Supporting Information

Electrochemistry of Bis-pyridine Cobalt Nitrophenylcorroles in Nonaqueous Media

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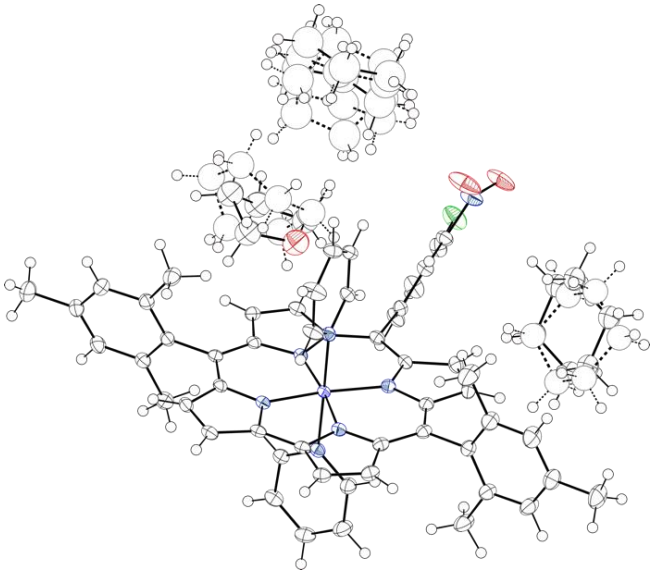
X-Ray Data of Compound [10-(4-F-3-NO_2)Ph-5,15-di-Mesityl]CorCo(Py)$_2$, 1



Compound	**Compound 1**
CCDC	1578032
Formula	$C_{69.38}H_{75.76}CoFN_7O_{2.81}$
$D_{calc.}$/ g cm^{-3}	1.276
μ/mm^{-1}	2.736
Formula Weight	1130.58
Colour	metallic dark violet
Shape	prism
Size/mm^3	0.48x0.21x0.14
T/K	100
Crystal System	monoclinic
Space Group	$P2_1/n$
a/Å	13.4928(6)
b/Å	14.9338(7)
c/Å	29.3778(14)
α/°	90
β/°	96.285(2)
γ/°	90
V/Å^3	5884.0(5)
Z	4
Z'	1
Wavelength/Å	1.541840
Radiation type	CuK_α
Θ_{min}/°	3.324
Θ_{max}/°	66.773
Measured Refl.	81064
Independent Refl.	10400
Reflections Used	9847
R_{int}	0.0383
Parameters	652
Restraints	6
Largest Peak	0.680
Deepest Hole	-0.940
GooF	1.036
wR_2 (all data)	0.1248
wR_2	0.1228
R_1 (all data)	0.0482
R_1	0.0460

Experimental Section. Single metallic dark violet prism-shaped crystals of (**Compound 1**) were recrystallized from a mixture of cyclohexane and THF by slow evaporation. A suitable crystal (0.48 x 0.21 x 0.14) mm^3 was selected and mounted on a MITIGEN holder oil on a Bruker D8 VENTURE diffractometer. The crystal was kept at T = 100 K during data collection. Using **Olex2**[1], the structure was solved with the **ShelXT**[2] structure solution program, using the Intrinsic Phasing solution method. The model was refined with version 2017/1 of **ShelXL**[2] using Least Squares minimization.

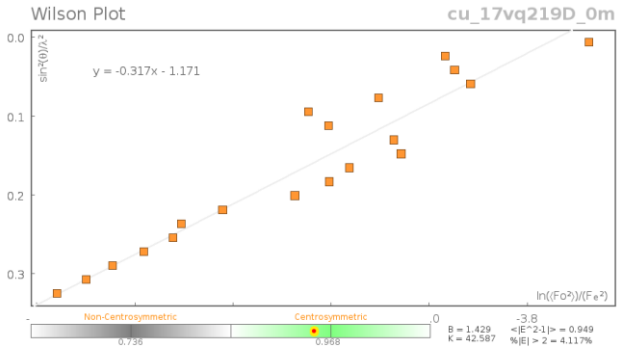
Crystal Data. $C_{69.38}H_{75.76}CoFN_7O_{2.81}$, M_r = 1130.58, monoclinic, $P2_1/n$ (No. 14), a = 13.4928(6) Å, b = 14.9338(7) Å, c = 29.3778(14) Å, β = 96.285(2)°, $\alpha = \gamma = 90$°, V = 5884.0(5) Å^3, T = 100 K, Z = 4, Z' = 1, μ(CuK_α) = 2.736, 81064 reflections measured, 10400 unique (R_{int} = 0.0383) which were used in all calculations. The final wR_2 was 0.1248 (all data) and R_1 was 0.0460 (I > 2σ(I)).

