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Phytochemical Screening and Docking-Based Evaluation of *A. sclerocarpa* Extracts Targeting 6OVA

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A B S T R A C T

Alphonsea sclerocarpa Thwaites, a member of the family Annonaceae, is a genus widely distributed across tropical regions. Traditionally, the whole plant of *A. sclerocarpa* has been valued for its significant therapeutic properties. The present study involved GC-MS analysis of plant extracts prepared using two different solvents: ethanol and petroleum ether. The ethanol extract identified 25 compounds, whereas the petroleum ether extract revealed 24 compounds. From each extract, four compounds were shortlisted for molecular docking studies against the target protein 6OVA.The binding energies of the ethanol-derived compounds were -1.8, -3.8, -1.9, and -1.5 kcal/mol, respectively. In contrast, the petroleum ether-derived compounds exhibited binding affinities of -1.1, -0.8, -1.6, and -2.0 kcal/mol. These results suggest that the compounds obtained from the ethanol extract have comparatively stronger binding affinities than those from the petroleum ether extract.

Introduction

Since ancient times, plants have been recognized as a primary source of medicinal compounds for the treatment of various diseases. Plant-derived medicines have played a crucial role in healthcare across both ancient and modern cultures (Petrovska, 2012). Similarly, *Alphonsea sclerocarpa*, which is widely distributed in Andhra Pradesh (India), is well recognized for its medicinal importance, particularly in cancer therapy and antimicrobial applications. Almost all parts of the plant, including its branches, bark, leaves, fruits, and flowers,

are extensively utilized for therapeutic purposes (Prasad, 2009; Suman Joshi *et al.,* 2017; Tacić *et al.,* 1987). They are rich in a wide array of bioactive compounds, including antioxidants, immunostimulants, cell proliferation enhancers, anti-inflammatory agents, anticancer constituents, and antimicrobial compounds. Several plants, such as green tea, cabbage, holy basil leaves, beets, and *aloe vera*, possess active functional groups with significant antimicrobial properties and the potential to aid in cancer treatment.

Materials and Methods

Collection of Plant Material: *A. sclerocarpa* leaves, a medicinal plant, were gathered from the Seshachalam forest area, verified by a taxonomist.

Gas Chromatography-Mass Spectrometry (GC-MS) Analysis: In this technique, the components of a mixture are first separated by gas chromatography and then individually analyzed using mass spectrometry. The analysis revealed the presence of both volatile and non-volatile compounds.

GC-MS serves as a powerful tool for understanding the metabolic activity of endophytic bacteria, including the nature of metabolites produced and the environmental factors influencing their growth. During the process, the sample is vaporized and passed through a gas chromatography column, where its constituents are separated. These separated compounds are then ionized and analyzed by the mass spectrometer, which identifies them based on their mass-to-charge ratio and quantifies their relative abundance.

Selection of Compounds for *In-silico* Studies: From each extract, four compounds possessing known or potential anticancer properties were chosen for molecular docking studies.

Molecular Docking Studies

Molecular docking is a computational approach used to predict the preferred orientation of a small molecule (ligand) when bound to a protein (receptor/target) and to estimate the binding affinity of this interaction.

In drug discovery, this method is crucial for identifying potential lead compounds that can modulate protein function (Pratistha Singh *et al.,* 2019). For this study, four compounds from each plant extract were shortlisted based on their relative abundance in GC-MS analysis and their reported bioactivity from previous studies.

Target Protein Preparation

- The 3D crystal structure of the target protein (6OVA) was retrieved from the Protein Data Bank (PDB).

The protein was prepared for docking by

- Removing bound water molecules, as they may interfere with ligand interaction.
- Adding polar hydrogens to account for hydrogen bonding possibilities.
- Assigning Kollman charges to accurately represent electrostatic interactions.

Ligand Preparation

- The selected compounds were chemically drawn and optimized using ChemSketch.
- The structures were energy-minimized through Open Babel to achieve the most stable conformation before docking, reducing steric clashes and ensuring biologically relevant configurations (Soumya Khare *et al.,* 2023).

