The Open Bioinformatics Journal
DOI: 10.2174/0118750362429534250911103350, 2025, 18, e18750362429534

ISSN: 1875-0362
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SUPPLEMENTARY MATERIAL OPEN ACCESS

In Silico Identification of Potential PD-L1 and VISTA Inhibitors in Ovarian Cancer: A Computational Approach Combining Virtual Screening and Molecular Dynamics Simulations

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Cite as: Ahmadi N, Hakmi M, Gaouzi Z, Elhafidi N, IBRAHIMI A. *In Silico* Identification of Potential PD-L1 and VISTA Inhibitors in Ovarian Cancer: A Computational Approach Combining Virtual Screening and Molecular Dynamics Simulations. Open Bioinform J, 2025; 18: e18750362429534. http://dx.doi.org/10.2174/0118750362429534250911103350

Published: September 15, 2025

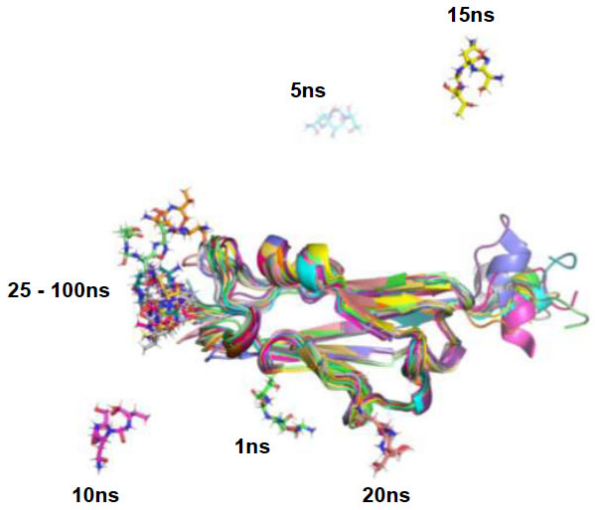

Fig. (4). Snapshots of the PD-L1/CA-170 complex from molecular dynamics simulation showing conformational evolution over time.

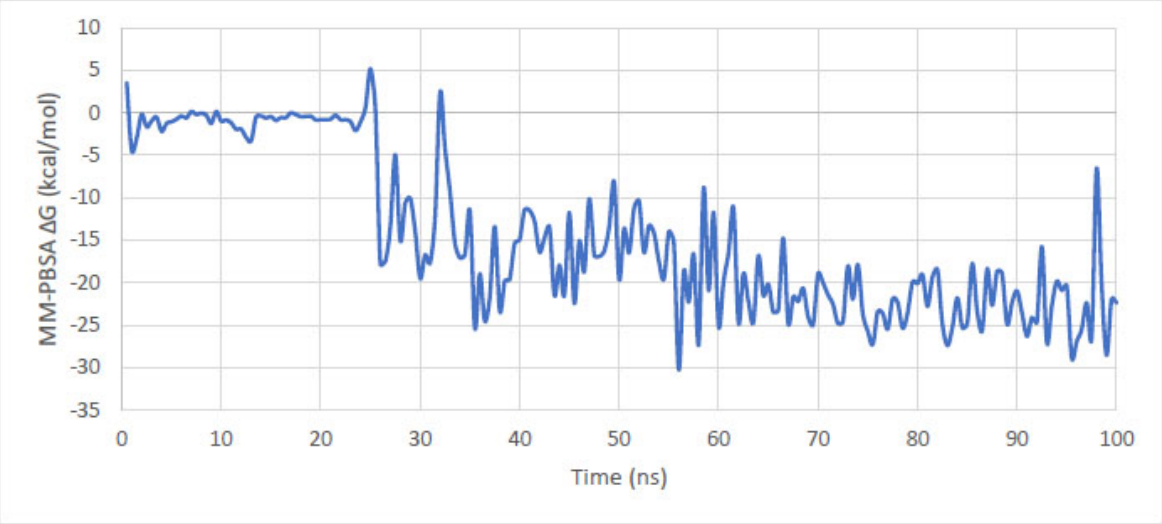

Fig. (4). Fluctuations of MM-PBSA Binding Free Energy as a Function of Time.