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In Silico study of nucleoside analogues as selective G9a/GLP inhibitors based on the skeleton of natural product Sinefungin.

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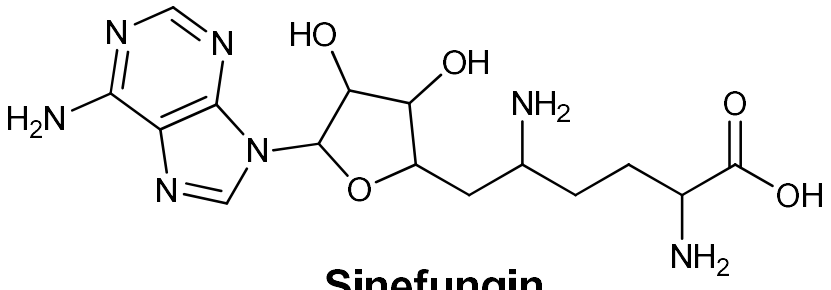
Abstract: Histone methyltransferases GLP/G9a are the potential targets for cancer therapy. Their gene mutations correlate closely with tumors, infectious diseases and neurogenerative disorders. To date, most of the reported small molecules are substrate-competitive inhibitors and own the same scaffold. Previously, it has reported that natural product sinefungin and a series of cycloalkyl substituted nucleoside analogues as selective GLP/G9a allosteric regulators. The present study aimed to design and optimize the structures from three aspects including the side chain on the ribofuranose, basic group and ribofuranose, and test their docking interactions. Mutations of amino acids(R1257/H1201/S1172/N1200/Y1242) will also be performed to confirm the key amino acids in the binding pocket. Lead compounds (2-3) are generated after research for later exploration of candidate drugs in cancer treatment.

Keywords *Histone methyltransferases, cancer, Sinefungin, Docking, Leads*



Sinefungin

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