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Mechanistic Insights into an Aloes Compound Veterinary Granules for Poultry as an ovarian activator

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ABSTRACT:

This study explores how the natural components of Aloes Compound Vet. Granules an age-old Ayurvedic remedy interact with important reproductive receptors in chickens. Using molecular docking techniques, we looked at how some of these key constituents bind to receptors like Estrogen receptor alpha (ESR1), Progesterone receptor (PGR), Thyroid hormone receptor beta (THRβ). These receptors play vital roles in follicle development, ovulation, hormone balance and early reproductive maturation. To give context, we included known ligands like estradiol, progesterone and liothyronine as controls. This way, we could compare how well the natural compounds performed. Certain compounds Rutin, Rubiadin and Friedelin stood out because they showed strong binding affinities, often mimicking how the control ligands fit into the receptors. These interactions hint that such molecules influences HPO's hormonal pathways and mineralization processes critical for reproductive health in poultry. Overall, the results support traditional claims about Aloes Granules, suggesting they have multiple targets within the body. To deepen our understanding, follow-up studies like molecular dynamics simulations or in-vitro testing are necessary. These steps will help clarify whether these interactions translate into meaningful biological effects.

KEYWORDS: Aloes Compound Granules; Molecular docking; Reproductive receptors; *Gallus gallus*; Phytoconstituents

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INTRODUCTION:

In commercial poultry farming it really matters, how efficiently hens lay eggs, which depends on a delicate balance between hormonal signals, metabolism, and structural processes inside the bird [7]. For chickens, egg production isn't just a simple act it's an energy-intensive, carefully choreographed event [7,8]. Hormones like estrogen, progesterone, thyroid play starring roles, guiding everything from reproductive readiness to follicle development and ovulation [7,4]. Even small hiccups in this system can cause fewer eggs, fragile shells, or broader reproductive issues [3,8]. As farmers and producers look for more natural ways to support their flocks' reproductive health, traditional medicine models are catching attention. Ayurveda, in particular, offers a treasure trove of herbal formulas believed to bolster fertility. One notable example is Aloes Compound Granules, a mix of herbs that includes Aloe indica, Rubia cordifolia, Balsamodendron myrrh, Peganum harmala, Bryonia patens and Leptadenia reticulata. These have long been considered rejuvenative and uterine tonics, said to enhance reproductive vigor and increase egg production [5,6]. While people have used these herbal remedies for centuries, understanding exactly how they work on a molecular level remains a challenge. That's where modern tools like molecular docking come in. This technology can predict how plant compounds might interact with key proteins involved in reproductive processes [10]. By simulating these interactions, scientists can start to uncover how herbal ingredients influence hormone signaling or structural proteins needed for egg formation [9,10]. It's a way to connect traditional wisdom with biochemical insights, shedding light on how these natural remedies might support poultry health at a molecular scale. This study aimed to explore how Aloes Compound Granules might work on a molecular level. We focused on three key receptors those together control critical aspects of reproductive readiness: genitals development, ovulation, hormone balance, energy metabolism etc. Estrogen receptor α (ESR1) is essential early on its involvement in making vitellogenin, a protein vital for yolk, and it helps the oviduct develop properly [7,9,11]. The progesterone receptor (PGR) plays a big role in deciding which follicle gets ready to ovulate and triggers the ovulation process itself also involved in oviposition in uterus [4,12]. The thyroid hormone receptor β (THRβ) controls overall metabolism, manages yolk precursor mobilization, and supports reproductive maturation [2,1,13]. All these receptors work together to connect hormonal signals with development. We docked phytochemicals from six different herbs to these receptors and compared their binding strengths to those of natural hormones like estradiol, progesterone and liothyronine [10]. Finding plant compounds that can bind just as well if not better than these native hormones could illuminate possible biochemical pathways through which Aloes Granules support egg production and growth [9]. This approach, combining molecular docking with traditional herbal knowledge, offers a fresh scientific perspective. It also paves the way for future studies whether in test tubes, animals, or computational models that might eventually lead to plant-based supplements aimed at boosting reproductive performance in poultry.

