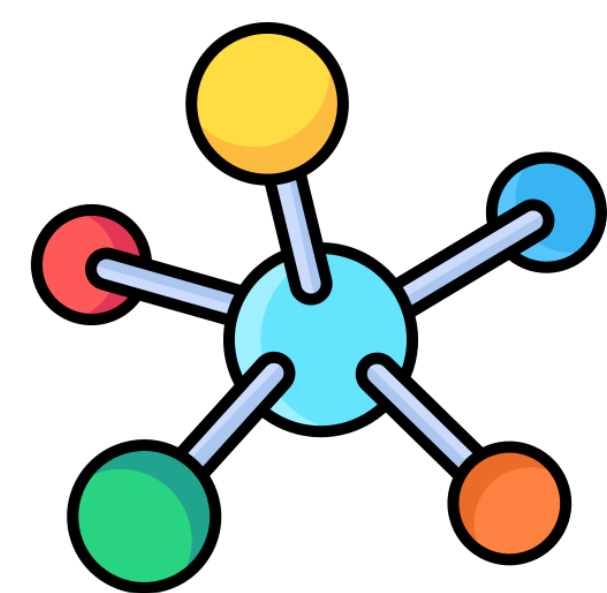
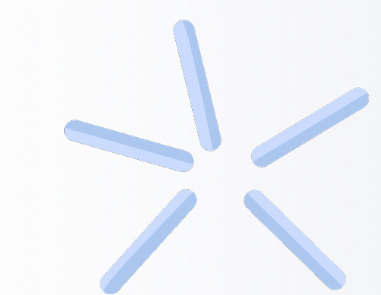


