Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

New sensitive and selective calixarene based fluorescent sensors for the detection of Cs^+ in an organoaqueous medium

Naresh Kumar,[a] Qui Pham-Xuan,[a] Alexis Depauw,[a] Miryana Hemadi,[b] Nguyet-Thanh Ha-Duong,[b] Jean-Pierre Lefevre,[a] Minh-Huong Ha-Thi*[ac] and Isabelle Leray*[a]

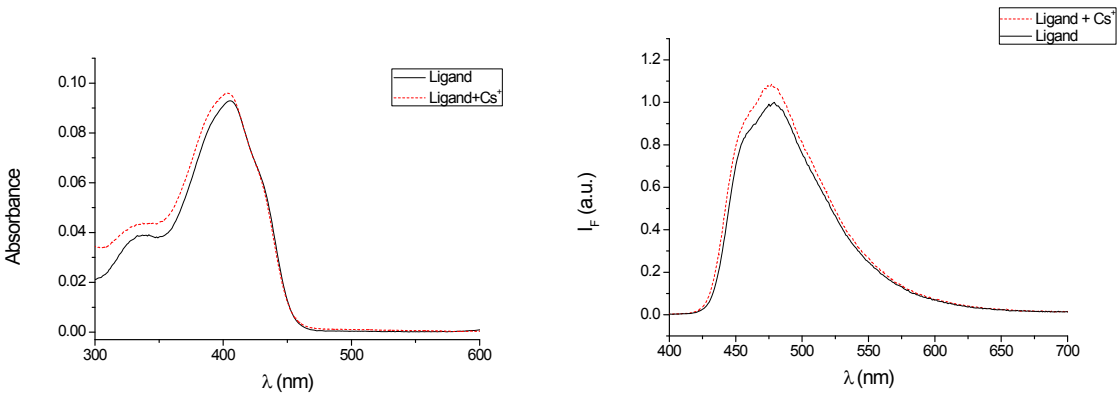

Figure S1. Absorption (a) and emission (b) spectra of Calix-COU-Benz (2.1 x 10^{-6} M) upon addition of a large excess of cesium acetate (9mM) in CH_3CN/H_2O (8/2; v/v). (λ_{exc} = 397 nm).

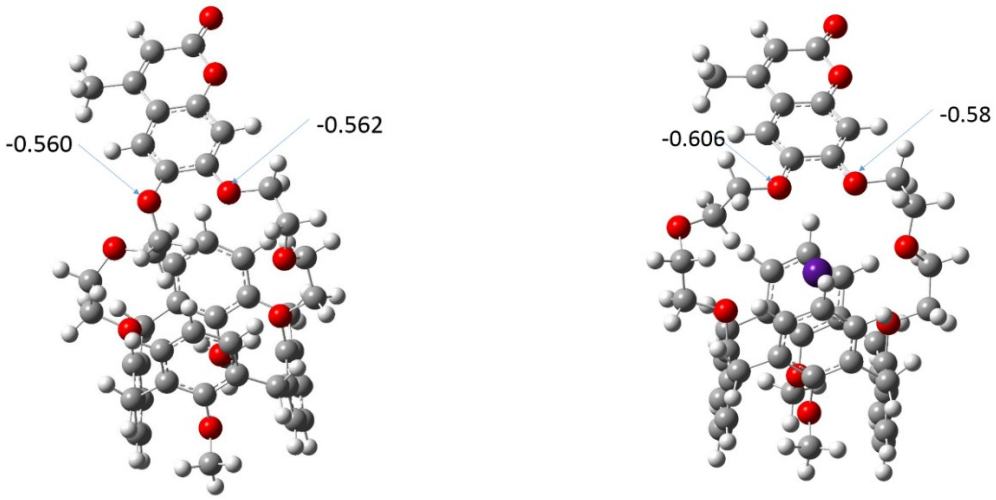

Figure S2: Calculated charges of oxygen atoms on optimized structures of the simplified calixarene and its Cs^+ complex. Calculations were performed with the Gaussian software. All calculations were performed using the B3LYP/6-31G and the B3LYP/LANL2DZ method.[1] Total energy are -2609.43 and -2629.24 a.u. for the ligand and the Cs^+ complex, respectively. A decrease of the charge on oxygen atoms on the 6 and 7 positions of the coumarin were observed on the Cs^+ complex.

