molecules

Identifying Novel ATX Inhibitors via Combinatory Virtual Screening Using Crystallography-Derived Pharmacophore Modelling, Docking Study, and QSAR Analysis

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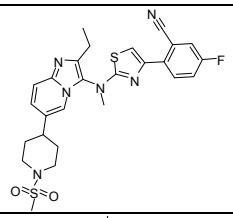
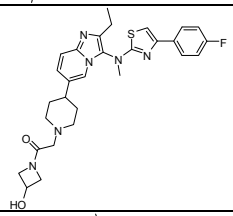
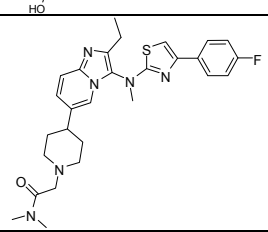
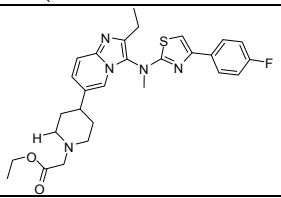
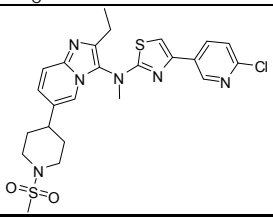
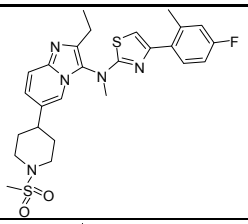
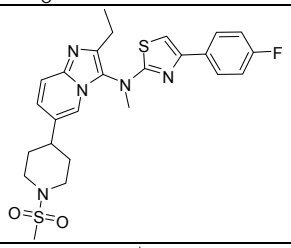
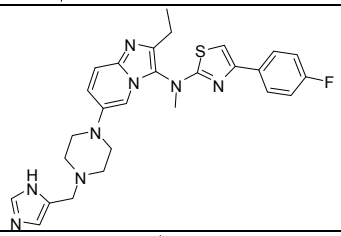
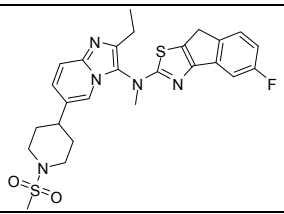
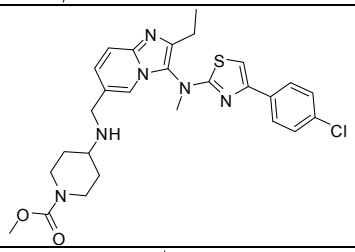
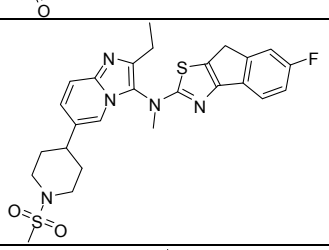
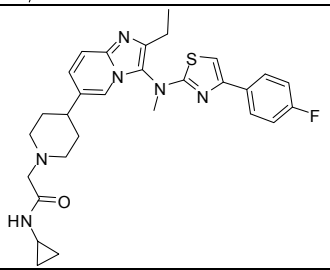
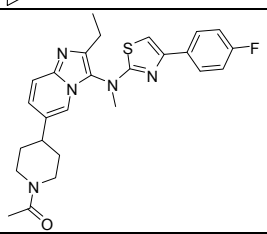
Supplementary Materials

Table S1. Chemical structures of the 22 training set inhibitors for building the 3D QSAR model with their IC_{50} and pIC_{50} values.

