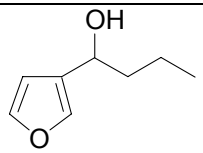
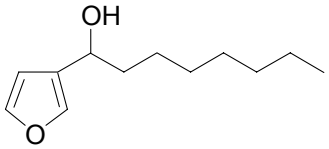
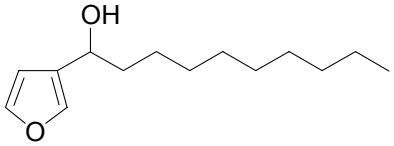
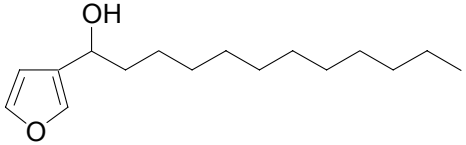
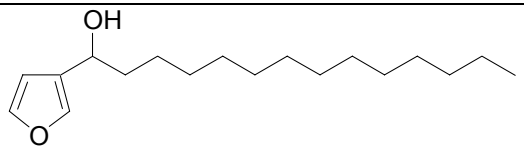
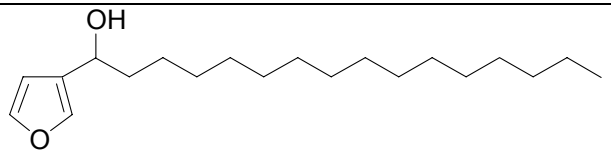
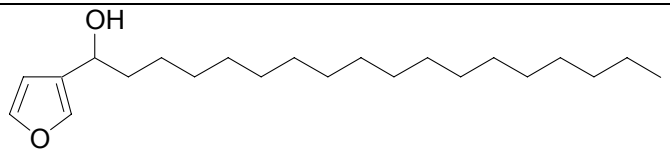
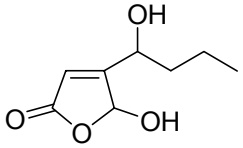
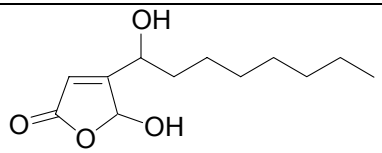
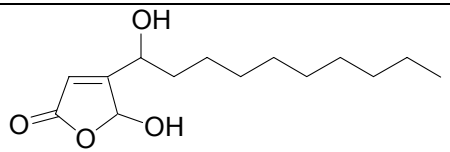
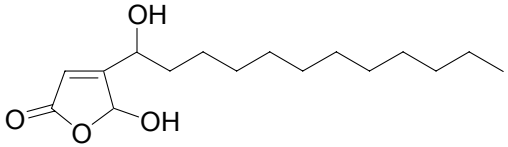
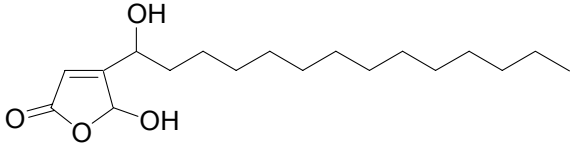
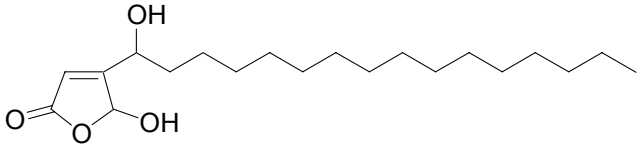
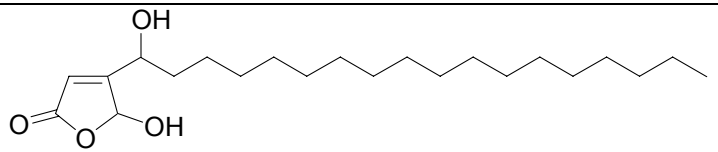
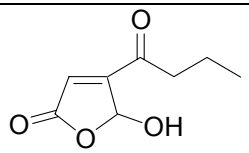
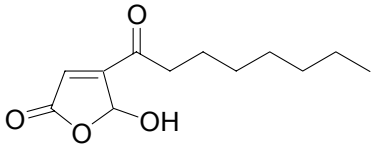
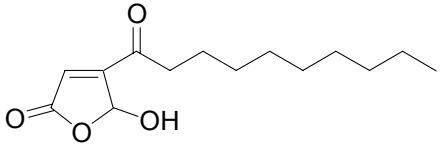
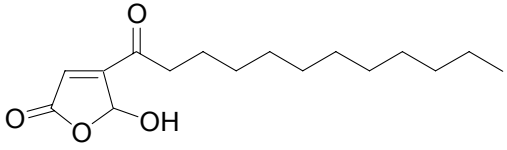
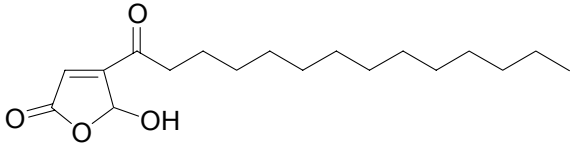
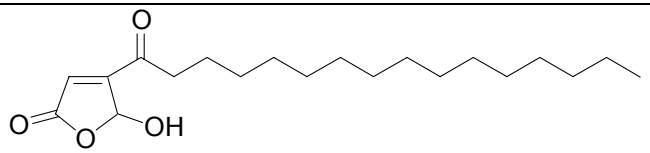
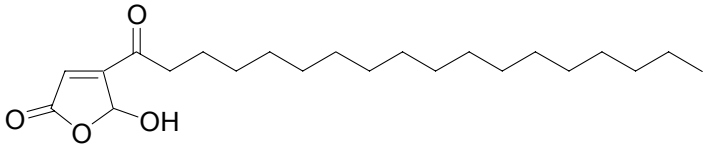
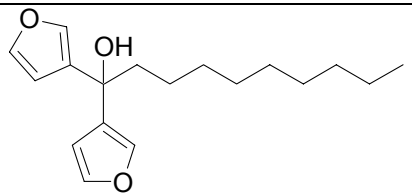
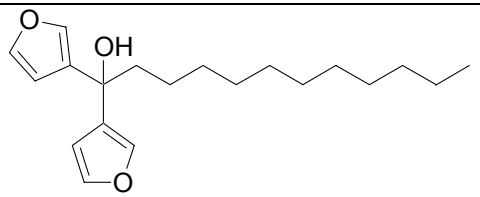
Table 2. Synopsis of inhibition data

