Please insert Figure S1

Figure S1 The root mean square deviation (RMSD) of the FGFR1/FGFR4 and their ligands' backbone heavy atoms along the 50 ns conventional MD simulations.

Please insert Figure S2

Figure S2 Molecular modeling analysis of AZD4547 to the activity cavity of FGFR1/4. (A) Alignment of crystal structure FGFR1/AZD4547 (yellow) and binding pose of FGFR1/AZD4547 (green) by molecular docking; (B) The alignment of last snapshots between FGFR1/AZD4547(yellow) and FGFR4/AZD4547(green) from conventional MD trajectories.

Table S1 Top 10 of residues contribution to the binding effective energy of FGFR1/AZD4547

Residue name	Decomposition energy	Standard error
Ala -640	-1.15	0.22
Val-492	-1.21	0.19
Lys-514	-1.34	0.29
Gly-567	-1.52	0.33
Tyr-563	-1.58	0.31
Val-561	-1.70	0.33
Leu-630	-1.80	0.26
Ile-545	-1.81	0.29
Phe-489	-1.90	0.36
Leu-484	-2.03	0.31

Table S2 Top 10 of residues contribution to the binding effective energy of FGFR4/AZD4547

Residue name	Decomposition energy	Standard error
Glu-551	-0.84	0.36
Ala-629	-0.88	0.29
Met-524	-1.09	0.19
Gly-556	-1.09	0.32
Ala-553	-1.11	0.85
Lys-503	-1.23	0.28
Leu-619	-1.47	0.24
Ile-534	-1.74	0.33
Leu-473	-2.02	0.37
Val-550	-2.14	0.29

Table S3 Top 10 of residues contribution to the binding effective energy of FGFR1/ponatinib

Residue name	Decomposition energy	Standard error
Leu-484	-1.49	0.24
His-621	-1.50	0.55
Ala-564	-1.70	0.38
Leu-630	-1.74	0.29
Val-561	-1.80	0.43
Phe-642	-1.86	0.62
Ile-545	-1.99	0.29
Tyr-563	-2.12	0.26
Ala-640	-2.17	0.30
Met-535	-2.20	0.32

Table S4 Top 10 of residues contribution to the binding effective energy of FGFR4/ponatinib

Residue name	Decomposition energy	Standard error
His-610	-1.62	0.37
Val-550	-1.66	0.42
Leu-473	-1.67	0.29
Arg-635	-1.68	0.35
Leu-619	-1.74	0.26
Ala-553	-1.75	0.37
Met-524	-1.82	0.66
Ile-534	-1.91	0.32
Asp-630	-1.91	0.49
Ala-629	-2.15	0.28