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Short term stability of the extracts of 22 emerging contaminants in different supporting media



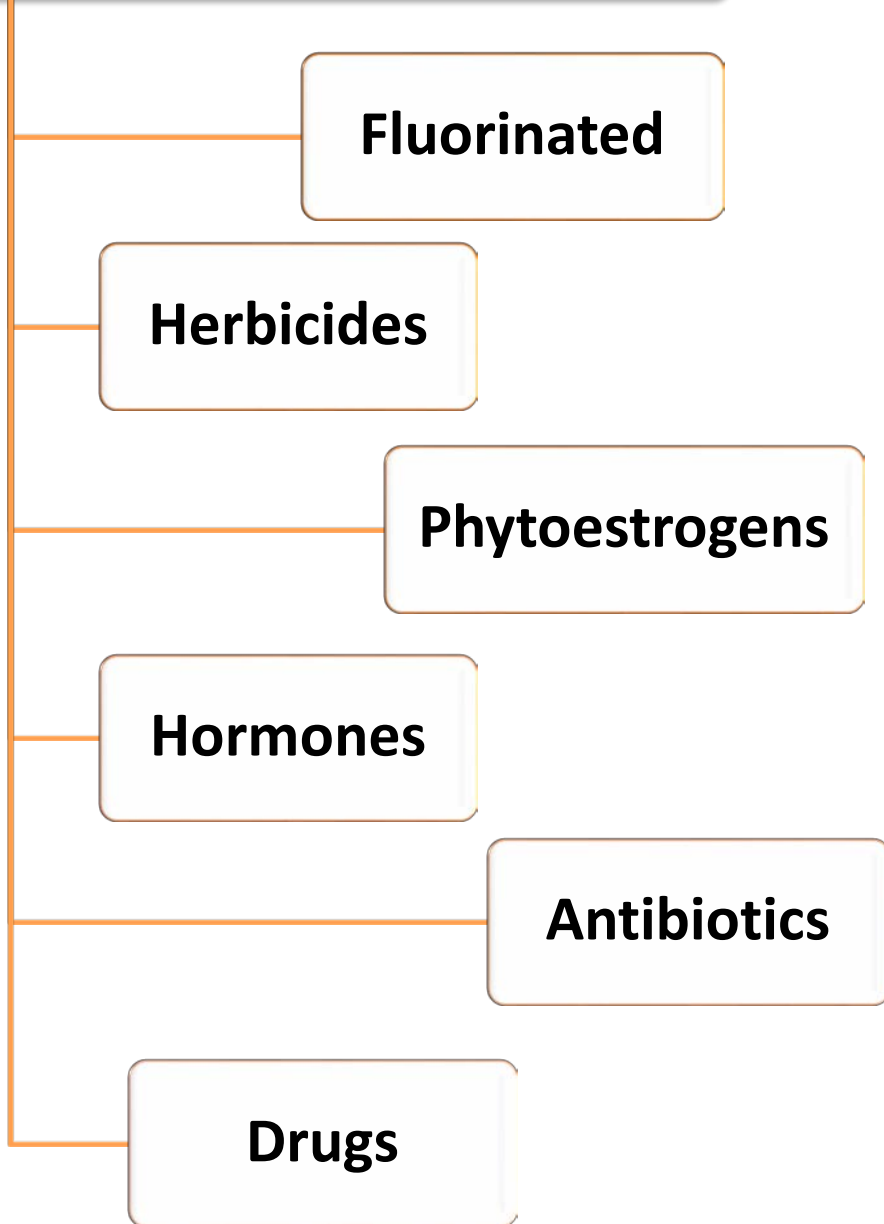
Context of the work



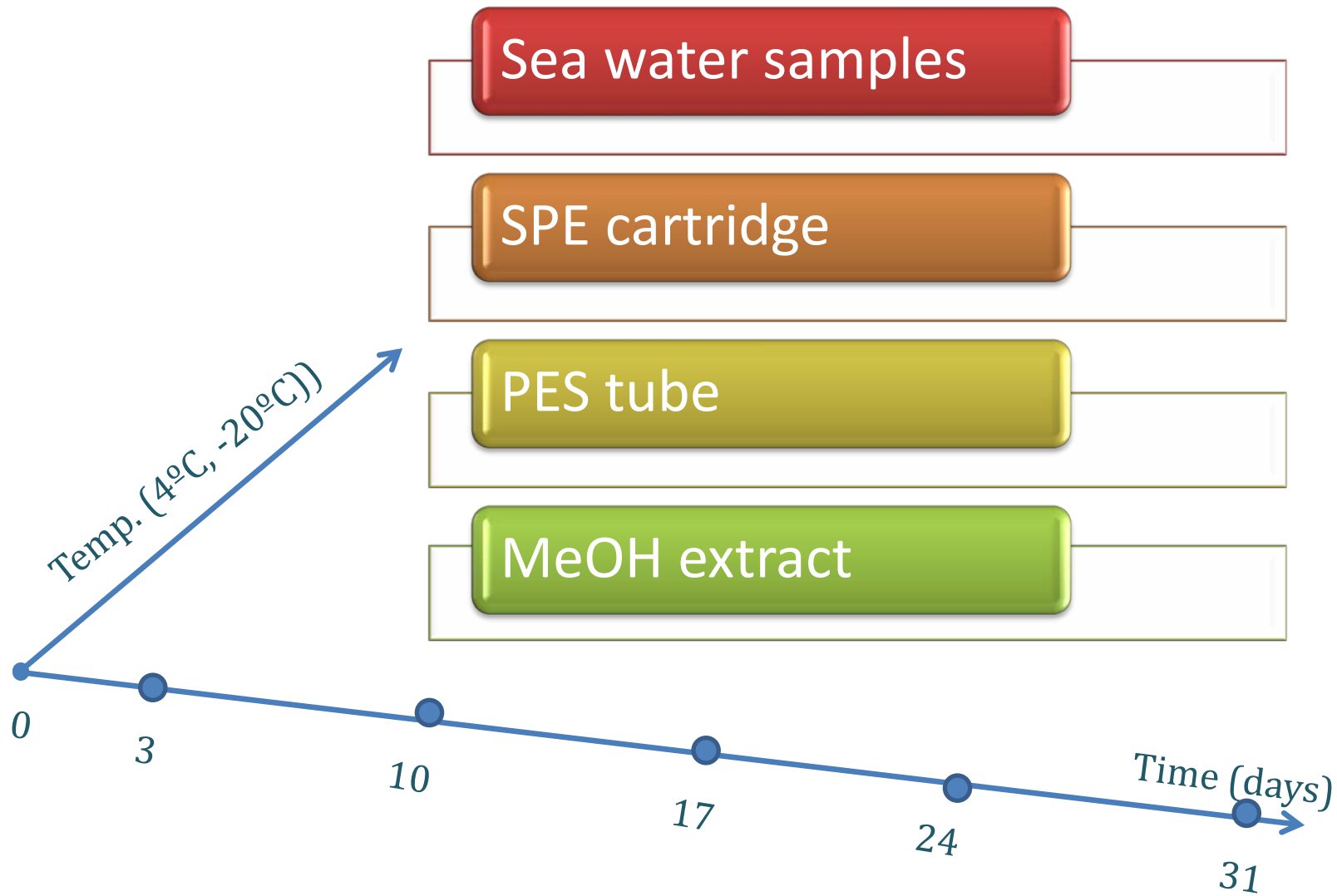




Analytes (>20)



- ACESULFAME
- AMITRIPTYLINE
- ATRAZINE
- BEZAFIBRATE
- CAFFEINE
- CARBAMAZEPINE
- DIURON
- GENISTEIN
- GENISTIN
- IMIPRAMINE
- IRBESARTAN
- KETOPROFEN
- NORFLOXACIN
- OXOBENZOTHIAZOLE
- PFOS
- PFOSA
- PFBS
- PG
- PROPANOLOL
- SULFADIAZINE
- SULFAMETHOXAZOLE
- TRIMETHOPRIM



Experimental approach

Sea Water



- 100 ml unfiltered sea water
- 500 ng/L each compound



- 4 °C
- < 31 days



- Oasis HLB 200 mg
- LC-MS/MS

SPE

- Spiked sea water soln. (100 ml)
- Strata-X-AW + Plexa-Bond Elut
100+100 mg

- -20 °C
- < 31 days

- Elution
- LC-MS/MS



PES polymer

Extrn.

