

Supporting Information

for

NDI integrated rotaxane/catenane and their interactions

with anions

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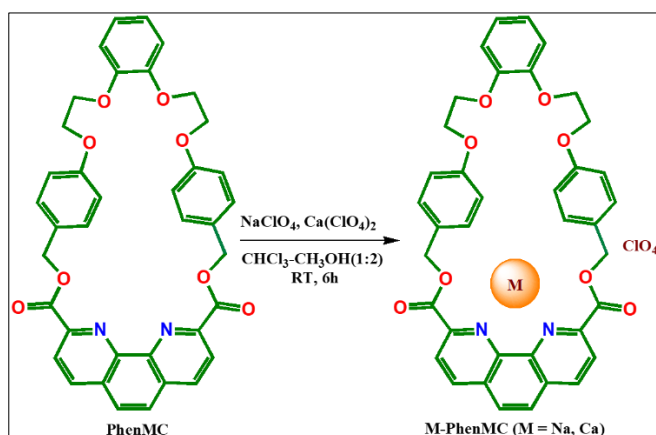
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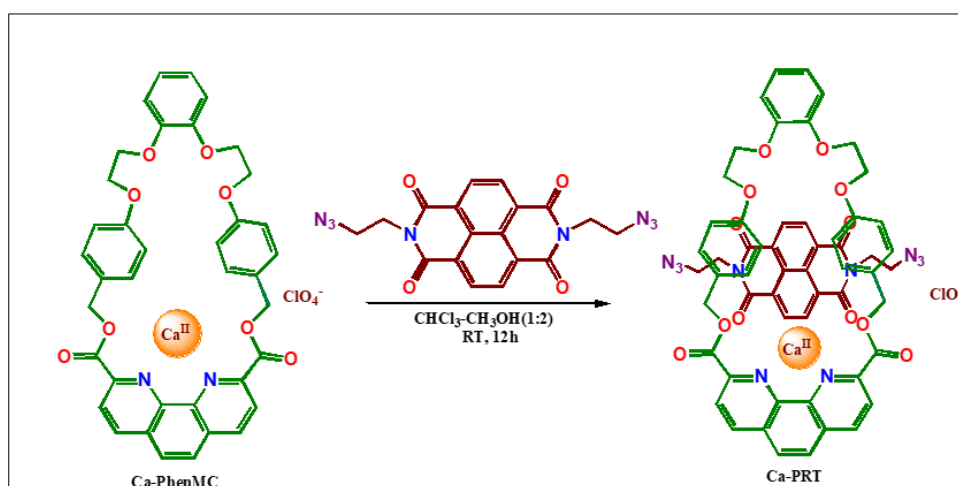
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Synthetic Scheme

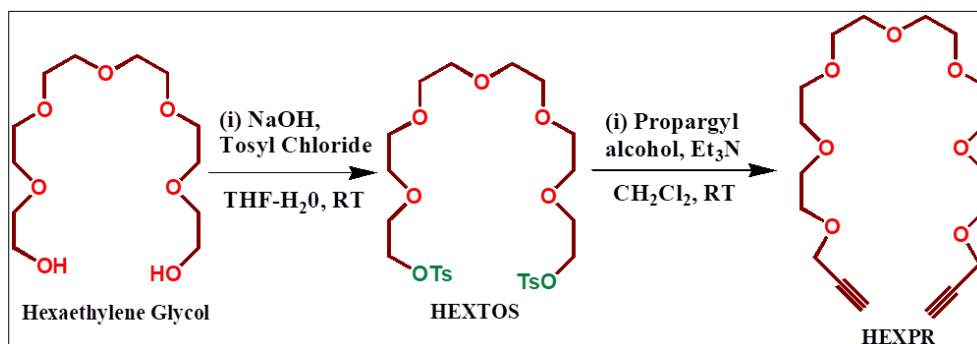
Scheme S1: Synthetic scheme of Na-PhenMC and Ca-PhenMC



Scheme S2: Synthetic scheme of Ca-PRT



Scheme S3: Synthetic scheme of HEXPR



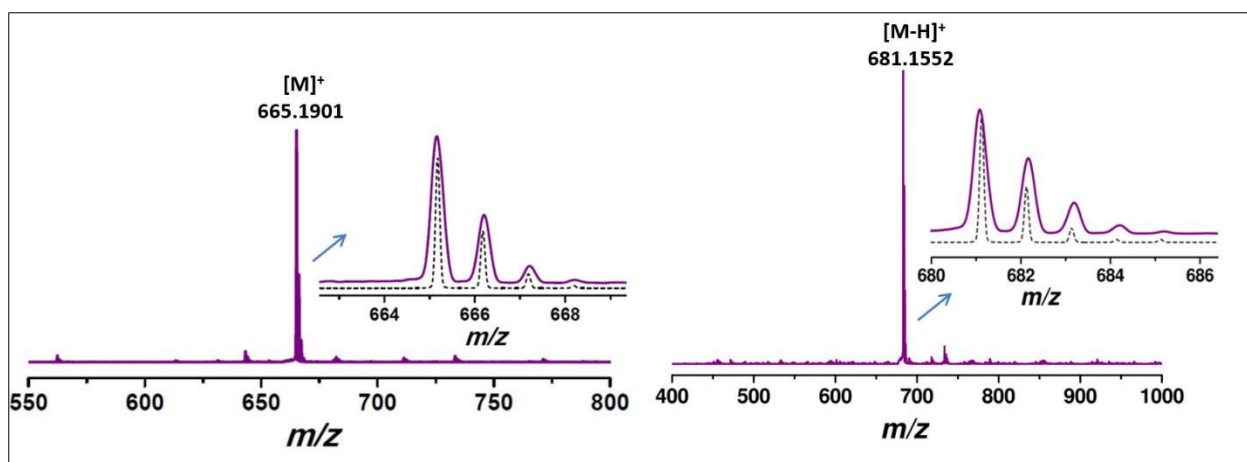


Figure S1: ESI-MS (+ve ion) spectra of i) *Na-PhenMC* and ii) *Ca-PhenMC* at 298K. Inset picture shows the similarity between isotopic distribution pattern (dotted) and the calculated (bold) one.

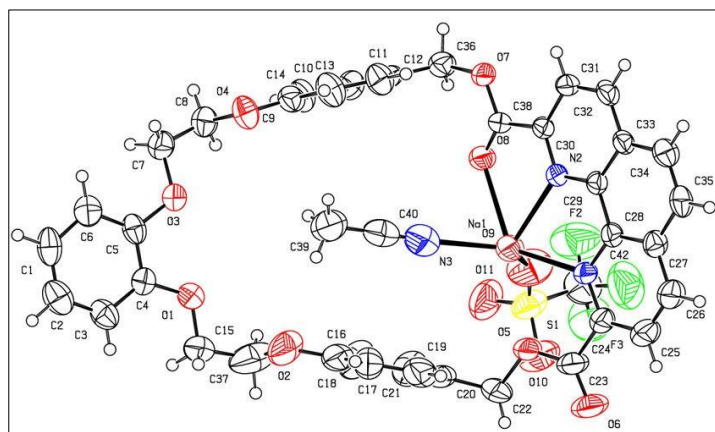


Figure S2: Single Crystal X-ray structure of *Na-PhenMC* (ellipsoid model using platon version)

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
$a/\text{\AA}$	9.632(5)
$b/\text{\AA}$	11.523(6)
$c/\text{\AA}$	18.177(10)
$\alpha/^\circ$	90.087(19)
$\beta/^\circ$	93.53(2)
$\gamma/^\circ$	94.613(17)
Unit cell volume/ \AA^3	2007.0(18)
Temperature/K	150(2)
Space group	<i>P</i> 1
No. of formula units per unit cell, <i>Z</i>	2
Radiation type	MoK α
Absorption coefficient, μ/mm^{-1}	0.170
No. of reflections measured	10968
No. of independent reflections	5249
R_{int}	0.0740
Final R_I values ($I > 2\sigma(I)$)	0.0679
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1670
Final R_I 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

...

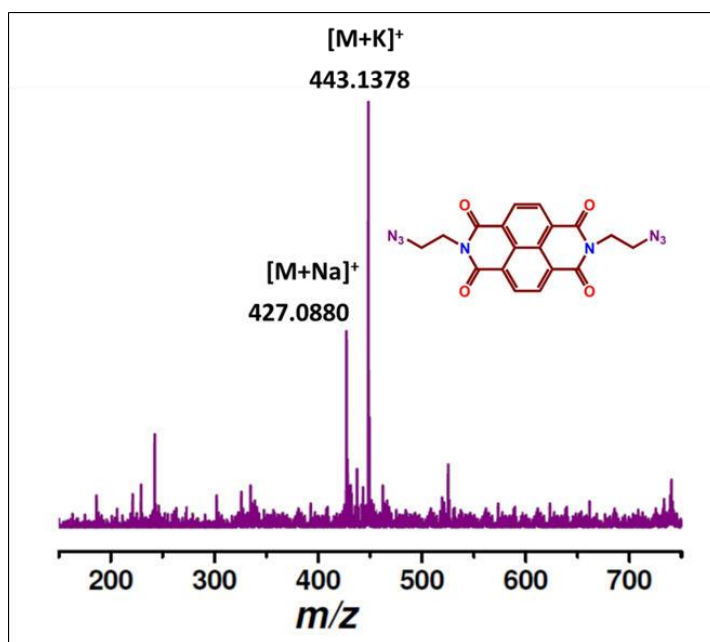


Figure S3. ESI-MS (+ve ion) spectrum of NDIAz at 298K.

