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Research Article

Molecular docking analysis of phyto compounds from *Acacia farnesiana* with protein targets linked to bronchitis

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Abstract:
Acute bronchitis is a lower respiratory tract lung infection that causes bronchial inflammation. The known protein drug targets are peptidoglycan D, D-transpeptidase, and DNA topoisomerase 4 subunit A for bronchitis linked infections. These are the membrane associated macromolecules which takes a major role in the formation of cell wall membrane by synthesising the cross-linked peptidoglycan. Therefore, it is of interest to design molecules with improved binding features with these protein targets. Hence, we document the molecular docking analysis data of four phytocompounds from *Acacia farnesiana* having optimal binding features with these targets linked to bronchitis for further consideration.

Keywords:
Acacia farnesiana, acute bronchitis, molecular docking, discovery studio, phytocompounds

Background:
More than 50% patients of are exposed to hospital borne bronchitis linked infections **[1].** Data in the drug bank database shows that the known protein targets for bronchitis **[2,3]** are the penicillin-binding

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proteins (PBP) **[4-8],** Peptidoglycan-D D-transpeptidase **[9,10],** DNA topoisomerase 4 subunit A **[11-14]** and DNA gyrase subunit **[15].** Therefore, it is of interest to document the molecular docking analysis of phytocompounds from *Acacia farnesiana* (**Figure 1 to Figure 11**) with the known protein targets **(Table 1)** linked to bronchitis.

Materials & Methods:

Target protein, sequences, structures, data preparation and validation:

The (1) Penicillin-binding protein 1A (PDB ID: 2WAF), (2) Peptidoglycan D, D-transpeptidase (PDB ID: 6HZQ), E.coli, (3) Penicillin-binding protein 1B (PDB ID: 3VMA) and (4) Penicillin-binding protein 1A(PDB: 2ZC6), were downloaded from the PDB database. The 3-dimensional structure models for DNA gyrase subunit A, DNA topoisomerase 4 subunit A and peptidoglycan D-D-transpeptidase (Clostridium perfringens (strain 13 / Type A)) developed using the Swiss-Model and Phyre2 web tool with sequences downloaded from the UniPort database. The Ramachandran plots **[16]** were drawn for the models (**Table 2**).

Ligand preparation and validation:

2D and 3D data on phytochemicals from *Acacia farnesiana* (sweet acacia) were retrieved from IMPPAT (Indian Medicinal Plants, Phytochemistry and Therapeutics) in data formats such as PDB, sdf, mol, and pdbqt. *Acacia farnesiana* has a total of 23 types of phytochemicals including flavonoids and other derivatives. We used 18 phyto chemicals excluding 5 flavonoids for this study.

Figure 1: Natural image of *Acacia farnesiana* fruit.

Molecular docking:

Discovery Studio Client Version 20.1 (-CDOCKER Module) is used for molecular docking analysis of protein targets with the selected ligands.

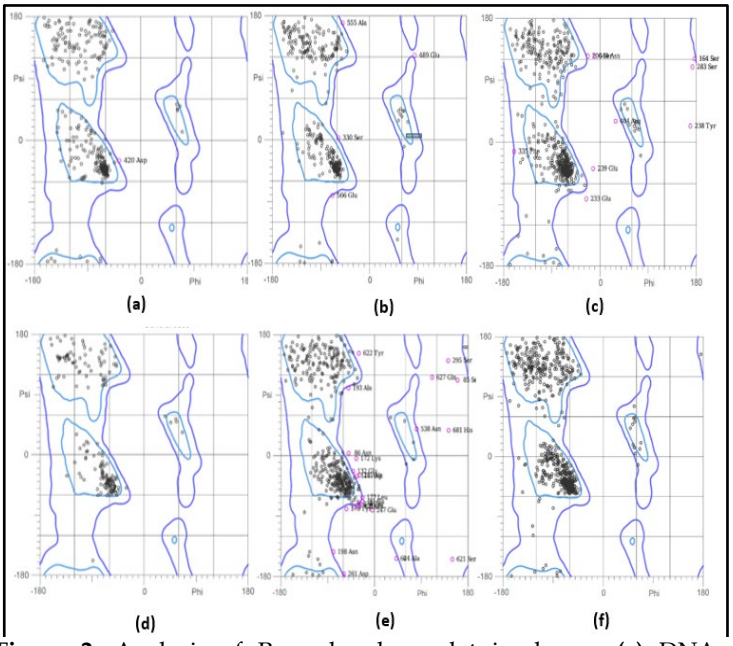

Figure 2: Analysis of Ramachandran plot is shown. **(a)** DNA topoisomerase 4 subunit, 96.1% (491/511) of all residues were in favored (98%) regions. 99.6% (509/511) of all residues were in allowed (>99.8%) regions. **(b)** Peptidoglycan_D_D-transpeptidase MrdA 96.4% (535/555) of all residues were in favored (98%) regions. 99.3% (551/555) of all residues were in allowed (>99.8%) regions. **(c)** Penicillin-binding protein 1B (PDB ID: 3VMA) 92.1% (645/700) of all residues were in favored (98%) regions. 98.3% (688/700) of all residues were in allowed (>99.8%) regions. **(d)** Peptidoglycan D, D-transpeptidase FtsI (PDB ID: 6HZQ) 95.5% (278/291) of all residues were in favored (98%) regions.99.7% (290/291) of all residues were in allowed (>99.8%) regions. **(e)** Penicillin-binding protein 1A (PDB ID-2WAF) 83.6% (514/615) of all residues were in favored (98%) regions. 94.8% (583/615) of all residues were in allowed (>99.8%) regions. **(f)** Penicillin-binding protein 1A (PDB -2ZC6) 95.1% (753/792) of all residues were in favored (98%) regions. 100.0% (792/792) of all residues were in allowed (>99.8%) regions.

