

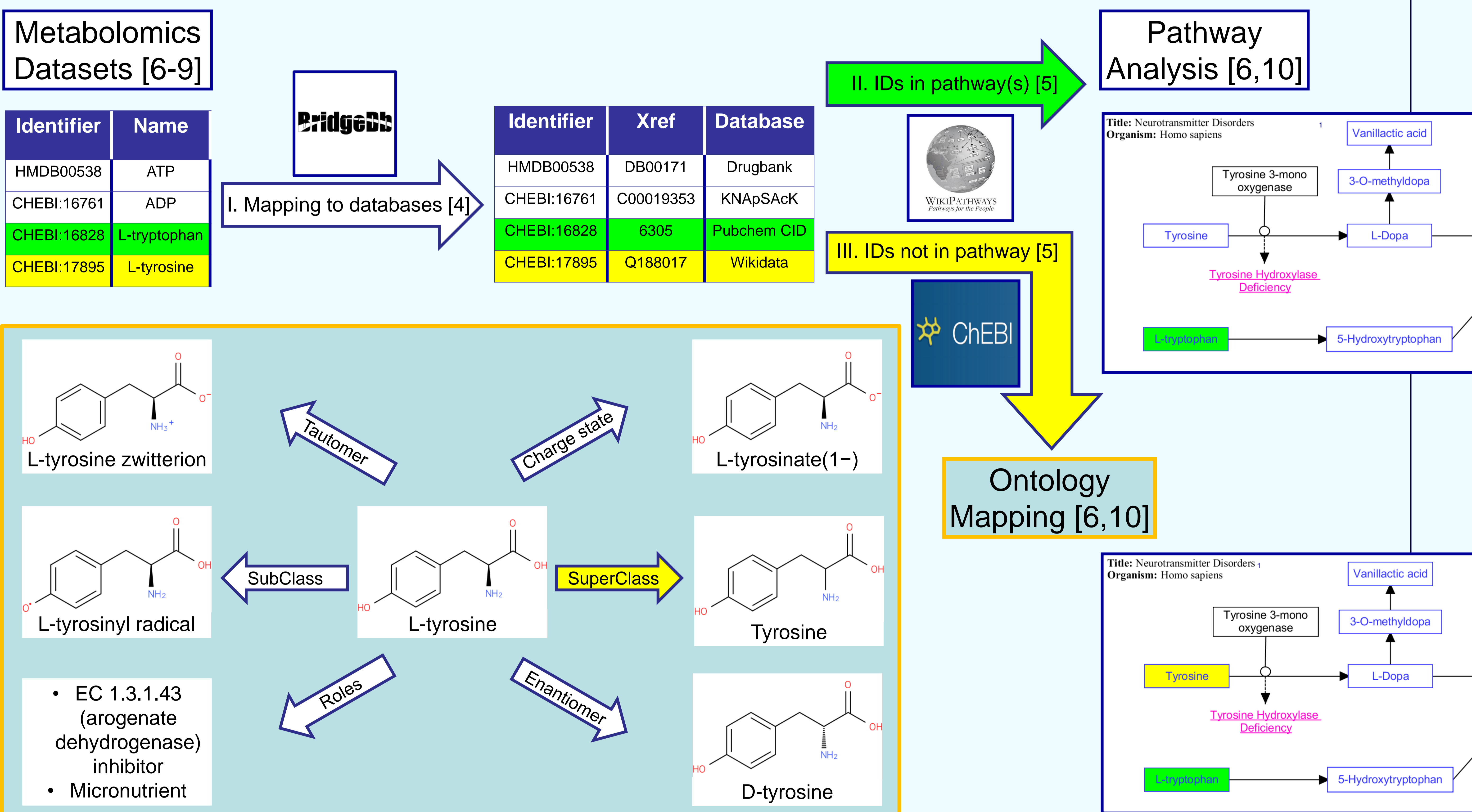
Chemistry Identifier Mapping to Pathway Databases using Ontologies: Expanding metabolomics analysis in WikiPathways with ChEBI

