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Supporting Information

Synthesis of 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetraarylporphyrins *via* a Clauson-Kaas reaction and the study of their electronic properties†

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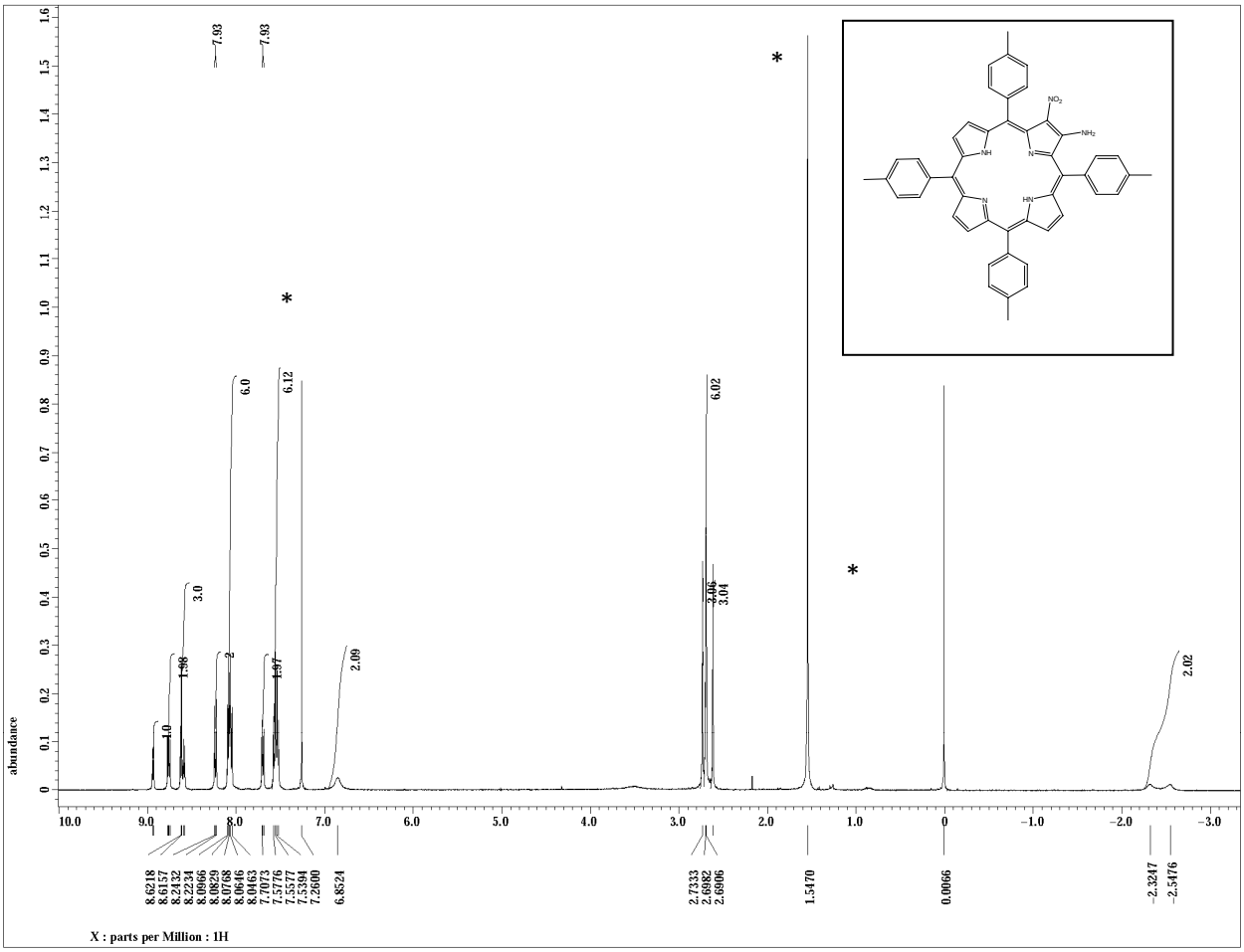


Figure S1. ^{1}H NMR spectrum of 2-amino-3-nitro-tetra-*p*-tolylporphyrin (**8**).

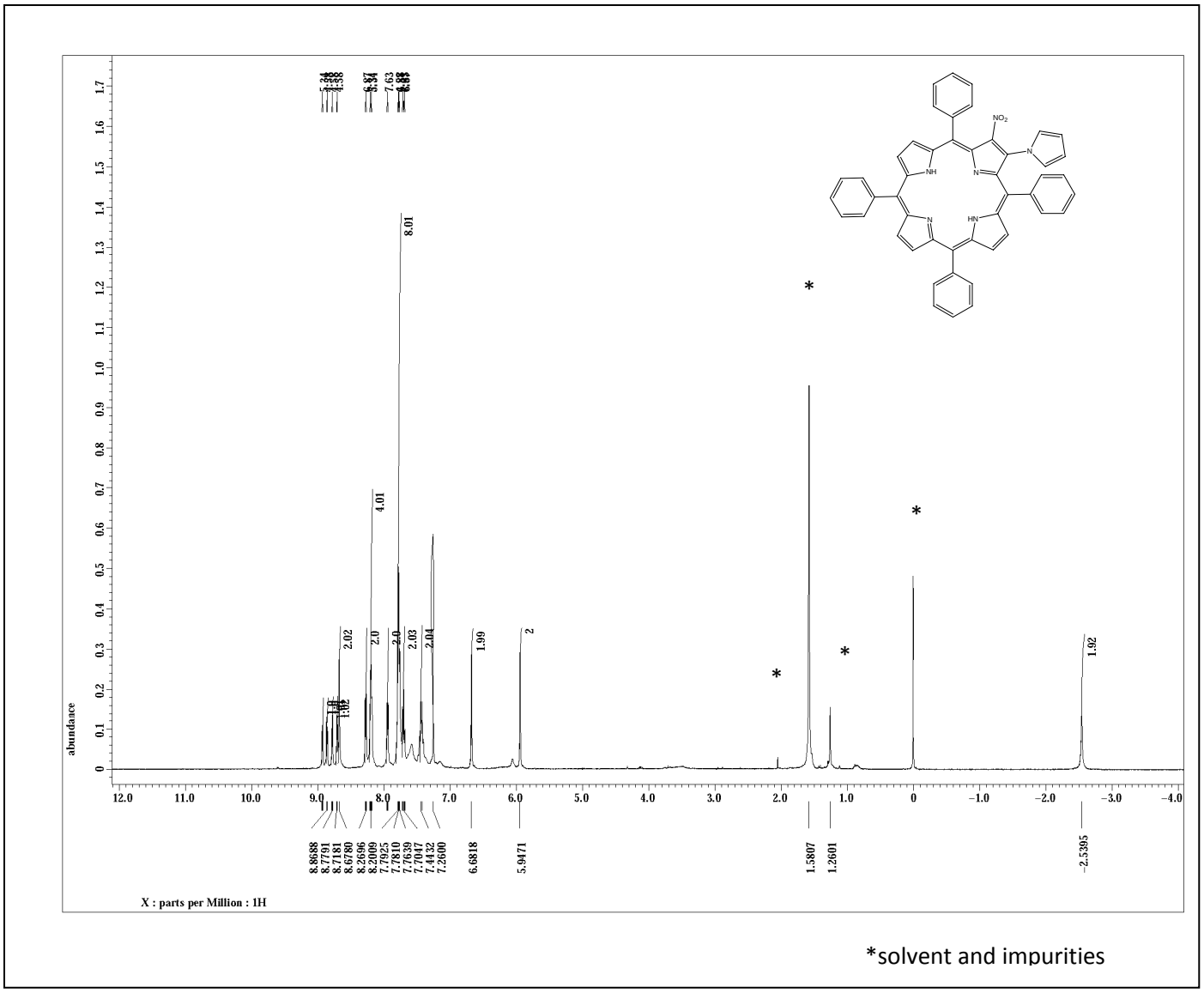


Figure S2. ^{1}H NMR spectrum of 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetraphenylporphyrin (**10**).

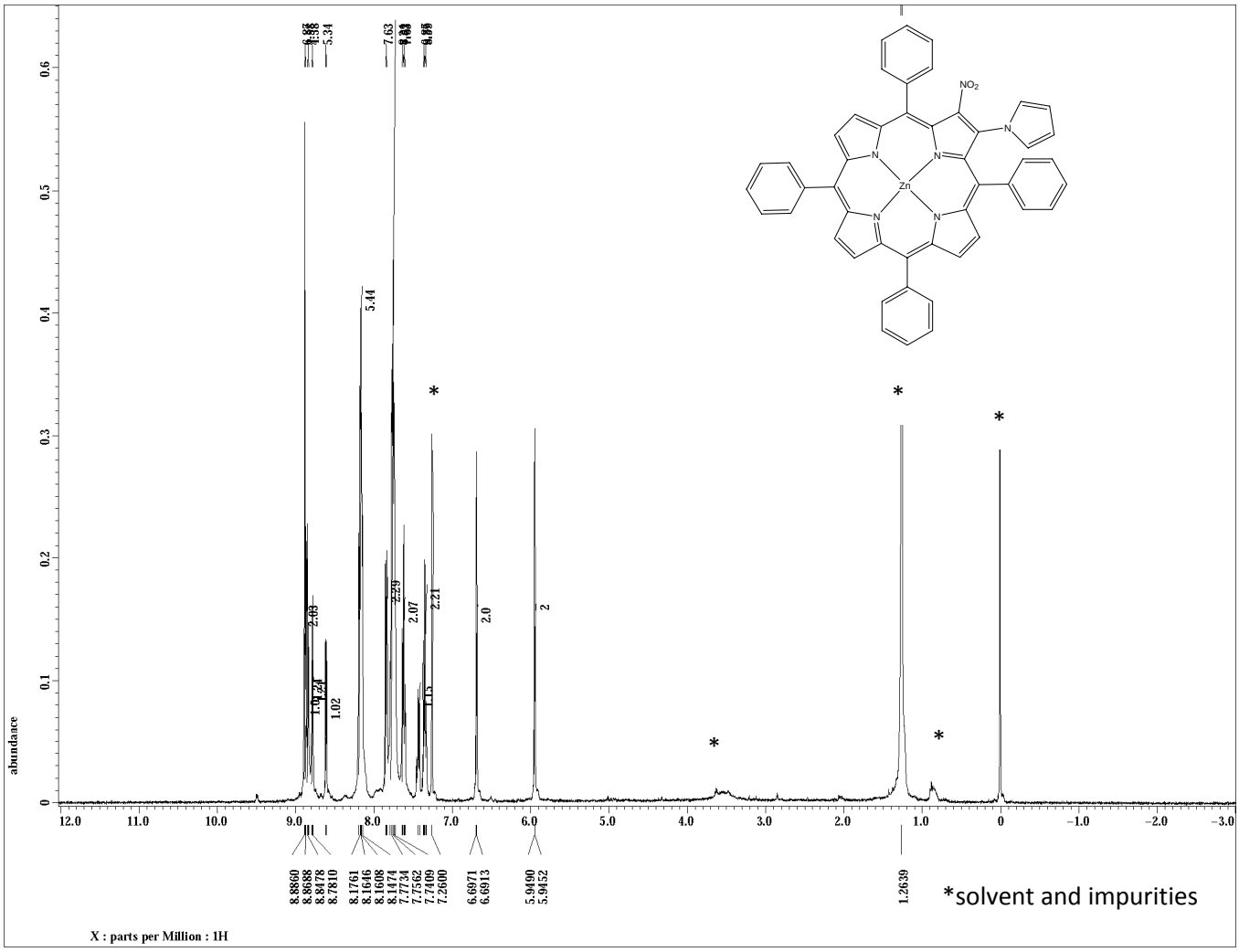


Figure S3. ^{1}H NMR spectrum of zinc(II) 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetraphenyl-porphyrin (**12**).

