

Electronic Supplementary Information

Encapsulation of divalent tetrahedral oxyanions of sulfur within rigidified dimeric capsular assembly of tripodal receptor: First crystallographic evidence of thiosulfate encapsulation

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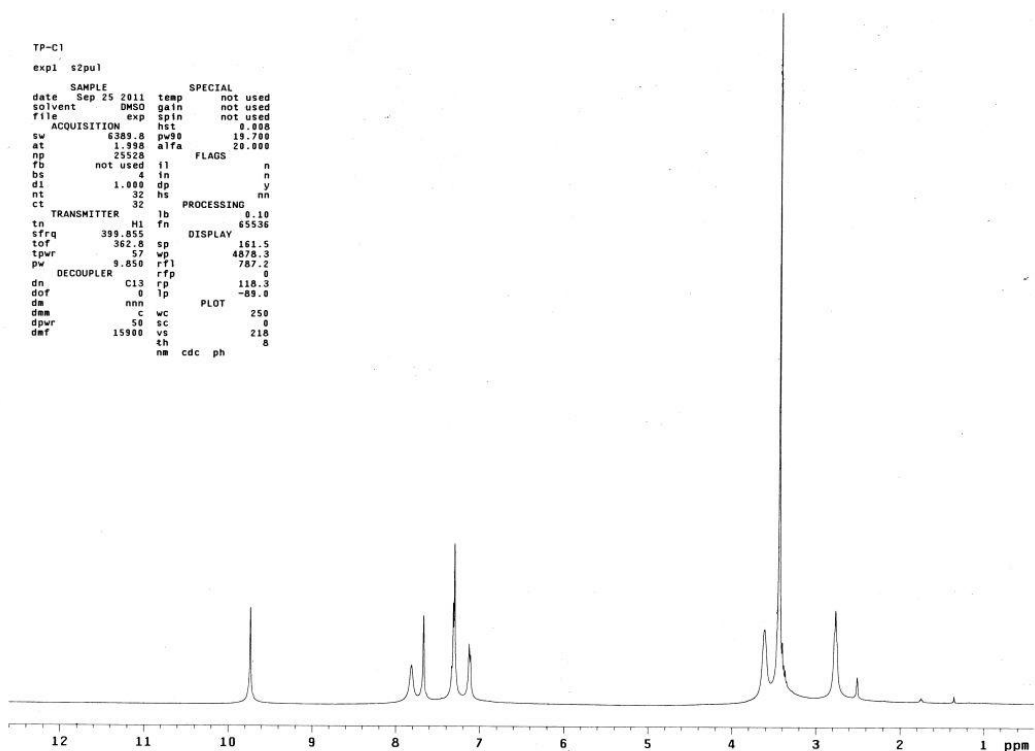


Fig. S1 ^1H NMR spectrum of receptor **L** in $\text{DMSO}-d_6$ at 298K.

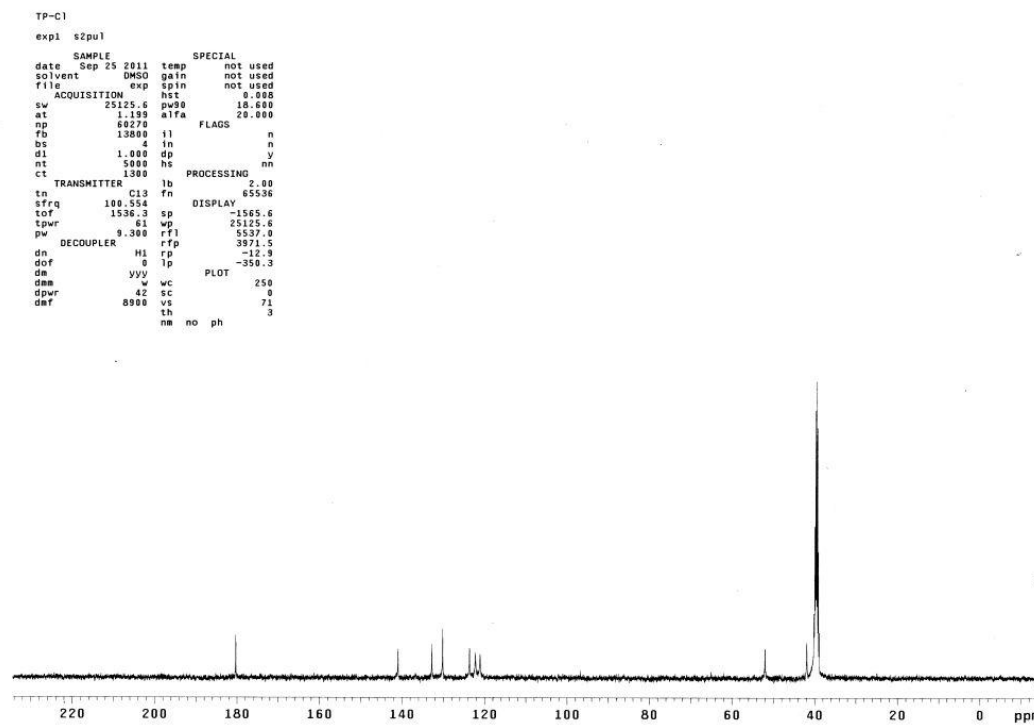


Fig. S2 ^{13}C NMR spectrum of receptor **L** in $\text{DMSO-}d_6$ at 298K.

