



DEPARTMENT : PHYSICS

ACTIVITY : INTERNSHIP TRAINING PROGRAM

YEAR : 2023-2024

**DEPARTMENT OF PHYSICS**

DATES	TIME	VENUE
18.12.2023 to 22.12.2023	10:00 a.m. to 05:00 p.m.	Nadar Mahajana Sangam S.Vellaichamy Nadar College, Madurai
Theme	Exploring Computational Chemistry and Molecular Modeling	
Nature of the Activity	Internship Training Program - PG Project	
Title	Gaussian 09w, Vasp, Molecular Docking Software and Characterization Techniques	
Convener & Coordinator	<b>Mrs.R.Kayalvizhi</b> Head, Assistant Professor of Physics E.M.G. Yadava Women's College	
No. of Beneficiaries	Students - 7	

**INTERNSHIP TRAINING PROGRAM ON "MOLECULAR DOCKING"**

**Objectives:**

The objective of the PG Project and Internship Training Program was to provide participants with a comprehensive understanding of computational chemistry tools and characterization techniques.

The program aimed to:

- Equip participants with practical skills in utilizing computational tools for theoretical calculations, molecular simulations, and molecular docking studies.
- Provide participants with the knowledge and expertise necessary to undertake independent research projects in the field of computational chemistry and molecular modelling.
- Bridge the gap between theoretical concepts and practical applications by offering hands-on training sessions and real-world research experiences.
- Prepare participants for careers in research and industry by imparting relevant skills and knowledge in computational chemistry and molecular modeling techniques.

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- Promote collaboration and networking among participants, faculty, and industry experts to encourage interdisciplinary research and knowledge exchange.

### **Activities:**

Participants engaged in a comprehensive PG Project and underwent hands-on training sessions on computational chemistry and molecular modeling. They explored Molecular Docking Software for studying ligand-receptor interactions and employed advanced characterization techniques to analyze molecular structures and properties. The students received guidance from experts in the field on the application of computational tools in research and industry. Practical sessions on advanced characterization techniques provided participants with valuable skills in experimental analysis.

### **Programme Outcomes:**

1. Participants gained a deeper understanding of computational chemistry principles and techniques, including quantum mechanics calculations, molecular dynamics simulations, and molecular docking studies.
2. Practical training sessions equipped participants with proficiency in using Gaussian 09w, VASP, and Molecular Docking Software for various applications in drug discovery, materials science, and chemical engineering.
3. The PG Project enabled participants to apply their knowledge and skills to real-world research projects, fostering innovation and scientific inquiry.
4. Interaction with experts and peers during the program facilitated networking and collaboration opportunities for future research endeavors.