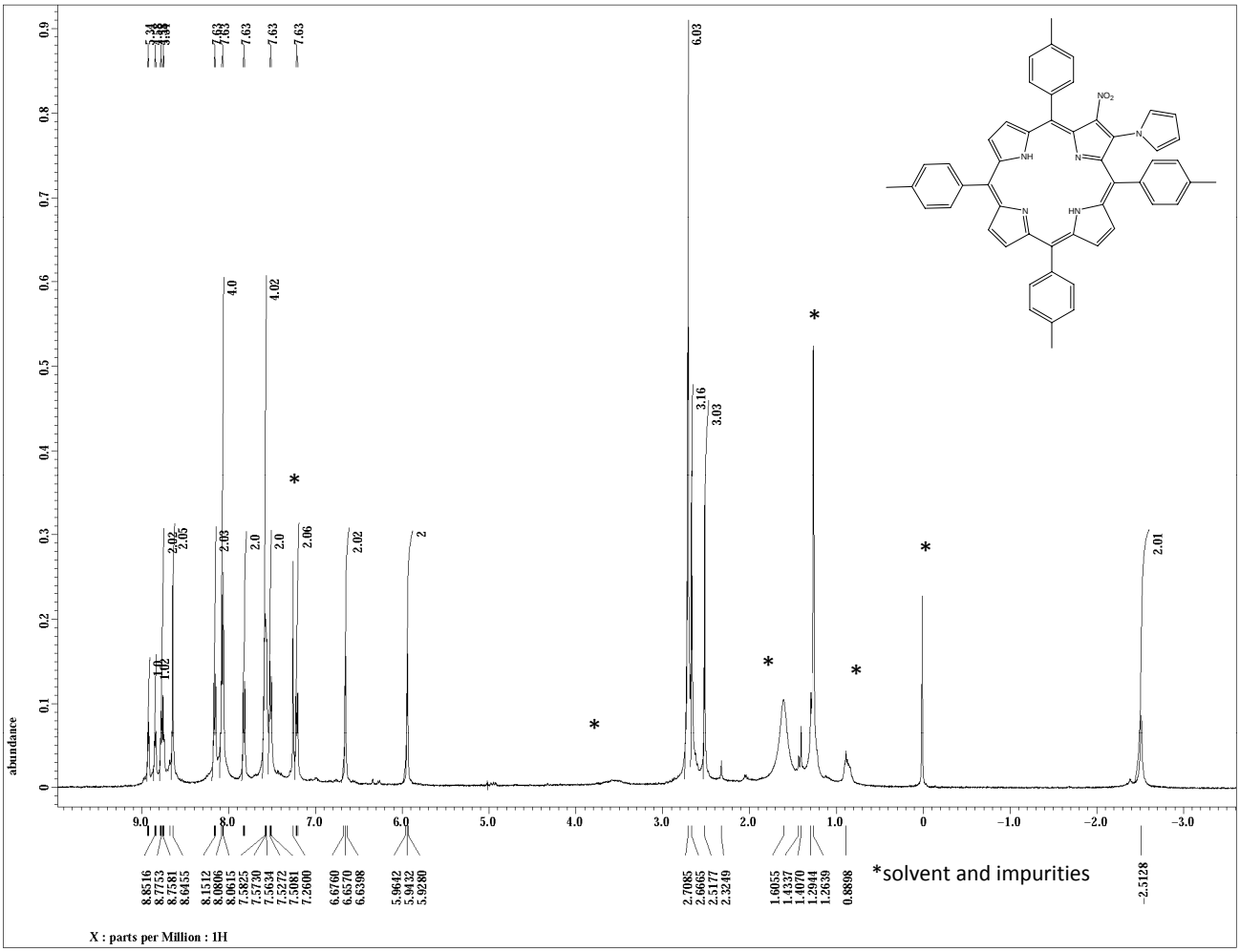


Figure S4. ^{1}H NMR spectrum of 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetra-*p*-tolylporphyrin (**14**).

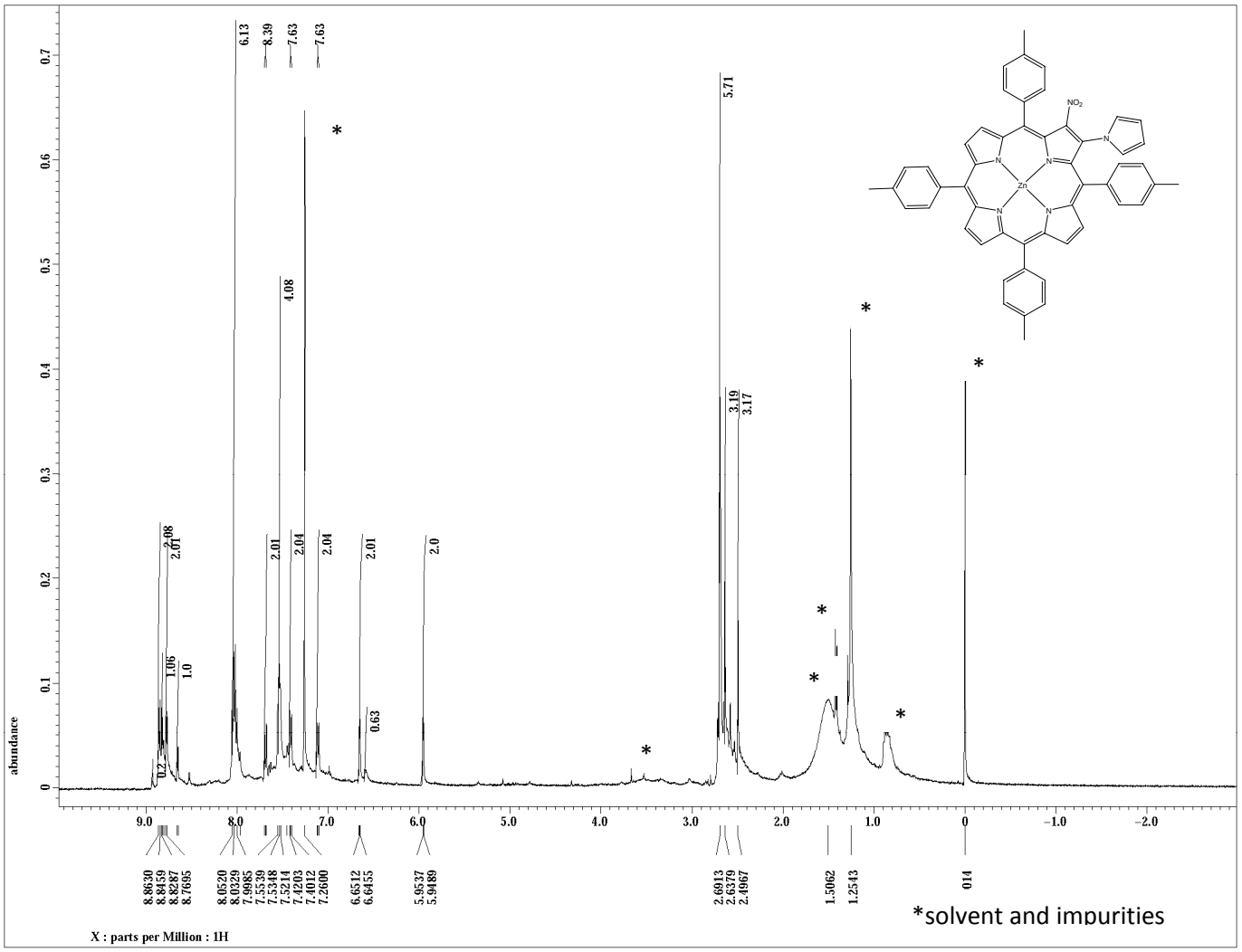


Figure S5. ^{1}H NMR spectrum of zinc(II) 2-nitro -3-(pyrrol-1-yl)-5,10,15,20-tetra-*p*-tolyl-porphyrin (**16**).

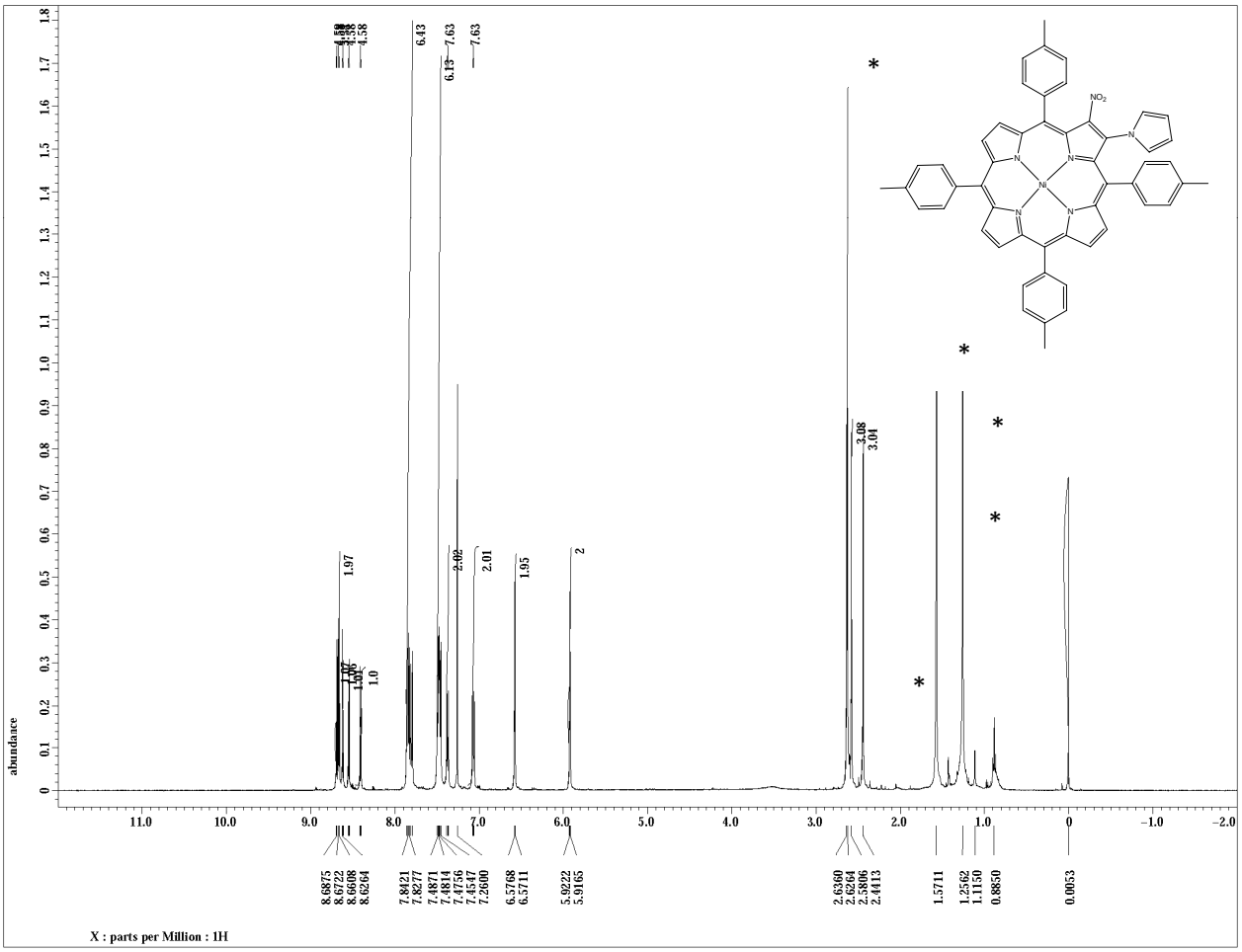


Figure S6. ^{1}H NMR spectrum of nickel(II) 2-nitro -3-(pyrrol-1-yl)-5,10,15,20-tetra-*p*-tolyl-porphyrin (**17**).

