Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Optical and electrochemical properties of heteroditopic ion receptors derived from crown ether-based calix[4]arene with amido-anthraquinone pendants

Benjamat Chailap and Thawatchai Tuntulani*

Department of Chemistry, Faculty of Science, Chulalongkorn University,Phayathai Road, Bangkok, Thailand
thawatchai.t@chula.ac.th

Supplementary data

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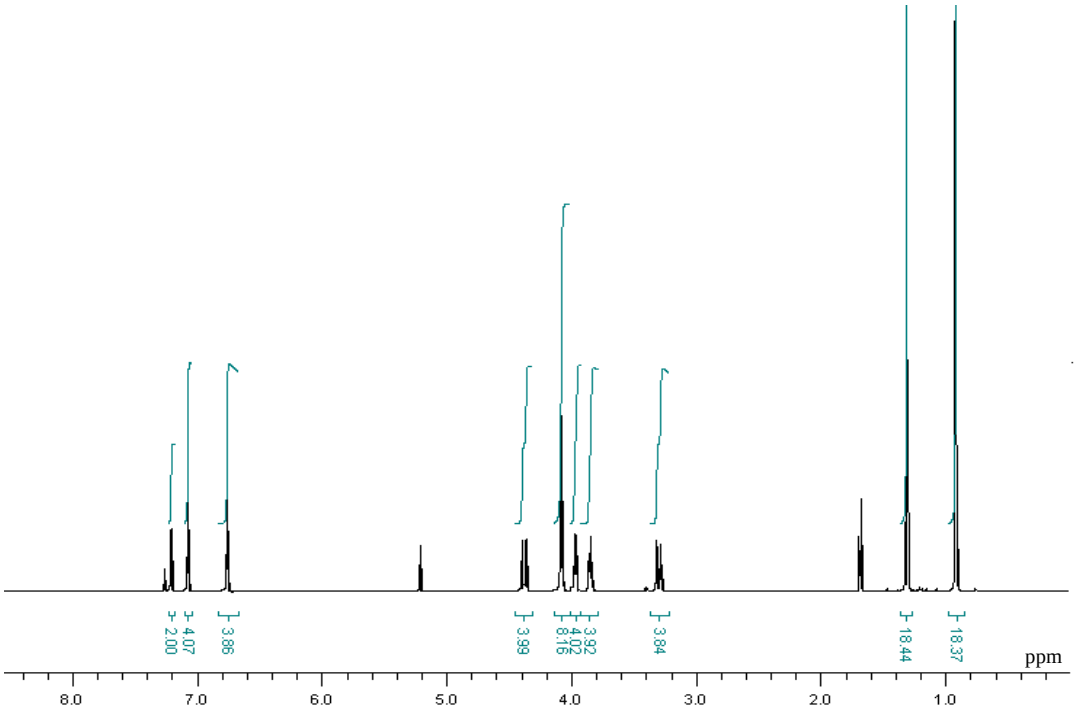


