



RESEARCH & POSTGRADUATE DEPARTMENT OF CHEMISTRY
ST. THOMAS' COLLEGE (AUTONOMOUS),

THRISSUR-680001, KERALA, INDIA.

**“COMPUTATIONAL QUANTUM MECHANICS &
MOLECULAR DESIGNING”**

NATIONAL WORKSHOP ON COMPUTATIONAL CHEMISTRY

28th & 29th September, 2015
Menachery Hall

Sponsored by



UNIVERSITY GRANTS COMMISSION

PROGRAMME SCHEDULE

28th September 2015

9:00 – 9:30 Registration
9:30 – 10:00 Inauguration Session
Mar Raphael Thattil,
(Manager)
Dr. P. O. Jenson
(Principal)
Dr. V Kumar
(C-MET Director)
10:00 – 11:00 Key note lecture
Dr. V. Kumar, Director
C-MET, Thrissur
11:00 – 11:15 Tea Break
11:15 – 12:45 Technical Session – I
“H-F, SCF methods”
Dr. Krishnamohan G.P
NIIST (Software Developer)
12:45 – 1:30 Lunch Break
1:30 – 04:00 Laboratory Session – I
“Molecular Designing”
Dr. Krishnamohan G.P
Dr. Resmi M.R,
Prof. Roy K.B.
Dr. Aneesh M.H.

29th September 2015

9:30 – 11:00 Technical Session – II
“Basis Sets, Z-matrix”
Dr. Krishnamohan G.P.
11:00 – 11:15 Tea Break
11:15 – 11:45 Technical Session – III
“Structure drawing softwares”
Dr. Resmi M.R,
SNGS College, Pattambi
11:45 – 12:15 Technical Session – IV
“Gaussian Programming”
Dr. Aneesh M.H.
PSMO College, Tirurangadi
12:15 – 12:45 Technical Session – V
“Computer simulation methods”
Prof. Roy K.B.
SNGS College, Pattambi
12:45 – 1:30 Lunch Break
1:30 – 3:30 Laboratory Session – II
“Optimization using Gaussian”
Dr. Krishnamohan G.P
Dr. Resmi M.R,
Prof. Roy K.B.
Dr. Aneesh M.H.
3:30 – 4:00 Valedictory Session

For registration and other details please contact:

Dr. Joby Thomas K (HOD, Chemistry)

Convener

Dr. Sunil Jose T

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Joint Conveners

Dr. Jency Thomas

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No Registration fee. No. of delegates restricted to 50.

Last date for registration: 25 September, 2015