

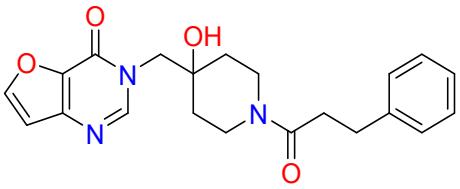
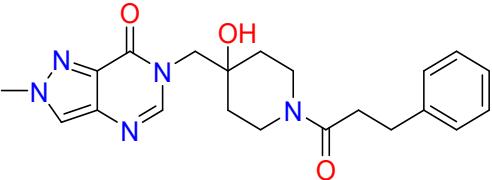
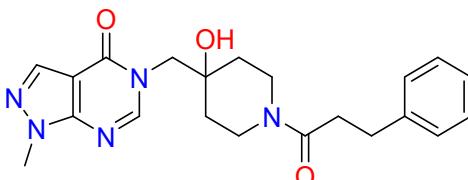
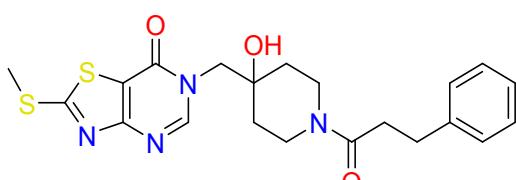
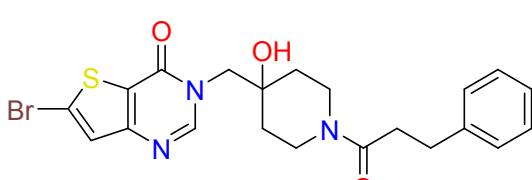
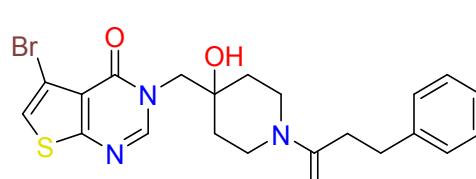
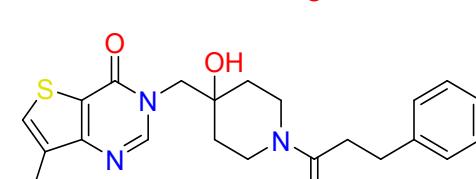
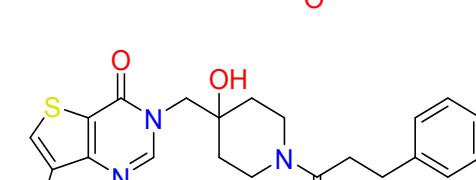
Supporting Information

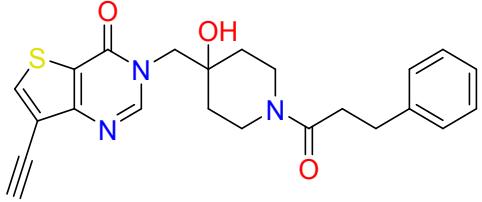
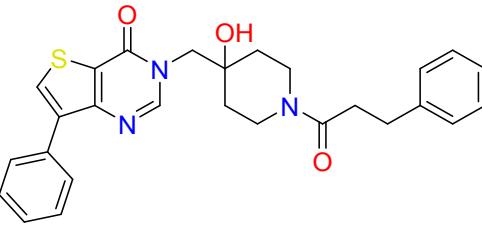
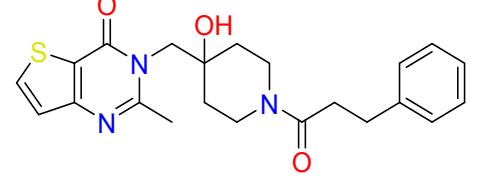
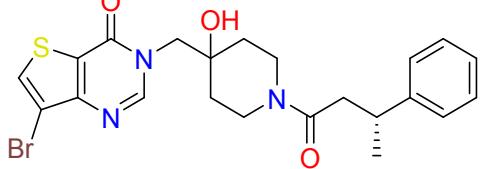
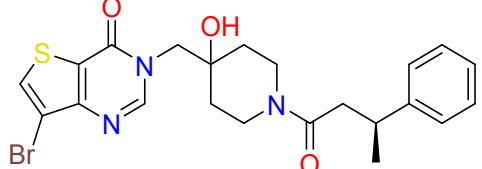
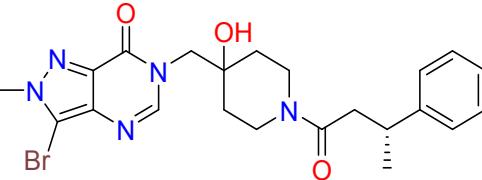
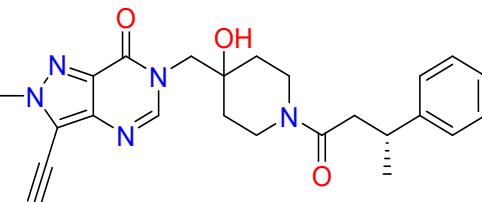
Supporting Information

Table S1. Compound structures and their corresponding biological activities; **Figure S2.** The scatter diagram of the PB1 scores versus experimental pIC_{50} values with the corresponding squared Pearson's correlation coefficient (R^2); **Figure S3.** The scatter diagram of the PB3 scores versus experimental pIC_{50} values with the corresponding squared Pearson's correlation coefficient (R^2); **Figure S4.** The scatter diagram of the PB4 scores versus experimental pIC_{50} values with the corresponding squared Pearson's correlation coefficient (R^2); **Figure S5.** The scatter diagram of the GB1 scores versus experimental pIC_{50} values with the corresponding squared Pearson's correlation coefficient (R^2); **Figure S6.** The scatter diagram of the GB2 scores versus experimental pIC_{50} values with the corresponding squared Pearson's correlation coefficient (R^2); **Figure S7.** The scatter diagram of the GB5 scores versus experimental pIC_{50} values with the corresponding squared Pearson's correlation coefficient (R^2); **Figure S8.** The scatter diagram of the GB6 scores versus experimental pIC_{50} values with the corresponding squared Pearson's correlation coefficient (R^2); **Figure S9.** The scatter diagram of the GB7 scores versus experimental pIC_{50} values with the corresponding squared Pearson's correlation coefficient (R^2).

