Supporting Information for:

Development of a Comprehensive, Validated Pharmacophore Hypothesis for Anthrax Toxin Lethal Factor (LF) Inhibitors Using Genetic Algorithms, Pareto Scoring, and Structural Biology

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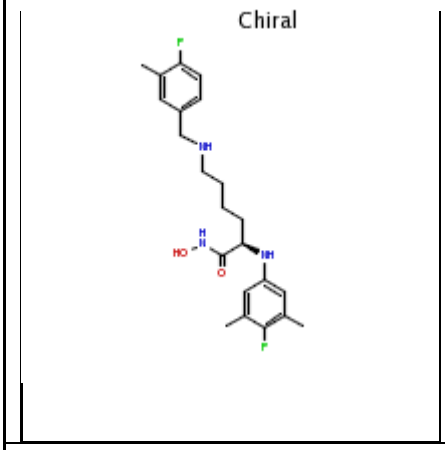
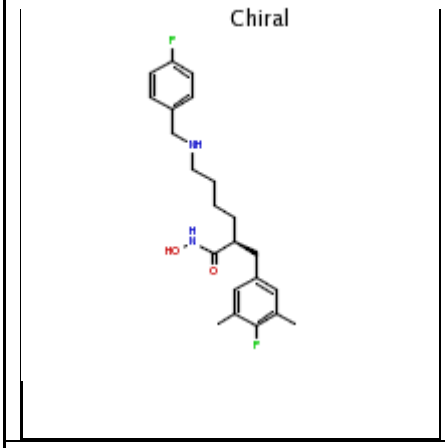
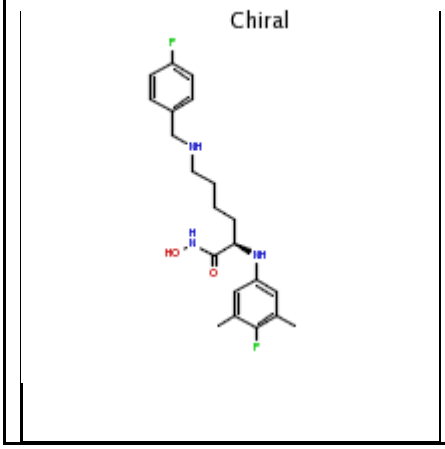
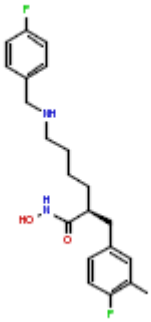
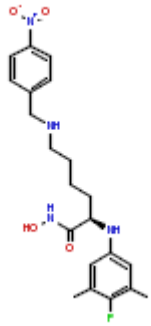
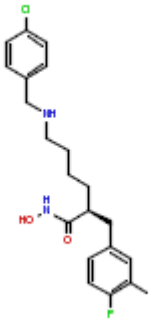
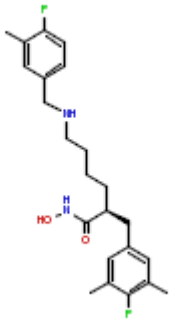
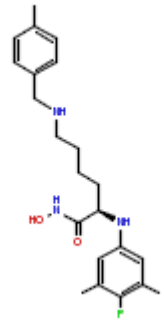
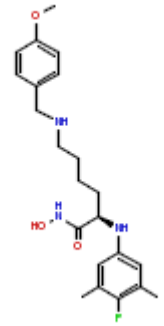
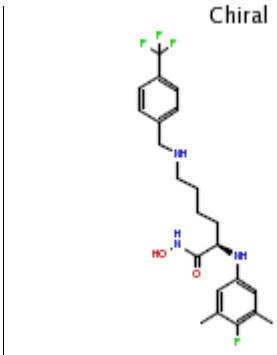
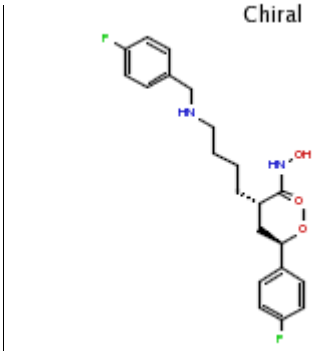
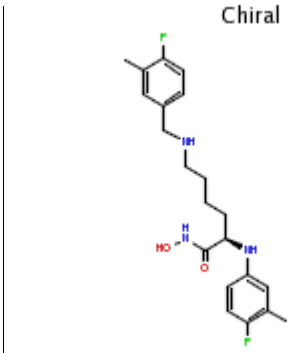
Contents:

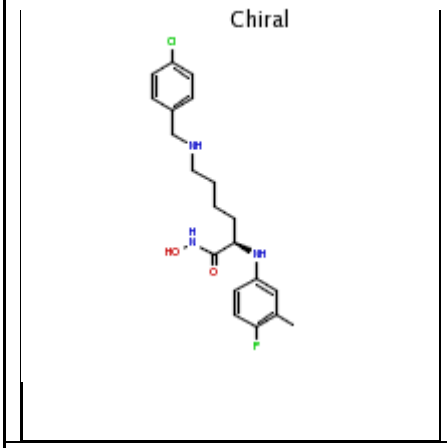
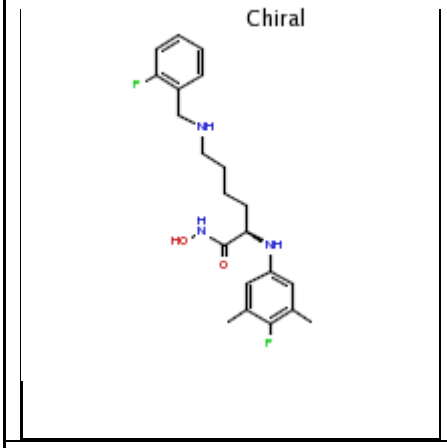
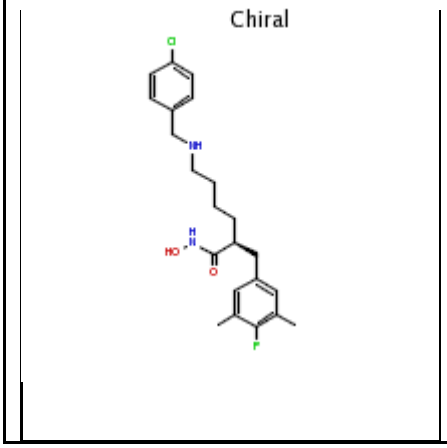
Table S1. Structures, LF biological activities, references, compound designators, and docking scores for screening set compounds in dataset **DB1A.** Asterisk next to biological activity value denotes inclusion in training set **DB1A_Training.**

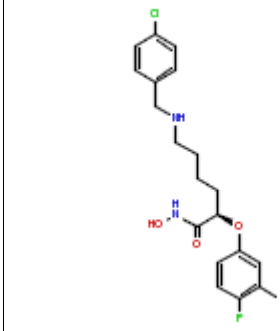
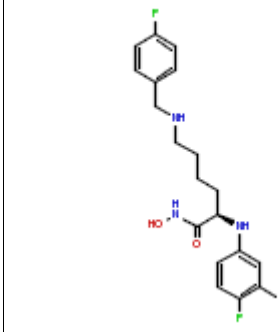
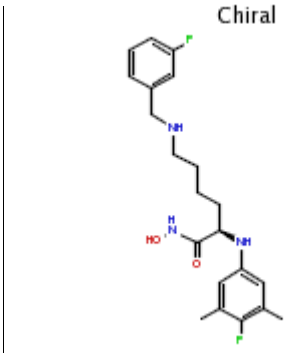
Structure	LF IC_{50} or K_i (μM)	Reference	Compound Designator	Docking Score (Surflex-Dock)
	0.00005	1	1a	12.69
	0.00013	1	5b	11.16
	0.00024	1	1b	12.11

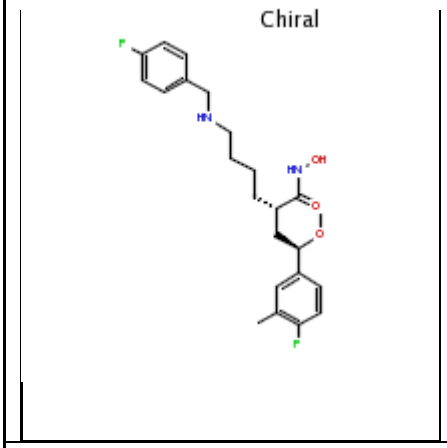
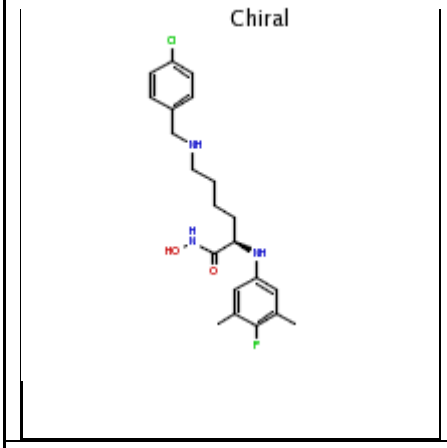
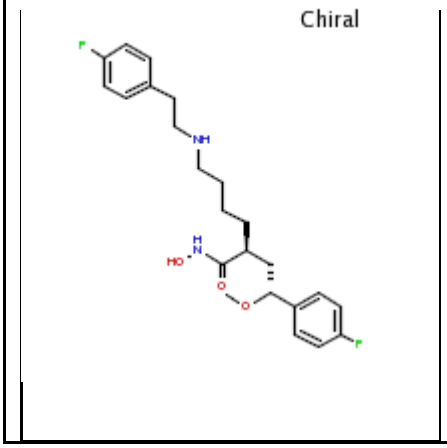
Chiral 	0.00025	1	9b	11.93
Chiral 	0.00030	2	25	12.63
Chiral 	0.00036	1	9c	10.36

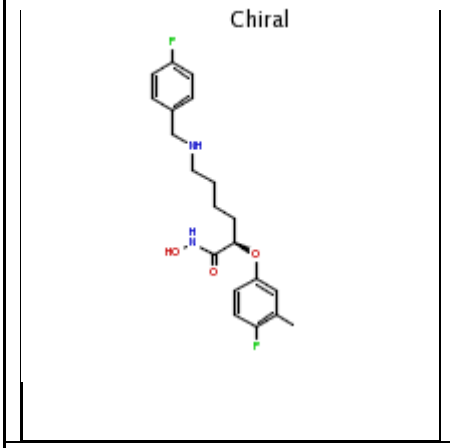
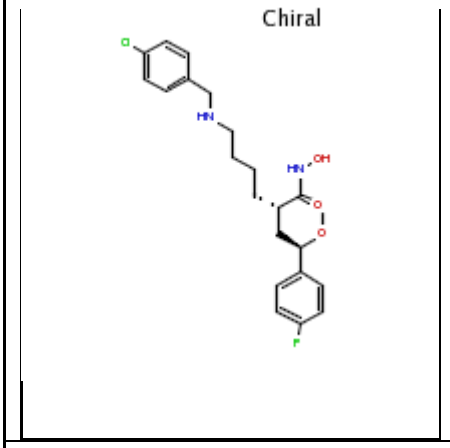
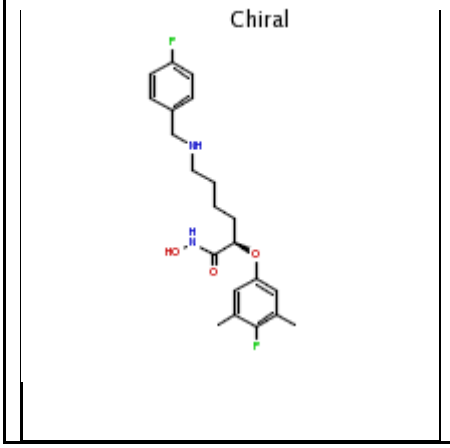
Chiral 	0.00039	1	5a	11.31
Chiral 	0.00041	2	22	11.53
Chiral 	0.00044	2	23	13.45

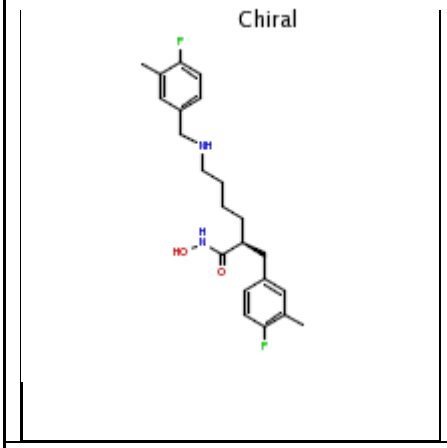
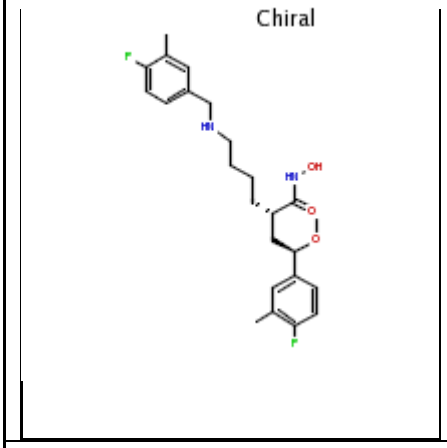
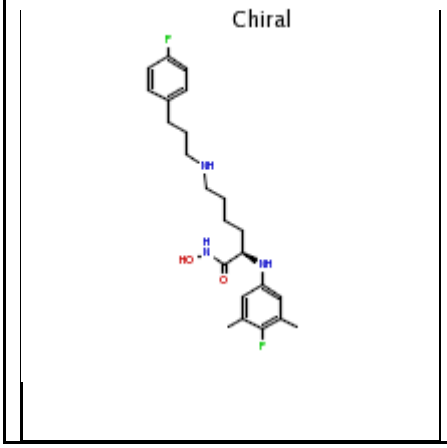
Chiral 	0.00047	2	24	12.53
Chiral 	0.00058	1	3b	12.69
Chiral 	0.00062	1	6a	12.20

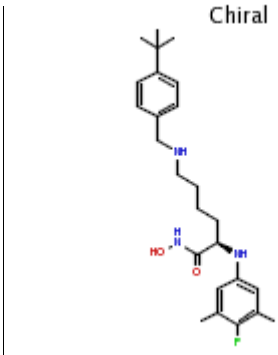
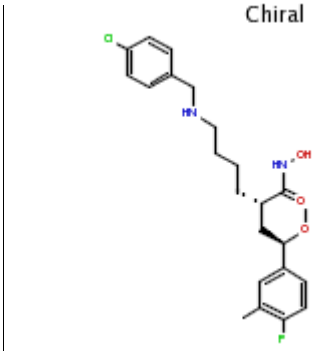
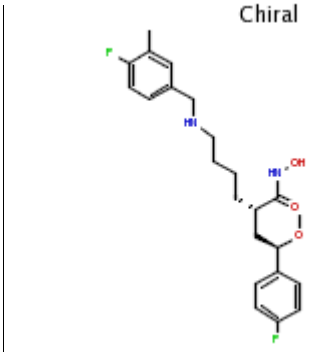
	0.00068	1	6c	11.98
	0.00069	2	18	11.43
	0.00071	1	5c	11.20

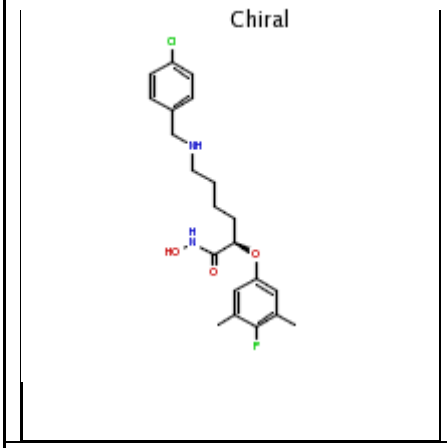
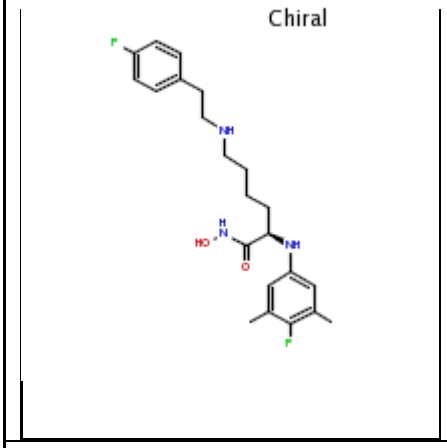
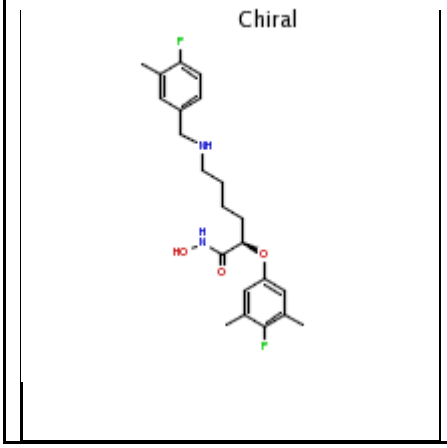
Chiral 	0.00075	1	8c	11.04
Chiral 	0.00081	1	6b	11.94
Chiral 	0.00085	2	19	11.92

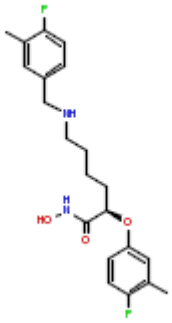
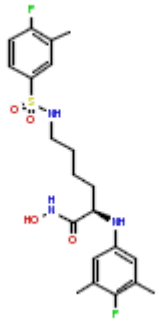
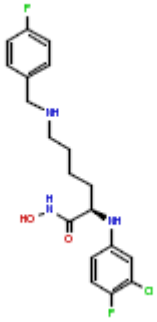
	0.00093	1	7b	12.61
	0.00100	1	1c	11.15
	0.00110	1	3d	12.20

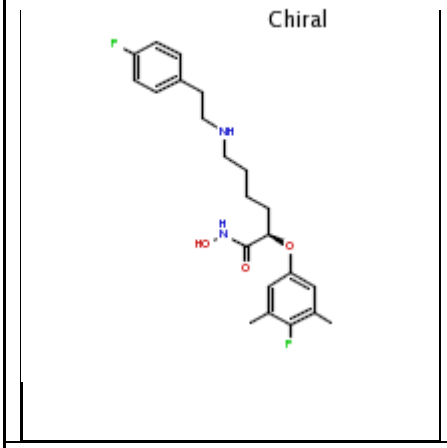
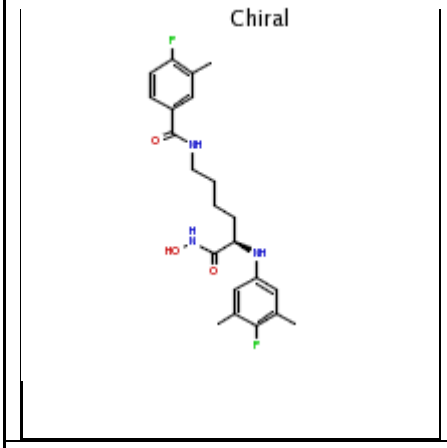
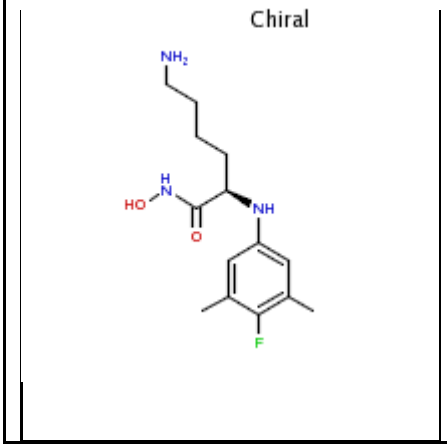
	0.00110	1	8b	12.78
	0.00120	1	3c	11.60
	0.00120	1	4b	11.79

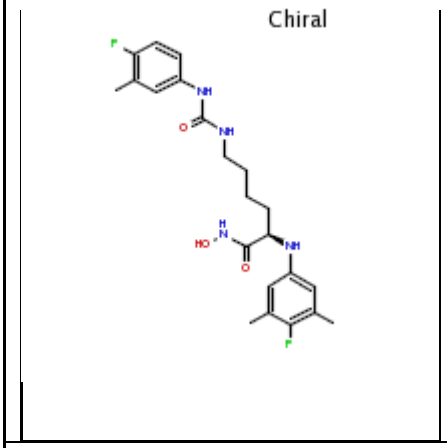
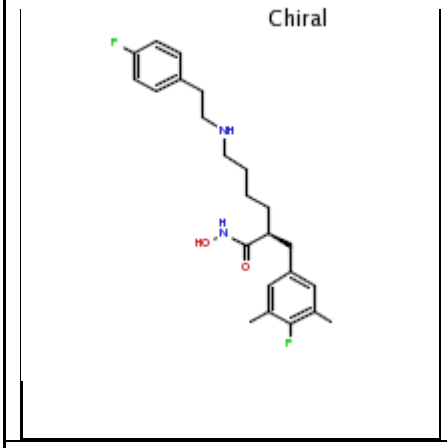
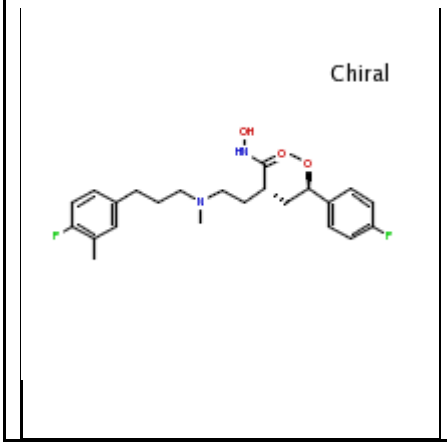
Chiral 	0.00120	1	9a	11.20
Chiral 	0.00130	1	7a	12.77
Chiral 	0.00130	2	28	11.27

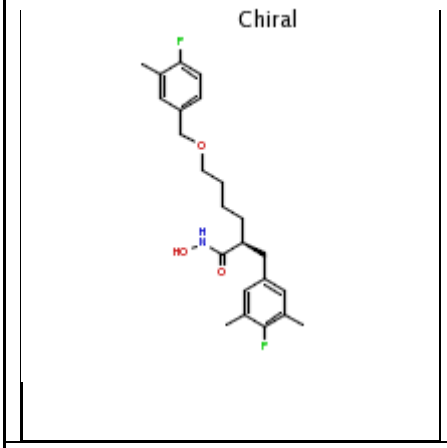
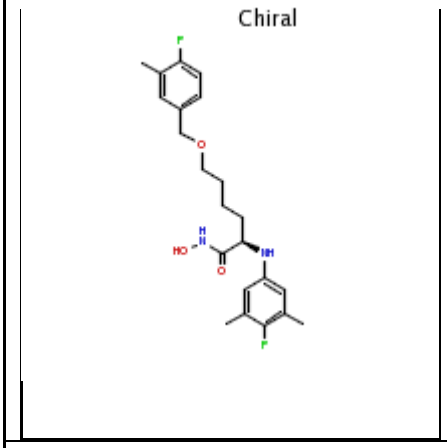
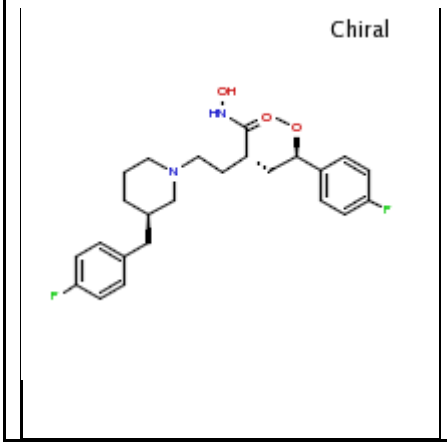
Chiral 	0.00140	2	26	12.78
Chiral 	0.00140	1	7c	11.97
Chiral 	0.00150	1	3a	12.67

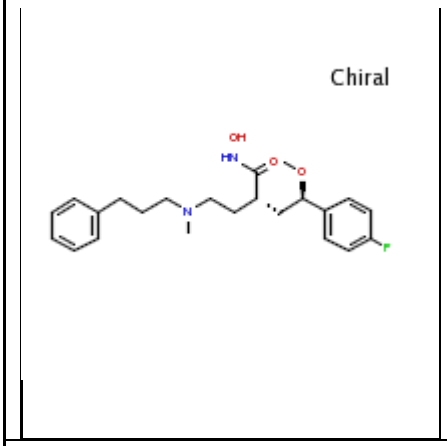
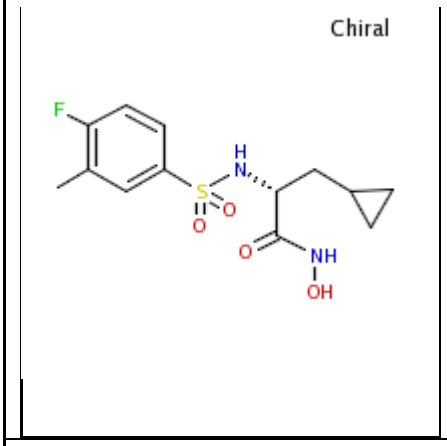
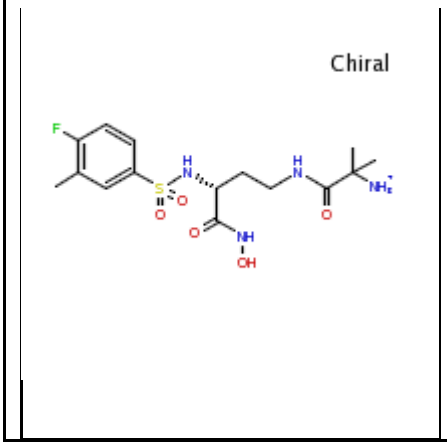
	0.00200	1	4c	11.79
	0.00210	1	1d	13.05
	0.00240	1	4a	11.55

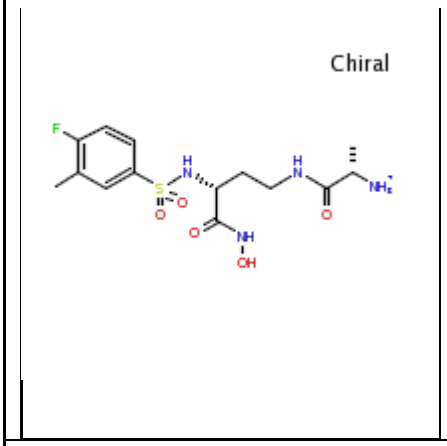
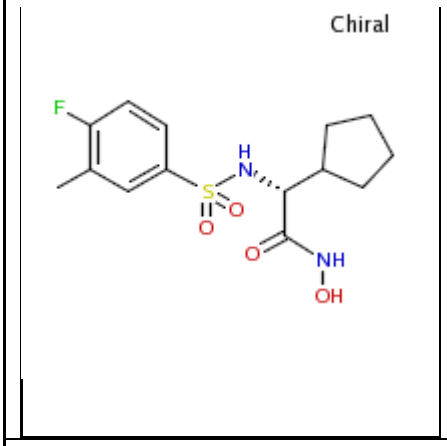
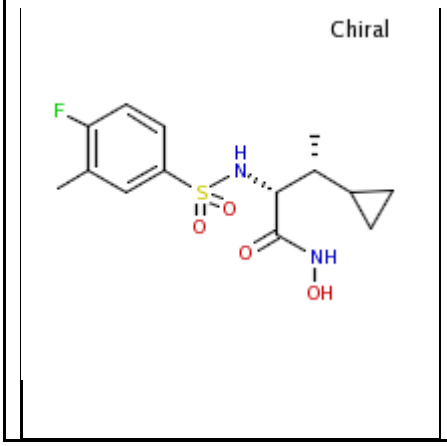
Chiral 	0.00300	1	8a	11.79
Chiral 	0.00310	2	15	12.41
Chiral 	0.00380	1	17	11.90

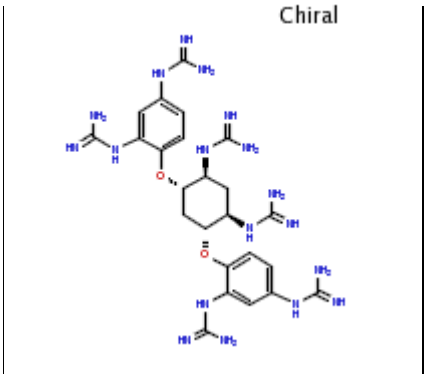
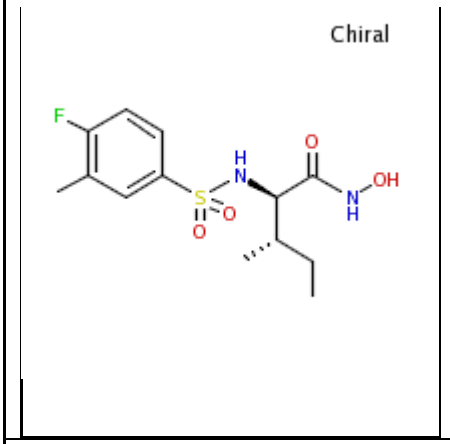
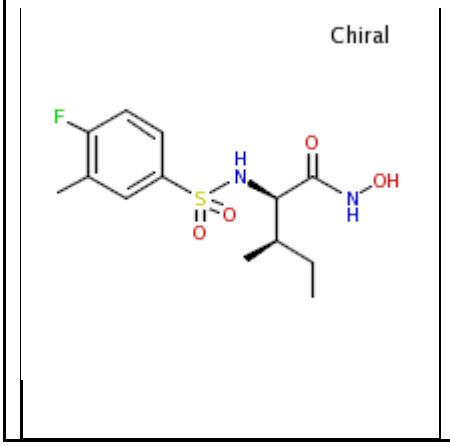
	0.00460	1	4d	11.50
	0.00730	2	14	11.30
	0.00820	2	13	10.61

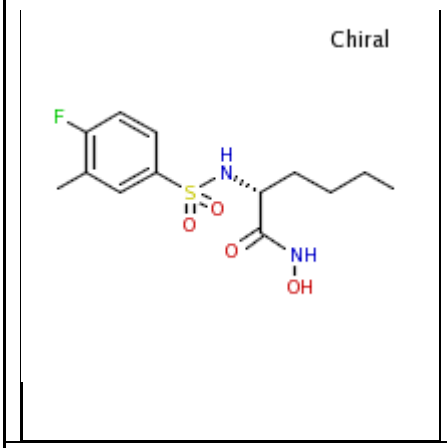
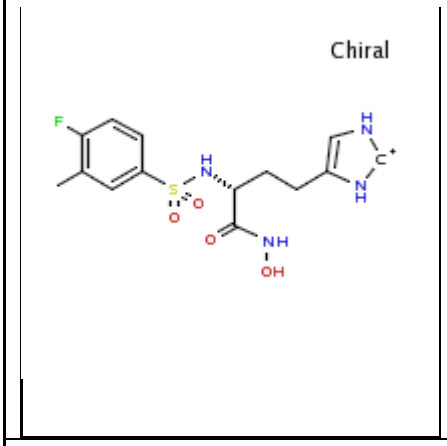
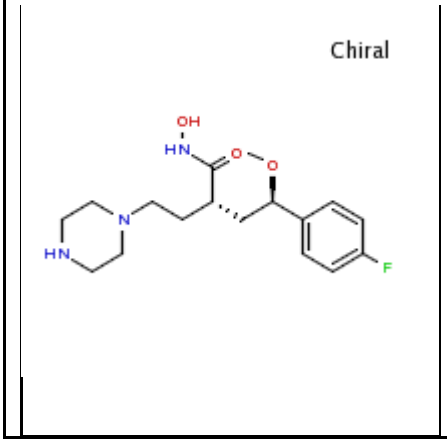
	0.00930	2	17	10.79
	0.00950	1	5d	12.18
	0.01100	2	40	13.02

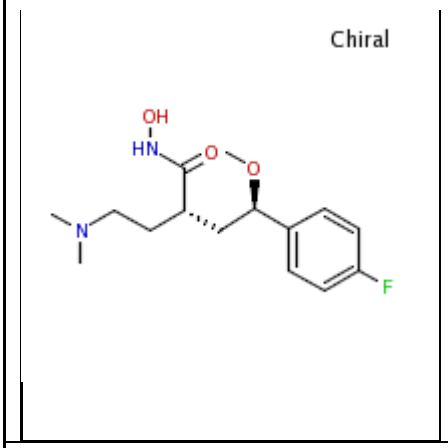
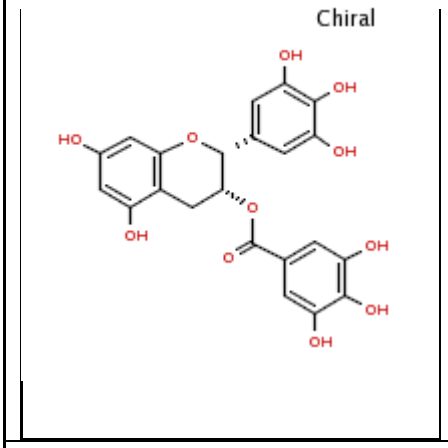
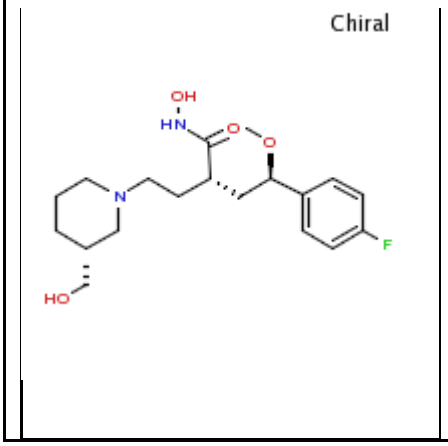
Chiral 	0.02500	1	15	12.09
Chiral 	0.03040	1	13	12.14
Chiral 	0.03300	2	34	11.34

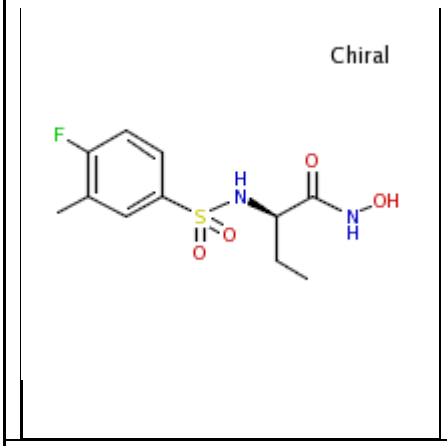
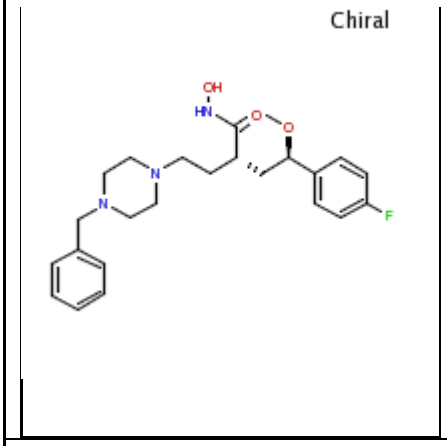
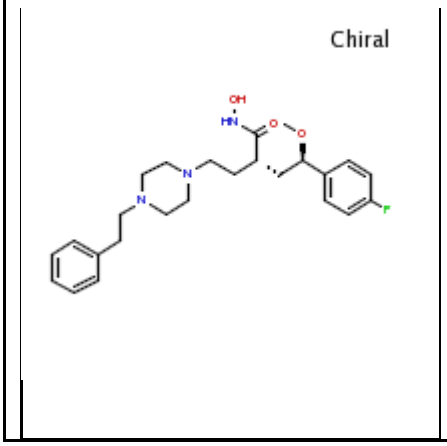
	0.04200	2	39	11.19
	0.05100*	3	44	10.35
	0.05700*	3	48	11.69

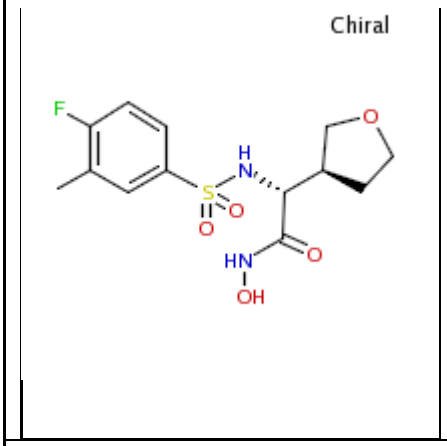
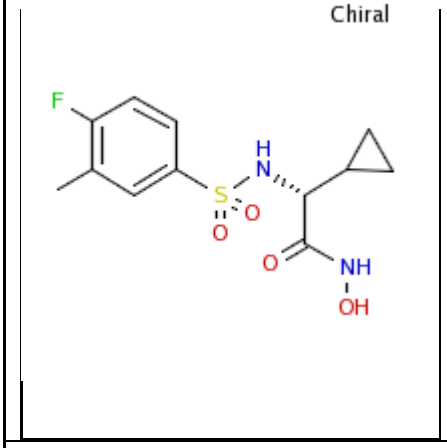
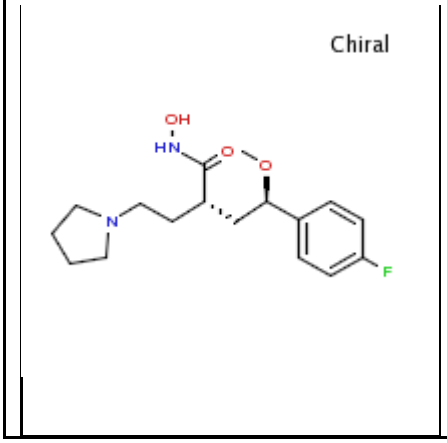
	0.05900*	3	47	11.64
	0.06400*	3	37	10.29
	0.06500*	3	45	10.51

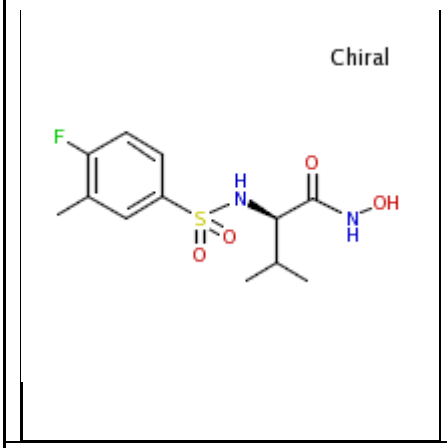
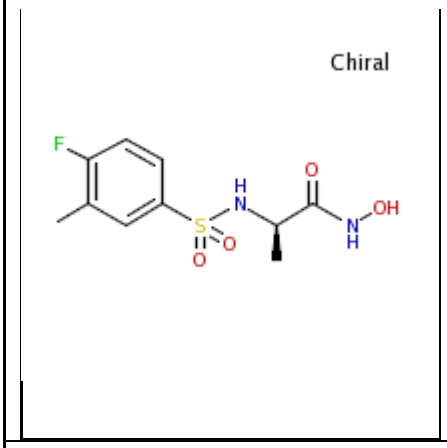
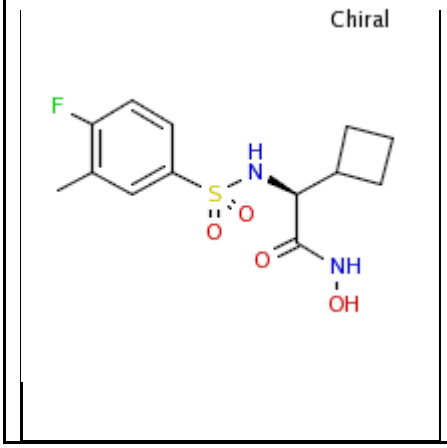
	0.06500	4	14	4.80
	0.06700*	3	42	10.55
	0.06700*	3	43	10.09

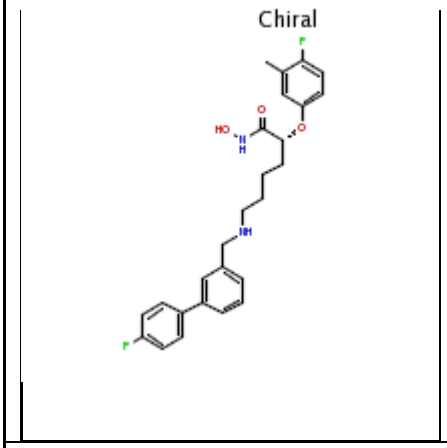
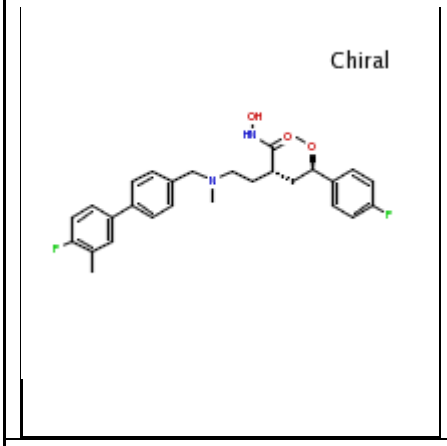
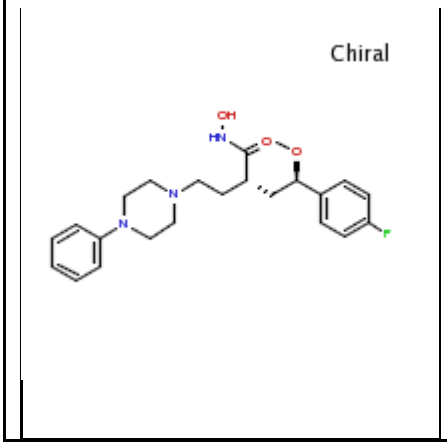
	0.07000*	3	33	11.23
	0.07500*	3	51	11.33
	0.09000	2	35	11.51

