Supplementary Materials

Molecular Mechanism of Food-Derived Polyphenols on PD-L1 Dimerization: A Molecular Dynamics Simulation Study

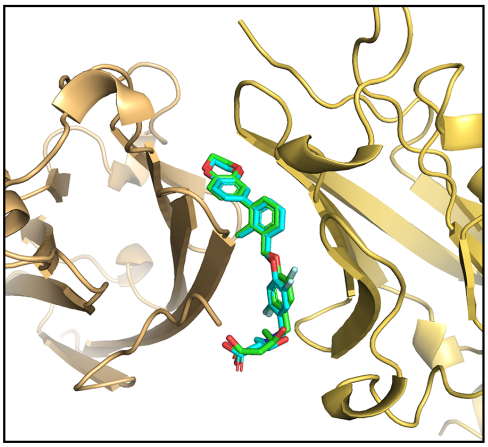


Figure S1. Overlap of the vina-docked pose and native conformation from the crystal structure (PDB ID: 5N2F). The docked pose and native confirmation are coloured cyan and green, respectively. ᴀPD-L1 and ʙPD-L1 are coloured orange and yellow, respectively.

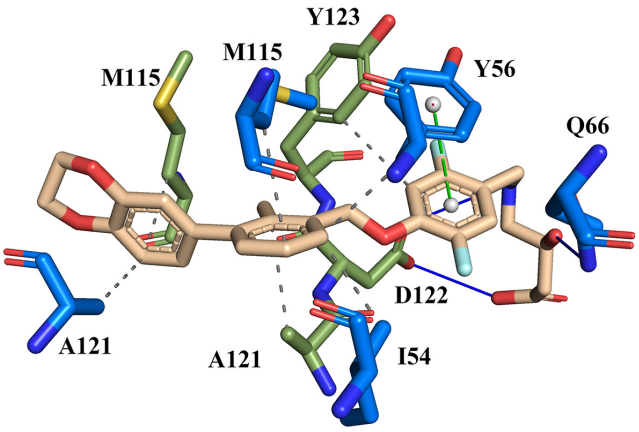


Figure S2. Binding modes and interactions between the docked BMS-200 and PD-L1 dimer. ᴀPD-L1 and ʙPD-L1 are coloured green and blue, respectively. BMS-200 is coloured beige. H bond, hydrophobic, and Π-stacking interactions are also shown.