

Contribution ID: 5 Contribution code: **Mo-II\_3**

Type: **Oral**

## Using FTMS to study PFAS reactions with peptides and proteins

*Monday, August 25, 2025 5:10 PM (20 minutes)*

PFASs are a diverse group of major emerging contaminants, with more than 7800 compounds identified to date. All of them possess at least one carbon atom, on which all the H substituents were replaced with F atoms. Due to the exceptional stability of the C-F bond, they are widely used as surfactants and stain repellents, in firefighting foams, cosmetics and surface coatings. The stability of the perfluorinated moiety makes it resistant to biodegradation and leads to accumulation of these substances in nature. PFASs are found in human blood, drinking water and biota in remote regions. Adverse effects such as hepatotoxicity, disturbances in lipid and protein metabolism and even carcinogenesis were attributed to these compounds. Yet the precise mechanisms by which these compounds interact with biological systems are unknown.

It is known that lipid-protein interactions can affect the functioning of the proteins. Due to structural similarity between the lipid chain and the perfluorinated chain it is reasonable to expect the interactions between PFASs and proteins to have a certain effect on the latter.

In this project, reactions between PFASs and peptides or proteins were studied. Each pair of compounds (a PFAS and a biomolecule) were incubated in aqueous medium for several hours, then the resulting solution measured by HRMS. The samples were analyzed by a 7-T LTQ FT-ICR with a resolving power of  $R = 400\,000$  at  $m/z$  400 and by LTQ-Orbitrap Elite mass spectrometer with mass resolving power of  $R = 480\,000$  (Thermo Fisher Scientific, Bremen, Germany) using ESI ionization.

Reactions between several PFASs and biomolecules were assessed. The results show that interactions are possible between the compounds, and they depend both on the PFAS and the biomolecule present. Most of the tested proteins and peptides interact with the PFSA compounds, as well as with perfluorophosphinic acids, but only a few exhibit interaction with PFCAs. Only GHK protein was found to interact with PFCAs. Each molecule of a protein or a peptide can interact with several PFAS molecules.

**Authors:** JARASHNELI, Andrei (Max-Planck-Institut für Kohlenforschung); VETERE, Alessandro (Max-Planck-Institut für Kohlenforschung); SCHRADER, Wolfgang (Max-Planck-Institut für Kohlenforschung)

**Presenter:** JARASHNELI, Andrei (Max-Planck-Institut für Kohlenforschung)

**Session Classification:** Monday

**Track Classification:** FTMS and High Resolution Mass Spectrometry