Electronic Supplementary Information

Dual-Controllable Stepwise Supramolecular Interconversions

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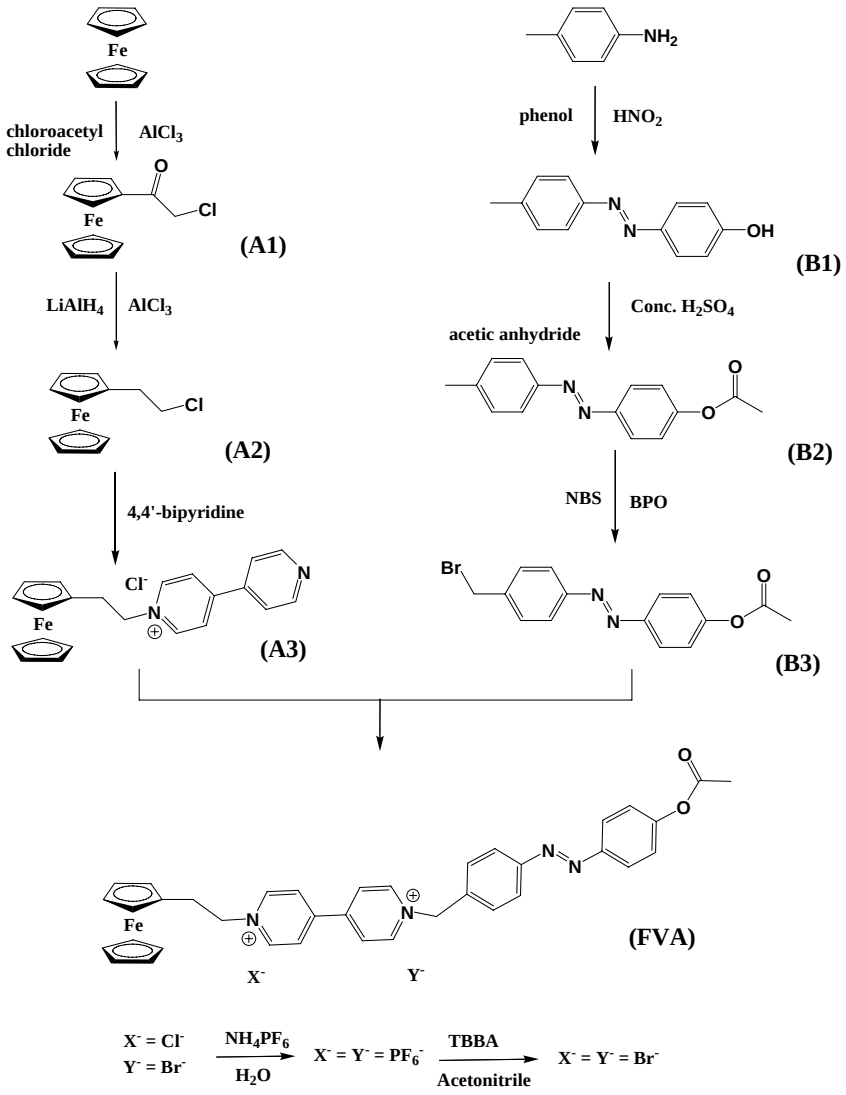
Instruments. ^{1}H NMR spectra were measured on a Brüker AV-400 spectrometer, and the ^{13}C NMR and 2D-NOESY NMR spectra were recorded on a Brüker AV-500 spectrometer. The electronic spray ionization (ESI) mass spectra were tested on a HP5989 mass spectrometer. Elemental analysis was performed on a vario EL III instrument. Absorption spectra were done on a Varian Cary 500 UV/Vis spectrophotometer (1-cm quartz cell used), while the ICD spectra were recorded on a Jasco J-815 CD spectrophotometer in a 1 mm quartz cell. The photoirradiation was carried on a CHF-XM 500-W high-pressure mercury lamp with a filter for 365 nm in a sealed Ar-saturated 1 cm quartz cell. The distance between the lamp and the sample cell was 20 cm. Melting points were determined by using an X-6 micro-melting point apparatus. Cyclic voltammetry (CV) experiments were performed with a CHI 660C electrochemical workstation using a normal three-electrode cell with a glassy carbon working electrode, a Pt wire auxiliary electrode, and saturated calomel electrode as reference. The experiments were carried out in solutions containing 0.1 M of NaCl as supporting electrolyte, and the curves were recorded at a scan rate of 50 mV/s.

Materials. *β*-cyclodextrin (*β*-CD), ferrocene, chloroacetyl chloride, *p*-toluidine, iodomethane, 4, 4'-bipyridine, N-bromosuccinimide (NBS), benzoyl peroxide (BPO) and the inorganic reagents were commercially available and used as received. Dichloromethane were dried over calcium hydride, and then distilled under reduced pressure. Acetonitrile were dried by 4A molecular sieve and distilled before used.



Scheme S1. Synthetic route to **FVA**

Synthesis of Chloroacetyl ferrocene (A1)

A solution of ferrocene (9.3 g, 0.05 mol) in CH_2Cl_2 (40 mL) was added to a stirred solution of chloroacetyl chloride (6.8 g, 0.06 mol) and $AlCl_3$ (8.0 g, 0.06 mol) in CH_2Cl_2 (80 mL) at 0 °C. After 3 hr, the reaction was quenched with water (200 mL). The solution was extracted three times with dichloromethane (180 mL) and the underlayer was washed with water (180 mL). After drying with anhydrous $MgSO_4$ and concentrated in vacuo, the residue was applied to silica gel chromatography (petroleum ether:

dichloromethane = 1:10) to afford orange compound **A1** (4.6 g, 35%). M.p. 91 ~ 93 ºC. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS): δ = 4.25 (s, 5H), 4.42(s, 2H), 4.60 (t, J = 2.4 Hz, 2H), 4.84 (t, J = 2.4 Hz, 2H).

Synthesis of Chloroethyl ferrocene (A2)

A solution of $LiAlH_4$ (0.6 g, 15.7 mmol) and $AlCl_3$ (2.03 g, 15.3 mmol) in Et_2O (50 mL) was added dropwise via filter cannula to a solution of **A1** (4.0 g, 15.3 mmol) in Et_2O (160 mL) at -10 °C. The mixture was continued stirring for 30 min at that temperature, followed by the color of the solution turning from wine to yellow. When the solvent was evaporated until ca. 30 mL remain, the mixture was applied to silica gel chromatography with petroleum ether elution to afford yellow compound **A2** (2.4 g, 63.3%). ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS): δ = 4.13 (s, 9H), 3.59 (t, J = 7.6 Hz, 2H), 2.81 (t, J = 7.6 Hz, 2H).

Synthesis of intermediate (A3)

A solution of **A2** (2.4 g, 9.7 mmol) and 4, 4'-bipyridine (10.6 g, 68 mmol) in acetonitrile (100 ml) was stirred for 2 days at 80°C. The solvent was removed in vacuo, and the residue was dissolved in some acetonitrile to applied to silica gel chromatography (dichloromethane: methanol = 50:3) to afford red compound **A3** (3.09 g, 78.8%). M.p. > 250 ºC. ^{1}H NMR (400 MHz, DMSO-d_6, 298K, TMS): δ = 9.13 (d, J = 6.8 Hz, 2H), 8.87 (d, J = 6.0 Hz, 2H), 8.61 (d, J = 6.8 Hz, 2H), 8.04 (d, J = 6.4 Hz, 2H), 4.74 (t, J = 7.6 Hz, 2H), 4.17 (s, 5H), 4.11 (d, J = 8.0 Hz, 4H), 3.03 (t, J = 7.6 Hz, 2H).

Synthesis of 4-hydroxyl-4'-methyl-azobenzene (B1)

$NaNO_2$ (52.25 g, 0.61 mol) dissolved in 387.5 mL H_2O, was added dropwise into *p*-toluidine (80 g, 0.75 mol) mixed with 225 mL HCl (36.5%) at 0 ~ 5°C. The final solution was kept stirring at 0°C for 15 min. Then a mixture of phenol (72 g, 0.76 mol) and 125 mL water was added dropwise into the above solution at 0 ~ 5 °C. The reaction was carried out at this temperature overnight and then NaOH was added until pH of 7–8 was achieved. A great deal of orange solid was gradually crystallized from the solution. The solid was filtered, washed with 700 mL CCl_4, dried in vacuo, and then gave out orange compound **B1** (87 g, 55%). M.p. 146 ~ 148 ºC. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS): δ = 7.86 (d, J = 8.4 Hz, 2H), 7.79 (d, J = 8.4 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 6.94 (d, J = 8.8 Hz, 2H), 5.35 (s, 1H), 2.43 (s, 3H).

