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Computational Elucidation of Phytochemicals Targeting Inflammatory and Hormonal Regulators in Gynecological Disorders.

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ABSTRACT:

Background: Gynecological disorders-including reproductive tract infections (RTIs), pelvic inflammatory disease (PID), endometriosis, polycystic ovary syndrome (PCOS), cervicitis, dysmenorrhea, and leucorrhoea are multifactorial conditions driven by infection, inflammation, and hormonal imbalance. MYRON, a traditional ayurvedic polyherbal formulation, is widely used for their management, though its molecular basis of action remains unclear. **Objective:** This study aimed to elucidate the multi-target molecular mechanisms of MYRON by evaluating interactions between its phytochemicals and key therapeutic targets involved in gynecological inflammation, infection, and hormonal regulation. **Methods:** Twenty-five phytochemicals were subjected to molecular docking against Estrogen Receptor Alpha (ER_α), Nuclear Factor Kappa B (*NF-κB*), Cyclooxygenase-2 (COX-2), Tumor Necrosis Factor Alpha (TNF_α), and DNA gyrase. Binding affinities and interaction profiles were analyzed and compared with standard control ligands. **Results:** MYRON phytochemicals exhibited notable multi-target binding across all five proteins. Several compounds showed strong affinity for ER_α, suggesting hormonal modulatory potential. Berberine, caffeic acid, ferulic acid, and triterpenoids demonstrated strong interactions with inflammatory mediators (*NF-κB*, COX-2, and TNF_α). Additionally, multiple phytochemicals overlapped with the DNA gyrase active site, indicating antibacterial activity relevant to RTIs. Ellagic acid, guggulsterone-E, and quercetin showed stable binding across hormonal, inflammatory, and antimicrobial targets.**Conclusion:** The findings provide molecular-level support for MYRON's traditional use in gynecological disorders through its coordinated multi-target actions, warranting further experimental and clinical validation.

Key words: Molecular Docking, Gynecological Disorders, Reproductive Tract Infections, Inflammation, Phytochemicals, MYRON

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Introduction:

Women's reproductive health is the core of public health as it directly correlates to the infant's health and its survival. The risk of biological diseases such as genetic variation, host defense mechanism, anatomical differences, sex steroid hormones, and reproduction effect differs between men and women which influences the sociocultural environment, psychological development and economic status generating the differences in disease risk among both the sexes.[1] Infertility, poor pregnancy outcomes, and increased HIV vulnerability are all consequences of reproductive tract infections (RTIs), making them a major global public health concern. RTIs include upper tract disorders like endometritis (endometrial inflammation), salpingitis (inflammation of the fallopian tube), and oophoritis (inflammation of the ovaries), as well as lower tract infections like vaginitis (vaginal inflammation) and cervicitis (cervical inflammation). Common symptoms associated with these infections encompass leucorrhoea (abnormal vaginal discharge), pruritis (intense vaginal itching), and dysuria (painful urination), which can exacerbate discomfort and signal underlying inflammation or infection. Untreated infections may progress to pelvic inflammatory disease (PID), ectopic pregnancy, or tubal infertility.[2] This not only causes physical discomfort but also profoundly impacts quality of life, reproductive health, and fertility outcomes. Numerous factors, such as bacterial infections, hormonal imbalances, chronic inflammatory responses, and compromised tissue integrity, often contribute to these disorders. As a result, comprehensive therapeutic approaches that address multiple pathological mechanisms simultaneously rather than focusing on individual symptoms are needed.[3] Traditional ayurvedic medicine has long understood the nature of gynecological issues and developed polyherbal formulations that restore physiological balance in multiple ways. In order to address the underlying causes of illness rather than just treating its symptoms, Ayurvedic medicines employ a multi-target therapeutic approach in which different bioactive substances act synergistically on various biological targets.[4] The current theories of systems pharmacology and network medicine recognize how complex diseases with multiple pathogens require multi-component, multi-target therapy approaches. Female reproductive health issues are often complex, involving a mix of ongoing inflammation, infections, oxidative stress, hormonal imbalances, impaired tissue healing, and immune system problems. Thus, treatments that can tackle multiple underlying pathways at the same time, rather than focusing on just one are important. MYRON, a traditional polyherbal Ayurvedic formulation, is commonly used to treat various illnesses, but the molecular processes behind its therapeutic effects are still unknown, leaving a significant gap between traditional knowledge and evidence-based therapy.[5] Finding these mechanisms is essential for the scientific validation of the traditional claims as well as for the identification of trustworthy biomarkers for monitoring patient reactions, improvement of the formulation, elucidation of possible drug interactions, and safe integration of this useful herbal remedy into modern healthcare procedures.[6] The current study utilizes molecular docking methods to systematically investigate the binding interactions of 25 major phytochemicals derived from MYRON's herbal components with 5 therapeutically relevant protein targets, with the goal of elucidating the multi-target molecular mechanisms that support the formulation of traditional therapeutic claims.[4] The study aims to characterize the binding affinities and interaction patterns of key phytoconstituents with

