Supplementary Materials

Table S1. PDB crystal structures of p38α MAPK in complex with TI-Is [1].

FAM	PDB ID Codes	TI-I Chemotypes
1	1A9U 1BL6, 1BL7, 1BMK, 1IAN, 1OUK, 1OZ1, 1YQJ, 1ZZL, 3C5U, 3FMJ, 3GCP, 3HVC, 3HL7, 3MPA, 3OBG, 3ZS5, 3ZSG, 4EWQ, 4F9W, 4F9Y, 4FA2	Pyridinyl and Pyrimidynilimidazoles, Pyridinylpyridazines and structurally related compounds
2	1DI9, 1M7Q, 1OUY, 1OVE, 2ZAZ, 3FC1, 3FLN, 3FLQ, 3FLS, 3FLW, 3FLY, 3FLZ, 3FMH, 3FMK, 3FSF, 3FSK, 3GC7, 3HP5, 3MW1, 3ZSI, 4EH2, 4EH3	Bicyclic 6,6-Heterocycles
3	1ZYJ, 1ZZ2, 4EH7	Diphenylethers
4	2BAL, 2BAQ, 2GFS, 2QD9, 3HRB, 3HUB, 3IW6, 3IW7, 3MPT, 3QUD, 3QUE, 3ZSH, 3ZYA	Diarylketones, piperazinylarylketones, and structurally related compounds
5	3FI4, 3FKN, 3FKO, 3FL4, 3FML, 3FMM, 3FMN, 3HA8, 3KF7	Pyrazolo-pyrimidines and analogues
6	1W7H, 1WBW, 3HLL, 3HP2, 3L8S, 3ROC, 4EH8	Benzylarylethers and structurally related compounds
7	3LFA, 4EH6	Diarylammides
8	1WBO, 1W84, 2I0H, 3HUC, 3IW5, 4DLJ, 4EH4, 4EH5	Miscellaneous

Table S2. SiteMap descriptors calculated for each ATP binding site crystallographic conformation.

Title	SiteScore	Volume	Exposure	Enclosure	Title	SiteScore	Volume	Exposure	Enclosure
1A9U	1.07	331.68	0.53	0.82	**3FLN-1W**	1.17	297.38	0.41	0.85
1BL6	1.07	406.46	0.55	0.80	**3FLQ**	0.96	239.41	0.58	0.80
1BL7	1.05	488.78	0.60	0.78	**3FLS**	1.12	355.01	0.50	0.80
1BMK	1.07	445.21	0.62	0.77	**3FLW**	1.13	365.30	0.51	0.84
1DI9	1.07	378.33	0.52	0.80	**3FLW-1W**	1.15	381.42	0.55	0.83
1M7Q	1.09	317.28	0.56	0.77	**3FLY**	1.14	331.68	0.53	0.82
1OUK	1.10	340.94	0.57	0.78	**3FLY-1W**	1.17	306.99	0.53	0.82
1OUY	1.10	344.72	0.51	0.80	**3FLZ**	1.14	331.68	0.50	0.82
1OVE	1.11	365.98	0.44	0.80	**3FLZ-1W**	1.17	334.77	0.52	0.82
1OZ1	0.98	280.57	0.64	0.74	**3FMH**	1.11	398.91	0.54	0.79
1W7H	1.11	356.72	0.34	0.84	**3FMH-1W**	1.14	322.42	0.51	0.79
1W84	1.08	533.02	0.56	0.82	**3FMJ**	1.07	399.25	0.57	0.80
1WBO	1.02	284.69	0.62	0.78	**3FMK**	1.17	274.06	0.38	0.85
1WBW	1.13	252.11	0.45	0.81	**3FMK-1W**	1.18	273.71	0.37	0.85
1YQJ	1.11	449.33	0.45	0.80	**3FML**	1.01	285.38	0.62	0.73
1ZYJ	1.11	273.37	0.50	0.80	**3FMM**	1.14	320.71	0.41	0.81
1ZZ2	1.11	312.47	0.46	0.81	**3FMN**	1.11	388.62	0.53	0.77
1ZZ2-1W	1.10	361.18	0.52	0.80	**3FSF**	1.04	326.19	0.60	0.74
1ZZL	1.13	353.63	0.42	0.85	**3FSK**	1.10	411.94	0.51	0.82
2BAL	1.06	298.41	0.46	0.79	**3GC7**	1.12	301.15	0.51	0.81
2BAL-1W	1.08	306.64	0.51	0.77	**3GCP**	1.08	212.66	0.50	0.75
2BAL-2W	1.10	271.31	0.45	0.79	**3HA8**	1.12	440.76	0.57	0.77
2BAQ	1.08	229.47	0.44	0.82	**3HL7**	1.10	311.79	0.41	0.80
2GFS	1.12	361.87	0.41	0.81	**3HLL**	1.08	402.68	0.47	0.82

Table S2. *Cont.*

Title	SiteScore	Volume	Exposure	Enclosure	Title	SiteScore	Volume	Exposure	Enclosure
2I0H	1.11	514.84	0.47	0.83	**3HP2**	1.16	189.68	0.38	0.81
2QD9	1.16	263.08	0.37	0.86	**3HP5**	1.10	349.86	0.46	0.80
2QD9-1W	1.17	267.54	0.37	0.87	**3HRB**	1.11	265.48	0.39	0.82
2ZAZ	0.98	230.50	0.46	0.79	**3HUB**	1.12	400.97	0.43	0.80
2ZAZ-1W	1.02	225.01	0.42	0.82	**3HUC**	1.11	305.96	0.53	0.75
3C5U	1.10	339.23	0.55	0.76	**3HVC**	1.13	293.27	0.36	0.85
3FC1	1.12	338.88	0.42	0.80	**3IW5**	1.12	326.54	0.33	0.86
3FI4	1.12	301.84	0.45	0.82	**3IW6**	1.11	313.50	0.37	0.81
3FI4-1W	1.14	299.10	0.47	0.81	**3IW7**	1.16	206.14	0.31	0.85
3FKN	1.11	416.06	0.47	0.80	**3KF7**	1.11	356.03	0.47	0.83
3FKN-1W	1.16	327.57	0.40	0.85	**3L8S**	1.11	356.72	0.49	0.76
3FKO	1.14	336.14	0.39	0.84	**3LFA**	0.99	275.43	0.59	0.78
3FKO-1W	1.20	249.02	0.31	0.88	**3MPT**	1.09	287.43	0.48	0.81
3FL4	1.14	394.45	0.44	0.81	**3MPT-1W**	1.14	265.83	0.49	0.81
3FL4-1W	1.17	336.83	0.42	0.83	**3MPT-2W**	1.15	273.37	0.44	0.82
3FLN	1.15	297.38	0.38	0.84	**3MW1**	1.09	261.37	0.47	0.78
3QUD	1.16	237.70	0.39	0.86	**4EH2**	1.10	455.85	0.59	0.78
3QUD-1W	1.19	218.49	0.33	0.87	**4EH3**	1.09	360.84	0.45	0.81
3QUE	1.20	285.03	0.33	0.88	**4EH4**	1.19	259.65	0.34	0.91
3QUE-1W	1.20	254.85	0.31	0.89	**4EH5**	1.11	411.94	0.57	0.75
3ROC	1.16	322.42	0.39	0.84	**4EH6**	1.15	363.58	0.48	0.83
3ZS5	1.06	268.23	0.57	0.70	**4EH7**	1.11	291.89	0.46	0.79
3ZSG	1.08	270.63	0.53	0.73	**4EH8**	1.21	350.20	0.47	0.86
3ZSH	1.07	394.79	0.39	0.80	**4EWQ**	1.10	358.44	0.54	0.81
3ZSI	1.11	295.67	0.32	0.85	**4F9W**	1.12	392.05	0.57	0.79
3ZYA	1.16	195.51	0.36	0.85	**4F9Y**	1.10	392.74	0.58	0.78
3ZYA-1W	1.16	190.02	0.38	0.86	**4FA2**	1.12	294.64	0.44	0.83
4DLJ	1.05	347.12	0.64	0.76	**4FA2-1W**	1.12	300.47	0.39	0.83

