

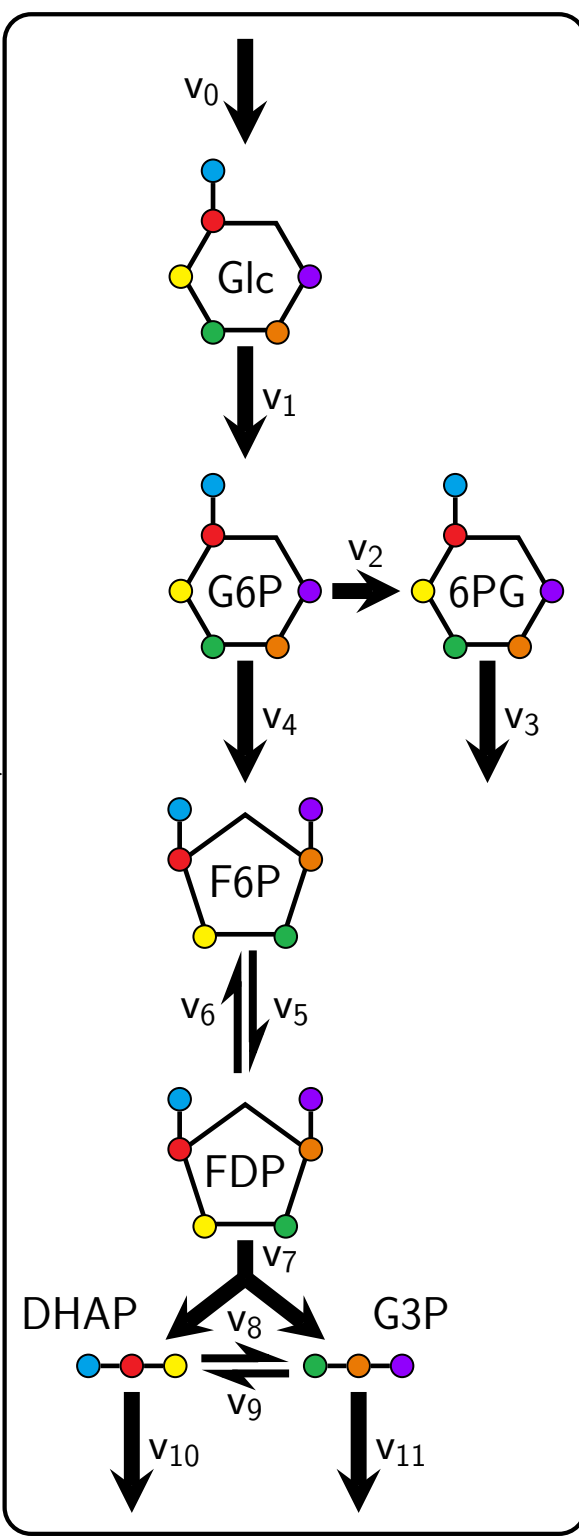
# 1. Pipeline inputs

$$\text{Stoichiometry} = \begin{bmatrix} 1 & -1 & 0 & 0 & \cdots \\ 0 & 1 & -1 & -1 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