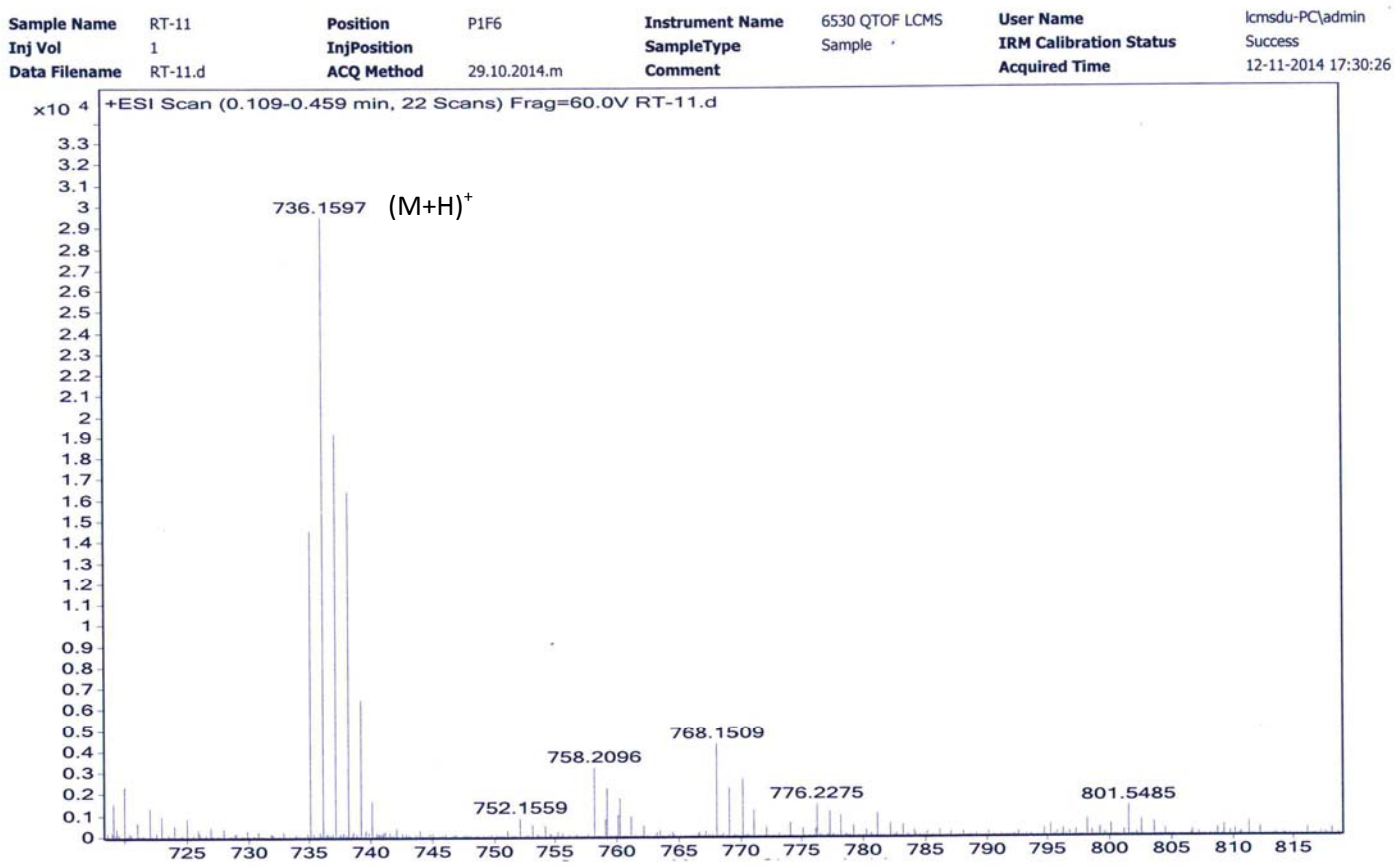


Figure S 7. ESI-HRMS of copper(II) 2-amino-3-nitro-5,10,15,20-tetraphenylporphyrin (**3**).

Qualitative Compound Report

Data File	RT47.d	**Sample Name**	RT47
Sample Type	Sample	**Position**	P1C8
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	19-09-2014 14:39:47
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

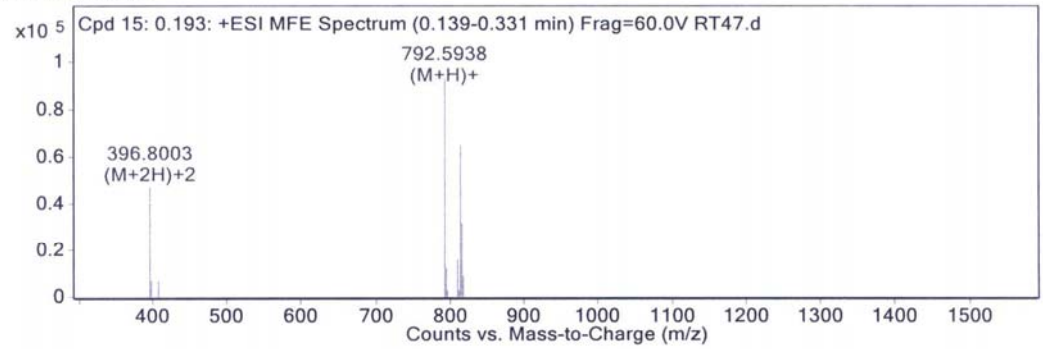
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	MFG Formula
Cpd 15: 0.193	0.193	791.5864	> limit

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 15: 0.193	792.5938	0.193	Find by Molecular Feature	791.5864

MFE MS Spectrum



MFE MS Zoomed Spectrum

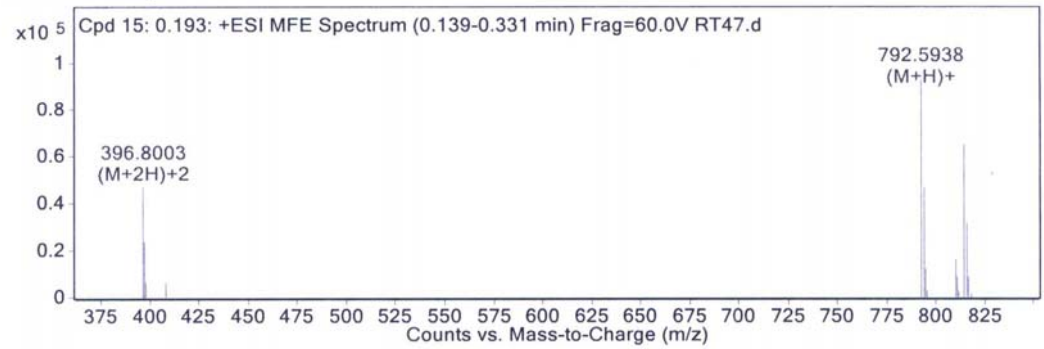


Figure S8. ESI-HRMS of copper(II) 2-amino-3-nitro-5,10,15,20-tetra-*p*-tolylporphyrin (**7**).

Qualitative Compound Report

Data File	RT26.d	**Sample Name**	RT26
Sample Type	Sample	**Position**	P1F2
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	22-09-2014 16:36:39
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

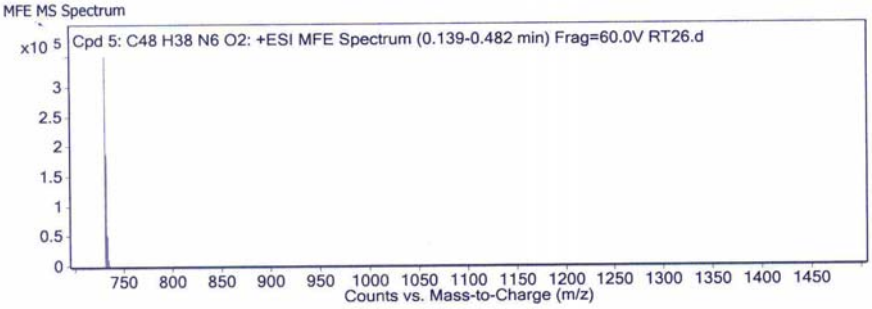
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C48 H38 N6 O2	0.227	730.3061	C48 H38 N6 O2	C48 H38 N6 O2	-0.63	C48 H38 N6 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C48 H38 N6 O2	731.3134	0.227	Find by Molecular Feature	730.3061

MFE MS Spectrum



MFE MS Zoomed Spectrum

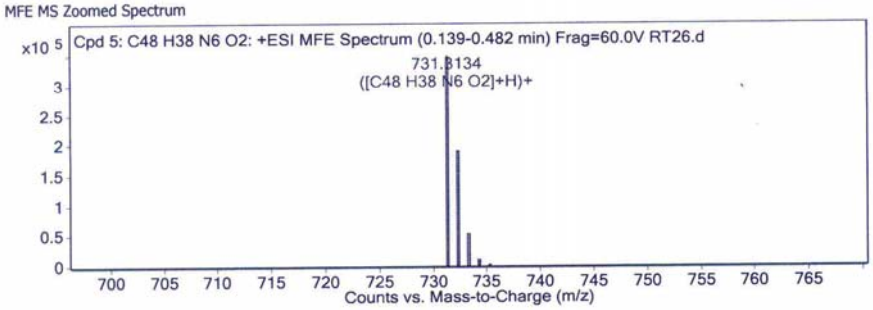


Figure S9. ESI-HRMS of 2-amino-3-nitro-5,10,15,20-tetra-*p*-tolylporphyrin (**8**).

