	1.05	0.05	0.37	0.9493	2.18	2.38
4-CHLOROPHENOL	II_3	258	2	2	2	-1.32	2.39		2.76	2.96		4.775	0.915	1.08	0.67	0.2	0.8975	2.72	2.29

Table S1B. FHM chemicals with a Specific MoA or Unsure MoA selected for IAM-HPLC measurements

Colour code: Ellison et al. 2015 evaluation of binning FHM narcotics (as listed in Enoch et al. 2008) via the Verhaar Scheme according to different filters:

Class 1 (narcosis or baseline toxicity)

Class 2 (less inert compounds)

Class 3 (unspecific reactivity)

Class 4 (compounds and groups of compounds acting by a specific mechanism)

Class 5 (Not possible to classify according to these rules)

FHM chemicals with a specific MoA	**US EPA-FHM MoA Class**	**ID in Enoch et al. 2008 REF [12]**	**Tox Tree 1.5 Ellison et al. 2015 REF [13]**	**Tox Tree 2.6 Ellison et al. 2015 REF [13]**	**Extra post filter Ellison et al. 2015 REF [13]**	**Log LC_{50} mM US EPA FHM**	**logP exper. Via EPI Suite**	**log K_{IAM} this study**	**Log K_{IAM} other study REF [16]**	**Log K_{MLW} Lipo-some 25°C REF [15]**	**CMB in mmol/kg based on average experi-mental LogK_{MLW}**	**ppLFER descriptors REF [17]**						**Log K_{MW} ppLFER REF [15]**	**Log K_{dmpc} COSMOMIC incl. -0.32 Offset as used in REF[18] This study**
												L	**E**	**S**	**A**	**B**	**Vx**		
CARBARYL (SEVIN) #2	ACHE_1	384	5	4	4	-1.35	2.36	2.98			42.0								
PROPOXUR (BAYGON)	ACHE_1	386	5	4	4	-1.38	1.52	2.27			7.84								
DIAZINON	ACHE_1	391	5	4	4	-1.51	3.81	4.04			**341**								
AMINOCARB	ACHE_1	394	5	4	4	-2.03	1.90	2.48			2.85								
ALDICARB	ACHE_1	388	5	4	4	-2.34	1.13	1.91			0.37								
CARBOFURAN	ACHE_1	393	5	4	4	-2.42	2.32	2.46			1.09	7.29		1.37	0.11	1.04	1.69	1.79	
O-ETHYL O-(P-NITROPHENYL	ACHE_1	395	5	5	5	-3.61	4.78	5.02			25.37								
AZINPHOS-METHYL	ACHE_1	385	5	4	4	-3.70	2.75	3.57			0.76								
ROTENONE	BLOCK_1					-4.94		4.58			0.43								
BUTANAL	REACTIVE_3	322	3	3	3	-0.65	0.88	1.02			2.34	2.27	0.19	0.65	0	0.45	0.69	0.48	
4-FLUOROANILINE	REACTIVE_4	285	2	5	5	-0.82	1.15	1.63			6.45	4.01	0.76	1.09	0.28	0.41	0.84	1.42	
2,4-DINITROTOLUENE	REACTIVE_4	347	3	5	5	-0.87	1.98	2.42			34.8	6.27	1.18	1.27	0.07	0.51	1.21	2.38	
4-NITROBENZALDEHYDE	REACTIVE_2	297	3	3	3	-1.18	1.56	1.90			5.25		1.08	1.53	0	0.51	1.05	1.55	
BENZALDEHYDE	REACTIVE_1	286	3	3	3	-1.14	1.48	1.80			4.48	4.01	0.82	1	0	0.39	0.87	1.61	
2,4,5-TRIBROMOIMIDAZOLE	REACTIVE_3	368	5	5	5	-1.58	1.96	2.27			4.86								
4-DIMETHYLAMINOCINNAMALDEHYDE	REACTIVE_2	308	3	3	3	-1.47		3.11			43.1								
SALICYLALDEHYDE	REACTIVE_3	315	3	3	3	-1.73	1.81	1.91			1.55	4.54	0.96	1.15	0.11	0.31	0.93	2.15	
4-CHLOROCATECHOL	REACTIVE_4	370	5	5	3	-1.96		1.60			0.43								
1-BENZOYLACETONE	REACTIVE_4	346	3	1	1	-2.17		2.57			2.52								
PENTAFLUOROBENZALDEHYDE	REACTIVE_3	330	3	3	3	-2.25		1.83			0.38								
A,A,A-TRIFLUORO-M-TOLUALDEHYDE	REACTIVE_3	326	3	3	3	-2.28	2.47	2.46			1.54								

1,3,5-TRICHLORO-2,4-DINITROBENZENE	REACTIVE_3	340	3	4	4	-3.09		4.04			8.88								
2-METHYL-1,4-NAPHTHOQUINONE	REACTIVE_2	288	3	5	5	-3.19	2.20	2.72			0.33	6.89	1.08				1.30		
A-BROMO-2',5'-DIMETHOXYACETOPHENONE	REACTIVE_3	334	3	5	5	-3.47		3.12			0.45								
1,3-DICHLORO-4,6-DINITROBENZENE	REACTIVE_3	337	3	5	5	-3.66		2.64			0.09								
N-VINYLCARBAZOLE	REACTIVE_2	362	5	5	5	-4.78		4.85			1.18								
2,4-DINITROANILINE	UNCOUPLER_1	373	3	5	5	-1.07		2.69			41.5								
2,4-DINITROPHENOL	UNCOUPLER_1	372	3	5	4	-1.14	1.67	1.90		2.64	13.5	6.04	1.20	1.50	0.10	0.55	1.12	1.80	
count											**28**								
average											**21**								
stdev											**64**								
min											**0.09**								
max											**341**								

FHM chemicals with an unsure MoA

AMPHETAMINE SULFATE	NEUROTOX_1	404	5	5	5	-1.11	1.76		2.31		16.0		0.85	0.88	0.16	0.73	1.24	1.70	2.47
NICOTINE SULFATE #1	NEUROTOX_1	406	5	5	5	-1.54	1.17		0.96		0.27								0.28
STRYCHNINE HEMISULPHATE SALT	NEUROTOX_1	405	5	5	5	-2.54	1.93		2.28		0.55								1.30
PHENYLTRIMETHYLAMMONIUM METHOSULFATE	UNSURE					0.00			0.64		4.4								0.27
BENZYLTRIETHYLAMMONIUM CHLORIDE	UNSURE					-0.15			1.37		16.6								0.76
N,N-DIMETHYLBENZYLAMINE	UNSURE_AMINE					-0.55			1.08		3.4		0.67	0.80	0.00	0.69	1.24	1.70	1.00
HEXYLAMINE	UNSURE_AMINE					-0.25	2.06		2.12		73.7								2.85
N-ETHYLBENZYLAMINE	UNSURE_AMINE					-0.37	1.82		1.64		18.4								1.41
BENZYLAMINE	UNSURE_AMINE					-0.02	1.09		1.73		51.1		0.83	0.88	0.10	0.72	0.96	0.74	2.17
N-HEPTYLAMINE	UNSURE_AMINE					-0.72	2.57		2.54		65.6								3.38
TERT-OCTYLAMINE	UNSURE_AMINE					-0.72			2.29		37.1								2.21
1-ADAMANTANAMINE	MIXED					-0.78	2.44		2.44		45.5								2.17
OCTYLAMINE	UNSURE_AMINE					-1.40	2.90		3.08		48.3								3.93
DI-N-HEXYLAMINE	UNSURE_AMINE					-2.38			3.28		8.0								2.99
N-DECYLAMINE	UNSURE_AMINE					-2.18	3.90		4.40		165								5.05
count											**12**								
average											**45**								
stdev											**45**								
min											**3**								
max											**165**								

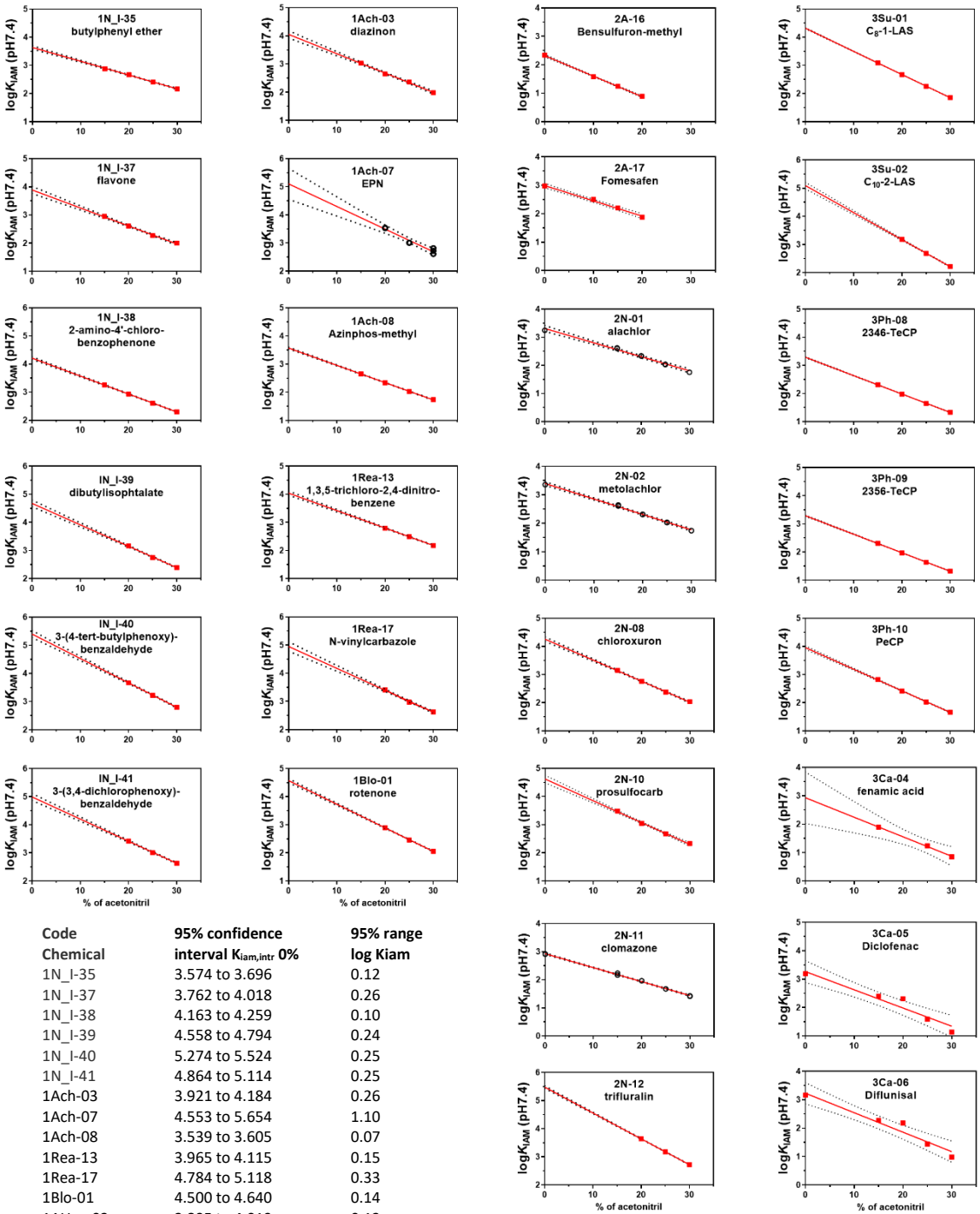
Table S2. Chemicals, CAS numbers, suppliers