Synthesis of 4-acetoxy-4'-methyl-azobenzene (B2)

A stirred mixture of **B1** (20 g, 94.3 mmol) and conc. sulfuric acid (0.4 ml) dissolved into acetic anhydride

(125 ml) was heated to 100 ºC for 3 h under argon, cooled and poured into ice water (700 ml) slowly with stirring. The solid was filtered and dried in vacuo. Thus gave out orange compound **B2** (20.8 g, 86.7%). M.p. 88 ~ 89 ºC. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS): δ = 7.94 (d, J = 8.4 Hz, 2H), 7.82 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 8.4 Hz, 2H), 7.25 (d, J = 8.8 Hz, 2H), 2.45 (s, 3H), 2.35 (s, 3H)

Synthesis of 4-acetoxy-4'-bromomethyl-azobenzene (B3)

A mixture of **B2** (10.4 g, 40.9 mmol), NBS (7.7 g, 43.3 mmol), BPO (0.6 g, 2.4 mmol) and CCl_4 (211 ml) were refluxed for 12 h under an atmosphere of Ar gas. The resulting solution was filtered while it was hot. The filtrate was cooling down to 0 °C to afford orange precipitate. The precipitate was filtered, washed with CCl_4 and gave pure **B3** (10.7 g, 78.6%). M.p. 120 ~ 121 ºC. ^{1}H NMR (400 MHz, $CDCl_3$, 298K, TMS): δ = 7.96 (d, J = 8.4 Hz, 2H), 7.89 (d, J = 8.0 Hz, 2H), 7.55 (d, J = 8.0 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 4.56 (s, 2H), 2.35 (s, 3H)

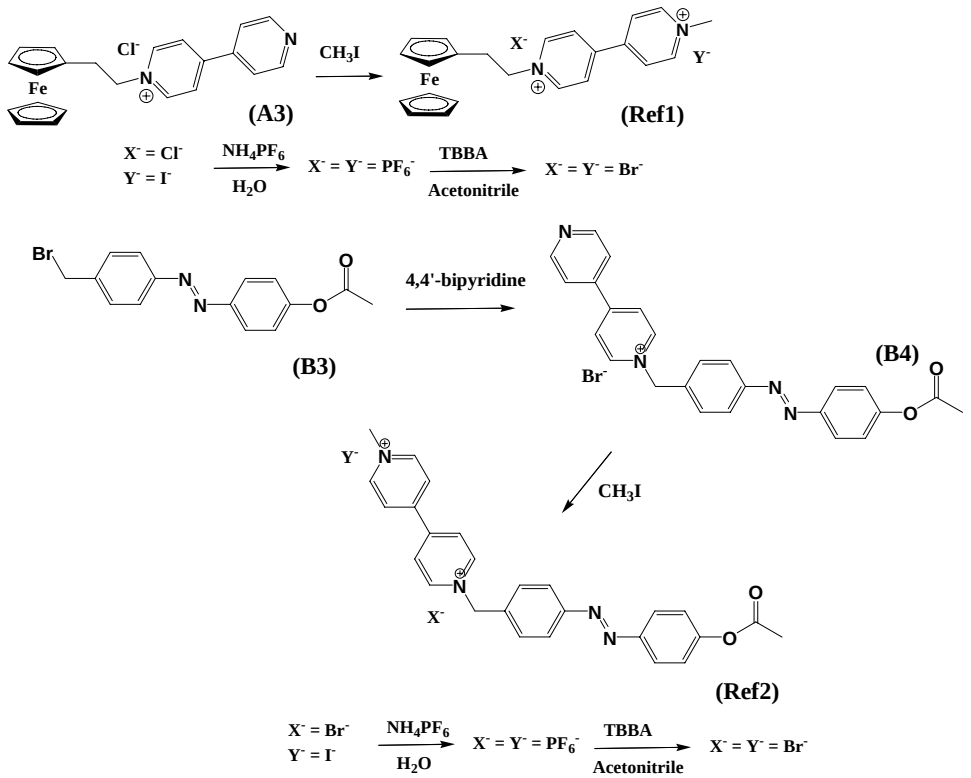
Synthesis of guest compound (FVA)

A3 (0.6 g, 1.48 mmol) was dissolved in acetonitrile (60 mL) at 70 °C. **B3** (3.5 g, 10.5 mmol) was added into the solution and the mixture was stirred at 70 °C for 5 hr. After cooling to room temperature, the mixture was filtered. And then the solid was washed with CH_2Cl_2 and gave a brown compound ca. 0.65 g. This compound was dissolved in water (1800 mL) and NH_4PF_6 (50 equiv.) was added to precipitate a brown solid. This solid was again dissolved in acetonitrile (150 mL) and TBAB (10 equiv.) was added to precipitate a brown solid. The solid was dried in vacuo and afford pure **FVA** (0.28 g, 24.3%). M.p. > 250 ºC. ^{1}H NMR (400 MHz, DMSO-d_6, 298K, TMS): δ = 9.58 (d, J = 1.6 Hz, 2H), 9.31 (d, J = 1.6 Hz, 2H), 8.84 (s, 2H), 8.77 (s, 2H), 7.95 (m, 4H), 7.84 (d, J = 7.2 Hz, 2H), 7.38 (d, J = 7.2 Hz, 2H), 6.09(s, 2H), 4.81 (s = 2H), 4.17 (s, 5H), 4.10 (s, 4H), 3.05 (s, 2H), 2.31 (s, 3H). ^{13}C NMR (500 MHz, DMSO-d_6, 298K, TMS): δ = 168.94, 153.01, 152.16, 149.41, 149.03, 148.47, 145.87, 145.75, 137.09, 130.23, 127.16, 126.42,

123.94, 123.11, 123.00, 82.37, 68.52, 68.25, 67.65, 62.60, 61.39, 30.99, 20.89. MS (ESI): m/z: 622.2 $[FVA-2Br]^+$ Elemental analysis calcd. for **FVA** $(C_{37}H_{34}Br_2FeN_4O_2)$ $(H_2O)_6$: C 52.53, H 5.48, N 6.62; found: C 52.57, H 5.36, N 6.45.

Preparation of the supramolecular ensemble (FVA⊂2CD):

FVA (78.1 mg, 0.1 mmol) and β-cyclodextrin (226.8 mg, 0.2 mmol) were mixed in an agate mortar, and were co-ground for 15 min under an infrared heat lamp. This uniform mixture would form 1:2 stoichiometric supramolecular assembly **FVA⊂2CD** rapidly in aqueous environment. ^{1}H NMR (400 MHz, D_2O, 298K): δ = 9.18 (d, J = 6.0 Hz, 2H), 8.78 (d, J = 6.0 Hz, 2H), 8.55 (d, J = 6.4 Hz, 2H), 8.43 (d, J = 6.4 Hz, 2H), 7.93 (d, J = 8.0 Hz, 2H), 7.88 (d, J = 8.8 Hz, 2H), 7.73 (d, J = 8.4 Hz, 2H), 7.35 (d, J = 8.4 Hz, 2H), 6.01(s, 2H), 5.00(s, 14H), 4.78 (s = 2H), 4.27 ~ 4.21 (m, 7H), 4.05 (m, 2H), 3.84 ~ 3.51 (m, 84H), 3.13 (s, 2H), 2.32 (s, 3H). MS (ESI): m/z: 1445.1 [**FVA⊂2CD** −2Br] $^{2+}$ Elemental analysis calcd. for **FVA⊂2CD** $(C_{121}H_{174}Br_2FeN_4O_{72})$ $(H_2O)_{27}$: C 41.59, H 6.58, N 1.60; found: C 41.50, H 6.42, N 1.46.



Scheme S2. Synthetic route to **Ref1** and **Ref2**

Synthesis of the reference compound (Ref1)

A3 (0.6 g, 1.48 mmol) was dissolved in acetonitrile (60 mL) at high temperature. The solution was then added upon iodomethane (1.5 g, 0.67 mL) and stirred for 1 day at 80°C. After cooling to room temperature, the mixture was filtered. The purple solid (ca. 0.68 g) was dissolved in water (50 mL) and NH_4PF_6 (10 mol equivalents) was added to precipitate a purple compound. This compound was again dissolved in acetonitrile (50 mL) and TBAB (10 mol equivalents) was added to precipitate a purple solid. The solid was dried in vacuo and afford pure **Ref1** (0.55 g, 68.6%). M.p. > 250 ºC. ^{1}H NMR (400 MHz, DMSO-d6, 298K, TMS): δ = 9.3 (m, 4H), 8.78 (s, 4H), 4.81 (t, J = 7.6 Hz, 2H), 4.44 (s, 3H), 4.18 (s, 5H), 4.11 (s, 4H), 3.05 (t, J = 7.6 Hz, 2H). ^{13}C NMR (400 MHz, DMSO-d_6, 298K, TMS): δ = 148.49, 147.96, 146.59, 145.79, 126.27, 126.10, 82.41, 68.54, 68.28, 67.67, 61.37, 47.98, 31.02. MS (ESI): m/z: 384.1 [**Ref1**−2Br]$^+$

Synthesis of intermediate (B4)

A solution of **B3** (6 g, 18.1 mmol) and 4, 4'-bipyridine (22.5 g, 144.2 mmol) in acetonitrile (300 mL) was stirred for 2 days at 80°C. The solvent was removed in vacuo, and the residue was washed by Et_2O (500 mL) to give a crude product. This crude solid was recrystallized by industrial ethanol to afford pure **B4** (6.2 g, 70.3%). M.p. > 250 ºC. ^{1}H NMR (400 MHz, DMSO-d6, 298K, TMS): δ = 9.40 (d, J = 6.8 Hz, 2H), 8.86 (d, J = 6.0 Hz, 2H), 8.67 (d, J = 6.8 Hz, 2H), 8.03 (d, J = 6.4 Hz, 2H), 7.94 (m, 4H), 7.79 (d, J = 8.4 Hz, 2H), 7.37 (d, J = 8.8 Hz, 2H), 6.01 (s, 2H), 2.30 (s, 3H)

Synthesis of the reference compound (Ref2)

