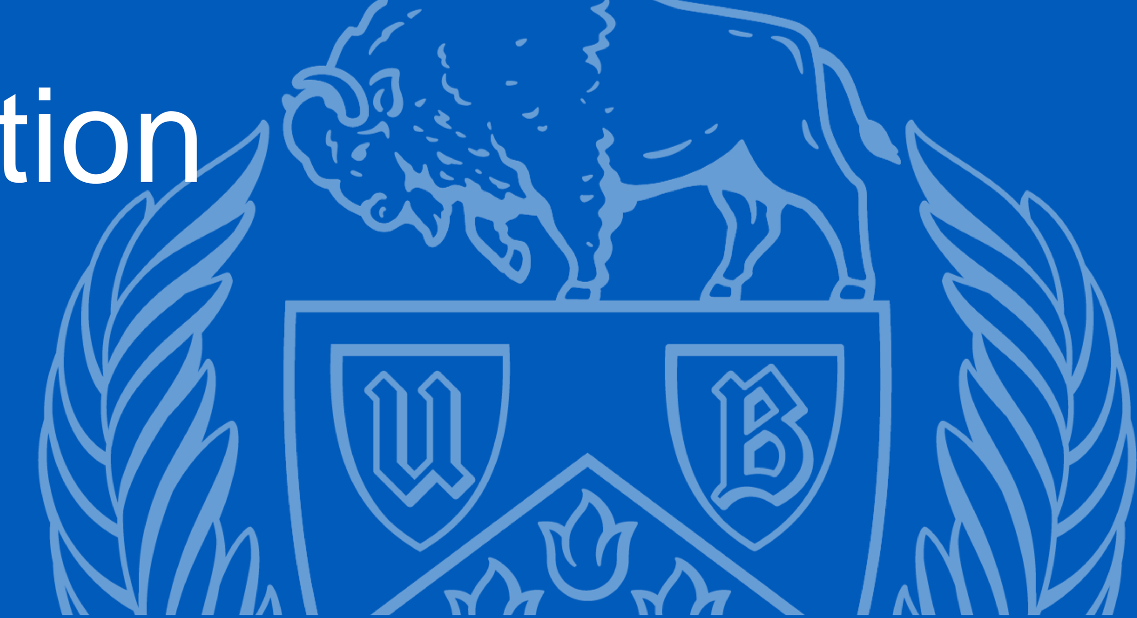
Bacterial degradation of perfluorooctane sulfonic acid (PFOS): detection of by-products by target and non-target analysis



Mindula K.Wijayahena[1], Irina S. Moreira[2], Joshua S. Wallace[1,3], Paula M. L. Castro[2], Diana S. Aga[1,3]

