Extension of Roles in the ChEBI Ontology

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Motivation

The Chemical Entities of Biological Interest (ChEBI [1]) ontology models chemicals, their classes, their roles, and their interrelations (Figure 1, left). While many roles correspond to how their substituent chemicals affect proteins, protein families, protein complexes, pathways, pathologies, or organisms, this information is unstructured. Yan et al. (2011) previously described how these correspondences could be theoretically formalized. This article proposes a concrete schema and axioms through which these roles can be linked to their target entities (Figure 1, right), a suite of open source, reusable curation tools, and ultimately a manually curated database of relationships between chemical roles and their targets.

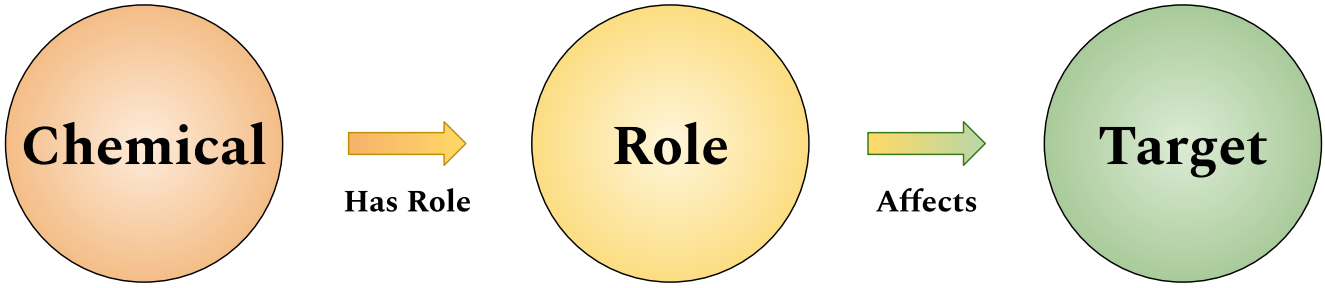

Figure 1: Schema for inference of chemicals' relations to targets via roles. Targets may be other chemicals, proteins, protein families, protein complexes, pathways, pathologies, or organisms.

Throughout this article, the term role (in the context of the ChEBI ontology) will be used in the colloquial sense described by Batchelor et al. (2010) rather than the formal sense prescribed by the Basic Formal Ontology (Smith et al., 2005).

References

1. **The ChEBI reference database and ontology for biologically relevant chemistry: enhancements for 2013.**
Janna Hastings, Paula de Matos, Adriano Dekker, Marcus Ennis, Bhavana Harsha, Namrata Kale, Venkatesh Muthukrishnan, Gareth Owen, Steve Turner, Mark Williams, Christoph Steinbeck
Nucleic acids research (2012-11-24) https://www.ncbi.nlm.nih.gov/pubmed/23180789
DOI: 10.1093/nar/gks1146 · PMID: 23180789 · PMCID: PMC3531142