Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

A Chiral Macrocyclic Molecule for Efficient Sensing of Sulfate Anion with CD Signals

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1 *Spectroscopic data of compound L*

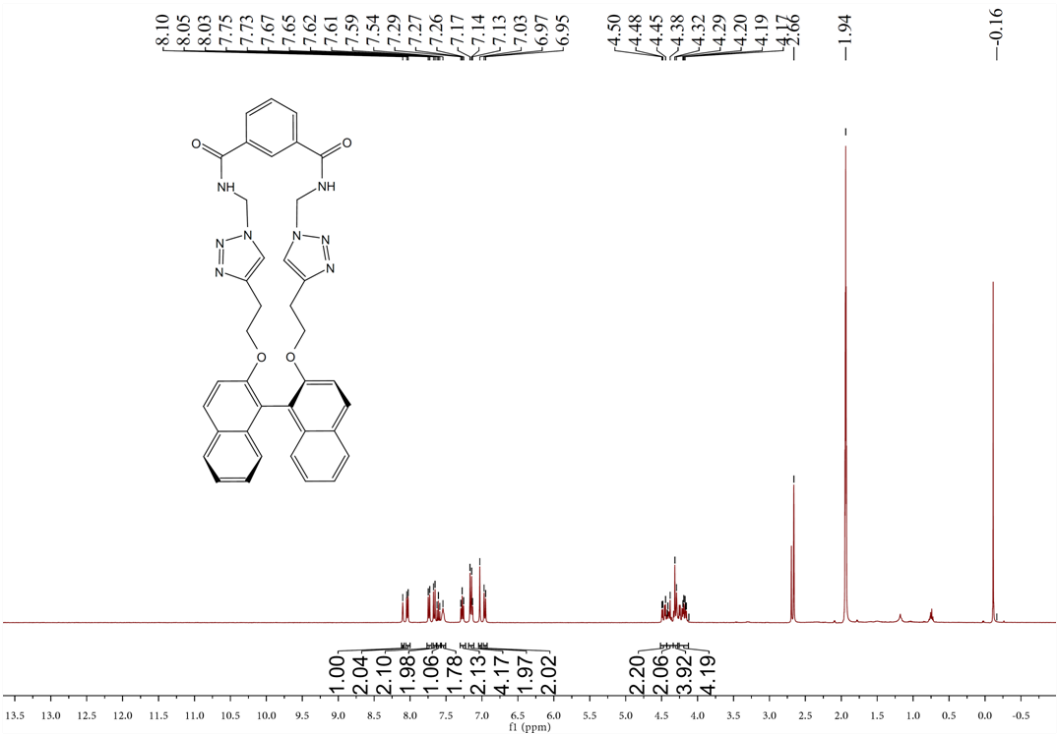

Figure S1

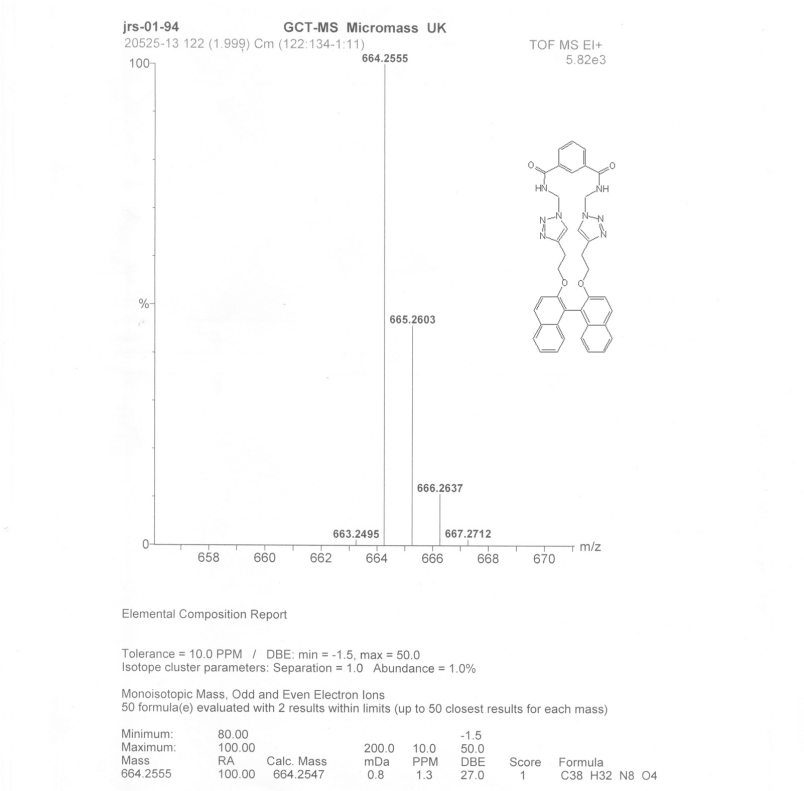

Figure S2

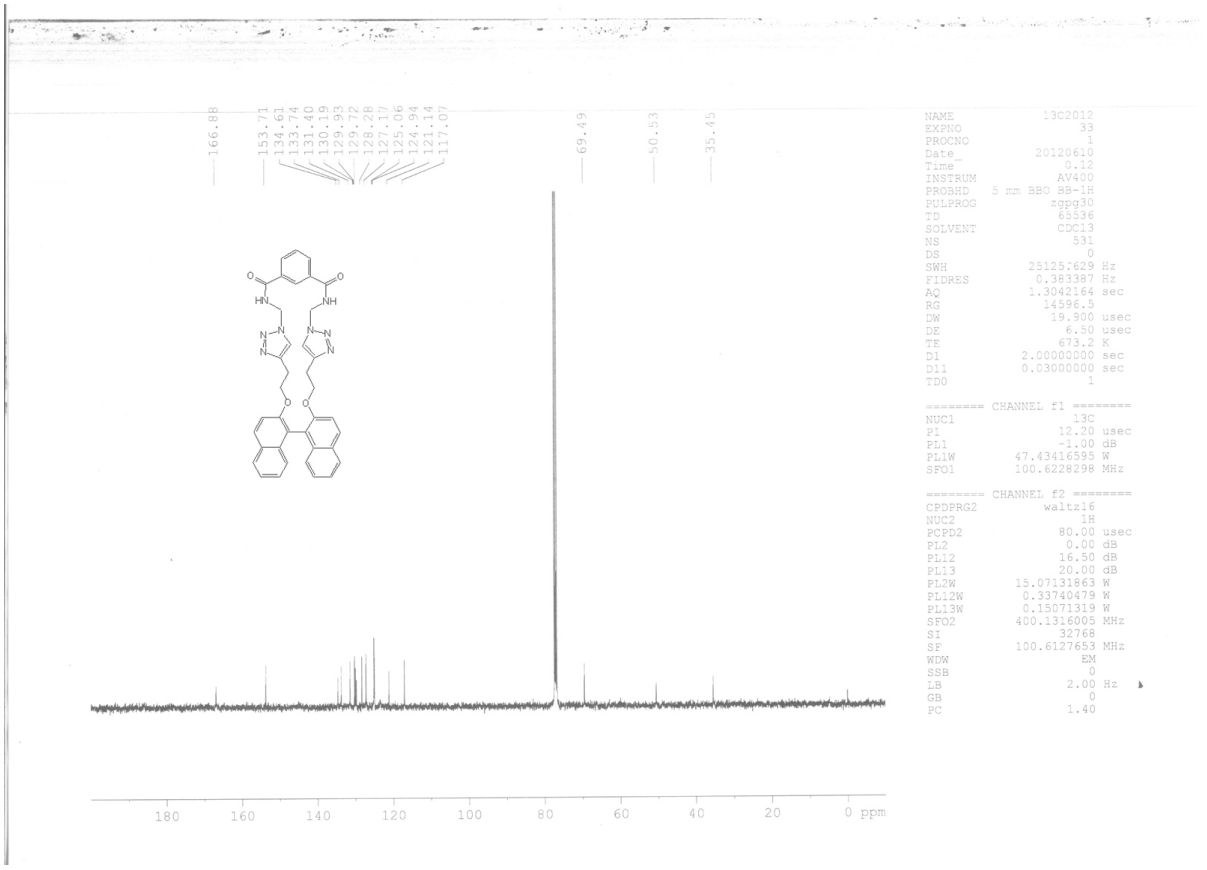

Figure S3

2 *UV-Vis Spectra and CD Spectra of compound L with aions*

