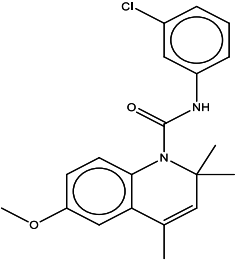
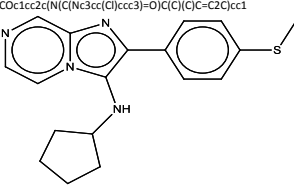
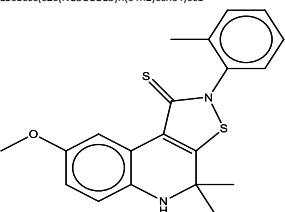
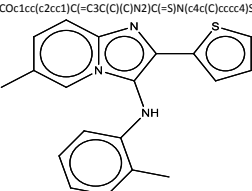
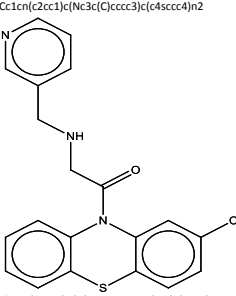
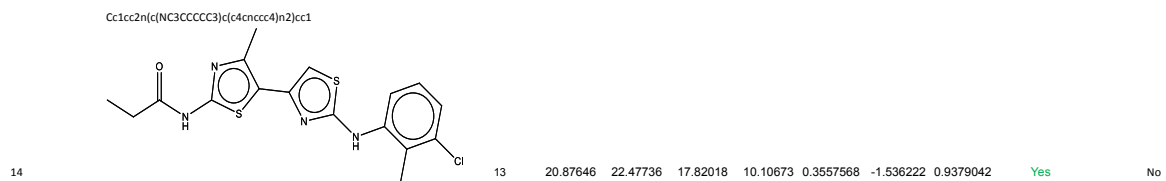
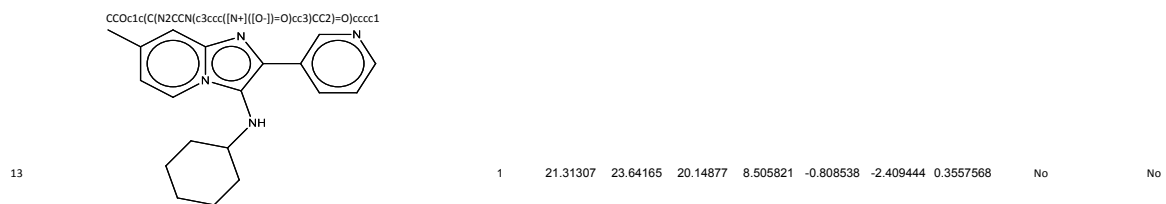
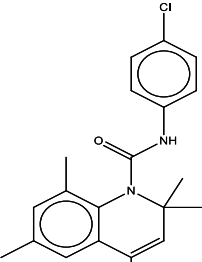
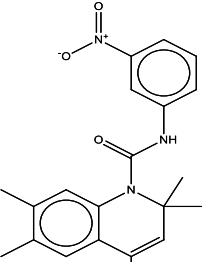
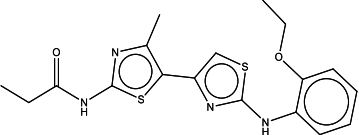
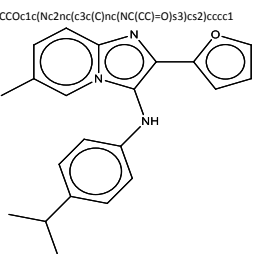
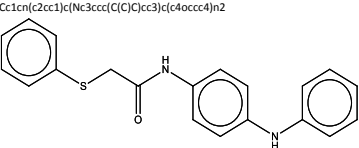
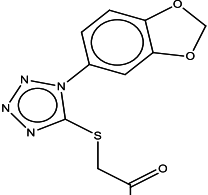
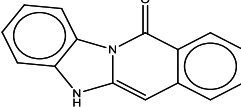
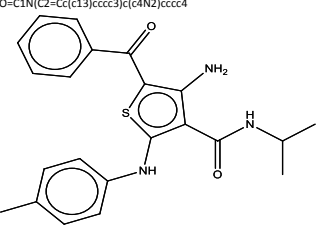
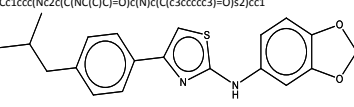
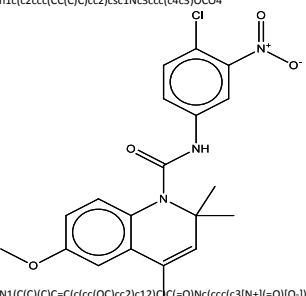


