

Electronic Supporting Information

Calix[4]amido Crown Functionalized Visible Sensors for Cyanide and Iodide Anions

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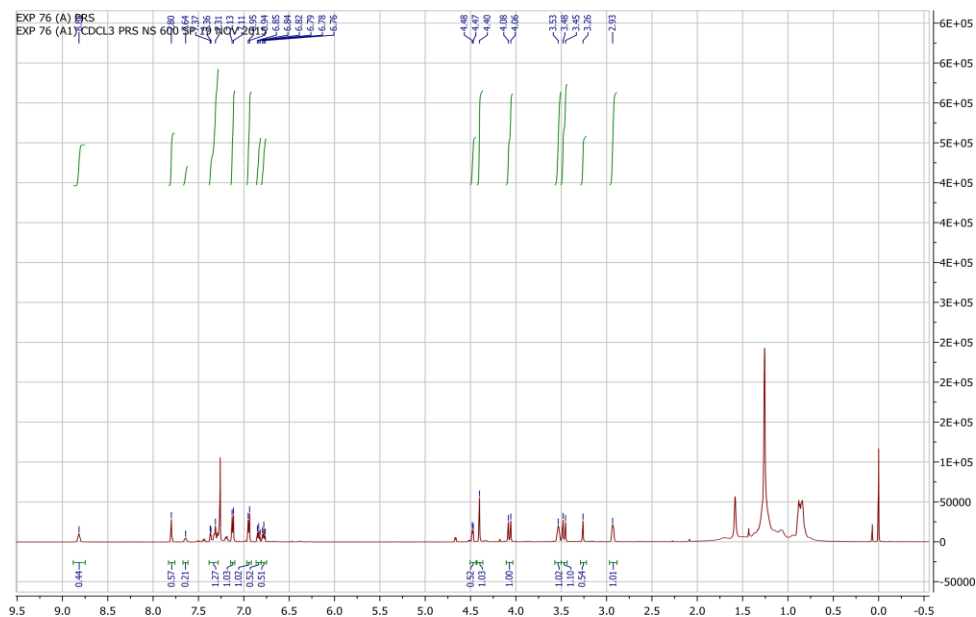


Figure S1. ¹H NMR spectrum of Ionophore I (500 MHz, CDCl₃ at 25 °C).

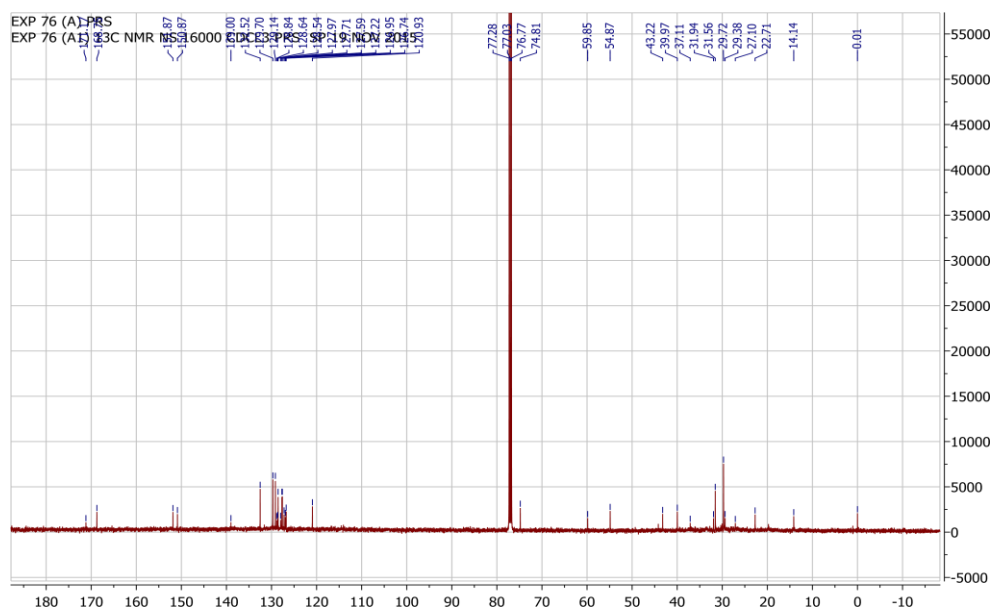


Figure S2. ¹³C NMR spectrum of Ionophore I (500 MHz, CDCl₃ at 25 °C).

