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3C-like 蛋白酶抑制剂的构效关系、分子对接和分子动力学

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QSAR, Molecular Docking and Molecular Dynamics of 3C-like Protease Inhibitors

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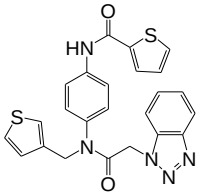
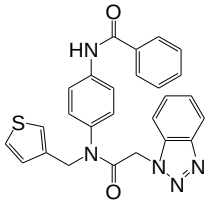
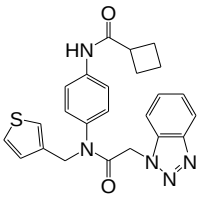
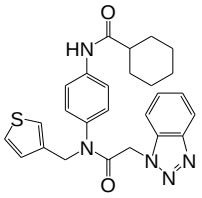
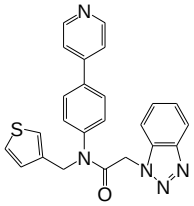
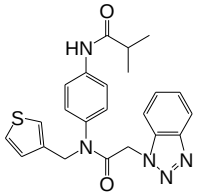
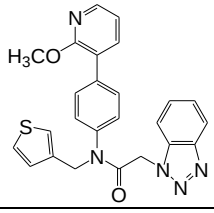
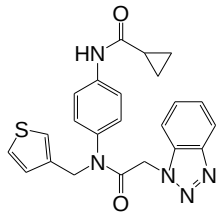
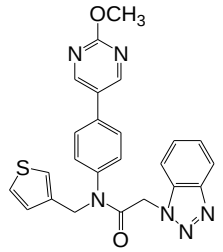
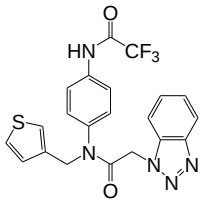
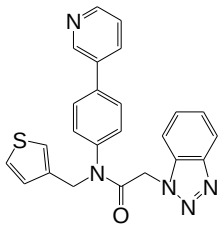
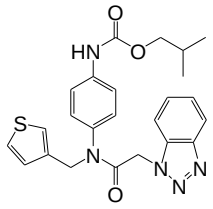
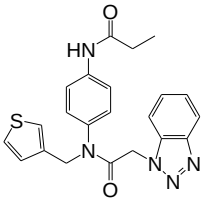
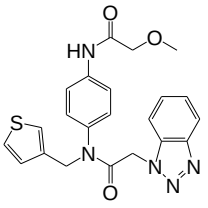
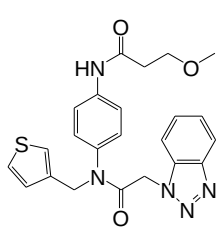
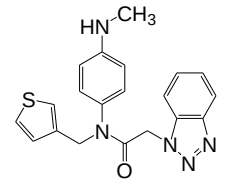
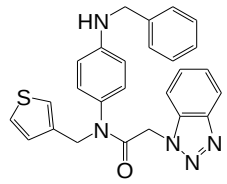
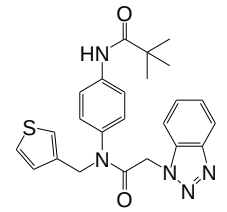
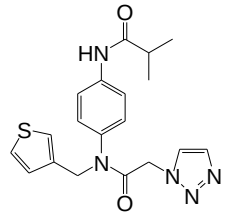
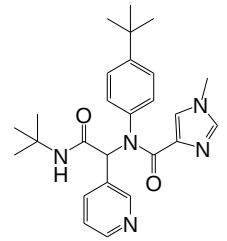
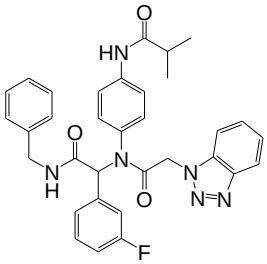
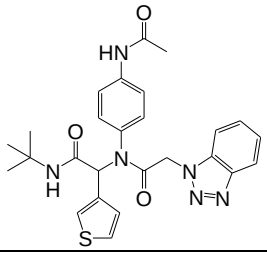
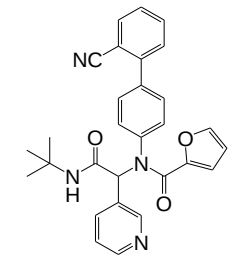
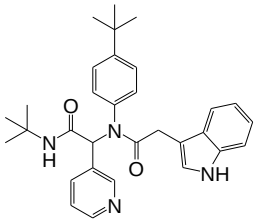
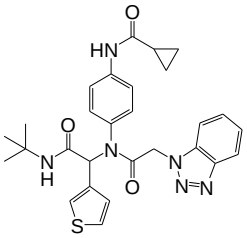
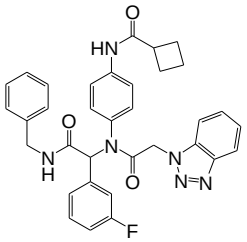
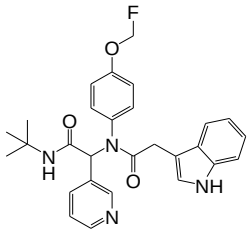
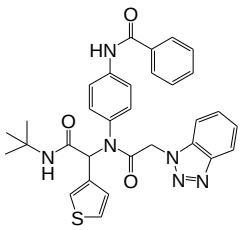
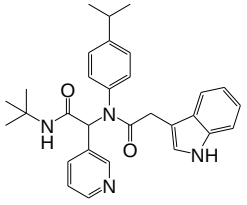
表 S1　所有的分子结构及其对应的生理活性