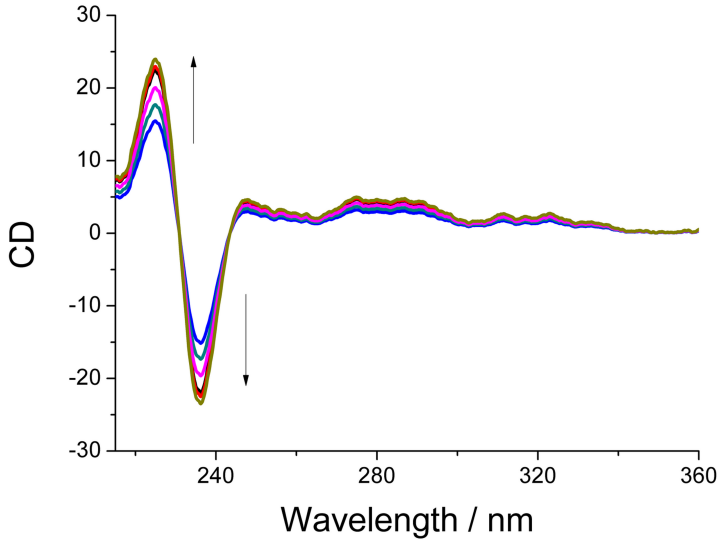

Figure S4 CD of Cycle-Binol molecule **L** (1.0×10^{-5} mol/L) upon addition of $H_2PO_4^-$ (0-100μM)

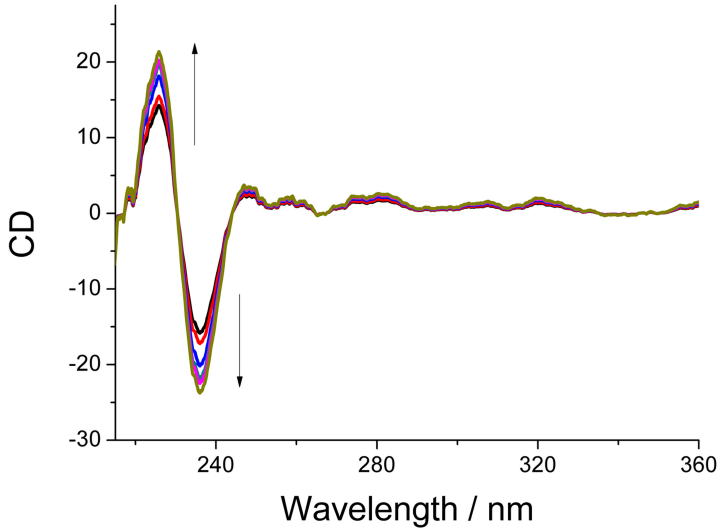

Figure S5 CD of Cycle-Binol molecule **L** (1.0×10^{-5} mol/L) upon addition of AcO^- (0-100μM)

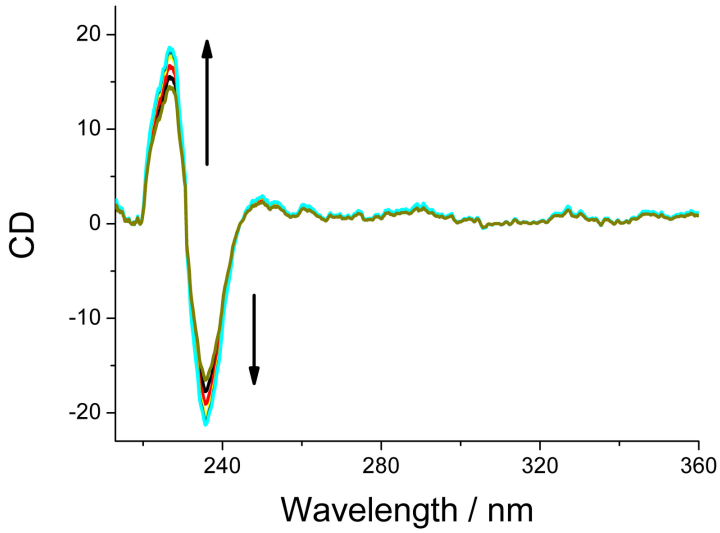

Figure S6 CD of Cycle-Binol molecule **L** (1.0×10^{-5} mol/L) upon addition of Br^- (0- 100µM)