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Known pharmacology properties of DL arginine, decanal, pyrocatechol, sulfoxide, benzaldehyde

L-arginine is a precursor to nitric oxide or NO and it is synthesized from L-arginine using the enzyme nitric oxide synthase **[17-18].** The naturally derived decanal has shown the capability of disrupting the permeability barrier of the cell membrane and it is responsible for the loss of chemiosmotic control **[19-21].** Pyrocatechol of Aloe vera extraction was exhibited to have maximum antibacterial activity **[22].** Sulfoxide in the form of dimethyl sulfoxide (DMSO) acts as an antibacterial and an anti-inflammatory agent against several bacteria such as *methicillin-resistant Staphylococcus aureus* (MRSA) and *Pseudomonas aeruginosa* **[23].** Benzaldehyde releases intracellular constituents and interacts with the cell surface; induce cell death by causing disintegration of the cell membrane **[24, 25].**

Results and Discussion:

The bronchitis affects the quality of human community **[26].** Penicillin-binding proteins 1B, 1A and Peptidoglycan D-D-transpeptidase, DNA topoisomerase 4 subunit A and DNA gyrase subunit A were taken as protein of target based on their role in disease-causing mechanism. 18 phytochemicals of *Acacia farnesiana* that have an anti-inflammation are docked and analyzed using Discovery studio v20.1 software with CHARMM module based on the -C-DOCKER energy. Seven phytochemicals of *Acacia farnesiana* have optimal interaction and binding energy with the seven-targeted proteins (**Table 3, Table 4 and Table 5**). The high -C-DOCKER energy shows high affinity of the compounds with targets **[27].** We observed that Pyridoxal phosphate, DL-Arginine, Decanal, and Sulfoxide have high -C-DOCKER energy compared to the rest of the phytochemicals. Therefore, the -C-DOCKER energy, Hydrogen bond and the position of ligand in the binding pockets of protein molecules are high for these molecules. Thus, these phytochemicals of *Acacia farnesiana* have potential modulatory functions against the bronchitis targets for further consideration.

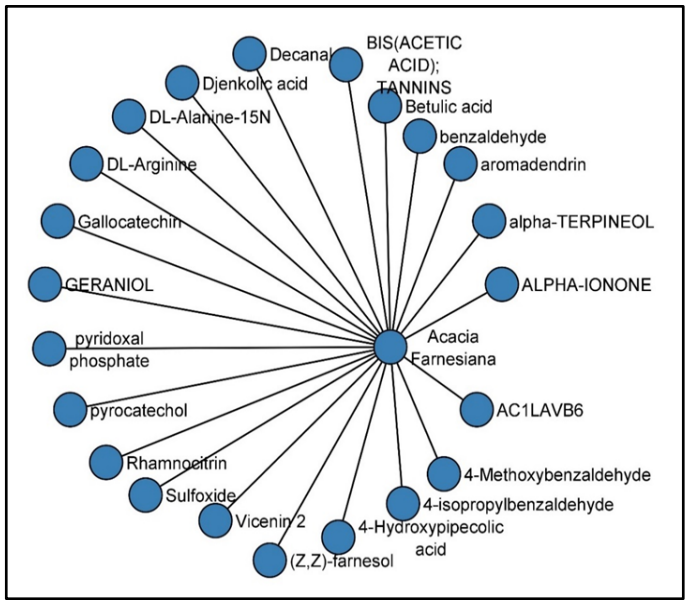

Figure 3: Phytochemicals of *Acacia farnesiana* retrieved from IMPPAT database.

Table 1: List of target proteins for bronchitis infection

S. No	Target Protein Name	Source of Organism
1	Penicillin-binding protein 1B (PDB ID: 3VMA)	*Haemophilus influenzae* (strain ATCC 51907 / DSM 11121 / KW20 / Rd)
2	Penicillin-binding protein 1A (PDB ID: 2WAF)	*Clostridium perfringens* (strain 13 / Type A)
3	Penicillin-binding protein 1A (PDB: 2ZC6)	*Escherichia coli* (strain K12)
4	Peptidoglycan D-D-transpeptidase (PDB ID: HZQ)	Escherichia coli (strain K12)
5	Peptidoglycan D-D-transpeptidase	*Clostridium perfringens* (strain 13 / Type A)
6	DNA topoisomerase 4 subunit A	*Streptococcus pneumoniae* serotype 4 (strain ATCC BAA-334 / TIGR4)
7	DNA gyrase subunit A	*Haemophilus influenzae* (strain ATCC 51907 / DSM 11121 / KW20 / Rd)

Table 2: Structural analysis scores of targeted proteins

Sl. No	Target Protein Name	Source of Organism	Clash Score	Ramachandran Region	Favoured	Ramachandran Outliers
1	DNA topoisomerase 4 subunit	Haemophilus influenzae (strain ATCC 51907 / DSM 11121 / KW20 / Rd)	1.84	96.09%		0.39%
2	Peptidoglycan D D-transpeptidase	Clostridium perfringens (strain 13 / Type A)	1.14	96.40%		0.72%
3	Penicillin-binding protein 1B (PDB ID: 3VMA)	Escherichia coli (strain K12)	16.82	92.145		1.71%
4	Peptidoglycan D D-transpeptidase	Escherichia coli (strain K12)	18.55	95.53%		0.34%

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	(PDB ID: 6HZQ)				
5	Penicillin-binding protein 1A (PDB ID: 2WAF)	Clostridium perfringens (strain 13 / Type A)	58.43	83.58%	5.20%
6	Penicillin-binding protein 1A (PDB : 2ZC6)	Streptococcus pneumoniae serotype 4 (strain ATCC BAA-334 / TIGR4)	4.21	95.08%	0.0%

Table 3: ADMET property of *Acacia farnesiana* phytochemicals.

