National and Kapodistrian University of Athens
School of Science
Department of Chemistry
Laboratory of Analytical Chemistry

TrAMS
Trace Analysis and Mass Spectrometry Group

Analytical advances for the comprehensive chemical hazard assessment in food chain under the One Health concept

Nikolaos S. Thomaidis

Prof. of Analytical Chemistry (NKUA)

Group Leader of Trace Analysis and Mass Spectrometry research group

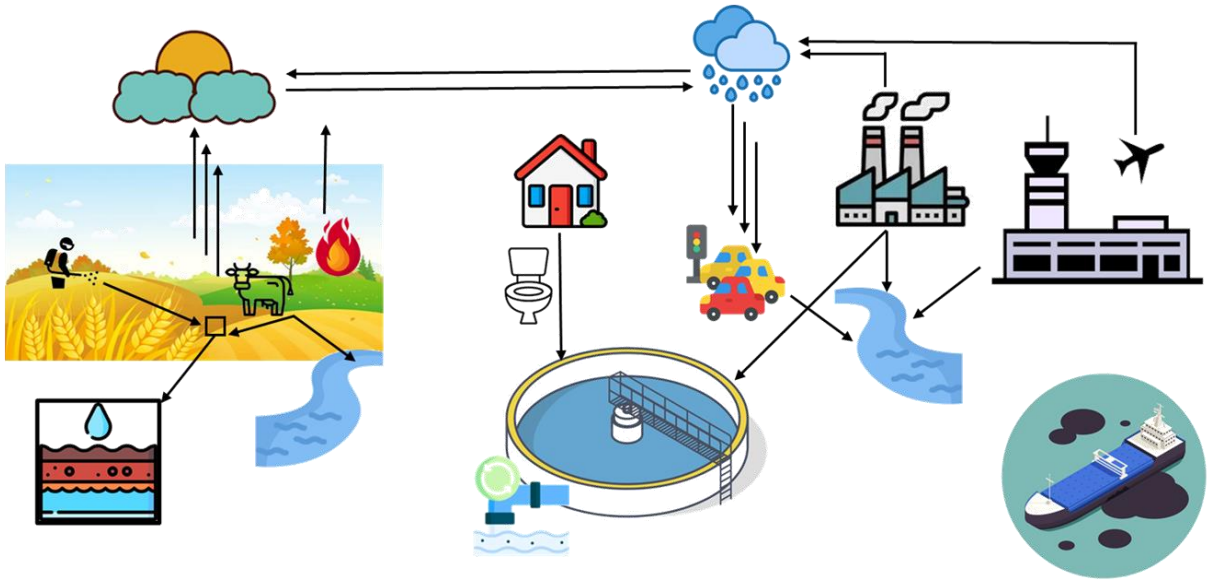
ΕΦΕΤ
ΕΘΝΙΚΟΣ ΦΟΡΕΑΣ ΕΛΕΓΧΟΥ ΤΡΟΦΙΜΩΝ

efsa
EUROPEAN FOOD SAFETY AUTHORITY

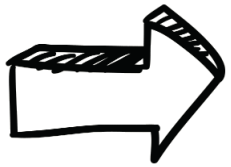
Risk Assessment and Ranking of Risks in European Food Safety Systems

Athens, 28th November 2024

Introduction



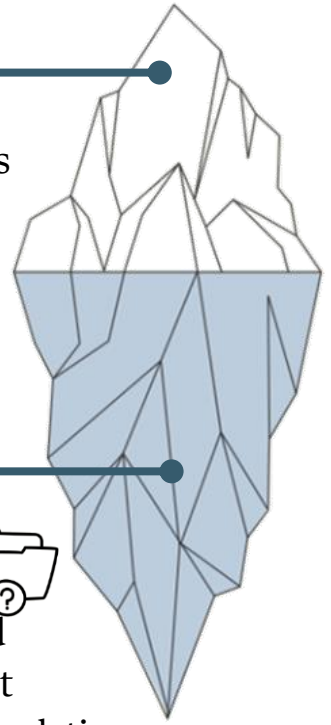
Sources of OPs in the environment



exposure of wildlife in hazardous chemicals

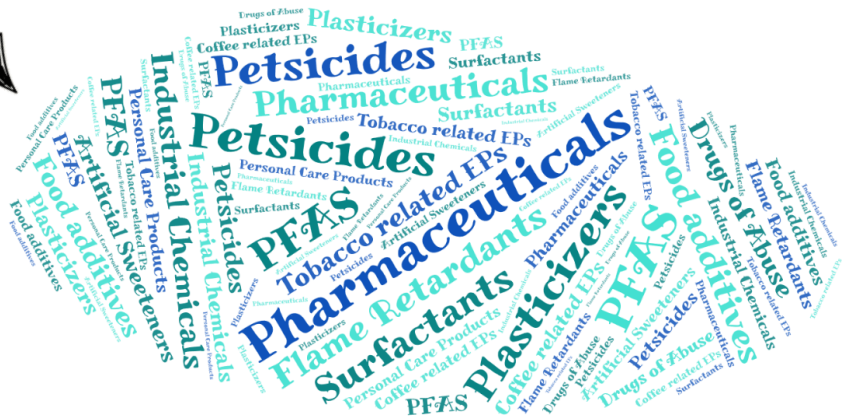
Persistent Organic Pollutants

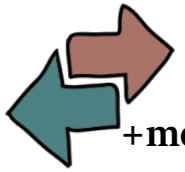
- known hazardous properties
- routinely monitored
- regulation



Emerging Pollutants

- unknown properties
- not routinely monitored
- detected in environment
- candidates for future regulation





+metabolites / transformation products

Our research group

Trace Analysis and Mass Spectrometry (**TrAMS**) group

- 5 Professors and Teaching associates
- 16 Post-doctoral researchers
- 13 PhD student
- 11 Master students
- 4 Undergraduate students
- 3 Analysts – Researchers
- 3 Administrative support

Development of advanced methodologies using state-of-the-art instrumentation

Applications in **Environmental Analysis**, **Life Science** and **Foodomics** studies

Long term collaborations with Universities & Research Institutes worldwide

Strong links with **regulatory bodies** for environmental quality and food safety issues

http://trams.chem.uoa.gr

@ThomaidisLab

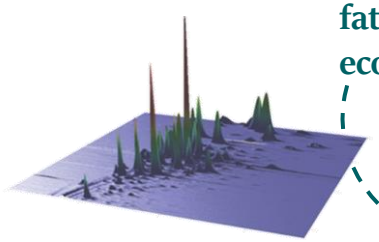
https://www.linkedin.com/groups/12717378

Our mission

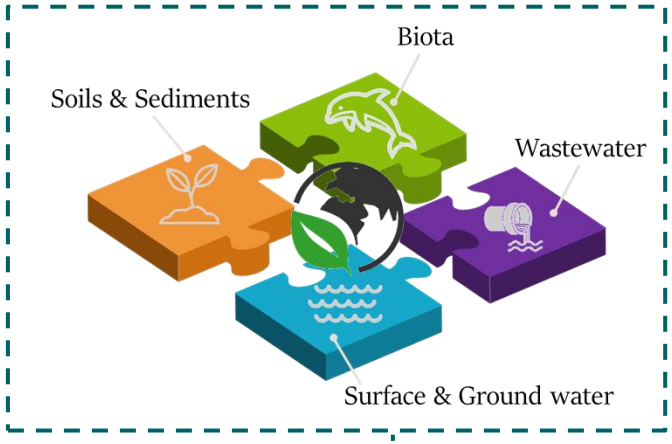
Answers in environmental problems on organic pollutants and their metabolites/ transformation products

holistic research approach

monitoring of thousands chemicals
fate studies
ecotoxicology



Monitoring "Big" Data



EU Regulatory bodies → new mitigation measures

*e.g. European Chemical Agency (**ECHA**)*
*European Commission Joint Research Centre (**JRC**)*
*Directorate-General for Environment (**DG ENV**)*

Development of novel analytical methodologies on sample preparation

State-of-the-art **mass spectrometric** instrumentation

Development of **advanced chemometric tools and data processing methods** (supporting non-target tools)

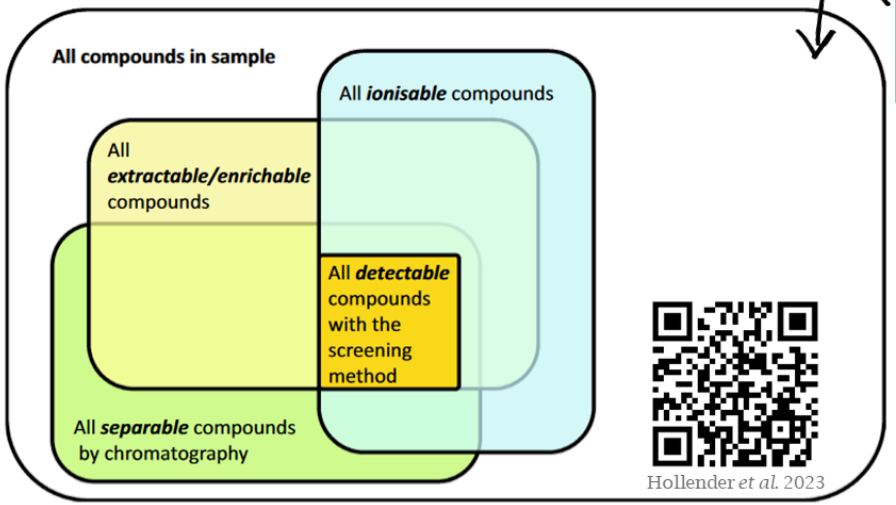
Holistic strategy of environmental monitoring

1. Analytical methodologies

2. Sources, fate, removal

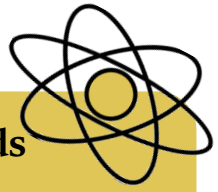
4. Risk Assessment

3. Metabolism & Transformation



Hollender *et al.* 2023

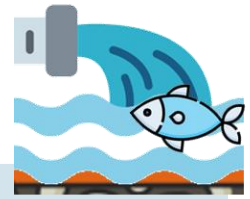
- ✓ Priority pollutants
- ✓ Emerging pollutants



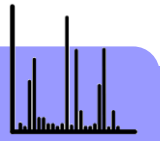
- ✓ Very polar compounds
- ✓ Polar to semi-polar compounds
- ✓ Non-polar compounds

- Target analysis
- Suspect screening
- Non-target screening

- ✓ Risk Assessment



- ✓ WW (influent, effluent, sewage sludge)
- ✓ Seawater
- ✓ Sediment /Soil
- ✓ Biota (different trophic levels)



- ✓ HRMS
- ✓ LRMS → higher sensitivity & selectivity

- ✓ (Semi-) Quantitative analysis
- ✓ Qualitative analysis
- ✓ Tentative identification

Instrumentation

LC-UV, LC-DAD
GC-FID
MS techniques

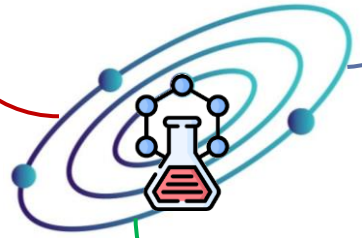
GC-APCI-QTOF

GC-EI-MS/MS

volatile
non-polar

LC-MS/MS

non-volatile
polar, semi-polar



inorganic

ICP-MS

LC-ESI-QToF MS

LC-VIP-HESI-**tims**-QToF MS

MALDI-ToF MS

State-of-the-art HRMS instrumentation

timsTOF fleX

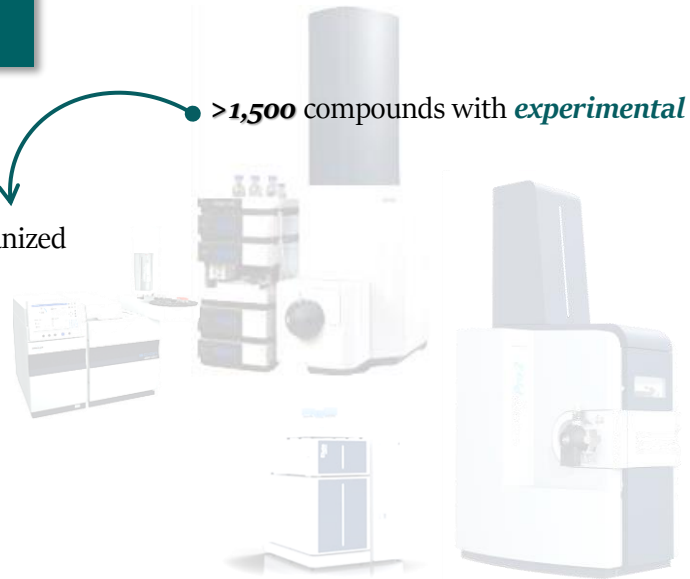
Multidimensional Chromatography–HRMS data

Wide-scope target screening

NKUA Databases

>3,200 organic micropollutants (*emerging contaminants and priority pollutants*) organized in 7 well-defined target datasets

>1,500 compounds with ***experimental CCS*** values!!!



The databases are continuously being **updated**!

