# NMAMIT NITTE
# Department of ISE
## MAJOR-PROJECT SYNOPSIS

| Student Name | USN | Student Signature |
|---|---|---|
| Saanvi U | NNM22IS133 | |
| Sanya Shresta Jathanna | NNM22IS141 | |
| Shachi Hegde | NNM22IS148 | |
| Shravya P Shetty | NNM22IS157 | |

| Guide Name | Signature with Date |
|---|---|
| Mr. Sharath Kumar | |

| | |
|---|---|
| **Project Title:** | AI-Powered Molecular Structure Generation and Visualization from Text, Images, and Video |

**Introduction:**

As students, understanding and visualizing molecular structures can be challenging, especially in experiments like acid-base titrations. Traditional learning methods often rely on theoretical explanations and static diagrams, making it difficult to grasp how molecules interact and change during chemical reactions. This lack of visualization can create a gap in understanding, especially in complex chemistry concepts.

To address this challenge and enhance the learning experience for students and educators, the app is proposed as a system that converts chemical names, photographed structures, and even video footage of chemical reactions into detailed 2D and 3D molecular models. By integrating advanced tools such as DeepChem, RDKit, OpenBabel, and computer vision algorithms, the app aims to provide accurate molecular representations for better interpretation.

This tool is particularly beneficial in educational settings, where instructors can use it to enhance chemistry demonstrations and experiments. Instead of relying solely on theoretical explanations, students can now see how molecules form, interact, and react in real-time, fostering a deeper understanding of chemical processes. With the app, learning chemistry becomes more interactive, engaging, and intuitive.

**Objective of the Project:**

- To develop a system that converts IUPAC and common chemical names into 2D and 3D molecular models for enhanced structure visualization.
- To develop a method for processing photographed chemical structures to generate precise 3D molecular models with detailed descriptions, improving molecular interpretation.
- To develop a video-based acid-base titration analysis system that detects color transitions (e.g., pink to colorless) and dynamically generates molecular structures to track reaction progress in real time.

**Problem Statement:**

This project aims to bridge this gap by developing a system that detects color transitions and dynamically generates molecular structures, while also converting IUPAC names, into representations. common names, and photographed images of chemical structures accurate 2D and 3D molecular representation .

**Methodology:**

**1. Data Collection and Preparation**

- Gather chemical data from public databases like **PubChem (using PUG REST API) and DeepChem's API**
- Collect images of molecular structures and titration reaction videos, and preprocess them to build datasets for training models.
- Clean and format data using **SMILES, SDF, and MOL file formats** for molecular representation.

**2. Model Development**

➢ **Chemical Name to 3D Structure:**

- Use RDKit and OpenBabel to convert IUPAC/common names into 2D and 3D molecular structures.
- Train deep learning models for name parsing and prediction of unknown structures.

➢ **Image to 3D Structure & Description:**

- Implement CNN-based deep learning models for chemical structure recognition.
- Use DeepChem and RDKit to convert recognized structures into 3D molecular models.
- Apply OCR (Optical Character Recognition) for extracting chemical information from images.

➢ **Video-Based Titration Analysis:**

- Utilize computer vision to detect color changes in acid-base titrations
- Train a deep learning model to analyze reaction progress and dynamically generate molecular structures.
- Implement regression models (MAE/RMSE) for accurate equivalence point detection.

**3. System Integration**

- Develop a **Flutter-based app** to integrate all three functionalities.
- Use **APIs (PubChem, DeepChem)** for chemical data retrieval.

- Implement **standardized data exchange formats (JSON, SMILES, SDF)** to ensure seamless communication between modules.

**4. Testing and Validation**

- Validate **name-to-structure accuracy** against PubChem and DeepChem datasets.
- Measure **image recognition performance** using the **Tanimoto similarity score**.
- Evaluate **titration video analysis** using MAE/RMSE to ensure accurate reaction tracking.

**5. Deployment and User Interface Design**

- Deploy the application on **Android & iOS** using **Flutter**.
- Implement a **user-friendly interface** with interactive 3D molecular visualization.
- Ensure real-time processing and responsiveness for an enhanced learning experience.

**Results / Conclusion:**

**Proposed Results:**

→ **Chemical Name to 3D Structure Conversion:** The system will effectively convert chemical names into accurate 2D and 3D structures using RDKit and OpenBabel, validated against PubChem and DeepChem databases.

→ **Image to 3D Structure & Description:** Deep learning models, especially CNNs, will accurately recognize molecular structures from images and convert them into 3D models. OCR integration will enhance chemical information extraction for improved accuracy.

→ **Video-Based Acid-Base Titration Analysis:** The system will successfully detect color changes in acid-base titration videos, track reaction progress, and dynamically generate molecular structures, with a focus on identifying equivalence points in real-time.

→ **System Integration:** All functionalities will be integrated into a Flutter-based app, with data exchanged in standardized formats like SMILES, SDF, and JSON, ensuring smooth communication across modules.

**References:**

**Major Reference:**

[1] O. S. Vasyutinskii, "Molecular reaction dynamics. By Raphael D. Levine," *J. Chem. Phys.*, vol. 122, no. 18, pp. 4664–4665, 2005.

**Other References:**

[2] K. Rajan, A. Zielesny, and C. Steinbeck, "STOUT V2.0: SMILES to IUPAC name conversion using transformer models," *J. Cheminformatics*, vol. 16, no. 1, p. 146, 2024.

[3] A. Fatemah, S. Rasool, and U. Habib, "Interactive 3D visualization of chemical structure diagrams embedded in text to aid spatial learning process of students," *J. Chem. Educ.*, vol. 97, no. 4, pp. 992–1000, 2020.

[4] F. Musazade, N. Jamalova, and J. Hasanov, "Review of techniques and models used in optical chemical structure recognition in images and scanned documents," *J. Cheminformatics*, vol. 14, no. 1, p. 61, 2022.

**_____ Only Office Use_____**

**Accepted/Rejected:**

**Suggestion/Corrections if any Specify:**

**Date:**

**Signature of the Project Coordinators:**