Modelling Structured Domains Using Description Graphs and Logic Programming

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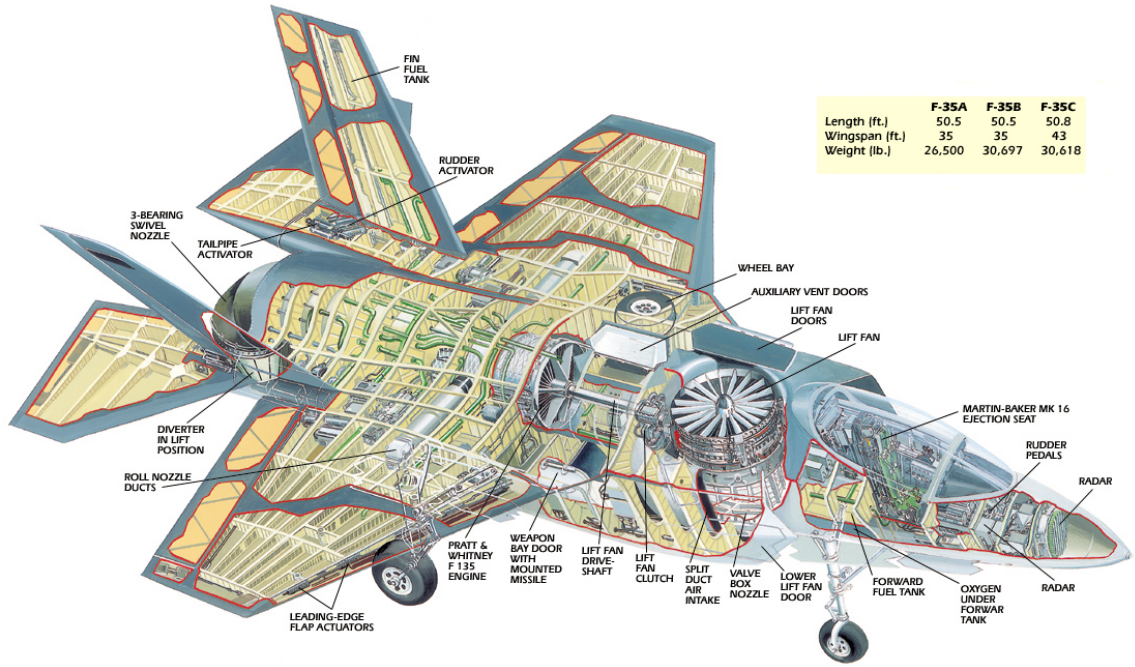

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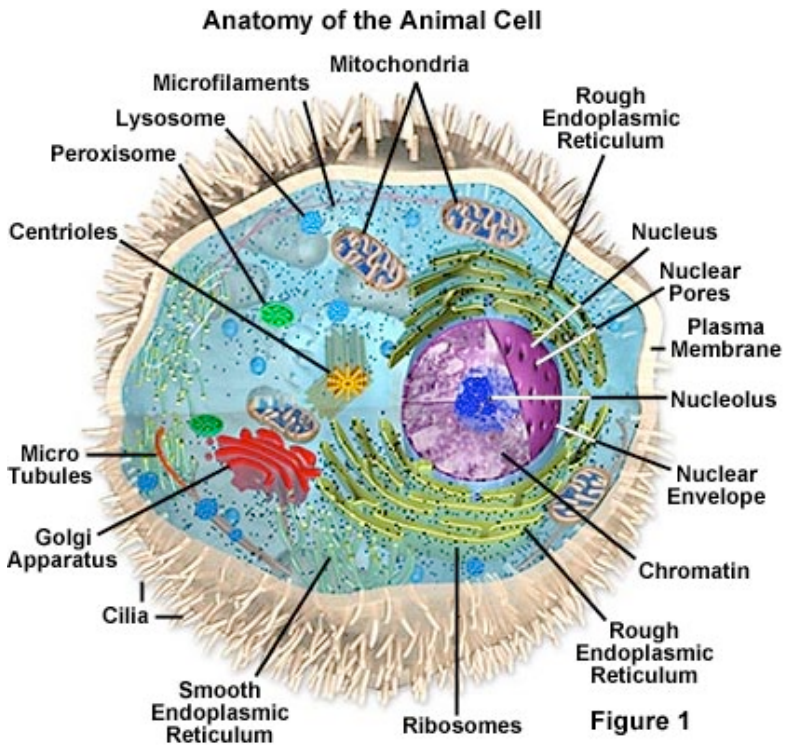

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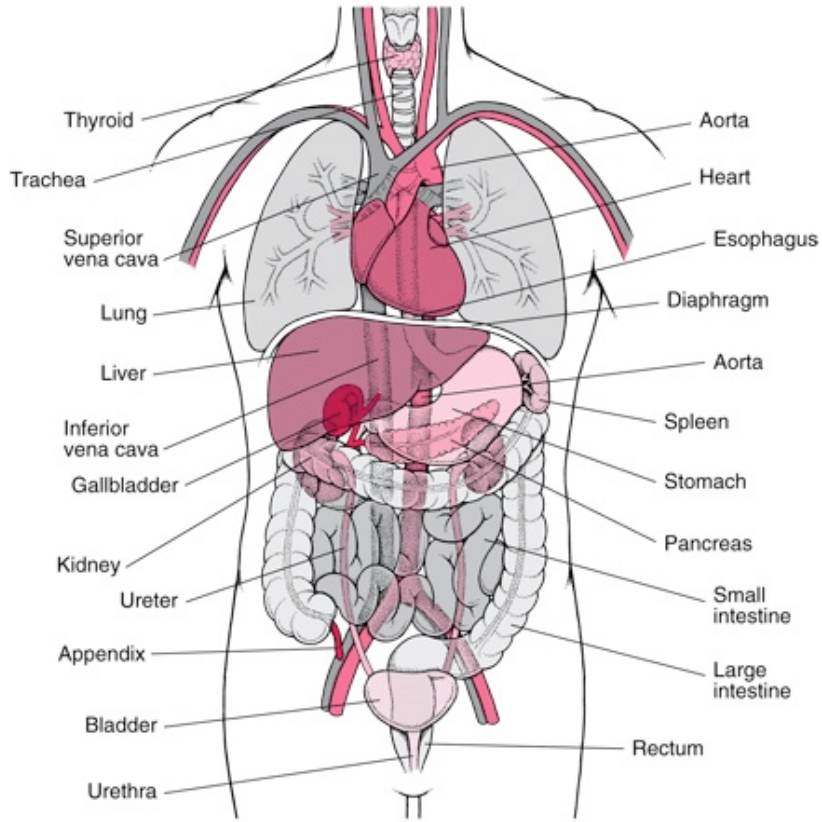

