

Molecular Modelling, Docking and Pharmacokinetic Studies of N-Arylidenequinoline-3-Carbohydrazides Analogs as Novel B-Glucuronidase Inhibitors

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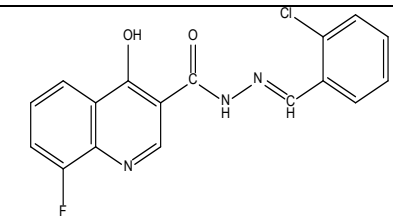
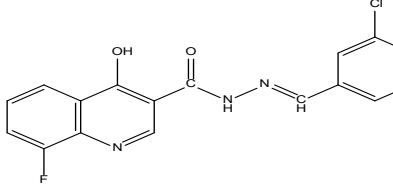
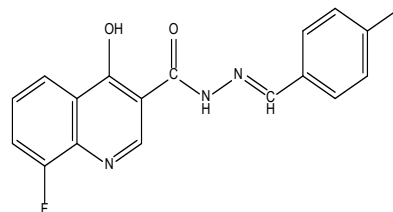
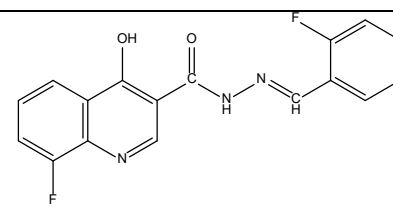
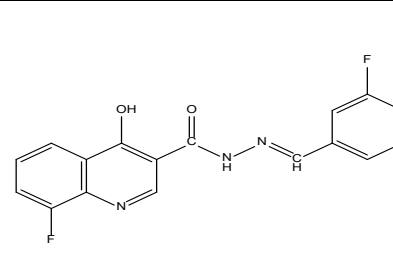
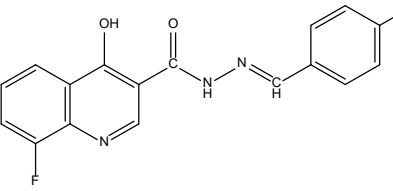
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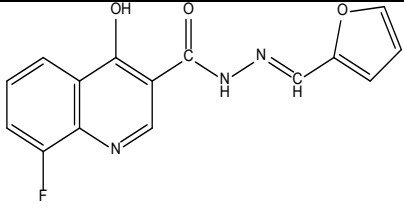
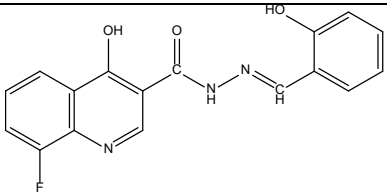
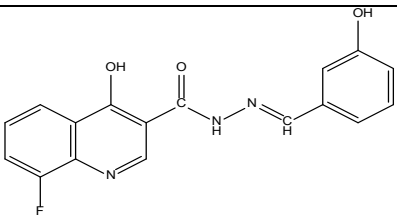
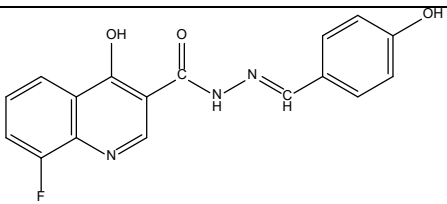
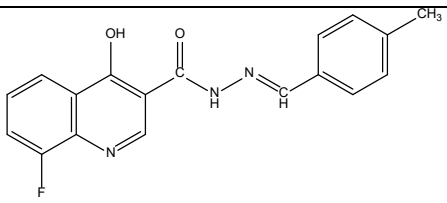
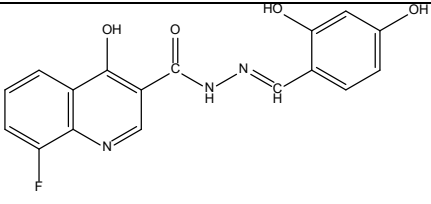
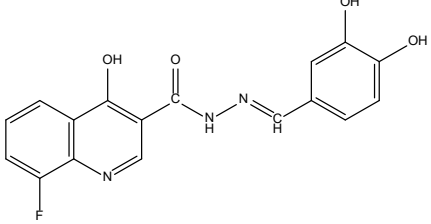
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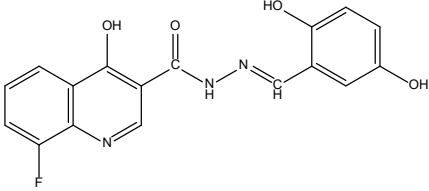
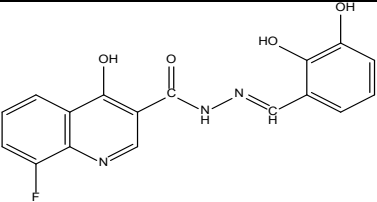
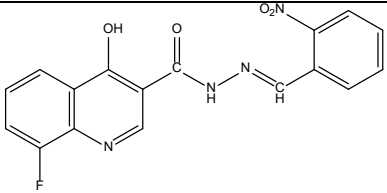
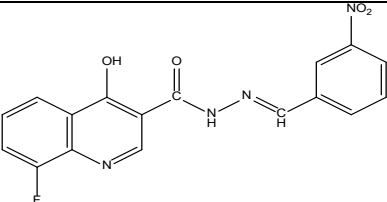
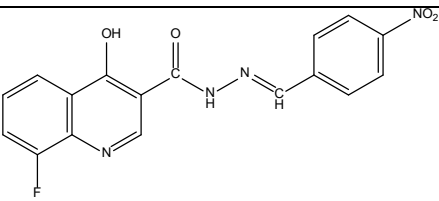
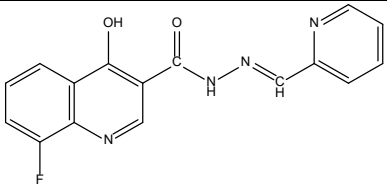
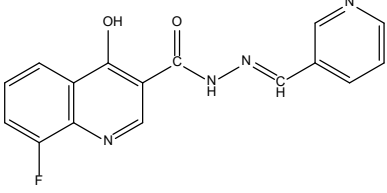
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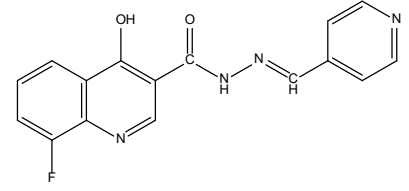
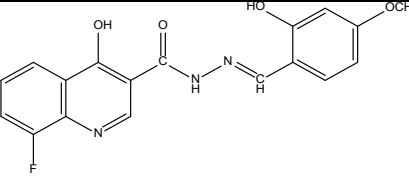
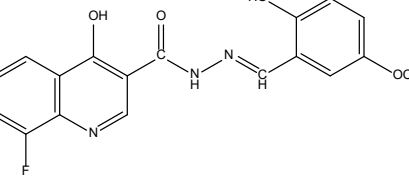
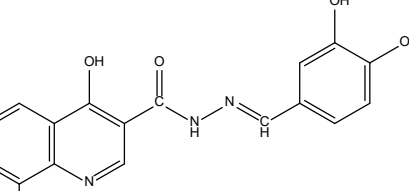
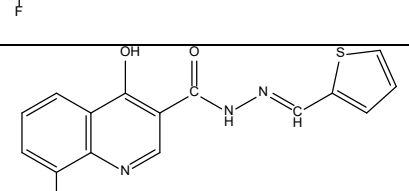
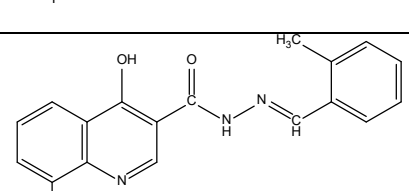
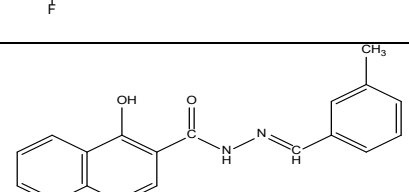
Supplementary Information

