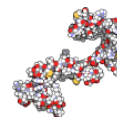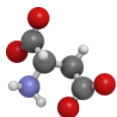# ARGET ATRP

1. Overview

The ARGET ATRP Dash app is a comprehensive tool designed to facilitate the understanding and application of the Atom Transfer Radical Polymerization (ATRP) technique, with a specific focus on the ARGET (Activators Regenerated by Electron Transfer) variation. This application serves as an educational and practical resource for chemists, researchers, and students engaged in polymer science, providing interactive visualizations, calculations, and literature references to enhance the learning and research experience.
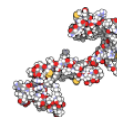
2. Key Features

- **Interactive Polymerization Simulations:** Visualize the polymerization process under various conditions.
- **Parameter Optimization Tool:** Experiment with different reactant concentrations, temperatures, and catalysts to find optimal conditions for your reactions.
- **Data Analysis:** Upload experimental data to compare with simulated results for validation and analysis.

3. Development Team

- Kauê Scaranari Alcantara <k175992@dac.unicamp.br> || UNICAMP
- Profa. Dra. Liliane Maria Ferrareso Lona <lona@unicamp.br> || UNICAMP
- Prof. Dr. Nicolas Spogis <nicolas.spogis@gmail.com> || UNICAMP || <https://linktr.ee/CascaGrossaSuprema>

ARGET ATRP

4. Installation

To install the necessary dependencies, you need to have Python installed on your system. If you don't have Python, you can download it (https://www.python.org/downloads/). After installing Python, follow the steps below:

- **Clone the Repository:** First, clone the ARGET ATRP App repository to your local machine (https://github.com/Spogis/ARGET_ATRP_MLP)
- **Install Dependencies:** Within the project directory, locate the `requirements.txt` file containing all necessary libraries. Install them by running: `pip install -r requirements.txt`. This will install all the dependencies required to run Easy DOE.
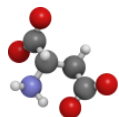
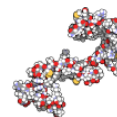## 5. Execution

To run the application, follow these steps:

- Navigate to the project directory where `main.py` is located.
- Execute the `main.py` file using Python: `python main.py`
- After running the command, Dash will start the local server and you can access the application through your browser. Normally, the URL will be something like `http://127.0.0.5:8080/`.

6. Support

If you encounter any problems or have any questions, do not hesitate to open an issue in the GitHub repository or contact us directly.

ARGET ATRP

7. License

This project is licensed under the Apache License - see the LICENSE.md file for details.

8. Contact: https://linktr.ee/CascaGrossaSuprema