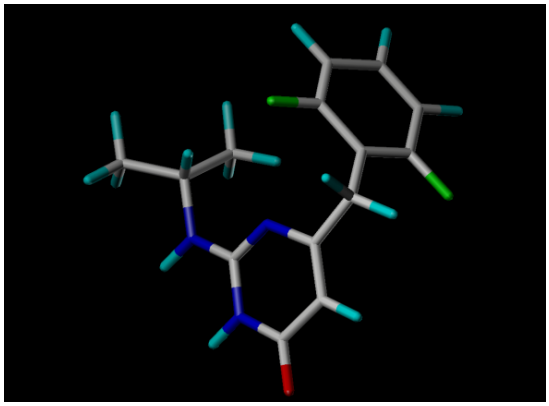
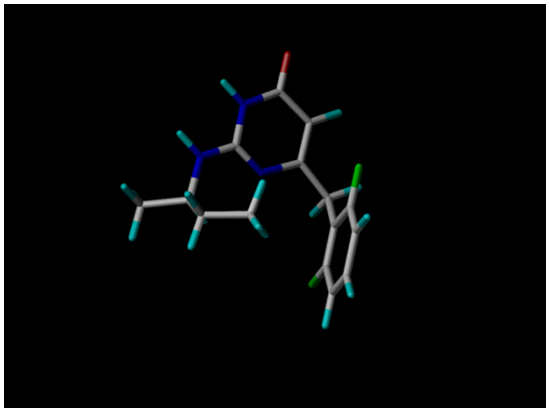
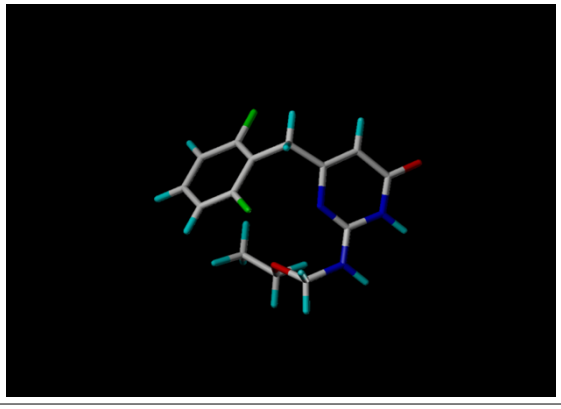
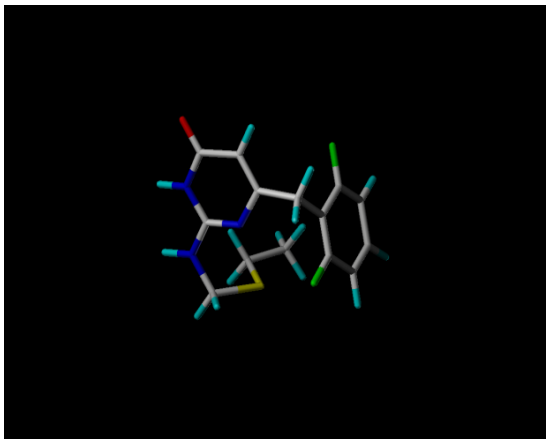
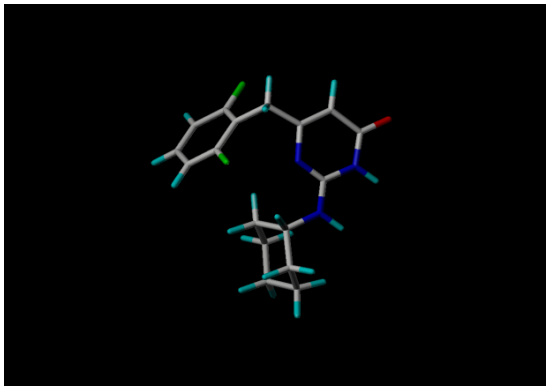
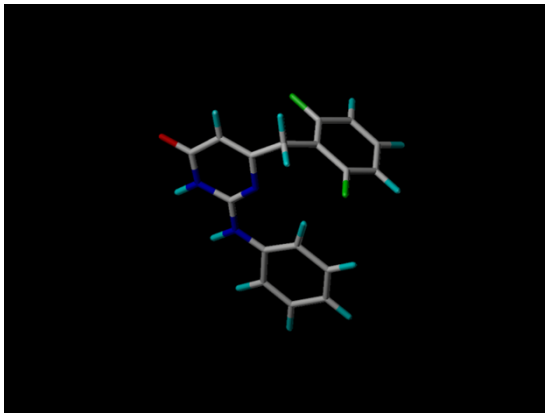
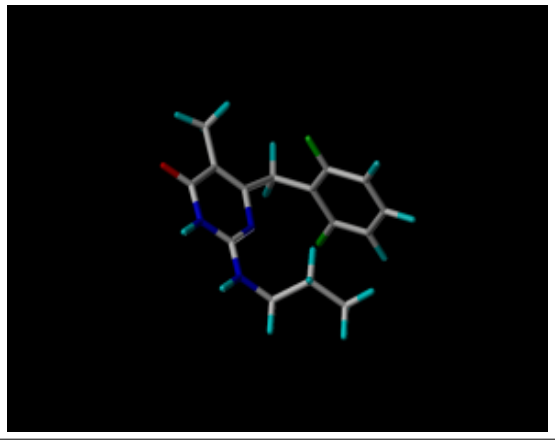
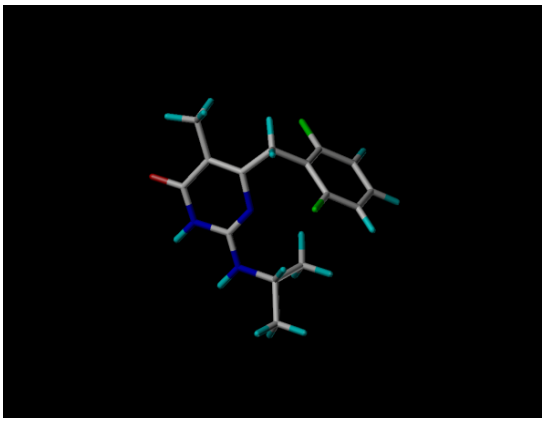
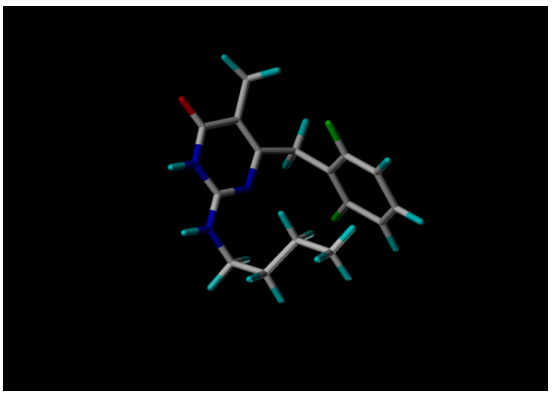
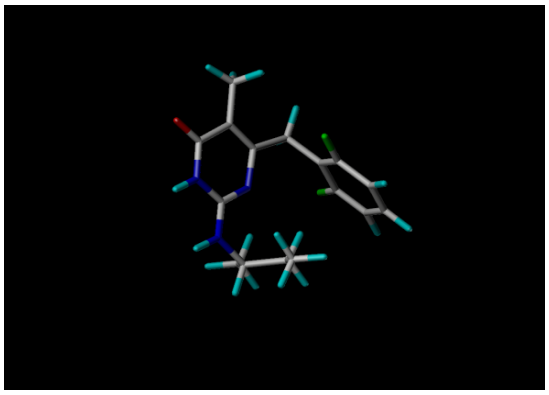
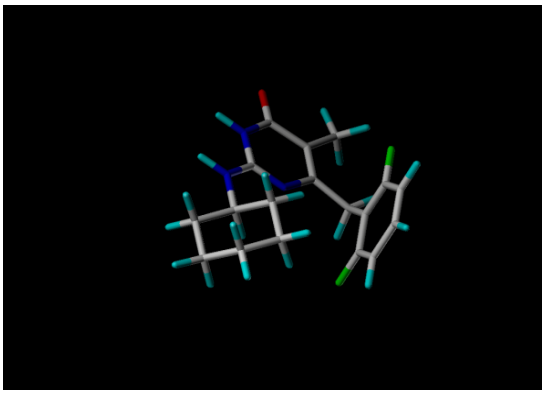
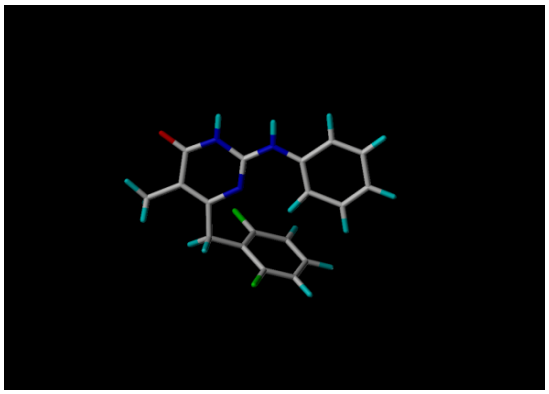
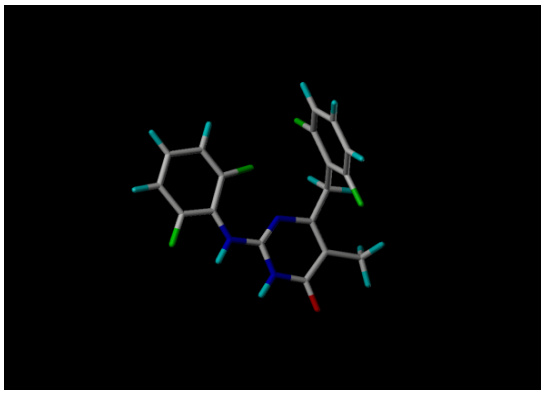
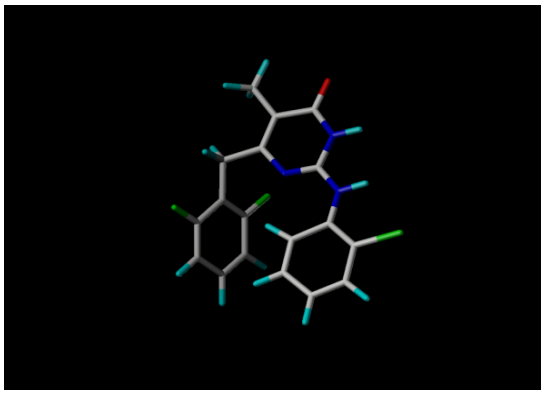
Electronic Supplementary Material (ESI) for RSC Advances.