[1]University at Buffalo, Chemistry Department, Buffalo, NY 14260

[2]Universidade Católica Portuguesa, 4169-005 Porto, Portugal

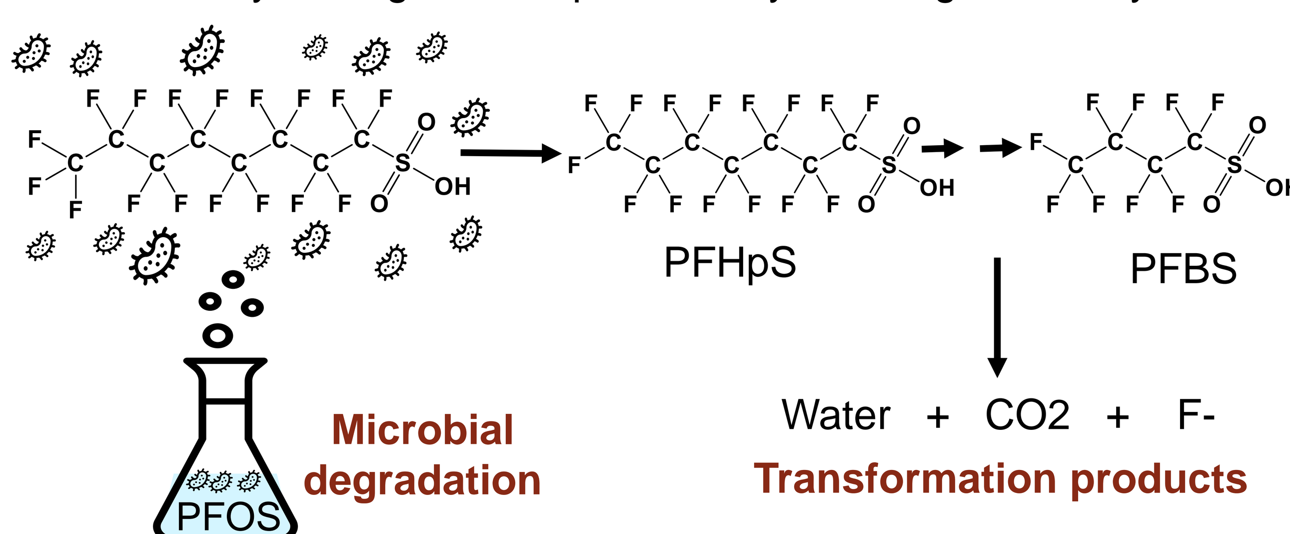
[3]RENEW Institute, University at Buffalo, Buffalo, NY 14260

Introduction

Per- and poly-fluoroalkyl substances (PFAS) are highly fluorinated synthetic chemicals with a wide variety of uses[1,2]. The carbon-fluorine bonds exhibit very high bond dissociation energies: around 536 kJ/mol, making PFAS generally resistant to degradation by oxidation, thermal treatment, and biological mechanisms, which has led to their classification as "forever chemicals"[3]. Strategies to enhance the biodegradation of these compounds are of great interest, such as identifying bacterial species that may be used for bioaugmentation. *Labrys portucalensis* F11 is an aerobic bacterium that has been isolated in Portugal and can degrade fluorinated pharmaceuticals, fluorobenzene, and fluoxetine[4,5]. This F11 strain has the ability to cleave C-F bonds in these fluorinated organic compounds and was therefore tested for its ability to degrade perfluorooctane sulfonate (PFOS), the most frequently detected PFAS in the environment.

Objectives

1. To determine whether the F11 bacteria strain can degrade PFOS
2. To identify biodegradation products by non-targeted analysis



Method

F11 + PFOS

Day 0 | Day 48 | Day 100 | Day 194

HLB / WAX

1. 0.1% NH4OH in methanol
2. Methanol
3. Acetonitrile

Volume	30 mL
Concentration	10 ppm
Temperature	25 °C
Condition	Aerobic
Growth medium	Minimal salts medium[1]

Non-target analysis: Liquid chromatography coupled to ion mobility separation and high-resolution time-of-flight mass spectrometry (LC-IMS-qToF-MS)

