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COMPARISSON OF THE AMINO ACIDS CO-EVOLUTION AND THE CORRELATED STRUCTURE DESCRIPTORS



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Short Abstract: The AA Co-evolution is a very powerful method of identifying those critical residues which are responsible for maintaining the minimum information for the specific function. By comparing the set of co evolving amino acids together with the variety of other structure parameters, couple of biologically important examples are presented.

Long Abstract:

By knowing if there are amino acids which are consistently preserved in very related and coupled fashion with other amino acids present in a chosen protein structure, we may be able to decipher which is the set of residues that contains a very concise and precise information so that the protein can preserve and maintain its primary function. So the method which defines the subsets of AA which are co-evolving in a coupled fashion is a very powerful way of defining the critical residues in the protein for the general and very specific structural or functional role. By following the description of the algorithm originally described by Rama Ranganathan et al (Russ, W. P., Lowery, D. M., Mishra, P., Yaffe, M. B. & Ranganathan, R. *Nature* 437, 579–583 (2005)), we have designed our own approach for identification of co-evolving residues so that the number of critical interactions can be observed among those AA. IN addition, having this algorithm and the results available in an integrated STING environment, we may observe how the other parameters which describe both the structure and the sequence, behave regarding this specific and exclusive set of co-evolving residues.

Typical exercise in this direction is: a) define co-evolving amino acids, b) compare contact type of that set of AA to all the other AA, c) see the possible correlation with the critical order of cross links and total energy of established and potentially available contacts and finally d) observe the variety of parameters describing the conservation of the residues such as the relative entropy and the evolutionary pressure.

In this work we present couple of biologically interesting examples where the structure study was completely dedicated to the determination of correlation of structure parameters among co-evolving set of residues and some other descriptors available among 310 of those which are available in STING_DB.