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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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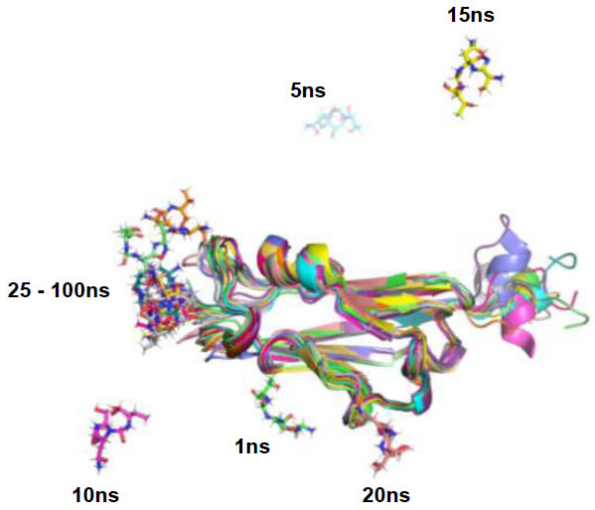

Fig. (4). Snapshots of the PD-L1/CA-170 complex from molecular dynamics simulation showing conformational evolution over time.

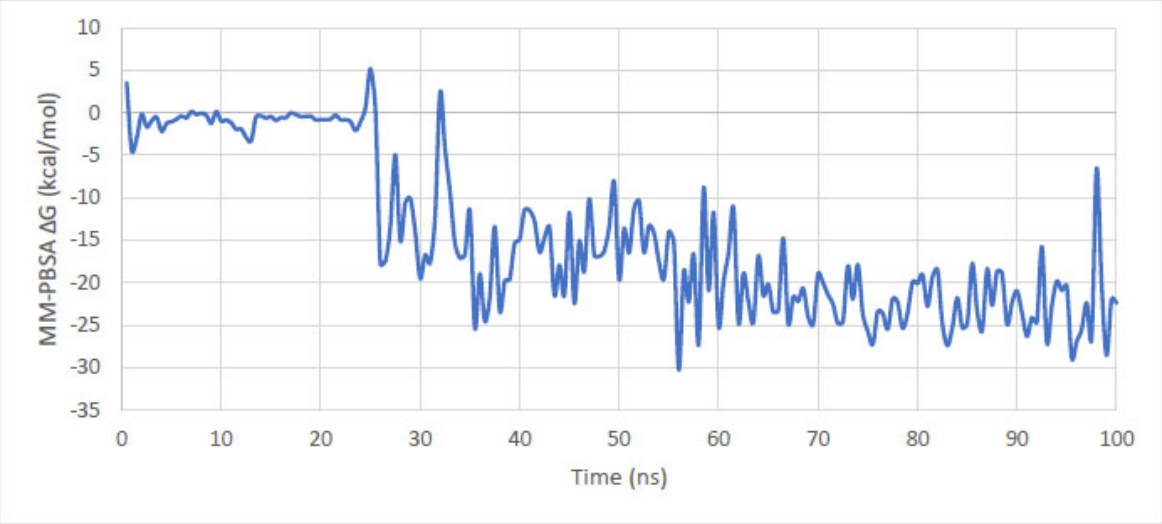

Fig. (4). Fluctuations of MM-PBSA Binding Free Energy as a Function of Time.