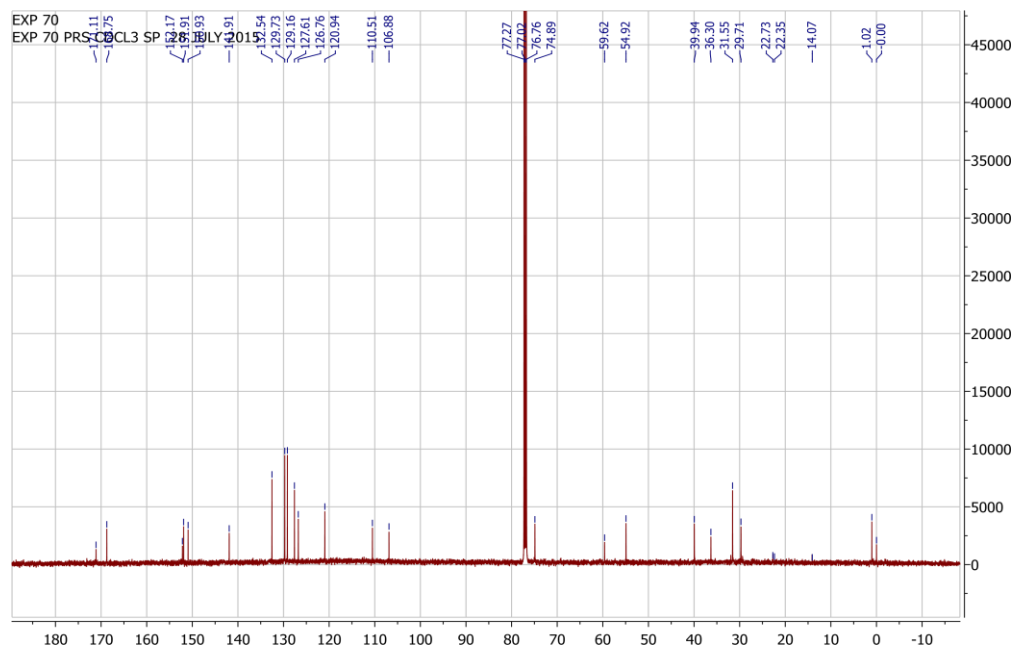


Figure S3. ^1H NMR spectrum of Ionophore II (500 MHz, CDCl_3 at 25°C).

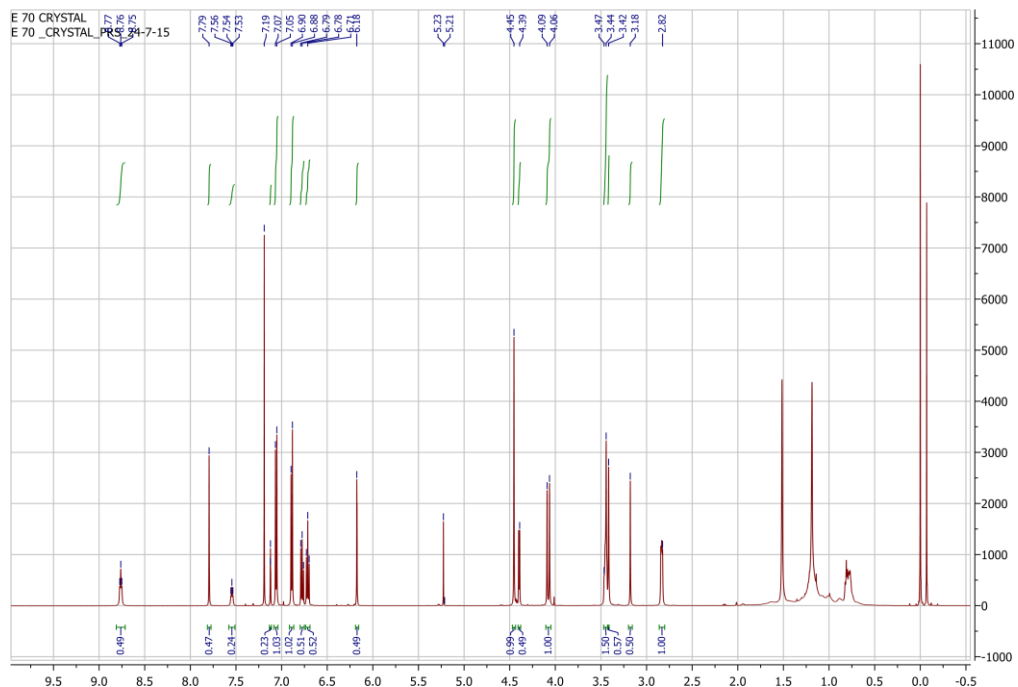


Figure S4. ^{13}C NMR spectrum of Ionophore II (500 MHz, CDCl_3 at 25°C).

