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Bioinformatics analysis of *Gymnema sylvestre* and *Withania somnifera* on insulin resistance pathway targets

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INTRODUCTION

Gymnema sylvestre *and* ***Withania somnifera*** are traditional medicinal plants with potential antidiabetic properties. This study employs molecular docking and bioinformatics approaches to investigate their interactions with key **insulin resistance** pathway targets. Insulin resistance represents a critical metabolic dysfunction underlying type 2 diabetes mellitus, characterized by impaired cellular response to insulin and disrupted glucose metabolism. Traditional medicinal plants offer promising therapeutic alternatives for managing metabolic disorders, with *Gymnema sylvestre* and *Withania somnifera* emerging as potential pharmacological interventions. *Gymnema sylvestre*, known as the "sugar destroyer" in Ayurvedic medicine, and *Withania somnifera*, commonly referred to as Ashwagandha, have demonstrated significant potential in modulating metabolic pathways. Despite extensive traditional use, their molecular mechanisms in addressing insulin resistance remain incompletely understood.

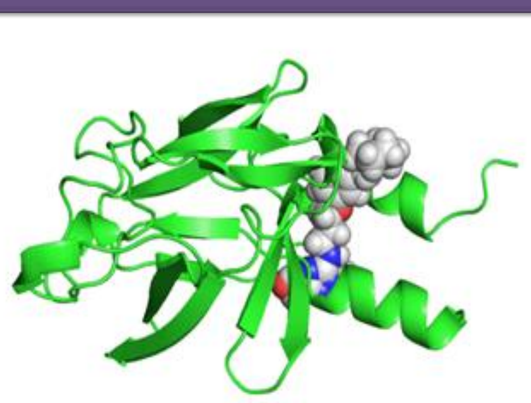
METHOD

Protein-protein interaction studies

Molecular Docking
AnalysisTargets: Insulin Receptor (IR), PPAR-γ, AKT/PKB
Molecular Docking Software: AutoDock Vina
Protein Structures: Obtained from Protein Data Bank (PDB)
Ligands: Active compounds from G. sylvestre and W. somnifera

Key Active Compounds
Gymnema sylvestre
Gymnemagenin
Gymnemic acids
Beta-carotene
Withania somnifera
Withaferin A
Withanolides
Withanone

RESULTS & DISCUSSION



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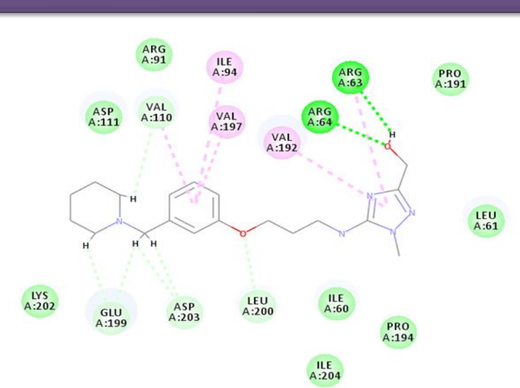

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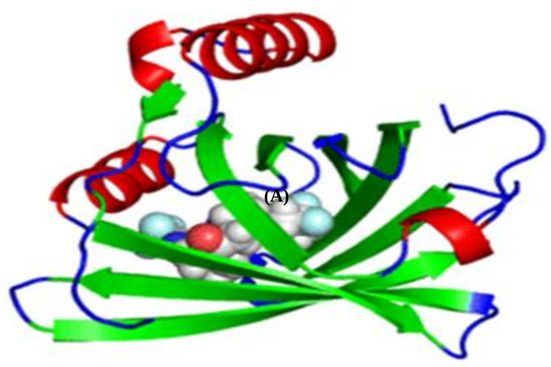

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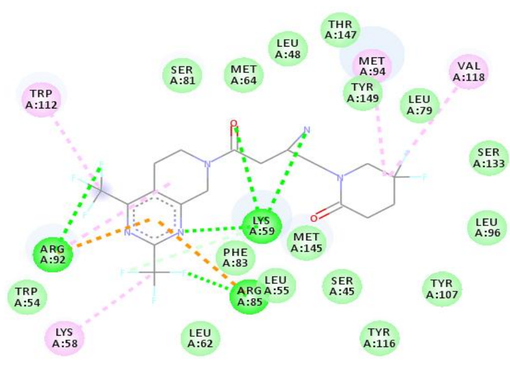