Table S3. Binding site residues defined by SiteMap for each protein structure.

PDB	Residues
1A9U	35, 38, 51, 53, 67, 71, 74, 75, 84, 86, 104, 105, 106, 107, 109, 167, 168, 169, 170, 171, 172, 173
1BL6	35, 38, 51, 53, 55, 67, 68, 71, 75, 84, 85, 86, 104, 106, 107, 108, 109, 110, 111, 112, 150, 152, 154, 155, 157, 165, 167, 168, 169, 170, 172, 173
1BL7	35, 38, 51, 53, 55, 67, 68, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 150, 152, 154, 155, 157, 165, 167, 168, 169, 170, 171, 172, 173
1BMK	35, 38, 51, 53, 67, 70, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 112, 155, 157, 167, 168, 169, 171, 172, 173
1DI9	30, 35, 38, 51, 53, 55, 67, 71, 74, 75, 78, 84, 104, 106, 107, 108, 109, 167, 168, 169, 170, 171, 172
1M7Q	30, 35, 38, 51, 53, 71, 75, 84, 86, 104, 106, 107, 108, 109, 110, 111, 112, 154, 157, 167, 168, 169, 171
1OUK	35, 38, 51, 53, 71, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 111, 112, 157, 165, 167, 168, 169, 171
1OUY	35, 38, 51, 52, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 154, 155, 157, 167, 168, 169, 171
1OVE	30, 34, 35, 38, 51, 53, 71, 75, 84, 86, 104, 106, 107, 108, 109, 110, 111, 112, 154, 155, 157, 167, 168, 169, 171
1OZ1	35, 38, 51, 53, 71, 75, 84, 86, 104, 106, 107, 108, 109, 110, 111, 112, 154, 155, 156, 157, 167, 168, 169, 171
1W7H	30, 35, 38, 51, 53, 71, 74, 75, 84, 104, 106, 107, 108, 109, 110, 111, 112, 115, 154, 157, 167, 168, 169, 171
1W84	30, 32, 33, 34, 35, 36, 38, 40, 51, 53, 55, 67, 71, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 110, 111, 150, 152, 155, 157, 158, 159, 163, 165, 167, 168, 169, 170, 171, 172, 174
1WBO	34, 35, 38, 51, 53, 55, 67, 71, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 165, 167, 168, 169, 171
1WBW	30, 31, 35, 38, 51, 52, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 154, 155, 167, 168, 169, 170, 171, 172
1YQJ	30, 35, 38, 51, 53, 70, 71, 74, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 111, 112, 115, 157, 165, 167, 168, 169, 171
1ZYJ	38, 51, 52, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 157, 167, 168, 169, 171
1ZZ2	30, 31, 35, 38, 51, 52, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 154, 155, 157, 165, 167, 168, 171
1ZZ2-1W	30,31,35,38,51,52,53,71,75,84,86,104,105,106,107,108,109,110,111,112,148,150,152,154,155,157,165,167,168
1ZZL	30, 31, 32, 35, 36, 38, 40, 51, 53, 55, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 155, 157, 167, 168, 169, 171, 173
2BAL	30, 32, 33, 34, 38, 51, 53, 71, 75, 84, 104, 106, 107, 108, 109, 111, 112, 152, 154, 155, 157, 167, 168, 169, 171
2BAL-1W	30,31,32,33,38,51,53,71,75,84,104,106,107,108,109,111,112,152,154,155,157,167,168,169,171
2BAL-2W	30,31,32,38,51,53,71,75,84,104,106,107,108,109,111,112,154,157,167,168,169,171
2BAQ	30, 33, 34, 35, 36, 38, 51, 53, 71, 75, 84, 104, 106, 107, 108, 109, 110, 111, 112, 154, 157, 165, 167, 168, 169, 170, 171
2GFS	30, 31, 35, 38, 51, 53, 71, 74, 75, 78, 84, 104, 106, 107, 108, 109, 110, 111, 112, 115, 154, 157, 167, 168, 169
2I0H	30, 31, 33, 34, 35, 36, 38, 39, 40, 51, 53, 71, 75, 84, 86, 104, 106, 107, 108, 109, 110, 111, 112, 152, 154, 155, 157, 167, 168, 169, 171, 173, 174