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antibacterial targets (DNA gyrase), hormonal receptors (ERα), and inflammatory mediators (NF-κB, COX-2, TNFα) to identify which bioactive compounds exhibit the strongest interaction with each target, potentially representing the principal active constituents responsible for specific therapeutic effects, and reveals the multi-target binding profile.[7,8,9] The findings of this study will contribute to the integration of traditional ayurvedic medicines into evidence-based healthcare, while demonstrating the power of computational methods in identifying the complex pharmacology of polyherbal formulations that have served humanity for centuries but remained mechanistically unexplored until the advent of modern molecular modeling technologies.[10]

Materials and Methods:

1. Selection of Target Proteins

Five therapeutically relevant protein targets representing key pathophysiological mechanisms in gynecological inflammatory disorders were selected: estrogen receptor alpha (ERα , PDB ID: 3ERT) for hormonal regulation and inflammatory modulation, cyclooxygenase-2 (COX-2, PDB ID: 5KIR) for prostaglandin-mediated inflammation, DNA gyrase (PDB ID: 1KZN) for antibacterial activity, nuclear factor kappa B (NF-κB, PDB ID: 3RZF) for inflammatory gene transcription, and tumor necrosis factor alpha (TNFα , PDB ID: 2AZ5) for pro-inflammatory cytokine signaling. All three-dimensional crystal structures were retrieved from the RCSB Protein Data Bank (https://www.rcsb.org/) based on high resolution, presence of relevant bound ligands, and structural quality. Each target structure was specifically selected with its co-crystallized control molecule intact, which served as a reference ligand for validation of the docking protocol and comparison with phytochemical binding affinities.[11]

2. Cleaning and Preparation of Targets

The target proteins were cleaned using UCSF Chimera. Briefly, the native ligand and all other non-standard atoms were deleted, the repeating chains of dimers were deleted to obtain monomeric target structure. Then, the targets were subsequently prepared using the 'Dock Prep' tool in Chimera which involved addition of hydrogen, fixing the structure, application of AM1-BCC Force Field. Finally, the targets were minimized by Steepest Descent. After cleaning and preparation, the target proteins were saved in .pdb format for docking.[12]

3. Molecular Docking:

Molecular Docking was performed using AutoDock Vina by PyRx (version 0.8).[13,14] Briefly, the target proteins and all the ligands were loaded. The ligands were minimized and converted to pdbqt format prior to docking. The grid box was maximized for blind docking and all the 25 ligands were then docked against each target proteins, respectively. The binding affinities obtained after docking were saved in .csv format for further analysis. The 2D and 3D receptor-ligand interactions were analyzed using PyMOL[15] and Biovia Discovery Studio.[16]

Results

1. Molecular docking against target receptors:

Molecular docking of all 25 ligands against 5 targets was performed and the respective binding affinities are given in the heatmap below (Figure 1). The binding affinities spanned from −5.5 to −9.8 kcal/mol, where darker blue shades denote stronger interactions (more negative values corresponding to favorable binding), while lighter blue shades indicate comparatively weaker interactions (less negative values).