Fig. S1-a ^{1}H-NMR spectrum of **1-a** in $CDCl_3$ plotted from mestrec program

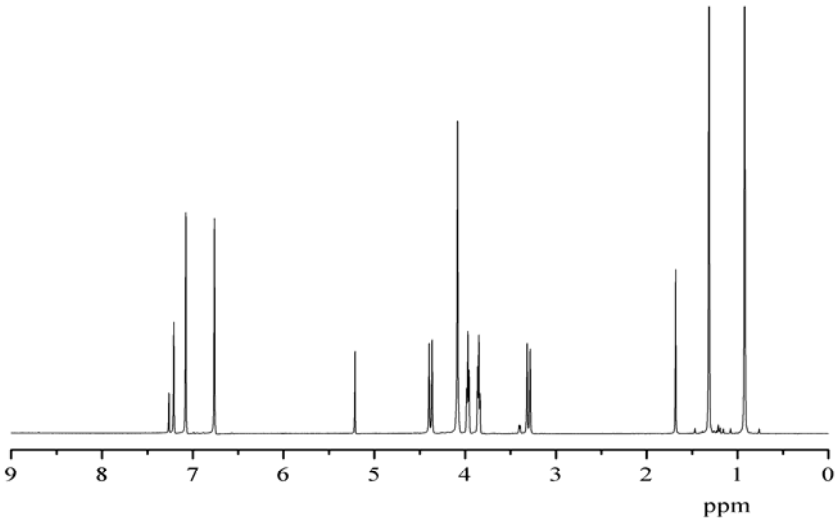


Fig. S1-b ^{1}H-NMR spectrum of **1-a** in $CDCl_3$ plotted from origin program

^{13}C-NMR spectrum of 1-a

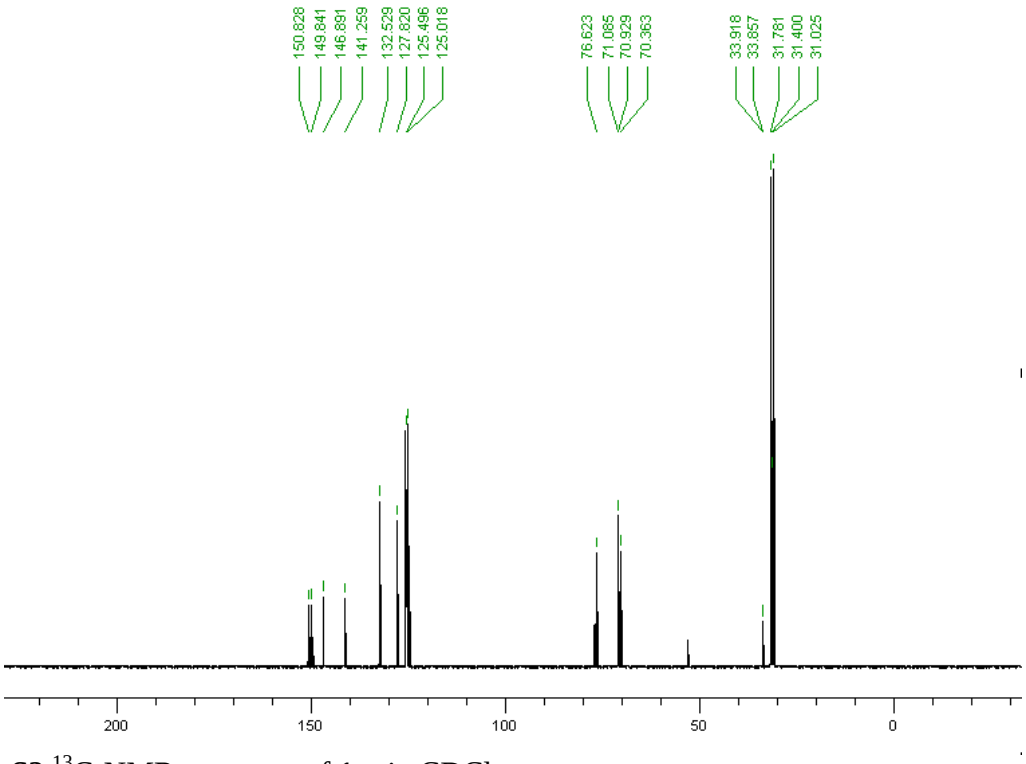


Fig. S2 ^{13}C-NMR spectrum of **1-a** in $CDCl_3$

