Scoring Functions Rescoring & Consensus Strategies — Hands-on

Go beyond black box docking scores and learn how to critically interpret, rescore and combine ranking strategies. This module covers the theory and practice of scoring functions, post docking pose analysis, rescoring workflows and consensus based prioritization so that virtual screening decisions become more defensible and better aligned with experimental follow up.

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Scoring Functions Landscape & Theory

Types of docking scoring functions and design goals

force field inspired scores | **empirical and knowledge based terms** | **machine learning augmented scoring**

Pose scoring vs binding affinity estimation

ranking poses vs ranking ligands | **relative vs absolute scales** | **limitations and common artifacts**

Benchmarking concepts for scoring functions

redocking and cross docking tasks **ROC curves and enrichment factors** **decoy sets and bias awareness**

Session 2
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Rescoring, Pose Filters & Interaction Checks

Rescoring with alternative engines or scoring schemes

using multiple docking engines **post processing scores with external tools** **speed vs accuracy trade offs**

Chemically sensible pose filters

steric clashes and strain checks **unsatisfied or broken hydrogen bonds** **buried polar atom flags**

Interaction pattern analysis

2D interaction diagrams **key anchor residues and motifs** **aligning poses across chemotypes**

Session 3
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Consensus Scoring & Multi Parameter Ranking

Consensus scoring strategies and combinations

rank based and score based fusion **voting and majority rules** **weighting schemes and calibration**

Adding basic property and liability filters to the score

simple physicochemical windows **alerts and PAINS filters** **flags for reactive or unstable motifs**

Multi parameter ranking and visualization of trade offs

score vs property scatter plots | simple desirability functions | short listing for different scenarios

Session 4

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Mini Capstone: Benchmark & Calibrate a Protocol

Designing a small benchmark with actives and decoys

Theory + Practical

Running docking, rescoring and consensus ranking

set up of scoring and rescoring steps | enrichment and ROC evaluation | parameter tuning for better recall

Deliverables: calibrated docking and scoring recipe

notebook or script with full pipeline | summary table of enrichment metrics | recommended settings for project use