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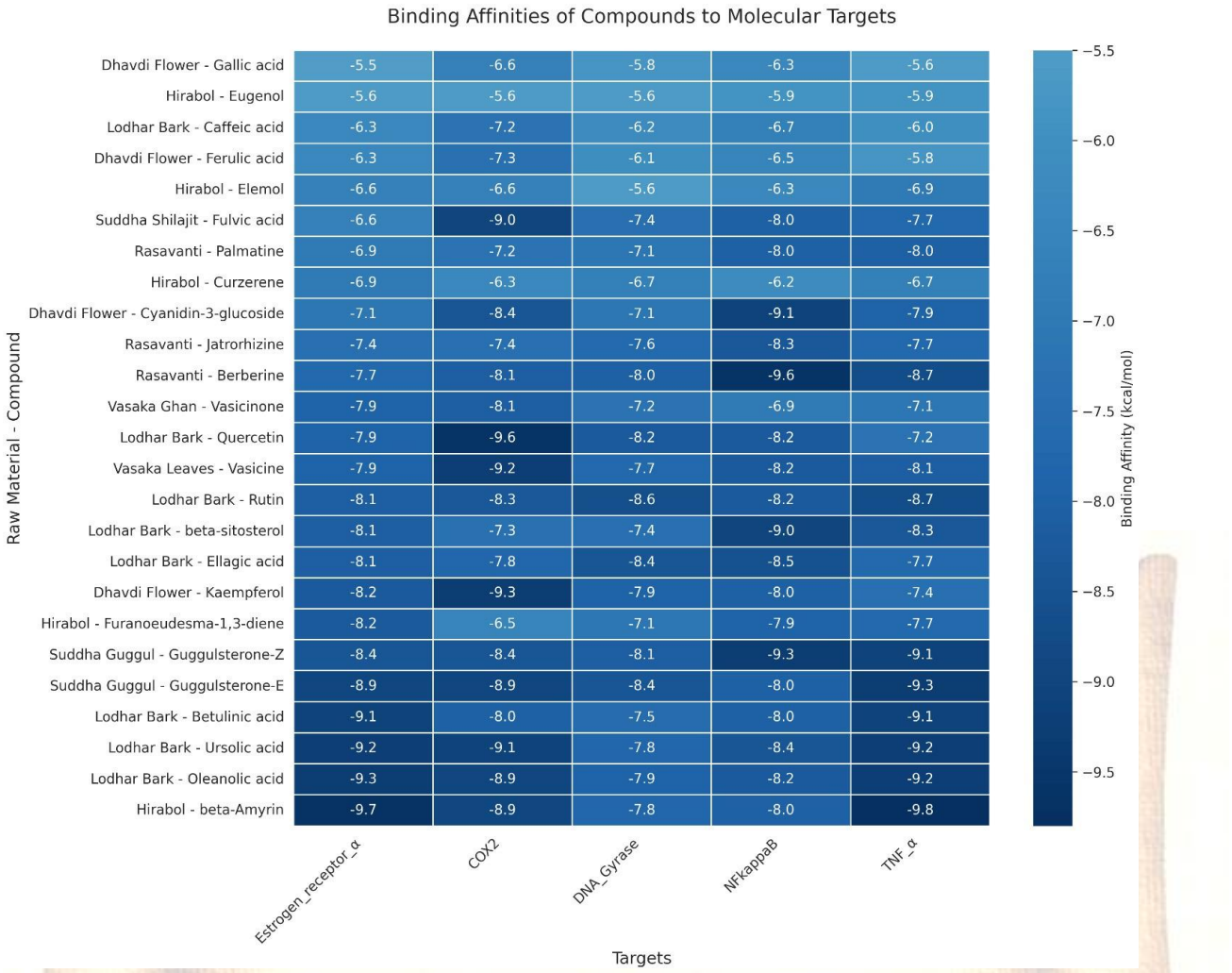

Figure 1: Heatmap of Binding Affinities of all the phytochemicals against five target receptors

2. 3D Interaction Analysis of MYRON Constituents:

Three-dimensional interaction analysis revealed that the screened phytochemicals from the formulation consistently occupied the binding sites of all five target proteins, namely *ERα*, COX-2, *NF-κB*, DNA gyrase, and *TNFα* (Figure 2). The docking protocol was validated by re-docking the native ligands of all 5 receptors and these native ligands were then used as controls for comparison. The top-ranked ligands for each target adopted stable conformations within the respective binding pockets and demonstrated substantial spatial overlap with the co-crystallized control ligands, indicating appropriate recognition of functionally relevant regions. For each receptor, the top-ranked ligand poses showing maximum overlap with the control (colored red) were selected and visualized (Figure 2).

