

SUPPLEMENTAL INFORMATION

The Influence of Molecular Structure on the Adsorption of PFAS to Fluid-Fluid Interfaces: Using QSPR to Predict Interfacial Adsorption Coefficients

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One table

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References

Table S1. Data included in study, along with acronyms and literature source (see notes below).

Acronym	Formula	Perfluorocarboxylates	Surface/Interfacial Tension Data Source
PFAA	CF ₃ CO ₂ Na	Na-Perfluoroacetate	Tamaki 1989
PFPrA	C ₂ F ₅ CO ₂ Na	Na-Perfluoropropanoate	Tamaki 1989
PFBA	C ₃ F ₇ CO ₂ Na	Na-Perfluorobutanoate	Tamaki 1989
PFPeA	C ₄ F ₉ CO ₂ Na	Na-Perfluoropentanoate	Tamaki 1989
PFHxA	C ₅ F ₁₁ CO ₂ Na	Na-Perfluorohexanoate	Lunkenheimer 2015
PFHpA	C ₆ F ₁₃ CO ₂ Na	Na-Perfluoroheptanoate	Lunkenheimer 2015/Tamaki 1989
PFOA	C ₇ F ₁₅ CO ₂ Na	Na-Perfluorooctanoate	Mean of 9 literature data sets
PFNA	C ₈ F ₁₇ CO ₂ Na	Na-Perfluorononanoate	Lunkenheimer 2015/Downer 1999/Dmowski 1990
PFDA	C ₉ F ₁₉ CO ₂ Na	Na-Perfluorodecanoate	Lunkenheimer 2015
PFUnA	C ₁₀ F ₂₁ CO ₂ Na	Na-Perfluoroundecanoate	Lunkenheimer 2015
		Branched PFCAs	
Iso-PFOA	(CF ₃) ₂ CF(CF ₂) ₄ CO ₂ Na	Na perfluoro-methyl-heptanoate	Meissner 1992/Shinoda 1972
Iso-PFDA	(CF ₃) ₂ CF(CF ₂) ₆ CO ₂ Na	Na-perfluoro-methyl-nonanoate	Meissner 1992
		Perfluorosulfonates	
PFBS	C ₄ F ₉ SO ₃ K	K-Perfluorobutanesulfonate	Campbell 2009
PFHxS	C ₆ F ₁₃ SO ₃ K	K-Perfluorohexanesulfonate	Campbell 2009
PFHpS	C ₇ F ₁₅ SO ₃ Na	Na-Perfluoroheptanesulfonate	Shinoda 1972
PFOS	C ₈ F ₁₇ SO ₃ K	K-Perfluorooctanesulfonate	Shinoda 1972
PFNS	C ₉ F ₁₉ SO ₃ K	K-Perfluorononanesulfonate	Shinoda 1972
		Polyfluoroalkyls	
9H-PFNA	C ₈ H _F 16CO ₂ Na	Na-9H Hexadecafluorononanoate	Downer 1999
7H-PFHpA	C ₆ H _F 12CO ₂ NH ₄	NH ₄ -7H-dodecafluoroheptanoate	Bernett 1959
SPBS	C ₉ F ₁₇ OC ₆ H ₄ SO ₃ Na	Na-p-perfluorononyloxy benzene sulfonate	Chen 2011
FC-53	CF ₃ (CF ₂) ₅ O(CF ₂) ₂ SO ₃ K	K-3-oxa-perfluorononane-sulfonate	He 1996
TDFHD	CF ₃ (CF ₂) ₃ CF(CF ₃)(CH ₂) ₁₀ CO ₂ Na	Na-tridecafluorohexadecanoate	Brace 1962
F9-CTAB	CF ₃ (CF ₂) ₃ (CH ₂) ₁₁ N(CH ₃) ₃ Br	Nonafluoropentadecyl-CTAB	Jackson 2015
F12-CTAB	(CF ₃) ₂ (CF ₂) ₃ (CH ₂) ₁₀ N(CH ₃) ₃ Br	Dodecafluoropentadecyl-CTAB	Jackson 2015
F17-CTAB	CF ₃ (CF ₂) ₇ (CH ₂) ₆ N(CH ₃) ₃ Br	Heptadecafluorotetradecyl-CTAB	Jackson 2015
UDFOS	CF ₃ (CF ₂) ₃ CH ₂ CF ₂ (CH ₂) ₂ SO ₃ Na	Na-undecafluorooctanesulfonate	Peng 2012
NFHES	CF ₃ CF ₂ O(CF ₂) ₂ (CH ₂) ₂ SO ₃ Na	Na-nonafluorohexylethersulfonate	Peng 2012
UDFHES	CF ₃ (CF ₂) ₂ O(CF ₂) ₂ (CH ₂) ₂ SO ₃ Na	Na-undecafluoroheptylethersulfonate	Peng 2012
TDFP	CF ₃ (CF ₂) ₂ C(CF ₃) ₂ CH ₂ CO ₂ Na	Na-tridecafluoropentanoate	Dmowski 1990
TDHP	CF ₃ (CF ₂) ₂ C(CF ₃) ₂ (CH ₂) ₂ CO ₂ Na	Na-tridecafluorohexanoate	Dmowski 1990
HDFPEC	CF ₃ (CF ₂) ₂ OCF(CF ₃)CF ₂ OCF(CF ₃)CO ₂ Na	Na-heptadecafluoropolyether carboxylate	Yin 2016
TDFBP	CF ₃ (CF ₂) ₂ C(CF ₃) ₂ CH ₂ C ₆ H ₄ PO ₃ Li ₂	Li-tridecafluoropentylbenzene phosphonate	Sha 2014