Table S3. *Cont.*

PDB	Residues
2QD9	30, 30, 32, 33, 34, 38, 51, 52, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 154, 157, 167, 168, 169, 171
2QD9-1W	30,32,33,38,51,52,53,71,74,75,84,86,104,105,106,107,108,109,110,111,112,154,157,167,168,169,171
2ZAZ	38, 51, 53, 71, 75, 84, 104, 106, 107, 108, 109, 112, 167, 168, 169, 171
2ZAZ-1W	38, 51, 53, 71, 75, 84, 104, 106, 107, 108, 109, 112, 167, 168, 169, 171
3C5U	30, 31, 34, 35, 36, 38, 51, 52, 53, 70, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 152, 154, 155, 157, 167, 168, 169, 170
3FC1	30, 38, 51, 52, 53, 67, 70, 71, 74, 75, 83, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 157, 166, 167, 168, 169
3FI4	30, 33, 34, 38, 51, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 115, 152, 154, 155, 157, 167, 168, 169, 171
3FI4-1W	30,32,33,34,38,51,53,71,75,84,86,104,105,106,107,108,109,111,112,115,152,154,155,157,167,168,169,171
3FKN	30, 31, 34, 35, 38, 51, 53, 71, 74, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 111, 112, 152, 154, 155, 157, 167, 168, 169, 170
3FKN-1W	30, 31, 35, 38, 51, 53, 71, 74, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 111, 112, 157, 167, 168, 169, 170
3FKO	30, 35, 38, 51, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 154, 155, 157, 167, 168, 169, 171
3FKO-1W	30, 35, 38, 51, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 154, 155, 156, 157, 167, 168, 169, 171
3FL4	30, 34, 35, 38, 51, 53, 67, 70, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 150, 152, 154, 155, 157, 167, 168, 169, 170
3FL4-1W	30, 35, 38, 51, 53, 67, 70, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 154, 155, 157, 167, 168, 169, 170
3FLN	30, 32, 33, 34, 38, 51, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 154, 155, 157, 167, 168, 169, 171
3FLN-1W	30, 32, 33, 38, 51, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 154, 155, 157, 167, 168, 169, 171
3FLQ	38, 51, 53, 71, 75, 84, 86, 104, 105, 106, 108, 109, 157, 167, 168, 169, 171
3FLS	30, 32, 32, 38, 51, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 115, 152, 155, 157, 167, 168, 169, 171, 174
3FLW	30, 33, 34, 35, 38, 51, 53, 67, 70, 71, 74, 75, 84, 86, 104, 106, 107, 108, 109, 111, 112, 154, 155, 157, 167, 168, 169, 170, 170
3FLW-1W	30, 33, 34, 35, 38, 51, 53, 71, 74, 75, 84, 86, 104, 106, 107, 108, 109, 111, 112, 154, 155, 157, 167, 168, 169, 170
3FLY	30, 32, 33, 34, 38, 51, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 157, 165, 167, 168, 169, 171
3FLY-1W	30, 32, 33, 34, 38, 51, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 157, 165, 167, 168, 169, 171
3FLZ	30, 33, 34, 38, 51, 52, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 154, 155, 157, 167, 168, 169, 171
3FLZ-1W	30, 33, 34, 38, 51, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 154, 155, 157, 167, 168, 169, 171
3FMH	30, 32, 33, 34, 38, 51, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 150, 152, 154, 155, 156, 157, 167, 168, 169, 171, 173, 174
3FMH-1W	30, 32, 33, 34, 38, 51, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 152, 154, 155, 157, 167, 168, 169, 171
3FMJ	30, 35, 38, 51, 53, 67, 70, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 154, 155, 167, 168, 169, 170, 170, 172

Table S3. *Cont.*

PDB	Residues
3FMK	30, 32, 33, 34, 38, 51, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 157, 167, 168, 169, 171
3FMK-1W	30, 32, 33, 33, 38, 51, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 155, 157, 167, 168, 169, 171
3FML	38, 51, 53, 67, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 157, 167, 168, 169, 171, 172
3FMM	30, 31, 34, 35, 38, 51, 53, 67, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 152, 154, 155, 157, 167, 168, 169, 171
3FMN	30, 38, 51, 53, 67, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 154, 155, 157, 167, 168, 169
3FSF	38, 51, 53, 67, 70, 71, 74, 75, 84, 104, 106, 107, 108, 109, 111, 112, 115, 157, 167, 168, 169, 170
3FSK	30, 32, 33, 34, 35, 38, 51, 53, 67, 70, 71, 74, 75, 78, 84, 104, 106, 107, 108, 109, 111, 112, 157, 167, 168, 169
3GC7	30, 35, 38, 51, 53, 71, 74, 75, 84, 85, 86, 104, 106, 107, 108, 109, 110, 111, 112, 157, 167, 168, 169, 171
3GCP	30, 31, 35, 38, 51, 53, 55, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 168, 169, 170, 171
3HA8	30, 35, 38, 51, 52, 53, 67, 70, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 154, 156, 157, 167, 168, 169
3HL7	29, 30, 31, 32, 33, 37, 50, 52, 70, 73, 74, 83, 85, 103, 105, 106, 107, 108, 109, 110, 111, 151, 153, 154, 156, 166, 167, 168, 170
3HLL	30, 33, 34, 35, 38, 51, 52, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 150, 152, 154, 155, 157, 165, 167, 168, 169, 171
3HP2	30, 33, 38, 51, 53, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 114, 115, 154, 157, 167, 168, 169, 170, 171
3HP5	30, 35, 38, 51, 52, 53, 67, 70, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 154, 157, 167, 168, 169, 170, 170
3HRB	30, 35, 38, 51, 53, 71, 74, 75, 84, 86, 104, 106, 107, 108, 109, 110, 111, 112, 157, 167, 168, 169, 171, 173
3HUB	30, 31, 35, 38, 51, 53, 70, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 155, 157, 167, 168, 169, 170, 170
3HUC	30, 31, 35, 38, 51, 52, 53, 71, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 111, 112, 154, 157, 165, 167, 168, 169, 170, 170
3HVC	30, 31, 32, 32, 38, 51, 53, 71, 74, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 111, 112, 152, 154, 155, 157, 165, 166, 167, 168, 169, 170
3IW5	30, 32, 32, 34, 35, 38, 40, 51, 52, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 154, 157, 165, 167, 168, 169, 170, 171, 171
3IW6	30, 31, 32, 32, 34, 35, 36, 37, 38, 40, 51, 52, 53, 71, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 154, 157, 167, 168, 169, 170, 171, 171
3IW7	30, 32, 38, 51, 53, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 154, 157, 167, 168, 169, 170, 171
3KF7	30, 33, 34, 38, 51, 52, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 152, 154, 155, 157, 165, 167, 168, 169, 171
3L8S	31, 32, 35, 38, 51, 53, 71, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 111, 112, 157, 165, 167, 168, 169, 169
3LFA	38, 51, 53, 71, 75, 84, 86, 104, 106, 107, 108, 109, 111, 112, 157, 167, 168, 168
3MPT	33, 34, 38, 51, 53, 71, 75, 84, 104, 106, 107, 108, 109, 111, 112, 157, 167, 168, 169, 171
3MPT-1W	33, 34, 38, 51, 53, 71, 75, 84, 104, 106, 107, 108, 109, 111, 112, 157, 167, 168, 169, 169, 171

