Supporting Information

Synthesis and Suzuki-Miyaura cross coupling reactions for post synthetic modification of a tetrabromo-anthracenyl porphyrin

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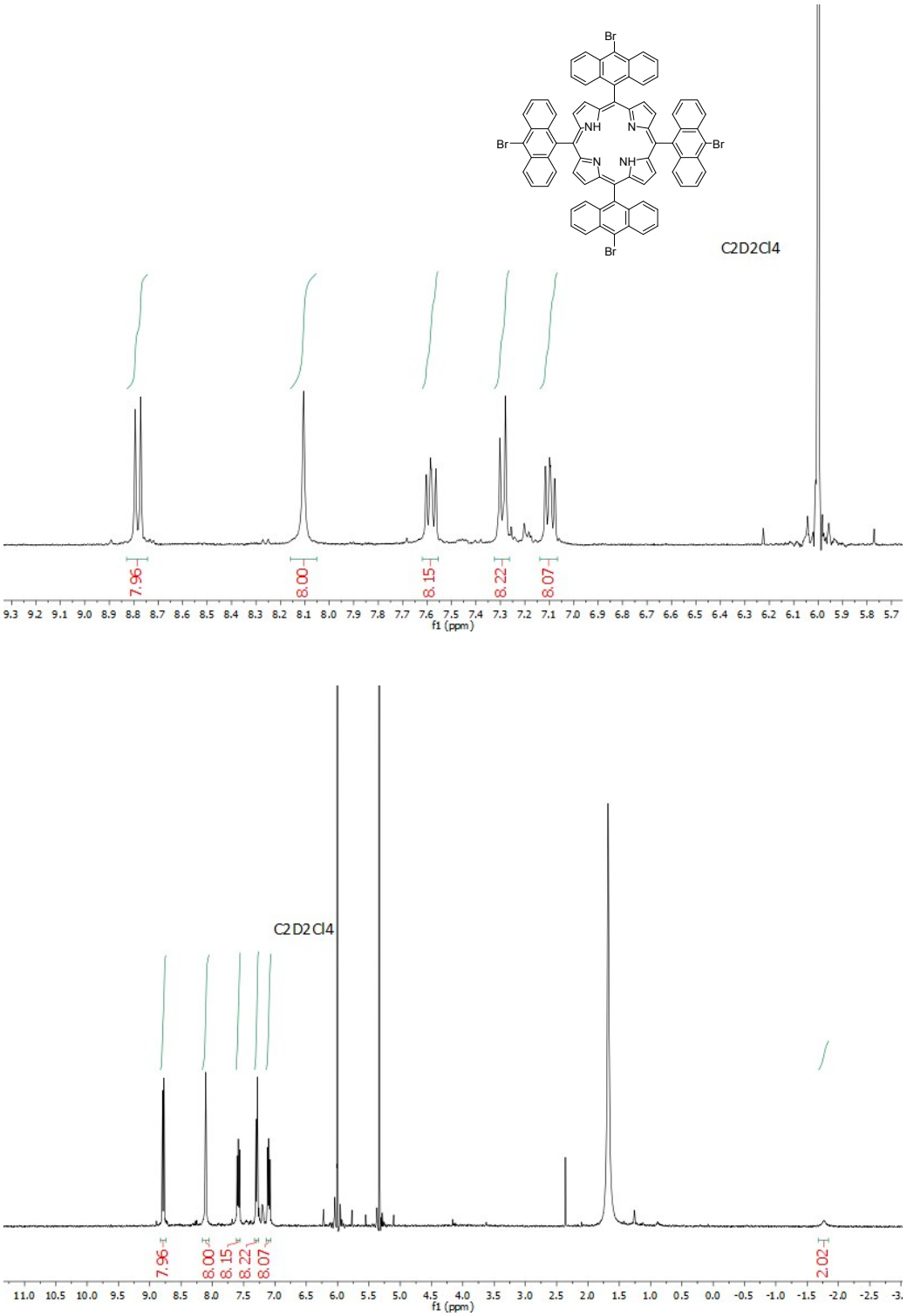


Figure S1. ^{1}H NMR spectra of **BrTAP** (400 MHz, $C_2D_2Cl_4$, 298K)

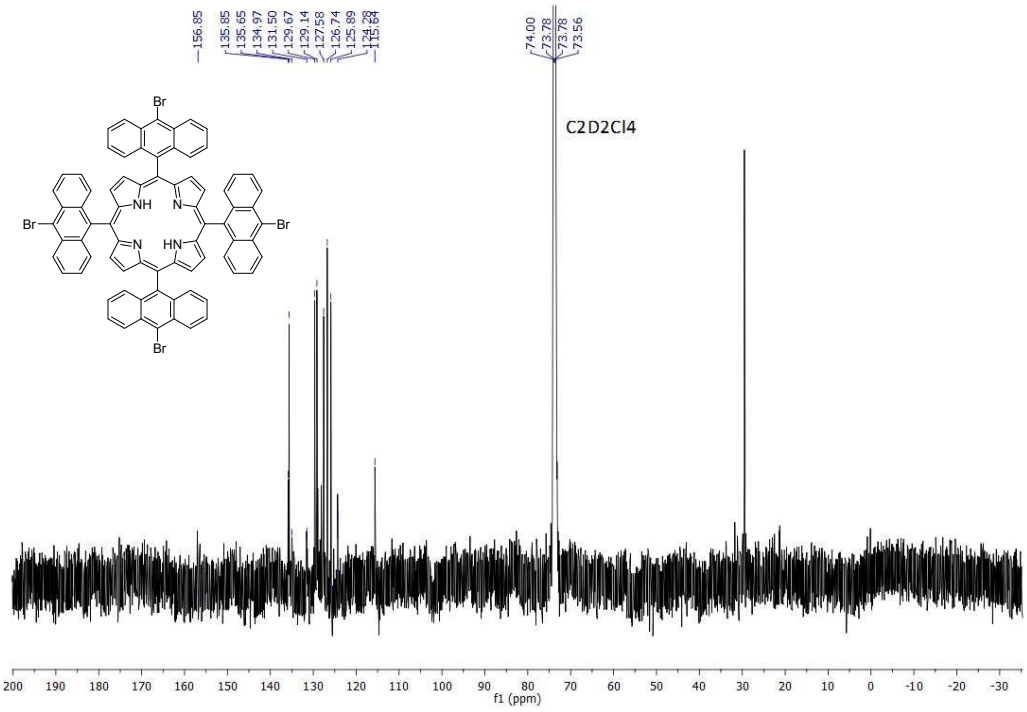


Figure S2. ^{13}C NMR spectra of **BrTAP** (125 MHz, $C_2D_2Cl_4$, 333K)

