Supporting Information

for

NDI integrated rotaxane/catenane and their interactions with anions

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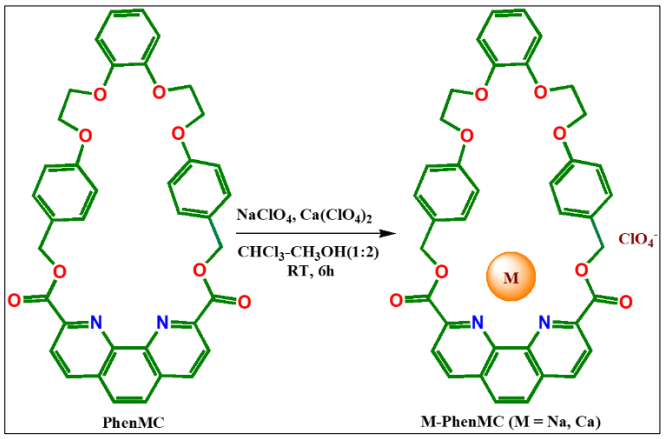
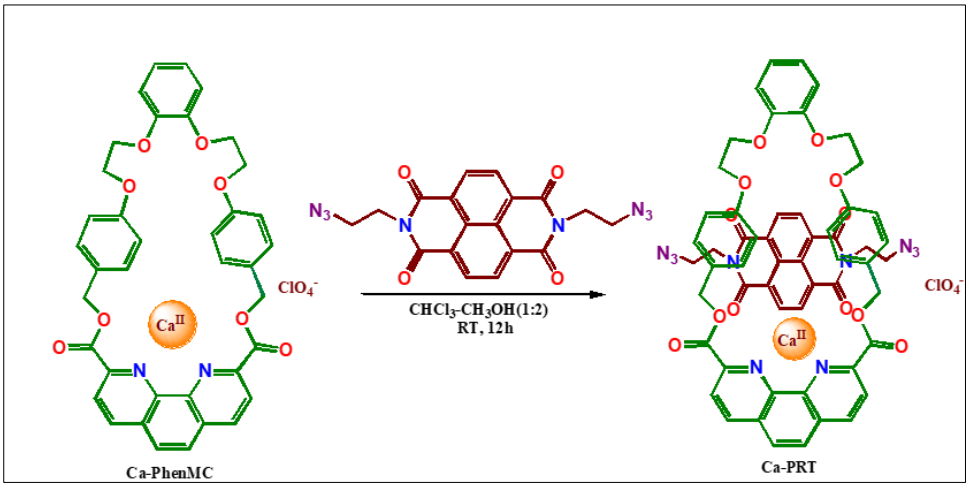
Synthetic Scheme

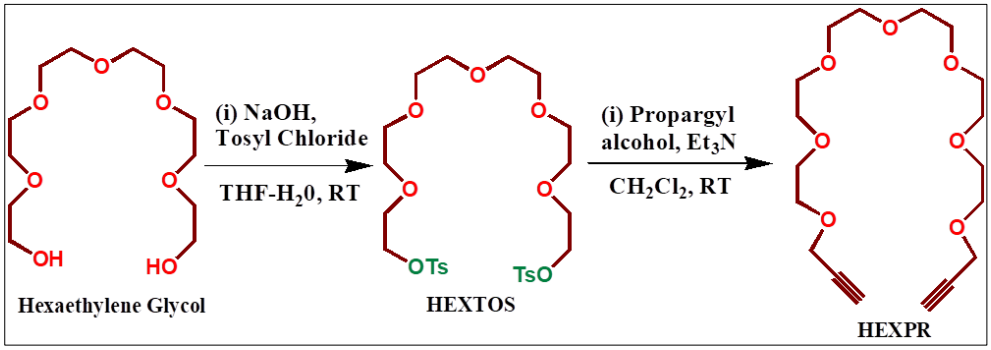
Scheme S1: Synthetic scheme of Na-**PhenMC** and Ca-**PhenMC**



Scheme S2: Synthetic scheme of Ca-**PRT**



Scheme S3: Synthetic scheme of **HEXPR**



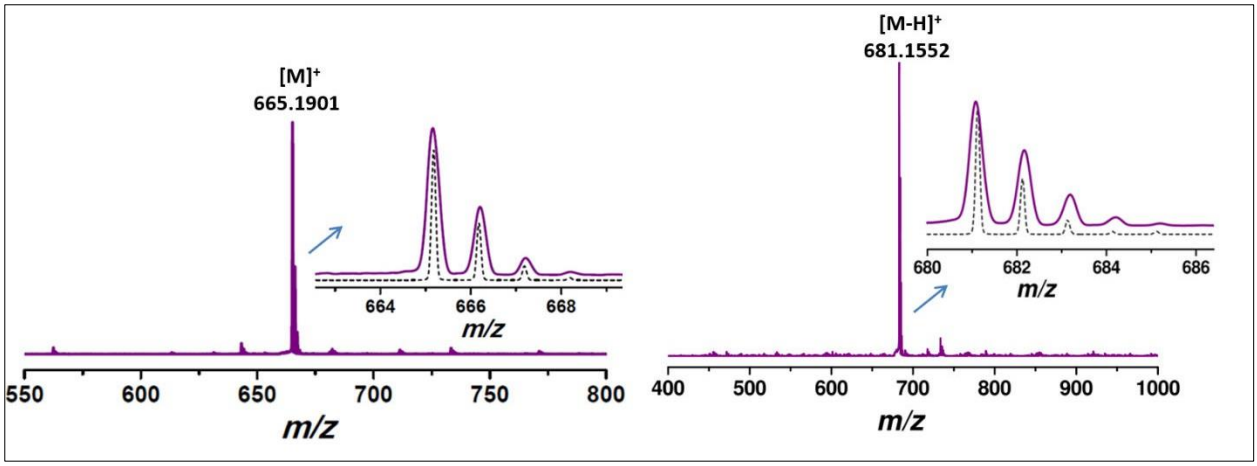


Figure S1: *ESI-MS (+ve ion) spectra of i)* ***Na-PhenMC*** *and ii)* ***Ca-PhenMC*** *at 298K. Inset picture shows the similarity between isotopic distribution pattern (dotted) and the calculated (bold) one.*

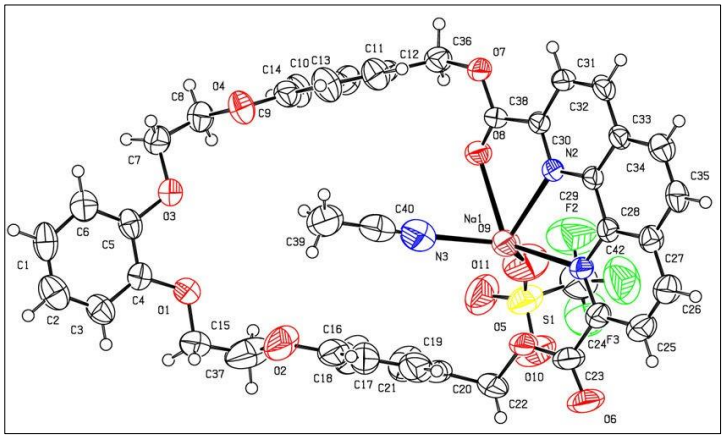


Figure S2: *Single Crystal X-ray structure of* ***Na-PhenMC*** *(ellipsoid model using platon version)*

Table S1: Crystallographic details of **Na-PhenMC**

Compound reference	PHENMCNa
Chemical formula	C41 H33 F3 N3 Na O11 S
Formula Mass	855.75
Crystal system	Triclinic
a/Å	9.632(5)
b/Å	11.523(6)
c/Å	18.177(10)
α/°	90.087(19)
β/°	93.53(2)
γ/°	94.613(17)
Unit cell volume/Å^3	2007.0(18)
Temperature/K	150(2)
Space group	$P\bar{1}$
No. of formula units per unit cell, *Z*	2
Radiation type	MoKα
Absorption coefficient, μ/mm^{-1}	0.170
No. of reflections measured	10968
No. of independent reflections	5249
R_{int}	0.0740
Final R_1 values ($I > 2\sigma(I)$)	0.0679
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1670
Final R_1 values (all data)	0.1391
Final $wR(F^2)$ values (all data)	0.2151
Goodness of fit on F^2	1.000
CCDC number	2167711

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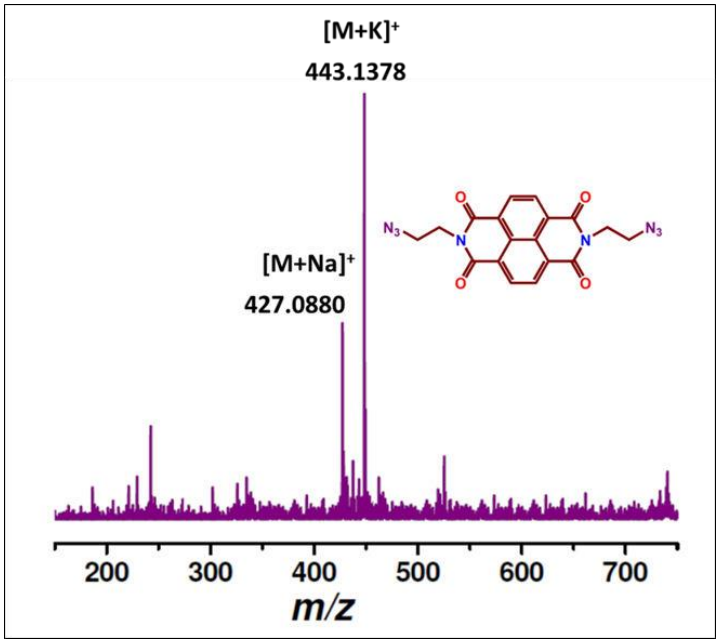

