

Virtual Combinatorial Peptide Screening Work-Flow

- Our virtual combinatorial peptide screening (VCPS) work-flow combines the modeling and scoring programs Ensemble, Transcend and Affinity
- Our VCPS work-flow enables us to search, score and rank the entire chemical and *a priori* reasonable physical space for a given peptide ligand (length N)
- Using the VCPS work-flow, we can quickly identify novel peptide ligand sequences for a given protein target
- These peptide ligands can then serve as starting points for peptide, peptidomimetic and small molecule drug discovery projects.

Crystallography, NMR, or
computational docking



protein-peptide (length N) complex



Systematic amino acid substitutions;
flexible side-chain optimization



MM-GB/SA scoring and ranking



Empirical free energy scoring and ranking
using *Affinity*



List of peptide sequences of length N that
are predicted to bind the protein target