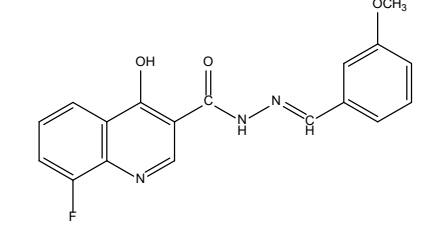
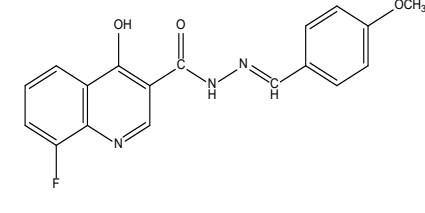
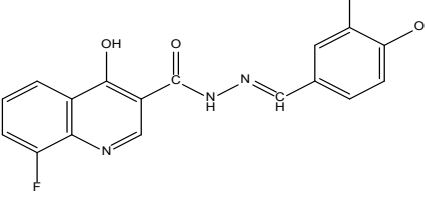
Table 1. The Substituents, pIC_{50} , Predicted pIC_{50} and residuals of the data set.

Sr No	R	pIC_{50}	Predicted IC_{50}	Residuals
1 ^x		1.264818	1.278745	-0.013927
2 ^x		1.625827	1.678489	-0.052662
3 ^x		1.383815	1.346263	0.037553
4 ^x		0.9638	0.936195	0.027593
5 ^y		1.5683	1.571916562	0.003597477
6 ^y		1.419956	1.419047	9.09E-04

7 ^y		1.585461	1.644859	-0.059399
8 ^x		0.826075	0.951784	-0.125709
9 ^x		1.257679	1.198934	0.058745
10 ^x		0.982271	1.022892	-0.040621
11 ^y		1.66407759	1.514579994	-0.15
12 ^x		0.491362	0.402842	0.08852
13 ^y		0.324282455	0.699263232	0.375

14 ^x		0.699838	0.560128	0.13971
15 ^x		0.414973	0.555802	-0.140829
16 ^y		1.220108088	1.631503	0.339
17 ^y		1.897077003	1.631503	-0.3
18 ^x		1.644439	1.631968	0.012471
19 ^y		1.281033367	1.769051	0.451
20 ^x		1.834929	1.70031	0.065878

21 ^x		1.693551	1.057709	-0.006759
22 ^x		0.982271	1.769051	-0.075438
23 ^y		0.919078092	1.160522472	0.241
24 ^x		1.255273	1.272427	-0.017155
25 ^x		1.348305	1.307547	0.040758
26 ^y		1.58546073	1.37902299	-0.21
27 ^y		1.707570176	1.740231206	0.033

28 ^x		1.903633	1.918551	-0.014919
29 ^x		1.841359	1.750816	0.090544
30 ^x		1.663701	1.678962	-0.015261

x= model building set and y= validation set