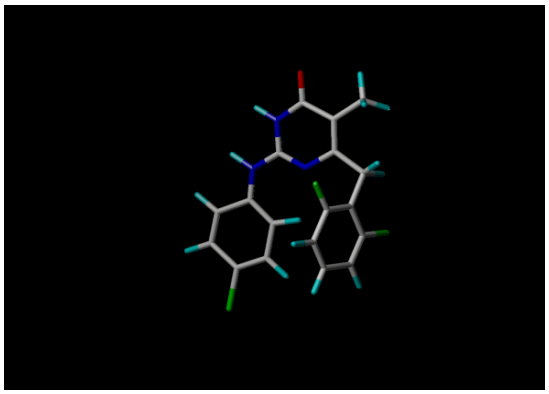
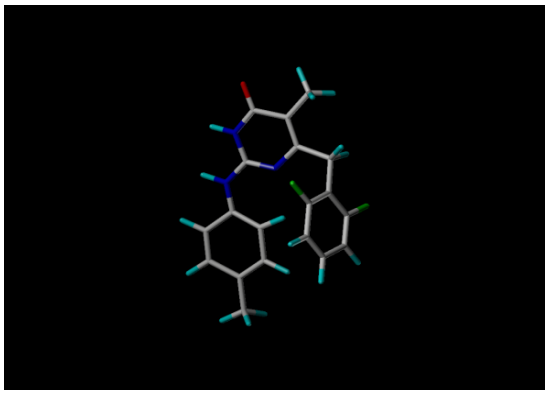
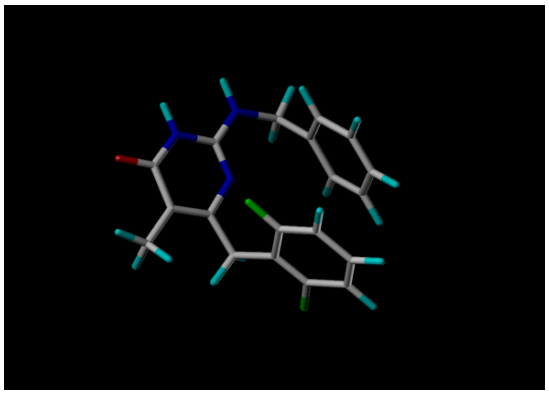
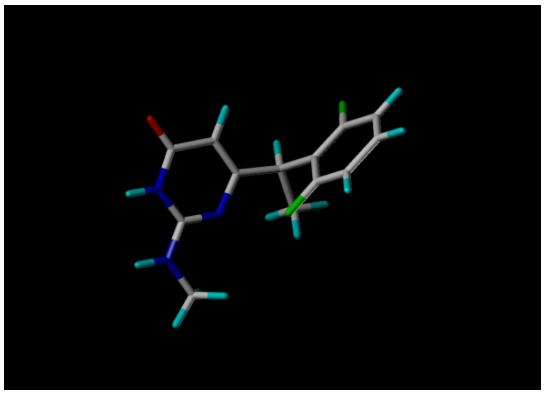
Supplementary Information 1: Table showing structure of lowest energy conformer obtained after conformational sampling for the DABO derivatives (Training, Test, Outlier, Approximate and Virtual Data set) and respective energy.

