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Drug likeness and ADMET screening of (*E*)-7-methyl-2-(5,6,7,8-tetrahydronaphthalen-2-yl)oct-5-en-3-one isolated from *Scoparia dulcis* L.

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Abstract: A chemical compound (E)-7-methyl-2-(5,6,7,8-tetrahydronaphthalen-2-yl)oct-5-en-3-one was isolated from solvent extract of Scoparia dulcis L. After characterization of the compound using different spectroscopic data analysis, the drug likeness screening was done using MolSoft server and the ADMET screening of the compound was done using Mobyle@RPBS software. The drug likeness screening of the compound revealed that the drug-likeness score of the compound was 1.17. The ADMET screening of the compound revealed that the compound did not possess any toxicity and passed successfully all the parameter of the screening. This result of drug likeness and ADMET screening will be helpful in conducting further analysis of the compound which might have the possibility of becoming a probable drug target for a specific disease.

Keywords: Scoparia dulcis L., (E)-7-methyl-2-(5,6,7,8-tetrahydronaphthalen-2-yl)oct-5-en-3-one, Drug likeness , ADMET screening, MolSoft server, Mobyle@RPBS

1. Introduction

The process of drug discovery is very complex, time and resource consuming. It requires an interdisciplinary effort to design effective and commercially viable drugs. Numerous technologies have been established and applied in drug R & D to minimize the research cycle and expenses (Ramulu and Goverdhan, 2012). Computer Aided Drug Design (CADD) is such a specialized discipline that provides an in depth discussion about the computer assisted techniques used to discover, design and optimize new, effective and safe drugs that can reduce time and expenses

associated with the process up to 50%. It uses computational methods to simulate drug-receptor interactions and are greatly dependent on bioinformatics tools, applications and databases (Ramulu and Goverdhan, 2012; DBM *et al.,* 2007).

A ketonic compound was isolated from an ethnomedicinal plant *Scoparia dulcis* L. After spectroscopic data analysis the compound structure was revealed to be (*E*)-7-methyl-2-(5,6,7,8-tetrahydronaphthalen-2-yl)oct-5-en-3-one. To study the bioactivity of the compound the compound was screened *in silico* using bioinformatics software and database.

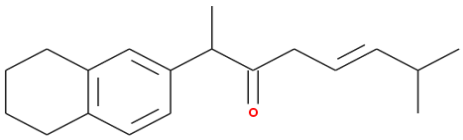

Fig 1: (E)-7-methyl-2-(5,6,7,8-tetrahydronaphthalen-2-yl)oct-5-en-3-one

The drug-likeness of a compound is a key factor during the initial phases of drug discovery. It is a concept in drug discovery assessing if a molecule has physicochemical properties like size, shape, solubility and structural features similar to existing drugs. Drug like compounds are more likely to be transformed into drugs. Descriptors of drug likeness include the classic Rule of Five (Ro5) as originally proposed by Lipinski in 1997. This is an effective guiding principle for the design of small-molecule drugs over 20 years. Ro5 highlights how some molecules have a tendency to be more easily optimized as drug candidates, leading researchers to consider the physicochemical properties of compounds systematically. However, emergence of beyond the Ro5 drugs shows that it is also possible to generate drugs outside of Lipinski space. Subsequently, during the successful transition from lead candidates to approved drugs, new descriptors have appeared, such as polar surface area (PSA) and lipophilic ligand efficiency (LLE). PSA describes the polarity and liposolubility of molecules, whereas LLE is a quality parameter related to molecule size. Both have improved the prediction accuracy of compound properties to some extent (Wenxiu Wei *et al.,* 2020).

ADMET refers to the properties of Absorption, Distribution, Metabolism, Excretion, and Toxicity of compounds, which are critical for predicting drug behavior in biological systems. It encompasses various metrics and data derived from numerous prediction servers that utilize machine learning and extensive ADMET databases. It helps weed out poor candidates early, saving time and money.

