Supporting Information for

An Effective Approach to Artificial Nucleases Using Copper(II) Complexes Bearing Nucleobases

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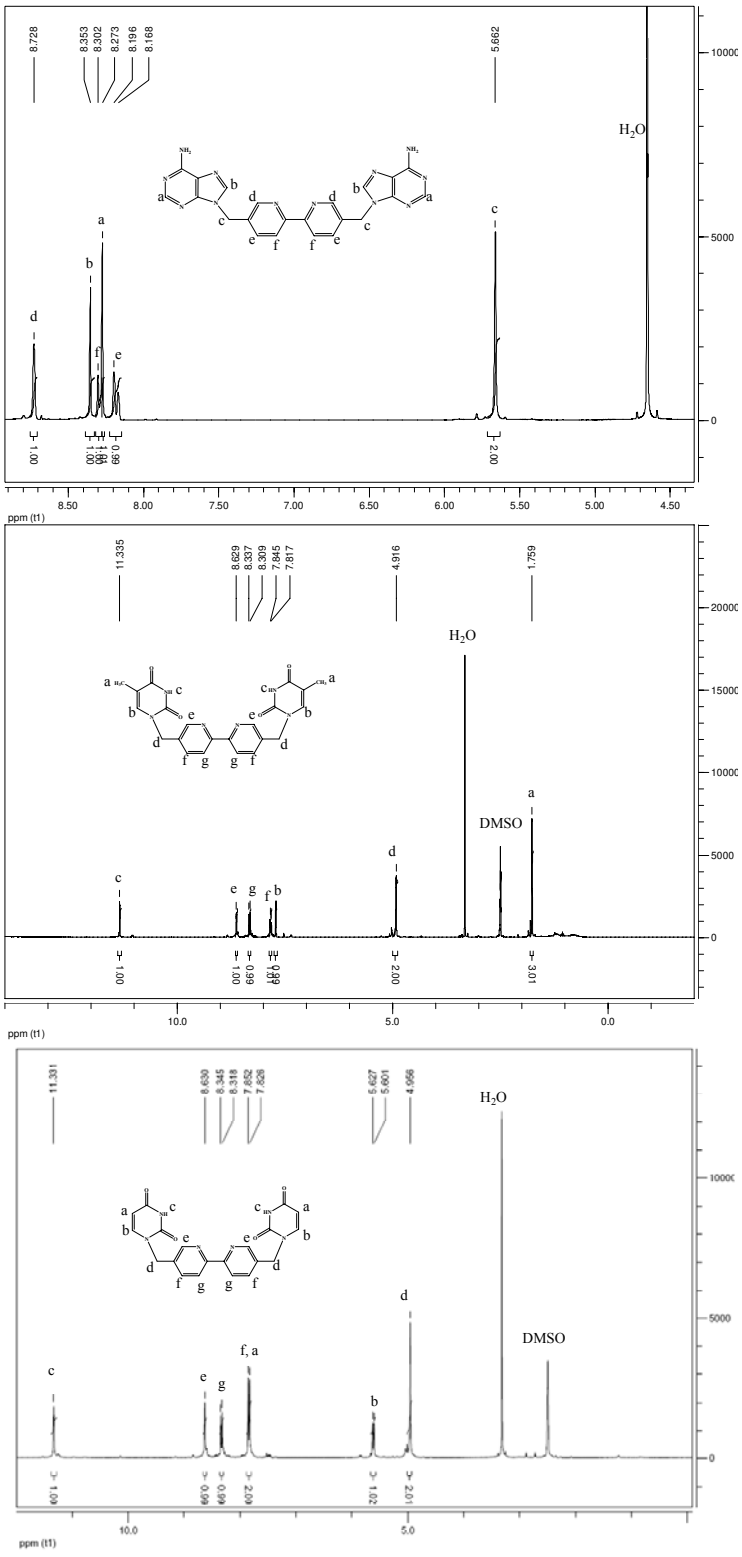

8.728
8.353
8.302
8.273
8.196
8.168
5.662
H2O
ppm (t1)
11.335
8.629
8.337
8.309
7.845
7.817
4.916
1.759
H2O
DMSO
ppm (t1)
11.331
H2O
DMSO
f, a
ppm (t1)

Fig. S1.

