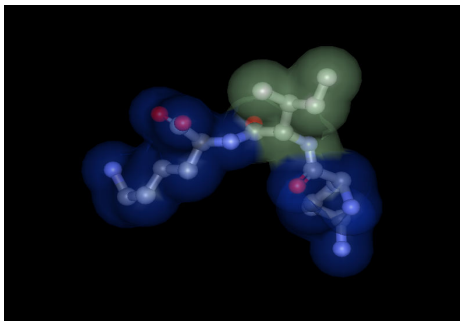
CMDBioscience, LLC

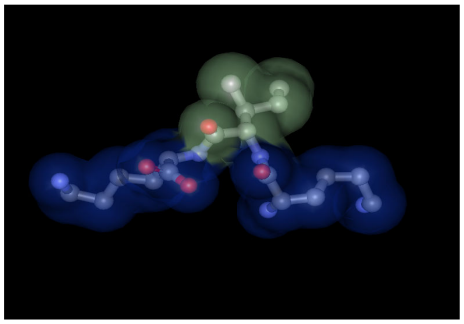
Custom designed peptides for use in the pharmaceutical, biotech & life science industries.

Ensemble:

The next generation in computational protein and peptide design technology.



Using Ensemble scientists can efficiently generate main chain and side chain peptide conformers for subsequent analysis.



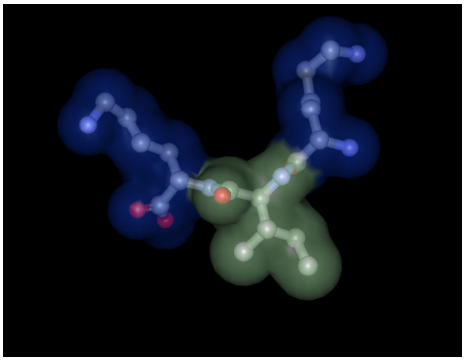
Improved accuracy: conformers generated by Ensemble are *a priori* physically realistic

High speed: Ensemble can be used to construct a database of peptide conformers for subsequent docking in a matter of seconds.

Versatility: Ensemble can be easily interfaced with other docking or ligand design programs and our other proprietary tools.

Given their small size, capacity for tight and specific binding, chemical versatility, and relative ease of synthesis, researchers are starting to focus on amino acids and small peptides as possible drug leads or as templates for more traditional small molecule drug projects. Thus, efficient computational tools are needed to analyze and simulate amino acids and peptides. More specifically, an essential ingredient in any computational approach to peptide design is the ability to efficiently model peptide and amino acid flexibility.

Ensemble is our proprietary algorithm for generating peptide or amino acid flexibility. The algorithm performs an intelligently constrained but deterministic search of phi, psi, and chi space to identify physically realistic peptide and amino acid conformers in a matter of seconds. In this way, Ensemble can be used to efficiently enumerate viable peptide conformers for subsequent study by docking or molecular simulation using commercially available software or using our other software applications, Transcend and Affinity.



In a recent study, CMD scientists used Ensemble, Transcend and Affinity to reproduce the native state binding modes for several OppA-tripeptide complexes, to within 1 $Å^2$ rmsd. Ensemble is thus a powerful and indispensable tool in structure-based peptide design. If you are interested in accessing the power of Ensemble, please don't hesitate to contact us.