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

Zakariyya Mughal

Insilica

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Problem space

Before you can answer a particular cheminformatics question:

P0 Many different data sources for cheminformatics and chemical safety.

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P2 Differences in how data are represented.

Solution: tabular data

multiple data sources

local analysis

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BioBricks

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interoperable data through common vocabularies, identifiers, and ontologies

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Working as part of NSF Proto-OKN program

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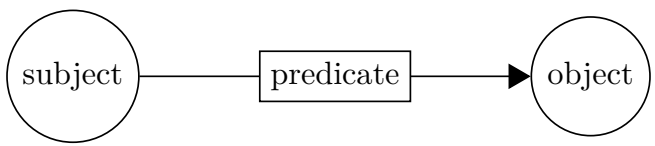
Built on RDF metadata standard

RDF

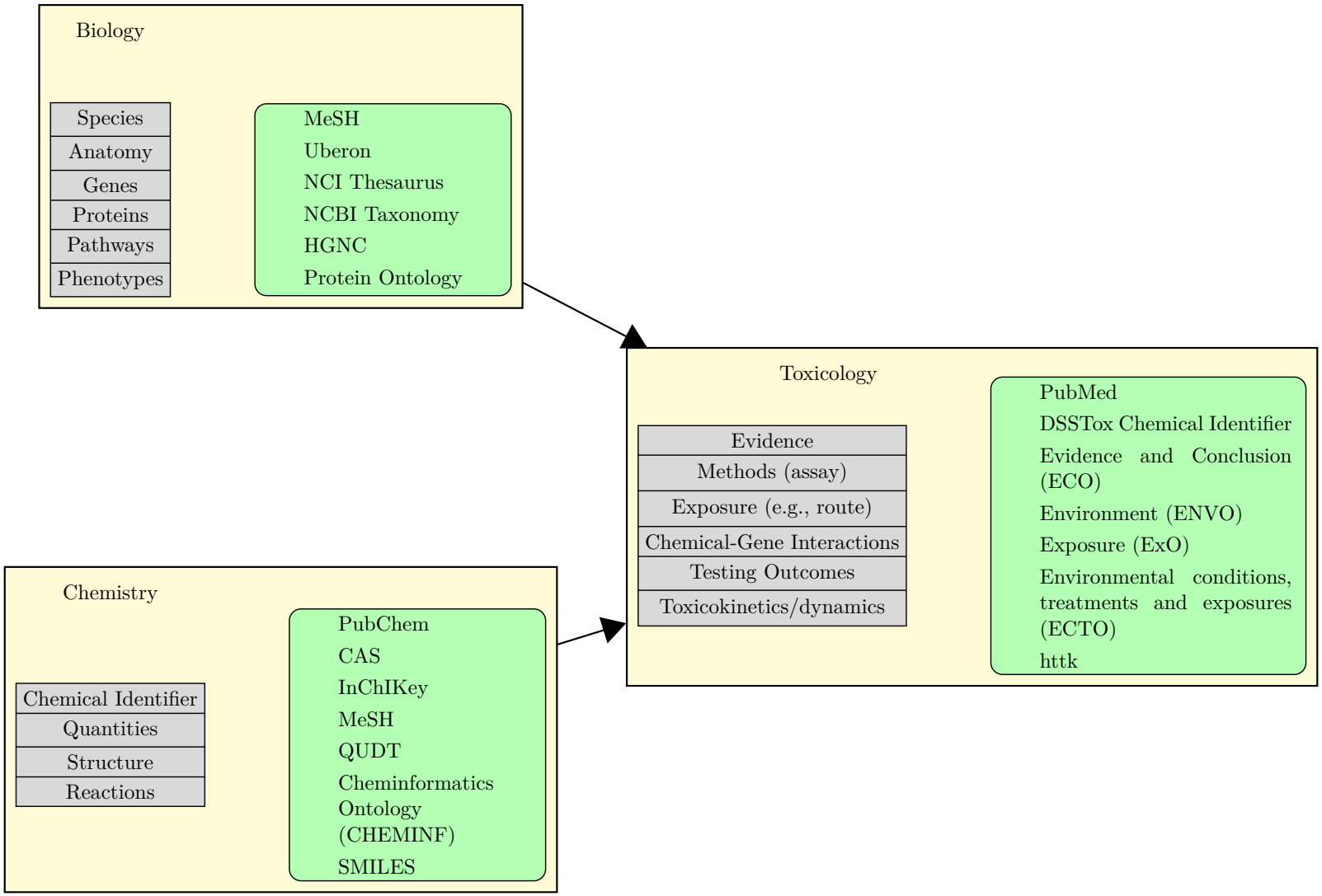
RDF based on triple relationships



Technology

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

Knowledge organization



Early prototype

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Looking for

- New datasets
- New use cases
- Improvements to data modeling