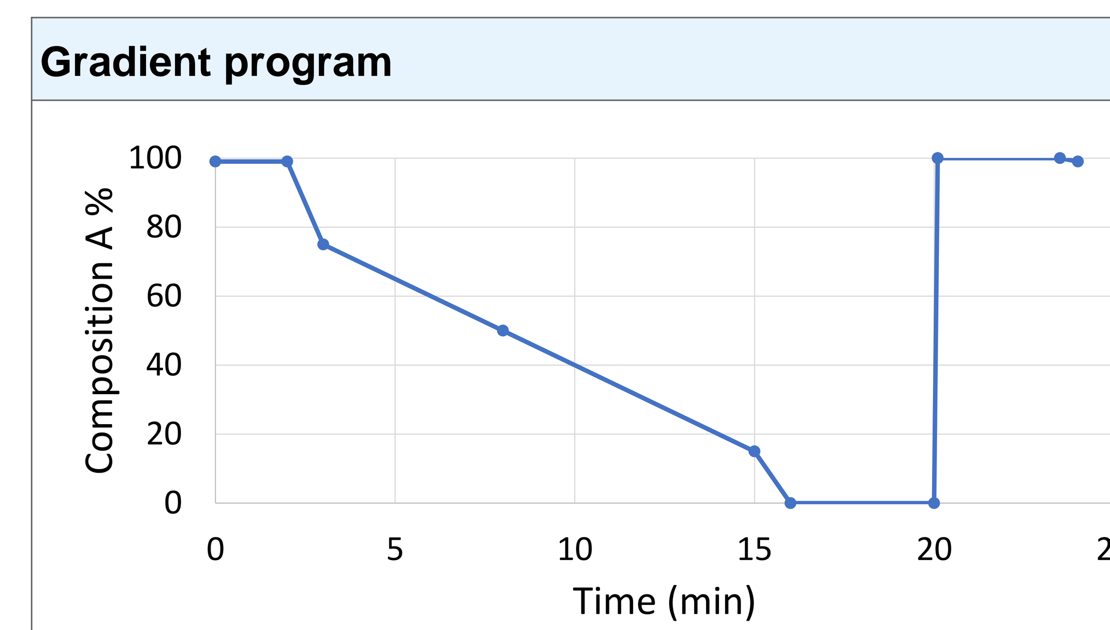
200 µL with ^{13}C labeled standard mix

SPE extract

LC-IMS-qToF-MS Instrumentation

Analytical column
Atlantis Premier BEH C18 AX, 1.7µm; 2.1mm x 100mm
Mobile phase A
Water + 2 mM Ammonium Acetate
Mobile phase B
Methanol + 0.1% Ammonium Hydroxide
Flow rate
0.30 mL/min
Injection volume
10.0 µL
Column Temperature
30 ˚C

