



Rhea RDF documentation

version: December 2019

Preliminary remarks

SPARQL endpoints:

- The Rhea SPARQL endpoint (<https://sparql.rhea-db.org/sparql>) is built from both **rhea.rdf** and **chebi.owl** (<ftp://ftp.expasy.org/databases/rhea/rdf/>). The datasets are synchronized with UniProt RDF data releases.
- **rhea.rdf** does not contain the cross-references to UniProt protein entries. They are available through the UniProt SPARQL endpoint (<https://sparql.uniprot.org/sparql>).

In Rhea RDF ([rhea.rdf](#)), all data are represented as subclasses of `rdfs:Class`, *i.e* there are no instances.

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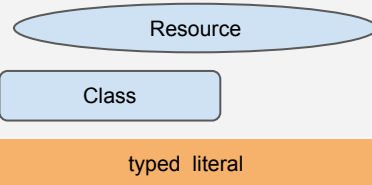
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Conventions

Namespaces / prefixes:

rh: <<http://rdf.rhea-db.org/>>
rdfs: <<http://www.w3.org/2000/01/rdf-schema#>>
ch: <<http://purl.obolibrary.org/obo/>>
ch2: <<http://purl.obolibrary.org/obo/chebi#>>
ch3: <<http://purl.obolibrary.org/obo/chebi/>>
up: <<http://purl.uniprot.org/core/>>
ec: <<http://purl.uniprot.org/enzyme/>>
pubmed: <<http://rdf.ncbi.nlm.nih.gov/pubmed/>>

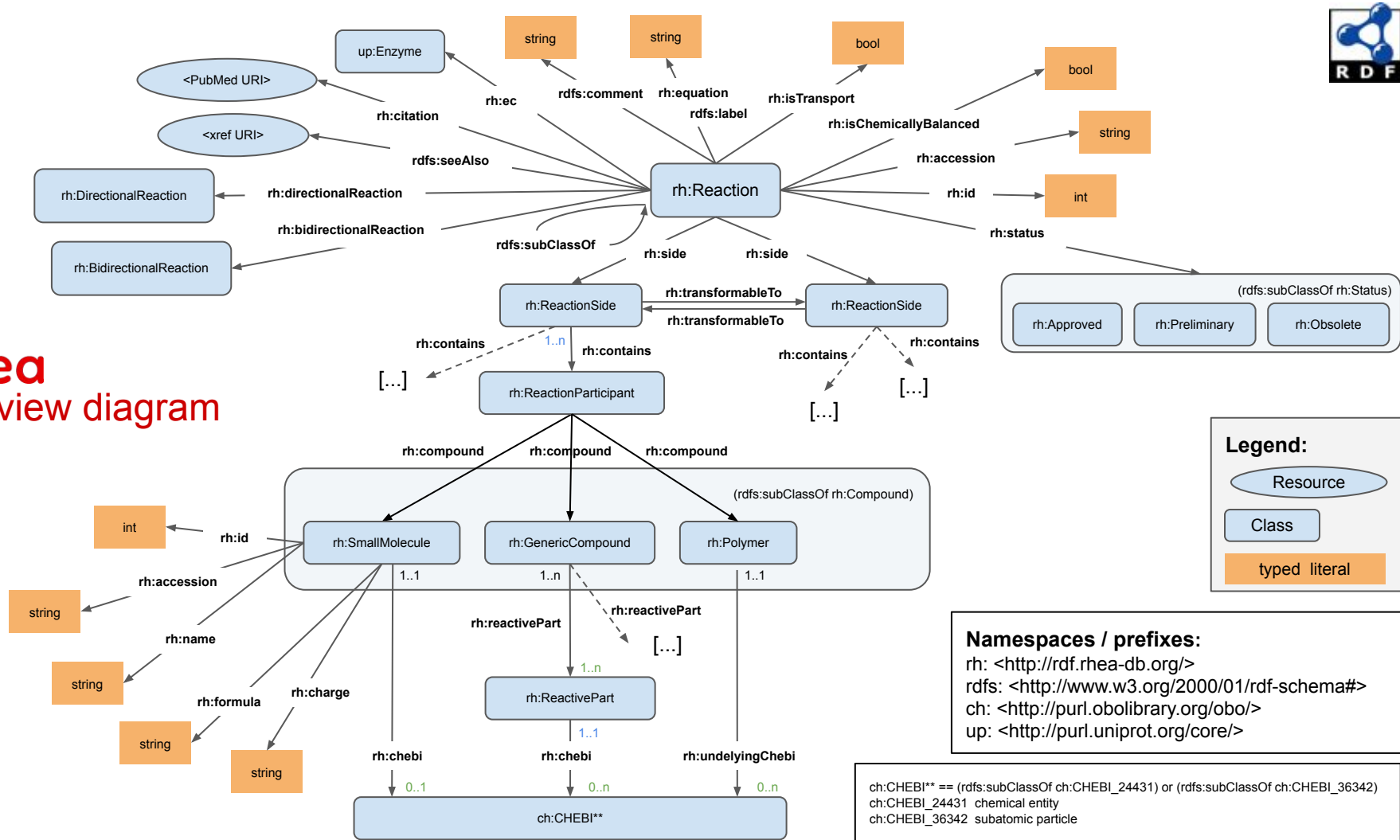
Legend:



ch:CHEBI** == (rdfs:subClassOf ch:CHEBI_24431) or (rdfs:subClassOf ch:CHEBI_36342)
ch:CHEBI_24431 chemical entity
ch:CHEBI_36342 subatomic particle



Rhea Overview diagram



Reactions, sides and participants

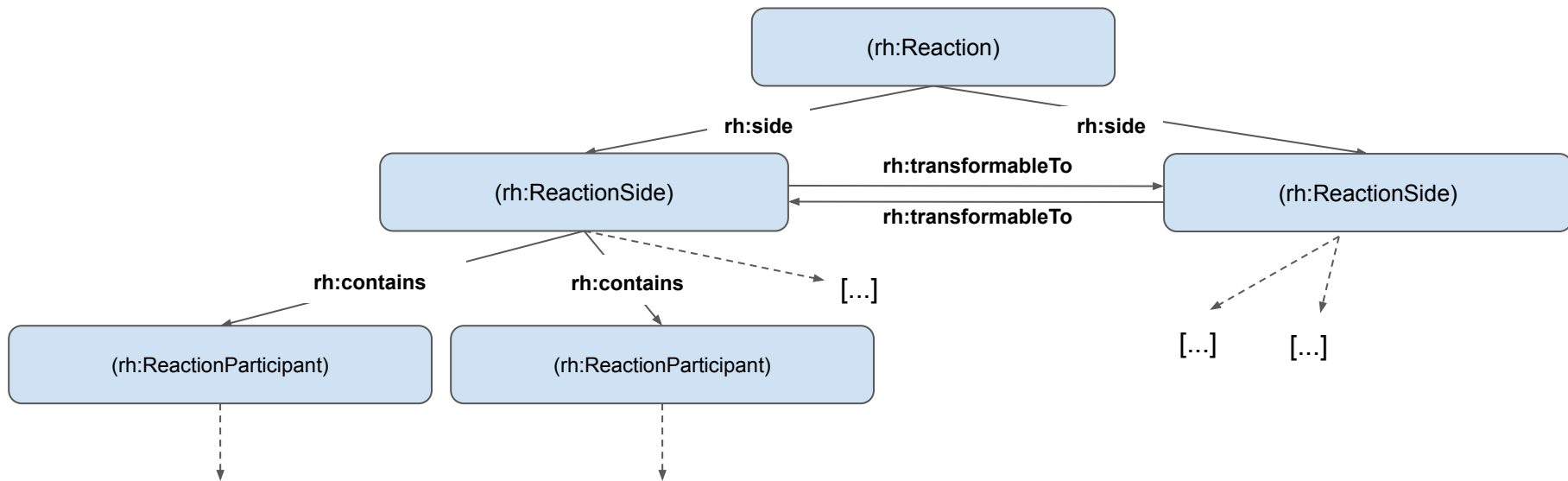
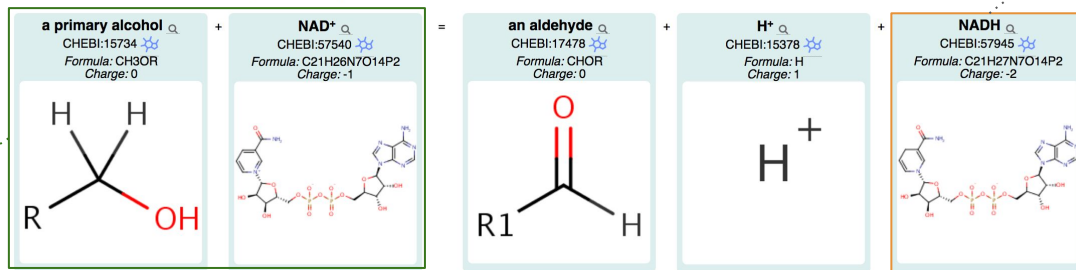
RHEA:10736 (APPROVED)

a primary alcohol + NAD(+) = an aldehyde + H(+) + NADH

Last modified: 2019-10-07. Chemically balanced: yes. Qualifiers: Class of reactions

reaction participant

reaction side



rh:Reaction



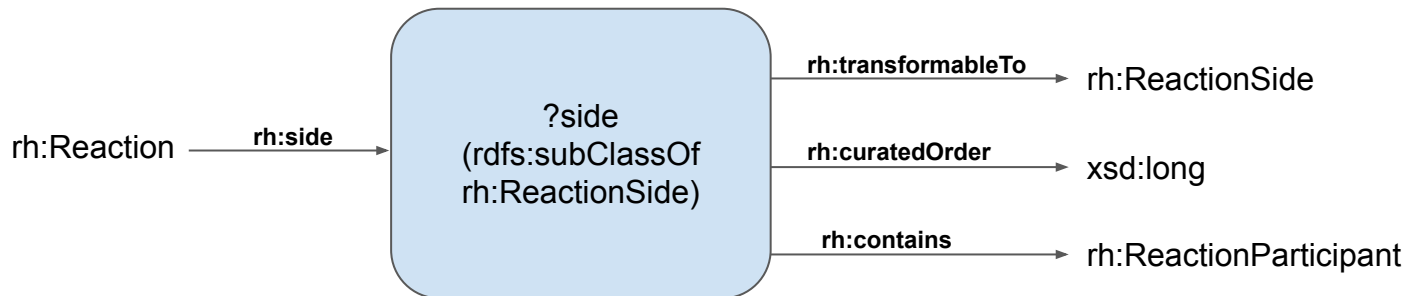
Definition:

A chemical or transport reaction of biological interest with unspecified direction. It is composed of two reaction sides.

rh:Reaction is a top class.

