

**A.S.D GOVT DEGREE COLLEGE FOR WOMEN (A), KAKINADA**

**(Re-Accredited with 'B' by NAAC)**

**DEPARTMENT OF CHEMISTRY**

**A Report on One Day International Webinar**



**“RECENT ADVANCES IN DRUG DISCOVERY**

**AND DEVELOPMENT”**

**ON**

**06<sup>TH</sup> DECEMBER 2023**



**A.S.D. GOVT. DEGREE COLLEGE FOR WOMEN(A)**

Kakinada-533002

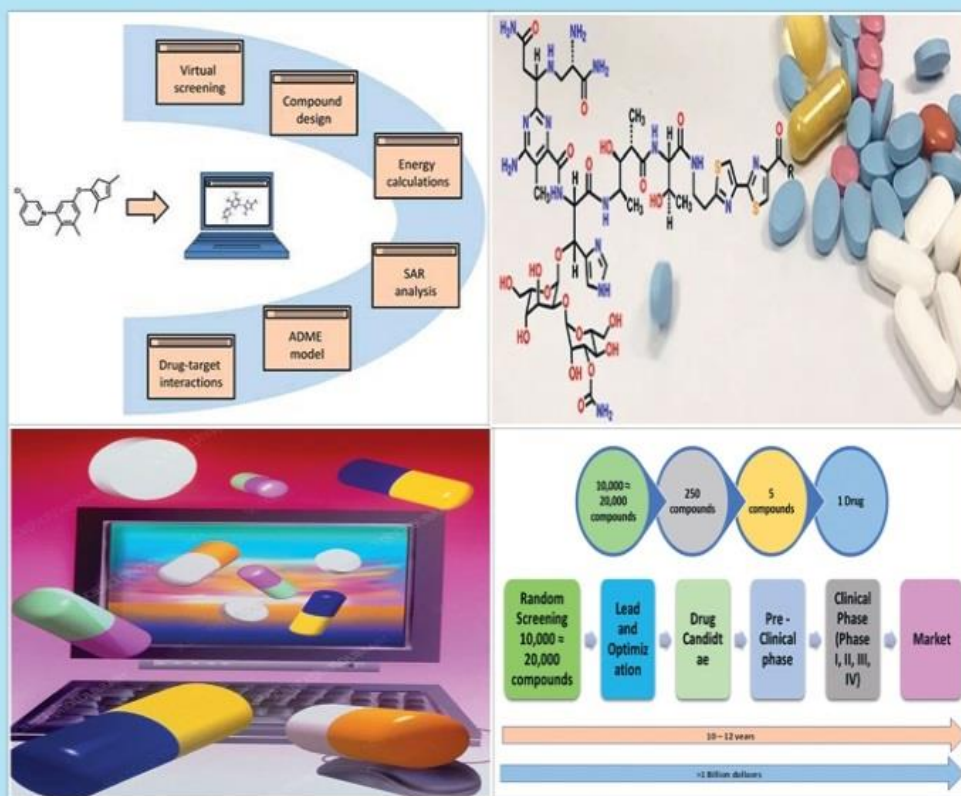
(Affiliated to Adikavi Nannaya University, Rajamahendravaram)

Re-accredited by NAAC with B Grade in Cycle III



# One Day International Webinar on Recent Advances in Drug Discovery and Development

**On 6<sup>th</sup> DECEMBER 2023**



**Organized By**

**DEPARTMENT OF CHEMISTRY**

**Under Internal Quality Assurance Cell (IQAC)**

### **About the College:**

Annavaram Satyavathi Devi Government Degree College for Women (Autonomous), Kakinada, Kakinada District, was started in 1962 with the motto : 'Sthree Vidya Pravardhataam' means 'Women Education Shall Prosper'. The idea came up with the inspiring words by Mahatma Gandhi, "If you educate a man, you educate an individual, but if you educate a woman, you educate an entire family". This is the only Government Degree College for Women in the entire coastal belt of Andhra Pradesh, with a Student Managed Hostel within the campus and 4 Social Welfare Hostels within a vicinity of 2 kilometres from the College. The College is mainly equipped with Smart Campus services like Virtual Classrooms, Digital Classrooms and LMS. At present, the college caters the education needs of nearly 1100 girl students at UG & PG level. The College has Adikavi Nannaya University recognized research center in the department of Commerce & Telugu

### **The college offers following 12 UG programmes :**

B.A Honours (Economics), B.A Honours (Political Science),  
B.Com Honours (General), B.Com Honours (Computer Applications) ,  
B.Com Honours (Digital Marketing), B.Sc.Honours (Home Science) B.Sc.Honours (Chemistry) B.Sc.Honours (Zoology), B.Sc.Honours (Botany), B.Sc.Honours (Physics)  
B.Sc.Honours (Computer Sciences), B.Sc.Honours (Mathematics)  
and 2 PG programmes: M.A.(Telugu) & M.Com. The College uses every opportunity with great care in strengthening the students to excel in their academics and get decent jobs.

### **About Chemistry Department :**

Chemistry Department is one of the oldest Department of this College, it is 61 years old department, established in the year 1962. In 1968, the Annavaram Devasthanam handed over the college to the Government of Andhra Pradesh. A.S.D. Govt. Degree and Junior College functioned as a composite institution till 1995.