^{1}H-NMR spectrum of **1**

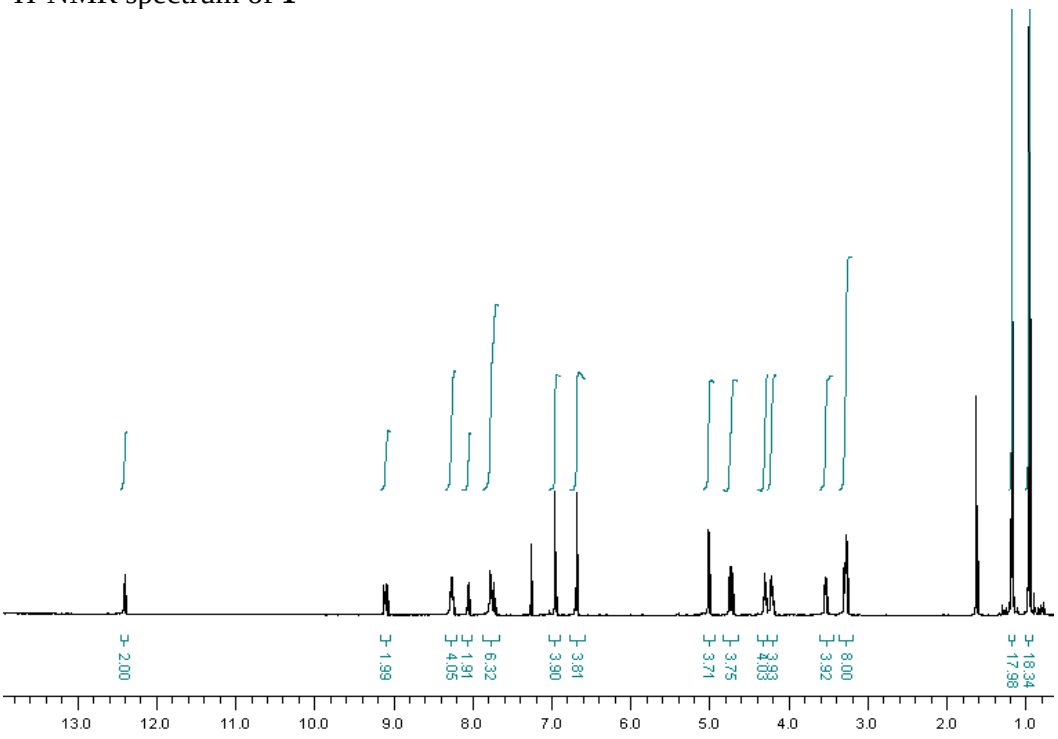


Fig. S3-a ^{1}H-NMR spectrum of **1** in $CDCl_3$ plotted from mestrec program

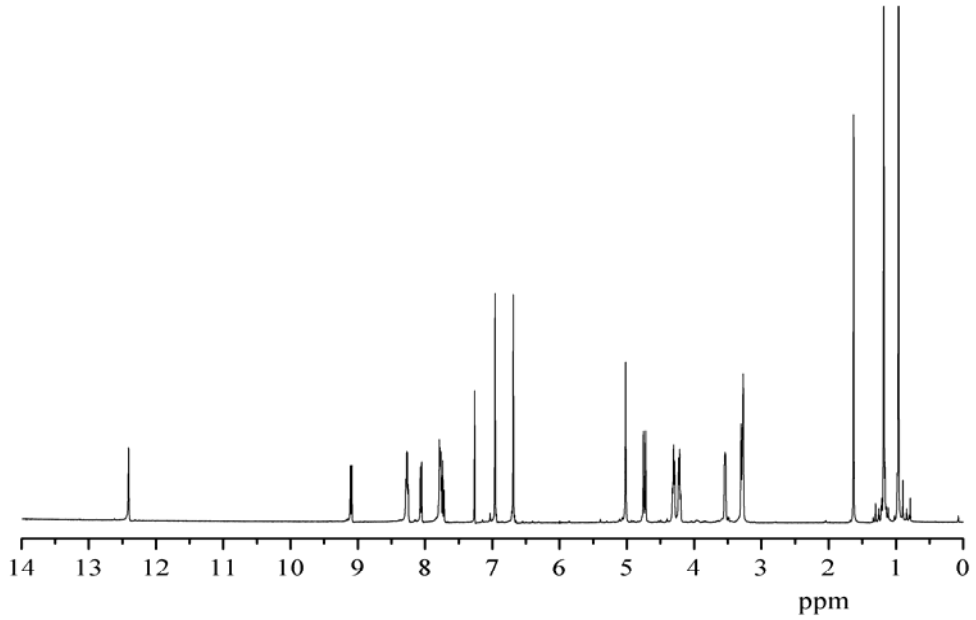


Fig. S3-b ^{1}H-NMR spectrum of **1** in $CDCl_3$ plotted from origin program

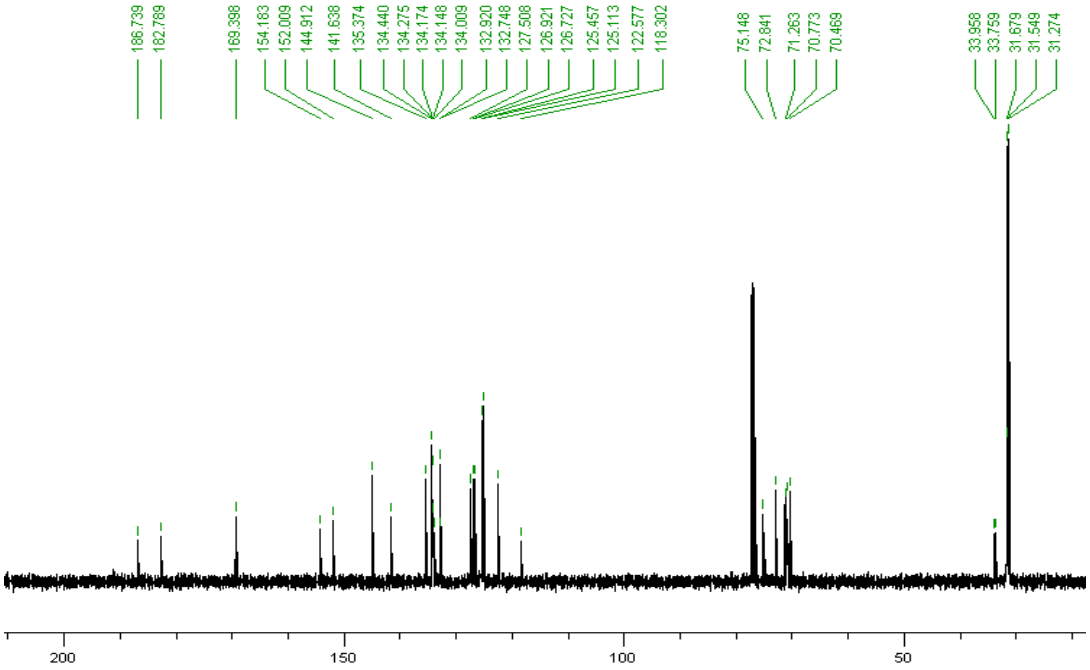


Fig. S4 ^{13}C-NMR spectrum of **1** in $CDCl_3$