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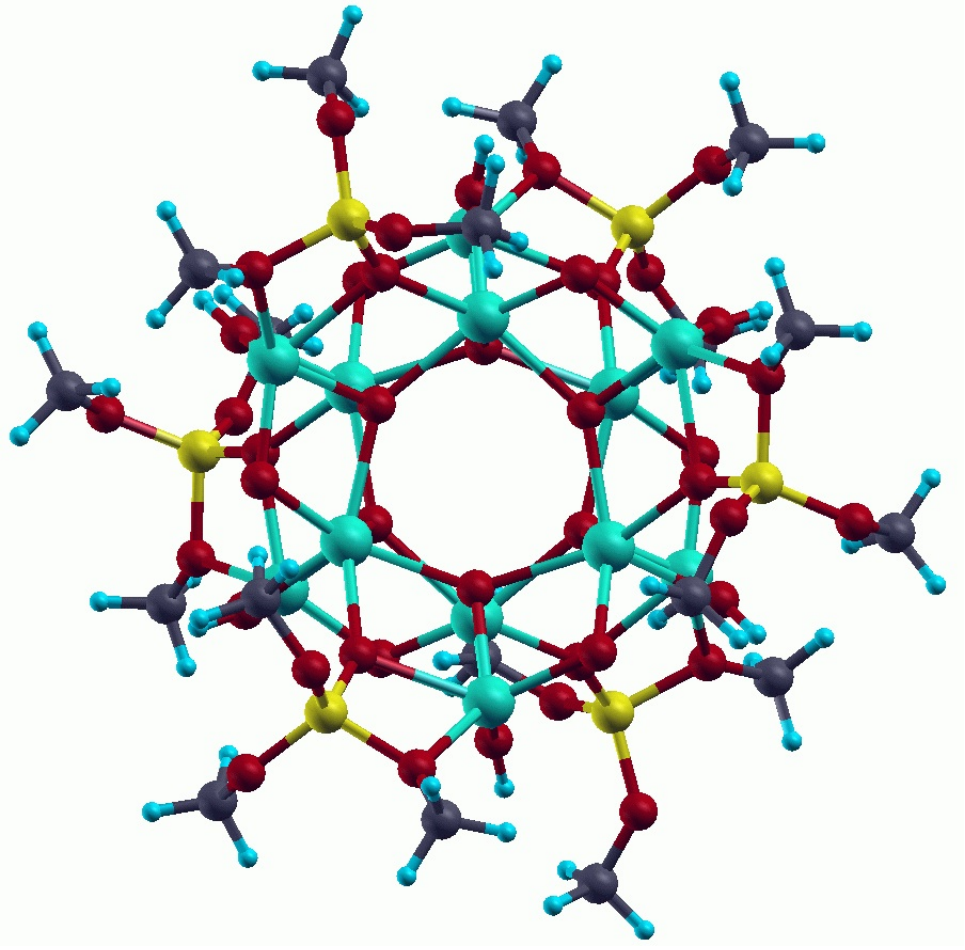

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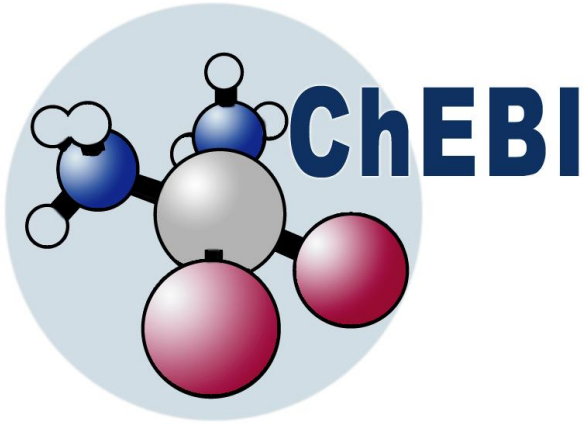

EMBL-EBI

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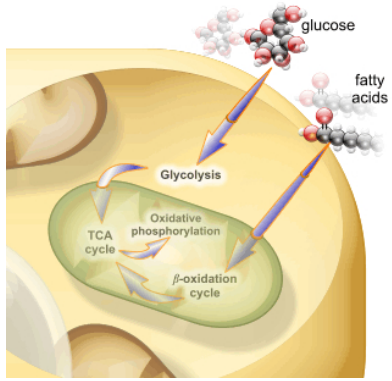

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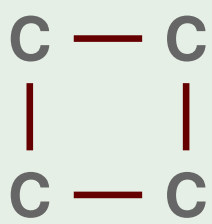

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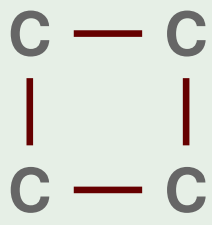

