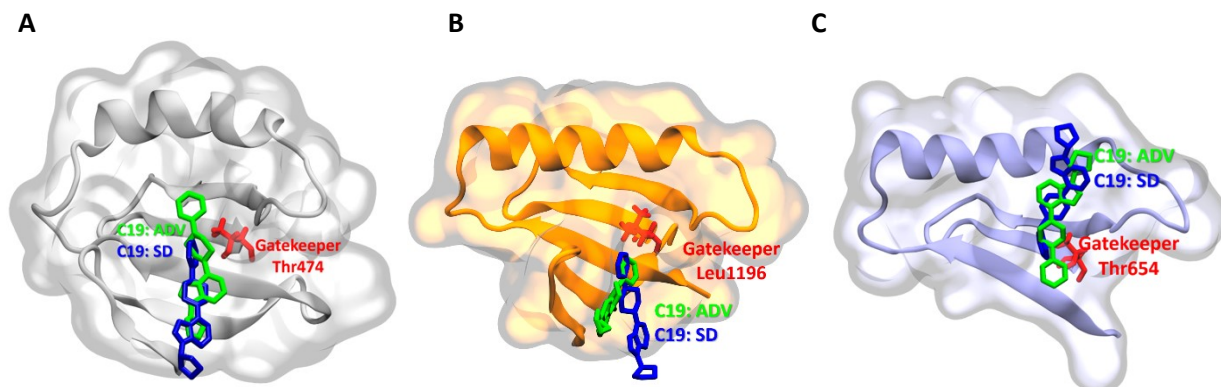## Supplementary Material

Figure S1. Compound **19**'s posed on the BTK (A), ALK (B), and DDR2 (C) to compare docking applications. The green and blue color show compound 19 poses in the active site of kinases. The red color shows the gatekeepers. ADV: AutoDock Vina, SD: SwissDock.

Table S1. The interactions between BTK and tested compounds, with the occupied binding pockets. The binding affinities of SwissDock are specified at the end of the table to compare the binding affinities of AutoDock Vina. FP: Front Pocket, GA: Gate Area, BL: Back Loop, BP: Back Pocket, GK: Gatekeeper, AL: Activation Loop.

BTK / *5P9J*	Compounds						
Residues	19	21	22	23	56*		
Leu408	✓	✓	✓	✓	✓	:	FP I
Val416					✓	:	FP II
Lys430	✓	✓			✓	:	GA
Val458		✓	✓	✓		:	BL
Leu460	✓	✓		✓		:	BP IV
Ile472	✓	✓	✓	✓		:	BP V
Thr474	✓	✓	✓	✓	✓	:	**GK**
Tyr476					✓	:	Hinge
Leu528					✓	:	FP VII
Phe540		✓		✓		:	D[F]G
Leu542	✓				✓	:	**AL**
Affinity (*kcal/mol*)	-9.2	-8.3	-9.3	-9.1	-10.3	:	Autodock Vina
	-7.9	-8.2	-8.0	8.1	-8.7	:	SwissDock