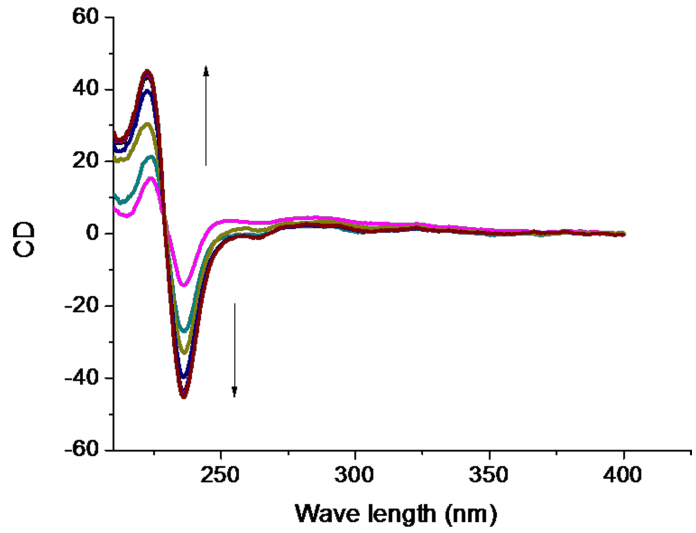

Figure S7 CD of Cycle-Binol molecule **L** (1.0×10^{-5} mol/L) upon addition of SO_4^{2-} (50-100 µM)

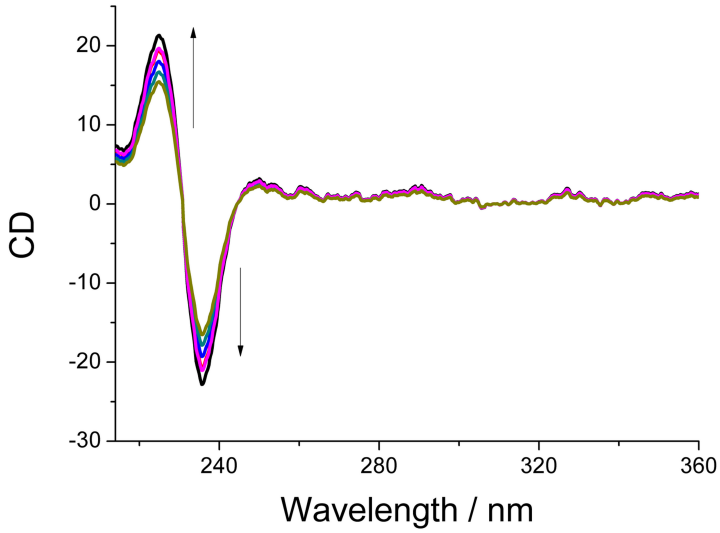

Figure S8 CD of Cycle-Binol molecule **L** (1.0×10^{-5} mol/L) upon addition of Cl^- (0-100 μM)

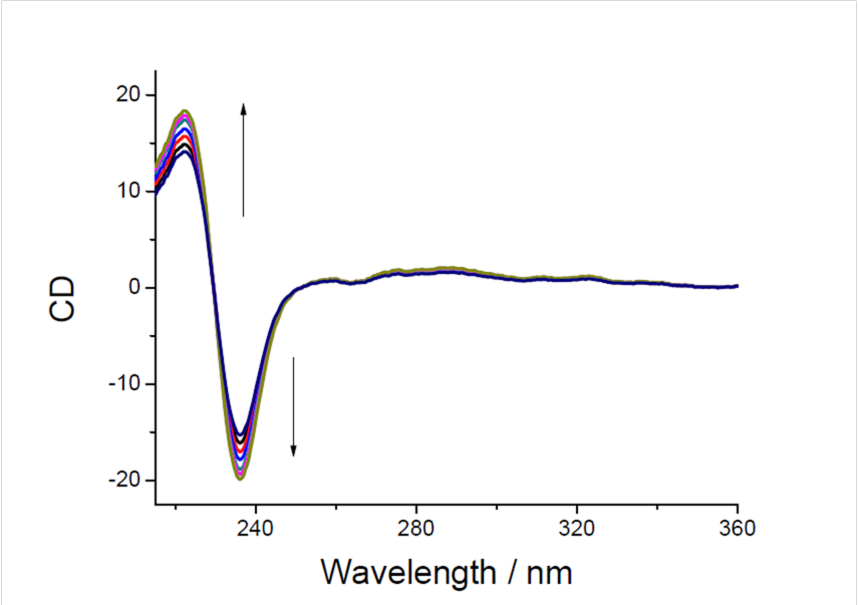

Figure S9 CD of Cycle-Binol molecule **L** (1.0×10^{-5} mol/L) upon addition of I^- (0-100 μM)

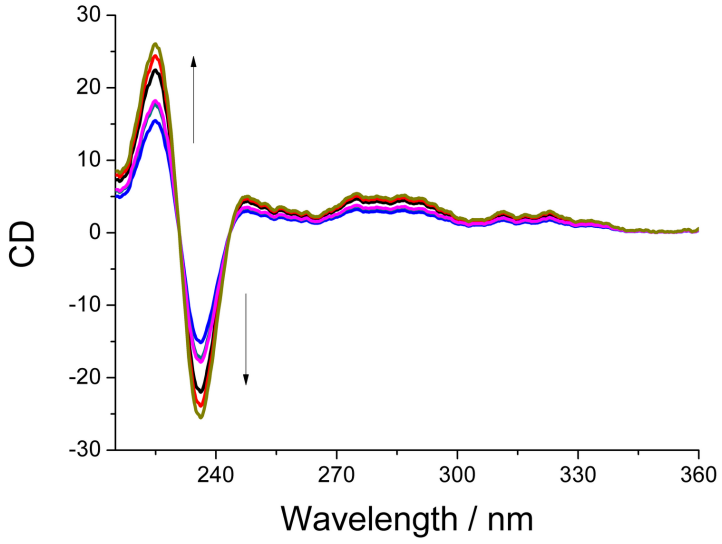

Figure S10 CD of Cycle-Binol molecule **L** (1.0×10^{-5} mol/L) upon addition of HSO_4^- (0-100 μM)