All the reactions published by Rhea are rdfs:subClassOf of rh:Reaction.

rh:ReactionSide



Definition:

A chemical or transport reaction (`rh:Reaction`) is composed of two reaction sides (`rh:ReactionSide`), sometimes denoted as left and right reaction sides.

In a **rh:Reaction**, the `rh:ReactionSide` are arbitrarily defined. They are linked by the predicate **rh:side**.

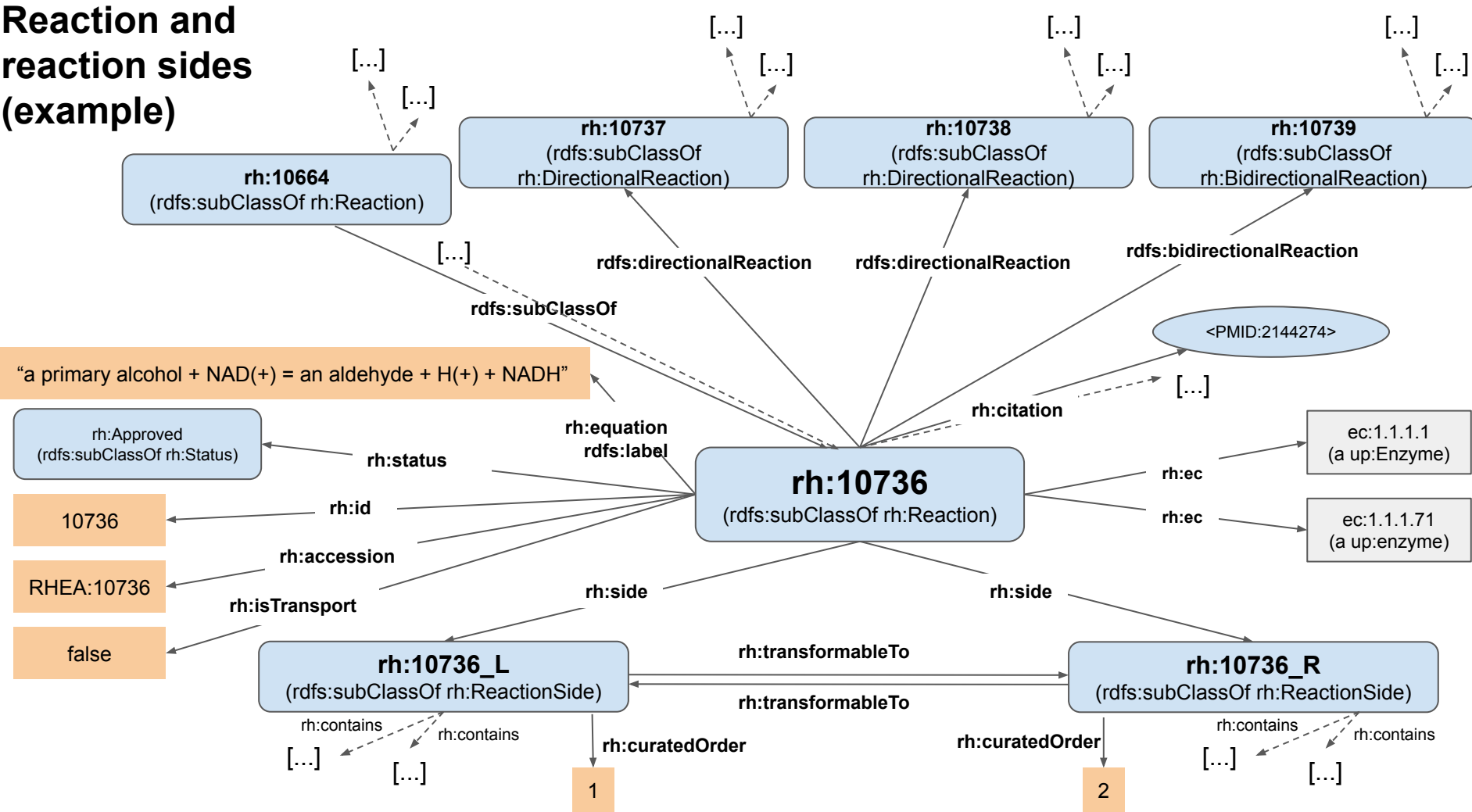
In a **rh:DirectionalReaction**, one `rh:ReactionSide` represents the substrate(s) (reactant(s), input) of the reaction, whereas the other represents the product(s) (output). In that case, the predicates **rh:substrate** and **rh:product** are used to denote the links.

In a **rh:BidirectionalReaction**, depending on the context, one `rh:ReactionSide` represents either the substrate(s) or the product(s). In that case, the predicate **rh:substrateOrProduct** is used to denote the links.

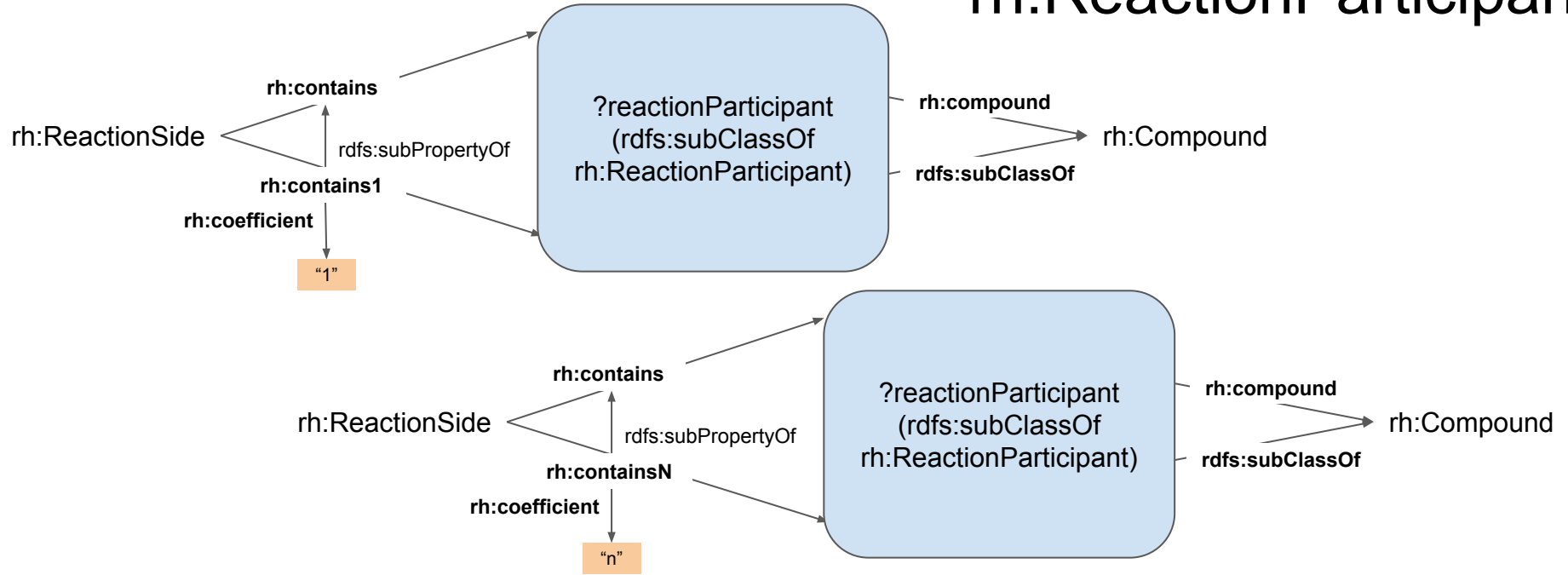
The link between the two reaction sides of a given reaction is denoted by the `rh:transformableTo` predicate.

A `rh:ReactionSide` gathers all the reaction participants (`rh:ReactionParticipant`) that are transformed into another `rh:ReactionSide`.

Reaction and reaction sides (example)



