

Baicalin And Caffeic Acid Target CLK1 To Mitigate Tau Hyperphosphorylation In Alzheimer's Disease

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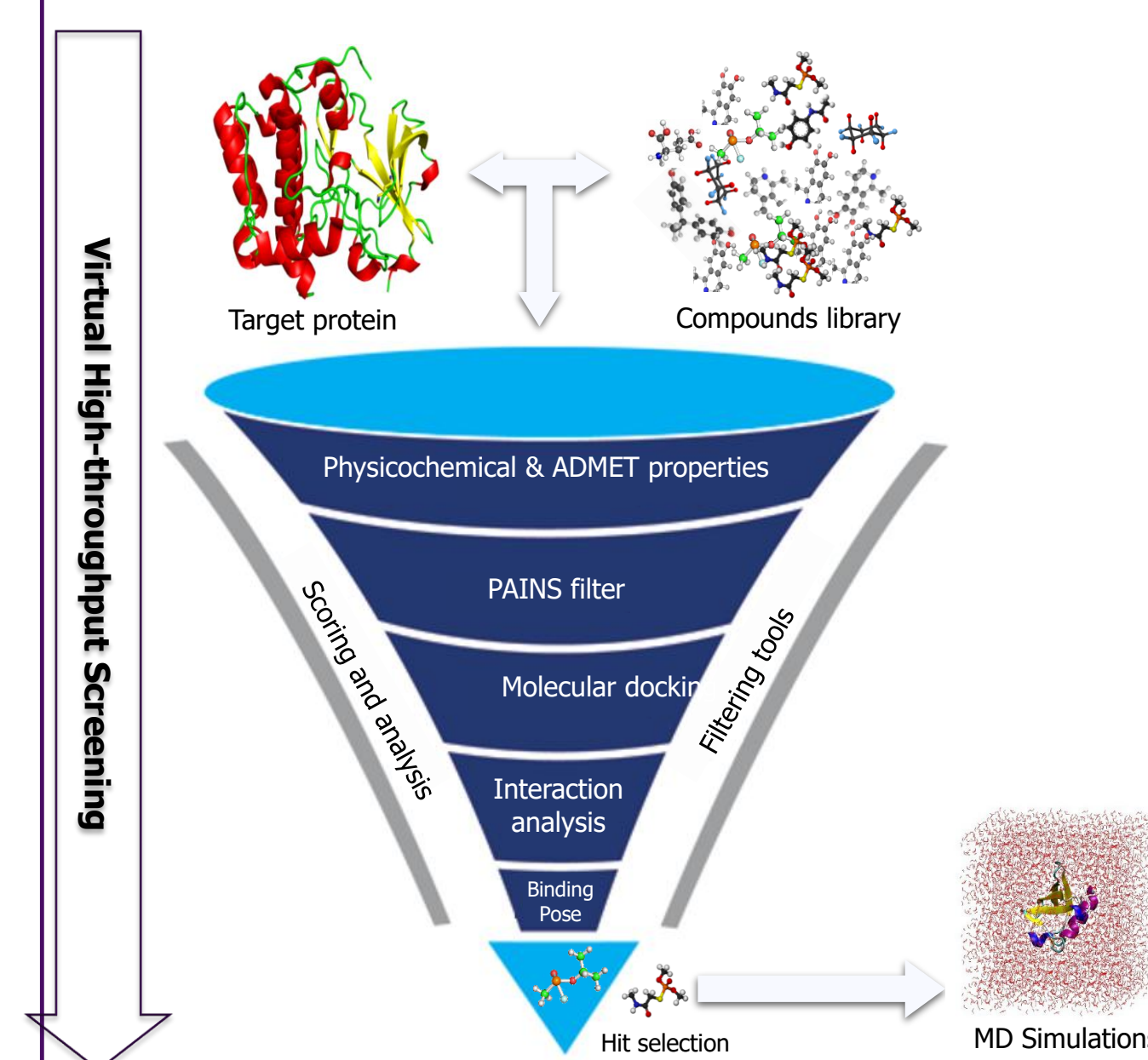
KEY TAKEAWAYS

- ✓ Baicalin and caffeic acid are novel CLK1 inhibitors.
- ✓ CLK1 inhibition reduces tau-associated toxicity.
- ✓ Natural compounds show promise for Alzheimer's disease therapy.