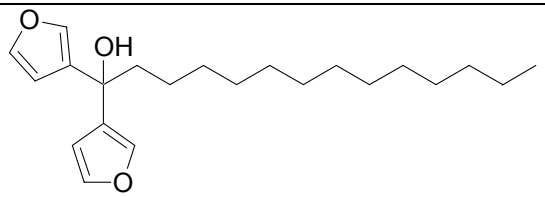
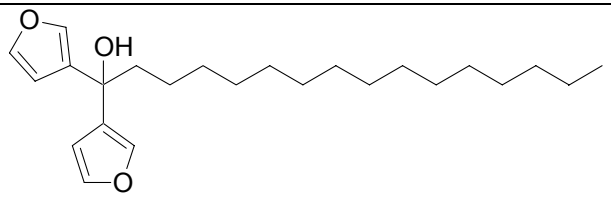
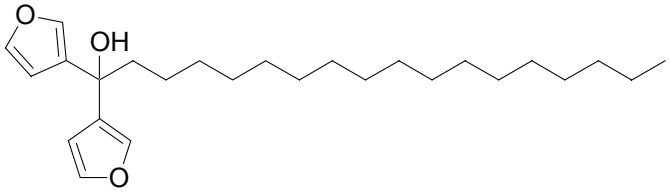
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
1		>100	>20	>20	>20
2		>100	>20	>20	>20
3		>100	>20	>20	>20
4		>100	>20	>20	>20

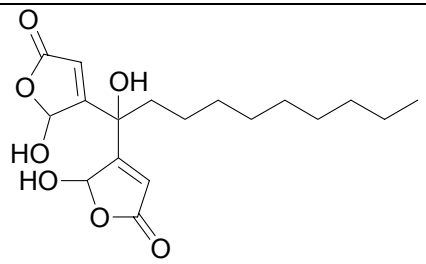
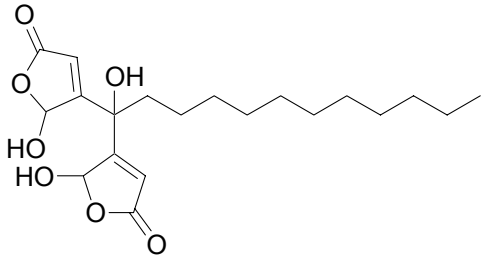
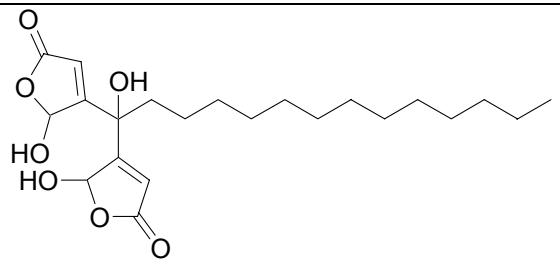
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
5		>100	>20	>20	>20
6		>100	>20	>20	>20
7		>100	>20	>20	>20
8		>100	>20	>20	>20
9		26	>20	>20	>20

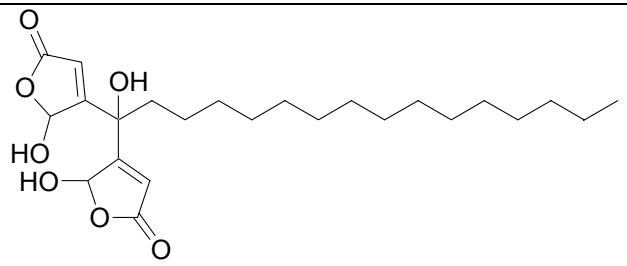
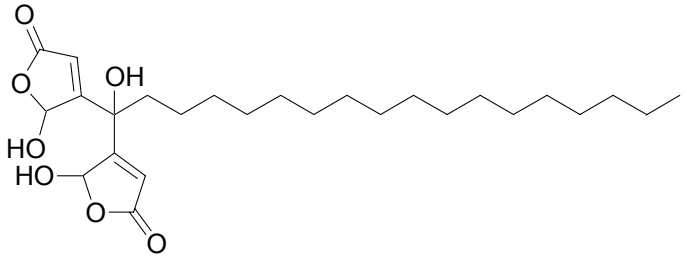
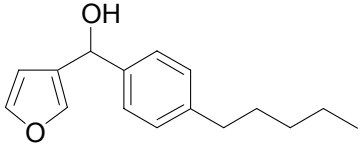
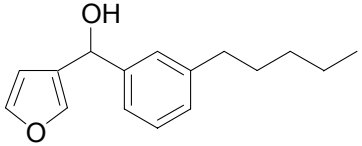
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
10		8.4	>20	>20	>20
11		2.3	>20	20.4 ± 1.5	16.7 ± 0.4
12		6.4 ± 2.4	>20	45 ± 15	10.2 ± 0.2
13		7	>20	>20	>20
14		2	>20	>20	>20

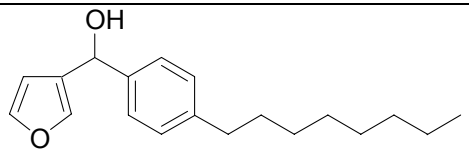
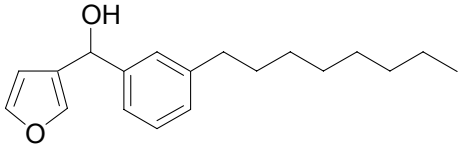
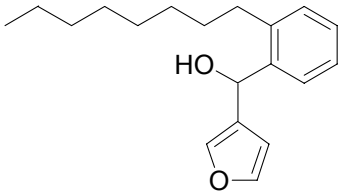
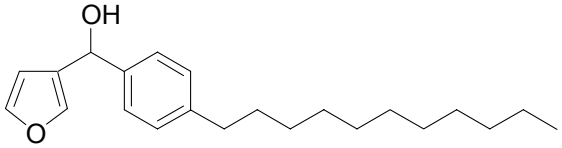
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
15		>100	>20	>20	>20
16		>100	>20	>20	>20
17		18	>20	>20	>20
18		5.9 ± 1.7	>20	84 ± 12	12.3 ± 1.0
19		4.5	>20	>20	>20

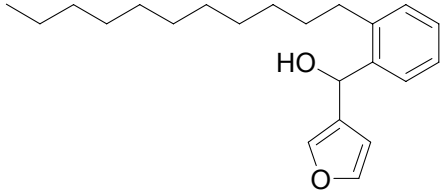
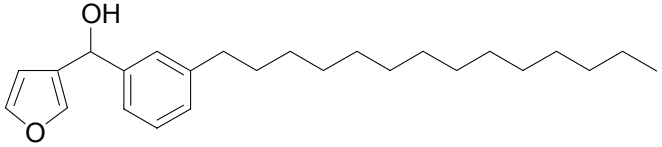
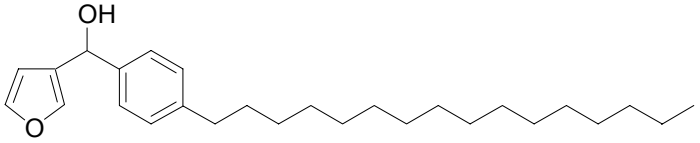
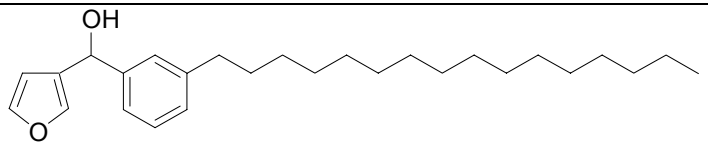
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
20		>100	>20	>20	>20
21		>100	>20	>20	>20
22		>100	>20	>20	>20
23		>100	>20	>20	>20

