Journal of Chemical Health Risks

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JCHR (2026) 16(2), 1247-1255 | ISSN:2251-6727

In Silico Molecular Docking Studies and Adme/T Analysis of *Semi Carpus Anacardium* Chemical Constituents for Psoriasis

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(Received: 16 January 2026 Revised: 25 February 2026 Accepted: 17 March 2026)

KEYWORDS

Semi Carpus Anacardium, Butein, Tetrahydroamento, In Silico Molecular Docking,.

ABSTRACT:

Progression in computational research has made it possible for the in-silico methods to offer epochal benefits to both regulatory needs and the pharmaceutical industry to assess the safety profile. The aim of the present study was In Silico Molecular Docking Studies and ADME/T Analysis of Semi Carpus Anacardium Chemical Constituent Flavones for Psoriasis. The docking method involves three steps, i.e.: preparation of proteins, identifying the GRID coordinates, and determining the bonding strength with the molecular docking score. Docking is a computational approach to know the binding affinity of the ligand molecule with the receptor proteins. Docking score indicated as Kcal/mol, the highest docking score indicates the higher binding affinity and it is compared with the standard drug molecule binding affinity which is used in psoriasis treatment, Molecular docking was done to the bioflavonoid; catechol ligands present in semi carpus anacardium chemical analysis. Butein and tetrahydroamento flavone compounds were docked against the 8 proteins such as TNF-alpha, IL-23, IL-17A, PDE-4, BTK, JAK-3, IL-6, p38MAPK. Semi carpus anacardium chemical constituents like Butein, Tetrahydroamento flavone shows better docking scores and suitable to deliver through the oral route of administration after performing the pharmacokinetic properties and Lipinski's rule of five evaluation. THAF shows highest docking score of -11.2 Kcal/ mol when comparing with the standard drug (-8.3Kcal/mol). Furthermore, formulations strategies improve the drug effectiveness and stability to increase the potential against psoriasis.

INTRODUCTION

Complementary and alternative medicine (CAM) is gaining importance nowadays due to the reduced efficacy and increased side effects of allopathic medication. Ayurveda is an ancient medical science that utilizes naturally available plant sources for the treatment of various diseases, requiring long-term therapy with minimal to no side effects (1).

Semi carpus anacardium Linn. (*Anacardiaceae* family), commonly known as marking nut tree (Nallajidi). This nut is well known for its anti-inflammatory and antioxidant effects, and it is used to treat skin conditions. Semi carpus word derived from the Greek word simeion, meaning marking, and carpus means nut. Anacardium means heart-shaped marking nut (2). The most promising components are bhilwanols, bioflavonoids, sterols, glycosides, and phenolic compounds. Nut milk is used in the siddha medicine called Kalpamrutha for the treatment of inflammation and ulceration (3). Flavonoids are the secondary plant metabolites, play a key role in the management of stress in plants and have a high relevance in human health, mainly due to their anti-inflammatory activity (4). The major constituents of Semi-carpus anacardium are biflavonoids, which are listed below. Butein (2',3,4,4'-

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Tetrahydroxy chalcone) is an important dietary flavonoid present in the semi-carpus plant nut, active against inflammation and oxidation (5). Tetrahydro amentoflavone is a potent inhibitor of xanthine oxidase, exhibiting antioxidant activity (6).

Psoriasis is an immune mediated inflammatory skin disorder with prevalence rate of 125 million throughout the worldwide suffering from this disease at various stages in different geographical regions. Clinical confirmation of psoriasis is done by the PASI score (Psoriasis area severity index) with the range of 0-72 with the clinical manifestation of erythema, thickening surface area involved (7). Skin scalability due to overproduction of keratinocytes and move towards the upper skin layers. Multiple therapies like oral, systemic, topical, photo, biological therapies were available to control the disease propagation mechanism, no certain therapy is available to cure the disease. As per WHO psoriasis is a rare immunological skin disorder and it can impact the physical, social, mental life of the person, change in diet and regular exercise improve the disease modification (8,9).

The present study deals with the natural treatment strategies to reduce the disease propagation of psoriasis by using semi carpus anacardium nut shell oil.

