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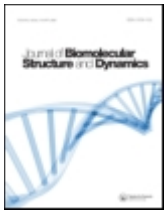

Original Articles

Investigation on critical structural motifs of ligands for triggering glucocorticoid receptor nuclear migration through molecular docking simulations

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Abstract

The glucocorticoid receptor (GR), a transcription factor regulating gene expression in a ligand-dependent fashion, is known for flexibility in adapting various ligands with their structures ranging from steroid to non-steroid. However, in our previous study, GR shows a stringent discrimination against a set of steroid ligands with highly similar structures for triggering its nuclear migration. In order to resolve this puzzle, we employed molecular docking simulations to investigate the origin of this structural discrimination. By analyzing the docking orientations and the related ligand–GR interaction patterns, we found that the hydrophilicity mismatch between the docking ligand and the GR ligand-binding site is the main cause combined with the steric hindrance and structural rigidness of these steroid ligands. Furthermore, we utilized this knowledge to rationalize how the structure –binding interaction of non-steroid ligands triggers GR nuclear migration with their structures available in Protein Data Bank.

Keywords

- glucocorticoid receptor,
- molecular docking simulation,
- solvent-exposed hydrophobic groove,
- nuclear migration

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