S. No	Phytochemical identifier	Phytochemical Name	BBB permeant	CYP2D6 inhibitor	Lipinski
1	CID:443158	(-)-Linalool	Yes	No	Yes; 0 violation
2	CID:1549107	(Z, Z)-farnesol	Yes	No	Yes; 0 violation.
3	CID:151907	4-Hydroxypipecolic acid	No	No	Yes; 0 violation.
4	CID:326	4-isopropylbenzaldehyde	Yes	No	Yes; 0 violation.
5	CID:31244	4-Methoxybenzaldehyde	Yes	No	Yes; 0 violation
6	CID:521229	AC1LAVB6	No	No	Yes; 1 violation: MLOGP>4.15
7	CID:5282108	ALPHA-IONONE	Yes	No	Yes; 0 violation
8	CID:17100	alpha-TERPINEOL	Yes	No	Yes; 0 violation.
9	CID:240	benzaldehyde	Yes	No	Yes; 0 violation.
10	CID:2371	Betulic acid	No	No	Yes; 1 violation: MLOGP>4.15.
11	CID:76419085	BIS (ACETIC ACID); TANNINS	No	No	No; 3 violations: MW>500, NorO>10, NHorOH>5
12	CID:8175	Decanal	Yes	No	Yes; 0 violation.
13	CID:51283	DL-Alanine-15N	No	No	Yes; 0 violation.
14	CID:232	DL-Arginine	No	No	Yes; 0 violation.
15	CID:637566	GERANIOL	Yes	No	Yes; 0 violation.
16	CID:1051	pyridoxal phosphate	No	No	Yes; 0 violation
17	CID:289	pyrocatechol	Yes	No	Yes; 0 violation
18	CID:8442	Sulfoxide	Yes	Yes	Yes; 0 violation.

Table 4: Molecular docking energy of all 18 ligands and protein.

S. No.	Protein	Source of Organism	Ligand CID ID	Phytochemical Name	-Cdocker energy (kcal/mol)
1	2WAF	Clostridium perfringens (strain 13 / Type A)	232	DL-Arginine	25.9683
			240	benzaldehyde	10.9988
			289	pyrocatechol	14.4266
			326	4-isopropyl benzaldehyde	13.6489
			1051	pyridoxal phosphate	32.8322
			8175	Decanal	22.5696
			8442	Sulfoxide	11.9438
			31244	4-Methoxybenzaldehyde	10.3737
			51283	DL-Alanine-15N	17.4873
			151907	4-Hydroxypipecolic acid	8.207
			443158	(-)-Linalool	-10.3739
			637566	GERANIOL	-25.0839
			1549107	(Z, Z)-farnesol	-43.1304
2	2ZC6	Streptococcus pneumoniae serotype 4 (strain ATCC BAA-334 /TIGR4)	240	Benzaldehyde	14.7887
			289	Pyrocatechol	16.0321
			326	4-isopropyl benzaldehyde pyridoxal	19.0869
			1051	phosphate	41.4751
			2371	4- Methoxybenzaldehyde	-89.6145
			8175	Decanal	31.9198
			8442	Sulfoxide	22.3133
			17100	Alpha-TERPINEOL	-4.83549
			31244	4-Methoxybenzaldehyde	13.8956
			51283	DL-Alanine-15N	18.0967
			151907	4-Hydroxypipecolic acid	13.5964
			443158	(-)-Linalool	-3.30347
			521229	AC1LAVB6	-48.8754
			637566	GERANIOL	-16.5693
			1549107	(Z,Z)-farnesol	-30.8338
			5282108	Alpha-Ionone	-10.3717
3	3VMA	Escherichia coli (strain K12)	232	DL-Arginine	34.2382
			240	Benzaldehyde	16.1819
			289	Pyrocatechol	17.7641
			326	4-isopropylbenzaldehyde	26.5843
			1051	pyridoxal phosphate	39.8335

