Ontology-Based Classification of Molecules: a Logic Programming Approach

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Department of Computer Science, University of Oxford

November 30, 2012

BIOINFORMATICS AND SEMANTIC TECHNOLOGIES

- Life sciences data deluge

Bioinformatics and Semantic Technologies

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- Hierarchical organisation of biochemical knowledge

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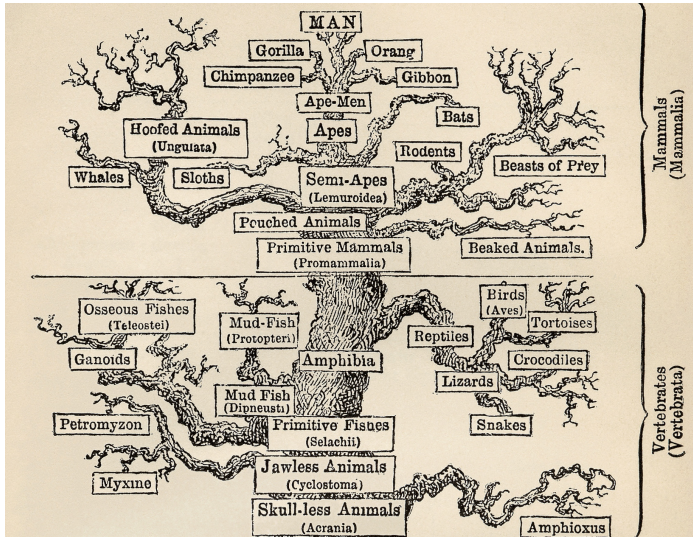

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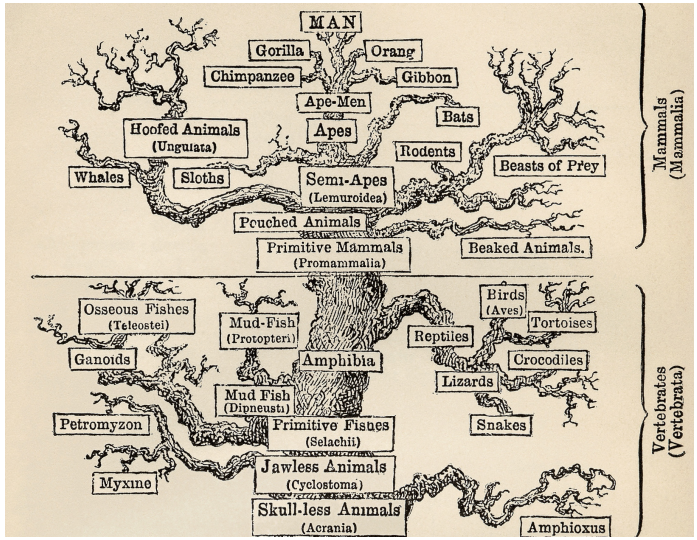

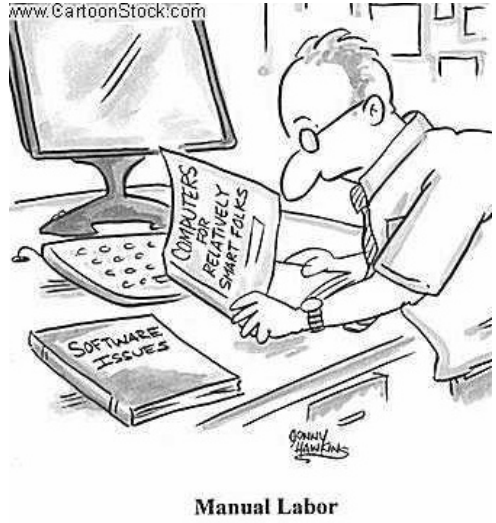

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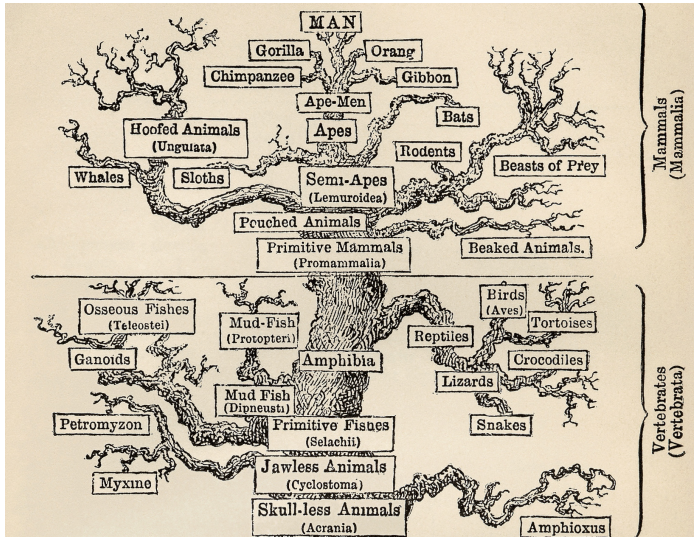

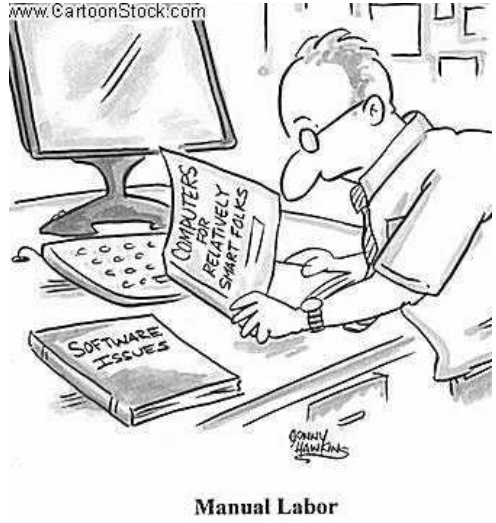

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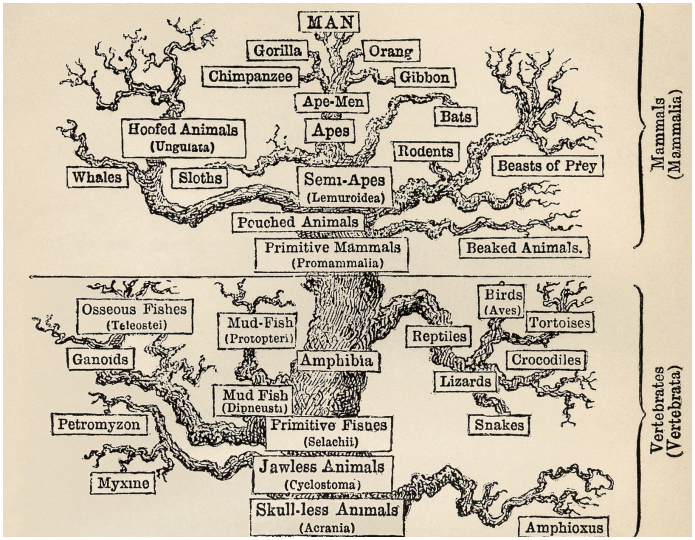