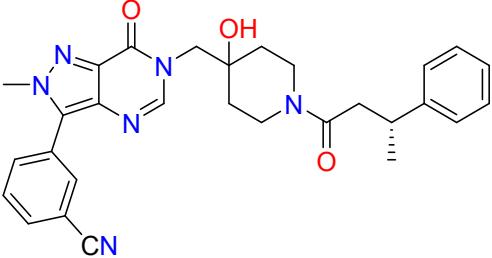
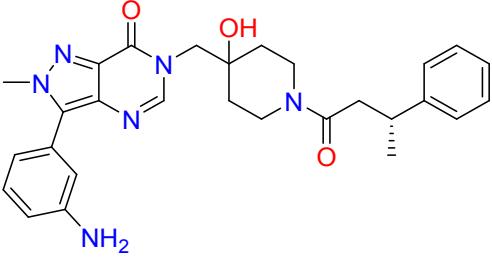
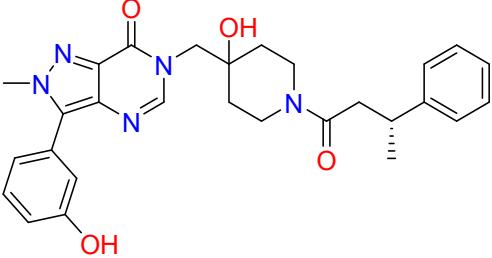
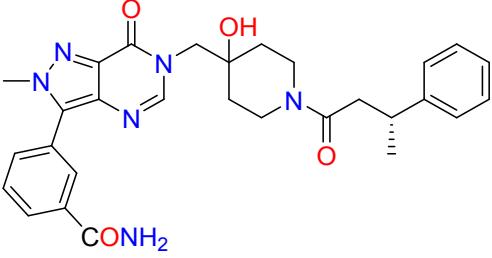
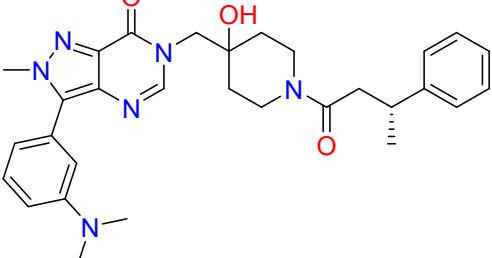
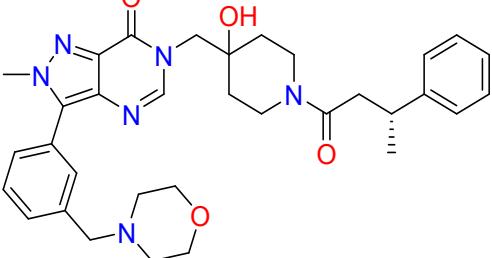
Table S1. Compound structures and their corresponding biological activities.

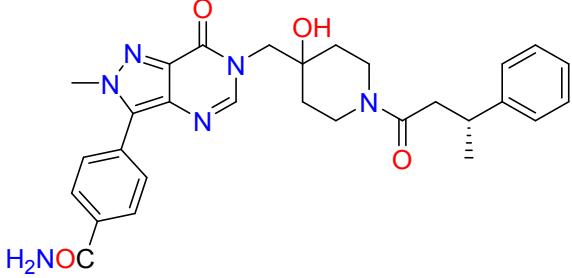
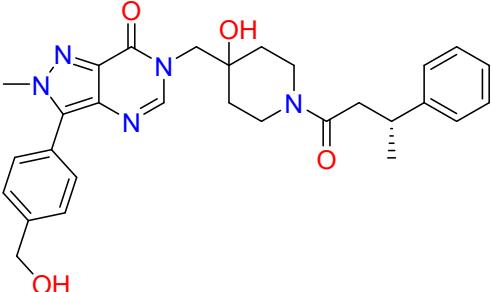
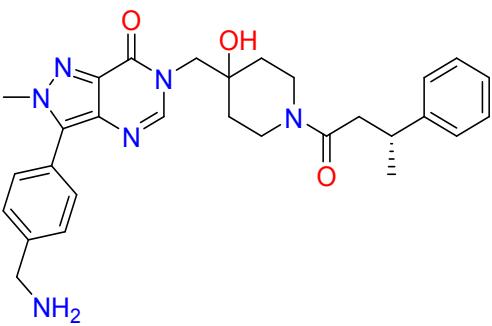
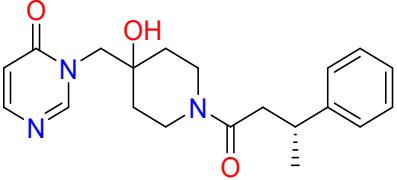
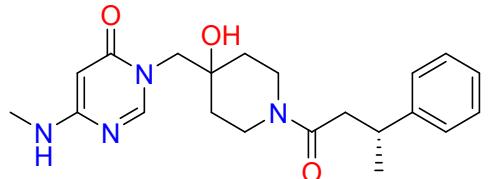
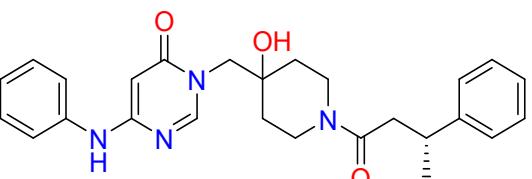
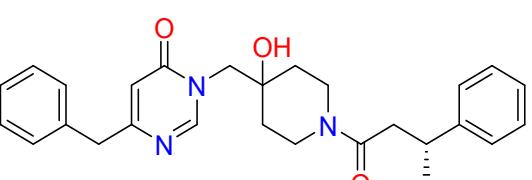
ID	Structure	IC_{50} (μM)	pIC_{50}
1 ^a		471 (K_D)	3.33
2		23	4.64
3		78	4.11
4		87	4.06

5		115	3.94
6		44	4.36
7		32	4.49
8		130	3.89
9		60	4.22
10		34	4.47
11		13	4.89
12		20	4.7

13		8	5.1
14		10	5
15 ^b		>200	#VALU E!
16 5N9R		0.3	6.52
ent-16		46	4.34
17		0.3	6.52
18		0.24	6.62