Compound code	Chemical structure	IC_{50} (nM)	pIC_{50}
1		126	6.89963
2		246	6.60907
3		261	6.58336
4		480	6.31876
5		493	6.30715

6		533	6.27327
7		710	6.14874
8		771	6.11295
9		804	6.09474
10		1,210	5.91721
11		1,212	5.9165
12		1,614	5.7921
13		1,624	5.78941

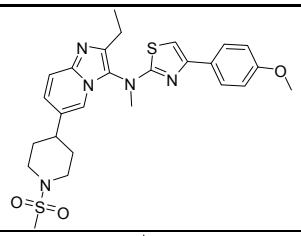
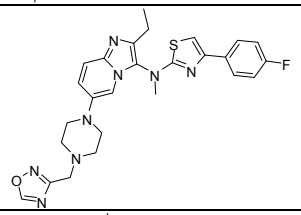
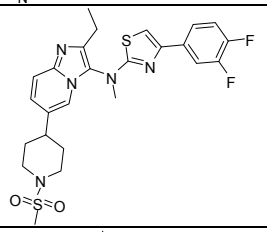
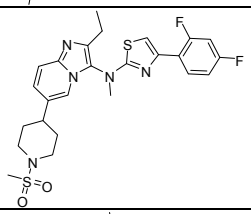
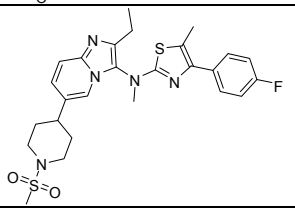
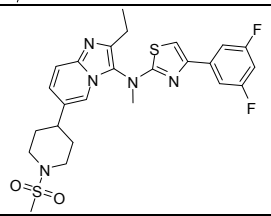
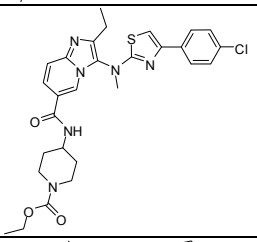
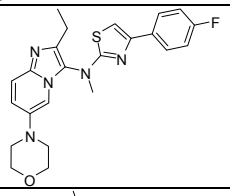
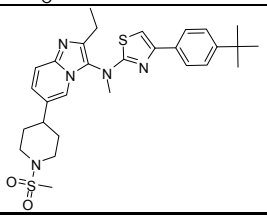
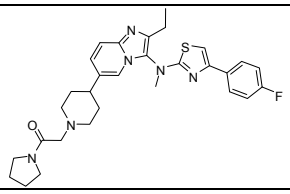
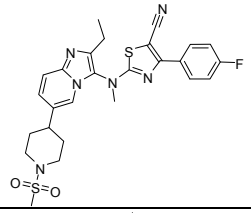
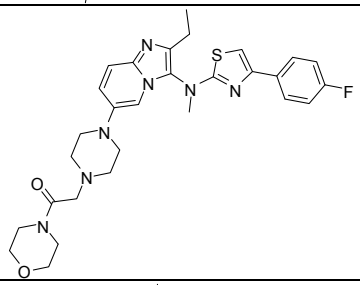
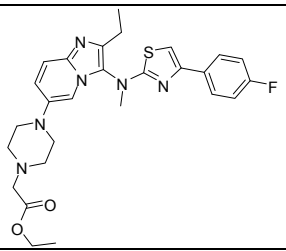
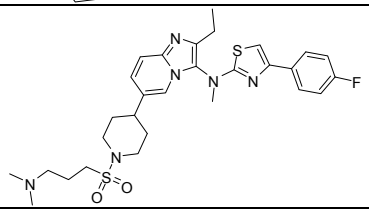
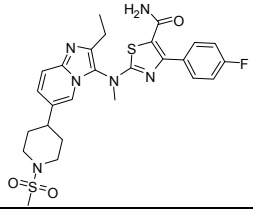
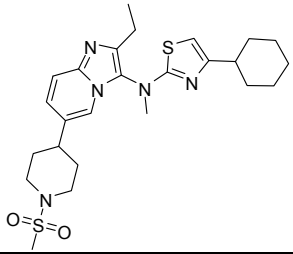
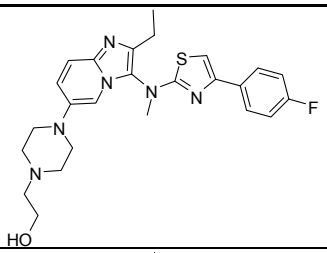
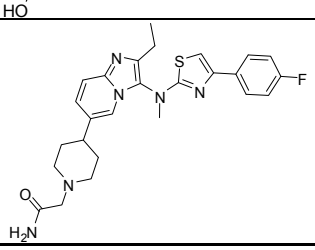
14		1,684	5.77366
15		1,708	5.76751
16		1,899	5.72148
17		2,021	5.69443
18		2,266	5.64474
19		4,246	5.37202
20		6,555	5.18343
21		6,800	5.16749
22		7,609	5.11867

