Supporting Information
For

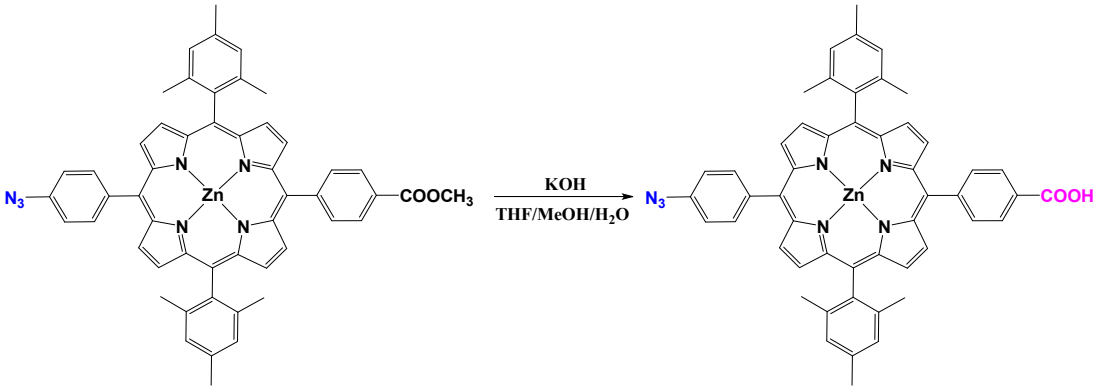
Click made porphyrin-corrole dyad: a system for photo-induced charge separation

Vasilis Nikolaou,[a] Kostas Karikis,[a] Yoann Farre,[b] Georgios Charalambidis,[a] F. Odobel,*[b] and Athanassios G. Coutsolelos.*[a]

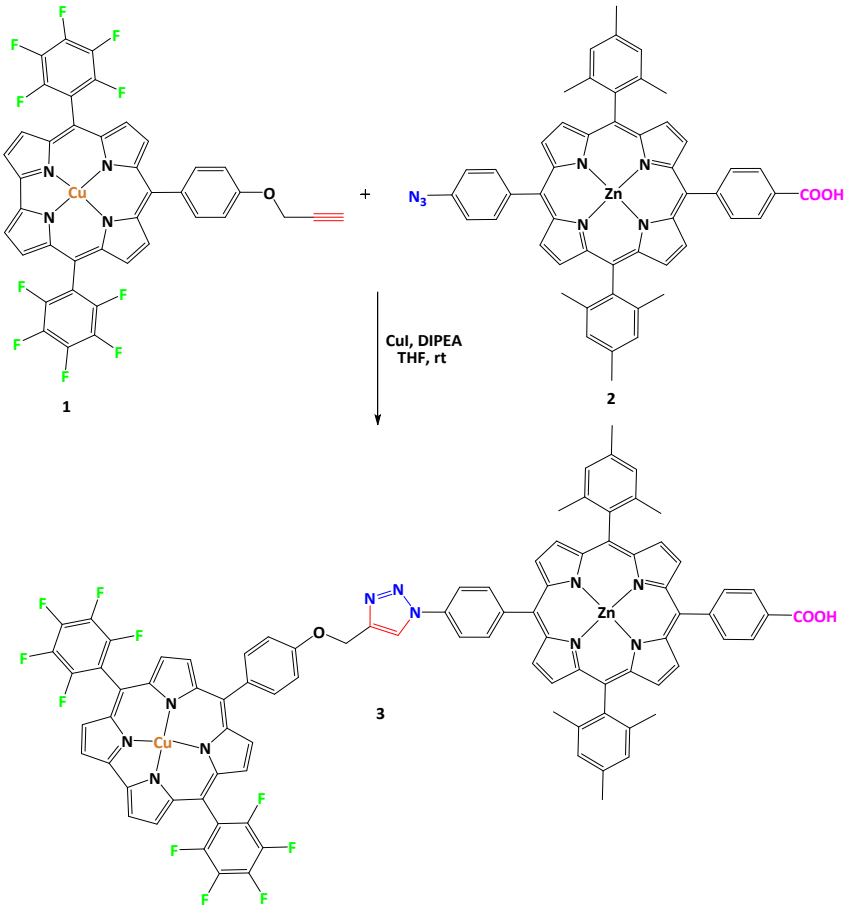
[a]*Department of Chemistry, University of Crete, Laboratory of Bioinorganic Chemistry, Voutes Campus, P.O. Box 2208, 71003, Heraklion, Crete, Greece*

[b]*Université LUNAM, Université de Nantes, CNRS, Chimie et Interdisciplinarité: Synthèse, Analyse, Modélisation (CEISAM), UMR 6230,2 rue de la Houssinière, 44322 Nantes cedex 3, France.*

Table of contents



Scheme S1: Synthesis of **2**.



Scheme S2: Synthesis of **3**.