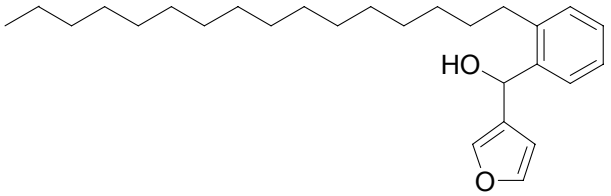
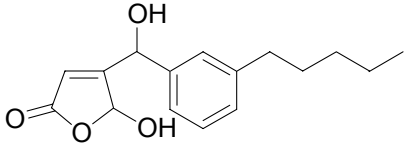
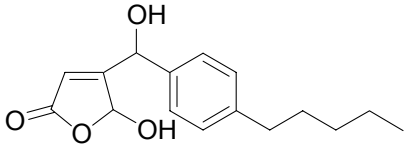
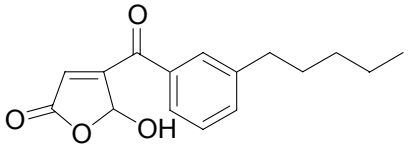
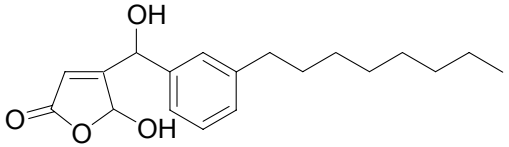
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
24		>100	>20	>20	>20
25		>100	>20	>20	>20
26		>100	>20	>20	>20

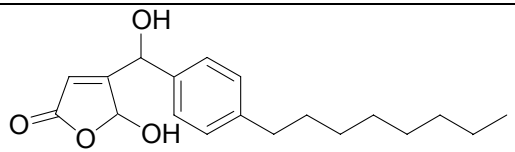
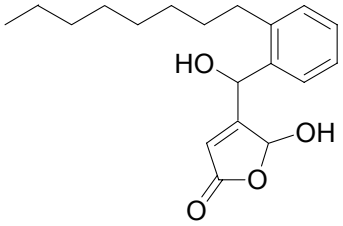
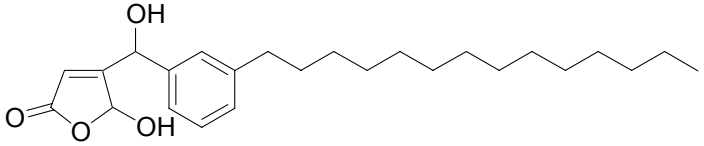
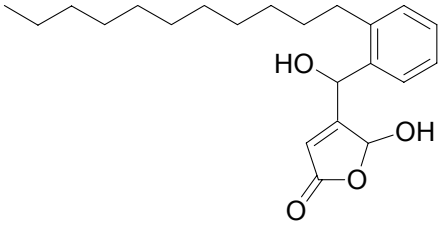
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
27		5.3	>20	>20	>20
28		3	>20	>20	>20
29		6	>20	>20	>20

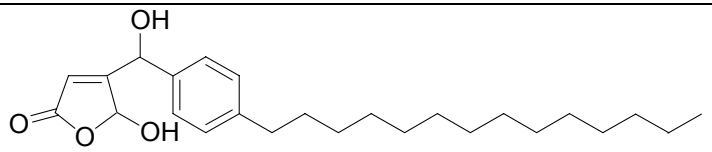
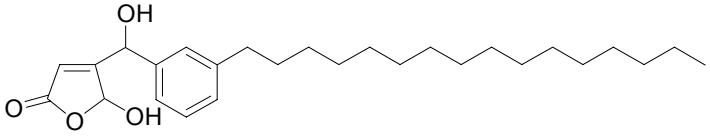
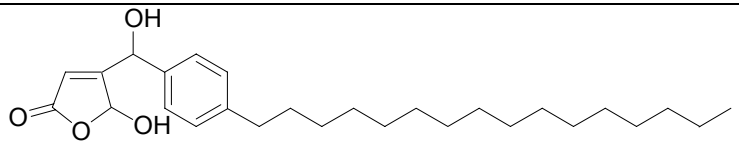
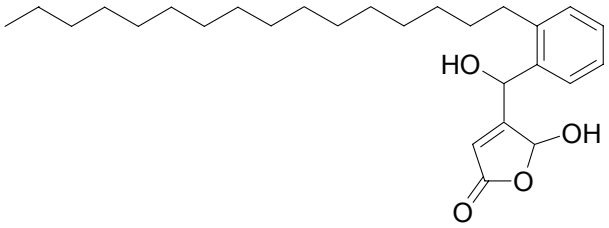
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
30		1.4 ± 0.5	>20	>20	>20
31		2	>20	>20	>20
32		>100	>20	>20	>20
33		>100	>20	>20	>20

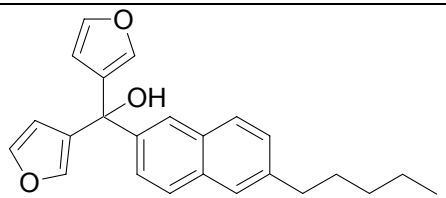
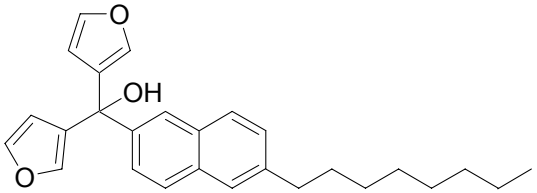
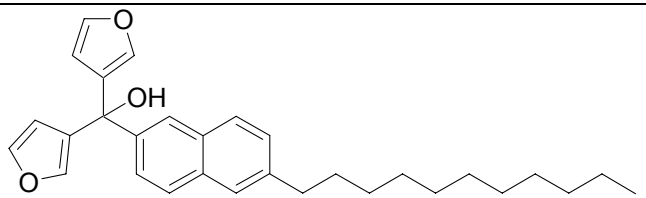
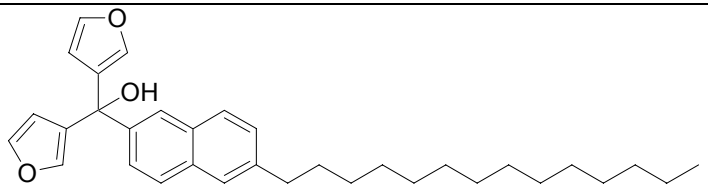
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
34		>100	>20	>20	>20
35		>100	>20	>20	>20
36		>100	>20	>20	>20
37		>100	>20	>20	>20