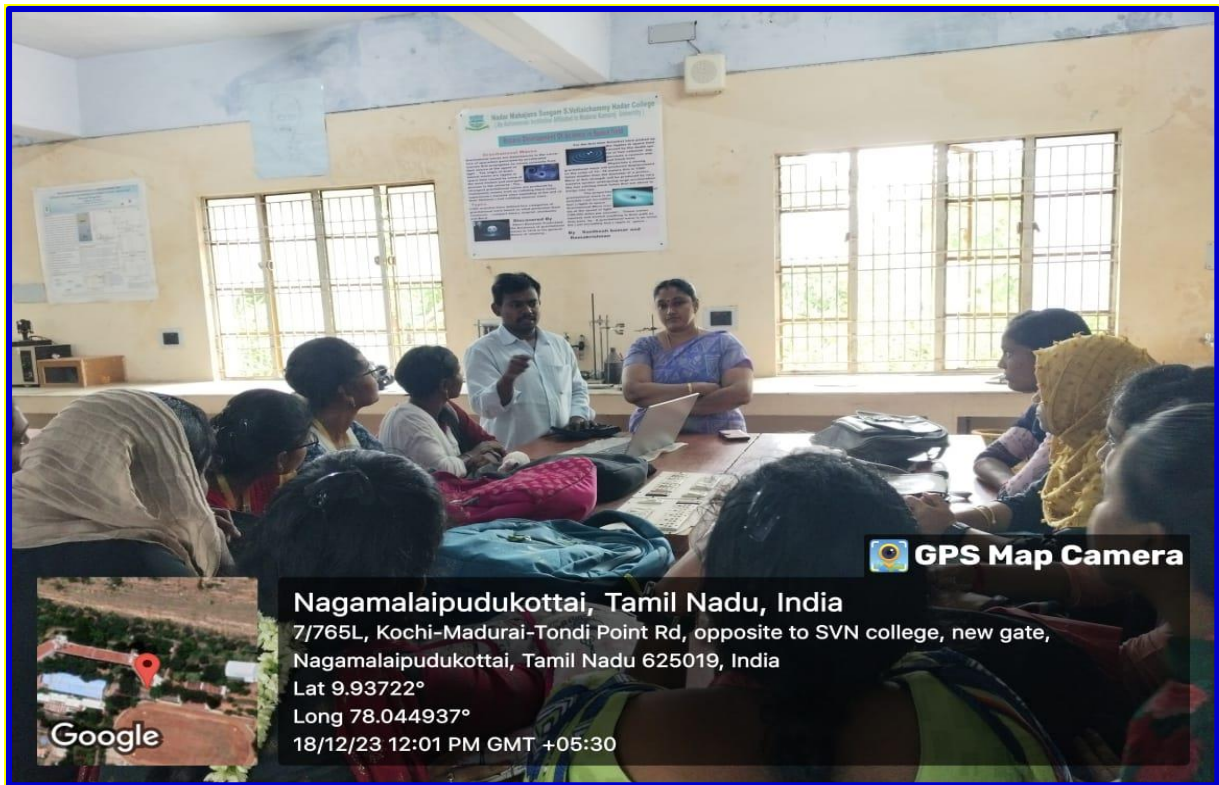
### **Feedback:**

Feedback from participants highlighted the following:

- Appreciation for the hands-on training sessions and practical exercises.
- Positive remarks on the expertise and guidance provided by faculty and industry professionals.
- Suggestions for more interactive sessions and opportunities for collaborative projects in future programs.

