Predicting function from structure: using a three-dimensional local main-chain binding motif and an environmental profile

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Abstract:

Structural genomics will lead to large-scale directed structure determination and a significant increase in the number of three-dimensional structures available prior to an understanding of their biological function. Methods that can make functional inferences through identification of structural similarity are likely to be of increasing importance as tools for structural biologists.

Recently, Russell (1998) reported a method for the detection of recurring 3D side-chain patterns as a means of inferring protein function and Kasuya & Thornton (1999) have identified maintenance of common 3D structure in several PROSITE sequence patterns. In many cases these structural patterns are common to proteins that are otherwise distantly related at both a sequence and a structural level.

Sequence similarity or the overall protein fold are not always sufficient criteria for inferring function. Here we report the use of conserved main-chain conformation and an environmental profile to detect similarities between protein binding sites. An example will be described as will its potential for use in database searching and implications for functional assignment from structure.

References:

Russell RB. Detection of protein three-dimensional side-chain patterns: new examples of convergent evolution. J Mol Biol. 1998 Jun 26;279(5):1211-27.

Kasuya A, Thornton JM. Three-dimensional structure analysis of PROSITE patterns. J Mol Biol. 1999 Mar 12;286(5):1673-91.