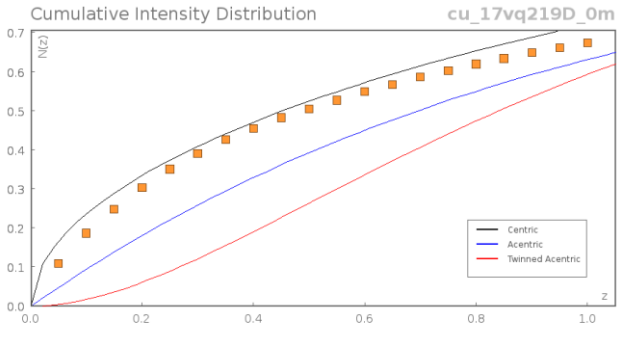
Structure Quality Indicators

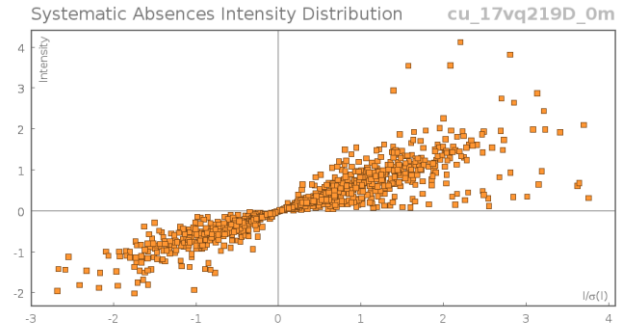
Reflections:	d min (Cu) 0.84	I/σ 33.4	Rint 3.83%	complete 100%
Refinement:	Shift 0.001	Max Peak 0.7	Min Peak -0.9	GooF 1.036

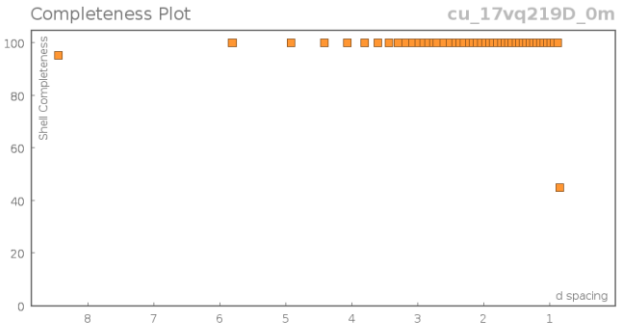
A metallic dark violet prism-shaped crystal with dimensions 0.48 x 0.21 x 0.14 mm^3 was mounted on a MITIGEN holder oil. X-ray diffraction data were collected using a Bruker D8 VENTURE diffractometer equipped with an Oxford Cryosystems low-temperature device, operating at T = 100 K. Data were measured using ϕ and ω scans of 1.00 ° per frame for 10.00 s using CuK_α radiation (sealed X-ray tube, 50 kV, 1 mA). The total number of runs and images was based on the strategy calculation from the program APEX3 (Bruker, 2015). The maximum resolution achieved was Θ = 66.773°. Cell parameters were retrieved using the **SAINT**[3] software and refined using **SAINT**[3] on 9270 reflections, 11 % of the observed reflections. Data reduction was performed using the **SAINT**[3] software which corrects for Lorentz polarization. The final completeness is 99.90 % out to 66.773° in Θ. A multi-scan absorption correction was performed using SADABS-2016/2[4] was used for absorption correction. wR_2 (int) was 0.0977 before and 0.0542 after correction. The Ratio of minimum to maximum transmission is 0.7323. The λ/2 correction factor is Not present. The absorption coefficient μ of this material is 2.736 mm^{-1} at this wavelength (λ = 1.54178Å) and the minimum and maximum transmissions are 0.4178 and 0.5705. The structure was solved in the space group $P2_1/n$ (# 14) by Intrinsic Phasing using the **ShelXT**[2] structure solution program and refined by Least Squares using version 2017/1 of **ShelXL**[2]. All hydrogen atoms and minor disordered part were refined isotopically. Hydrogen atom positions were calculated geometrically and refined using the riding model. For each solvent, disordered parts were found in the crystal structure and some geometric parameters of disordered components in each group were restrained by using EADP constraints, SADI restraints or some rigid fragment taken from the literature. One site is partially occupied by a mixture of THF/cyclohexane (81%/19%), other disordered cyclohexane was found in ratio 31%/69% and over three positions in ration 37%/32%/31%. (For more detail see the .res file included in the cif. files). SADABS-2016/2[4] was used for absorption correction. wR_2 (int) was 0.0977 before and 0.0542 after correction. The Ratio of minimum to maximum transmission is 0.7323. There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 4 and Z' is 1.

