



# **JMOL APPLICATION**

## **C\_CHE2201**



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# ALL SAINTS' COLLEGE THIRUVANANTHAPURAM

*Affiliated to University of Kerala*

**Re-accredited with A+ Grade by NAAC**

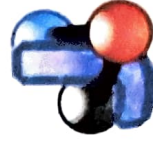
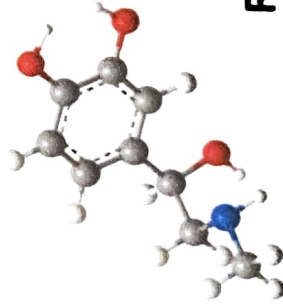


**spoken-tutorial**

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Ministry of Human Resources and  
Development, Government of India.

**Certificate Course conducted by  
The Department of Chemistry, All Saints' College, Thiruvananthapuram  
in Association with Spoken Tutorial Programme IIT Bombay  
for the academic year 2022-23**



*On Jmol Application*

**Duration – 30 hours**

**Registration starts on 26/2/23 and ends on 28/2/23  
Event Date: 3/3/23 to 10/4/23**

Srigowri M P  
Training Manager  
Spoken Tutorial - IIT Bombay

Event coordinator

Dr. Siji V L

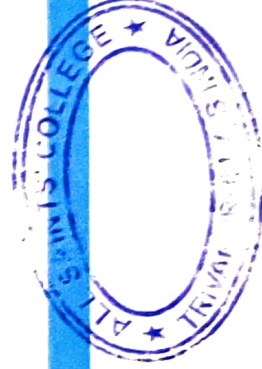
HOD

Dr. Sunita Kurur

*Reshmi*  
Principal

Dr. Reshmi R Prasad  
Principal

All Saints' College  
Thiruvananthapuram-7





## ALL SAINTS' COLLEGE

Thiruvananthapuram-695007, Kerala, India

Phone: 0471-2501153

E-mail: [allsaintscollegeasc@gmail.com](mailto:allsaintscollegeasc@gmail.com)

2022-2023

Name of Course	Certificate on Course on "Jmol Application"
Department offering the Course	Department of Chemistry
Course Duration	30 Hours
Start date	03/03/2023
End date	10/04/2023
Faculty In Charge	Dr. Siji V L

### SYLLABUS

Jmol is an open-source Java viewer for chemical structures and biomolecules in 3D. It does not require 3D acceleration plugins. 3D models created by using Jmol may be used as a teaching tool or for research in chemistry and biochemistry. It is free and open source software, written in Java, it runs on Windows, Mac OS X, Linux and Unix systems.

The Spoken Tutorial Effort for Jmol Application has being contributed by Dr. Snehalatha Kaliappan with domain reviews done by faculty and research scholars from the Chem Engg Dept, IIT Bombay.

#### Basic Level

##### 1. Overview of Jmol Application

- Learn about Jmol Application
- Important uses of Jmol
- Official website to download Jmol
- Information regarding Installation on various operating systems
- Download, extract and run Jmol Application on Ubuntu Linux OS
- Salient features of Jmol
- Show Jmol Wiki main page
- Advantages of Jmol
- Various uses of Jmol
- Play video clippings of Jmol Application tutorials available on ST website

##### 2. Introduction to Jmol Application

- Brief description about Jmol Application
- Software requirements
- Prerequisites
- Open the Jmol Application on Ubuntu/ Linux system
- Explain program interface (Menu Bar, Tool bar, Pop-up menu and display area)



  
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- Change the size of the display area
- Create models of simple organic molecules (alkanes)
- Energy Minimization
- Save the image as .mol file

### 3. Create and Edit Molecular Models

- Substitute the hydrogen in molecular model with a functional group
- Add and delete bonds
- Add and delete atoms
- Pop-up-menu (Contextual menu)

### 4. Modify Display and View

- Rotate, zoom, move and spin the model
- Modify the view
- Change the style of the display
- Change the size and color of atoms and bonds
- Axes and bound box
- Save the image in various file formats