**a**

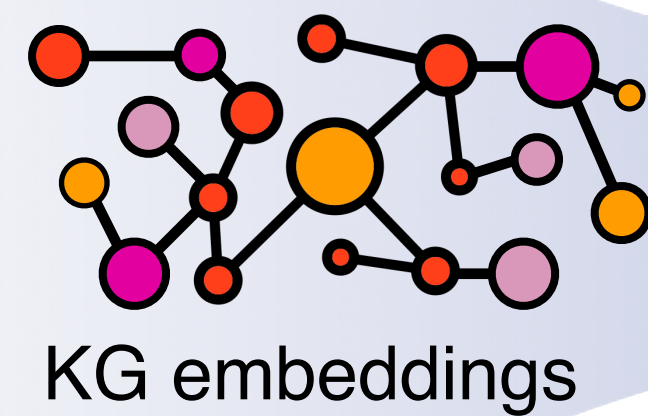
Drug Molecular



Atom features

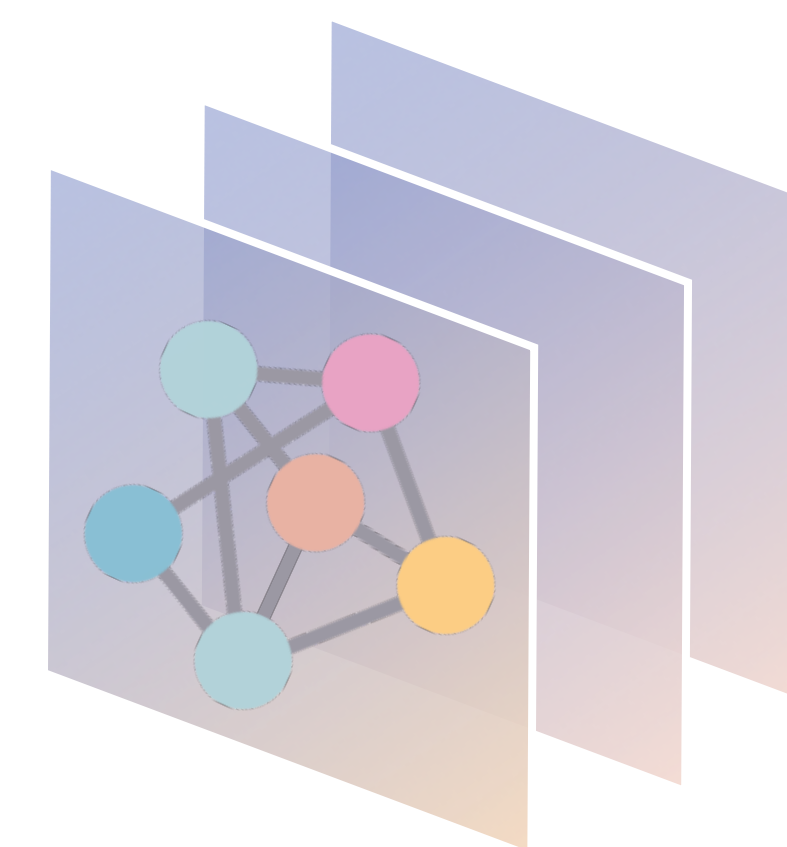


Bond features



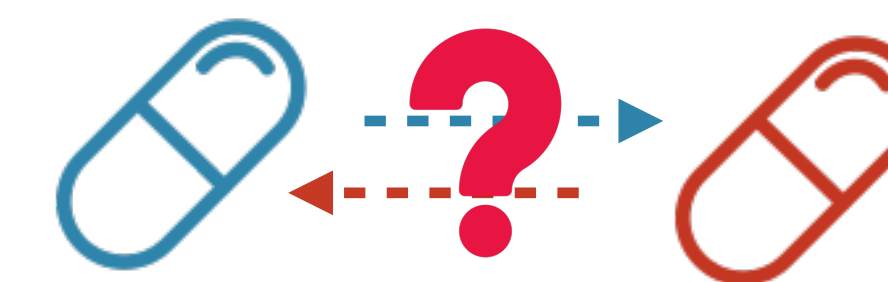
KG embeddings

### KG-embedded Molecular Graph Construction



### Graph Transformer

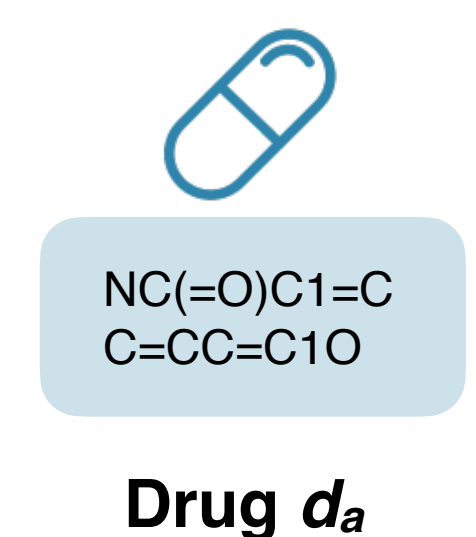
Drug Molecular Characterization



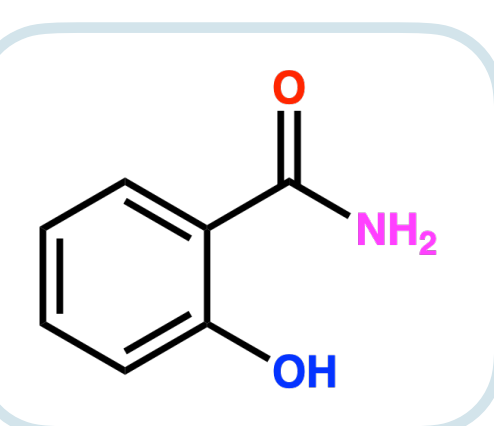
Interaction / No Interaction

**b**

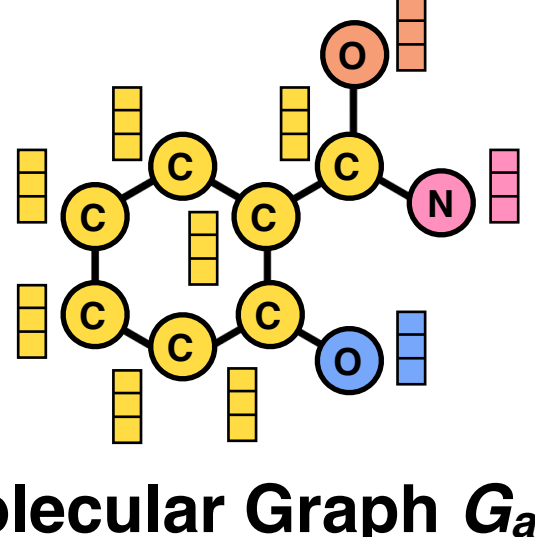
### KG-embedded Molecular Graph Construction