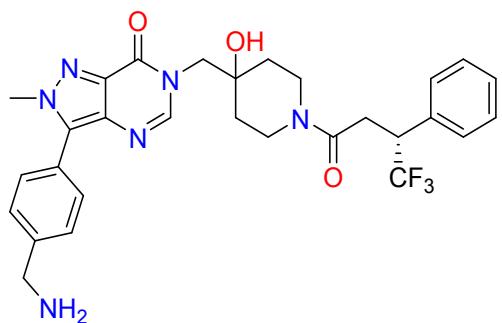
19		0.3	6.52
20		0.33	6.48
21		0.56	6.25
22		0.035	7.46
23		0.03	7.52
24		0.09	7.05
25		1.4	5.85

26		0.15	6.82
27		0.024	7.62
28		0.039	7.41
29		0.03	7.52
30		0.075	7.12
31		0.25	6.6

32		0.05	7.3
33		0.04	7.4
34		0.006	8.22
35		23	4.64
36		4.2	5.38
37		1.9	5.72
38		90	4.05

39		2.8	5.55
40		0.12	6.92
41		7.2	5.14
42		0.39	6.41
43		12	4.92
44		1.4	5.85
45		1.1	5.96
46 6F5H		0.09	7.05

47
5N9T



0.022 7.66

^aThe initial binding fragment (compound 1) was not used in our study.

^bBecause there is no exact activity value, compound 15 was not used in our study.

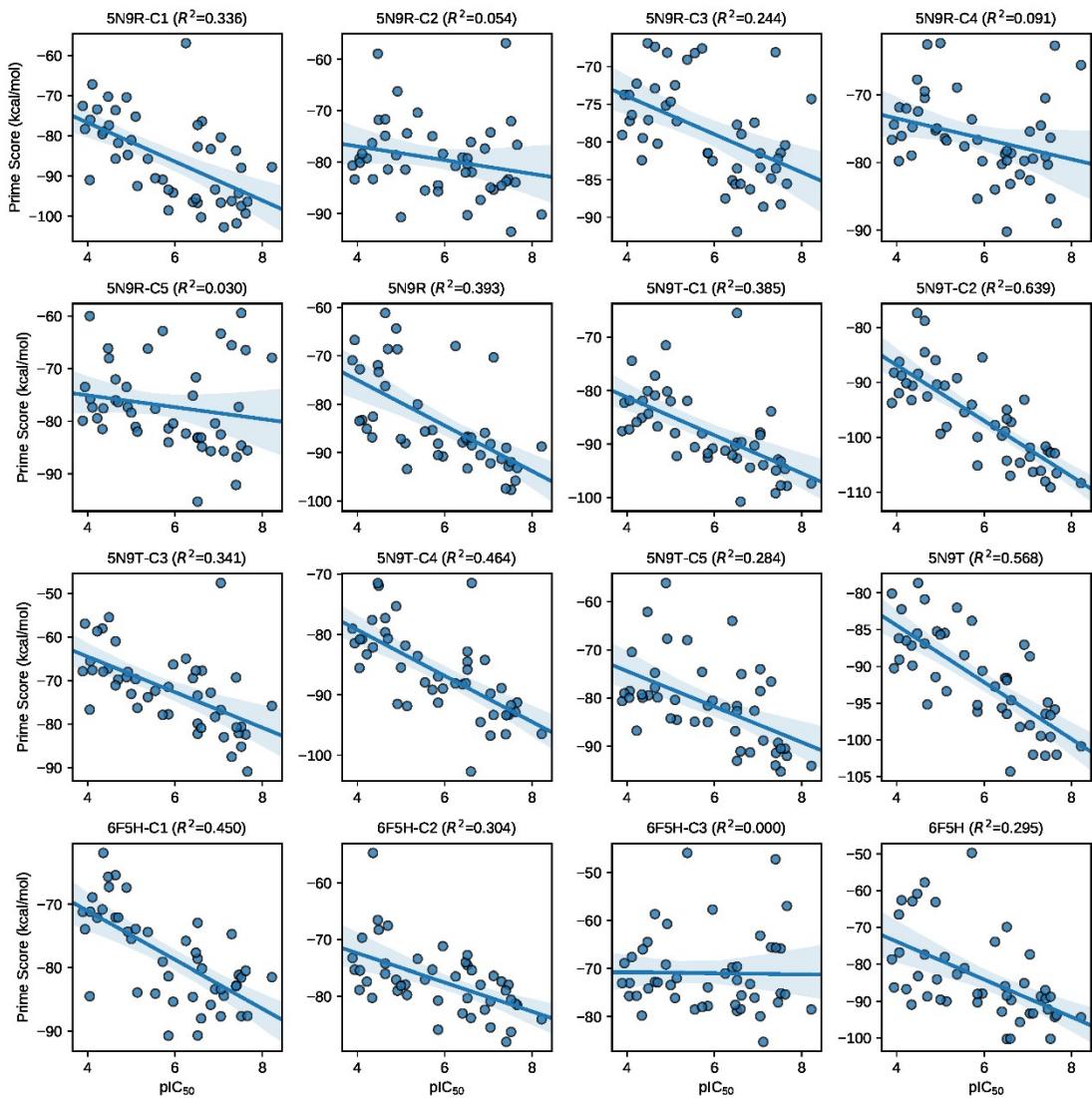


Figure S1. The scatter diagram of the Prime score versus experimental pIC₅₀ values with the corresponding squared Pearson's correlation coefficient (R^2).