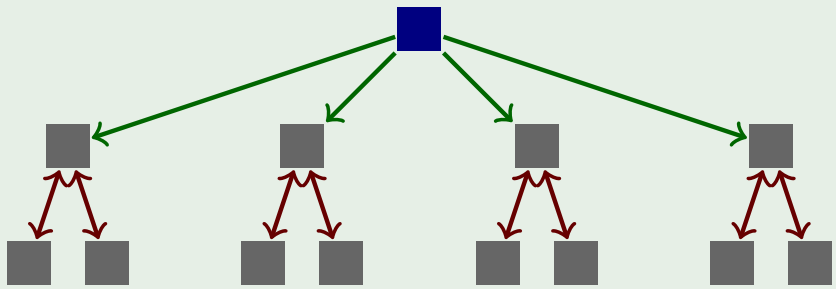

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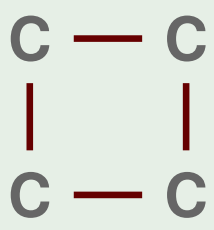

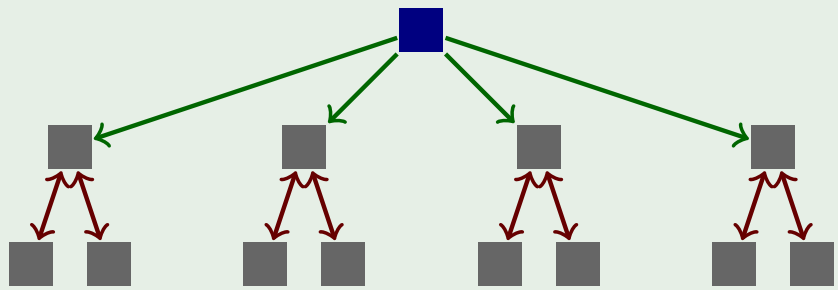

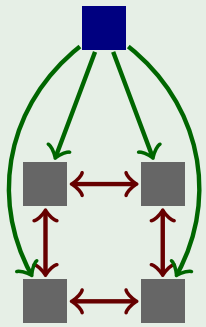

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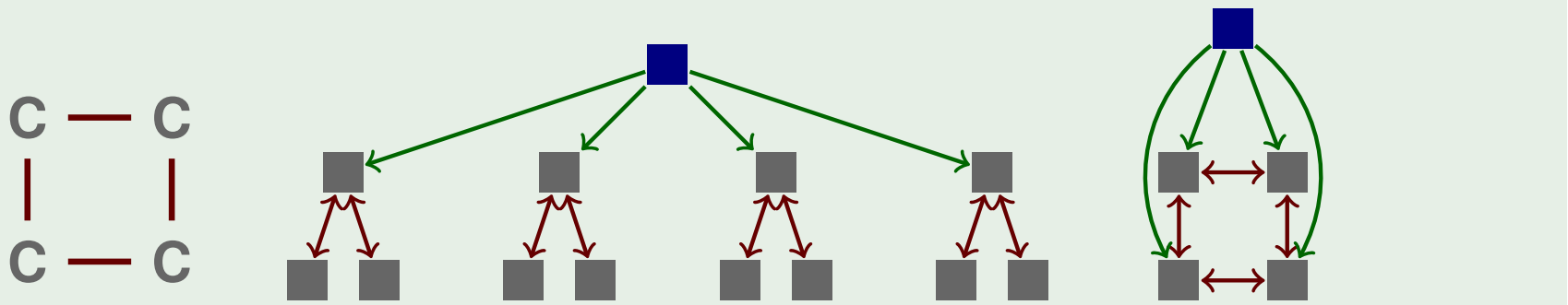

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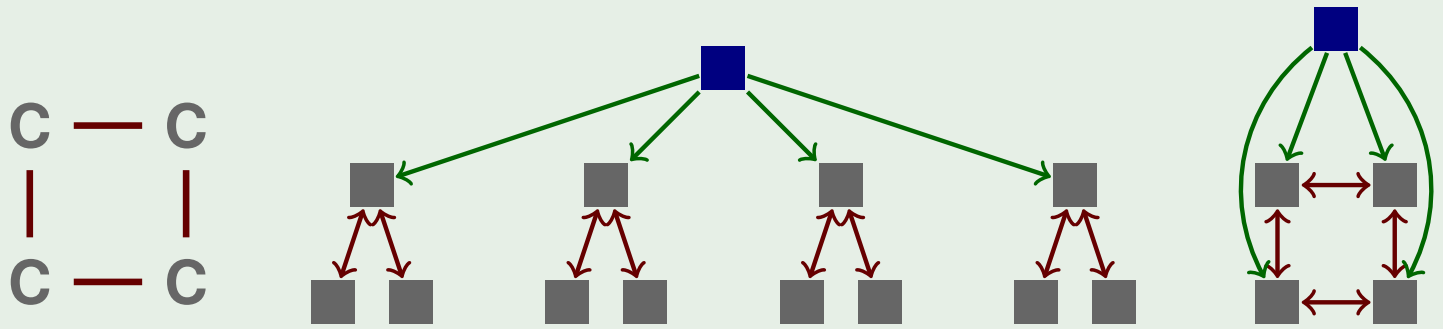