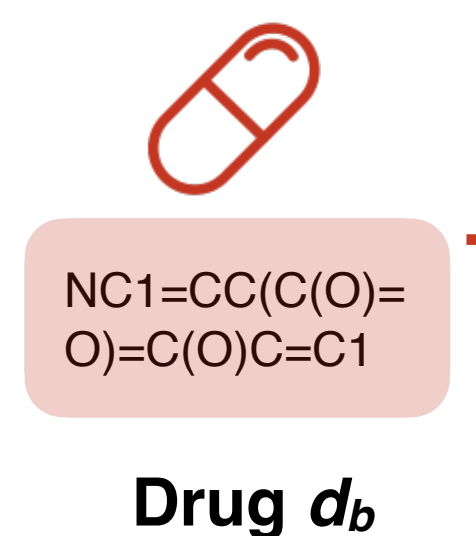
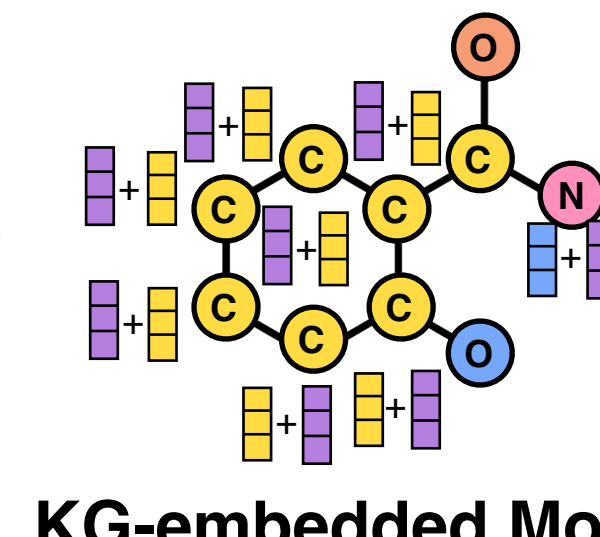
Rdkit



