

Organized by
Department of Pharmaceutical Chemistry,
JSS College of Pharmacy, Ooty

A Brief Report

AICTE Sponsored, One week Short Term Training Programme (STTP) on “**Recent advances in Drug Discovery, Development and Lead Optimization**” was conducted by virtual mode in three modules organized by Department of Pharmaceutical chemistry, JSS College of Pharmacy, Ooty.

Course duration: One week

Online Module-I (10-08-2020 to 15-08-2020)

Online Module-II (07-09-2020 to 12-09-2020)

Online Module-III (05-10-2020 to 10-10-2020)

Course Timings: 10.00 AM to 1.00 PM & 2.00 PM to 5.00 PM

The **First module** of the programme was inaugurated on **10-08-2020 at 10 pm** by **Dr. S.P. Dhanabal**, Principal, JSSCP, Ooty and **Dr. R. Kalirajan**, Asst. Professor and coordinator of STTP delivered the welcome address. **Dr. Md. Afzal Azam**, Professor & Head highlighted the importance of computational chemistry tools in modern day to day research and explain about the programme. **Dr. R. Raghu**, Vice President, Schrodinger LLC, Bengaluru briefed about the importance of computational tools in the modern drug discovery. **Col B Venkat, Director, (Faculty Development Cell), AICTE, New Delhi** also participated in the inaugural function through virtual mode.

The external experts from various reputed organizations such as **Mr. Surojit Sadhu**, Advent Informatics, Pune, **Dr. Girinath Pillai**, Zastra Innovations, Bengaluru, **Dr. P. Bharathidasan**, Chief Technical Manager Bio Pharma Labs, Hyderabad **Dr. Karthikeyan M**, Senior scientist,

National Chemical Laboratory, Pune **Dr. N. Ayyadurai**, Senior Scientist, Biotechnology Division, Central Leather Research Institute, Chennai and **Dr. S. Murugesan**, Associate Professor, BITS, Pilani, are given lectures and demo on various computational tools. As per schedule, the department of pharmaceutical chemistry faculties are moderate and introduce each resource person. Also some of our internal resource persons also delivered lectures on various topics.

About 40 delegates (faculties) from various parts of India were selected from 100 applications received for the I-module. The delegates attended all the lectures from 10 am to 01 pm in the forenoon session and 2-5 pm in the afternoon session. The feedback about all the lectures and demo presentation was collected on daily basis and was highly appreciated by all delegates.

At the last day (15-08-2020) of the module-I, the online assessment was conducted by posting the questions delegates from all the lecture topics. The E-certificates were issued to all the delegates and resource persons. At the end of module-I, in the valedictory, **Dr. Afzal Azam**, Head of the department was consolidated about programme and feedback was given by some of the delegates. **Dr. R. Kalirajan**, coordinator of STTP delivered the vote of thanks.

Some snapshots for STTP I-Module

The screenshot shows a Zoom meeting interface. The main content is a slide titled "P450 Regioselectivity" featuring a chemical structure of a complex molecule with various carbon atoms labeled. The following table summarizes the regioselectivity data shown on the slide:

Label	Percentage
C2	91%
C1, C3	1%
C7	2%
C10, C12	0%
N11	0%
N8	4%
C9, C13	0%
C19	0%
C24	3%
C25, C26	0%
C23	0%

Text on the slide:

- These results show **where** a molecule is likely to be metabolised **if** it is a substrate
- Regioselectivity can be calculated CYP3A4, CYP2D6, CYP2C9, CYP2C19, CYP2C8, CYP1A2, CYP2E1

At the bottom of the slide, it says "Zastra 11/09/20 11:42 AM Girinath, Zastra Innovations 2017 Slide 62 of 58".

The Zoom interface includes a video feed of a participant (Girinath Pillai), a list of other participants (RAJKUMAR.S, Jayanthi koppula), and a toolbar with options like Unmute, Stop Video, Security, Participants (25), Polls, Chat, Share Screen, Record, Support, Reactions, More, and End.

