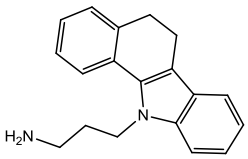
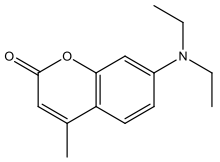
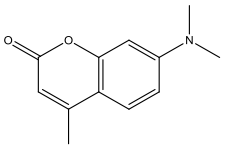
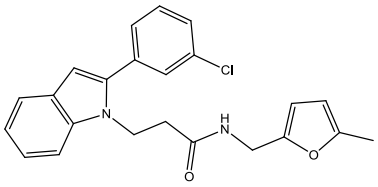
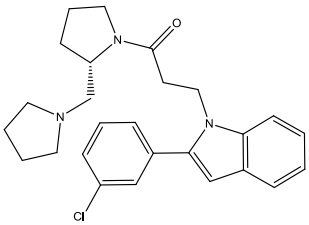
Table S1 Chemical structures of training molecules.

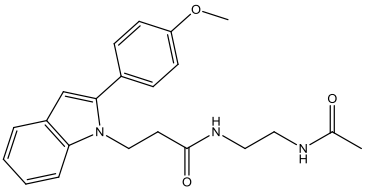
1. 

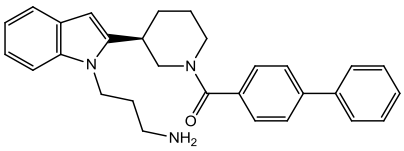
2. 

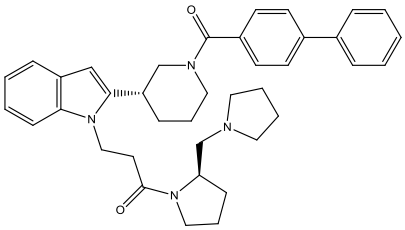
3. 

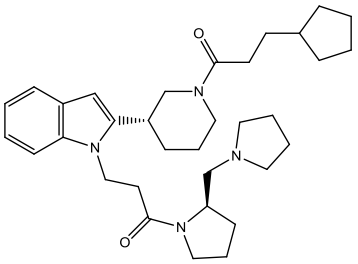
4. 

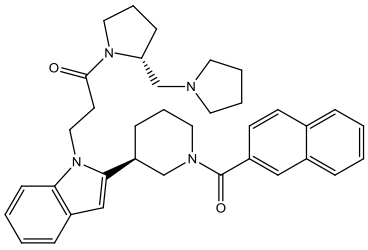
7. 

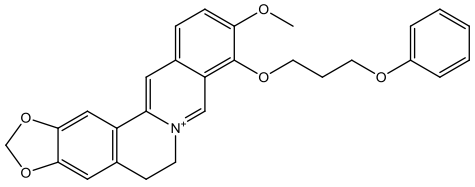
8. 

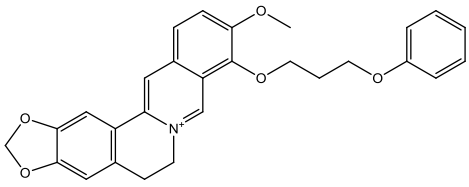
9. 

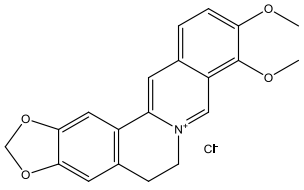
10. 

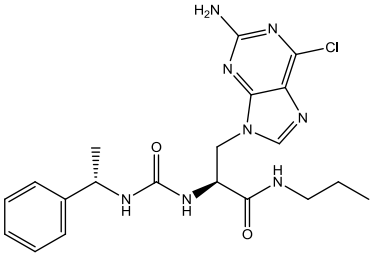
11. 

