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ADMET Prediction And Molecular Docking Of Constituents From *Wedelia Chinensis* For Anticancer Activity

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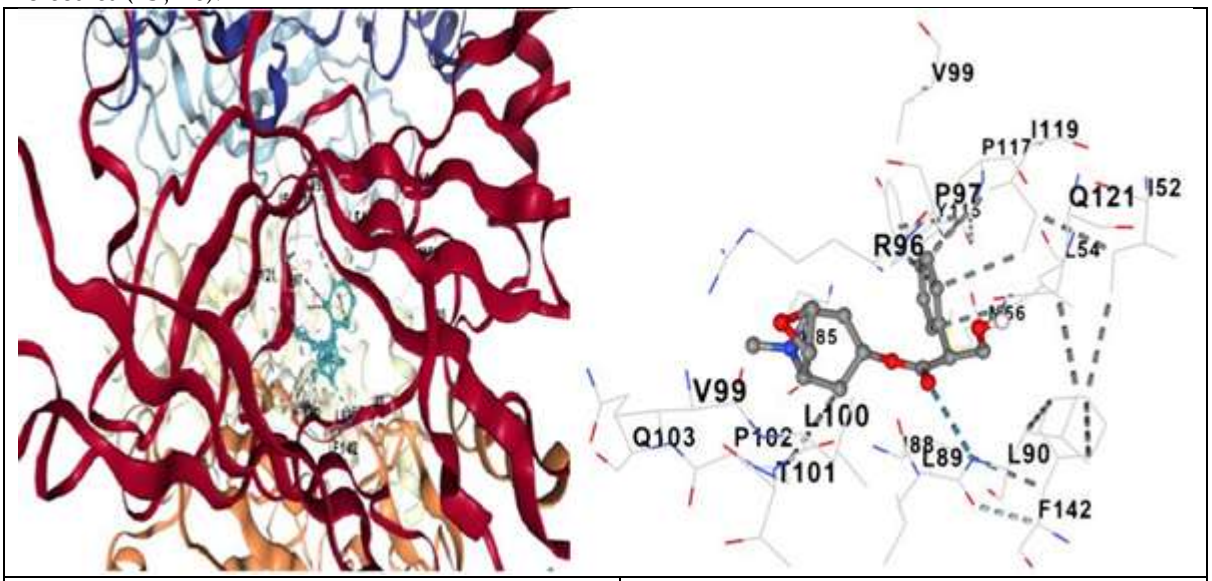
ABSTRACT:
Wedelia chinensis is a soft, hairy plant that spreads out and has branches that are less than 50 cm long. Checking how well phytochemicals bond and how amino acids interact with each other. In silico, phytochemicals that have anticancer properties were matched up with the standard drug. We looked at ADMET (adsorption, distribution, metabolism, excretion, and toxicity) and ADMET filter-passing polyphenols. AutoDock Vina was used for a preliminary docking study. The results were then confirmed by AutoDock 4.2.6 and SwissDock. Scientists did a study and found that stigmasterol interacts best with solid structures. The structure of the Cyclophilin Colon Cancer Antigen 10 from Homo Sapiens (PDB: 2HQ6) and a comparison with caffeine, a standard drug with a binding affinity of -6 kcal/mol, and stigmasterol, a naturally occurring chemical constituent with a binding affinity of -10.7 kcal/mol. Based on molecular docking, ADMET modeling, and active site interactions, this drug can help fight cancer. These showed that the molecule worked as a cancer receptor drug.
KEYWORDS: Cancer, Wedelia chinensis, caffeine, Molecular Docking, ADMET.

