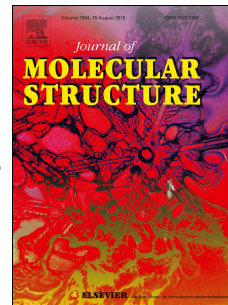


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Spectroscopic investigation, hirshfeld surface analysis and molecular docking studies on anti-viral drug entecavir

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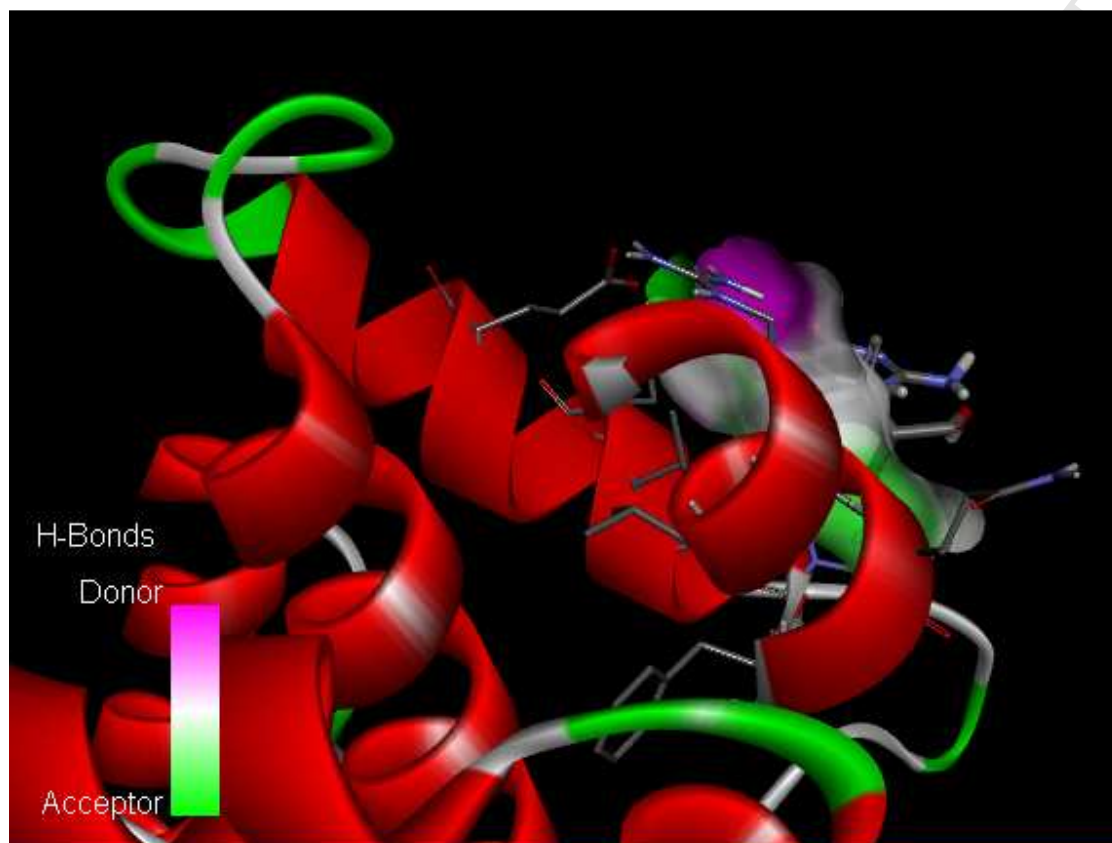
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Graphical Abstract

In this work, we have reported a combined theoretical and experimental spectroscopic investigation on molecular structure, NBO, Hirshfield Surface analysis, NLO, Fukui and molecular docking studies on Entecavir.



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