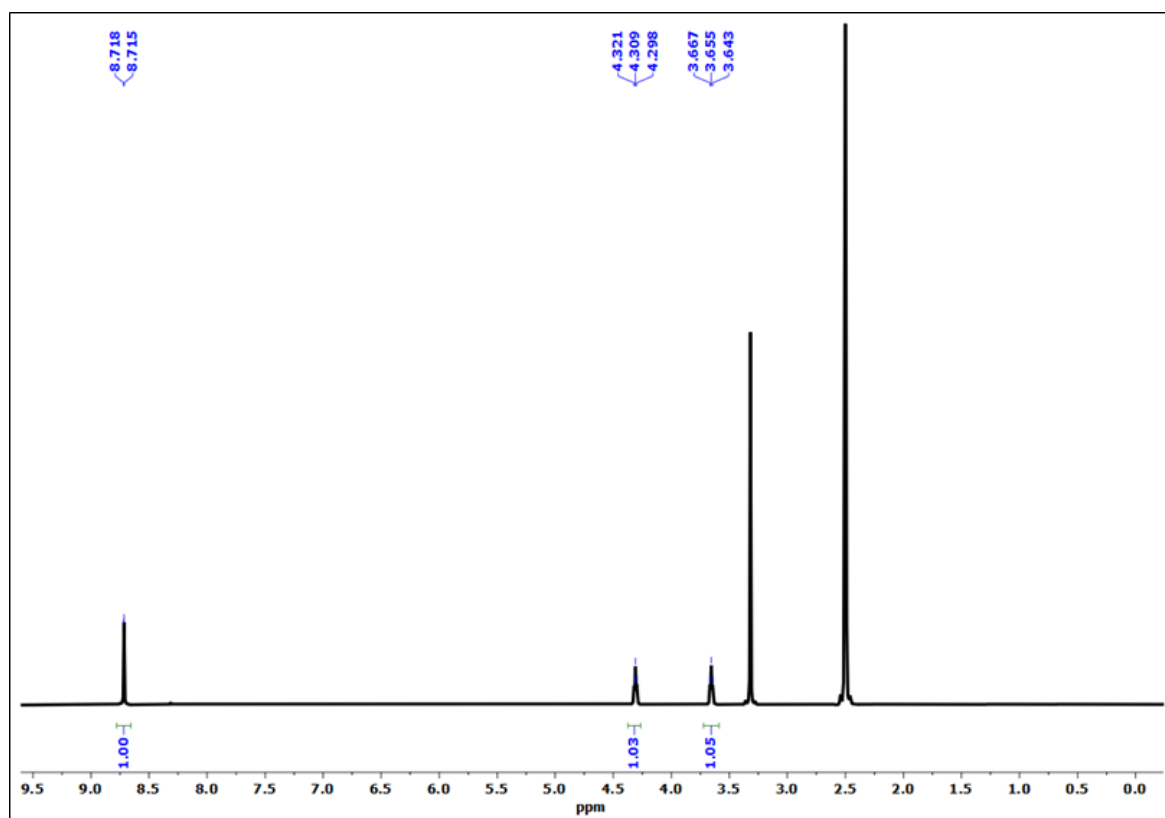


Figure S4. 1H NMR spectrum of NDIAz in $DMSO-d_6$ (400MHz) at 298 K.

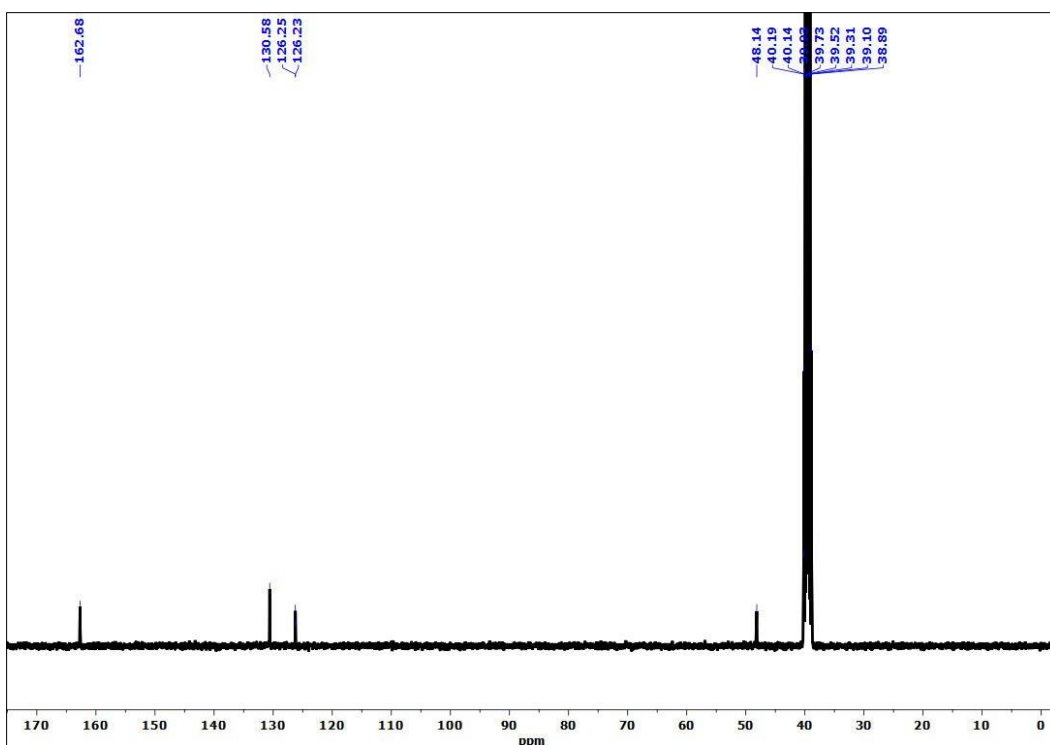


Figure S5. ^{13}C NMR spectrum of NDIAz in DMSO- d_6 (100MHz) at 298 K

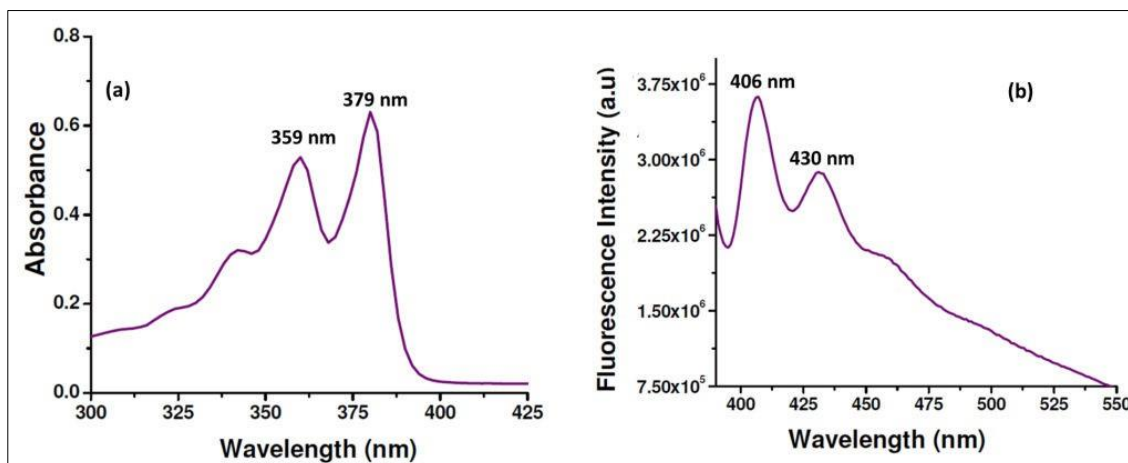


Figure S6. (a) UV-Vis and (b) PL spectrum of NDIAz in CHCl_3 -DMF (4:1) at 298 K.

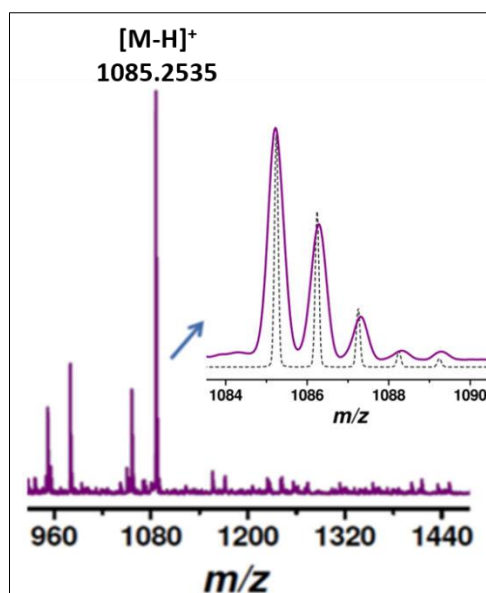


Figure S7. ESI-MS (+ve ion) spectra of **Ca-PRT**. Inset picture shows the similarity between isotopic distribution pattern (dotted) and the calculated (bold) one.