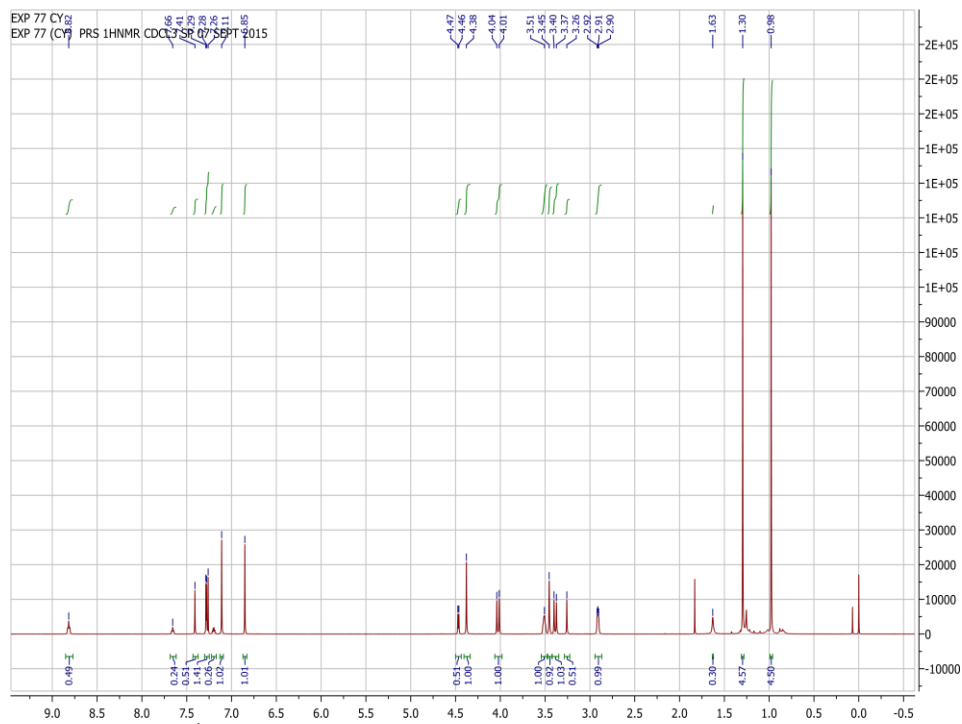


Figure S5. ¹H NMR spectrum of Ionophore III (500 MHz, CDCl₃ at 25 °C).

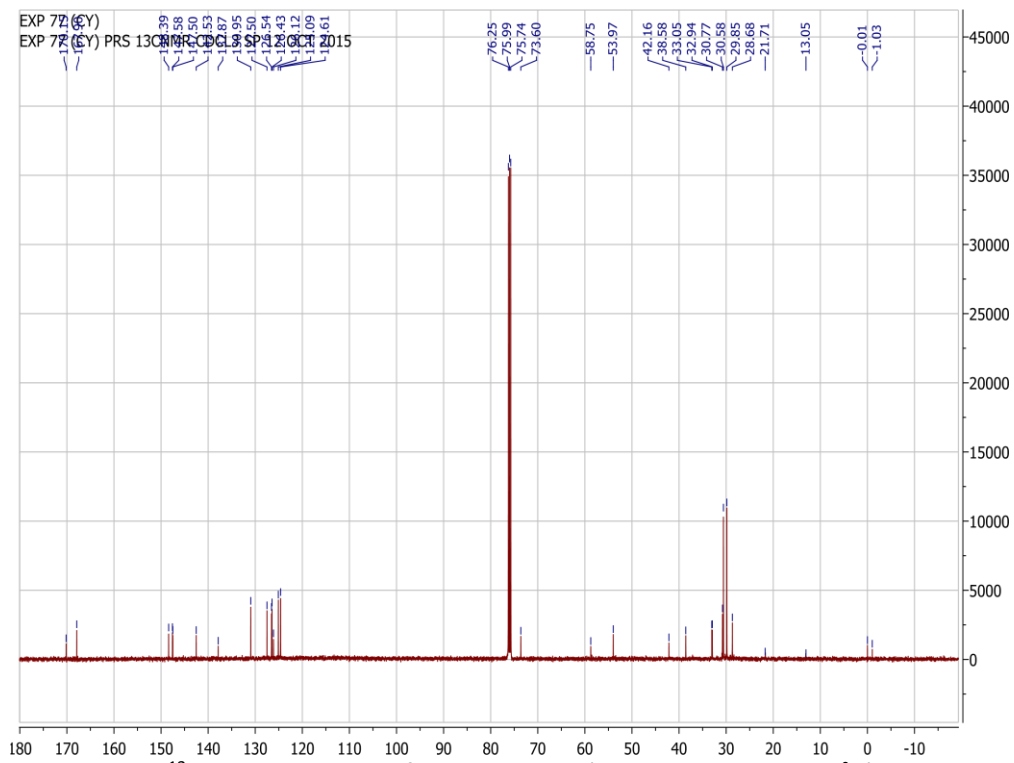


Figure S6. ¹³C NMR spectrum of Ionophore III (500 MHz, CDCl₃ at 25 °C).

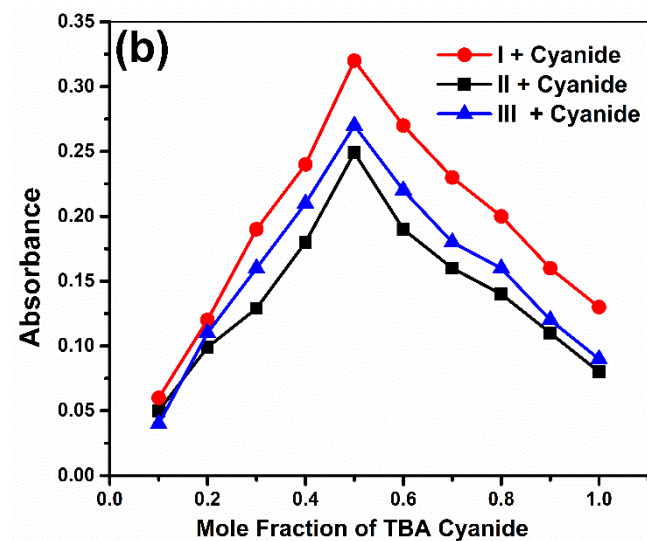
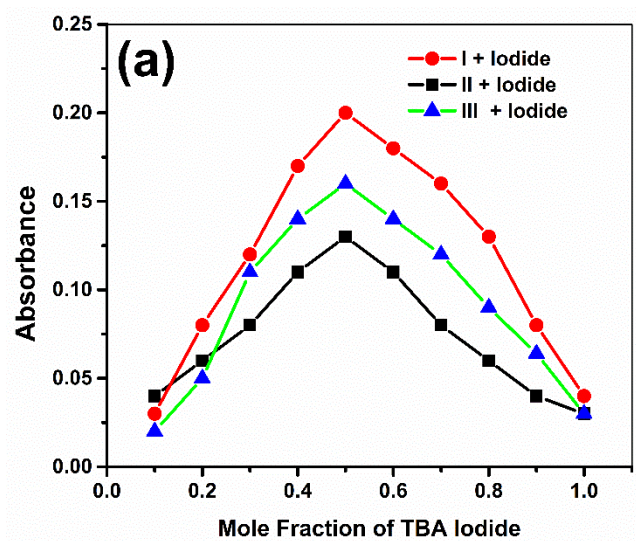