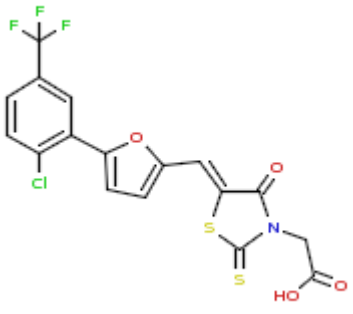
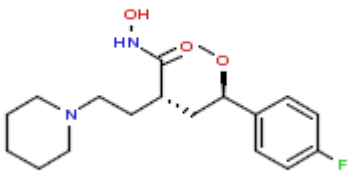
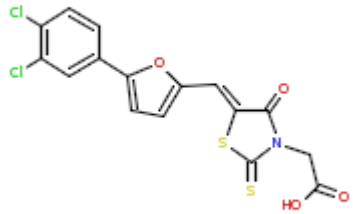
	0.09600	2	29	10.21
	0.09700	5	EGCG	2.78
	0.09900	2	33	12.53

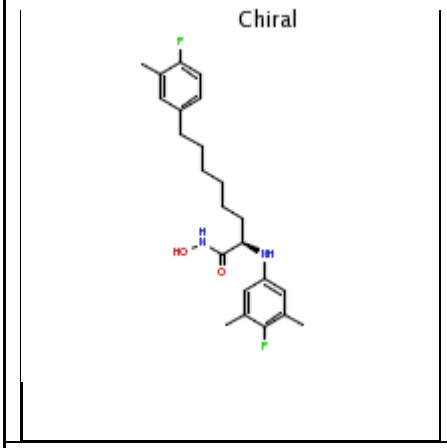
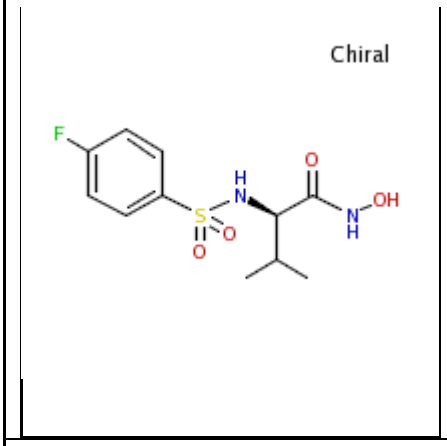
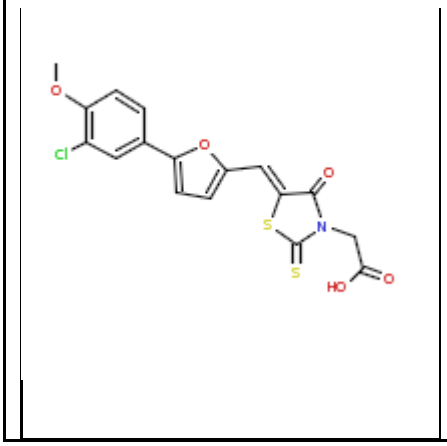
	0.10000*	3	32	9.40
	0.11500	2	37	10.56
	0.11800	2	38	10.92

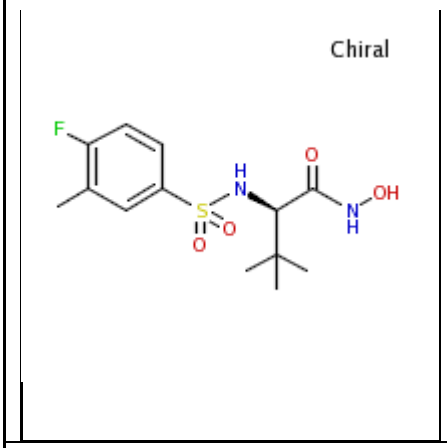
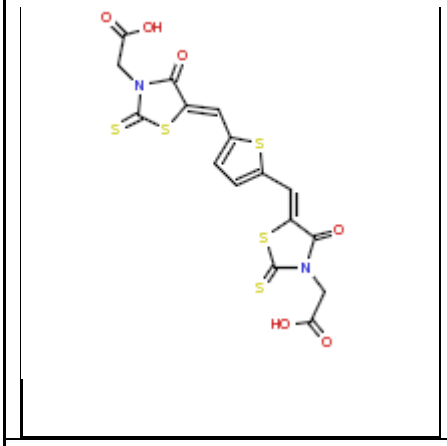
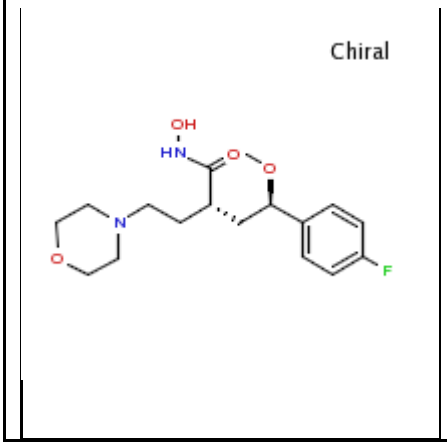
	0.12000*	3	41	9.81
	0.12000*	3	35	10.16
	0.12200	2	30	10.50

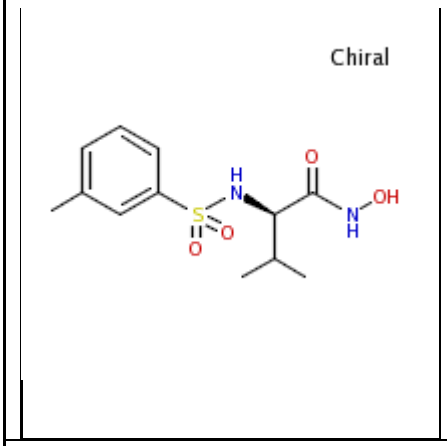
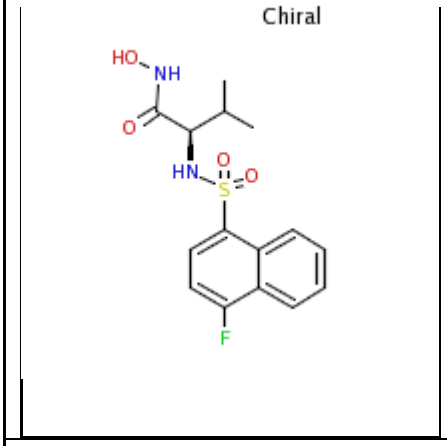
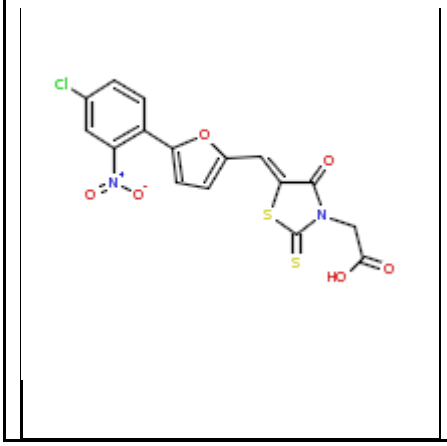
	0.13000*	3	16	10.20
	0.13000*	3	31	8.79
	0.13000*	3	36	9.92

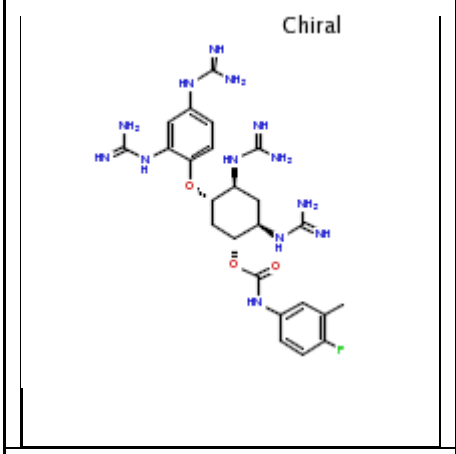
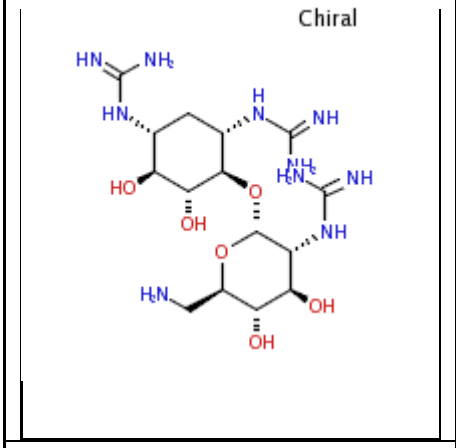
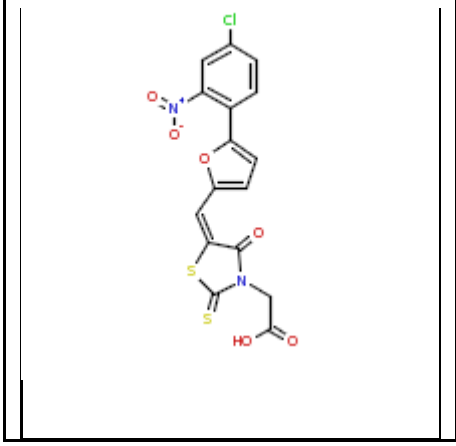
	0.13000	6	18	12.68
	0.13500	2	41	12.25
	0.15100	2	36	10.81

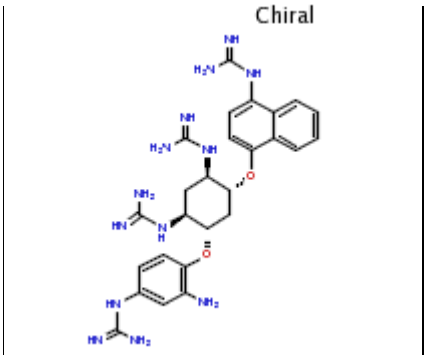
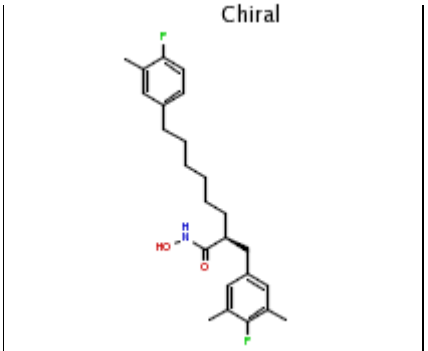
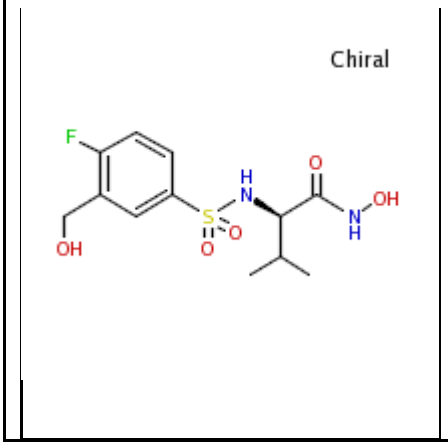
	0.19000*	7	65	6.14
Chiral 	0.23000	2	31	10.93
	0.26000*	7	64	5.85

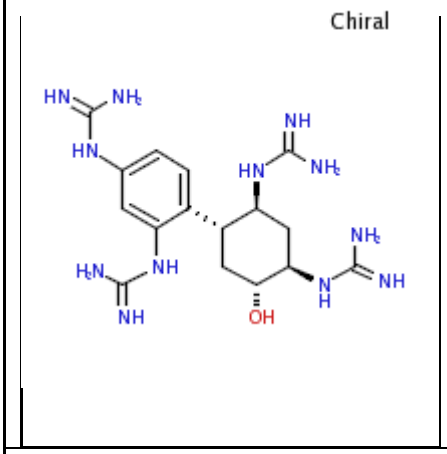
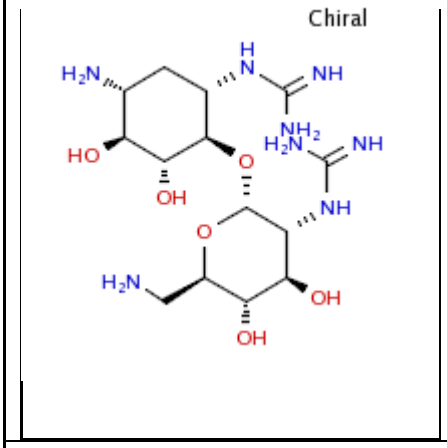
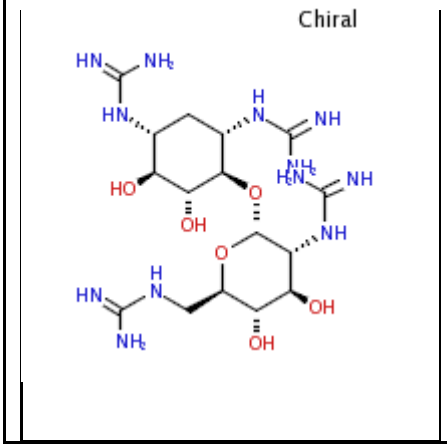
	0.27300	1	14	11.98
	0.29000*	3	13	9.00
	0.29800*	8	BI-11B1	5.94

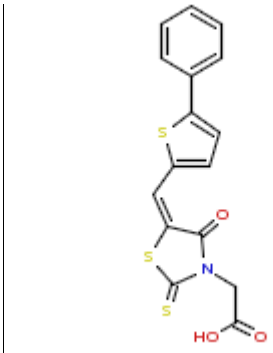
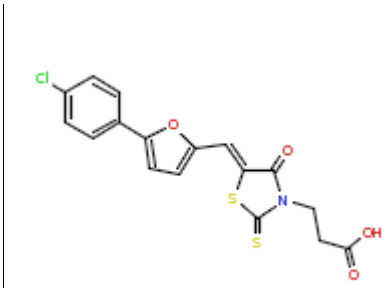
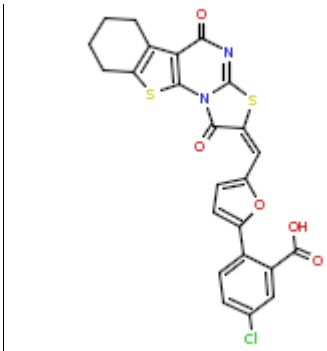
	0.30000*	3	34	10.23
	0.32000*	7	67	6.53
	0.35000	2	32	10.60

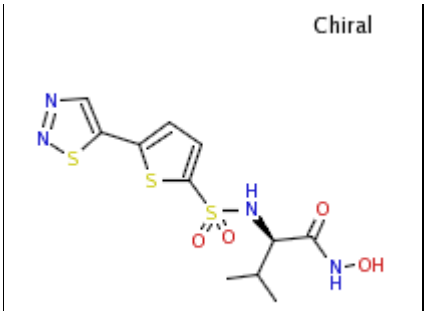
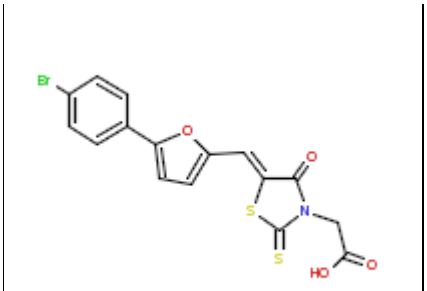
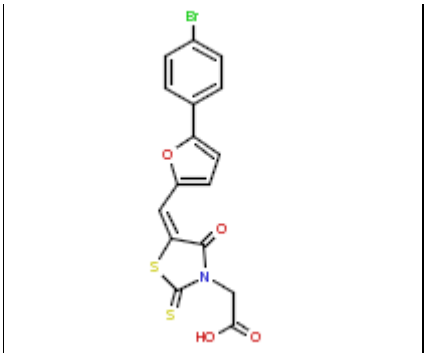
	0.40000*	3	15	9.73
	0.46000*	3	25	10.48
	0.50000*	8	BI-11A11	6.50

	0.50000	4	12	9.28
	0.50000	9	23	8.51
	0.50000*	10	30	5.87

	0.56000	11	1d	7.56
	0.57700	1	16	11.37
	0.60000*	3	27	10.76

	0.60000	4	8c	7.55
	0.70000	9	21	8.69
	0.70000	9	4	7.14

	0.74000*	10	9	6.52
	0.80000*	8	BI-MFM3	5.57
	0.80000	12	1	6.67

	0.81000*	3	30	8.31
	0.85000*	8	BI-11A10	6.04
	0.85000*	10	4	6.12

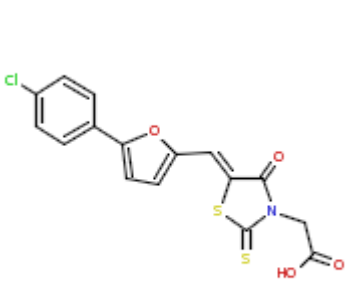
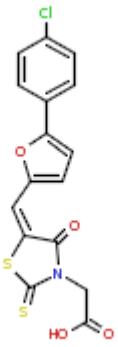
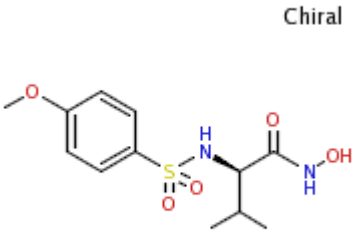
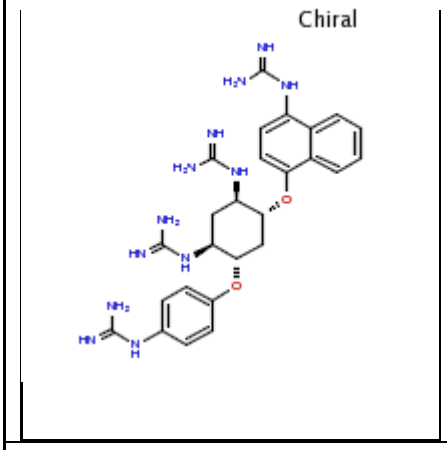
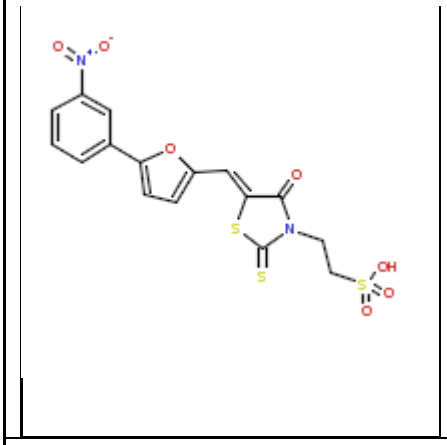
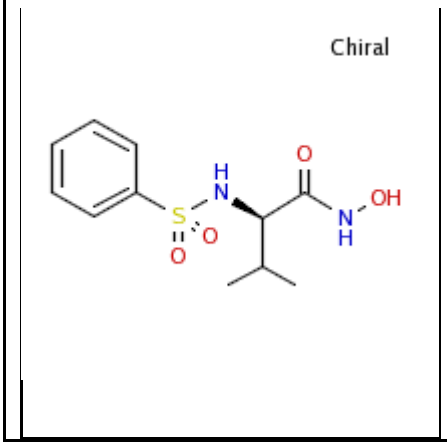
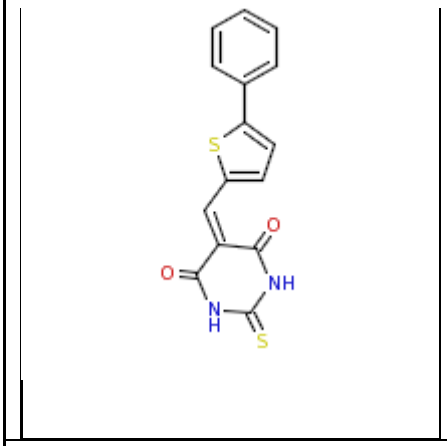
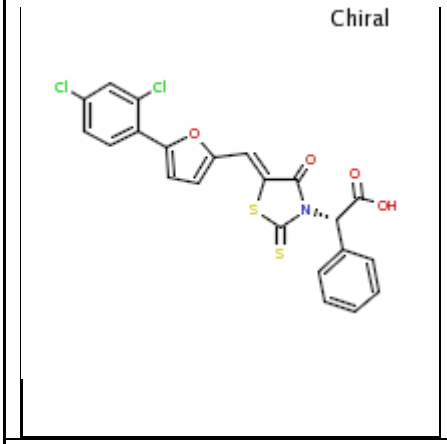
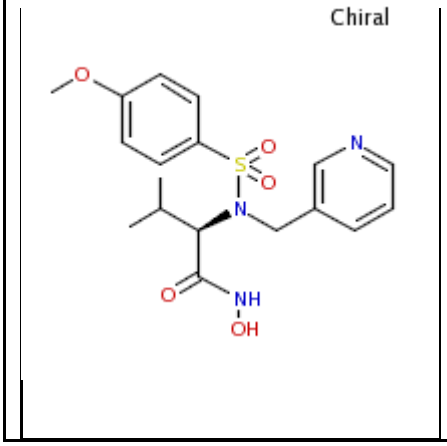
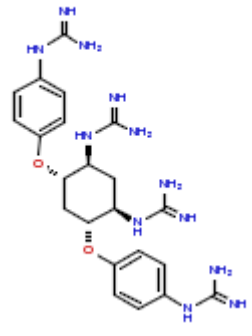
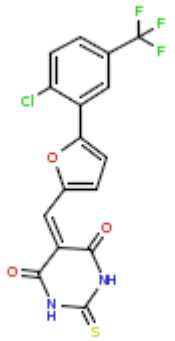
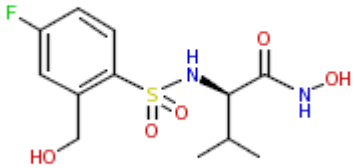
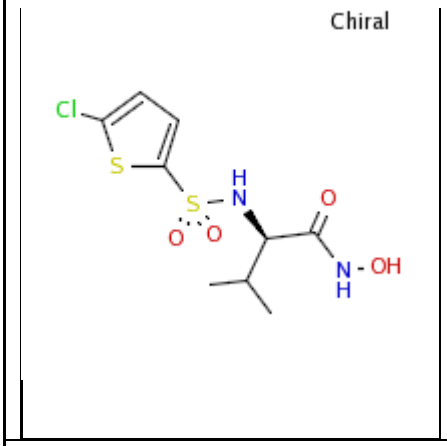
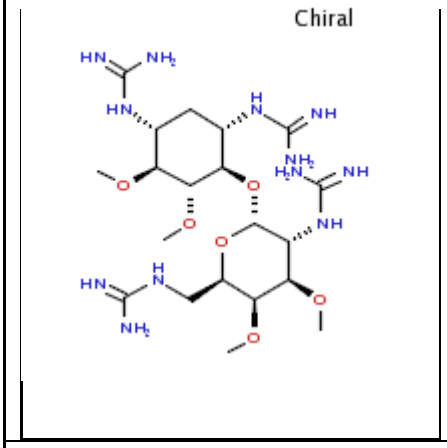
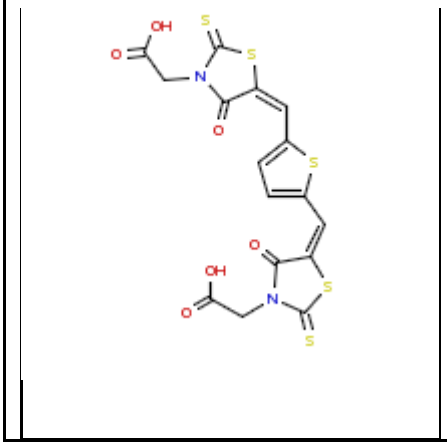
	0.90000*	8	BI-11A9	6.05
	0.90000*	10	3	5.63
	0.90000*	3	2	9.65

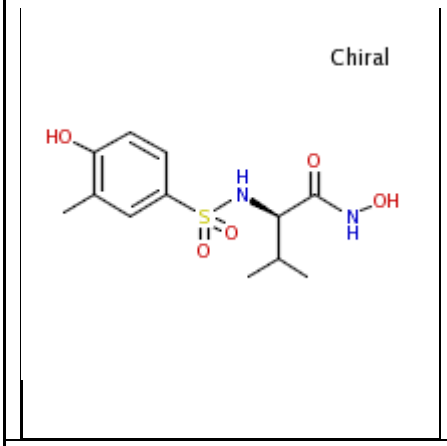
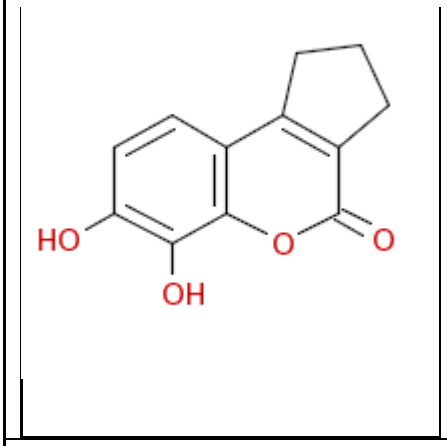
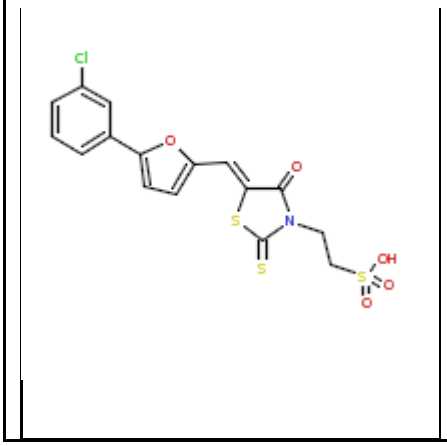
Table S2. Structures, LF biological activities, references, compound designators, and docking scores for screening set compounds in dataset **DB1B.**

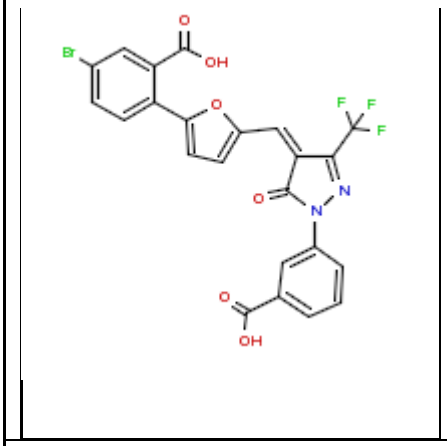
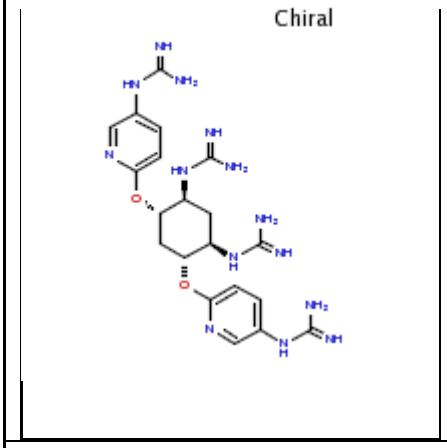
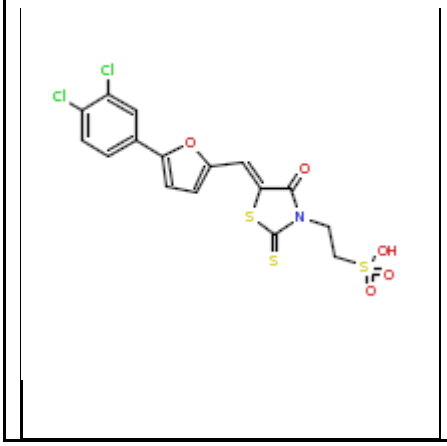
Structure	LF IC_{50} or K_i (μM)	Reference	Compound Designator	Docking Score (Surflex-Dock)
	1.002	4	1e	8.63
	1.090	7	9	5.95
	1.100	3	10	8.36

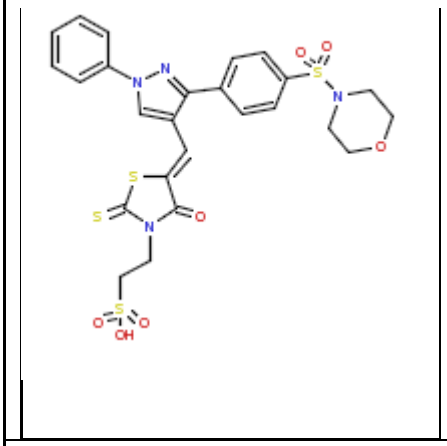
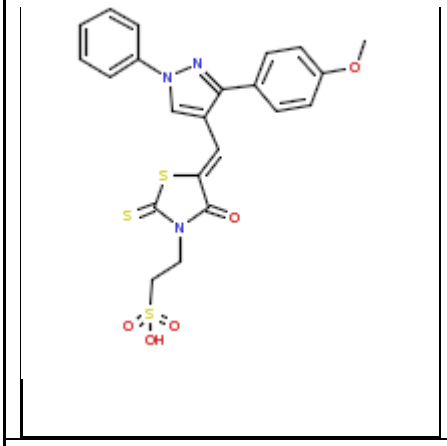
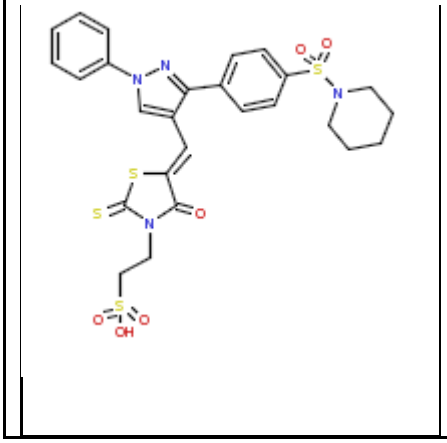
	1.200	10	23	4.36
Chiral 	1.200	7	13	6.16
Chiral 	1.200	3	1	9.57

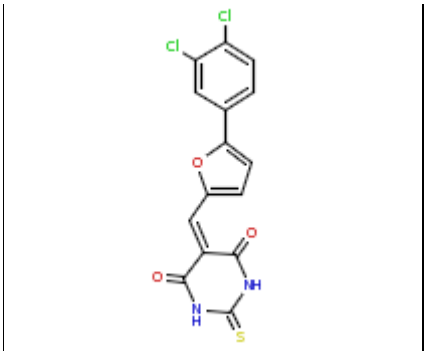
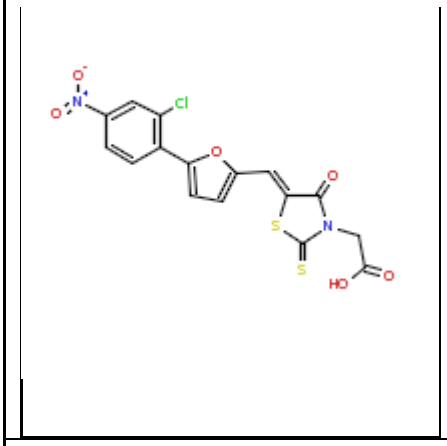
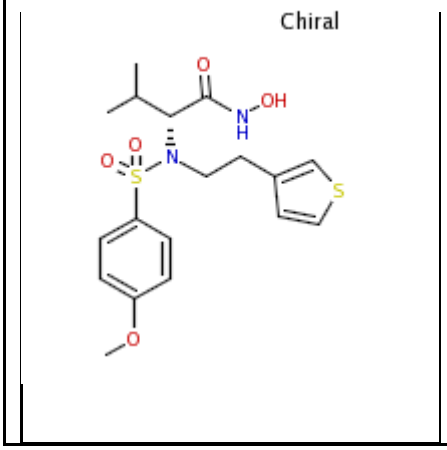
Chiral 	1.241	4	1g	9.81
	1.300	10	21	5.05
Chiral 	1.310	3	28	10.18

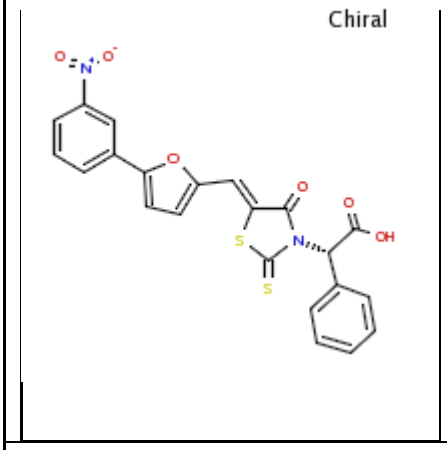
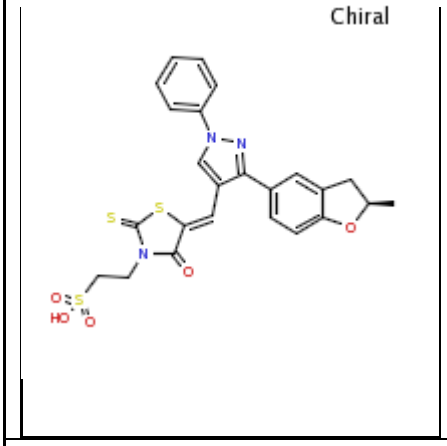
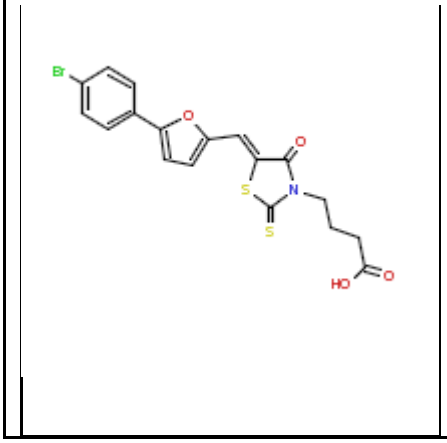
	1.310	3	29	7.65
	1.500	9	29	7.05
	1.600	10	12	4.99

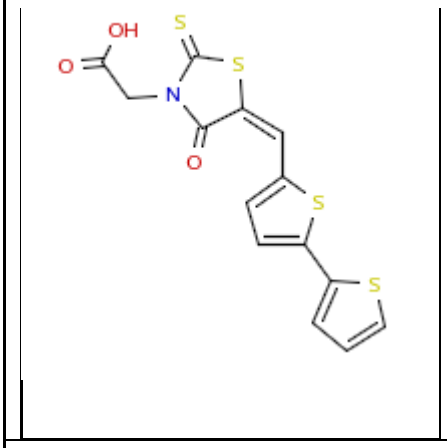
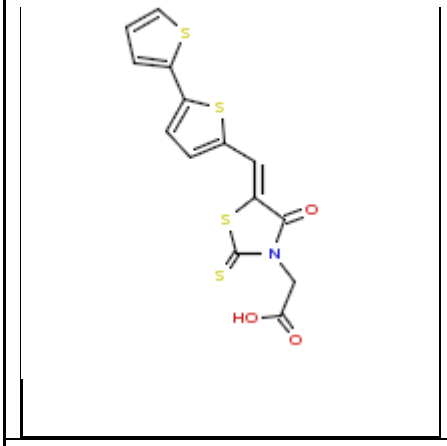
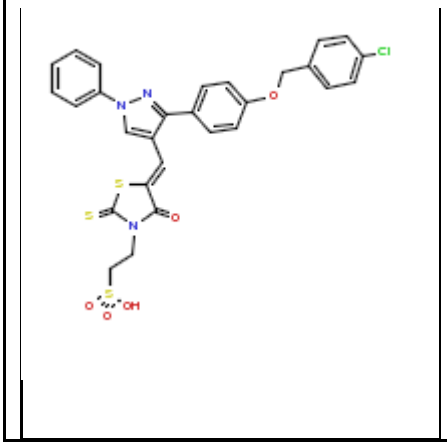
	1.640	3	26	9.41
	1.700	13	6	7.03
	1.700	7	10	6.07

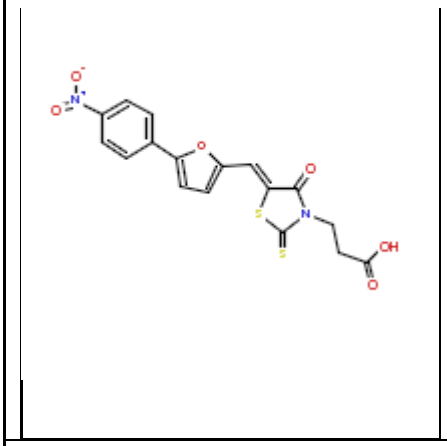
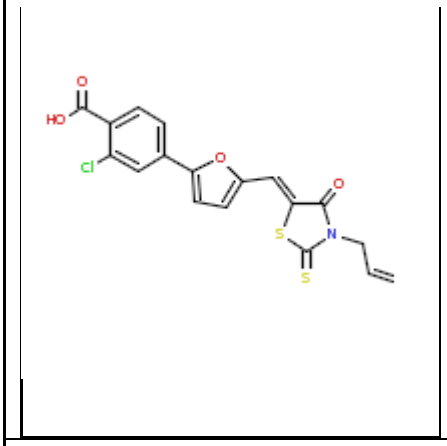
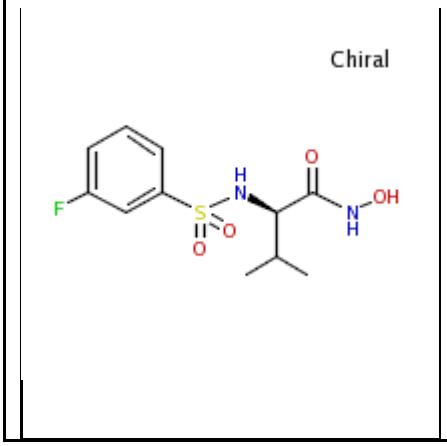
	1.700	12	2	6.97
	1.716	4	1i	9.88
	1.780	7	11	5.64

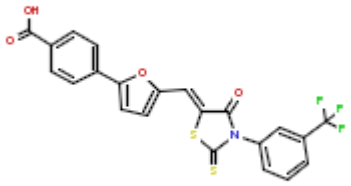
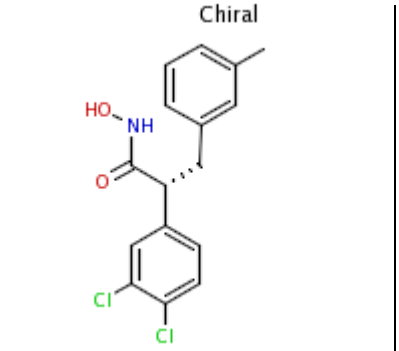
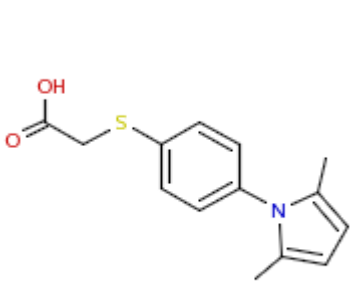
	1.860	7	42	7.33
	2.040	7	40	6.90
	2.070	7	43	6.80

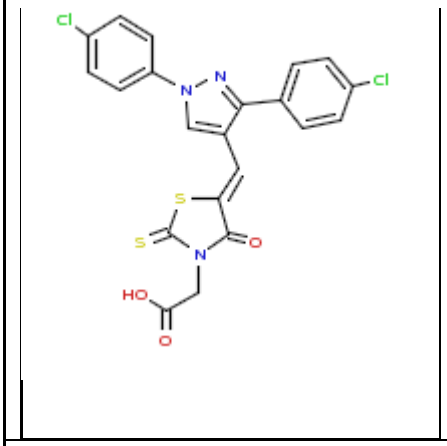
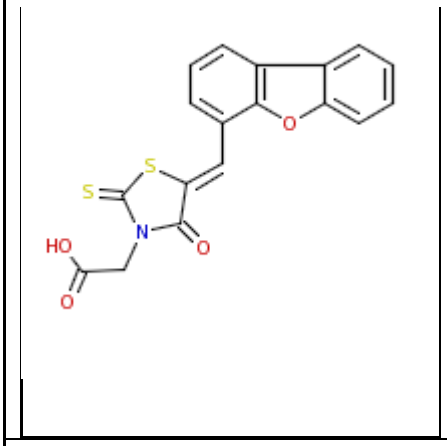
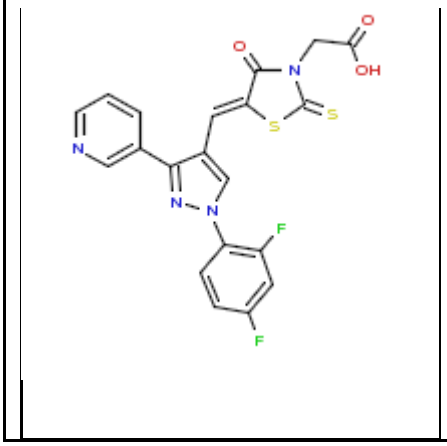
	2.100	10	22	4.45
	2.100	7	4	5.87
	2.100	3	8	8.38

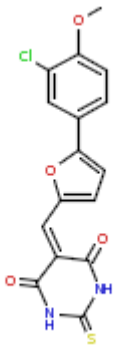
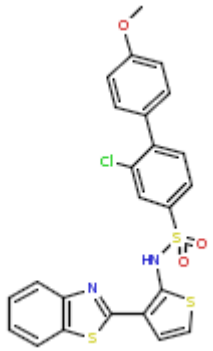
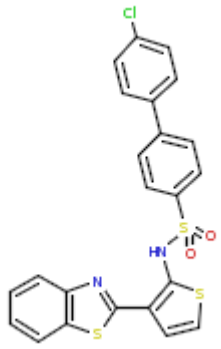
	2.180	7	7	5.94
	2.290	7	39	6.80
	2.300	8	21	6.59

