

Biodegradation of perfluorooctane sulfonic acid (PFOS) by the bacterial strain *Labrys portucalensis* F11 and identification of metabolites

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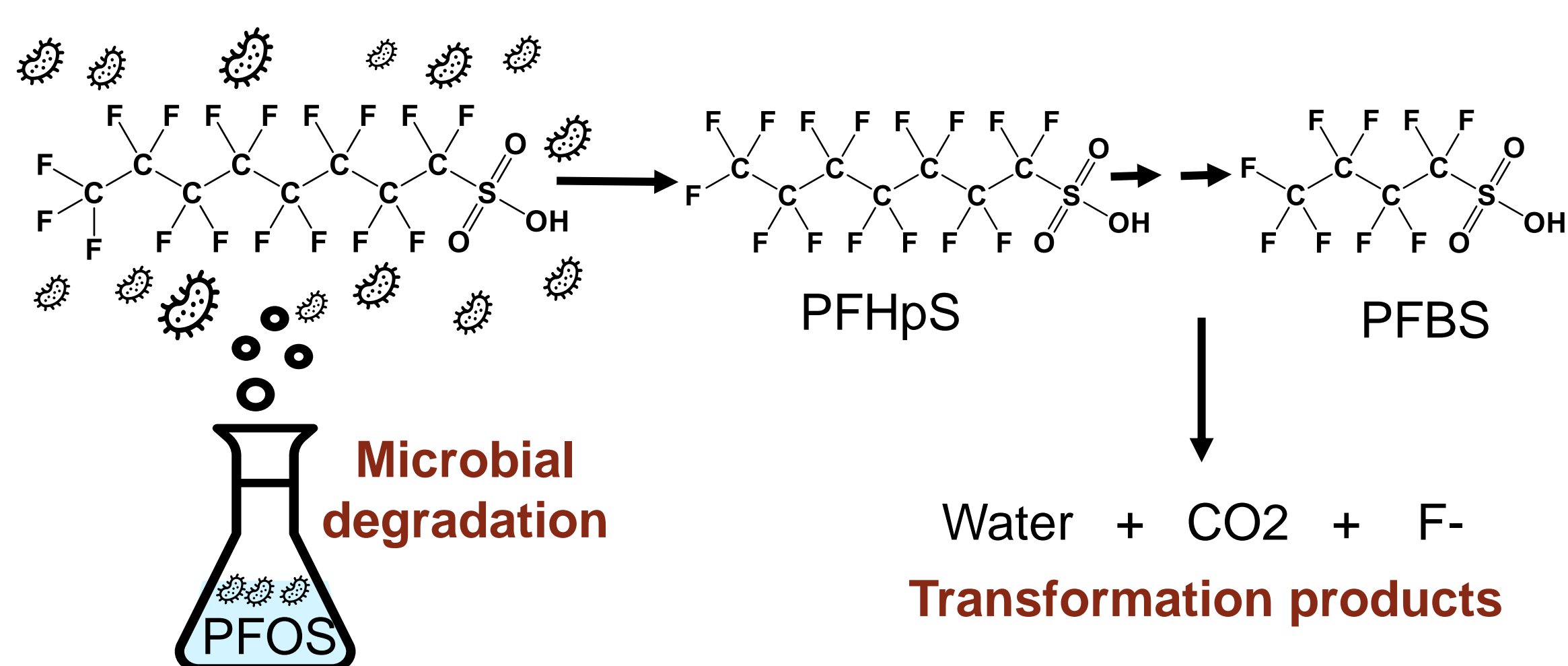
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Introduction

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.

