Extending Logic Programming for Life Sciences Applications

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Department of Computer Science, University of Oxford

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Bioinformatics and Semantic Technologies

- Life sciences data deluge

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- Hierarchical organisation of biochemical knowledge

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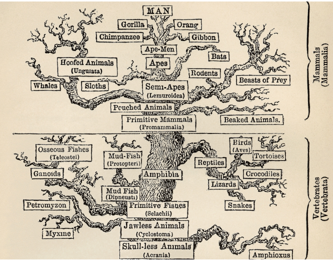

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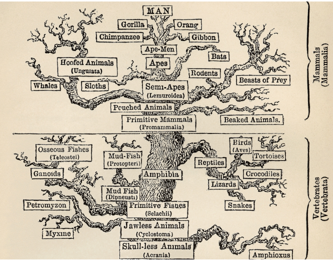

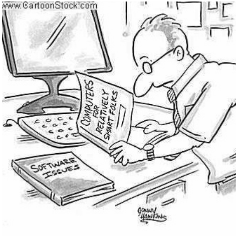

Manual Labor

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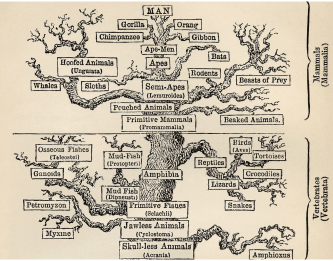

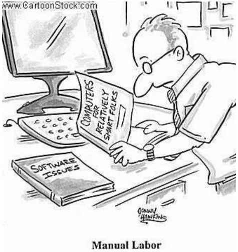

- Fast, automatic and repeatable classification driven by Semantic technologies

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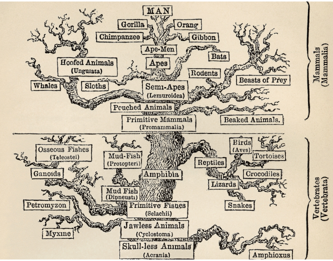

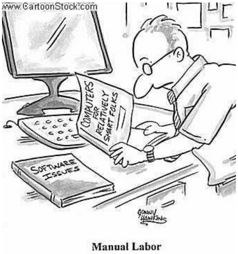

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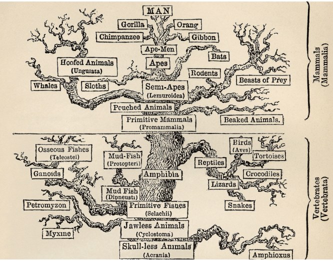

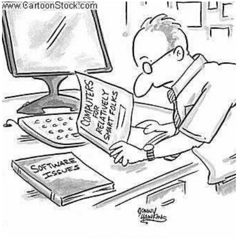

Manual Labor

- Fast, automatic and repeatable classification driven by Semantic technologies
- Web Ontology Language, a W3C standard family of logic-based formalisms
- OWL bio- and chemo-ontologies widely adopted

The ChEBI Ontology

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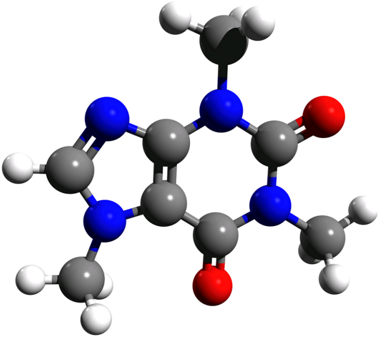

$\rightsquigarrow$ caffeine is a cyclic molecule

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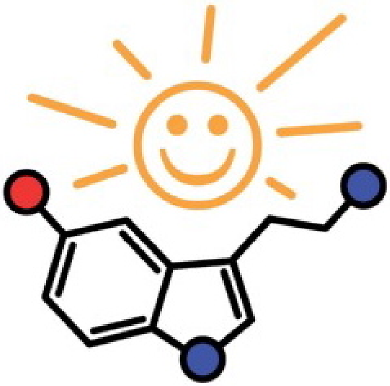

$\rightsquigarrow$ serotonin is an organic molecule

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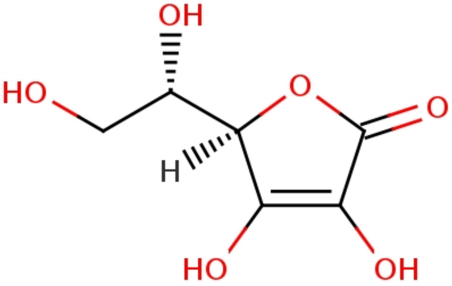

$\rightsquigarrow$ ascorbic acid is a carboxylic ester

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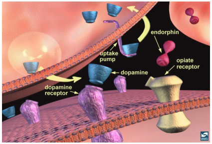

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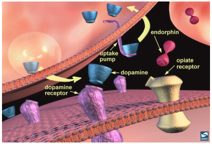

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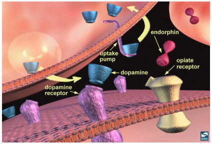

