

Synthesis, Characterization of N-phenylpropan-2-imine and its effect on the anti-oxidant and In-silico docking studies with (2S)-1-{2-[(2S)-2,6-dicarboxy-2,3-dihydropyridin-4(1H)-ylidene]ethylidene}-5-(β-d-glucopyranosyloxy)-6-hydroxy-2,3-dihydro-1H-indol-1-ium-2-carboxylate

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ABSTRACT

Schiff bases continue to attract significant interest as versatile ligands in coordination chemistry due to their structural tunability, ease of synthesis, and strong donor capabilities. This study explores and evaluates the reactivity patterns of a series of Schiff bases in the formation of stable metal complexes relevant to catalytic applications. By systematically varying the electronic and steric properties of the imine framework, we investigate how ligand architecture influences metal coordination behavior, complex stability, and catalytic performance. Spectroscopic and analytical techniques including FTIR, AAS and various chemical analysis techniques were employed to characterize ligand–metal interactions and identify key structural features governing reactivity. Catalytic assessments in representative organic transformations demonstrated that Schiff-base metal complexes exhibit enhanced activity and selectivity when optimal electronic balance and chelation geometry are achieved. The findings highlight the critical role—that the Schiff base can be authentically used as a preservative, antimicrobial and color preservation for fruits and veggies as a replacement of different synthetic and hazardous chemical Schiff-base-derived metal catalysts with improved stability and of ligand design in modulating catalytic efficiency and provide a framework for developing next functional versatility.

Keywords: Schiff base, FTIR, AAS, chemical analysis, catalytic stable complex, ligand-metal interaction, fruits and veggies, preservatives

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INTRODUCTION

Schiff bases, a versatile class of imine-containing organic ligands, have attracted significant attention in coordination chemistry due to their structural flexibility, synthetic accessibility, and tunable electronic properties. Their ability to readily form stable complexes with a wide range of metal ions makes them valuable candidates for catalytic applications across chemical, environmental, and biological systems. Understanding and assessing the reactivity patterns of Schiff bases is therefore essential for designing efficient catalytic processes, optimizing metal–ligand stability, and tailoring functional complexes for targeted applications. In recent years, the catalytic activity of Schiff base–metal complexes has been explored in oxidation, reduction, polymerization, and enzymatic mimic reactions, where ligand structure and electronic characteristics play

vital roles in determining reaction pathways and efficiencies. By evaluating how structural modifications influence reactivity—such as donor atom variations, steric hindrance, and electronic effects—catalysts. Beyond catalysis, Schiff bases are emerging as promising agents in the development of food enhancement products due to their antioxidant, antimicrobial, and chelating properties. These characteristics enable them to stabilize food matrices, inhibit spoilage, and improve nutritional or sensory attributes. However, maximizing their potential requires comprehensive analytical assessment to ensure safety, stability, and performance in complex food systems. A major aspect of Schiff base chemistry lies in understanding their reactivity patterns, which govern their ability to bind metals, participate in electron-transfer processes, and influence catalytic reaction pathways. Factors such as the

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nature of the substituents, conjugation, steric bulk, and the presence of additional coordinating sites significantly alter the ligand's electronic environment, thereby affecting its reactivity. Furthermore, the configuration of the imine group and the presence of aromatic or heterocyclic rings enhance delocalization and stabilize the resulting metal complexes. These structural features are central to developing Schiff base-metal complexes exhibiting high catalytic efficiency, selectivity, and stability in various chemical transformations. Catalytic processes mediated by Schiff base complexes encompass a broad range, including oxidation, hydrogenation, polymerization, cross-coupling, and biomimetic reactions. Transition-metal complexes of Schiff bases— particularly those containing Cu, Co, Ni, Mn, Fe, and Zn—have demonstrated remarkable activity and robustness under diverse reaction conditions. Their catalytic behavior is strongly influenced by ligand design, metal coordination geometry, and

surrounding electronic environment. Therefore, exploring and assessing the reactivity patterns of different Schiff bases becomes essential for rational catalyst development. Through systematic investigation, chemists can correlate structural attributes with reactivity and thereby optimize the catalyst's performance for specific chemical processes. In addition to their classical role in catalysis, Schiff bases are gaining prominence in food science and food enhancement technologies. This emerging interest stems from their inherent antioxidant, antimicrobial, and metal-chelating abilities. These properties are crucial in food preservation, enhancement of nutritional value, color stabilization, prevention of lipid oxidation, and inhibition of microbial contamination.

