Supporting Information

Enantioselective separation of chiral ofloxacin using functional Cu(II)-coordinated G-rich oligonucleotides

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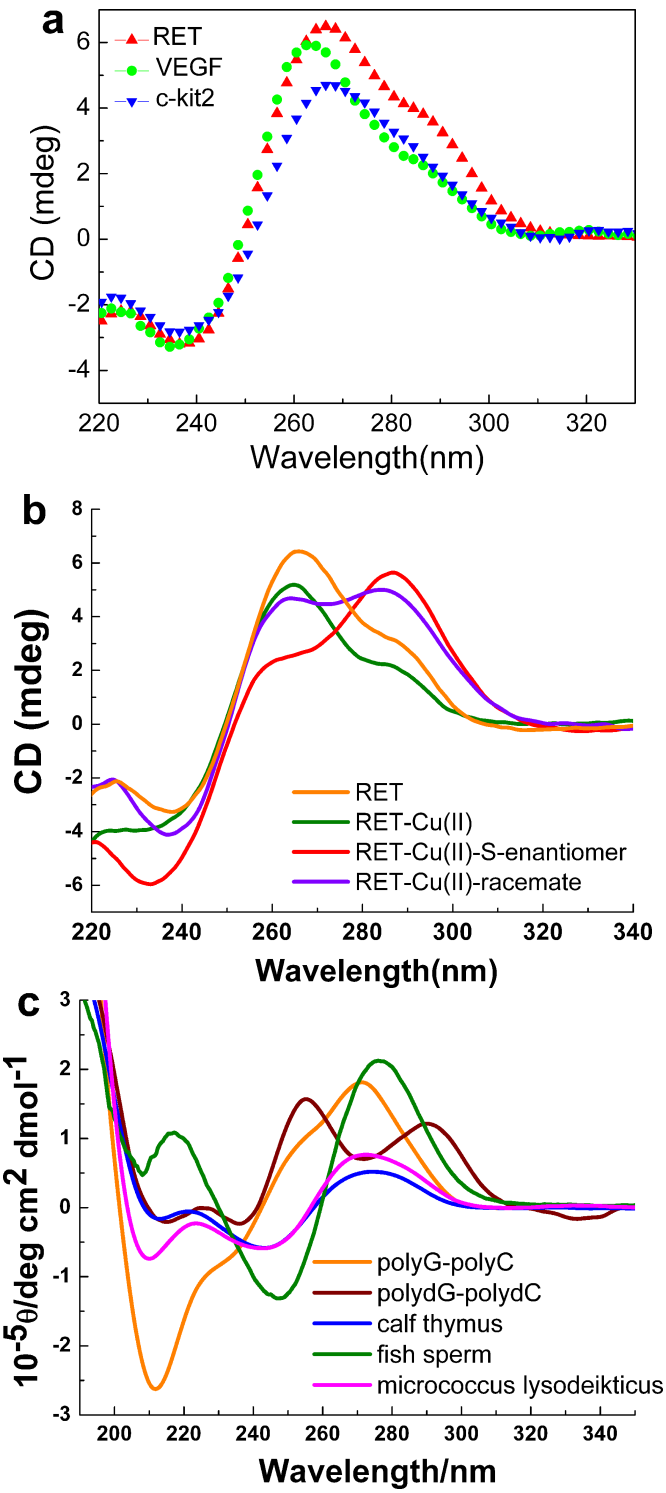

Fig. S1. (a) CD spectra of 20 μM G-rich oligonucleotides in 10 mM Tris-HCl buffer at pH 7.0; (b) CD spectra of 20 μM RET, RET-Cu(II) ([Cu^{2+}]/base=0.1), as well as RET-Cu(II) in the presence of 50 μM S- and racemic ofloxacin respectively at pH 7.0; (c) CD spectra of the polynucleotides used in this study at pH 7.0.