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					2371	Betulic acid	-133.497
					8175	Decanal	34.7661
					8442	Sulfoxide	29.6826
					17100	alpha-TERPINEOL	1.15522
					31244	4-Methoxybenzaldehyde	18.6867
					51283	DL-Alanine-15N	19.0834
					151907	4-Hydroxypipecolic acid	16.2281
					443158	(-)-Linalool	-1.31029
					521229	AC1LAVB6	-44.8457
					637566	GERANIOL	-14.3766
					1549107	(Z,Z)-farnesol	-26.7187
					5282108	Alpha-Ionone	-4.36655
4	6HZQ			Escherichia coli (strain K12)	232	DL-Arginine	35.582
					240	Benzaldehyde	18.2039
					289	Pyrocatechol	20.6657
					326	4-isopropylbenzaldehyde	19.8501
					1051	pyridoxal phosphate	44.6154
					8175	Decanal	34.5847
					8442	Sulfoxide	18.4343
					17100	alpha-TERPINEOL	-2.41484
					31244	4-Methoxybenzaldehyde	15.8058
					51283	DL-Alanine-15N	23.3154
					151907	4-Hydroxypipecolic acid	18.5808
					443158	(-)-Linalool	-3.27398
					637566	GERANIOL	-19.1135
					1549107	(Z, Z)-farnesol	-31.8632
					5282108	Alpha-Ionone	-7.3133
5	Peptidoglycan transpeptidase	D	D-	Clostridium perfringens (strain 13 / Type A)	232	DL-Arginine	28.9364
					240	Benzaldehyde	11.084
					289	pyrocatechol	14.7133
					326	4-isopropylbenzaldehyde	18.7276
					1051	pyridoxal phosphate	40.0006
					2371	Betulic acid	-77.9329
					8175	Decanal	27.8622
					8442	Sulfoxide	24.1085
					17100	alpha-TERPINEOL	-6.48147
					31244	4-Methoxybenzaldehyde	12.1121
					51283	DL-Alanine-15N	13.3479
					151907	4-Hydroxypipecolic acid	10.0444
					443158	(-)-Linalool	-5.48512
					521229	AC1LAVB6	-40.4713
					637566	GERANIOL	-24.0682
					1549107	(Z, Z)-farnesol	-34.9516
					5282108	ALPHA-IONONE	-7.21031
6	DNA gyrase subunit			Haemophilus influenzae (strain ATCC 51907 / DSM 11121 / KW20 / Rd)	240	Benzaldehyde	14.4452
					289	Pyrocatechol	16.4871
					51283	DL-Alanine-15N	14.8384
7	DNA topoisomerase 4 subunit			Haemophilus influenzae (strain ATCC 51907 / DSM 11121 / KW20 / Rd)	240	Benzaldehyde	15.9759
					289	Pyrocatechol	17.9047
					51283	DL-Alanine-15N	15.4779

The three topmost ranked molecules were chosen and visualized using Discovery Studio v20.1 software based on their binding energy and hydrogen interactions between the ligand and protein. To understand the interactions between the molecules, the 2-dimensional molecular interaction were plotted using the same software.

Table 5. The binding residues, -C-DOCKER energy between the amino acid and ligand molecule

S. No	Target Protein	Ligand Name	Binding Residues	-C-DCOKER energy
1	2WAF	Pyridoxal phosphate	ASN-A:334, ASN-A:659	25.9683
		DL-Arginine	ASN-A656, ASN-A:334, ASN-A:659, GLU-A:331	32.8322
		Decanal	ASN-A:659	22.5696
2	2ZC6	Pyridoxal phosphate	THR-560, ASN-562, TRP-411, TYR-409, ASN-430, LYS-373, SER-370, SER-428	41.4751
		Decanal	LYS-557, SER-370	31.9198
		Sulfoxide	ASN-430	22.3133
3	3VMA	Pyridoxal phosphate	LEU-A:201, THR-A:203, MET-A:204	
		Decanal	ASN-A:322, ILE-A:408	34.7661
		DL-Arginine	THR-A:203, ILE-A:408, VAI-A:407, SER-A:319, ASN-A:322, LEU-A:201, ILE-A:202	34.2382
4	6HZQ	Pyridoxal phosphate	VAI-A:344, TYR-A:419, GLY-A:306, SER-A:307, ASN-A:361, LYS-A:310, GLY-A;496, LYS-A:358	44.6154
		DL-Arginine	THR-A:497, TYR-A:419, LYS-A:310, PHE-A:417, SER-A:359, LYS-A:358	35.582

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		Decanal	LYS-A:310, SER-A:307, PHE-A:417	34.5847
5	Peptidoglycan	Pyridoxal phosphate	ASP-A:204, ARG-A:163, HIS-A:203, TYR-A:161, GLY-A:160, LYS-A:162, ALA-A:201	40.0006
	D D-transpeptidase	Dl-Arginine	ASP-A:204, ALA-A:201, GLY-A:160, LYS-A:162, ARG-A:163	28.9364
		Decanal	LYS-A:159	27.8622
6	DNA gyrase subunit	Benzaldehyde	ARG-A:459, ARG-A:387	14.4452
		Pyrocatechol	ARG-A: 459, ARG-A:387	16.4871
		DL-Alanine-15N	ALA-A: 386	14.8384
7	DNA topoisomerase 4 subunit	Pyrocatechol	GLY-A: 41	15.9759
		Benzaldehyde	HIS-A: 46, SER-A:172	17.9047
		DL-Alanine-15N	GLY-A: 171, ASN-A:170	15.4779

