

Supporting Information

Acid Dissociation versus Molecular Association of Perfluoroalkyl Oxoacids: Environmental Implications

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Isotope ratios of PFO species observed by ESI-MS

	m/z	$I_{m/z}$ a.u	$I_{(m+1)/z}$ a.u.	$100 \times I_{(m+1)/z} / I_{m/z}$ measured	$100 \times I_{(m+1)/z} / I_{m/z}$ calculated
PFO ⁻	413	7027	619	8.8	9.0
PFO-CO ₂ ⁻	369	2212	165	7.5	7.9
(PFO) ₂ H ⁻	827	1564	283	18.1	18.0

- ESI-MS signal intensities at m/z= 369, 370, 413, 414, 827, 828 from 5 μM PFOA solutions at pH 1.5.
- Last column, calculated as $100 \times I_{(m+1)/z} / I_{m/z} = 100 \times n \times 0.0111 / 0.9889$ for C_n-species