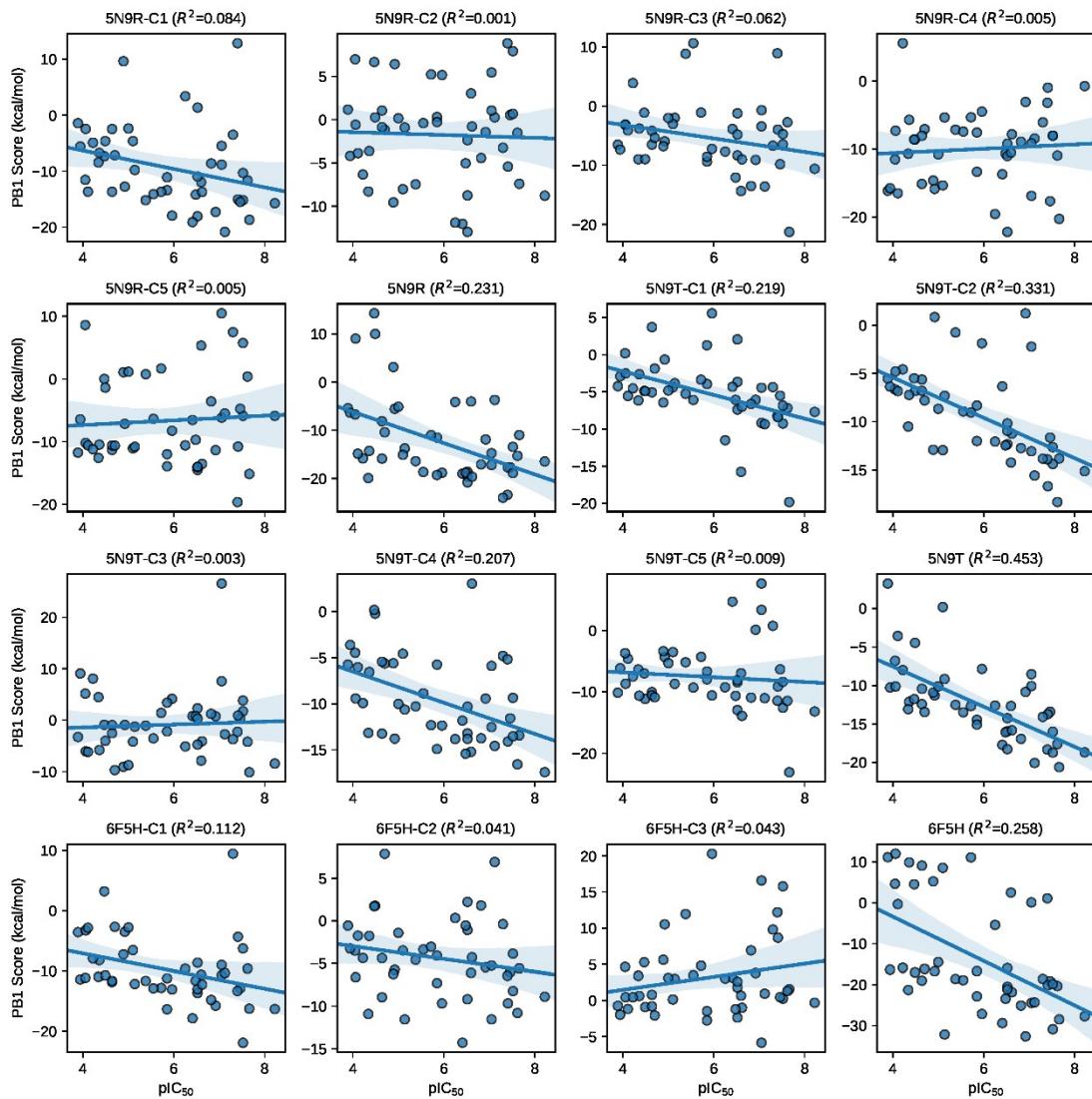


Figure S2. The scatter diagram of the PB1 scores versus experimental pIC₅₀ values with the corresponding squared Pearson's correlation coefficient (R^2).

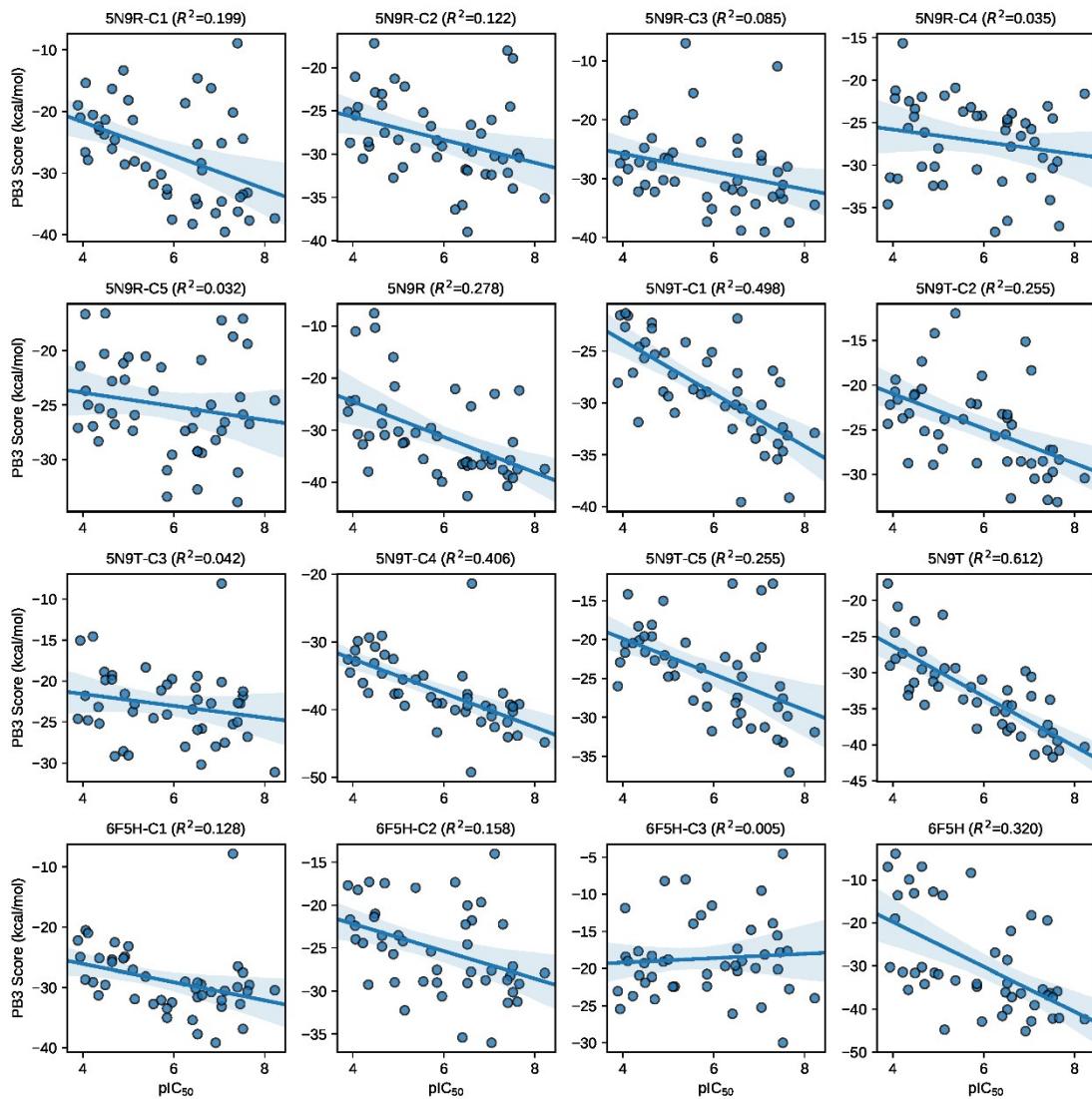


Figure S3. The scatter diagram of the PB3 scores versus experimental pIC₅₀ values with the corresponding squared Pearson's correlation coefficient (R^2).