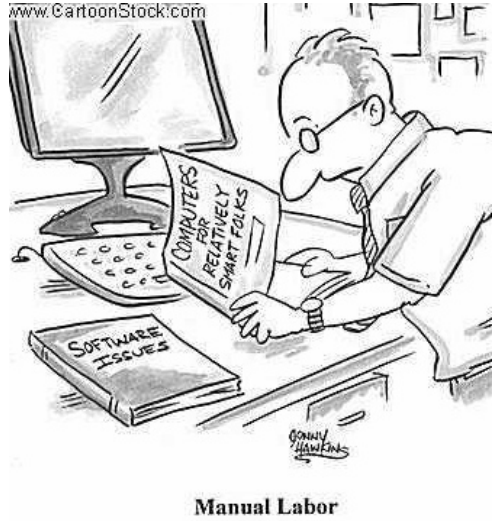

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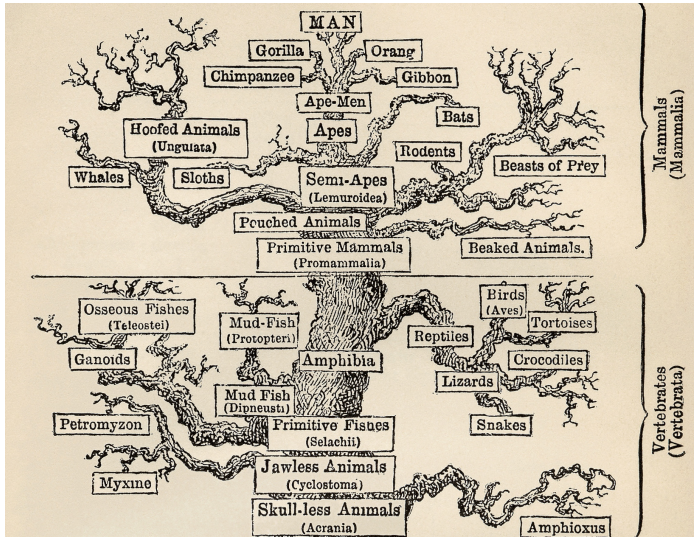

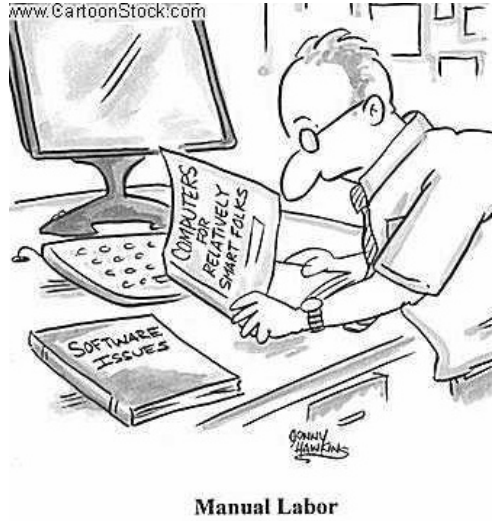

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- Web Ontology Language, a W3C standard family of logic-based formalisms
- OWL bio- and chemo-ontologies widely adopted

THE CHEBI ONTOLOGY

- OWL ontology Chemical Entities of Biological Interest

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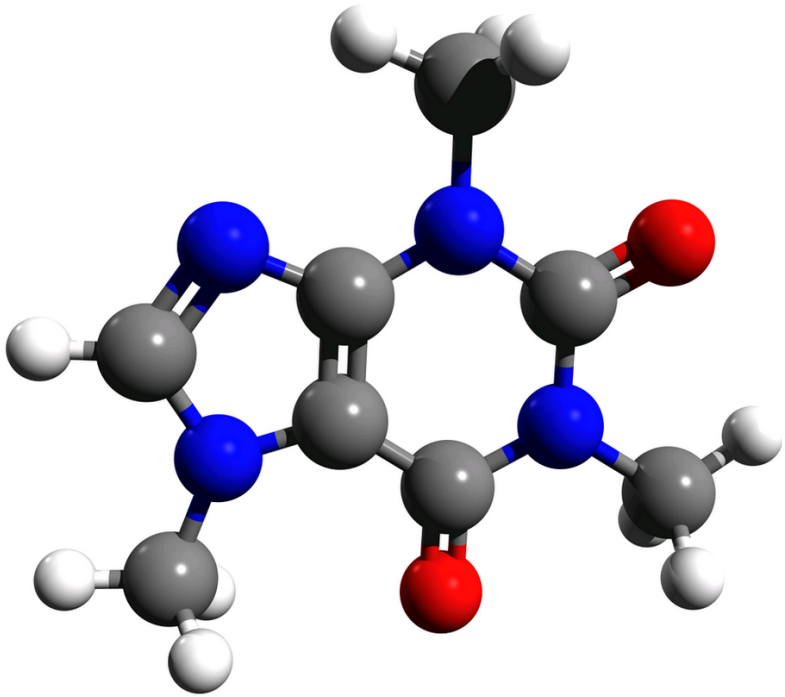

⇝ caffeine is a cyclic molecule

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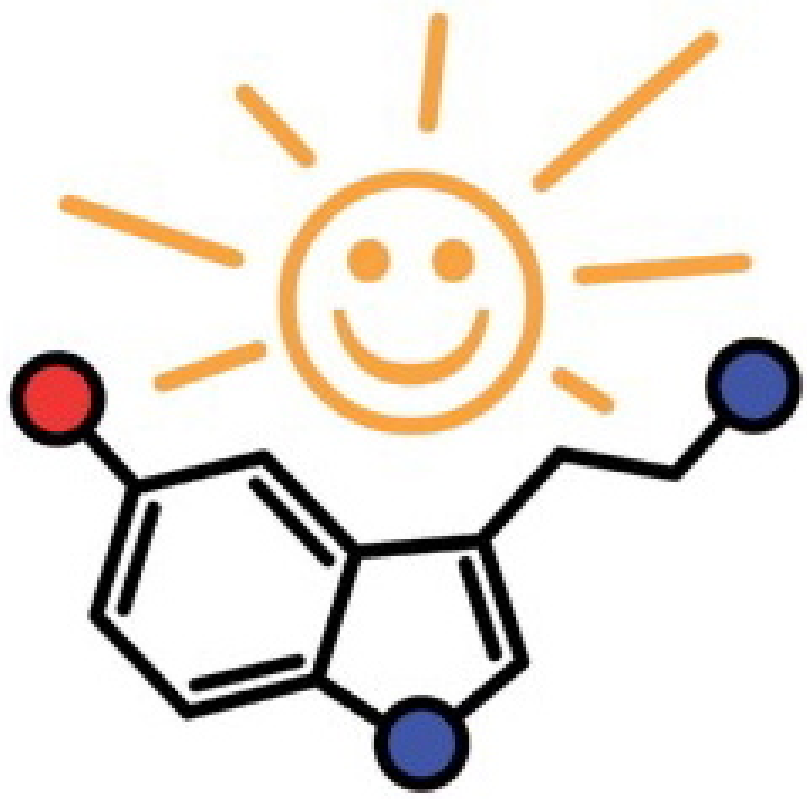