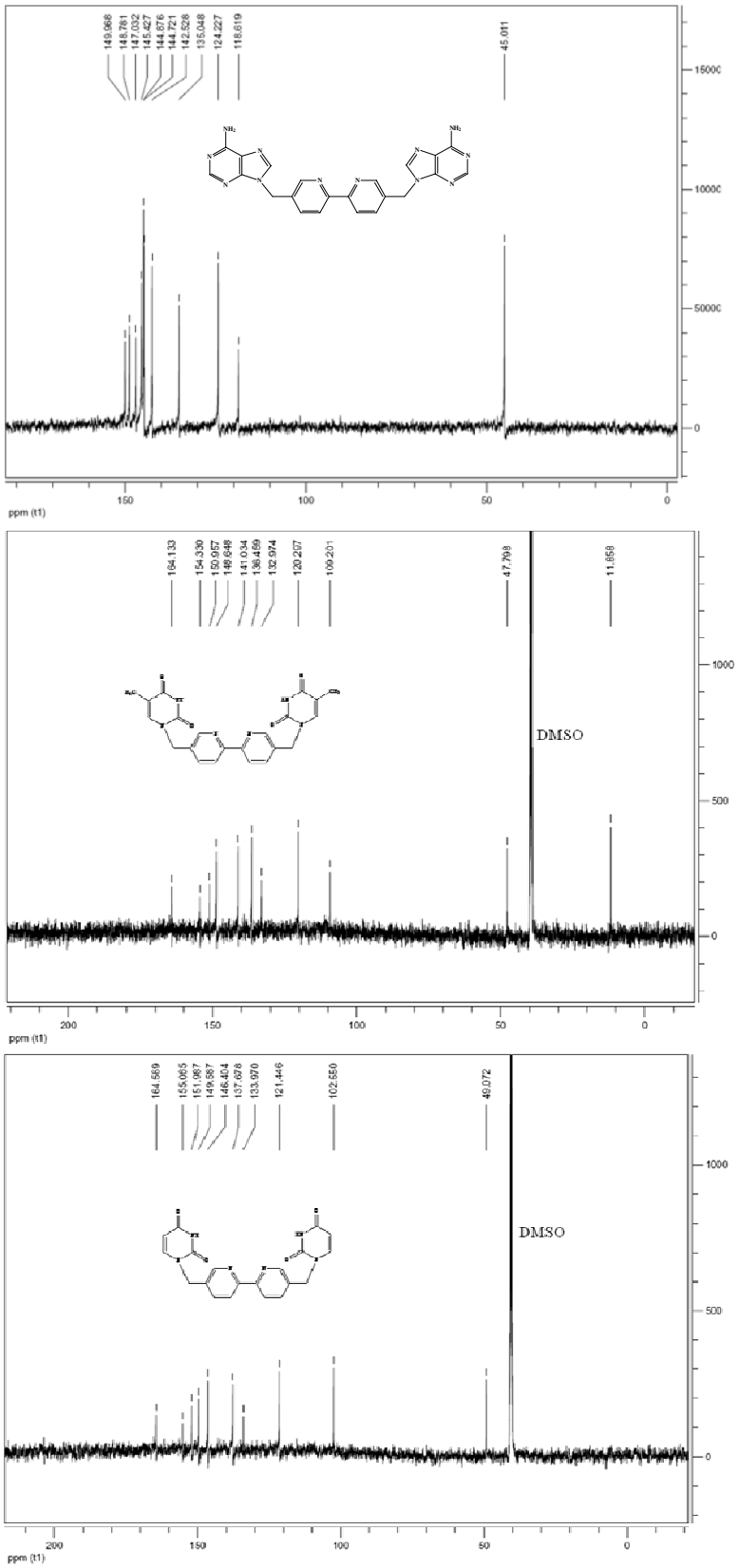

149.968
148.781
147.032
145.427
144.676
144.721
142.526
135.048
124.227
118.619
45.011
ppm (t1)
164.133
154.330
150.957
148.648
141.034
136.459
132.974
120.257
109.201
47.798
11.858
DMSO
ppm (t1)
164.569
155.065
151.987
149.597
146.404
137.678
133.920
121.446
102.550
49.072
DMSO
ppm (t1)

Fig. S2.

