Reaction Networks – Directed Hypergraphs

Visualization as a bipartite graph.

Example:

$g_1 + g_2 \xrightarrow{p} g_3$ $\quad g_4 \xrightarrow{p} g_5$ $\quad 2g_6 \xrightarrow{p} g7$

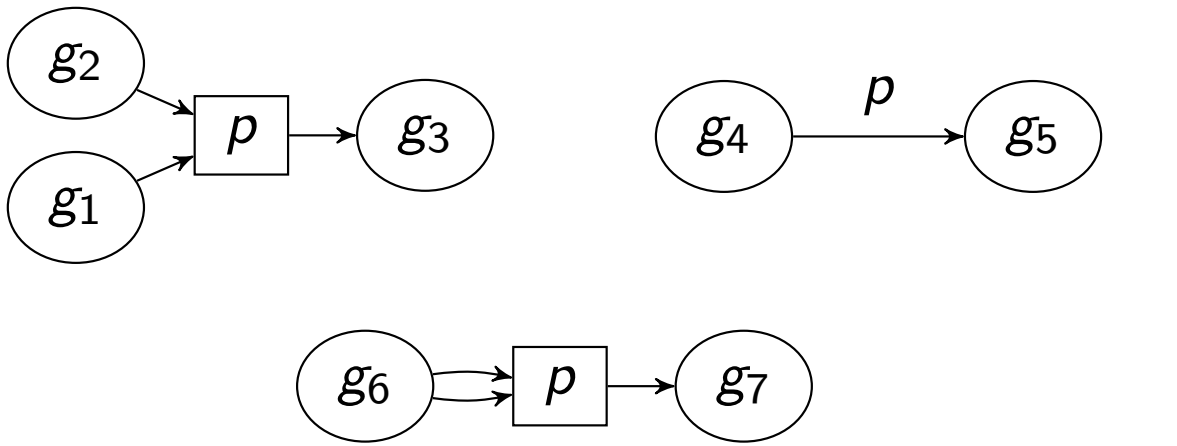


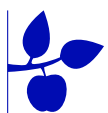
Figure : Examples of reaction network visualization.

Exploration Strategies

Given a set of starting molecules and a set of reaction patterns, how to explore the implied reaction network?
Brute-force? (combinatorial explosion)

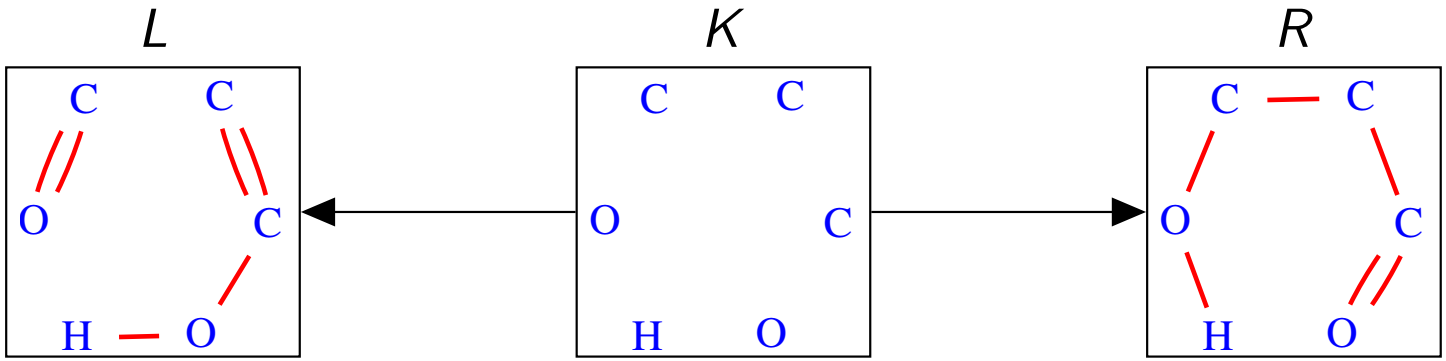
Strategy Interface: A strategy is (almost) a function transforming a set of molecules into a set of molecules.
Examples:

- A reaction pattern; e.g., p
  Try to transform all combinations of educts.
- Parallelization; e.g., $\texttt{parallel}[p_1, p_2]$
  Apply p_1 and p_2 simultaneously.
- Sequencing; e.g., $p_1 \rightarrow p_2$
  First apply p_1, on the result apply p_2.