### 5. Measurements and Labelling

- Create a model of Carboxylic acid. Example, Acetic acid
- Create a model of Nitroalkane. Example, Nitroethane
- Label atoms in a model with symbol of the element
- Label atoms in a model with number
- Label atoms in a model with both symbol and number
- Measure bond lengths in a model
- Examples : Carbon-Carbon single bond
- Carbon-Oxygen single and double bonds
- Measure bond angles in a model
- Measure dihedral angles in a model

## Intermediate Level

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### 6. Script Console and Script Commands

- About Script Commands
- How to write Script commands
- How to use Script console
- Change display of propane by using script commands
- Change the color of atoms and bonds
- Change the size of bonds and atoms



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- Display lines of text on panel
- Change color, font and size of font of the text

## 7. Surfaces and Orbitals

- Create models of alicyclic molecules. Example: Cyclohexane
- Create models of aromatic molecules. Example: Benzene
- Display Surface topology of molecules. Example: Molecular surface and Dot surface
- Create models of Atomic orbitals s, p, d and f
- Create models of Molecular Orbitals sp<sup>3</sup>, sp<sup>2</sup> and sp
- Create molecular orbitals for methane molecule
- Create molecular orbitals for ethene molecule

## 8. Structures from Database

- Load chemical structures from chemical structure database (PubChem)
- Load structure of Phenol and convert it to Para-amino Phenol
- Load structure of cholesterol and highlight the double-bond and side-chain
- Convert 2D structures drawn in GChemPaint to 3D models in Jmol
- Convert 2D structures of Alanine, Adenosine, Alpha-d-glucopyranose to 3D models in Jmol

## 9. Crystal Structure and Unit Cell

- Download CIF (Crystallographic Information File) from Crystallography Open Database (COD)
- Open CIF files in Jmol
- Display unit cell and unit cell parameters on Jmol panel
- Display crystal structures of different crystal systems. For example Cubic (sodium chloride), Hexagonal (graphite) and Rhombohedral (calcite)

## Advance Level

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### 10. Proteins and Macromolecules

- Load structures of proteins from Protein Data Bank (PDB)
- Download .pdb files from the database
- View the 3D structure of Insulin using PDB code (4EX1)
- View the structure without water molecules
- Modify the display of secondary structure
- Highlight hydrogen bonds and disulfide bonds

### 11. 3D Models of Enzymes



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- Load structure of Hexokinase using PDB code
- Modify the display of secondary structure
- Highlight amino acid residues at the active site
- Highlight the substrate
- Highlight the co-factors
- View Ramachandran plot for proteins

## 12. Symmetry and Point Groups

- Draw lines (C<sub>2</sub> and C<sub>3</sub> rotational axes) through atoms in methane molecule
- Spin and rotate the molecule along the axis
- Draw reflection plane through atoms in methane molecule
- Demonstration of point group classification using examples of methane and allene


## 13. Animation using Script Commands

- Jmol animation using script commands.
- Demonstration of animation using ethane and hemoglobin as examples.
- Script commands with keywords, move, delay, slab, loop and capture.
- Save the animation as GIF file.

## Course outcome:


Upon completion of the course the student will be able to

- Create and visualize chemical structures in 3D.
- Render secondary structures of proteins and nucleic acids.
- View crystal structure and unit cell parameters.
- Display structures in various display formats such as ball-and-stick, CPK, sticks etc.
- Change the thickness of bonds, colour of atoms and bonds.
- Rotate and view the molecule from various angles.
- Display interatomic distances, bond-angles, dihedral-angles, dipoles, charges and symbols.
- Display surfaces, atomic and molecular orbitals.
- Produce animations and create GIF files.

