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In Silico Design, Synthesis and In Vitro Evaluation of Quinazolinone Derivatives as Dipeptidyl Peptidase-4 (DPP-IV) Inhibitors

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Abstract : Taking into account the important role of DPP-IV in diabetes mellitus, inhibitors for DPP-IV were designed, synthesized and evaluated for the activity. From amongst various nitrogen containing heterocycles, quinazolinones were selected for testing the DPP-IV inhibition. The synthesized molecules were characterized by melting point, infrared spectra and ¹H-NMR, elemental analysis and ¹³C-NMR. Two best molecules [PS-3 & PS-6] were chosen on the basis of Vlife score of -45.78 and -51.7 2 respectively and when tested for *in vitro* DPP-IV inhibition, the activity was concomitant to the docking scores. These molecules may therefore serve as the lead for further modification to design potent DPP-IV inhibitors. **Keywords:** *In silico*, Quinazolinone, In-Vitro, DPP-IV inhibition activity.

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