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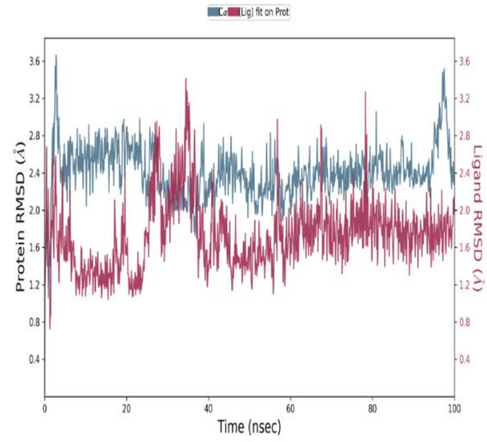
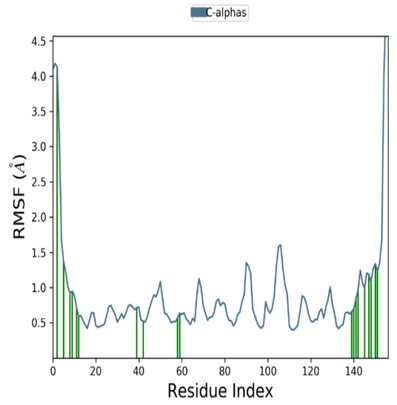
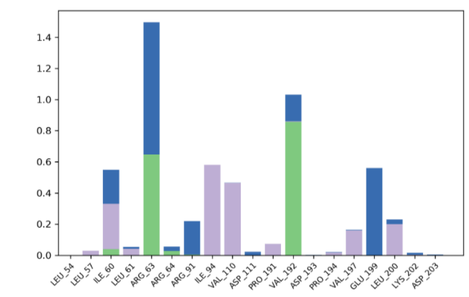
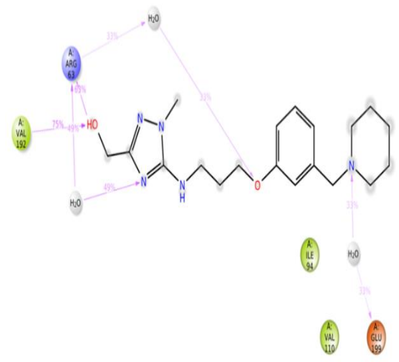




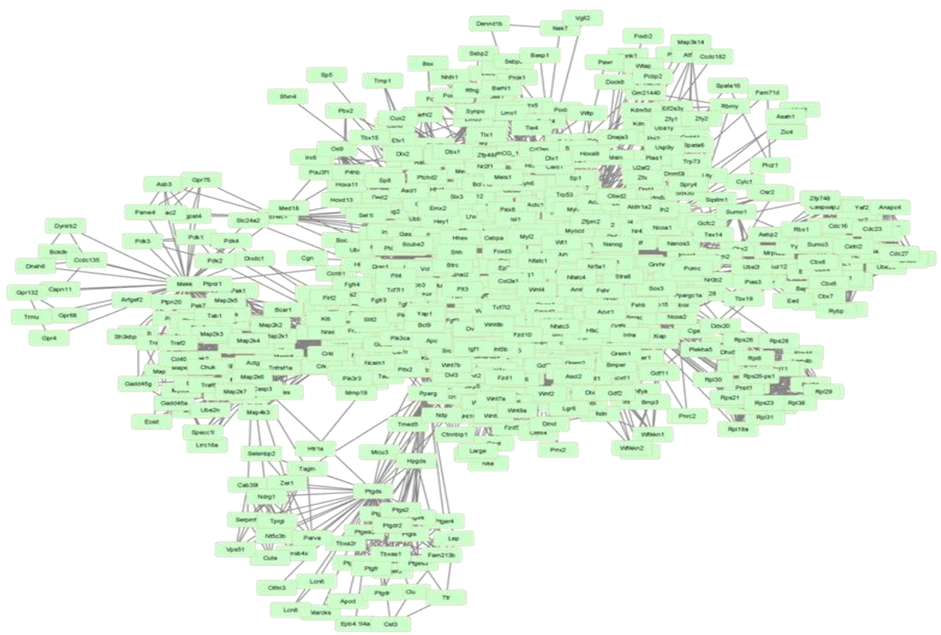




Binding Affinity (kcal/mol)

Compound	Insulin Receptor	PPAR-γ	AKT/PKB
Gymnemagenin	-7.2	-6.8	-7.5
Withaferin A	-8.1	-7.6	-8.3

PPI for the analyzing few proteins involved in the pathway



CONCLUSION

Both plants demonstrate significant molecular interactions with insulin resistance pathway targets. Withaferin A shows stronger binding affinity compared to Gymnemagenin. Molecular docking suggests potential therapeutic applications in managing insulin resistance. The increased prevalence of IR and its critical role in a number of diseases has created an urgent need to better understand the mechanisms underlying the pathogenesis of IR and how they interplay with genetics and different environments, particularly dietary.

FUTURE WORK

In vitro validation
Comprehensive clinical trials
Detailed mechanism of action studies