A solution of **B4** (6 g, 12 mmol) dissolved in DMSO (70 mL), was mixed by a solution of iodomethane (12 g, 5.4 mL) acetonitrile (300 mL). The mixture was stirred for 1 day at 60 °C and an orange solid was filtered out. The solid (ca. 5.8 g) was dissolved in water (500 mL) and NH_4PF_6 (10 mol equivalents) was added to precipitate a yellow compound. This compound was again dissolved in acetonitrile (350 mL) and TBAB (10 mol equivalents) was added to precipitate an orange solid. The solid was dried in vacuo and afford pure **Ref2** (4.2 g, 60%). M.p. > 250 ºC. ^{1}H NMR (400 MHz, DMSO-d_6, 298K, TMS): δ = 9.56 (d, J = 6.4 Hz, 2H), 9.29 (d, J = 6.6 Hz, 2H), 8.82 (d, J = 6.4 Hz, 2H), 8.75 (d, J = 6.4 Hz, 2H), 7.97 (m, 4H), 7.84 (d, J = 8.4 Hz, 2H), 7.40 (d, J = 8.8 Hz, 2H), 6.07 (s, 2H), 4.44 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (400 MHz, DMSO-d6, 298K, TMS): δ = 168.96, 153.04, 152.19, 149.42, 149.19, 148.10, 146.58, 145.90, 137.08, 130.23, 127.10, 126.19, 123.95, 123.14, 123.02, 62.68, 48.01, 20.89. MS (ESI): m/z: 424.2 [**Ref2**−2Br]$^+$

Association constant K between the reference compounds and *β*-CD

The association constant between **Ref1**, **Ref2** and *β*-CD in aqueous solution was determined by following the UV absorption at 370 nm and 320 nm, as shown in Figure S1 and S2, respectively. The concentration of **Ref1** and **Ref2** were both kept at 2.0×10^{-4} M. Upon addition of excess *β*-CD, the absorption of the reference compounds varied remarkably. With a 1:1 stoichiometry, the inclusion complexation of *β*-CD with the reference compounds is expressed by the following equation:

$$[\text{Ref}] + [\beta\text{-CD}] \underset{}{\overset{K}{\rightleftharpoons}} [\text{Ref-CD}]$$

We employed the usual double reciprocal plot according to the modified Hidebrand-Benesi equation:

$$\frac{1}{[\Delta A]} = \frac{1}{K[\Delta\varepsilon][\text{Ref}][\beta\text{-CD}]} + \frac{1}{[\Delta\varepsilon][\text{Ref}]}$$

where ΔA denotes the absorbance difference before and after *β*-CD were added and $\Delta\varepsilon$ denotes the difference of the molar extinction coefficient between the reference compounds and Ref-CD complexes at the same wavelength. The association constant K can be obtained from the double reciprocal plot of $1/\Delta A$ versus $1/[\beta\text{-CD}]$, and the value we obtained here is 2.42×10^3 M^{-1} and 1.63×10^3 M^{-1} for **Ref1⊂CD** and **Ref2⊂CD** complex system, respectively.

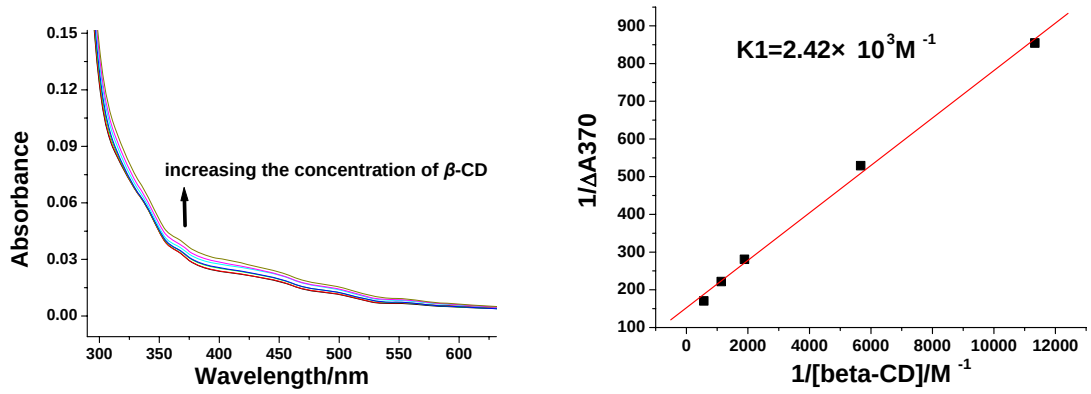


Figure S1. The UV absorption of **Ref1** upon stepwise addition of excess *β*-CD. The concentration of **Ref1** keeps 2.0×10^{-4} M (298K).

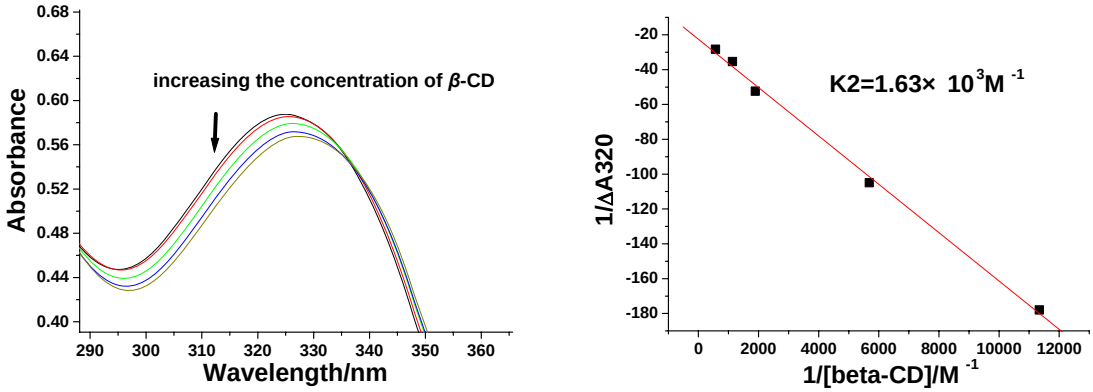


Figure S2. The UV absorption of **Ref2** upon stepwise addition of excess *β*-CD. The concentration of **Ref2** keeps 2.0×10^{-4} M (298K).

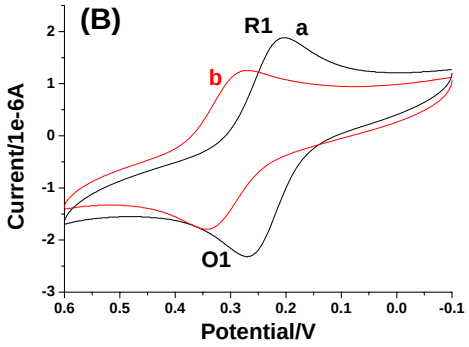


Figure S3. Cyclic voltammograms (CV) of **Ref1** (1.01×10^{-4}) in water at 298K a) in the absence and b) presence of 20 equiv. *β*-CD.

Electrochemical method for determination of the association constants between ferrocene and *β*-CD ($K1_0$) and between ferrocenium and *β*-CD ($K1_+$)

The electrochemical determination for the association constants of **Ref1⊂CD** complex was evaluated in H_2O by plotting the variation of the half-wave potential of Ref1 in the presence of *β*-CD with respect to the half-wave potential in the absence of *β*-CD as a function of the total concentration of *β*-CD (Figure S13). The relationship between $\Delta E_{1/2}$ and [*β*-CD] can be depicted as follows:[5d]

$$\Delta E_{1/2} = \frac{RT}{2F} \ln\left(\frac{(1+K1_0*[\beta\text{–}CD])\,(1+K1_0*\,r\,*[\beta\text{–}CD])}{(1+K1_+*[\beta\text{–}CD])\,(1+K1_+*\,r\,*[\beta\text{–}CD])}\right)$$

$K1_0$ and $K1_+$ are the complexation constants between *β*-CD and **Ref1** or **Ref1**$^+$, respectively. The value of r, 0.503, was estimated by using the equation $r=(M1/M1{\cdot}CD)^{1/2}$, in which M1 and M1·CD are the molecular

weights of **Ref1** and **Ref1⊂CD** complex, respectively. The data fitting was conducted using Matlab (R2007a) and got the values for $K1_0$ = 4910 M^{-1} and $K1_+ < 3$ M^{-1}. Although the values here have a little deviation with the one obtained via the method in determining absorption, they can be employed to fully demonstrate that the station in ferrocene form can be efficiently complexed with *β*-CD ring in water, whereas ferrocenium complexed with *β*-CD ring is unfavourable.

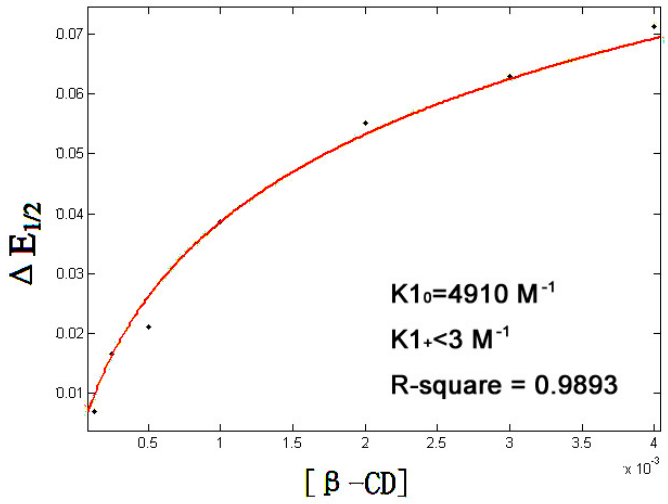


Fig. S4. Half-wave potential difference of **Ref1** in H_2O in the presence of *β*-CD and in the absence of *β*-CD as a function of the total concentration of *β*-CD, recorded at a glassy carbon electrode at a scan rate of 50 mV/s.