Table S3. *Cont.*

PDB	Residues
3MPT-2W	30, 38, 51, 53, 71, 74, 75, 84, 104, 106, 107, 108, 109, 111, 112, 154, 157, 167, 168, 169, 171, 171
3MW1	30, 38, 51, 53, 71, 75, 84, 104, 106, 107, 108, 109, 110, 111, 112, 154, 157, 165, 167, 168, 169, 171
3QUD	30, 32, 33, 38, 51, 53, 71, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 154, 157, 165, 167, 168, 169, 170, 171, 174
3QUD-1W	30, 38, 51, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 154, 157, 165, 167, 168, 169, 170, 171, 174
3QUE	30, 33, 36, 38, 51, 53, 71, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 154, 157, 165, 167, 168, 169, 170, 171, 174
3QUE-1W	30, 38, 51, 53, 71, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 154, 157, 165, 167, 168, 169, 170, 171, 174
3ROC	30, 32, 33, 38, 51, 52, 53, 71, 74, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 154, 155, 157, 167, 168, 169, 171
3ZS5	30, 31, 35, 38, 51, 53, 55, 67, 70, 71, 74, 75, 78, 84, 86, 104, 105, 106, 107, 108, 109, 110, 168, 169, 170, 171
3ZSG	30, 31, 35, 38, 51, 53, 55, 71, 74, 75, 78, 84, 86, 104, 105, 106, 107, 108, 109, 110, 168, 169, 170, 171
3ZSH	30, 35, 38, 51, 53, 70, 71, 74, 75, 78, 83, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 152, 154, 155, 157, 166, 167, 168, 168
3ZSI	30, 32, 33, 34, 35, 36, 37, 38, 40, 49, 51, 52, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 154, 157, 167, 168, 169, 170, 171, 171
3ZYA	30, 33, 35, 37, 38, 51, 52, 53, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 157, 167
3ZYA-1W	30, 33, 35, 37, 38, 51, 52, 53, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 157, 167, 168, 169
4DLJ	35, 38, 51, 53, 71, 75, 84, 86, 104, 106, 107, 108, 109, 111, 112, 154, 155, 157, 167, 168, 168
4EH2	32, 35, 36, 38, 51, 53, 70, 71, 74, 75, 84, 104, 106, 107, 108, 109, 111, 112, 154, 157, 167, 168, 169, 170, 170
4EH3	30, 32, 35, 36, 38, 51, 53, 71, 75, 84, 104, 106, 107, 108, 109, 110, 111, 112, 114, 115, 118, 152, 154, 157, 165, 167, 168, 169, 170, 171, 172, 183, 184, 185
4EH4	30, 31, 32, 35, 38, 51, 52, 53, 71, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 157, 165, 167, 168, 169, 170, 171
4EH5	35, 38, 51, 53, 71, 74, 75, 78, 84, 85, 86, 87, 104, 105, 106, 107, 108, 109, 110, 111, 112, 152, 155, 157, 165, 167, 168, 168
4EH6	30, 31, 32, 32, 35, 38, 51, 53, 71, 74, 75, 78, 83, 84, 104, 106, 107, 108, 109, 111, 112, 157, 167, 168, 169, 169
4EH7	30, 31, 32, 35, 36, 38, 51, 53, 71, 75, 84, 104, 106, 107, 108, 109, 110, 111, 112, 157, 165, 167, 168, 169, 170, 170
4EH8	30, 35, 38, 51, 53, 71, 74, 75, 78, 83, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 154, 155, 156, 157, 165, 167, 168, 169, 169
4EWQ	30, 31, 35, 38, 51, 52, 53, 71, 74, 75, 84, 86, 104, 105, 106, 107, 108, 109, 111, 112, 152, 154, 155, 157, 165, 167, 168, 169, 169, 171, 172
4F9W	30, 31, 32, 33, 35, 36, 37, 38, 51, 53, 71, 75, 84, 85, 86, 104, 105, 106, 107, 108, 109, 111, 112, 155, 157, 167, 168, 171
4F9Y	30, 33, 34, 35, 36, 38, 51, 52, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 157, 167, 168, 169, 171
4FA2	30, 38, 51, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 154, 155, 157, 167, 168, 169, 170, 171
4FA2-1W	30, 38, 51, 53, 71, 75, 84, 86, 104, 105, 106, 107, 108, 109, 110, 111, 112, 115, 154, 155, 157, 167, 168, 169, 170, 171

Table S4. C-lobe and N-lobe RMSD matrix.

Alignment Set					
		AS-Clobe	AS-Nlobe	All-Clobe	All/Nlobe
RMSD Calculation Set	AS-Clobe	5.27 Å	6.49 Å	-	-
	AS-Nlobe	5.44 Å	1.27 Å	-	-
	All-Clobe	-	-	12.54 Å	12.84 Å
	All-Nlobe	-	-	5.93 Å	0.96 Å