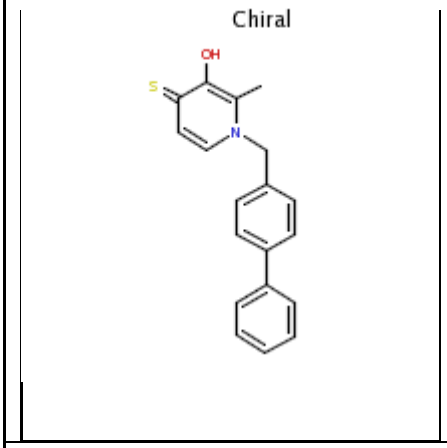
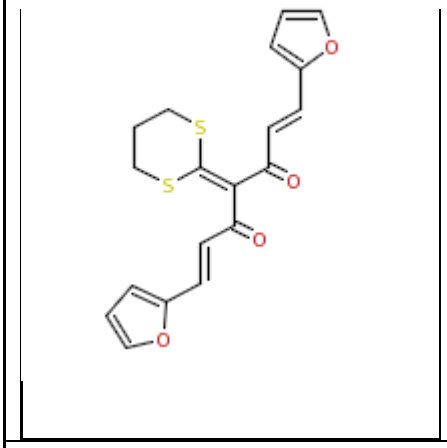
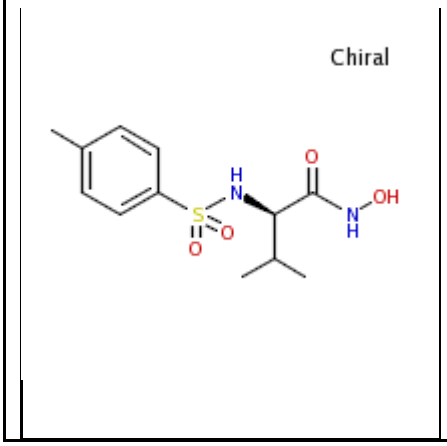
	2.300	10	24	6.83
	2.300	7	66	5.52
	2.450	7	38	6.63

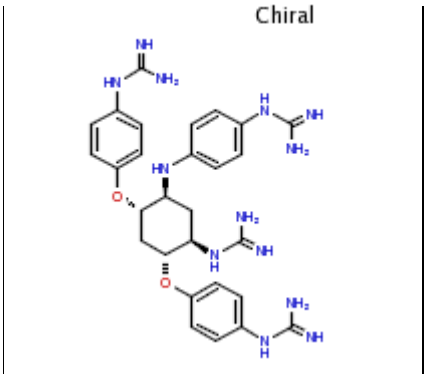
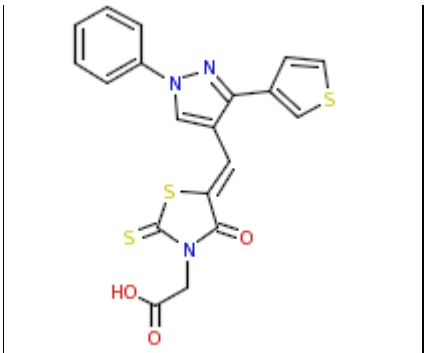
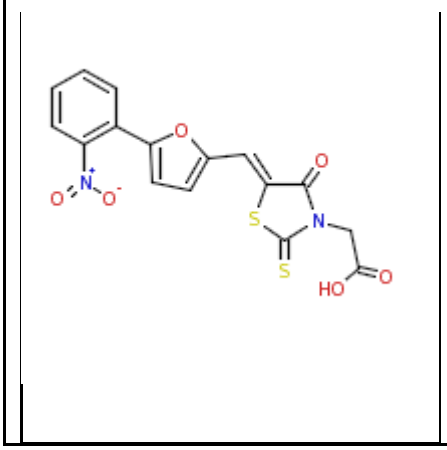
	2.700	8	19	6.13
	2.700	8	20	5.90
Chiral 	2.800	3	12	9.24

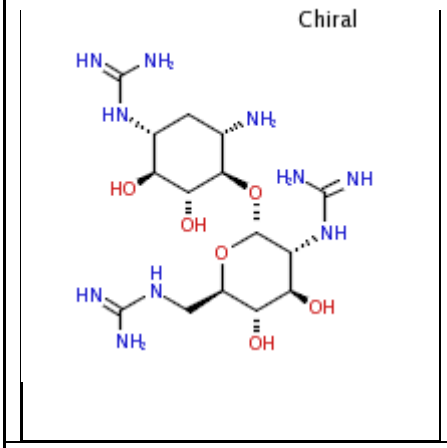
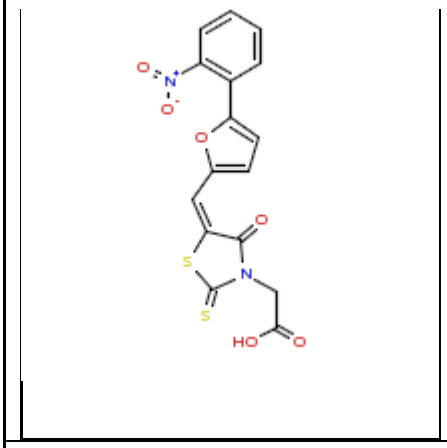
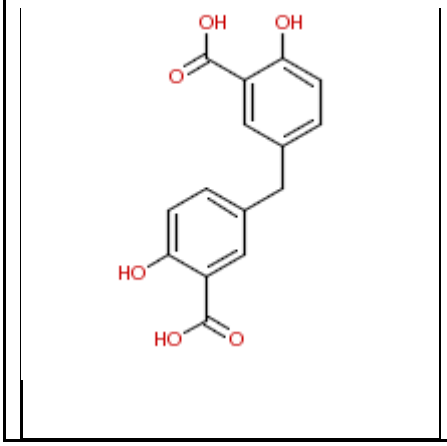
	2.900	8	18	4.15
	2.900	6	22	10.59
	2.900	12	56	5.27

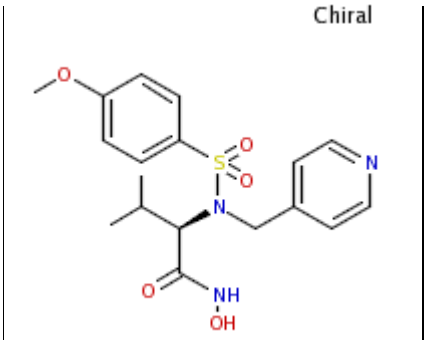
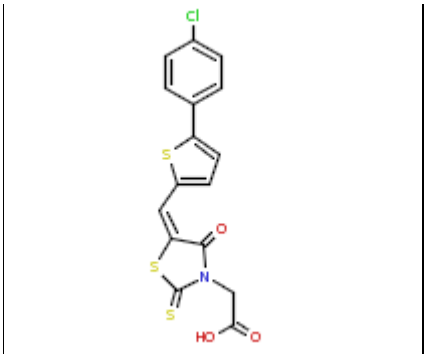
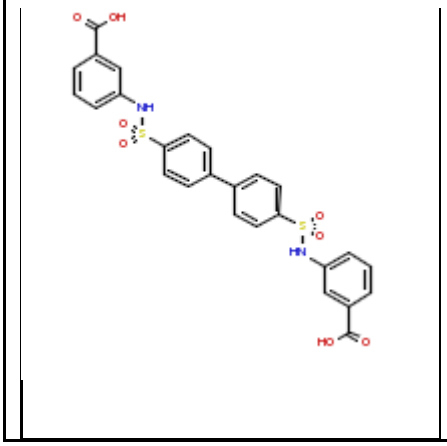
	2.950	7	34	6.17
	2.960	7	55	6.00
	2.990	7	32	8.05

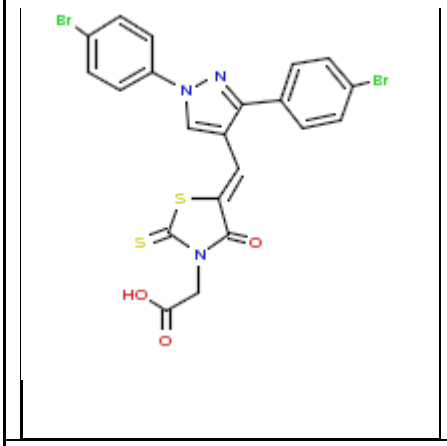
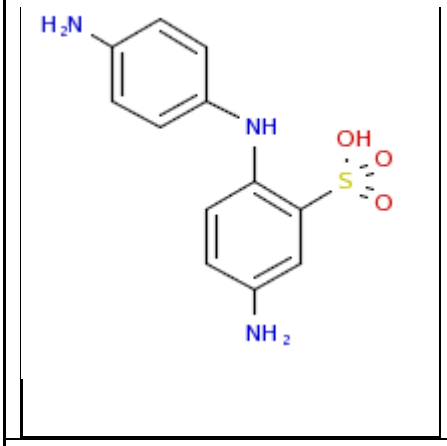
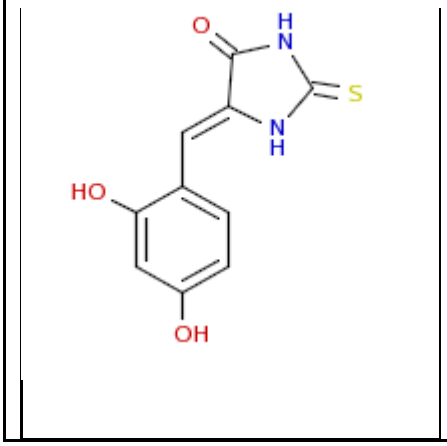
	3.000	10	29	4.89
	3.000	14	124	6.21
	3.000	14	71	7.24

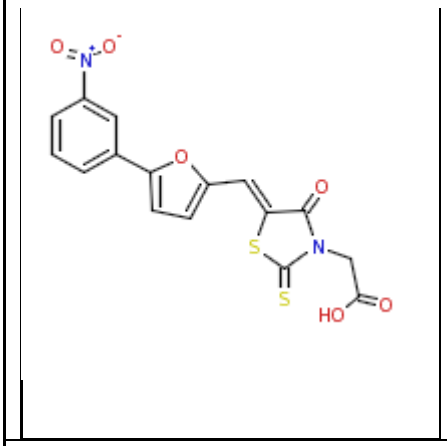
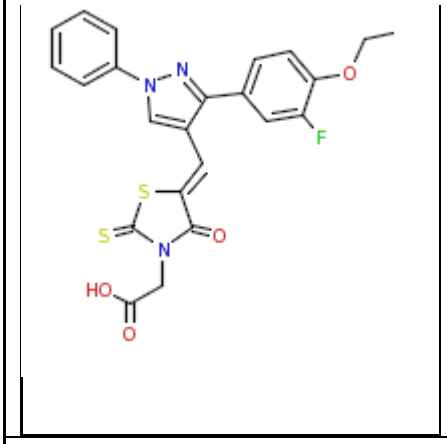
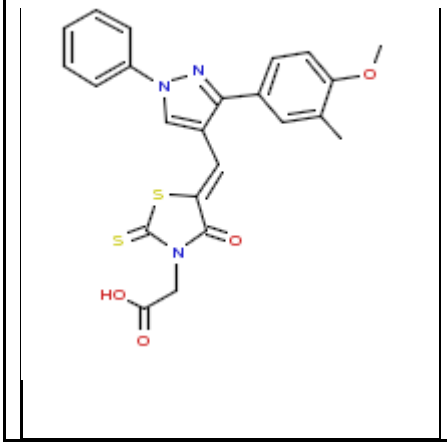
Chiral 	3.000	6	11	7.92
	3.000	12	3	5.95
Chiral 	3.000	3	14	8.96

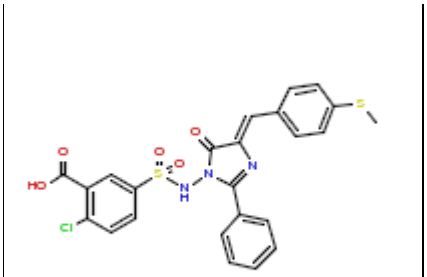
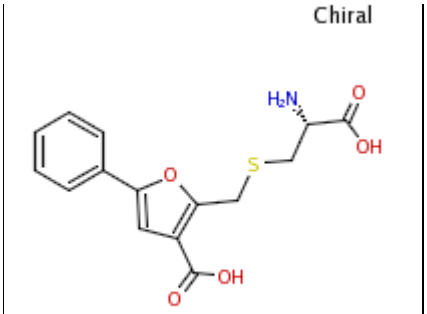
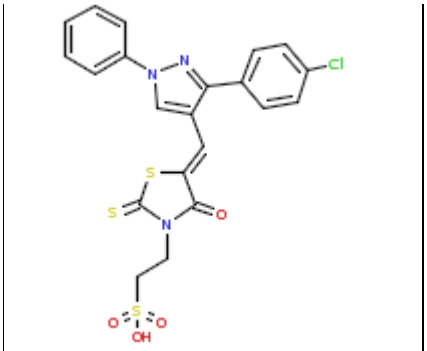
	3.053	4	1n	8.56
	3.070	7	29	7.34
	3.100	8	BI-11A12	6.22

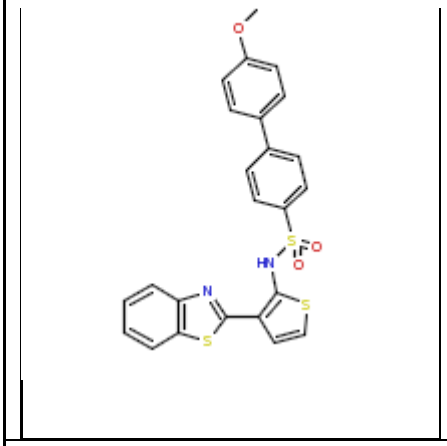
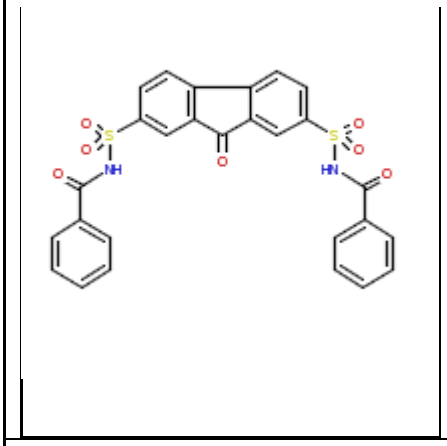
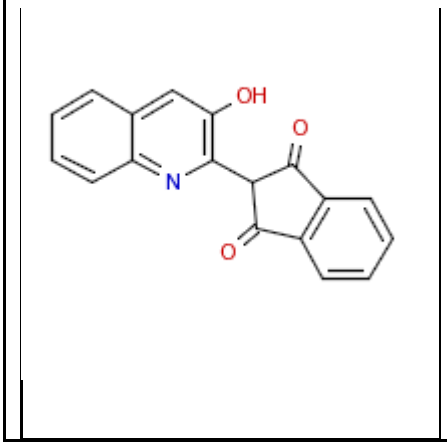
	3.100	9	17	8.44
	3.100	10	5	7.57
	3.100	12	4	9.72

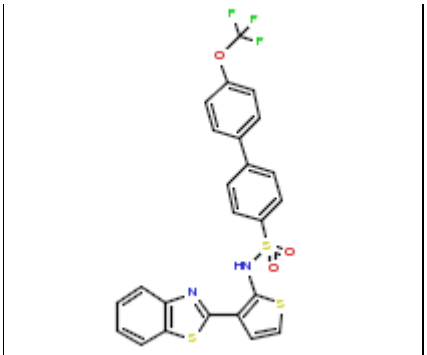
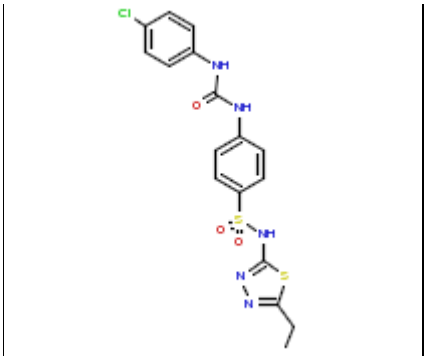
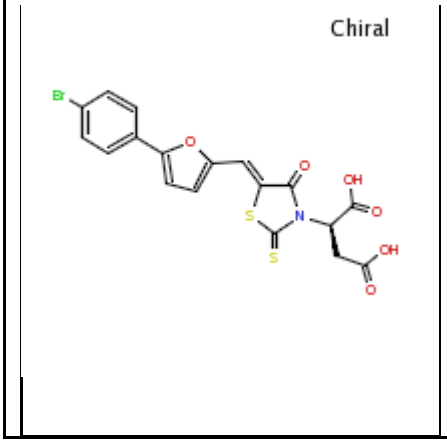
	3.100	3	7	10.64
	3.200	10	11	5.89
	3.200	15	9	7.96

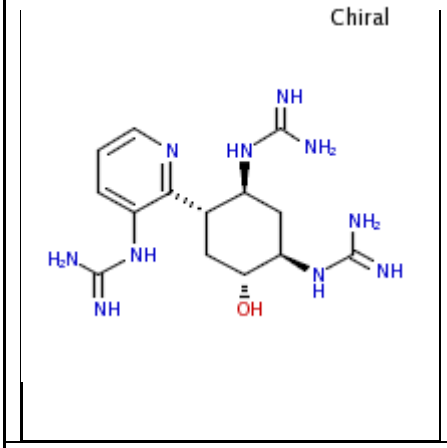
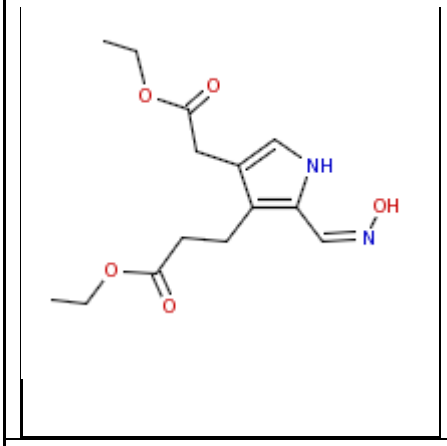
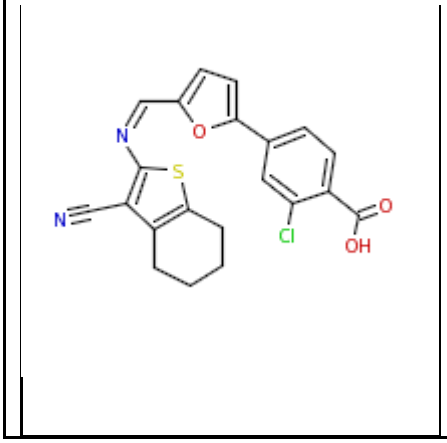
	3.350	7	35	3.94
	3.400	14	1	7.17
	3.400	12	5	6.96

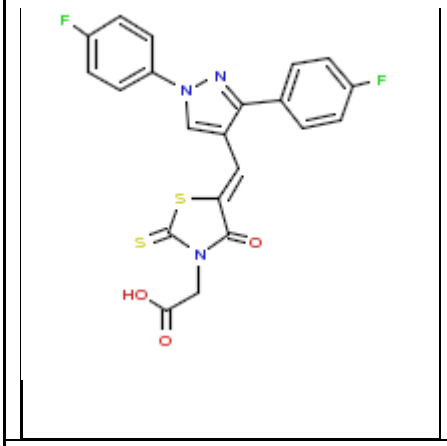
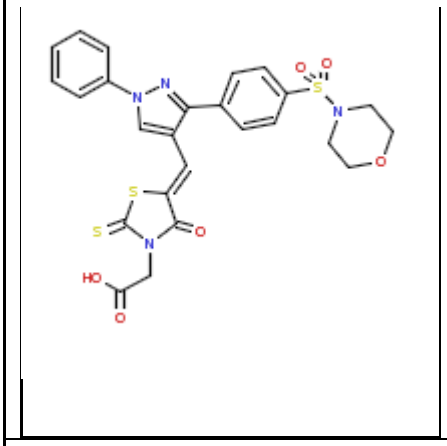
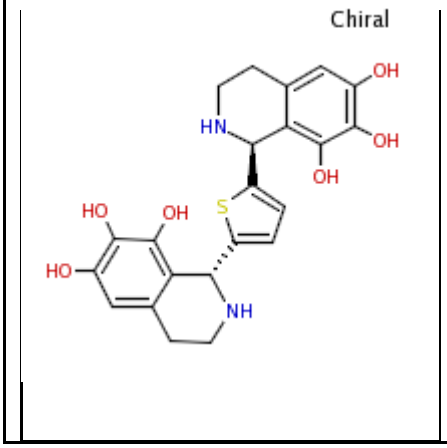
	3.450	7	3	6.28
	3.450	7	46	4.86
	3.580	7	36	4.81

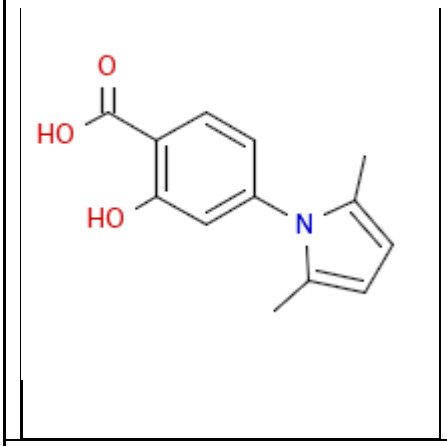
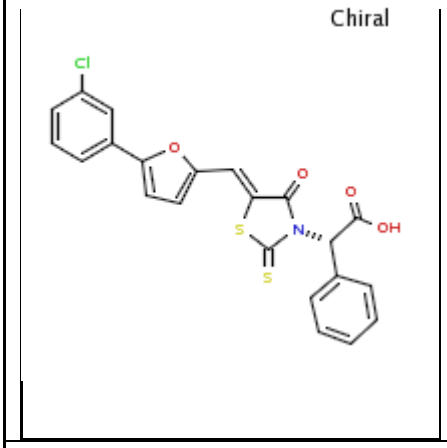
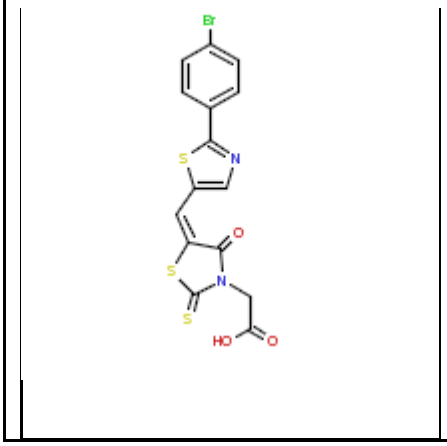
	3.600	12	6	6.98
	3.600	12	7	6.61
	3.660	7	41	5.47

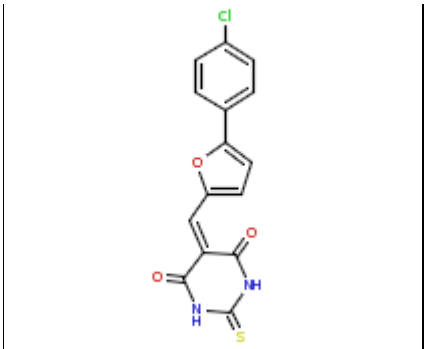
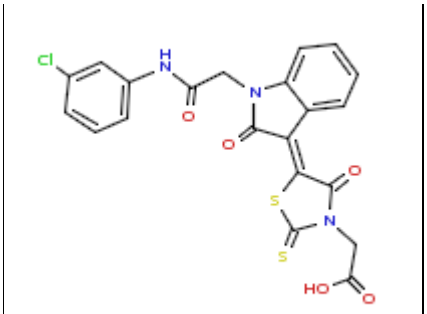
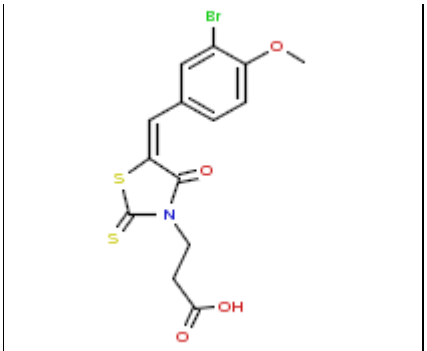
	3.800	14	70	8.01
	3.800	15	18	8.34
	3.890	13	5	7.43

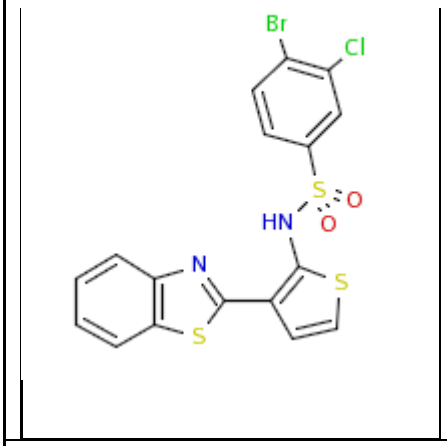
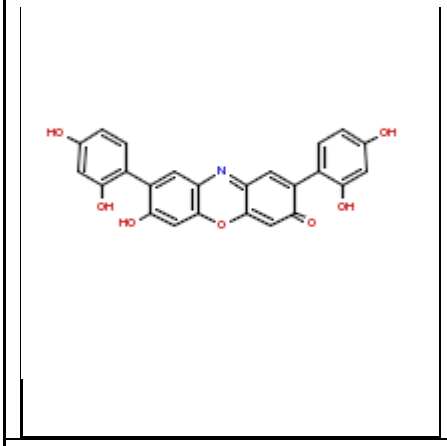
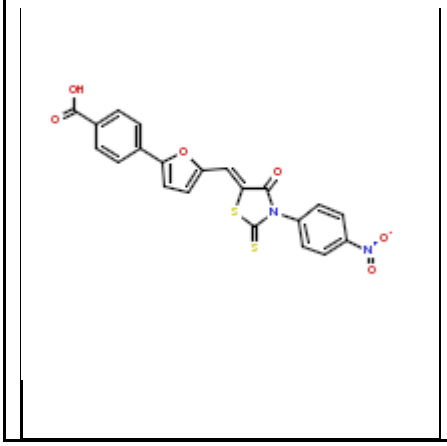
	3.900	14	72	7.91
	3.900	12	8	7.14
	3.980	7	5	6.08

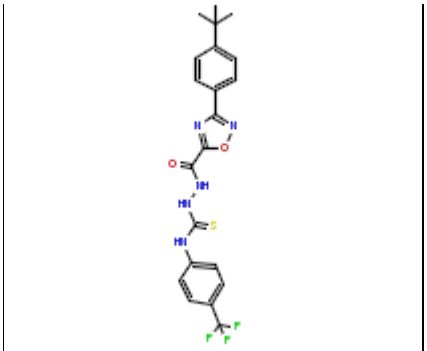
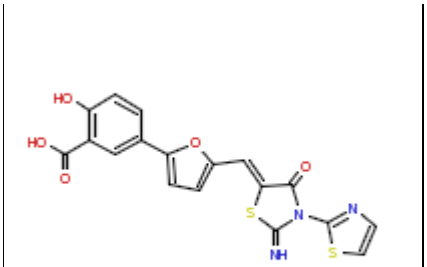
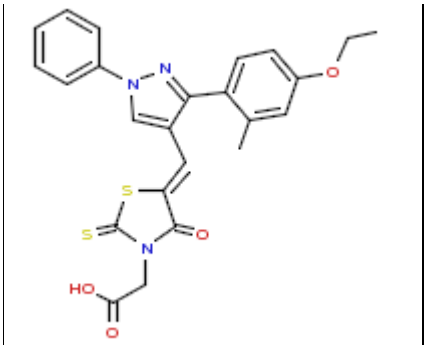
	4.100	4	8e	7.76
	4.200	14	2	10.76
	4.200	12	9	4.91

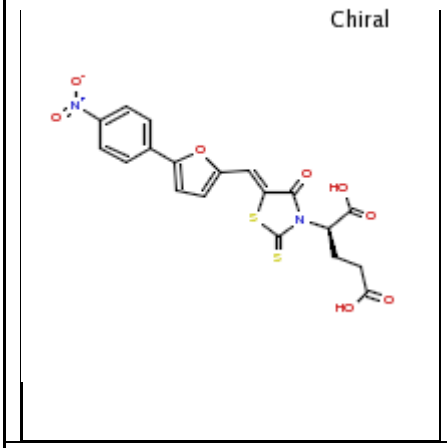
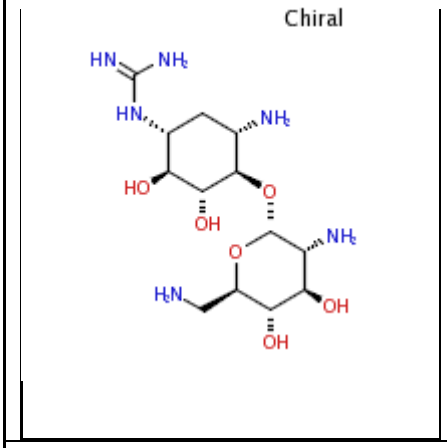
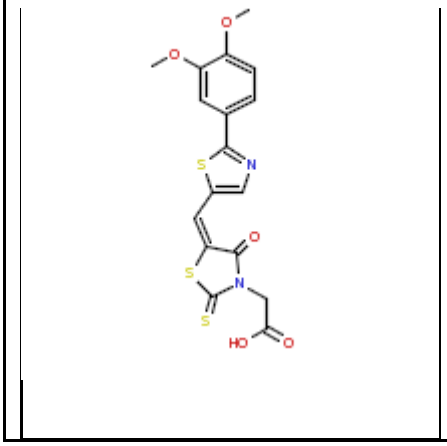
	4.220	7	33	7.92
	4.260	7	31	6.20
	4.300	16	5a	5.63

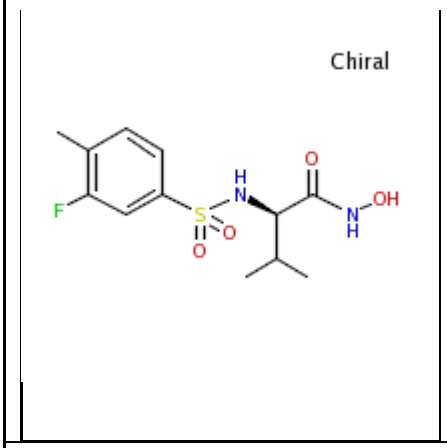
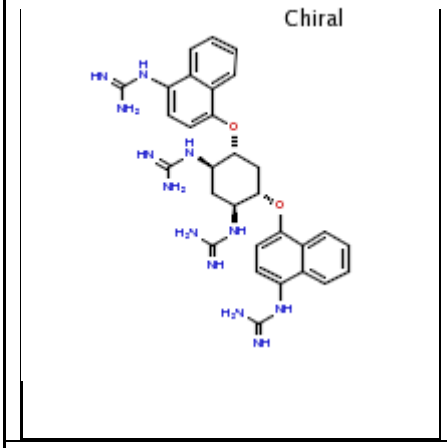
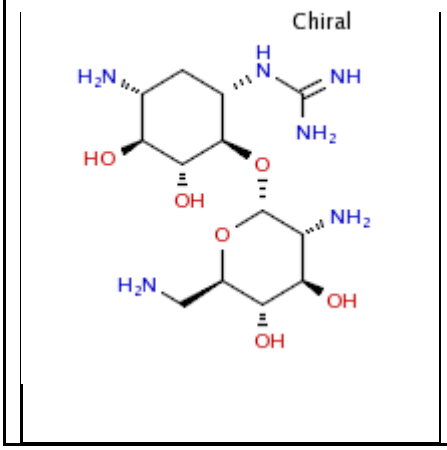
	4.300	12	10	5.18
	4.340	7	8	6.19
	4.400	10	16	5.40

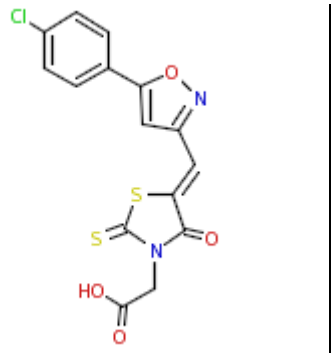
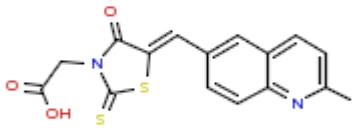
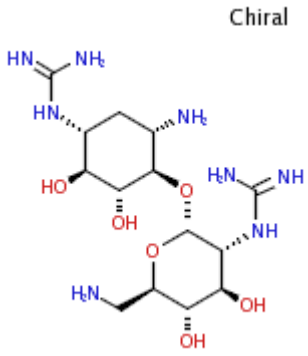
	4.400	10	25	4.73
	4.400	7	62	5.47
	4.400	12	11	6.50

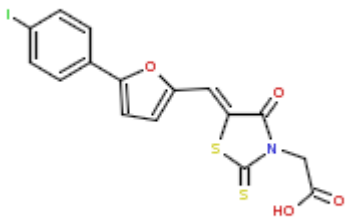
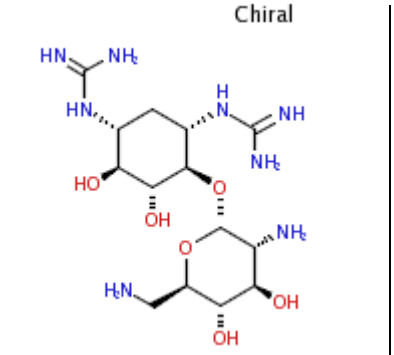
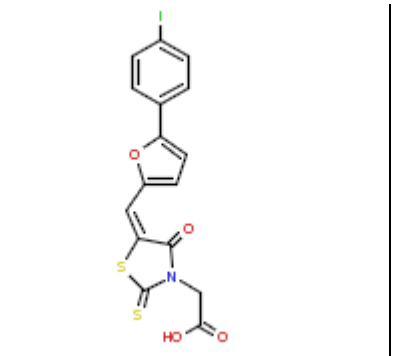
	4.500	14	123	6.50
	4.500	16	2	6.63
	4.800	8	16	4.68

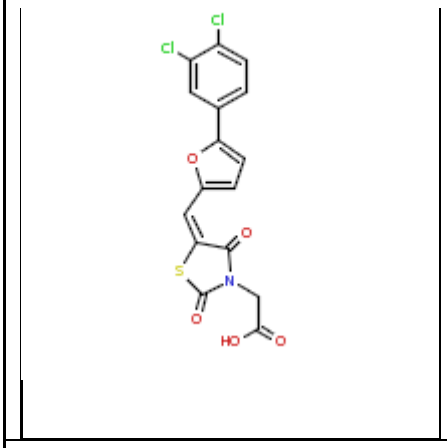
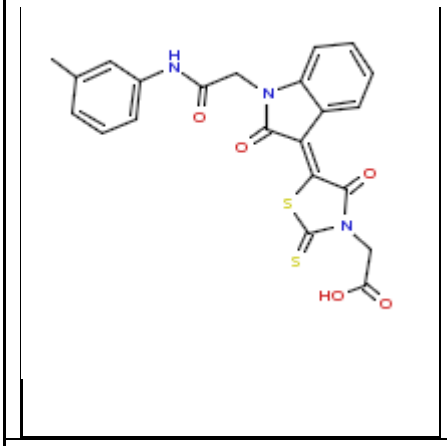
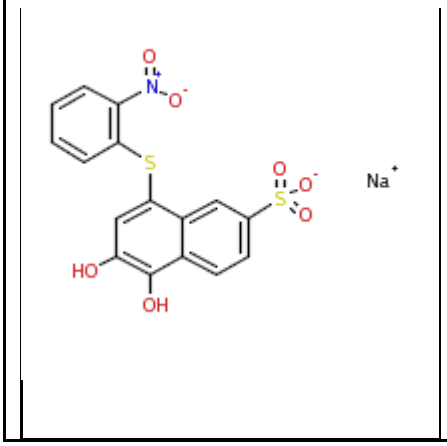
	4.800	14	3	7.08
	4.800	12	12	4.29
	4.870	7	37	6.46

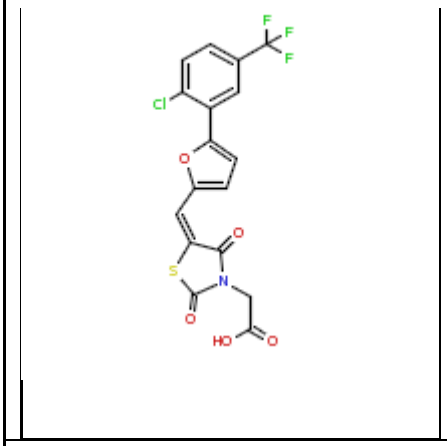
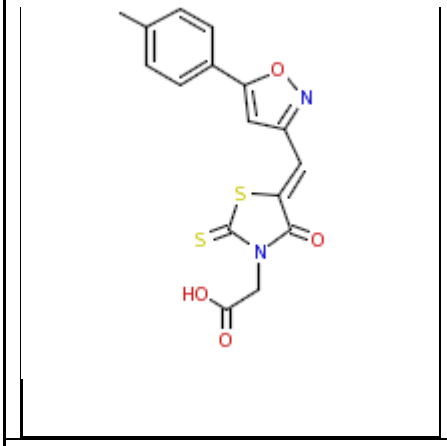
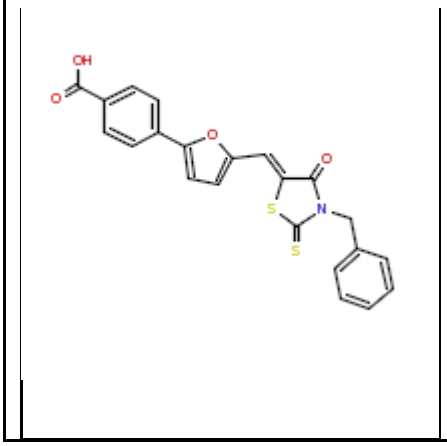
	4.910	7	6	6.36
	5.000	9	9	5.83
	5.000	10	15	6.59

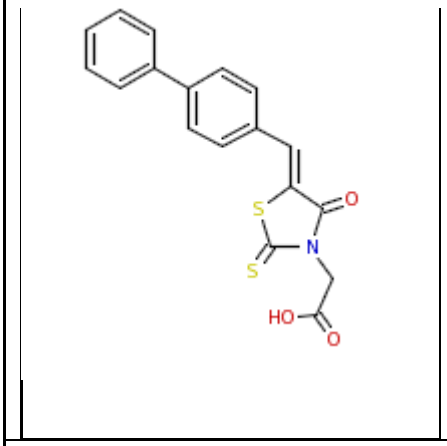
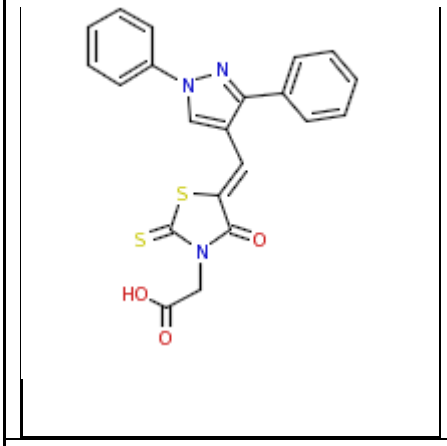
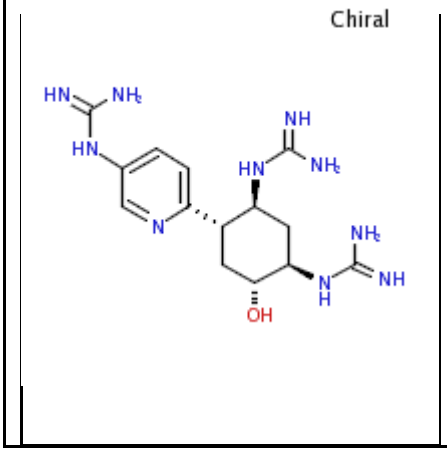
	5.180	3	18	9.42
	5.188	4	1f	5.74
	5.200	9	11	8.36

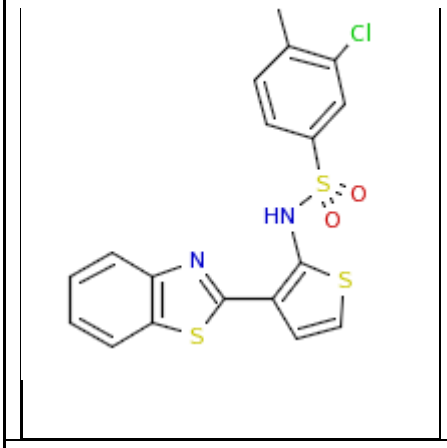
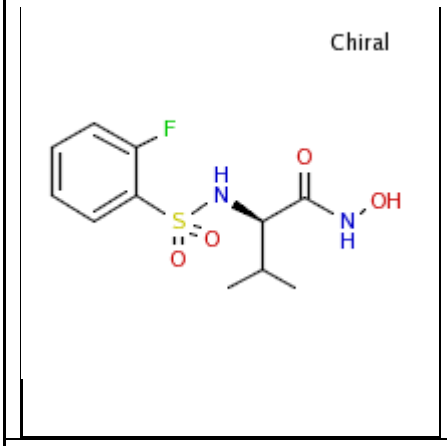
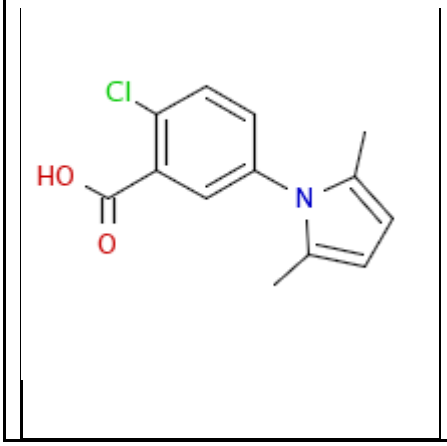
	5.200	7	24	6.40
	5.260	7	54	4.92
	5.300	9	20	8.92

