Article

Identification of Potential Multitarget Compounds against Alzheimer's Disease through Pharmacophore-Based Virtual Screening

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Table S1. Scores of the three best compounds selected through molecular docking by AutoDock Vina 1.1.2.

Molecule	AChE *	BChE *	BACE-1 *
ZINC45068352	-9.6	-10.4	-9.9
ZINC03873986	-10.6	-11.2	-12.2
ZINC71787288	-9.6	-10.6	-9.6

*kcal/mol - lower energy indicates better docking

Table S2. Scores of the three best compounds selected through molecular docking by GOLD.

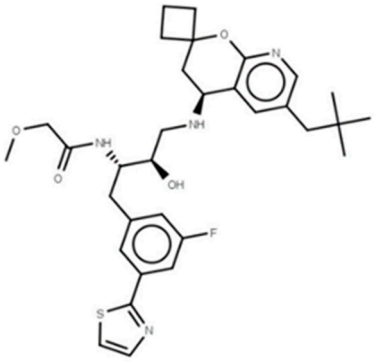
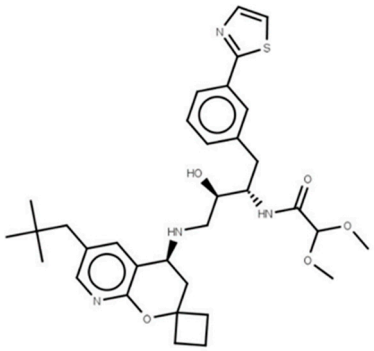
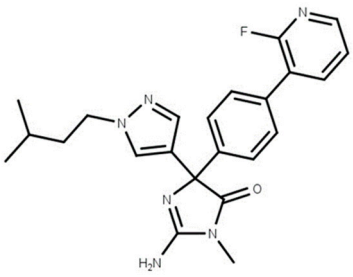
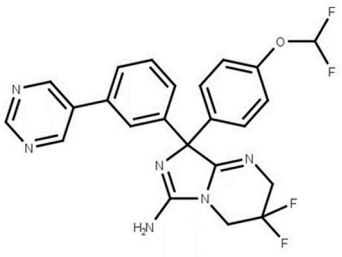
Molecule	AChE *	BChE *	BACE-1 *
ZINC45068352	58.82	63.25	43.32
ZINC03873986	68.49	37.38	41.54
ZINC71787288	57.65	56.64	41.91

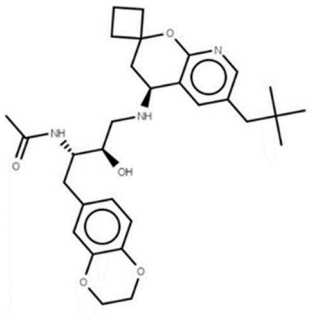
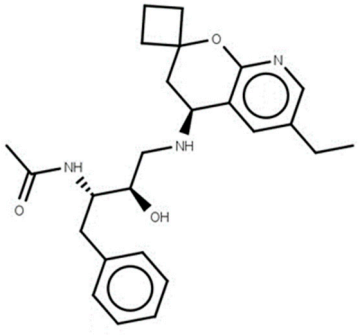
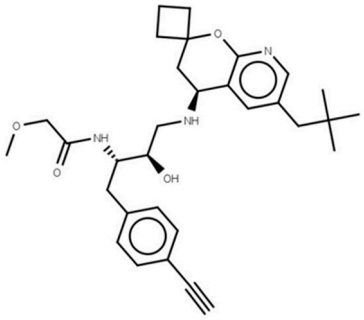
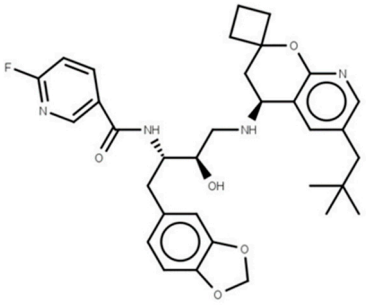
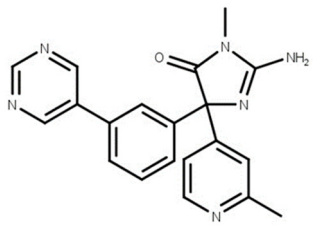
*dimensionless - Higher numbers indicate better docking

Table S3. Toxicological analysis of the remaining molecules.

