

Preliminary appreciation biodegradation of formate and fluorinated ethers by means of Raman spectroscopy coupled with chemometrics

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1- Airport facilities context

The safety of passengers in particular relying on intensive use of de-icers (formate, acetate, ...), anti-icing (glycol-related chemicals), fire-fighting foams (fluorinated ethers, ...)

⇒ local pollution due to the accumulation in soil and water resources

⇒ large organic charges in water treatment facilities and in water courses



Objectives and expected chemometrics benefits

- detection of these chemicals (example: fluorinated ethers < 1%, when specified)
- evaluation of pollutants and their environmental concentrations for water management (product choice, cleanup solution)
- evaluation of their biodegradation (levels and kinetics) using cost-effective, reliable and quick techniques

2- Biodegradation and Raman spectroscopy

Selection of a formate and of a fluorinated ether

Commercial products = mixtures of chemicals, some presenting higher toxicity

Implementation of a simplified OECD 301F protocol for the screening of chemicals for ready biodegradability in an aerobic aqueous medium, with an inoculum made of sewage domestic effluents

Data collection with Raman spectrometer (Kaiser Optics RXN-2, 785 nm laser light)

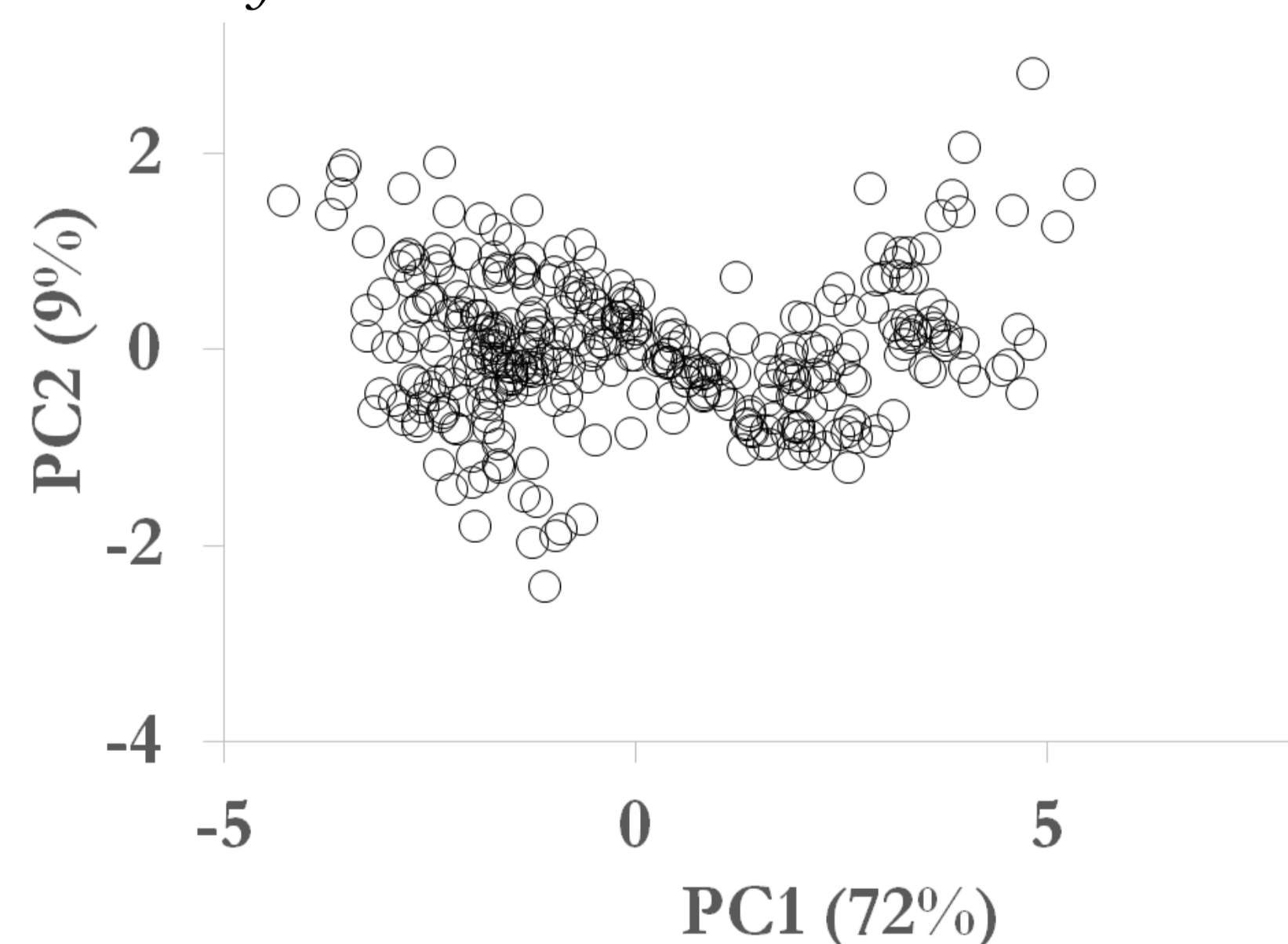
over 28 days, every 15 minutes, with a 30 s integration time (⇒ over 2500 spectra/test)