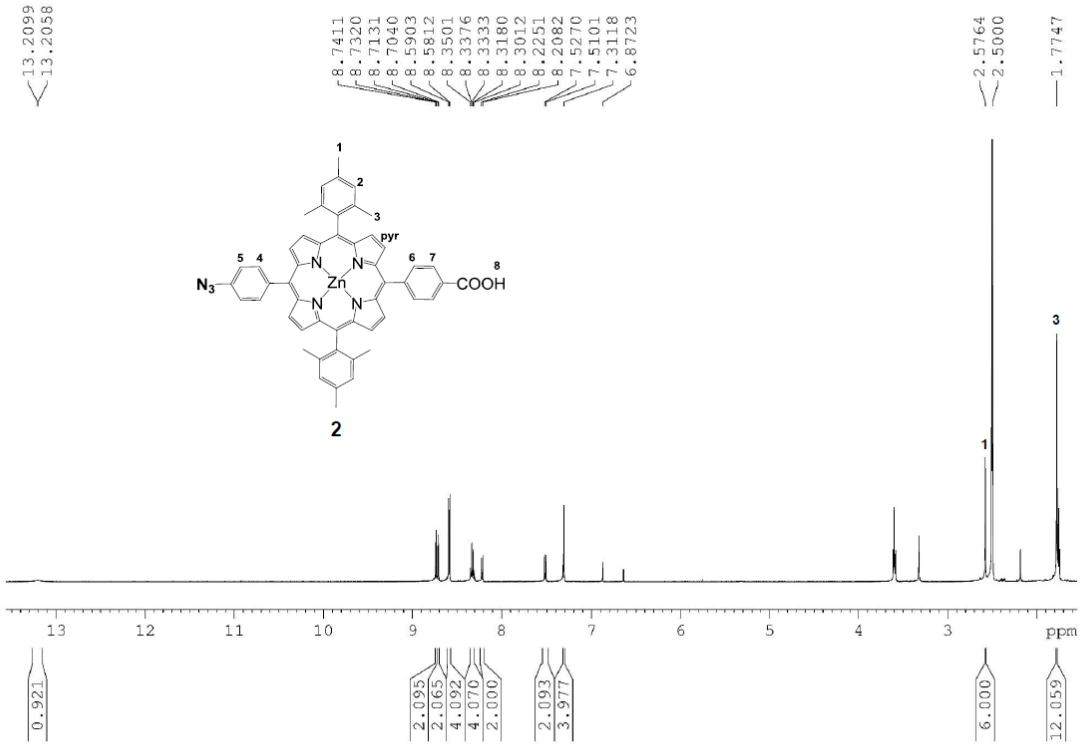


Figure S1: ^{1}H NMR spectrum of **2** (500MHz, DMSO-d^{6}).

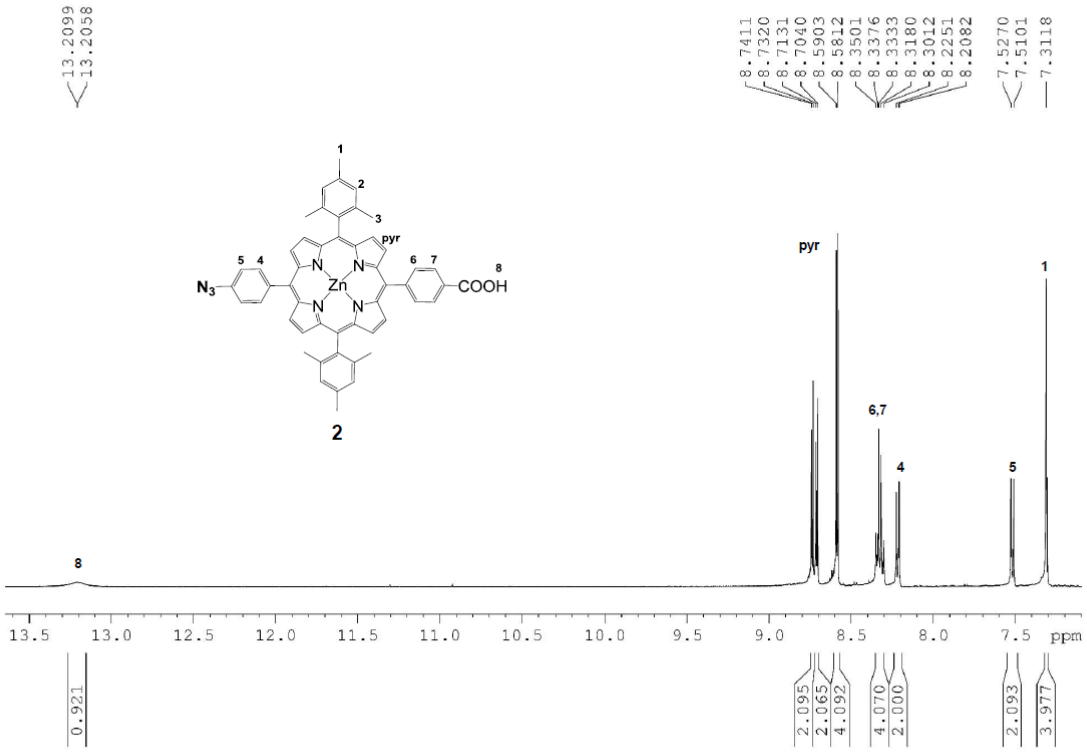


Figure S2: Focus on aromatic region of ^{1}H NMR spectrum of **2** (500MHz, DMSO-d^{6}).