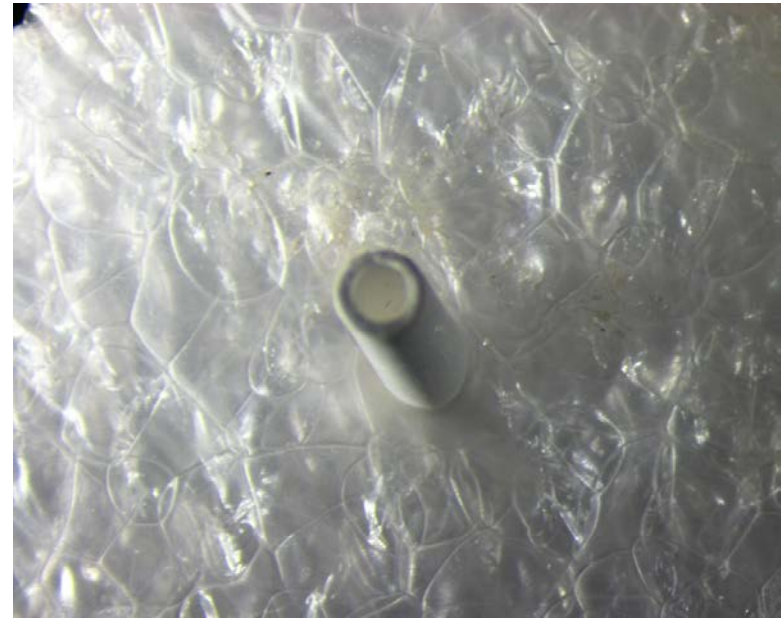
- 4 PES tubes (x4 cm)
- Overnight extr.
- Washed & dried

