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Design, synthesis, biological evaluation and molecular docking studies of phenylpropanoid derivatives as potent anti-hepatitis B virus agents

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A series of phenylpropanoid derivatives were discovered as potent anti-HBV agents. Compound 4c-1 showed the most potent anti-HBV activity, demonstrating potent inhibitory effect not only on the secretion of HBsAg (IC_{50} = 14.18 μM, SI = 17.85) and HBeAg (IC_{50} = 6.20 μM, SI = 40.82) secretion but also HBV DNA replication (IC_{50} = 23.43 μM, SI = 10.80). The structure-activity relationships of were analysed and docking study was carried out to explore the molecular interactions and a molecular target by MOE.