Molecule	Maximum Tolerated dose (human)	hERG I inhibitor	Oral Rat Acute Toxicity (LD50)	Oral Rat Chronic Toxicity (LOAEL)	Hepatotoxicity	Skin Sensitization	T.Pyriformis toxicity	Minnow toxicity
ZINC03873986	0.695	No	2.499	3.126	No	No	0.286	-0.457
ZINC71787288	0.639	No	2.709	2.23	Yes	No	0.321	-0.361

Table S4. Chemical structure and biological activity of inhibitors against BACE-1 used in generating pharmacophore models.

Nº	Chemical structure	IC_{50} (nM)
1		1.9
11		9.1
17		16
19		19.5

22		22.8
28		39
31		47
32		48
38		79.98

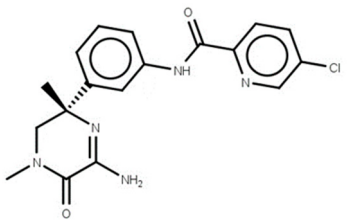
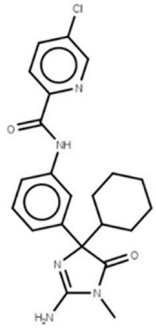
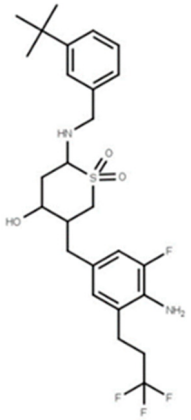
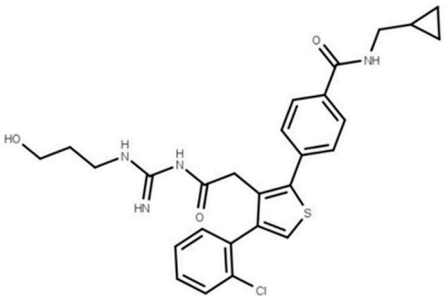
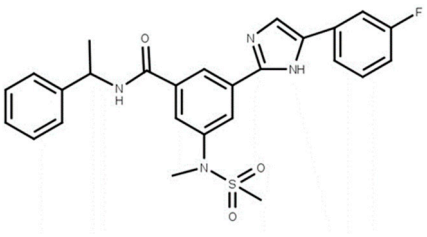