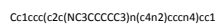
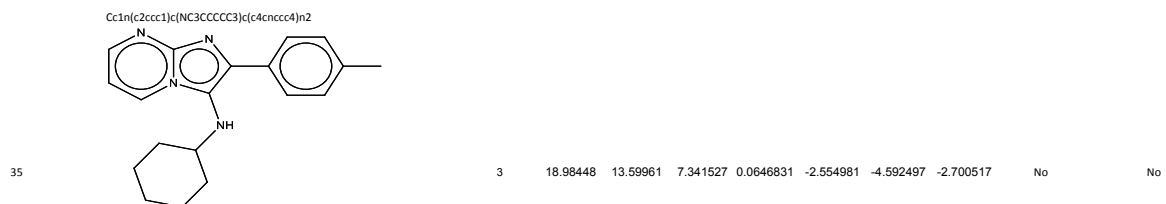
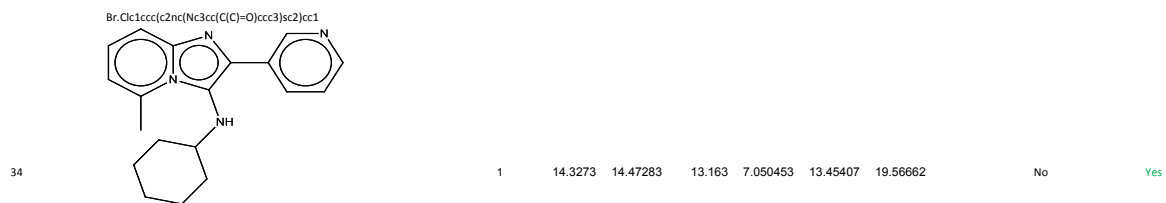
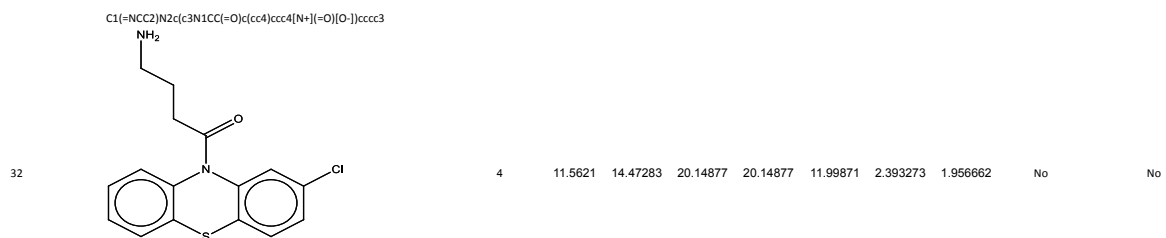
6	 <chem>COc1ccc2c(N(C(C)C)C(=O)Nc3ccc(Cl)cc3)cc(C)c1</chem>	2	25.67917	20.73092	23.93273	22.47736	13.163	5.30401	-0.808538	Yes	Yes
7	 <chem>COc1cc2c(N(C)C3CC3)cc(C)=O(C)C(C)C=C2C1</chem>	12	18.40233	25.09702	14.3273	3.848642	-0.517465	-2.11837	-0.226391	Yes	No
8	 <chem>CS1ccc(c2c(NC3CCCC3)n(c4n2)ccnc4)c1</chem>	2	24.80595	15.49159	13.45407	19.27555	7.6326	5.30401	1.811126	Yes	No
9	 <chem>COc1cc(c2cc1)C(=C3C(C)C(N2)C(=S)N(c4c(C)cccc4)S3</chem>	1	24.2238	13.163	6.177232	-3.137128	-1.827296	-3.719275	-0.808538	Yes	Yes
10	 <chem>Cc1cn(c2cc1)c(Nc3c(C)cccc3)c(c4cccc4)n2</chem> <chem>Clc1cc(c2cc1)N(C(C)C)C(=O)Nc3ccc(Cl)cc3</chem>	4	21.16753	24.2238	17.38357	11.99871	5.740621	0.3557568	3.848642	Yes	No