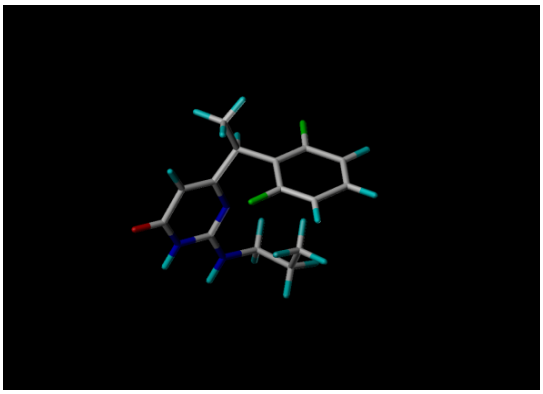
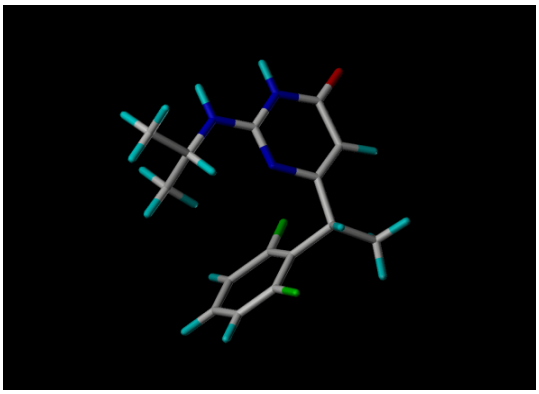
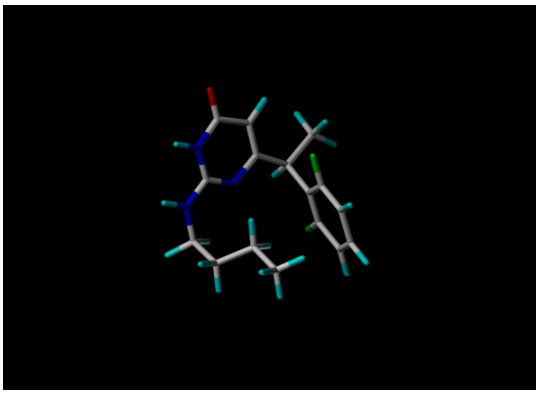
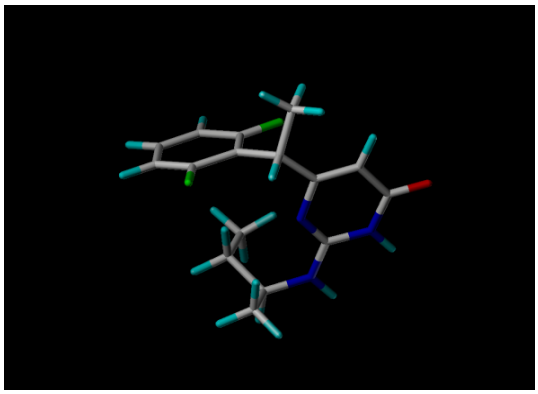
Comp. No.	Conformer no.	Structure	Energy(KJ/mol)
Training Set			
1	DABO_0400040		2.280
2	DABO_0700023		1.851
3	DABO_0800022		1.134

