Centurion University
Shaping Lives... Empowering Communities...

Drug Research Using Biovia

Event Description: Drug Research using BIOVIA, webinar was organized on the year of 2017-18. By Centurion University of Technology and Management, It Gives idea about prediction of drugs by molecular docking,

Course Objectives:

- To know about the tools of discovery studio Biovia software
- Ligand-protein interaction
- Drug designing

Learning Outcomes:

- Prediction of drug by molecular docking
- Pharmacophore modelling
- Publication/product

Pre-requisites: Nil
Course Type : Audit (Workshop)
Duration : 30 Hours

Module	Contents	Duration
Module1	• Discovery of phytochemicals as potential drug substitute • Practice: Use of discovery studio for drug design • Practice: Phytochemicals present in a particular plant and download its molfile • Practice: Identification of enzyme molecules of a microbe using Brenda enzyme database • Practice: Downloads PDB file of different enzymes • Practice: Study of different parts of an enzyme molecule in a molecular window. • Practice: Liganeprotein molecular docking.	10 hours
Module2	• Identification of pharmacophore (Automatic/Manually) • Practice: Automatic identification of structural feature of a pharmacophore • Practice: Identification of a pharmacophore manually • Practice: ADMET and Toxicity report analysis of a drug molecule.	10 hours
Module3	• Functionalization of a molecule and study its potential as a drug • Practice:Forcefieldof a protein molecule using simulation. • Identification of a specific phytochemical for a disease. • Identification of a chemical drug based on structural similarity with a phytochemical for a specific disease.	10 hours
	TOTAL	**30 hours**

Convenor

Dr. Anita Patra, Registrar, CUTM

Name of the event:

Drug Research using Biovia

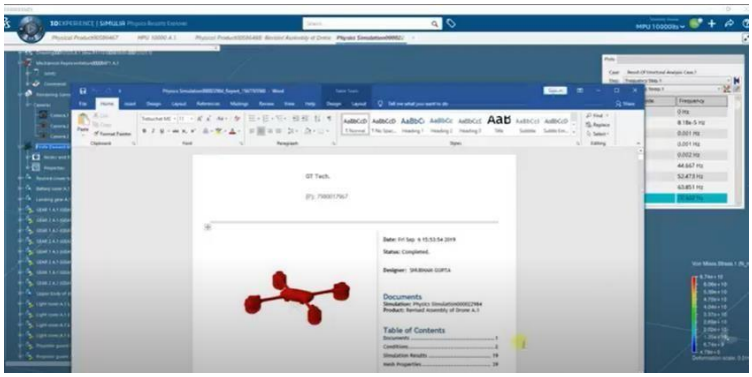
Total number of

participants: 53

Date: 17/03/2018

Computer-Aided drug design accelerates and economizes drug discovery and drug manufacturing processes; it is considered an effective strategy. With the significant rise in the availability of information on small molecule and biological macromolecule, the efficiency of computer-aided drug discovery has been enhanced and is being extensively applied to almost every phase in drug discovery and manufacturing activities such as detecting targets, validation, lead discovery, and optimization & preclinical tests. Since the last few years, substantial developments have been observed in computer-aided drug discovery techniques including molecular similarity calculation, de novo design, pharmacophore modelling and mapping, molecular docking, and sequence-based virtual screening, etc. Industries and also Government laboratories and Research centers are utilizing ampoule funding after computer-aided drug discovery.

The programme intended to find out the tools of discovery studio Biovia software, ligand-protein interaction and drug designing.



Basics of Drug Designing on 17.03.2018

Main objective of this programme is

- To know about the tools of discovery studio Biovia software
- Ligand-protein interaction

• Drug designing and Prediction of drug by molecular docking

• Pharmacophore modelling

• Publication/product

The learners were made familiarize with the following key aspects

- Prediction of drug by molecular docking
- Pharmacophore modelling
- Publication/product

The followings were the major concepts discussed in the programme:

1. Discovery of phytochemicals as potential drug substitute
2. Identification of pharmacophore (Automatic/Manually)
3. Functionalization of a molecule and study its potential as a drug

Through this programme participants would learnt about:

- Biovia Tools and their application in drug discovery processes.
- Identify potential biological molecules from synthetic and natural sources by using Biovia.
- Recognize and comprehend various disease targets and select an ideal target for drug discovery.
- Design novel drug candidates for various diseases by using Biovia Discovery Studio.
- Repurpose the already existing drugs for safe and effective medication for various diseases.