Instant JChem 20.15.0

File Edit View Search Data Lists Chemistry Tools Window Help

45671872318

7/94

Form view for approved 2 Grid view for approved Charts and Analysis Grid view for approved

Design Query Browse Code

Structure, Mol Weight

Structure, Mol Weight

1

2

Mol Weight 445.4

3

Mol Weight 749.0

4

Mol Weight 475.5

00:42:38

00:43:32

The screenshot shows the JChem 20.15.0 software interface. On the left, there is a 'Projects' pane with 'approved' selected, showing a list of queries and lists. The main area contains a grid of four scatter plots: 1) Mol Weight vs JCHEM_REFRACTIVITY, 2) ALDOPS_LOOP vs ALDOPS_LOOP, 3) JCHEM_NUMBER_OF_RINGS vs JCHEM_NUMBER_OF_RINGS, and 4) JCHEM_PWA_STRONGEST_BASIC vs JCHEM_PWA_STRONGEST_BASIC. On the right, a 'Structure, Mol Weight' list shows four chemical structures with their respective molecular weights: 445.4, 749.0, and 475.5. The bottom of the window shows a Windows taskbar with various icons and a system tray.

Role of Chemoinformatics in Drug Discovery

M Karthikeyan
Principal Scientist

CSIR-National Chemical Laboratory

Gmail
karthincl

<http://moltable.ncl.res.in>
+91-9767427981

8/14/2020

02:09:45

The slide features a blue and white header with the CSIR logo. The main title is 'Role of Chemoinformatics in Drug Discovery'. Below the title, there is a red circle with a diagonal slash over a monkey sitting on a laboratory bench, symbolizing the replacement of animal testing by computational methods. The presenter's name and title are listed: M Karthikeyan, Principal Scientist, CSIR-National Chemical Laboratory. Contact information is provided: Gmail (karthincl), website (http://moltable.ncl.res.in), and phone number (+91-9767427981). The date 8/14/2020 is shown in the bottom left, and the time 02:09:45 is in the bottom right. A cartoon illustration of a robot sitting at a desk with a computer monitor displaying a grid of colored squares is also present.

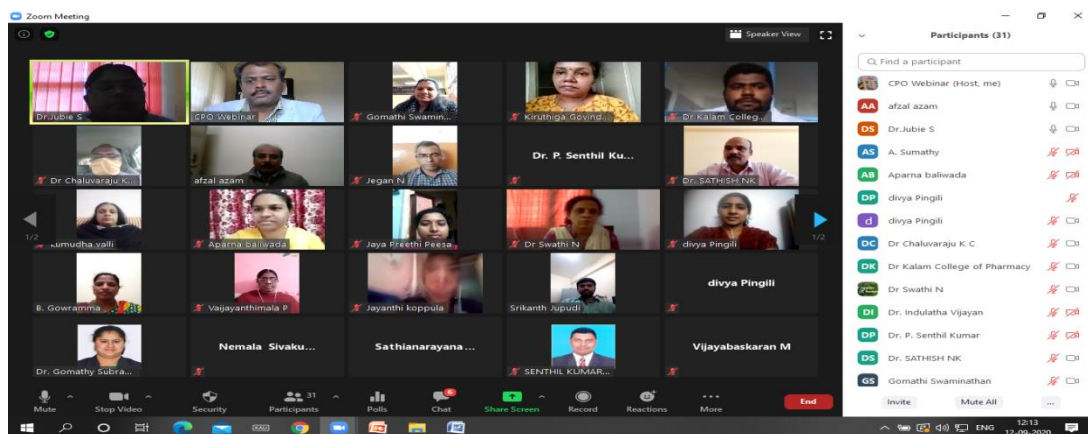
The **Second module** of the programme was inaugurated on **07-09-2020 at 10 pm** by **Dr. S.P. Dhanabal**, Principal, JSSCP, Ooty and explain the highlights of the college. **Dr. R. Kalirajan**, Asst. Professor and coordinator of STTP delivered the welcome address. **Dr. Md. Afzal Azam**, Professor & Head highlighted the importance of computational tools.

