



HAL
open science

Exploring Non-Target Screening and Differential Analysis in Assessing Nature-Based Reactive Barrier Treatment of Micropollutants in Treated Wastewater

Charlotte Guy, Geoffroy Duporté, Linda Luquot, Elena Gomez

► **To cite this version:**

Charlotte Guy, Geoffroy Duporté, Linda Luquot, Elena Gomez. Exploring Non-Target Screening and Differential Analysis in Assessing Nature-Based Reactive Barrier Treatment of Micropollutants in Treated Wastewater. SETAC Europe 34th Annual Meeting, May 2024, Séville, Spain. . hal-04581270

HAL Id: hal-04581270

<https://hal.science/hal-04581270>

Submitted on 21 May 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Exploring Non-Target Screening and Differential Analysis in Assessing Nature-Based Reactive Barrier Treatment of Micropollutants in Treated Wastewater



C.Guy¹, G. Duporté¹, L. Luquot², E. Gomez¹

¹HydroSciences Montpellier, Université de Montpellier, CNRS, IRD, Montpellier, France

²Géosciences Montpellier, Université de Montpellier, CNRS, Montpellier, France



Context

- **Reuse of treated wastewater (REUSE):** interesting alternative in response of global water scarcity. Risks due to the presence of **contaminants of emerging concern (CECs)** in **treated wastewater (TWW)**.
- Recent studies (Valhondo et, 2023; Patel et al., 2021) have shown the potential of **reactive barriers (RB)** made of natural materials (**Nature based Solution**) easy to access and low cost as recharge system to eliminate contaminants present in TWW.
- Evaluating RB process effectiveness remain challenging.