$\rightsquigarrow$ serotonin is an organic molecule

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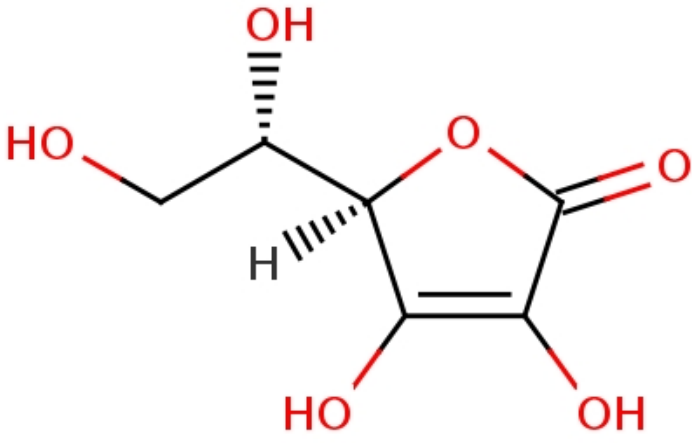

$\rightsquigarrow$ ascorbic acid is a carboxylic ester

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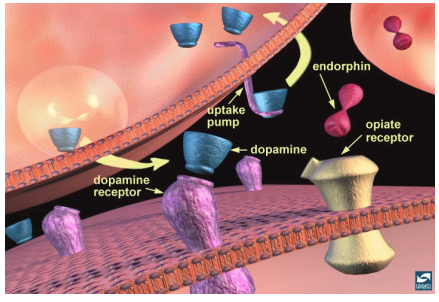

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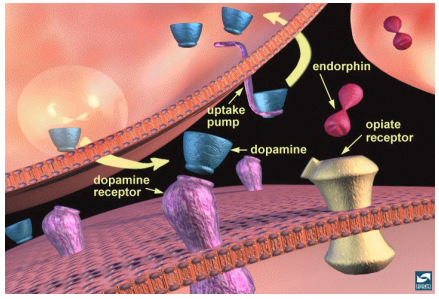

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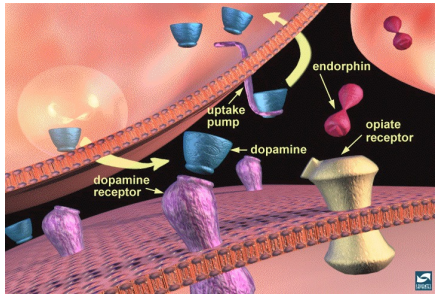

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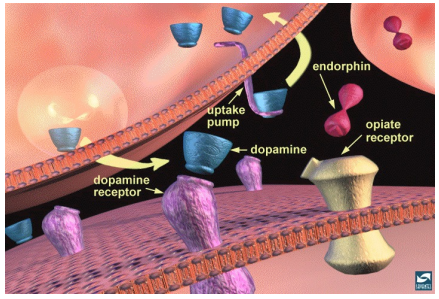

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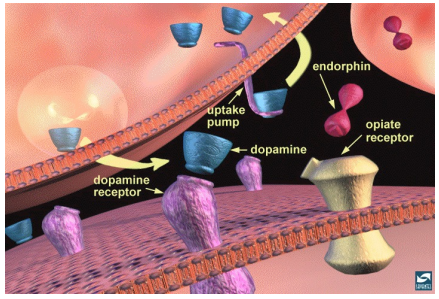

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- Speed up growth by automating chemical classification

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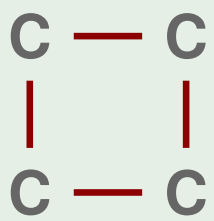

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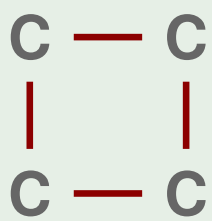
$$\text{Cyclobutane} \sqsubseteq \exists(=4)\text{hasAtom}.(\text{Carbon} \sqcap \exists(=2)\text{hasBond}.\text{Carbon})$$



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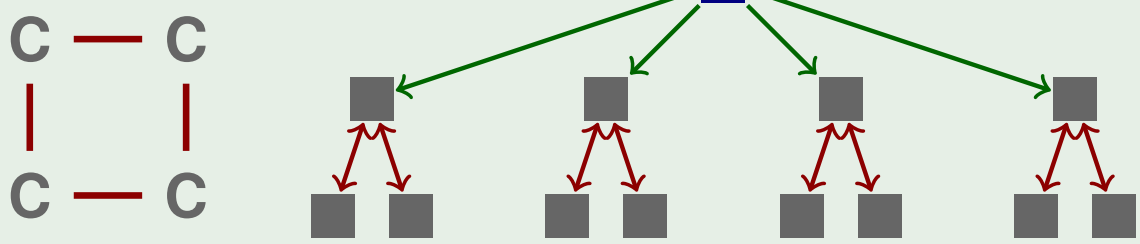

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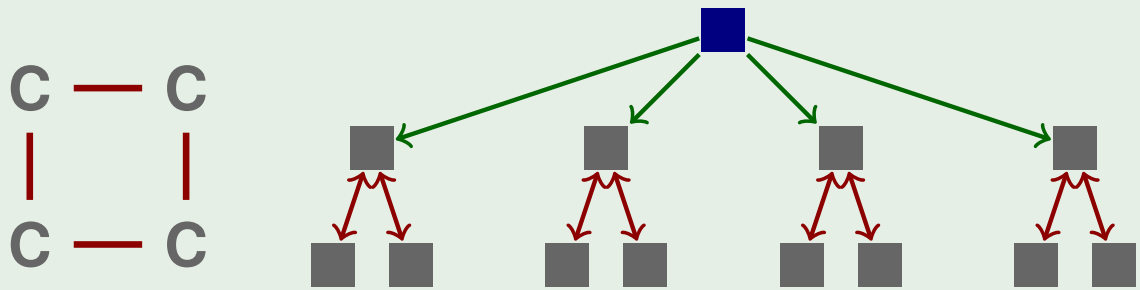

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  1. Is cyclobutane a cyclic molecule? ✘