The external experts from various reputed organizations such as **Ravikumar Muttenini and Dr. Kranthi raj** from Immunocure, **Dr. Pritesh Bhat, Dr. Sudarsan, Dr. Prajwal Nandekar, Mr. Vinod Devaraji**, Senior Scientist - Applications, Schrodinger LLC., Bengaluru, **Dr. Girinath Pillai**, Zastra Innovations, Bengaluru, **Dr. Dhivya Shanmugam**, from Altem Technologies (P), Ltd, Bengaluru, and **Dr. S. Murugesan**, Associate Professor, BITS, Pilani, are given lectures and demo on various computational tools. As per schedule, the department of pharmaceutical chemistry faculties are moderate and introduce each resource person. Also some of our internal resource persons also delivered lecture on various topics.

About 40 delegates (faculties) from various parts of India are selected from the applications received for the II-module. Delegates attended all lectures from 10 am to 01 pm in the forenoon session and 2-5 pm afternoon session. The feedback about all the lectures and demo was collected on daily basis and was highly appreciated by all delegates.

At the last day (12-09-2020) of the module-II, the online assessment was conducted by posting questionnaires to all delegates from all the lecture topics. The E-certificates are issued to all delegates and resource persons. At the end of module-II, in the valedictory, **Dr. Afzal Azam**, Head of the department was consolidated about the programme, feedback was given by some delegates. **Dr. R. Kalirajan**, coordinator of STTP delivered the vote of thanks.

Some snapshots for STTP II-Module



Zoom Meeting You are viewing Sudharsan Pandiyar's screen View Options

Recording... Participants (35)

Find a participant

CPO Webinar (Host, me) Sudharsan Pandiyar A. Sumathy Aparna Baliwada bodhya sri vullisi divya Pingili Dr Chaluvaraju K C Dr N Swathi Dr T Durai Ananda Kumar Dr. Indulatha Vijayan Dr. SATHISH NK Hariram Singh Jaya Preethi Peesa, Tirupati Jayanthi koppula

Workflow for a Jaguar DFT calculation

Draw 3D Structure

Specify Basis Set
6-31G**, cc-pVTZ, ...

Specify Functional
B3LYP-MM, M06-2X-D3, PW6B95-D3, ...

Specify calculation type
Single point, optimization, torsional scan, ...

Solve Schrödinger Equation
 $\hat{H}\phi = E\phi$

Solve self consistent field (SCF) equations iteratively to obtain energy and wave function

Compute and print desired properties

Use wavefunction to obtain densities, atomic charges, orbitals, ...

Specify desired properties
ESP charges, surfaces, orbitals, ...

Specify other options
Print level, numerical accuracy, ...

SCHRÖDINGER. MATERIALS NOT FOR PUBLIC DISTRIBUTION 11

Unmute Stop Video Security Participants 35 Polls Chat Share Screen Reactions More End

Windows taskbar: 12:34 08-09-2020

You are viewing Prajwal Nandekar's screen View Options

Stop Video Participants Stop Share Please Share Remote Control More

You are screen sharing Stop Share

CPO Webinar Prajwal Nandekar Dr. Gomathy Subra... Koushik

SCHRÖDINGER.

Molecular Dynamics
Applications in Drug Discovery

Prajwal Nandekar, Ph.D
Sr. Scientist, Schrödinger Inc. Bangalore

prajwal@schrodinger.com
Mobile: 9900090033

Mute Stop Video Security Participants 28 Polls Chat Share Screen Record Support Reactions More End

The **Third module** of the programme was inaugurated on **05-10-2020 at 10 pm** by **Dr. S.P. Dhanabal**, Principal, JSSCP, Ooty and explain the highlights of the college. **Dr. R. Kalirajan**, Asst. Professor and coordinator of STTP delivered the welcome address. **Dr. Md. Afzal Azam**, Professor & Head highlighted the importance of computational tools.