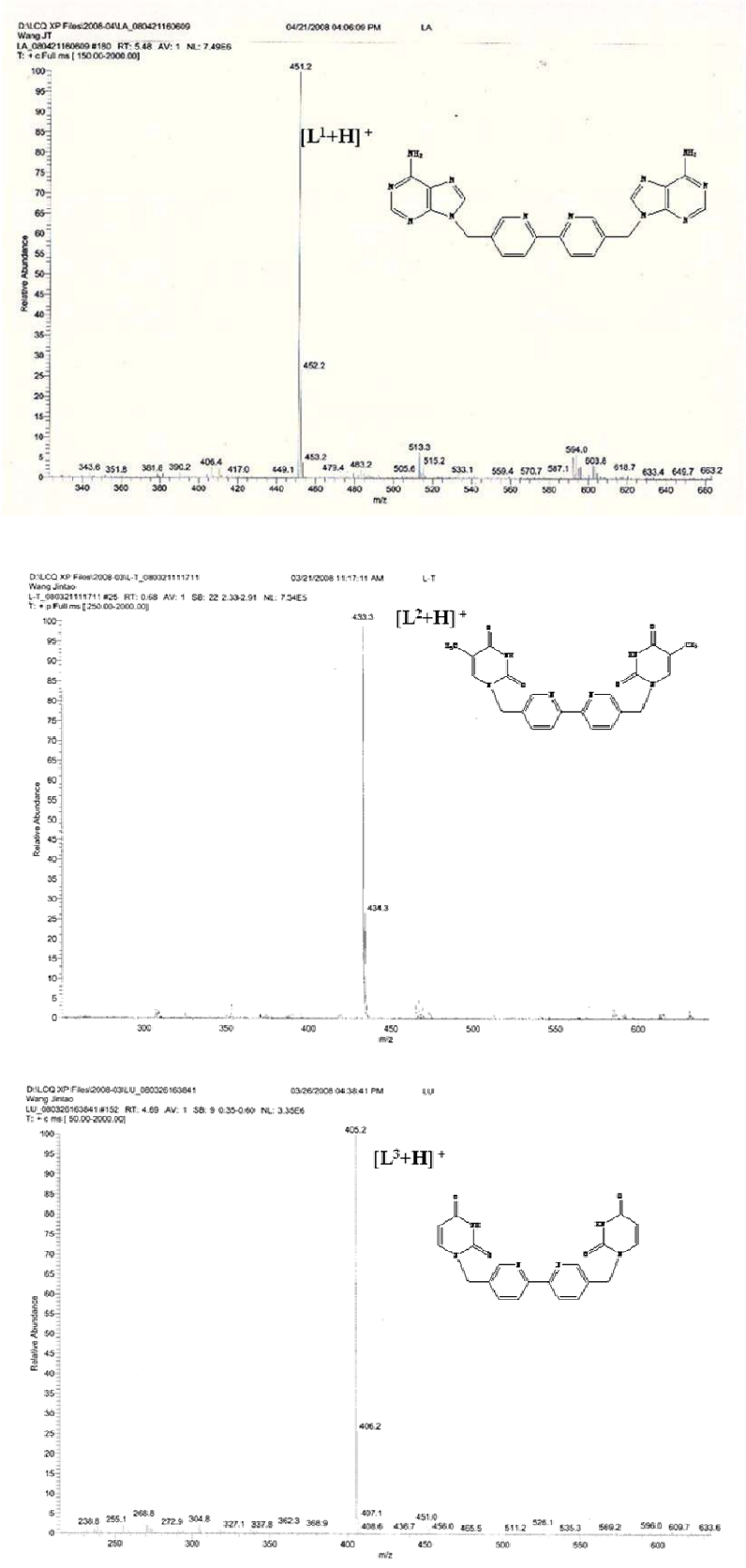

[L1+H]+
451.2
452.2
[L2+H]+
433.3
434.3
[L3+H]+
405.2
406.2
Relative Abundance
m/z

Fig. S3.

