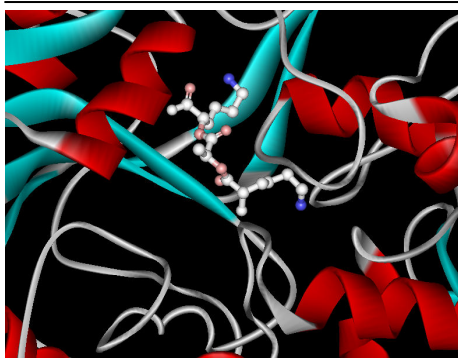


CMDBioscience, LLC

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

Transcend:

The next generation in computational protein and peptide design technology.



Using Transcend scientists can predict if proteins (or peptides) will associate and suggest three dimensional models for the complex.

Improved accuracy: Rigid-body binding modes refined by Transcend better approximate reality.

High speed: Transcend can be used to refine hundreds of rigid body docking solutions in minutes.

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

Docking studies are an integral part of many rational drug design projects. Most protein docking algorithms, however, are incapable of truly predictive docking. Rather, they are limited to suggesting model structures, given prior knowledge that the two proteins will associate. This is because most protein docking algorithms do not score binding poses according to the binding free energy ΔG_{bind} . Moreover, most docking algorithms are limited to rigid-body docking and thus fail to model the structural rearrangements that accompany binding. Truly predictive docking, then, requires a scoring function that ranks complexes according to ΔG_{bind} and that provides for flexibility.

Transcend is our proprietary algorithm for truly predictive docking. Starting from binding poses generated using conventional docking software, Transcend employs an iterative conformational search and rigid body minimization protocol to identify native-like binding modes on a potential energy surface. The binding modes can then be scored and ranked using MM-GB/SA scoring and our Affinity empirical free energy function for true predictive docking. Our results indicate that Transcend can be used to discriminate native and native-like binding modes for a range of protein and peptide interactions. Transcend also includes a flexible side chain substitution engine for accurate mutant modeling. To access the predictive power of Transcend, please don't hesitate to contact us.