The external experts from various reputed organizations such as **Ravikumar Muttenini and Dr. Kranthi raj** from Immunocure, **Dr. Girinath Pillai** , Zastra Innovations, Bengaluru, **Mr. Surojit Sadhu**, Advent Informatics, Pune, **Dr. Karthikeyan M**, Senior scientist, National Chemical Laboratory, Pune **Dr. Dhivya Shanmugam**, from Altem Technologies (P), Ltd, Bengaluru, and **Dr. P. K. Krishnan Namboori**, CEO, Biopharma solutions, are given lectures and demo on various computational tools. As per schedule, the department of pharmaceutical chemistry faculties are moderate and introduce each resource person. Also some of our internal resource persons also delivered lecture on various topics.

About 40 delegates (faculties) from various parts of India are selected from the applications received for the III-module. The delegates attended all lectures from 10 am to 01 pm in the forenoon session and 2-5 pm in the afternoon session. The feedback about all the lectures and demo was collected on daily basis and was highly appreciated by all delegates.

At the last day (**10-10-2020**) of the module-III, the online assessment was conducted by posting questionnaires to delegates from all the lecture topics. The E-certificates are issued to all the delegates and resource persons. At the end of module-III, in the valedictory, **Dr. Afzal Azam**, Head of the department was consolidated about programme and feedback was given by some delegates. **Dr. R. Kalirajan**, coordinator of STTP delivered the vote of thanks.

Some snapshots for STTP II-Module



Recording... You are viewing 1760511 MADHAVA M.'s screen View Options

What does Immunocure Do?

Immunocure is a CRO, discovering small molecules and formulations employing AI & CADD technologies for our clients

Established in 2019

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Participants: 28

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Participants: Dhanabalan, CPO Webinar, 1760511 MADH..., Dr. Aneeesh T.P., Deepa Mandlik, Chiranjeevi Pon...

Recording... PenAttention

PenAttention

Mouse Pointer Highlighter

Free Windows program that displays a highlight the pencil or pointer at the location of the pen

How to....

- ★ Download and Install
- ★ Click on system tray
- ★ Select highlight pen and mouse option

PenAttention 10

Highlight Settings

Quantity: 1, Color: Yellow, Radius: 1, Width: 1, Height: 1, Display Scaling Factor: Auto-detect

Preview

Radius: 10, Width: 50, Height: 50

This is sample text
This is sample text
This is sample text
This is sample text
This is sample text

Highlight mouse as well as pen
Hotkey Highlight Toggle: ON, CTRL + F9, CTRL + ALT + F9

chenniah.jayakumar

Mute Stop Video Security Participants Polls Chat Share Screen Pause/Stop Recording Support Reactions More End

Participants: CPO Webinar, Dr. Zaranappa, Dr. Aneeesh T.P.

Herewith we take this opportunity to thank, **All India Council for Technical Education**, New Delhi for financial support under STTP scheme, especially **Col B Venkat**, Director (Faculty Development), AICTE, NewDelhi for supporting us for successful organizing of this STTP programme.

We also thank the Honorable Chancellor **His Holiness Jagadguru Sri Shivarathri Deshikendra Mahaswamijigalavuru**, Honorable Pro chancellor **Dr. B. Suresh**, Honorable Vice chancellor **Dr. Surinder Singh.**, Registrar **Dr. B. Manjunatha**, JSS Academy of Higher Education Research, Mysuru and especially chief information officer **Dr. Ravindra** and his team for their IT support for the smooth conduct of this STTP through ZOOM platform.

Our heartily thanks to **Dr. S. P. Dhanabal**. Principal, **Mr. C.Jayakumar**, Asst. prof and all our colleagues from JSS College of Pharmacy, Ooty for their kind support to organize the Short Term Training programme successfully.

Last but not least, our heartily thanks to all the resource persons from various reputed organizations and delegates who are all joined from various states of our country for Scientific learning.

