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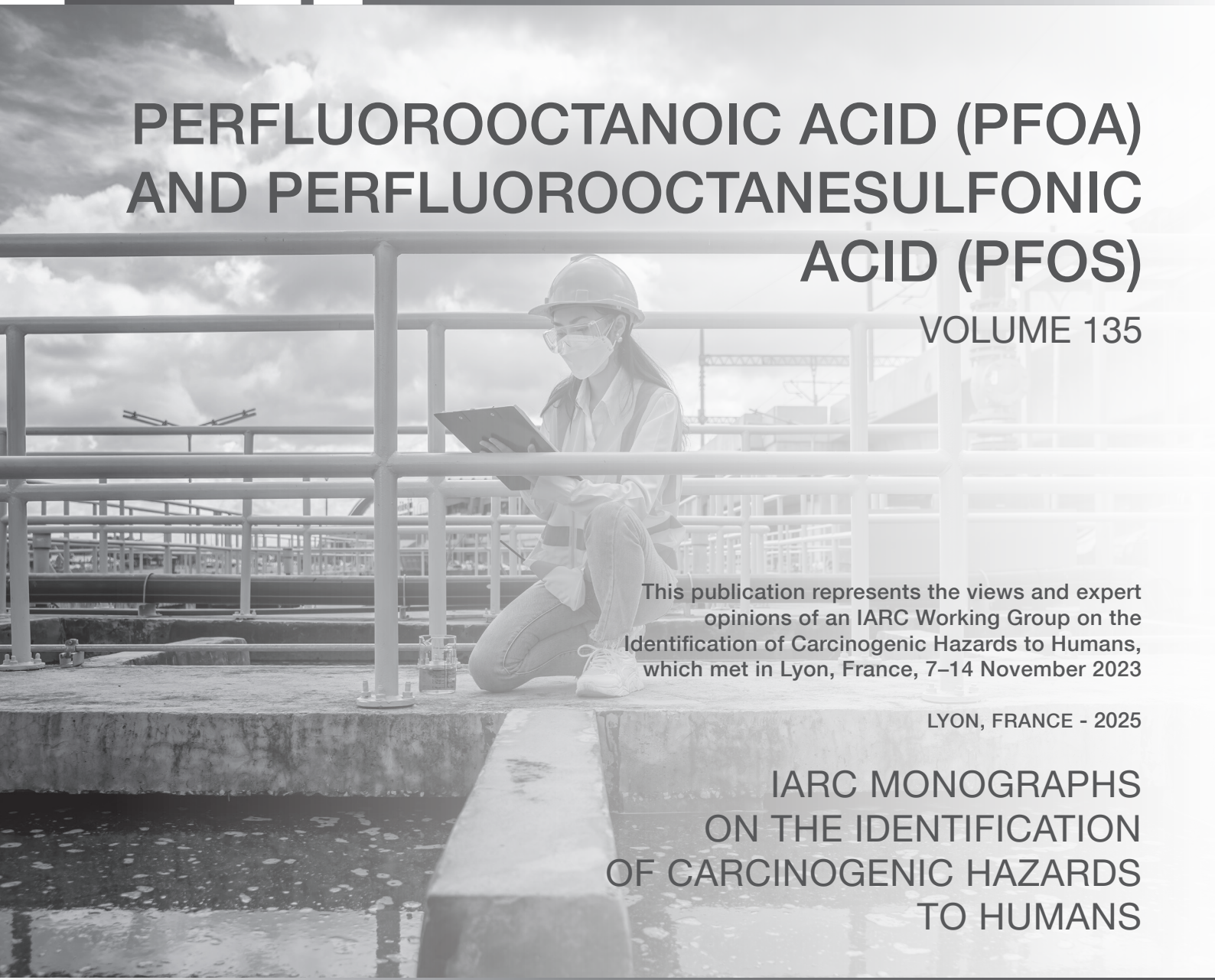

PERFLUOROOCTANOIC ACID (PFOA) AND PERFLUOROOCTANESULFONIC ACID (PFOS)

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International Agency for Research on Cancer

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Table S4.1 Calculations to derive dissociation constants, by the Working Group