INTRODUCTION

Since cancer is still one of the major causes of death worldwide, there is a constant need to find safer and more effective treatment options (Gowtham, *et al.,* 2023). Traditional medicinal plants have gained attention in drug discovery due to their diverse bioactive phytochemicals with potential anticancer properties (Yadav, *et al.,* 2017). Traditional medicine has long used *Wedelia chinensis*, a well-known plant in Ayurvedic and traditional Chinese practices, to treat inflammation, liver disorders, and tumor-related ailments (Mani, *et al.,* 2024). Many studies have shown that it contains a lot of flavonoids, sterols, and coumarins, which are thought to help with its medicinal effects, including fighting cancer (Mali, *et al.,* 2022). Advances in computational biology provide helpful instruments for early-stage drug discovery, including the prediction of absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties, which are critical for evaluating drug-likeness and safety profiles of bioactive compounds (Bibi, F., Nouroz, F., Ahmad, A., Noreen, S., & Khan, S. (2023). Additionally, molecular docking studies offer analyses of the binding affinity and interaction patterns of phytochemicals with target proteins involved in cancer progression, facilitating the identification of promising lead compounds (6). In this study, important plant compounds from Wedelia chinensis were analyzed using computer simulations to predict their ADMET properties and how well they bind to proteins related to cancer (7). The goal was to assess how these compounds behave in the body, their possible toxicity, and how well they can bind to target proteins, helping to find promising anticancer candidates for further research

MATERIALS AND METHOD

Software and programs:
ChemSketch, a program for drawing chemistry molecules, was used to show the ligand compounds. Avogadro software was used to change the.mol file to the.pdb format. This is version 4.0 of Autodock (9). The study on the semi-flexible protein ligand docking was done with preliminary docking tools. The Molinspiration online property tool was used to look at the molecule's chemical properties (10). Researchers used the protein database to figure out the crystal structure of the cyclophilin CeCYP16-like region of the human colon cancer antigen 10 that was found by testing with a blood test. It had the PDB code [PDB: 2HQ6]. The goal of the computer studies will be to look at the solid structure (11). Pyrx software was used to virtually screen a library of variations. Discovery Studio 3.5 was used to see how molecules communicate and move (12).
Preparation of ligand:
The structure of the ligand was made with the clean structure tool and the ChemSketch program. It was saved as an a.mol file in the working area. Then, the Avogadro program was used to open the.mol file and make the structure better. The improved structure was in the a.pdb file in the working directory (13, 14).
Preparation of receptor:
The anticancer drug's crystal structure was rectified using Autodock v4.0 software after it was downloaded from an online database in.pdb format. The energy was decreased by dispersing the charges throughout the receptor. The water molecules connected to the receptor were swapped out for polar hydrogen molecules (15, 16).



(a) (b)

Figure 1: Ligand interaction diagram of protein and chemical constituent (A) Stigmasterol with PDB ID 2HQ6 in receptor region (b) Stigmasterol with PDB ID 2HQ6 in hide receptor
Receptor-Ligand Interaction:
Using Autodock v4.0, we were able to find the binding sites and the energies that went with them. The idea that energy and stability are opposites means that a shape with more binding energy is less stable (17-19). The software has been set up so that it works with the way the protocol is used in other places. The Lamarckian Genetic Algorithm (LGA) was used to find the energy level, with X = 24.320, Y = 25.140, and Z = 26.480 as the values and a grid point spacing of 0.375 angstroms. It came with 126 grid boxes (x, y, and z) that were set up in 60:60:60 ratios for atomic saving settings. The grid box was carefully made so that the active ligand binding area of the receptor was in the middle and the grid went all the way around it (20-23).
Physiochemical Properties:
The ligand's properties were computed using the Molinspiration online property calculator. The ligand's structure was sketched and certain properties were ascertained using an internal tool. The attributes were grouped into broad categories, such as bioactivity and structural feature. It was anticipated that using the

Protox III web server would cause acute oral toxicity (24-27).

RESULT AND DISCUSSION:

Docking scores indicate binding strength with the target, where more negative values suggest stronger binding. Stigmasterol (−10.7), Wedelolactone (−10), and Luteolin (−9.5) have strong binding to the target, meaning they are likely to interact well with it. Limonene (−5.2) and Phellandrene (−5.7) have less favorable scores, indicating weaker binding. All molecules obey Lipinski's rule except stigmasteryl glucoside, which violates it due to high MW (574.42) and excessive rotatable bonds (8). Despite this, other large lipophilic compounds like melissic acid (MW 452.46, LogP 12.31) and lignoceric acid (MW 368.37, LogP 9.98) technically "obey" due to favorable hydrogen bond counts, but LogP exceeds the ideal. Compounds like stigmasterol, wedelolactone, and luteolin show strong binding and obey Lipinski's rules, making them promising drug candidates. Stigmasteryl glucoside, while showing moderate binding (−7), fails Lipinski, suggesting poor oral bioavailability or permeability. Highly lipophilic compounds (e.g., lignoceric acid, melissic acid) may pose solubility issues, despite rule compliance. TPSA < 140 $Å^2$ generally predicts good absorption.Wedelolactone (113.27), luteolin (111.13), and quercetin (131.36) have high TPSA but are still under the threshold, indicating moderate permeability. Compounds like limonene, phellandrene, and α-humulene have TPSA = 0, indicating extreme lipophilicity, possibly affecting solubility.

