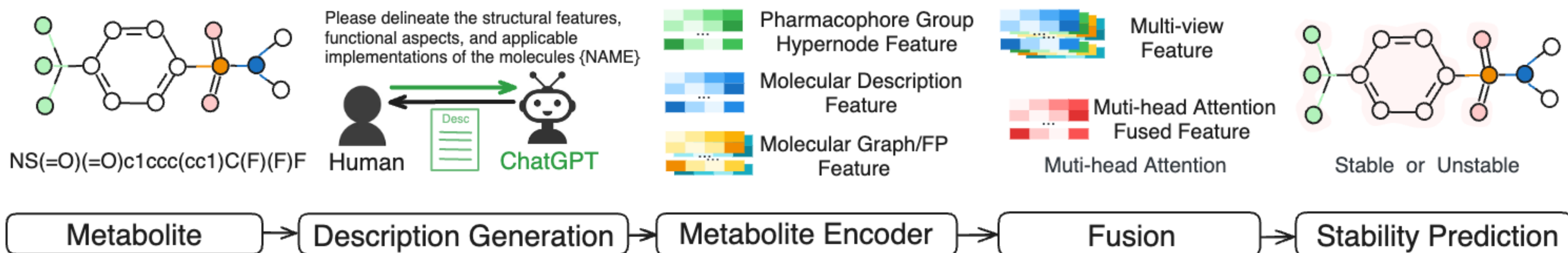
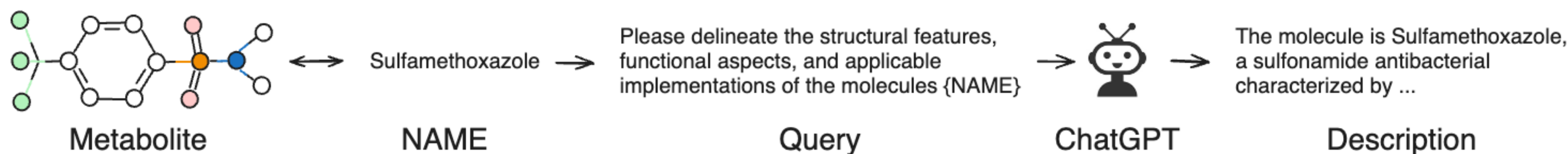


A. Workflow Overview

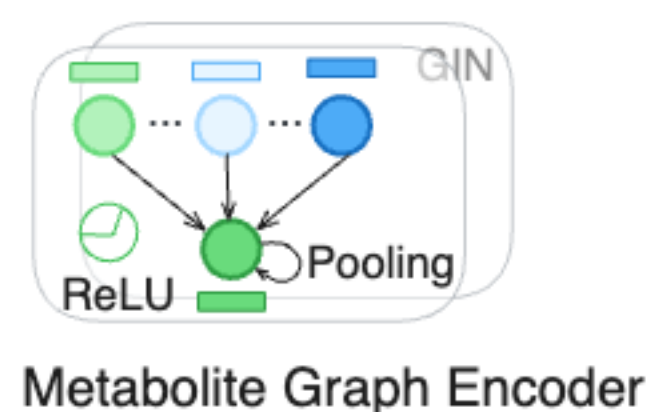
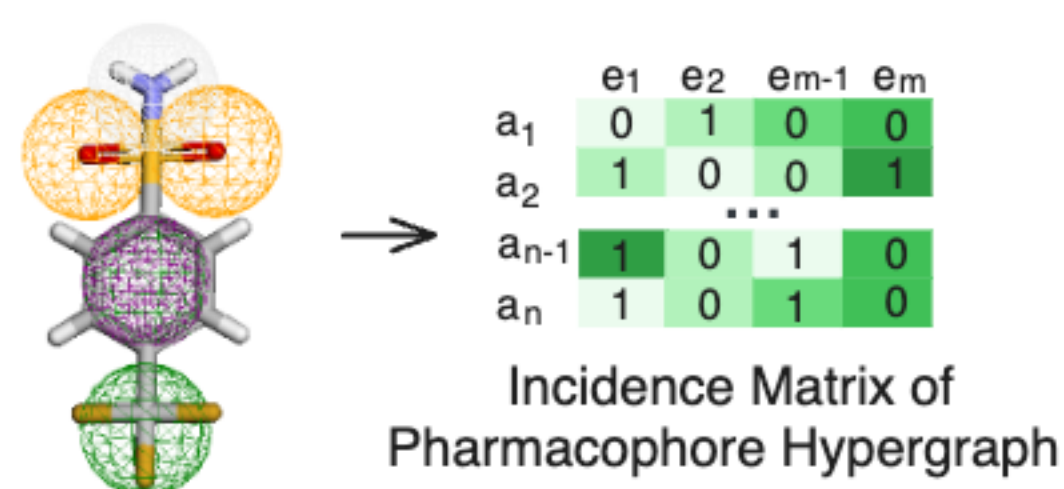