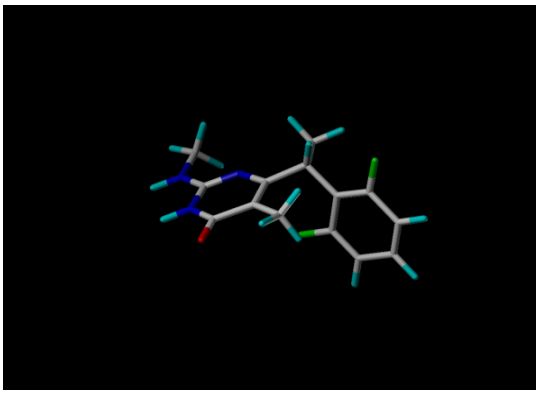
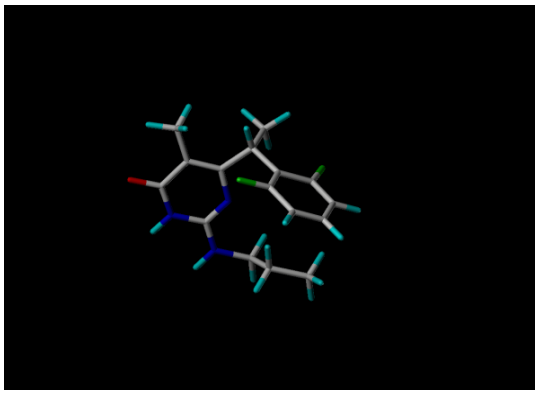
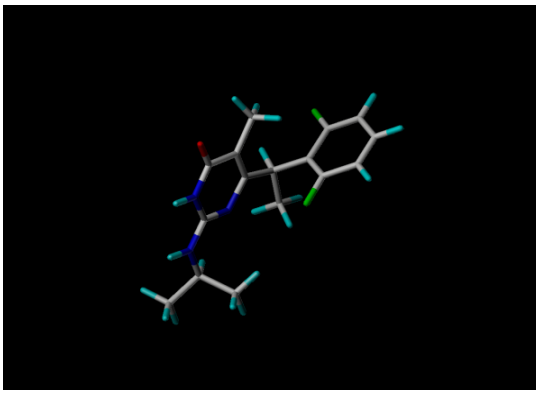
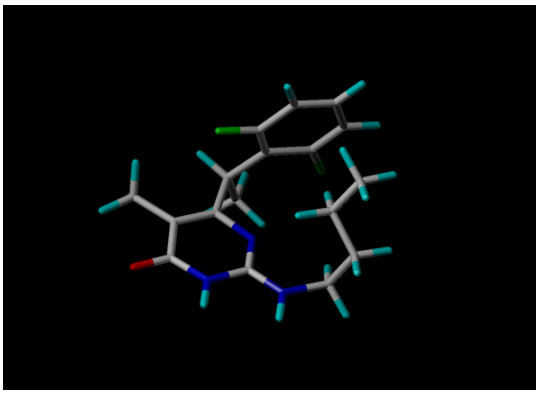
4	DABO_0900095		-0.150
5	DABO_1000005		2.989
6	DABO_1100001		9.831
7	DABO_1300053		2.869