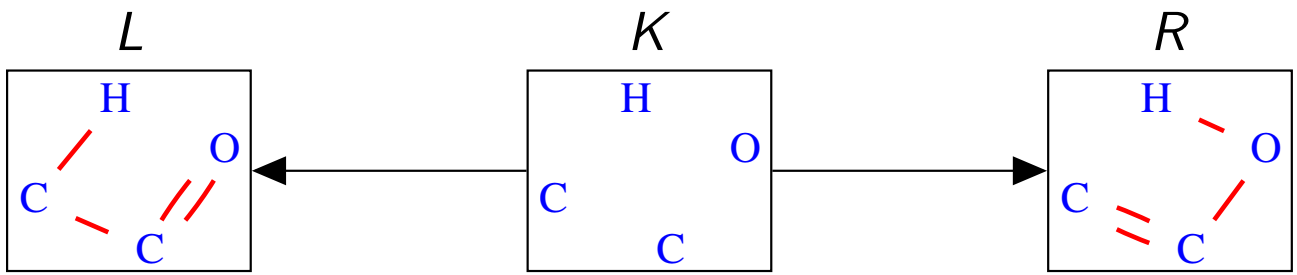


The Formose Chemistry

4 reaction patterns:



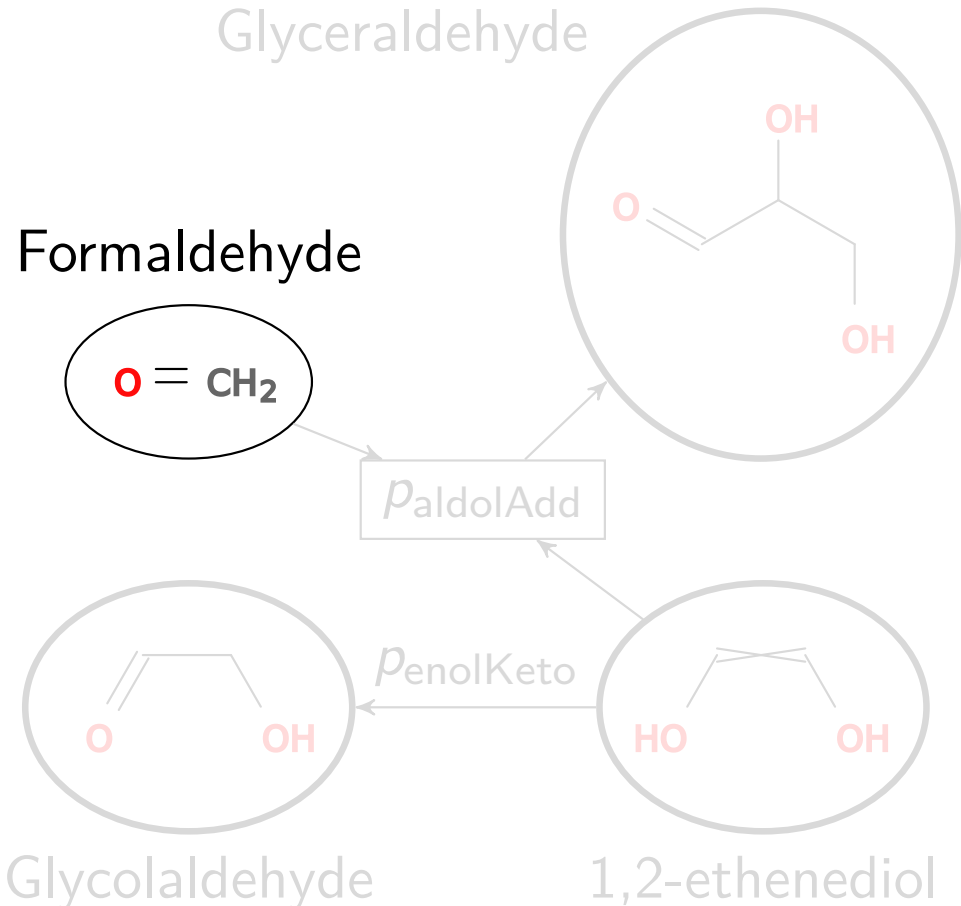
(a) Aldol addition (p_{aldolAdd}). (Reverse aldol addition ($p_{\text{aldolSplit}}$))



(b) Keto-to-enol (p_{ketoEnol}). (Enol-to-keto (p_{enolKeto}))

Parallelization and Sequencing

addUniverse[formaldehyde] → addSubset[1,2-ethenediol]
→ parallel[{p_{aldolAdd}, p_{enolKeto}}]