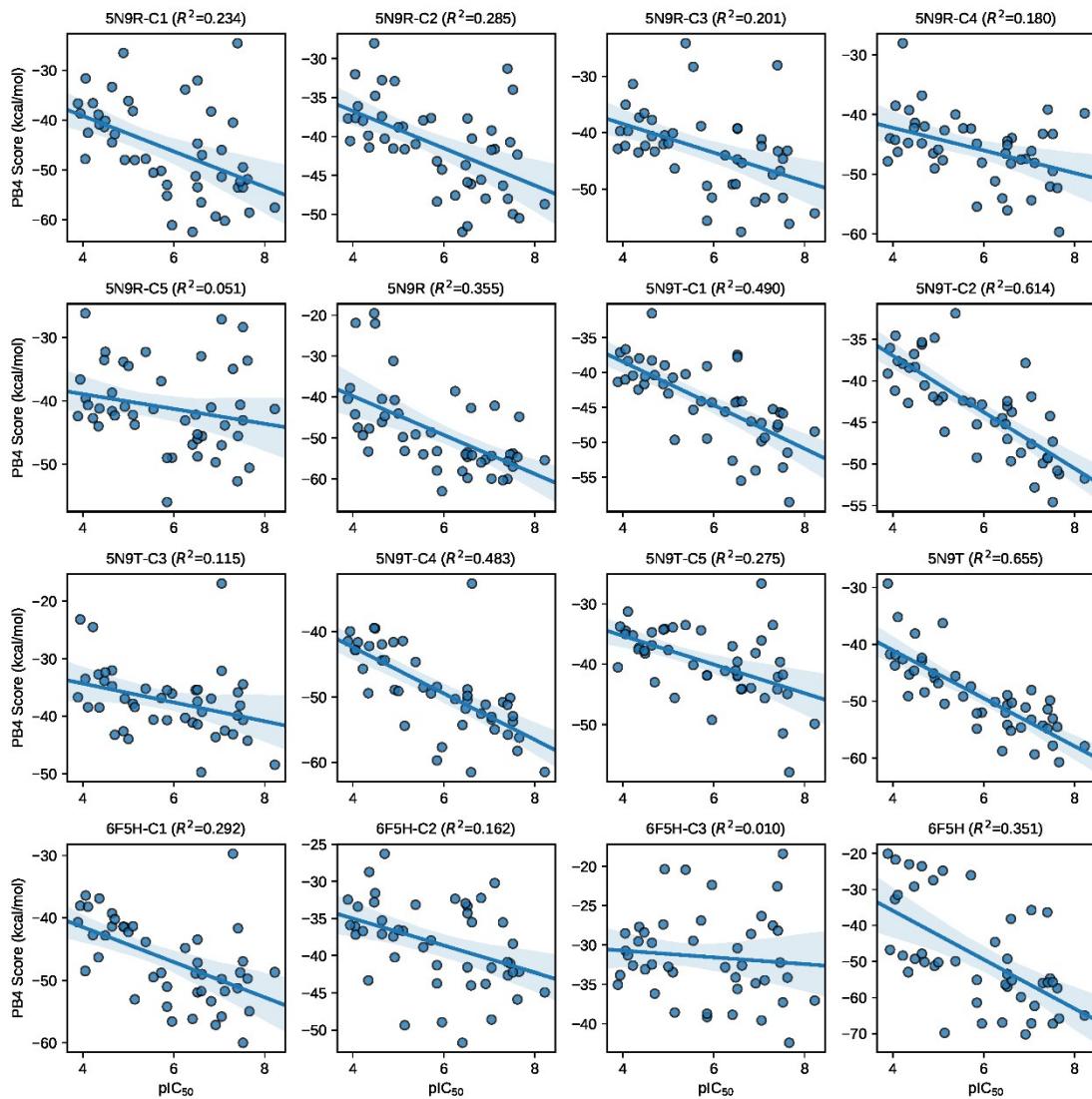


Figure S4. The scatter diagram of the PB4 scores versus experimental pIC₅₀ values with the corresponding squared Pearson's correlation coefficient (R^2).