Figure S7. Showings Job's Plot for anions capture by ionophore's (a) TBA salt of iodide and (b) TBA salt of cyanide.

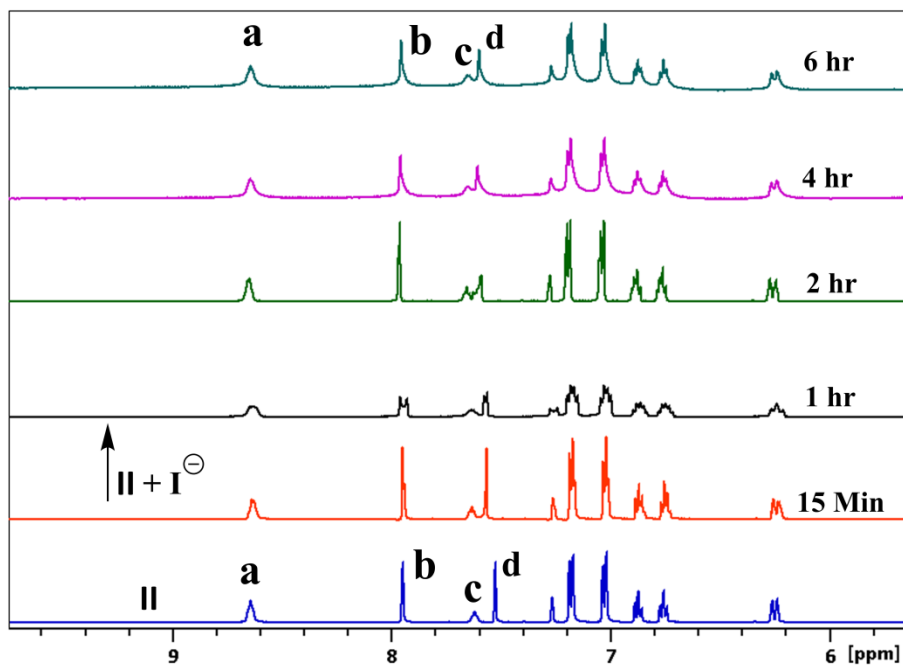


Figure S 8. A part of time-dependent ^1H NMR spectra (500 MHz) in $\text{CDCl}_3:\text{CD}_3\text{CN}$ at 25°C showing protons of lonophore II in the absence and the presence of iodide anion.

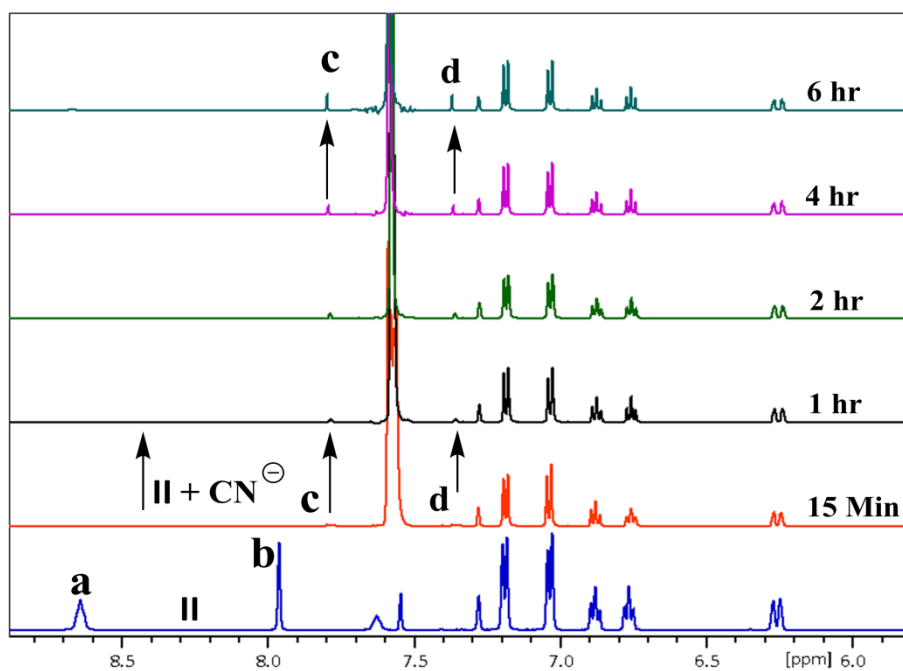


Figure S 9. A part of time-dependent ^1H NMR spectra (500 MHz) in $\text{CDCl}_3:\text{CD}_3\text{CN}$ at 25°C showing protons of lonophore II in the absence and the presence of cyanide anion.

