INTERNSHIP PROGRAMME FOR UG DEGREE (SEMESTER-V)

(For the students admitted under New Curriculum and Credit Framework from the academic session 2023-24)

Course Title: Computer Aided Drug Designing (CADD)	
Internship Providing Organization (IPO):	**Department of Chemistry, Bankura Sammilani College**
Category of Course:	**For UG DEGREE (SEM-V)**
Duration:	**60 Hours**
Course Coordinator and Contact Details:	**Dr. Mrinmoy Shannigrahi Mob: 9732343790**
Mentors:	**Dr. Shantanu Hazra Dr. Pinaki Mandal Dr. Samaresh Ghosh Dr. Sabir Ahamed Dr. Susovan Bhowmik Dr. Swadesh Mandal Dr. Swapnadip Roy**
Intake Capacity:	**40 Students**
Course Fees:	**Rs. 100/- (Students from Host Institution) Rs. 400/- (Students from Other Institution)**

SYLLABUS

Course Title: Computer Aided Drug Designing (CADD)
[50 Marks/2 Credits/60 Hours]

Learning Outcomes (LO)
• Understanding of the rational drug design principles. • Mastering In-silico Drug design. • Developing skills in molecular modelling techniques and in docking.

Module I (Theory: 20 hours)		
Unit 1	**Introduction to Drug Discovery & Types of Drugs** Overview of the process of drug discovery and its development, basic principles and challenges in drug discovery, Target and lead identification. Analgesic, antipyretic, antibiotics, anti-inflammatory, antiviral, Cardiovascular, anti HIV-AIDS and anti-cancer drugs.	**4 hours**
Unit 2	**Structure –Property & ADME** Relationship between molecular structure and various properties of drugs- such as solubility, permeability, and drug likeness. Principles of Absorption, Distribution, Metabolism, and Excretion (ADME) of drugs.	**4 hours**
Unit 3	**SAR and QSAR** Quantitative Structure-Activity Relationships (QSAR) and their use in predicting drug activity based on molecular structure.	**3 hours**
Unit 4	**Pharmacophore Modeling** Concept of pharmacophores and how they are used in drug design. **Target-Based Drug Design** This section focuses on designing drugs that specifically target a particular biological target, such as an enzyme or receptor.	**4 hours**
Unit 5	**Molecular Modeling** Various techniques for simulating and modeling molecules-molecular mechanics, force fields, quantum mechanics, and conformational analysis. **Docking** Simulating the interaction between a drug molecule and its target protein.	**5 hours**

Module II (In-silico Lab: 40 hours)		
Unit 6	Different available softwares for Drug designing Screening libraries of compounds against potential drug targets through PyRx Web-based chemical structure editor Ketche	**10 hours**
Unit 7	AutoDock and AutoDock Vina (structure-based drug design)	**10 hours**
Unit 8	ChemMaster (QSAR modelling)	**10 hours**
Unit 9	PDBinder and eFindSite (identifying ligand-binding sites in protein structures)	**10 hours**