

Neem for PCOS: Computational Docking Insights



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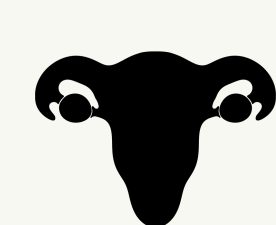
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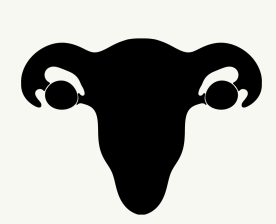
INTRODUCTION

PCOS impacts 8-13% of women during their reproductive age. It contributes to menstrual irregularities, hirsutism, anovulatory infertility, and poses risks like endometrial cancer and metabolic disturbances. Neem leaf and its constituents have been demonstrated to exhibit immunomodulatory, anti-inflammatory, antihyperglycaemic, antiulcer, antimalarial, antifungal, antibacterial, antiviral, antioxidant, antimutagenic and anticarcinogenic properties. TNF - α (Tumor Necrosis Factor alpha) and TNFR2 (Tumor Necrosis Factor Receptor 2) are the target proteins involving the pathways for the elevated levels of PCOS. Their inhibition would maintain the blood brain barrier and permit promising outcome.

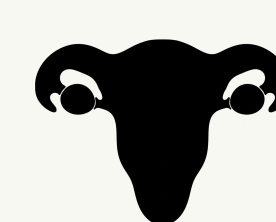
METHODOLOGY



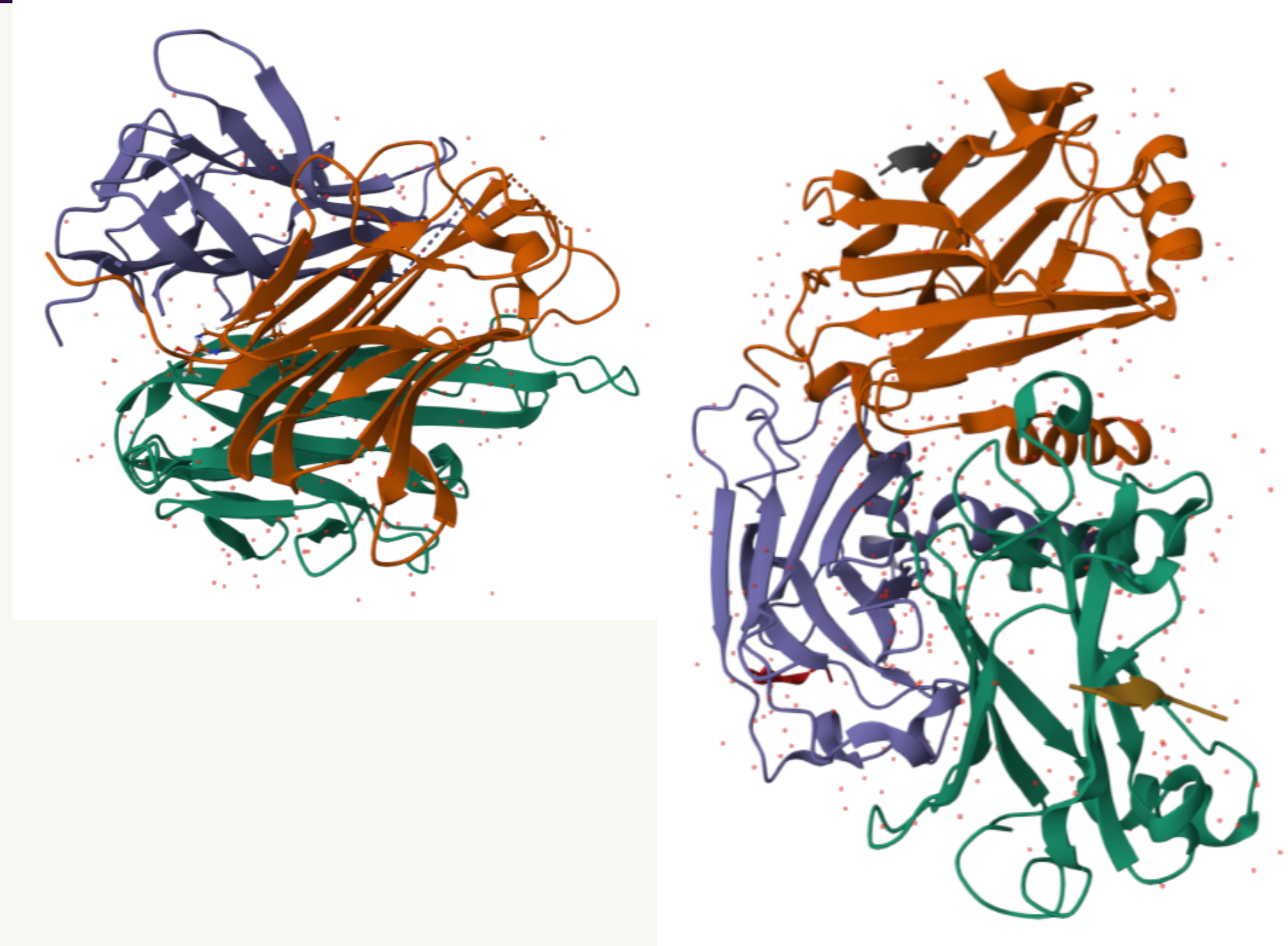
Protein and Ligand Preparation



Docking Analysis



MM - GBSA Analysis



RESULTS

Protein	Compound	Docking score	Glide score
TNF - α	Scopoletin	-7.914	-7.927
TNFR - 2	Nimocinolide	-6.898	-6.797

Protein	Compound	Binding energy (kcal/mol)
TNF - α	Scopoletin	-46.27
TNFR - 2	Nimocinolide	-68.535

CONCLUSION

The 55 phytochemicals obtained from Neem leaf revealed promising outcomes for potential therapeutic interventions in Polycystic Ovarian Disorder (PCOD). Notably, Scopoletin and Nimocinolide emerged as standout candidates, exhibiting remarkable efficacy in the analyses. Moreover, the Molecular mechanics with generalised born and surface area solvation (MM/GBSA) highlighted that Nimocinolide has a potential binding energy specificity and then Scopoletin. As we venture into future research endeavors, Neem holds promise as a valuable asset in the ongoing pursuit of effective treatments for PCOD.

REFERENCES

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