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IIT-M finds way for more effective drugs to treat HIV-AIDS

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Indian Institute of Technology Madras (IIT-M) researchers are working on a revolutionary new idea that can pave the way to effective drugs for treating HIV/AIDS. Using molecular dynamics simulations, the research team have shown that introducing electrostatic interaction sites on potential drug molecules can enhance the efficacy of the antiviral drug against the HIV virus.

This research was led by Prof Sanjib Senapati, Department of Biotechnology, IIT Madras, along with his research scholars, Mohammed Ahsan and Chinmai Pindi. The results of their ground-breaking work have recently been published in the prestigious peer-review Journal of the American Chemical Society – Biochemistry.

Elaborating on this research, Prof Senapati, said, “Current inhibitors that target HIVPR make use of the weak forces of attraction called ‘van der Waal’s forces’ to attach themselves to the protease molecule. Given that these forces are weak, the efficacy of the drug is variable and the virus will soon become resistant to them.”

One of the routes that drug developers work on is to attack is HIV-1 protease (HIVPR), an essential enzyme that is used by the AIDS virus for growth and maturation. Drug designers have aimed at developing efficient inhibitors of the enzyme – inhibitors are molecules that bind with the enzyme, thereby making it unavailable to the virus for growth and maturation.

The molecular dynamics (MD) simulation studies conducted by IIT Madras researchers showed the presence of a strong and asymmetrical electric charge in the active site of the HIVPR. If a drug molecule can be designed with a complementary charge, so that it can bind tightly with this active site through electrostatic attraction, it can permanently deactivate/inhibit the enzyme.

“Current drugs lack this electrostatic complementarity. This must be investigated because it is well-known that electrostatic forces between molecules are much stronger than van der Waals forces,” added Prof Senapati.

Thus, Prof Senapati and his team propose that drug design strategies should embrace both electrostatics and van der Waals interactions to complement the HIVPR active site architecture.