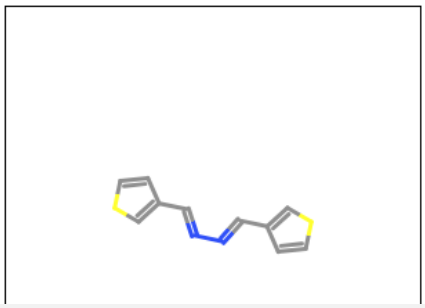
Oral toxicity prediction results for input compound



Predicted LD50: 1460mg/kg

Predicted Toxicity Class: 4

1	2	3	4	5	6

Average similarity: 37.99%

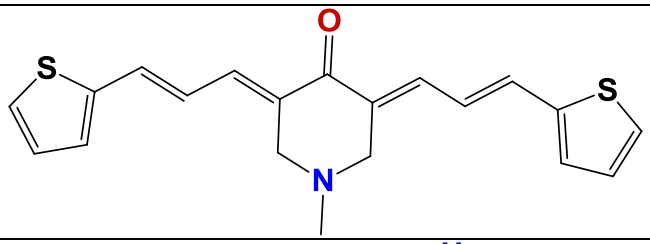
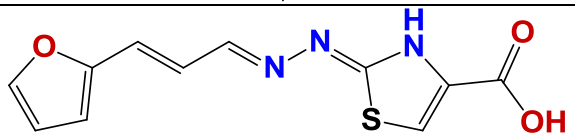
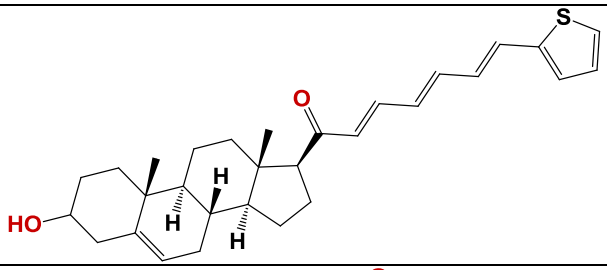
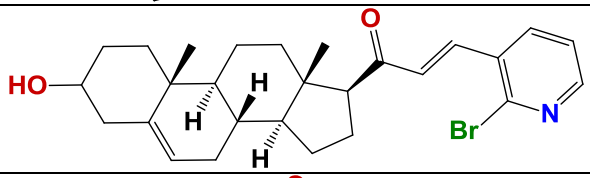
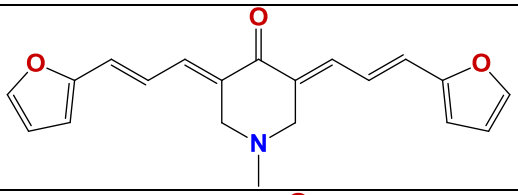
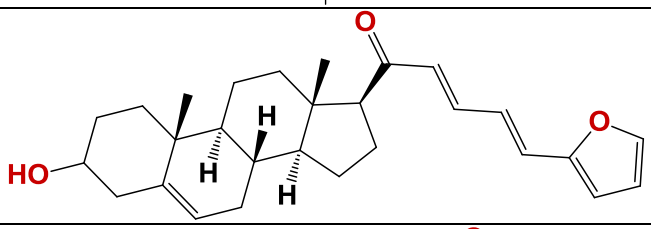
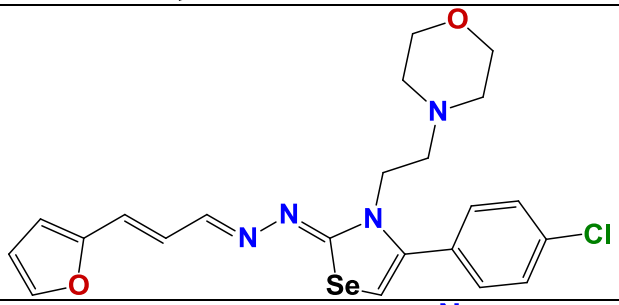
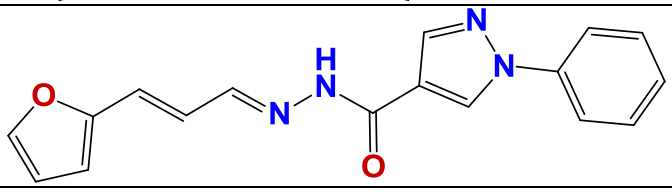
Prediction accuracy: 23%

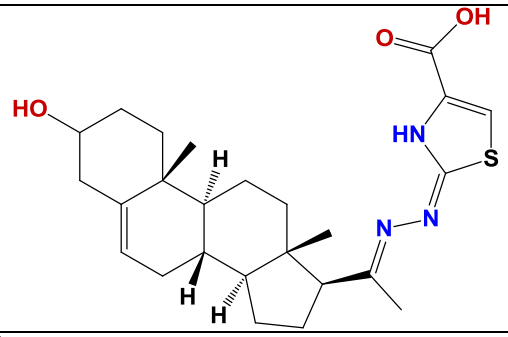
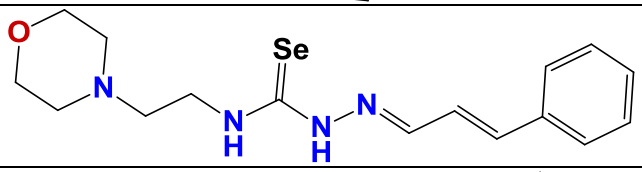
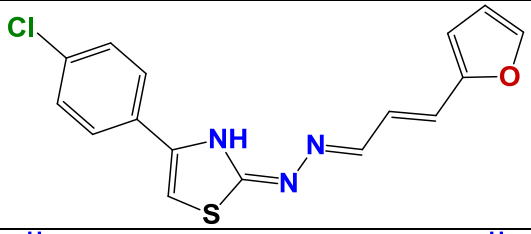
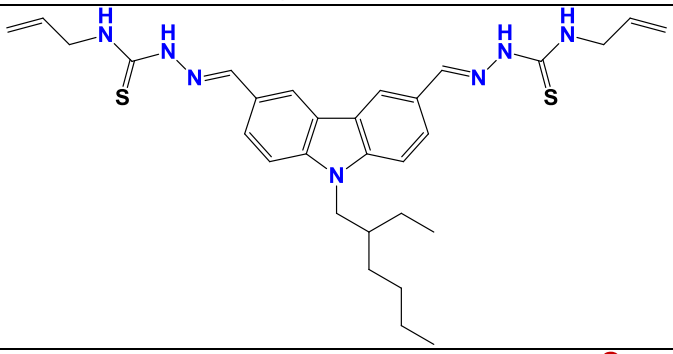
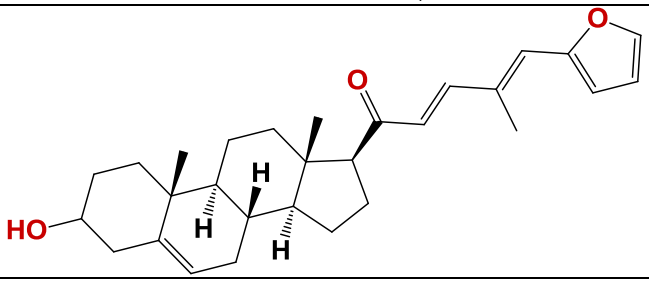
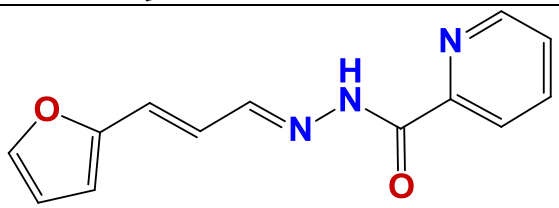
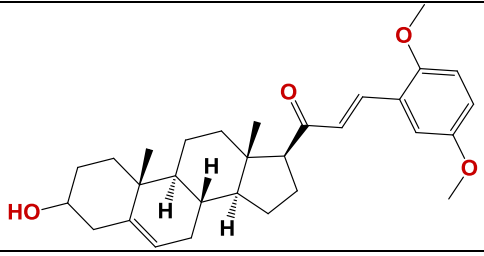
Name	C1(/C=N/N=C/C2=CSC=
Molweight	220.31
Number of hydrogen bond acceptors	2
Number of hydrogen bond donors	0
Number of atoms	14
Number of bonds	15
Number of rings	2

