

基于分子描述符和机器学习方法预测和虚拟筛选乳腺癌靶向蛋白 HEC1 抑制剂

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Predicting and Virtually Screening Breast Cancer Targeting Protein HEC1 Inhibitors by Molecular Descriptors and Machine Learning Methods

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表 S1 本文中用到的所有描述符
Table S1 All descriptors in the paper

simple molecular properties(18)

1	W_{mol}	Molecular weight
2	nhyd	Count of hydrogen atoms
3	nhal	Count of halogen atoms
4	nhet	Count of hetero atoms
5	nhev	Count of heavy atoms
6	ncof	Count of F atoms
7	ncocl	Count of Cl atoms
8	ncobr	Count of Br atoms
9	ncoi	Count of I atoms
10	ncarb	Count of C atoms
11	nphos	Count of P atoms
12	nsulph	Count of S atoms
13	noxy	Count of O atoms
14	nnitro	Count of N atoms
15	nring	Numbers of rings
16	nrot	Number of rotatable bonds
17	ndonr	Number of H-bond donors
18	naccr	Number of H-bond acceptors
19	${}^0\chi$	Simple molecular connectivity Chi indices for path order 0
20	${}^1\chi$	Simple molecular connectivity Chi indices for path order 1
21	${}^2\chi$	Simple molecular connectivity Chi indices for path order 2
22	${}^3\chi_{\text{P}}$	Simple molecular connectivity Chi indices for path order 3
23	${}^3\chi_{\text{C}}$	Simple molecular connectivity Chi indices for cluster
24	${}^4\chi_{\text{PC}}$	Simple molecular connectivity Chi indices for path/cluster
25	${}^3\chi_{\text{CH}}$	Simple molecular connectivity Chi indices for cycles of 3 atoms
26	${}^4\chi_{\text{CH}}$	Simple molecular connectivity Chi indices for cycles of 4 atom
27	${}^5\chi_{\text{CH}}$	Simple molecular connectivity Chi indices for cycles of 5 atom

28	${}^6\chi_{\text{CH}}$	Simple molecular connectivity Chi indices for cycles of 6 atom
29	χ^{v}	Valence molecular connectivity Chi indices for path order 0
30	χ^{v}	Valence molecular connectivity Chi indices for path order 1
31	χ^{v}	Valence molecular connectivity Chi indices for path order 2
32	$\chi^{\text{v}}_{\text{P}}$	Valence molecular connectivity Chi indices for path order 3
33	$\chi^{\text{v}}_{\text{C}}$	Valence molecular connectivity Chi indices for cluster
34	$\chi^{\text{v}}_{\text{PC}}$	Valence molecular connectivity Chi indices for path/cluster
35	$\chi^{\text{v}}_{\text{CH}}$	valence molecular connectivity Chi indices for cycles of 3 atoms
36	$\chi^{\text{v}}_{\text{CH}}$	valence molecular connectivity Chi indices for cycles of 4 atoms
37	$\chi^{\text{v}}_{\text{CH}}$	valence molecular connectivity Chi indices for cycles of 5 atoms
38	$\chi^{\text{v}}_{\text{CH}}$	valence molecular connectivity Chi indices for cycles of 6 atoms
39	κ	Molecular shape Kappa indices for one boned fragments
40	κ	Molecular shape Kappa indices for two boned fragments
41	κ	Molecular shape Kappa indices for three boned fragments
42	κ_{α}	Kappa alpha indices for one boned fragments
43	κ_{α}	Kappa alpha indices for two boned fragments
44	κ_{α}	Kappa alpha indices for three boned fragments
45	phi	Kier molecular flexibility index
46	S_{hev}	Sum of electrotopological state (Estate) indices of heavy atoms
47	S_{car}	Sum of Estate indices of carbon atoms
48	S_{het}	Sum of Estate indices of hetero atoms
49	S_{hal}	Sum of Estate indices of halogen atoms
50	$S(1)$	Atom-type H Estate sum for -OH
51	$S(2)$	Atom-type H Estate sum for =NH
52	$S(3)$	Atom-type H Estate sum for -SH
53	$S(4)$	Atom-type H Estate sum for -NH₂
54	$S(5)$	Atom-type H Estate sum for > NH
55	$S(6)$	Atom-type H Estate sum for : NH:
56	$S(7)$	Atom-type H Estate sum for #CH (sp)
57	$S(8)$	Atom-type H Estate sum for =CH₂ (sp ²)
58	$S(9)$	Atom-type H Estate sum for =CH- (sp ²)
59	$S(10)$	Atom-type H Estate sum for :CH: (sp ² , aromatic)
60	$S(11)$	Atom-type H Estate sum for CH_n X (sp ³ , X= F, Cl, Br, I)
61	$S(12)$	Atom-type H Estate sum for CH_n (Saturated)
62	$S(13)$	Atom-type H Estate sum for CH_n (unsaturated)
63	$S(14)$	Atom-type H Estate sum for CH_n (aromatic)

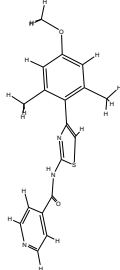
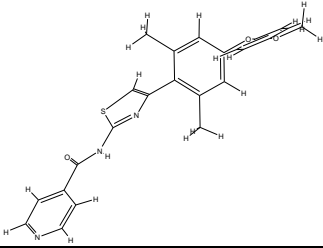
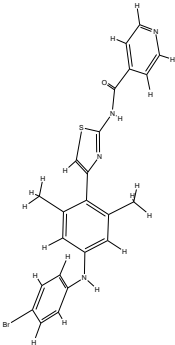
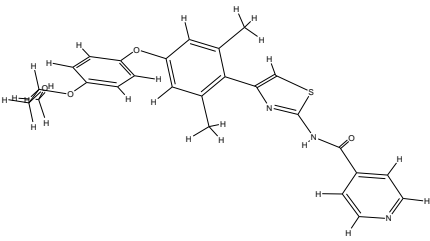
64	S(15)	Atom-type H Estate sum for AH_n (not C, N, O, S)
65	S(16)	Atom-type Estate sum for $-\text{CH}_3$
66	S(17)	Atom-type Estate sum for $=\text{CH}_2$
67	S(18)	Atom-type Estate sum for $>\text{CH}_2$
68	S(19)	Atom-type Estate sum for $\equiv\text{CH}$
69	S(20)	Atom-type Estate sum for $=\text{CH}-$
70	S(21)	Atom-type Estate sum for $:\text{CH}:$ (aromatic)
71	S(22)	Atom-type Estate sum for $>\text{CH}-$
72	S(23)	Atom-type Estate sum for $=\text{C}=\text{C}$
73	S(24)	Atom-type Estate sum for $\equiv\text{C}-$
74	S(25)	Atom-type Estate sum for $=\text{C}<$
75	S(26)	Atom-type Estate sum for $:\text{C}:-$
76	S(27)	Atom-type Estate sum for $:\text{C}::$
77	S(28)	Atom-type Estate sum for $>\text{C}<$
78	S(29)	Atom-type Estate sum for $-\text{NH}_2$
79	S(30)	Atom-type Estate sum for $=\text{NH}$
80	S(31)	Atom-type Estate sum for $>\text{NH}$
81	S(32)	Atom-type Estate sum for $:\text{NH}:$
82	S(33)	Atom-type Estate sum for $\equiv\text{N}$
83	S(34)	Atom-type Estate sum for $=\text{N}-$
84	S(35)	Atom-type Estate sum for $:\text{N}:$
85	S(36)	Atom-type Estate sum for $>\text{N}-$
86	S(37)	Atom-type Estate sum for $-\text{N}<<$ (NO_2)
87	S(38)	Atom-type Estate sum for $:\text{N}:-$
88	S(39)	Atom-type Estate sum for $-\text{OH}$
89	S(40)	Atom-type Estate sum for $=\text{O}$
90	S(41)	Atom-type Estate sum for $-\text{O}-$
91	S(42)	Atom-type Estate sum for $:\text{O}:$
92	S(43)	Atom-type Estate sum for $-\text{F}$
93	S(44)	Atom-type Estate sum for $-\text{SiH}_3$
94	S(45)	Atom-type Estate sum for $-\text{SiH}_2-$
95	S(46)	Atom-type Estate sum for $>\text{SiH}-$
96	S(47)	Atom-type Estate sum for $>\text{Si}<$
97	S(48)	Atom-type Estate sum for $-\text{PH}_2$
98	S(49)	Atom-type Estate sum for $-\text{PH}-$
99	S(50)	Atom-type Estate sum for $>\text{P}-$
100	S(51)	Atom-type Estate sum for $-\text{>P=}$ (P.O)
101	S(52)	Atom-type Estate sum for $-\text{=P=}$ (P. O_2)
102	S(53)	Atom-type Estate sum for $-$
103	S(54)	Atom-type Estate sum for $-\text{SH}$
104	S(55)	Atom-type Estate sum for $=\text{S}$
105	S(56)	Atom-type Estate sum for $-\text{S}-$
106	S(57)	Atom-type Estate sum for $:\text{S}:$

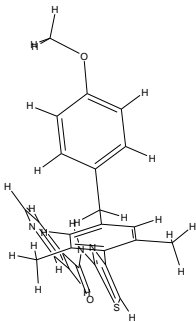
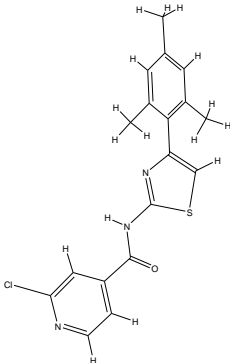
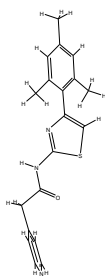
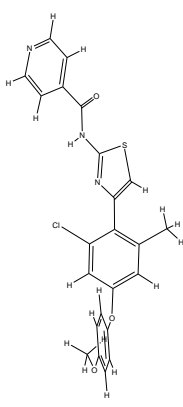
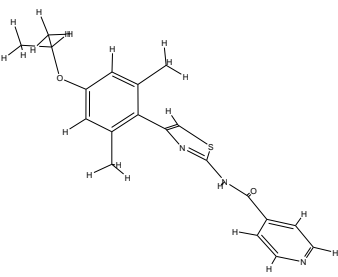
107	<i>S</i> (58)	Atom-type Estate sum for >S=O
108	<i>S</i> (59)	Atom-type Estate sum for >S<<
109	<i>S</i> (60)	Atom-type Estate sum for -Cl
110	<i>S</i> (61)	Atom-type Estate sum for GeH ₃
111	<i>S</i> (62)	Atom-type Estate sum for -GeH ₂ -
112	<i>S</i> (63)	Atom-type Estate sum for >GeH-
113	<i>S</i> (64)	Atom-type Estate sum for >Ge<
114	<i>S</i> (65)	Atom-type Estate sum for -AsH ₂
115	<i>S</i> (66)	Atom-type Estate sum for -AsH-
116	<i>S</i> (67)	Atom-type Estate sum for >As-
117	<i>S</i> (68)	Atom-type Estate sum for ->As=
118	<i>S</i> (69)	Atom-type Estate sum for -SeH
119	<i>S</i> (70)	Atom-type Estate sum for =Se
120	<i>S</i> (71)	Atom-type Estate sum for -Se-
121	<i>S</i> (72)	Atom-type Estate sum for :Se:
122	<i>S</i> (73)	Atom-type Estate sum for >Se=
123	<i>S</i> (74)	Atom-type Estate sum for -=Se=-
124	<i>S</i> (75)	Atom-type Estate sum for -Br
125	<i>S</i> (76)	Atom-type Estate sum for -SnH ₃
126	<i>S</i> (77)	Atom-type Estate sum for -SnH ₂ -
127	<i>S</i> (78)	Atom-type Estate sum for >SnH-
128	<i>S</i> (79)	Atom-type Estate sum for >Sn<
129	<i>S</i> (80)	Atom-type Estate sum for -I
130	Twien	Weiner Index
131	Tcent	Centric Index
132	Talte	Altenburg Index
133	Tbala	Balaban Index
134	Thara	Harary Number
135	Tschl	Schultz Index
136	Tradi	PetitJohn R2 Index
137	Tdiam	PetitJohn D2 Index
138	Tbmdd	Mean Distance Index
139	Tpeti	PetitJohn I2 Index
140	Tiwie	Information Weiner
141	Trmsd	Balaban RMSD Index
142	Tigdi	Graph Distance Index
143	π_i	Polarizability index
144	μ	Molecular dipole moment
145	$Q_{H, Max}$	Most positive charge on H atoms
146	$Q_{C, Max}$	Most positive charge on C atoms
147	$Q_{N, Max}$	Most positive charge on N atoms
148	$Q_{O, Max}$	Most positive charge on O atoms
149	$Q_{H, Min}$	Most negative charge on H atoms

