



ADITYA COLLEGE OF PHARMACY

Aditya nagar, Surampalem,
Andhra Pradesh 533437



A Certificate course on "Molecular docking studies using Autodock Vina Software"

Eligibility: IV B.Pharm

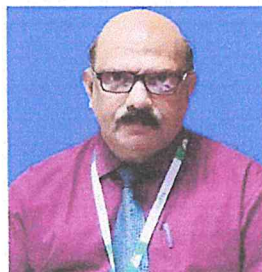
Students who are interested to join the certificate course should contact the respective coordinator



Coordinator: B.N.B. Vidhei
Asst. Professor,
Aditya College of Pharmacy



Resource Person: Dr. K. RamaKrsihna
Asst. Professor,
Aditya College of Pharmacy



Convener: Dr. K. Ravishankar
Principal,
Aditya College of Pharmacy



Patron: Dr. N. Satish Reddy
Vice-Chairman,
Aditya Educational Institutions



Sema
PRINCIPAL
Aditya College of Pharmacy
SURAMPALAM-533 437

All the students enrolled in this course will be provided with a certificate



ADITYA COLLEGE OF PHARMACY

(Affiliated to JNTUK, Approved by AICTE)



(ADITYA NAGAR, ADB ROAD, SURAMPALEM 533 437, E.G.Dt, Ph.9949876664, 08852-200005)

Website: www.acop.edu.in, Email: office@acop.edu.in

COURSE SYLLABUS

DURATION: 30Hrs

COURSE NAME: Molecular Docking studies using Autodock Vina Software

Course Objective:

- To Understand the Molecular docking studies
- To perform the Molecular Docking studies using **AutoDock Vina** software
- To analyze the docking results obtained with help of **AutoDock Vina**

Course Outcome:

- To learn the installation of Molecular docking software like **AutoDock Vina**
- To learn the molecular docking studies theory and its practical application by performing docking studies using **AutoDock Vina** software.
- To learn and understand the various docking parameters

Day 1: 07-11-2020, 6Hrs

Module I:

- ✓ Basics of Computational chemistry
- ✓ Basics of Molecular simulations

Day 2: 21-11-2020, 6Hrs

Module II:

- ✓ Installation of **AutoDock Vina** software in Window and Mac OS
- ✓ Understand the hands on experience of GUI and various options of **AutoDock Vina** software

Day 3: 28-11-2020, 6Hrs

Module III:



Sanjay
PRINCIPAL
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- ✓ Online exploration of databases for Protein and Ligand search
- ✓ Preparation Protein and ligand for molecular docking studies by **AutoDock Vinasoftware**

Day 4: 05-12-2020, 6Hrs

Module IV:

- ✓ Docking studies like docked structure and its interactions and binding energy using **AutoDock Vinasoftware**
- ✓ Molecular dynamic studies like potential energy, RMSD, RMSF plots etc by using **AutoDock Vinasoftware**

Day 5: 12-12-2020, 6Hrs

Module V:

- ✓ Protein –ligand structure determination through topology file
- ✓ 2D and 3D surface mapping using molecular simulations
- ✓ Analysis and interpretation of docking results obtained by **AutoDock Vinasoftware**

REFERENCE:

1. Myers, N. (2015). *Rendering life molecular*. Duke University Press.
2. Morris, G. M., & Lim-Wilby, M. (2008). Molecular docking. In *Molecular modeling of proteins* (pp. 365-382). Humana Press.
3. Valdés-Tresanco, M. S., Valdés-Tresanco, M. E., Valiente, P. A., & Moreno, E. (2020). AMDock: a versatile graphical tool for assisting molecular docking with Autodock Vina and Autodock4. *Biology direct*, 15(1), 1-12.
4. Nguyen, N. T., Nguyen, T. H., Pham, T. N. H., Huy, N. T., Bay, M. V., Pham, M. Q., ... & Ngo, S. T. (2019). Autodock vina adopts more accurate binding poses but autodock4 forms better binding affinity. *Journal of Chemical Information and Modeling*, 60(1), 204-211.



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ADITYA

COLLEGE OF PHARMACY

Approved by AICTE & PCI - NEW DELHI, Affiliated to JNTUK KAKINADA
(Formerly known as Sri Sai Aditya Institute of Pharmaceutical Sciences & Research)

Ph: 99498 76664

Email: office@acop.edu.in

Website: www.acop.edu.in

CERTIFICATE COURSE SUMMARY 2020-21

COURSE CODE AND NAME : CMDS and Molecular docking studies using
Autodock Vina Software

COURSE DURATION : 30Hrs

YEAR AND BRANCH OFFERED: IV B.Pharmacy

COURSE INSTRUCTORS : Dr.K.Rama Krishna, Asso.Professor

COURSE OUTCOME

The student would be able to learn the installation of Molecular docking software like **AutoDock Vina**, molecular docking studies theory and its practical application by performing docking studies using **AutoDock Vina** software, and understand the various docking parameters

COURSE TYPE : Self framed course

ASSESSMENT MODE

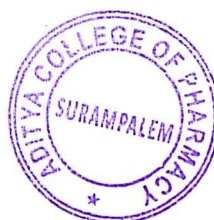
ATTENDANCE : 30 Hours

NO.OF PARTICIPANTS : 49

SCHEME OF EXAM : MCQ Offline

DATE OF EXAM : 14-12-2020

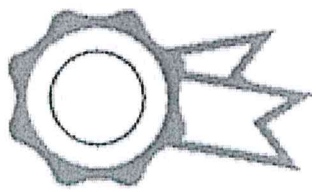

Course coordinator




Principal
Aditya College of Pharmacy
SURAMPALAM-533 437



Sample



CERTIFICATE OF COMPLETION



This is to certify that Mr./Ms.

bearing roll number _____ has successfully
completed the certificate course entitled
“Molecular Docking Studies Using Autodock Vina Software”
held in Aditya College of Pharmacy, Surampalem
from 07th November to 12th December, 2020

N. Saha Dasgupta
Chairman

N. Subudhakar Dasgupta

Vice-Chairman

PRINCIPAL
Aditya College of Pharmacy
SURAMPALAM-533 437

K. Venkateshwar

Director & Principal

