

Methodological improvements in docking: are we actually getting better?

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One of the long-standing methods for validation of a docking engine/scoring function is self- or cognate docking; re-docking a crystallographic ligand into its cognate protein receptor. Several problems have made it difficult to determine if new scoring functions/docking engines genuinely do improve cognate docking. We present a comparison of a variety of docking/scoring methods found in our docking engine OEDocking on our recently released dataset, Iridium. We apply rigorous statistical analyses to the data to determine if, and with what likelihood, a given technique outperforms another. With a well validated approach to cognate docking available we expect the field will be able to turn to the problem of genuine interest, cross-docking, with greater confidence.