

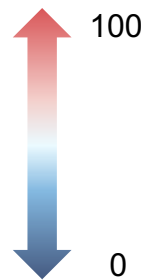
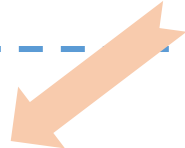
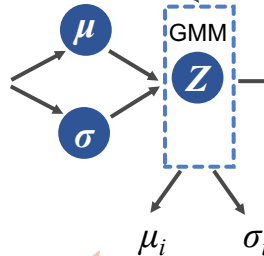
Datasets

- Candidate drug
- ChEMBL
- ZINC
- GDB

Encoder

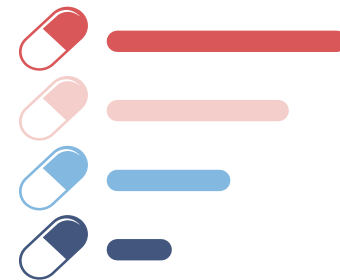
Decoder

$$\varepsilon \sim N(0,1)$$

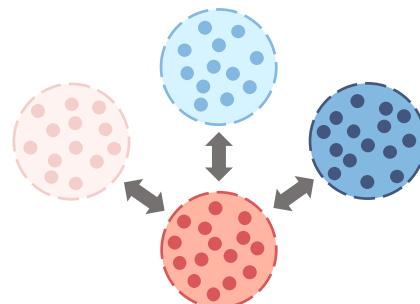
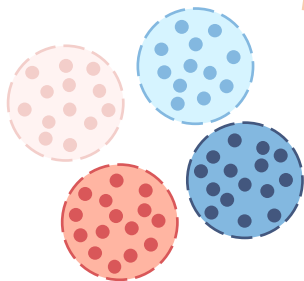
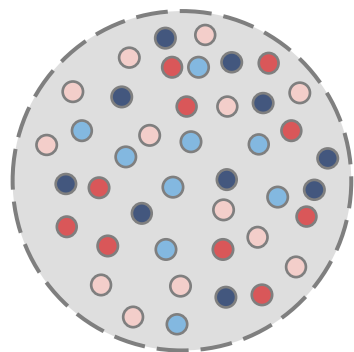
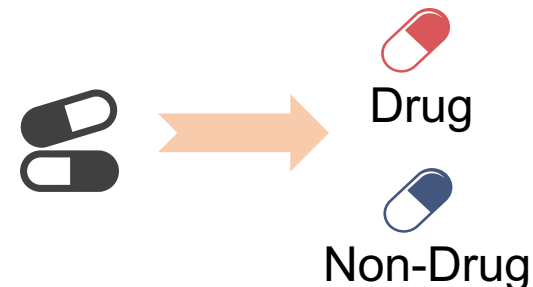


Applications

Drug-likeness scoring



Drug Classification



Scoring based on
Wasserstein Distance

Original space

Latent space