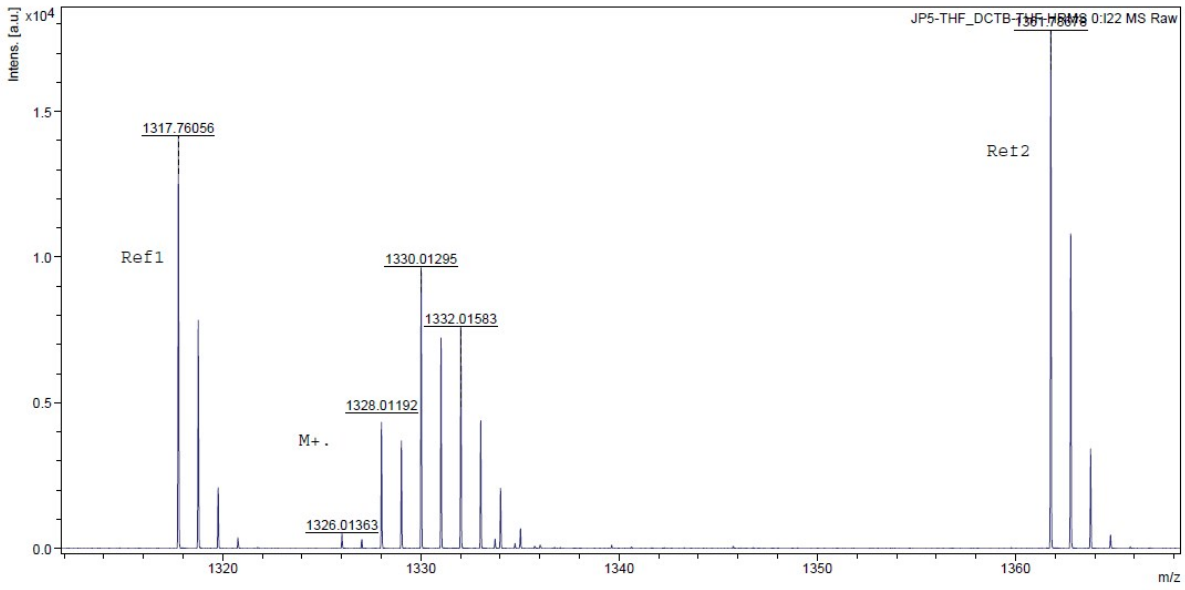


Figure S3. HRMS, MALDI-TOF for **BrTAP**

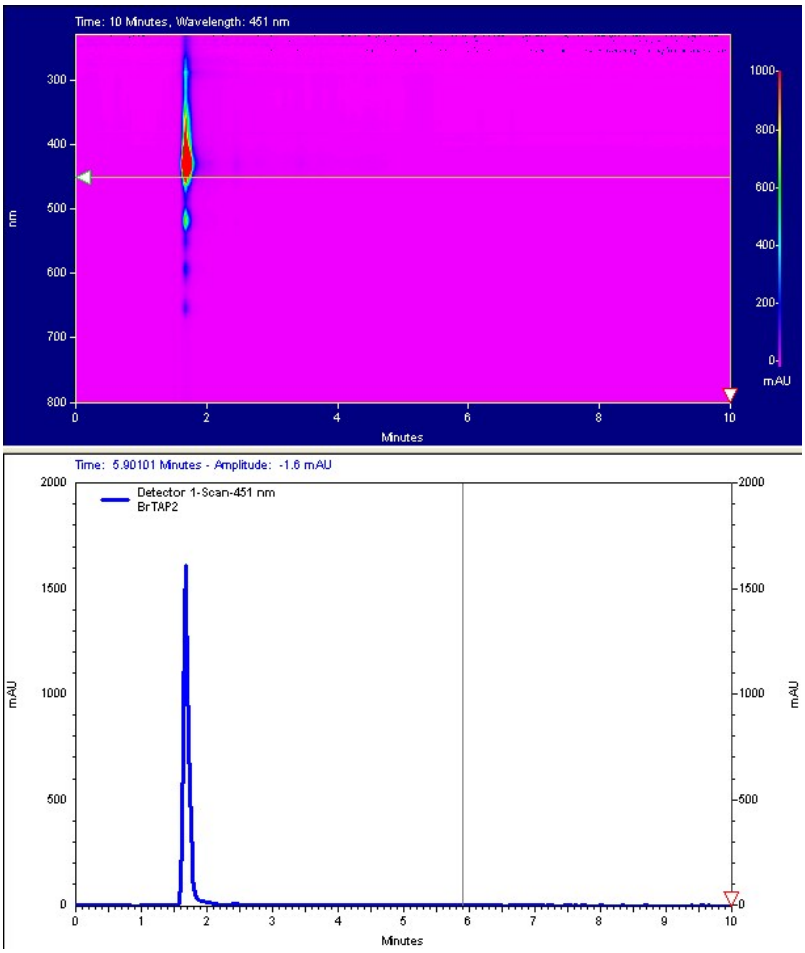
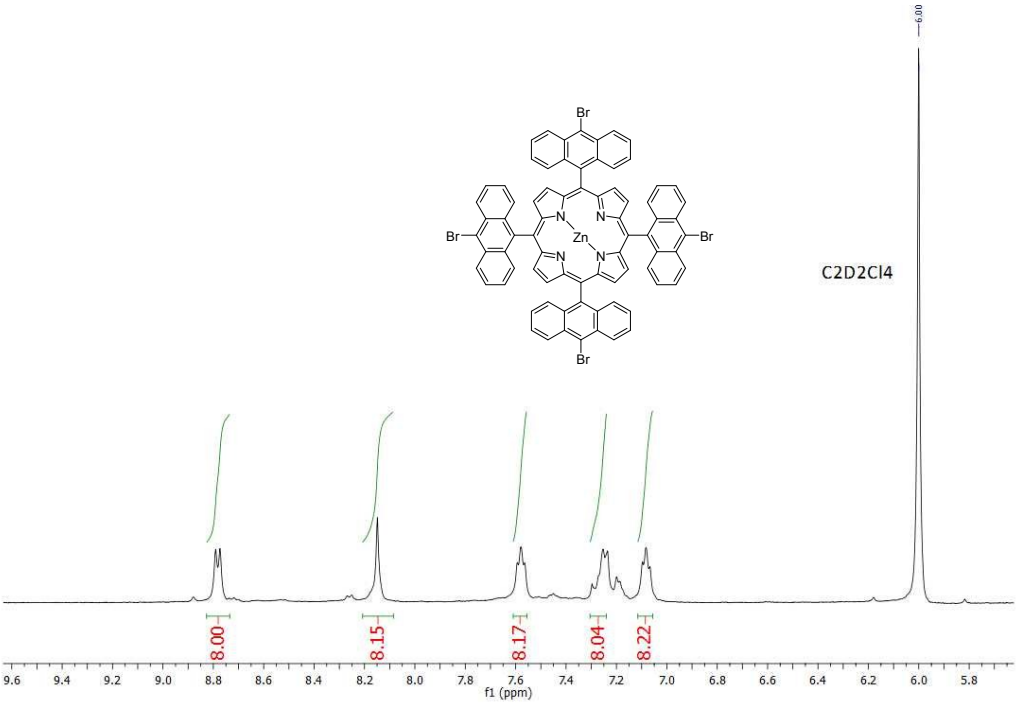


Figure S4. HPLC chromatogram for **BrTAP**, elution with toluene/heptane 1:1



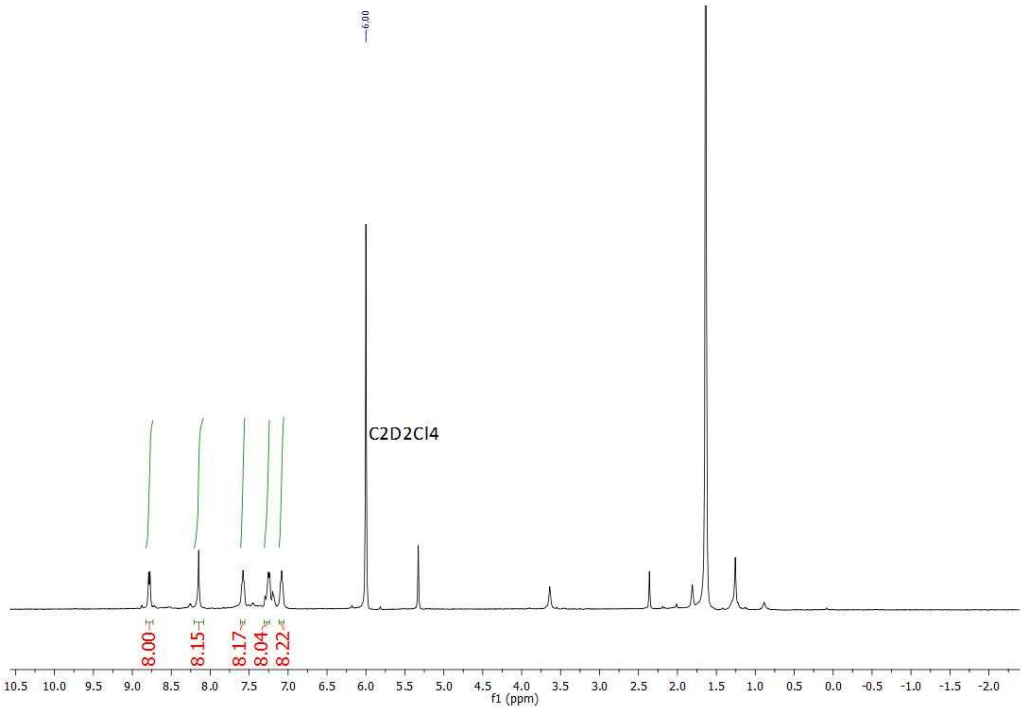


Figure S5. ^{1}H NMR spectra of **ZnBrTAP** (400 MHz, $C_2D_2Cl_4$, 298K)

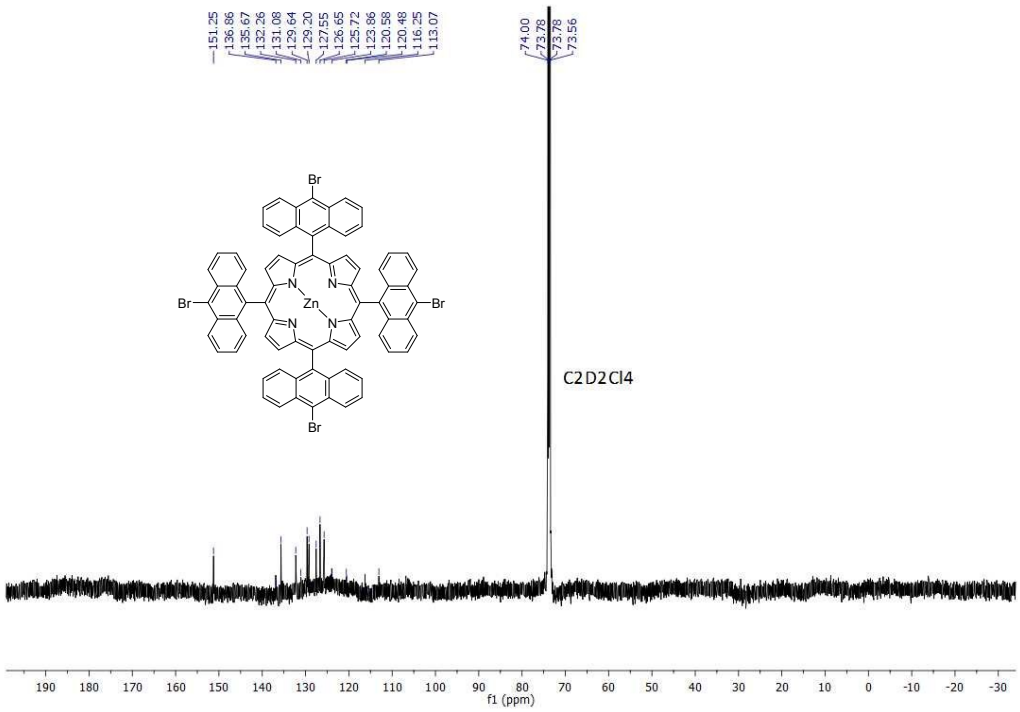


Figure S6. ^{13}C NMR spectra of **ZnBrTAP** (125 MHz, $C_2D_2Cl_4$, 333K)