Storage

- -20 °C
- < 31 days

Analysis

- MeOH desorption
- LC-MS/MS



MeOH

- A mixed soln.
- 500 ng/l each compound

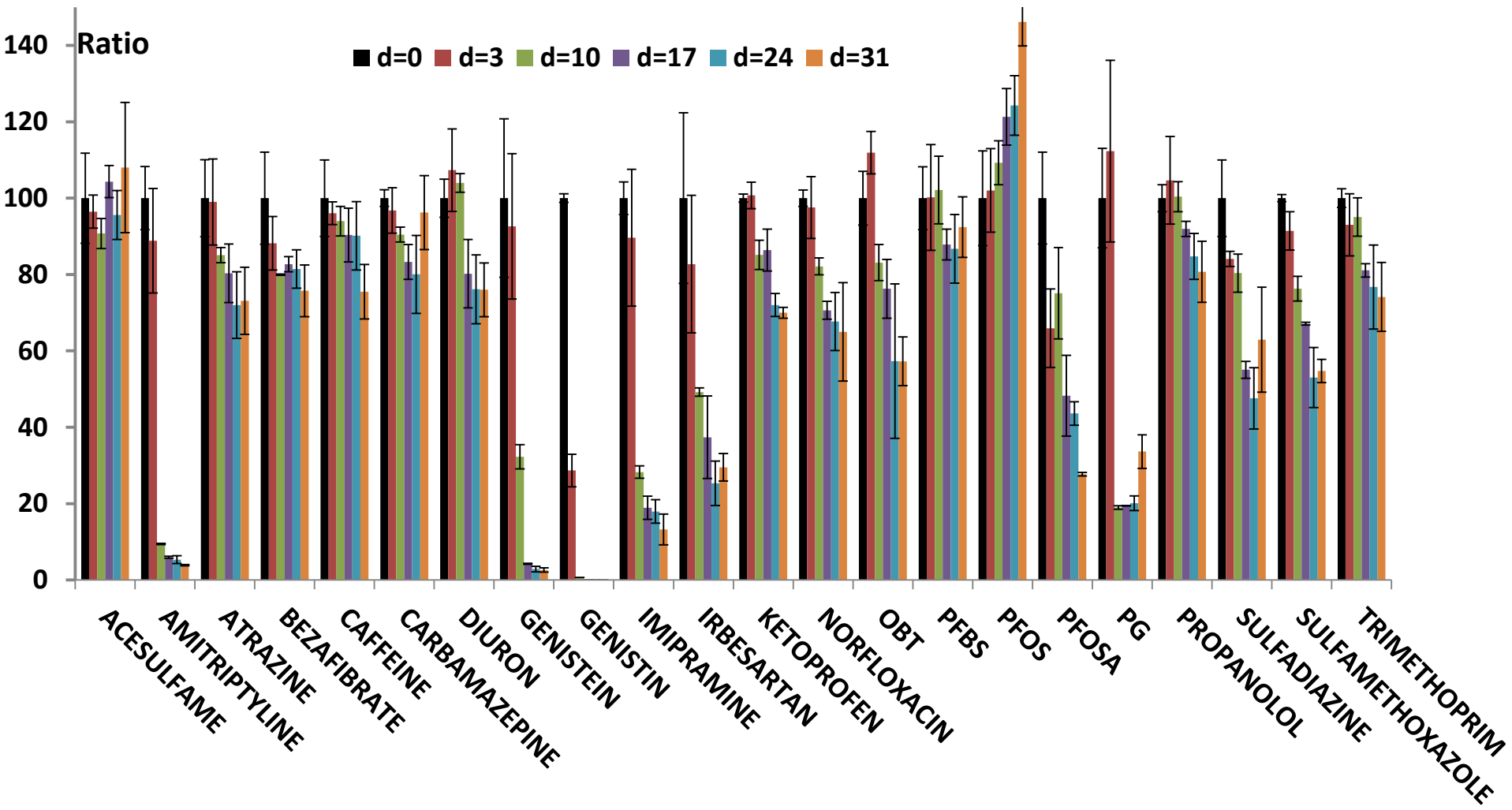
- -20 °C
- < 31 days

- Evaporation
- LC-MS/MS



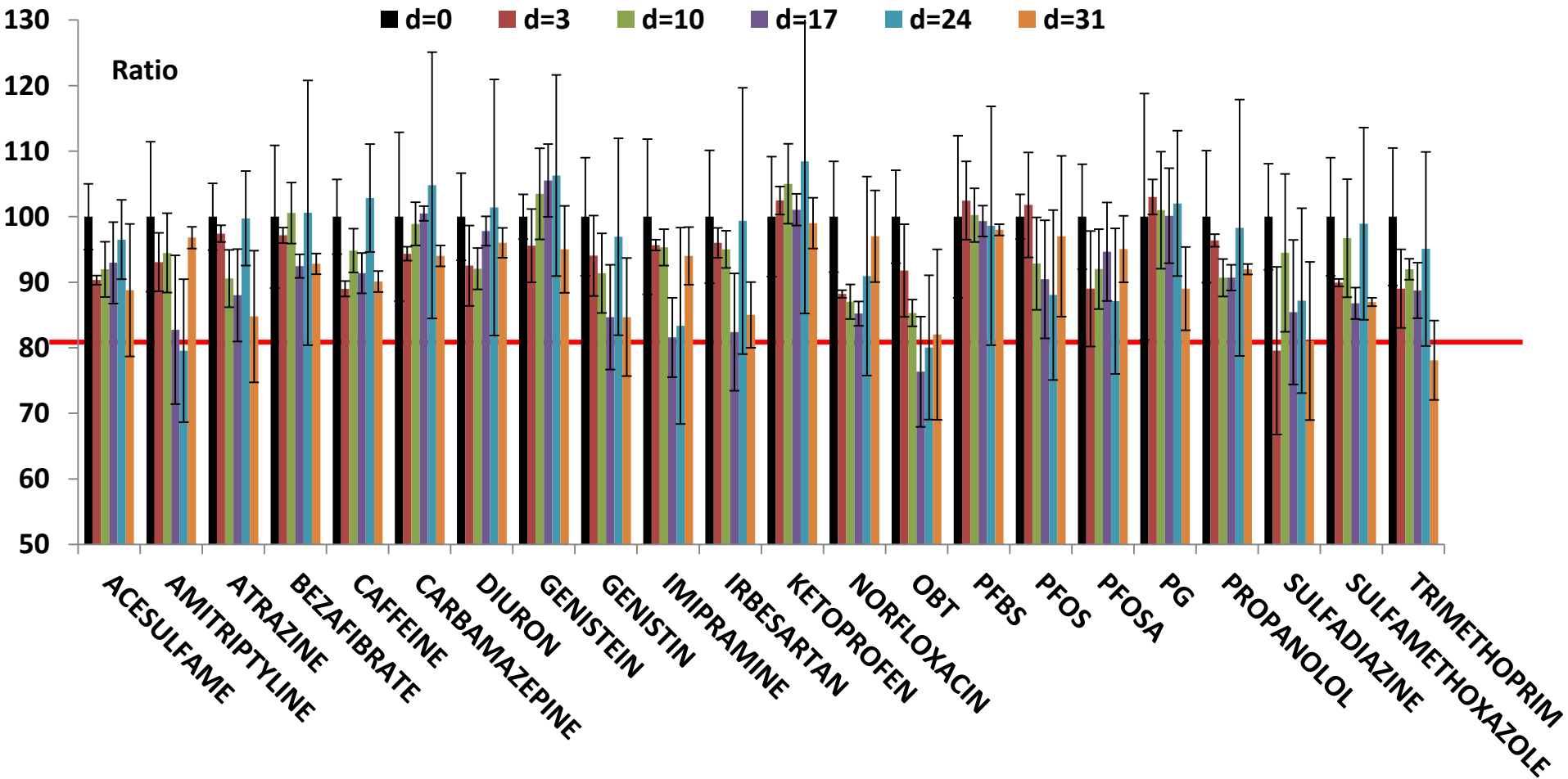
Results: Sea Water

(T_{ref} 4°C)