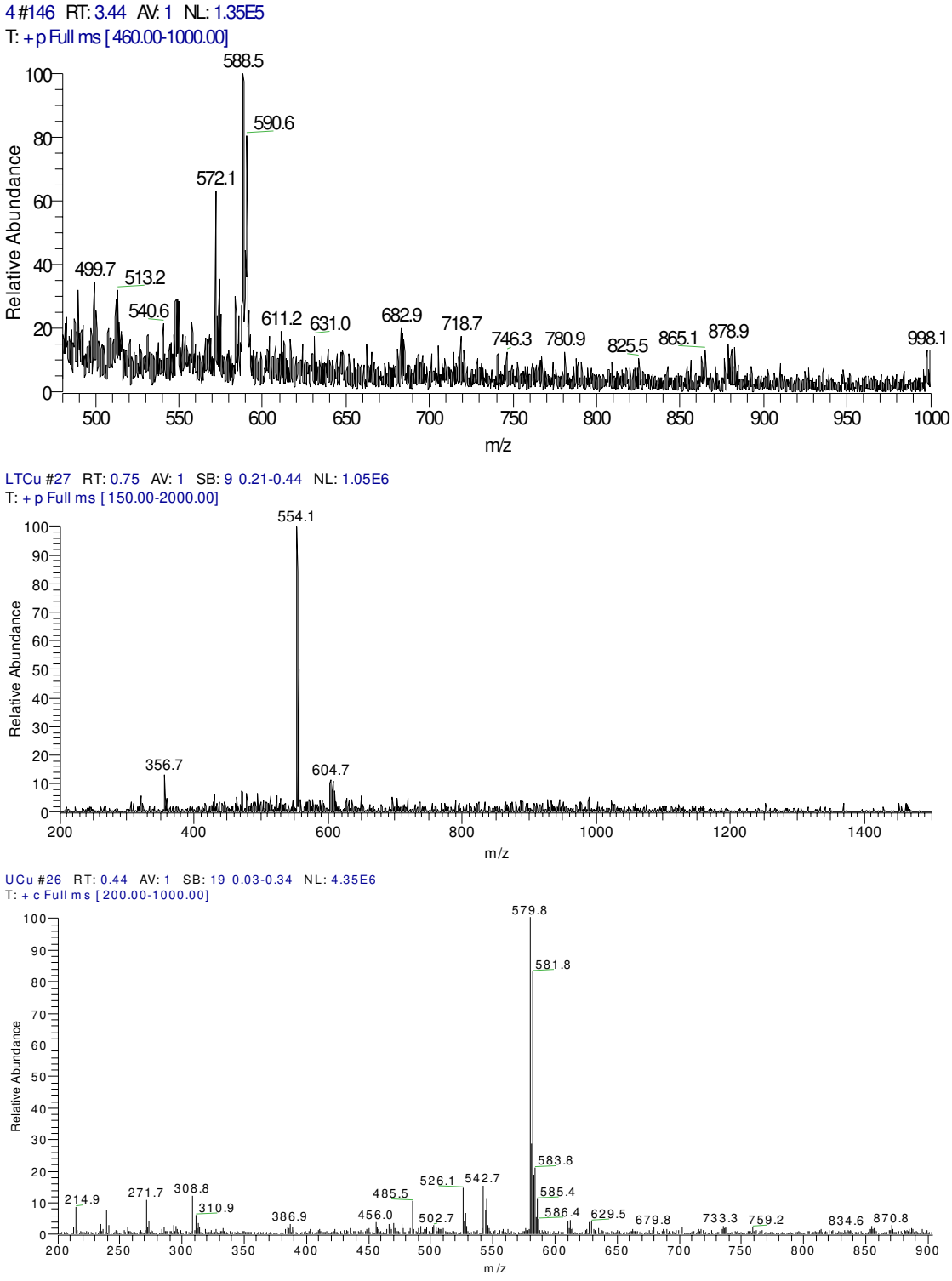

4 #146 RT: 3.44 AV: 1 NL: 1.35E5
T: + p Full ms [460.00-1000.00]
Relative Abundance
m/z
588.5
590.6
572.1
499.7
513.2
540.6
611.2
631.0
682.9
718.7
746.3
780.9
825.5
865.1
878.9
998.1
LTCu #27 RT: 0.75 AV: 1 SB: 9 0.21-0.44 NL: 1.05E6
T: + p Full ms [150.00-2000.00]
554.1
356.7
604.7
UCu #26 RT: 0.44 AV: 1 SB: 19 0.03-0.34 NL: 4.35E6
T: + c Full ms [200.00-1000.00]
579.8
581.8
583.8
585.4
586.4
214.9
271.7
308.8
310.9
386.9
456.0
485.5
502.7
526.1
542.7
629.5
679.8
733.3
759.2
834.6
870.8

Fig. S4.

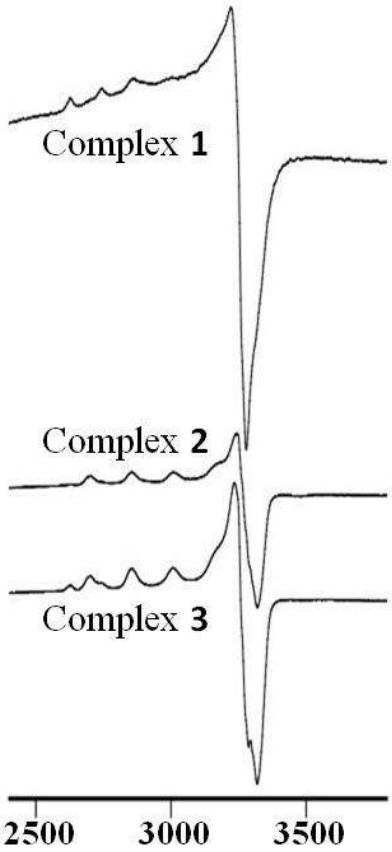


Fig. S5.

