

PROGRAM 1. ONE DAY WEBINAR REPORT

DATE: 27-06-2020

CONDUCTED BY: P.G ORGANIC CHEMISTRY & ANALYTICAL CHEMISTRY DEPARTMENTS

TOPIC: ^1H NMR SPECTROSCOPY

NO. OF STUDENTS AND FACULTY REGISTERED AND PARTICIPATED: 750

Keshav Memorial Institute of Commerce & Sciences
(Affiliated to Osmania University)
Narayanaguda, Hyderabad-29

Department of Chemistry(PG) & IQAC

WEBINAR
on
 ^1H -NMR Spectroscopy

10-11 AM
June 27

Guest Speaker

Prof. S. Satyanarayana, Ph.D, FRSC
Former Vice-Chancellor,
Osmania University

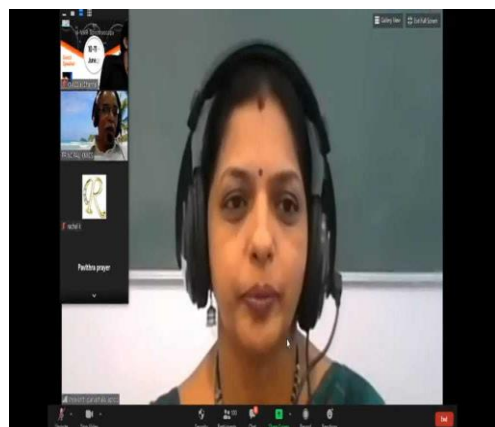
Convener
Mrs. P. Shravanthi
Head
Dept. of Organic Chemistry
Ph: 9849543563

Co-ordinator
Mrs. M. Sangeetha Lawrence
Head, Dept. of Analytical Chemistry
Ph: 9573219565

Webinar Chairperson
Dr. J. Nageswara Rao
Principal

E-Certificates will be provided to the participants

REGISTER NOW AT





PROGRAM 2. NATIONAL SCIENCE DAY 2020-2021

Date :02/03/2021

Venu :Sardar Patel Hall

Chief Guest :Sir Neil Gogte

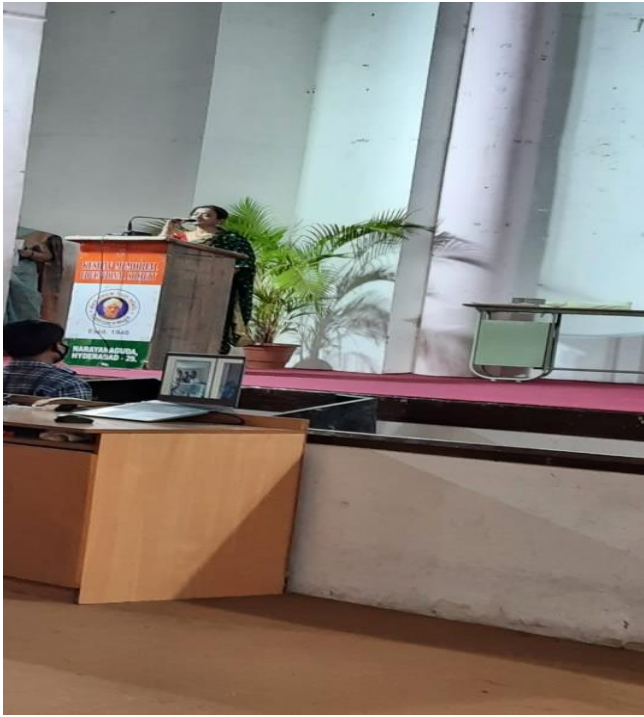
Time of The Programme : 12:00 P.M

Theme of The Programmme : “ Future of STI : Impact on Education Skills & Work”

















PROGRAM 3 .ONE DAY WEBINAR

DATE : 10-05-2021

CHIEF GUEST : Prof M.Vijjulatha

TIME OF THE PROGRAMME : 11:00 AM

Topic : Quantitative Structure – Activity Relationship and Molecular Modeling.


KESHAV MEMORIAL INSTITUTE OF COMMERCE AND SCIENCES
 (Affiliated to Osmania University) Narayanaguda, Hyderabad, 500029.

Department of Chemistry (PG) & IQAC is organizing a
 One Day Webinar on
**QUANTITATIVE STRUCTURE – ACTIVITY RELATIONSHIP AND
 MOLECULAR MODELLING**

Date: 10-05-2021 Time: 11:00 am - 1:00 pm

Guest Speaker
Prof. Vijjulatha Manga
 Dean, Development of UGC Affairs,
 Dept of Chemistry,
 Osmania University.





Click here to join the Webinar on 010/05/2021
<https://meet.google.com/cvw-wdhg-yma>

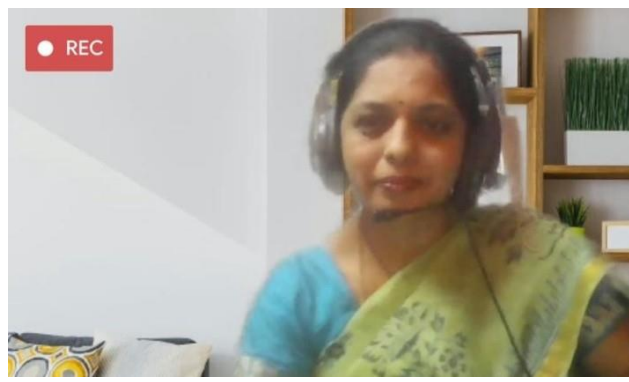
Organised by
 Department of Chemistry (PG) & IQAC
 Keshav Memorial Institute of Commerce and Sciences
Dr. Annadanam Subramanyam
 Secretary, KMES

Prof. K. Someswara Rao **Prof. J. Nageswara Rao**
 Principal Director, KMES

DEPARTMENT OF CHEMISTRY (PG)

P. Shrivanthi Convenor	V. Anjaneyulu Member	N. Krishna Prasad Member
M. Sangeetha Lawrence Member	S. Pranitha Member	G. Sindhuri Member

e-Certificate will be provided for the participants.





Quantitative structure-activity relationships (QSAR)
&
Molecular Modelling

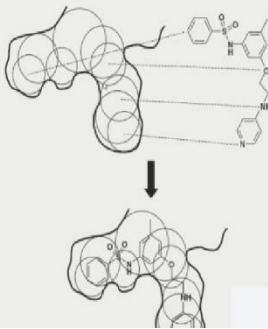
PROF. M. VIJULATHA

Dept. of Chemistry
University College of Science
Dean, Development & UGC Affairs
Osmania University

REC

The DOCK algorithm – Rigid docking

- The DOCK algorithm developed by Kuntz and co-workers is generally considered one of the major advances in protein-ligand docking [Kuntz et al., *JMB*, 1982, 161, 269]
- The earliest version of the DOCK algorithm only considered rigid body docking and was designed to identify molecules with a high degree of shape complementarity to the protein binding site.
- The first stage of the DOCK method involves the construction of a "negative image" of the binding site consisting of a series of overlapping spheres of varying radii, derived from the molecular surface of the protein

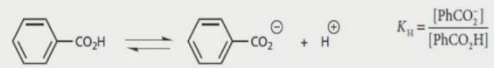


REC

Hammett substituent constant (σ_p)

Electronic effects of the substituents in Aromatic rings

Ionization of benzoic acid in water.



Electronic effects

