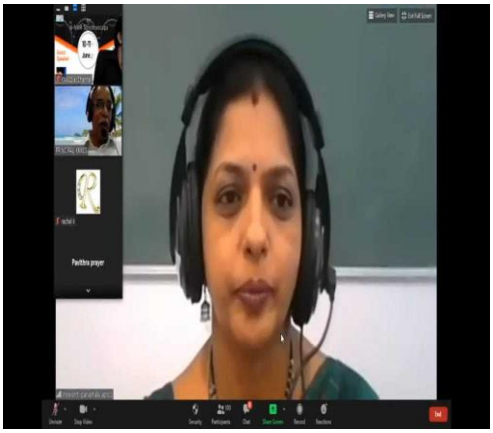
PROGRAM 1. ONE DAY WEBINAR REPORT

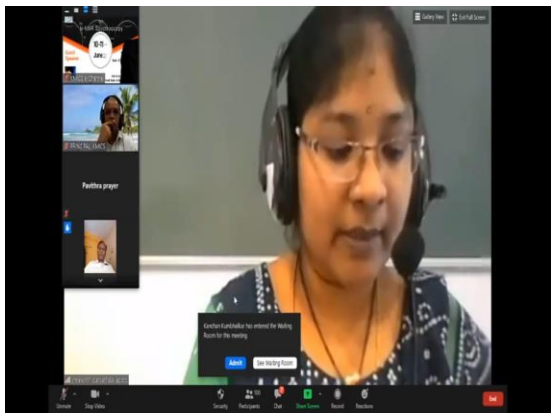
DATE: 27-06-2020

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

TOPIC: ^{1}H NMR SPECTROSCOPY

NO. OF STUDENTS AND FACULTY REGISTERED AND PARTICIPATED: 750




Gallery View
Full Full Screen
Pavithra prayer
Admit
See Waiting Room
Unmute
Stop Video
Security
Participants
Chat
Share Screen
Record
Reactions
End

***PROGRAM 2. NATONAL SCIENCE DAY* 2020-2021**

Date :*02/03/2021*

Venu :*Sardar Patel Hall*

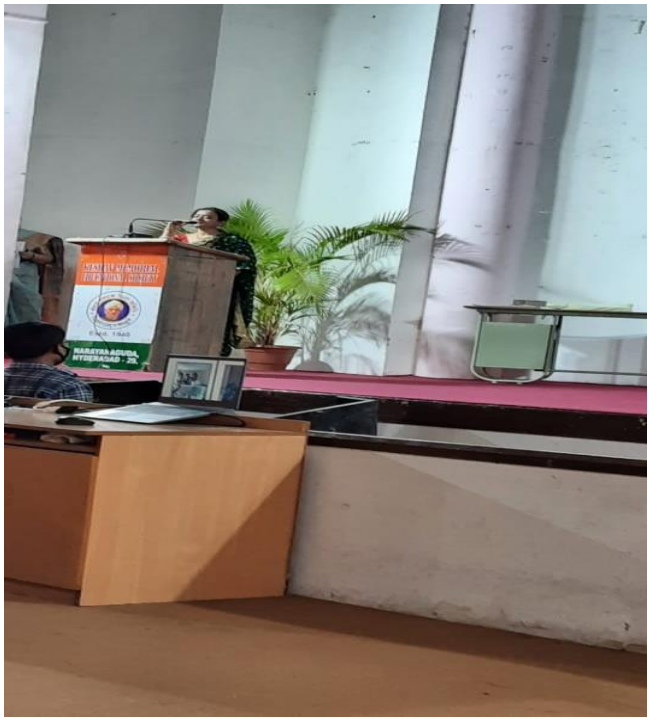
Chief Guest :*Sir Neil Gogte*

Time of The Programme :*12:00 P.M*

Theme of The Programmme : " *Future of STI : Impact on Education Skills & Work"*


"Future of STI: Impact on Education Skills &
02 - 03 - 2021
Sri Dr. A.V.Subrahm
Secretary, KME
mittee & IQAC


KESHAV MEMORIAL INSTITUTE OF COMMERCE AND SCIENCES
SCIENCE DAY

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NATIONAL SCIENCE
"Future of STI: Impact on Education
02 - 03 - 2021
Prof. K. Someshwer Rao
Prof. J. Nageswara Rao
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NARAYANAGUDA,


welcome
KESHAV MEMORIAL INSTITUTE OF COMMERCE AND SCIENCES
(Affiliated to Osmania University) Narayanaguda, Hyderabad-29
NATIONAL SCIENCE DAY
"Future of STI: Impact on Education Skills & Work"
02 - 03 - 2021
Chief Guest
Sri Nellgogta
(Founder, Director KMIT)
Prof. K. Someshwer Rao
Principal, KMICS
Prof. J. Nageswara Rao
Director, KMFS
Sri Dr. A.V.Subrahmanyam
Secretary, KMLS
Organized by
Science Asso ion Committee & IQAC


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Director, KMICS


KESHAV MEMORIAL INSTITUTE OF COMMERCE AND SCIENCE
NATIONAL SCIENCE
Prof. K. Sameshwer Rao
Principal KMICS
Organized by

PROGRAM 3 .ONE DAY WEBINAR

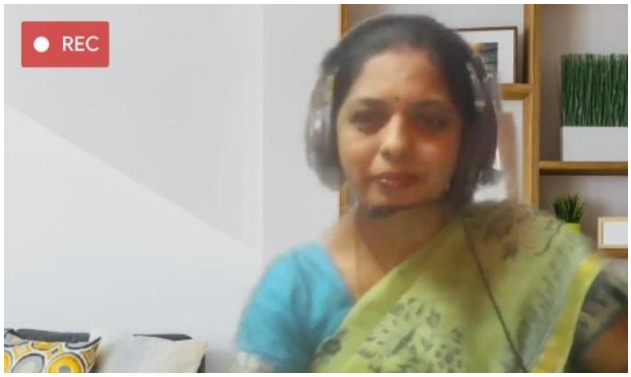
DATE : 10-05-2021

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 Register
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. Someshwer Rao
Principal
Prof. J.Nageswara Rao
Director, KMES
DEPARTMENT OF CHEMISTRY (PG)
P.Shravanthi
Convenor
V.Anjaneyulu
Member
N.Krishna Prasad
Member
M.Sangeetha Lawerence
Member
S.Pranitha
Member
G.Sindhuri
Member
e-Certficate will be provided for the participants


REC


REC

Quantitative structure–activity relationships (QSAR)
&
Molecular Modelling

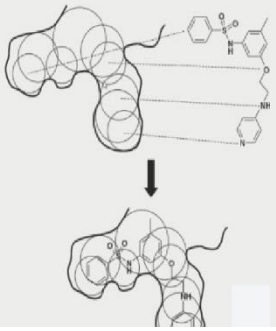
PROF. M. VIJJULATHA

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



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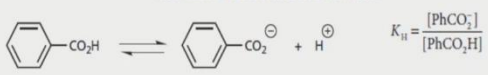
Hammett substituent constant (σ_X)

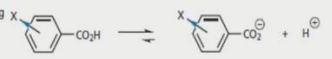
Electronic effects of the substituents in Aromatic rings

Ionization of benzoic acid in water.



Electronic effects

Electron-withdrawing group



Larger K_x

Electron-donating group

Smalle