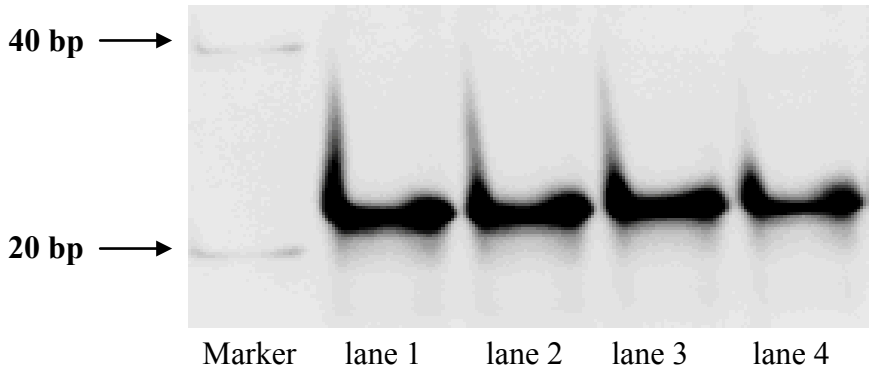

Fig. S2. PAGE image of double-stranded RET in 10 mM Tris-HCl buffer (pH 7.0) in the absence (lane 1) and presence of Cu^{2+} at the [Cu^{2+}]/[base] ratio of 0.1 (lane 2), 1 (lane 3) and 5 (lane 4) respectively.