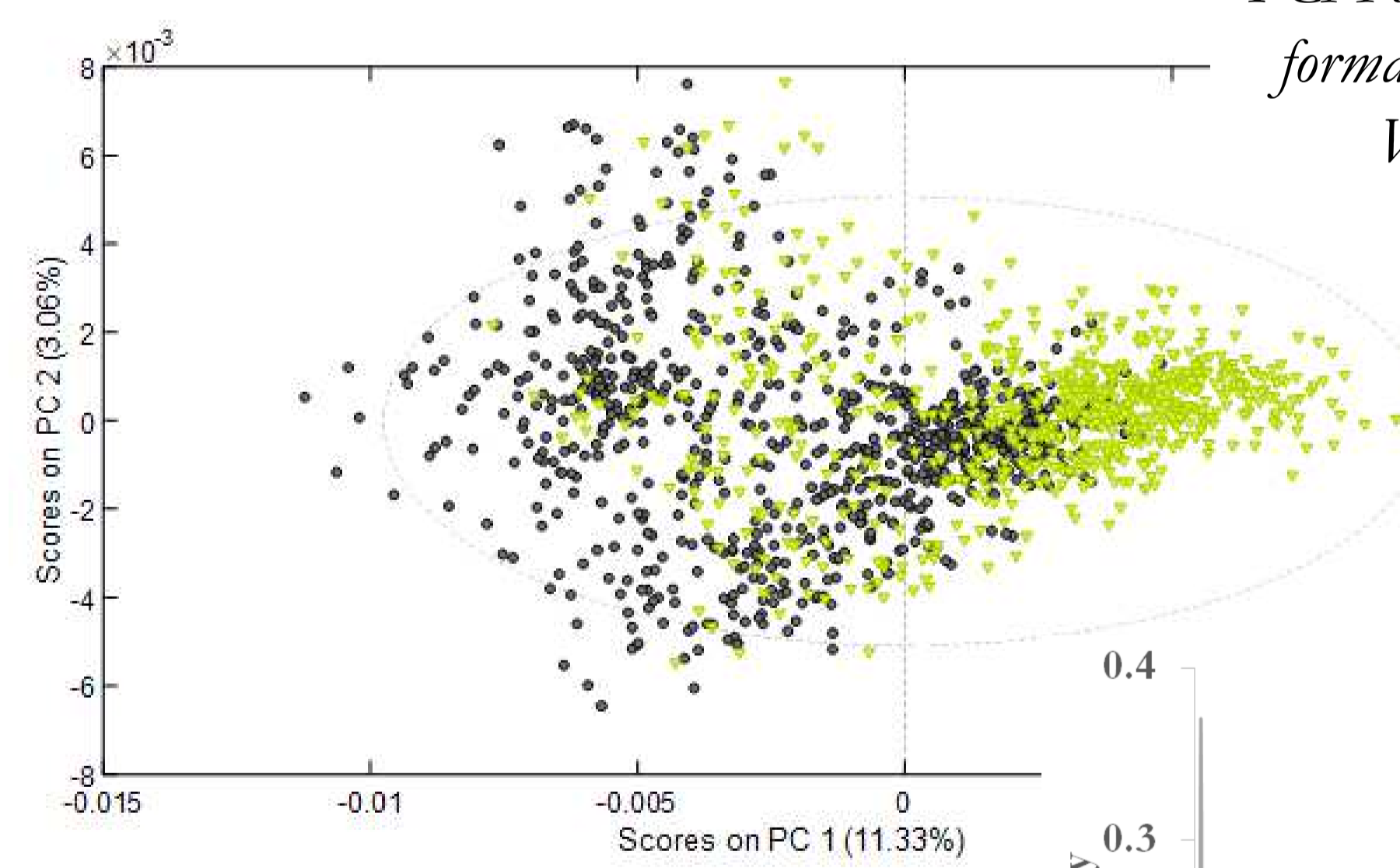
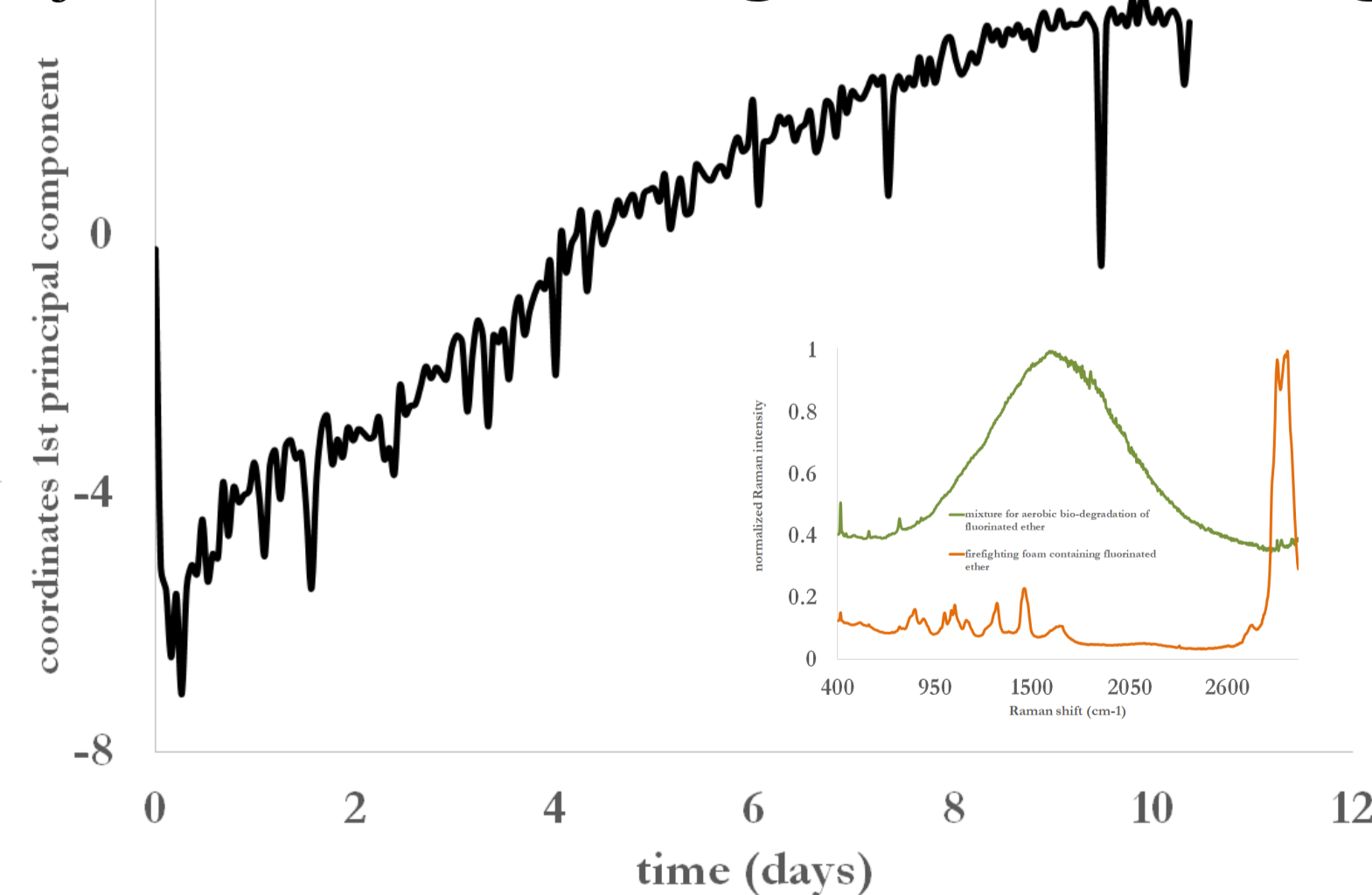
Raman immersion probes during the biodegradation test of a fluorinated ether