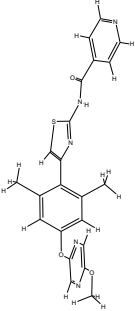
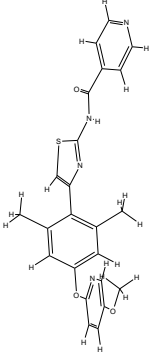
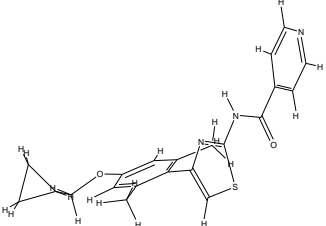
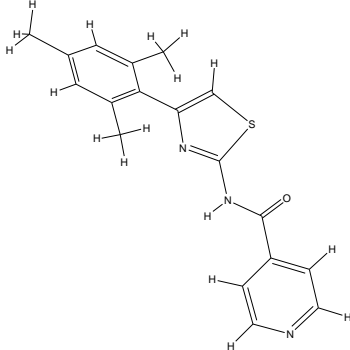
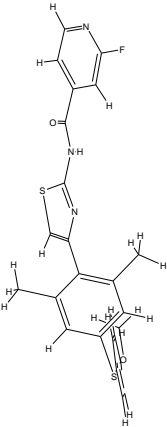
150	$Q_{C, \text{Min}}$	Most negative charge on C atoms
151	$Q_{N, \text{Min}}$	Most negative charge on N atoms
152	$Q_{O, \text{Min}}$	Most negative charge on O atoms
153	$A_{Q, \text{max}}$	Most positive charge in a molecule
154	$A_{Q, \text{min}}$	Most negative charge in a molecule
155	$Q_{H, \text{SS}}$	Sum of squares of charges on H atoms
156	$Q_{C, \text{SS}}$	Sum of squares of charges on C atoms
157	$Q_{N, \text{SS}}$	Sum of squares of charges on N atoms
158	$Q_{O, \text{SS}}$	Sum of squares of charges on O atoms
159	$Q_{A, \text{SS}}$	Sum of squares of charges on all atoms
160	Mpc	Mean of positive charges
161	Mnc	Mean of negative charges
162	Mac	Mean absolute charge
163	Rpc	Relative positive charge
164	Rnc	Relative negative charge
165	dis1	Length vectors (longest distance)
166	dis2	Length vectors (longest third atom)
167	dis3	Length vectors (4 th atom)
168	V_{mc}	Van der Waals molecular volume
169	AS	Solvent accessible surface area
170	VS	van der Waals surface area
171	MS	Molecular surface area
172	PSA	Polar molecular surface area
173	Sapc	Sum of solvent accessible surface areas of positively charged atoms
174	Sanc	Sum of solvent accessible surface areas of negatively charged atoms
175	Sapcw	Sum of charge weighted solvent accessible surface areas of positively charged atoms
176	Sancw	Sum of charge weighted solvent accessible surface areas of negatively charged atoms
177	Svpc	Sum of van der Waals surface areas of positively charged atoms
178	Svnc	Sum of van der Waals surface areas of negatively charged atoms
179	Svpcw	Sum of charge weighted van der Waals surface areas of positively charged atoms
180	Svncw	Sum of charge weighted van der Waals surface areas of negatively charged atoms
181	Rugty	Molecular rugosity
182	Gloty	Molecular globularity
183	Shpl	Hydrophilic region
184	Shpb	Hydrophobic region
185	Capy	Capacity factor
186	Hlb	Hydrophilic-Hydrophobic balance
187	Hiwpl	Hydrophilic Intery Moment
188	Hiwpb	Hydrophobic Intery Moment

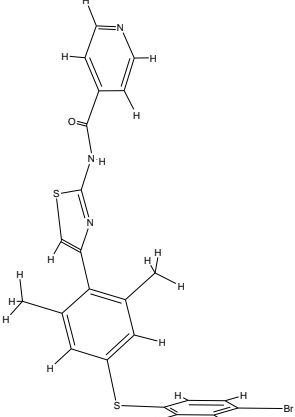
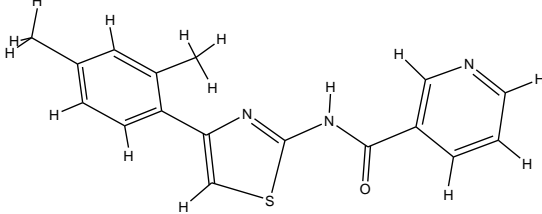
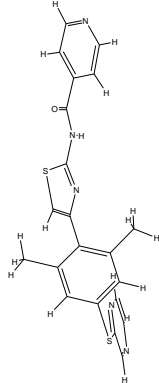
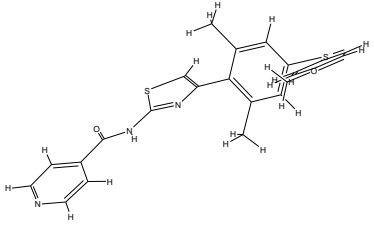
表S2 训练集中化合物的结构、类别和来源 (I: HEC1抑制剂, N: HEC1非抑制剂)

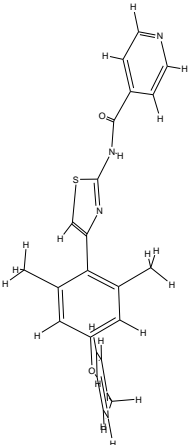
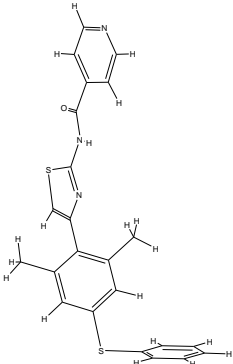
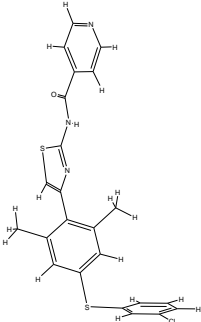
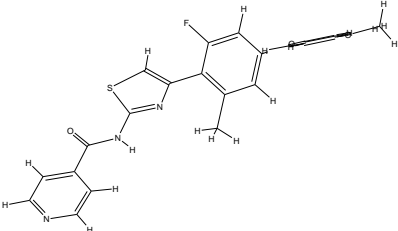
Table S2 Structure, categories and sources of training set compounds
(I: HEC1 inhibitors, N: HEC1 non-inhibitor)

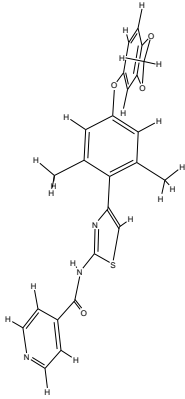
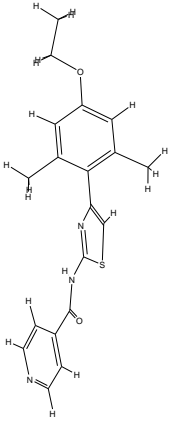
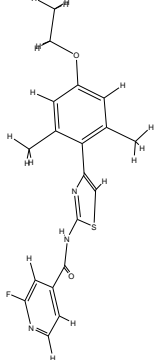
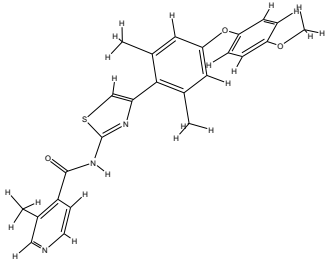
No.	ID	结构	类别	来源
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2	48		I	[1]
3	52		I	[1]
4	12		I	[1]

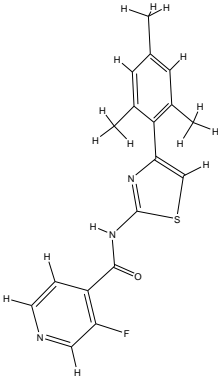
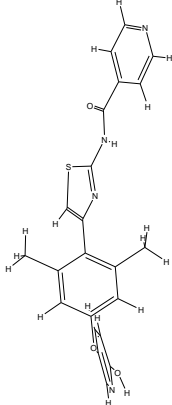
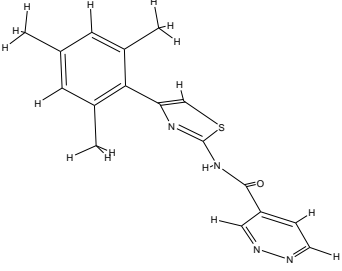
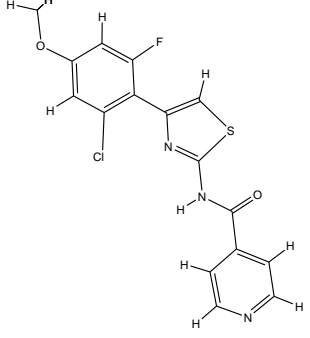
5	51		I	[1]
6	II-64		I	[1]
7	47		I	[1]
8	53		I	[1]
9	46		I	[1]

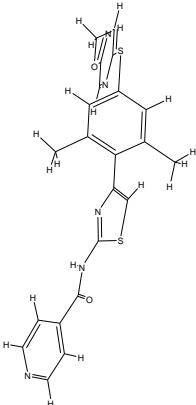
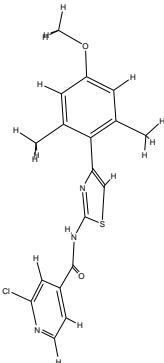
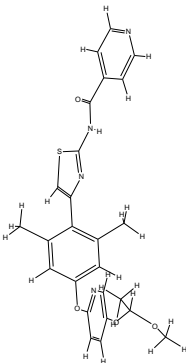
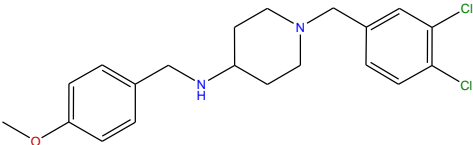
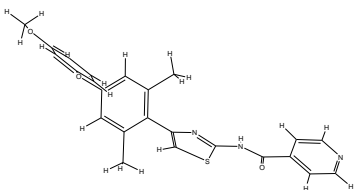
10	15		I	[1]
11	18		I	[1]
12	4		I	[1]
13	II-1		I	[1]
14	II-126		I	[1]

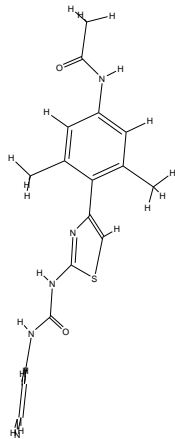
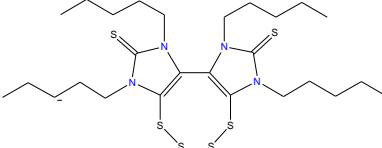
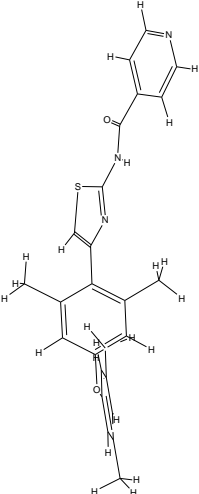
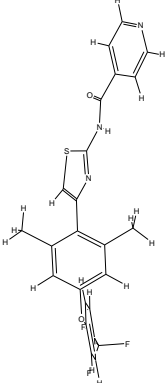
15	37		I	[1]
16	JMC-11		I	[2]
17	11		I	[1]
18	II-117		I	[1]

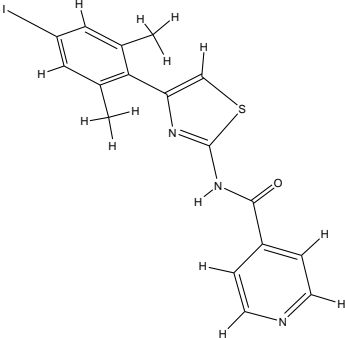
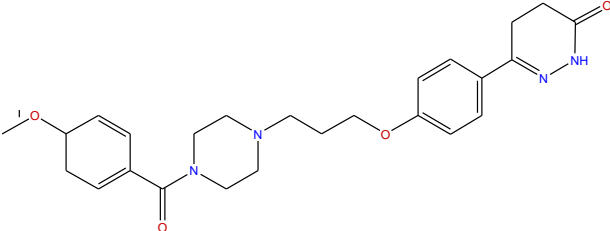
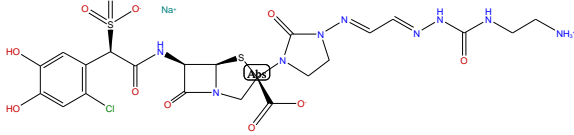
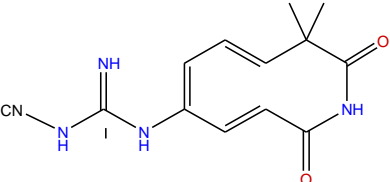
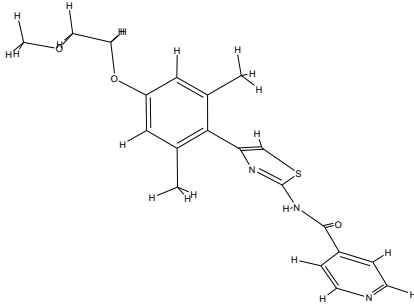
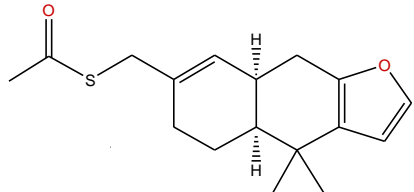
19	II-112		I	[1]
20	II-115		I	[1]
21	38		I	[1]
22	30		I	[1]

