Dynamic Molecular Structure Generation from Text, Visual, and Video Inputs

Synopsis Presentation

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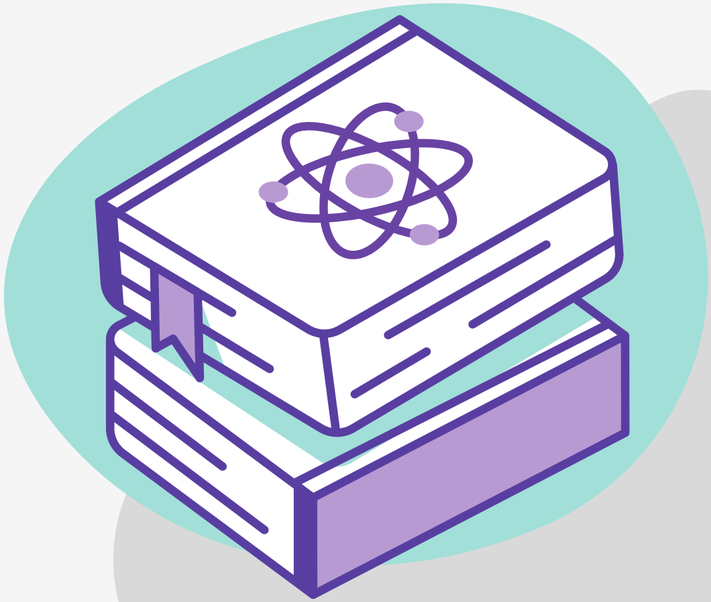


Introduction

- Difficult to visualize molecular interactions
- Static diagrams and theory limit understanding
- Complex concepts lack real-time representation
- Converts chemical names, images, and videos into **2D & 3D molecular models**

Introduction

- Uses **DeepChem, RDKit, OpenBabel, and computer vision** for accuracy
- Bridges the gap between theory and practical learning
- Enhances teaching with dynamic demonstrations
- Makes chemistry engaging & intuitive

Literature Survey

Literature Review

Research Gap

[1] D**istorted molecular structures** – Difficulty in recognizing distorted chemical structures, affecting **image-to-structure conversion accuracy**.

[11] No standardized datasets for chemical structure training – Lack of **well-curated datasets** affects model **generalization and accuracy** in molecular structure generation.

[18] Real-time molecular visualization & cheminformatics integration – Lack of seamless **real-time visualization** and integration with **cheminformatics tools** for molecular analysis.

[28] Lack of AI-driven error correction in computer vision for chemistry – Need for **enhanced recognition accuracy** in **molecular structure identification** from images and videos.

Motivation

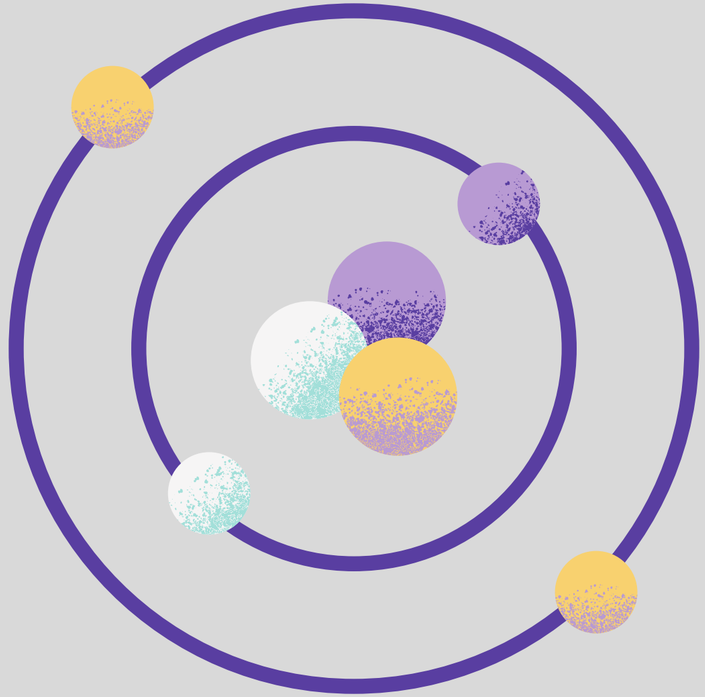
- The difficulty in accurately recognizing distorted molecular structures in low-quality images motivated us to find a more reliable solution for molecular analysis.
- The lack of standardized datasets in cheminformatics inspired us to work on improving model generalization and accuracy.
- The need for real-time molecular visualization in research and education drove us to explore interactive and dynamic solutions.
- The frequent errors in image-based molecular recognition highlighted the importance of AI-driven error correction to enhance efficiency and accuracy.