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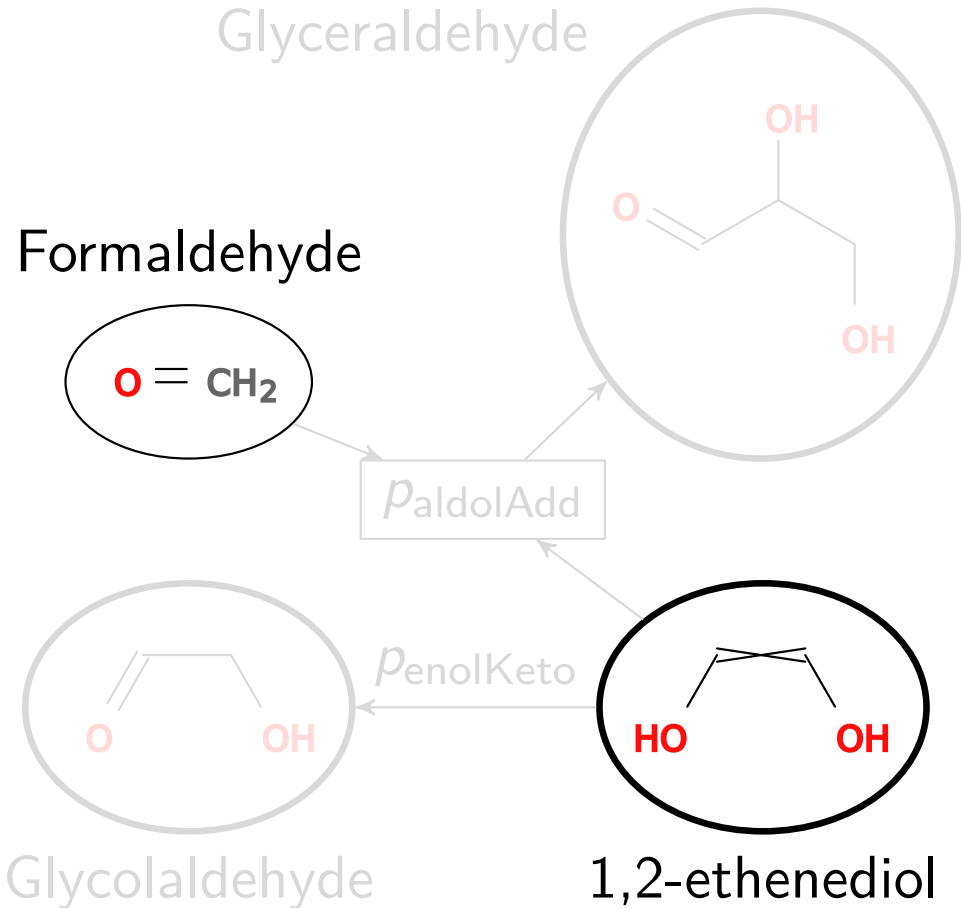

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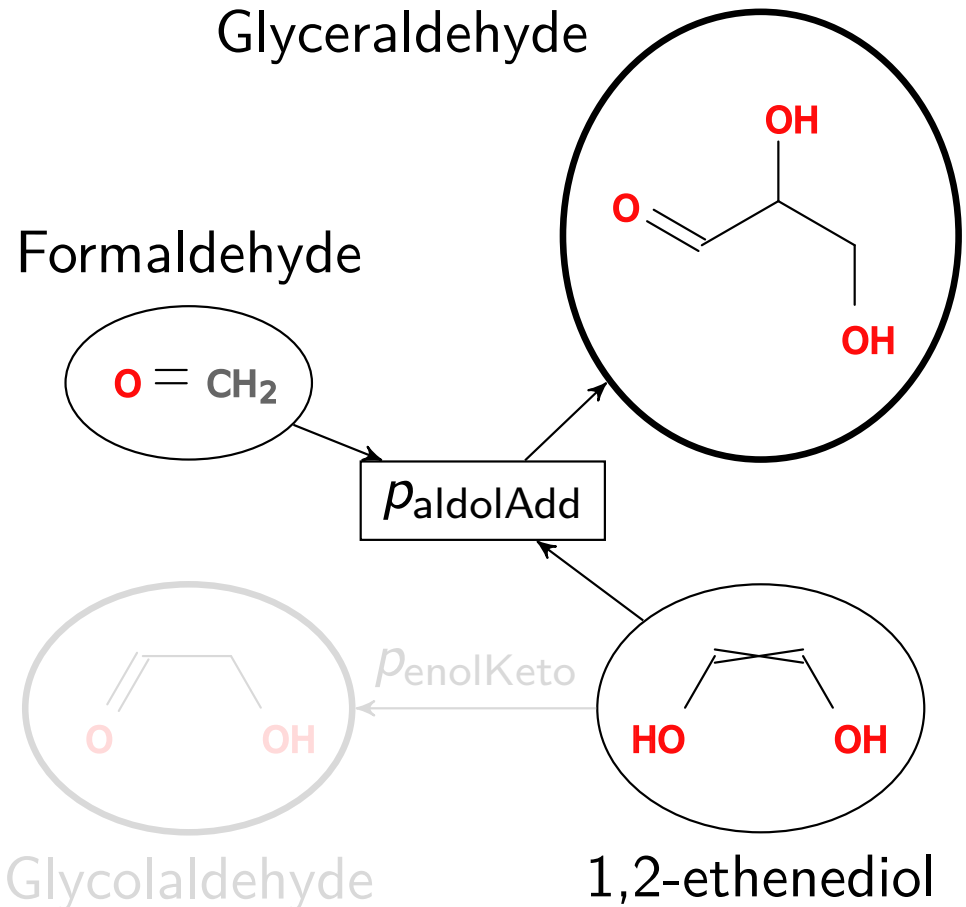