Docking Procedure

- Docking simulations were carried out using AutoDock Vina integrated in PyRx, a widely used platform for virtual screening.
- A grid box was generated that covered the active/binding site of the protein, defining the search space where potential ligand binding orientations could be explored.
- The docking software evaluated multiple binding poses (orientations and conformations) of each ligand within the active site.
- Binding affinity values were calculated in kcal/mol. Higher negative values indicate stronger ligand–protein interactions, reflecting a more stable complex.

Binding Analysis and Visualization

The docked complexes were visualized using Discovery Studio Visualizer, which enabled the identification of (Ayesha Khanum *et al.,* 2024).

- Hydrogen bonds formed between the ligand and amino acid residues.

- Hydrophobic interactions that stabilize nonpolar regions of ligands.
- Pi–pi or pi–cation interactions, especially relevant for aromatic compounds.

Significance of Docking

Molecular docking not only provides binding affinity scores but also highlights the specific molecular interactions responsible for stability. This helps in:

- Predicting the biological activity of novel compounds.
- Understanding how structural features of phytochemicals contribute to anticancer activity.
- Prioritizing compounds (such as Azulene in your case) for further *in vitro* and in vivo evaluations in cancer cell lines and animal models

Results and Discussion

Ethanol Extract Analysis

The ethanolic extract of *Alphonsea sclerocarpa* was used for GC–MS analysis. Ethanol, being a polar solvent, is highly effective in dissolving a wide range of phytochemicals. The study revealed the presence of 25 phytoconstituents, among which four compounds- 4H-Pyran-4-one, Azulene, Hexadecanoic acid, and Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-were identified as having notable anticancer potential.

Molecular Docking

These selected compounds were further evaluated through molecular docking studies against the target protein 6OVA (Actin-like protein 6A, also known as BAF53a). This protein is strongly implicated in cancer progression, particularly ovarian cancer, where its overexpression is associated with poor prognosis, metastasis, chemoresistance, and enhanced tumour cell survival through promotion of cell cycle progression.

The binding affinities obtained from docking were:

- 4H-Pyran-4-one: –1.8 kcal/mol
- Azulene: –3.8 kcal/mol
- Hexadecanoic acid: –1.9 kcal/mol
- Pyrrolo[1,2-a] pyrazine-1,4-dione, hexahydro: –1.5 kcal/mol

Among these, Azulene exhibited the strongest binding affinity (–3.8 kcal/mol), suggesting a more promising interaction with the target protein compared to other ethanol-derived compounds as well as those from the petroleum ether extract. Azulene has been reported for its activity against human pancreatic cancer cell lines and human oral squamous cell carcinoma, supporting its potential as a candidate for anticancer drug development.

From the Table. 3: *Physicochemical properties show the number of atoms, molecular weight, fraction CSP3, topological polar surface area, and number of rotatable bonds, molar refractivity.* 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl, Azulene, Hexadecanoic acid, ethyl ester, Pyrrolo[1,2-a] pyrazine-1,4-dione, hexahydro*, representing their importance, have good oral bioavailability properties.*

From the Table. 4 *Lipophilicity and hydrophilicity demonstrate the octanol-water partition coefficient values of* 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl, Azulene, Hexadecanoic acid, ethyl ester, Pyrrolo[1,2-a] pyrazine-1,4-dione, hexahydro*. As indicated in this table, these values were within the permissible range of -0.4 to +5.6, implying a good lipophilic compound*

Petroleum ether

Petroleum Ether Extract of *A. sclerocarpa*

The petroleum ether extract of *A. sclerocarpa* was prepared using petroleum ether as a nonpolar solvent. Non-polar solvents are primarily used to extract non-polar compounds present in plant materials. In this study, two solvents were employed for extraction: one polar (ethanol) and one non-polar (petroleum ether), to obtain a wider range of phytoconstituents.