Table 1: Results of binding affinity of molecule and physiochemical properties and Lipinski rules.

Sr. No.	Ligand	Docking score	MW (g/mol)	Rotatable bonds	H-bond acceptor	H-bond donors	TPSA	LOGP	Follow Lipinski
1.	Standard caffeine	-6	194.08	0	6	0	61.82	0.048	Obey
2.	Stigmasterol	-10.7	412.37	5	1	1	20.23	7.436	Obey
3.	Wedelolactone	-10	314.04	1	7	3	113.27	3.194	Obey
4.	Luteolin	-9.5	286.05	1	6	4	111.13	2.902	Obey
5.	Quercetin	-9.3	302.04	1	7	5	131.36	2.155	Obey
6.	ρ- Cymene	-7.1	134.11	1	0	0	0	3.994	Obey
7.	a-humulene	-7	204.19	0	0	0	0	5.194	Obey
8.	Stigmasteryl glucoside	-7	574.42	8	6	4	99.38	5.738	Not Obey
9.	Germacrene	-6.7	206.2	1	0	0	0	5.393	Obey
10.	Indole-3-carbaldehyde	-6.7	145.05	1	2	1	32.86	2.02	Obey
11.	Norwedelic acid	-6.7	318.04	2	8	6	151.59	2.041	Obey
12.	Phenacetin	-6.6	179.09	4	3	1	38.33	1.677	Obey
13.	Lignoceric acid	-6.4	368.37	22	2	1	37.3	9.98	Obey
14.	Melissic acid	-6.4	452.46	28	2	1	37.3	12.313	Obey

15.	Spathulenol	-6.3	220.18	0	1	1	20.23	4.032	Obey
16.	Phellandrene	-5.7	136.13	1	0	0	0	3.857	Obey
17.	Limonene	-5.2	136.13	1	0	0	0	4.368	Obey

Table 2: Absorption characteristics of the selected phytochemical

Sr. No.	Ligand	Caco-2 Permeability	MDCK Permeability	Pgp-inhibitor	Pgp-substrate	HIA	F20%	F30%
1.	Standard caffeine	-4.668	7.52E-06	0.066	0.001	0.005	0.008	0.185
2.	Stigmasterol	-5.096	1.15E-05	0.009	0.868	0.154	0.042	0.998
3.	Wedelolactone	-5.028	1.00E-05	0.004	0.274	0.047	0.998	1
4.	Luteolin	-5.204	7.69E-06	0.004	0.005	0.014	0.93	0.997
5.	Quercetin	-4.302	1.96E-05	0.011	0.005	0.004	0.211	0.931
6.	ρ- Cymene	-4.613	1.64E-05	0.068	0.001	0.016	0.012	0.003
7.	a-humulene	-4.816	2.10E-05	0.051	0.004	0.035	0.012	0.17
8.	Stigmasteryl glucoside	-4.539	2.04E-05	0.092	0.005	0.008	0.94	0.975
9.	Germacrene	-4.492	9.89E-06	0	0.004	0.008	0.011	0.967
10.	Indole-3 carbaldehyde	-6.127	5.46E-06	0	0.013	0.591	0.996	1
11.	Norwedelic acid	-4.298	1.71E-05	0.003	0.063	0.003	0.003	0.993
12.	Phenacetin	-5.196	1.04E-05	0	0	0.005	0.258	0.999
13.	Lignoceric acid	-5.272	3.82E-06	0	0	0.006	0.124	1
14.	Melissic acid	-4.567	1.93E-05	0.001	0	0.004	0.008	0.012
15.	Spathulenol	-4.383	2.39E-05	0.001	0.013	0.005	0.014	0.146
16.	Phellandrene	-4.32	1.93E-05	0.002	0	0.003	0.818	0.798
17.	Limonene	-4.668	7.52E-06	0.066	0.001	0.005	0.008	0.185

The absorption characteristics of the selected phytochemical ligands were compared against the standard drug, caffeine, using key pharmacokinetic indicators including Caco-2 and MDCK permeability, P-glycoprotein (Pgp) interaction, Human Intestinal Absorption (HIA), and oral bioavailability fractions (F20% and F30%).

