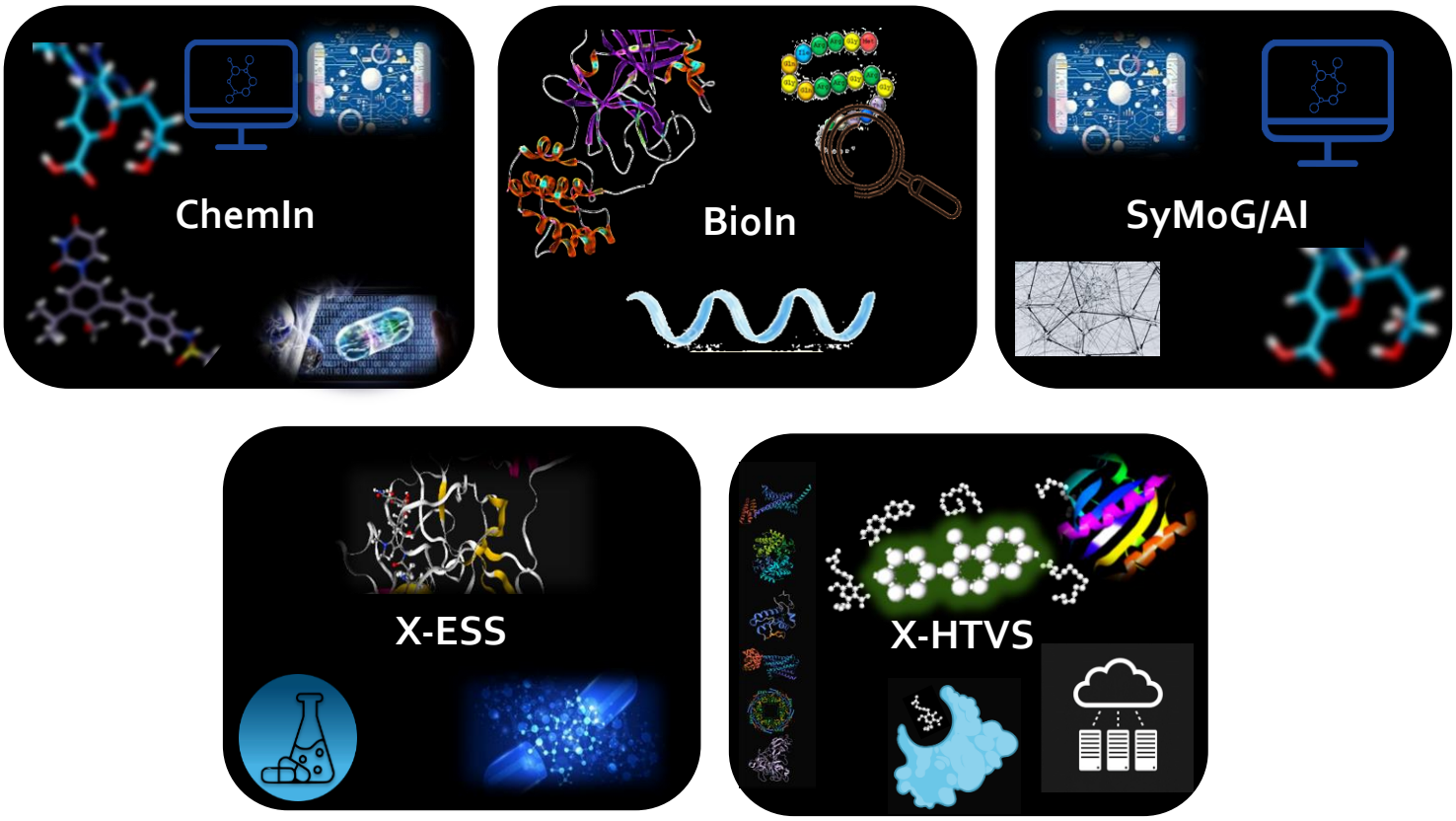
PRESCIENCE
INSILICO

Applying Deep Tech to Scientific Research

Prescience *in silico* Solution Suite
PRinS$^{3®}$

AI/HPC Driven Solutions Suite for Drug Discovery and Materials Research



Innovate | Accelerate | Discover

Discovering the Future: Creating solutions and paving the way for the new possibilities

Contact us

Prescience welcomes your question and App evaluation/ Demo requests. Email support@presience.in and visit https://www.prescience.in for more details

Key Features of PRinS^{3}®

Integrated Platform Provides Ready Solutions

PRinS^{3} is a new age platform developed to host applications (APPs) to perform the scientific computations and directly provide solutions. Scientific solutions are designed for industries working in materials, chemicals, energy, and pharmaceutical domains.

