

MaMEA User's Guide

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1 Introduction

MaMEA (MacroMolecular Evolutionary Algorithm) is a genetic algorithm (GA) for chemistry. It aims to be as general as possible, being suitable for use with any class of molecules. While it does not support all types of molecules out of the box it is designed to be easily extended. This is made easier by being written in Python. For notes on how to extend MaMEA to a new class of molecules or add GA operations, see the developer's guide.

2 Installing MaMEA

3 Input Files

4 Running MaMEA

4.1 From the command line.

5 Output

6 MaMEA as a Library