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Supplementary material

SUPPLEMENTARY MATERIAL TO

Application of an R-group search technique in the molecular design of dipeptidyl boronic acid proteasome inhibitors

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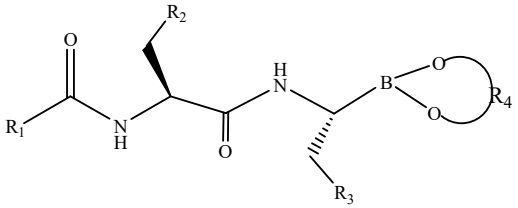
TABLE S-I. Structures and bioactivities of the 40 dipeptidyl boronic acid derivatives



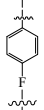
No.	R_1	R_2	R_3	R_4	Exp. pIC_{50}	Pred. pIC_{50}
1					–0.28	–0.27
2					–0.68	–0.66
3[a]					–0.51	–0.60
4					–0.62	–0.58
5					–0.049	0.080
6					–0.71	–0.39
7					–0.28	–0.26

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TABLE S-I. Continued

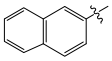
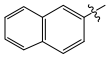
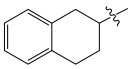
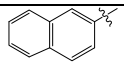
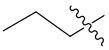
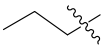
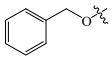
No.	R_1	R_2	R_3	R_4	Exp. pIC_{50}	Pred. pIC_{50}
8					–0.72	–0.84
9					–0.83	–0.81
10					–0.10	–0.32
11		CH_3,CH_3			–1.59	–1.32
12					–1.15	–1.32
13[a]		CH_3,CH_2CH_3			–1.24	–1.21
14					–0.63	–0.69
15					–0.88	–0.79
16					–0.79	–0.79
17					–0.56	–0.31
18					–0.16	–0.02
19					–0.53	–0.46
20					–0.064	–0.061
21					–0.061	–0.051
22		CH_3,CH_3			–0.84	–0.68
23					0.12	0.25
24					–0.13	–0.06

TABLE S-I. Continued

No.	R_1	R_2	R_3	R_4	Exp. pIC_{50}	Pred. pIC_{50}
25					–0.39	–0.44
26					–0.064	–0.105
27	CH_3				–0.93	–0.81
28	CH_3				–0.37	–0.56
29[a]	CH_3				–0.44	–0.64
30					–1.21	–1.12
31[a]					–2.06	–1.73
32					–1.69	–1.94
33					–2.08	–2.23
34					–2.67	–2.17
35[a]					–1.61	–1.53
36					–0.52	–0.61
37[a]					–0.04	–0.06
38				H,H	–0.21	–0.13
39				H,H	0.08	–0.39
40				H,H	–0.29	–0.26

[a]Test set samples