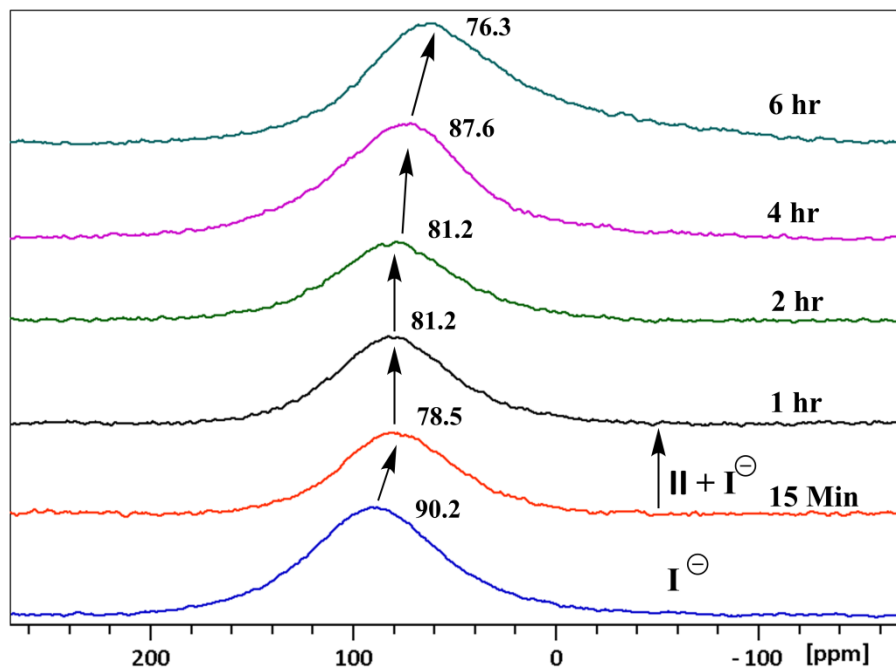


Figure S10. Time-dependent ^{127}I NMR spectra (500 MHz) in CDCl_3 : CD_3CN at 25°C showing ^{127}I peaks of Tetrabutylammonium iodide the absence, as well as in the presence, of Ionophore II.

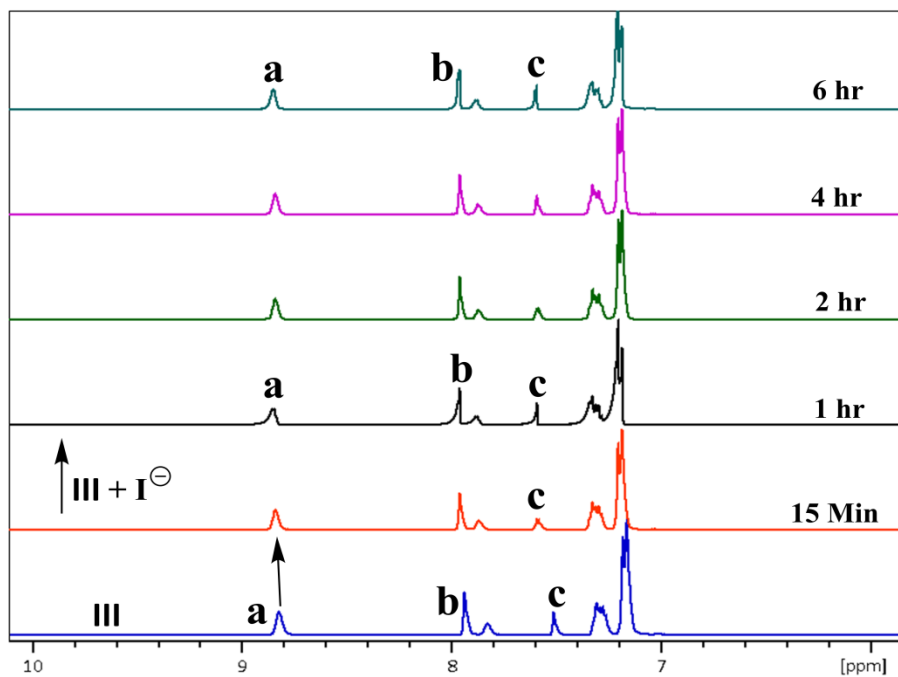


Figure S11. A part of time-dependent ^1H NMR spectra (500 MHz) in CDCl_3 : CD_3CN at 25°C showing protons of Ionophore III in the absence, as well as in the presence, of Iodide anion.