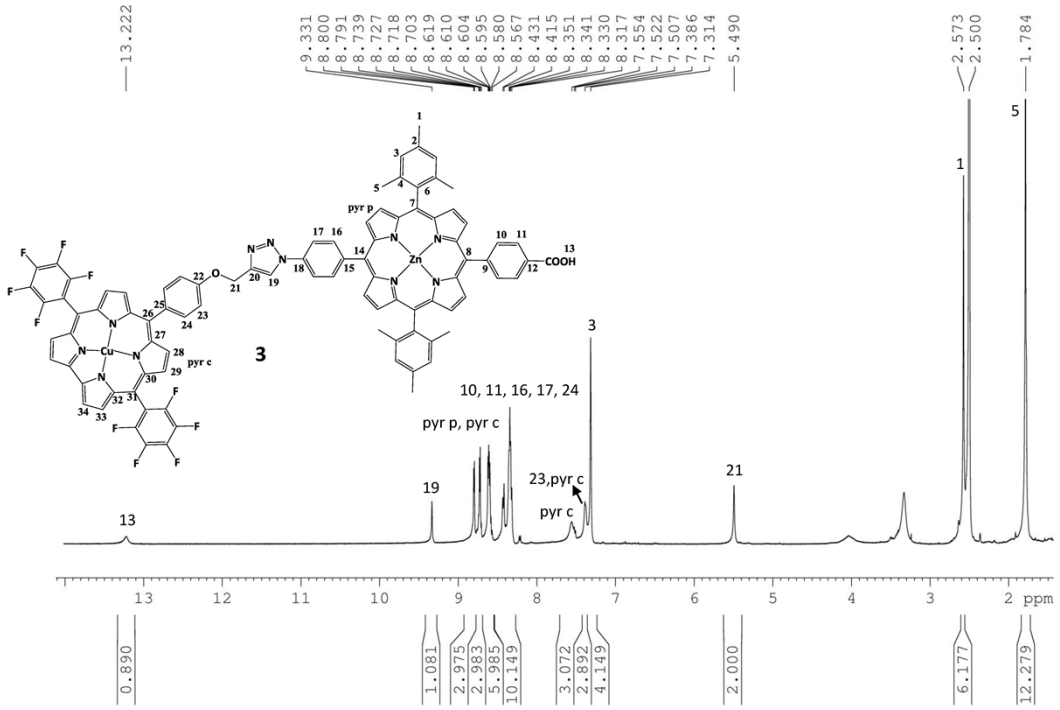


Figure S3: ^{1}H NMR spectrum of **3** (500MHz, DMSO-d^{6}).

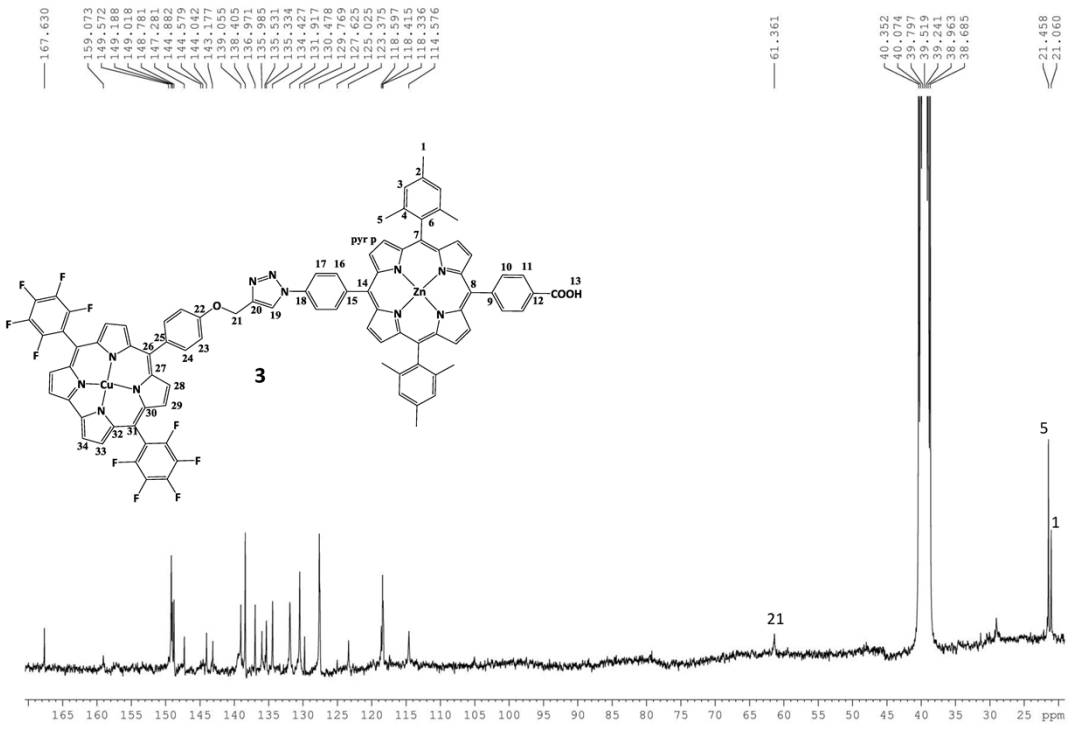


Figure S4: ^{13}C NMR spectrum of **3** (75MHz, DMSO-d^{6})

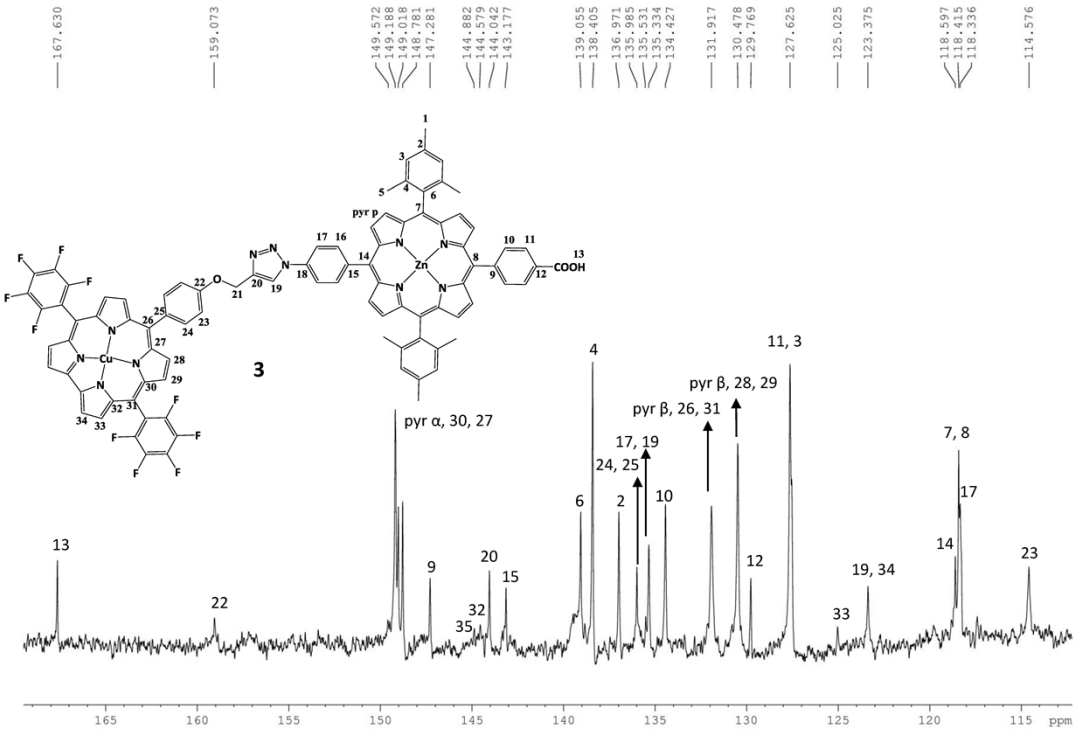


Figure S5: Focus on the aromatic region of ^{13}C NMR spectrum of **VK** (500MHz, DMSO-d^6).

