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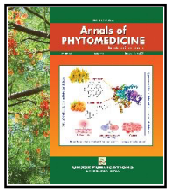

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In silico assessment of NF-κB protein inhibitors through molecular docking studies

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Abstract

Nuclear factor kappa B (NF-κB) is a pivotal transcription factor involved in inflammation, immune responses, and cancer progression. In the quest for safer and more effective therapeutic agents, this study employed molecular docking to screen 313 bioactive phytochemicals against NF-κB, aiming to identify potential natural inhibitors. Ligands were sourced from literature and public databases and prepared using ChemDraw, V Conf, and Open Babel, while the NF-κB protein (PDB ID: 1SVC) was retrieved from the RCSB Protein Data Bank and refined using BIOVIA Discovery Studio. Binding site prediction was achieved via PrankWeb and literature data. Docking was conducted with PyRx 0.8 using AutoDock Vina, and binding interactions were analysed in Discovery Studio. Results revealed that hypericin and withanolide exhibited the strongest binding affinities (–8.4 kcal/mol), surpassing standard NF-κB inhibitors such as olmesartan (–6.3 kcal/mol) and disulfiram (–3.5 kcal/mol). Other top-performing compounds included diosmin (– 8.3 kcal/mol), tomatidine, tubeimoside-I, and solanine (all –8.0 kcal/mol), each interacting with key NF-κB residues through hydrogen bonding and hydrophobic interactions. These phytochemicals, available from diverse medicinal plants, showed superior binding profiles, highlighting their therapeutic potential. Overall, the study underscores the promise of natural compounds in modulating NF-κB activity and supports their further investigation through molecular dynamics simulations and experimental validation. These findings provide a foundation for the development of phytochemical-based NF-κB inhibitors with potential applications in inflammation and cancer therapy.

1. Introduction

The nuclear factor kappa-light-chain-enhancer of activated B cells (NF-κB) protein complex plays a critical role in the regulation of various biological processes, including DNA transcription, cytokine production, immune responses, and cell survival (Liu *et al.,* 2017). This protein complex is essential for maintaining normal cellular function and is actively involved in the modulation of cell differentiation, proliferation, and immunological defense mechanisms (Egbuna *et al.,* 2022). However, dysregulation of the NF-κB pathway, whether through aberrant activation, over expression, or persistent signaling has been strongly associated with the onset and progression of numerous pathological conditions (Jayab *et al.,* 2024).

Specifically, abnormal NF-κB activity has been implicated in a wide range of diseases, including various cancers, inflammatory bowel disease, autoimmune disorders, chronic inflammation, gastritis, atherosclerosis, septic shock, viral infections, rheumatoid arthritis, and asthma (Vlahopoulos, 2017; de Gregorio *et al.,* 2020; Adetuyi *et al.,* 2022) (Figure 1). The broad involvement of NF-κB in these conditions is partly due to its ubiquitous presence in nearly all animal cell types and its complex interactions with numerous signaling pathways. These pathways are triggered by a variety of stimuli such as proinflammatory cytokines, reactive oxygen species (ROS), physical and chemical stress, ultraviolet (UV) radiation, heavy metals, oxidized low-density lipoprotein (LDL), and microbial or viral antigens (Adetuyi *et al.,* 2022).

Furthermore, constitutive activation of NF-κB has been shown to promote the transcription of anti-apoptotic and pro-survival genes, such as Bcl-2 and Bcl-XL, thereby contributing to tumour cell resistance to apoptosis and chemotherapeutic agents (Godwin *et al.,* 2013; Mehta *et al.,* 2013). This phenomenon is particularly evident in haematological malignancies such as acute myeloid leukaemia (AML), where more than 50% of patients exhibit constitutively active NF-κB, which enables leukemic cells to evade programmed cell death and supports their uncontrolled proliferation (Darwish *et al.,* 2019). In a study involving 103 AML patients, Darwish *et al.* (2019) used quantitative real-time polymerase chain reaction (RT-PCR) to evaluate NF-κB expression in bone marrow samples. Their findings revealed that 80.5% of the patients (83 out of 103) had elevated NF-κB expression levels compared to the control group, suggesting a strong correlation between NF-κB overexpression and AML pathogenesis.

Given its central role in disease mechanisms, NF-κB has emerged as a promising molecular target for therapeutic intervention. Notably, several herbal and dietary plant extracts have demonstrated potential *in vitro* for inhibiting NF-κB activity (Paur *et al.,* 2010). Among these, the citrus flavonoid nobiletin has been reported to suppress NF-κB signalling in experimental mouse models, highlighting the potential of natural products in modulating this critical pathway (Lin *et al.,* 2019).