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.

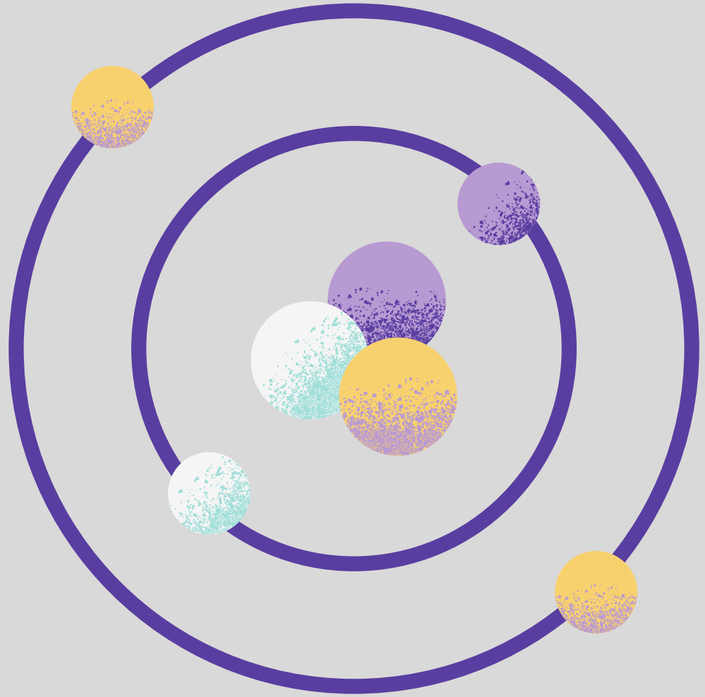
Problem Statement

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, common names, and photographed images of chemical structures into accurate 2D and 3D molecular representations .

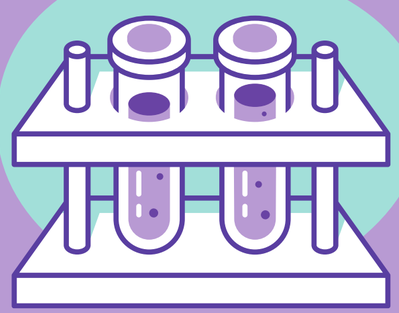


Methodology

1. Data Collection and Preparation
2. Model Development
3. System Integration
4. Testing and Validation
5. Deployment and User Interface Design



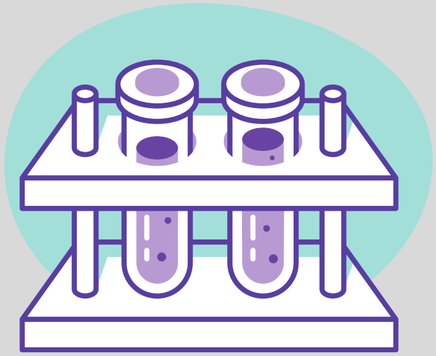
Methodology



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

Methodology



2. Model Development

- Chemical Name to 3D Structure
- Image to 3D Structure & Description
- Video-Based Titration Analysis

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

Methodology

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.

