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Supplementary material

Experimental hydrophobicity parameters of perfluorinated alkylated substances from reversed-phase HPLC

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Table S1. Characteristics of perfluorinated compounds employed

Chemical abbreviations are according to Buck et al.[1]

Compound Name	Chemical abbreviation	Chemical structure	*m/z* ESI^-	Purity (%)	CAS-Nr	Supplier
Perfluorobutyl sulfonate	PFBS	$C_4F_9SO_3^-$	299	98	59933–66–3	ABCR, Karlsruhe, Germany
Perfluorohexyl sulfonate	PFHxS	$C_6F_{13}SO_3^-$	399	97	45285–51–6	ABCR, Karlsruhe, Germany
Perfluorooctyl sulfonate	PFOS	$C_8F_{17}SO_3^-$	499	98	45298–90–6	Fluka, Buchs, Switzerland
Perfluorooctane sulfonamide	FOSA	$C_8H_2F_{17}SO_2N$	428	97	754–91–6	ABCR, Karlsruhe, Germany
6:2 Fluorotelomer sulfonate	6:2 FTS	$C_8H_4F_{13}SO_3^-$	499	98	27619–97–2	Interchim, Montlucon, France
Perfluorobutanoic	PFBA	$C_4HF_9CO_2$	213	99	375–22–4	ABCR, Karlsruhe, Germany
Perfluorohexanoic	PFHxA	$C_6HF_{13}CO_2$	313	98	307–24–4	ABCR, Karlsruhe, Germany
Perfluoroheptanoic	PFHpA	$C_7HF_{15}CO_2$	363	96	375–85–9	Acros, Geel, Belgium
Perfluorooctanoic	PFOA	$C_8HF_{17}CO_2$	413	96	335–67–1	Acros, Geel, Belgium
Perfluorononanoic	PFNA	$C_9HF_{17}CO_2$	463	97	375–95–1	Aldrich, Milwood, WI, USA
Perfluorodecanoic	PFDA	$C_{10}HF_{21}CO_2$	513	98	335–76–2	ABCR, Karlsruhe, Germany
Perfluoroundecanoic	PFUnA	$C_{11}HF_{23}CO_2$	563	97	2058–94–8	Acros, Geel, Belgium
Perfluorododecanoic	PFDoA	$C_{12}HF_{25}CO_2$	613	96	307–55–1	ABCR, Karlsruhe, Germany
Perfluorotetradecanoic	PFTeDA	$C_{14}HF_{29}CO_2$	713	99	376–06–7	Acros, Geel, Belgium
2-oxy-4-oxypyrimidine	Uracil	$C_4H_4N_2O_2$	111	9	66–22–8	Acros, Geel, Belgium

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Table S2. log k_0 values obtained from isocratic HPLC elution using MeOH–water as mobile phase

Results from Lichrospher column are from two independent runs at pH = 2.2 and one run at pH = 2.4

Column stationary phase	Fluorinated C	Aqua	Lichrospher			Aqua	Lichrospher	
pH		2.2	2.2–1	2.2–2	2.4	5.2	6.0	7.6
PFBA	3	1.21			2.07		2.04	2.01
PFHxA	5	2.85	2.76	3.45	2.81	3.22	2.18	2.87
PFHpA	6	3.52	3.42	3.84	3.35	3.53	3.06	3.34
PFOA	7	4.20	4.59	4.50	4.03	4.25	3.75	4.23
PFNA	8	4.78	5.33	5.06	4.76	4.88	4.62	5.11
PFDA	9	5.38	6.24	6.01	5.65	5.53	5.64	5.65
PFUnA	10	6.13	6.79	6.57	5.61	6.26	5.78	6.37
PFDoA	11		7.65	6.35	6.61			7.47
PFBS	4	2.14	2.23	2.5	2.44	2.63	2.15	2.12
PFHxS	6	3.66	3.95	4.18	3.31	3.68	3.16	3.45
PFOS	8	4.93	5.47	5.29	4.80	4.88	4.69	5.11
FOSA	8	5.85	5.46	5.70	6.00	5.72	6.03	5.88
6:2FTS	6	3.54	4.55	4.04	3.96	4.11	3.73	4.20