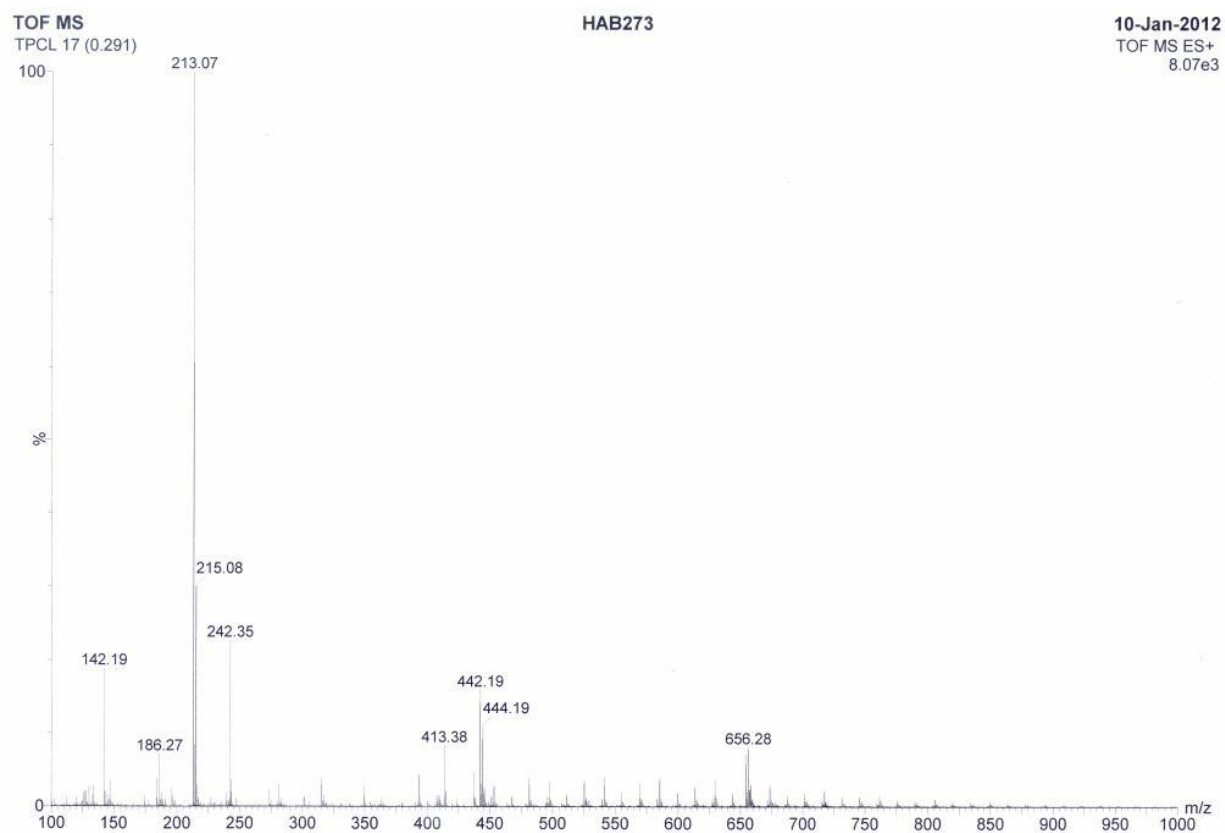


Fig. S3 ESI Mass spectrum of **L**.

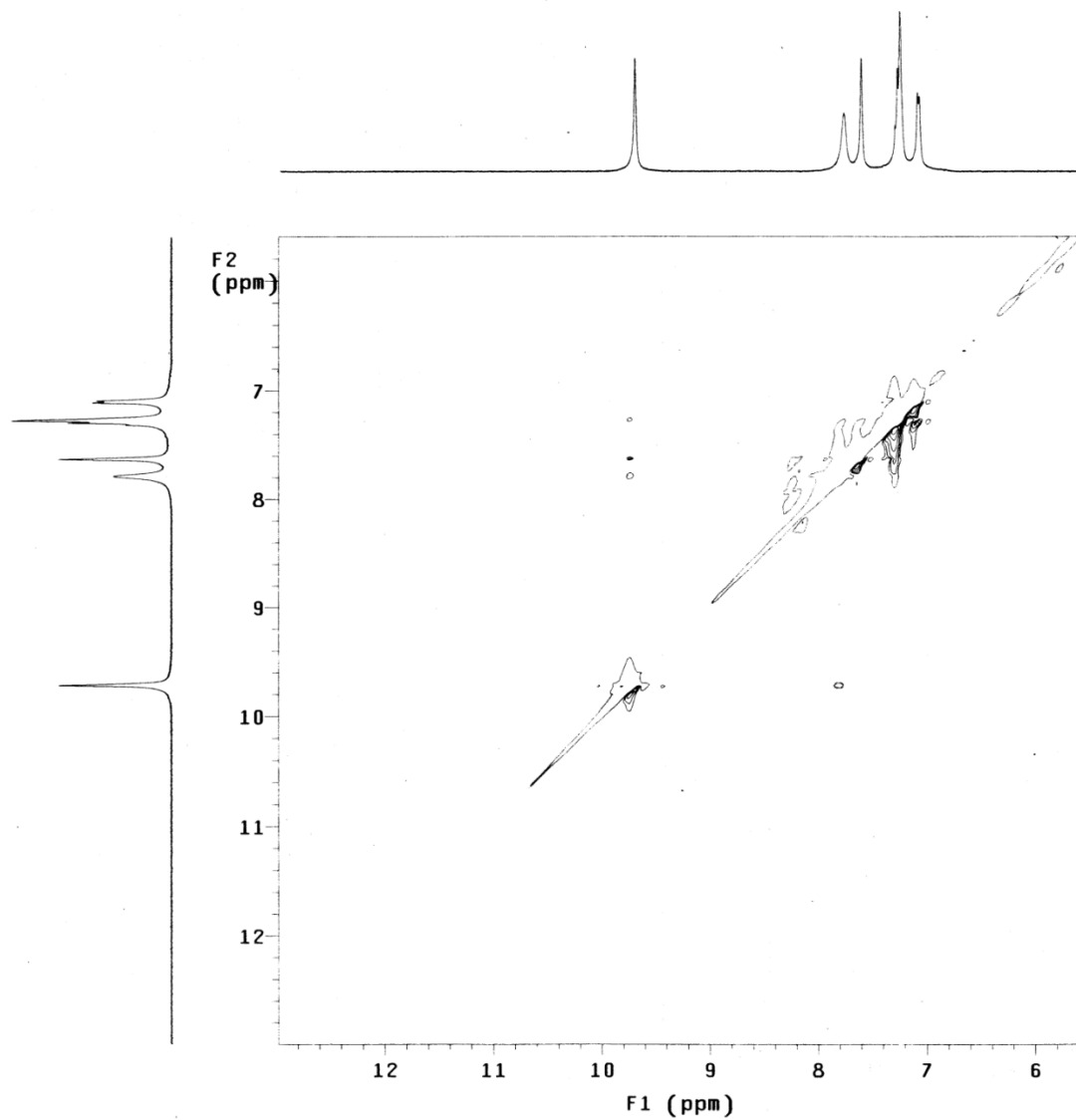


Fig. S4 NOESY spectrum of **L**.