Later in tune with the policy of U.G.C, the Government of Andhra Pradesh has bifurcated this institution into Junior and Degree Colleges in 1996. Since then the Chemistry Department is handling only U.G. level teaching. In 2015, the U.G.C. conferred Autonomy status to the institution, and from the academic year 2015-16, the Department switched over to semester system under CBCS pattern.

In addition to the conventional courses (B.Sc. - MPC/CBZ), restructured courses such as Chemistry, Botany and Microbiology (CBMB) in 1998-99 and market-oriented course such as Chemistry, Zoology, Aquaculture Technology, (CZAqT, Chemistry, Botany and Horticulture were introduced in 2018-19. At present the Department is offering B.Sc Honours (Chemistry) as single major system and five other UG programmes M.P.C, B.Z.C, CBMB, CZAQUA, CBHC and one Certificate course. At present, the department caters the education needs of nearly 300 girl students at UG level. The Department implementing microscale experiments for qualitative analysis and conducts Field trips. extension activities regularly.

### About the Programme :

This webinar intends to create interest towards research among faculty and students on Drug discovery and development . It provides talks on advanced drug discovery and development with eminent Scientists across the globe. Computer-aided drug design (CADD) is a modern computational technique used in the drug discovery process to identify and develop a new therapeutic drugs. It includes computational Chemistry, molecular modeling, molecular design and rational drug design. CADD is used to optimize identified leads and its approach saves time, it is fast and cost-effective. Therefore, today, in the fast-moving world with technological advancement, CADD has become inevitable. The Webinar focuses on Computer Aided Drug Discovery and Development, Advances in Drug Discovery & Development, Chemical biology.

### SPEAKERS



**Dr Vijaya Hinge**

CADD Scientist for Haares Chem Tech Inc.,  
Canada.



**Dr. Nagarjun Narayanaswamy**

Scientist, Rajiv Gandhi Centre for Biotechnology (RGCB),  
Thiruvananthapuram Kerala, India-695014.



**Dr. Vadde Ramu**, Msc.,PhD.

Marie-Curie Individual Postdoctoral Fellow  
Ruhr-University Bochum 44801, Germany

### PROGRAMME OUTLINE

#### Session 1 :

10.00 to 10.30 : Inauguration

#### Session 2:

10.30 to 11.45 : Computer Aided Drug Discovery and Development by  
Dr Vijaya Hinge, CADD scientist for Haares Chem Tech Inc., Canada.

#### Session 3:

12 noon to 1pm : Chemical biology by Dr. Nagarjun Narayanaswamy, Scientist, RGCB,  
Thiruvananthapuram.

#### Session 4:

2.30 to 4.00pm: Advances in Drug Discovery and development by Dr. Vadde  
Ramu, Marie-Curie Individual Postdoctoral Fellow, Ruhr-University Bochum 44801,  
Germany.

**No Registration Fee:-**

Regeneration Link : <https://forms.gle/tJDY28Avm81NhDnT6>

A.S.D.GOV'T. DEGREE COLLEGE FOR WOMEN  
(Re-Accredited with 'B' by NAAC)  
KAKINADA



**One Day International Webinar**  
**on**  
**“Recent Advances in Drug Discovery and Development on 6<sup>th</sup> December 2023”**

**PROGRAMME SCHEDULE**

1. Prayer : Students
2. Welcome by (10.02AM) : **Dr.K.Anitha,**  
Lecturer In-Charge of Chemistry
3. Inaugural Address (10.07AM) : **Dr.V.Ananthalakshmi,**  
Principal, A.S.D.Govt.Degree College (W)(A)
4. About the Seminar : **Mrs. M. Suvarchala,**  
Vice-Principal
- Technical Session-1** : 10.30 to 11.45AM
5. Introduction of Resource person : Dr.K.Jhansi Lakshmi, Lecturer in Chemistry
6. **Dr.Vijaya Hinge**  
CADD Scientist for Haares  
Chem Tech Inc, Canada : Computer aided Drug discovery & Development
- 7. Technical Session- 2** : 12.00 Noon to 1.00PM
8. Introduction of Resource person : P.Leena, Lecturer in Chemistry
9. **Dr.Nagarjuna Narayanaswamy**  
Scientist, RGCB : Chemical Biology  
Tiruvananthapuram
10. **LUNCH BREAK** : 1.00PM to 2.00PM
11. **Technical Session- 3** : 2.30PM to 4.00PM
12. Introduction of Resource person: M.Subbalakshmi, Lecturer in Chemistry
13. **Dr.Vadde Ramu**, M.Sc., Ph.D  
Marie- Curie Individual Post doctoral Fellow  
Ruhr-University Bochum 44801 : Advances in Drug Discovery and  
Development Germany.
14. Vote of Thanks : Dr.K.Anitha

## Introduction :

On the 6<sup>th</sup> of December 2023, the auditoriums of “A.S.D. Govt Degree College for Women” in Kakinada came alive with the spirit of exploration and knowledge – sharing during the International Webinar on “Recent Advances in Drug Discovery and Development.” 514 members actively participated in the webinar. This collaborative gathering provided a unique platform for students, Professionals, and experts to delve into the forefront of Pharmaceutical research.