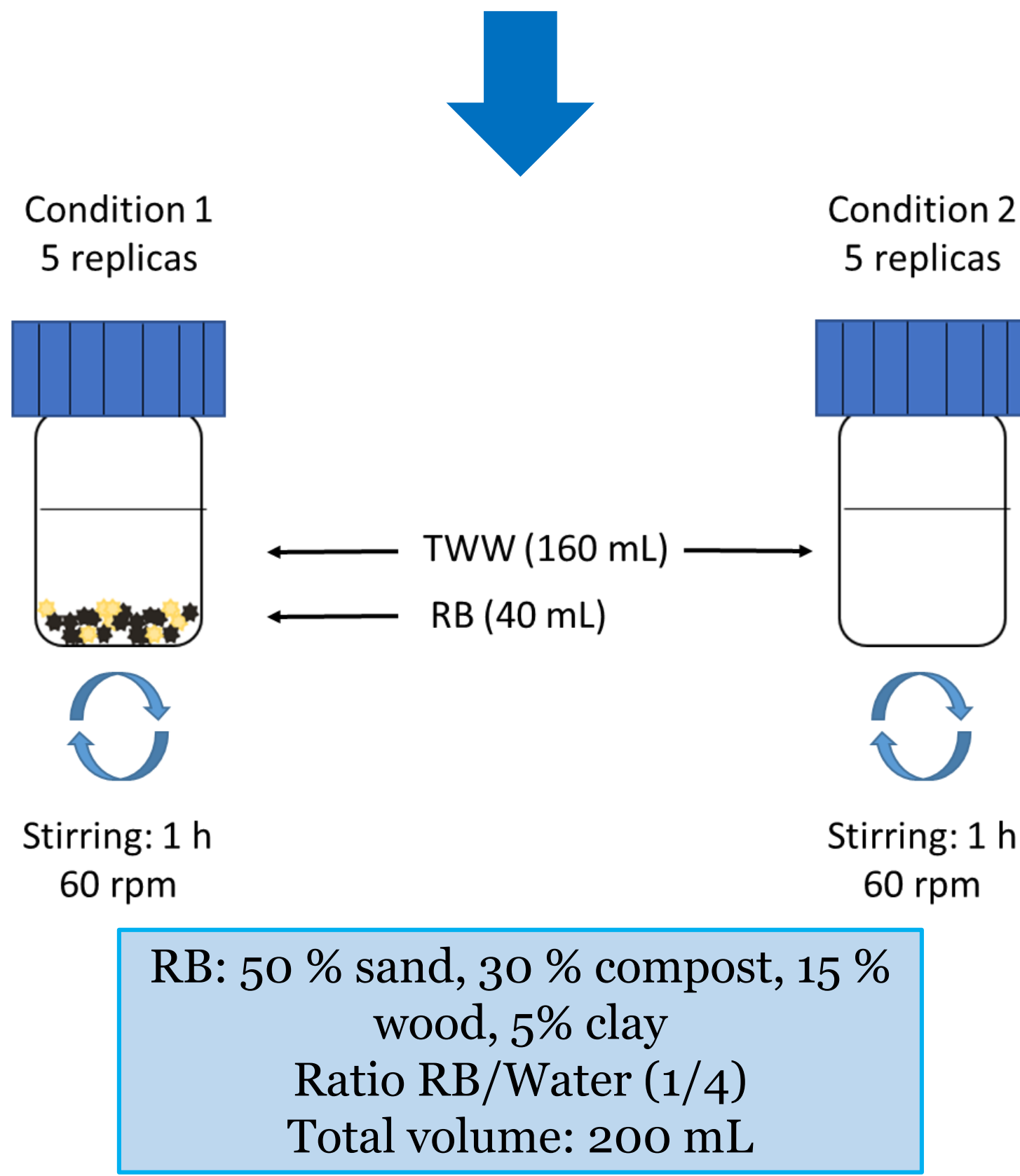
Goals

- Develop **differential approach** based **non-targeted analysis (NTA)** to evaluate **nature-based reactive barrier** effectiveness
- Study the **NTA contribution** for broadening perspectives on the **impact of RB** treatment

Materials and Methods



Sampling TWW at wastewater treatment plant of Murviel lès Montpellier (34, France)



Extraction on solid phase (SPE, Oasis HLB)



HPLC – HRMS

- Resolution: 70 000
- Targeted (38 CECs) and non-targeted analysis
- Internal databases made of 109 CECs for non-targeted identification