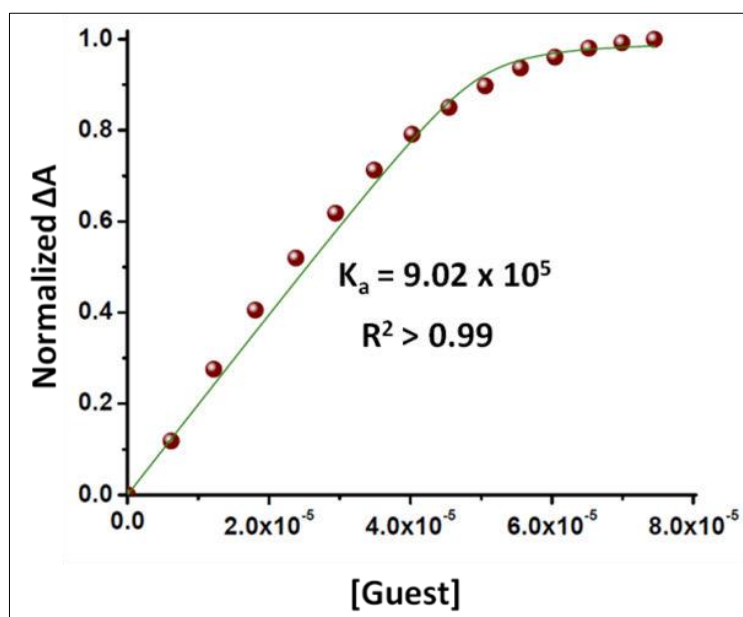


Figure S8. Non-linear 1:1 curve fitting plot from UV titration experiment to determine binding constant for the formation of **NDIAz** ($2 \times 10^{-5} M$) and **Ca-PhenMC** ($2 \times 10^{-4} M$) in $CHCl_3$ -DMF (4:1) at 298 K.

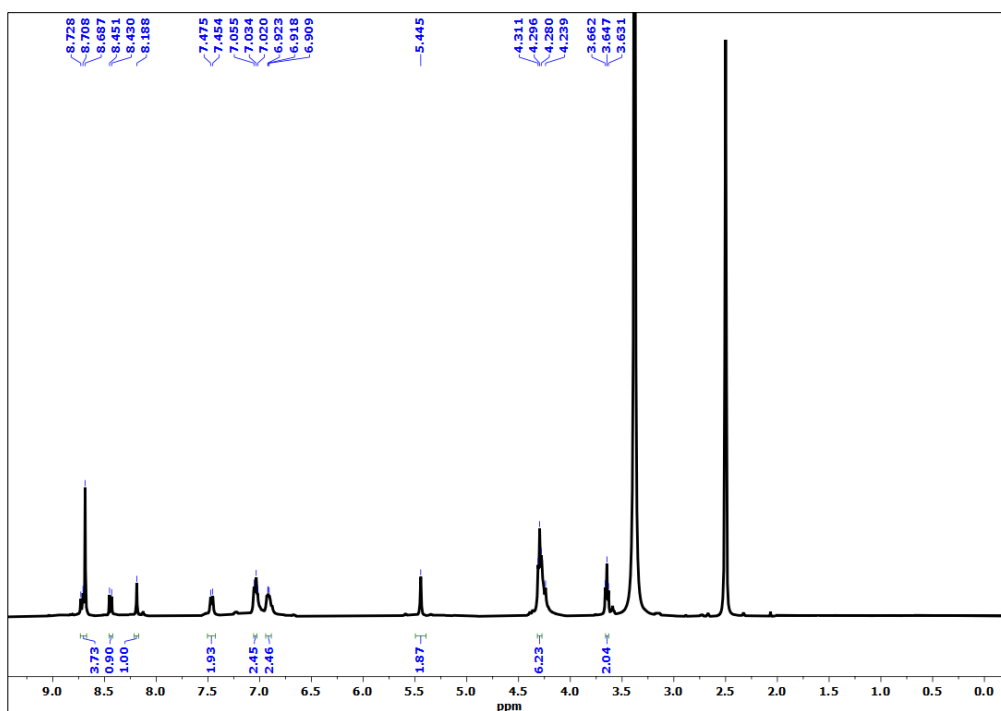


Figure S9. ^1H NMR spectrum of Ca-PRT in DMSO- d_6 (400MHz) at 298 K.

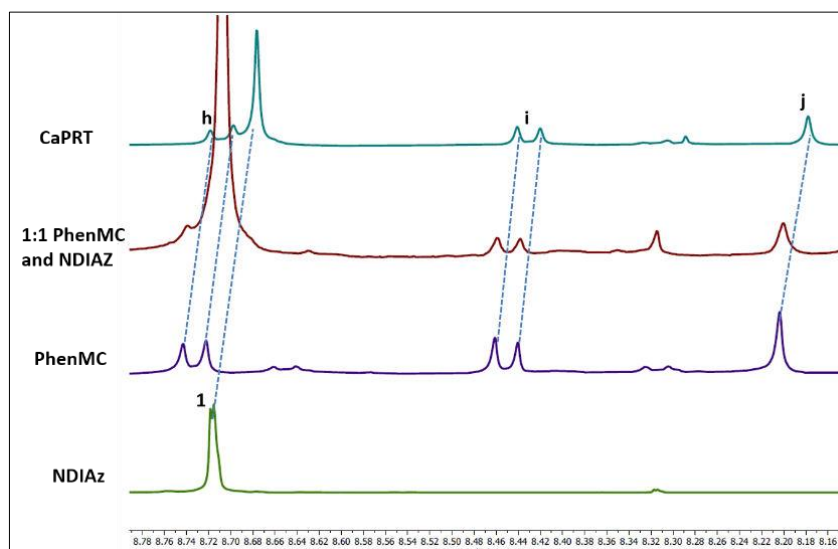


Figure S9a. Comparative ^1H NMR of Ca-PRT, 1:1 PhenMC-NDIAz, PhenMC and NDIAz in DMSO- d_6 (400 MHz) at 298 K.

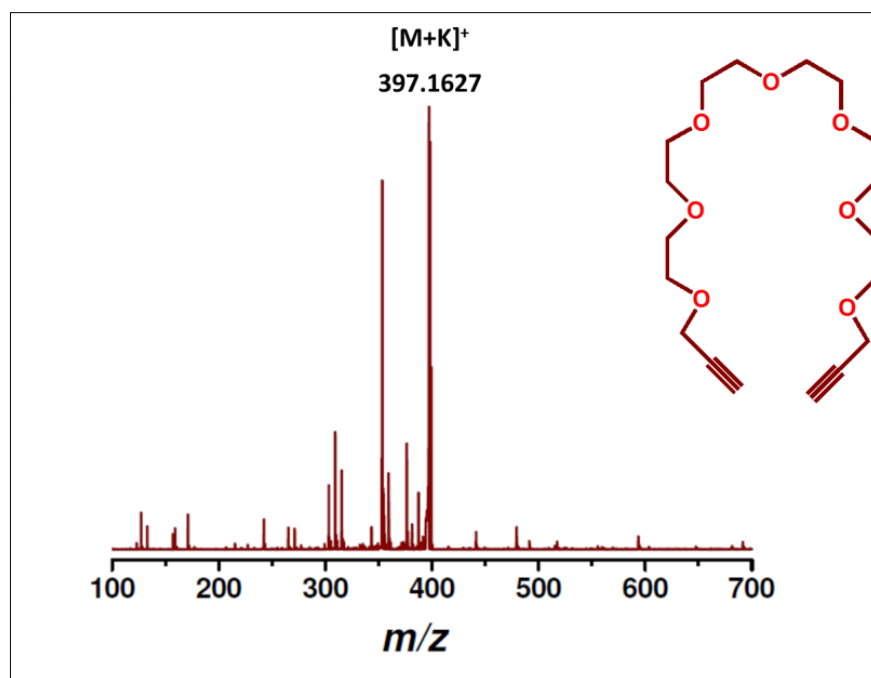


Figure S10. ESI-MS (+ve ion) spectrum of **HEXPR**.