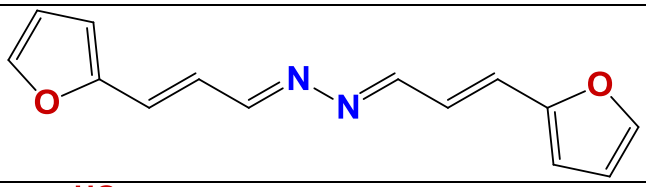
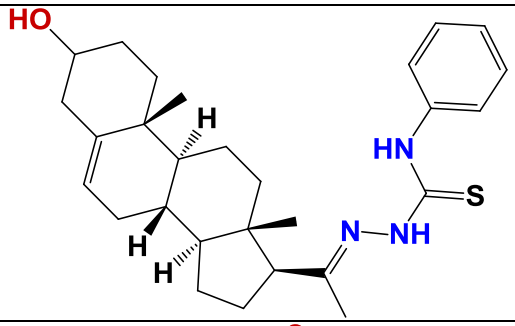
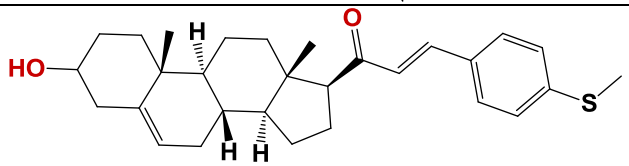
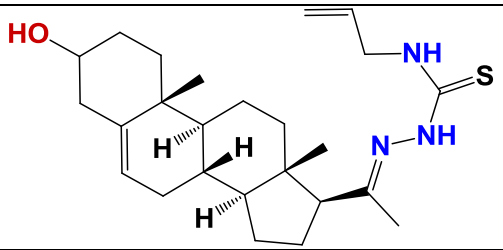
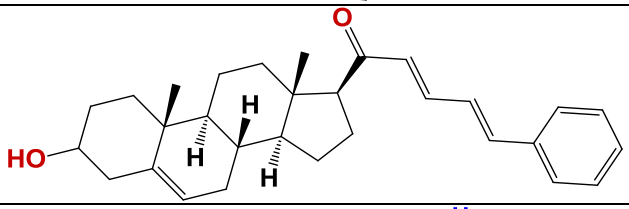
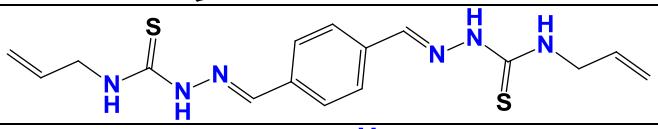
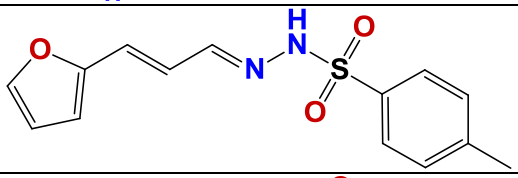
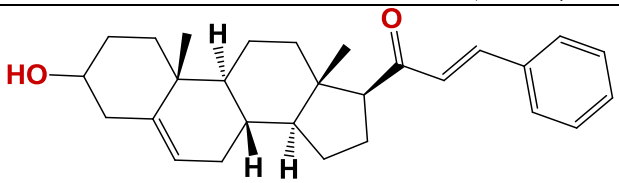
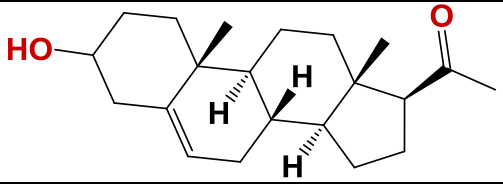
Toxicity Model Report

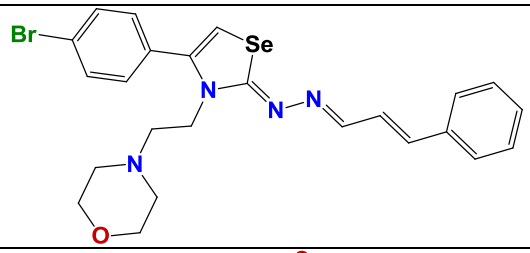
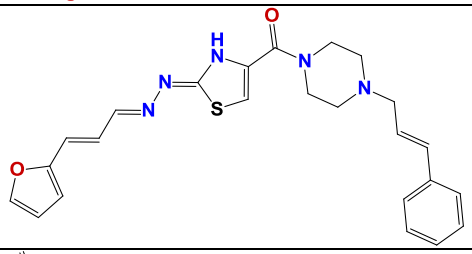
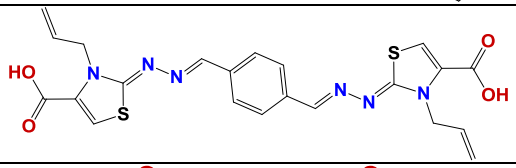
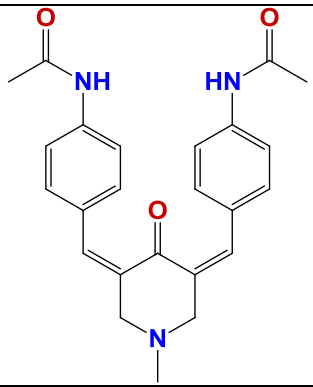
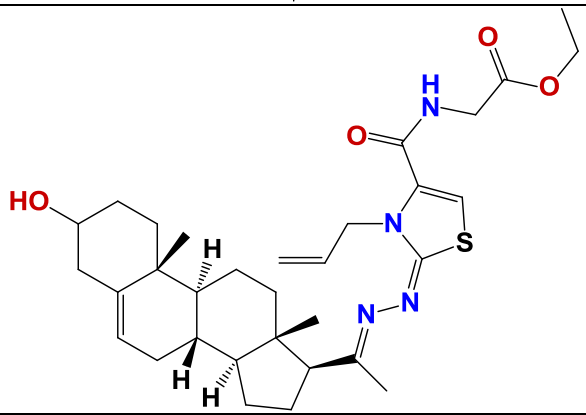
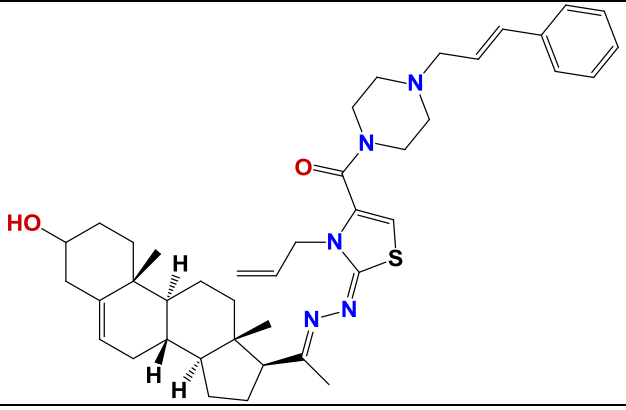
Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.53
Toxicity end points	Carcinogenicity	carcino	Active	0.58
Toxicity end points	Immunotoxicity	immuno	Inactive	0.99
Toxicity end points	Mutagenicity	mutagen	Inactive	0.54
Toxicity end points	Cytotoxicity	cyto	Inactive	0.80
Tox21-Nuclear receptor signalling pathways	Aryl hydrocarbon Receptor (AhR)	nr_ahr	Inactive	0.57
Tox21-Nuclear receptor signalling pathways	Androgen Receptor (AR)	nr_ar	Inactive	0.82
Tox21-Nuclear receptor signalling pathways	Androgen Receptor Ligand Binding Domain (AR-LBD)	nr_ar_lbd	Inactive	0.8
Tox21-Nuclear receptor signalling pathways	Aromatase	nr_aromatase	Inactive	0.94
Tox21-Nuclear receptor signalling pathways	Estrogen Receptor Alpha (ER)	nr_er	Inactive	0.54
Tox21-Nuclear receptor signalling pathways	Estrogen Receptor Ligand Binding Domain (ER-LBD)	nr_er_lbd	Inactive	0.97
Tox21-Nuclear receptor signalling pathways	Peroxisome Proliferator Activated Receptor Gamma (PPAR-Gamma)	nr_ppar_gamma	Inactive	0.77
Tox21-Stress response pathways	Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE)	sr_are	Inactive	0.68
Tox21-Stress response pathways	Heat shock factor response element (HSE)	sr_hse	Inactive	0.68
Tox21-Stress response pathways	Mitochondrial Membrane Potential (MMP)	sr_mmp	Inactive	0.86
Tox21-Stress response pathways	Phosphoprotein (Tumor Supressor) p53	sr_p53	Inactive	0.73
Tox21-Stress response pathways	ATPase family AAA domain-containing protein 5 (ATAD5)	sr_atad5	Inactive	0.74

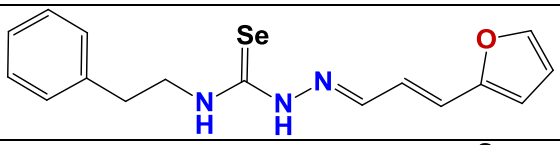
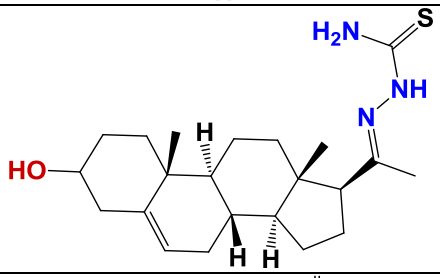
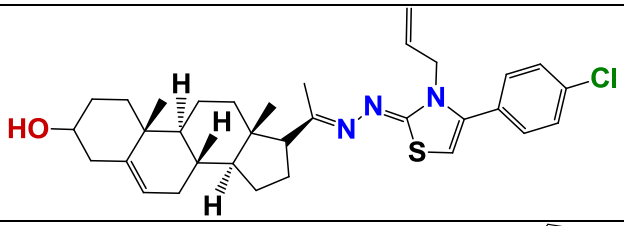
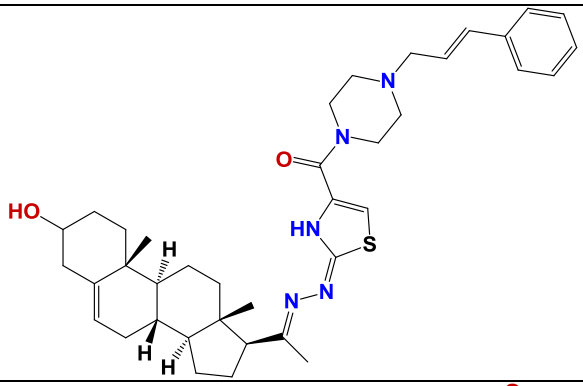
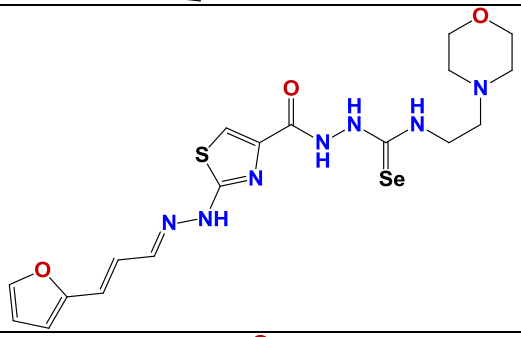
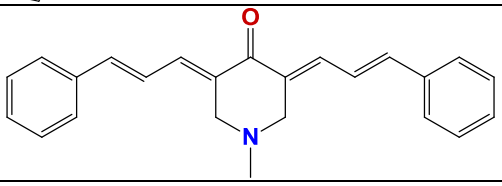
Table S1. List of the 175 selected molecules from the in house library (LIDENSA Chemolibrary) examined in this work and their activity on *C. elegans* motility. The compound code number, structural formula, concentration used and remaining motility are shown. Color code: yellow for moderate activity (65-25% of motility), green for potent activity (25-0% of motility).