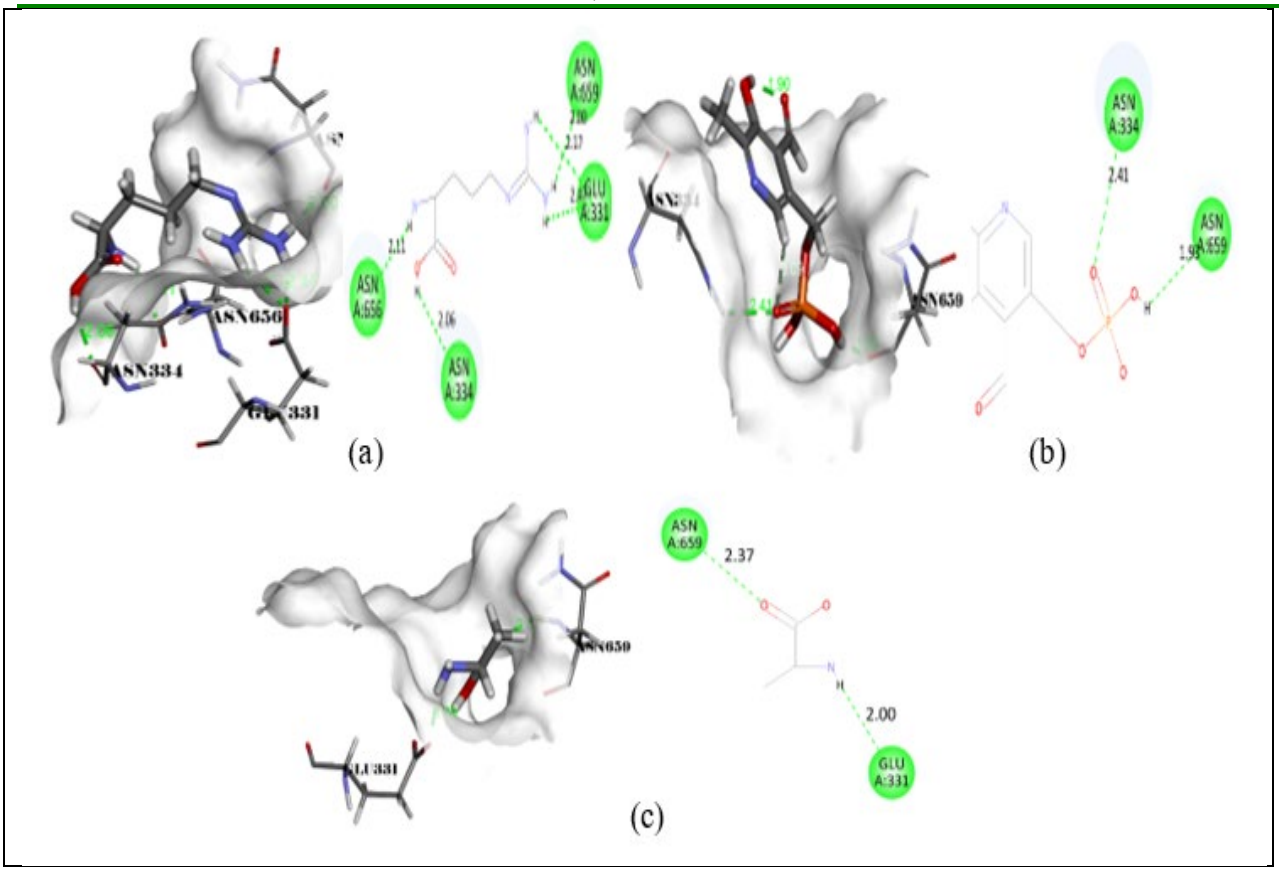

Figure 4: Graphical representation of bioavailability radar of all 18 phytocompounds of *Acacia farnesiana*.

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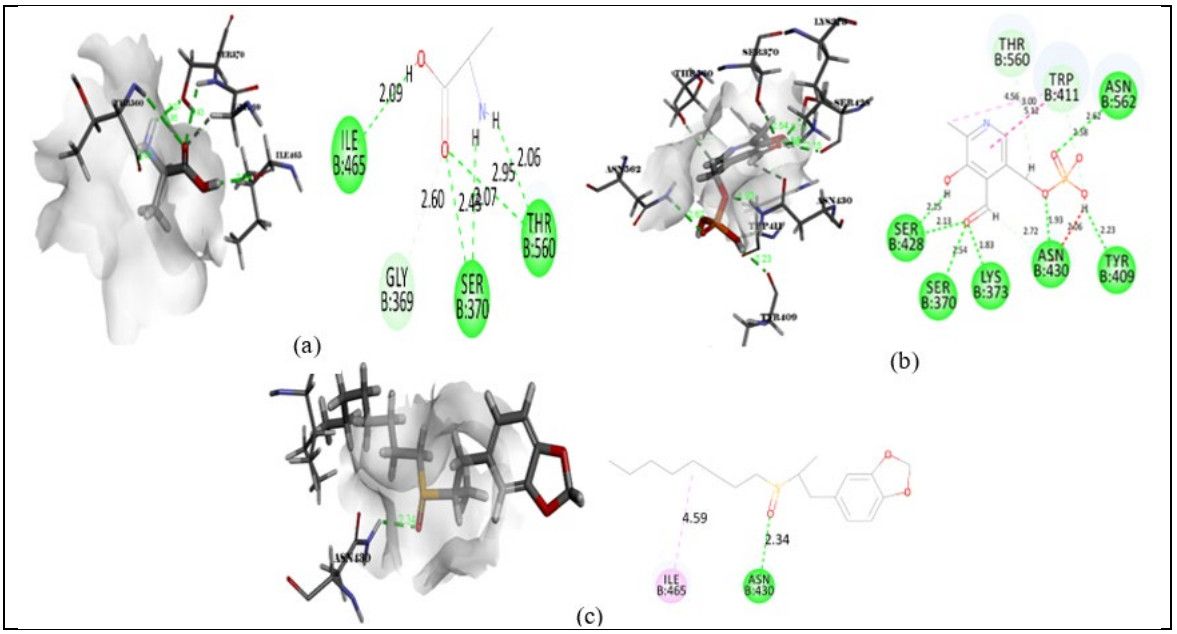

