METRIN-KG: A knowledge graph integrating plant metabolites, traits, and biotic interactions

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Abstract

Background

In recent years, biodiversity data management has emerged as a critical pillar in global conservation efforts. Today, the ability to efficiently collect, structure, and analyze biodiversity data is central to breakthroughs in conservation, drug development, disease monitoring, ecological forecasting, and agri-tech innovation. However, due to the vastness and heterogeneity of biodiversity data, it is often confined to databases for specific research areas in isolated formats and disconnected from other relevant resources. Crucial components of such data in kingdom Plantae comprise of metabolomes - the vast array of compounds produced by plants; traits - measurable characteristics of plants that influence their growth, survival, and reproduction, and that affect ecosystem processes; and biotic interactions - relationships of plants with other living organisms, affecting the ecosystem functions.

Results

In this work, we present METRIN-KG (MEtabolomes, TRaits, and INteractions-Knowledge Graph) a powerful data resource simplifying the integration of diverse and heterogeneous data resources such as plant metabolomes, traits, and biotic interactions.

Conclusions

The proposed knowledge graph provides an interface to interactively search for data relating plant metabolomes, traits, and interactions. This, in turn, will facilitate development of research questions in life-sciences. In this context, we provide representative case studies on how to frame queries that can be used to search for relevant data in the knowledge graph.

Keywords: Knowledge Graphs, Plant Metabolomes, Plant Traits, Biotic Interactions

Context

Interplay of metabolomes, traits, and biotic interactions

All species of our planet are connected by means of shared resources for sustenance, response to environmental effects, and multi-level biotic and abiotic interactions. An in-depth understanding of this multi-scale network of interactions enables researchers from natural sciences, chemistry, microbiology, ecology, plant biology, and climate change to address critical questions in ecology, biodiversity conservation, agriculture, and human health. As referenced by studies before [1–3], there are seven main shortfalls of biodiversity knowledge. Amongst these shortfalls, Raunkiæran and Eltonian emphasize *lack of connected knowledge on species' traits and interactions, as well as their corresponding relation to ecological functions*. The chemistry of life, by governing biotic interactions, resource access, environmental adaptation, and individual phenotype, provides a link to building the mechanistic network required to understand species' processes underlying ecosystem functioning [4].

The metabolome, a key component of the chemistry of life, refers to all metabolites forming the substrates or products of enzymatic reactions in an organism. To a certain extent, the metabolome provides a bridge between the ecosystem functioning and the contextual information of species' states across multiple scales (spatial, temporal, and environmental) [5–7]. In the Plantae kingdom, the sheer magnitude of metabolite diversity produced by plants is estimated to be between 1.5 and 25.7 million collectively for 400,000 plants [8], which poses significant challenges for metabolomic data analysis [9,10].

It has been shown that metabolomes can provide a proxy for the estimation of the plant functions, thus revealing the cause-and-effect relationship between external environmental factors and plant fitness [9]. However, exploring the metabolome structure across spatial, temporal, and environmental scales requires extensive studies to unravel the interplay of hundreds of compound classes and their potential biological and ecological functions.

Since experimental approaches alone cannot provide such comprehensive datasets, aggregating data across multiple studies that combine metabolome with physiological or environmental data appears as a necessary solution. Such information can include functional data like traits and co-dependence data like interactions.

Plant ecology focuses on how an organism's traits influence its interactions with and in response to environmental conditions throughout its life cycle. Traits like plant height, seed mass, leaf area, leaf carbon, nitrogen, and phosphorus contents have been used to define plant processes across taxonomic (tree of life) [11–13], spatial (e.g.: subalpine regions) [14], environmental (e.g.: weather changes) [15], and temporal (e.g.: reproduction during the life of plant or life history) scales [15–17]. However, the mechanistic understanding behind the effect of traits on plant fitness and functioning is not clear [18–21] because of the unexplained or ambiguous relation of traits and variation in ecosystem functioning.

Plant biotic interactions, including relationships with other plants, fungi, bacteria, and soil organisms, have been shown to influence ecosystem structure and function, ultimately shaping biodiversity patterns [22–24]. As sessile organisms, plant biotic

interactions also rely heavily on chemical mediation, involving both volatile and non-volatile compounds to compensate for their lack of mobility. Such interactions, particularly those involving insects, such as defense mechanisms or pollinator attraction, have been closely linked to the diversity of plant metabolites through evolutionary processes [25–29].

Challenges in integrating high-dimensional data

In recent years, efforts have been made to include chemistry into the functional traits framework to resolve plant functions in ecosystems [30,31]. Many studies have tried to combine the traits with specific compounds or classes of compounds [30–34], biotic interactions with traits [35–38], and biotic interactions with metabolomes [39–42]. Some studies have combined the three to decipher ecosystem functioning. For instance, they have examined plant traits, their interactions with soil biota, and related chemodiversity [43,44]. Some have explored the effect of insect herbivory on plant traits and their secondary metabolite concentrations [45–47]. Others investigated links between plant root traits, nutrient foraging, chemodiversity, and their symbiotic relationship with mycorrhizal fungi [48–50]. Additional research has focussed on allelopathic interactions and nutrient mobilization during intercropping in agriculture [51,52]. Studies also cover plant root traits, exudates (metabolites produced by roots), and its interactions with the rhizosphere microbiome [53]. Further examples include links between biotic interactions, elevation gradients, and metabolomics [54]; climate-induced plant host shift in insects [55]; plant microbe interactions and chemical defense mechanisms [56]; as

well as insect herbivory and defense mechanisms facilitated by secondary metabolites [57–59]. Moreover, several reviews published during the last decade have stressed the importance of combining plant traits, interactions, and metabolomes [33,60–67]. The main challenge in studies that combine these three components is the high dimensionality of each, coupled with limited resources available to characterize such complexity, which poses analytical limitations (e.g. incomplete spectral libraries, detection limits), suboptimal data availability, and cross-links across the three components.

The experimental approaches commonly used in functional ecology are powerful tools for exploring and describing specific mechanisms. However, they remain limited when it comes to disentangling complex processes operating at larger scales. Linking chemical pathways, compound classes, or molecular structures to ecological functions remains a major challenge in ecological research. Recent development of databases and advances in data science offer a new potential to reach this goal. A data-driven approach is required to first map the existing knowledge in all three areas followed by the development of research hypotheses. Building on the few previous studies in this direction, we explored various datasets and databases related to traits, interactions, and metabolomics, which ultimately inspired the core idea of this study.

Much information on the heterogeneity of metabolites biosynthesized by organisms lies locked in isolated tabular formats, excel sheets, and pdf documents (as discussed in [68]). Few databases provide comprehensive information on metabolites or natural products [68–72]. The Earth Metabolome Initiative (EMI) [73] and its pilot project Digital Botanical Gardens Initiative (DBGI) [74], were launched in 2022. They aim to document

metabolic content for all known species on Earth (initiating point being botanical gardens living collections), following the Findable, Accessible, Interoperable, Reusable (FAIR) guidelines [75]. Under the EMI umbrella, comes the Experimental Natural Products Knowledge Graph (ENPKG) [69], a published resource of metabolomes from 1600 tropical plant extracts. ENPKG uses a sample-centric approach comprising semantic annotations to structure large, heterogeneous metabolomics datasets into knowledge graphs. It also enables harmonization of experimental data with publicly available resources. However, no ecological metadata was integrated in ENPKG.

Like metabolite data, multi-species level interaction data also lies locked as pairwise correlation metrics in peer-reviewed research papers. While Global Biotic Interactions (GloBI) [76] and tools like BiotXplorer [77] have succeeded in collecting this information in a FAIR resource [78], they allow only partial multi-species level interaction mapping and are limited to pairwise interactions. Such documentation of interactions is remarkable, yet it suffers from the lack of providing complete multi-species level interactions. Furthermore, higher-order interaction structures (e.g. multi-trophic or trait-mediated interactions) are often analyzed post hoc using correlation-based summaries that abstract away mechanistic or phenotypic information. Similarly, data on plant trait heterogeneity is limited to few resources like TRY [79,80] and global plant trait network [81].

There are individual databases listing organism traits [80,82], metabolite-pathway relations of a limited number of plant species [83] as well as microbes [84,85], pairwise interaction maps [76], medicinal herbs [86], and food [87]. However, there is no single resource available that combines knowledge across organisms, detailing their traits,

interactions, and their complete/partial metabolomes, all of which are important for the in-depth understanding of the complex network of life.

MEtabolomes, TRaits, and INteractions - Knowledge Graph (METRIN-KG)

In this Data Note, we present the first efforts in combining publicly available data on plant traits, interactions, and metabolome from peer-reviewed research and databases in METRIN-KG. We have linked enriched metabolome datasets behind ENPKG [69] with high dimensional data on plant traits from TRY database [80], pairwise interaction data from GloBI [76], and annotated data on natural products from LOTUS [68] (available through Wikidata). To ensure semantic interoperability, we have used ontologies for knowledge representation like the Earth Metabolome Initiative Ontology (EMI Ontology) [88,89], and the ENPKG ontology for natural product-specific concepts [69]. We used Ontop [90–92] and Python rdflib library [93] to materialize the Resource Description Framework (RDF) triples. We further implemented a SPARQL Protocol and RDF Query Language (SPARQL) editor to query METRIN-KG and retrieve results.

We anticipate METRIN-KG to be useful for interactively searching related information on traits, interactions, and metabolome, thus guiding and inspiring the development of future research questions in the fields of ecology, biodiversity conservation, agriculture and human health. Moreover, we believe this information could also be valuable to a wider audience beyond researchers, such as policymakers and public health

professionals, by enhancing their understanding of the broader implications of research within their respective fields.

In the following sections we provide details on how the datasets used in METRIN-KG were retrieved, structured, and linked. We also provide a brief overview of the construction of the EMI Ontology, discuss potential reuse of METRIN-KG, and present representative queries for exploring the knowledge graph.

Methods

Data retrieval from TRY database

For this study, the pilot dataset was retrieved from the TRY website [94] by requesting data for 41 traits based on the most used functional trait categories in plant physiology studies [30] - plant height, seed mass, leaf area, leaf carbon content, leaf nitrogen content, leaf phosphorus content, stem specific density, leaf lifespan, leaf respiration rate, and photosynthesis rate (**Table-1**). Scientific names of the species from this dataset were mapped to Wikidata as listed in the section 'Taxonomy mapping'. The retrieved data is archived publicly in file 'TRYdb_40340.txt.gz' in a Zenodo repository [95].