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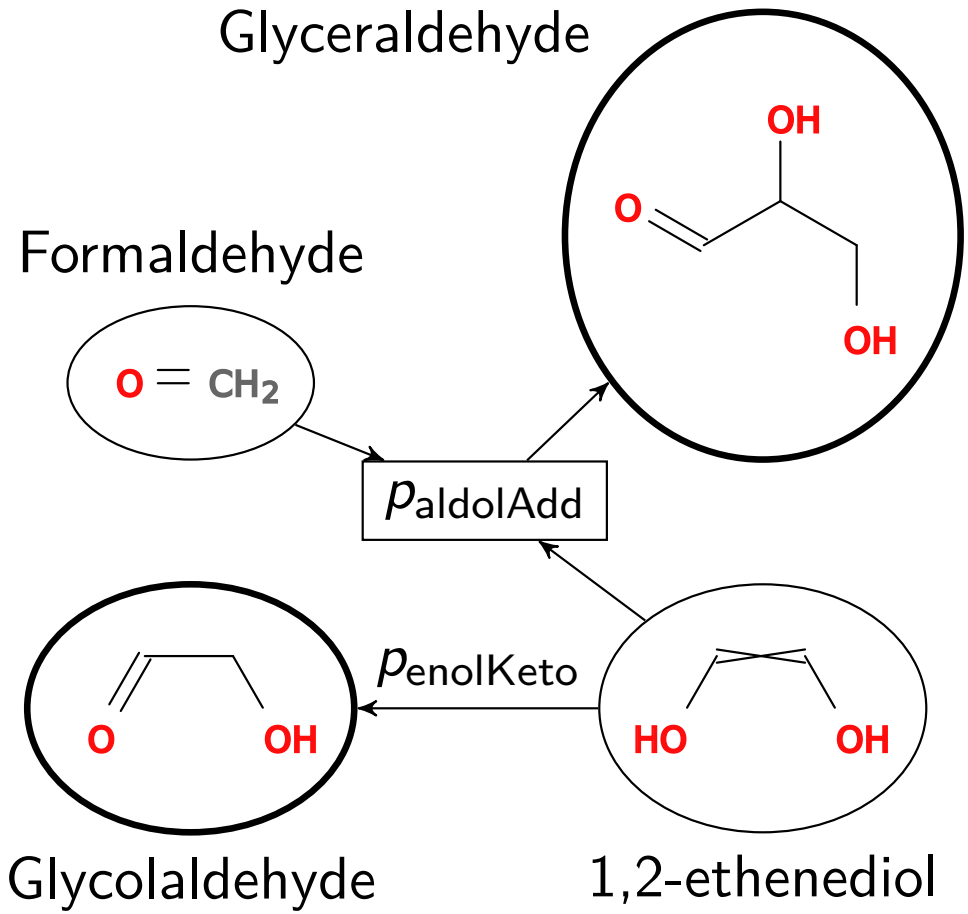
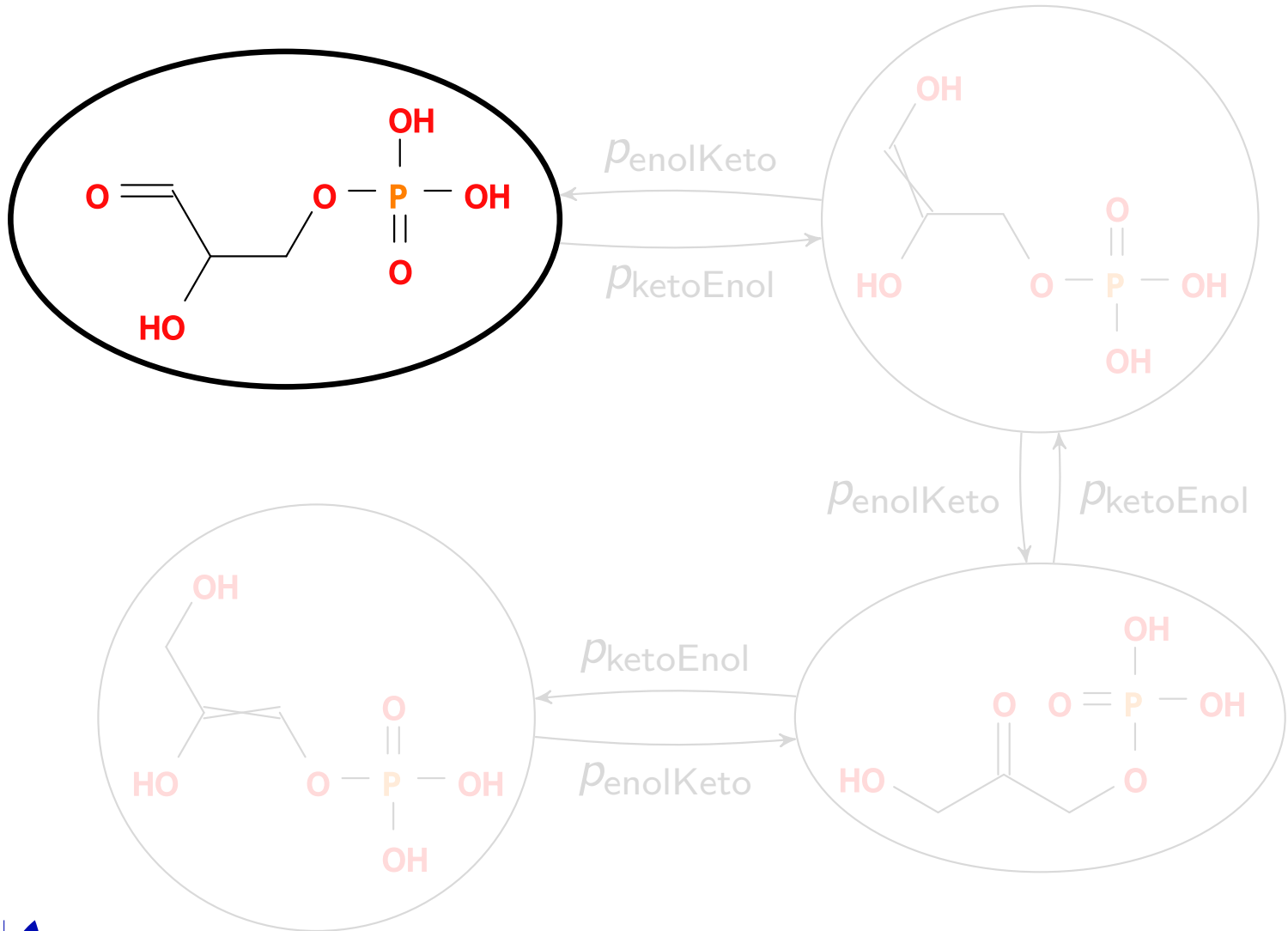


