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Theoretical Prediction Of Medicinal Properties Of Fucoidan - A Swissadme Analysis

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ABSTRACT

Fucoidan (I) have been modelled using SwissADME web tool and physicochemical, pharmacokinetics, drug-likeness and medicinal properties of I were analyzed. The results reveal that the selected candidate (I) possesses high gastrointestinal (GI) absorption and positive result to Lipinski's rule. It exhibits good bioavailability score and notable synthetic accessibility.

KEYWORDS: Fucoidan, Theoretical analysis, ADME properties, Pharmacology and SwissADME web tool

I. INTRODUCTION

Several studies have been conducted on clinical applications of fucoidan in recent years, especially regarding its oral drug delivery. Fucoidan is well known to have various biological functions and is often investigated for pharmaceutical applications. Although fucoidan has shown promising results in various dosage forms, its potential applications as a dietary supplement have been demonstrated, and recent studies show that oral administration of fucoidan is preferred[1].

Fucoidan, produced by the cell walls of brown seaweed, possesses biological effects, covering anticancer, antiviral, anti-inflammatory, antioxidant, and a potential for promoting angiogenesis and osteogenesis. Many research studies show diverse scientific results on fucoidan's therapeutic prospect in dentistry and the mechanism of action in the therapy of oral diseases. A literature search was carried out using keywords with Boolean operators, including fucoidan (AND) oral (OR) dental (OR) dentistry, to identify related publications from PubMed, ScienceDirect, and Google Scholar databases. The results showed that fucoidan had various therapeutic potentials in the field of dentistry, including anticancer, anti-inflammatory, radioprotection, protection of dental pulp tissue, and bone regeneration. These characteristics were related to the sulfate composition and molecular weight. Fucoidan has various therapeutic potentials crucial for oral health. Hence, it might be used for material development and drug production in dentistry[2].

Fucoidan is a polysaccharide largely made up of l-fucose and sulphate groups. Fucoidan is favourable worldwide, especially amongst the food and pharmaceutical industry as a consequence of its promising therapeutic effects. It's applaud able biological functions are ascribed to its unique biological structure. Classical bioactivities associated with fucoidan include antioxidant antitumor, anticoagulant, antithrombotic, immunoregulatory, antiviral and anti-inflammatory effects. Many variety of in vitro and in vivo studies have been carried out to further highlight its therapeutic potentials[3].

The marine environment based studies and reviews have been done in the past on the bioactivity of fucoidan e.g., by producing anti-oxidant, anti-tumor, immunoregulation, anti-viral and anti-coagulant activities [4-11].

Even though several studies have been documented on Fucoidan, there has been no SwissADME[12] analysis performed to the best of our knowledge. Therefore, this work focuses on the physicochemical properties, pharmcokinetics, drug-likeness and medicinal properties of Fucoidan using SwissADME web tool.

II. Methodology

Computational software and web-servers were utilized to study the physicochemical and pharmacokinetic properties of metformin. SwissADME, is publicly accessible web servers that suggest various properties of the active chemical entity by using accurate algorithms. Swiss ADME, free web tool was utilized to study the physicochemical properties, bio-availability radar, pharmacokinetics, Druglikeness and medicinal Chemistry of Fucoidan in this present work.

Physicochemical properties

The physicochemical properties of I, such as canonical SMILES, molecular formula, molecular weight, number of such as canonical SMILES, formula, molecular weight, rotatable bonds, H-bond acceptors, H-bond donors, etc. were collected from web-based online server such as SwissADME.