Materials And Methods

Ayurvedic Formulation

For this study, we focused on Aloes Compound Granules, a classic Ayurvedic mixture traditionally used to boost reproductive health. The formulation contains six herbs: *Aloe indica, Rubia cordifolia, Balsamodendron myrrh, Peganum*

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harmala, Bryonia patens, and *Leptadenia reticulata*. In Ayurvedic texts, these plants are classified as *rasayana* or *garbhashaya poshaka* terms that point to their rejuvenative qualities, support for the uterus, and their role in enhancing oocyte. We chose these herbs specifically to capture the full range of their phytochemicals, giving us a comprehensive picture of the formulation's potential effects.

Selecting the Target Proteins

To understand how these herbs might influence reproductive functions, we zeroed in on three key receptors involved in genitals development and hormonal balance in chickens (Gallus gallus). These include the estrogen receptor α (ESR1), progesterone receptor (PGR) and thyroid hormone receptor β (**THRβ**). We pulled their structures from the uniprot database, along with their associated PDB complexes, so we could look at their three-dimensional shapes. Basically, they're the core switches that Reproductive modulators need to influence if they're going to make a difference.

Ligand Identification and Preparation

We looked up the active compounds in six different herbs using trusted phytochemical databases. To visualize their shapes, downloaded their 3D structures from pubchem, saved as .pdb files. But before testing how these molecules might interact with targets, each one was carefully prepared. Added hydrogen atoms, assigned Gasteiger charges, and ran a quick energy minimization. This process helps ensure that the molecules are in stable, low-energy forms making the docking results more reliable and realistic.

Docking Controls

To check how well the docking worked, we used the original ligands that were crystallized with each receptor as positive controls. For ESR1, we looked at estradiol; progesterone was used for PGR; liothyronine (T3) for THRβ. These familiar molecules helped us see what typical binding looks like and provided a benchmark for how strongly other compounds might interact. Basically, they gave us a point of comparison to gauge the phytochemicals' binding behavior.

Molecular Docking Procedure

First, the receptor molecules were prepared by cleaning up a few things removing water molecules, adjusting protonation states to make sure everything's balanced, and setting up grid boxes around the native ligand binding sites. Then, each plant-derived compound was docked into its respective receptor's active site. We looked at how well they fit by checking the binding energies, but also paid closer attention to the hydrogen bonds they formed, the hydrophobic contacts they made, and any π-interactions present. We also checked how closely their poses matched the original ligand's position in the crystal structure, giving us a better idea of how promising each interaction might be.

RESULTS

Molecular Docking

Docking analyses revealed distinct interaction patterns between phytochemicals from Aloes Compound Granules and three reproductive targets in *Gallus gallus*. The strongest interactions were observed with ESR1 and PGR (–10 to –5 kcal/mol), approximating affinities of native ligands and indicating a high probability of receptor engagement. Moderate binding occurred with THRβ. Notably, many ligands converged around ~ –7 kcal/mol for ESR1 and PGR, suggesting preferential affinity toward pathways governing vitellogenesis, follicular development, and ovulation. Collectively, the docking profiles support selective engagement of endocrine and biomineralization pathways relevant to avian reproduction. ESR1 interactions were dominated by Rubiadin, Luteolin, Aloeemodin, and Kaempferol (–9.3 to –8.0

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kcal/mol), although estradiol remained the highest-affinity ligand (~ –10 kcal/mol). In PGR, Friedelin displayed the tightest binding (–8.7 kcal/mol), exceeding progesterone, with Ellagic acid, Lupeol, and Rutin clustering between –7.6 and –7.0 kcal/mol. THRβ binding was led by Rutin (–9.5 kcal/mol), followed by Lupeol, Stigmasterol, β-sitosterol, and Friedelin each outperforming liothyronine (~ –7.3 kcal/mol).