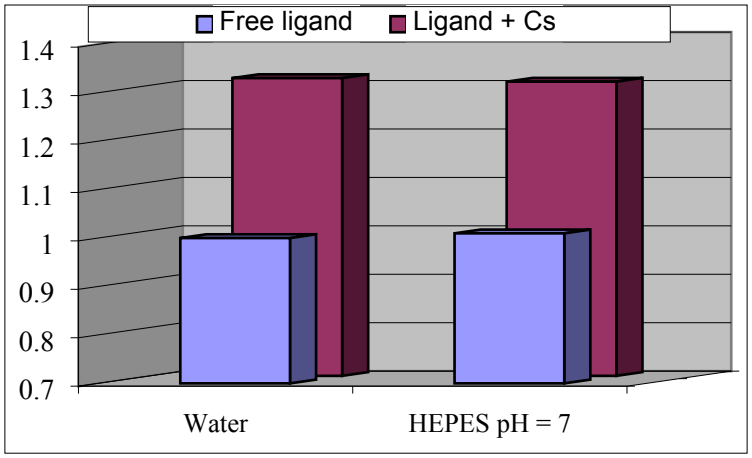

Figure S3. Fluorescence response at 562 nm of Calix-COU-Benz-CN (3.1 x 10^{-6} M) in the presence of Cs^+ 100 µM in CH_3CN/H_2O 8/2 and in CH_3CN/HEPES buffer 10 mM (pH = 7) 8/2.

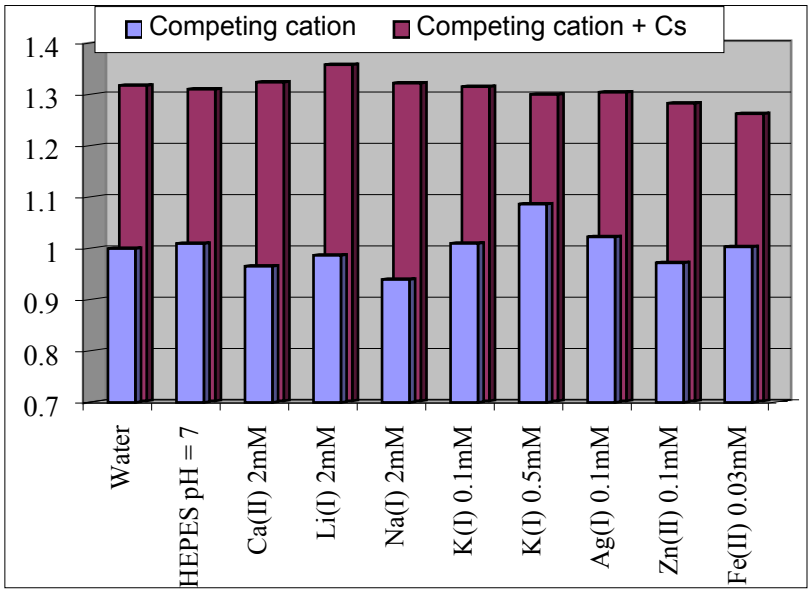

Figure S4. Selectivity diagram of Calix-COU-Benz-CN (3.1 x 10^{-6} M) in the presence of selected competitive metal ions in CH_3CN/H_2O 8/2. [Cs+] = 100 µM, , λ_{exc} = 456 nm, λ_{em} = 562 nm