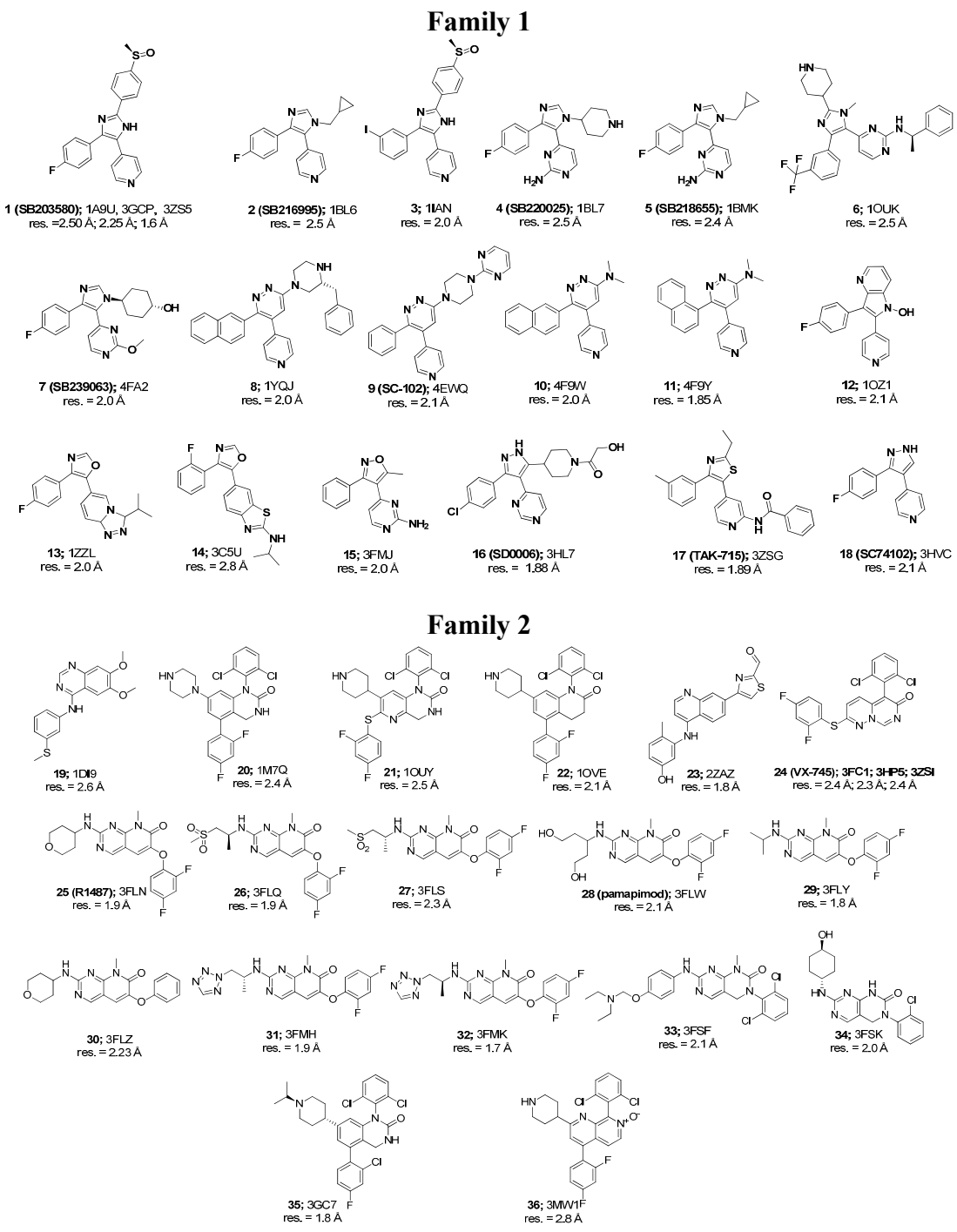

Figure S1. *Cont.*

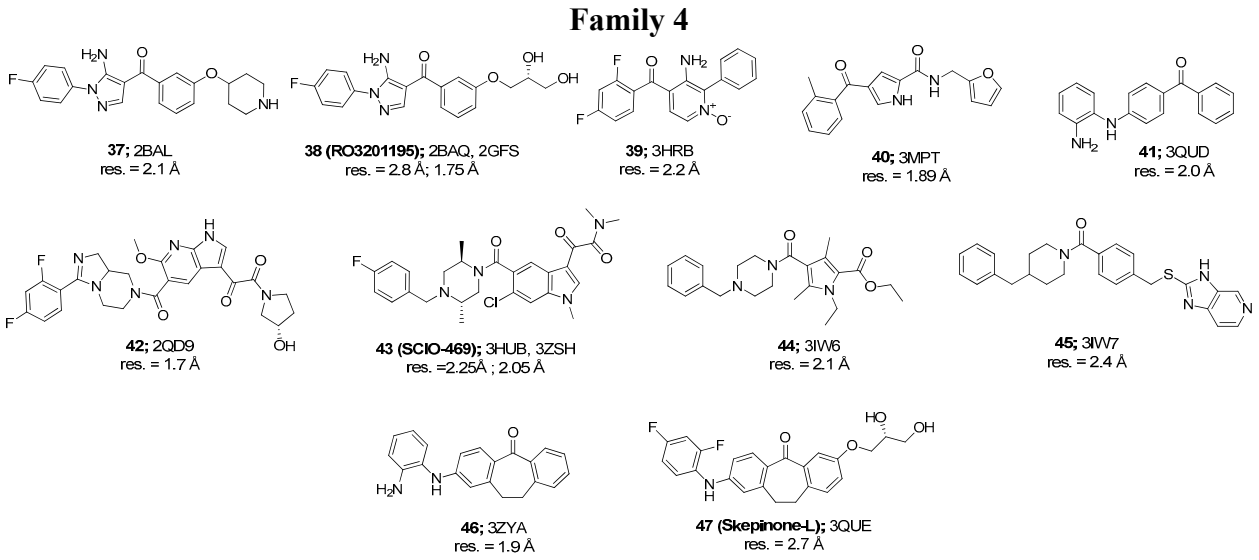

Figure S1. 2D structures of TI-Is with the corresponding PDB ID of the ligand/p38α MAPK complex. res. = PDB resolution.

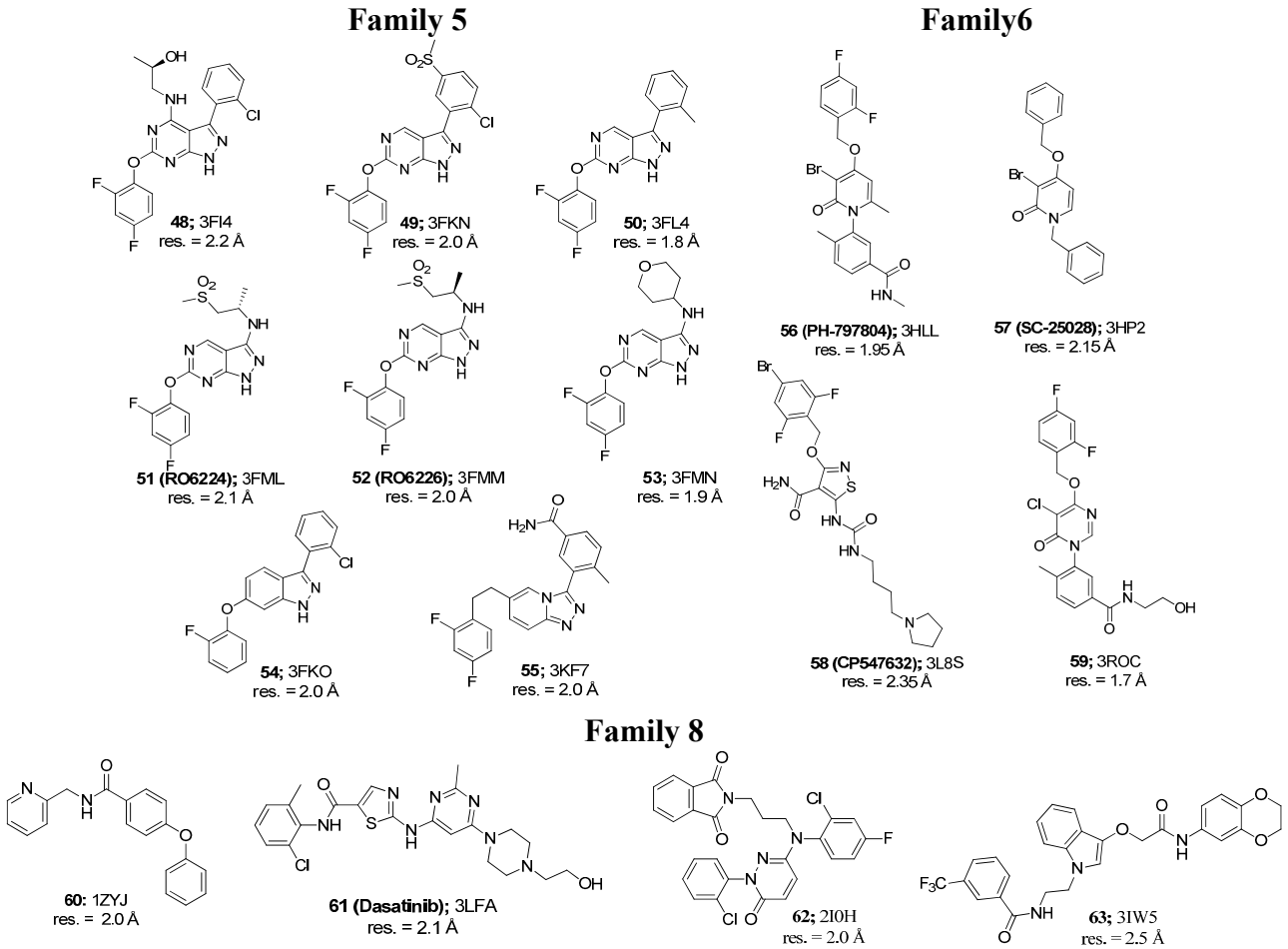

Figure S2. 2D structures of TI-Is with the corresponding PDB ID of the ligand/p38α MAPK complex. res. = PDB resolution. Ligands **60** and **61** were originally included in families 3 and 7, respectively.

