DeCAF – Discriminatic

1. Introduction

Predicting biological activity of small molecules is a key element of computer-aided drug design. Existing methods often fa
similar physicochemical properties but different structures. Many of the current approaches rely on generating 3D conf
sampling problems and unacceptably high computational costs for large sets of molecules. Herein we present DeCAF – a n
ligand properties and a fast and effective tool for comparing multiple molecules, and merging them into a single pharmacophor
as an open source Python module (**http://bitbucket.org/marta-sd/decaf**) and can be easily combined with RDKit to f
design.