

Supplementary Material

Classification Model for Benzo[*c*]phenanthridine Analogues with Topoisomerase-I Inhibitory Activity by Support Vector Machine

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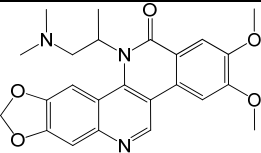
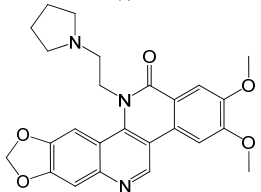
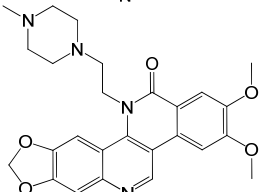
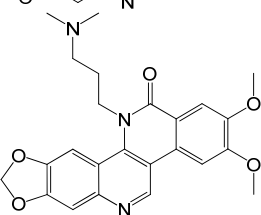
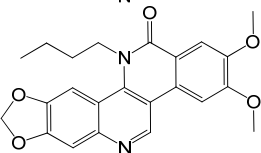
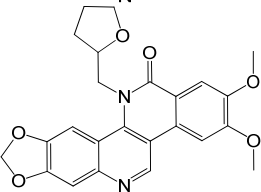
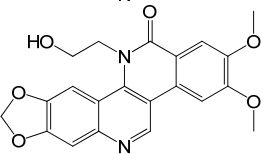
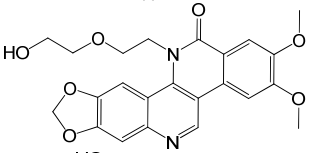
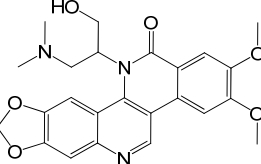
Table S1. Chemical structure of 82 benzo[*c*]phenanthridine derivatives and their topoisomerase I inhibitory activity REC and classification results from the final SVM model.

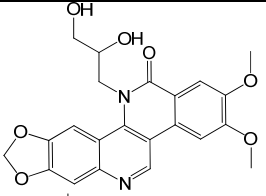
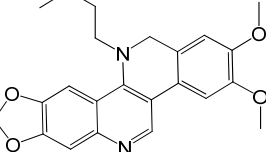
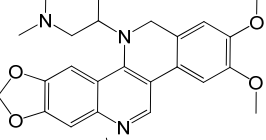
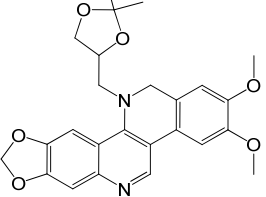
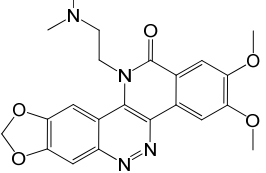
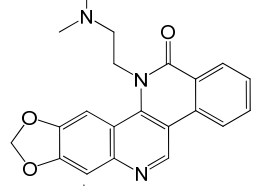
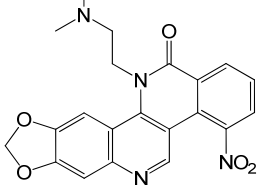
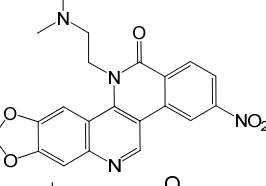
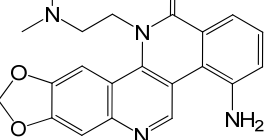
Table S2. Chemical structure of 10 benzo[*c*]phenanthridine derivatives in the application set and their topoisomerase I inhibitory activity REC and classification results from the final SVM model.

Table S1. Chemical structure of 82 benzo[*c*]phenanthridine derivatives and their topoisomerase I inhibitory activity REC and classification results from final SVM model.

Classification: «+» presented stronger than topotecan; «−» presented weaker than topotecan