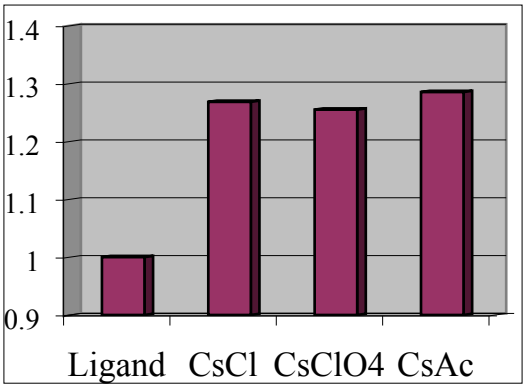

Figure S5. Fluorescence intensity at 562 nm of Calix-COU-Benz-CN (3.1 x 10^{-6} M) in CH_3CN/H_2O 8/2, in the presence of Cs^+ 100 µM from various cesium salts.

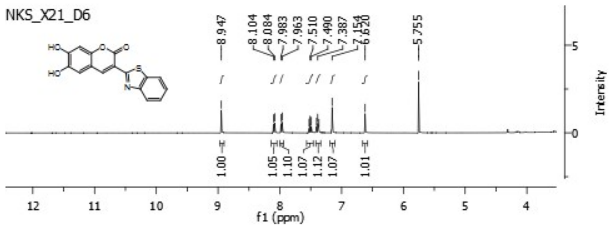

Figure S6: ^{1}H NMR Spectrum of **1** (DMSO-d_6, 400 MHz).

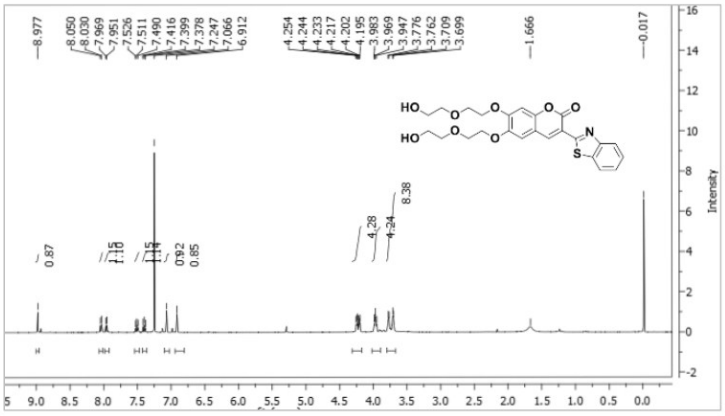

Figure S7: ^{1}H NMR Spectrum of **COU-Benz** ($CDCl_3$, 400 MHz).

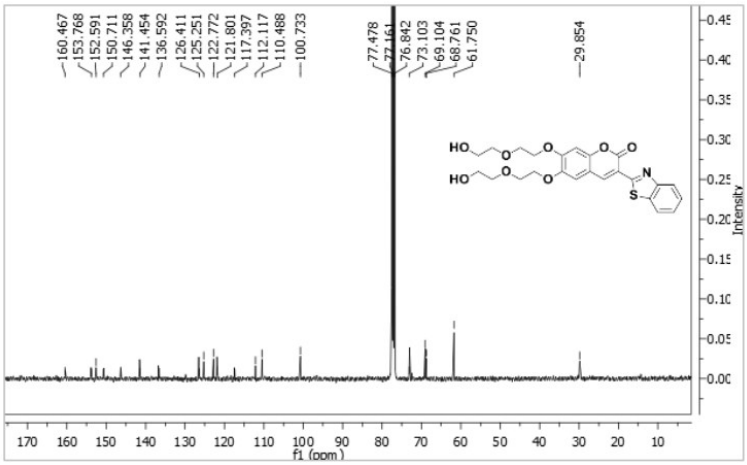

Figure S8: ^{13}C NMR Spectrum of **COU-Benz** ($CDCl_3$, 100 MHz).

