Fluorescence Quantum Yield Prediction

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1 Introduction

2 Data preparation

Step 1

The first step is to prepare the data, at the first stage we are going to prepare the data encounter in the article writen by [**Ju2021**]. For this purpose we are going to take the SMILES structures, transform them to a 3D structures using the RDKit module, after that we are going to optimize the structures using the MN15/6-311+G(d,p) method and basis. Using the optimized structures a set of descriptors are going to be calculated.

- Take the SMILES structures
- Transform them to 3D structures
- Optimize the structures using the MN15/6-311+G(d,p) method and basis

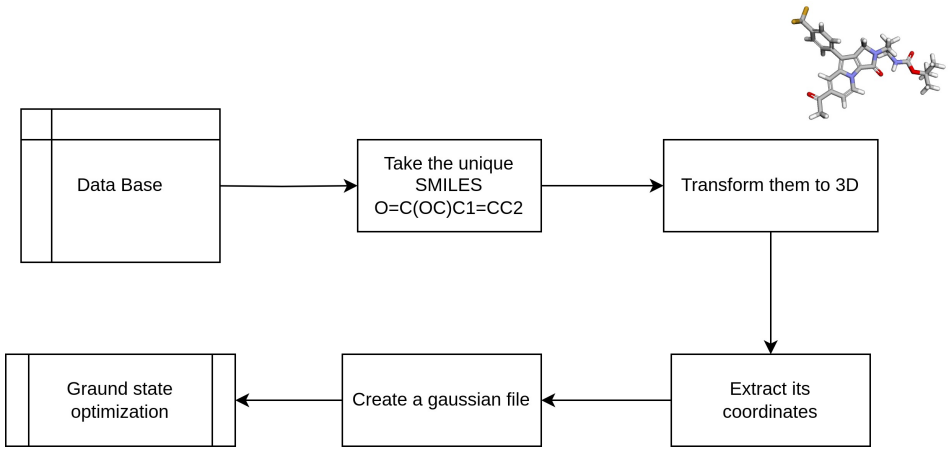

Figure 1: Molecular structures preparation

- Calculate the descriptors

q q

3 Results

4 Conclusion