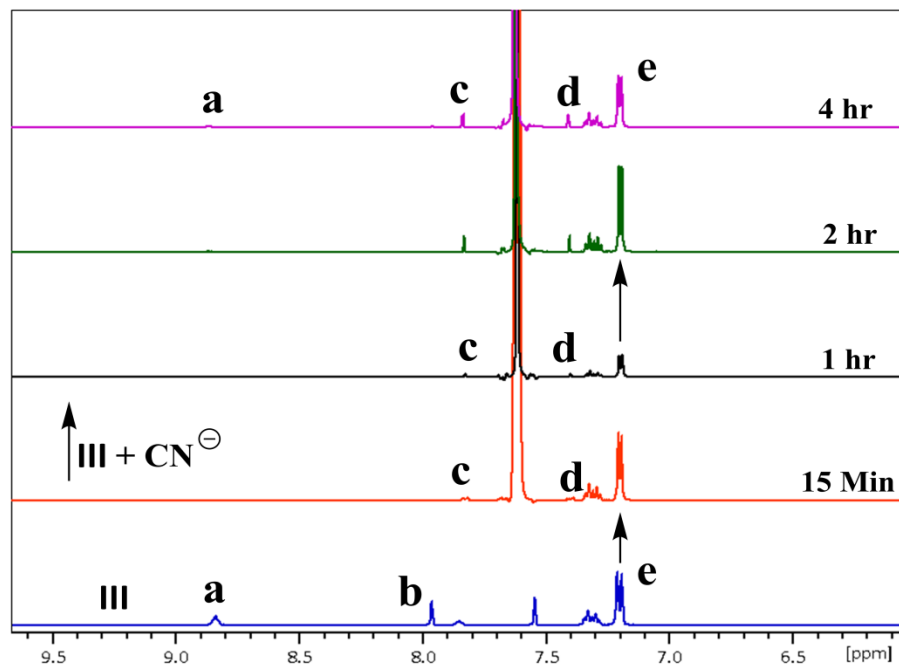


Figure S12. A part of time dependent ^1H NMR spectra (500 MHz) in CDCl_3 : CD_3CN at 25°C showing protons of lonophore III in the absence, as well as in the presence, of cyanide anion.

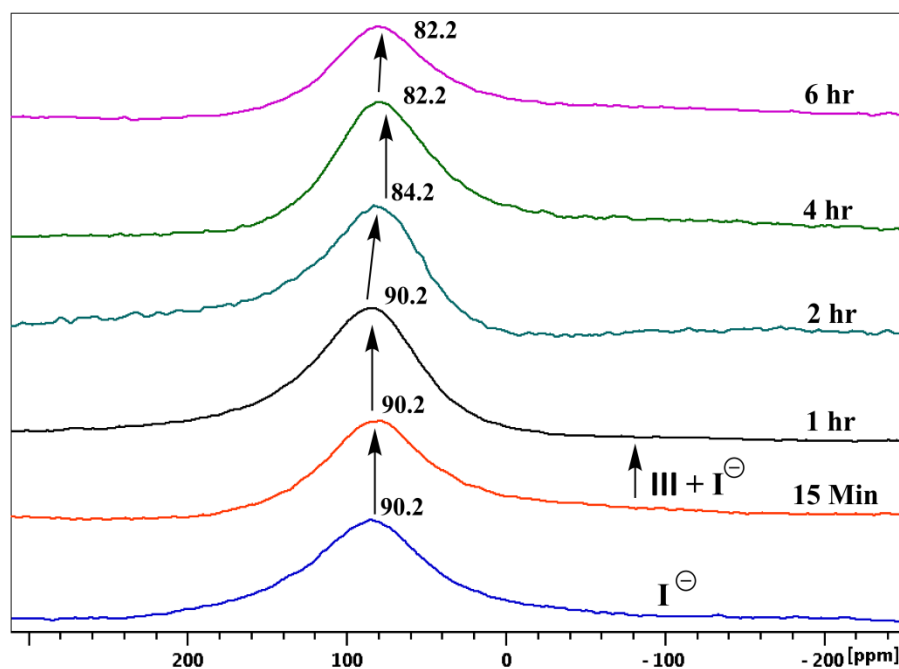


Figure S13. Time-dependent ^{127}I NMR spectra (500 MHz) in CDCl_3 : CD_3CN at 25°C showing ^{127}I peaks of Tetrabutylammonium iodide absence, as well as in the presence, of lonophore III.

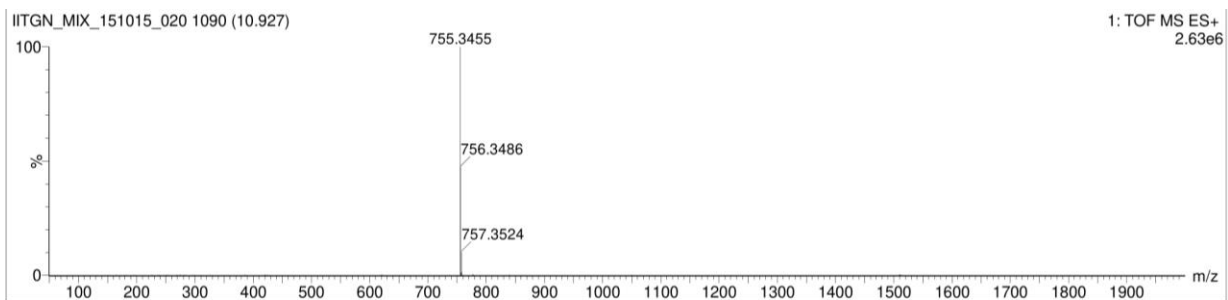


Figure S14. Mass Spectra of ionophore I.

