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Department of Chemistry

ChemDraw Activity Report

Title: Introduction to ChemDraw for Chemical Structure Drawing and Reaction Mechanism Representation

Date: 20/01/2025

Venue: Chemistry Department

Conducted by: Jayashari Jasud

Objective of the Activity:

The primary objective of this activity was to familiarize students and researchers with the ChemDraw software, a widely used chemical structure drawing tool, and to enhance their ability to:

- Accurately draw chemical structures, including organic molecules, heterocycles, and reaction intermediates.
- Create and label reaction schemes and mechanisms.
- Calculate molecular properties such as molecular weight, IUPAC names, and elemental analysis.
- Generate and export publication-quality chemical drawings for research articles, theses, and presentations.

Methodology:

Participants were introduced to the basics of ChemDraw via a live demonstration, followed by hands-on practice. The session covered the following key activities:

1. **Introduction to ChemDraw Interface:**

Understanding toolbars, templates, atom and bond types, and shortcut keys.

2. **Drawing Simple and Complex Structures:**

Construction of aliphatic and aromatic compounds, heterocyclic systems (e.g., pyridine, quinoline), and functional groups.

3. **Reaction Mechanism Representation:**

Drawing curved arrows, electron flow, lone pairs, and transition states.

4. Use of Templates:

Using pre-built structure templates such as amino acids, nucleotides, and ring systems.

5. Structure to Name / Name to Structure Conversion:

Using the IUPAC naming tool and reverse structure prediction features.

6. Spectroscopic Features:

Generating predicted NMR shifts and chemical formulas.

7. Exporting for Publication:

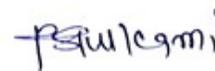
Creating high-resolution images in TIFF, PNG, and EPS formats for journal submission.

Outcome of the Activity:

- All participants successfully created chemical structures and reaction schemes using ChemDraw.
- Students learned how to generate IUPAC names and use atom numbering for spectral assignment.
- Participants appreciated the utility of ChemDraw in organizing and presenting synthetic schemes for research publications and thesis documentation.
- The activity improved overall understanding of chemical structure representation and encouraged the adoption of digital tools in academic and research writing.

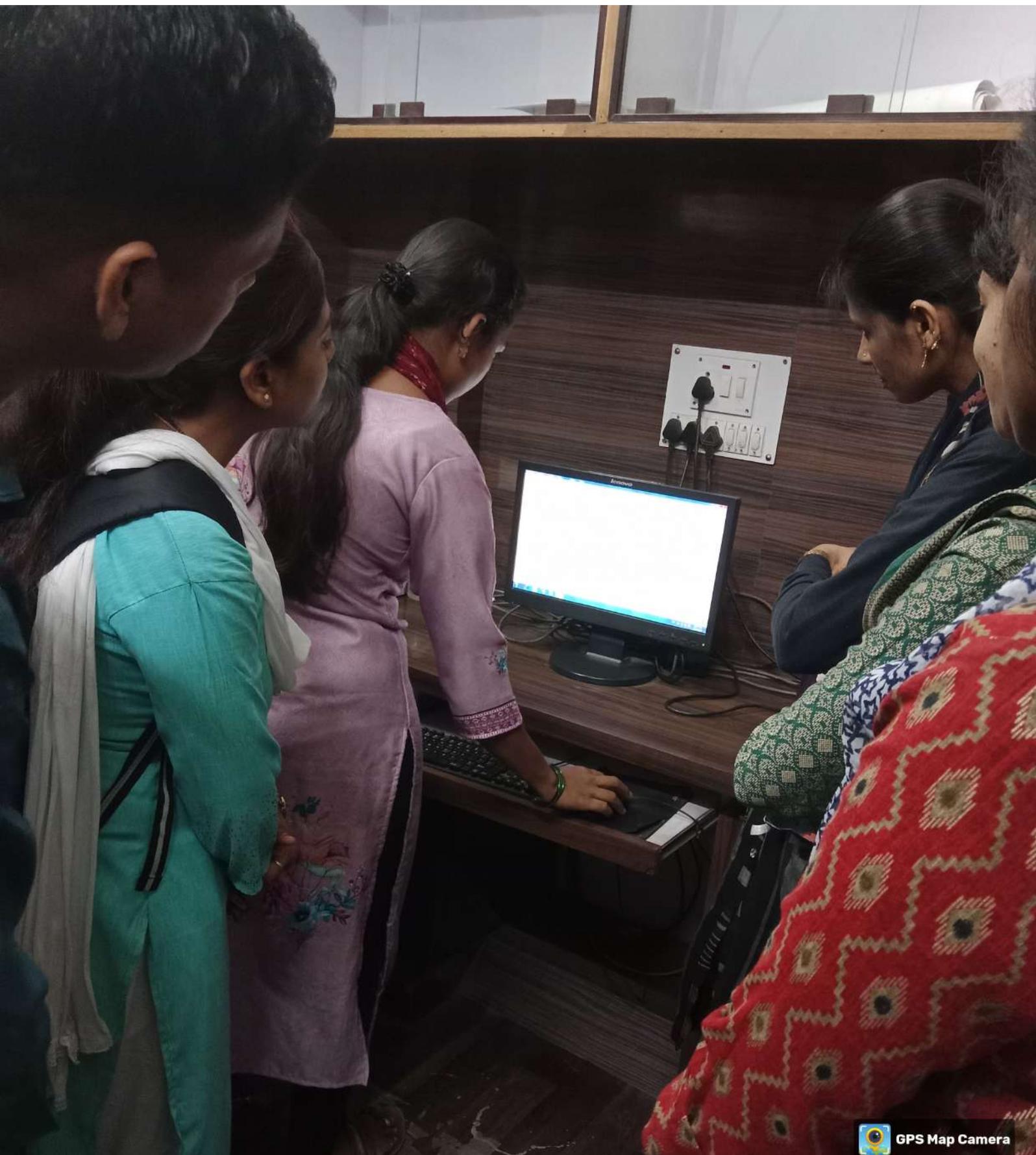
Conclusion:

The ChemDraw activity proved to be an effective educational and research-support tool. It helped bridge the gap between traditional hand-drawn chemical structures and modern digital representation, essential for scientific communication. Continued practice and advanced workshops are recommended to further enhance proficiency in using ChemDraw, especially for preparing high-quality graphical abstracts, mechanisms, and compound libraries.



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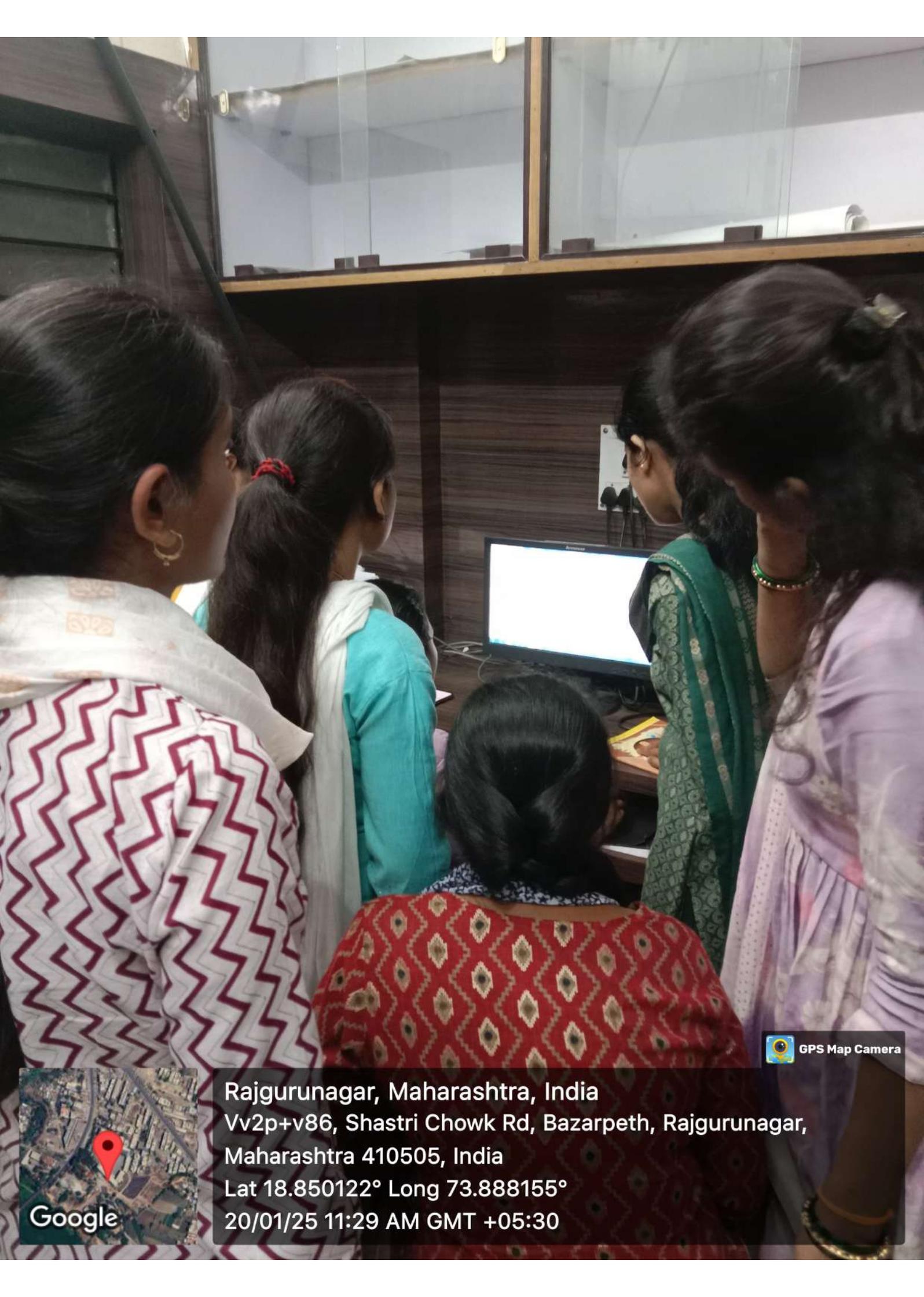