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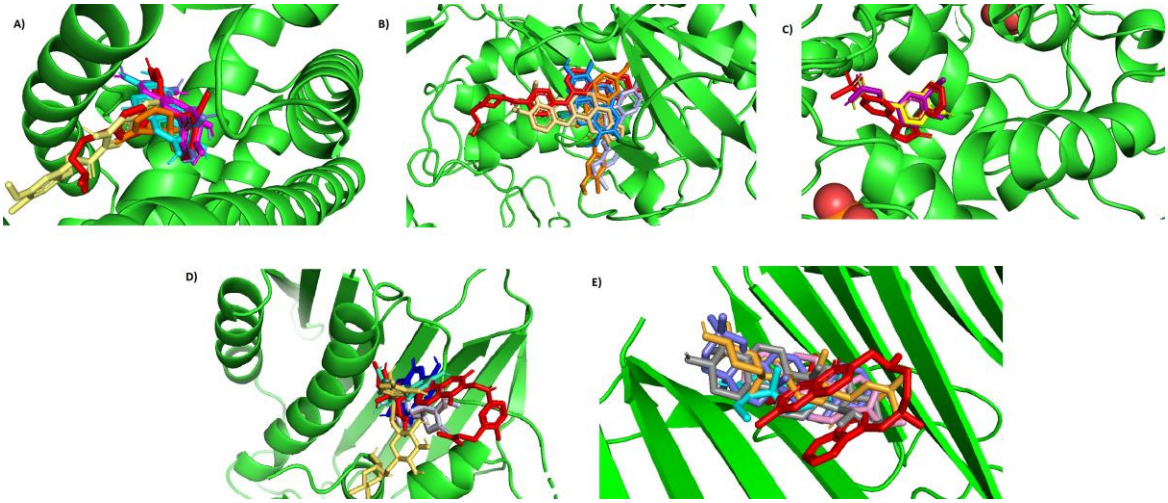

Figure 2: 3D Interaction maps of the ligands interacting with the active sites of the receptors

For ERα (Figure 2A), kaempferol (magenta), furanoeudesma-1,3-diene (orange), ellagic acid (cyan), vasicine (pale yellow), and quercetin (slate) overlapped with control 4-hydroxytamoxifen (red; −9.5 kcal/mol). In NF-κB (Figure 2B), the fifth redocked pose of the control ligand XNM (red; −8.6 kcal/mol) showed a clear spatial overlap with berberine (light orange; −9.6 kcal/mol), ellagic acid (marine), jatrorhizine (light blue), and vasicine (orange). COX-2 docking (Figure 2C) revealed that caffeic acid (yellow) and ferulic acid (purple) occupied the control rofecoxib-binding channel (red; −9.9 kcal/mol). For DNA gyrase (Figure 2D), rutin (yellow-orange; −8.6 kcal/mol), ellagic acid (blue), guggulsterone E (dirty violet), quercetin (green-cyan), and guggulsterone Z (blue- white) overlapped with control chlorobiocin (red). In TNFα (Figure 1E), β-amyrin (slate; −9.8 kcal/mol), guggulsterone E (cyan), guggulsterone Z (pink), oleanolic acid (bright orange), and ursolic acid (gray) showed extensive overlap with the control chromenone derivative (red; −8.0 kcal/mol). The consistent overlap of phytochemical binding poses with their respective control ligands across all targets indicates potential multi-target modulatory activity.

3. 2D interaction analysis against *ERα*

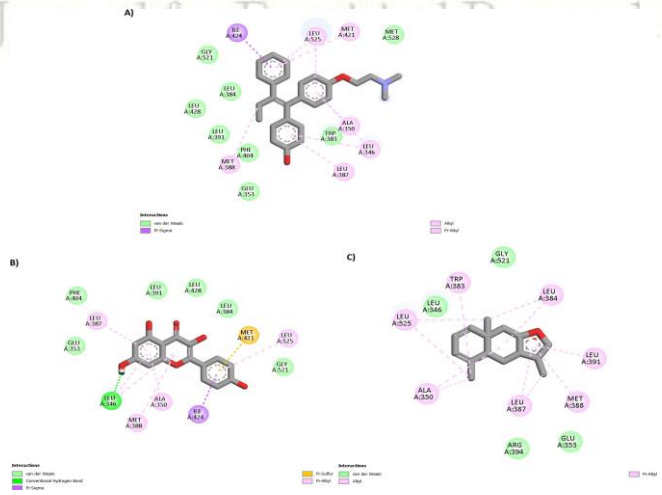

Figure 3: Two-dimensional interaction map of *ERα* with (A) 4-hydroxytamoxifen, (B) kaempferol, and (C) furanouedesma-1,3-diene.

