

1.00p.m-2.00p.m : Lunch Break  
 Session X : 2.00pm-3.00pm

**Hands on Session on Protein Preparation and Ligand Preparation**

**Dr.U.C. Jaleel,**

Assistant Professor, Chemoinformatics,  
 Malabar Christian College, Calicut  
 3.00pm-4.00pm

Session XI : **Hands on training on ADME Prediction**

**Dr. Prasad M Alex**

Associate Professor in Chemistry,  
 Marthoma College, Chungathara

4.00pm-4.15pm : Tea Break  
 Session XII : 4.15pm-5.30 pm

**Paper Presentation**

Chair : **B.Rema Devi**  
 Assistant Professor, Dept.of Chemistry,  
 S.N.College, Chengannur

**Sequence Alignment Methods**

**Salman Zaheer**

(Department of Biotechnology, Amity University , Noida, UP)

**Virtual Screening**

**Susheel Kumar**

(Sastra University, Thanjavur , Tamilnadu)

**Algorithms in Molecular Docking**

**Pankaj Singh**

(Chemoinformatics, NIT, Bhopal)

**Synthesis, Characterization and Singlet Oxygen**

**Generation Capacity of meso-tetraaryl porphycene**

**K.S.Anju**

(Photosciences and Photonics Section, Chemical Sciences and  
 Technology Division, NIIST (CSIR), Trivandrum)

**GUI for CDK Tools**

**Hareesh Shanker**

(OSDD Chemoinformatics,  
 Malabar Christian College, Calicut)

**Development of QSAR Tuberculosis Data Sets**

**Nufail.M**

(OSDD Chemoinformatics,  
 Malabar Christian College, Calicut)

**SATURDAY 19-03-2011**

Invocation : College Choir  
 Session XIII : 9.00am-10.00am  
**Poster Presentation**  
 Session XIV : 10.00am-11.00am  
**Hands on training on Binding Site Prediction**  
**Dr. Prasad M Alex**  
 Associate Professor in Chemistry,  
 Marthoma College, Chungathara  
 11.00am-11.15am : Tea Break  
 Session XV : 11.15am-1pm  
**Hands on session on Grid Generation with Constraints and Docking**  
**Dr.U.C. Jaleel**  
 Assistant Professor, Chemoinformatics,  
 Malabar Christian College, Calicut  
 1.00 pm-2.00 pm : Lunch Break  
 Session XVI : 2.00pm-3.00pm  
**Hands on session on QSAR**  
**Vijay H. Masand**  
 Department of Chemistry, Vidya Bharati  
 College, Amravati, Maharashtra  
 3.00 pm-3.15 pm : Tea Break  
 3.15 pm-3.30 pm : **Evaluation**  
 3.30 pm -5.00 pm : **Valedictory Session**  
 Invocation : College Choir  
 Welcome : **Dr.V.L.Pushpa**  
 Convenor, Work Shop  
 Presidential Address : **Dr.V.K.Gopi**  
 Principal, S.N.College, Chengannur  
 Inaugural Address : **Dr.M.Jayaprakas**  
 Director, CDC, University of Kerala  
 Felicitations : **Smt.Veena.C**  
 HOD, Economics  
**Dr.S.R.Jitha**  
 Associate Professor, Dept.of Politics  
 Vote of Thanks : **Dr.S.Sujatha**  
 Associate Professor, Dept.of Chemistry

**National Anthem**

**CADD-2011**

**NATIONAL WORKSHOP ON COMPUTER AIDED DRUG DESIGNING**

**From 17<sup>th</sup> to 19<sup>th</sup> March 2011**

Organized by:

**THE POST GRADUATE DEPARTMENT OF CHEMISTRY**

**SREE NARAYANA COLLEGE**  
 CHENGANNUR, ALAPPUZHA, KERALA, INDIA  
*Affiliated to University of Kerala*

Sponsored by

**UNIVERSITY GRANTS COMMISSION**

**VENUE: COLLEGE AUDITORIUM**

**PROGRAMME**

**THURSDAY 17-03-2011**

9am-9.30am : **Registration**  
 9.45am : **Inaugural Session**  
 Invocation : **College Choir**  
 Welcome : **Dr.K.B.Manoj**  
 Co-ordinator  
 Presidential address : **Dr.V.K.Gopi**  
 Principal, S.N.College,  
 Chengannur  
 Inaugural Address : **Dr.S.V.Sudheer**  
 Director, Academic Staff College,  
 University of Kerala  
 Felicitations : **Mr.V.K.Vasudeva Panicker**  
 RDC Convenor  
**Dr.I.G.Shibi**  
 General Secretary, ACT  
**Mr.T.M.Philip**  
 HOD, Commerce  
 Vote of Thanks : **Dr.M.S.Latha**  
 HOD, Chemistry  
 10.30am-10.45am : Tea Break