MATERIALS AND METHODS:

All the ligand molecules related to this study were downloaded from https://pubchem.ncbi.nlm.nih.gov site in 3D SDF format. Protein molecules were downloaded from the Protein Data Bank repository (https://www.rcsb.org/). Software tools like Biovia Discovery, Autodock Vina, Open Babel, pkCSM, and SWISSADME were used for the visualization, conversion to predict pharmacokinetic properties. System specifications are Windows 11, 64-bit, with Intel @ Core TM i5-6200U CPU 2.30 G Hz. SMILES (simplified molecular input line entry system) of every ligand should be provided in the specified box of the sites to predict the detailed molecular level parameters.

Autodock Vina:

This docking software is a freely available tool to perform the molecular docking mechanism, with a set of algorithms. Vina software runs with Java and Python programming, and blind docking is possible with a space adjustment of 0.5 A^0.

pkCSM and SWISSADME:

Predicting small molecule properties is of utmost importance to know the fate of drug molecules, and there is a chance to improve their characteristics. By using this web server, we can access the absorption, distribution, metabolism, and excretion-related parameters. Toxicity and safety dosage regimens were also included in these servers. Radar plots are also included to exhibit the physicochemical characteristics of the drugs.

Methods:

The docking method involves three steps, i.e.: preparation of proteins, identifying the GRID coordinates, and determining the bonding strength with the molecular docking score. Docking is a computational approach to know the binding affinity of the ligand molecule with the receptor proteins. Docking score indicated as Kcal/mol, the highest docking score indicates the higher binding affinity and it is compared with the standard drug molecule binding affinity which is used in psoriasis treatment (10).

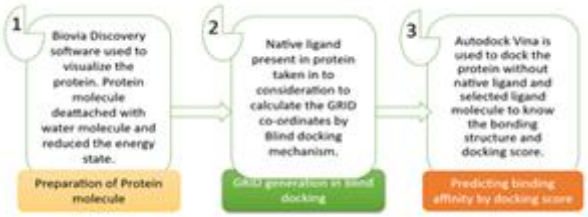

Figure 1: Molecular docking mechanism represented in step-by-step explanation.

RESULTS AND DISCUSSION:

Molecular docking was done to the bioflavonoid; catechol ligands present in semi carpus anacardium chemical analysis. In this present study the ligands were docked against the proteins involved in the psoriasis disease propagation mechanism. As per the study conducted by the Pentu et al., (2025) the proteins were selected to understand the psoriasis mechanism and the importance of proteins involved in it. Butein and tetrahydroamento flavone compounds were docked

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JCHR (2026) 16(2), 1247-1255 | ISSN:2251-6727

against the 8 proteins such as TNF-alpha, IL-23, IL-17A, PDE-4, BTK, JAK-3, IL-6, p38MAPK.

(a) (b)

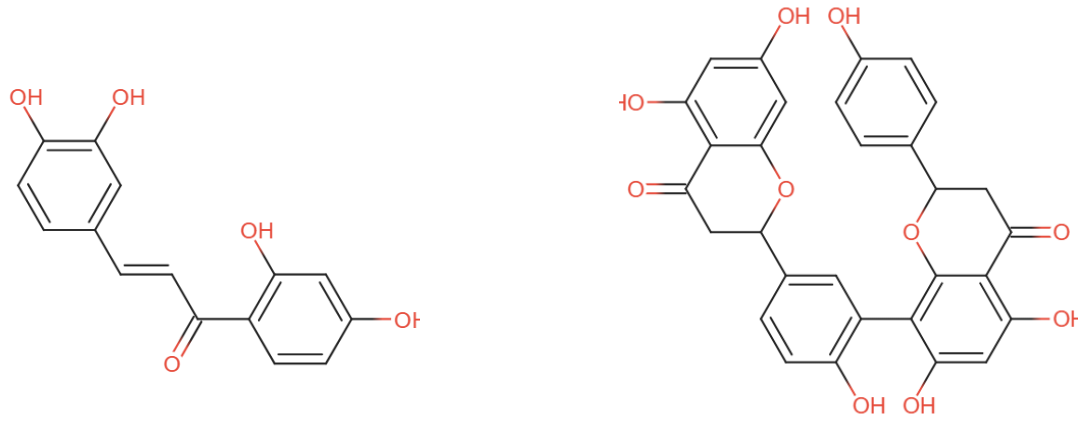

Figure 2: Molecular structures of (a) Butein and (b) Tetrahydroamento flavone

Table 1: Molecular descriptor properties of ligands.