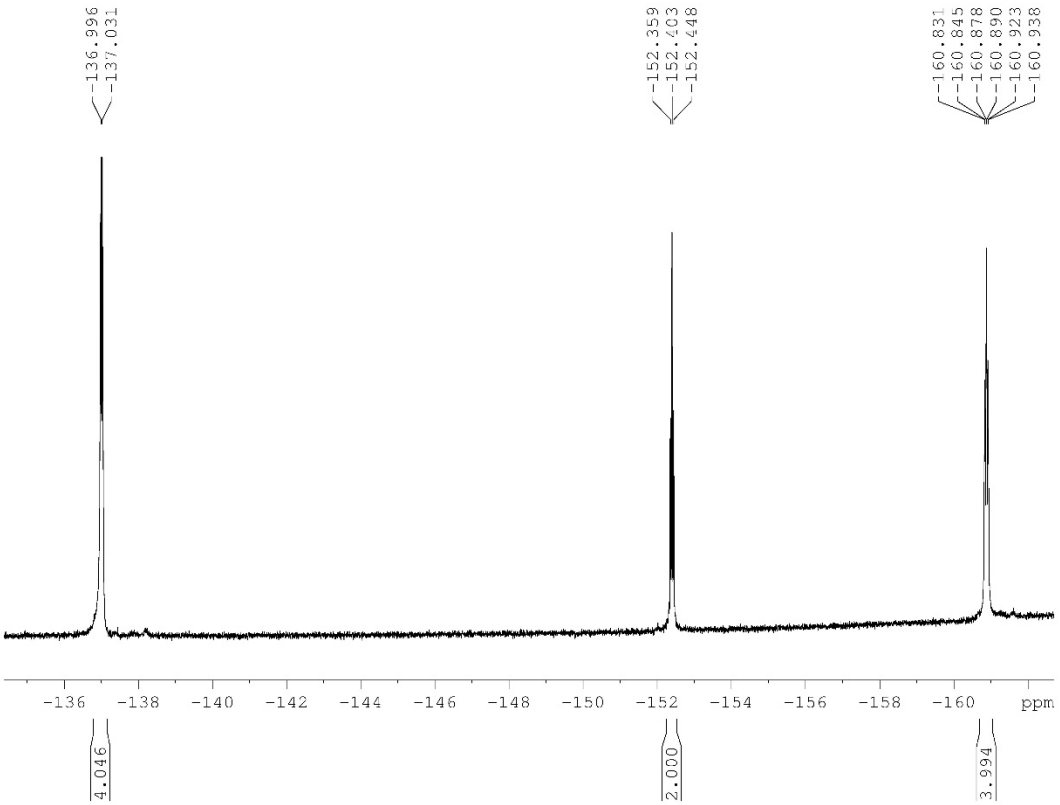


Figure S6: ^{19}F NMR spectrum of **VK** (470MHz, DMSO-d^6).

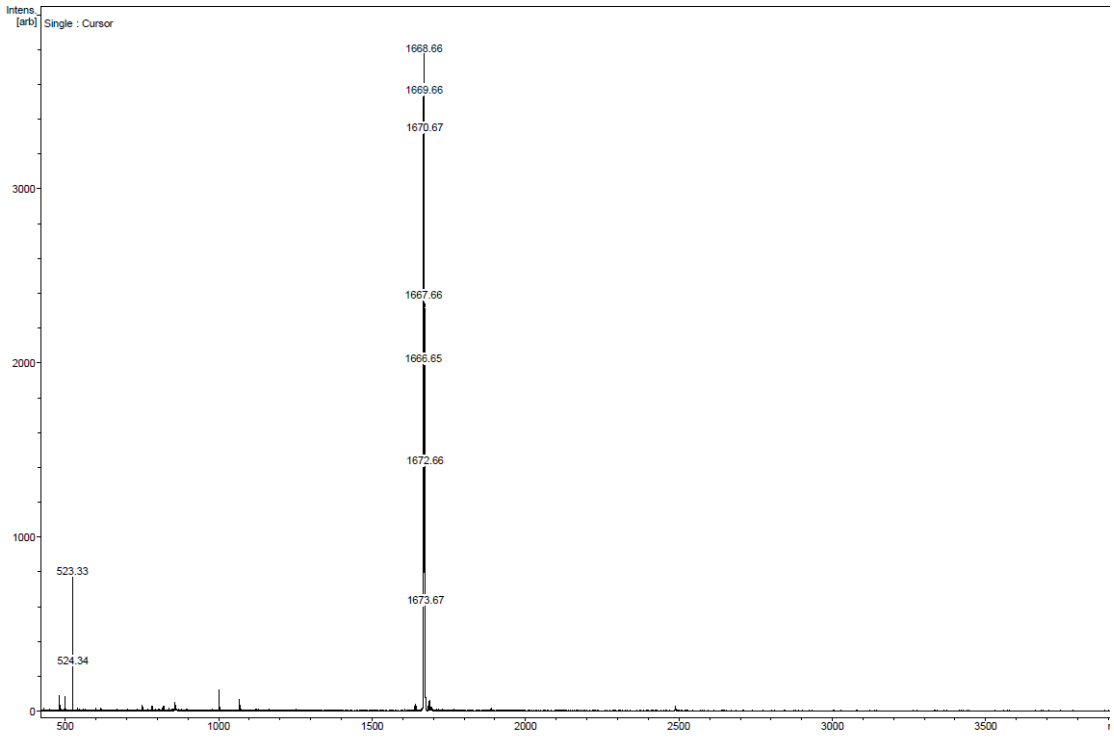


Figure S7: Maldi-TOF spectrum of **3**.

