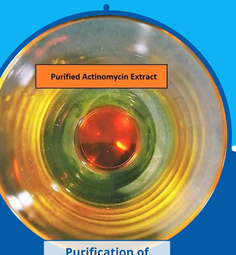
***In vitro* and *in silico* evaluations** of actinomycin X_2 and actinomycin D as potent anti-tuberculosis agents

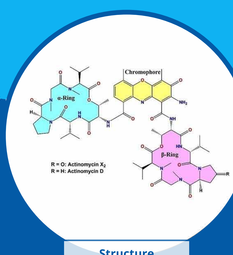
Production of Actinomycins



Purification of Actinomycins

BACKGROUND

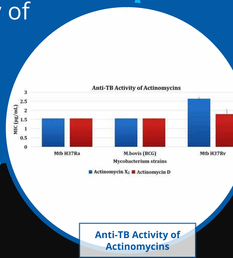
Multidrug-resistant tuberculosis (MDR-TB) is one of the world's most devastating contagious diseases and is caused by the *MDR-Mycobacterium tuberculosis* (MDR-Mtb) bacteria. It is essential to identify novel anti-TB drug candidates and target proteins to treat MDR-TB.



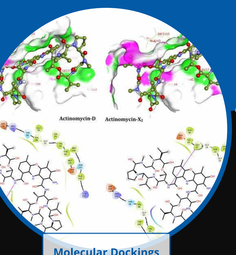
Structure Elucidation of Actinomycins

METHODS

In vitro and *in silico* studies were used to investigate the anti-TB potential of two newly sourced actinomycins, actinomycin-X_2 (act-X_2) and actinomycin-D (act-D), from the *Streptomyces smyrnaeus* strain UKAQ_23 (isolated from the Jubail industrial city of Saudi Arabia).



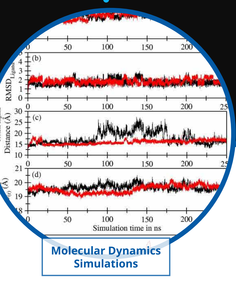
Anti-TB Activity of Actinomycins



Molecular Dockings

RESULTS

Our results suggest that both actinomycins X_2 and D are highly potent anti-TB drug candidates.



Molecular Dynamics Simulations

CONCLUSION

Our results show that act-X_2 is better able to antagonistically interact with the protein kinase PknB target than act-D, and thus has more potential as a new anti-TB drug candidate.

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