Compound Discoverer software

Statistical analysis (ANOVA, p-value ...)
Differential analysis

Results and discussion

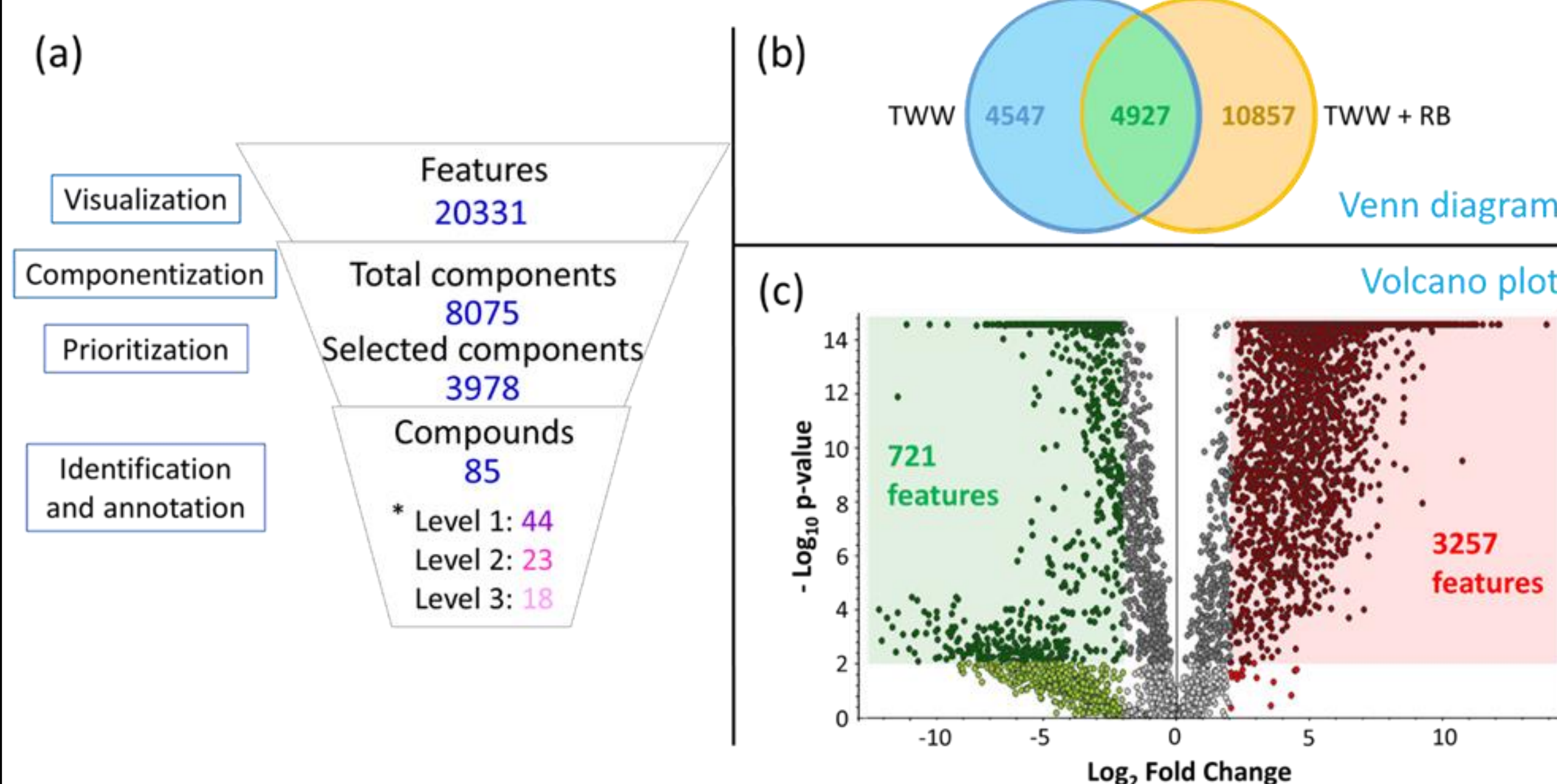


Fig 1: Analytical signals (Venn Diagram), prioritized features (Volcano plot) and annotated or identified compounds from NTA data