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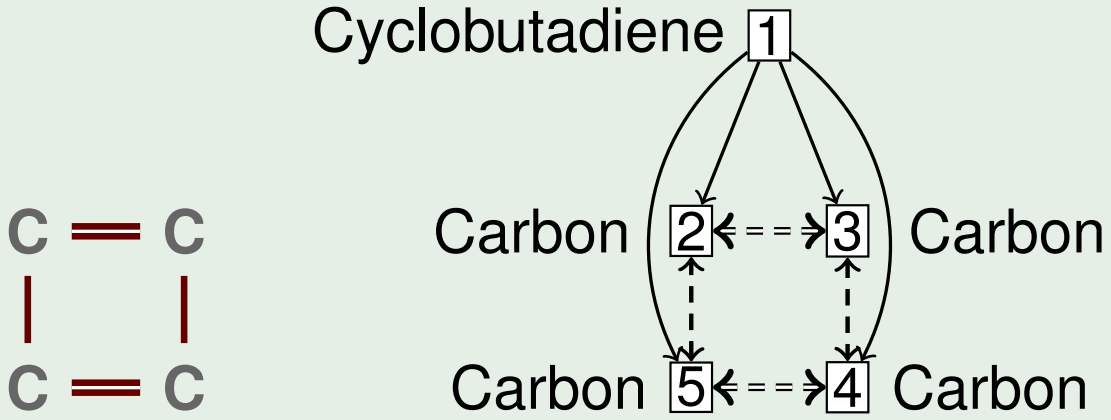

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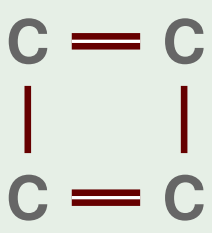

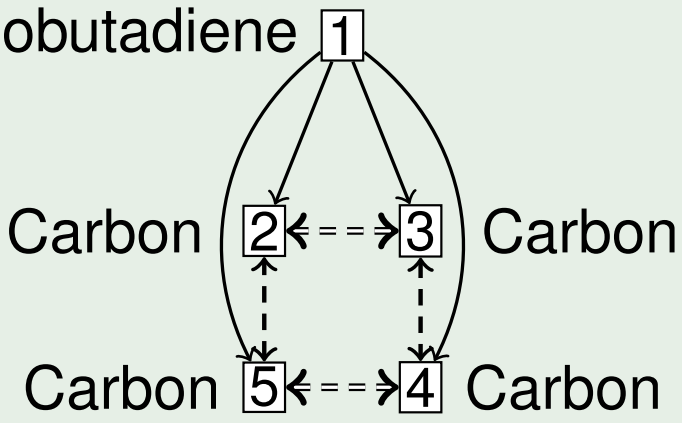

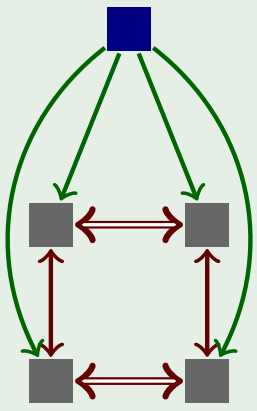

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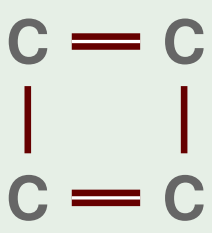

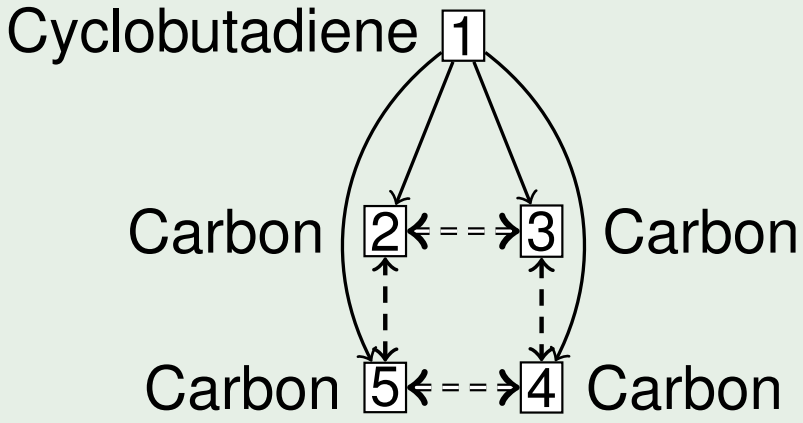

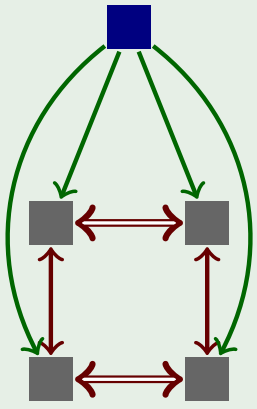

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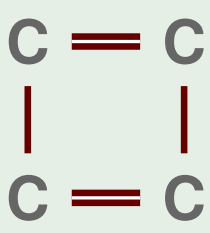

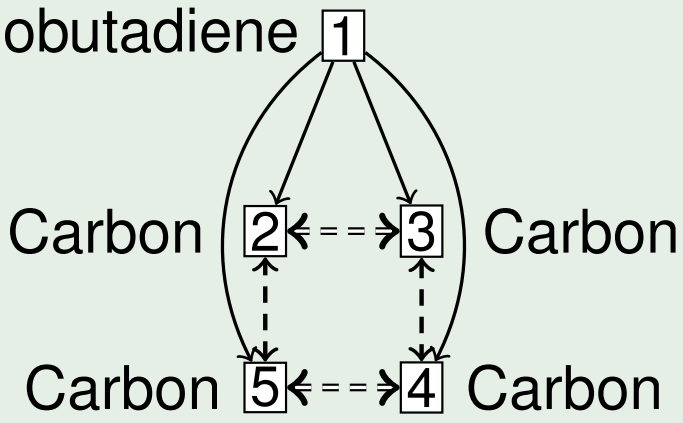

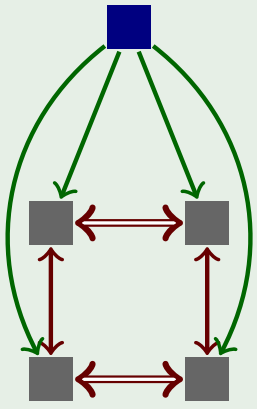

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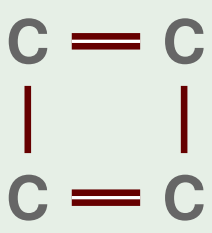