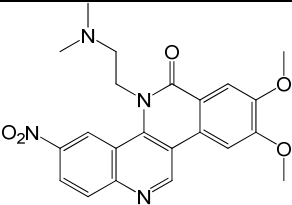
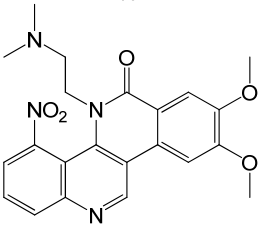
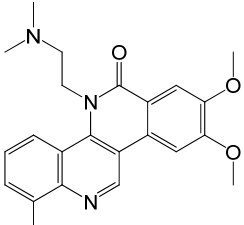
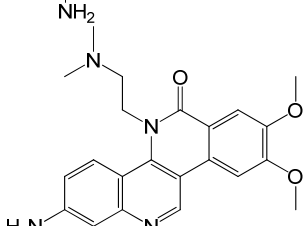
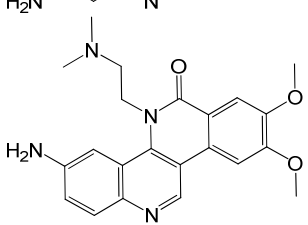
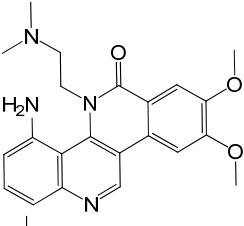
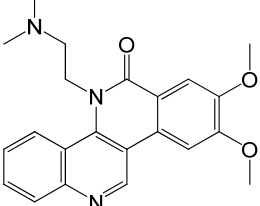
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			Topo I mediated DNA cleavage (Experimental)	
1		Nitidine	10	—
2		BMC_03_3795_10a	8	—
3		BMC_03_3795_10b	200	—
4		BMC_03_3795_10c	200	—
5		BMC_03_3795_10d	>1000	—
6		BMC_03_3795_10e	500	—
7		BMC_03_3795_10f	10	—
8		BMC_03_3795_11a	>1000	—
9		BMC_03_3795_11b	100	—
10		BMC_03_3795_12d	>1000	—
11		BMC_03_2061_03a	0.5	—

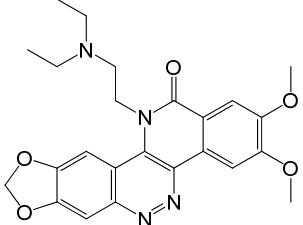
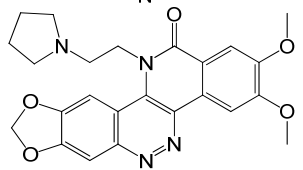
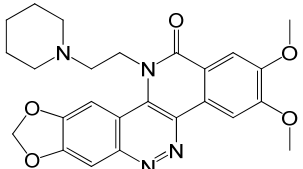
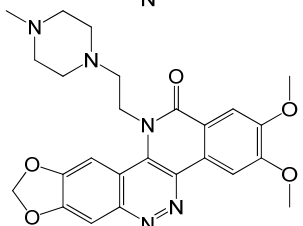
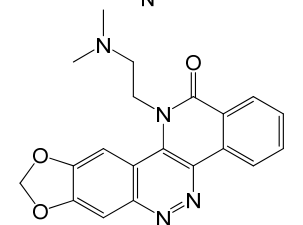
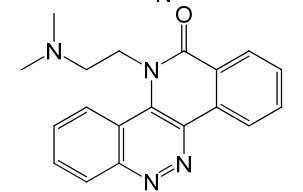
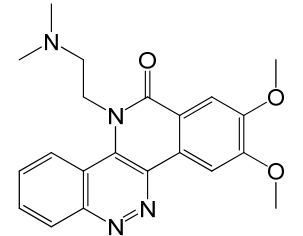
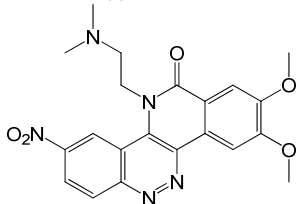
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			Topo I mediated DNA cleavage (Experimental)	
12		BMC_03_2061_03b	>1000	—
13		BMC_03_2061_03c	0.3	+
14		BMC_03_2061_03d	1000	—
15		BMC_03_2061_03e	1	—
16		BMC_03_2061_03f	1000	—
17		BMCL_02_3333_03c	10	—
18		BMC_03_2061_03h	50	—
19		BMC_03_2061_03i	1	—
20		BMC_03_2061_03j	>1000	—