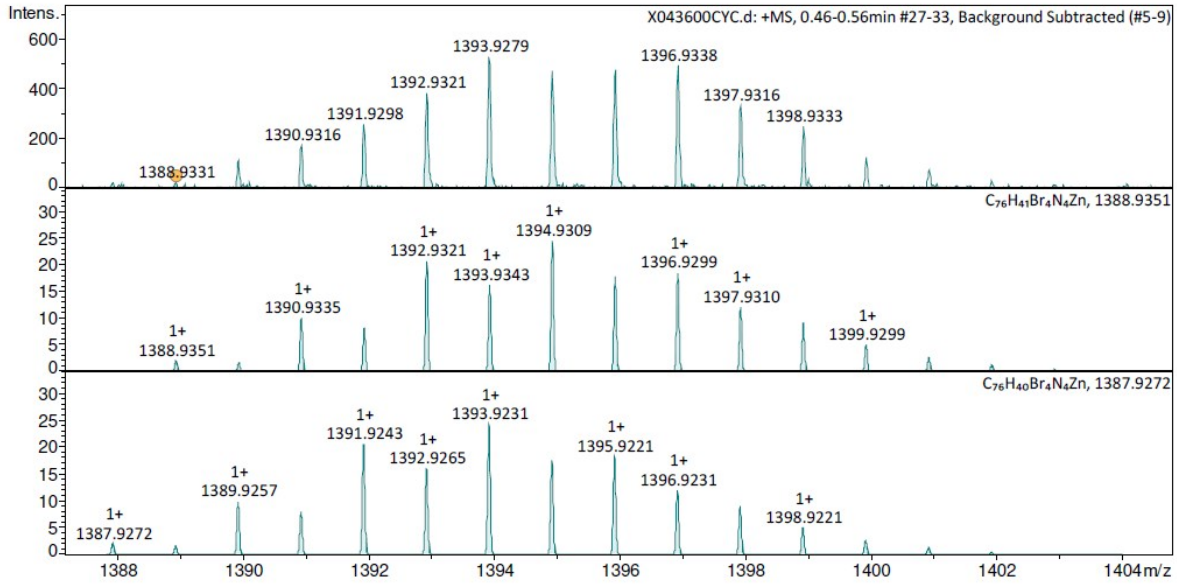


Figure S7. HRMS, ESI-QTOF for **ZnBrTAP,** fingerprint of experimental spectrum (top) corresponded to a mix of MH+ and M+ as compared with simulated spectra (middle and bottom)

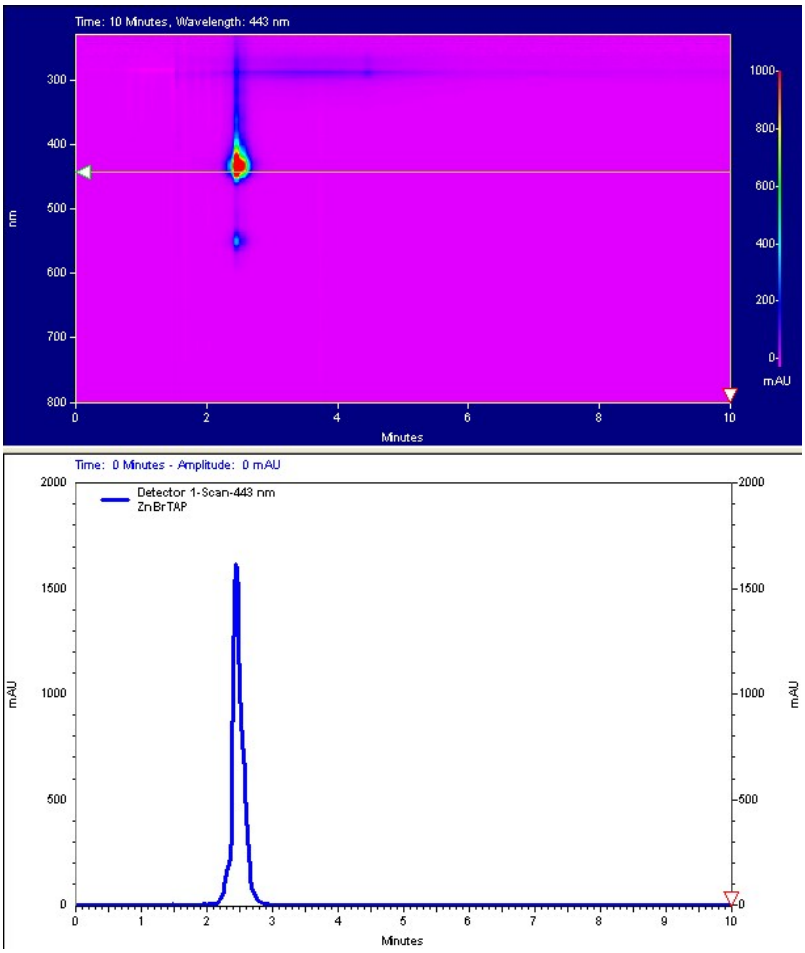


Figure S8. HPLC chromatogram for **ZnBrTAP**, elution with toluene/heptane 1:1

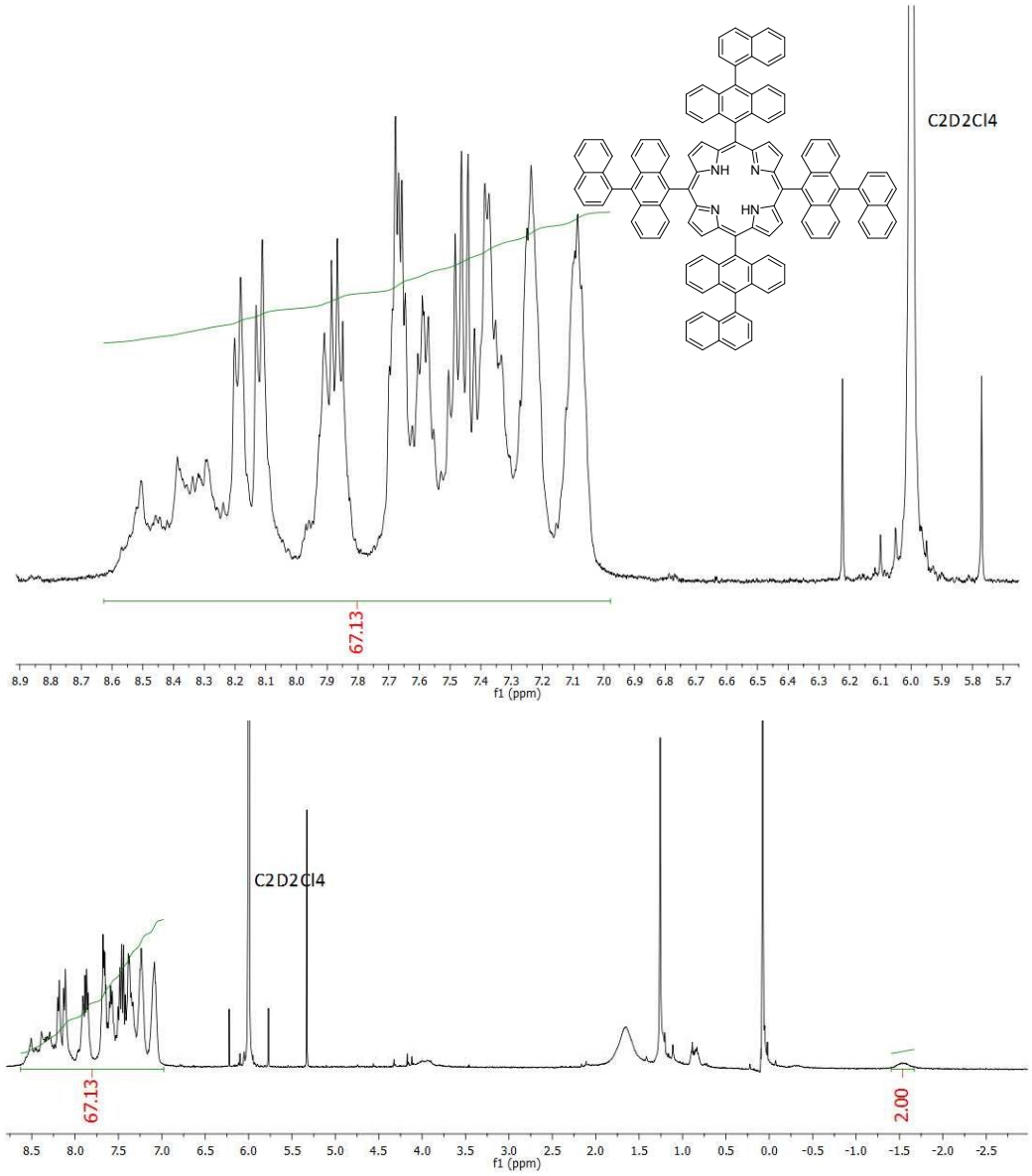


Figure S9. ^{1}H NMR spectra of **TNAP** (400 MHz, $C_2D_2Cl_4$, 298K)

