

Swiss Institute of  
Bioinformatics

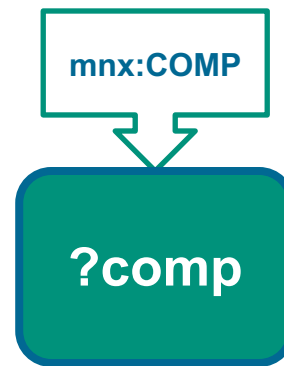
MetaNetX/MNXref rel. 4.3

A few diagrams to document the RDF schema

# Notation

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



which means `?comp rdf:type mnx:COMP`

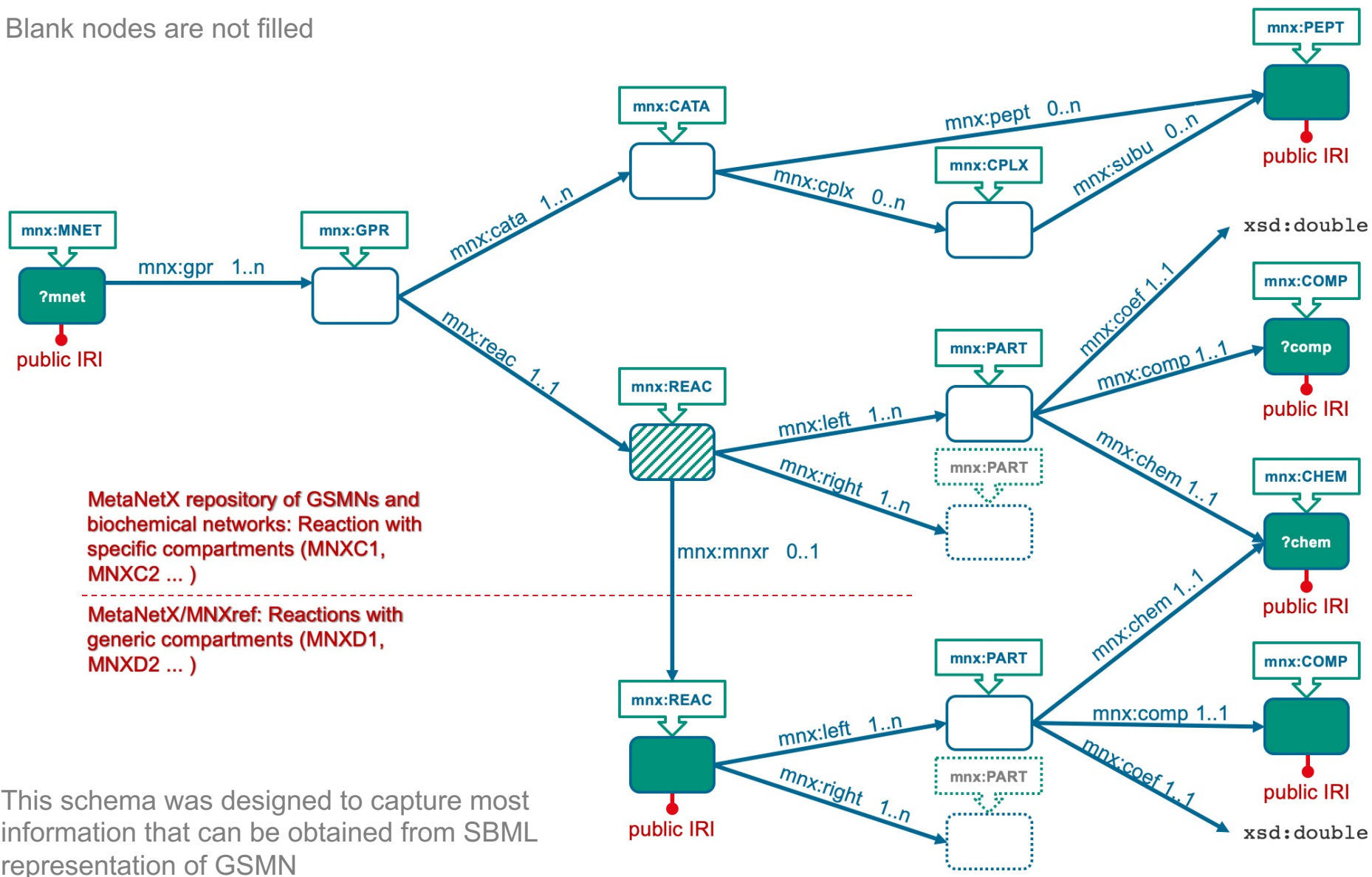
- GSMN stands for Genome-Scale Metabolic Network (GEM is another frequently used acronym for the same beast).