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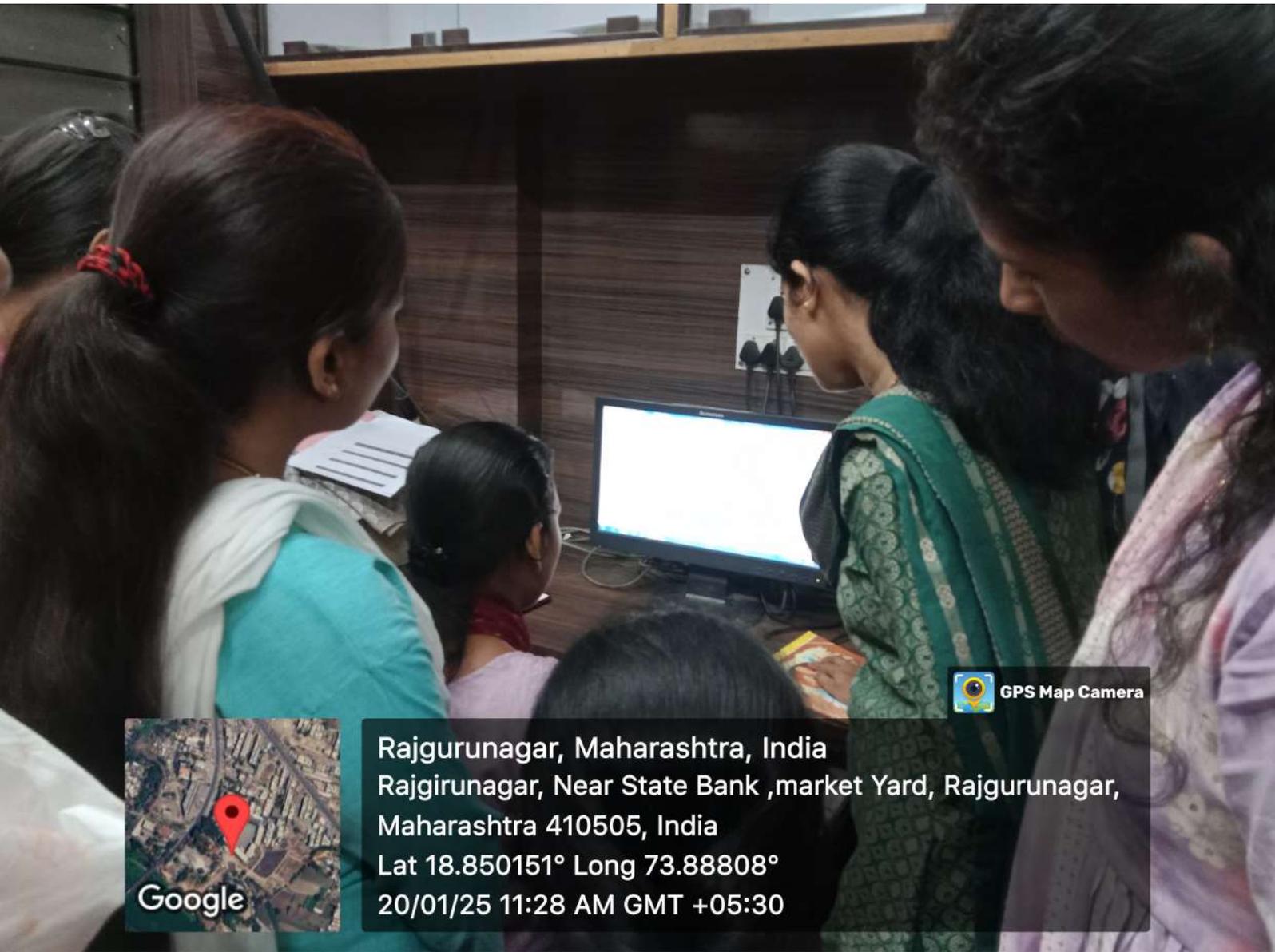
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