

## Supplementary information

Table1. The compound structures of the training set

Compound No.	R <sup>3</sup>	R <sup>4</sup>	R <sup>5</sup>	IC <sub>50</sub> (nM)
<b>1</b>	H	H	H	66
<b>2</b>	2-F	H	H	175
<b>3</b>	3-F	H	H	62
<b>4</b>	3-Cl	H	H	62
<b>5</b>	3-Br	H	H	19
<b>6</b>	3-OMe	H	H	140
<b>7</b>	4-F	3-F	H	21
<b>8</b>	4-F	3-Me	H	86
<b>9</b>	4-F	3-Cl	H	28
<b>10</b>	4-F	3-Br	H	44

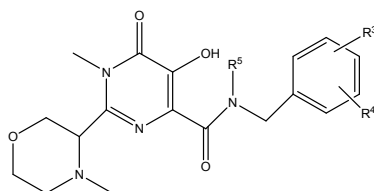


Table1 (continued)

Compound No.	R <sup>1</sup>	R <sup>2</sup>	R <sup>3</sup>	IC <sub>50</sub> (nM)
11	H		Me	80
12	H		H	120
13	H		Me	90
14	H		H	70
15	H		Me	20
16	H		H	40
17	H		H	130
18	H		H	20
19	H		Me	20
20	H		H	50
21	Me		Me	550
22	H		Me	100
23	H		H	30

Table1 (continued)

Compound No.	R <sup>1</sup>	R <sup>2</sup>	R <sup>3</sup>	IC <sub>50</sub> (nM)
24	H		Me	100
25	H		H	60
26	Me		Me	4
27	Me		Me	20
28	Me		Me	15
29	Me		--	440
30	Me		--	180
31	Me		--	200
32	Me		--	130
33	Me		--	30
34	Me		--	61
35	Me		--	20
36	Me		--	30

Table1 (continued)

Compound No.	R <sup>1</sup>	R <sup>2</sup>	R <sup>3</sup>	IC <sub>50</sub> (nM)
37	Me		--	21
38	Me		--	62
39	Me		--	60
40	Me		--	70
41	Me		--	140
42	Me		--	200
43	Me		--	250
44	Me		--	130
45	Me		--	41
46	Me		--	32
47	Me		--	15
48	Me		--	20
49	Me		--	52

Table1 (continued)

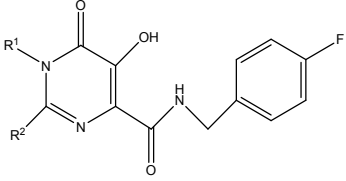
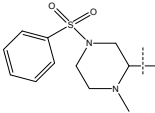
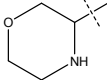
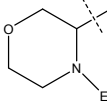
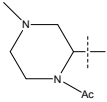
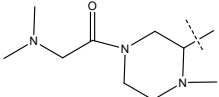
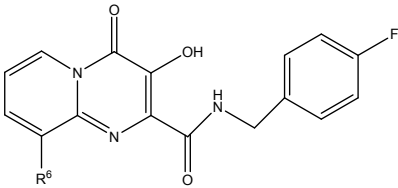
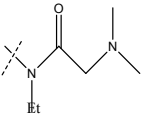
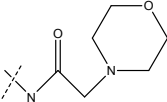
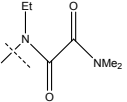
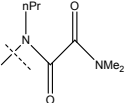
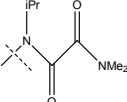
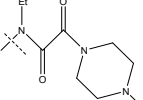
Compound No.	R <sup>1</sup>	R <sup>2</sup>	R <sup>3</sup>	IC <sub>50</sub> (nM)
				
<b>50</b>	Me		--	7
<b>51</b>	Me		--	50
<b>52</b>	H		--	33
<b>53</b>	Me		--	4000
<b>54</b>	Me		--	4

Table 2. The compound structures of the test set

Compound No.	R <sup>1</sup>	R <sup>2</sup>	R <sup>3</sup>	IC <sub>50</sub> (nM)
71	H		Me	20
72	H		Me	250
73	H		H	220
74	H		Me	14
75	Me		H	6
76	Me		--	100
77	Me		--	100
78	Me		--	50
79	Me		--	12
80	H		--	30

Table 3 The compound structures of the test set

Compound No.	R <sup>6</sup>	IC <sub>50</sub> (nM)
		
81	NHEt	36
82	NHCOPh	18
83		185
84		23
85		36
86		18
87		21
88		21