GC-MS Analysis

Gas Chromatography–Mass Spectrometry (GC-MS) analysis of the petroleum ether extract revealed the presence of 24 phytoconstituents. Out of these, four compounds were selected for further evaluation based on their reported anticancer properties:

- Butanoic acid
- Oxirane-2-carboxylic acid
- Sorbitol
- 3-Methylmannoside

Molecular Docking Studies

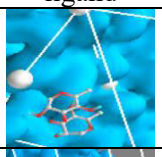
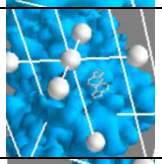
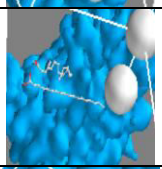
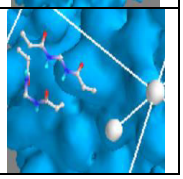
The selected compounds were studied through molecular docking against the 6OVA protein, which is identified as Actin-like protein 6A (ACTL6A), also known as BAF53a. This protein plays a key role in cancer progression, including promoting tumour cell survival, metastasis, and chemoresistance, particularly in ovarian cancer.

The binding affinities obtained were as follows:

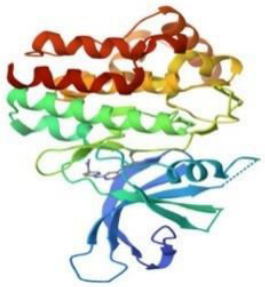
- Butanoic acid: -1.1 kcal/mol
- Oxirane-2-carboxylic acid: -0.8 kcal/mol
- Sorbitol: -1.6 kcal/mol
- 3-Methylmannoside: -2.0 kcal/mol

Among the tested compounds, 3-Methylmannoside showed the highest binding affinity (-2.0 kcal/mol), indicating a stronger and potentially more stable interaction with the protein target.

Table.1 Results of docking between the drug targets with Ligand using the software programs iGEMDOCK and AutoDockVina

Name of the compound	Ligand	Binding Affinity Kcal/mol	rmsd/ub	rmsd/lb	Binding of protein and ligand
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl	6OVA_119838_uff_E=117.53	-1.8	0	0	
Azulene	6OVA_9231_uff_E=281.09	-3.8	0	0	
Hexadecanoic acid, ethyl ester	6OVA_5281_uff_E=4383.69	-1.9	0	0	
Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro	6OVA_8041_uff_E=54.91	-1.5	0	0	

Structure of PDB Protein 6OVA



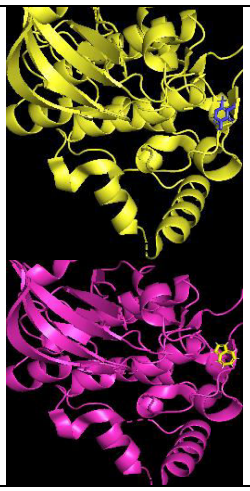
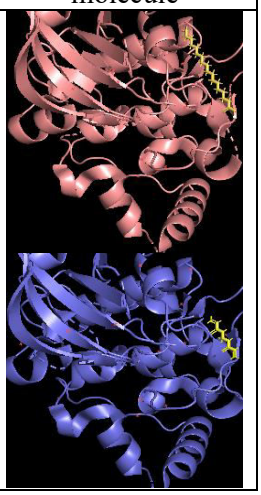
Ligand +protein	3Dvisual of protein and ligand molecule	Ligand+protein	3D visual of protein and ligand molecule
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl Azulene		Hexadecanoic acid, ethyl ester Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro	

Table.2 General properties of (4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl, Azulene, Hexadecanoic acid, ethyl ester, Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro) such as molecular formula, canonical smiles, and IUPAC name.