chem code	chem name	CAS nr	purity	supplier
1N_I-01	2-hydroxyethyl ether	111-46-6	99%	Alfa Aesar
1N_I-02	triethylene glycol	112-27-6	99%	Alfa Aesar
1N_I-03	2-methyl-2,4-pentanediol	107-41-5	98%	Alfa Aesar
1N_I-04	urethane	51-79-6	>99%	Aldrich
1N_I-05	3-methyl-1-pentyn-3-ol	77-75-8	98%	Aldrich
1N_I-06	n-phenyldiethanolamine	120-07-0	97%	Alfa Aesar
1N_I-07	3-methyl-3-pentanol	77-74-7	CERTIFIED	Ehrenstorfer Gmbh
1N_I-08	2,4,5-trimethyloxazole	20662-84-4	97%	Alfa Aesar
1N_I-09	cis-3-hexen-1-ol	928-96-1	98%	Alfa Aesar
1N_I-10	2-methyl-3,3,4,4-tetrafluoro-2-butanol	29553-26-2	AldrichCPR	Aldrich
1N_I-11	trans-3-hexen-1-ol	928-97-2	97%	Alfa Aesar
1N_I-12	2-phenoxyethanol	122-99-6	puriss., >=99.0%	Fluka
1N_I-13	2,6-dichlorobenzamide	2008-58-4	98%	Alfa Aesar
1N_I-14	1-ethynyl-cyclohexanol	78-27-3	99%	Alfa Aesar
1N_I-15	3,4-dimethyl-1-pentyn-3-ol	1482-15-1	94%	Alfa Aesar
1N_I-16	diethyl benzylphosphonate	1080-32-6	99%	Sigma
1N_I-17	2-(bromomethyl)tetrahydro-2h-pyran	34723-82-5	ampule of 1 mL	Supelco
1N_I-18	2',3',4'-trimethoxyacetophenone	13909-73-4	96%	Aldrich
1N_I-19	2-dimethylaminopyridine	5683-33-0	97%	Alfa Aesar
1N_I-20	2-amino-4-chloro-6-methylpyrimidine	5600-21-5	98%	Alfa Aesar
1N_I-21	2-phenyl-3-butyn-2-ol	127-66-2	98%	Alfa Aesar
1N_I-22	2,5-dimethylfuran	625-86-5	98+%	Alfa Aesar
1N_I-23	2,3-dihydrobenzofuran	496-16-2	99%	Aldrich
1N_I-24	5-ethyl-2-methylpyridine	104-90-5	97%	Alfa Aesar
1N_I-25	benzyl-tert-butanol	103-05-9	97%	Aldrich
1N_I-26	benzyl sulfoxide	621-08-9	zur Synthese	Merck Millipore
1N_I-27	2-(n-ethyl-m-toluidino)ethanol	91-88-3	98%	Aldrich
1N_I-28	A,A,A-trifluoro-o-tolunitrile	447-60-9	97%	Alfa Aesar
1N_I-29	A,A,A-4-tetrafluoro-m-toluidine	2357-47-3	99%	Aldrich
1N_I-30	A,A,A-4-tetrafluoro-o-toluidine	393-39-5	97%	Alfa Aesar
1N_I-31	4-ethoxy-2-nitroaniline	616-86-4	AldrichCPR	Aldrich
1N_I-32	4-(diethylamino)benzaldehyde	120-21-8	97%	Alfa Aesar
1N_I-33	4-phenylpyridine	939-23-1	97%	Aldrich
1N_I-34	1,1-diphenyl-2-propyn-1-ol	3923-52-2	99%	Alfa Aesar
1N_I-35	butyl phenyl ether	1126-79-0	99%	Alfa Aesar
1N_I-36	4-(diethylamino)salicylaldehyde	17754-90-4	98%	Aldrich
1N_I-37	flavone	525-82-6	99%	Alfa Aesar
1N_I-38	2-amino-4'-chlorobenzophenone	2894-51-1	AldrichCPR	Aldrich
1N_I-39	di-n-butylisophthalate	3126-90-7	98.7%	Riedel-deHaen
1N_I-40	3-(4-tert-butylphenoxy)benzaldehyde	79124-76-8	94%	Aldrich
1N_I-41	3-(3,4-dichlorophenoxy)benzaldehyde	69770-23-6	98	Aldrich
1N_II-01	6-chloro-2-pyridinol	16879-02-0	98%	Aldrich
1N_II-02	2-amino-5-bromopyridine	1072-97-5	98%	Alfa Aesar
1N_II-03	2-chloro-4-methylaniline	615-65-6	98%	Alfa Aesar

1N_II-04	4-amino-2-nitrophenol	119-34-6	97%	Alfa Aesar
1N_II-05	2-chloro-4-nitroaniline #2	121-87-9	Certified	Ehrenstorfer Gmbh
1N_II-06	3-trifluoromethyl-4-nitrophenol	88-30-2	97%	Alfa Aesar
1Ach-01	carbaryl	63-25-2	pestanal	Aldrich
1Ach-02	propoxur	114-26-1	pestanal	Aldrich
1Ach-03	diazinon	333-41-5	pestanal	Aldrich
1Ach-04	aminocarb	2032-59-9	pestanal	Aldrich
1Ach-05	aldicarb	116-06-3	pestanal	Aldrich
1Ach-06	carbofuran	1563-66-2	Pestanal 99%	Riedel-deHaen
1Ach-07	EPN (o-ethyl o-(4-nitrophenyl) phenylphosphonothioate)	2104-64-5	pestanal	Aldrich
1Ach-08	azinphos-methyl	86-50-0	Pestanal, 98,9%	Fluka
1Rea-01	butanal	123-72-8	>99%	Aldrich
1Rea-02	4-fluoroaniline	371-40-4	99%	Aldrich
1Rea-03	2,4-dinitrotoluene	121-14-2	97%	Aldrich
1Rea-04	4-nitrobenzaldehyde	555-16-8	98%	Aldrich
1Rea-05	benzaldehyde	100-52-7	Reagent Plus >99%	Aldrich
1Rea-06	2,4,5-tribromoimidazole	2034-22-2	97%	Alfa Aesar
1Rea-07	4-dimethylaminocinnamaldehyde	6203-18-5	>98%	Aldrich
1Rea-08	salicylaldehyde	90-02-8	analytical standard	Aldrich
1Rea-09	4-chlorocatechol	2138-22-9	97%	Aldrich
1Rea-10	1-benzoylacetone	93-91-4	99%	Aldrich
1Rea-11	pentafluorobenzaldehyde	653-37-2	98%	Aldrich
1Rea-12	A,A,A-trifluoro-m-tolualdehyde	454-89-7	97%	Aldrich
1Rea-13	1,3,5-trichloro-2,4-dinitrobenzene	6284-83-9	CPR	Aldrich
1Rea-14	2-methyl-1,4-naphthoquinone	58-27-5	Crystalline	Aldrich
1Rea-15	a-bromo-2',5'-dimethoxyacetophenone	1204-21-3	97%	Aldrich
1Rea-16	1,3-dichloro-4,6-dinitrobenzene	3698-83-7	97%	Aldrich
1Rea-17	n-vinylcarbazole	1484-13-5	98%	Aldrich
1Blo-01	rotenone	83-79-4	Pestanal 98.1%	Fluka
1Unc-01	2,4-dinitroaniline	97-02-9	98%	Ehrenstorfer Gmbh
2A-01	Clopyralid	1702-17-6	Pestanal	Aldrich
2A-02	Fluroxypyr	69377-81-7	Pestanal	Aldrich
2A-03	Triclopyr	55335-06-3	Pestanal	Aldrich
2A-04	MCPA	94-74-6	Pestanal	Aldrich
2A-05	2,4-D	94-75-7	Pestanal	Aldrich
2A-06	MCPP (mecoprop)	93-65-2	Pestanal	Aldrich
2A-07	2,4-DP	142-28-9	Pestanal	Aldrich
2A-08	MCPB	94-81-5	Pestanal	Ehrenstorfer Gmbh
2A-09	2,4-DB	94-82-6	Pestanal	Ehrenstorfer Gmbh
2A-10	2,4,5-T	93-76-5	Pestanal	Aldrich
2A-11	DNOC	497-56-3	Pestanal	Supelco
2A-12	Dinoseb	88-85-7	Pestanal	Aldrich
2A-13	Bromoxynil	1689-84-5	Pestanal	Aldrich
2A-14	Ioxynil	1689-83-4	Pestanal	Supelco
2A-15	Triasulfuron	82097-50-5	Pestanal	Aldrich
2A-16	Bensulfuron-methyl	83055-99-6	Pestanal	Aldrich
2A-17	Fomesafen	72178-02-0	Pestanal	Aldrich
2N-01	Alachlor	15972-60-8	Pestanal	Aldrich

2N-02	Metolachlor	51218-45-2	Pestanal	Aldrich
2N-03	Simazine	122-34-9	Pestanal	Aldrich
2N-04	Ametryn	834-12-8	Pestanal	Aldrich
2N-05	Terbutylazine	5915-41-3	Pestanal	Aldrich
2N-06	Diuron	330-54-1	Pestanal	Aldrich
2N-07	Linuron	330-55-2	Pestanal	Aldrich
2N-08	Chloroxuron	1982-47-4	Pestanal	Supelco
2N-09	Ethofumesate	26225-79-6	Pestanal	Aldrich
2N-10	Prosulfocarb	52888-80-9	Pestanal	Aldrich
2N-11	Clomazone	81777-89-1	Pestanal	Aldrich
2N-12	Trifluralin	1582-09-8	Pestanal	Aldrich
3Ca01	Salicylic acid sodium	54-21-7	Reagent+ 99.5%	Aldrich
3Ca02	5-Phenylvaleric acid	2270-20-4	99%	Aldrich
3Ca03	Ibuprofen	15687-27-1	99%	Acros
3Ca04	Fenamic acid	91-40-7	98%	Aldrich
3Ca05	Diclofenac sodium	15307-79-6	Lot BCBS5961V	Sigma R&D
3Ca06	Diflunisal	22494-42-4	An.standard	Aldrich
3Su01	4-octylbenzene-1-sulfonate	6149-03-7	97%	Aldrich
3Su02	C10-2-LAS	no CAS	custom synthesized	J. Tolls[19]
3Ph01	Warfarin	129-06-6	Certified Ref.Material	Aldrich
3Ph02	Pentafluorophenol	771-61-9	>99%	Aldrich
3Ph03	2,4-Dinitrophenol	51-28-5	Pestanal, 99.9%	Fluka
3Ph04	Bromoxynil	1689-84-5	Pestanal	Aldrich
3Ph05	2-Methyl-4,6-dinitrophenol	534-52-1	neat	Aldrich
3Ph06	4-Tert-butyl-2,6-dinitrophenol	4097-49-8	AldrichCPR	Aldrich
3Ph07	Dinoseb	88-85-7	Pestanal	Aldrich
3Ph08	2,3,4,6-tetrachlorophenol	58-90-2	92%	Ehrenstorfer Gmbh
3Ph09	2,3,5,6-tetrachlorophenol	935-95-5	98%	Janssen
3Ph10	Pentachlorophenol	87-86-5	99%	Aldrich