***Figure S3**. ESI-MS (+ve ion) spectrum of **NDIAz** at 298K.*

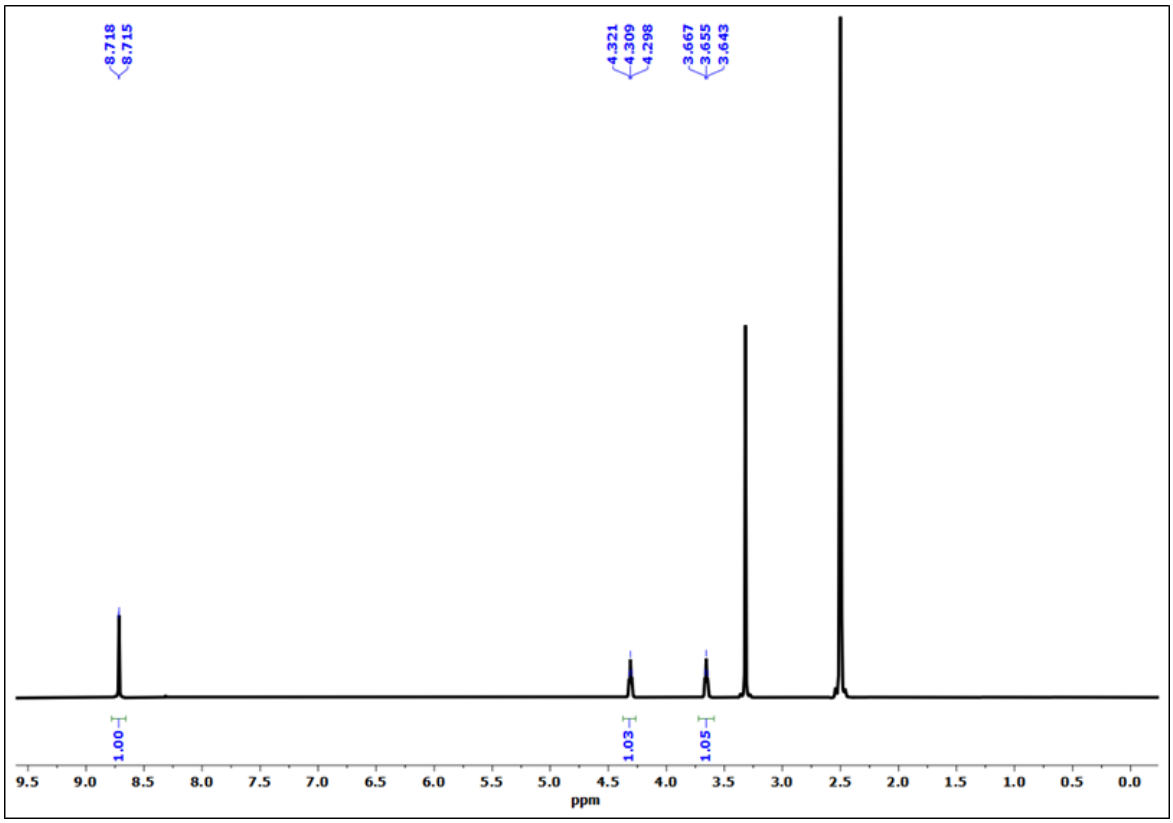

***Figure S4.** ^{1}H NMR spectrum of **NDIAz** in DMSO-d_6 (400MHz) at 298 K.*

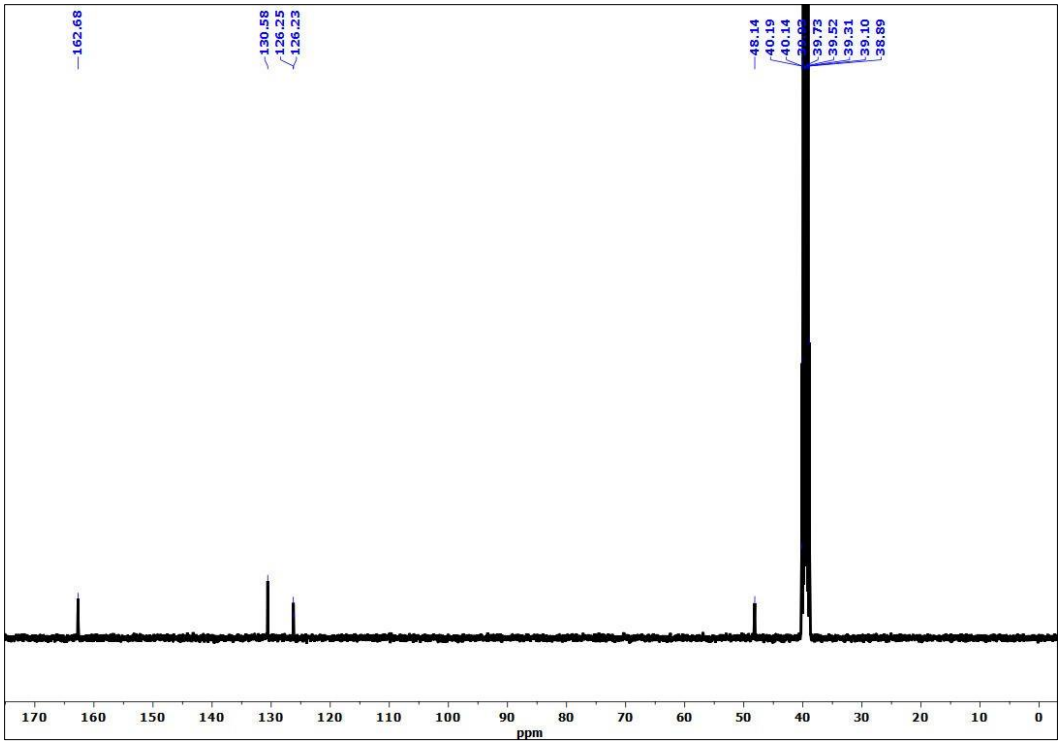

Figure S5. *^{13}C NMR spectrum of* ***NDIAz*** *in DMSO-d_6 (100MHz) at 298 K*

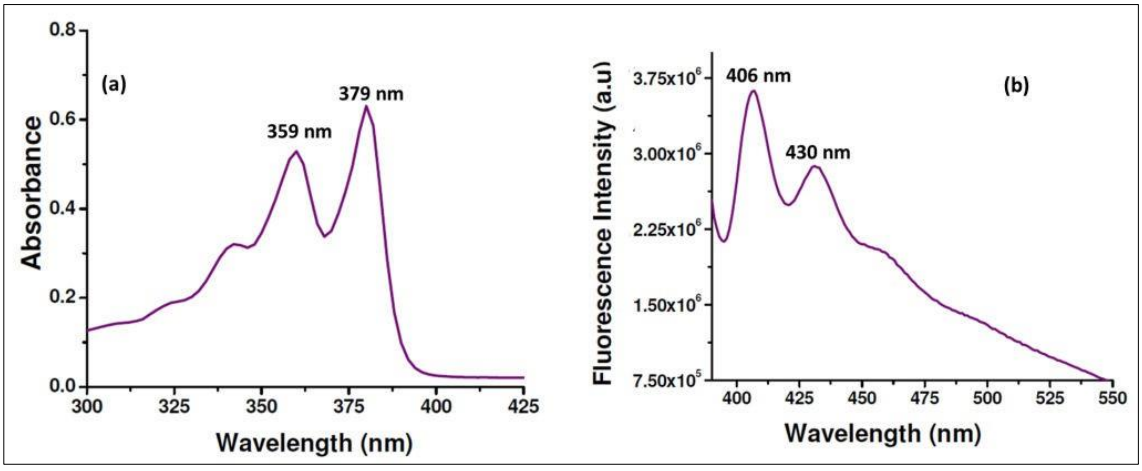

Figure S6. ***(a)*** *UV-Vis and* ***(b)*** *PL spectrum of* ***NDIAz*** *in $CHCl_3$-DMF (4:1) at 298 K.*

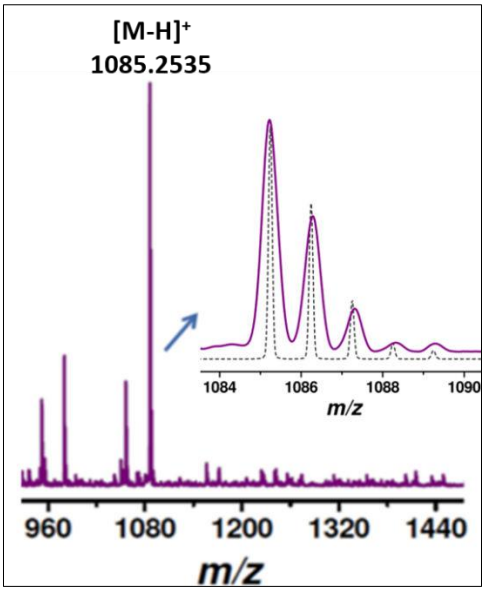

Figure S7. *ESI-MS (+ve ion) spectra of* ***Ca-PRT****. Inset picture shows the similarity between isotopic distribution pattern (dotted) and the calculated (bold) one.*

