Towards Predicting Pesticide Degradation: A Molecular Scaffolding Approach to Environmental Hazards

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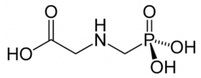
What is Roundup?

Glyphosate



Why is it important?

Glyphosate or Roundup is used as a pesticide to kill pests, insects, weeds, rodents, etc.

What are the consequences?

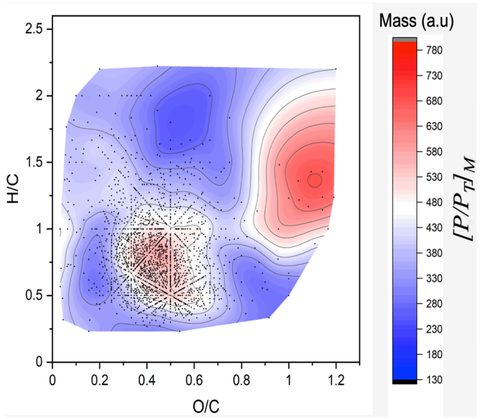
Glyphosate affects soil chemistry and can lead to cancer carninogens.

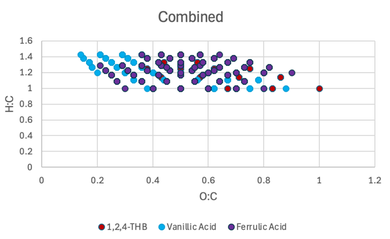
Purpose

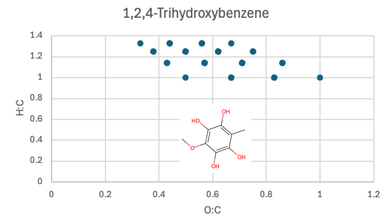
- When Roundup is used on plants and soils, Glyphosate has different effects on the solubility (LogKow) and degradation pathways of molecules based on soil factors.
- These soil factors have to do with the organic composition of the soil.
- Organic matter in soils comes from 1,2,4-Trihydroxybenzene, Ferulic Acid, and Vanillic Acid.
- Pesticides degrade these molecules and make daughter molecules.
- This allows me to assess how glyphosate alters degradation by comparing parent–daughter product distributions and LogKow.

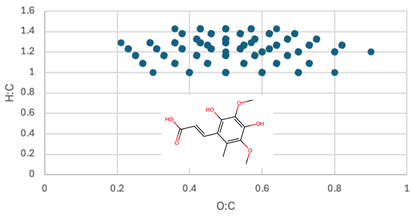
Methods

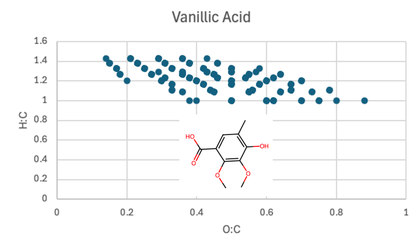
- A computational approach using Jupyter Notebooks and Python 3 for simulated parent-daughter molecules was used.
- FTICR-MS of soil that shows around 6-8 thousand molecules.

