Supporting Information

β-Functionalized Dibenzoporphyrins with Mixed Substituents Pattern: Facile Synthesis, Structural, Spectral and Electrochemical Redox Properties

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Table of contents:

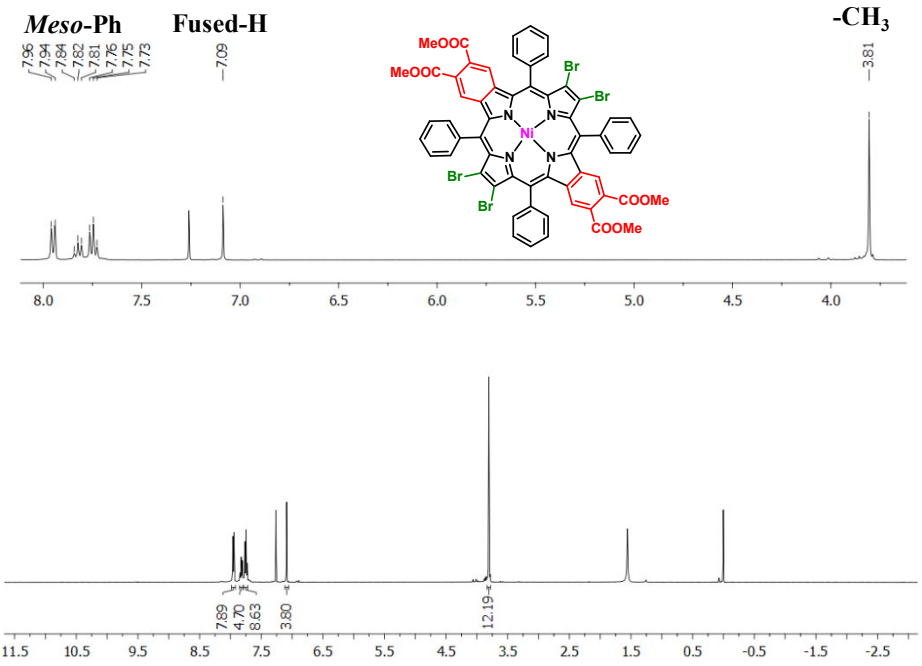


Figure S1. ^{1}H NMR spectrum of NiTPP(Benzo)$_2$Br$_4$ in $CDCl_3$ at 298 K.

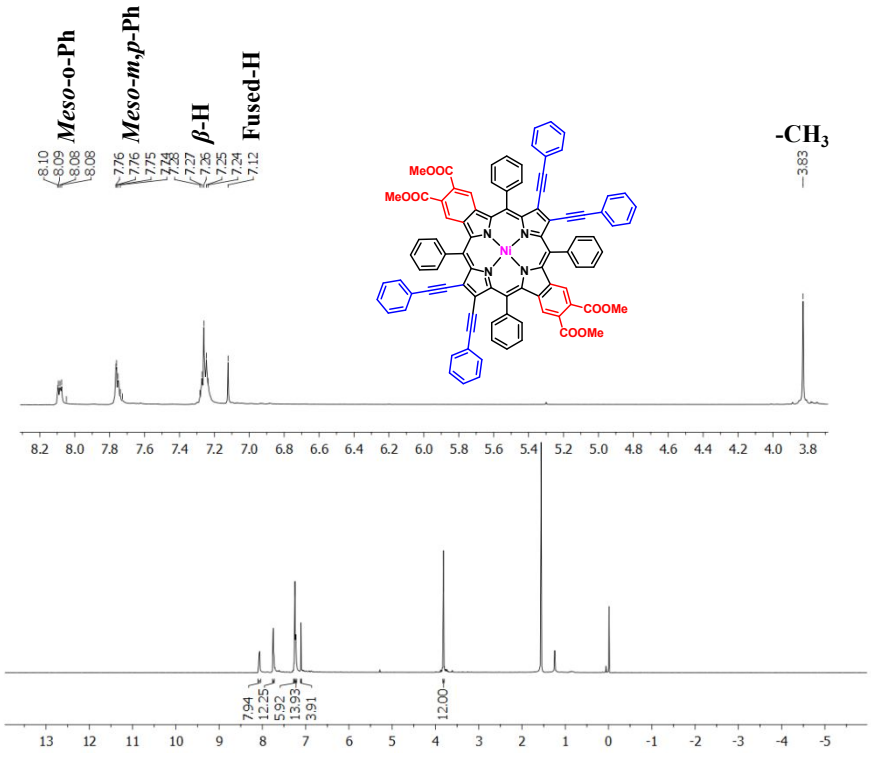


Figure S2. ^{1}H NMR spectrum of NiTPP(Benzo)$_2$(PE)$_4$ in $CDCl_3$ at 298 K.