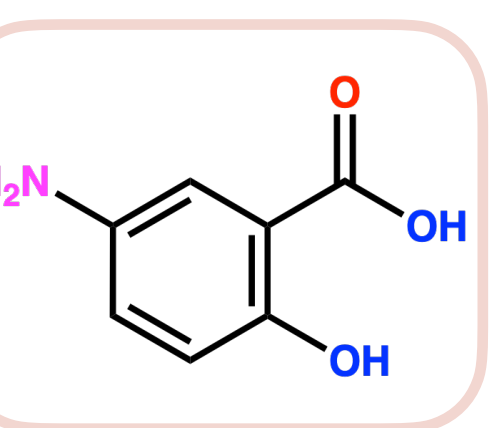
DGL



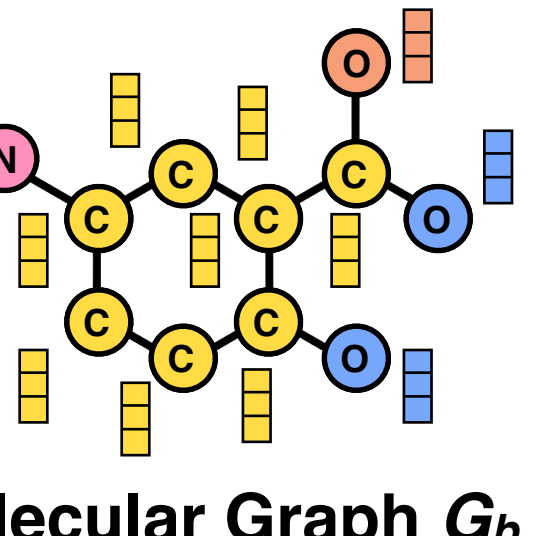
+



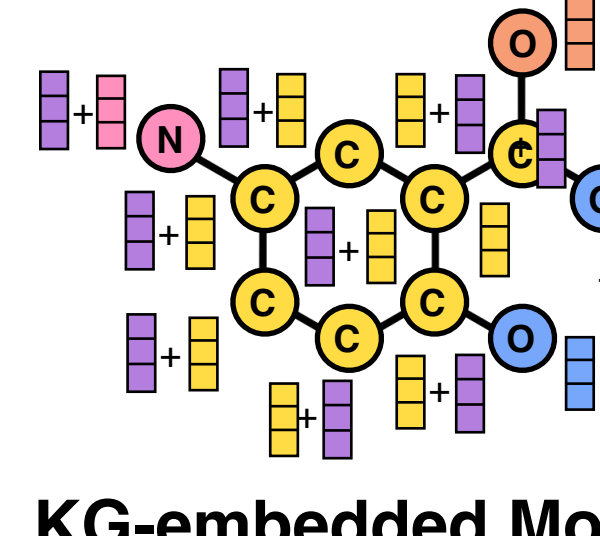
Rdkit



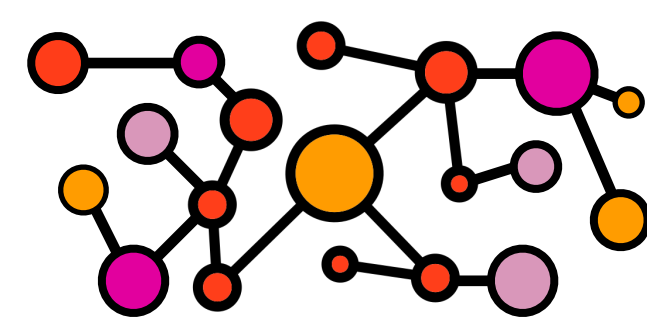
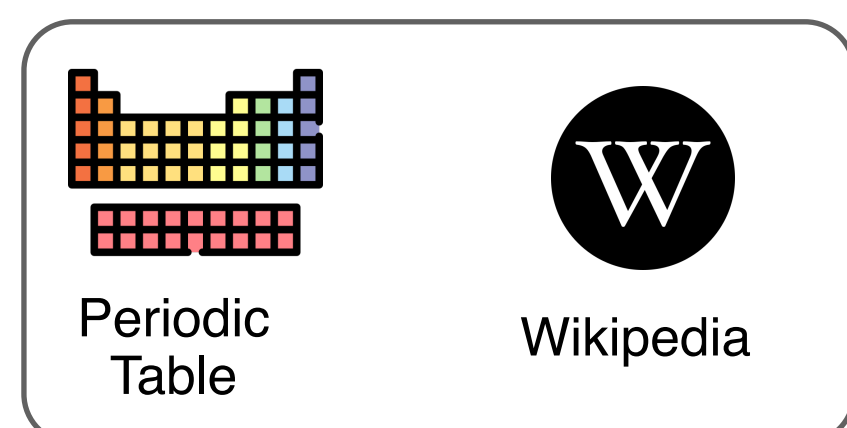
DGL