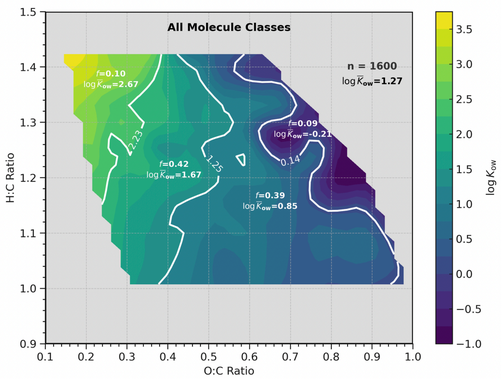


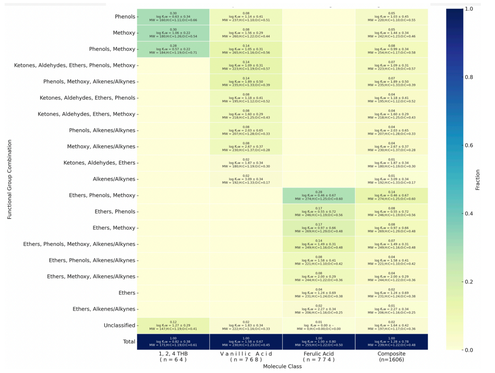


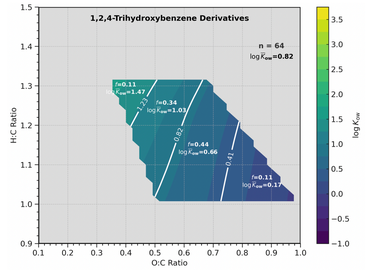


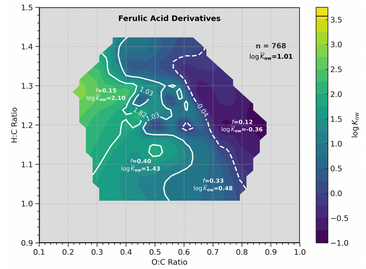


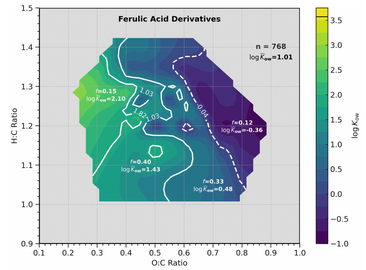






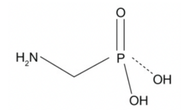






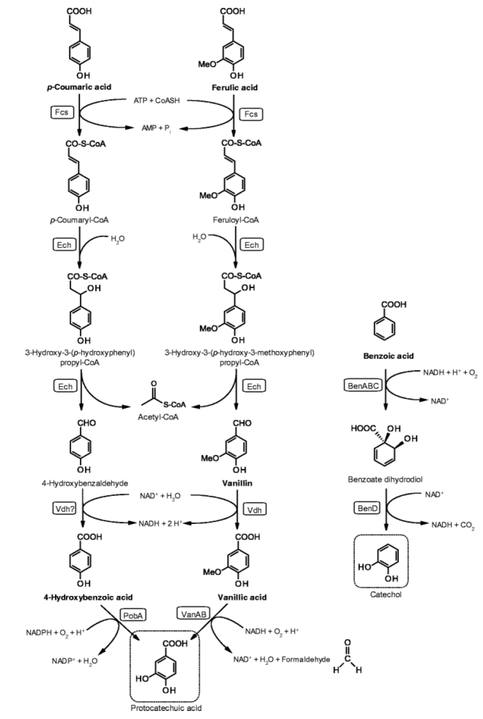
Future Work

AMPA LogKow: -1.63

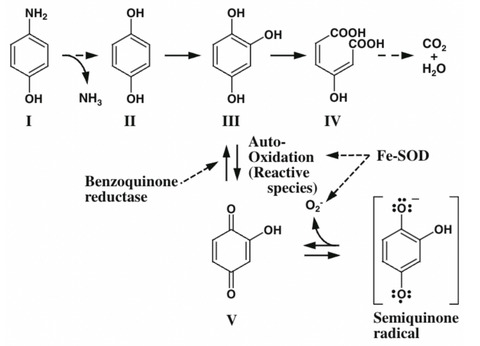


- Since different soils have different distributions of Octanol Water Partitioning Coefficients, I will derive the solubility of the daughter compounds of Glyphosate, like AMPA, using FTICR-MS.
- Furthermore, we can use AI machine learning to tag molecules from my simulated dataset to unknown molecules in soils across the country.

Degradation Pathways



Ravi, Krithika, et al. "Conversion of lignin model compounds by pseudomonas putida KT2440 and isolates from compost." *Applied Microbiology and Biotechnology*, vol. 101, no. 12, 15 Mar. 2017, pp. 5059–5070, https://doi.org/10.1007/s00253-017-8211-y.



Takenaka, Shinji, et al. "Fe-superoxide dismutase and 2-hydroxy-1,4-benzoquinone reductase preclude the auto-oxidation step in 4-aminophenol metabolism by Burkholderia sp. strain AK-5." *Biodegradation*, vol. 22, no. 1, 18 May 2010, pp. 1–11, https://doi.org/10.1007/s10532-010-9569-5.