rh:ReactionParticipant

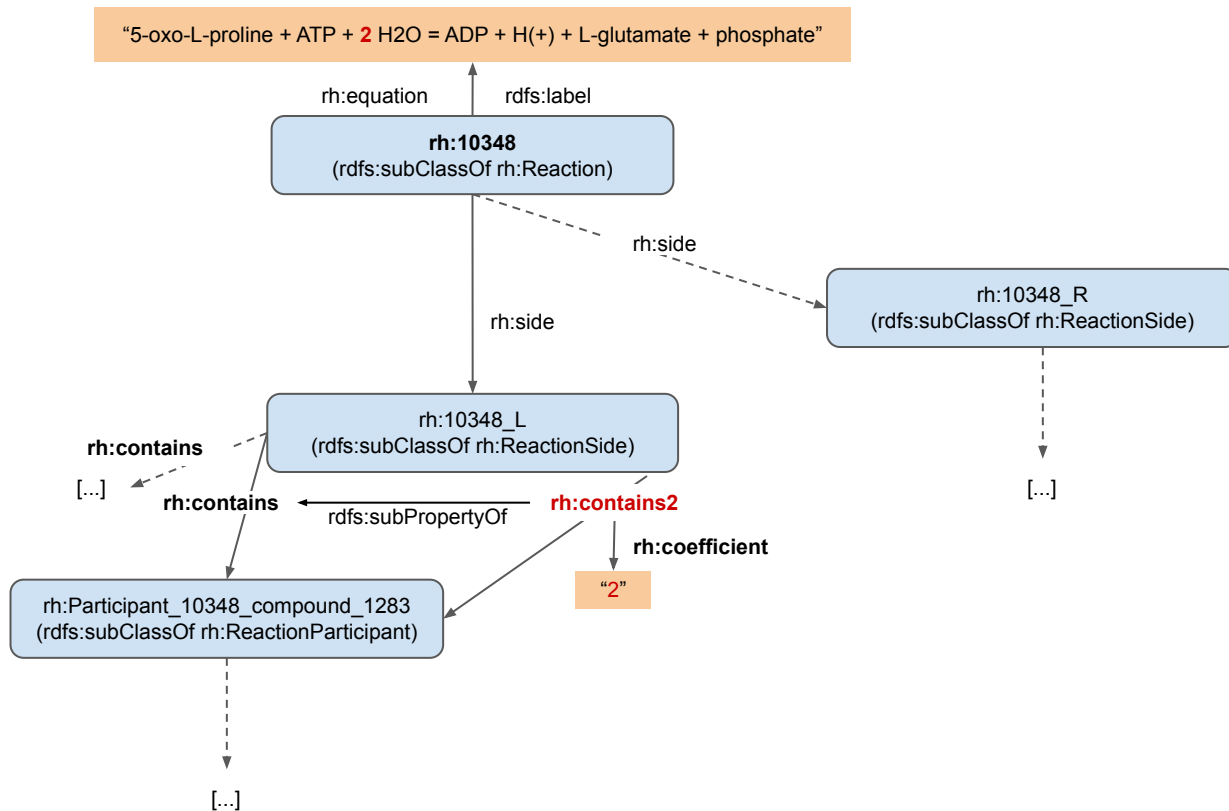


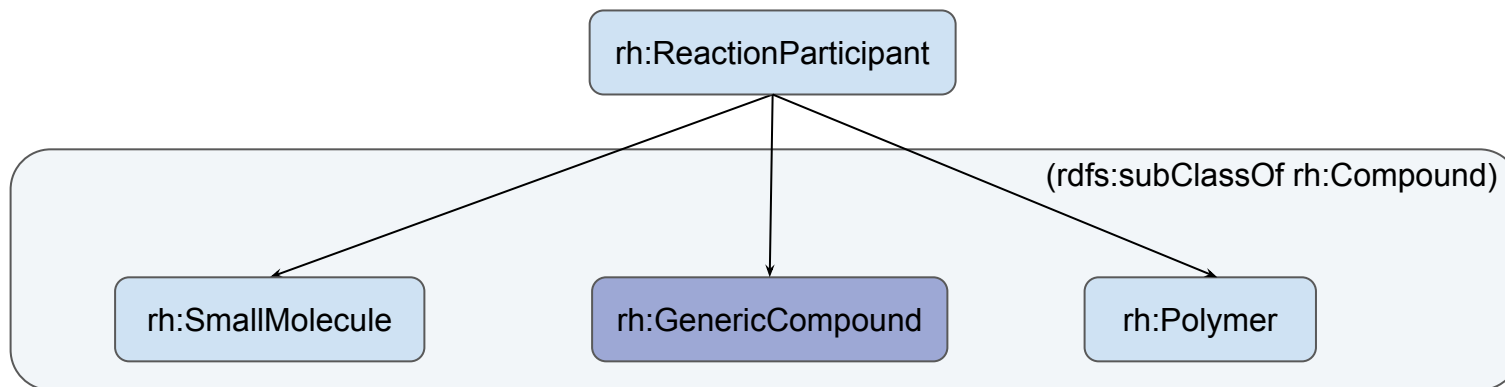
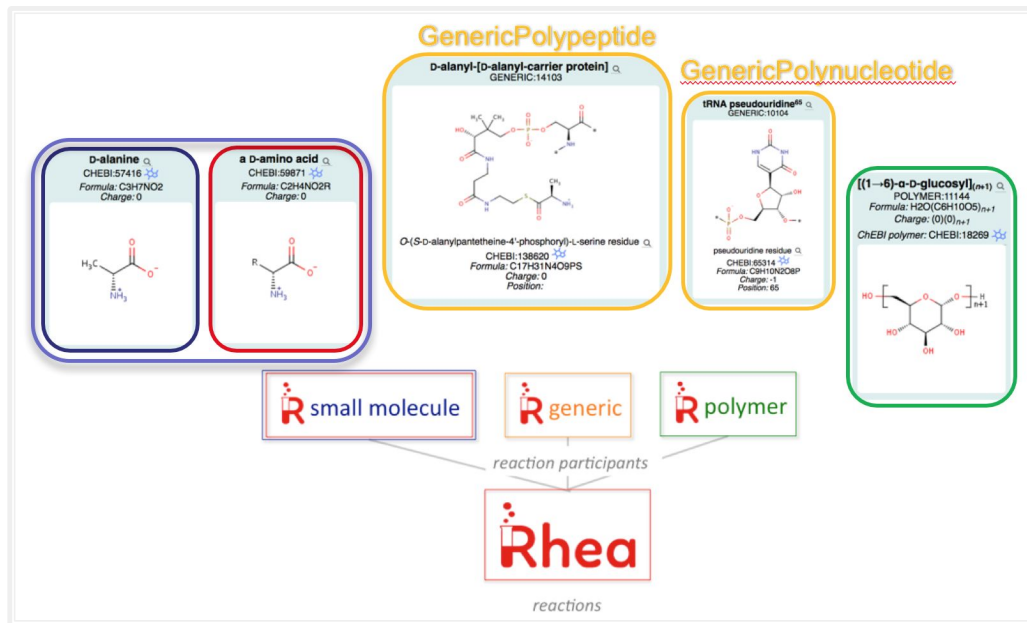
Definition: A chemical entity (subclass of `rh:Compound`) that is transformed in a chemical reaction or translocated in a transport reaction. There are three kind of participants: small molecules (`rh:SmallMolecule`), macromolecules (`rh:GenericCompound`) and polymers (`rh:Polymer`).

A reaction side (`rh:ReactionSide`) contains (`rh:contains`) participants (`rh:ReactionParticipant`).

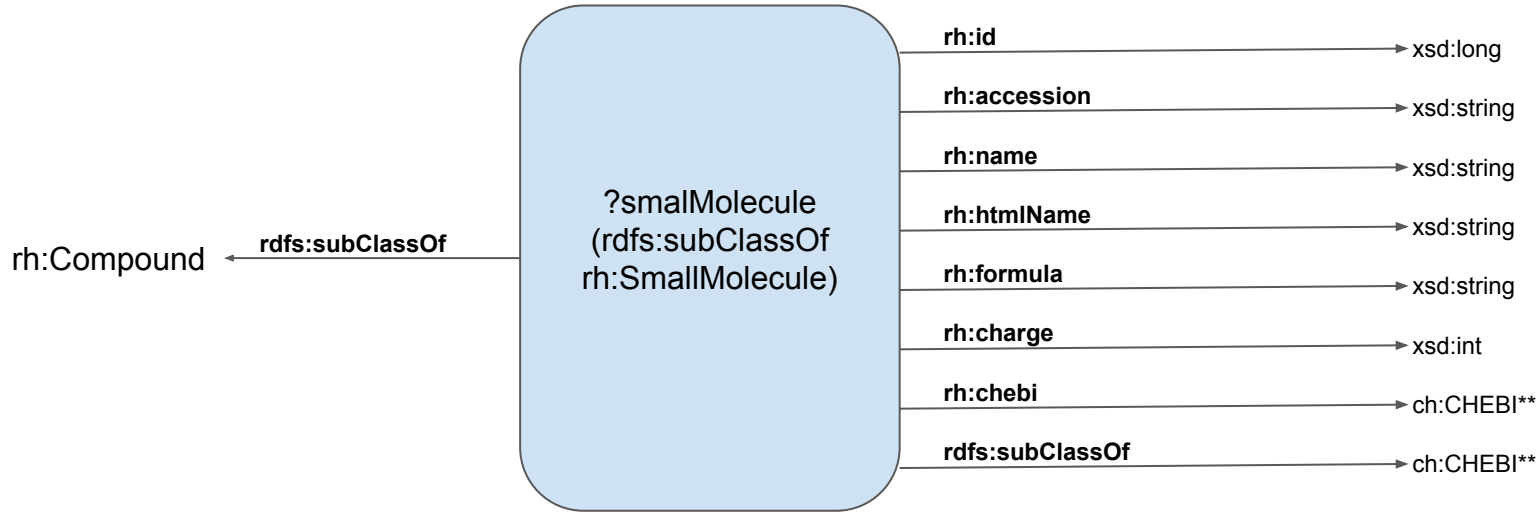
The stoichiometric coefficient of a participant is defined in a subproperty of `rh:contains` (`rh:contains1`, `rh:contains2`, `rh:containsN`,...).

rh:contains & rh:contains2 (example)





rh:SmallMolecule



Definition:

A chemical compound that is a low molecular weight (MW) molecule involved as participant, in a chemical or transport reaction.

