

1

Protein  
databases

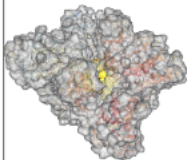
UniProt  
Protein Data Bank



2

Pocket  
selection

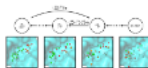
Binding site  
extraction



3

Generative  
models

Diffusion



Genetic



Transformer



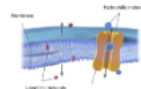
4

Evaluation  
metrics



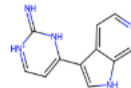
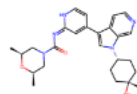
Toxicity screening

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40
41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60



5

Output



Potential  
drug  
candidates  
with optimal  
properties