Schiff base derivatives and their metal complexes have been evaluated for their potential to extend shelf life, improve sensory qualities, and contribute to safer food storage systems. As the demand for natural or semi-synthetic additives grows, Schiff bases offer an attractive solution for designing multifunctional food enhancement products. However, the introduction of such compounds into food systems necessitates a thorough understanding of their stability, reactivity, compatibility with food matrices, and potential toxicological implications. Schiff bases form highly stable complexes with transition metals due to internal chelation. Stability arises from Chelate effect (thermodynamic stabilization), Planar or near-planar geometry enabling delocalization, π -back bonding between ligand and metal, Rigid frameworks limiting decomposition. Influence of Metal Ions on Stability Cu(II), Ni(II), Co(II) \rightarrow Strong d-p orbital overlap, forming highly stable square-planar or octahedral complexes. Zn(II) \rightarrow Forms stable complexes but remains catalytically inert (useful for food applications due to low toxicity). Fe(III) and Mn(II) \rightarrow Allow redox- active catalytic pathways. Reactivity-Stability Correlation Metal complexes with electron-rich Schiff bas...

Electronic Effects Electron-donating substituents increase electron density, thereby enhancing: Coordination efficiency Redox activity Catalytic speed Electron-withdrawing groups improve A Schiff base metal complex

may catalyze reactions by Activating substrates through coordination Facilitating electron transfer Stabilizing reactive intermediates Enabling proton abstractions via imine nitrogen

Significant applications of Schiff base :

Coordination Chemistry

Schiff bases are excellent ligands because the azomethine group ($-C=N-$) can bind to metal ions.

Schiff base condensation reactions can produce macrocyclic ligands. These complexes often mimic: Porphyrins and Corrins, Biomimetic chemistry Oxygen transport studies. Schiff bases form highly stable chelate complexes (chelation effect). Stability arises from: Ring formation, Electronic donation, Planarity of the ligand. These stable complexes are suitable for: Catalysis ,Industrial synthesis

Bioinorganic Chemistry

Schiff base complexes are Metalloproteins and Metalloenzymes like: Catalase ,Superoxide dismutase,(SOD),Cytochrome P450 and used in Enzyme mechanism studies, Artificial enzyme development

Pharmaceutical industry

Schiff bases, characterized by the azomethine functional group ($-C=N-$), have gained wide attention in pharmaceutical research due to their chemical versatility, bioactivity, and ability to form stable complexes with metal ions. These properties make them valuable scaffolds for drug design, synthesis, and therapeutic applications. Azomethine Group ($-C=N-$) The azomethine linkage enhances Electron density on nitrogen, Ability to interact with biomolecules, Lipophilicity, improving membrane permeability, Biological binding activity, These factors significantly increase pharmacological potential.

MATERIALS AND METHODOLOGY

Step 1 involves Dissolution of aniline : 0.01 mol of aniline is dissolved in 15mL of ethanol.

Step 2 involves addition of acetone (0.01 mol) to the solution of aniline. Step 3 involves the addition of 5 mL of glacial acetic acid to catalyze the reaction by dehydration. The mixture was then stirred and refluxed at 60 °C for 60 minutes. The Schiff base imine usually appears the reddish-brown color in the liquid state. The product obtained was filtered under suction.

Reaction Scheme:

Step I

Preparation of N-phenylpropan-2-imine from Aniline & Acetone

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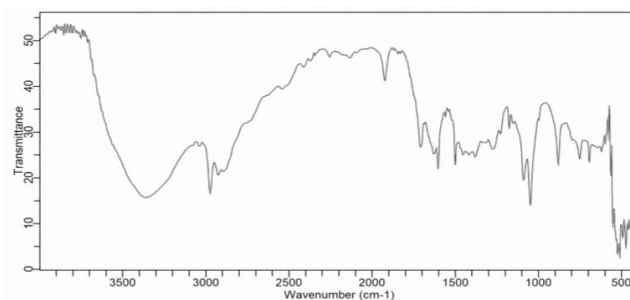
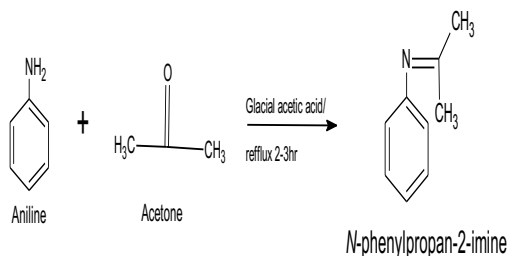
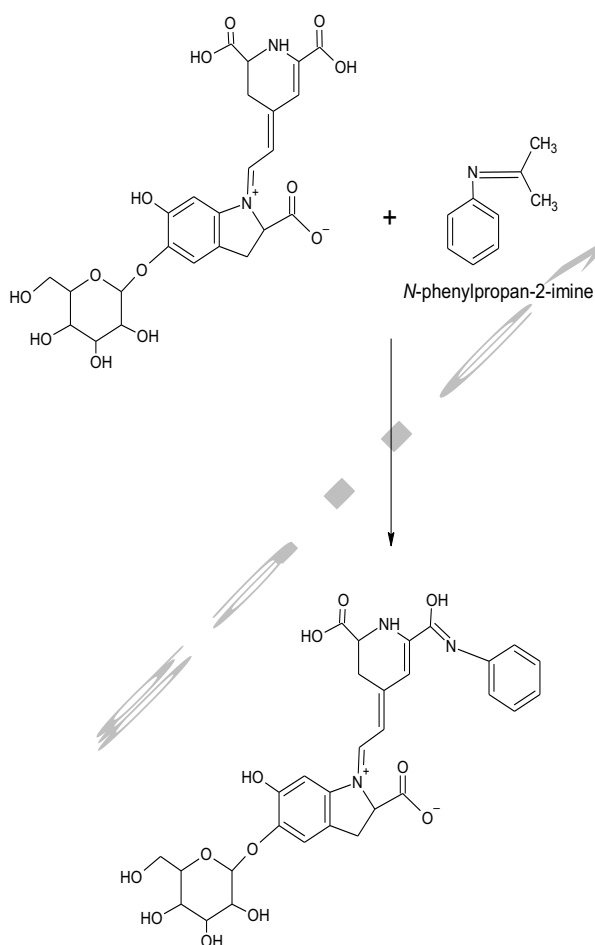


Fig.1 FTIR Spectra of N-phenylpropan-2-imine

Step II

Preparation of Z)-1-((Z)-2-(2-carboxy-6-((Z)-hydroxy(phenylimino)methyl)-2,3-dihydropyridin-4(1H)-ylidene)ethylidene)-6-hydroxy-5-((3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)indolin-1-ium-2-carboxylate from (2S)-1-{2-[(2S)-2,6-dicarboxy-2,3-dihydropyridin-4(1H)-ylidene]ethylidene}-5-(β-d-glucopyranosyloxy)-6-hydroxy-2,3-dihydro-1H-indol-1-ium-2-carboxylate and N-phenylpropan-2-imine (Betanin).



Interpretation of FTIR Spectra

Based on the displayed FTIR spectrum (4000–400 cm^{-1}), the following characteristic absorptions can be interpreted. Exact peak positions may vary slightly due to resolution and baseline, but the assignments are reliable for a Schiff base.

Major Absorption Bands and Assignments

~3400–3300 cm^{-1} (broad, weak–moderate)
→ O–H stretching (phenolic –OH, if present) or N–H stretching (trace/unreacted amine).
Broad nature suggests hydrogen bonding.

~3050–3000 cm^{-1} (weak)
→ Aromatic C–H stretching.

~2950–2850 cm^{-1} (moderate)
→ Aliphatic C–H stretching (–CH₃ / –CH₂ groups).

~1620–1640 cm^{-1} (strong, sharp)
→ C=N stretching (azomethine group)

This is the diagnostic peak confirming Schiff base formation.

~1580–1500 cm^{-1} (moderate)

→ Aromatic C=C stretching vibrations.