Figure 5: Intermolecular interaction of 2WAF with (a) pyridoxal phosphate, (b) DL-Arginine, (c) Decanal

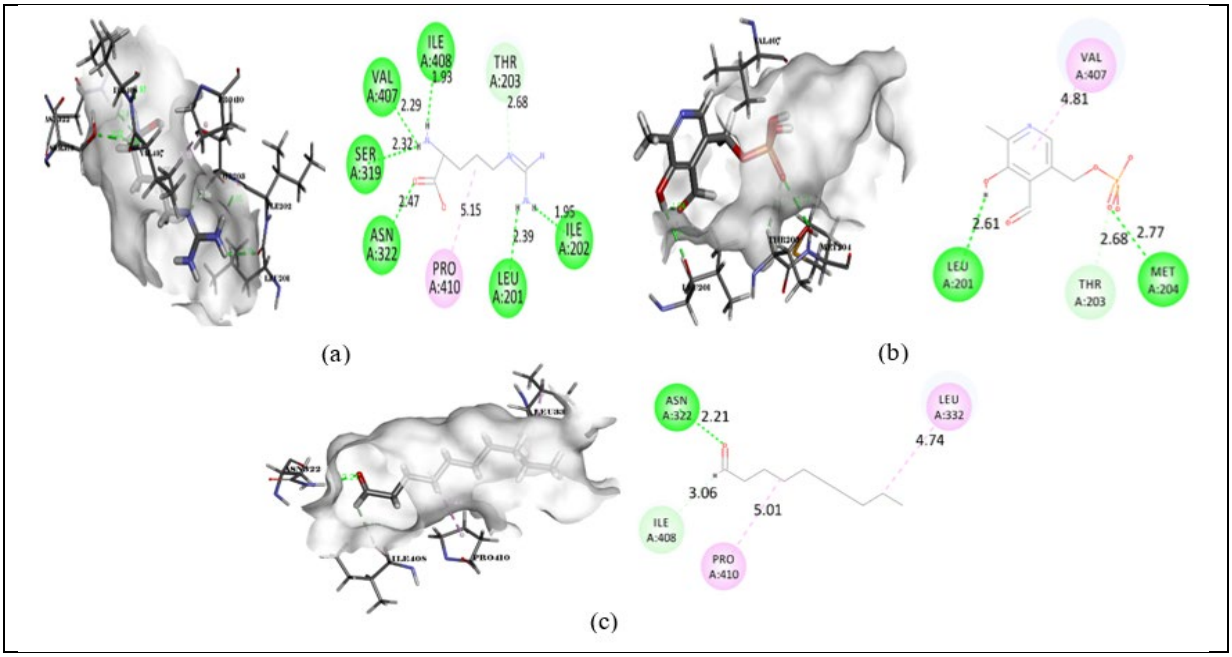

Figure 6: Intermolecular interaction of 2ZC6 with (a) Pyridoxal phosphate, (b) Decanal, (c) Sulfoxide.

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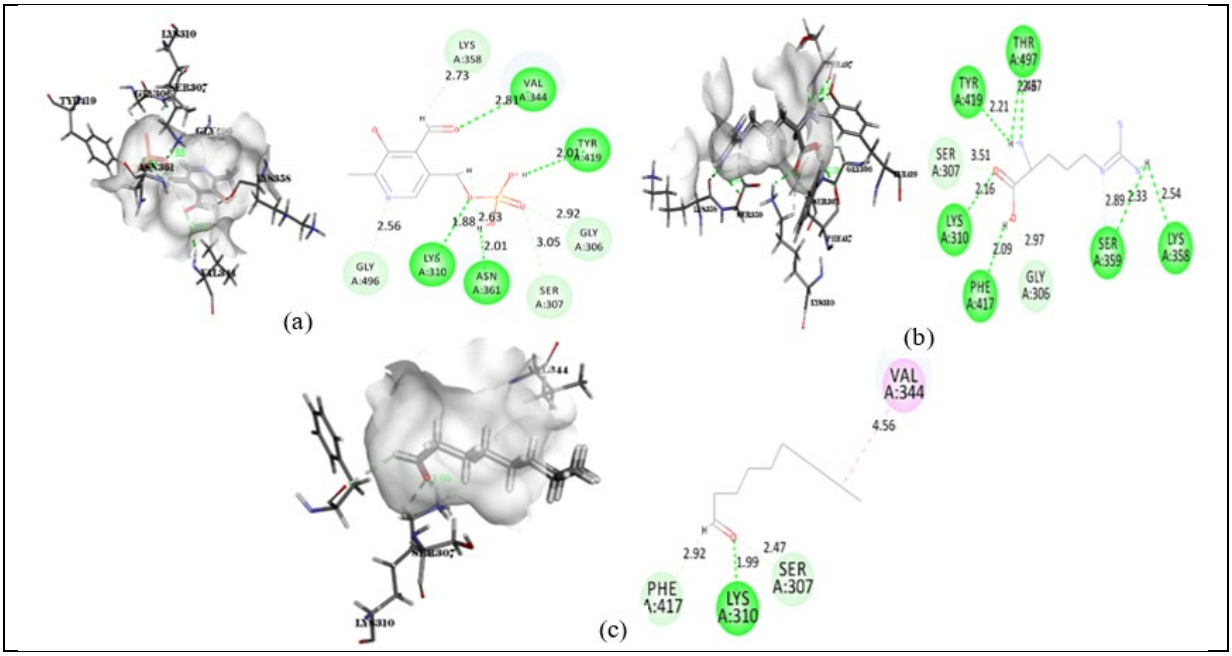

Figure 7: Intermolecular interaction of 3VMA with (a) Pyridoxal phosphate, (b) Decanal, (c) DL-Arginine.

