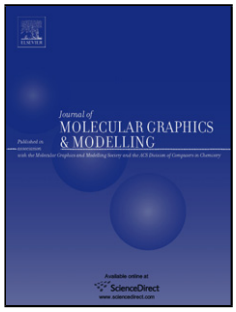

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New generation of docking programs: supercomputer validation of force fields and quantum-chemical methods for docking

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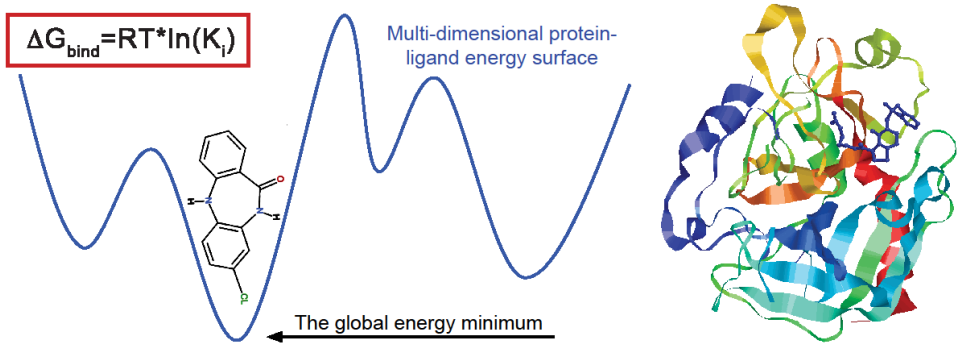
Graphical abstract



Highlights

- Docking accuracy is compared for CHARMM, MMFF94, PM7, PM6-D3H4X with solvent models
- The highest docking accuracy is found for PM7 with the COSMO solvent
- Docking positioning accuracy for PM7/COSMO is better than for PM6-D3H4X/COSMO
- Docking positioning accuracy for CHARMM with GBSW solvent and PM7/COSMO are close