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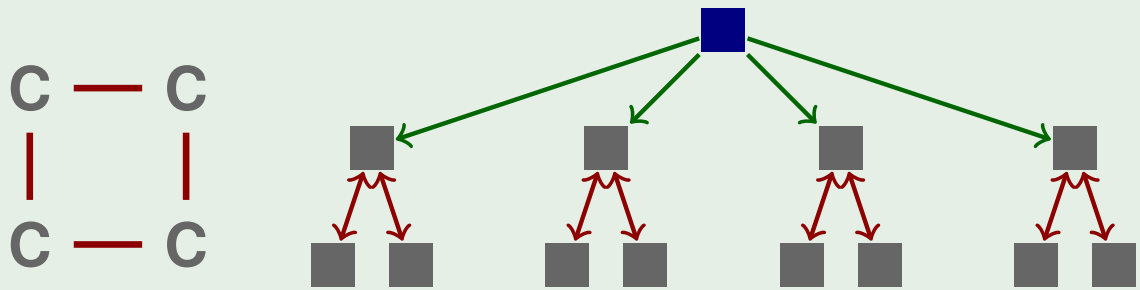

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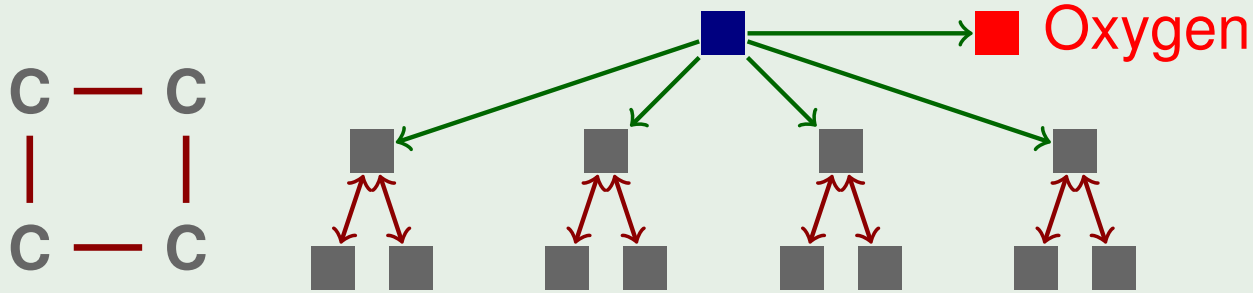

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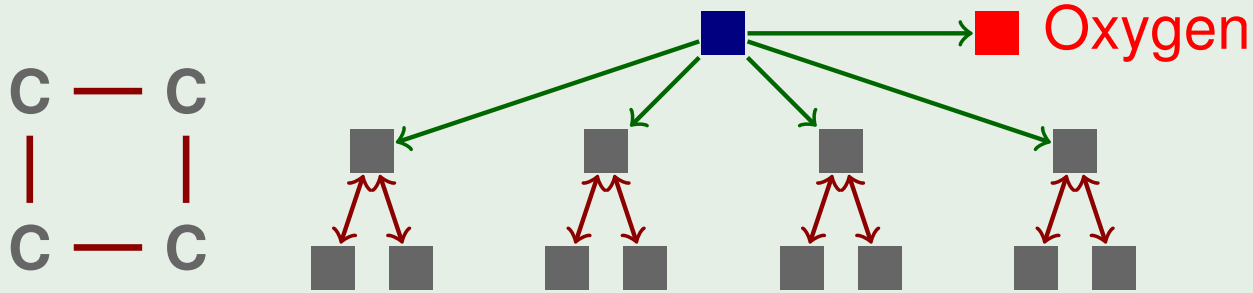

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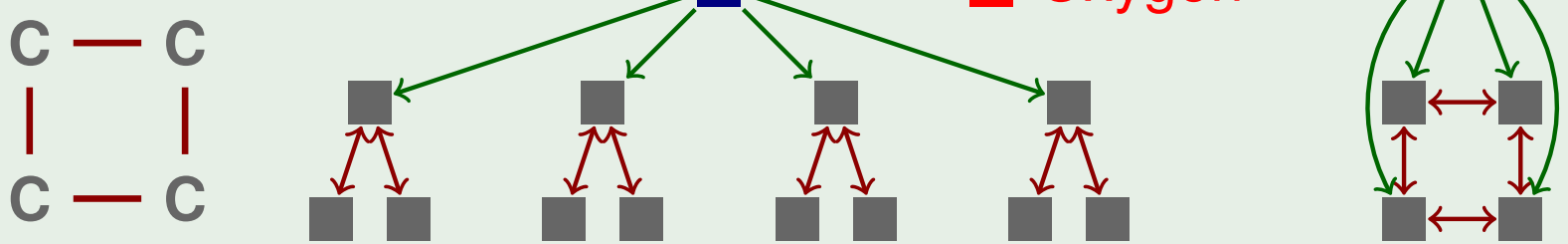

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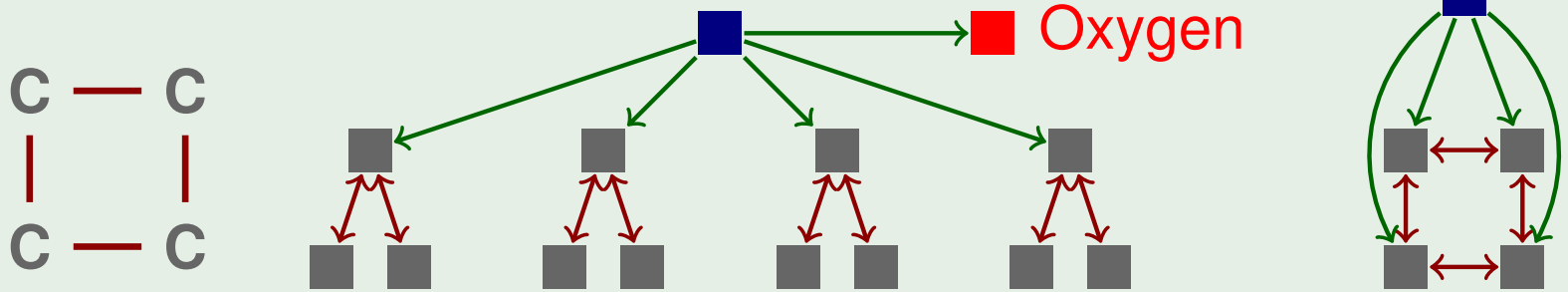

