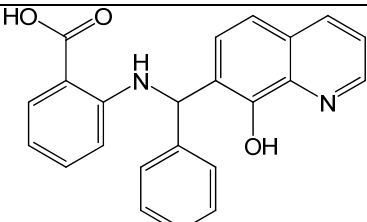
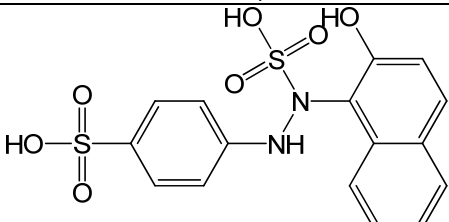
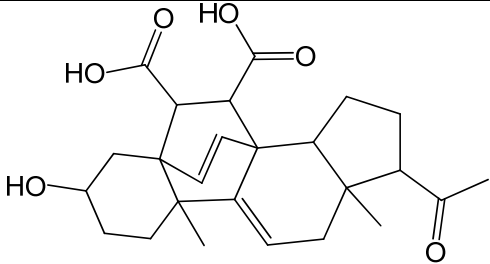
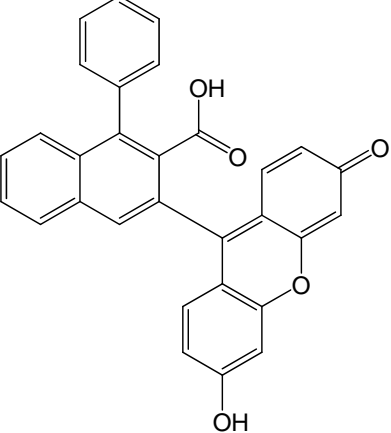
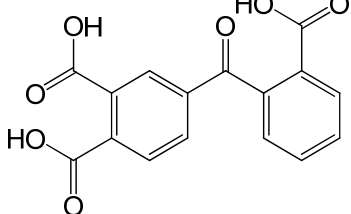
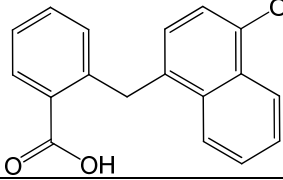
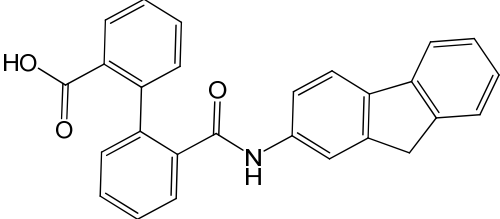
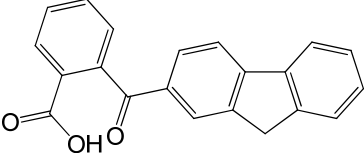
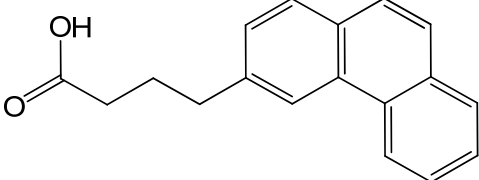
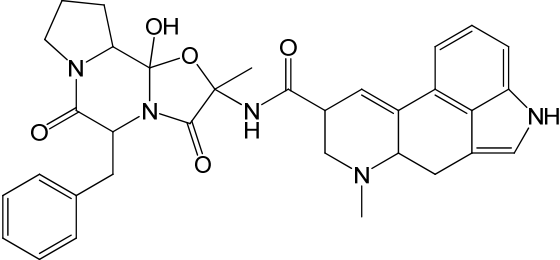
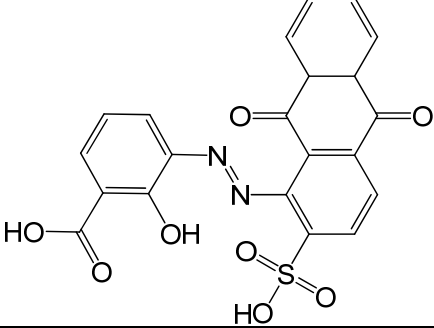
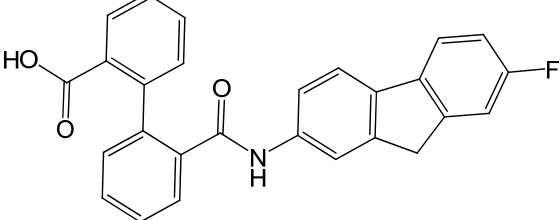
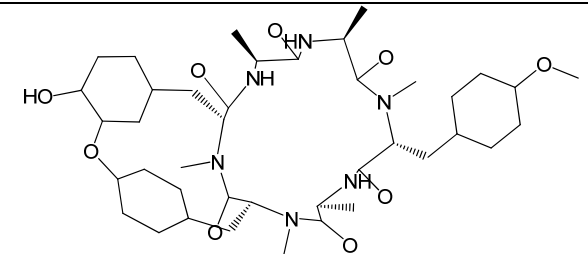
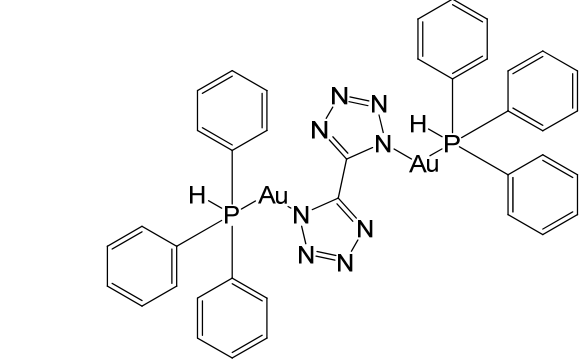
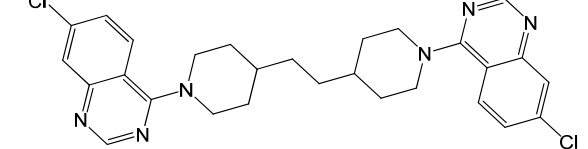
