Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Co(II)Tetraphenyltetraphenanthroporphyrin@MWCNTs: Enhanced ππ Interaction for Robust Electrochemical Catalysis

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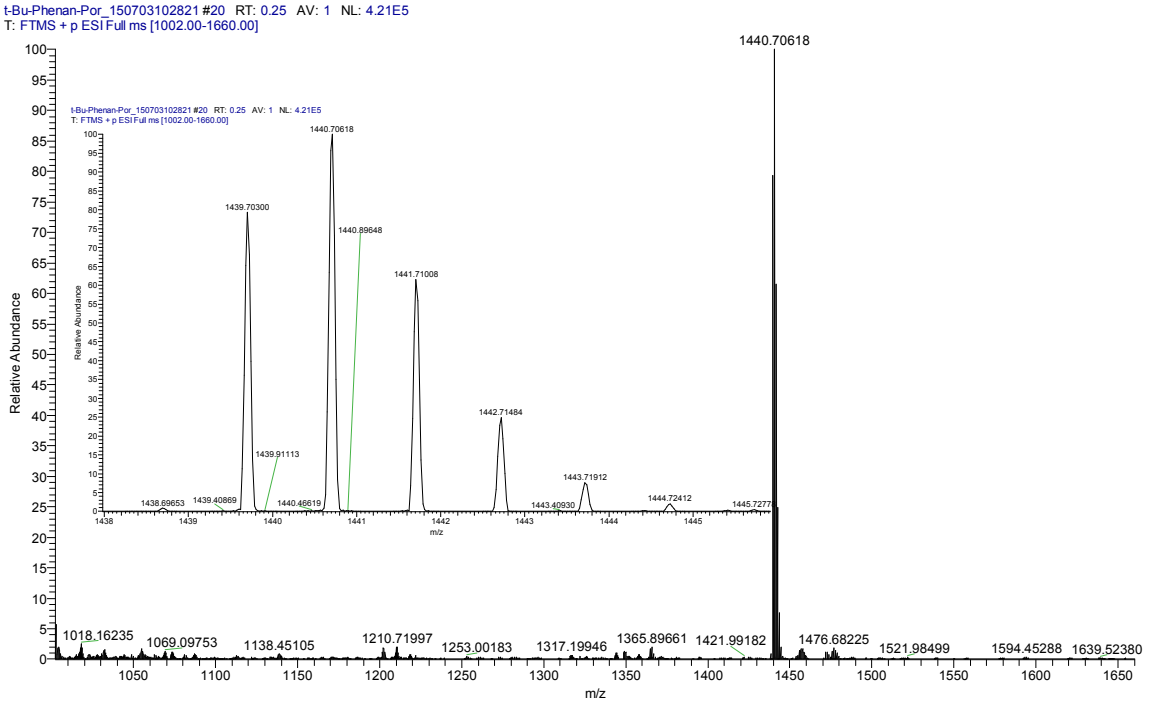

Figure S1 High-resolution mass spectra of H_2TPTPP **1**.