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Docking analysis showed that the reference ligand 4-hydroxytamoxifen (OHT) had the highest binding affinity for estrogen receptor alpha (ERα), with a docking score of −9.5 kcal/mol (Figure 2A). OHT fit well in the ERα ligand-binding pocket. It formed strong hydrophobic and π-alkyl interactions with key residues like Leu346, Leu384, Met388, and Ala350 (Figure 3A). Among the phytochemicals, kaempferol (Figure 2B) and furanouedesma-1,3-diene (Figure 2C) had similar binding energies of −8.2 kcal/mol. Kaempferol formed hydrogen bonds and had hydrophobic interactions, which improved the stability of the complex. In contrast, furanouedesma-1,3-diene mainly interacted through π-alkyl and van der Waals interactions.

4. 2D interaction analysis against COX-2:

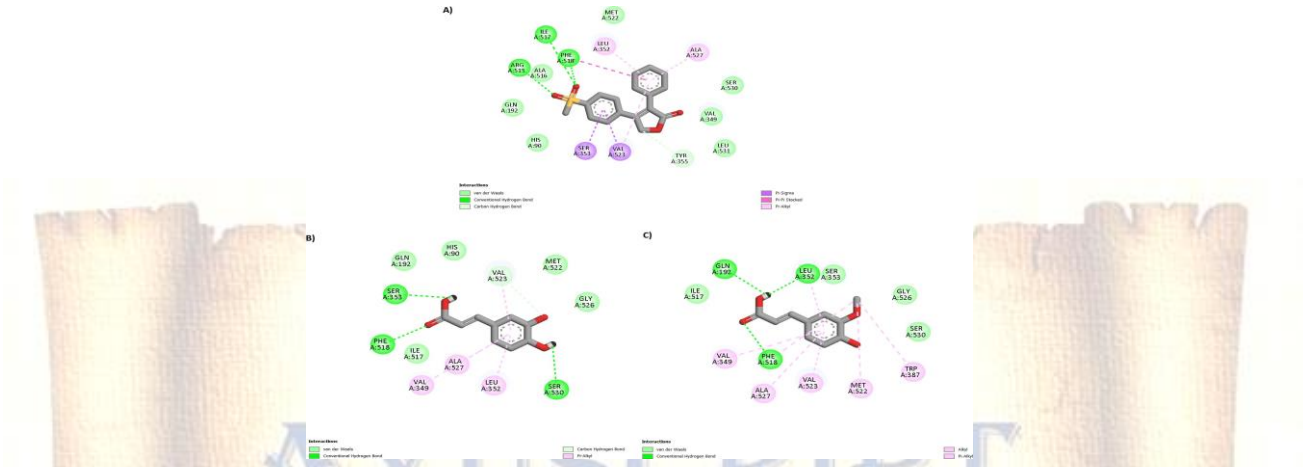

Figure 4:2D interaction diagrams of COX-2 with (A) rofecoxib, (B) caffeic acid, and (C) ferulic acid.

Docking analysis against cyclooxygenase-2 (COX-2) showed that the reference inhibitor rofecoxib exhibited the strongest binding affinity, with a docking score of −9.9 kcal/mol (Figure 4A). Rofecoxib was well accommodated within the COX-2 active site and formed extensive hydrophobic and π−alkyl interactions with key residues such as Val349, Leu352, Val523, Ala527, and Met522 consistent with its selective COX-2 inhibitory profile. Among the phytochemicals, caffeic acid (Figure 4B) and ferulic acid (Figure 4C) demonstrated moderate binding affinities of −7.2 and −7.3 kcal/mol respectively. Both compounds occupied the same catalytic pocket as the control ligand and were primarily stabilized by multiple hydrogen-bond interactions, particularly involving residues Ser353, Gln192, Phe518, and Ser530 along with additional van der Waals contacts. The shared binding region with rofecoxib suggests that caffeic acid and ferulic acid may modulate COX-2 activity through interactions within the enzyme's active site.

