Designing potential extensions from G-SRS to ChEBI ontology to identify natural product-drug interactions

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Introduction

- Complementary health approaches involving the use of natural products (NPs) are increasing in popularity in the US.
- Limited information about NPs exists in drug databases and biomedical ontologies
- There is a need to integrate data in existing biomedical resources including NP substances, constituents, and pharmacokinetic knowledge.
- We used kratom and green tea as NP cases to design potential logical extensions to map NPs to the ChEBI ontology
- The goal of this work is to advance computational research on NP-drug interactions.

For more details:

https://github.com/dbmi-pitt/NaPDI-pv/tree/master/ontology_map.

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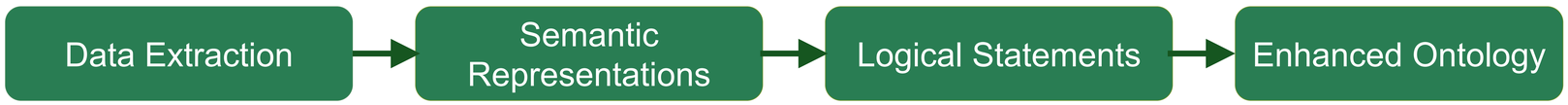
NaPDI
Center of Excellence for Natural Product-Drug Interaction Research

Objective

To integrate natural products (NPs) in the Open Biological and Biomedical Ontology (OBO) Foundry ontologies by designing logical extensions to include NPs, NP constituents, and related pharmacokinetic information in the ontologies. This will facilitate discovery of potential natural product-drug interactions (NPDIs).

Workflow

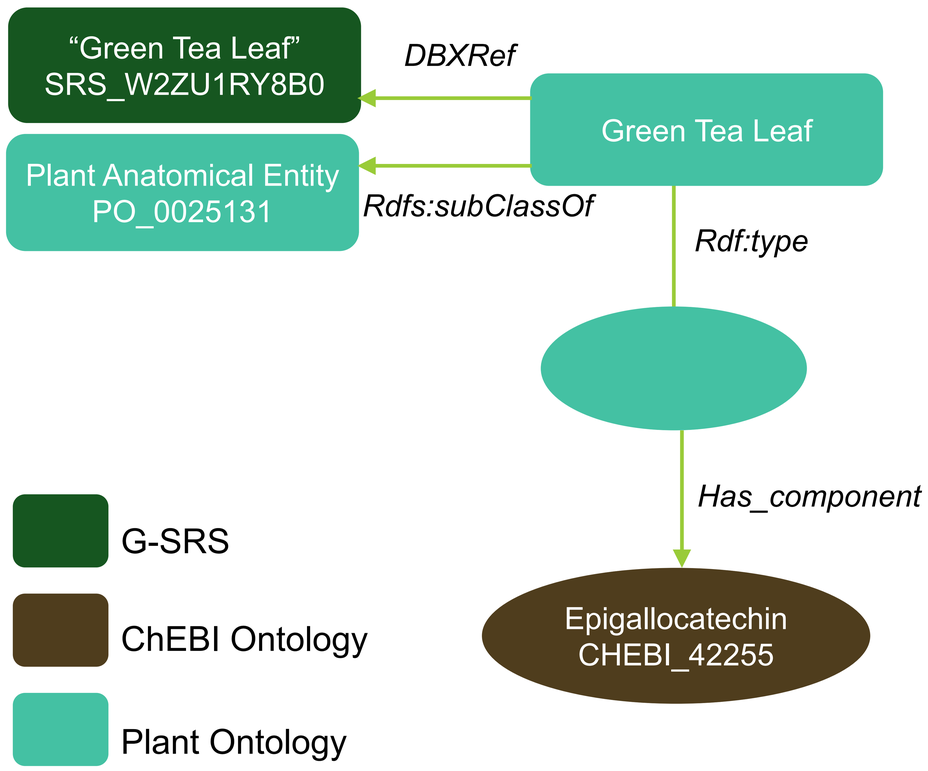


Global Substance Registration System (G-SRS)

G-SRS harmonizes chemical identification for drug development and safety research using an ISO standard and is the primary substance identification system for the Food and Drug Administration (FDA).

- Over 25000 structurally diverse substances with organism family and part, constituents and metabolites
- References to other NP-data sources such as Dietary Supplement Label Database, NCIT
- Verification of information by experts
- Standard identifiers
- Pharmacokinetic information

Semantic Representation



Logical Statements

```
BNode1
OBO:database_cross_reference
SRS:Green Tea Leaf

BNode1 RDFS:subClassOf
PO:Plant Anatomical Entity

BNode1 rdf:type UUID2

BNode2 RO:has_component
CHEBI:Epigallocatechin
```

Semantic Representation - Green Tea