Ligand	Molecular weight	LogP	HBA	HBD	Rotatable bonds	LV
Butein	272.256	2.4051	5	4	3	0
Tetrahydroamento flavone	542.496	5.0002	10	6	3	2 (Molecular weight >500; HBD >5)

LV-Lipinski's violation; Yellow colour indicates violation of molecular descriptors.

Mol. Wt <500; LogP <5; HBA < 10; HBD <5 as per the Lipinski's rule of five.

Lipiski's rule of five describes the properties of the drug molecules decides its fate, weather it is deliver through oral route or not. More than one deviation in lipinski's violation leads to less bioavailability when it is given in oral route (11).

Table 2: Hydrogen and non-hydrogen bond representation between Ligand and receptor interaction mechanism.

Protein	Ligands	Hydrogen Bonds	Non-hydrogen bonds
TNF-α (2AZ5)	Butein (5281222)	THR A:77	ASN A:137
	Tetrahydroamentoflavanone (326004)	-	-
	Methotrexate (126941)	-	TYR B:119, TYR A:119, GLY B:121
IL-23 (3QWR)	Butein (5281222)	-	-
	Tetrahydroamentoflavanone (326004)	ASN A:200, THR A:202	MET A:189

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	Methotrexate	-	-
IL-17A (5HI4)	Butein (5281222)	LEU A:97	ILE A:96, ILE B;96
	Tetrahydroamentoflavanone (326004)	TYR A:6.02	LEU B:97, GLU B:95, PRO A:63
	Methotrexate	LEU B:97	ILE B;96, LEU A:97
PDE-4 (5K1I)	Butein (5281222)	-	PRO A:322, PHE A:372, LEU A:319, ILE A:336, TYR A:159, ASN A:321, ASP A:318.
	Tetrahydroamentoflavanone (326004)	ASN A:209, SER A:208	GLU A:230, MET A:273, HIS A:160, MG A:1003, HIS A:204, LEU A:229, GLN A;210,
	Methotrexate	-	PHE A:340, HIS A:160, ILE A:336, SER A:208
BTK (4OTF)	Butein (5281222)	-	THR A;410, LYS A:430, GLY A:411, VAL A:416
	Tetrahydroamentoflavanone (326004)	MET A:477	VAL A:416, LEU A:528, ALA A:428, LEU A: 408, GLY A:408, TYR A:476, LYS A:430, THR A:474.
	Methotrexate	-	OCS A:481, GLY A:411, THR A:410, ASN A:526, ARG A:525.
JAK-3 (5TTS)	Butein (5281222)	-	LYS A:855, ASP A:967, VAL A:836.
	Tetrahydroamentoflavanone (326004)	CYC A:909	LEU A:828, GLY A:908, LEU A:956, ARG A:953, ARG A:911, ASP A:912.
	Methotrexate	-	LEU A:956, LEU A :828, VAL A; 836, GLY A:908, LEU A:905, TYR A:904.
IL-6 (5FUC)	Butein (5281222)	ASN C:202	THR C:204
	Tetrahydroamentoflavanone (326004)	ASN E:74	ASP E:73. THR C:218, GLN E:72, GLN C:220, ASN C:202.
	Methotrexate	THR C:218	ALA E:75, THR C:204, THR C:206, ASN E:74, ASP E:73
p38MAPK (2C6O)	Butein (5281222)	LEU A:83	GLU A:81, PHE A:82, ALA A:31, ILE A: 10, LEU A:134.
	Tetrahydroamentoflavanone (326004)	PHE A:82	VAL A:18, ALA A:31, LEU A:134, ILE A:10, Leu A:83, GLU A:81, PHE A:80, ALA A:144, ASP A:145, LYS A:33.

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	Methotrexate	-	VAL A:18; GLN A:131; ASP A:86; LEU A:134; ILE A:10

Purple colour indicates Pi-Sigma bonds # Pink colour indicates Pi-alkyl bonds # Orange colour indicates π-π-sulfur interactions between the ligand and sulfur-containing residues.