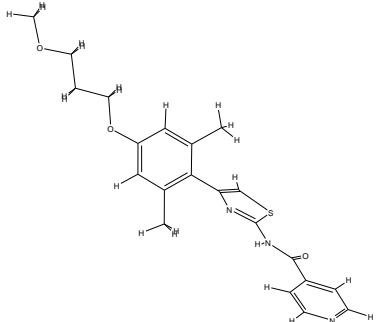
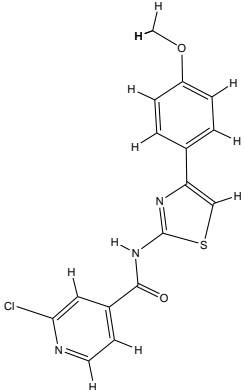
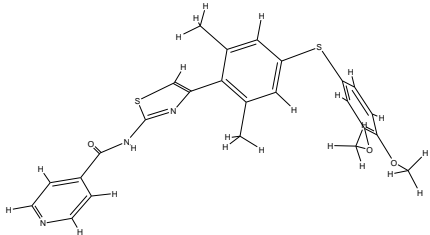
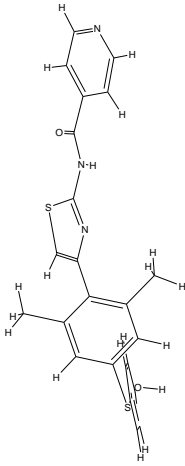
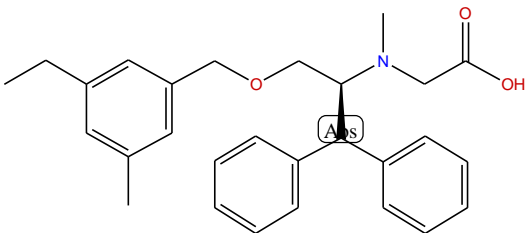
23	II-101		I	[1]
24	II-52		I	[1]
25	II-70		I	[1]
26	II-121		I	[1]

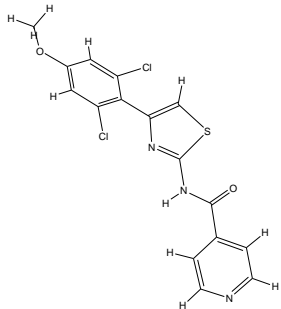
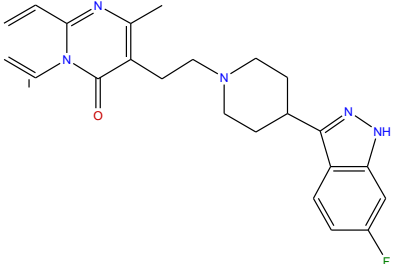
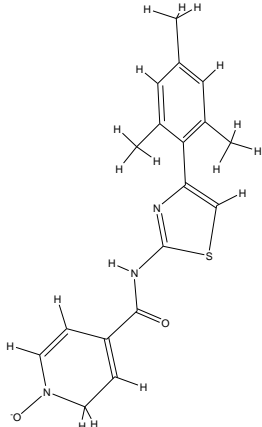
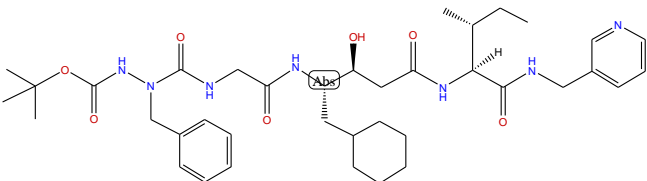
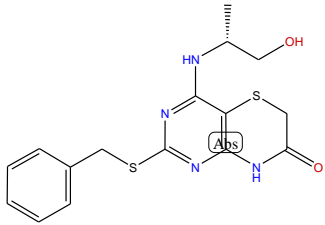
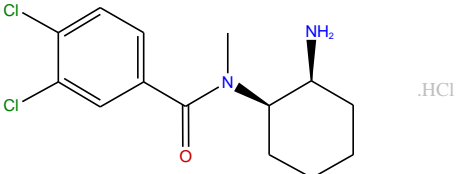
27	II-77	 <p>The structure shows a thiazole ring connected via its nitrogen atom to a carbonyl group. This carbonyl group is further attached to a pyridine ring. The pyridine ring has a fluorine atom at the 3-position and a hydrogen atom at the 4-position. The thiazole ring has a methyl group at the 4-position and a hydrogen atom at the 5-position.</p>	I	[1]
28	5	 <p>The structure features a thiazole ring connected to a pyridine ring. The pyridine ring has a nitro group (-NO2) at the 3-position. The thiazole ring has a methyl group at the 4-position and a hydrogen atom at the 5-position.</p>	I	[1]
29	II-8	 <p>The structure shows a thiazole ring connected via its nitrogen atom to a carbonyl group. This carbonyl group is attached to a pyridine ring. The pyridine ring has a methyl group at the 3-position. The thiazole ring has a methyl group at the 4-position and a hydrogen atom at the 5-position.</p>	I	[1]
30	13	 <p>The structure depicts a thiazole ring connected to a pyridine ring. The pyridine ring has a chlorine atom at the 3-position and a methoxy group (-OCH3) at the 4-position. The thiazole ring has a methyl group at the 4-position and a hydrogen atom at the 5-position.</p>	I	[1]

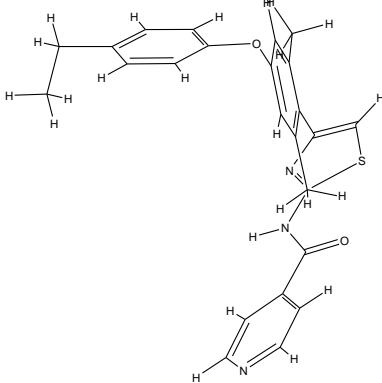
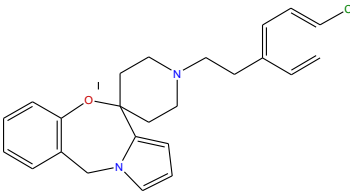
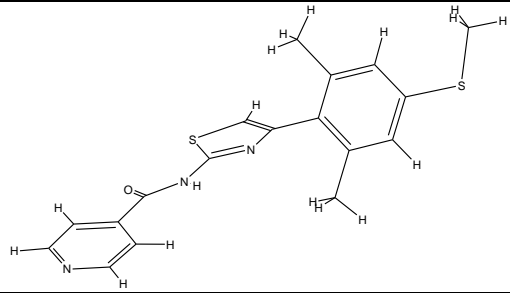
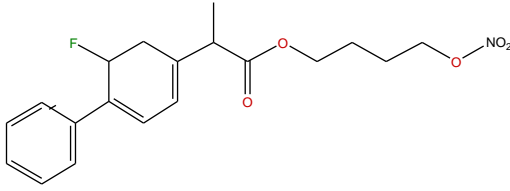
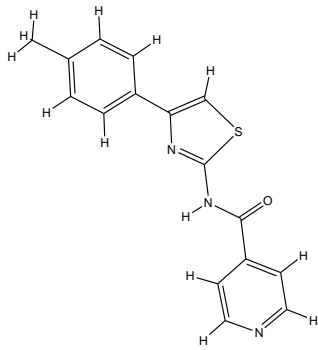
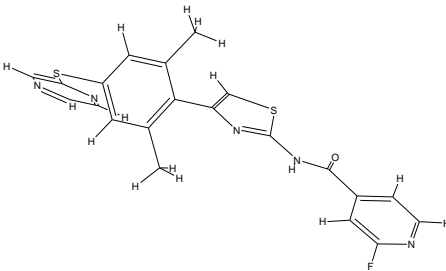
31	25		I	[1]
32	II-65		I	[1]
33	17		I	[1]
34	124178	 .HCl .HCl	N	MDDR
35	II-107		I	[1]

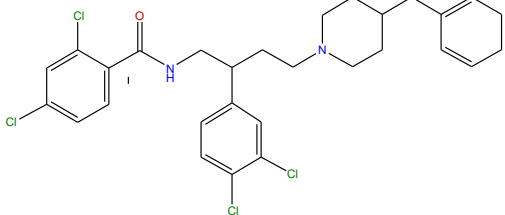
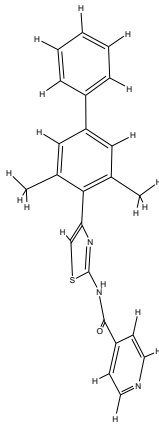
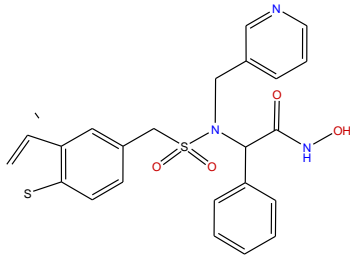
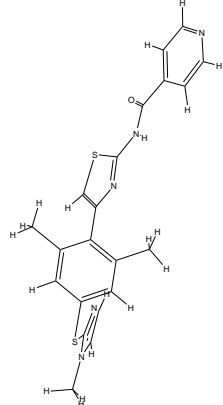
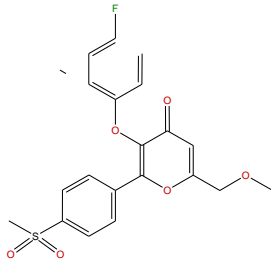
36	II-68		I	[1]
37	71941		N	MDDR
38	II-102		I	[1]
39	II-108		I	[1]

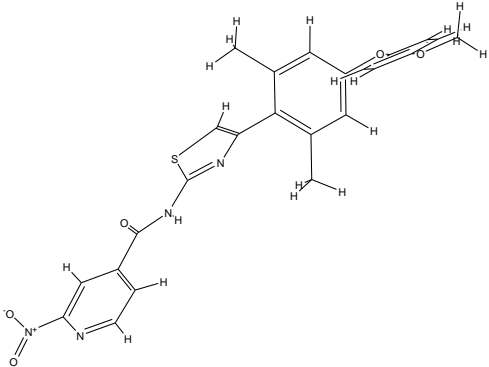
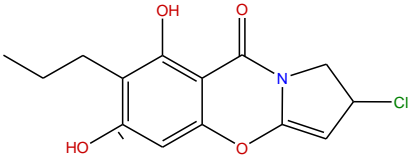
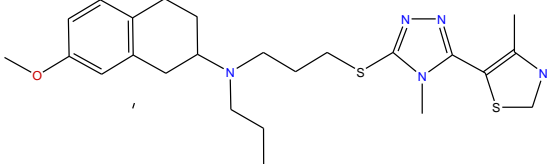
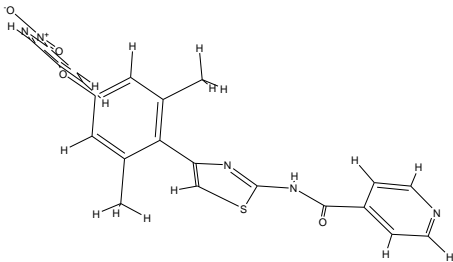
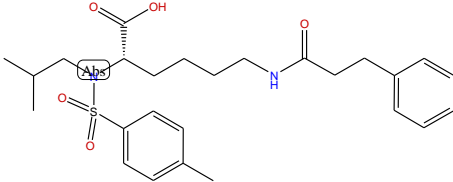
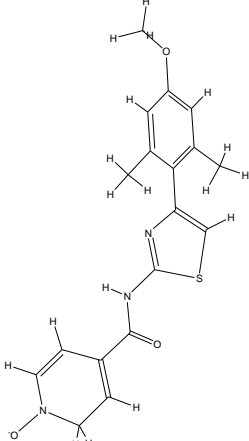
40	II-114		I	[1]
41	10837		N	MDDR
42	74544		N	MDDR
43	2759		N	MDDR
44	II-109		I	[1]
45	27339		N	MDDR

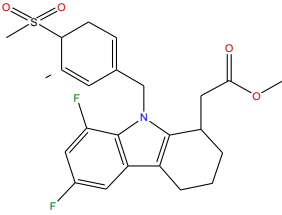
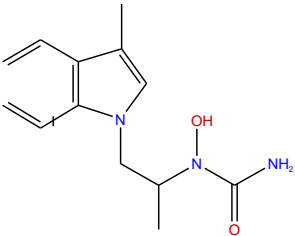
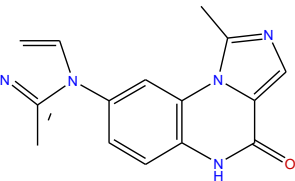
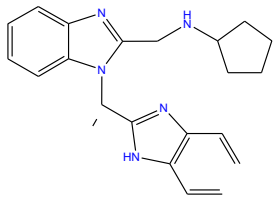
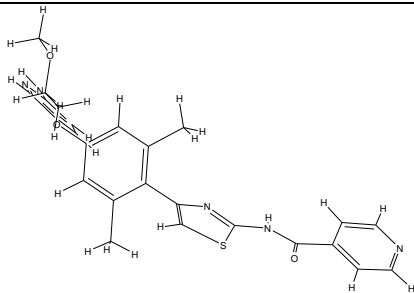
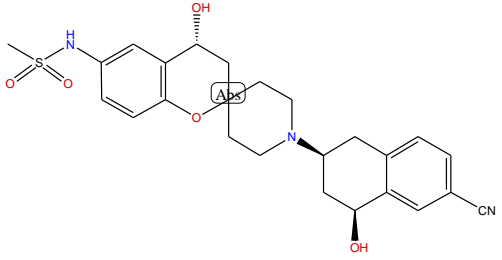
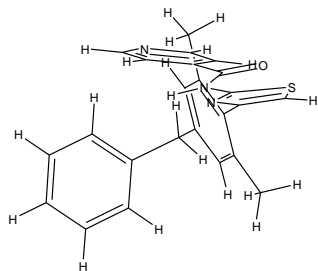
46	II-110		I	[1]
47	II-54		I	[1]
48	33		I	[1]
49	34		I	[1]
50	62858		N	MDDR

