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Title:	Unraveling the structural landscape of intra-chain domain interfaces: Implication in the evolution of domain-domain interactions
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Abstract:	Intra-chain domain interactions are known to play a significant role in the function and stability of multidomain proteins. These interactions are mediated through a physical interaction at domain-domain interfaces (DDIs). With a motivation to understand evolution of interfaces, we have investigated similarities among DDIs. Even though interfaces of protein-protein interactions (PPIs) have been previously studied by structurally aligning interfaces, similar analyses have not yet been performed on DDIs of either multidomain proteins or PPIs. For studying the structural landscape of DDIs, we have used iAlign to structurally align intra-chain domain interfaces of domains. The interface alignment of spatially constrained domains (due to inter-domain linkers) showed that ~88% of these could identify a structural matching interface having similar C-alpha geometry and contact pattern despite that aligned domain pairs are not structurally related. Moreover, the mean interface similarity score (IS-score) is 0.307, which is higher compared to the average random IS-score (0.207) suggesting domain interfaces are not random. The structural space of DDIs is highly connected as ~84% of all possible directed edges among interfaces are found to have at most path length of 8 when 0.26 is IS-score threshold. At this threshold, ~83% of interfaces form the largest strongly connected component. Thus, suggesting that structural space of intra-chain domain interfaces is degenerate and highly connected, as has been found in PPI interfaces. Interestingly, searching for structural neighbors of inter-chain interfaces among intra-chain interfaces showed that ~86% could find a statistically significant match to intra-chain interface with a mean IS-score of 0.311. This implies that domain interfaces are degenerate whether formed within a protein or between proteins. The interface degeneracy is most likely due to limited possible ways of packing secondary structures. In principle, interface similarities can be exploited to accurately model domain interfaces in structure prediction of multidomain proteins.
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