Thanking You

Dr. R. Kalirajan

(Co-ordinator, STTP)

Dr. Md. Afzal Azam

(Head, Department of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty)

Encl – Programme schedules with topics for all three modules of STTP and Brochure



**AICTE Sponsored, One week
Short Term Training Programme (STTP) on
Recent advances in Drug Discovery,
Development and Lead Optimization
[Online Module-1]**



JSS College of Pharmacy, Ooty, Tamilnadu

Programme Schedule

Date	Time	Resource Person	Topic
10-08-2020 Monday	10.00 - 10.30 am	Inauguration	
	10-30 am – 01.00pm	Mr. Surojit Sadhu Advent Informatics +91 9833050178 surojit@adventinformatics.com	Use of Chem Axon tools in Drug Discovery
	02.00 – 3.00 pm	Dr. Asish D Wadhvani, Asst. Professor & Head Dept. of Pharmaceutical Biotechnology, JSS College of Pharmacy, Ooty	<i>In Vitro</i> cell culture models for high-throughput drug screening and toxicity
	03.00 – 4.00 pm	Dr. Md. Afzal Azam, Professor & Head Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Binding more Investigations by Molecular dynamics
	04.00 – 5.00 pm	Dr. R. Vadivelan, Professor Dept. of Pharmacology, JSS College of Pharmacy, Ooty	Ethical Guidelines In Preclinical Testing: Key Perspectives
11-08-2020 Tuesday	10.00 am – 01.00pm	Mr. Surojit Sadhu Advent Informatics +91 9833050178 surojit@adventinformatics.com	Use of ChemAxon tools in Drug Discovery – Software demo
	2.00 pm – 3.00 pm	Dr. Praveen T K, Professor & Head Dept. of Pharmacology, JSS College of Pharmacy, Ooty	Animal Testing: History and alternative methods
	3.00 pm – 4.00 pm	Dr. B. Gowamma, Asst. Professor Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Basics of chiral separation
	4.00 pm – 5.00 pm	Dr. MJN. Chandrasekar Professor & Coordinator School of Life Sciences, Ooty campus JSS Academy of Higher Education & Research,	Understanding Proposal Writing For Grants
12-08-2020 Wednesday	10.00 am – 11.30 am	Dr. Girinath Pillai, Chief Scientific Officer Zastra Innovations, Bengaluru, gpillai@zastrain.com 9448367493, 9995981141	Role of ADME/Toxicity in the Drug Candidate Selection using Multi Parameter Optimization
	11-30 am – 01.00 pm	Dr. Suresh Mohan Kumar Professor & Research Director Dept. of Pharmacognosy, JSS College of Pharmacy, Ooty	Vocal for Herbal: Drug Discovery Approaches for Innovative & Society Impacting Healthcare Solutions

	02.00 – 03.00 pm	Dr. S. Jubie , Asst. Professor Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Fatty acids and their analogues as anticancer agents
	03.00 – 04.00 pm	Dr. B. Babu , Lecturer Dept. of Pharmaceutical Analysis, JSS College of Pharmacy, Ooty	LC-MS/MS - "An Hyphenated tool in Identification and Characterization of Synthesized Small molecules"
	04.00 – 5.00 pm	Dr. Gomathy Subramaniyan Asst. Professor Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Activation of SIRT-3 enzyme in Neurological disorders
13-08-2020 Thursday	10.00 am – 01.00 pm	Dr. Girinath Pillai , Zastra Innovations, Bengaluru, gpillai@zastrain.com 9448367493, 9995981141	Role of ADME/Toxicity in the Drug Candidate Selection using Multi Parameter Optimization – Software Demo
	02.00 – 03.00 pm	Mr. C. Jayakumar Asst. Professor & IT Coordinator JSS College of Pharmacy, Ooty	Digital tools for Effective Presentation : A Demonstration
	03.00 – 04.00 pm	Dr. P. Bharathidasan Chief Technical Manager Bio Pharma Labs, Hyderabad	An Update on Recent Research & Developments on Natural products
	04.00 – 5.00 pm	Dr. Kalirajan Rajagopal Asst. Professor Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	COVID19 activity of Phytochemical constituents of some Natural Remedies : A computational approach
14-08-2020 Friday	10.00 am – 01.00 pm	Dr. Karthikeyan M , National Chemical Laboratory, Pune Cell- 9767427981 karthincl@gmail.com	Free online Chem informatics tools-lecture and Demo
	2.00 – 5.00 pm		
15-08-2020 Saturday	10.00 - 11.30 am	Dr. N.Ayyadurai , Senior Scientist, Biotech division Central Leather Research Institute, Chennai ayyadurai@clri.res.in 9566715100	Next Generation Target Missiles for Cancer Prepared By Expanding the Genetic Code
	11-30 am – 01.00 pm	Dr. S. Murugesan , Associate Professor BITS, Pilani murugesan@pilani.bits-pilani.ac.in 9413489684	Identification of potential SARS-CoV-2 inhibitors from natural product databases using CADD techniques
	02.00 – 4.00 pm	Valedictory & Online Assessment	

