The ChEBI Ontology: an ontology for chemistry within a biological context

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Abstract

Chemical Entities of Biological Interest (ChEBI) is a freely available database of molecular entities and chemical concepts, which is manually annotated to a high standard of quality and is non-redundant, thus differentiating it from other publicly available chemistry resources. It focuses specifically on those chemical entities which are of interest to the life sciences community, including metabolites and drugs. ChEBI is a reference database for chemical nomenclature and structures, and provides a chemical ontology.

The ChEBI ontology provides a classification for all entities in ChEBI according to their chemical structures, and where applicable their biological or applied roles. The ontology is composed of the individual ChEBI entities and the relationships between them. The types of relationships include *is a*, which is used to relate a specialised entity to a more general one which subsumes it, *has part*, which is used to indicate the constituents of a composite entity, *has role*, which is used to link a molecular entity to a role which it performs in some contexts, and various chemical relationships including *is enantiomer of* and *is tautomer of*. The ChEBI ontology is widely used for such purposes as text mining (recognition of chemical names in the literature) and unambiguous annotation of chemical entities in biological databases.

Recent developments in the ontology include the introduction of the *has part* and *has role* relationships to resolve previously ambiguous usage of *is part of* and *is a* respectively, and the classification of all previously unclassified checked entities. Future directions include enriching the semantic definition of terms so as to facilitate the use of a description logic based reasoner to assist the ontology editing process.

ChEBI may be accessed and browsed online at `http://www.ebi.ac.uk/chebi`, or programmatically via a SOAP-based web service documented at `http://www.ebi.ac.uk/chebi/webServices.do`, and the full dataset is available for download in several formats including the popular OBO ontology format.