B. Generating Molecular Description with ChatGPT

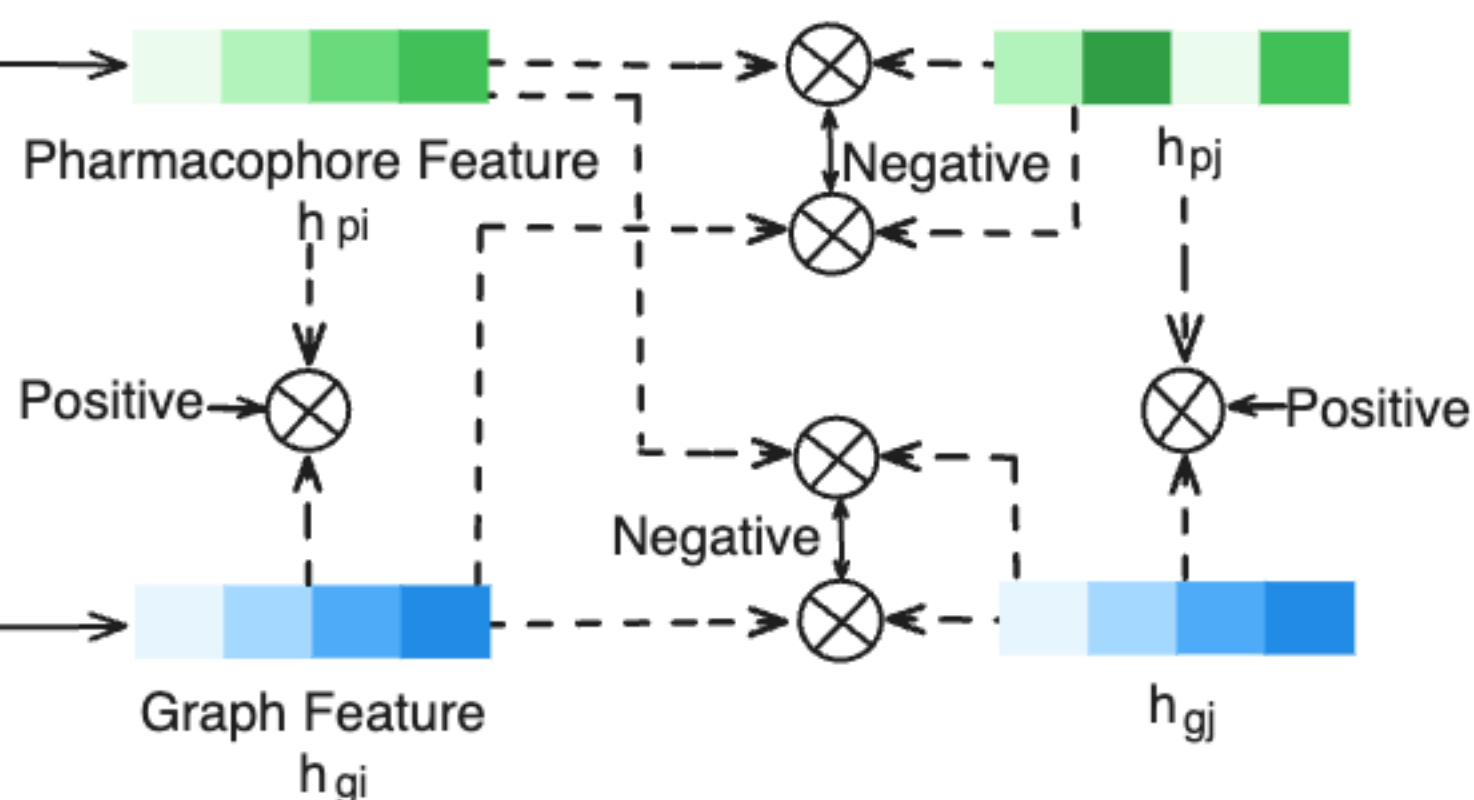


C. Processing and Predicting

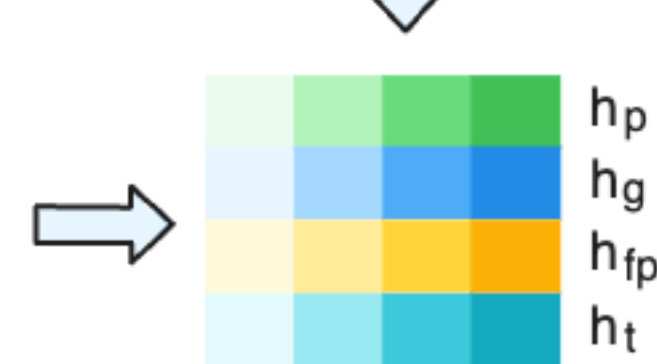
C.1. Feature Initialization