Table S5. Cross-docking performance. For overall ligands and for each family, the $RMSD_{avg}$ and success rate (% success) are reported.

PDB	All		FAM1		FAM2		FAM4		FAM5		FAM6		FAM8	
	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success
1A9U	2.78	34.9	1.86	61.1	2.15	44.4	7.11	0.0	1.89	37.5	0.00	0.0	9.77	0.0
1BL6	2.61	23.8	2.02	38.9	2.78	33.3	4.84	0.0	1.79	25.0	0.00	0.0	7.00	0.0
1BL7	3.09	27.0	2.42	55.6	2.33	22.2	6.00	9.1	2.40	25.0	0.00	0.0	10.21	0.0
1BMK	2.69	22.2	1.94	38.9	2.82	27.8	2.93	0.0	2.61	12.5	1.45	25.0	10.31	0.0
1DI9	4.58	17.5	2.85	38.9	4.83	16.7	6.69	9.1	6.04	0.0	2.08	0.0	7.12	0.0
1M7Q	3.33	23.8	2.58	22.2	3.94	38.9	2.73	27.3	2.06	12.5	2.57	0.0	5.73	0.0
1OUK	2.02	46.0	1.45	66.7	1.95	61.1	2.62	0.0	1.88	62.5	2.56	25.0	5.98	0.0
1OUY	4.35	7.9	1.98	5.6	5.97	5.6	3.71	18.2	2.03	12.5	2.42	0.0	4.08	0.0
1OVE	3.89	31.7	3.57	22.2	5.19	33.3	3.18	54.5	3.10	25.0	1.57	50.0	2.34	0.0
1OZ1	2.65	30.2	2.28	61.1	2.24	38.9	5.87	0.0	2.52	12.5	0.00	0.0	4.58	0.0
1W7H	5.15	4.8	1.65	11.1	4.60	5.6	5.30	0.0	5.39	0.0	6.81	0.0	7.00	0.0
1W84	2.81	20.6	2.49	27.8	2.89	27.8	2.58	0.0	4.52	12.5	1.90	50.0	0.00	0.0
1WBO	2.44	39.7	2.12	50.0	1.71	50.0	4.33	0.0	1.58	75.0	2.70	25.0	2.99	0.0
1WBW	4.91	6.3	4.23	11.1	4.32	11.1	3.07	0.0	7.87	0.0	3.30	0.0	3.25	0.0
1YQJ	2.46	27.0	1.81	44.4	2.71	27.8	4.05	0.0	2.36	50.0	0.00	0.0	3.20	0.0
1ZYJ	3.38	30.2	3.90	22.2	3.18	55.6	2.62	27.3	3.68	0.0	2.24	25.0	4.63	25.0
1ZZ2-1W	6.18	6.3	6.65	0.0	6.55	5.6	5.59	9.1	0.00	0.0	4.97	25.0	5.43	25.0
1ZZ2	4.51	11.1	5.15	5.6	4.80	16.7	5.03	0.0	1.43	12.5	1.93	25.0	2.39	25.0
1ZZL	5.49	9.5	6.85	0.0	7.27	0.0	4.35	18.2	1.61	37.5	8.11	0.0	6.17	25.0
2BAL-1W	2.86	31.7	3.54	5.6	1.70	61.1	4.27	18.2	1.54	62.5	2.40	25.0	5.51	0.0
2BAL-2W	4.03	9.5	6.20	0.0	3.27	0.0	4.53	9.1	1.80	50.0	2.40	25.0	5.96	0.0
2BAL	2.99	39.7	3.08	38.9	1.77	61.1	4.67	9.1	1.70	62.5	4.35	25.0	6.28	0.0
2BAQ	5.31	15.9	7.10	11.1	5.56	5.6	3.83	27.3	4.94	37.5	5.85	25.0	2.15	0.0
2GFS	3.90	17.5	0.00	0.0	4.99	11.1	2.99	45.5	2.66	50.0	4.34	0.0	10.46	0.0
2I0H	4.11	25.4	3.83	33.3	5.90	11.1	2.40	27.3	3.00	37.5	2.89	25.0	5.44	25.0
2QD9-1W	2.78	25.4	3.84	16.7	2.72	27.8	1.92	27.3	1.77	37.5	2.10	25.0	4.55	25.0