~1450–1380 cm^{-1} (weak–moderate)

→ C–H bending (alkyl and aromatic).

~1300–1200 cm^{-1} (moderate)

→ C–N stretching vibration (supports imine linkage).

~1150–1000 cm^{-1} (weak–moderate)

→ C–O stretching (phenolic C–O, if derived from plant-based aldehydes).

~900–700 cm^{-1} (weak)

→ Aromatic C–H out-of-plane bending.

Key Conclusions

The strong band near ~1620–1640 cm^{-1} confirms the presence of the azomethine (–C=N–) group, which is definitive evidence for Schiff base formation.

Absence (or significant reduction) of a strong C=O band (~1700 cm^{-1}) indicates successful condensation of the aldehyde/ketone with an amine.

Aromatic and aliphatic bands suggest the molecule contains aromatic rings and alkyl substituents, consistent with typical Schiff base structures.

Overall spectral features confirm the successful synthesis of a Schiff base compound.

Characterization of N-phenylpropan-2-imine:

Characterization of the Schiff base was done by IR spectroscopy.

Characterization of Complex between Schiff base, β-Carotene and Betanin by AAS

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3.	Zinc	mg/kg	1.29
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Samples were prepared as follows:

Sample A) 60ml Schiff base + 90ml β-carotene + 90ml betanin.

Sample B) 60ml Schiff base + 180ml betanin.

Sample C) 60ml Schiff base + 180ml β-carotene.

Results & Discussion for Sample A)

Sr. No	Test parameters	Unit	Test Result
1.	Iron	mg/100g	1.67
2.	Copper	mg/kg	1.34
3.	Zinc	mg/kg	4.34

When Schiff base was treated with β-carotene and betanin it was shown that the concentration of essential metals such as Fe, Cu and Zn detected were within the normal range. The unitary methods for detection of metal concentration is done at mg/kg. Therefore, the data evaluated is 1.67 in iron, 1.34 in copper, 4.34 in zinc.

Results & Discussion for Sample B)

Sr. No	Test parameters	Unit	Test Result
1.	Iron	mg/100g	0.80
2.	Copper	mg/kg	0.58
3.	Zinc	mg/kg	2.20

When Schiff base was treated with betanin, it was shown that the concentration of essential metals such as Fe, Cu and Zn detected were within the normal range. The unitary methods for detection of metal concentration is done at mg/kg. Therefore, this data evaluates the presence of iron about 0.80, copper around 0.58 and zinc about 2.20

Results & Discussion for Sample C)

Sr. No	Test parameters	Unit	Test Result
1.	Iron	mg/100g	1.14
2.	Copper	mg/kg	0.63
3.	Zinc	mg/kg	1.29

When Schiff base was treated with β-carotene , it was shown that the concentration of essential metals such as Fe, Cu and Zn detected were within the normal range. The unitary methods for detection of metal concentration is done at mg/kg. Therefore this data evaluates the presence of iron about 1.14, copper about 0.63 and zinc at 1.29.

Concentration of Fe,Cu and Zinc in β-carotene

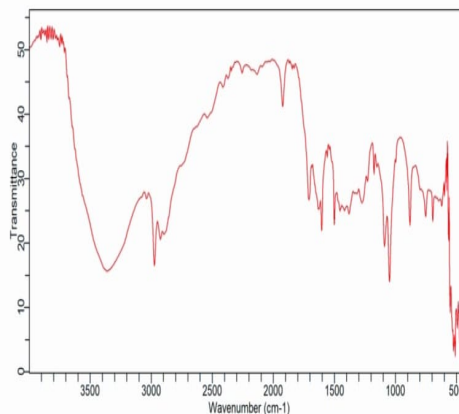
Sr. No	Test parameters	Unit	Test Result
1.	Iron	mg/100g	1.14
2.	Copper	mg/kg	0.63

Concentration of Fe,Cu and Zinc in Betanin

Sr. No	Test parameters	Unit	Test Result
1.	Iron	mg/100g	0.80
2.	Copper	mg/kg	0.58
3.	Zinc	mg/kg	2.20



Sample ID: schiff base 1
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 User: admin
 Sample Scans: 32
 Background Scans: 32
 Resolution: 8
 System Status: Good
 File Location: C:\Users\Public\Documents\Agilent\MicroLab\Results\schiff base 1_2025-12-02T12:41:52.a2r
 Date/Time: 12/02/2025 12:41:52 PM
 Range: 4000 - 400
 Apodization: Happ-Genzel



Peak Number	Wavenumber (cm ⁻¹)	Intensity
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Conclusion : The results indicate that the presence of Schiff base along with β-carotene and betanin does not change the concentration of essential elements such as Fe, Cu and Zn. These results further suggest that Schiff base effectively binds with the essential elements forming coordination complexes.