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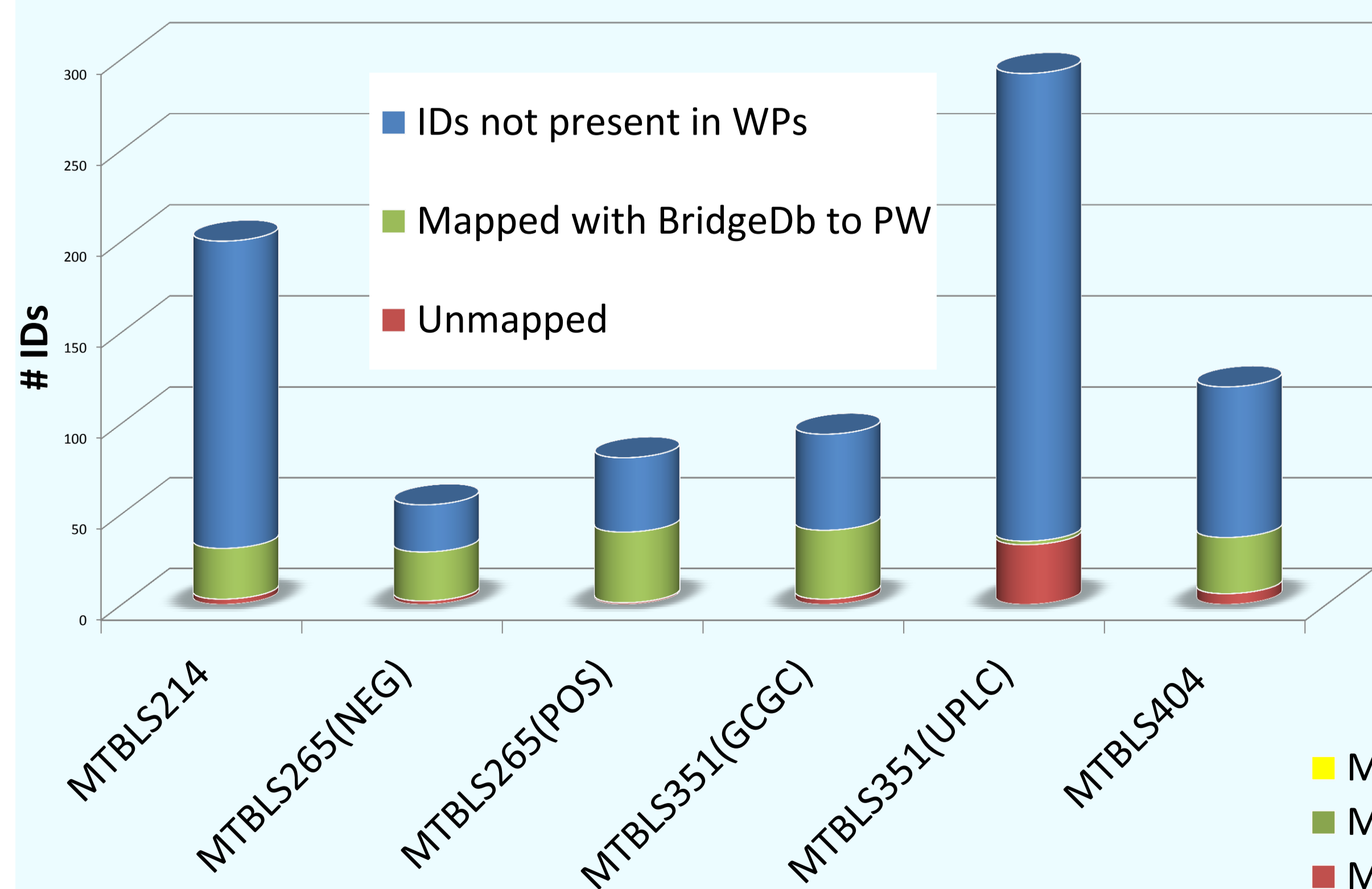
Abstract

Health research uses large scale data collection methods, such as metabolomics, to study the state of an individual, organs, and increasingly tissues and single cells. Changes in metabolism are relevant for many diseases. Pathway and network approaches are extensively used to integrate various data types to understand measurements and results in their biological context. Unfortunately, not all measured metabolites can be linked to metabolite identities present in biological pathway models. In order to overcome this problem, we use the ontological information from ChEBI [1] to create additional mappings for metabolites in the pathway database WikiPathways [2]. By applying this method on various publicly available datasets in the MetaboLights [3] repository, we want to estimate the increased mapping that chemical ontologies can provide.