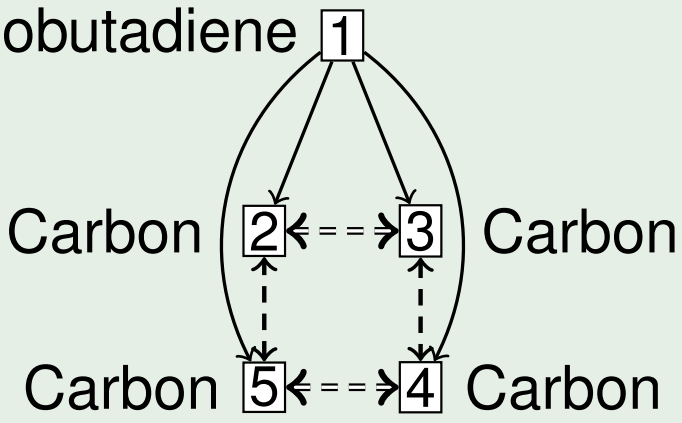

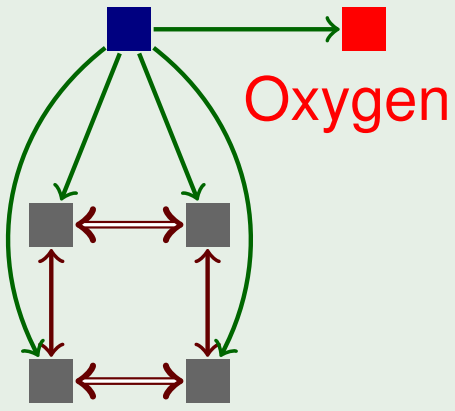

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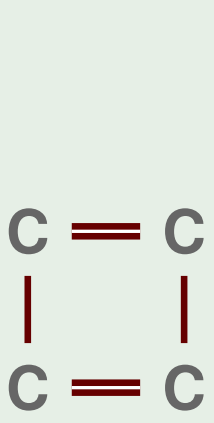

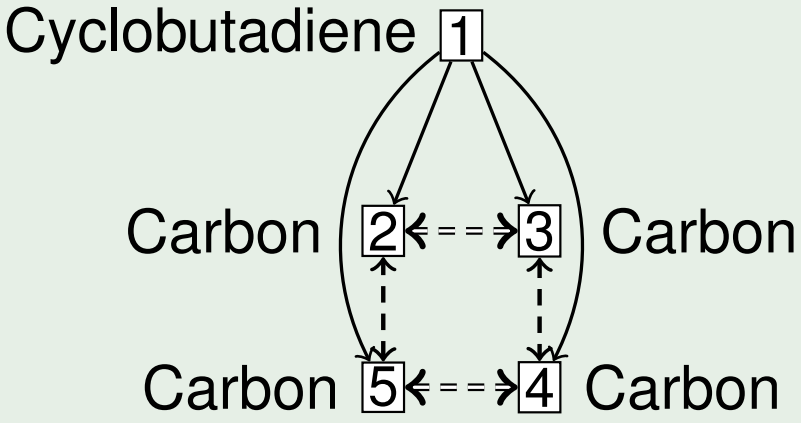

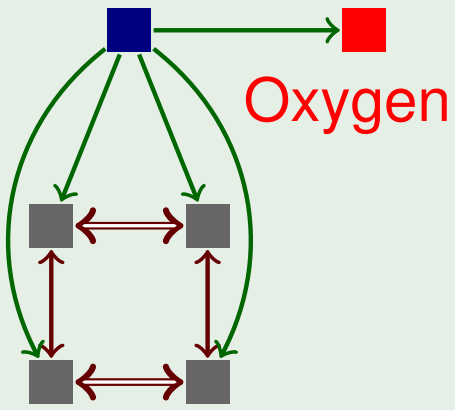

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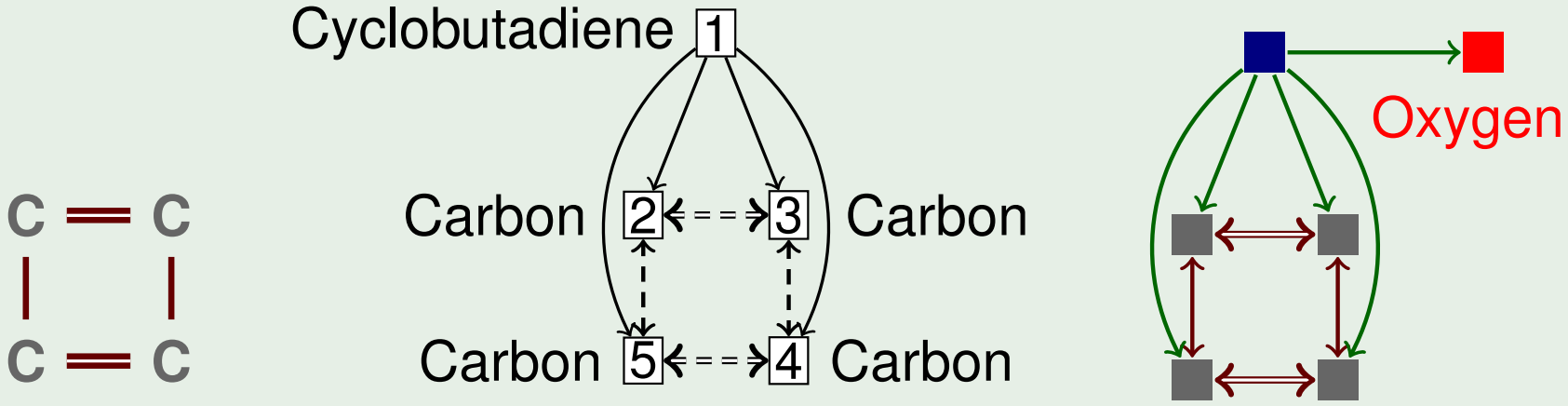

