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



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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 al., 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.

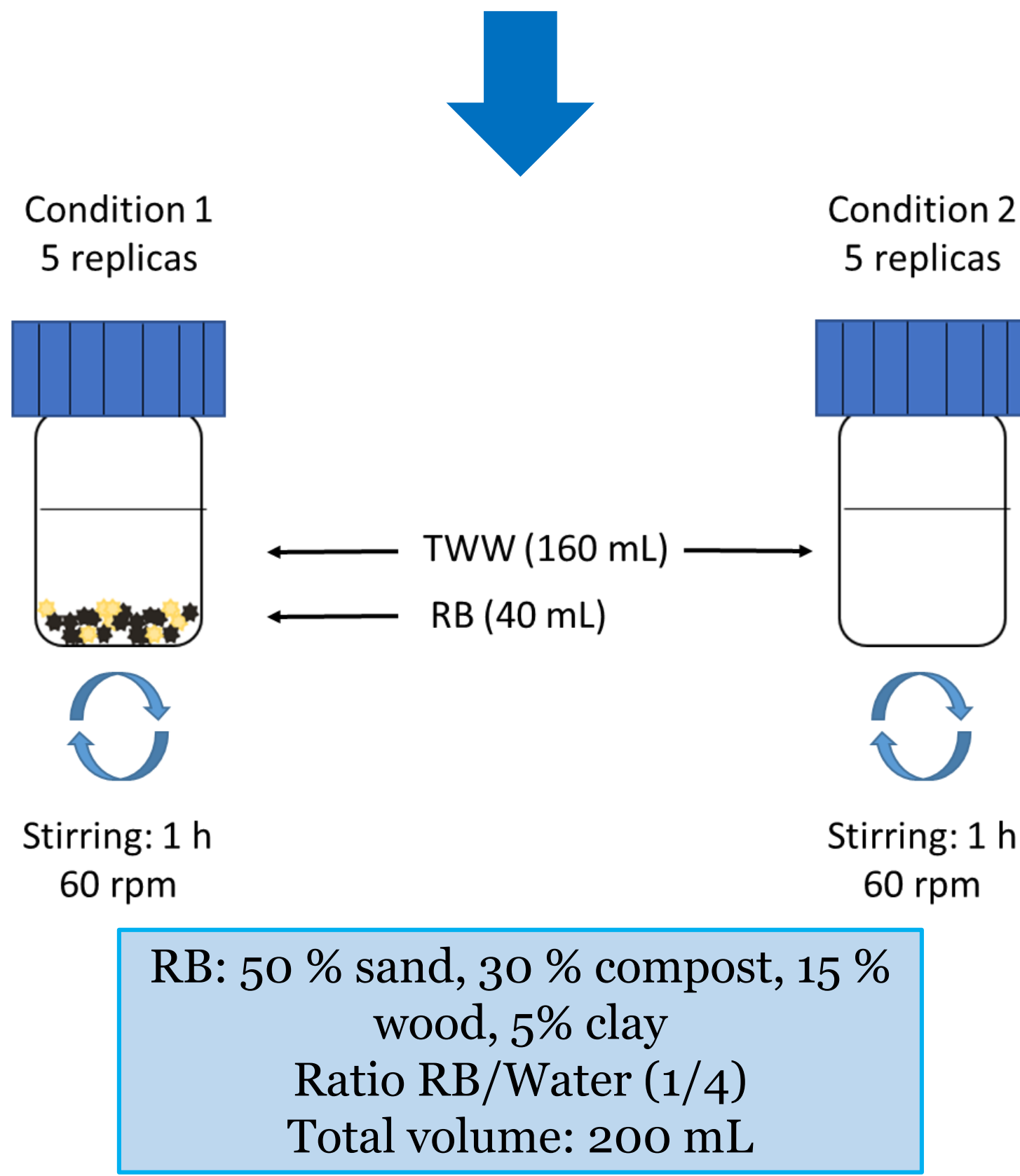