In-built Cloud Computing

By design, PRinS^{3} is cloud enabled, although also works on a suitable workstation. Even in absence of in-house HPC compute power, users can execute all the calculations in cloud from the graphical user interface. Prescience helps the user in setting up cloud account of their choice.

High Throughput Calculation

PRinS^{3} is inherently designed for high throughput. It can screen millions of compounds against multiple targets. The integrated process is built to perform high throughput docking for thousands to millions of compounds and materials design in fully automated way. All the applications and solution are ready to produce meaningful results derived from large set of calculations.

Design New Drugs and Materials

The standard solutions available in PRinS$_{3}$ are designed to solve research problems in drugs discovery and materials research for diverse industries like life-sciences, Energy and Chemical/Materials industries. PRinS^{3} architecture allows for designing custom solutions for several industries on-demand. Our consulting team is prepared to deliver them at a short time-frame.

Compatible with Linux, Windows and MacOS

PRinS$_{3}$ platform is operating system agnostic. The client interface is developed for Linux, Windows and MacOS (Intel Only) and works seamlessly in any of these OS. The server-side implementation is done on docker, so it is very simple to install and use in any server running any OS.

Fully Automated Solutions

The process flow is in-built and designed for automation, requiring least manual intervention from the user. Modular architecture allows creating additional features on demand within a very short time-span.

At Scale - High Performance Computing

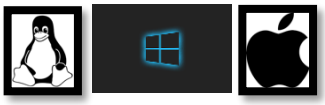
PRinS^{3} provides easy access from the user-interface to the on-premise high performance computing infrastructure and helps in managing all the calculations in parallel. The calculations scale automatically according to the size of the infrastructure. Calculations can be also be executed in hybrid i.e., in-house infra and cloud at the same time.

Easy and Intuitive Interface

Minimalistic design of user- interface of PRinS$_{3}$ is highly intuitive and facilitates short learning-curve. New users can quickly setup and perform calculations, and visualize results generated in the interface or use for publications, patents, whitepapers and presentations.

Ready Visualization of Structures and Data

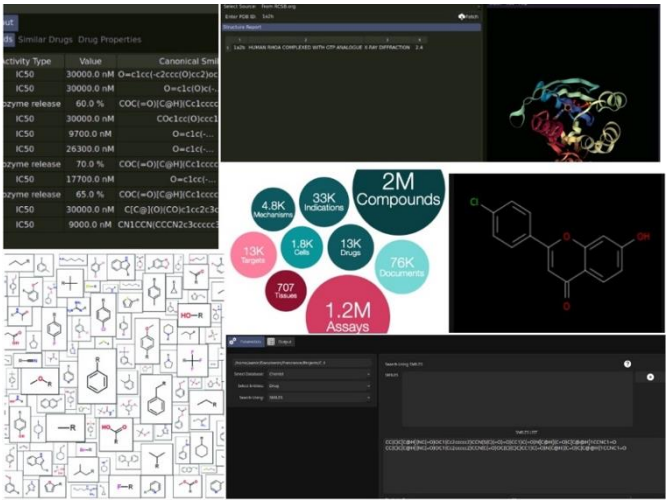
The visualization tools for structures and plotting interfaces for data are integrated in PRinS^{3}. These tools are utilized by each of the applications to visualize every step of the process flow towards the solutions. The user interventions are limited, and the graphs/structures generated are high quality.