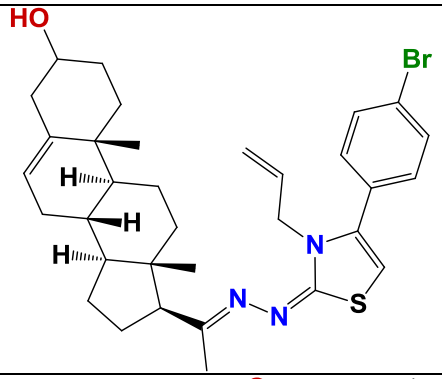
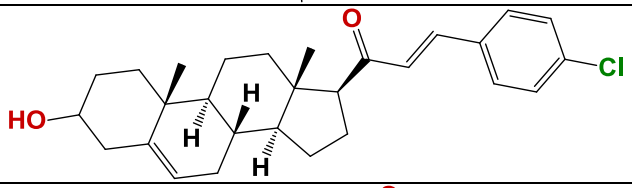
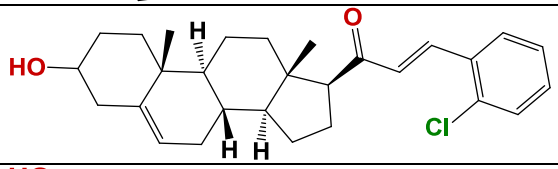
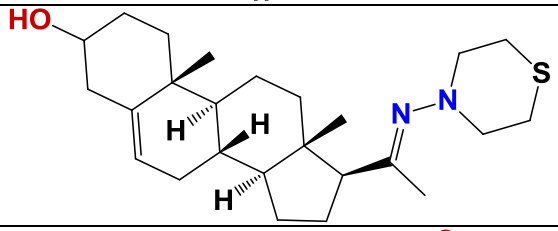
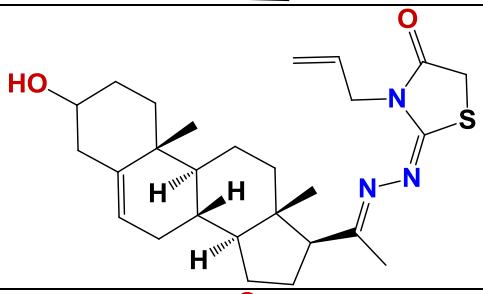
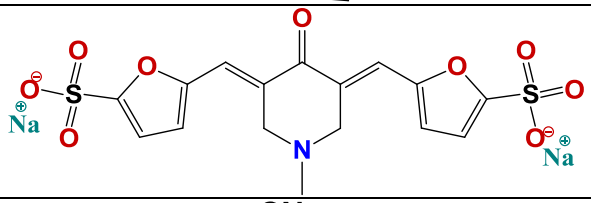
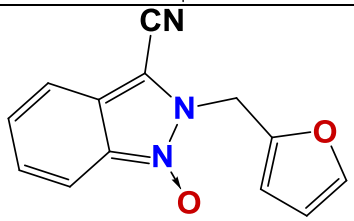
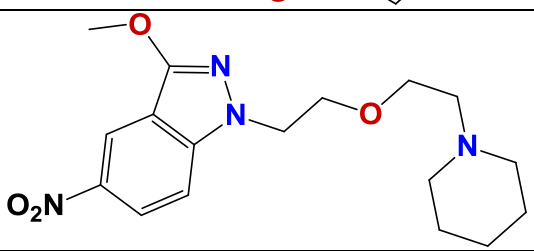
Chemolibrary code	Structure	Concentration (μM)	Motility (%)
1285		24	72
1311		24	68
1319		18	100
1257		21	108
1282		28	62
1289		17	99
1097		27	87
1366		29	111

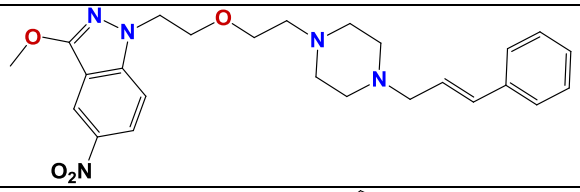
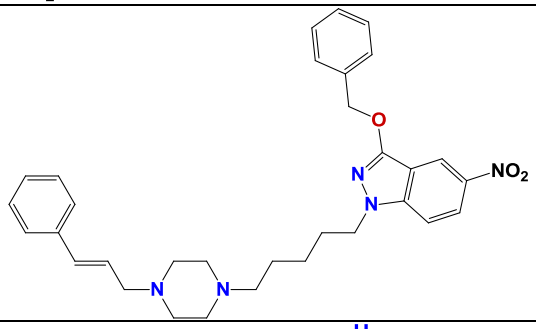
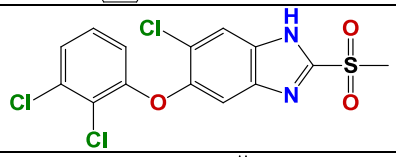
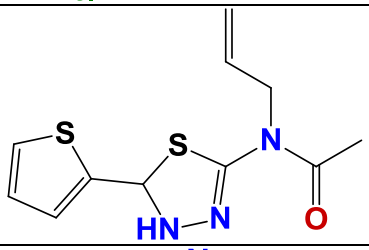
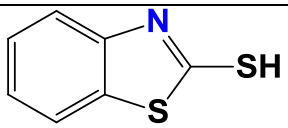
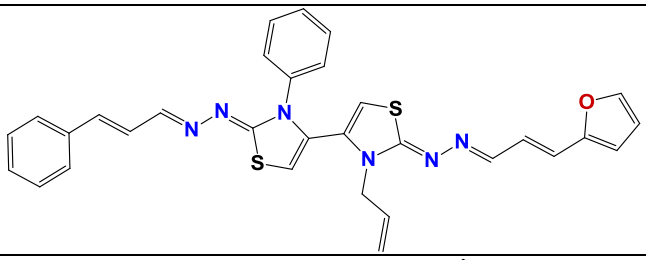
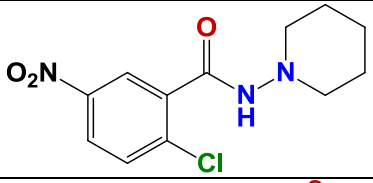
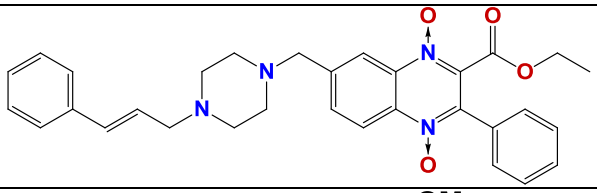
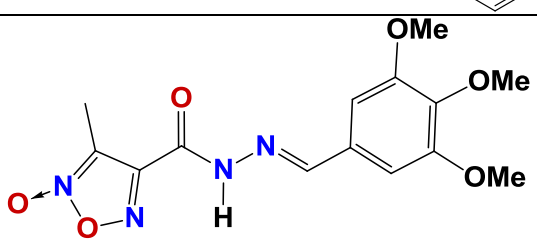
1258		27	116
1219		40	62
1312		50	94
1368		19	105
1287		50	61
1367		50	63
1316		21	106

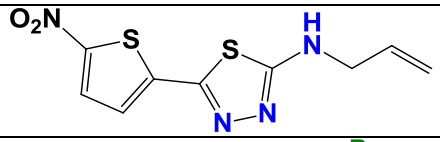
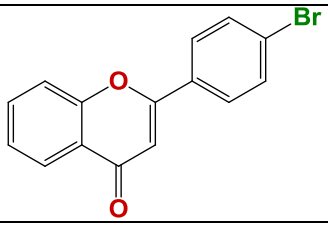
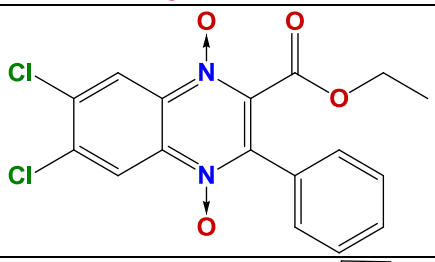
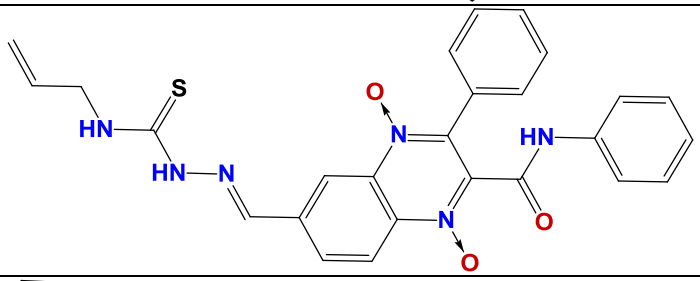
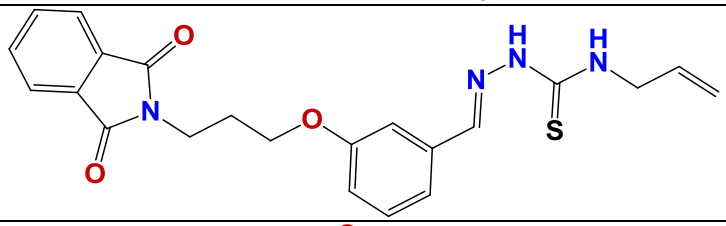
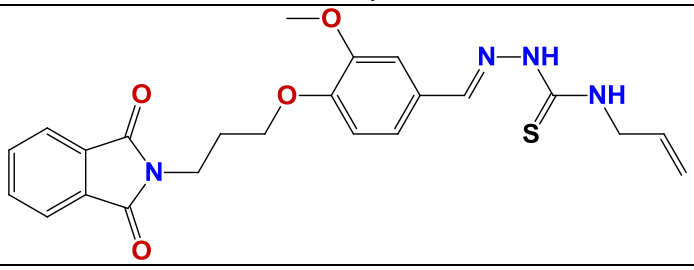
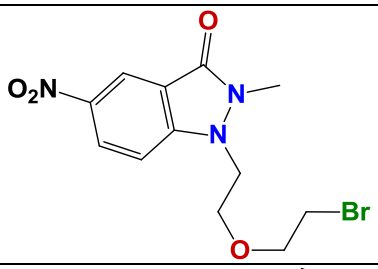
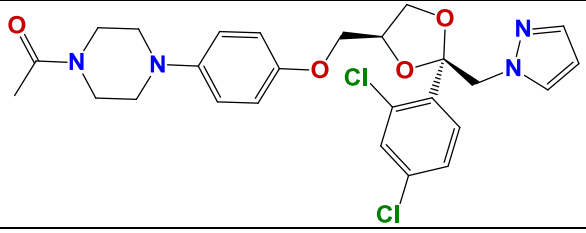
1140		50	23
1291		20	216
1262		17	200
1154		43	107
1279		20	109
1307		14	107
1369		37	84
1288		18	126
1290		19	148