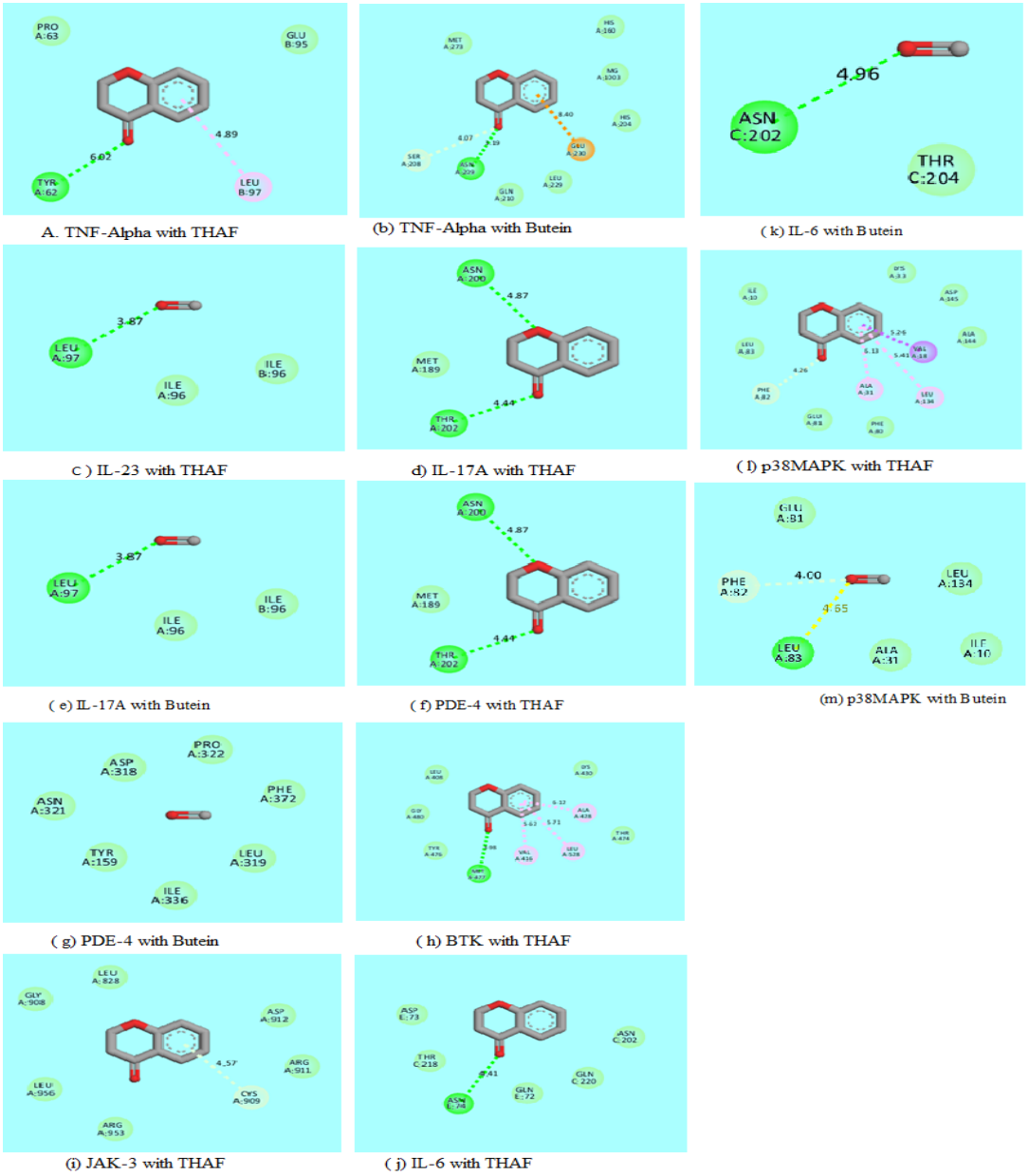

Figure 3: 2D images of the proteins docked with ligands.

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Docking mechanism reveals the structural features of the receptor with its hydrogen and non-hydrogen bonds interactions. In this blind docking mechanism ligand docked at the position of GRID co-ordinates which are collected from the native ligand of the protein. Individual protein has identical values of GRID. IL-6, IL-17A and IL-23 showed remarkable bonding interactions with the Butein and THAF when compared with the methotrexate.

Table 3: Docking scores of ligands with specific protein molecules.