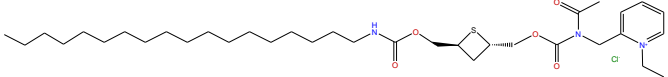
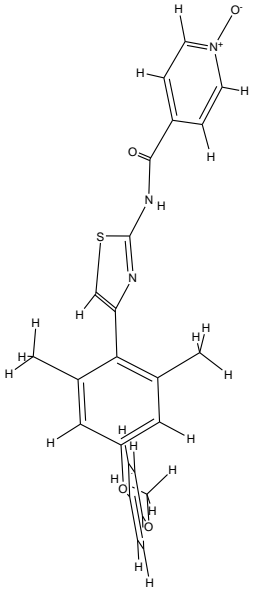
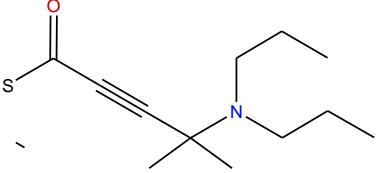
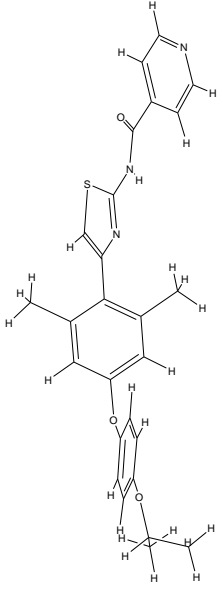
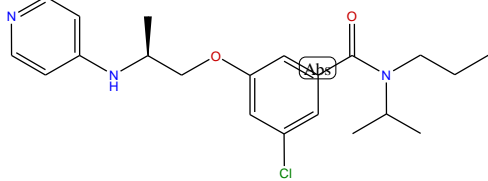
57	10		I	[1]
58	20063		N	MDDR
59	II-71		I	[1]
60	19345		N	MDDR
61	127666		N	MDDR
62	40174		N	MDDR

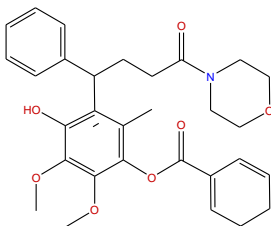
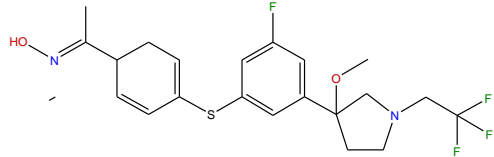
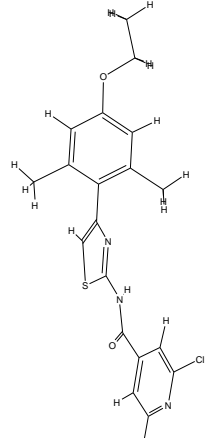
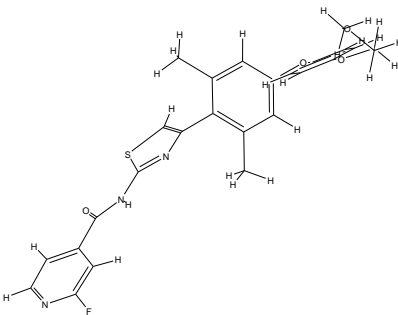
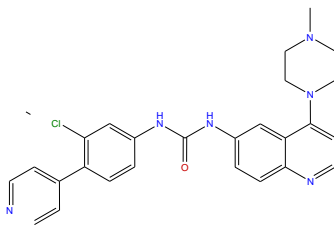
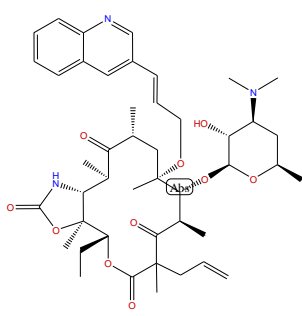
63	II-113		I	[1]
64	8833		N	MDDR
65	II-125		I	[1]
66	71186		N	MDDR
67	II-6		I	[1]
68	19		I	[1]

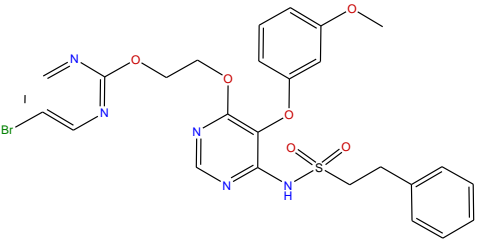
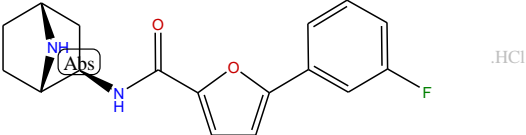
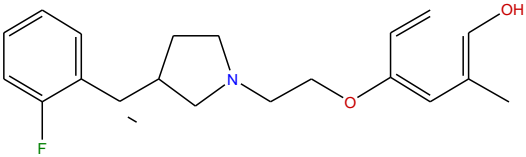
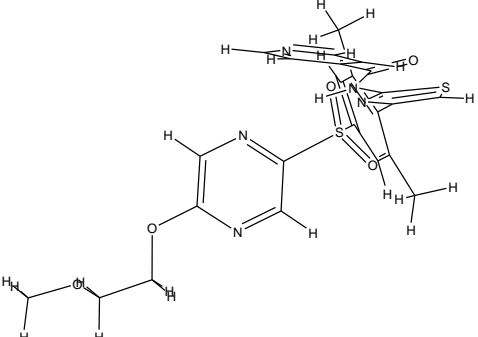
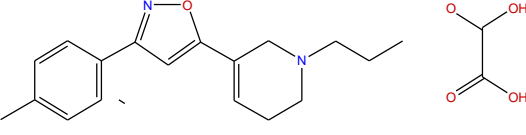
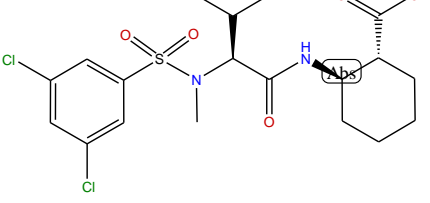
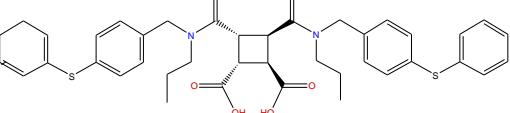
69	37522		N	MDDR
70	II-53		I	[1]
71	128043		N	MDDR
72	41		I	[1]
73	128182		N	MDDR

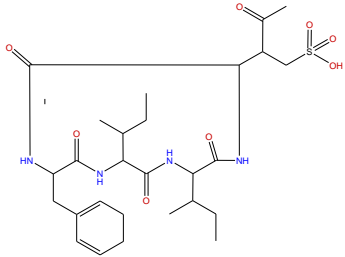
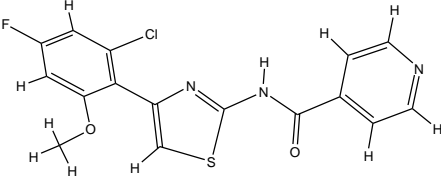
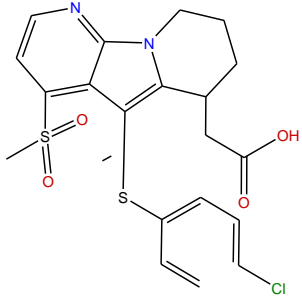
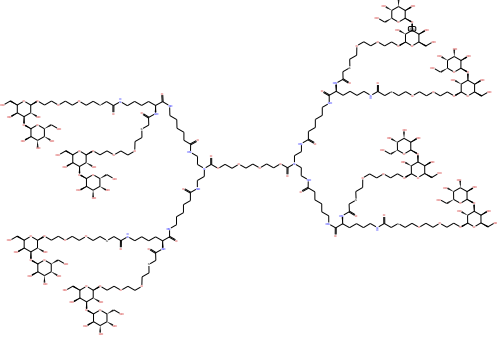
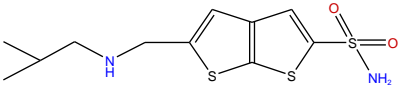
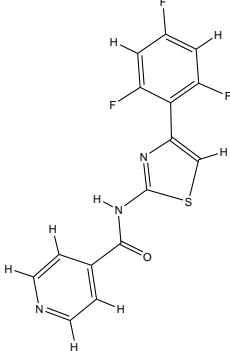
74	II-124		I	[1]
75	112512		N	MDDR
76	117716		N	MDDR
77	24		I	[1]
78	128435		N	MDDR
79	II-72		I	[1]

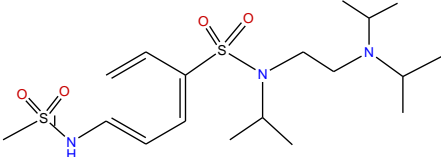
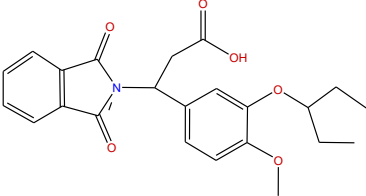
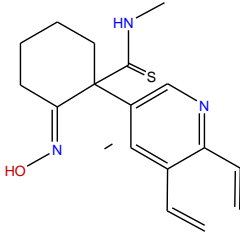
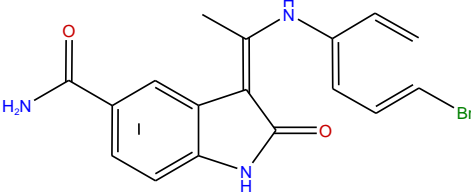
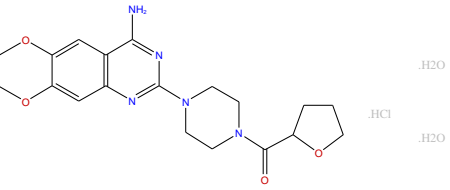
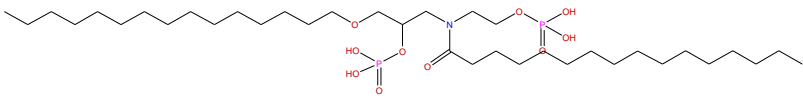
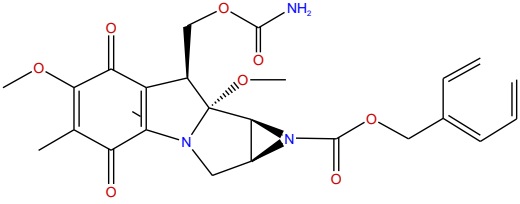
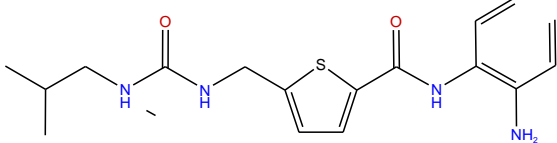
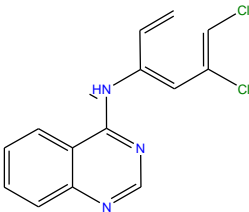
80	10556		N	MDDR
81	43999		N	MDDR
82	26422		N	MDDR
83	140405		N	MDDR
84	29		I	[1]
85	80602		N	MDDR
86	II-118		I	[1]

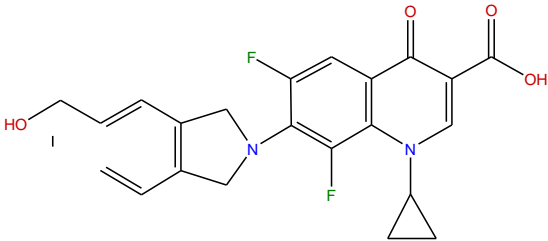
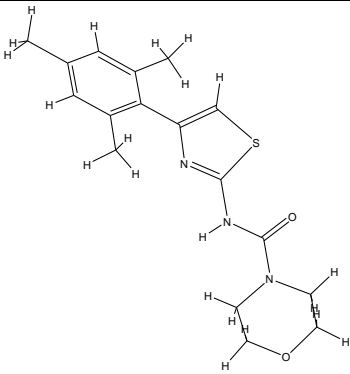
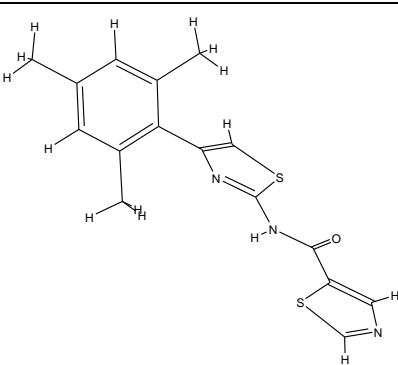
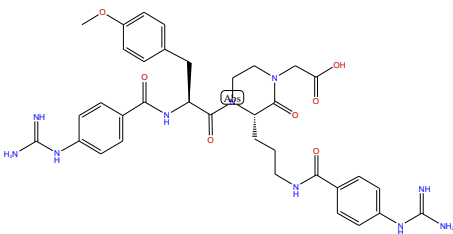
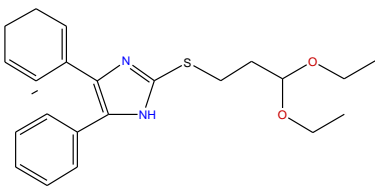
87	93314		N	MDDR
88	II-120		I	[1]
89	130010		N	MDDR
90	16		I	[1]
91	115093		N	MDDR