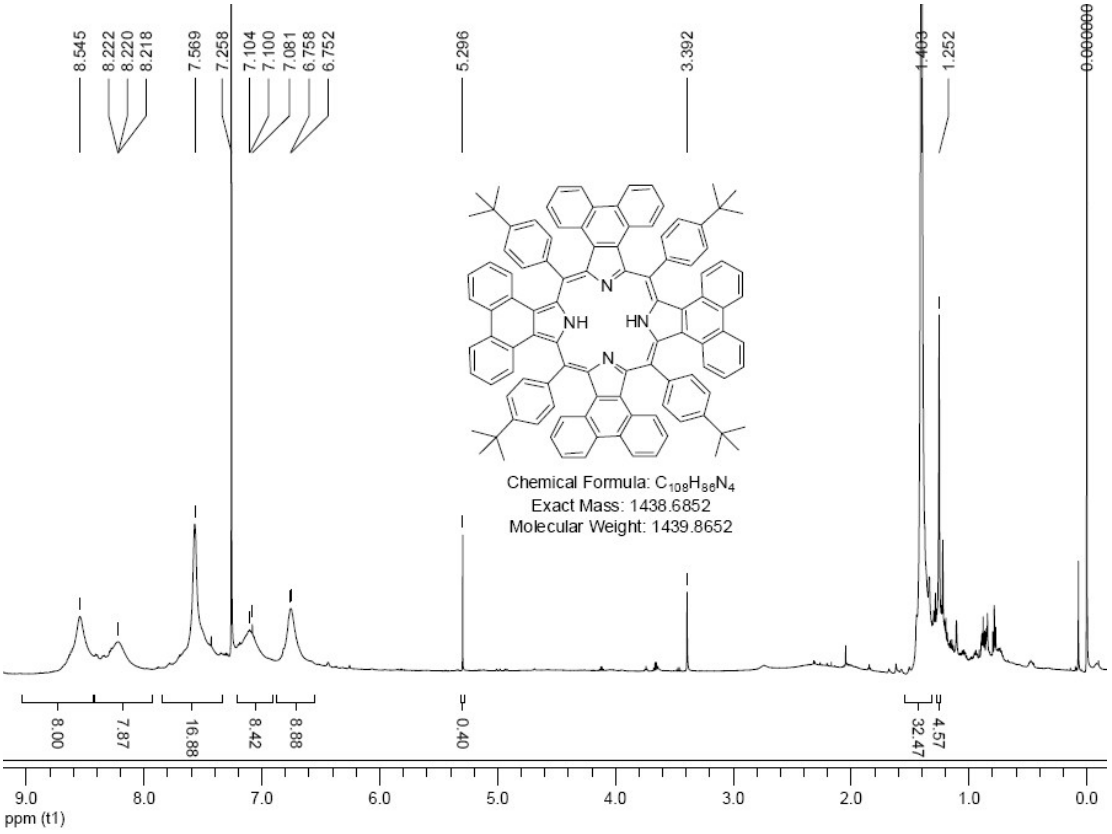

Figure S2 ^{1}HNMR spectra of H_2TPTPP **1**.