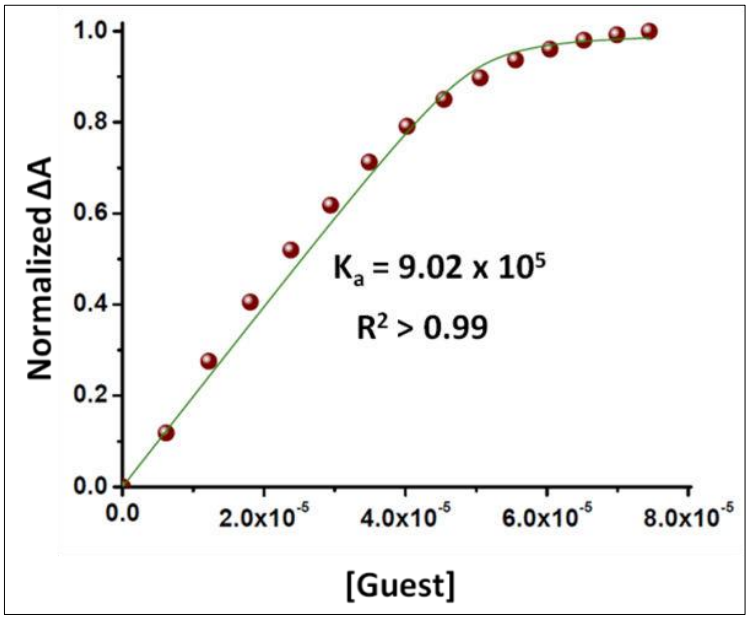

Figure S8. *Non-linear 1:1 curve fitting plot from UV titration experiment to determine binding constant for the formation of* ***NDIAz*** *($2X10^{-5}$M) and* ***Ca-PhenMC*** *($2X10^{-4}$M) in $CHCl_3$- DMF (4:1) at 298 K.*

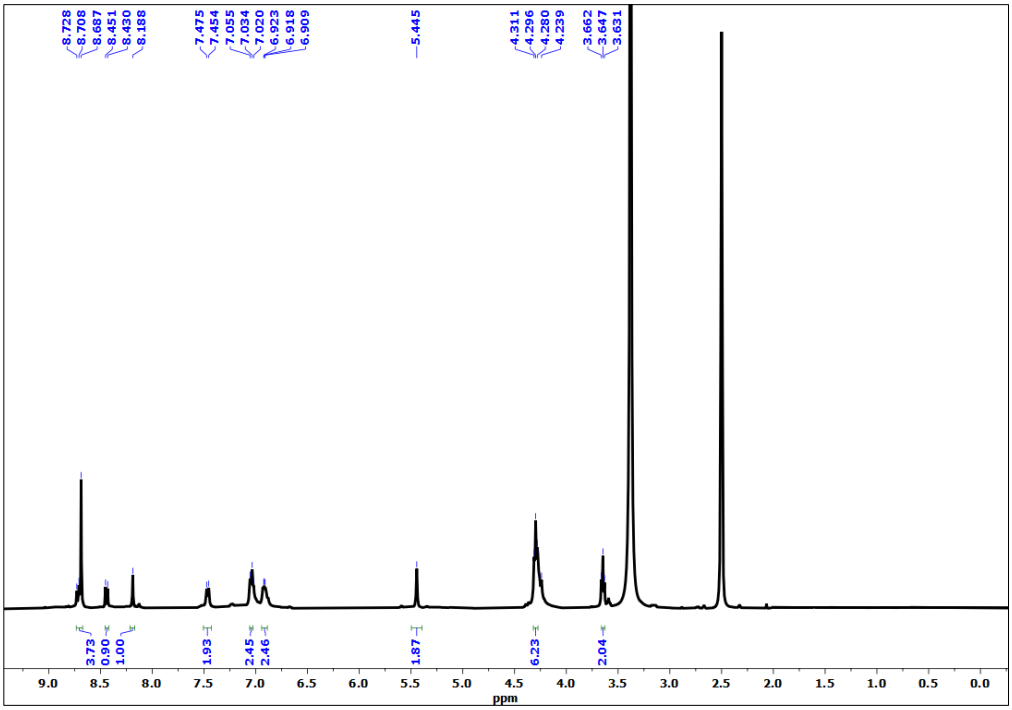

Figure S9. *^{1}H NMR spectrum of Ca-**PRT** in DMSO-d_6 (400MHz) at 298 K.*

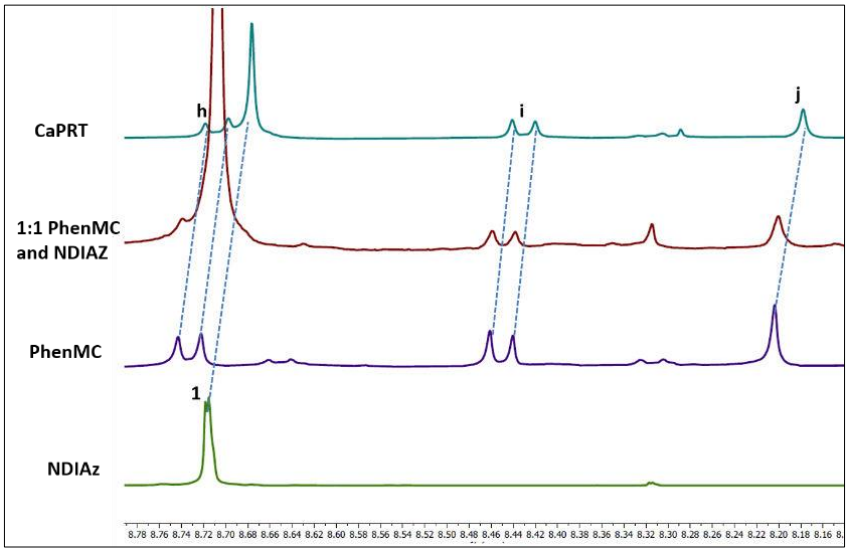

Figure S9a. *Comparative ^{1}H NMR of Ca-PRT, 1:1 PhenMC-NDIAz, PhenMC and NDIAz in DMSO-d_6 (400 MHz) at 298 K.*