Table S2. Chemical structures of the 9 test set inhibitors for building the 3D QSAR model with their IC_{50} and pIC_{50} values.

Compound code	Chemical structure	IC_{50} (nM)	pIC_{50}
23		86	7.0655
24		138	6.86012
25		231	6.63639
26		280	6.55284
27		357	6.44733
28		1,410	5.85078
29		1,904	5.72033

30		2,359	5.62727
31		2,372	5.62489

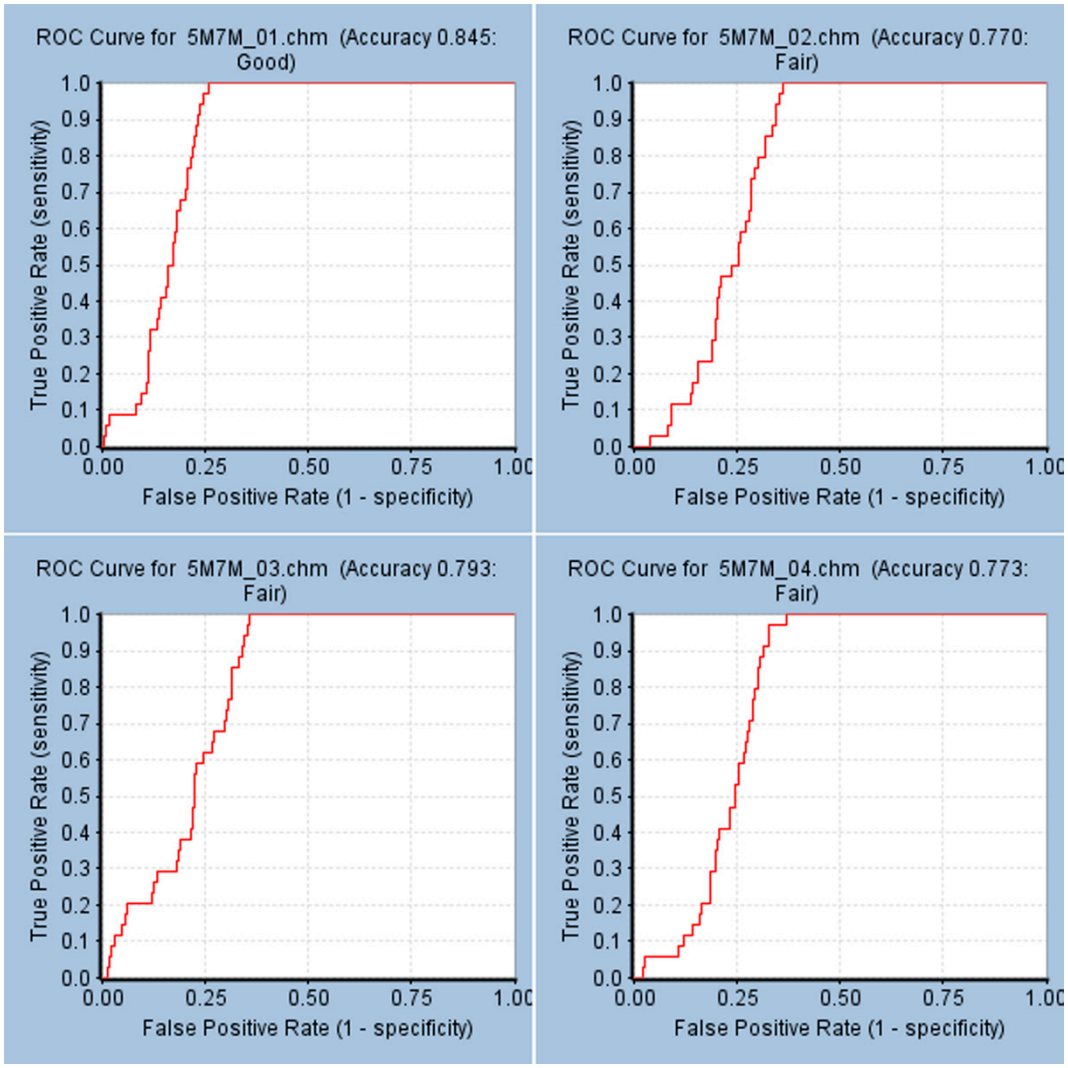


Figure S1. ROC curves of pharmacophore models 5M7M 01-04.

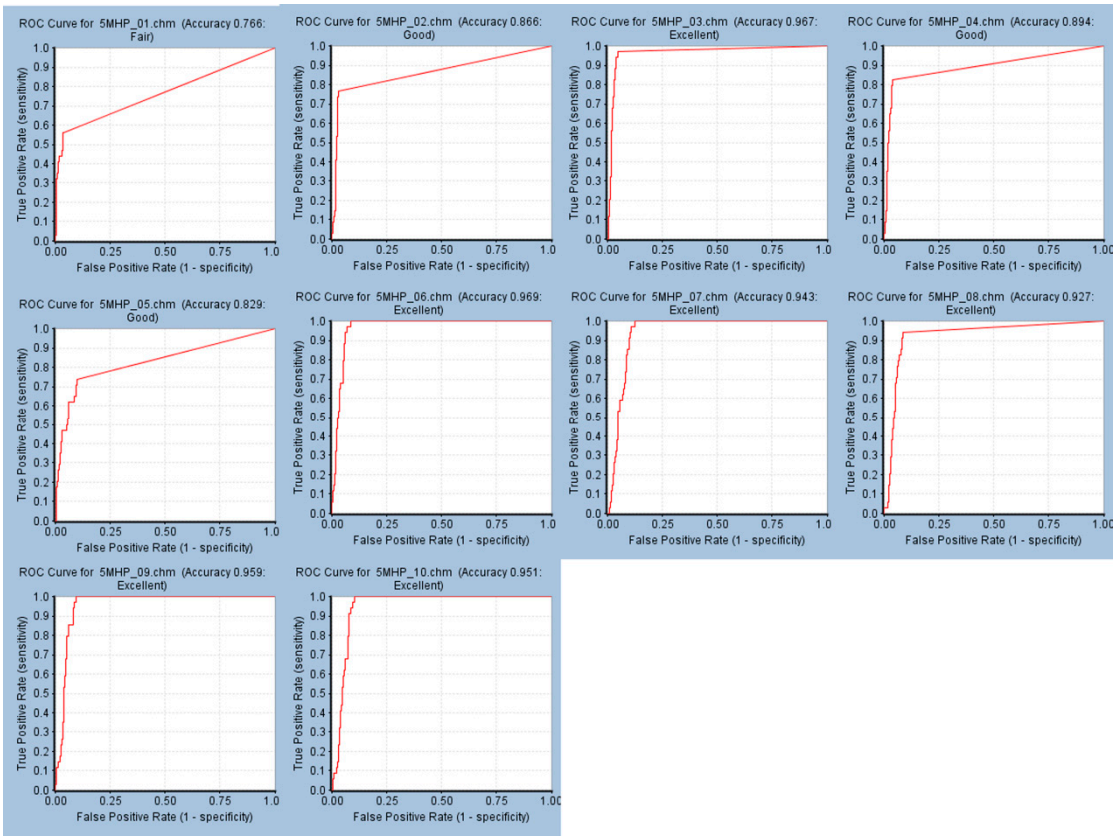


Figure S2. ROC curves of pharmacophore models 5MHP 01-10.