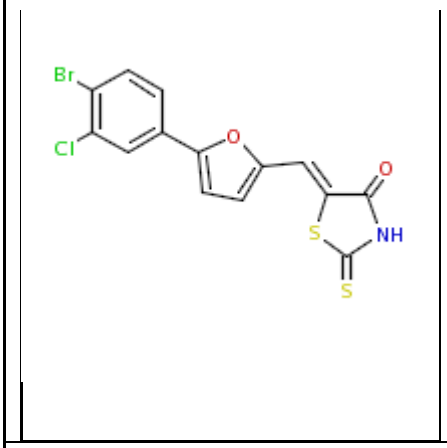
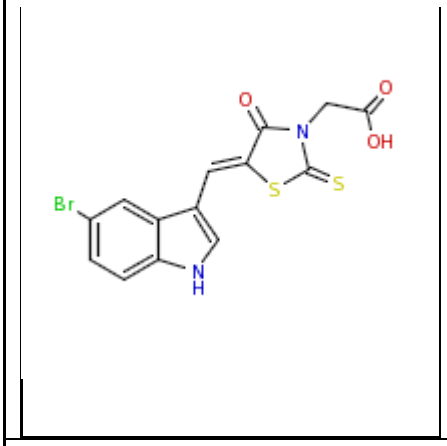
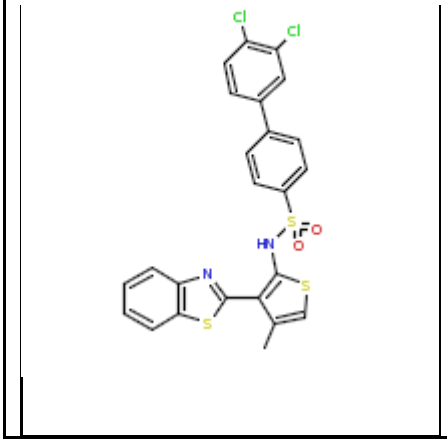
	5.500	8	15	6.01
	5.600	9	19	7.11
	5.600	10	2	5.76

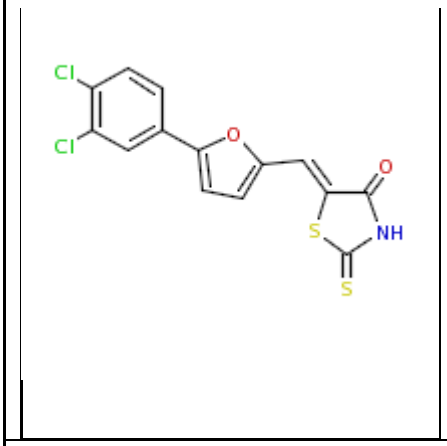
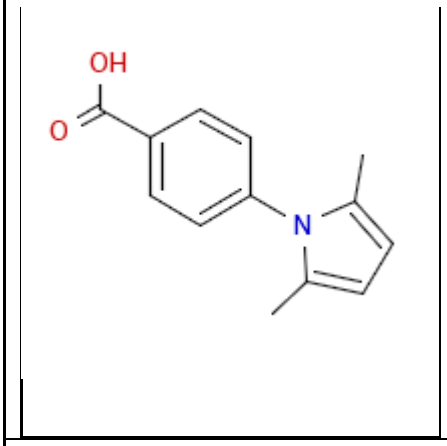
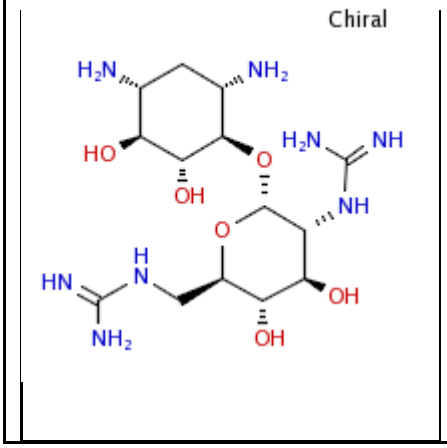
	5.600	10	28	6.22
	5.710	7	63	6.28
	5.890	13	4	8.06

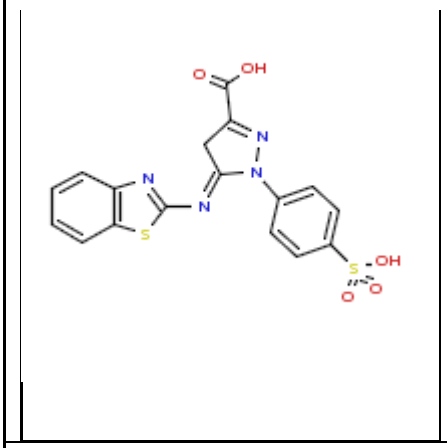
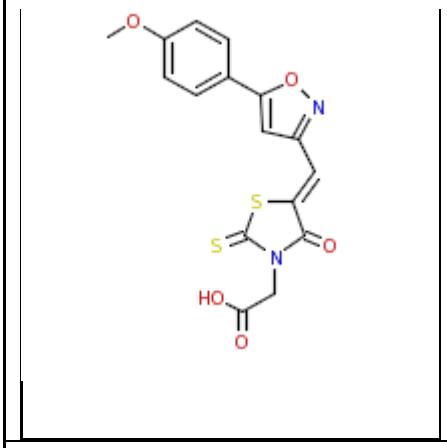
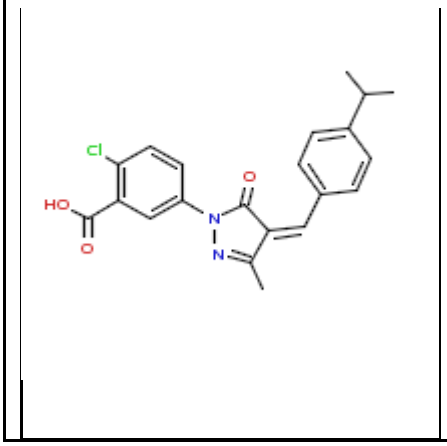
	5.900	10	17	6.97
	5.900	7	22	6.63
	6.000	8	14	5.51

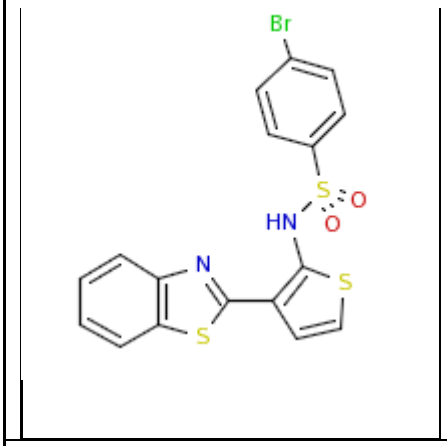
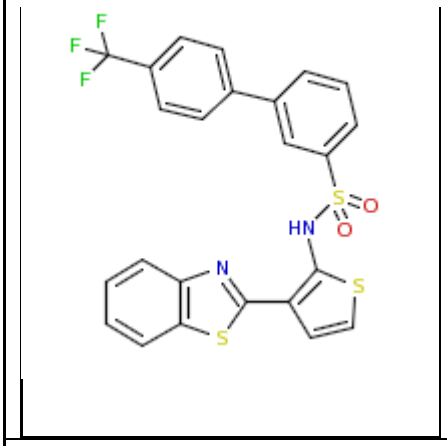
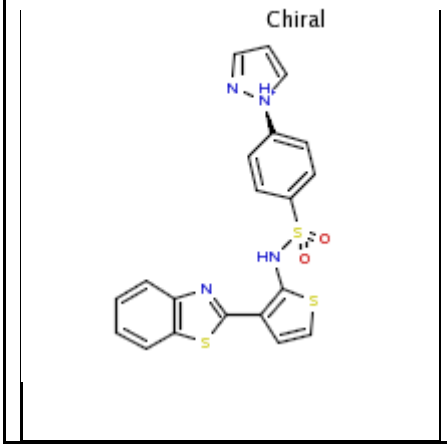
	6.200	7	49	5.62
	6.250	7	30	8.36
	6.600	4	8d	10.03

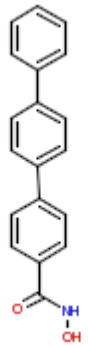
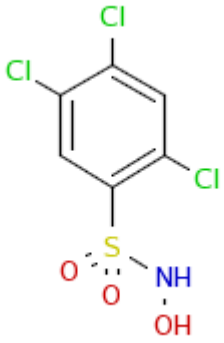
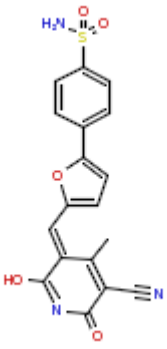
	6.600	14	55	6.47
	6.600	3	11	8.62
	6.800	12	57	4.60

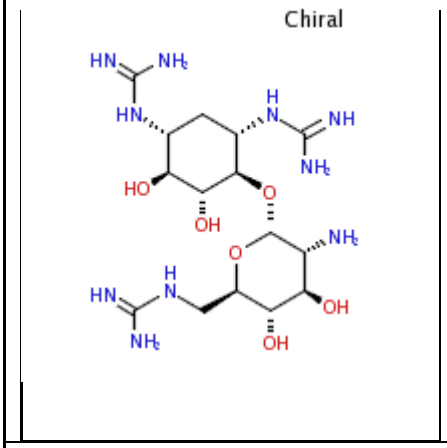
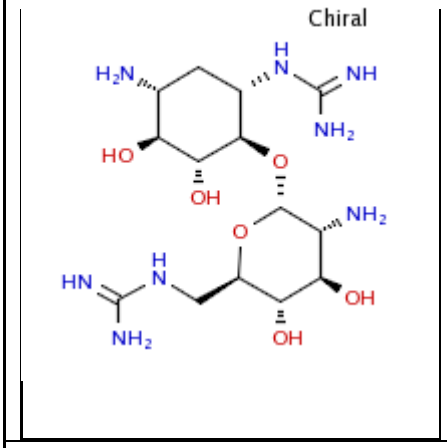
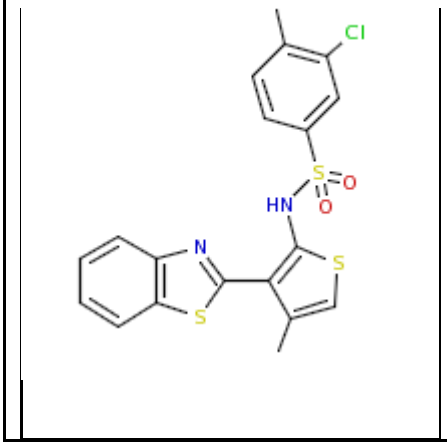
	7.000	8	13	4.01
	7.040	7	61	6.80
	7.200	14	75	7.05

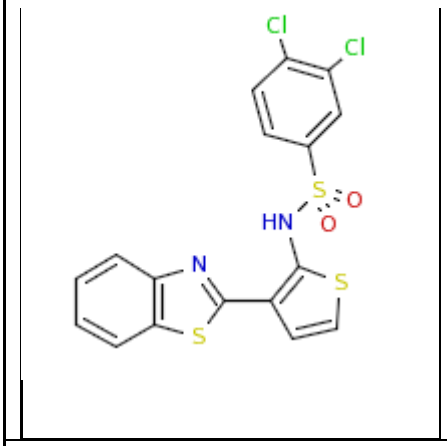
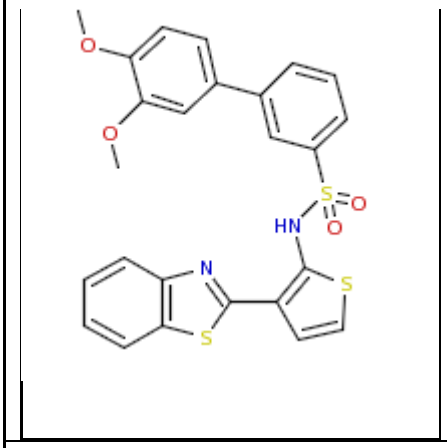
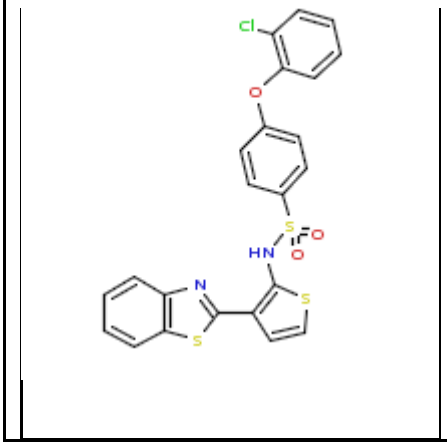
	7.400	8	12	4.09
	7.600	12	58	5.40
	7.700	9	22	8.63

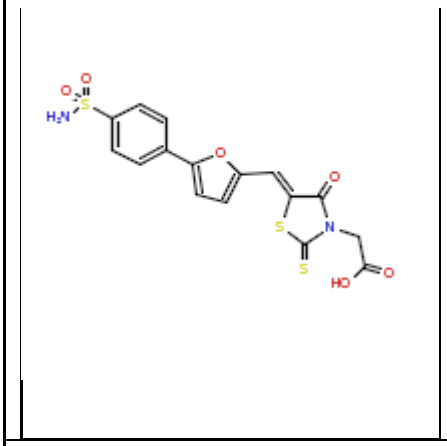
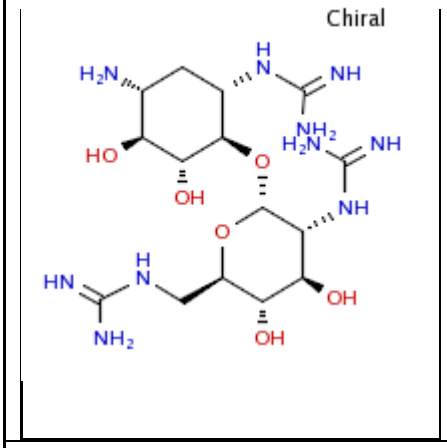
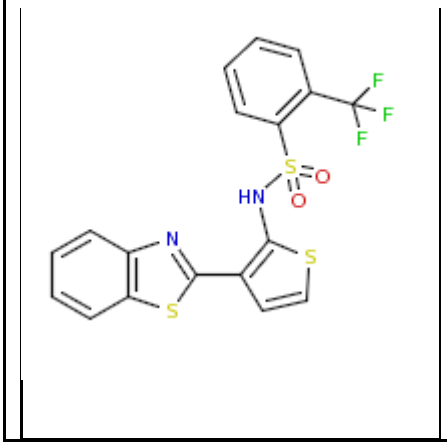
	7.700	12	13	5.34
	7.800	7	23	7.58
	7.900	12	14	6.96

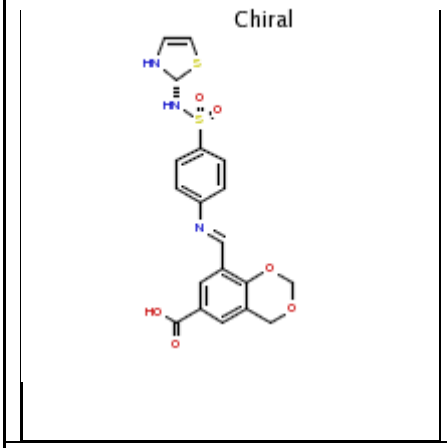
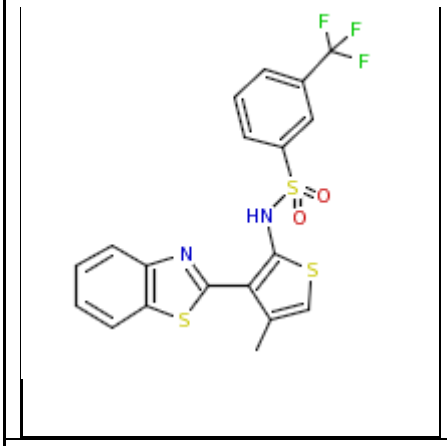
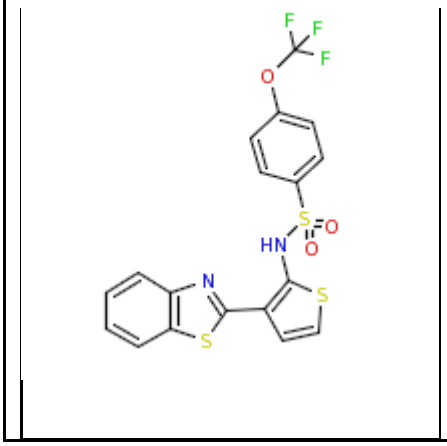
	8.000	14	68	6.49
	8.000	14	77	6.76
	8.000	14	85	6.54

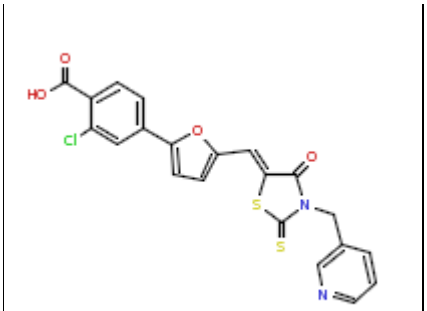
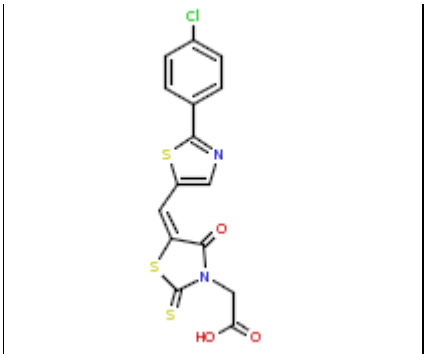
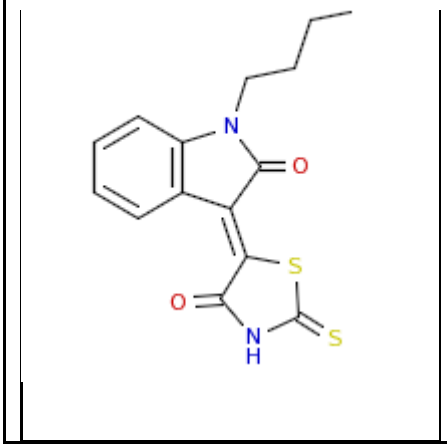
	8.000	6	1	6.63
	8.300	6	2	5.34
	8.300	12	15	7.73

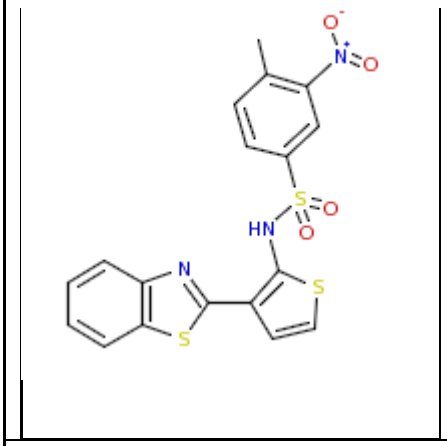
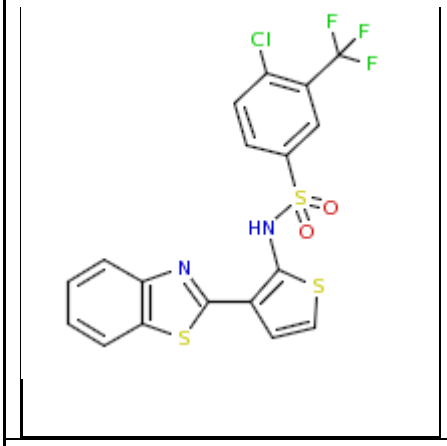
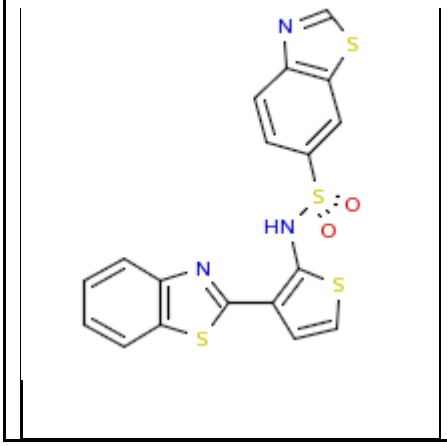
	8.700	9	16	8.60
	8.800	9	15	7.64
	8.900	14	21	6.24

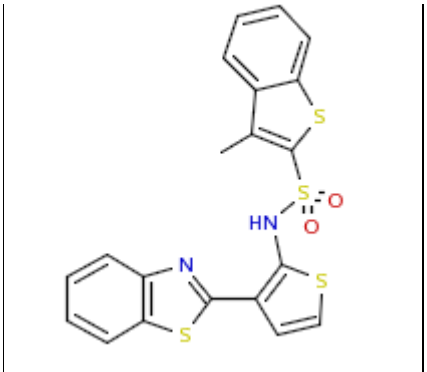
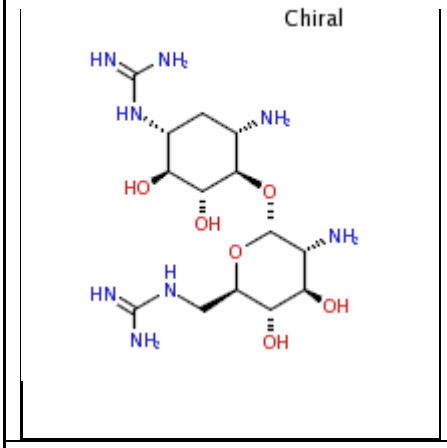
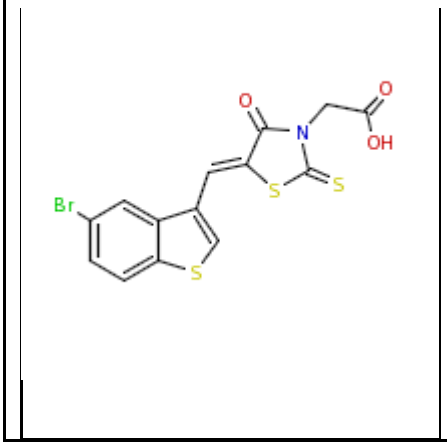
	9.000	14	60	6.61
	9.000	14	78	6.57
	9.000	14	79	6.91

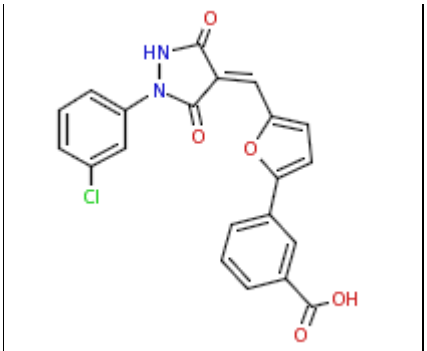
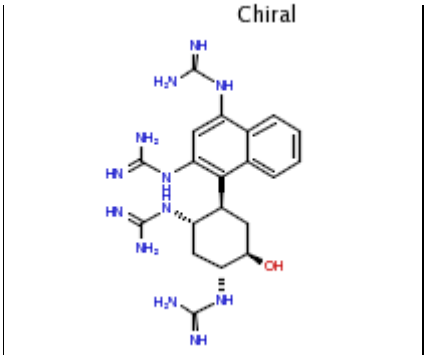
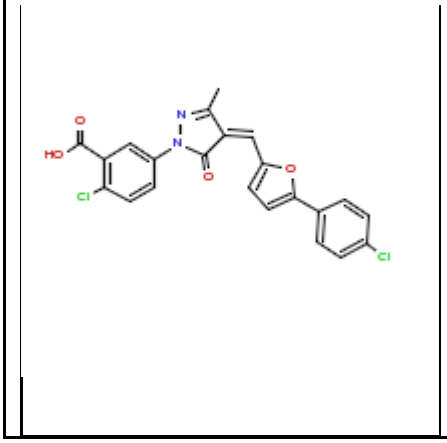
	9.100	8	11	7.45
	9.200	9	25	8.81
	9.300	14	45	5.58

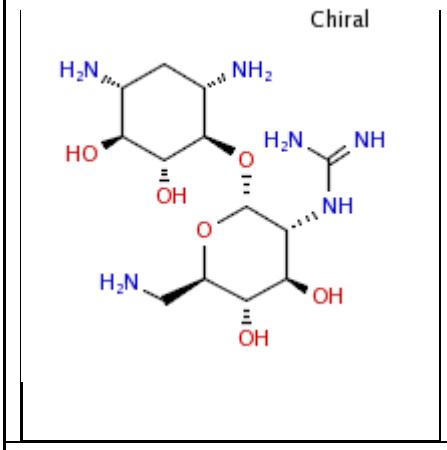
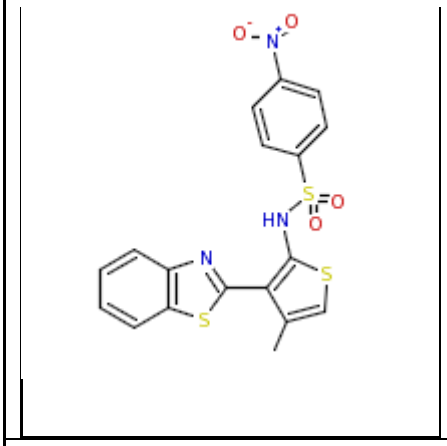
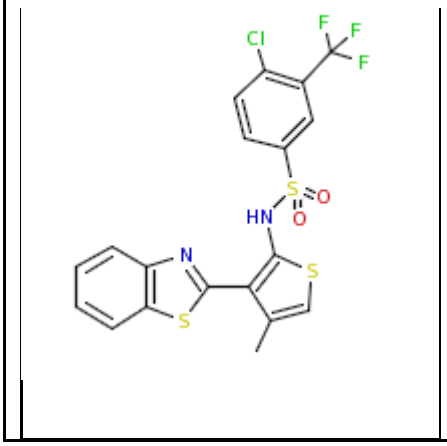
	9.300	12	16	6.45
	9.400	14	10	6.48
	9.600	14	46	6.53

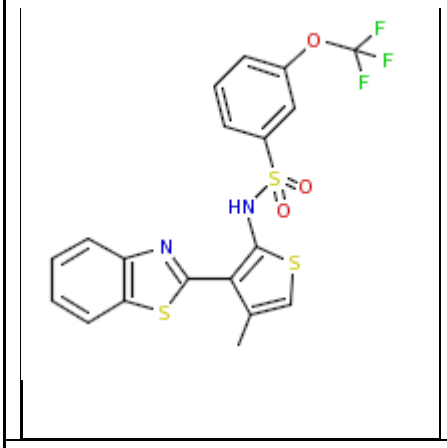
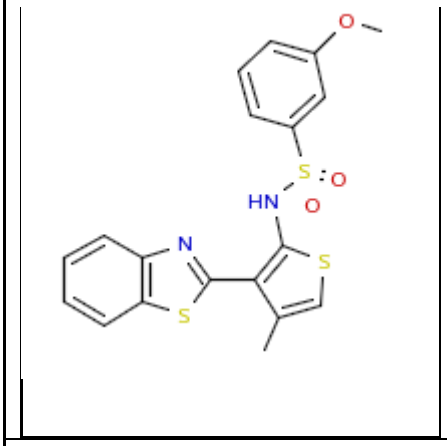
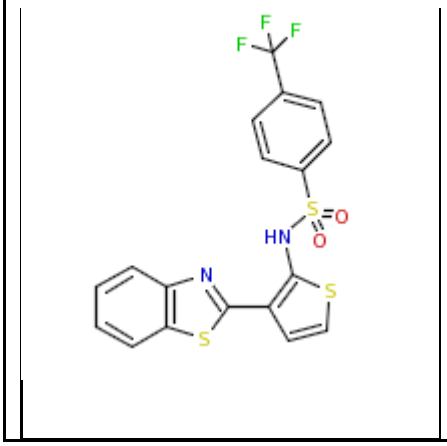
	9.900	8	10	6.27
	10.000	10	14	5.64
	10.000	13	3	4.02

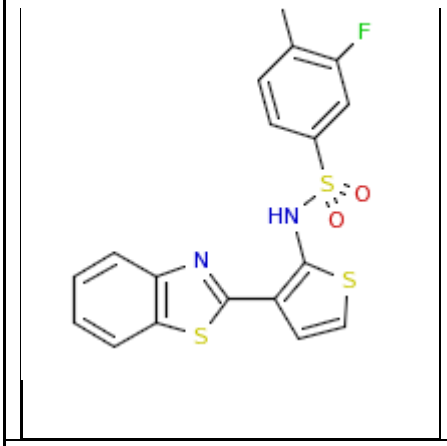
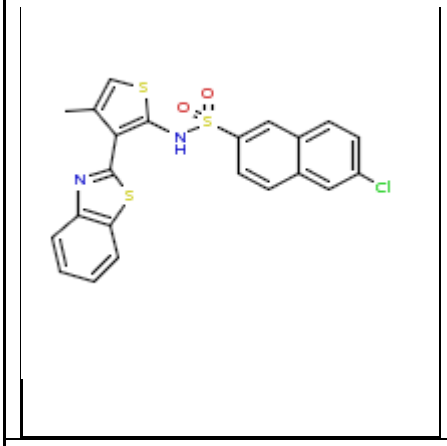
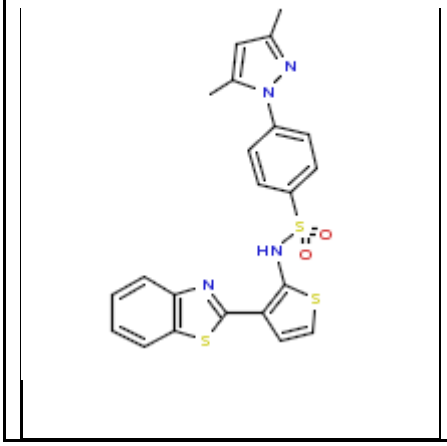
	10.000	14	63	5.86
	10.000	14	64	6.52
	10.000	14	92	6.86

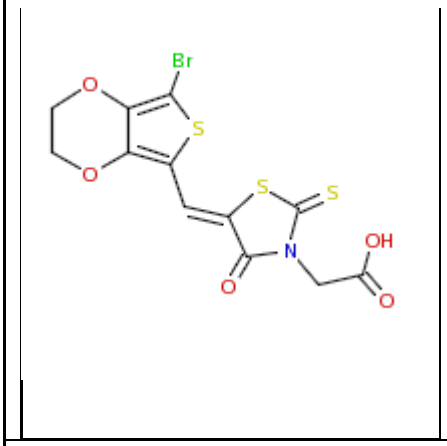
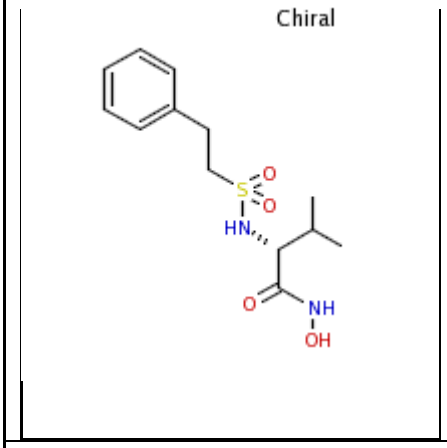
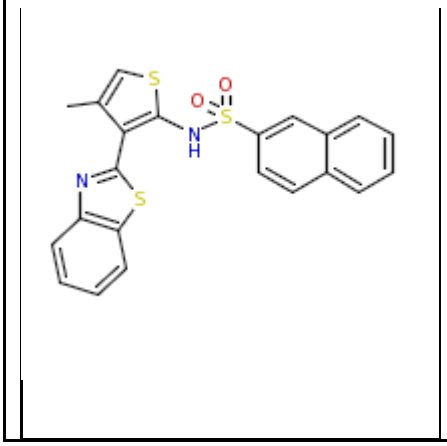
	10.000	14	96	6.83
	10.200	9	14	7.56
	10.400	7	58	4.49

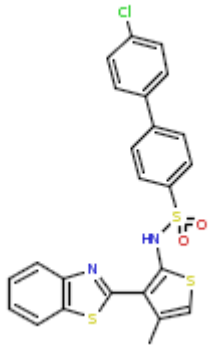
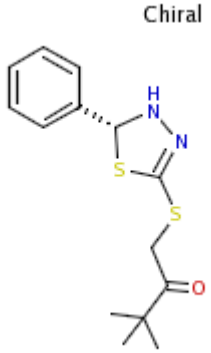
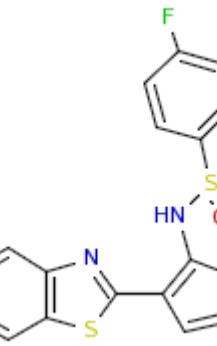
	10.500	12	17	7.59
Chiral 	10.700	4	8g	3.55
	10.700	12	18	6.73

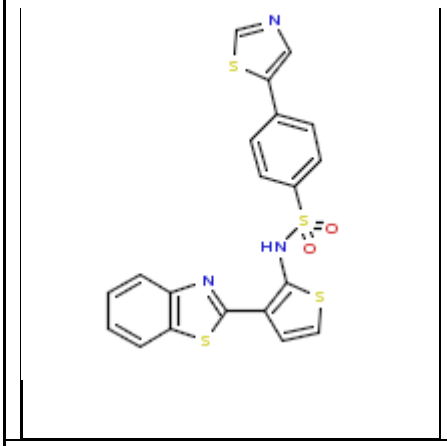
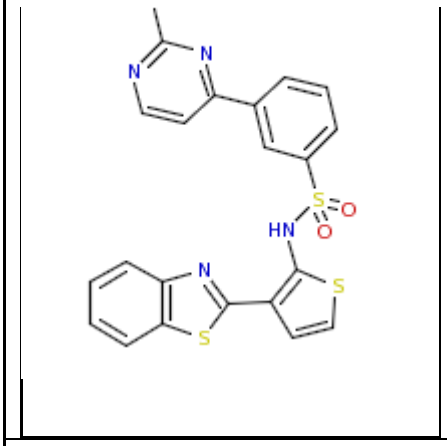
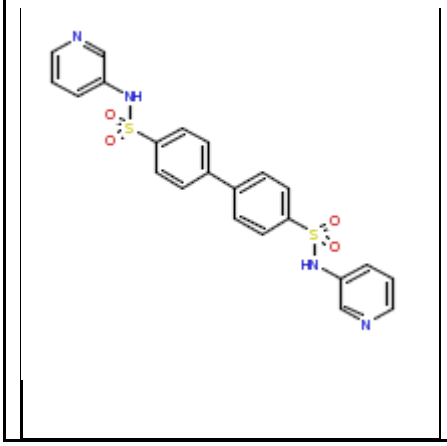
	10.900	9	13	8.04
	11.000	14	17	7.79
	11.000	14	30	6.25

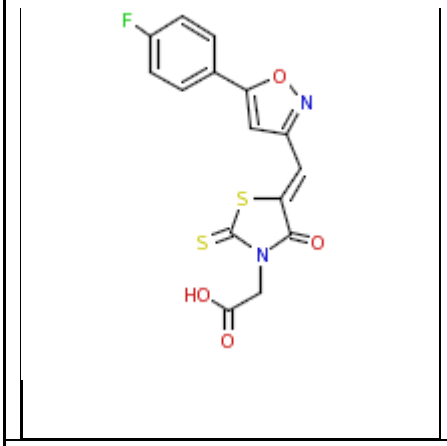
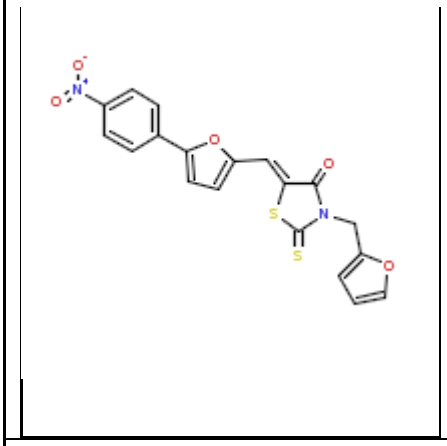
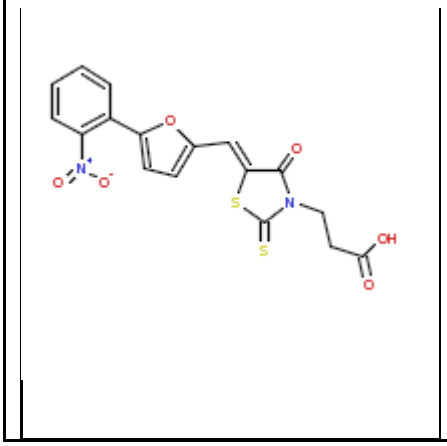
	11.000	14	32	7.08
	11.000	14	33	6.50
	11.000	14	51	6.43

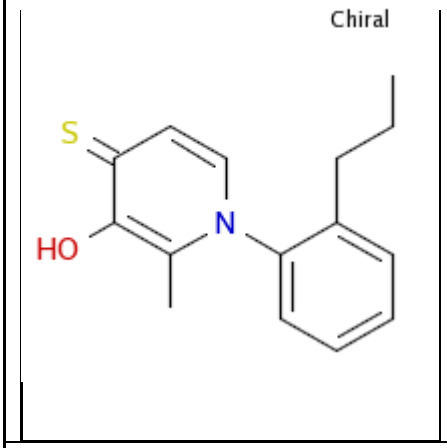
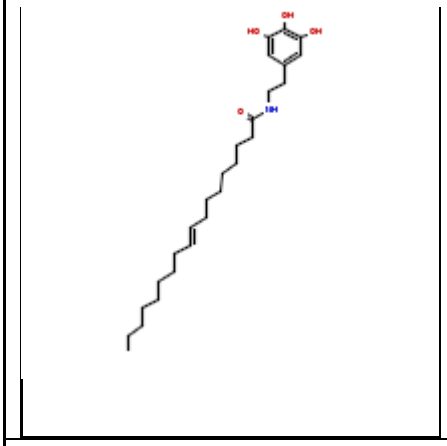
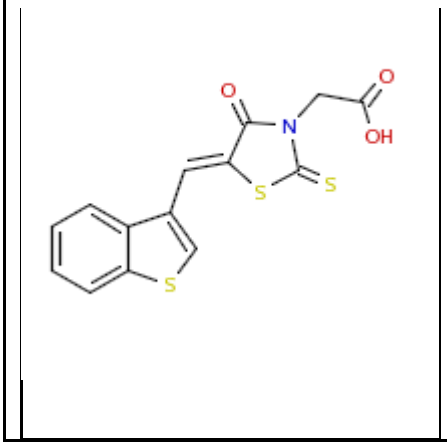
	11.000	14	53	6.37
	11.000	14	67	7.04
	11.000	14	89	6.22

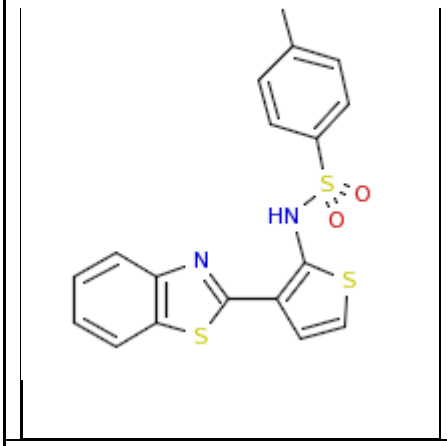
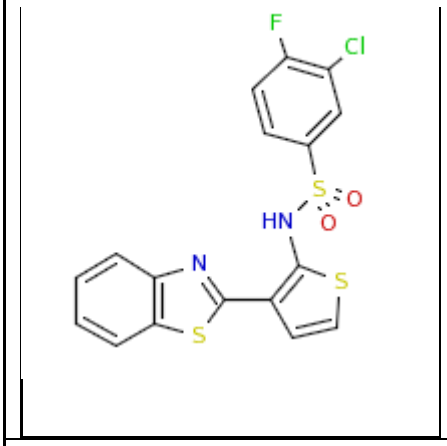
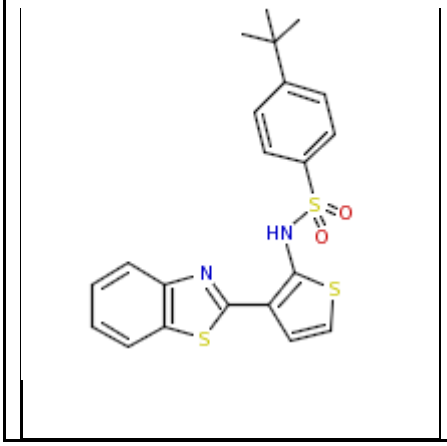
	11.400	7	47	4.87
	11.880	3	19	11.05
	12.000	14	34	7.22