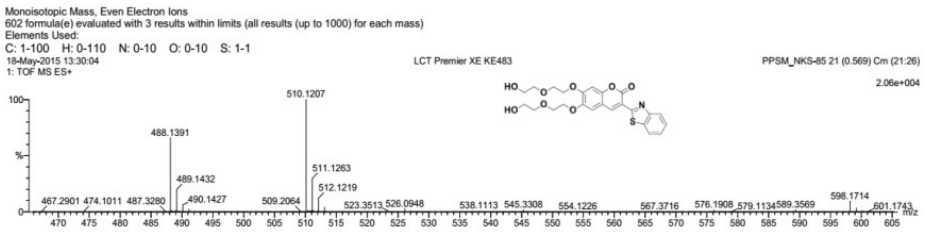

Figure S9: Mass spectrum (HRMS: TOF MS ES+) of **COU-Benz**.

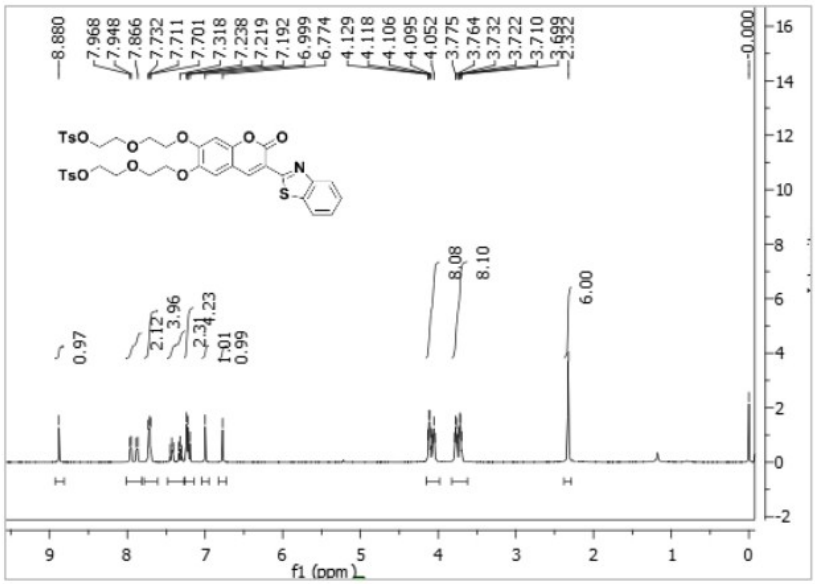

Figure S10: ^{1}H NMR Spectrum of **2** ($CDCl_3$, 400 MHz).

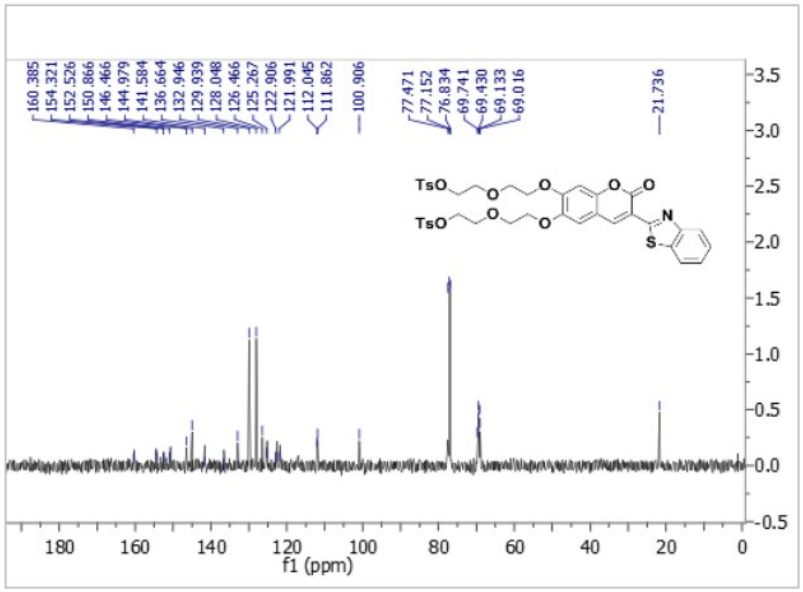

Figure S11: ^{13}C NMR Spectrum of **2** ($CDCl_3$, 100 MHz).

