MetaNetX/MNXref rel. 4.3
A few diagrams to document the RDF schema
Notation

- IRI and blank nodes are systematically typed in the MetaNetX RDF schema. In the following diagrams this is represented as:

  ![Diagram](image)

  which means

  $$\text{?comp} \text{ rdf:type mnx:COMP}$$

- GSMN stands for Genome-Scale Metabolic Network (GEM is another frequently used acronym for the same beast).
## Main node types

<table>
<thead>
<tr>
<th>mnx:CHEM</th>
<th>A metabolite</th>
</tr>
</thead>
<tbody>
<tr>
<td>mnx:COMP</td>
<td>A sub-cellular compartment</td>
</tr>
<tr>
<td>mnx:PART</td>
<td>A &quot;part&quot; in a chemical equation, made of a stoichiometric coefficient and a metabolite in a sub-cellular compartment</td>
</tr>
<tr>
<td>mnx:REAC</td>
<td>A chemical equation made of the above parts, assigned to its left or right side</td>
</tr>
<tr>
<td>mnx:PEPT</td>
<td>A gene or gene product, <em>i.e.</em> a polypeptide. Most published GSMNs are using gene identifiers from an organism-specific nomenclature. The corresponding UniProt identifiers are recovered when possible</td>
</tr>
<tr>
<td>mnx:CPLX</td>
<td>A protein complex or multiprotein complex is a group of one, two or more associated polypeptide chains. In Systems Biology, the word <em>protein</em> is usually used to designate the quaternary structure of enzymes and transporters, not their primary structure, <em>i.e.</em> the polypeptidic chains.</td>
</tr>
<tr>
<td>mnx:CATA</td>
<td>A catalyst contains the list of the involved protein complexes together with constraints on the flux carried by the implied reaction.</td>
</tr>
<tr>
<td>mnx:GPR</td>
<td>Gene-Protein-Reaction: A particular reaction with zero, one, or several catalysts, in the context of a particular GSMN</td>
</tr>
<tr>
<td>mnx:MNET</td>
<td>A Genome-Scale Metabolic Network (GSMN) or a metabolic network or a biochemical pathway, which are essentially sets of GPRs</td>
</tr>
</tbody>
</table>
This schema was designed to capture most information that can be obtained from SBML representation of GSMN.
mnx:COMP - sub-cellular compartment
Example of a compartment instance: Cytoplasm

```turtle
@PREFIX mnx: <https://rdf.metanetx.org/schema/>
@PREFIX comp: <https://rdf.metanetx.org/comp/>
@PREFIX go: <http://purl.obolibrary.org/obo/GO_>
@PREFIX biggC: <https://identifiers.org/bigg.compartment/>
comp:MNXC3 a mnx:COMP;
  rdfs:label 'MNXC1';
  rdfs:comment 'cytoplasm';
  mnx:compSource go:0005737;
  mnx:compXref go:0005737, biggC:c, seed:c.
```

The diagram illustrates the RDF representation of the Cytoplasm compartment, with properties such as the label "MNXC1" and the comment "cytoplasm".
mnx:PEPT - gene or gene product (e.g. polypeptide)

- Most published GSMNs are using gene identifiers from an organism-specific nomenclature
- The corresponding UniProt identifiers are recovered at MetaNetX, when possible
mnx:CHEM - metabolite

Nota Bene: mnx:chemRefer or at least one mnx:chemReplacedBy always exists
MetaNetX repository of GSMNs and biochemical networks: Reaction with specific compartments (MNXC1, MNXC2 ... ). These identifiers may change in the near future!

MetaNetX/MNXref: Reactions with generic compartments (MNXD1, MNXD2 ... ). Stable identifiers
GPR stands for Gene-Protein-Reaction
Large GSMNs contain thousands of GPR
mnx:GPR – GPR are the building block of GSMN

GSMNs
specific compartments
MNXC1, MNXC2...

MetaNetX/MNXref
generic compartments
MNXD1, MNXD2...

Reaction name(s) in the original model

xsd:string

rdfs:label 1..1

rdfs:comment 1..1

Summary of catalysis info in the original model

xsd:string

mnx:GPR

mnx:REAC

mnx:REAC

mnx:mnxr 0..1

?MNXR

mnx:REAC

mnx:CATA

mnx:GPR

mnx:REAC

?rea

mnx:reac 1..1

mnx:cata 1..n
Subunits are all required to produce a functional protein complex
Public cross-references are documented