## Inauguration and Opening Sessions :

### Prayer :

The day began with a solemn prayer, symbolizing unity and purpose as participants readied themselves for a day of enriching discourse.

### Welcome Note :

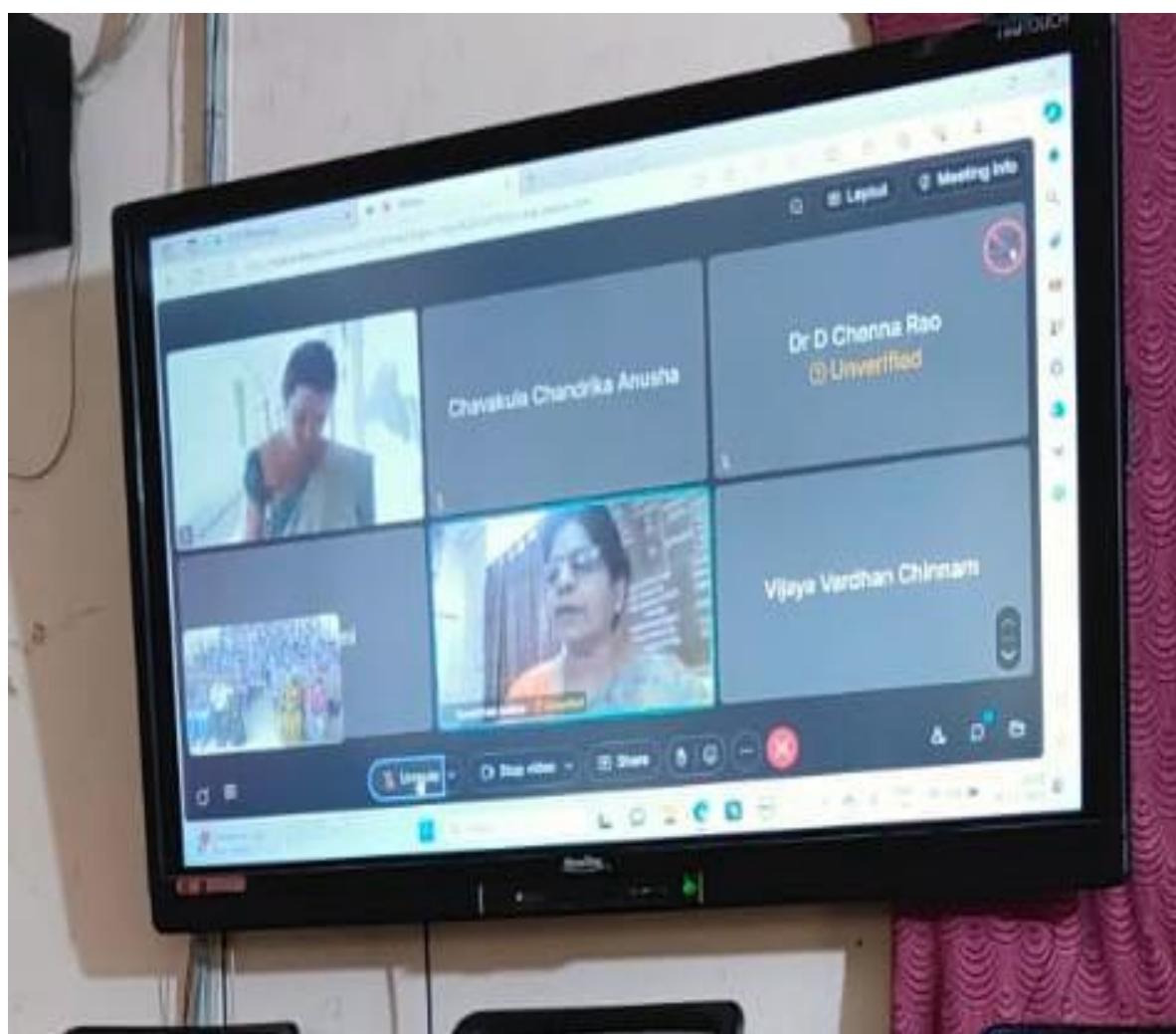
Dr.K.Anitha, the meticulous Lecturer In – Charge of Chemistry, extended a warm welcome, emphasizing the collaborative ethos that defines the scientific community.



## Inaugural Address :

Vice Principal Mrs.M.Suvarchala delivered an illuminating inaugural address, highlighting the transformative role of drug discovery in shaping the future of healthcare and provided a comprehensive webinar introduction, setting the stage for the day's proceedings.

Dr.V.Anantha Lakshmi, Principal and Mrs.M.Suvarchala, Vice Principal actively participated and encouraged the students throughout the event.



## Technical Sessions - 1

Resource Person : Dr.Vijaya Hinge

Topic : “Advancements in Computer – Aided Drug Discovery”

Time : 10:30 AM to 11:45 AM

### Introduction of Resource Person :

Dr.K.Jhansi Lakshmi introduced the first speaker , Dr.Vijaya Hinge, a seasoned CADD Scientist at Haares Chem Tech Inc., Canada.

