Certificate course on molecular docking studies using Auto Dock Vina Software

6th -11th October 2023

Course Duration- 30Hr's

Organized By

Department of Pharmaceutical Chemistry

SEVEN HILLS COLLEGE OF PHARMACY

(AUTONOMOUS)

Venkatramapuram, R C Puram (Mandal), Tirupati (Dist), Tirupati, 517 561, A.P, INDIA
Accredited "A" Grade by NAAC
Approved by, PCI, New Delhi and Awarding Univeristy: JNT University Anantapur - Ananthapuramu
Recognized by UGC Under Sections 2(f) & 12(B) of UGC Act 1956
Recognized Research Centre by JNTUA, Ananthapuramu
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In association with

Glory pharma Chem India Private Limited, Tirupati.

Convener:

Dr.M.Niranjan Babu
Principal
Seven Hills College of Pharmacy
(Autonomous), Tirupati

Course Co-ordinator:

Ms.M. Reddemma
Assistant Professor
Seven Hills College of Pharmacy
(Autonomous), Tirupati

Course Syllabus

Course Objectives

The goal of Molecular docking studies using Auto Dock Vina Software is

- **To understand the molecular docking studies.**
- **To perform molecular docking studies using Auto Dock Vina software.**
- **To analyze the docking results obtained with the help of Auto Dock Vina.**

Course Outcomes

By the completion of the course, Student can be able

- **To install the molecular docking software like Auto Dock Vina.**
- **To learn the molecular docking studies theory and its practical application by Performing docking studies using Auto Dock Vina software.**
- **To learn and understand various docking parameters.**

Module 1 : Introduction to Molecular docking

Basics of computational chemistry
Basics of Molecular simulations

Module 2: Installation of docking software

Installation of Auto Dock Vina software in window and Mac OS
Understand the hands on experience of GUI and various options of Auto dock Vina software

Module 3: Preparation of ligand and protein

Online exploration of databases for Protein and Ligand search
Preparation of Protein and Ligand for molecular docking studies by Auto Dock Vina software

Module 4: Molecular docking using Auto Dock Vina

Docking studies like docked structures and tits interaction and binding energy using Auto Dock Vina software
Molecular dynamic studies like potential energy, RMSD,RMSF plots etc. using Auto Dock Vina software

Module 5: Analysis and interpretation of docking results

Protein ligand structure determination through topology file
2D, 3D surface mapping using molecular simulations

Syllabus And Course Description

S.No	Date and Module	Module	Description	No of Hours	Resource Person
1	06.10.2023 Day 1	Module 1 Introduction to Molecular docking	• Basics of computational chemistry • Basics of Molecular simulations	06	Dr P. R. Logesh, Professor Department of Pharmaceutical Chemistry Sri Krishna Chaitanya college of Pharmacy, Madanapalli, Andhra Pradesh, Pin:517 325
2	07.10.2023 Day 2	Module 2 Installation of docking software	• Installation of Auto Dock Vina software in window and Mac OS • Understand the hands on experience of GUI and various options of Auto dock Vina software	06	Mr. Y. Rajendra Associate Professor, Department of Pharmaceutical Chemistry, Seven Hills College Of Pharmacy Tirupathi, Andhra Pradesh – 517 561
3	09.10.2023 Day 3	Module 3 Preparation of ligand and protein	• Online exploration of databases for Protein and Ligand search • Preparation of Protein and Ligand for molecular docking studies by Auto Dock Vina software	06	Ms. M. Reddemma Assistant Professor Department of Pharmaceutical Chemistry, Seven Hills College Of Pharmacy Tirupathi, Andhra Pradesh –517 561
4	10.10.2023 Day 4	Module 4 Molecular docking using Auto Dock Vina	• Docking studies like docked structures and tits interaction and binding energy using Auto Dock Vina software • Molecular dynamic studies like potential energy, RMSD,RMSF plots etc. using Auto Dock Vina software	06	Dr.G. Satheesh Kumar Professor, Department of Pharmaceutical Chemistry, Seven Hills College Of Pharmacy Tirupathi, Andhra Pradesh –517 561
5	11.10.2023 Day 5	Module 5 Analysis and interpretation of docking results	• Protein ligand structure determination through topology file • 2D, 3D surface mapping using molecular simulations	06	Dr.R. Radha Professor Department of Pharmaceutical Chemistry, Seven Hills College Of Pharmacy Tirupathi, Andhra Pradesh –517 561

TOTAL LECTURE HOURS – 30Hrs

Course References

- **Beginner's guide to protein-ligand docking using AUTODOCK VINA by VISHAL MEVADA**
- **Computational Chemistry, introduction to the theory and applications of Molecular and quantum Mechanics by Errol G. Lewars.**
- **Essentials of computational Chemistry by Christopher J. cramer.**

Programme Framing Committee

S.No	Name of the Faculty	Designation	Name of the College	Role
1	Dr. B. Ravi Teja	Professor	Seven Hills College of Pharmacy	Course Co-Ordinator
2	Ms. M. Reddemma	Assistant Professor	Seven Hills College of Pharmacy	Course Co-Ordinator
3	Dr. G. Satheesh Kumar	Professor	Seven Hills College of Pharmacy	Member
4	Dr.R. Radha	Professor	Seven Hills College of Pharmacy	Member
5	Mr.Y. Rajendra	Associate Professor	Seven Hills College of Pharmacy	Member

Participants will receive a Course Completion certificate upon attaining the 80% ofattendance and 60% of Marks in the End Test.

Course Type: Self-Made course with the Approval of statutory Bodies

Course Offered to: B Pharmacy IV Year

Assessment Mode: Offline

Internal Assessment Exam Pattern: Multiple Choice Questions

Eligible students can enroll your name with Department of Pharmaceutical Chemistry

For other details contact Course coordinator

NO REGISTRATION FEE