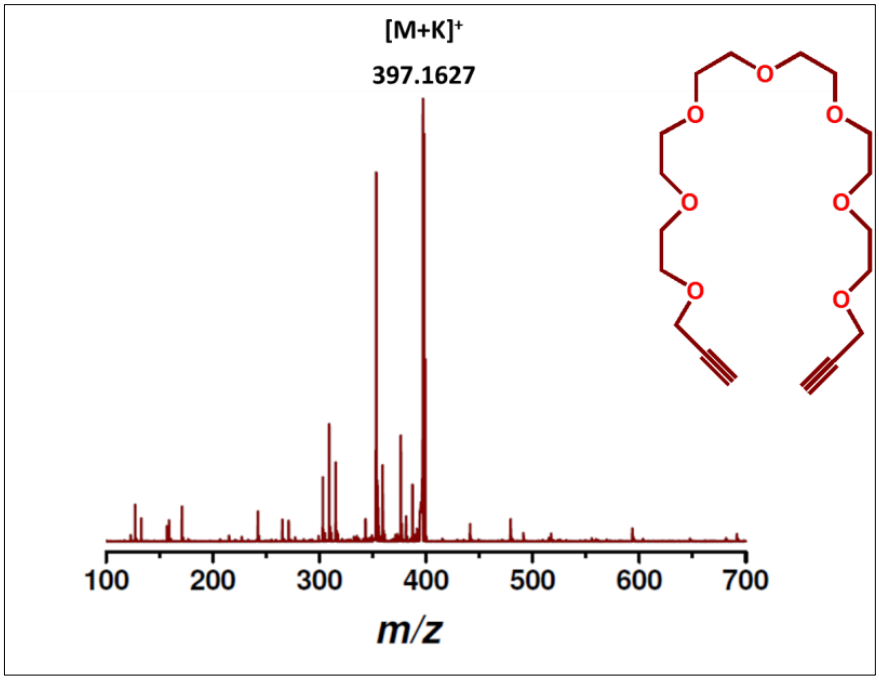

Figure S10. *ESI-MS (+ve ion) spectrum of* ***HEXPR.***

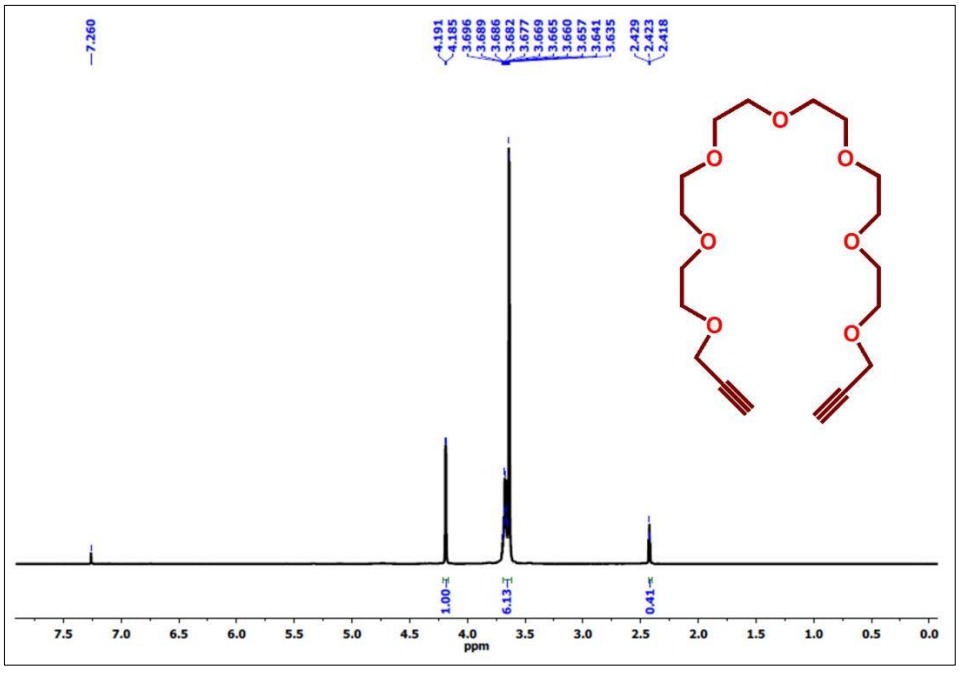

Figure S11. *^{1}H NMR spectrum of* ***HEXPR*** *in $CDCl_3$ (400MHz) at 298 K*

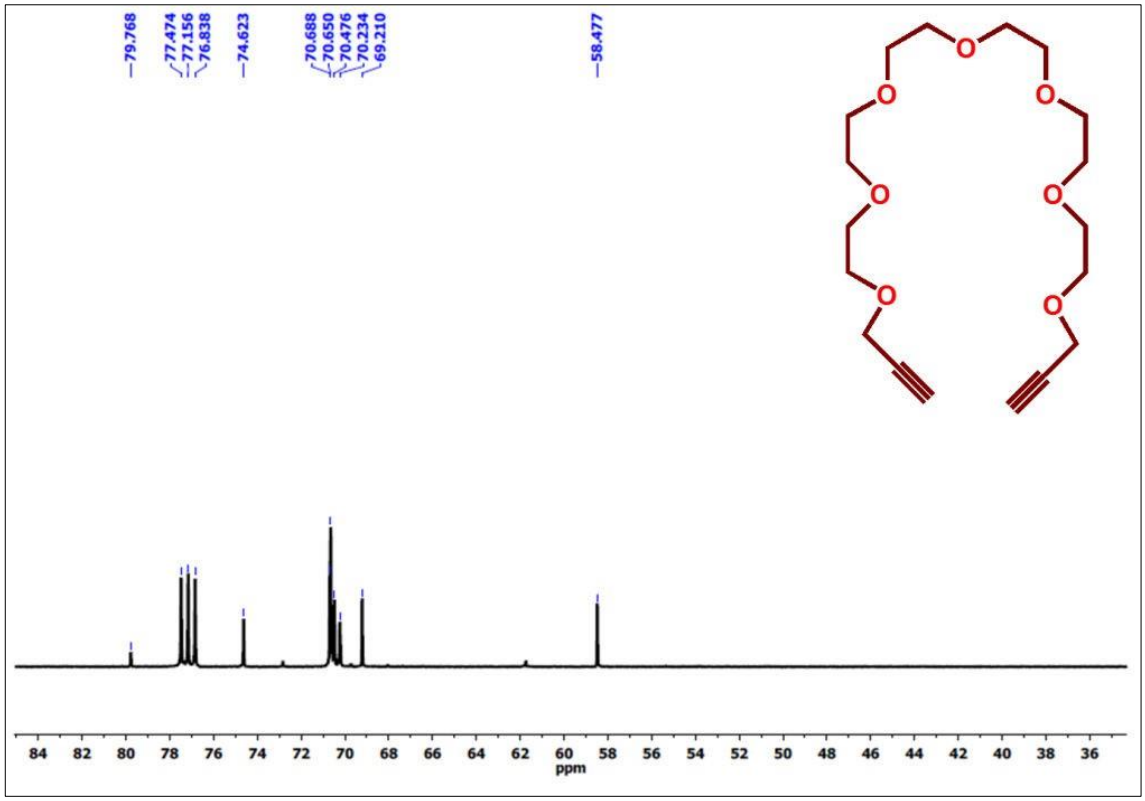

Figure S12. *^{13}C NMR spectrum of **HEXPR** in $CDCl_3$ (100MHz) at 298 K*

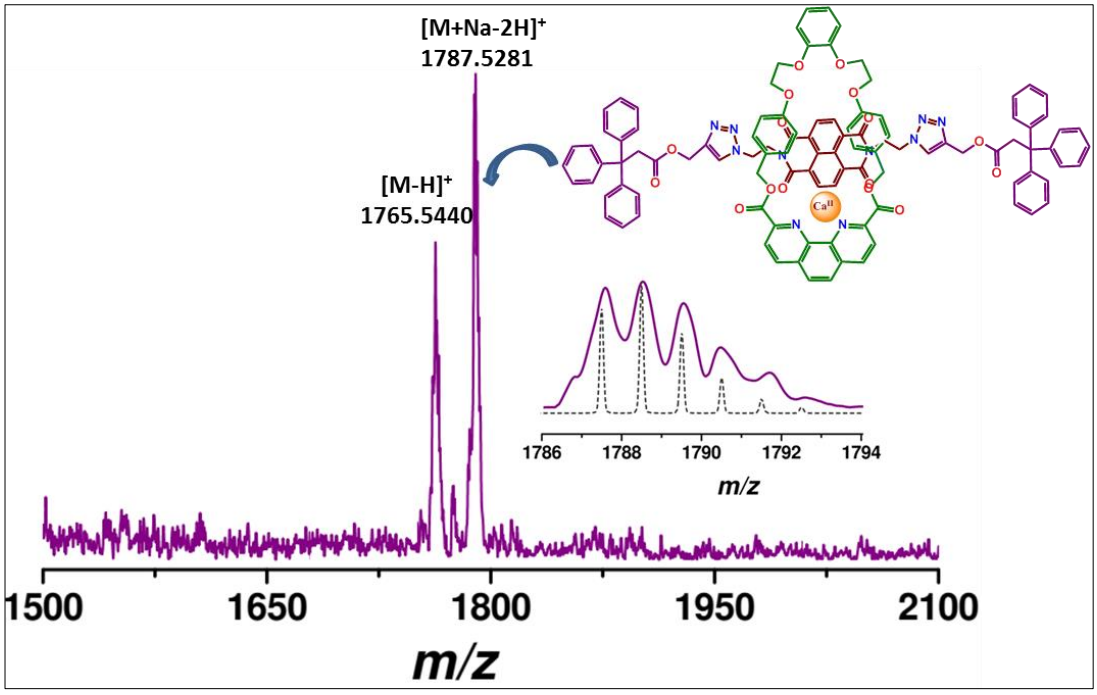

Figure S13. *ESI-MS (+ve ion) spectrum of Ca-**NDIROT***