Dr.Vijaya Hinge unfolded the intricacies of computer – Aided Drug Discovery, elucidating the audience on the fusion of computational methods and medicinal chemistry. The session explored the role of molecular docking, virtual screening and AI – driven algorithms in identifying potential drug candidates. Dr.Hinge’s engaging discourse emphasized the transformative impact of technology on the pharmaceutical industry, paving the way for a future where computational tools expedite drug development.

The screenshot shows a Cisco Webex meeting interface. The main content is a presentation slide titled "QSAR models". The slide is divided into two columns. The left column is titled "Prediction of P-glycoprotein inhibitors with machine learning classification models and 3D-RISM-KH theory based solvation energy descriptors". The right column is titled "Predicting skin permeability using the 3D-RISM-KH theory based solvation energy descriptors for a diverse class of compounds". Below the text, there is a list of three models: 1. P-Glycoprotein inhibitors model, 2. BBB permeability model, and 3. Skin Permeability model. The meeting interface includes a top bar with navigation icons, a top right corner with "Layout" and "Meeting info" buttons, a top left corner with a back arrow, and a top center area with participant thumbnails for "Vijaya Hinge", "awdc,rjy", "LEENA PENNETI", "Dr M sudhakar", and "Dr D Chenna Rao". A right sidebar shows "Participants (84)" with a search bar and a list of participants including "JKCMC :: CCE, AP", "Vijaya Hinge", "ADC KKD", "ADCGPT", "aditya degree college...", "anantha lakshmi", "Andhra University", "annapurna.srcm@gm...", and "Asheesh gcrjy". At the bottom, there are controls for "Unmute", "Start video", "Share", "Participants", "Chat", and "Content". The Windows taskbar is visible at the very bottom with the search bar and various application icons.



Cisco Webex

cceap.webex.com/wbxmjs/joinservice/sites/cceap/meeting/download/30c42f372f934a37bee8c2276a628107?siteurl=cceap&MTID=m468d44765fad7a9d256bafab83c9403

Layout Meeting info

Participants (85)

Invite people

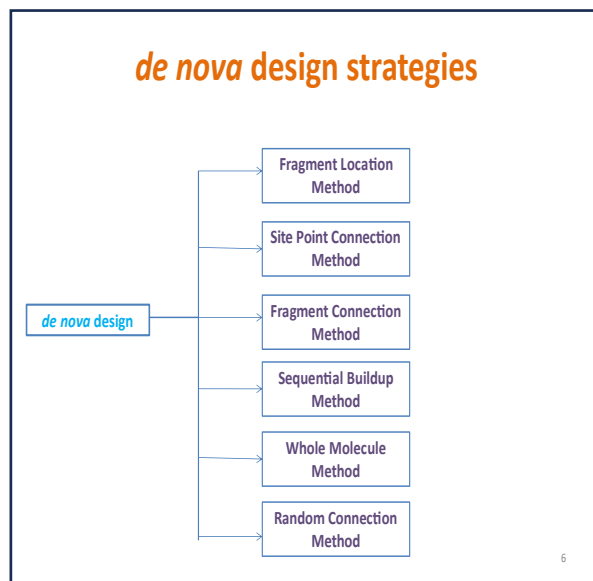
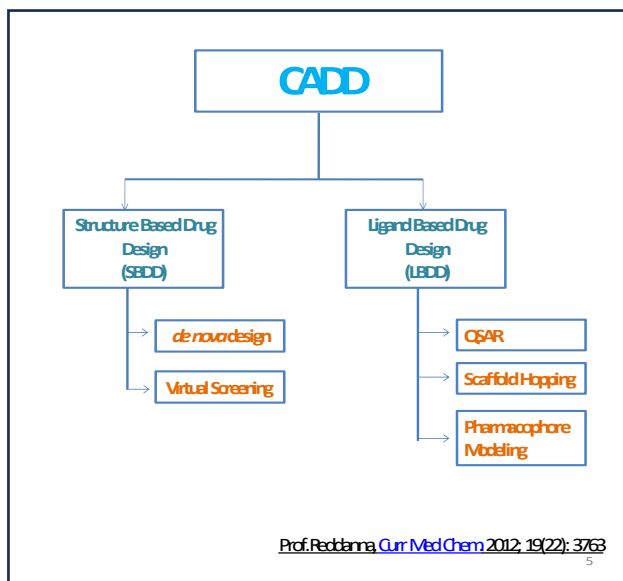
In the meeting (85)

- JKCMC :: CCE, AP Host, me
- Vijaya Hinge Presenter @gmail.com
- ADC KKD Unverified
- ADCGPT Unverified
- aditya degree college... Unverified
- anantha lakshmi @gmail.com
- Andhra University @andhrauniversity.edu
- annapurna.srcm@gm... @gmail.com
- Athili Durga Bhavani ...