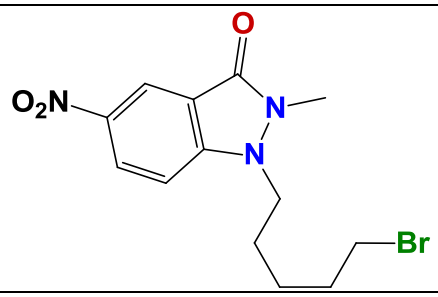
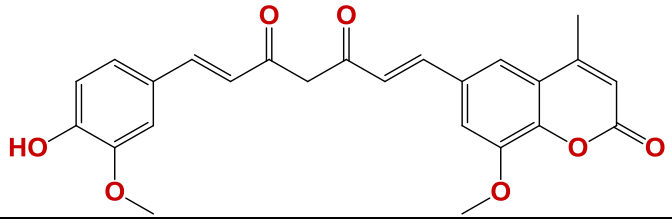
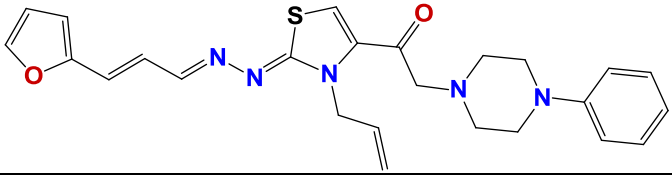
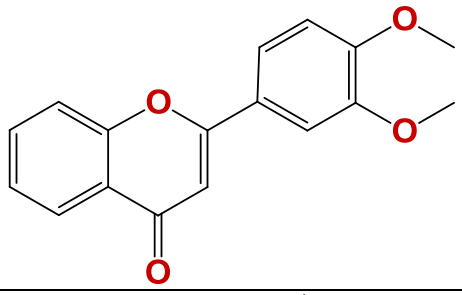
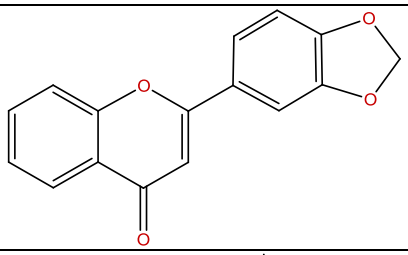
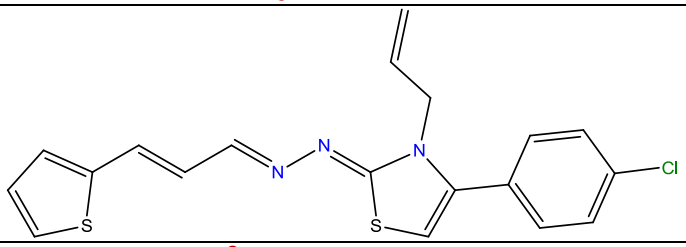
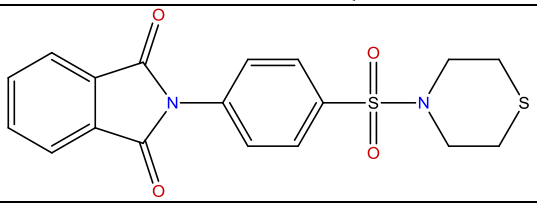
1222		13	145
1364		29	61
1310		30	115
1281		20	122
1263		18	120
1261		19	119

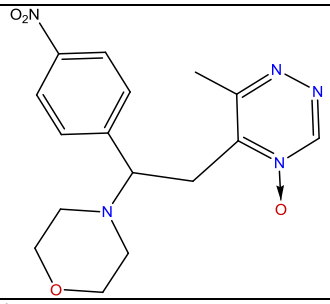
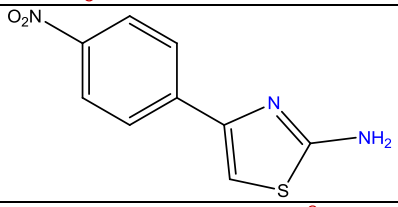
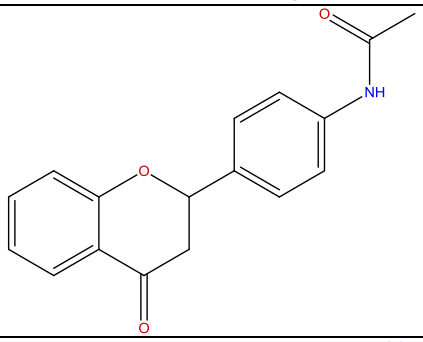
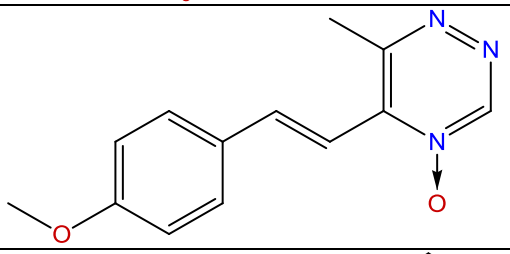
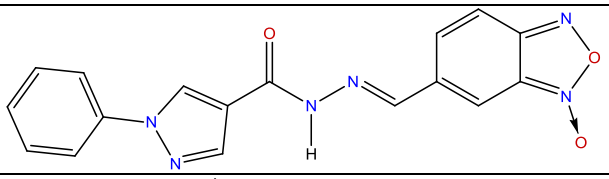
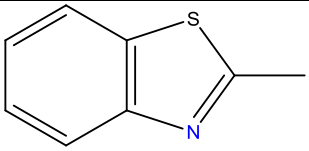
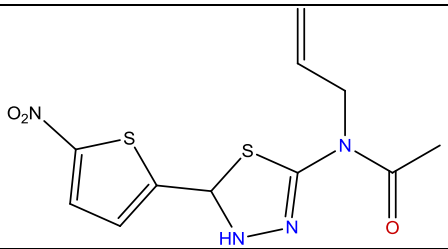
1145		19	139
1260		27	161
1144		30	86
1317		27	142
1365		33	105
1284		38	98

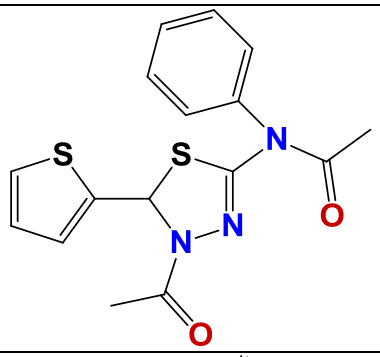
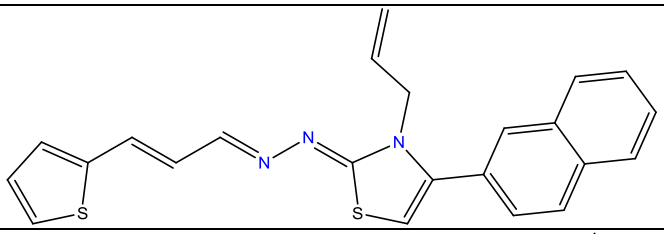
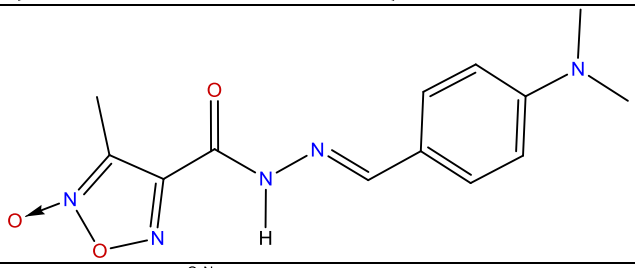
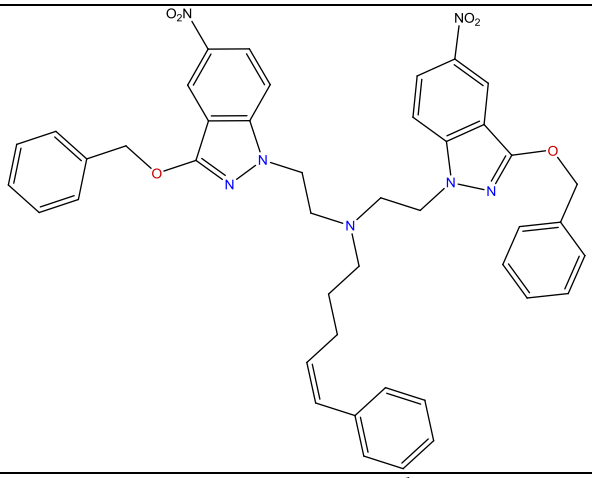
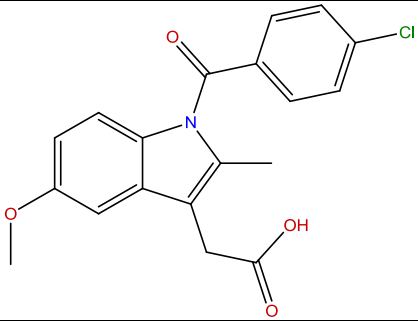
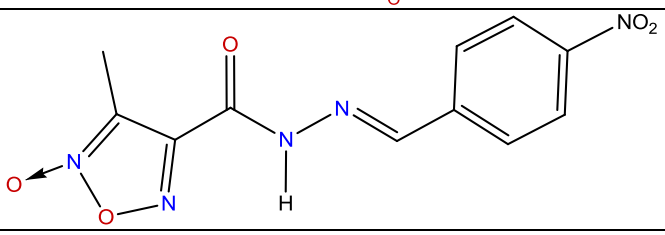
1272		25	55
1256		23	105
1259		35	110
1087		20	112
1125		23	134
1286		17	139
463		44	173
458		17	142