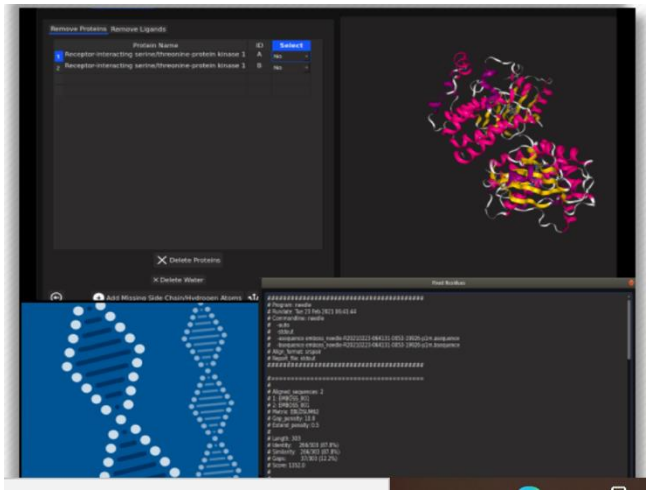


PRinS³®: Drug Discovery Apps

Features of ChemIn: Cheminformatics

- Integrated ChEMBL and Uniportkb-Swissprot database for searching chemicals based on targets
- Sequence similarity search for targets using NCBI-BLAST and FASTA
- Expand chemical space with similarity search and Artificial Intelligence
- Fully integrated SMILE structure search and conversions
- Create input ligand structures in PDB format for X-ESS





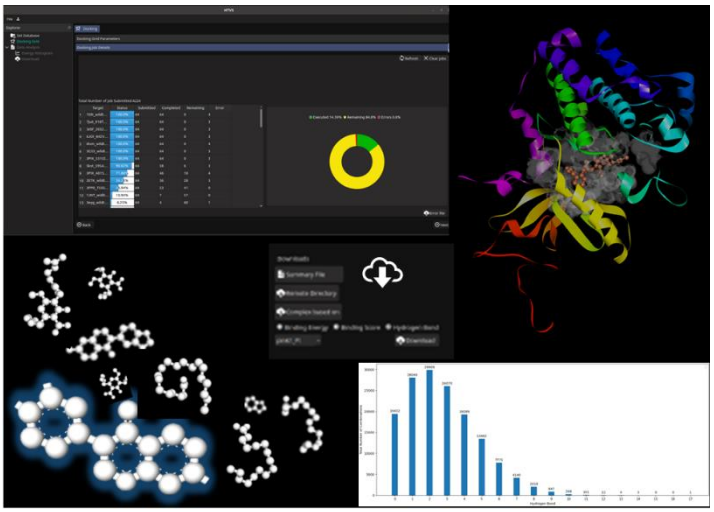
Features of BioIn: Bioinformatics

- Integrated RSCB database for searching targets
- Clean target structures by deleting unwanted protein chains, ligands, ions, water
- Model missing residues and loops
- Model numeric and alpha-numeric residue ID
- Homology modelling for unknown structures
- Adding various mutant to proteins
- Clean/rectify target biomolecules for input in X-ESS

Features of SyMoG/AI: Artificial Intelligence-Synthetic Molecule Generator

- SyMoG/AI is a state of the art Artificial Intelligence-based molecules generator
- 7 pre-trained models for drug targets are available
- Graphical Neural Network based AI model implemented
- Interactive GUI for visualization of predicted physicochemical properties such as synthesizability, solubility, drug-likeliness, logP, etc.
- All post-processing is done at the server-side and users can visualize the structural similarity between inputs and AI-generated compounds
- Clustering of the generated compounds based on scaffolds/motifs and creation of compound libraries as per selected scaffold
- Users get access to all the raw data for any additional analysis, visualization and post processing
- Users can export the structures of AI-generated compounds, input compounds, the scaffold-based clusters of the compounds in PDB, image, and pdf format
- Now users could request for addition of new customized pre-trained models to this App via email: support@prescience.in

