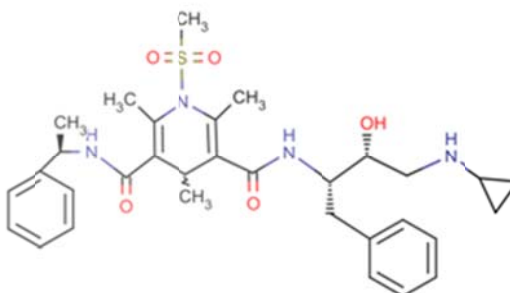
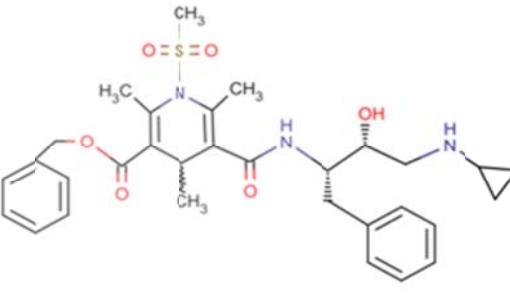
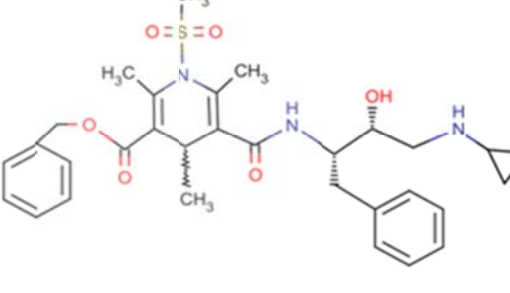
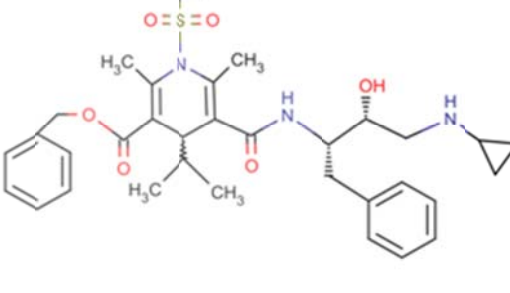