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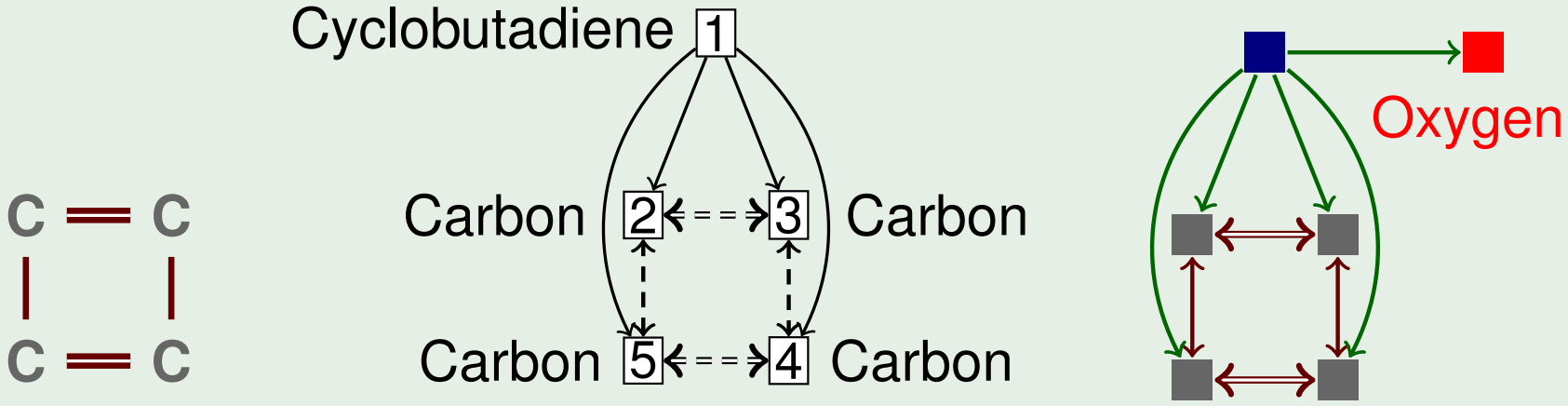

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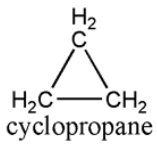

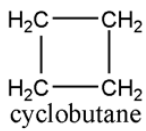

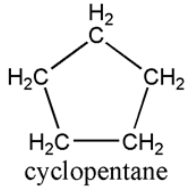

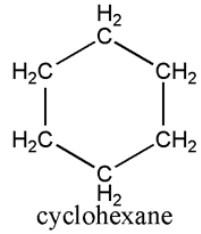

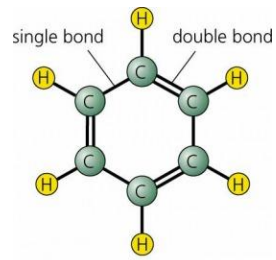

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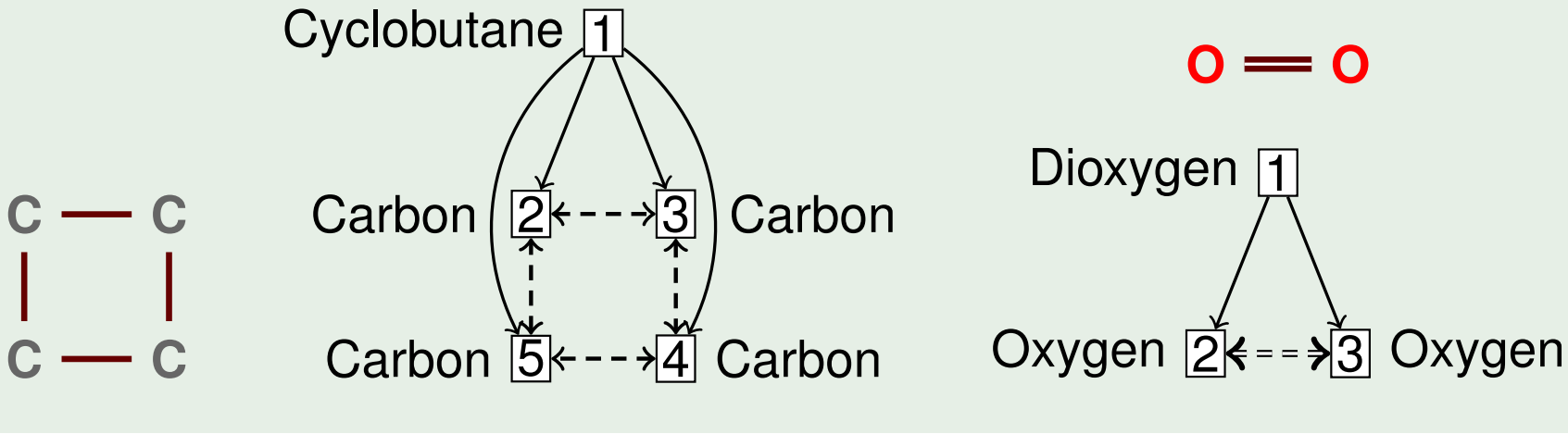

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$$\text{Cyclobutane}(c_1), \quad \text{Dinitrogen}(c_2), \ldots$$