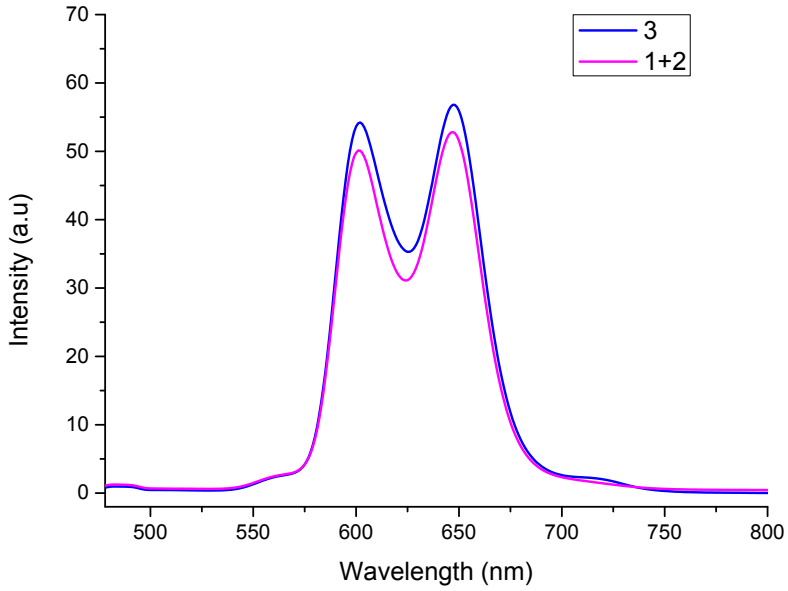


Figure S8: Emission spectra of equal concentration solutions of alkyne corrole -azide porphyrin (magenta) and **3** (blue) when excited at the porphyrin chromophore (420 nm).

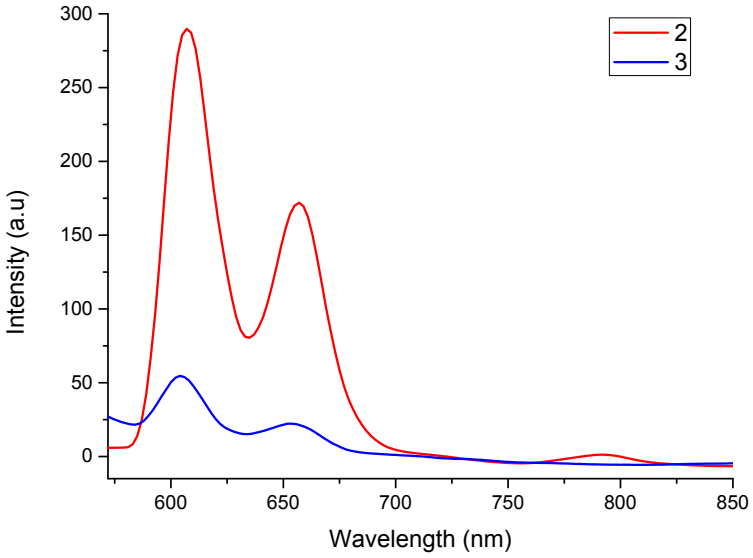


Figure S9: Emission spectra at 77K of **2** (red) and **3** (blue) when excited at the porphyrin chromophore (550 nm).

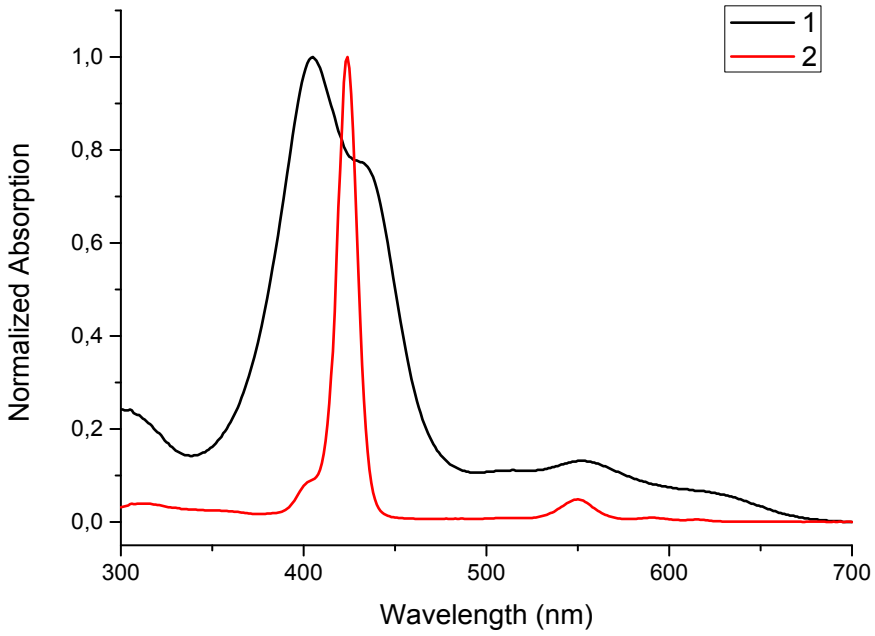


Figure S10: Normalized absorption spectra of **1** (black) and **2** (red) in THF.