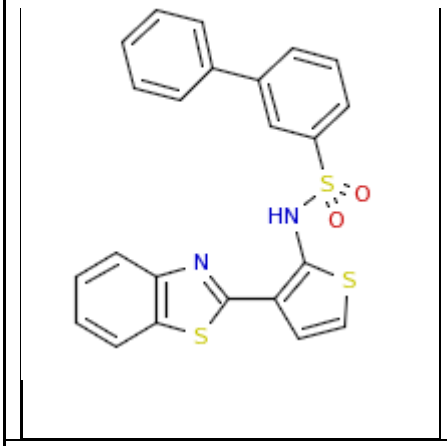
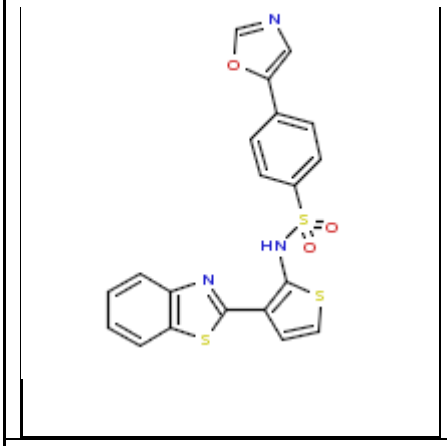
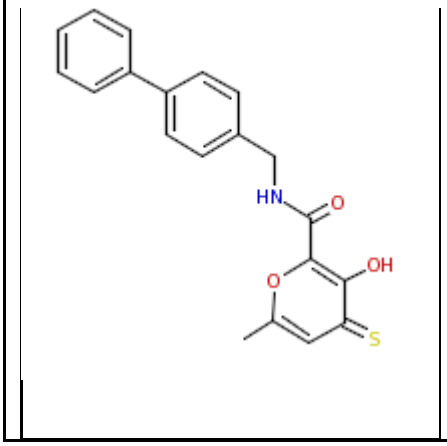
	12.000	14	37	7.29
	12.000	14	4	5.95
	12.000	14	54	6.83

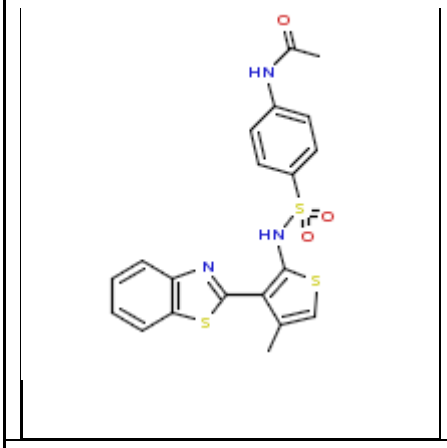
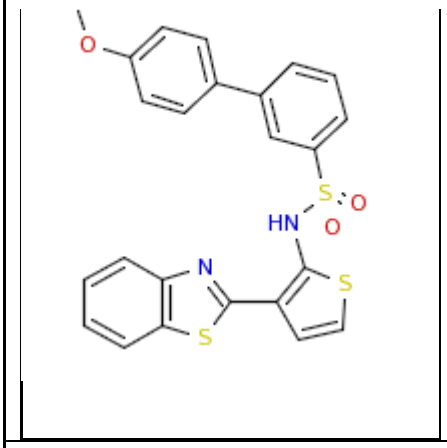
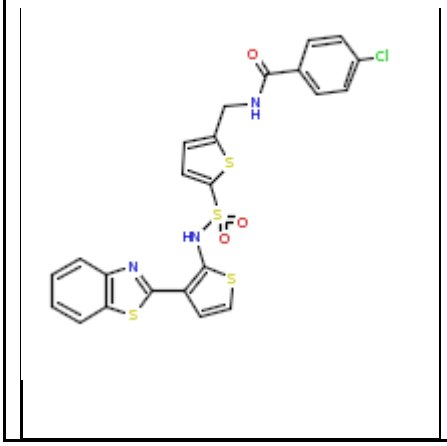
	12.000	14	82	7.17
	12.000	14	88	7.42
	12.000	15	8	8.19

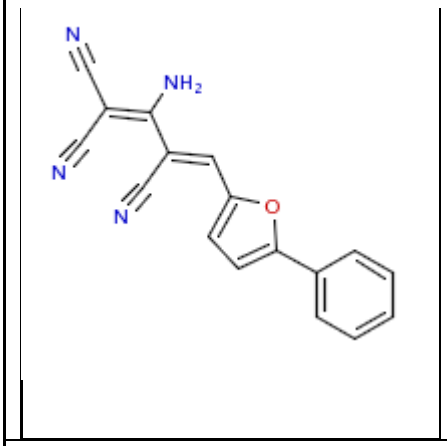
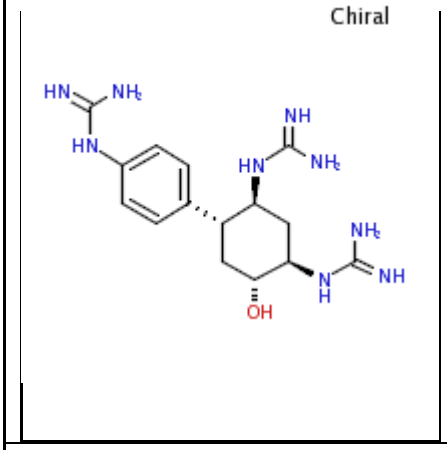
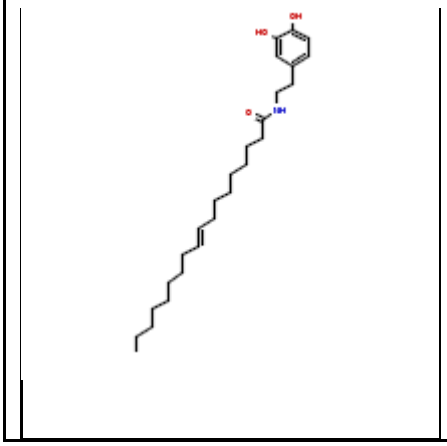
	12.400	7	25	6.48
	12.600	8	9	5.42
	12.800	8	8	7.02

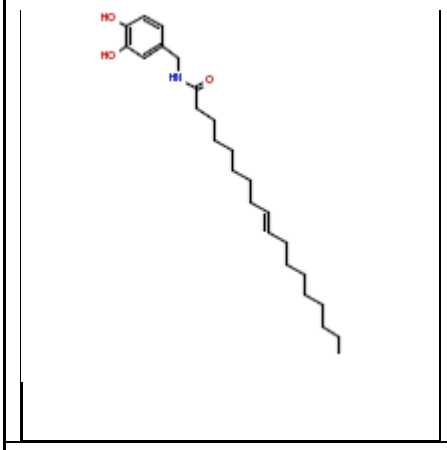
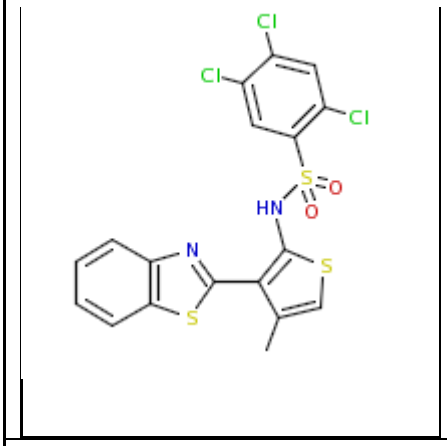
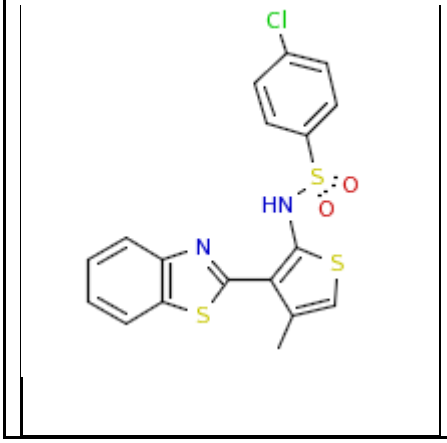
	13.000	17	94F8	6.72
	13.000	18	4	10.75
	13.000	7	57	4.82

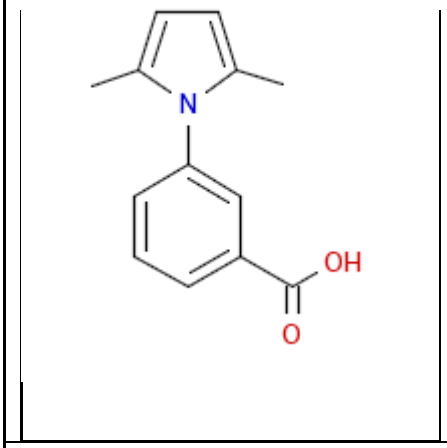
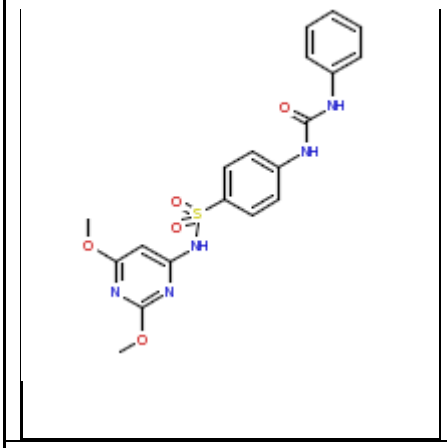
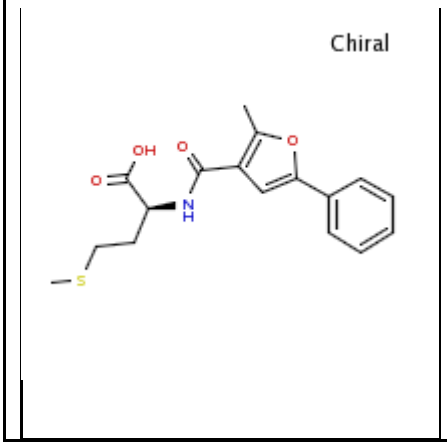
	13.000	14	48	6.56
	13.000	14	57	6.51
	13.000	14	59	7.37

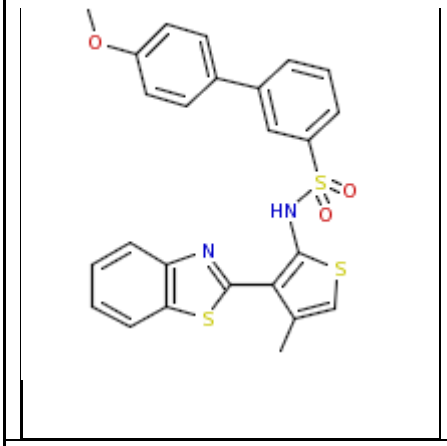
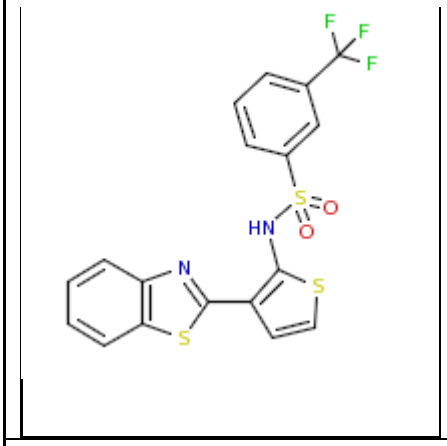
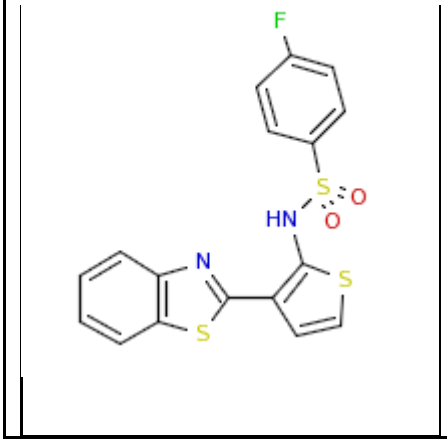
	13.000	14	76	7.81
	13.000	14	83	6.27
	13.900	19	AM-2S	6.28

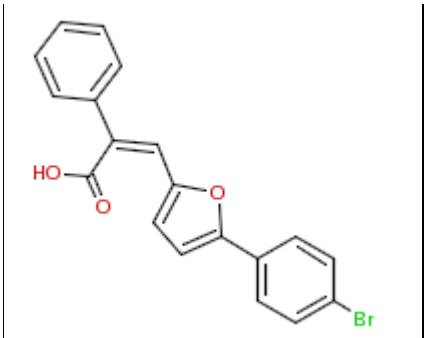
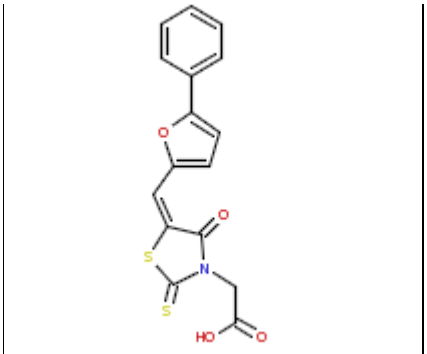
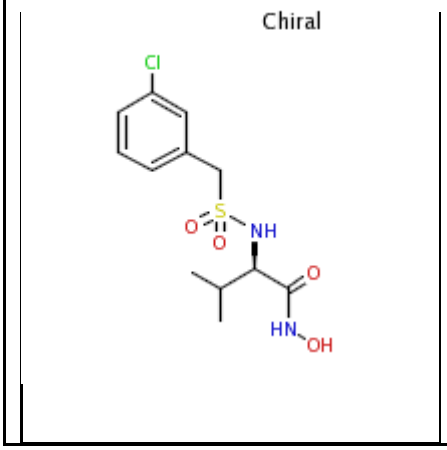
	14.000	14	16	8.00
	14.000	14	73	6.92
	14.000	14	98	7.40

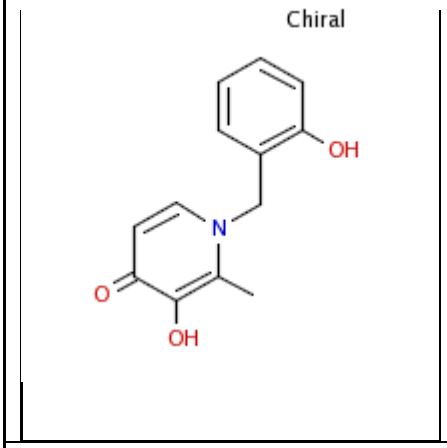
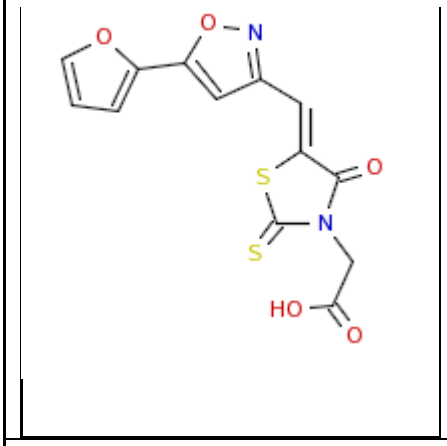
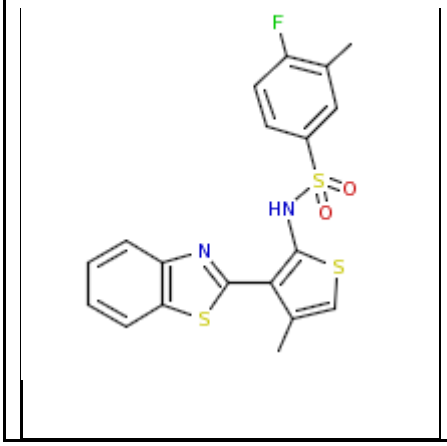
	14.800	12	19	5.27
	14.900	4	8a	9.38
	15.000	18	1	9.78

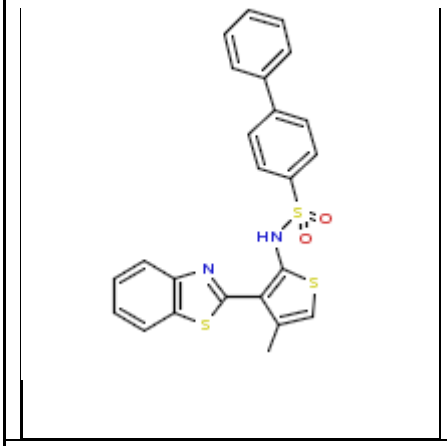
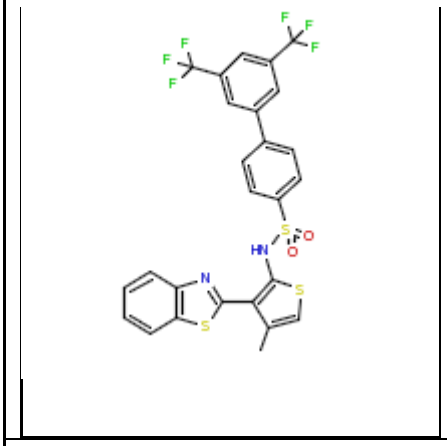
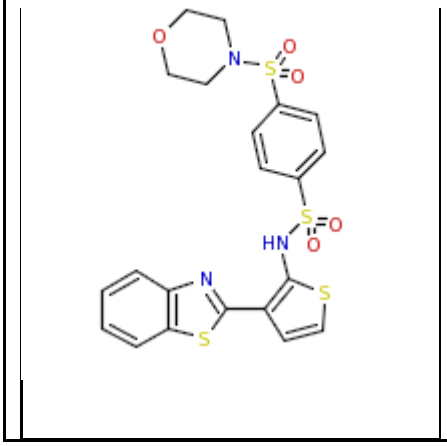
	15.000	20	5	11.56
	15.000	14	22	5.92
	15.000	14	5	6.46

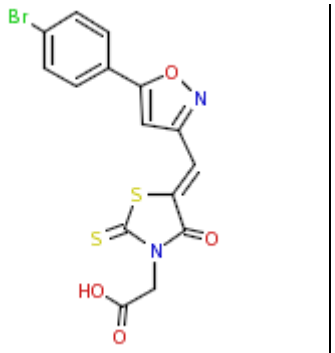
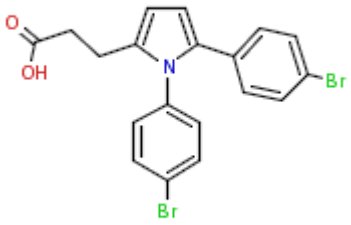
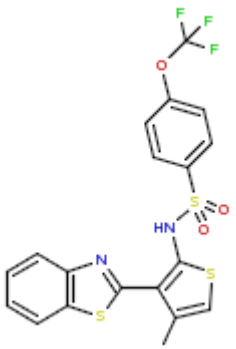
	15.000	12	59	5.13
	15.300	12	Table2_6	8.24
	15.900	12	20	6.51

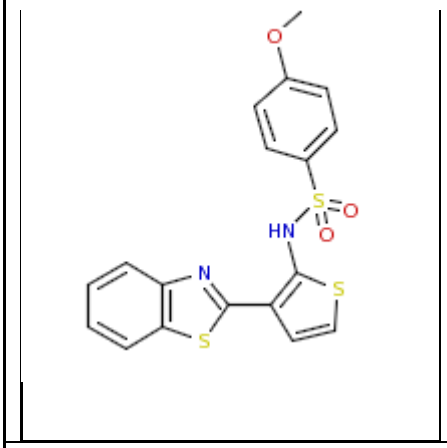
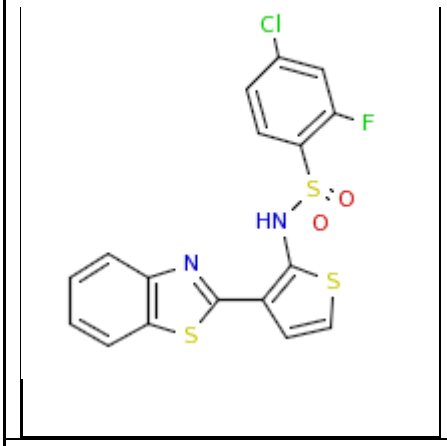
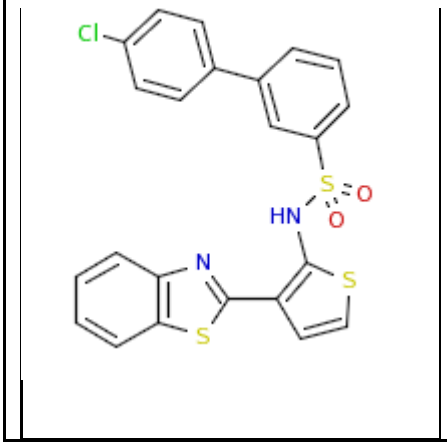
	16.000	14	38	7.09
	16.000	14	44	7.10
	16.000	14	49	6.56

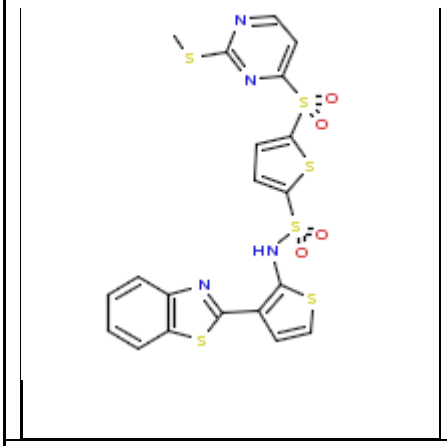
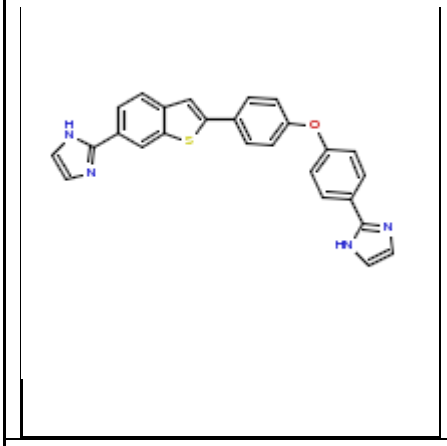
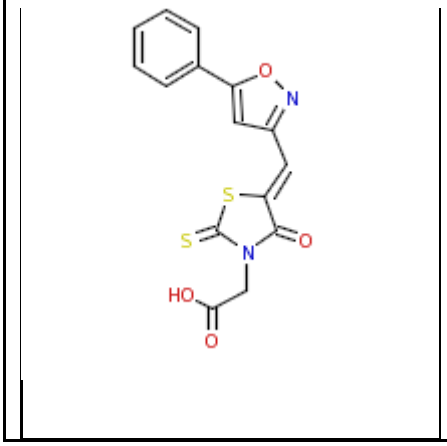
	16.500	12	21	6.54
	16.600	10	26	7.80
Chiral 	16.600	3	20	9.67

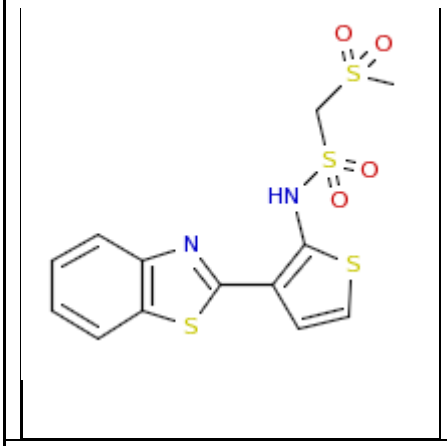
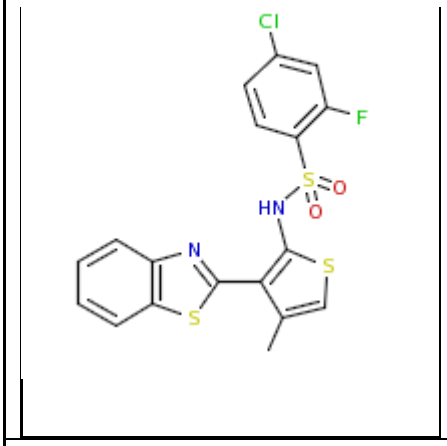
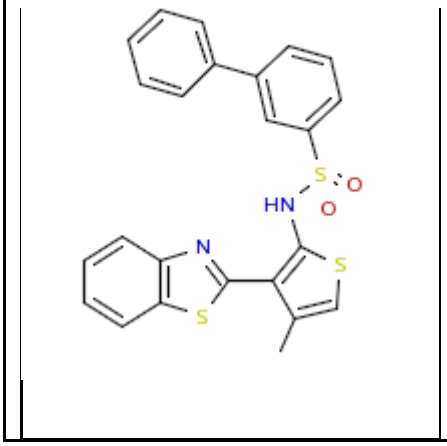
	17.000	17	94D8	6.81
	17.000	7	20	6.27
	17.000	14	20	6.51

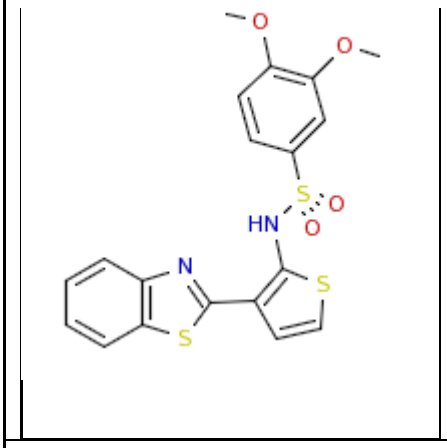
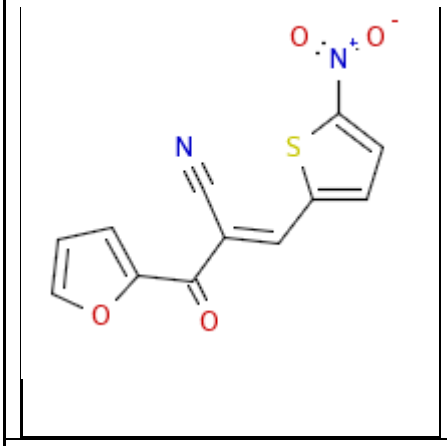
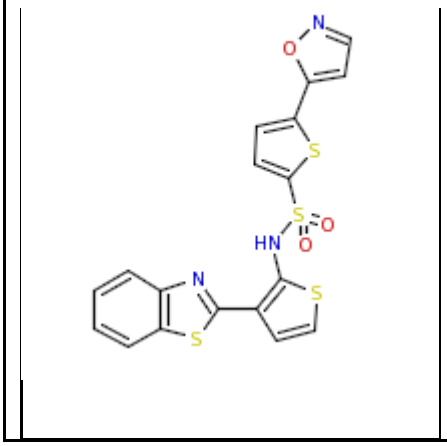
	17.000	14	35	7.53
	17.000	14	40	6.92
	17.000	14	87	7.81

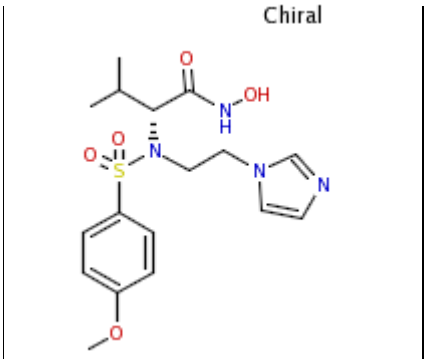
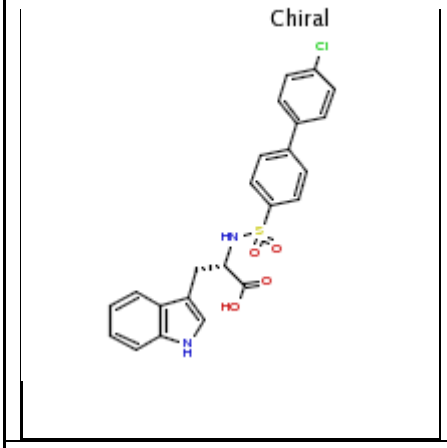
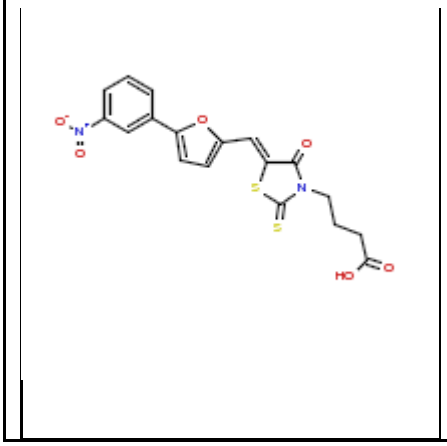
	17.300	7	26	6.43
	17.700	12	60	6.79
	18.000	14	12	7.12

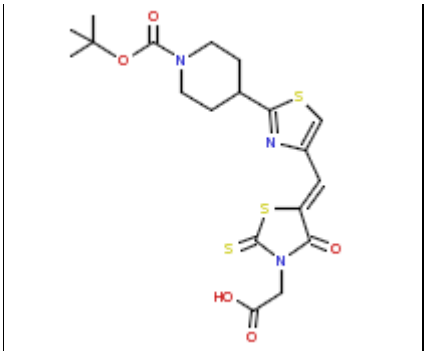
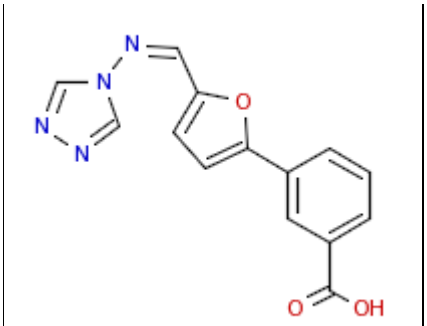
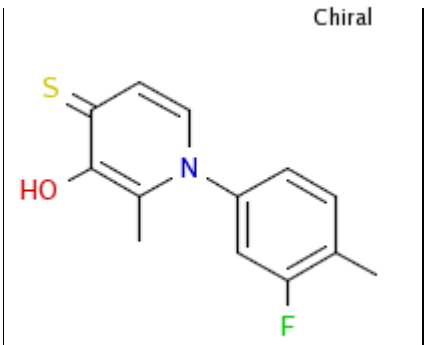
	18.000	14	47	6.23
	18.000	14	52	6.40
	18.000	14	74	7.93

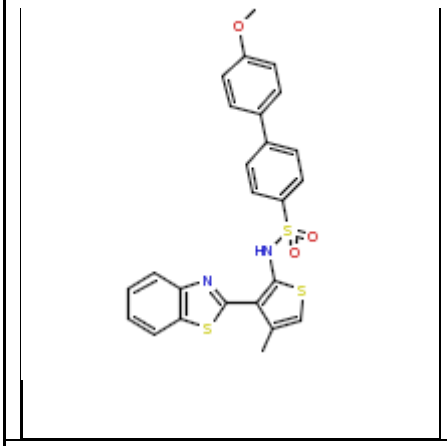
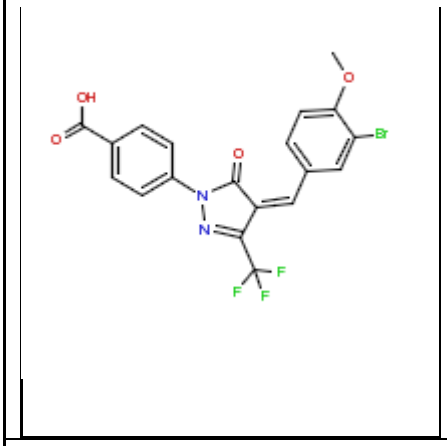
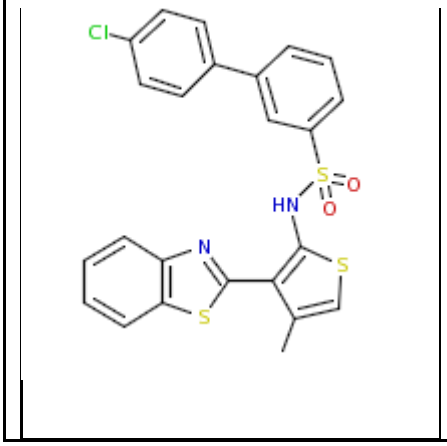
	18.000	14	99	8.80
	18.000	21	25a	6.95
	18.700	7	21	6.48

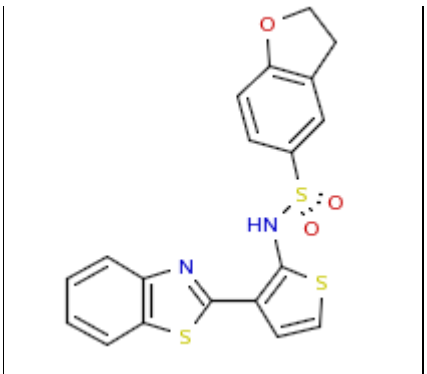
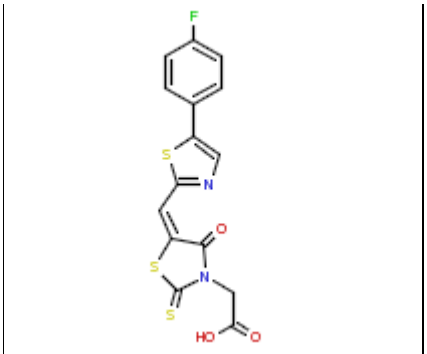
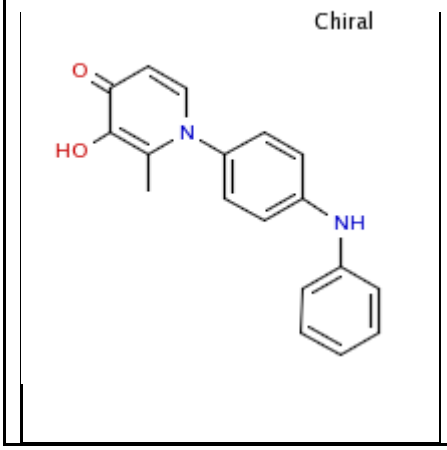
	19.000	14	101	6.57
	19.000	14	18	6.30
	19.000	14	41	8.31

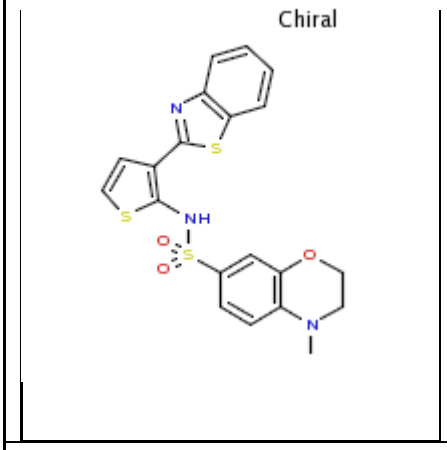
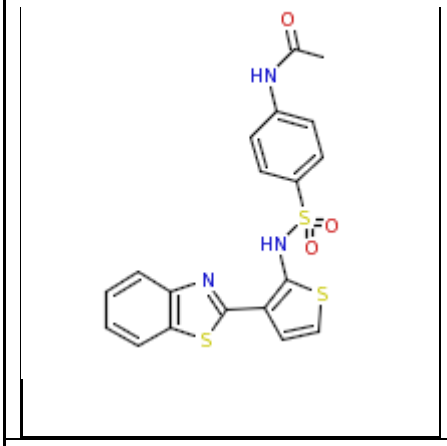
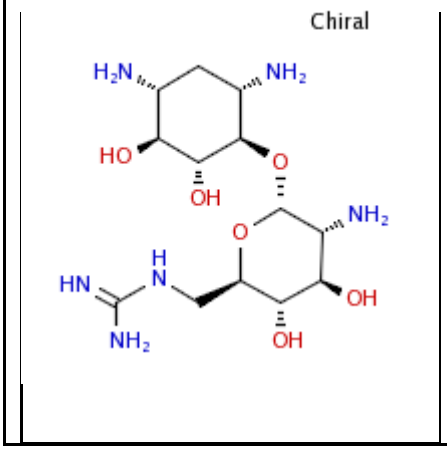
	19.000	14	58	6.37
	19.000	14	6	5.15
	19.000	14	97	8.22

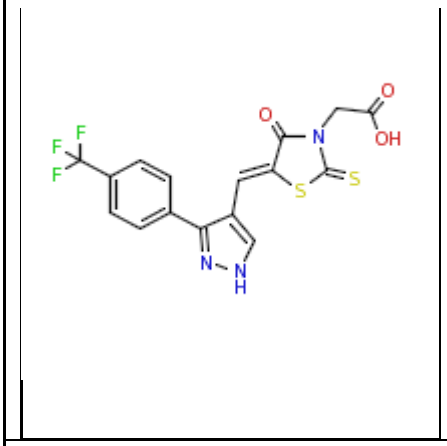
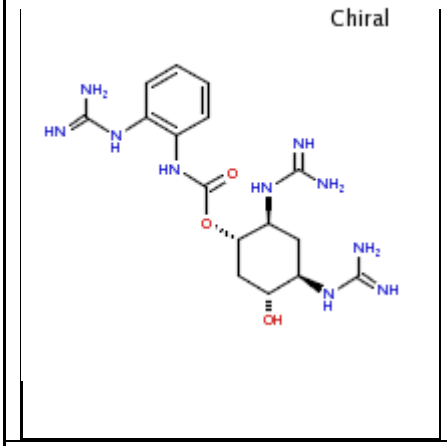
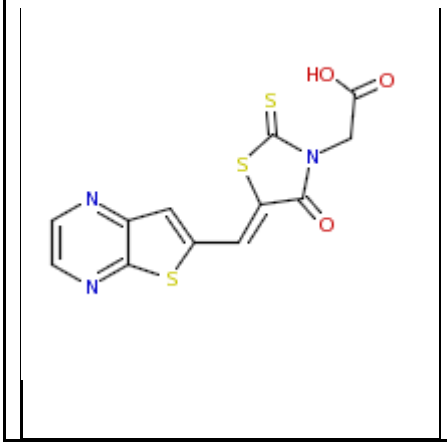
	19.100	3	9	8.08
	19.700	6	16	7.98
	20.000	8	7	6.89

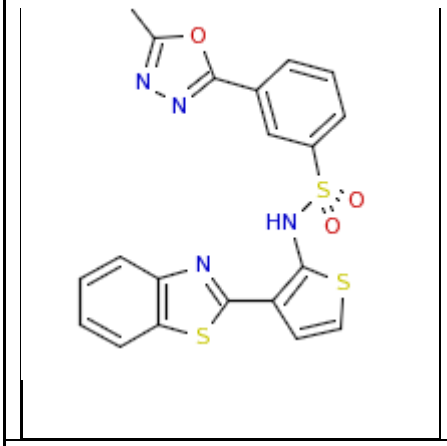
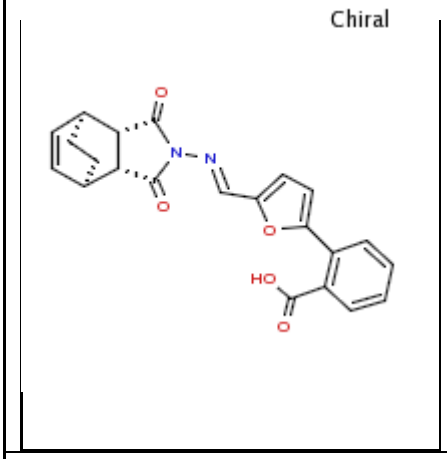
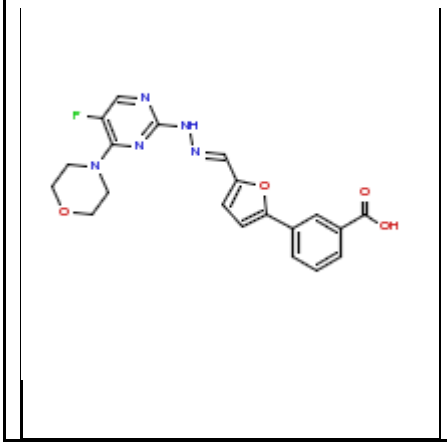
	20.000	7	18	4.40
	20.900	12	22	5.77
	21.000	17	94G10	6.78

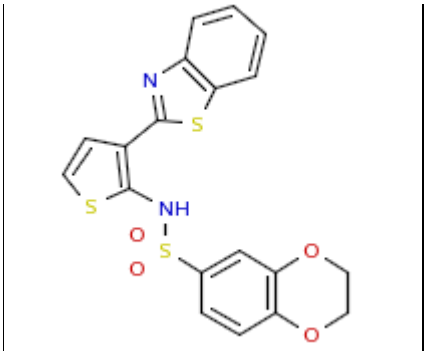
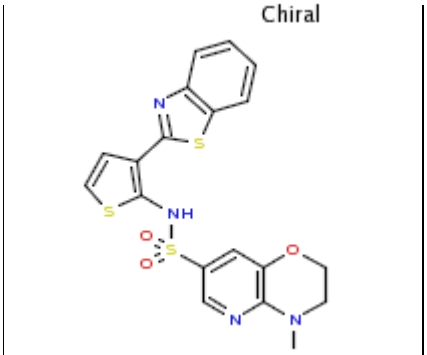
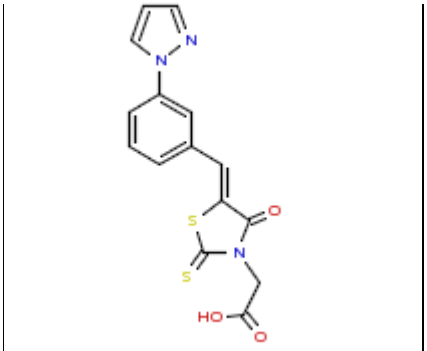
	21.000	14	36	8.29
	21.300	12	45	5.59
	22.000	14	39	8.50