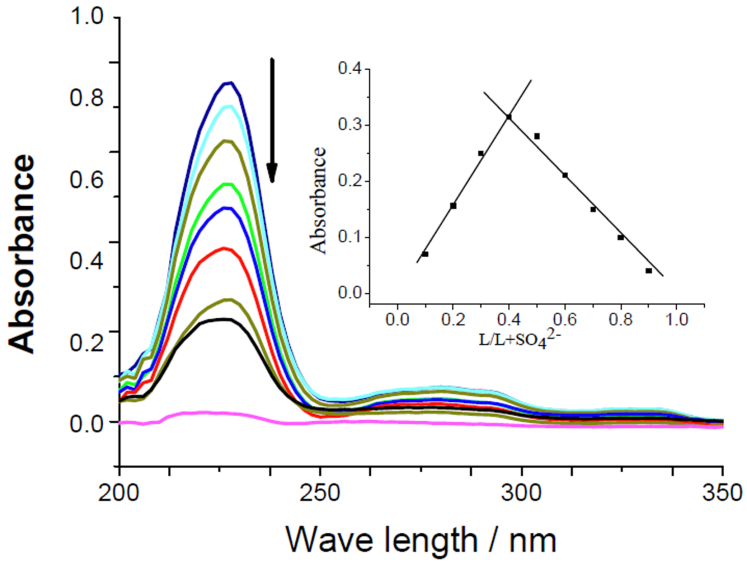

Figure S11 The job plot showing formation of a **L**-SO_4^{2-} complex

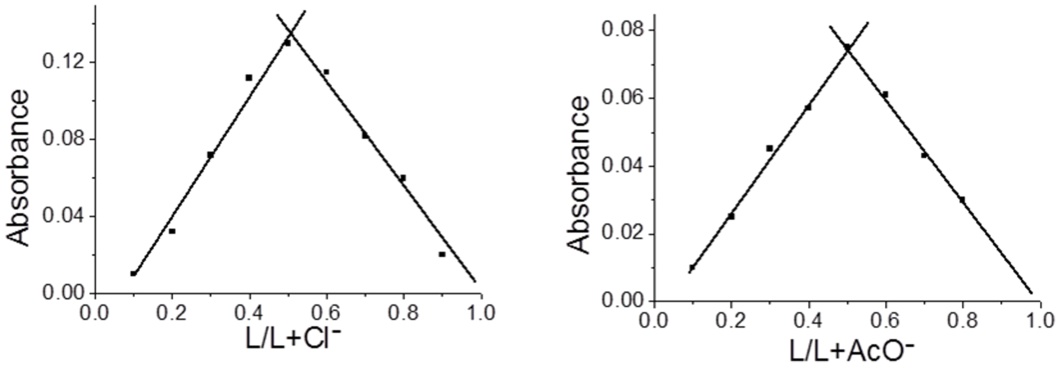

Figure S12 Job plot showing formation of a Cl^--**L** complex and AcO^--**L** complex

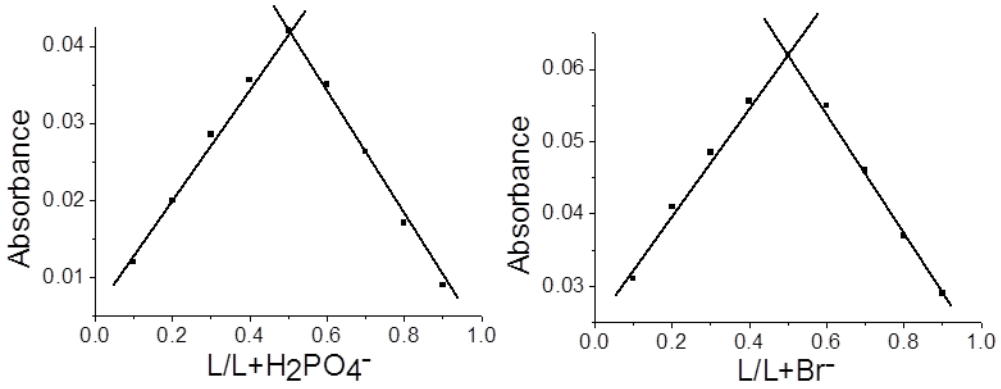

Figure S13 Job plot showing formation of a $H_2PO_4^-$-**L** complex and Br^--**L** complex.

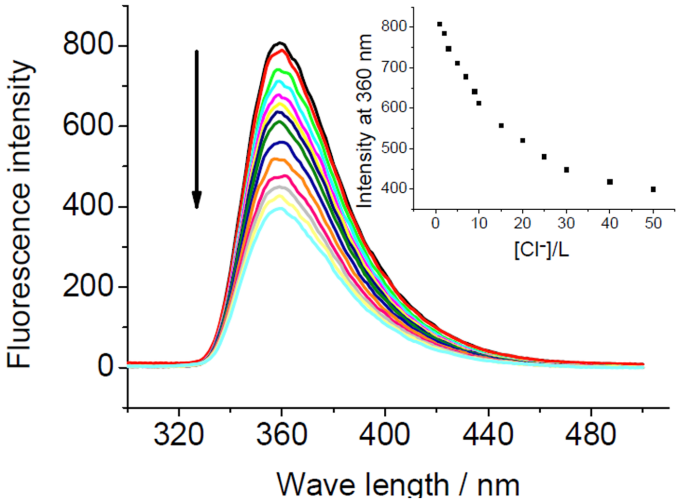

Fig S14 Fluorescence spectra (excitation at 358 nm) of receptor **L** (1.0×10^{-5} mol/L) in CH_3CN solution upon addition of 0–50 equiv. of Cl^-

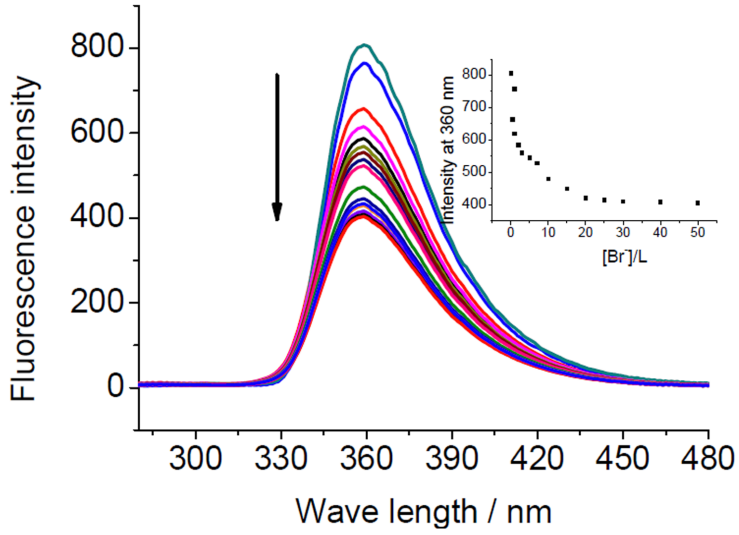

Fig S15 Fluorescence spectra (excitation at 358 nm) of receptor **L** (1.0×10^{-5} mol/L) in CH_3CN solution upon addition of 0–50 equiv. of Br^-

