

In Silico Design of Novel *Artocarpus altilis*-Derived Compounds Targeting the c-Myc/Max Heterodimer

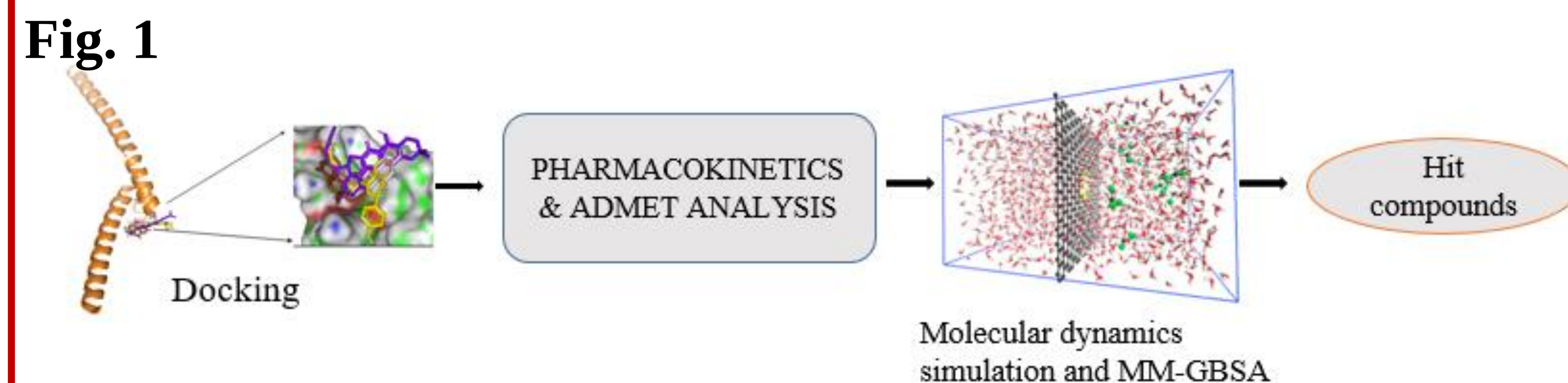
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Background and Objectives

- The c-Myc transcription factor is overexpressed in up to 70% of human cancers, but its unstructured nature makes it undrugable. (Miller *et al.*, 2012)
- c-Myc Must form heterodimer with Max protein to drive cancer. (Duffy *et al.*, 2021)
- We investigate a novel therapeutic approach by screening natural compounds from breadfruit (*Artocarpus altilis*) to inhibit the c-Myc/Max interaction.