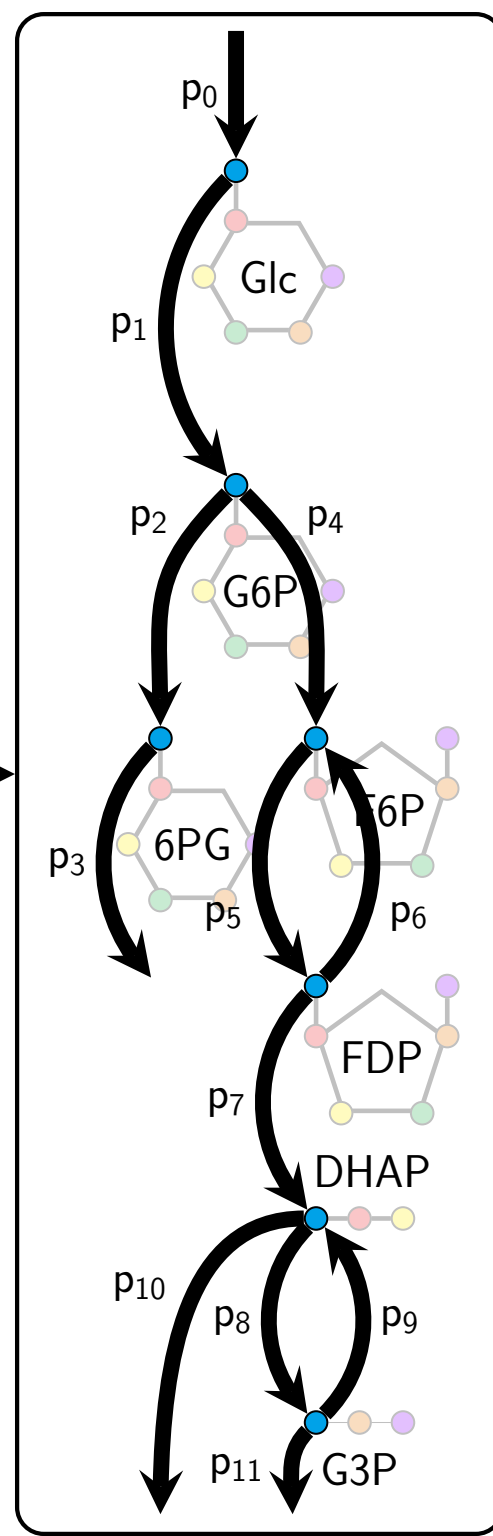
$$\text{SMILES} = \begin{bmatrix} \text{C}([\text{C}@\text{H}]1[\text{C}@\text{H}]([\text{C}@\text{H}]([\text{C}@\text{H}](\text{C}(\text{O}1)\text{O})\text{O})\text{O})\text{O})\text{O} \\ \text{C}([\text{C}@\text{H}]1[\text{C}@\text{H}]([\text{C}@\text{H}]([\text{C}@\text{H}](\text{C}(\text{O}1)\text{O})\text{O})\text{O})\text{O})\text{OP}(=\text{O})(\text{O})\text{O} \\ \text{C}([\text{C}@\text{H}]([\text{C}@\text{H}]([\text{C}@\text{H}]([\text{C}@\text{H}](\text{C}(=\text{O})\text{O})\text{O})\text{O})\text{O})\text{O})\text{OP}(=\text{O})(\text{O})[\text{O}-] \\ \vdots \end{bmatrix}$$

$$\text{Element} = \begin{bmatrix} \text{Carbon} \\ \text{Nitrogen} \\ \vdots \end{bmatrix} \quad \text{Flux} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ \vdots \end{bmatrix}$$

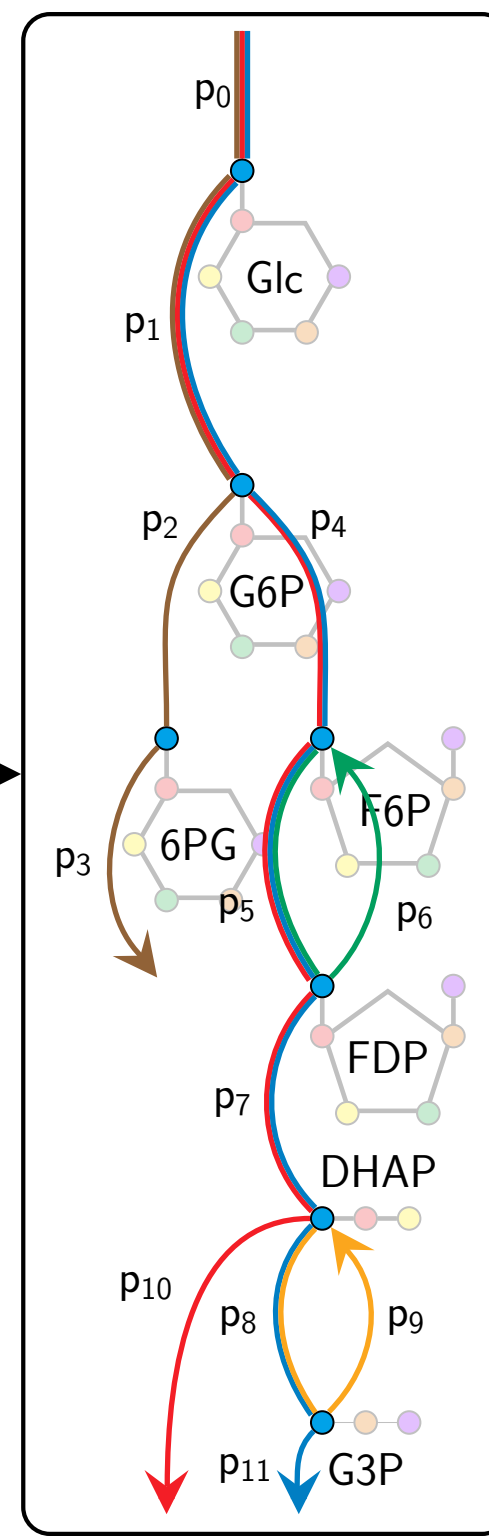
## 2. Model processing and validation



## 3. Atomic flux graph construction



## 4. ACHMC construction



## 5. Output estimated AEFM weights