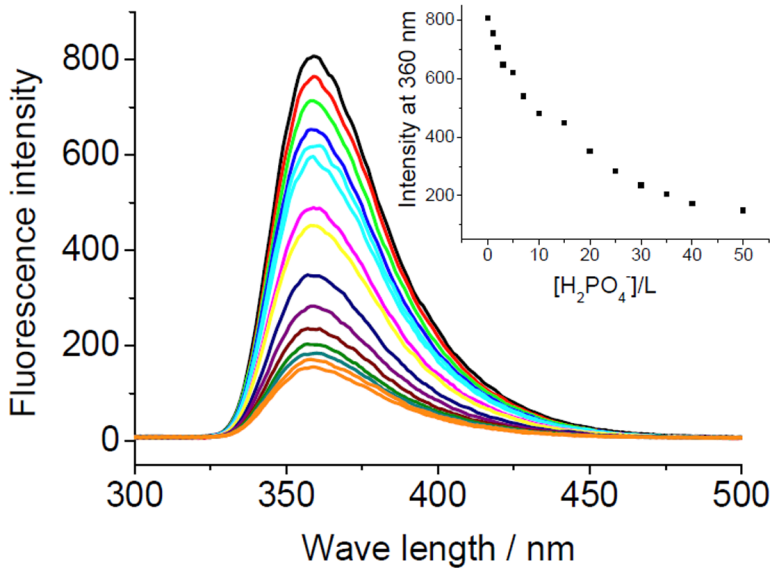

Fig S16 Fluorescence spectra (excitation at 358 nm) of receptor **L** (1.0×10^{-5} mol/L) in CH_3CN solution upon addition of 0–50 equiv. of $H_2PO_4^-$

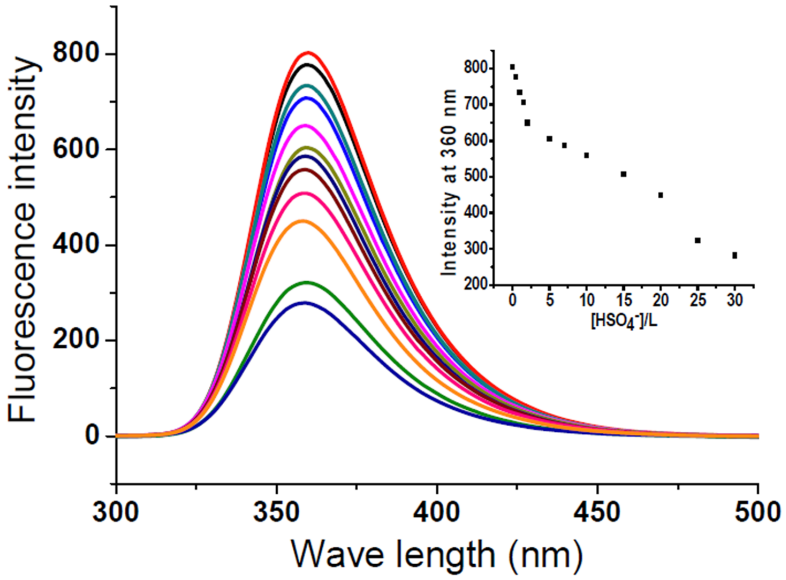

Fig S17 Fluorescence spectra (excitation at 358 nm) of receptor **L** (1.0×10^{-5} mol/L) in CH_3CN solution upon addition of 0–50 equiv. of HSO_4^-

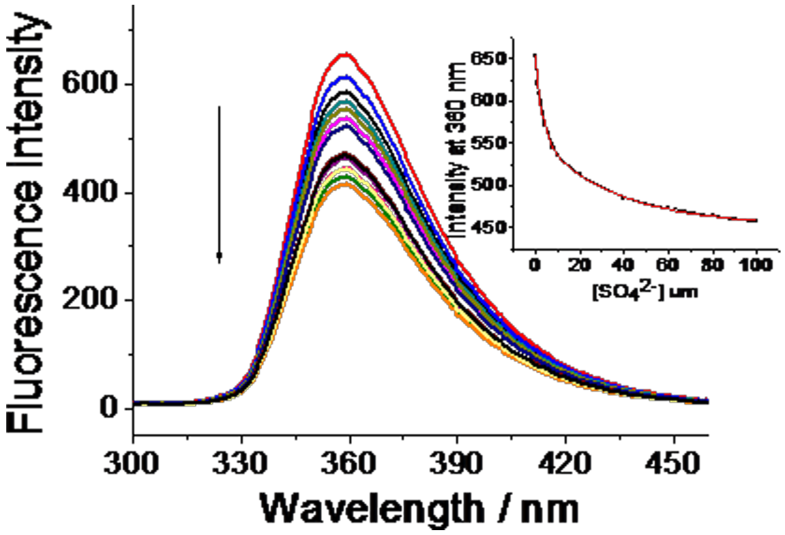

Fig S18 Fluorescence spectra (excitation at 358 nm) of receptor L (1.0 × 10−5 mol/L) in CH3CN solution upon addition of 0–50 equiv. of SO_4^{2-}