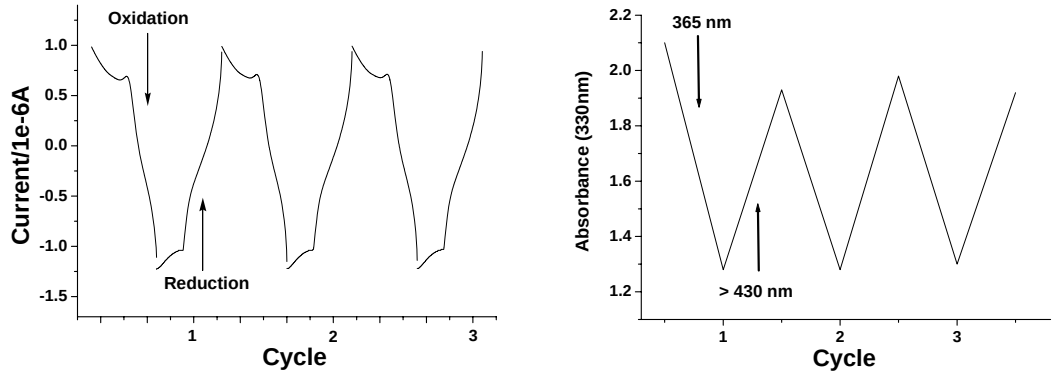


Figure S5. The representation of the reversibility and repeatability of **FVA⊂2CD.** Left) Change of the current in cyclic voltammetry (CV) test of **FVA⊂2CD** in water**.** Right) Changes in absorbance at 330 nm of **FVA⊂2CD** in water, along with changes in alternation of full irradiation by 365-nm UV light and visible light.

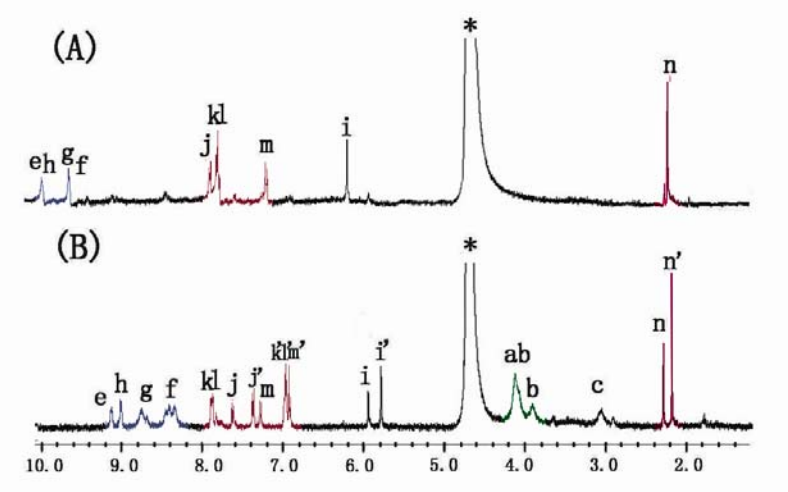
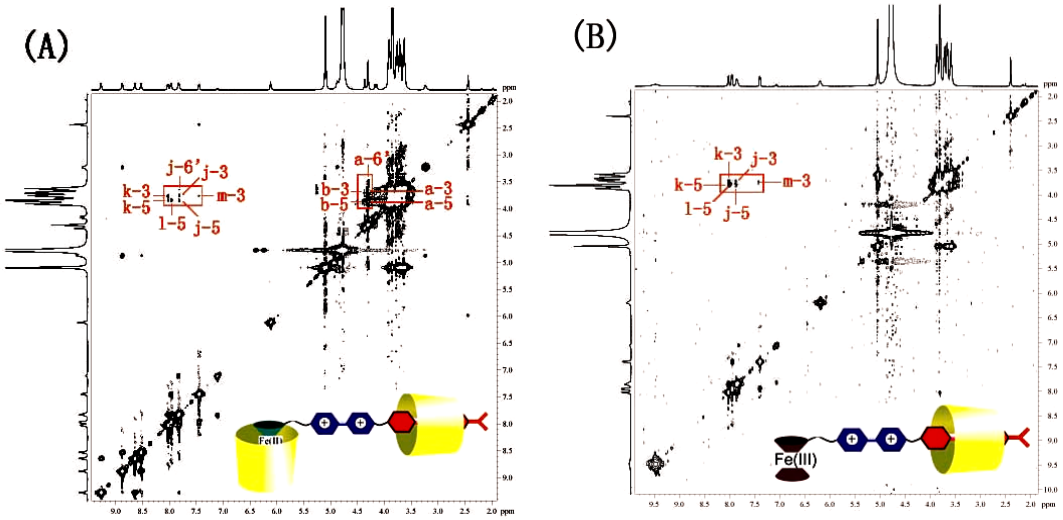


Fig. S6 ^{1}H NMR spectra (400 MHz in D_2O at 298 K) of (A) **FVA-o**, addition of 1.2 equiv. ferric chloride to **FVA**; (B) **FVA-p**, irradiation on **FVA** by 365 nm for 2 h *in situ*. The proton peaks of $H_{k,l}$ in **FVA-o** (δ = 7.80, $H_{k,l}$ in Fig. S6A) and the proton peaks of $H_{a,b}$ in **FVA-p** (δ = 4.11, $H_{a,b}$ in Fig. S6B) are overlapped, compared with the corresponding splitting ones in **Fig.2C** and **2D**. These results give the circumstantial evidence of the assembly/disassembly behaviors of the *β*-CD complexes.



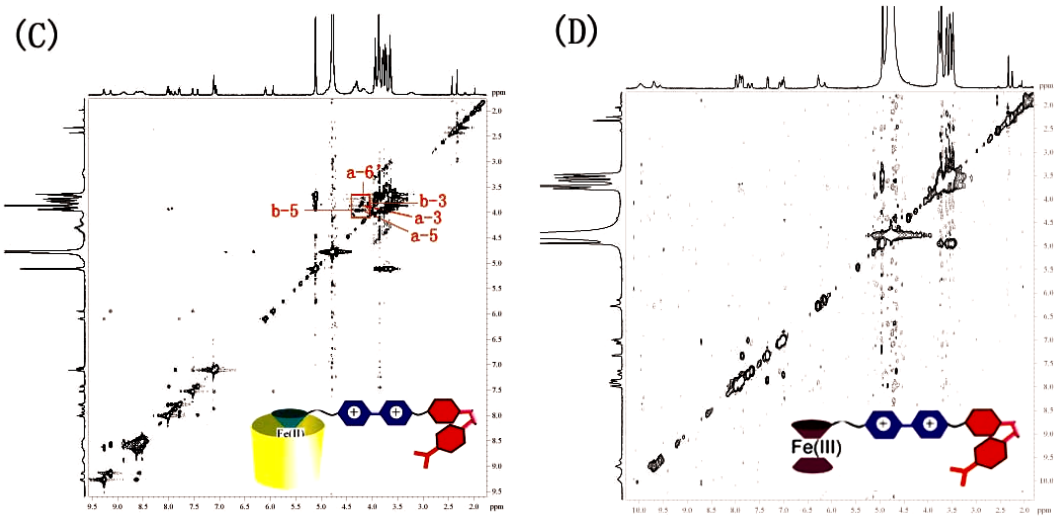


Figure S7. The two-dimensional ^{1}H NOESY NMR spectra (500 MHz in D_2O at 298 K) of (A) **FVA⊂2CD**; (B) **FVA-o ⊂CD**, addition of 1.2 equiv. ferric chloride to **FVA⊂2CD**; (C) **FVA-p ⊂CD**, irradiation on **FVA⊂2CD** by 365 nm for 2 h; (D) **FVA-op**, irradiation on **FVA⊂2CD** by 365 nm for 2 h, then addition of 1.2 equiv. ferric chloride.

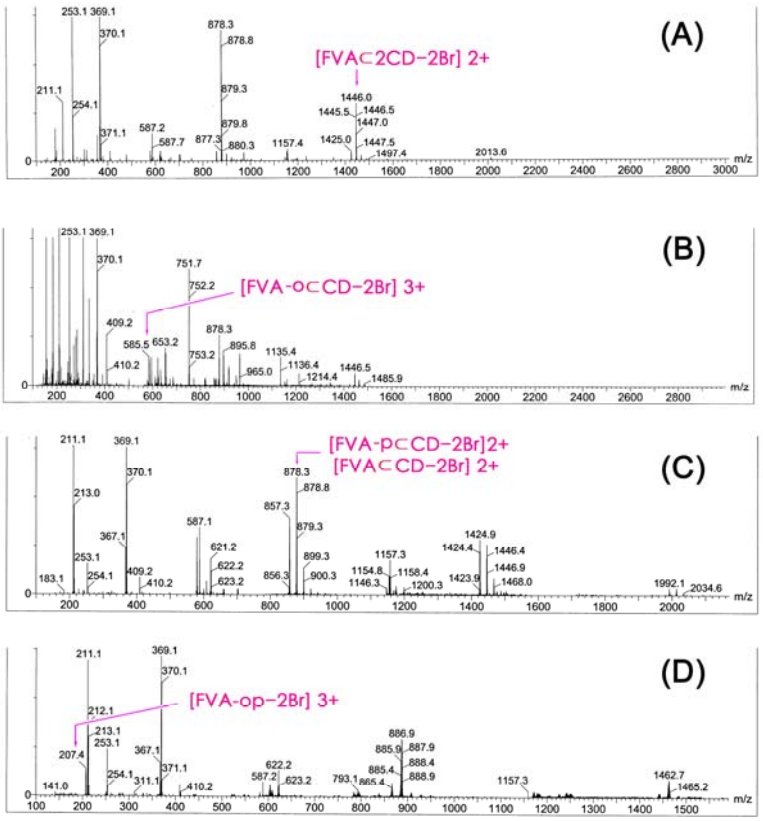


Figure S8. ESI-MS spectra in aqueous solution of (A) **FVA⊂2CD**; (B) **FVA-o ⊂CD**, addition of 1.2 equiv. ferric chloride to **FVA⊂2CD**; (C) **FVA-p ⊂CD**, irradiation on **FVA⊂2CD** by 365 nm for 2 h; (D) **FVA-op**, irradiation on **FVA⊂2CD** by 365 nm for 2 h, then addition of 1.2 equiv. ferric chloride.