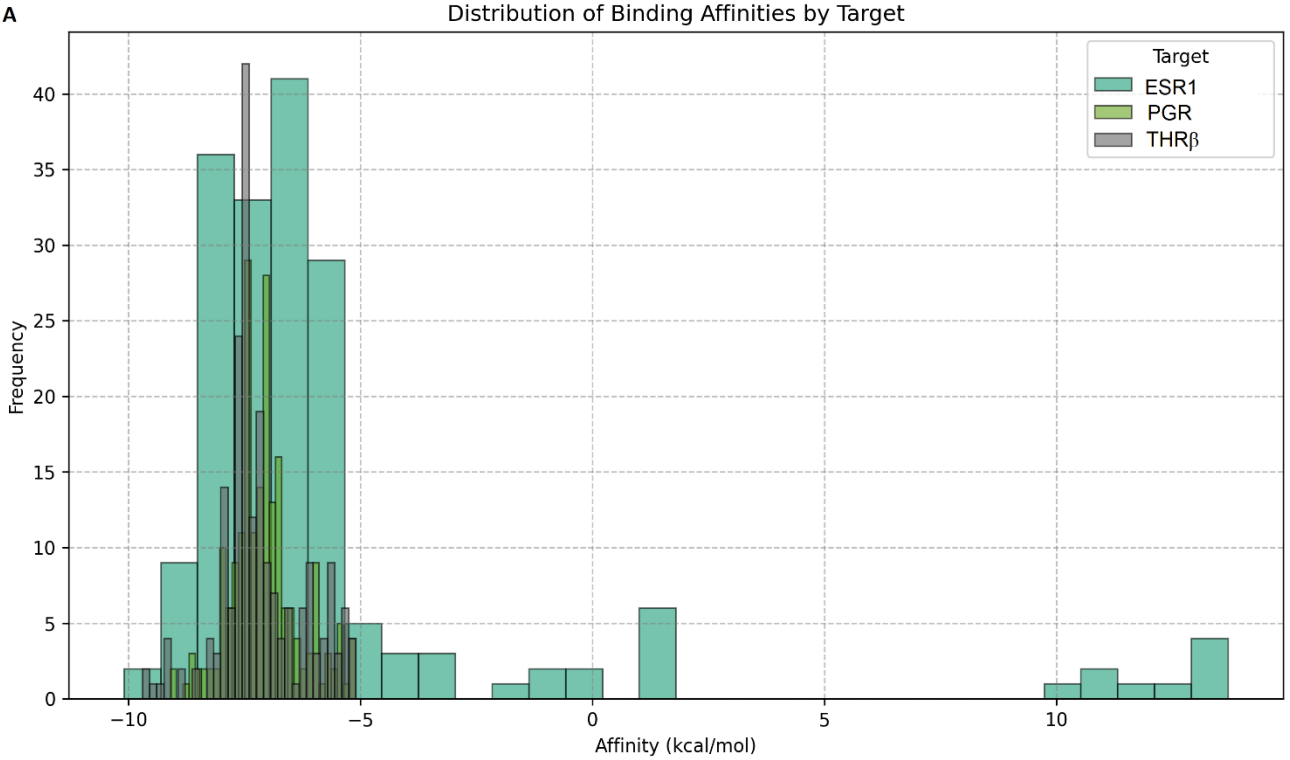

Figure 1: A) Distribution of binding affinities (kcal/mol) for phytoconstituents docked against three reproductive targets in Gallus gallus.

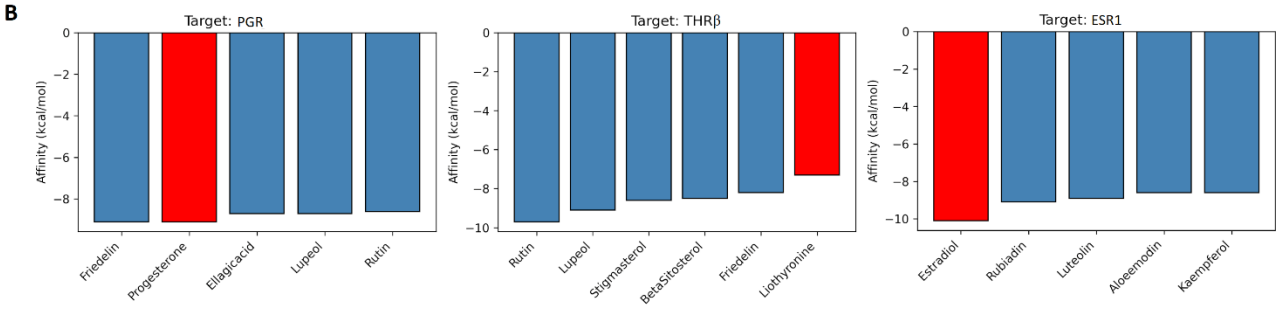

Figure 2: B) Top phytoconstituent hits and corresponding hormonal controls across each reproductive target.