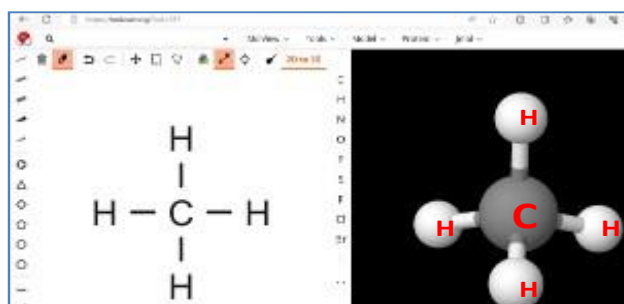
Unmute Start video Share

Participants Chat Content

22°C 11:06 06-12-2023



## Methane: Molecular structure

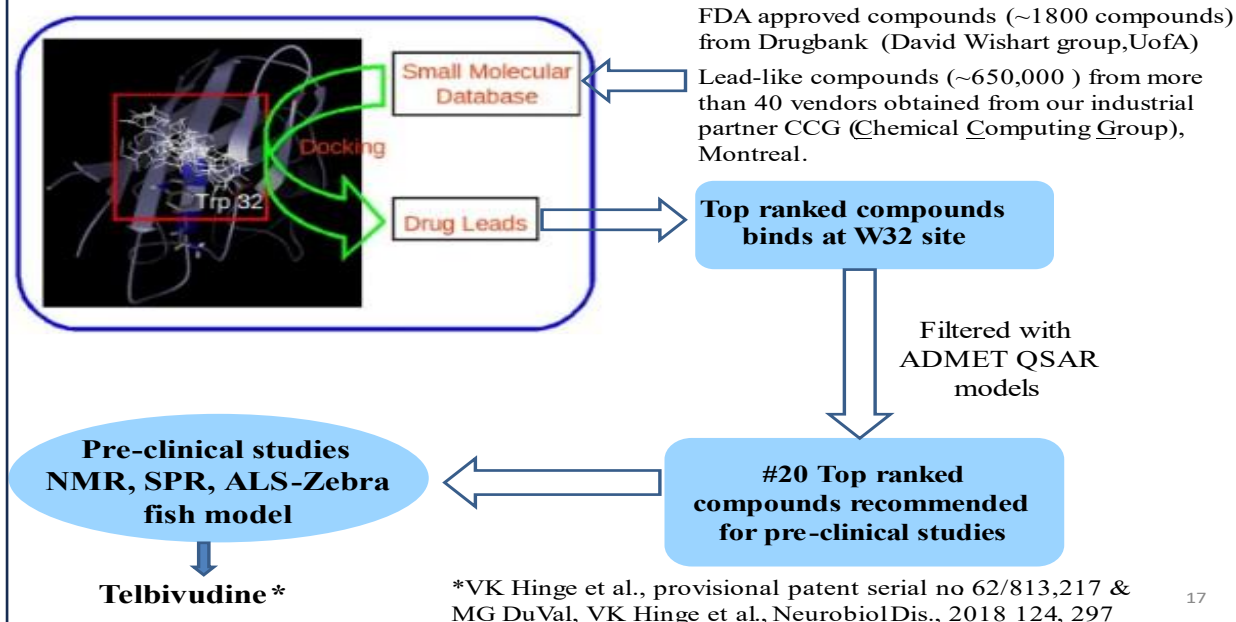


### Methane atoms its 3D coordinates

		atoms	3D-coordinates
1			
2	5		
3	1 Meth	CT	1 0.116 0.116 0.116
4	1 Meth	HC1	2 0.061 0.061 0.061
5	1 Meth	HC2	3 0.171 0.171 0.061
6	1 Meth	HC3	4 0.171 0.061 0.171
7	1 Meth	HC4	5 0.061 0.171 0.171
8			0.232109 0.232109 0.232109

Ref: <https://molview.org/?cid=297>

## Virtual screening at Trp32 site of SOD1



## Technical Session - 2

Resource person : Dr.Nagarjuna Narayanaswamy

Topic : “Chemical Biology”

Time : 12PM to 1PM

### Introduction of Resource Person :

P.Leena, Lecturer in Chemistry, introduced the captivating world of Chemical Biology through the expertise of Dr.Nagarjuna Narayanaswamy, a distinguished Scientist at RGCB, Thiruvananthapuram.

Dr.Nagarjuna Narayanaswamy navigated through the interdisciplinary landscape of drug development, shedding light on the intricate interplay between chemical compounds and biological systems. The session explored innovative strategies in target identification, emphasizing the synergy between chemistry and biology in creating targeted and effective therapeutics. Dr.Narayanaswamy's insights deepened the audience's understanding of the collaborative nature of modern drug discovery.

The screenshot displays a Cisco Webex meeting interface. At the top, the browser address bar shows the URL: [ccep.webex.com/wbxmjs/joinservice/sites/ccep/meeting/download/30c42f372f934a37bee8c2276a628107?siteurl=ccep&MTID=m468d44765fad7a9d256bafafb83c9403](https://ccep.webex.com/wbxmjs/joinservice/sites/ccep/meeting/download/30c42f372f934a37bee8c2276a628107?siteurl=ccep&MTID=m468d44765fad7a9d256bafafb83c9403). The meeting title is "Viewing Dr. Nagarjun Narayanaswamy's shared content". The interface shows a grid of participants: srinivas nerella, JKCMC :: CCE, AP, awdc,rjy, ADC KKD, and Suvarchala Mallela. A central window displays a presentation slide titled "Fluorescence probe". The slide content includes: "Fluorescence probe is a molecule that absorbs the light and emit the light in longer wavelength region." Below this is a diagram of Jablonski diagrams showing energy levels (S0, S1, T1) and transitions (excitation, emission, non-radiative relaxation, intersystem crossing). A text box at the bottom states: "Fluorescence probes are extremely useful in cell imaging, protein labeling, flow cytometry, DNA sequencing and forensics applications." The meeting controls at the bottom include "Unmute", "Start video", "Share", and "Participants" (54). The system tray at the bottom shows the date and time as 06-12-2023, 12:06.