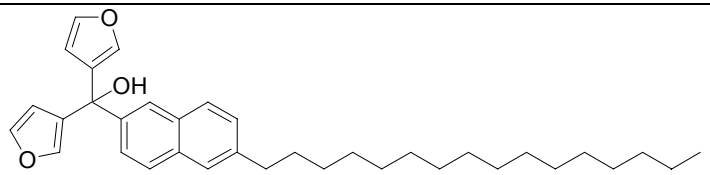
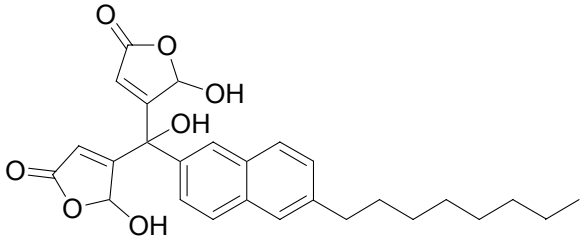
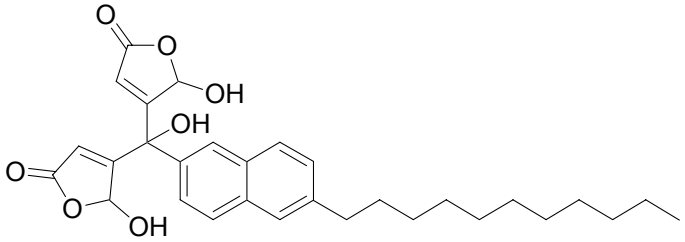
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
38		>100	>20	>20	>20
39		>100	>20	>20	>20
40		>100	>20	>20	>20
41		>100	>20	>20	>20

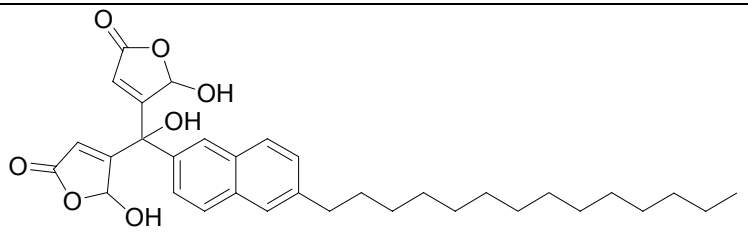
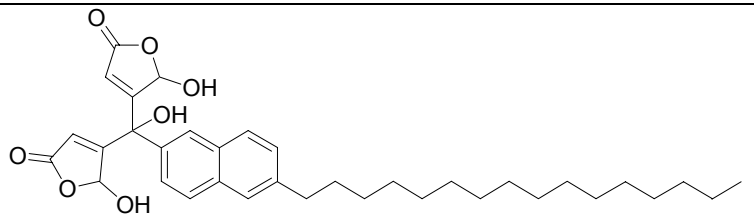
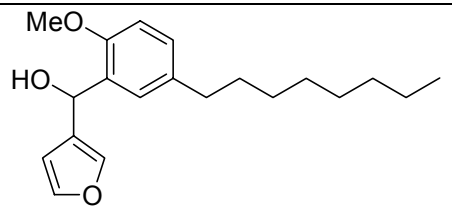
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
42		>100	>20	>20	>20
43		8	>20	>20	>20
44		13	>20	>20	>20
45		23	>20	>20	>20
46		8.5	>20	>20	>20

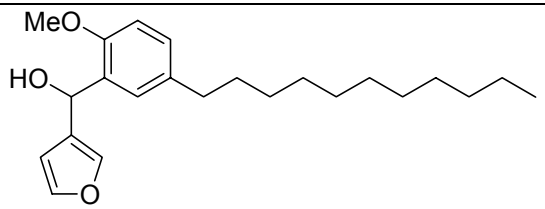
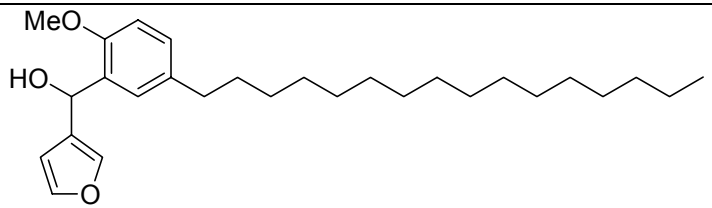
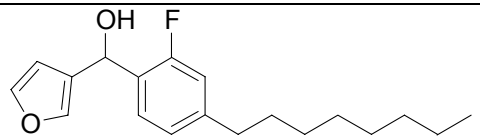
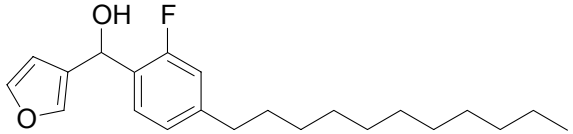
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
47		6.4	>20	>20	>20
48		5.4	>20	>20	>20
49		3.5	>20	>20	>20
50		5.7	>20	>20	>20

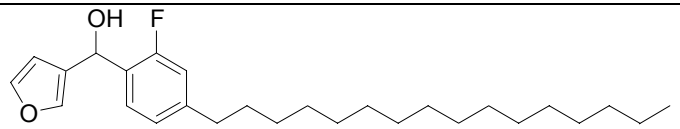
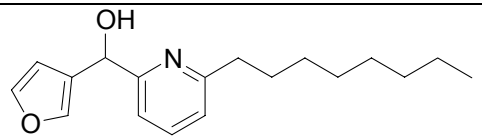
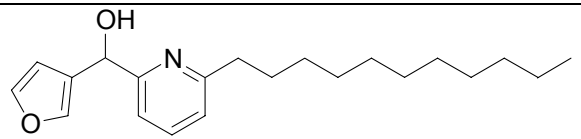
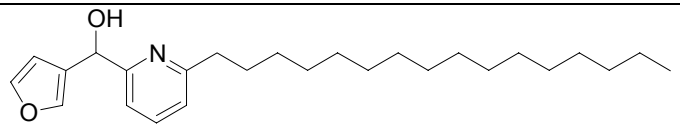
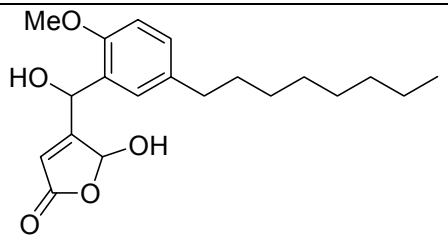
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
51		4.8	>20	>20	>20
52		4	>20	>20	>20
53		1.7	>20	>20	>20
54		>100	>20	>20	>20

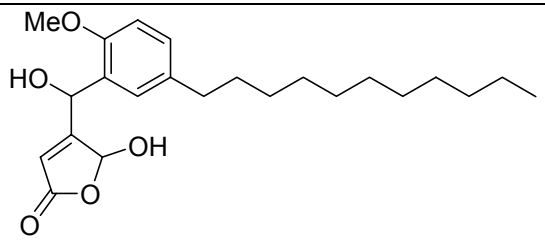
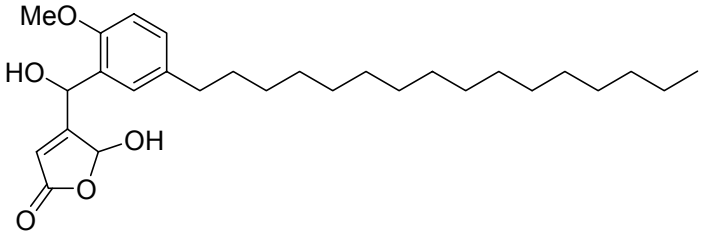
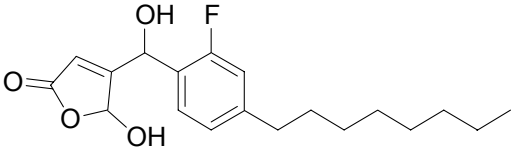
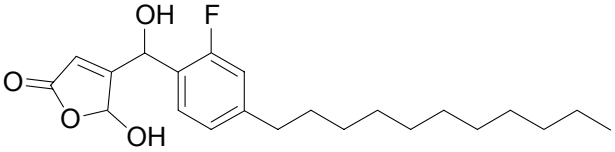
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
55		>100	>20	>20	>20
56		>100	>20	>20	>20
57		>100	>20	>20	>20
58		>100	>20	>20	>20