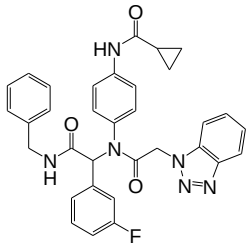
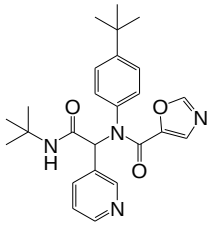
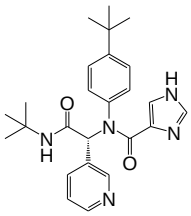
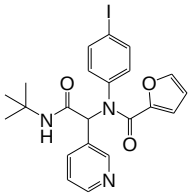
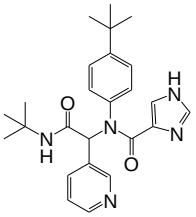
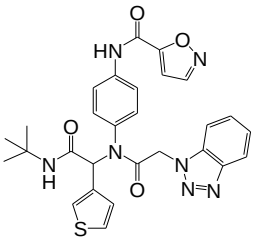
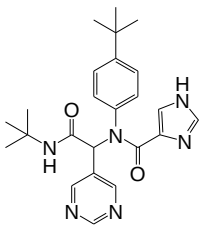
Table S1　All structures and inhibitory activities of the dataset

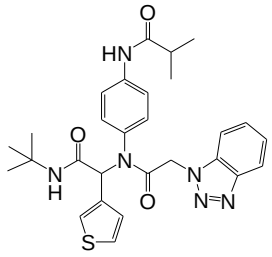
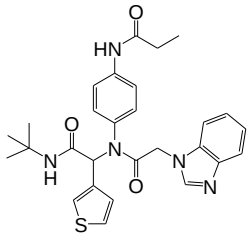
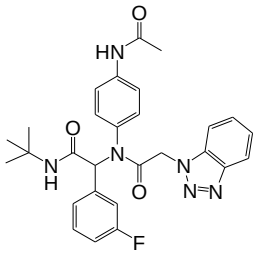
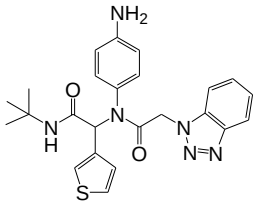
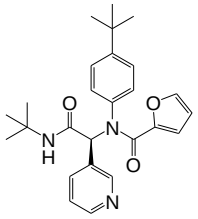
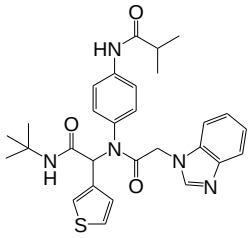
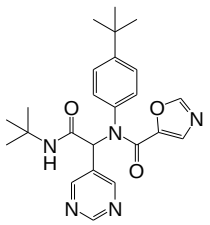
No.	Molecular structure	Actual pIC_{50}	Predicted pIC_{50}					
			Alignment-I		Alignment-II		Alignment-III	
			CoMFA	**CoMSIA**	CoMFA	CoMSIA	CoMFA	CoMSIA
1		6.48	5.97	**6.54**	6.31	6.10	6.23	5.91
2		6.39	5.90	**6.33**	6.45	6.10	6.46	5.87
3		5.92	5.79	**5.87**	5.70	5.77	5.89	5.69
4[t]		5.92	5.75	**6.02**	5.58	5.36	4.85	5.51
5[t]		5.82	5.48	**5.73**	5.66	5.70	5.82	5.69
6[t]		5.80	5.80	**5.80**	5.12	5.22	4.89	5.50
7		5.77	5.76	**5.80**	5.64	5.71	5.75	5.69