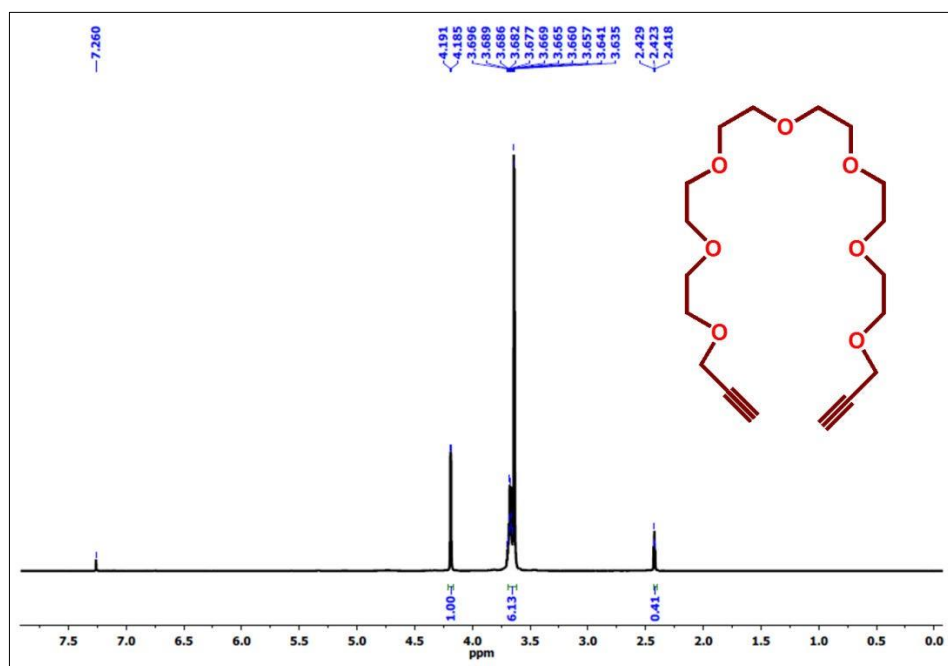


Figure S11. ^1H NMR spectrum of **HEXPR** in CDCl_3 (400MHz) at 298 K

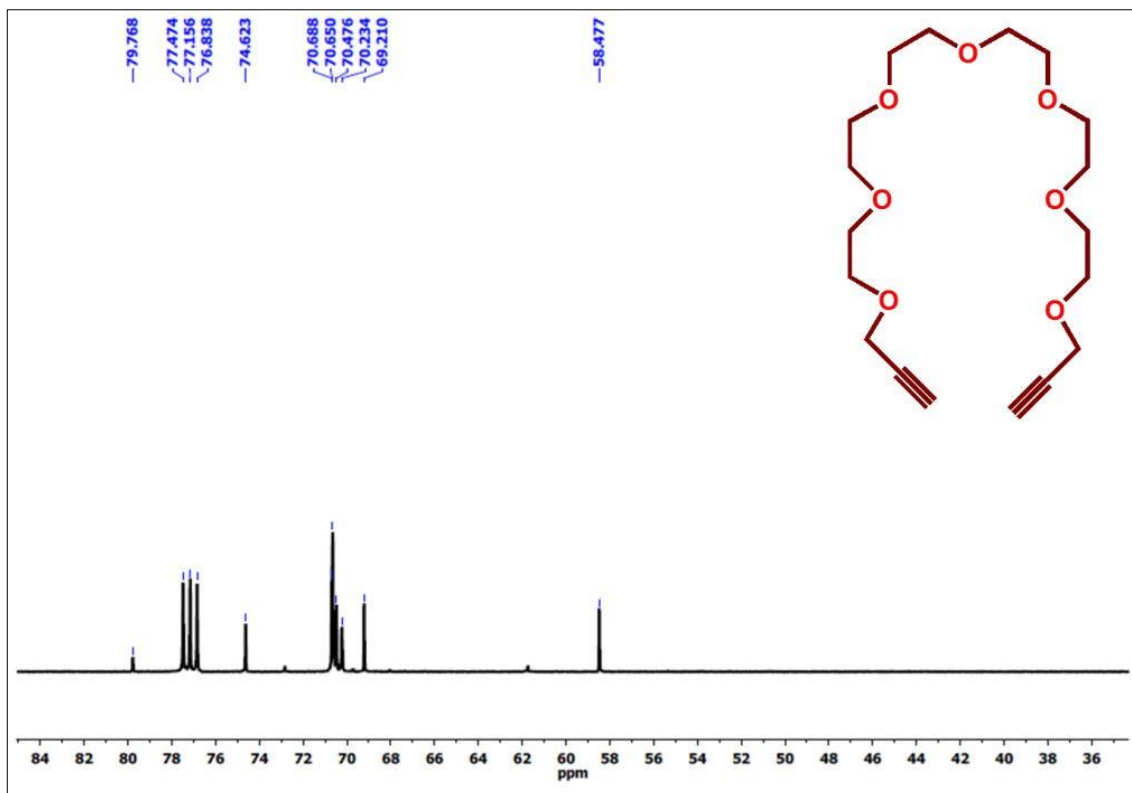


Figure S12. ^{13}C NMR spectrum of **HEXPR** in CDCl_3 (100MHz) at 298 K

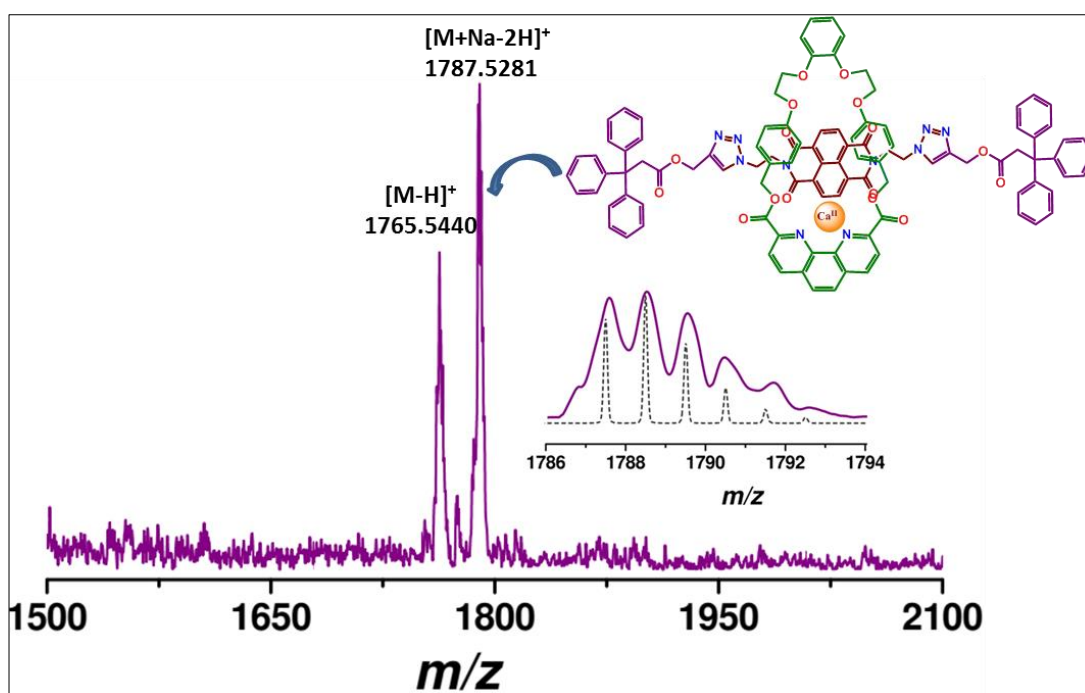


Figure S13. ESI-MS (+ve ion) spectrum of **Ca-NDIROT**

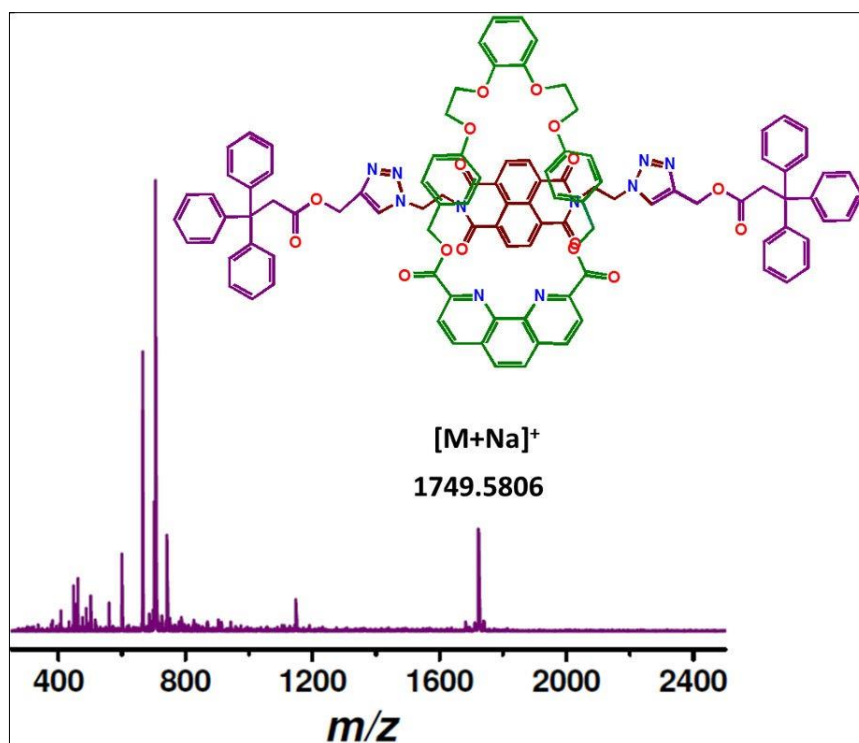