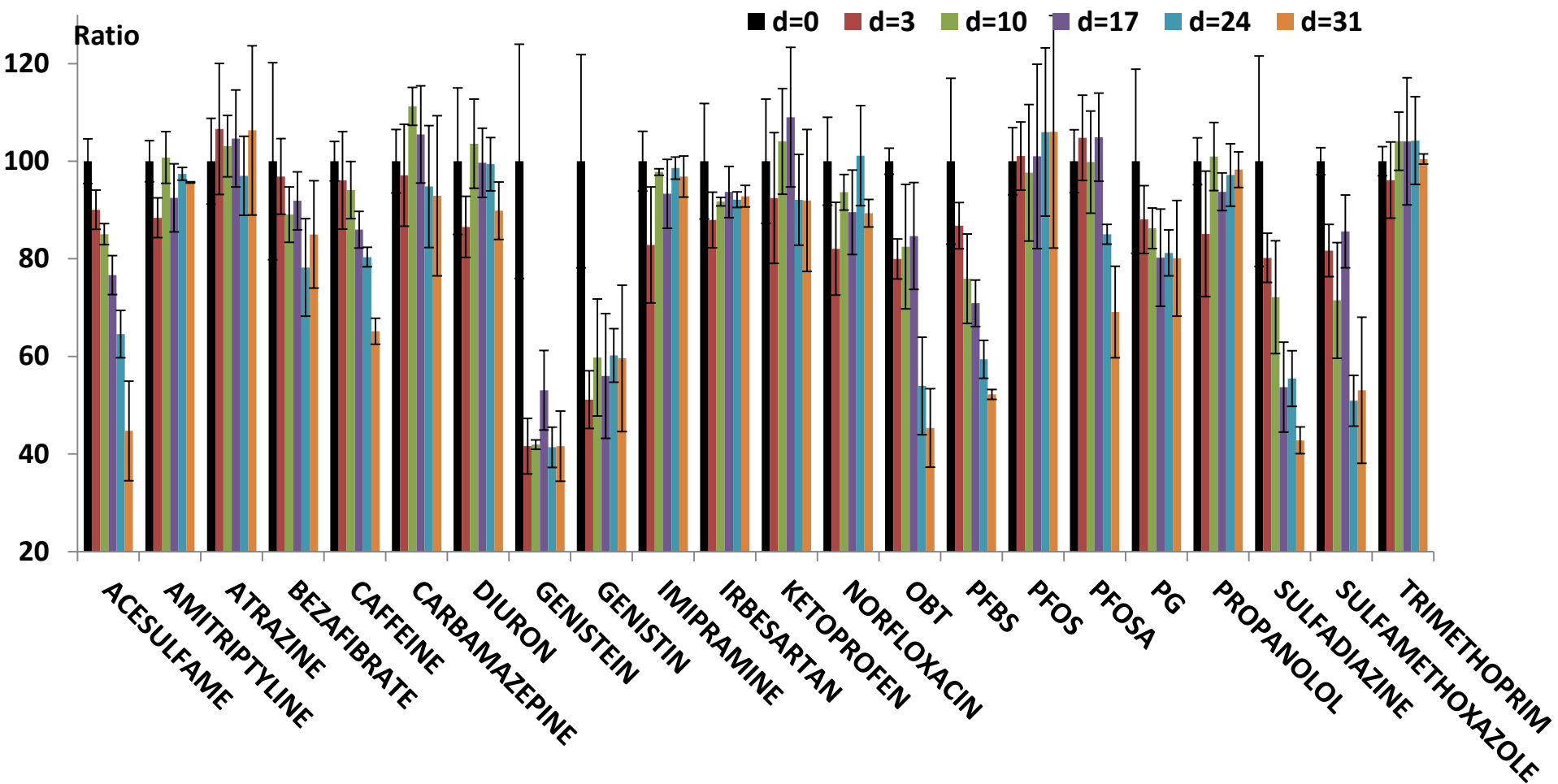


Results: SPE

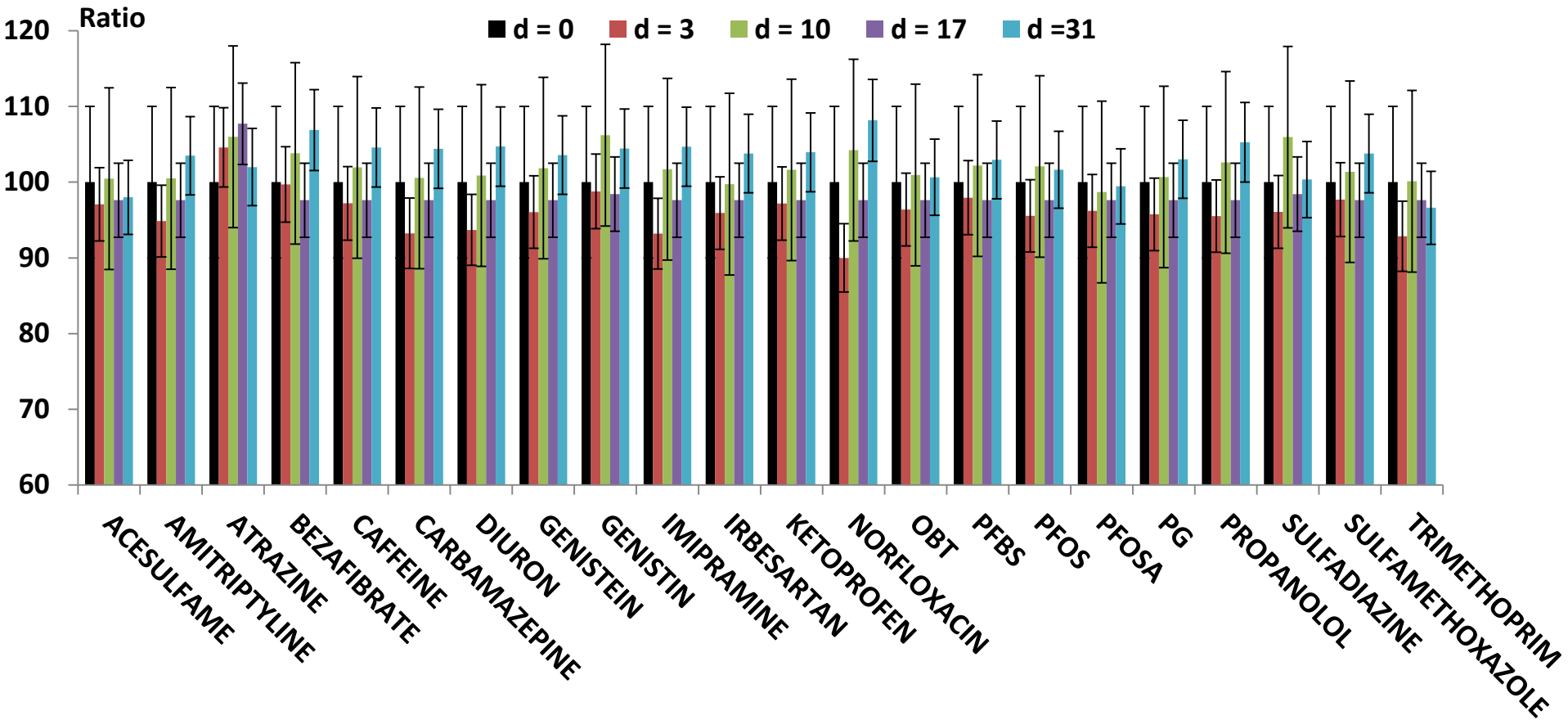
($T_{ref} -20^{\circ}C$)



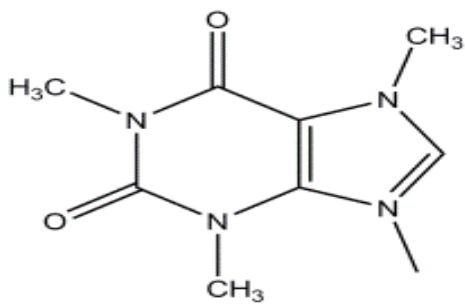
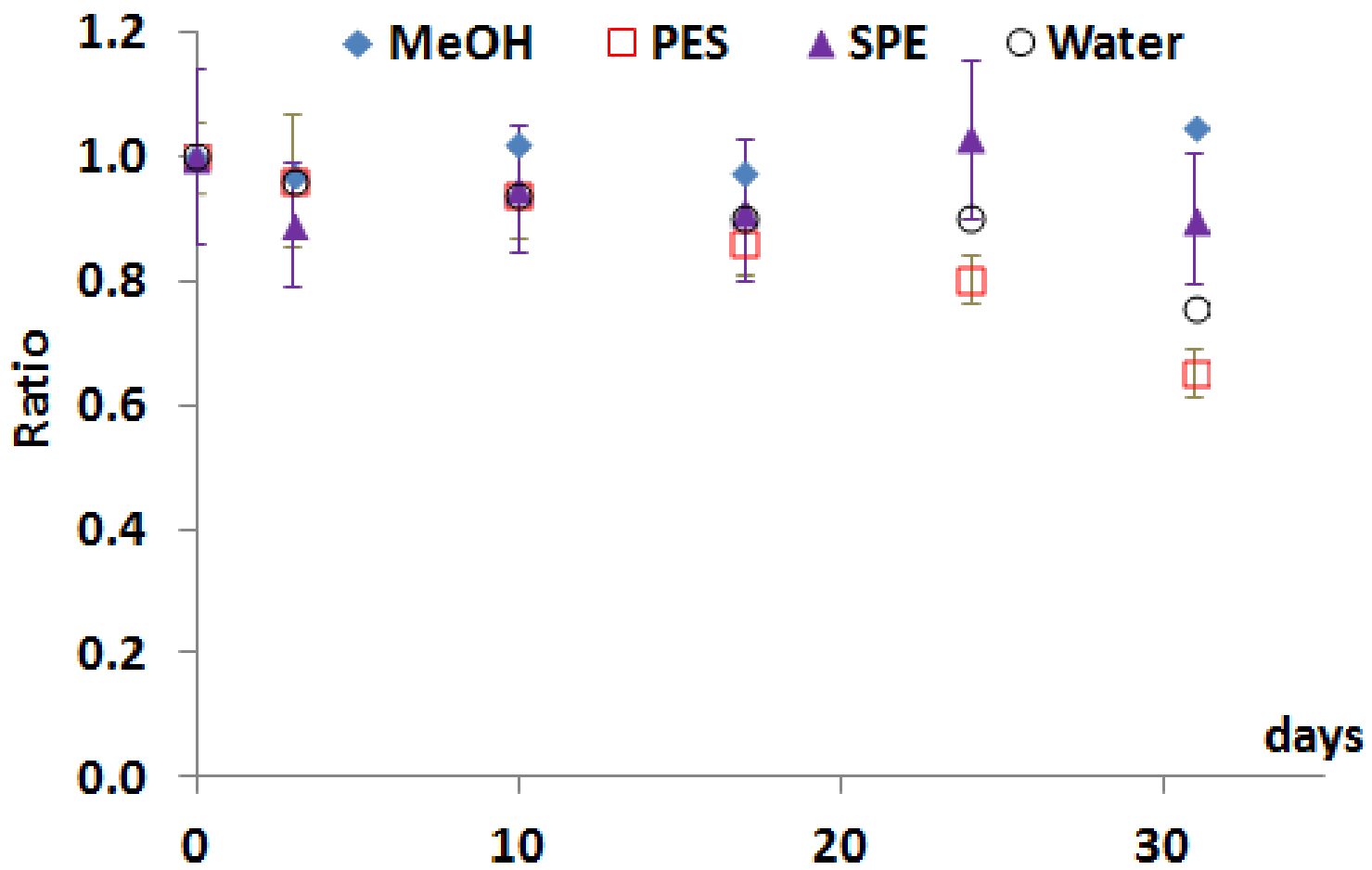
Results: PES