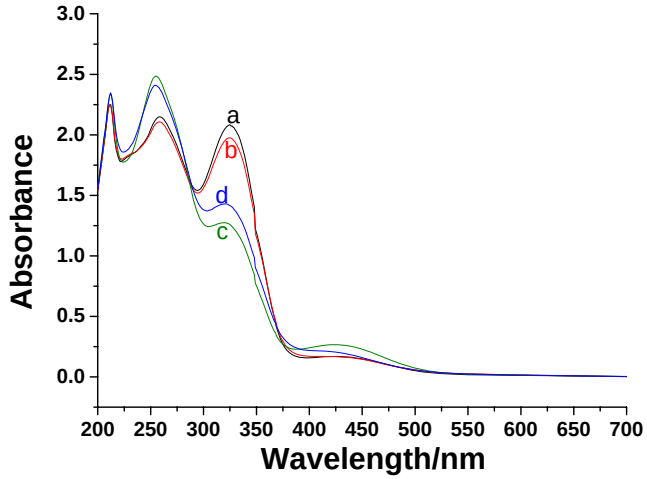


Figure S9. Absorption spectra of **FVA⊂2CD** a) in the initial state, b) after addition of 1.2 mol equivalents ferric chloride **(FVA-o⊂CD)**, c) after irradiation at 365 nm for 30 min **(FVA-p⊂CD)**, and d) after irradiation at 365 nm for 30 min, then addition of 1.2 mol equivalents ferric chloride **(FVA-op)**. These optical spectra were measured in water with the complex concentration of 1.01×10^{-4} M at 298K.

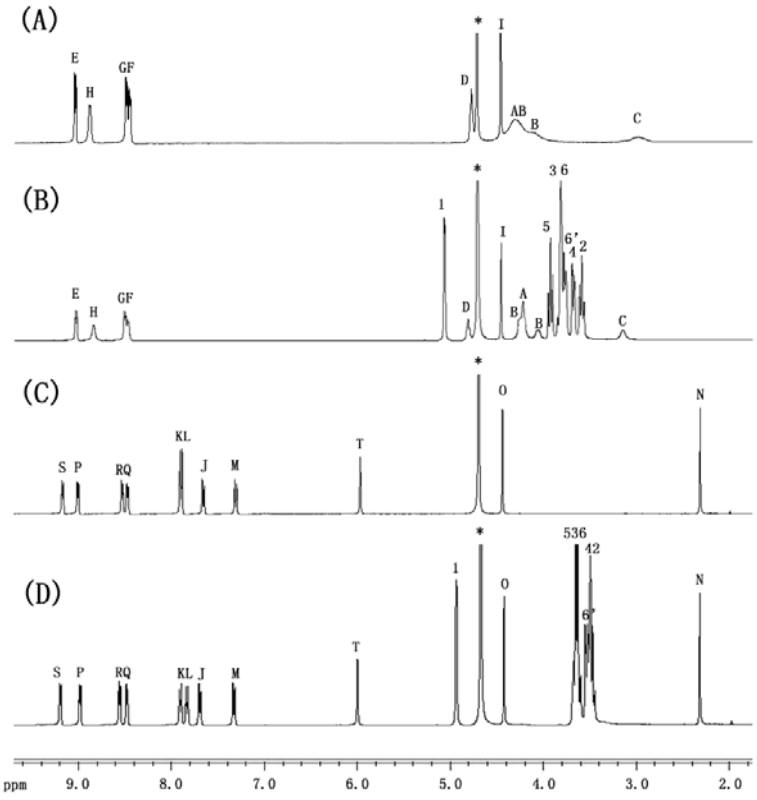


Figure S10. ^{1}H NMR spectra (400MHz, 298K) of A) **Ref1** in D_2O, B) **Ref1** in D_2O after addition of 1 equiv. *β*-CD (**Ref1⊂CD**), C) **Ref2** in D_2O, and D) **Ref2** in D_2O after addition of 1 equiv. *β*-CD (**Ref2⊂CD**). The concentration of **Ref1** and **Ref2** was maintained at 1.5×10^{-2} M.

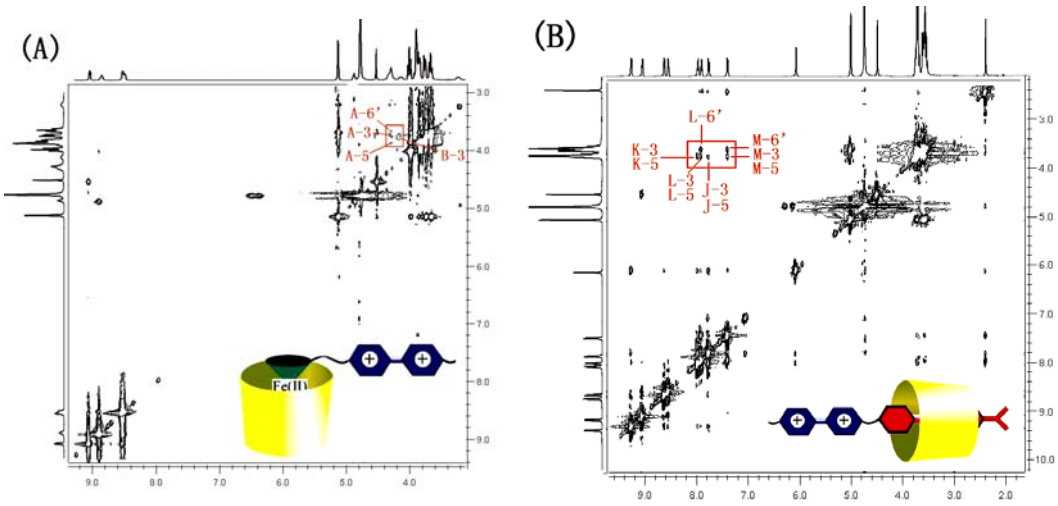


Figure S11. Two-dimensional ROESY NMR spectra (500 MHz, D_2O, 298 K) of A) **Ref1** in D_2O after addition of 1 mol equivalent *β*-CD (**Ref1⊂CD**) and B) **Ref2** in D_2O after addition of 1 mol equivalent *β*-CD (**Ref2⊂CD**). The concentration of **Ref1** and **Ref2** was maintained at 2.0×10^{-2} M.

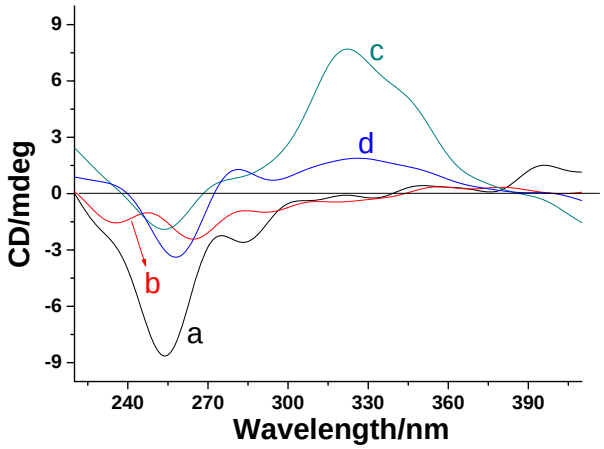


Figure S12. Induced circular dichroism (ICD) spectra (1.01×10^{-3} M in water, 298K) for (A) **Ref1⊂CD**; (B) addition of 1.2 equiv. ferric chloride to **Ref1⊂CD**; (C) **Ref2⊂CD**; (D) irradiation on **Ref2⊂CD** by 365 nm for 2 h.

