

Atom Mapping with Constraint Programming

Supplementary Material

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1 Reaction R01440

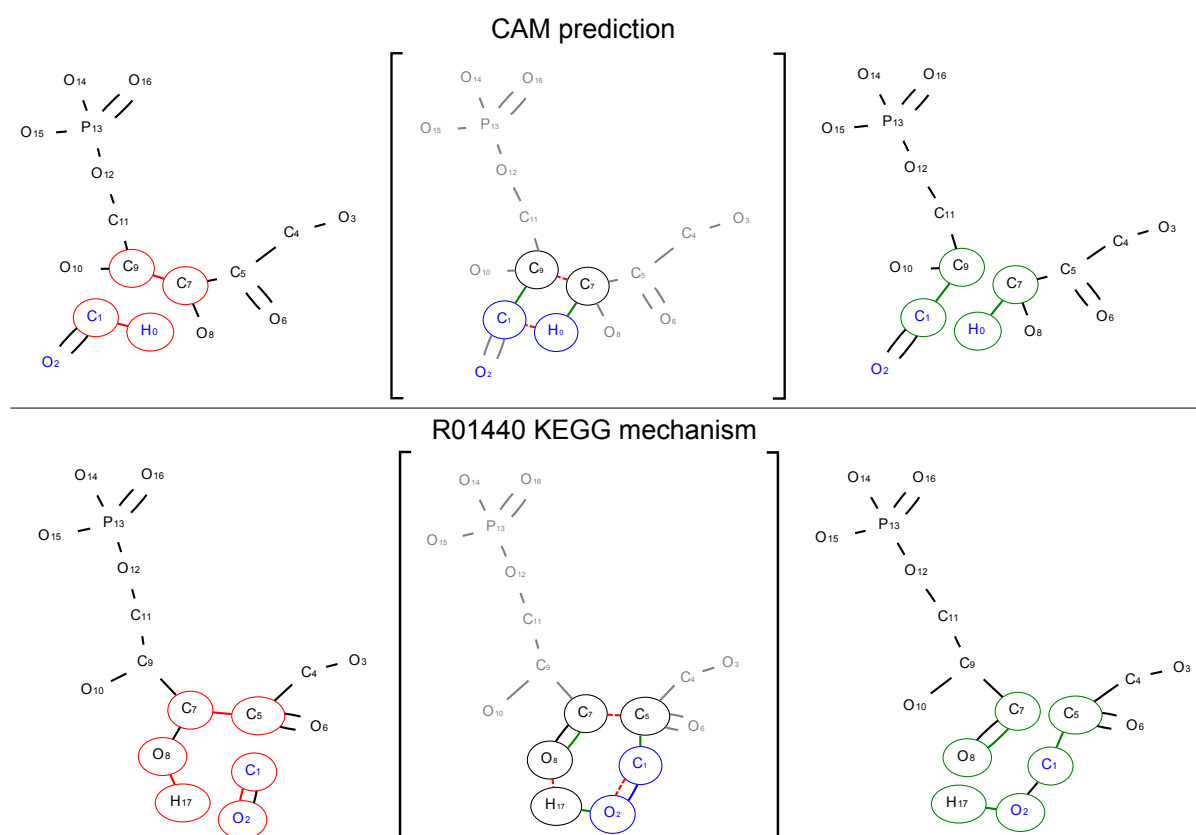


Figure 1: Reaction R01440 (top) CAM-predicted mechanism based on a homovalent ITS cycle of 4 atoms and (bottom) the 6-atom cycle according to the mechanism stored in the KEGG database. The center graph represents the ITS. Red bond are broken from left to right while green bonds are formed. Blue atoms belong to the $\text{C}=\text{O}$ molecule from the left side.