Table S1. Continued.

Nonionic PFAS			
TDFTE	CF ₃ (CF ₂) ₅ C ₂ H ₄ SC ₂ H ₄ (CH ₂ CH ₂ O) ₂ OH	Tridecafluoro thiodiethoxylate	Matos 1989
TDFTE	CF ₃ (CF ₂) ₅ C ₂ H ₄ SC ₂ H ₄ (CH ₂ CH ₂ O) ₃ OH	Tridecafluoro thiotriethoxylate	Matos 1989
TDFTE	CF ₃ (CF ₂) ₅ C ₂ H ₄ SC ₂ H ₄ (CH ₂ CH ₂ O) ₅ OH	Tridecafluoro thiopentaethoxylate	Matos 1989
PFOA-amide	CF ₃ (CF ₂) ₆ CONHCH ₂ CH ₃ CHOH	N-(2-hydroxypropyl)perfluorooctane amide	Dai 2013
NFTME	CF ₃ (CF ₂) ₃ CH ₂ O(CH ₂ CH ₂ O) ₃ CH ₃	Nonafluoro triethyleneoxide methyl ether	Eastoe 2001
TDFTE	CF ₃ (CF ₂) ₅ CH ₂ O(CH ₂ CH ₂ O) ₃ CH ₃	Tridecafluoro triethyleneoxide methyl ether	Eastoe 2001
HOFTME	CF ₂ H(CF ₂) ₃ CH ₂ O(CH ₂ CH ₂ O) ₃ CH ₃	H-octafluoro triethyleneoxide methyl ether	Eastoe 2001
HDDFTME	CF ₂ H(CF ₂) ₅ CH ₂ O(CH ₂ CH ₂ O) ₃ CH ₃	H-dodecafluoro triethyleneoxide methyl ether	Eastoe 2001
Alcohols			
8:1 FTOH	CF ₃ (CF ₂) ₇ CH ₂ OH	8:1 Fluorotelomer alcohol	Casandra 2018
FC8diol	(CF ₂) ₆ (CH ₂) ₂ (OH) ₂	Perfluorooctane-1,8-diol	Takiue 2009
Hydrocarbons			
SDBS	C ₁₈ H ₂₉ SO ₃ Na	Na-dodecylbenzene sulfonate	Zimoch 1999
SDS	C ₁₂ H ₂₅ SO ₄ Na	Na-dodecyl sulfate	Zdziennicka 2012
CTAB	C ₁₉ H ₄₂ NBr	Hexadecyltrimethylammonium bromide	Nakahara 2011
Triton 45	(CH ₃) ₃ CCH ₂ C(CH ₃) ₂ C ₆ H ₄ -(OCH ₂ CH ₂) _n OH, n=4.5	Octylphenol Ethoxylate	Fainerman 2009
OIL-Water			
PFOA	C ₇ F ₁₅ CO ₂ Cs	Cs-PFOA Decane-Water	Janczuk 1997
PFOA	C ₇ F ₁₅ CO ₂ Cs	Cs-PFOA Benzene-Water	Janczuk 1997
PFOA	C ₇ F ₁₅ CO ₂ Na	Na-PFOA Heptane-Water	Dmowski 1990
PFNA	C ₈ F ₁₇ CO ₂ Na	Na-PFNA Heptane-Water	Dmowski 1990
TDFP	CF ₃ (CF ₂) ₂ C(CF ₃) ₂ CH ₂ CO ₂ Na	Na-TDFP Heptane-Water	Dmowski 1990
TDHP	CF ₃ (CF ₂) ₂ C(CF ₃) ₂ (CH ₂) ₂ CO ₂ Na	Na-TDHP Heptane-Water	Dmowski 1990
SDBS	C ₁₈ H ₂₉ SO ₃ Na	SDBS Tetrachloroethene-Water	Kim 1999/Zhong 2016
SDBS	C ₁₈ H ₂₉ SO ₃ Na	SDBS Decane-Water	Kim 1999