For all sessions Join Zoom Meeting with following link

<https://us02web.zoom.us/j/84396261831> [Meeting ID: 843 9626 1831]

For Any Queries Kindly contact

Dr. R. Kalirajan

Co-ordinator –STTP, JSS College of Pharmacy, Ooty, Tamilnadu

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**AICTE Sponsored, One week
Short Term Training Programme (STTP) on
Recent advances in Drug Discovery, Development
and Lead Optimization
[Online Module-II]
JSS College of Pharmacy, Ooty, Tamilnadu**



Programme Schedule

Date	Time	Resource Person	Topic
07-09-2020 Monday	10.00 - 10.30 am	Inauguration	
	10-30 am – 01.00pm	Ravikumar Muttanini Immunocure ravi@immunocure.us 8722160669	Computer Aided Drug Designing Techniques from Hit Identification to Lead Optimization (Lecture & Demo)
	02.00 – 5.00 pm	Dr. Kranthi Raj Immunocure raj@immunocure.us	Computer Aided Drug Designing Techniques from Hit Identification to Lead Optimization (Lecture & Demo)
08-09-2020 Tuesday	10.00 am – 12.00noon	Dr. Pritesh Bhat, <i>Senior scientist,</i> Schrödinger LLC, Bengaluru pritesh.bhat@schrodinger.com	Advances in Computational Structure-Based Drug Design Methods
	12.00Noon – 1.00 PM	Dr. Sudharsan Pandiyan <i>Senior scientist,</i> Schrödinger LLC, Bengaluru sudharsan.pandiyan@schrodinger.com	Quantum mechanics in computational drug discovery
	2.00 pm – 5.00 pm	Dr. Md. Afzal Azam, Professor & Head Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Molecular docking Vs Molecular dynamics simulation - analysis of MD trajectory
09-09-2020 Wednesday	10.00 am– 12.00noon	Dr Prajwal Nadekar <i>Senior scientist,</i> Schrödinger LLC, Bengaluru prajwal.nandekar@schrodinger.com	Molecular Dynamics Simulations: Applications in Drug Discovery
	12.00Noon – 1.00 PM	Dr. B. R. Prasanthkumar JSS College of Pharmacy, Mysuru	CoMFA and CoMSIA a 3D QSAR Techniques: A 40 years old but still promising
	02.00 – 03.00 pm	Dr. S. Jubie Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Fatty acids and their analogues as anticancer agents
	03.00 – 04.00 pm	Mr. Jayakumar C JSS College of Pharmacy, Ooty	Digital tools for Effective Presentation : A Demonstration
	04.00 – 5.00 pm	Dr. Justin A Dept. of Pharmacology, JSS College of Pharmacy, Ooty	Glitazones show neuroprotection by PGC-1 α signalling activation via PPAR- γ agonism: A fleeting look at the promising <i>in silico</i> hypothesis