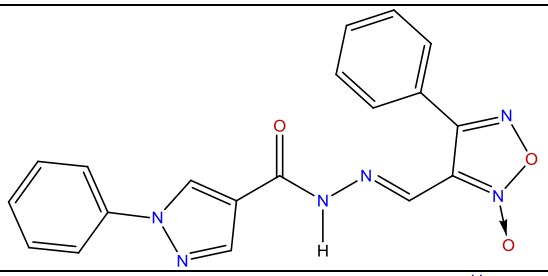
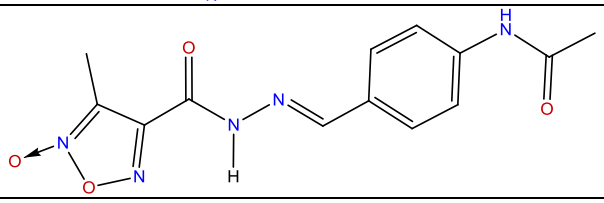
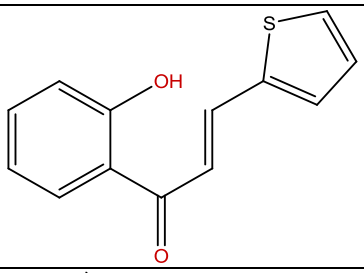
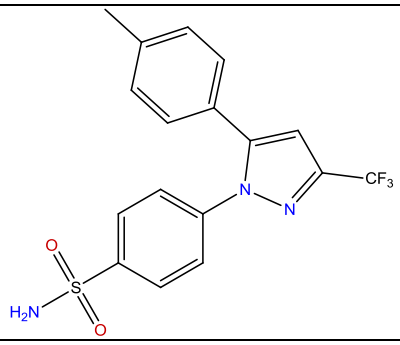
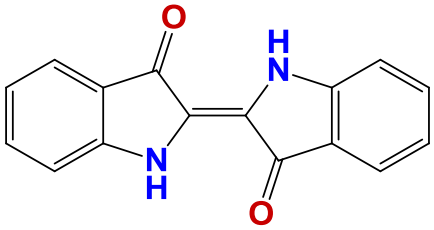
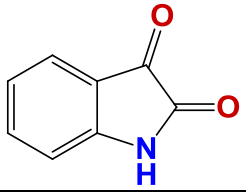
198		15	120
505		50	174
1293		18	146
286		28	107
1318		30	104
791		50	116
523		28	92
221		15	185
1184		18	127

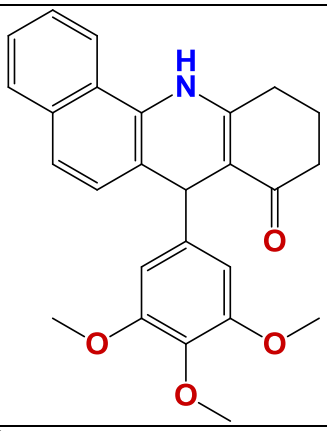
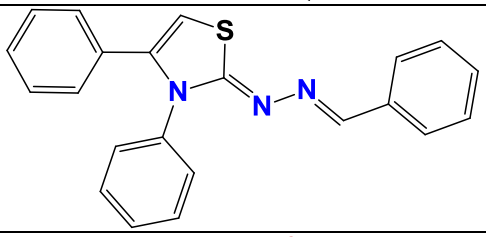
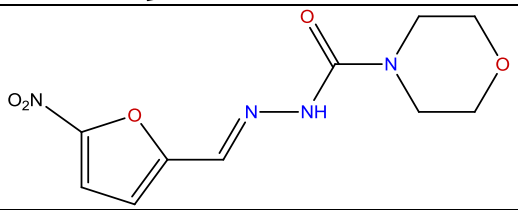
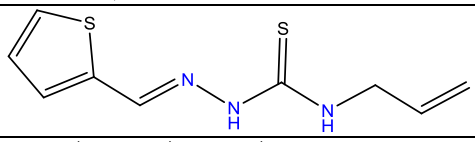
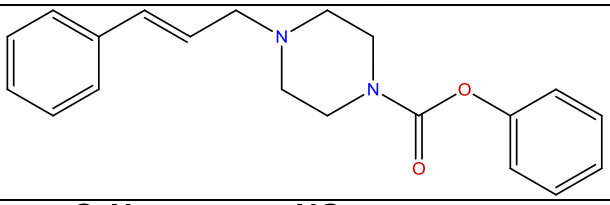
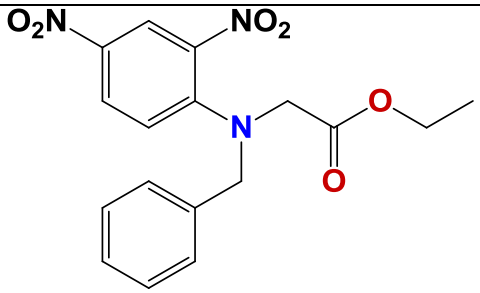
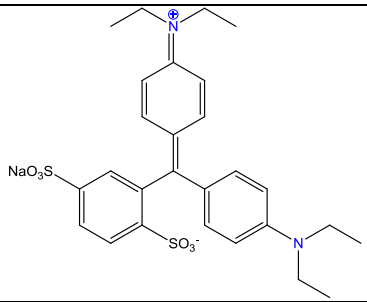
292		14	85
691		24	76
658		14	111
297		50	178
421		20	107
423		18	106
519		45	106
486		13	99

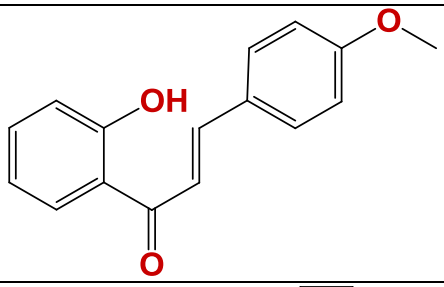
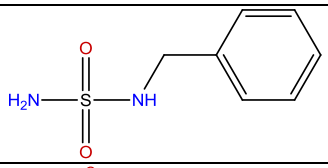
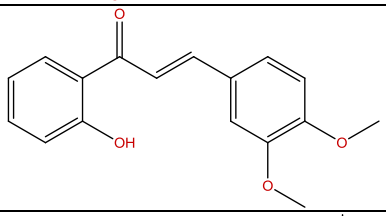
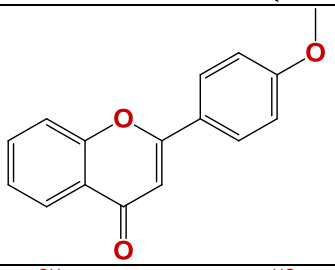
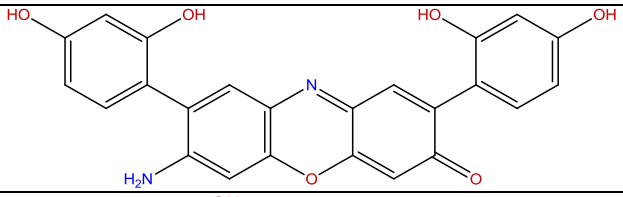
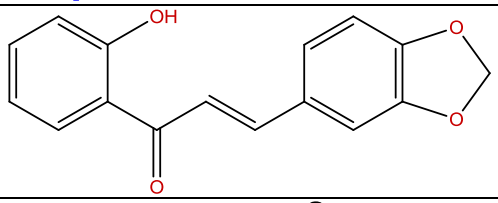
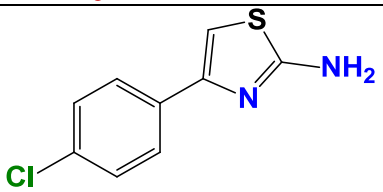
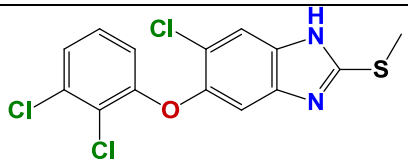
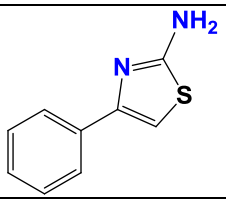
520		40	87
915		50	187
1099		50	80
734		21	119
882		42	137
1134		13	112
1170		24	110