Convenor

Dr. Anita Patra, Registrar, CUTM

Name of Event: Drug Research Using Biovia
Organized by: Centurion University of Technology and Management
Date: 17 March 2018

Event Description: Drug Research using BIOVIA, webinar was organized in the year of 2017-18. By Centurion University of Technology and Management, It Gives idea about prediction of drugs by molecular docking.

List of Participants:

S. No.	Name	Reg. No.	Presence/Absent
1	DIGVIJAY BEHERA	170101120001	Present
2	YEDLA DEEPIKA	170101120002	Present
3	DEBASIS PADHY	170101120003	Present
4	ANKADALA KARUNAKAR	170101120004	Present
5	VALLA PRIYANKA	170101120005	Present
6	REVALLA VIDYA SRI	170101120006	Present
7	DIBYA SAMBIT SAHU	170101120007	Present
8	SEPHALI PANDA	170101120011	Present
9	SOUMYA DEEPTO DASH	170101120012	Present
10	YALALA SANDEEP KUMAR	170101120013	Absent
11	M. SAI SPANDANA	170101120014	Present
12	SIRIPURAM LAKSHMI PRASANNA	170101120015	Present
13	CHIKATI DIVYA TEJA	170101120016	Present
14	T. GREESHMA	170101120017	Present
15	VOONA SRIJA	170101120019	Present
16	P. HARSHAVARDHAN	170101120020	Present
17	PRANAY RAJ	170101120021	Present
18	BADAL CHOUDHURY	170101120022	Present
19	G. PAVAN KALYAN	170101120023	Present
20	MONALISA PRADHAN	170101120024	Present
21	SAASWAT PANIGRAHI	170101120025	Present
22	KOTTURU SAI	170101120026	Present
23	ROUTHU DIVYA	170101120028	Present
24	POREDDI PRIYANKA	170101120029	Present
25	METTA DEVENDRA PRASAD	170101120030	Present
26	ALIBILLI MAHESH	170101120032	Present

27	AYUSHI MISHRA	170101120034	Present
28	DEVARACHETTY SRIYA	170101120035	Present
29	POTNURU MANIKANTA	170101120036	Present
30	KILLAMSETTY PRAVEENA	170101120038	Present
31	TULUGU RAHUL	170101120039	Present
32	DARAPU ABHISHEK	170101120040	Present
33	HRUDANAND NIAL	170101120041	Present
34	DAYA SHANKAR ROUT	170101120043	Present
35	VYSYA RAJU SAI SIRISHA	170101120044	Present
36	ROUTH KARTHIK	170101120045	Present
37	AMOSH KHURA	170101120046	Present
38	ROSHAN KAJUR	170101120047	Present
39	MAJJI REENA	170101120048	Present
40	B.NAGA SATISH KUMAR REDDY	170101120049	Present
41	LAKSHMI NARAYANA MANUKONDA	170101120050	Present
42	ANDHAVARAPU ANUSHA	170101120051	Present
43	PINTU KARJEE	170101120052	Present
44	DHARAM NISHAN MISHAL	170101120053	Present
45	AYUBA BHUYAN	170101120054	Present
46	GONDRU KIRAN KUMAR	170101120055	Present
47	SANJANA SINGH	170101120056	Present
48	PREETI PADMA PATRO	170101120057	Present
49	PADALA VENKATESH	170101120058	Present
50	SAROJ KUMAR NAYAK	170101120059	Absent
51	KALAMATA AVINASH	170101120060	Present
52	EPPILI CHATRAPATHI	170101120061	Present
53	BOMMALI VARA PRASAD	170101120062	Present

Convenor

Dr. Anita Patra, Registrar, CUTM