Repetition

addSubset[G3P] $\rightarrow$ `repeat[parallel[{`$p_{\text{ketoEnol}}, p_{\text{enolKeto}}$`}]]`



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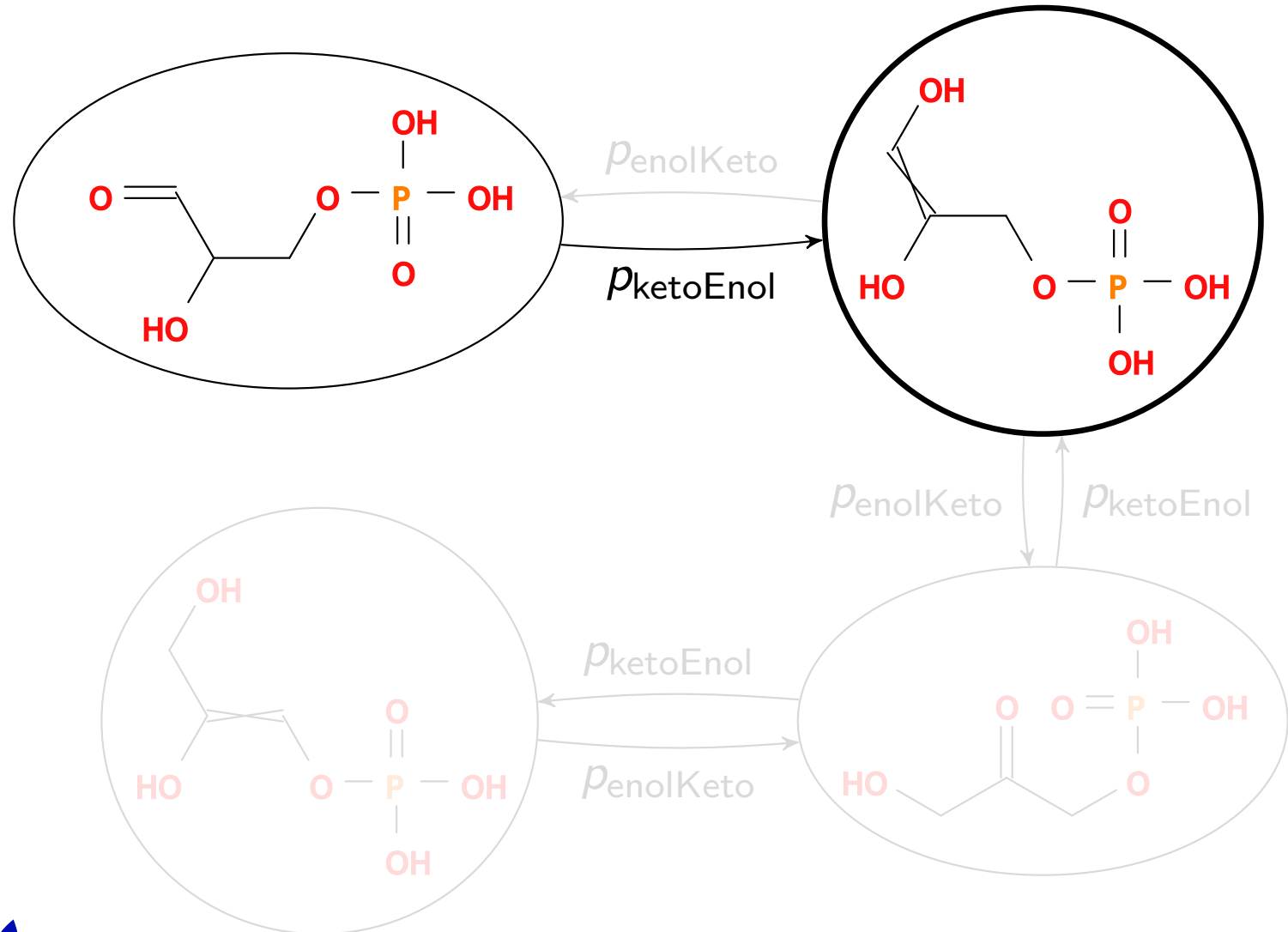