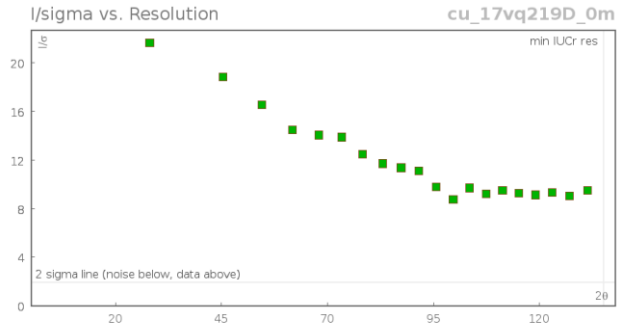
Data Plots: Diffraction Data



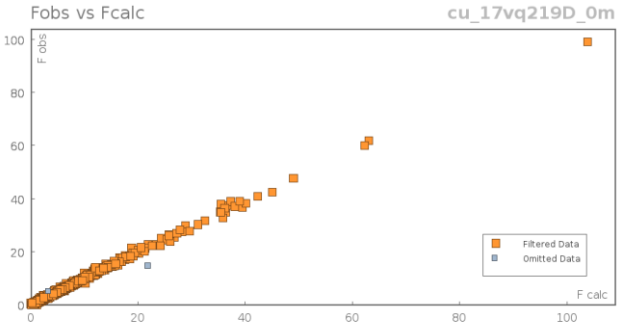


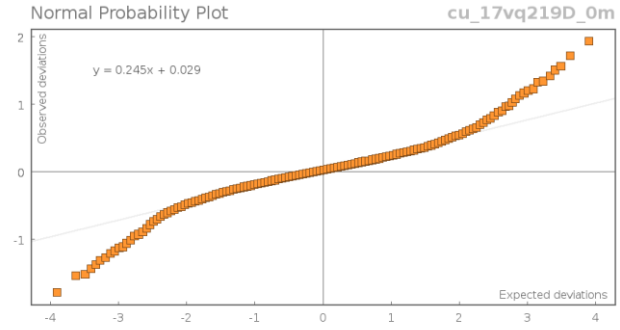






Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	82959	Unique reflections	10400
Completeness	0.999	Mean I/σ	33.36
hkl_{max} collected	(14, 17, 34)	hkl_{min} collected	(-16, -17, -35)
hkl_{max} used	(15, 17, 34)	hkl_{min} used	(-16, 0, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.77
d_{max} used	14.6	d_{min} used	0.84
Friedel pairs	14556	Friedel pairs merged	1
Inconsistent equivalents	0	R_{int}	0.0383
R_{sigma}	0.0203	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	6
Multiplicity	(11495, 11137, 6268, 3410, 1756, 805, 312, 110, 8)	Maximum multiplicity	21
Removed systematic absences	1889	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer

Table S1. Fractional atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for **compound 1**. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij}.