Table-1: List of traits used for retrieving data from TRY database

Trait identifier in TRY	Trait Name

1	Leaf area
3108	Leaf area (in case of compound leaves: leaf, petiole excluded)
3109	Leaf area (in case of compound leaves: leaflet, petiole excluded)
3110	Leaf area (in case of compound leaves: leaf, petiole included)
3111	Leaf area (in case of compound leaves: leaflet, petiole included)
3112	Leaf area (in case of compound leaves: leaf, undefined if petiole in- or excluded)
3113	Leaf area (in case of compound leaves: leaflet, undefined if petiole is in- or excluded)
3114	Leaf area (in case of compound leaves undefined if leaf or leaflet, undefined if petiole is in- or excluded)
11	Leaf area per leaf dry mass (specific leaf area, SLA or 1/LMA)
3115	Leaf area per leaf dry mass (specific leaf area, SLA or 1/LMA): petiole excluded
3116	Leaf area per leaf dry mass (specific leaf area, SLA or 1/LMA): petiole included
3117	Leaf area per leaf dry mass (specific leaf area, SLA or 1/LMA): undefined if petiole is in- or excluded)
3085	Leaf area per leaf dry mass (specific leaf area, SLA or 1/LMA) of leaf lamina
3086	Leaf area per leaf dry mass (specific leaf area, SLA or 1/LMA) petiole, rhachis, and midrib excluded
3106	Plant height vegetative
3107	Plant height generative
26	Seed dry mass
3660	Seed fresh mass
3836	Seed mass per fruit
4	Stem specific density (SSD, stem dry mass per stem fresh volume) or wood density
3452	Stem specific density (SSD, stem dry mass per stem fresh volume) or wood density: heartwood
3764	Stem specific density (SSD, stem dry mass per stem fresh volume) or wood density: stem
13	Leaf carbon (C) content per leaf dry mass
14	Leaf nitrogen (N) content per leaf dry mass
15	Leaf phosphorus (P) content per leaf dry mass

12	Leaf lifespan (longevity)
663	Leaf respiration rate in light per dry mass
512	Leaf respiration rate in light per leaf area
664	Leaf respiration rate in light per leaf respiration rate in the dark
2943	Leaf respiration rate in the dark as a fraction of photosynthetic carboxylation capacity (Vcmax)
665	Leaf respiration rate in the dark minus respiration in light, mass based
54	Leaf respiration rate in the dark per leaf area
41	Leaf respiration rate in the dark per leaf dry mass
500	Leaf respiration rate in the dark per leaf nitrogen (N) content
272	Leaf respiration rate in the dark temperature dependence
53	Photosynthesis rate per leaf area
974	Photosynthesis rate per leaf area: transition to TPU limited photosynthesis
40	Photosynthesis rate per leaf dry mass
135	Photosynthesis rate per leaf nitrogen (N) content (photosynthetic nitrogen use efficiency, PNUE)
134	Photosynthesis rate per leaf transpiration (photosynthetic water use efficiency: WUE)
3128	Photosynthesis rate per stomatal conductance

Abbreviations - SLA: Specific Leaf Area; LMA: Leaf dry Mass per Area; SSD: Stem Specific Density; TPU: Triose Phosphate Utilisation; PNUE: Photosynthetic Nitrogen Use Efficiency; WUE: Water Use Efficiency

Data retrieval from GloBI

The compressed stable release of interaction data was downloaded from the Zenodo archive of GloBI, version 0.8 from January 2025 [96], representing ‘species interactions tabulated as pairwise interactions in a zipped tab-separated values format.’ (as described on the GloBI website [97]). The creators of GloBI mention that ‘included taxonomic names are not interpreted, but included as documented in their sources’. The

taxonomic identifiers and names were mapped to Wikidata as listed in the section 'Taxonomy mapping'. The data is available publicly in file 'verbatim-interactions.tsv.gz' at GloBI Zenodo repository [96].

Taxonomy mapping

GloBI collates interaction information from standardized data from numerous sources including online repositories and projects (e.g.: Encyclopedia of Life) as well as data entered by individual projects through GloBI's dataset-template [98]. The full list of data sources is available on its website [99]. The combination of these two approaches resulted in taxonomic identifiers from around 15 taxonomy databases (**Supplementary Table 1**) to be present in GloBI. The initial taxonomic mappings from these 15 resources as well as their scientific names to Wikidata identifiers were done using QLever's [100] SPARQL user interface (UI) for Wikidata [101]. SPARQL queries used for mapping are as follows:

a) Query [102] for mapping Wikidata identifiers to ones from 15 taxonomy databases (**Supplementary Table 1**).
b) Query [103] for retrieving Wikidata identifiers and their lineage.

The full queries are listed in **Supplementary data.**

The retrieved data is available publicly in 'wdTax' files at METRIN-KG Zenodo repository [104].

For the TRY database, the scientific names were directly matched to ones obtained from Wikidata, to obtain corresponding Wikidata identifiers.

Metadata mapping

GloBI provides limited mappings of life stages and body parts to Uber-Anatomy Ontology (UBERON) [105], Plant Ontology (PO) [106], Environment Ontology (ENVO) [107], Gene Ontology (GO; body parts only) [108], and Phenotype and Trait Ontology (PATO; body parts only) [109] for organisms involved in interactions (**Supplementary Table 2**). For biological sex, the names are provided in GloBI, but no specific mapping to existing ontologies.

With such limited mappings, it was crucial to map the raw text in metadata columns- body part, life stage, and biological sex. Such unmapped text was not single standardized terms, rather it contained compound expressions, abbreviations, counts, symbols, or multiple entities within a single field. For example, body part entries included values such as “2 guts”, “abdominal cavity”, “abo”, “abomasum/si”. Biological sex fields contained symbolic or aggregated values (e.g. “+”, “-”, “?”), numeric summaries (e.g. “10M,9F”, “11 males, 4 females, 2 juveniles”), or multilingual expressions (e.g. “11 machos | 9 hembras”). Life stage fields similarly contained compound or inconsistent representations, such as “adult; adult; egg”, “adult; larvae”, “0, I, II, III”, or mixed capitalization and punctuation.

As part of the metadata mapping process, such entries were first parsed using delimiters and normalization rules to separate them into individual candidate terms, which were then mapped independently to ontology entities.

To semantically match candidate terms with ontology concepts, we developed a script using ontology parsing and sentence embeddings. The code including the parsing and semantic matching [110] is publicly available at the METRIN-KG github repository. We utilized the Python Owlready2 library version-0.47 [111] to load a suite of biomedical and environmental ontologies, namely the ones originally present in GloBI, as well as others from their Persistent Uniform Resource Locators (PURL) (see **Supplementary Table 2**). For life stages and body parts, the full suite was considered, whereas for biological sex, only UBERON [105] and PATO [109] were considered.

From each ontology, we extracted class labels and associated synonyms (including exact, broad, and related synonyms where available) as candidate terms for matching. Synonyms were collected from Web Ontology Language (OWL) annotation properties such as `hasExactSynonym`, `hasBroadSynonym`, and `hasRelatedSynonym`. Each candidate term was paired with its primary label and class Internationalized Resource Identifier (IRI) for traceability.

To compute semantic similarity, we used the pre-trained `all-MiniLM-L6-v2` model from Python SentenceTransformers library version-3.3.1 [112]. This model is a lightweight transformer trained to generate 384-dimensional dense vector embeddings that reflect the semantic content of short text spans. It is particularly suited for tasks such as semantic textual similarity and clustering.

All ontology terms (labels and synonyms) were encoded into dense vector representations using this model. Similarly, each user-provided input term for unmapped life stages, body parts, and biological sex was independently embedded into the same vector space. Term embeddings were computed using the model's `encode()` method with `convert_to_tensor=True`, which produced PyTorch-compatible tensors suitable for high-performance vector operations.

Cosine similarity was computed between each input term vector and all ontology term vectors using the `util.pytorch_cos_sim` function in SentenceTransformers. For each input term, the ontology term with the highest cosine similarity score was identified as the top candidate match. Cosine similarity is a common metric for comparing the orientation, rather than magnitude of two vectors. Given two vectors A and B, cosine similarity is defined as:

$$\text{cosine_similarity}(A,B)=A.B \,/\, |A|.|B|$$

Values range from -1 to 1, where 1 indicates identical direction (i.e., maximum similarity) and 0 indicates orthogonality (no similarity). For each input term, we computed its similarity against all ontology terms. The term with the highest similarity score was selected as the top candidate match. While all terms receive a candidate match, only matches with a similarity score ≥ 0.7 were flagged for manual review. This threshold ensures that low-confidence suggestions are carefully examined, while very low-similarity terms are treated as unmatched.

All results were output to a comma-separated values (CSV) file, including the input term, matched ontology label, its primary label, the ontology class IRI, and the similarity score.

While the automated process provided high-quality initial suggestions, all matches were manually reviewed and corrected to ensure semantic appropriateness. Corrections were informed by domain-specific knowledge and contextual relevance, particularly in cases where terms had multiple meanings or where high similarity scores did not guarantee ontological alignment. This two-stage process, automated semantic matching followed by manual curation, ensured both scalability and accuracy in aligning non-standardized input terms with controlled ontology concepts.

The above workflow was also run for matching the units of measure for trait data from TRY to the units vocabulary [113] provided by Quantities, Units, Dimensions, and Types (QUDT 2.1 schema) [114], followed by manual correction.

The mapped data is archived in the folders ‘globi’ and ‘trydb’ under processed data at METRIN-KG Zenodo repository [104].

EMI Ontology

EMI [73] is a global effort to profile the metabolic content of all currently known species on our planet. Here, knowledge representation plays a key role to correctly capture, contextualize, and structure the vast amount of chemical diversity data that have been and will be generated in the upcoming years. Consequently, this will facilitate data

(re)use and interoperability. To accurately represent the EMI knowledge, we explored several general-purpose and domain-specific ontologies to design a framework to describe chemical compounds (e.g., natural products) and their related data such as geolocation, provenance, organism sample metadata, and organism interactions. The EMI ontology reuses and repurposes, where applicable, several other ontologies beyond the life sciences such as World Wide Web Consortium's (W3C) [115] Sensor, Observation, Sample, and Actuator (SOSA) ontology [116], that was primarily designed for other applications including the Open Geospatial Consortium (OGC) use cases. OGC is a consortium that aims to improve access to geospatial and location information [117]. Furthermore, semantic reconciliation powered by biocuration is at the core of our proposed ontology. For example, by applying the EMI ontology version 1.0, we can accommodate and harmonize different organismal, chemical and material sample taxonomies as well as vocabularies such as the Relation Ontology (RO) [118] to define interactions between organisms (e.g., "has pathogen"). The other ontologies reused in EMI are those of Simple Knowledge Organization System (SKOS) [119], standard units of measures from QUDT [114], geo-locations from the basic geo (World Geodetic System 1984 (WGS84) lat/long) vocabulary [120], and natural product-specific concepts from the ENPKG ontology [121]. Moreover, in addition to making several existing ontologies interoperable for the EMI knowledge representation, we created more than 100 new concepts and relations that can be easily identified since they start with the https://w3id.org/emi# (*emi:*) prefix in the EMI ontology [88], for example, the term *emi:NonTrait*, a non trait structured value. All new and reused terms that constitute the

EMI ontology are documented and available online [88]. The code and a tutorial to build the metabolite-specific knowledge graph component of METRIN-KG with this ontology are available at the EMI Ontology GitHub repository [122]. **Figure-1** shows the EMI ontology schema.

