

## Iit-Ism Team Identifies A Common Spice That Has The Potential To Cure Covid-19



Professor Umakanta Tripathy

Ashis Sinha IDhanbad: IIT-ISM Scientists identified a common spice that has the potential to cure COVID-19.

A computational study conducted by the researchers from the Department of Physics, Indian Institute of Technology- Indian School of Mines (ISM), Dhanbad has identified piperine, found in black pepper that can bind and inhibit the SARS-Cov-2 virus.

This study was led by Professor Umakanta Tripathy and his team of Ph.D. Students, Janmejaya Rout and Bikash Chandra Swain, and was recently published in the "Journal of Biomolecular Structure and Dynamics" titled "In silico investigation of spice molecules as a potent inhibitor of SARS-CoV-2".

The Covid-19 pandemic has already claimed 1 lakh lives in India and 1 million worldwide. There are concerted efforts by scientists worldwide to develop therapeutic drugs to cure those who are infected by the SARS-CoV-2 virus.

Several vaccine candidates are also under trial in different parts of the world, including in India.

"The virus uses proteins present on its surface to enter cells of our body and start causing damage," explains Prof. Tripathy. His team started looking for natural compounds that could bind to the virus proteins and stop it from entering our cells.

The ISM team used computer-based techniques such as molecular docking and molecular dynamics (MD) simulation to hunt for potential inhibitors. "We picked up 30 molecules present in common kitchen spices and started exploring their role as a therapeutic agent," adds Professor Tripathy.

It turns out that out of all the molecules tested, piperine, an alkaloid present in pepper and responsible for its pungency, emerged as a strong inhibitor of the virus proteins. As pepper is consumed in the diet, its antiviral properties will act as a boon as we will not have to deal with side effects seen with chemical drugs.

"Our results look very promising. Although the study is purely computational and requires testing in laboratories for further confirmation, it is still an important lead," opines Prof. Tripathy. The molecule is now being tested experimentally in the laboratory in collaboration with Dr. Ashok Kumar Patra, Director, Biologics Development, IMGENEX India Pvt. Ltd., an Odisha based Biotech Company.

The computer-based studies are often considered as the first step before these get tested in

laboratories and undergo subsequent trials if found efficient.

Professor Umakanta Tripathy is an Assistant Professor in the Department of Physics, Indian Institute of Technology (Indian School of Mines), Dhanbad. Janmejaya Rout and Bikash Chandra Swain are Ph.D. Scholars in the same department.



Scientists Develop A Machine To Identify Protein Species That Trigger Parkinson's Disease



ASHis Sinha I Dhanbad: IIT-ISM Dhanbad Prof. Umakanta Tripathy and his team developed a Z-scan machine to provide a solution for the treatment of Parkinson's disease in collaboration with Prof. Krishnananda Chattopadhyay and his team from CSIR-Indian Institute of Chemical Biology (IICB) Kolkata. The other team members are Sumanta Ghosh, Sakshi, Bikash Chandra Swain, and Ritobrita

Chakraborty.

Prof. Umakanta said the accumulation of an inherently disordered protein Alpha-synuclein aggregates in brain tissue plays a pivotal role in the pathology and etiology of Parkinson's disease. Aggregation of Alpha-synuclein has been found to be complex and heterogeneous. Because of the inherent complexity and large dynamic range (between few microseconds to several days), it is difficult for the conventional biophysical and biochemical techniques to sample the entire time window of Alpha-synuclein aggregation.

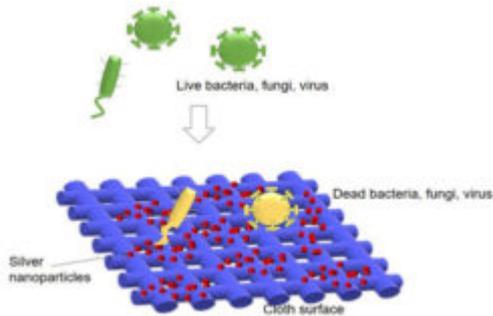
Here, for the first time, we have introduced the Z-scan technique as a novel tool to investigate different conformations formed in the aggregation kinetics of Alpha-synuclein, in which different species showed its characteristic nonlinear features, said Prof. Umakanta. "A switch in the sign of the nonlinearity has been observed for the first time as a signature of the late oligomeric conformation, a prime suspect that triggers neuronal cell death associated with Parkinson's disease, and a device, which monitors this conveniently can be beneficial for both pharmaceutical as well as clinical research," he added.

For example, in the near future, this tool can be used to screen blood plasma to find the aggregated toxic species of the protein, Alpha-Synuclein, for a possible diagnosis of Parkinson's disease because the Alpha-Synuclein protein is also present in the plasma of human blood, said Prof. Umakanta.

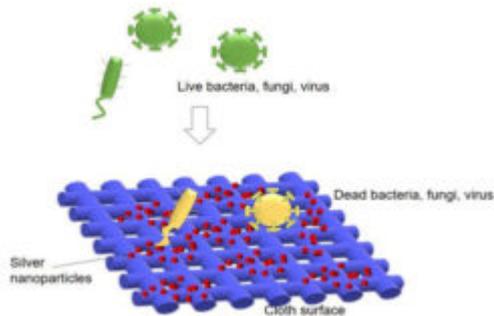
Besides, this tool can also be used for drug screening to find a suitable candidate to cure Parkinson's disease. Here, the drug that can inhibit the aggregation process of the Alpha-Synuclein protein from preventing to form the toxic species can be easily identified through our device, he said.

