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Supplementary Material

Supramolecular Interaction Between Cucurbit[8]uril and the Quinolone Antibiotic Ofloxacin

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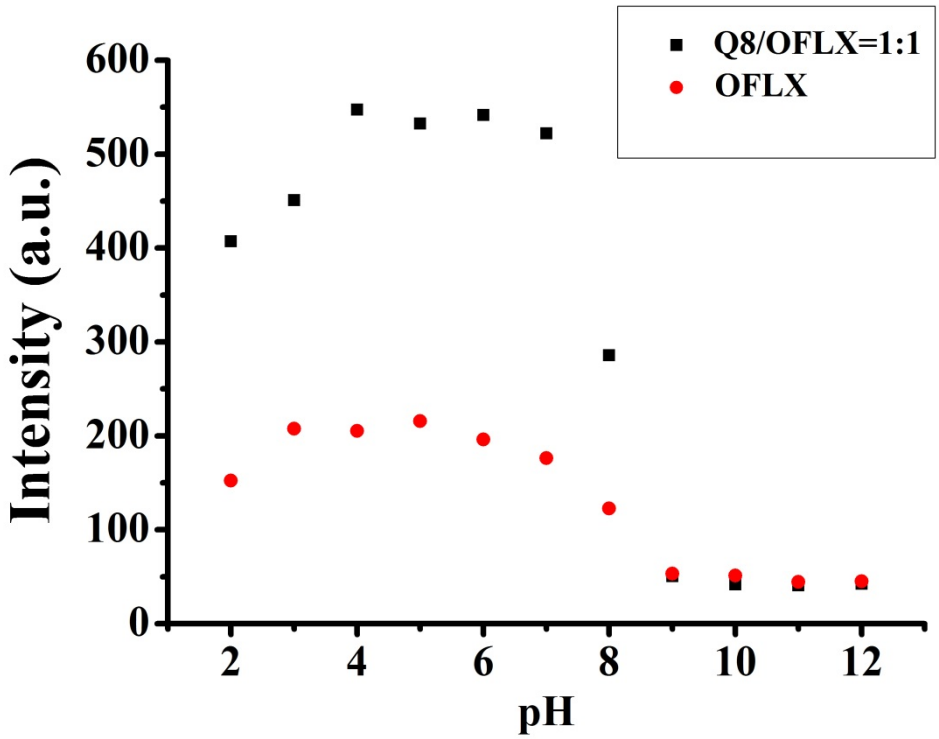

Figure S1 pK_a studies. Fluorescence emission spectra of OFLX (2.0×10^{-5} mol·L^{-1}) and in the presence of 1.0 equiv of Q[8] at different pH values.