# Main node types

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

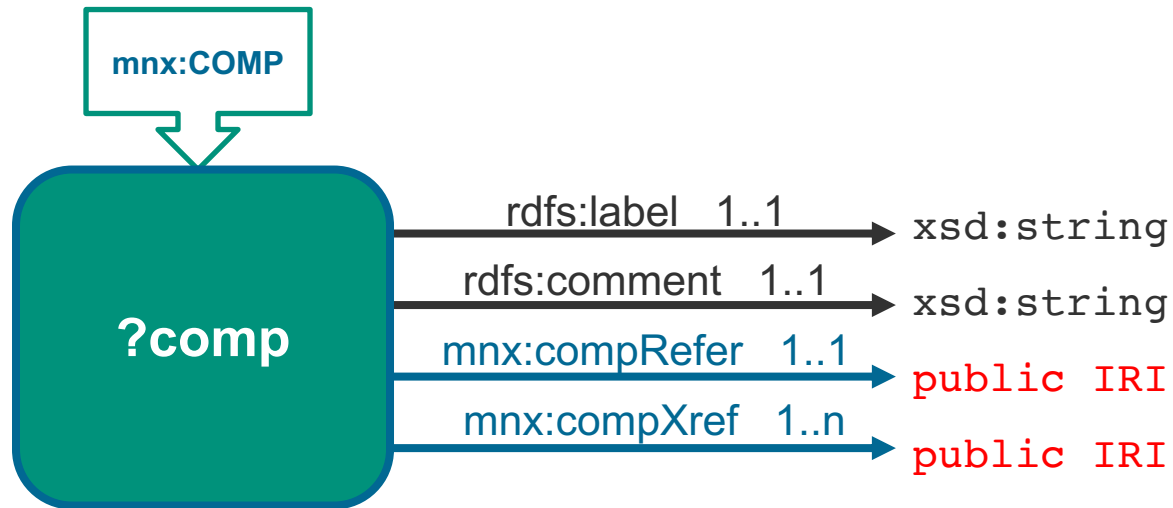
# Schema overview

Blank nodes are not filled



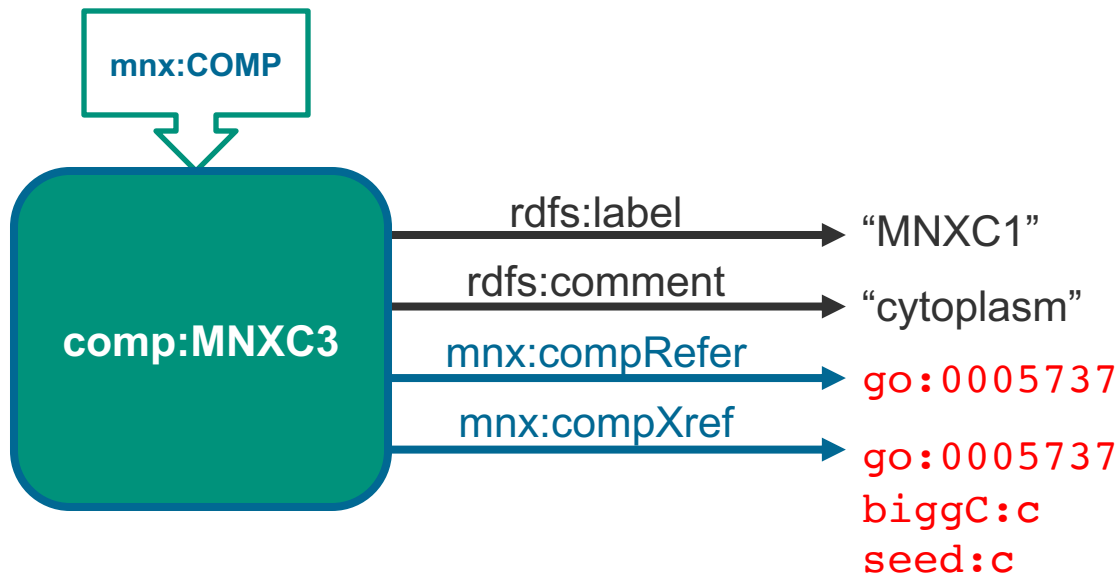