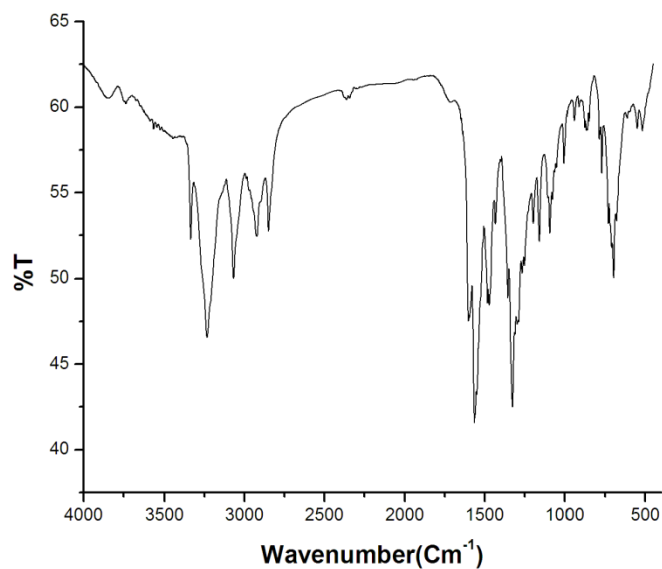


Fig. S5 IR spectrum of receptor **L**.

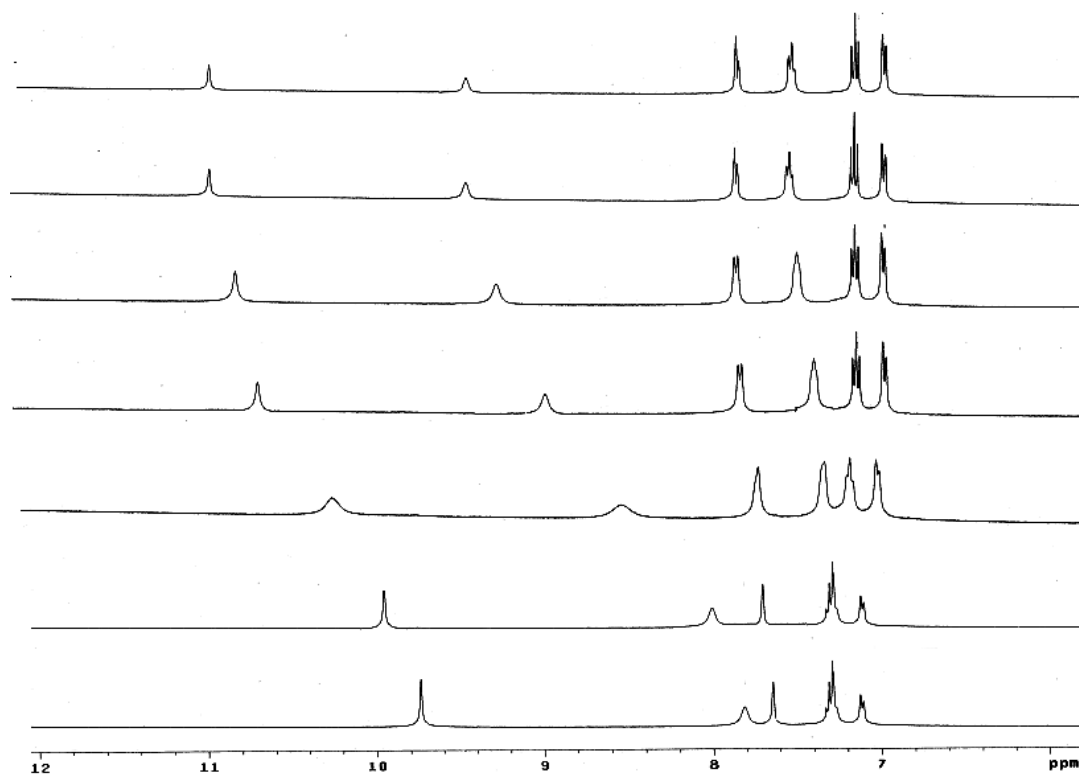


Fig. S6 Stack plot of the ¹H NMR spectra of receptor **L** in the presence of increasing amounts of [n-Bu₄N⁺]₂SO₄²⁻ recorded in DMSO-*d*₆ at 298 K.

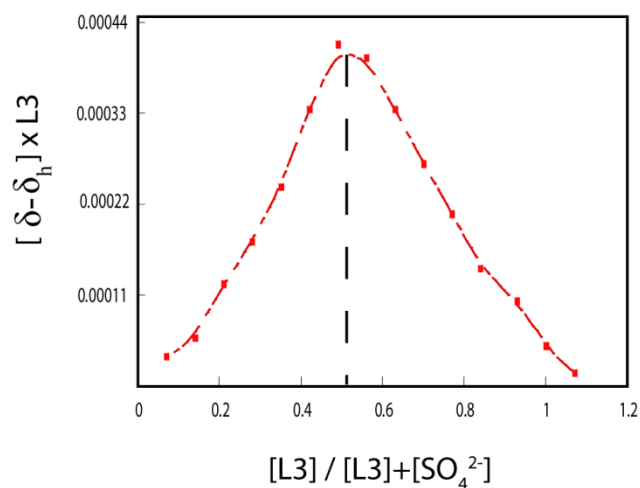


Fig. S7 Job's plot for **L** with $[n\text{-Bu}_4\text{N}^+]_2\text{SO}_4^{2-}$ in $\text{DMSO-}d_6$ at 298K.

