Aurora's Degree & PG College

(Accredited by NAAC with 'B++' grade)
Chikkadpally, Hyderabad- 500020
Department of Genetics

EVENT REPORT

NAME OF THE EVENT	Workshop on Molecular docking and Protein visualization
TYPE OF EVENT	Department
FACULTY INCHARGE	P Sangha Mokshavi
DEPARTMENT	Genetics
DATE	29 – 31 May, 2020
VENUE	Google Meet
TARGET AUDIENCE	Life science students, faculty & research scholars

OBJECTIVE:

In view of the current research need the workshop is intended to learn the underlying principles behind molecular interactions of various proteins.

BRIEF ABOUT THE EVENT:

Molecular Docking is a well-established computational technique which predicts the interaction energy between two molecules. This technique mainly incorporates algorithms like molecular dynamics, Monte Carlo stimulation, fragment-based search methods. Molecular docking studies are used to determine the interaction of two molecules and to find the best orientation of ligand which would form a complex with overall minimum energy.

In view of the current research need and adaptable methods that can used without moving place to place, bioinformatics takes its highest place in learning. The event was split into 3 days for 3hours per day. Each day was taken up with 2 to 3 tasks to be done for the following steps next

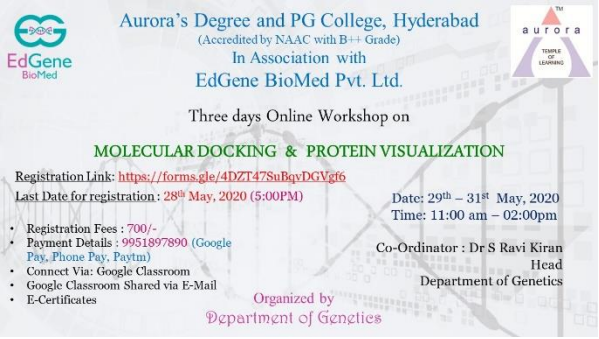
day. The company assigned a trainee who first gave the basics of bioinformatics followed by the ground terminology that is used for the docking process.

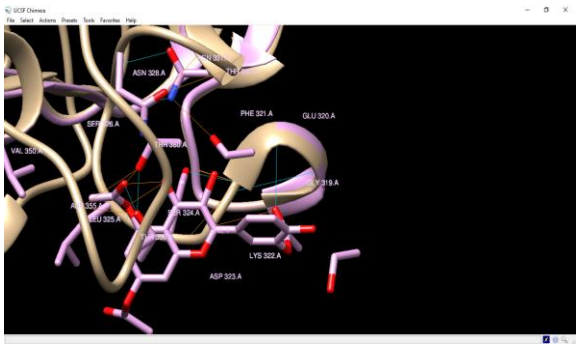
The method employed was ligand – protein docking. The first step starts with preparing the structure of the Ligand using the software ChemSketch tool. These prepared ligand molecules are stored in. mol format. These ligands are further converted to PDB format using Open Babble tool. Protein of interest is further downloaded from Protein Data Bank in PDB format. The edit of protein molecules to trim the heteroatoms is followed by SPDV.exe software. Once the ligand and molecule are placed into PDB format Docking is done by using AutoDock tools followed by AutoGrid where Ligand and Protein are docked for understanding the interactions. The last step is done with Chimera tool where a protein along with ligand is pictorially represented where active site binding is checked followed by analysing toxicity.

OUTCOME:

Participants have been trained on how molecules interact by docking protein and ligand. These techniques help us to do rapid progress on effective drug screening and mechanisms behind it.

PHOTOGRAPHS:



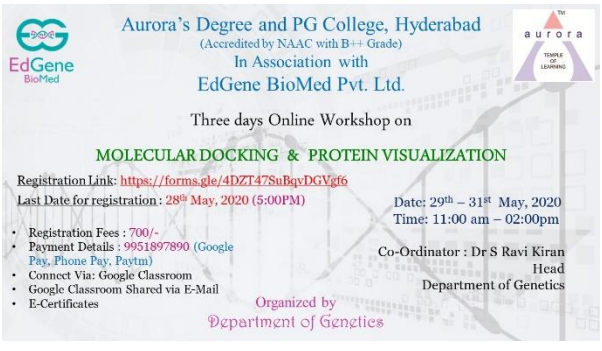


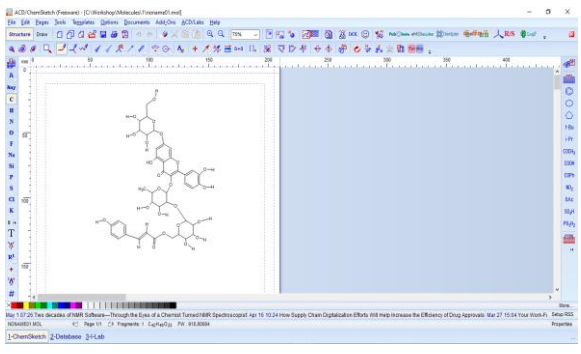
DETAILED REPORT:

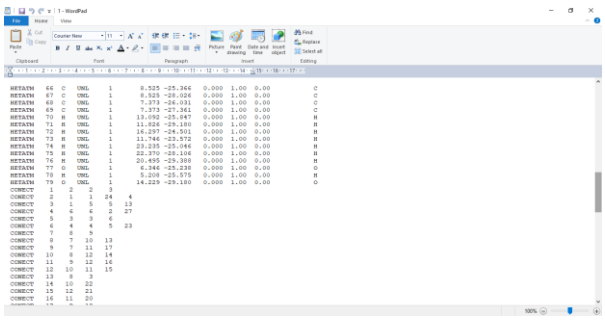
LIST OF PARTICIPANTS:

Name	College Name
P S S Ashwin kumar	Aurora's Degree and PG College
Ms. S VANITHA	Bhavan's Vivekananda College of Science, Humanities and Commerceommerce
Metla sai pavan kalyan	AURORA DEGREE AND PG COLLEGE
Marri Sandeep	Osmania University
Vishnu Prasad Nair R U	University of Hyderabad
Sangha Mokshavi Peddibhotla	Aurora Degree and PG College
Chandravamshi Kulakarni	Aurora degree and pg College
Krishnendhu Mavila	Jss academy of higher education and research , Mysore
Sree varshini	IISER Tirupathi
Pooja V Chandran	BITS Pilani,Hyderabad Campus
Neha Jahan	Aurora’s Degree and PG College
Gayathri Madishetty	Aurora’s Degree and PG College
V.Rohini	Government Degree college for women, Begumpet
M.Emmnauel Raj	Central University of Tamilnadu
Akhila Patlori	Aurora's Degree & PG College
Apoorva Namburi	Central University of Tamil Nadu

PHOTOGRAPHS:







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