- new compounds of interest
- regulated compounds
- frequently identified chemicals
- literature

Main chemical classes

LC-amenable chemicals

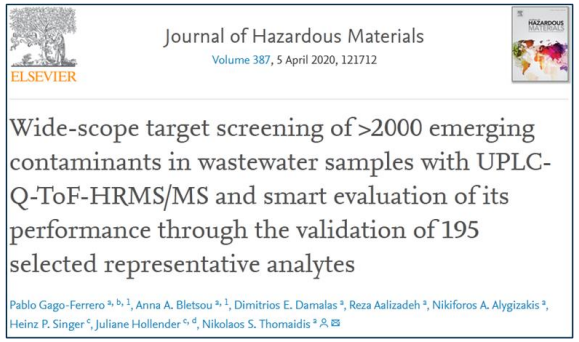
- Plant Protection Products (>900)
- Pharmaceuticals & Veterinary Drugs (>700)
  - Antibiotics (>50)
- Illicit drugs & New Psychoactive Substances (>500)
- Personal care products
- Industrial Chemicals (>150)
  - Benzothiazoles
  - Benzotriazoles
  - Flame Retardants
  - Quaternary ammonium compounds (QACs)
  - Surfactants
  - Tire additives
- Per- and Polyfluoroalkyl Substances (PFAS) (>60)
- Sweeteners
- Preservatives
- Steroids/Hormones

+

- ***Transformation Products / Metabolites (~200)***

GC-amenable chemicals

- Polycyclic Aromatic Hydrocarbons (PAHs)
- Polychlorinated Biphenyls (PCBs)
- Plant Protection Products
  - Organochlorine Pesticides (OCPs)
- Polychlorinated Naphthalenes (PCNs)
- Polybrominated Diphenyl Ethers (PBDEs)
- Explosives


Journal of Hazardous Materials
Volume 387, 5 April 2020, 121712
ELSEVIER

Wide-scope target screening of >2000 emerging contaminants in wastewater samples with UPLC-Q-ToF-HRMS/MS and smart evaluation of its performance through the validation of 195 selected representative analytes

Pablo Gago-Ferrero [a, b, 1], Anna A. Bletsou [a, 1], Dimitrios E. Damalas [a], Reza Aalizadeh [a], Nikiforos A. Alygizakis [a], Heinz P. Singer [c], Juliane Hollender [c, d], Nikolaos S. Thomaidis [a, *]

Database structure

- Analyte name & Chemical identifiers
- Retention time (**RT**)
- Full-scan MS
  - pseudomolecular ion
  - adduct ions
  - in-source fragment ions

  (most abundant: precursor ion, other MS ions: qualifier ions)
- bbCID MS/MS
  - fragment ions as **qualifier ions**

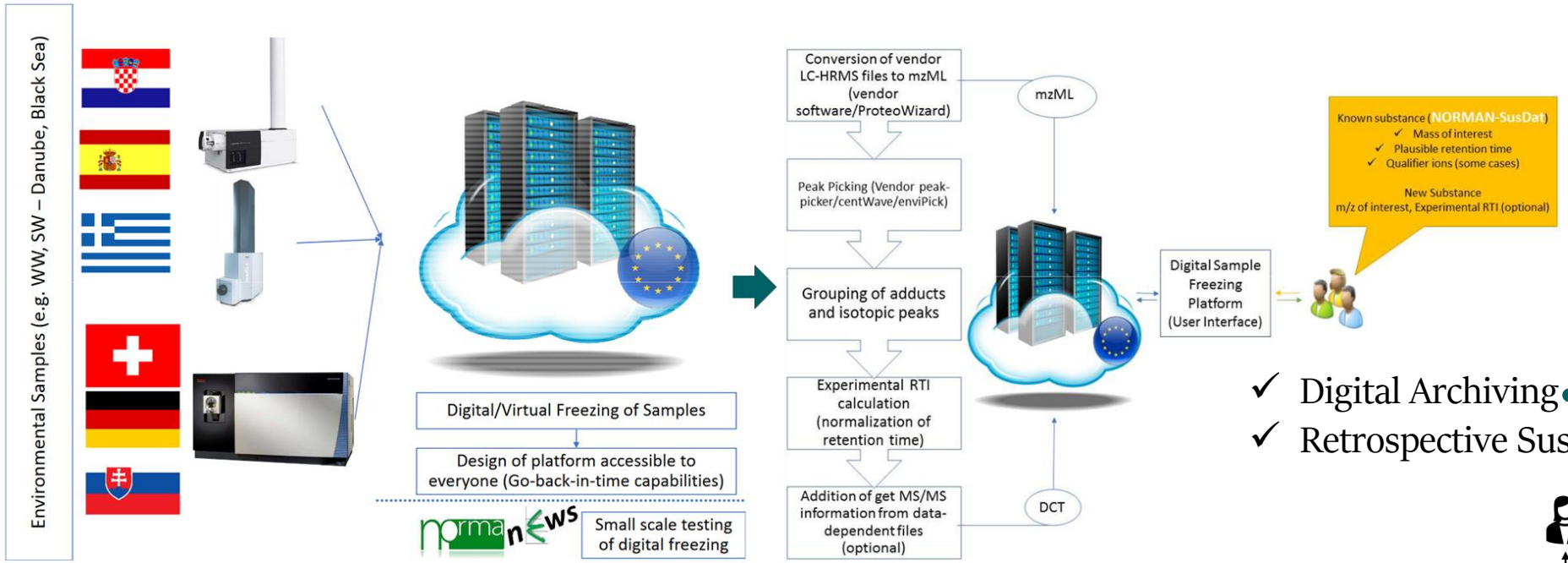
  (mandatory ions: ions with > 50% relative intensity)

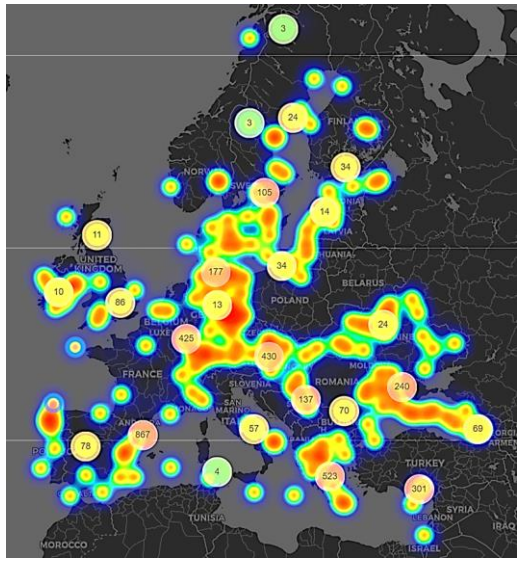
LC-TIMS-HRMS database

- **$1/K_0$** and calculated **CCS** for each ion species

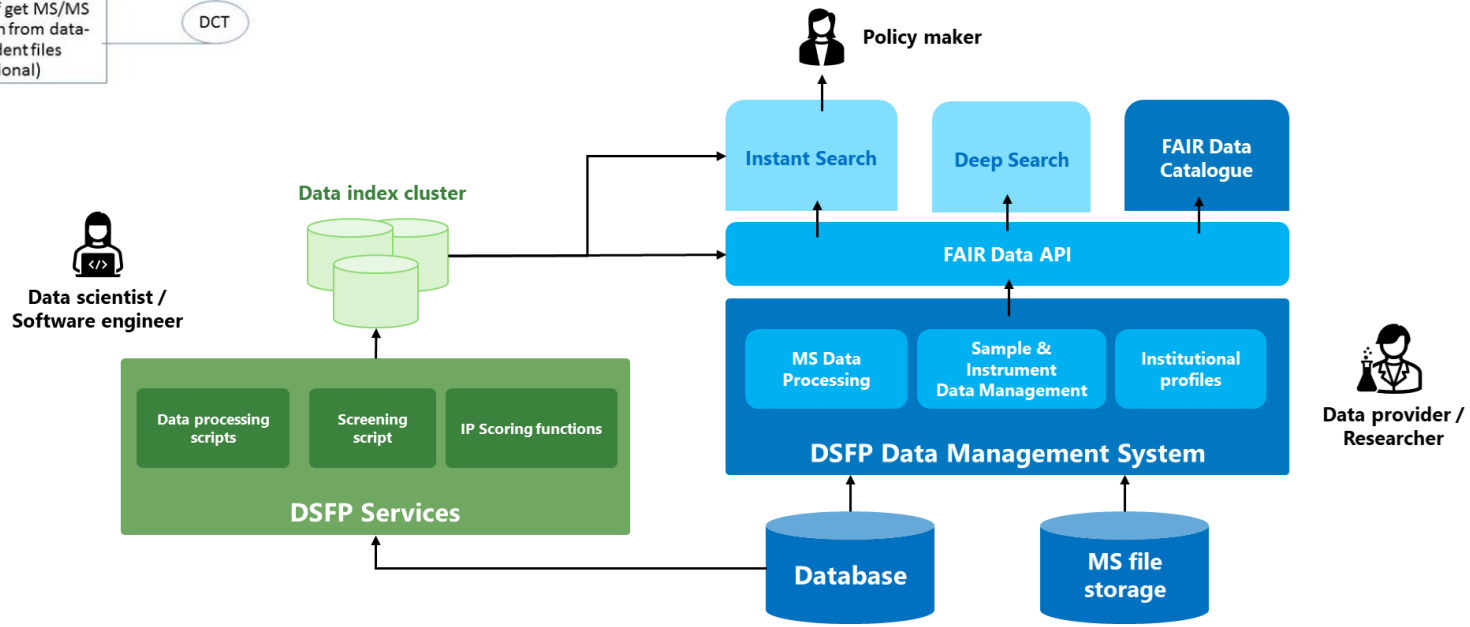
In-house developed tools supporting environmental analysis by HRMS

NORMAN Digital Sample Freezing Platform (DSFP)



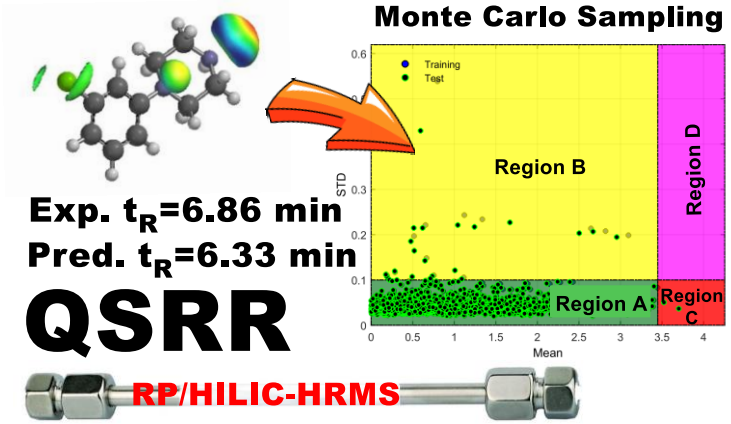


✓ Digital Archiving
✓ Retrospective Suspect Screening

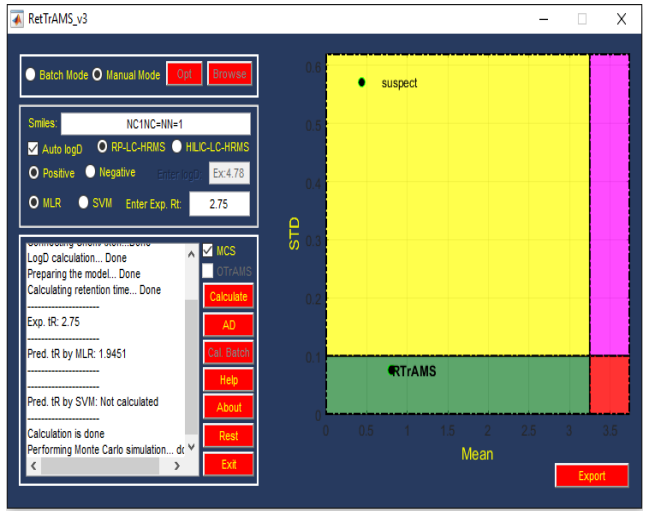


In-house developed tools supporting environmental analysis by HRMS

Retention time prediction model



RetTrAMS software v.3



Journal of Hazardous Materials 363 (2019) 277–285

Contents lists available at ScienceDirect

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journal homepage: www.elsevier.com/locate/jhazmat

Development and application of retention time prediction models in the suspect and non-target screening of emerging contaminants

Reza Aalizadeh, Maria-Christina Nika, Nikolaos S. Thomaidis*

Not secure | rti.chem.uoa.gr

Development and Prediction of Retention Time Indices for LC-HRMS (version 2.0.0)

National and Kapodistrian UNIVERSITY OF ATHENS

Retention Time Indices for LC-HRMS (version 2.0.0):

About | Calibrants | Single compound | Batch mode | Comparison of Experimental RTIs | Chemical Curation | FAQ

Select the target ESI:
- +ESI
- -ESI

Select the RTI versus tR calibration mode:
- Prediction limits
- Auto-calibrate
- Manual

Upload RTI calibrants data...

Browse... No file selected

Defalut max. file size 1MB (*.csv file)

Click here to build the calibration curve...

Click here to restart the current session...