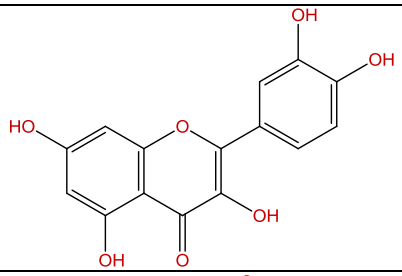
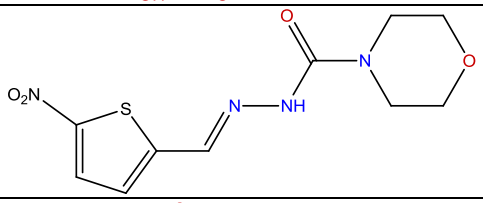
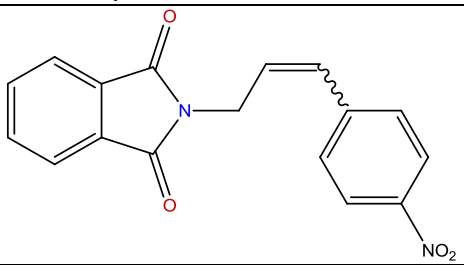
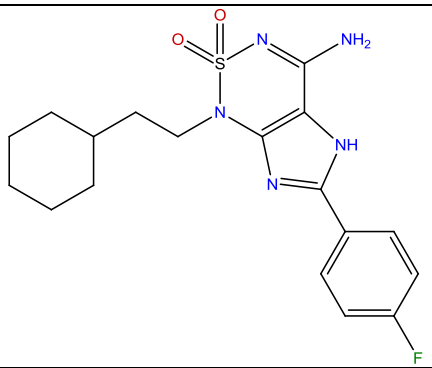
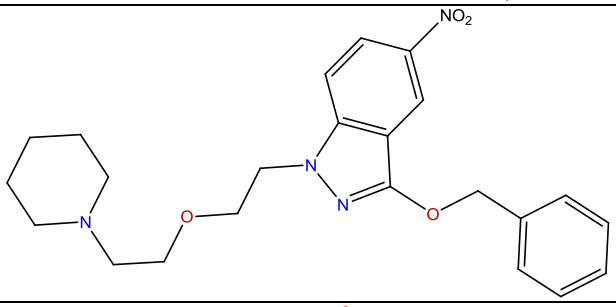
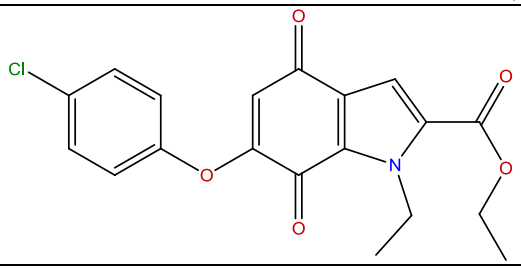
360		50	101
1098		50	188
1342		20	193
210		17	135
1204		22	156
1308		50	113
287		28	75

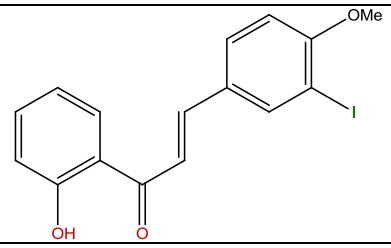
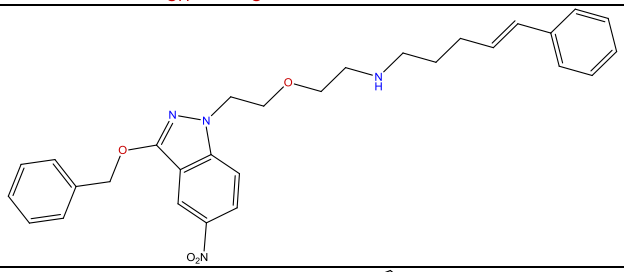
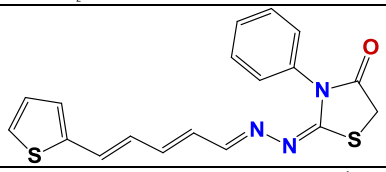
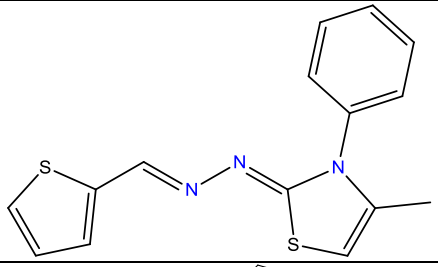
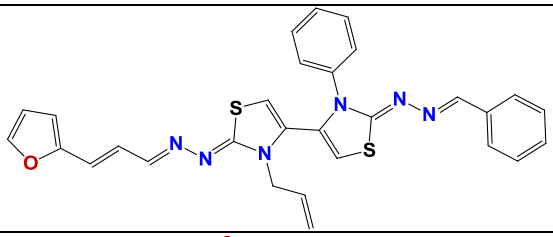
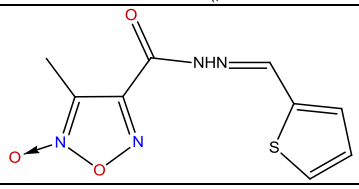
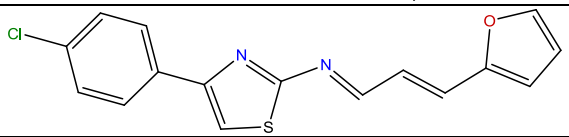
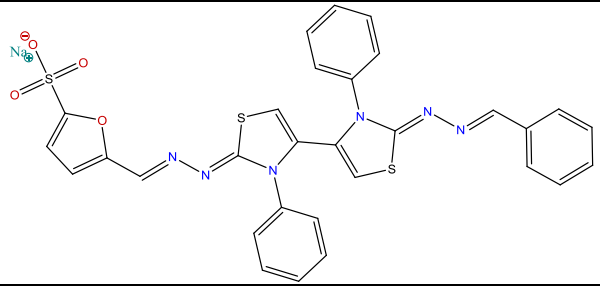
284		25	102
1218		23	107
1199		50	116
503		50	70
1122		15	99
1183		39	194

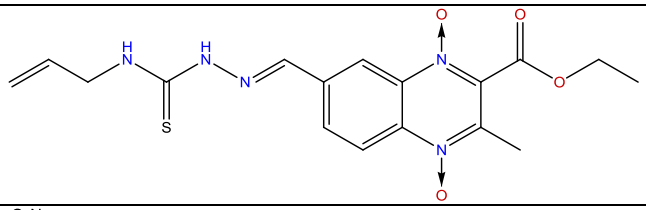
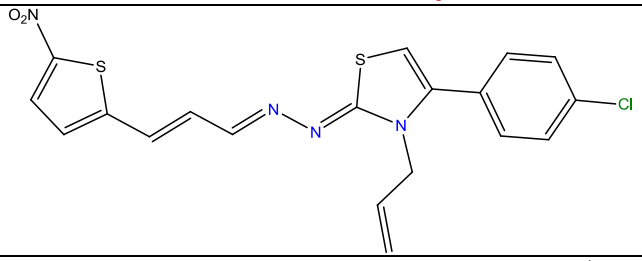
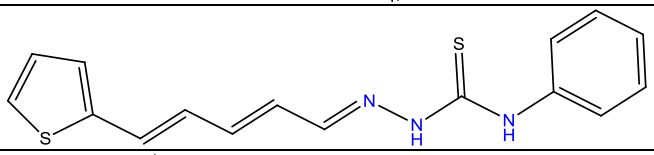
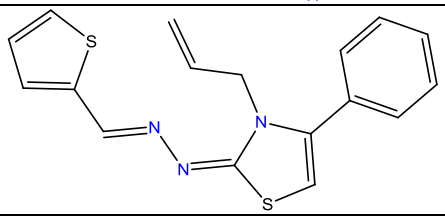
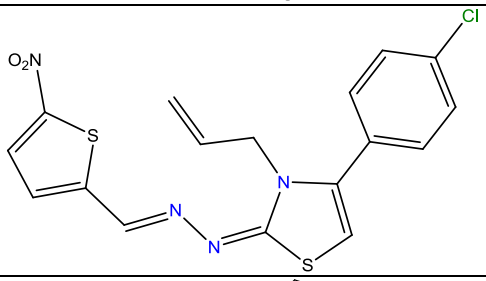
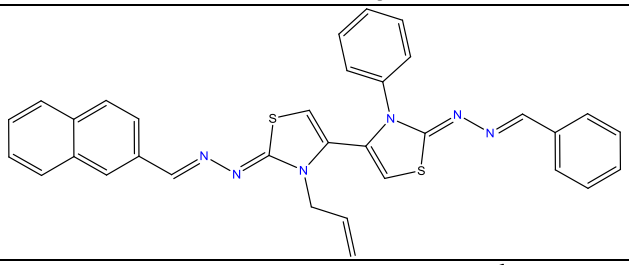
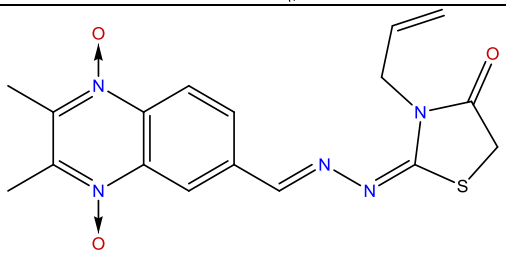
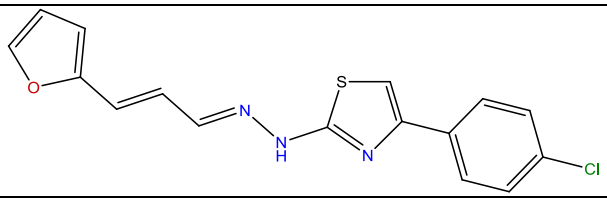
1206		50	101
1187		44	89
150		37	78
1121		38	69
879		35	67
385		50	83

