

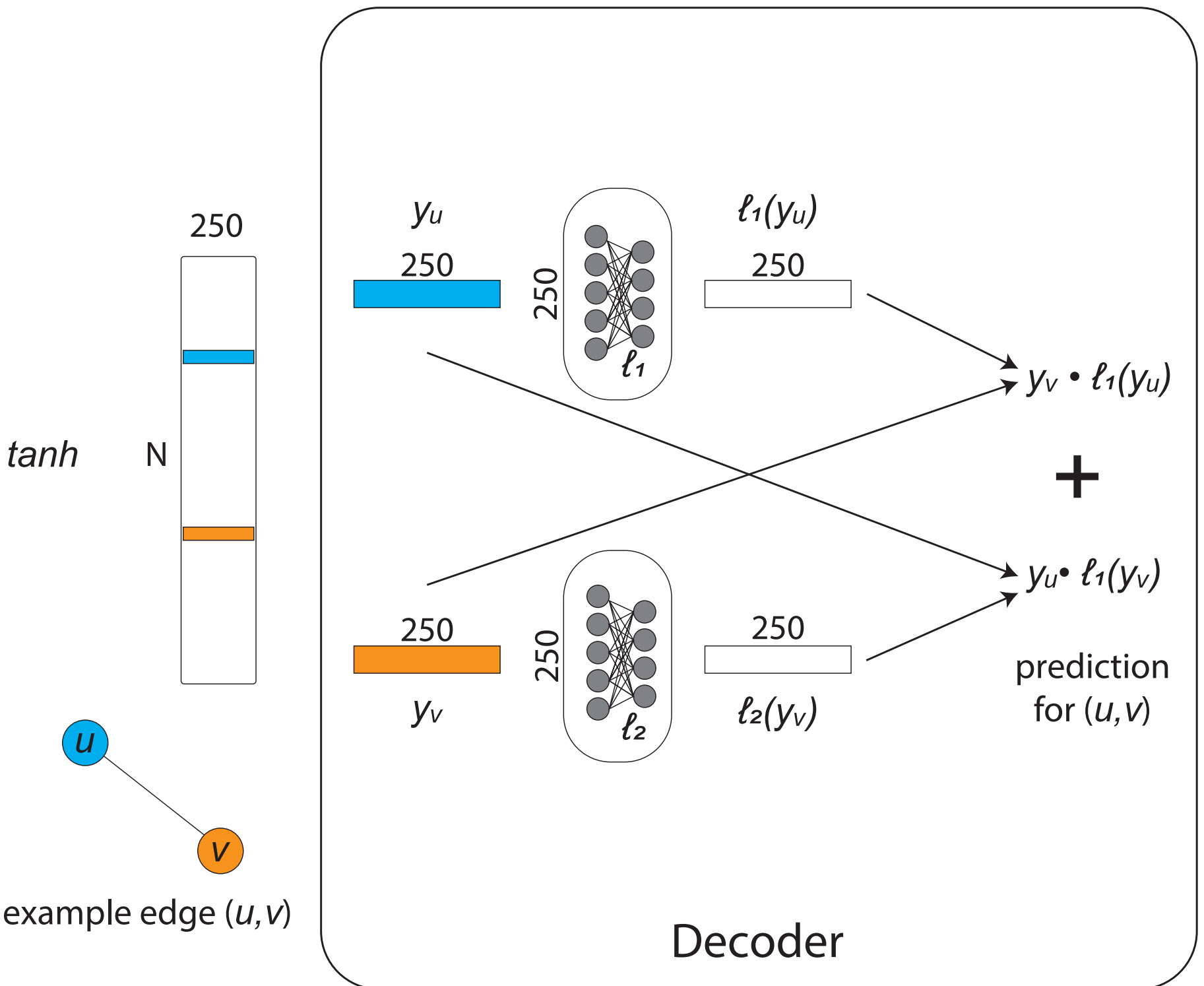
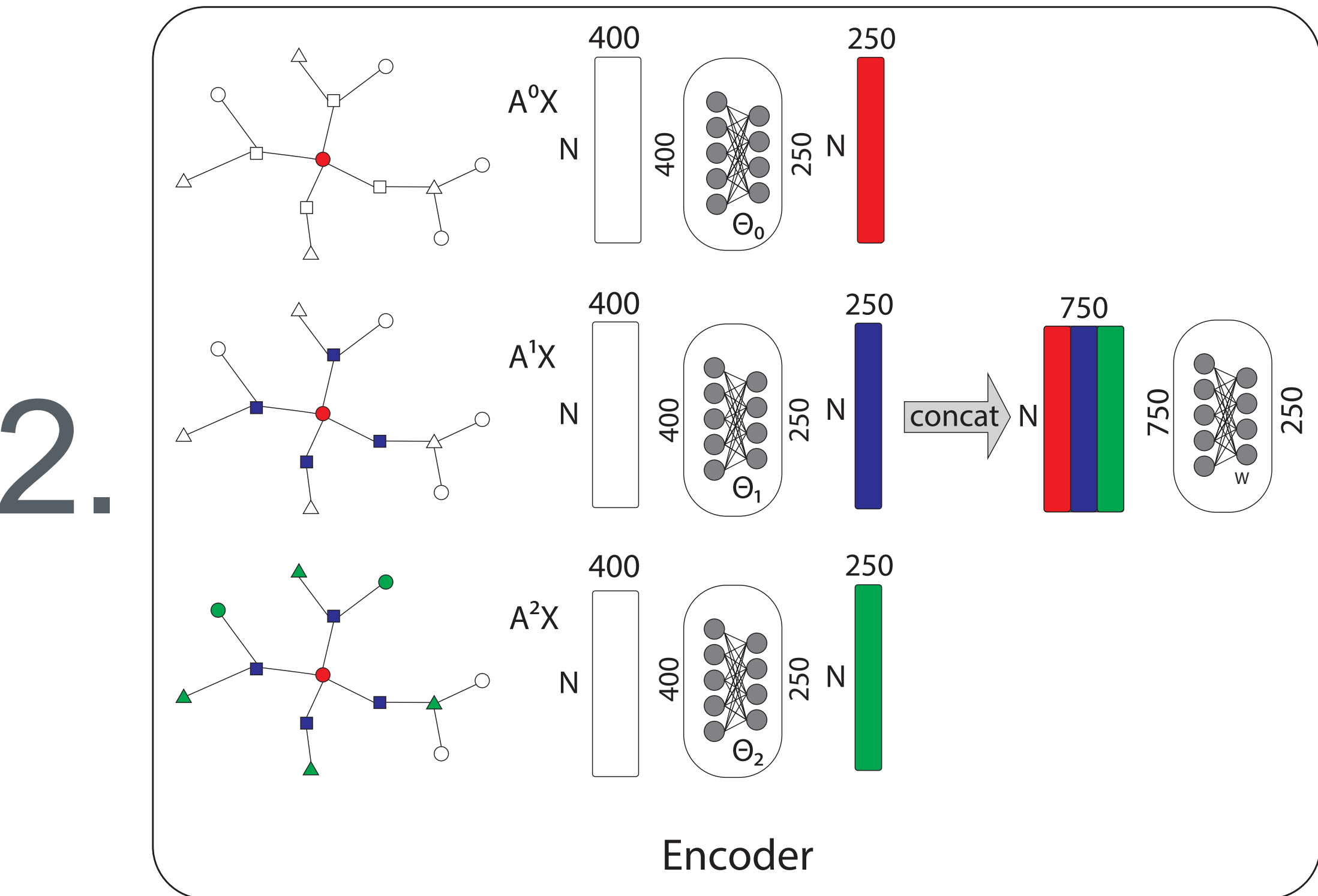
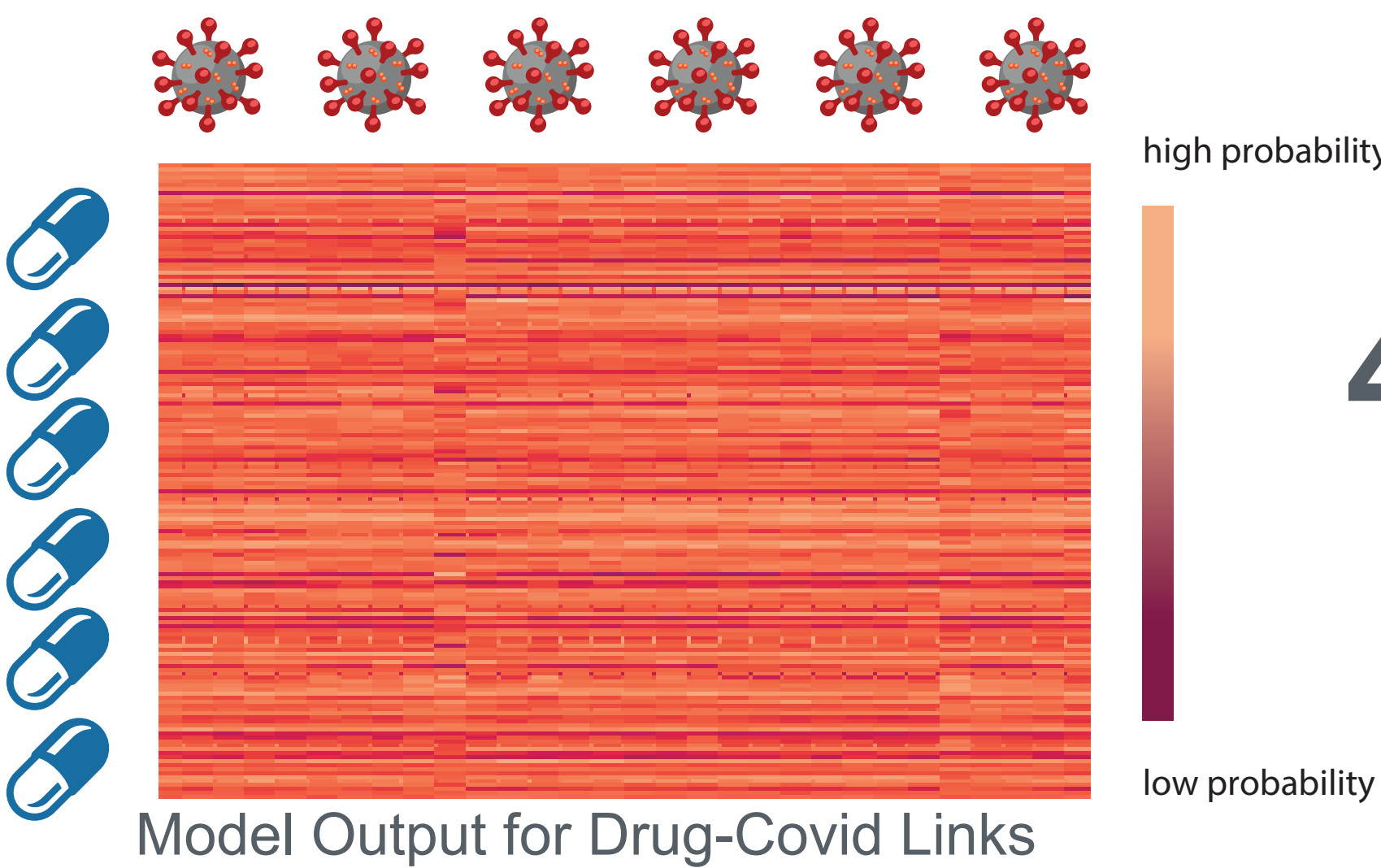
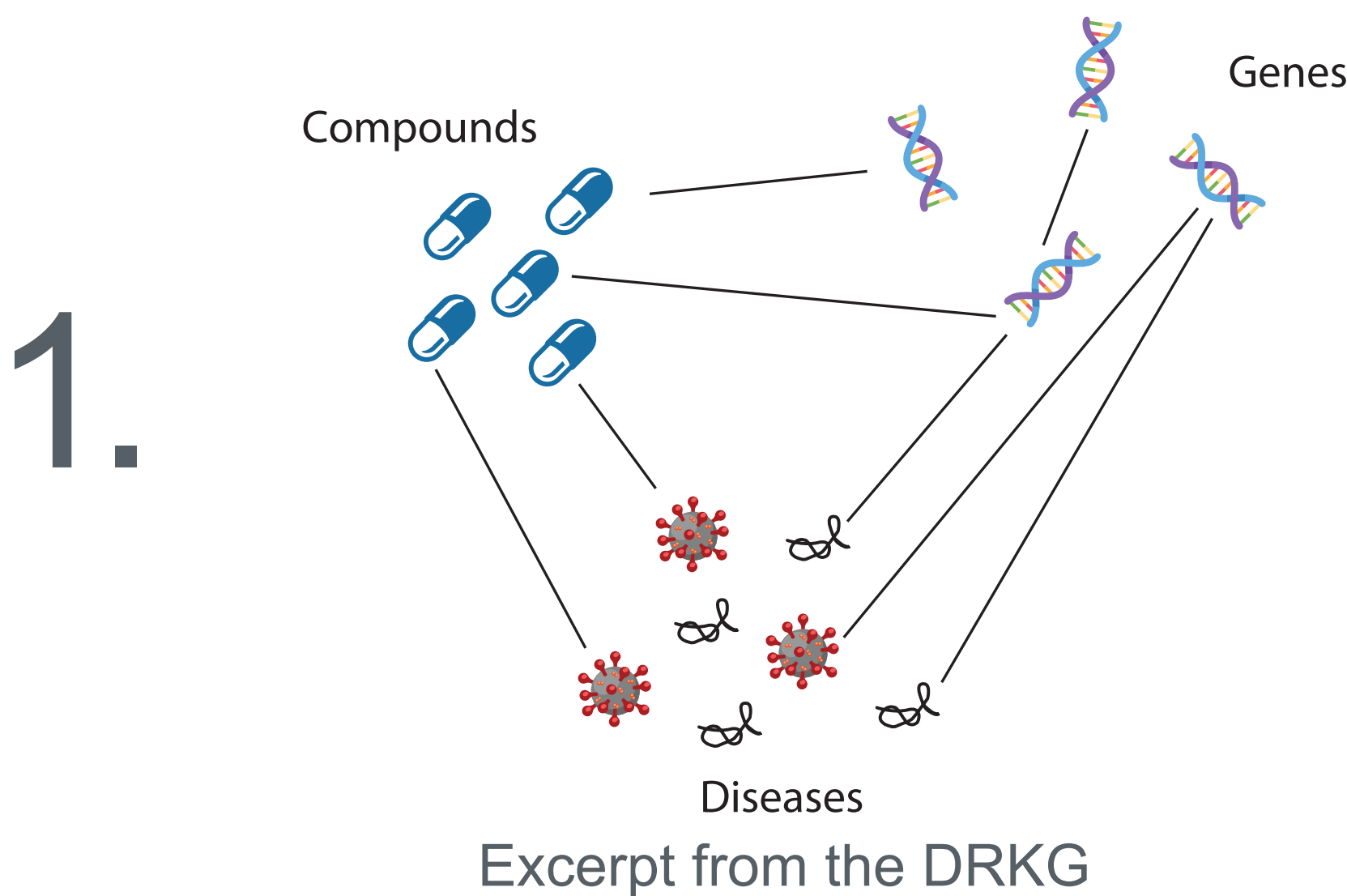
Drug Repurposing for Multiple COVID Strains using Collaborative Filtering

Otto Kißig, Martin Taraz, Sarel Cohen, Vanja Doskoč, Tobias Friedrich

From Knowledge Graph to Drug Candidates

1. Prepare the Drug Repurposing Knowledge Graph (DRKG)
2. Derive neighborhood-aware embeddings
3. Predict probability for all Drug-Covid links
4. Map probability matrix to scores per drug
5. Derive a ranking and select top-100 drug candidates

Aggregation Strategy	# Hits
Single Disease (median)	20
Global Score Maximum	22
Global Score Mean	30
Cluster Score Maximum with KMeans (k=8)	18
Cluster Score Maximum with KMeans (k=3)	20
Union over Disease Rankings (Dr COVID)	21
Union over Cluster Rankings with KMeans (k=8)	24
Union over Cluster Rankings with KMeans (k=3)	32



Encoder Decoder Architecture