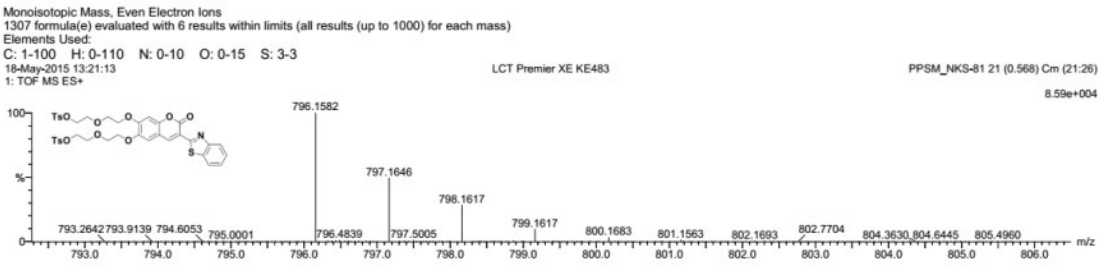

Figure S12: Mass spectrum (HRMS: TOF MS ES+) of **2**.

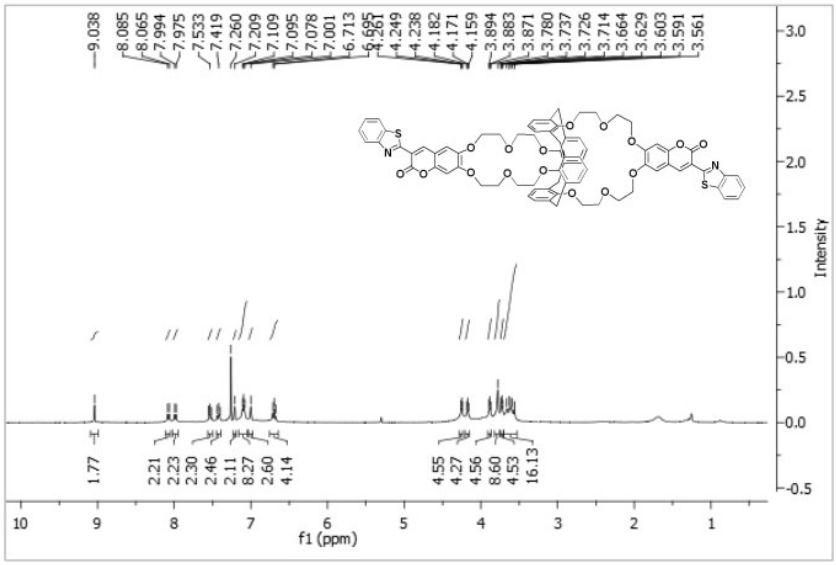

Figure S13: ^{1}H NMR Spectrum of **Calix-COU-Benz** ($CDCl_3$, 400 MHz).