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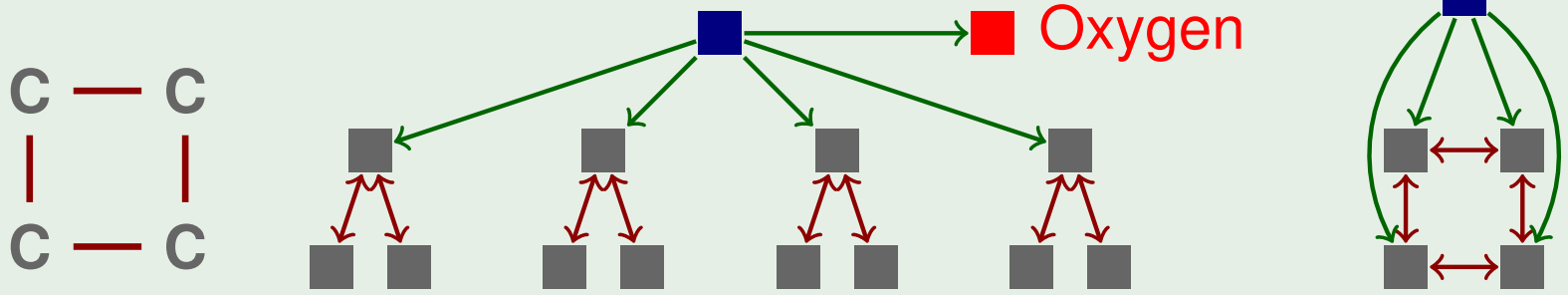

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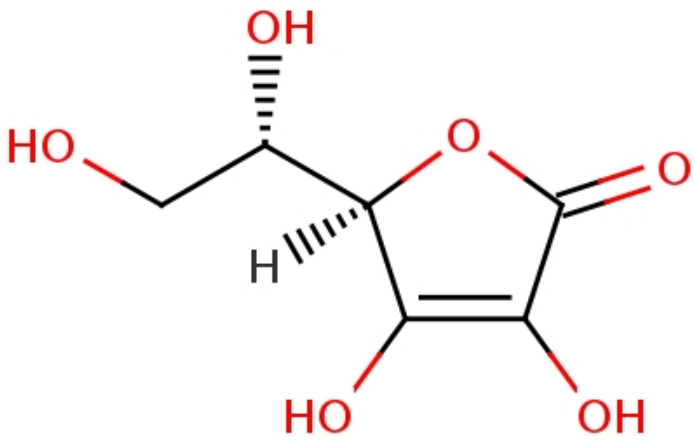
Language for representing biochemical structures with a favourable performance/expressivity trade-off

CLASSIFYING STRUCTURED OBJECTS



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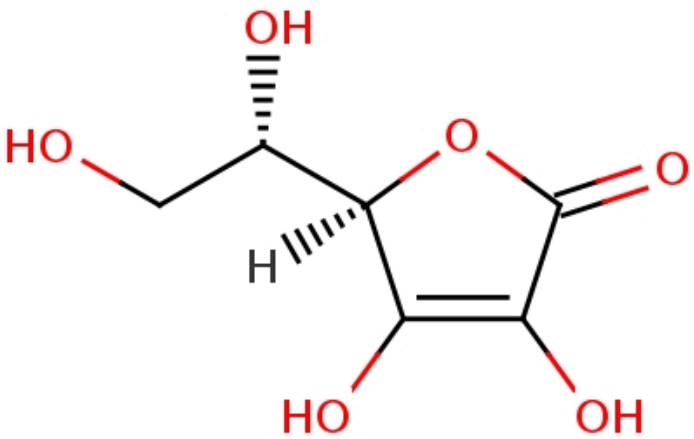

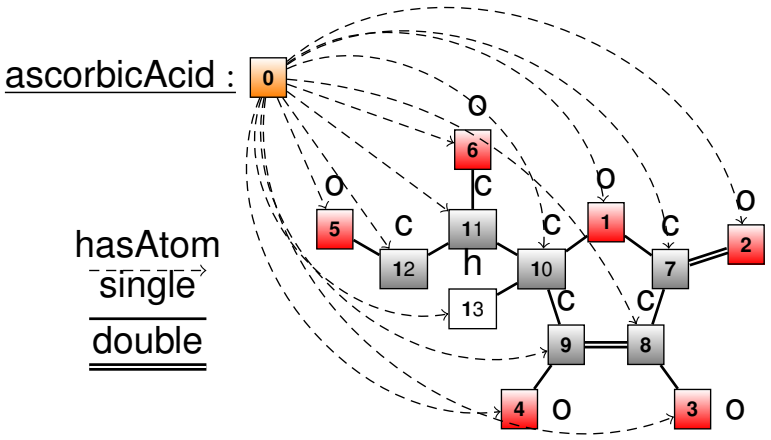

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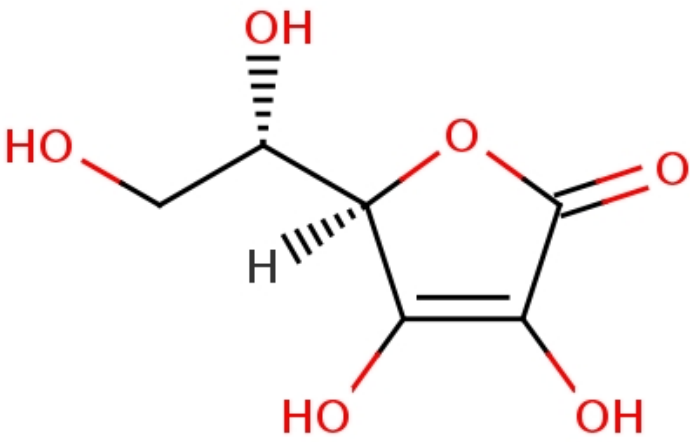

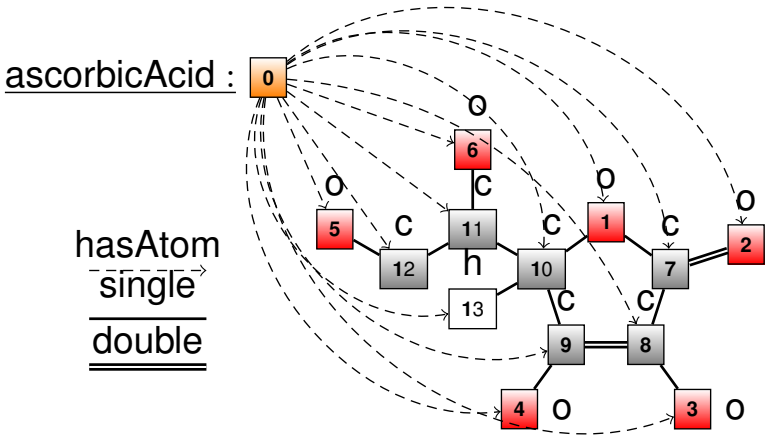

$$\text{ascorbicAcid}(x) \rightarrow \text{hasAtom}(x, f_1(x)) \wedge \ldots \wedge \text{hasAtom}(x, f_{13}(x))$$
$$\text{o}(f_1(x)) \wedge \ldots \wedge \text{c}(f_7(x)) \wedge \ldots \wedge$$
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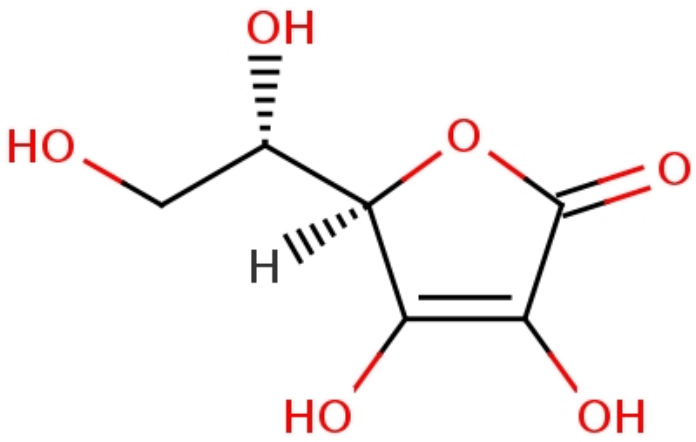