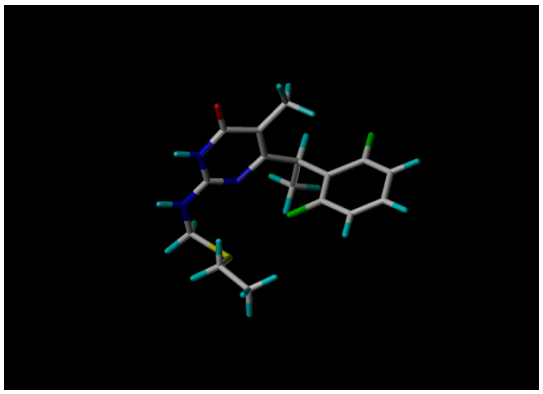
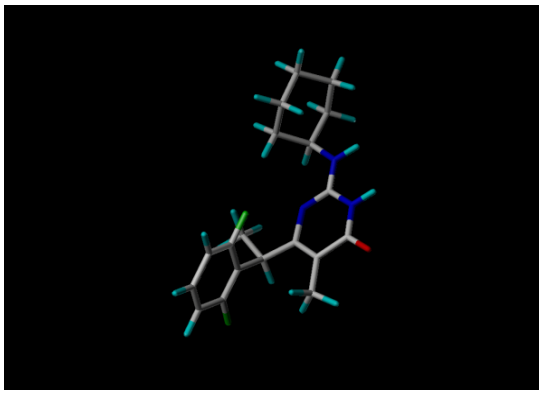
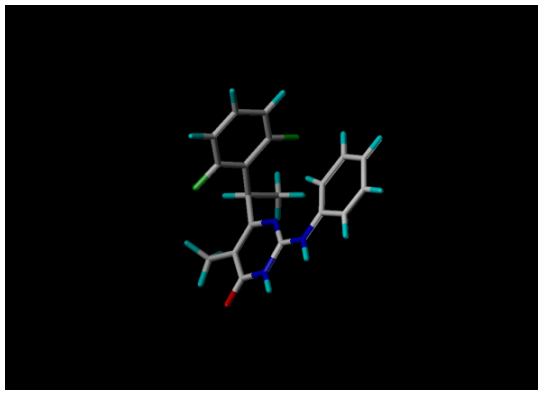
8	DABO_1400048		3.376
9	DABO_1500041		2.574
10	DABO_1600025		3.136
11	DABO_1800019		2.922

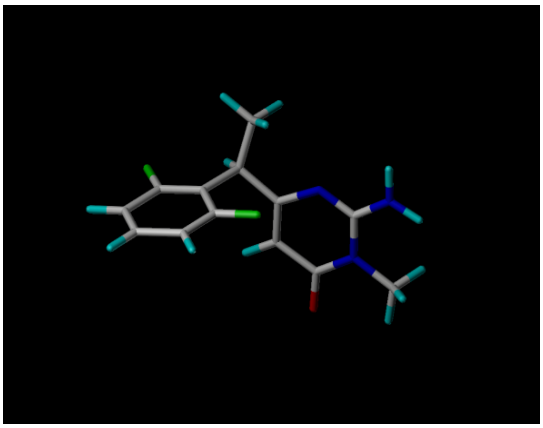
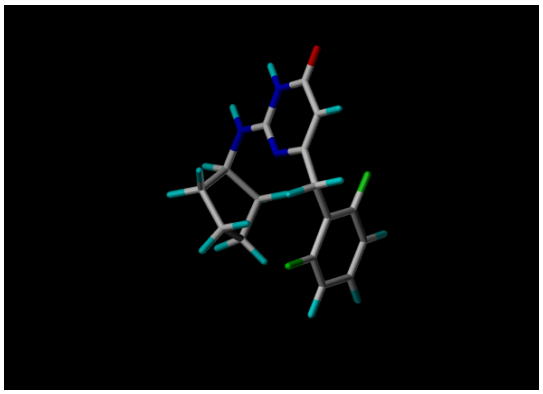
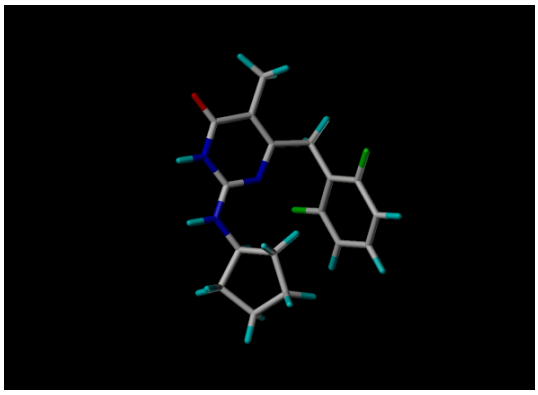
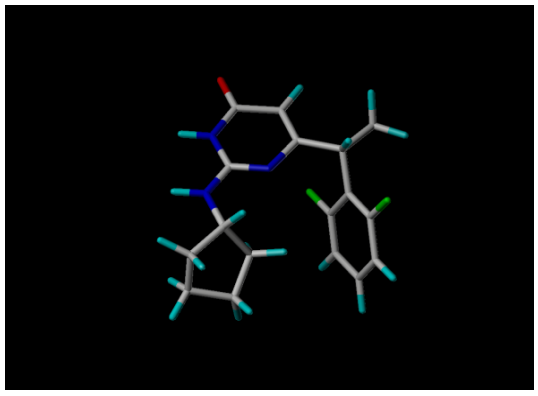
12	DABO_1900016		10.836
13	DABO_2000042		10.886
14	DABO_2100019		12.586
15	DABO_2200018		9.880