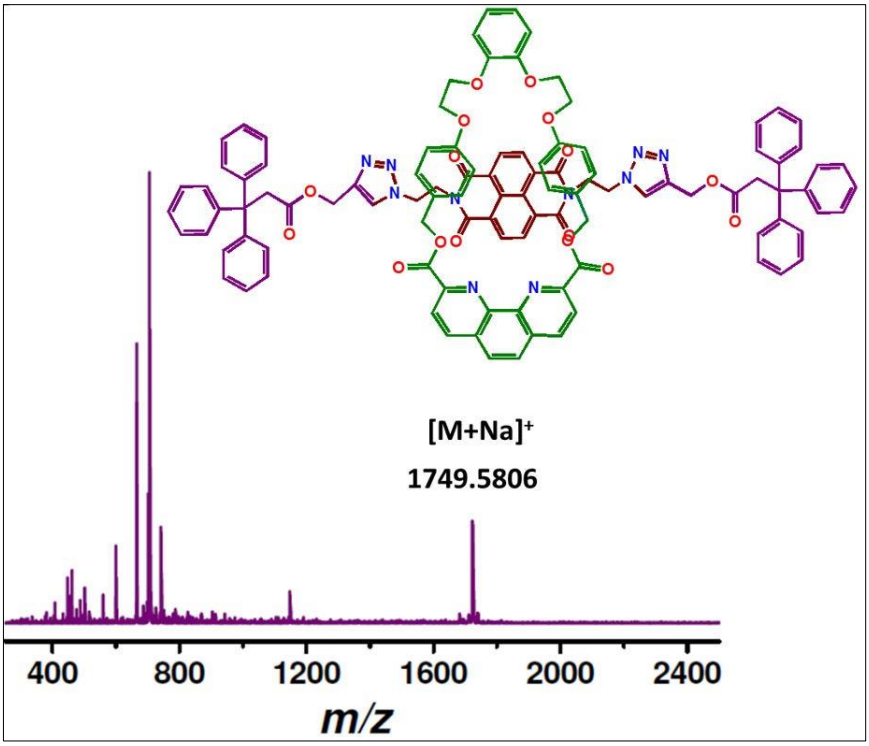

Figure S14. *ESI-MS (+ve ion) spectrum of* ***NDIROT***

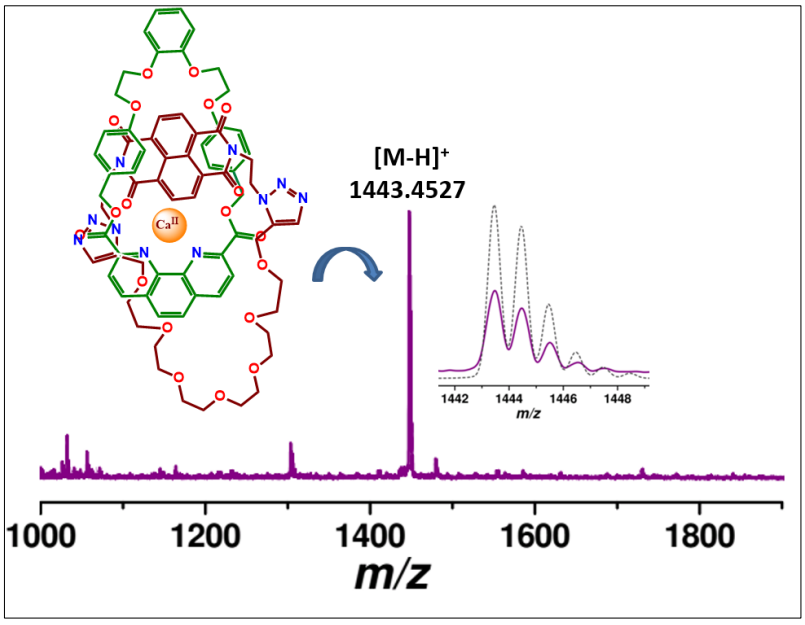

Figure S15. *ESI-MS (+ve ion) spectrum of Ca-* ***NDICAT***

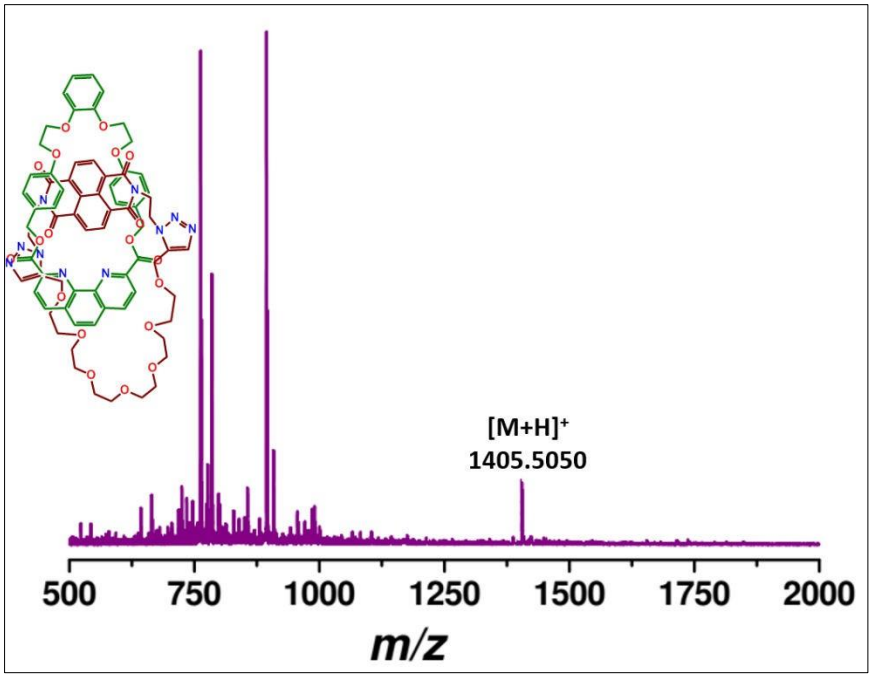

Figure S16. *ESI-MS (+ve ion) spectrum of* ***NDICAT***

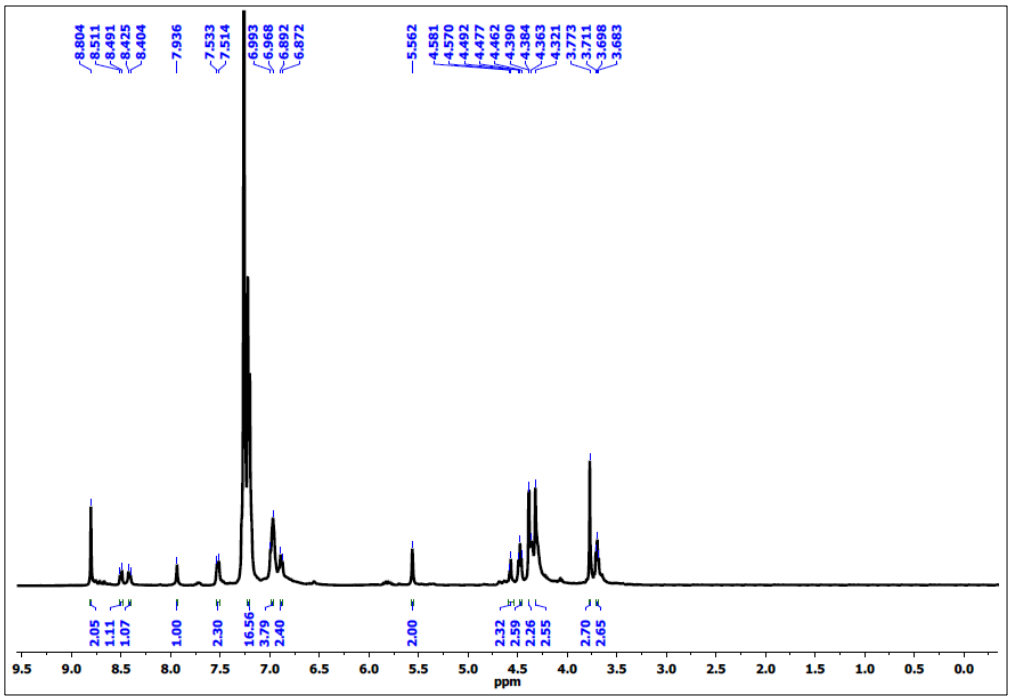

Figure S17. *^{1}H NMR spectrum of* ***NDIROT*** *in $CDCl_3$ (400MHz) at 298 K*