Goals

- 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

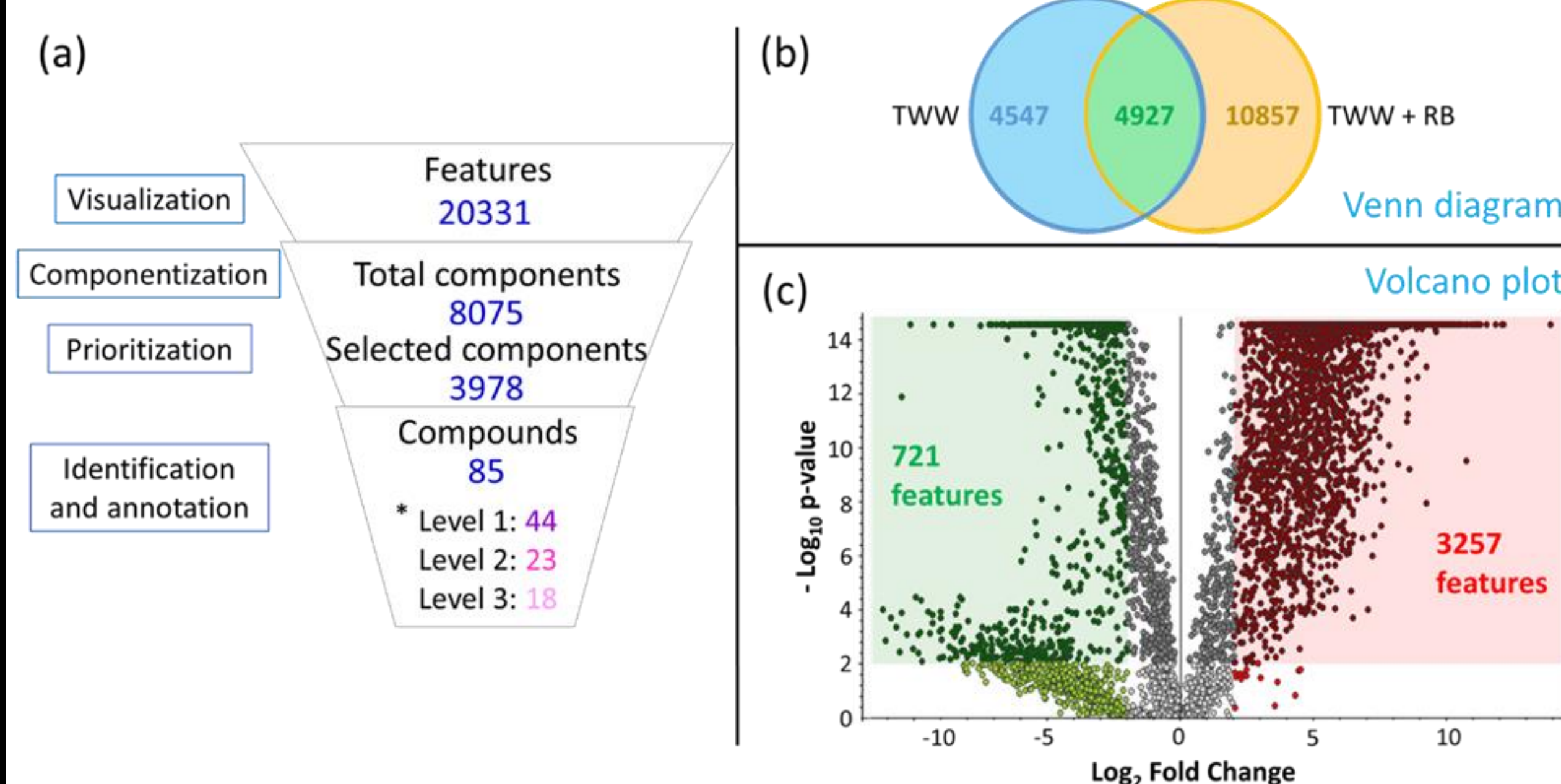


Fig 1: Analytical signals (Venn Diagram), prioritized features (Volcano plot) and annotated or identified compounds from NTA data

