1 Evaluación EC1

Parte 1. Software y Licencias

1a. Crear su software aplicado a quiralidad (como se desarrolló en clase) y verificar su correcta operatividad (funcional en streamlit). Asignar el nombre inchiral-apellido.streamlit.app a su enlace en streamlit (8 puntos)

1b. Agregar una tabla con 2 posibles licencias y justificar porqué las considera pertinente para este trabajo (2 puntos)

Parte 2. Reporte académico del trabajo

De acuerdo al formato IMRyD, trabaje el manuscrito desde la plantilla sugerida en overleaf:

2a. Agregue al menos 1 imagen en resultados, haciendo uso del software en streamlit. (1 punto)

2b. Agregue contenido en todas las secciones donde se indica "EDITAR". Agregar comentarios en color (6 puntos):

- Rojo para partes que considere que están incompletas o se deben modificar.
- Azul para partes que considere que estan listas pero que Ud no trabajó.
- Verde para las partes que están listas y que Ud. realizó o que realizará en esta evaluación. Sugerencia: Puede usar por ejemplo: "el texto que quiero colorear de azul"

2c. Agregue citas bibliográficas a cada comentario que agregó en "2b". (3 puntos)

Web Generator of 3D Stereoisomeric Structures

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Abstract

(Recuerde que este trabajo tiene el formato IMRyD, es decir, Introducción, Metodología, Resultados y Discusiones. No es necesario que intervenga en el Abstract. Las ediciones para la evaluación EC1 inician desde la "Introducción") Stereochemistry is a critical aspect of the structure-function relationship between organic molecules, given that stereoisomers of the same compound can exhibit radically different physicochemical and biological properties. However, a recurring limitation in molecular modeling databases and tools is the underrepresentation of stereochemical space. These databases typically only include previously reported or synthesized structures, which restricts computational exploration and rational drug design. In this work, we present a freely accessible web-based platform, developed in Python, that allows the automatic generation of all three-dimensional stereoisomeric structures from the SMILES code of organic molecules. To this end, the RDKit and Open Babel toolkits were integrated, enabling systematic stereochemical enumeration and construction of 3D geometries. The generated structures can be freely downloaded in standard formats, facilitating their application in molecular docking studies, QSAR, molecular dynamics, and virtual database exploration. The platform's source code is also available on GitHub under the GPLv3 license, promoting reproducibility and open collaboration within the scientific community. This tool contributes to closing the gap in the comprehensive representation of stereochemical space, boosting research in cheminformatics, computational chemistry, and drug design.

Keywords

Stereoisomeric, chirality, streamlit, cheminformatics

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2 Introduction

Despite advances in molecular representation, one of the main limitations in the modeling and rational design of organic compounds is the underrepresentation of stereochemical space [1]. A molecule with multiple chiral centers can give rise to a large number of three-dimensional stereoisomers (theoretically up to 2^n, with n chiral centers) [2]. However, most chemical databases only record those that have been synthesized or experimentally reported. This limitation creates a knowledge gap, as there is no complete representation of all possible stereochemical variants [3].

This gap has important implications for the prediction of physicochemical and biological properties. The literature has shown that stereoisomers of the same molecule can exhibit drastic differences in solubility, reactivity, metabolism, toxicity, and pharmacological activity; one enantiomer may be therapeutic, while its mirror image may be inactive or even harmful. In this context, the lack of a systematic inventory of stereoisomers compromises the validity of molecular docking studies, QSAR, molecular dynamics, and artificial intelligence-based models, which critically depend on the correct 3D geometry of the evaluated isomer.

Therefore, the computational generation of all three-dimensional stereoisomeric structures of an organic molecule seeks to close this gap by providing a comprehensive and accurate representation of the stereochemical space. This not only expands the coverage of candidate compound screening but also increases the reliability of predictive models in cheminformatics, drug design, and computational chemistry, decisively contributing to the identification of the stereoisomer responsible for the desired biological activity.

3 Methodology

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3.1 Workflow

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4 Results

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5 Discusion

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6 Conclusions

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Acknowledgments

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