"Nevertheless, we believe that this simple, inexpensive, and sensitive device can also have potential future applications in detecting or monitoring conformations in other essential

proteins related to different neurodegenerative and other human diseases,” he added. Notably, until now, Parkinson’s disease is incurable, and it is a common neurodegenerative disorder.



### Iit-Ism Develops Nanoparticles Coating For Cloths To Kill Novel Coronavirus



IIT-ISM develops Silver nanoparticles coating for textiles to combat COVID-19

Ashis Sinha I Bokaro: Indian Institute of Technology (IIT-ISM) Dhanbad has developed a wash-resistant antiviral and antibacterial coating of silver nanoparticles for textiles. This coating makes the textile (cloth) super-hydrophobic may also kill Novel Coronavirus when the virus comes in contact.

A three-member team of ISM scientists headed by Aditya Kumar, professor of chemical engineering, Kalpita Nath and Poonam Chauhan conducted successful research on the efficacy of the coating on E. coli (bacteria) and A. Niger (fungus). Though, tests on COVID-19 are yet to be conducted, informed a Media Cell official of IIT (ISM).

Now, we are at the final stage of testing the coated cloth for its anti-viral property, specifically for COVID-19. After up-scaling of this technology at IIT(ISM) Dhanbad, these coated clothes can be made available at affordable prices to the mass, said the official.

We have started the study soon after the WHO recommended the use of triple-layered masks and PPE kits for COVID-19 prevention, said Aditya.

“These PPE kits can only be used one time and health care workers get infected while removing PPEs and also during disposal of the infected PPEs. Additionally, it is not easy to work with PPE kits put on over multilayered clothing, particularly, in hot and humid seasons,” he added. If, the clothes themselves are made anti-bacterial and anti-viral, then multi-layered clothing and full body cover PPE kits will not be needed; also the spread of the virus by transferring from one surface to the other will get reduced considerably, said Aditya.

Keeping above in mind, we have developed a method to prepare a facile and durable super-hydrophobic coating of silver nanoparticles on the surface of cloth using an in-situ UV irradiation method followed by its modification with the Perfluorodecyltriethoxysilane, he said.

Explaining the facts of their research Aditya said, “Super-hydrophobicity is a phenomenon which shows that the water droplet does not stick to the surface at all and rolls off easily from it. At lab-scale, this coating is found to have excellent chemical and thermal stability making it reusable multiple times even after repeated washing.”

The coated cloth exhibits exceptional self-cleaning and stain-resistant properties leading to complete non-adherence of dirt, liquid droplets and stain (for example, food, rust, ink, etc.) on the cloth surface, he said.

He said, anti-bacterial and anti-fungal properties of the coated cloth were confirmed by carrying out E. coli (bacteria) and A. Niger (fungus) culture studies, respectively. “This coating is imbued with silver nanoparticles, which is a proven anti-viral agent. It inhibits the attachment of the virus on the surface of the cell itself,” stated Aditya.

“When microbes come in contact with the coated cloth, they are repelled by the superhydrophobic nature of the coating. If they somehow touched the cloth surface, they get killed by Ag<sup>+</sup> (silver) ions present in the coating.

The Ag<sup>+</sup> ions strongly inhibit microbial growth through suppression of the respiratory enzymes and electron transport components and interference with the DNA functions,” Aditya explained. Since silver is also non-toxic in nature to humans at very low concentrations, the silver nano-particle coating becomes human friendly. The super-hydrophobic nature of the coating combined with the anti-viral agent silver, makes it a potential anti-COVID-19 coating, he said.



Ism Dhanbad Develops Uvc System To Curtail Covid-19 Spread



IIT-ISM, Dhanbad develops UVC system to curtail COVID-19 spread

Ashis Sinha I Dhanbad: IIT-ISM, Dhanbad has developed a UVC radiation-based disinfectant chamber to address the concern raised for rapid transmission of the COVID-19 virus within the country. The system is designed by the faculty members of the departmental of Mechanical Engineering and fabricated in the “Central Fabrication Facility” of ISM.

Professor A R Dixit, the Project Coordinator said that the UVC (200-280nm) could be an effective measure for decontaminating surfaces that may be contaminated by the SARS-CoV-2 virus by inducing photodimers in the genomes of microorganisms. The current global SARS-CoV2

pandemic is of serious concern with its extraordinary transmission rate and rapid spread throughout the country.

Although the mortality rate in India is reported low as compared to other countries, currently, no antiviral drugs or vaccine is available to the public. It has been reported that structurally this virus is similar to other coronaviruses such as severe acute respiratory syndrome (SARS) and the Middle East respiratory syndrome (MERS), and can be addressed with existing disinfection methods such as disinfectant chemicals, drying heating, and ultra-violet radiations (UVC).

Ultraviolet light has been demonstrated to be capable of destroying viruses, bacteria, and fungi, In view of the above, a team comprising of Professor Dixit, Professor Arun Dayal Udai, Ashish Kumar, and Ashish Sidharth has designed UVC based sterilizer, he said.

It consists of two chambers (440x400x400 and 440x400x100mm) to accommodate different size items. The time required to disinfect the items depends upon the size of the item and type of material, said Prof Dixit. "The UVC dose is fixed based on data reported in the leading journal papers. The estimated time required disinfecting the item in the big and small chamber is 3 minutes and 1 minute, respectively," he added.

The system has the provision to set desired sterilizing time, chamber selection, hand sanitizing station, LED lights, warning signals, etc. In addition to its functionality, the aesthetic look of the UVC chamber is also carefully designed, he said.

"The developed prototype is ready to be commercialized in case any interested industry or organization approaches the institute," added Prof. Dixit.