Facilitating Data Curation: a Solution Developed in the Toxicology Domain

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Context

- The goal of toxicology is to understand the adverse effects of chemical compounds or physical agents on living organisms.
- The IVTD Group in the VUB aims to collect safety testing data of cosmetic ingredients available in publicly available safety evaluation reports with the goal of creating a knowledge base.

Structure of a Spreadsheet



Test: Skin Absorption In Vitro Non-OECD

Problem

- Subject matter experts currently rely on spreadsheets, which causes problems for: data curation, data analysis, and data exploration.
- Semantic Technologies can overcome these challenges and furthermore allows data to be linked with external datasets.
- But semantic technologies are not easily accessible to these subject matter experts [1]
- How can we facilitate the creation of a knowledge base for the available safety evaluation reports by subject matter experts in the domain of toxicology?

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method of analysis	observations (free text)	absorption data (bioavaliability %)	tabulated data over each cellular compartment	absorption profile (graph)	test substance									test conditions															
					lomogeneity	Н	oncentration (%)	composition	ourity (%)	olubility in receptor fluic	chemical batch nr	additional info (free text)				method			additional info (free text)				Variables						
					1		0	0	U.	S	C	0		skintype & source		group size (donors/repl	cell design	receptor fluid		temperature (*C)	humidity	exposed area (cm ²)	dose (mg/cm²)	sampling fractions (h)	duration of exposure (h				
													thickness um	source	treatment														

Proposed Solution: Using the Jigsaw Metaphor to Guide Experts in Creating Resources

- An interface metaphor [2] is drawing upon the knowledge of familiar concepts to facilitate learning and using a system.
- ► The Jigsaw Metaphor is proven successful for other tasks.
- In our proposed solution, the Jigsaw puzzle pieces guide subject matter experts in creating valid data entries.



The prototype is built on top of Google Blockly for the metaphor and Apache Jena for the knowledge base.

Knowledge Organization

The knowledge architecture consists of:

- A lightweight ontology containing few axioms for extensibility.
- ► The structure of jigsaw pieces in separate named graphs.
- The knowledge base containing the data of safety evaluation reports—one graph per report.

Both the creation of the ontology and the structure of the jigsaw pieces are currently driven by the existing spreadsheets.



Conclusions and Future Work

References

We proposed the adoption of a jigsaw metaphor to facilitate data curation by subject matter experts. Future work is twofold:

- Use of the tool by subject matter experts for foreseen in 2020
- Adoption of the jigsaw metaphor defining and maintaining the various blocks
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