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Design and synthesis of novel viral capsid disassembly inhibitors as anti-HIV agents

Ramya Krishna N, Sridhar Goud and M Mallika

National Institute of Pharmaceutical Education and Research, Hyderabad, India

Globally, about 36.9 million people were reported to be living with HIV in the year 2014. There is a need to produce alternatives with novel mechanism of action. HIV is a grueling disease with irreparable consequences such as Kaposi's sarcoma and other opportunistic infections. Viral capsid forms an attractive target due to its evolutionarily conserved restriction mechanisms. Also, mutations do not affect the viral capsid, i.e., resistance shown by currently used drugs is not observed. There are no drugs currently used in HIV therapy with this mechanism and viral capsid as target is a scarcely ventured area. The aim of the present study is to design specific viral capsid uncoating inhibitors leading to development of anti-HIV agents with high efficiency and safety. Executing various computer-assisted drug design techniques, several molecules were designed using structure based and pharmacophore based drug design. ADME properties, drug likeness studies have also been performed. All the experiments were performed using Schrödinger Suite 2014. The designed molecules are being synthesized and biological activity testing is underway.