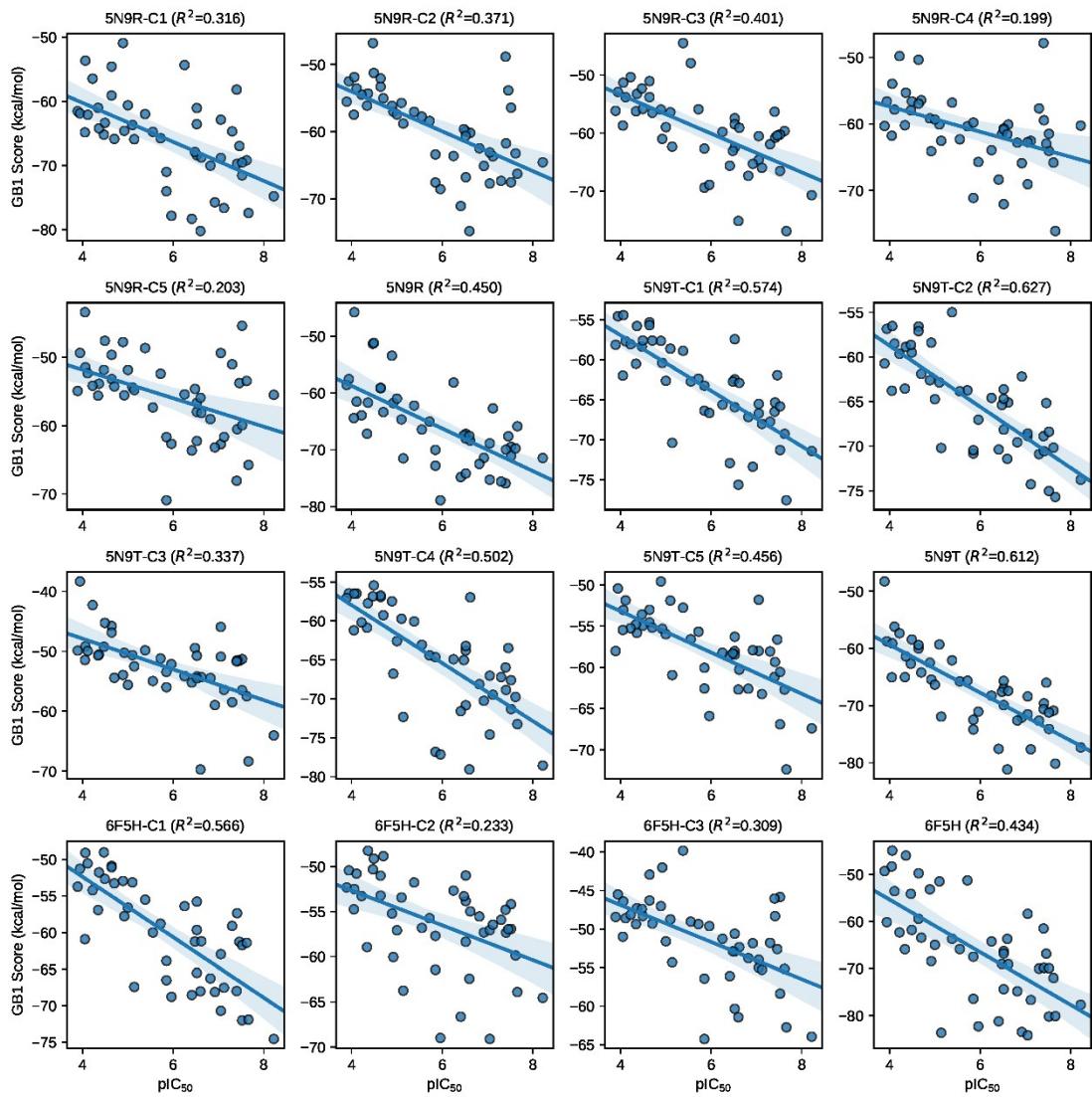


Figure S5. The scatter diagram of the GB1 scores versus experimental pIC₅₀ values with the corresponding squared Pearson's correlation coefficient (R^2).

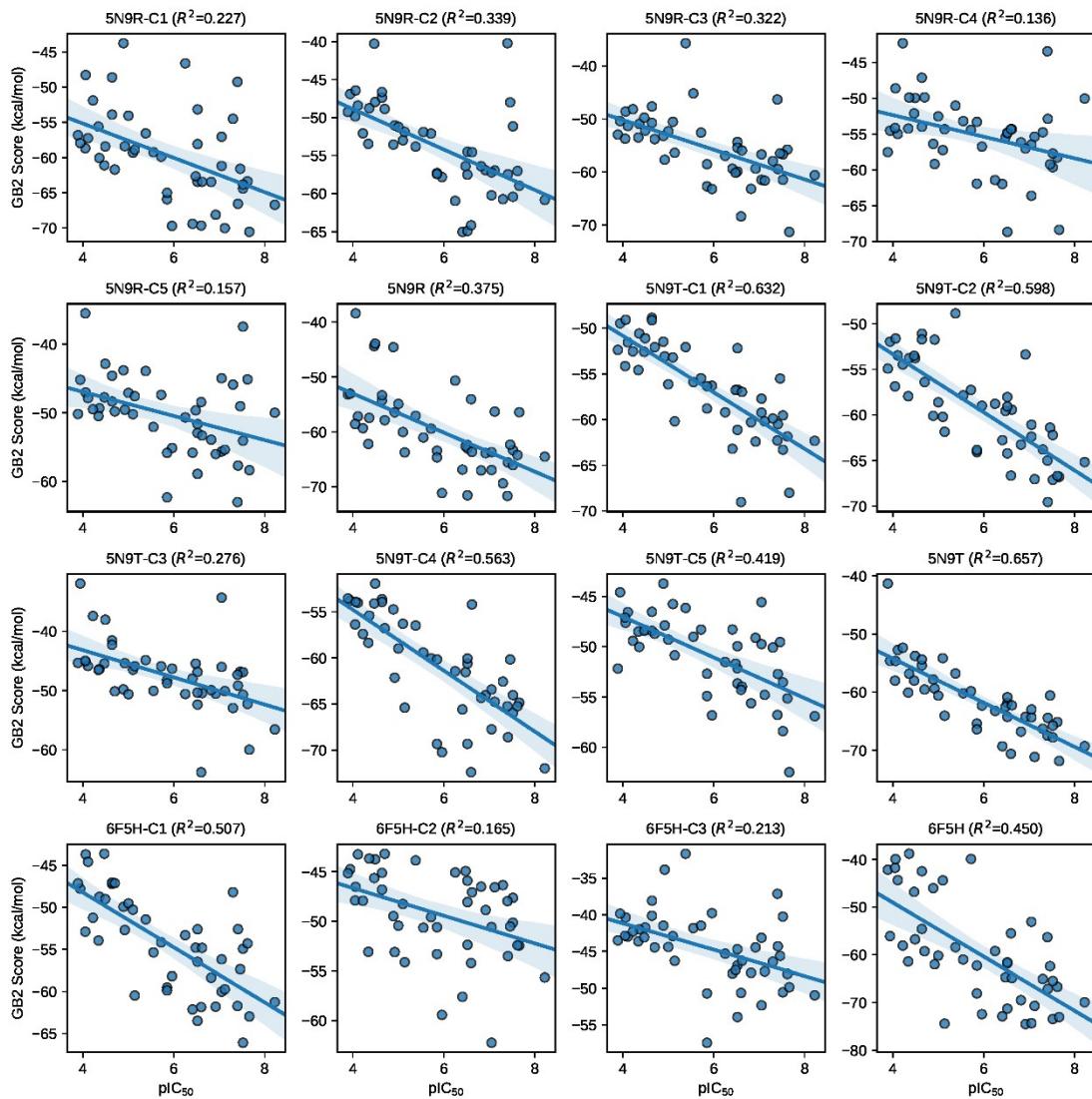


Figure S6. The scatter diagram of the GB2 scores versus experimental pIC₅₀ values with the corresponding squared Pearson's correlation coefficient (R^2).