Atom	x	y	z	U_{eq}
Co1	7303.4(2)	6782.9(2)	6668.7(2)	13.13(10)
O1	5327.0(19)	9265.7(12)	4513.5(7)	54.0(6)
F1	4534.4(12)	7055.7(11)	3785.8(5)	41.5(4)
N4	6041.7(12)	6473.5(11)	6360.3(5)	15.0(3)
N3	7903.3(12)	7054.8(11)	6129.7(6)	16.2(3)
N2	8485.6(12)	7038.4(11)	7038.2(6)	16.6(3)
N1	6869.9(12)	6538.3(11)	7239.7(6)	15.6(3)
O2	5183.0(17)	8715.8(13)	3838.0(6)	48.9(5)
N6	7740.7(12)	5508.4(11)	6640.2(5)	17.3(3)
N5	6857.3(12)	8043.1(11)	6704.7(6)	15.7(3)
C15	5796.3(15)	6474.5(13)	5895.3(7)	15.8(4)
C14	6450.8(16)	6725.0(13)	5574.6(7)	17.3(4)
C13	7445.0(15)	7001.1(13)	5691.9(7)	16.7(4)
C10	8867.9(15)	7375.4(13)	6112.3(7)	17.6(4)
C11	8999.1(16)	7518.0(14)	5641.0(7)	20.8(4)
C12	8137.6(16)	7291.0(14)	5383.5(7)	20.7(4)
C9	9581.2(15)	7519.4(13)	6488.8(7)	18.0(4)
C8	9394.4(15)	7341.5(13)	6942.2(7)	17.7(4)
C5	8500.5(15)	6900.7(13)	7498.3(7)	17.3(4)
C4	7551.9(15)	6621.7(13)	7616.1(7)	17.0(4)
C1	5961.9(15)	6317.3(13)	7367.4(7)	16.7(4)
C19	5132.8(15)	6179.4(13)	7038.6(7)	17.1(4)
C18	5195.8(14)	6252.5(12)	6568.2(7)	16.0(4)
C17	4405.1(15)	6094.0(13)	6208.3(7)	18.1(4)
C16	4758.8(15)	6236.1(13)	5800.4(7)	19.0(4)
C20	4155.9(15)	5929.6(14)	7200.0(7)	18.5(4)
C25	3840.2(16)	5034.3(14)	7180.7(7)	21.7(4)
C26	4473.4(18)	4315.3(15)	6995.7(9)	28.7(5)
C24	2935.9(16)	4808.9(15)	7339.3(8)	25.5(5)
C23	2336.6(16)	5444.1(16)	7516.9(8)	26.6(5)
C27	1359.6(18)	5188.0(18)	7685.1(10)	38.5(6)
C22	2659.7(16)	6327.9(16)	7531.0(8)	25.7(5)
C21	3557.9(16)	6583.1(15)	7375.4(7)	21.4(4)
C28	3860.0(18)	7557.9(15)	7394.6(9)	28.7(5)
C2	6076.9(16)	6253.2(13)	7857.5(7)	19.7(4)
C3	7059.5(16)	6443.3(13)	8010.6(7)	20.1(4)
C6	9465.9(15)	7124.3(14)	7710.5(7)	20.8(4)
C7	10017.5(16)	7397.1(14)	7366.4(7)	21.9(4)
C29	10589.0(15)	7867.5(14)	6410.6(7)	19.6(4)
C34	10769.4(17)	8788.9(15)	6411.9(9)	28.4(5)
C33	11712.2(18)	9101.1(16)	6334.3(9)	33.9(6)
C32	12475.3(17)	8524.2(17)	6259.7(9)	30.8(5)
C36	13490.0(19)	8858(2)	6168.8(10)	41.3(6)
C31	12287.0(17)	7612.1(16)	6271.8(9)	30.2(5)
C30	11361.8(16)	7268.9(15)	6346.5(8)	24.0(5)
C35	11201.8(18)	6270.6(16)	6360.8(10)	34.3(6)
C37	9968(2)	9444.2(17)	6505.2(12)	48.5(8)
C38	6009.2(15)	6797.9(13)	5088.6(7)	18.5(4)
C43	5676.3(17)	6050.1(15)	4830.5(7)	25.0(5)
C42	5179.9(19)	6140.7(16)	4393.7(8)	29.9(5)
C41	5035.2(17)	6978.0(16)	4203.7(7)	25.8(5)
C40	5389.9(16)	7729.7(15)	4447.8(7)	22.8(4)
N7	5284.9(16)	8631.7(13)	4252.4(7)	32.1(5)
C39	5863.2(16)	7639.2(14)	4890.2(7)	20.5(4)
C53	7112.0(15)	4829.1(14)	6699.8(7)	18.9(4)
C52	7416.9(17)	3940.1(14)	6718.6(7)	23.5(5)
C51	8405.8(18)	3738.4(15)	6680.5(8)	29.0(5)
C50	9049.3(18)	4438.4(16)	6619.6(9)	30.5(5)
C49	8695.6(16)	5304.2(15)	6596.8(8)	23.7(4)
C48	6367.2(15)	8446.6(14)	6338.3(7)	18.9(4)
C47	5998.0(15)	9308.8(14)	6350.4(7)	20.2(4)
C46	6141.7(16)	9787.9(14)	6752.8(8)	23.7(5)
C45	6660(2)	9385.0(16)	7128.0(8)	32.1(5)