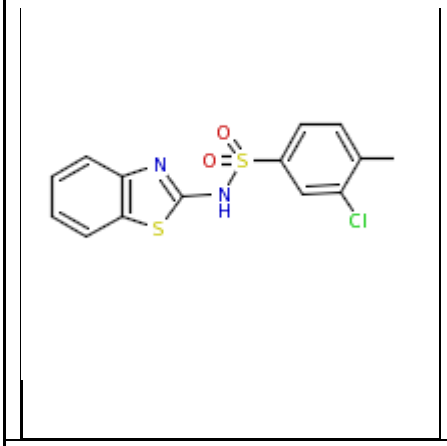
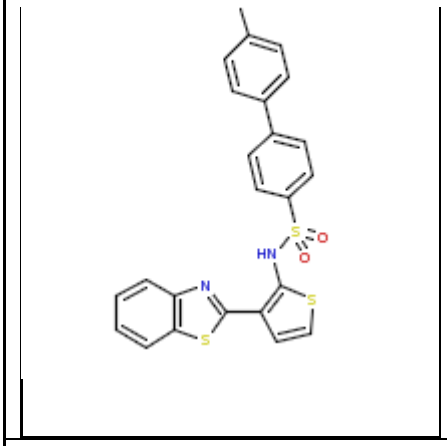
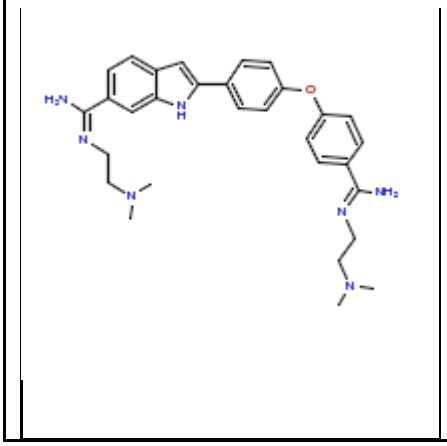
	22.000	14	90	6.49
	22.400	10	27	5.82
	23.000	17	94F10	8.18

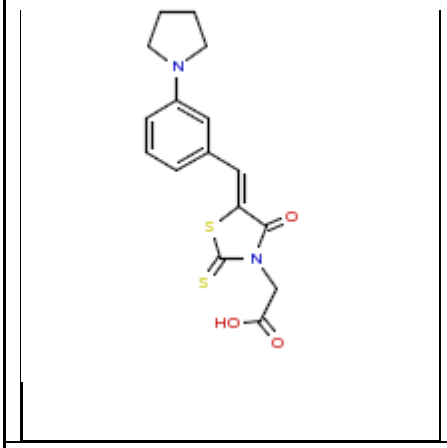
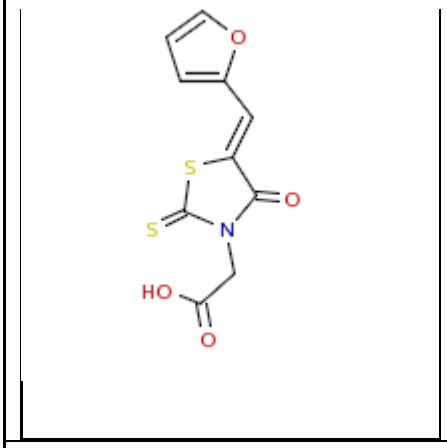
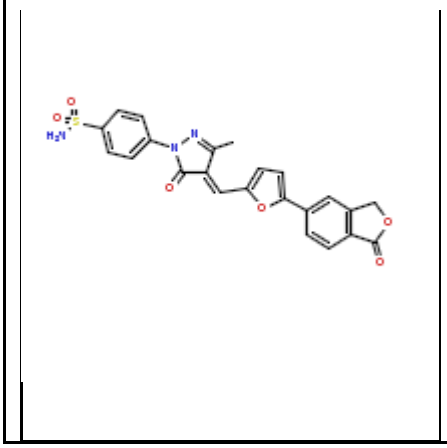
	23.000	14	95	6.02
	24.000	14	50	7.68
	24.300	9	7	7.58

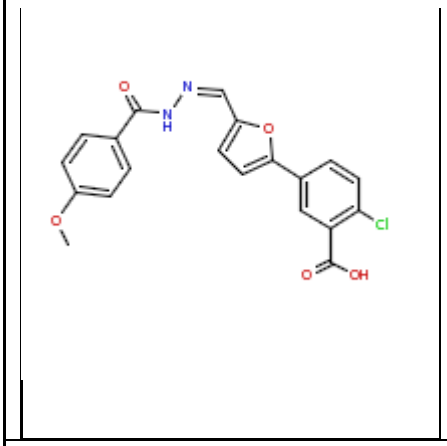
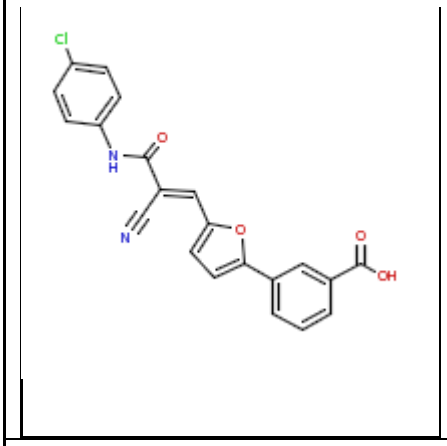
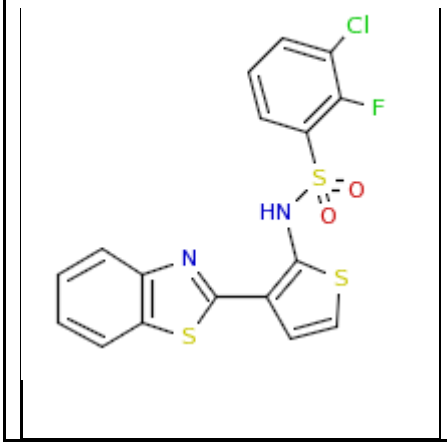
	24.600	7	27	6.99
	24.800	4	10	8.57
	24.900	7	59	5.40

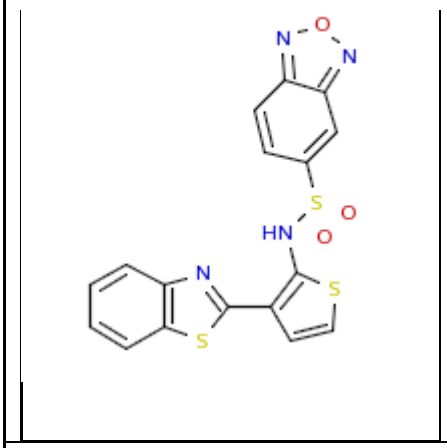
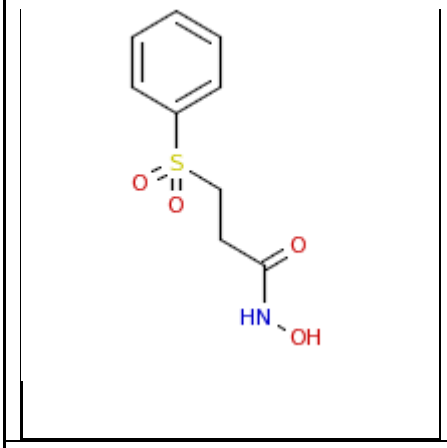
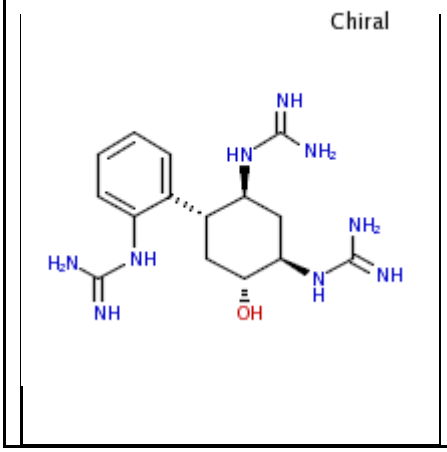
	25.000	14	84	6.06
	25.600	12	23	6.71
	26.600	12	24	6.12

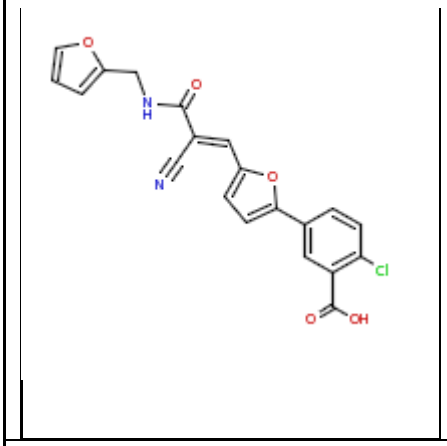
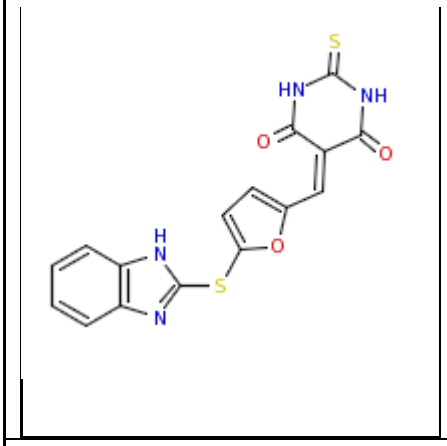
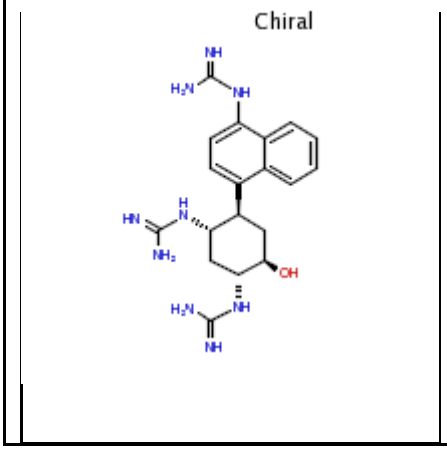
	27.000	14	93	6.93
Chiral 	27.000	14	94	7.63
	27.900	7	52	6.44

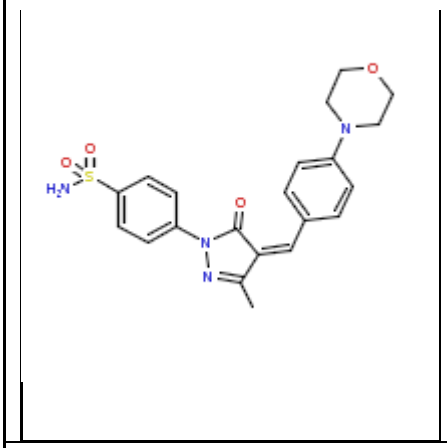
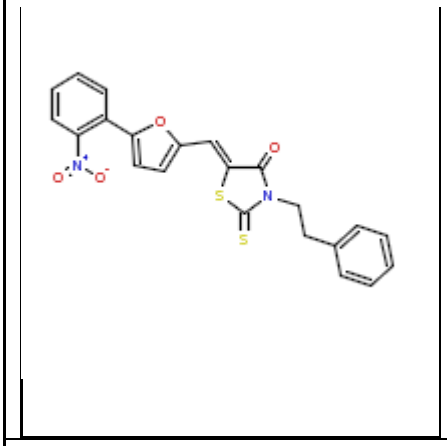
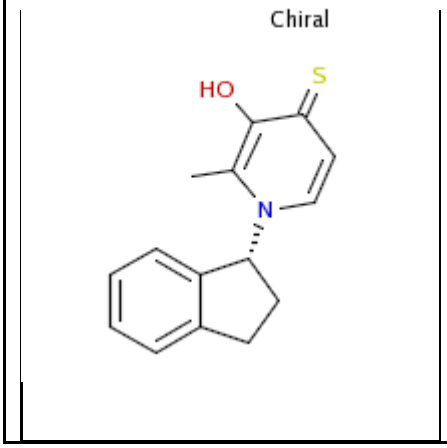
	28.000	14	102	6.52
	28.000	14	69	7.84
	28.000	21	12	8.30

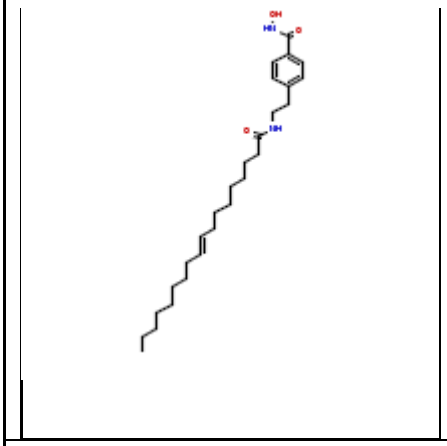
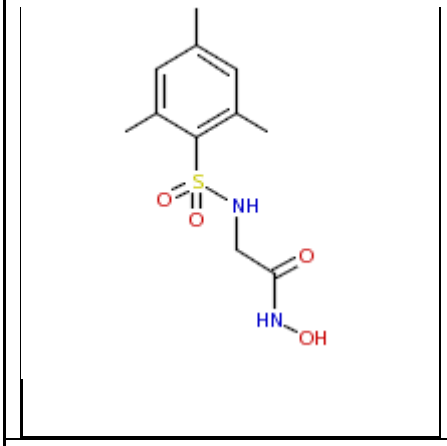
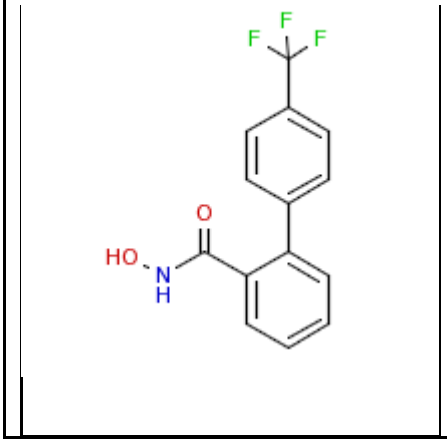
	28.100	7	50	5.27
	28.300	12	Table2_3	4.78
	29.600	12	52	5.19

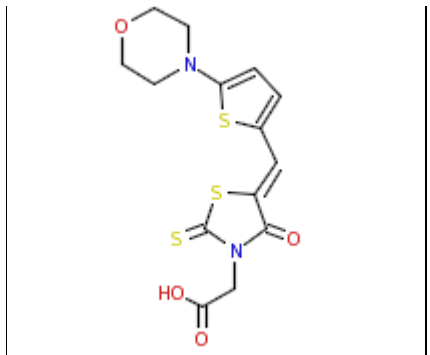
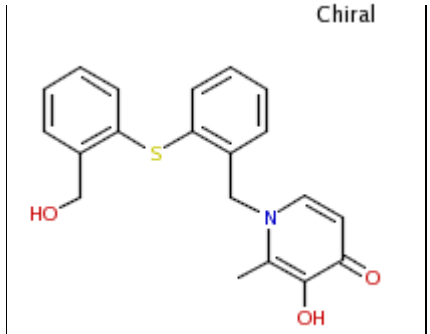
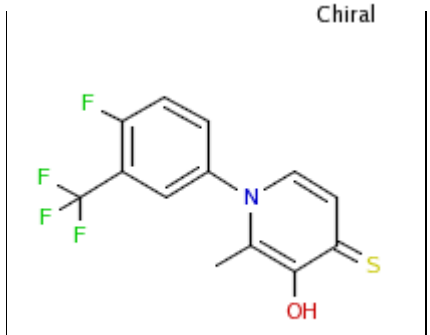
	29.700	12	25	6.16
	29.900	12	26	5.39
	30.000	14	61	6.49

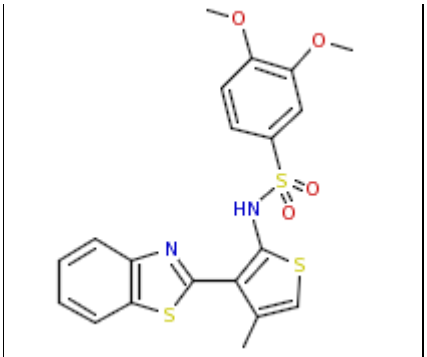
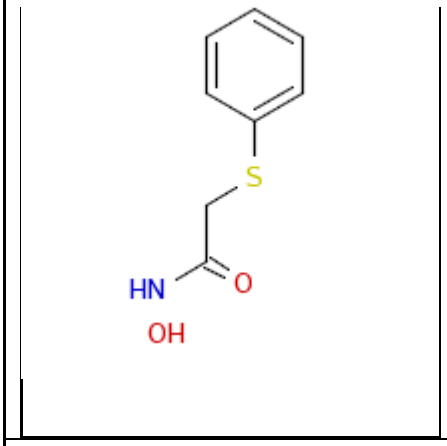
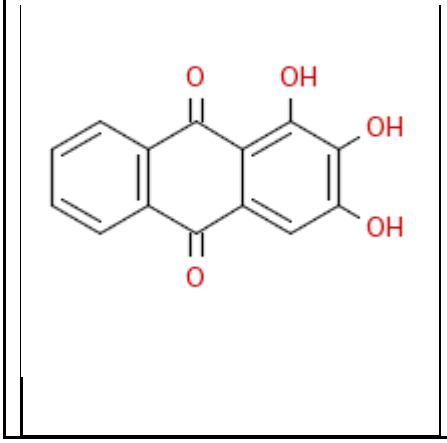
	30.000	14	91	6.52
	30.000	6	7	8.54
	30.600	4	8b	6.56

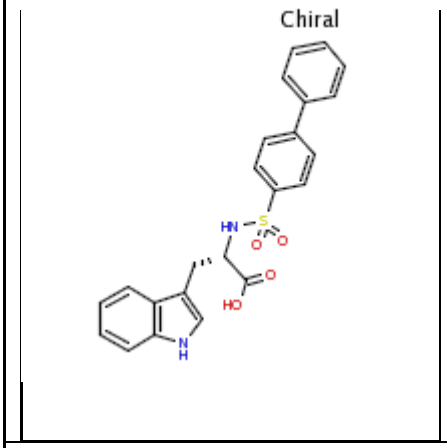
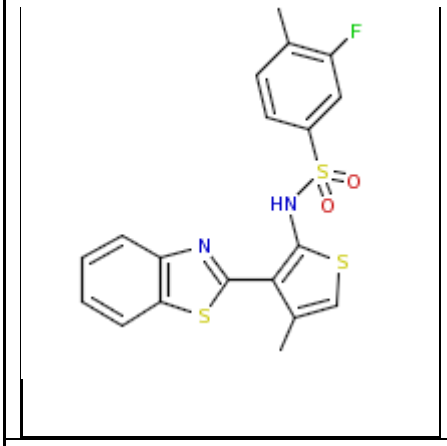
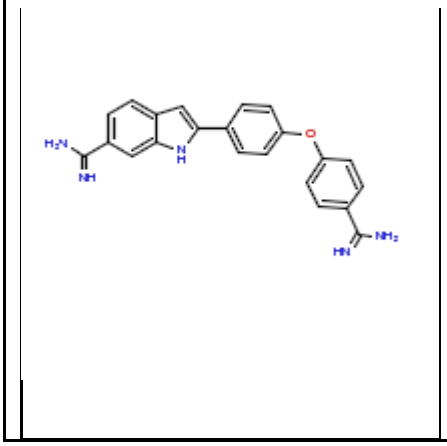
	30.700	12	27	6.79
	30.900	12	Table2_5	6.55
	31.400	4	8f	8.00

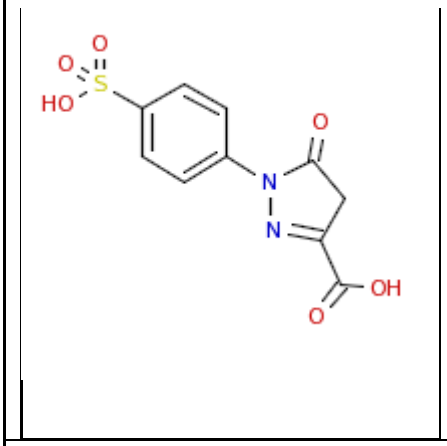
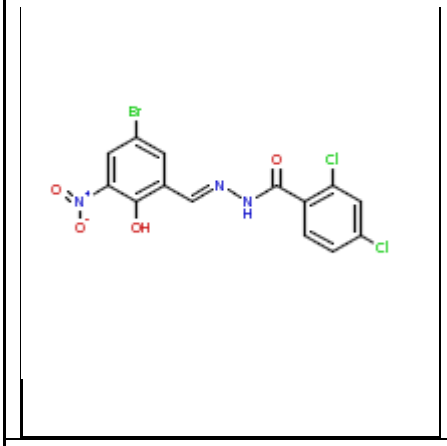
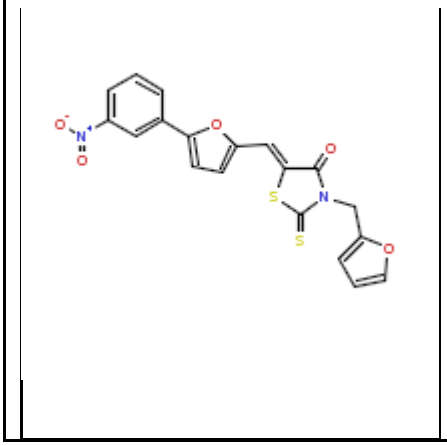
	31.700	12	53	5.53
	31.900	8	6	5.97
Chiral 	32.000	17	94F12	6.08

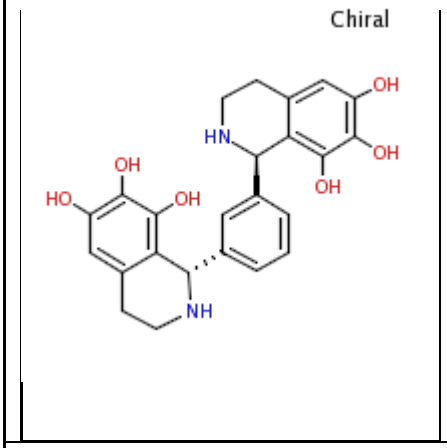
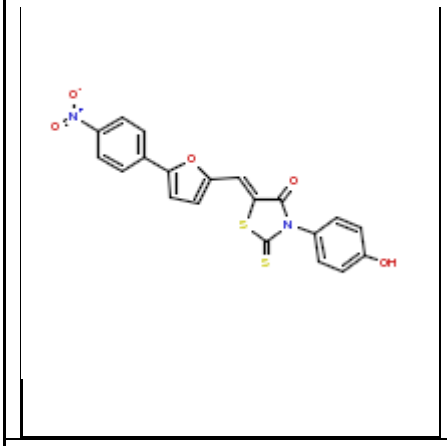
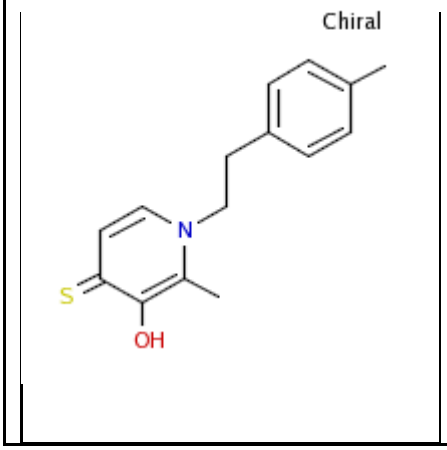
	32.000	18	6	9.07
	32.000	6	5	9.41
	32.000	6	6	9.08

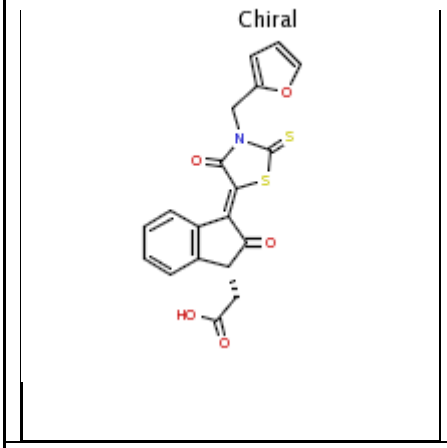
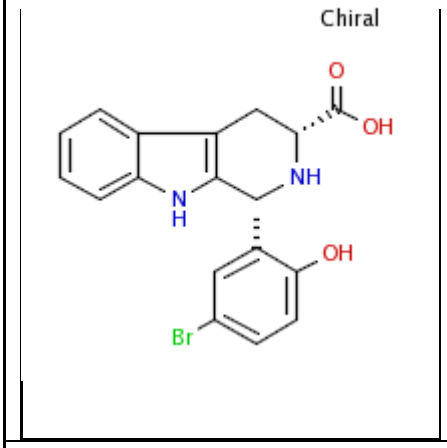
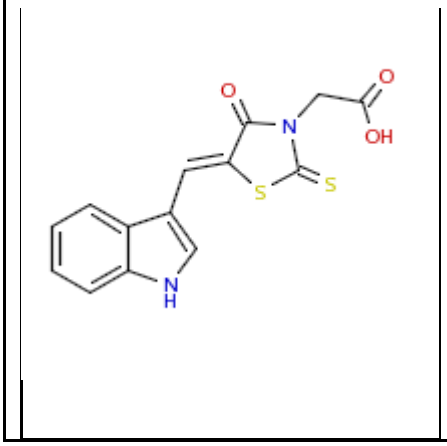
	32.500	7	48	5.76
	34.000	17	94B11	7.93
	34.000	17	9.40E+13	6.38

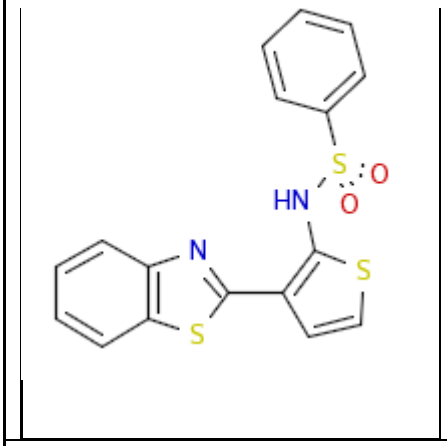
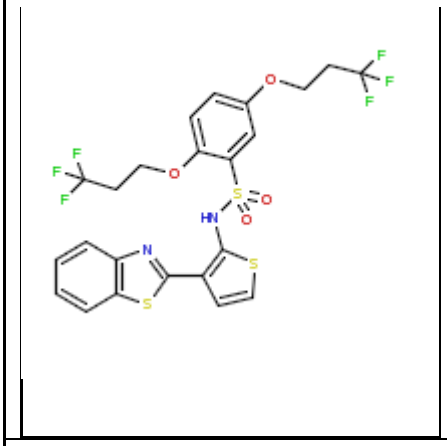
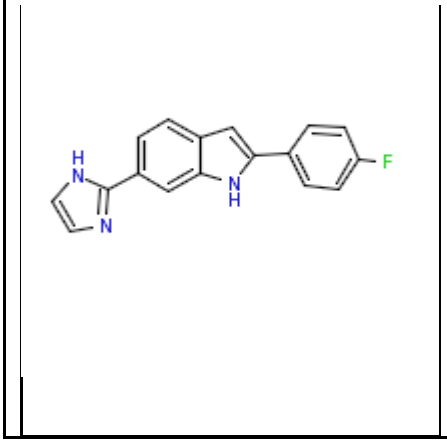
	34.000	14	24	7.41
	34.000	6	4	7.03
	34.000	16	1	6.65

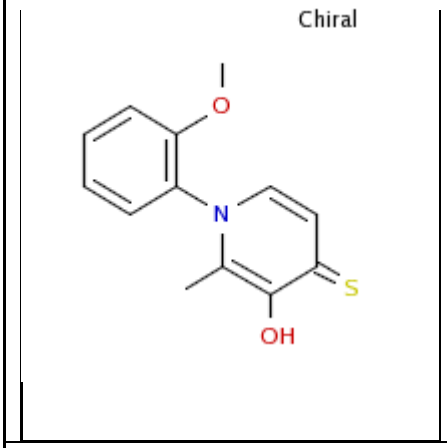
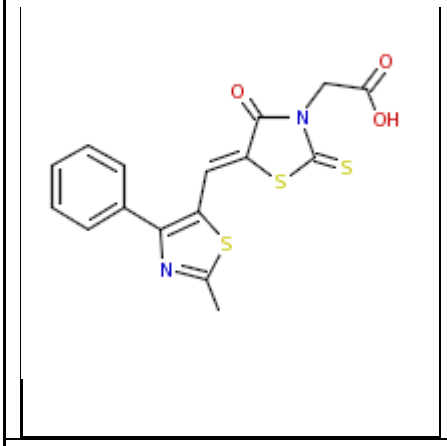
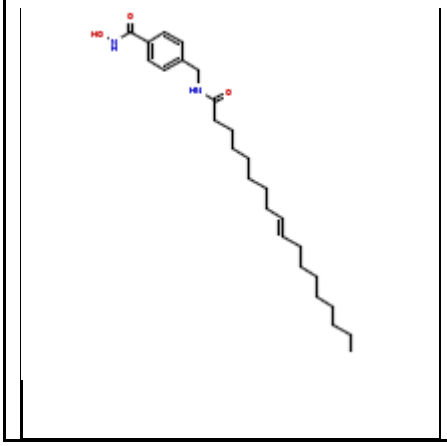
	34.900	6	15	8.82
	35.000	14	19	6.62
	35.000	21	5	6.56

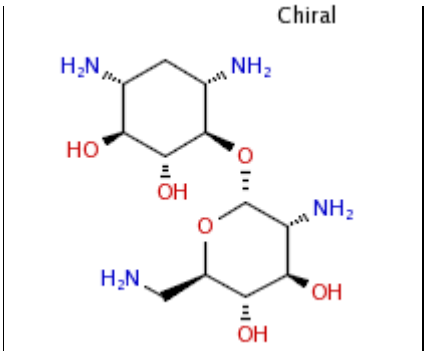
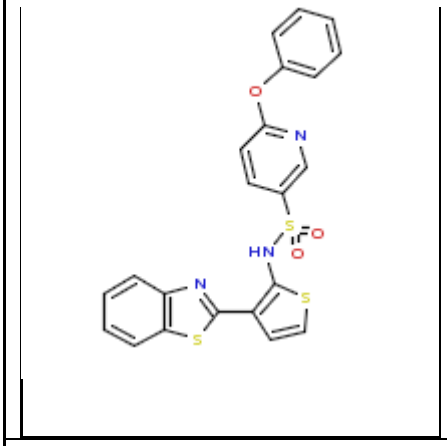
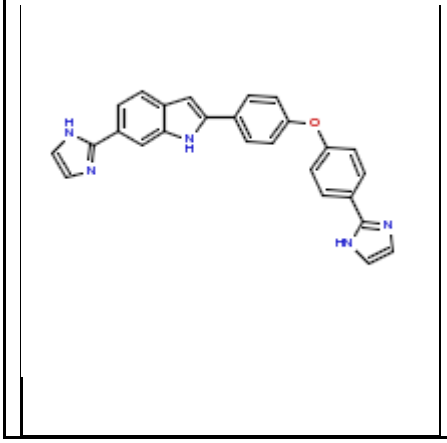
	35.200	12	46	6.14
	35.500	12	Table2_1	5.91
	36.300	8	5	6.69

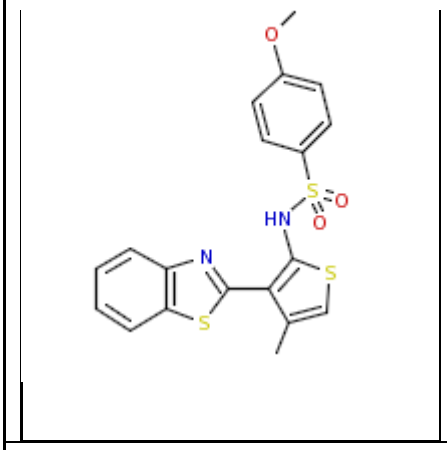
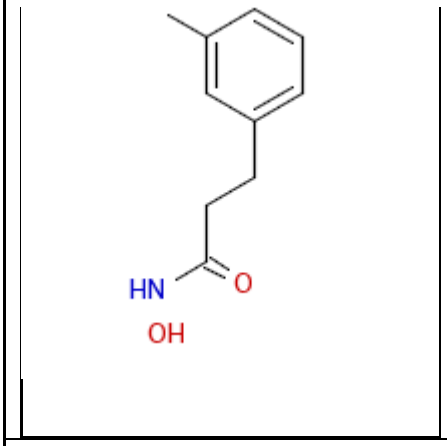
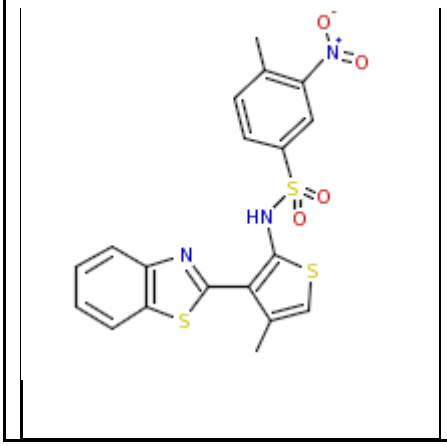
	36.700	16	6a	5.72
	37.700	8	4	5.09
	38.000	17	94G8	7.23

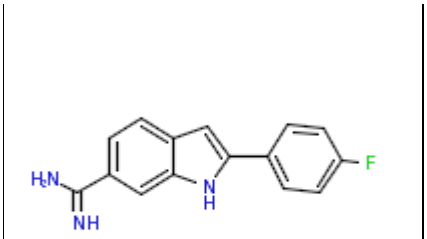
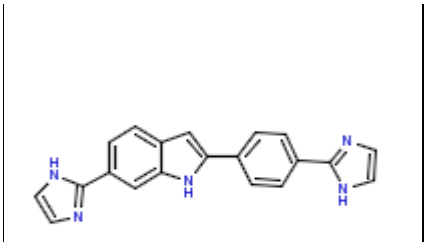
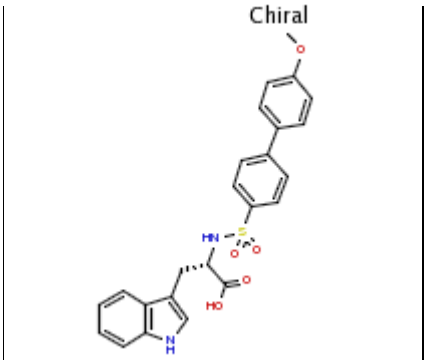
	38.000	13	2	5.58
	38.200	13	1	5.80
	38.700	7	60	5.19

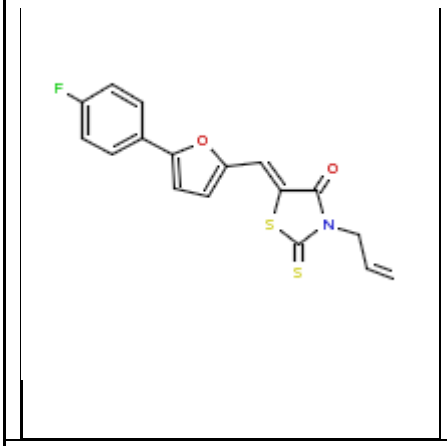
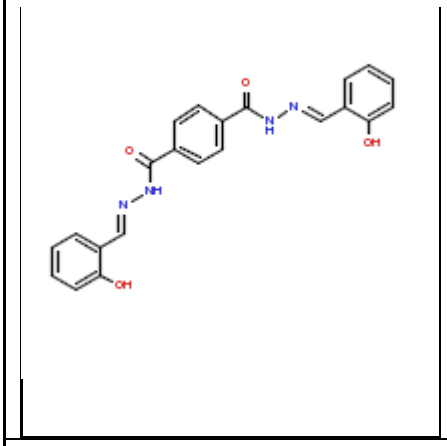
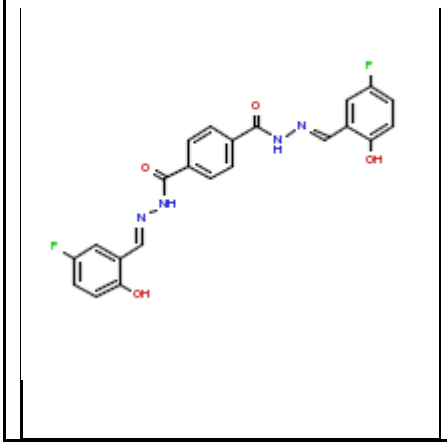
	39.000	14	43	6.71
	39.000	14	56	7.70
	40.000	21	40c	7.06

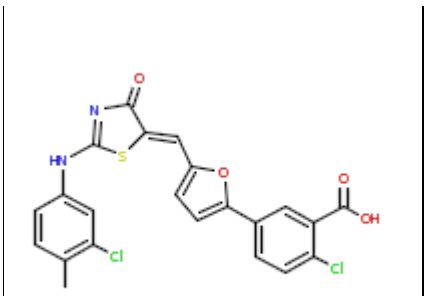
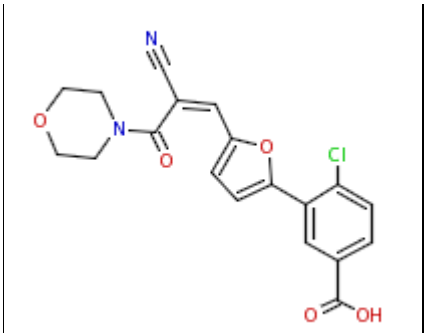
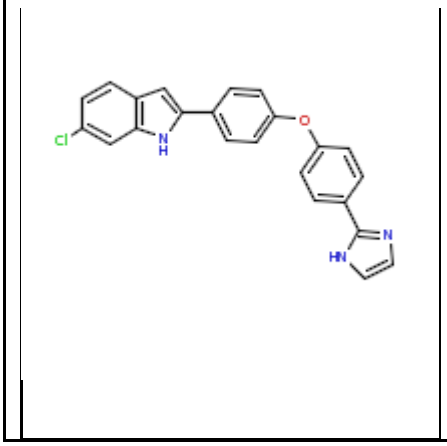
	41.000	17	9.40E+10	4.86
	41.000	7	19	7.73
	42.000	20	6	9.04

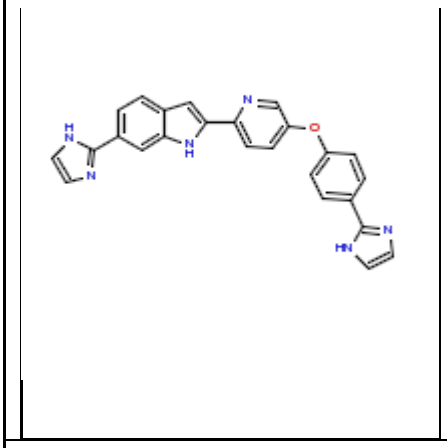
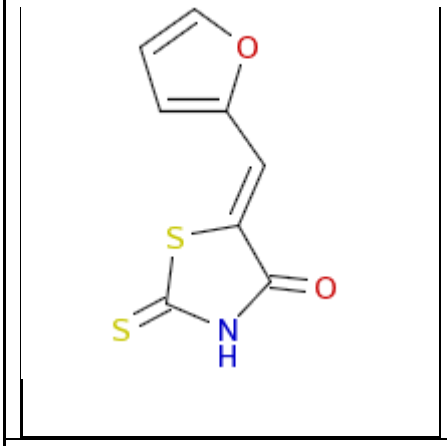
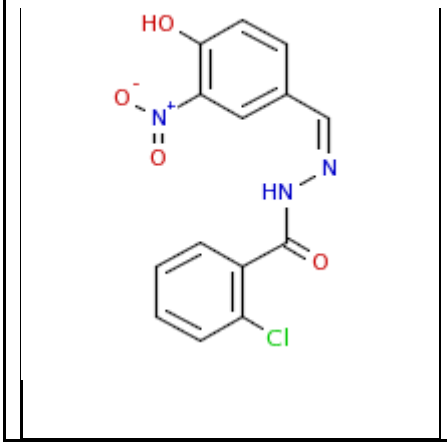
	42.900	9	2_neamine	8.78
	43.000	14	81	7.67
	43.000	21	13	6.26