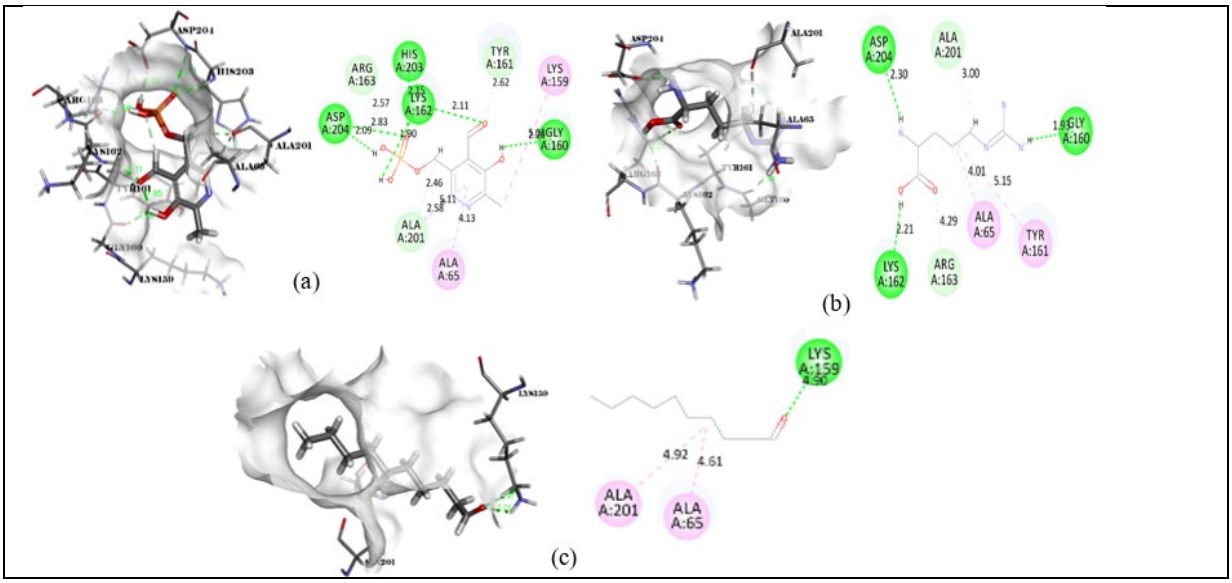

Figure 8: Intermolecular interaction of 6HZQ with (a) Pyridoxal phosphate, (b) DL-Arginine, (c) Decanal

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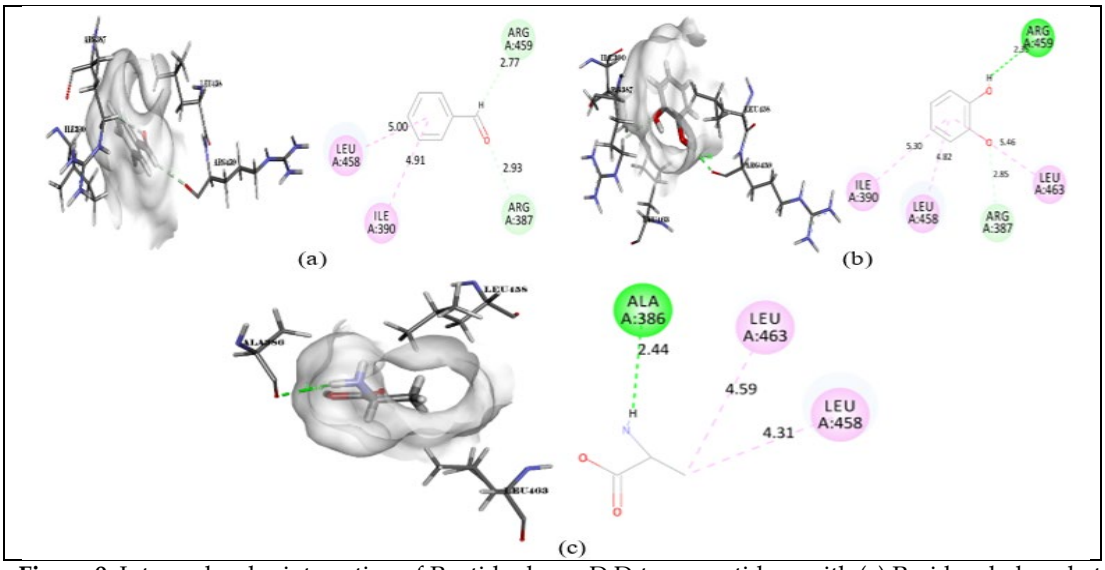

Figure 9: Intermolecular interaction of Peptidoglycan D D-transpeptidase with (a) Pyridoxal phosphate, (b) DL-Arginine, (c) Decanal