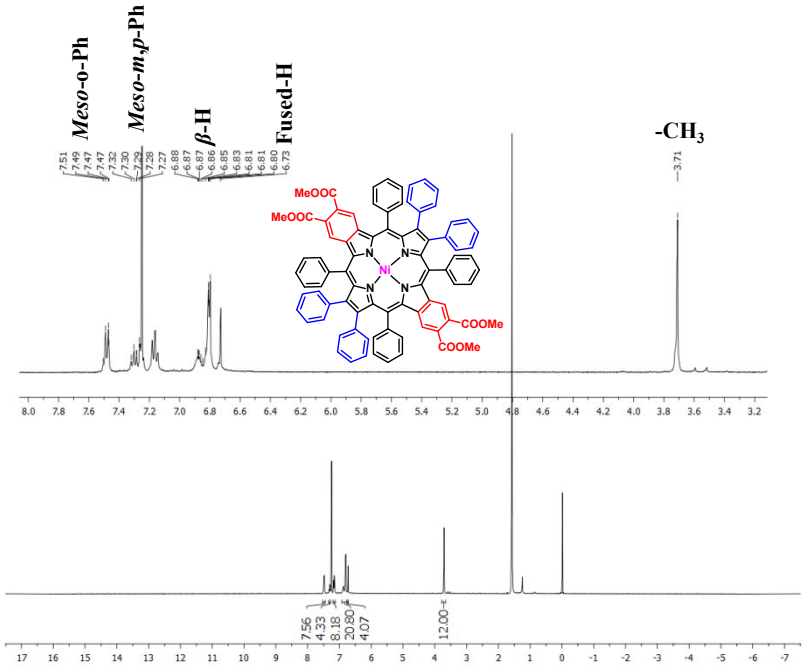


Figure S3. ^{1}H NMR spectrum of NiOPP(Benzo)$_2$ in $CDCl_3$ at 298 K.

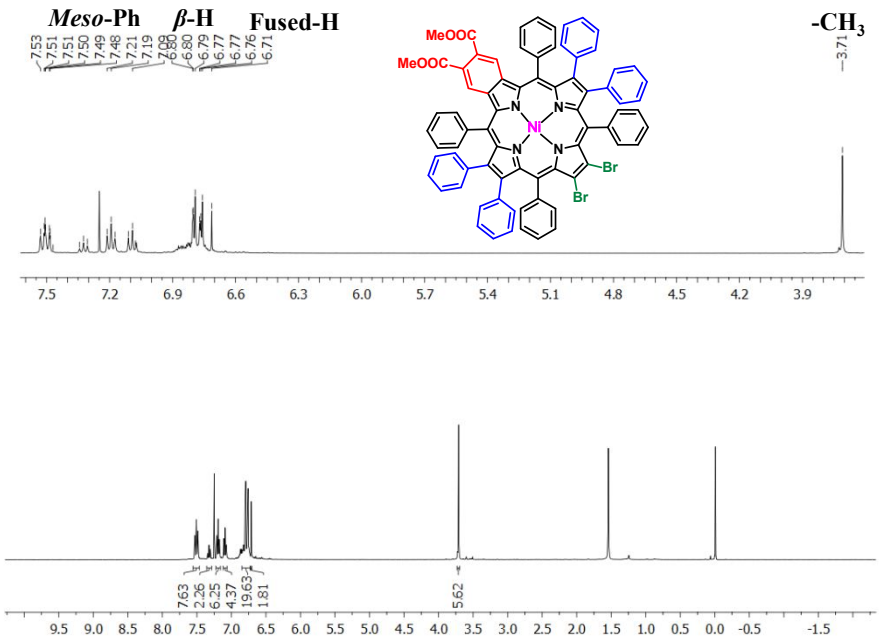


Figure S4. ^{1}H NMR spectrum of NiOPP(Benzo)Br_2 in $CDCl_3$ at 298 K.

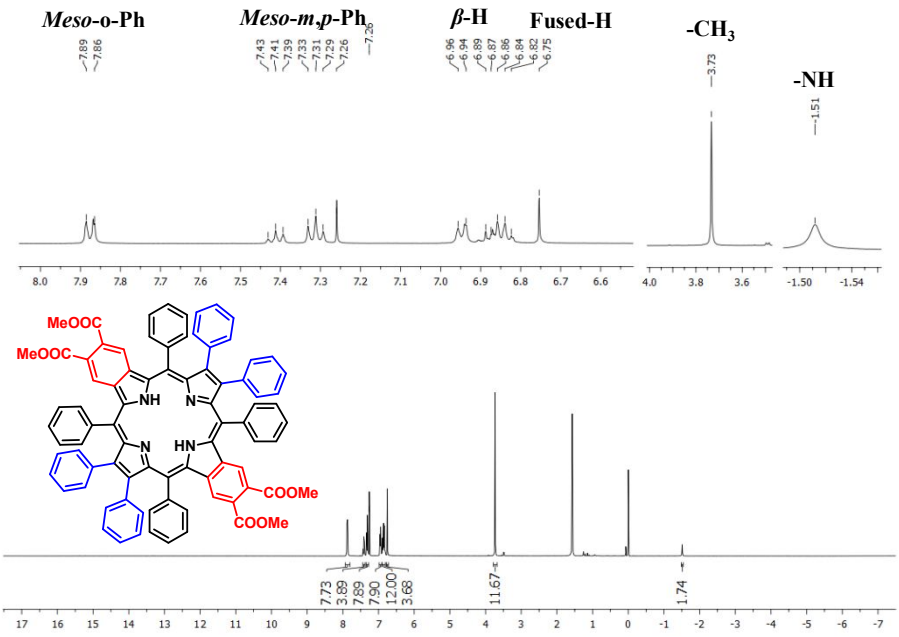


Figure S5. ^{1}H NMR spectrum of H_2OPP(Benzo)$_2$ in $CDCl_3$ at 298 K.