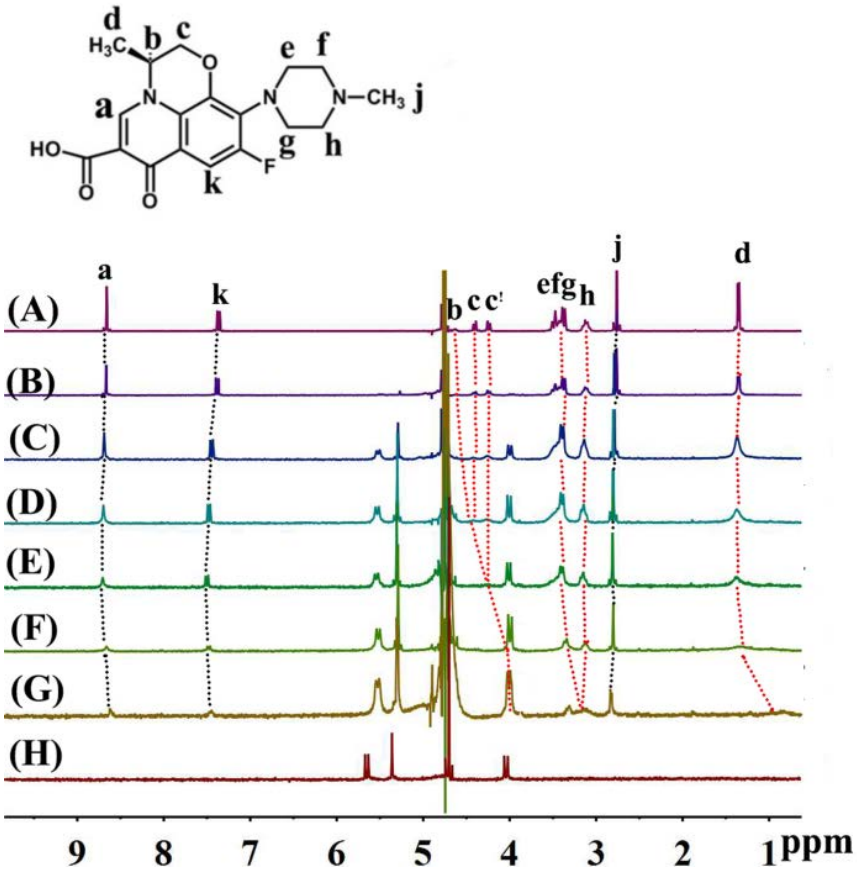

Figure S2 ^{1}H NMR spectra of free OFLX (A), OFLX in the presence of 0.03 equiv of Q[8] (B), 0.09 equiv of Q[8] (C), 0.15 equiv of Q[8] (D), 0.20 equiv of Q[8] (E), 0.58 equiv of Q[8] (F), 1.02 equiv of Q[8] (G) and host Q[8] (H) in pD = 2.5.

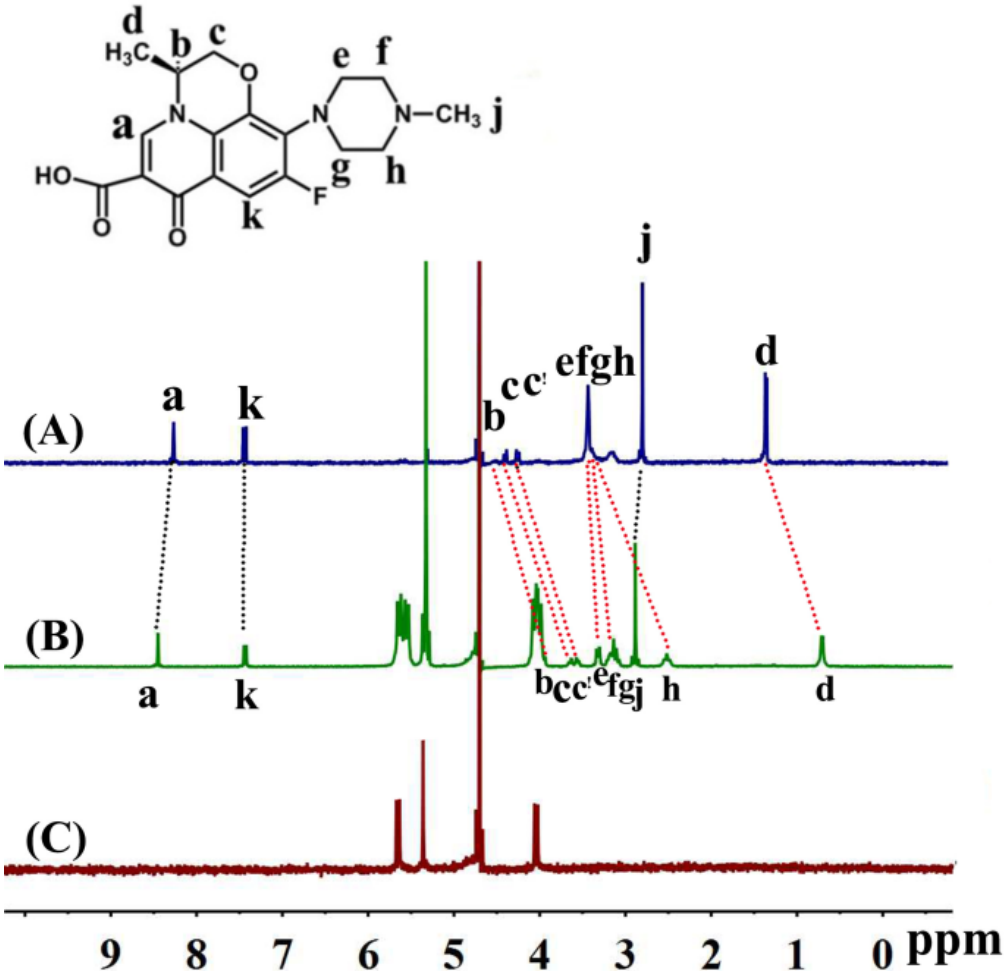

Figure S3 ^{1}H NMR spectra of free OFLX (A), OFLX in the presence of 1.05 equiv of Q[8] (B), and host Q[8] (C) in pD = 8.0.

