**SUPPORTING INFORMATION**

# Response to Comment on "Comparative assessment of the global fate and transport pathways of long-chain perfluorocarboxylic acids (PFCAs) and perfluorocarboxylates (PFCs) emitted from direct sources".

James M. Armitage,[†] Matthew MacLeod,[§] Ian T. Cousins,[†]*

[†] Department of Applied Environmental Science (ITM), Stockholm University, SE-10691 Stockholm, Sweden

[§] Institute for Chemical and Bioengineering, Swiss Federal Institute of Technology, ETH Zurich, HCI G129, CH-8093 Zürich, Switzerland.

* corresponding author: ian.cousins@itm.su.se; +46 (0)8 16 4012

3 pages, 2 tables

**Section S1. Brief description of data presented in Jing et al. (1)**

Jing et al. (1) assessed the lipophilicity of a series of perfluoroalkyl carboxylates and sulfonates through the application of an experimental technique known as ion-transfer cyclic voltammetry. The main purpose of the electrochemical experiments is to obtain estimates of the formal ion transfer potential (FTP) which, as discussed in ref *1–3*, can be related to a formal partition coefficient based on the relationship between the FTP and the Gibbs energy of transfer of the anion. Since the partitioning data presented in ref *6* were calculated from formal ion transfer potentials, our interpretation of these data is that they represent estimates of the lipophilicity of the anions only (i.e. log P of $PFO^-$, $PFN^-$, etc.) and not the distribution coefficients (log D). Furthermore, the measurements reported in ref *1* were conducted using n-octanol with an organic supporting electrolyte (TDDATFAB) present at a concentration of 40 mM and water containing 1 mM $MgSO_4$. An external current was also being carried by a negative charge from the aqueous to octanol phase. Because the SPARC calculations do not account for the experimental conditions (e.g. 'charged' octanol vs. neutral octanol, presence of electrolytes) we are not convinced that the empirical and SPARC values are directly comparable with respect to absolute values (even at pH $\geq$ 6 where SPARC predicts that these compounds are present almost entirely in ionized form in the aqueous phase).

**Table S1**. Comparison of log $K_{AW}$ values generated by COSMOtherm v2.1 accessed on 2009 07 21 ('New') and used in ref *4* ('Old')

| Homologue | 'New' | 'Old' |
|---|---|---|
| C6 | -2.76 | -3.04 |
| C7 | -2.49 | -2.66 |
| C8 | -2.18 | -2.37 |
| C9 | -1.81 | -2.03 |
| C12 | -0.92 | -1.23 |

**Table S2**. Comparison of log $K_{OW}$ (dry octanol/water) values generated by COSMOtherm v2.1 accessed on 2009 07 21 ('New') and used in ref *4* ('Old')

| Homologue | 'New' | 'Old' |
|---|---|---|
| C6 | 3.40 | 3.26 |
| C7 | 3.94 | 3.82 |
| C8 | 4.45 | 4.30 |
| C9 | 4.99 | 4.84 |
| C12 | 6.54 | 6.26 |

## Literature Cited


1. Jing, P.; Rodgers, P.J.; Ameniya, S. High lipophilicity of perfluoroalkyl carboxylate and sulfonate: Implications for their membrane permeability. *J. Am. Chem. Soc.* **2009**, 131, 2290–2296.
2. Reymond, F.; Steyaert, G.; Carrupt, P-A.; Testa, B.; Girault, H. Ionic partition diagrams: A potential-pH representation. *J. Am. Chem. Soc.* **1996**, 118, 11951–11957.
3. Reymond, F.; Chopineaux-Courtois, V.; Steyaert, G.; Bouchard, G.; Carrupt, P-A.; Testa, B.; Girault, H.H. Ionic partition diagrams of ionisable drugs: pH-lipophilicity profiles, transfer mechanisms and charge effects on salvation. *J. Electroanal. Chem.* **1999**, 235–299.
4. Armitage, J.M.; Macleod, M.; Cousins, I.T. Comparative assessment of the global fate and transport pathways of long-chain perfluorocarboxylic acids (PFCAs) and perfluorocarboxylates (PFCs) emitted from direct sources. *Environ. Sci. Technol.* **2009**, doi:10.1021/es900753y.