SARST - Structure Alignment by Ramachandran Search Tool

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Abstract

Comparing 3D structures may reveal biologically interesting similarities that are not detectable by comparing sequences. The structural alignment of proteins has become increasingly important with the growing number of known protein structures. The number of deposited structures in PDB increased exponentially after 1994, especially several structural genomics projects launched recently. Several techniques are currently available that attempt to find the structure similarity between protein structures, including Dali, FLASH, CE and VAST. All the existing methods are converting protein 3D structure into 2D information, and compare structure similarity in 2D space. We have developed a new algorithm, SARST – Structure Alignment by Ramachandran Search Tool, to further convert 2D information into linear codes (1D), and compare structure in 1D level. The algorithm first calculate dihedral angles (Φ, ψ) from the coordinates of protein structure (3D→2D), and then translate these angles (Φ, ψ) into Ramachandran codes (2D→1D). SARST is not only a quick way to compare similarity between protein structure, but also an effective way to perform structural homology searching in database.