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In Silico Study of Gallic AcidDerivatives as Novel AntiviralAgents of Hepatitis C

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Abstract: In this paper, we report in silico study of gallic acid derivativesas novel antihepatitis C virus agents. The derivatives were designed by expanding the carboxyl group of gallic acid with open-chain moiety of L-threonine-allyl esters, as well as to modify the hydroxy groups on the aromatic ring of gallic acid with methoxy group in the derivatives. Designed compounds and the original gallic acid were docked based on their interaction with hepatitis C virus receptor binding target NS5B. Compared to gallic acid, all the twenty designed compounds, exhibited higher binding energy, affinity, and hydrogen bond interaction on receptor target of NS5B, indicating that the designed compounds have a stronger inhibitory activity against NS5B.
Keywords : In silico docking, gallic acid, stereocentre derivative, antiviral, Hepatitis C.

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