Dr. Manish Kumar Gupta

Associate fellow
email: manish.gupta@teri.res.in
Homepage: https://www.researchgate.net/profile/Manish_K_Gupta
URL: https://scholar.google.co.in/citations?user=r-e0d1gAAAAJ&hl=en

Research focus:

Dr. Gupta has a Masters Degree in Pharmacy, and subsequently obtained his PhD in 2008 from Central Drug Research Institute, Lucknow, India. Dr. Gupta has core expertize in computational chemistry and biology. His research activities focus on 3D modeling and characterization of protein structures, study on mechanistic aspects of proteins, development of activity and toxicity prediction models for small organic molecules and design of novel agonists/antgonists for enzymes. He is well versed in various computational approaches used in chemical biology such as molecular dynamics simulations, *in silico* structure optimization and characterization, docking and virtual screening. He has established a molecular modeling lab at TD-NBC which have following software:
Gromacs 5.1.4: Molecular dynamics simulation studies
Modeller 9.15: 3D modeling of proteins
Bioedit 7.2.5: Biological sequence alignment editor
Gaussian 9w: Small molecule structure optimization using quantum chemistry calculations/DFT
GMDH shell: Artifecial neural networks based non-linear modeling
PyMol: Structural graphics

Current Research :

1. Structural studies on abscisic acid (ABA) receptors to design novel ABA receptor antagonists for the control of reproductive stage stress tolerance in crop plants
2. Study on proteolytic enzymes involved in pathogenesis of *Rhizoctonia solani* and inhibitors thereof for the control of sheath blight in rice
3. Development of beetroot red formulation (Ntural red color) for the application in food industry