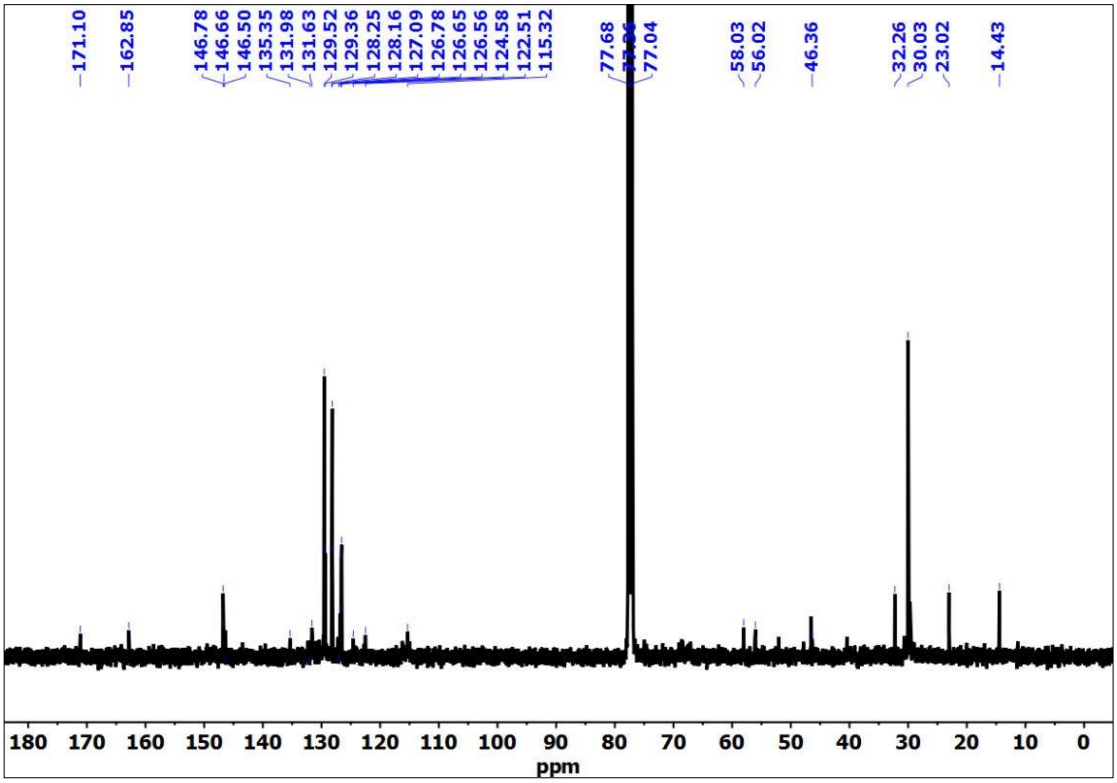

Figure S18. *^{13}C NMR spectrum of **NDIROT** in $CDCl_3$ (100MHz) at 298 K*

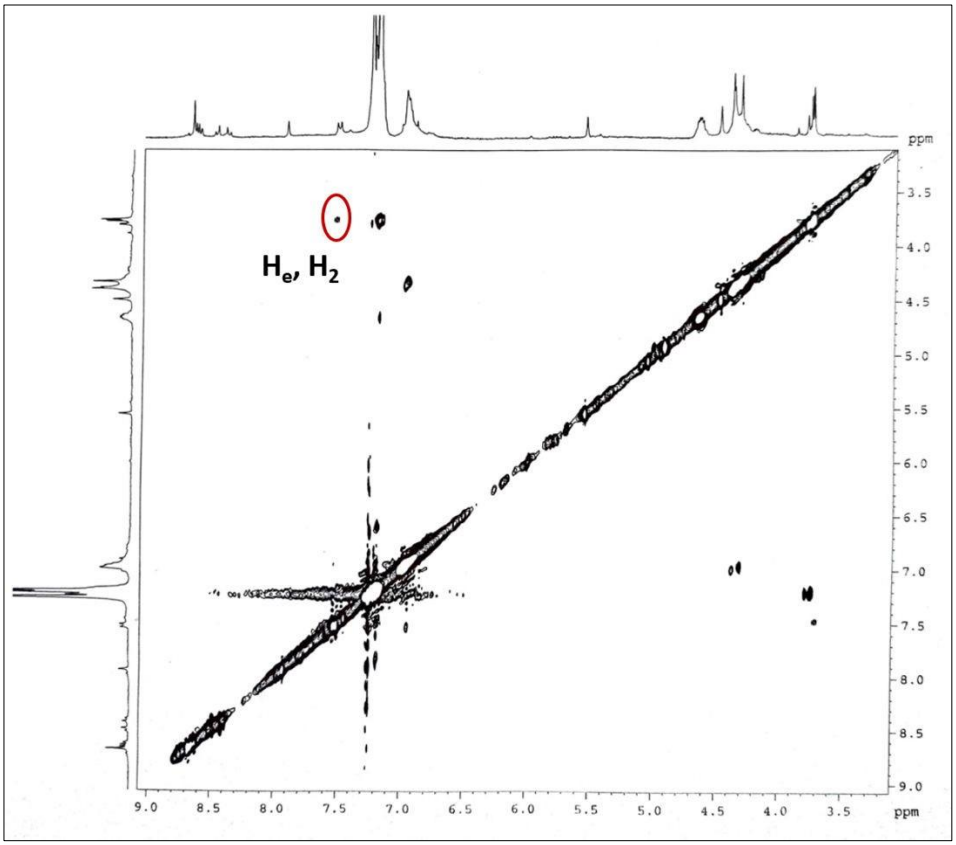

Figure S18a. *ROESY spectrum of **NDIROT** in $CDCl_3$ (300MHz) at 298 K*

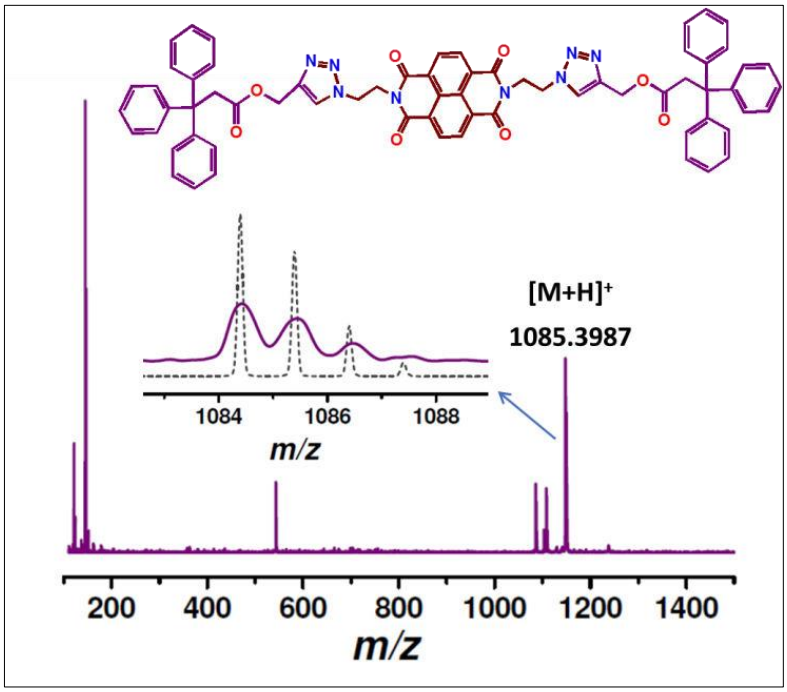

Figure S19. *ESI-MS (+ve ion) spectrum of* **NDI-AXSTP**

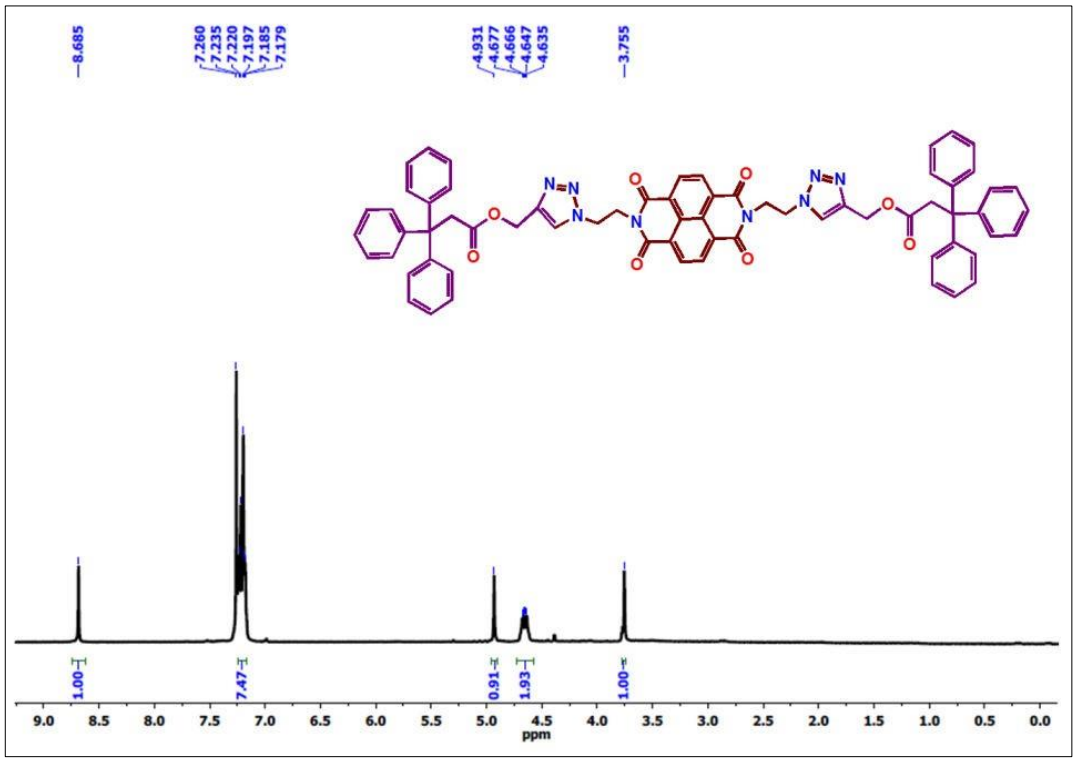

Figure S20. *^{1}H NMR spectrum of* **NDI-AXSTP** *in $CDCl_3$ (400MHz) at 298 K*