Objectives

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



Method

F11 + PFOS

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

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

SPE extract

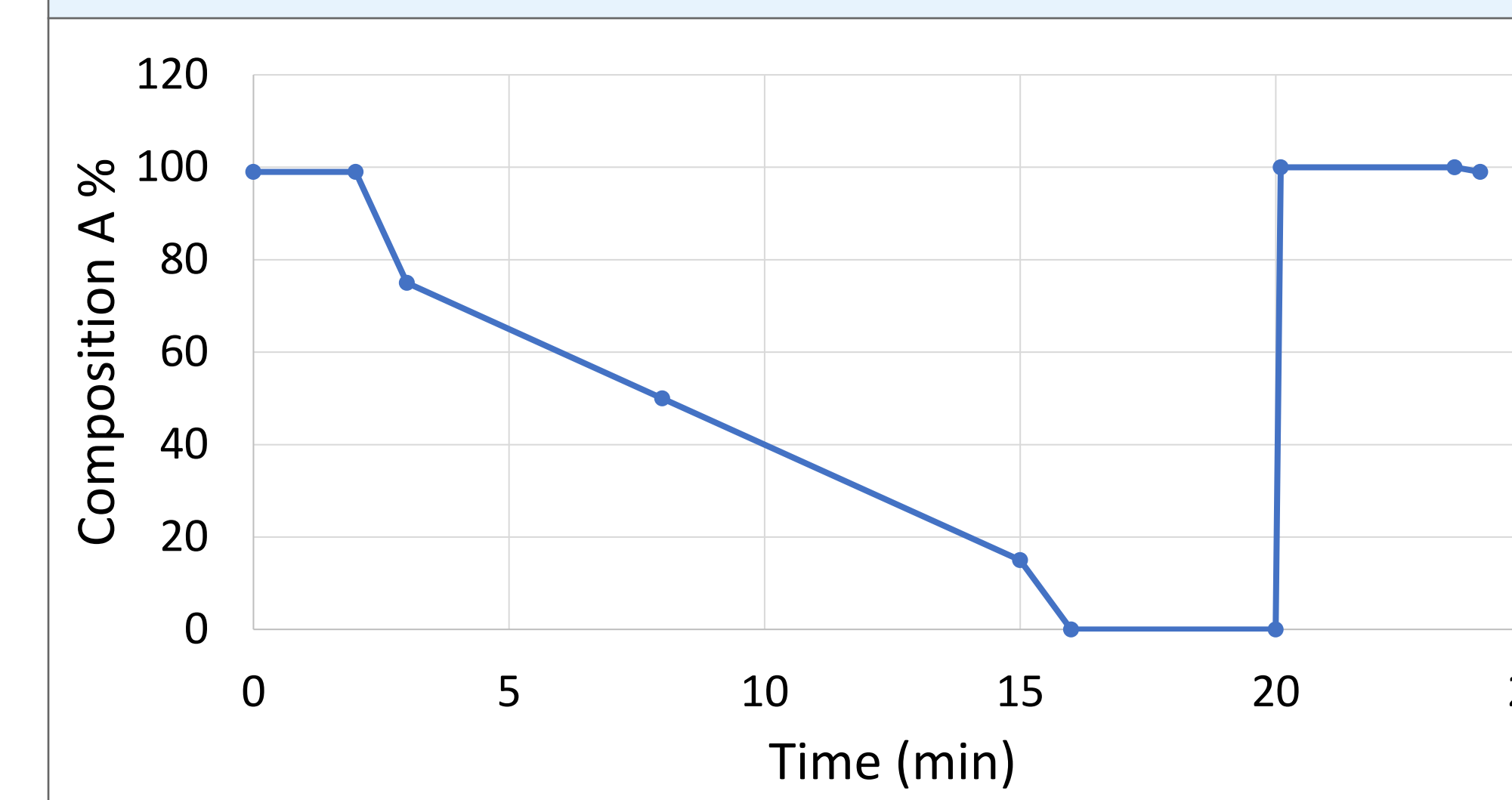
200 µL with ¹³C labeled standard mix

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

LC-IMS-qToF Instrumentation

Analytical column
Atlantis Premier BEH C18 AX, 1.7µm; 2.1mm x 100mm
Mobile phase A
Water + 2mM 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 Analysis