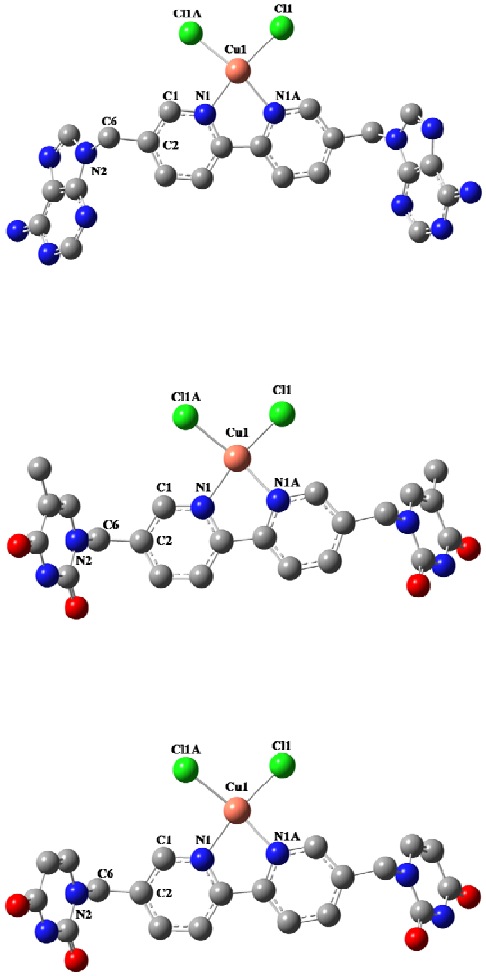


Fig. S6.

Table S1.

	Complex **1**	Complex **2**	Complex **3**
Cu(1)-N(1)	2.08	2.08	2.08
Cu(1)-N(1A)	2.08	2.08	2.08
Cu(1)-Cl(1)	2.29	2.29	2.29
Cu(1)-Cl(1A)	2.29	2.29	2.29
C(1)-N(1)	1.35	1.35	1.35
C(6)-C(2)	1.52	1.52	1.52
C(6)-N(2)	1.47	1.49	1.49
N(1)-Cu(1)-N(1A)	78.64	78.67	78.60
N(1A)-Cu(1)-Cl(1)	93.65	93.71	93.66
Cl(1)-Cu(1)-Cl(1A)	97.39	98.20	98.01
N(1)-Cu(1)-Cl(1A)	93.65	93.71	93.66
N(1)-Cu(1)-Cl(1)	163.23	161.47	162.06
N(1A)-Cu(1)-Cl(1A)	163.23	161.46	162.07
C(1)-C(2)-C(6)	120.39	120.17	120.12
C(2)-C(6)-N(2)	113.35	112.87	112.97

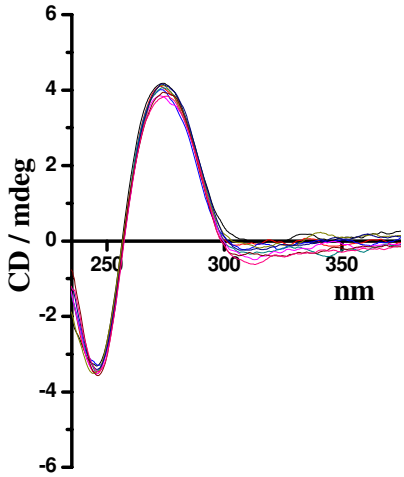


Fig. S7.

Table S2.

Complex **3** (μM)	Reaction time (min)	Fraction of DNA			*n* 1	*n* 2	*n* 1/*n* 2
		Supercoiled	Nicked	Linear			
50	10	0.296	0.680	0.024	1.193	0.025	48.099
50	20	0.207	0.734	0.059	1.512	0.063	24.173
70	28	0.185	0.745	0.071	1.615	0.076	21.232
70	35	0.447	0.531	0.022	0.784	0.023	34.655
70	42	0.327	0.596	0.077	1.037	0.083	12.512
250	12	0.282	0.675	0.044	1.223	0.046	26.855
250	18	0.150	0.745	0.105	1.786	0.117	15.258