Bioavailability Radar

Bioavailability radar for the Studied molecules have been obtained from SwissADME database. All the parameters in bioavailability radar have been analysed and the results were shown accordingly. The bioavailability radar gives graphical interpretation of properties such as lipophilicity, compound size, insolubility, polarity, instaurations and flexibility in its six hexagonal vertices which help to evaluate scopes of improvement of bioavailability score. The radar images for metformin and its methylated derivatives (Table. 2) were collected from SwissADME web-server. SwissADME is a free web application on a website (http:// www.swissadme.ch/, accessed on 20 July 2022). ADME supports the development of new drugs by precisely pre-dicting the medicinal chemistry, drug-like properties, solubility, lipophilicity (LIPO), physicochemical properties, and pharmacokinetic parameters of small molecules. SwissADME also exhibited the structure and bioavailability- 3.1 In ability radar using canonical SMILES. The first part showed the chemical structure in two dimensions. The second part 3.1.1 Antioxidant is the bioavailability radar, which allows for a rapid peek at how much the target compounds resemble medicines. For each feature anticipated to be orally accessible, the optimum physicochemical environment is illustrated by the pink area as LIPO: -0.7 < XLOGP3 < +5.0, SIZE (Molecular weight (MW)) 150 g/mol < MW < 500 g/mol, POLAR (Polarity) 20A Molecular polar surface area (TPSA) < 130 A2, INSOLU (Insolubility) -6 < Log S(ESOL) < 0, INSATU (Insaturation) 0.25 < FractionCsp3 < 1 and FLEX (Flexibility) 0 < RP (Number of rotatable bonds) < 9 are the six physicochemical qualities that are taken into consideration.

Pharmacokinetics

The Pharmacokinetics study of the selected molecule was performed by the utilization of Swiss ADME web server. In particular, Gastrointestinal absorption and Brain Blood Barrier permeation were studied.

Druglikeness

In this work, druglikeness was studied for the selected candidate whether Lipinski rule was obeyed and bioavailability score was noted for I using web tool.

Medicinal Chemistry

The SwissADME web tool was very much useful to analyse the Medicinal Chemistry of the molecules in this work. Leadlikeness and Synthetic accessibility of the chosen candidate has been noticed for analysis.

III. Results and Discussion

The chosen molecule have been modelled and analysed for its medicinal properties using SwissADME server. The modelled structure and its Bio-availability Radar are shown in Fig. 1.

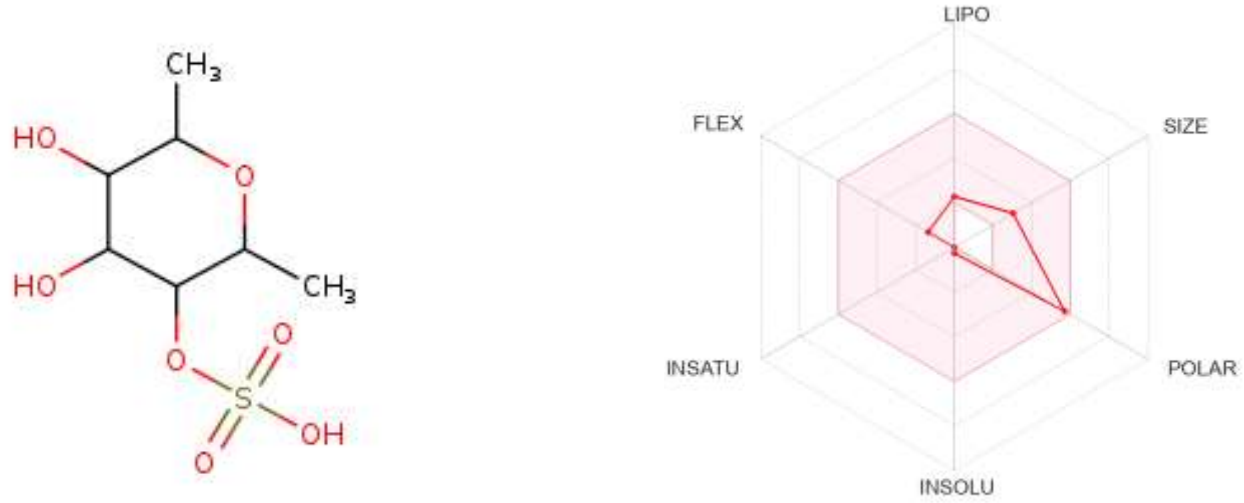

Fig. 1 Modelled structure and Bio-availability Radar of Fucoidan by SwissADME web tool