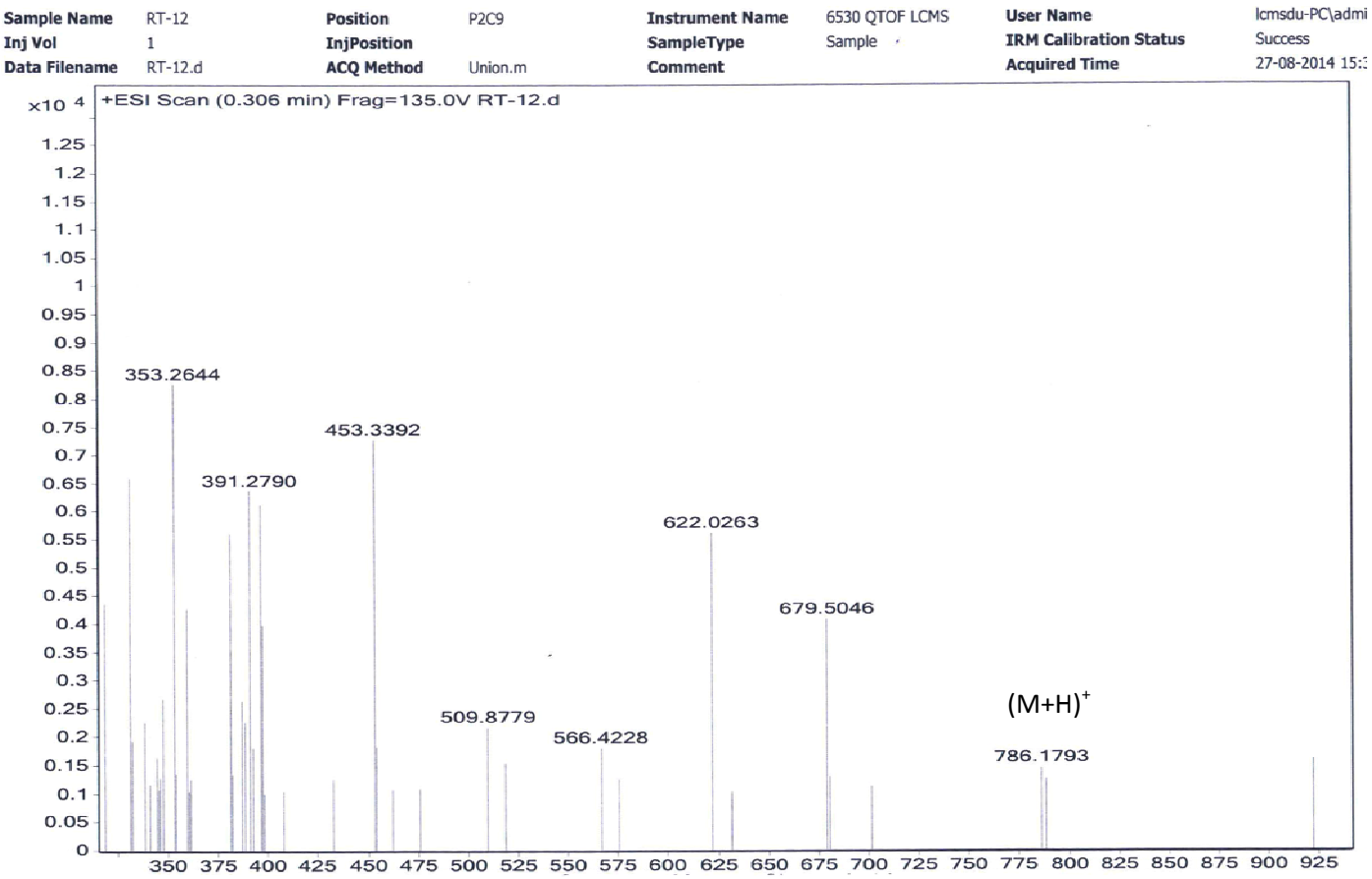


Figure S10. ESI-HRMS of copper(II) 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetraphenylporphyrin (**9**).

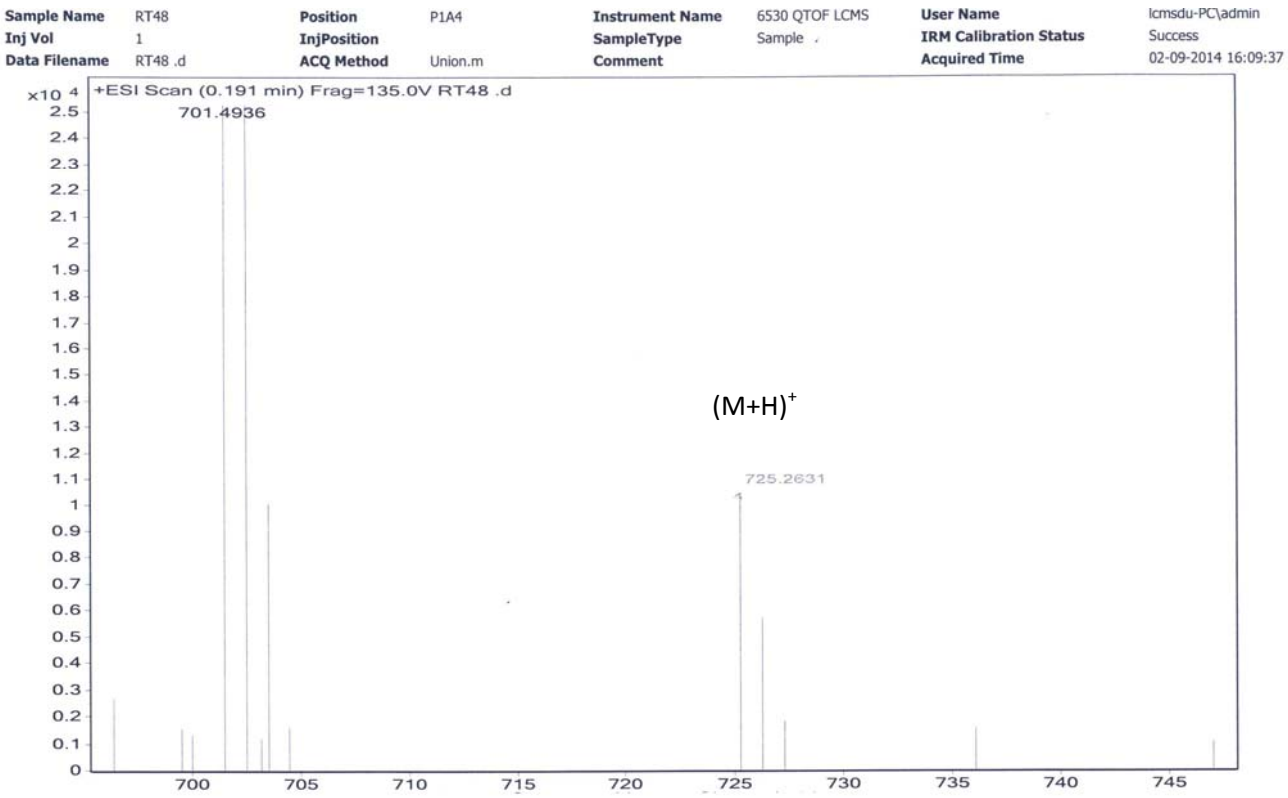


Figure S11. ESI-HRMS of 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetraphenylporphyrin (**10**).

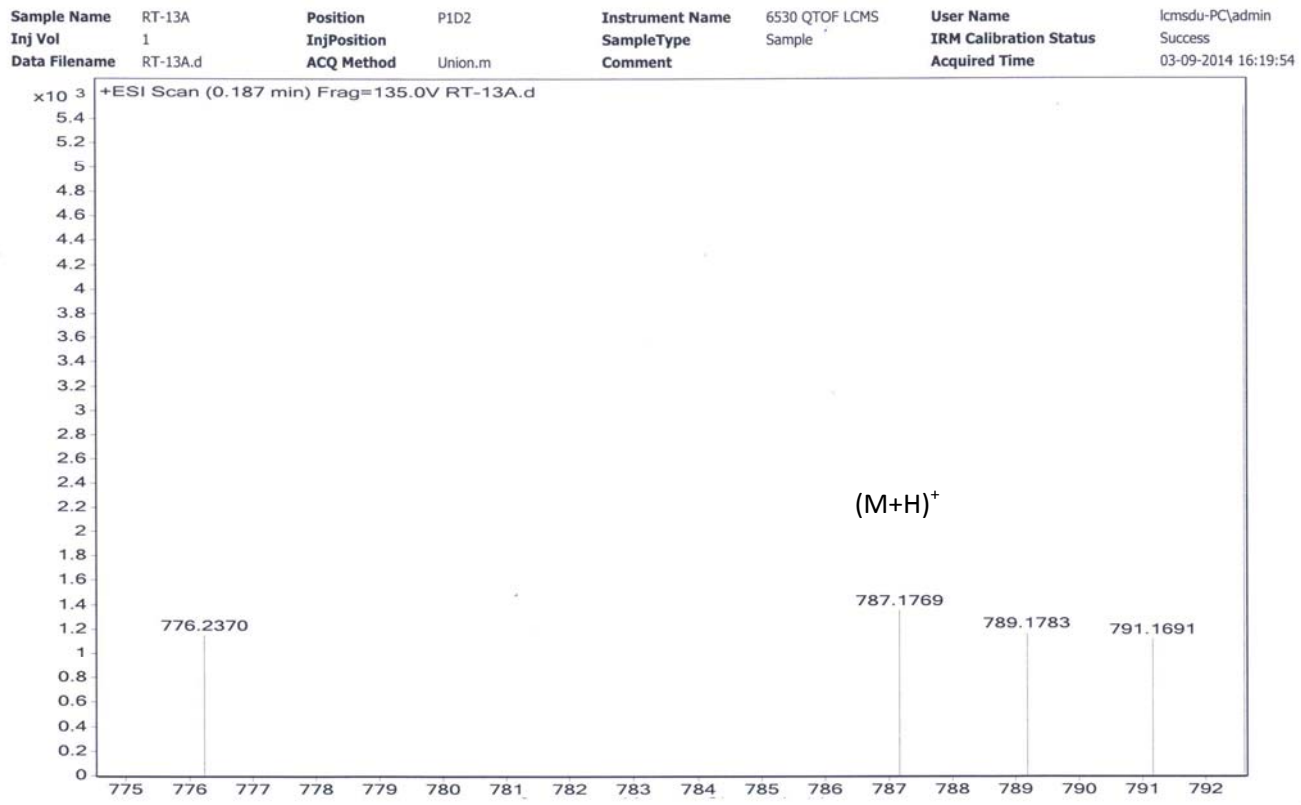


Figure S12. ESI-HRMS of zinc(II) 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetraphenylporphyrin (**12**).

