

**DEPARTMENT OF CHEMISTRY**

**CERTIFICATE COURSE IN**

**MOLECULAR MODELLING  
TECHNIQUES AND DRUG DESIGN**

**DURATION : 3 MONTHS (32 HOURS)**

POST GRADUATE DEPARTMENT OF CHEMISTRY

ST.STEPHENS COLLEGE

PATHANAPURAM

CERTIFICATE COURSE IN

**“MOLECULAR MODELLING TECHNIQUES AND DRUG DESIGN”**

Course Code - CHE 2020

(32 hours)

Syllabus

**MODULE 1 Basics of cheminformatics**

(6 hours)

Chemical-biological databases and data sources; (Pubchem & PDB) Chemical file formats ; (MOL, SDF, PDB formats), File format conversion using OPEN BABEL.

**MODULE 2 Software Training**

(8 hours)

Chemistry related softwares - Structure drawing softwares, molecular modelling softwares, Molecular visualization tools (Avogadro ,Chemdraw, Pymol & Discovery Studio).

**MODULE 3 Computer assisted drug design**

(8 hours)

Drug Likeness Prediction – Properties of small molecules , structural features, ADME prediction, Bioavailability, Toxicity studies, Pharmacokinetics and Pharmacodynamics of drugs(Swiss ADME & PreADMET servers).

**MODULE 4 Computational quantum chemistry**

(3 hours)

Potential energy surface- stationary point, saddle point or transition state, local and global minima, Basis sets , Quantum mechanical computational methods-Ab initio methods, Semiempirical methods, DFT methods. Non-quantum mechanical computational methods.

**MODULE 5 Computational Chemistry Experiments**

(7 hours)

Single point energy and vibrational frequency calculation of simple molecules, Calculation of energy of HOMO and LUMO of simple organic molecules, Ionisation energy and electron affinity calculations.

  
Renu Thomas  
HoD & Associate Professor  
Department of Chemistry  
St. Stephen's College, Pathanapuram

## Course Outcomes

Through this course, the students will be able to

1. Apply computer-based calculations to determine the geometry, energies and properties of molecules.
2. Get hands-on experience in various insilico tools.

## Aim of the Course

The certificate course, “**MOLECULAR MODELLING TECHNIQUES AND DRUG DESIGN**” aims to bring an idea on the basic principles of computer aided drug design and about computational quantum chemistry.

## Scope of the course

Computational chemistry is a branch of chemistry that uses computer simulation to assist in solving complex chemical problems. It exploits methods of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures, the interactions, and the properties of molecules. Computational chemistry methods are fairly cheap, fast compared to experiments, and it is environmentally safe also. The process of drug development and drug discovery is very challenging, expensive and time consuming. It has been accelerated due to development of computational tools and methods. *In silico* screening paves path for the synthesis and screening of selected compounds as better therapeutic agents.

  
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## EVALUATION AND GRADING

The evaluation scheme of this course includes an internal evaluation. The components involved in evaluation include a written test and attendance. The marks assigned to various components for internal evaluation is as follows.

Sl.No.	Components	Marks
1	Test	20
2	Attendance	5
	Total	25

### **Evaluation of Attendance**

Percentage of attendance	Mark
Above 90%	5
Between 85 and below 90	4
Between 80 and below 85	3
Between 76 and below 80	2
75	1

### **Grading Scale**

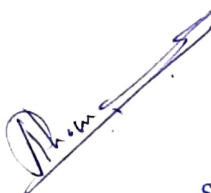
Percentage of marks	Grade
90 and above	A
Between 80 and below 90	B
Between 70 and below 60	C
Between 60 and below 50	D

## Grading and Evaluation

No.	Name of student	Attendance Percentage	Marks	Test Marks	Total	Grade
1	Anna Neha Roy	93	5	20	25	A
2	Athira M.S	100	5	20	25	A
3	Hiba Fathima Anzar	100	5	18	23	A
4	Neena Lekshmi	100	5	20	25	A
5	Nishana Nizar	100	5	20	25	A
6	Fidha Fathima	93	5	20	25	A
7	Ameena S.	100	5	18	23	A
8	Annie Koshy	100	5	20	25	A
9	Anusha .A	100	5	20	25	A
10	Archana N.M	93	5	20	25	A
11	Raji E.R	100	5	20	25	A
12	Jerin K Raju	100	5	20	25	A
13	Ullas Mohan	100	5	20	25	A
14	Abijith R J	100	5	19	24	A
15	Athira Vikraman	100	5	20	25	A

  
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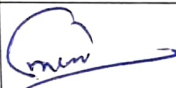
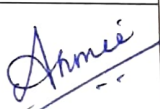

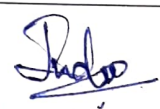







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## Details of Students Enrolled



No.	Name of student	Class	Email	Signature
1	Anna Neha Roy	B.Sc Chemistry (Sem 1)	annaneha25@gmail.com	
2	Athira M.S	B.Sc Chemistry (Sem 1)	athirameenu85@gmail.com	
3	Hiba Fathima Anzar	B.Sc Chemistry (Sem 1)	hibaanzar785@gmail.com	
4	Neena Lekshmi	B.Sc Chemistry (Sem 1)	neenalekshmi59@gmail.com	
5	Nishana Nizar	B.Sc Chemistry (Sem 1)	nishananisar4@gmail.com	
6	Fidha Fathima	B.Sc Chemistry (Sem 1)	fidhafathimaa2002@gmail.com	
7	Ameena S.	B.Sc Chemistry (Sem 1)	ameenaams4@gmail.com	
8	Annie Koshy	M.Sc Chemistry (Sem 1)	anniekoshy81@gmail.com	
9	Anusha .A	M.Sc Chemistry (Sem 1)	anushaias97@gmail.com	
10	Archana N.M	M.Sc Chemistry (Sem 1)	indooachu@gmail.com	
11	Raji E.R	M.Sc Chemistry (Sem 1)	rajimgr234@gmail.com	
12	Jerin K Raju	M.Sc Chemistry (Sem 1)	k.jerin.1998@gmail.com	
13	Ullas Mohan	M.Sc Chemistry (Sem 1)	ullasmohan1998ptpm@gmail.com	



  
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14	Abijith R J	M.Sc Chemistry (Sem 1)	abijithrj@gmail.com	
15.	Athira Vikraman	M.Sc Chemistry (Sem 1)	athiravishnu1999@gmail.com	



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