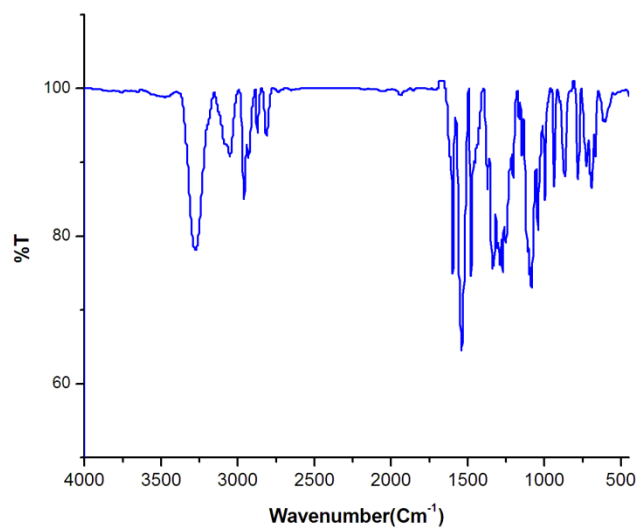


Fig. S8 IR Spectrum of the complex **1**.

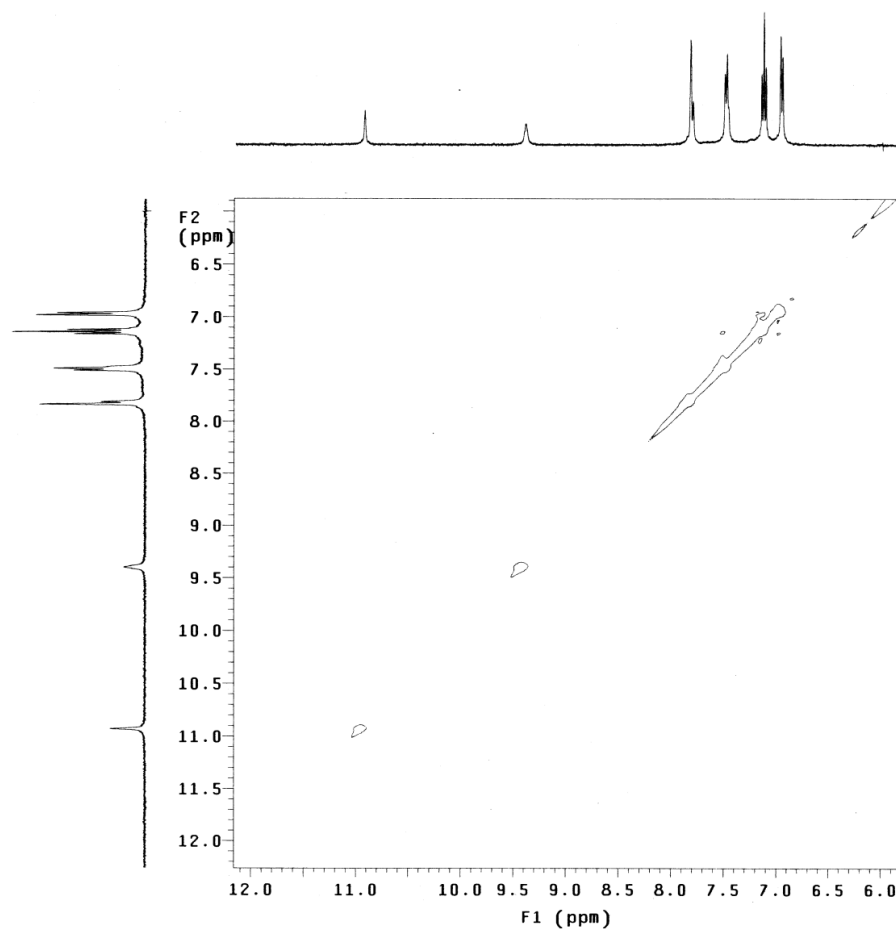


Fig. S9 NOESY spectrum of **L** in presence of one equivalent SO_4^{2-} anion.

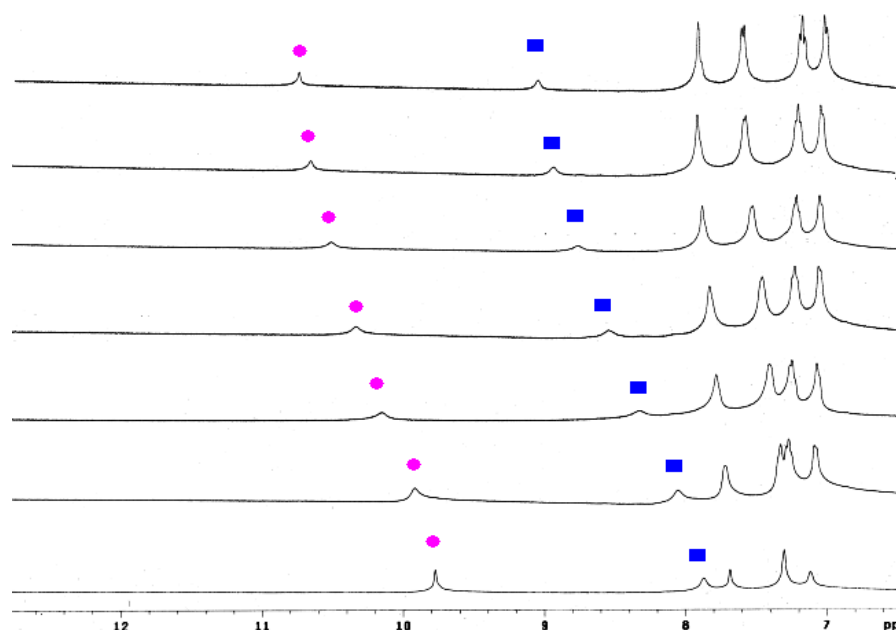


Fig. S10 Stack plot of the ^1H NMR spectra of receptor **L** in the presence of increasing amounts of $\text{Na}_2\text{S}_2\text{O}_3$ recorded in $\text{DMSO}-d_6$ at 298 K.