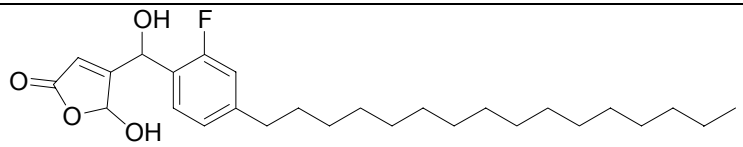
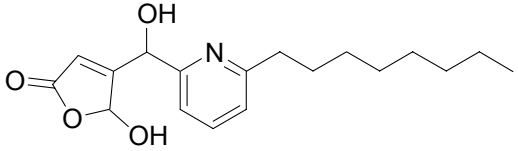
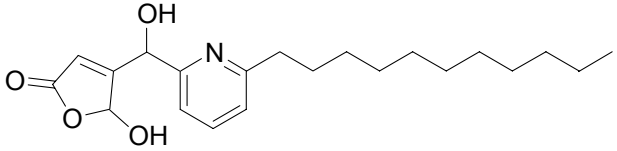
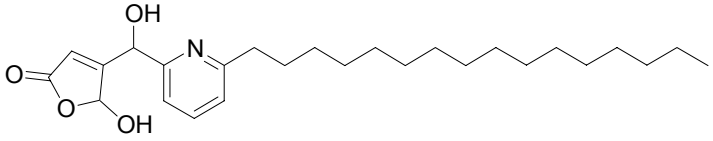
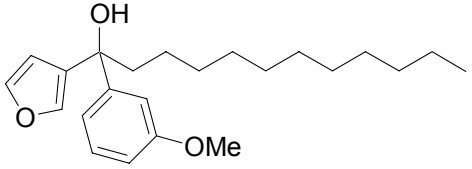
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
59		>100	>20	>20	>20
60		4.8	>20	>20	>20
61		0.35 ± 0.18 0.49 ± 0.18	>20	14 ± 3 19 ± 4	2.4 ± 0.3

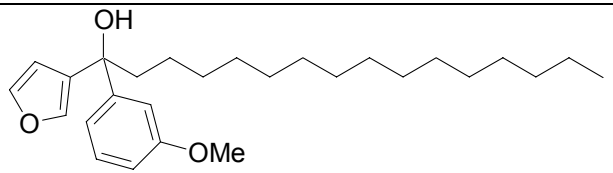
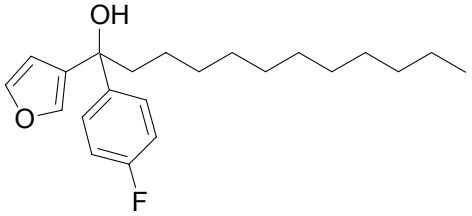
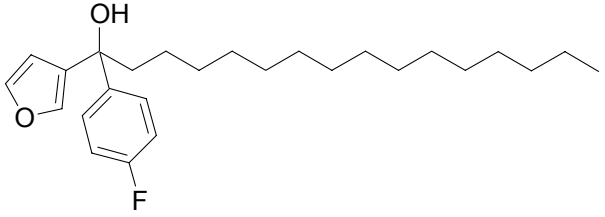
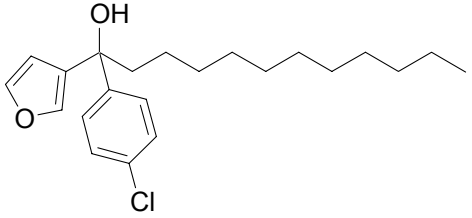
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
62		10	>20	>20	>20
63		3.9	>20	>20	>20
64		>100	>20	>20	>20

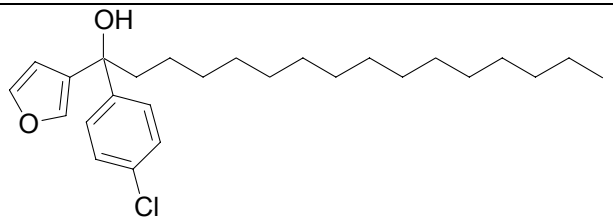
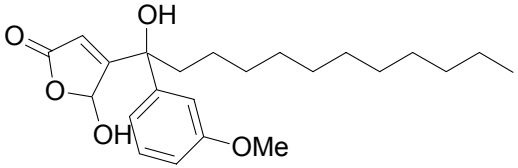
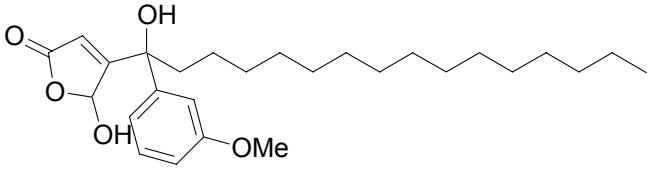
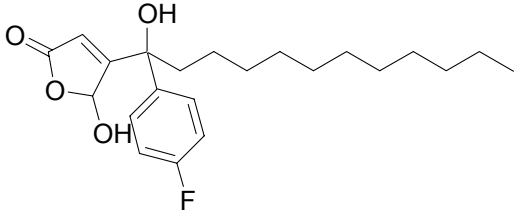
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
65		>100	>20	>20	>20
66		1.8 ± 0.7 1.1 ± 0.1	>20	19 ± 3 22 ± 4	6.7 ± 0.9
67		>100	>20	>20	>20
68		>100	>20	>20	>20

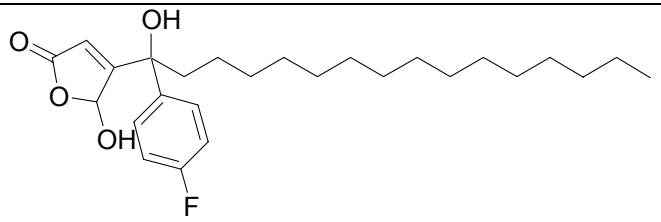
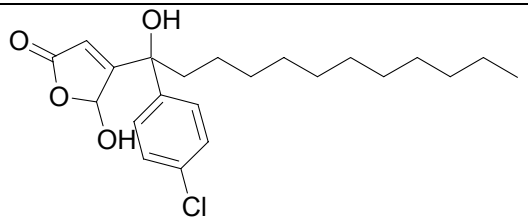
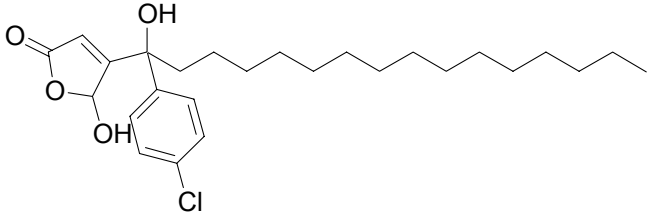
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
69		>100	>20	>20	>20
70		>100	>20	>20	>20
71		>100	>20	>20	>20
72		>100	>20	>20	>20
73		5.4	>20	>20	>20

