

Supplementary Information

Figure S1. Comparison of the induced-fit poses predicted for **SW155246** (carbon atoms in green), **SW155246-1** (carbon atoms in pink) and **SW155246-2** (carbon atoms in light blue). The co-crystal sinefungin (carbon atoms in yellow) is shown for reference. Hydrogen bonds between **SW155246** and the protein are shown in dashed pink lines.

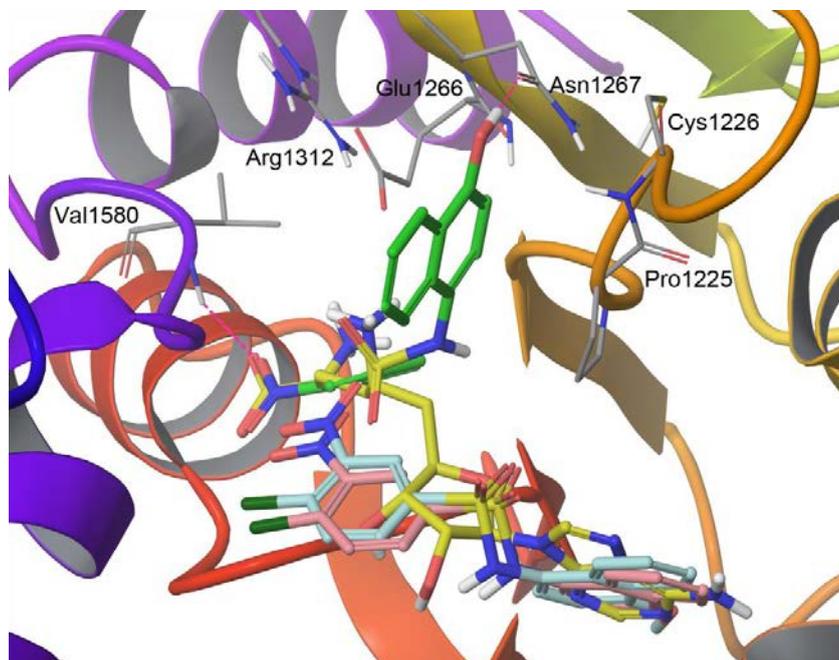


Figure S2. Predicted binding mode for **SW155246** with induced-fit docking (carbon atoms in light green) and regular docking (carbon atoms in dark green).