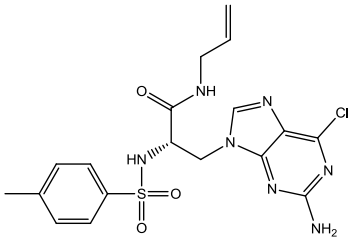
12. 

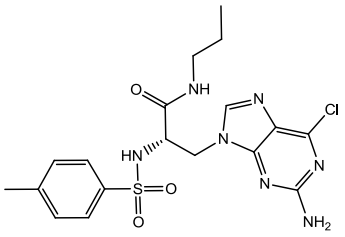
14. 

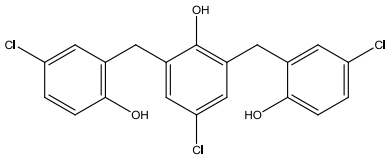
15. 

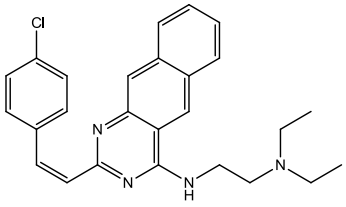
18. 

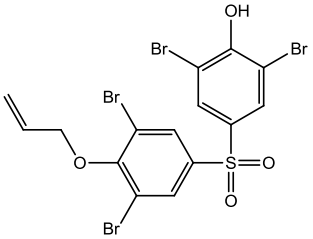
21. 

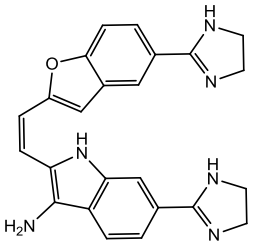
22. 

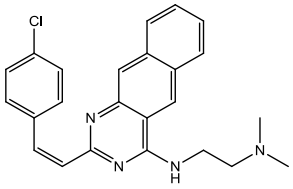
23. 

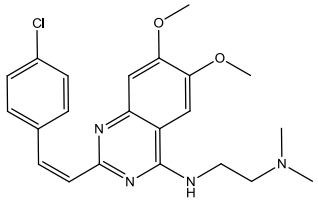
24. 

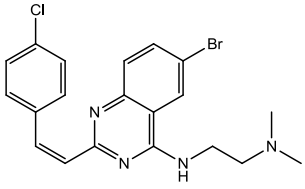
26. 

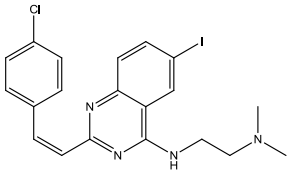
27. 

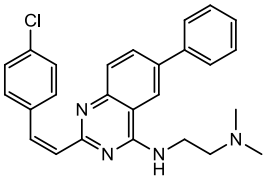
28. 

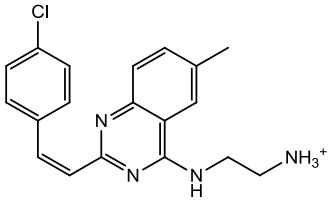
30. 

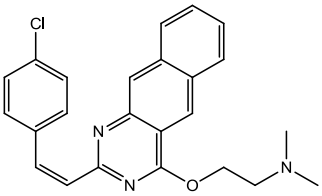
32. 

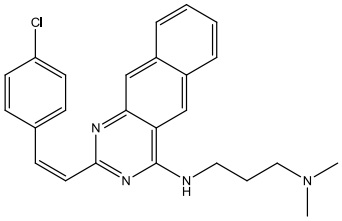
33. 

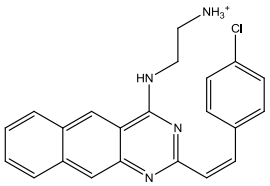
34. 

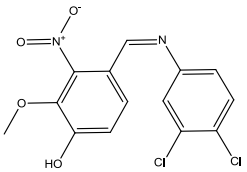
35. 

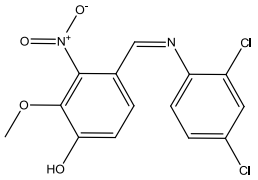
39. 