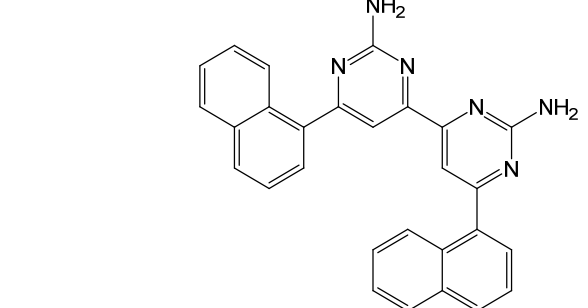
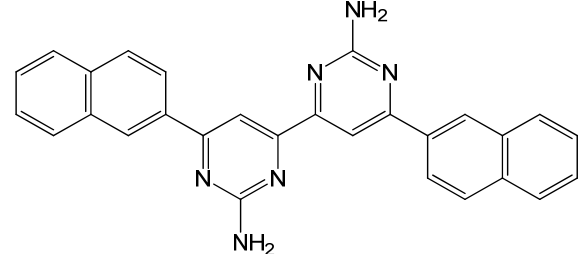
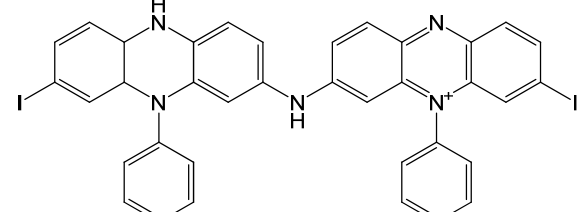


**Table S1. Chemical structures of NCI Compounds tested and their inhibitory activity against BoNT/E.**

S. No.	Div. No.	NSC No.	Structure	Inhibition of BoNT/E at 250 $\mu$ M
1	4	1012		63.1
2	98	9600		49.7
3	100	9746		25.1
4	133	12181		6.8
5	355	28620		71.1

6	628	50155		21.3
7	775	67690		37.2
8	834	77053		83.4
9	969	92828		28.3
10	991	95090		3.9
11	1279	125908		51.4
12	1292	128598		69.1

13	1618	259969		0.0
14	1633	274547		91.6
15	1792	343227		31.5
16	1853	371876		0.0
17	1854	371878		33.6
18	1896	402959		0.0