Atom	x	y	z	U_{eq}
C44	7007.2(18)	8522.1(15)	7093.7(7)	25.4(5)
C55	8685(2)	6391.6(15)	3884.0(12)	44.4(5)
C54	9244.0(17)	7217.6(19)	4077.0(11)	44.4(5)
C59	8864(2)	8064.8(16)	3826.4(11)	44.4(5)
C58	7741(2)	8170.7(15)	3831.0(11)	44.4(5)
C57	7182.6(18)	7343.7(19)	3637.1(11)	44.4(5)
C56	7563(2)	6497.5(16)	3887.7(11)	44.4(5)
O3	2929.9(12)	5832.8(17)	4930.8(7)	51.9(4)
C69	2290.7(17)	5827(2)	5293.8(5)	51.9(4)
C68	1215.9(14)	5809(2)	5060.5(8)	51.9(4)
C67	1340.2(15)	5276(2)	4622.2(8)	51.9(4)
C66	2349.8(16)	5623(2)	4501.7(6)	51.9(4)
C70	2792(6)	10153(6)	4632(4)	81.4(9)
C71	2326(7)	10323(6)	5074(3)	81.4(9)
C72	1232(6)	10047(6)	5028(3)	81.4(9)
C73	1101(6)	9076(6)	4875(3)	81.4(9)
C74	1567(6)	8907(5)	4432(3)	81.4(9)
C75	2660(6)	9182(6)	4478(3)	81.4(9)
C59A	9293(5)	7878(5)	3834(3)	51.6(12)
C58A	8204(6)	8166(4)	3751(3)	51.6(12)
C57A	7520(5)	7368(5)	3632(3)	51.6(12)
C56A	7670(5)	6643(5)	3997(3)	51.6(12)
C55A	8758(6)	6355(4)	4080(3)	51.6(12)
C54A	9442(5)	7153(5)	4199(2)	51.6(12)
C65	1225(10)	6671(10)	5130(7)	60.0(19)
C60	2344(10)	6681(12)	5114(6)	60.0(19)
C62	2172(13)	5298(10)	4696(6)	60.0(19)
C61	2639(14)	6228(10)	4686(6)	60.0(19)
C63	1506(11)	5124(12)	5073(6)	60.0(19)
C64	652(11)	5791(9)	5069(7)	60.0(19)
C72A	1640(8)	9479(6)	5203(3)	81.4(9)
C73A	1528(7)	10125(5)	4799(3)	81.4(9)
C74A	2389(8)	10035(6)	4507(3)	81.4(9)
C75A	2505(8)	9073(7)	4349(3)	81.4(9)
C70A	2619(7)	8427(5)	4753(3)	81.4(9)
C71A	1756(8)	8517(5)	5045(3)	81.4(9)
C70B	2883(7)	8944(7)	4514(4)	81.4(9)
C75B	1884(8)	8459(6)	4463(3)	81.4(9)
C74B	1332(7)	8593(6)	4883(3)	81.4(9)
C73B	1207(7)	9583(7)	4988(4)	81.4(9)
C72B	2206(8)	10068(6)	5038(4)	81.4(9)
C71B	2757(8)	9935(6)	4618(5)	81.4(9)