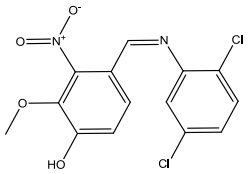
40. 

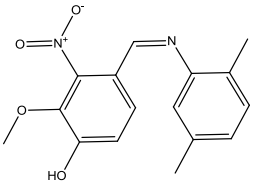
41. 

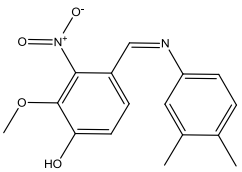
43. 

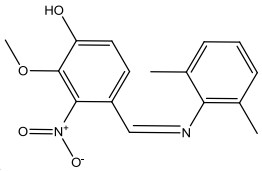
44. 

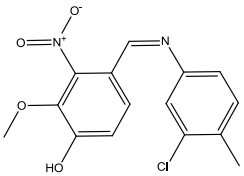
45. 

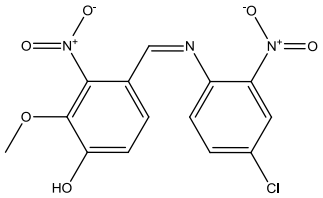
46. 

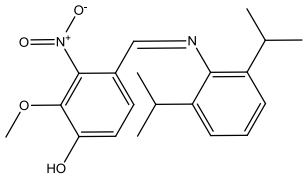
47. 

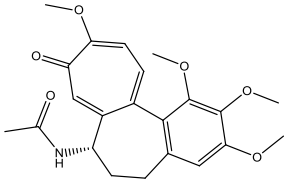
48. 

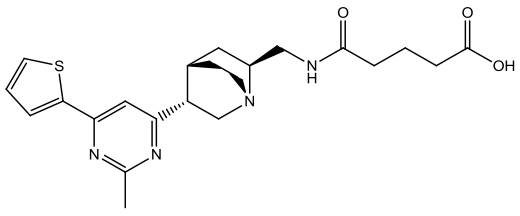
49. 

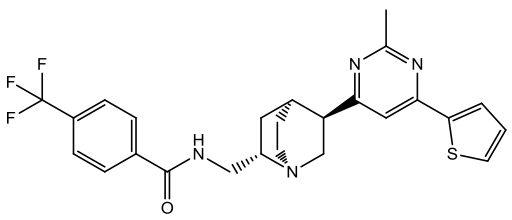
50. 

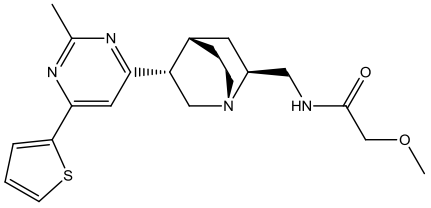
51. 

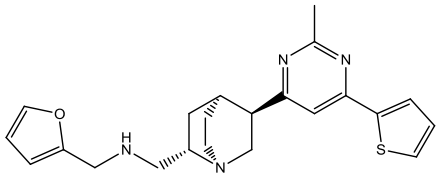
52. 

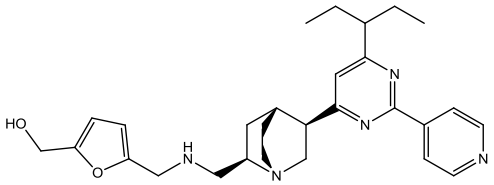
53. 

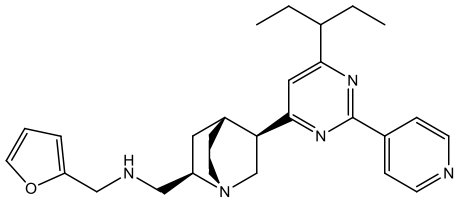
54. 