Figure S14. ESI-MS (+ve ion) spectrum of NDIROT

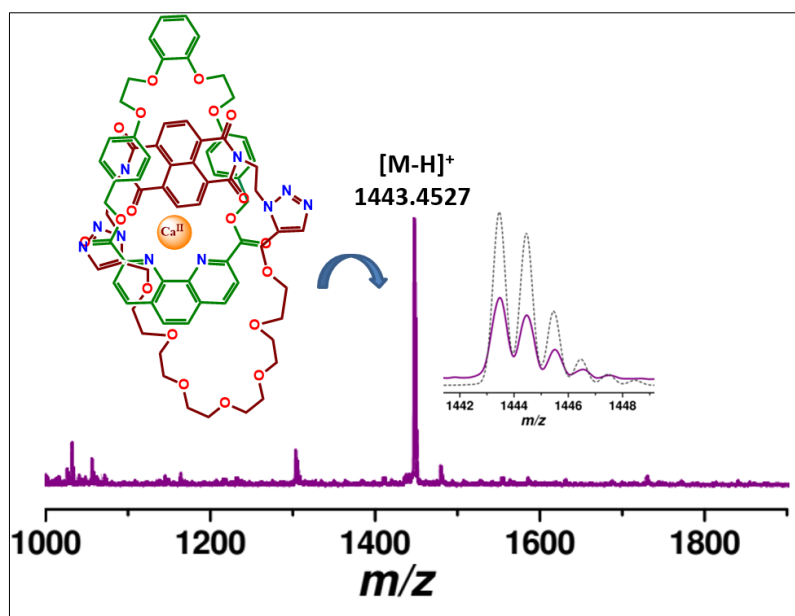


Figure S15. ESI-MS (+ve ion) spectrum of Ca-NDICAT

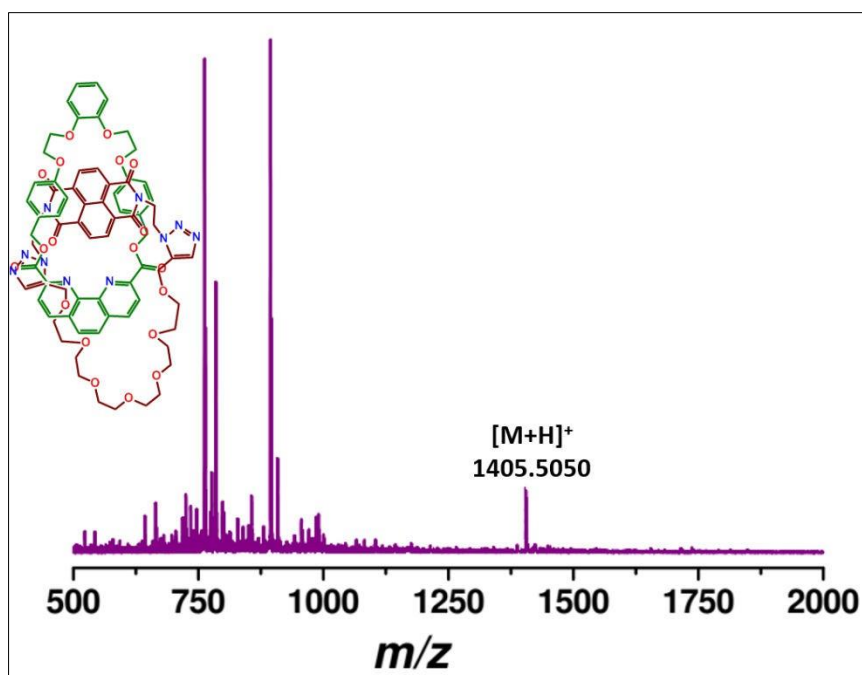


Figure S16. ESI-MS (+ve ion) spectrum of NDICAT

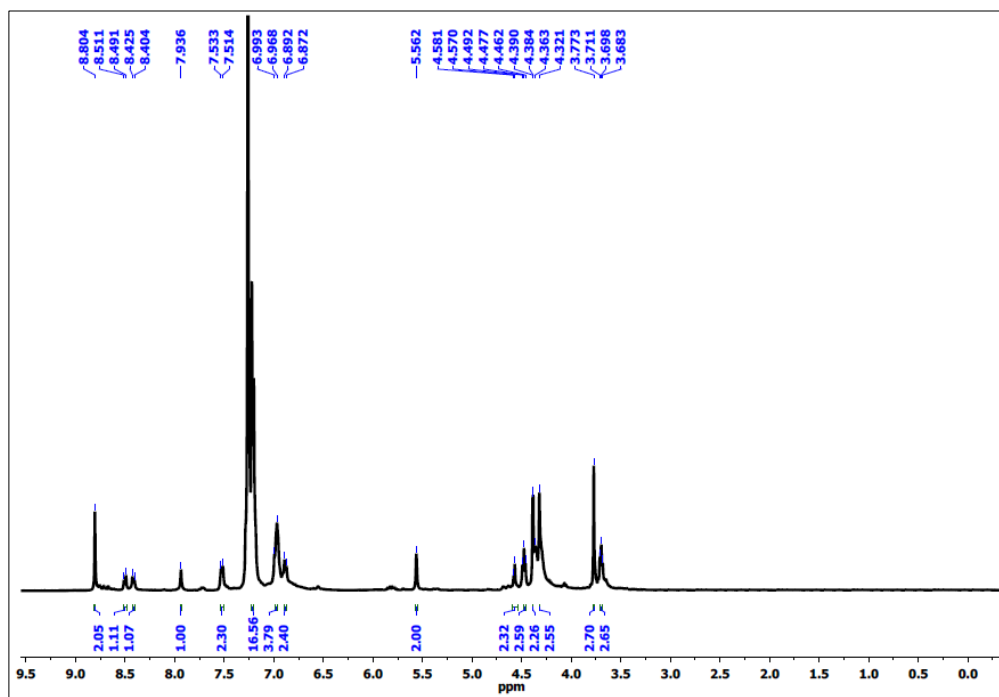


Figure S17. 1H NMR spectrum of NDIROT in $CDCl_3$ (400MHz) at 298 K

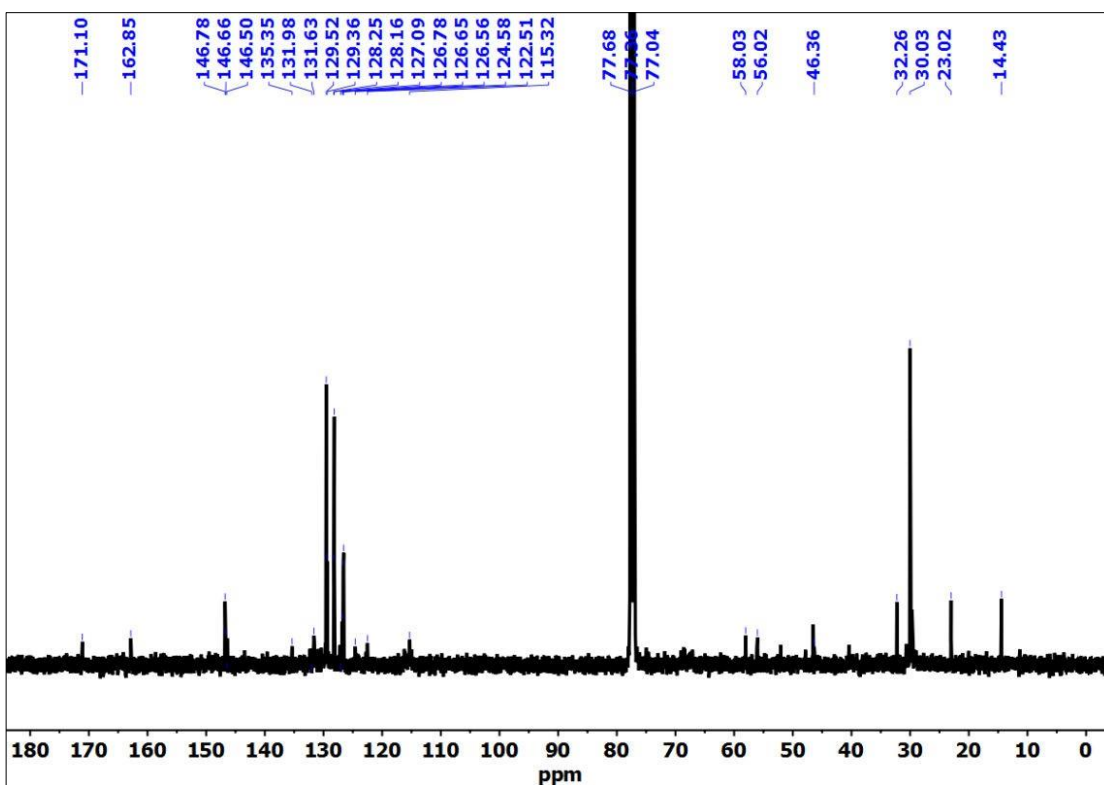