INTRODUCTION

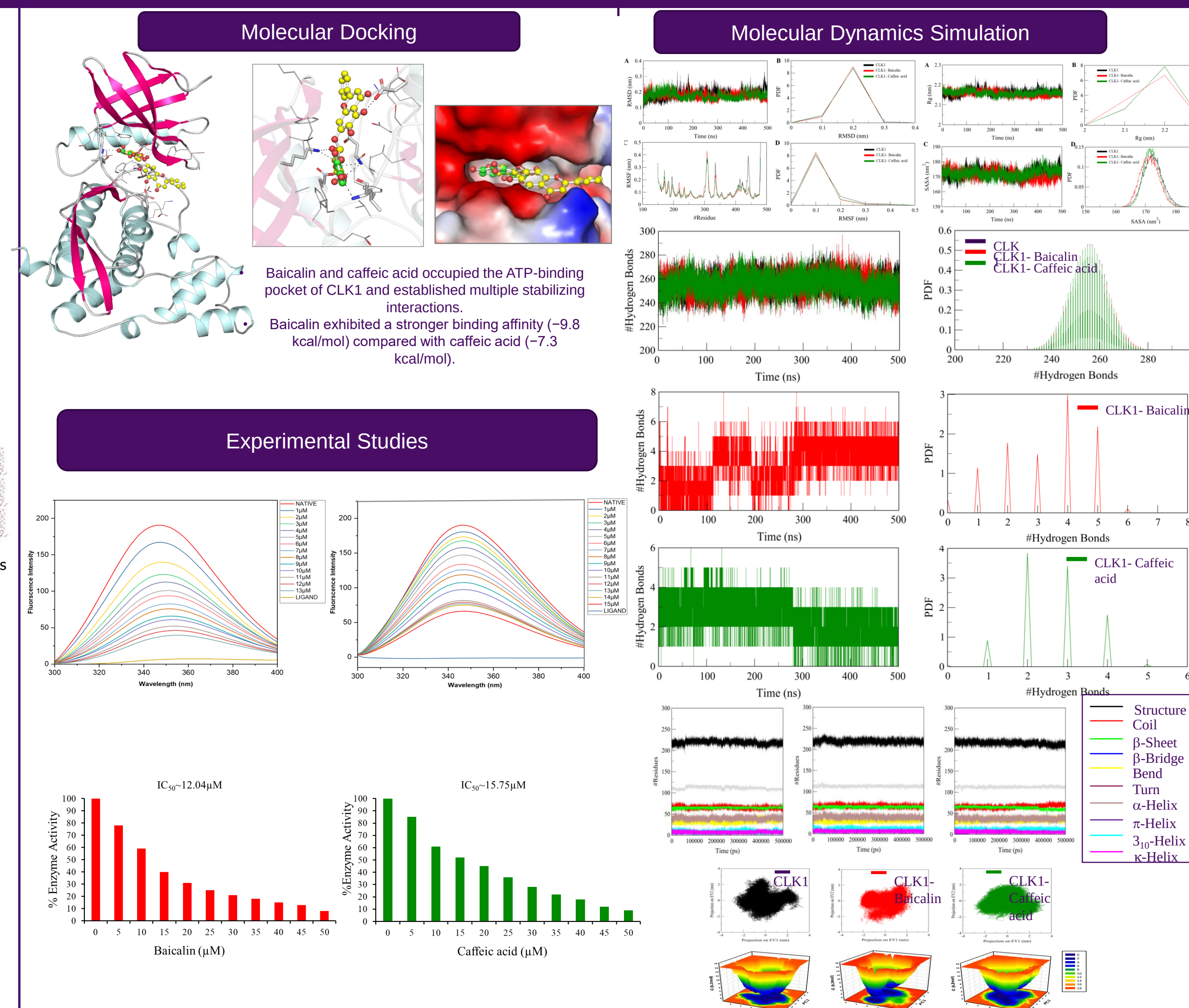
Alzheimer's disease (AD) is characterized by progressive cognitive decline and pathological tau hyperphosphorylation. Cdc2-like kinase 1 (CLK1), a serine/threonine kinase involved in RNA splicing regulation, has emerged as a potential therapeutic target due to its role in tau phosphorylation. This study investigated natural phytochemicals as CLK1 inhibitors and identified baicalin (BA) and caffeic acid (CA) as promising lead compounds.

METHODS



- Phytochemicals were screened against CLK1 using molecular docking.
- Binding stability was assessed through 500 ns molecular dynamics simulations.
 - Protein–ligand interactions were validated by fluorescence spectroscopy.
 - ATPase and kinase inhibition assays were performed to evaluate CLK1 inhibition.
 - Binding affinity and inhibitory potency were determined experimentally.

RESULTS



CONCLUSION

- BA and CA exhibited strong binding affinity and stable interactions with the catalytic pocket of CLK1, as supported by molecular docking and molecular dynamics simulations.
- Experimental studies, including fluorescence binding, ATPase inhibition, kinase inhibition, and cell viability assays, confirmed the effective inhibition of CLK1 and demonstrated protection against tau-associated cytotoxicity.
- The study identified BA and CA as promising natural CLK1 inhibitors that may reduce tau hyperphosphorylation and represent potential lead compounds for AD therapy.

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