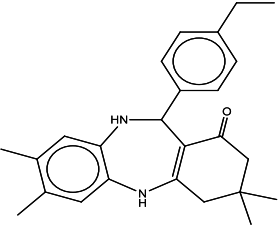
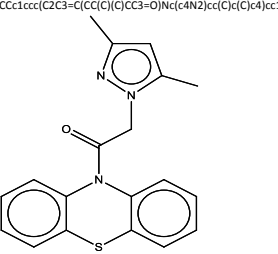
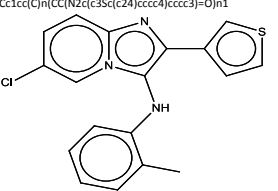
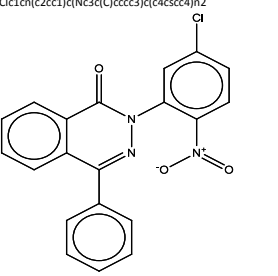
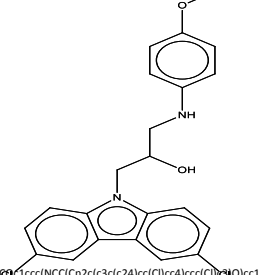


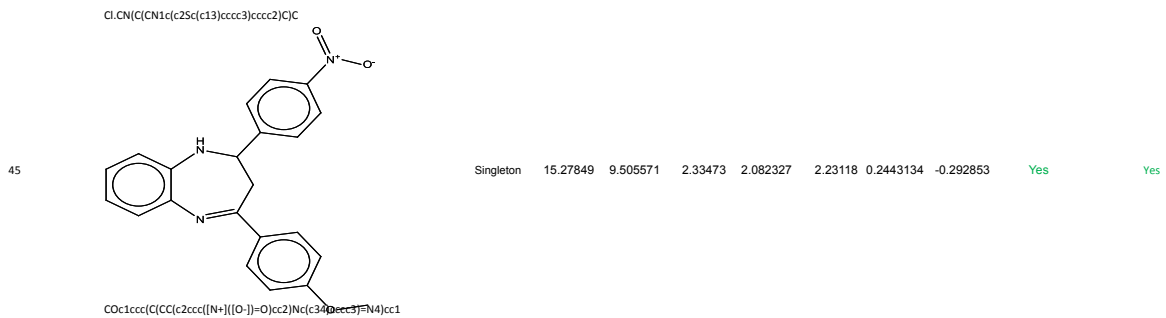
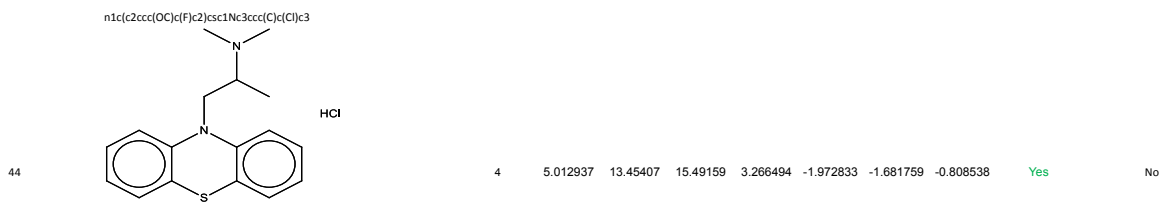
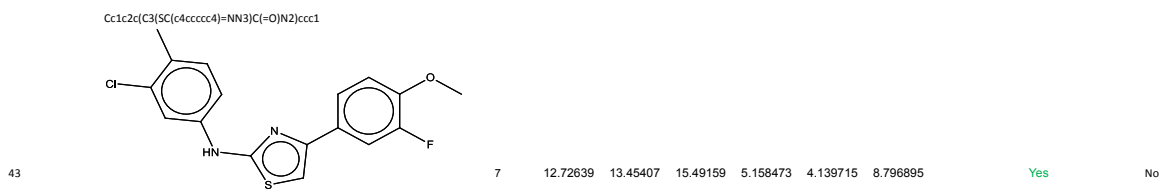
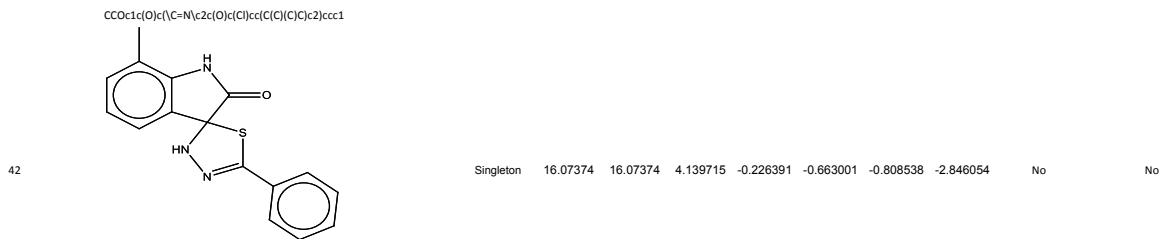
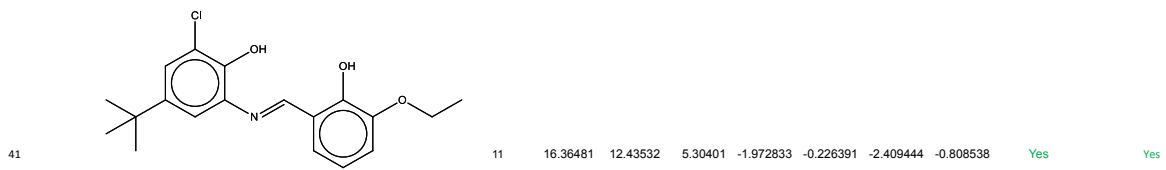
16	 <chem>Clc1ccc(NC(=O)Nc2c(C)c(C)C=C(C)cc2C)cc1</chem>	2	20.43984	20.14877	22.04075	16.65589	8.796895	0.7923674	0.7923674	Yes	No
17	 <chem>CC(c1cN(C)Nc2cc([N+](=O)[O-])ccc2=O)C3(C)C)cc(C)C(C)c1)=C3</chem>	2	18.54786	17.23803	21.89521	16.07374	15.49159	5.30401	6.177232	Yes	No
18	 <chem>CCOC1=CC=C(C=C1)Nc2nc(C)sc2Nc3c(C)sc3C(=O)NCC</chem>	13	21.60414	17.23803	5.30401	1.083441	-0.226391	1.520052	-0.517465	No	Yes
19	 <chem>CCOC1=CC=C(C=C1)Nc2nc(C)sc2Nc3c(C)sc3C(=O)NCC</chem>	1	12.58085	12.28978	15.49159	15.49159	21.31307	18.40233	21.02199	No	Yes
20	 <chem>Cc1cn(c2cc1)c(Nc3ccc(C)cc3)c4occcc4n2</chem>	Singleton	20.43984	21.31307	12.14424	3.412031	-2.846054	-0.808538	-1.827296	Yes	Yes