Knowledge graph construction

Based on the EMI ontology as a data schema (**Figure-1**), we built a knowledge graph (KG) that semantically enriches, integrates, and interoperates 3 data sources - enriched metabolome datasets behind the ENPKG, trait data from TRY-db, and interaction data from GloBI. We developed the KG by combining subgraphs in two stages:

a) Ontop tool [90–92] was applied for developing the subgraph from enriched datasets (metabolite annotation, molecular networks, and taxonomical resolution results) originally used to build the ENPKG graph [123,124]. Ontop is a virtual knowledge graph system where SPARQL queries are translated into Structured Query Language (SQL) queries based on the predefined mappings. Ontop also provides means to materialize a KG according to these mappings. Therefore, to build the graph, one table for each tabular file was created in a relational database with a simplistic data schema. The files were loaded in this database through mysql version-8.2 [125]. Finally, to construct the KG, mappings were defined between the relational schema and the EMI ontology using the Ontop mapping language [90]. With these mappings [126], the EMI ontology [88], and

the relational database, the RDF triples were materialized with Ontop to compose the KG.

b) For developing the subgraphs from TRY database and GloBI, Python rdflib library version-7.0.0 [93,127] was used. To construct them, the tab-separated value (TSV) files obtained for each of these two resources were used. These tables were then connected through Wikidata identifiers (**Figure-2**) for taxonomy, whenever they were available as indicated in section 'Taxonomy mapping'. Mappings were defined between the relational schema and the EMI ontology using rdflib's inherent capability to map ontology elements.

   The process for incorporating mappings to metadata for GloBI (source/target taxonomy, life stage renamed to developmental stage, body part renamed to anatomical entity, and biological sex) and TRY database (taxonomy and trait's units of measure) was performed before generating the RDF triples.

   The code to develop the subgraphs is available at the METRIN-KG GitHub repository [128].

The RDF files can be downloaded at METRIN-KG Zenodo repository [104] in the folder 'KG' under processed data.

Indexing the knowledge graph and implementing the SPARQL end-point

We used Qlever [100], a SPARQL engine, to index our knowledge graph by implementing the steps described in qlever-control [129]. A SPARQL editor to query the indexed graph is available at [130]. This endpoint can also be accessed through https://kg.earthmetabolome.org/metrin/api [131] for programmatic purposes. An example for the programmatic access is provided on METRIN-KG's github wiki [132]. The underlying operational endpoint is currently available at [133]. The stable URL [130], functions as a long-term and stable identifier to safeguard accessibility should the operational endpoint be modified in the future. This interface includes several examples covering specific use-cases for the three datasets (ENPKG metabolites, TRY-db traits, and GloBI interactions). Some of these use-cases are presented as case studies in the section 'Data re-use and case studies'.

To provide the SPARQL editor user-interface for the indexed graph, we implemented qlever-ui [134,135] with few changes. To improve the user experience when navigating entities in the knowledge graph, we extended the qlever-ui interface to support fallback representations for non-available or missing web pages. This was achieved by incorporating SPARQL DESCRIBE queries into the frontend of the UI. The modified interface attempts to retrieve a minimal RDF-based summary of the requested entity when the original resource is not accessible (e.g., due to missing data in the knowledge graph). When such a condition is met, the interface automatically issues a SPARQL

DESCRIBE query for the corresponding IRI. The result is rendered in a simplified RDF triple view, providing context about the entity based on available data in the backend knowledge base. The implementation is available via a fork of the official qlever-ui GitHub repository here [136].

Data Description

Mapping of TRY data

The original structure of the TRY datasets is modelled as plant species mapping to trait and non-trait data as well as related metadata like information on studies from which the data was obtained, as shown in **Figure-3**. The column names depicted in the figure are taken directly from the CSV table retrieved from TRY, the description of which is provided in **Supplementary Table 3**. Columns retained in the knowledge graph are indicated in the table and the figure. Overall, 20,272,589 records for 70,748 unique plant species were retrieved in a TSV format. (**Supplementary Table 4**).

The dataset was refined to a minimal form by removing columns that contained redundant or ambiguous information. For example, author first and last names were excluded, as this information is already available in the retained ‘Reference’ field. Likewise, the ‘OriginalName’ column duplicated data present in ‘DataName’ and was therefore omitted. ‘Replicates’ is also an entity mentioned in ‘DataName’ and therefore not retained. The TRY database includes standardized values for certain traits in the

columns ‘ErrorRisk’, ‘StdValue’, ‘StdValueStr’, ‘OrigUncertainityStr’, ‘UncertaintyName’, ‘ValueKindName’, and ‘RelUncertainityPercent’. However, these were excluded due to their limited coverage across the dataset. This selective retention helped minimize redundancy and ensured consistency within the constructed knowledge graph. The metrics of the dataset following this refinement are as follows:

A) 65,675 unique species names (‘AccSpeciesName’; see **Supplementary Table 4**) out of 70,748 from TRY database were mapped to Wikidata (see section Taxonomy mapping).
B) Overall 1,826,445 traits & 17,212,303 non-trait (e.g.: number of replicates, latitude, longitude) records, data values, and corresponding units (**Supplementary Table 4**) were retained after mapping 65,672 species to Wikidata identifiers.

Query to retrieve metrics is described in [137].

Mapping of GloBI data

The original structure and column descriptions of the GloBI data are described in **Figure-4** and **Supplementary Table 5**. The column descriptions are also provided on the github account of GloBI as depicted on its website [138]. Columns retained in the knowledge graph are indicated in the table and the figure. Lineage information was not retained, as it can be retrieved via federated queries through Wikidata. Physiological stage data was omitted due to the absence of reliable mappings to established ontologies or controlled vocabularies. The ‘eventDateTime’ field was removed owing to

ambiguity - specifically, it was not clear whether it referred to the timing of the interaction event or the time of observation.

Overall, 20,480,925 records were obtained from 1,747,254 unique taxonomic identifiers and/or names (**Supplementary Table 4**), out of which 609,087 were mapped to 337,293 unique Wikidata identifiers. Overall, 12,872,681 GloBI records for only the mapped taxonomic identifiers were retained.

Query for the number of unique Wikidata identifiers and the number of records are provided in [139] and [140], respectively.

At the time of writing this manuscript, 1867 body part names were mapped to 996 ontology terms. 621 life stage names were mapped to 227 ontology terms. 57 biological sex names were mapped to 10 ontology terms.

Bias

Biases in the mapped GloBI data in our knowledge graph reflect those documented for GloBI, including taxonomic and geographic skews, which are extensively discussed in the GloBI literature [76].

Metabolite coverage is primarily derived from two sources: (i) untargeted metabolomics data from approximately 1,600 plant extracts from the Pierre Fabre collection, as described in the ENPKG paper [69], and (ii) compound–taxon associations curated via Wikidata/LOTUS, which are also known to be biased toward well-studied taxa and compounds [68].

Data re-use and case studies

Potential re-use and expansion of data

The current state of the knowledge graph provides a solid foundation. Its utility can be significantly enhanced by incorporating additional data sources and refining its structure.

a) Data re-use for studies in life sciences research

Researchers can query METRIN-KG to identify potential relationships between plant traits, interactions, and the presence or bioactivity of specific natural products. For example, one could query for plants with specific traits known to be associated with defense mechanisms and then explore the natural products they produce. The integrated data can be used to build predictive models for natural product occurrence or bioactivity based on plant traits and ecological context. This information can help prioritize plant species or natural product classes with a higher likelihood of possessing desired bioactivities. In addition, by analyzing trait-interaction-metabolome associations, researchers can prioritize plant species or ecological contexts that are more likely to yield novel or interesting natural products. Investigating such ecological roles of natural products can provide clues about their potential mechanisms of action and possible drug targets.

METRIN-KG can also facilitate the investigation of how natural products mediate species interactions. For instance, one could explore how specific compounds are associated with pollination or defense against herbivores in plants with particular traits. The understanding of the evolutionary pressures that shape the diversity of natural products can be investigated by linking them with the respective host traits and interactions.

In the context of potential data re-use for studies in life sciences research, we aimed to retrieve data from METRIN-KG on a few known questions in plant ecology, agriculture, and biodiversity. **Table-2** lists the questions and the respective links to the SPARQL queries.

Table-2: Examples of SPARQL queries for METRIN-KG and links to queries

Query	Title	Subject	Direct link to queries	Snapshot github commit link to queries
1 (CS1)	List interactions of all species which have an IUCN status of near threatened.	Conservation science	https://kg.earthmetabolome.org/metrin/11 [141]	https://kg.earthmetabolome.org/metrin/11/v/53581b1 [142]
2 (CS1)	List traits of all species which have an IUCN status of near-threatened.	Conservation science	https://kg.earthmetabolome.org/metrin/12 [143]	https://kg.earthmetabolome.org/metrin/12/v/53581b1 [144]
3 (CS1)	List all metabolites produced by species with near-threatened IUCN status and with values available (or greater than a specific value) for trait 'Seed dry mass'.	Conservation science	https://kg.earthmetabolome.org/metrin/13 [145]	https://kg.earthmetabolome.org/metrin/13/v/53581b1 [146]
4 (CS2)	List traits (and their values) of plants producing Diterpenoids	Functional ecology	https://kg.earthmetabolome.org/metrin/14 [147]	https://kg.earthmetabolome.org/metrin/14/v/53581b1 [148]
5 (CS3)	Natural producers (and their interactions that might be useful in agriculture) of onopordopicrin (wd:Q27107580), which might exhibit antimicrobial and	Human health	https://kg.earthmetabolome.org/metrin/20 [149]	https://kg.earthmetabolome.org/metrin/20/v/53581b1 [150]

	cytotoxic activities, especially against human-derived macrophages and against epidermoid carcinoma cells.			
6 (CS4)	List links between host-parasite and host-allelopathic interactions, where host is an agricultural crop, allelopath is usually a plant that inhibits growth of parasites which are usually insects. Inhibition happens by root/stem/leaf exudates of the allelopath.	Sustainable agriculture	https://kg.earthmetabolome.org/metrin/18 [151]	https://kg.earthmetabolome.org/metrin/18/v/53581b1 [152]
7 (CS5)	Retrieve data of 4 traits in leaf economics spectrum	Theoretical ecology	https://kg.earthmetabolome.org/metrin/22 [153]	https://kg.earthmetabolome.org/metrin/22/v/53581b1 [154]
8 (CS5)	Retrieve metabolites of organisms with data available from 4 traits in leaf economics spectrum	Theoretical ecology	https://kg.earthmetabolome.org/metrin/23 [155]	https://kg.earthmetabolome.org/metrin/23/v/53581b1 [156]
9	List of possible natural locations of plants, which produce senkyunolide which is a thalide for cerebral disorders	Human health	https://kg.earthmetabolome.org/metrin/16 [157]	https://kg.earthmetabolome.org/metrin/16/v/53581b1 [158]
10	List metabolites of plants that interact with plant parasite moth Orgyia postica	Functional ecology	https://kg.earthmetabolome.org/metrin/17 [159]	https://kg.earthmetabolome.org/metrin/17/v/53581b1 [160]
11	A list of interactions depicting connections between parasitoids harmful for insects living as parasites on plants.	Functional ecology	https://kg.earthmetabolome.org/metrin/19 [161]	https://kg.earthmetabolome.org/metrin/19/v/53581b1 [162]
12	List possible interactions of plants that can produce Norhyocyamine, a plant secondary metabolite	Functional ecology	https://kg.earthmetabolome.org/metrin/21 [163]	https://kg.earthmetabolome.org/metrin/21/v/53581b1 [164]

Abbreviations - CS: Case Study; IUCN: International Union for Conservation of Nature

b) User-friendly approach to add queries as examples within METRIN-KG

We devised a method for the users of METRIN-KG to propose a query and incorporate it within the examples (e.g. queries listed in **Table-2**) using the SPARQL query-editor

proposed in [165,166]. Once a user proposes a query on EMI's sparql-examples GitHub repository's issues section, it will allow us to review it for inclusion in the examples. Once the review and corrections are complete, the query will be available on the SPARQL query endpoint [130]. While the examples listed in **Table-2** provide several complex queries, this option allows the users to provide context-specific queries useful for building research questions.