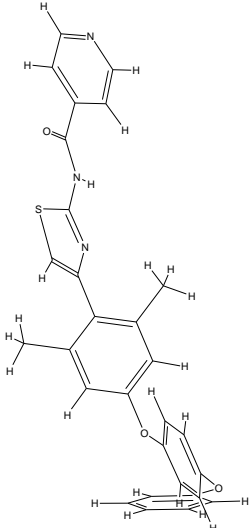
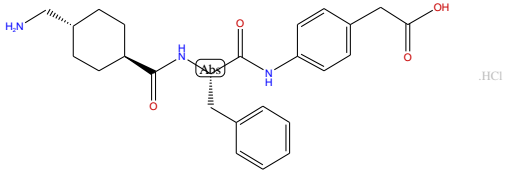
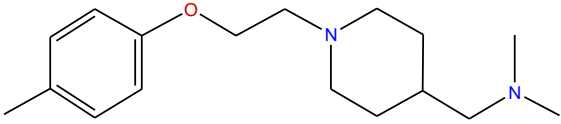
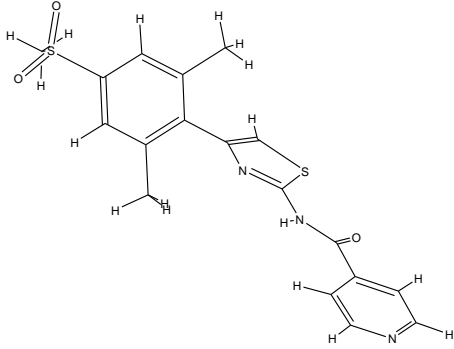
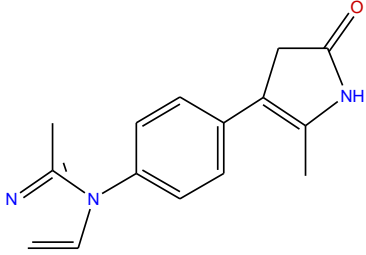
92	8320		N	MDDR
93	59024		N	MDDR
94	II-66		I	[1]
95	20		I	[1]
96	106931		N	MDDR
97	121496		N	MDDR

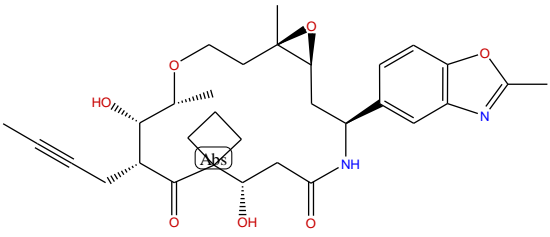
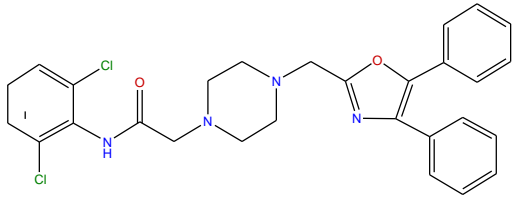
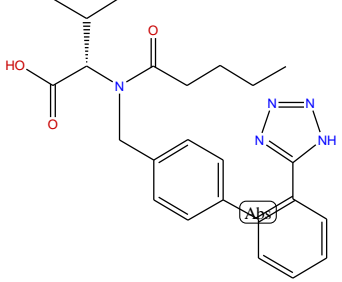
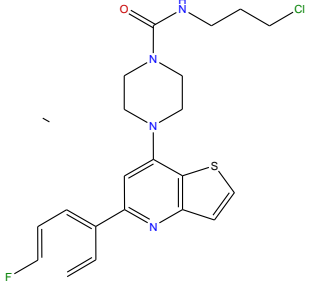
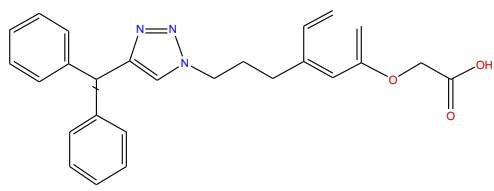
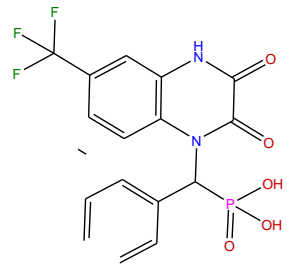
98	132998		N	MDDR
99	141920		N	MDDR
100	91528		N	MDDR
101	31		I	[1]
102	55038		N	MDDR
103	107919		N	MDDR
104	71844		N	MDDR

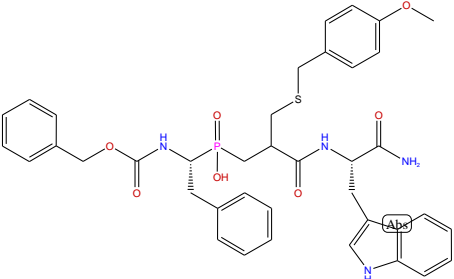
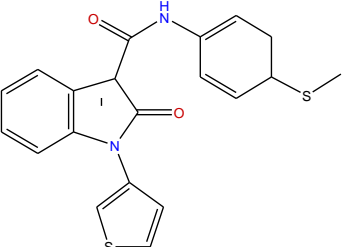
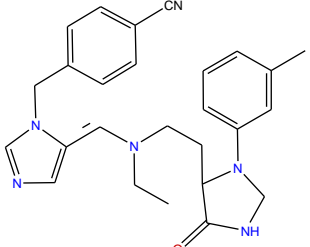
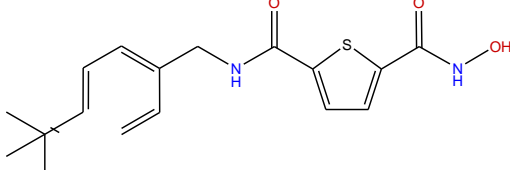
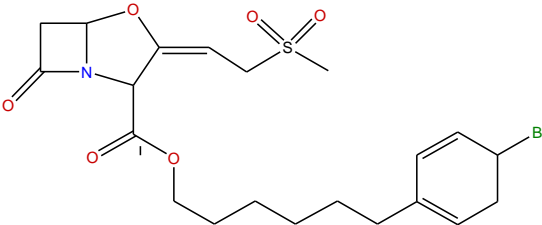
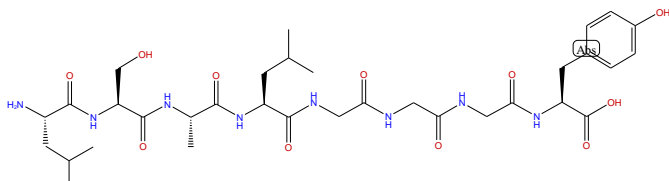
105	148432		N	MDDR
106	14		I	[1]
107	153912		N	MDDR
108	127210		N	MDDR
109	10478		N	MDDR
110	II-76		I	[1]

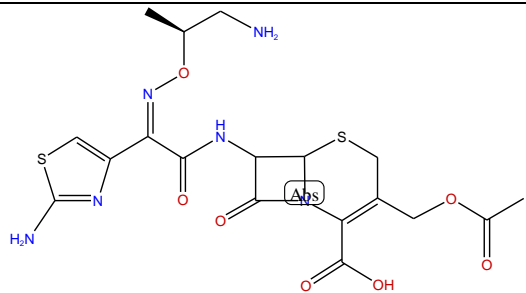
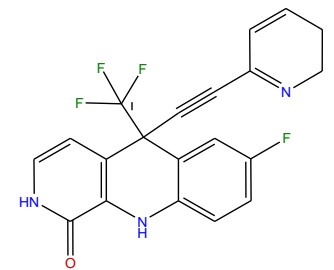
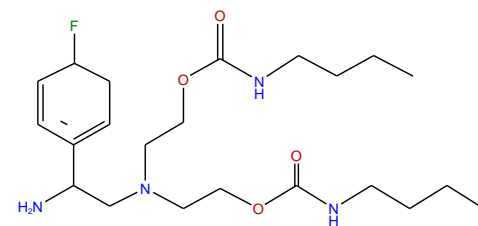
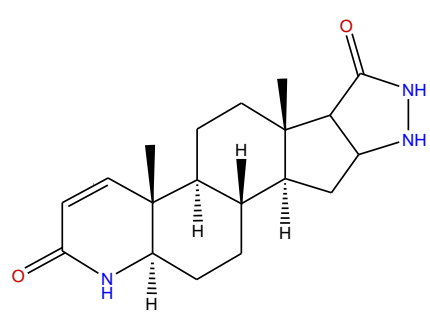
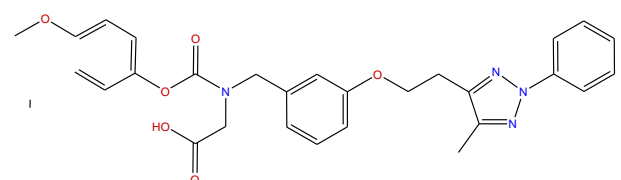
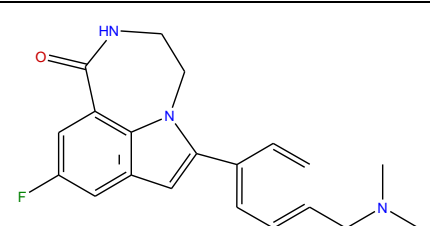
111	4451		N	MDDR
112	91294		N	MDDR
113	13920		N	MDDR
114	112113		N	MDDR
115	73175		N	MDDR
116	52640		N	MDDR
117	12415		N	MDDR
118	155479		N	MDDR
119	159615		N	MDDR

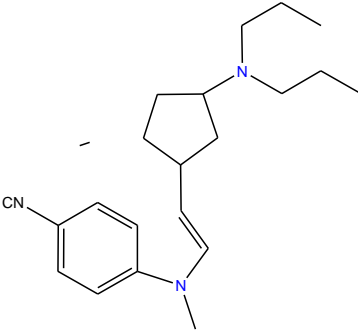
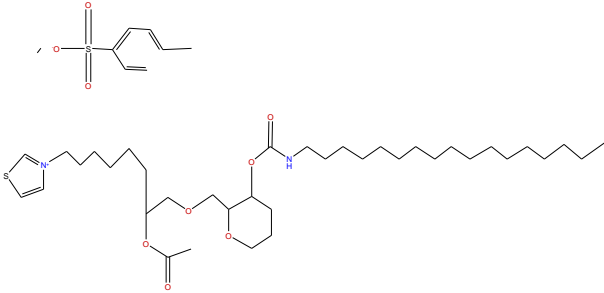
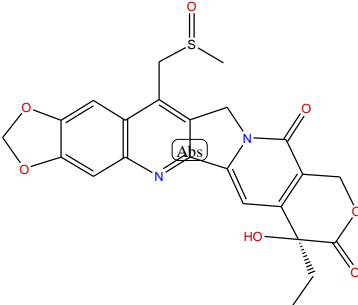
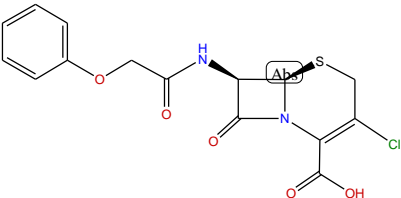
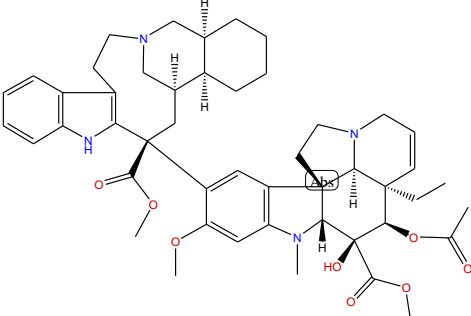
120	17459		N	MDDR
121	JMC-21		I	[2]
122	II-9		I	[1]
123	85410		N	MDDR
124	37268		N	MDDR