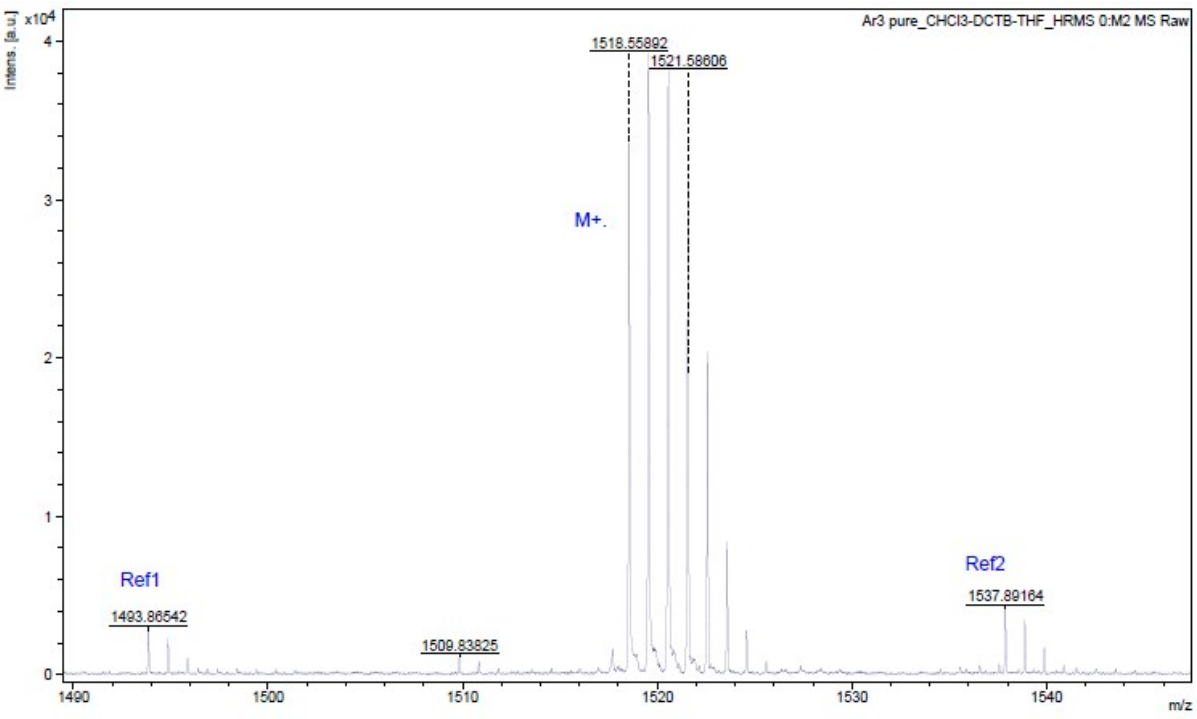


Figure S10. HRMS, MALDI-TOF for **TNAP**

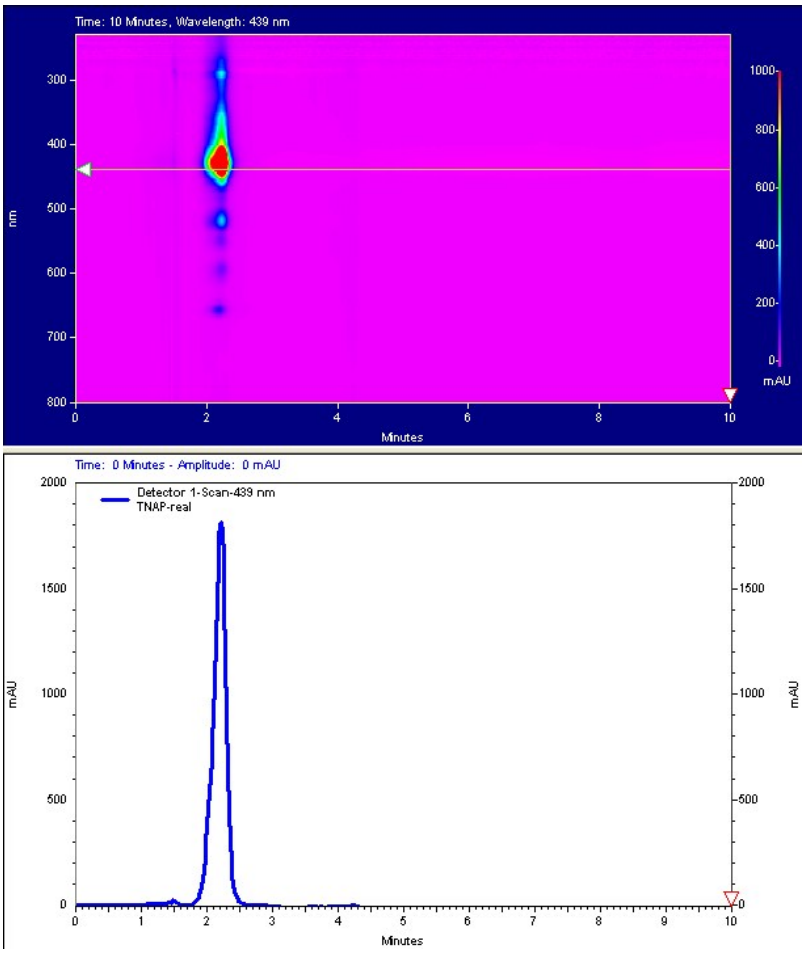


Figure S11. HPLC chromatogram for **TNAP**, elution with toluene/heptane 1:1

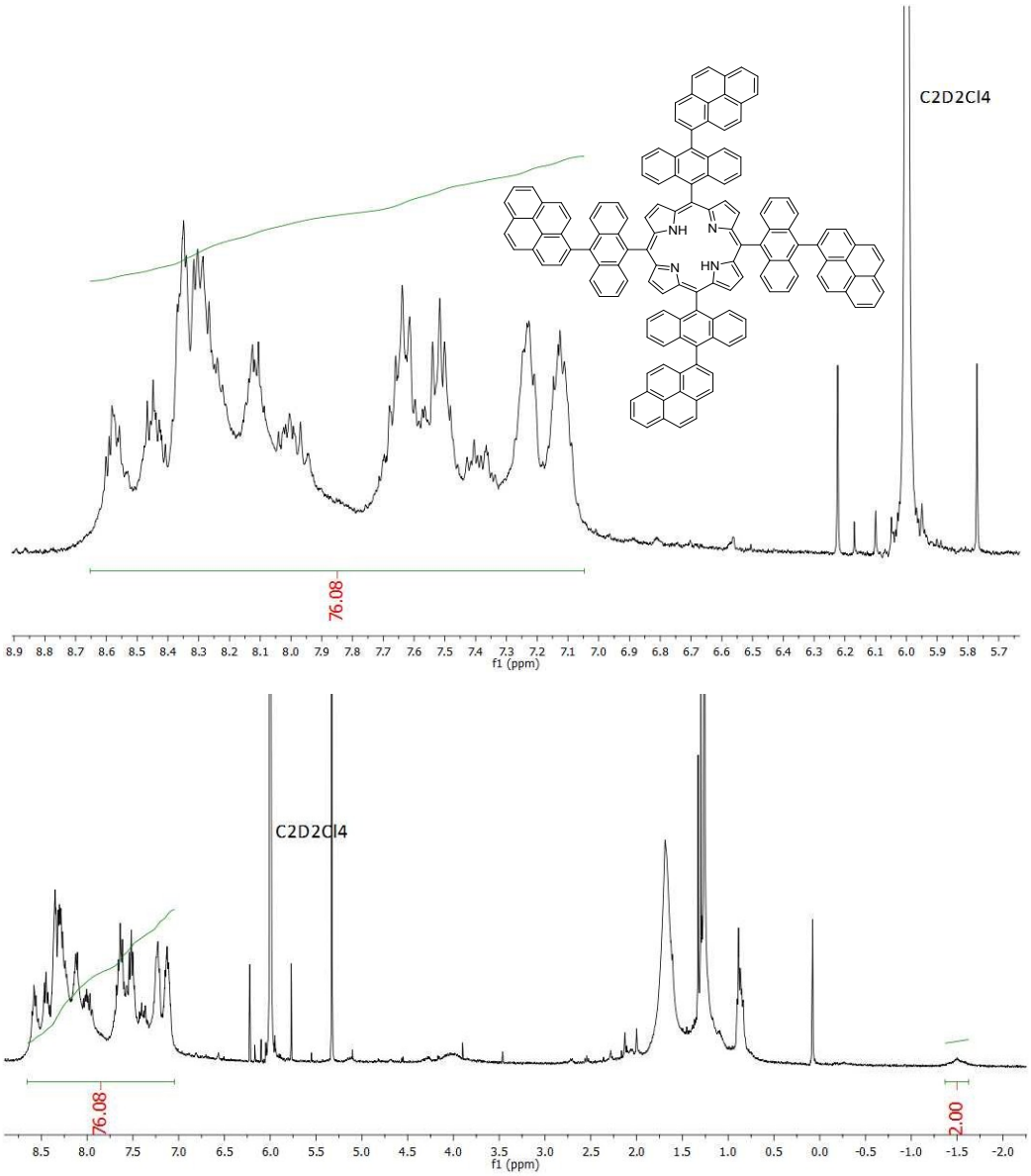


Figure S12. ^{1}H NMR spectra of **TPyAP** (400 MHz, $C_2D_2Cl_4$, 298K)