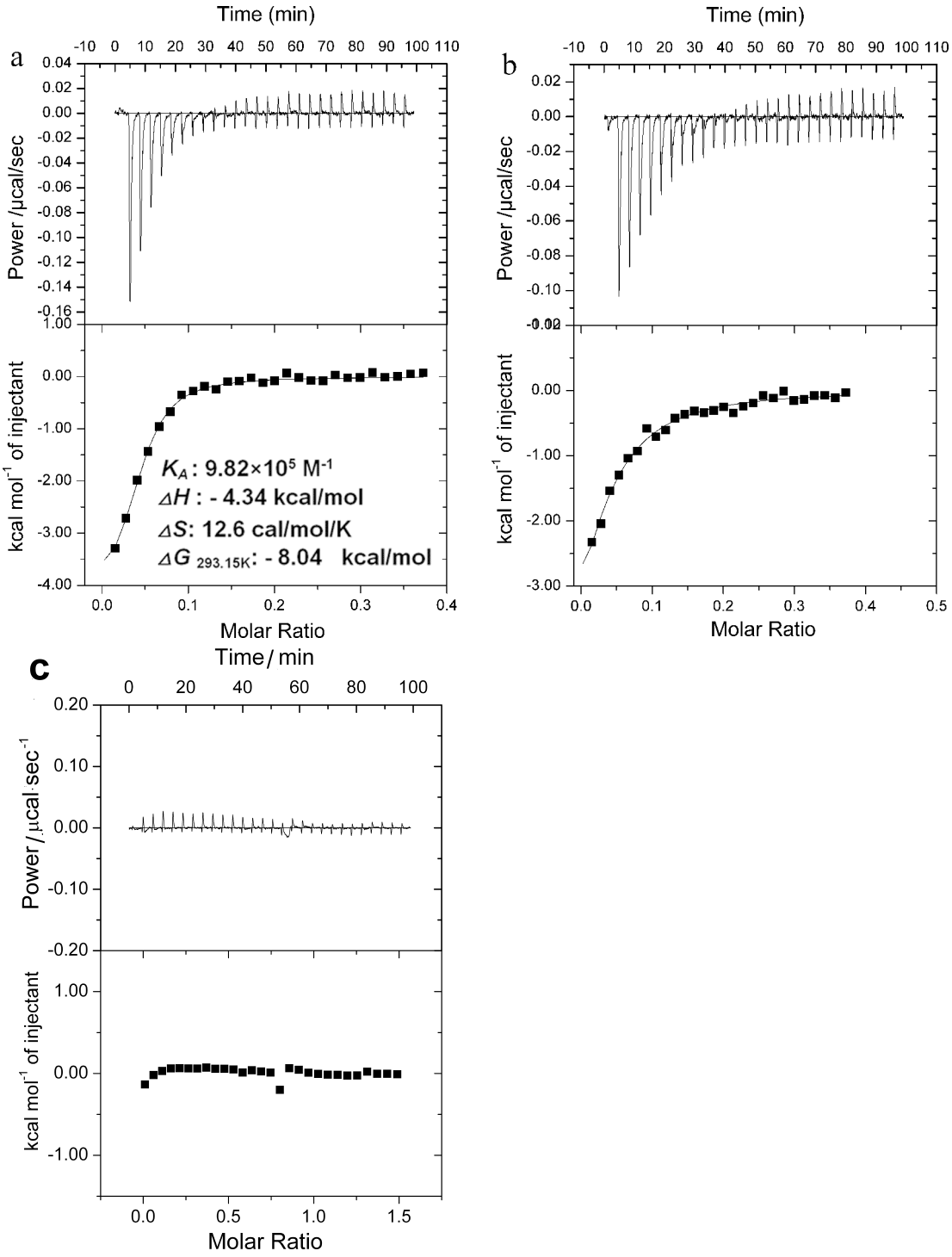

Fig. S3. Calorimetric titrations of 5 µM RET-Cu(II) complex ([Cu^{2+}]/[base]=0.1) with 0.2 mM S-ofloxacin (a) and racemic ofloxacin (b) at pH 7.0 at 20 ^{o}C, a standard nonlinear least-squares regression binding model, involving a single class of non-interacting sites fitted best to the data; (c) Calorimetric titrations of 5 µM RET in the absence of Cu^{2+} with 0.8 mM S-ofloxacin.

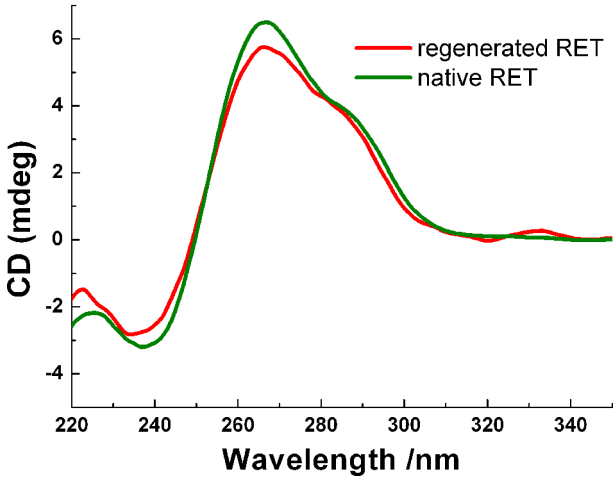

Fig. S4. Comparable CD spectra of native and regenerated RET at pH 7.0, regenerated RET was prepared from RET-Cu(II)-ofloxacin complex by adding EDTA, through ultrafiltration the filtered residue was resuspended by equivalent volume buffer.

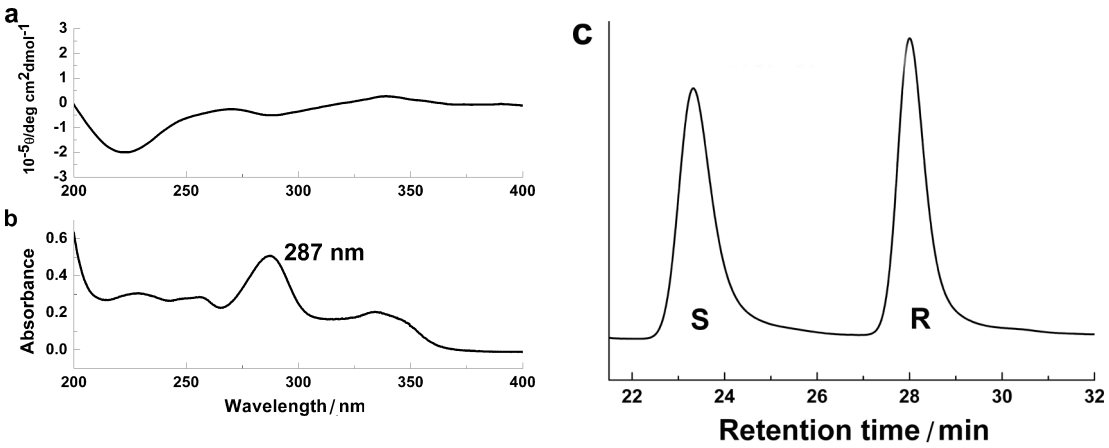

Fig. S5. CD (a) and UV (b) spectra of S-ofloxacin in 10 mM Tris-HCl buffer (pH 7.0); (c) HPLC analysis of racemic ofloxacin.