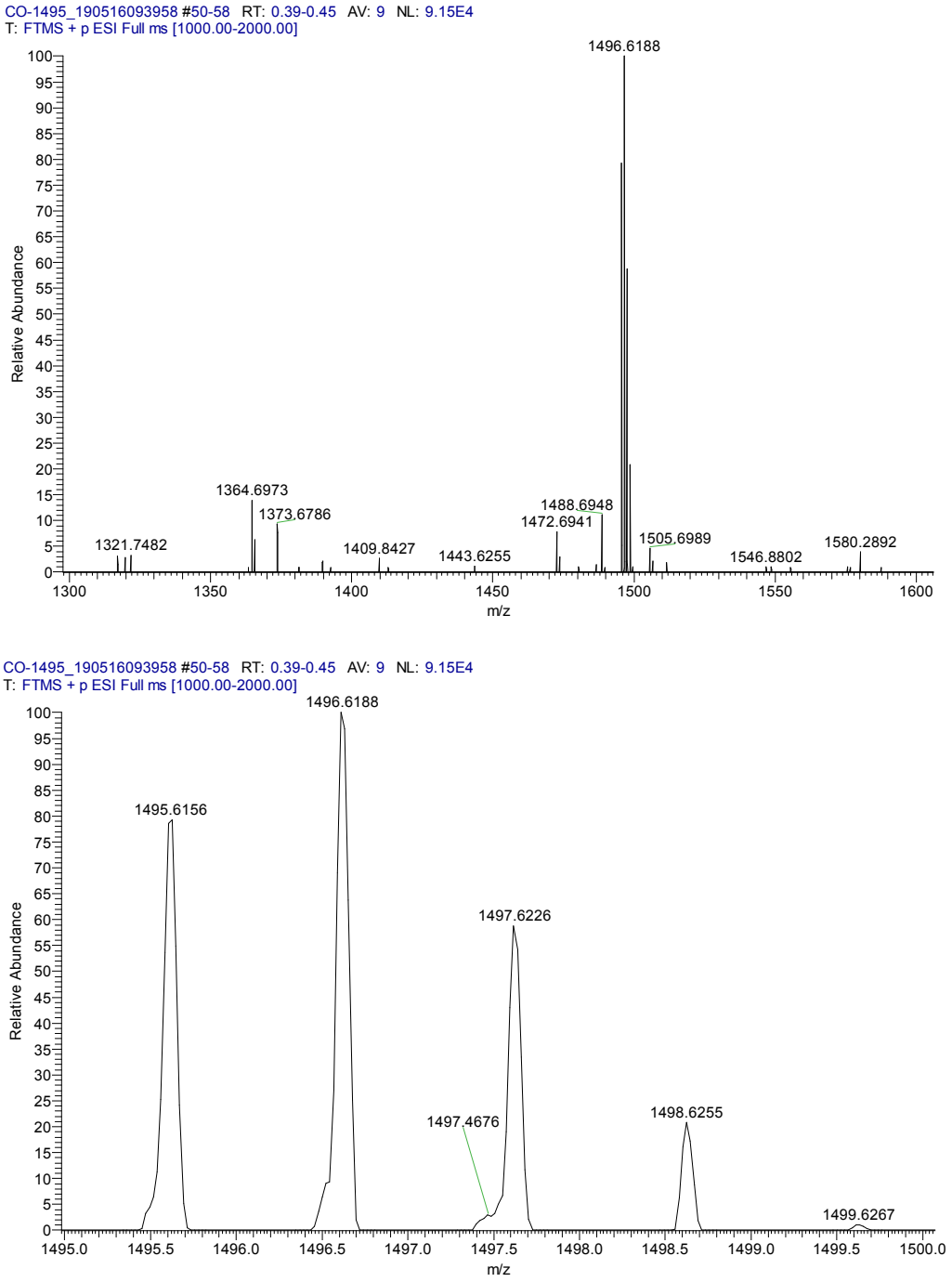

Figure S3 High-resolution mass spectra of Co(II)TPTPP **2**.