2. Methodology

The drug likeness screening of the compound was done using Molsoft L.L.C server. It is a free web server used to screen the drug likeness property of a molecule and also to study whether the molecule satisfy all the Lipinski rule of 5.

ADMET screening of the compound was done using Mobyle@RPBS online portal. The compound was loaded in SMILES format using parameters *viz.*, molecular weight, logP, logSw, tPSA, Rotable Bonds, Rigid Bonds, Flexibility, HBD, HBA, HBD_HBA, Rings, MaxSizeRings, NumCharges, Total Charges, Heavy atoms, Carbon atoms, Hetero atoms, Ratio R/C, Lipinski violation, Solubility (mg/l), SolubilityForecastIndex, Oral Bioavailability VEBER, Oral Bioactivity EGAN, Traffic lights, 4_400, Phospholipidosis, Fsp^3 and Stereocenters.

3. Result and Discussion

Drug likeness Screening:

The compound (*E*)-7-methyl-2-(5,6,7,8-tetrahydronaphthalen-2-yl)oct-5-en-3-one successfully passed the drug likeness screening and exhibited a drug likeness model score of 1.17.

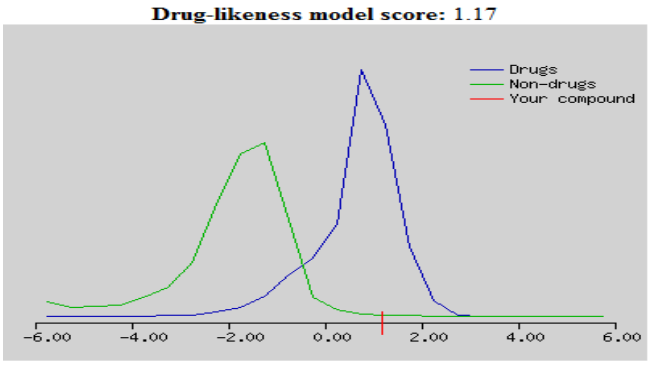

Fig 2: Graph showing Drug likeness

Table 1: Lipinski Rule of 5 and other parameters

Sl. No.	Lipinski RO5 and other parameters	Values
1.	Molecular weight	270.20
2.	Number of HBA	1
3.	Number of HBD	0
4.	MolLogP	5.13 (>5)
5.	MolLogS	-5.73 (in Log(moles/L))0.51(in mg/L)
6.	MolPSA	13.41 A^2
7.	MolVol	317.46 A^3
8.	Number of stereo centers	1

ADMET Screening:

ADMET screening of the compound was performed and revealed that the compound possessed no toxicity risk and passed successfully all the ADMET parameters.

Table 2: ADMET screening result of the compound

Sl. No.	ADMET parameters	Values
1.	Molecular weight	270.4091
2.	logP	5.23
3.	logSw	-4.57796
4.	tPSA	17.07
5.	Rotable Bonds	5
6.	Rigid Bonds	13
7.	Flexibility	0.277778
8.	HBD	0
9.	HBA	1
10.	HBD_HBA	1
11.	Rings	1
12.	MaxSizeRings	10
13.	NumCharges	0
14.	Total Charges	0
15.	Heavy atoms	20
16.	Carbon atoms	19
17.	Hetero atoms	1
18.	Ratio R/C	0.052632
19.	Lipinski_violation	1
20.	Solubility (mg/l)	2778.684844
21.	SolubilityForecastIndex	Reduced solubility
22.	Oral_Bioavailability_VEBER	Good
23.	Oral_Bioactivity_EGAN	Good
24.	Traffic lights	2
25.	4_400	Good
26.	3_75	Bad
27.	Phospholipidosis	nonInducer
28.	Fsp^3	0.526316
29.	Stereocenters	1
30.	Result	Accepted