A tutorial for contributing queries to METRIN-KG is provided on its GitHub repository wiki [167].

c) Adding data or federating over knowledge graphs presenting datasets from other publicly available resources

Incorporating environmental data (e.g., climate data and soil data) could allow for the analysis of how environmental factors influence traits, interactions, and natural product production and distribution. Including data on the timing of biological events (e.g., flowering times) could add a temporal dimension to the analysis of interactions and natural product occurrence. In addition, incorporating image data (e.g., plant morphology) and spectral data (e.g., metabolomic profiles) could provide richer characterizations of the entities within the knowledge graph. Integrating broader ecological context, such as community composition and ecosystem dynamics, could provide a more holistic understanding of the relationships. Where ethically and legally appropriate, incorporating curated traditional knowledge related to plant uses and natural products could add valuable perspectives. Moreover, including data from other

natural product databases (e.g.: PubChem [70], ChEMBL [71,168]) could broaden the coverage of chemical compounds and their properties.

d) Enhancing ontological structure and semantics:

For developing more granular relationship types, moving beyond simple pairwise interactions to include more specific relationship types (e.g., pollination, herbivory, symbiosis) with associated properties (e.g., strength, specificity) could be useful. The first efforts in this direction are taken by GloBI [76] and BiotXplorer [77]. However, they are limited to pairwise interactions and not connected to other types of data, which our knowledge graph provides. A useful step in this direction could be to implement semantic reasoning, hence inferring new relationships and knowledge that are not explicitly stated in the data.

e) Democratizing METRIN-KG access: querying in natural language

In order to make available the knowledge in the METRIN-KG for non-SPARQL savvy users, we applied ExpasyGPT [169], a Large Language Model (LLM)-driven tool based on lightweight metadata that allows for querying knowledge graphs in natural language. This tool facilitates querying METRIN-KG as well as various other life-science databases in plain English. In other words, ExpasyGPT aids in constructing SPARQL queries in response to user's text-format questions. Therefore, the final response is not given by the LLM but by querying METRIN-KG, which contains curated and high quality data, mitigating well-known LLM issues such as hallucinations, lack of domain specific

knowledge and black-box behaviour. Consequently, this makes answers verifiable and reproducible. More precisely, ExpasyGPT implements a context-optimization approach that relies on two main sources of metadata: (i) pairs of question-query examples and (ii) automatically generated description of used classes and predicates. Both (i) and (ii) should be defined using well-known W3C vocabularies such as Vocabulary of Interlinked Datasets (VoID) and Shapes Constraint Language (SHACL), accessible through the SPARQL endpoint. Applying ExpasyGPT is straightforward thanks to the fact that the metadata already exists as described in **Table 2** and is automatically done. A tutorial of how to use ExpasyGPT is provided on METRIN-KG GitHub repository wiki [170].

Case studies

Out of the 12 examples listed in **Table-2**, we built 5 case study (CS) summaries for 8 as listed below.

CS1: List traits, interactions, and metabolites of all species which have an International Union for Conservation of Nature (IUCN) status of near threatened.

Subject - Conservation science

The queries are described in [141], [143], [145] (**Table 2**)

Some studies have addressed the need to identify the threat status of plants by studying their functional traits [171–173]. Moreover, one study has suggested

approaches for conservation of threatened plant species using functional trait patterns [174]. Some other studies have used predictive modelling to enhance knowledge of interacting species pairs (e.g.: predator-prey interactions) [175,176] in the context of their habitat and traits. In addition, some researchers have suggested and reviewed ecological restoration strategies for threatened ecosystems based on functional traits and plant-animal interactions [177–179].

Keeping such broad studies in mind, we developed 3 SPARQL queries retrieving the traits, interactions, and metabolites of plant species with IUCN status of near threatened. Such queries would aid the researchers in collecting data relevant to near threatened plant species (in some cases, insects) and develop strategies to model patterns specific to climate change, thereby developing ecological restoration plans.

Basic metrics obtained from the results of the queries are provided in **Table 3**. The results obtained from the three queries contain 9,299 unique species with highly heterogeneous data coverage. While interaction data were available for the majority of species (8,598), trait measurements were substantially sparser (1,051 species, 19,279 measurements across 98 traits), and metabolite data were limited to only 47 species (818 unique InChIKeys and 1,000 records). 37 species possessed all three data types.

While these 3 queries can be combined into one, we kept them separate to improve efficiency and retain modularity.

Table-3: Metrics for CS1

Metric	**Value**

Total unique species (all data)	9299
Unique species with trait data	1051
Unique species with metabolite data	47
Unique species with interaction data	8598
Unique species with traits and metabolites	47
Unique species with all three data types	37
Total unique traits	98
Total unique metabolites (InChIKeys)	818
Total unique interaction types	24
Total trait measurements	19279
Total metabolite records	1000
Total interaction records	12396

CS2: List traits and their values for plants producing diterpenoids

Subject - Functional ecology

The query is described in [147] (**Table 2**).

Recent studies have utilized trait data to understand the implications of diterpenoids producing invasive plant species and their allelopathic relationships with agricultural crops [180–185]. In the context of agriculture, there have been reviews of plant traits and their effects on insect herbivory [186], crop resilience (e.g.: rice) of plants producing diterpenoids [187–189], and the implications of drought stress on diterpenoid producing plants and their traits [190]. In the context of biodiversity conservation, there have been studies on plant traits and their metabolic profile [191]. In addition, there has been

research on plant interactions with microbial communities of plants where leaf surface has been reported to contain diterpenoids (tobacco and phyllosphere) [192].

Considering such diverse research on diterpenoids-producing plants or where diterpenoids are known to be extracted from plant surfaces, we developed a simple query to list traits of plants which have been known to produce or harbor diterpenoids.

Figure-5 provides the trait coverage of top 30 species selected based on measurement frequency from the results. **Supplementary Tables 6** and **7** provide complete summaries of species and trait distributions. The dataset contains 98 traits measured across 2,131 species, with photosynthesis per leaf area being the most frequently measured trait (16,472 measurements) followed by leaf nitrogen content (14,841 measurements) and specific leaf area (14,698 measurements). *Pinus sylvestris* has the highest number of trait measurements (14,557 records), followed by *Qualea grandiflora* (5,260 records) and *Fagus sylvatica* (4,978 records).

CS3: Natural producers and their biotic interactions that might be useful in agriculture of onopordopicrin.

Subject - Human health

The query is described in [149] (**Table 2**).

Onopordopicrin is a metabolite produced by several plants like *Arctium lappa* and genus *Shangwua.* It has been shown to potentially exhibit antimicrobial and cytotoxic activities, especially against human-derived macrophages and against epidermoid carcinoma

cells [193]. There is less scientific evidence to support these claims and research in this area has only recently been enhanced [194–197], making onopordopicrin an appropriate and timely subject for prospective research studies in human health and pharmacology.

To specifically target the research in this area, we developed a query to retrieve the natural producers of onopordopicrin and their biotic interactions.

The results comprise of 98 diterpenoid-producing species connected through 101 biotic interactions. While we did not find *Arctium lappa* and genus *Shangwua* in the results, *Eriophyllum confertiflorum*, emerges as a hub species with 77 incoming connections, that interacts with numerous other organisms (**Figure-6**). The network shows a highly skewed degree distribution where a small number of plant species (like *Centaurea melitensis* with 14 connections) dominate interactions, while the majority of species participate in only one or two interactions each.

CS4: Allelopathy interactions in push-pull agriculture

Subject - Sustainable agriculture

The query is described in [151] (**Table 2**).

Studies on allelopathy have advanced our knowledge of plant interactions with other organisms, particularly in agriculture [198–200] and invasion ecology [180]. For instance, species of genera *Desmodium*, through their root and stem exudates, may protect crops of maize (*Zea mays*) and sorghum (*Sorghum*) against attack from

stemborer arthropods and weed *Striga hermonthica* [201,202]. Besides focussed research [203], there are few studies exploring the allelopathic properties and the plant metabolites responsible for them.

We developed a query to target such interactions and the metabolites produced by the protective allelopathic plants.

In the original GloBI dataset, several fungal genera (e.g., *Fusarium*, *Puccinia*, *Claviceps, Sclerotinia sclerotiorum*) were misidentified as allelopath, likely resulting from automated inverse relationship generation where Plant 'hasPathogen' Fungus was inverted to Fungus 'allelopathOf' Plant. In the result obtained for CS4, we removed 55 interactions (45% of the original dataset) where fungi were incorrectly classified as allelopaths, as these organisms represent direct pathogenic relationships rather than plant-mediated chemical interference. After applying this filter, the results show 67 tripartite interactions involving 46 parasites, 11 allelopathic plants, and 10 crops (**Figure-7, Supplementary Table 8**).

CS5: Retrieve traits and metabolites for organisms for which traits from Leaf Economic Spectrum (LES) are available

Subject - Theoretical ecology

Queries are described in [153] and [155] (**Table 2**).

Leaf Economic Spectrum is a foundational concept in plant ecology, describing coordinated variation in leaf traits across species, typically forming a trade-off between

resource-acquisitive and resource-conservative strategies [81,204]. Resource-acquisitive species have traits like high specific leaf area (SLA), high nitrogen content, short leaf lifespan, which are optimized for rapid growth in resource-rich environments. Resource-conservative species show traits like low SLA, low nutrient content, long leaf lifespan, which are better suited for resource-poor environments with conservative growth. These relationships are global, cross-taxonomic, and continuous. They help predict ecosystem functions, species distributions, and responses to environmental changes.

We developed a query to retrieve values for four traits (including their sub-categories totalling to six) relevant for LES - specific leaf area, leaf dry matter content, leaf nitrogen content, and lead phosphorus content. Further, we developed another query to retrieve metabolites produced by species with data for four LES traits available in the knowledge graph. While we were unable to identify plant species with both metabolite data and complete trait coverage across all four categories, this limitation itself reinforces the value of our knowledge graph approach and the importance of continued data integration efforts.

Table-4 depicts LES trait data from 1,058 plant species with metabolite profiles from 627 species, identifying 49 species (with incomplete trait coverage) with both datasets available for comparative analysis. The data encompassed 6 key functional traits across 2,324 measurements and 11,313 unique metabolites across 16,587 associations.

Table-4: Metrics for CS4

Metric	**Value**
Unique species with traits	1058

Unique traits	6
Unique species with metabolites	627
Unique metabolites	11313
Unique species with both traits and metabolites	49
Total trait records	2324
Total metabolite records	16587

At the time of writing this manuscript, the results of our queries reflect the state of METRIN-KG and the federated sources available. As these underlying datasets are continuously updated and expanded, the query outputs presented here may evolve over time. All scripts used to generate the tables and figures for case studies are available at METRIN-KG GitHub repository [128].

