Poster presentation

Secbase - secondary structure elements and ligand binding
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Relibase is an object-oriented data management system [1] that stores structures of three dimensional protein-ligand complexes deposited in the PDB. Secbase is a modular extension of Relibase that integrates information about secondary structural elements assigned to each individual protein structure in Relibase. In addition to information about helices and β-sheets retrieved from the PDB, we have integrated a new uniform classification of all turn families, based on recent clustering methods. Highly accurate sequence-based protein turn prediction has confirmed this new categorization as consistent and well defined [2].

As shown using Secbase [3], backbone hydrogen bonds show cooperative effects in α-helices and parallel β-sheets leading to a decrease of the mean hydrogen-bond length with increasing number of turns in α-helices and number of strands in parallel β-sheets, respectively. We are analysing protein-ligand complexes using Secbase to ascertain if a similar difference in hydrogen bonding strength between a ligand and the backbone of secondary structural elements exists.

Secbase could be used for knowledge discovery, protein structure prediction and comparison of complex secondary structural patterns up to motifs or domains. In combination with existing Relibase functionality, analysis of the interactions between ligands and reoccurring patterns of secondary structural elements in proteins is possible. In particular the analysis of the new turn classification could be of interest, since β-turns are known to play a central role as molecular recognition elements in protein-protein interfaces and binding of peptide hormones to their receptors [4] and could be essential for the optimal sidechain conformation within ligand binding. Additionally, cross-reactivity between related protein families with similar folding but insignificant sequence homology could be detected by this approach [5].

References
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