Department of Chemical Sciences

A REPORT ON

Collaboration of Bioinformatics Group, Ganeshkhind, Pune University Campus, Pune with Professor R. C. Deka

1. Name of the Collaborative Activity: Collaboration of Bioinformatics Group, Ganeshkhind, Pune University Campus, Pune with Professor R. C. Deka
2. Nature of Activity: R&D
3. Name of the Collaborating Agency/ Individual with affiliation, and contact details: Dr. Uddhavesh B Sonavane Bioinformatics Group, Ganeshkhind, Pune University Campus, Pune – 411007
4. Summary of collaboration: We have used Beck-Lee-Yang-Parr (BLYP) functional along with DNP basis set to obtain more accurate geometrical parameters, charges and electronic energies of the various conformers. We have then compared these structural parameters with the available experimental structural parameters. We have also performed frequency calculations of the different conformers at the same level of theory. These frequency calculations provided us about all the possible modes of vibrations and thermo-chemical parameters. Apart from this, the reaction enthalpies and Gibbs free energies are also helpful to calculate the feasibility of reactions. We have further carried out orbital and population analysis calculations of HOMO and LUMO energies for the conformers. Moreover, the Fukui function analysis carried out in this work gave an idea about the active sites and susceptibility of nucleophilic, electrophilic and radical attack.
5. List of year-wise activities under the collaboration:
   Activity 2017-18: Computational studies of anti-cancer drug mediated by graphene and reaction mechanism of drug generated alkyl radical with guanine
   Activity 2018-19: Structural insight into antisense gapmer-RNA oligomer duplexes through molecular dynamics simulations
   Activity 2019-20: Structural insight into locked nucleic acid based novel antisense modifications: A DFT calculations at monomer and MD simulations at oligomer level

Signature and Seal of Head of Department/ Centre/ Cell

Name: Professor Ruli Borah
Designation: Professor & Head