compounds developed in our lab, enabled machine learning models to predict bitterness from molecular structure alone. Yet the vast majority of published chemosensory data remains fragmented across tens of thousands of papers, reported in heterogeneous formats, scales, and terminology, and largely inaccessible to computational analysis.
Alongside recent initiatives to create community-wide standards, and encouraging data sharing in platforms such as the Zenodo ChemoSensoryData Community, we aim to unearth the wealth of chemosensory knowledge currently buried in historical literature.
Specifically, we are developing an AI-powered pipeline that leverages large language models to discover, classify, and extract structured sensory data from published papers. Drawing on recent advances in LLM-based scientific information extraction, our system extracts experimental details including substances, concentrations, food matrices, and sensory attributes ratings. Next, organize them into a standardized, ingredient-centric knowledge base. I will present the challenges of parsing heterogeneous sensory literature and the role of manually curated data cohorts in validating automated data extractions. Finally I will illustrate how integrating extracted data opens new avenues for cross-compound generalization, mixture prediction, and the generation of novel, testable hypotheses in chemosensory science.

LC-ESI-MS/MS characterization of organic selenium compounds in red wine

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Selenium, in the form of selenoamino acids and selenoproteins, is an essential component of the immune system reducing free radicals, which may lead to chronic diseases, such as cancer and heart disease. Selenomethionine (SeMet) and Se-methylselenocysteine (MeSeCys) are the major selenium-containing amino acids in dietary sources. SeMet is a bioactive form of selenium with antioxidant properties, playing a significant role in cardiovascular health, autoimmune conditions, and the prevention of certain cancers. Additionally, selenomethionine oxide (SeMetO), which possesses a protective mechanism against oxidative stress, is the oxidized form of amino acid selenomethionine. In this study, a rapid and sensitive HPLC-ESI-MS/MS technique was applied for the first time to identify and quantify organic selenium compounds, including: selenomethionine, selenomethionine oxide and selenium methylselenocysteine in Kratošija wines (a synonym of Zinfandel, Primitivo and Crljenak Kaštelanski). The wines were produced by inoculating two commercial yeasts: ZymafloreTM Xpure (Laffort) and Lalvin ICVD80 (Lallemand) in order to study the effect of yeasts on selenium compounds content in the final wines. The effect of the yeasts on the selenium compounds in both wines was observed. Thus, wine fermented with Lalvin ICVD80 contained higher amounts of SeMet and MeSeCys, probably due to a better ability to transform the inorganic selenium into organic selenium compounds (especially selenomethionine). Both wines contained high levels of SeMetO, produced as a result of the oxidation of SeMet during fermentation and/or storage. The obtained results suggest that the red wine Kratošija can be considered as an adequate source of SeMet and SeMetO, possessing healthy properties.