Figure S2. Extrapolation of $K_{iam,intr}$ values from IAM-HPLC measurements at different acetonitrile fractions to fully aqueous buffer (0% solvent)



Code Chemical	95% confidence interval $K_{iam,intr}$ 0%	95% range log Kiam
1N_I-35	3.574 to 3.696	0.12
1N_I-37	3.762 to 4.018	0.26
1N_I-38	4.163 to 4.259	0.10
1N_I-39	4.558 to 4.794	0.24
1N_I-40	5.274 to 5.524	0.25
1N_I-41	4.864 to 5.114	0.25
1Ach-03	3.921 to 4.184	0.26
1Ach-07	4.553 to 5.654	1.10
1Ach-08	3.539 to 3.605	0.07
1Rea-13	3.965 to 4.115	0.15
1Rea-17	4.784 to 5.118	0.33
1Blo-01	4.500 to 4.640	0.14
1AUnc-03	3.895 to 4.019	0.12
1AN_01	3.265 to 3.313	0.05
2A-16	2.278 to 2.367	0.09
2A-17	2.908 to 3.069	0.16
2N-01	3.208 to 3.420	0.21
2N-08	4.178 to 4.335	0.16
2N-10	4.485 to 4.755	0.27
2N-11	2.902 to 2.955	0.05
2N-12	5.432 to 5.526	0.09
3Su01	4.297 to 4.339	0.04
3Su02	4.975 to 5.205	0.23
3Ph08	3.265 to 3.313	0.05
3Ph09	3.259 to 3.317	0.06
3Ph10	3.895 to 4.019	0.12

Table S3. Comparison between Liposome D_{MLW} and IAM-HPLC based $K_{iam,intr}$

Chemical	$logK_{mlw}$ neutral	liposome $logK_{MLW}$	log $K_{IAM,intr}$	diff	log $K_{IAM,intr}$ + $\delta_{IAM-SSLM}$		
Organic anions Dataset used to derive $\delta_{IAM-SSLM}$		Droge 2019 [2]	Droge 2019 [2]		-0.47		
PFBA		1.00	1.50	-0.50	**1.03**		
PFPA		1.73	2.09	-0.36	**1.62**		
PFHxA		2.31	2.67	-0.36	**2.20**		
PFHpA		2.87	3.35	-0.48	**2.88**		
PFOA		3.51	4.04	-0.53	**3.57**		
PFBS		2.63	2.93	-0.30	**2.46**		
C_8SO3		1.74	2.40	-0.66	**1.93**		
$C_{10}SO3$		3.01	3.60	-0.59	**3.13**		
C_8SO4		2.58	3.10	-0.52	**2.63**		
$C_{10}SO4$		3.79	4.10	-0.31	**3.63**		
		average	$\delta_{IAM-SSLM}$	-0.47			
Dataset to check $\delta_{IAM-SSLM}$		Bittermann 2016 [18]	This study				
Salicylic acid		1.03	1.56	-0.53	**1.09**		
Diflunisal		2.73	3.7	-0.97	**3.23**		
5-Phenylvaleric acid		1.66	1.89	-0.23	**1.42**		
Ibuprofen		1.81	2.82	-1.01	**2.35**		
Fenamic acid		2.28	3.42	-1.14	**2.95**		
Diclofenac		2.64	3.73	-1.09	**3.26**		
4-octylbenzene-1-sulfonate*		3.63	4.82	-1.19	**4.35**		
C10-2-LAS*		4.79	5.1	-0.31	**4.63**		
Pentafluorophenol		1.74	2.23	-0.49	**1.76**		
Pentachlorophenol*		4.35	4.45	-0.10	**3.98**		
2,3,4,6-tetrachlorophenol*		3.46	3.74	-0.28	**3.27**		
2,3,5,6-tetrachlorophenol*		3.49	3.77	-0.28	**3.3**		
2,4-Dinitrophenol		1.9	2.37	-0.47	**1.9**		
2-Methyl-4,6-dinitrophenol		2.35	2.81	-0.46	**2.34**		
4-Tert-butyl-2,6-dinitrophenol		3.23	3.41	-0.18	**2.94**		
Dinoseb		3.35	3.78	-0.43	**3.31**		
Bromoxynil		2.1	2.88	-0.78	**2.41**		
Warfarin		1.4	3.09	-1.69			
Count all anions listed except warfarin				27			
Average difference K_{mlw}-$K_{iam,intr}$ 28 anions				-0.54			
organic cations		Liposome $logK_{MW}$	log $K_{IAM.intr}$ cation	diff	log $K_{IAM,intr}$ + $\delta_{IAM-SSLM}$	Amine type	$\delta_{IAM-SSLM}$ average
Dataset used to derive $\delta_{IAM-SSLM}$		Timmer 2017 [1]	Timmer 2017 [1]				
octylamine		3.1	2.32	0.78	**3.1**	1°	
decylamine		4.3	3.57	0.73	**4.35**	1°	0.8
dodecylamine		5.58				1°	
N-methyloctylamine		2.76	2.32	0.44	**2.8**	2°	
N-methyldecylamine		3.98	3.59	0.39	**4.07**	2°	
N-methyldodecylamine		5.39	4.8	0.59	**5.28**	2°	

dihexylamine		3.15	2.87	0.28	**3.35**	2°	
dioctylamine		4.65	5.03	-0.38	**5.51**	2°	0.5
N,N-dimethyloctylamine		2.35	2.38	-0.03	**2.35**	3°	
N,N-dimethyldecylamine		3.65	3.62	0.03	**3.59**	3°	0.0
N,N-dimethyldodecylamine		5.3				3°	
N,N,N-trimethyloctylammonium		2.18	2.18	0.00	**2.07**	4°	
N,N,N-trimethyldecylammonium		3.34	3.44	-0.10	**3.33**	4°	
N,N,N-trimethyldodecylammonium		4.35	4.57	-0.22	**4.46**	4°	-0.1
N,N,N-trimethyltetradecylammonium		5.46				4°	
C6-benzalkonium		2.12	2.42	-0.30	**2.31**	4°	
C8-benzalkonium		3.11	3.3	-0.19	**3.19**	4°	
C10-benzalkonium		4.01	4.47	-0.46	**4.36**	4°	-0.2
C12-pyridinium		4.89				4°	
	$logK_{mlw}$ neutral	**Log K_{mlw} cation**	**log $K_{IAM.intr}$ cation**	**diff**	**log $K_{IAM,intr}$ + $\delta_{IAM-SSLM}$**	**Amine type**	**diff**
Dataset to check $\delta_{IAM-SSLM}$	**Bittermann 2016 [18]**	**Bittermann 2016 [18]**	**Droge 2017 [4]**				average per amine type
3,4-dimethylaniline	2.11	1.99	1.55	0.44	2.33	1°	
2,4,6-trimethylaniline	2.38	2.12	1.86	0.26	2.64	1°	
4-phenylbutylamine	2.41	2.12	1.98	0.14	2.76	1°	
amlodipine	3.75	3.75	4.15	-0.40	4.93	1°	0.1
atenolol		1.01	1.26	-0.25	1.73	2°	
nadolol		0.95	1.88	-0.93	2.35	2°	
metoprolol		1.28	2.06	-0.78	2.53	2°	
pindolol		1.40	2.11	-0.71	2.58	2°	
acebutolol		0.66	2.40	-1.74	2.87	2°	
alprenolol		2.17	2.79	-0.62	3.26	2°	
propranolol		2.74	3.12	-0.38	3.59	2°	
fluoxetine		4.03	4.28	-0.25	4.75	2°	-0.7
procaine		0.73	1.57	-0.84	1.54	3°	
lidocaine		1.07	1.66	-0.59	1.63	3°	
chlorpromazine		3.40	4.34	-0.94	4.31	3°	-0.8
Neutral chemicals	**$logK_{mlw}$ neutral**		**Log K_{iam}**	**diff**			
Dataset to check $\delta_{IAM-SSLM}$	**Endo 2011 [15]**		**Sprunger 2007 [20]**				
1-Propanol	0.12		0.86	0.74			
Cyclohexanone	0.54		1.35	0.81			
1-Pentanol	1.08		1.61	0.53			
1-Hexanol	1.72		2.11	0.39			
Diethyl phthalate	1.77		2.91	1.14			
Phenol	1.95		1.96	0.01			
Estriol	1.96		2.93	0.97			
4-Fluorophenol	2.32		2.23	-0.09			
3-Methylphenol	2.34		2.33	-0.01			
4-Methylphenol	2.42		2.29	-0.13			
2-Methylphenol	2.45		2.30	-0.15			
2,6-Dimethylphenol	2.47		2.53	0.06			
4-Nitrophenol	2.72		2.56	-0.16			
3-Chlorophenol	2.78		2.98	0.20			

4-Ethylphenol	2.85		2.82	-0.03			
4-Chlorophenol	2.89		2.76	-0.13			
Chlorobenzene	3.00		2.86	-0.14			
Progesterone	3.28		4.26	0.98			
4-Phenylphenol	3.69		3.84	0.15			
1,3-Dichlorobenzene	3.71		3.76	0.05			
Estradiol	3.79		3.93	0.14			
Hexane	3.8		3.25	-0.55			
Heptane	4.55		4.47	-0.08			
Diazepam	2.99		3.47	0.48			
Average difference K_{mlw}-K_{iam} 24 neutrals				-0.21			