# mnx:COMP - sub-cellular compartment

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# Example of a compartment instance: Cytoplasm

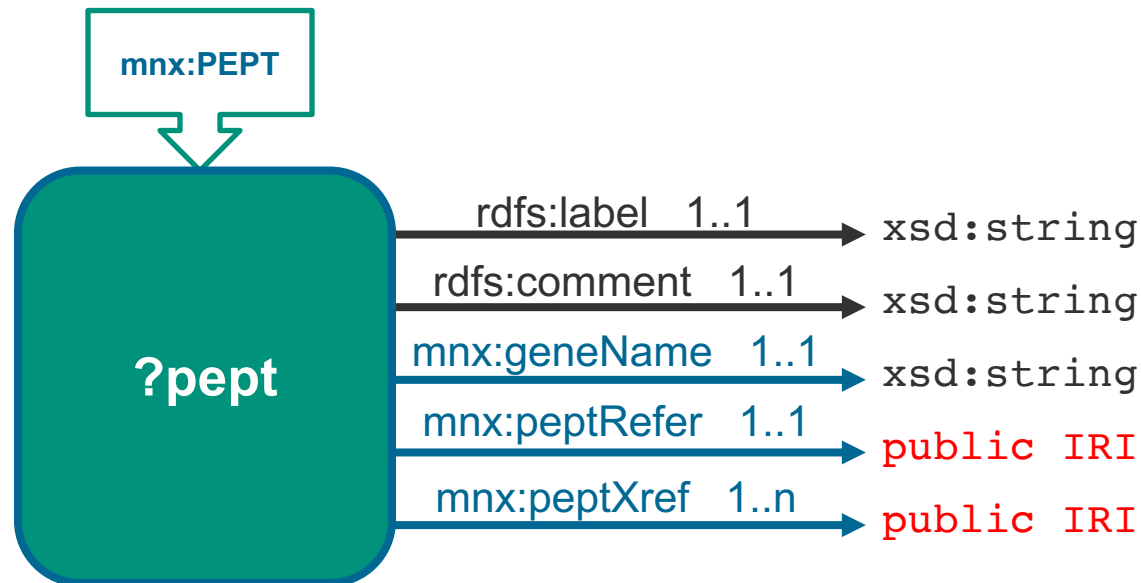
```
@PREFIX mnx: <https://rdf.metanetx.org/schema/>