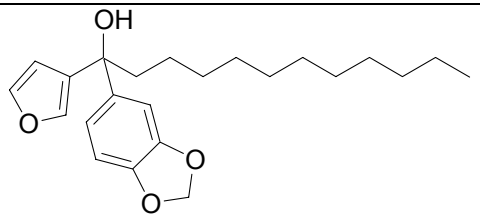
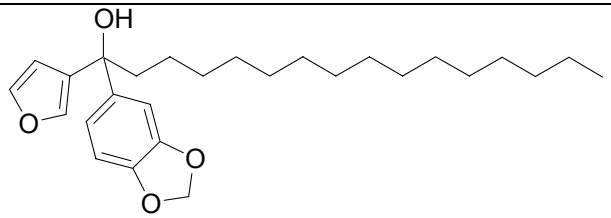
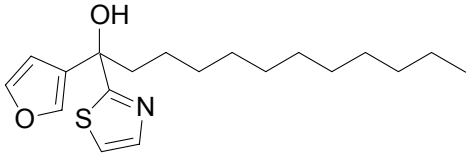
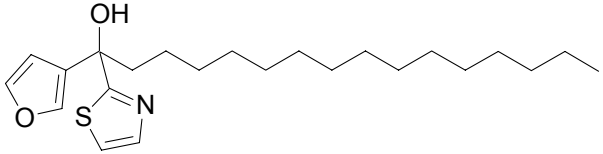
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
74		2.0 ± 1.0	>20	13.2 ± 0.5	13.9 ± 0.8
75		2.2	>20	>20	>20
76		1.9 ± 0.7	>20	11.2 ± 0.3	13.5 ± 1.0
77		4	>20	>20	>20

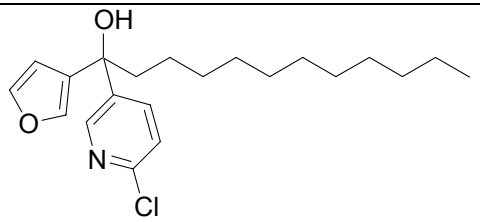
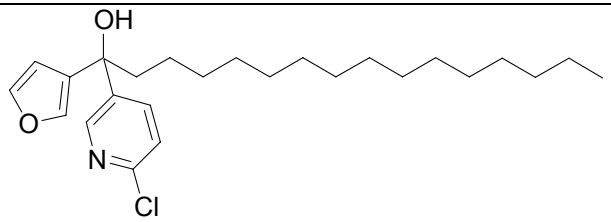
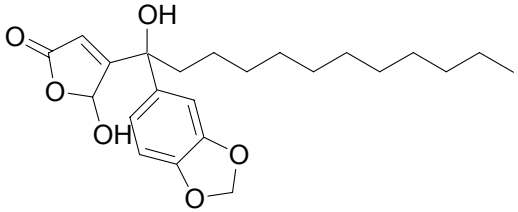
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
78		>100	>20	19 ± 3 21 ± 3	5.3 ± 1.1
79		14	>20	>20	>20
80		12	>20	>20	>20
81		11	>20	>20	>20
82		>100	>20	>20	>20

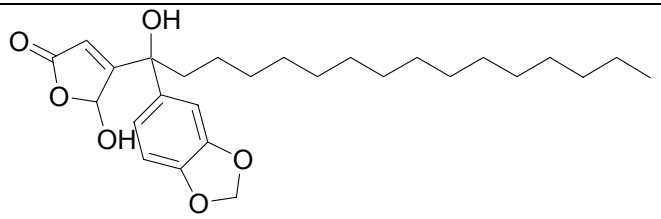
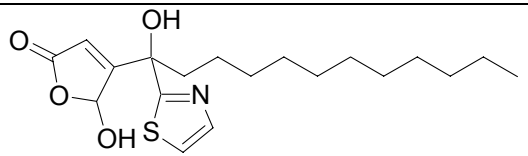
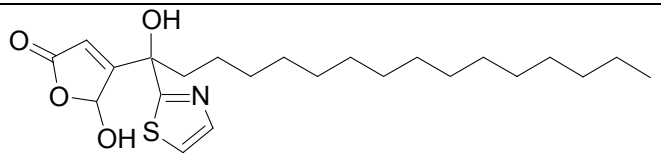
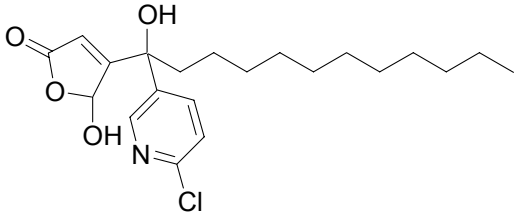
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
83		>100	>20	>20	>20
84		>100	>20	>20	>20
85		>100	>20	>20	>20
86		>100	>20	>20	>20

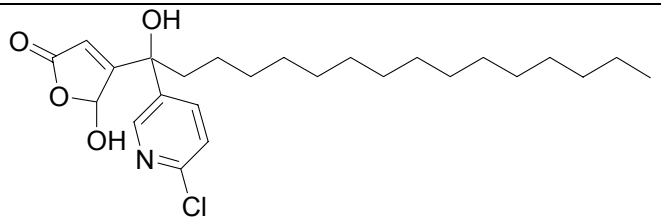
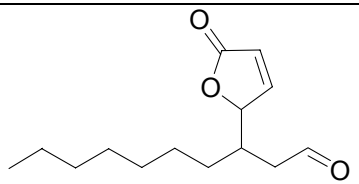
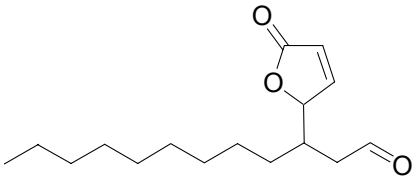
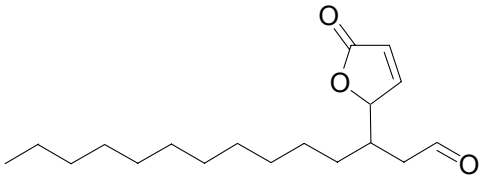
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
87		>100	>20	>20	>20
88		1.6 ± 0.6	4.5 ± 0.3	10 ± 1	14 ± 2
		1.0 ± 0.1	4.5 ± 0.3	10 ± 2	
89		4.5 ± 2.1	21 ± 3	>20	>20
90		1.5 ± 0.2	2.1 ± 0.5	13 ± 3	34 ± 4
		1.4 ± 0.01	1.6 ± 0.1		