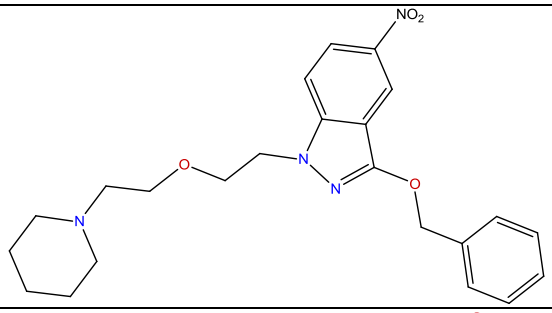
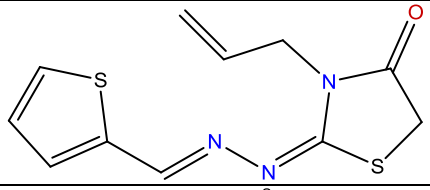
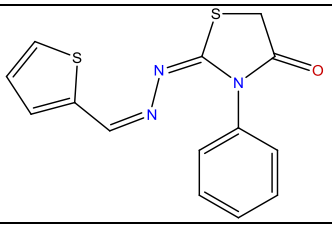
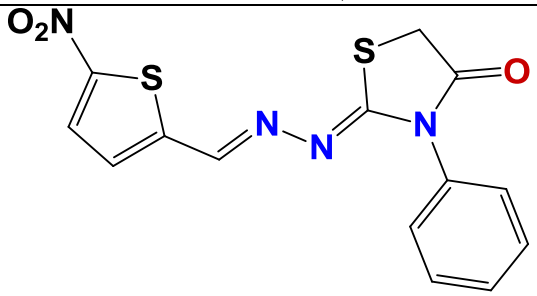
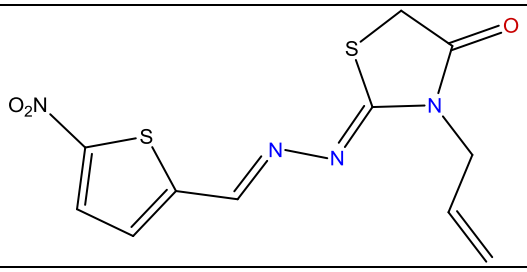
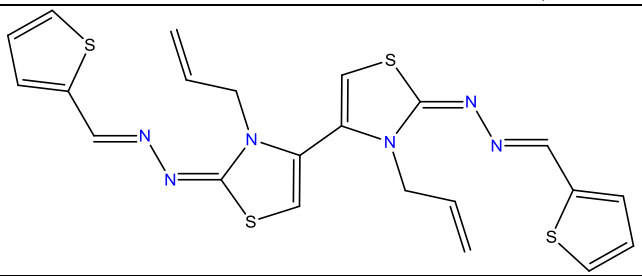
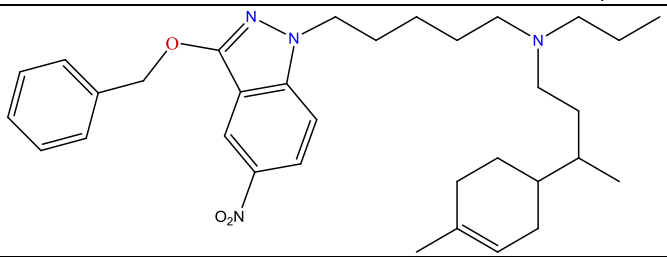
1234		13	80
270		33	78
63		50	80
137		50	98
240		50	128
568		50	58
940		50	102

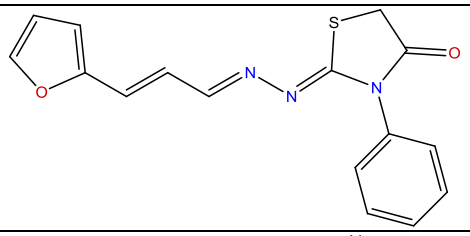
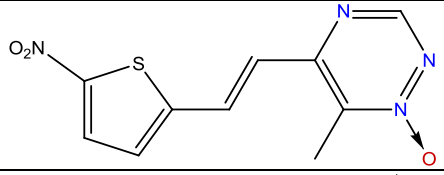
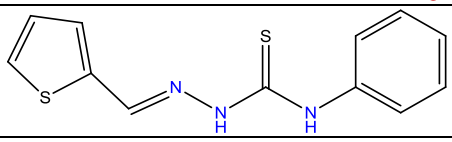
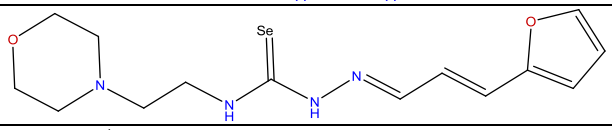
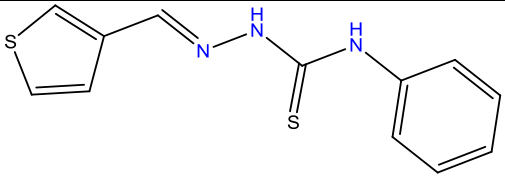
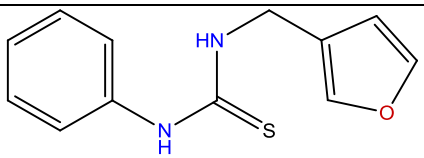
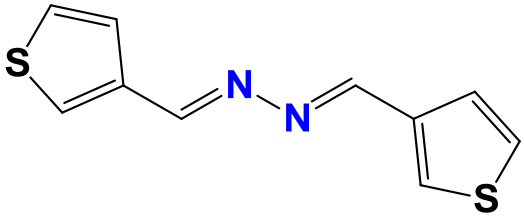
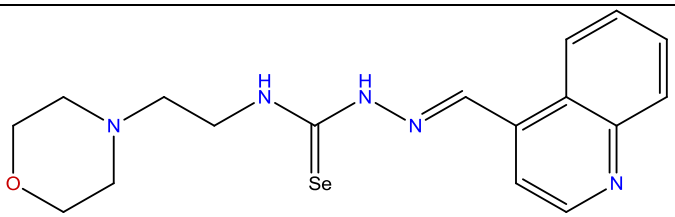
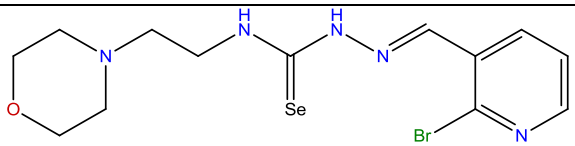
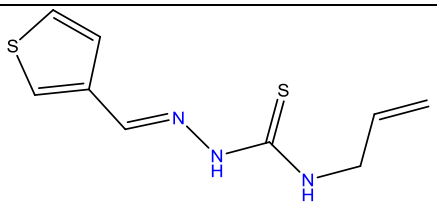
731		50	8
124		50	95
884		50	74
724		50	63
990		50	86
151		50	83
813		50	50
1278		50	60
810		50	93

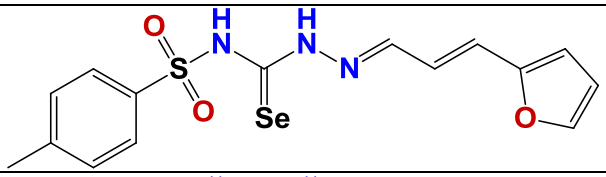
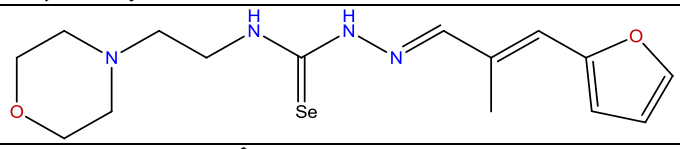
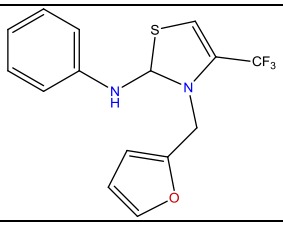
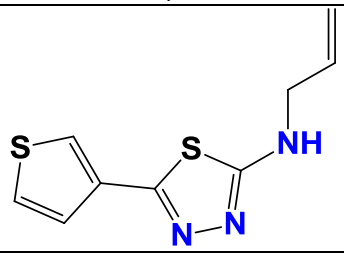
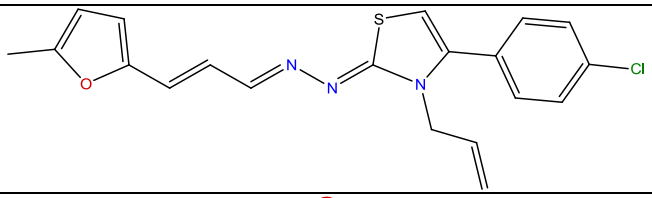
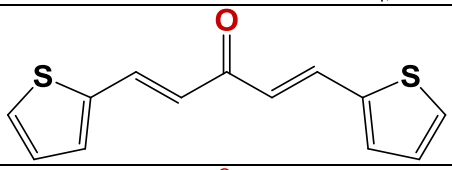
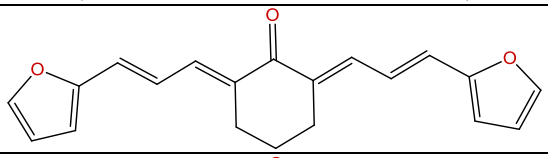
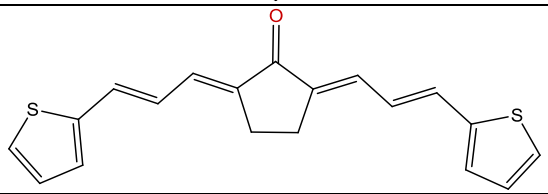
1337		50	101
139		50	120
608		39	68
706		50	79
457		38	87
1129		50	87