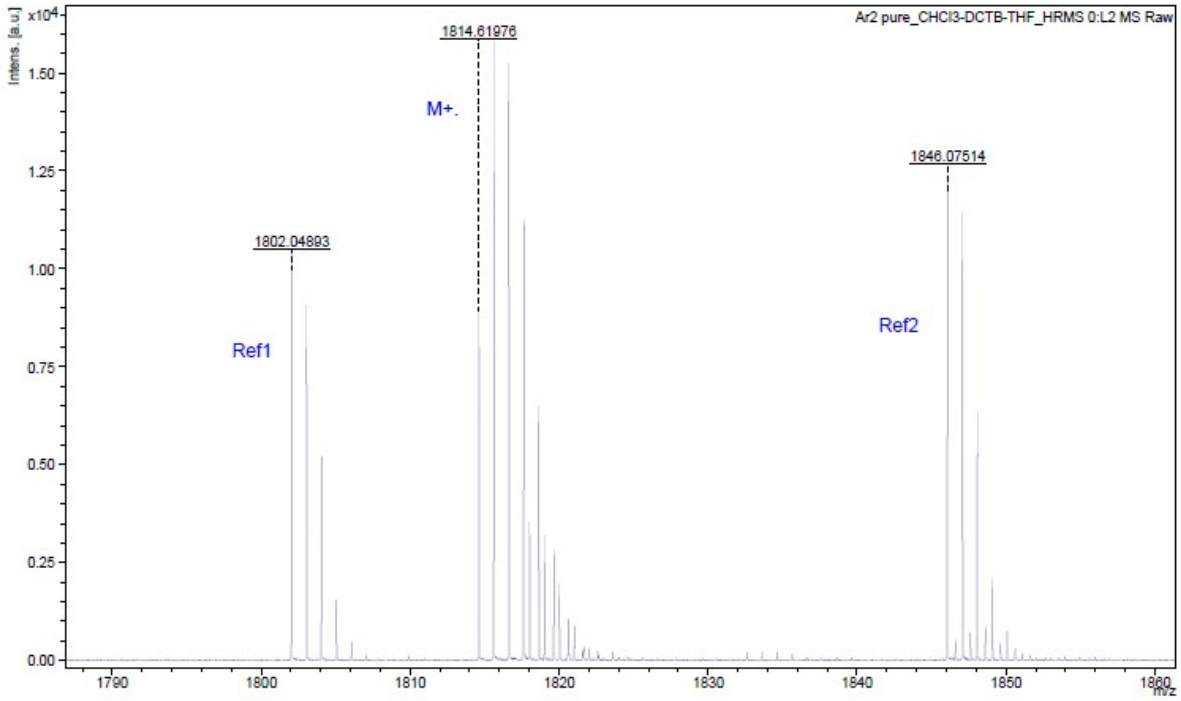


Figure S13. HRMS, MALDI-TOF for **TPyAP**

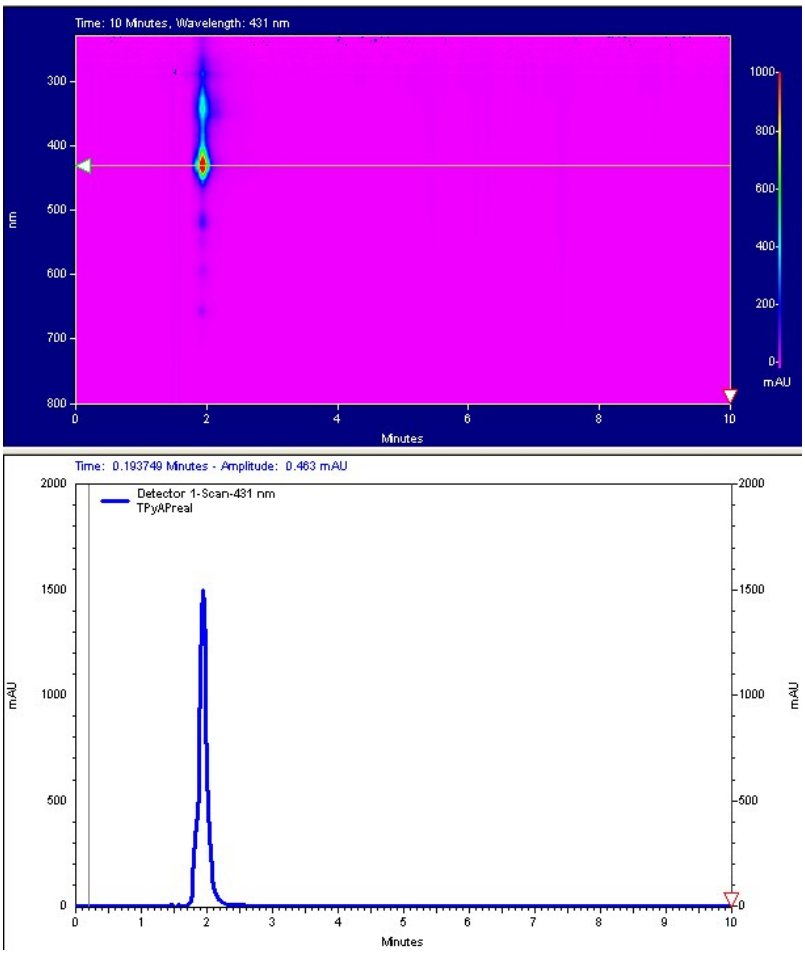


Figure S14. HPLC chromatogram for **TPyAP**, elution with toluene/heptane 1:1

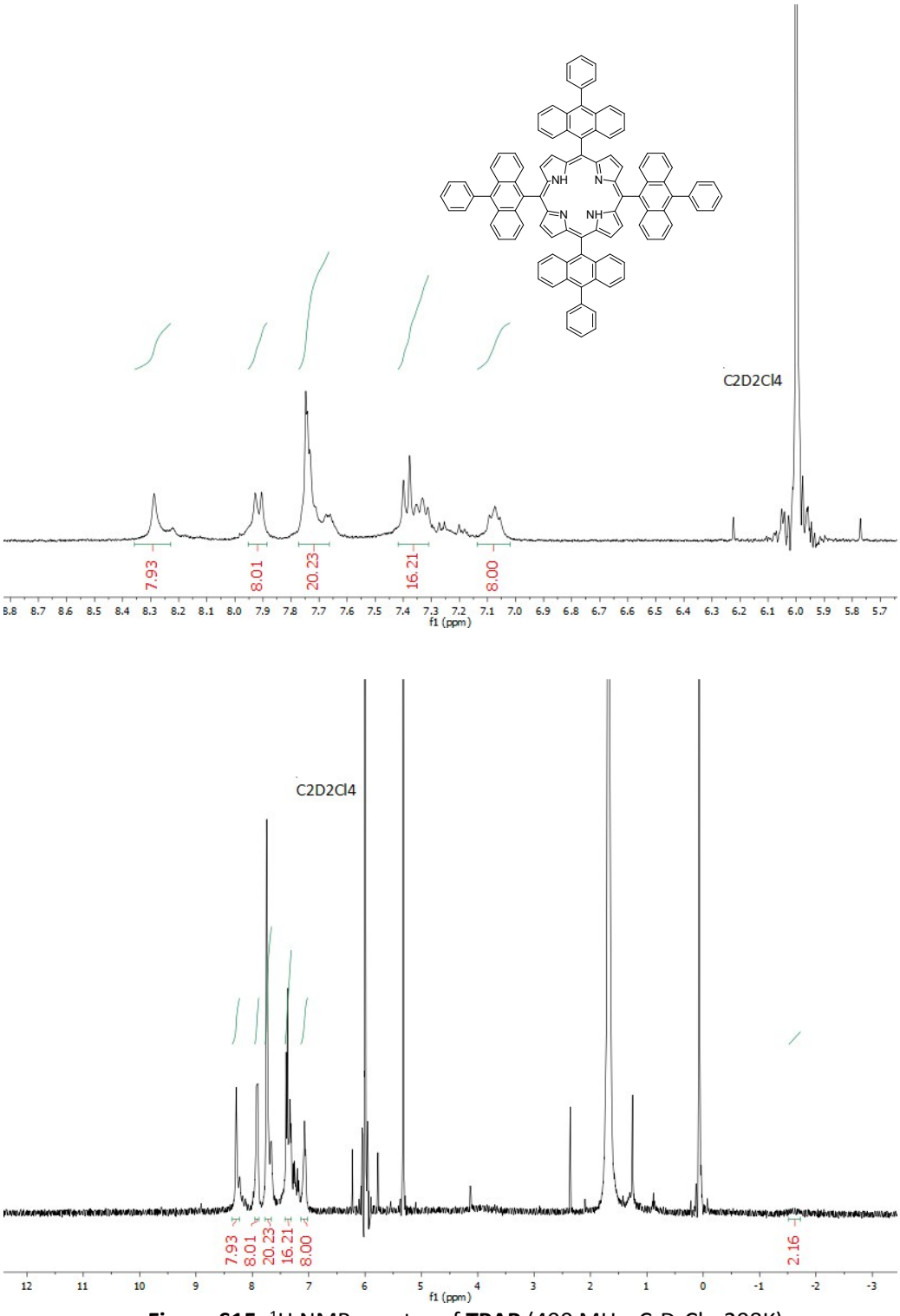


Figure S15. ^{1}H NMR spectra of **TPAP** (400 MHz, $C_2D_2Cl_4$, 298K)