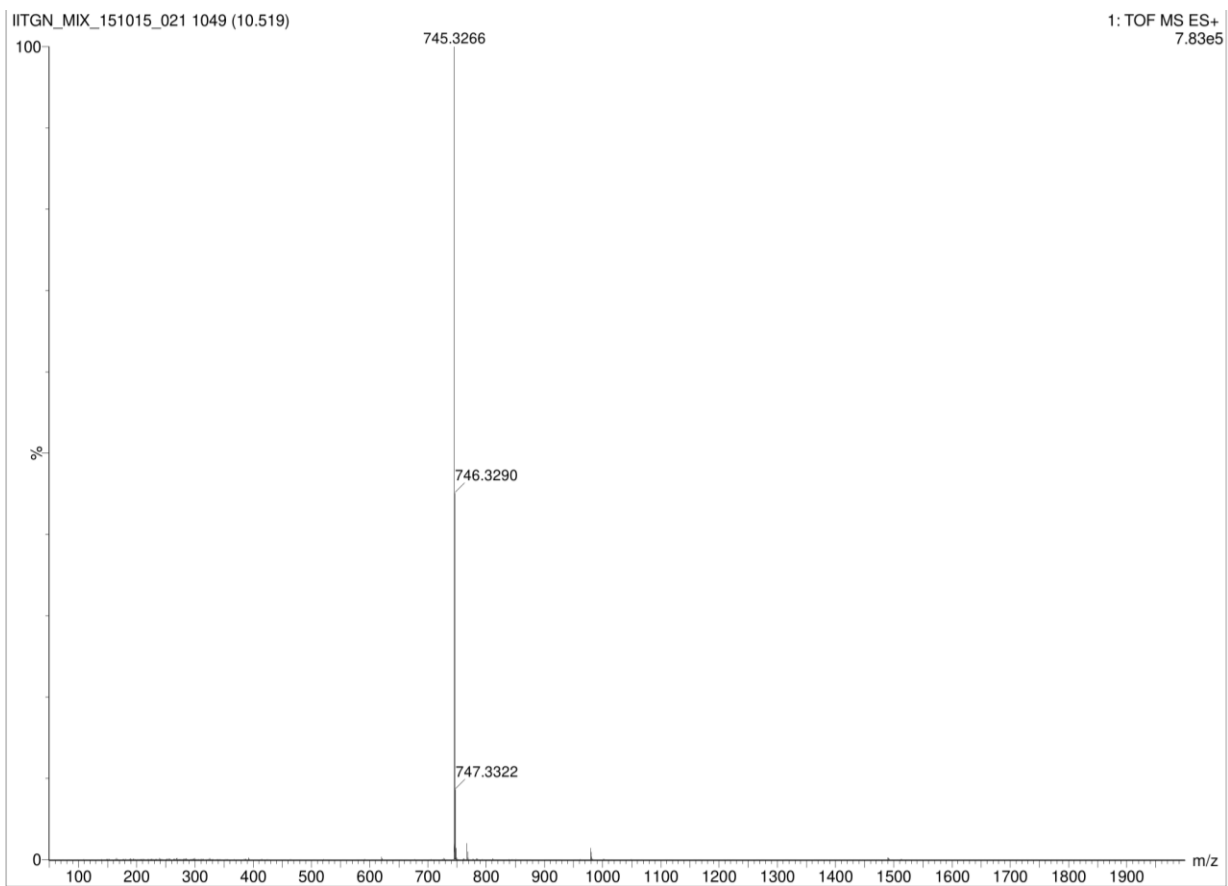


Figure S15. Mass Spectra of ionophore II.