Ligand	TNF-α	IL-23	IL-17A	PDE-4	BTK	JAK-3	IL-6	p38 MAPK
Butein	-5.3	-5.7	-7.1	-8.7	-7.5	-7.9	-6.8	-8.4
THAF	-7	-7.8	-9.7	-11.2	-10.8	-9.3	-7.8	-10.3
Methotrexate	-8.1	-7.7	-6.7	-8.2	-6.4	-8.3	-7.9	-7.1

PDE-4 protein binding with THAF recorded as highest binding score of -11.2 Kcal/mol and the bonding amino acid sequence is ASN A:209, SER A:208 conventional hydrogen bonds. All most all the proteins with THAF docking score are higher than the standard one. Butein has lacking in docking score when compared with the standard and THAF.

Table 4: Ligands with SMILES string.

S. No.	Ligand	PubChem ID	SMILES
1	**Butein**	5281222	C1=CC(=C(C=C1/C=C/C(=O) C2=C(C=C(C=C2) O) O) O) O
2	**Tetrahydroamento flavone**	326004	C1C(OC2=C(C(=CC(=C2C1=O) O) O) C3=C(C=CC(=C3) C4CC(=O) C5=C(C=C(C=C5O4) O) O) O) C6=CC=C(C=C6) O

Pharmacokinetic properties:

Pharmacokinetic properties decide the fate of the drug molecule with ADME properties (Absorption, distribution, Metabolism, Excretion). Absorption related properties like water solubility, CaCo2 permeability, intestinal absorption, skin permeability, P-glycoprotein substrate and P-glycoprotein inhibitor shows the absorption related characteristics. CaCo2 permeability > 0.9 indicates good permeation through epithelial barriers, Butein and THAF exhibits good water solubility and intestinal absorption (it should be always > 30 %). Both the ligands show the good skin permeability, P-glycoprotein functions like a biological barrier to expel out the xenobiotics. Butein is No Pgp inhibitor and THAF acts as Pgp inhibitor action (12).

Distribution related characteristics like, VDss indicates the volume of distribution mechanism, Butein has higher distribution, THAF has lesser volume of distribution mechanism. All ligands were not permeable through BBB and CNS. Fraction of unbound drug concentration was mentioned in the table column. CYP3A4 substrate is Butein and THAF as CYP1A2. OCT2 (organic clearance transporter 2) act as renal clearance system, both the ligands have higher clearance with kidneys. (Table 6 shows the data related to the pharmacokinetic properties of ligands)

AMES toxicity (mutagenic nature), Hepatotoxicity, skin sensitization was recorded as zero. hERG inhibition leads to increase in QT interval of cardiac rhythm (13).

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Table 5: Drug pharmacokinetic properties

Properties	Butein	Tetrahydroamento flavone	
PSA	114.232	226.096	
AlogP	2.4051	5.002	
Water Solubility (Log mol/L)	-3.177	-2.946	Absorption
CaCo2 Permeabilit(Log Papp in 10-6 cm/s)	-0.021	0.219	
Interstinal absorption (human % absorbed)	72.567	63.381	
Skin Permeability (log Kp)	-2.736	-2.735	
P-Glycoprotein substrate	YES	Yes	
P-Glycoprotein I Inhibitor	NO	Yes	
P-Glycoprotein II Inhibitor	NO	Yes	
VDss (log L/Kg)	0.741	-1.392	Distribution
Fraction unbound (Fu)	0.232	0.112	
BBB Permeability (log BB)	-0.895	-1.136	
CNS Permeability (log PS)	-2.395	-3.315	
CYP2D6 substrate	No	No	Metabolism
CYP3A4 substrate	NO	Yes	
CYP1A2 inhibitor	Yes	NO	
CYP2C19 inhibitor	NO	NO	
CYP2C9 inhibitor	NO	NO	
CYP2D6 inhibitor	NO	No	
CYP3A4 inhibitor	NO	No	
Total clearance (Log ml/min/kg)	0.015	-0.134	Excretion
Renal OCT2 substrate	No	No	
AMES toxicity	No	No	Toxicity
Max. tolerable dose	0.117	0.428	
hERG I inhibitor	No	No	

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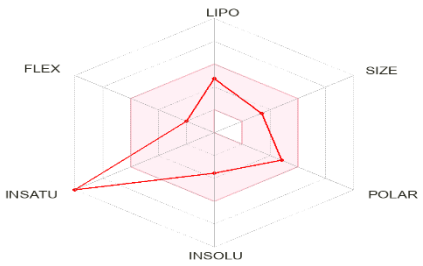
hERG II inhibitor	No	Yes	
Hepatotoxicity	No	No	
Skin Sensitization	NO	NO	
Oral rat acute toxicity (LD50) mol/ kg	2.456	2.613	
Oral rat Chronic toxicity (LOAEL) log mg/kg_ bw/day	2.578	4.09	