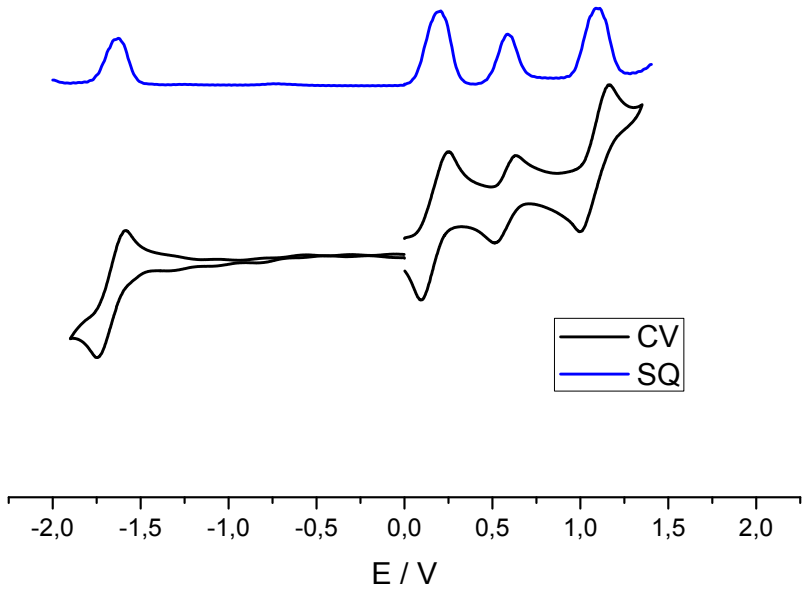


Figure S11: Cyclic and square wave voltammograms of **1** in THF. All potentials are reported vs. SCE and FcH/FcH^+ was used as internal standard ($E_{1/2}Ox$ = 0.55 V).

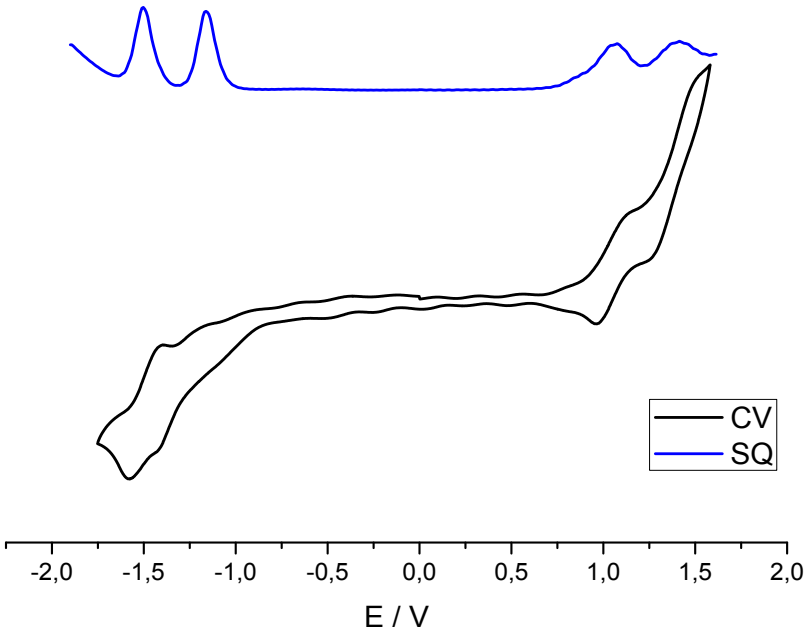


Figure S12: Cyclic and square wave voltammograms of **2** in THF. All potentials are reported vs. SCE and FcH/FcH^+ was used as internal standard ($E_{1/2}Ox$ = 0.55 V).

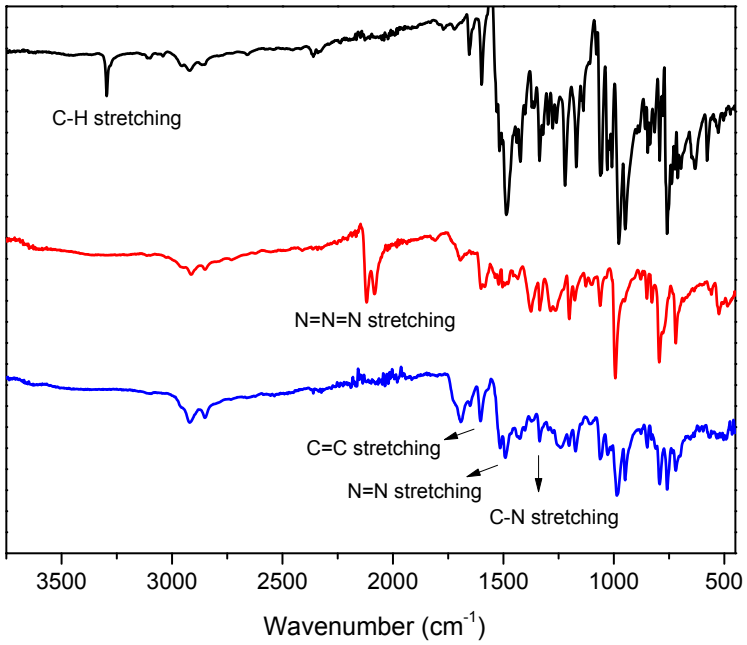


Figure S13: AT-FTIR spectra of **1** (black), **2** (red) and **3** (blue).