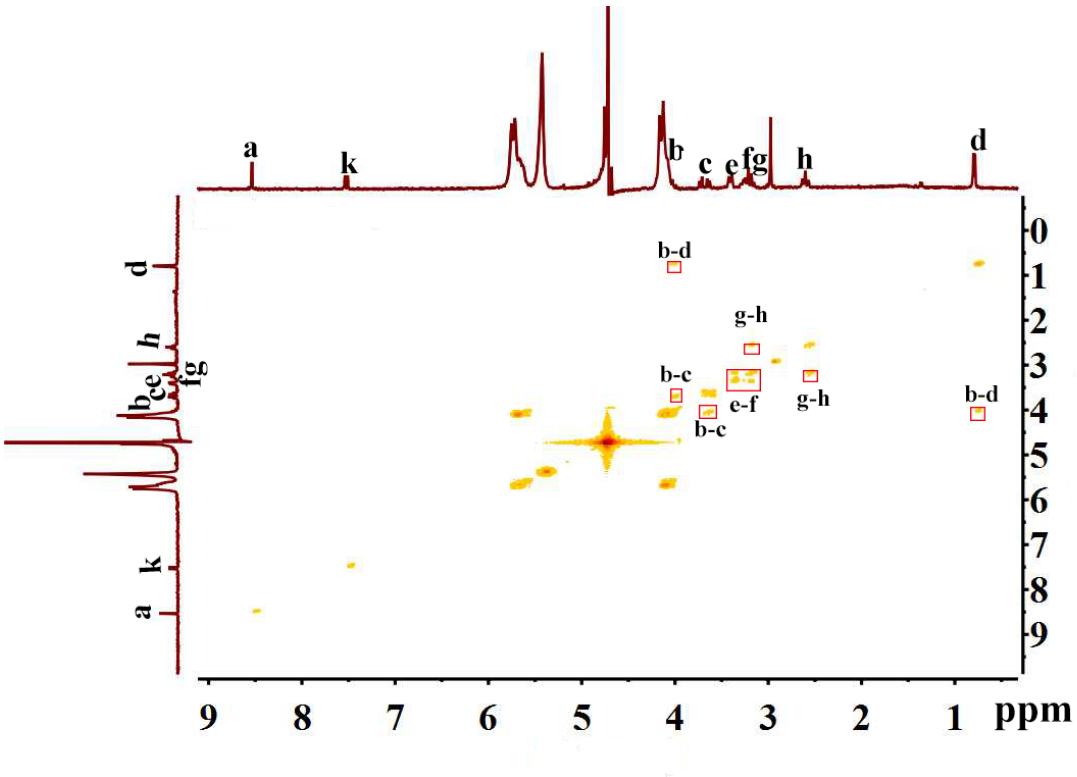

Figure S4 The ^{1}H-^{1}H COSY spectrum (400MHz, D_2O) of Q[8]@OFLX.

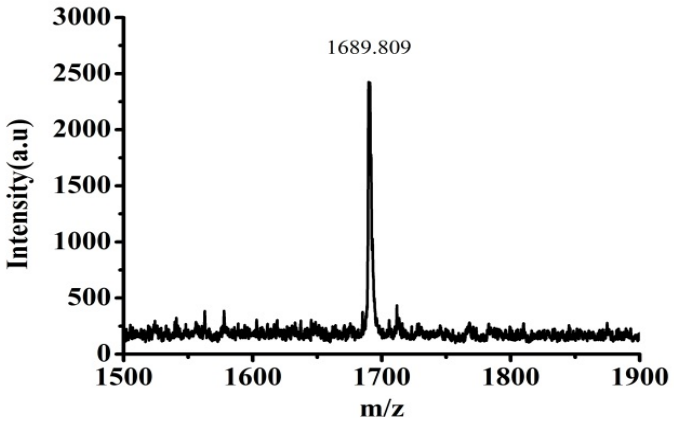

Figure S5 MALDI-TOF mass spectrum of the complex OFLX@Q[8]

MALDI-TOF mass spectrometry is a common technique used for assessing the interaction between host and guest molecules. As demonstrated in Figure 5, the principal mass spectrometry signal was observed at *m*/*z* 1689.809, and identified as OFLX@Q[8] (calculated *m*/*z*: 1689.536). These data provide direct support for the formation of a 1:1 stoichiometric Q[8]-OFLX inclusion complex.