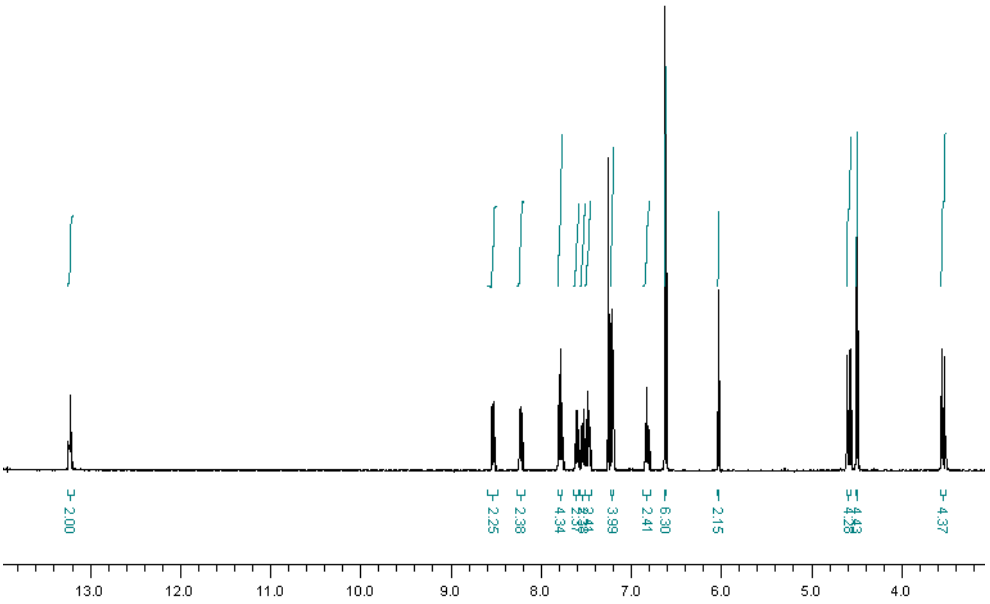


Fig. S5-a ^{1}H-NMR spectrum of **2-a** in $CDCl_3$ plotted from mestrec program

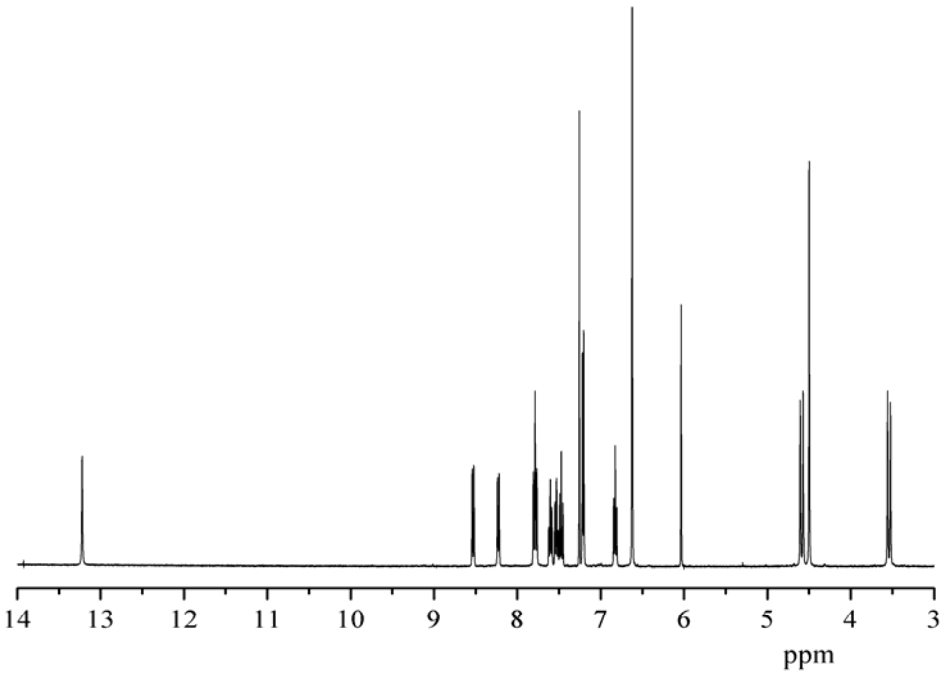


Fig. S5-b ^{1}H-NMR spectrum of **2-a** in $CDCl_3$ plotted from origin program

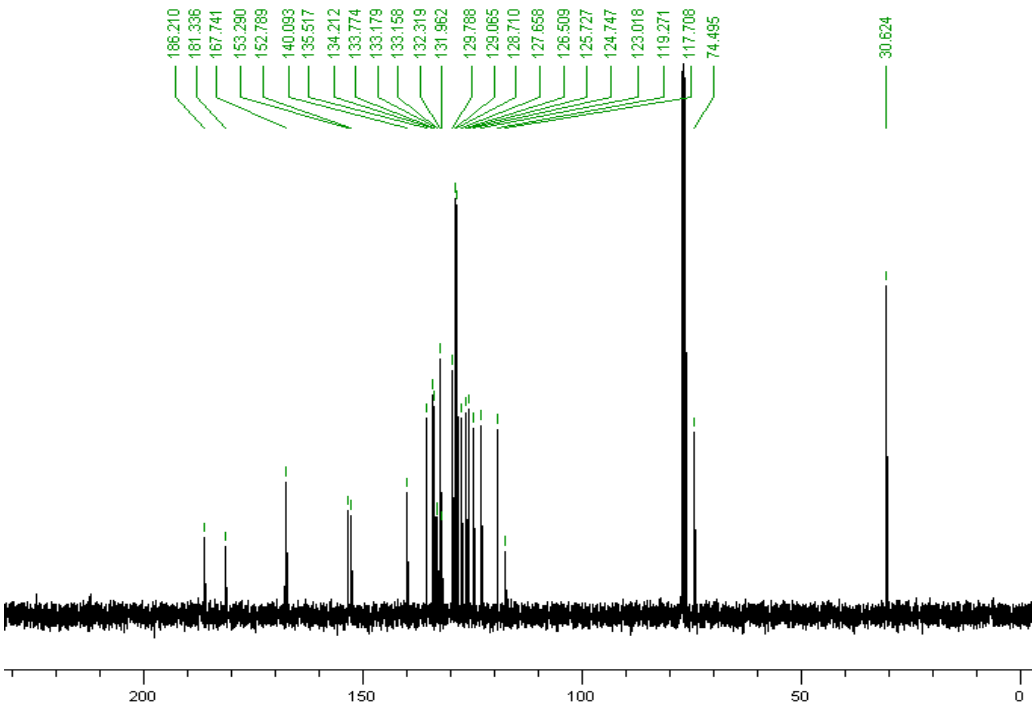


