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Title Analysis of Tertiary Contact Conservation among Structurally Related Proteins

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Abstract:

Protein tertiary structures, despite insignificant sequence similarity, show remarkable structural similarity. However, it is not clearly known whether tertiary contacting residues of structurally equivalent residues are also structurally equivalent. Moreover, whether such residues are conserved in homologous sequences is also unclear. In the present study, we have systematically studied the contact conservation of structurally conserved residues at various levels of structural similarities. Further, we hypothesized that structurally and functionally important residues should have high contact conservation even in distantly related proteins. The analyses showed that there is significant contact conservation, however, coverage of these structurally equivalent residues diminishes from closely to distantly related proteins. We also computed the correlation of contact conservation with various features such as sequence conservation, secondary structure and residue accessibility. This showed that contact conservation is observed mostly in regular secondary structures, as expected, however, coil regions show variable conservation. We found that both buried/exposed residues have comparable contact conservation of structurally equivalent residues. Surprisingly, we observed that structurally equivalent residues do not show residue conservation. This could be mainly because of the co-evolution of interacting residues.

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