3. Conformation study of L, L_2SO_4 complex by VT NMR, COSY NNR

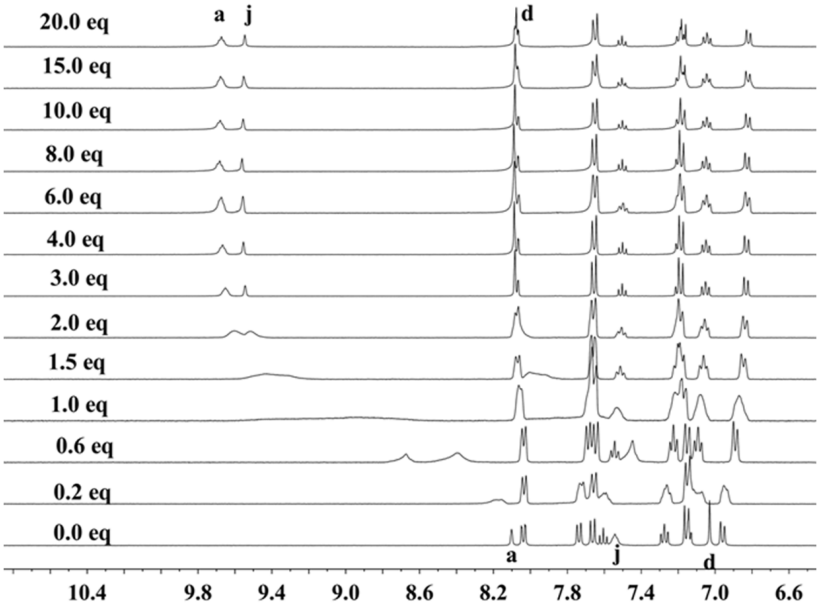

Fig S19 Portion of ^{1}HNMR traces of **L** in CD_3CN in the presence of Cl^-

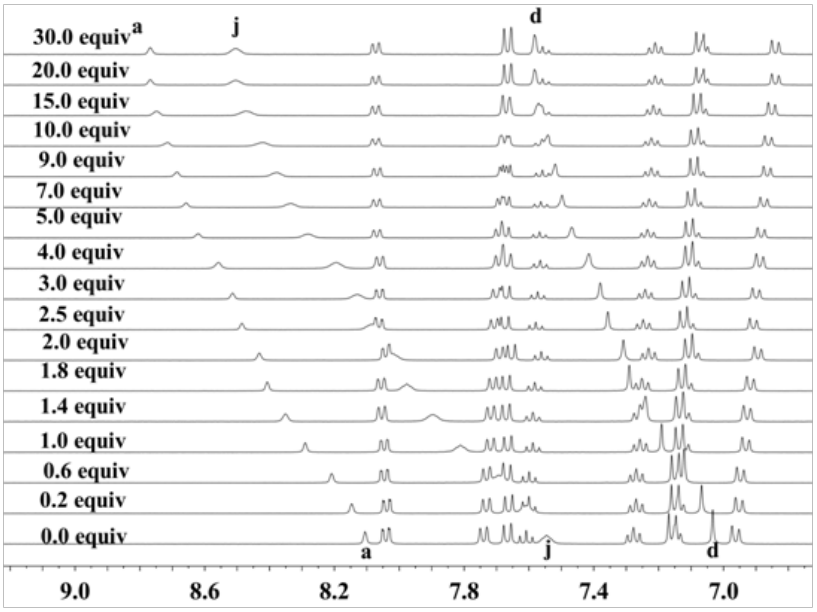

Fig S20 Portion of ^{1}HNMR traces of **L** in CD_3CN in the presence of I^-

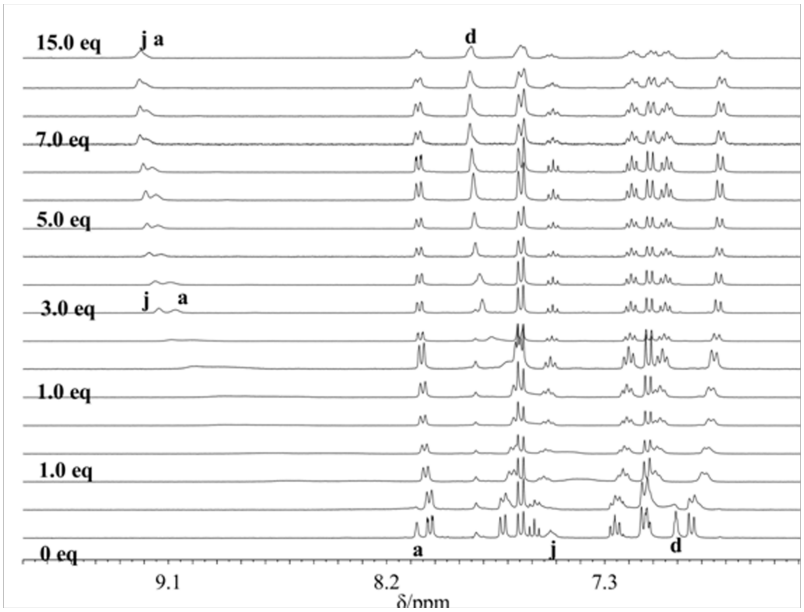

Fig S21 Portion of ^{1}HNMR traces of **L** in CD_3CN in the presence of Br^-

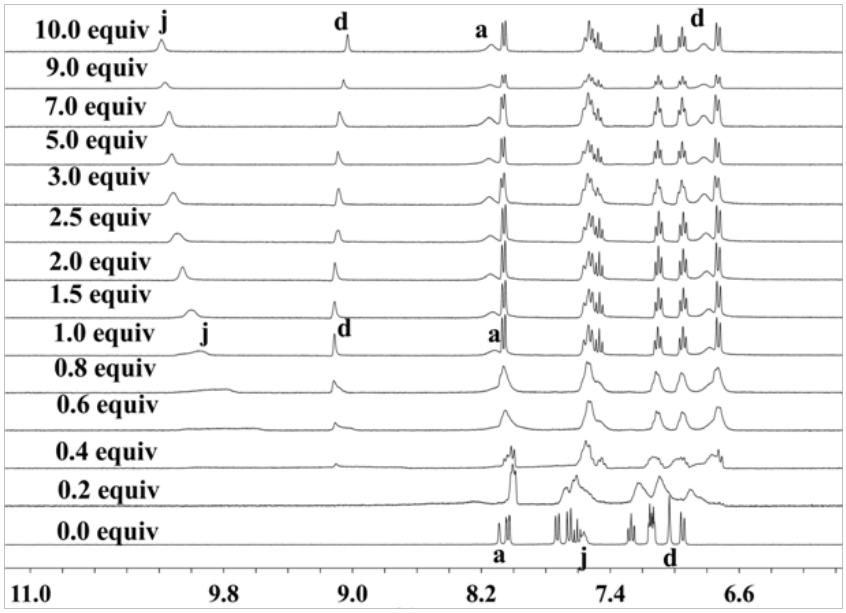

Fig S22 Portion of ^{1}HNMR traces of **L** in CD_3CN in the presence of $H_2PO_4^-$