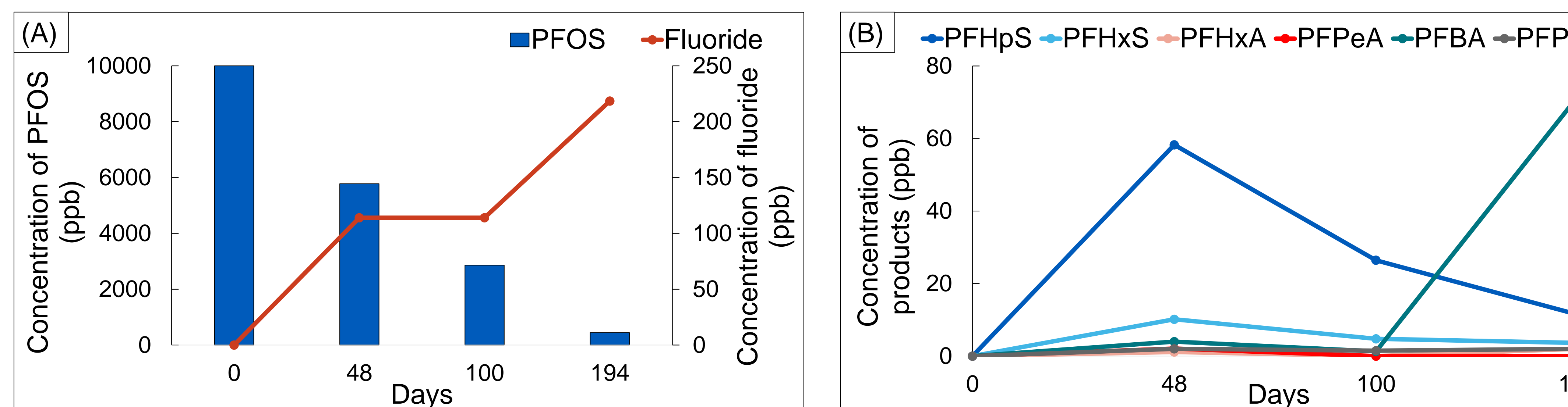
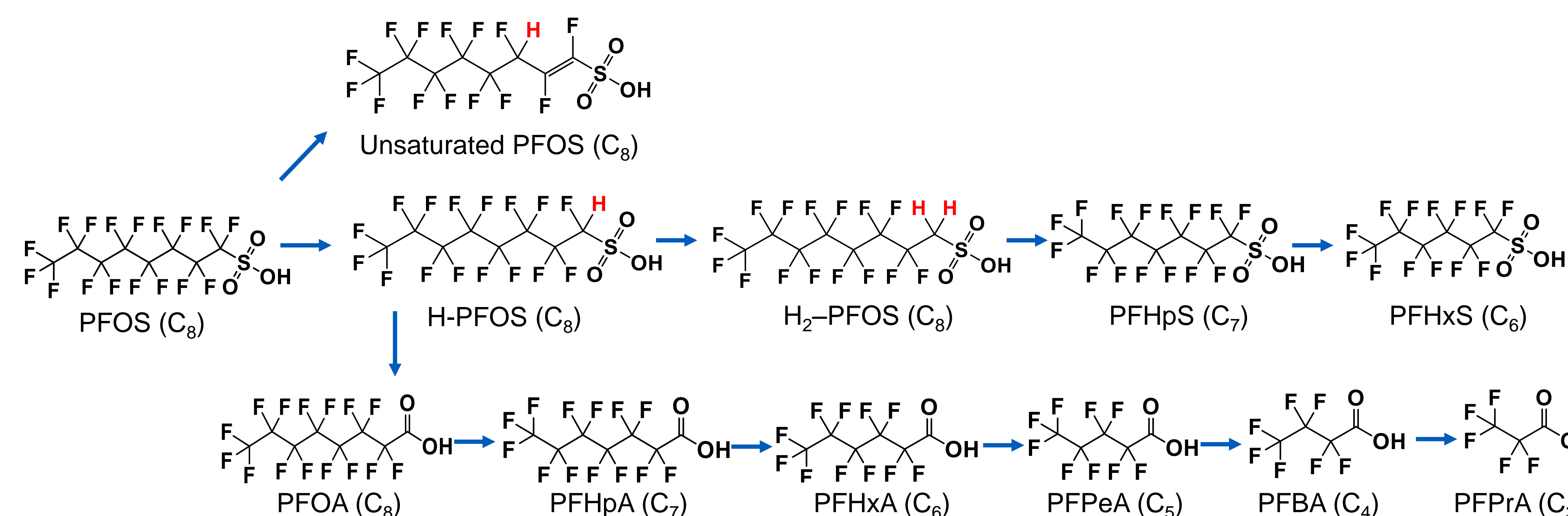


Figure 1: Plot showing a decrease in PFOS and a corresponding increase in fluoride (A) and targeted metabolites, PFHpS, PFHxS, PFHxA, PFPeA, PFBA and PFPrA (B) detected across 4 time points (0, 48, 100 and 194 days).

