Sri Sankara Arts & Science College
Autonomous
A Unit of Sri Kanchi Kamakoti Peetam Charitable Trust
Affiliated to University of Madras
Accredited by NAAC with 'A' Grade

24/11/2022

MINUTES OF MEETING OF THE BOARD OF STUDIES

Department: Biotechnology

Venue: Board Room

Date: November 24th, 2022

Agenda: Approval to establish the Centre for Drug Design and Discovery and Centre for Medicinal and aromatic plants Research to take effect from the even semester of 2022-23. Approval of Syllabus of Advanced Diploma in Computer Aided Drug Design and Discovery (CADDD) – Value Added Program to take effect from 2023 -2024.

The following members were present in the meeting:

1. Prof.R.Puvanakrishnan, Ph.D., Professor, CSIR Emeritus, Central Leather Research Institute, Adyar, Chennai - External Subject Expert.

2. Prof.N.Munuswamy, D.Sc., Professor Emeritus, Department of Zoology, University of Madras, Guindy Campus, Chennai-600025- External Subject Expert.

3. Prof.B.Ramesh, Ph.D., Professor and Head, Dept. of Biotechnology, Sri Sankara Arts and Science College, Enathur, Kanchipuram – Chairman.

4. Dr.V.Guruchandran, Ph.D., Assistant Professor, Dept. of Biotechnology, Sri Sankara Arts and Science College, Enathur, Kanchipuram – Member.

5. Dr.A.Shyamala, Ph.D., Assistant Professor, Dept. of Biotechnology, Sri Sankara Arts and Science College, Enathur, Kanchipuram – Member.

6. Dr.P.Saravanan, Ph.D., Assistant Professor, Dept. of Biotechnology, Sri Sankara Arts and Science College, Enathur, Kanchipuram – Member.

7. Dr.D.Chitra, Ph.D., Assistant Professor, Dept. of Biotechnology, Sri Sankara Arts and Science College, Enathur, Kanchipuram – Member.

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8. Dr.S.Malathi, Ph.D., Assistant Professor, Dept. of Biotechnology, Sri Sankara Arts and Science College, Enathur, Kanchipuram - Member.

9. Dr.K.R.Venkatesan, Ph.D., Principal, Sri Sankara Arts and Science College, Enathur, Kanchipuram – Special invitee.

- The Board of Studies unanimously approved the establishment of the Centre for Drug Design and Discovery and the Centre for Medicinal and Aromatic Plants Research to take effect from the even semester of 2022-23 **(Annexure I).**

- Board of Studies unanimously approved the Syllabus of Advanced Diploma in Computer Aided Drug Design and Discovery (CADDD) – Value Added Program to take effect from the academic year 2023-24 **(Annexure II).**

Signature of members:

1. Prof.R.Puvanakrishnan -

2. Prof.N.Munuswamy -

3. Prof.B.Ramesh -

4. Dr. V.Guruchandran -

5. Dr.A.Shyamala -

6. Dr.P.Saravanan -

7. Dr.D.Chitra -

8. Dr.S.Malathi -

9. Dr.K.R.Venkatesan -

CENTRE FOR DRUG DESIGN AND DISCOVERY

Coordinator: Dr.B. Ramesh, Ph.D.,

Proposed Activities

- Screening and identification of novel bioactive compounds by using in silico studies.
- Optimization of the affinity, potency and selectivity of the existing drugs and reducing the side effects of existing drugs using CADD, artificial intelligence and high-power computing tools.
- Drug repurposing studies involving high throughput screening.
- Experimental validation screened bioactive compounds by in vitro studies.
- Publication of the results in reputed international journals.
- Patenting of novel molecules and technology transfer.
- Making the drug into a therapeutic product.
- Creating scientific linkages with other institutes and industries by signing MOUs for collaborative research in Theoretical Biology.
- Offering value-added courses and organizing various short-term training programs.

Course Proposed to take effect from 2023-2024

ADVANCED DIPLOMA IN COMPUTER AIDED DRUG DESIGN AND DISCOVERY (CADDD)

CENTRE FOR MEDICINAL AND AROMATIC PLANT RESEARCH

Coordinator: Dr.V.Guruchandran, Ph.D.,

Proposed Activities

- Research on economically important medicinal and aromatic plants.
- Standardization of the protocol for invitro culturing of rare endangered species.
- Publication of the results in reputed international journals, patenting and technology transfer.
- Creating scientific linkages with other institutes and industries by signing MOUs for collaborative research.
- Offering value-added courses and organizing various short-term training programs.

ADVANCED DIPLOMA IN

COMPUTER AIDED DRUG DESIGN AND DISCOVERY (CADDD)

Duration: 1 Year

Module 1

Databases for screening studies, ZINC, Indian Medicinal Plants, Phytochemistry And Therapeutics 2.0 (IMPPAT 2.0), DRUGBANK, Pubchem.

Various formats of molecules, SDF, SMILES, PDB, PDBQT, MOL, MOL2 and their conversion using Open Babel, DataWarrior – OpenMolecules, BIOVIA Discovery Studio Visualizer, Marvinview, and Avogadro. Drawing chemical molecules using MarvinSketch.

Module 2

Target protein databases, PDB and AlphaFold Protein Structure Database. Handling protein and ligand in editing software, RasWin, UCSF Chimera, PyMOL. Fixing the structure using Swiss PDB Viewer.

Highthrouput screening and docking using Autodock Vina, PyRx, and docking using iGEMDOCK – BioXGEM. Prediction of ADME parameters, pharmacokinetic properties, druglike nature and medicinal chemistry friendliness by SwissADME and admetSAR. Optimization of the lead compound with consideration of ADMET properties using ADMETopt.

Module 3

Quantitative structure-activity relationship (QSAR), Data division for training and testing sets, Descriptor calculation by PaDEL software, regression and classification-based QSAR modelling by DTC-QSAR software, validation of the QSAR model, screening large database of ligands using the model developed.

Molecular dynamics simulation by GROMACS, Protein structure preparation and force field generation, Ligand force field calculation by PRODRG 2.5 and CGenFF. Complex generation and building the topology, Solvation, the addition of ions, Energy Minimization, Restraining the Ligand, NVT equilibration, NPT simulation, production MD, and MD Analysis by RMSD, RMSF, Rg, HBOND and Protein-Ligand Interaction Energy.

Module 4

Literature search and designing a research project, Mendeley reference manager software for writing dissertation and publication. Project execution and submission of dissertation. Project Viva Voce.