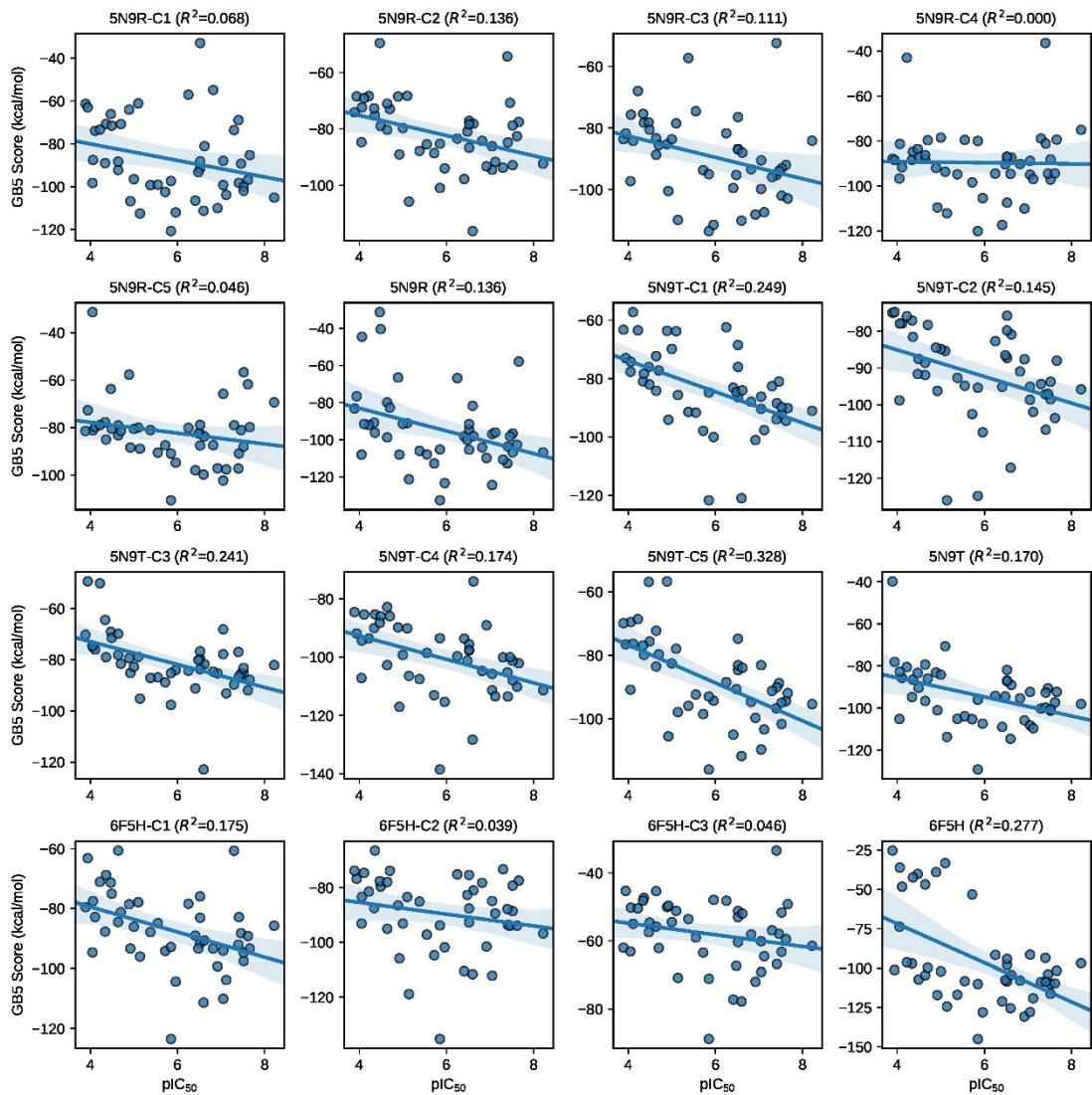


Figure S7. The scatter diagram of the GB5 scores versus experimental pIC₅₀ values with the corresponding squared Pearson's correlation coefficient (R^2).