+

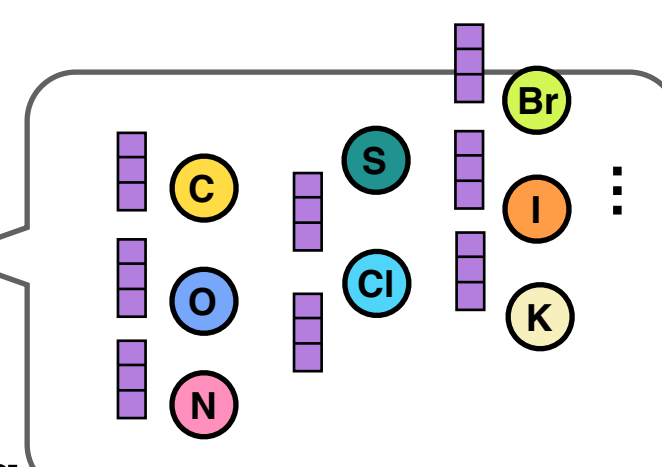


### ElementKG embedding

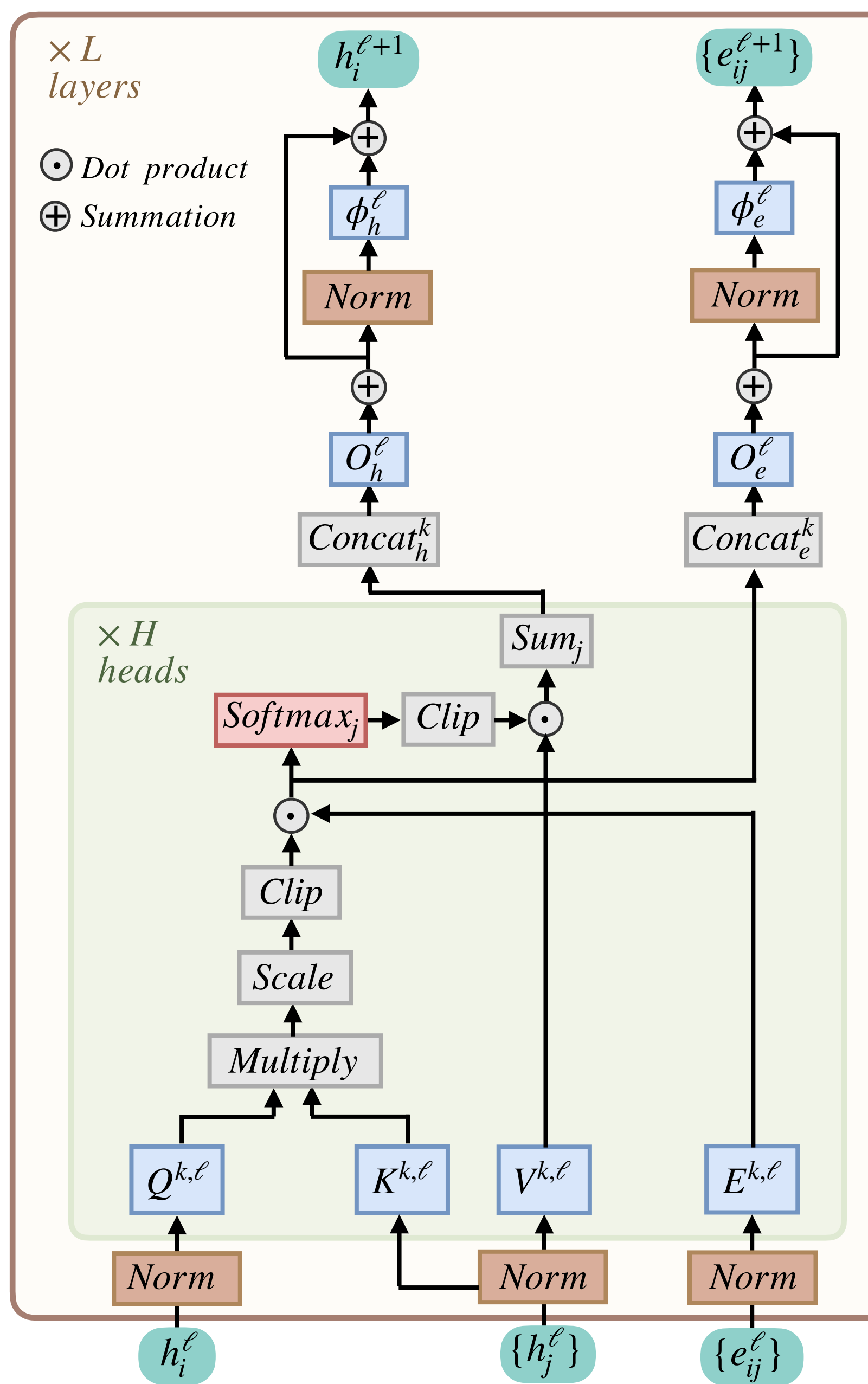


ElementKG

KG embedding

**c**

### Graph Transformer Architecture



### DDI prediction