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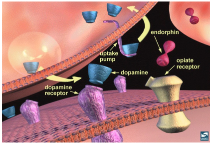

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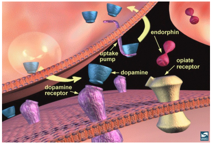

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- Speed up growth by automating chemical classification

Expressivity Limitations of OWL

1. At least one tree-shaped model for each consistent OWL ontology $\rightsquigarrow$ problematic representation of cycles

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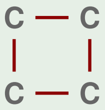

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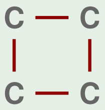
$$\text{Cyclobutane} \sqsubseteq \exists(=4)\text{hasAtom}.(\text{Carbon} \sqcap \exists(=2)\text{hasBond}.\text{Carbon})$$



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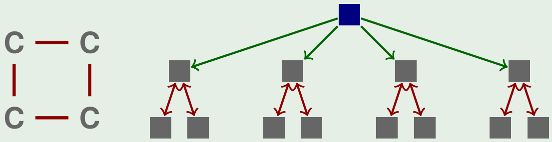

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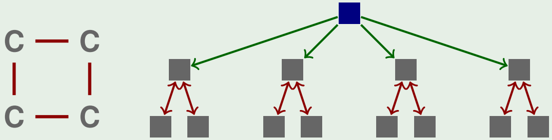

- OWL-based reasoning support
  1. Is cyclobutane a cyclic molecule? ✘

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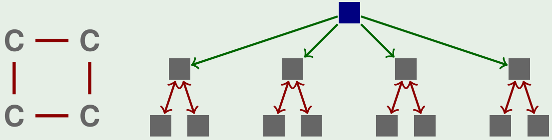

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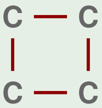

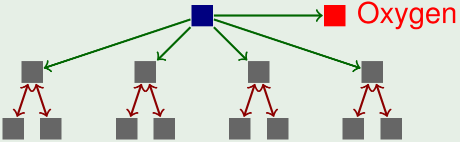

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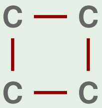

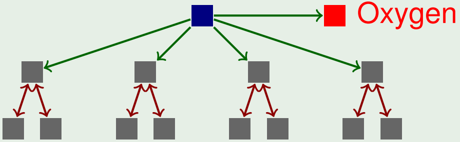

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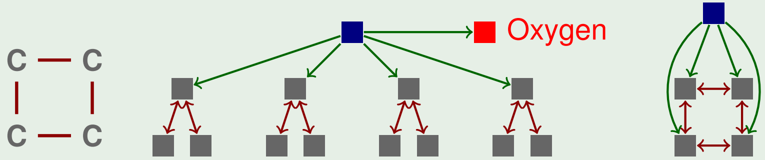

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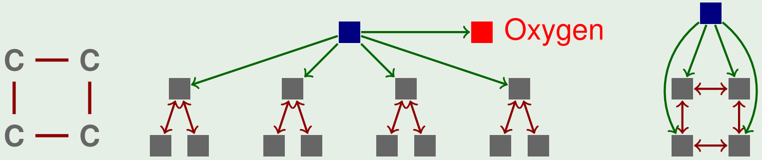

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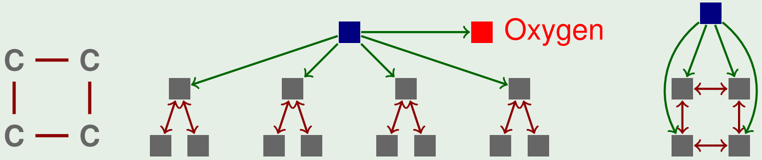

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Results overview

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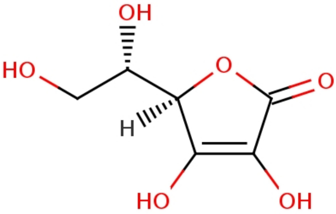
Language for representing complex objects with a favourable performance/expressivity trade-off

Classifying Structured Objects



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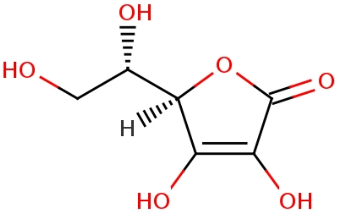

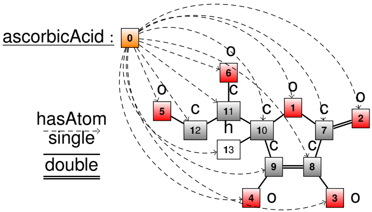

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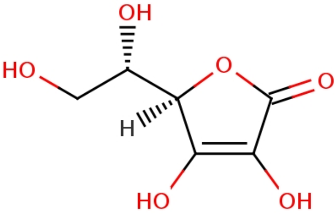