Gradient program



LC-IMS-qToF-MS Analysis

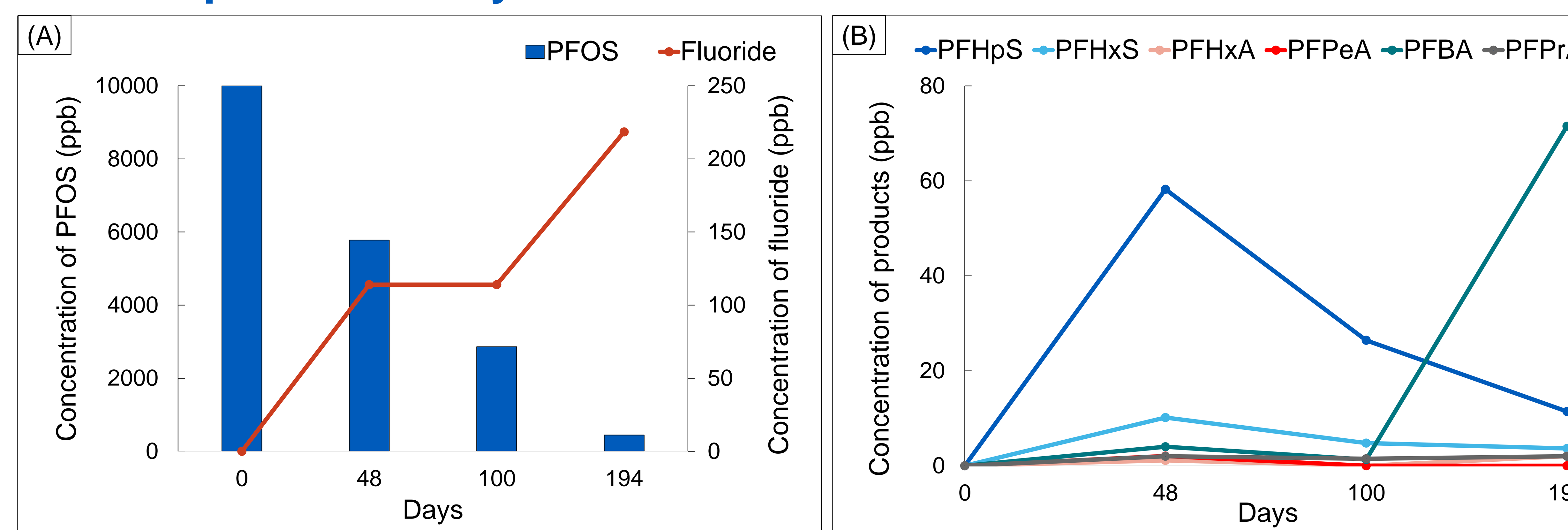
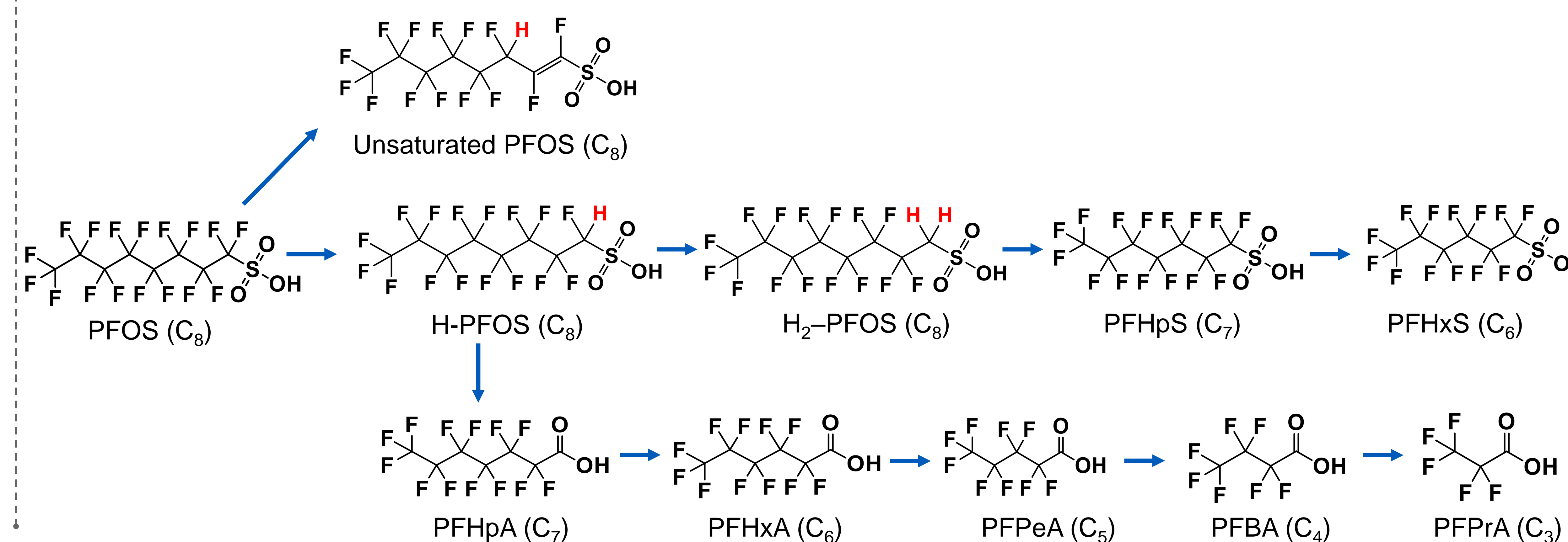


Figure 1: Plot showing a decrease in PFOS and a corresponding increase in fluoride (A) and targeted metabolites, PFHpS, PFHxS, PFHxA, PFPeA, PFBA and PFPrA (B) detected across 4 time points (0, 48, 100 and 194 days).