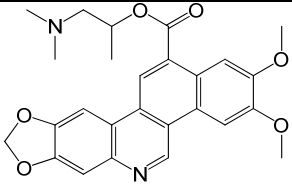
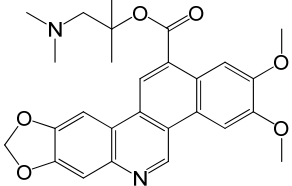
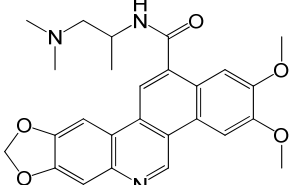
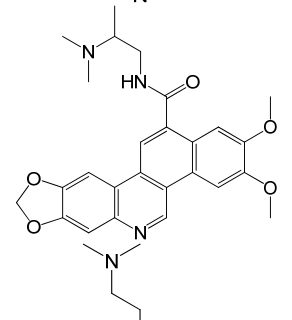
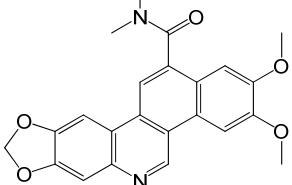
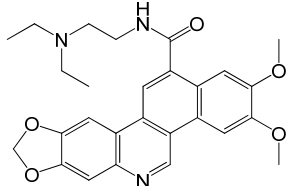
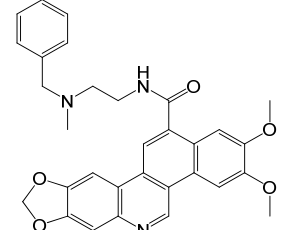
No	Chemical structure	Name	REC	Topo I classified result (Predictive)
			Topo I mediated DNA cleavage (Experimental)	
21		BMC_03_2061_03k	0.8–1.0	+
22		BMC_03_2061_04a	0.8	–
23		BMC_03_2061_04b	100	+
24		BMC_03_2061_09k	10	–
25		JMC_03_2254_02	0.3	–
26		JMC_03_2254_03	6	–
27		JMC_03_2254_05a	1000	+
28		JMC_03_2254_05b	0.1	+
29		JMC_03_2254_06a	15	–

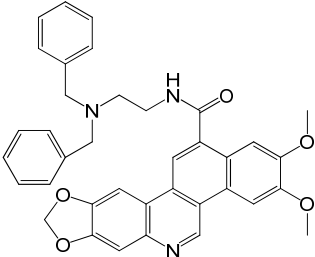
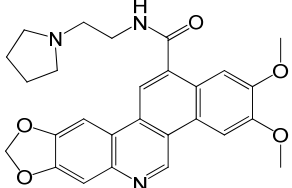
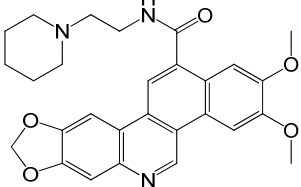
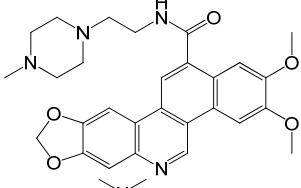
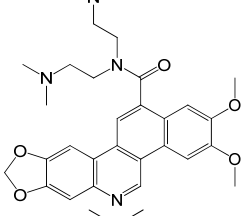
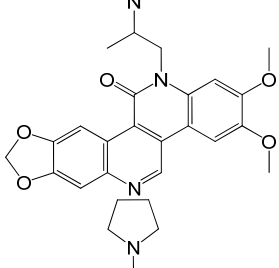
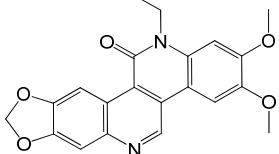
No	Chemical structure	Name	REC	Topo I mediated DNA cleavage (Experimental)	Topo I classified result (Predictive)
			Topo I mediated DNA cleavage (Experimental)		
30		JMC_03_2254_06b	0.5	—	—
31		JMC_03_2254_05c	0.2	—	—
32		JMC_03_2254_06c	8.0	—	—
33		JMC_03_2254_16a	10	+	+
34		JMC_03_2254_17a	500	—	—
35		JMC_03_2254_02	0.5	+	+
36		BMCL_02_3333_02	>1000	—	—
37		BMCL_02_3333_03	200	—	—
38		BMCL_02_3333_04a	0.3	+	+

No	Chemical structure	Name	REC	Topo I mediated DNA cleavage (Experimental)	Topo I classified result (Predictive)
39		BMCL_02_3333_04b	1000	—	—
40		BMCL_02_3333_04c	30	—	—
41		BMCL_02_3333_04d	1.0	—	—
42		LDDD_04_198_01	0.03	—	—
43		LDDD_04_198_02	2.0	—	—
44		LDDD_04_198_03	2.0	—	—
45		BMC_04_3731_03a	9	—	—
46		BMC_04_3731_03b	6	—	—