## Technical Session

|                  |   |  |
|------------------|---|--|
| Session I        | : | 10.45am-11.30am  |
| Chair            | : | <b>Dr.U.C.Jaleel</b><br>Assistant Professor, Chemoinformatics,<br>Malabar Christian College, Calicut   |
| Topic            | : | <b>Open Source Drug Discovery</b>  |
| Resource Person  | : | <b>Dr.Zakir Thomas</b><br>Project Director, OSDD, CSIR, New Delhi                                      |
| Session II       | : | 11.30am-12.30pm  |
| Topic            | : | <b>QSAR: Introduction, Methodology and Successes</b>   |
| Resource Person  | : | <b>Vijay H. Masand</b><br>Department of Chemistry, Vidya Bharati<br>College, Amravati, Maharashtra     |
| 12.30 pm-1.30 pm | : | Lunch Break  |
| Session III      | : | 1.30pm-2.15pm  |
| Chair            | : | <b>Dr.M.S.Latha</b><br>HOD, P.G.Dept.of Chemistry,<br>S.N.College, Chengannur                          |
| Topic            | : | <b>Molecular Modelling</b>   |
| Resource Person  | : | <b>Mr.R.Raghu</b><br>Senior Director, Schrödinger, USA   |
| Session IV       | : | 2.15pm-3.15pm  |
| Chair            | : | <b>Dr.Desy P.Koruthu</b><br>Dept of Chemistry, Christian College,<br>Chengannur                        |
| Topic            | : | <b>Introduction to Drug Designing</b>  |
| Resource Person  | : | <b>Dr.U.C.Jaleel</b><br>Assistant Professor, Chemoinformatics,<br>Malabar Christian College, Calicut   |
| Session V        | : | 3.15pm-4.00pm  |
| Chair            | : | <b>Smt.Laila Ganagadharan</b><br>Associate Professor, Dept.of Chemistry,<br>D.B.College, Sasthamkottah |
| Topic            | : | <b>Molecular Dynamics</b>  |
| Resource Person  | : | <b>Dr. Prasad M Alex</b><br>Associate Professor, Dept of Chemistry,<br>Marthoma College, Chungathara   |
| 4.00 pm-4.15 pm  | : | Tea Break  |
| Session VI       | : | 4.15pm-5.30pm  |
|                  | : | <b>Paper Presentation</b>  |

Chair : **Dr.S.Sujatha**  
Associate Professor, Dept.of Chemistry,  
S.N.College, Chengannur

### Docking Studies on Some Quinazoline Analogues

**Dr.Kesav Mohan**  
(Director, Vellappally Natesan College of Engineering, Kattachira,  
Alappuzha)

### Why Computer Aided Drug Designing?

**Girinath G Pillai**  
(Researcher, State Inter University Centre for Bioinformatics,  
UoK, Kerala)

### A Novel Method for The Upper Rim Alkoxy-substitution of Calix[4] arene via a Bis(spirodienone) Route

**Sreeja Thulasi**  
(Organic Chemistry Section,  
Chemical Sciences and Technology Division, NIIST(CSIR), Trivandrum)

### Synthesis and Crystal Growth of 3-(2-morpholinyl-4-phenylthiazol-5-oyl) Coumarin

**R. Reshmy**  
(Department of Chemistry,  
Bishop Moore College, Mavelikara, Alappuzha)

### In Silico Development of Inhibition of Lanosterol Synthase Cholesterol Management

**A.S. Soubhagya**  
(Dept.of Chemistry, NIT Calicut)

### Studies on the Synthesis and Characterisation of a New Series of Biologically Active Transition Metal Schiff Base Complexes.

**Preetha G. Prasad**  
(Department of Basic Sciences, Sree Buddha College of Engineering,  
Pattoor, Alleppey)

### Novel Targets for Parkinson Disease

**Jayan.K**  
(Dept of Chemoinformatics, Malabar Christian College, Calicut)

## FRIDAY 18-03-2011

Invocation : College Choir  
Session VII : 9.00am-10.00am  
**Paper Presentation**

Chair : **Sreeja Thulasi**  
Assistant Professor, Dept of Chemistry,  
T.K.M.M.College, Nangiarkulangara

### Novel Multicomponent Reaction Involving Isoquinoline, DMAD and Isatilidenes Leading to the Synthesis of Functionalized Spiro-Oxindoles

#### B. Rema Devi

(Department of Chemistry, Sree Narayana College, Ala,  
Chengannur, India)

#### Molecular Descriptors

**Abhik Seal**  
(OSDD Chemoinformatics,  
DOEACC Centre, Kolkata (JU campus))

#### Personalised Medicine

**Kamini Raithatha**  
(OSDD Chemoinformatics, M S University, Baroda)

### Boarding from PubChem Compound Database to Weka

#### Ranjeet Singh

(Department of Biotechnology & Molecular Biology,  
Bangalore University, Bangalore)

### Data Mining Studies on Cytochrome P450 Activity of Functionalized Compounds-Molecular Descriptors in Modelling Activity

**Chiranjeevi Lakavath**  
(Indian Institute of Toxicology Research, Lucknow)

### Designing of Drugs through Computer followed by an Attempt for Synthesis

**Dr. G. M. Nazeruddin**  
(Department of Chemistry (P.G. Centre), Poona College Camp, Pune)

Session VIII : 10.00am-11.00am  
Chair : **Dr. Prasad M Alex**  
Associate Professor in Chemistry,  
Marthoma College, Chungathara

Topic : **Ligand Based Drug Design**  
**Dr.Anshu Bharadwaj**  
Scientist, IGIB, New Delhi

11.00am-11.15am : Tea Break  
Session IX : 11.15am-12.00pm  
Chair : **Dr.Kesav Mohan**  
Director, Vellappally Natesan College of  
Engineering, Kattachira, Alappuzha

Topic : **Protein Modelling, ADME and Binding Site Prediction**  
**Dr.Vinod Scaria**  
Scientist, IGIB, New Delhi

12.00pm-1.00pm : **Hands on training on Data Mining**  
**Vijay H. Masand**  
Department of Chemistry, Vidya Bharati  
College, Amravati, Maharashtra