



The CHaMP web-app:an interactive tool to infer biotransformation pathways from your MS peaks

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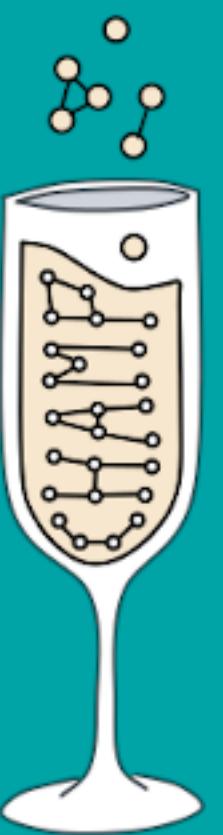
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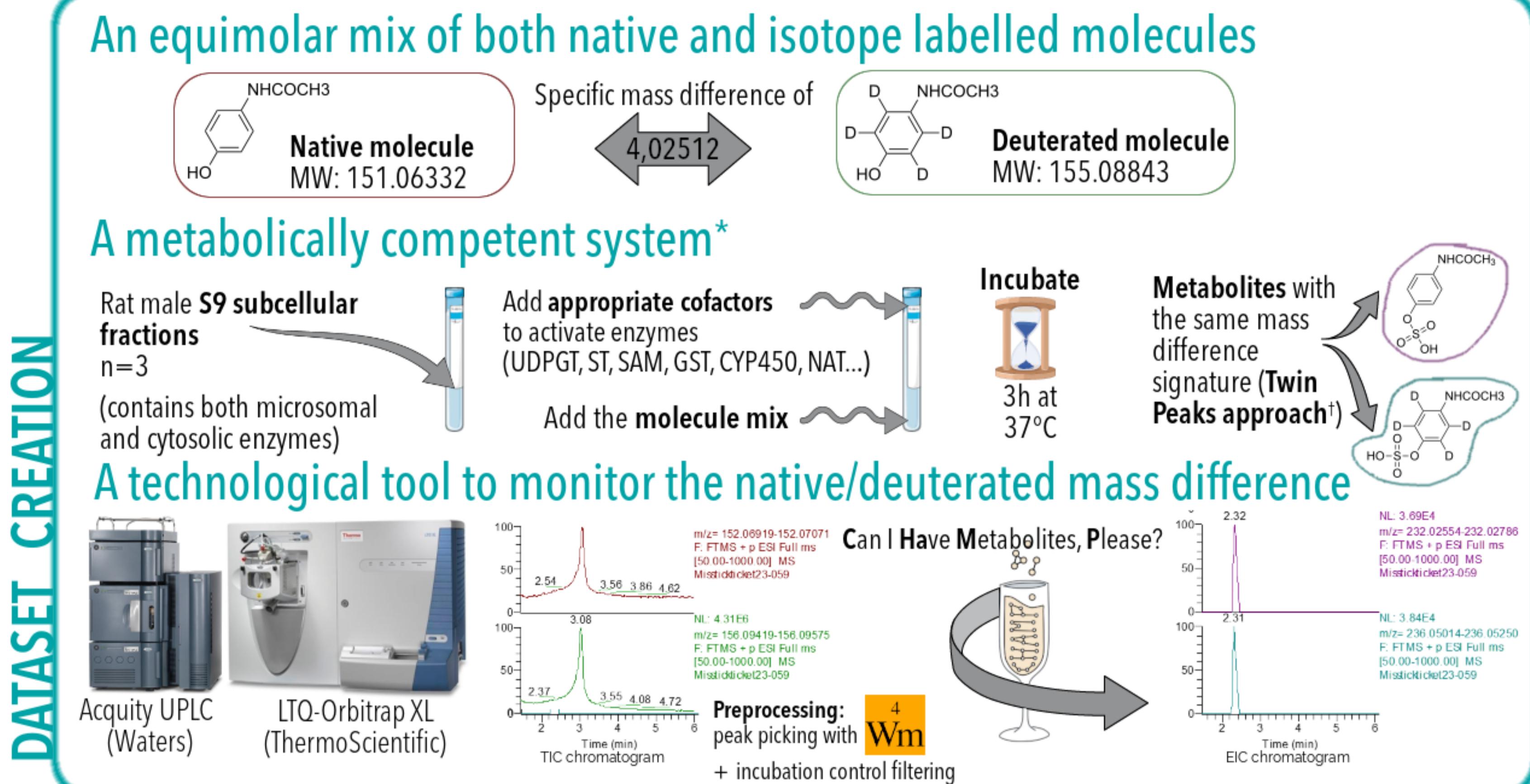
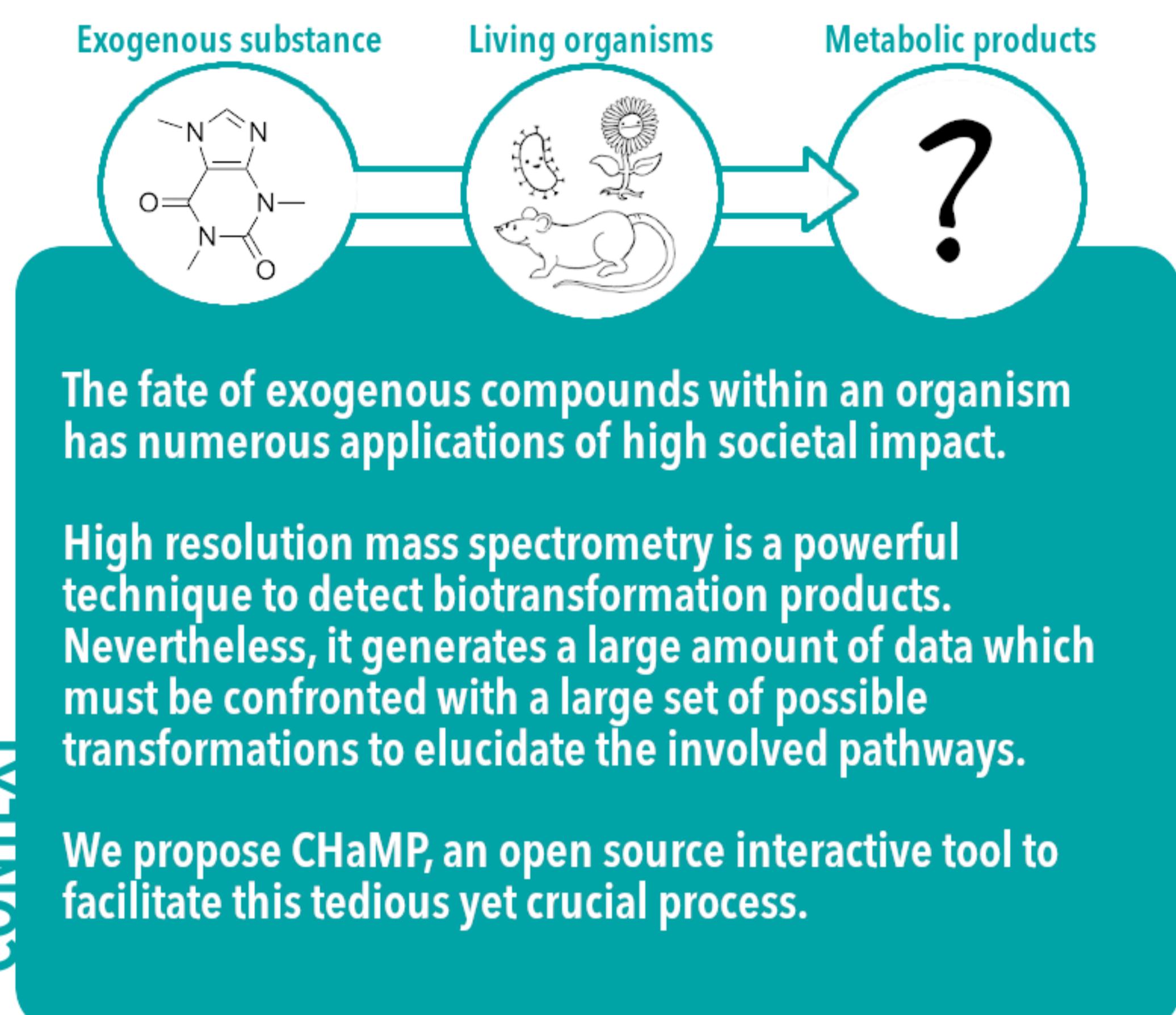
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The CHaMP web-app: an interactive tool to infer biotransformation pathways from your MS peaks