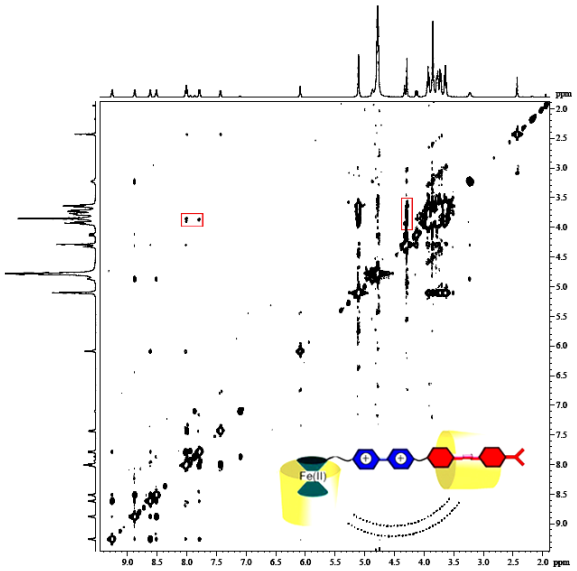
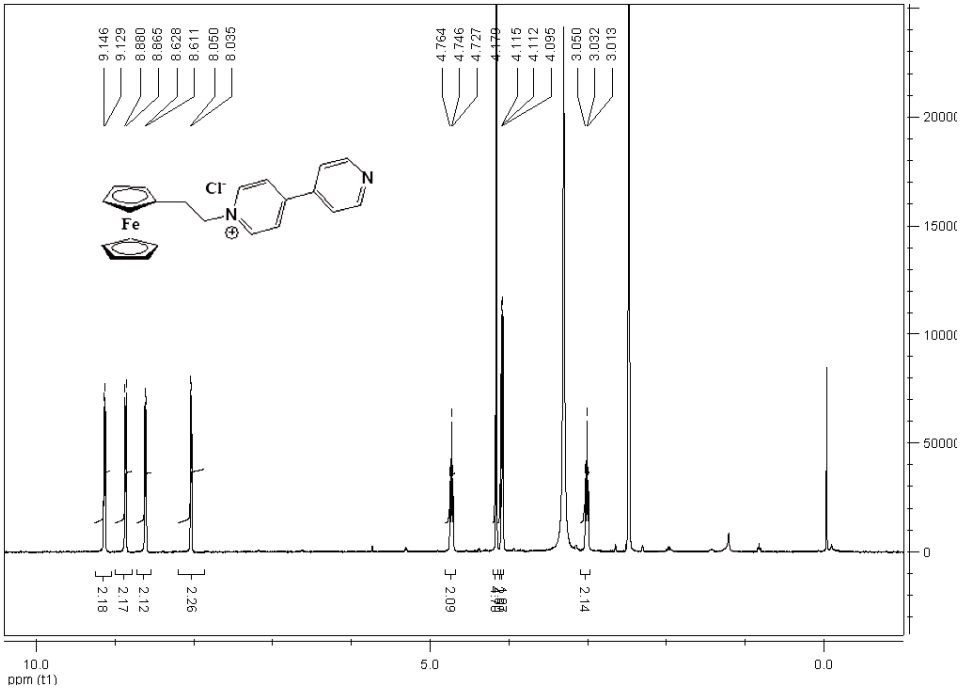
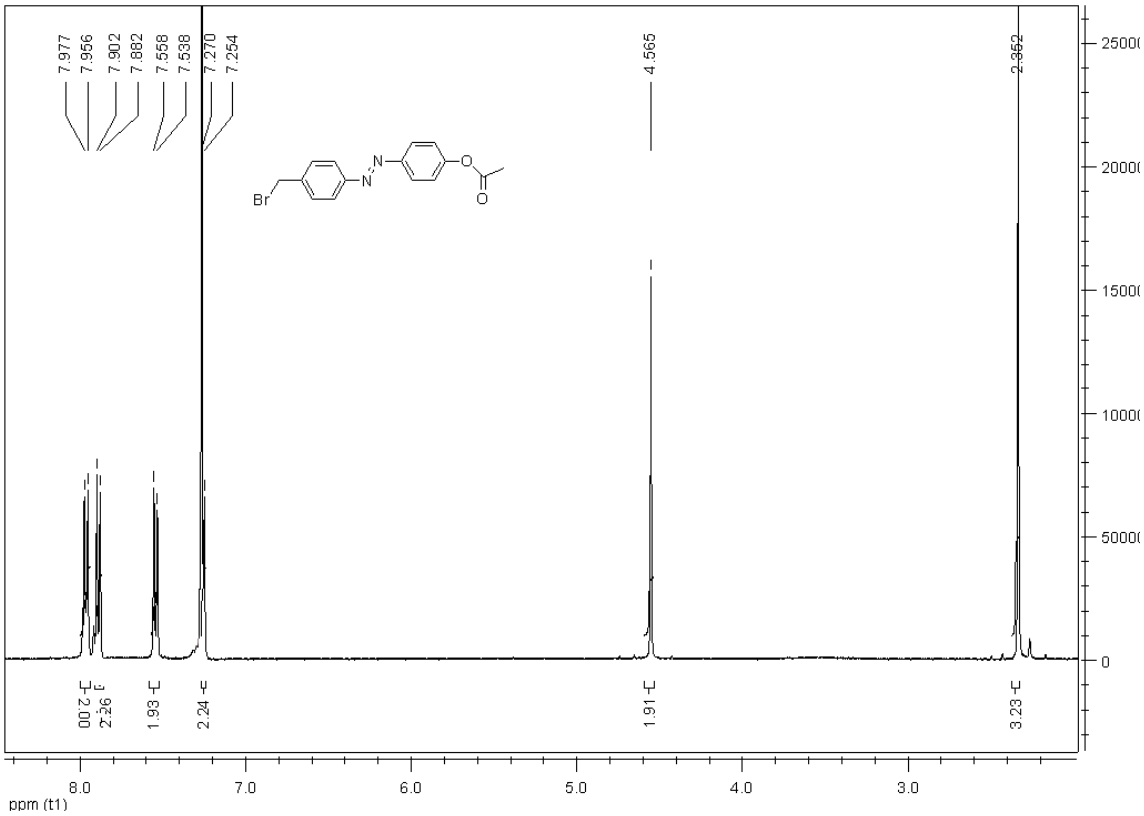


Figure S13. The two-dimensional ^{1}H NOESY NMR spectrum (500 MHz in D_2O at 298 K) of **FVA⊂CD** (1:1 complex). NOEs are observed from ferrocenyl protons $H_{a, b}$, and also from the azobenzenyl protons $H_{j, k, l}$ to the internal protons of *β*-CD, which have elucidated that the 1 equiv. *β*-CD here is oscillating between the two stations. The stronger NOEs signals (from ferrocenyl protons to the protons of *β*-CD) indicate the bigger association constant K1.

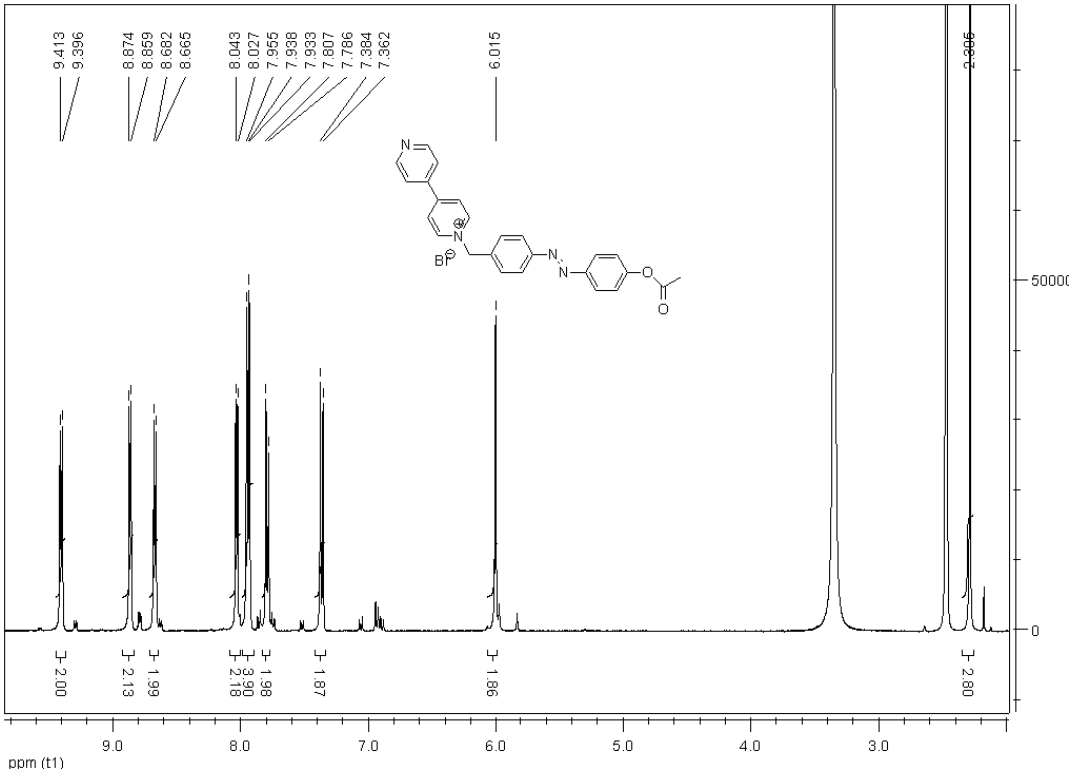
^{1}H NMR spectrum of **A3** in DMSO-d_6 (400MHz)