Structural Basis of High-Affinity Binding

Estrogen Receptor α (ESR1)

Rubiadin aligned closely with estradiol's pose in the receptor's hydrophobic pocket (Figure 3). Both ligands shared interactions with Arg388 a residue essential for helix-12 stability while Rubiadin additionally engaged Met337 and Leu340. The overlap in residues stabilizing the ligand-binding domain supports Rubiadin's ability to mimic aspects of ESR1 activation.

eISSN : 2582 - 7634
International Journal of Indian Medicine, 2025; 6(12):76-84 ISSN: 2582-7634

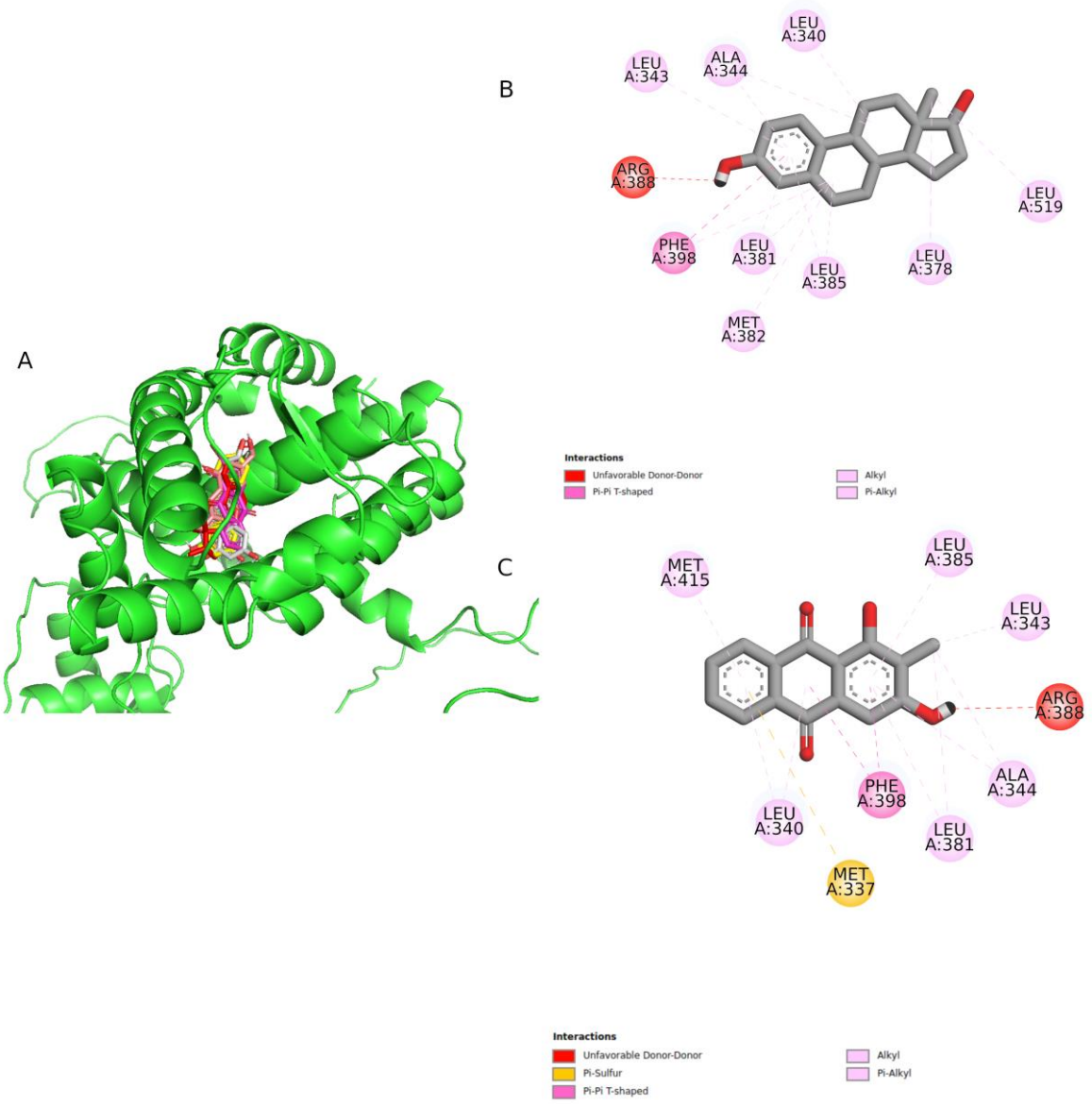

Figure 3: Structural alignment and interaction profiles of estradiol and Rubiadin within the estrogen receptor α (ESR1).

