3D Metabolism DB: RDF Format Reference

This is a documentation to express the RDF ontology within 3D Metabolism's Database

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How is this data structured

RDF tripes are expressed as <subject, predicate, object>.

In Wikidata terms, <subject, predicate, object> becomes <item, property, value>

For reference, this is what the data can be thought of when imported to our database

3DMetabolism Wikidata

Identifier	instanceOf	reactionWithin	partOf
Q2340523	Biological Reaction	glycolysis	

Subjects/Objects

- `Biological Pathway` **Q9** :

  Overview : An instance of a pathway involved within a *process*

  Examples:

  - glycolysis
  - gluconeogenesis
  - citric-acid-cycle

- `Biological Reaction` **Q10**:

  Overview: An instance of a biological reaction

  Examples:

  - 1,3-bisphospho-D-glycerate + ADP ⇔ 3-phospho-D-glycerate + ATP
  - D-fructose 6-phosphate + ATP ⇒ D-fructose 1,6-bisphosphate + ADP
  - 3-Phospho-D-glycerate ⇔ 2-Phospho-D-glycerate

- `Chemical Compound` **Q11**:

  Overview: An instance of a chemical compound

  Examples:

  - 3-phosphonato-D-glyceroyl phosphate(4-)
  - ADP(3-)
  - 3-phosphonato-D-glycerate(3-)

- `Chemical formula` **Q12**:

  Overview: An instance of a *chemical compound's* formula

Examples:

- $C_3H_4O_7P^{-3}$

Predicates

- `instanceOf` **P1 :**

  Subject: Any

  Object: *Subject Class*

  Overview: A predicate intended to relate the subject to the type of subject class

- `reactionWithin` **P3**:

  Subject: *Biological Reactions*

  Object: *Biological Pathways*

  Overview: A predicate intended for biological reactions to relate it to its respected biological pathway

- `hasPart` **P4:**

  Subject: *Any*

  Object: *Any*

  Overview: A predicate intended to classify the subjects' children objects

- `partOf` **P5:**

  Subject: *Any*

  Object: *Any*

  Overview: A predicate intended to relate it's itself to its parent object

- `chemicalFormula` **P6:**

  Subject: *Chemical Compound*

  Object: Chemical Formula

  Overview: A predicate intended to relate the chemical compound to the chemical formula

- `containReaction` **P7:**

  Subject: *Chemical Compound*

  Object: Chemical Formula

  Overview: A predicate intended to relate the chemical compound to the chemical formula

- `containReactant` **P8:**

  Subject: *Biological Pathway; Biological Compound*

  Object: *Chemical Compound*

  Overview: A predicate used to identify the reactants involved within the subject

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WikiData example queries

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working code

```
#Get child of glycolysis
SELECT ?Pathway ?PathwayLabel
WHERE
{
```

```
  wd:Q45317172 wdt:P527 ?Pathway. #Glycolysis has part
  SERVICE wikibase:label { bd:serviceParam wikibase:language "[AUTO_LANGUAGE]". }
}
GROUP BY ?Pathway ?PathwayLabel
```

```
#get child of Glycolysis' child
SELECT ?child ?childLabel ?parentLabel ?parent
WHERE
{
   wd:Q45317172 wdt:P527 ?parent.
  ?parent wdt:P527 ?child
  SERVICE wikibase:label { bd:serviceParam wikibase:language "[AUTO_LANGUAGE]". }
}
group by ?parent ?parentLabel ?childLabel ?child
```

References/Resources

RDF syntax: https://www.w3.org/TR/turtle/

Representation Learning on RDF: https://towardsdatascience.com/representation-learning-on-rdf-and-lpg-knowledge-graphs-6a92f2660241

RDF Tutorial- An Introduction to the Resource Description Framework: https://www.youtube.com/watch?v=zeYfT1cNKQg

carbohydrate metabolic process - WikiData: https://www.wikidata.org/wiki/Q2734081

creating RDF schema: https://www.w3schools.com/xml/xml_rdf.asp

https://www.europeandataportal.eu/sites/default/files/d2.1.2_training_module_2.4_designing_and_developing_vocabularies_i