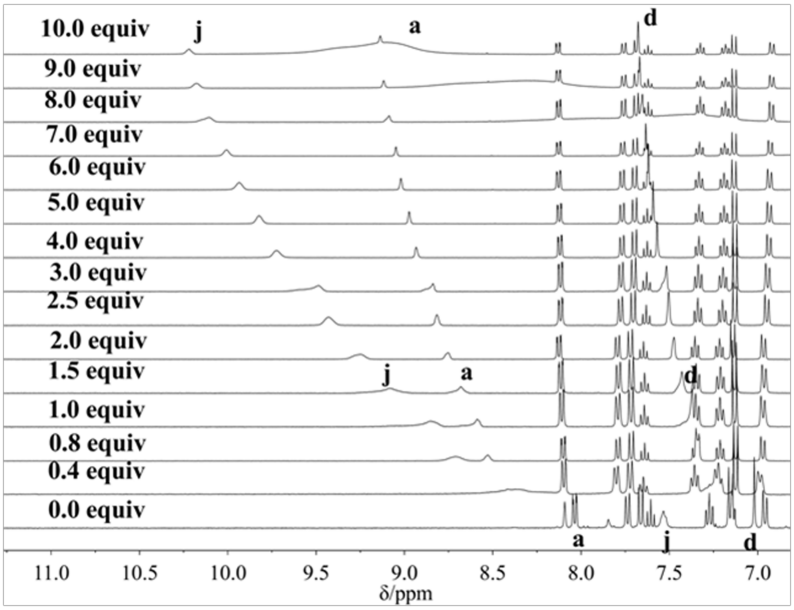

Fig S23 Portion of ^{1}HNMR traces of **L** in CD_3CN in the presence of AcO^-

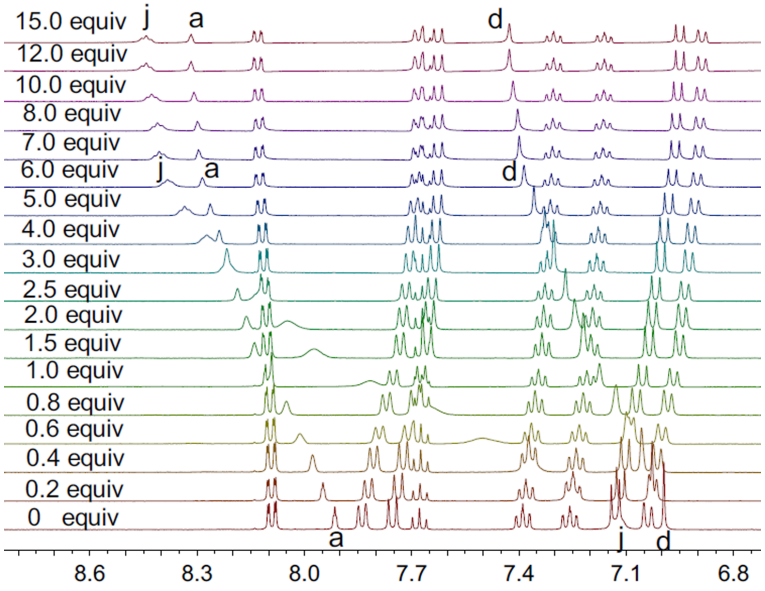

Fig S24 Portion of ^{1}HNMR traces of **L** in CD_3CN in the presence of HSO_4^-

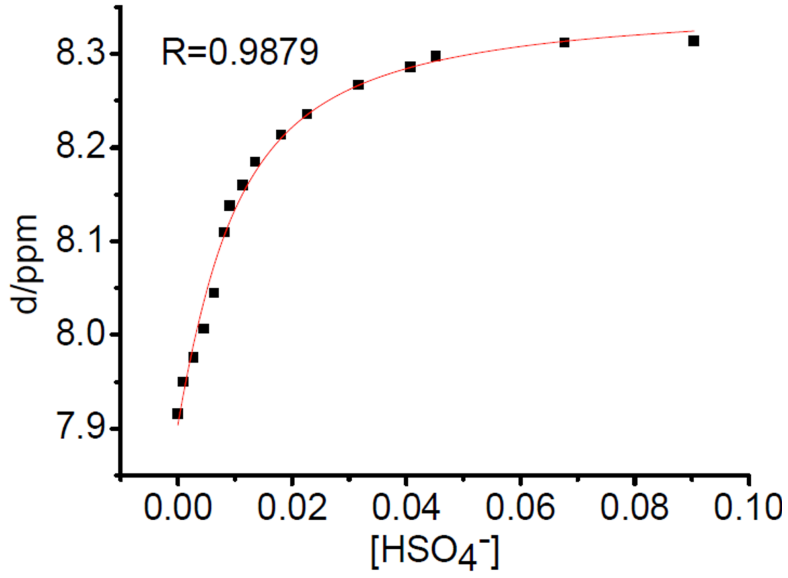

Figure S25 curve fitting of Proton Ha chemical shift

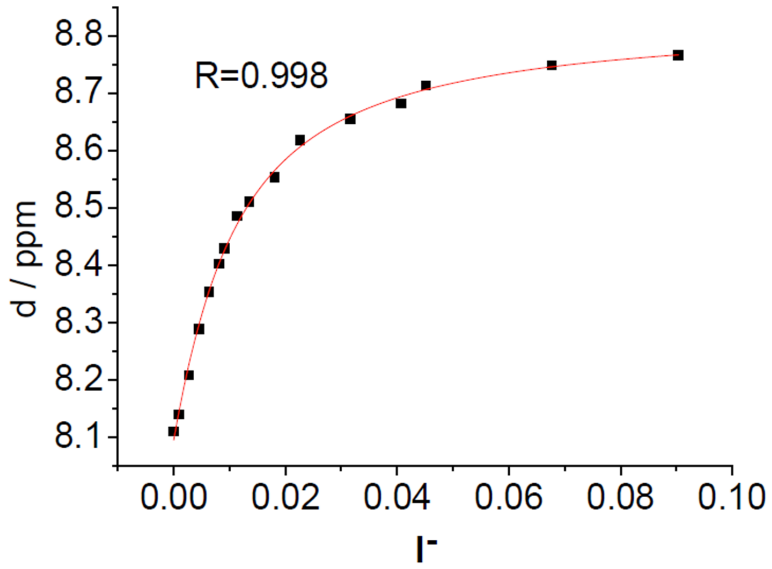

Figure S26 curve fitting of Proton Hj chemical shift

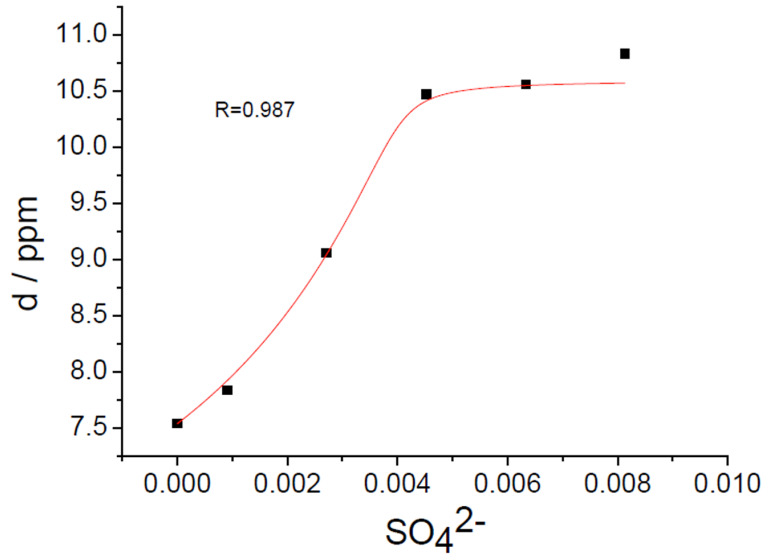