@PREFIX comp: <https://rdf.metanetx.org/comp/>
@PREFIX go: <http://purl.obolibrary.org/obo/GO_>
@PREFIX biggC: <https://identifiers.org/bigg.compartment/>
comp:MNXC3 a mnx:COMP ;
  rdfs:label 'MNXC1' ;
  rdfs:comment 'cytoplasm' ;
  mnx:compSource go:0005737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



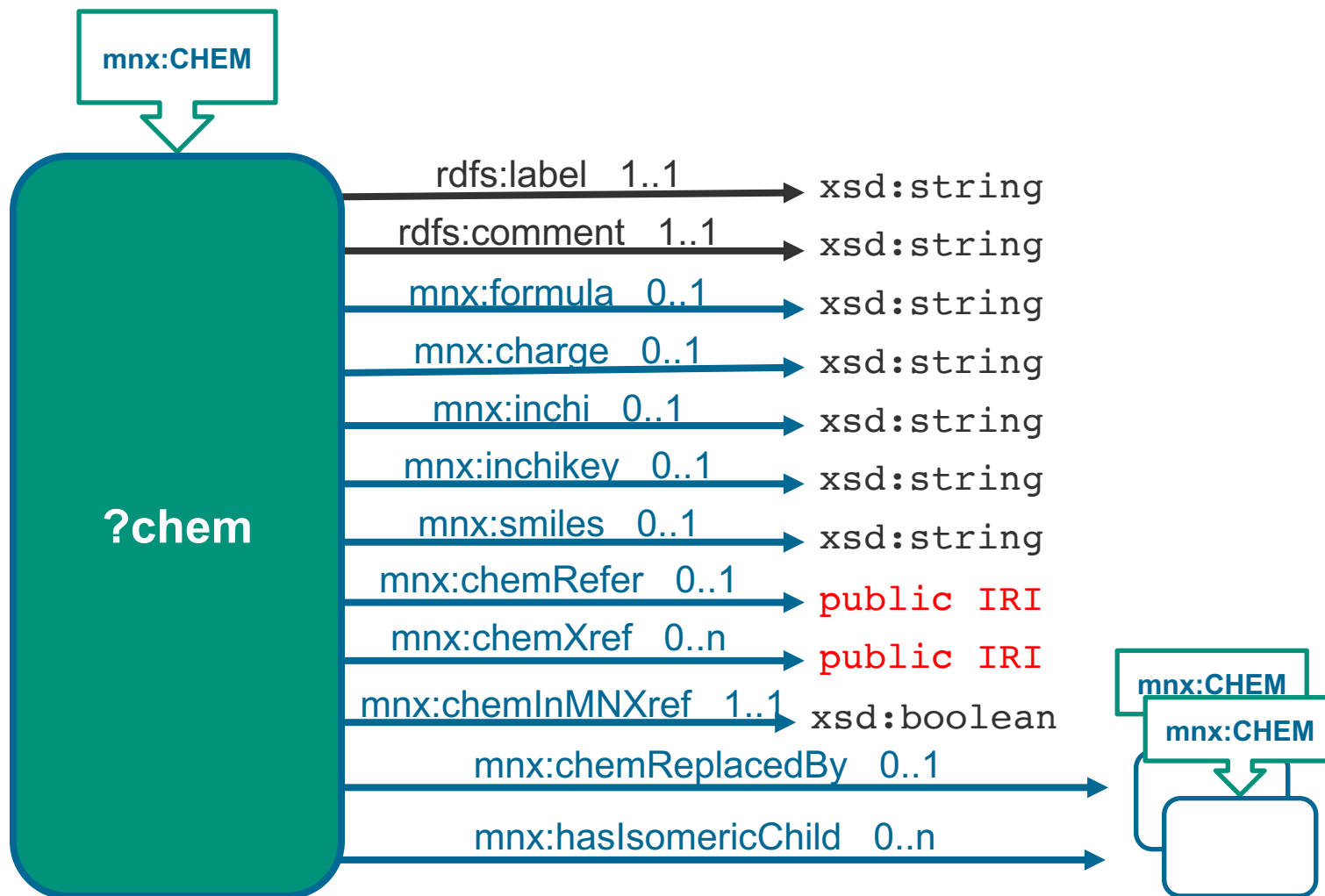
# mnx:PEPT - gene or gene product (e.g. polypeptide)

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