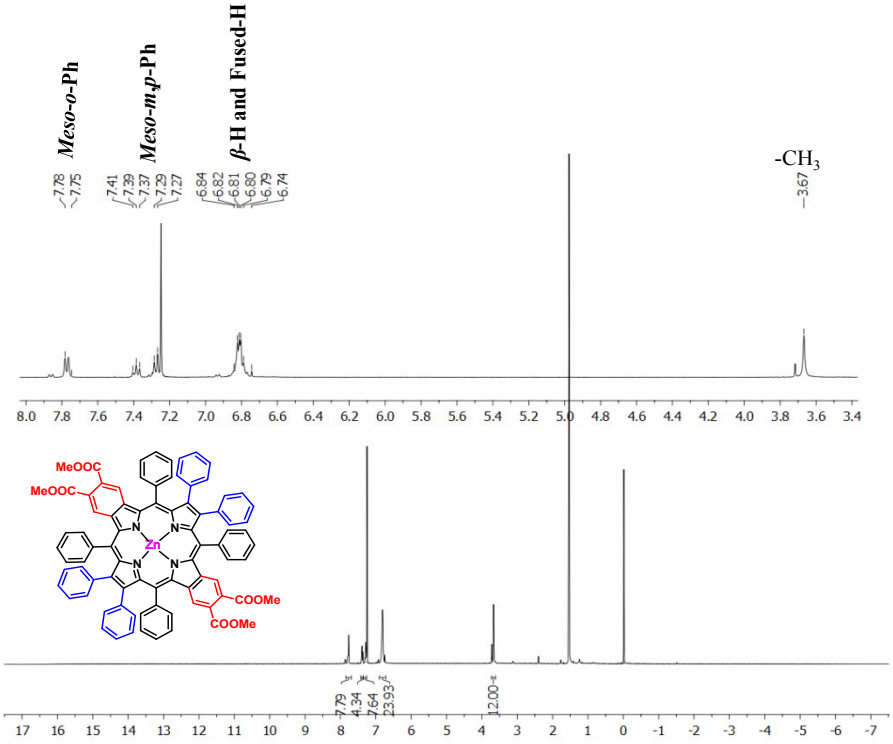


Figure S6. ^{1}H NMR spectrum of ZnOPP(Benzo)$_2$ in $CDCl_3$ at 298 K.

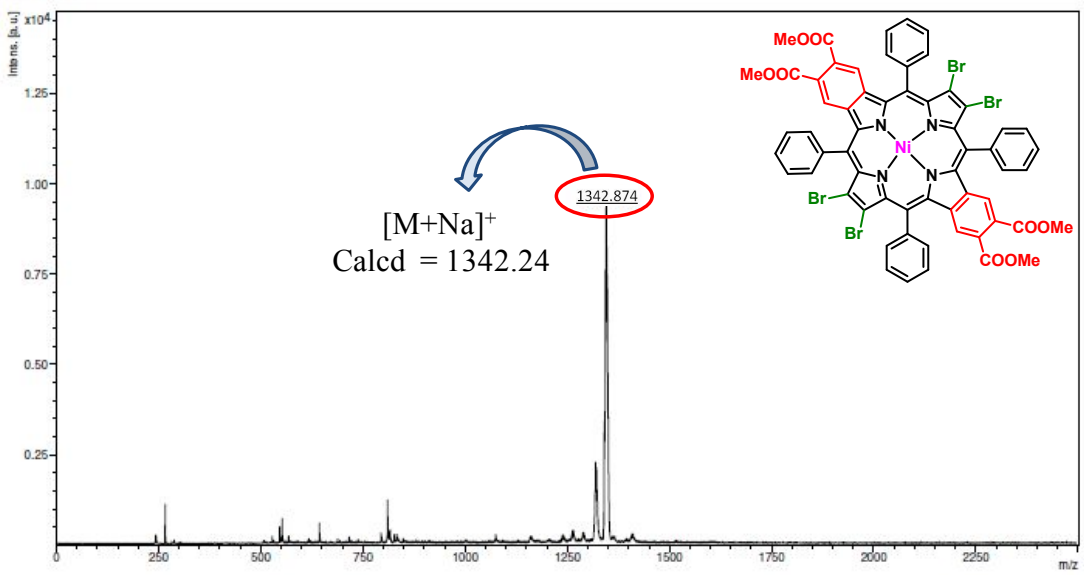


Figure S7. MALDI-TOF mass spectrum of NiTPP(Benzo)$_2$Br$_4$.

