

Supplementary Materials

Molecular Mechanism of Small-molecule Inhibitors in Blocking the PD-1/PD-L1 Pathway through PD-L1 Dimerization

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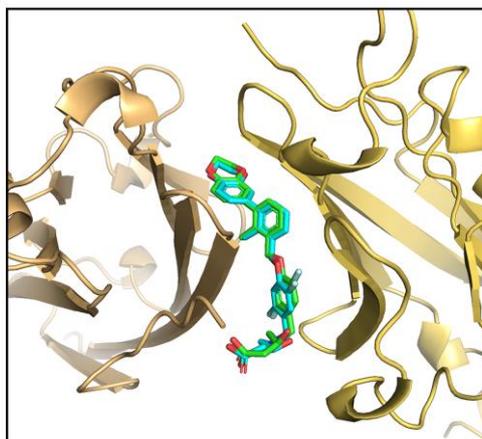


Figure S1. Overlap of the vina-docked pose and native conformation from the crystal structure (PDB ID: 5N2F). The docked pose and native conformation are coloured cyan and green, respectively. The α PD-L1 and β PD-L1 are coloured orange and yellow, respectively.

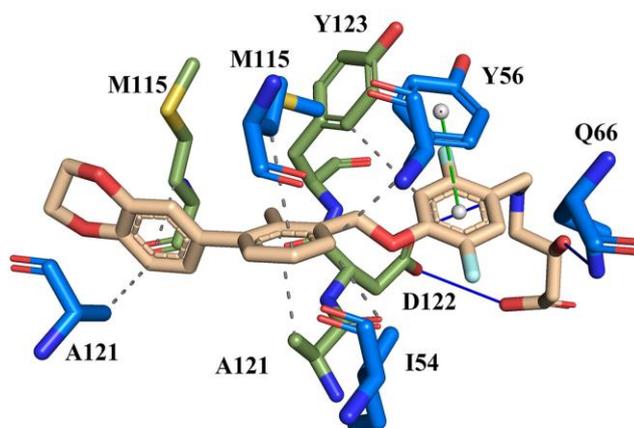


Figure S2. Binding modes and interactions between the docked BMS-200 and PD-L1 dimer. The α PD-L1 and β PD-L1 are coloured green and blue, respectively. BMS-200 is coloured beige. The H bond, hydrophobic and Π -stacking interactions are also shown.