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Pharmacological Properties Of APTMS And GPTMS- A Swissadme Prediction

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ABSTRACT
APTMS and GPTMS have been modelled using SwissADME web tool and physicochemical, pharmacokinetics, drug-likeness and medicinal properties were studied. The results show that APTMS and GPTMS possess high gastrointestinal (GI) absorption and GPTMS especially shows blood brain barrier (BBB) permeation. Both exhibit good bioavailability score and great synthetic accessibility.

KEYWORDS: APTMS, GPTMS, Pharmacology, SwissADME web tool and ADME properties

I. INTRODUCTION

Biofouling is an undesirable process in which biological molecules and organisms adhere to a surface which causes severe negative effects in various fields including healthcare, water distillation, and marine transportation. Therefore, its prevention is highly explored by thin films, based on different sol–gel precursors, 3-aminopropyltrimethoxysilane (APTMS) using spin-coating on glass. The APTMS film showed, as expected, antibacterial properties and it led to a significant prevention of protein and bacterial adsorption [1].

Antimicrobial photodynamic therapy (aPDT) and antimicrobial photothermal therapy (aPTT) are promising local and effective alternative therapies for antibiotic resistant bacterial infections and biofilms. A combination of nanoparticles and organic photosensitizers offers a great opportunity to combine PDT and PTT for effective eradication of both planktonic bacteria and their biofilms. Photo-induced antibacterial activity of indocyanine green (ICG), 3-aminopropylsilane coated superparamagnetic iron oxide nanoparticles (APTMS@SPIONs) and ICG loaded APTMS@SPIONs was evaluated on planktonic cells and biofilms of Gram-negative (E. coli, K. pneumoniae, P. aeruginosa) and Gram-positive (S. epidermis) bacteria. APTMS@SPION/laser treatment completely eliminated P. aeruginosa and provided 7-log reduction in the colony forming unit (CFU) of E. Coli. This is the first example for antibacterial phototoxicity of this nanoparticle [2]. ZIF-8 was synthesized and functionalized with 3-aminopropyl trimethoxy silane. Antibacterial activity was investigated with Staphylococcus aureus, and *Escherichia coli*. Bacterial decrease in the viable cell count method was 92 % on S. aureus and 20 % on *E. coli*. The maximum adsorption capacities were obtained 2159 mg/g for ZIF-8@APTMS [3].

The emergence and spread of pathogenic microbes with resistance to multiple antibiotics necessitates the development of new broad-spectrum microbicides. Metal nanoparticles are one such microbicide and they have been recognized for their potential value in fighting harmful microbes. The Cu-APTMS NPs showed a significant in vitro degradation activity against bacterial DNA, which is important in vivo microbicidal

activity. In addition, pathogenic fungi (*Candida tropicalis* and *Fusarium verticillioides*) were irreversibly deactivated by treatment with Cu-APTMS NPs [4].

It is documented that both APTMS and GPTMS are very fruitful in the catalytic synthesis of nanoparticles [5,6]. The synthesis of palladium (PdNPs) and its bimetallic (Pd-Au/Au-Pd) nanoparticles of controlled nanogeometry, polycrystallinity and functional ability is challenging task. The synthesized PdNPs shows peroxidase mimetic activity as a function of 3-APTMS concentration [7].

The suitable composition of 3-APTMS and organic reducing agents not only control the dispersibility in variety of solvents but also enable the formation of organic-inorganic hybrid that facilitated catalytic activity of as synthesized nanomaterials [8].

Functional textile coatings containing embedded dyestuff were synthesized by sol–gel method. 3-Glycidoxypropyltrimethoxysilane (GPTMS) is a useful organofunctional trialkoxysilane precursor for the development of wearable sensors [9].

To the best of our knowledge, in silico study of ADME properties [10] of APTMS and GPTMS have not been reported so far by SwissADME web tool [11]. Therefore, this work mainly focuses on theoretical analysis of medicinal properties of APTMS and GPTMS.

II. METHODOLOGY

The Swiss ADME database was utilized to evaluate the physicochemical properties, pharmacokinetics, drug-likeness and to study the medicinal Chemistry of the selected compounds namely APTMS and GPTMS for this present work. The 2D structure of the studied compounds were first modelled and converted into corresponding SMILES (Simplified Molecular Input Line Entry System) and the program was further performed for efficient screening and analysis of potential drug molecules.

III. RESULTS AND DISCUSSION

Bio-availability Radar

The selected candidates have been subjected to SwissADME web tool in order to evaluate the physicochemical as well as ADME properties [10]. Initially the selected compounds were modelled on the monitor of the SwissADME database and converted into SMILES. The chemical structure and bioavailability radar of the selected compounds have been shown in Figure 1 & 3. In bioavailability radar of the compounds Pink / Red area is seen in the plot which reflects the maximum range of lipophilicity, Size, Polarity, insolubility, instauration and flexibility. By analysing the radar of the selected molecules, it is showing good range for all the characteristics and thereby considered to be promising candidates to proceed for further drug development.