Iteration 1

Repetition

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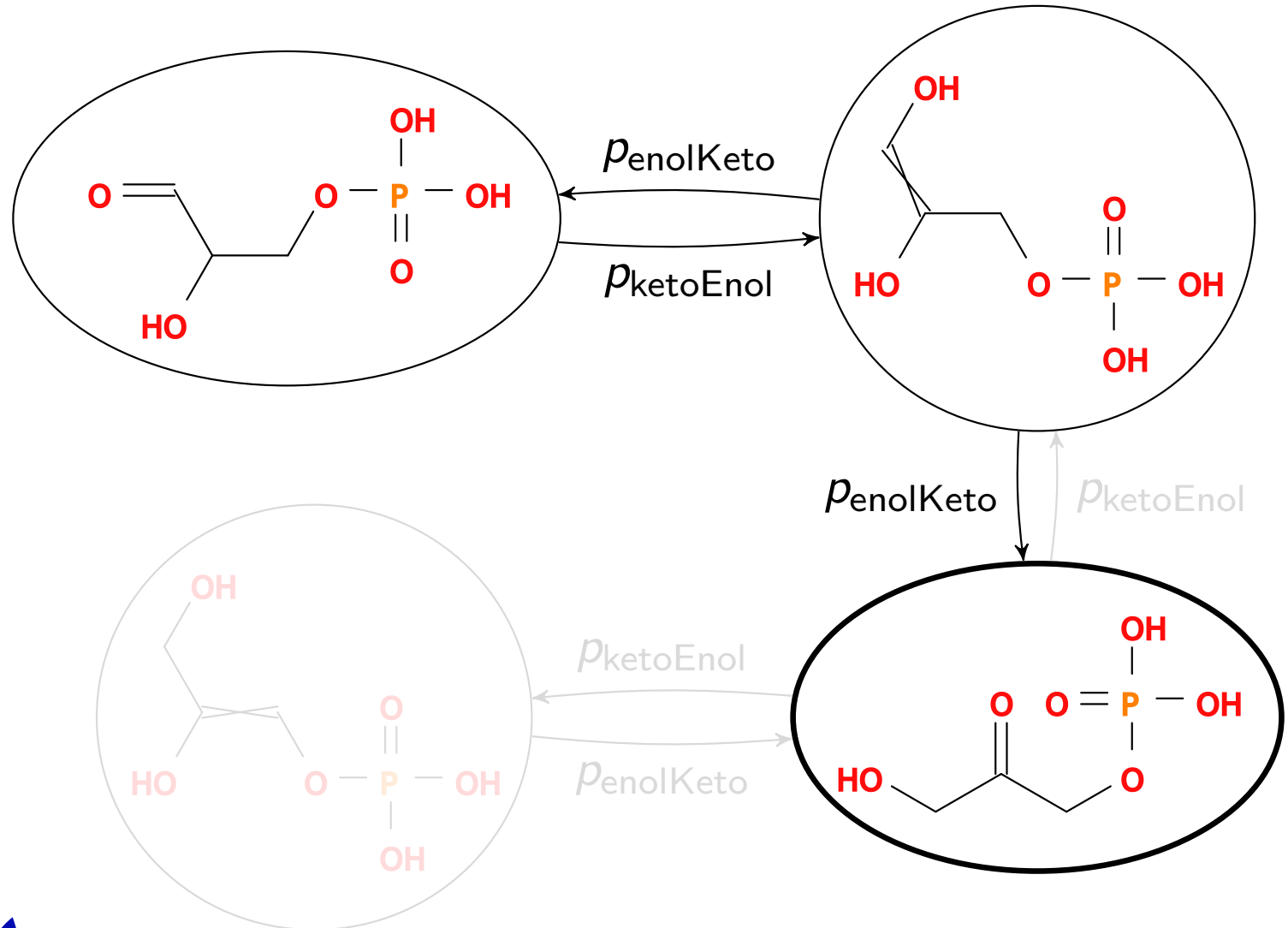
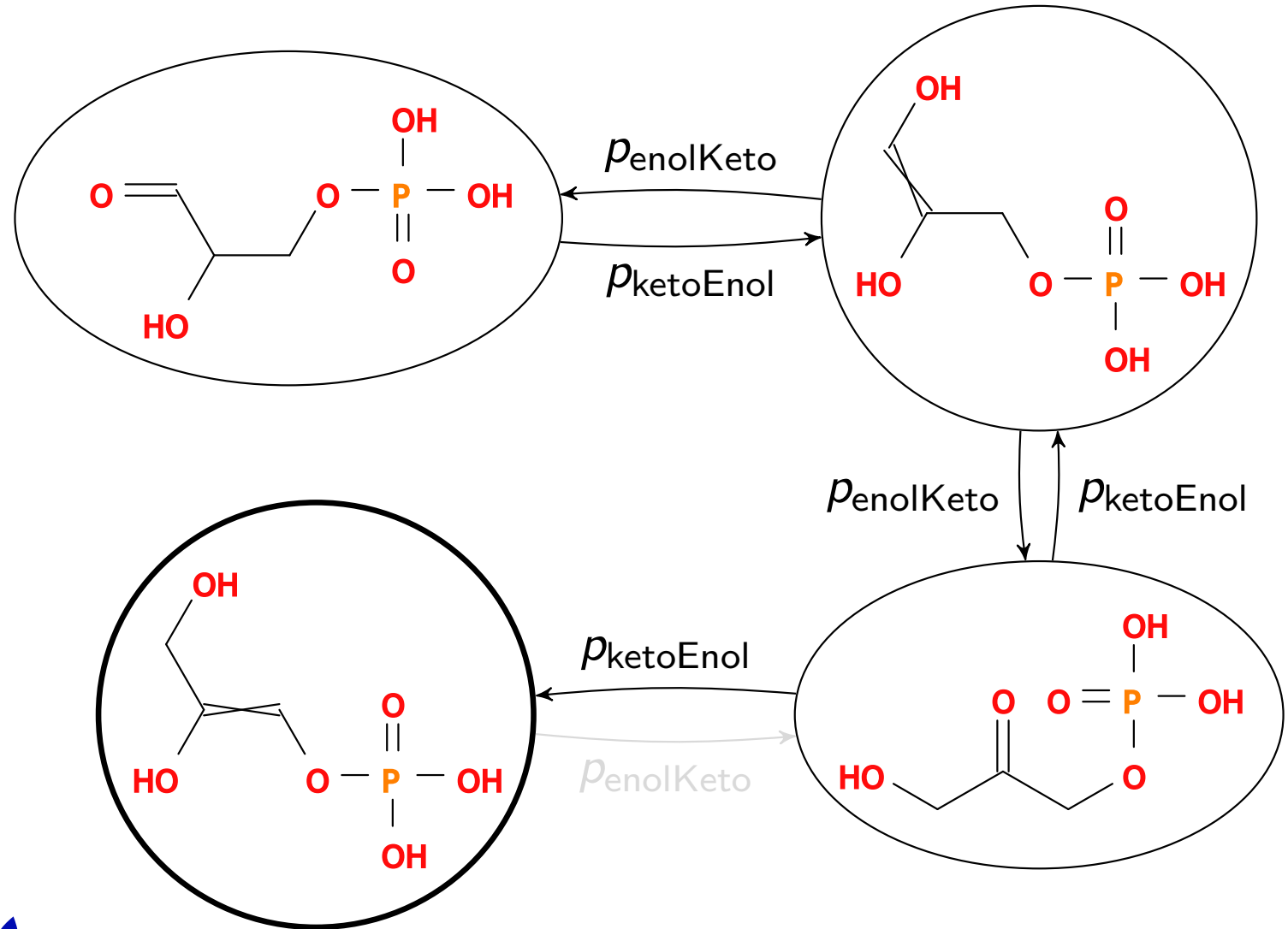