Trace Analysis & Mass Spectrometry Group

NORMAN Suspect list Exchange website

Sign out

Download the Calibrants files (generic files for reporting):

Download calibrants info for +ESI

Download calibrants info for -ESI

Download the example files for chemical curation:

Download example file for chemical curation

Download the example files (input files for UOA-RTI):

Download example file for the suspect list

Download example file for the calibrants (-ESI)

Download example file for the calibrants (+ESI)

Download the example files of the multiple comparison procedure for

Download example file for the calibrants

Download example file for the suspect list

Download example file for the name of institutes

+ESI (calibrants):

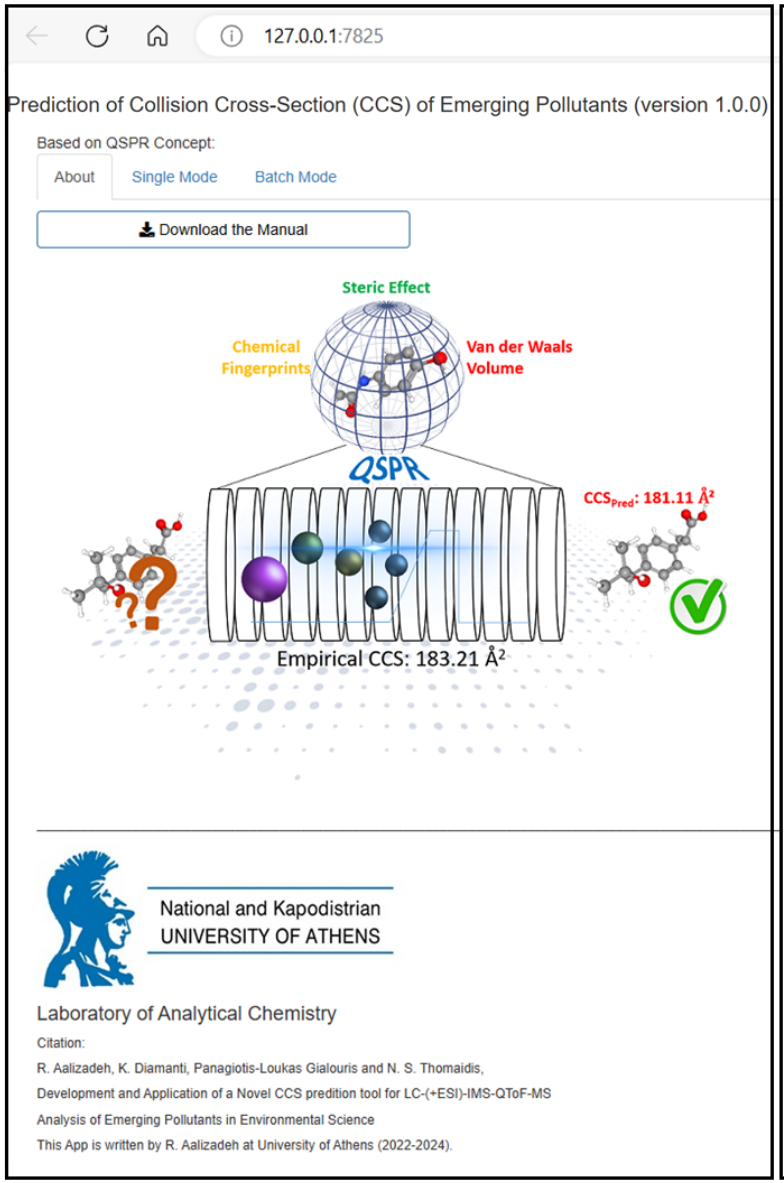
	A	B
1	Calibrants	tR
2	Guanylurea	1.33
3	Amitrole	1.21
4	Histamine	1.2
5	Chlormequate	1.1
6	Methamidophos	2.64
7	Vancomycin	5.36
8	Cefoperazone	6.12
9	Trichlorfon	7.02
10	Butocarboxim	8.46
11	Dichlorvos	
12	Tylosin	8.79
13	TCMTB	12.34
14	Rifaximin	11.94
15	Spinosad_A	11.11
16	Emamectin	12.01
17	Avermectin	16.71
18	Nigericin	16.01
19	Ivermectin	17.01

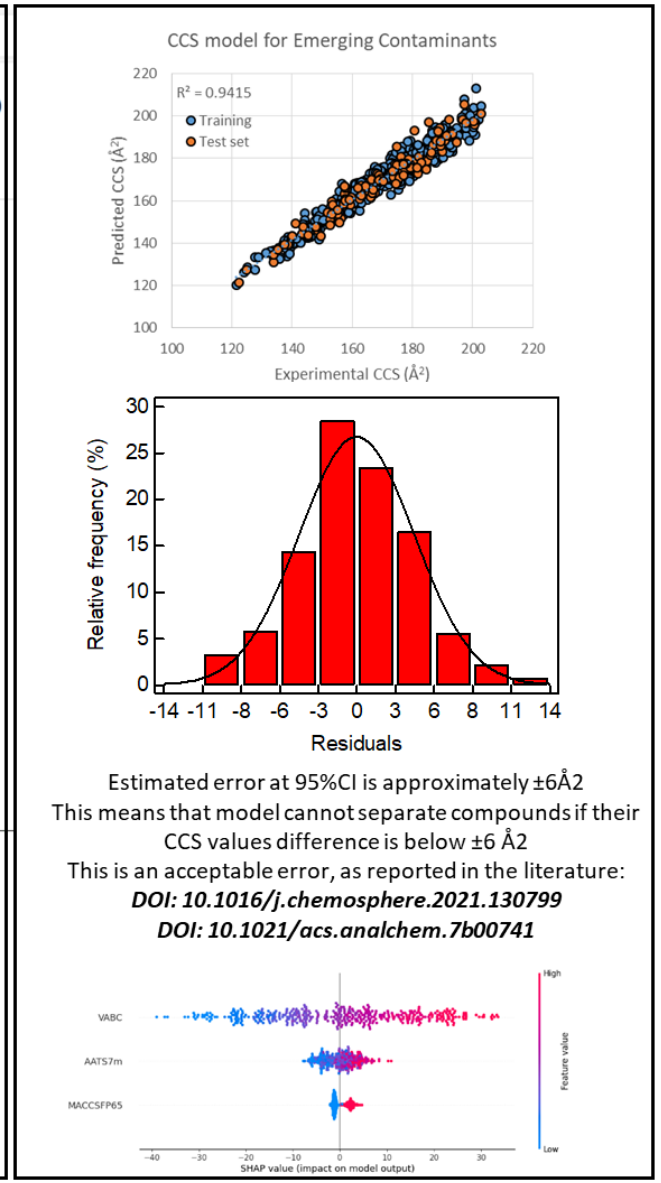
-ESI (calibrants):

	A	B
1	Calibrants	tR
2	Amitrole	
3	Benzoic_acid	
4	Acephate	4.3
5	Salicylic_acid	
6	Simazine_2_Hydroxy	6.23
7	Tepraloxydim	7.9
8	Bromoxynil	7.65
9	MCPA	7.39
10	Valproic_acid	10.16
11	Phenytoin	9.47
12	Flamprop	8.91
13	Benodanil	11.43
14	Dinoterb	11
15	Inabenfide	11.08
16	Coumaphos	14.04
17	Triclosan	14.15
18	Abamectin	16.5
19	Salinomycin	17.45

In-house developed tools supporting environmental analysis by HRMS

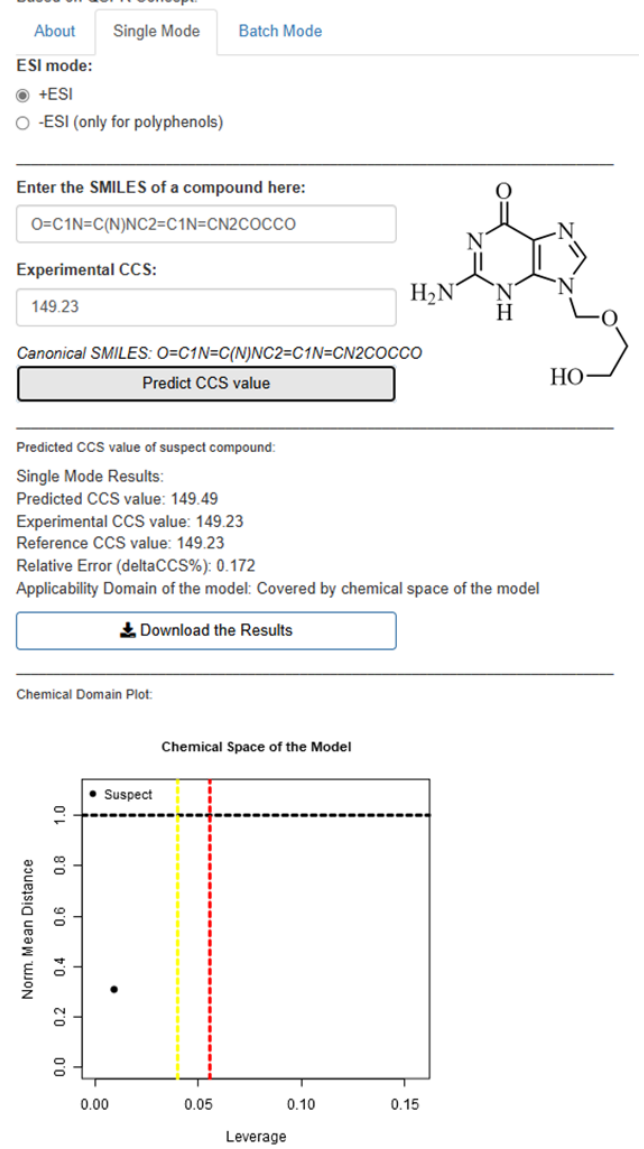
CCS prediction model





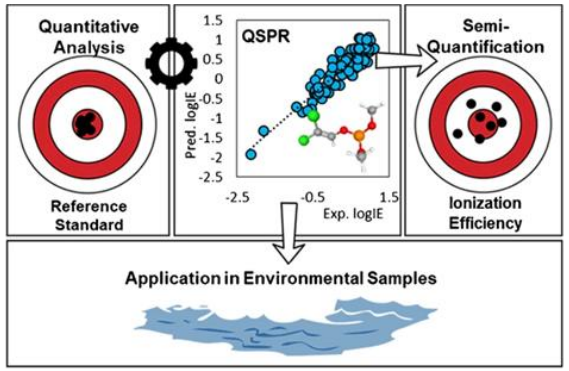
Using CCSpro app for prediction of CCS for Aciclovir

Example for Aciclovir:



In-house developed tools supporting environmental analysis by HRMS

Semi quantification workflows (LC-ESI-HRMS)

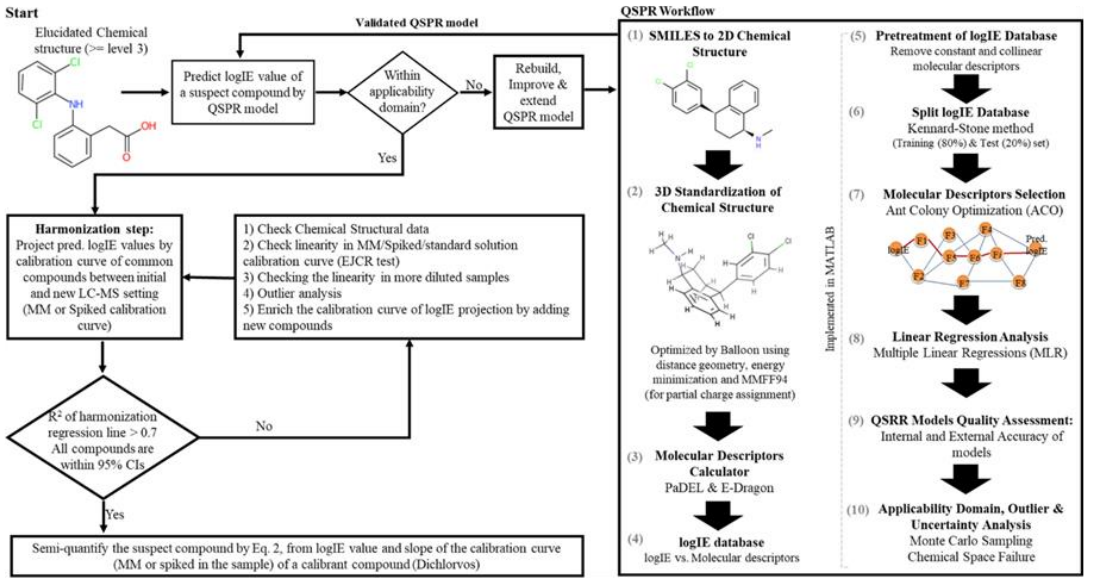


1 Creation of logIE database for LC-+ESI-HRMS (for various emerging contaminants)

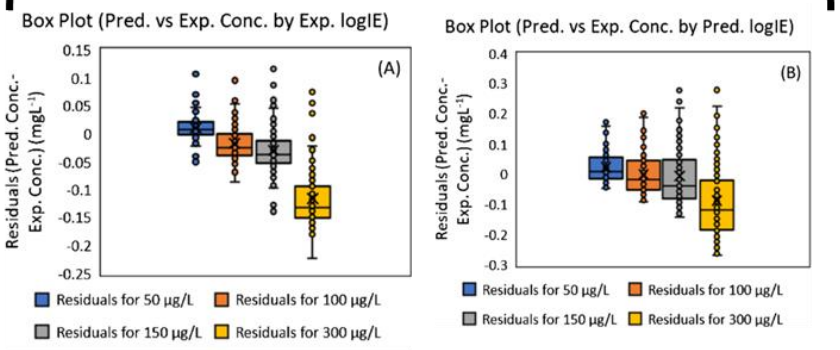
Table 1 List of 103 emerging contaminants with experimental and predicted logIE values

ID	Subset	Compound name	CAS	Exp. logIE
M002 [a]	Training	Niflumic acid	4394–00-7	0.496
M004	Training	Colchicine	64–86-8	0.412
M005	Training	Levamisol	14,769–73-4	0.964
M006 [a]	Training	Trimethoprim	738–70-5	0.641
M007	Training	Methimazole	60–56-0	0.479
M008	Training	Brompheniramine	86–22-6	0.702
M010	Training	Oxyphenylbutazone	129–20-4	−0.334
M011	Training	Sulfanilamide	63–74-1	−0.571
M013	Training	Norfloxacin	70,458–96-7	0.564
M014	Training	Sarafloxacin	98,105–99-8	0.105
M015	Training	Tilmicosin	108,050–54-0	−0.793
M016	Training	Prednisolone	50–24-8	−0.232
M017 [a]	Training	Mabuterol	56,341–08-3	0.506
M020 [a]	Training	Valsartan	137,862–53-4	−0.540
M021 [a]	Training	Theophylline	58–55-9	−0.474
M022 [a]	Training	Ranitidine	66,357–35-5	0.794
M024 [a]	Training	Carbamazepine	298–46-4	0.855
M025	Training	Piperazine	110–85-0	0.286
M027 [a]	Training	Paracetamol	103–90-2	0.420
M028	Training	Simvastatin	79,902–63-9	−0.280
M029	Training	Morantel	20,574–50-9	0.754
M030	Training	Diaveridine	5355–16-8	0.803
M031	Training	Sulfathiazole	72–14-0	0.009
M032 [a]	Training	Sulfadiazine	68–35-9	0.095
M033	Training	Sulfamethoxypyridazine	80–35-3	0.317
M034	Training	Sulfamerazine	127–79-7	0.204
M035 [a]	Training	Sulfamethoxazole	723–46-6	0.081
M037	Training	Ciprofloxacin	85,721–33-1	0.288
M038	Training	Ofloxacin	82,419–36-1	0.531
M039	Training	Difloxacin	98,106–17-3	0.270
M041	Training	Flumequine	42,835–25-6	0.617
M042	Training	Marbofloxacin	115,550–35-1	0.417
M043	Training	Lincomycin	154–21-2	−0.099
M044	Training	Chlorpromazine	50–53-3	0.800
M045	Training	1-OH-Benzotriazole	2592–95-2	−0.051
M046	Training	5-methyl-Benzotriazole	136–85-6	0.650