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5. 2D interaction analysis against *NF-κB*:

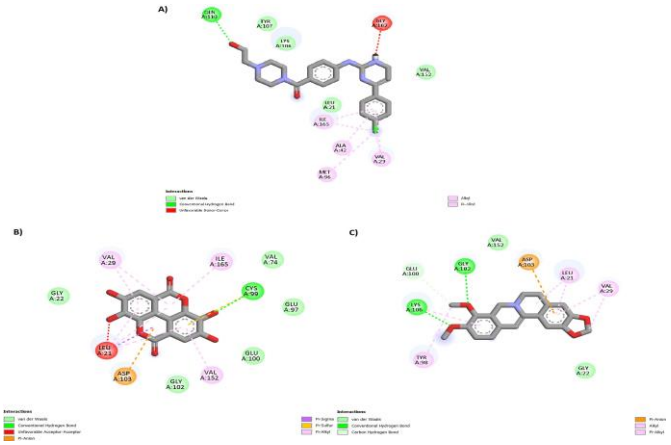

Figure 5: 2D interaction diagrams of NF-κB with (A) XNM, (B) ellagic acid, and (C) berberine.

Docking against NF-κB indicated that berberine exhibited the highest binding affinity with a docking score of −9.6 kcal/mol, followed by the control ligand XNM (−8.6 kcal/mol) and ellagic acid (−8.5 kcal/mol) (Figure 4). Two-dimensional interaction analysis revealed that the control compound XNM (Figure 5A) binds within the NF-κB DNA-binding region through a combination of hydrophobic and polar interactions, including contacts with residues Lys106, Tyr107, Gln110, Val29, and Leu21. Ellagic acid (Figure 5B) established multiple stabilizing hydrogen bonds with residues such as Cys99, Gly102, and Asp103, in addition to hydrophobic interactions, indicating strong polar complementarity within the binding pocket. In contrast, berberine (Figure 5C) interacted predominantly through electrostatic and aromatic interac- tions, including hydrogen bonding with Gly102 and Lys106 and π–anion interactions involving Asp103, along with extensive π–alkyl contacts with Leu21 and Val29.The overlap in binding regions and conservation of key interacting residues across all ligands suggest that ellagic acid and berberine occupy binding sites comparable to the control compound, supporting their potential to modulate NF-κB activity.

6. 2D interaction analysis against DNA gyrase:

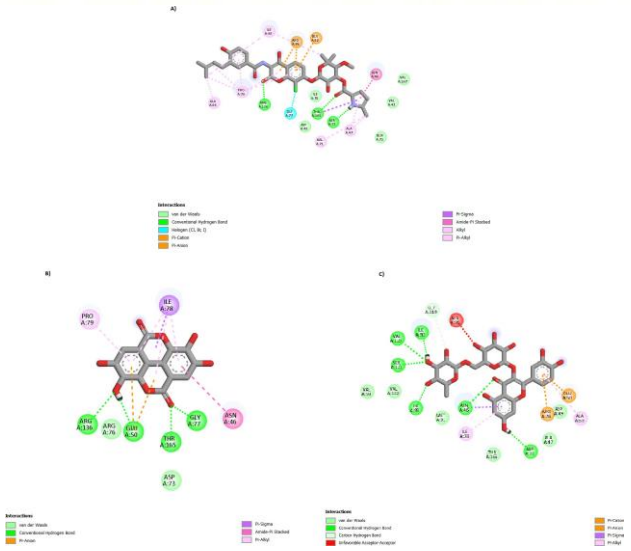

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Figure 6: 2D interaction diagrams of DNA gyrase with (A) chlorobiocin, (B) ellagic acid, and (C) rutin.

Docking studies against DNA gyrase showed that the reference inhibitor **chlorobiocin** exhibited the highest binding affinity **(−9.1 kcal/mol;** Figure 6A). Chlorobiocin occupied the **ATP-binding pocket** and was stabilized by a combination of **hydrogen bonding, π–cation/π–anion, and hydrophobic interactions,** involving key residues such as **Arg76, Glu50, Arg136, Thr165, Asp73, and Gly77.** Among the phytochemicals**, ellagic acid (Figure 6B)** and **rutin (Figure 6C)** displayed favorable binding energies of **−8.4 and −8.6 kcal/mol,** respectively. Ellagic acid interacted mainly through **hydrogen bonds and π–anion interactions,** while rutin formed **multiple hydrogen bonds and extensive van der Waals contacts,** consistent with its larger molecular structure. The shared binding region and conserved interacting residues suggest that both phytochemicals may interfere with ATP binding and inhibit DNA gyrase activity.