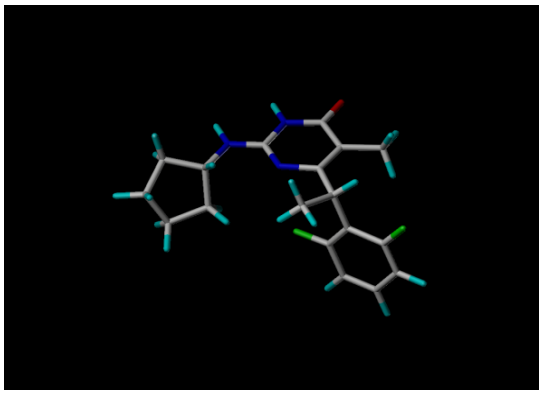
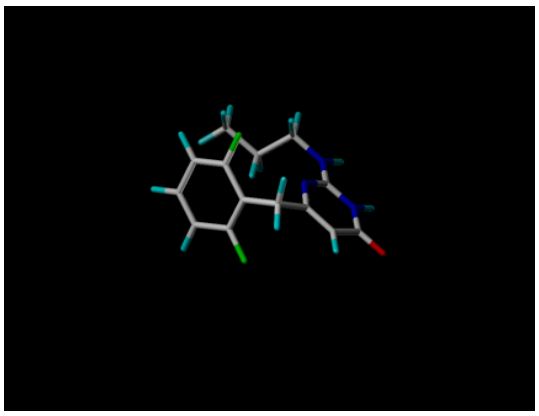
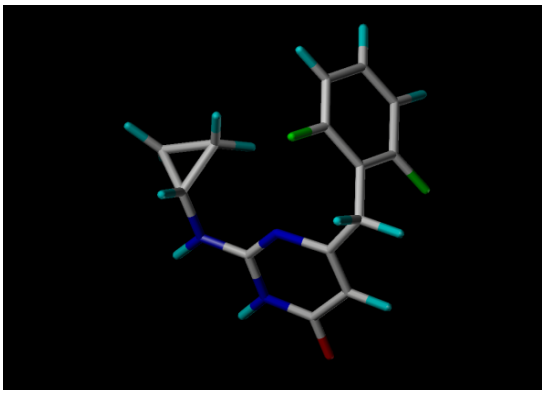
16	DABO_2300016		10.364
17	DABO_2400003		11.486
18	DABO_2600031		1.757
19	DABO_2700030		3.780

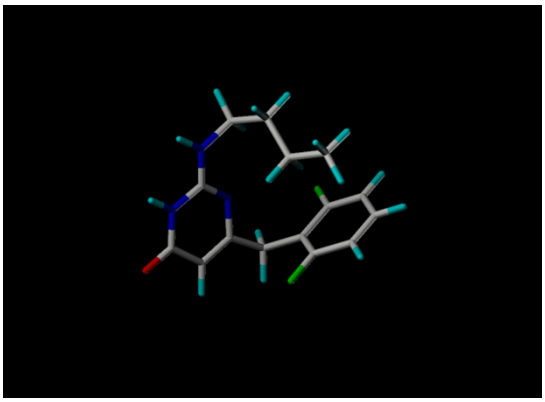
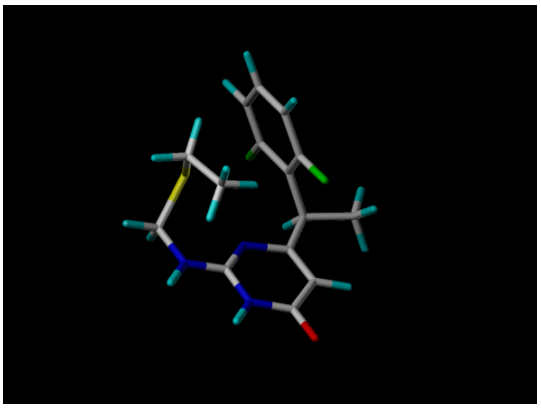
20	DABO_2800053		2.035
21	DABO_2900043		2.918
22	DABO_3000034		1.555
23	DABO_3100032		2.198

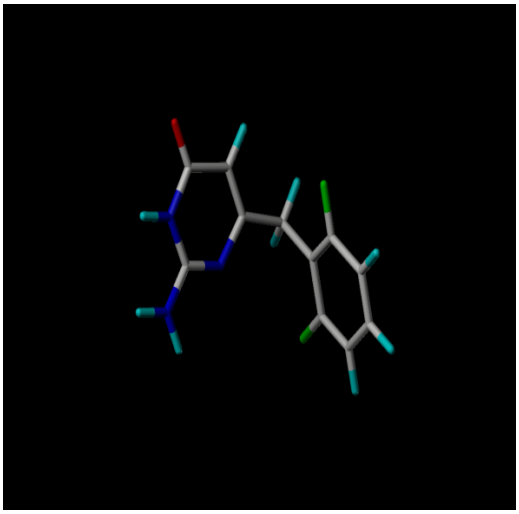
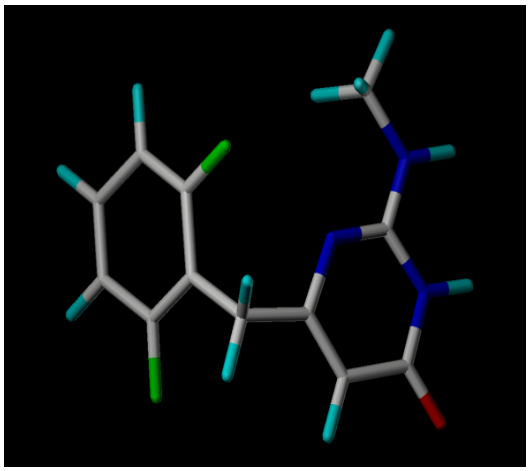
24	DABO_3400018		4.223
25	DABO_3500024		3.561
26	DABO_3600036		3.775
27	DABO_3700081		3.255