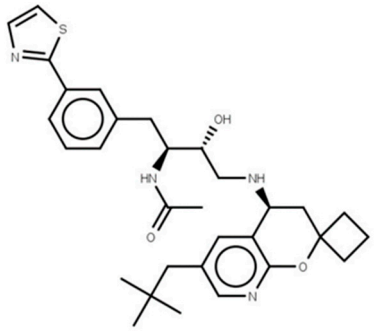
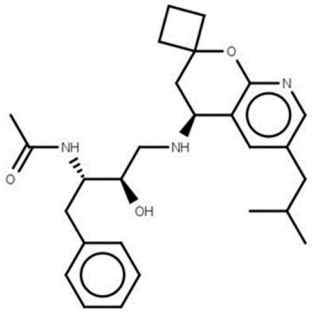
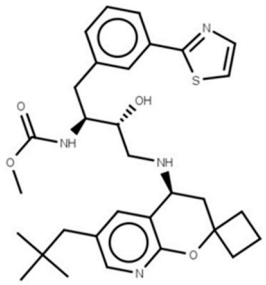
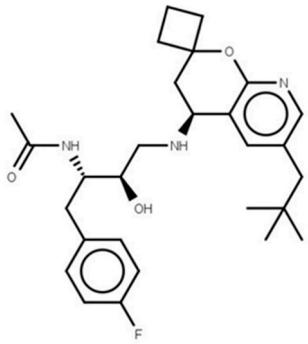
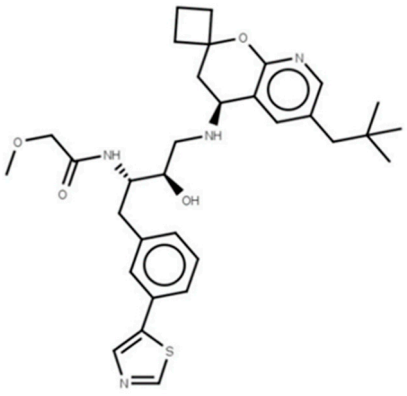
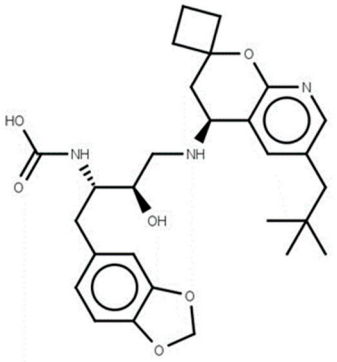
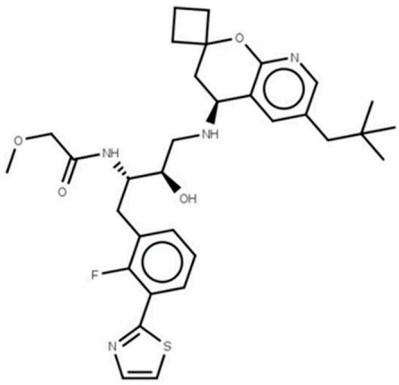
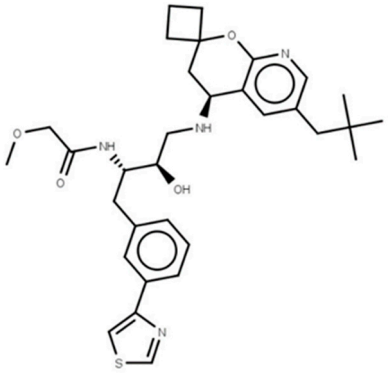
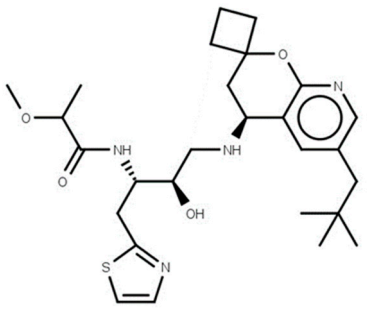
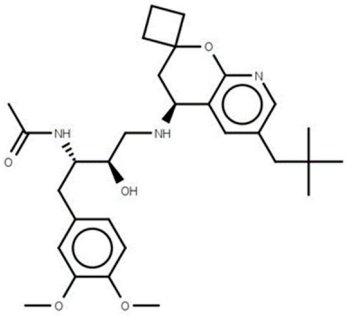
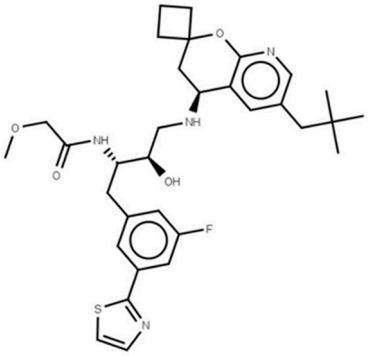
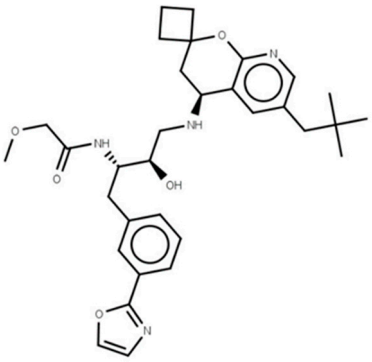
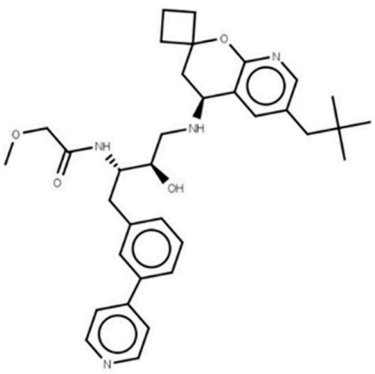
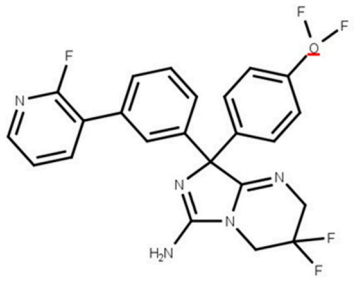
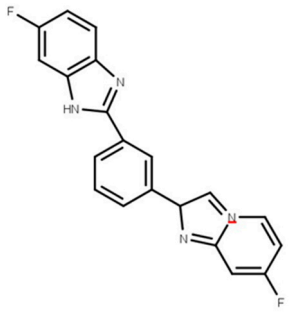
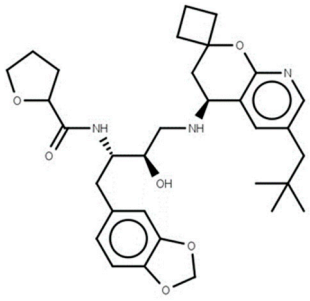
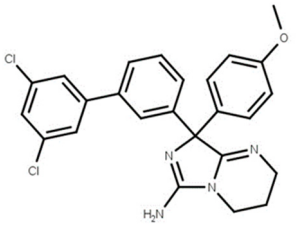
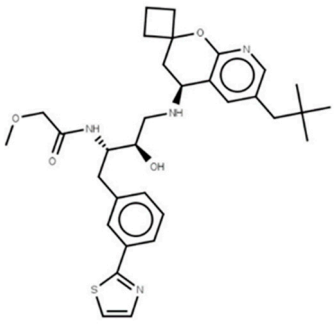
39		83
40		100
41		130
42		140
44		187