Proposed biotransformation pathway



Isomer separation

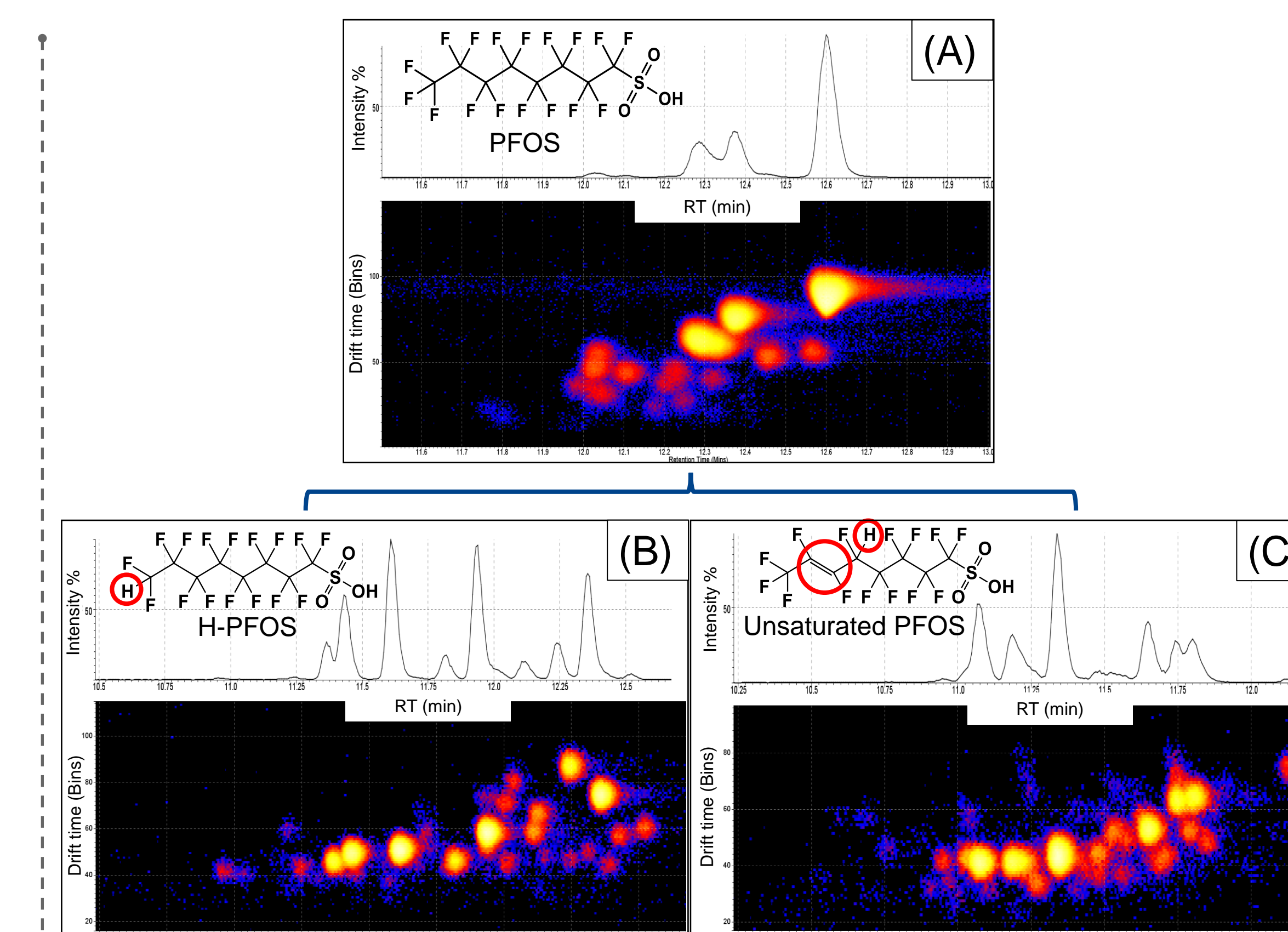


Figure 2: IMS chromatograms exhibiting isomer separation of (A) PFOS (m/z 498.932); (B) H-PFOS (m/z = 480.940); (C) unsaturated PFOS (m/z = 442.942)

Conclusions

- *Labrys portucalensis* strain F11 can degrade PFOS under aerobic conditions.
- Microbial degradation products were identified for PFOS from C₈ to C₃ compounds.
- Non-target analysis facilitated the identification of the unsaturated and hydrogenated C₈ 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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