Name of the Ligand/compound	Chemical formula	SMILES	IUPAC Name
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl,	$C_6H_8O_4$	CC1=C(C(=O)C(CO1)O)O	dimethyl (E)-but-2-enedioate
Azulene	C10H8	C1=CC=C2C=CC=CC2=C1	naphthalene
Hexadecanoic acid, ethyl ester,	C18H36O2	CCCCCCCCCCCCCCCC(=O)O	octadecanoic acid
Pyrrolo[1,2-a] pyrazine-1,4-dione, hexahydro	C7H10N2O2	C=CC(=O)NCNC(=O)C=C	N-[(prop-2-enoylamino) methyl] prop-2-enamide

Table.3

Molecules	Molecular Weight (g/mol)	No. heavy atoms	No. atom. heavy atoms	Fraction CSP3	No. rotatable bonds	No.H-bond acceptors	No. H-bond donors	Molar refractivity	TPSA (oA2)
1	144	10	0	0.50	0	4	2	32.39	66.76 Å²
2	128	10	10	0.00	0	0	0	43.95	00.00Å²
3	284	19	0	0.94	16	1	0	88.84	17.07Å²
4	154	11	0	0.14	6	2	2	40.82	58.20 Å²

Table.4 Lipophilicity and hydrophilicity of 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl, Azulene, Hexadecanoic acid, ethyl ester, Pyrrolo [1,2-a] pyrazine-1,4-dione, hexahydro

Lipophilicity		**Hydrophilicity**											
Molecules	Consensus Log P	ESOL Log S	ESOL Solubility (mg/ml)	ESOL Solubility (mol/l)	ESOL Class	Ali Log S	Ali Solubility (mg/ml)	Ali Solubility (mol/l)	Ali Class	Silicos-IT LogSw	Silicos-IT Solubility (mg/ml)	Silicos-IT Solubility (mol/l)	Silicos-IT class
1	0.22	-0.50	4.55e+01	3.16e-01	Very soluble	-0.57	3.89e+01	2.70e-01	Very soluble	0.15	2.03e+02	1.41e+00	soluble
2	3.10	-3.45	4.51e-02	3.52e-04	soluble	-2.98	1.36e-01	1.06e-03	Soluble	-4.03	1.19e-02	9.27e-05	moderately soluble
3	6.17	-5.58	7.11e-04	2.65e-06	Moderately soluble	-8.36	1.18e-06	4.40e-09	Poorly soluble	-6.69	5.44e-05	2.03e-07	poorly soluble
4	0.18	-0.48	5.08e+01	3.30e-01	Very soluble	-0.91	1.90e+01	1.24e-01	Very soluble	-1.16	1.06e+01	6.87e-02	soluble

Octanol/Water

Table.5 Pharmacokinetics properties of 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl, Azulene, Hexadecanoic acid, ethyl ester, Pyrrolo[1,2-a] pyrazine-1,4-dione, hexahydro

Molecules	**GI absorption**	**BBB permeant**	**P-gp substrate**	**CYP1A2 inhibitor**	**CYP2C19 inhibitor**	**CYP2C9 inhibitor**	**CYP2D6 inhibitor**	**CYP3A4 inhibitor**	**Log-Kp (cm/s)**
1	High	No	No	No	No	No	No	No	-7.44
2	Low	Yes	No	Yes	No	No	No	No	-4.74
3	Low	No	No	Yes	No	No	No	No	-2.16
4	High	No	No	No	No	No	No	No	-7.15

Table.6 Druglikeness and lead likeness of 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl, Azulene, Hexadecanoic acid, ethyl ester, Pyrrolo[1,2-a] pyrazine-1,4-dione, hexahydro

Molecules	Lipinski #violations	Ghose #violations	Veber	Egan	Muegge #violations	Bioavailability Score	PAINS #alerts	Brenk #alerts	Leadlikeness #violations	Synthetic Accessibility
1	1	No	No	No	No	0.55	0	0	No	3.32
2	1	No	Yes	Yes	No	0.55	0	0	No	1.00
3	1	No	No	No	No	0.55	0	1	No	2.49
4	1	No	Yes	Yes	No	0.55	0	2	No	1.84

Table.7 Tabulates the toxicity profile of the compounds of 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl, Azulene, Hexadecanoic acid, ethyl ester, Pyrrolo[1,2-a] pyrazine-1,4-dione, hexahydrowhich were non-toxic in hERG,AMES toxicity, Acute oral toxicity and Human oral bioavailability.

