Target Identification using Computational Supreme (COMP-S™) - Docking Based Target Identification)

Small-molecule Target-ID Premises, Problem Statement and Value

Discovery Program Identified a *bioactive* (small-molecule, peptide, protein, antibody) however the target(s), the cellular binding partners, and Action Mechanism of *bioactive* is not known

- Information of Target of *bioactive* will allow
  - Rational optimization of *bioactive*
  - Early 'de-risking' of program by characterizing 'off-target(s)' of the *bioactive*
  - Drug-Efficacy biomarker discovery, patient stratification and commercial differentiation by clarifying the action mechanism of *bioactive*

Our Focus = Target Identification

Target Identification / Deconvolution is not Trivial
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A single Tool / Technology May Not necessarily solve the problem for all

Our >10 years expertise allows us to evaluate the 'fit-for-purpose' technology for every program
and
then we deploy appropriate Technology for **right target** from a portfolio of Technology

Different Technologies
1) UPT = Unique Polymer Technology, 2) SCLS = Subcellular Location Specific Target Capture Technology, 3) COMP = 'in-silico' target ID workflows, 4) TBB = Traditional Bead/Biotinylated Molecule Based Method, 5) TPP = Thermal Proteome Profiling

Computational Supreme (COMP-S™) - Docking Based Target Identification)

COMP

- **Key Advantages**
- Utilizes Structural and Functional Features of ‘test-molecule’ when comparing historical database
- Target deconvolution can be completed in 2-3 weeks.

COMP is Shantani's proprietary method for target identification using mining of historical ligand-target data sets.

[2D/3D molecular structure and molecule-target pair linked funtion based filter leading to increased chance of right target identifications.]

Working Principle

This computation bait-molecule-protein docking-based method relies on historical data-set that ‘X’ kind of molecular structure interacts with ‘Y’ kind of targets to provide ‘Z’ kind of phenotype.

Workflow

In COMP, the 2-D and 3-D structures of the 'bait-molecule' along with this function is searched in historical databases for similarity. A custom based algorithm is developed for every specific molecule to compare it with historical data-set and based on comparison score, targets identity is predicted.