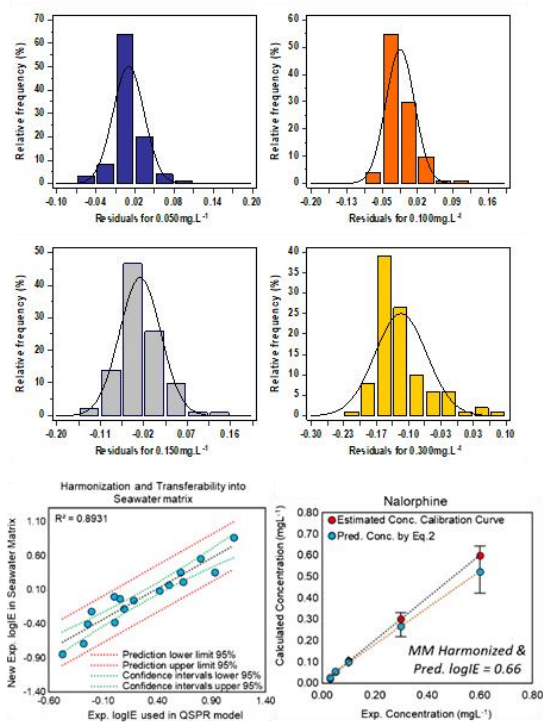
2 *Workflow for application of QSPR and validation of logIE concept in LC-ESI-HRMS*



3 *Prediction error*



4 *Transferability to searwater sample/matrix*



Analytical and Bioanalytical Chemistry (2022) 414:7435–7450
https://doi.org/10.1007/s00216-022-04084-6

RESEARCH PAPER

A novel workflow for semi-quantification of emerging contaminants in environmental samples analyzed by LC-HRMS

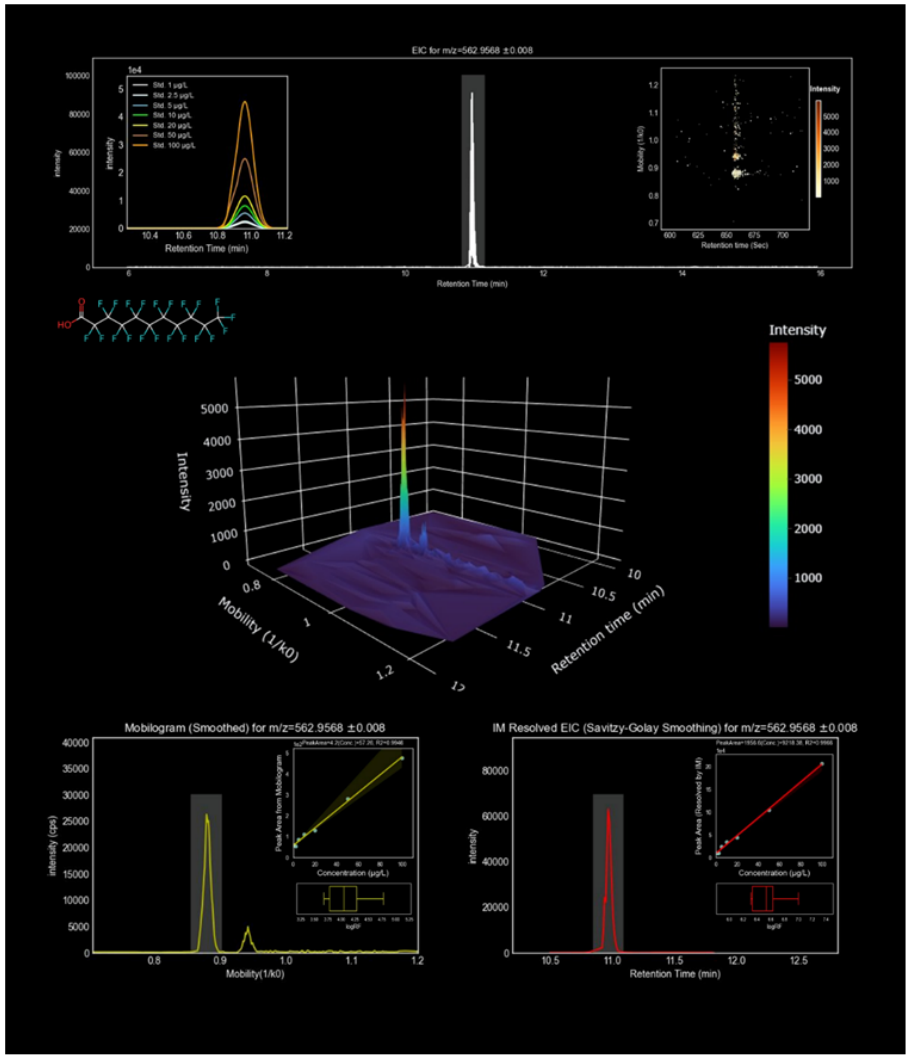
Reza Aalizadeh[1] · Varvara Nikolopoulou[1] · Nikiforos Alygizakis[1,2] · Jaroslav Slobodnik[2] · Nikolaos S. Thomaidis[1]

Received: 19 February 2022 / Revised: 31 March 2022 / Accepted: 11 April 2022 / Published online: 26 April 2022

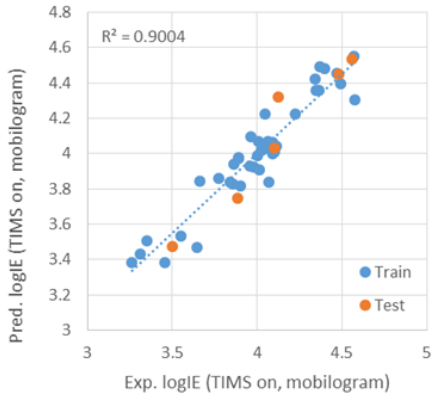
In-house developed tools supporting environmental analysis by HRMS

Semi quantification workflows (LC-ESI-IMS-HRMS)

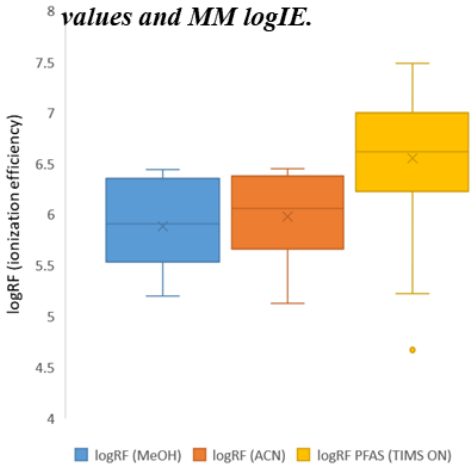
1 Creation of logIE database for LC- +/-ESI-IMS-HRMS (for various emerging contaminants)



2 *Using QSPR for developing logIE concept in LC-ESI-IMS-HRMS directly from Mobilogram*

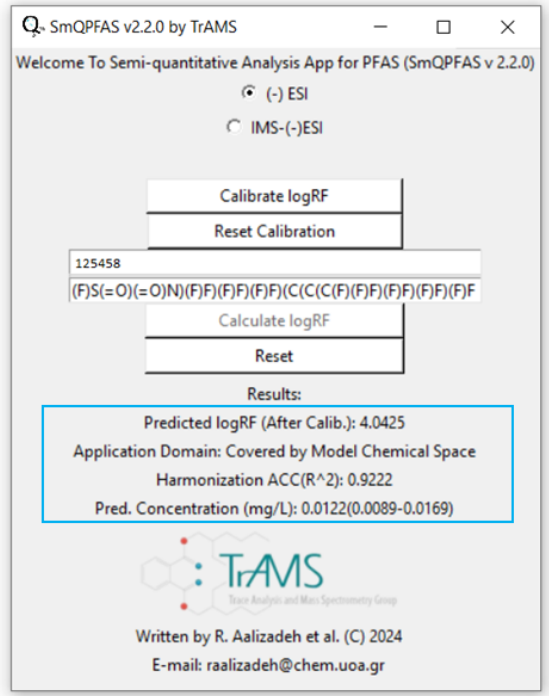


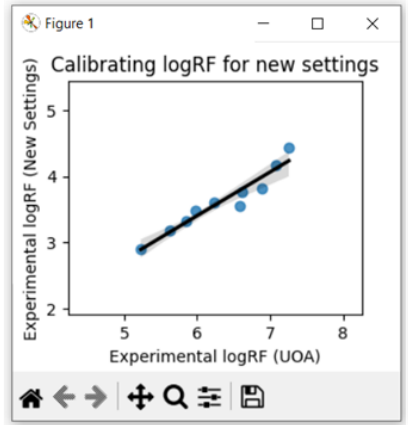
3 *Matrix Matched Ionization Efficiency is significantly improved by resolving the peaks using ion mobility dimension. It purifies relevant peaks from the background and promotes the great transferability between reference logIE values and MM logIE.*

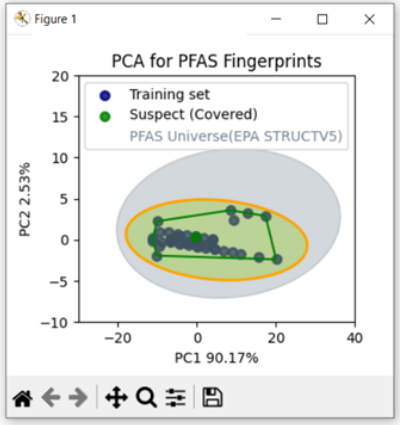


4 *Executable software to perform ESI-IMS-HRMS semiQ*

SmQPFAS.exe

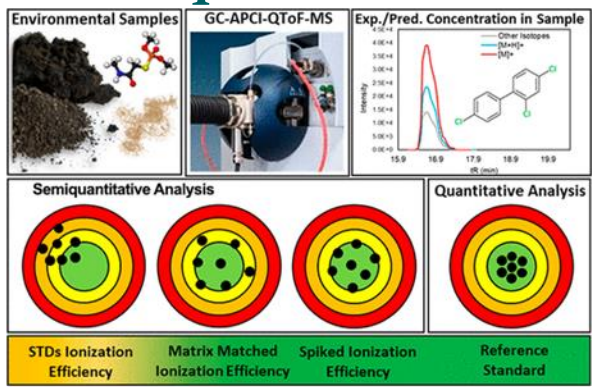


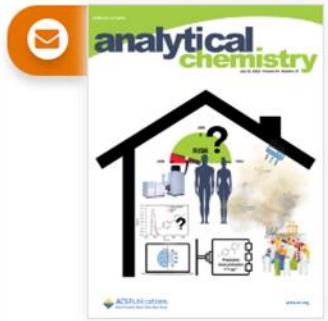




In-house developed tools supporting environmental analysis by HRMS

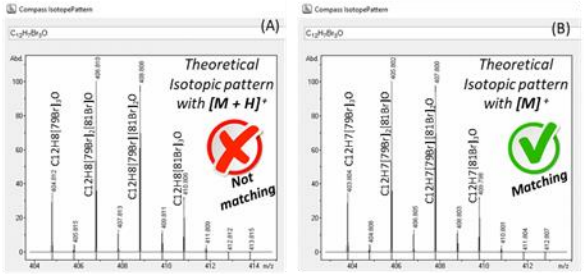
Semi quantification workflows (GC-APCI-HRMS)

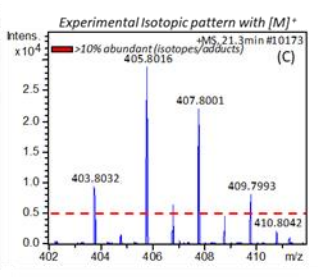


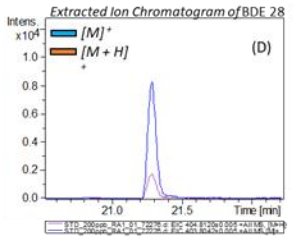


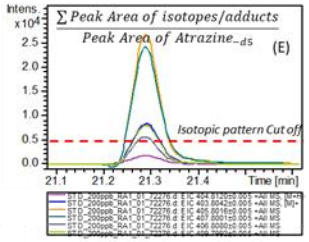
Analytical Chemistry

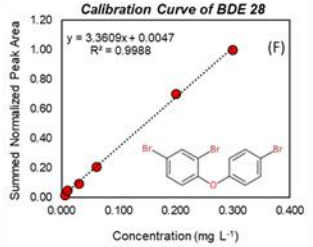
1 Creation of logIE database for GC-APCI-HRMS (for various emerging contaminants)

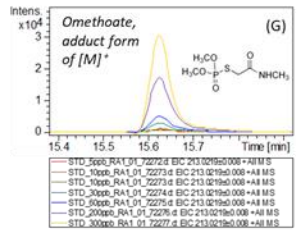


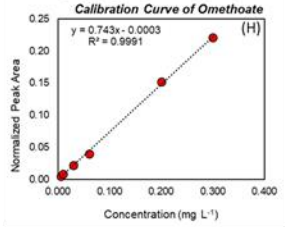












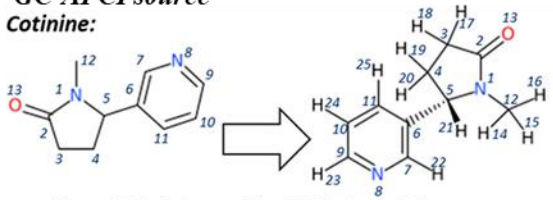
$$Exp.APCI\ logIE = log_{10}\left(\frac{slope_{BDE-28}}{slope_{Omethoate}} \times \frac{MW_{Omethoate}}{MW_{BDE-28}}\right)$$

$$= log_{10}\left(\frac{3.3609}{0.743} \times \frac{213.192}{406.895}\right)$$

$$= 0.3747$$

2 Simple ionization mechanism of compounds in GC-APCI source

Cotinine:



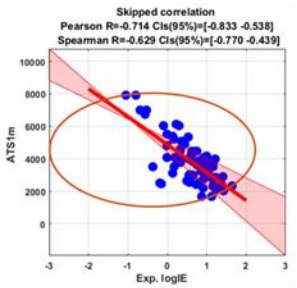
Connectivity in terms of "explicit hydrogen" atoms

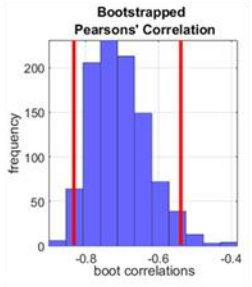
ATS1ω= (ω1 x ω2) + (ω2 x ω3) + (ω3 x ω4) + (ω4 x ω5) + (ω5x ω6) + (ω6 x ω7) + (ω7 x ω8) + (ω8 x ω9) + (ω9 x ω10) + (ω10 x ω11) + (ω11 x ω6) + (ω5 x ω1) + (ω1 x ω12) + (ω2 x ω13) + (ω12 x ω14) + (ω12 x ω15) + (ω12 x ω16) + (ω3 x ω17) + (ω3 x ω18) + (ω4 x ω19) + (ω4 x ω20) + (ω5 x ω21) + (ω7 x ω22) + (ω9 x ω23) + (ω10 x ω24) + (ω11 x ω25)

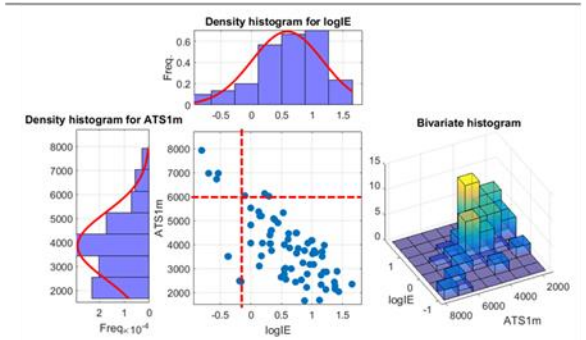
***ω is atomic masses in ATS1m**

ATS1m= (14.007 x 12.011) + (12.011 x 12.011) + (12.011 x 12.011) + (12.011 x 12.011) + (12.011 x 12.011) + (12.011 x 12.011) + (12.011 x 12.011) + (12.011 x 14.007) + (14.007 x 12.011) + (12.011 x 12.011) + (12.011 x 12.011) + (12.011 x 12.011) + (12.011 x 14.007) + (14.007 x 12.011) + (12.011 x 15.9994) + (12.011 x 1.008) + (12.011 x 1.008) + (12.011 x 1.008) + (12.011 x 1.008) + (12.011 x 1.008) + (12.011 x 1.008) + (12.011 x 1.008) + (12.011 x 1.008) + (12.011 x 1.008) + (12.011 x 1.008) + (12.011 x 1.008) + (12.011 x 1.008)

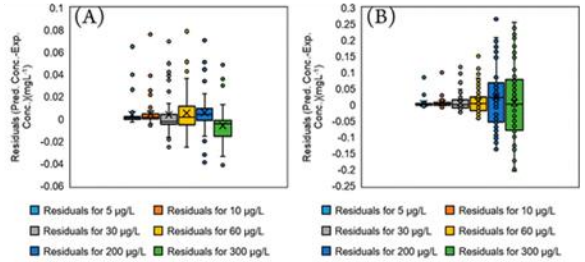
ATS1m=2332.75

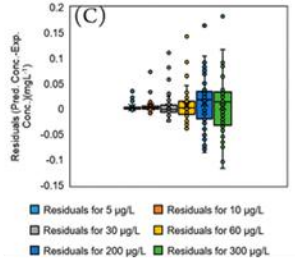




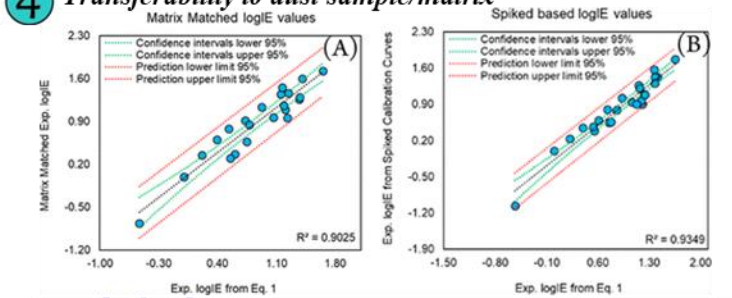


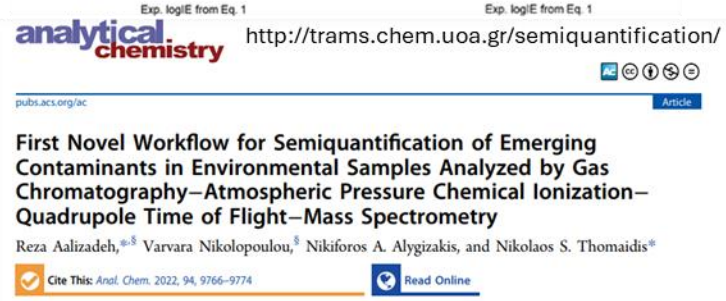
3 Prediction error





4 Transferability to dust sample/matrix





In-house developed tools supporting environmental analysis by HRMS

Non-target screening approaches

Pretreatment step

- **Data Independent Acquisition mode** (DIA) (Raw data), **MS calibration** + conversion to **mzML**
- **XCMS+ IPO package + Peaks annotation by CAMERA and Non-target R package**
- **Subtraction of analytical procedural blank from samples**
- **Prioritization of the peak list by Chemometrics**

Level 5

- **m/z of interest $[M+H]^+$ & $[M-H]^-$**
- **Search databases for match ("Known Unknown")**

Level 4

- **Mass accuracy threshold (Molecular Formula)** (< 2 mDa)
  Isotopic pattern of the precursor ion (> 50)
  Characteristic adduct ions ($[M + NH_4]^+$, $[M + Na]^+$, etc.)

Level 3

- **MS/MS spectral interpretation & prediction**
  In silico fragmentation platforms (MetFrag)
  QSRR models for tR prediction

Level 2

- 2b) **Diagnostic evidence (diagnostic ion, etc)**
  GC/LC retention time indices (RI)
- 2a) **MS/MS spectral match**
  Literature or library spectrum (MassBank)

Level 1

- Confirmation by **authentic reference standard**

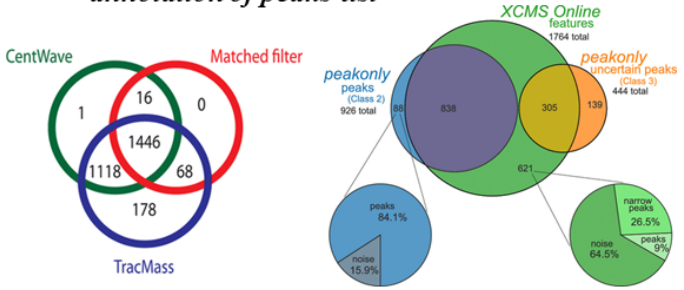
- **Semi-quantification and Risk Assessment**

---

1 ***Lessons learned from Norman News***

Checklist:
Quality control for mass accuracy of spiked IS considering:
Type of mass analyzer, method of ms-calibration, age of equipment, scan sampling rate of the detector

2 ***Use of complementary tools for peak picking and annotation of peaks-list***



DOI: 10.1021/ac403905h DOI:10.1021/acs.analchem.9b04811

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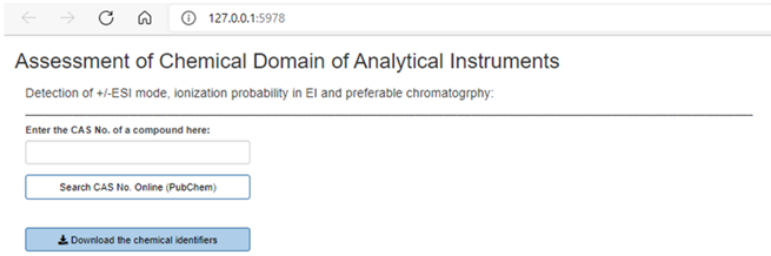
1 ***Application domain evaluation***



2 **Ionization/tR prediction**

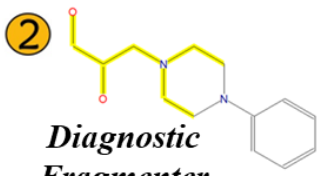
---

1 ***LRI: Harmonization of tR data***

NIST National Institute of Standards and Technology U.S. Department of Commerce

Direct n-alkane Exp. LRI comparison (<50 RI unit)

2 ***Diagnostic Fragmenter***



---

1 ***Norman Initiative for evaluation and validation of semi-quantitation approach***

2 ***UOA approach: EJCR test, injection volume test etc.***

In-house developed tools supporting environmental analysis by HRMS

Non-target screening approaches

Pretreatment step

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- **Mass accuracy threshold (Molecular Formula)** (< 2 mDa)
- **Isotopic pattern of the precursor ion** (> 50)
- **Characteristic adduct ions** ($[M + NH_4]^+$, $[M + Na]^+$, etc.)

Level 3

- **MS/MS spectral interpretation & prediction**
- ESI-HRMS spectra prediction via CFM-ID
- QSRR models for tR prediction
- **QSRR models for CCS prediction**

Level 2

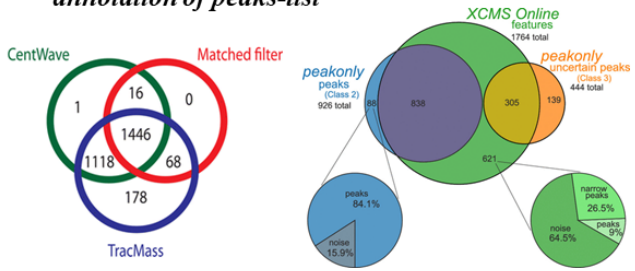
- 2b) **Diagnostic evidence (diagnostic ion, etc)**
- **Experimental LC retention time indices (RTI)**
- **Experimental Collisional Cross Section (CCS)**
- 2a) **MS/MS spectral match**
- Literature or library spectrum (MassBank)

Level 1

- Confirmation by **authentic reference standard**

- **Semi-quantification and Risk Assessment (oral and aquatic acute toxicity)**

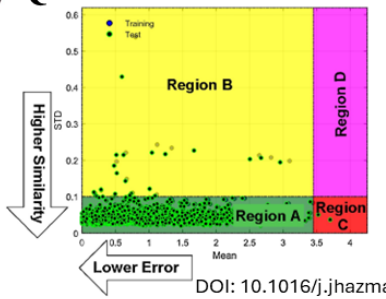
1. *Use of complementary tools for peak picking and annotation of peaks-list*



2. *Norman SusDat activity: Chemical Curation*

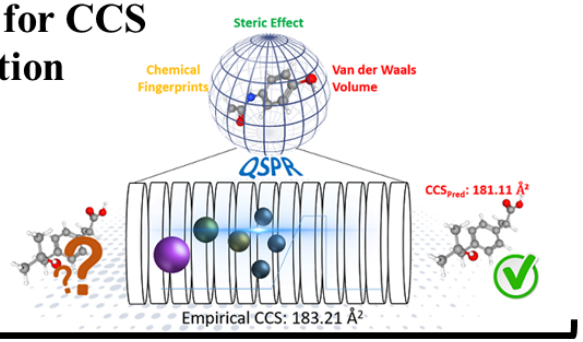
DOI: 10.1021/ac403905h DOI:10.1021/acs.analchem.9b04811

1. **QSRR validation**

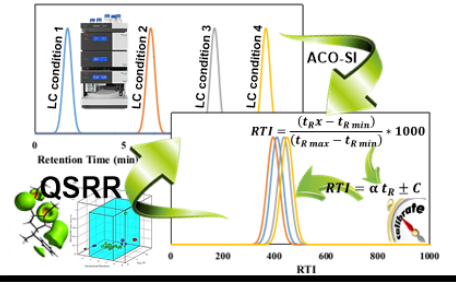


DOI: 10.1016/j.jhazmat.2018.09.047

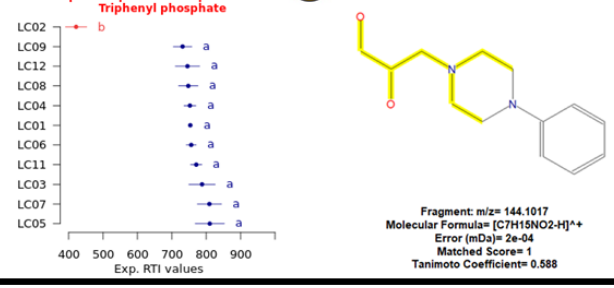
2. **QSPR for CCS prediction**



1. *RTI: Harmonization of LC settings*



2. *Diagnostic Fragmenter*



1. *Norman Initiative for evaluation and validation of semi-quantitation approach*
2. *UOA approach: EJCR test, injection volume test etc.*

In-house developed tools supporting environmental analysis by HRMS

Prioritization tools

Contents lists available at ScienceDirect

Journal of Hazardous Materials

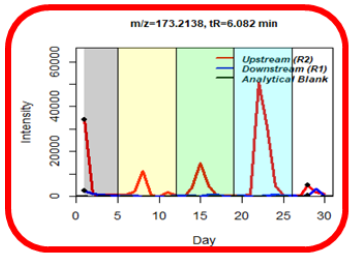
journal homepage: www.elsevier.com/locate/jhazmat