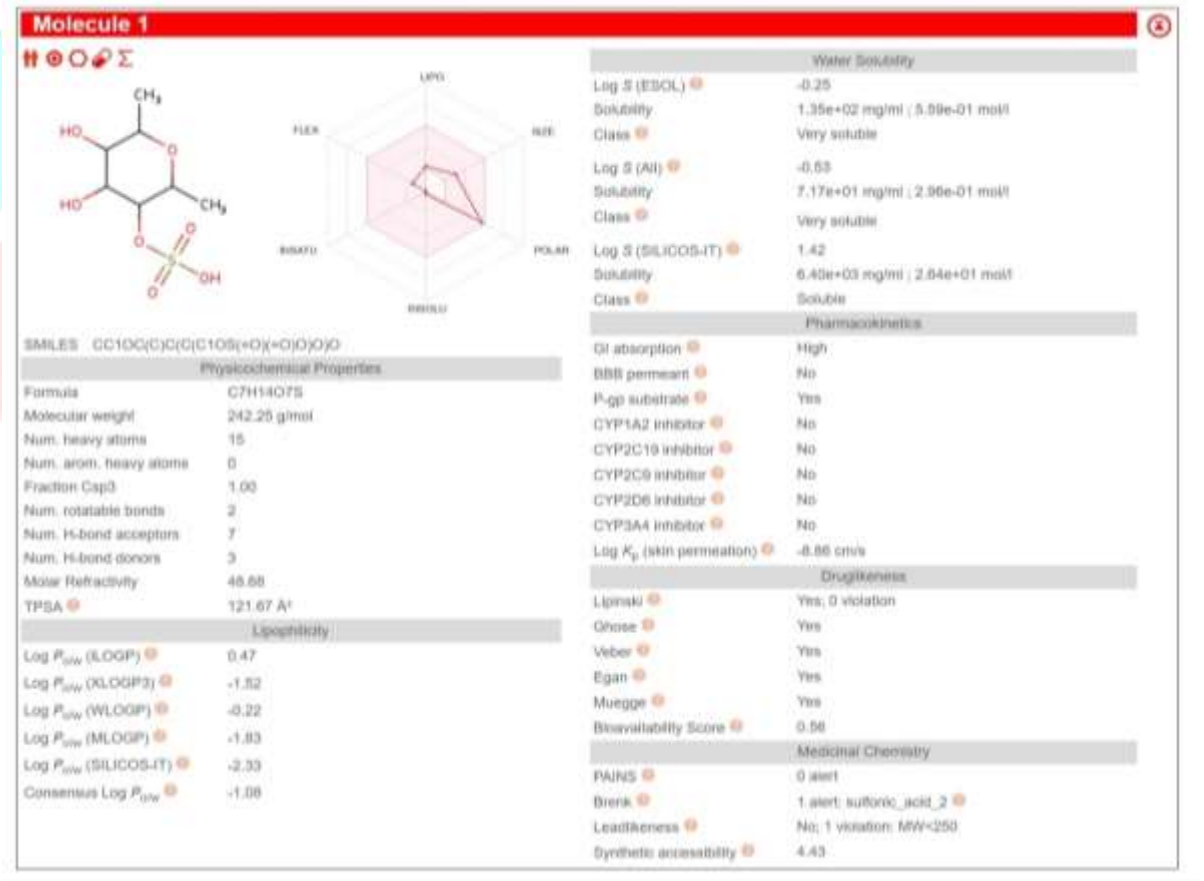

Fig. 2 SwissADME analysis of Fucoidan

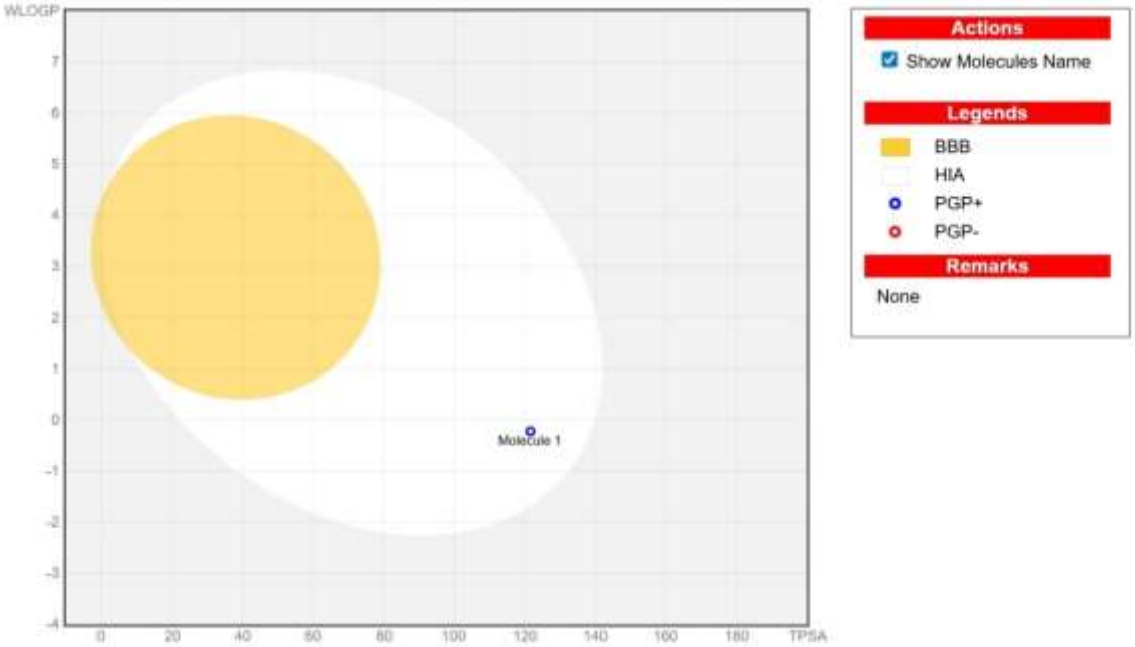

Fig. 3 BOILED Egg of Fucoidan by SwissADME server

Table 1. ADME properties of Fucoidan by SwissADME software

Descriptors	Fucoidan
SMILES	CC1OC(C)C(C(C1OS(=O)(=O)O)O)O
Molecular Formula	$C_7H_{14}O_7S$
Molecular Weight	242.25 g/mol
Number of rotatable bonds	2
Number of Hydrogen bond acceptor	7
Number of Hydrogen bond donor	3
Molar Refractivity	48.68
TPSA	121.67 $Å^2$
Log $P_{o/w}$	-1.08
Log S (ESOL)	-0.25 (very soluble)
GI absorption	High
BBB permeant	No
Log K_p (skin permeation)	-8.86 cm/s
Lipinski	Yes; 0 violation
Bioavailability Score	0.56
Leadlikeness	No; 1 violation : MW < 250
Synthetic accessibility	4.43

By analysing the bioavailability radar of Fucoidan (shown in Fig. 1) it is inferred that all the parameters namely lipophilicity, size, polarity, insolubility, insaturation and flexibility are responding to the standard level, i.e.,within the pink / red area of the radar for a molecule to be of an oral drug. Hence the studied molecule (I) is good enough to be acting as an oral drug. In this work, the whole computational informations collected from SwissADME web tool has been shown in Fig. 2. The Table 1. shows the pharmacokinetics study of the selected system. Gastrointestinal absorption and Blood Brain Barrier (BBB) permeantion are noted in the table for analysis. As the candidate is having high GI absorption and no BBB permeant value, the chosen molecule would have good pharmacokinetic properties and the BOILED Egg diagram (shown in Fig. 3) is also a good evidence for the same.

The druglikeness properties of the I are shown in the Table 1. In general, an orally active drug has no more than one violation of the following criteria, i.e., Lipinski's rule of five[13-19].

- No more than 5-H bond donors (the total no. of N-H and O-H bonds)
- No more than 10 H-bond acceptors (all N/O atoms)
- A molecular was less than 500 daltons.
- A Calculated octanol-water partition coefficient (log P) that does not exceed 5.

From the result it has been inferred that the selected candidate is also obeying Lipinki's rule thereby offering promising point for the system to be acting as an oral drug and the bioavailability score is 0.56.

The Table 1. denotes the Medicinal Chemistry of the selected candidate and showing that zero alerts to PAINS (Potential interference compounds) and better synthetic availability for the chosen system.

IV. CONCLUSION

The computational simulations of the selected candidate (I) by SwissADME server was conducted on their physicochemical, pharmacokinetic, drug-likeness and therapeutic properties. The results established that I has significant GI absorption and no BBB penetration in particular. Fucoidan has great synthetic accessibility and positive bioavailability score. The results of Fucoidan obtained from this preliminary study of in silico analysis provide the promising value to be an oral drug and could be extended for the in vitro study to elaborate significant therapeutic potential of the studied system.

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