

Integrative computational approach to farnesyltransferase inhibition toward anti-liver cancer drug candidate from *Syzygium cumini* essential oils

Wira Eka Putra^{1*}, Arief Hidayatullah², Diana Widiastuti³, Hary Isnanto⁴,
Muhammad Fikri Heikal⁵, Sustiprijatno⁶

- 1) Biotechnology Study Program, Department of Applied Sciences, Faculty of Mathematics and Natural Sciences, Universitas Negeri Malang, East Java, 65145, Indonesia
- 2) Democratic Governance and Poverty Reduction Unit, United Nations Development Programme, Eijkman-RSCM Building, Jakarta, 10430, Indonesia
- 3) Department of Chemistry, Faculty of Mathematics and Natural Science, Universitas Pakuan, West Java, 16129, Indonesia
- 4) Department of Biochemical Technology, School of Bioresources and Technology, King Mongkut's University of Technology Thonburi, Bangkok, 10140, Thailand
- 5) Tropical Medicine Graduate Program, Faculty of Medicine, Khon Kaen University, Khon Kaen, 40002, Thailand
- 6) Research Center for Applied Botany, National Research and Innovation Agency, West Java, 16911, Indonesia

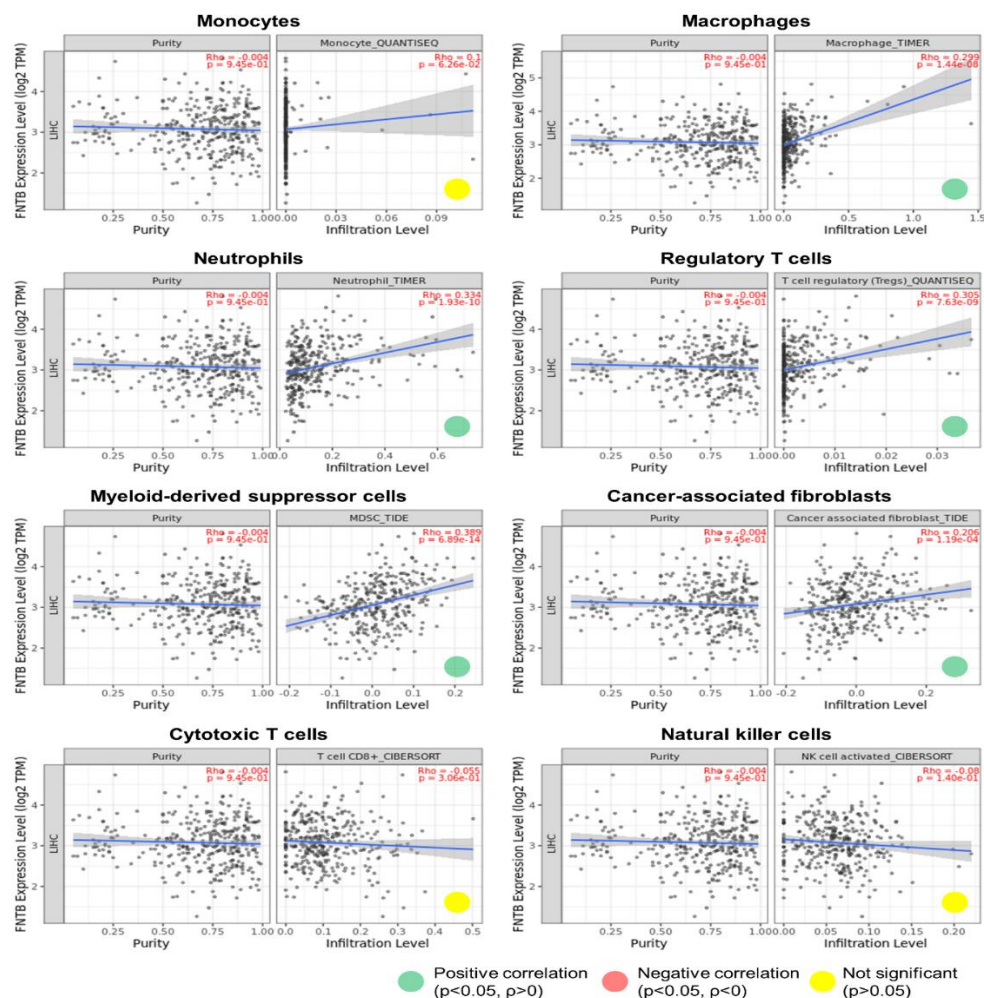


Figure S1: Analysis of the correlation between FNTB gene expression and tumor microenvironment component infiltration in liver cancer patients using publicly available datasets.