Iteration 2

Repetition

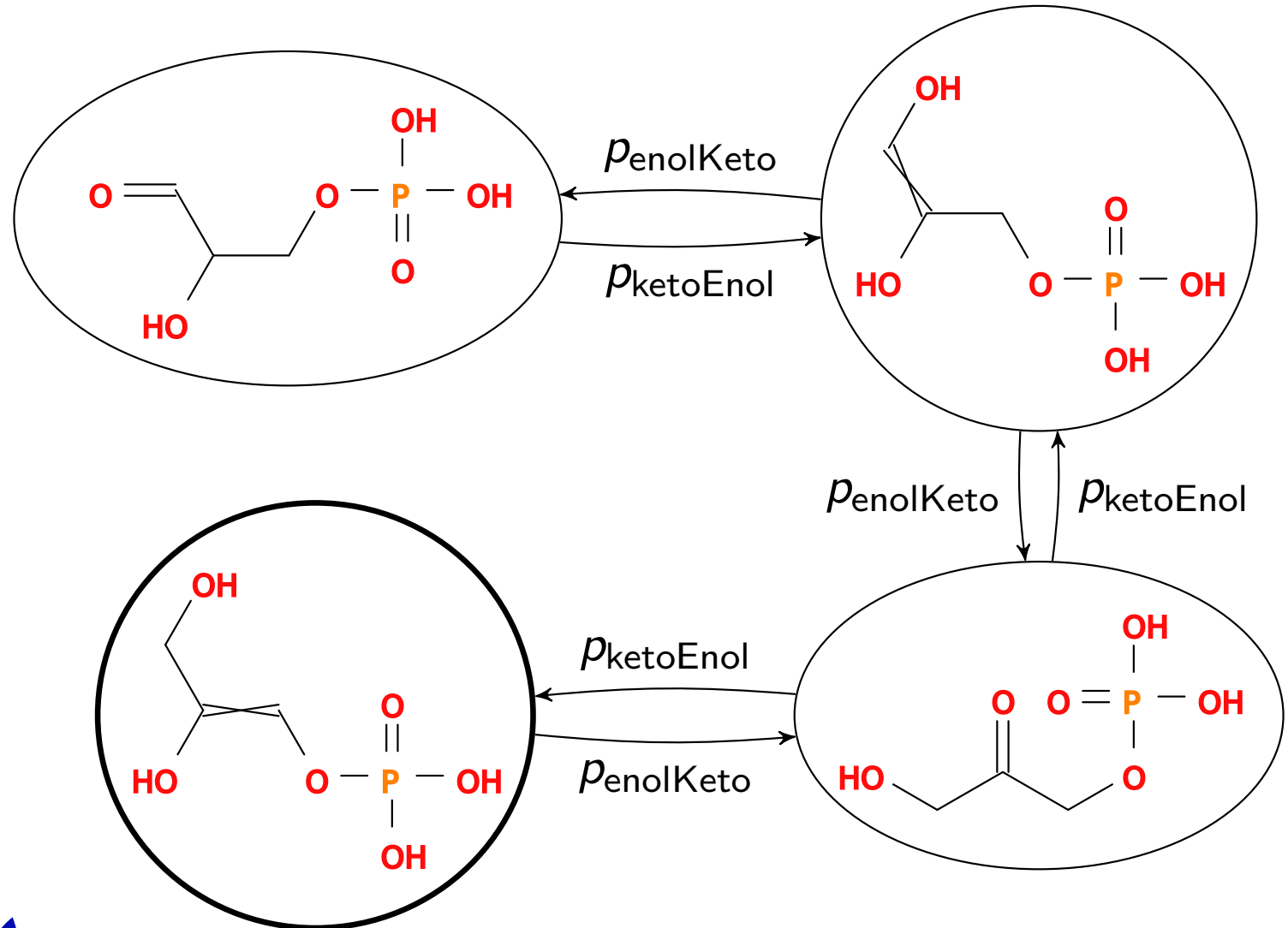
$$\texttt{addSubset}[\text{G3P}] \rightarrow \texttt{repeat}[\texttt{parallel}[\{p_{\text{ketoEnol}}, p_{\text{enolKeto}}\}]]$$



Iteration 3

Repetition

$$\texttt{addSubset}[\text{G3P}] \rightarrow \texttt{repeat}[\texttt{parallel}[\{p_{\text{ketoEnol}}, p_{\text{enolKeto}}\}]]$$



Iteration 4