Physicochemical properties

The physicochemical properties of the selected compounds obtained using SwissADME database have been listed in Table 1 & 2. From the result it is inferred that APTMS has one hydrogen bond donor which is absent in GPTMS. This may be one of the reasons for APTMS which is present in more acceptable range of pink area in bio-availability radar thereby can act as an oral drug. Molar refractivity of both the compounds are good.

Pharmacokinetics study

The pharmacokinetics and drug-likeness of the selected compounds are shown in Table 1 & 2. It is indicating that the gastrointestinal (GI) absorption is high for both the selected molecules and it is indicated in yellow region of the BOILED egg (Figure 2 & 4). APTMS is not possessing Blood Brain barrier (BBB) Permeation. However, GPTMS showing positive result for BBB permeant which is evidently pointed in white region of the BOILED egg (Figure 4) thereby very suitable remedy for the betterment of central nervous system.

Lipinski rule

Lipinski rule of 5 helps to distinguish between drug-like and non drug-like molecules [10]. It predicts high probability of success or failure due to drug likeness for molecules complying with 2 or more of the following rules.

- Molecular mass less than 500 Dalton
- High lipophilicity (expressed as LogP less than 5)
- Less than 5 hydrogen bond donors
- Less than 10 hydrogen bond acceptors
- Molar refractivity should be between 40-130

APTMS and GPTMS are obeying Lipinski's rule thereby eligible for being an Oral drug at the preliminary stage of drug discovery. Bioavailability score is also good for both the compounds.

Medicinal chemistry

The Table 1 & 2 reveal that both the selected molecules are having MW less than 250 and good synthetic accessibility. GPTMS is especially showing enhanced synthetic accessibility than APTMS.

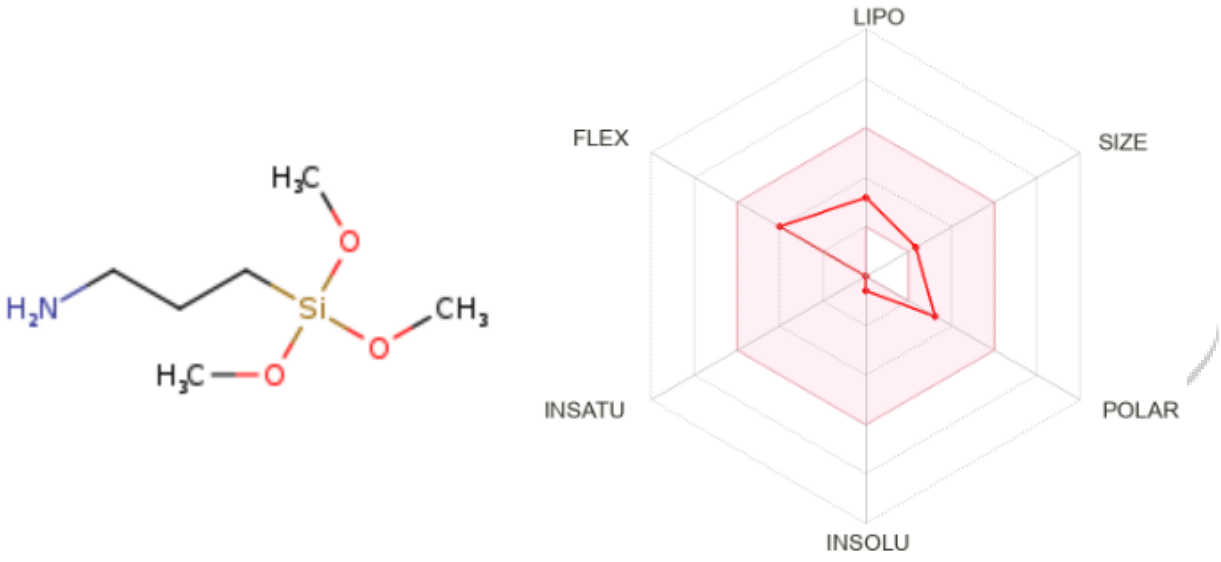

Figure. 1 The modelled structure and Bio-availability Radar of APTMS by SwissADME

Table 1. ADME properties of APTMS by SwissADME web tool

SMILES	NCCC[Si](OC)(OC)OC
Molecular Formula	$C_6H_{17}NO_3Si$
Molecular Weight	179.29 g/mol
Number of rotatable bonds	6
Number of Hydrogen bond acceptor	4
Number of Hydrogen bond donor	1
Molar Refractivity	44.79
TPSA	53.71 $Å^2$
Log $P_{o/w}$	0
Log S (ESOL)	-0.60 (poorly soluble)
GI absorption	High
BBB permeant	No
Log K_p (skin permeation)	-7.34 cm/s
Lipinski	Yes; 0 violation
Bioavailability Score	0.55
Leadlikeness	No; 1 violation MW < 250
Synthetic accessibility	3.70