Figure S18. ^{13}C NMR spectrum of NDIROT in CDCl_3 (100MHz) at 298 K

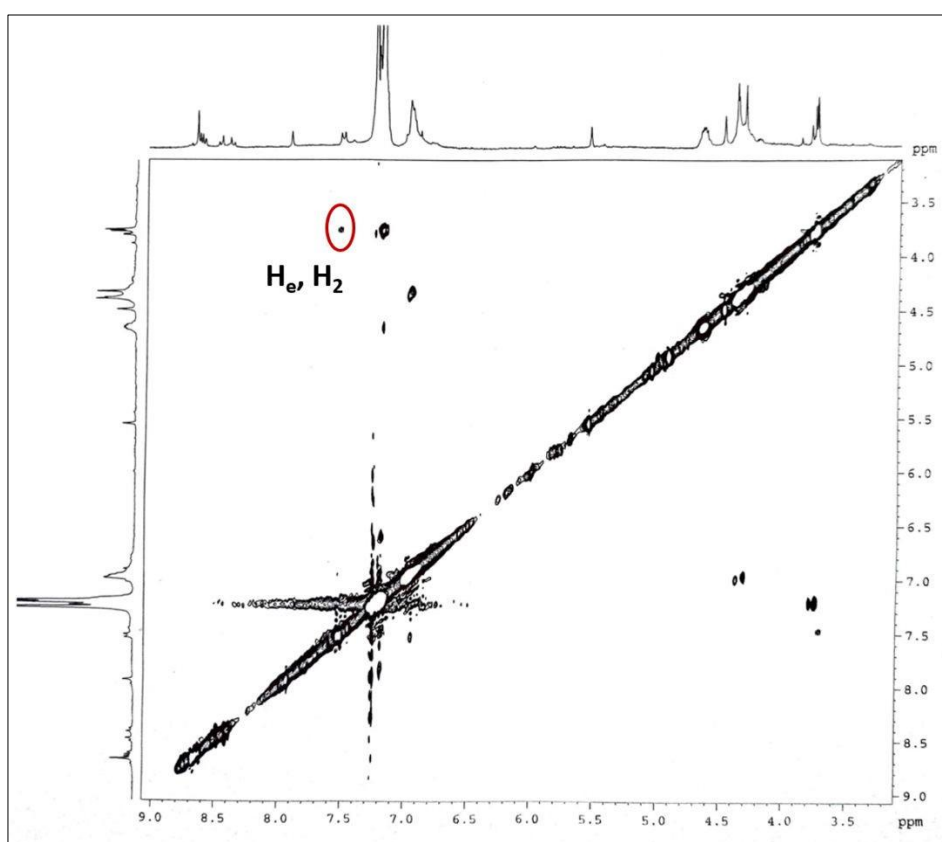


Figure S18a. ROESY spectrum of NDIROT in CDCl_3 (300MHz) at 298 K

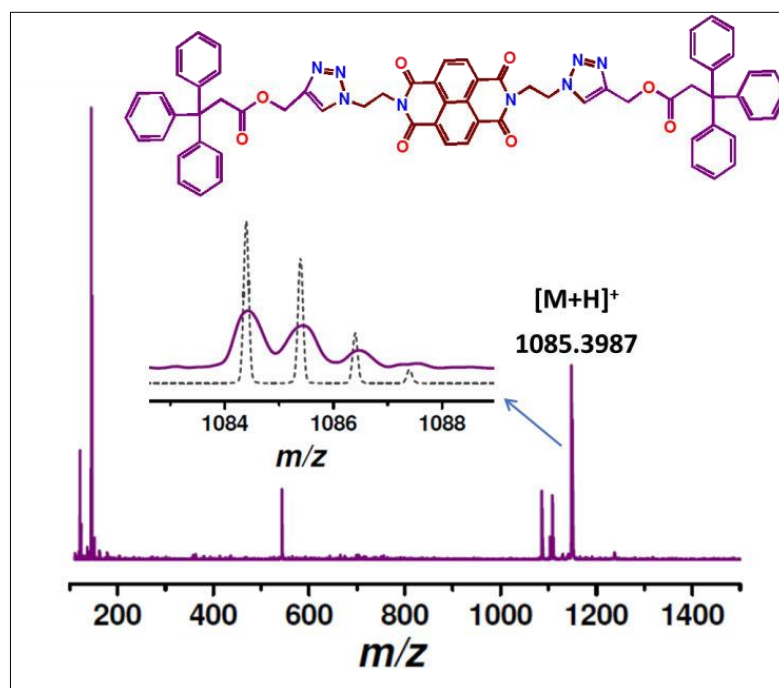


Figure S19. ESI-MS (+ve ion) spectrum of NDI-AXSTP

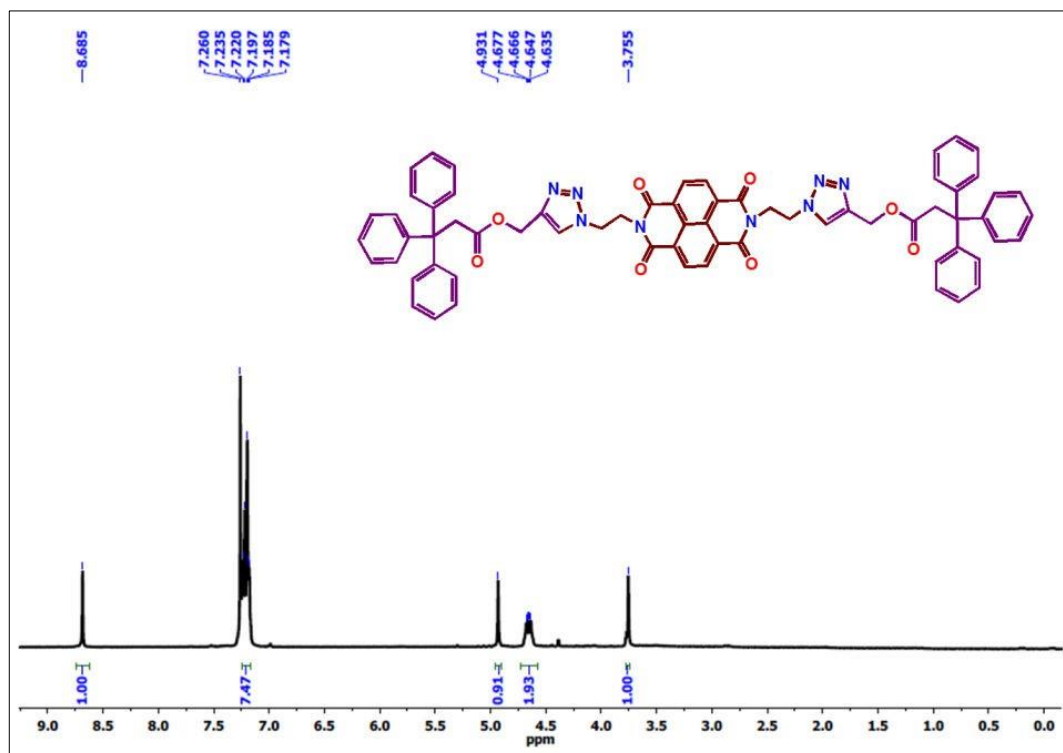


Figure S20. ^1H NMR spectrum of NDI-AXSTP in CDCl_3 (400MHz) at 298 K

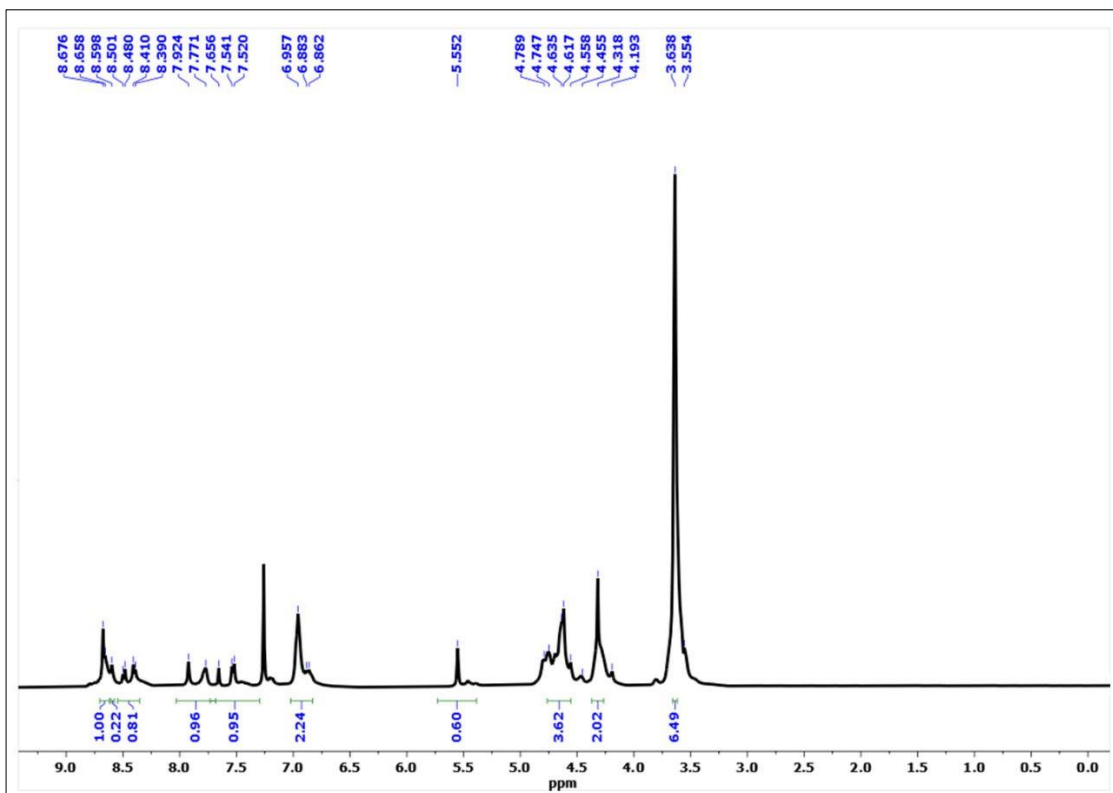