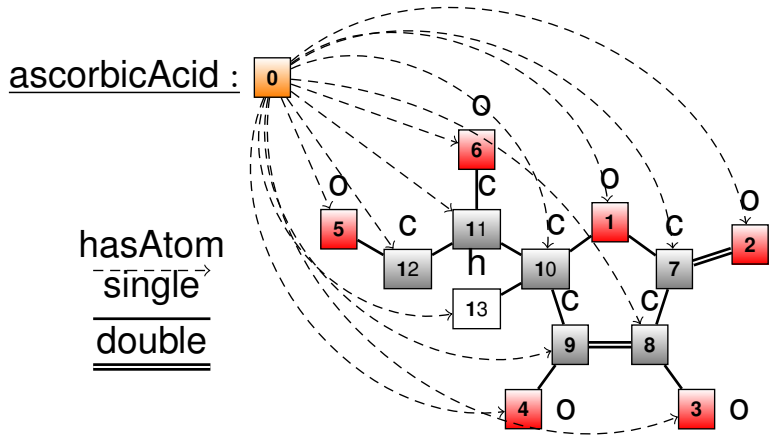

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$$\text{hasAtom}(x, y_1) \wedge \text{hasAtom}(x, y_2) \wedge y_1 \neq y_2 \rightarrow \text{polyatomicEntity}(x)$$

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

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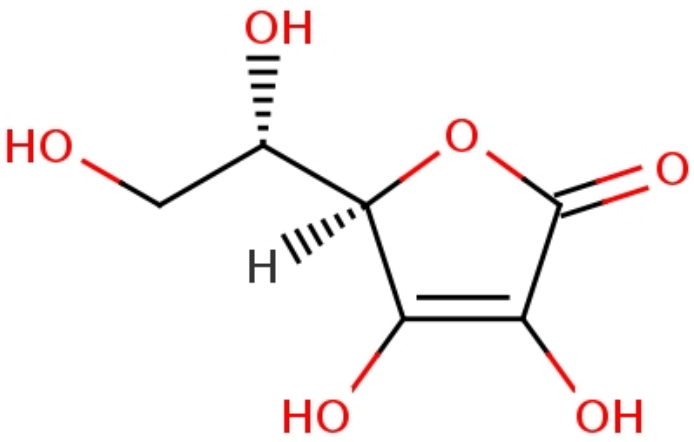
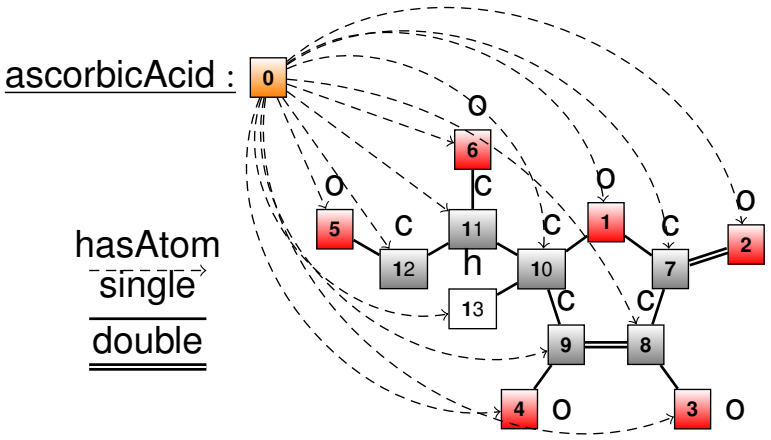
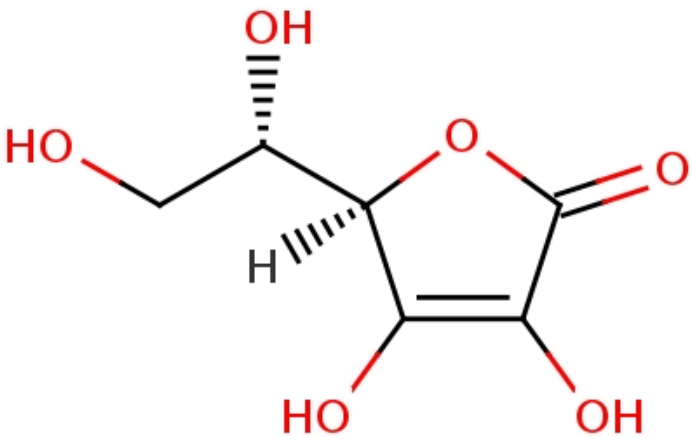


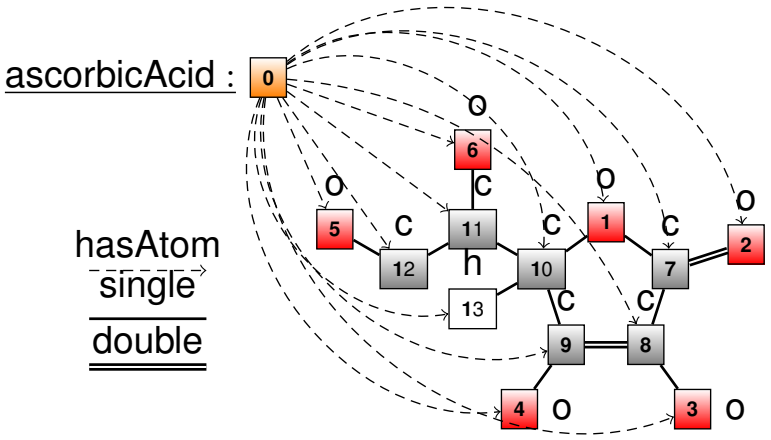


Input fact: ascorbicAcid(a)