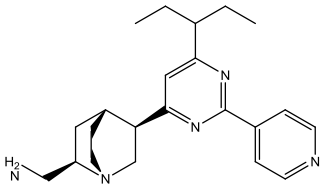
55. 

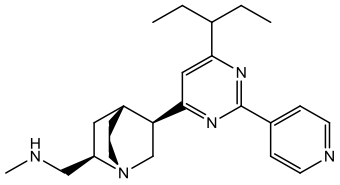
56. 

58. 

59. 

60. 

61. 

62. 

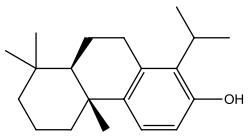
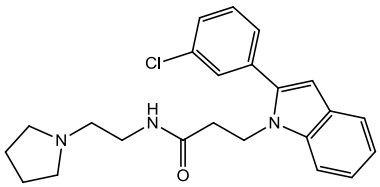
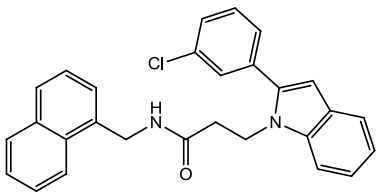
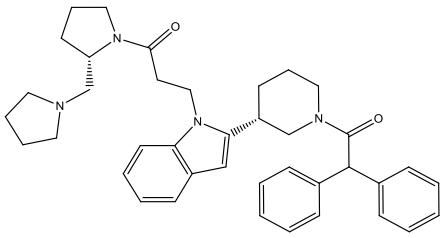
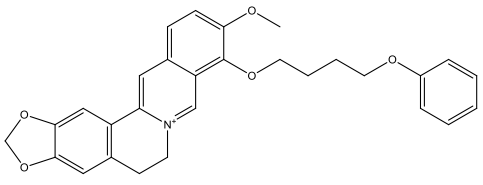
63. 

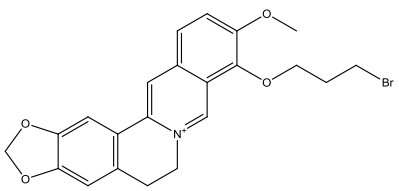
Table S2 Chemical structures of test molecules.

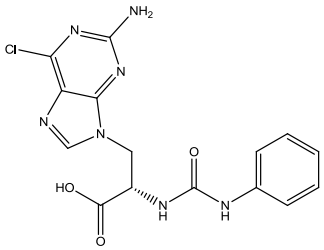
5. 

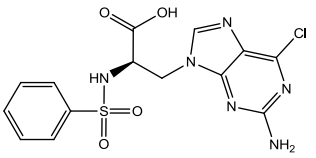
6. 

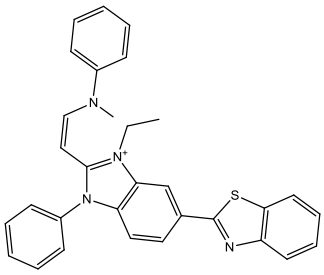
13. 

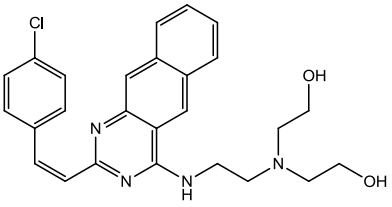
16. 

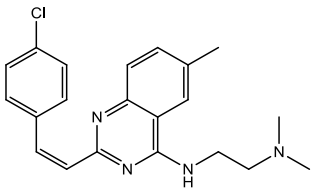
17. 

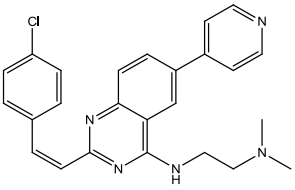
19. 

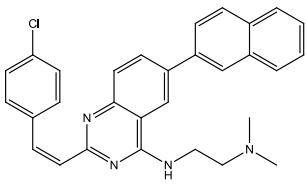
20. 