C.2. Contrastive Learning

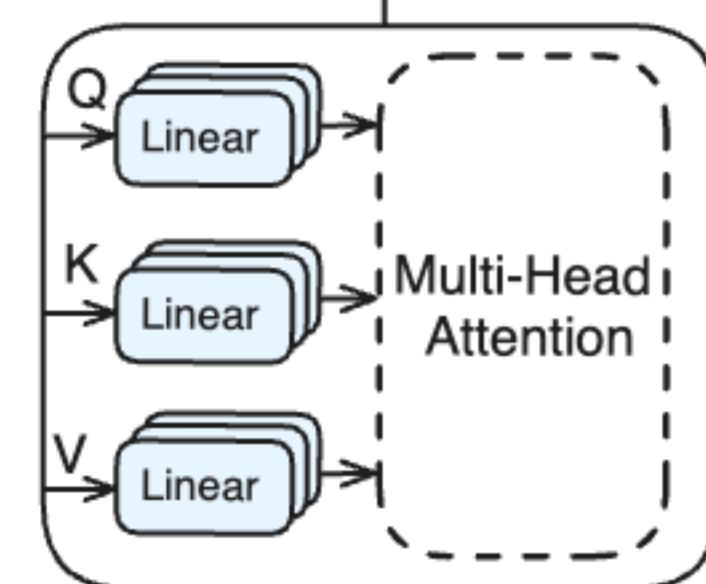
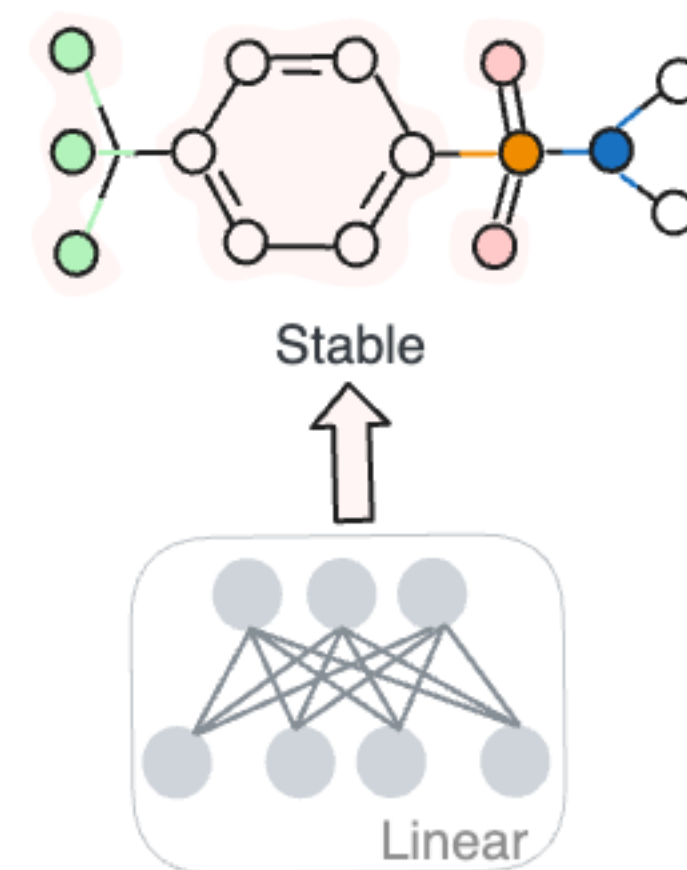


Metabolite j in a batch



$$Z \in \mathbb{R}^{4 \times d}$$

C.3. Scoring



Attention-based Fusion