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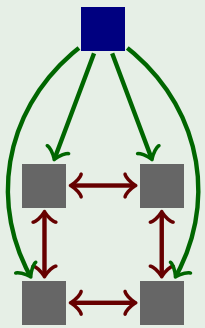

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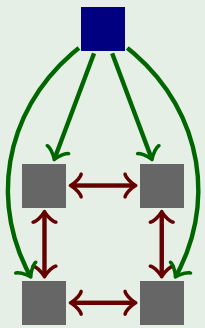

$$\begin{aligned}
\text{Cyclobutane}(x) &\rightarrow G_{cb}(x, f_1(x), f_2(x), f_3(x), f_4(x)) \\
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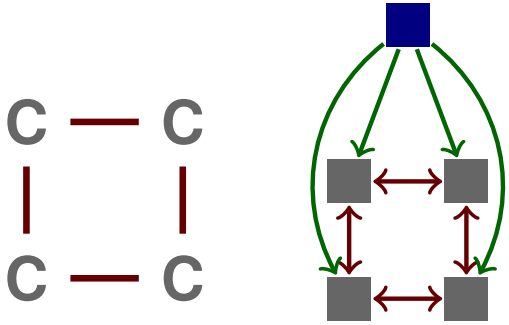

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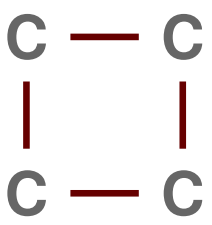

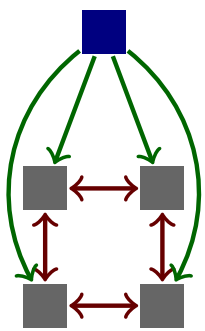

- Is cyclobutane a hydrocarbon? ✓

Classifying Objects

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$$\text{Molecule}(x) \wedge \bigwedge_{1 \le i \le 4} \text{HasAtom}(x, y_i) \wedge \bigwedge_{1 \le i \le 3} \text{Bond}(y_i, y_{i+1}) \wedge$$

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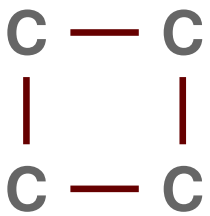

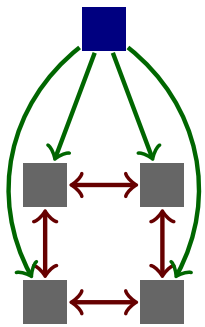

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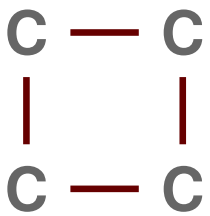

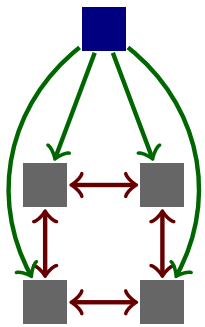

- Does cyclobutane contain a four-membered ring? ✓

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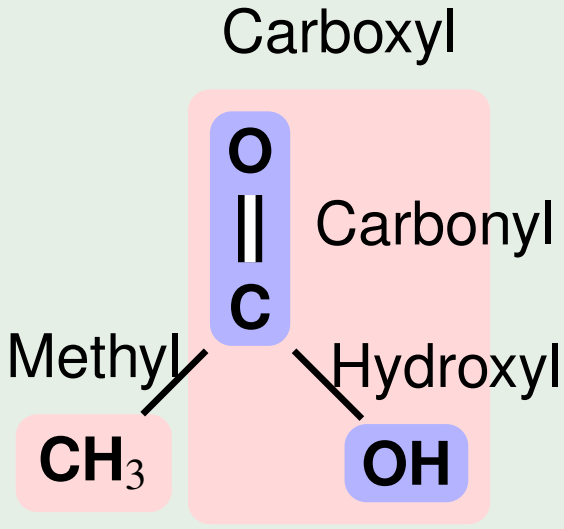