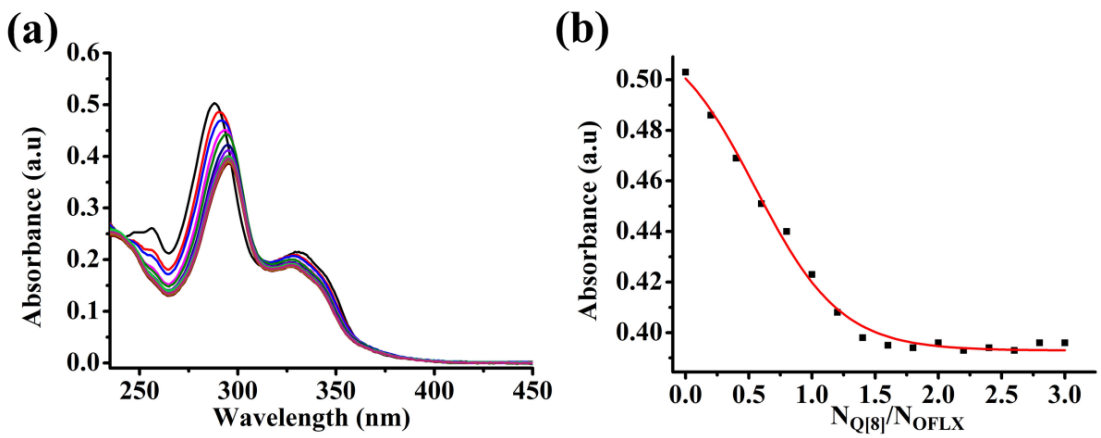

Figure S6. (a) UV absorption of OFLX (2.0×10^{-5}mol·L^{-1}) upon the addition of increasing amounts (0, 0.1, 0.2...2.8, 3.0 equiv) of Q[8], (b) plot of maximum absorption *vs*. $N_{Q[8]}/N_{OFLX}$.