 Dr. Siji VL  
Coordinator



*Sumita K*  
Dr. Sumita Kukur  
HOD Dept of Chemistry

  
Principal  
All Saints' College  
Thiruvananthapuram-7



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2022-2023

Name of Course	Certificate on Course on "Jmol Application"
Department offering the Course	Department of Chemistry
Course Duration	30 Hours
Start date	03/03/2023
End date	10/04/2023
Faculty In Charge	Dr. Siji V L

### Course summary

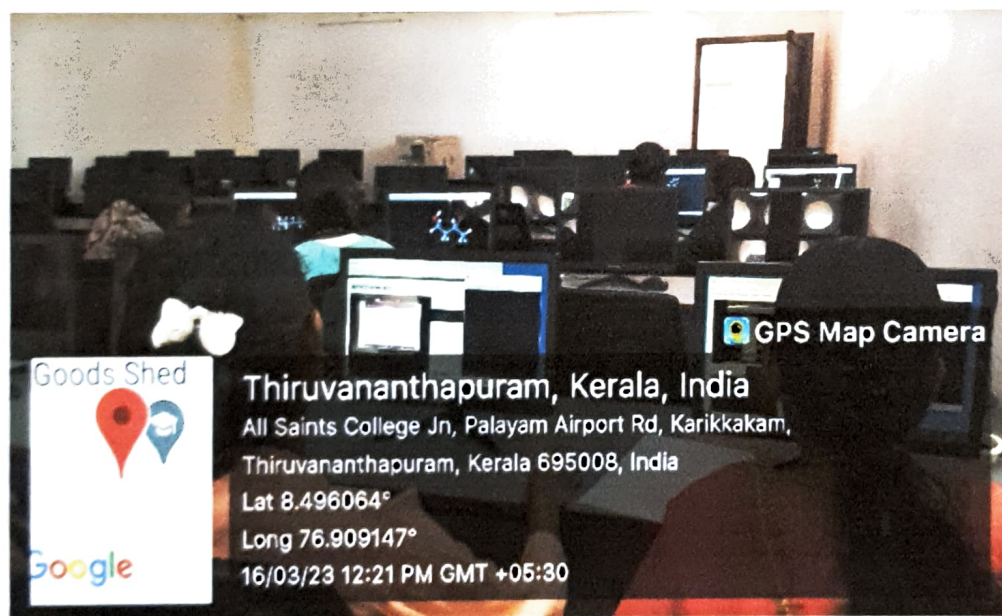
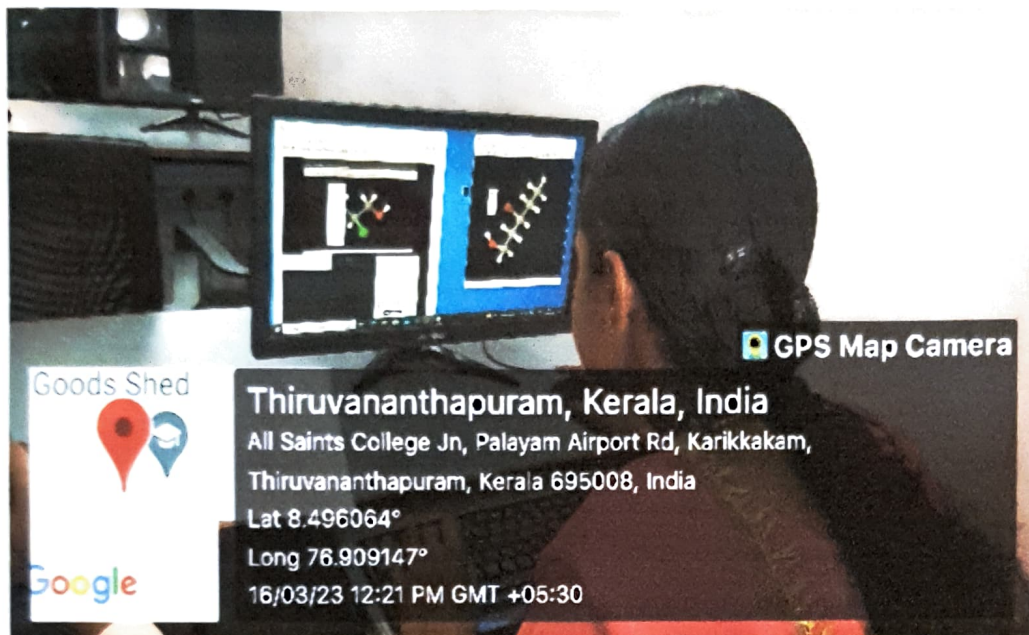
The certificate course "Jmol Application" has been organized by the Department of Chemistry, All Saints' College, Thiruvananthapuram, coordinated by Dr. Siji V L, Assistant Professor in the Department of Chemistry. The course was conducted in association with IIT Bombay, Spoken Tutorial Program, powered by MoE, Govt. of India. 44 students enrolled for the program. The course registration started on 26/02/2023 and ended on 28/02/2023. The event started on 03/03/2023 and ended on 10/04/2023. After completion of the course the students appeared for the online exam by IIT Bombay, Spoken Tutorial on 18/6/23. All students passed in the examination and obtained Participation certificate and Course completion certificate.