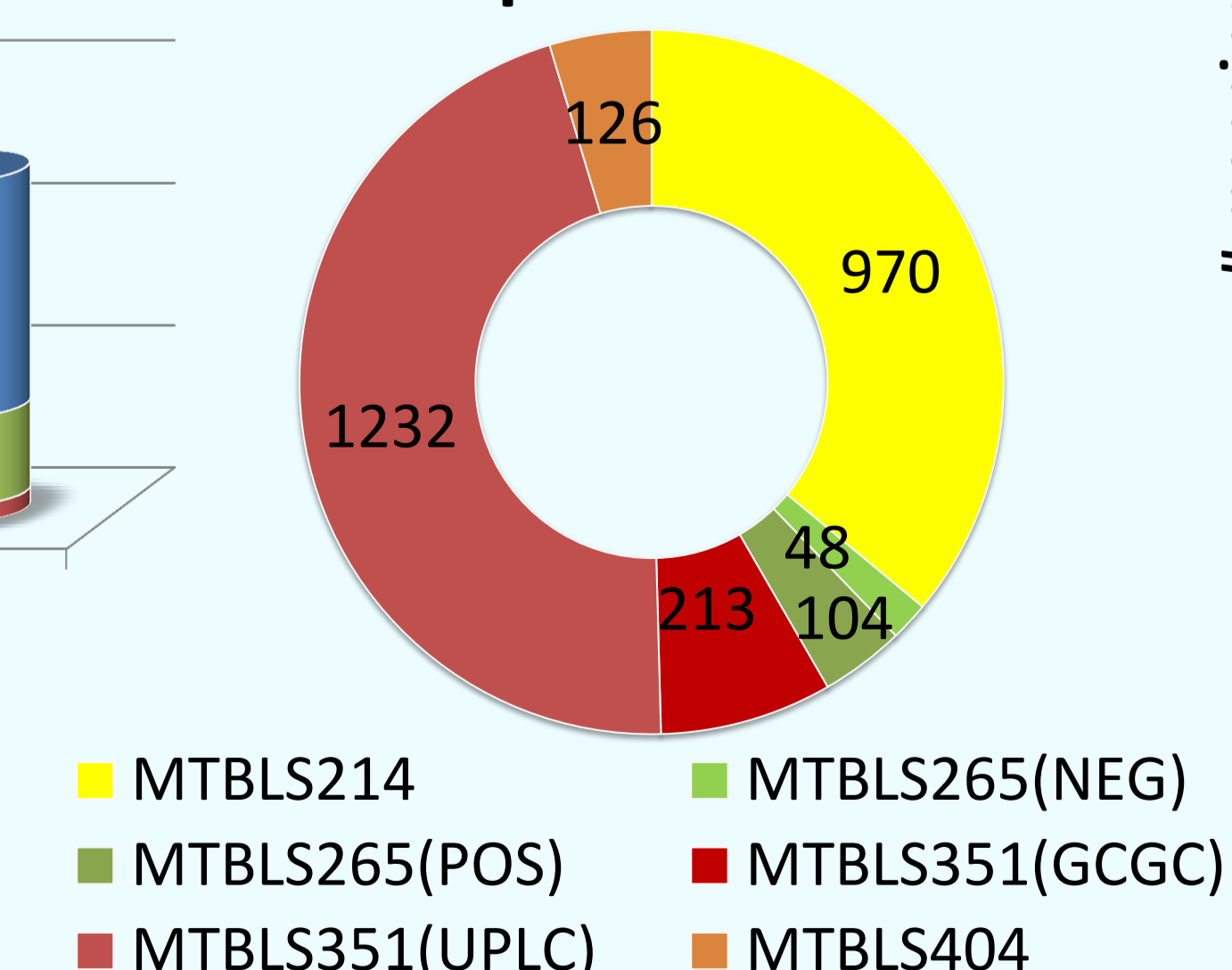
Results I + II

Mappings through BridgeDb and WikiPathways



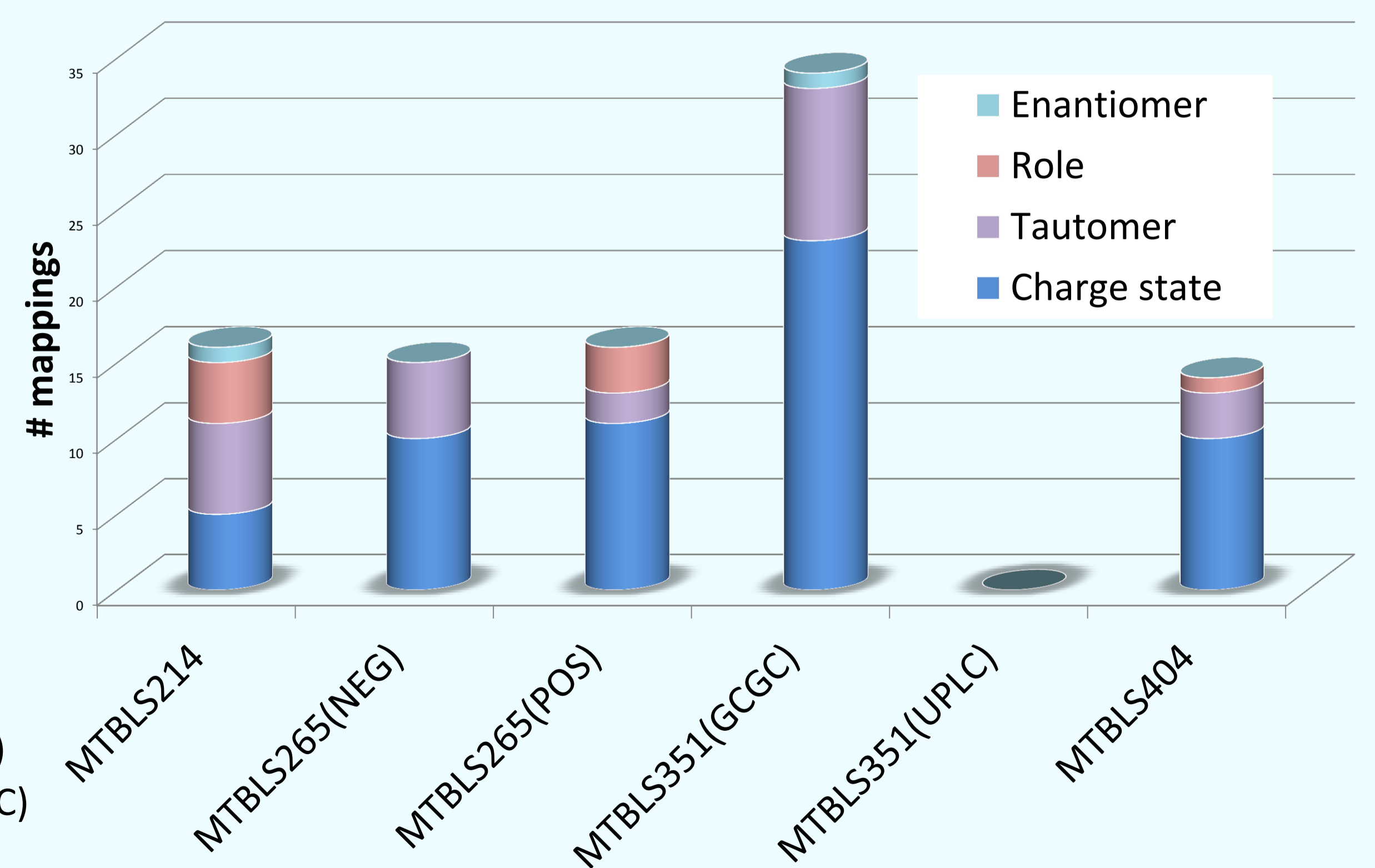
Ontology Mapping

SuperClasses



Results III

Additional Mappings through Ontologies



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References:

- [1] Hastings J. *et al.* Nucl. Acids Res. 2016
- [2] Slenter D.; *et al.* Nucl. Acids Res. 2018
- [3] Haug K; *et al.* Nucl. Acids Res. 2013
- [4] BridgeDb metabolites mapping file DOI: 10.6084/m9.figshare.6260003.v1
- [5] WikiPathways pathways accession number: <http://data.wikipathways.org/20180410/>

Metabolomics datasets from MetaboLights:

- [6] MTBLS124, DOI: 10.1371/journal.pgen.1004801
- [7] MTBLS265, DOI: 10.1073/pnas.1603023113
- [8] MTBLS351, DOI: 10.1038/nature18646
- [9] MTBLS404, DOI: 10.1021/acs.jproteome.5b00354

Pathway analysis for MTBLS214 on:

- [10] WP4220_r97366, neurotransmitter disorders; Friesacher A., Slenter D., Willighagen E.