Table S5. *Cont.*

PDB	all		FAM1		FAM2		FAM4		FAM5		FAM6		FAM8	
	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success
2QD9	2.82	22.2	0.90	16.7	3.74	16.7	3.06	18.2	1.40	50.0	1.91	50.0	5.60	0.0
2ZAZ-1W	4.29	9.5	5.20	0.0	3.99	11.1	4.33	0.0	4.75	37.5	2.47	25.0	3.31	0.0
2ZAZ	3.68	30.2	1.95	55.6	3.57	33.3	5.46	9.1	5.58	25.0	3.12	0.0	4.99	0.0
3C5U	4.31	14.3	4.25	11.1	6.18	0.0	1.75	27.3	4.26	37.5	5.80	0.0	6.48	25.0
3FC1	4.21	27.0	3.31	16.7	5.91	22.2	3.52	45.5	1.72	50.0	4.50	25.0	5.78	0.0
3FI4-1W	2.31	30.2	2.50	11.1	1.65	38.9	3.42	27.3	1.73	62.5	2.34	50.0	2.21	0.0
3FI4	2.49	36.5	2.51	38.9	1.91	55.6	4.54	9.1	1.73	62.5	2.84	0.0	2.67	0.0
3FKN-1W	3.21	17.5	8.05	0.0	6.41	5.6	3.08	27.3	1.10	62.5	3.30	25.0	1.68	25.0
3FKN	3.44	22.2	1.30	27.8	5.19	5.6	2.83	27.3	4.78	50.0	2.74	0.0	1.08	25.0
3FKO-1W	3.13	17.5	6.96	0.0	1.91	16.7	4.34	18.2	1.13	62.5	2.56	25.0	5.47	0.0
3FKO	2.36	30.2	1.39	11.1	2.71	22.2	2.58	45.5	2.03	75.0	2.68	25.0	1.80	25.0
3FL4-1W	2.55	22.2	0.00	0.0	5.73	11.1	2.03	45.5	1.38	62.5	2.07	50.0	2.54	0.0
3FL4	3.72	14.3	3.66	5.6	6.01	5.6	2.04	27.3	2.46	50.0	3.13	0.0	6.83	0.0
3FLN-1W	2.76	31.7	2.84	11.1	2.03	44.4	5.34	9.1	1.45	87.5	1.59	50.0	5.03	0.0
3FLN	2.09	44.4	1.87	44.4	1.60	55.6	4.02	27.3	1.42	87.5	3.46	0.0	2.57	0.0
3FLQ	2.60	38.1	1.70	50.0	1.70	55.6	4.25	0.0	2.09	50.0	2.62	25.0	6.26	0.0
3FLS	2.35	42.9	1.41	44.4	1.56	61.1	3.89	18.2	1.77	62.5	4.43	25.0	4.63	0.0
3FLW-1W	2.21	39.7	2.45	22.2	1.87	61.1	3.45	18.2	1.30	75.0	1.92	50.0	2.44	0.0
3FLW	2.83	38.1	2.36	38.9	1.54	50.0	5.85	0.0	1.36	87.5	4.48	25.0	8.99	0.0
3FLY-1W	2.71	38.1	3.65	27.8	1.40	55.6	4.70	9.1	1.51	62.5	1.88	75.0	2.43	0.0
3FLY	2.60	38.1	2.70	27.8	1.46	61.1	4.29	9.1	1.43	75.0	3.69	25.0	7.88	0.0
3FLZ-1W	2.23	46.0	2.32	50.0	1.84	66.7	3.19	9.1	1.36	62.5	1.85	50.0	4.64	0.0
3FLZ	2.44	38.1	1.48	38.9	1.42	55.6	4.87	0.0	1.36	75.0	5.01	25.0	6.18	0.0
3FMH-1W	2.22	46.0	2.14	50.0	2.33	55.6	2.43	36.4	1.83	62.5	2.38	25.0	2.35	0.0
3FMH	2.09	49.2	1.86	50.0	1.92	66.7	2.66	27.3	1.57	62.5	1.45	50.0	5.64	0.0
3FMJ	3.39	23.8	2.17	55.6	2.55	22.2	5.14	0.0	5.90	0.0	2.78	25.0	8.66	0.0

Table S5. *Cont.*

PDB	all		FAM1		FAM2		FAM4		FAM5		FAM6		FAM8	
	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success
3FMK-1W	2.88	38.1	2.46	27.8	3.58	44.4	3.56	18.2	1.21	87.5	2.23	50.0	4.63	0.0
3FMK	2.37	52.4	2.09	55.6	2.68	55.6	2.87	36.4	1.16	87.5	2.44	50.0	4.47	0.0
3FML	2.69	33.3	1.36	44.4	2.20	33.3	3.28	9.1	1.92	75.0	8.38	0.0	8.05	0.0
3FMM	3.21	17.5	5.47	5.6	5.60	5.6	2.50	45.5	0.98	50.0	4.32	0.0	2.21	0.0
3FMN	2.23	46.0	1.94	50.0	1.60	61.1	3.39	18.2	1.13	62.5	1.50	50.0	9.28	0.0
3FSF	3.02	30.2	2.85	33.3	2.22	33.3	2.74	27.3	3.02	37.5	4.48	25.0	6.66	0.0
3FSK	3.10	36.5	2.44	27.8	2.23	55.6	3.22	27.3	1.34	50.0	7.60	25.0	8.71	0.0
3GC7	3.62	31.7	2.44	50.0	5.03	27.8	3.81	27.3	2.86	25.0	2.63	25.0	4.84	0.0
3GCP	3.08	17.5	2.00	61.1	5.35	0.0	5.63	0.0	0.00	0.0	9.53	0.0	0.00	0.0
3HA8	2.85	33.3	2.14	66.7	2.51	38.9	4.83	0.0	2.79	25.0	0.00	0.0	6.87	0.0
3HL7	2.88	15.9	2.39	27.8	3.34	11.1	3.69	9.1	2.08	25.0	2.76	0.0	7.13	0.0
3HLL	3.85	28.6	3.02	33.3	5.45	22.2	2.85	36.4	3.13	25.0	1.24	50.0	4.28	0.0
3HP2	5.36	12.7	6.18	0.0	7.51	5.6	3.03	27.3	3.68	25.0	1.90	25.0	1.80	25.0
3HP5	4.30	28.6	3.69	22.2	5.68	16.7	5.15	27.3	1.63	75.0	2.59	25.0	4.78	25.0
3HRB	3.74	22.2	2.22	38.9	5.36	16.7	2.19	18.2	3.78	25.0	5.80	0.0	5.53	0.0
3HUB	5.22	12.7	3.64	5.6	8.35	0.0	2.52	27.3	1.81	50.0	5.91	0.0	9.25	0.0
3HUC	3.63	7.9	2.39	11.1	5.87	0.0	3.94	9.1	3.41	25.0	0.00	0.0	0.00	0.0
3HVC	2.79	22.2	2.43	38.9	2.21	11.1	3.90	9.1	3.22	50.0	2.03	0.0	0.00	0.0
3IW5	4.46	9.5	3.32	16.7	6.97	0.0	3.76	9.1	3.70	25.0	2.45	0.0	2.28	0.0
3IW6	4.61	20.6	5.62	11.1	7.25	5.6	3.29	45.5	1.54	50.0	2.10	25.0	2.54	0.0
3IW7	4.37	20.6	7.08	0.0	7.22	5.6	2.37	54.5	1.06	50.0	1.69	50.0	2.20	0.0
3KF7	4.21	22.2	2.06	33.3	6.58	16.7	3.62	9.1	4.93	37.5	1.85	25.0	0.00	0.0
3L8S	3.33	19.0	4.51	5.6	2.58	33.3	3.90	0.0	3.54	50.0	2.42	25.0	2.91	0.0
3LFA	2.65	39.7	2.52	44.4	2.15	38.9	4.58	18.2	1.57	75.0	2.37	50.0	3.90	0.0
3MPT-1W	3.01	20.6	3.63	5.6	2.37	27.8	3.45	36.4	1.98	37.5	0.00	0.0	3.79	0.0
3MPT-2W	3.31	22.2	4.17	0.0	2.57	38.9	3.38	18.2	1.96	50.0	2.03	25.0	5.63	0.0