Registration link for the certificate course



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All Saints' College  
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Students attending the course

*[Signature]*  
 Dr. SIVIL  
 Coordinator



*[Signature]*  
 Dr. Sumita Kurer  
 HOD Dept of chemistry

*[Signature]*  
 Principal  
 All Saints' College  
 Thiruvananthapuram-7





भारतीय प्रौद्योगिकी संस्थान मुंबई  
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**Indian Institute of Technology Bombay**  
Powai, Mumbai-400 076, India

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फैक्स/Fax : (+91-22) 2572 3480

वेबसाइट/Website : [www.iitb.ac.in](http://www.iitb.ac.in)

IIT Bombay

### **Letter of Association.**

Ref.No. STIITB/2023/1212

Date 19-04-2023

To,  
Principal  
All Saints' College  
Thiruvananthapuram, Kerala.

We are delighted to provide your Institute the Letter of Association for the training you organised for students and faculties. **All Saints' College, Thiruvananthapuram, Kerala** engaged 44 Students and 2 Faculties in taking the IIT Bombay- ST courses on Jmol Application in association with **IIT Bombay, Spoken Tutorial Program** powered by MoE, Govt. of India.

The Certificate course on **Jmol Application** was conducted to the students and faculties, organised by **Dr. Sunita Kurur**, HOD, the Department of Chemistry from **3rd March to 10th April 2023** with 44 students and 2 faculties. The event was coordinated by **Dr. Siji V L** for the FDP and SDP and **Devika C S** for the SDP

In deep acknowledgement of your stellar efforts. We wish to collaborate many more times in this manner with you in coming years.

Yours Sincerely,

Yours Sincerely,  
For and On behalf of Spoken Tutorials  
Indian Institute of Technology, Bombay

*Akanksha Saini*



Mrs. Akanksha Saini  
National Coordinator  
Spoken Tutorial Project, IIT Bombay



भारतीय प्रौद्योगिकी संस्थान मुंबई  
पवई, मुंबई-400 076, भारत

**Indian Institute of Technology Bombay**  
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वेबसाइट/Website : www.iitb.ac.in

IIT Bombay

### Letter of Certification

Ref.No. STIITB/2023/1213

Date 19-04-2023

To,  
Principal  
All Saints' College  
Thiruvananthapuram, Kerala.

We are happy to provide your Institute the Letter of Certification for the training you organised for students and faculties. **All Saints' College, Thiruvananthapuram, Kerala** engaged 44 Students and 2 Faculties in taking the IIT Bombay- ST courses on Jmol Application in association with **IIT Bombay, Spoken Tutorial Program** powered by MoE, Govt. of India.

### Details of Participants enrolled in various Software Training Workshops under Spoken Tutorial, IIT Bombay.

Sl No:	Name of Student	Sl No:	Name of Student
1	Devika CS	23	Gowri S R
2	Gopika GS	24	Aditya A J
3	Ashini T M	25	Athira i
4	ASHMITHA D G	26	Anjali Sunny
5	Kesiya Salvador	27	Aswathy PL
6	Keerthi Krishna	28	SB. Sandra Rani
7	Aswasree B	29	Ganga V Anilkumar
8	Anjali Suresh S	30	Ardra krishnan k
9	DEVI S A	31	Aiswarya S
10	Revathy S A	32	Arya R
11	Anjana Stephen	33	Shabana.H
12	Amina S Muncer	34	Heera SJ