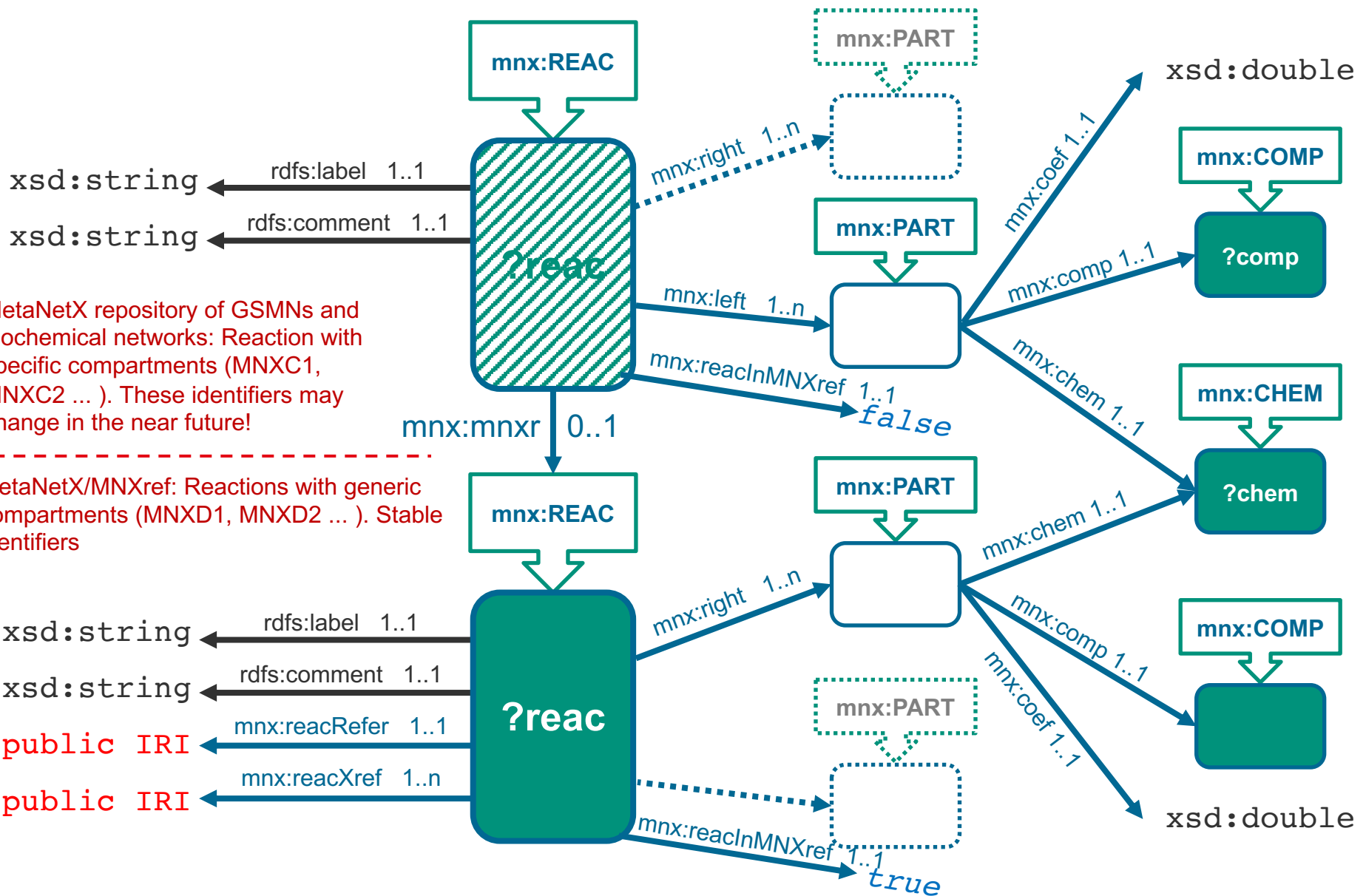
# mnx:CHEM - metabolite



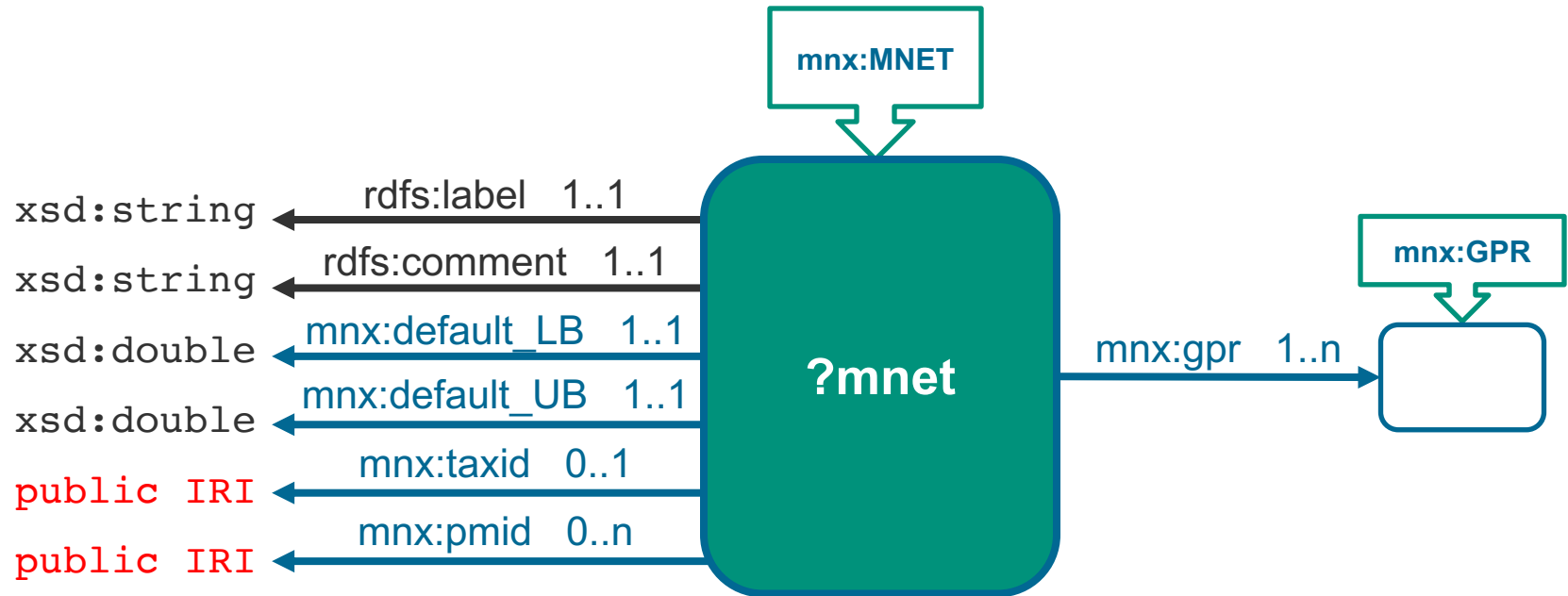
**Nota Bene:** `mnx:chemRefer` or at least one `mnx:chemReplacedBy` always exists



# mnx:REAC - reactions, two flavours

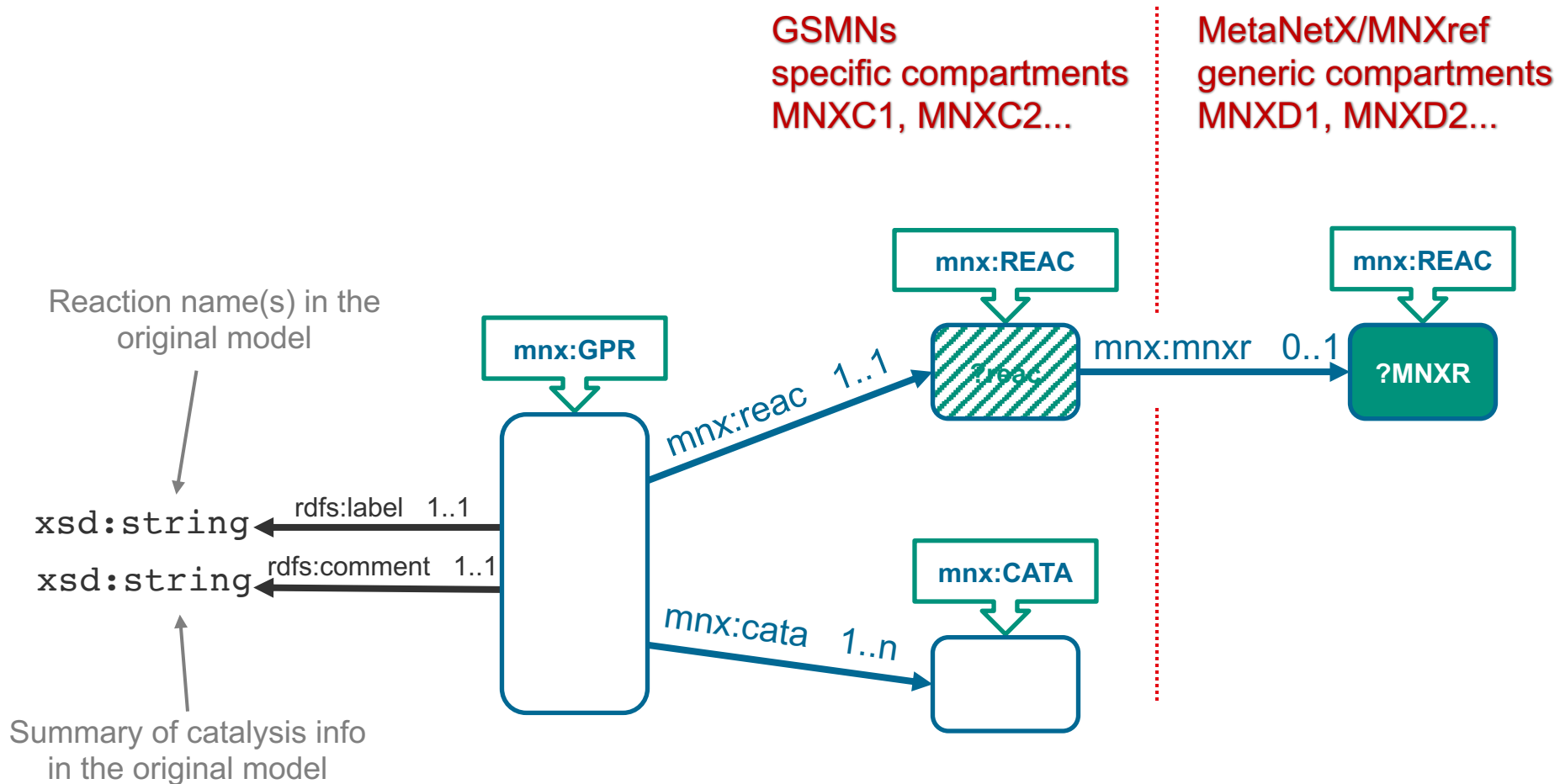