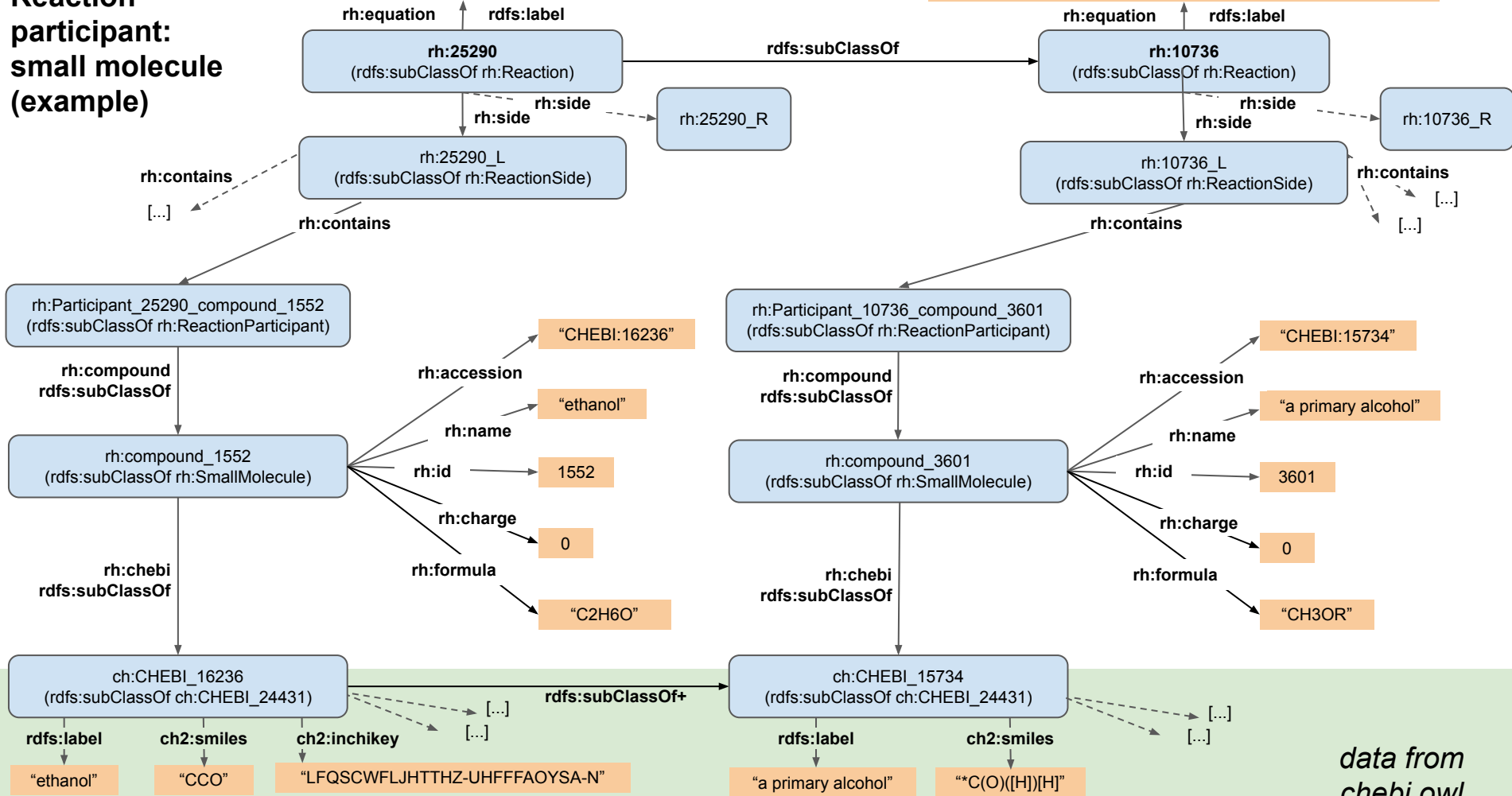
It is a subclass of rh:Compound.

It is a subclass of a given ChEBI chemical entity.

Reaction participant: small molecule (example)

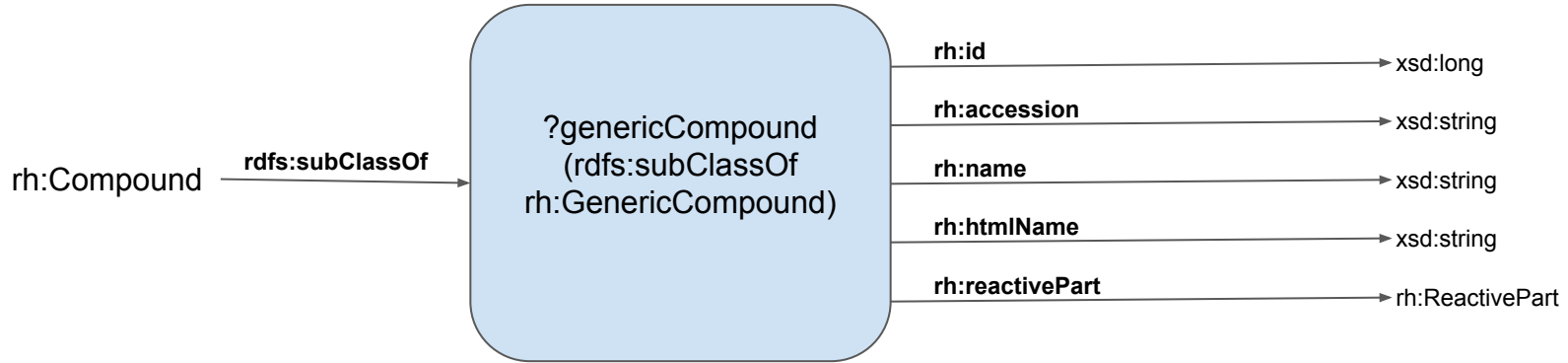
"ethanol + NAD(+) = acetaldehyde + H(+) + NADH"

"a primary alcohol + NAD(+) = an aldehyde + H(+) + NADH"



*data from
chebi.owl*

rh:GenericCompound

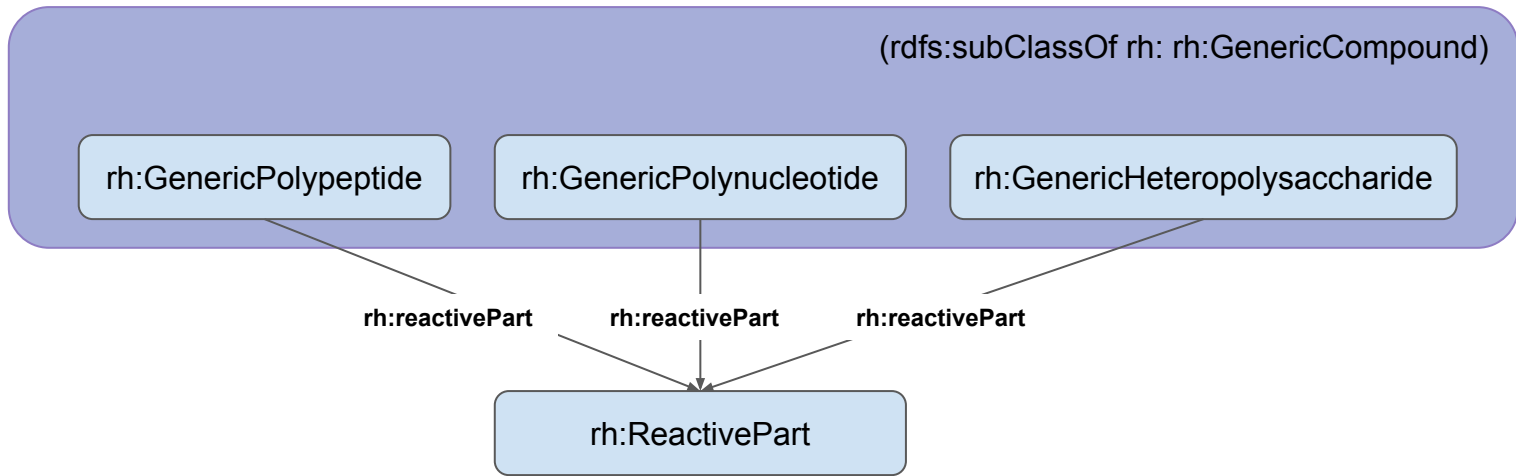


Definition:

A macromolecule involved as participant, in a chemical or transport reaction. Its chemical structure is not fully described but simplified to the functional group(s) involved in the reaction. These reactive part(s) are chemically defined.

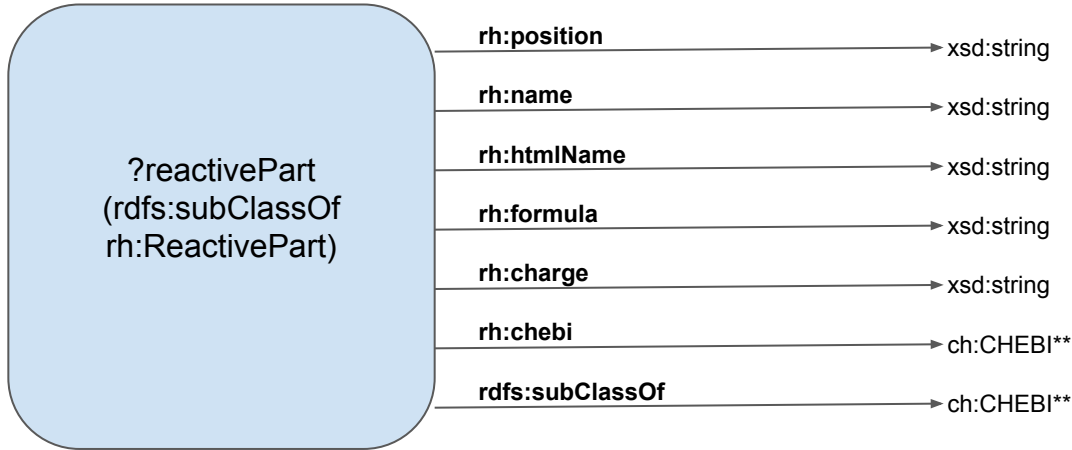
`rh:GenericCompound` represents three kind of macromolecules: proteins (`rh:GenericPolypeptide`), nucleic acids (`rh:GenericPolynucleotide`) and heteropolysaccharides (`rh:GenericHeteropolysaccharide`).

`rh:GenericCompound` is a subclass of `rh:Compound` and is subclassed in `rh:GenericPolypeptide`, `rh:GenericPolynucleotide`, `rh:GenericHeteropolysaccharide`.



rh:GenericPolypeptide	A protein (polypeptide sequence). It is a subclass of rh:GenericCompound.
rh:GenericPolynucleotide	A DNA or RNA nucleic acid (polynucleotide sequence). It is a subclass of rh:GenericCompound.
rh:GenericHeteropolysaccharide	An heteropolysaccharide. It is a subclass of rh:GenericCompound.