Progesterone Receptor (PGR)

Friedelin and progesterone overlapped within PGR's hydrophobic core (Figure 4). Progesterone relied on hydrogen bonding with His734 and Tyr606, whereas Friedelin lacking polar groups achieved stable packing via hydrophobic interactions with Thr682, Val778, and Lys738. These findings indicate that Friedelin may partially mimic progesterone's binding mode despite its non-polar structure.

eISSN : 2582 - 7634
International Journal of Indian Medicine, 2025; 6(12):76-84 ISSN: 2582-7634

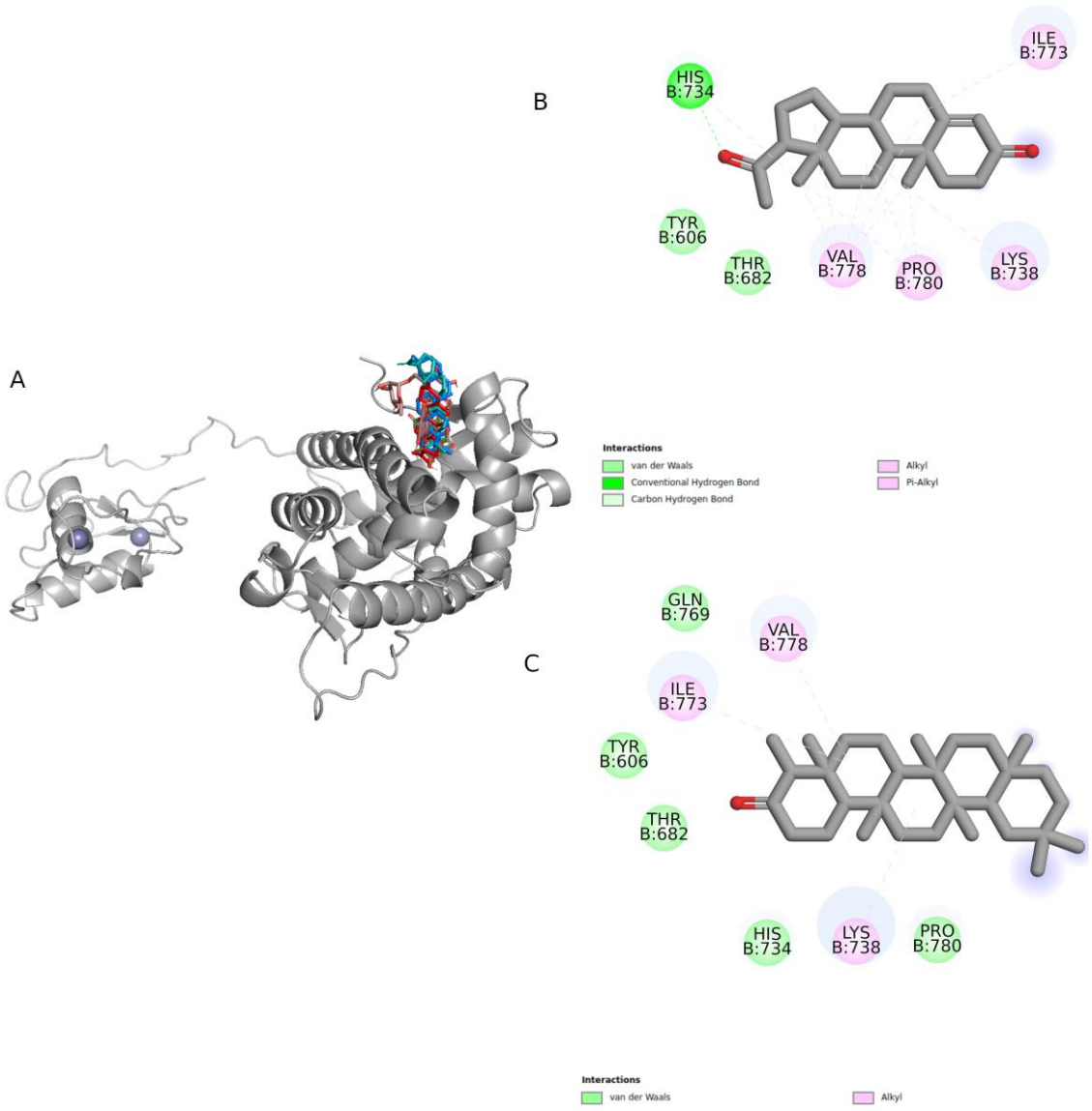

Figure 4: Binding conformations and interaction profiles of progesterone and Friedelin within the progesterone receptor (PGR).