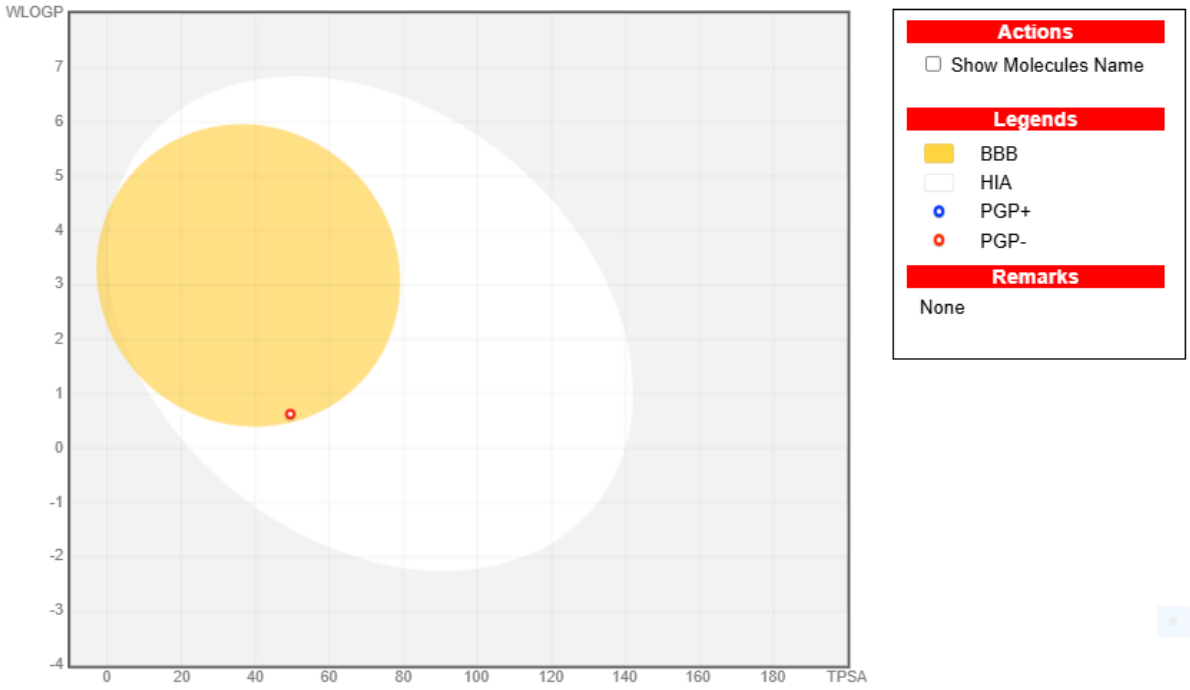

Figure. 2 BOILED Egg of APTMS by SwissADME

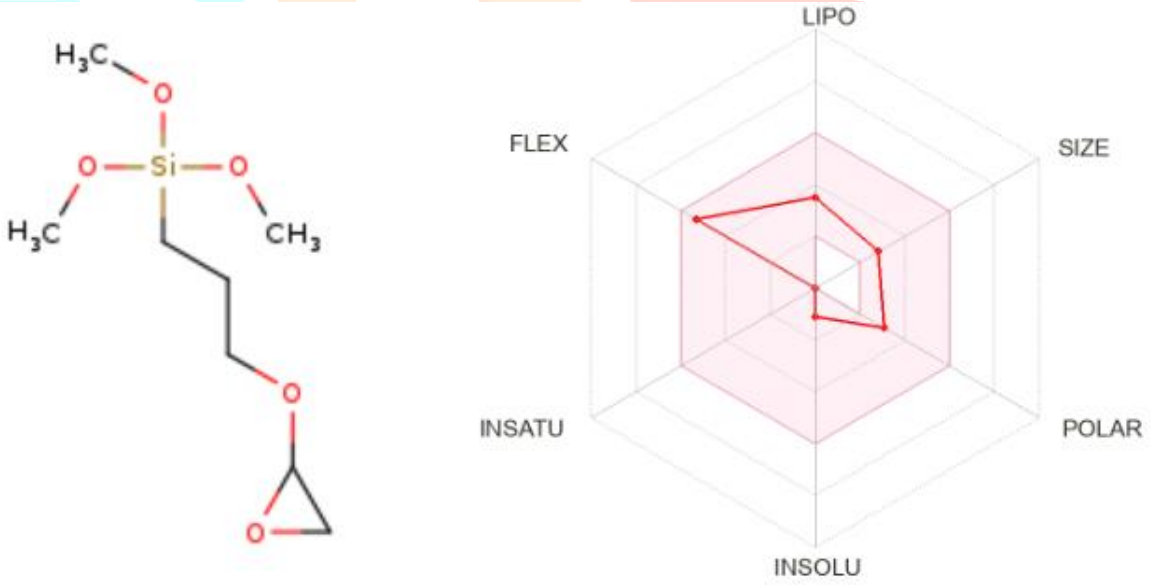

Figure. 3 The modelled structure and Bio-availability Radar of GPTMS by SwissADME