Figure S21. ^1H NMR spectrum of NDICAT in CDCl_3 (400MHz) at 298 K

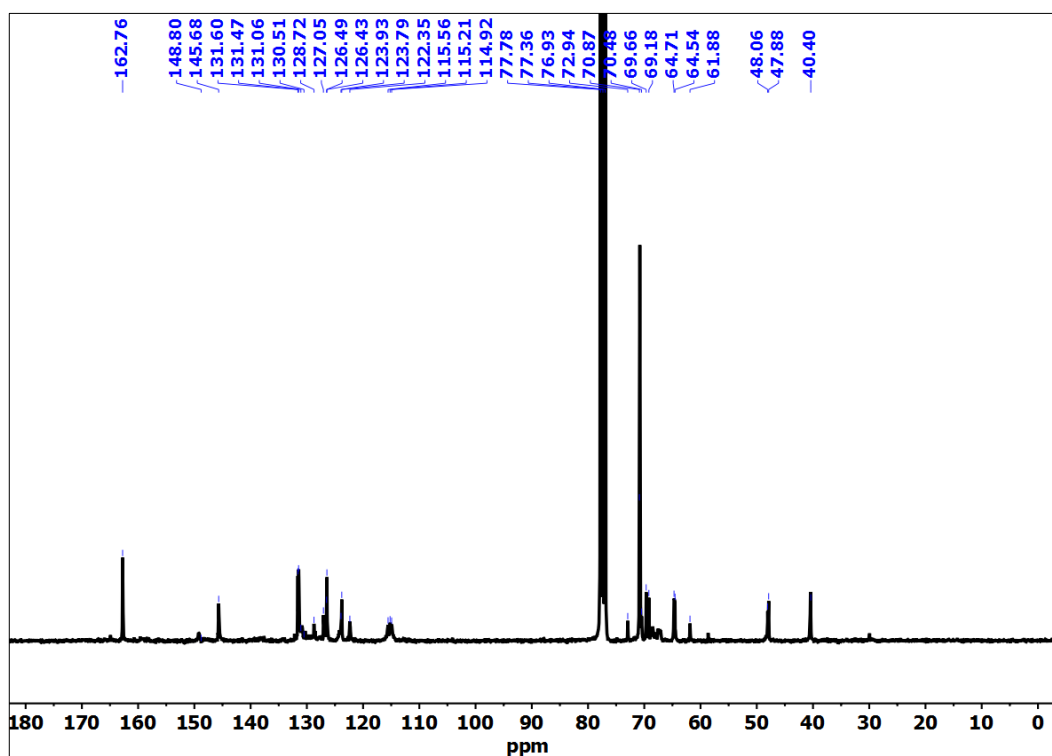


Figure S22. ^{13}C NMR spectrum of NDICAT in CDCl_3 (75MHz) at 298 K

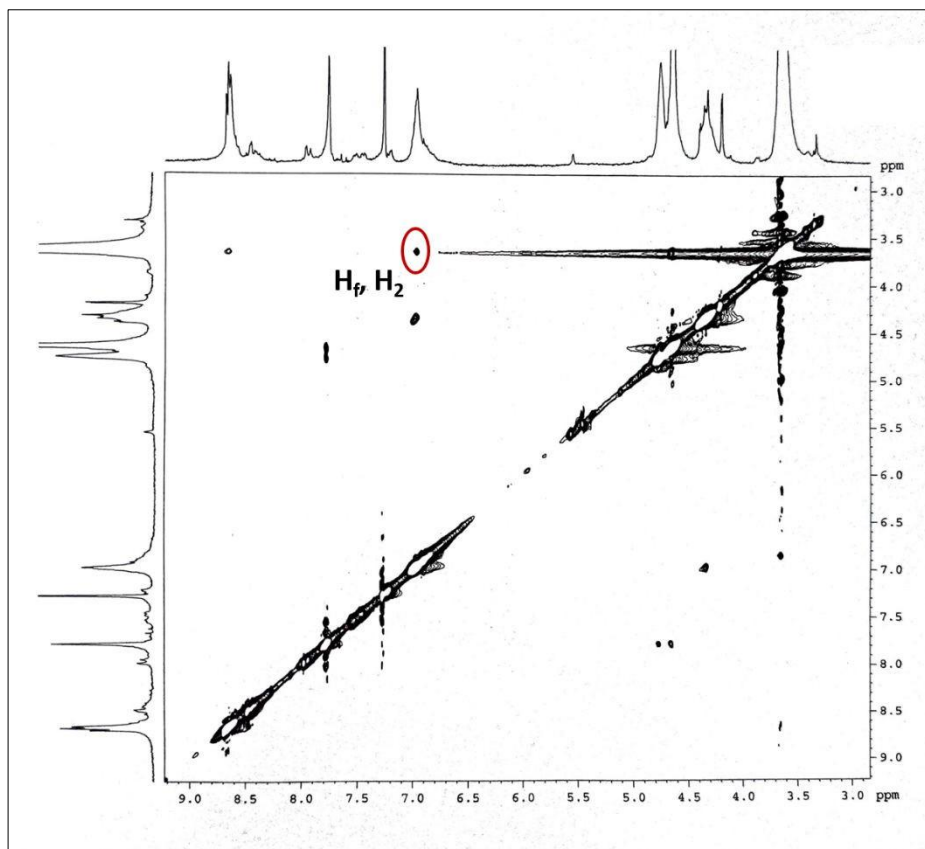


Figure S22a. ROESY spectrum of NDICAT in $CDCl_3$ (300MHz) at 298 K

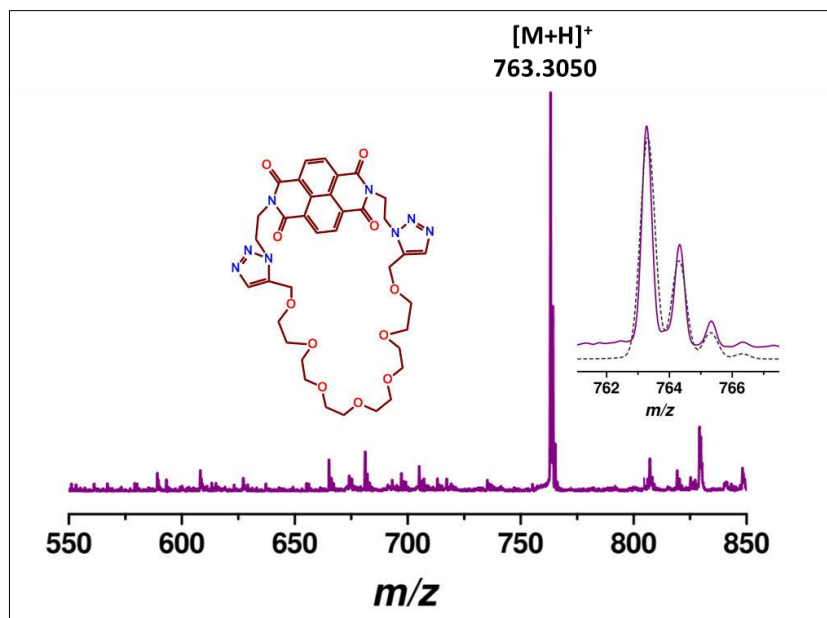


Figure S23. ESI-MS (+ve ion) spectrum of NDIMC.