8		5.72	5.55	**5.71**	5.97	6.14	5.62	5.79
9		5.70	5.53	**5.70**	5.95	5.76	5.85	5.70
10		5.66	5.80	**5.65**	5.49	5.25	5.53	5.70
11		5.62	5.49	**5.51**	5.50	5.70	5.65	5.70
12		5.55	5.77	**5.53**	5.74	5.76	5.63	5.69
13		5.51	5.53	**5.55**	5.67	5.82	5.71	5.80
14		5.51	5.80	**5.53**	5.58	5.46	5.68	5.77
15		5.43	5.82	**5.44**	5.35	5.15	5.34	5.59

16		5.32	5.61	**5.34**	5.38	5.66	5.20	5.67
17[t]		5.28	5.37	**5.13**	5.70	5.70	5.79	5.65
18[t]		5.06	5.41	**5.29**	5.59	5.38	5.34	5.71
19		4.80	5.55	**4.82**	4.66	4.99	4.68	5.27
20		5.89	5.10	**5.90**	5.85	5.66	5.81	5.11
21		5.82	5.15	**5.83**	5.65	5.78	5.94	5.53
22		5.74	5.23	**5.74**	5.44	5.39	5.55	5.51

23		5.66	5.17	**5.60**	5.59	5.10	5.68	4.93
24		5.66	4.95	**5.63**	5.57	5.26	5.68	5.02
25		5.57	5.25	**5.61**	5.60	5.39	5.51	5.40
26		5.47	5.20	**5.50**	5.38	5.51	5.50	5.38
27[t]		5.41	4.98	**5.37**	5.03	4.90	4.99	5.00
28[t]		5.38	5.41	**5.23**	5.06	4.79	5.87	5.49
29		5.16	4.95	**5.22**	5.36	5.33	5.38	5.04

30		5.15	5.55	**5.17**	5.06	4.89	5.11	4.91
31		5.07	4.85	**5.08**	4.75	4.80	4.98	4.79
32[t]		5.03	5.36	**4.90**	4.66	5.11	5.43	5.13
33		5.02	5.11	**5.04**	5.15	5.48	4.91	5.22
34		4.95	5.11	**4.96**	4.79	4.86	4.75	4.75
35[t]		4.83	5.07	**4.83**	5.66	5.54	5.11	5.43
36		4.81	5.12	**4.80**	4.81	4.79	4.75	4.72

37		4.76	4.94	**4.73**	4.57	4.52	4.80	5.10
38[t]		4.74	5.02	**4.61**	4.35	4.39	4.38	5.07
39		4.73	5.01	**4.77**	5.16	5.33	4.92	5.38
40		4.66	4.96	**4.63**	4.68	4.90	4.46	5.09
41		4.45	4.98	**4.47**	4.43	4.90	4.49	4.84
42		4.28	4.86	**4.25**	4.72	4.51	4.47	5.16
43		4.25	5.15	**4.26**	4.56	4.73	4.60	4.75

[t] means the molecule belonged to the test set. The optimal results are shown in bold.