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POSTER COMMUNICATION · PHARMACOLOGY & THERAPEUTICS

AI-Powered Ligand-Based Design Targeting YCK1 and YCK2 in Saccharomyces cerevisiae: Implications for Modulating Kinase Signaling Pathways in Drug Discovery

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KEY MESSAGES

1. AI-powered ligand-based design effectively identifies potential inhibitors targeting YCK1 and YCK2 kinases.
2. Molecular docking and dynamics simulations confirm strong and stable ligand binding to YCK1 active sites.
3. ADMET analysis supports favorable pharmacokinetic properties, making these ligands promising drug candidates.

ABSTRACT

Introduction. This study utilizes AI-powered ligand-based design to target YCK1 and YCK2 in Saccharomyces cerevisiae to discover small-molecule inhibitors that modulate kinase signaling pathways. These kinases are potential drug targets due to their role in critical signaling pathways involved in cancers and neurodegenerative diseases.

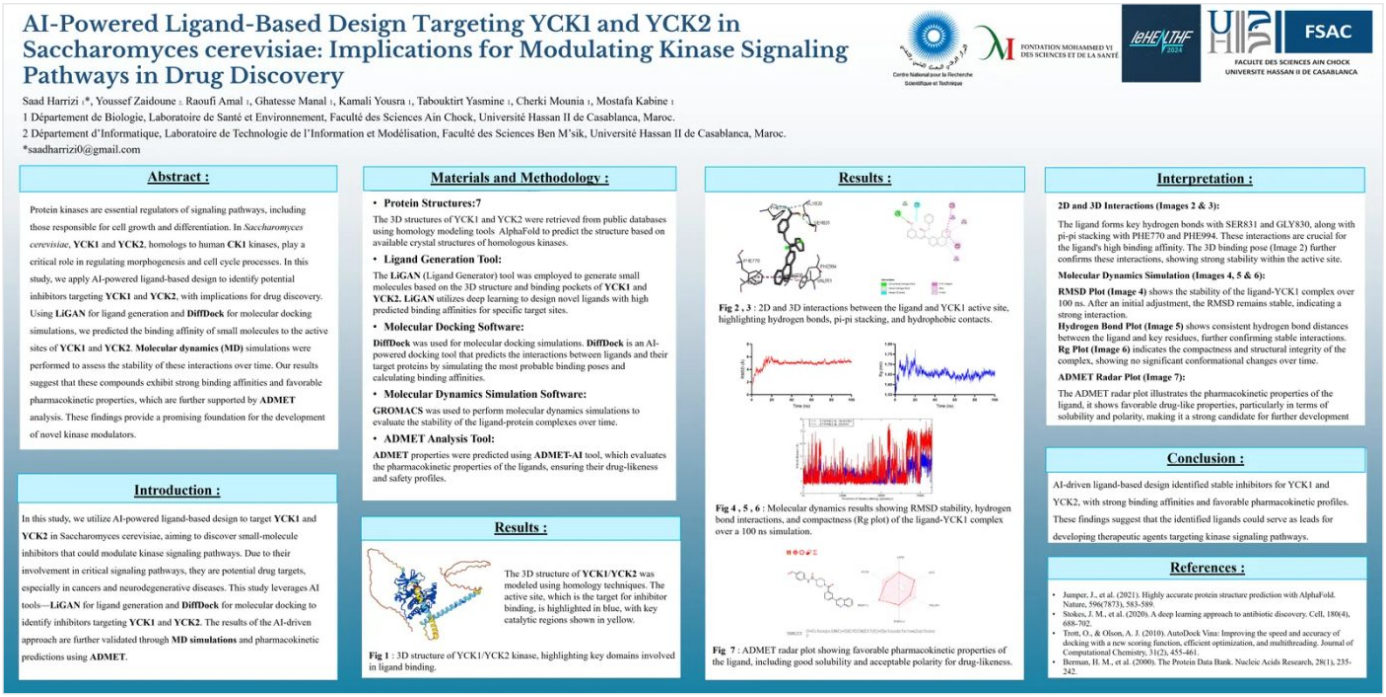
Materials and methods. The 3D structures of YCK1 and YCK2 were obtained using homology modeling with AlphaFold. Ligands were generated using the LiGAN tool, which employs deep learning to design novel ligands with predicted high binding affinities. Molecular docking simulations were performed using DiffDock to predict ligand-protein interactions. Molecular dynamics simulations with GROMACS assessed the stability of ligand-protein complexes. ADMET properties were predicted using the ADMET-AI tool to evaluate pharmacokinetic profiles and drug-likeness.

Results. The 3D structure of YCK1/YCK2 was modeled highlighting key domains for ligand binding. Docking and molecular dynamics simulations showed strong binding affinities and stable interactions between ligands and YCK1 active site residues SER831 and GLY830, supported by hydrogen bonding, pi-pi stacking, and hydrophobic contacts. RMSD, hydrogen bond, and Rg plots confirmed complex stability over 100 ns. ADMET radar plots indicated favorable pharmacokinetic properties, including good solubility and polarity, supporting drug-like characteristics.

Conclusion. AI-driven ligand-based design identified stable inhibitors for YCK1 and YCK2 with strong binding affinities and favorable pharmacokinetic profiles. These ligands could serve as leads for developing therapeutic agents targeting kinase signaling pathways.

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