3- PCA and MCR biodegradation analysis

PCA scores plot for Raman spectra obtained during formate biodegradation monitoring after SNV and baseline correction

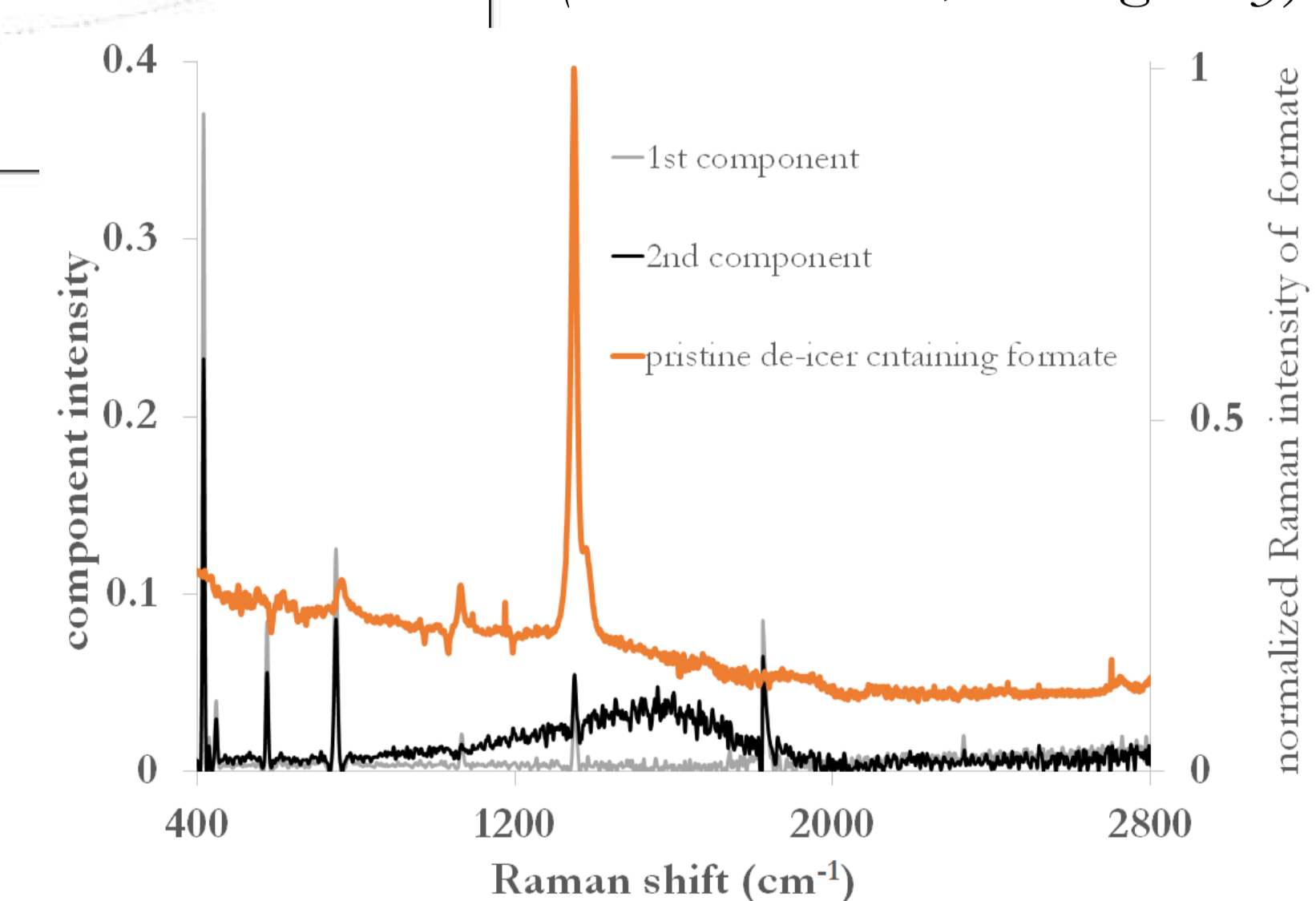


PC1 coordinates as a function of time for PCA on Raman spectra obtained during fluorinated ether biodegradation monitoring



PCA scores plot on Raman spectra during formate degradation after application of Whittaker filter (0,01 / 100)

MCR-ALS results on Raman spectra of formate degradation (SIMPSSIMA, non-negativity)



4- Conclusion

Successful implementation of Raman spectroscopy in the monitoring of the biodegradation of chemicals according to OECD protocol in spite turbidity of the fluid

Biodegradation identified through time evolution of 1st PC- coordinates dispersion in the scores plot

Remaining peaks representative of the pristine chemicals, indicating biodegradation not fully completed

Method to be applied to other molecules with conventional analysis (HPLC, ...)