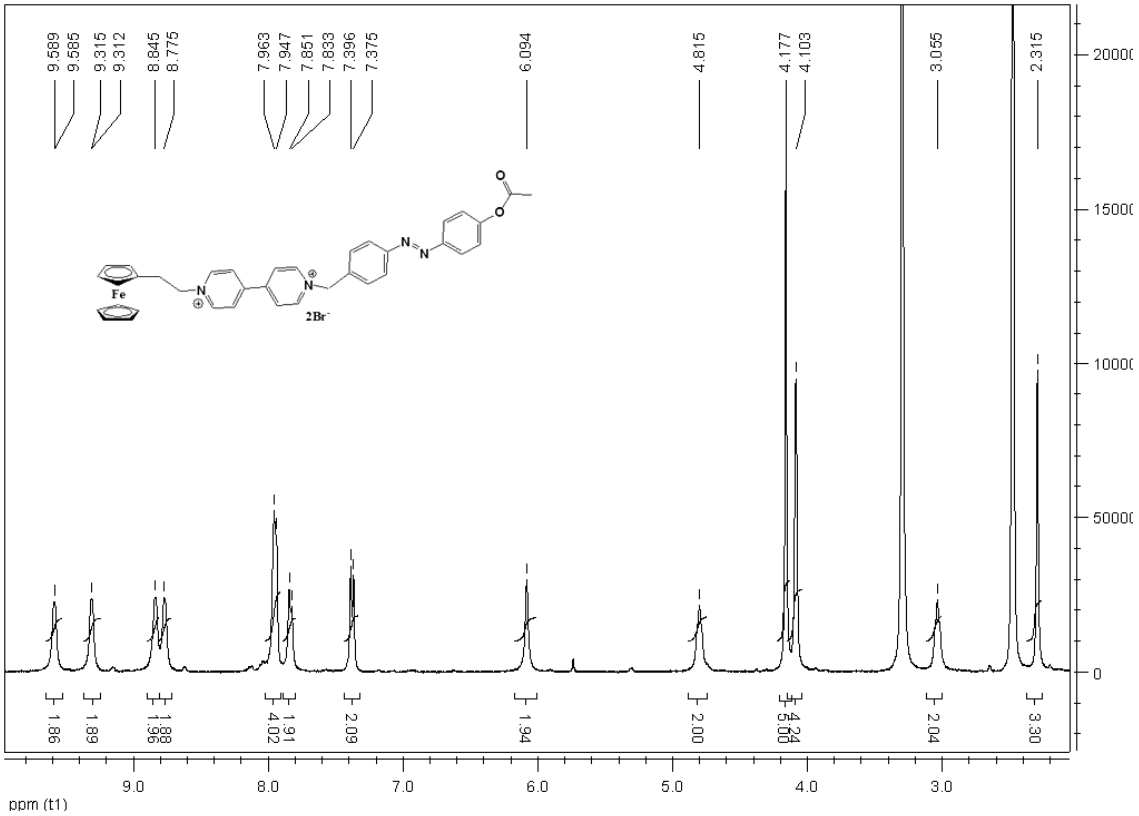
^{1}H NMR spectrum of **B3** in $CDCl_3$ (400MHz)



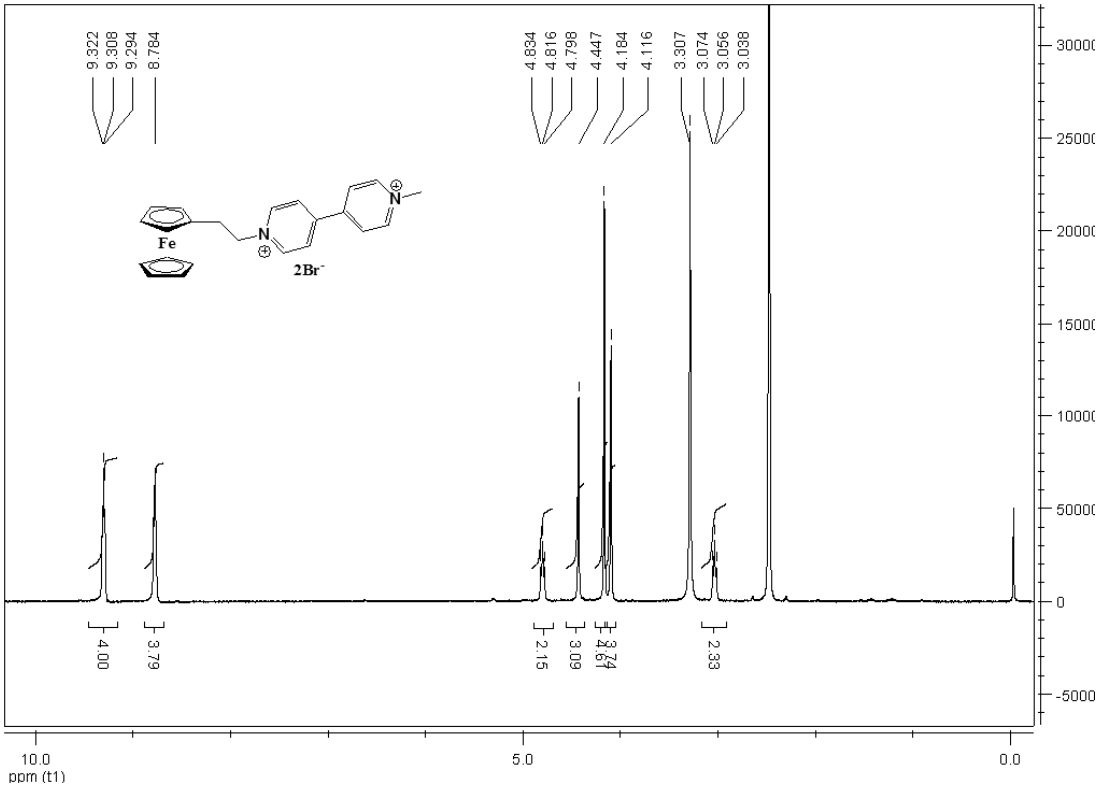
^{1}H NMR spectrum of **B4** in DMSO-d_6 (400MHz)



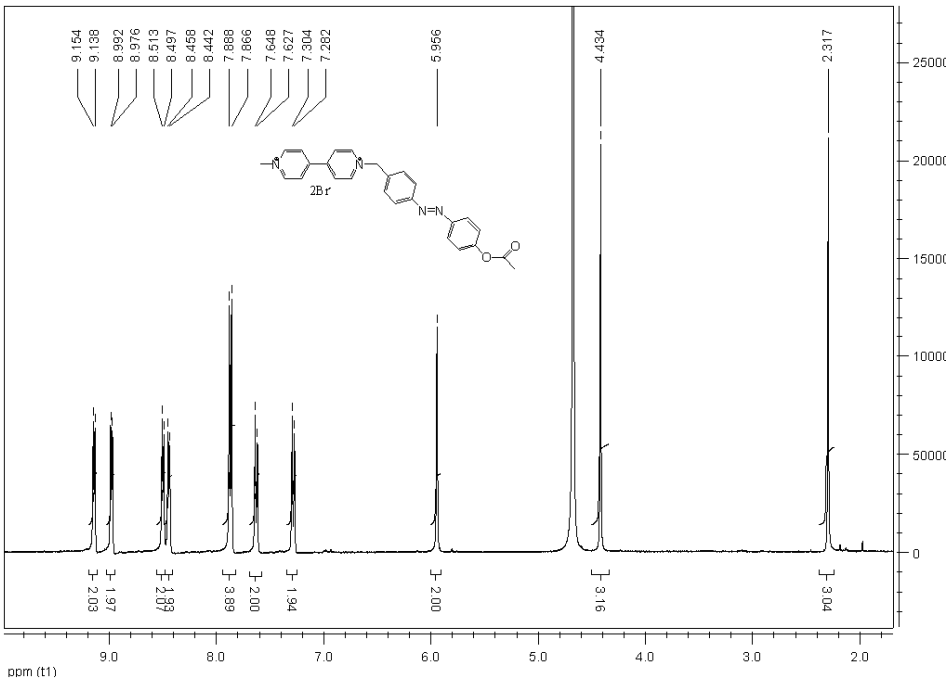
^{1}H NMR spectrum of **FVA** in DMSO-d_6 (400MHz)



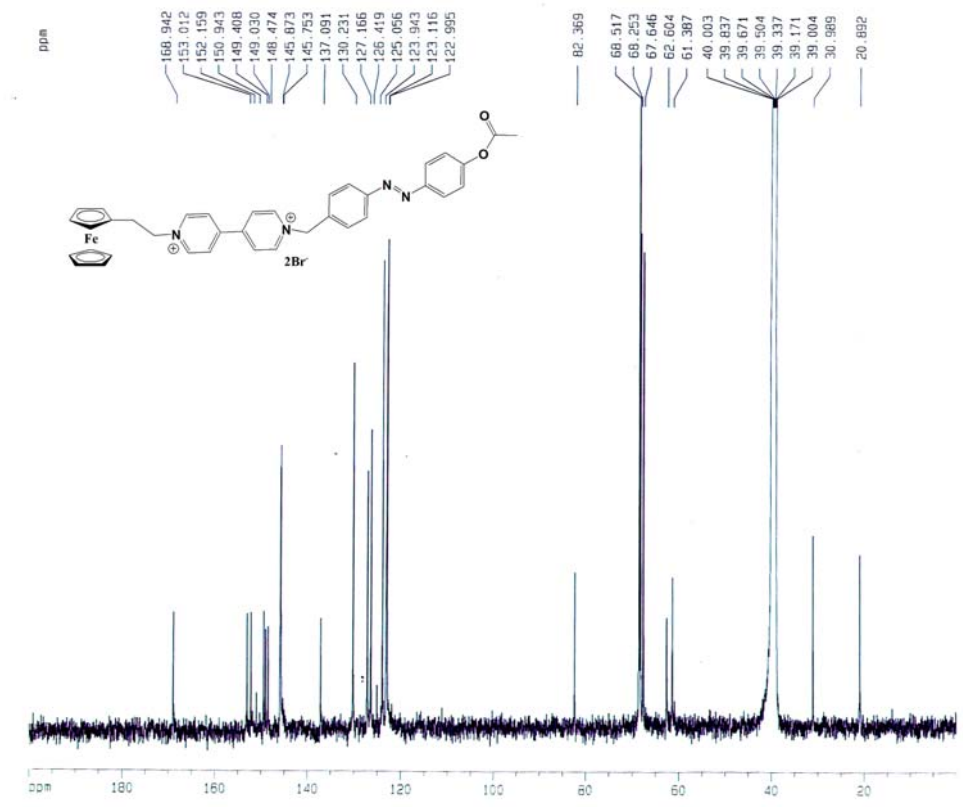
^{1}H NMR spectrum of **Ref1** in DMSO-d_6 (400MHz)