Conclusions

We provide METRIN-KG aiming to integrate seemingly disconnected databases of plant metabolomes, plant traits, and interactions. To facilitate exploration of this resource, we provide a way to search for those connections through a user interface. We aspire to draw the attention of researchers in areas of drug-discovery, ecology, human health, biodiversity conservation, and agriculture to the power of knowledge graphs in integrating life-sciences datasets. We wish to increase awareness amongst researchers to include as varied data as possible, so as to approach research questions from

multiple perspectives. In this context, we provide representative case studies to retrieve data for different research projects. We plan to extend METRIN-KG to incorporate the full breadth of metabolome data from plants in the near future. In the distant long-term, we plan to extend it, adding more information on metabolite data for other kingdoms beyond Plantae, while updating the trait and interaction data from TRY and GloBI, respectively, as new versions are released. We hope that our efforts will encourage other researchers to use and contribute to this resource.

Availability of source code and requirements

a) METRIN-KG

Project name: metrin-kg

Project homepage: https://github.com/earth-metabolome-initiative/metrin-kg

License: GPL-3.0 license

Operating system(s): Ubuntu 24.04.2 LTS

Programming language: Python

Hardware requirements: 32 GB RAM, 500 GB disk-capacity

RRID: SCR_027914

biotools: metrin_kg

METRIN-KG's code is also available through Zenodo [205].

b) Earth Metabolome Initiative Ontology

Project name: Earth Metabolome Initiative Ontology, illustrated with an example of knowledge-graph construction

Project homepage: https://github.com/earth-metabolome-initiative/earth_metabolome_ontology

License: Software code under GPL-3.0 license, Ontology under CC0-1.0 license

Operating system(s): modern Linux/Windows/Unix distribution (64-bit OS)

Programming language: OWL, Python

Hardware requirements: any x86_64 or ARM64 CPU with at least 2 cores, and a minimum of 8 GB RAM and 60 GB disk are recommended for functional setups

RRID: SCR_027915

biotools: earth_metabolome_initiative_ontology

Data availability

All input and output files used in mapping taxonomy, metadata, ontology, and knowledge graph construction as well as RDF files are available on EMI's Zenodo repository for METRIN-KG (CC0-1.0) [104] and TRY (CC-BY-4.0) [95] .

Abbreviations

AO: Agronomy Ontology; APO: Ascomycete Phenotype Ontology; BRENDA: Braunschweig Enzyme Database; BSPO: Biological Spatial Ontology; BTO: BRENDA Tissue Ontology; CEPH: Cephalopod Ontology; ChEBI: Chemical Entities of Biological Interest; CL: Cell Ontology; CLAO: Collembola Anatomy Ontology; CS: Case Study; CSV: Comma-Separated Values; DBGI: Digital Botanical Gardens Initiative; DDANAT: Dictyostelium Discoideum Anatomy; ECOCORE: Ecology Core Ontology; EFO: Experimental Factor Ontology; EMI: Earth Metabolome Initiative; ENPKG: Experimental Natural Products Knowledge Graph; ENVO: Environment Ontology; FAIR: Findable, Accessible, Interoperable, and Reusable; FAO: Fungal Anatomy Ontology; FLOPO: Flora Phenotype Ontology; FMA: Foundational Model of Anatomy; FOODON: Food Ontology; GallOnt: ontology for plant gall phenotypes; GloBI: Global Biotic Interactions; GO: Gene Ontology; HAO: Hymenoptera Anatomy Ontology; IDO: Infectious Disease Ontology; IDOMAL: Infectious Disease Ontology for Malaria; IRI: Internationalized Resource Identifier; IUCN: International Union for Conservation of Nature; KG: Knowledge Graph; LES: Leaf Economic Spectrum; LMA: Leaf dry mass per area; LOTUS: *not an acronym*; METRIN-KG: MEtabolomes, TRaits, and INteractions-Knowledge Graph; NCIT: National Cancer Institute Thesaurus; OBI: Ontology for Biomedical Investigations; OGC: Open Geospatial Consortium; OMIT: Ontology for MIcroRNA Target Prediction; OWL: Web Ontology Language; PATO: Phenotype and Trait Ontology; PHIPO: Pathogen-Host Interaction Phenotype Ontology; PNUE: Photosynthetic Nitrogen Use Efficiency; PO: Plant Ontology; PORO: Porifera

Ontology; QUDT: Quantities, Units, Dimensions, and Types; RDF: Resource Description Framework; RO: Relation Ontology; SHACL: Shapes Constraint Language; SKOS: Simple Knowledge Organization System; SLA: Specific Leaf Area; SOSA: Sensor, Observation, Sample, and Actuator; SPARQL: SPARQL Protocol and RDF Query Language; SSD: Stem Specific Density; SQL: Structured Query Language; TGMA: Mosquito gross anatomy ontology; TPU: Triose Phosphate Utilisation; TRY: *not an acronym*; TSV: Tab-Separated Values; UBERON: Uber-Anatomy Ontology; UI: User Interface; URL: Uniform Resource Locators; VoID: Vocabulary of Interlinked Datasets; W3C: World Wide Web Consortium; WGS84: World Geodetic System 1984; WUE: Water Use Efficiency

Competing Interests

The authors declare that they have no competing interests.

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Authors' Contributions

D.T., P.M.A., T.M.F., and E.D. conceptualized the study. D.T. and T.M.F curated the data, designed the methodology and developed the knowledge graph. T.M.F. designed and developed the Earth Metabolome Initiative Ontology with inputs from D.T. and P.M.A.. D.T. and T.M.F. prepared the visualization. D.T. and E.D. identified the example case-studies relevant to the knowledge graph. T.M.F and P.M.A. provided computing resources for the project. P.M.A, T.M.F., and E.D. acquired the funding for the project. D.T. and T.M.F. wrote the original draft. All authors reviewed and edited the manuscript.

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Figure titles and legends

Figure-1: **Snapshot of the data schema of the Earth Metabolome Initiative (EMI) ontology.** Classes are represented in round-edged rectangles. Entity relationships are represented by directional arrows.

Figure-2: Schema of relations between different entities of integrated datasets of metabolome, traits, and interactions. Entities mapped are represented in bold and the corresponding relationship is represented by directional arrows.

Figure-3: Original structure of traits dataset retrieved from TRY database. Purple-shaded rectangles represent columns retained for METRIN-KG. Gray-shaded rectangles represent columns not retained for METRIN-KG. Column relationships are represented by directional arrows.

Figure-4: Original structure of interactions dataset retrieved from GloBI. Purple-shaded rectangles represent columns retained for METRIN-KG. Gray-shaded rectangles represent columns not retained for METRIN-KG. Column relationships are represented by directional arrows.

Figure-5: CS2 - Trait coverage of top 30 species selected based on measurement frequency from the results. Blue shows measured traits for a species; white shows no trait measured.

Figure-6: CS3 - Interaction network for diterpenoid producing plant species. Node size and color represent connection count. Only top-20 species with the highest connection count are labelled.

Figure-7: CS4 - Sankey plot representing the flow of allelopathy interactions in push-pull agriculture. Parasites are shown in red, allelopathic plants in green, and protected crops in orange.

Supplementary Table titles and legends

Supplementary Table 1: List of taxonomy databases used in GloBI

Supplementary Table 2: List of ontologies used in METRIN-KG.

Supplementary Table 3: **Column descriptions of data retrieved from TRY database.** Column names and descriptions were retained from the files provided by TRY database managers

Supplementary Table 4: **Metrics for TRY database and GloBI.**

Supplementary Table 5: **Column descriptions of data retrieved from GloBI.** Column names and descriptions obtained from GloBI dataset template repository [158].

Supplementary Table 6: CS2 - Summary of species distributions.

Supplementary Table 7: CS2 - Summary of trait distributions.

Supplementary Table 8: Filtered data without fungi species for CS4.