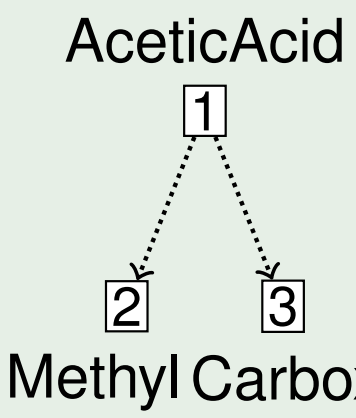

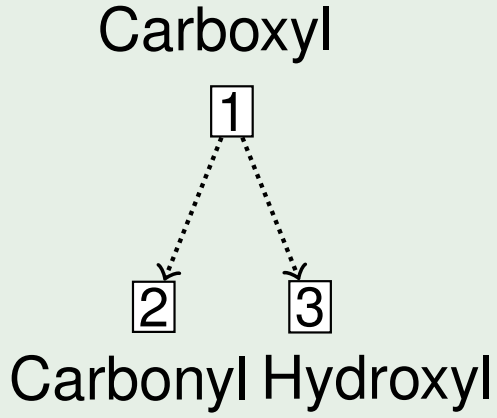

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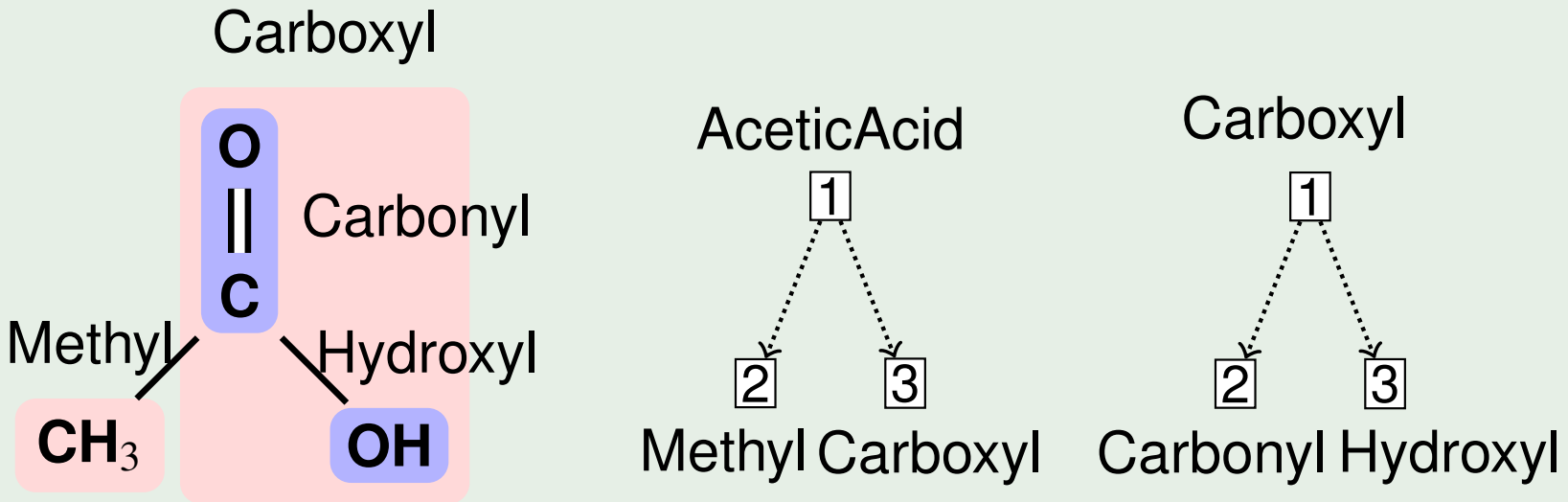

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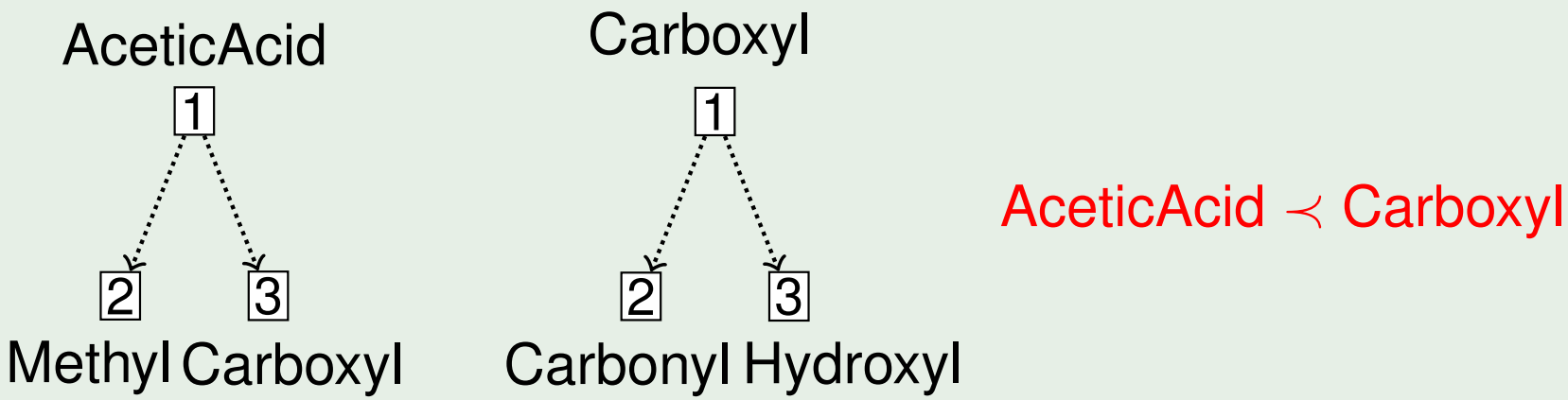

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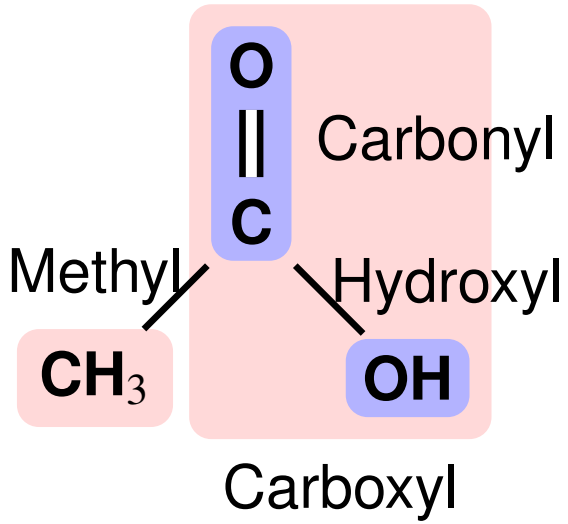

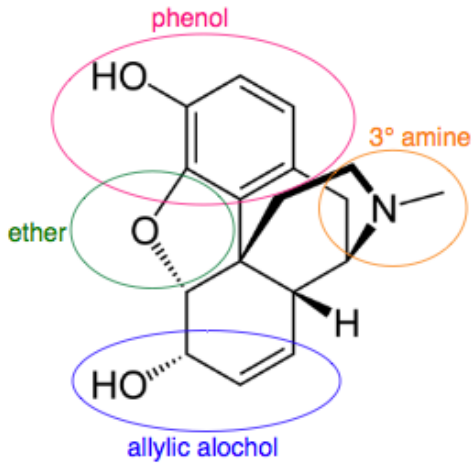

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- Thank you for listening. Questions?