Name of ligand	hERGinhibition	AMES toxicity	Carcinogenicity (Class III)	Acute oral toxicity (kg/mol)	Human oral bioavailability
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl	0.31	0.266	0.314	-3.746	0.465
Azulene	0.482	0.293	0.645	-3.324	0.112
Hexadecanoic acid, ethyl ester,	0.875	0.084	0.127	-3.824	0.215
Pyrrolo[1,2-a] pyrazine-1,4-dione, hexahydro	0.126	0.784	1.263	-2.393	0.032

Table.8 Results of docking between the drug targets with Ligand using the softwareprograms iGEMDOCK and AutoDock Vina

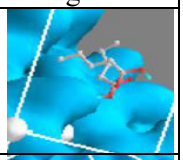
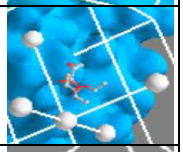
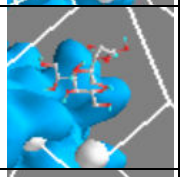
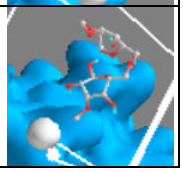
Name of the compound	Ligand	Binding Affinity Kcal/mol	rmsd/ub	rmsd/lb	Binding of protein and ligand
Butanoic acid, 2-methyl	6OVA_7991_uff_E=21.16	-1.1	0	0	
Oxirane-2-carboxylic acid, ethyl ester	6OVA_107319_uff_E=1421.88	-0.8	0	0	
Sorbitol	6OVA_5780_uff_E=150.40	-1.6	0	0	
3-Methylmannoside	6OVA_247323_uff_E=352.99	-2.0	0	0	

Table.9

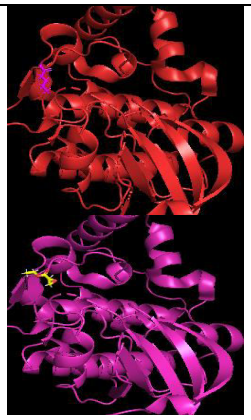
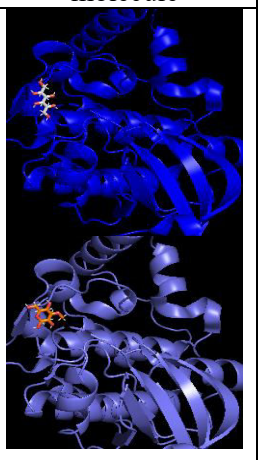
Ligand +protein	3Dvisual of protein and ligand molecule	Ligand+protein	3D visual of protein and ligand molecule
Butanoicacid, 2-methyl Oxiranecarboxlic acid, ethyl ester		Sorbitol 3-Methylmannoside	

Table.10 General properties of (Butanoic acid, 2-methyl, Oxirane-2-carboxylic acid, ethyl ester, Sorbitol, 3-Methylmannoside) such as molecular formula, canonical smiles, and IUPAC name.

Name of the Ligand/compound	Chemical formula	SMILES	IUPAC Name
Butanoic acid, 2-methyl	C5H10O2	CCCCC(=O)O	Pentatonic acid
Oxirane-2-carboxylic acid, ethyl ester,	C5H8O3	C=CC(=O)OCCO	2-hydroxyethyl prop-2-enoate
Sorbitol	C6H14O6	C([C@H] ([C@H] ([C@@H] ([C@H] (CO)O)O)O)O)O	(2R,3R,4R,5S)-hexane-1,2,3,4,5,6-hexol
3-Methylmannoside	C7H14O6	COC1[C@@H] ([C@H] (C([C@@H] ([C@@H]1O) O)O)O)O	(1R,2S,4S,5S)-6-methoxycyclohexane-1,2,3,4,5-pentol

Table.11 Lipophilicity and hydrophilicity of Butanoic acid, 2-methyl, Oxirane-2-carboxylic acid, ethyl ester, Sorbitol, 3-Methylmannode.

