Protein-protein docking and dynamics of peptide from *Clitoria ternatea* with *Daboia ruselli* viper venom PLA $_2$

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Abstract

Molecular docking outshines other approaches at creating a surfeit of potential models of protein-protein complexes. It is highly challenging to distinguish the favourable, native-like models from the newly discovered ones. We propose here a protocol based on molecular dynamics (MD) simulations that would allow distinguishing native from non-native models to complement scoring functions used in docking. The initial part of the study concentrated on modelling the protein-protein complex of a cyclic peptide (cter M) from *Clitoria ternatea* with *Daboia ruselli* snake venom PLA $_2$ receptor using docking in Discovery Studio, which was complemented with molecular dynamic simulations to discriminate between native protein and the investigated complex to report its stability. The peptide complex showed almost similar stability in nearly all measured properties, such as Root Mean Square Deviation (RMSD), Root Mean Square Fluctuation (RMSF), and Radius of Gyration (Rg) of native contacts from the initial docked model. A reasonably short simulation of 100 ns is sufficient to achieve this accuracy, making this approach practical.

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