Fig. S6 ^{13}C-NMR spectrum of **2-a** in $CDCl_3$

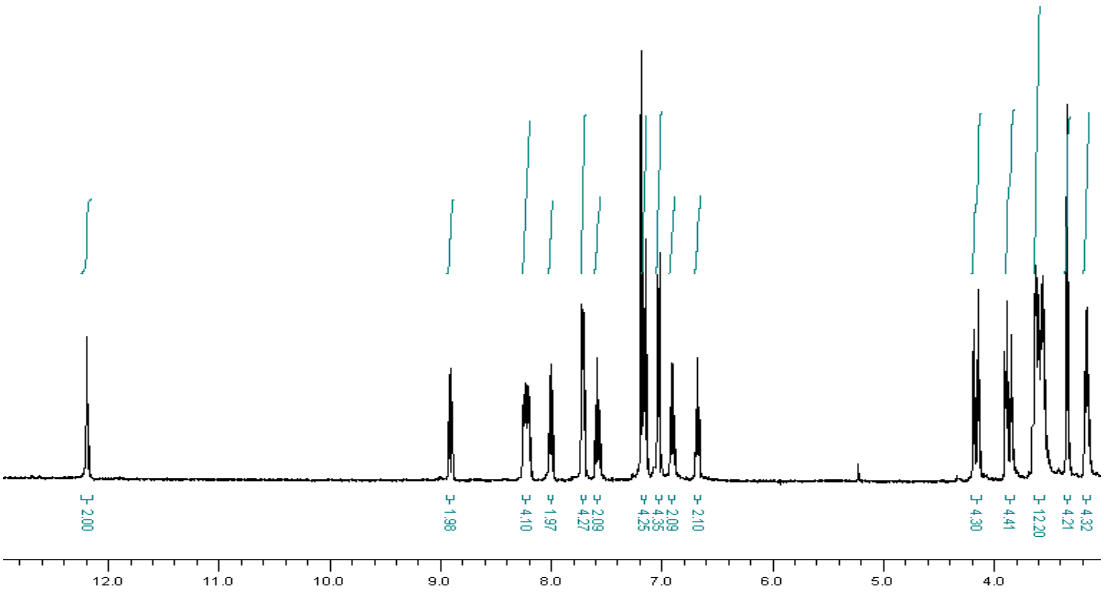


Fig. S7-a ^{1}H-NMR spectrum of **2** in $CDCl_3$ plotted from mestrec program

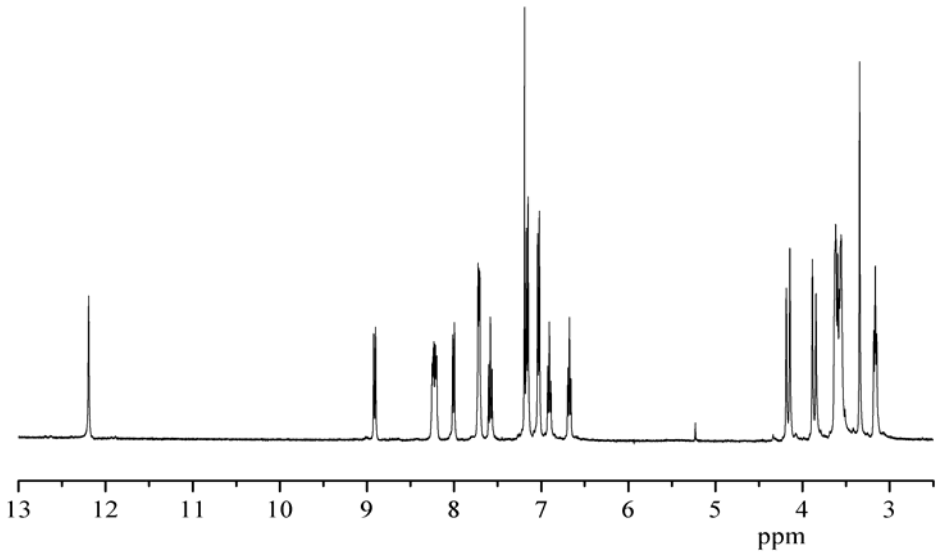


Fig. S7-b ^{1}H-NMR spectrum of **2** in $CDCl_3$ plotted from origin program

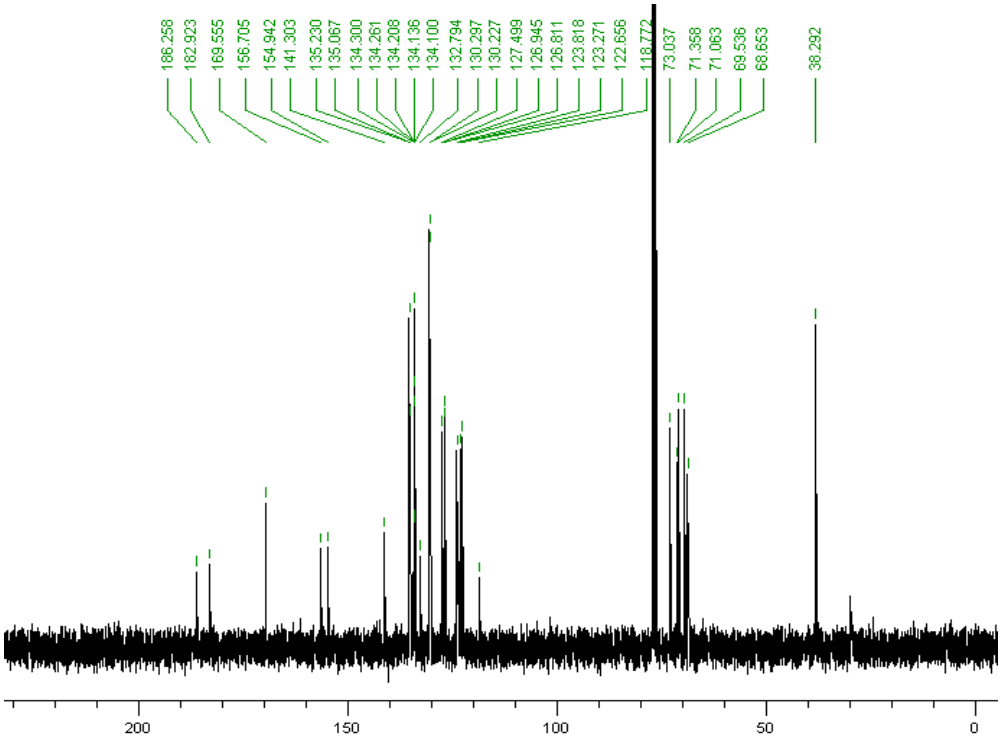


