ENHANCING SENSITIVITY AND RESOLUTION OF ^{19}F NMR SPECTRA OF PFAS THROUGH BAND-SELECTIVE HOMONUCLEAR DECOUPLING

Markus Rotzinger,[a] Viktoria Müller[b,c], Armin Macher[a], Jörg Feldmann, Klaus Zangger

[a] Institute of Chemistry, University of Graz, Heinrichstraße 28, Graz, Austria
[b] Institute of Chemistry/Analytical Chemistry, University of Graz, Universitätsplatz 1, Graz, Austria
[c] The James Hutten Institute, Aberdeen, United Kingdom
markus.rotzinger@uni-graz.at

Per- and polyfluoroalkyl substances (PFAS) are a diverse class of substances defined by the presence of perfluorinated carbon atoms.[1] PFAS, which were developed more than 70 years ago, exhibit several favorable properties which made them indispensable in the manufacturing of various items such as non-stick coatings of pans, food-packaging and firefighting foams.[2] However, several of the compounds have been identified to bioaccumulate at alarming levels and are potentially toxic.[3–5] To better establish NMR in the analysis of these compounds, we developed a method which maximizes resolution as well as sensitivity for acquiring decoupled ^{19}F NMR spectra of PFAS. The experiment uses band-selective homonuclear decoupling[6-9] of the CF_3 spectral region (around -82.4 ppm) and results in spectra showing both enhanced resolution and enhanced signal intensities for perfluorinated compounds. PFAS mixtures, which show highly overlapped multiplett signals in conventional ^{19}F NMR spectra are reduced to individual separated singlets enabling not only their identification, but also quantification at concentrations of less than 10 mg/L.

Acknowledgements. Financial support to K.Z. by the Austrian Science Foundation (FWF) through the DocFunds project BioMolStruct is gratefully acknowledged.

REFERENCES

[1] C. F. Kwiatkowski, D. Q. Andrews, L. S. Birnbaum, T. A. Bruton, J. C. DeWitt, D. R. U. Knappe, M. V. Maffini, M. F. Miller, K. E. Pelch, A. Reade, A. Soehl, X. Trier, M. Venier, C. C. Wagner, Z. Wang, A. Blum, *Environ. Sci. Technol. Lett.* **2020**, *7*, 532–543.

[2] S. Das, A. Ronen, *Membranes* **2022**, *12*, 662.

[3] H. Brunn, G. Arnold, W. Körner, G. Rippen, K. G. Steinhäuser, I. Valentin, *Environ. Sci. Eur.* **2023**, *35*, 20.

[4] M. E. Solan, J.-A. Park, *Front. Toxicol.* **2024**, *6*, 1423449.

[5] F. Coperchini, L. Croce, G. Ricci, F. Magri, M. Rotondi, M. Imbriani, L. Chiovato, *Front. Endocrinol.* **2021**, *11*, DOI 10.3389/fendo.2020.612320.

[6] L. Castañar, P. Nolis, A. Virgili, T. Parella, *Chem. – Eur. J.* **2013**, *19*, 17283–17286.

[7] L. Castañar, J. Saurí, P. Nolis, A. Virgili, T. Parella, *J. Magn. Reson.* **2014**, *238*, 63–69.

[8] J. Ying, J. Roche, A. Bax, *J. Magn. Reson. San Diego Calif 1997* **2014**, *241*, 97–102.

[9] R. W. Adams, L. Byrne, P. Király, M. Foroozandeh, L. Paudel, M. Nilsson, J. Clayden, G. A. Morris, *Chem. Commun.* **2014**, *50*, 2512–2514