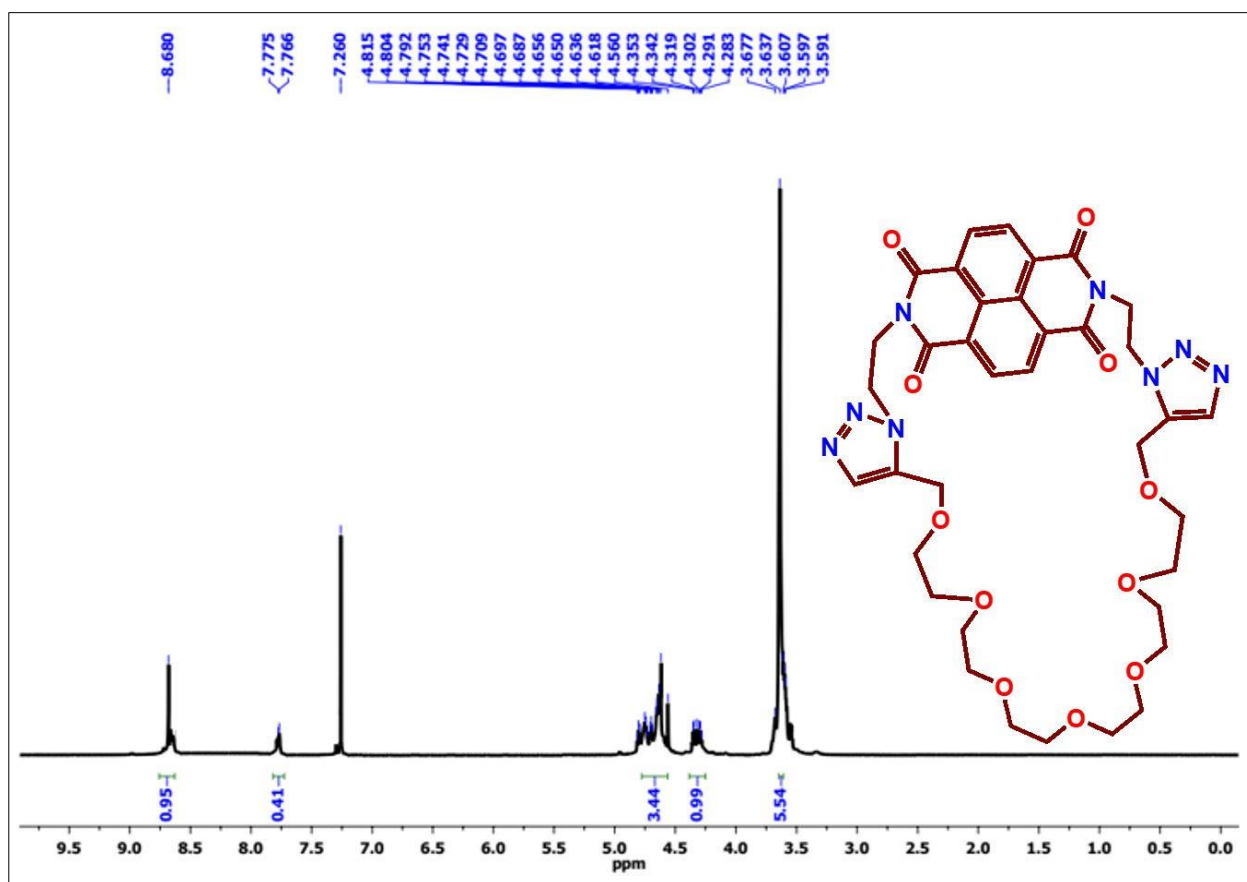


Figure S24. ^1H NMR spectrum of NDIMC in CDCl_3 (400MHz) at 298 K

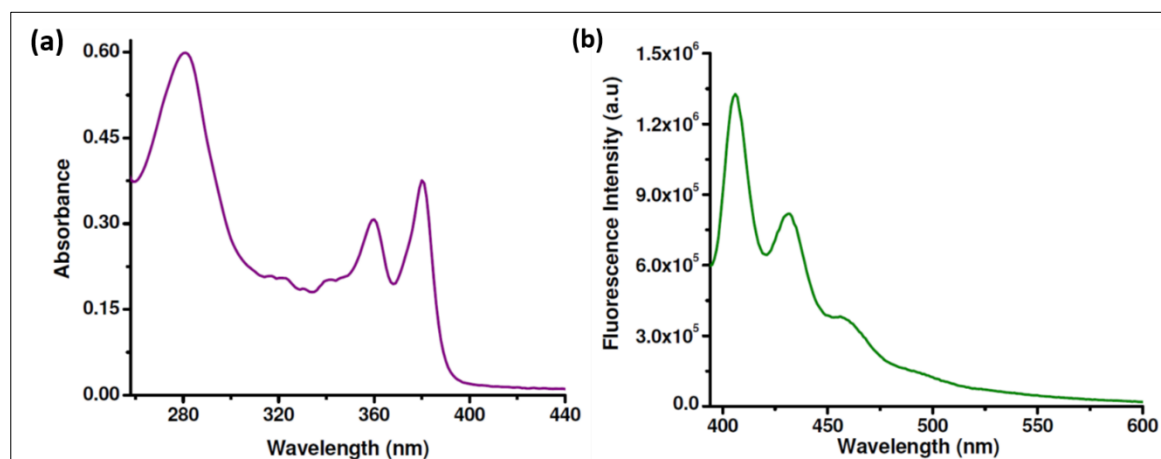


Figure S25. a) UV-Vis and b) PL spectrum of NDIROT in CHCl_3 at 298K

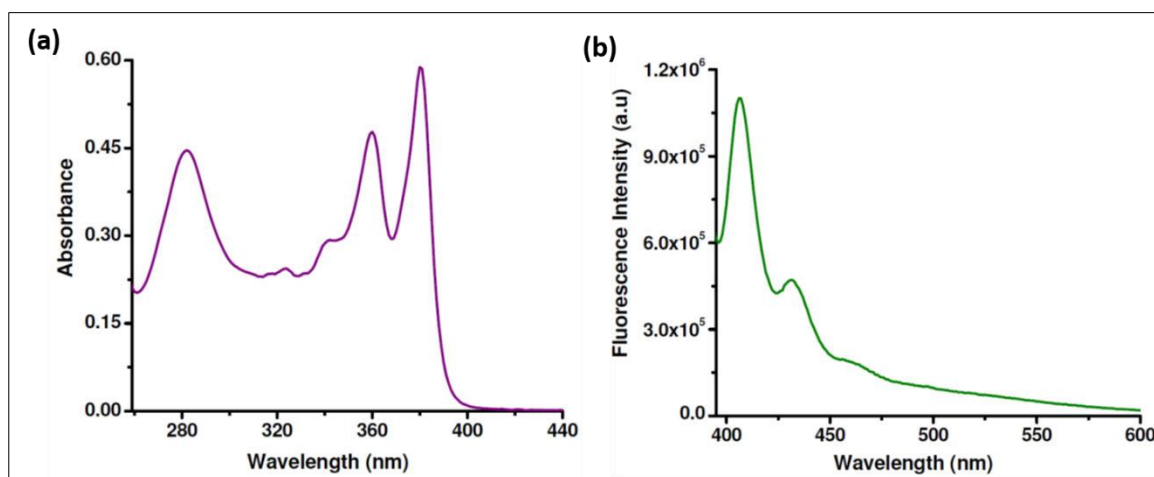


Figure S26. a) UV-Vis and b) PL spectrum of **NDICAT** in CHCl_3 at 298K

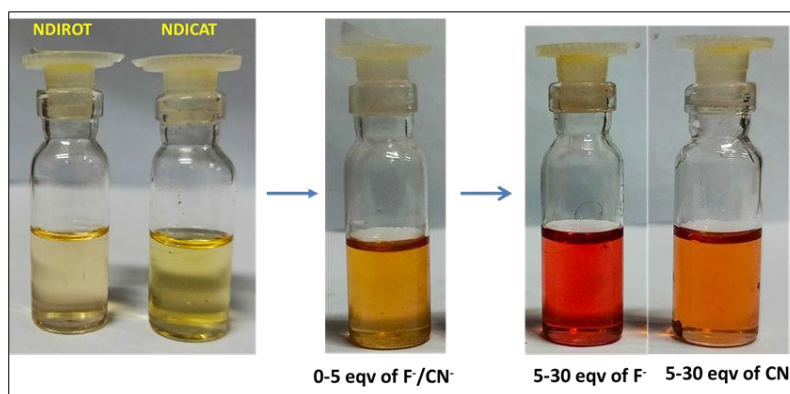


Figure S27. Snapshot of characteristic colour changes of (a) **NDIROT** and (b) **NDICAT** during addition 0.5 to 100 eqv. of F^- and CN^- in DMSO.

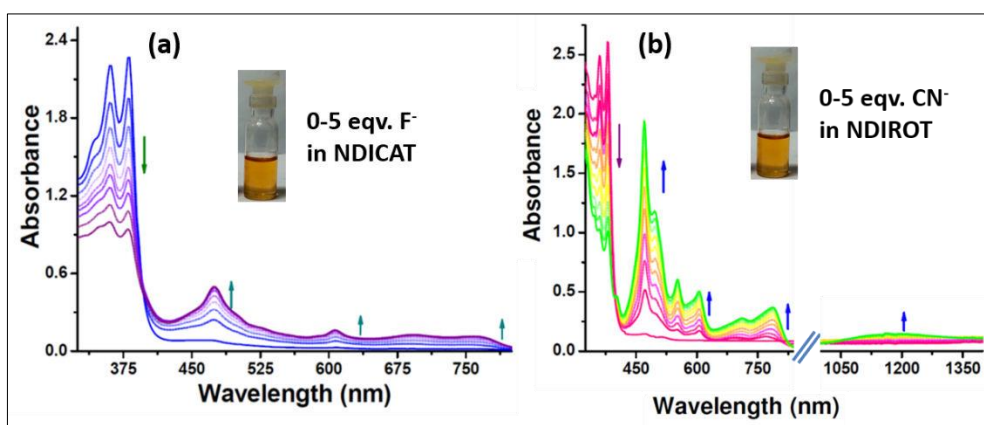


Figure S28. UV-Vis-NIR changes of (a) **NDICAT** (0.2mM) upon addition of F^- and (b) **NDIROT** (0.2mM) upon addition of CN^- in DMSO at 298K.

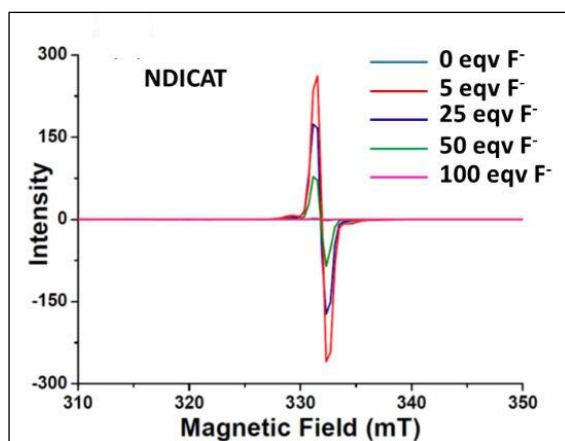


Figure S29. X-band EPR spectra of **NDICAT** (0.2 mM) in DMSO at 298 K.

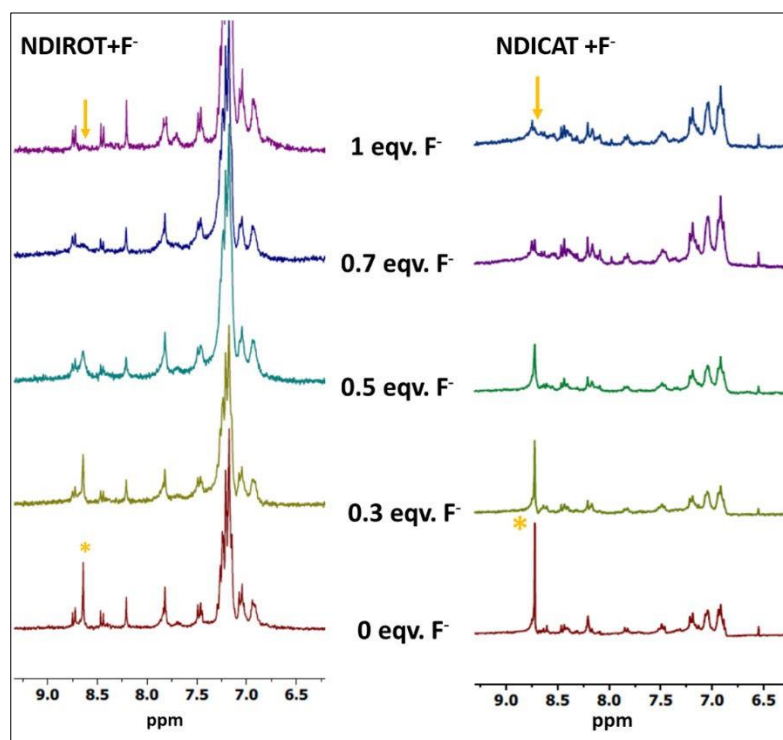


Figure S30. ^1H NMR spectra of NDIROT/NDICAT (0.2 mM) after treatment with different equivalents of F^- in d_6 -DMSO at 298 K.

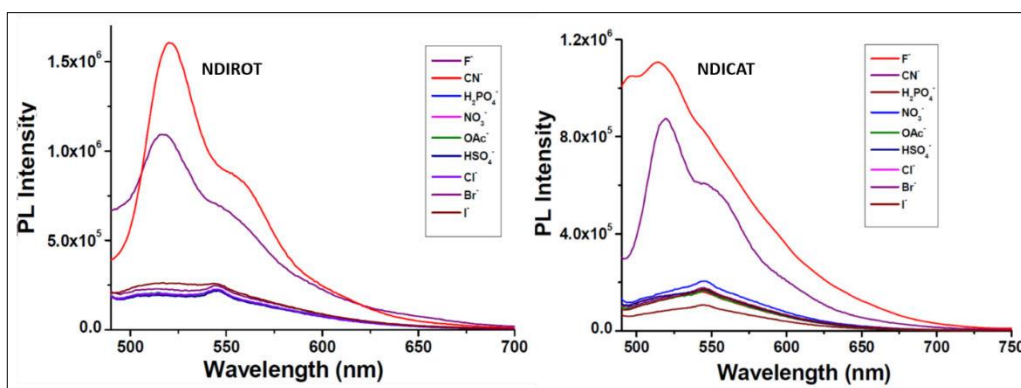


Figure S31. Comparative PL spectra of **NDIROT** (0.2mM) and **NDICAT** (0.2mM) upon addition of various anions of TBA salts at 298K in DMSO.