Lipophilicity		Hydrophilicity											
Molecules	Consensus Log P	ESOL Log S	ESOL Solubility (mg/ml)	ESOL Solubility (mol/l)	ESOL Class	Ali Log S	Ali Solubility (mg/ml)	Ali Solubility (mol/l)	Ali Class	Silicos-IT LogSw	Silicos-IT Solubility (mg/ml)	Silicos-IT Solubility (mol/l)	Silicos-IT class
1	1.08	-1.15	7.22e+00	7.06e-02	Very soluble	-1.78	1.71e+00	1.67e-02	Very soluble	-0.78	1.69e+01	1.66e-01	soluble
2	0.18	-0.16	7.97e+01	6.86e-01	Very soluble	-0.31	5.68e+01	4.89e-01	Very Soluble	-0.20	7.39e+01	6.37e-01	soluble
3	-1.90	1.31	3.75e+03	2.06e+01	Highly soluble	1.12	2.38e+03	1.31e+01	Highly soluble	2.57	6.71e+04	3.68e+02	soluble
4	-2.38	1.02	2.03e+03	1.05e+01	Highly soluble	1.42	5.11e+03	2.63e+01	Highly soluble	2.58	7.37e+04	3.79e+02	soluble

O/W: Octanol/Water

Table.12 Pharmacokinetic properties of Butanoic acid, 2-methyl, Oxirane-2-carboxylic acid, ethyl ester, Sorbitol, 3-Methylmannoside.

Molecules	GI absorption	BBB permeant	P-gp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Log-Kp (cm/s)
1	High	Yes	Yes	No	No	No	No	No	-6.16
2	High	Yes	No	Yes	No	No	No	No	-7.05
3	Low	No	No	No	No	No	No	No	-9.61
4	Low	No	Yes	No	No	No	No	No	-9.74

Table.13 Druglikeness and leadlikeness of Butanoic acid, 2-methyl, Oxirane-2-carboxylic acid, ethyl ester, Sorbitol, 3-Methylmannoside,

Molecules	Lipinski #violations	Ghose #violations	Veber	Egan	Muegge #violations	Bioavailability Score	PAINS #alerts	Brenk #alerts	Leadlikeness #violations	Synthetic Accessibility
1	1	No	Yes	Yes	No	0.85	0	0	No	1.00
2	1	No	Yes	Yes	No	0.55	0	1	No	1.72
3	1	No	Yes	Yes	No	0.55	0	0	No	3.30
4	1	No	Yes	Yes	No	0.55	0	0	No	3.76

Table.14 Tabulates the toxicity profile of the compounds ofButanoic acid, 2-methyl, Oxirane-2-carboxylic acid, ethyl ester, Sorbitol, 3-Methylmannoside, which were non-toxic in hERG, AMES toxicity, acute oral toxicity, and Human oral bioavailability.

Name of ligand	hERGinhibition	AMES toxicity	Carcinogenicity (Class III)	Acute oraltoxicity (kg/mol)	Human oral bioavailability
Butanoic acid, 2-methyl	0.211	0.008	0.19	-3.331	0.137
Oxirane-2-carboxylic acid, ethyl ester	0.211	0.475	0.475	-2.342	0.086
Sorbitol	0.202	0.217	0.171	-4.084	0.178
3-Methylmannoside	0.253	0.136	0.146	-3.881	0.376

Author Contributions

Ashwini: Investigation, formal analysis, writing—original draft. Prerana Pramod Dange: Validation, methodology, writing—reviewing. Pawar Sagar Namdeo:—Formal analysis, writing—review and editing. Y. R. Karthik: Investigation, writing—reviewing. Padmalatha. S. Rai: Resources, investigation writing—reviewing. Y. L. Ramachandra: Validation, formal analysis, writing—reviewing.

Data Availability

The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

Ethical Approval Not applicable.

Consent to Participate Not applicable.

Consent to Publish Not applicable.

Conflict of Interest The authors declare no competing interests.

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