Determination of Antioxidant properties of the samples

The following samples were analyzed for their anti-oxidant activities using DPPH assay. Free radical scavenging activity (% RSA) was measured at 517 nm.

Sample	Contents
A	N-phenylpropan-2-imine
B	β-carotene
C	(2S)-1-{2-[(2S)-2,6-dicarboxy-2,3-dihydropyridin-4(1H)-ylidene]ethylidene}-5-(β-d-glucopyranosyloxy)-6-hydroxy-2,3-dihydro-1H-indol-1-ium-2-carboxylate
D	N-phenylpropan-2-imine + β-carotene
E	N-phenylpropan-2-imine + (2S)-1-{2-[(2S)-2,6-dicarboxy-2,3-dihydropyridin-4(1H)-ylidene]ethylidene}-5-(β-d-glucopyranosyloxy)-6-hydroxy-2,3-dihydro-1H-indol-1-ium-2-carboxylate
F	N-phenylpropan-2-imine + (2S)-1-{2-[(2S)-2,6-dicarboxy-2,3-dihydropyridin-4(1H)-ylidene]ethylidene}-5-(β-d-glucopyranosyloxy)-6-hydroxy-2,3-dihydro-1H-indol-1-ium-2-carboxylate + β-carotene

Results & Discussion:

Anti-oxidant assay of Test sample A

Dilution	O.D	%RSA
Undiluted	0.39	54.6
10:10dil	0.43	46.5
1:100dil	0.76	11.6
1:1000dil	0.8	6.97
Control	0.86	

Test sample B

Dilution	O.D	%RSA
Undiluted	0.35	75
Dil 1:2	0.46	67
Dil 1:4	0.58	58
Dil 1:6	0.76	46
Dil 1:8	0.97	30
Control	1.4	

Test sample C :- shows no antioxidant property

Test sample D

Dilution	O.D	%RSA
Undiluted	0.22	74.71
10:10dil	0.3	65.51
1:100dil	0.87	0

1:1000dil	0.87	0
Control	0.87	0

Test sample E

Dilution	O.D	%RSA
Undiluted	0.21	76.91
Dil 1:2	0.45	48.86
Dil 1:4	0.7	20.45
Dil 1:6	0.88	0
Dil 1:8	0.88	0
Control	0.88	

Test sample F

Dilution	O.D	%RSA
Undiluted	0.46	48
10:10dil	0.46	48
1:100dil	0.81	10
1:1000dil	0.83	7
Control	0.9	

From the above results following conclusions can be drawn:

Test Sample A (Schiff base)

Showed moderate antioxidant activity. Maximum %RSA at undiluted sample (54.6%). Activity decreased sharply with dilution. Indicates dose-dependent antioxidant activity, but not very strong at higher dilutions.

Test Sample B (β-carotene)

Exhibited strong antioxidant activity. High %RSA even after dilution: Undiluted: 75% 1:2: 67% 1:4: 58%. Activity decreases gradually → good antioxidant potential.

Test Sample C (Betanin)

No antioxidant activity detected. %RSA ≈ 0% at all concentrations.

Test Sample D (Schiff base+ β-carotene)

Good activity at low dilution: Undiluted: 74.71% .10:10 dilution: 65.51%. At 1:100 and higher dilutions, no activity observed (%RSA = 0). Indicates activity only at higher concentration.

Test Sample E (Schiff base +Betanin)

Highest antioxidant activity among all samples. %RSA values: Undiluted: 76.1% 1:2: 48.86% 1:4: 20.45% Clear concentration-dependent response. Calculated values suggest IC₅₀ lies between undiluted and 1:2 dilution, confirming strong antioxidant potency.