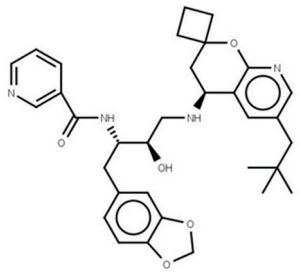
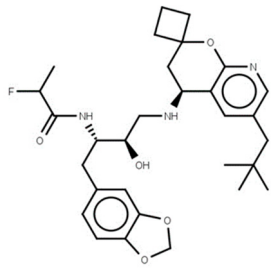
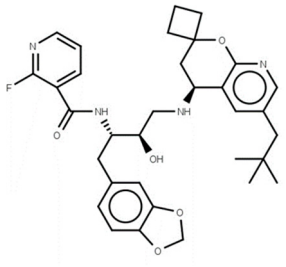
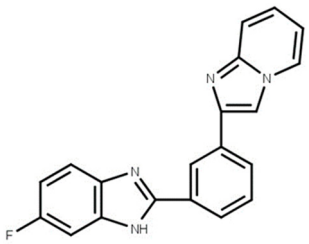
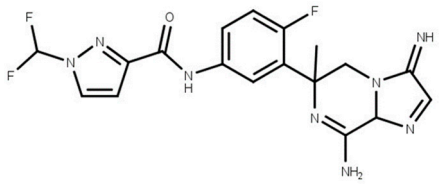
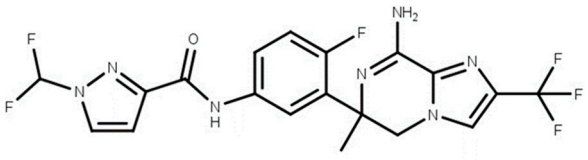
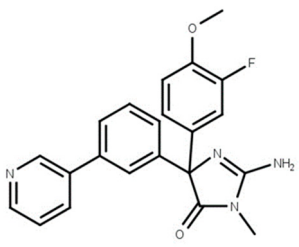
Table S5. Chemical structure and biological activity of inhibitors against BACE-1 that were used in evaluating pharmacophore models.

Nº	Chemical structure	IC_{50} (nM)
2		3.7
3		4
4		4.1
5		5

6		5.2
7		5.4
8		6.1
9		6.9

10		7.2
12		9.3
13		9.5
14		9.6
15		9.8

16		12.59
18		18
20		20.4
21		22.39
23		26

24		26.1
25		28.9
26		33.2
27		35
29		46.67
30		46.77
33		50

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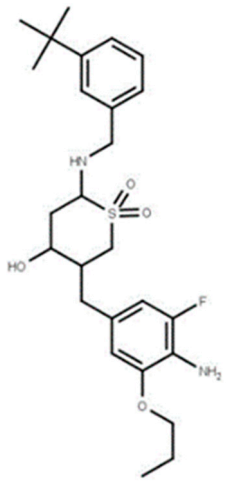

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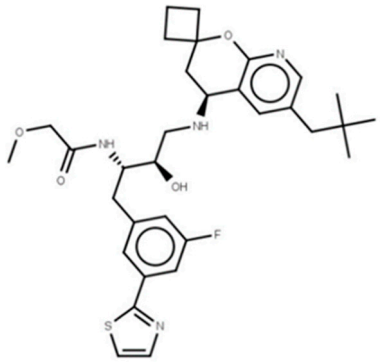

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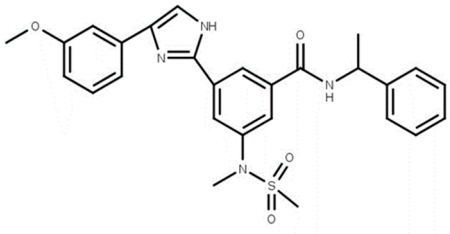

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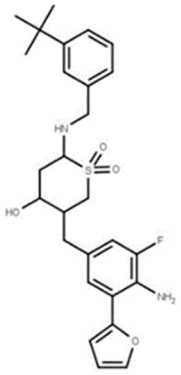