1. Caco-2 and MDCK Permeability:
Caco-2 and MDCK cell models serve as in vitro surrogates for intestinal permeability. Compounds with higher permeability (less negative log values) are generally better absorbed. Quercetin (-4.302), Norwedelic acid (-4.298), and Spathulenol (-4.383) demonstrated superior Caco-2 permeability compared to caffeine (-4.668), indicating better potential for intestinal absorption. MDCK values were notably higher in Spathulenol (2.39E-05) and **a**-humulene (2.10E-05), suggesting favorable membrane permeability.

2. P-glycoprotein (Pgp) Inhibition and Substrate Recognition:
Pgp plays a key role in effluxing drugs out of cells, affecting their intracellular concentration. Most compounds were non-inhibitors and non-substrates of Pgp, minimizing concerns about efflux-related absorption issues. Stigmasterol (0.868) and Wedelolactone (0.274) showed moderate substrate interaction, which may influence bioavailability due to efflux activity.

3. Human Intestinal Absorption (HIA):
HIA values show the extent to which compounds can be absorbed through the intestine. Indole-3-carbaldehyde (0.591) and Stigmasterol (0.154) had relatively high HIA values, suggesting better intestinal uptake. Most other compounds, including standard caffeine (0.005), exhibited very low HIA, indicating poor absorption.

4. Oral Bioavailability (F20% and F30%):
Oral bioavailability (F20% and F30%) estimates the percentage of the compound that reaches systemic circulation. Wedelolactone (0.998, 1.0) and Indole-3-carbaldehyde (0.996, 1.0) showed excellent oral bioavailability, suggesting high potential as orally active agents. In contrast, compounds like p-cymene (0.012, 0.003) and Melissic acid (0.008, 0.012) exhibited poor bioavailability.

5. Comparative Insights:
Among all phytochemicals, Wedelolactone, Indole-3-carbaldehyde, and Stigmasteryl glucoside stand out with favorable absorption, permeability, and bioavailability properties. Despite being the standard, caffeine shows poor HIA and bioavailability, which may limit its comparative absorption performance in this context.

Table 3: *Insilico* Metabolism study of chemical constituents

Sr. No.	Ligand	CYP1A2-inhibitor	CYP1A2-substrate	CYP2C 19- inhibitor	CYP2C19 - substrate	CYP2 C9- inhibitor	CYP2C9-substrate	CYP2D6-inhibitor
1.	Standard caffeine	0.135	0.974	0.024	0.312	0.003	0.545	0.002
2.	Stigmasterol	0.981	0.862	0.076	0.057	0.615	0.908	0.282
3.	Wedelolactone	0.981	0.154	0.124	0.046	0.576	0.842	0.568
4.	Luteolin	0.943	0.115	0.053	0.041	0.598	0.643	0.411
5.	Quercetin	0.941	0.944	0.855	0.864	0.574	0.61	0.778
6.	ρ- Cymene	0.691	0.515	0.529	0.426	0.429	0.948	0.728
7.	a-humulene	0.002	0.337	0.007	0.891	0.035	0.106	0.001
8.	Stigmasteryl glucoside	0.441	0.502	0.326	0.361	0.535	0.917	0.177
9.	Germacrene	0.977	0.45	0.559	0.285	0.12	0.911	0.081
10.	Indole-3-carbaldehyde	0.492	0.071	0.026	0.034	0.424	0.126	0.038
11.	Norwedelic acid	0.841	0.94	0.479	0.824	0.065	0.843	0.033
12.	Phenacetin	0.102	0.155	0.214	0.054	0.051	0.995	0.028
13.	Lignoceric acid	0.046	0.127	0.108	0.046	0.02	0.997	0.042
14.	Melissic acid	0.139	0.587	0.085	0.895	0.227	0.604	0.009
15.	Spathulenol	0.258	0.471	0.178	0.93	0.142	0.337	0.059
16.	Phellandrene	0.678	0.652	0.223	0.834	0.06	0.804	0.02
17.	Limonene	0.678	0.652	0.223	0.834	0.06	0.804	0.02

The metabolism of a compound is significantly influenced by cytochrome P450 enzymes (CYPs), which

are responsible for drug metabolism, interactions, and clearance. The predictive values in Table 3 represent the probability of inhibition or substrate behavior for key CYP enzymes.