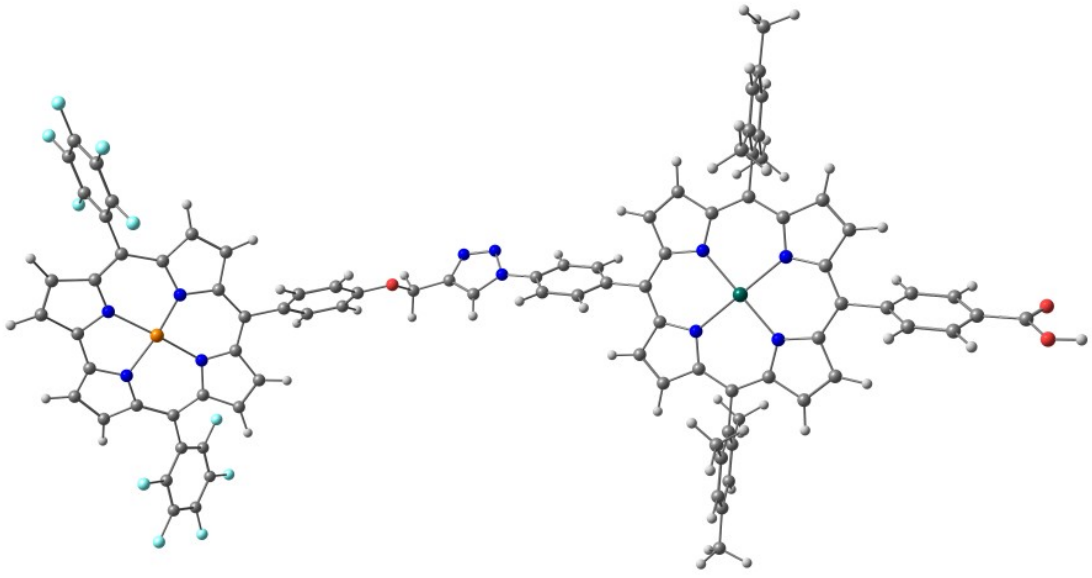


Figure S14: Gas phase geometry optimized structure of **3**. Carbon, nitrogen, hydrogen, oxygen, fluoro, zinc and copper atoms correspond to grey, blue, white, red, light blue, green and orange spheres, respectively.

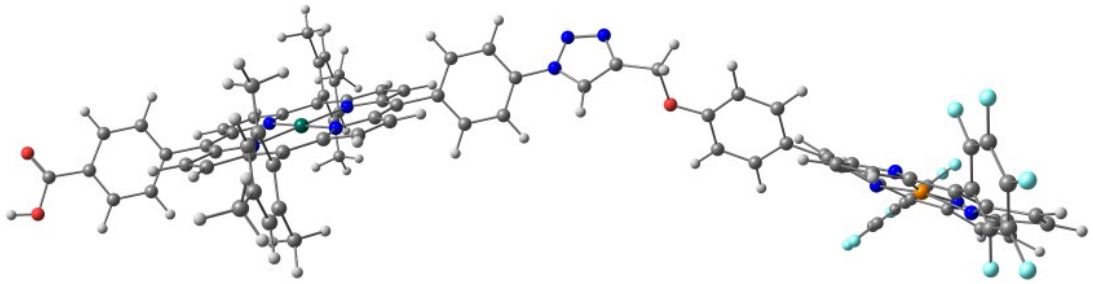


Figure S15: Different view perspective of the gas phase geometry optimized structure of **3**. Carbon, nitrogen, hydrogen, oxygen, fluoro, zinc and copper atoms correspond to grey, blue, white, red, light blue, green and orange spheres, respectively.

Table S1 Coordinates of gas phase geometry optimized structure of **3** calculated by DFT at the B3LYP / 6-31G(d) level. E = - 5588.2265805 Hartree / particle.

	x	**y**	**z**
C	-4.522786000	-0.715040000	0.218792000
C	-2.207990000	-5.057277000	0.105398000
C	1.691551000	-2.629074000	1.871184000
C	-1.557748000	0.759244000	1.494739000
C	-2.286837000	1.971400000	1.266860000
C	-3.534429000	1.608436000	0.802652000
C	-3.571396000	0.168815000	0.736887000
N	-2.376436000	-0.294926000	1.238029000
C	-4.278928000	-2.112222000	0.066750000
C	-5.277726000	-3.123667000	-0.131062000
C	-4.639635000	-4.336558000	-0.157599000
C	-3.235339000	-4.086513000	0.014753000
N	-3.042997000	-2.720853000	0.118045000
C	-0.889252000	-4.782288000	0.541932000
C	0.255386000	-5.640279000	0.407917000
C	1.336344000	-4.961019000	0.906680000
C	0.875829000	-3.674409000	1.345522000
N	-0.486064000	-3.604121000	1.144074000
C	1.257976000	-1.303107000	1.964279000
C	1.827538000	-0.151479000	2.617941000
C	0.905137000	0.871369000	2.536239000
C	-0.227938000	0.355354000	1.827387000

N	0.045389000	-0.918270000	1.438875000
C	3.068644000	-2.965216000	2.315504000
C	-2.535401000	-6.452936000	-0.281549000
C	-5.855532000	-0.185300000	-0.168734000
C	4.195784000	-2.342186000	1.760782000
C	5.489085000	-2.647919000	2.177712000
C	5.685191000	-3.600272000	3.174857000
C	4.587601000	-4.239509000	3.747151000
C	3.303003000	-3.918003000	3.317651000
C	-2.257722000	-7.533728000	0.581097000
C	-2.571652000	-8.836750000	0.225392000
C	-3.164791000	-9.108069000	-1.018687000
C	-3.438759000	-8.050435000	-1.896195000
C	-3.130976000	-6.742678000	-1.518789000
C	-6.348928000	-0.324404000	-1.474131000
C	-7.592968000	0.173244000	-1.852190000
C	-8.383397000	0.835430000	-0.915452000
C	-7.924530000	0.991685000	0.390182000
C	-6.677735000	0.484769000	0.748528000
F	4.055853000	-1.436745000	0.784306000
F	6.542271000	-2.040911000	1.619848000
F	6.920681000	-3.899404000	3.581366000
F	4.773453000	-5.147207000	4.711765000
F	2.274762000	-4.539601000	3.908104000
F	-8.027660000	0.029796000	-3.109031000
F	-5.612240000	-0.936065000	-2.409719000
F	-9.576797000	1.318188000	-1.267677000
F	-8.687287000	1.617080000	1.293555000
F	-6.287111000	0.638506000	2.020004000
O	-3.431397000	-10.419435000	-1.271032000
C	-4.045411000	-10.760116000	-2.520262000
C	-4.248675000	-12.237340000	-2.563347000
C	-5.050303000	-13.046378000	-1.788276000
N	-4.843304000	-14.299445000	-2.274386000
N	-3.956310000	-14.262431000	-3.308626000
N	-3.601332000	-13.023485000	-3.474624000
C	-5.421240000	-15.532246000	-1.861144000
C	-5.514137000	-16.586338000	-2.775001000
C	-6.087457000	-17.789905000	-2.374328000
C	-6.588022000	-17.966233000	-1.073539000
C	-6.478935000	-16.894143000	-0.174349000
C	-5.894128000	-15.687872000	-0.555337000
C	-4.955550000	-20.394490000	-0.840428000
C	-4.517966000	-21.673679000	-0.669257000
C	-5.668809000	-22.473289000	-0.311401000
N	-6.785004000	-21.670126000	-0.274350000
C	-6.383714000	-20.395980000	-0.598177000
C	-10.717114000	-18.473120000	-0.131352000
C	-9.460856000	-18.079213000	-0.483619000
C	-8.602188000	-19.240421000	-0.373412000
N	-9.352772000	-20.318777000	0.030497000