Table S4. IAM-HPLC measurement details

Code	Chemical	Mobile phase	Detec-tor RI = refract-ometer	% sol-ven t	pH	tracer Rt (min)	tracer	Sor-bate Rt (min)	Log Kiam sor-bate	Log Kiam aver-age	Log Kiam, intr
1N_I-01	2-hydroxyethyl ether	10 mM NH4 acetate	RI	0	5	1.38	water	1.41	-0.47	-0.46	
		10 mM NH4 acetate	RI	0	5	1.38	water	1.41	-0.45		
1N_I-02	Triethylene glycol	10 mM NH4 acetate	RI	0	5	1.38	water	1.46	0.01	0.01	
1N_I-03	2-methyl-2,4-pentanediol	10 mM NH4 acetate	RI	0	5	1.38	water	1.80	0.75	0.75	
1N_I-04	Urethane	10 mM NH4 acetate	RI	0	5	1.38	water	1.62	0.51	0.48	
		10 mM NH4 acetate	RI	0	5	1.38	water	1.63	0.52		
		10 mM NH4 acetate	UV	0	5	1.33	KBr	1.50	0.38		
1N_I-05	3-methyl-1-pentyn-3-ol	10 mM NH4 acetate	RI	0	5	1.38	water	2.53	1.19	1.19	
1N_I-06	n-phenyldiethanolamine	10 mM NH4 acetate	RI	0	5	1.38	water	6.49	1.84	1.85	
		10 mM NH4 acetate	RI	0	5	1.38	water	6.40	1.84		
		10 mM NH4 acetate	UV	0	5	1.33	KBr	6.49	1.87		
		10 mM NH4 acetate	UV	0	5	1.89	KBr	8.96	1.85		
		10 mM NH4 acetate	UV	0	5	1.85	KBr	8.73	1.85		
1N_I-07	3-methyl-3-pentanol	10 mM NH4 acetate	RI	0	5	1.38	water	3.36	1.43	1.43	
		10 mM NH4 acetate	RI	0	5	1.38	water	3.36	1.43		
1N_I-08	2,4,5-trimethyloxazole	10 mM NH4 acetate	UV	0	5	1.33	water	5.65	1.79	1.78	
		10 mM NH4 acetate	UV	0	5	1.90	KBr	7.83	1.77		
		10 mM NH4 acetate	UV	0	5	1.90	KBr	7.84	1.77		
1N_I-09	*cis*-3-hexen-1-ol	10 mM NH4 acetate	*RI*	0	5	1.38	water	4.20	1.58	1.58	
		10 mM NH4 acetate	RI	0	5	1.38	water	4.20	1.58		
1N_I-10	2-methyl-3,3,4,4-tetrafluoro-2-butanol	10 mM NH4 acetate	RI	0	5	1.38	water	3.86	1.53	1.53	
1N_I-11	*trans*-3-hexen-1-ol	10 mM NH4 acetate	*RI*	0	5	1.38	water	4.45	1.62	1.62	
		10 mM NH4 acetate	RI	0	5	1.38	water	4.45	1.62		
1N_I-12	2-phenoxyethanol	10 mM NH4 acetate	RI	0	5	1.38	water	5.02	1.70	1.70	
		10 mM NH4 acetate	RI	0	5	1.38	water	5.04	1.70		
		10 mM NH4 acetate	UV	0	5	1.33	KBr	5.08	1.73		
		10 mM NH4 acetate	UV	0	5	1.89	KBr	6.94	1.70		
		10 mM NH4 acetate	UV	0	5	1.89	KBr	6.77	1.69		
1N_I-13	2,6-dichlorobenzamide	10 mM NH4 acetate	UV	0	5	1.33	KBr	3.39	1.47	1.52	
		10 mM NH4 acetate	UV	0	5	1.89	KBr	5.34	1.54		
		10 mM NH4 acetate	UV	0	5	1.89	KBr	5.33	1.54		
1N_I-14	1-ethynyl-cyclohexanol	10 mM NH4 acetate	RI	0	5	1.38	water	6.06	1.80	1.80	
		10 mM NH4 acetate	RI	0	5	1.38	water	6.06	1.80		
1N_I-15	3,4-dimethyl-1-pentyn-3-ol	10 mM NH4 acetate	RI	0	5	1.38	water	4.27	1.60	1.60	
		10 mM NH4 acetate	RI	0	5	1.38	water	4.27	1.60		
1N_I-16	Diethyl benzylphosphonate	10 mM NH4 acetate	UV	0	5	1.33	KBr	20.22	2.43	2.41	
		10 mM NH4 acetate	UV	0	5	1.89	KBr	27.17	2.40		
		10 mM NH4 acetate	UV	0	5	1.89	KBr	27.14	2.40		
1N_I-17	2-(bromomethyl)-tetrahydro-2h-pyran	10 mM NH4 acetate	RI	0	5	1.38	water	5.66	1.77	1.79	
		PBS	UV	0	7.4	1.26	KBr	5.49	1.80		
		PBS	UV	0	7.4	1.26	KBr	5.48	1.80		
		PBS	UV	0	7.4	1.26	KBr	5.49	1.80		
1N_I-18	2',3',4'-trimethoxy-acetophenone	10 mM NH4 acetate	UV	0	5	1.33	KBr	19.47	2.41	2.40	
		10 mM NH4 acetate	UV	0	5	1.89	KBr	26.36	2.39		
		10 mM NH4 acetate	UV	0	5	1.89	KBr	26.35	2.39		
1N_I-19	2-dimethylaminopyridine	PBS	UV	0	7.4	1.44	KBr	8.36	1.96	1.96	
		PBS	UV	0	7.4	1.44	KBr	8.34	1.96		
		PBS	UV	0	7.4	1.44	KBr	8.33	1.96		
		10 mM NH4 acetate	UV	0	5	1.33	KBr	1.87	0.89		
		10 mM NH4 acetate	UV	0	5	1.90	KBr	2.63	0.87		
		10 mM NH4 acetate	UV	0	5	1.90	KBr	2.64	0.87		
		150 mM NaCl	UV	0	3	1.90	KBr	2.28	0.57		
		150 mM NaCl	UV	0	3	1.90	KBr	2.26	0.55		

Code	Chemical	Mobile phase	Detec-tor RI = refract-ometer	% sol-ven t	pH	tracer Rt (min)	tracer	Sor-bate Rt (min)	Log Kiam sor-bate	Log Kiam aver-age	Log Kiam, intr
		150 mM NaCl	UV	0	3	1.90	KBr	2.24	0.52		
1N_I-20	2-amino-4-chloro-6-methylpyrimidine	10 mM NH4 acetate	UV	0	5	1.33	KBr	5.56	1.78	1.76	
		10 mM NH4 acetate	UV	0	5	1.89	KBr	7.58	1.76		
		10 mM NH4 acetate	UV	0	5	1.89	KBr	7.56	1.75		
1N_I-21	2-phenyl-3-butyn-2-ol	10 mM NH4 acetate	UV	0	5	1.33	KBr	11.82	2.17	2.16	
		10 mM NH4 acetate	UV	0	5	1.89	KBr	15.78	2.14		
1N_I-22	2,5-dimethylfuran	PBS	UV	0	5	1.44	KBr	10.44	2.07	2.05	
		PBS	UV	0	5	1.44	KBr	10.44	2.07		
		PBS	UV	0	5	1.44	KBr	10.44	2.07		
		10 mM NH4 acetate	UV	0	5	1.45	water	9.13	2.00		
1N_I-23	2,3-dihydrobenzofuran	PBS	UV	0	7.4	1.44	KBr	14.28	2.23	2.22	
		PBS	UV	0	7.4	1.44	KBr	14.24	2.22		
		PBS	UV	0	7.4	1.44	KBr	14.23	2.22		
		10 mM NH4 acetate	UV	0	5	1.33	water	12.42	2.20		
1N_I-24	5-ethyl-2-methylpyridine	PBS	UV	0	5	1.44	KBr	22.36	2.44	2.51	
		PBS	UV	0	5	1.44	KBr	22.20	2.43		
1N_I-25	benzyl-tert-butanol	10 mM NH4 acetate	UV	0	5	1.45	water	31.15	2.59	2.58	
		10 mM NH4 acetate	UV	0	5	1.90	KBr	39.91	2.58		
		10 mM NH4 acetate	UV	0	5	1.90	KBr	39.84	2.58		
		PBS	UV	0	5	1.44	KBr	22.14	2.43		
1N_I-26	Benzyl sulfoxide	10 mM NH4 acetate	UV	0	5	1.33	water	40.60	2.75	2.73	
		10 mM NH4 acetate	UV	0	5	1.90	KBr	54.78	2.72		
		10 mM NH4 acetate	UV	0	5	1.90	KBr	54.78	2.72		
1N_I-27	2-(n-ethyl-m-toluidino)ethanol	PBS	UV	0	7.4	1.44	KBr	43.64	2.74	2.74	
		PBS	UV	0	7.4	1.44	KBr	43.42	2.74		
		PBS	UV	0	7.4	1.44	KBr	43.28	2.74		
		10 mM NH4 acetate	UV	0	5	1.45	KBr	7.80	1.92		
		10 mM NH4 acetate	UV	0	5	1.87	KBr	10.31	1.93		
		10 mM NH4 acetate	UV	0	5	1.87	KBr	10.30	1.93		
		150 mM NaCl	UV	0	3	1.90	KBr	3.67	1.24		
		150 mM NaCl	UV	0	3	1.90	KBr	3.62	1.23		
		150 mM NaCl	UV	0	3	1.90	KBr	3.61	1.23		
1N_I-28	A,A,A-trifluoro-o-tolunitrile	10 mM NH4 acetate	UV	0	5	1.45	water	28.27	2.54	2.54	
		10 mM NH4 acetate	UV	0	5	1.90	KBr	36.43	2.54		
		10 mM NH4 acetate	UV	0	5	1.90	KBr	36.24	2.53		
1N_I-29	A,A,A-4-tetrafluoro-*m*-toluidine	PBS	UV	0	7.4	1.44	KBr	35.79	2.65	2.64	
		PBS	UV	0	7.4	1.44	KBr	35.86	2.65		
		PBS	UV	0	7.4	1.44	KBr	35.82	2.65		
		10 mM NH4 acetate	UV	0	5	1.45	KBr	32.76	2.61		
1N_I-30	A,A,A-4-tetrafluoro-*o*-toluidine	PBS	UV	0	7.4	1.44	KBr	28.37	2.55	2.53	
		PBS	UV	0	7.4	1.44	KBr	28.39	2.55		
		PBS	UV	0	7.4	1.44	KBr	28.38	2.55		
		10 mM NH4 acetate	UV	0	5	1.45	KBr	25.72	2.50		
		150 mM NaCl	UV	0	3	1.90	KBr	34.99	2.52		
		150 mM NaCl	UV	0	3	1.90	KBr	34.59	2.51		
		150 mM NaCl	UV	0	3	1.90	KBr	34.47	2.51		
1N_I-31	4-ethoxy-2-nitroaniline	10 mM NH4 acetate	UV	0	5	1.45	water	50.50	2.81	2.87	
		PBS	UV	0	5	1.44	KBr	60.90	2.89		
		PBS	UV	0	5	1.44	KBr	61.20	2.89		
1N_I-32	4-(diethylamino)-benzaldehyde	PBS	UV	0	7.4	1.44	KBr	99.30	3.11	3.10	
		PBS	UV	0	7.4	1.44	KBr	99.00	3.11		
		10 mM NH4 acetate	UV	0	5	1.45	KBr	95.50	3.09		
		10 mM NH4 acetate	UV	0	5	1.50	KBr	101.0	3.10		
		10 mM NH4 acetate	UV	0	5	1.46	KBr	100.4	3.11		
		10 mM NH4 acetate	UV	0	5	1.46	KBr	100.0	3.10		
		150 mM NaCl	UV	0	3	1.90	KBr	89.60	2.94		