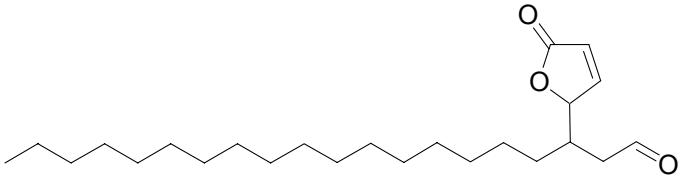
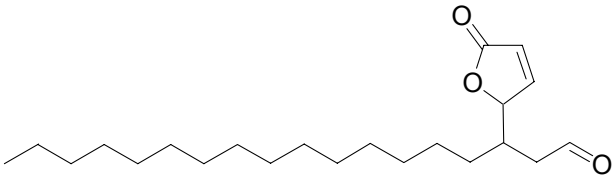
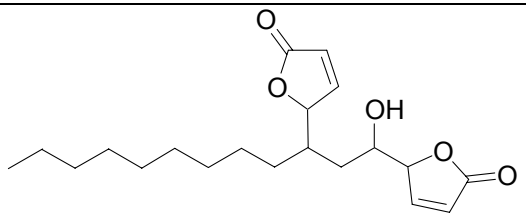
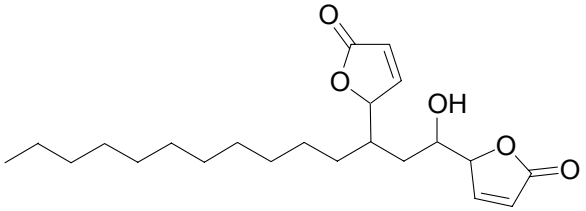
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
91		2.9 ± 1.1	24 ± 6	>20	>20
92		1.2 ± 0.2	16 ± 2	93 ± 10	23 ± 8
93		2.3 ± 0.5	1.3 ± 0.1	7.8 ± 1.8	2.8 ± 0.4
		1.9 ± 0.1	1.9 ± 0.1	5.0 ± 2.1	

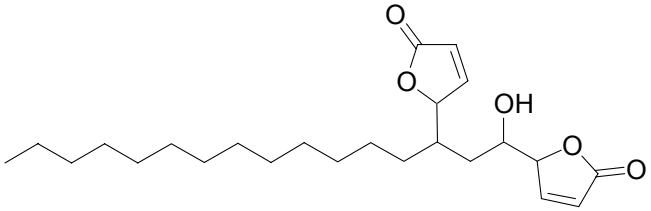
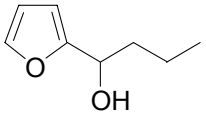
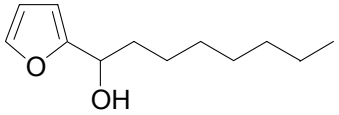
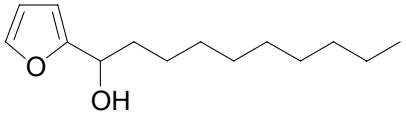
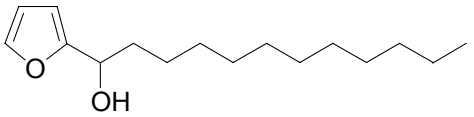
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
94		>100	>20	>20	>20
95		>100	>20	>20	>20
96		>100	>20	>20	>20
97		>100	>20	>20	>20

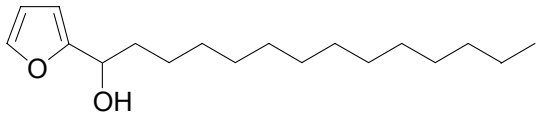
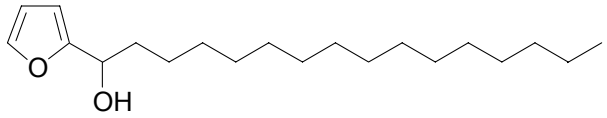
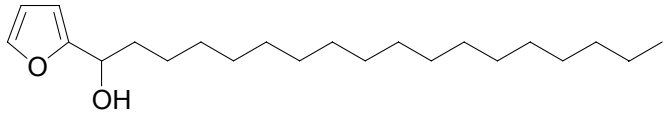
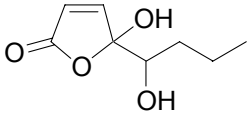
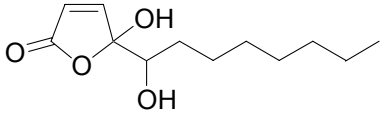
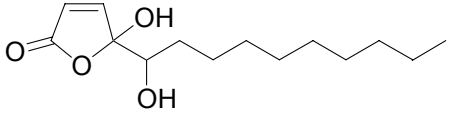
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
98		>100	>20	>20	>20
99		>100	>20	>20	>20
100		30	>20	>20	>20

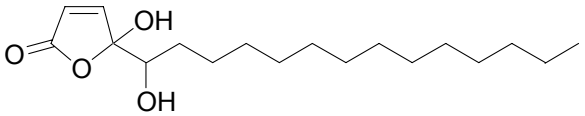
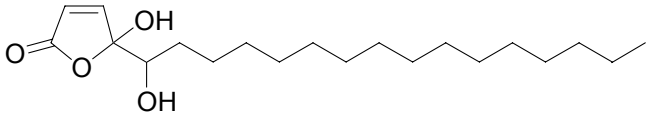
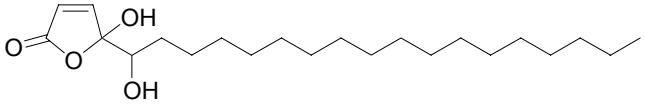
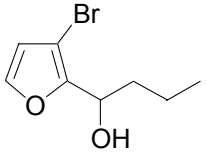
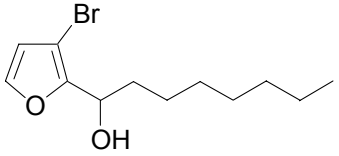
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
101		19	>20	>20	>20
102		35	>20	>20	>20
103		12	>20	>20	>20
104		2.8 ± 0.3	15 ± 1	>20	>20

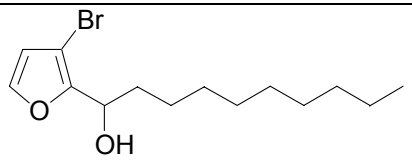
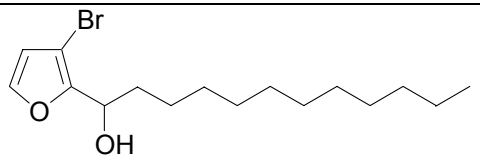
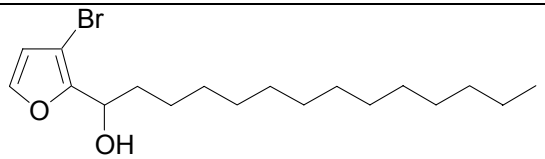
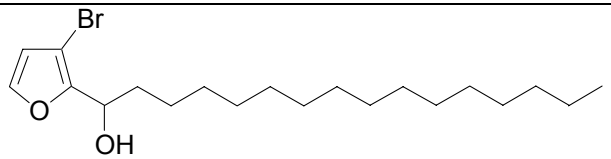
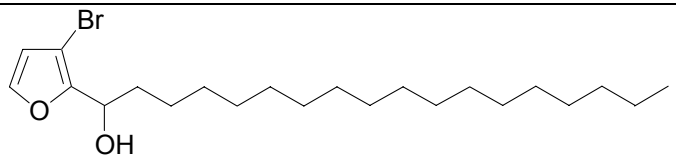
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
105		5.1 ± 2.1	23 ± 5	>20	>20
106		7.9 ± 0.8	>20	5.8 ± 0.7	52 ± 9
107		3.1 ± 0.3	>20	3.8 ± 0.4	39 ± 6
108		10.7	>20	>20	>20