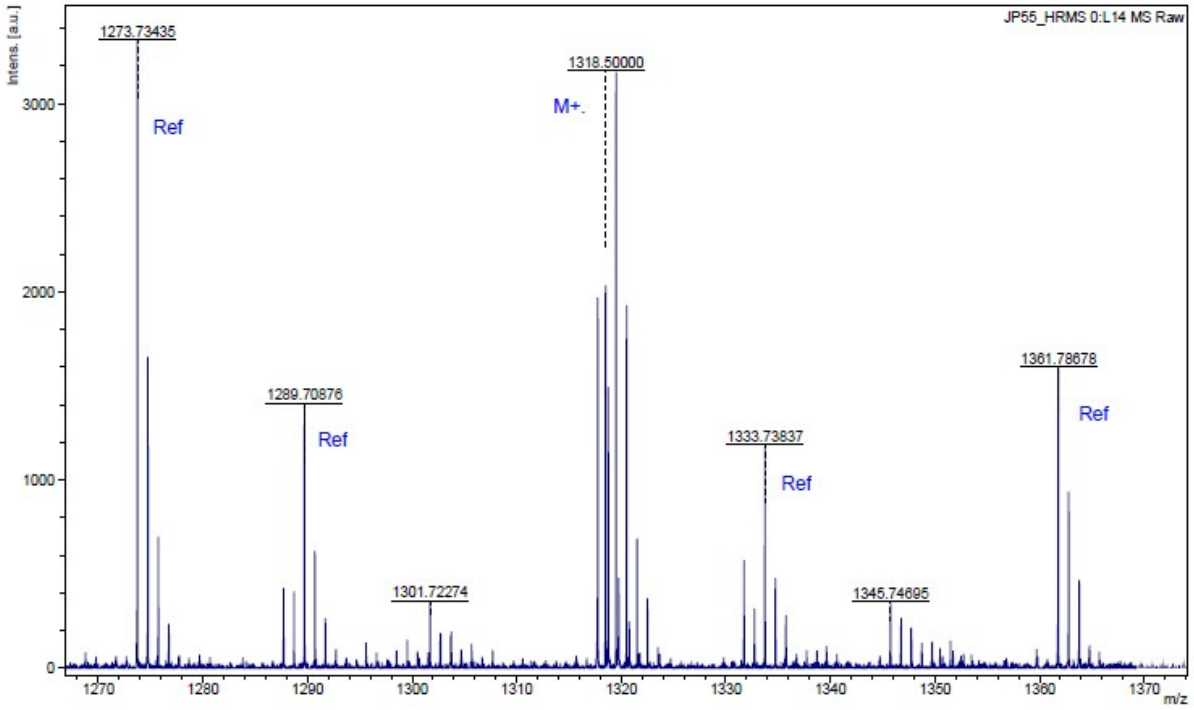


Figure S16. HRMS, MALDI-TOF for **TPAP**

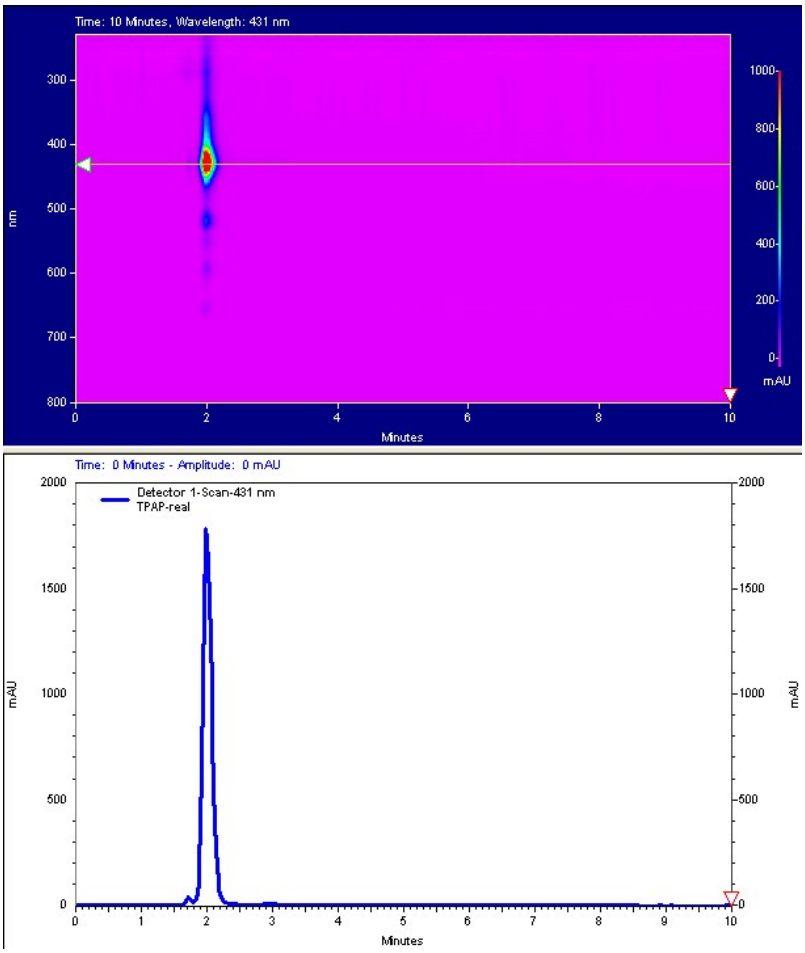


Figure S17. HPLC chromatogram for **TPAP**, elution with toluene/heptane 1:1

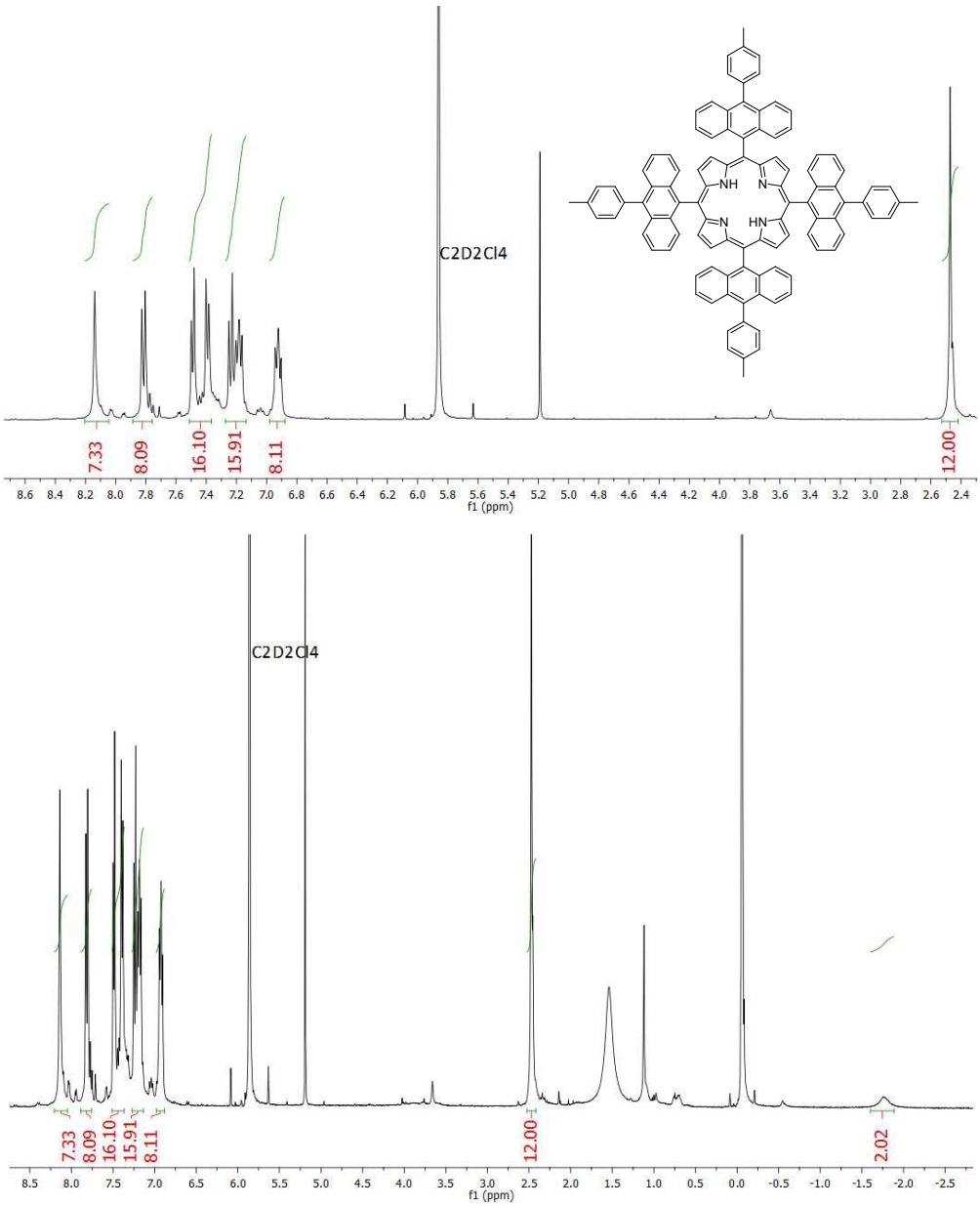


Figure S18. ^{1}H NMR spectra of **TTAP** (400 MHz, $C_2D_2Cl_4$, 298K)