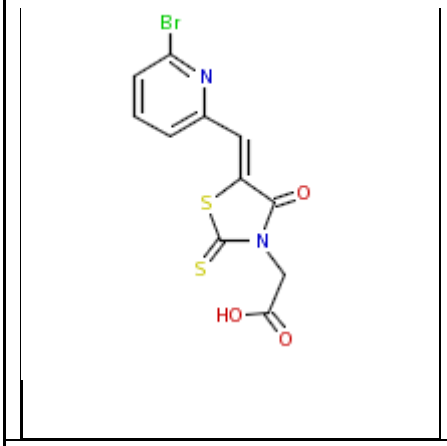
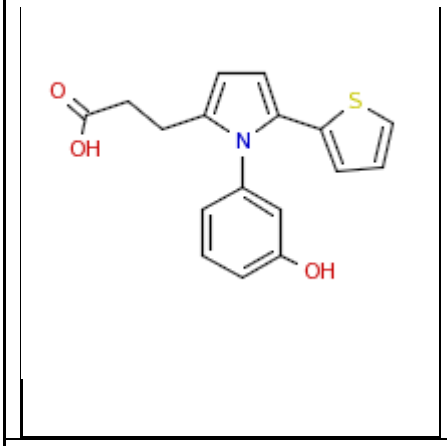
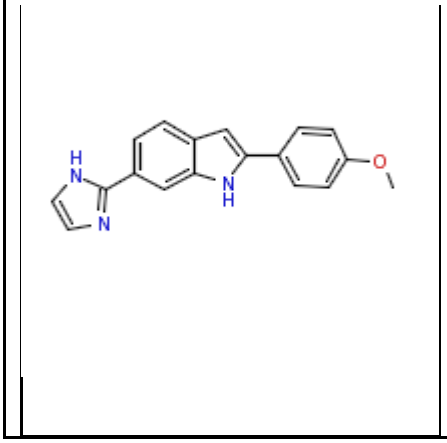
	46.000	14	13	7.00
	47.000	6	3	7.30
	48.000	14	29	7.12

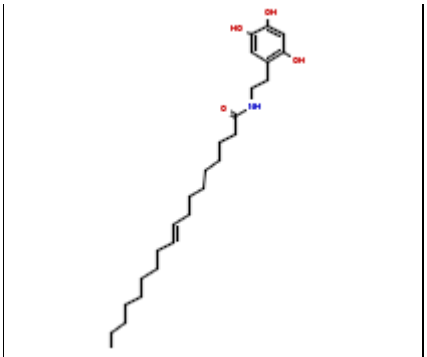
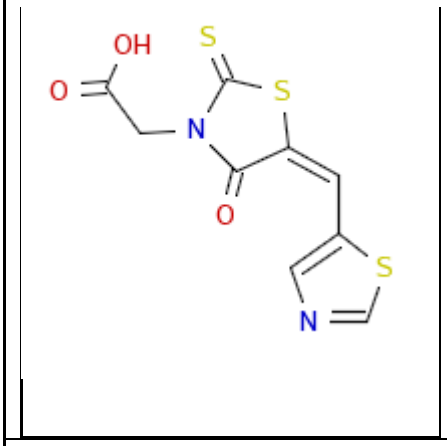
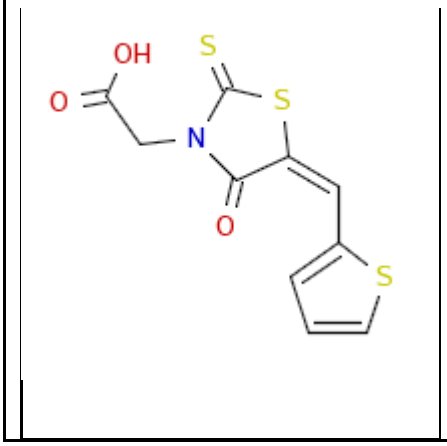
	48.000	21	40b	6.29
	49.000	21	44a	5.75
	49.100	6	17	9.27

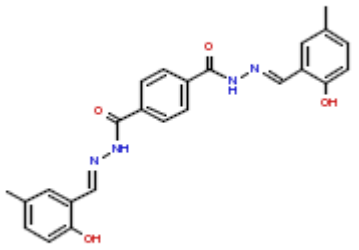
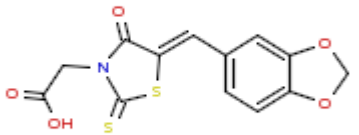
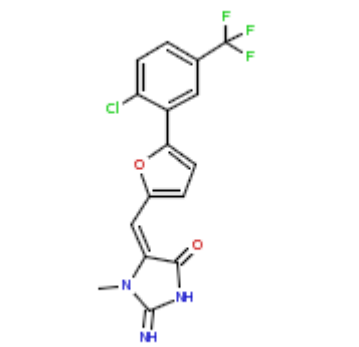
	50.000	8	3	4.48
	50.000	22	3h	8.25
	50.000	22	7h	7.98

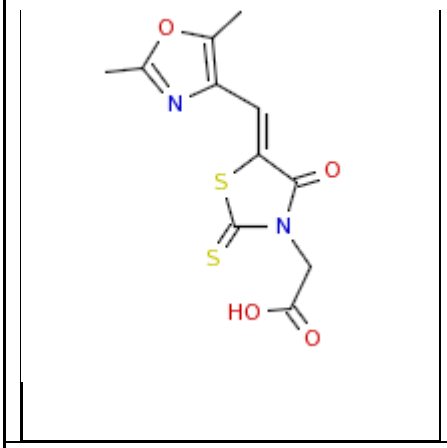
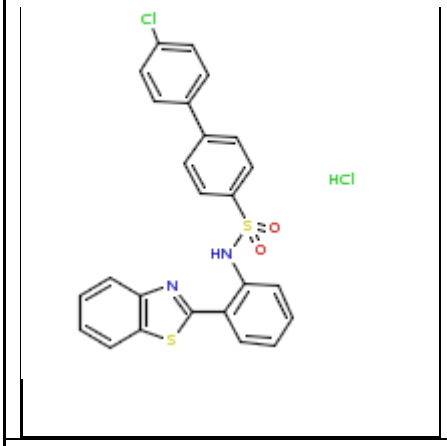
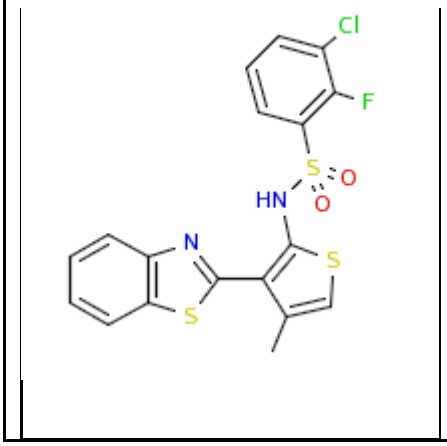
	50.000	12	29	6.71
	50.000	12	30	4.89
	51.000	21	32	6.41

	55.000	21	24a	5.45
	56.400	12	Table2_4	3.23
	56.900	12	Table2_2	6.09

	58.000	7	56	5.58
	60.000	12	61	8.62
	61.000	21	43c	7.38

	70.000	17	5	9.55
	72.400	10	13	6.05
	79.400	10	10	5.75

	80.000	22	2h	8.63
	83.300	7	53	5.67
	100.000	10	19	5.95

	100.000	7	17	6.01
	100.000	14	112	8.03
	100.000	14	27	6.33

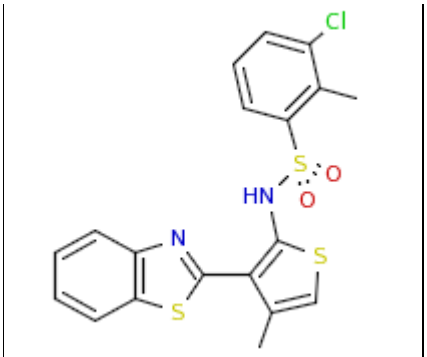
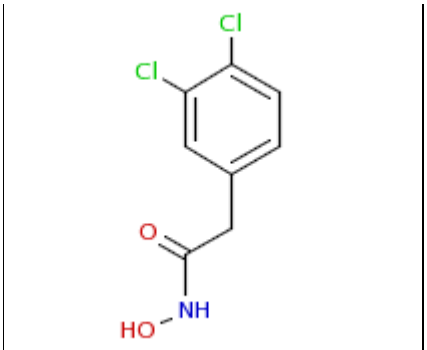
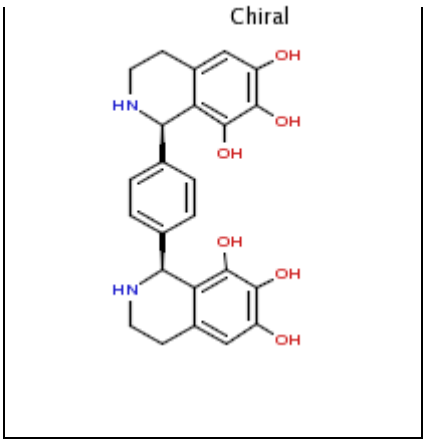
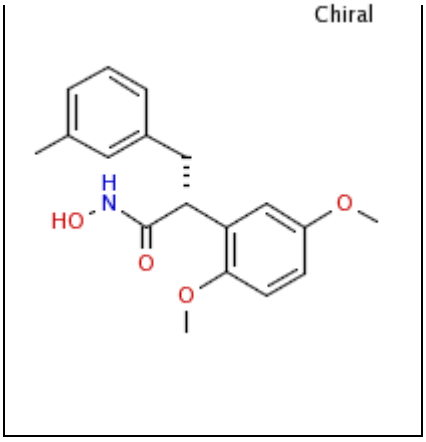
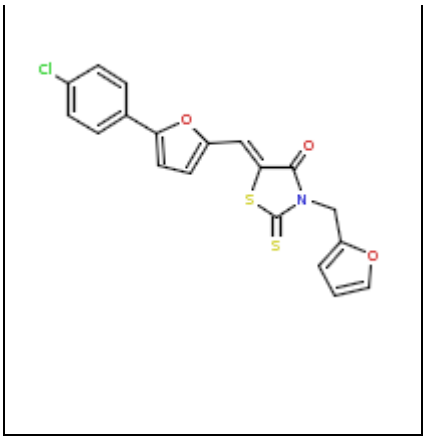
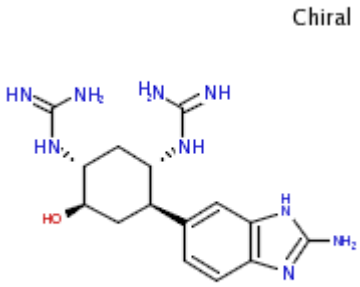
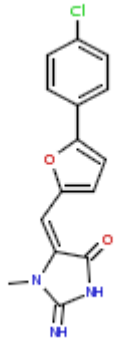
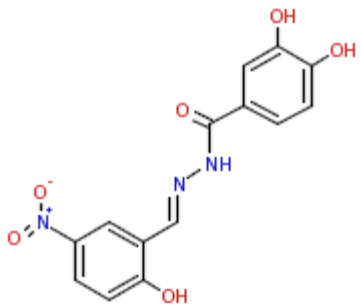
	100.000	14	28	6.85
	100.000	6	20	6.29

Table S3. Structures, LF biological activities, references, compound designators, and docking scores for screening set compounds in dataset **DB1C.**

Structure	LF IC_{50} or K_i (μM)	Reference	Compound Designator	Docking Score (Surflex-Dock)
	123.8	16	7a	5.95
	130.0	6	23	9.83
	150.0	8	2	4.91

	153.7	4	8h	8.09
	200.0	10	18	5.08
	200.0	22	1a	7.69

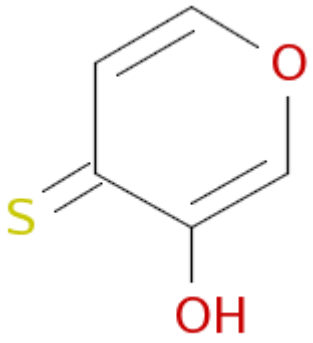
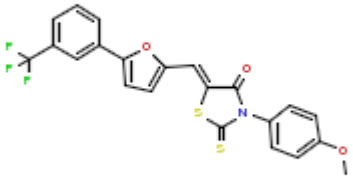
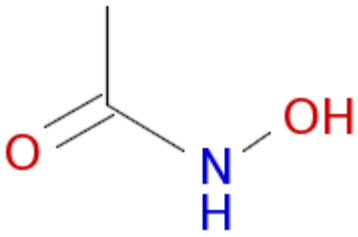
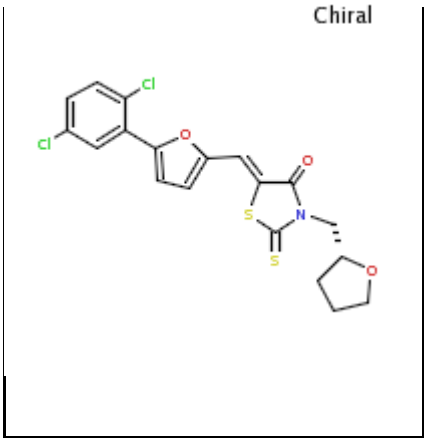
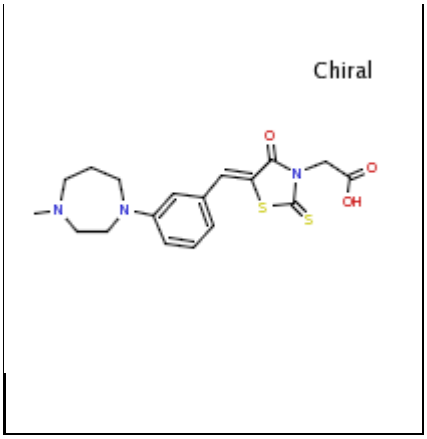
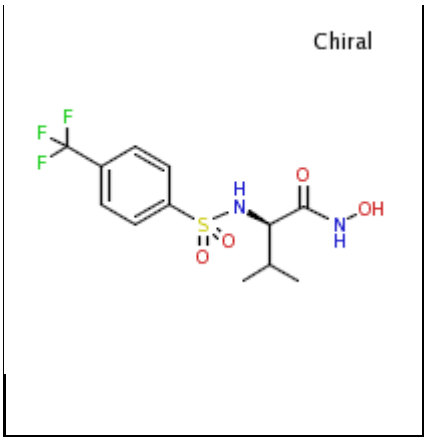
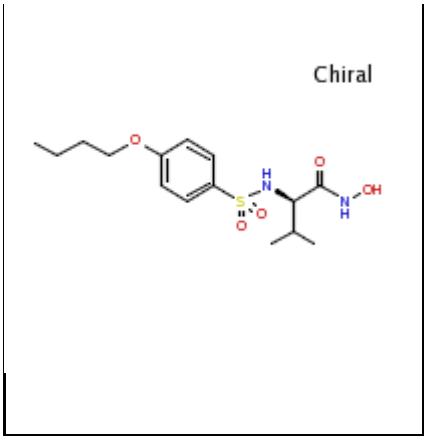
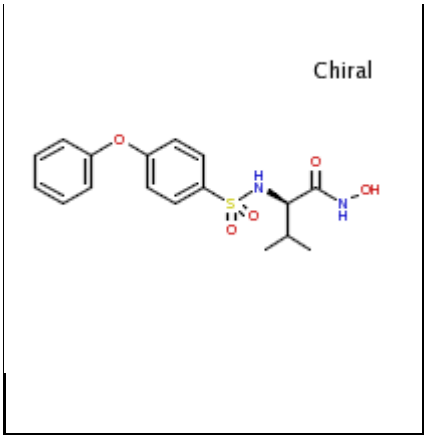
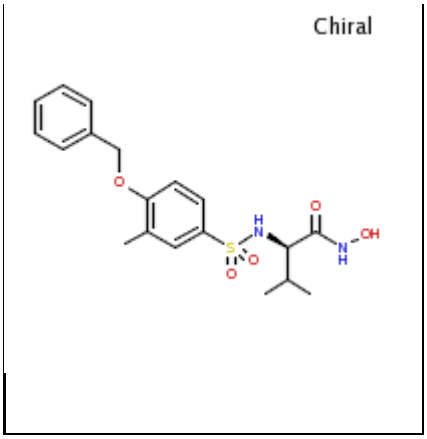
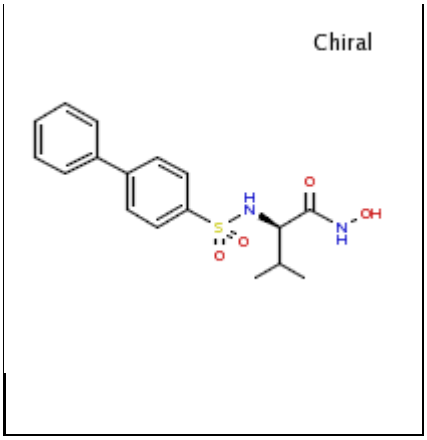
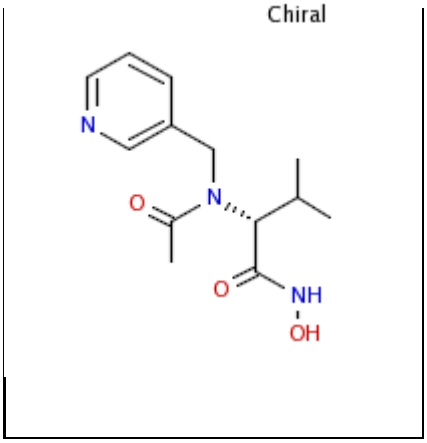
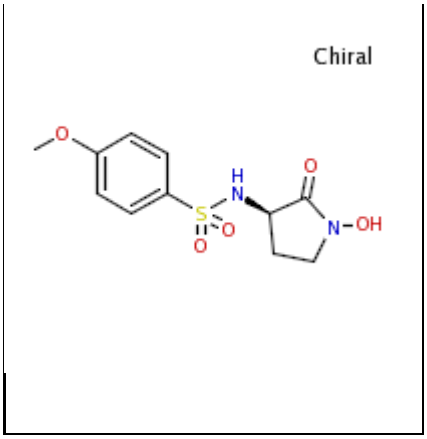
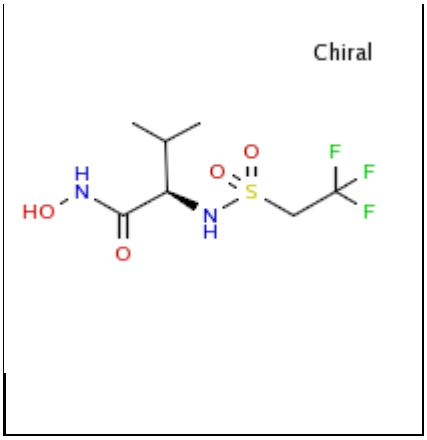
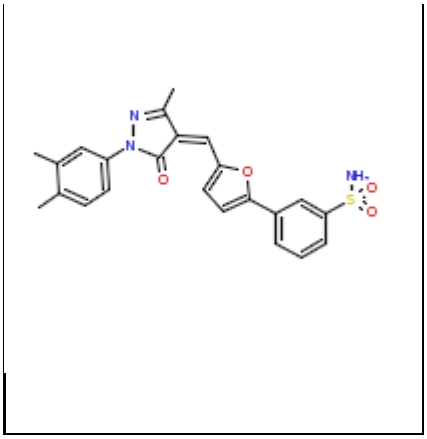
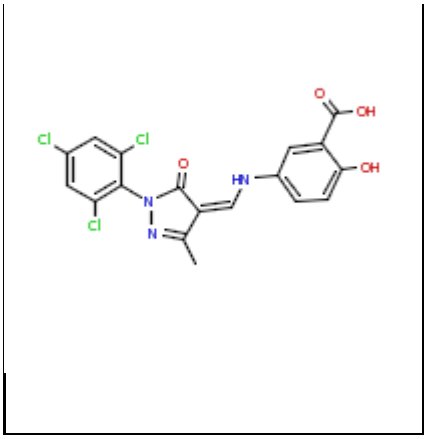
	204.0	23	2d	4.65
	300.0	8	1	5.29
	11400.0	23	1g	4.72

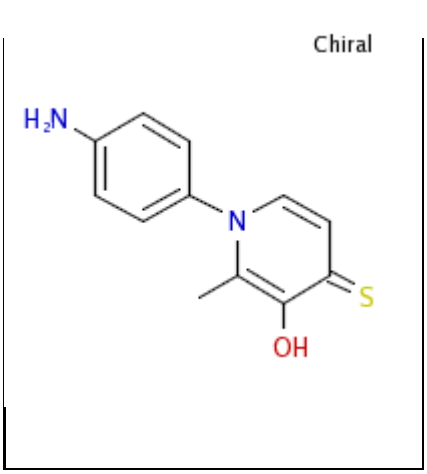
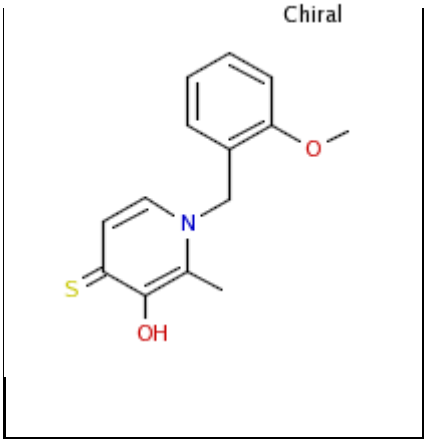
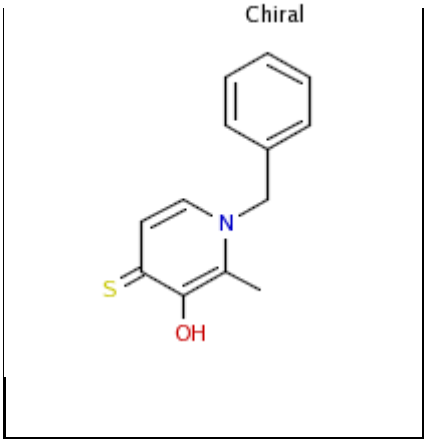
Table S4. Structures, LF biological activities, references, compound designators, and docking scores for screening set compounds in dataset **DB1D.**

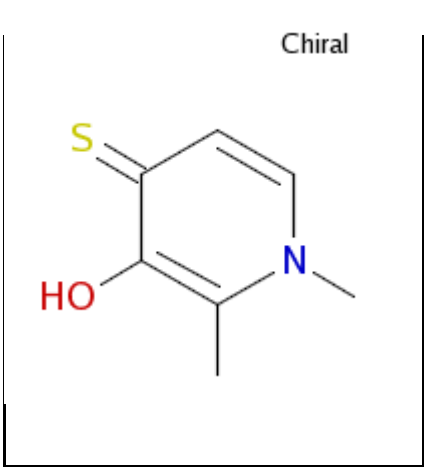
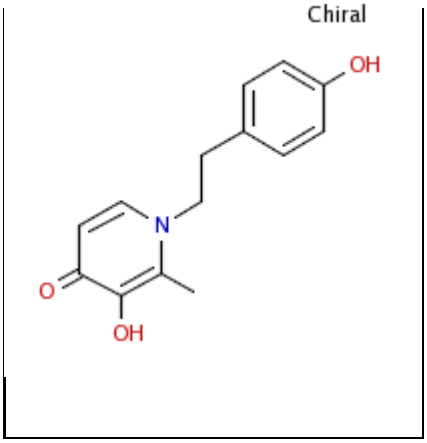
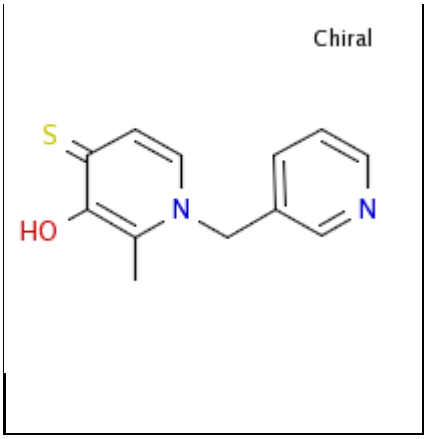
Structure	LF IC_{50} or K_i (μM)	Reference	Compound Designator	Docking Score (Surflex-Dock)
	>25	7	16	5.55
	>25	7	51	7.45
	>40	3	17	9.92

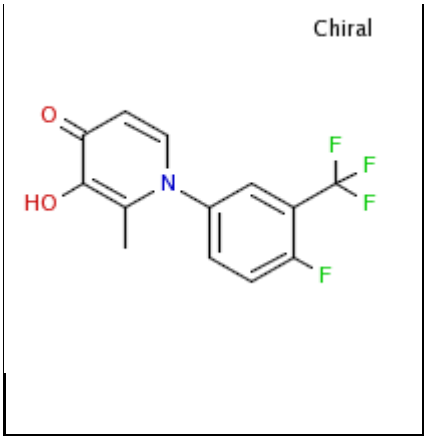
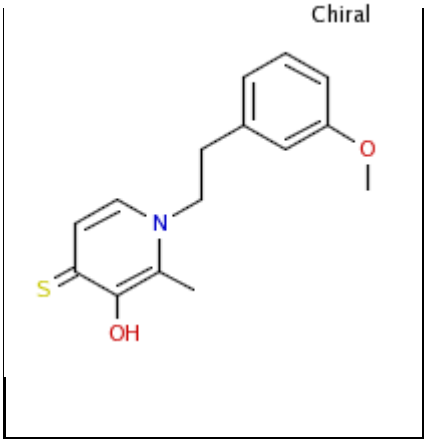
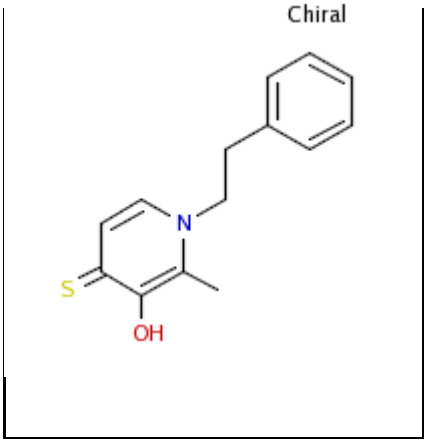
	>40	3	21	11.68
	>40	3	22	9.27
	>40	3	23	10.25

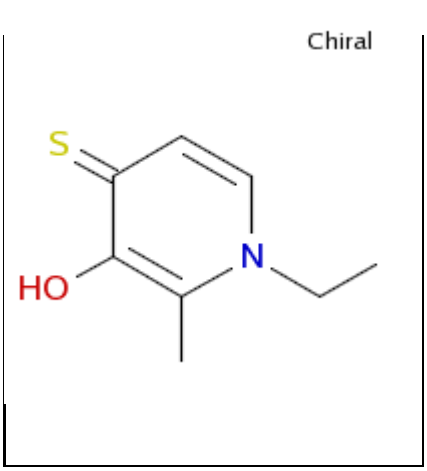
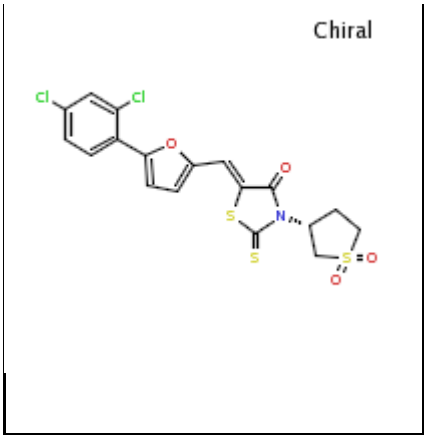
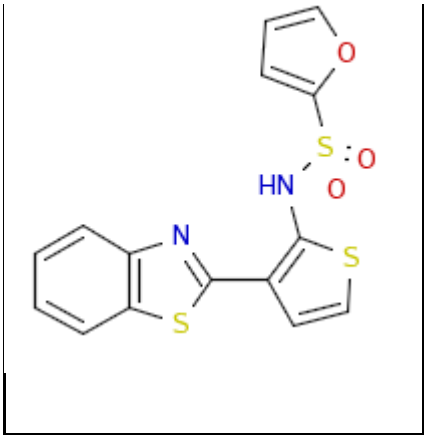
	>40	3	24	9.96
	>40	3	3	9.35
	>40	3	5	7.42

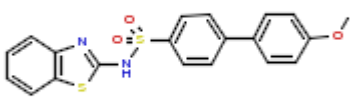
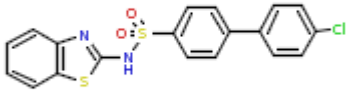
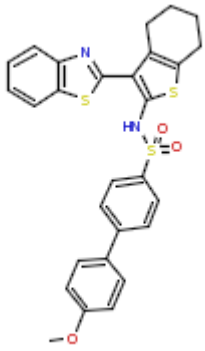
	>40	3	6	8.26
	>45	12	38	5.84
	>45	12	47	6.23

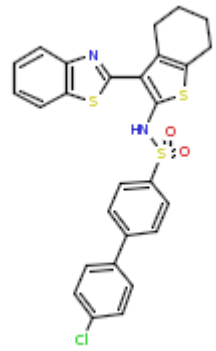
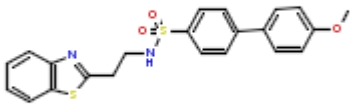
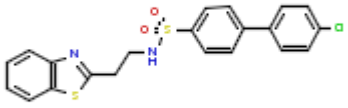
	>50	17	94C7	6.34
	>50	17	94F5	6.01
	>50	17	94F9	6.21

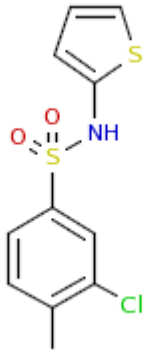
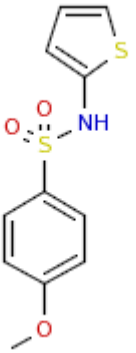
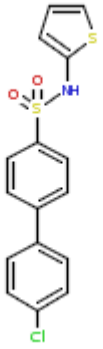
	>50	17	94G11	5.52
	>50	17	94G12	7.31
	>50	17	94G4	6.25

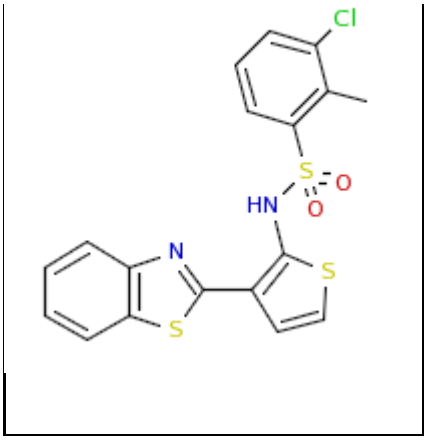
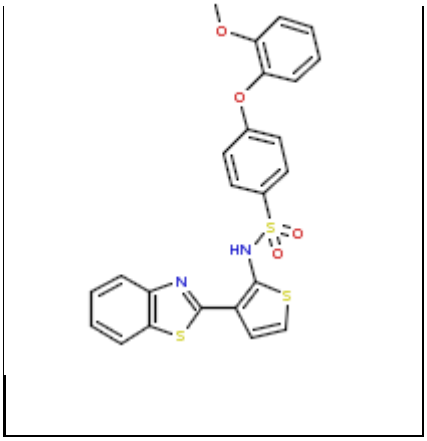
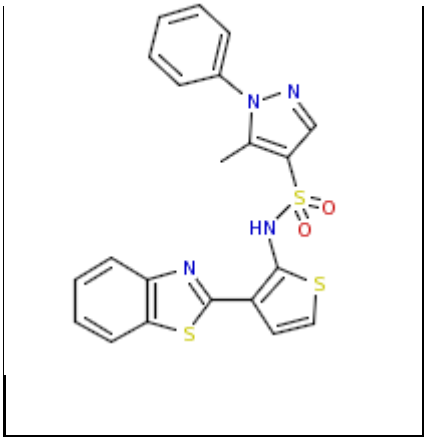
	>50	17	94G6	6.06
	>50	17	94G7	8.84
	>50	17	94H2	7.18

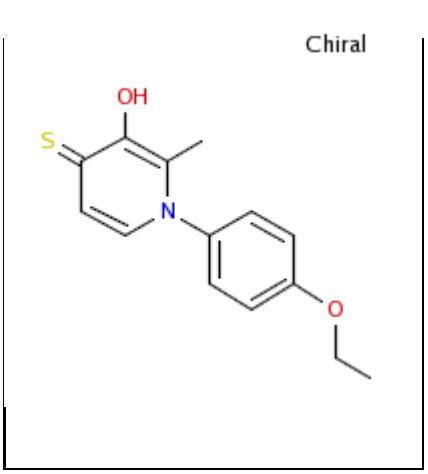
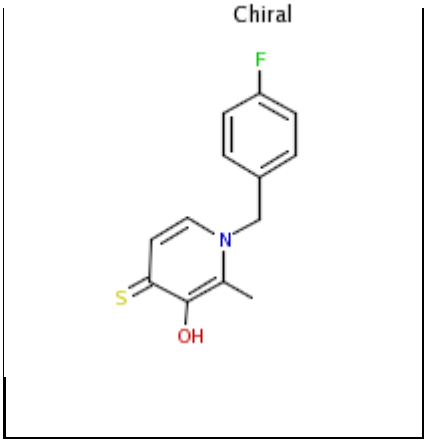
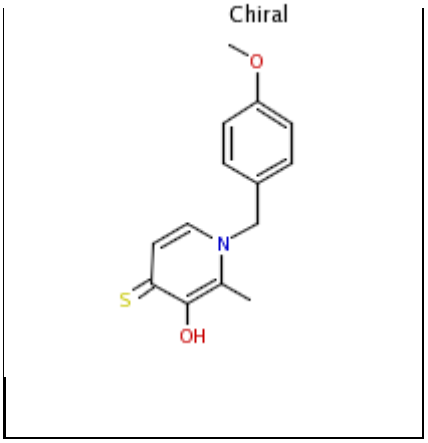
	>50	17	94H3	5.56
	>50	7	15	4.31
	>50	14	100	7.55

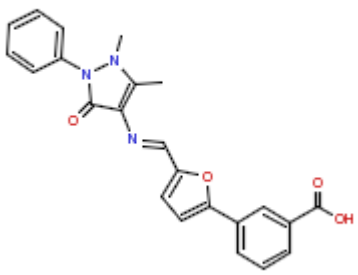
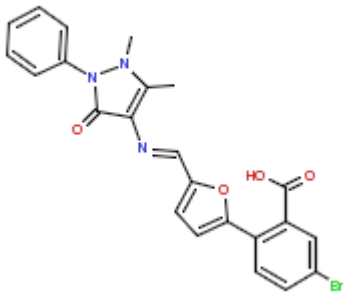
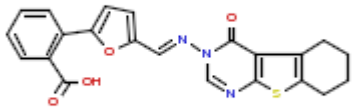
	>50	14	103	7.83
	>50	14	104	7.52
	>50	14	105	8.25

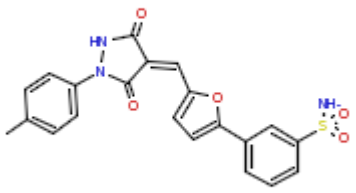
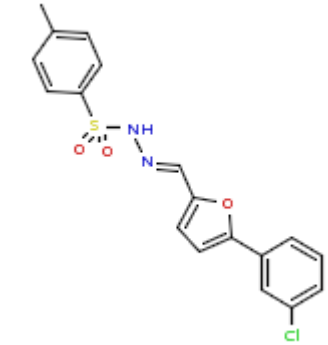
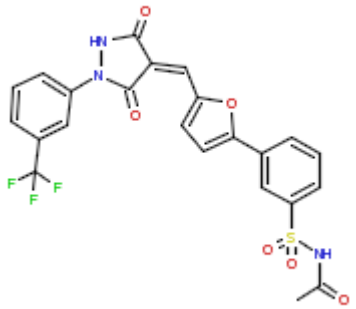
	>50	14	106	7.44
	>50	14	109	7.66
	>50	14	110	7.87

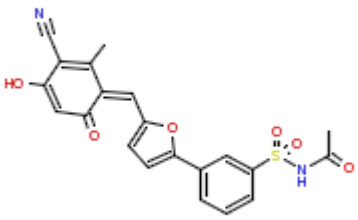
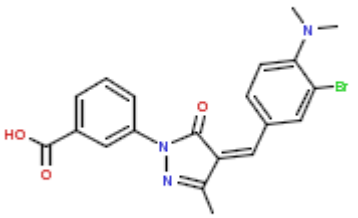
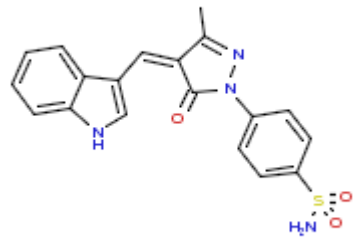
	>50	14	113	6.09
	>50	14	114	4.97
	>50	14	115	6.37

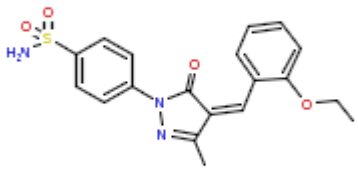
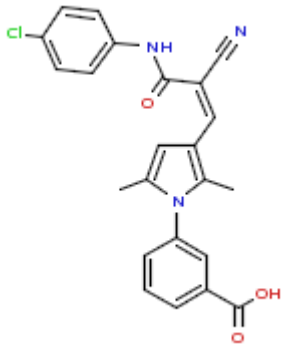
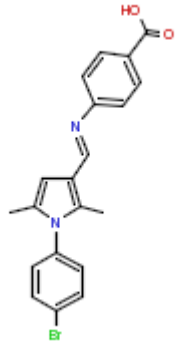
	>50	14	62	6.68
	>50	14	80	8.45
	>50	14	86	7.11

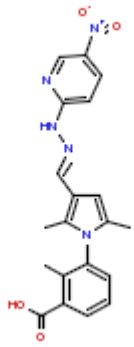
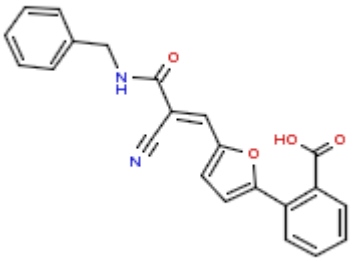
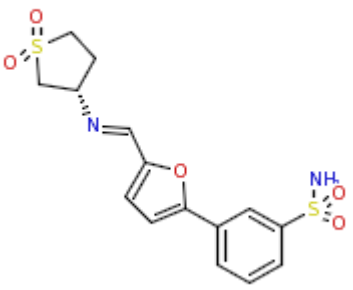
	>50	6	12	6.70
	>50	6	13	6.62
	>50	6	14	6.94

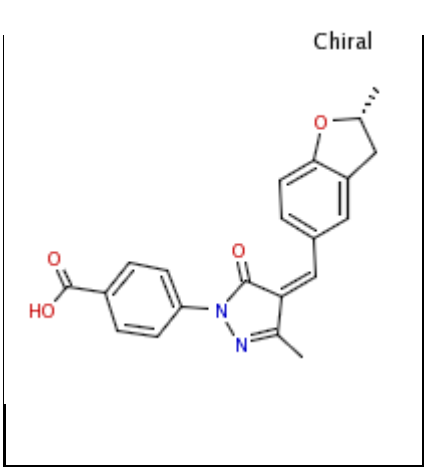
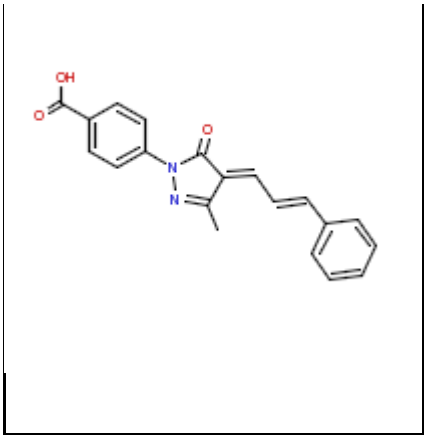
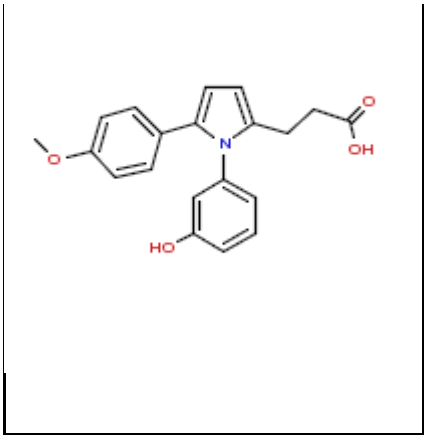
Chiral 	>50	12	31	6.68
Chiral 	>50	12	32	6.88
	>50	12	33	7.75

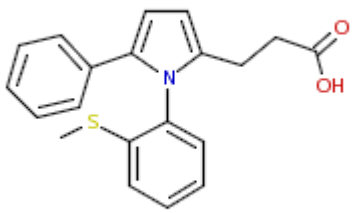
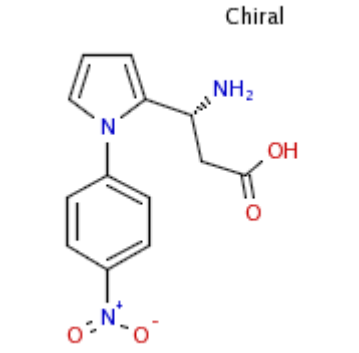
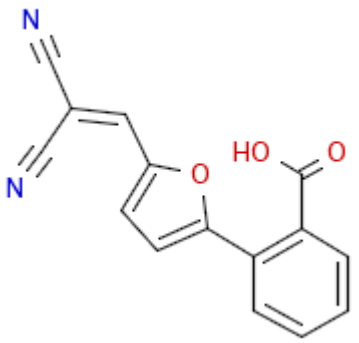
	>50	12	39	7.10
	>50	12	40	6.83
	>50	12	41	7.90

