

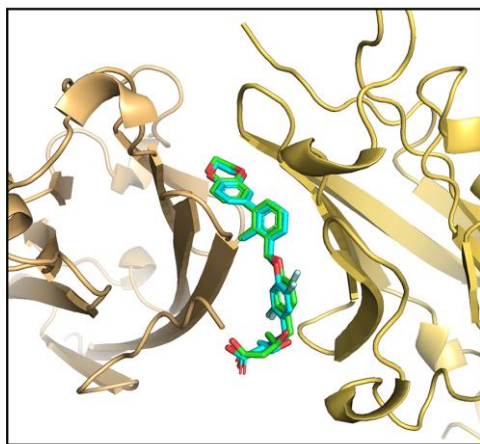
# Supplementary Materials

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

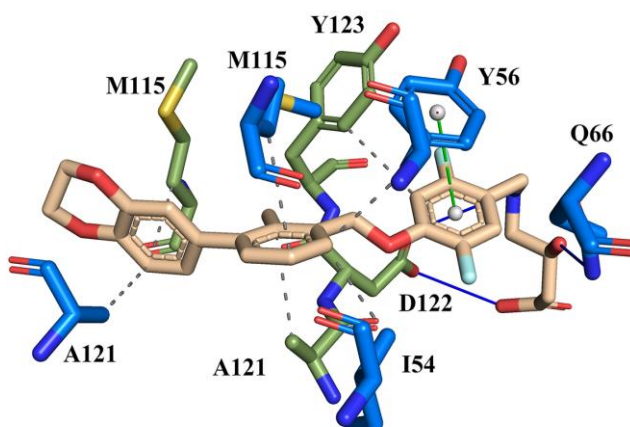
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**Figure S1.** Overlap of the vina-docked pose and native conformation from the crystal structure (PDB ID: 5N2F). The docked pose and native conformation are coloured cyan and green, respectively. The  $\alpha$ PD-L1 and  $\beta$ PD-L1 are coloured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



**Figure S2.** Binding modes and interactions between the docked BMS-200 and PD-L1 dimer. The  $\alpha$ PD-L1 and  $\beta$ PD-L1 are coloured green and blue, respectively. BMS-200 is coloured beige. The H bond, hydrophobic and  $\pi$ -stacking interactions are also shown.