(a)



(b)

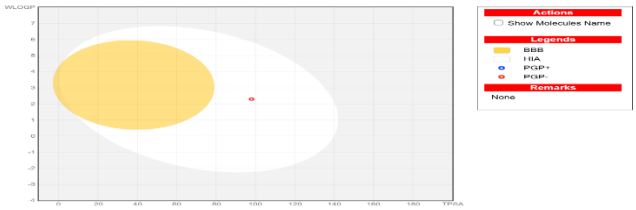
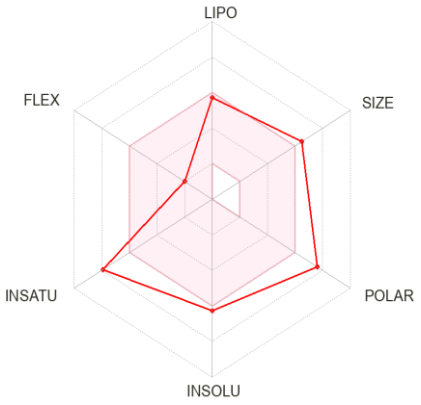


Figure 4: Physicochemical properties by (a) radar maps and (b) Boiled egg prediction of Butein.

Butein exhibit excellent physicochemical properties to deliver through oral route of administration. Radar map indicates, shaded region is the favorable properties to formulate oral formulation. LIPO- Lipophilicity region should be within the range of -0.7 to +5, Molecular weight in the range of 150 to 500 mg/mol, TPSA (total polar surface area) should be 20 to 130 $A^{0\,2}$, Insolubility between -6 to 0, insaturation (Fraction of CSp^3) in the range of 0.25 to 1, flexibility (no. of rotatable bonds) within 0 to 9. As per the figure __ only properties like insaturation deviated from the shaded region due to higher unsaturated bonds. Boiled egg indicates, egg yolk yellow is the region of permeable through the BBB, white yolk permeable through GI tract, red dot indicates not to be effluated from the CNS from the P-glycoprotein.

(a)



(b)

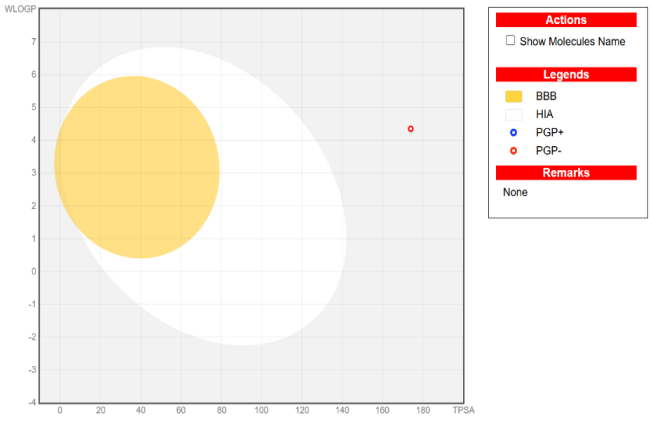


Figure 5: Physicochemical properties by (a) radar map and (b) Boiled egg prediction of Tetrahydroamento flavone.

Tetrahydroamento flavone physicochemical properties description indicated by the radar map describes, there is only one deviation in insaturation due to higher unsaturation bonds. Boiled egg explains the BBB

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permeation of yellow yolk; white yolk permeates through Gi tract and red dot indicated effluent of CNS by P-glycoproteins.

CONCLUSION:

Psoriasis is not a life-threatening disorder, but it requires regular care and nourishment of skin layers with regular moisturizing agents and diet. Synthetic compounds are not preferable for long term therapies and these can be replaced with the plant related alternative treatment mechanisms. *Semi carpus anacardium* chemical constituents like Butein, Tetrahydroamento flavone shows better docking scores and suitable to deliver through the oral route of administration after performing the pharmacokinetic properties and Lipinski's rule of five evaluation. THAF shows highest docking score of -11.2 Kcal/ mol when comparing with the standard drug (-8.3Kcal/mol). Furthermore, formulaitons strategies improve the drug effectiveness and stability to increase the potential against psoriasis.

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