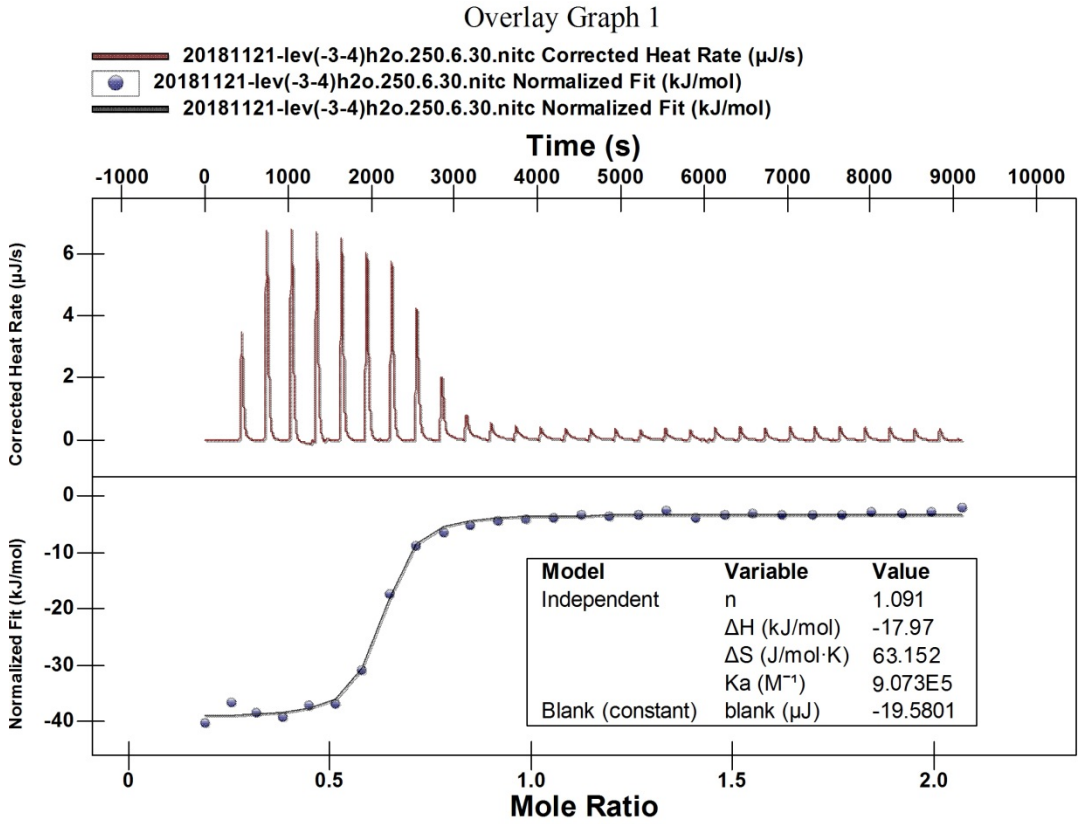

Figure S7 ITC profile of Q[8] with OFLX in aqueous solution at 298.15 K

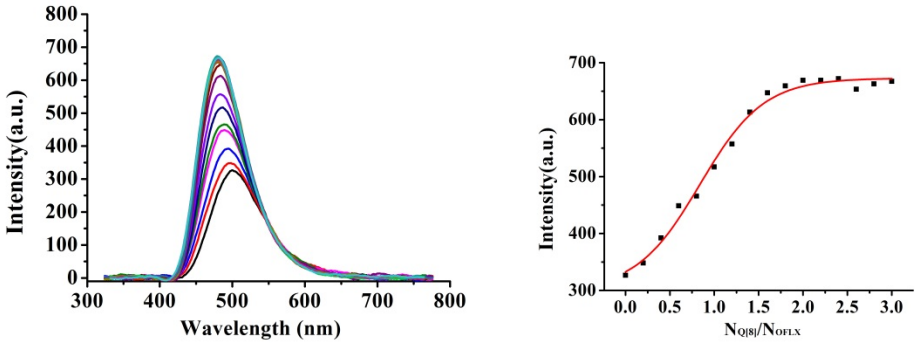

Figure S8. (a) Fluorescence emission spectra of OFLX (2.0×10^{-5} mol·L^{-1}) upon the addition of increasing amounts (0, 0.1, 0.2...2.8, 3.0 equiv.) of Q[8] at pH 3.5; (b) plot of maximum intensity vs. $N_{Q[8]}/N_{OFLX}$ at pH 3.5.

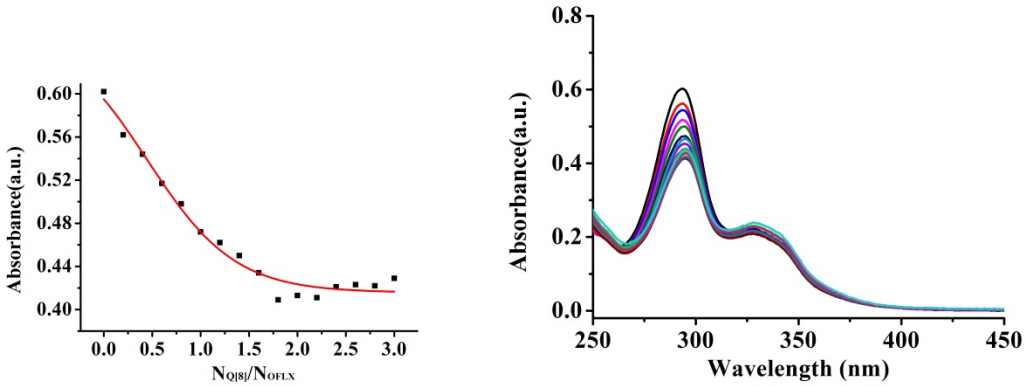

Figure S9. (a) UV absorption of OFLX (2.0×10^{-5}mol·L^{-1}) upon the addition of increasing amounts (0, 0.1, 0.2...2.8, 3.0 equiv) of Q[8] at pH 3.5, (b) plot of maximum absorption vs. $N_{Q[8]}/N_{OFLX}$ at pH 3.5.