7. 2D interaction analysis against *TNFα*:

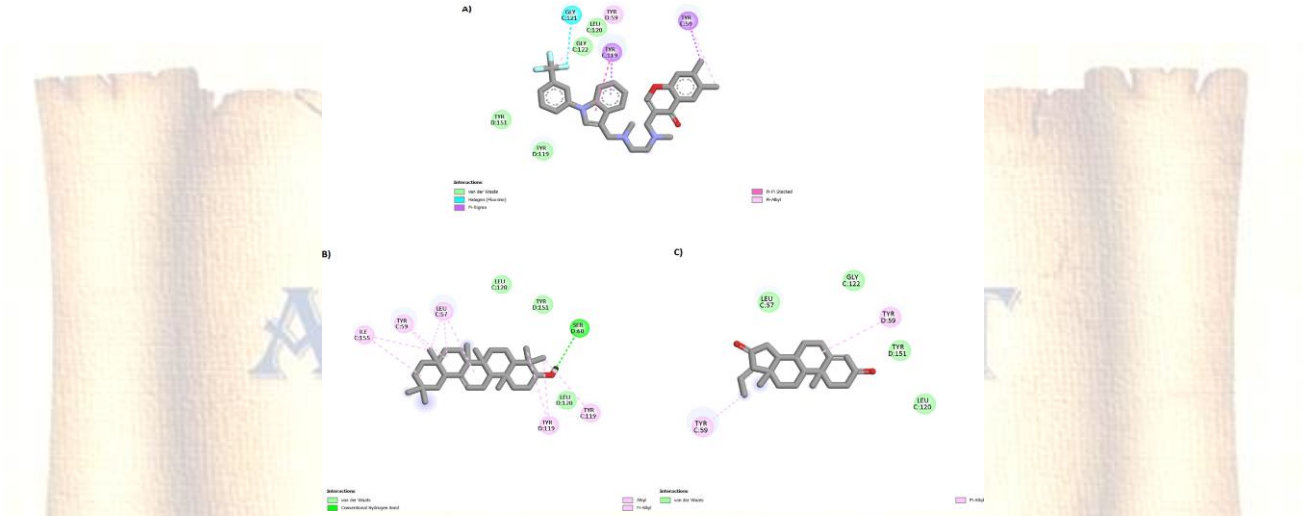

Figure 7: 2D interaction diagrams of *TNFα* with (A) chromenone derivative, (B) β-amyrin, and (C) guggulsterone E.

Docking analysis against tumor necrosis factor alpha (*TNFα*) revealed that the phytochemicals **β-amyrin** and **guggulsterone E** exhibited stronger binding affinities than the reference **chromenone derivative**, with docking scores of **−9.8 and −9.3 kcal/mol**, respectively, compared to **−8.0 kcal/mol** for the control (Figure 7). Two-dimensional interaction analysis showed that the chromenone derivative **(Figure 7A)** bound at the **TNF receptor-binding interface**, forming **π–π stacking, π–alkyl, and van der Waals interactions** with key residues such as **Tyr59, Tyr119, Leu120, and Gly122**. **β-Amyrin (Figure 7B)** occupied an overlapping region and was stabilized mainly by **hydrophobic and π–alkyl interactions**, with an additional **hydrogen bond with Ser60**, which may contribute to its enhanced affinity. **Guggulsterone E (Figure 7C)** also bound within the same interface, engaging predominantly through **hydrophobic and π–alkyl interactions** involving conserved residues including **Tyr59 and Leu120**.The shared binding region and conservation of interacting residues suggest that β-amyrin and guggulsterone E may interfere with **TNF–TNF receptor interactions**, supporting their potential role as *TNFα* modulators.