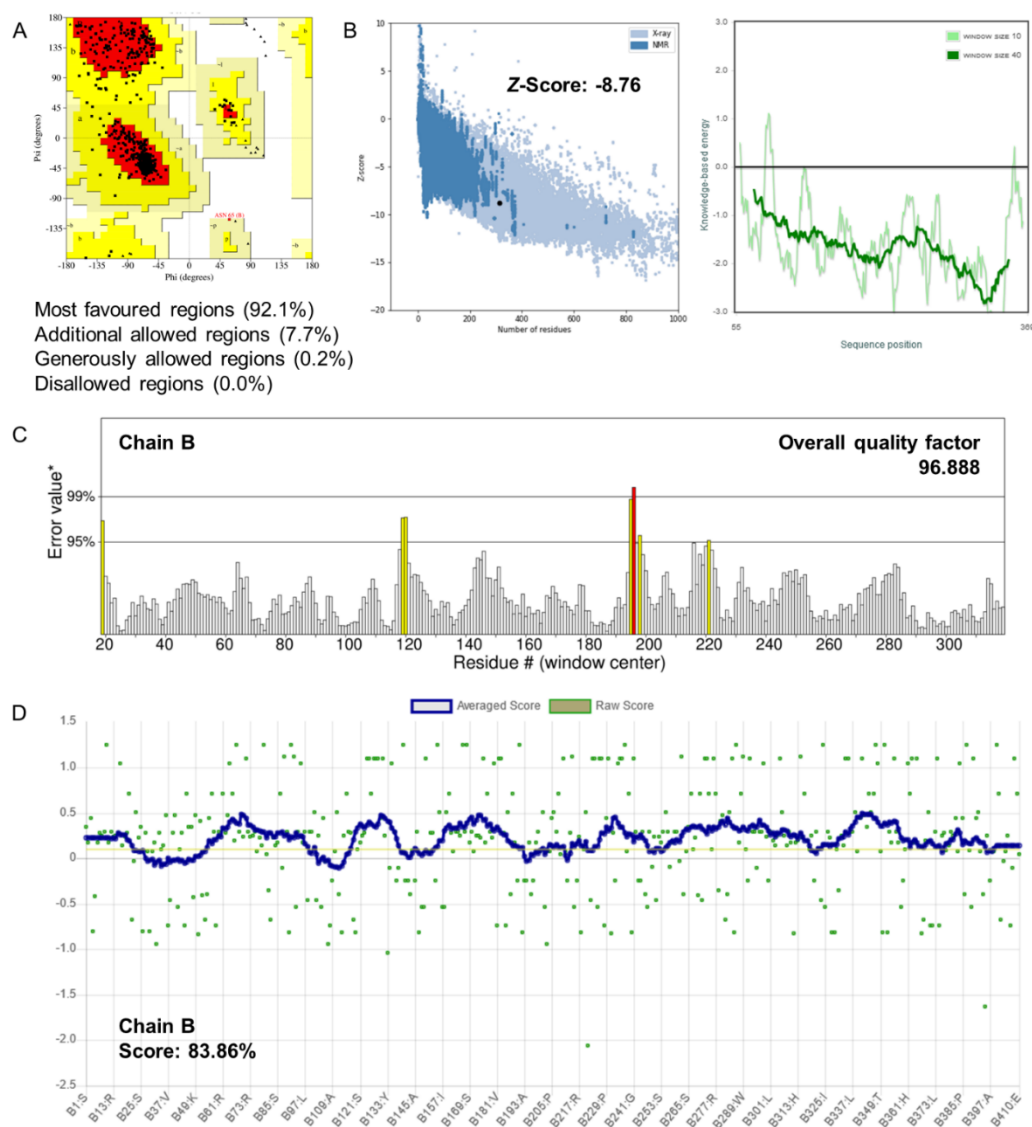


Figure S2: Validation of the FNTB protein structure using various assessment web-tools. (A) Ramachandran plot analysis via SAVES. (B) Protein structure evaluation through ProSA-web. (C) ERRAT plot assessment using SAVES. (D) VERIFY 3D plot analysis via SAVES.

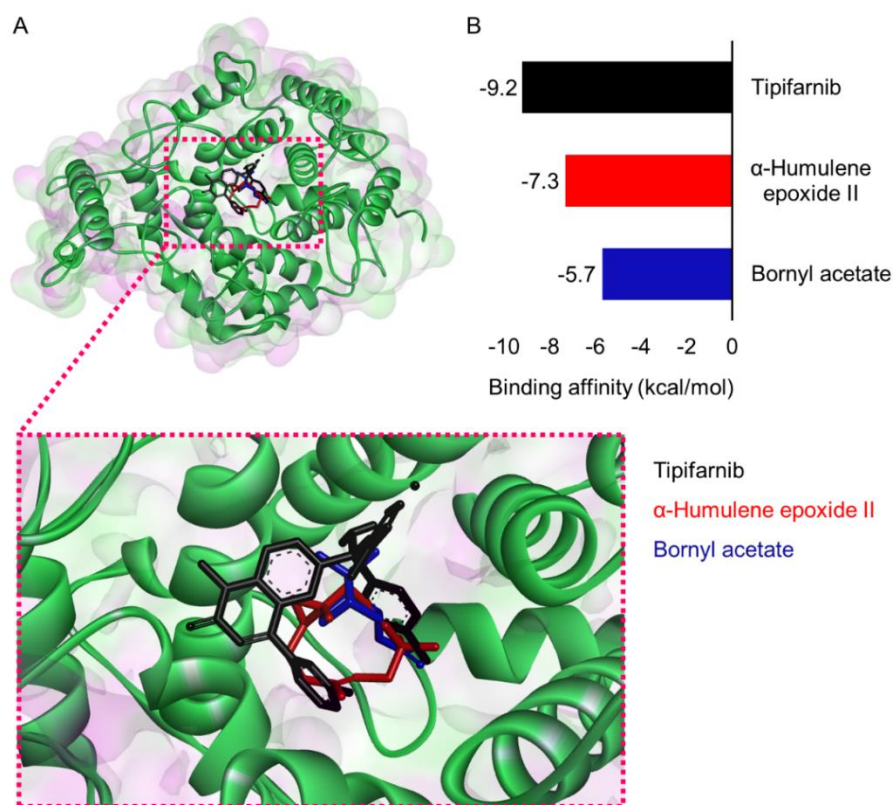


Figure S3: Docking analysis of ligand binding with the target protein. (A) Evaluation of binding affinity scores. (B) 3D visualization of the FNTB-ligand complex.