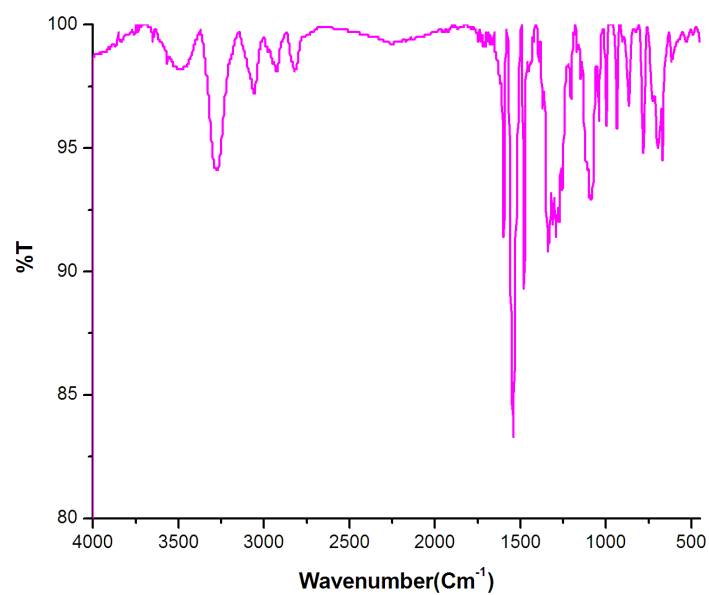


Fig. S11 IR Spectrum of the complex **2**.

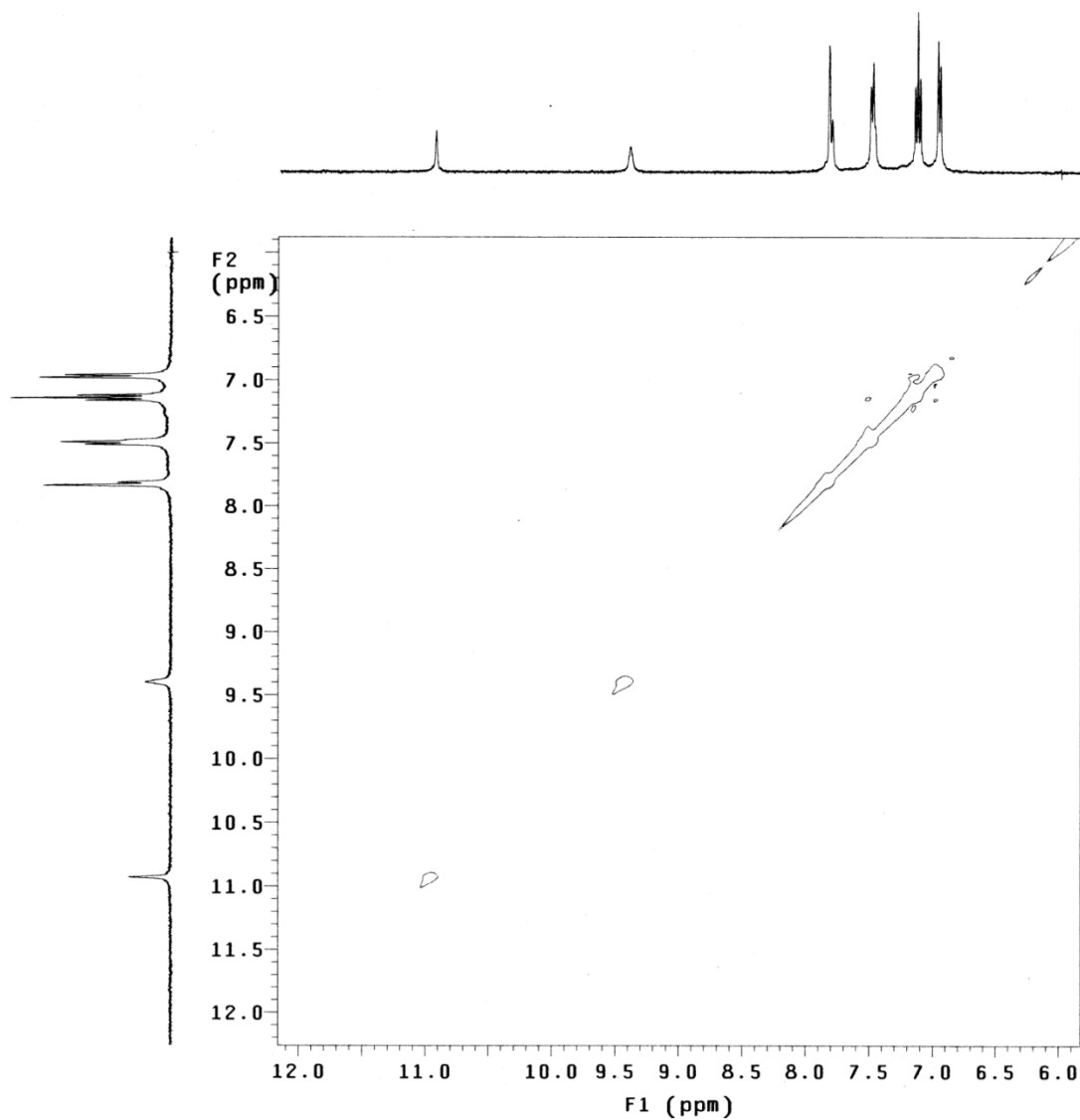


Fig. S12 NOESY spectrum of **L** in presence of one equivalent $\text{S}_2\text{O}_3^{2-}$ anion recorded in $\text{DMSO-}d_6$ at 298 K.