C	-10.648137000	-19.882345000	0.185798000
C	-7.219499000	-19.259536000	-0.660903000
C	-12.428668000	-24.135224000	1.353404000
C	-12.864412000	-22.854241000	1.191963000
C	-11.712337000	-22.053499000	0.840956000
N	-10.596847000	-22.857571000	0.800217000
C	-10.999923000	-24.133629000	1.114377000
C	-11.752053000	-20.670963000	0.568942000
C	-6.664864000	-26.054568000	0.658271000
C	-7.923106000	-26.451086000	0.999279000
C	-8.781340000	-25.289198000	0.889518000
N	-8.028715000	-24.208199000	0.496614000
C	-6.732542000	-24.643909000	0.346226000
C	-5.627980000	-23.854823000	-0.033715000
C	-10.165473000	-25.271877000	1.170083000
C	-10.801973000	-26.570149000	1.558900000
C	-11.326664000	-26.755838000	2.849288000
C	-11.918940000	-27.961923000	3.215559000
C	-11.999535000	-29.013003000	2.291686000
C	-11.480104000	-28.838633000	1.001841000
C	-10.888727000	-27.632205000	0.641592000
Cu	-1.485606000	-1.971857000	0.960814000
Zn	-8.690793000	-22.264081000	0.263229000
C	-12.619618000	-30.321004000	2.625315000
O	-12.711423000	-31.263369000	1.863169000
O	-13.091941000	-30.377594000	3.897770000
H	-1.914096000	2.976243000	1.417377000
H	-4.321197000	2.273334000	0.472048000
H	-6.342040000	-2.944479000	-0.200733000
H	-5.092155000	-5.313907000	-0.243236000
H	0.251074000	-6.619390000	-0.049007000
H	2.363459000	-5.298684000	0.932941000
H	2.774452000	-0.129728000	3.140668000
H	1.001483000	1.870253000	2.941513000
H	-1.808050000	-7.338282000	1.549871000
H	-2.371704000	-9.666598000	0.895824000
H	-3.877378000	-8.229054000	-2.870958000
H	-3.338548000	-5.931915000	-2.210609000
H	-3.401188000	-10.471695000	-3.359267000
H	-5.000143000	-10.224015000	-2.612688000
H	-5.732902000	-12.833770000	-0.981366000
H	-5.142638000	-16.450752000	-3.783748000
H	-6.166054000	-18.604524000	-3.087919000
H	-6.840562000	-17.013461000	0.842464000
H	-5.786543000	-14.886952000	0.169353000
H	-4.363203000	-19.527783000	-1.095645000
H	-3.507990000	-22.046628000	-0.765499000
H	-11.615168000	-17.872343000	-0.099186000
H	-9.147107000	-17.095075000	-0.799986000
H	-13.021869000	-25.003627000	1.600175000
H	-13.874188000	-22.480934000	1.288961000

H	-5.766639000	-26.655112000	0.628241000
H	-8.239332000	-27.437365000	1.306252000
H	-11.258869000	-25.946793000	3.570575000
H	-12.314257000	-28.094180000	4.216655000
H	-11.554196000	-29.658391000	0.294770000
H	-10.495349000	-27.499760000	-0.361936000
H	-13.469149000	-31.271496000	3.996981000
C	-13.085735000	-19.982045000	0.688272000
C	-13.937861000	-19.887784000	-0.432857000
C	-13.483830000	-19.426480000	1.922808000
C	-15.171155000	-19.240893000	-0.297115000
C	-14.725986000	-18.788499000	2.013303000
H	-15.823039000	-19.167777000	-1.165695000
H	-15.026432000	-18.358803000	2.967095000
C	-15.587181000	-18.687253000	0.917185000
C	-4.293162000	-24.542590000	-0.146267000
C	-3.444286000	-24.629699000	0.978331000
C	-3.886714000	-25.095770000	-1.378709000
C	-2.206817000	-25.268790000	0.848122000
C	-2.639955000	-25.726250000	-1.463573000
H	-1.554666000	-25.330106000	1.717449000
H	-2.329981000	-26.148259000	-2.417651000
C	-1.785380000	-25.826898000	-0.362683000
C	-4.771162000	-25.013921000	-2.603365000
H	-4.296361000	-25.501110000	-3.460616000
H	-5.740030000	-25.498129000	-2.433324000
H	-4.981388000	-23.973894000	-2.879773000
C	-3.849033000	-24.041766000	2.312257000
H	-4.774463000	-24.494332000	2.687855000
H	-3.067601000	-24.201437000	3.061628000
H	-4.031077000	-22.962971000	2.238842000
C	-0.456143000	-26.538313000	-0.469030000
H	0.307303000	-26.057625000	0.152720000
H	-0.534986000	-27.581628000	-0.134774000
H	-0.091465000	-26.554168000	-1.501503000
C	-16.937921000	-18.021611000	1.046730000
H	-17.244741000	-17.550124000	0.106771000
H	-17.716438000	-18.749196000	1.313430000
H	-16.932887000	-17.252340000	1.826405000
C	-12.591145000	-19.507797000	3.141520000
H	-13.059439000	-19.018851000	4.001400000
H	-12.381003000	-20.547937000	3.417537000
H	-11.622365000	-19.025955000	2.964401000
C	-13.538623000	-20.469383000	-1.771200000
H	-12.612404000	-20.018558000	-2.146866000
H	-13.360548000	-21.549202000	-1.703905000
H	-14.321484000	-20.302986000	-2.517598000