



NATIONAL INSTITUTE OF TECHNOLOGY ANDHRA PRADESH
Department of Biotechnology
BIOTECHNICAL ENGINEERING ASSOCIATION

A Report on One day Hands-on Workshop

on

“Basic Tools & Techniques in Bioinformatics using VLifeMDS”

by

Mr. Amit Bedi

Manager, VLife Sciences Technologies (A division of NovaLead Pharma Pvt. Ltd)

Program Date: 18th April 2018

Venue: DBMS Lab, First Floor, Main building, NIT Andhra Pradesh

Time: 11:00 am to 4:00 pm

Audience: Students and Faculty, Department of Biotechnology, NIT Andhra Pradesh

Programme details:

A workshop on “**Basic Tools & Techniques in Bioinformatics using VLifeMDS**” was organized by the Biotechnical Engineering Association (BEA) for students and faculty of Department of Biotechnology.

The session is started with an introduction to the VLifeMDS software. Students and faculties were enlightened about the possible requirement of the software and its tools for understanding and solving several biological complications. This session also focussed on discussion about various applications of this software.



Mr. Amit Bedi giving introduction to the VLifeMDS

Post-introduction, hands on training was conducted for students and faculty on

- Design of small molecules, visualization and analysis using VLifeBase.
- All molecular operations and key activity of conformer generation using VLife Engine.
- Homology modelling with options for manual and automated template based modelling using ProModel.
- Molecular Docking studies with multiple scoring functions and options for rapid and high precision docking using VLifeDock.
- 2D/ 3D QSAR with multi variable selection options and regressions methods using VLifeQSAR.
- Exploring databases with multiple search options including property, fingerprint and pharmacophore based using ChemDBS.
- Pharmacophore generation and application in optimization and searches using MolSign.
- Creating combinatorial library with a choice of substitutions using LeadGrow.
- Calculating and visualizing molecular properties on the surface of a molecule using ProViz.



Mr. Amit Bedi training the students on various tools available in VLifeMDS

Mr. Amit had also given a brief introduction to the following

- To obtain site specific clues for new molecule design and optimization using GQSAR.
- To optimize lead design based on interaction between the molecule and interacting residues in the active site using VLifeSCOPE.
- An extension to the combinatorial library generation capability that ensures that molecules which can be synthesized can only be generated in a library using LeadGrow+.
- Shape Based Screening using Aakar.
- Customized workflows for research protocols using VLife Workflow.



Students performing the hands on workshop on Bioinformatics

Mr. Amit has introduced the students to Bioinformatics, which is a theory and laboratory subject in their fourth year, first semester. This software is very useful for the staff and faculty, can be used for carrying out laboratory classes and several student projects.