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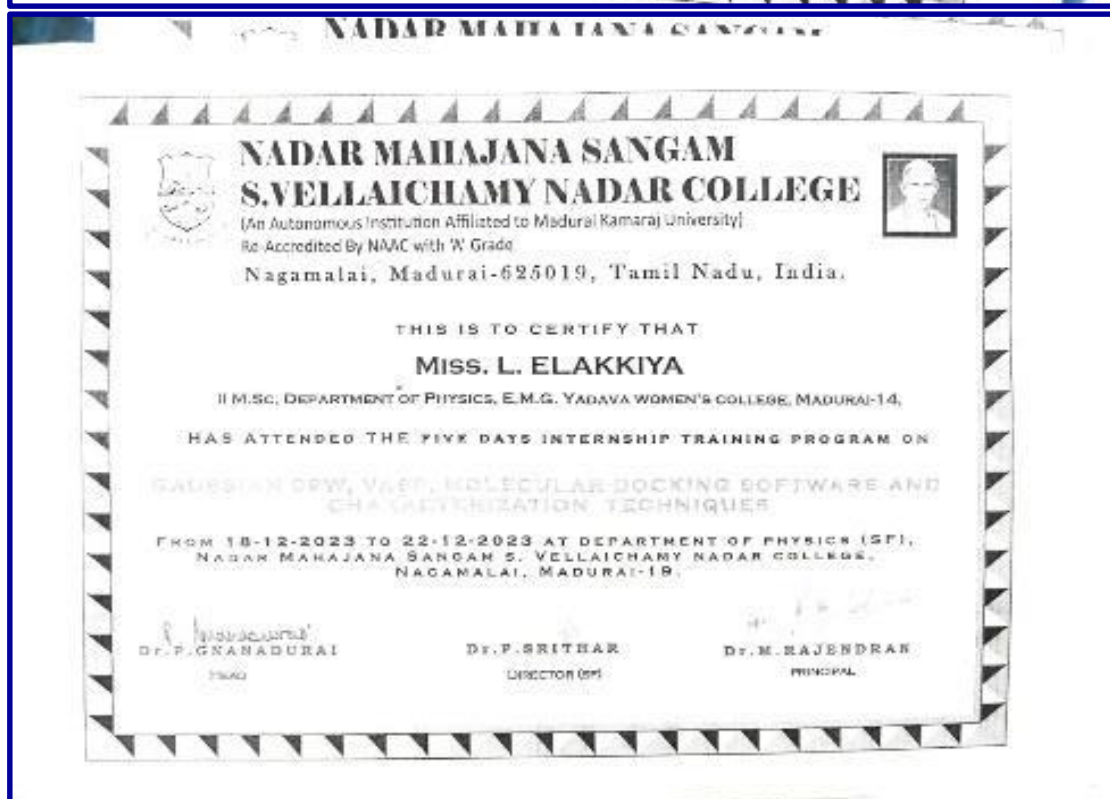
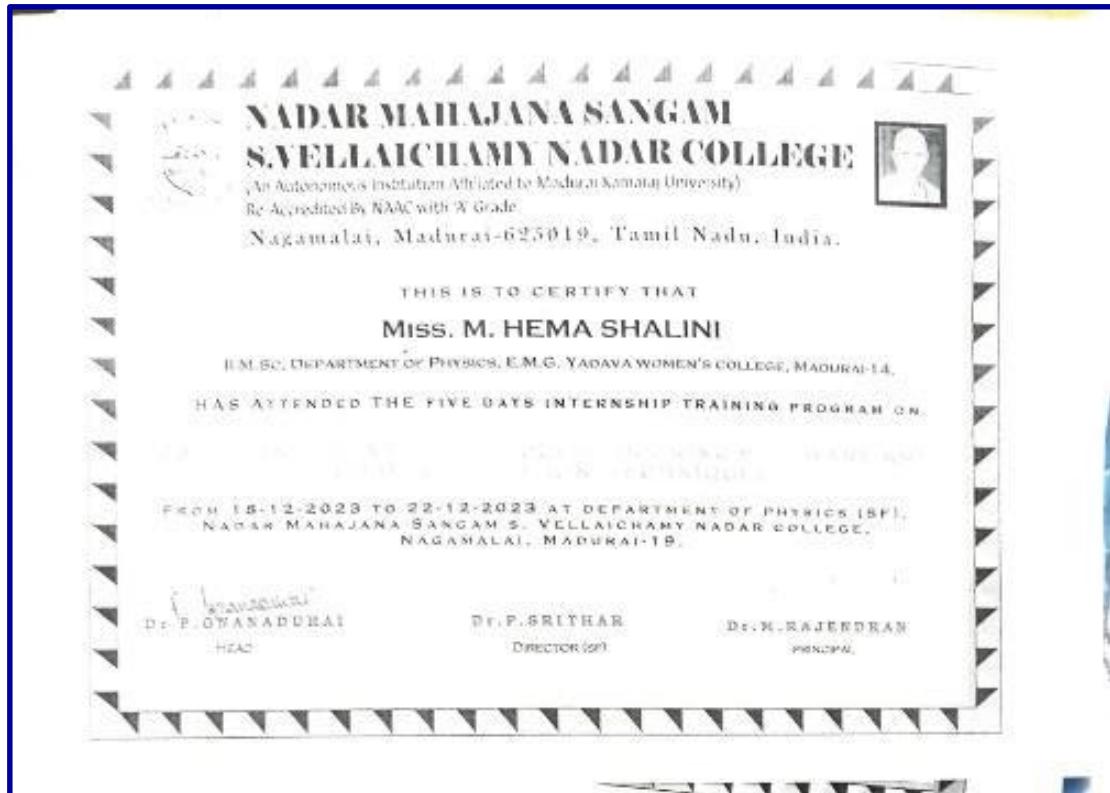
Photographs:



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## E.M. GOPALAKRISHNA KONE YADAVA WOMEN'S COLLEGE

### Student Participants:

 <b>E.M.G. YADAVA WOMEN'S COLLEGE, MADURAI – 625 014.</b> (An Autonomous Institution – Affiliated to Madurai Kamaraj University) Re-accredited (3 <sup>rd</sup> Cycle) with Grade A <sup>+</sup> and CGPA 3.51 by NAAC		
<b>Internship Training Program on “Gaussian 09w, Vasp, Molecular Docking Software and Characterization Techniques” - 18.12.2023 to 22.12.2023</b>		
<b>S.NO</b>	<b>Name of the Students</b>	<b>Register Number</b>
1.	L.Elakkiya	22PPH03
2.	M.Hemashalini	22PPH06
3.	S.Heeba Nasrin	22PPH05
4.	M.Kaviya	22PPH08
5.	M.Leena	22PPH09
6.	G.Pradeepa	22PPH10
7.	A.Rahini	22PPH12