10-09-2020 Thursday	10.00 am – 12.00noon	Mr Vinod Devaraji <i>Senior scientist,</i> Schrödinger LLC, Bengaluru Vinod.Devaraji@schrodinger.com	Hit or Lead Optimization of small molecules using 3D QSAR for screening small molecule derivatives.
	12.00Noon – 1.00 PM	Dr. Srikanth Jupudi Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Introduction to different docking techniques and demo on free docking and molecular dynamics tools- “PyRx and GROMACS”
	02.00 – 03.00 pm	Dr. Asish D Wadhvani Asst. Professor & Head Dept. of Pharm. Biotechnology, JSS College of Pharmacy, Ooty	<i>In Vitro</i> cell culture models for high-throughput drug screening and toxicity
	03.00 – 5.00 pm	Dr. S. Murugesan, Associate Professor, BITS, Pilani murugesan@pilani.bits-pilani.ac.in 9413489684	Identification of potential SARS-CoV-2 inhibitors from natural product databases using CADD techniques
11-09-2020 Friday	10.00 am – 1.00 PM	Dr. Girinath Pillai, Zastra Innovations, Bengaluru, gpillai@zastrain.com 9448367493, 9995981141	Role of ADME/Toxicity in the Drug Candidate Selection using Multi Parameter Optimization
	2.00 – 3.00 pm	Dr. B. Gowramma Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Basics of chiral separation
	3.00 – 4.00 pm	Dr. Gomathi Swaminathan Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	New Perspectives on Outstanding Role of Traditional Medicines For Modern Therapeutics
	4.00 – 5.00 pm	Dr. Kalirajan Rajagopal Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	COVID19 activity of Phytochemical constituents of some Natural Remedies : A computational approach
12-09-2020 Saturday	10.00 am - 12.00noon	Dhivya shanmugarajan Application Scientist (Accylyr’s) Altem Technologies (P) Ltd, Bengaluru dhivya.shanmugarajan@altem.com 9003288384	Unravelling the utility of Structure-based pharmacophore mapping for lead optimization – “New Advances in Drug Discovery “
	12.00noon– 01.00 pm	Dr. S.P. Dhanabal Principal, JSSCP, Ooty	Natural products in drug discovery
	02.00 – 4.00 pm	Valedictory & Online Assessment	

For all sessions Join Zoom Meeting with following link

<https://us02web.zoom.us/j/89945708424>

For Any Queries Kindly contact

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[Online Module-III]**

JSS College of Pharmacy, Ooty, Tamilnadu



Programme Schedule

Date	Time	Resource Person	Topic
05-10-2020 Monday	10.00 - 10.15 am	Inauguration	
	10-15 am – 01.1pm	Ravikumar Muttineni Immunocure ravi@immunocure.us 8722160669	Computer Aided Drug Designing Techniques from Hit Identification to Lead Optimization (Lecture & Demo)
	02.00 – 03.00 pm	Dr. Anand Vijayakumar Dept. of Pharmacology, JSS College of Pharmacy, Ooty	Clinical trial protocol development
	03.00 – 04.00 pm	Dr. S. Jubie Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Fatty acids and their analogues as anticancer agents
	04.00 – 05.00 pm	Dr. Srikanth Jupudi Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Introduction to different docking techniques and demo on free docking and molecular dynamics tools- “PyRx and GROMACS”
06-10-2020 Tuesday	10-00 am – 01.00pm	Ravikumar Muttineni Immunocure ravi@immunocure.us 8722160669	Computer Aided Drug Designing Techniques from Hit Identification to Lead Optimization (Lecture & Demo)
	2.00 pm – 5.00 pm	Dr. Girinath Pillai, Zastra Innovations, Bengaluru, gpillai@zastrain.com 9448367493, 9995981141	Role of ADME/Toxicity in the Drug Candidate Selection using Multi Parameter Optimization
07-10-2020 Wednesday	10.00 am – 1.00 PM	Surojit Sadhu, Advent Informatics +91 9833050178 surojit@adventinformatics.com	Use of Chem Axon tools in Drug Discovery
	02.00 – 03.00 pm	Mr. Jayakumar C JSS College of Pharmacy, Ooty	Digital tools for Effective Presentation : A Demonstration
	03.00 – 04.00 pm	Dr. Gomathi Swaminathan Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	New Perspectives on Outstanding Role of Traditional Medicines For Modern Therapeutics
	04.00 – 5.00 pm	Dr. Kalirajan Rajagopal Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	COVID19 activity of Phytochemical constituents of some Natural Remedies : A computational approach