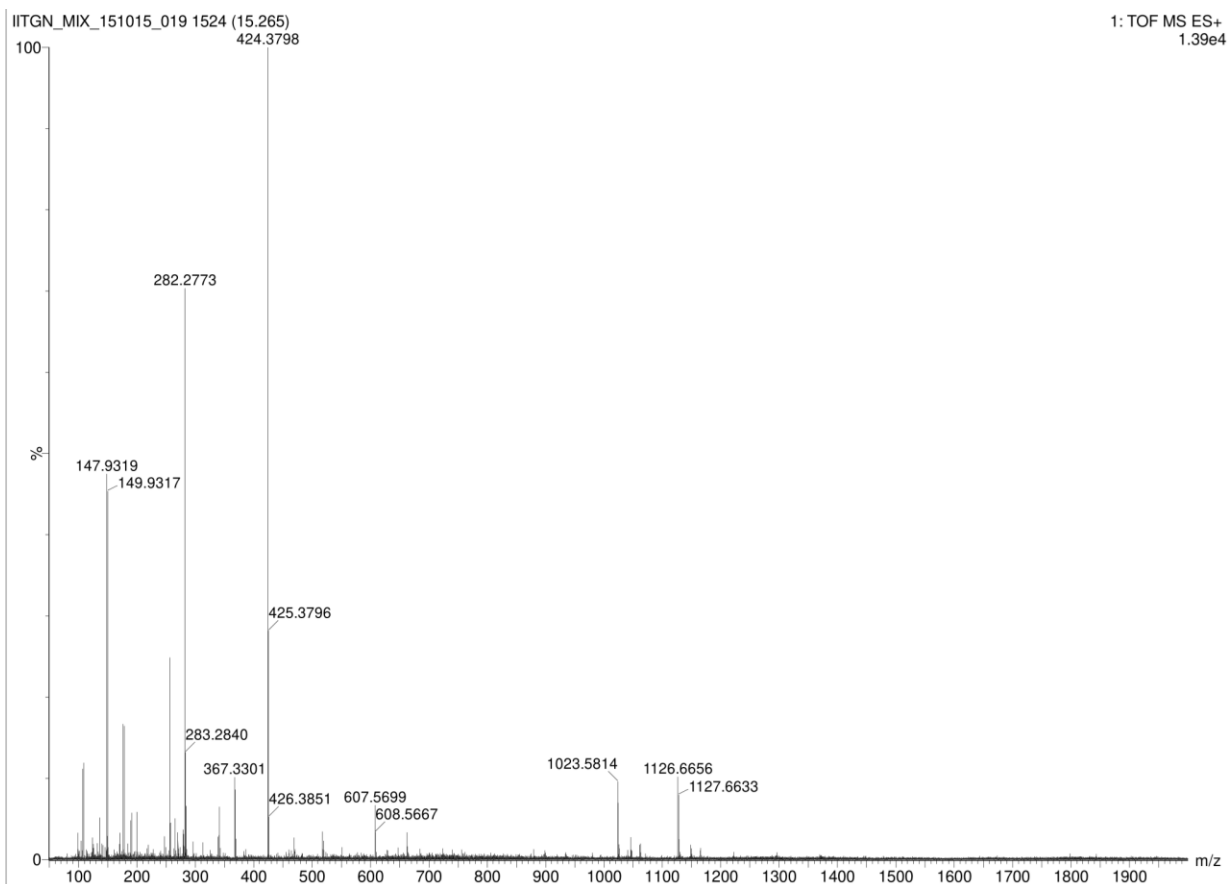


Figure S16. Mass Spectra of ionophore III

Table S1. X-ray crystal structure data of Ionophore I

Ionophore	I
Empirical Formula	$C_{46}H_{47}Cl_3N_4O_{10}$
Formula mass	922.23
Crystal color	Colorless
Crystal size	0.21x0.12x0.11
Temperature (K)	298 (2)
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	$a = 14.3406(8) \text{ \AA}$, $b = 17.5842(11) \text{ \AA}$, $c = 19.2583(11) \text{ \AA}$
Cell Angles	$\alpha = 90.00^\circ$, $\beta = 105.478(3)^\circ$, $\gamma = 90.00^\circ$

Cell Volume	4680.2(5) Å ³
Z	4
Calculated Density	1.309 g/cm ³
Abs. Coeff. (mm ⁻¹)	0.256
F(000)	1928
Reflection no. total	8217
Reflection got	5666
No. of parameter	570
S (GOF)on F2	1.925
Final R1 WR2(>21)weighted R1, WR2 (all data)	0.3244 , 0.2791
R _{all}	0.1390
CCDC Number	1506051

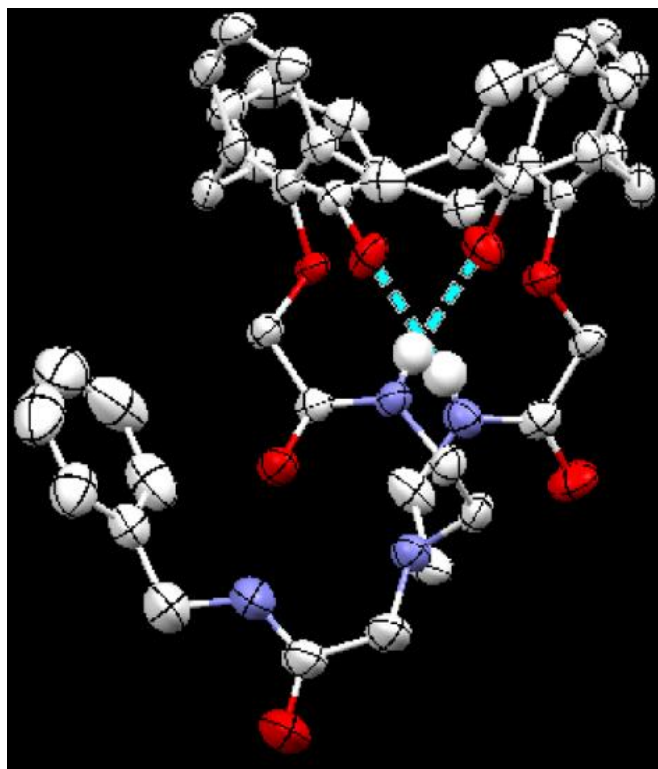


Figure S17. Single Crystal X-ray Structure of ionophore I (50% probability)

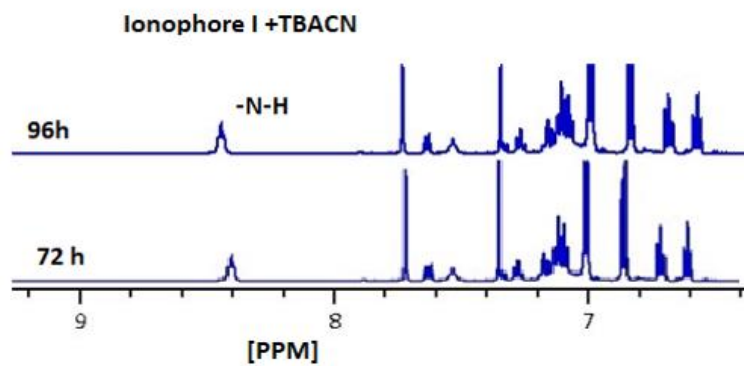


Figure S18: Time dependent NMR when color is reappearing after 72 hrs.