O=C(Nc1ccc(Nc2ccccc2)cc1)CSc3ccccc3

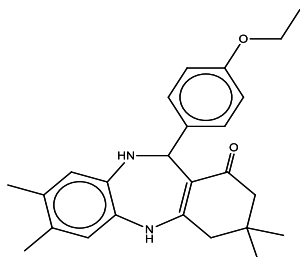
26	 <chem>Clc1cc2cc3n(C(CSc3n(C(=O)C)C4=CC=CC=C4)OC(=O)C)nn3=O)c(c652)cccc6</chem>	6	15.49159	20.58538	10.83441	-0.371928	-0.808538	-4.44696	-0.808538	No	Yes
27	 <chem>Clc1cc2cc3n(C(CSc3n(C(=O)C)C4=CC=CC=C4)OC(=O)C)nn3=O)c(c652)cccc6</chem>	Singleton	20.58538	15.49159	10.83441	1.811126	0.2102199	0.3557568	-3.137128	Yes	Yes
28	 <chem>O=C1N(C2=Cc(c13)cccc3)c(c4N2)cccc4</chem>	Singleton	14.61837	20.43984	14.90944	-2.263907	-3.137128	-3.137128	-2.409444	No	Yes
29	 <chem>Cc1ccc(Nc2c(C(NC(C)C)=O)c(N)c(C3=CC=CC=C3)=O)s2)cc1</chem>	7	15.49159	20.43984	19.56662	18.11126	13.59961	6.613842	3.412031	Yes	Yes
30	 <chem>n1c(c2ccc(CC(C)C)cc2)sc1Nc3ccc(c4c3)OC(=O)C</chem>	2	18.98448	19.13001	17.82018	20.43984	8.796895	1.520052	0.9379042	Yes	Yes