Table S1. DNA sequences used in the experiments

Name	Sequence	Molecular weight ($g \cdot mol^{-1}$)	Extinction coefficient $L \cdot (mol \cdot cm)^{-1}$
htelo	5'-$AG_3(T_2AG_3)_3$-3'	6966.5	228500
	5'-$(C_3TA_2)_3C_3T$-3'	6504.3	193700
RET	5'-$A(G_4C)_3G_5C$-3'	7004.5	212500
	5'-$GC_5(GC_4)_3T$-3'	6475.2	169100
c-kit2	5'-$C(C_3T)_2(CG)_2(C_3G)_2$-3'	6201.0	163500
	5'-$(CG_3)_2(CG)_2(AG_3)_2G$-3'	6659.3	205600
VEGF	5'-$CG_4CG_3CCG_5CG_4T$-3'	6955.5	205000
	5'-$AC_4GC_5GGC_3GC_4G$-3'	6524.2	178400

Table S2. The $e.e._R$ (S-enantiomer excess) of ofloxacin enantiomers in the residues at each operational stage in the enrichment process of R-enantiomer through three-stage operation [a]

Sequence	Stage	$e.e._R$ (%)	As (%)
RET-Cu(II)	1^{st}	29.3	48.0
	2^{nd}	13.2	33.2
	3^{rd}	– 23.2	15.9
c-kit2-Cu(II)	1^{st}	38.9	52.2
	2^{nd}	13.3	34.2
	3^{rd}	– 40.4	12.1
VEGF-Cu(II)	1^{st}	26.6	55.3
	2^{nd}	2.0	33.7
	3^{rd}	– 44.9	9.7

[a] Experimental conditions: 100 μM racemic ofloxacin, 20 μM DNA, pH 7.0.

Table S3. The $e.e._R$ (S-enantiomer excess) of ofloxacin enantiomers in the residues at each operational stage in the enrichment process of R-enantiomer through three-stage operation [a]

Sequence	Stage	$e.e._R$ (%)	As (%)
RET	1st	23.7	28.5
	2nd	21.9	18.2
	3rd	13.9	13.1
c-kit2	1st	38.8	23.3
	2nd	34.0	18.2
	3rd	23.9	11.8
VEGF	1st	30.9	25.1
	2nd	19.1	20.4
	3rd	10.5	12.9

[a] Experimental conditions: 100 μM racemic ofloxacin, 20 μM DNA, pH 7.0.

Table S4. The $e.e._R$ (S-enantiomer excess) of ofloxacin enantiomers in the residues at each operational stage in the enrichment process of S-enantiomer through three-stage operation [a]

Sequence	Stage	$e.e._R$ (%)	As (%)
RET-Cu(II)	1st	29.3	48.0
	2nd	39.9	31.4
	3rd	49.5	27.1
c-kit2-Cu(II)	1st	38.9	52.2
	2nd	61.1	44.1
	3rd	78.1	30.3
VEGF-Cu(II)	1st	26.6	55.3
	2nd	43.1	40.1
	3rd	57.6	31.7

[a] Experimental conditions: 100 μM racemic ofloxacin, 20 μM DNA, pH 7.0.

Table S5. The $e.e._R$ (S-enantiomer excess) of ofloxacin enantiomers in the residues at each operational stage in the enrichment process of S-enantiomer through three-stage operation [a]

Sequence	Stage	$e.e._R$ (%)	As (%)
RET	1st	23.7	28.5
	2nd	36.0	10.6
	3rd	n.d.[b]	n.d.[b]
c-kit2	1st	38.8	23.3
	2nd	59.3	8.3
	3rd	n.d.[b]	n.d.[b]
VEGF	1st	30.9	25.1
	2nd	52.8	12.7
	3rd	n.d.[b]	n.d.[b]

[a] Experimental conditions: 100 μM racemic ofloxacin, 20 μM DNA, pH 7.0; [b] The concentration is too low to be determined.