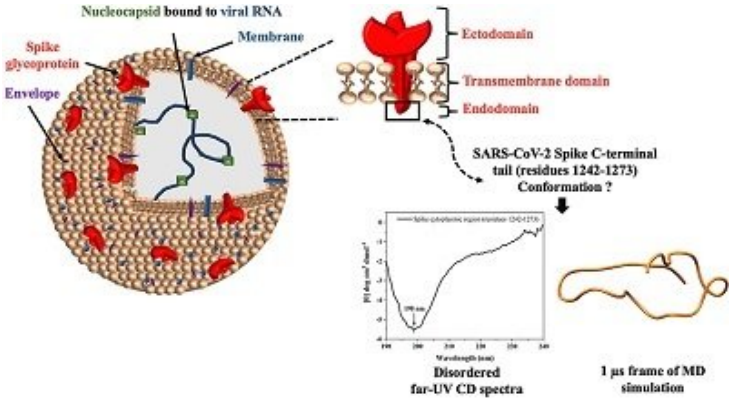
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IIT-Mandi gives further understanding on basic science of COVID-19 and related infections

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Researchers use advanced computational algorithms and laboratory techniques



Researchers from the Indian Institute of Technology (IIT) Mandi, using spectroscopy and simulation methods, unravelled the molecular structure of a functional protein region of the COVID-19 virus. The team has established the structure of one section of an important spike protein responsible for the virus's infectivity.

The unique and pioneering observations have been recently published in the journal Virology. The research was led by Dr Rajanish Giri, Associate Professor, School of Basic Sciences, IIT Mandi, and co-authored by his Prateek Kumar, Taniya Bhardwaj, and Dr Neha Garg, Assistant Professor at Banaras Hindu University.

Dr Giri’s research team has used CD spectroscopy and molecular dynamics simulations to investigate the shape or conformation of the spike glycoprotein’s intravirion region, also known as the C-terminal region or endodomain.

The researchers have validated the simulation results with experimental studies and have shown that the structure of the intravirion region of the spike protein i.e. endodomain is an intrinsically disordered region in isolation. Also, solvent dependent studies suggest the conformational or shape-changing capabilities of this endodomain. Prateek Kumar, Ph.D. scholar, IIT Mandi posits that the structural malleability of this region can help identify many new targets inside the host cell, which, in turn, could help in understanding the basic science of COVID-19 and other coronavirus infections.