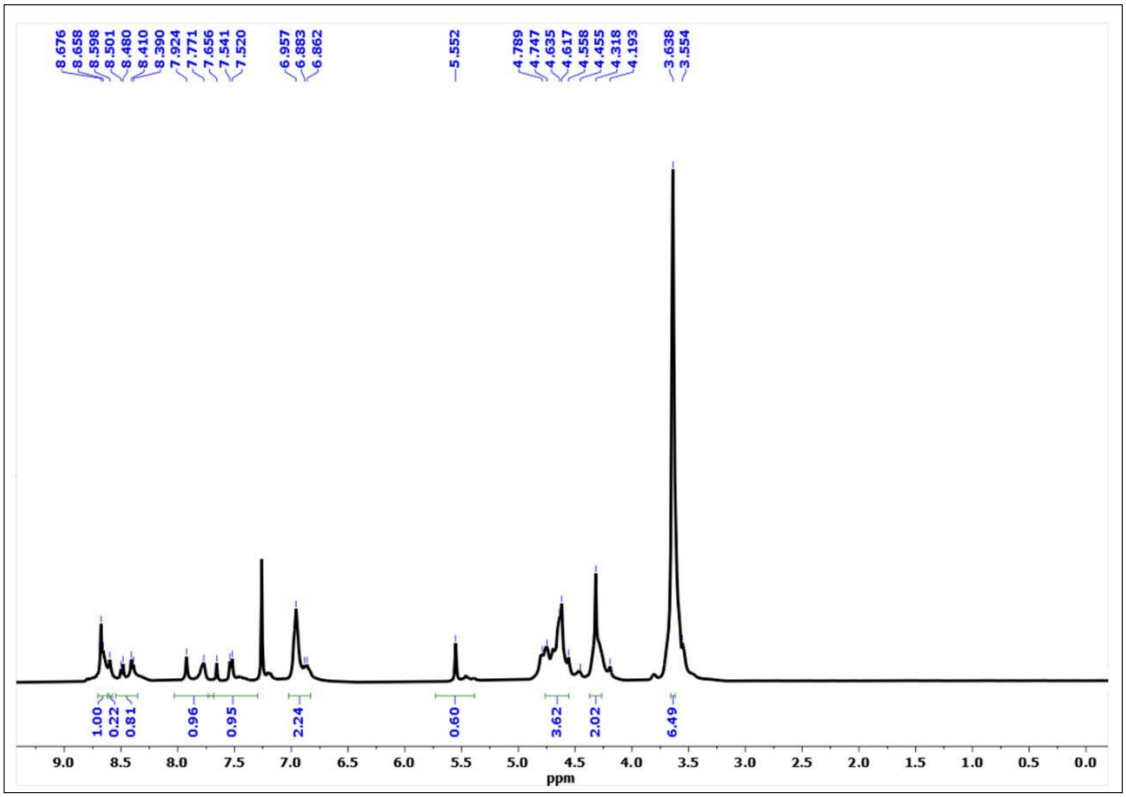

Figure S21. *^{1}H NMR spectrum of* ***NDICAT*** *in $CDCl_3$ (400MHz) at 298 K*

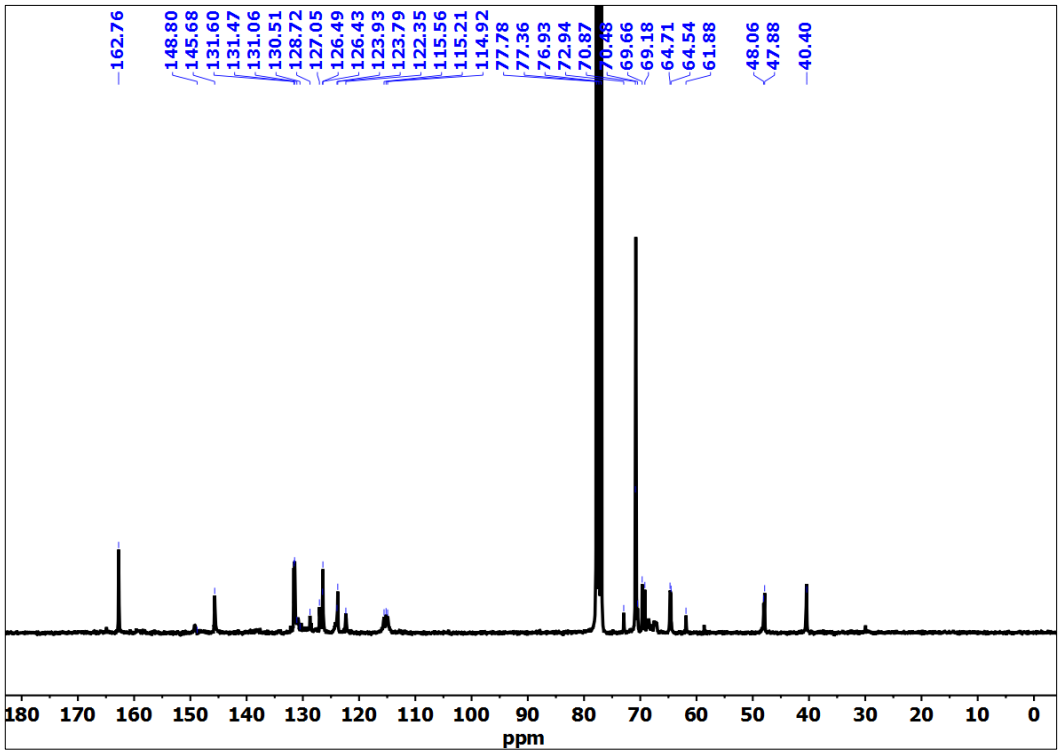

Figure S22. *^{13}C NMR spectrum of* ***NDICAT*** *in $CDCl_3$ (75MHz) at 298 K*

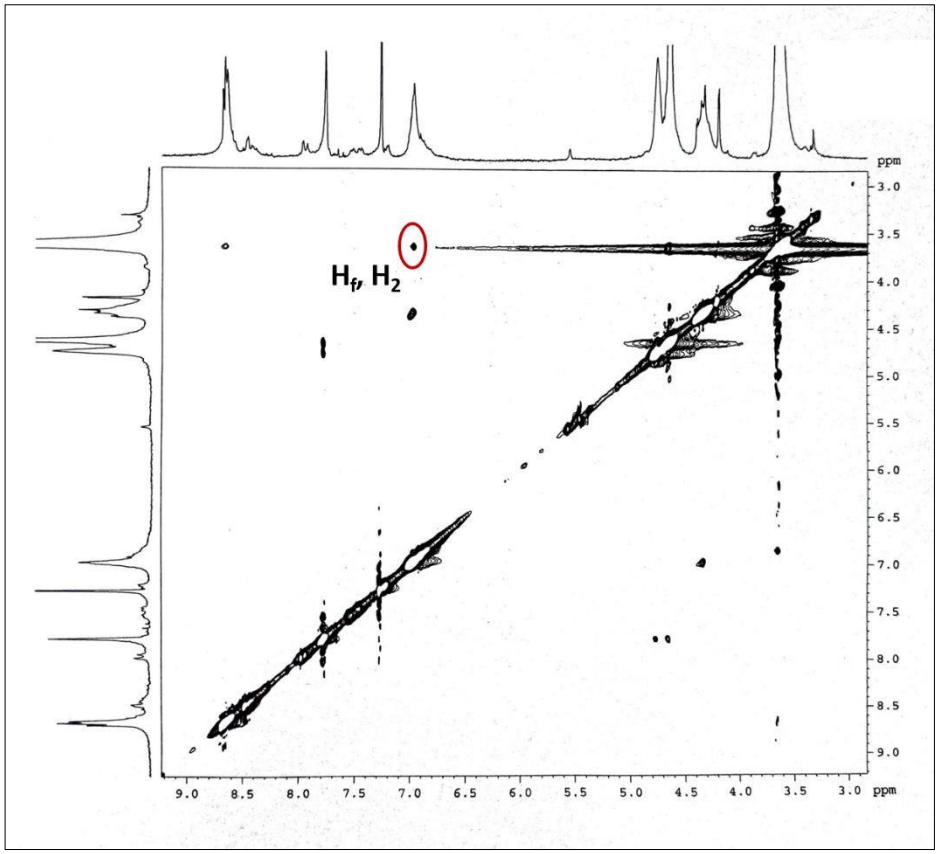

Figure S22a. *ROESY spectrum of* ***NDICAT*** *in* $CDCl_3$ *(300MHz) at 298 K*

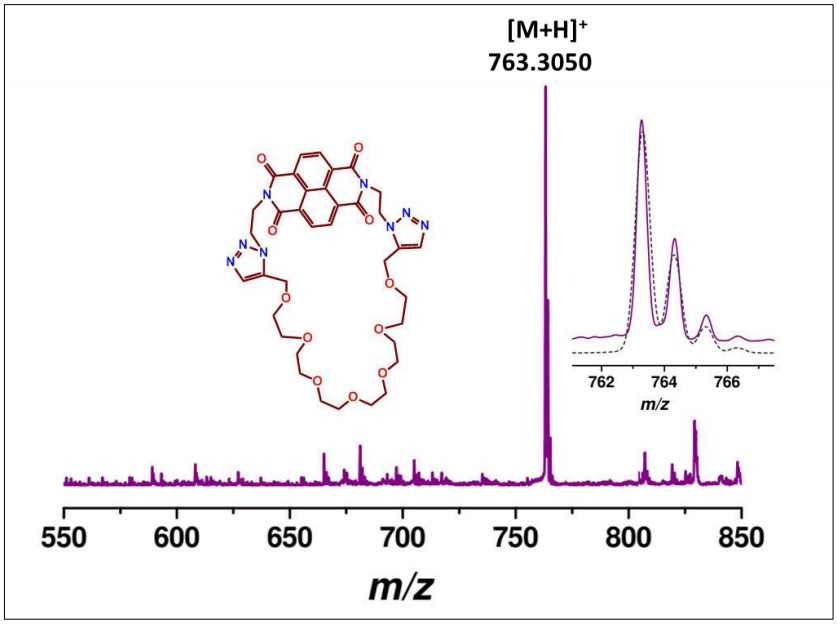

Figure S23. *ESI-MS (+ve ion) spectrum of* ***NDIMC.***

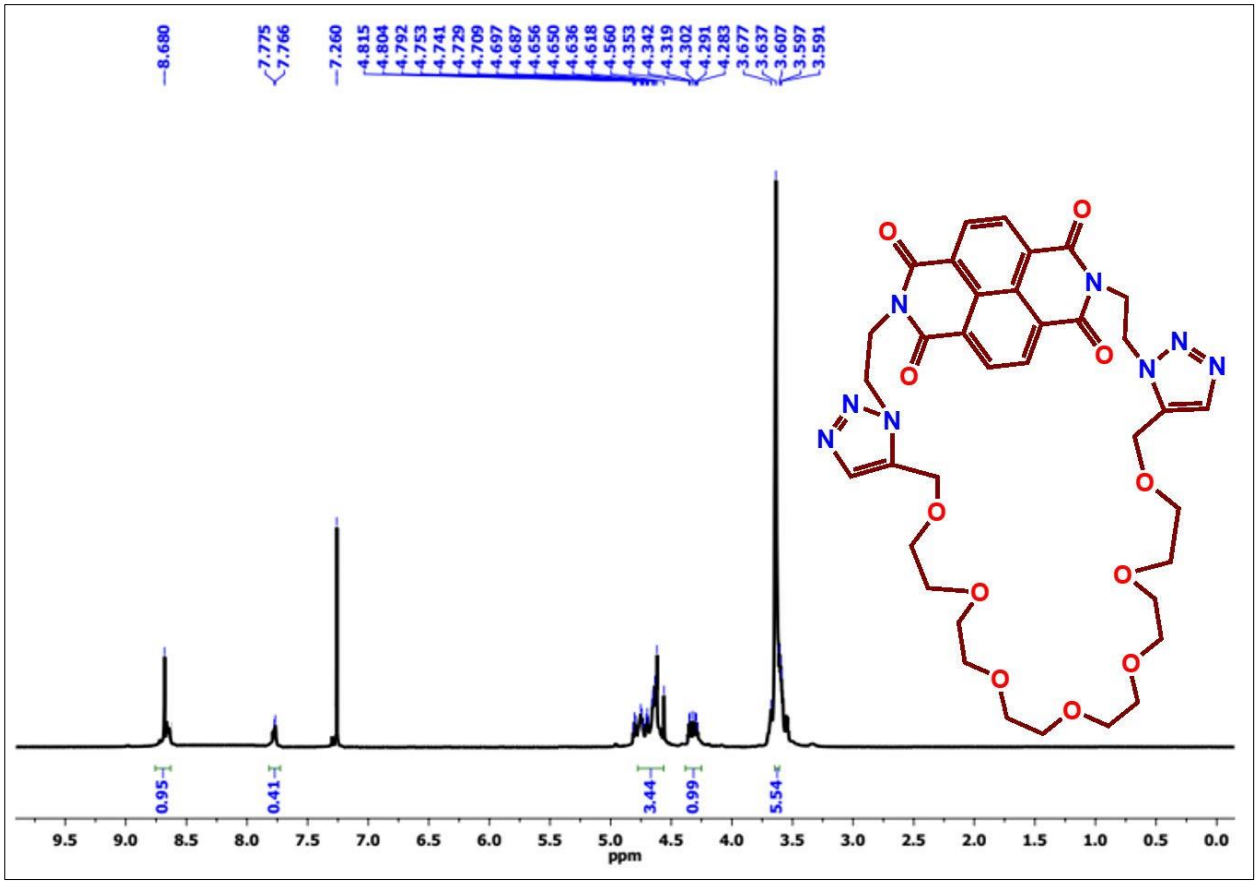

Figure S24. *^{1}H NMR spectrum of **NDIMC** in $CDCl_3$ (400MHz) at 298 K*

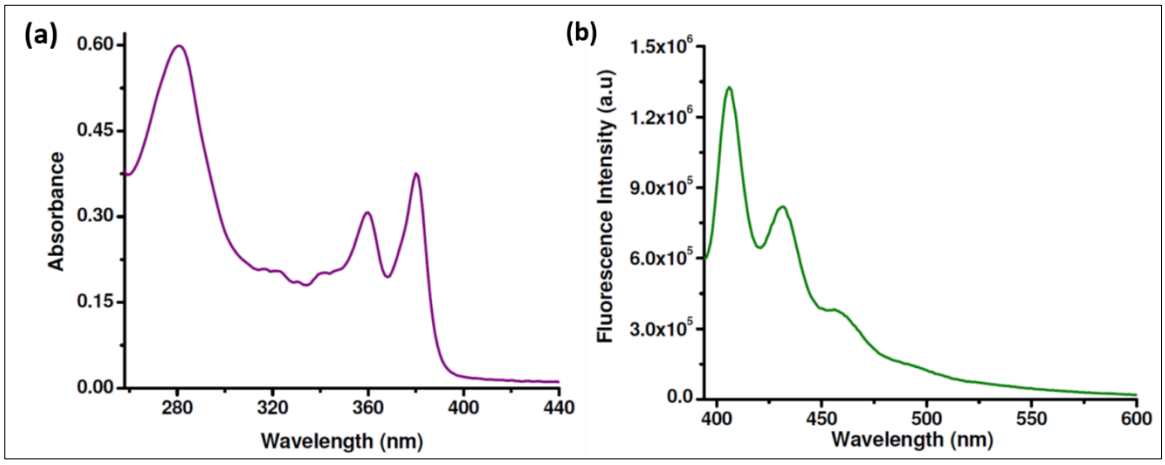

Figure S25. *a) UV-Vis and b) PL spectrum of **NDIROT** in $CHCl_3$ at 298K*

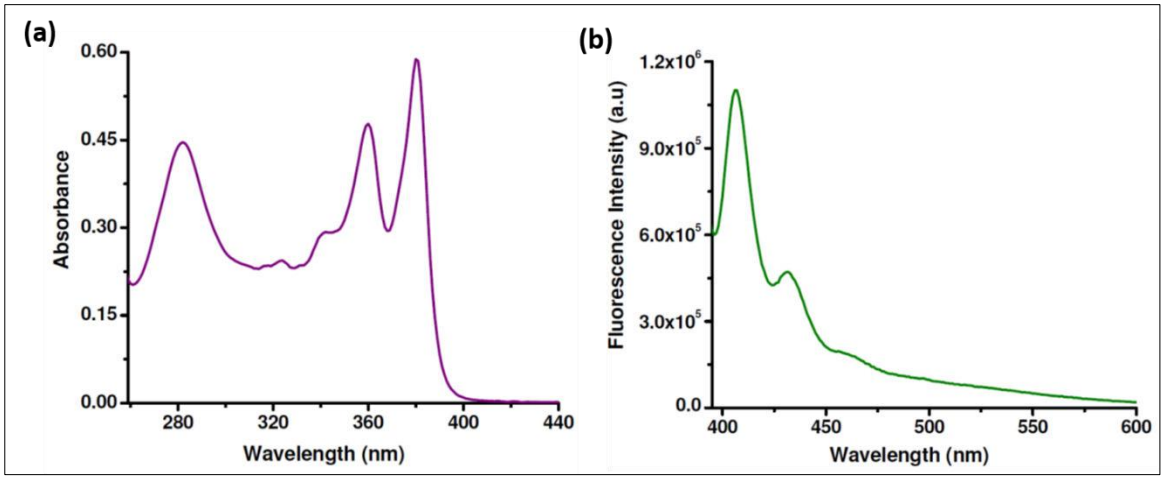

Figure S26. *a) UV-Vis and b) PL spectrum of* ***NDICAT*** *in $CHCl_3$ at 298K*