Cisco Webex

cccap.webex.com/wbxmjs/joinservice/sites/cccap/meeting/download/30c42f372934a37bee8c2276a628107?siteurl=cceap&MTID=m468d44765fad7a9d256bafab83c9403

Layout Meeting info

Participants (45)

Invite people

In the meeting (45)

- JKMC :: CCE, AP Host, me
- Dr. Nagarjun Narayan... Presenter Unverified
- ADCGPT Unverified
- Andhra University @andhrauniversity.edu
- AWDC-GWK Unverified
- awdc,rjy Unverified
- awdcgpt Unverified
- Chandra sekhar @gmail.com
- Degala Pallamraju Mute All Unmute All

Viewing Dr. Nagarjun Narayanaswamy's shared content

100%

Video stopped

Förster resonance energy transfer (FRET)

- Förster resonance energy transfer (FRET): FRET is energy transfer mechanism between two fluorescent molecules (Donor and acceptor).
- In FRET, A Donor fluorescence molecule transfer its excited state energy to an acceptor fluorescent molecule in nonradiative manner through dipole-dipole interactions.
- FRET mainly depends on dipole-dipole interactions and distance between the donor/acceptor molecules

Unmute Start video Share Participants Chat Content

Type here to search

26°C 12:20 06-12-2023

Cisco Webex

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Layout Meeting info

Participants (43)

Invite people

In the meeting (43)

- JKMC :: CCE, AP Host, me
- Dr. Nagarjun Narayan... Presenter Unverified
- ADCGPT Unverified
- Akula kranthi sowjanya Unverified
- Andhra University @andhrauniversity.edu
- AWDC-GWK Unverified
- awdc,rjy Unverified
- Chandra sekhar @gmail.com
- Degala Pallamraju Mute All Unmute All

Viewing Dr. Nagarjun Narayanaswamy's shared content

100%

Video stopped

Nucleotide and DNA structure with minor and major grooves

Major groove

Minor groove

2 nm

3.4 nm

Unmute Start video Share Participants Chat Content

Type here to search

26°C 12:29 06-12-2023



## Lunch Break : (1PM to 2PM)

The midday break provided a valuable opportunity for participants to engage in informal discussions, fostering collaboration and networking among attendees.

## Technical Session – 3

Resource Person : Dr.Vadde Ramu

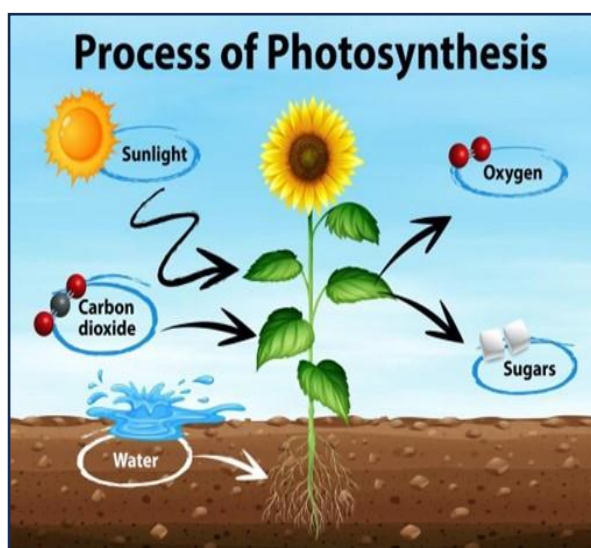
Topic : “Advances in Drug Discovery and Development”