Code	Chemical	Mobile phase	Detec-tor RI = refract-ometer	% sol-vent	pH	tracer Rt (min)	tracer	Sor-bate Rt (min)	Log Kiam sor-bate	Log Kiam aver-age	Log Kiam, intr
1N_I-33	4-phenylpyridine	PBS	UV	0	7.4	1.44	KBr	88.10	3.05	3.05	
		PBS	UV	0	7.4	1.44	KBr	87.50	3.05		
		PBS	UV	0	7.4	1.44	KBr	87.00	3.05		
		10 mM NH4 acetate	UV	0	5	1.45	KBr	29.75	2.57		
		150 mM NaCl	UV	0	3	1.90	KBr	6.38	1.65		
		150 mM NaCl	UV	0	3	1.90	KBr	6.29	1.64		
		150 mM NaCl	UV	0	3	1.90	KBr	6.24	1.63		
1N_I-34	1,1-diphenyl-2-propyn-1-ol	10 mM NH4 acetate	UV	0	5	1.45	KBr	167.0	3.34	3.34	
		10 mM NH4 acetate	UV	0	5	1.50	KBr	177.5	3.34		
		10 mM NH4 acetate	UV	0	5	1.50	KBr	176.0	3.34		
1N_I-35	Butyl phenyl ether	30% ACN / 150 mM NaCl	UV	30	5	1.69	KBr	14.58	2.16	3.64	
		30% ACN / 150 mM NaCl	UV	30	5	1.69	KBr	14.56	2.16		
		25% ACN / 150 mM NaCl	UV	25	5	1.76	KBr	25.64	2.41		
		25% ACN / 150 mM NaCl	UV	25	5	1.76	KBr	25.56	2.41		
		20% ACN / 150 mM NaCl	UV	20	5	1.74	KBr	44.50	2.67		
		20% ACN / 150 mM NaCl	UV	20	5	1.74	KBr	44.70	2.67		
		15% ACN / 150 mM NaCl	UV	15	5	1.76	KBr	73.00	2.88		
1N_I-36	4-(diethylamino)-salicylaldehyde	10 mM NH4 acetate	UV	0	5	1.45	KBr	174.5	3.35	3.35	
		10 mM NH4 acetate	UV	0	5	1.45	KBr	172.0	3.35		
1N_I-37	Flavone	30% ACN / 150 mM NaCl	UV	30	5	1.61	KBr	10.05	2.00	3.90	
		25% ACN / 150 mM NaCl	UV	25	5	1.76	KBr	19.29	2.27		
		25% ACN / 150 mM NaCl	UV	25	5	1.76	KBr	19.18	2.27		
		20% ACN / 150 mM NaCl	UV	20	5	1.76	KBr	38.98	2.60		
		20% ACN / 150 mM NaCl	UV	20	5	1.74	KBr	39.19	2.61		
		15% ACN / 150 mM NaCl	UV	15	5	1.76	KBr	85.70	2.95		
1N_I-38	2-amino-4'-chloro-benzophenone	30% ACN / 150 mM NaCl	UV	30	5	1.77	KBr	20.53	2.30	4.21	
		30% ACN / 150 mM NaCl	UV	30	5	1.77	KBr	20.47	2.30		
		25% ACN / 150 mM NaCl	UV	25	5	1.76	KBr	38.76	2.60		
		25% ACN / 150 mM NaCl	UV	25	5	1.76	KBr	39.78	2.61		
		20% ACN / 150 mM NaCl	UV	20	5	1.74	KBr	81.00	2.93		
		15% ACN / 150 mM NaCl	UV	15	5	1.76	KBr	171.00	3.26		
1N_I-39	Di-n-butylisophthalate	30% ACN / 150 mM NaCl	UV	30	5	1.57	KBr	21.81	2.39	4.68	
		30% ACN / 150 mM NaCl	UV	30	5	1.57	KBr	21.69	2.39		
		30% ACN / 150 mM NaCl	UV	30	5	1.23	KBr	17.32	2.39		
		30% ACN / 150 mM NaCl	UV	30	5	1.23	KBr	17.97	2.41		
		25% ACN / 150 mM NaCl	UV	25	5	1.55	KBr	49.50	2.77		
		25% ACN / 150 mM NaCl	UV	25	5	1.55	KBr	48.80	2.76		
		25% ACN / 150 mM NaCl	UV	25	5	1.22	KBr	35.38	2.72		
		20% ACN / 150 mM NaCl	UV	20	5	1.22	KBr	93.50	3.16		
		20% ACN / 150 mM NaCl	UV	20	5	1.22	KBr	97.00	3.17		
1N_I-40	3-(4-tert-butylphenoxy)-benzaldehyde	30% ACN / 150 mM NaCl	UV	30	5	1.61	KBr	55.20	2.80	5.41	
		30% ACN / 150 mM NaCl	UV	30	5	1.77	KBr	60.80	2.80		
		25% ACN / 150 mM NaCl	UV	25	5	1.76	KBr	156.2	3.22		
		20% ACN / 150 mM NaCl	UV	20	5	1.74	KBr	437.0	3.67		
1N_I-41	3-(3,4-dichlorophenoxy)-benzaldehyde	30% ACN / 150 mM NaCl	UV	30	5	1.77	KBr	42.00	2.63	4.98	
		30% ACN / 150 mM NaCl	UV	30	5	1.77	KBr	41.50	2.63		
		25% ACN / 150 mM NaCl	UV	25	5	1.76	KBr	97.20	3.01		
		20% ACN / 150 mM NaCl	UV	20	5	1.74	KBr	243.0	3.42		
1N_II-01	6-chloro-2-pyridinol	10 mM NH4 acetate	UV	0	5	1.33	KBr	2.99	1.37	1.35	
		10 mM NH4 acetate	UV	0	5	1.90	KBr	4.07	1.33		
		10 mM NH4 acetate	UV	0	5	1.90	KBr	4.07	1.33		
1N_II-02	2-amino-5-bromopyridine	PBS	UV	0	7.4	1.44	KBr	11.47	2.12	2.12	
		PBS	UV	0	7.4	1.44	KBr	11.41	2.12		
		PBS	UV	0	7.4	1.44	KBr	11.40	2.12		

Code	Chemical	Mobile phase	Detec-tor RI = refract-ometer	% sol-ven t	pH	tracer Rt (min)	tracer	Sor-bate Rt (min)	Log Kiam sor-bate	Log Kiam aver-age	Log Kiam, intr
		10 mM NH4 acetate	UV	0	5	1.45	KBr	7.17	1.87		
		10 mM NH4 acetate	UV	0	5	1.85	KBr	9.87	1.91		
		10 mM NH4 acetate	UV	0	5	1.85	KBr	9.86	1.91		
		150 mM NaCl	UV	0	3	1.90	KBr	2.98	1.03		
		150 mM NaCl	UV	0	3	1.90	KBr	2.95	1.02		
		150 mM NaCl	UV	0	3	1.90	KBr	2.93	1.01		
1N_II-03	2-chloro-4-methylaniline	PBS	UV	0	7.4	1.44	KBr	30.64	2.58	2.56	
		PBS	UV	0	7.4	1.44	KBr	30.74	2.58		
		PBS	UV	0	7.4	1.44	KBr	30.65	2.58		
		10 mM NH4 acetate	UV	0	5	1.45	KBr	26.99	2.52		
		10 mM NH4 acetate	UV	0	5	1.85	KBr	34.87	2.53		
		10 mM NH4 acetate	UV	0	5	1.85	KBr	34.88	2.53		
1N_II-04	4-amino-2-nitrophenol	10 mM NH4 acetate	RI	0	5	1.38	water	5.36	1.73	1.74	
		10 mM NH4 acetate	RI	0	5	1.38	water	5.35	1.73		
		10 mM NH4 acetate	UV	0	5	1.33	KBr	5.36	1.76		
		10 mM NH4 acetate	UV	0	5	1.90	KBr	7.39	1.74		
		10 mM NH4 acetate	UV	0	5	1.90	KBr	7.19	1.72		
1N_II-05	2-chloro-4-nitroaniline	10 mM NH4 acetate	UV	0	5	1.33	KBr	53.00	2.87	2.84	
		10 mM NH4 acetate	UV	0	5	1.50	KBr	55.60	2.83		
		10 mM NH4 acetate	UV	0	5	1.50	KBr	55.20	2.83		
		10 mM NH4 acetate	UV	0	5	1.50	KBr	55.20	2.83		
1N_II-06	3-trifluoromethyl-4-nitrophenol	10 mM NH4 acetate	UV	0	5	1.50	KBr	149.0	3.27	3.27	
		10 mM NH4 acetate	UV	0	5	1.50	KBr	149.0	3.27		
		10 mM NH4 acetate	UV	0	5	1.50	KBr	149.0	3.27		
1Ach-01	Carbaryl	PBS	UV	0	7.4	1.26	water	64.50	2.98	2.98	
		PBS	UV	0	7.4	1.26	water	64.34	2.98		
		PBS	UV	0	7.4	1.26	water	64.09	2.97		
1Ach-02	Propoxur	PBS	UV	0	7.4	1.79	KBr	20.00	2.28	2.27	
		PBS	UV	0	7.4	1.65	KBr	17.77	2.27		
		PBS	UV	0	7.4	1.65	KBr	17.60	2.26		
1Ach-03	Diazinon	30% ACN / PBS	UV	30	7.4	1.29	water	7.81	1.98	4.04	
		25% ACN / PBS	UV	25	7.4	1.29	water	16.34	2.34		
		25% ACN / PBS	UV	25	7.4	1.29	water	17.23	2.37		
		20% ACN / PBS	UV	20	7.4	1.27	water	31.21	2.65		
		20% ACN / PBS	UV	20	7.4	1.27	water	31.18	2.65		
		15% ACN / PBS	UV	15	7.4	1.29	water	70.60	3.01		
		15% ACN / PBS	UV	15	7.4	1.29	water	78.10	3.05		
1Ach-04	Aminocarb	PBS	UV	0	7.4	1.79	KBr	31.00	2.49	2.48	
		PBS	UV	0	7.4	1.65	KBr	28.53	2.49		
		PBS	UV	0	7.4	1.65	KBr	28.08	2.48		
		PBS	UV	0	7.4	1.65	KBr	27.79	2.48		
1Ach-05	Aldicarb	PBS	UV	0	7.4	1.57	KBr	8.37	1.91	1.91	
		PBS	UV	0	7.4	1.57	KBr	8.35	1.91		
		PBS	UV	0	7.4	1.57	KBr	8.32	1.91		
		PBS	UV	0	7.4	1.57	KBr	8.28	1.91		
1Ach-06	Carbofuran	PBS	UV	0	7.4	1.46	KBr	25.22	2.49	2.46	
		PBS	UV	0	7.4	1.46	KBr	24.99	2.48		
		PBS	UV	0	7.4	1.46	KBr	25.50	2.49		
		PBS	UV	0	7.4	1.57	KBr	20.51	2.36		
1Ach-07	EPN	30% ACN / 150 mM NaCl	UV	30	5	1.57	KBr	35.70	2.61	5.10	
		30% ACN / 150 mM NaCl	UV	30	5	1.23	KBr	35.50	2.72		
		30% ACN / 150 mM NaCl	UV	30	5	1.23	KBr	44.50	2.82		
		25% ACN / 150 mM NaCl	UV	25	5	1.22	KBr	67.00	3.01		
		25% ACN / 150 mM NaCl	UV	25	5	1.22	KBr	67.20	3.01		
		20% ACN / 150 mM NaCl	UV	20	5	1.22	KBr	226.0	3.54		
		20% ACN / 150 mM NaCl	UV	20	5	1.22	KBr	221.0	3.53		
1Ach-08	Azinphos-methyl	30% ACN / 150 mM NaCl	UV	30	5	1.53	KBr	5.94	1.74	3.58	
		25% ACN / 150 mM NaCl	UV	25	5	1.53	KBr	10.17	2.03		
		25% ACN / 150 mM NaCl	UV	25	5	1.53	KBr	10.22	2.03		
		20% ACN / 150 mM NaCl	UV	20	5	1.53	KBr	19.36	2.34		
		20% ACN / 150 mM NaCl	UV	20	5	1.53	KBr	19.38	2.34		