Note 1: The number of citations listed under the data source for a given PFAS reflects the number of data sets available for that specific compound.

Note 2: Data sources for Na-PFOA are An et al., 1996, Chen et al. 2005, Dmowski et al., 1990, Lopez-Fontan et al. 2005, Lunkenheimer et al. 2015, Lunkenheimer et al. 2017, Lyu et al., 2018 (denoted as “UAZ” in Figure 1), Shinoda et al. 1972, and Tamaki et al. 1989.

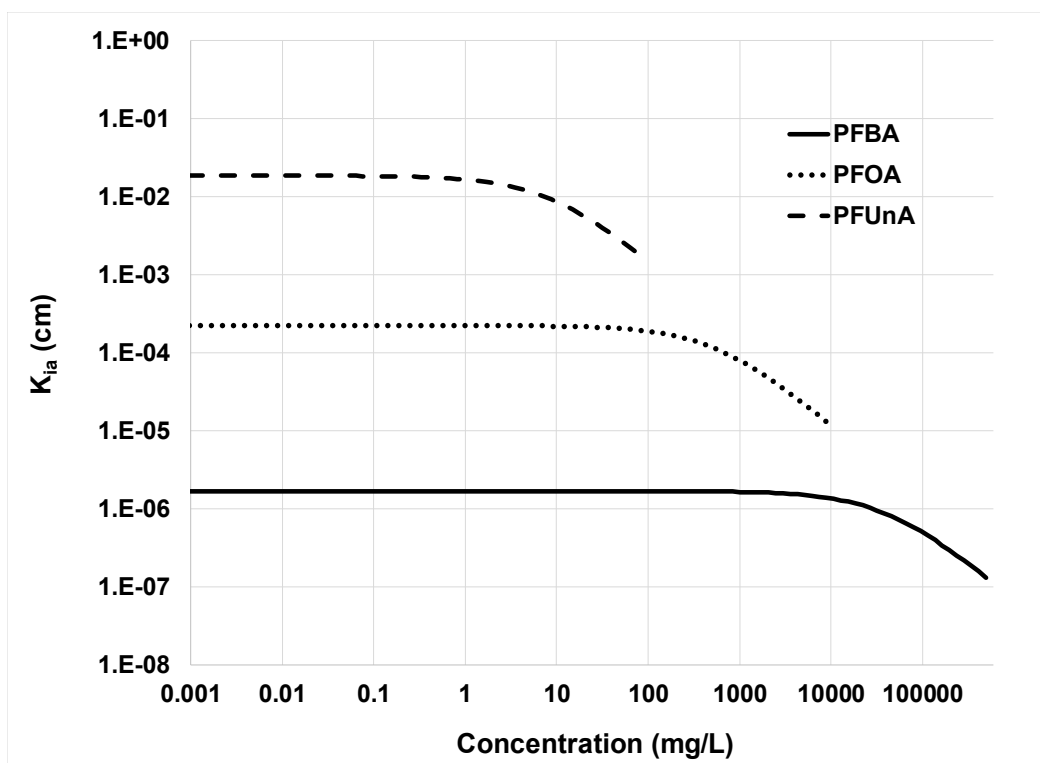


Figure S1. Air-water interfacial adsorption coefficient (K_{ia}) versus solution concentration of three selected PFAS (Na-forms as reported in Table S1). Acronyms referenced to Table S1.

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