Results: MeOH

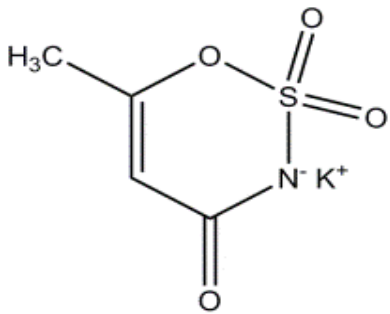
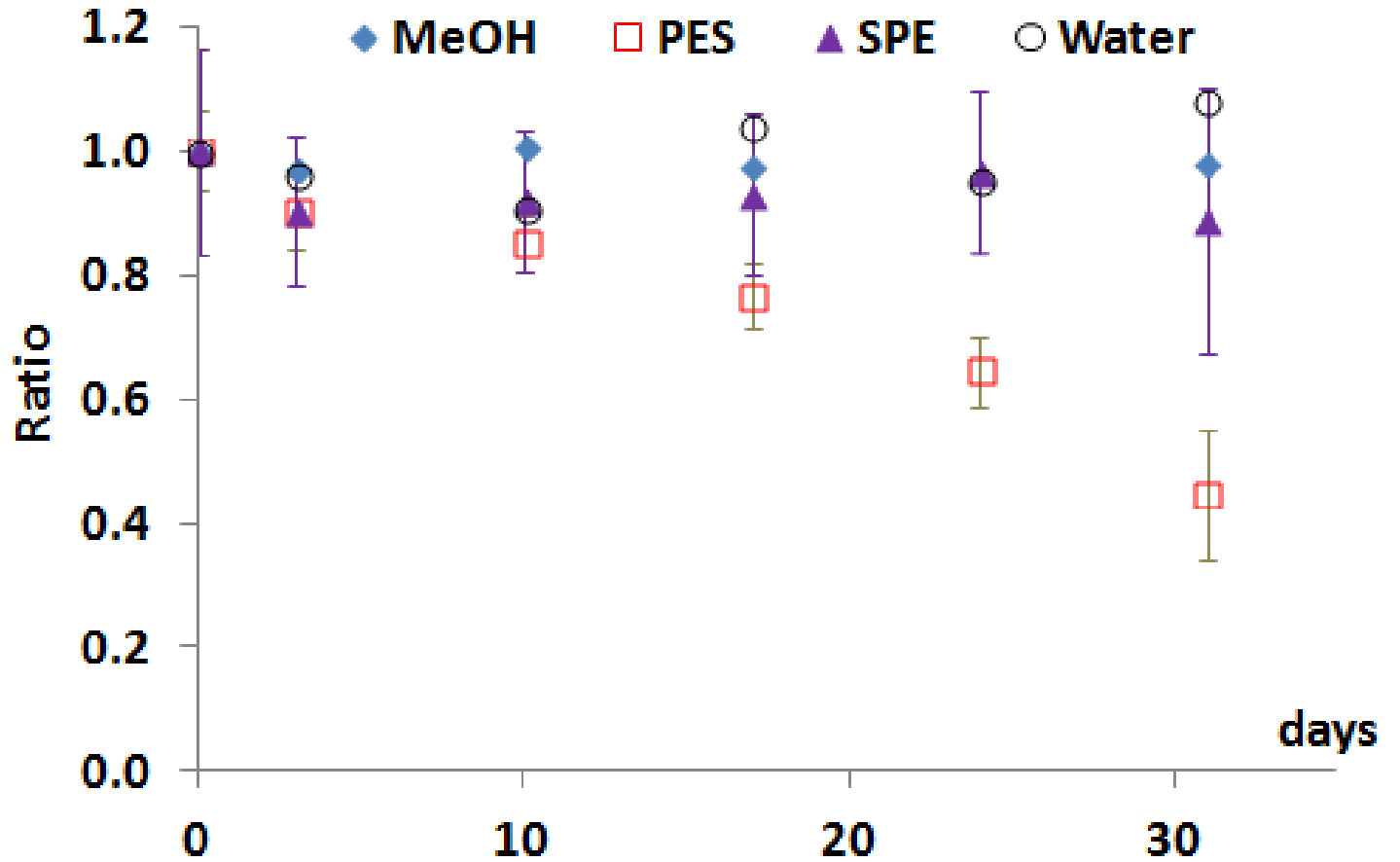


CAFFEINE



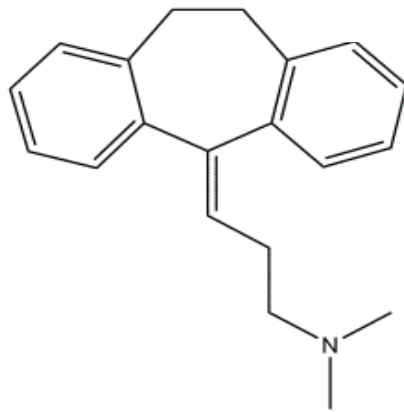
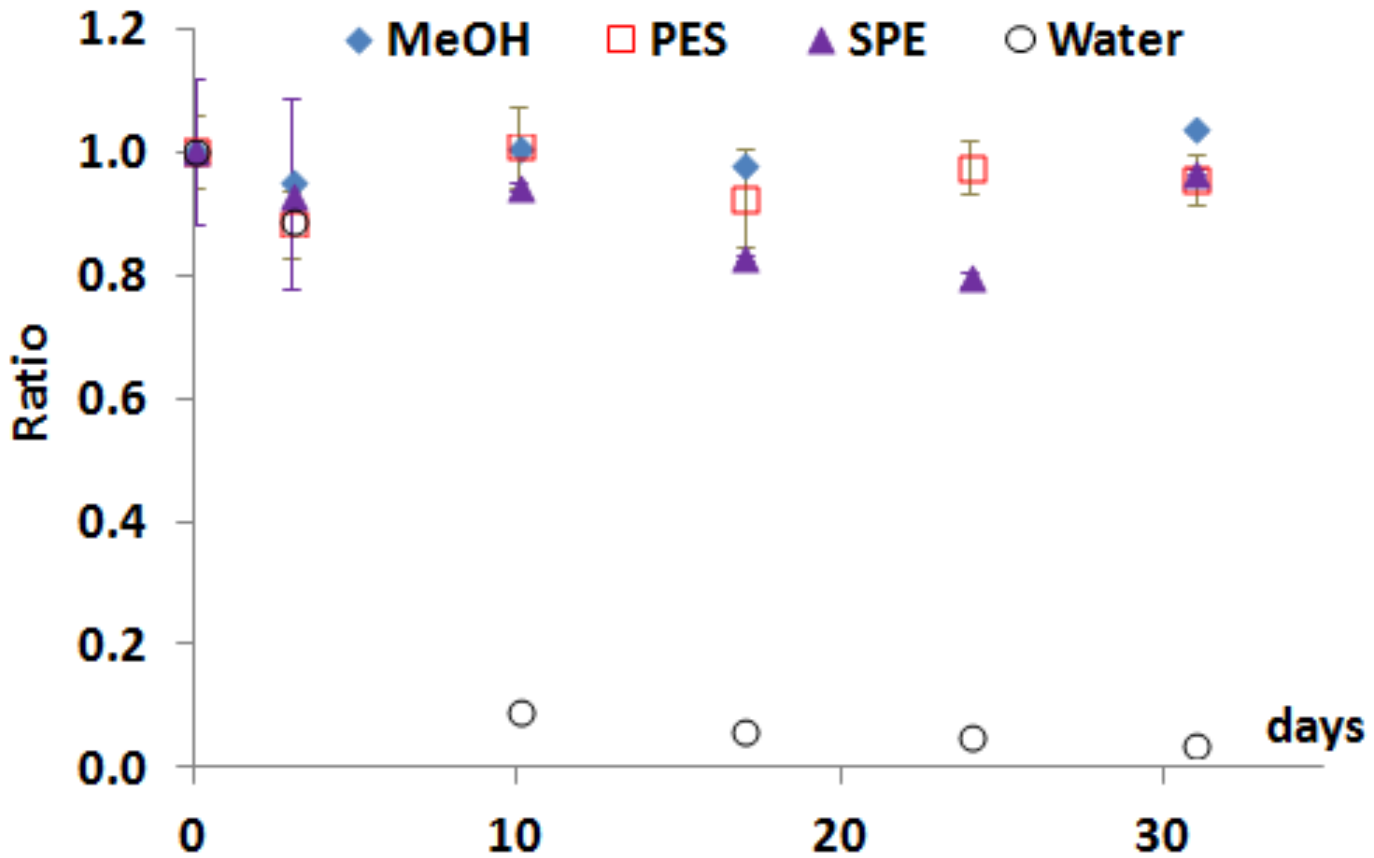
MW (g/mol)	log K _{ow}	pKa	W _{sol} (mg/l)
194.19	-0.60	0.9	2.2 x 10 ⁴