1. Standard Drug – Caffeine:

Caffeine shows a high substrate probability for CYP1A2 (0.974) and moderate interaction as a substrate with CYP2C9 (0.545). It has minimal inhibitory roles across all enzymes, indicating a low potential to interfere with the metabolism of co-administered drugs.

2. High CYP Inhibitors:

Stigmasterol, Wedelolactone, Luteolin, and Quercetin show strong inhibition for CYP1A2, which may affect the metabolism of drugs like caffeine. Quercetin exhibits a broad inhibitory profile: high inhibition of CYP1A2 (0.941) and CYP2C19 (0.855), suggesting a higher risk for drug-drug interactions. Germacrene and Norwedelic acid also demonstrate potent inhibition of multiple CYPs, suggesting potential metabolic competition and possible accumulation of co-administered substrates.

3. Strong Substrate Candidates:

Quercetin and Norwedelic acid show high substrate probability for CYP1A2, 2C19, and 2C9, indicating extensive metabolism via these enzymes. Phenacetin and Lignoceric acid exhibit strong CYP2C9 substrate activity (0.995 and 0.997), which may make them prone to enzyme-based variability in metabolic rate.

4. Low Interactors (Minimal CYP interaction):

α-Humulene and Indole-3-carbaldehyde show low inhibitory and substrate probabilities for most CYPs, indicating they are less likely to cause metabolic interference or competition.

5. Moderate Metabolizers:

ρ-Cymene, Phellandrene, and Limonene exhibit moderate substrate and inhibitory interactions, mainly for CYP2C9 and CYP2C19, which may cause mild to moderate interactions depending on dosage and combinations.

Table 4: Excretion parameters of various phytochemicals

Sr. No.	Ligand	CL	T1/2
1.	Standard caffeine	1.83	0.774
2.	Stigmasterol	15.958	0.014
3.	Wedelolactone	8.454	0.819
4.	Luteolin	8.146	0.898
5.	Quercetin	8.284	0.929
6.	ρ- Cymene	7.38	0.276
7.	a-humulene	3.4	0.403
8.	Stigmasteryl glucoside	4.455	0.017
9.	Germacrene	5.488	0.253
10.	Indole-3-carbaldehyde	6.548	0.798
11.	Norwedelic acid	9.177	0.938
12.	Phenacetin	6.297	0.684
13.	Lignoceric acid	2.761	0.21
14.	Melissic acid	2.897	0.079
15.	Spathulenol	14.582	0.064
16.	Phellandrene	12.66	0.617
17.	Limonene	11.517	0.233

Table 4 presents the excretion parameters of various phytochemicals in comparison with the standard drug caffeine, focusing on two key pharmacokinetic values: Clearance (CL) and Half-life (T1/2).

Clearance (CL): Standard caffeine shows a clearance of 1.83 mL/min, which is relatively low. Most phytochemicals, such as Stigmasterol (15.958), Spathulenol (14.582), and Phellandrene (12.66), exhibit much higher clearance, indicating faster systemic elimination. A few compounds like Lignoceric acid (2.761) and Melissic acid (2.897) have moderate clearance, suggesting slower excretion rates more comparable to caffeine.

Half-life (T1/2): Caffeine's half-life is 0.774 hours, indicating moderate retention in the body.

Compounds such as Quercetin (0.929), Norwedelic acid (0.938), and Luteolin (0.898) have longer half-lives than caffeine, suggesting they may exert prolonged biological effects. In contrast, several constituents like Stigmasterol (0.014) and Stigmasteryl glucoside (0.017) have very short half-lives, indicating rapid degradation or excretion from the body.