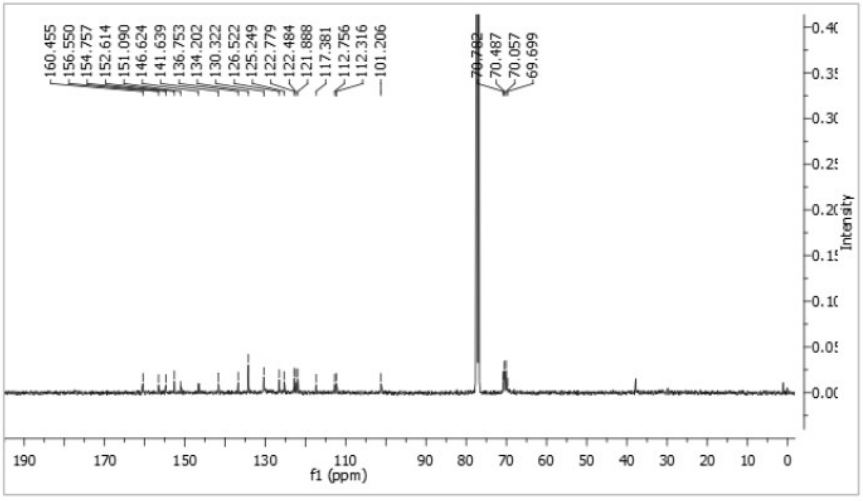

Figure S14: ^{13}C NMR Spectrum of **Calix-COU-Benz** ($CDCl_3$, 100 MHz).

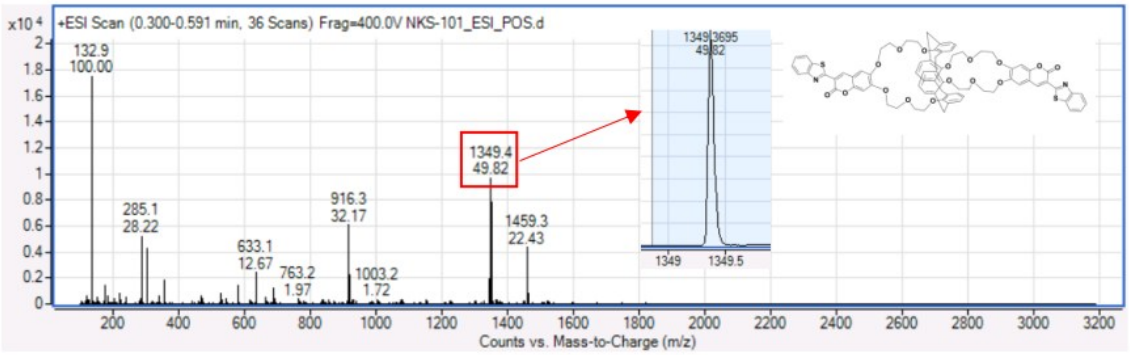

Figure S15: Mass spectrum (HRMS: TOF MS ES+) of **Calix-COU-Benz**.

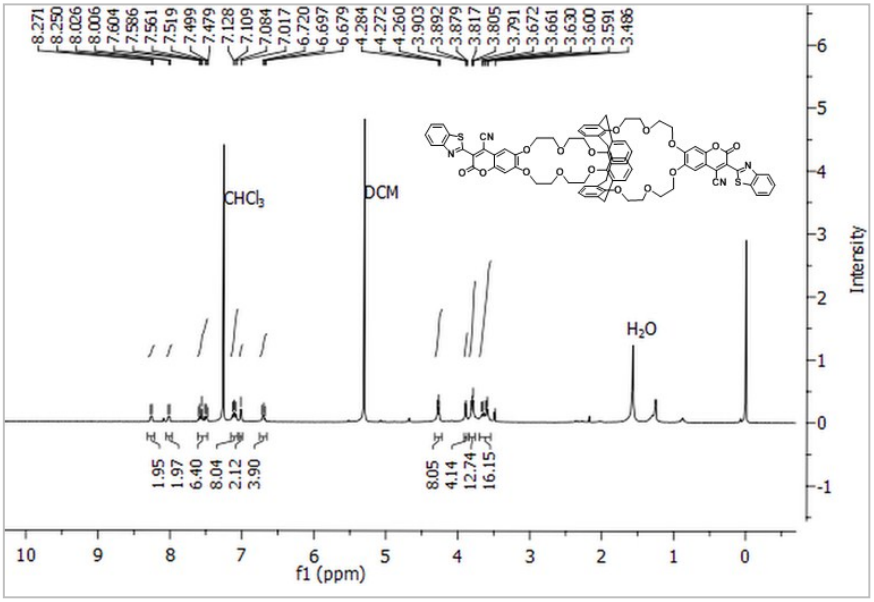

Figure S16: ^{1}H NMR Spectrum of **Calix-COU-Benz-CN** ($CDCl_3$, 400 MHz).