ACESULFAME



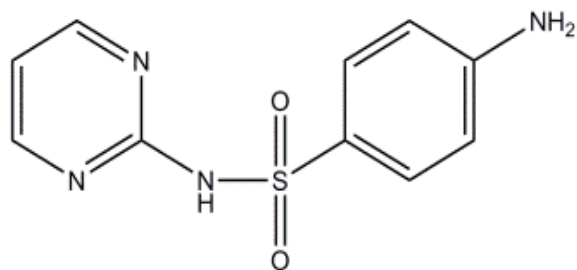
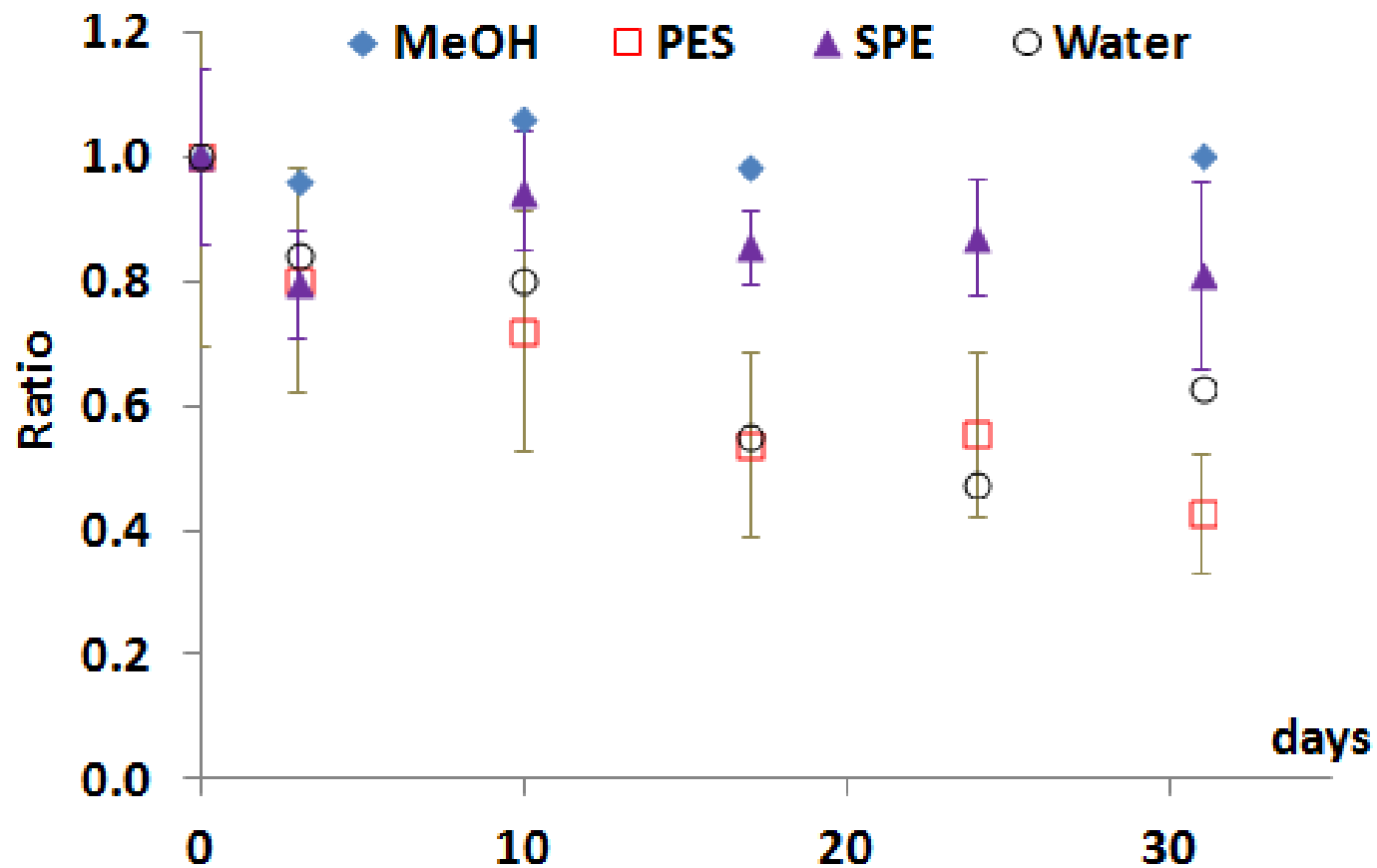
MW (g/mol)	log K _{ow}	pKa	W _{Sol} (mg/l)
163.15	-1.20	3.0	5.9 x 10 ⁵

AMITRIPTYLINE



MW (g/mol)	log K _{ow}	pKa	W _{Sol} (mg/l)
277.40	2.30	9.8	10.8

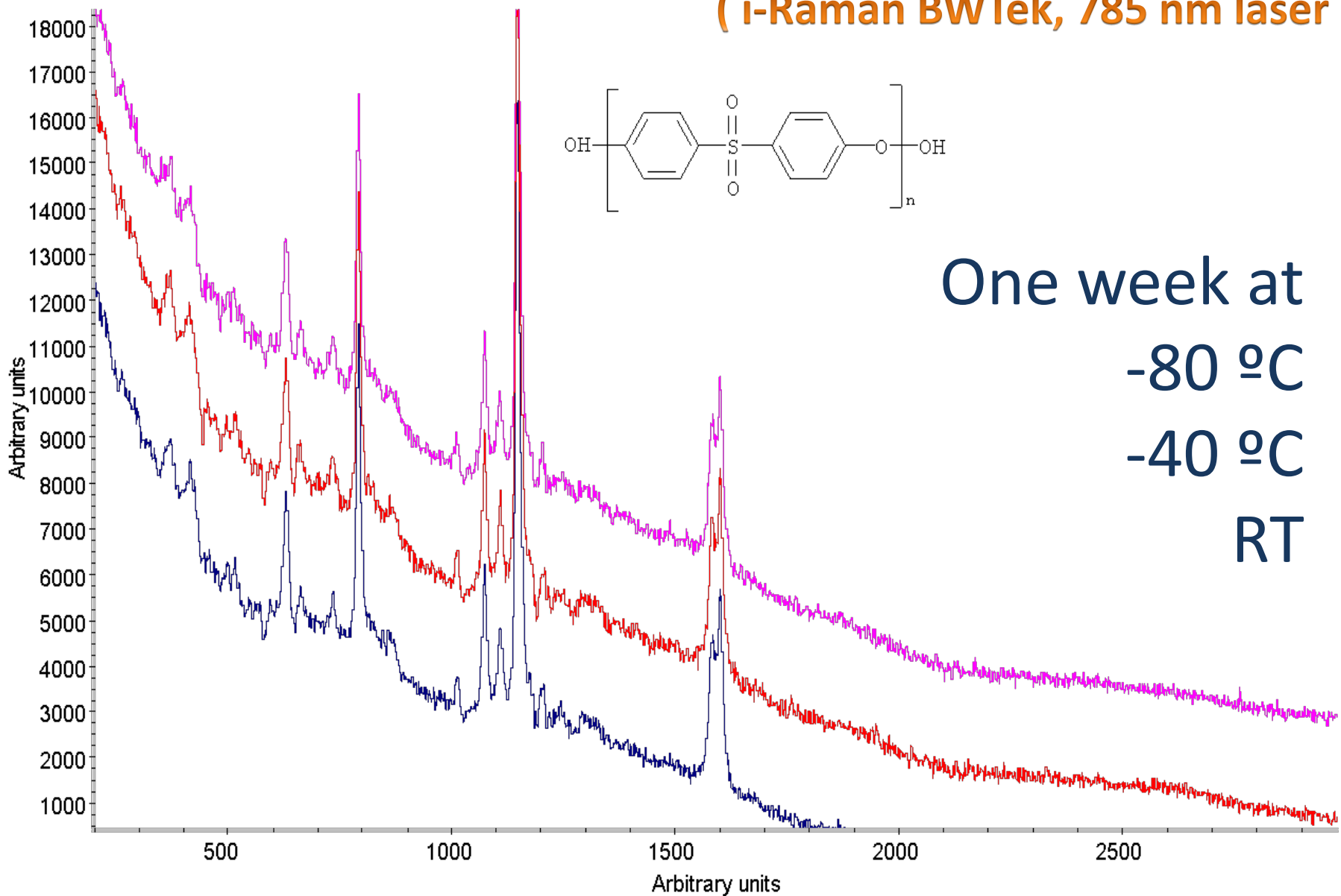
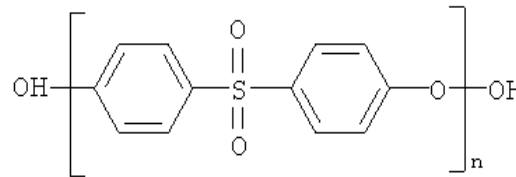
SULFADIAZINE