Fig. S8 ^{13}C-NMR spectrum of **1** in $CDCl_3$ plotted from mestrec program

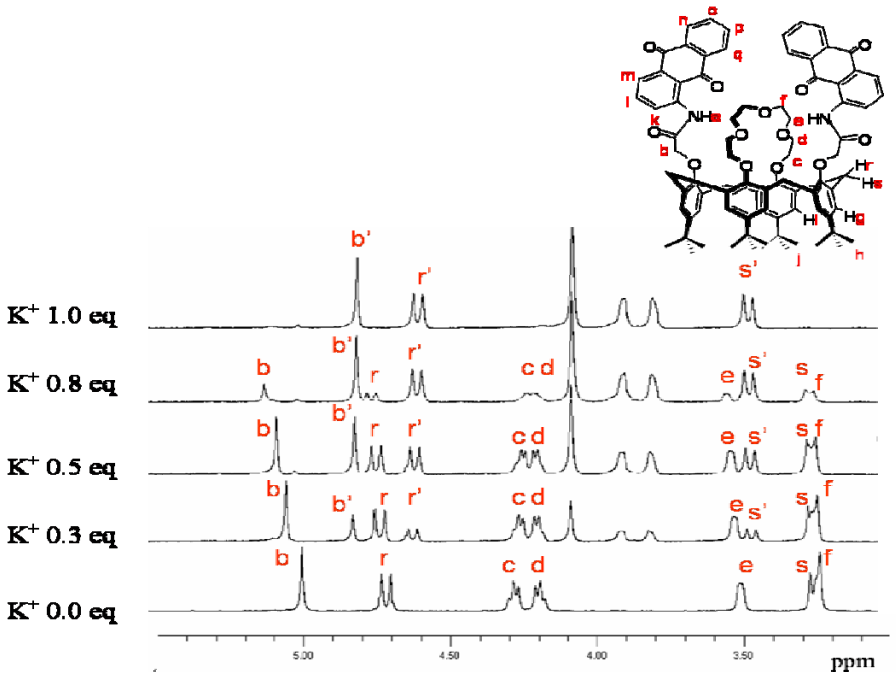


Fig. S9 ^{1}H NMR titration spectrum between receptor **1** and potassium ions in 5% v/v CD_3CN in $CDCl_3$ showed slow complexation/decomplexation process. X and X' represented protons of decomplexes and complexes with K^+, respectively.