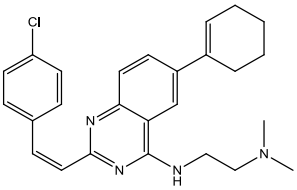
25. 

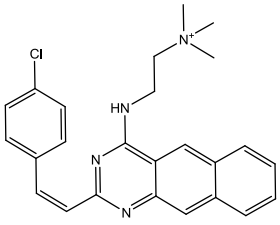
29. 

31. 

36. 

37. 

38. 

42. 

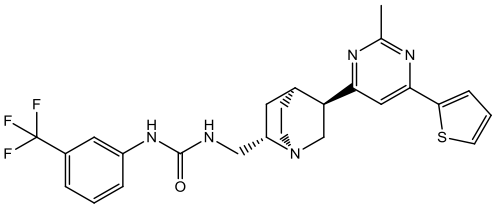
57. 

Table S3 Ligands with their activities (pIC_{50}), predicted activity(pIC_{50}) and fitness scores.

No.	QSAR Set	Activity	Predicted Activity	Pharm Set	Fitness
1	Training	2.686	2.52	+	1.72
2	Training	3.978	3.49	+ +	1.81
3	Training	4.069	4.45	+ +	1.73
4	Training	2.597	2.78	+	1.47
5	Test	2.789	3.21	+	1.16
6	Test	2.483	3.18	+	1.13
7	Training	2.491	2.87	+	1.79
8	Training	2.608	3.18	+	1.49
9	Training	3.529	3.67	+	0.88
10	Training	3.567	3.75	+ +	1.30
11	Training	3.096	2.97	+	1.39

No.	QSAR Set	Activity	Predicted Activity	Pharm Set	Fitness
12	Training	3.263	3.30	+	1.52
13	Test	2.959	3.06	+	1.25
14	Training	4.246	4.27	+ +	0.73
15	Training	4.196	3.98	+ +	1.47
16	Test	4.197	3.88	+ +	1.33
17	Test	3.619	3.39	+ +	1.69
18	Training	3.565	3.24	+ +	1.24
19	Test	4.347	3.94	+ +	0.65
20	Test	3.921	3.91	+ +	0.74
21	Training	3.745	3.65	+ +	0.58
22	Training	3.770	3.77	+ +	0.69
23	Training	3.585	3.71	+ +	1.58
24	Training	5.301	5.40	+ + +	1.38
25	Test	5.000	3.74	+ + +	1.19
26	Training	4.824	4.68	+ + +	1.59
27	Training	4.602	4.64	+ + +	1.76
28	Training	5.398	5.37	+ + +	1.40
29	Test	4.620	4.22	+ + +	1.66
30	Training	4.921	4.63	+ + +	1.54
31	Test	4.620	4.52	+ + +	1.63
32	Training	4.000	4.29	+ +	1.55
33	Training	4.523	4.52	+ + +	1.69
34	Training	4.022	4.31	+ +	1.62
35	Training	4.553	4.52	+ + +	1.60
36	Test	4.523	4.76	+ + +	1.56
37	Test	4.237	4.7	+ +	1.57
38	Test	4.310	4.46	+ +	1.52
39	Training	4.569	4.52	+ + +	1.70
40	Training	4.585	4.45	+ + +	1.64
41	Training	4.187	4.46	+ +	1.61
42	Test	4.284	4.39	+ +	1.68
43	Training	5.046	4.81	+ + +	1.66
44	Training	4.067	3.92	+ +	2.05
45	Training	4.110	4.29	+ +	1.70
46	Training	4.142	4.62	+ +	2.48
47	Training	4.811	4.70	+ + +	3.00
48	Training	4.639	4.69	+ + +	2.28
49	Training	5.027	4.99	+ + +	1.88
50	Training	4.387	4.14	+ + +	1.84
51	Training	4.300	3.99	+ +	1.29
52	Training	5.678	5.60	+ + +	1.13
53	Training	3.983	3.80	+ +	1.59