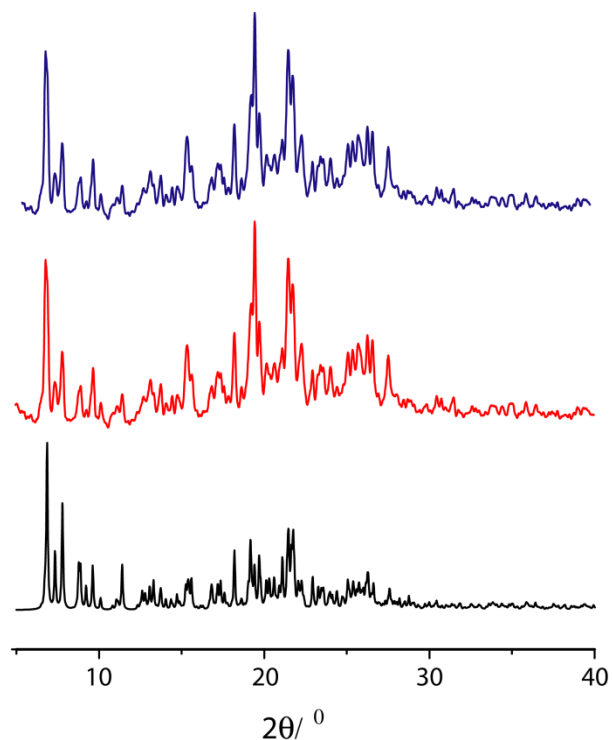


Fig. S13 Powder X-ray diffraction: simulated pattern from the single-crystal X-ray of complex **1** (black), experimental pattern from the crystalline solid obtained in presence of sulfate anion (red), experimental pattern from the crystalline solid obtained in presence of hydrogensulfate anion (blue).

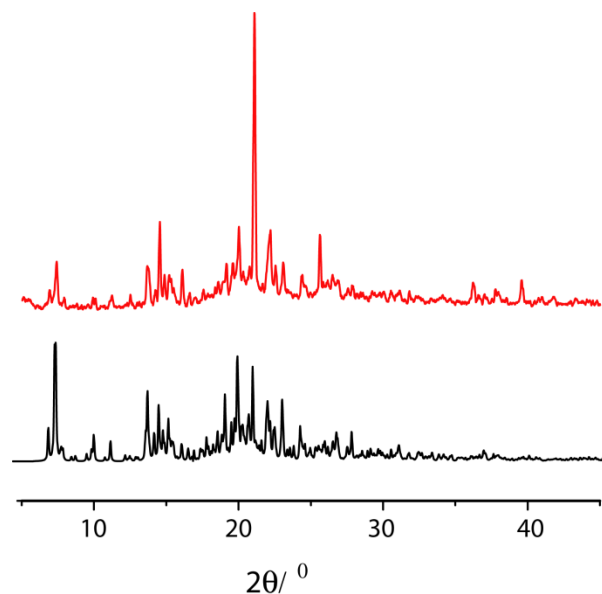


Fig. S14 Powder X-ray diffraction: simulated pattern from the single-crystal X-ray of complex **2** (black), experimental pattern from the crystalline solid of complex **2** (red),

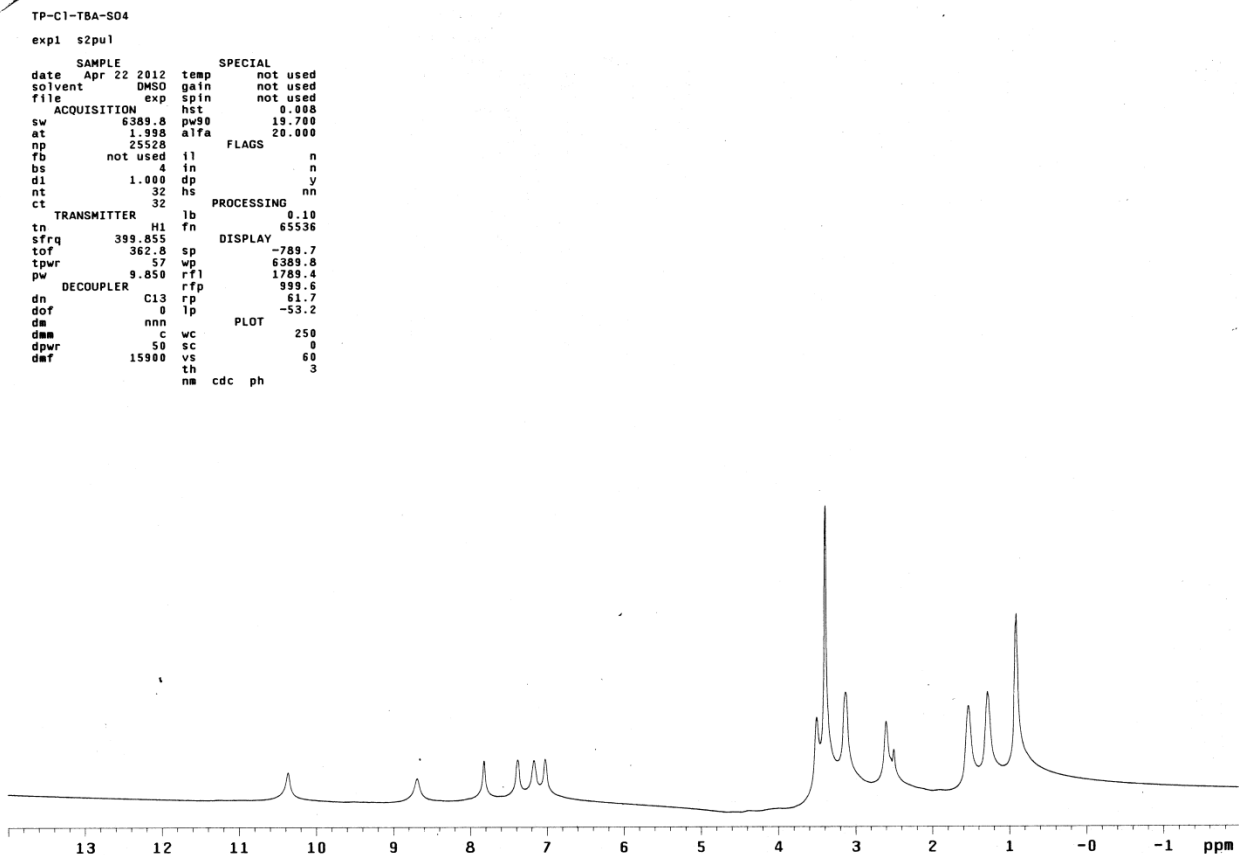


Fig. S15 ^1H NMR spectrum of complex **1** recorded in DMSO- d_6 at 298 K.

