

Supporting information

Table S1. Reproduction of the binding modes of the co-crystallized ligands.

ABL			ALK			BRA ^F		
PDB	Resolution	RMSD	PDB	Resolution	RMSD	PDB	Resolution	RMSD
2E2B	2.20	0.91	2XB7	2.50	1.16	3C4C	2.57	0.59
2G2H	2.00	1.53	2XBA	1.95	1.71	3IDP	2.70	0.54
2HIW	2.20	0.66	3LCS	1.95	0.91	3PPK	3.00	1.27
2HYY	2.40	0.25	4DCE	2.03	0.89	3PRF	2.90	0.54
2HZI	1.70	0.52	4FOB	1.90	1.59	4E26	2.55	4.43
3CS9	2.21	0.34	4FOC	1.70	2.25	4FK3	2.65	0.72
3UE4	2.42	1.66	4FOD_1 ^a	2.00	1.45			
3QRI	2.10	0.59	4FOD_2 ^a	2.00	2.46			
3QRK	2.30	0.83						

^aTwo binding modes were found in the co-crystallized ligand, which were named by _1 and _2.