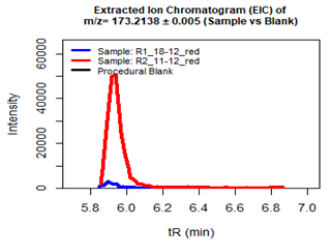
Research Paper

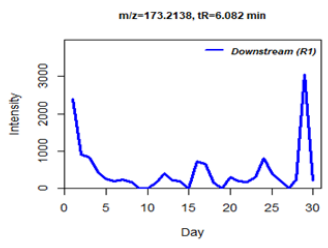
TrendProbe: Time profile analysis of emerging contaminants by LC-HRMS non-target screening and deep learning convolutional neural network

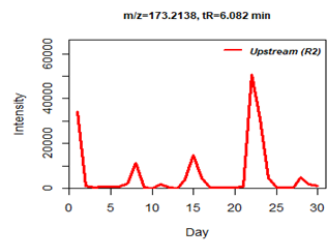
Varvara Nikolopoulou, Reza Aalizadeh*, Maria-Christina Nika, Nikolaos S. Thomaidis*

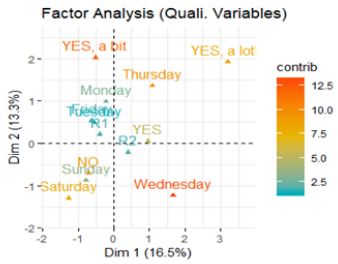
Laboratory of Analytical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, 15771 Athens, Greece

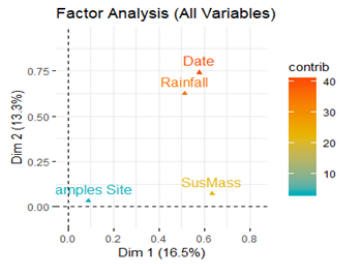


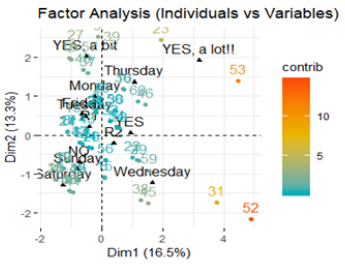


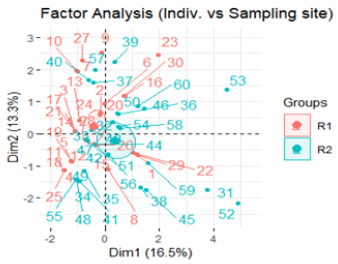


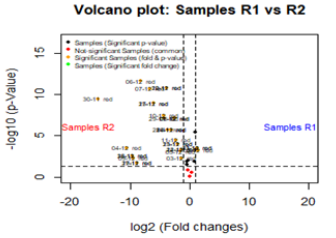


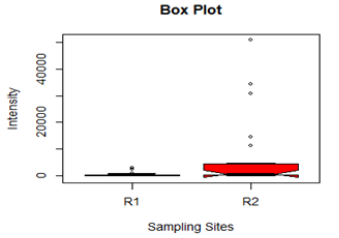


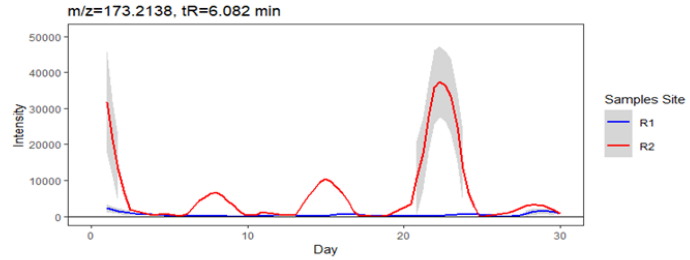












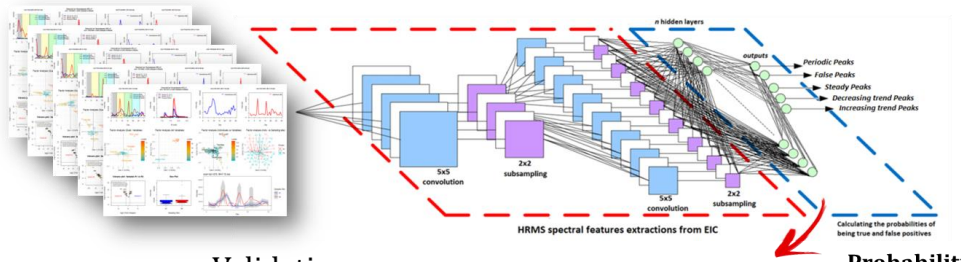
Trimethyloctylammonium, industrial chemical, manufacture of plastics products

Periodic trend → **periodic industrial discharges ?**

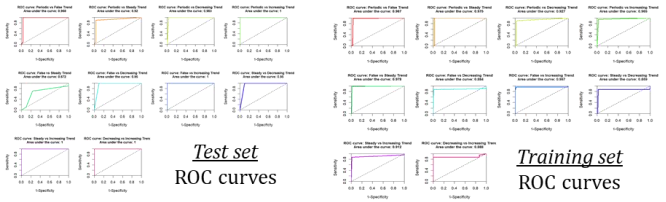
Training set
1000 features

Test set
50 features

For every [m/z, tR] of HRMS Peaklist



Validation



Test set
ROC curves

Training set
ROC curves

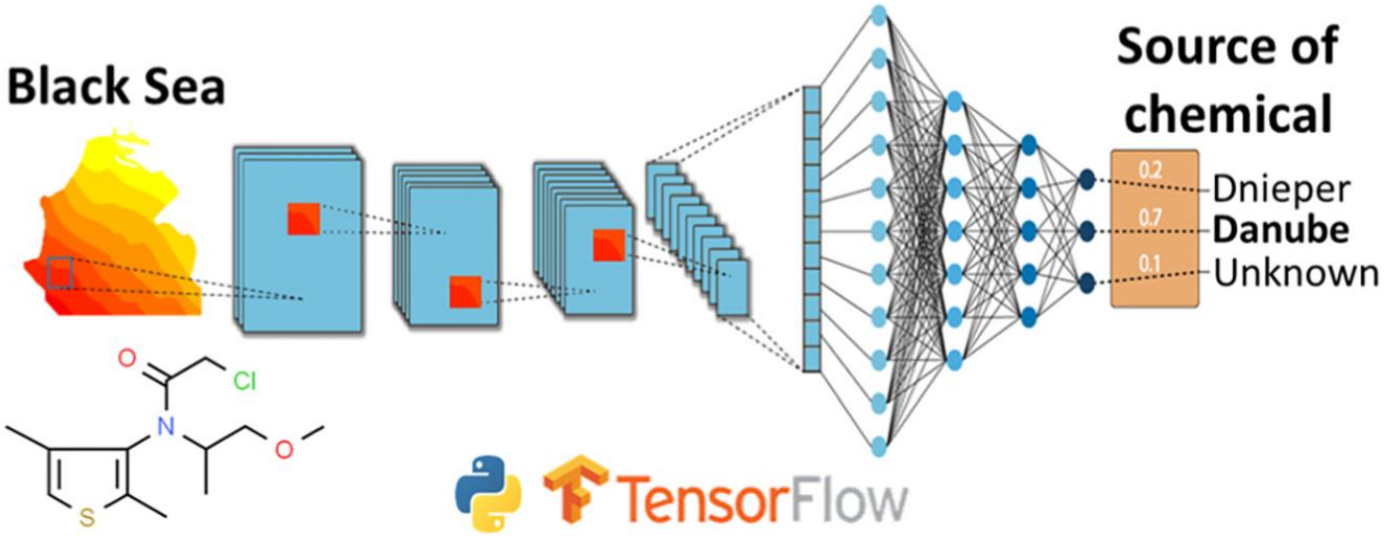
Probabilities

P(False Trend)= 0.000
P(Steady Trend)= 0.000
P(Periodic Trend)= 0.630
P(Decreasing)= 0.335
P(Increasing)= 0.035

*TrendProbe (alpha version)

In-house developed tools supporting environmental analysis by HRMS

Prioritization tools



Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

Detecting the sources of chemicals in the Black Sea using non-target screening and deep learning convolutional neural networks

Nikiforos Alygizakis [a,b,*], Theodoros Giannakopoulos [c], Nikolaos S. Thomaidis [a,*], Jaroslav Slobodnik [b]

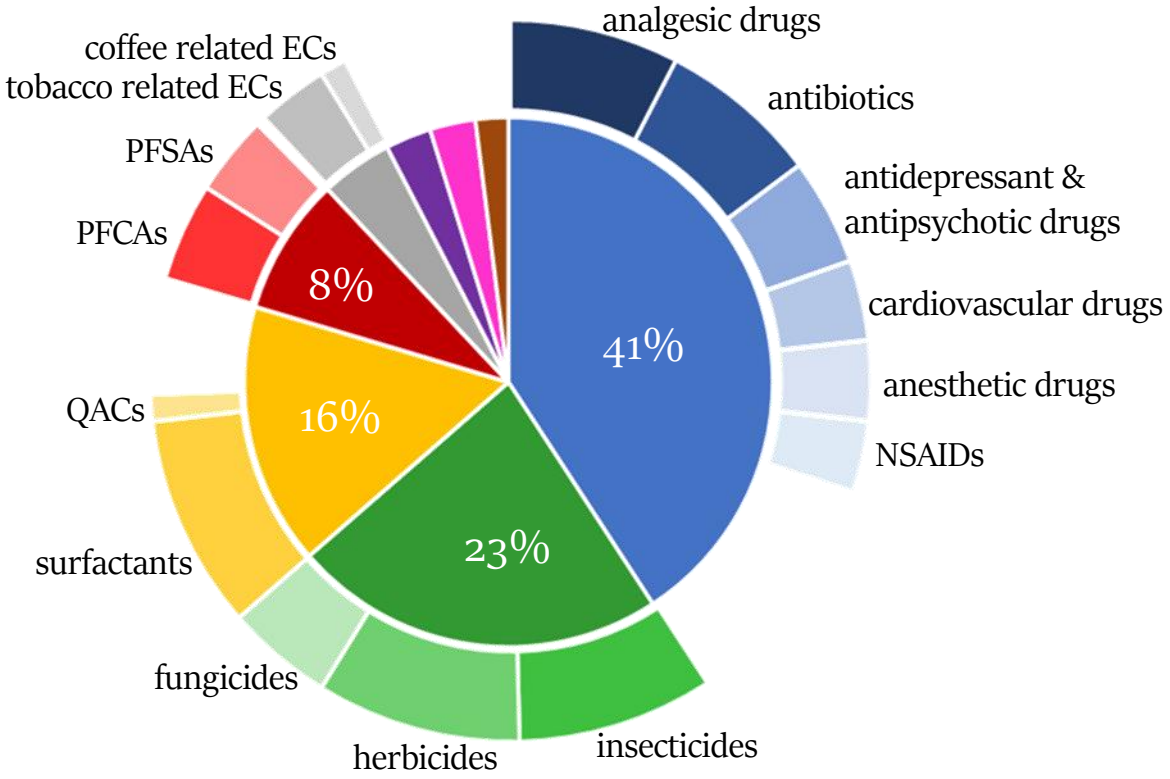
HIGHLIGHTS

- Deep learning model that detects the **sources** of chemicals in the **Black Sea**.
- Interactive dash application that filters and **visualize** the chemicals.
- **Spatial distribution** was used as a non target screening **prioritization** approach.
- Large rivers proved to be among important sources of chemicals in the Black Sea.
- 48.2 ± 1.5 % and 31.1 ± 3.0 % of signals originated from Danube and Dnieper respectively

LIFE APEX

250 chemicals were determined through wide-scope target analysis in LIFE APEX samples

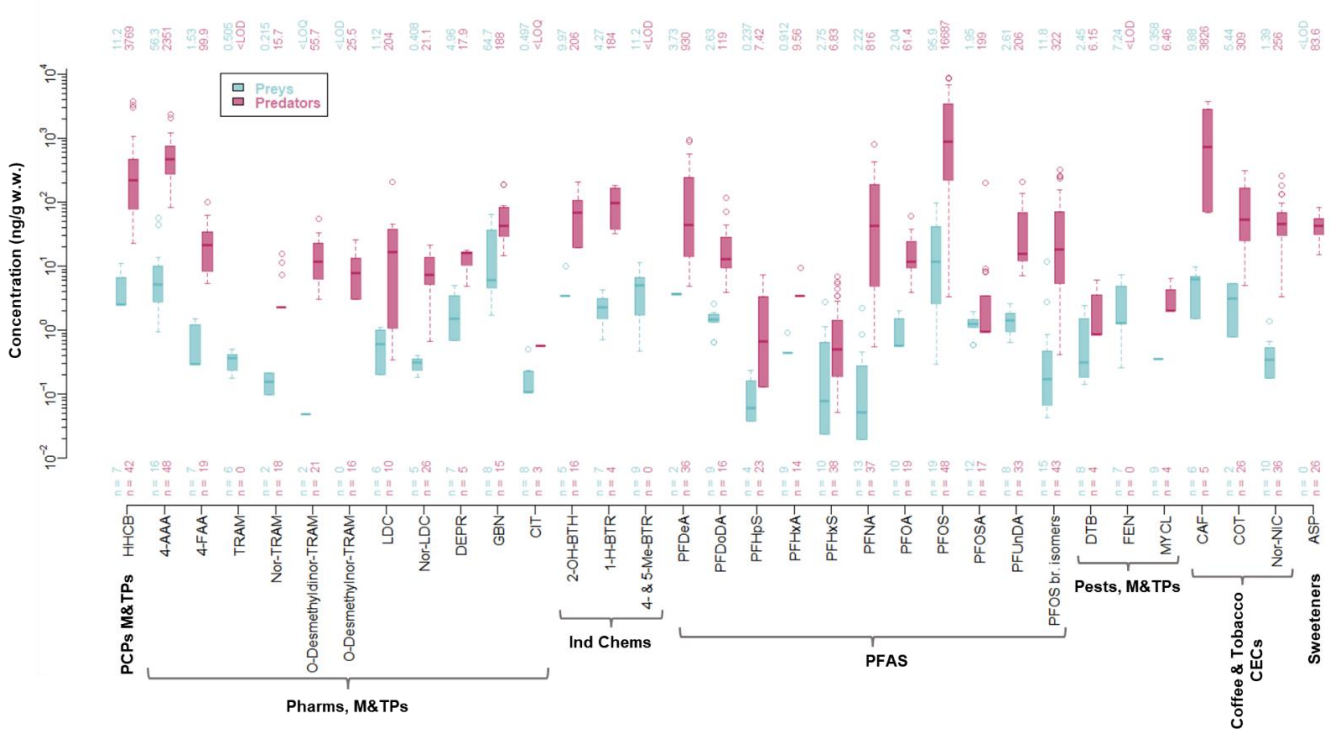
→ *97* in more than 2 tiers of LIFE APEX project



LIFE APEX

Highlights

- **67 apex predator & prey** samples from 4 European countries
- **145 contaminants of emerging concern** from various chemical classes were detected
- 30% of the prioritized compounds were **PFAS**, indicating their widespread presence in the environment & bioaccumulative properties
- Parent compounds & TPs (tramadol, lidocaine and their M&TPs) in the list of the prioritized compounds
- **Elevated concentration levels in apex predators** (liver) Vs prey (muscle tissue) samples
- Data suitable to prioritize chemicals for PBT assessment and evaluation of mitigation measures.