Methodology



TARGET DETAILS

PDB ID :6G6K

Reference: Alisertib

Validation: 100 ns MD simulation

POST SIMULATION ANALYSIS

RMSD, RMSF,ROG,SASA

Key results

Fig.2

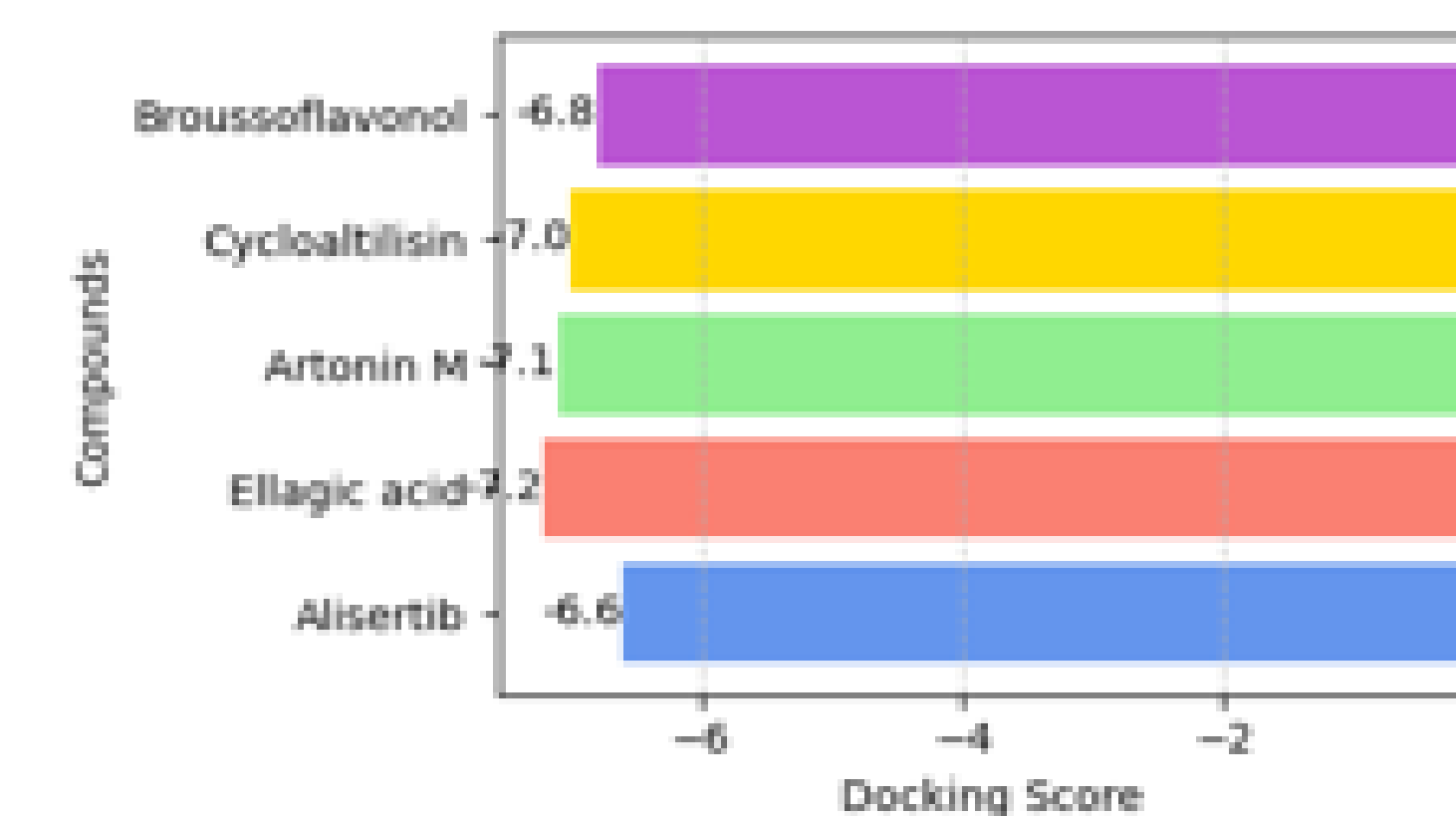


Fig.3

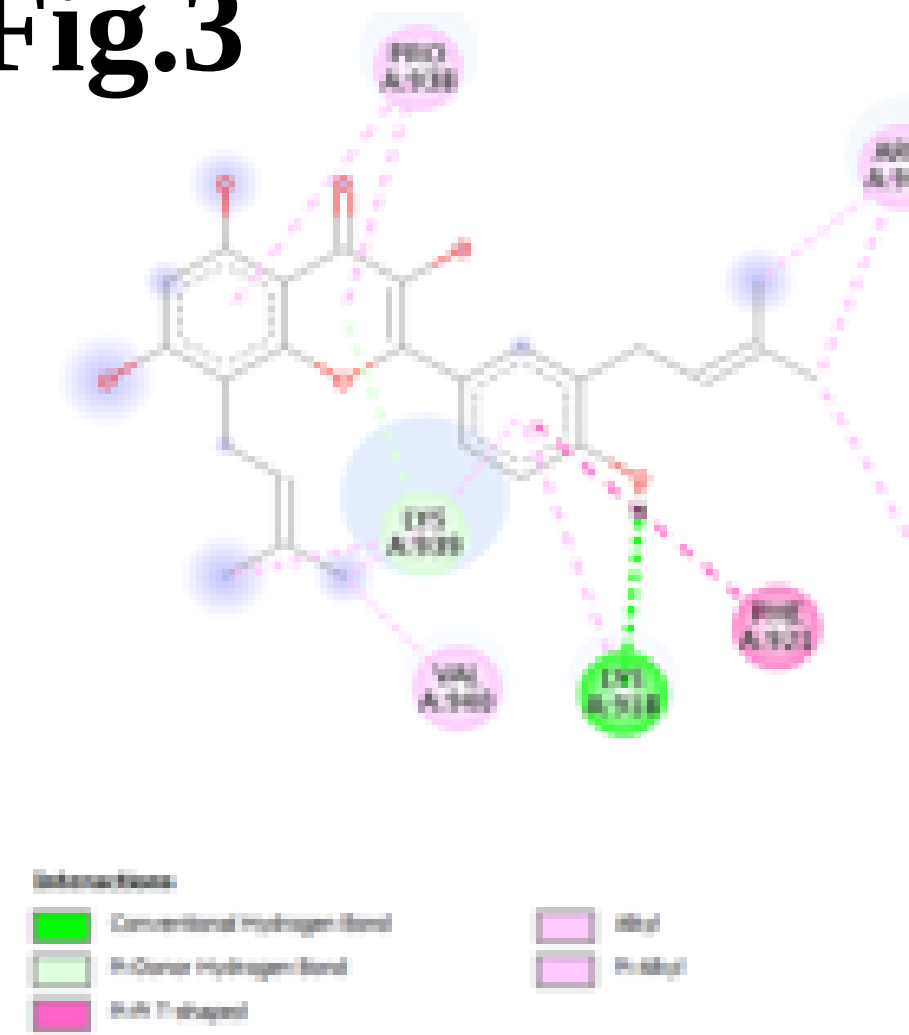


Fig.6

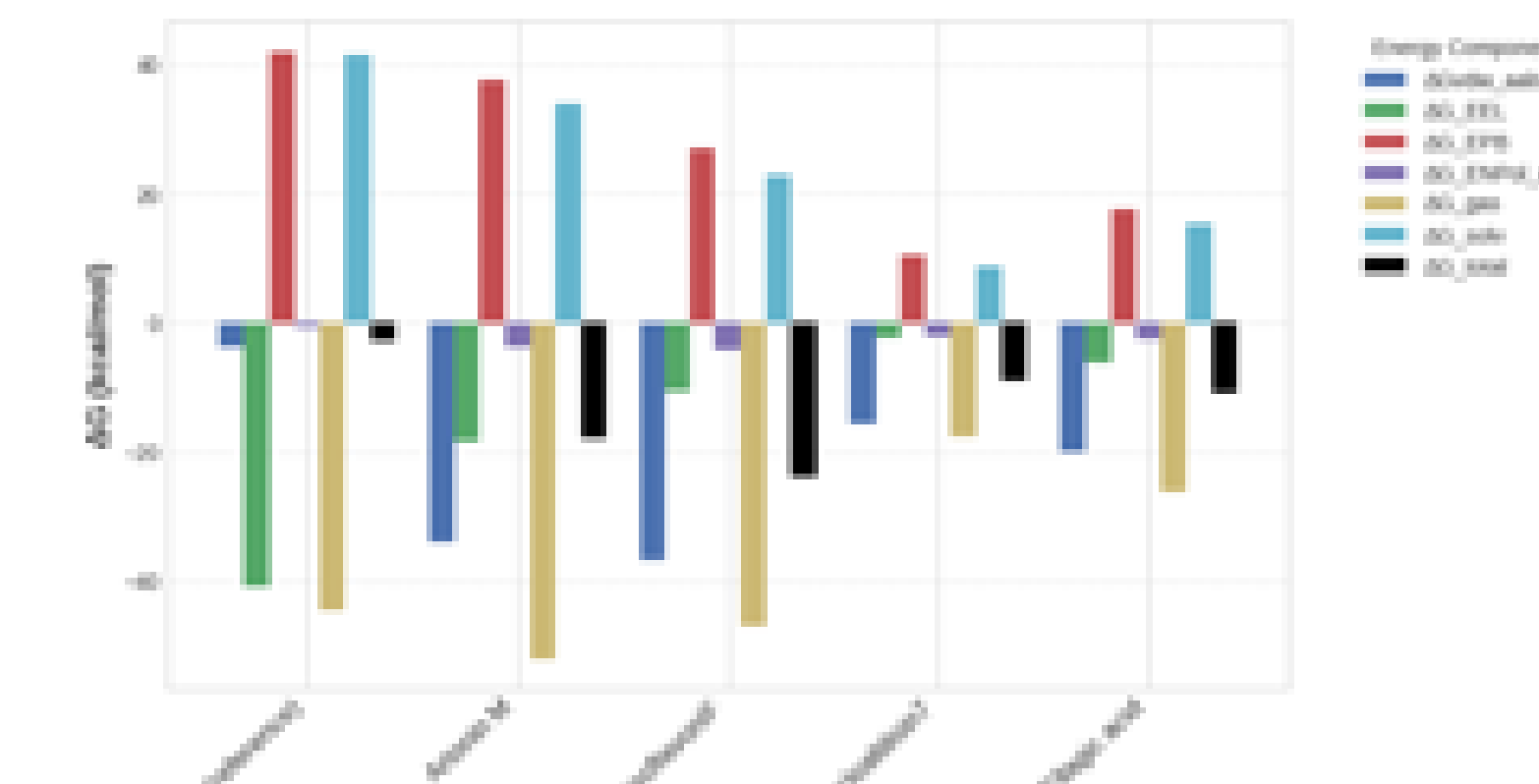


Fig.4