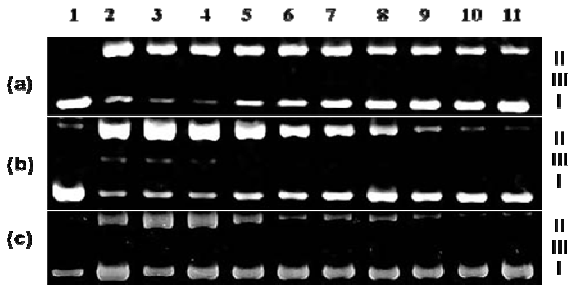
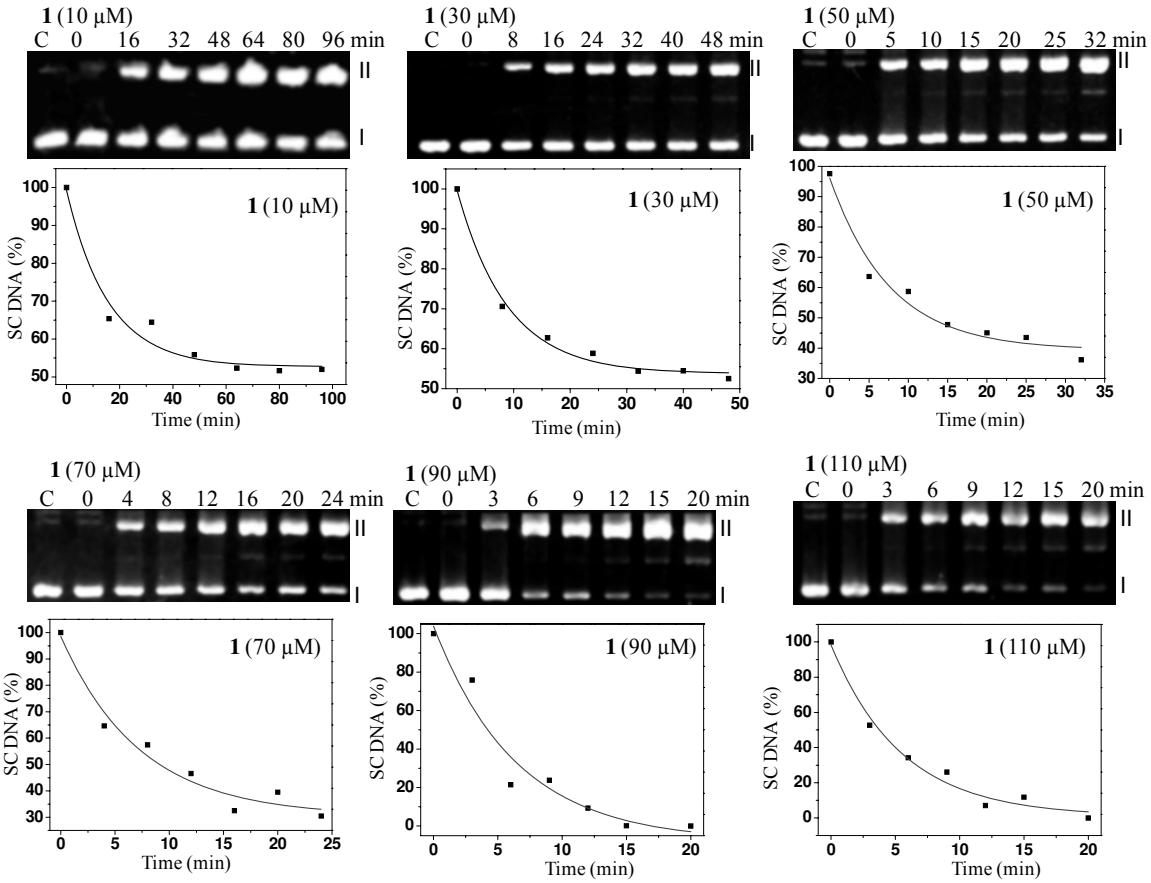


Fig. S8.


1 (10 μM)
C 0 16 32 48 64 80 96 min
II
I
1 (10 μM)
SC DNA (%)
Time (min)
1 (30 μM)
C 0 8 16 24 32 40 48 min
II
I
1 (30 μM)
SC DNA (%)
Time (min)
1 (50 μM)
C 0 5 10 15 20 25 32 min
II
I
1 (50 μM)
SC DNA (%)
Time (min)
1 (70 μM)
C 0 4 8 12 16 20 24 min
II
I
1 (70 μM)
SC DNA (%)
Time (min)
1 (90 μM)
C 0 3 6 9 12 15 20 min
II
I
1 (90 μM)
SC DNA (%)
Time (min)
1 (110 μM)
C 0 3 6 9 12 15 20 min
II
I
1 (110 μM)
SC DNA (%)
Time (min)