This study aims to conduct an *in silico* assessment of NF-κB protein inhibitors through molecular docking studies. By computationally

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evaluating the binding affinity and interaction profiles of selected compounds with the NF-κB protein, this study seeks to identify potential lead molecules that could serve as effective inhibitors of NF-κB activity. This approach offers a cost-effective and time-efficient strategy for the preliminary screening of therapeutic candidates prior to experimental validation.

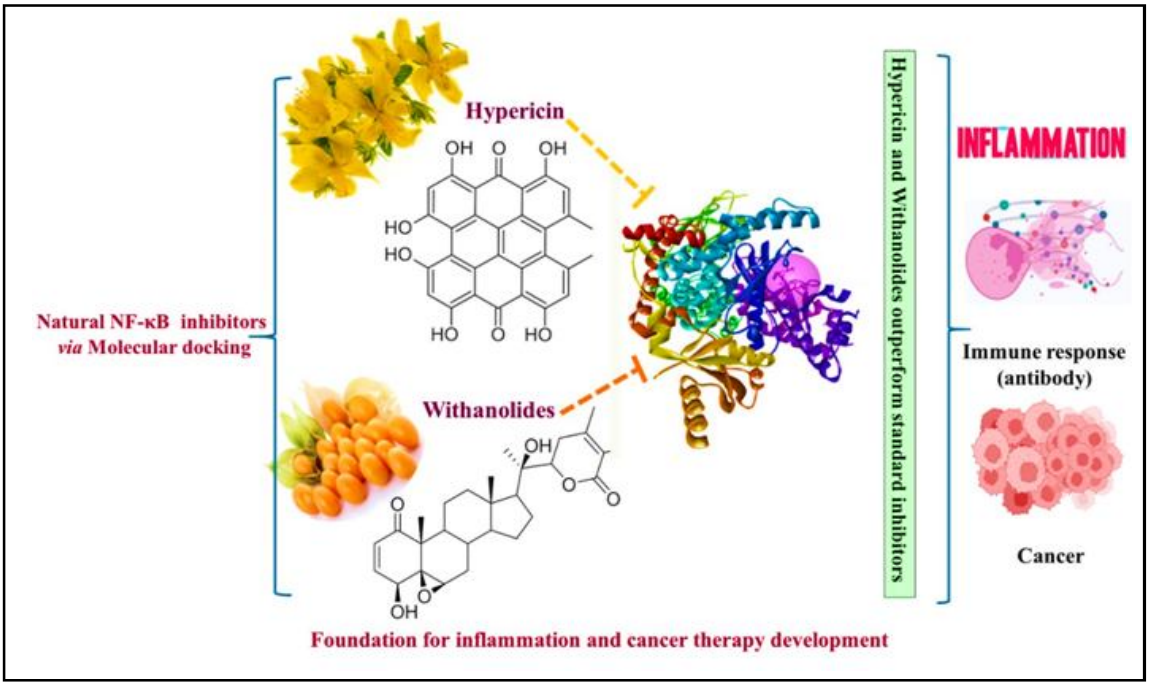

Figure 1: Effect of natural NF-κB inhibitors on inflammation, cancer and immune responses.

2. Materials and Methods

2.1 *In silico* study (Computational study)

2.1.1 Ligand curation and preparation

A comprehensive literature review was undertaken to identify phytochemicals previously reported to exhibit anticancer properties. Key references included works edited by Kumar and Egbuna (2018), Egbuna *et al.* (2019), and Saravanan *et al.* (2020). Based on this review, 313 phytochemicals and several conventional anticancer drugs were selected for further analysis. The 3D structures of these compounds, along with their corresponding compound IDs (CIDs), were retrieved from the NCBI PubChem database in SDF format.

For compounds that were not available in the PubChem or ChemSpider databases, their chemical structures were manually drawn using ChemDraw Ultra 12.0 (Cambridge Soft). To ensure compatibility with docking software, all ligands were converted from 2D to 3D SDF format using VConf software (Vera Chem LLC). Subsequently, all prepared ligand structures were merged into a single SDF file using Open Babel, to facilitate integration into the PyRx platform.

2.1.2 Protein preparation

The crystal structure of the NF-κB protein (specifically the p50 subunit) was obtained from the RCSB protein data bank (PDB) in .pdb format, using the PDB ID: 1SVC at a resolution of 2.6 Å. Protein preparation was carried out using BIOVIA Discovery Studio Visualizer 2021 (v21.1.0.20298; Dassault Systèmes), following the protocol described by Qasayme *et al.* (2019). During this process, all water molecules and heteroatoms were removed, while polar hydrogens were added to optimise the protein structure for docking (Banu *et al.,* 2025). The co-crystallised ligands within the protein were used to identify and model the active site. This modelled binding site was further validated by comparing it with experimental references and binding data.