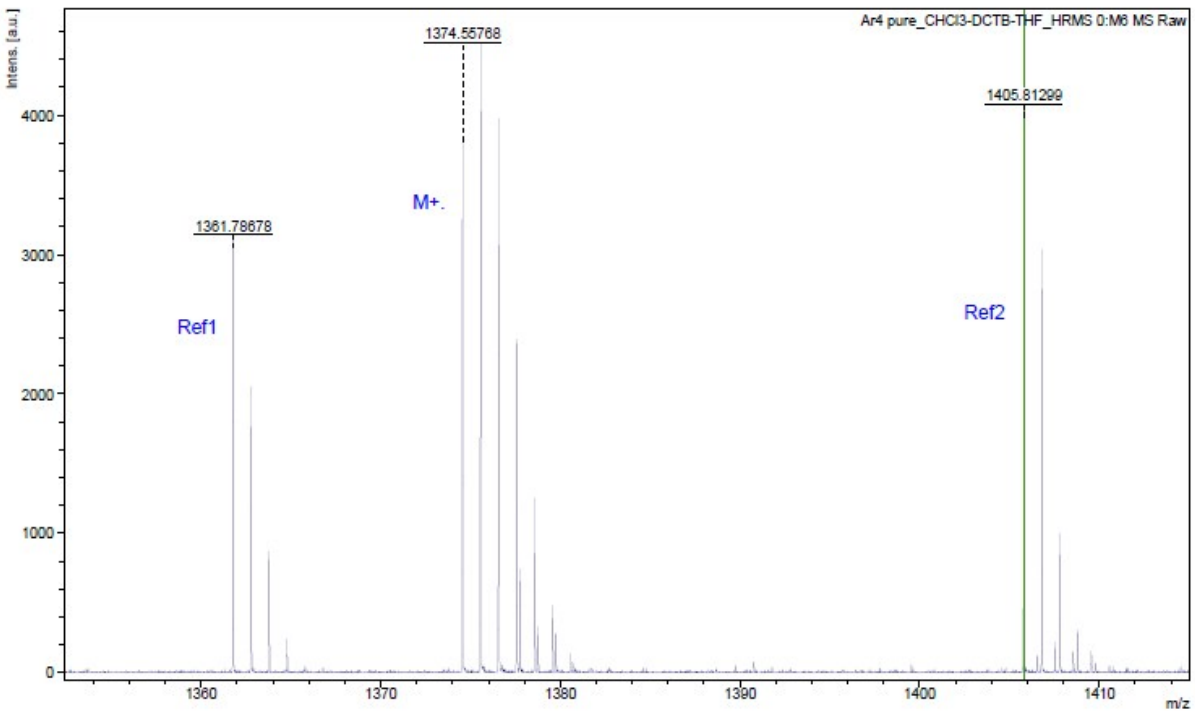


Figure S19. HRMS, MALDI-TOF for **TTAP**

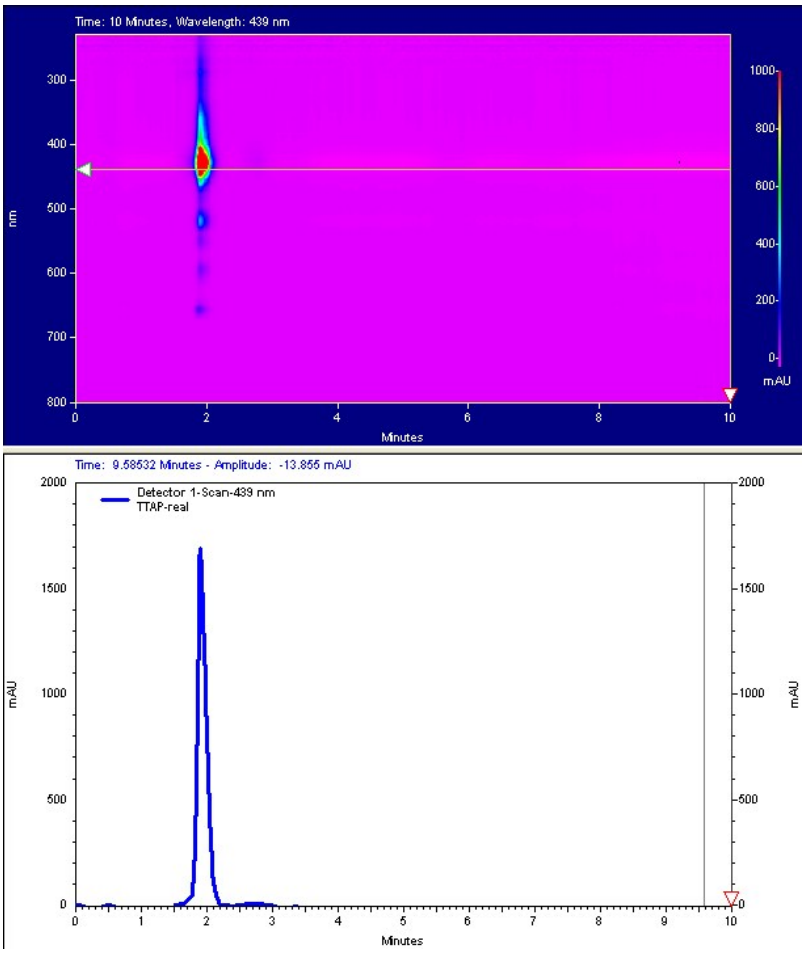


Figure S20. HPLC chromatogram for **TTAP**, elution with toluene/heptane 1:1

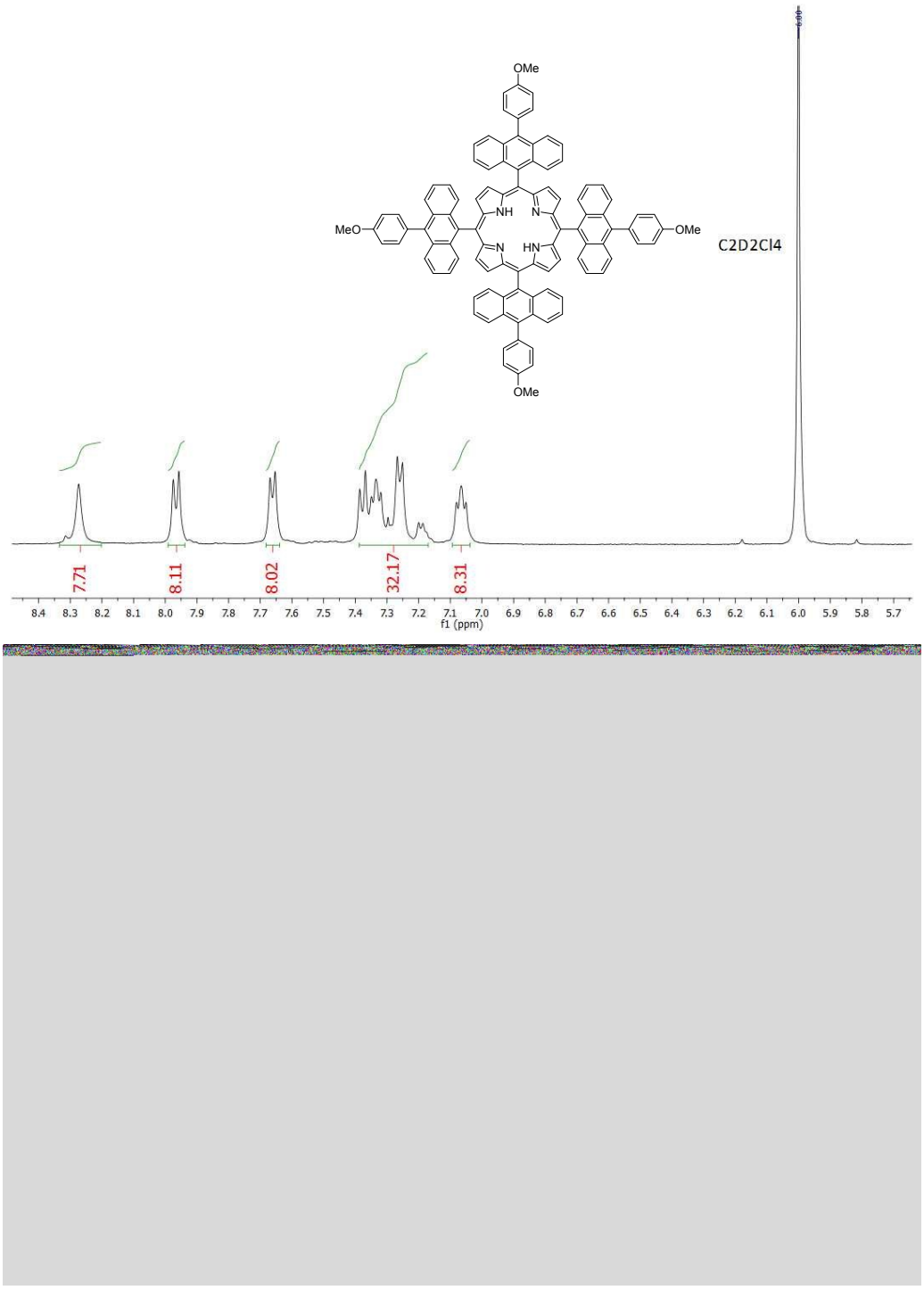


Figure S21. ^{1}H NMR spectra of **TMPAP** (400 MHz, $C_2D_2Cl_4$, 298K)

