PyMolDat - Molecule Viewing Software

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Abstract

Abstract 1:

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1. *Concept*

1.1 Introduction

What did we do? How can one access the software (GitHub link)?

1.2 Motivation

Adding polarisation graphics/Van der Waals interactions on a software package is easier than added plugins to PyMol etc.

1.3 Week 2-3

I chose to use matplotlib due to it's ease in integrating into a GUI window, and for its numerous methods to create interactive objects.

2. *Week 1-3*

2.1 Prototyping Molecule Viewer

2.2 Database

2.3 Molecular Connectivity Algorithm

2.3.1

3. *Chapter 3*

3.1 Chapter 3

4. *Conclusion*

4.1 Summary and Final Thoughts for the Reader

5. *References*