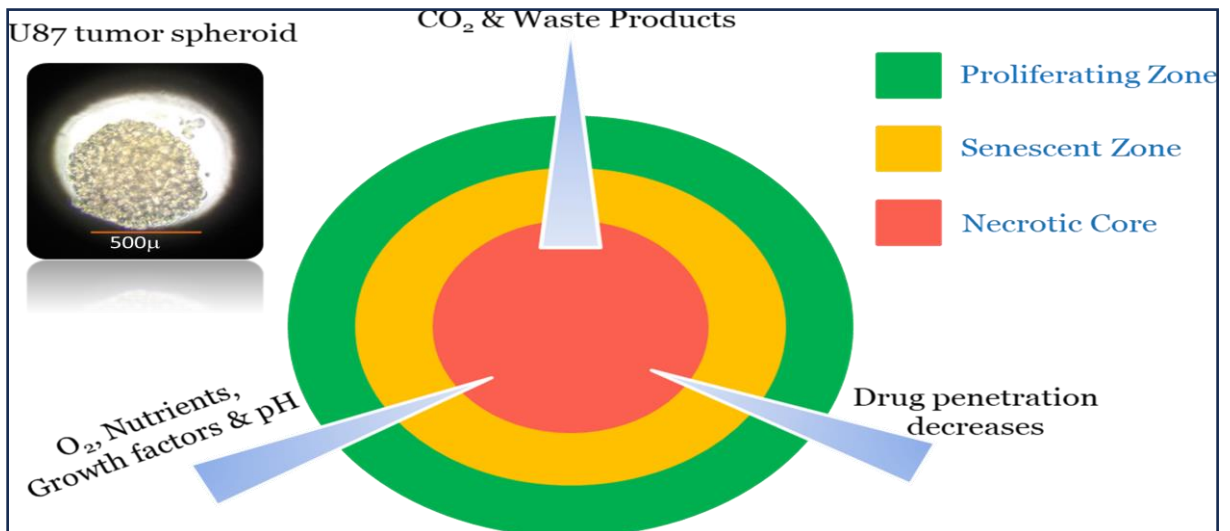
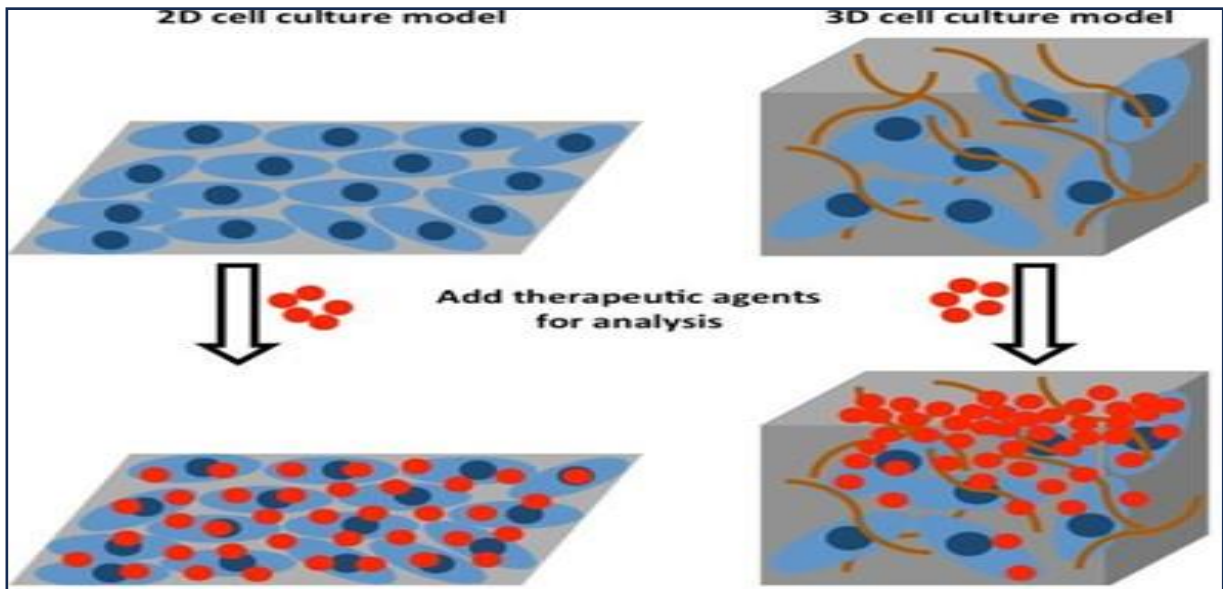
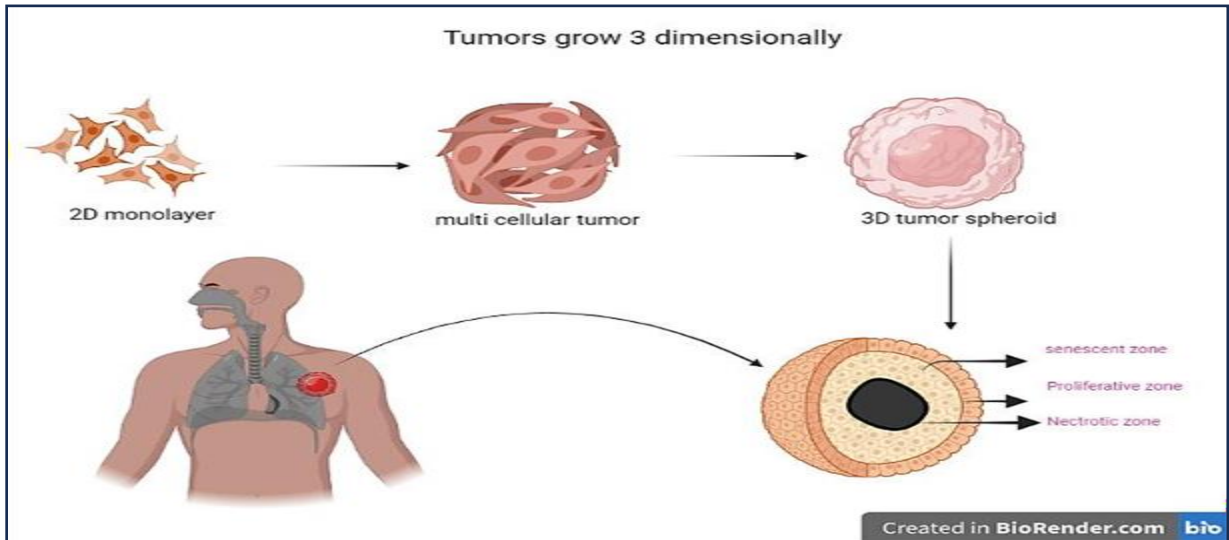
Time : 2:30 PM to 4 PM

