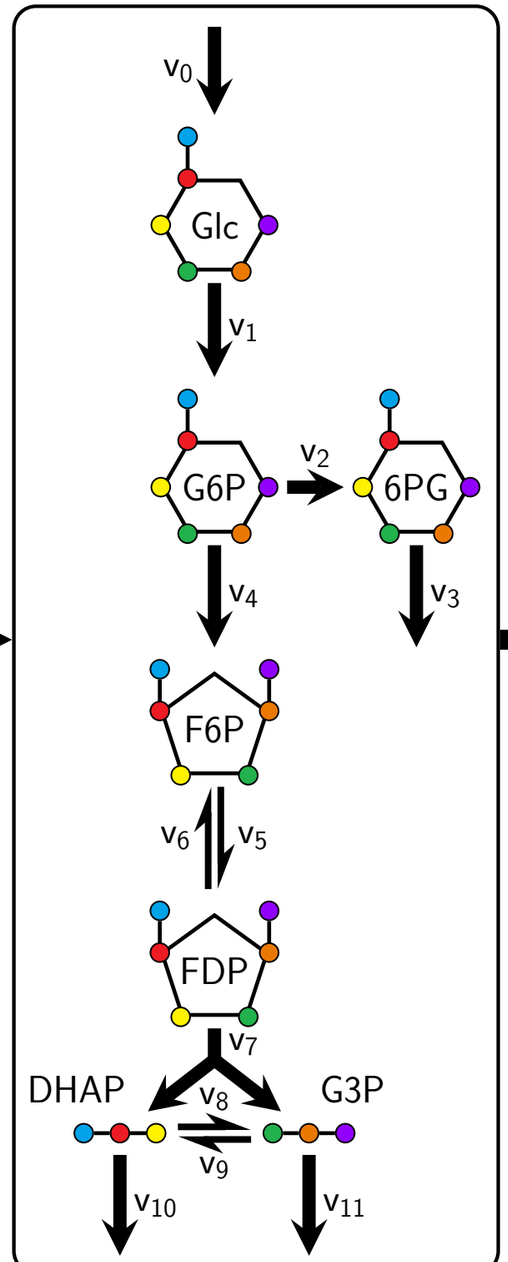
1. Pipeline inputs

$$\text{Stoichiometry} = \begin{bmatrix} 1 & -1 & 0 & 0 & \cdots \\ 0 & 1 & -1 & -1 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \quad \text{SMILES} = \begin{bmatrix} \text{C([C@@H]1[C@H]([C@@H]([C@H](C(O1)O)O)O)O)O} \\ \text{C([C@@H]1[C@H]([C@@H]([C@H](C(O1)O)O)O)O)OP(=O)(O)O} \\ \text{C([C@H]([C@H]([C@@H]([C@H](C(=O)O)O)O)O)O)OP(=O)(O)[O-]} \\ \vdots \end{bmatrix}$$

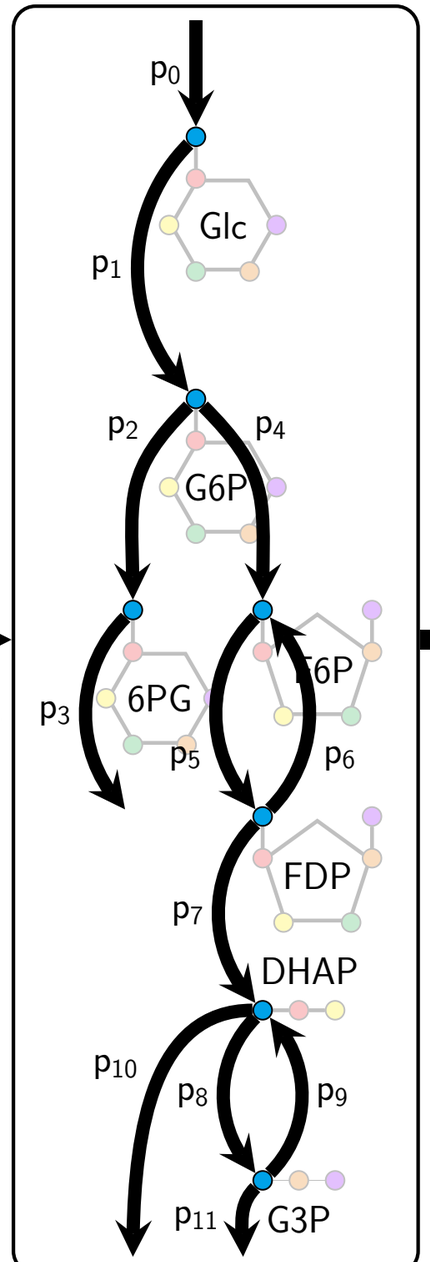
$$\text{Element} = \text{Carbon (C)} \qquad \text{Flux} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ \vdots \end{bmatrix}$$

2. Model processing and validation



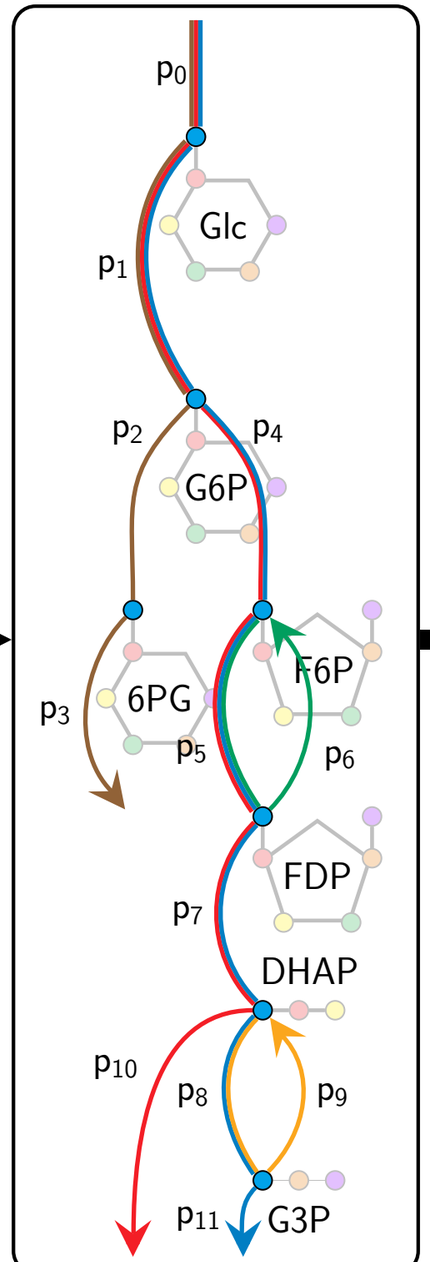
Trace atoms via RXNMapper

3. Atomic flux graph construction



Enumerate AEFMs for source metabolite atoms

4. ACHMC construction



Compute AEFM weights for source metabolite atoms

5. Output estimated AEFM weights