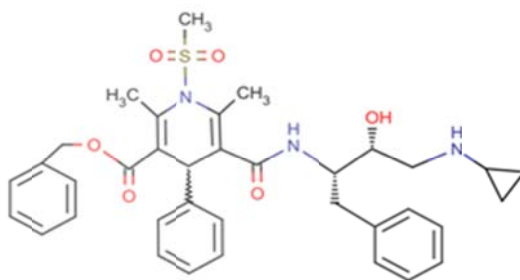
Supplementary Tables

Supplementary Table 1

S. No.	Molecular Structure (2D)	pIC ₅₀ (nm)
Training Set		
1		4.80
2		5.02
3		5.10
4		4.90

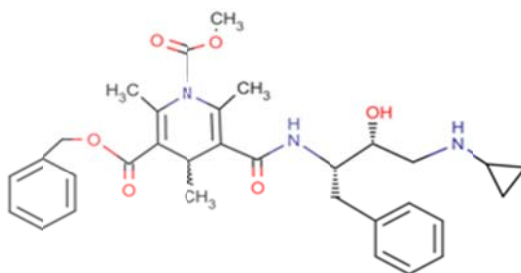
5

4.70



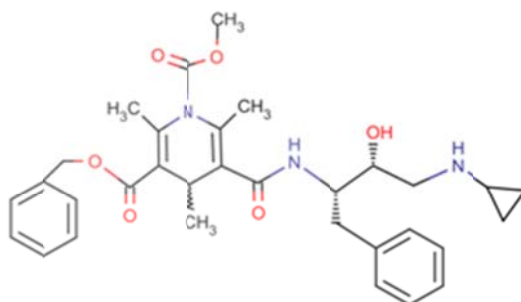
6

4.82



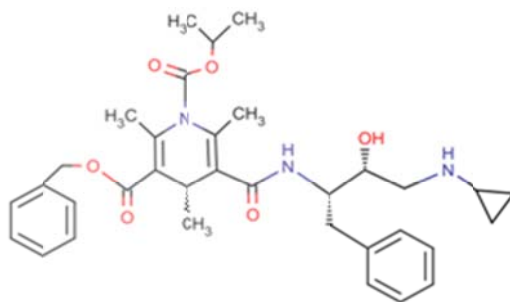
7

4.81



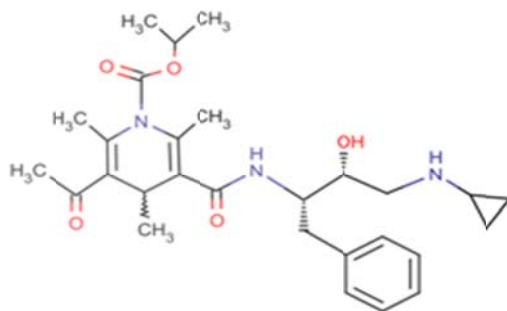
8

5.05

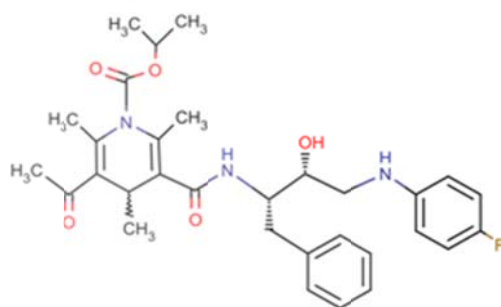


9

4.53

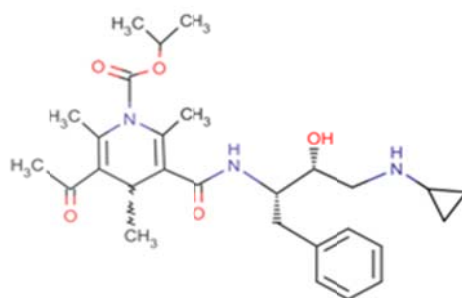


10



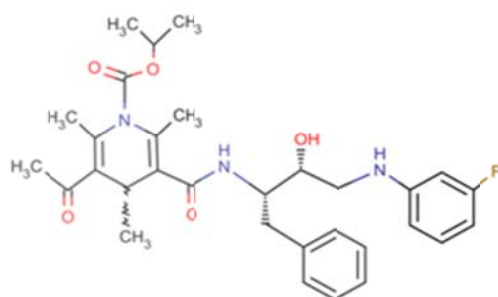
4.60

11



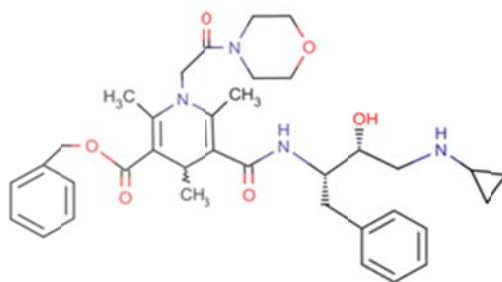
4.50

12



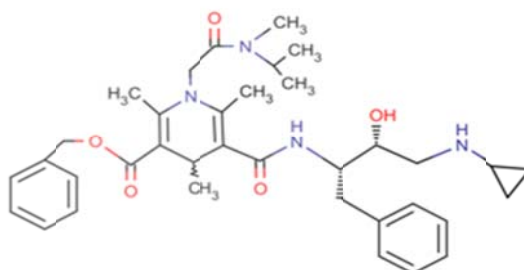
4.60

13



4.55

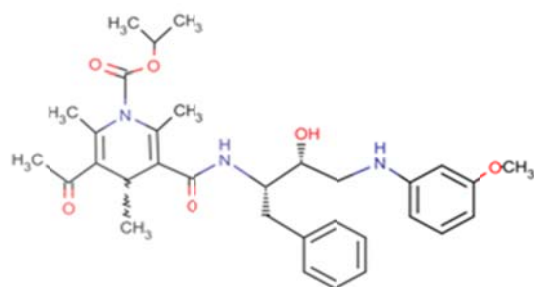
14



4.55

15

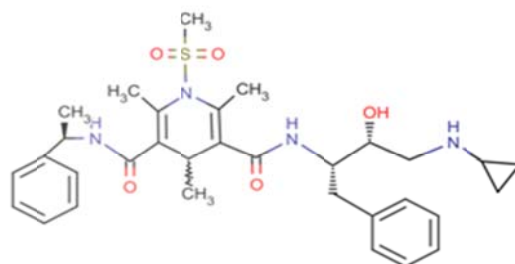
4.60



Test Set