Marine Valleix^{1,2}, Clément Frainay^{1@}, Elodie Person¹, Jean-François Martin², Laurent Debrauwer², Daniel Zalko¹, Fabien Jourdan¹ and Sylvie Chevolleau²

CONTEXT



Explore putative network
drag nodes to create publication-ready figures

Upload masses, select compound of interest and set mass matching tolerance

Going further: check for missing links, add custom transitions to fill the gaps

Try it here

https://champ.sk8.inrae.fr

Behind the curtain:

1. Load a list of compound masses (ideally from twin-peaks analysis) and explore putative degradation or metabolism routes, using a mass difference network rooted toward a mass of interest.

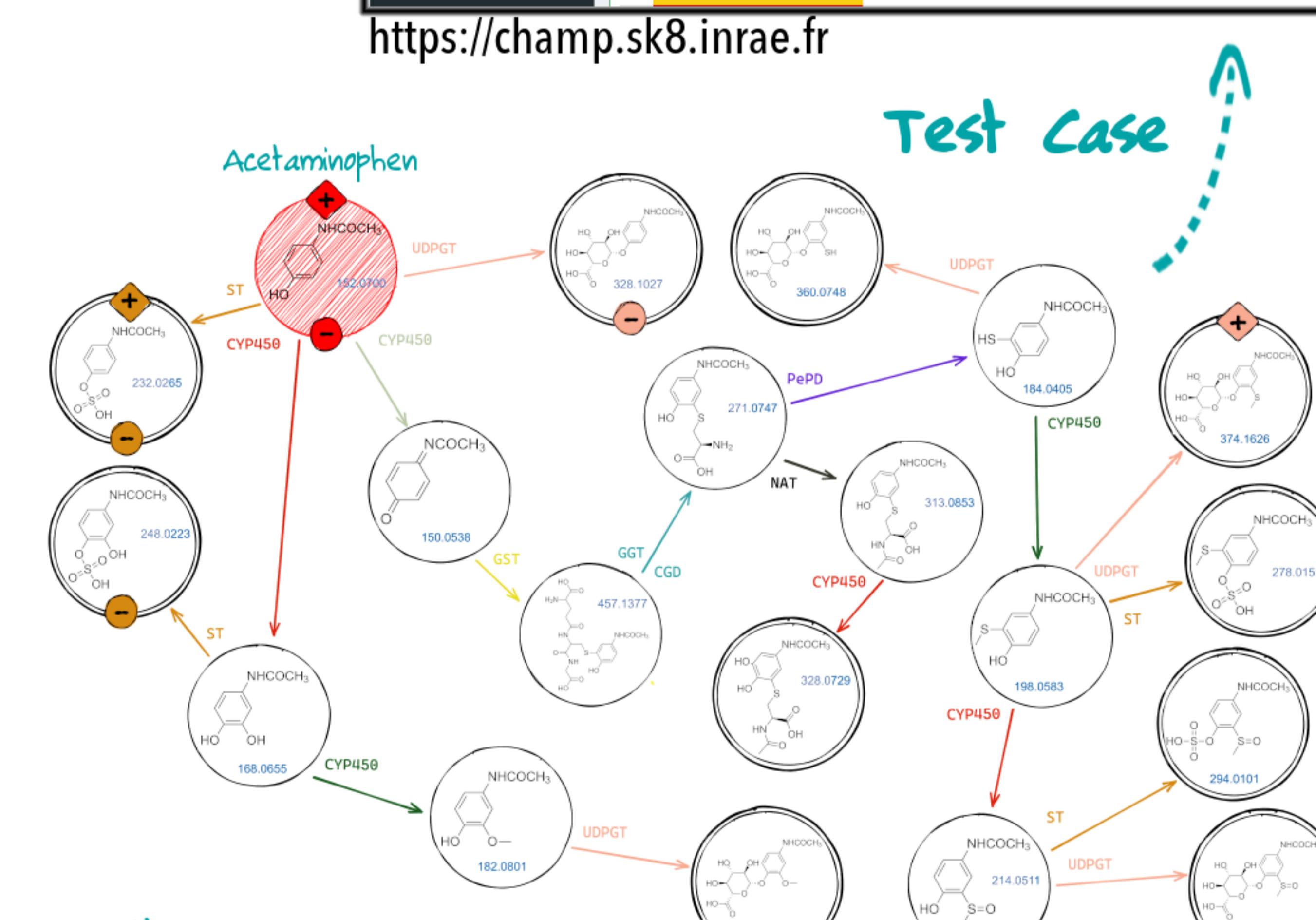
2. Degradation/Metabolization Network

3. See biotransformations, select relevant ones

4. Transformation list

5. Network Table

6. Get transformation info from the table, Download valuable data



DISCUSSION / CONCLUSION

- Test case: CHaMP proved to be a very efficient tool for retrieving and reconstructing acetaminophen metabolic pathways from a mass list using a combination of experimental data and knowledge from literature†.

- Higher concentration of acetaminophen mix could bring some routes to saturation (phase II pathways) and yield more terminal nodes (such as phase I products) from experimental data.
- Kinetic experiments could help detect intermediate compounds from experimental data.

- CHaMP's visual and interactive approach made more efficient the reconstruction process of biotransformation pathways from mass data.

Challenges

- A few missing links remaining due to specific mass shifts, which can be added manually.
- Less relevant alternative routes require manual pruning.

Perspectives

- Inference of missing intermediates using Steiner Tree pruning.
- Organic pollutants whose metabolic pathways are yet partly unknown are currently being investigated using CHaMP.

* C. Al-Ayoubi, et al. Metabolism of versicolorin A, a genotoxic precursor of aflatoxin B1: Characterization of metabolites using in vitro production of standards. Food and Chemical Toxicology, 2022

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‡ A. David, et al. Acetaminophen metabolism revisited using non-targeted analyses: Implications for human biomonitoring. Environment International, 2021

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