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Validation of Ligand-Protein Docking Simulations

([1]Tokai University School of Medicine, [2]Ryoka Systems Inc.) ○Noriaki Hirayama (1), Ryoichi Kataoka (2), Jyunichi Goto (2)

Docking simulation between drug molecules and their target molecules is a highly useful technique in drug discovery. Although several software programs for docking simulations have been published, the docking problems are not solved yet and none of the currently available programs are perfect in predicting the correct binding modes. To evaluate the potential of the newly developed docking program Ph4Dock, we have selected 44 reliable crystal structures of protein-ligand complexes. The diffraction-component precision index (DPI) originally used in crystallography was applied in this study in order to evaluate the docking results quantitatively. The root-mean-square deviation (rmsd) between non-hydrogen atoms of the ligand in the prediction and experimental results were analyzed using DPI. The rmsd values for 25 structures, consisting of almost 60% of the dataset, are less than three times of the corresponding DPI values. It means that the precision of docking results obtained by Ph4Dock is mostly equivalent to the experimental error in these cases.