Contents lists available at ScienceDirect

Environment International

journal homepage: www.elsevier.com/locate/envint

Full length article

Assessment of contaminants of emerging concern in European apex predators and their prey by LC-QToF MS wide-scope target analysis

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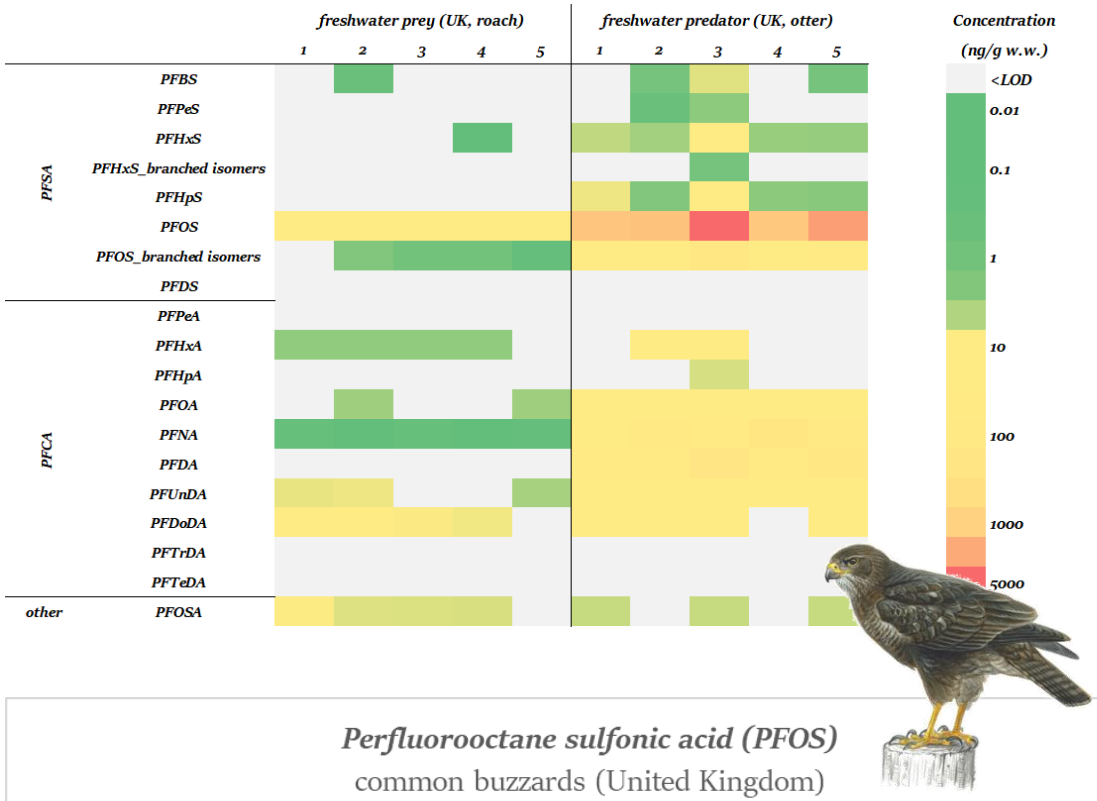
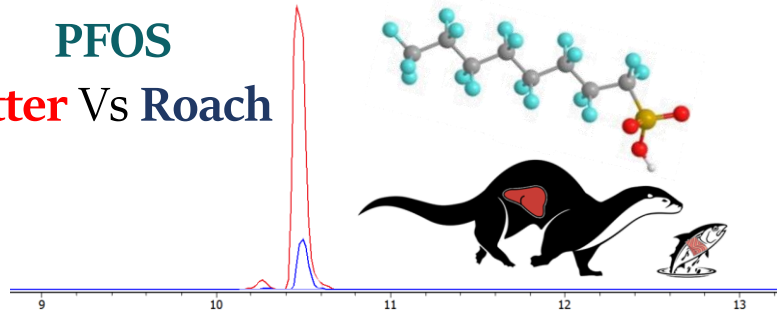
LIFE APEX

higher concentration levels in **freshwater predators** Vs the respective prey



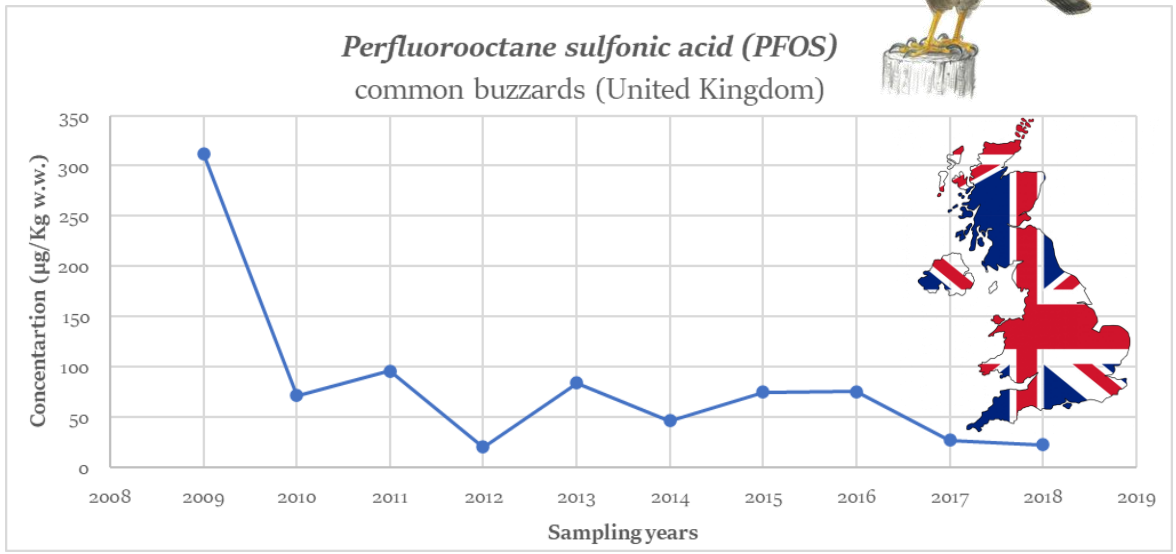
PFOS
Otter Vs Roach

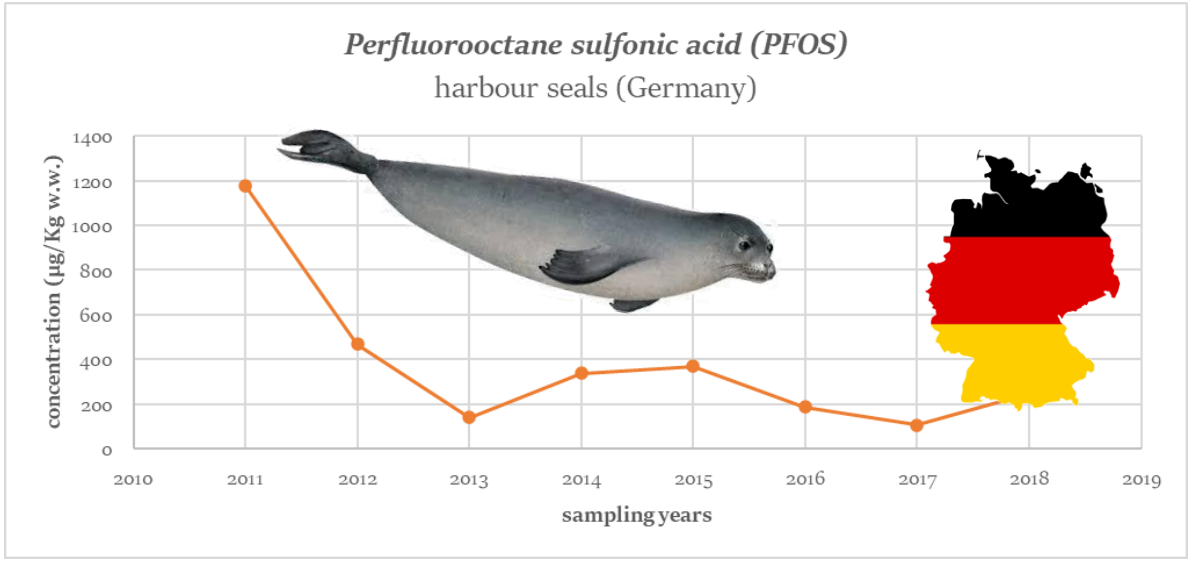


time-trend analysis

2010-2018 → **trend** to lower concentrations of PFOS

Attributed to PFOS replacement compounds?

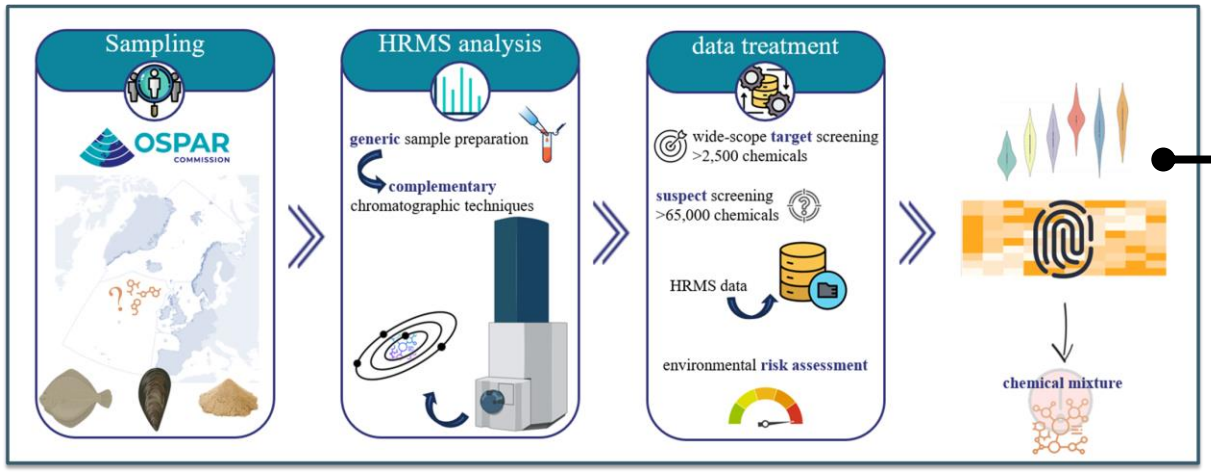


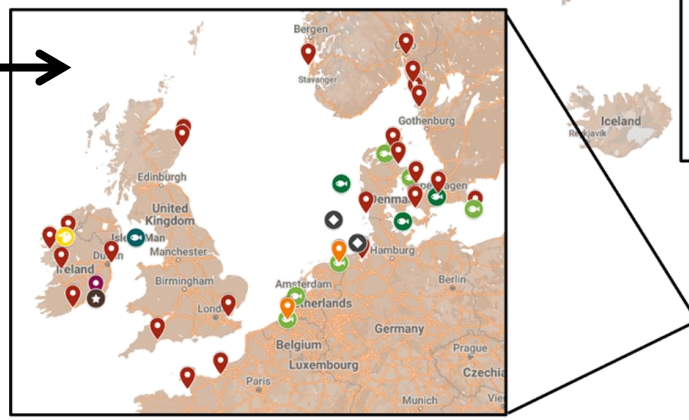


CONnECT

OSPAR COMMISSION

NORMAN





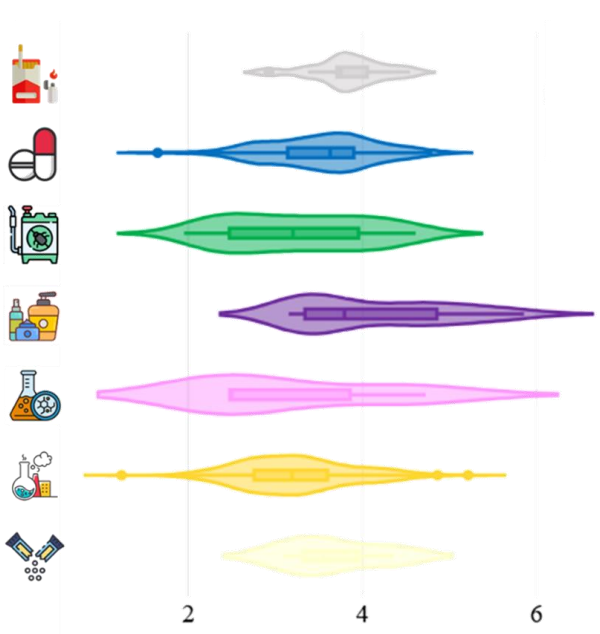
molluscs (*Mytilus edulis*, *Crassostrea gigas*, *Mytilus galloprovincialis*, *Ostrea edulis*)