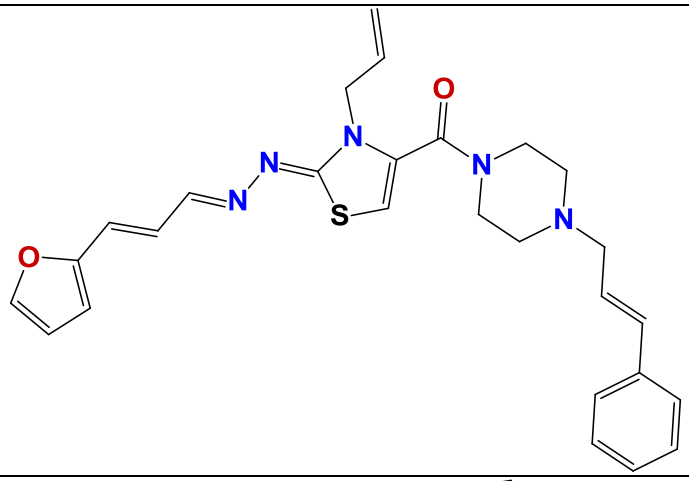
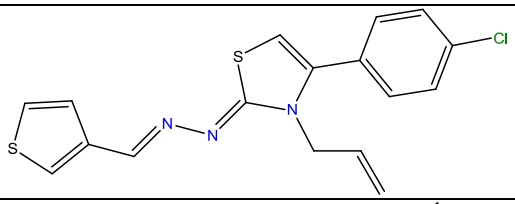
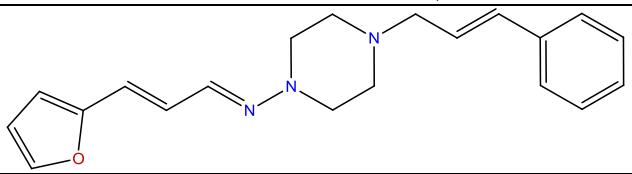
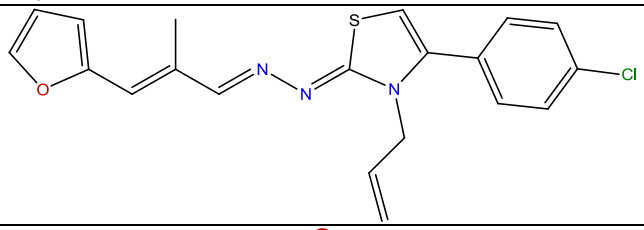
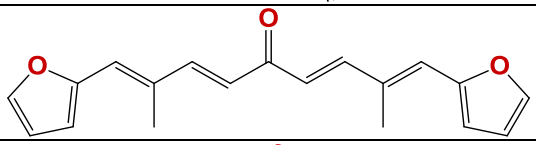
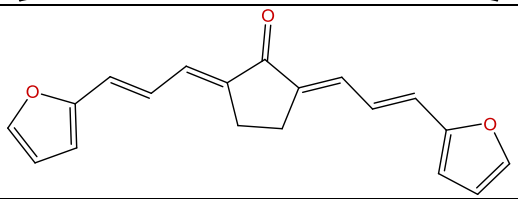
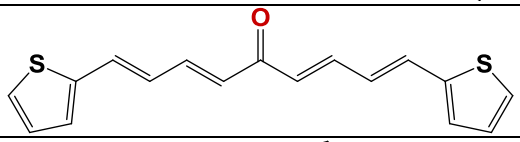
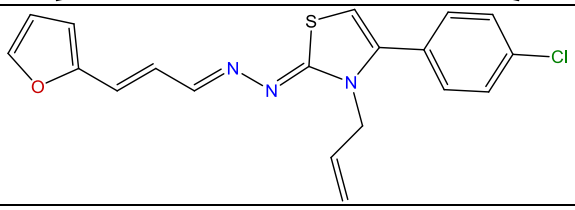
1336		50	113
485		50	76
313		44	63
1103		36	68
782		50	61
1174		50	105
910		50	84
784		50	102

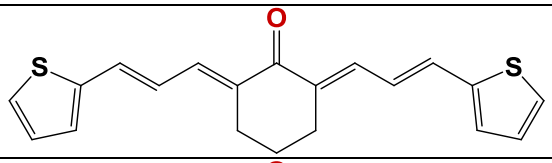
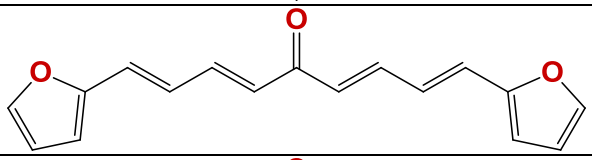
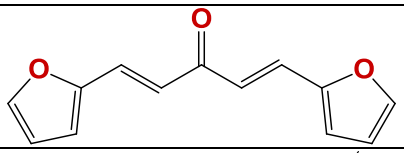
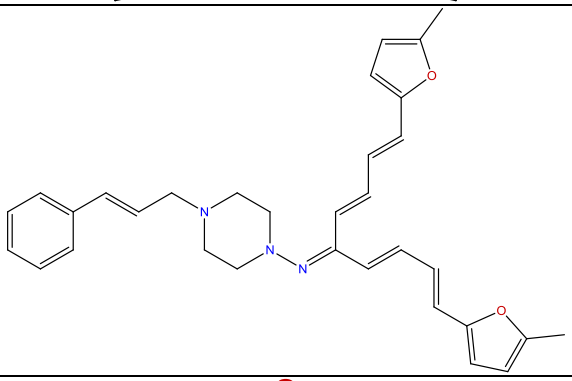
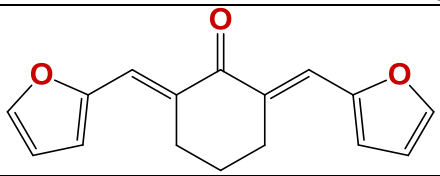
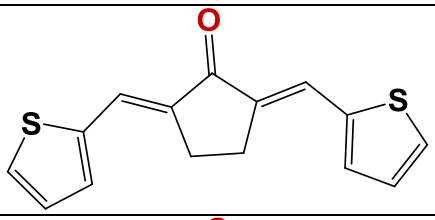
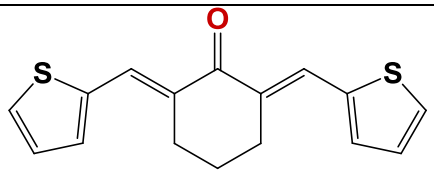
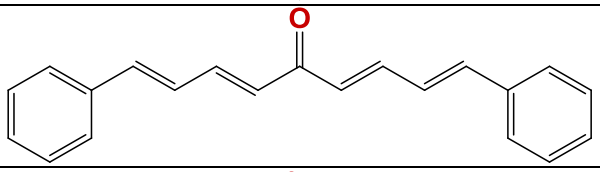
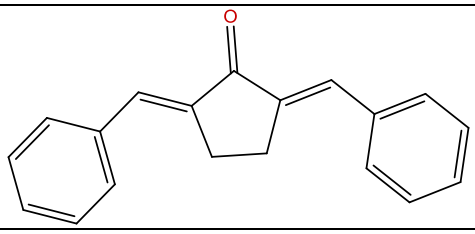
489		45	85
144		50	89
310		50	169
272		50	71
145		50	60
783		50	83
301		36	94
901		50	87

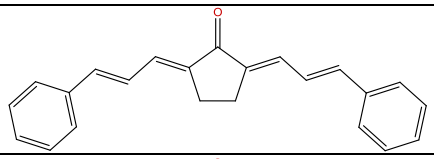
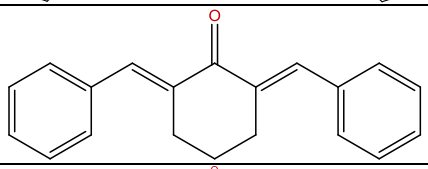
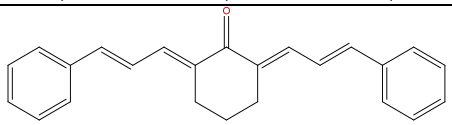
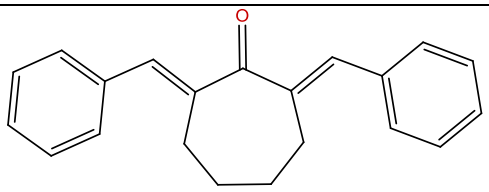
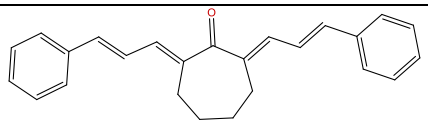
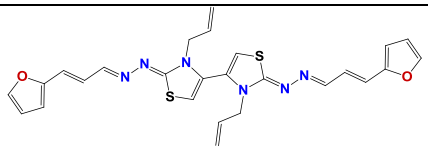
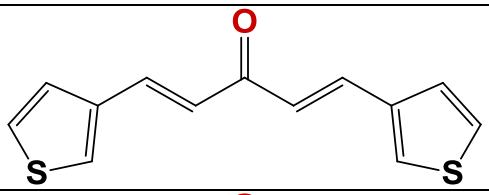
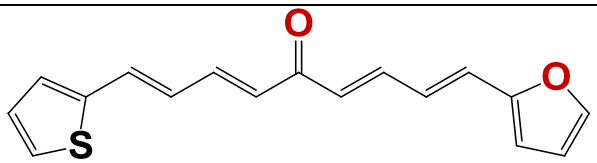
194		50	78
273		50	93
293		50	111
262		47	59
129		50	105
288		50	110
199		50	104

282		50	75
214		50	94
279		50	89
1147		50	90
1383		50	90
694		50	64
1381		50	2
1379		50	100
1380		50	132
911		50	168

1377		50	45
1378		50	84
1385		50	85
1384		50	55
872		50	82
796		50	7
1019		50	74
1018		34	115

314		45	60
877		50	68
912		50	92
873		50	67
809		50	55
1223		50	96
798		39	63
266		36	124

1245		50	23
793		50	68
795		50	0
1102		50	114
808		50	53
1248		50	64
807		50	82
797		50	82
1247		50	80

1246		50	86
799		50	83
800		50	73
803		50	78
804		50	63
295		50	86
1387		50	69
1414		50	73