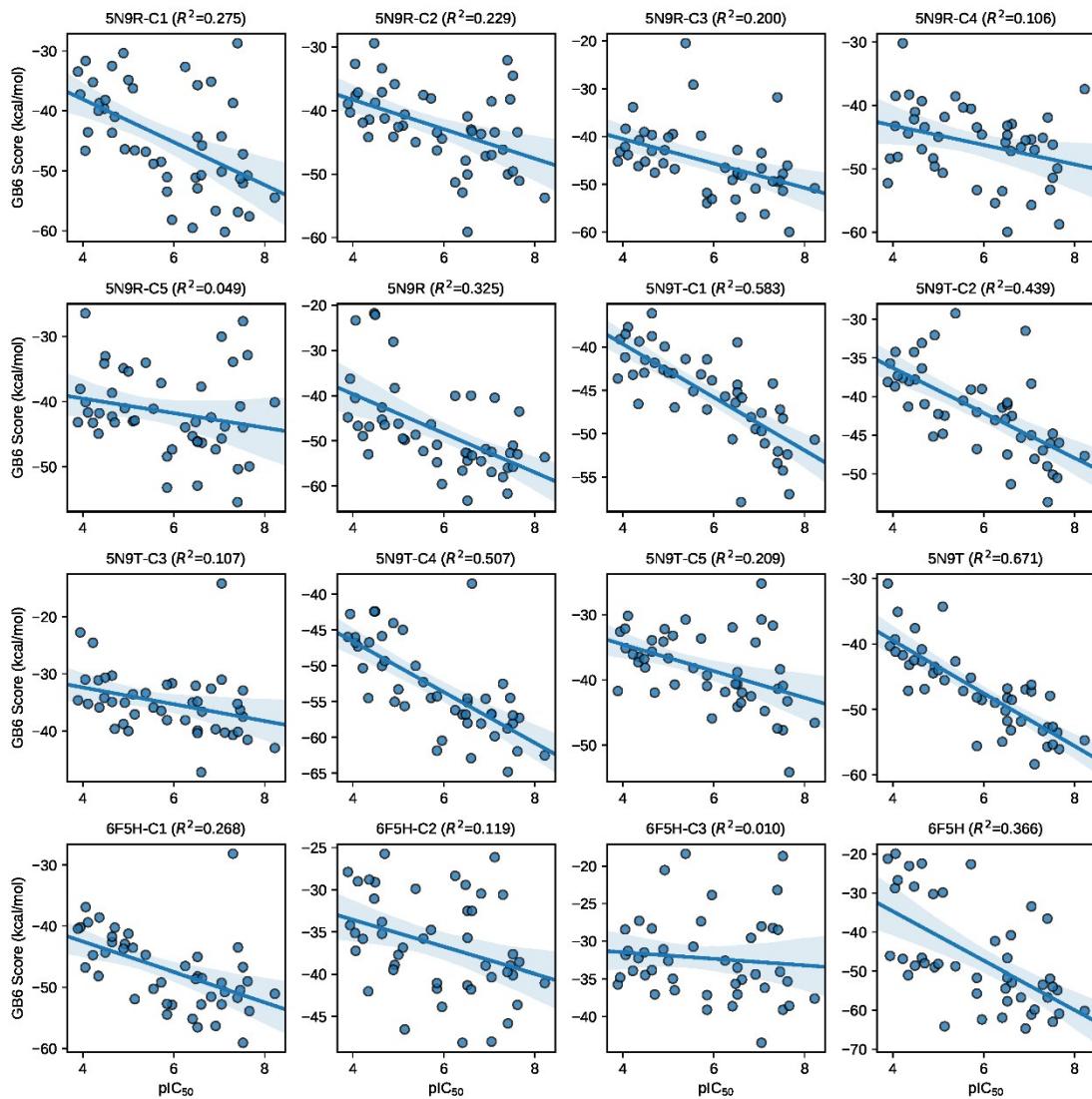


Figure S8. The scatter diagram of the GB6 scores versus experimental pIC₅₀ values with the corresponding squared Pearson's correlation coefficient (R^2).

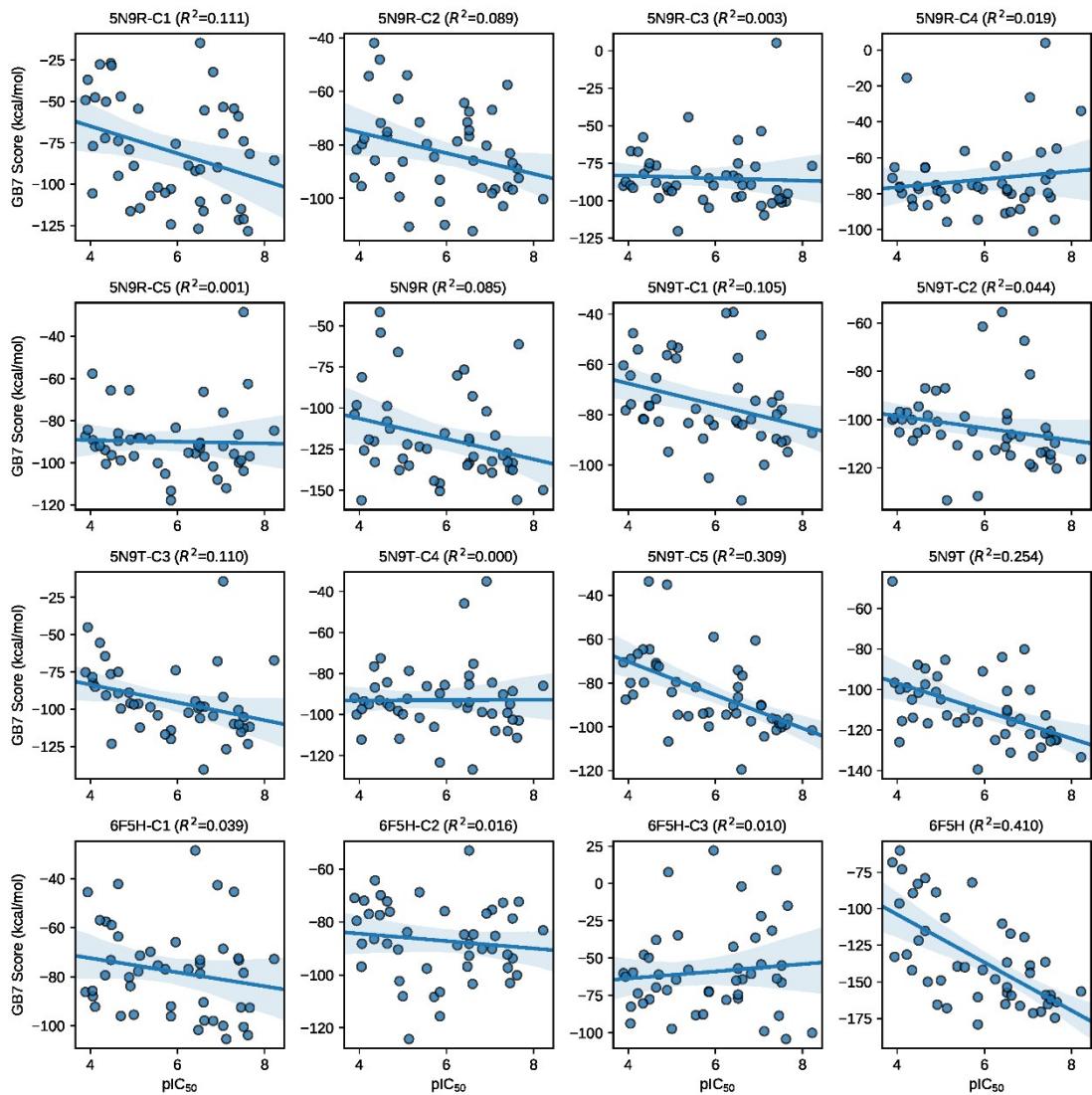


Figure S9. The scatter diagram of the GB7 scores versus experimental pIC₅₀ values with the corresponding squared Pearson's correlation coefficient (R^2).