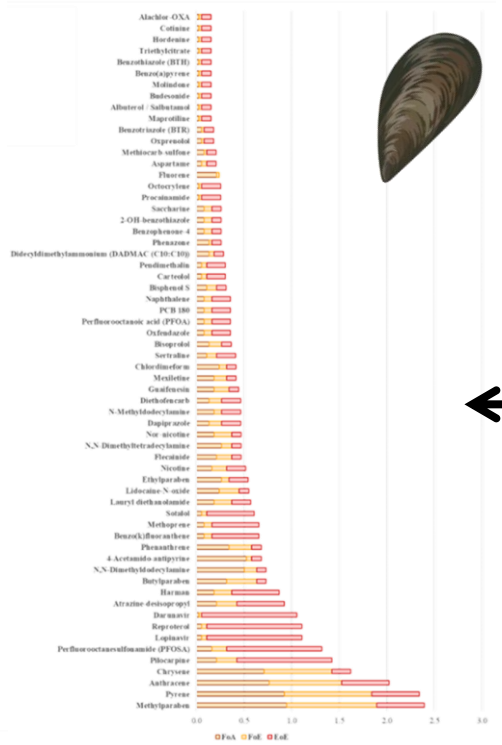
fish (*Pleuronectes platessa*, *Platichthys flesus*, *Gadus Morhua*)

arthropods (*Nephrops norvegicus*)

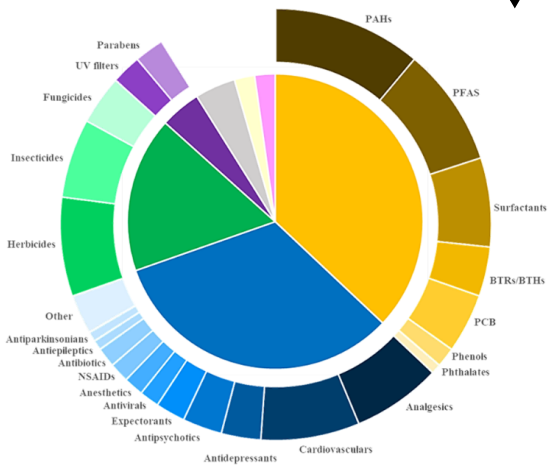
eggs (*Uria aalge*)

sediments

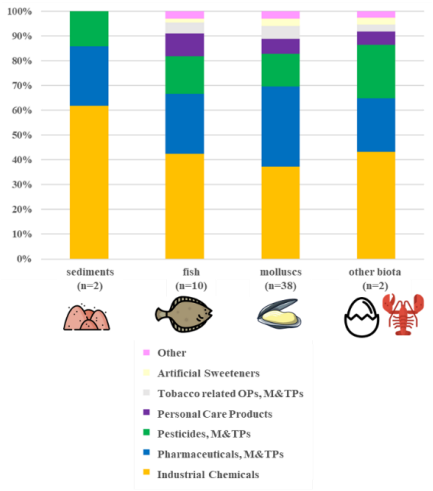




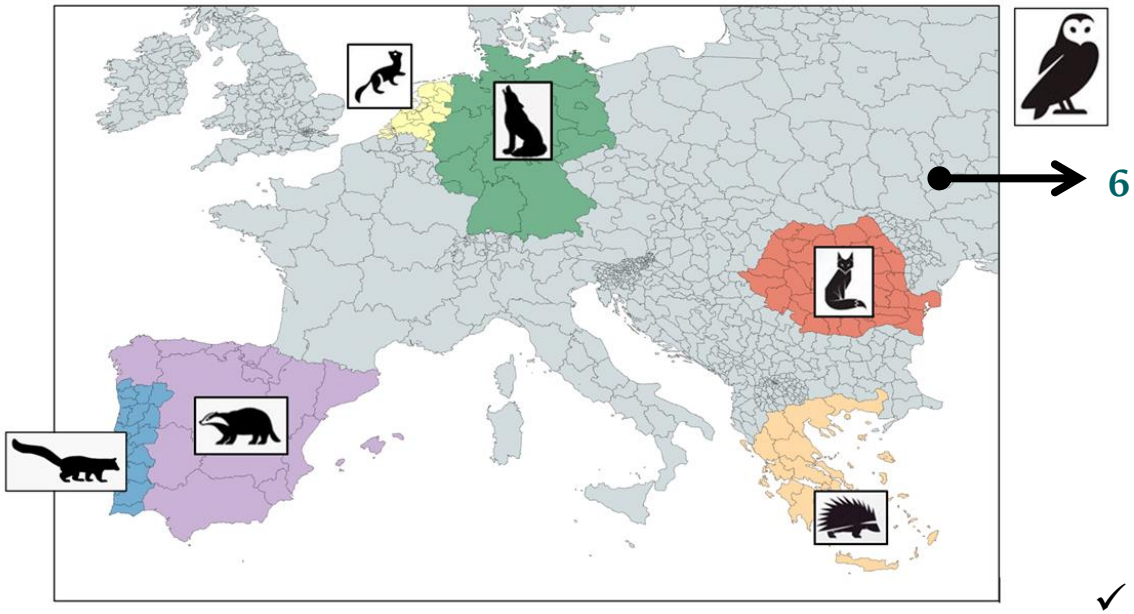
(a)



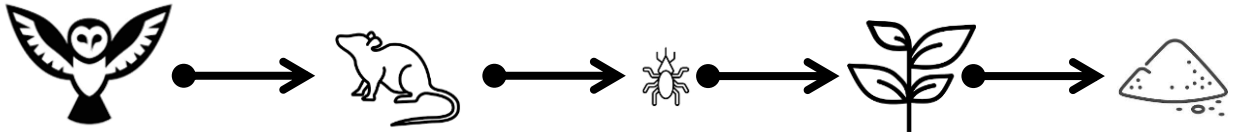
(b)



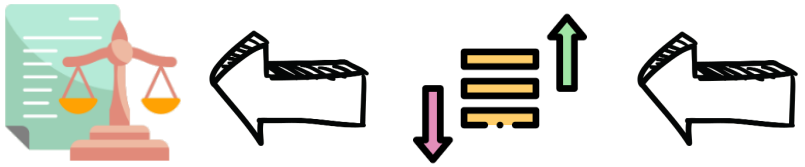
TerraChem



6 case studies (different **terrestrial** food chain) + **1 pan-European case study** (barn owl)
environmental samples from different trophic levels



- ✓ Wide-scope target analysis of >3,500 environmentally relevant organic pollutants
- ✓ Suspect screening of >100,00 chemicals
- ✓ GC-MS/MS for the determination of priority pollutants
- ✓ elemental analysis using ICP-MS



in-silico tools for the prediction of the toxicity, hazardous properties and fate of these chemicals in the terrestrial environment

Barn owl *Tyto alba* J. Dekker © 2023

Beech marten *Martes foina* Gg. Any, CC BY-SA 4.0 via Wikimedia Commons

Grey wolf *Canis lupus* C. Brück, CC BY-SA 4.0 via Wikimedia Commons

European badger *Meles meles* Caroline Legg, CC BY 2.0 via Wikimedia Commons

Egyptian mongoose *Herpestes ichneumon* CC BY-SA 4.0 via Wikimedia Commons

European hedgehog *Erinaceus europaeus* Touno Erik, CC BY-SA 4.0 via Wikimedia Commons

Red fox *Vulpes vulpes* Henrik Mollke, CC BY 2.0 via Wikimedia Commons

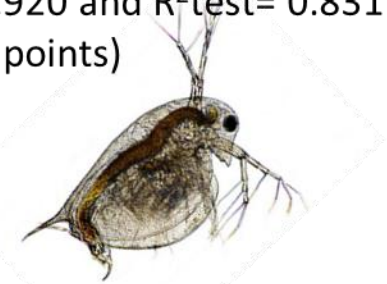
Toxicity prediction models

Tox TrAMS Version 1.0
Trace Analysis and Mass Spectrometry Group

ToxTrAMS v1.0 (acute and oral toxicity assessment toolbox)

Daphnia Magna

(R^2fitting= 0.920 and R^2test= 0.831
n=2174 end points)

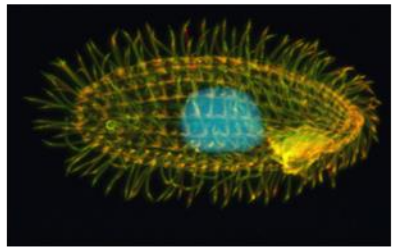


Pimephales promelas (Fish)

(R^2fitting= 0.982 and R^2test= 0.839
n=5953 end points)

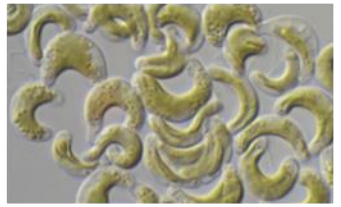
Tetrahymena pyriformis

(R^2fitting= 0.902 and R^2test= 0.856
n=1053 end points)



Selenastrum capricornutum (Algae)

(R^2fitting= 0.865 and R^2test= 0.759
n=538 end points)



Oral LD_{50} in rat

(R^2fitting= 0.821 and R^2test= 0.789
n=5743 end points)

Environmental Science
Processes & Impacts

PAPER

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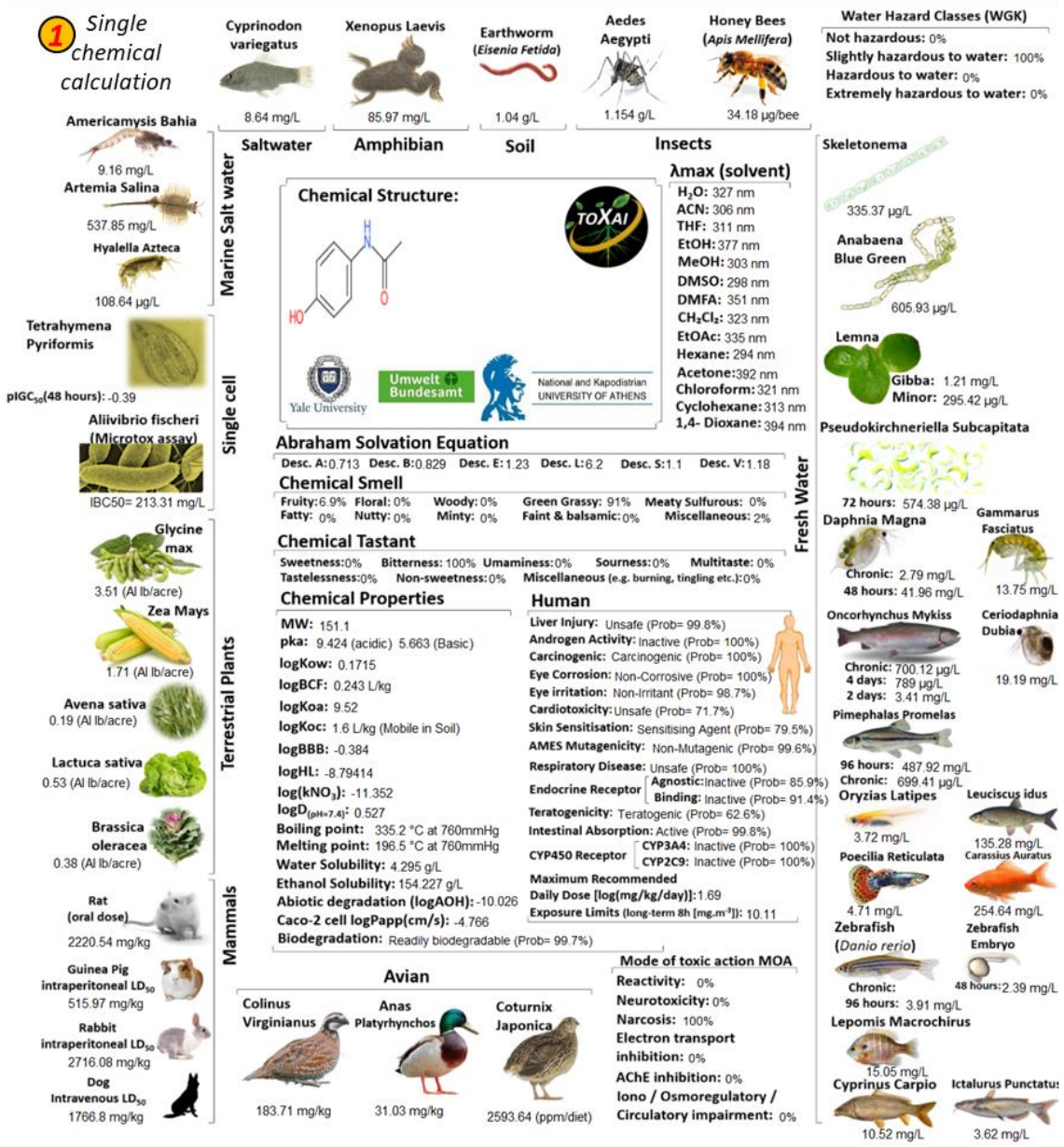
Prediction of acute toxicity of emerging contaminants on the water flea *Daphnia magna* by Ant Colony Optimization–Support Vector Machine QSTR models†

Reza Aalizadeh,[a] Peter C. von der Ohe[b] and Nikolaos S. Thomaidis*[a]

Toxicity prediction models

ToxAI; Open source R and Python-based app to perform in silico risk characterization and environmental fate analysis towards more than 105 end points



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Trace Analysis and Mass Spectrometry Group

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Thank you very much for your attention!

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