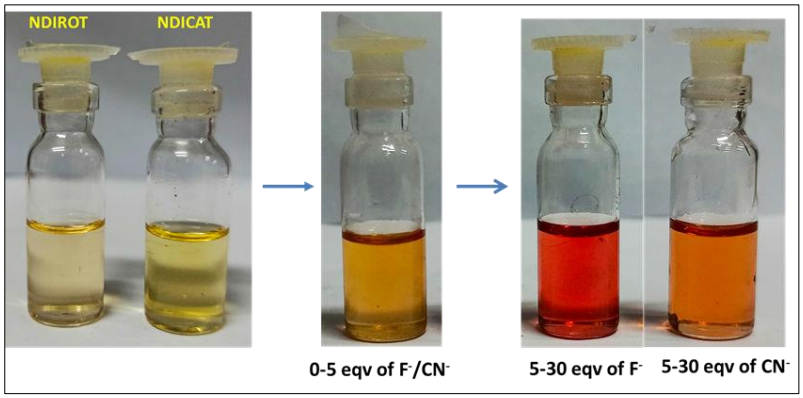

Figure S27. Snapshot of characteristic colour changes of (a) **NDIROT** and (b) **NDICAT** during addition 0.5 to 100 eqv. of F^- and CN^- in DMSO.

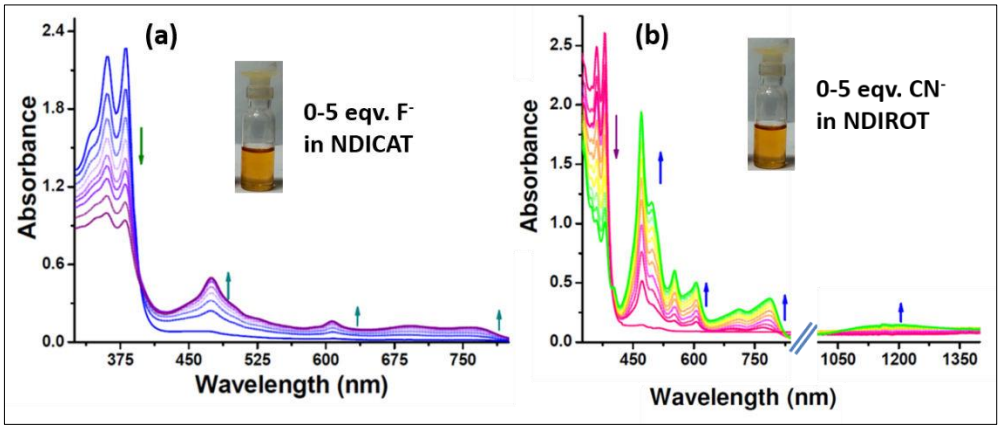

Figure S28. UV-Vis-NIR changes of (a) **NDICAT** (0.2mM) upon addition of F^- and (b) **NDIROT** (0.2mM) upon addition of CN^- in DMSO at 298K.

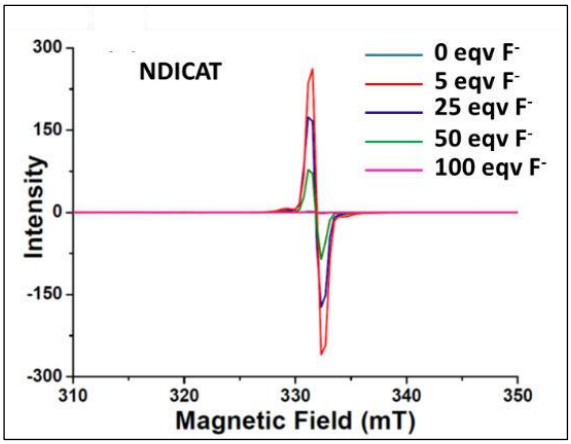

Figure S29. X-band EPR spectra of **NDICAT** (0.2 mM) in DMSO at 298 K.

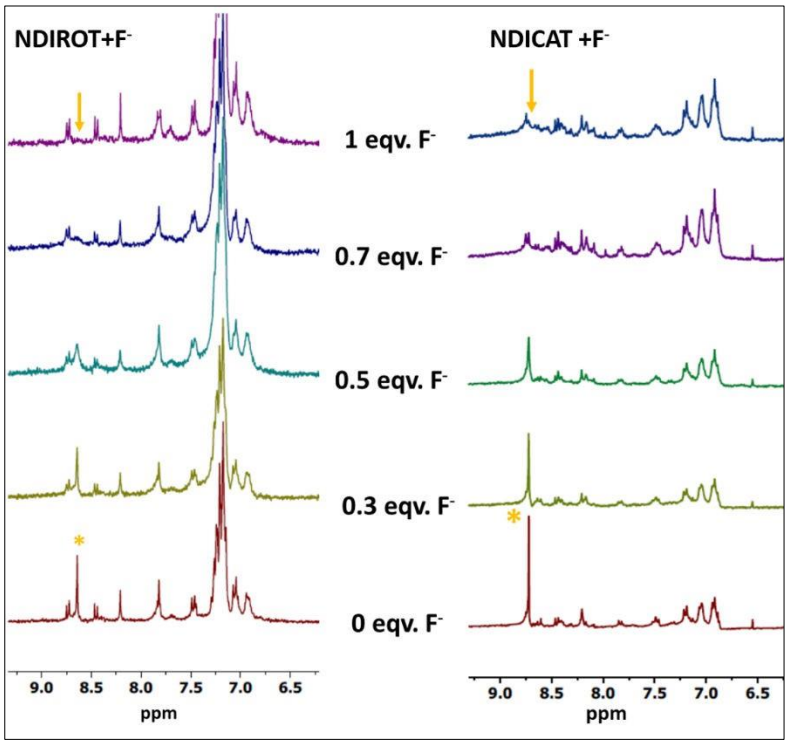

Figure S30. ^{1}H NMR spectra of NDIROT/NDICAT (0.2 mM) after treatment with different equivalents of F^{-} in d_6- DMSO at 298 K.

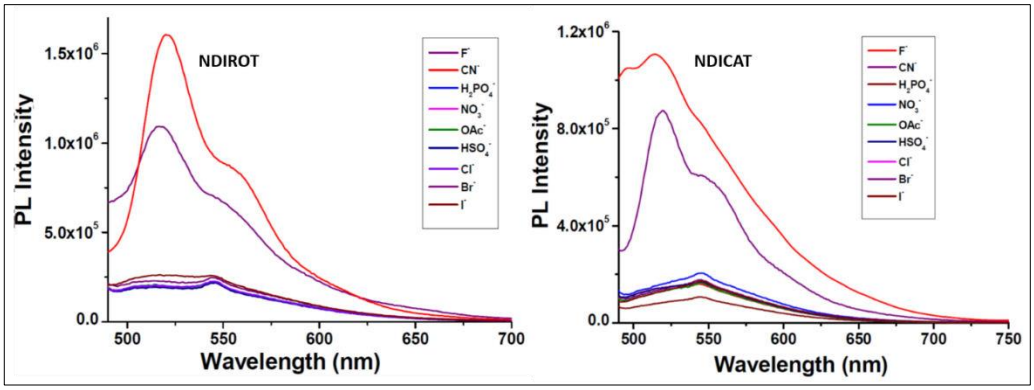

Figure S31. Comparative PL spectra of **NDIROT** (0.2mM) and **NDICAT** (0.2mM) upon addition of various anions of TBA salts at 298K in DMSO.