# mnx:MNET - GSMN and other metabolic networks

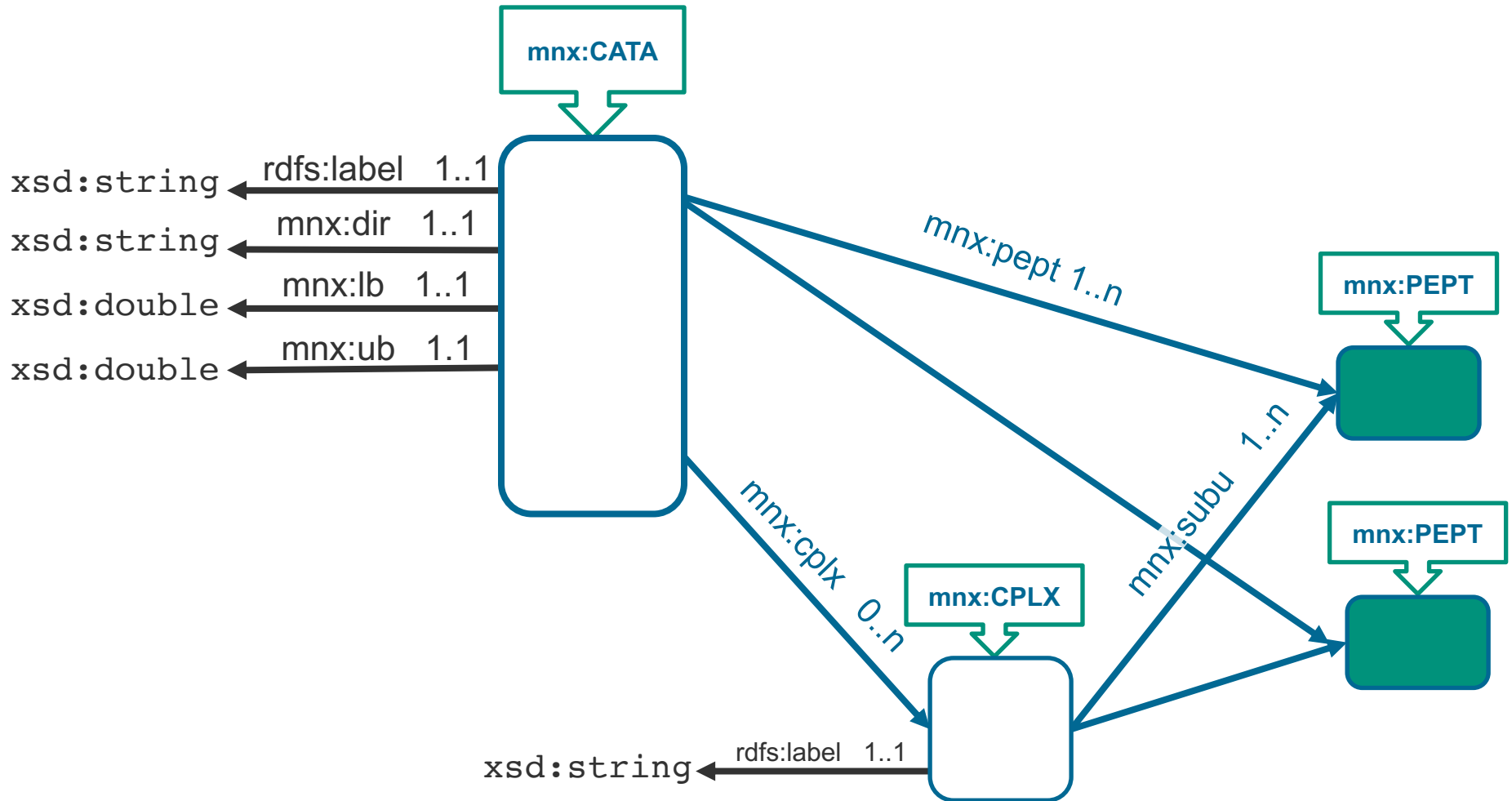


GPR stands for Gene-Protein-Reaction  
Large GSMNs contain thousands of GPR

# mnx:GPR – GPR are the building block of GSMN



# mnx:CATA – catalyst and complex description



Subunits are all required to produce a functional protein complex

# Public cross-references are documented

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