08-10-2020 Thursday	10.00 am – 01.00pm	Dr. Karthikeyan M , National Chemical Laboratory, Pune Cell- 9767427981 karthincl@gmail.com	Free online Chem informatics tools- lecture and Demo
	02.00 – 5.00 pm		
09-10-2020 Friday	10.00 am – 12.00 noon	Dr. Md. Afzal Azam Professor & Head Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Molecular docking Vs Molecular dynamics simulation - analysis of MD trajectory
	12.00noon – 01.00 pm	Dr. B. Gowramma Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Basics of chiral separation
	02.00 – 04.00 pm	Dr. P.K.Krishnan Namboori Amrita Molecular Modeling And Synthesis (AMMAS) Research lab, Amrita Vishwa Vidyapeetham- University, Coimbatore-641112 CEO-Biopharma Solutions n_krishnan@cb.amrita.edu	Integrated multi-scale screening strategy forLead Optimization- principles and applications
	4.00 – 5.00 pm	Dr. S. Gomathy Dept. of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty	Activation of SIRT-3 enzyme in Neurological disorders
10-10-2020 Saturday	10.00 am - 12.30noon	Dhivya shanmugarajan Application Scientist (Accylr's) Altem Technologies (P) Ltd, Bengaluru dhivya.shanmugarajan@altem.com 9003288384	Unravelling the utility of Structure-based pharmacophore mapping for lead optimization – “New Advances in Drug Discovery “
	12.30noon– 01.30 pm	Dr. S.P. Dhanabal Principal, JSSCP, Ooty	Natural products in drug discovery
	02.00 – 4.00 pm	Valedictory & Online Assessment	

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Co-ordinator –STTP, JSS College of Pharmacy, Ooty, Tamilnadu

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AICTE Sponsored

**One Week Short Term Training Programme (STTP) Series on
Recent advances in Drug Discovery, Development and Lead Optimization**



Organized by
**Department of Pharmaceutical Chemistry,
JSS College of Pharmacy, Ooty, Tamilnadu
(JSS Academy of Higher Education & Research, Mysuru)**

Duration: One week (10.00 am to 1.00 pm & 2.00 to 5.00 pm)
Online Module-I : 10-08-2020 to 15-08-2020
Online Module-II : 07-09-2020 to 12-09-2020
Online Module-III : 05-10-2020 to 10-10-2020

JSS College of Pharmacy, Ooty, is one of the pioneering research institutions in the country imparting quality pharmacy education at Diploma, graduate, post graduate and doctoral levels. The college is affiliated to JSS Academy of Higher Education & Research, Mysuru, which is accredited A⁺ Grade by NAAC. The College is ranked 9th in India by NIRF, MHRD and certified by the ISO-9001:2015.

Department of Pharmaceutical Chemistry was established in the year 1988 and has well equipped research laboratories with several advanced instruments and software's for CADD. Several research projects have been sanctioned by the government agencies like DBT, AICTE, UGC, CSIR, ICMR, DST etc. Our broad research areas are Green chemistry, Drug Design and Discovery, Synthesis of Biological active Heterocyclic compounds.

One week Short Term Training Programme (STTP) series on "Recent advances in Drug Discovery, Development and Lead Optimization" has been designed to provide the theoretical background as well as demonstration on approach in the latest developments across the broad and diverse fields of Drug Design, Discovery and Development of novel drugs using various computational tools, machine learning tools etc.

Who can Attend

Faculties / Industrialists from Pharmaceutical chemistry, Pharmacology, Biotechnology, Pharmaceutical Analysis and Pharmacognosy background.

Benefits

- ❖ Eminent resource persons from reputed Academicians, Industrialists and Software professionals in CADD.
- ❖ Certificate will be issued to all the registered participants

Instructions to the Participants for Online Course:

- ❖ Filling the registration form is mandatory.
- ❖ Attendance is mandatory for all sessions.
- ❖ All sessions will be conducted by online mode and the Link will be sent in advance.
- ❖ Online Assessment will be conducted on the last day by online mode.
- ❖ Limited seats are available on First-Come-First-Serve basis.
- ❖ The list of selected participants for each module will be intimated through E-mail.

Address for all Correspondence:

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Click the Link Below for Registration

<https://forms.gle/QXC6GAkJTJ69tx7fU6>