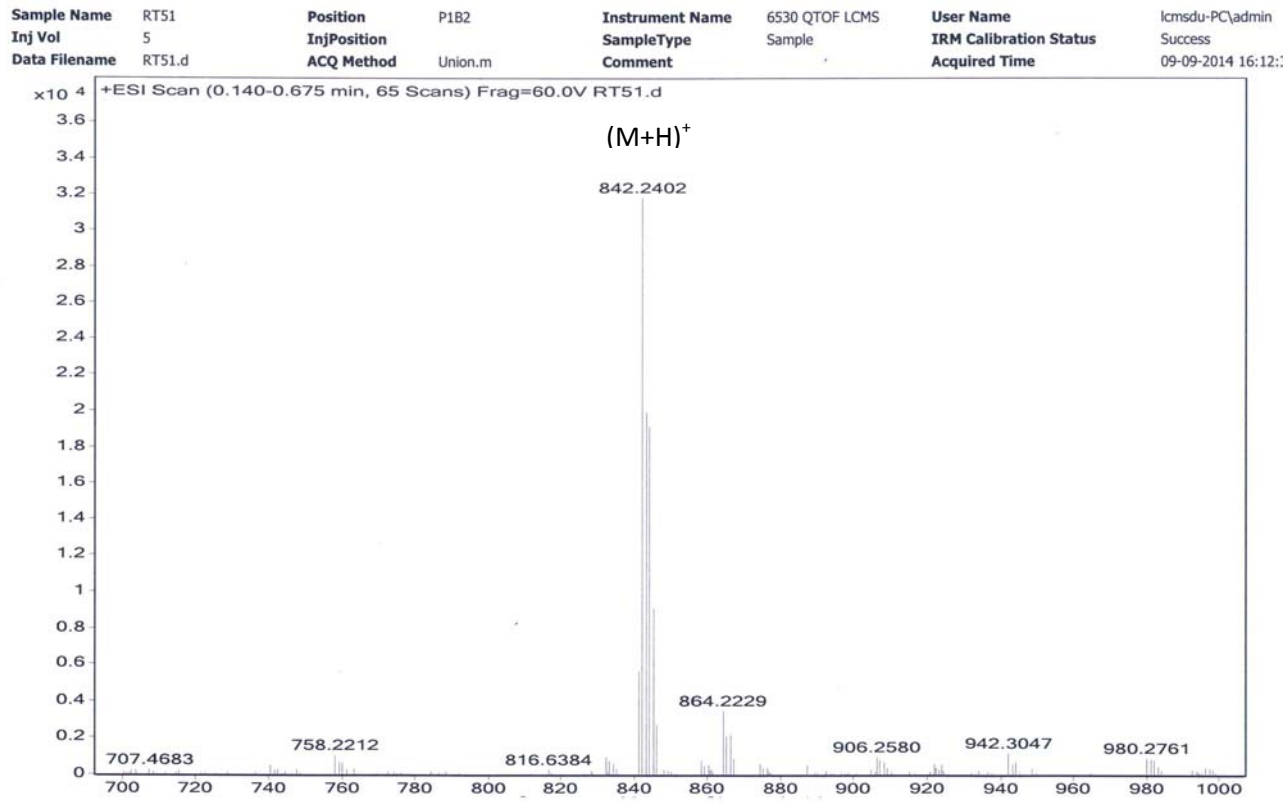


Figure S13. ESI-HRMS of copper(II) 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetra-*p*-tolylporphyrin (**13**).

Qualitative Compound Report

Data File	RT54.d	**Sample Name**	RT54
Sample Type	Sample	**Position**	P2A2
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	10-09-2014 15:55:17
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

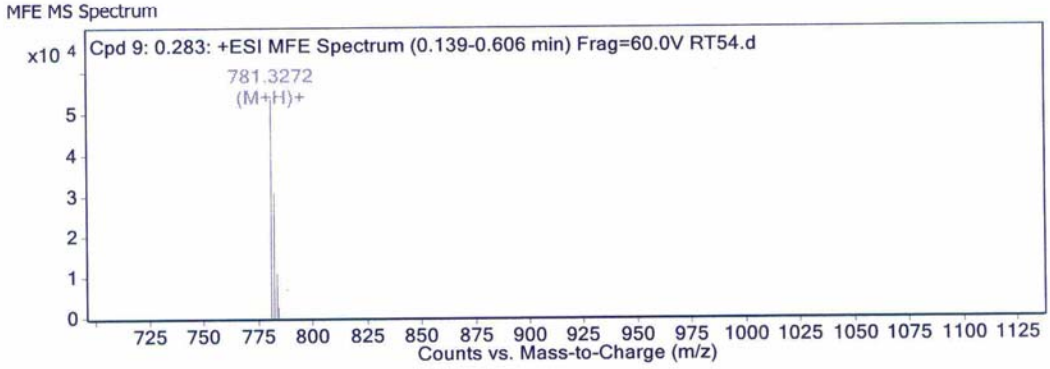
Sample Group		**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)	

Compound Table

Compound Label	RT	Mass	MFG Formula
Cpd 9: 0.283	0.283	780.3199	> limit

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: 0.283	781.3272	0.283	Find by Molecular Feature	780.3199

MFE MS Spectrum



MFE MS Zoomed Spectrum

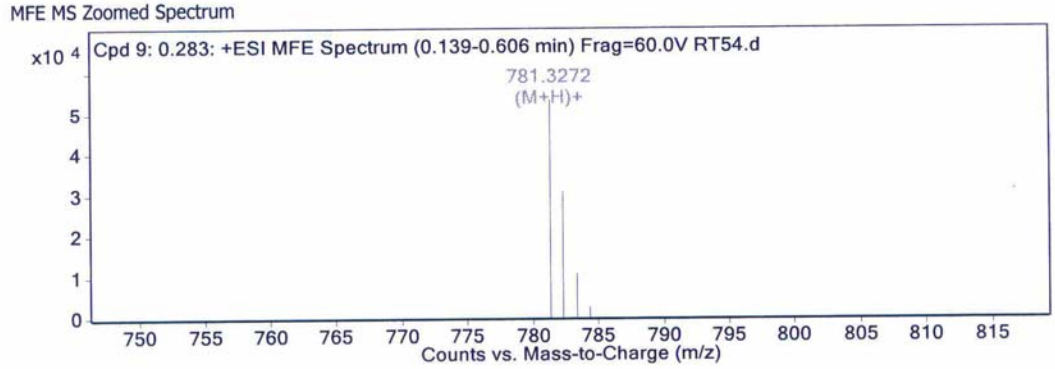


Figure S14. ESI-HRMS of 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetra-*p*-tolylporphyrin (**14**).

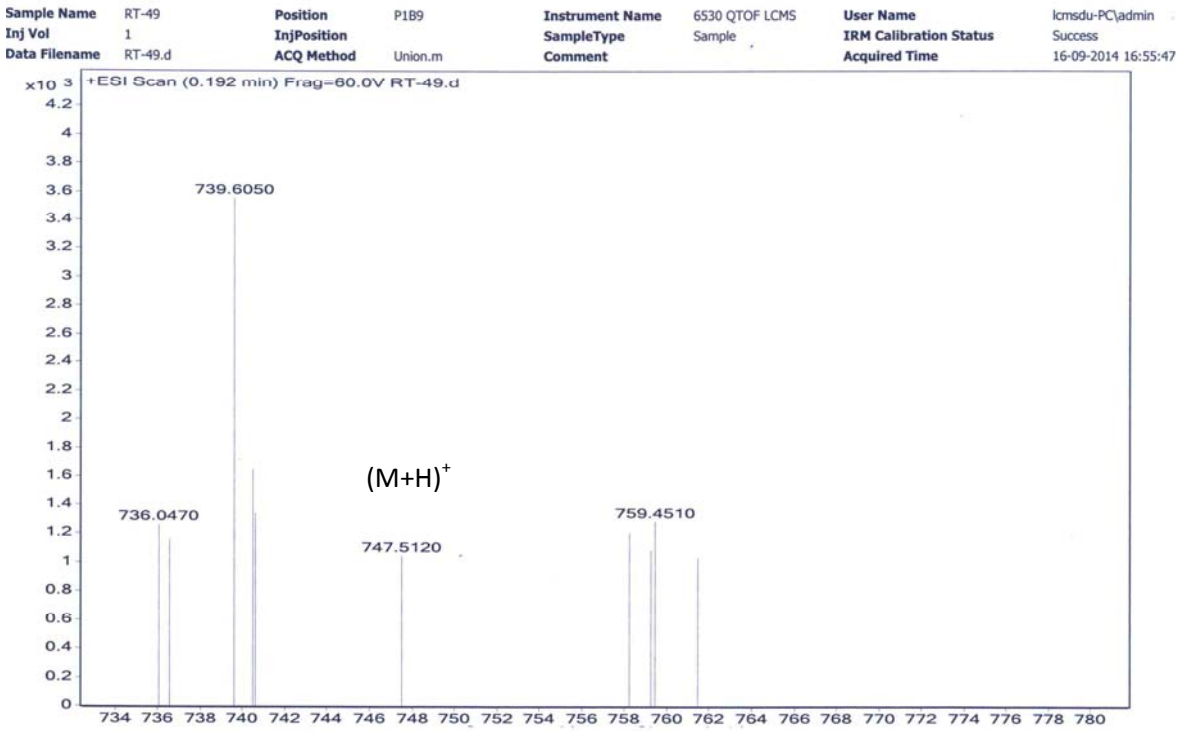


Figure S15. ESI-HRMS of magnesium(II) 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetraphenyl-porphyrin (**15**).

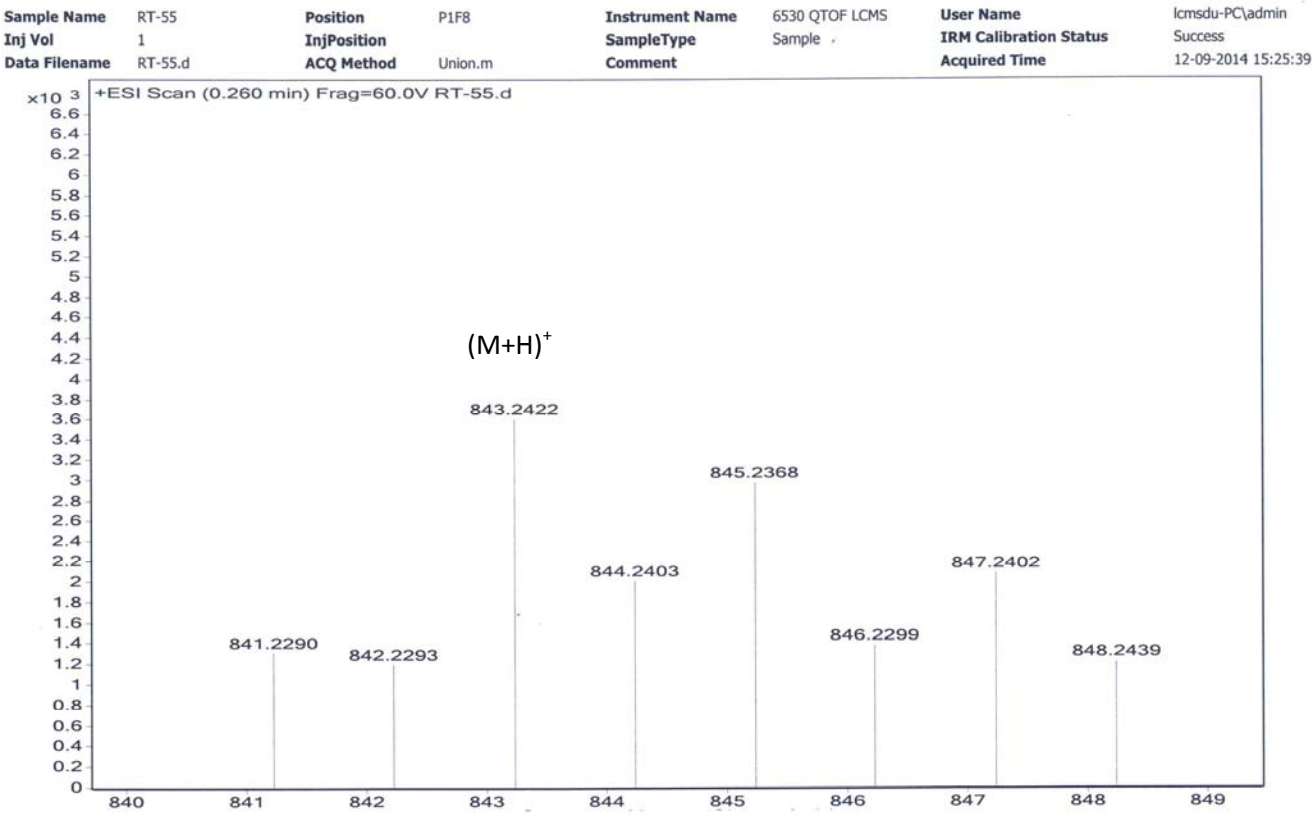


Figure S16. ESI-HRMS of zinc(II) 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetra-*p*-tolylporphyrin (**16**).