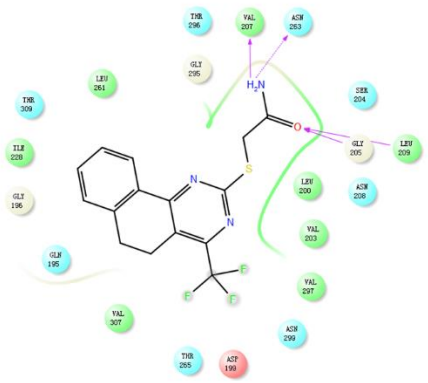
No.	QSAR Set	Activity	Predicted Activity	Pharm Set	Fitness
54	Training	3.499	3.52	+	1.21
55	Training	3.157	3.27	+	1.25
56	Training	3.399	3.42	+	1.25
57	Test	3.264	3.16	+	1.47
58	Training	3.721	3.27	+ +	1.18
59	Training	4.135	4.20	+ +	0.76
60	Training	4.254	4.17	+ +	0.80
61	Training	4.426	4.19	+ + +	0.84
62	Training	3.724	3.99	+ +	1.09
63	Training	4.389	4.42	+ + +	1.71

+ + + represents Activity, + + represent Moderate Activity, + represents Inactivity.

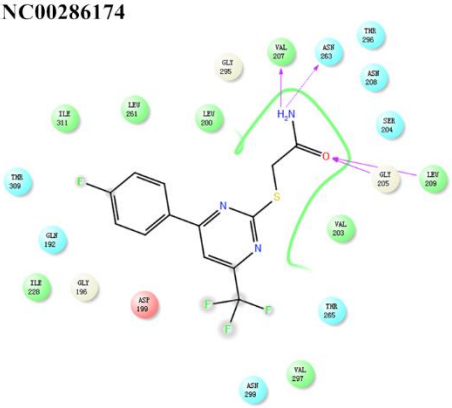
Table S4 $\Delta G_{\text{Bind\_Coulomb}}$ and $\Delta G_{\text{Bind\_Solv\_GB}}$ of selected molecules

ZINC	$\Delta G_{\text{Bind\_Coulomb}}$	$\Delta G_{\text{Bind\_Solv\_GB}}$
ZINC00309019	-7.70	14.87
ZINC00286174	-10.76	13.02
ZINC05706598	140.57	-106.20
ZINC00669639	-21.95	23.75
ZINC00662372	-12.43	14.75
ZINC41498620	-8.12	18.22
ZINC02366906	-142.38	150.70
ZINC04968357	-11.75	16.87

ZINC00309019



ZINC00286174



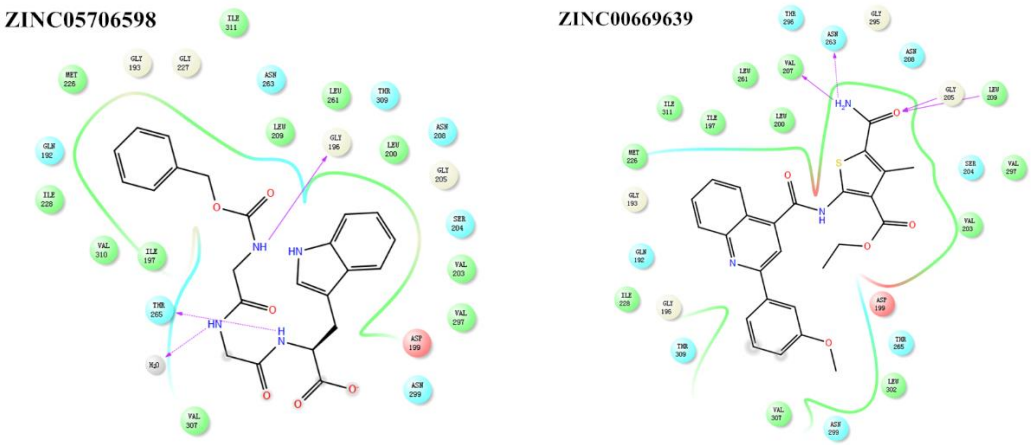


Figure S1 2D interaction of selected ZINC00309019, ZINC00286174, ZINC05706598 and ZINC00669639.