Stable model: ascorbicAcid(a), hasAtom(a, a_i^f) for $1 \leq i \leq 13$, o(a_i^f) for $1 \leq i \leq 6$, c(a_i^f) for $7 \leq i \leq 12$, h(a_{13}^f), single(a_8^f, a_3^f), single(a_9^f, a_4^f), single(a_{12}^f, a_i^f) for $i \in \{5, 11\}$, single(a_{11}^f, a_6^f), single(a_{10}^f, a_i^f) for $i \in \{1, 9, 11, 13\}$, single(a_7^f, a_i^f) for $i \in \{1, 8\}$, double(a_2^f, a_7^f), double(a_8^f, a_9^f), horc(a_i^f) for $7 \leq i \leq 13$, polyatomicEntity(a), carboxylicEster(a), cyclic(a)

Classifying Structured Objects





Input fact: ascorbicAcid(a)
Stable model: ascorbicAcid(a), hasAtom(a, a_i^f) for $1 \leq i \leq 13$, o(a_i^f) for $1 \leq i \leq 6$, c(a_i^f) for $7 \leq i \leq 12$, h(a_{13}^f), single(a_8^f, a_3^f), single(a_9^f, a_4^f), single(a_{12}^f, a_i^f) for $i \in \{5, 11\}$, single(a_{11}^f, a_6^f), single(a_{10}^f, a_i^f) for $i \in \{1, 9, 11, 13\}$, single(a_7^f, a_i^f) for $i \in \{1, 8\}$, double(a_2^f, a_7^f), double(a_8^f, a_9^f), horc(a_i^f) for $7 \leq i \leq 13$, polyatomicEntity(a), carboxylicEster(a), cyclic(a)

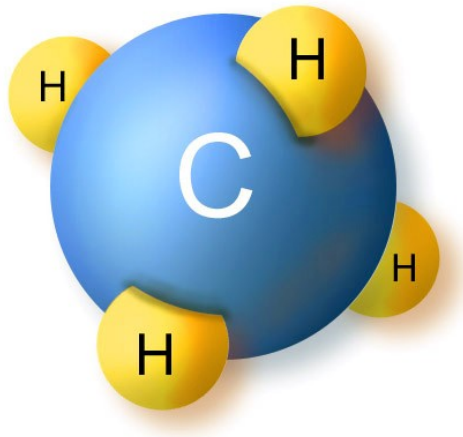
$\rightsquigarrow$ Ascorbic acid is a cyclic polyatomic entity and a carboxylic ester

Chemical Classes We Covered

1. Existence of subcomponents

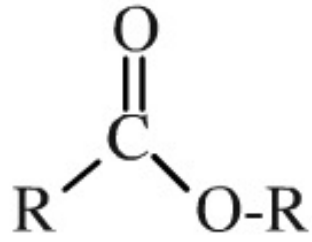
Chemical Classes We Covered

1. Existence of subcomponents
   - Carbon molecules



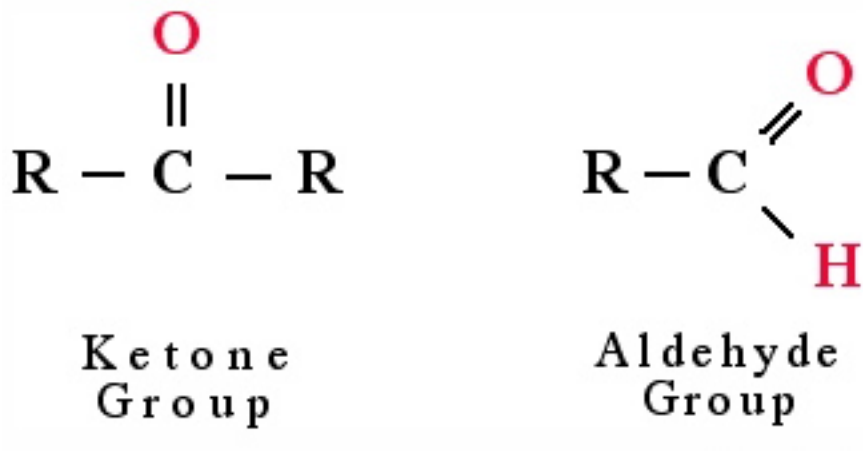
Chemical Classes We Covered

1. Existence of subcomponents
   - Carbon molecules
   - Carboxylic acids and carboxylic esters



Chemical Classes We Covered

1. Existence of subcomponents
   - Carbon molecules
   - Carboxylic acids and carboxylic esters
   - Ketones and aldehydes



Chemical Classes We Covered

1. Existence of subcomponents
   - Carbon molecules
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2. Exact cardinality of parts

Chemical Classes We Covered

1. Existence of subcomponents
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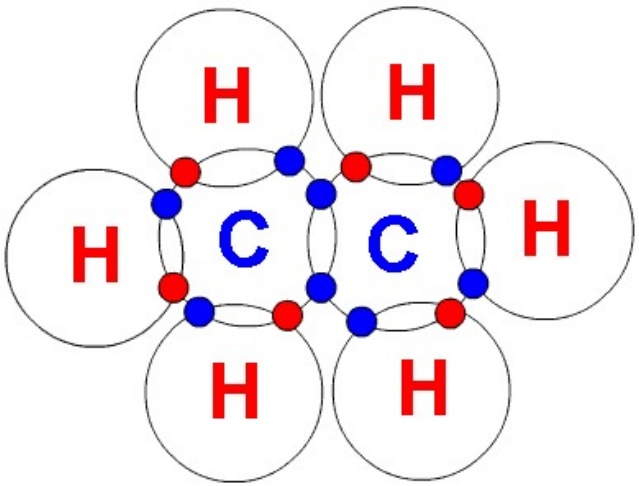
2. Exact cardinality of parts
   - Exactly two carbons



Chemical Classes We Covered

1. Existence of subcomponents
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2. Exact cardinality of parts
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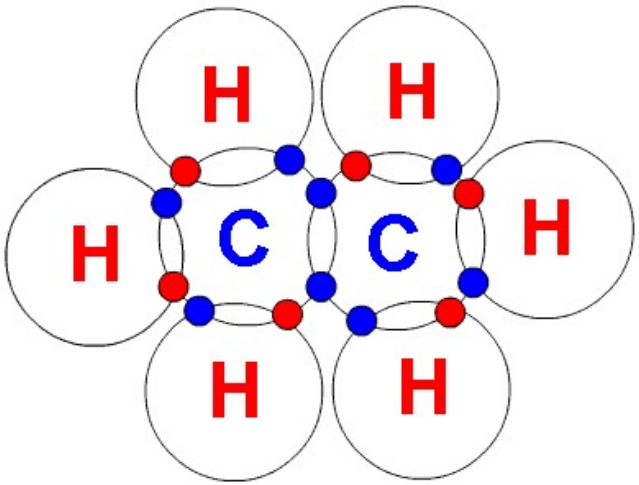
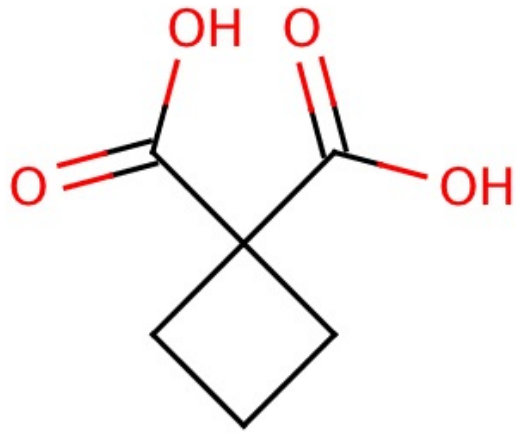
   - Dicarboxylic acid