Expected Outcomes

- Chemical Name to 3D

Converts chemical names into 2D/3D structures using RDKit & OpenBabel, validated with PubChem & DeepChem

- Image to 3D Model

Uses CNNs & OCR to extract and convert molecular structures from images

- Video-Based Titration Analysis

Detects color changes, tracks reaction progress, and identifies equivalence points in real time

- System Integration

Flutter-based app using SMILES, SDF, and JSON for seamless communication

References

[1] Y. Chen *et al.*, "MolNexTR: A Generalized Deep Learning Model for Molecular Image Recognition," *J. Cheminformatics*, vol. 16, no. 1, p. 141, 2024.

[2] J. Correia, J. Capela, and M. Rocha, "DeepMol: An Automated Machine and Deep Learning Framework for Computational Chemistry," *J. Cheminformatics*, vol. 16, no. 1, pp. 1–17, 2024.

[3] T. Wu *et al.*, "Molecular Joint Representation Learning via Multi-Modal Information of SMILES and Graphs," *IEEE/ACM Trans. Comput. Biol. Bioinf.*, vol. 20, no. 5, pp. 3044–3055, 2023.

[4] P. Liu *et al.*, "GIT-Mol: A Multi-Modal Large Language Model for Molecular Science with Graph, Image, and Text," *Comput. Biol. Med.*, vol. 171, p. 108073, 2024.

[5] M. Maria *et al.*, "VTX: Real-Time High-Performance Molecular Structure and Dynamics Visualization Software," *arXiv preprint arXiv:2501.12750*, 2025.

[6] K. Seshadri, P. Liu, and D. R. Koes, "The 3Dmol.js Learning Environment: A Classroom Response System for 3D Chemical Structures," *J. Chem. Educ.*, vol. 97, no. 11, pp. 3872–3876, 2020.

[7] A. A. Alharbi, "Cognitive Learning Approach to Enhance University Students' Visualization of Molecular Geometry in Chemical Compounds: A Case Study in Saudi Arabia," *J. Radiat. Res. Appl. Sci.*, vol. 18, no. 1, p. 101283, 2025.

[8] N. Hazarika, R. K. Roy, H. K. Singh, and T. Bezboruah, "On the Use of Computer Vision to Estimate Chemical Concentration Based on Colorimetric Analysis," *International Journal of Computer Applications*, vol. 174, no. 21, pp. 1–7, 2022.

[9] A. K. Shah *et al.*, "ChemScraper: Leveraging PDF graphics instructions for molecular diagram parsing," *Int. J. Document Anal. Recognit. (IJDAR)*, vol. 27, no. 3, pp. 395–414, 2024.

[10] J. Li *et al.*, "ChemVLM: Exploring the power of multimodal large language models in chemistry area," *arXiv preprint arXiv:2408.07246*, 2024.

References

[11] 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.

[12] M. Hirohara *et al.*, "Convolutional neural network based on SMILES representation of compounds for detecting chemical motif," *BMC Bioinformatics*, vol. 19, pp. 83–94, 2018.

[13] T. N. Astuti, K. H. Sugiyarto, and J. Ikhsan, "Effect of 3D visualization on students' critical thinking skills and scientific attitude in chemistry," *Int. J. Instruction*, vol. 13, no. 1, pp. 151–164, 2020.

[14] X. Wu *et al.*, "Graph neural networks for molecular and materials representation," *J. Mater. Informatics*, vol. 3, no. 2, 2023.

[15] A. Fatemah, S. Rasool, and U. Habib, "Interactive 3D visualization of chemical structures embedded in text to aid spatial learning process of students," 2023.

[16] K. Zhang, Y. Lin, G. Wu, Y. Ren, X. Zhang, B. Wang, X. Zhang, and W. Du, "Sculpting Molecules in Text-3D Space: A Flexible Substructure-Aware Framework for Text-Oriented Molecular Optimization," *Nature Communications*, vol. 15, pp. 1–15, 2024.