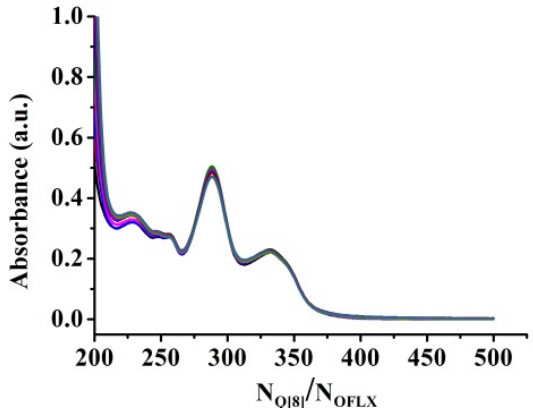

Figure S10. (a) UV absorption of OFLX (2.0×10^{-5}mol·L^{-1}) upon the addition of increasing amounts (0, 0.1, 0.2...2.8, 3.0 equiv) of Q[8] at pH 10.0

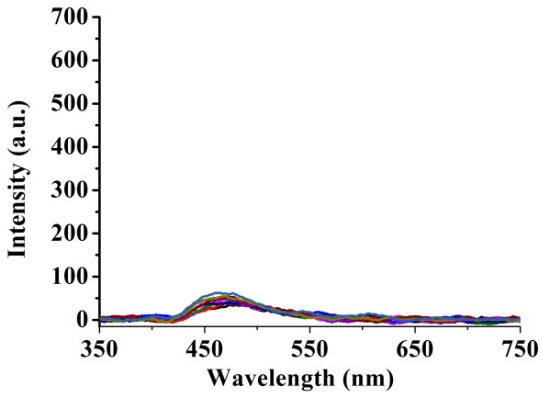

Figure S11. (a) Fluorescence emission spectra of OFLX (2.0×10^{-5} mol·L^{-1}) upon the addition of increasing amounts (0, 0.1, 0.2...2.8, 3.0 equiv.) of Q[8] at pH 10.0

Table S1. The thermodynamic parameters of Q[8]@OFLX.

Complex	K_a (M^{-1})	$\Delta H°$ (kJ mol^{-1})	$T\Delta S°$ (kJ mol^{-1})
Q[8]@OFLX	$(9.07 \pm 0.64) \times 10^5$	(-17.97 ± 1.23)	(18.82 ± 1.49)

Table S2 Binding constant values of some hosts with ofloxacin and other fluoroquinolones at different pH values.

Host	**guest**	**K_a (M^{-1})**	**Calculated from determined data**	**Ref**
methyl β-cyclodextrin (Me-β-CD)	Ofloxacin	7.8×10^3	Fluorescence	[22](c)
methyl β-cyclodextrin (Me-β-CD)	Ofloxacin	1.0×10^3	Fluorescence (pH=7.53)	[26]
methyl β-cyclodextrin (Me-β-CD)	Ofloxacin	0.2×10^3	Fluorescence (pH=10.53)	[26]
methyl β-cyclodextrin (Me-β-CD)	Ofloxacin	0.167×10^3	Fluorescence (pH=3.05)	[26]
β-CD	Ofloxacin	4.5×10^5	Fluorescence	[27]
β-CD	Ofloxacin	1.17×10^4	UV-Vis	[28]
Q[7]	Danofloxacin (DOFL)	$(2.1 \pm 0.2) \times10^4$	Fluorescence (pH=3.5)	[21]
Q[7]	Danofloxacin (DOFL)	$(1.6 \pm 0.9) \times10^5$	Fluorescence (pH=7.5)	[21]
Q[7]	Danofloxacin (DOFL)	$(6.5 \pm 0.5) \times10^3$	Fluorescence (pH=10.2)	[21]
Q[7]	Danofloxacin (DOFL)	$(2.1 \pm 0.2) \times10^5$	ITC (pH=3.5)	[21]
Q[7]	Danofloxacin (DOFL)	$(1.7 \pm 0.1) \times10^5$	ITC (pH=7.5)	[21]
Q[7]	Danofloxacin (DOFL)	$(7.3 \pm 0.5) \times10^3$	ITC (pH=10.2)	[21]
Q[8]	Ofloxacin	$(9.07 \pm 0.64) \times10^5$	ITC (pH=7.0)	In this work
Q[8]	Ofloxacin	7.24×10^4 M^{-1}	UV-Vis (pH=7.0)	In this work
Q[8]	Ofloxacin	1.18×10^5 M^{-1}	Fluorescence (pH=7.0)	In this work
Q[8]	Ofloxacin	4.76×10^4 M^{-1}	Fluorescence (pH=3.6)	In this work
Q[8]	Ofloxacin	Not get K value	Fluorescence (pH=10.2)	In this work