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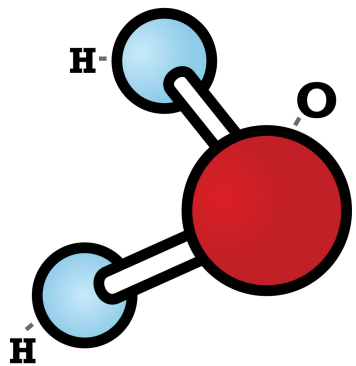

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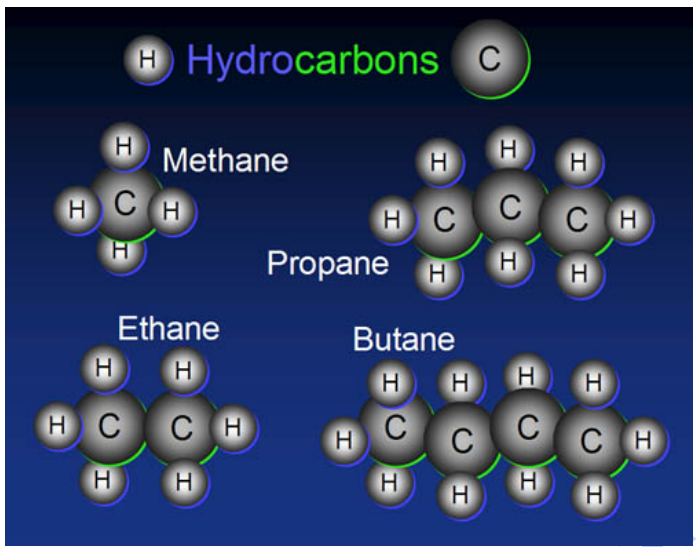

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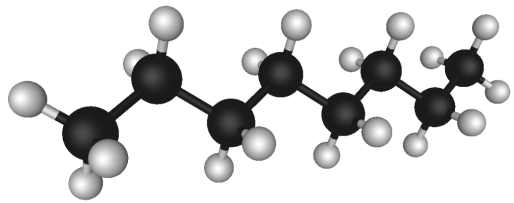

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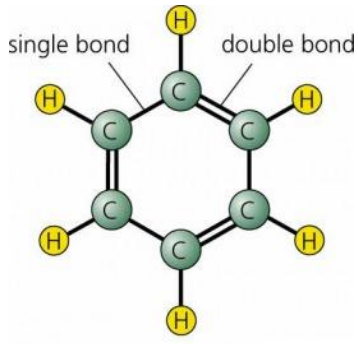

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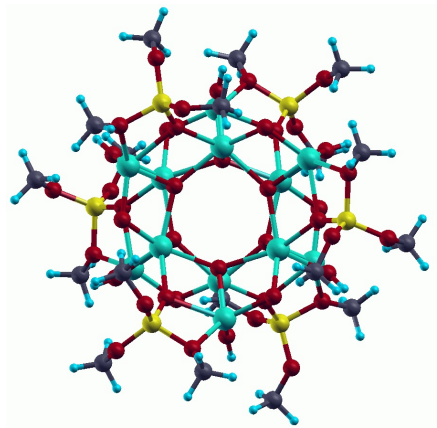

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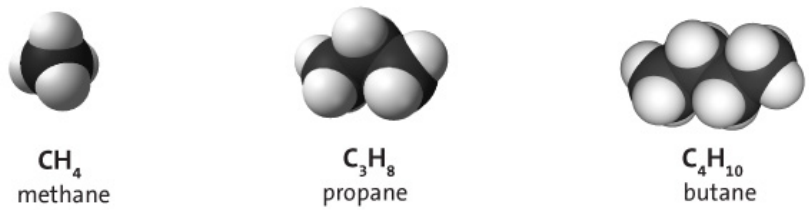

Empirical Evaluation

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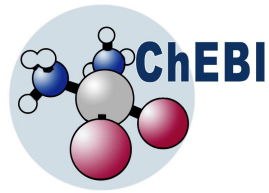

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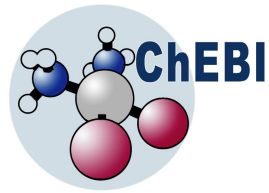

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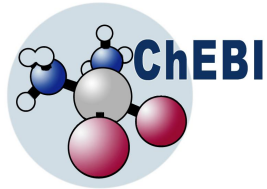

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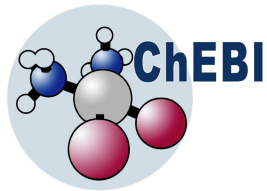

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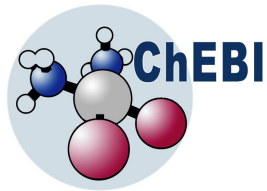

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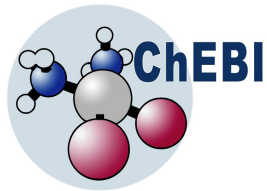

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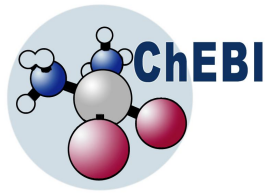

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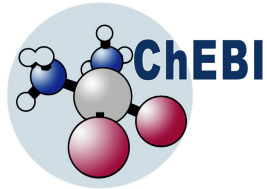

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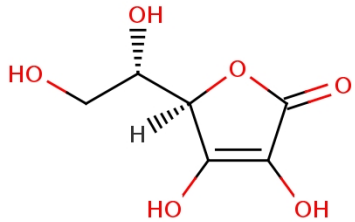
- Contradictory subclass relation from ChEBI:
  - Ascorbic acid is asserted to be a carboxylic acid (release 95)
  - Not listed among the subsumptions derived by our prototype



Conclusion and Further Research

- Results
  1. Expressive and decidable formalism for complex objects

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Language for representing biochemical structures with a favourable performance/expressivity trade-off

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

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define carboxylicEster
some hasAtom SMILES(COC(=O)[*])
end.

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

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    E.g., Small molecules if they weigh less than 800 daltons

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- Thank you! Questions?!?