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Notes: AI application for azophotoswitches' optimization with pharmacological interest

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"The dumbest people I know are those who know it all."

Malcolm S. Forbes

Abstract

Insert abstract

I Introduction

The impact of Artificial Intelligence on science has being nothing but an outstanding breakthrough without many comparable predecessors. This projects aims to develop an implementation of artificial intelligence in computational chemistry, more concretely we aim to use artificial intelligence - based algorithms to predict the inhibition potential of a molecules for a certain protein.

Now a days one of the main goals of computational chemistry is the capability of predicting certain properties of unstudied substances without the experimental costs. Moreover we do focus on the *cyclooxygenase-2* (COX-2) since is well known to be related to cancer development.