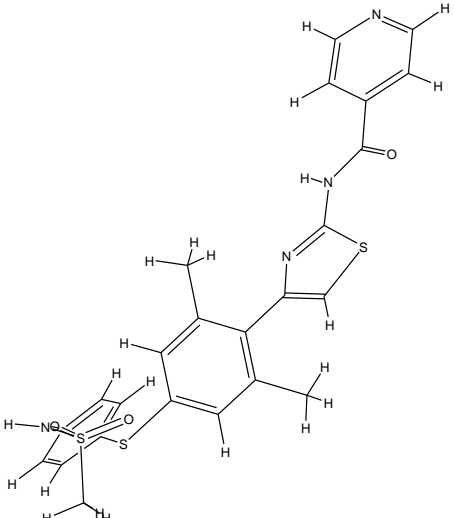
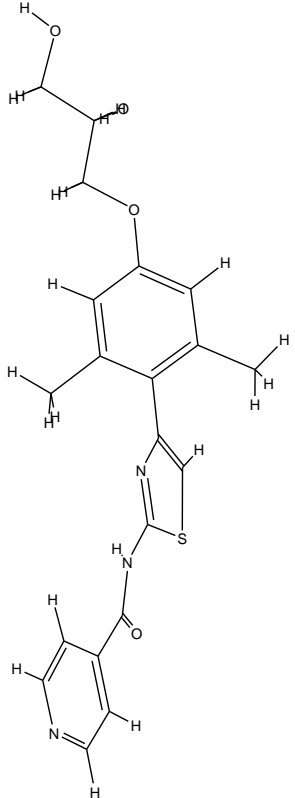
125	26		I	[1]
126	16610		N	MDDR
127	69946		N	MDDR
128	II-127		I	[1]
129	2019		N	MDDR

130	129758		N	MDDR
131	58260		N	MDDR
132	41020		N	MDDR
133	109676		N	MDDR
134	53680		N	MDDR
135	115482		N	MDDR

136	122540		N	MDDR
137	22933		N	MDDR
138	111911		N	MDDR
139	142114		N	MDDR
140	89007		N	MDDR
141	70295		N	MDDR

142	8754		N	MDDR
143	131154		N	MDDR
144	5685		N	MDDR
145	62059		N	MDDR
146	149752		N	MDDR
147	124472		N	MDDR

148	152439		N	MDDR
149	4166		N	MDDR
150	61796		N	MDDR
151	6141		N	MDDR
152	29367		N	MDDR

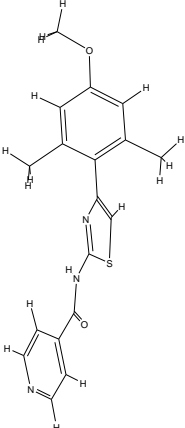
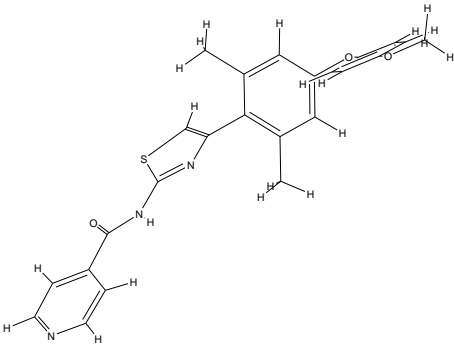
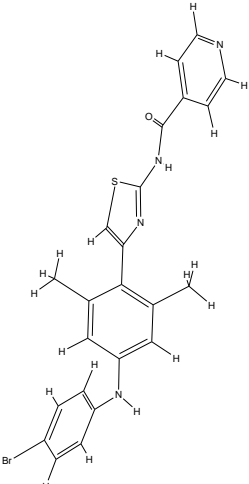
153	43		I	[1]
154	II-97		I	[1]

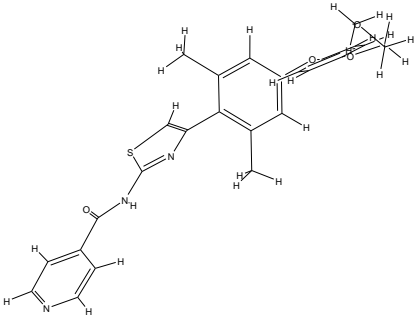
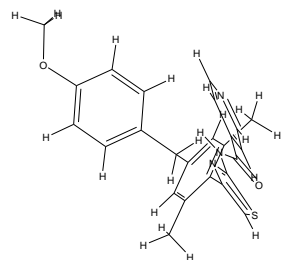
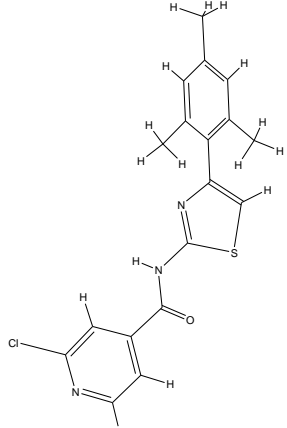
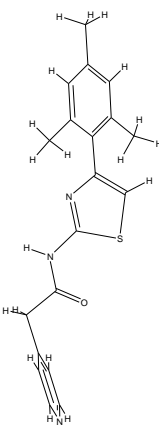
表S3 测试集中化合物的结构、类别和来源

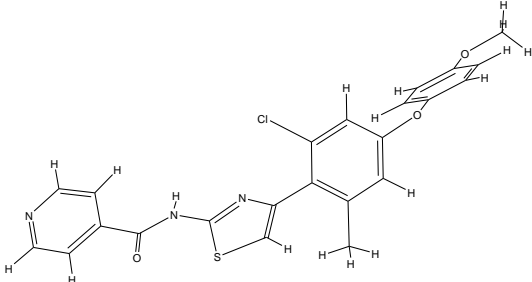
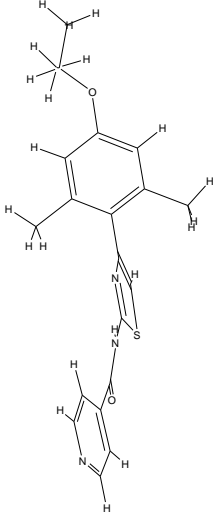
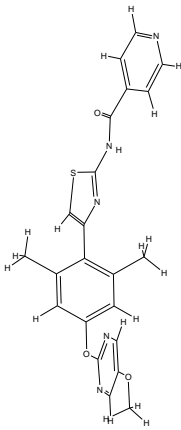
(I: HEC1抑制剂, N: HEC1非抑制剂)

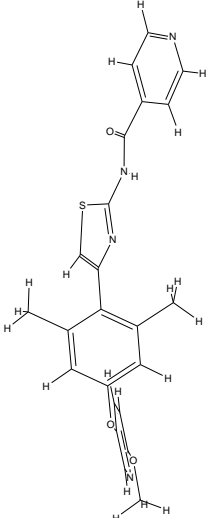
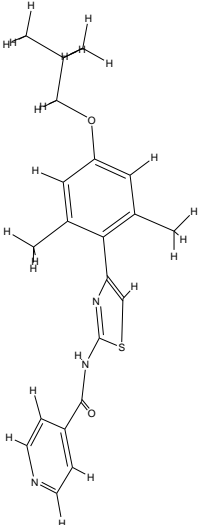
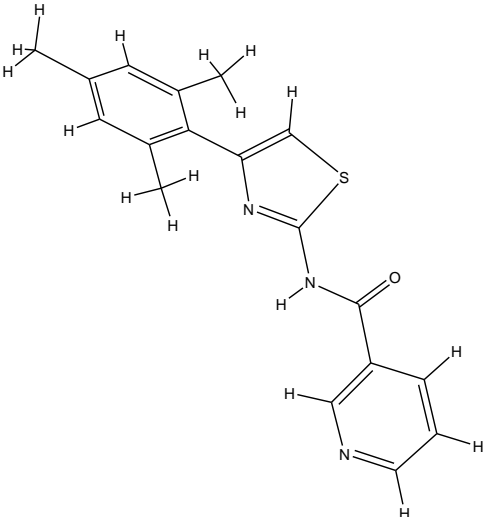
Table S3 Structure, category and source of the test set compounds

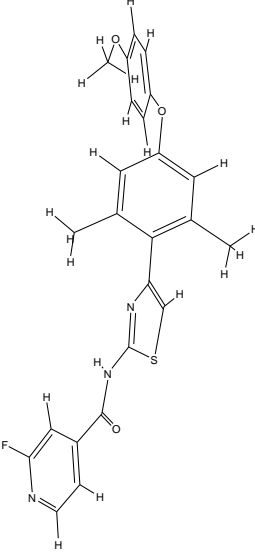
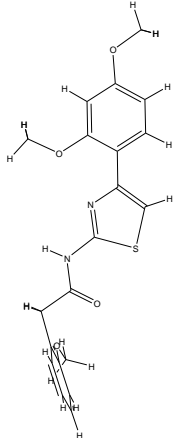
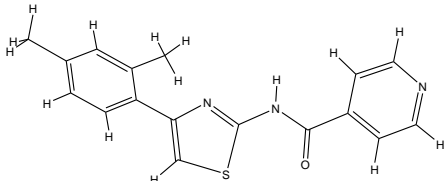
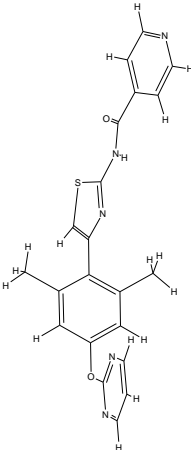
(I: HEC1 inhibitor, N: HEC1 non inhibitor)

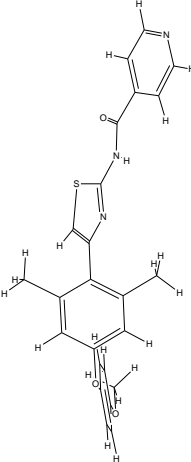
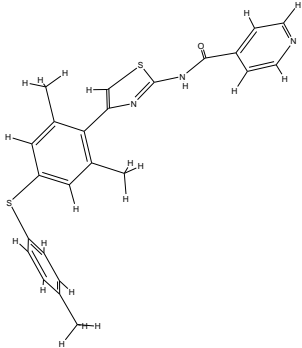
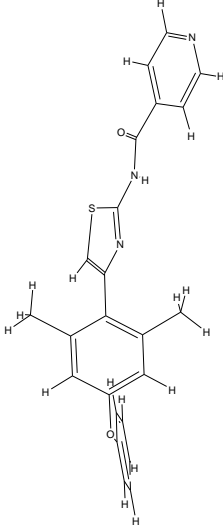
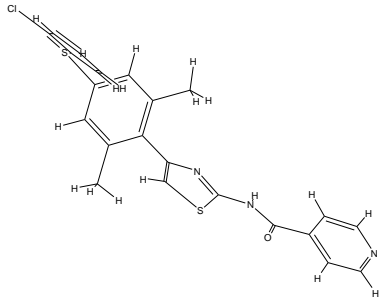
No.	ID	结构	类别	来源
1	II-42		I	[1]
2	49		I	[1]
3	II-122		I	[1]

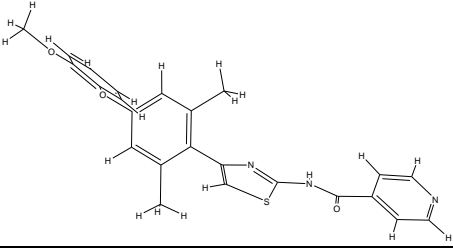
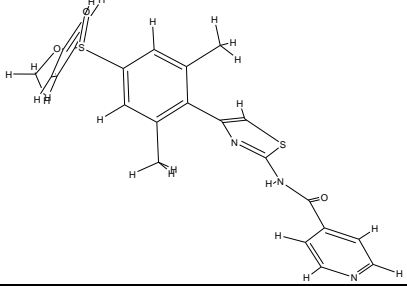
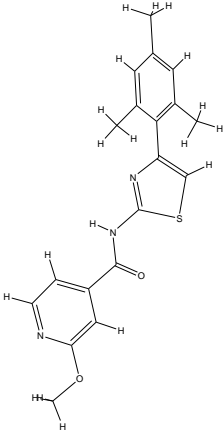
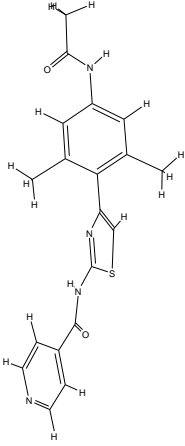
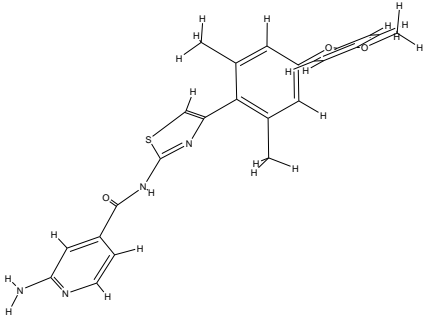
4	21		I	[1]
5	II-119		I	[1]
6	II-81		I	[1]
7	II-93		I	[1]

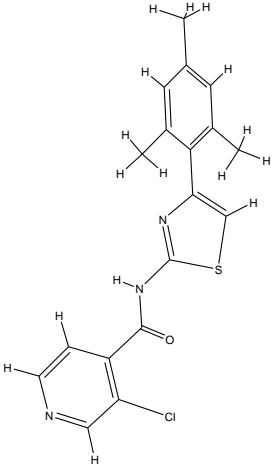
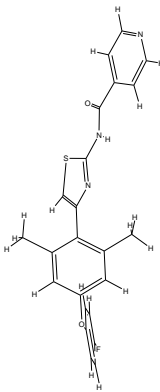
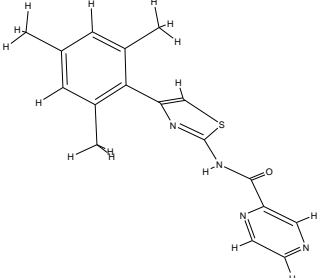
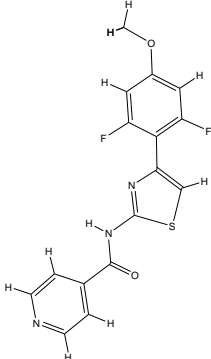
8	II-131		I	[1]
9	II-82		I	[1]
10	8		I	[1]

