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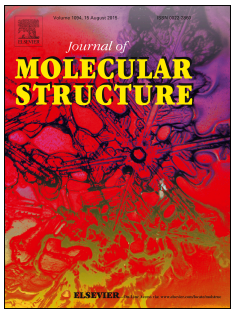

Spectroscopic (FT-IR, FT Raman) and quantum mechanical study on N-(2,6-dimethylphenyl)-2-{4-[2-hydroxy-3-(2-methoxyphenoxy)propyl]piperazin-1-yl}acetamide

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Graphical Abstract

The current study investigate upon the structural, vibrational, electronic, non linear optical, thermodynamic and docking studies on the title compound using (DFT/B3LYP) method with 6–311 ++ G (d, p) basis set. The compound under study was docked into the active site of protein 3TTJ which associated with Myocardial Ischemia.