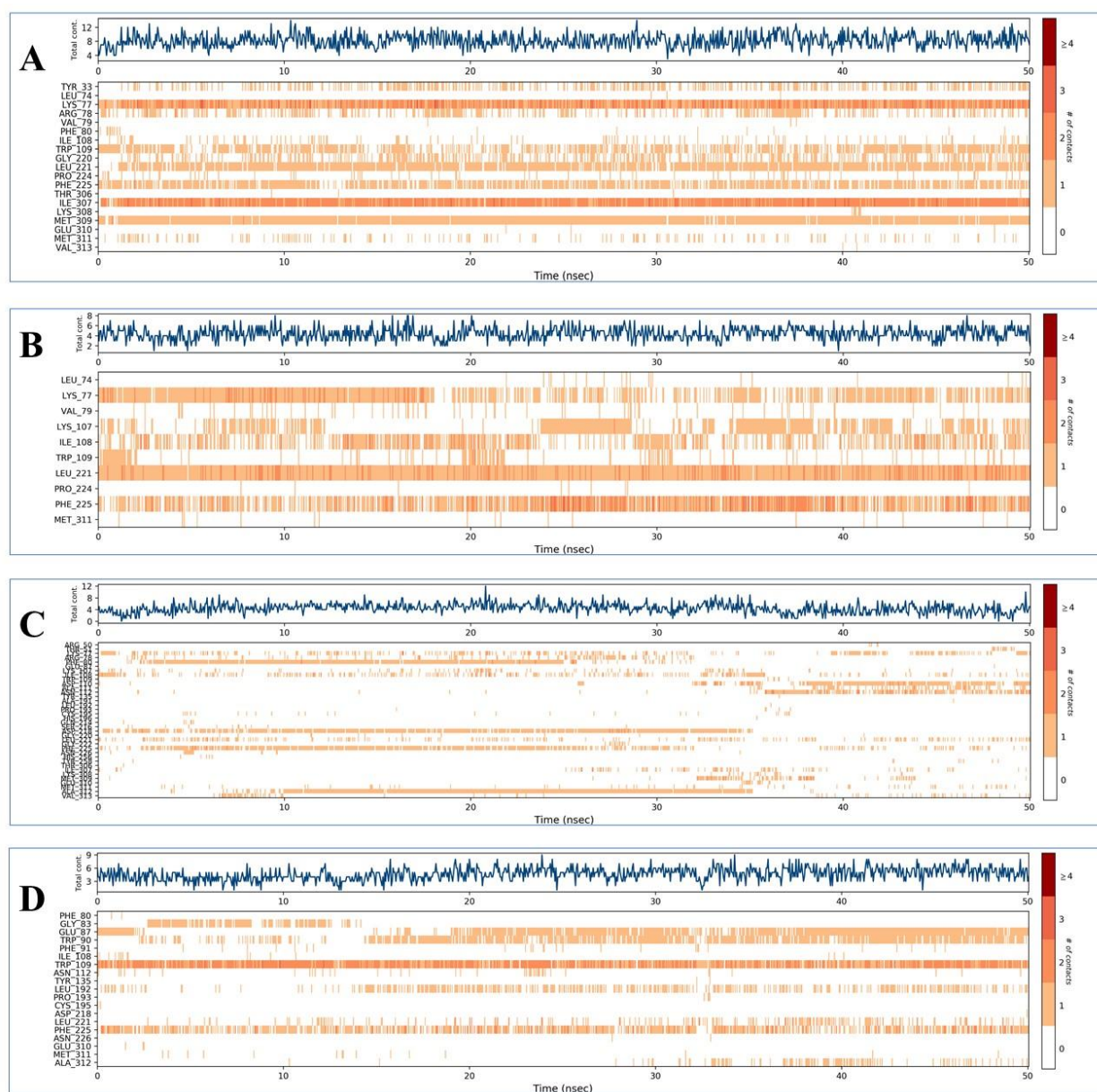
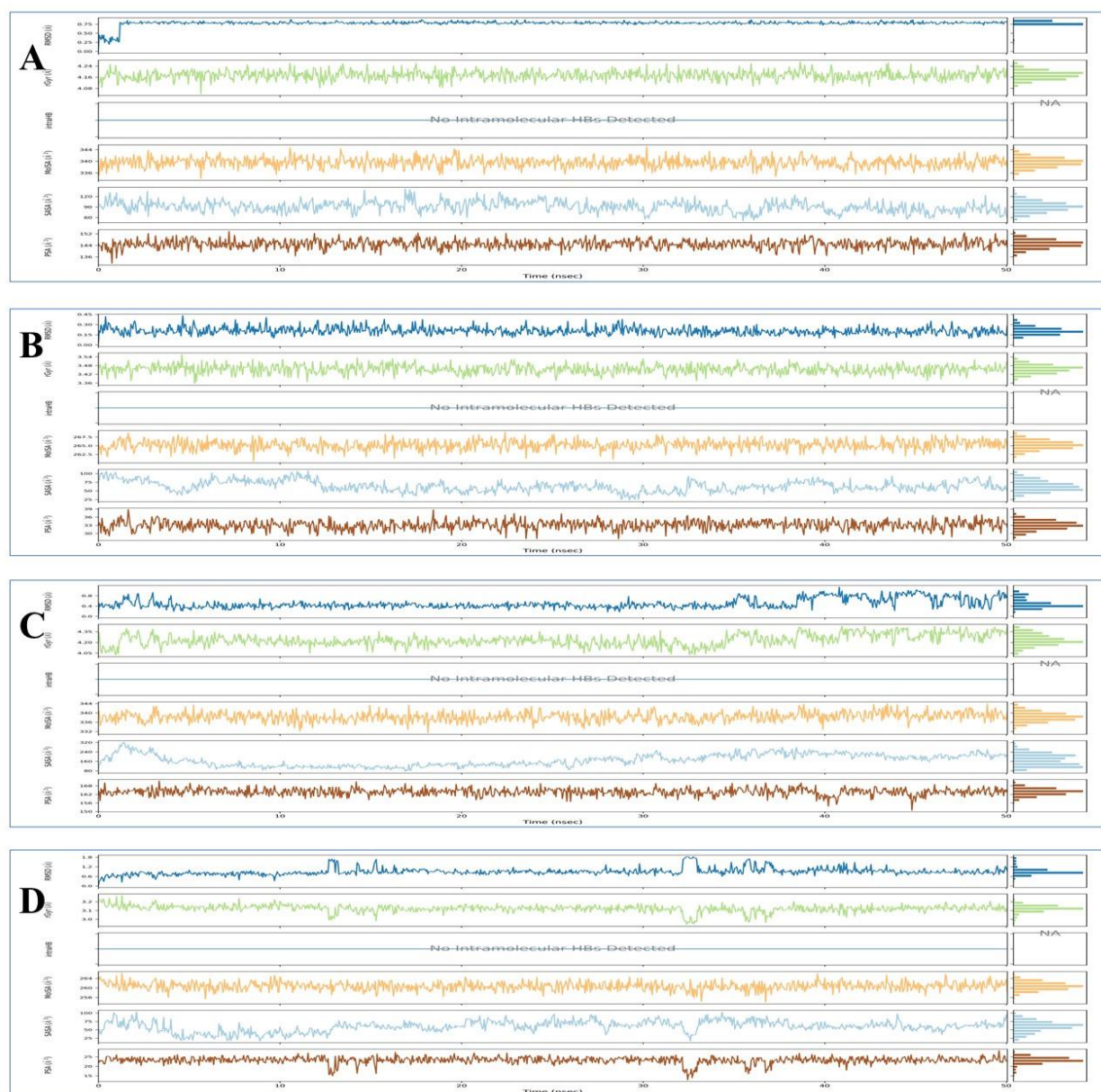


## Computational Identification of Druggable Bioactive Compounds from *Catharanthus roseus* and *Avicennia marina* against Colorectal Cancer by Targeting Thymidylate Synthase

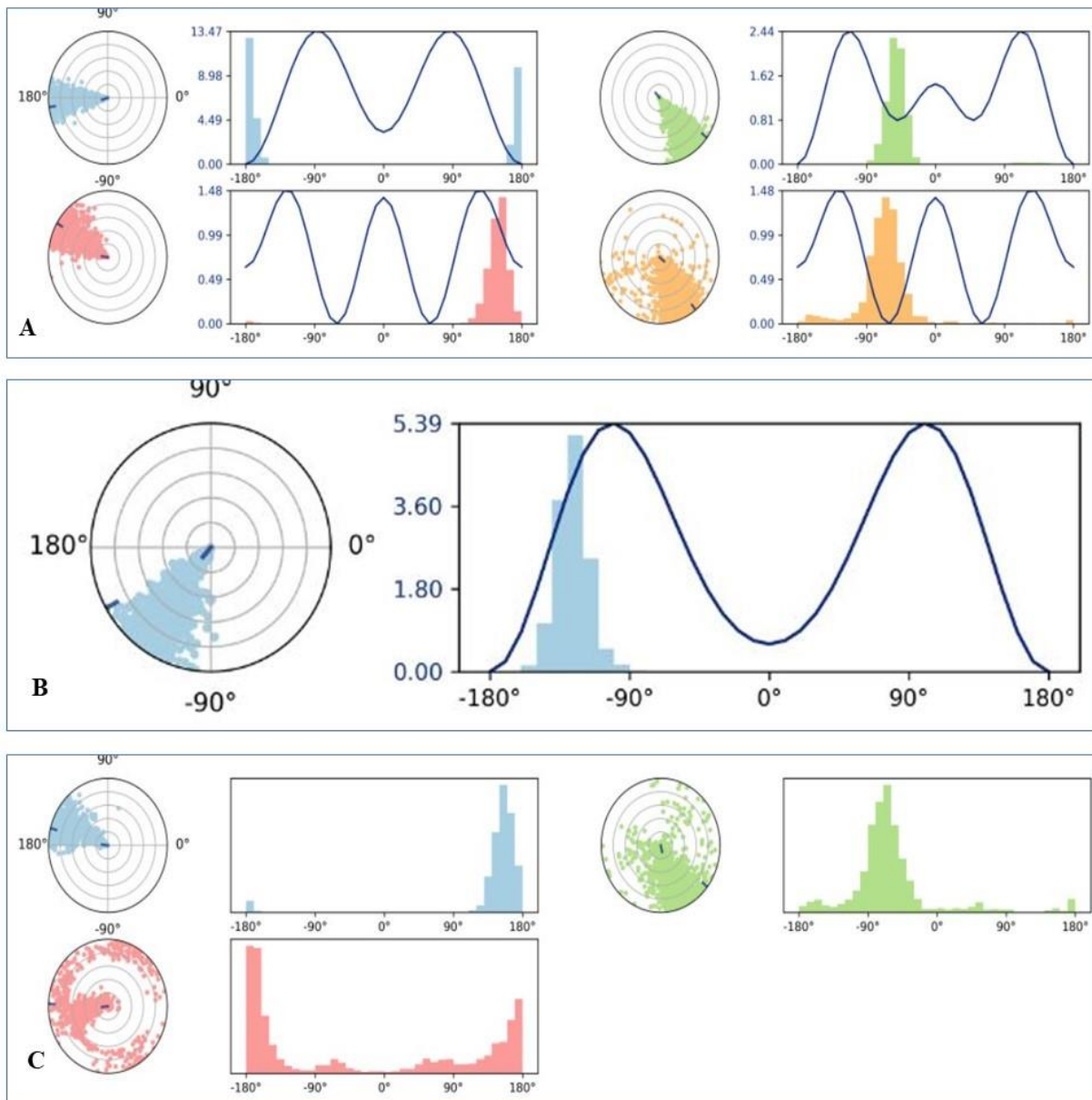
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**Figure S1:** Showing the contact mapping of the protein-ligands interactions for the selected four compounds found during the 50 ns simulation run. Herein, showing the selected four ligands A. PubChem CID: 102004710, B. PubChem CID: 198912, C. PubChem CID: 11969465, and D. PubChem CID: 5281349 contact map with target protein.



**Figure S2:** Depicted the RMSD (Å), rGyr (Å), intra-HB, MolSA(Å<sup>2</sup>), SASA(Å<sup>2</sup>), and PSA (Å<sup>2</sup>) of the selected four compounds in complex with TS protein. Herein, showing the value of the compounds A. PubChem CID: 102004710, B. PubChem CID: 198912, C. PubChem CID: 11969465, and D. PubChem CID: 5281349.



**Figure S3:** Depicted the torsion properties of the selected three compounds A. PubChem CID: 102004710, B. PubChem CID: 198912, C. PubChem CID: 11969465.