Code	Chemical	Mobile phase	Detec-tor RI = refract-ometer	% sol-ven t	pH	tracer Rt (min)	tracer	Sor-bate Rt (min)	Log Kiam sor-bate	Log Kiam aver-age	Log Kiam, intr
		15% ACN / 150 mM NaCl	UV	15	5	1.54	KBr	38.11	2.65		
		15% ACN / 150 mM NaCl	UV	15	5	1.53	KBr	38.29	2.66		
1Rea-01	Butanal	PBS	UV	0	7.4	1.57	KBr	2.45	1.02	1.02	
1Rea-02	4-fluoroaniline	PBS	UV	0	7.4	1.46	KBr	4.86	1.64	1.63	
		PBS	UV	0	7.4	1.86	KBr	5.92	1.62		
		PBS	UV	0	7.4	1.57	KBr	5.10	1.63		
1Rea-03	2,4-dinitrotoluene	PBS	UV	0	7.4	1.46	KBr	22.33	2.43	2.42	
		PBS	UV	0	7.4	1.86	KBr	27.07	2.41		
		PBS	UV	0	7.4	1.57	KBr	23.13	2.41		
1Rea-04	4-nitrobenzaldehyde	PBS	UV	0	7.4	1.50	KBr	7.78	1.90	1.90	
		PBS	UV	0	7.4	1.50	KBr	7.77	1.90		
		PBS	UV	0	7.4	1.50	KBr	7.74	1.89		
1Rea-05	Benzaldehyde	PBS	UV	0	7.4	1.79	KBr	7.70	1.80	1.80	
		PBS	UV	0	7.4	1.51	KBr	6.52	1.80		
		PBS	UV	0	7.4	1.51	KBr	6.50	1.80		
1Rea-06	2,4,5-tribromoimidazole	PBS	UV	0	7.4	1.50	KBr	16.37	2.27	2.27	
		PBS	UV	0	7.4	1.50	KBr	16.36	2.27		
		PBS	UV	0	7.4	1.50	KBr	16.29	2.27		
1Rea-07	4-dimethylamino-cinnamaldehyde	PBS	UV	0	7.4	1.60	KBr	111.5	3.11	3.11	
		PBS	UV	0	7.4	1.60	KBr	110.0	3.11		
		PBS	UV	0	7.4	1.60	KBr	109.0	3.10		
1Rea-08	Salicylaldehyde	PBS	UV	0	7.4	1.79	KBr	9.80	1.93	1.91	
		PBS	UV	0	7.4	1.65	KBr	8.72	1.91		
		PBS	UV	0	7.4	1.65	KBr	8.71	1.91		
1Rea-09	4-chlorocatechol	PBS	UV	0	7.4	1.79	KBr	5.56	1.60	1.60	
1Rea-10	1-benzoylacetone	PBS	UV	0	7.4	1.79	KBr	37.00	2.57	2.57	
		PBS	UV	0	7.4	1.51	KBr	31.30	2.57		
		PBS	UV	0	7.4	1.51	KBr	31.06	2.57		
1Rea-11	Pentafluorobenzaldehyde	PBS	UV	0	7.4	1.50	KBr	6.88	1.83	1.83	
		PBS	UV	0	7.4	1.50	KBr	6.88	1.83		
		PBS	UV	0	7.4	1.50	KBr	6.87	1.83		
1Rea-12	A,A,A-trifluoro-*m*-tolualdehyde	PBS	UV	0	7.4	1.50	KBr	24.80	2.47	2.46	
		PBS	UV	0	7.4	1.50	KBr	24.60	2.46		
		PBS	UV	0	7.4	1.50	KBr	24.70	2.46		
1Rea-13	1,3,5-trichloro-2,4-dinitro-benzene	30% ACN / 150 mM NaCl	UV	30	5	1.57	KBr	14.02	2.18	4.04	
		30% ACN / 150 mM NaCl	UV	30	5	1.57	KBr	14.01	2.18		
		30% ACN / 150 mM NaCl	UV	30	5	1.23	KBr	10.88	2.17		
		30% ACN / 150 mM NaCl	UV	30	5	1.23	KBr	11.00	2.18		
		25% ACN / 150 mM NaCl	UV	25	5	1.55	KBr	27.86	2.51		
		25% ACN / 150 mM NaCl	UV	25	5	1.55	KBr	28.01	2.51		
		25% ACN / 150 mM NaCl	UV	25	5	1.22	KBr	20.09	2.47		
		20% ACN / 150 mM NaCl	UV	20	5	1.22	KBr	41.00	2.79		
		20% ACN / 150 mM NaCl	UV	20	5	1.22	KBr	42.01	2.80		
1Rea-14	2-methyl-1,4-naphtho-quinone	PBS	UV	0	7.4	1.51	KBr	42.26	2.71	2.72	
		PBS	UV	0	7.4	1.51	KBr	42.38	2.71		
		PBS	UV	0	7.4	1.51	KBr	44.99	2.74		
1Rea-15	A-bromo-2',5'-dimethoxy-acetophenone	PBS	UV	0	7.4	1.79	KBr	125.0	3.11	3.12	
		PBS	UV	0	7.4	1.46	KBr	106.0	3.13		
		PBS	UV	0	7.4	1.46	KBr	106.0	3.13		
1Rea-16	1,3-dichloro-4,6-dinitro-benzene	PBS	UV	0	7.4	1.79	KBr	42.28	2.63	2.64	
		PBS	UV	0	7.4	1.46	KBr	35.32	2.64		
		PBS	UV	0	7.4	1.46	KBr	35.09	2.64		
		PBS	UV	0	7.4	1.46	KBr	35.07	2.64		
1Rea-17	N-vinylcarbazole	30% ACN / 150 mM NaCl	UV	30	5	1.57	KBr	37.80	2.64	4.95	

Code	Chemical	Mobile phase	Detec-tor RI = refract-ometer	% sol-vent	pH	tracer Rt (min)	tracer	Sor-bate Rt (min)	Log Kiam sor-bate	Log Kiam aver-age	Log Kiam, intr
		30% ACN / 150 mM NaCl	UV	30	5	1.57	KBr	37.90	2.64		
		30% ACN / 150 mM NaCl	UV	30	5	1.57	KBr	34.40	2.60		
		25% ACN / 150 mM NaCl	UV	25	5	1.22	KBr	62.40	2.98		
		25% ACN / 150 mM NaCl	UV	25	5	1.22	KBr	61.80	2.97		
		20% ACN / 150 mM NaCl	UV	20	5	1.22	KBr	166.0	3.41		
		20% ACN / 150 mM NaCl	UV	20	5	1.22	KBr	166.5	3.41		
1Blo-01	Rotenone	30% ACN / 150 mM NaCl	UV	30	5	1.53	KBr	10.84	2.06	4.58	
		30% ACN / 150 mM NaCl	UV	30	5	1.53	KBr	10.63	2.05		
		25% ACN / 150 mM NaCl	UV	25	5	1.53	KBr	24.90	2.46		
		25% ACN / 150 mM NaCl	UV	25	5	1.53	KBr	24.96	2.46		
		20% ACN / 150 mM NaCl	UV	20	5	1.52	KBr	64.60	2.89		
		20% ACN / 150 mM NaCl	UV	20	5	1.53	KBr	66.00	2.90		
1Unc-01	2,4-dinitroaniline	PBS	UV	0	7.4	1.50	KBr	40.60	2.69	2.69	
1AUns-01	Salicylic acid	PBS	UV	0	7.4	1.40	water	2.13	0.99	0.99	1.49
1AUnc-01	2,4-Dinitrophenol	PBS	UV	0	7.4	1.40	water	6.33	1.82	1.86	2.36
		10 mM NH4 acetate	UV	0	5	1.46	KBr	7.65	1.90		
1AUnc-02	Dinoseb	PBS	UV	0	7.4	1.40	water	135.6	3.26	3.26	3.76
		PBS	UV	0	7.4	1.40	water	136.3	3.26		
1AUnc-03	Pentachlorophenol	30% ACN / PBS	UV	30	7.4	1.38	thiourea	4.76	1.66	3.95	4.45
		30% ACN / PBS	UV	30	7.4	1.38	thiourea	4.80	1.67		
		25% ACN / PBS	UV	26	7.4	1.39	thiourea	9.28	2.03		
		25% ACN / PBS	UV	25	7.4	1.39	thiourea	9.27	2.03		
		20% ACN / PBS	UV	20	7.4	1.40	thiourea	20.63	2.41		
		20% ACN / PBS	UV	20	7.4	1.40	thiourea	20.69	2.42		
		15% ACN / PBS	UV	15	7.4	1.41	thiourea	51.27	2.82		
1AN-01	2,3,4,6-tetrachlorophenol	30% ACN / PBS	UV	30	7.4	1.38	thiourea	2.95	1.33	3.29	3.79
		30% ACN / PBS	UV	30	7.4	1.38	thiourea	2.97	1.33		
		25% ACN / PBS	UV	25	7.4	1.39	thiourea	4.65	1.64		
		25% ACN / PBS	UV	25	7.4	1.39	thiourea	4.66	1.65		
		20% ACN / PBS	UV	20	7.4	1.40	thiourea	8.40	1.98		
		20% ACN / PBS	UV	20	7.4	1.40	thiourea	8.43	1.98		
		15% ACN / PBS	UV	15	7.4	1.41	thiourea	16.68	2.31		
		15% ACN / PBS	UV	15	7.4	1.41	thiourea	16.75	2.31		
2A-01	Clopyralid	100 mM NH4 acetate	UV	0	5.5	1.34	water	1.66	0.64	0.64	0.64
2A-02	Fluroxypyr	PBS	UV	0	7.4	1.44	thiourea	3.38	1.41	1.40	1.90
		PBS	UV	0	7.4	1.44	thiourea	3.34	1.40		
		PBS	UV	0	7.4	1.44	thiourea	3.34	1.40		
2A-03	Triclopyr	PBS	UV	0	7.4	1.44	thiourea	4.98	1.67	1.66	2.16
		PBS	UV	0	7.4	1.44	thiourea	4.92	1.66		
		PBS	UV	0	7.4	1.44	thiourea	4.92	1.66		
2A-04	MCPA	PBS	UV	0	7.4	1.44	thiourea	4.87	1.65	1.64	2.14
		PBS	UV	0	7.4	1.44	thiourea	4.81	1.65		
		PBS	UV	0	7.4	1.44	thiourea	4.81	1.65		
		PBS	UV	0	7.4	1.44	thiourea	4.66	1.63		
		PBS	UV	0	7.4	1.44	thiourea	4.64	1.62		
		PBS	UV	0	7.4	1.44	thiourea	4.64	1.62		
2A-05	2,4-D	PBS	UV	0	7.4	1.44	thiourea	4.72	1.63	1.63	2.13
		PBS	UV	0	7.4	1.44	thiourea	4.70	1.63		
		PBS	UV	0	7.4	1.44	thiourea	4.71	1.63		
2A-06	MCPP (mecoprop)	PBS	UV	0	7.4	1.44	thiourea	6.16	1.79	1.78	2.28
		PBS	UV	0	7.4	1.44	thiourea	6.07	1.78		
		PBS	UV	0	7.4	1.44	thiourea	6.07	1.79		
		PBS	UV	0	7.4	1.44	thiourea	5.87	1.77		
		PBS	UV	0	7.4	1.44	thiourea	5.88	1.77		
		PBS	UV	0	7.4	1.44	thiourea	5.84	1.76		
2A-07	2,4-DP	PBS	UV	0	7.4	1.44	thiourea	6.13	1.79	1.79	2.29
		PBS	UV	0	7.4	1.44	thiourea	6.14	1.79		
		PBS	UV	0	7.4	1.44	thiourea	6.10	1.79		
2A-08	MCPB	PBS	UV	0	7.4	1.44	thiourea	14.65	2.24	2.24	2.74
		PBS	UV	0	7.4	1.44	thiourea	14.72	2.24		
		PBS	UV	0	7.4	1.44	thiourea	14.60	2.24		
2A-09	2,4-DB	PBS	UV	0	7.4	1.44	thiourea	15.98	2.28	2.28	2.78