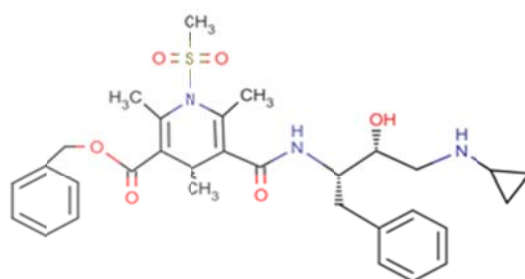
1

4.80



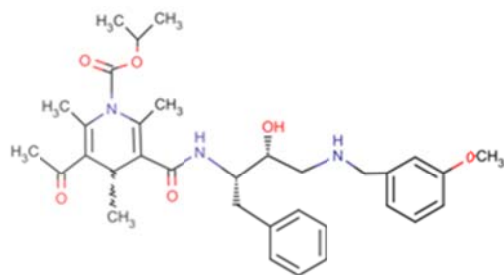
2

4.83



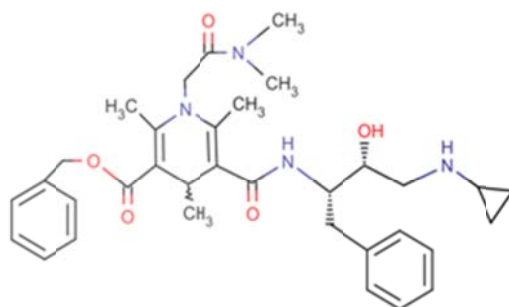
3

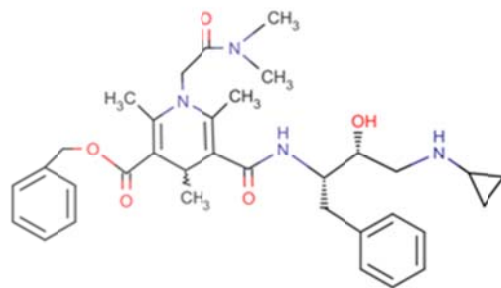
4.63



4

4.60





Supplementary Table 2

S. No.	Actual activity (pIC ₅₀ in nm)	Selected Descriptors			Predicted activity (pIC ₅₀ in nm)
		R1- NitrogenCount	R2- DeltaEpsilonA	R3- k3alpha	
1	4.80	1	0	0	4.80
2	4.80	1	0	0	4.80
3	4.83	0	0	0	4.95
4	5.02	0	0	0	4.95
5	5.10	0	0	0	4.95
6	4.90	0	0	0	4.95
7	4.70	0	0.067	0	4.71
8	4.82	0	0	3.63	4.95
9	4.81	0	0	5.01	4.95
10	5.05	0	0	5.63	4.95
11	4.53	0	0	5.63	4.57
12	4.60	0	0	5.63	4.57
13	4.50	0	0	5.63	4.57
14	4.60	0	0	5.63	4.60
15	4.60	0	0	5.63	4.57
16	4.63	0	0	5.63	4.57
17	4.60	0	0	2.63	4.54
18	4.41	0	0	2.63	4.54
19	4.55	0	0	1.77	4.54
20	4.55	0	0	2.52	4.54