

# National Level Competition For Students

Association with BECon Fest(IIT Delhi Event)

## Workshop Details

Topic: Cheminformatics &  
its application in research  
and Drug Industry

15th & 16th October 2018

Registration Fee - INR 1150/-

## Benefits

Industry Expert Faculty.  
Certificate to each participant.  
Medals & Certificates of Excellence  
for Top 5 students  
Top 5 Outstanding selected students  
get the chance to participate in the  
final round @IIT Delhi campus

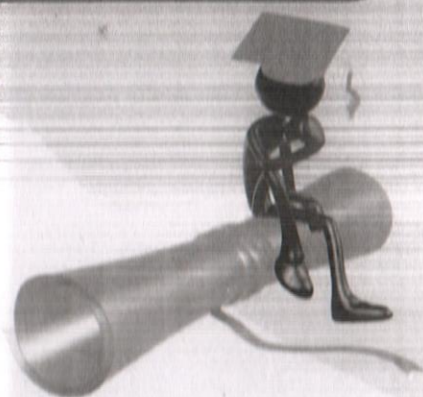
## Mode of Selection

### 1st Round:

Karpagam Academy of  
Higher Education.

### 2nd Round:

IIT Campus



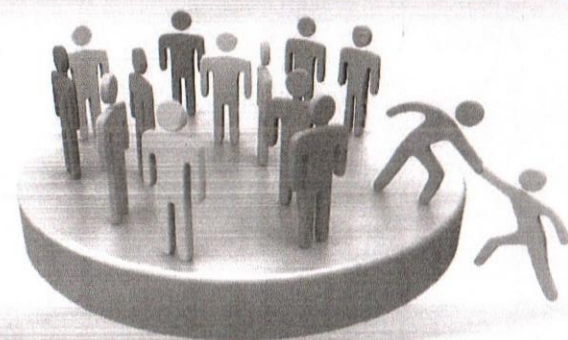
Organized by: Karpagam Academy of Higher Education

Co-ordinator : Dr.M.Gopalakrishnan - 8189849030

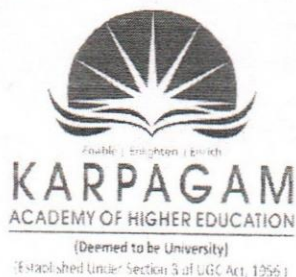
Co-ordinators : 1) N. Nivetha-7373178204

2) G. Lakshmipriya-9566945010

Prizes worth  
50k







## DEPARTMENT OF CHEMISTRY

We cordially invite you for the Workshop on  
*Cheminformatics & Its Application in Research and  
Drug Industry*

*On 15 & 16<sup>th</sup> October, 2018.*

**Dr. S. SUDALAIMUTHU**

Vice-Chancellor,

Karpagam Academy of Higher Education  
has kindly consented to preside over the function

**Ms. Kirthana M. V. Sindhe**

Professional research scientist & project ladder in Biomedical Research,  
Drug Discovery

*Will inaugurate the Workshop activities*

**Venue: Barathi Hall**

**Time: 9.30 am**

**All are invited**

# *Cheminformatics & Its Application in Research and Drug Industry*

## **Agenda**

**15.10.2018 – Monday**

**Prayer Song**

**Lighting the Kuthuvilakku**

**Welcome Address :**

**Dr. S. Ravi**  
Professor and Head  
Department of chemistry

**Presidential Address :**

**Dr. S. SUDALAIMUTHU**  
Vice-Chancellor,  
Karpagam Academy of Higher Education,  
Coimbatore.

**Inaugural Address :**

**Ms. Kirthana M. V. Sindhe**  
Professional research scientist & project  
ladder in Biomedical Research, Drug  
Discovery

**Felicitation :**

**Dr. R. SUNDARARAJAN**  
Registrar,  
Karpagam Academy of Higher Education,  
Coimbatore

**Dr. M. PALANISWAMY**

Dean, FASH  
Karpagam Academy of Higher Education,  
Coimbatore

**Vote of thanks :**

**SHUHAIL IRRFAN AHAMED.J**  
I M.Sc Chemistry



## A REPORT ON THE WORKSHOP PROGRAMME ON "CHEMINFORMATICS AND ITS APPLICATION IN RESEARCH AND DRUG INDUSTRY"

IIT Delhi in an effort to give an awareness about the "Future Scope of Chemist science" as an initiative for "Chemistry-Science Field" has organized a programme called MAKEINTERN - BECON EVENT IIT-DELHI. The programme was planned for two rounds

1. First round: To be conducted in 30 zonal centers (our institution as one of the center)
2. Second round: Finale round would be held at BECON EVENT IIT-DELHI

MakeIntern is the official training partner of Becon event IIT-Delhi. The first round of the programme was conducted in our University (KAHE) on 15-10-2018 & 16-10-2018 (from 9.30 am to 4.00 pm). Students from KAHE and from other institutions were permitted to participate in the programme. Ms. Kirthana M.V.Sindhe was the resource person for the two days.