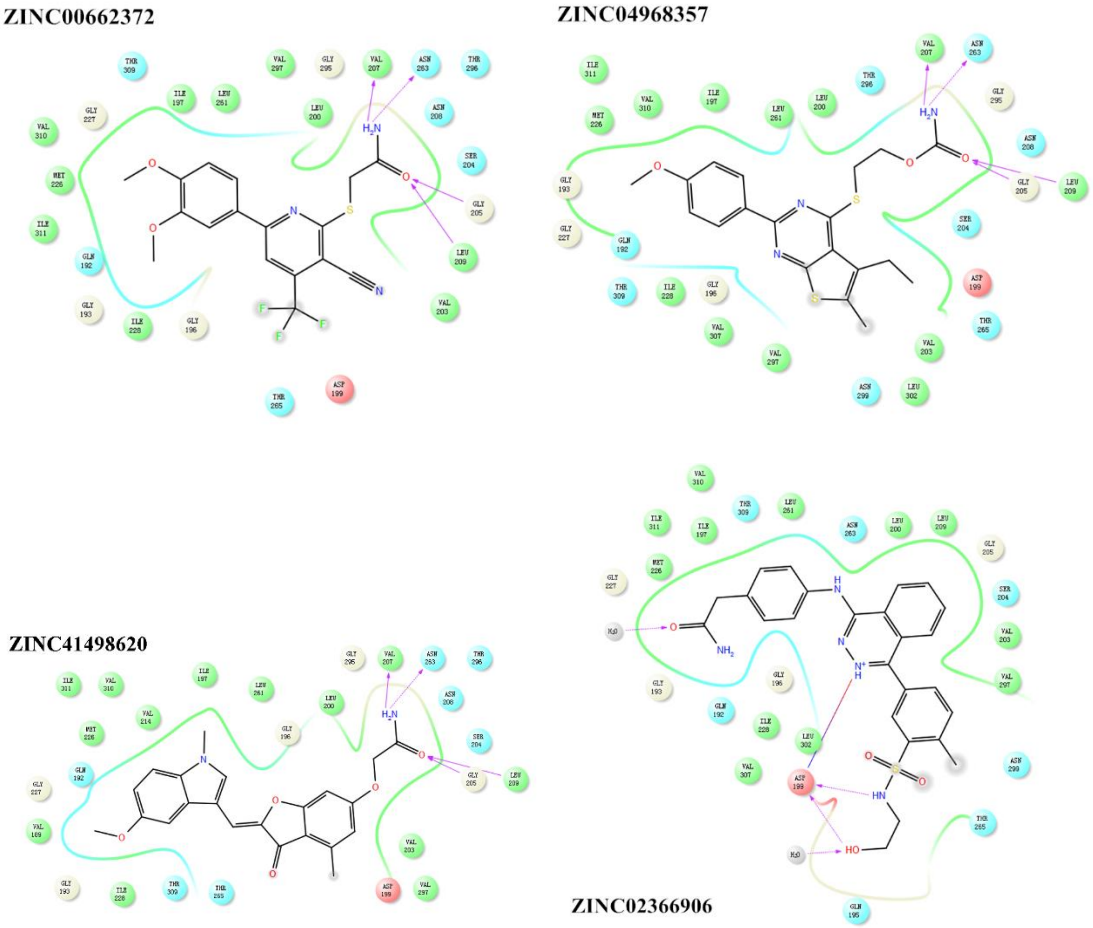


Figure S2 2D interaction of selected seven hitsZINC00662372, ZINC02366906 ZINC41498620 and ZINC04968357