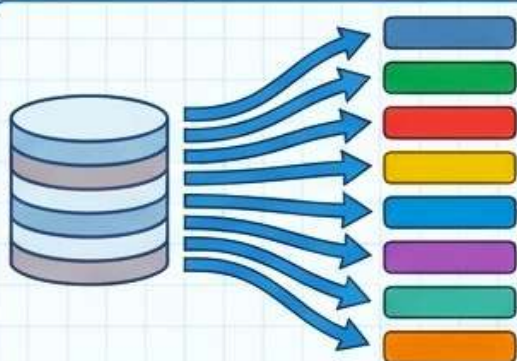
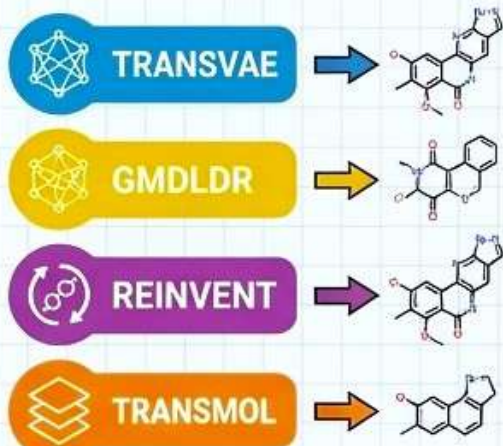


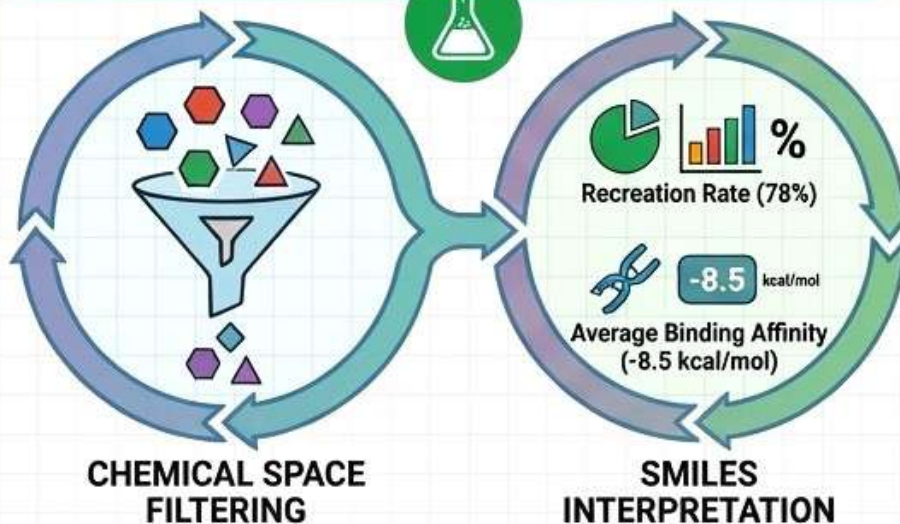
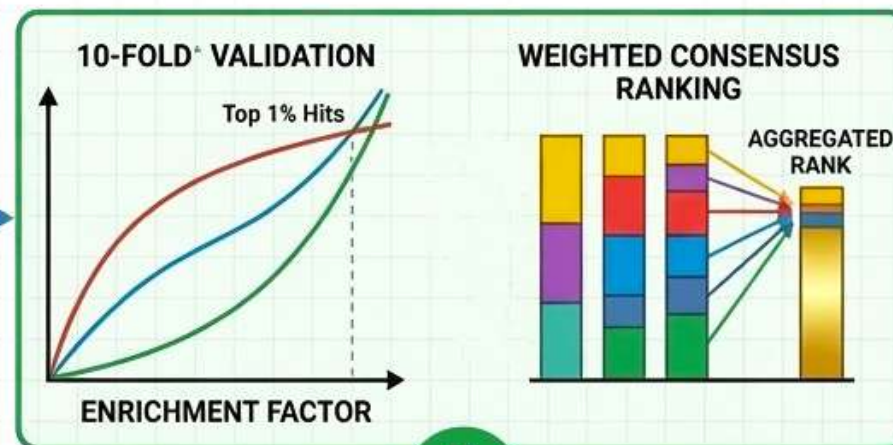
## 10-FOLD DATA SPLIT



## IN-SILICO COMPOUND GENERATION



## ENRICHMENT FACTOR, RRA & CROSS-VALIDATION



## GENERATIVE MODELS & OPTIMIZATION

