

Table S1. Proteins used for molecular docking

Protein	Grid box size	Grid box position
CDK3	25Å × 25Å × 25Å	center x = 23,955 center y = -98,581 center z = 12,749
CDK4	27,954Å × 26,138Å × 30,130Å	center x = 15,176 center y = -38,529 center z = 10,612
CDK6	32,632Å × 32,701Å × 34,77Å	center x = 21,980 center y = 37,150 center z = -3,829
CDK8	32,557Å, 29,804 Å × 30,578Å	center x = -6,19 center y = 11,504 center z = -11,722

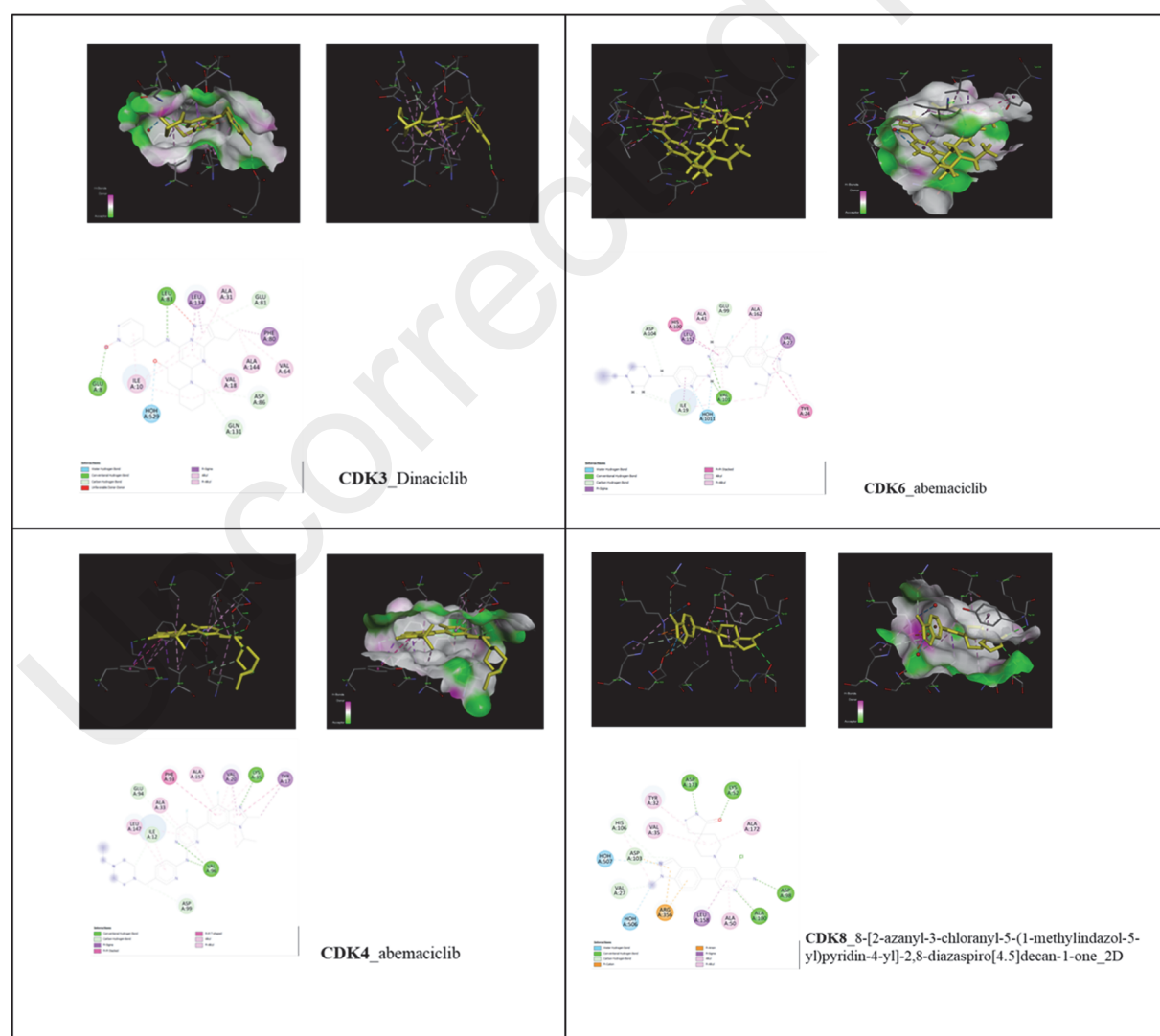


Fig. S1. Images of the target protein with the co-crystal ligand