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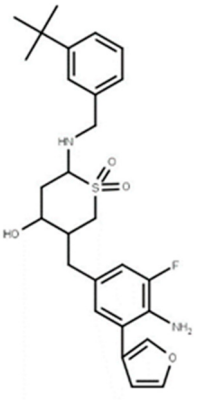
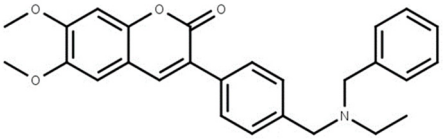
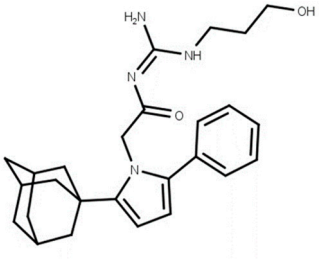
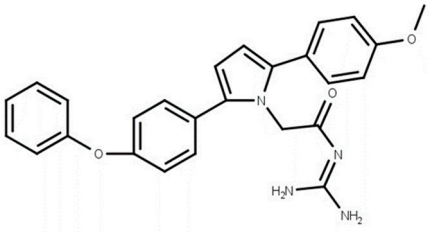
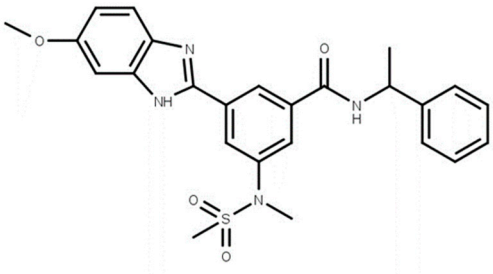
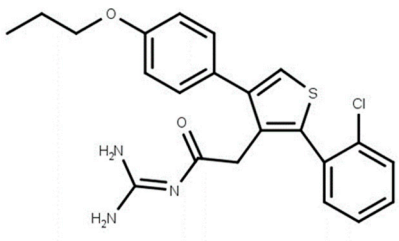
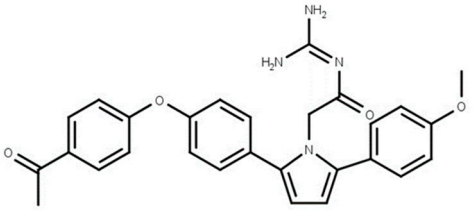
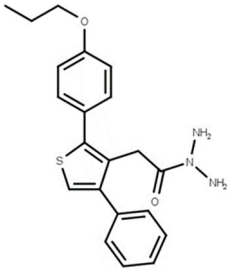
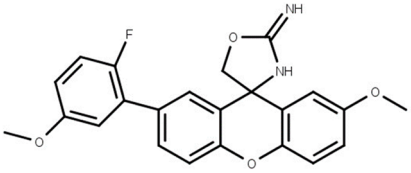
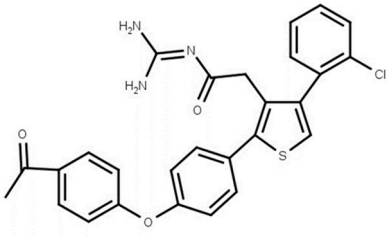
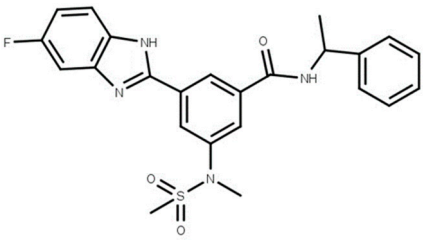
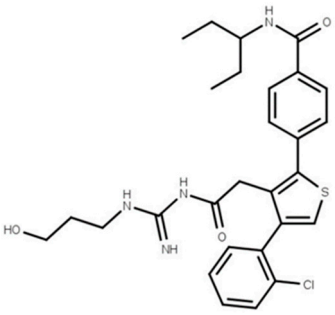
43		150
45		238
46		239
47		500
48		545
49		590

50		600
51		680
52		740
53		750
54		786
55		930

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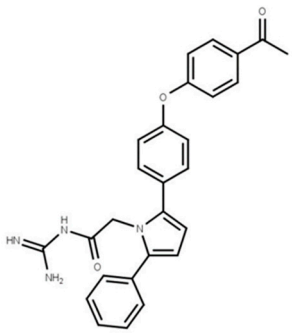

1000