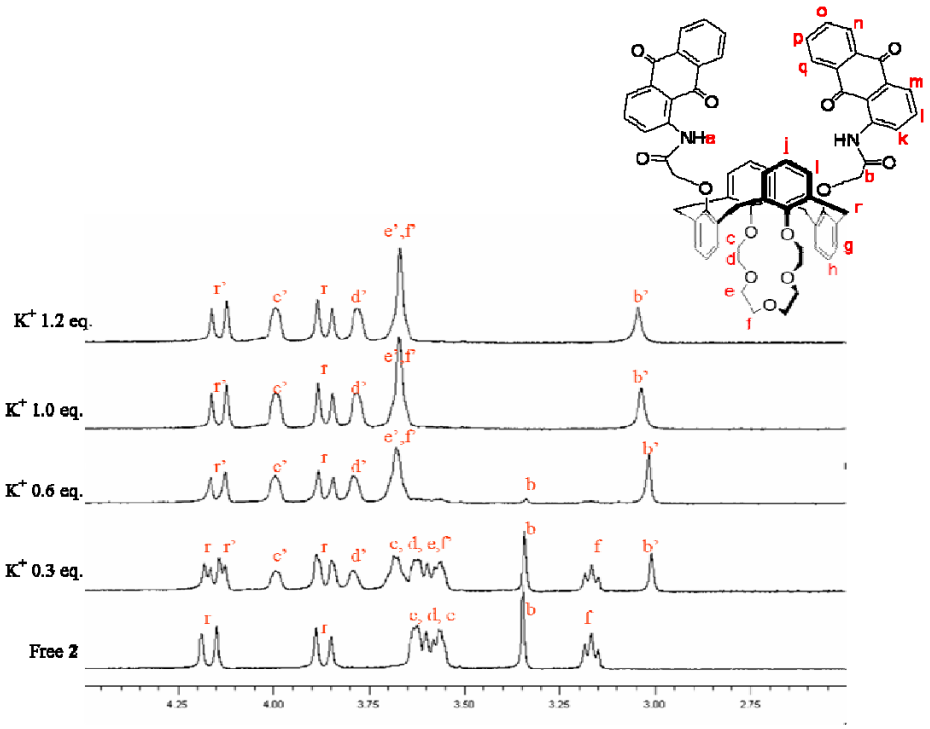
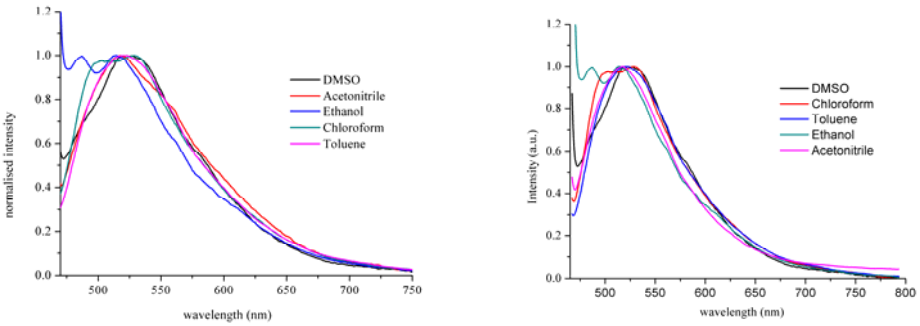


Fig. S10 ^{1}H NMR titration spectrum between receptor **2** and potassium ions in 5% v/v CD_3CN in $CDCl_3$ showed slow complexation/decomplexation process. X and X' represented protons of decomplexes and complexes with K^+, respectively.

Remark: The AB signals of methylene protons r' and s' of compound **1** upon complexing K^+ shifted more upfield and downfield, respectively as compared to the AB signals of 1,3-alternate compound **2**. This indicates a large cone angle change in the cone conformation of compound **1** upon binding K^+.



(a) (b)

Fig. S11 Normalized fluorescence emission spectra spectra of (a) **1** (50 μM) and (b) **2** (50 μM) in various solvents.

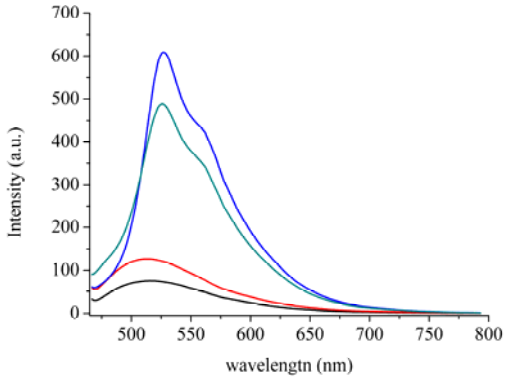
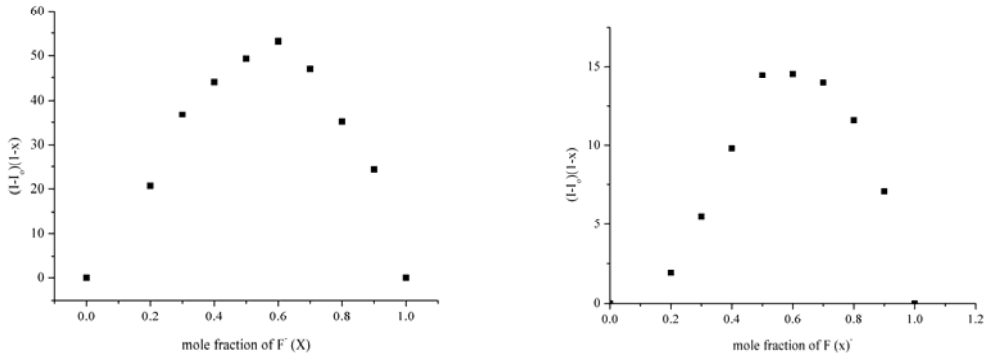


Fig. S12 Fluorescence emission spectra of **2** (50 μM) and TBAF·3H_2O (100 equiv.) in the absence (blue spectrum) and presence (green spectrum) of KPF_6 (1.2 equiv.) in CH_3CN.