Table S5. *Cont.*

PDB	all		FAM1		FAM2		FAM4		FAM5		FAM6		FAM8	
	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success	$RMSD_{avg}$	% success
3MPT	3.04	22.2	3.57	5.6	2.54	38.9	3.48	27.3	2.13	25.0	2.50	0.0	5.64	25.0
3MW1	3.93	22.2	3.15	27.8	6.25	16.7	2.99	27.3	3.01	25.0	1.84	25.0	4.89	0.0
3QUD-1W	4.05	17.5	0.00	0.0	7.25	5.6	4.33	27.3	1.60	62.5	1.81	50.0	5.31	0.0
3QUD	4.44	20.6	4.96	5.6	7.38	11.1	2.62	36.4	2.67	50.0	1.65	50.0	2.33	0.0
3QUE-1W	5.59	7.9	3.15	5.6	9.07	0.0	3.47	18.2	1.77	12.5	0.88	25.0	0.00	0.0
3QUE	4.08	27.0	2.96	16.7	7.44	11.1	3.29	36.4	2.59	62.5	1.68	75.0	2.60	0.0
3ROC	4.04	14.3	4.33	5.6	6.41	5.6	1.91	27.3	2.13	12.5	1.86	75.0	3.73	0.0
3ZS5	2.47	28.6	2.46	55.6	1.89	33.3	4.17	9.1	2.14	12.5	2.65	0.0	2.65	0.0
3ZSG	2.32	25.4	1.98	55.6	2.96	22.2	2.61	0.0	1.70	25.0	4.09	0.0	0.00	0.0
3ZSH	4.88	17.5	5.80	5.6	7.78	0.0	3.37	27.3	3.19	62.5	1.81	25.0	4.57	25.0
3ZSI	4.72	19.0	5.35	0.0	7.34	11.1	3.94	27.3	2.49	62.5	1.90	50.0	2.28	0.0
3ZYA-1W	3.64	15.9	11.15	0.0	6.99	5.6	2.88	18.2	2.26	50.0	1.57	75.0	2.43	0.0
3ZYA	3.77	22.2	1.39	11.1	7.94	5.6	2.82	36.4	1.79	50.0	1.56	75.0	2.77	0.0
4DLJ	2.18	54.0	1.82	83.3	1.96	55.6	4.01	18.2	1.37	50.0	2.53	50.0	1.74	25.0
4EH2	3.35	42.9	2.02	55.6	2.70	50.0	5.85	9.1	2.34	75.0	4.64	25.0	6.11	0.0
4EH3	3.43	31.7	4.79	11.1	4.80	16.7	2.31	63.6	2.34	62.5	2.32	50.0	1.99	25.0
4EH4	3.01	12.7	3.19	16.7	4.18	5.6	1.72	27.3	2.82	12.5	0.00	0.0	0.00	0.0
4EH5	3.52	28.6	3.22	33.3	2.49	50.0	5.09	0.0	3.21	37.5	3.05	0.0	8.35	0.0
4EH6	2.80	25.4	2.90	22.2	2.10	33.3	3.59	27.3	2.20	37.5	8.20	0.0	3.25	0.0
4EH7	3.05	30.2	3.72	16.7	3.43	16.7	2.95	54.5	1.58	62.5	2.18	50.0	3.38	0.0
4EH8	3.62	14.3	5.40	0.0	4.58	5.6	4.28	18.2	1.88	50.0	2.48	50.0	4.82	0.0
4EWQ	2.44	20.6	1.97	55.6	0.00	0.0	0.00	0.0	1.84	25.0	3.15	25.0	10.00	0.0
4F9W	2.06	41.3	1.40	72.2	2.73	22.2	3.82	9.1	1.10	87.5	2.16	25.0	3.20	0.0
4F9Y	2.01	46.0	1.44	77.8	2.03	27.8	4.00	18.2	1.25	75.0	1.86	50.0	2.91	0.0
4FA2-1W	2.78	20.6	1.74	44.4	5.59	5.6	1.69	18.2	1.99	25.0	3.14	0.0	0.00	0.0
4FA2	2.36	23.8	1.78	44.4	3.93	16.7	2.16	9.1	2.44	25.0	1.95	25.0	0.00	0.0

Table S6. Original residue numbers of retained water molecules for each solvated protein target as defined in the PDB file.

Protein	W1	W2	Protein	W1	W2
1ZZ2	374		3FLY	1154	
2BAL	468	416	3FLZ	2021	
2QD9	365		3FMH	1183	
2ZAZ	560		3FMK	1045	
3FI4	435		3MPT	395	614
3FKN	2019		3QUD	369	
3FKO	1078		3QUE	364	
3FL4	363		3ZYA	2076	
3FLN	381		4FA2	594	
3FLW	1002				

Table S7. Maximum (MAX) and mean RMSD values (MEAN) for every binding site residues across crystallographic conformations.

Residue	MAX	MEAN	Residue	MAX	MEAN	Residue	MAX	MEAN
Pro29	1.561	1.035	Leu75	1.553	1.392	Lys152	5.040	3.627
Val30	2.188	1.833	Met78	1.653	1.375	Pro153	4.921	3.641
Gly31	5.404	4.650	Val83	2.148	1.570	Ser154	4.224	3.202
Ser32	7.012	6.486	Ile84	3.169	2.415	Asn155	3.821	2.869
Gly33	7.947	6.624	Gly85	1.943	1.353	Leu156	3.755	2.756
Ala34	10.166	9.195	Leu86	1.490	1.431	Ala157	3.702	2.713
Tyr35	13.823	11.621	Leu87	1.425	1.356	Val158	4.407	3.293
Gly36	6.221	5.546	Tyr103	0.636	0.464	Asn159	4.264	3.259
Ser37	2.605	2.172	Leu104	0.680	0.498	Glu163	3.906	2.941
Val38	0.988	0.709	Val105	1.420	1.393	Lys165	2.834	2.057
Cys39	0.663	0.474	Thr106	1.640	1.485	Ile166	2.841	2.104
Ala40	0.744	0.535	His107	3.510	3.037	Leu167	3.758	2.907
Val50	0.623	0.441	Leu108	1.676	1.130	Asp168	5.987	4.996
Ala51	0.740	0.486	Met109	5.187	4.113	Phe169	10.870	9.810
Val52	1.524	1.413	Gly110	3.746	2.964	Gly170	14.154	13.062
Lys53	1.298	1.030	Ala111	4.433	3.216	Leu171	19.251	15.720
Leu55	1.624	1.358	Asp112	4.639	3.452	Ala172	17.153	14.755
Arg67	5.150	4.078	Asn114	6.971	4.839	Arg173	23.264	20.150
Thr68	1.133	0.779	Asn115	6.018	4.566	His174	24.979	18.560
Arg70	3.788	3.411	Lys118	11.021	8.645	Val183	13.070	9.210
Glu71	1.586	1.294	His148	3.703	2.629	Ala184	12.399	9.757
Arg73	1.715	1.267	Asp150	4.920	3.560	Thr185	9.048	6.856
Leu74	2.314	1.928	Leu151	4.390	3.306			

Reference

1 Astolfi, A.; Iraci, N.; Manfroni, G.; Barreca, M.L.; Cecchetti, V. A Comprehensive Structural Overview of p38α MAPK in Complex with Type I Inhibitors. *ChemMedChem* **2015**, *10*, 957–969.