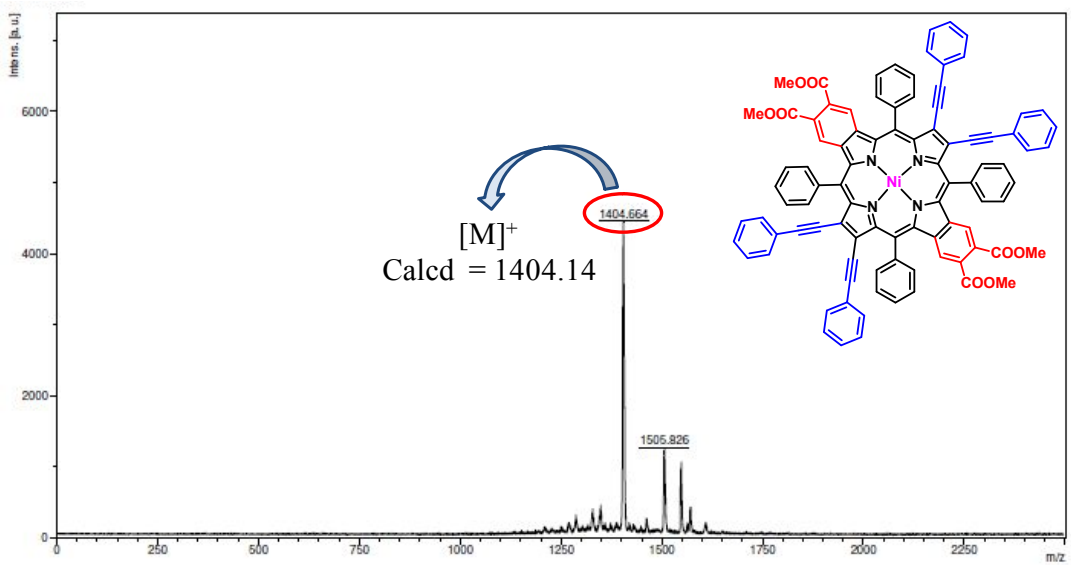


Figure S8. MALDI-TOF mass spectrum of NiTPP(Benzo)$_2$(PE)$_4$.

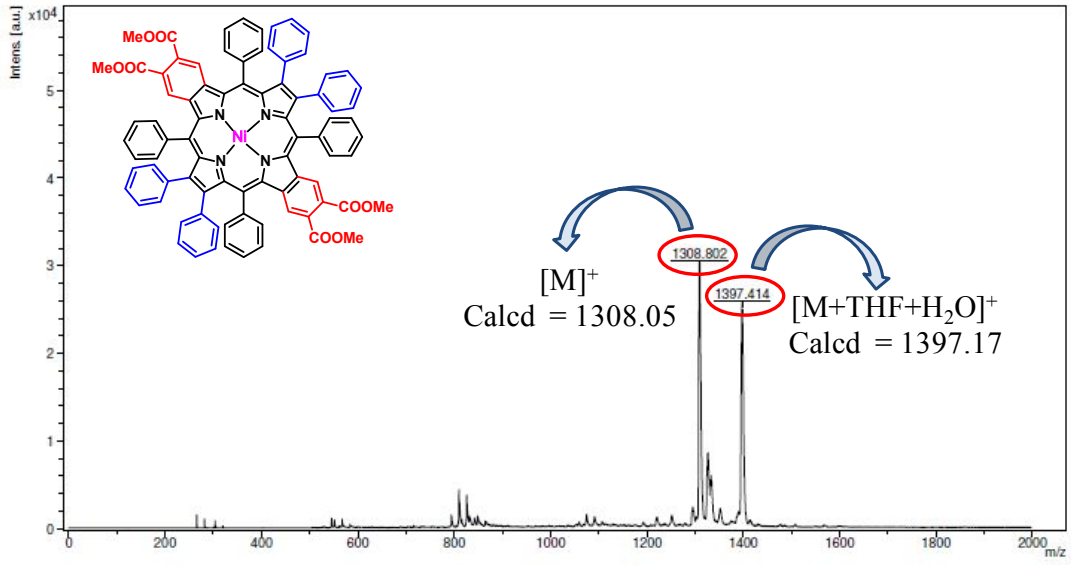


Figure S9. MALDI-TOF mass spectrum of NiOPP(Benzo)$_2$.

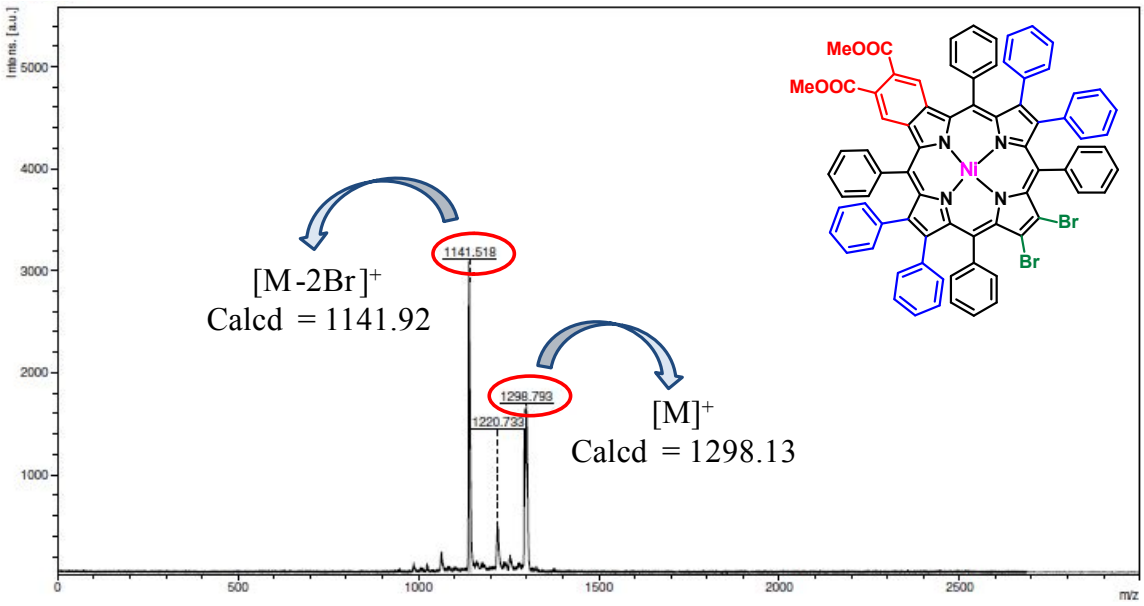


Figure S10. MALDI-TOF mass spectrum of NiOPP(Benzo)Br_2.

