CHEMICAL KNOWLEDGE REPRESENTATION WITH DESCRIPTION GRAPHS AND LOGIC PROGRAMMING

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December 9, 2011



OWL for the representation of molecular structures



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- OWL for the representation of molecular structures
- OWL ontology Chemical Entities of Biological Interest





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- OWL for the representation of molecular structures
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 - High quality annotation and taxonomy of chemical compounds

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Interoperability between researchers

- OWL for the representation of molecular structures
- OWL ontology Chemical Entities of Biological Interest
 - High quality annotation and taxonomy of chemical compounds
 - Interoperability between researchers
 - Drug discovery and elucidation of metabolic pathways





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ChEBI is manually incremented

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ChEBI is manually incremented

Currently ~ 27,000 fully annotated entries

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Is dinitrogen inorganic?

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- Each new molecule is subsumed by several chemical classes
 - Is dinitrogen inorganic?
 - Does cyclobutane contain a four-membered ring?

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Is acetylene a hydrocarbon?

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- Is acetylene a hydrocarbon?
- Does benzaldehyde contain a benzene ring?

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Speed up curating tasks with automated reasoning tools

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- Each new molecule is subsumed by several chemical classes
 - Is dinitrogen inorganic? ~> Yes
 - Does cyclobutane contain a four-membered ring? ~ Yes

- Is acetylene a hydrocarbon? ~ Yes
- Does benzaldehyde contain a benzene ring? ~> Yes

Speed up curating tasks with automated reasoning tools

Chemical compounds are highly cyclic



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- Chemical compounds are highly cyclic
- OWL fundamentally inable to represent cycles
 - Does cyclobutane contain a four-membered ring? ×



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EXAMPLE

Cyclobutane \sqsubseteq (= 4)hasAtom.(Carbon \sqcap (= 2)hasBond.Carbon)

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(MIS) representing chemicals with OWL

- Chemical compounds are highly cyclic
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 - Does cyclobutane contain a four-membered ring? ×
- Limitations of OWL (partially) remedied by extension of OWL with Description Graphs and rules [Motik et al., 2009]



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Switch to logic programming

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 - Replace classical negation with negation-as-failure

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 - Translate DGs into logic programs with function symbols

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 Expressive and decidable logic-based formalism for chemical knowledge representation

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- Encouraging results of a preliminary evaluation

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- Encouraging results of a preliminary evaluation
- Thank you. See you in the poster session!