Table S3. Reported log K_{ow} values from two calculation models by Arp. et al.,[2] Kelly et al.[3] (table S3 of the their supporting information) and Wang et al.,[4] and from experiments by Jing et al.[5]

Method	Calculated log K_{ow}				log $P^{0'}$
	COSMO-therm		Sparc		Voltammetry
Reference	Arp. et al.[2]	Wang et al.[4]	Arp. et al.[2]	Kelly et al.[3]	Jing et al.[5]
PFBA	–	2.82	–	–	–0.68
PFHxA	3.26	3.42	3.12	–	0.54
PFHpA	3.82	4.06	3.82	2.8	1.15
PFOA	4.30	4.67	4.59	3.6	1.76
PFNA	4.84	5.30	5.45	4.5	2.37
PFDA	5.30	6.50	6.38	5.4	2.98
PFUnA	5.76	7.15	7.40	6.4	3.59
PFDoA	–	7.77	–	7.1	4.20
PFBS	–	3.90	–	–	–
PFHxS	–	5.17	–	–	–
PFOS	5.25	6.43	5.26	4.3	2.57

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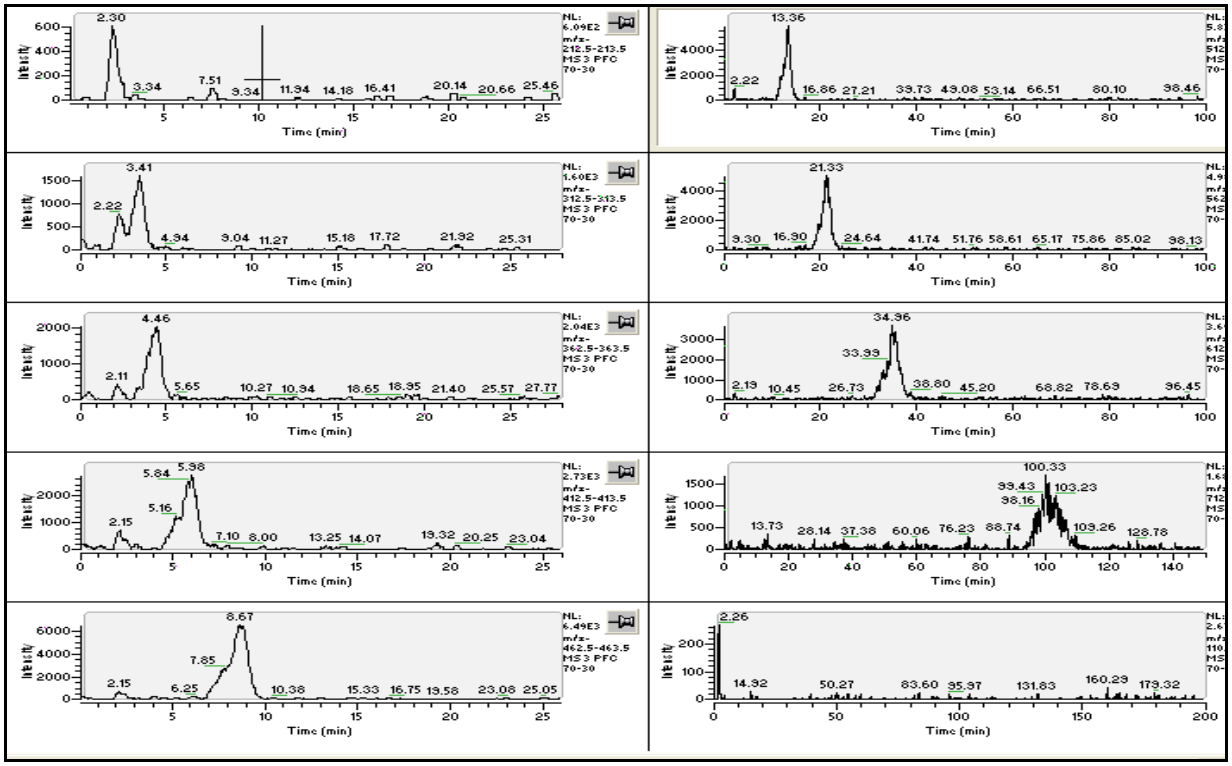

Fig S1. Example chromatograms of all PFCAs and uracil obtained by LC-MS.

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