### Introduction of Resource Person :

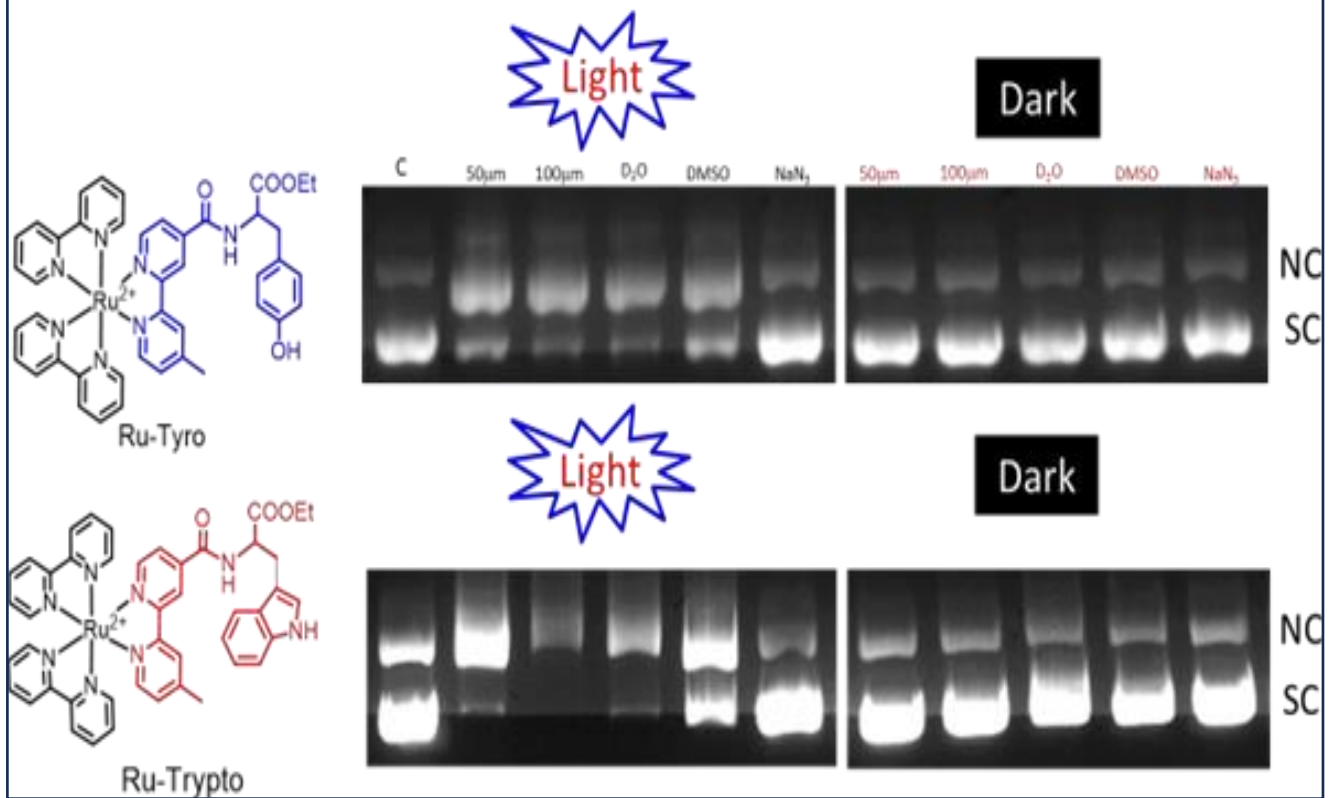
M.Subba Lakshmi, Lecturer in Chemistry, introduced the final technical session featuring Dr.Vadde Ramu, a Marie – Curie individual post – doctoral fellow from Ruhr University, Bochum, Germany.

Dr.Vadde Ramu comprehensive exploration of Advances in Drug Discovery Spanned Multiple Dimensions. He delved into the innovative use of nanotechnology for targeted drug delivery, providing a glimpse into the future of precision medicine. Furthermore, Dr.Vadde discussed the integration of data – driven strategies in optimizing clinical trials, showcasing the transformative potential of big data in pharmaceutical research. His session not only presented cutting – edge technologies but also emphasized the ethical considerations and regulatory challenges associated with these novel approaches.





## Photo-cleavage of plasmid DNA by generation of $^1O_2$





### **Conclusion :**

The one – day international webinar emerged as a pivotal platform for knowledge exchange, pushing the boundaries of understanding in drug discovery and development. The technical sessions not only showcased the latest advancements but also ignited a spark of curiosity and inspiration among the participants, fostering a shared commitment to advancing pharmaceutical research.

### **Vote of Thanks :**

The event concluded with Dr.K.Anitha expressing heartfelt gratitude to the speakers, participants, and the organizing committee. Her words encapsulated the collective appreciation for a day filled with intellectual stimulation and collaborative learning.