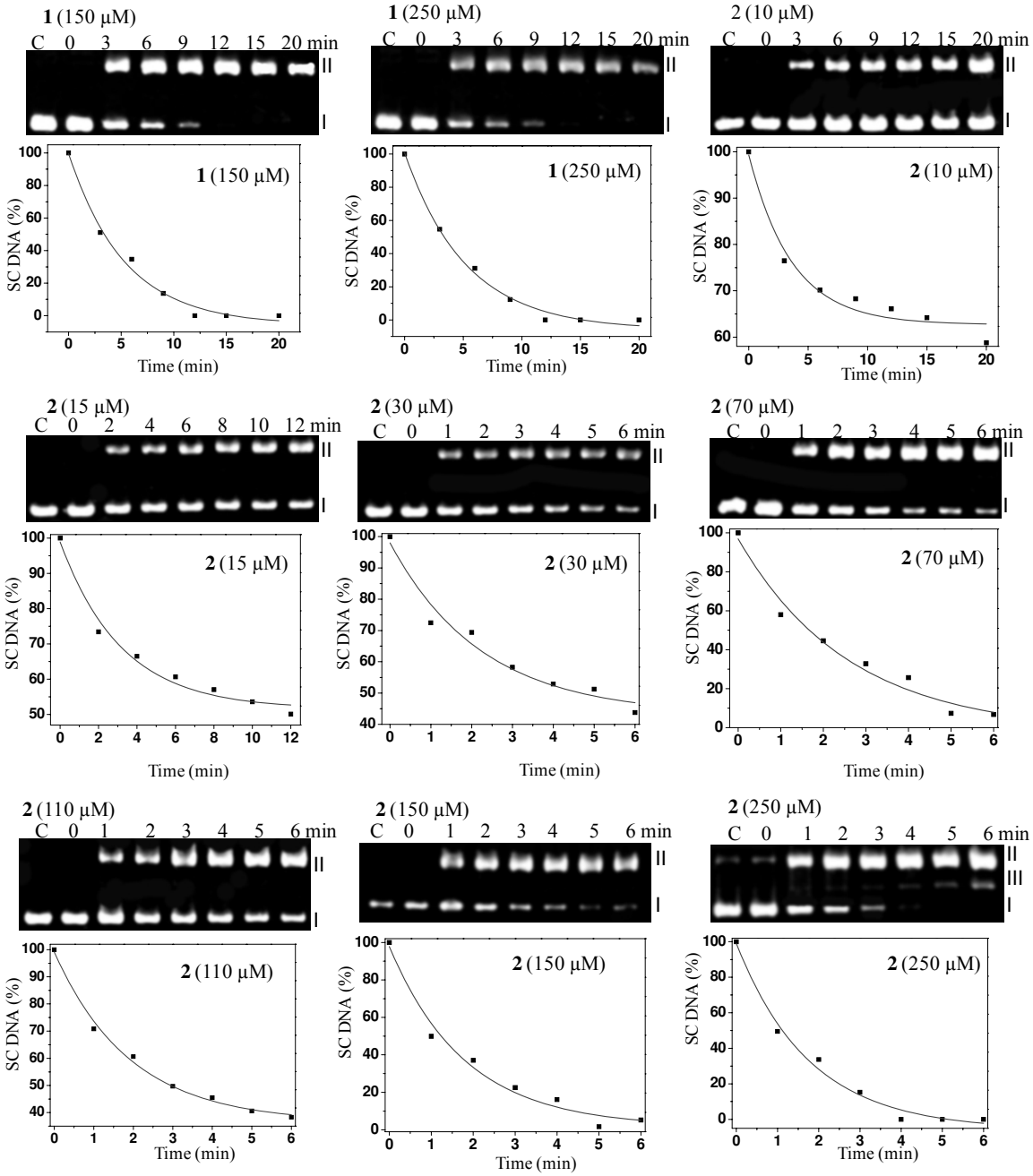

1 (150 μM)
C 0 3 6 9 12 15 20 min
II
I
SC DNA (%)
1 (150 μM)
Time (min)
1 (250 μM)
C 0 3 6 9 12 15 20 min
II
I
SC DNA (%)
1 (250 μM)
Time (min)
2 (10 μM)
C 0 3 6 9 12 15 20 min
II
I
SC DNA (%)
2 (10 μM)
Time (min)
2 (15 μM)
C 0 2 4 6 8 10 12 min
II
I
SC DNA (%)
2 (15 μM)
Time (min)
2 (30 μM)
C 0 1 2 3 4 5 6 min
II
I
SC DNA (%)
2 (30 μM)
Time (min)
2 (70 μM)
C 0 1 2 3 4 5 6 min
II
I
SC DNA (%)
2 (70 μM)
Time (min)
2 (110 μM)
C 0 1 2 3 4 5 6 min
II
I
SC DNA (%)
2 (110 μM)
Time (min)
2 (150 μM)
C 0 1 2 3 4 5 6 min
II
I
SC DNA (%)
2 (150 μM)
Time (min)
2 (250 μM)
C 0 1 2 3 4 5 6 min
II
III
I
SC DNA (%)
2 (250 μM)
Time (min)

Fig. S9.