Figure S27 curve fitting of Proton Hj chemical shift

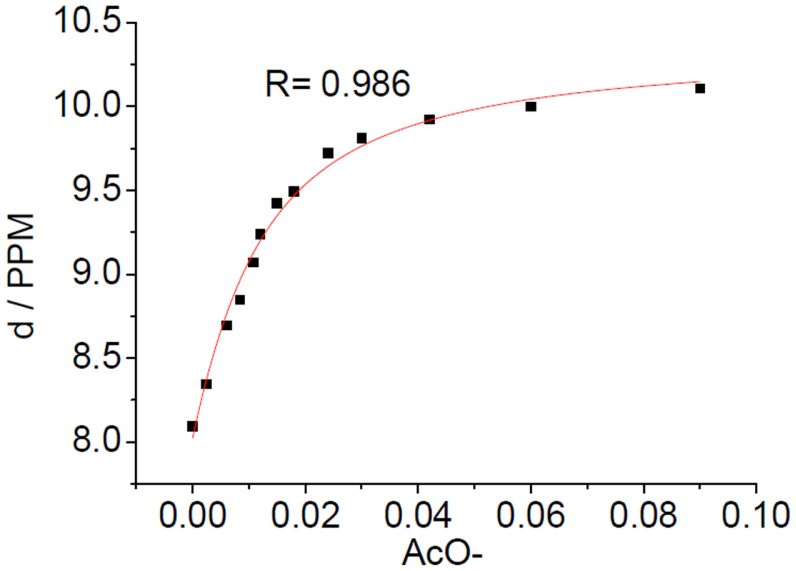

Figure S28 curve fitting of Proton H_j chemical shift

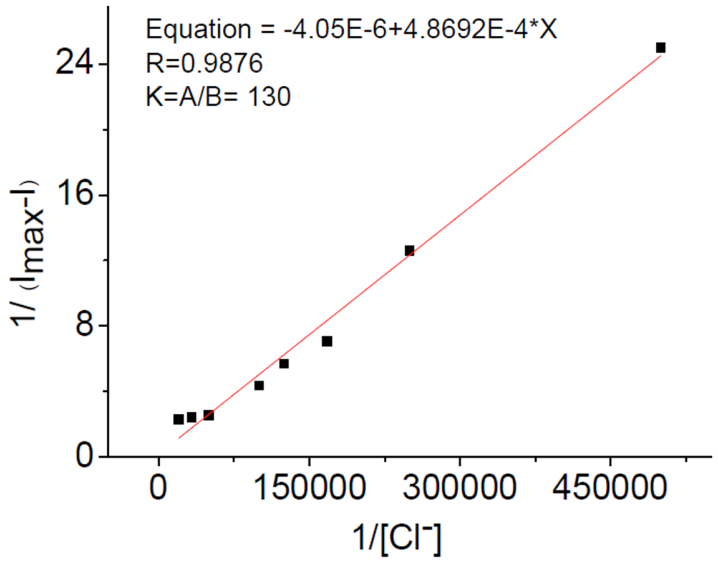

Figure S29 The binding constants (K) from Benesi–Hildebrand plots

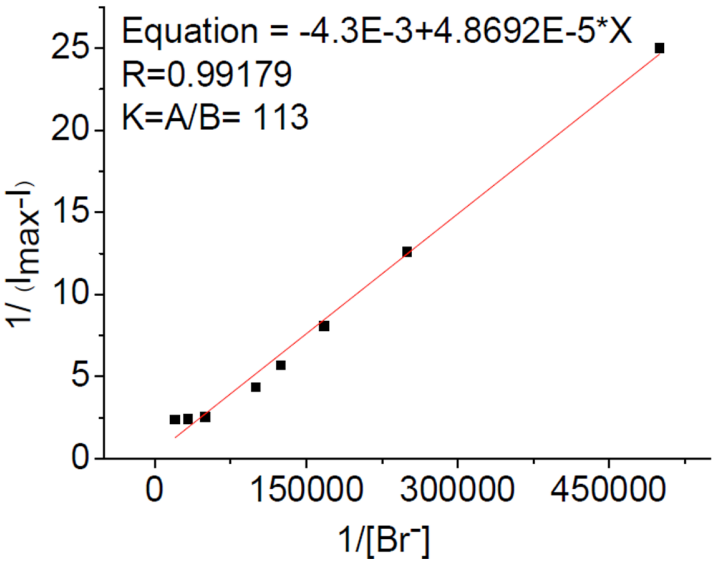

Figure S30 The binding constants (K) from Benesi–Hildebrand plots

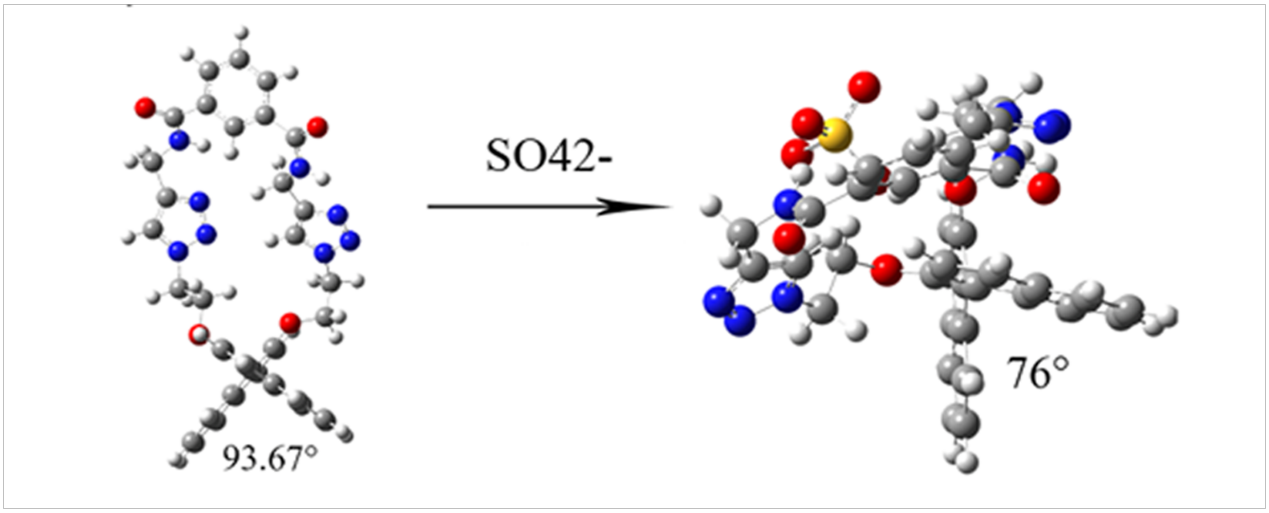

Figure S31 Computation for **L**-SO_4^{2-} complex conducted at the B3LYP/6-31G* theory.