

Theoretical study of zeatin - a plant hormone and potential drug for neural diseases - on the basis of DFT, MP2 and target docking.

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Zeatin, a cytokinin of the adenine family, originally isolated from *Zea mays* L., exhibits also bioeffects towards human cells: it is a potent acetylcholinesterase inhibitor and can potentially inhibit amyloid β -protein formation. The role of zeatin in neural disease treatment is yet to be established. This computational study describes a hierarchy of interactions between zeatin and a receptor, a protein from the nodulin family. DFT in hybrid and dispersion-corrected form as well as MP2 approaches were used to derive interaction energies. Docking procedure was employed to investigate the role of selected interaction for anchoring the ligand.

Adres publiczny

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<http://www.elsevier.com>