Comprehensive Virtual Screening

Chemspace Virtual Screening Services

CHEMSPACE
Delivering Discovery Solutions®

INPUT

What do we expect as Input?

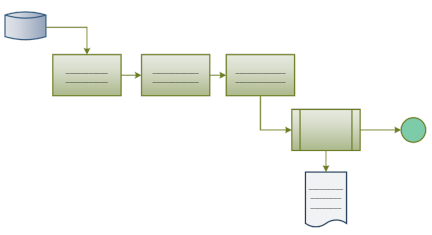
- Desired protein target
- Better results are expected if an X-ray structure is available
- If the structure of the selected protein was not determined, one would need a list of closest analog proteins for corresponding homology modeling
- Known active compounds (optional)
- Preferred ligand chemotype (optional)

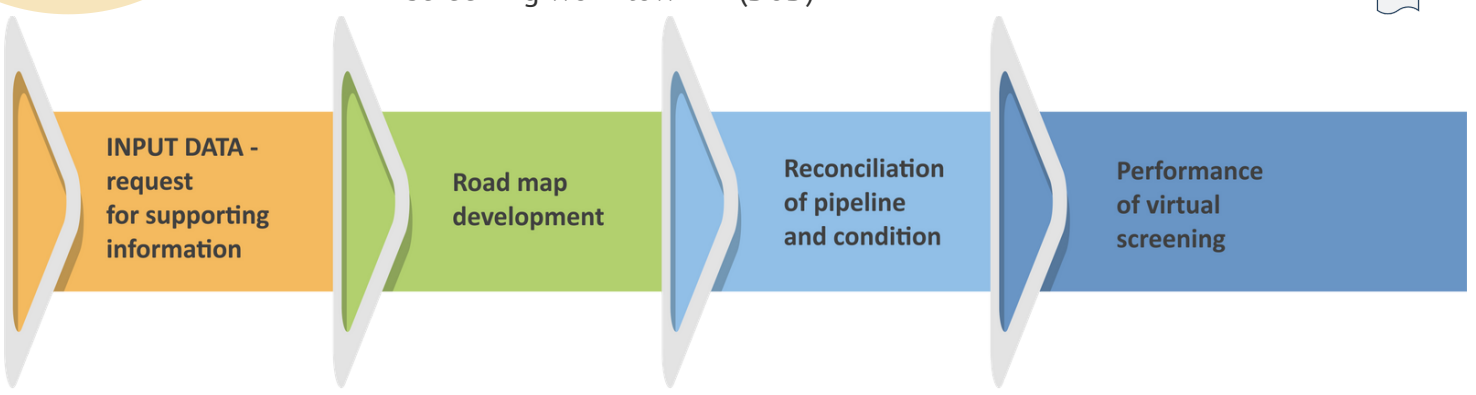
PIPELINE

Virtual Screening Pipeline

Expectation of all accessible information Planning and developing a virtual screening workflow

Reconciliation of composition of the workflow and the definition of done (DoD)





OUTPUT

RESULTS

- List of perspective hit compounds, having the highest affinity to the selected receptor and preferred of diversified chemotypes
- Report with several illustrations and workflow descriptions
- Fine-tuning of the approach for large databases screening
- Combinations of different tools or virtual screening as a complete task to find picked set of compounds requested size (Analogs Searching, MedChemfilters, Molecular Docking, Molecular Dynamics, Homology Modeling, QSAR, etc.)
- Finding biologically active molecules that show activity against a specific protein
- Also applicable for fast screening of multi-million compound libraries

MISSION OF VIRTUAL SCREENING

- When dealing with enormous-sized datasets as inputs in any study, optimizing computational resources used while retaining prediction accuracy becomes defining factor when building the workflows.
- Offering various computational services, Chemspace confidently relies on its valuable experience and successfully completed projects.
- These services can be contracted under confidentiality terms as well as other specific conditions agreed with the customer