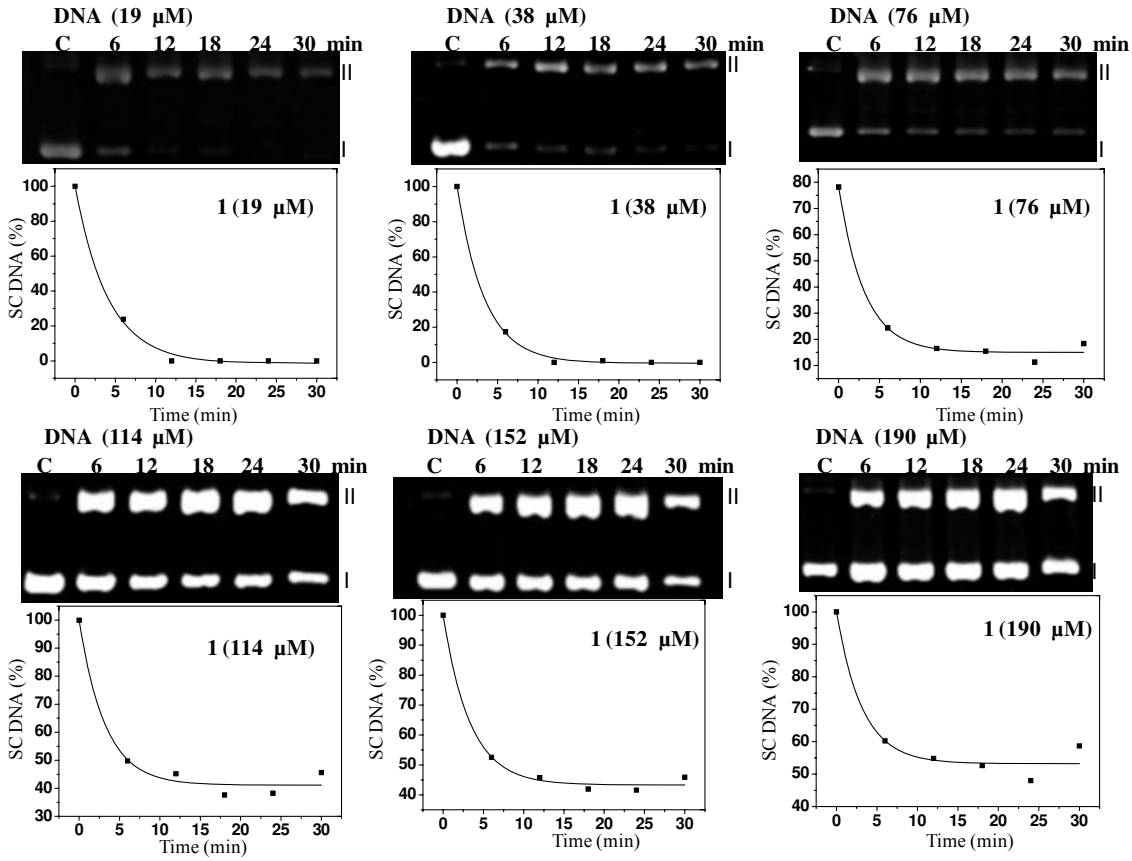

DNA (19 μM)
C 6 12 18 24 30 min
II
I
1 (19 μM)
SC DNA (%)
Time (min)
DNA (38 μM)
C 6 12 18 24 30 min
II
I
1 (38 μM)
SC DNA (%)
Time (min)
DNA (76 μM)
C 6 12 18 24 30 min
II
I
1 (76 μM)
SC DNA (%)
Time (min)
DNA (114 μM)
C 6 12 18 24 30 min
II
I
1 (114 μM)
SC DNA (%)
Time (min)
DNA (152 μM)
C 6 12 18 24 30 min
II
I
1 (152 μM)
SC DNA (%)
Time (min)
DNA (190 μM)
C 6 12 18 24 30 min
II
I
1 (190 μM)
SC DNA (%)
Time (min)

Fig. S10.

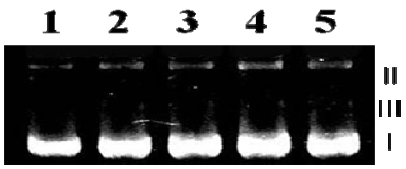


Fig. S11.

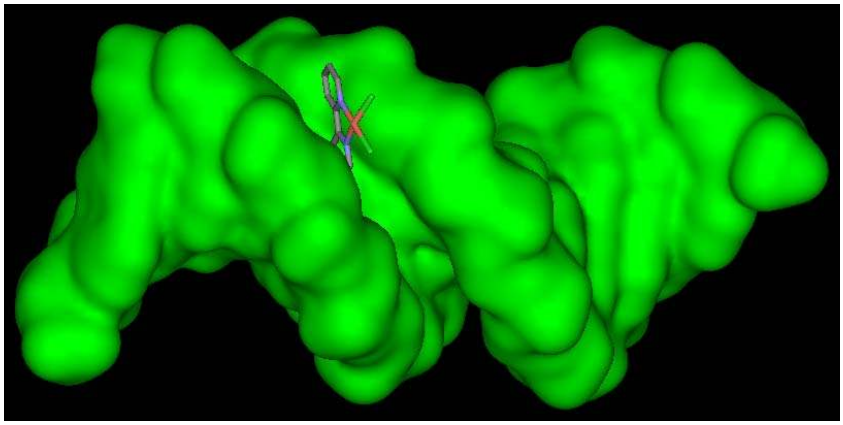


Fig. S12.