U.S.-Based Researcher Amena Khatun Manica Advances Computational Drug Discovery for Schizophrenia

U.S.:: Amena Khatun Manica, a U.S.-based chemistry researcher with advanced academic training in both Bangladesh and the United States, is contributing to the growing field of computational medicinal chemistry through research focused on molecular modeling and structure-based drug discovery.Manica earned her Bachelor of Science and first Master of Science in Chemistry from Comilla University in Bangladesh before pursuing a second Master of Science in Chemistry at the University of New Haven in Connecticut.

Her academic training has provided her with a strong foundation in chemistry, computational modeling, molecular dynamics, and biomedical research.One of her notable research contributions is the 2025 first-author study, “Computational Modeling Design of Novel NMDAR Agonist for the Treatment of Schizophrenia,” published in Neurogenetics. The research explores the N-methyl-D-aspartate receptor (NMDAR), an important molecular target associated with neurological function and the pathophysiology of schizophrenia.


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The study applied a multi-stage computational drug-discovery approach involving virtual screening, molecular modeling, ADMET assessment, blood-brain barrier prediction, and molecular dynamics simulation. Through this process, the researchers identified Compound_8, Compound_15, and Compound_945 as promising computational candidates for further investigation.

The findings demonstrate how computational chemistry can help researchers evaluate potential therapeutic molecules before moving toward more resource-intensive laboratory and preclinical studies. By examining molecular interactions, pharmacological properties, predicted toxicity, and molecular stability, computational methods can improve early-stage drug candidate selection.Manica’s broader research interests include computational medicinal chemistry, molecular dynamics, virtual screening, pharmacological prediction, blood-brain barrier analysis, and machine-learning-assisted drug discovery. Her continuing research direction focuses particularly on central nervous system disorders, including schizophrenia and related neuropsychiatric conditions.Through her interdisciplinary research, Manica aims to contribute to the development of safer and more effective therapeutic candidates while advancing the use of computational technologies in modern drug discovery. Her work reflects a continuing commitment to scientific research, computational innovation, and biomedical applications with potential relevance to significant unmet medical needs.