To dock, or not to dock… how to deal with the quality assessment strategy of protein-ligand docking protocols comparing their performances.

Stefano Moro
Molecular Modeling Section (MMS)
Dept. of Pharmaceutical and Pharmacological Sciences
Via Marzolo 5, 35131 Padova - IT
stefano.moro@unipd.it

The progress made in the field of bio-crystallography has increased the adoption of docking-driven approaches for the identification or the optimization of novel potent and selective ligands.(1) As routinely demonstrated, docking programs are usually successful in generating multiple poses that include binding modes similar to the crystallographically determined bound structure, whereas scoring functions are much less successful at correctly identify the corresponding "bioactive" binding mode. (1) This intrinsic limitation generally implies the need for the calibration of the docking protocol through benchmark studies prior to applying it. Traditionally, these benchmarks have focused on redocking the cognate ligand of a crystallographic receptor–ligand complex to measure geometric pose prediction accuracy. (1) In our research group, we have recently proposed an alternative assessment strategy to compare performances of protein-ligand docking protocols, named DockBench. This tool is an integrate informatics platform to automatically perform and compare RMDS-based molecular docking performances (benchmark) of different docking/scoring methods. An intuitive graphical analysis can help docking users, including non-expert users, to identify the best docking/scoring combination to perform a docking-based virtual screening campaign. (2-5)

References
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