rh:ReactivePart

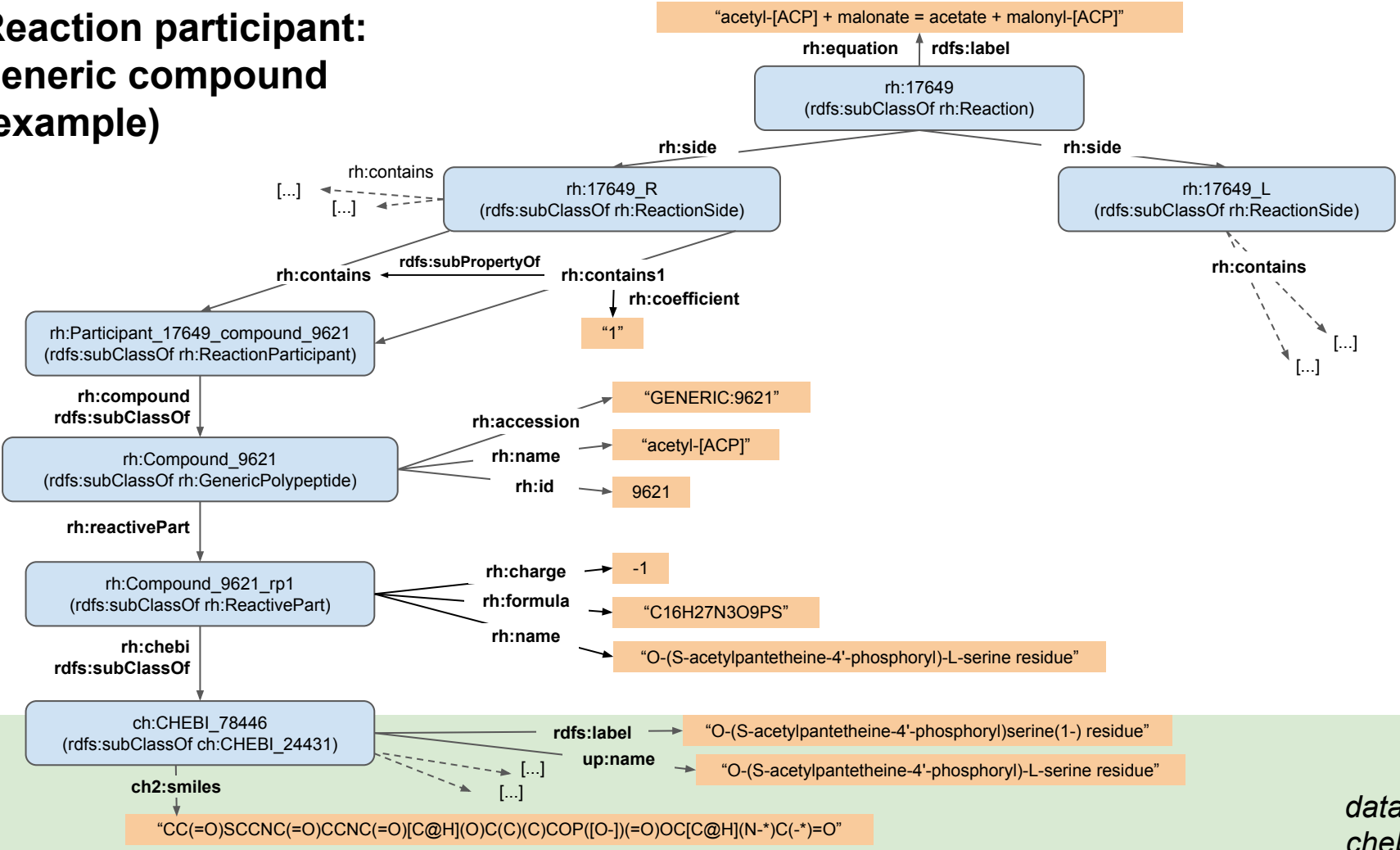


Definition:

The reactive part of a macromolecule (`rh:GenericCompound`). It has a defined chemical structure.

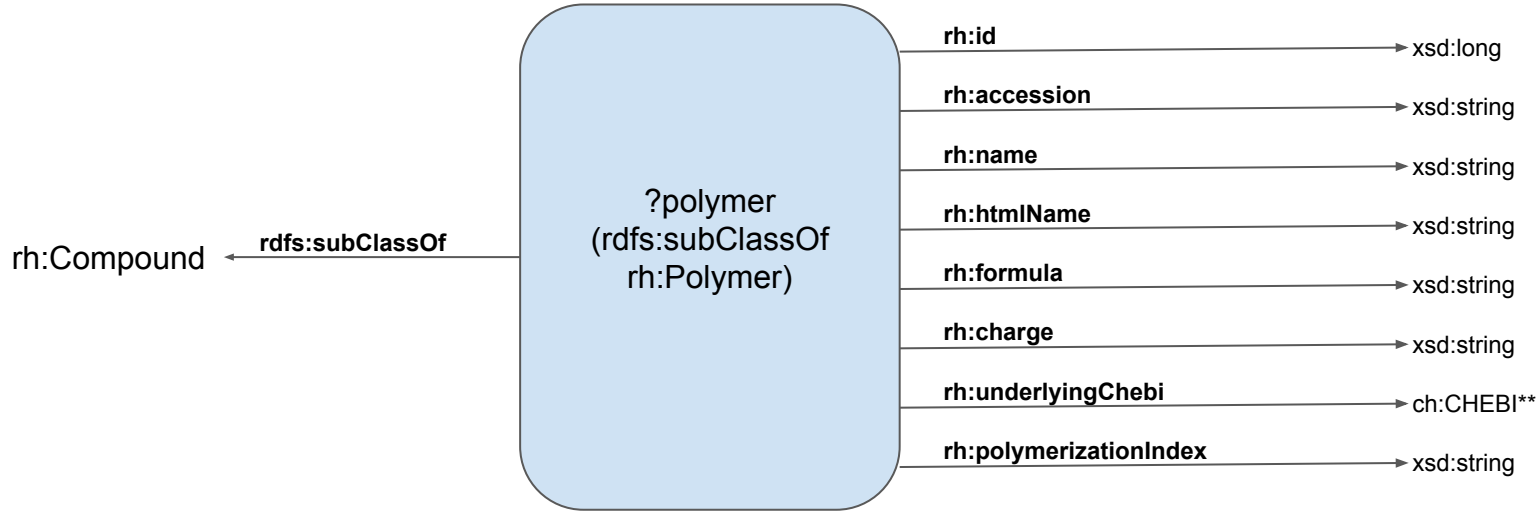
It is a subclass of a given ChEBI chemical entity.

Reaction participant: generic compound (example)



*data from
chebi.owl*

rh:Polymer



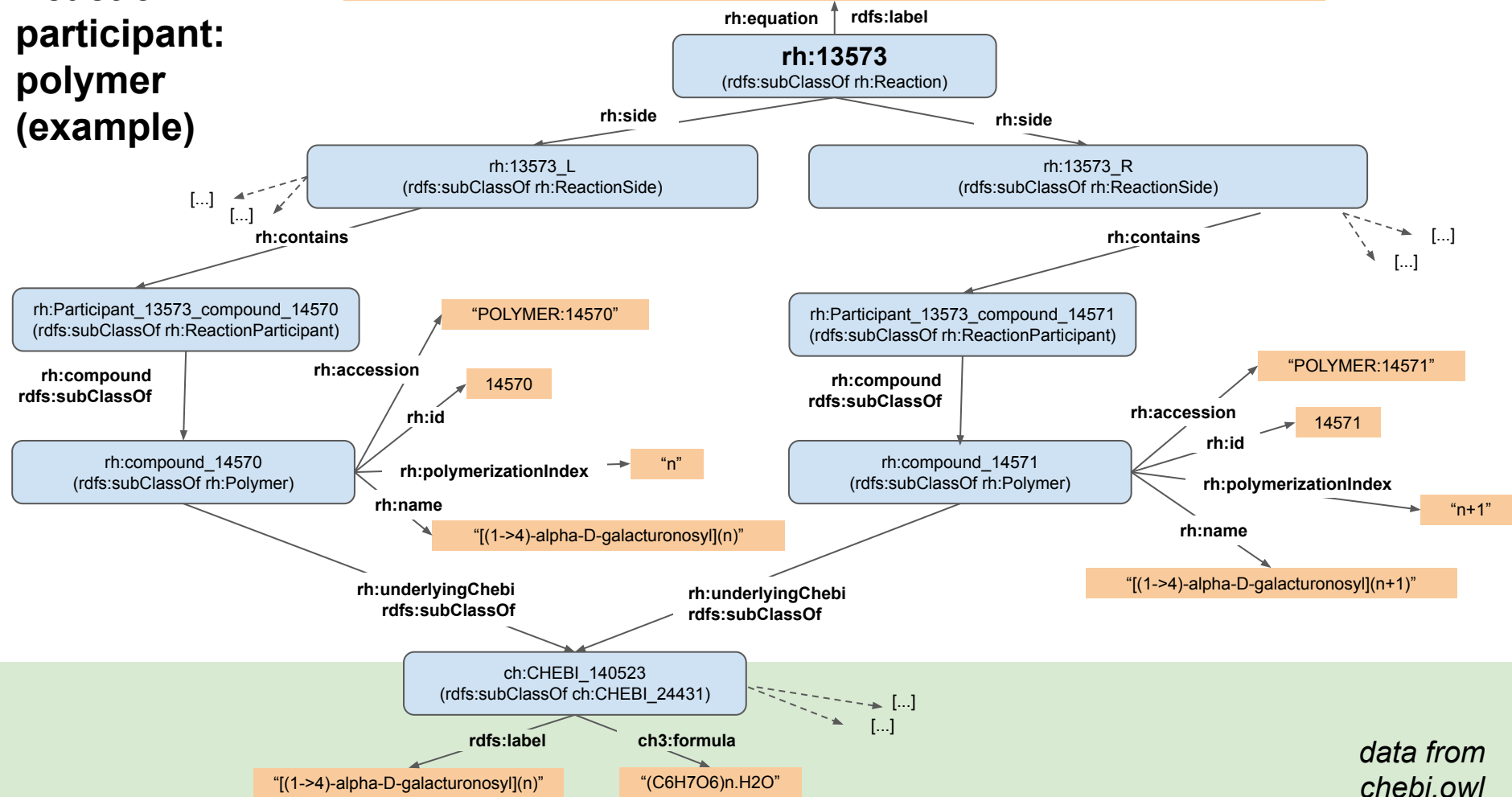
Definition:

A simple polymer (a molecule with defined repeated unit(s) and polymerization index (PI) involved as participant, in a chemical or transport reaction. It is defined by an underlying ChEBI polymer and a PI (n, n+1, n-1, etc).

It is a subclass of rh:Compound.

