BioBricks-OKG: An Open Knowledge Graph for Cheminformatics and Chemical Safety

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Award: NSF SBIR 2333728

Problem space

Before you can answer a particular cheminformatics question:

P0 Many different data sources for cheminformatics and chemical safety.

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- **P0** Many different data sources for cheminformatics and chemical safety.
- P1 Retrieving data sources for local analysis.
- **P2** Differences in how data are represented.

Solution: tabular data

multiple data sources local analysis

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BioBricks

Solution: graph data

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multiple data sources local analysis interoperable data through common vocabularies, identifiers, and ontologies

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Built on RDF metadata standard

RDF

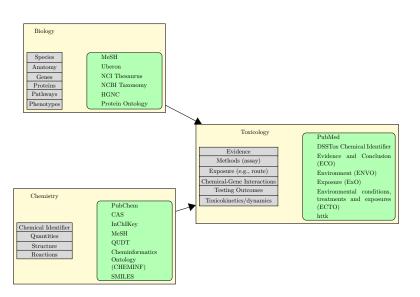
RDF based on triple relationships



Technology

- 1. Build on existing BioBricks infrastructure
- 2. Use tabular data as a data source (tabular brick)
- 3. Map tabular data to graph data (triple brick)
- 4. Load this triple brick into a triplestore graph database or use directly

Knowledge organization



Early prototype

datasets: ICE, tox21, CTDbase, MeSH, HGNC, CosIng

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New datasets

New use cases

Improvements to data modeling