Proposed biotransformation pathway



Isomer separation

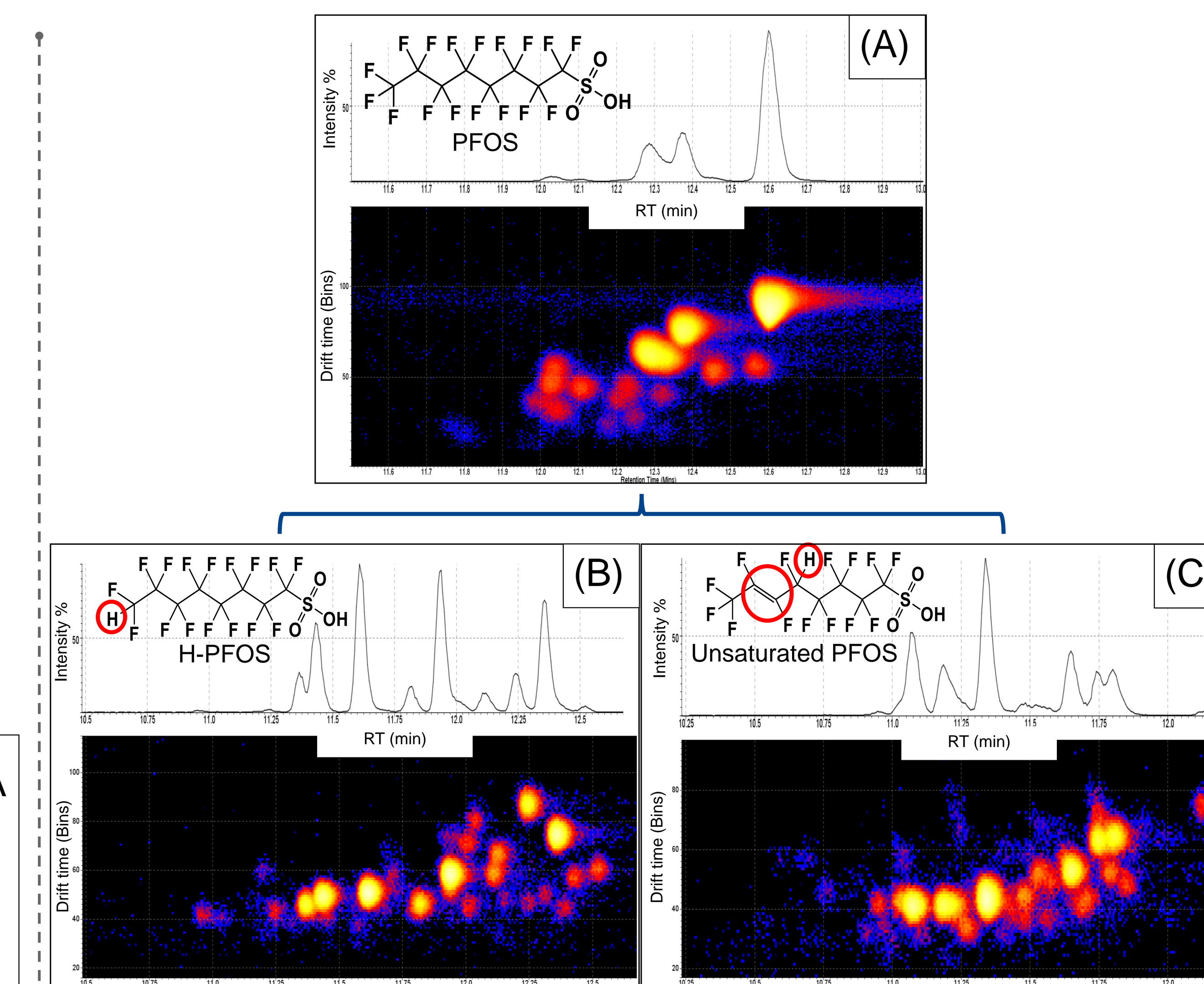


Figure 2: IMS chromatograms exhibiting isomer separation of (A) PFOS (m/z 498.932); (B) H-PFOS (m/z = 480.940); (C) unsaturated PFOS (m/z = 442.942)

Conclusions

- *Labrys portucalensis* strain F11 degraded PFOS.
- Shorter-chain PFAS, from C_7 to C_3 were formed as metabolites.
- Non-target analysis facilitated the identification of the unsaturated and hydrogenated C_8 compounds.
- IMS separation exhibited the separation of isomers of PFOS as well as defluorinated PFOS isomers including isomers of H-PFOS and isomers of unsaturated PFOS.

Acknowledgements

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University at Buffalo The State University of New York

Department of Chemistry
College of Arts and Sciences

Contact: **mindulaw@buffalo.edu**