13	Amritha.m.k	35	Midhula M.M
14	Haripriya S	36	Ananniya Antony
15	Ajna Sakeensha	37	Geethu S
16	Hema Hegin	38	S AMINA
17	Archa P R	39	Drishya J R
18	Daliya S	40	Nandhana Terry
19	Anjitha. A. S	41	Neethu P V
20	Jincy.J	42	Anu .A
21	SARA ABEL	43	Soumya S S
22	Shivani	44	Anna Elizabeth
<b>Sl No:</b>	<b>Name of Faculty</b>	<b>Sl No:</b>	<b>Name of Faculty</b>
1	Dr. Shamla	2	RENJU K

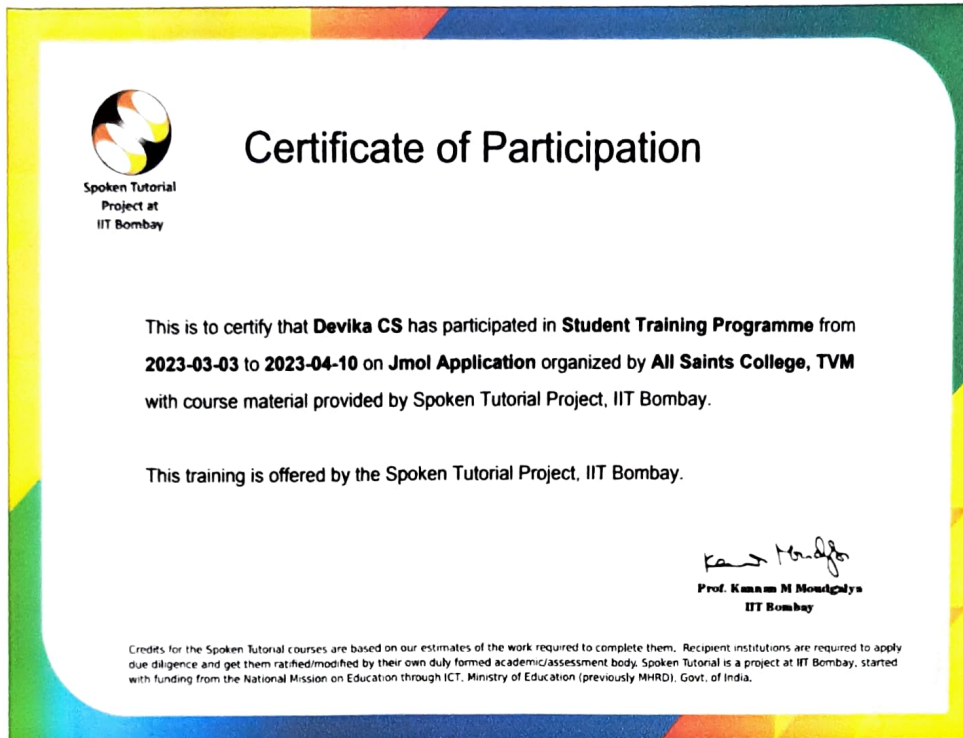
We congratulate the efforts taken in training the faculties and students. We wish to collaborate many more times in this manner with you in coming years.

Yours Sincerely,  
For and On behalf of Spoken Tutorials  
Indian Institute of Technology, Bombay

*Akanksha Saini* 

Mrs. Akanksha Saini  
National Coordinator  
Spoken Tutorial Project, IIT Bombay

## Sample Certificates



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All Saints' College  
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Project at  
IIT Bombay

## Certificate of Participation

This is to certify that **Kesiya Salvador** has participated in **Student Training Programme** from **2023-03-03 to 2023-04-10** on **Jmol Application** organized by **All Saints College, TVM** with course material provided by Spoken Tutorial Project, IIT Bombay.

This training is offered by the Spoken Tutorial Project, IIT Bombay.

  
Prof. Kannan M. Moudgal  
IIT Bombay

Credits for the Spoken Tutorial courses are based on our estimates of the work required to complete them. Recipient institutions are required to apply due diligence and get them ratified/modified by their own duly formed academic/assessment body. Spoken Tutorial is a project at IIT Bombay, started with funding from the National Mission on Education through ICT, Ministry of Education (previously MHRD), Govt. of India.