2.1.3 Active site prediction

Active site prediction was conducted using a combination of structural data and bioinformatic tools. The active binding residues of NF-κB were predicted using a blend of scholarly references, the PDB database, BIOVIA Discovery Studio, and PrankWeb (P2Rank), an advanced machine learning-based web server designed for ligand binding site prediction. PrankWeb provided both visual prediction and center coordinates for potential binding pockets. Predictions from all sources were cross-compared, and consensus residues were selected for defining the active binding site. These predicted residues were used to configure the grid box for docking in PyRx, ensuring comprehensive coverage of the target binding site.

2.2 Molecular docking studies

Molecular docking simulations were performed using PyRx version 0.8, in accordance with the protocol described by Dallakyan and Olson (2015). PyRx is an integrated virtual screening tool that facilitates molecular docking of large compound libraries against target proteins. Ligands in 3D SDF format were loaded into the platform using its built-in Open Babel graphical interface. Energy minimisation of ligands was executed using the universal force field (UFF) and the

conjugate gradient algorithm, with 200 total steps. The step size was initially set to 1 and subsequently refined to 0.1 for greater precision.

Following minimisation, all ligands were converted to AutoDock-compatible pdbqt format to prepare for docking. The docking protocol was executed with an exhaustiveness level of 8, allowing for thorough exploration of potential binding conformations. Ligands were ranked based on binding affinity, with the most negative binding energy values indicating the strongest interaction. The ligand with the highest affinity was identified as the best potential inhibitor of NF-κB, based on its binding energy (Prasanth *et al.,* 2020).

Visualization and analysis of ligand protein interactions at the optimal docking poses were carried out using BIOVIA Discovery Studio Visualizer 2021. Validation of the docking procedure was also undertaken to ensure the accuracy and reliability of the results.

NF-κB X: 32.7472, Y: 23.9276, Z: 35.4777 X: 35.9463, Y: 35.3993, Z: 31.5206 60, 243, 244, 246, 274, 275

3. Results

The molecular docking analysis of 313 bioactive phytochemicals against the NF-κB protein (PDB ID: 1SVC) identified several compounds with strong binding affinities, highlighting their potential as natural inhibitors. Hypericin and withanolide exhibited the highest binding energies (– 8.4 kcal/mol), surpassing standard inhibitors olmesartan (– 6.3 kcal/mol) and disulfiram (– 3.5 kcal/mol). Other top-performing compounds included diosmin (-8.3 kcal/mol), tomatidine, tubeimoside-I, and solanine (all -8.0 kcal/mol). These ligands interacted with key residues in the NF-κB binding pocket, such as Arg60, Lys244, and Glu275, through hydrogen bonds and hydrophobic interactions. Table 1 summarises the molecular docking scores, PubChem IDs, and natural sources of the top 20 phytochemicals and reference drugs. Notably, phytochemicals consistently demonstrated stronger binding affinities compared to synthetic controls. For instance, venetoclax (-9.1 kcal/mol) and daunorubicin (-8.0 kcal/mol), conventional anticancer drugs, showed competitive binding but are associated with higher toxicity profiles.