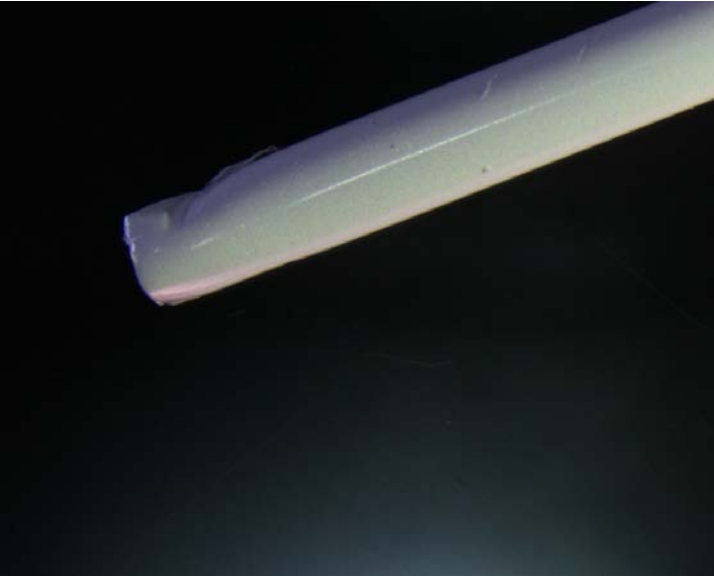
MW (g/mol)	log K _{ow}	pKa	W _{Sol} (mg/l)
250.28	0.10	2.0; 7.5	77

Raman analysis

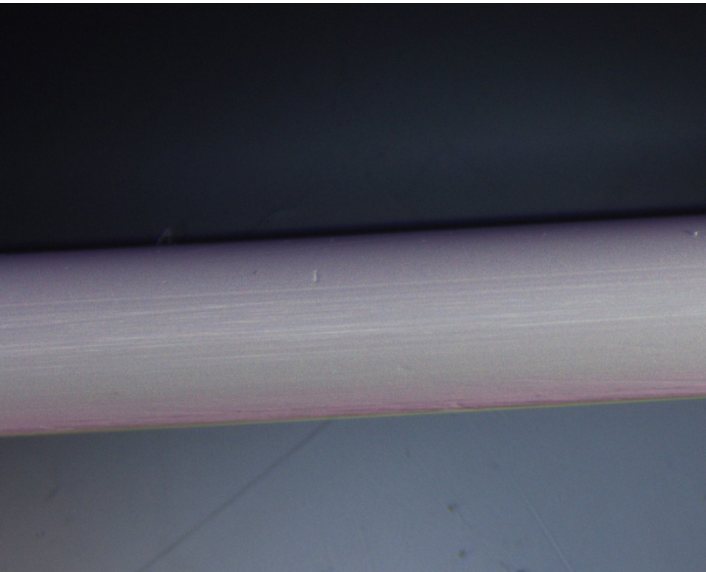
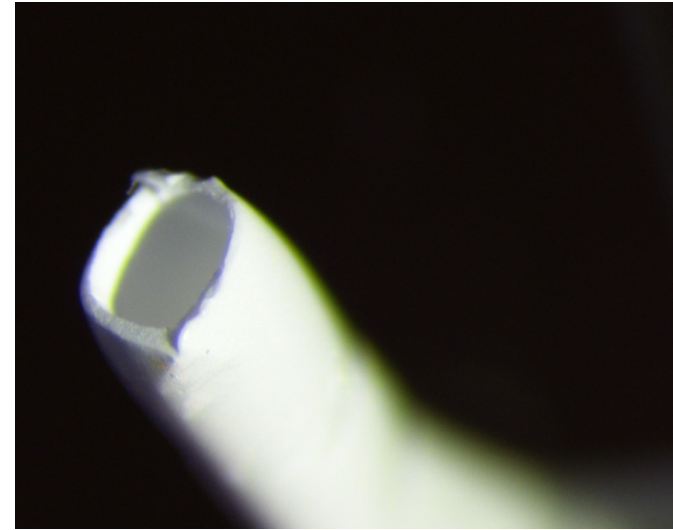
(i-Raman BWTek, 785 nm laser)