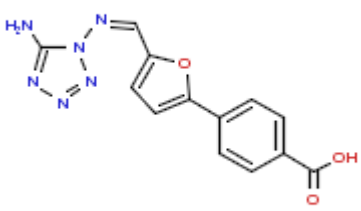
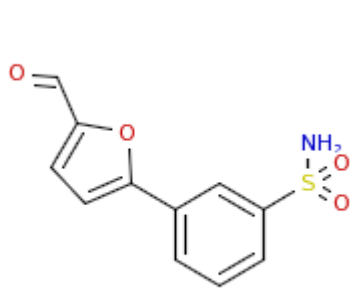
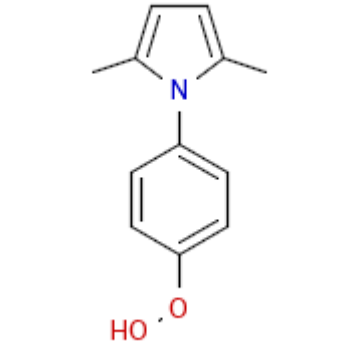
	>50	12	42	7.80
	>50	12	48	5.68
	>50	12	54	8.83

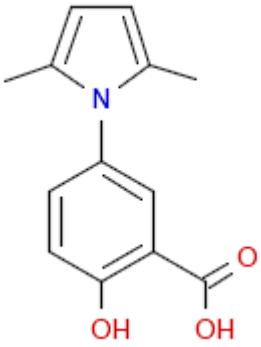
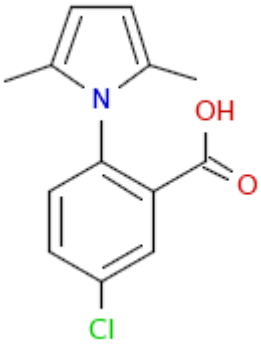
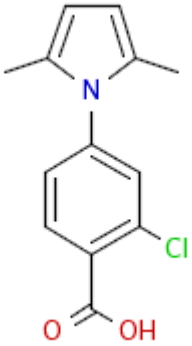
	>50	12	55	6.68
	>50	12	62	5.80
	>50	12	63	5.61

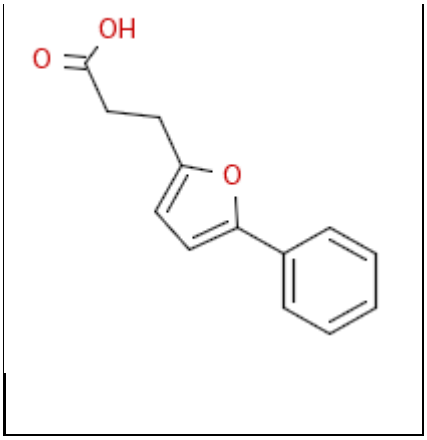
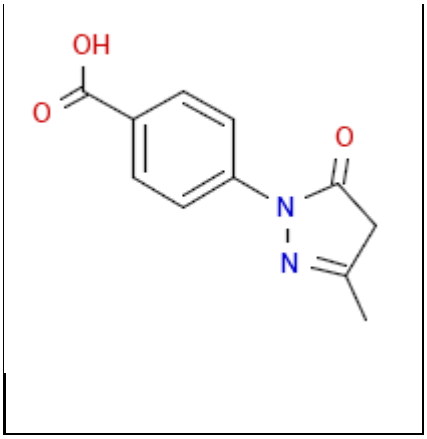
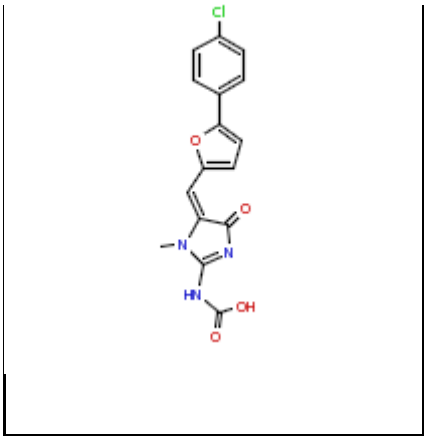
	>50	12	64	6.98
	>55	12	34	7.78
Chiral 	>55	12	43	5.94

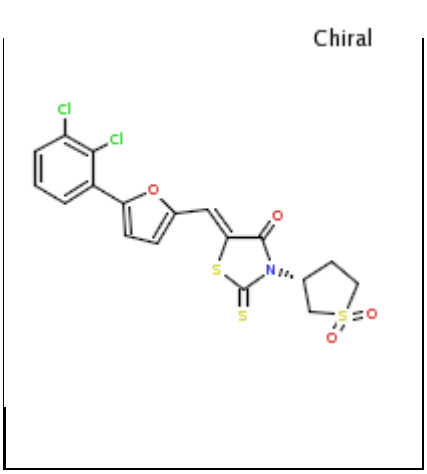
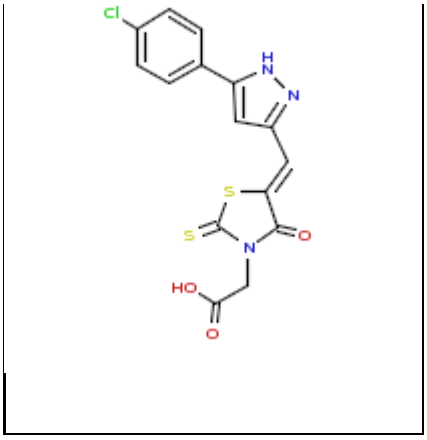
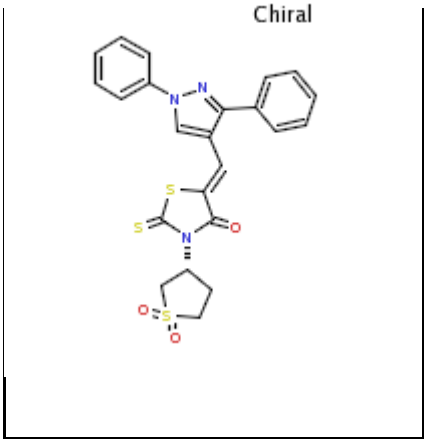
	>55	12	49	6.53
	>60	12	50	5.35
	>60	12	65	8.17

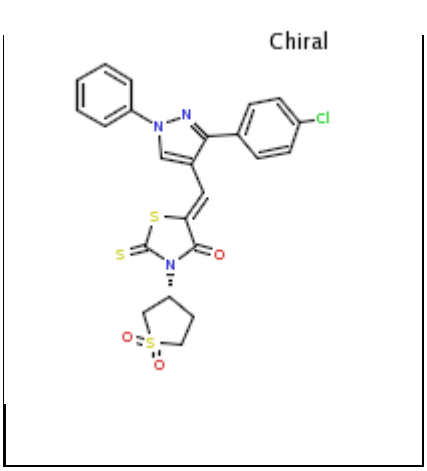
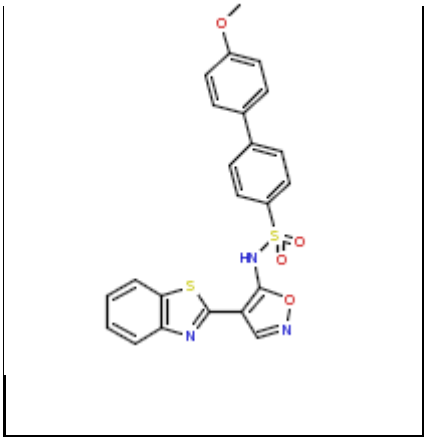
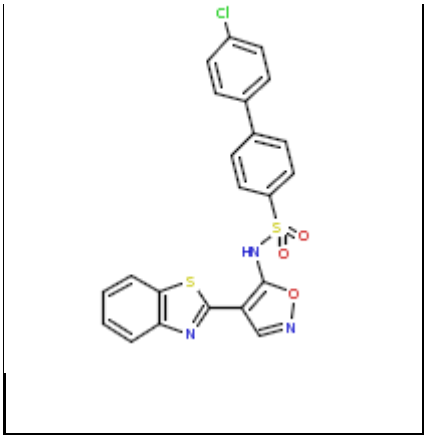
	>60	12	66	7.20
	>70	12	67	7.24
	>75	12	35	6.13

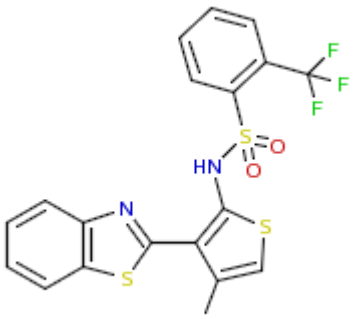
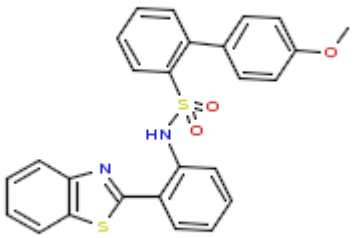
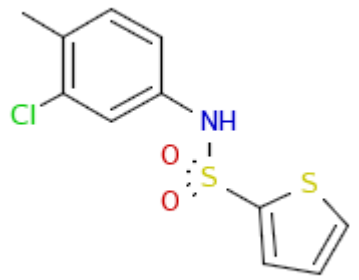
	>80	12	36	6.22
	>80	12	44	4.14
	>85	12	68	7.29

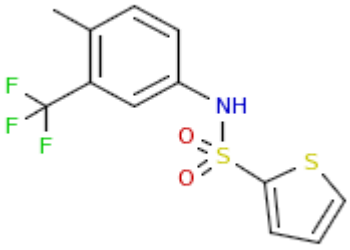
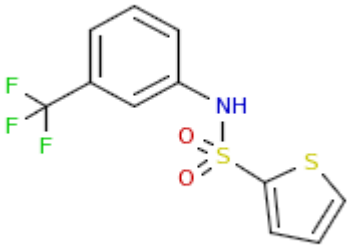
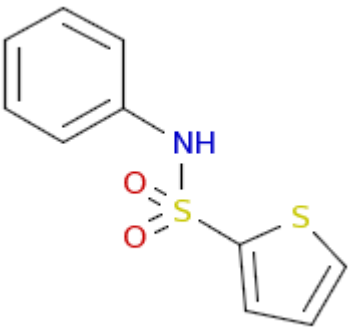
	>85	12	69	6.31
	>85	12	70	3.29
	>85	12	71	4.94

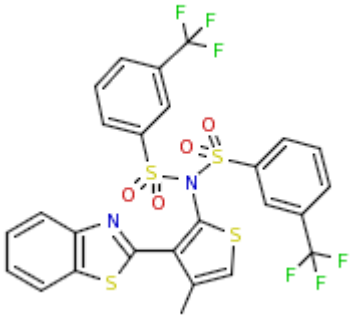
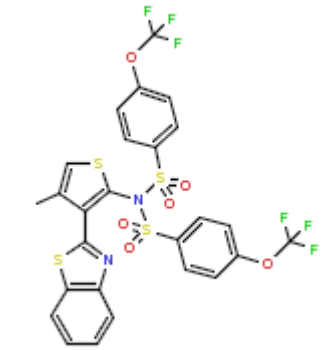
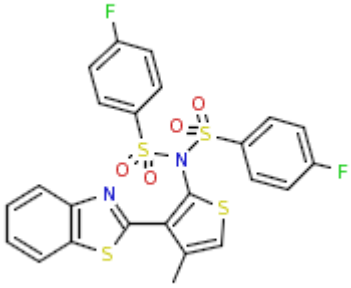
	>90	12	37	6.60
	>90	12	51	4.45
	>100	10	20	4.86

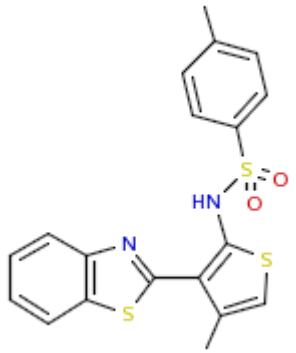
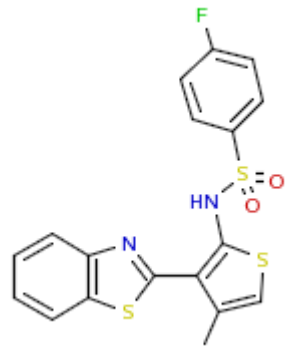
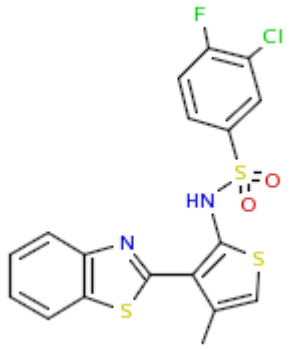
	>100	7	14	4.98
	>100	7	28	6.56
	>100	7	44	4.84

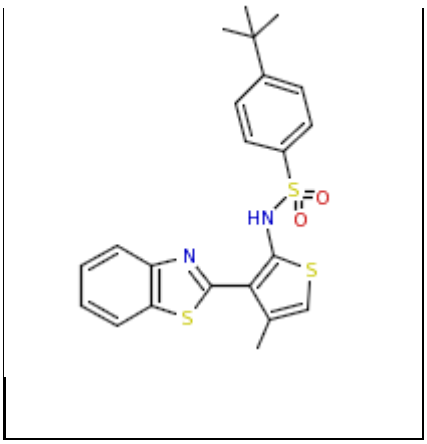
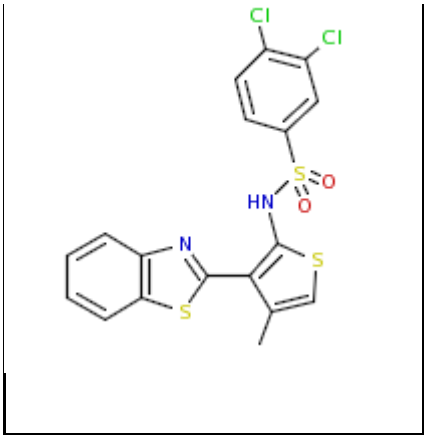
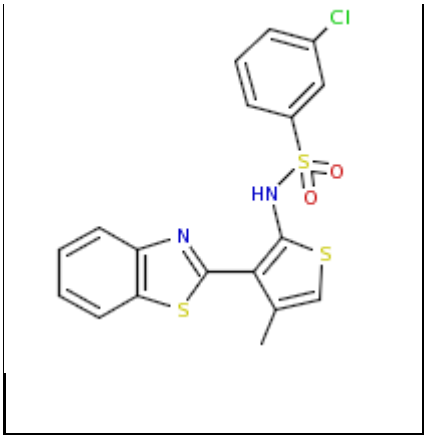
	>100	7	45	4.76
	>100	14	107	8.58
	>100	14	108	7.11

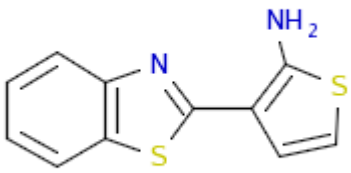
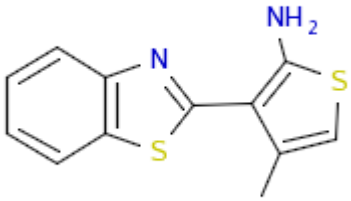
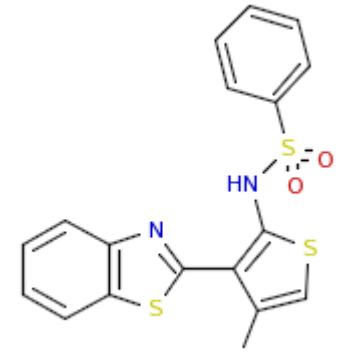
	>100	14	11	6.06
	>100	14	111	7.32
	>100	14	116	5.30

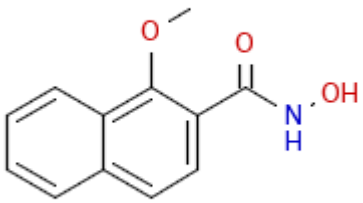
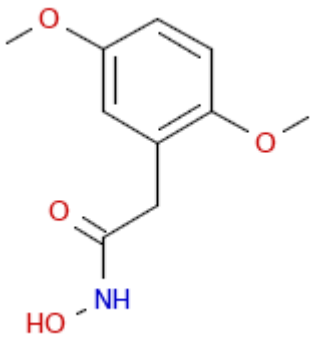
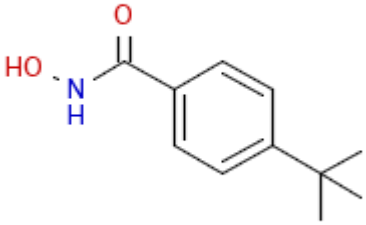
	>100	14	117	5.70
	>100	14	118	5.53
	>100	14	119	5.22

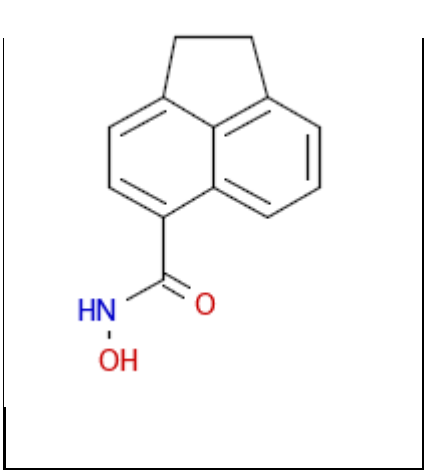
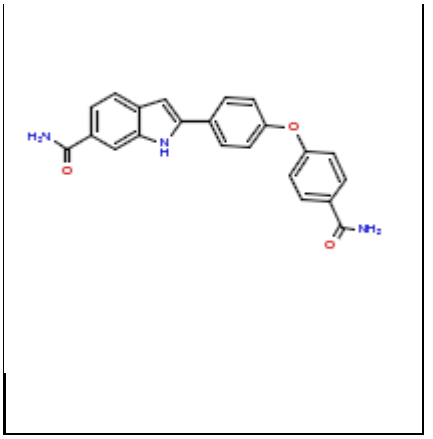
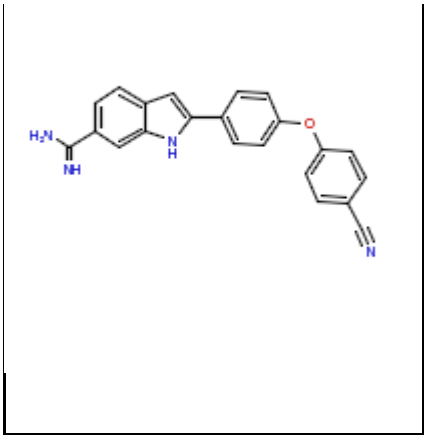
	>100	14	120	5.45
	>100	14	121	4.45
	>100	14	122	4.29

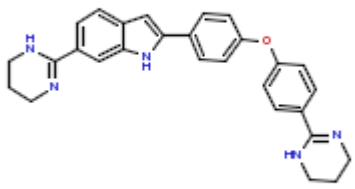
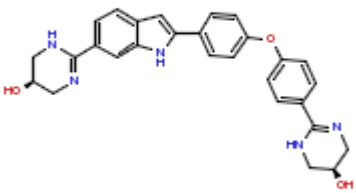
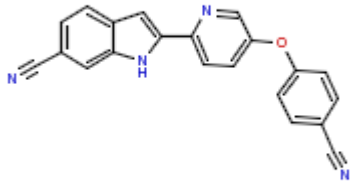
	>100	14	14	6.83
	>100	14	15	6.21
	>100	14	23	6.43

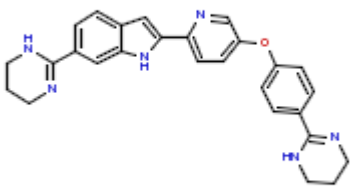
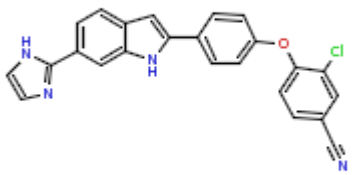
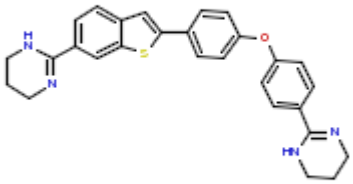
	>100	14	25	7.22
	>100	14	26	6.16
	>100	14	31	6.13

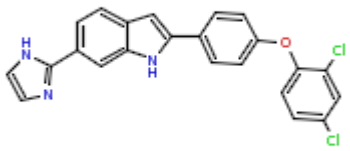
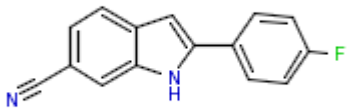
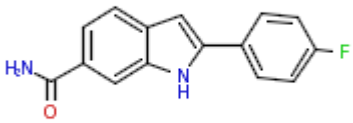
	>100	14	42	4.00
	>100	14	8	4.14
	>100	14	9	5.94

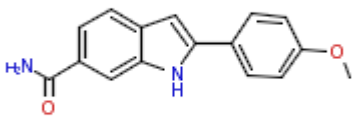
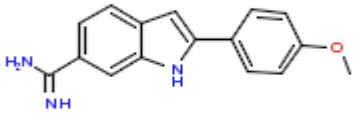
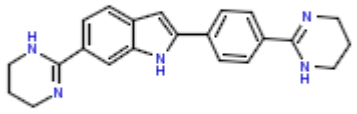
	>100	6	10	5.26
	>100	6	21	6.94
	>100	6	8	5.15

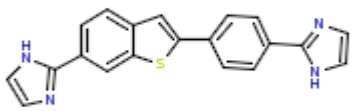
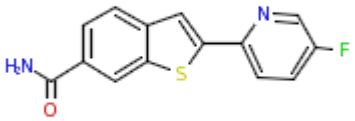
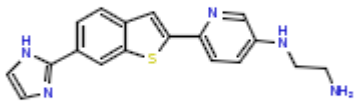
	>100	6	9	7.23
	>100	21	10	6.79
	>100	21	11	6.27

	>100	21	14	7.65
Chiral 	>100	21	15	5.41
	>100	21	23a	7.02

	>100	21	24b	5.50
	>100	21	24c	6.21
	>100	21	25b	7.20

	>100	21	29	6.38
	>100	21	39	6.37
	>100	21	40a	5.66

	>100	21	43a	6.48
	>100	21	43b	6.19
	>100	21	44b	6.98

	>100	21	46a	5.97
	>100	21	49	5.46
	>100	21	50	7.72

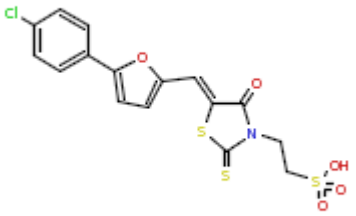
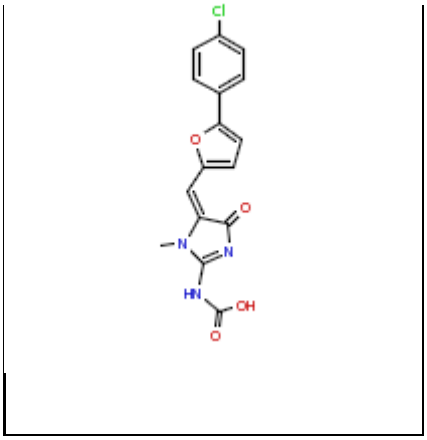
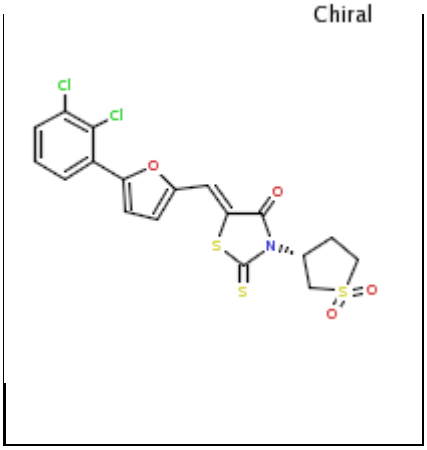
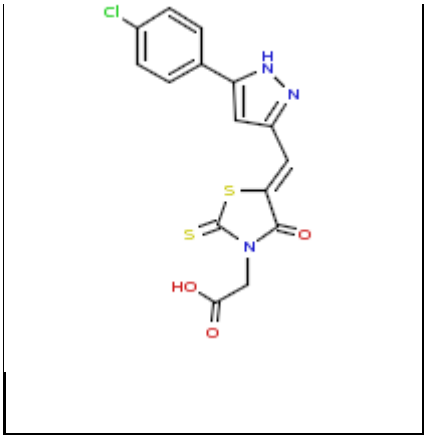
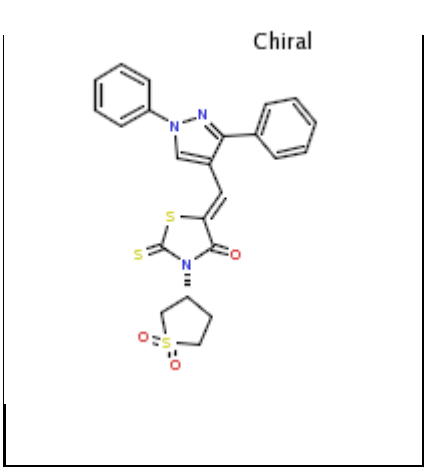
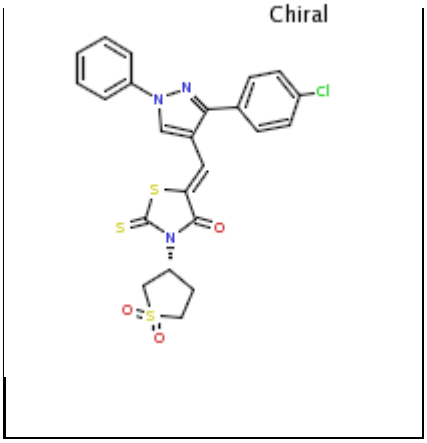
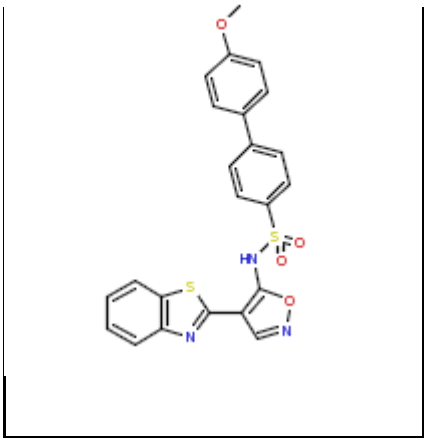
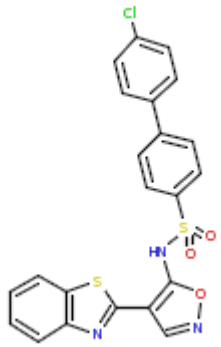
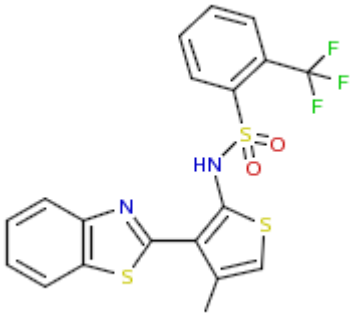
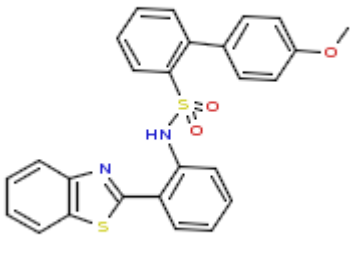
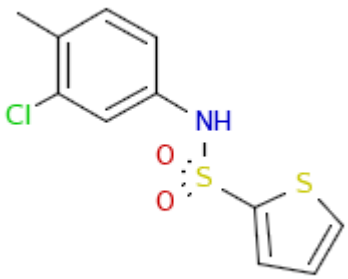
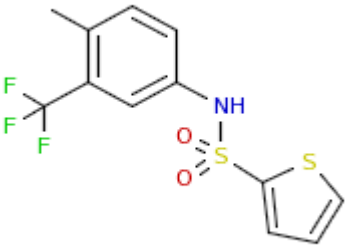
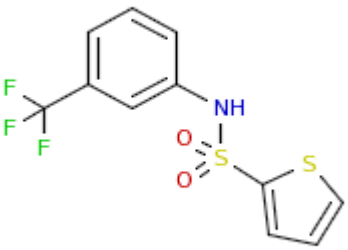
	>200	7	12	5.77

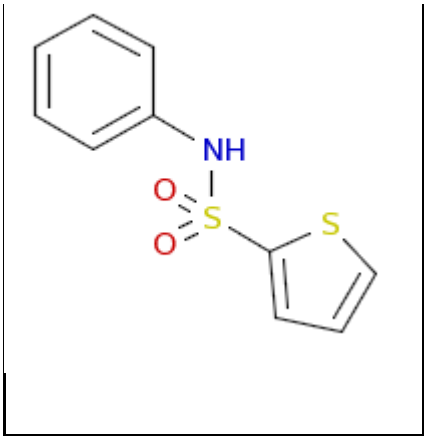
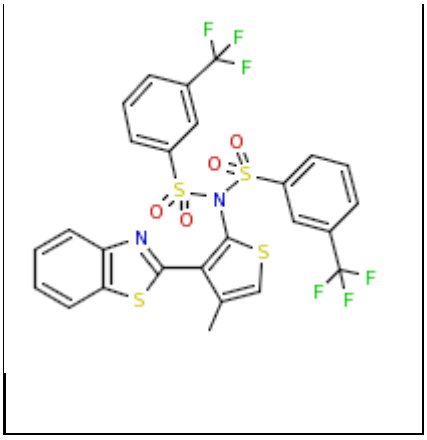
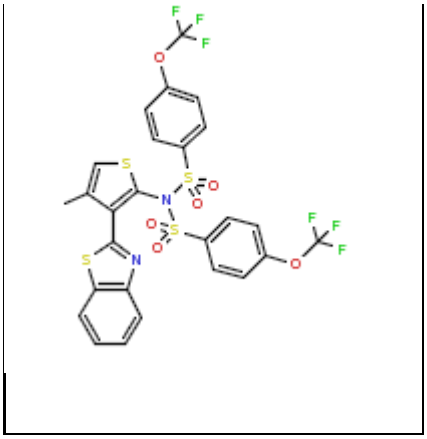
Table S5. Structures, LF biological activities, references, compound designators, and docking scores for screening set compounds in dataset **DB1E.**

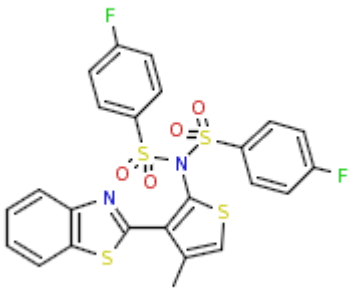
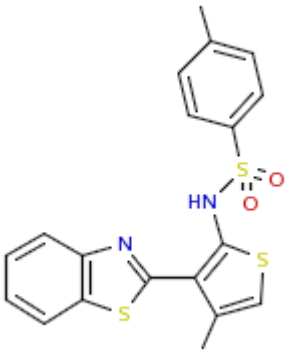
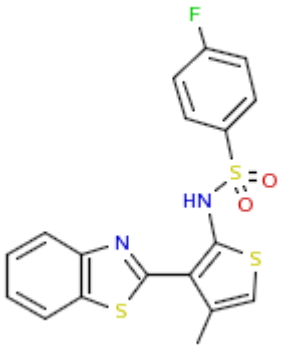
Structure	LF IC_{50} or K_i (μM)	Reference	Compound Designator	Docking Score (Surflex-Dock)
	>100	10	20	4.86
Chiral 	>100	7	14	4.98
	>100	7	28	6.56

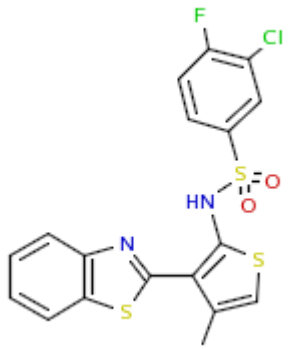
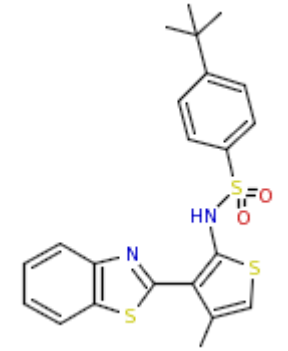
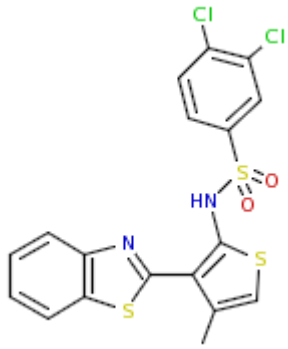
	>100	7	44	4.84
	>100	7	45	4.76
	>100	14	107	8.58

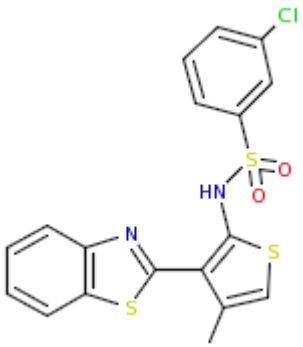
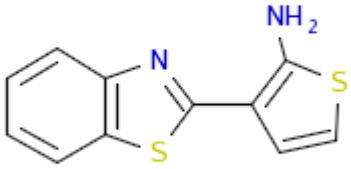
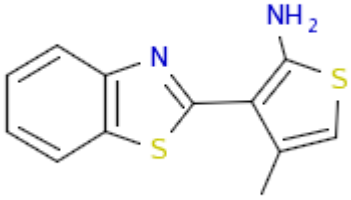
	>100	14	108	7.11
	>100	14	11	6.06
	>100	14	111	7.32

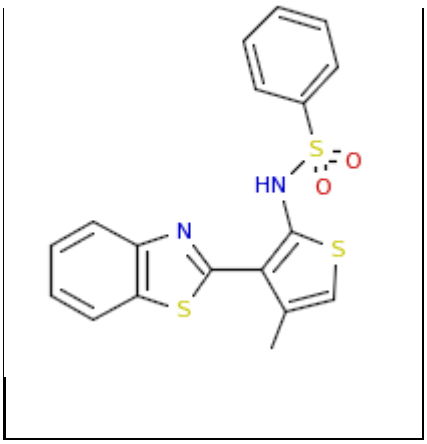
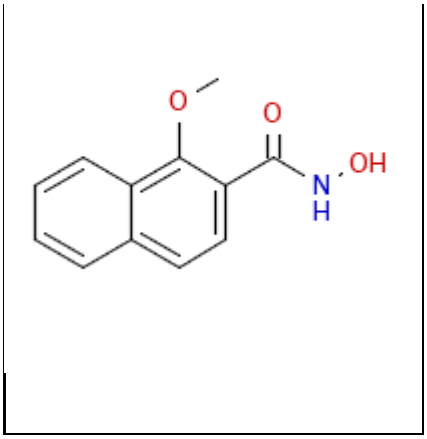
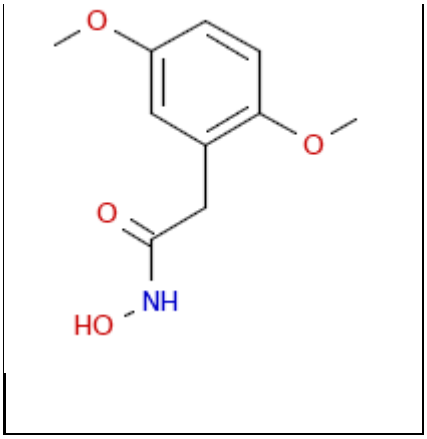
	>100	14	116	5.30
	>100	14	117	5.70
	>100	14	118	5.53

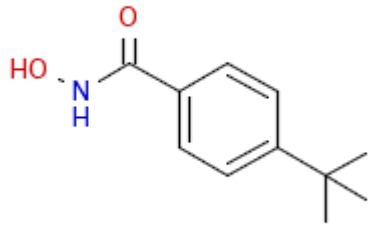
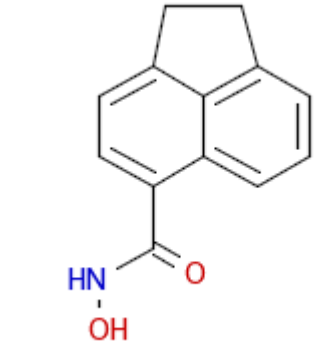
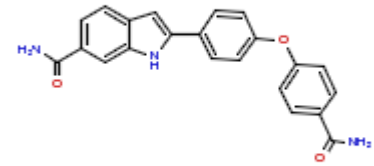
	>100	14	119	5.22
	>100	14	120	5.45
	>100	14	121	4.45

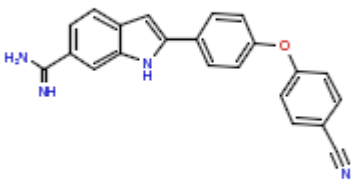
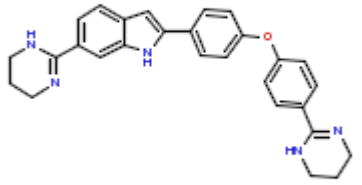
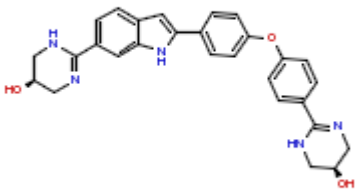
	>100	14	122	4.29
	>100	14	14	6.83
	>100	14	15	6.21

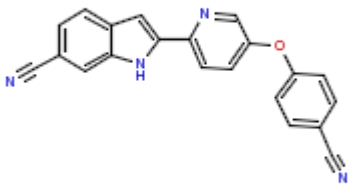
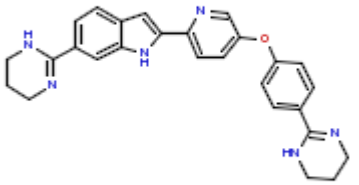
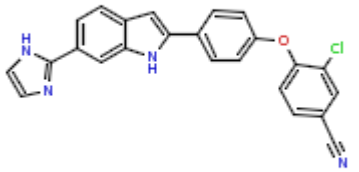
	>100	14	23	6.43
	>100	14	25	7.22
	>100	14	26	6.16

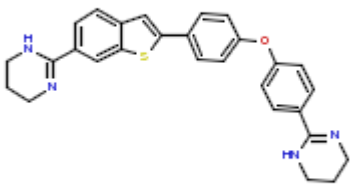
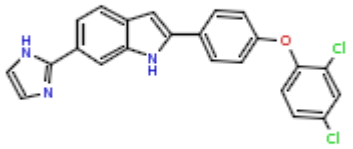
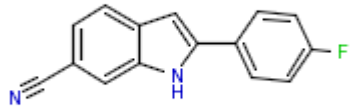
	>100	14	31	6.13
	>100	14	42	4.00
	>100	14	8	4.14

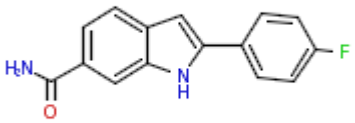
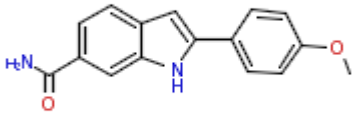
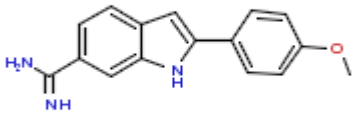
	>100	14	9	5.94
	>100	6	10	5.26
	>100	6	21	6.94

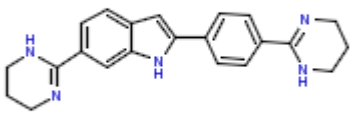
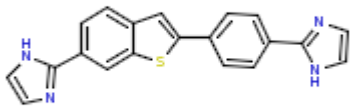
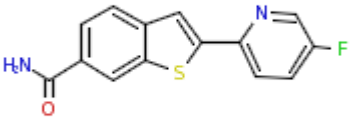
	>100	6	8	5.15
	>100	6	9	7.23
	>100	21	10	6.79

	>100	21	11	6.27
	>100	21	14	7.65
Chiral 	>100	21	15	5.41

	>100	21	23a	7.02
	>100	21	24b	5.50
	>100	21	24c	6.21

	>100	21	25b	7.20
	>100	21	29	6.38
	>100	21	39	6.37

	>100	21	40a	5.66
	>100	21	43a	6.48
	>100	21	43b	6.19

	>100	21	44b	6.98
	>100	21	46a	5.97
	>100	21	49	5.46

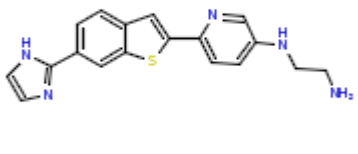
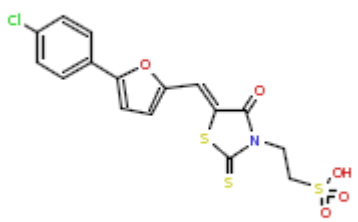
	>100	21	50	7.72
	>200	7	12	5.77

Table S6. Pairwise distances (Å) between features in final pharmacophore hypothesis **UM1.**

Pairwise Distance (Å)	F6 Hyd	F7 Hyd	F8 Hyd	F13 Acc	F20 Hyd	F21 Acc	F22 Acc	F23 Don
F6 Hyd[a]		4.63	8.45	1.69	6.06	1.55	5.03	1.12
F7 Hyd			3.89	4.43	10.53	5.86	9.20	5.36
F8 Hyd				8.03	14.42	9.75	12.78	9.06
F13 Acc					6.96	2.78	6.26	1.48
F20 Hyd						4.67	4.32	5.81
F21 Acc							4.53	1.92
F22 Acc								4.79
F23 Don								

[a]Hyd = hydrophobic; Aro = aromatic; Acc = hydrogen-bond acceptor; Don = hydrogen-bond donor

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