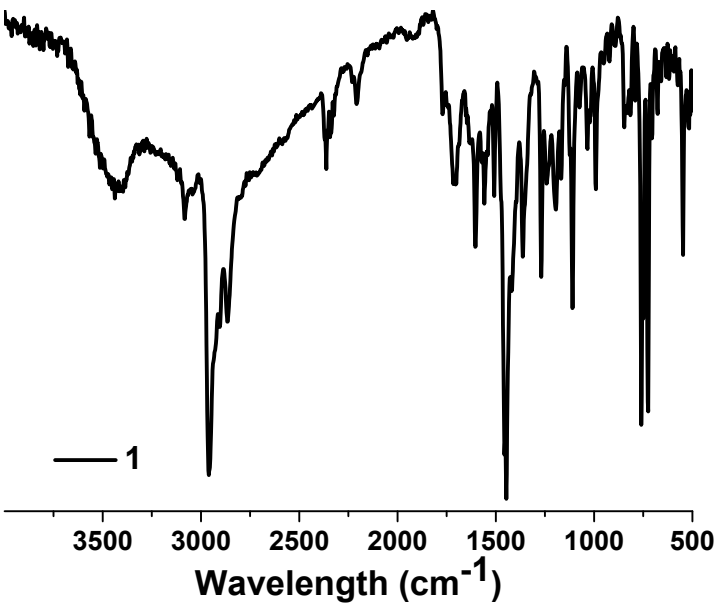

Figure S4 FT-IR spectra H_2TPTPP **1**,

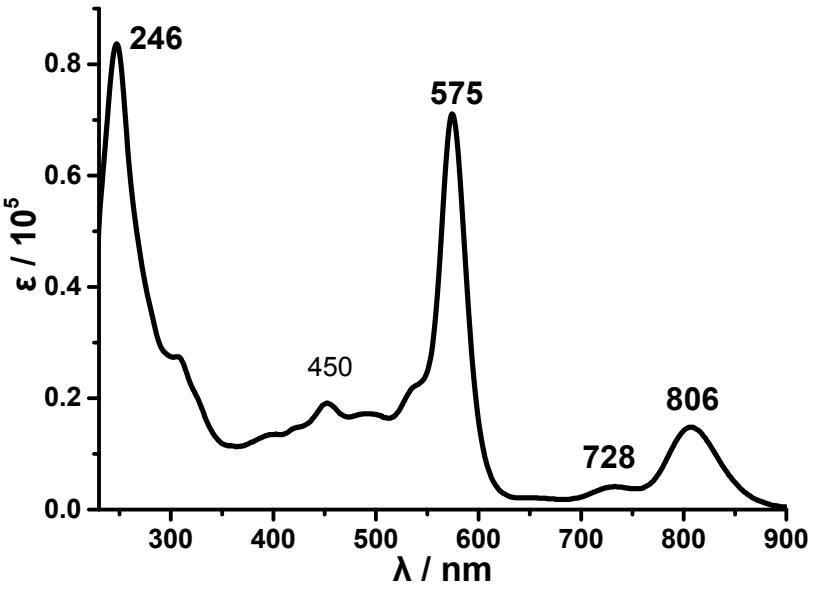

Figure S5 UV-vis absorption spectra H_2TPTPP **1**

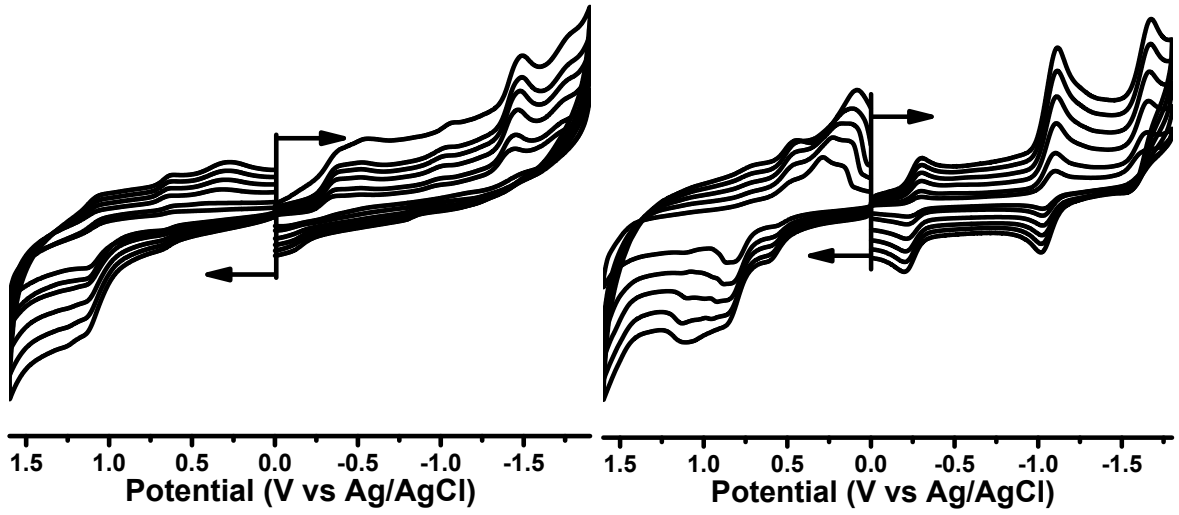

Figure S6 Cyclic voltammetry of H_2TPTPP **1** (left) and Co(II)TPTPP **2** (right) at scan speed v = 50 mV/s, 100 mV/s, 200 mV/s, 300 mV/s, 400 mV/s, 500 mV/s in CH_2Cl_2 containing 0.1M TBAP.

Table S1: The calculated TD-DFT spectra of B3LYP optimized geometry for the methyl-substituted model complexes of Co(II)TPP and Co(II)TPTPP **2** obtained using Gaussian 09 software package using the B3LYP functional with 6-31G(d) basis set.

Co(II)TPP							
Band[a]	**#[b]**	**Calc[c]**			**Exp[d]**		**Wave Function[e] =**
----	**1**	----	----	----	----	----	Ground State
Q	**13, 14**	19.2	520	(0.01)	18.9	529	**56% s→ -a/-s; 43% a → -a/-s;** …
B	**28, 29**	25.7	388	(0.49)	24.3	412	44% d_{xy} → -a/-s; **22% a → -a/-s; 22% s → -a/-s;** …
Co(II)TPTPP							
Band[a]	**#[b]**	**Calc[c]**			**Exp[d]**		**Wave Function[e] =**
----	**1**	----	----	----	----	----	Ground State
Q_x	**13**	14.9	671	(0.00)	14.7	680	**56% s→ -a/-s; 41% a → -a/-s;** …
Q_y	**14**	15.2	658	(0.00)			**52% a → -a/-s; 44% s→ -a/-s;** …
B_x	**21**	18.5	541	(0.48)	19.2	521	**47% a → -a/-s; 33% s→ -a/-s;** …
B_y	**25**	19.2	520	(0.65)			**46% s→ -a/-s; 34% a → -a/-s;** 12% d_{z^2} → -a/-s; …

[a] − Band assignment described in the text. [b] − The number of the state assigned in terms of ascending energy within the TD-DFT calculation [c] − Calculated band energies ($10^3.cm^{-1}$), wavelengths (nm) and oscillator strengths in parentheses (f). [d] − Observed energies ($10^3.cm^{-1}$) and wavelengths (nm) in CH_2Cl_2 for Co(II)TPP and **2**. [e] − The wave functions based on the eigenvectors predicted by TD-DFT. One-electron transitions associated with the **a**, **s**. **-a** and **-s** MOs of Michl's perimeter model[2] are highlighted in bold.

References

1. S. B. Piepho and P. N. Schatz, In *Group Theory in Spectroscopy with Applications to Magnetic Circular Dichroism*, Wiley: New York, 1983.
2. Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.