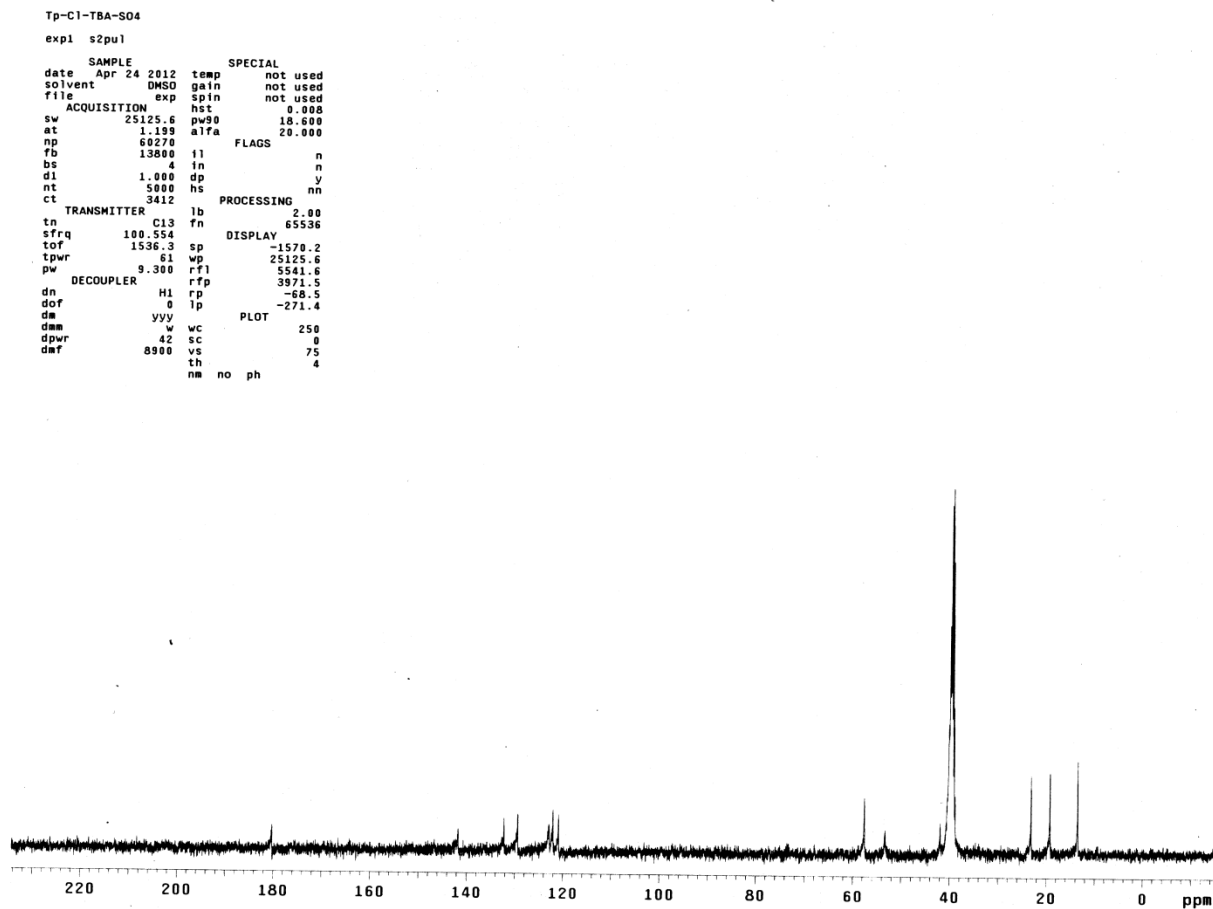


Fig. S16 ^{13}C NMR spectrum of complex **1** recorded in $\text{DMSO-}d_6$ at 298 K.