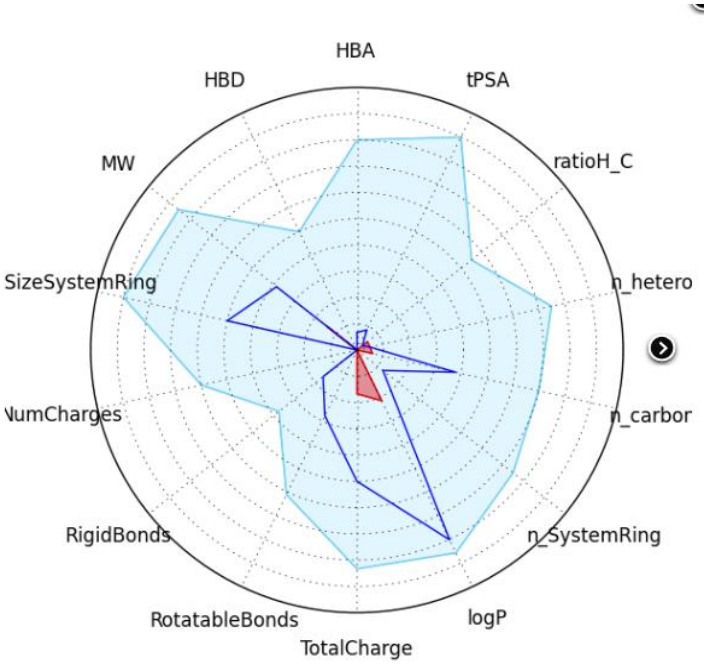

Fig 3: PhysChem filter positioning

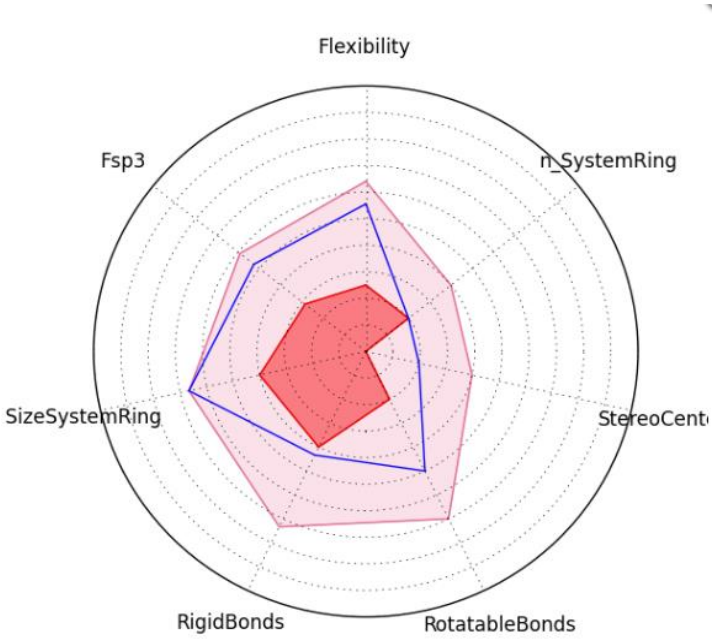

Fig 4: Compound Complexity

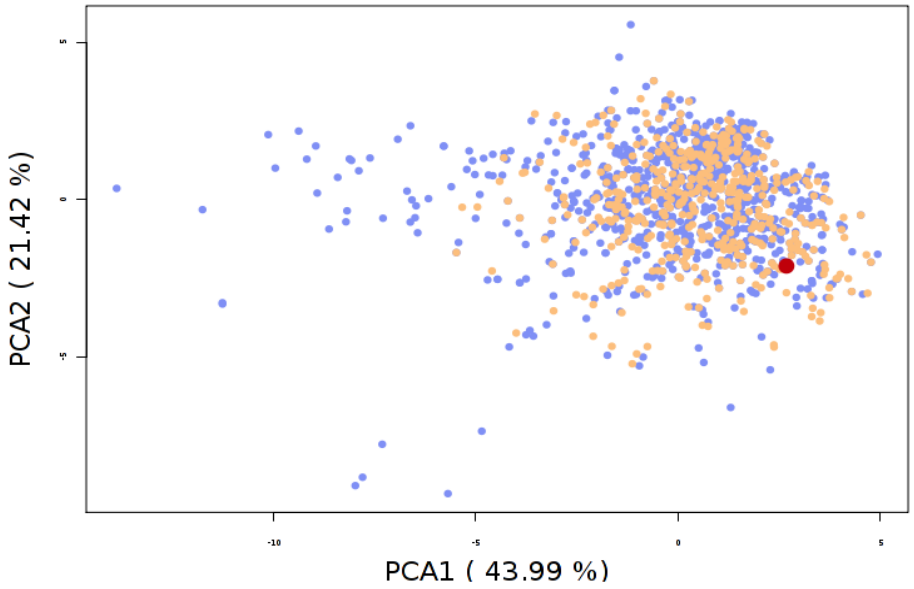

Fig 5: Oral Property Space

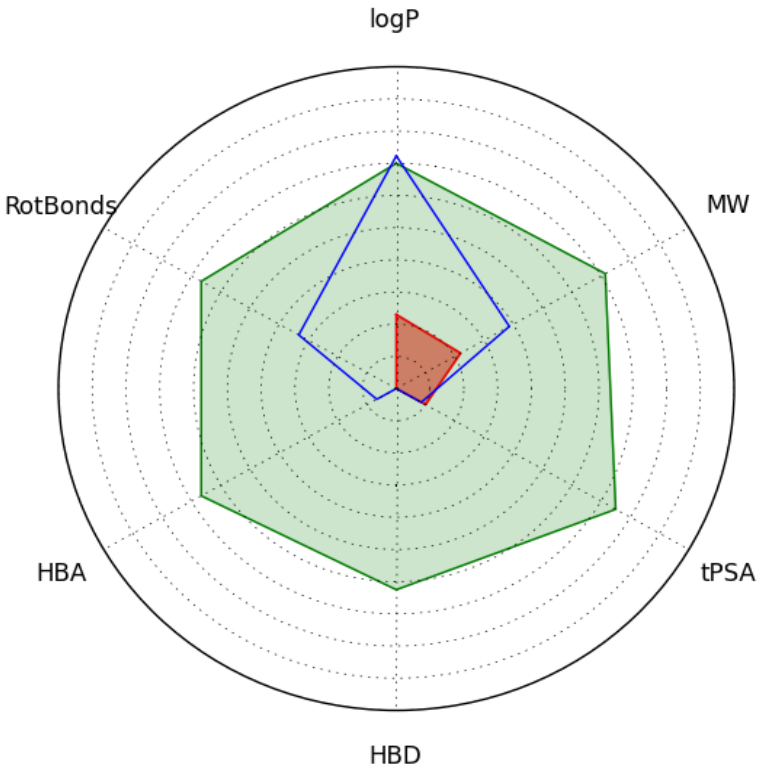

Fig 6: Oral absorption estimation

4. Conclusion

Computer aided drug design is a very promising tool for designing and optimizing new, effective and safe lead molecule which can reduce the time as well as expenses associated with the process of drug discovery. Hence, before proceeding to in vivo approaches, the in silico screening of the compound is ideal for predicting probable bioactivity, evaluating the actual mechanism of action and other pharmacological parameters which could be beneficial in designing a lead molecule for a definite therapeutic utility.

After isolation of the chemical compound, before proceeding to in vivo screening, the in silico screening of the compound was done to evaluate the drug likeness and ADMET properties of the compound. The results revealed that the compound passed successfully all the parameters of the screening. After confirming the non toxicity of the compound, we can move to the next step of target fishing based on the data of the screening. Therefore, this piece of work will be helpful in conducting further analysis of the compound that have the possibility of becoming a probable lead molecule of a specific disease.

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