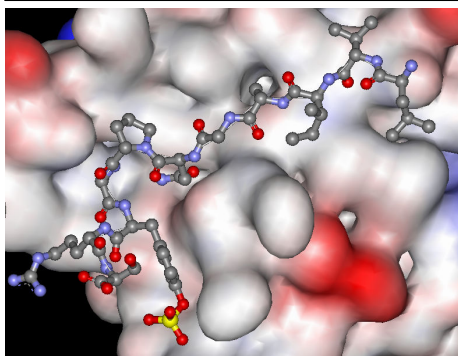


# CMDBioscience, LLC

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

## *Affinity:*

*The next generation in computational protein and peptide design technology.*



Affinity was used to blindly predict  $\Delta G_{\text{bind}}$  to within  $0.92 \text{ kcal}\cdot\text{mol}^{-1}$  for 9 different Sh2-pTyr and PTB-pTYR complexes. The picture is of IRS

*Improved accuracy:* Testing shows that Affinity outperforms existing functions

*High speed:* Affinity can serve as a scoring function for docking algorithms, providing for true predictive docking.

*Versatility:* Affinity can be interfaced with docking, ligand design and other protein modeling algorithms. Affinity can also be symbiotically combined with more costly and rigorous free energy methodologies, such as MM-GB/SA scoring.

Non-covalent protein-protein and protein-peptide recognition is essential to life. Hence, protein-protein interactions are attractive targets for therapeutic intervention. There is also considerable interest in developing protein and peptide-based drugs and in using peptide ligands as starting points for small molecule drug discovery projects. Because protein and peptide interactions are ultimately controlled by free energy changes, what researchers desperately need is a fast, accurate and intuitive function for explaining and predicting protein-protein binding affinities ( $\Delta G_{\text{bind}}$ ).

**Affinity** is our proprietary, novel and physics-based empirical free energy function for predicting and explaining  $\Delta G_{\text{bind}}$ . Because Affinity calculates  $\Delta G_{\text{bind}}$  from static structures it can be used to calculate binding free energies in a matter of seconds on a single workstation. This speed, however, does not come at the expense of predictive accuracy. Extensive testing has shown that Affinity can be used to blindly predict  $\Delta G_{\text{bind}}$  for diverse proteins with a 90% success rate and to within  $\approx 1.0 \text{ kcal}\cdot\text{mol}^{-1}$  of the experimental binding affinity. Affinity is consistent with the intuitions of medicinal chemists and can thus serve as an invaluable tool in interpreting results and guiding molecular design projects. Affinity, our core technology, is a powerful tool for solving a range of protein and peptide design problems. If you are interested in accessing the revolutionary power of Affinity, please don't hesitate to contact us.