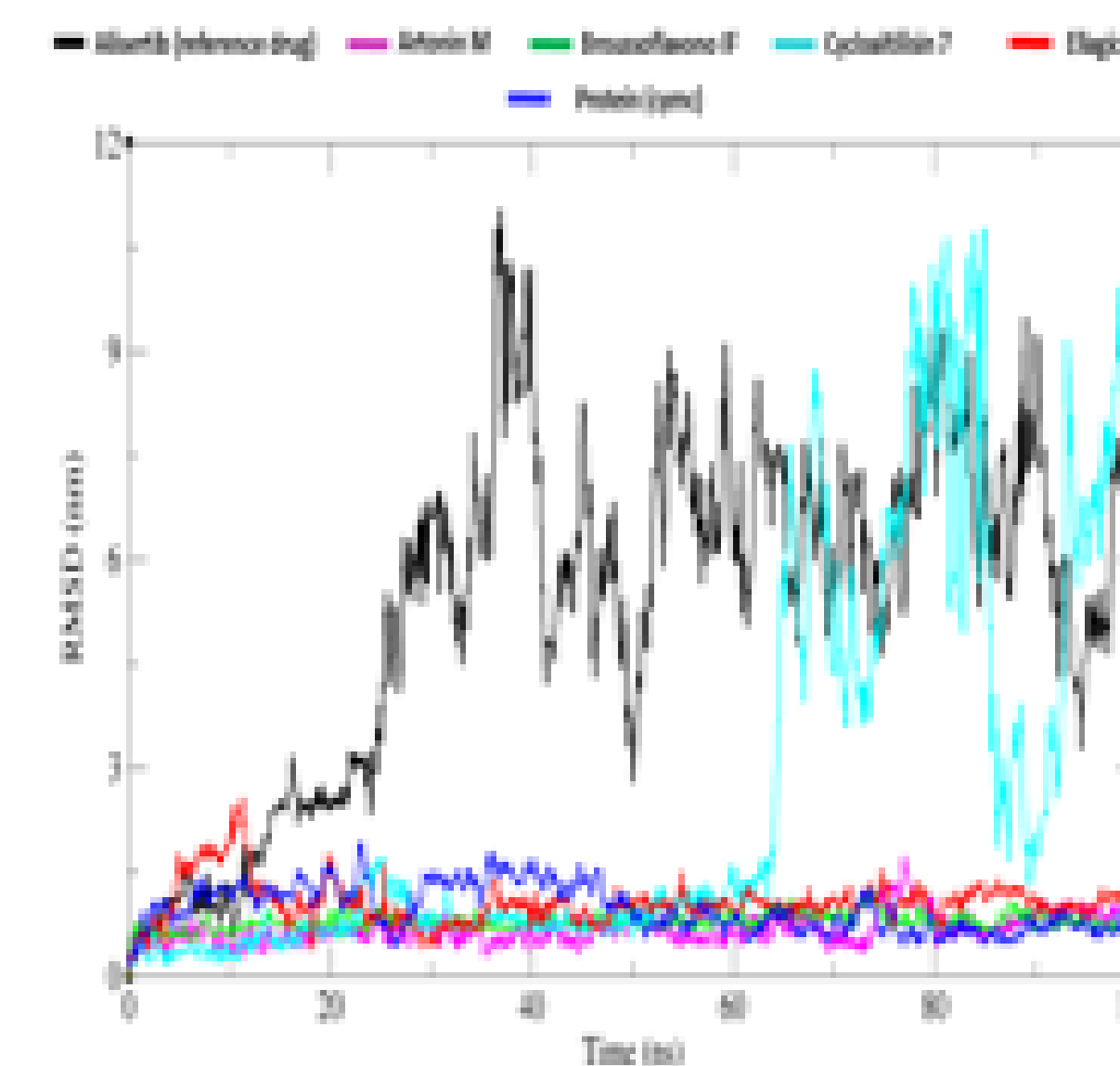
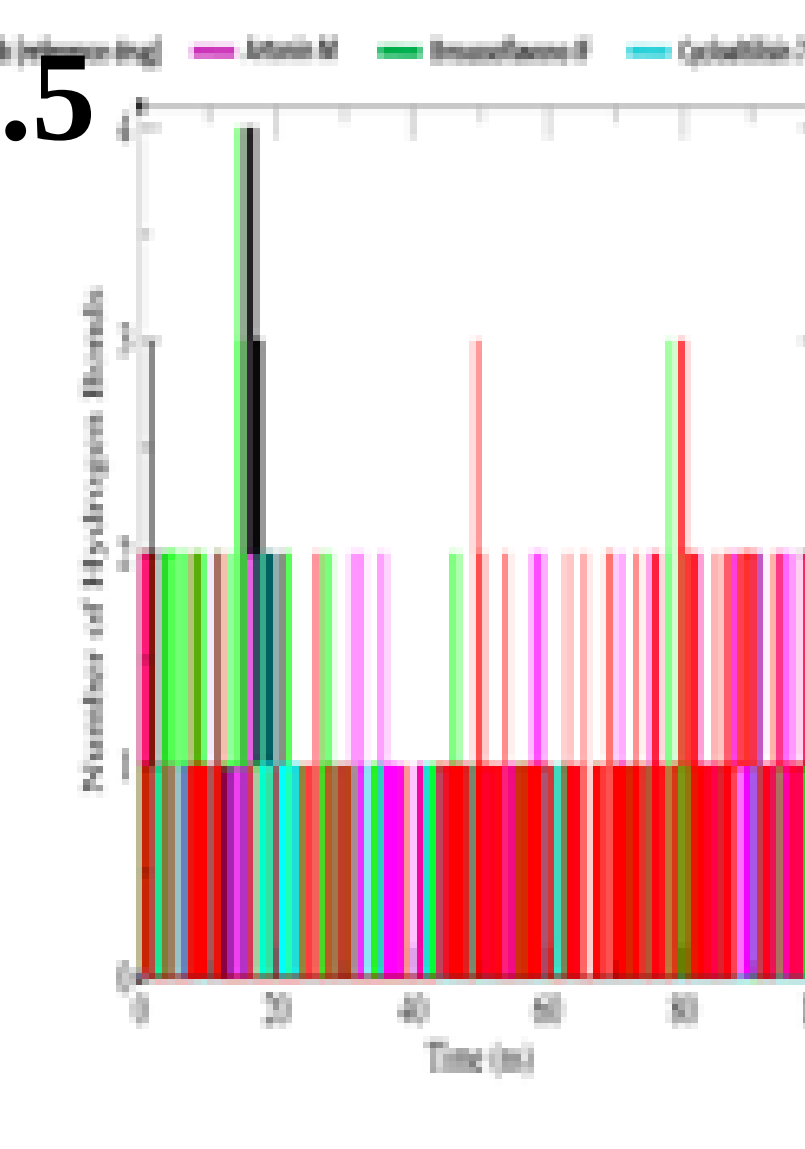


Fig.5



Breakthrough Discovery

Brousoflavonol F emerges as the most promising natural c-Myc inhibitor with superior binding affinity and exceptional stability compared to existing inhibitors

References

1. Miller, D. M., Thomas, S. D., Islam, A., Muench, D., & Sedoris, K. (2012). c-Myc and cancer metabolism. *Clinical Cancer Research*, 18(20), 5546–5553. <https://doi.org/10.1158/1078-0432.CCR-12-0977>
2. Duffy, M. J., O'Grady, S., Tang, M., & Crown, J. (2021). MYC as a target for cancer treatment. *Cancer Treatment Reviews*, 94, 102154. <https://doi.org/10.1016/j.ctrv.2021.102154>

SDG 3 Impact

- Novel cancer therapeutics
- Sustainable drug sources
- Affordable treatment potential
- Reduced cancer mortality

Future Directions

- Experimental validation in vitro
- Lead optimization studies
- Preclinical testing
- Clinical development

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