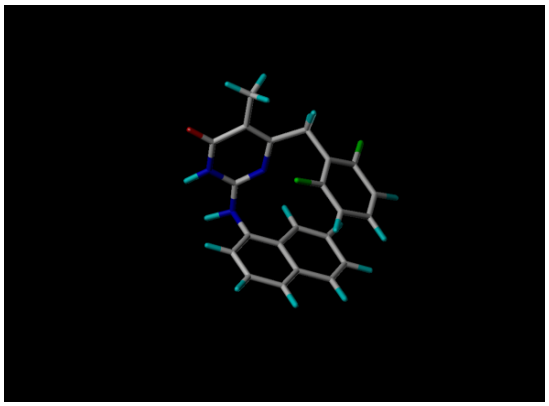
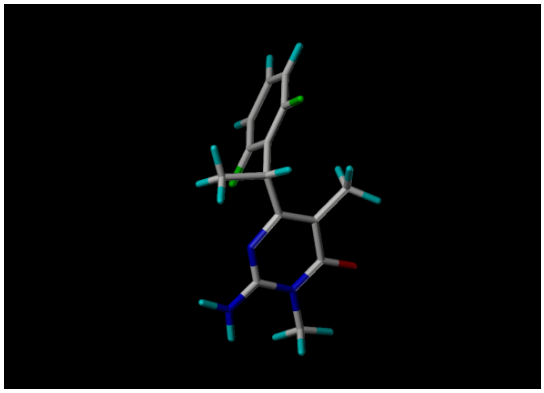
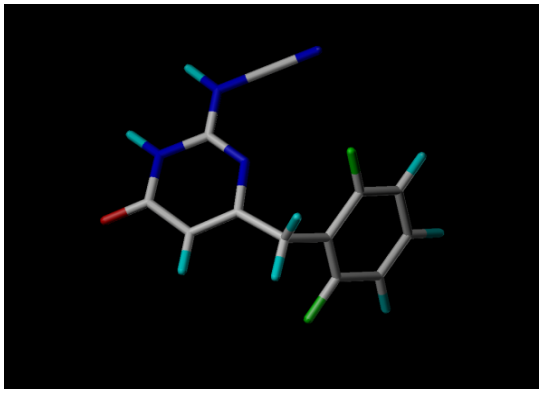
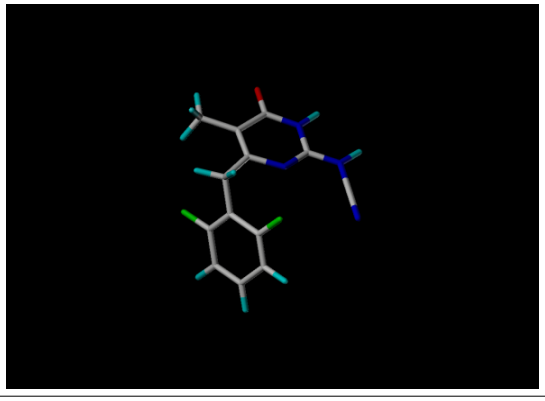
28	DABO_3800003		1.622
29	DABO_3900018		4.642
30	DABO_4000013		11.634
31	DABO_4100005		6.337

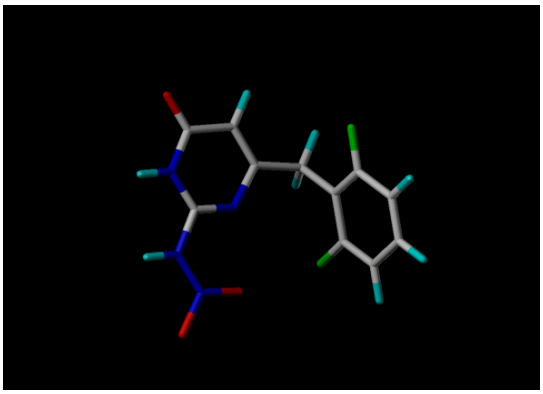
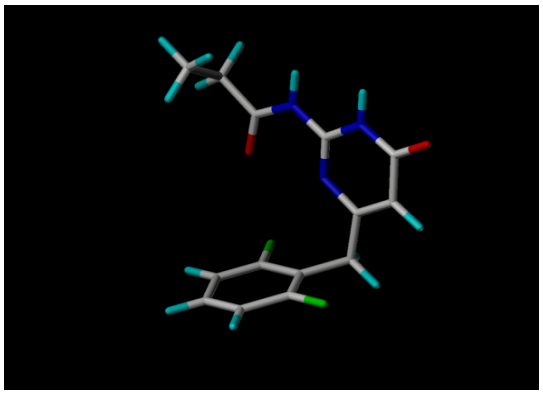
32	DABO_4200006		6.682
33	DABO_5000011		11.591
34	DABO_5100055		12.820
35	DABO_5200047		12.234

