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Medicinal Properties of Palladium Nanoparticles-A SwissADME screening

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ABSTRACT

Palladium nanoparticles (**A**), as a result of APTMS and THF-HPO with Pd salt, have been modelled using SwissADME server and physicochemical, pharmacokinetics, drug-likeness and medicinal properties were screened. The results show that **A** possess high gastrointestinal (GI) absorption with no blood brain barrier (BBB) permeation. It displays worthy bioavailability score and moderate synthetic accessibility.

KEYWORDS: APTMS, THF-HPO, Pd nanoparticles, Medicinal properties and SwissADME

I. INTRODUCTION

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 [1,2].

The redox electrochemistry of ormosil-encapsulated Fc-COOH in both cases was found to display sluggish reversible electrochemistry mainly due to restricted mobility of ferrocenium ions within nano structured domain. In addition to that Fc-COOH loses its mediation capability required for designing mediated electrochemical sensors under such condition. These findings directed to design or mosil film fulfilling the requirement of ferrocene-mediated bio-electrochemical sensing and the choice of electrocatalyst in combination with encapsulated mediator for facilitating electron transfer process became significant. Fortunately, the interaction of palladium chloride (PdCl2) and GPTMS while making ormosil film with TMS has been recorded. It was found that palladium chloride/tetrachlorpalladate (PdCl2/K2PdCl4) opens the epoxide ring of glycidoxy residue and in turn gets reduced into palladium followed by subsequent co-ordination within two glycidoxy residue [3-11].

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 [12]. Therefore, this work mainly focuses on theoretical analysis of medicinal properties of APTMS and GPTMS.

II. METHODOLOGY

The Swiss ADME server was used to screen the physicochemical properties, pharmacokinetics, drug-likeness and to study the Medicinal Chemistry of **A** for this paper. The 2D structure of **A** was first modelled and converted into corresponding SMILES (Simplified Molecular Input Line Entry System) and the simulations were further performed for efficient screening and analysis of its therapeutic properties.

III. RESULTS AND DISCUSSION

Analysis of Bio-availability Radar

The selected candidates have been subjected to SwissADME web tool in order to evaluate the physicochemical as well as ADME properties [12]. 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. 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.

Study of Physicochemical properties

The physicochemical properties of the selected compounds obtained using SwissADME database have been listed in Table 1. From the result it is inferred that **A** has two hydrogen bond donors, seven HBA and seven RB. This may be one of the reasons for **A** which is present in more favourable range of pink area in bio-availability radar thereby can act as an oral drug. Molar refractivity of the studied compound is good.

Screening of Pharmacokinetics

The pharmacokinetics and drug-likeness of the selected compound is shown in Table 1. It is indicating that the gastrointestinal (GI) absorption is high and it is indicated in white region of the BOILED egg (Figure 3). **A** is not possessing Blood Brain barrier (BBB) Permeation. Therefore, **A** is suitable remedy without the disturbance 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

A is obeying Lipinski's rule thereby eligible for being an Oral drug at the preliminary stage of drug discovery. Bioavailability score is also the studied compound.

Medicinal chemistry

The Table 1 shows that the selected molecule is having zero alert to PAINS, MW more than 250 and good synthetic accessibility. It is especially showing moderate synthetic accessibility.

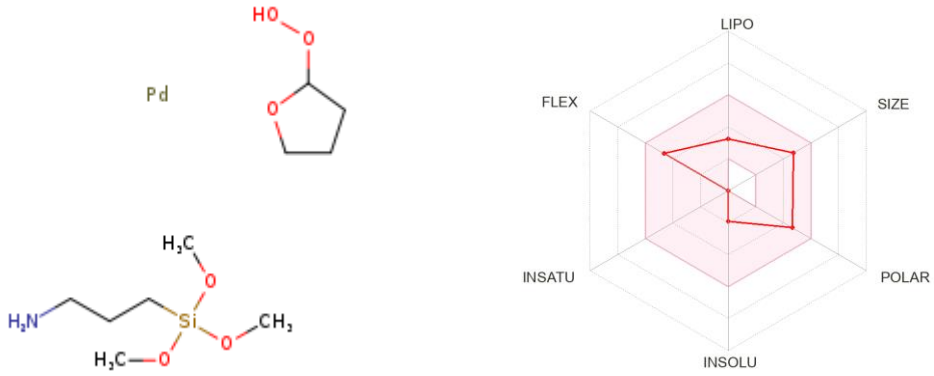

Figure. 1 The modelled structure and Bio-availability Radar of A by SwissADME server