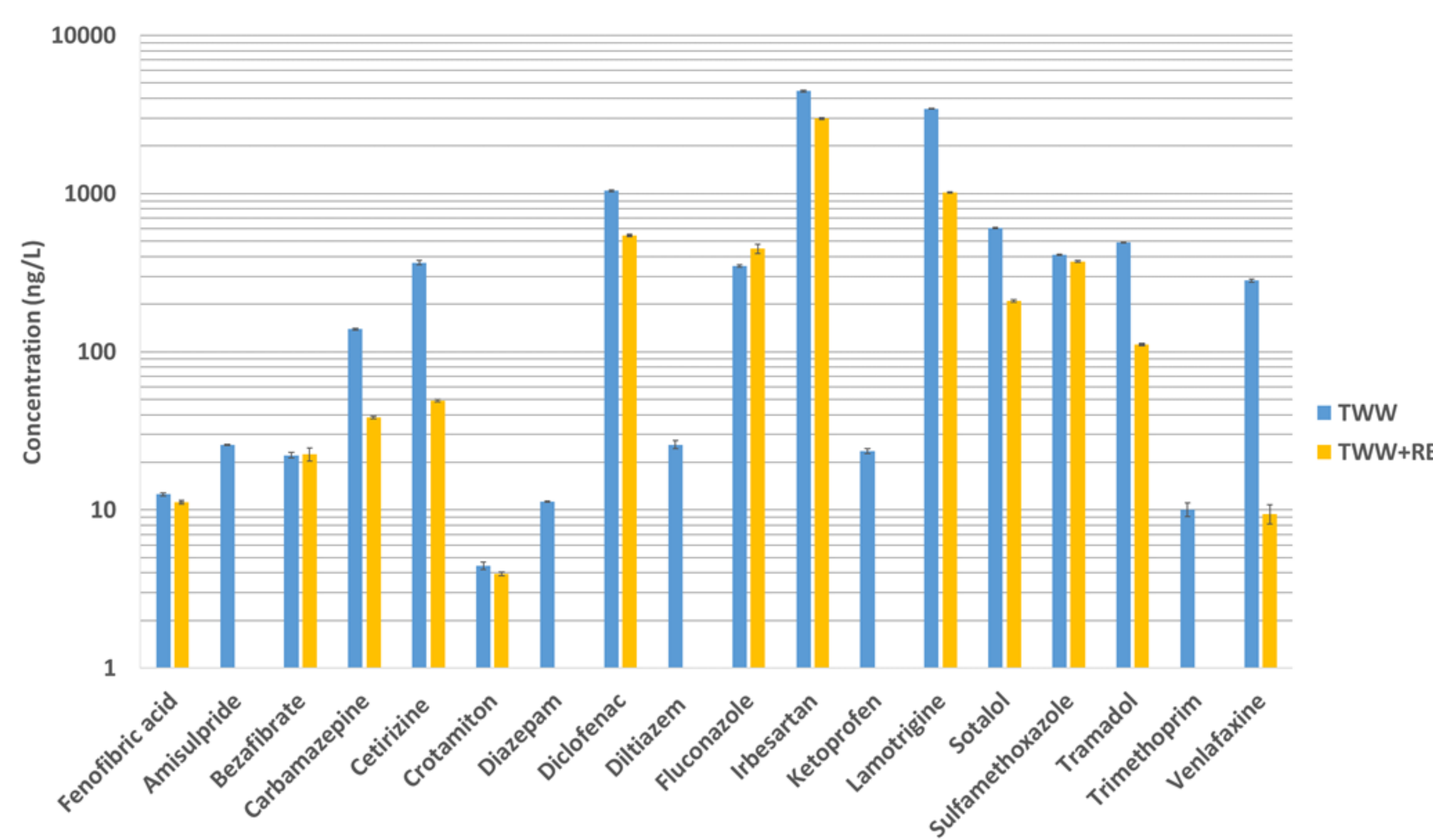


Fig 2: Concentrations of 18 targeted compounds found in TWW and TWW + RB

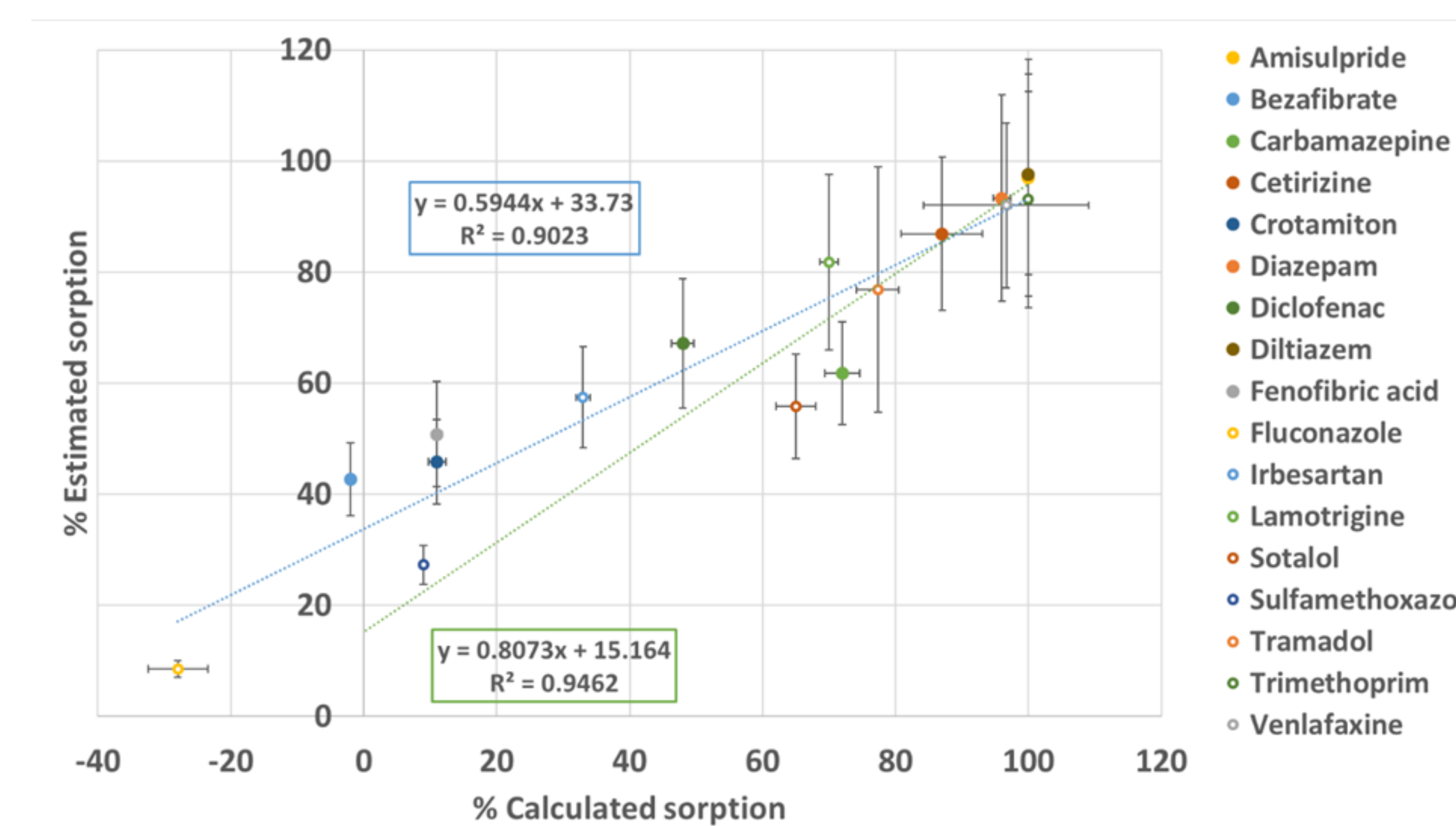


Fig 3: Percentage of sorption estimated by NTA in function of percentage of sorption calculated for target analysis; in blue: linear regression accounting all the compounds, in green: linear regression accounting compounds with $S > 75\%$

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**

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