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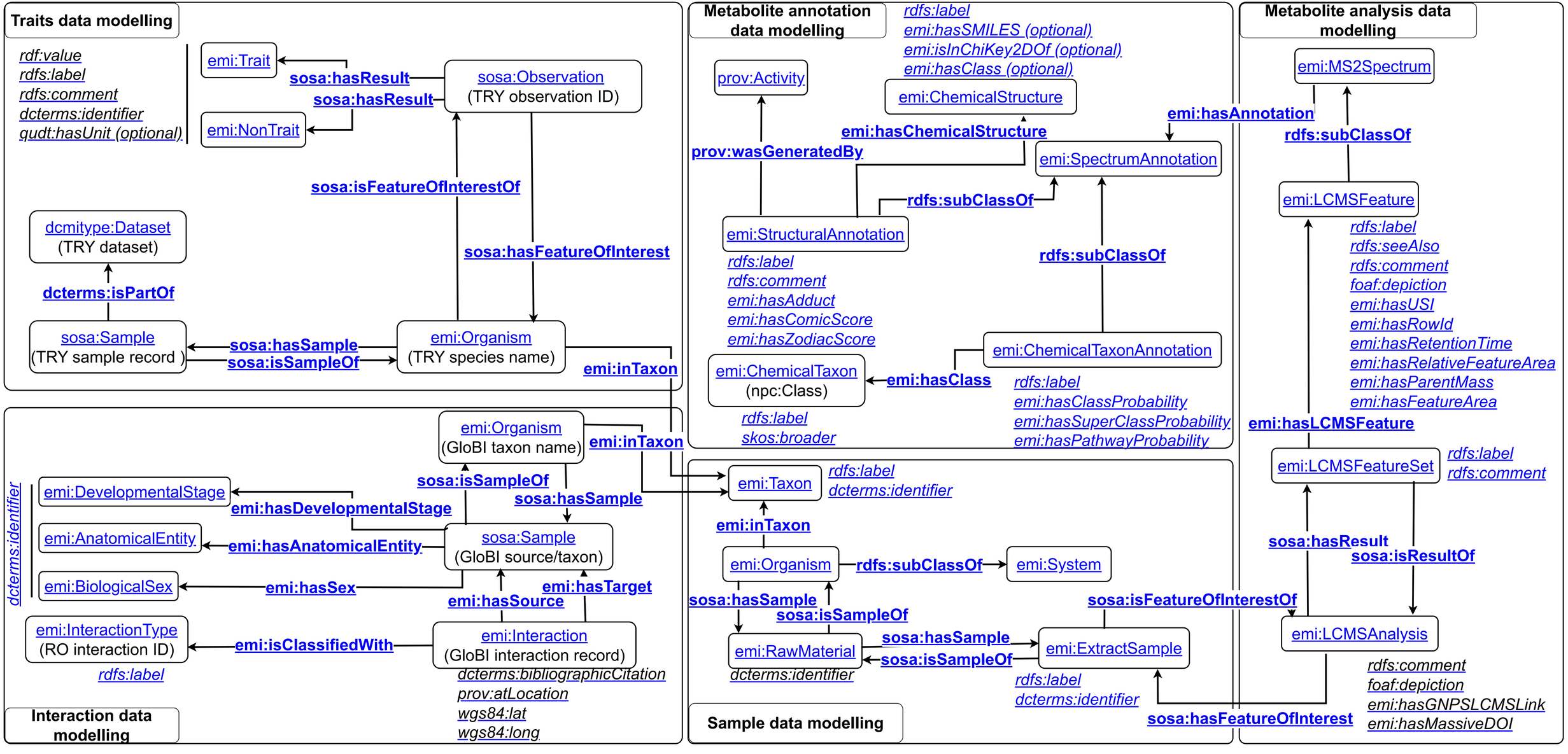
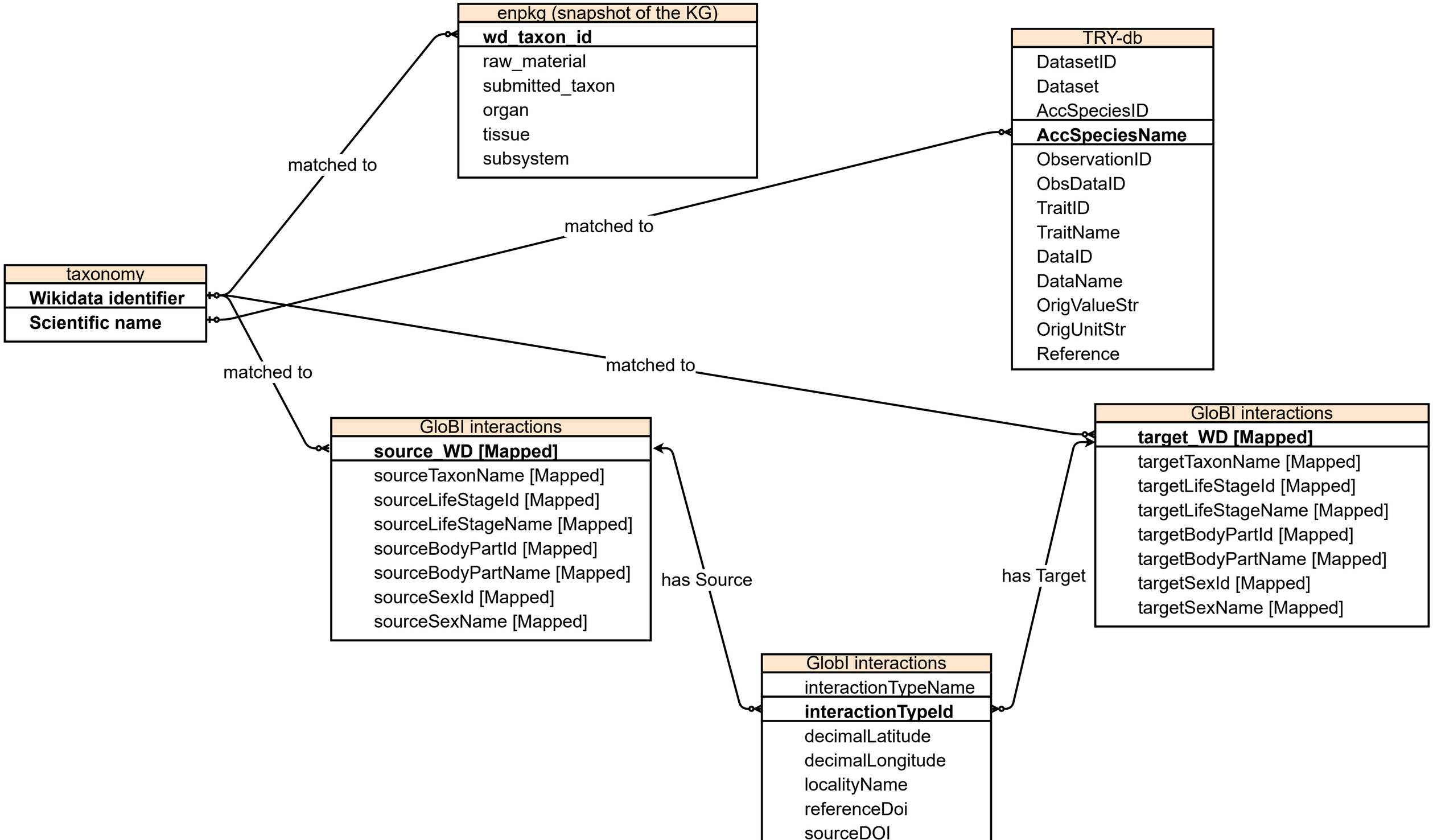

Traits data modelling
rdf:value
rdfs:label
rdfs:comment
dcterms:identifier
qudt:hasUnit (optional)
emi:Trait
emi:NonTrait
sosa:hasResult
sosa:hasResult
sosa:Observation
(TRY observation ID)
sosa:isFeatureOfInterestOf
sosa:hasFeatureOfInterest
dcmitype:Dataset
(TRY dataset)
dcterms:isPartOf
sosa:Sample
(TRY sample record)
sosa:hasSample
sosa:isSampleOf
emi:Organism
(TRY species name)
emi:inTaxon
Metabolite annotation data modelling
rdfs:label
emi:hasSMILES (optional)
emi:isInChiKey2DOf (optional)
emi:hasClass (optional)
prov:Activity
emi:ChemicalStructure
emi:hasChemicalStructure
emi:hasAnnotation
prov:wasGeneratedBy
emi:SpectrumAnnotation
rdfs:subClassOf
emi:StructuralAnnotation
rdfs:subClassOf
rdfs:label
rdfs:comment
emi:hasAdduct
emi:hasComicScore
emi:hasZodiacScore
emi:ChemicalTaxonAnnotation
emi:ChemicalTaxon
(npc:Class)
emi:hasClass
rdfs:label
emi:hasClassProbability
emi:hasSuperClassProbability
emi:hasPathwayProbability
rdfs:label
skos:broader
Metabolite analysis data modelling
emi:MS2Spectrum
rdfs:subClassOf
emi:LCMSFeature
rdfs:label
rdfs:seeAlso
rdfs:comment
foaf:depiction
emi:hasUSI
emi:hasRowId
emi:hasRetentionTime
emi:hasRelativeFeatureArea
emi:hasParentMass
emi:hasFeatureArea
emi:hasLCMSFeature
emi:LCMSFeatureSet
rdfs:label
rdfs:comment
sosa:hasResult
sosa:isResultOf
emi:LCMSAnalysis
rdfs:comment
foaf:depiction
emi:hasGNPSLCMSLink
emi:hasMassiveDOI
emi:Organism
(GloBI taxon name)
emi:inTaxon
sosa:isSampleOf
sosa:hasSample
dcterms:identifier
emi:DevelopmentalStage
emi:hasDevelopmentalStage
emi:AnatomicalEntity
emi:hasAnatomicalEntity
sosa:Sample
(GloBI source/taxon)
emi:BiologicalSex
emi:hasSex
emi:hasTarget
emi:hasSource
emi:InteractionType
(RO interaction ID)
emi:isClassifiedWith
emi:Interaction
(GloBI interaction record)
rdfs:label
dcterms:bibliographicCitation
prov:atLocation
wgs84:lat
wgs84:long
Interaction data modelling
emi:Taxon
rdfs:label
dcterms:identifier
emi:inTaxon
emi:Organism
rdfs:subClassOf
emi:System
sosa:hasSample
sosa:isSampleOf
sosa:isFeatureOfInterestOf
emi:RawMaterial
sosa:hasSample
sosa:isSampleOf
emi:ExtractSample
dcterms:identifier
rdfs:label
dcterms:identifier
sosa:hasFeatureOfInterest
Sample data modelling