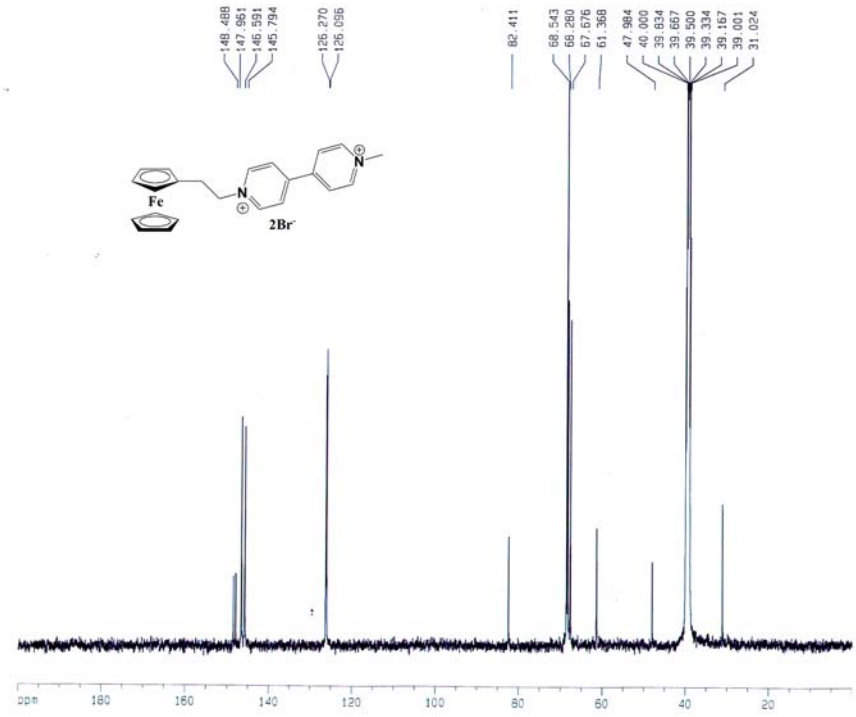
^{1}H NMR spectrum of **Ref2** in D_2O (400MHz)



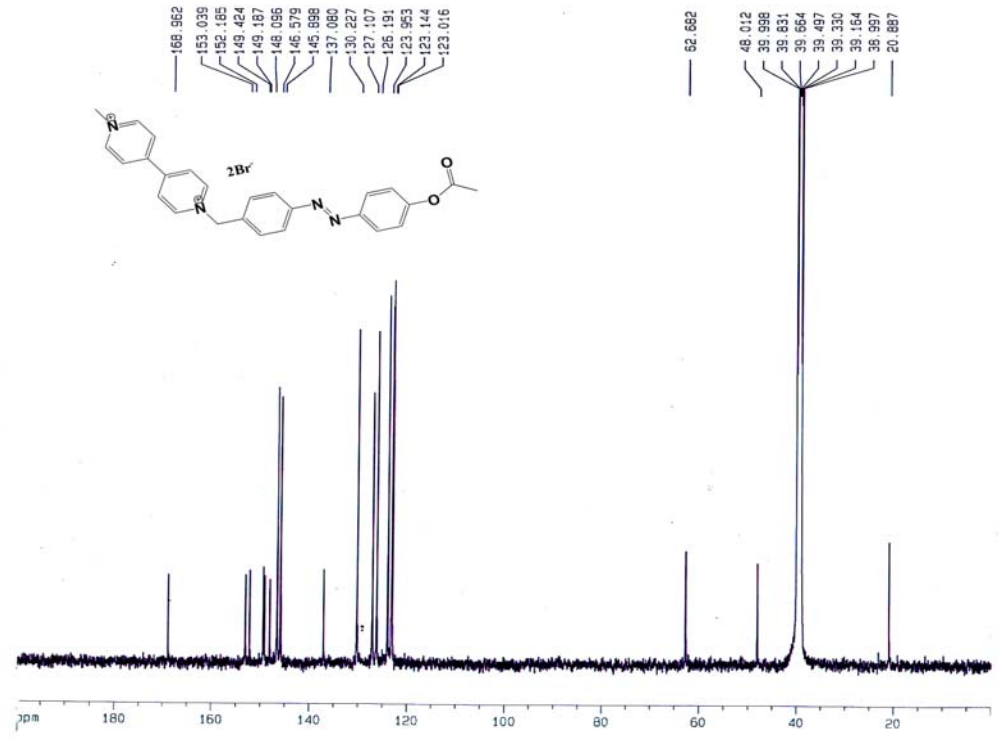
^{13}C NMR spectrum of **FVA** in DMSO-d_6 (500MHz)



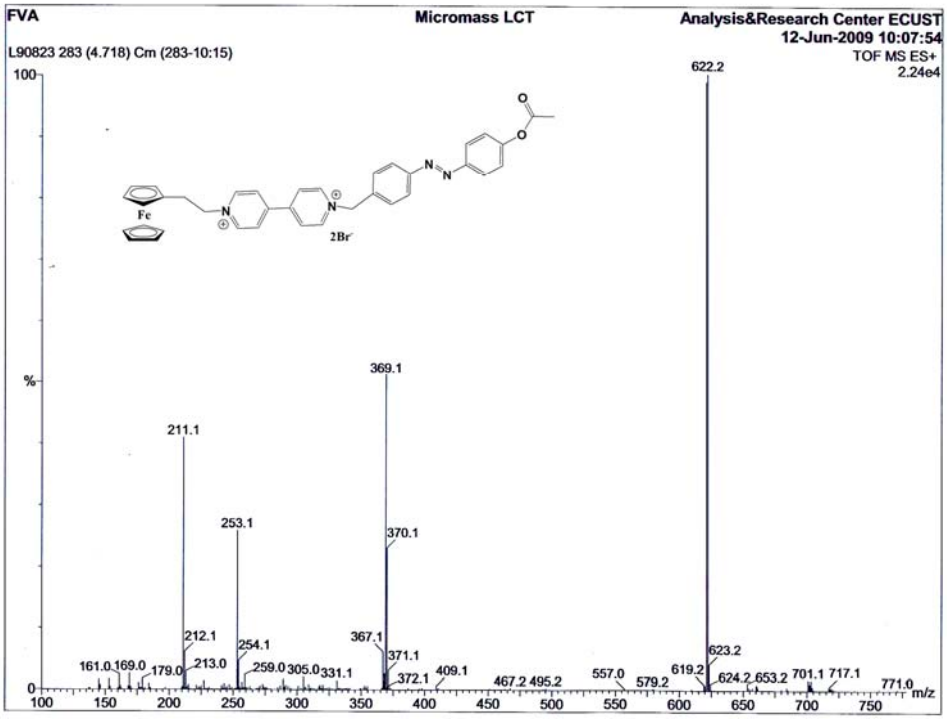
^{13}C NMR spectrum of **Ref1** in DMSO-d_6 (500MHz)



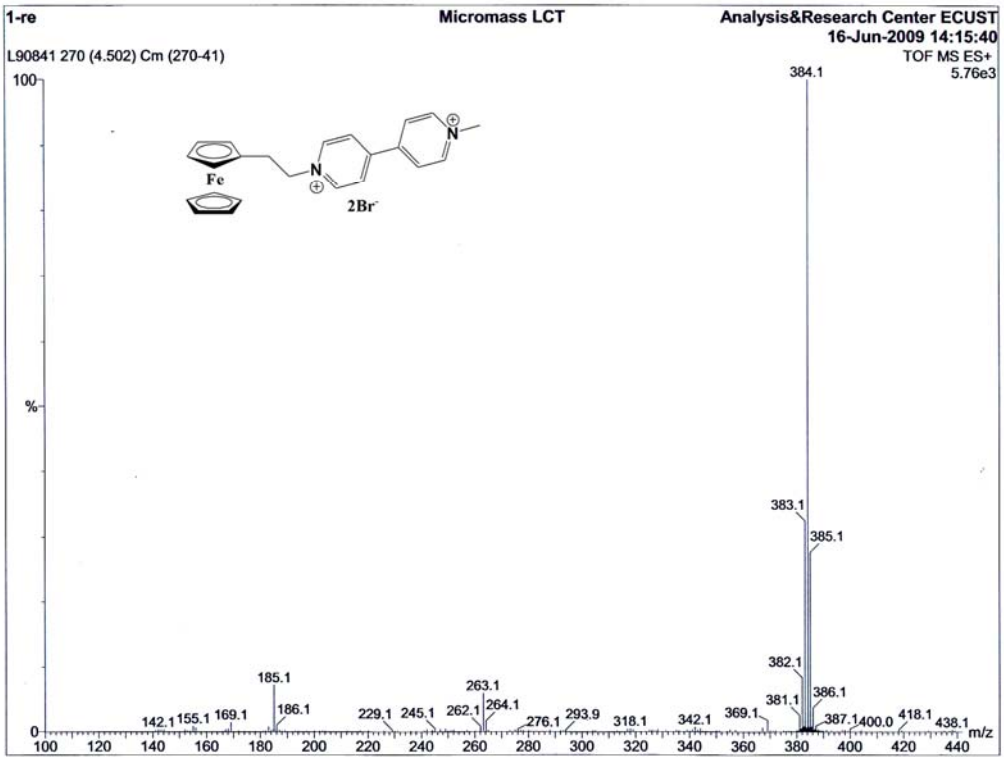
^{13}C NMR spectrum of **Ref2** in DMSO-d_6 (500MHz)



MS spectrum (ESI) of **FVA**



MS spectrum (ESI) of **Ref1**



MS spectrum (ESI) of **Ref2**