Reference	Information available in the paper	Working Group calculation[a]	Information reported in the Monograph[a]
Han et al. (2003)	Dissociation constant between PFOA and HSAs: 0.38 mM (micro-desalting columns)	No (used as reported - rounded)	Highest value for PFOA-HSA (4×10^{-4} M)
Messina et al. (2005)	Hill binding constants for two HSA-PFOA binding sites:	Reverse	
	1.44×10^{5} M^{-1}	6.9×10^{-6} M	Included in the range
	3.17×10^{4} M^{-1}	3.2×10^{-5} M	Included in the range
Chen and Guo (2009)	Binding constant to human HSA (by fluorescent quenching)	Reverse	
	PFOA, 2.7×10^{5} M^{-1}	3.7×10^{-6} M	Lowest values for PFOA-HSA
	PFOS, 2.2×10^{4} M^{-1}	4.5×10^{-5} M	PFOS-HSA
Li et al. (2009)	Absorption constant for PFOS with HSA	Reverse	
	5.01×10^{3} M^{-1}	2.0×10^{-4} M	Highest value for PFOS-HSA
Wu et al. (2009)	Absorption constant K_a (dialysis, Temkin isothermal model)	Reverse	Included in the range
	3.12×10^{4} M^{-1}	3.2×10^{-5} M	
Luo et al. (2012)	Crystal structure of PFOS with HSA		Direct evidence of PFOS interacting with HSA
	No binding experiments		
Zhang et al. (2013a)	K_d for displacement from hL-FABP (fluorescence displacement assay)	No (used as reported)	
	PFOA, 50.4 µM		Included (high value)
	PFOS, 18.5 µM		Included
Sheng et al. (2016)	K_d for PFOA-hL-FABP for wt	No (used as reported)	Lower value for PFOA-LFABP 2.4×10^{-6} M)
	2.36×10^{-6} M		
Maso et al. (2021)	Crystal structure of PFOA with HSA		Direct evidence of PFOA interacting with HSA

Table S4.1 Calculations to derive dissociation constants, by the Working Group

Reference	Information available in the paper	Working Group calculation[a]	Information reported in the Monograph[a]
Bischel et al. (2010)	Association constant of BSA with PFOA equals	Reverse	BSA not HSA
	1.4×10^6 M^{-1} (dialysis)	7.1×10^{-7} M	
	1.3×10^5 M^{-1} (nanoESI-MS)	7.7×10^{-6} M	
	References		
	(PFOA-HSA):		
	2.4×10^4 M^{-1} (Sabín et al., 2006)	4.2×10^{-5} M	
	2.6×10^3 M^{-1} (Han et al., 2003)	3.8×10^{-4} M	Only new value (in range)
	3.12×10^4 M^{-1} (Wu et al., 2009)	3.2×10^{-5} M	
	1.44×10^5 M^{-1} (Messina et al., 2005)	6.9×10^{-6} M	
	3.17×10^4 M^{-1} (Messina et al., 2005)	3.1×10^{-5} M	Study not included because a review and considered redundant
Fedorenko et al. (2021)	BSA study (non-human protein)		Study not included

BSA, bovine serum albumin; hL-FABP, human liver-type fatty acid-binding protein; L-FABP, liver-type fatty acid-binding protein; HSA, human serum albumin; nanoESI-MS, nano-electrospray ionization-mass spectrometry; PFOA, perfluorooctanoic acid; PFOS, perfluorooctanesulfonic acid; wt, wildtype.

[a] This table reports on toxicokinetic constants reported in the individual references cited in Section 4.1, and whether the value was recalculated by the Working Group to obtain a dissociation constant.

For association, binding, or absorption constants, the recalculation procedure uses a reverse value (… = $1/K_a$).

K_d = 3.7×10^{-6} to 4×10^{-4} M for PFOA and 4.5–20×10^{-5} M for PFOS, and L-FABP, with K_d = 2.4–50.4×10^{-6} M for PFOA and 18.5×10^{-6} M for PFOS.

Values are colour-coded:

K_d = 3.7– 400 µM for PFOA and 45–200 µM for PFOS, and L-FABP, with K_d = 2.4–50.4 µM for PFOA and 18.5 µM for PFOS.