enpkg (snapshot of the KG)
wd_taxon_id
raw_material
submitted_taxon
organ
tissue
subsystem
TRY-db
DatasetID
Dataset
AccSpeciesID
AccSpeciesName
ObservationID
ObsDataID
TraitID
TraitName
DataID
DataName
OrigValueStr
OrigUnitStr
Reference
taxonomy
Wikidata identifier
Scientific name
matched to
matched to
matched to
matched to
GloBI interactions
source_WD [Mapped]
sourceTaxonName [Mapped]
sourceLifeStageId [Mapped]
sourceLifeStageName [Mapped]
sourceBodyPartId [Mapped]
sourceBodyPartName [Mapped]
sourceSexId [Mapped]
sourceSexName [Mapped]
GloBI interactions
target_WD [Mapped]
targetTaxonName [Mapped]
targetLifeStageId [Mapped]
targetLifeStageName [Mapped]
targetBodyPartId [Mapped]
targetBodyPartName [Mapped]
targetSexId [Mapped]
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has Target
GloBI interactions
interactionTypeName
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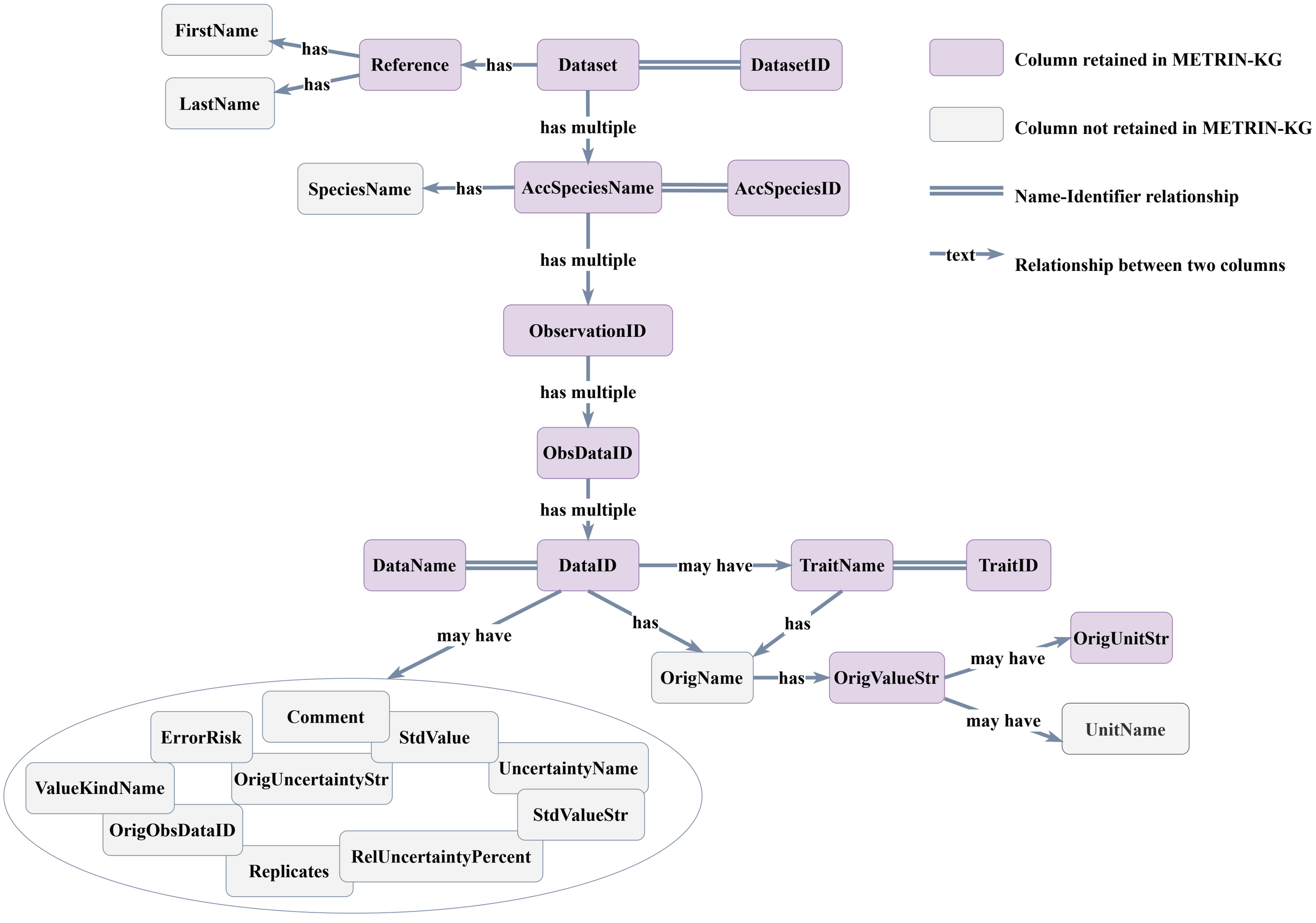
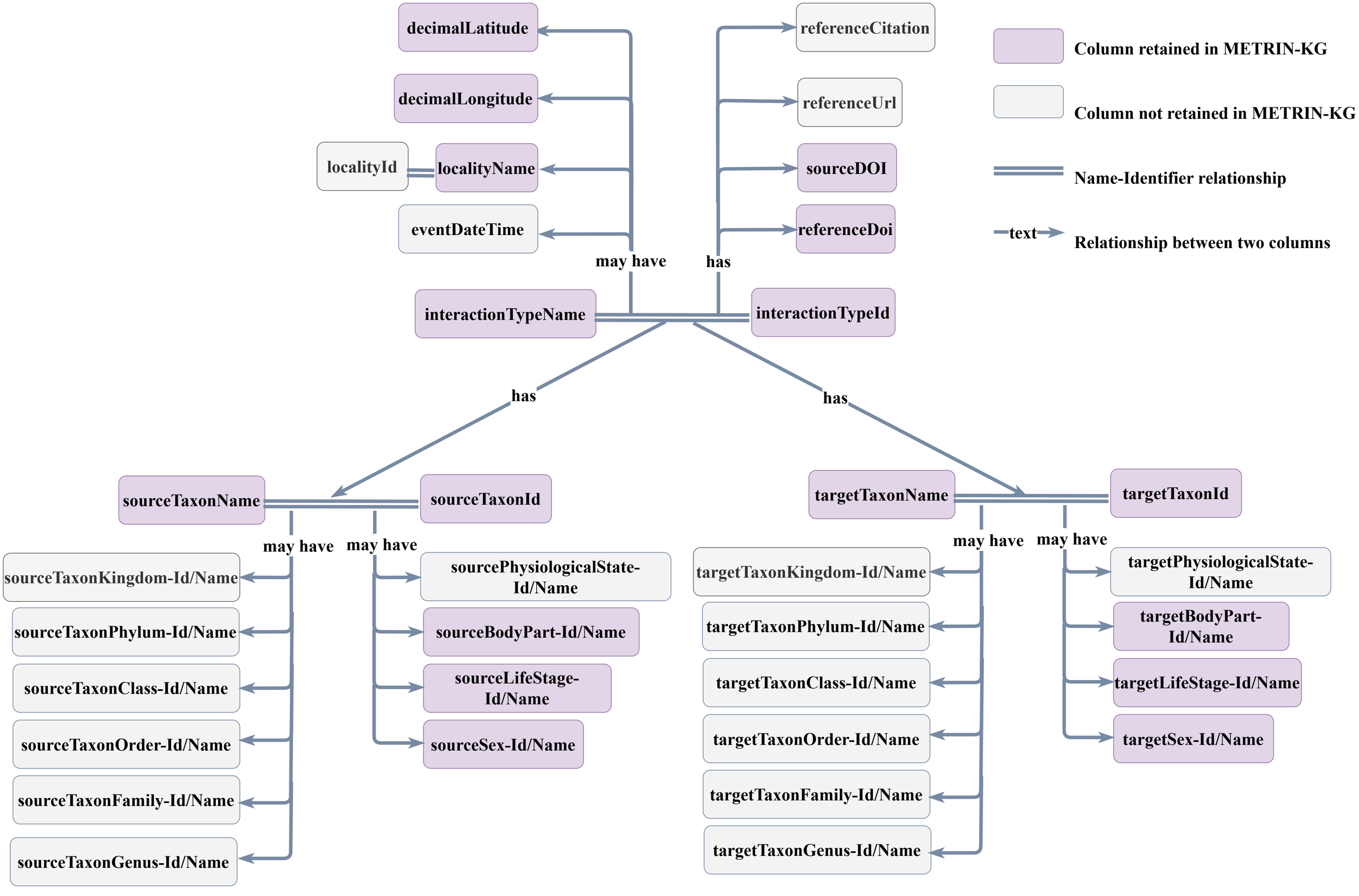
decimalLatitude
decimalLongitude
localityName
referenceDoi
sourceDOI


FirstName
has
Reference
has
Dataset
DatasetID
LastName
has
has multiple
SpeciesName
has
AccSpeciesName
AccSpeciesID
has multiple
ObservationID
has multiple
ObsDataID
has multiple
DataName
DataID
may have
TraitName
TraitID
may have
has
has
OrigUnitStr
OrigName
has
OrigValueStr
may have
may have
UnitName
Comment
ErrorRisk
StdValue
ValueKindName
OrigUncertaintyStr
UncertaintyName
StdValueStr
OrigObsDataID
RelUncertaintyPercent
Replicates
Column retained in METRIN-KG
Column not retained in METRIN-KG
Name-Identifier relationship
text
Relationship between two columns