Test Sample F (Schiff base + β-carotene + Betanin)

Moderate to low antioxidant activity. %RSA: Undiluted & 10:10 dilution: 48% 1:100: 10% 1:1000: 7% Activity rapidly decreases with dilution.

Overall Comparison (Antioxidant Strength Order)

Sample E > Sample B > Sample D ≈ Sample A > Sample F > Sample C

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CONCLUSION

Sample E shows the strongest antioxidant activity. Sample B also demonstrates good and stable activity. Samples A & D exhibits moderate antioxidant activities. Sample F exhibits minimal antioxidant activity. Sample C shows no antioxidant activity. Antioxidant activity in all active samples is concentration dependent. These results indicate that Schiff base enhances the anti-oxidant activity of Betatin, which also indicates greater coordination. However the anti-oxidant activity of β-carotene is significantly reduced when combined with Schiff base indicating poor coordination.

Summary:

Sample	Anti-Oxidant Activity	Contents
A	Moderate	N-phenylpropan-2-imine
B	Good & Stable	β-carotene
C	Nil	(2S)-1-{2-[(2S)-2,6-dicarboxy-2,3-dihydropyridin-4(1H)-ylidene]ethylidene}-5-(β-d-glucopyranosyloxy)-6-hydroxy-2,3-dihydro-1H-indol-1-ium-2-carboxylate
D	Moderate	N-phenylpropan-2-imine + β-carotene
E	Strongest	N-phenylpropan-2-imine + (2S)-1-{2-[(2S)-2,6-dicarboxy-2,3-dihydropyridin-4(1H)-ylidene]ethylidene}-5-(β-d-glucopyranosyloxy)-6-hydroxy-2,3-dihydro-1H-indol-1-ium-2-carboxylate
F	Low	N-phenylpropan-2-imine + (2S)-1-{2-[(2S)-2,6-dicarboxy-2,3-dihydropyridin-4(1H)-ylidene]ethylidene}-5-(β-d-glucopyranosyloxy)-6-hydroxy-2,3-dihydro-1H-indol-1-ium-2-carboxylate + β-carotene

In-silico docking studies:

In the molecular docking study, ErbB family members human epidermal growth factor 2 (HER2) (PDB ID: 3PP0) that compound A demonstrated superior binding affinity and more favorable interaction profiles with the target protein compared to the positive control, indicating stronger molecular interactions, improved stability within the binding site, and potentially enhanced inhibitory activity, highlighting its promise as a more effective candidate for further investigation. Significant interactions were determined using the energy score (S= -8.4 kcal/mol). Indolin based

carboxylate anion (COO⁻) engaged in a conventional hydrogen bond interaction with VAL797 and C-H bond with GLN795. Additionally, dihydropyridine like compound containing hydroxy group participates in conventional hydrogen bond interaction namely SER728 and ALA730. Similarly pyridine like moiety containing more three conventional hydrogen bond interaction with GLU766, GLU865 and ALA867. In the similar manner this moiety shows hydrophobic pi-alkyl interaction with ILE788 and ALA771 engaged in benzylic aromatic region. A detailed molecular interaction analysis can be found in Figure 1.

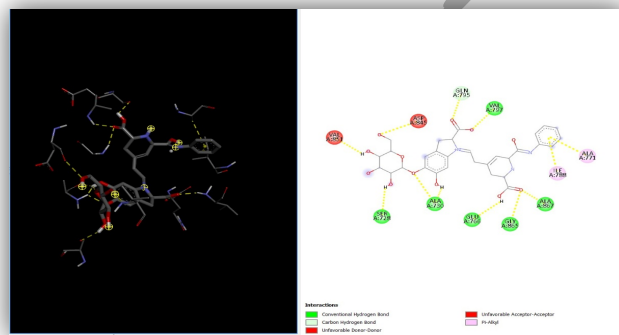


Fig. 2: 2D and 3D-interactions of compound and control with 3PP0 protein binding pockets.

Conclusion : From the above docking studies it refers that the molecule under study may be an anti-lung and anti-breast cancer moiety.

Conflict of Interest: The authors have no competing interest to declare.

Data Availability: All data generated or analyzed during this study will be made available upon request.

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