Evaluation of Docking Results by Diffraction-component Precision Index (DPI)

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Since efficient docking technique can be a powerful tool for the computer-aided drug design, many different approaches to solving the docking problems have been proposed. The reliability of the docking results has not been quantitatively discussed. Relatively subjective criteria have been generally applied to evaluate the docking results so far. The DPI introduced by Cruickshank[1] is 'a good and rough guide' to coordinate precision and can be used to evaluate the reliability of the docking results.

In the docking study the most useful quantity to consider the docking results is an rmsd between predicted and experimental heavy-atom coordinates of the ligand structure. Suppose the standard uncertainty of the observed and predicted molecular model is the same in magnitude and equals to σ, the estimated standard uncertainty of the rmsd between the corresponding atoms in the observed and predicted molecule can be approximated to be $\sqrt{2}\ \sigma$. Therefore the magnitude of the rmsd value can be evaluated using the estimated uncertainty.

We have recently developed a unique docking algorithm named Ph4Dock[2] and the docking results obtained by Ph4Dock were evaluated using DPI. The present study has demonstrated that DPI is a good measure to judge the quality of docking results.

[1] Cruickshank D.W.J., *Acta Crystallogr*., 1999, **D44**, 583. [2]Goto J., Kataoka R., Hirayama N., *J. Med. Chem.*, 2004, **47**, 6804.

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