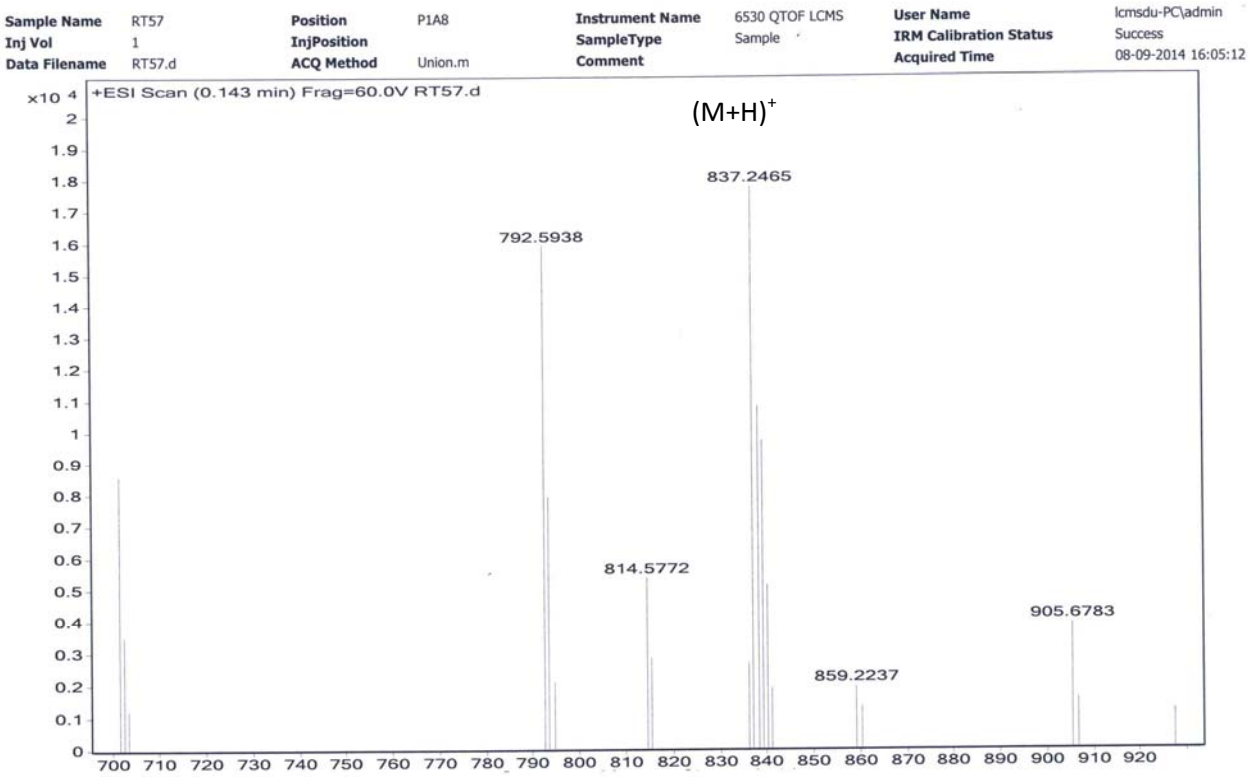


Figure S17. ESI-HRMS of nickel(II) 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetra-*p*-tolylporphyrin (**17**).

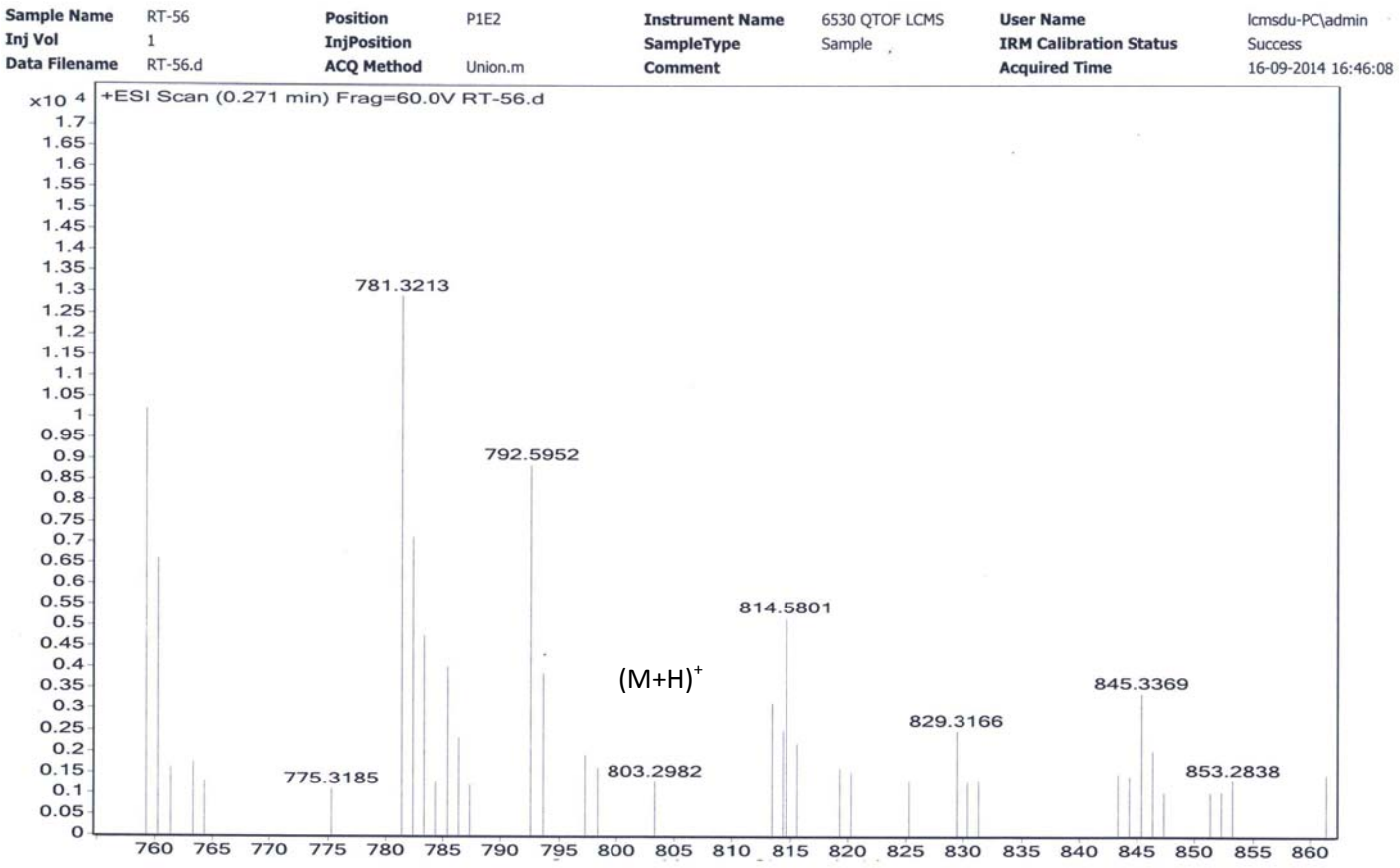


Figure S18. ESI-HRMS of magnesium(II) 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetra-*p*-tolyl-porphyrin (**18**).

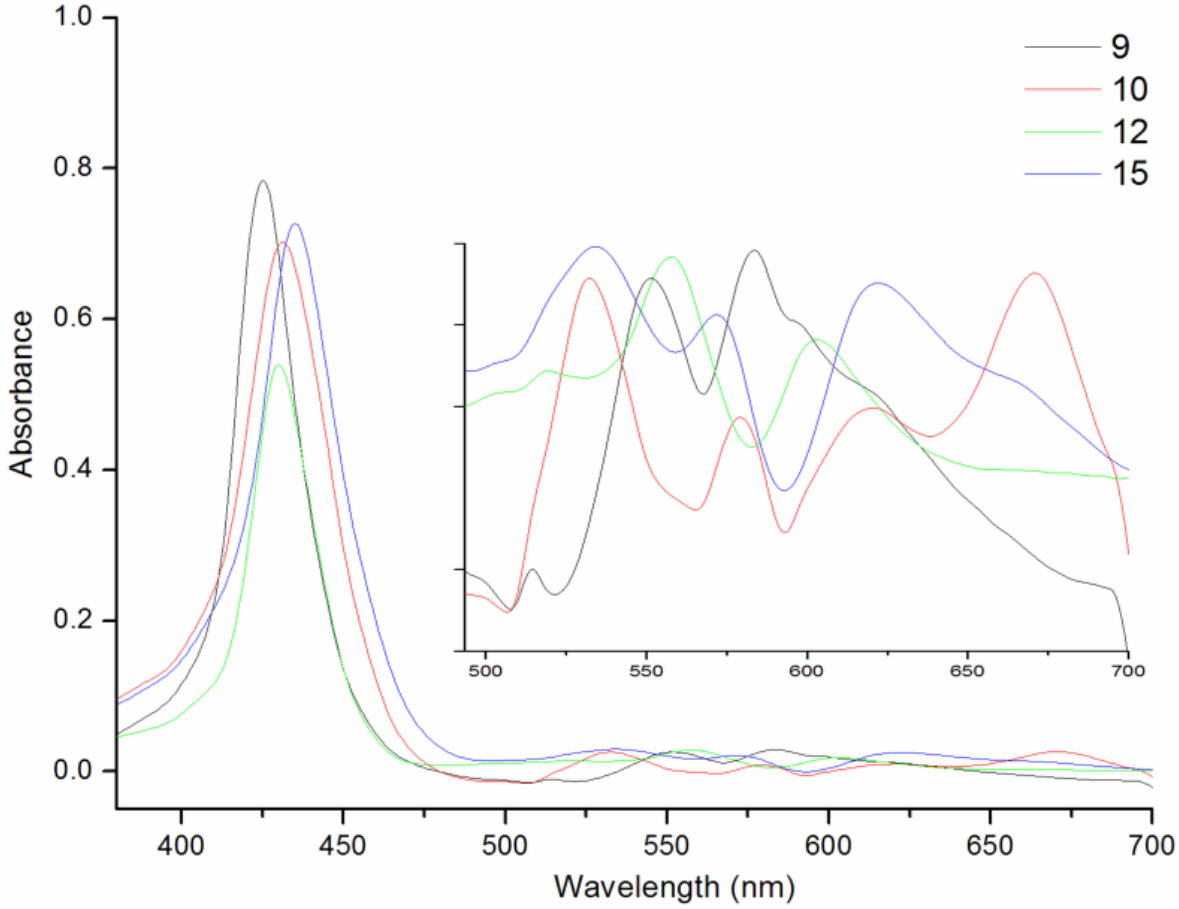


Figure S 19. UV-Vis spectra of *meso*-tetraphenylporphyrins (**9**, **10**, **12** and **15**).