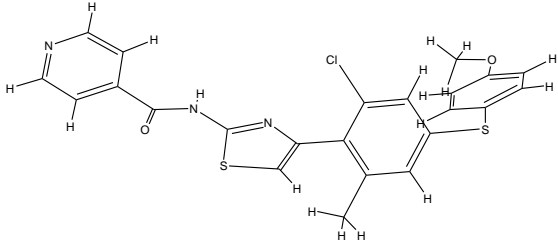
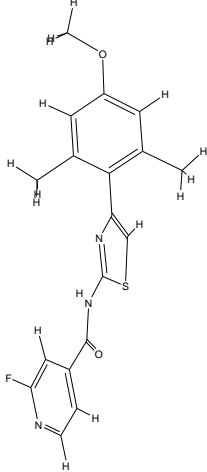
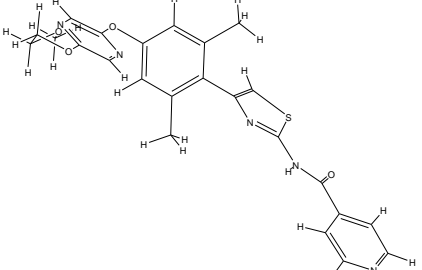
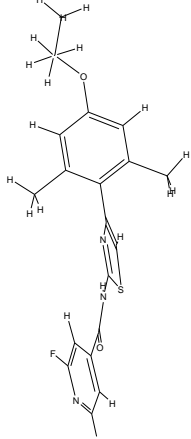
11	9		I	[1]
12	II-100		I	[1]
13	JMC-12		I	[2]

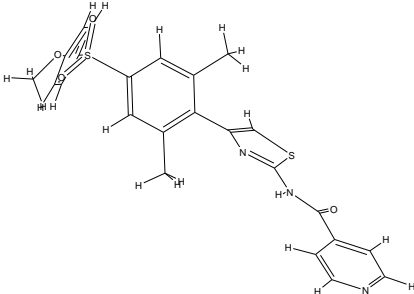
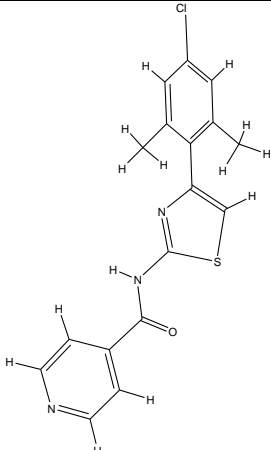
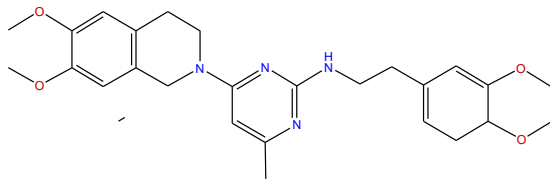
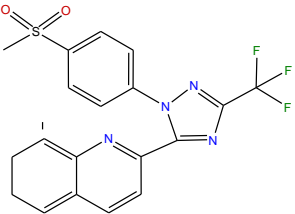
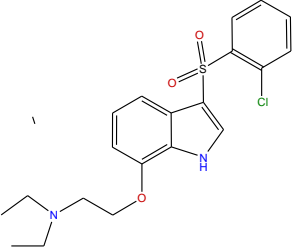
14	II-98		I	[1]
15	40		I	[1]
16	JMC-13		I	[2]
17	6		I	[1]

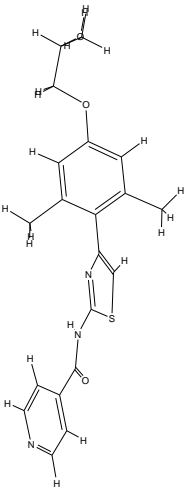
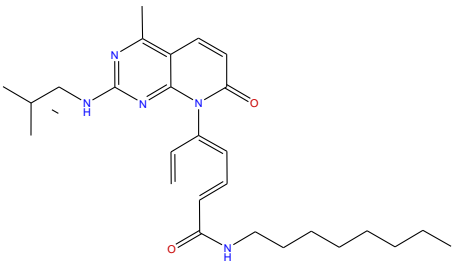
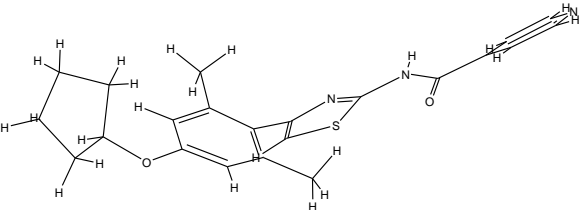
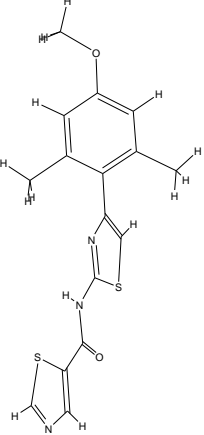
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19	II-116		I	[1]
20	II-79		I	[1]
21	39		I	[1]

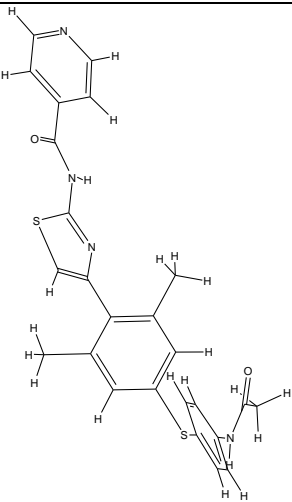
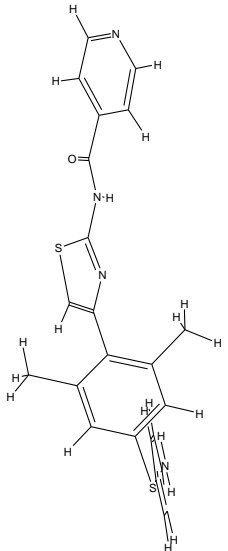
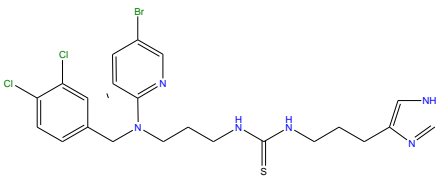
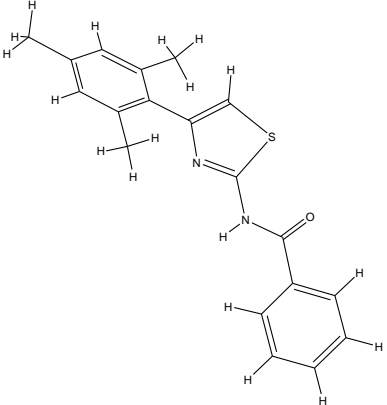
22	II-111		I	[1]
23	II-130		I	[1]
24	II-86		I	[1]
25	II-74		I	[1]
26	II-128		I	[1]

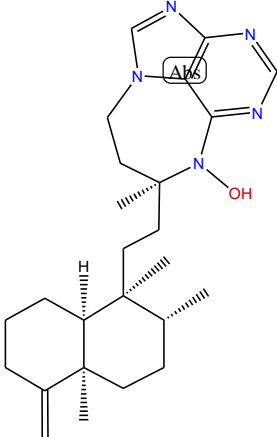
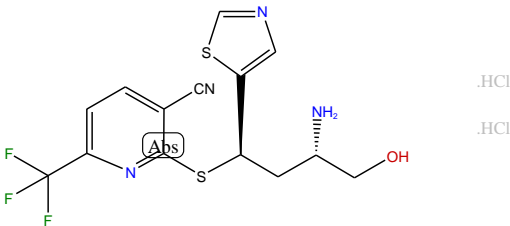
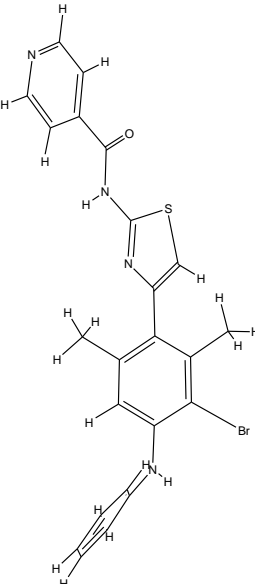
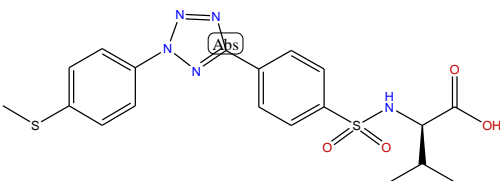
27	II-80		I	[1]
28	II-96		I	[1]
29	JMC-15		I	[2]
30	II-78		I	[1]

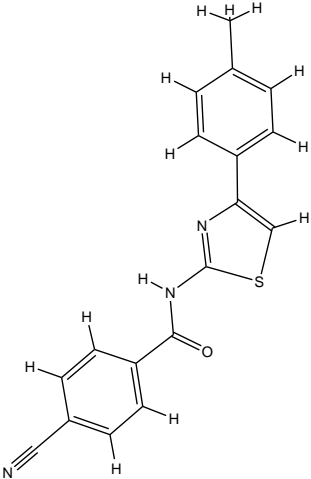
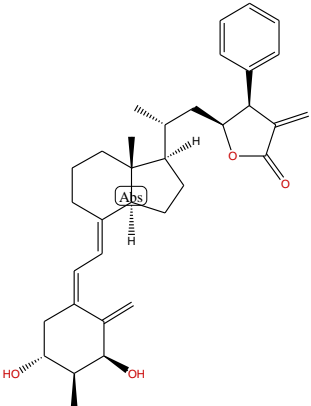
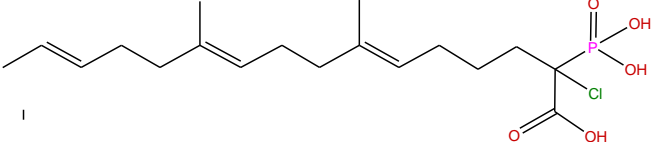
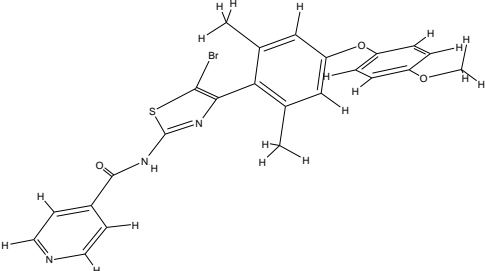
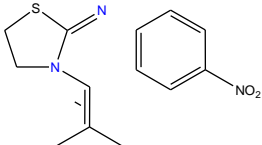
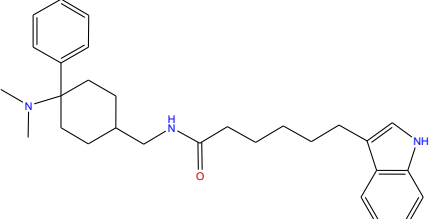
31	3		I	[1]
32	II-69		I	[1]
33	22		I	[1]
34	II-99		I	[1]

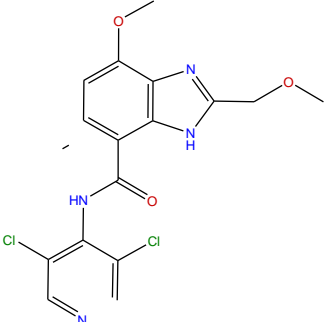
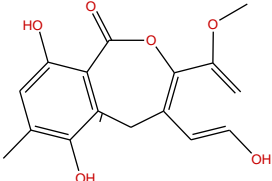
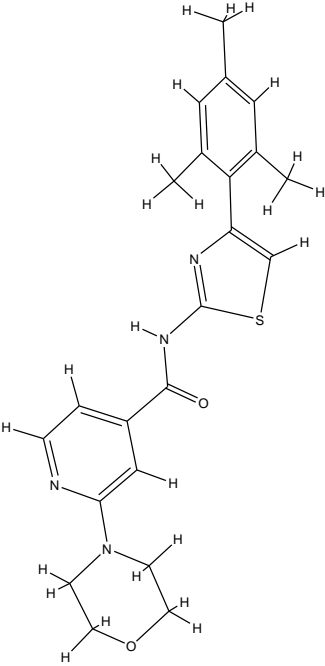
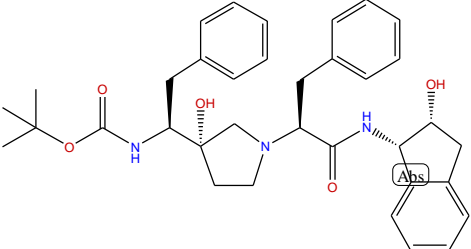
35	II-129		I	[1]
36	II-55		I	[1]
37	46347		N	MDDR
38	155173		N	MDDR
39	155602		N	MDDR

