Supplementary Information

Table S1. The similarity between 19 ligands by the Tanimoto coefficient (FCFP4) [a].

	2BMC	2C6E	2J50	2NP8	2W1C	2W1E	2W1F	2W1G	2X6D	2X6E	2XRU	3COH	3FDN	3H0Y	3H0Z	3M11	3MYG	3NRM	3P9J
2BMC	100	28	32	17	20	18	25	16	26	28	54	23	24	21	27	28	17	11	23
2C6E	28	100	21	15	18	16	22	17	21	16	32	19	20	20	32	20	19	16	18
2J50	32	21	100	18	21	19	24	17	25	25	34	15	14	20	20	19	8	5	28
2NP8	17	15	18	100	16	19	19	16	13	14	22	13	21	31	14	19	7	6	19
2W1C	20	18	21	16	100	69	64	71	26	17	23	19	20	21	26	16	15	15	18
2W1E	18	16	19	19	69	100	59	75	20	13	21	19	20	16	18	26	13	15	19
2W1F	25	22	24	19	64	59	100	53	18	14	28	20	24	21	25	21	15	18	25
2W1G	16	17	17	16	71	75	53	100	19	13	22	21	16	11	15	19	13	15	17
2X6D	26	21	25	13	26	20	18	19	100	66	28	21	12	20	22	20	19	15	13
2X6E	28	16	25	14	17	13	14	13	66	100	29	18	10	16	17	15	27	23	9
2XRU	54	32	34	22	23	21	28	22	28	29	100	25	23	25	27	28	18	14	21
3COH	23	19	15	13	19	19	20	21	21	18	25	100	18	16	18	20	14	13	17
3FDN	24	20	14	21	20	20	24	16	12	10	23	18	100	22	23	22	15	16	22
3H0Y	21	20	20	31	21	16	21	11	20	16	25	16	22	100	26	25	6	5	22
3H0Z	27	32	20	14	26	18	25	15	22	17	27	18	23	26	100	30	12	12	21
3M11	28	20	19	19	16	26	21	19	20	15	28	20	22	25	30	100	12	14	20
3MYG	17	19	8	7	15	13	15	13	19	27	18	14	15	6	12	12	100	60	8
3NRM	11	16	5	6	15	15	18	15	15	23	14	13	16	5	12	14	60	100	8
3P9J	23	18	28	19	18	19	25	17	13	9	21	17	22	22	21	20	8	8	100
IC_{50} [b]	**27.0**	**0.8**	**24.0**	**42.0**	**10.0**	**12.0**	**5.9**	**3.0**	**12.0**	**15.0**	**9.0**	**4.0**	**33.0**	**6.0**	**4.3**	**43.0**	**4.0**	**4.0**	**31.0**

[a] For simplicity, absolute values × 100 are represented; and [b] Enzyme inhibition IC_{50} (nM).

Table S2. The cross-docking scores of 19 crystal structures.

	2BMC	2C6E	2J50	2NP8	2W1C	2W1E	2W1F	2W1G	2X6D	2X6E	2XRU	3COH	3FDN	3H0Y	3H0Z	3M11	3MYG	3NRM	3P9J
2BMC	79.9	-[a]	79.5	27.8	65.1	60.0	55.9	61.1	70.2	74.2	65.1	36.3	40.5	-	-	34.6	56.3	32.1	44.7
2C6E	4.4	72.3	30.3	-	-	-	-	-	46.6	-	9.2	34.5	-	-	-	-	20.4	-	-
2J50	88.0	-	85.1	64.6	87.8	86.8	76.6	88.6	85.6	87.2	80.0	71.7	74.6	-	19.0	17.2	67.7	52.3	47.3
2NP8	41.8	-	50.2	39.3	44.0	41.2	36.6	38.6	44.6	42.3	37.0	42.0	39.4	43.4	23.3	-	40.6	32.1	42.5
2W1C	-	-	49.3	37.4	44.7	41.1	36.1	43.7	76.3	27.4	-	48.5	40.9	-	36.3	-	48.6	31.2	33.4
2W1E	26.5	-	43.0	26.8	31.1	24.7	27.3	25.5	60.9	-	-	40.6	25.8	19.0	1.59	-	18.1	20.6	27.6
2W1F	-	-	-	61.7	-	60.9	61.8	-	-	-	-	55.4	61.5	57.0	-	-	-	61.2	60.8
2W1G	32.2	-	43.6	32.1	42.3	32.1	28.6	38.1	59.7	25.6	24.6	45.8	31.9	-	26.6	-	36.4	29.7	29.3
2X6D	70.3	-	71.2	70.4	73.4	77.6	59.7	73.0	78.0	-	59.0	-	70.9	62.5	35.0	57.2	-	-	75.5
2X6E	56.0	-	55.0	65.8	66.4	61.6	47.7	63.4	66.5	55.5	41.1	-	60.2	51.6	26.7	46.9	-	-	59.8
2XRU	84.6	50.1	88.1	73.6	86.7	87.8	72.1	84.8	92.9	88.4	84.6	81.3	69.6	-	68.7	37.6	74.9	62.1	49.2
3COH	-	-	58.8	-	53.0	61.2	-	55.1	-	-	-	61.5	62.4	-	-	-	64.1	60.0	55.8
3FDN	-	-	-	-	-	-	-	-	-	-	-	1.2	23.5	-	21.0	-	-	-	-
3H0Y	26.6	-	27.3	8.6	-	29.9	39.7	19.6	43.1	18.5	32.0		22.8	44.4		48.0	-	-	43.8
3H0Z	78.1	38.5	68.1	59.2	65.3	66.6	36.7	67.0	51.1	65.4	57.2	62.7	62.0	40.3	51.8	42.1	49.1	7.0	63.5
3M11	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	54.5	-	-	-
3MYG	53.5	-	65.3	38.4	65.9	57.3	-	65.1	42.6	70.0	54.4	67.9	64.4	-	37.7	-	59.4	57.9	23.1
3NRM	-	-	57.4	55.3	60.9	59.1	56.4	59.7	-	-	-	56.8	57.3	-	-	-	69.6	67.0	60.7
3P9J	-	-	46.2	60.2	13.7	57.1	54.8	32.9	-	-	-	57.2	53.0	52.8	-	-	39.9	49.4	60.9

[a] A ligand does not bind to a protein.