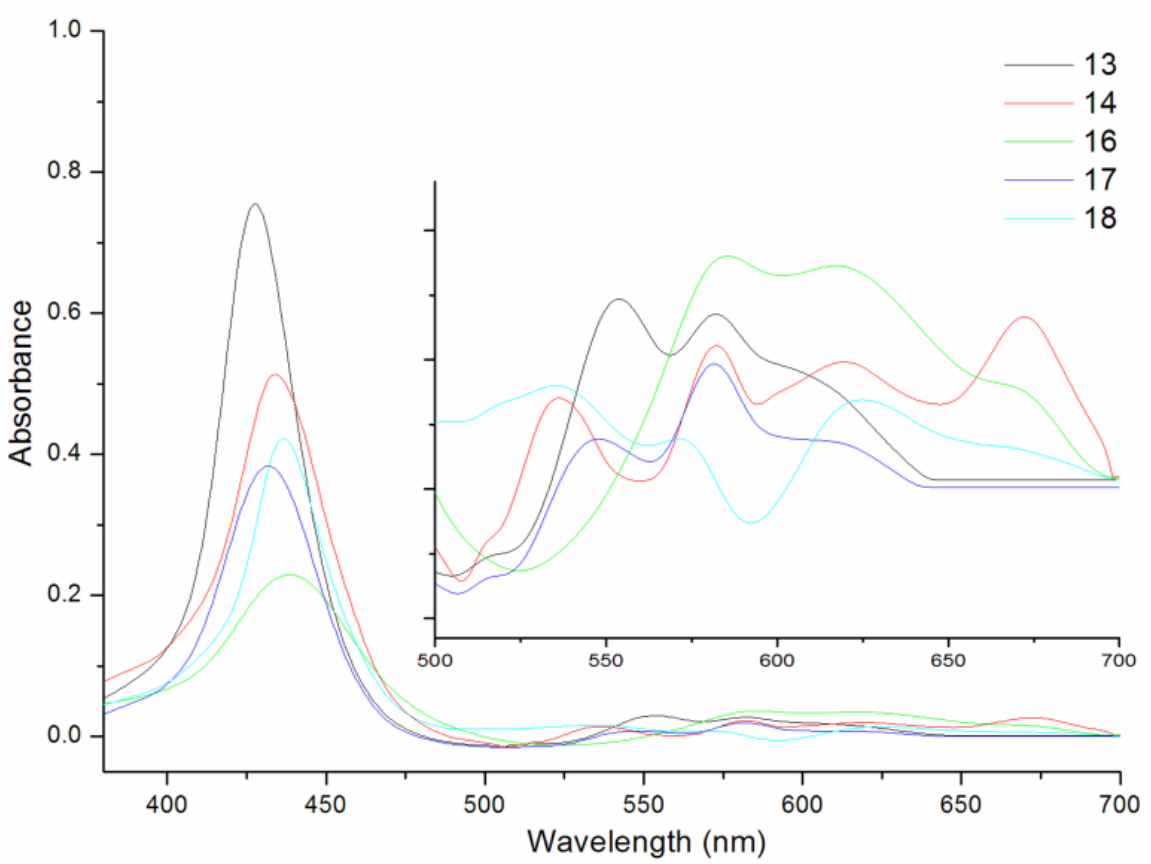


Figure S 20. UV-Vis spectra of *meso*-tetra-*p*-tolylporphyrins (**13, 14, 16, 17** and **18**).

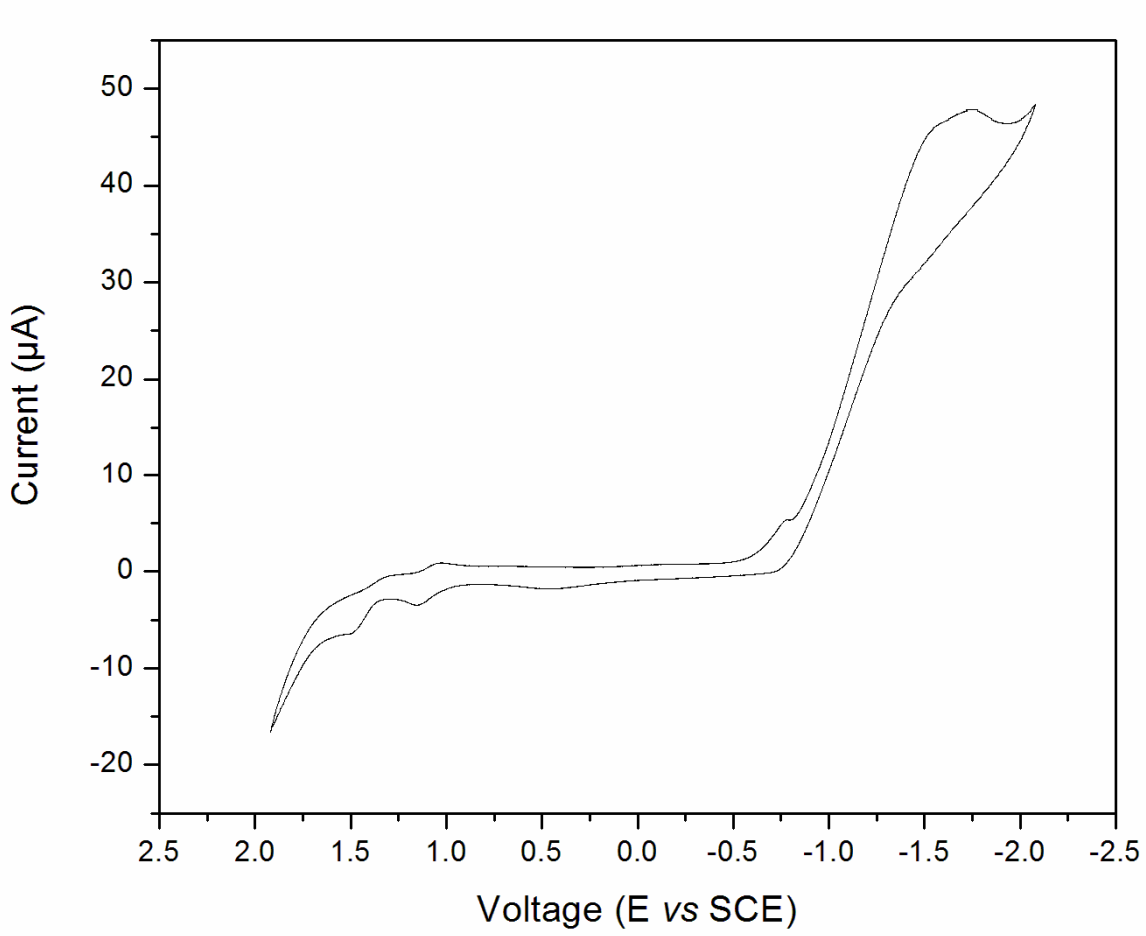


Figure S 21. Cyclic voltammograms of copper (II) 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetra-phenylporphyrin (**9**) in CH_2Cl_2 + 0.1M Bu_4NPF_6 at a scan rate v = 0.05Vs^{-1}.

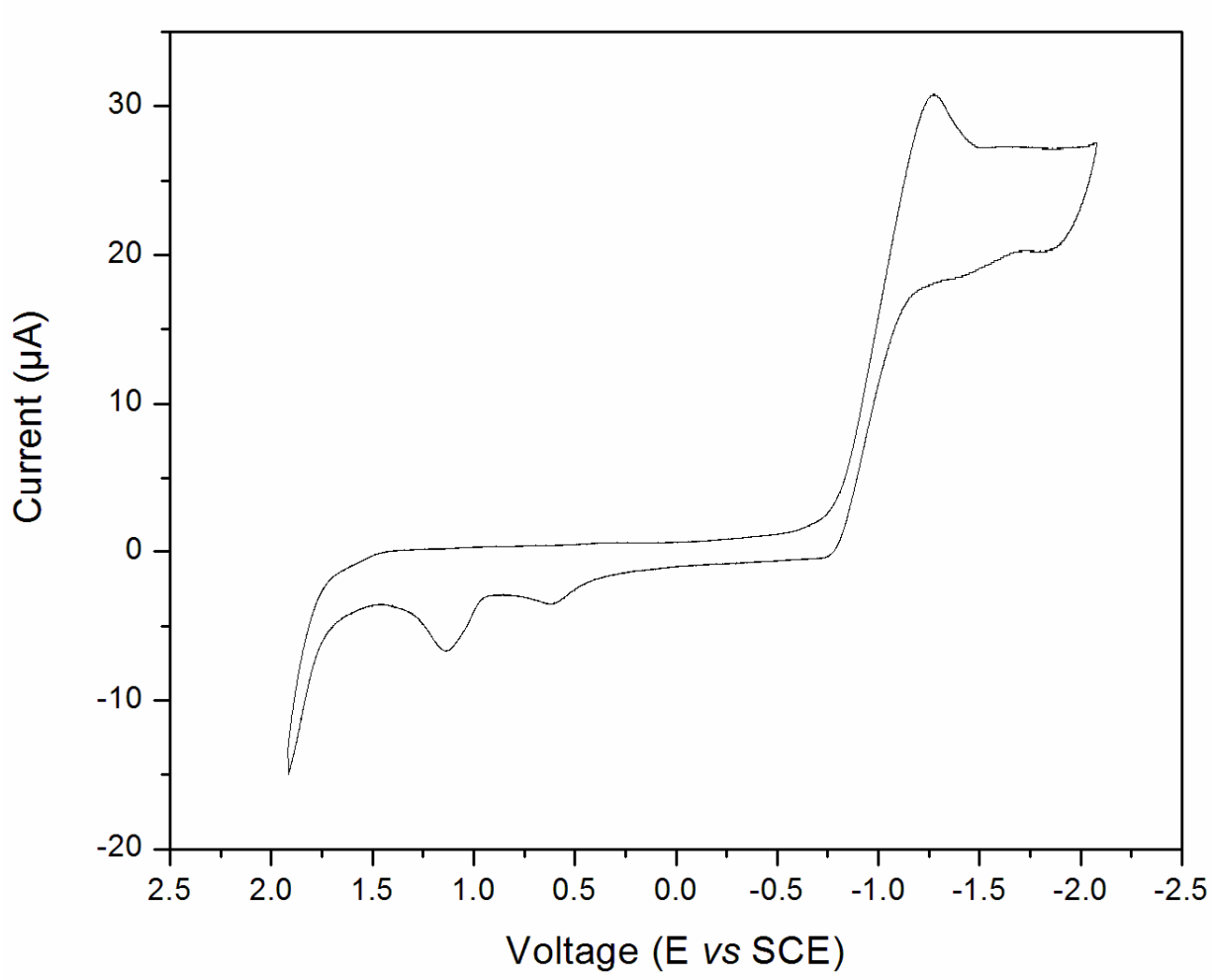


Figure S 22. Cyclic voltammograms of 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetraphenylporphyrin (**10**) in CH_2Cl_2 + 0.1M Bu_4NPF_6 at a scan rate v = 0.05Vs^{-1}.