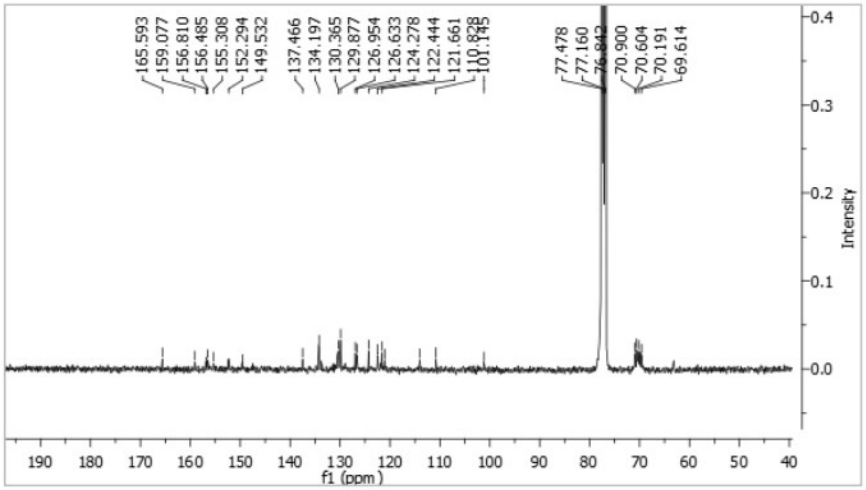

Figure S17: ^{13}C NMR Spectrum of **Calix-COU-Benz-CN** ($CDCl_3$, 100 MHz).

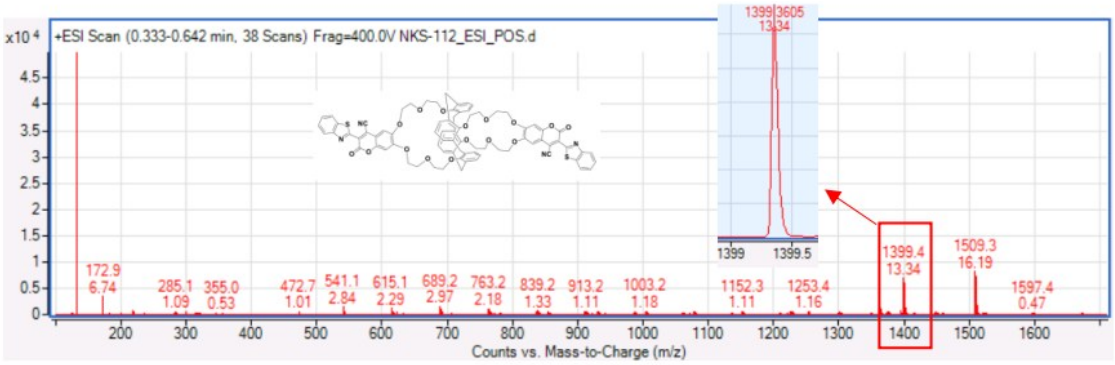

Figure S18: Mass Spectrum (HRMS: TOF MS ES+) of **Calix-COU-Benz-CN**.

