SPECIAL INTEREST GROUP

DRUG-DESIGN

DERIVATED OF DIBENZOYLMETHANE: IN SILICO ANALYSIS FOR DRUG DEVELOPMENT

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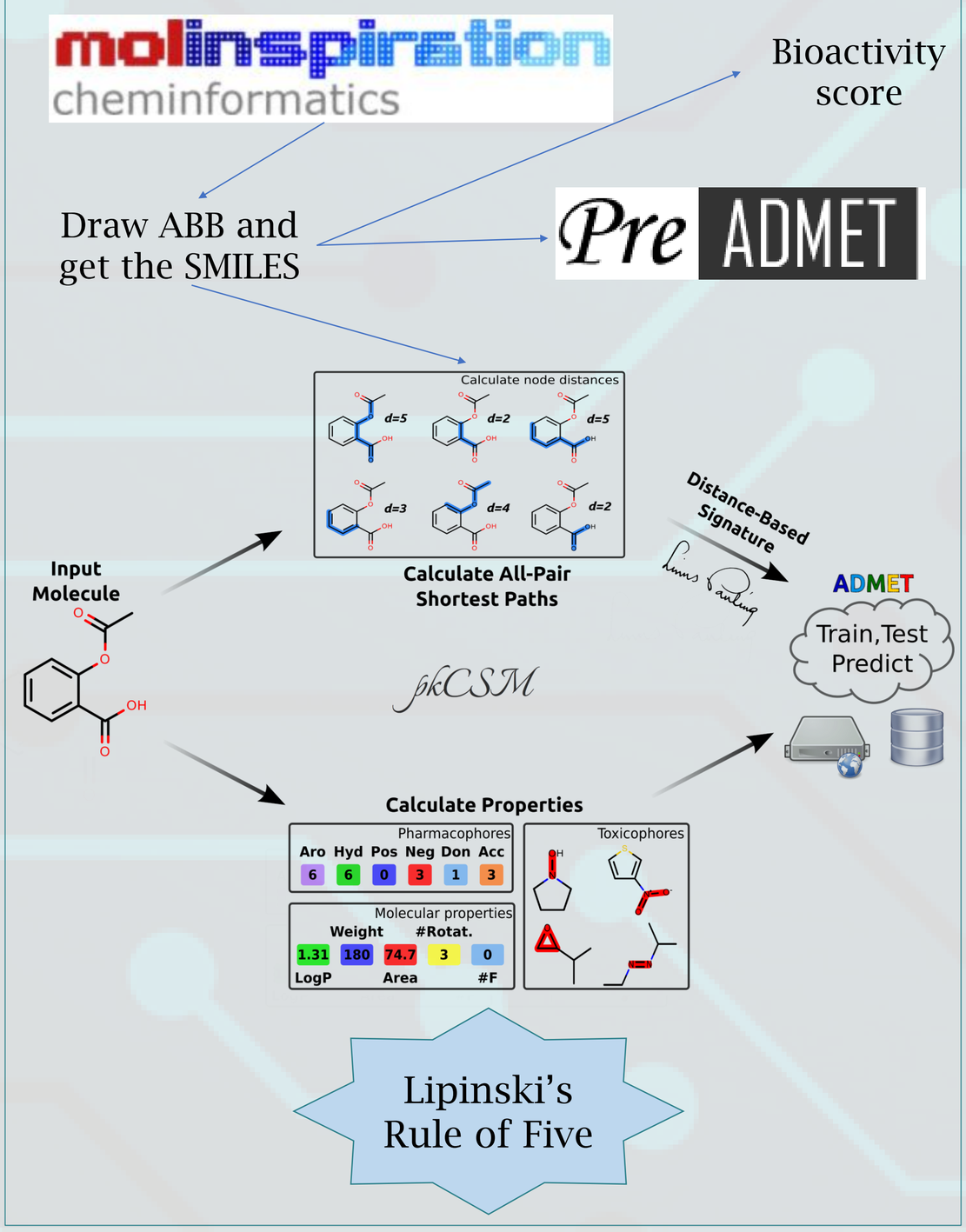
INTRODUCTION

In silico analysis is the beginning of many researches and it can predict which way follow it's possible to evaluate the promisor compounds and the pathways of action. Most drugs for the treatment of cancer have limited efficacy and tumor recurrence rapidly follows. Therefore, the search for new molecules is necessary for the development of more effective clinical therapies. The family of beta-diketones, including dibenzoylmethane, is known by the large bioactivity, such as antitumor, antibacterial, and anti-inflammatory activities.

OBJECTIVE

The aim of this study was evaluating in silico the derivate of dibenzoylmethane (ABB), one beta-diketone, as pharmacokinects, physicochemical and toxicity by ADMET and bioactivity score methods to a drug development.

METHODS



RESULTS

Table 1: Predictions obtained by pkCSM, preADMET and Molinspiration.

	Variable	Predict Value	Reference Value
Cytochrome p450 isoforms - CYP (pkCSM)	CYP2D6 substrate	**No**	Yes or No
	CYP3A4 substrate	**Yes**	
	CYP1A2 inhibitior	**No**	
	CYP2C19 inhibitior	**Yes**	
	CYP2C9 inhibitior	**Yes**	
Cardiotoxicity (pkCSM)	hERG I inhibitor	**No**	
	hERG II inhibitor	**Yes**	
Toxicity (preADMET)	Carcinogenicity Mouse	**No**	
	Carcinogenicity Rat	**No**	
	Ames Mutagenicity	**No**	
Bioactivity Score (Molinspiration)	GPCR ligand	**0.02**	**Active** (score > 0) **Moderately active** (score: -5.0-0.0) **Inactive** (score < -5.0)
	Ion channel modulator	**-0.01**	
	Kinase inhibitor	**-0.17**	
	Nuclear receptor ligand	**0.08**	
	Protease inhibitor	**-0.01**	
	Enzyme inhibitor	**-0.02**	

CONCLUSION

These results showed that the ABB compound has great potencial to provide us with a potent drug in medical clinic and *in vivo* tests should be performed.

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