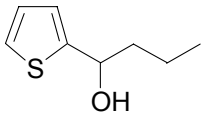
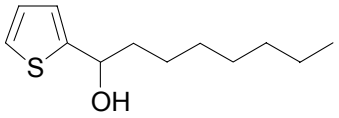
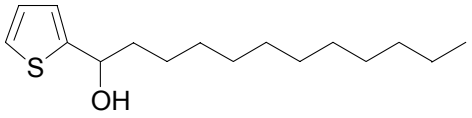
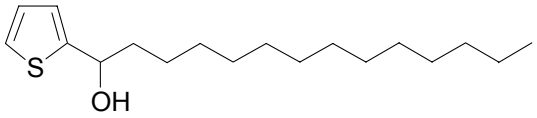
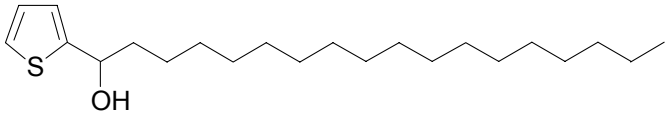
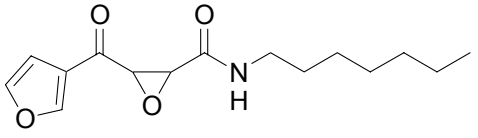
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
109		>100	>20	90	117
110		>100	>20	88	85
111		43	>20	38	83
112		45	>20	10 ± 2 12 ± 2	95 ± 4

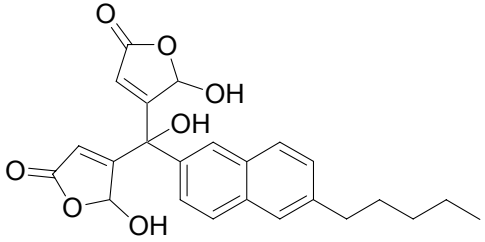
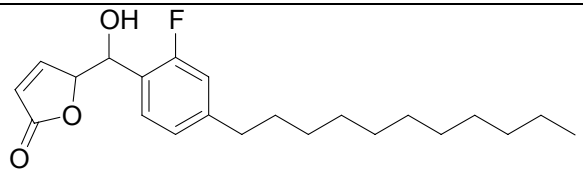
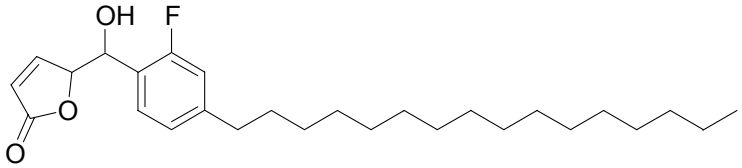
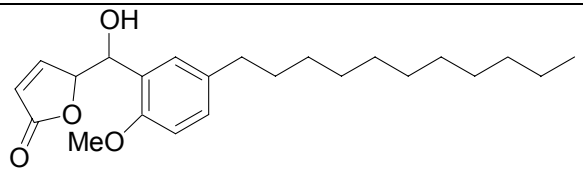
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
113		30	>20	>20	>20
114		>100	>20	>20	>20
115		>100	>20	>20	>20
116		>100	>20	>20	>20
117		>100	>20	>20	>20

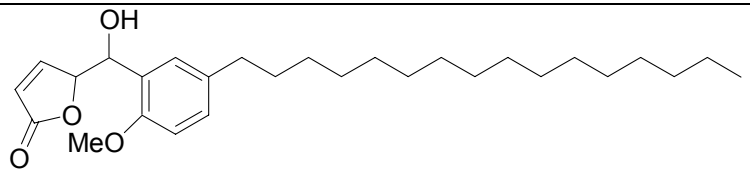
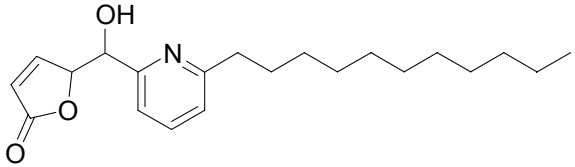
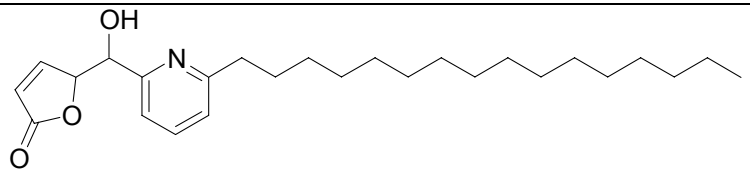
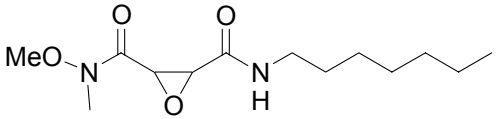
Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
118		>100	>20	>20	>20
119		>100	>20	>20	>20
120		>100	>20	>20	>20
121		>100	>20	>20	>20
122		20	>20	>20	>20
123		12	>20	>20	>20

Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
124		13	>20	>20	>20
125		14	>20	>20	>20
126		3.7	>20	>20	>20
127		>100	>20	>20	>20
128		>100	>20	>20	>20

Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
129		>100	>20	>20	>20
130		>100	>20	>20	>20
131		>100	>20	>20	>20
132		>100	>20	>20	>20
133		>100	>20	>20	>20

Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
134		>100	>20	>20	>20
135		>100	>20	>20	>20
136		>100	>20	>20	>20
137		>100	>20	>20	>20
138		>100	>20	>20	>20
139		90	>20	>20	>20

Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
140		>100	>20	>20	>20
141		>20	>20	>20	>20
142		40	>20	>20	>20
143		100	>20	>20	>20

Entry	Structure	Cdc25A IC_{50}/IC_{50} in 0.001% T*	AChE IC_{50}/IC_{50} in 0.01% T*	11βHSD1 IC_{50}/IC_{50} in 0.01% T*	11βHSD2 IC_{50}, μM
144		>100	>20	>20	>20
145		>100	>20	>20	>20
146		50	>20	>20	>20
147		>100	>20	>20	>20

*Control experiments with 0.001% or 0.01% Triton X-100, respectively, according to McGovern *et al.* [McGovern, S. L., Helfand, B. T., Feng, B. & Shoichet, B. K. (2003) *J. Med. Chem.* **46,** 4265-4272]. All IC_{50} values are in μM.