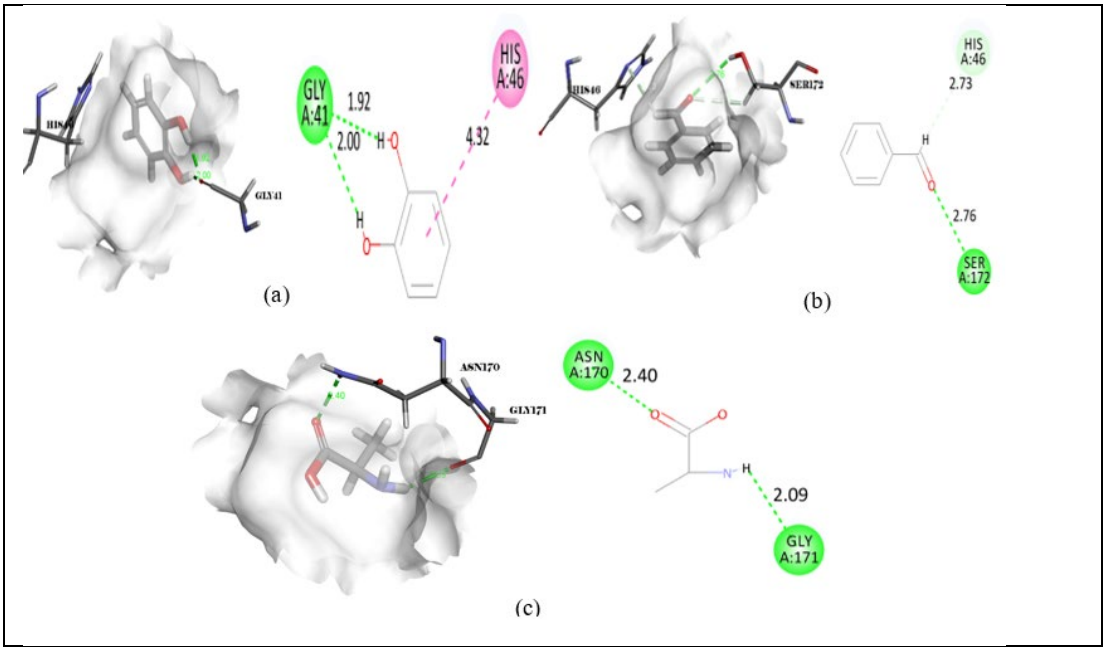

Figure 10: Intermolecular interaction of DNA *Gyrase* subunit with (a) Benzaldehyde, (b) Pyrocatechol, (c) Alanine-15N

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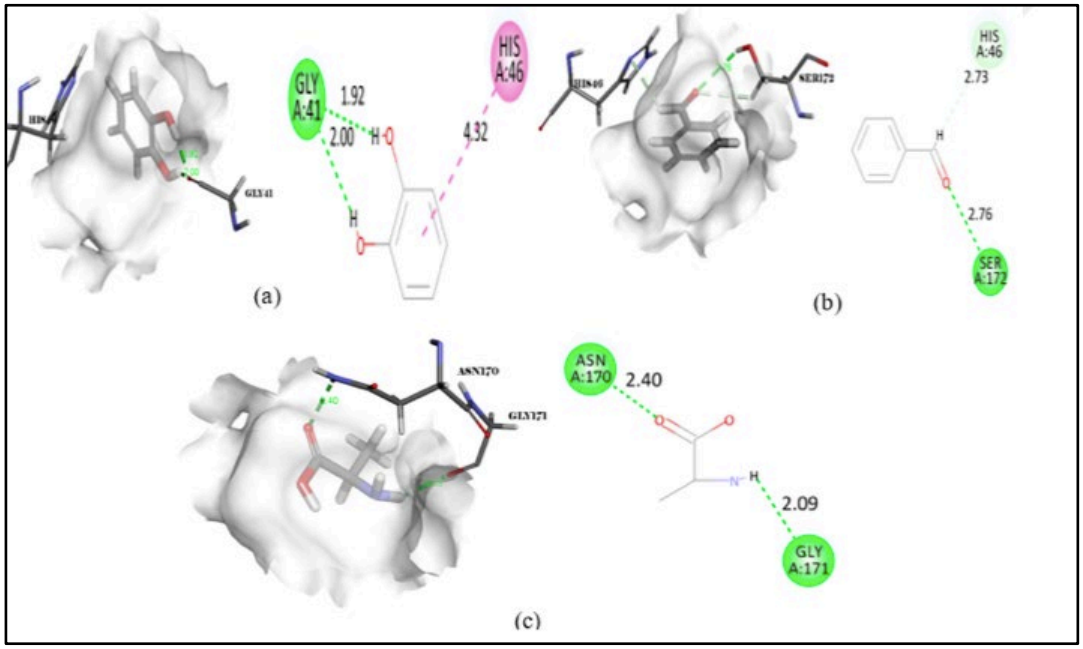

Figure 11: Intermolecular interaction of DNA topoisomerase 4 subunit with (a) Pyrocatechol, (b) Benzaldehyde, (c) DL-Alanine-15N

Conclusion:

We document the molecular docking analysis of four phytocompounds (Pyridoxal phosphate, DL-Arginine, Decanal, and Sulfoxide) from *Acacia farnesiana* having optimal binding features with targets linked to bronchitis for further consideration.

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Conflicts of Interest: There is no conflict of interest to declare.

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