Thyroid Hormone Receptor β (THRβ)

Rutin and T3 bound within the same deep hydrophobic pocket (Figure 5). While T3 interacted through Thr276 and Asp274, Rutin formed an expanded hydrogen-bond network involving Ser91, Asp89, Asp275, Tyr314, Arg318, and Lys96, supported by π–alkyl and π–anion contacts. The interaction density is consistent with Rutin's stronger binding affinity and suggests potential modulation of THRβ -dependent metabolic processes.

eISSN : 2582 - 7634
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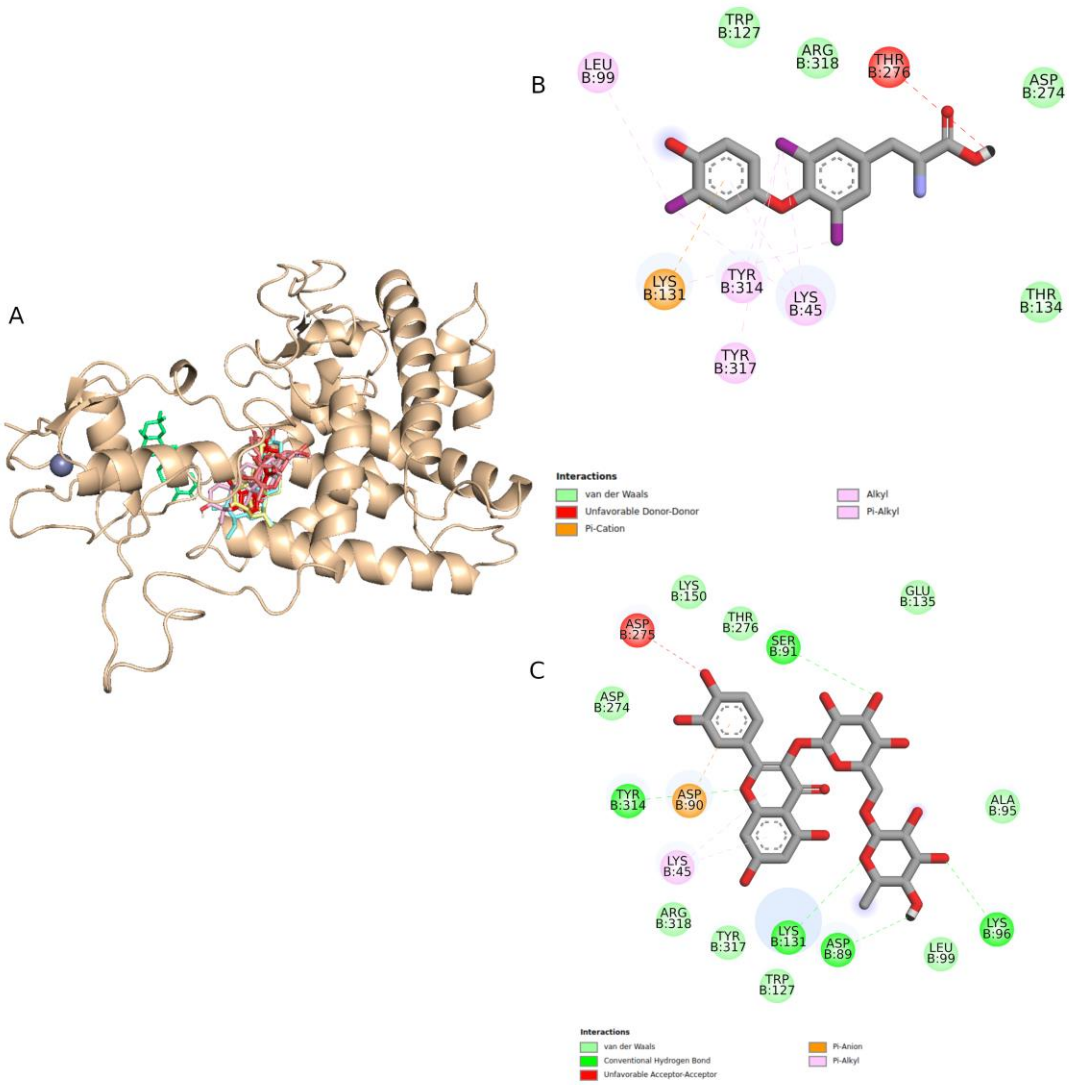