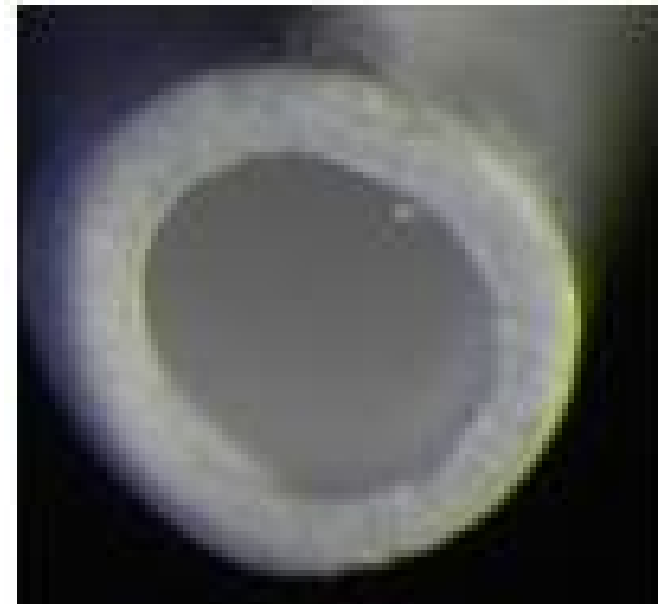
Microscopic Images



-40 °C

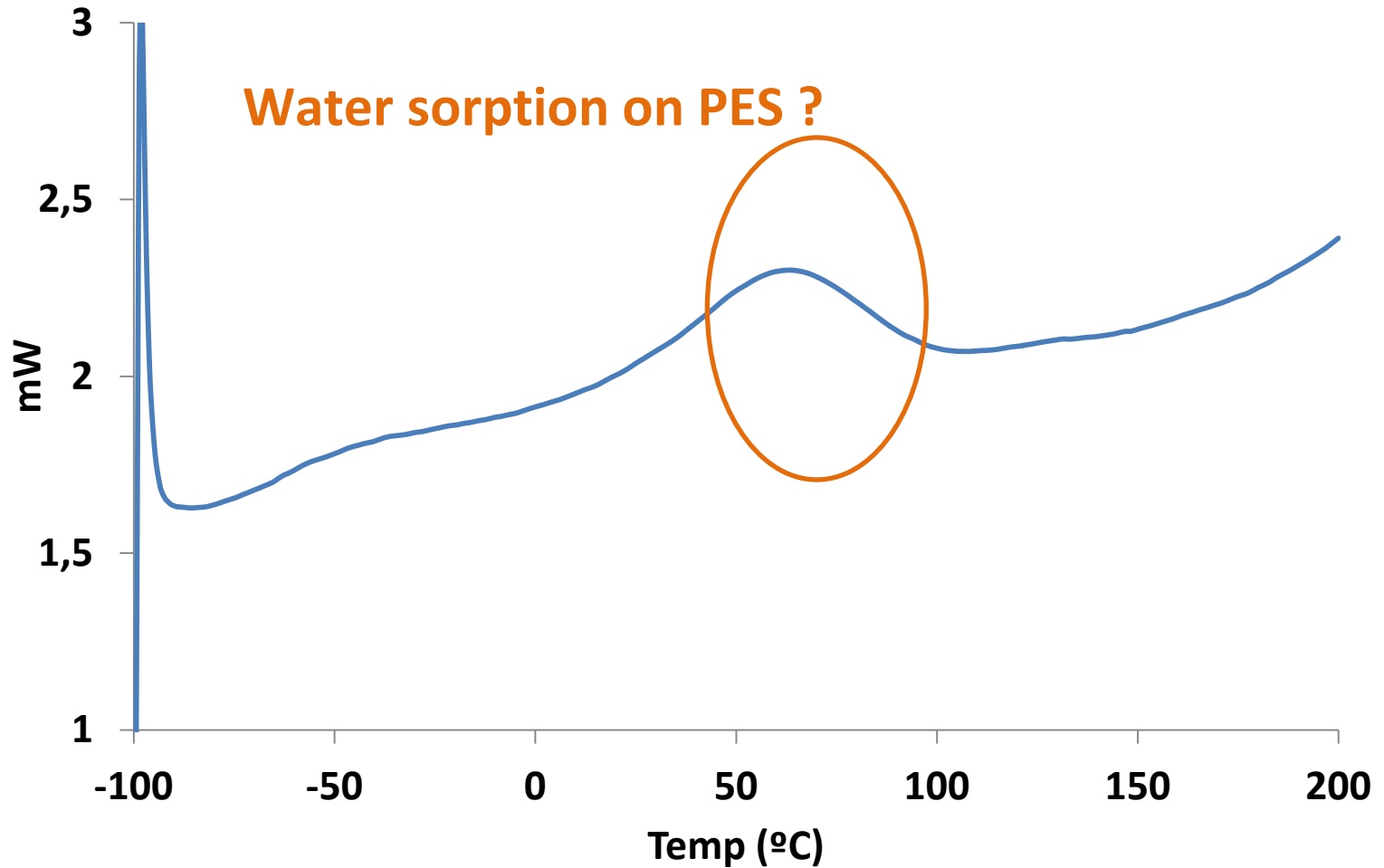


RT

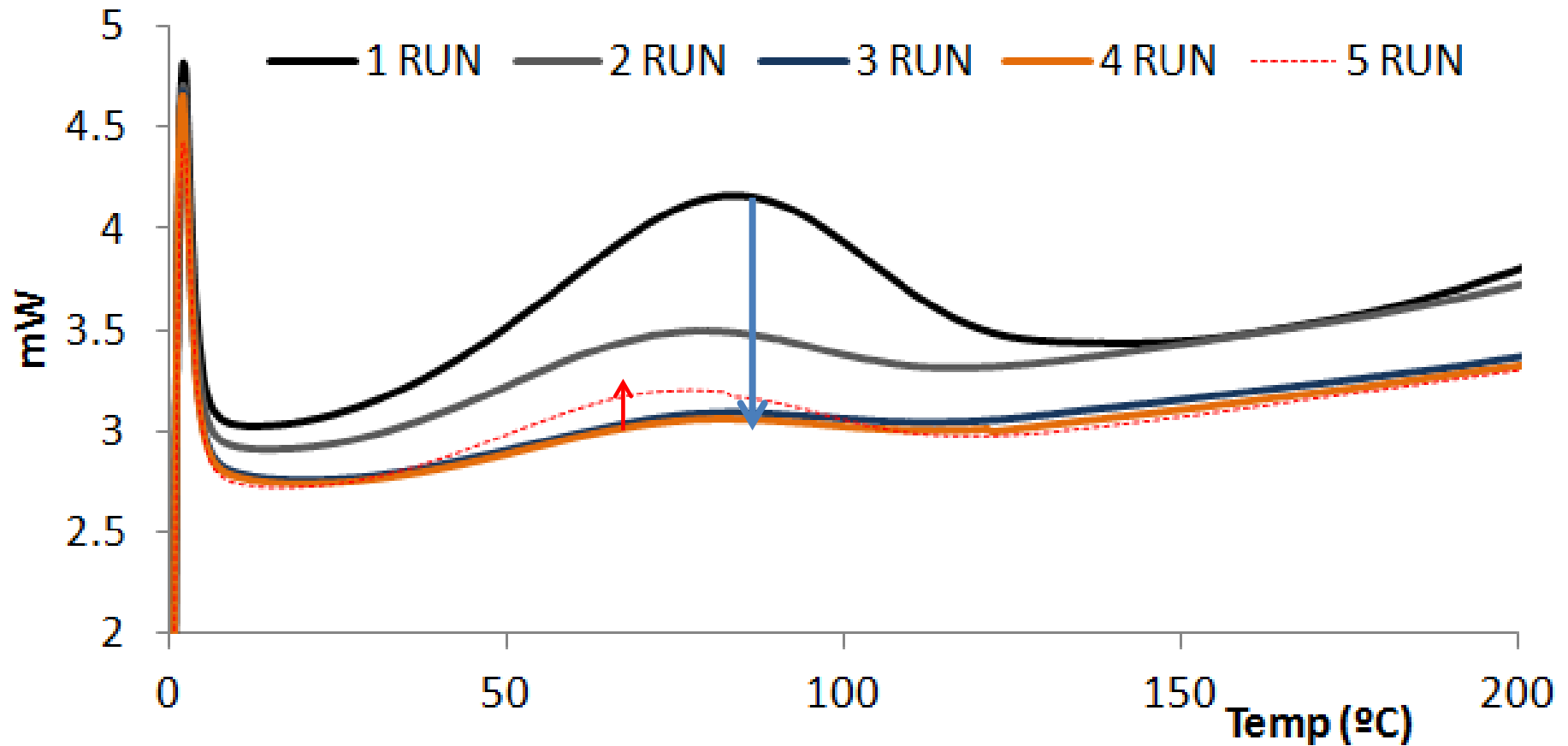


DSC analysis of PES

(Mettler-Toledo DSC822)



Sequential analysis



Conclusions



- ✓ The safest option is to keep the extracts in methanol.
- ✓ The SPE cartridges are a good option because we can assure recoveries > 80%.
- ✓ Water and PES samples should be processed as soon possible because many compounds are lost.

Thank you!