Reaction participant: polymer (example)

"[(1->4)-alpha-D-galacturonosyl](n) + UDP-alpha-D-galacturonate = [(1->4)-alpha-D-galacturonosyl](n+1) + H(+) + UDP"



data from
chebi.owl

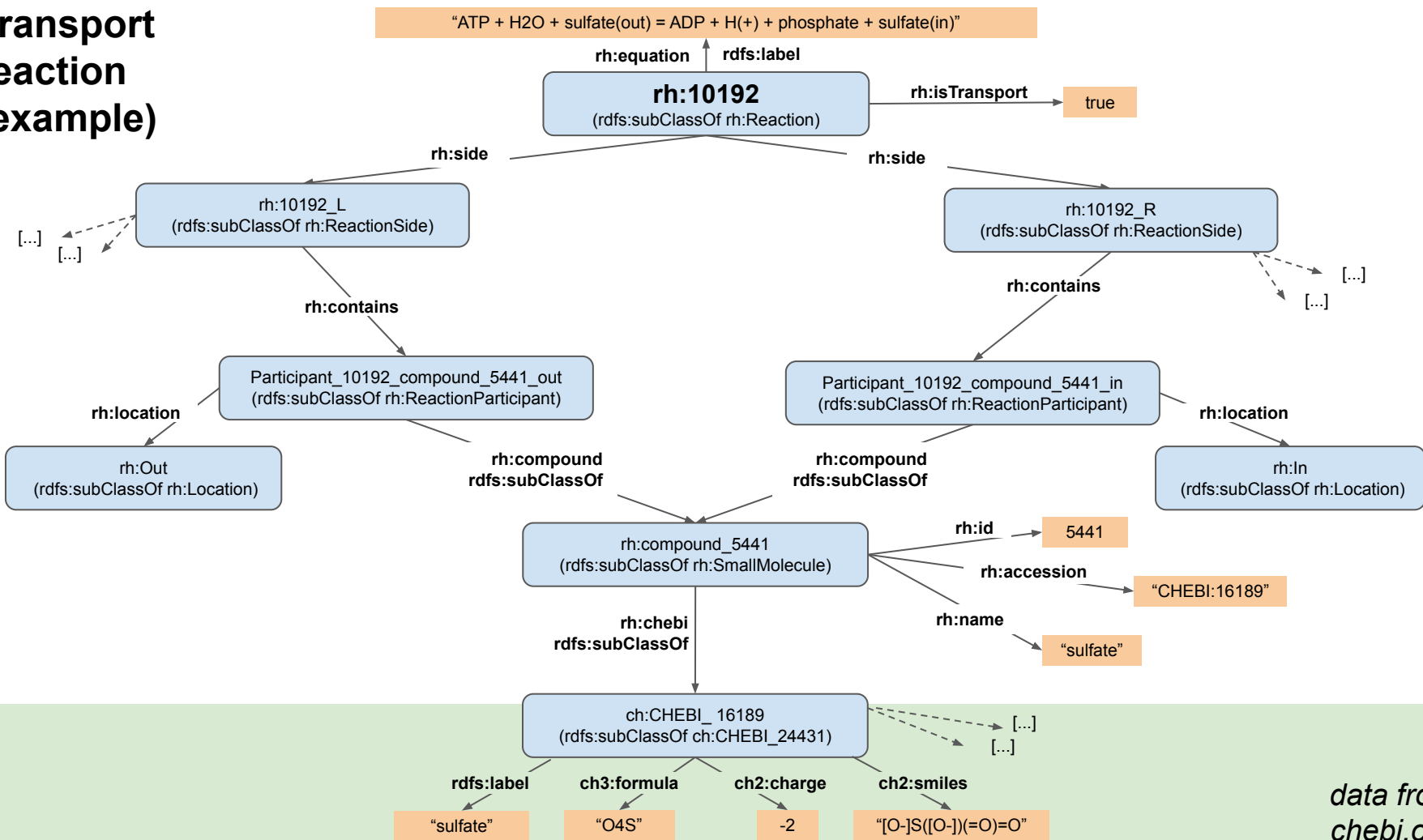
Transport reaction and Location

rh:isTransport	Boolean flag indicating if a reaction is a transport reaction. In transport reaction, the same compound is found in both reaction sides but with a different location.
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rh:Location	The location of a reaction participant (rh:ReactionParticipant) in a transport reaction.
rh:In	It is a subclass of rh:Location.
rh:Out	It is a subclass of rh:Location.



Transport reaction (example)

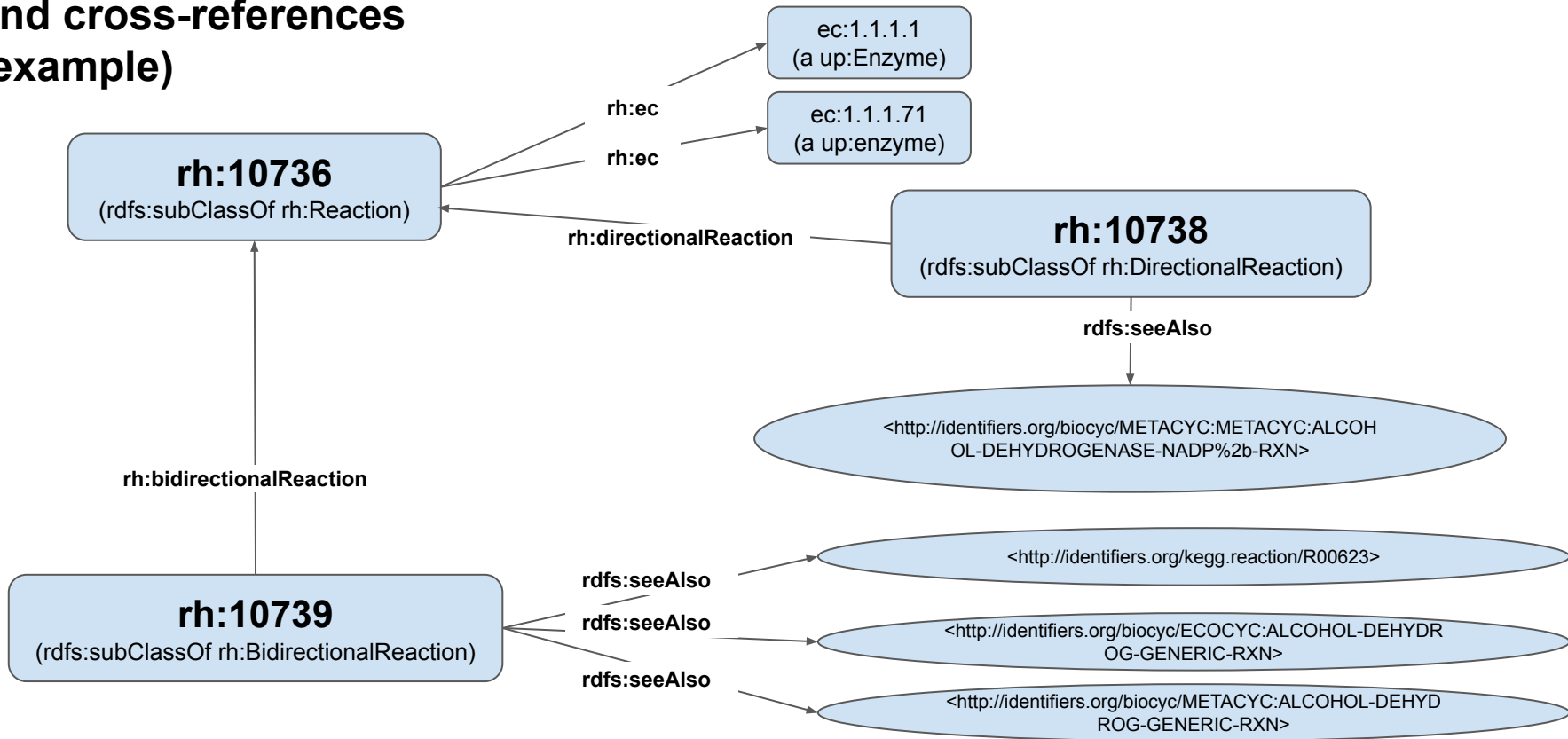


data from
chebi.owl

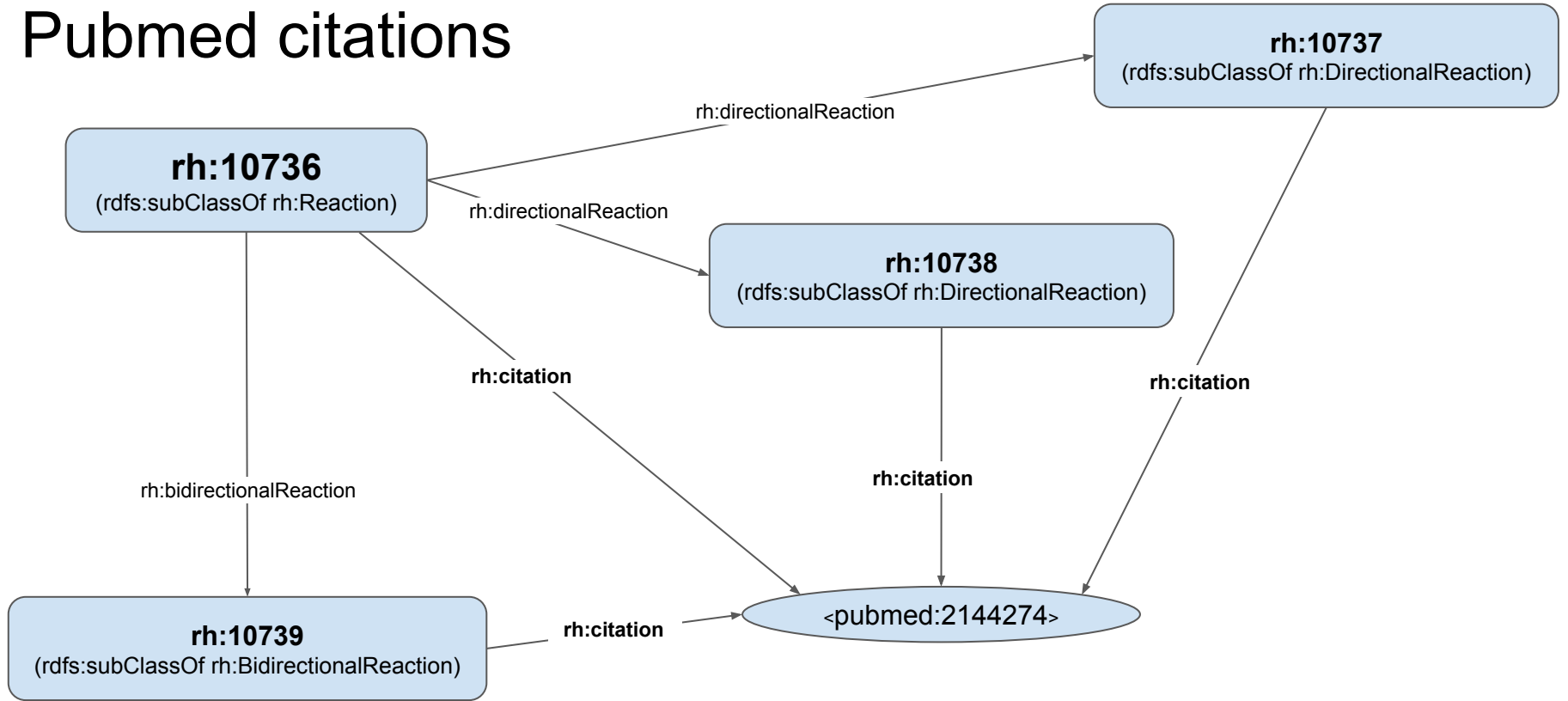
Links to EC numbers and cross-references