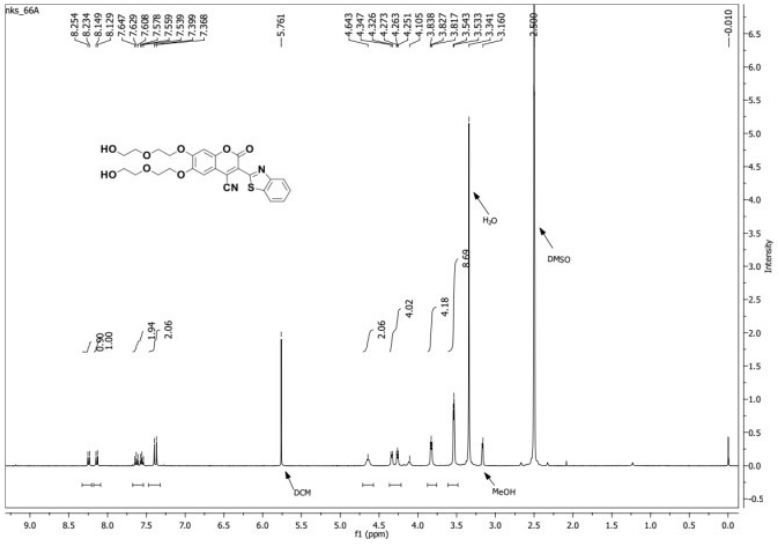

Figure S19: ^{1}H NMR Spectrum of **COU-Benz-CN** (DMSO-d_6, 400 MHz).

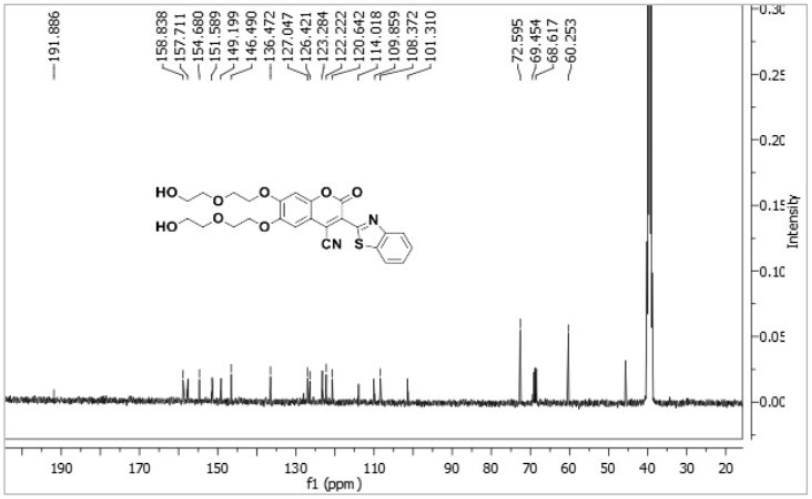

Figure S20: ^{13}C NMR spectrum of **Benz-CN** (DMSO-d_6, 100 MHz).

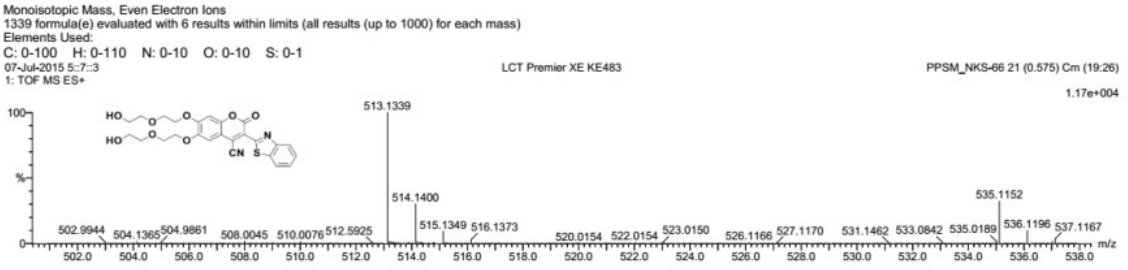

Figure S21: Mass spectrum (HRMS: TOF MS ES+) of **Benz-CN**.

Reference

(1) Korovitch, A.; Mulon, J. B.; Souchon, V.; Lion, C.; Valeur, B.; Leray, I.; Ha-Duong, N. T.; Chahine, J. *J. Phys. Chem. B* **2009**, *113*, 14247.