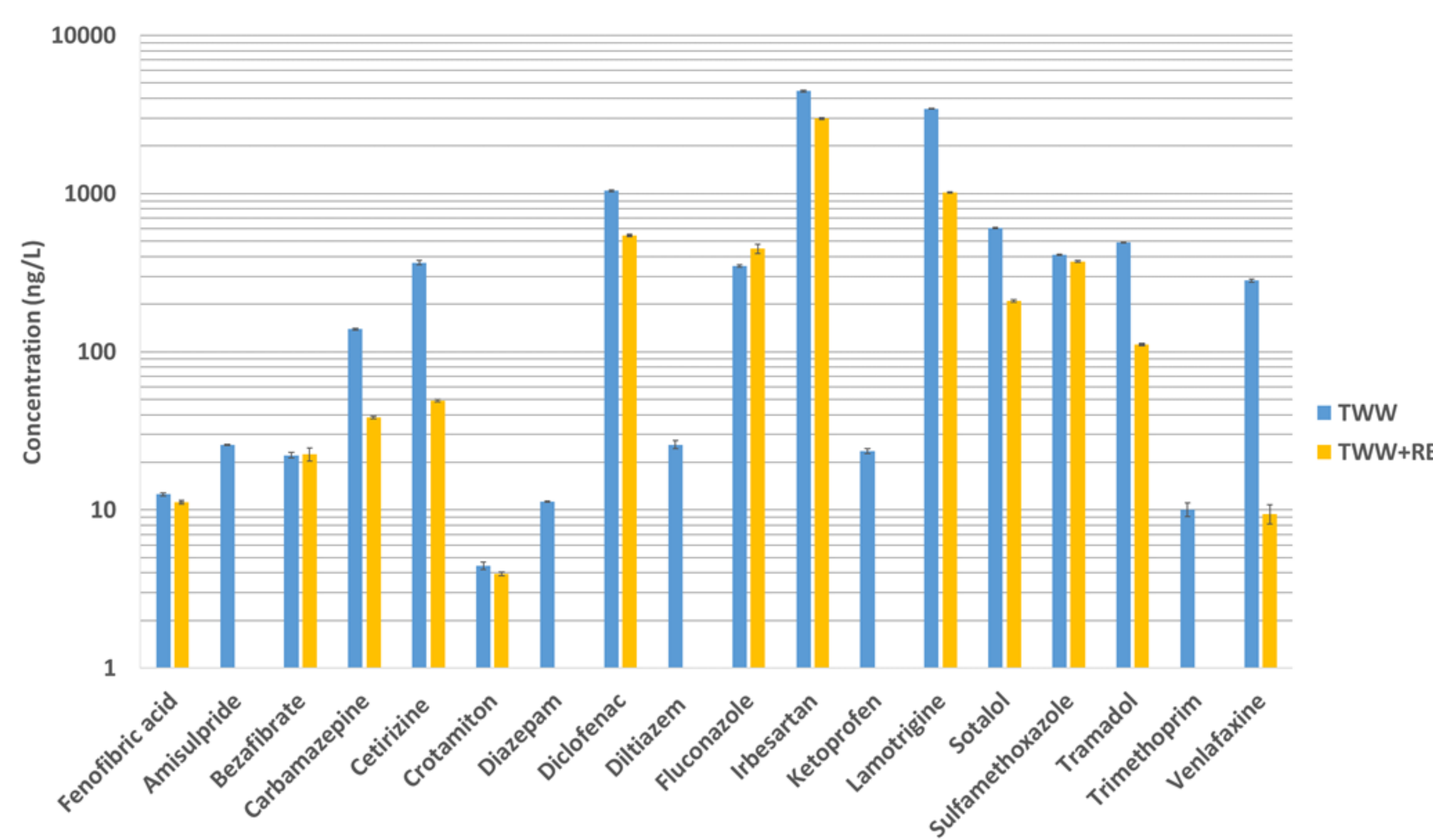


Fig 2: Concentrations of 18 targeted compounds found in TWW and TWW + RB

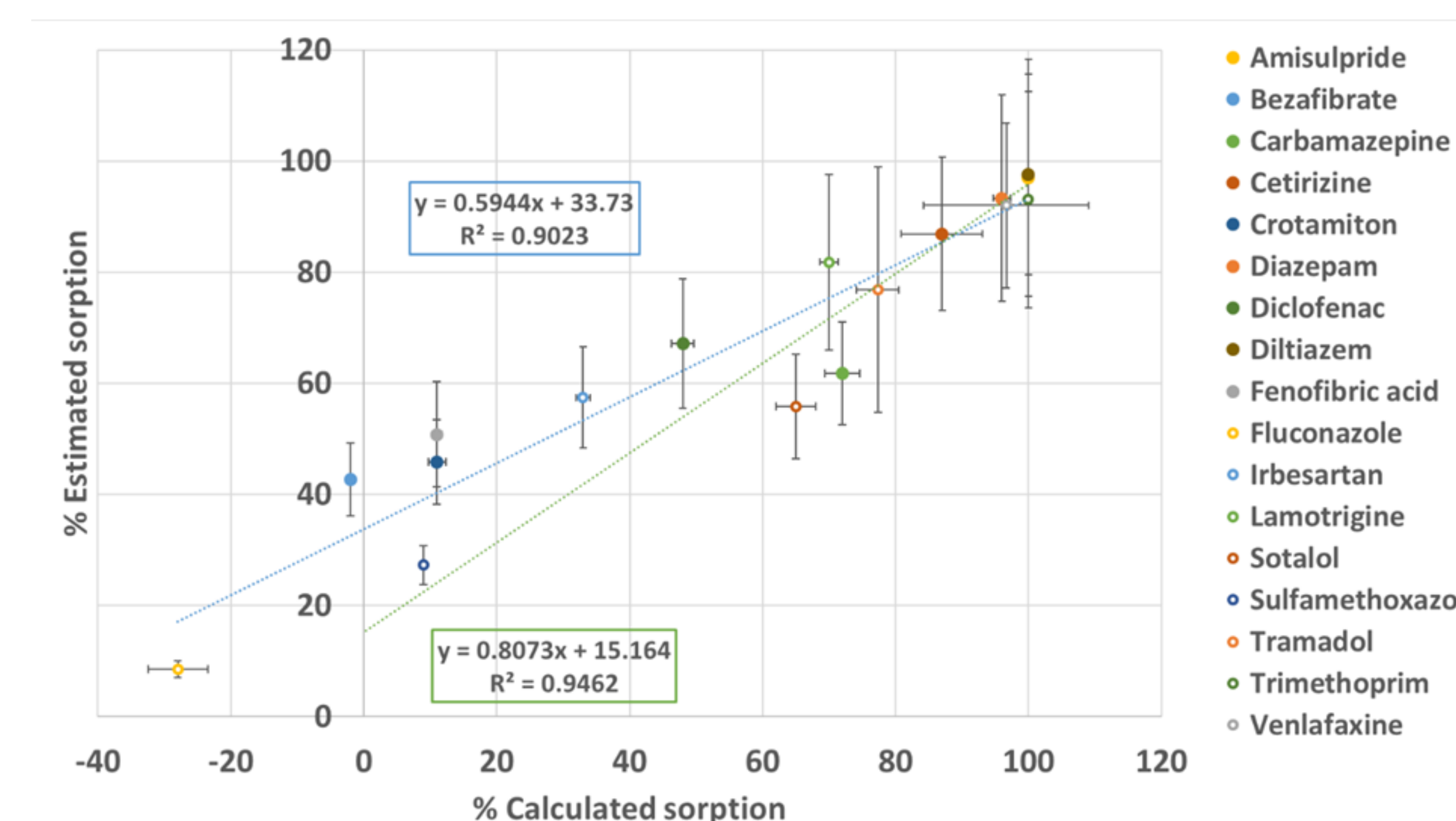


Fig 3: Percentage of sorption estimated by NTA in function of percentage of sorption calculated for target analysis; in blue: linear regression accounting all the compounds, in green: linear regression accounting compounds with $S > 75\%$

Comprehensive analysis in positive mode (Fig 1):

- 85 compounds identified or tentatively annotated
- 49 compounds with peak area increasing after contact with RB and 43 compounds with peak area decreasing after contact with RB
- Decreasing: pharmaceuticals and pharmaceutical metabolites
- Increasing: natural products and transformation products

Compound identification challenges:

- false positives and false negatives
- quality criteria: analytical stability, contamination, reproducibility
- matrix effect

Concentrations and CECs sorption (Fig 2):

- 18/28 targeted compounds found in TWW
- Irbesartan, lamotrigine and diclofenac $> 1 \mu\text{g/L}$
- Sorption: 61% compounds $> 50\%$
39% compounds $> 80\%$

$$S (\%) = \frac{C_{TWW+RB}}{C_{TWW}} * 100$$

- Sorption consistent with other studies (Valhondo et al., 2023; Patel et al., 2021)
- Sorption is the main process in this study

NTA applicability for sorption estimation (Fig 3):

- Satisfactory correlation but matrix effect vigilance is needed
- Estimated sorption overestimate by 34 % calculated sorption
- Improved correlation for compound sorbing $> 75\%$

- NTA reveals numerous compounds in TWW but also after contact with RB
- Differential analysis provide valuable information on the effectiveness of RB

Conclusion and perspectives

- **110 compounds identified or tentatively annotated** in positive and negative mode
- NTA provides a broad and complete **view of the performances of nature-based RB** treatment, giving information on the **compounds released** by the barrier in addition to **RB sorption capacity**
- **Prospects:**
 - pursue investigations using RB made with the studied materials in column experiments exploring other parameters such as flow, duration, redox conditions, microbiological activity and in real-life situations
 - approach allowing the study of released compounds by the RB with the identification of potential **transformation products**

Work published in *Frontiers in Environmental Science*

Guy et al., 2024

doi:

[10.3389/fenvs.2024.1385806](https://doi.org/10.3389/fenvs.2024.1385806)