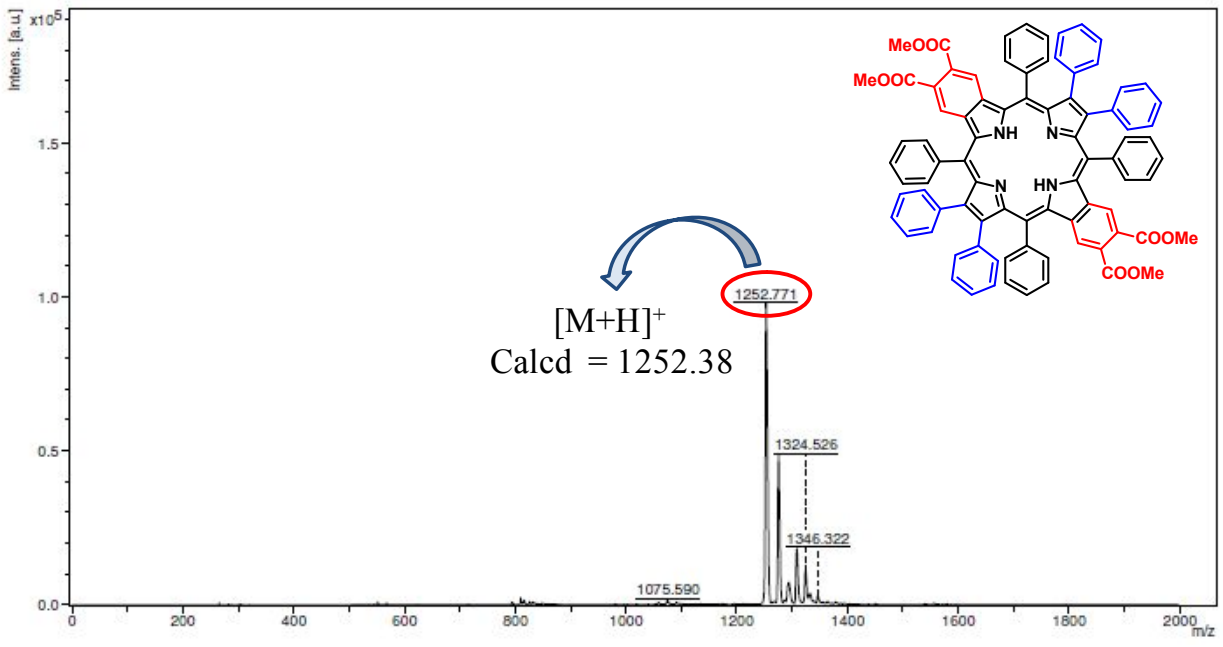


Figure S11. MALDI-TOF mass spectrum of H_2OPP(Benzo)$_2$.

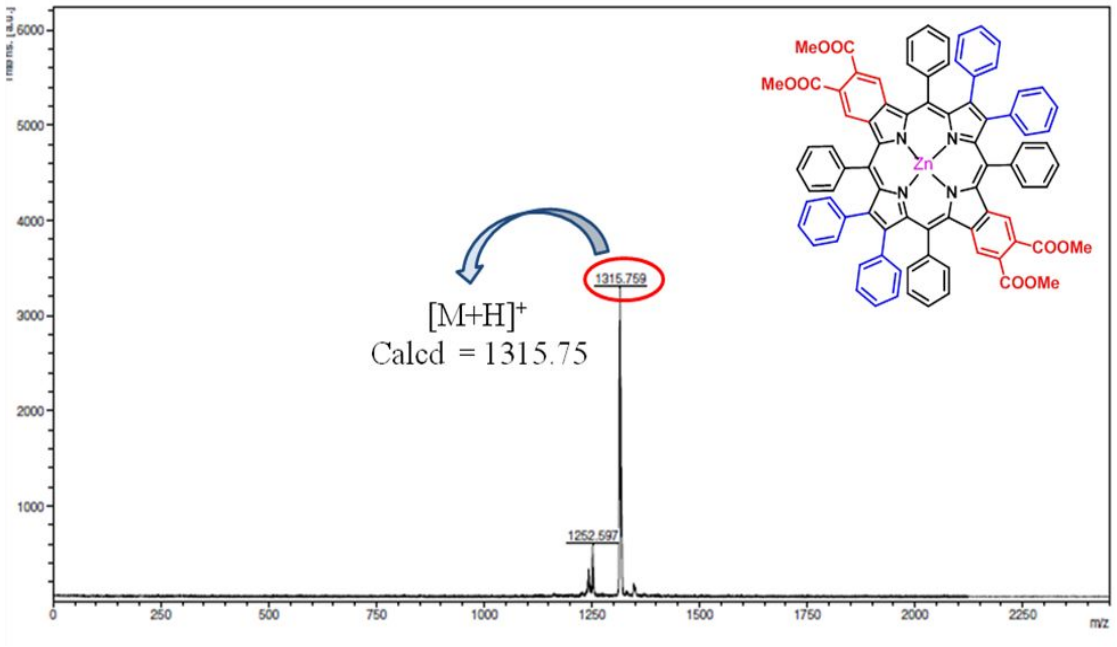


Figure S12. MALDI-TOF mass spectrum of ZnOPP(Benzo)$_2$.