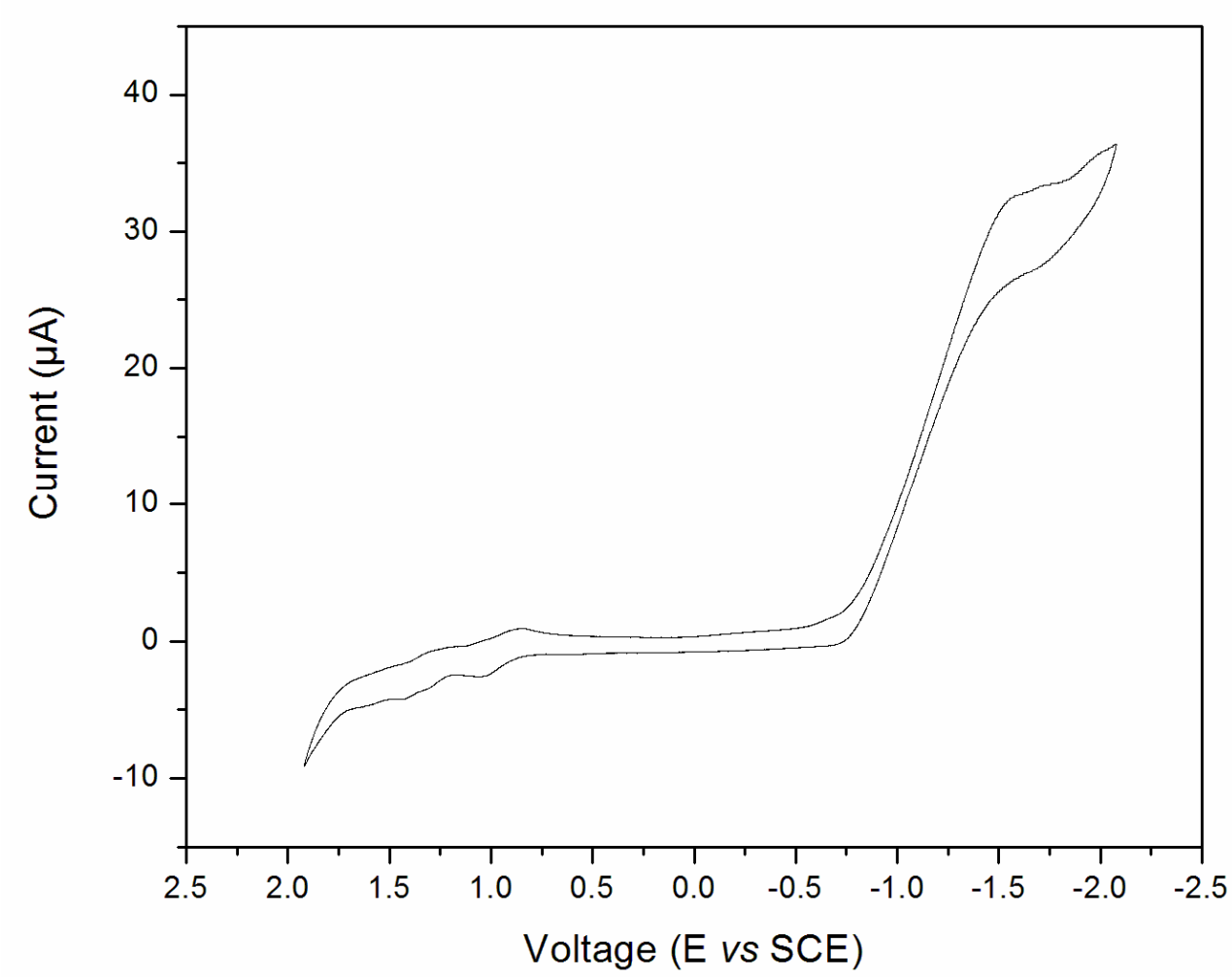


Figure S 23. Cyclic voltammograms of zinc (II) 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetraphenylporphyrin (**12**) in CH_2Cl_2 + 0.1M Bu_4NPF_6 at a scan rate v = 0.05Vs^{-1}.

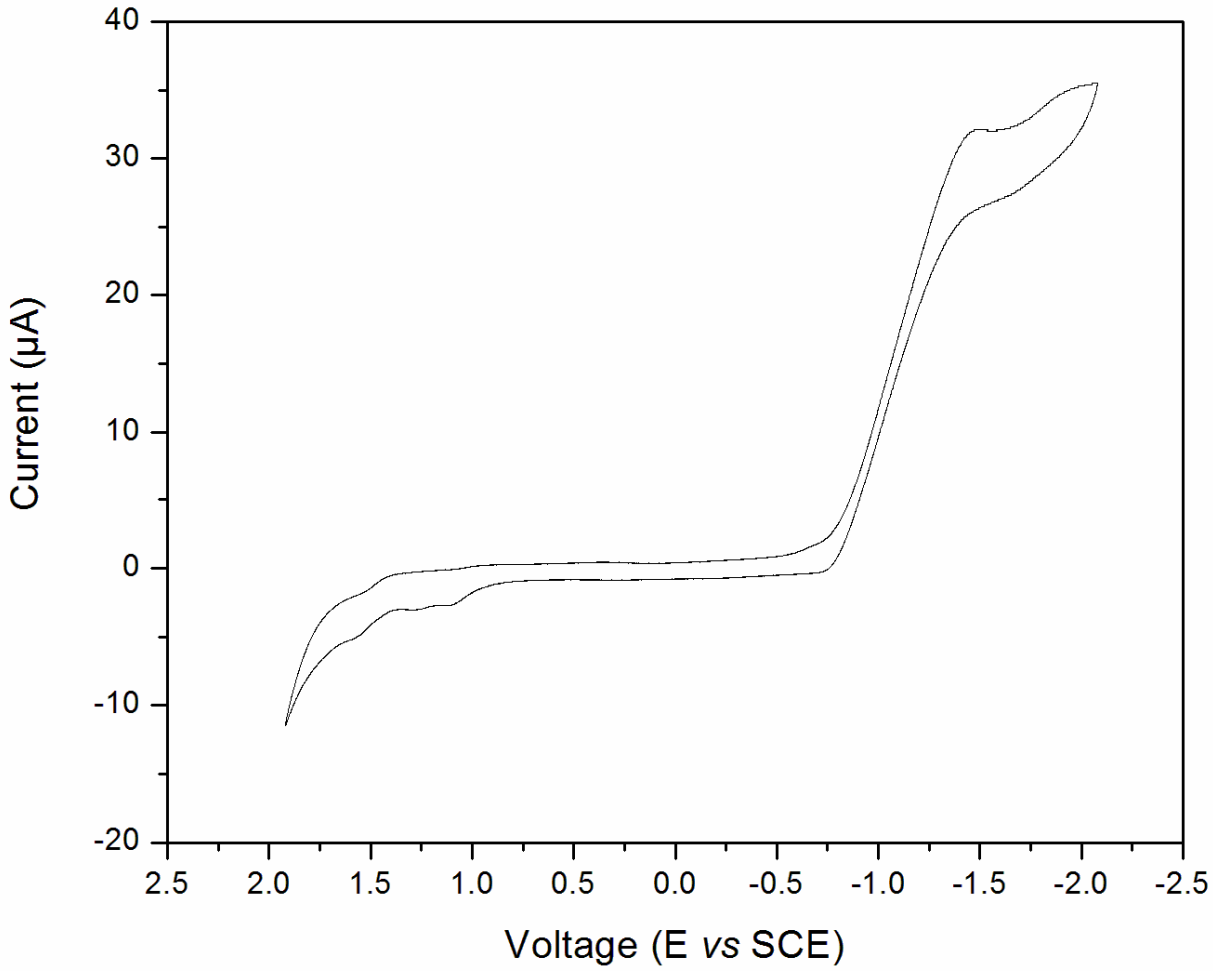


Figure S 24. Cyclic voltammograms of 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetra-*p*-tolylporphyrin (**14**) in CH_2Cl_2 + 0.1M Bu_4NPF_6 at a scan rate $v = 0.05Vs^{-1}$.

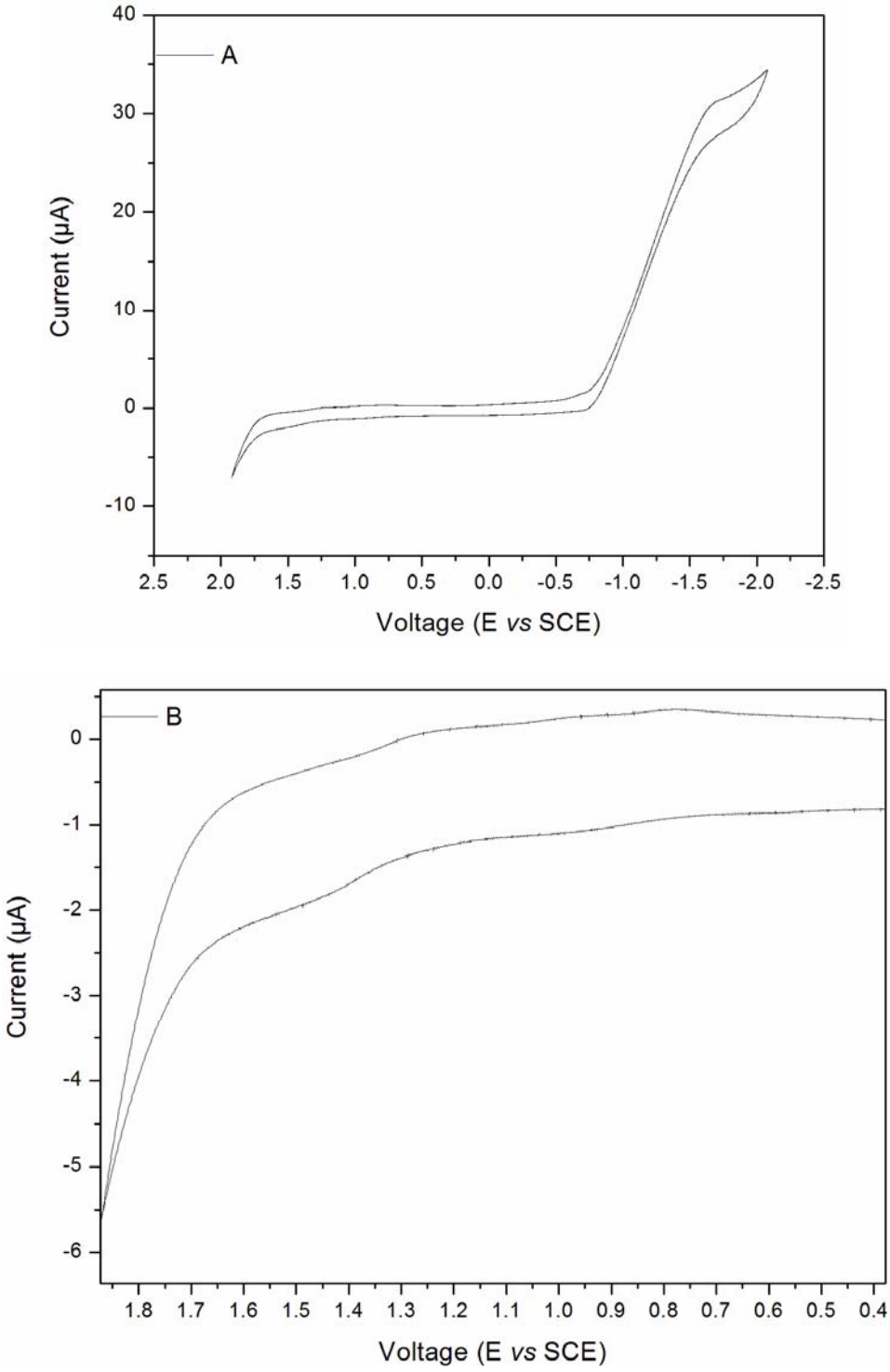


Figure S 25. Cyclic voltammograms of zinc (II) 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetra-*p*-tolylporphyrin (**16, Fig. A**) in CH_2Cl_2 + 0.1M Bu_4NPF_6 at a scan rate $v = 0.05Vs^{-1}$. Figure B shows the expansion of cyclic voltammograms from 0.4 -1.8 V.