- a. Sixty students participated in the programme.
- b. A hand on experiment based workshop was held for the students
- c. Towards the end of the programme based on the students presentation and quiz programme five students were selected from our programme, so that they can participate in the second round
- d. The following Students were selected.
  1. DHARANI.J (Karpagam Acadmey of Higher Educatiun)
  2. MAITHREYAN.V.V (Bharathidasan University)
  3. SHUHAIL IRRFAN AHAMED J (Karpagam Acadmêy of Higher Educatiun)
  4. ASHIF MOHAMED. A (Karpagam Acadmey of Higher Educatiun)
  5. SHARMIR. A (Karpagam Acadmey of Higher Educatiun)

Training was provided in the following areas

- a. Introduction and scope of Chemo Informatics
- b. Cheminformatics resources
- c. Chemical databases, Chemical Library preparation
- d. Chemical structure design
- e. Molecular modeling, molecular dynamics
- f. Structure based drug design
- g. Ligand based drug design
- h. Pharmacophore analysis, QSAR
- i. Pharmacokinetic analysis
- j. Molecular docking, Virtual screening.

On the first day the registration was between 9.00 am to 9.30 pm. To begin with an inaugural function was planned between 9.30 am and 10.00 am. The programme was started with a prayer song by the participants followed by lighting of the kuthuvillake by the dignitaries. Then Dr.S.Ravi, Professor & Head, Department of Chemistry welcomed the gathering and briefed about the programme. Mrs. Kirthana M.V.Sindhe the resource person from "MakeIntern" delivered the Inaugural address. Dr.S.P.Rajendran, Adjunct Professor, Department of Chemistry felicitated the programme.

### Programme Schedule

#### Day I

S.No	Day/Timings	Program details
1	9.30 am to 10.30 am	Inaugural function
2	10.00 am to 11.00am	Introduction and scope of Chemoinformatics
3	11.00 am to 11.15 am	Tea break
4	11.15 am to 12.15 am	Chemical databases, Chemical library preparation, Chemical structure design
5	12.15 pm to 1.00 pm	Molecular modeling, molecular dynamics
6	1.00 pm to 2.00 pm	Lunch break
7	2.00pm to 3.00 pm	Database search, Chem draw & structure design (Lab)
8	3.00 pm to 4.00 pm	Structure based drug design (Lab)

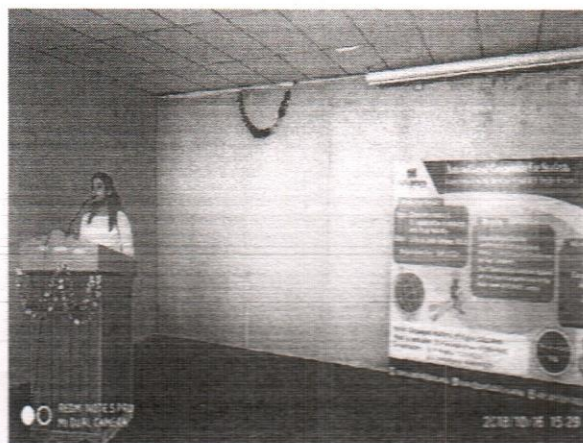
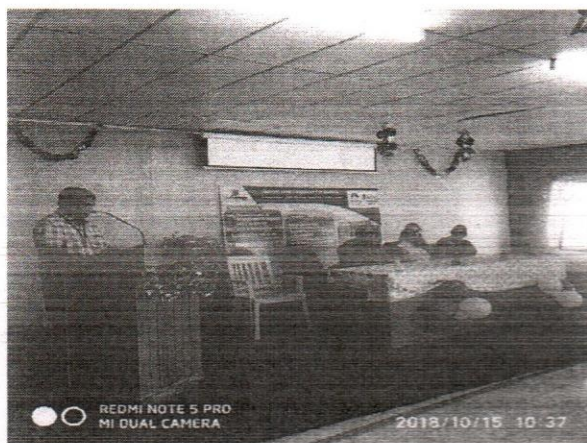
#### Day II

S.No	Day/Timings	Program details
1	9.30 am to 11.00 am	Ligand based drug design, Pharmacophore analysis, QSAR
2	11.00 am to 11.15am	Tea break
3	11.15 am to 1.00 pm	Pharmacokinetic analysis
4	1.00 pm to 2.00 pm	Lunch break
5	2.00 pm to 3.00	Molecular docking, Virtual screening. (Lab)



	pm	
6	3.00 pm to 4.00 pm	Students presentation & Quiz Programme
7	4.00 pm to 4.15 pm	Valedictory function

The Valedictory function started with a prayer song. The students were requested to give their feedback about the programme. Five students offered the feedback. The selected five students were congratulated and this was followed by the certificate distribution to the students by the resource person Mrs. Kirthana M.V.Sindhe. The programme was completed after the National Anthem.



S.P.M.  
8/11