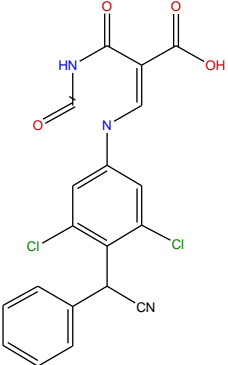
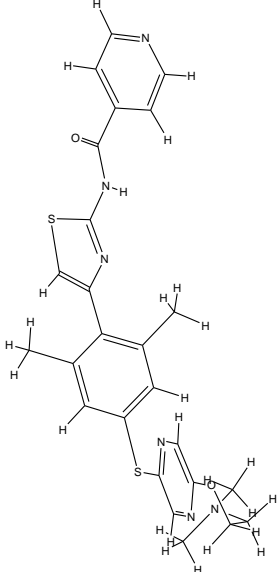
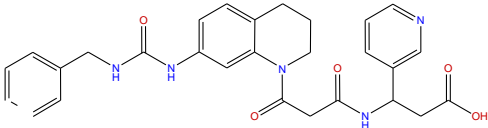
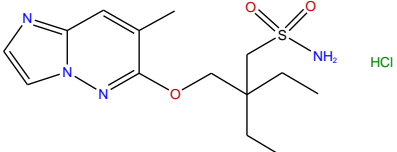
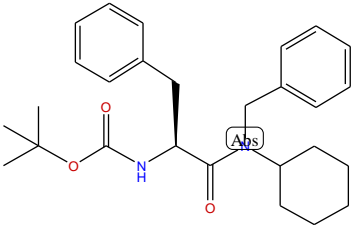
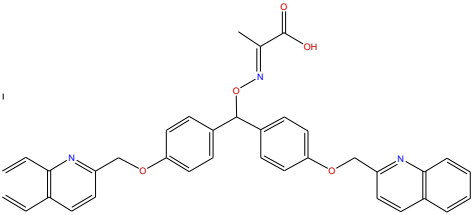
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41	149343		N	MDDR
42	II-85		I	[1]
43	II-75		I	[1]

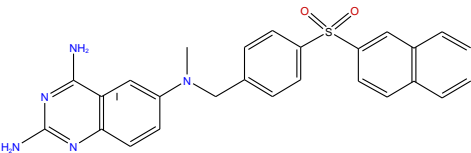
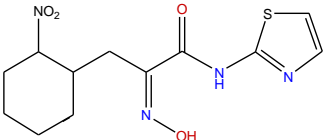
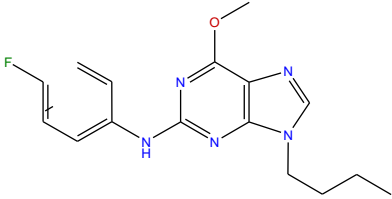
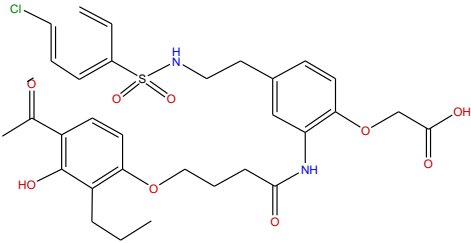
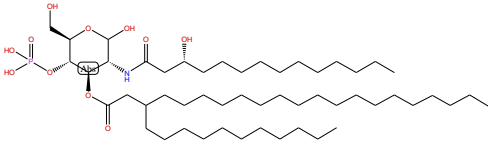
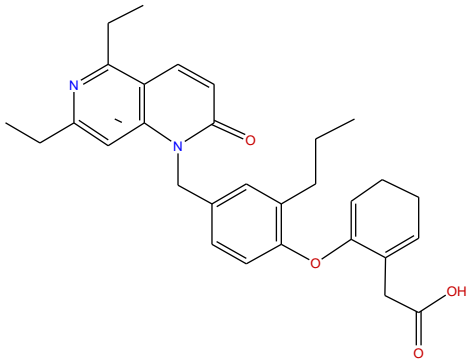
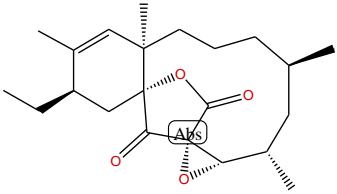
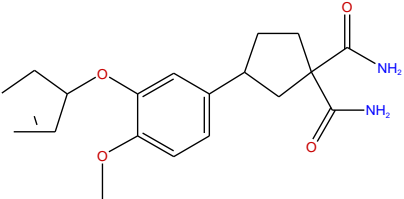
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45	35		I	[1]
46	94137		N	MDDR
47	JMC-6		I	[2]

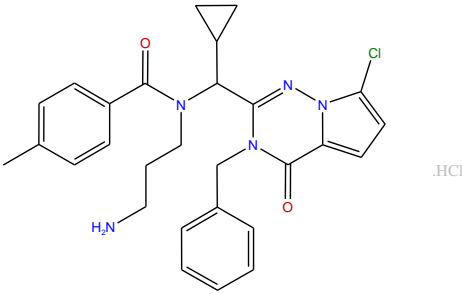
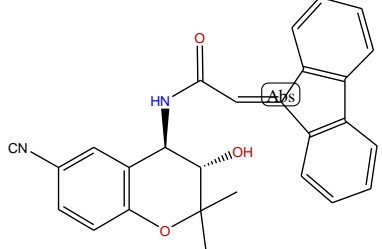
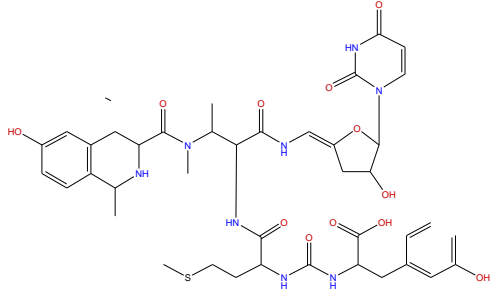
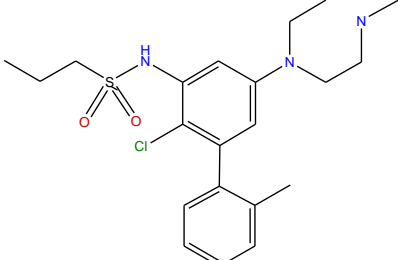
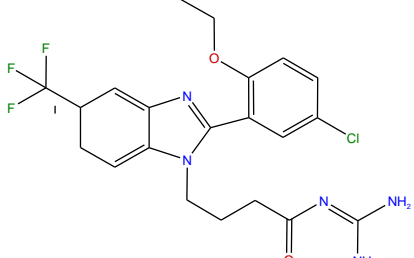
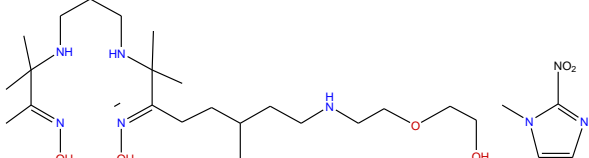
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49	154193		N	MDDR
50	II-123		I	[1]
51	95361		N	MDDR

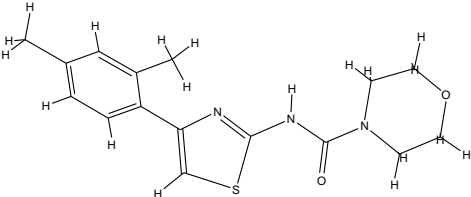
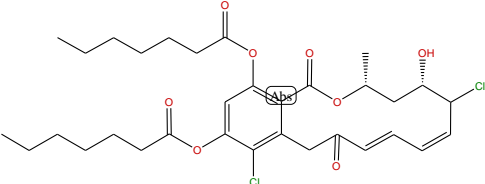
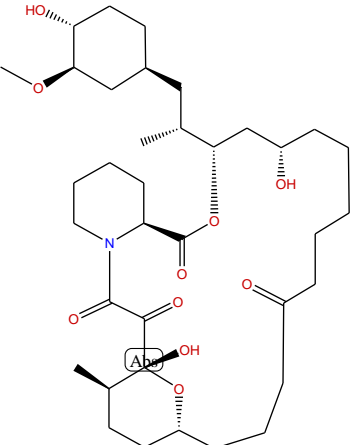
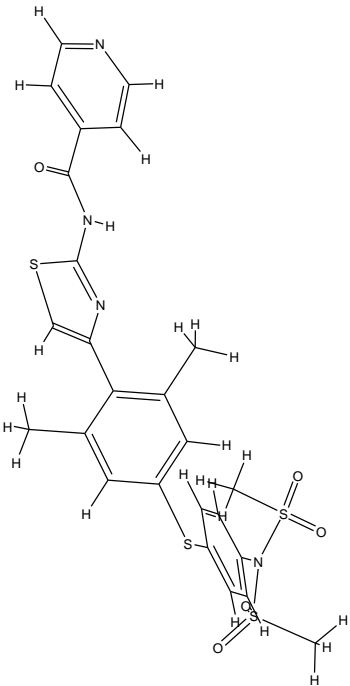
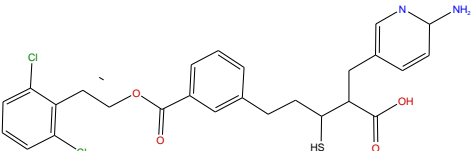
52	7		I	[1]
53	157791		N	MDDR
54	60755		N	MDDR
55	2		I	[1]
56	117843		N	MDDR
57	154534		N	MDDR

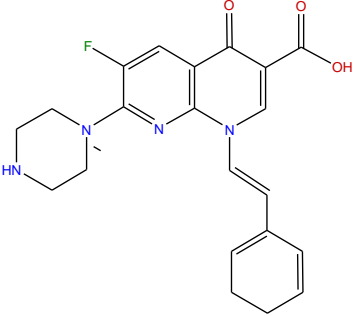
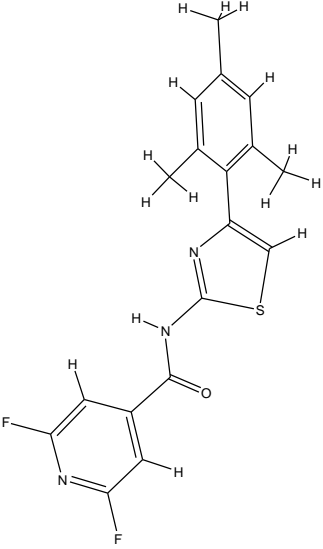
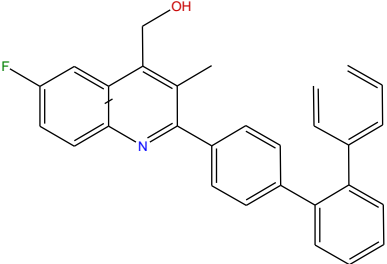
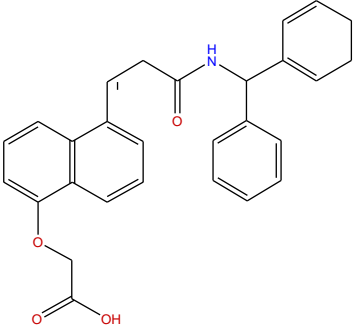
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59	141027		N	MDDR
60	II-83		I	[1]
61	57952		N	MDDR

62	33224		N	MDDR
63	28		I	[1]
64	108193		N	MDDR
65	54228		N	MDDR
66	59232		N	MDDR
67	88748		N	MDDR

68	53251		N	MDDR
69	59319		N	MDDR
70	117573		N	MDDR
71	54211		N	MDDR
72	37044		N	MDDR
73	50925		N	MDDR
74	58188		N	MDDR
75	50594		N	MDDR

76	148205		N	MDDR
77	58917		N	MDDR
78	44283		N	MDDR
79	76783		N	MDDR
80	138720		N	MDDR
81	68512		N	MDDR

82	JMC-20		I	[2]
83	92386		N	MDDR
84	45438		N	MDDR
85	42		I	[1]
86	147932		N	MDDR

87	2717		N	MDDR
88	II-90		I	[1]
89	150503		N	MDDR
90	81691		N	MDDR

experiment 1

实验1 细胞增殖抑制实验

Experiment 1 The anti-proliferative activity of compounds

外增殖抑制实验运用 MTT 法进行检测。收集传代培养中处于对数生长期的细胞，以 2000~5000 个细胞/孔的密度接种到 96 孔板，置于 37℃，5%CO₂ 细胞培养箱内培养 24h；再将药物按浓度梯度加入，培养 96h；避光条件下每孔加入 20μL 的 MTT 溶液 (5 mg mL⁻¹)，继续培养 2~4h，倾去上清液，每孔加入 150μL 的 DMSO，摇床上振摇 10~20min；待结晶充分溶解，设定波长为 570nm，在酶标仪 Spectra MAX M5 上测定每孔光密度，数据用 Graphpad Prism 5 测定，实验至少重复 3 次，选用紫杉醇作为阳性对照药物。

参考文献

- [1] Qiu X L, Li G, Wu G, et al. J Med Chem., 2009, 52(6): 1757-1767.)
[2] J.刘, J-J.黄,CN 103038231 A,2013