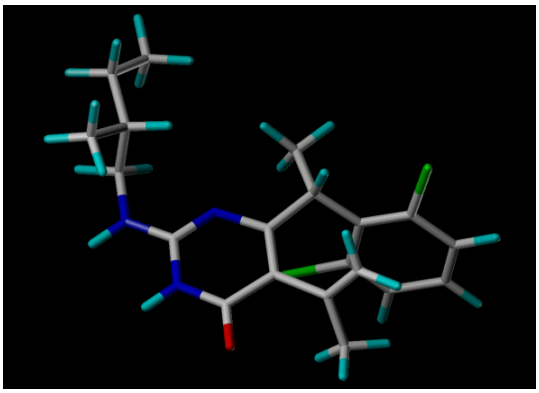
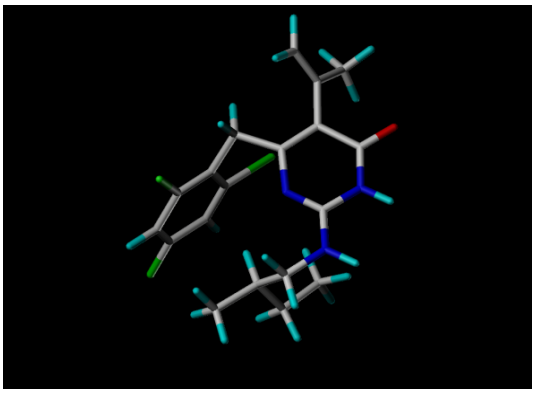
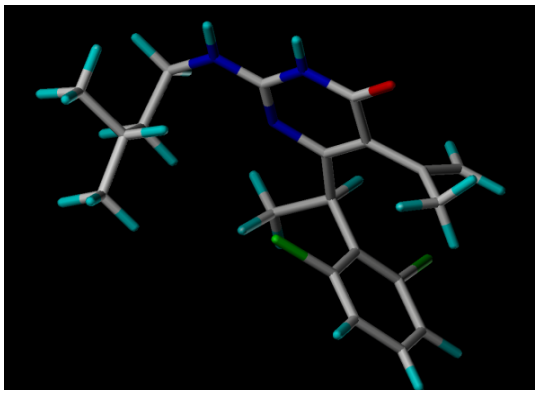
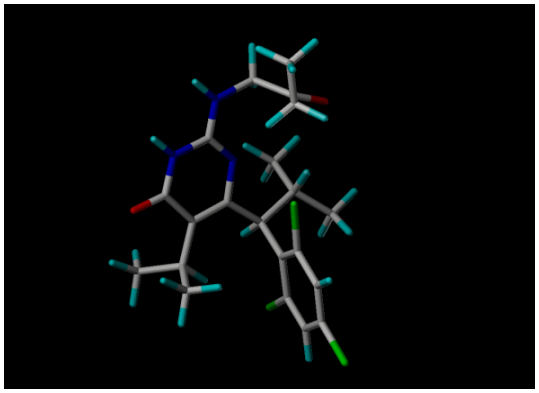
36	DABO_5300038		13.588
Test set			
37	DABO_0200020		2.377
38	DABO_0300052		1.819
39	DABO_0500019		86.582

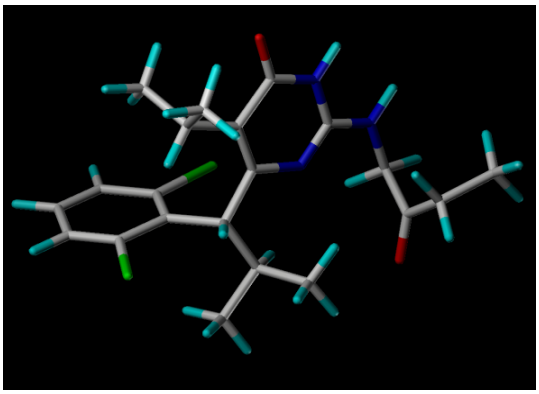
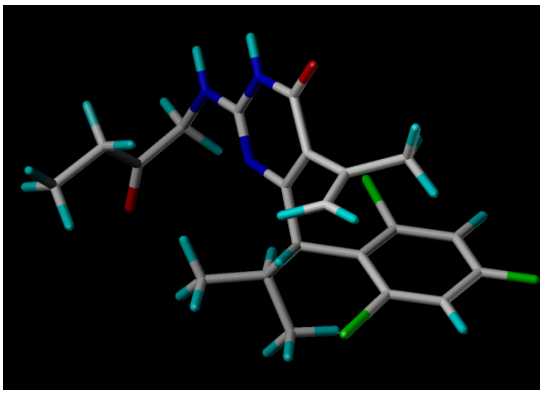
40	DABO_0600023		1.243
41	DABO-1200003		4.470
43	DABO_3200076		0.265

44	DABO_3300045		-13.393
45	DABO-4400002		2.299
Outlier			
46	DABO_0100002		3.251

Approximate Data set			
47	DABO_2500005		-0.474
48	DABO_4300013		7.198
49	DABO_4500022		1.698
50	DABO_4600035		2.929

51	DABO_4700018		1.200
52	DABO_4800007		2.424
53	DABO_4900014		2.845

Virtual Data Set			
54	DABO_VDS_11400034		-5.170
55	DABO_VDS_12200008		-8.622
56	DABO_VDS_15000041		-5.957
57	DABO_VDS_15400011		-8.500

58	DABO_VDS_15600033		-6.324
59	DABO_VDS_15800052		-7.006