No	Chemical structure	Name	REC	Topo I classified result (Predictive)
			Topo I mediated DNA cleavage (Experimental)	
47		BMC_04_3731_03c	2	—
48		BMC_04_3731_03d	>300	—
49		BMC_04_3731_04a	100	—
50		BMC_04_3731_04b	12	—
51		BMC_04_3731_04c	6	—
52		BMC_04_0795_04	>300	—
53		BMC_04_3731_05	10	—

No	Chemical structure	Name	REC	Topo I classified result (Predictive)
			Topo I mediated DNA cleavage (Experimental)	
54		BMC_04_0795_01b	0.3	—
55		BMC_04_0795_01f	0.2	+
56		BMC_04_0795_01g	2.0	—
57		BMC_04_0795_01h	20	—
58		BMC_04_0795_03	10	—
59		BMC_04_0795_02	>1000	—
60		BMC_04_0795_04	0.8	+
61		BMC_04_0795_05	5	—

No	Chemical structure	Name	REC	Topo I classified result (Predictive)
			Topo I mediated DNA cleavage (Experimental)	
62		BMC_05_6782_07c	1.0	—
63		BMC_05_6782_07d	8	—
64		BMC_05_6782_08	0.6	+
65		BMC_05_6782_09c	0.4	—
66		BMC_05_6782_09d	10	—
67		BMC_05_6782_09e	0.7	+
68		BMC_05_6782_09f	12	—

No	Chemical structure	Name	REC	Topo I classified result (Predictive)
			Topo I mediated DNA cleavage (Experimental)	
69		BMC_05_6782_09g	60	—
70		BMC_05_6782_09h	0.6	+
71		BMC_05_6782_09i	1.5	—
72		BMC_05_6782_09j	0.3	+
73		BMC_05_6782_10	3	+
74		BMC_06_3131_10c	1.2	—
75		BMC_06_3131_10d	0.07	+

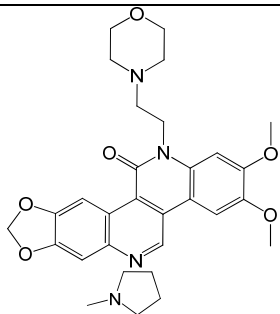
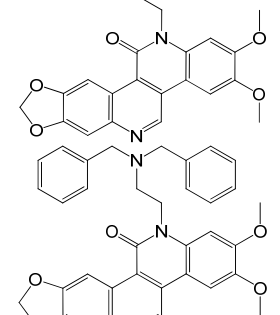
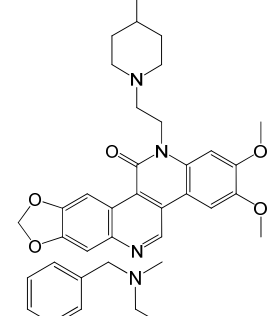
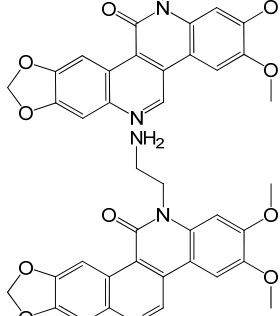
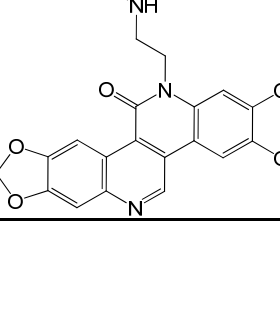
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			Topo I mediated DNA cleavage (Experimental)	
76		BMC_06_3131_10g	9	—
77		BMC_06_3131_10i	0.45	+
78		BMC_06_3131_10j	>100	—
79		BMC_06_3131_10f	3	—
80		BMC_06_3131_10k	13	—
81		BMC_06_3131_10l	0.35	+
82		BMC_06_3131_10m	0.15	+

Table S2. Chemical structure of 10 benzo[*c*]phenanthridine derivatives in application set and their topoisomerase I inhibitory activity REC and classification results from final SVM model.

Classification: «+» presented stronger than topotecan; «-» presented weaker than topotecan

No	Chemical structure	Name	REC Topo I mediated DNA cleavage (Experimental)	Topo I classified result (Predictive)
A1-		BMC_08_7824_7a	0.03	+
A2		BMC_08_7824_7b	0.08	+
A3		BMC_08_7824_9	0.2	+
A4		BMC_08_7824_11	0.1	+
A5		BMC_08_8598_9	>10	-
A6		BMC_08_8598_10	0.2	-
A7		BMC_08_8598_12	0.2	-
A8		BMC_08_8598_13	0.2	+
A9		BMC_08_8598_14	>10	-
A10		BMC_08_8598_15	>10	-