Figure 5: Binding orientations and interaction profiles of liothyronine (T3) and Rutin within the thyroid hormone receptor β (THRβ).

DISCUSSION:

The docking studies of Aloes Compound vet. Granules offer initial molecular clues supporting their traditional claims of boosting reproductive health in Gallus gallus. The phytochemicals within the formulation show strong affinities for three key receptors: ESR1, PGR and THRβ. These receptors are crucial for hormone regulation, follicle development. The interaction pattern suggests that the formulation operates through multiple pathways relevant to avian reproductive physiology. Among the compounds tested, Rutin, Rubiadin, Friedelin stood out as the highest-affinity ligands. Interestingly, some of these molecules bind as tightly as or even more tightly than endogenous controls like estradiol, progesterone and liothyronine. Structural analysis indicates that these phytochemicals fit snugly into the ligand-binding sites of their target receptors, forming a network of hydrogen bonds, hydrophobic contacts, and π-interactions with key residues that stabilize and activate the receptors. Rutin, for example, showed notable affinity for THRβ, hinting at possible roles in calcium transport and metabolic regulation. Rubiadin and

eISSN : 2582 - 7634
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Friedelin, on the other hand, displayed binding modes similar to natural steroid hormones, implying potential estrogenic or progestogenic activity. This multi-receptor engagement aligns well with Ayurvedic descriptions of Aloes Compound Granules as uterine-supporting (*garbhashaya poshaka*) and egg-enhancing (*anda-vriddhikara*) formulations. The docking results across receptors involved in hormone signaling, nutrient processing, and shell formation form a plausible mechanistic picture one that correlates with observed improvements in reproductive performance and eggshell quality. That said, these findings are purely computational and need to be validated experimentally. Future research should include molecular dynamics simulations to assess complex stability, receptor-binding assays to test affinity in vitro, and cell-based studies to examine downstream biological effects. Combining these approaches will be essential to determine whether the predicted interactions translate into real physiological benefits. Such work will clarify the therapeutic potential of this traditional formulation within the context of modern reproductive biology.

CONCLUSION:

This research offers molecular-level insight into why Aloe-based formulations are traditionally used to boost reproductive performance and improve ovarian strength in chickens. The docking studies identified several key plant compounds such as Rutin, Rubiadin and Friedelin that show strong binding to receptors vital to avian HPO axis, including ESR1, PGR, THRβ**.** These molecules didn't just stick loosely; they interacted in a stable manner within the active sites of these proteins, with affinities comparable to natural hormones. Such interactions hint at the potential to influence processes like follicle development, reproductive readiness, and egg holding capacity for healthy hatching. Interestingly, the compounds seem to target multiple pathways involving both hormonal regulation and structural components, offering a mechanistic explanation consistent with traditional Ayurvedic concepts of *garbhashaya poshaka* and *anda-vriddhikara*. Of course, these findings are purely predictive at this stage. To truly understand the biological effects, follow-up studies such as molecular dynamics simulations and cellular assays are necessary to confirm activity and functional impact. Altogether, these results set a promising stage for further research into Aloes Compound vet. granules as natural, multi-target options to support ovarian health and enhance reproductive ability in poultry. They bridge age-old traditional knowledge with insights from modern molecular science, opening new avenues for sustainable farming practices.

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CONFLICT OF INTEREST

This research was conducted as part of the ongoing scientific initiatives of Alarsin, Mumbai. The authors declare that there are no conflicts of interest beyond their professional affiliation with the organization.

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