

Press Release

IIT Mandi researchers elucidate the molecular structure of Endodomain of the spike protein of the COVID-19 virus

Using advanced computational algorithms and laboratory techniques, the researchers have deciphered the structural flexibilities of the C-terminal region

Mandi, 5th April 2022: Researchers from IIT Mandi, using spectroscopy and simulation methods, unraveled 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 Ph.D. scholars, Mr. Prateek Kumar, Ms. Taniya Bhardwaj, and Dr. Neha Garg, Assistant Professor at Banaras Hindu University.

The SARS Coronavirus 2, the cause of the ongoing COVID-19 pandemic, is so-called because of the spikes on its surface that give it the appearance of a crown (or corona). The proteins that make up the spikes are responsible for the penetration of these viruses into the host cells of the infected lifeform.

Speaking about his recent work, Dr. Rajanish Giri, Associate Professor, School of Basic Sciences, IIT Mandi, said, “Our team has deciphered the shape of the endodomain of spike protein, in isolation, as a reductionist approach. We found that there is no order or structure, and this is an intrinsically disordered region. The endodomain is an important part of spike protein as it contains transporting signals that help in movement of protein inside host cells and thus play a crucial role in infection.”

Further, Dr. Rajanish Giri, mentioned, “Due to absence of specific order or structure, this is the part of Dark Proteome of the virus. It also suggests that endodomain can adopt a fully disordered or partially disordered structure under different conditions. For studying the SARS-CoV-2 spike endodomain, we have used advanced computational algorithms and laboratory techniques. We have also proved, what have only remained speculations so far, the structural flexibilities of the C-terminal region or endodomain.”

Given the importance of the spike protein in the virus' infectivity, considerable research work is being carried out all over the world on characterizing their molecular structure. It is now known that the spike protein comprises a section that is outside the main virus body (the extravirion) known as ectodomain; a



section that crosses the viral membrane (transmembrane); and a section that is inside the viral structure (the intravirion), known as endodomain.

Most studies only focus on the extravirion, and there is much less information available on the transmembrane and intravirion parts of the spike protein. 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.

“Our findings provide direction to the scientific community for the exploration of drugs that can target this region of the spike protein, keeping in mind, its structural flexibility,” **says Mr. Prateek Kumar, Ph.D. scholar, IIT Mandi.** He further 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.

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.

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About [IIT Mandi](#)

IIT Mandi has four Academic Schools and three major Research Centers. The Schools are: School of Computing and Electrical Engineering, School of Basic Sciences, School of Engineering, and School of Humanities and Social Sciences. The Centers are: Advanced Materials Research Centre (AMRC; set up with an investment of Rs. 60 crores), Centre for Design and Fabrication of Electrical Devices (C4DFED; has Rs. 50 crores worth of fabrication tools), and BioX Centre (has acquired research equipment worth Rs. 15 crores).

The unique, project-oriented B.Tech. curriculum is centred around its 4-year long Design and Innovation stream. From August 2019, IIT Mandi started 3 new and unique B. Tech. programmes in Data Science and Engineering, Engineering Physics, and Dual Degree in Bioengineering. Since the inception of the Institute, IIT Mandi faculty have been involved in over 275 Research and Development (R&D) projects worth more than Rs. 120 crore.

IIT Mandi set up the IIT Mandi iHub and HCI Foundation (iHub; a section-8 company) on its campus at Kamand with significant funding of INR 110 crores from the Department of Science and Technology (DST), Government of India. The iHub is planned to fuel research and technology development, skill development, startup and innovation, and collaborations in the HCI and allied AI/ML areas in India. IIT Mandi is the only second-generation IIT to be featured at rank no. 7 in the Atal Ranking of Institutions on Innovation Achievements of the Innovation Cell, Ministry of Education, Govt. of India.

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