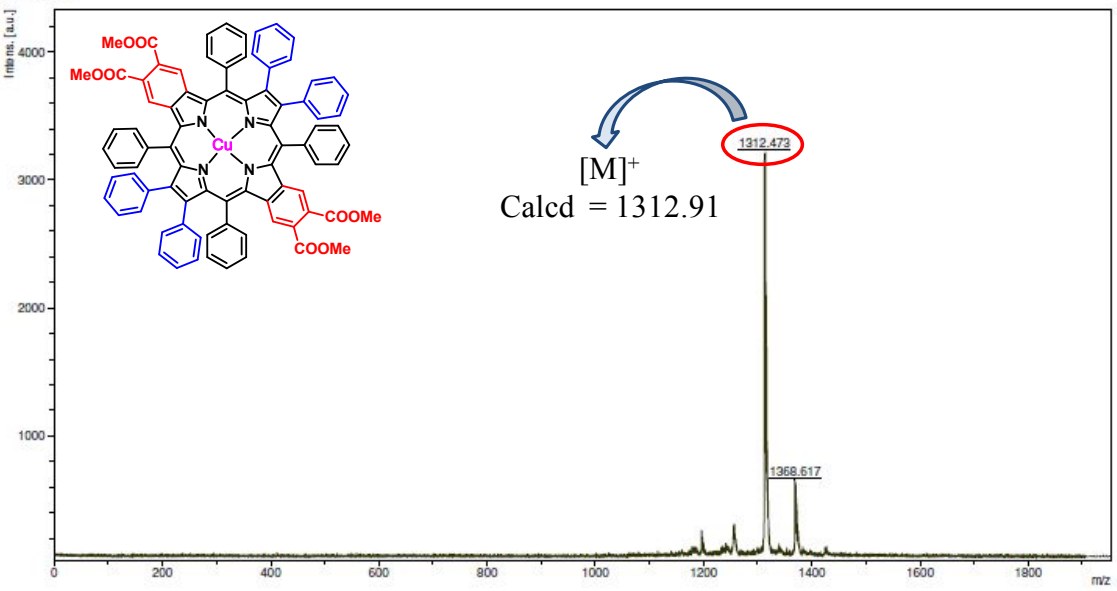


Figure S13. MALDI-TOF mass spectrum of CuOPP(Benzo)$_2$.

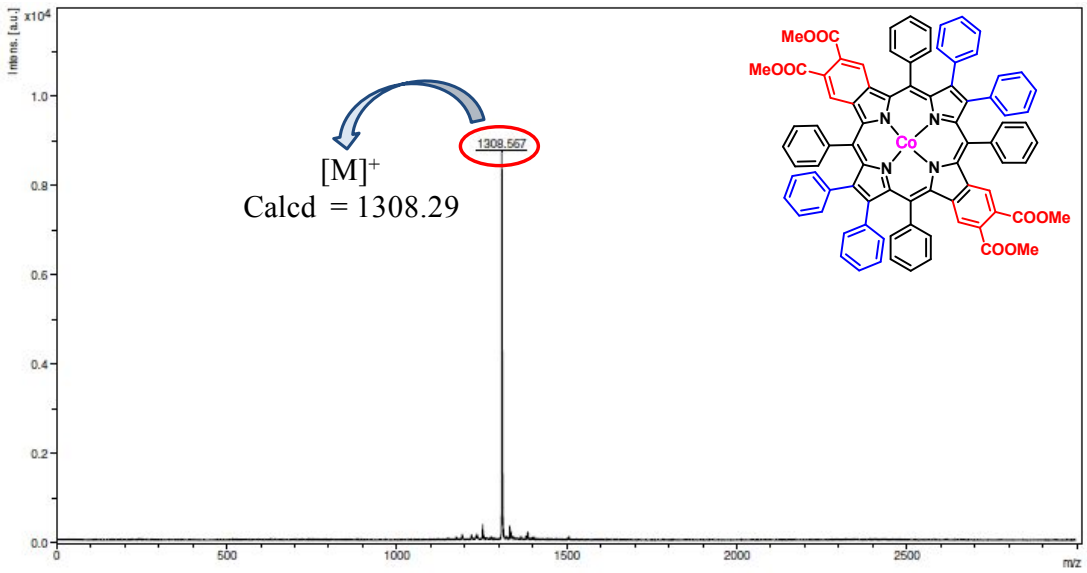


Figure S14. MALDI-TOF mass spectrum of CoOPP(Benzo)$_2$.

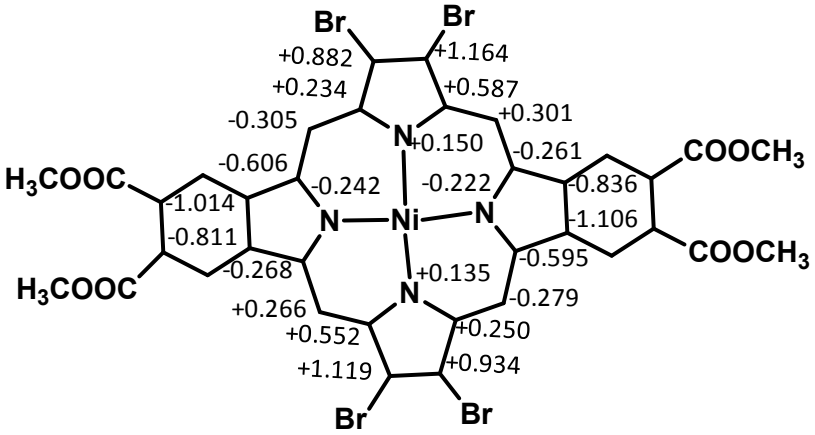
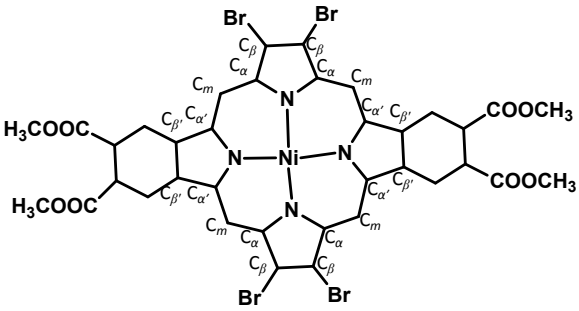