Code	Chemical	Mobile phase	Detec-tor RI = refract-ometer	% sol-ven t	pH	tracer Rt (min)	tracer	Sor-bate Rt (min)	Log Kiam sor-bate	Log Kiam aver-age	Log Kiam, intr
		PBS	UV	0	7.4	1.44	thiourea	16.07	2.28		
		PBS	UV	0	7.4	1.44	thiourea	15.98	2.28		
2A-10	2,4,5-T	PBS	UV	0	7.4	1.44	thiourea	10.87	2.09	2.09	2.59
		PBS	UV	0	7.4	1.44	thiourea	10.92	2.10		
		PBS	UV	0	7.4	1.44	thiourea	10.88	2.09		
2A-11	DNOC	PBS	UV	0	7.4	1.44	thiourea	12.06	2.14	2.15	2.65
		PBS	UV	0	7.4	1.44	thiourea	12.17	2.15		
		PBS	UV	0	7.4	1.44	thiourea	12.14	2.15		
2A-12	Dinoseb	PBS	UV	0	7.4	1.40	water	135.6	3.26	3.26	3.76
		PBS	UV	0	7.4	1.40	water	136.3	3.26		
2A-13	Bromoxynil	PBS	UV	0	7.4	1.44	thiourea	13.50	2.20	2.20	2.70
		PBS	UV	0	7.4	1.44	thiourea	13.56	2.20		
2A-14	Ioxynil	PBS	UV	0	7.4	1.44	thiourea	50.73	2.81	2.81	3.31
		PBS	UV	0	7.4	1.44	thiourea	51.01	2.81		
2A-15	Triasulfuron	PBS	UV	0	7.4	1.43	thiourea	4.14	1.55	1.55	2.05
		PBS	UV	0	7.4	1.44	thiourea	4.13	1.55		
		PBS	UV	0	7.4	1.44	thiourea	4.13	1.55		
2A-16	Bensulfuron-methyl	PBS	UV	0	7.4	1.44	thiourea	18.18	2.34	2.32	2.82
		20% ACN / PBS	UV	20	7.4	1.44	thiourea	2.04	0.89		
		15% ACN / PBS	UV	15	7.4	1.44	thiourea	2.79	1.25		
		15% ACN / PBS	UV	15	7.4	1.44	thiourea	2.76	1.24		
		10% ACN / PBS	UV	10	7.4	1.44	thiourea	4.32	1.58		
		10% ACN / PBS	UV	10	7.4	1.44	thiourea	4.31	1.58		
2A-17	Fomesafen	PBS	UV	0	7.4	1.44	thiourea	74.00	2.98	2.98	3.48
		PBS	UV	0	7.4	1.44	thiourea	72.82	2.97		
		PBS	UV	0	7.4	1.44	thiourea	72.98	2.97		
		20% ACN / PBS	UV	20	7.4	1.44	thiourea	7.15	1.88		
		15% ACN / PBS	UV	15	7.4	1.44	thiourea	13.60	2.20		
		10% ACN / PBS	UV	10	7.4	1.44	thiourea	25.32	2.50		
2N-01	Alachlor	30% ACN / PBS	UV	30	7.4	1.29	water	5.19	1.76	3.32	
		25% ACN / PBS	UV	25	7.4	1.29	water	8.67	2.03		
		25% ACN / PBS	UV	25	7.4	1.29	water	8.44	2.02		
		20% ACN / PBS	UV	20	7.4	1.27	water	15.97	2.34		
		20% ACN / PBS	UV	20	7.4	1.27	water	15.98	2.34		
		20% ACN / PBS	UV	20	7.4	1.27	water	15.82	2.34		
		20% ACN / PBS	UV	20	7.4	1.27	water	15.82	2.34		
		15% ACN / PBS	UV	15	7.4	1.29	water	28.40	2.60		
		15% ACN / PBS	UV	15	7.4	1.29	water	29.40	2.61		
		0% ACN / PBS	UV	0	7.4	1.27	water	122.0	3.25		
2N-02	Metolachlor	30% ACN / PBS	UV	30	7.4	1.29	water	5.08	1.74	3.40	
		25% ACN / PBS	UV	25	7.4	1.29	water	8.54	2.03		
		25% ACN / PBS	UV	25	7.4	1.29	water	8.52	2.03		
		20% ACN / PBS	UV	20	7.4	1.27	water	14.98	2.31		
		20% ACN / PBS	UV	20	7.4	1.27	water	14.97	2.31		
		15% ACN / PBS	UV	15	7.4	1.29	water	29.04	2.61		
		15% ACN / PBS	UV	15	7.4	1.29	water	31.33	2.64		
		0% ACN / PBS	UV	0	7.4	1.27	water	155.5	3.36		
2N-03	Simazine	PBS	UV	0	7.4	1.26	water	21.80	2.49	2.49	
		PBS	UV	0	7.4	1.26	water	21.80	2.49		
		PBS	UV	0	7.4	1.26	water	21.90	2.49		
2N-04	Ametryn	PBS	UV	0	7.4	1.26	water	94.50	3.15	3.14	
		PBS	UV	0	7.4	1.26	water	94.40	3.15		
		PBS	UV	0	7.4	1.26	water	94.00	3.14		
2N-05	Terbutylazine	PBS	UV	0	7.4	1.26	water	154.5	3.36	3.36	
		PBS	UV	0	7.4	1.26	water	154.0	3.36		
		PBS	UV	0	7.4	1.26	water	153.0	3.36		
2N-06	Diuron	PBS	UV	0	7.4	1.26	water	162.0	3.38	3.38	
		PBS	UV	0	7.4	1.26	water	162.5	3.38		
		PBS	UV	0	7.4	1.26	water	163.0	3.38		
2N-07	Linuron	PBS	UV	0	7.4	1.26	water	220.0	3.52	3.51	
		PBS	UV	0	7.4	1.26	water	216.0	3.51		
		PBS	UV	0	7.4	1.26	water	209.5	3.49		
2N-08	Chloroxuron	30% ACN / PBS	UV	30	7.4	1.29	water	8.73	2.04	4.25	

Code	Chemical	Mobile phase	Detec-tor RI = refract-ometer	% sol-vent	pH	tracer Rt (min)	tracer	Sor-bate Rt (min)	Log Kiam sor-bate	Log Kiam aver-age	Log Kiam, intr
		25% ACN / PBS	UV	25	7.4	1.29	water	17.47	2.37		
		25% ACN / PBS	UV	25	7.4	1.29	water	17.41	2.37		
		20% ACN / PBS	UV	20	7.4	1.27	water	40.61	2.77		
		20% ACN / PBS	UV	20	7.4	1.27	water	39.79	2.76		
		15% ACN / PBS	UV	15	7.4	1.29	water	96.20	3.14		
2N-09	Ethofumesate	PBS	UV	0	7.4	1.26	water	120.0	3.25	3.25	
		PBS	UV	0	7.4	1.26	water	118.5	3.25		
		PBS	UV	0	7.4	1.26	water	118.0	3.24		
2N-10	Prosulfocarb	30% ACN / PBS	UV	30	7.4	1.29	water	15.92	2.33	4.61	
		25% ACN / PBS	UV	25	7.4	1.29	water	33.64	2.68		
		25% ACN / PBS	UV	25	7.4	1.29	water	32.56	2.66		
		20% ACN / PBS	UV	20	7.4	1.27	water	76.00	3.05		
		20% ACN / PBS	UV	20	7.4	1.27	water	75.90	3.05		
		15% ACN / PBS	UV	15	7.4	1.29	water	191.8	3.45		
		15% ACN / PBS	UV	15	7.4	1.29	water	218.0	3.50		
2N-11	Clomazone	30% ACN / PBS	UV	30	7.4	1.29	water	3.10	1.42	2.93	
		30% ACN / PBS	UV	30	7.4	1.29	water	3.01	1.40		
		25% ACN / PBS	UV	25	7.4	1.29	water	4.55	1.68		
		25% ACN / PBS	UV	25	7.4	1.29	water	4.42	1.66		
		20% ACN / PBS	UV	20	7.4	1.27	water	7.42	1.96		
		20% ACN / PBS	UV	20	7.4	1.27	water	7.57	1.97		
		15% ACN / PBS	UV	15	7.4	1.29	water	12.55	2.22		
		15% ACN / PBS	UV	15	7.4	1.29	water	11.25	2.16		
		15% ACN / PBS	UV	15	7.4	1.29	water	13.04	2.24		
		15% ACN / PBS	UV	15	7.4	1.29	water	11.28	2.17		
		0% ACN / PBS	UV	0	7.4	1.27	water	57.10	2.92		
		0% ACN / PBS	UV	0	7.4	1.27	water	56.20	2.91		
		0% ACN / PBS	UV	0	7.4	1.27	water	56.70	2.92		
		0% ACN / PBS	UV	0	7.4	1.27	water	56.00	2.91		
2N-12	Trifluralin	30% ACN / PBS	UV	30	7.4	1.29	water	37.20	2.72	5.48	
		25% ACN / PBS	UV	25	7.4	1.29	water	104.0	3.18		
		25% ACN / PBS	UV	25	7.4	1.29	water	102.0	3.17		
		20% ACN / PBS	UV	20	7.4	1.27	water	295.0	3.64		
3Ca01	Salicylic acid	PBS	UV	0	7.4	1.40	water	2.13	0.99	0.99	1.49
3Ca02	5-Phenylvaleric acid	PBS	UV	0	7.4	1.40	water	3.61	1.47	1.47	1.97
3Ca03	Ibuprofen	PBS	UV	0	7.4	1.40	water	15.61	2.28	2.28	2.78
3Ca04	Fenamic acid	PBS	UV	30	7.4	1.40	water	1.93	0.85	2.93	3.43
		PBS	UV	25	7.4	1.47	water	2.82	1.24		
		PBS	UV	15	7.4	1.47	water	7.53	1.89		
3Ca05	Diclofenac	PBS	UV	0	7.4	1.40	water	117.5	3.20	3.26	3.76
		PBS	UV	0	7.4	1.40	water	115.4	3.19		
		PBS	UV	30	7.4	1.40	water	2.43	1.14		
		PBS	UV	25	7.4	1.47	water	4.47	1.59		
		PBS	UV	20	7.4	1.47	water	17.47	2.31		
		PBS	UV	15	7.4	1.47	water	20.89	2.40		
3Ca06	Difflunisal	PBS	UV	0	7.4	1.40	water	108.2	3.16	3.23	3.73
		PBS	UV	0	7.4	1.40	water	108.8	3.16		
		PBS	UV	30	7.4	1.40	water	2.10	0.98		
		PBS	UV	25	7.4	1.47	water	3.62	1.44		
		PBS	UV	20	7.4	1.47	water	13.30	2.18		
		PBS	UV	15	7.4	1.47	water	16.19	2.28		
3Su01	4-octylbenzene-1-sulfonate	30% ACN / PBS	UV	30	7.4	1.38	thiourea	6.64	1.86	4.31	4.81
		30% ACN / PBS	UV	30	7.4	1.38	thiourea	6.64	1.86		
		25% ACN / PBS	UV	26	7.4	1.39	thiourea	14.61	2.25		
		25% ACN / PBS	UV	25	7.4	1.39	thiourea	14.80	2.26		
		20% ACN / PBS	UV	20	7.4	1.40	thiourea	35.91	2.67		
		20% ACN / PBS	UV	20	7.4	1.40	thiourea	36.27	2.67		
		15% ACN / PBS	UV	15	7.4	1.41	thiourea	92.99	3.09		
		15% ACN / PBS	UV	15	7.4	1.41	thiourea	92.74	3.09		
3Su02	C_{10}-2-LAS	30% ACN / PBS	UV	30	7.4	1.38	thiourea	13.55	2.22	5.11	5.61
		30% ACN / PBS	UV	30	7.4	1.38	thiourea	13.16	2.21		
		25% ACN / PBS	UV	26	7.4	1.39	thiourea	36.82	2.68		