Table 1: Molecular docking scores of NF-κB protein inhibitors

S.No.	Compound	Pub Chem ID	Binding energy (kcal/mol)	Sources
1.	Hypericin	3663	– 8.4	Genera *Hypericum* (Saint John's wort)
2.	Withanolide	53477765	– 8.4	Nightshade plant family, *e.g., Datura, Solanum, Withania, Jaborosa*
3.	Diosmin	5281613	– 8.3	Citrus fruits (oranges and lemons) and peel extracts, hyssop, figwort
4.	Tomatidine	65576	-8.0	Stems and leaves of tomato plants, and in the fruits at low concentrations
5.	Tubeimoside-I	51346132	– 8.0	*Bolbostemma paniculatum*
6.	Solanine	262500	– 8.0	Nightshade family, *e.g.,* genus *Solanum e.g.* potato, tomato, eggplants
7.	Mezerein	24832075	– 7.8	*Daphne mezereum* (Thymelaeaceae) and related plants
8.	Vicenin-2	442664	– 7.8	Sweet oranges, *Ocimum sanctum,* buckwheats, fenugreeks
9.	Neohesperidin	442439	– 7.8	Citrus fruits (*e.g.,* oranges and lemons), peel extracts and inedible ones
10.	Polyphyllin	72960700	– 7.7	*Paris polyphylla*
11.	Cycloartocarpesin	15224382	– 7.6	Genera *Artocarpus, e.g., Artocarpus heterophyllus* (Jackfruit)
12.	Platycodin	162859	-7.6	*Platycodon grandiflorus*
13.	Hypoxoside	13785311	-7.5	*Hypoxis obtuse,* star-grass
14.	Glycyrrhizic acid	14982	– 7.5	Licorice (Root extract), *Glycyrrhiza glabra* (Fabaceae)
15.	Isovitexin	162350	-7.5	Pigeon pea, Passion flower, bamboo, mimosa (champagne + citrus juice), wheat leaves, rice hull of *Oryza sativa*
16.	Baicalin	64982	– 7.4	Plants in Genus *Scutellaria* and in *Oroxylum indicum*
17.	α-Carotene	6419725	– 7.4	Carrots, sweet potatoes, pumpkin, avocado, green beans, spinach
18.	Cleistanthin	4485134	– 7.4	*Cleistanthus collinus*
19.	Silymarin	5213	– 7.4	Seeds of milk thistle *Silybum marianum* (L.)
20.	Verbascoside	5281800	– 7.4	Plants of Verbenaceae, Olive, Lamiaceae family
21.	Vitexin	5280441	– 7.4	Leaves of *Phyllostachys nigra* (Bamboo), passion flower, Pearl millet
Standard NF-κBdrug				
1.	Olmesartan	158781	– 6.8	NF-κB inhibitor
2.	Disulfiram	3117	– 3.5	NF-κB inhibitor
Other top performing anticancer drugs				
3.	Venetoclax	49846579	– 9.1	Bcl-2 inhibitor
4.	Daunorubicin	30323	_ 8.0	DNA intercalation and inhibits macromolecular biosynthesis
5.	Guadecitabine	135564655	– 7.8	DNA (cytosine-5)-methyltransferase 1 (DMNT1) inhibitor
6.	Sonidegib	24775005	– 7.6	SMO inhibitor

The docking results also revealed structural diversity among the top ligands, including flavonoids (*e.g.,* diosmin, vicenin), glycoalkaloids (*e.g.,* solanine, tomatidine), and triterpenoids (*e.g.,* withanolide). These compounds originated from medicinal plants such as *Hypericum perforatum*, *Withania somnifera*, and *Solanum* species.

4. Discussion

The superior binding affinities of hypericin and withanolide suggest their potential to competitively inhibit NF-κB activation. Hypericin's mechanism aligns with prior studies showing its suppression of IκBα phosphorylation, thereby blocking NF-κB nuclear translocation (Novelli *et al.,* 2020). Similarly, withanolide's interaction with residues critical for IKK binding may explain its anti-inflammatory and anticancer effects (White *et al.,* 2016). The strong performance of diosmin (– 8.3 kcal/mol) correlates with its documented role in downregulating proinflammatory cytokines *via* NF-κB inhibition in hepatic models (Hassanein *et al.,* 2025).

The glycoalkaloids tomatidine and solanine, though less studied, showed binding profiles comparable to established inhibitors. Their predicted suppression of p65 nuclear translocation and COX-2 expression (Chiu and Lin, 2008) underscores the need for experimental validation. Similarly, tubeimoside-I's affinity (– 8.0 kcal/mol) supports its reported dual inhibition of NF-κB and PI3K/Akt pathways in cancer (Wang *et al.,* 2022).

Notably, the phytochemicals' binding energies exceeded those of synthetic drugs like olmesartan, suggesting natural compounds may offer safer alternatives with fewer off-target effects. However, computational results must be contextualised with pharmacokinetic and toxicity data. For example, solanine, while poteoptimisent, has known toxicities at high doses, necessitating structure-activity relationship studies to optimise safety.

The diversity of plant sources from citrus peels to nightshades highlights the untapped potential of natural products in drug discovery. These findings align with trends advocating phytochemicals as adjuncts to synthetic therapies, particularly for chronic inflammatory diseases (Paur *et al.,* 2010). Future work should integrate molecular dynamics simulations to assess binding stability and *in vitro* assays to confirm NF-κB suppression.

5. Conclusion

This study demonstrates the high binding affinity of several phytochemicals to the NF-κB protein, particularly hypericin, withanolide, and diosmin, which showed superior docking scores compared to conventional inhibitors. These results, supported by existing literature, provide a scientific basis for further *in vitro* and *in vivo* evaluations of these compounds as natural NF-κB inhibitors. Their application could be pivotal in managing inflammation-driven diseases such as cancer, arthritis, and autoimmune disorders. It is also recommended that the natural sources of these compounds be explored further for therapeutic purposes, while edible sources should be consumed regularly as a preventive mechanism against diseases.

Conflict of interest

The authors declare no conflicts of interest relevant to this article.

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