decimalLatitude
decimalLongitude
localityId
localityName
eventDateTime
referenceCitation
referenceUrl
sourceDOI
referenceDoi
Column retained in METRIN-KG
Column not retained in METRIN-KG
Name-Identifier relationship
text
Relationship between two columns
may have
has
interactionTypeName
interactionTypeId
has
has
sourceTaxonName
sourceTaxonId
targetTaxonName
targetTaxonId
may have
may have
may have
may have
sourceTaxonKingdom-Id/Name
sourceTaxonPhylum-Id/Name
sourceTaxonClass-Id/Name
sourceTaxonOrder-Id/Name
sourceTaxonFamily-Id/Name
sourceTaxonGenus-Id/Name
sourcePhysiologicalState-Id/Name
sourceBodyPart-Id/Name
sourceLifeStage-Id/Name
sourceSex-Id/Name
targetTaxonKingdom-Id/Name
targetTaxonPhylum-Id/Name
targetTaxonClass-Id/Name
targetTaxonOrder-Id/Name
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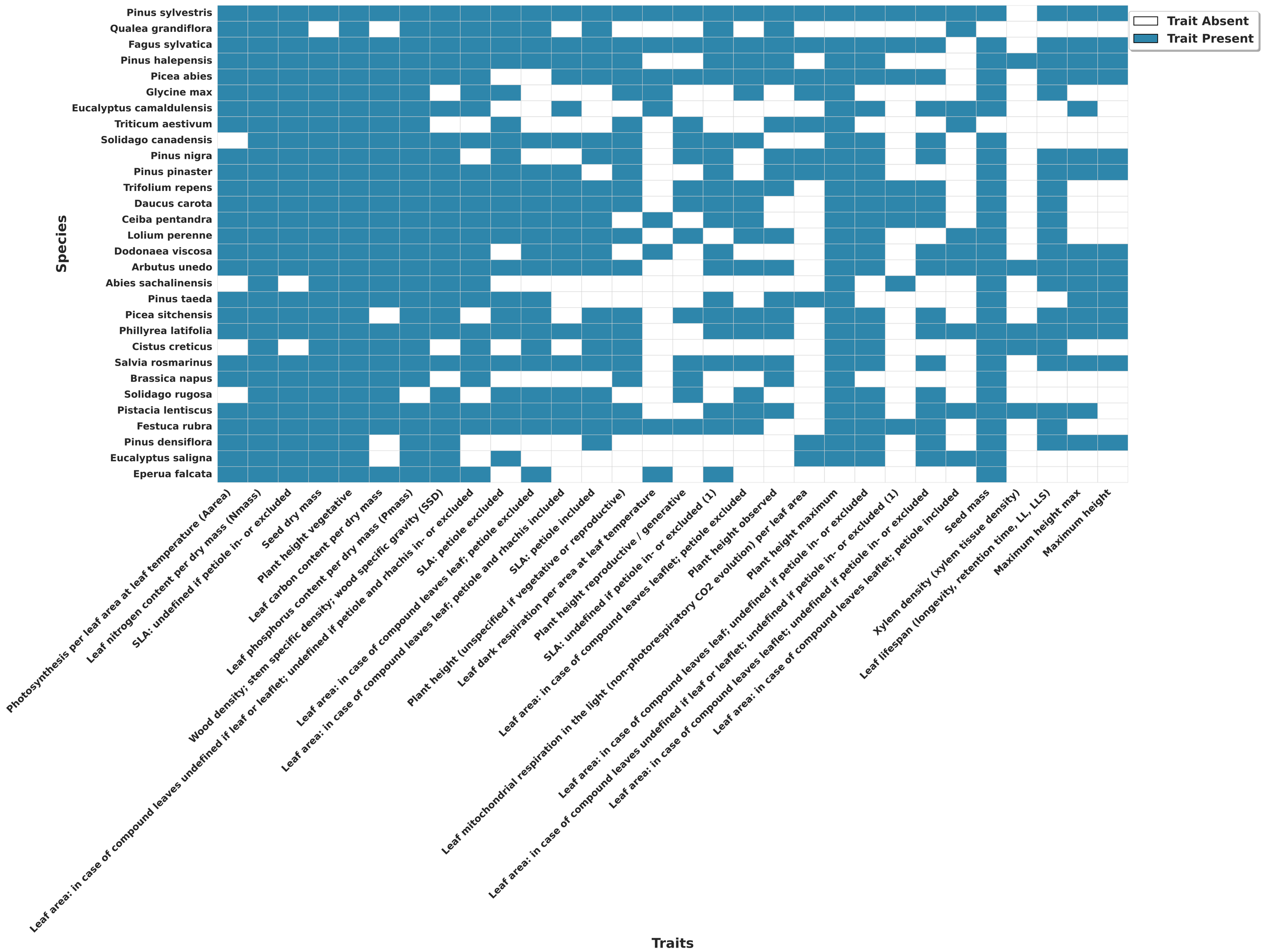
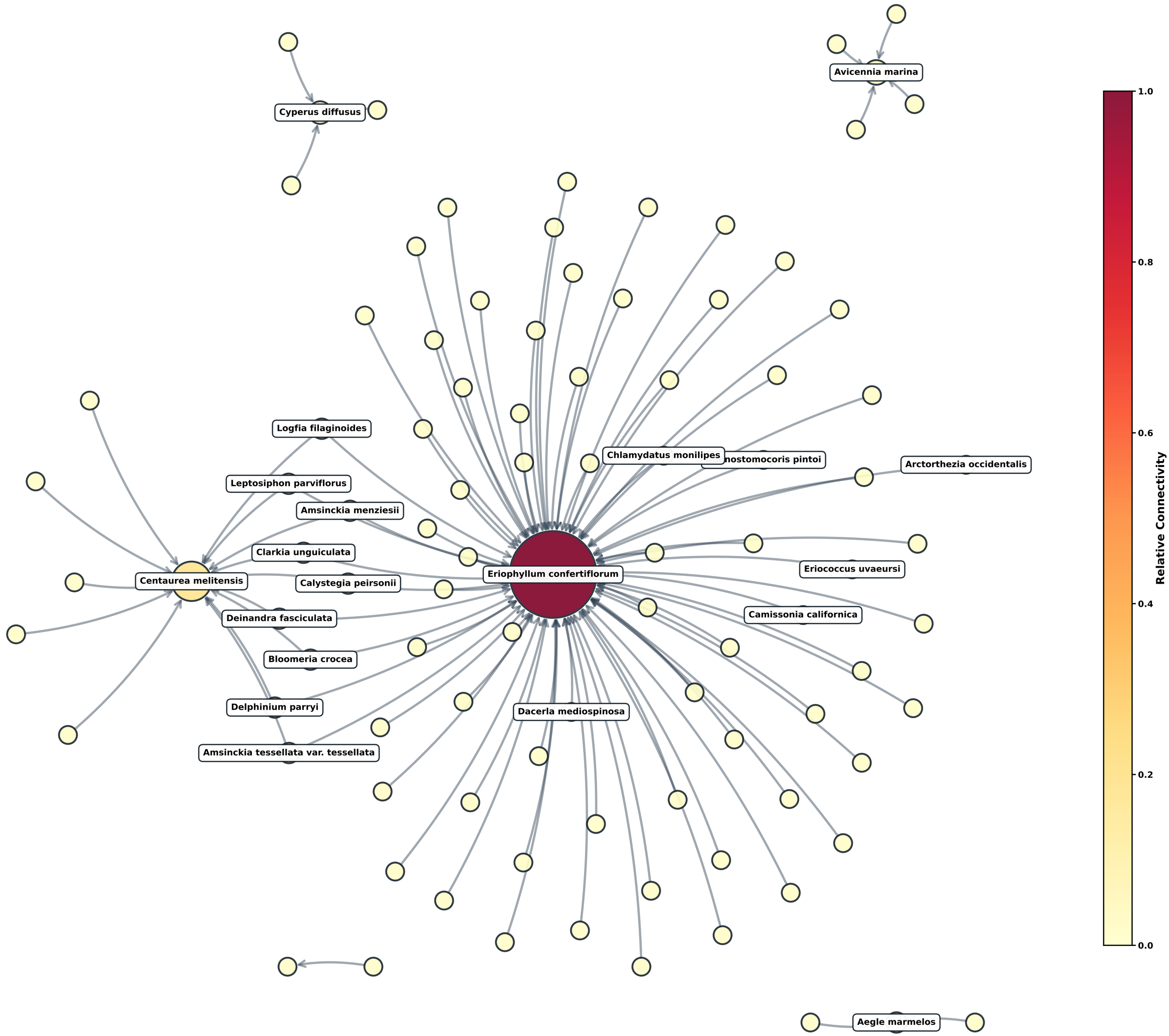
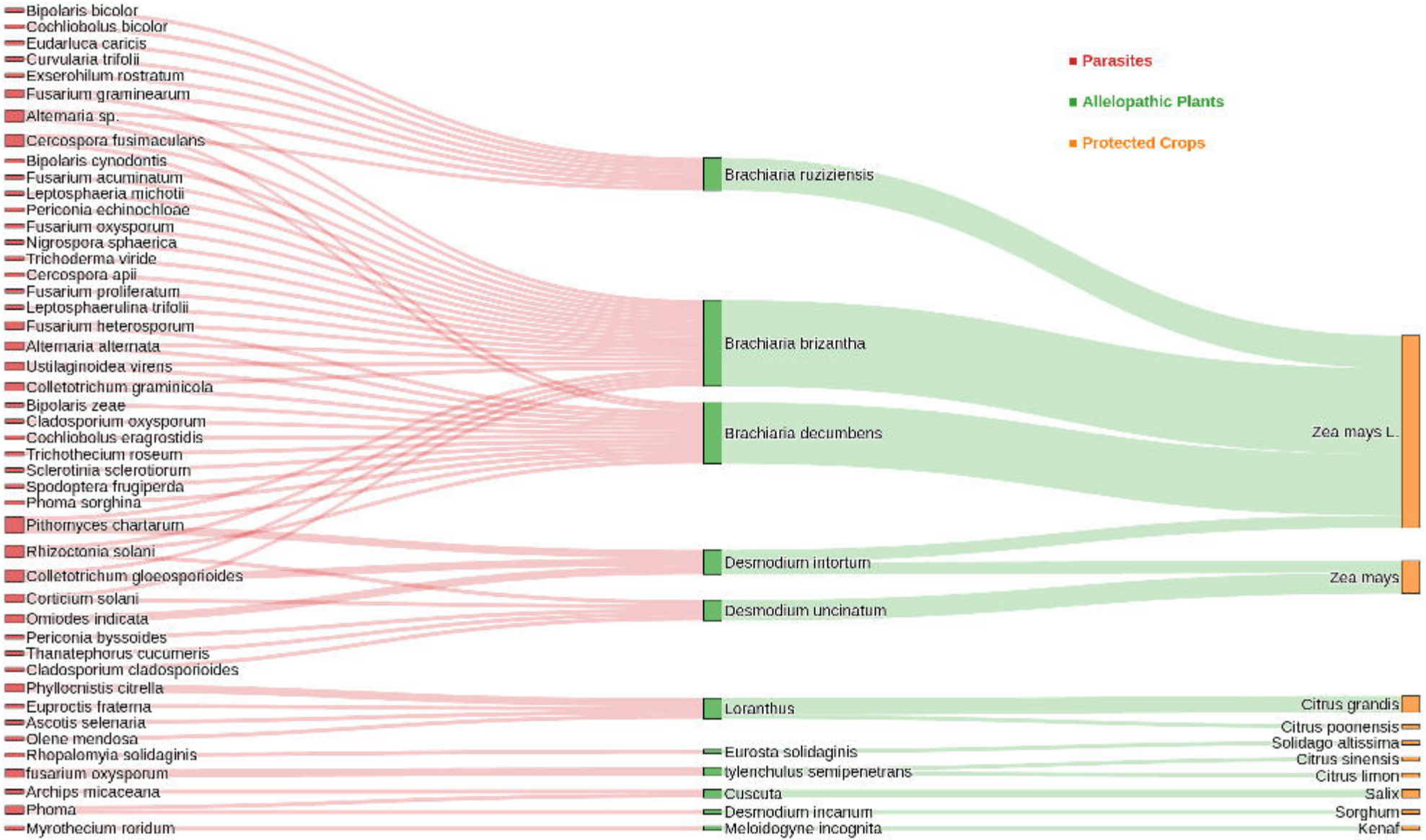
targetSex-Id/Name


Trait Absent
Trait Present
Species
Pinus sylvestris
Qualea grandiflora
Fagus sylvatica
Pinus halepensis
Picea abies
Glycine max
Eucalyptus camaldulensis
Triticum aestivum
Solidago canadensis
Pinus nigra
Pinus pinaster
Trifolium repens
Daucus carota
Ceiba pentandra
Lolium perenne
Dodonaea viscosa
Arbutus unedo
Abies sachalinensis
Pinus taeda
Picea sitchensis
Phillyrea latifolia
Cistus creticus
Salvia rosmarinus
Brassica napus
Solidago rugosa
Pistacia lentiscus
Festuca rubra
Pinus densiflora
Eucalyptus saligna
Eperua falcata
Photosynthesis per leaf area at leaf temperature (Aarea)
Leaf nitrogen content per dry mass (Nmass)
SLA: undefined if petiole in- or excluded
Seed dry mass
Plant height vegetative
Leaf carbon content per dry mass
Leaf phosphorus content per dry mass (Pmass)
Wood density; stem specific density; wood specific gravity (SSD)
Leaf area: in case of compound leaves undefined if leaf or leaflet; undefined if petiole and rhachis in- or excluded
SLA: petiole excluded
Leaf area: in case of compound leaves leaf; petiole excluded
Leaf area: in case of compound leaves leaf; petiole and rhachis included
SLA: petiole included
Plant height (unspecified if vegetative or reproductive)
Leaf dark respiration per area at leaf temperature
Plant height reproductive / generative
SLA: undefined if petiole in- or excluded (1)
Leaf area: in case of compound leaves leaflet; petiole excluded
Plant height observed
Leaf mitochondrial respiration in the light (non-photorespiratory CO2 evolution) per leaf area
Plant height maximum
Leaf area: in case of compound leaves leaf; undefined if petiole in- or excluded
Leaf area: in case of compound leaves undefined if leaf or leaflet; undefined if petiole in- or excluded (1)
Leaf area: in case of compound leaves leaflet; undefined if petiole in- or excluded
Seed mass
Xylem density (xylem tissue density)
Leaf lifespan (longevity, retention time, LL, LLS)
Maximum height max
Maximum height
Traits


Cyperus diffusus
Avicennia marina
Logfia filaginoides
Leptosiphon parviflorus
Amsinckia menziesii
Clarkia unguiculata
Centaurea melitensis
Calystegia peirsonii
Deinandra fasciculata
Bloomeria crocea
Delphinium parryi
Amsinckia tessellata var. tessellata
Chlamydatus monilipes
nostomocoris pintoi
Arctorthezia occidentalis
Eriophyllum confertiflorum
Eriococcus uvaeursi
Camissonia californica
Dacerla mediospinosa
Aegle marmelos
Relative Connectivity
1.0
0.8
0.6
0.4
0.2
0.0


Parasites
Allelopathic Plants
Protected Crops
Bipolaris bicolor
Cochliobolus bicolor
Eudarluca caricis
Curvularia trifolii
Exserohilum rostratum
Fusarium graminearum
Alternaria sp.
Cercospora fusimaculans
Bipolaris cynodontis
Fusarium acuminatum
Leptosphaeria michotii
Periconia echinochloae
Fusarium oxysporum
Nigrospora sphaerica
Trichoderma viride
Cercospora apii
Fusarium proliferatum
Leptosphaerulina trifolii
Fusarium heterosporum
Alternaria alternata
Ustilaginoidea virens
Colletotrichum graminicola
Bipolaris zeae
Cladosporium oxysporum
Cochliobolus eragrostidis
Trichothecium roseum
Sclerotinia sclerotiorum
Spodoptera frugiperda
Phoma sorghina
Pithomyces chartarum
Rhizoctonia solani
Colletotrichum gloeosporioides
Corticium solani
Omiodes indicata
Periconia byssoides
Thanatephorus cucumeris
Cladosporium cladosporioides
Phyllocnistis citrella
Euproctis fraterna
Ascotis selenaria
Olene mendosa
Rhopalomyia solidaginis
fusarium oxysporum
Archips micaceana
Phoma
Myrothecium roridum
Brachiaria ruziziensis
Brachiaria brizantha
Brachiaria decumbens
Desmodium intortum
Desmodium uncinatum
Loranthus
Eurosta solidaginis
tylenchulus semipenetrans
Cuscuta
Desmodium incanum
Meloidogyne incognita
Zea mays L.
Zea mays
Citrus grandis
Citrus poonensis
Solidago altissima
Citrus sinensis
Citrus limon
Salix
Sorghum
Kenaf