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Discussion:

Complicated gynecological syndromes have the features of abnormal hormonal, immune and microbial pathways, which make multi-target therapy inevitable. For instance, endometriotic lesions are under estrogen (ER_α) control and during chronic inflammation, NF-κB is hyperactivated in ectopic endometrium that enhances COX-2 and prostaglandin synthesis.[17] Endocrine disturbance and low-level inflammation are observed in PCOS. High TNF_α was reported in PCOS patients from a meta-analysis linking inflammatory cytokines to insulin resistance and hyperandrogenism. [18]. Inhibiting NF-κB, TNFα and COX-2 would also suppress cytokine storms and pain (e.g. by inhibiting prostaglandin synthesis), while inhibiting ER_α prevents estrogen-driven proliferation. It has been shown that one agent like curcumin can suppress together NF-κB, COX-2 and TNF_α[19], further indicating how a single agent can intervene into several cascades. For genital tract infections such as cervicitis and pelvic inflammatory disease, suppression of pathogen growth is an important therapeutic approach. Pathogens such as *Mycoplasma genitalium* are treated with antibiotics that target bacterial DNA gyrase, an enzyme with a critical role in bacterial DNA replication.[20] In practice, a drug or formulation that combines DNA-gyrase inhibition with host anti-inflammatory properties would target both the infection and its aftermath. The quinolone antibiotics are great at killing bacteria that use gyrase to replicate DNA, but uncontrolled inflammation can still damage the tissue and induce painful sensation. Simultaneous inhibition of the host NF-κB and TNF_α pathways acts to restrict this damage. As a consequence, the best treatments have to eliminate the infection while also dialing down the immune overreaction. This research demonstrates the interaction of MYRON's phytochemical binding poses with control ligands in at least one of five important targets; ER_α, COX-2, DNA gyrase, NF-κB and TNF_α providing molecular basis for ayurvedic formulation to be used traditionally on gynecological disorders. Broad-spectrum antibacterial activity of MYRON through DNA gyrase inhibitory multi-target polypharmacological profile explains its therapeutic efficacy in the treatment of reproductive tract infections by compounds like rutin, ellagic acid quercetin and guggulsterones. In the case of pelvic inflammatory disease, endometriosis and dysmenorrhea, MYRON showed higher activity at modulating the inflammation-related pathways, such as NF-κB (berberine), COX-2 (caffeic and ferulic acids) or TNF_α (triterpenoids like β-amyrin). In both endometriosis and PCOS, binding with ER_α by flavonoids and ellagic acid adds to hormone management in addition to anti-inflammatory effects and combined antibacterial/anti-inflammatory action is found for cervicitis and leucorrhea. Key compounds in MYRON, like ellagic acid and quercetin, interact with a wide range of biological targets. This multi-target approach demonstrates the kind of pharmacological redundancy, chemical diversity, and synergy that often gives natural formulations an edge over single-target synthetic drugs, potentially leading to better effectiveness, a broader safety margin, and fewer side effects. However, predictions from molecular docking studies have limitations and hence, further research will focus on biochemical, functional, cellular, pharmacokinetic, and clinical validation. These results provide a solid molecular basis for MYRON's traditional holistic benefits and hence could serve as a valuable complementary option alongside conventional therapies.

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Conclusion:

This molecular docking study successfully elucidates MYRON's multi-target mechanisms in gynecological disorders, demonstrating that 25 phytochemical constituents modulate five critical therapeutic targets with binding affinities from -9.8 to -5.5 kcal/mol. Key findings include β-amyrin's exceptional *TNFα* binding (-9.8 kcal/mol), berberine's potent NF-κB inhibition (-9.6 kcal/mol), and quercetin's strong COX-2 interaction (-9.6 kcal/mol), with several compounds exceeding pharmaceutical controls. The identification of multi-target modulators (ellagic acid, quercetin) validates MYRON's polypharmacological approach for managing RTIs (DNA gyrase inhibition), inflammatory conditions (NF-κB, COX-2, TNFα modulation), and hormonal disorders (ERα regulation). This computational validation bridges traditional ayurvedic wisdom with evidence-based medicine, positioning MYRON as an accessible solution for women's reproductive health. Future experimental validation, pharmacokinetic studies, and clinical trials will translate these molecular insights into optimized therapeutic protocols for gynecological care worldwide.

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Conflict of Interest

This study was carried out within the framework of the continuing research programs at Alarsin, Mumbai. The authors declare no conflicts of interest other than their employment with the organization. All authors participated in the conception and design of the study, analysis of data, and preparation of the manuscript, free from any external commercial influence.

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