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Project at  
IIT Bombay

## Certificate for Completion of Training

This is to certify that **Kesiya Salvador** successfully passed a **Jmol Application** test, remotely conducted by the Spoken Tutorial project, IIT Bombay, under an honour invigilation system.

Self learning through Spoken Tutorials and passing an online test completes the training programme.

**Credits: 1    Score: 97.50%**

  
Prof. Kannan M. Moudgal  
IIT Bombay

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Project at  
IIT Bombay

## Certificate of Participation

This is to certify that **Arya RS** has participated in **Student Training Programme** from **2023-03-03 to 2023-04-10** on **Jmol Application** organized by **All Saints College, TVM** with course material provided by Spoken Tutorial Project, IIT Bombay.

This training is offered by the Spoken Tutorial Project, IIT Bombay.

Prof. Kannan M Moudgal  
IIT Bombay

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## Certificate for Completion of Training

This is to certify that **Arya RS** successfully passed a **Jmol Application** test, remotely conducted by the Spoken Tutorial project, IIT Bombay, under an honour invigilation system. Self learning through Spoken Tutorials and passing an online test completes the training programme.

**Credits: 1    Score: 97.50%**

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Principal  
All Saints' College  
Thiruvananthapuram.



## Certificate of Participation

This is to certify that **Anu .A** has participated in **Student Training Programme** from **2023-03-03 to 2023-04-10** on **Jmol Application** organized by **All Saints College, TVM** with course material provided by Spoken Tutorial Project, IIT Bombay.

This training is offered by the Spoken Tutorial Project, IIT Bombay.

  
Prof. Kannan M Moudgalya  
IIT Bombay

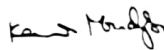
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## Certificate for Completion of Training

This is to certify that **Anu .A** successfully passed a **Jmol Application** test, remotely conducted by the Spoken Tutorial project, IIT Bombay, under an honour invigilation system. Self learning through Spoken Tutorials and passing an online test completes the training programme.

**Credits: 1    Score: 97.50%**

  
Prof. Kannan M Moudgalya  
IIT Bombay

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## Certificate of Participation

This is to certify that **Anna Elizabeth** has participated in **Student Training Programme** from **2023-03-03 to 2023-04-10** on **Jmol Application** organized by **All Saints College, TVM** with course material provided by Spoken Tutorial Project, IIT Bombay.

This training is offered by the Spoken Tutorial Project, IIT Bombay.

  
Prof. Kannan M Moudgalys  
IIT Bombay

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## Certificate for Completion of Training

This is to certify that **Anna Elizabeth** successfully passed a **Jmol Application** test, remotely conducted by the Spoken Tutorial project, IIT Bombay, under an honour invigilation system.

Self learning through Spoken Tutorials and passing an online test completes the training programme.

**Credits: 1 Score: 95.00%**

  
Prof. Kannan M Moudgalys  
IIT Bombay

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Admission No.	NAME	Days		Total Hours																										MARKS		Fees		Students' Initials	Class Teacher's Initials	Remarks																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
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Dr. Siji VL  
Teacher in charge

Dr. Sunita Kumar  
Head of Department

Dr. Reshmi R. Prasad  
Principal  
All Saints' College  
Thiruvananthapuram-7



INCREASE	On Register at the beginning	...	DECREASE	Promotions	...	No. at the end of the month	...	Attendance Total	...	Checked
	Promotions	...		Transfers	...	No. of Schedule caste, Hill Tribes & Other Backward Commu:	...	Average age	...	
	Transfers	...		Non-Payment	...	No. other full fee concession holders	...	No. of Hindus	...	
	New Admission	...		Temporary	...	Average Daily Strength	...	No. of Christians	...	
	Re-admission	...		Permanent	...	Do Do Attendance	...	No. of Mohammedans	...	
	Total Admission	...		Total Removal	...	Percentage of Attendance	...	No. of Jews	...	