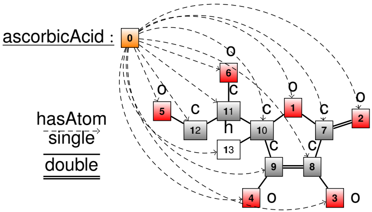

$$\text{ascorbicAcid}(x) \rightarrow \text{hasAtom}(x, f_1(x)) \wedge \ldots \wedge \text{hasAtom}(x, f_{13}(x))$$
$$\text{o}(f_1(x)) \wedge \ldots \wedge \text{c}(f_7(x)) \wedge \ldots \wedge$$
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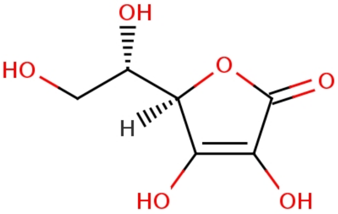
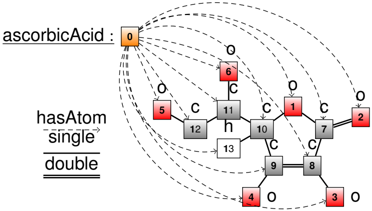
CLASSIFYING STRUCTURED OBJECTS





$$\textcolor{orange}{\mathrm{ascorbicAcid}}(x) \rightarrow \mathrm{hasAtom}(x, f_1(x)) \wedge \ldots \wedge \mathrm{hasAtom}(x, f_{13}(x))$$
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$$\mathrm{single}(f_1(x), f_7(x)) \wedge \mathrm{double}(f_7(x), f_2(x)) \wedge \ldots$$

$$\mathrm{hasAtom}(x, y_1) \wedge \mathrm{hasAtom}(x, y_2) \wedge y_1 \neq y_2 \rightarrow \mathrm{polyatomicEntity}(x)$$

$$\wedge_{i=1}^{5} \mathrm{hasAtom}(x, y_i) \wedge \textcolor{gray}{\mathrm{c}}(y_1) \wedge \textcolor{red}{\mathrm{o}}(y_2) \wedge \textcolor{red}{\mathrm{o}}(y_3) \wedge$$
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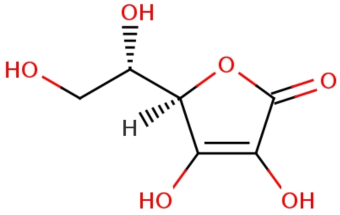
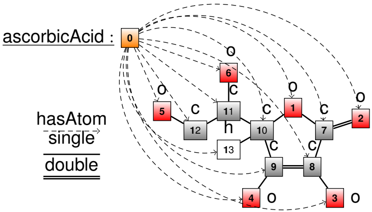
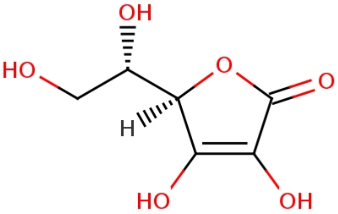
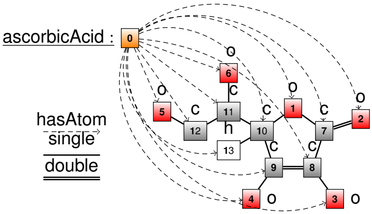




Input fact: ascorbicAcid(a)
Stable model: ascorbicAcid(a), hasAtom(a, a^f_i) for $1 \le i \le 13$, o(a^f_i) for $1 \le i \le 6$, c(a^f_i) for $7 \le i \le 12$, h(a^f_{13}), single(a^f_8, a^f_3), single(a^f_9, a^f_4), single(a^f_{12}, a^f_i) for $i \in \{5, 11\}$, single(a^f_{11}, a^f_6), single(a^f_{10}, a^f_i) for $i \in \{1, 9, 11, 13\}$, single(a^f_7, a^f_i) for $i \in \{1, 8\}$, double(a^f_2, a^f_7), double(a^f_8, a^f_9), horc(a^f_i) for $7 \le i \le 13$, polyatomicEntity(a), carboxylicEster(a), cyclic(a)





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$\rightsquigarrow$ Ascorbic acid is a cyclic polyatomic entity and a carboxylic ester

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- Model-faithful and model-summarising acyclicity (MFA and MSA): capture as generally as possible class of programs with models of finite size

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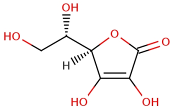
  - Ascorbic acid is asserted to be a carboxylic acid (release 95)
  - Not listed among the subsumptions derived by our prototype



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$$\wedge_{i=1}^{5} \mathsf{hasAtom}(x, y_i) \wedge \mathsf{c}(y_1) \wedge \mathsf{o}(y_2) \wedge \mathsf{o}(y_3) \wedge \mathsf{c}(y_4) \wedge$$
$$\mathsf{double}(y_1, y_2) \wedge \mathsf{single}(y_1, y_3) \wedge \mathsf{single}(y_3, y_4) \wedge \mathsf{single}(y_1, y_5)$$
$$\rightarrow \mathsf{carboxylicEster}(x)$$

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    define carboxylicEster
    some hasAtom SMILES$(\mathrm{C}-\mathrm{O}-\mathrm{C}(=\mathrm{O})-*)$
    end.

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    E.g., Carboxylic ester is an organic molecular entity

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- Thank you! Questions?!?