rh:ec	<p>The nomenclature committee of the IUBMB defines enzyme classes based, among others, on the catalyzed reaction(s). The enzyme classes are identified by an Enzyme Commission number (EC number).</p> <p>rh:ec is used between a rh:Reaction (the catalyzed reaction) and a complete EC number (the enzyme class).</p>
rdfs:seeAlso	<p>The cross-references to other metabolic/protein resources.</p> <p>There are two kind of cross-references:</p> <ul style="list-style-type: none">- Manually curated (KEGG reaction, MetaCyc reaction, EcoCyc reaction)- Computed based on ChEBI participants (Reactome (hsa reaction), MACiE reaction) <p>The MetaCyc/EcoCyc reactions are linked to either rh:Reaction (no define direction), rh:DirectionalReaction or rh:BidirectionalReaction.</p> <p>The KEGG reactions are linked to rh:BidirectionalReaction.</p> <p>The cross-references to UniProt protein entries are not part of the rhea.rdf distribution. They are available from the uniprot.rdf distribution.</p>

EC numbers and cross-references (example)

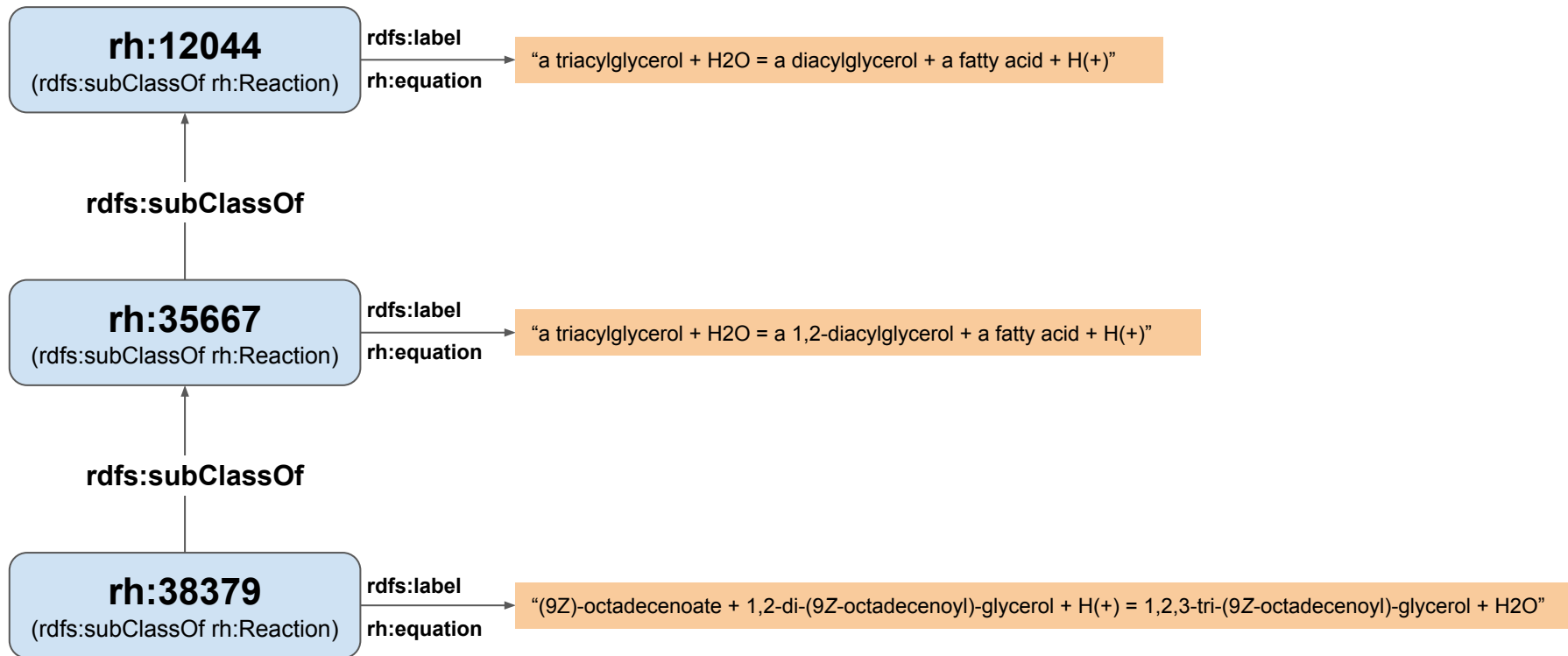


Pubmed citations



rh:citation	The relation between a rh:Reaction, a rh:DirectionalReaction or rh:BidirectionalReaction and a PubMed URI.
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Reaction hierarchical classification



Rhea curation status

rh:Status	Curation status of a reaction (rh:Reaction).
rh:Approved	Manually curated reaction. The reaction is evidenced and is chemically balanced at the level of mass and charge. It is a subclass of rh:Status.
rh:Preliminary	Manually curated reaction. The reaction is indirectly evidenced and/or some knowledge is missing (e.g it has some undefined participant(s)). The reaction is possibly not balanced at the level of mass and charge. It is a subclass of rh:Status.
rh:Obsolete	The reaction is no more valid.

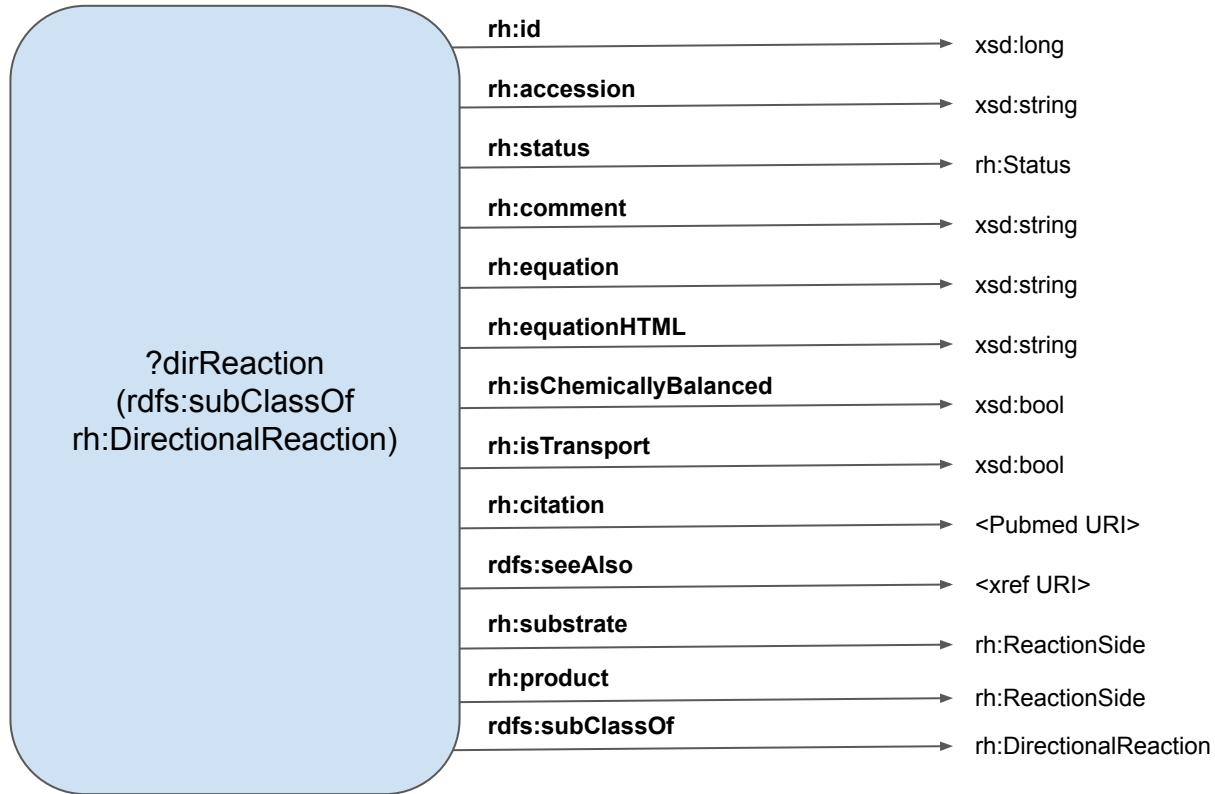
(rdfs:subClassOf rh:Status)

rh:Approved

rh:Preliminary

rh:Obsolete

rh:DirectionalReaction



Definition:

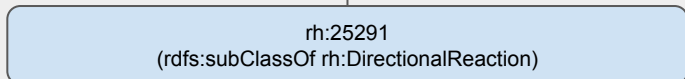
A chemical or transport reaction of biological interest with a direction specified by substrates and products.

All the directional reactions published by Rhea are rdfs:subClassOf rh:DirectionalReaction.

rh:DirectionalReaction (example1)

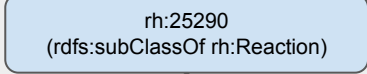
"ethanol + NAD(+) => acetaldehyde + H(+) + NADH"

rh:equation
rdfs:label



"ethanol + NAD(+) = acetaldehyde + H(+) + NADH"

rh:equation
rdfs:label



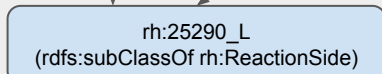
rh:directionalReaction

rh:substrate

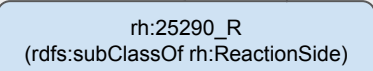
rh:side

rh:side

rh:product



rh:transformableTo



rh:contains

[...]

[...]

rh:transformableTo

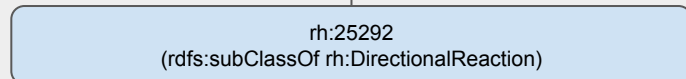
rh:contains

[...]