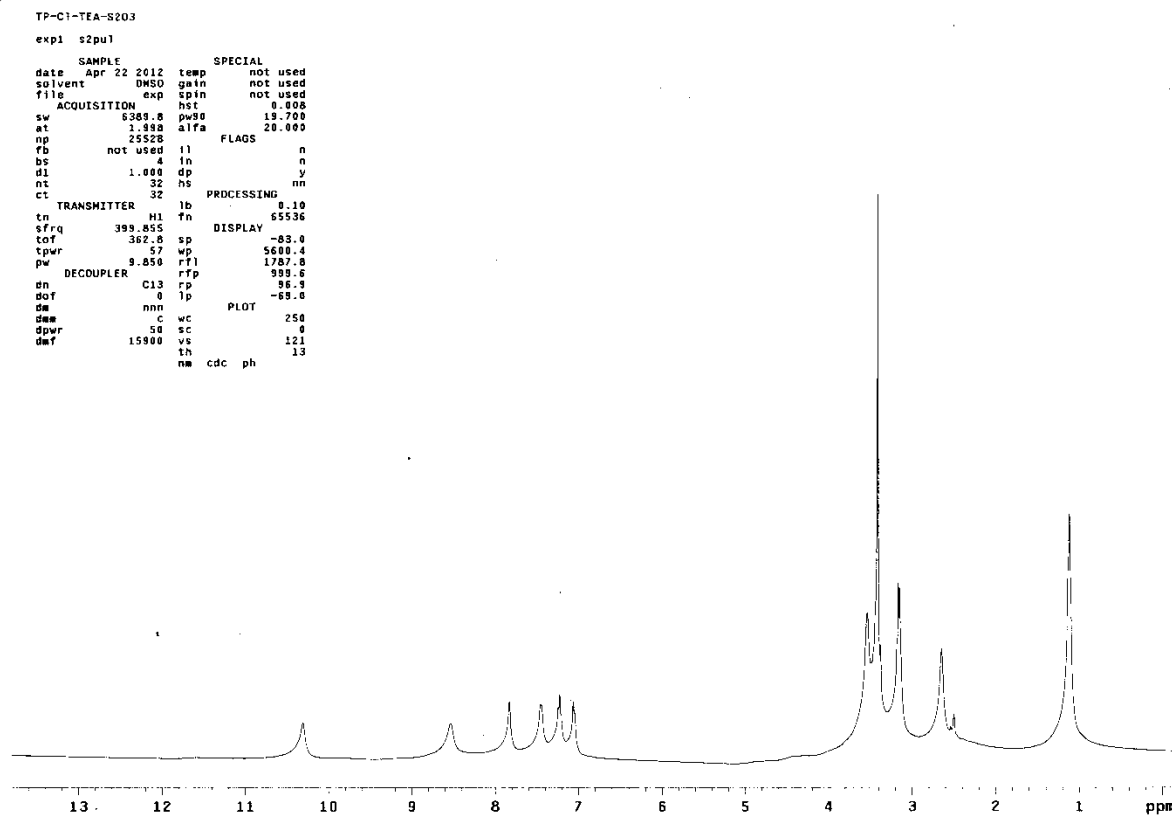


Fig. S17 ^1H NMR spectrum of complex **2** recorded in $\text{DMSO}-d_6$ at 298 K.

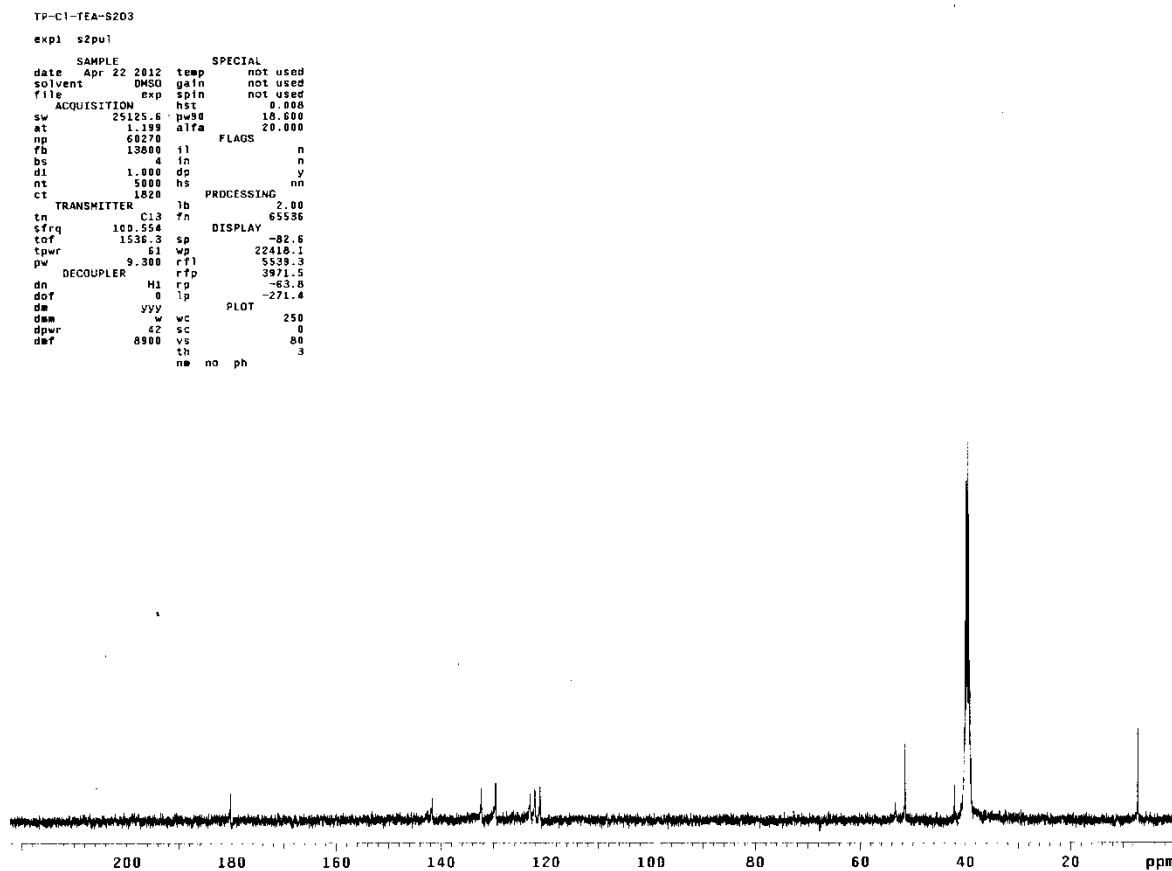


Fig. S18 ^{13}C NMR spectrum of complex 2 recorded in $\text{DMSO-}d_6$ at 298 K.

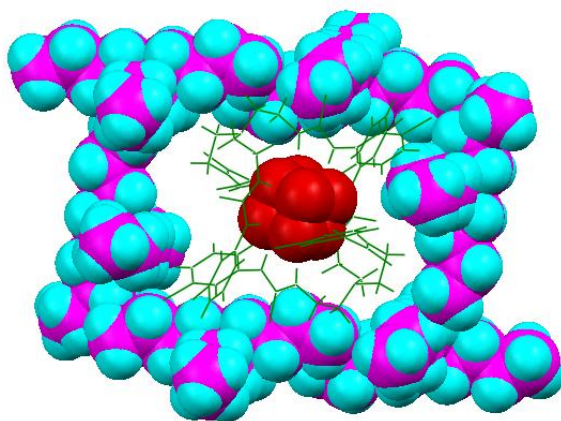


Fig. S19 Depicting sulphate encapsulated receptor segment is present in the hydrophobic pocket of TBA counter cations in complex **1**.