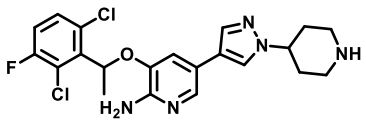
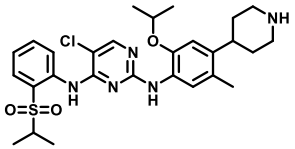
SYNERGY OF ADVANCED MACHINE LEARNING AND DEEP NEURAL NETWORKS WITH CONSENSUS MOLECULAR DOCKING FOR ENHANCED POTENCY PREDICTION OF ALK INHIBITORS

FDA APPROVED ALK INHIBITORS

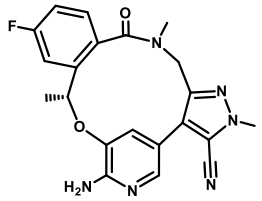
Crizotinib



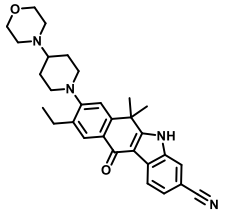
Ceritinib



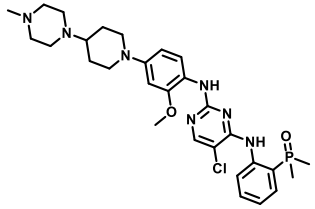
Lorlatinib



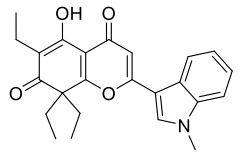
Alectinib



Brigatinib



POTENTIAL ALK INHIBITORS CANDIDATES



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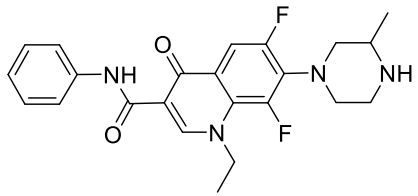

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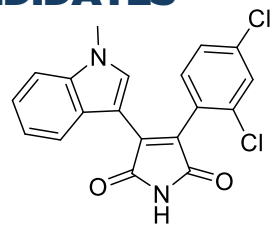

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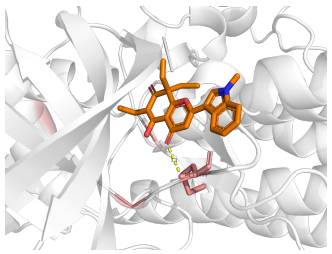
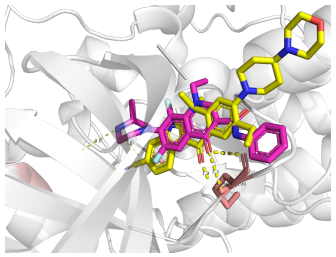
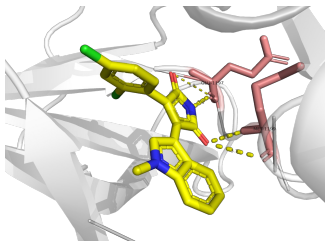
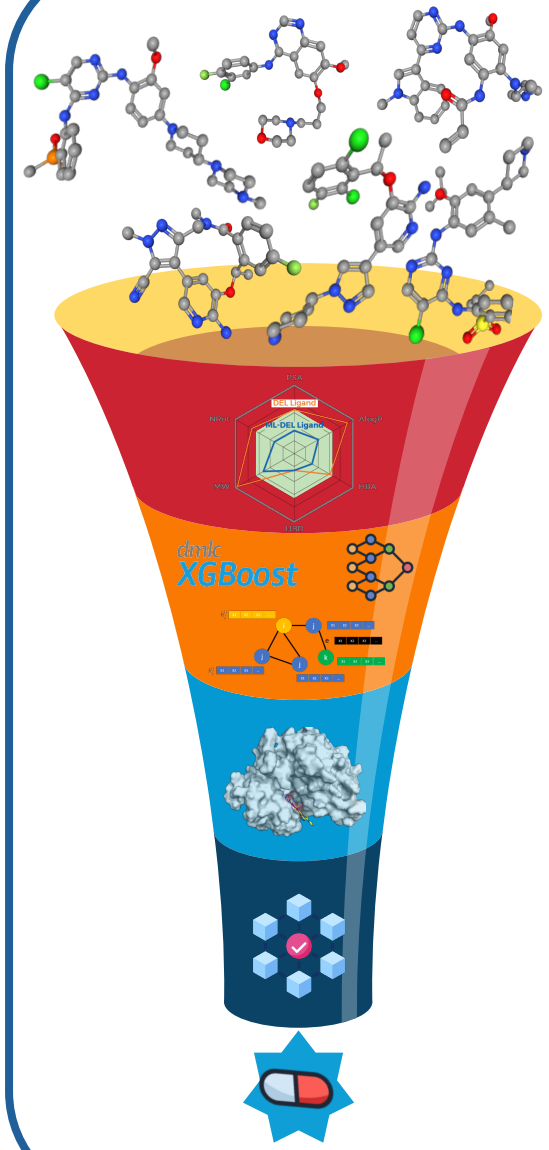






VIRTUAL SCREENING FUNNEL



Potential ALK inhibitors

Screening dataset:
120,571 compounds

1 **Druglikeness screening**

8742 compounds pass Druglikeness screening

2 **Ensemble AI models**

2491 compounds satify the ensemble models

3 **Molecular docking**

GNINA, Vina-GPU, Autodock-GPU

4 **Consensus docking**

8 compounds satify consensus docking