[17] K. Rajan, A. Zielesny, and C. Steinbeck, "STOUT V2.0: SMILES to IUPAC Name Conversion Using Transformer Models," *Journal of Cheminformatics*, vol. 14, no. 1, pp. 1–10, 2024.

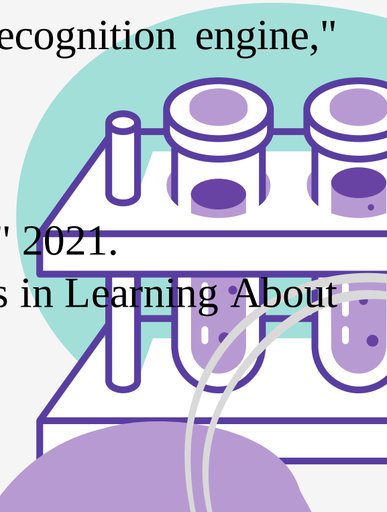
[18] M. Sandje, S. Ouattara, D. D. Jerome, and A. Clément, "Method of Estimation of Chemical Compounds of a Solution by Analysis of Video Images of Titration from a Semi-Automatic Approach," *International Journal of Chemical Sciences*, vol. 36, no. 4, pp. 455–469, 2022.

[19] R. Kumar, M. P. Chaudhary, and N. Chauhan, "Recent Advances and Current Strategies of Cheminformatics with Artificial Intelligence for Development of Molecular Chemistry Simulations," *Journal of Molecular Graphics and Modelling*, vol. 114, pp. 108145, 2022.

[20] D. S. Wigh, J. M. Goodman, and A. A. Lapkin, "A Review of Molecular Representation in the Age of Machine Learning," *Chemical Reviews*, vol. 122, no. 10, pp. 11154–11192, 2022.

References

[21] Y. Xu, J. Xiao, C.-H. Chou, J. Zhang, J. Zhu, Q. Hu, H. Li, N. Han, B. Liu, S. Zhang, J. Han, Z. Zhang, S. Zhang, W. Zhang, L. Lai, and J. Pei, "MolMiner: You Only Look Once for Chemical Structure Recognition," *Chemical Science*, vol. 13, no. 24, pp. 7168–7180, 2022.
[22] I. I. Salame, A. Montero, and D. Eschweiler, "Examining Some of the Students' Challenges and Alternative Conceptions in Learning About Acid-Base Titrations," *Journal of Chemical Education*, vol. 99, no. 7, pp. 2567–2575, 2022.
[23] J. Mao, J. Wang, K.-H. Cho, and K. T. No, "IUPAC-GPT: IUPAC-based large-scale molecular pre-trained model for property prediction and molecule generation," 2023.
[24] B. Zhang, L. Meng, Q. Song, J. Zhang, and L. Xu, "HSV color space-based automated chemical titrator," 2023.
[25] K. Rajan, H. O. Brinkhaus, A. Zielesny, and C. Steinbeck, "Advancements in hand-drawn chemical structure recognition through an enhanced DECIMER architecture," 2024.
[26] I. Khokhlov, L. Krasnov, M. V. Fedorov, and S. Sosnin, "Image2SMILES: Transformer-based molecular optical recognition engine," 2023.
[27] B. Baillif, J. Cole, P. McCabe, and A. Bender, "Deep generative models for 3D molecular structure," 2023.
[28] Y. Kosenkov and D. Kosenkov, "Computer vision in chemistry: Automatic titration," 2021.
[29] Y. Fan, J. Li, Y. Guo, L. Xie, and G. Zhang, "Digital image colorimetry on smartphones for chemical analysis: A review," 2021.
[30] I. I. Salame, A. Montero, and D. Eschweiler, "Examining Some of the Students' Challenges and Alternative Conceptions in Learning About Acid-Base Titrations," *Journal of Chemical Education*, vol. 99, no. 7, pp. 2567–2575, 2022.



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