Table 2. ADME properties of GPTMS by SwissADME web tool

SMILES	CO[Si](CCCOC1CO1)(OC)OC
Molecular Formula	$C_8H_{18}O_5Si$
Molecular Weight	222.31 g/mol
Number of rotatable bonds	8
Number of Hydrogen bond acceptor	5
Number of Hydrogen bond donor	0
Molar Refractivity	51.75
TPSA	49.45 $Å^2$
Log $P_{o/w}$	0.53
Log S (ESOL)	-1.11 (very soluble)
GI absorption	High
BBB permeant	Yes
Log K_p (skin permeation)	-7.19 cm/s
Lipinski	Yes; 0 violation
Bioavailability Score	0.55
Leadlikeness	No; 1 violation MW < 250
Synthetic accessibility	4.20

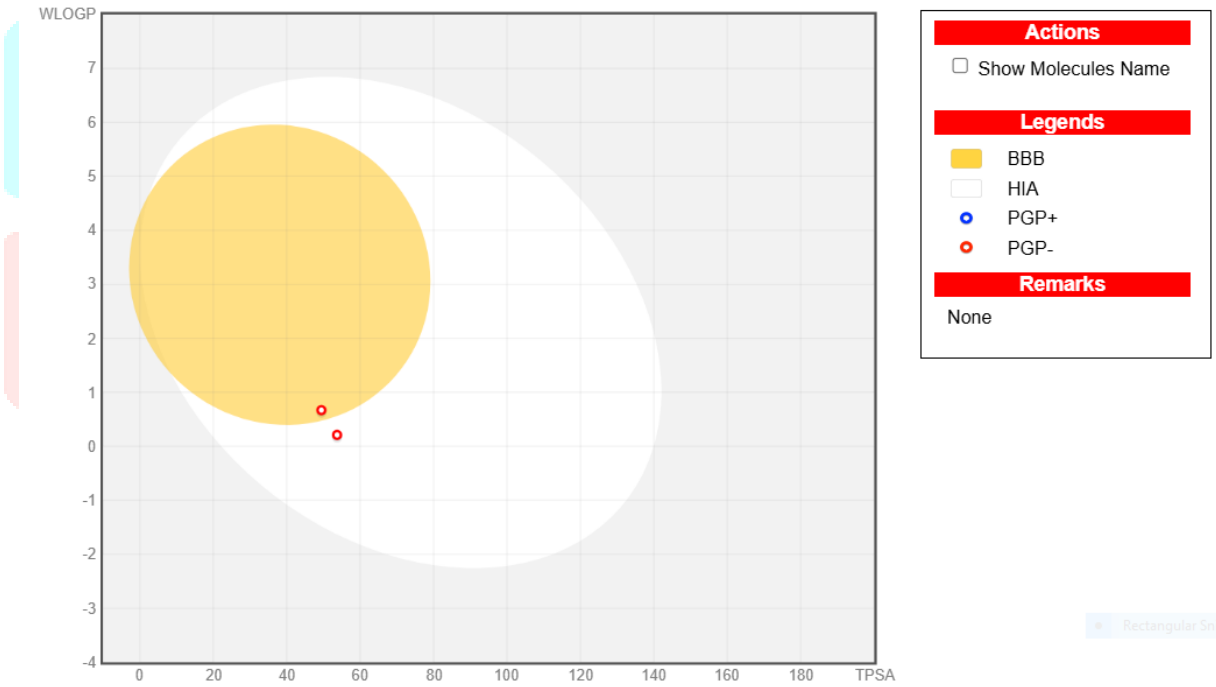

Figure. 4 BOILED Egg of GPTMS by SwissADME

IV. CONCLUSION

The simulation of APTMS and GPTMS by SwissADME server was conducted on their physicochemical, pharmacokinetic, drug-likeness and therapeutic properties. The findings demonstrate that both APTMS and GPTMS have substantial GI absorption and GPTMS exhibiting BBB penetration in particular. Both have high synthetic accessibility and favourable bioavailability score. The results obtained from this initial step of in silico study could be considered for the in vitro analysis to produce significant therapeutic potential of these compounds.

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