Figure S15 Deviation of the core atoms from the mean plane.

Table S1. Crystal structure data of NiTPP(Benzo)$_2$Br$_4$.	
Empirical formula	$C_{60}H_{36}Br_4N_4NiO_8$
Formula wt.	1319.22
Crystal system	Monoclinic
Space group	C12/c1
a (Å)	38.09
b (Å)	12.91
c (Å)	25.86
α (º)	90
β (º)	105.4
γ (º)	90
Volume (Å^3)	12260
Z	8
$D_{cald.}$ (mg/m^3)	1.429
λ (Å)	0.710
T (K)	293
No. of total reflns.	34335
No. of indepnt. reflns.	4667
R	0.043
R_w	0.112
GOOF	1.065
CCDC	**1830920**

Table S2. Selected average bond lengths and bond angles.



Bond Length (Å)	
Ni -N	1.92(5)
Ni -N’	1.92(7)
N -C_α	1.38(1)
N’-C_α’	1.37(1)
C_α-C_β	1.44(1)
C_α’-C_β’	1.45(1)
C_β- C_β	1.36(1)
C_β’-C_β’	1.38(1)
C_α-C_m	1.38(1)
C_α’-C_m	1.39(1)
ΔC_β	0.987
Δ24	0.548
ΔNi	0.064
Bond Angles (°)	
N- Ni-N	167.64(3)
N’-Ni-N’	169.93(3)
Ni -N-C_α	125.72(5)
Ni -N’-C_α’	125.96(6)
N- C_α-C_m	123.64(8)
N’-C_α’-C_m	123.92(8)
N-C_α -C_β	109.02(7)
N’-C_α’-C_β’	109.65(7)
C_β-C_α-C_m	126.64(8)
C_β’-C_α’-C_m	125.64(8)
C_α-C_β-C_β	107.28(7)
C_α’-C_β’- C_β’	106.48(7)
C_α-N-C_α	106.59(7)
C_α’- N’- C_α’	107.00(7)
C_α-C_m-C_α’	120.86(8)

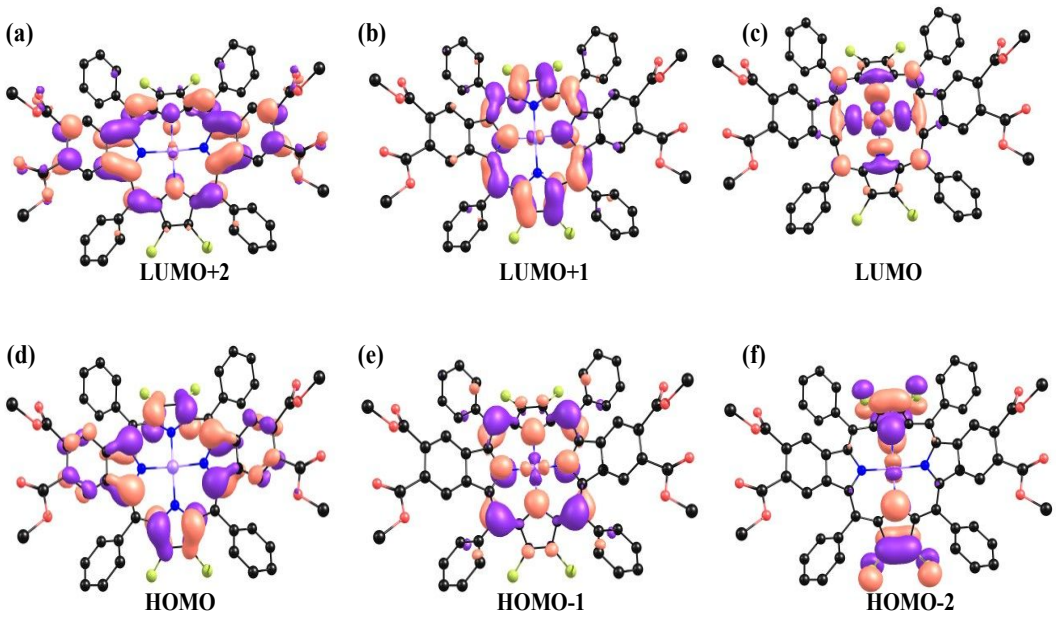


Figure S16. Frontier molecular orbitals (FMOs) of NiOPP(Benzo)$_2$Br$_4$.