[...]

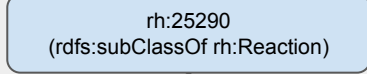
"acetaldehyde + H(+) + NADH => ethanol + NAD(+)"

rh:equation
rdfs:label



"ethanol + NAD(+) = acetaldehyde + H(+) + NADH"

rh:equation
rdfs:label



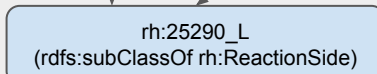
rh:directionalReaction

rh:product

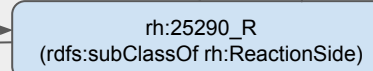
rh:side

rh:side

rh:substrate



rh:transformableTo



rh:contains

[...]

[...]

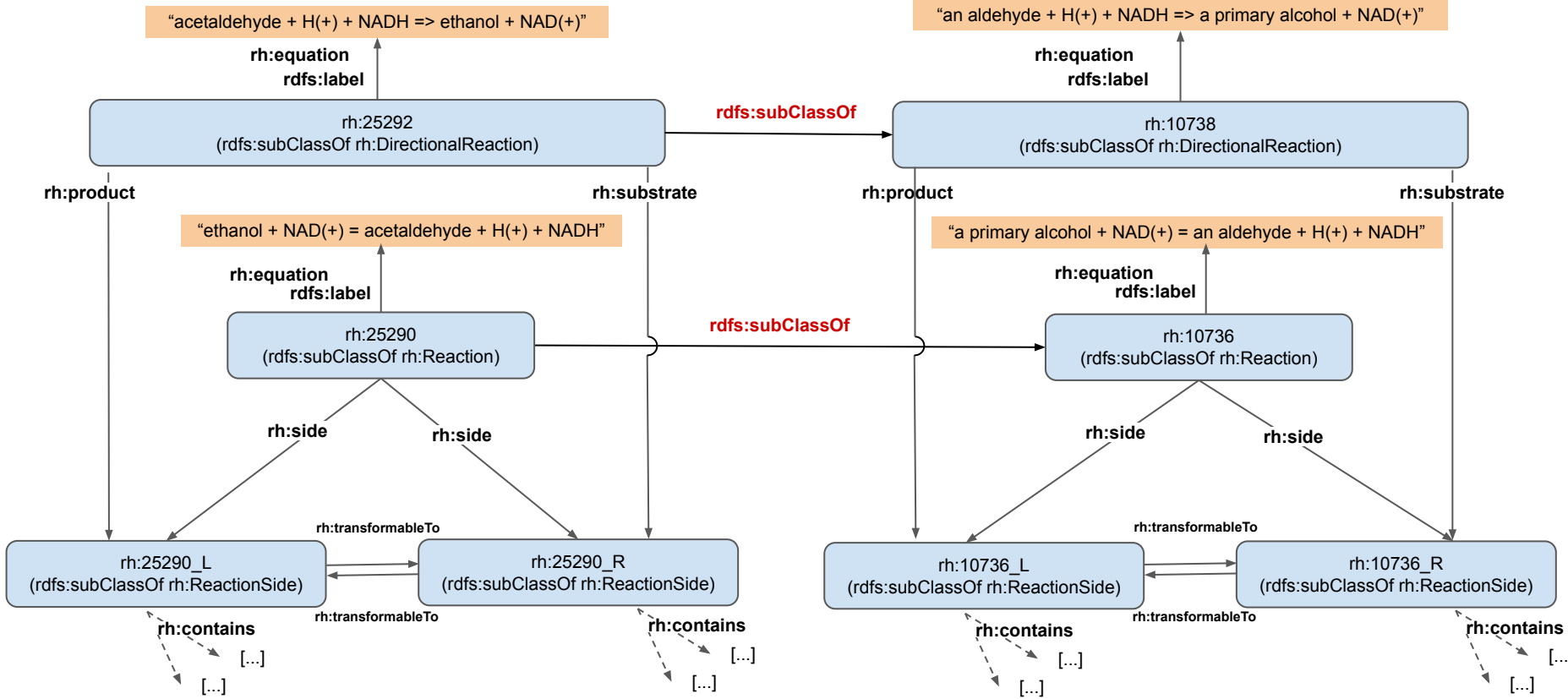
rh:transformableTo

rh:contains

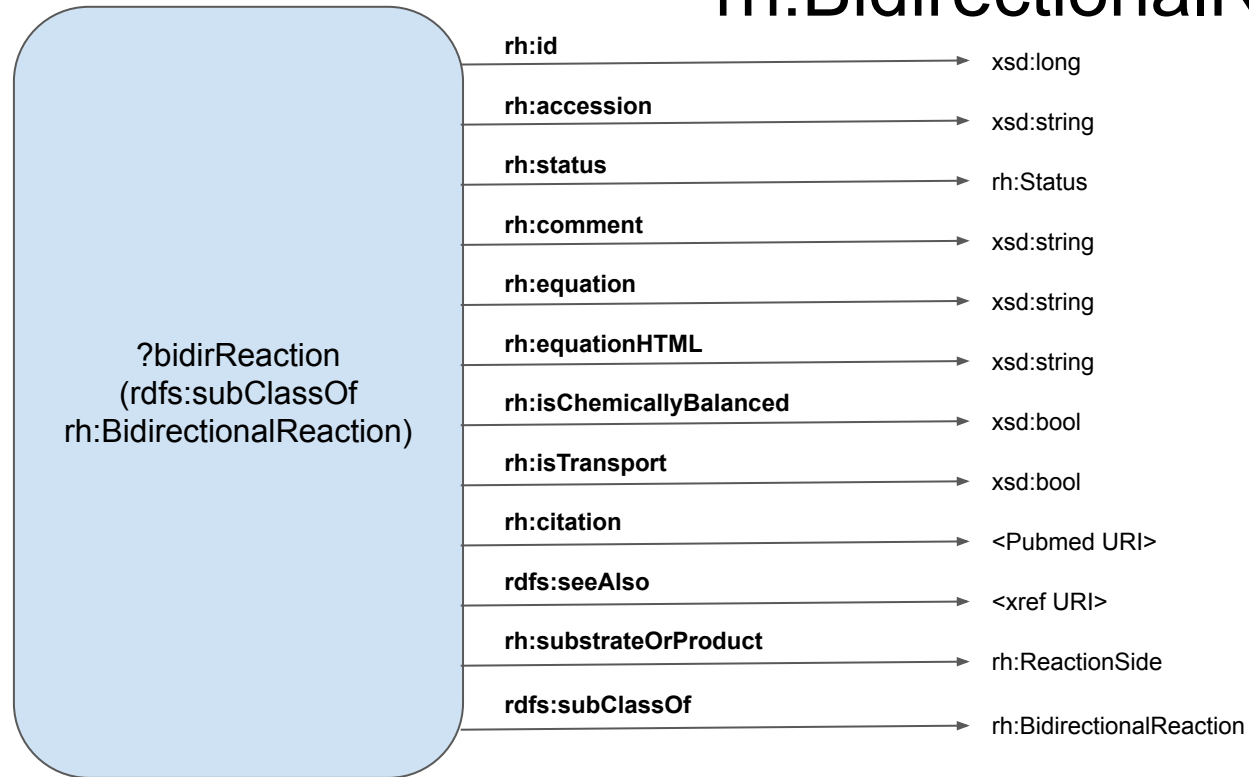
[...]

[...]

rh:DirectionalReaction (example2)



rh:BidirectionalReaction

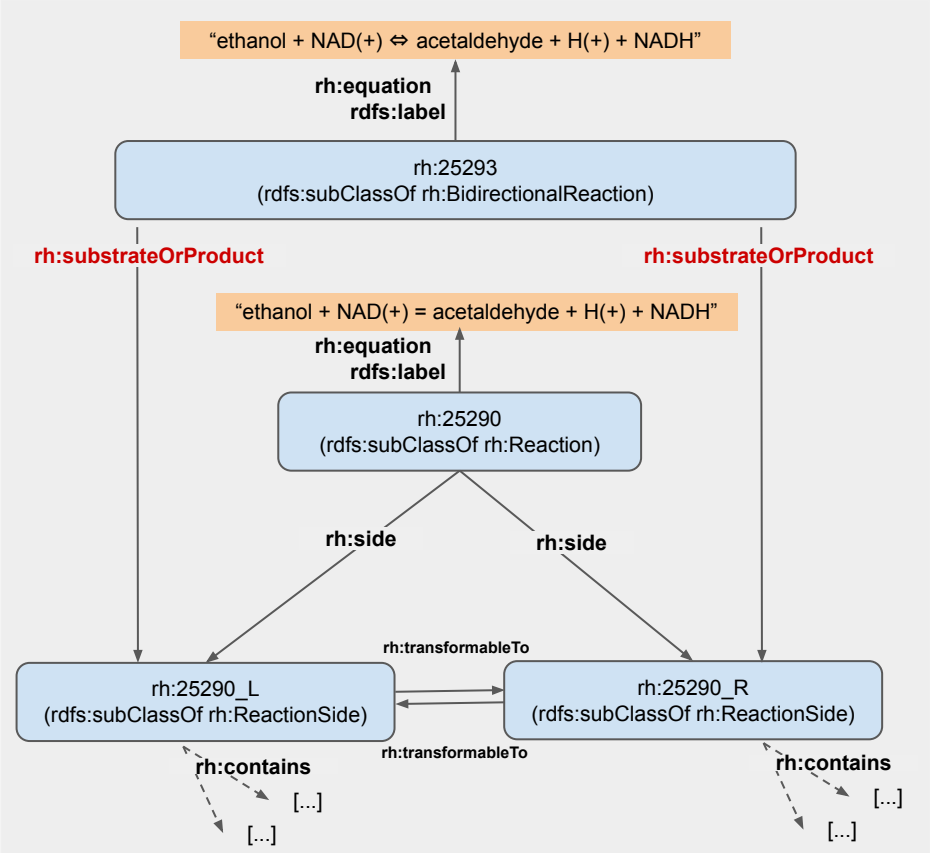


Definition:

A chemical or transport reaction of biological interest which can happen in one direction or the other, depending on the physiological conditions.

All the bidirectional reactions published by Rhea are `rdfs:subClassOf rh:BidirectionalReaction`.

rh:BidirectionalReaction (example1)



rh:BidirectionalReaction (example2)

