

Metabolomics Ontologies: SKOS-ified the ArMet specification

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Abstract

The MetWare project is going to make use of ontology technologies to control the content of the database, and a first step is to convert our MetWare database design into something using a formal ontology language. I have played with OWL in the past (see for example its use in Bioclipse), but was not overly happy with it in all situations.

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chem-bla-ics

The MetWare project is going to make use of ontology technologies to control the content of the database, and a first step is to convert [our MetWare database design](#) into something using a formal ontology language. I have played with [OWL](#) in the past (see for example [its use in Bioclipse](#)), but was not overly happy with it in all situations.

Then I read about [SKOS](#), Simplified Knowledge Organisation System. Unlike OWL, SKOS is less strict on relations between concepts being marked up. Often these concepts are loosely bound, instead following a strict *is_a* hierarchy. [ArMet](#) is a Metabolomics knowledge system which does not have a strong hierarchy, and SKOS seemed to me to be the most suitable markup candidate. So, I SKOS-ified the ArMet specification, resulting in [this rather simple document](#). The document is SKOS, but has an associated [skos2html.xsl XSLT stylesheet](#), so that Firefox converts it to XHTML on the fly.

An entry looks like:

```
<skos:Concept rdf:about="GenotypeID">
  <skos:prefLabel>genotypeID</skos:prefLabel>

  <skos:definition>A unique identifier for the genotype.</skos:definition>
  <skos:broader rdf:about="GenotypeProperty"/>
</skos:Concept>
```

The full SKOS specification allows capturing much of what we want to do, including i18n via the label system, loose hierarchical relations via *skos:broader*, and the concepts of *skos:Collection* to aggregate concepts. Where needed, it allows borrowing from other languages. For example, to link concepts from MetWare to the original ArMet specification *owl:sameAs* can be used.