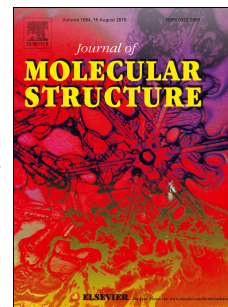


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Vibrational spectroscopic (FT-IR, FT-Raman) and quantum mechanical study of 4-(2-chlorophenyl)-2-ethyl-9-methyl-6H-thieno[3,2-f] [1,2,4]triazolo[4,3-a][1,4] diazepine

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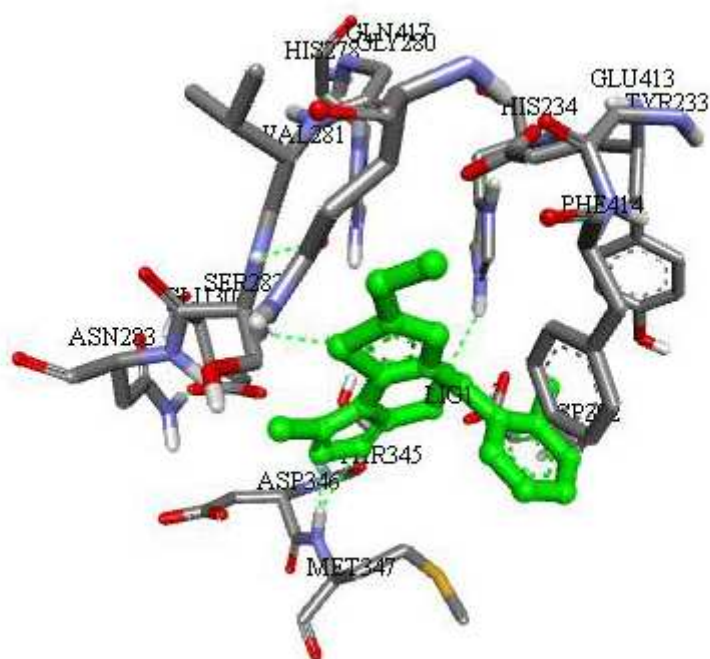
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GRAPHICAL ABSTRACT

Experimental and theoretical calculations on the molecular structure, electronic and vibrational characteristics of 4-(2-chlorophenyl)-2-ethyl-9-methyl-6H-thieno[3,2-*f*] [1,2,4] triazolo [4,3-*a*][1,4] diazepine are presented. The theoretical calculations are obtained by DFT/B3LYP method with 6-311++G(d,p) as basis set. Molecular docking studies are performed and shows that the compound exhibit antidepressant property.



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