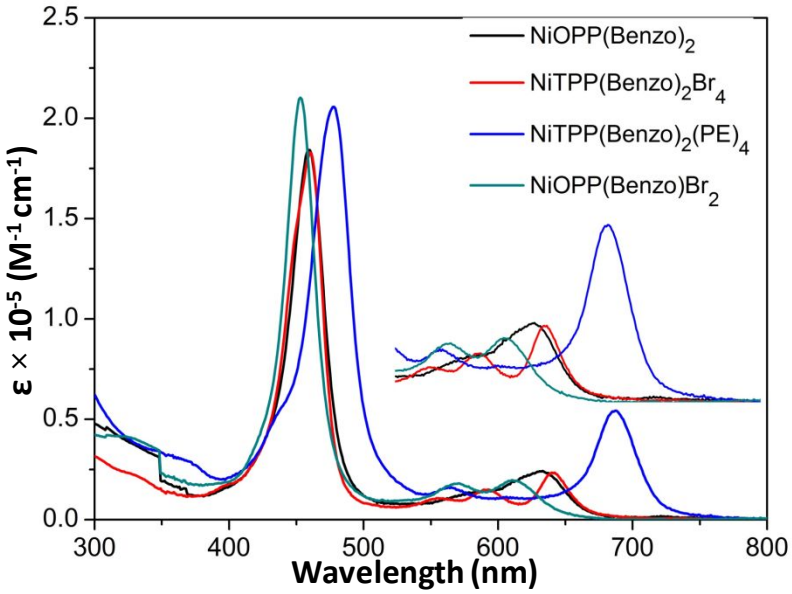


Figure S17. Comparative absorption spectra of Ni(II) benzoporphyrins in CH_2Cl_2 at 298 K.

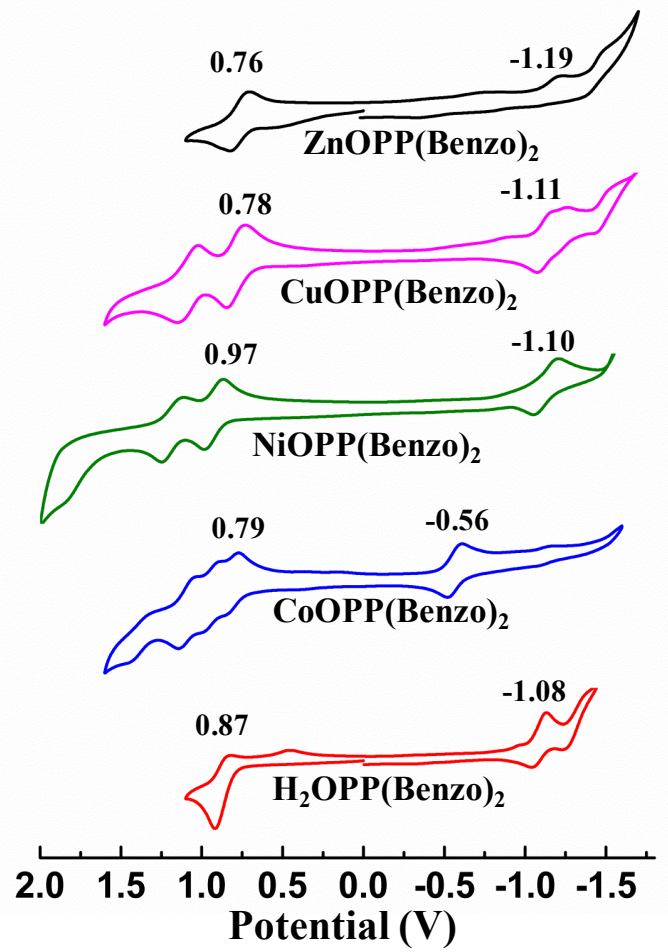


Figure S18. Comparative cyclic voltammograms of MOPP(Benzo)$_2$.

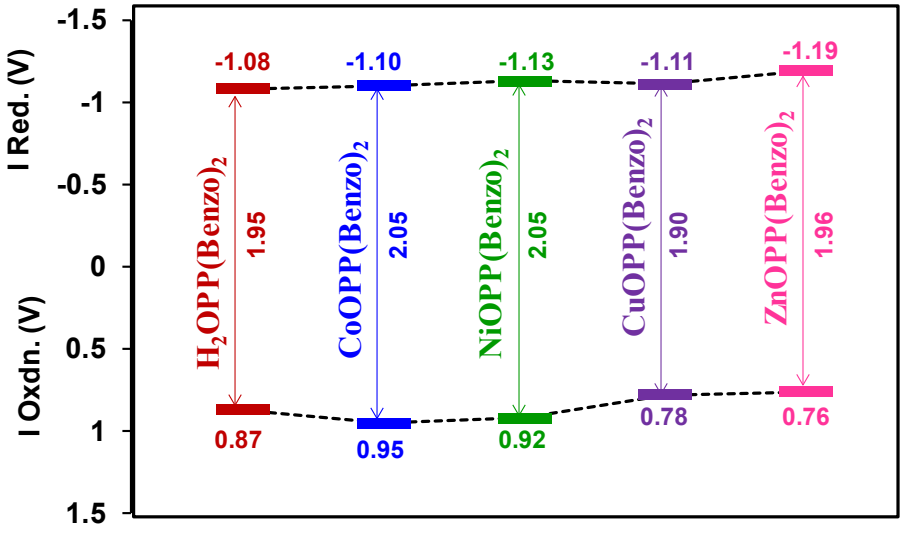


Figure S19. Variation in the HOMO-LUMO gap of MOPP(Benzo)$_2$.