Overall Trends and Implications: Fast-clearing and short half-life compounds (e.g., stigmasterol, spathulenol) may need frequent dosing or formulation modifications to maintain therapeutic levels. Compounds with longer half-lives and moderate clearance (e.g., quercetin, norwedelic acid) might offer sustained activity and be beneficial in reducing dosage frequency. Balanced excretion profiles such as that of Wedelolactone (CL: 8.454, T1/2: 0.819) suggest potential as a bioactive compound with effective systemic duration.

Table 5: *Insilico* Toxicity predication of chemical constituents

Sr. No.	Ligand	Carcinogenicity	Skin Sensitization	Acute Aquatic Toxicity	Toxicophores
1.	Standard caffeine	0.039	0	0	1
2.	Stigmasterol	0.054	0	1	0
3.	Wedelolactone	0.032	6	0	4
4.	Luteolin	0.095	7	0	2
5.	Quercetin	0.05	8	0	2
6.	ρ- Cymene	0.386	0	1	0
7.	a-humulene	0.028	0	1	0
8.	Stigmasteryl glucoside	0.045	1	2	0
9.	Germacrene	0.029	0	1	0
10.	Indole-3-carbaldehyde	0.25	2	0	3
11.	Norwedelic acid	0.029	7	0	3
12.	Phenacetin	0.783	4	0	1
13.	Lignoceric acid	0.03	0	0	0
14.	Melissic acid	0.02	0	0	0
15.	Spathulenol	0.065	0	1	0
16.	Phellandrene	0.344	0	1	0
17.	Limonene	0.922	0	1	0

The toxicity prediction data for the phytochemicals, along with the standard drug caffeine, provides significant insight into their potential safety profiles for therapeutic application. The analysis is based on five key toxicity parameters: carcinogenicity, skin sensitization, acute toxicity, aquatic toxicity, and presence of toxicophores.

Carcinogenicity: Carcinogenicity scores ranged widely across the tested compounds. Caffeine, the standard, exhibited a low carcinogenicity score (0.039), similar to many natural constituents like melissic acid (0.020), α-humulene (0.028), and norwedelic acid (0.029). However, compounds such as limonene (0.922) and phenacetin (0.783) displayed high carcinogenic potential, suggesting caution in their therapeutic application due to potential long-term cancer risks.

Skin Sensitization: Most compounds showed minimal to no skin sensitization risk (score of 0), indicating favorable dermal safety. However, quercetin (8), luteolin (7), and norwedelic acid (7) showed high scores, which may indicate the potential to trigger allergic or immunogenic skin reactions and therefore may require formulation modifications or delivery strategies to mitigate this risk.

Acute Toxicity: The majority of compounds did not exhibit acute toxicity (score 0). Exceptions include stigmasterol, ρ-cymene, α-humulene, stigmasteryl glucoside, germacrene, spathulenol, phellandrene, and limonene, all showing mild acute toxicity (score 1–2). These compounds might require dosage optimization or further toxicological testing in preclinical models.

Aquatic Toxicity: Aquatic toxicity was primarily low or absent across most phytochemicals, which is favorable from an environmental toxicity perspective. However, wedelolactone (4) and indole-3-

carbaldehyde (3) presented moderate aquatic toxicity, suggesting potential ecological concerns if used in large-scale applications or formulations.

Toxicophores: Toxicophore analysis revealed that most compounds carried minimal or no structural alerts for toxicity. High counts were noted for wedelolactone (4), indole-3-carbaldehyde (3), and norwedelic acid (3). These toxicophore-containing compounds may possess reactive functional groups or substructures known to be associated with toxicity and thus warrant further structural optimization.

CONCLUSION

Caffeine has a binding affinity of -6 kcal/mol for stigmasterol, whereas the naturally occurring chemical components have a binding affinity of -10.7 kcal/mol. One naturally occurring chemical component is caffeine. Additionally, the study showed that stigmasterol interacted most well with the receptor crystalline structure of the cyclophilin CeCYP16-like domain of the human colon cancer antigen 10 (PDB: 2HQ6). The most significant link was found to be this one. Based on molecular docking, ADMET prediction, and interactions with active sites, this specific medication is used as an anticancer agent. This allowed us to confirm that the chemical does, in fact, interact with anticancer receptors in a way that is effective.

Declarations:

Consent for publication:

All the authors approved the manuscript for publication.

Competing interests:

All authors declare no competing interests.

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