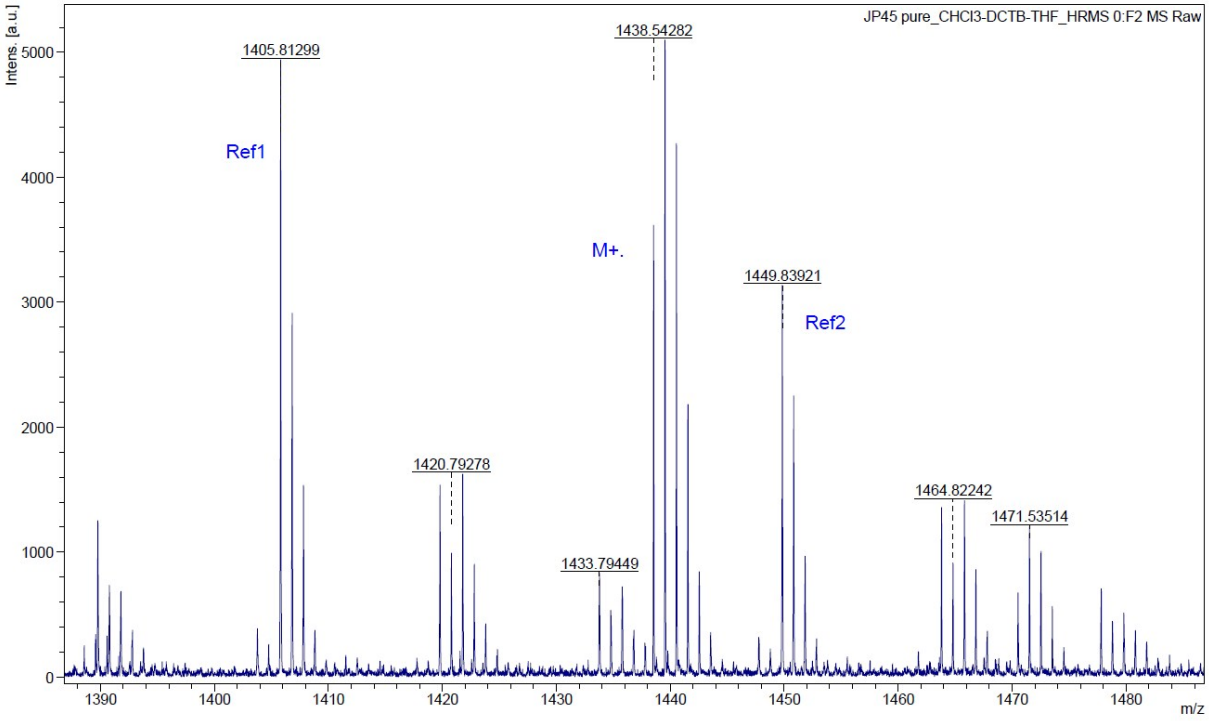


Figure S22. HRMS, MALDI-TOF for **TMPAP**

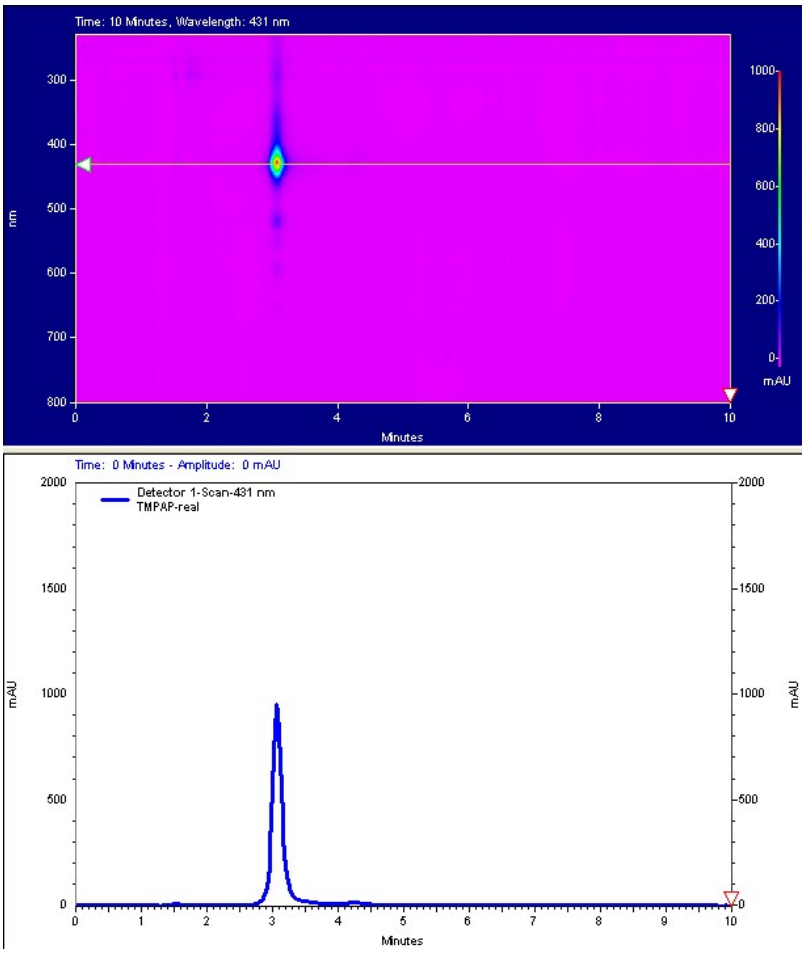
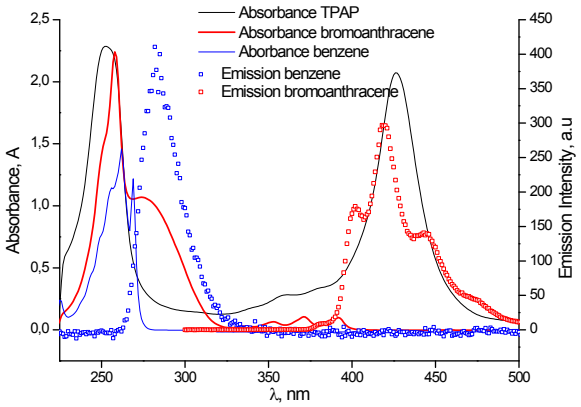
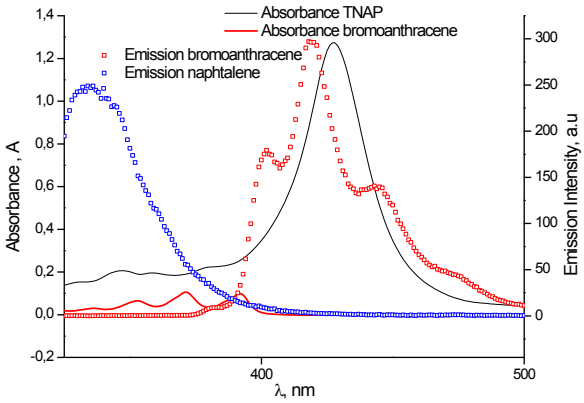


Figure S23. HPLC chromatogram for **TMPAP**, elution with toluene/heptane 80:20

a



b



c

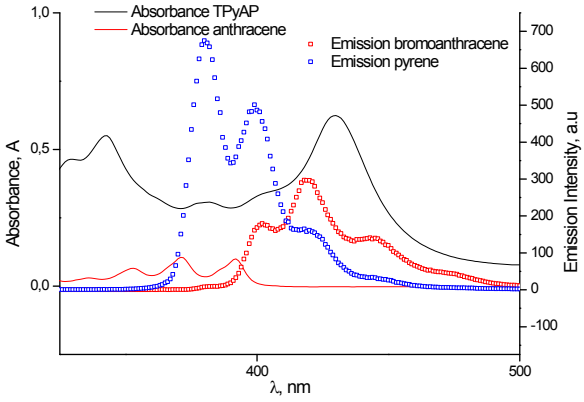


Figure S24. Spectral overlap in DCM of emission spectrum of free external PAH (phenyl/naphthalene/pyrene, blue), absorption and emission spectra of anthracene (red) and absorption spectrum (black) of **TPAP** (a**), TNAP** (b) and **TPyAP** (c).

DFT Data. Molecular coordinates (Å) and corresponding total energies (eV) for the molecular optimized geometries, calculated from DFT.

TPAP

166

ETOT = -17342.731948

C	64.866519	-25.396045	7.972914
C	65.743458	-26.221443	7.388750
C	66.412914	-25.443412	6.325461
N	65.924232	-24.161219	6.282548
C	64.975900	-24.098823	7.273434
C	64.183485	-22.972778	7.599476
C	67.422867	-25.978849	5.491312
C	64.234176	-21.724277	6.949520
C	68.103866	-25.272365	4.480710
C	69.148322	-25.759102	3.623553
C	69.528582	-24.757194	2.784087
C	68.738163	-23.591816	3.066872
N	67.888588	-23.948831	4.109296
N	65.057784	-21.379120	5.882623
C	64.811497	-20.069790	5.481878
C	63.783796	-19.575622	6.354874
C	63.441534	-20.560404	7.230261
C	68.794426	-22.340484	2.422537
C	67.972038	-21.227531	2.720262
C	65.452738	-19.379881	4.434063
C	66.476692	-19.908198	3.612821
C	68.049238	-19.944566	1.990229
C	67.130391	-19.137698	2.534387
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H	62.697872	-20.510014	8.018845
H	68.730159	-19.732072	1.171076
H	66.889100	-18.113930	2.263539
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C	63.876937	-17.717186	3.358032
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C	64.089437	-15.275545	3.767962
C	63.418173	-16.358566	3.139583
C	67.098887	-28.426917	4.953816
C	68.862040	-27.788096	6.535257
C	69.230001	-29.182654	6.693384
C	68.528266	-30.186196	5.972944
C	67.465087	-29.822445	5.103138
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C	62.267024	-16.181066	2.296714
C	70.326479	-29.475483	7.576213
C	66.707065	-30.784323	4.349848
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H	67.184865	-23.319835	4.543536
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C	61.863228	-23.546599	8.434200
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C	65.341525	-29.039852	3.368243
C	65.690760	-30.412711	3.516938
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C	71.001972	-28.492706	8.241621

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C	64.304302	-22.154019	12.694677
C	68.915660	-31.648794	6.127325
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H	65.608960	-13.447702	5.111950
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H	69.310181	-25.748672	7.130823
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H	62.319051	-22.685924	13.266559
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H	71.832536	-28.746767	8.901486
H	72.913693	-20.527880	4.346507
H	74.645629	-20.259634	2.573413
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H	60.747736	-17.071693	1.090715
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H	67.535967	-13.921486	6.568809
H	66.255712	-21.676678	11.850072
H	64.611884	-21.904443	13.710960
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C	68.857762	-33.732603	7.392391
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C	70.029211	-33.649833	5.290078
C	69.679886	-32.308131	5.146444
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C	72.805503	-20.655524	-2.698864
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H	68.530086	-34.286279	8.273381
H	69.888351	-35.419005	6.520893
H	70.625411	-34.138142	4.517938
H	70.004652	-31.756867	4.262562
H	62.629112	-13.676662	5.468017
H	61.845299	-11.359206	5.095002
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H	60.679289	-25.625263	12.281937
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TNAP

190

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N	65.732418	-24.247627	6.118426
C	64.629529	-24.277522	6.937968
C	63.776242	-23.184604	7.239532
C	67.393479	-25.981150	5.456681
C	63.922545	-21.875762	6.730434
C	68.194052	-25.186369	4.605175
C	69.358855	-25.592719	3.871244
C	69.811580	-24.535510	3.140085
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222

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H	71.528541	-35.540163	2.485162

H	66.414895	-33.317889	7.132574
H	70.668793	-37.461462	3.769808
H	69.129481	-38.379685	5.518464
H	67.360957	-38.028661	7.219064
H	66.449109	-35.761011	7.637687
C	79.213642	-21.122393	-1.086953
C	79.584875	-23.599582	-0.967523
C	79.130370	-24.870895	-0.626112
H	78.762552	-19.040380	-1.126191
H	77.523849	-26.046566	0.204746
H	80.202696	-21.001397	-1.533386
H	80.573167	-23.473320	-1.412265
H	79.767375	-25.738032	-0.806388