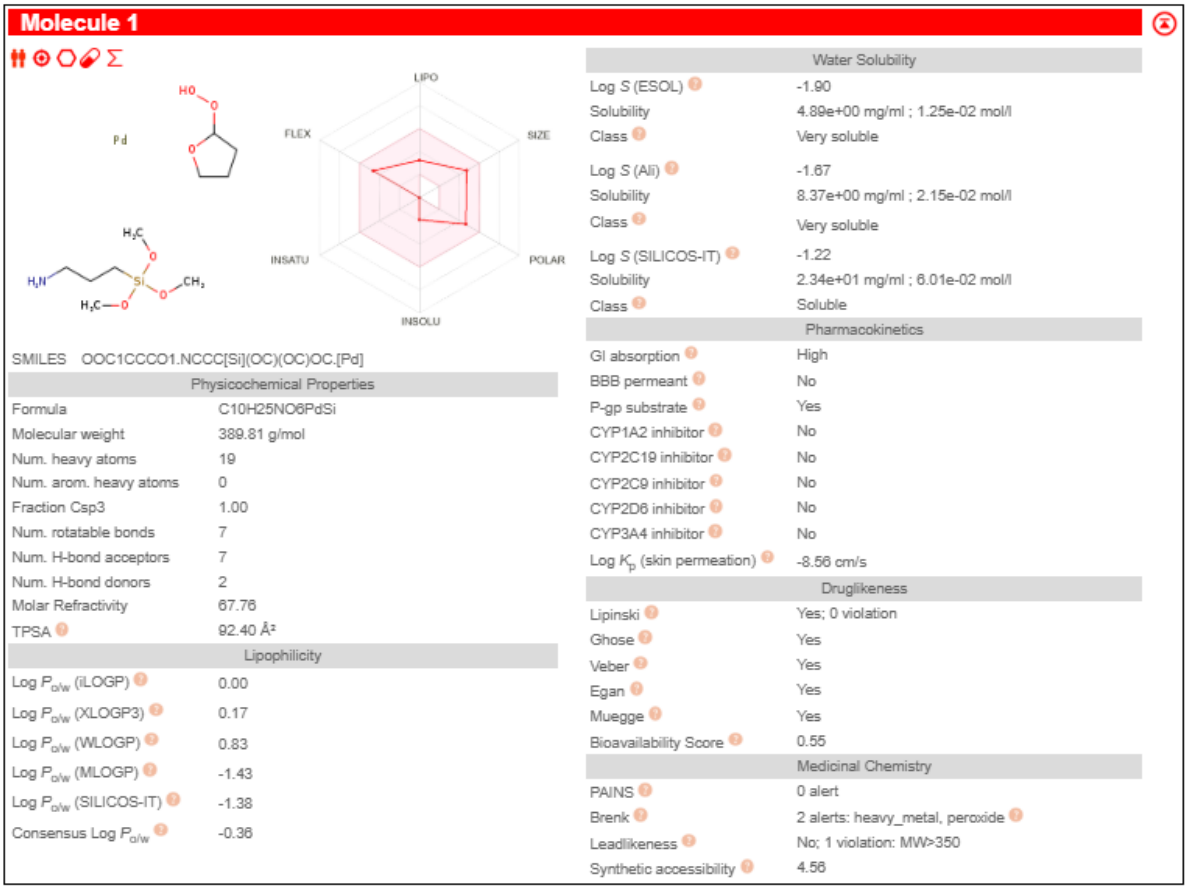

Figure. 2 SwissADME screening of A

Table 1. ADME properties of A by SwissADME server

SMILES	OOC1CCCO1.NCCC[Si](OC)(OC)OC.[Pd]
Molecular Formula	$C_{10}H_{25}NO_6PdSi$
Molecular Weight	389.81 g/mol
Number of rotatable bonds	7
Number of Hydrogen bond acceptor	7
Number of Hydrogen bond donor	2
Molar Refractivity	67.76
TPSA	92.40 $Å^2$
Log $P_{o/w}$	0
Log S (ESOL)	-1.90 (very soluble)
GI absorption	High
BBB permeant	No
Log K_p (skin permeation)	-8.56 cm/s
Lipinski	Yes; 0 violation
Bioavailability Score	0.55
Leadlikeness	No; 1 violation: MW>350
Synthetic accessibility	4.56

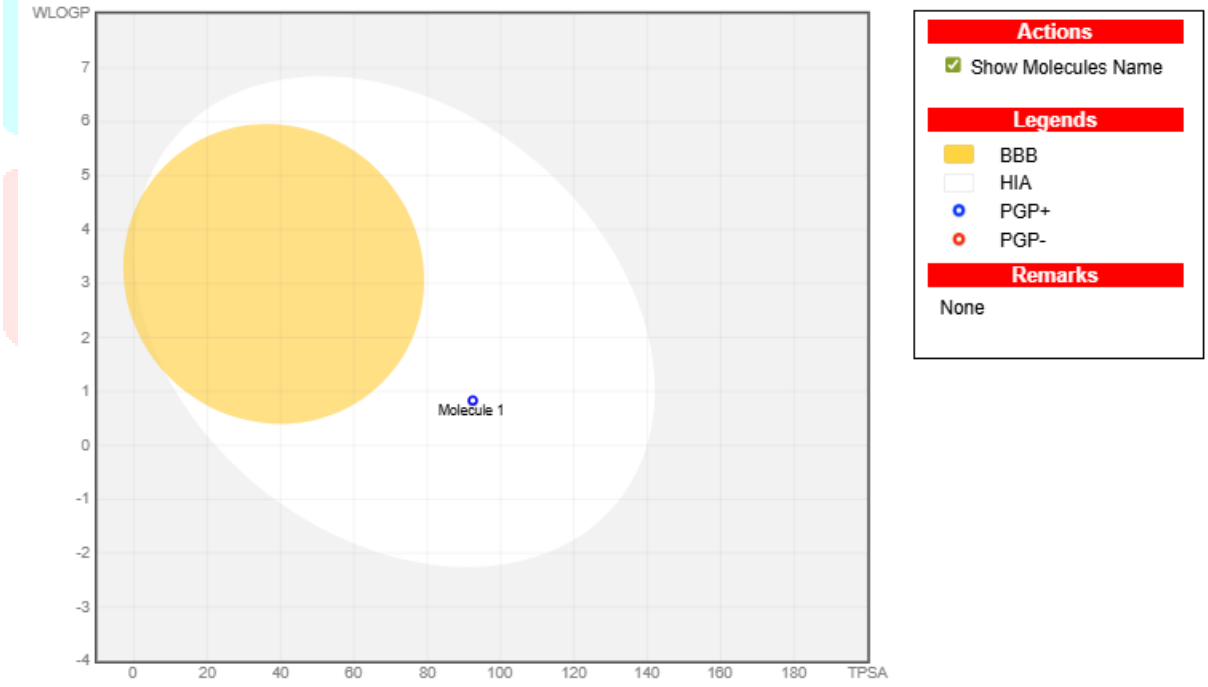

Figure. 3 BOILED Egg of A by SwissADME server

IV. CONCLUSION

The screening of **A** by SwissADME web tool was performed on their physicochemical, pharmacokinetic, drug-likeness and therapeutic properties. The results show that the selected molecule has high GI absorption and no BBB penetration in particular. High bioavailability score and favourable synthetic accessibility have been observed for the studied compound. The findings obtained from this study could be thrown light for the experimentalists to proceed further with the medicinal properties of **A** in the drug designing.

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