Table S3. *In vitro* kinase inhibition assay of benzo[*d*]midazole-4,7-dione analogues.
(a) Compound **16** at Aurora-A(h) [a].

Concentration	Counts	Mean (Counts-Blanks)	Activity (% Inhibition)	Mean (%)	SD [b]
0.01 μM	3932	3847	4		
0.03 μM	3566	3481	13		
0.10 μM	3932	3847	4		
0.30 μM	3609	3524	12		
1.00 μM	3159	3074	23	/	/
3.00 μM	3236	3151	21		
10.0 μM	1731	1646	59		
30.0 μM	541	456	89		
100.0 μM	149	64	98		
Control	4068	4005	1	0	3
	4116		−1		
	4226		−3		
	3951		9		
Blank	72	/	/	/	/
	98				

[a] ATP Concentration: 15 μM; [b] Standard deviation.

Table S4. (a) Compound **17** at Aurora-A(h) [a].

Concentration	Counts	Mean (Counts-Blanks)	Activity (% Inhibition)	Mean (%)	SD [b]
0.01 μM	3488	3366	10		
0.03 μM	3682	3560	5		
0.10 μM	3658	3536	6		
0.30 μM	3632	3510	6		
1.00 μM	3212	3090	18	/	/
3.00 μM	3177	3055	18		
10.0 μM	1328	1206	68		
30.0 μM	434	312	92		
100.0 μM	121	−1	100		
Control	3839	3747	1	0	8
	3568		8		
	4255		−10		
	3814		1		
Blank	111	/	/	/	/
	133				

[a] ATP Concentration: 15 μM; and [b] Standard deviation.

Table S5. Aurora-B(h) [a].

Compound	Counts	Mean (Counts-Blanks)	Activity (% Inhibition)	Mean (%)	SD [b]
12	1265 1115	998	68 72	70	3
16	681 723	510	85 84	84	1
17	969 1013	799	77 75	76	1
Control	3948 3306 3561 3301	3337	−13 7 −1 7	0	9
Blank	204 180	/	/	/	/

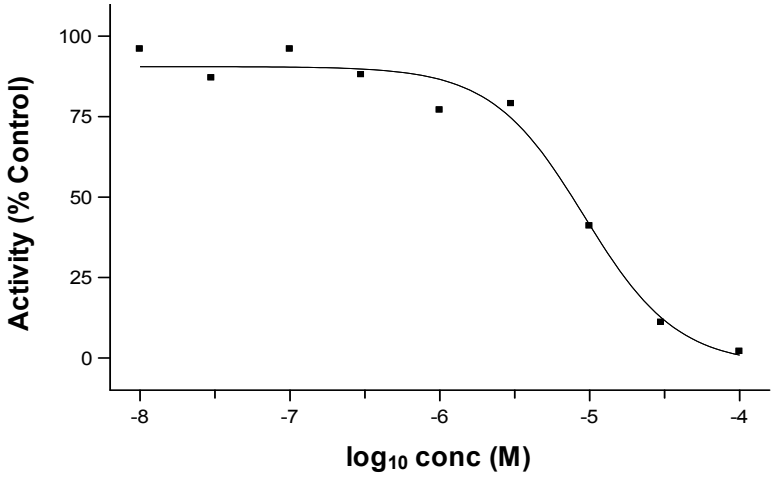
[a] ATP Concentration: 10 μM; [b] Standard deviation.

Table S6. Aurora-C(h) [a].

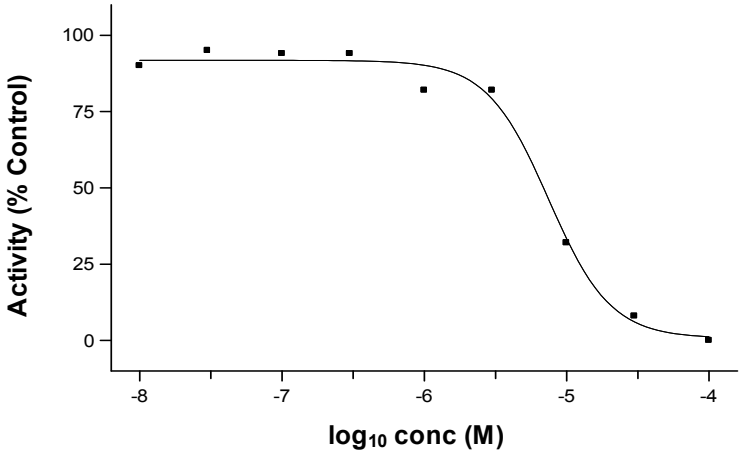
Compound	Counts	Mean (Counts-Blanks)	Activity (% Inhibition)	Mean (%)	SD [b]
12	6890 6112	6313	2 13	7	8
16	6097 6859	6290	14 2	8	8
17	6049 5677	5675	14 20	17	4
Control	7347 7527 6956 6256	6834	−5 −7 1 11	0	8
Blank	208 168	/	/	/	/

[a] ATP Concentration: 15 μM; and [b] Standard deviation.

Figure S1. Logarithm of concentration *vs.* activity (%) of aurora-A (h) for Compound **16** and **17**.



Compound **16**



Compound **17**