36		8	17.82018	14.61837	0.6468305	-4.155886	-5.029108	-0.808538	-0.808538	Yes	Yes
37	<chem>Cc1ccc(C2C3=C(C(C)C)CC3=O)Nc(c4N2)cc(C)C)c1</chem> 	4	17.82018	16.07374	5.449547	-5.029108	-3.573739	-2.554981	-2.846054	Yes	Yes
38	<chem>Cc1cc(C)n(CC(N2c(c3Sc(c24)cccc4)cccc3)=O)n1</chem> 	1	17.0925	7.923674	-0.226391	-4.155886	-1.972833	6.177232		Yes	Yes
39	<chem>Clc1cn(c2cc1)c(Nc3c(C)cccc3)c(c4cccc4)n2</chem> 	Singleton	16.36481	10.3978	-0.517465	0.2102199	4.8674	14.03622		Yes	Yes
40	<chem>Clc1cc(N2C(=O)c(c3c(c4cccc4)=N2)cccc3)c([N+](=[O-])=O)cc1</chem> 	Singleton	14.61837	16.36481	14.03622	13.163	1.520052	-1.681759	-0.371928	Yes	Yes



46

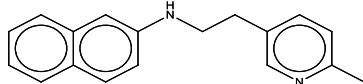


8

11.70763 10.97995 6.177232 6.468305 10.97995 14.90944

Yes

Yes

CCOc1ccc(C2C3=C(C(C)C)CC3=O)Nc1c4N2)cc(C)C(C)C4)cc1


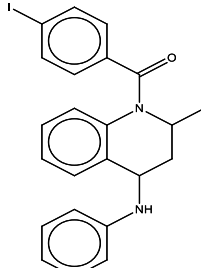
47

Singleton 10.97995 14.3273 13.163 0.5012937 -2.554981 -4.010349 -3.137128

No

Yes

48

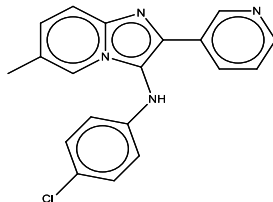
Cc1nc(CCNc2cc(c3cc2)cccc3)cc1


Singleton 14.3273 9.96119 0.9379042 1.520052 -1.827296 -1.681759 -0.663001

Yes

Yes

49

Ic1ccc(C(N2c(c3C(Nc4cccc4)CC2)cccc3)=O)cc1


1

13.74515 1.811126 0.7923674 -5.029108 -5.465718 -3.573739 -0.808538

No

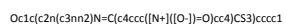
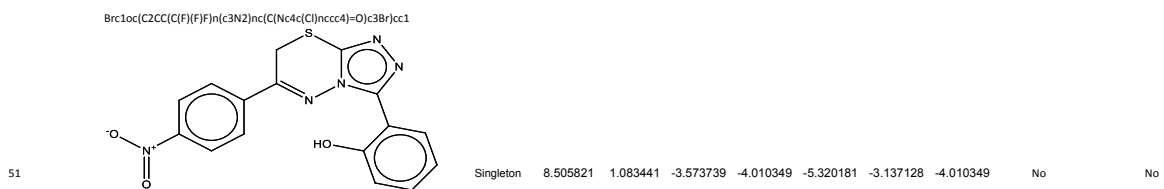
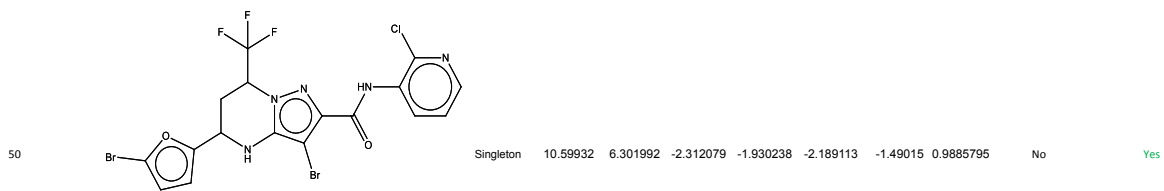
Yes

Clc1ccc(Nc2n(c3nc2c4cccc4)cc(C)cc3)cc1

α-Tocopherol

11.99871 6.759379 -0.226391 -0.808538 -2.700517 -4.44696 -0.226391

No



Vitamin K2

3.120957 -2.263907 -0.517465 -0.371928 -0.371928 0.0646831

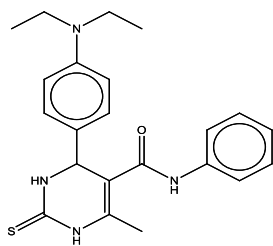
Ethoxyquin

1.739317 3.09194 -1.412488 0.4967167 -0.331684 -1.496622 -0.370515

Ethopropazine hydrochloride

2.451224 1.389836 -0.771772 -0.435234 -1.393072 0.2184259 -0.325212

52



Singleton -1.245149 -0.517465 -0.517465 1.811126 -1.681759 2.102199 -1.390686 No No

CCN(C)Cc1ccc(cc1)C2C(C)NC(=S)N2