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Unraveling the Anti-diabetic Potential of *Annona squamosa*: GC-MS and Molecular Docking Insights

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SUMMARY. The global burden of diabetes demands exploration of novel therapeutic options. Traditional plants offer untapped potential, with *Annona squamosa* showing promising anti-diabetic activity. This study aimed to identify bioactive compounds from these plants and evaluate their potential interaction with key anti-diabetic targets using GC-MS and molecular docking. Plant extracts were analysed by GC-MS to identify and characterize bioactive compounds. The identified compounds were docked with insulin receptor protein associated with type 2 diabetes mellitus pathogenesis. Binding affinities and interaction patterns were analysed. GC-MS revealed diverse bioactive compounds in methanolic extracts of *Annona squamosa,* including phenolic acids, terpenes and alkaloids. Molecular docking demonstrated promising binding affinities of several compounds with the target proteins. Key interactions included hydrogen bonding, hydrophobic interactions, and π-π stacking. This study identified potential anti-diabetic compounds from *Annona squamosa.* The docking and network pharmacological results suggest their potential to modulate key enzymes and receptors involved in glucose homeostasis. Further *in vitro* and *in vivo* studies are warranted to validate these findings and explore their therapeutic potential for diabetes management.

RESUMEN. La carga mundial de diabetes exige la exploración de nuevas opciones terapéuticas. Las plantas tradicionales ofrecen un potencial sin explotar, y *Annona squamosa* muestra una prometedora actividad antidiabética. Este estudio tuvo como objetivo identificar compuestos bioactivos de estas plantas y evaluar su posible interacción con dianas antidiabéticas clave mediante GC-MS y acoplamiento molecular. Los extractos de plantas se analizaron mediante GC-MS para identificar y caracterizar compuestos bioactivos. Los compuestos identificados se acoplaron con la proteína del receptor de insulina asociada con la patogénesis de la diabetes mellitus tipo 2. Se analizaron las afinidades de unión y los patrones de interacción. La GC-MS reveló diversos compuestos bioactivos en extractos metanólicos de Annona squamosa, incluidos ácidos fenólicos, terpenos y alcaloides. El acoplamiento molecular demostró afinidades de unión prometedoras de varios compuestos con las proteínas diana. Las interacciones clave incluyeron enlaces de hidrógeno, interacciones hidrofóbicas y apilamiento π-π. Este estudio identificó posibles compuestos antidiabéticos de *Annona squamosa*. Los resultados farmacológicos de acoplamiento y de red sugieren su potencial para modular enzimas y receptores claves involucrados en la homeostasis de la glucosa. Se justifican más estudios *in vitro* e *in vivo* para validar estos hallazgos y explorar su potencial terapéutico para el manejo de la diabetes.

KEYWORDS: *Annona squamosa*, anti-diabetic, GC-MS, insulin, molecular docking, network pharmacology, protein.

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