PRinS³®: Drug Discovery Apps

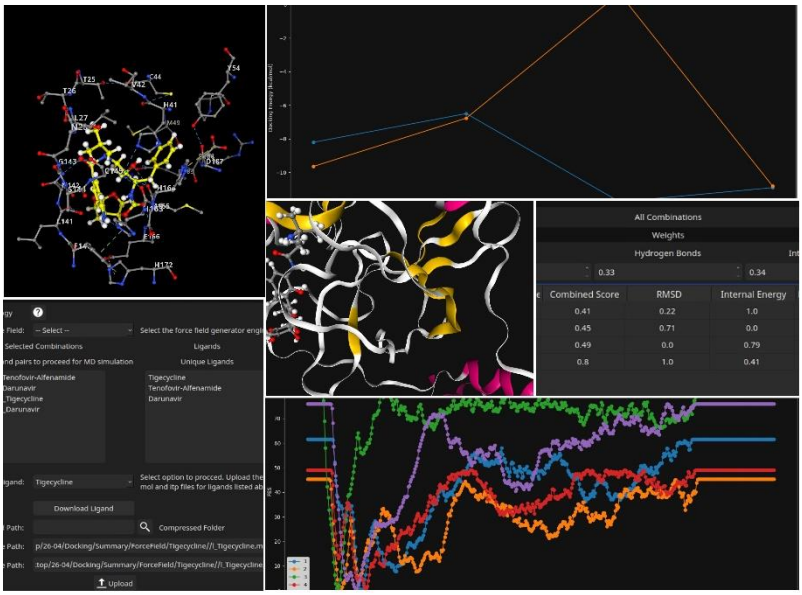


Features of X-HTVS: Multi-Target Multi-Ligand High-Throughput Virtual Screening

- Discover lead-like compounds from gigantic chemical space
- Docking-based app to screen multiple targets with thousands to millions of compounds at one go
- Run calculations on cloud and/or in-house servers
- Options for algorithms - Lamarckian Genetic Annealing (LGA) and Local Search (LS)
- Choice of partial charges, Model type (Bound, Extended), Number of GA runs (Coarse grain, Highly coarse grain, fine-grain and user -defined)
- Control output with docking scores, binding energy and H-bonds represented histogram plots
- Investigate the binding mode of lead-like compounds by further refining with X-ESS

Features of X-ESS: Multi-Target Multi-Ligand Enhanced Sampling Screening

- Fully automated, high throughput screening in parallel novel drug designing platform with state-of-the-art free energy of binding calculator
- Process flow includes docking, molecular dynamics (MD) and free energy calculations
- Efficient scoring algorithms for screening at each stage
- Choose Protein, Nucleic Acid and Peptides as target and small molecules, peptides, peptides as ligand
- Takes your already docked structure as input for further MD and FES analysis
- Fast MD Engine (powered by GROMACS) is fully integrated and GPU enabled
- Options for simultaneous fully automated blind docking and active site docking for multiple targets
- Additional segment for calculation of state-of-the-art enhanced sampling Even Tempered Meta-dynamics based free energy of binding predictions for finding combinations of target-ligand with higher selectivity
- Binding Free Energy analysis by Molecular Mechanics Poisson-Boltzmann Surface Area (MMPBSA)
- Interactive GUI for visualization of structure, interacting residues and ligand; ready plots for energy, H-bond, free energy and scoring
- In addition to the default values, get full control of the calculations through advanced parameter sections
- Run calculations in local machine, in-house server, HPC, and on public cloud (Google Cloud) directly from the interface

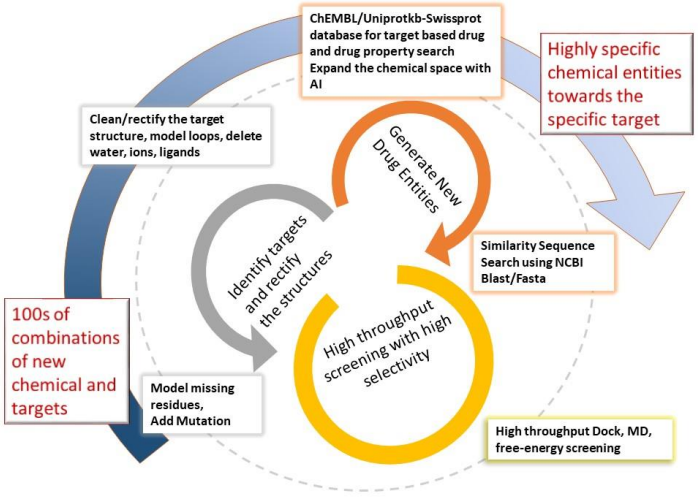


- All post processing is done at server side and users get access to all the raw data for any additional analysis, visualization and post processing
- Standard Force fields are integrated, ligand force fields can be generated from the interface using well tested opensource algorithms

Note: Customized force fields in bulk numbers can be obtained from prescience team on-demand
Customize analysis tools for specific output can be added by Prescience team on request

Request for DEMO

Request for Evaluation



Contact us

Email support@presience.in and visit https://www.prescience.in