Code	Chemical	Mobile phase	Detec-tor RI = refract-ometer	% sol-ven t	pH	tracer Rt (min)	tracer	Sor-bate Rt (min)	Log Kiam sor-bate	Log Kiam aver-age	Log Kiam, intr
		25% ACN / PBS	UV	25	7.4	1.39	thiourea	36.74	2.68		
		20% ACN / PBS	UV	20	7.4	1.4	thiourea	112.4	3.18		
3Ph01	Warfarin	PBS	UV	0	7.4	1.4	water	28.24	2.56	2.56	3.06
3Ph02	Pentafluorophenol	PBS	UV	0	7.4	1.4	water	5.08	1.70	1.70	2.20
3Ph03	2,4-Dinitrophenol	PBS	UV	0	7.4	1.4	water	6.33	1.82	1.86	2.36
		10 mM NH4 acetate	UV	0	5	1.46	KBr	7.65	1.90		
3Ph04	Bromoxynil	PBS	UV	0	7.4	1.43	thiourea	13.50	2.20	2.20	2.70
		PBS	UV	0	7.4	1.43	thiourea	13.56	2.20		
3Ph05	2-Methyl-4,6-dinitrophenol	PBS	UV	0	7.4	1.40	water	15.25	2.27	2.27	2.77
3Ph06	4-Tert-butyl-2,6-dinitrophenol	PBS	UV	0	7.4	1.40	water	57.30	2.88	2.88	3.38
3Ph07	Dinoseb	PBS	UV	0	7.4	1.40	water	135.6	3.26	3.26	3.76
		PBS	UV	0	7.4	1.40	water	136.3	3.26		
3Ph08	2,3,4,6-tetrachlorophenol	30% ACN / PBS	UV	30	7.4	1.38	thiourea	2.95	1.33	3.29	3.79
		30% ACN / PBS	UV	30	7.4	1.38	thiourea	2.97	1.33		
		25% ACN / PBS	UV	25	7.4	1.39	thiourea	4.65	1.64		
		25% ACN / PBS	UV	25	7.4	1.39	thiourea	4.66	1.65		
		20% ACN / PBS	UV	20	7.4	1.40	thiourea	8.40	1.98		
		20% ACN / PBS	UV	20	7.4	1.40	thiourea	8.43	1.98		
		15% ACN / PBS	UV	15	7.4	1.41	thiourea	16.68	2.31		
		15% ACN / PBS	UV	15	7.4	1.41	thiourea	16.75	2.31		
3Ph09	2,3,5,6-tetrachlorophenol	30% ACN / PBS	UV	30	7.4	1.38	thiourea	2.91	1.32	3.28	3.78
		30% ACN / PBS	UV	30	7.4	1.38	thiourea	2.94	1.33		
		25% ACN / PBS	UV	26	7.4	1.39	thiourea	4.58	1.63		
		25% ACN / PBS	UV	25	7.4	1.39	thiourea	4.58	1.64		
		20% ACN / PBS	UV	20	7.4	1.40	thiourea	8.29	1.97		
		20% ACN / PBS	UV	20	7.4	1.40	thiourea	8.29	1.97		
		15% ACN / PBS	UV	15	7.4	1.41	thiourea	16.50	2.31		
		15% ACN / PBS	UV	15	7.4	1.41	thiourea	16.57	2.31		
3Ph10	Pentachlorophenol	30% ACN / PBS	UV	30	7.4	1.38	thiourea	4.76	1.66	3.95	4.45
		30% ACN / PBS	UV	30	7.4	1.38	thiourea	4.80	1.67		
		25% ACN / PBS	UV	26	7.4	1.39	thiourea	9.28	2.03		
		25% ACN / PBS	UV	25	7.4	1.39	thiourea	9.27	2.03		
		20% ACN / PBS	UV	20	7.4	1.40	thiourea	20.63	2.41		
		20% ACN / PBS	UV	20	7.4	1.40	thiourea	20.69	2.42		
		15% ACN / PBS	UV	15	7.4	1.41	thiourea	51.27	2.82		

1. Timmer, N.; Droge, S. T. J., Sorption of cationic surfactants to artificial cell membranes: comparing phospholipid bilayers with monolayer coatings and molecular simulations. *Environmental Science & Technology* **2017,** *51*, 2890-2898.
2. Droge, S. T. J., Membrane-water partition coefficients to aid risk assessment of perfluoroalkyl anions and alkyl sulfates. *Environmental Science & Technology* **2019,** *53*, 760-770.
3. Droge, S. T. J., Dealing with Confounding pH-Dependent Surface Charges in Immobilized Artificial Membrane HPLC Columns. *Analytical Chemistry* **2016,** *88*, (1), 960-967.
4. Droge, S. T. J.; Hermens, J. L. M.; Gutsell, S.; Rabone, J.; Hodges, G., Predicting the phospholipophilicity of monoprotic positively charged amines. *Environ. Sci. Process. Impacts* **2017,** *19*, 307-323.
5. Droge, S. T. J.; Hermens, J. L. M.; Rabone, J.; Gutsell, S.; Hodges, G., Phospholipophilicity of CxHyN+ amines: Chromatographic descriptors and molecular simulations for understanding partitioning into membranes. *Environmental Science: Processes & Impacts* **2016,** *18*, 1011-1023.
6. Yang, Y. X.; Zhang, Q.; Li, Q. Q.; Xia, Z. N.; Chen, H.; Zhou, K.; Yang, F. Q., pH-dependent surface electrostatic effects in retention on immobilized artificial membrane chromatography: Determination of the intrinsic phospholipid-water sorption coefficients of diverse analytes. *Journal of Chromatography A* **2018,** *1570*, 172-182.
7. Rhee, D.; Markovich, R.; Chae, W. G.; Qiu, X.; Pidgeon, C., Chromatographic surfaces prepared from lyso phosphatidylcholine ligands. *Analytica Chimica Acta* **1994,** *297*, (3), 377-386.
8. Ong, S.; Liu, H.; Qiu, X.; Bhat, G.; Pidgeon, C., Membrane partition coefficients chromatographically measured using immobilized artificial membrane surfaces. *Analytical Chemistry* **1995,** *67*, (4), 755-762.
9. Ong, S.; Pidgeon, D., Thermodynamics of solute partitioning into immobilized artificial membranes. *Analytical Chemistry* **1995,** *67*, (13), 2119-2128.
10. Escher, B. I.; Schwarzenbach, R. P.; Westall, J. C., Evaluation of liposome-water partitioning of organic acids and bases. 2. Comparison of experimental determination methods. *Environmental Science & Technology* **2000,** *34*, (18), 3962-3968.
11. Yen, T. E.; Agatonovic-Kustrin, S.; Evans, A. M.; Nation, R. L.; Ryand, J., Prediction of drug absorption based on immobilized artificial membrane (IAM) chromatography separation and calculated molecular descriptors. *Journal of Pharmaceutical and Biomedical Analysis* **2005,** *38*, (3), 472-478.
12. Enoch, S. J.; Hewitt, M.; Cronin, M. T. D.; Azam, S.; Madden, J. C., Classification of chemicals according to mechanism of aquatic toxicity: An evaluation of the implementation of the Verhaar scheme in Toxtree. *Chemosphere* **2008,** *73*, (3), 243-248.
13. Ellison, C. M.; Madden, J. C.; Cronin, M. T. D.; Enoch, S. J., Investigation of the Verhaar scheme for predicting acute aquatic toxicity: Improving predictions obtained from Toxtree ver. 2.6. *Chemosphere* **2015,** *139*, 146-154.
14. Vaes, W. H. J.; Ramos, E. U.; Verhaar, H. J. M.; Hermens, J. L. M., Acute toxicity of nonpolar versus polar narcosis: Is there a difference? *Environmental Toxicology and Chemistry* **1998,** *17*, (7), 1380-1384.
15. Endo, S.; Escher, B. I.; Goss, K. U., Capacities of membrane lipids to accumulate neutral organic chemicals. *Environmental Science and Technology* **2011,** *45*, (14), 5912-5921.
16. Ledbetter, M. R.; Gutsell, S.; Hodges, G.; Madden, J. C.; O'Connor, S.; Cronin, M. T. D., Database of published retention factors for immobilized artificial membrane HPLC and an assessment of the effect of experimental variability. *Environmental Toxicology and Chemistry* **2011,** *30*, (12), 2701-2708.
17. Ulrich, N.; Endo, S.; Brown, T. N.; Watanabe, N.; Bronner, G.; Abraham, M. H.; Goss, K. U., UFZ-LSER database v 3.2.1 [Internet], Leipzig, Germany, Helmholtz Centre for Environmental Research-UFZ. In 2017; Vol. 2018.

18. Bittermann, K.; Spycher, S.; Goss, K. U., Comparison of different models predicting the phospholipid-membrane water partition coefficients of charged compounds. *Chemosphere* **2016,** *144*, 382-391.
19. Tolls, J. Thesis: Bioconcentration of Surfactants. Utrecht University, Utrecht, 1998.
20. Sprunger, L.; Blake-Taylor, B. H.; Wairegi, A.; Acree Jr, W. E.; Abraham, M. H., Characterization of the retention behavior of organic and pharmaceutical drug molecules on an immobilized artificial membrane column with the Abraham model. *Journal of Chromatography A* **2007,** *1160*, (1-2), 235-245.