(a) (b)

Fig. S13 Job's plot of (a) **1** and (b) **1** + K^+ (1.2 eq.) with TBAF·$3H_2O$ in $CHCl_3$

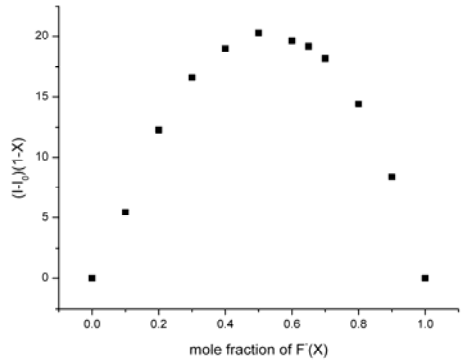


Fig. S14 Job's plot of **2** with TBAF·$3H_2O$ in $CHCl_3$

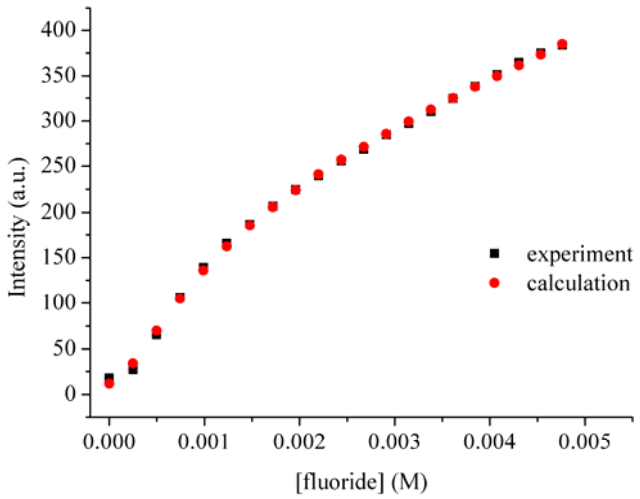


Fig. S15 Fitting graph of emission titration at 542 nm between **1** and TBAF·3H_2O calculated from SPECFIT32 software

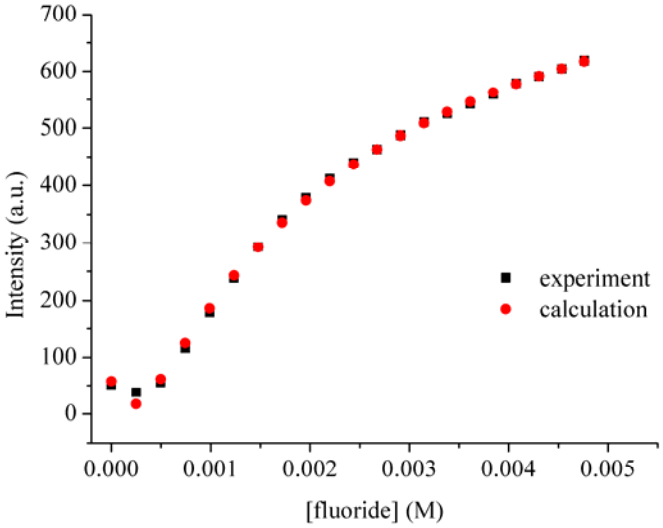


Fig.S16 Fitting graph of emission titration at 542 nm between **1**+$\mathbf{K}^+$ and TBAF·3H_2O calculated from SPECFIT32 software

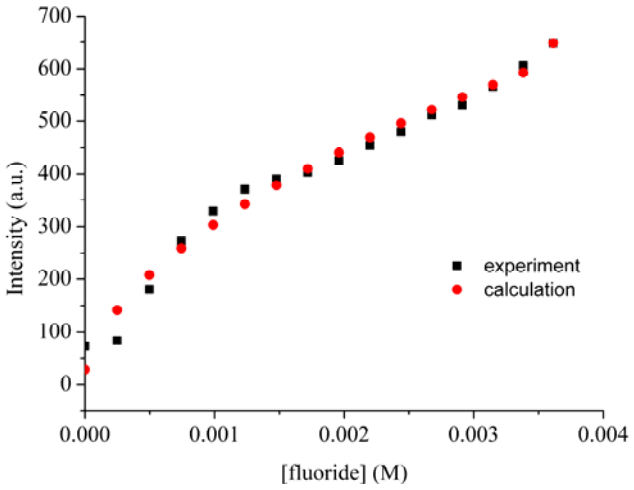


Fig.S17 Fitting graph of emission titration at 542 nm between **2** and TBAF·$3H_2O$ calculated from SPECFIT32 software

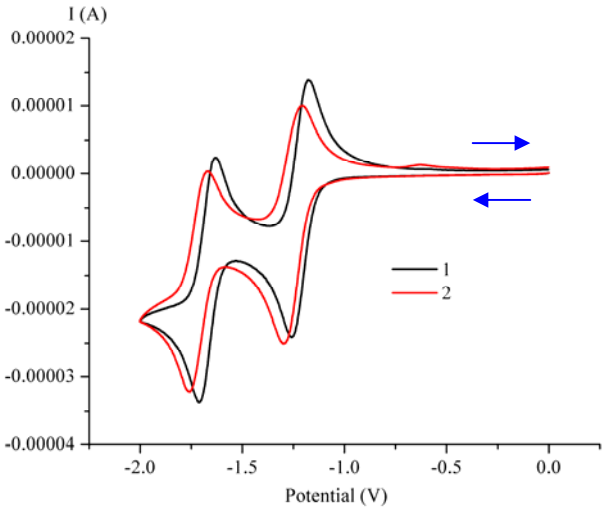


Fig. S18 Cyclic voltammograms of **1** (1 mM) and **2** (1 mM) in 40% CH_3CN:CH_2Cl_2 with 0.1 M $TBAPF_6$ at scan rate 50 mV. Blue arrows represent scaned direction.