Table S2. Anisotropic displacement parameters (x10^4) **compound 1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co1	14.46(17)	12.64(17)	12.01(17)	0.60(11)	0.15(12)	0.25(12)
O1	99.3(17)	22.9(9)	35.1(10)	0.2(8)	-14(1)	8.9(10)
F1	52.7(9)	46.2(9)	21.8(7)	3.2(6)	-12.8(6)	-9.5(7)
N4	17.2(8)	13.3(8)	14.4(8)	1.0(6)	1.3(6)	0.2(6)
N3	16.8(8)	14.8(8)	16.7(8)	-0.3(7)	1.0(6)	0.4(6)
N2	18.1(8)	15.8(8)	15.4(8)	0.5(6)	0.1(6)	1.4(7)
N1	18.5(8)	13.2(8)	14.8(8)	1.1(6)	0.6(6)	0.8(6)
O2	86.3(16)	34.3(10)	23.3(9)	8.5(7)	-6.1(9)	13.9(10)
N6	19.9(8)	17.8(8)	13.8(8)	0.1(6)	0.5(6)	0.3(7)
N5	15.0(8)	15.6(8)	16.4(8)	1.2(6)	1.1(6)	-1.4(6)
C15	19.6(10)	11.6(9)	15.8(9)	0.7(7)	-1.0(7)	0.3(7)
C14	21.7(10)	13.1(9)	16.6(10)	-0.3(7)	0.3(8)	0.2(7)
C13	21.6(10)	14.2(9)	14.2(9)	1.0(7)	2.0(8)	0.6(8)
C10	18(1)	13.4(9)	21.7(10)	-0.6(8)	3.7(8)	0.8(7)
C11	20.5(10)	21(1)	21.8(11)	-0.2(8)	6.3(8)	-1.9(8)
C12	24.6(11)	22.3(11)	15.4(10)	-0.1(8)	3.8(8)	-0.9(8)
C9	17.4(10)	14.4(9)	22.3(10)	-2.4(8)	2.1(8)	1.1(8)
C8	17.2(10)	14.3(9)	21.2(10)	-2.9(8)	0.5(8)	0.6(8)
C5	21.7(10)	13.8(9)	15.9(10)	-0.5(7)	-0.8(8)	3.7(8)
C4	22.6(10)	12.0(9)	15.5(10)	0.2(7)	-1.1(8)	3.1(8)
C1	21(1)	11.4(9)	18.3(10)	1.9(7)	4.3(8)	1.7(7)
C19	19.2(10)	11.6(9)	20.7(10)	1.9(7)	3.3(8)	2.2(7)
C18	17.0(9)	10.3(9)	20.6(10)	0.9(7)	1.4(8)	0.5(7)
C17	15.7(9)	15.4(10)	22.8(10)	0.7(8)	-0.1(8)	-0.6(7)
C16	21.4(10)	15.7(10)	18.7(10)	0.3(8)	-3.2(8)	-0.7(8)
C20	19.4(10)	18.7(10)	17.4(10)	2.9(8)	1.7(8)	-0.7(8)
C25	22.6(10)	19.5(10)	23(1)	3.6(8)	2.4(8)	0.2(8)
C26	31.5(12)	16.8(10)	38.9(13)	1.7(9)	9.4(10)	-0.7(9)
C24	25.7(11)	20.3(11)	30.7(12)	6.3(9)	3.7(9)	-4.8(9)
C23	22.5(11)	29.8(12)	28.0(11)	8.5(9)	5.2(9)	-1.9(9)
C27	27.6(13)	37.3(14)	53.0(16)	9.7(12)	15.7(11)	-1.7(11)
C22	24.0(11)	27.6(12)	26.6(11)	0.7(9)	7.6(9)	3.5(9)
C21	23.4(11)	21.2(10)	19.8(10)	1.3(8)	3.6(8)	0.6(9)
C28	28.7(12)	21.4(11)	37.6(13)	-3.5(10)	11.1(10)	0.8(9)
C2	25.3(10)	15.9(10)	18.7(10)	3.1(8)	6.2(8)	1.7(8)
C3	28.1(11)	16.5(10)	15.2(10)	1.5(8)	0.6(8)	4.1(8)
C6	21.9(10)	22.2(11)	16.9(10)	-1.5(8)	-3.4(8)	2.0(8)
C7	17.9(10)	22.6(11)	24.0(11)	-4.0(9)	-2.7(8)	0.0(8)
C29	17.5(10)	21.5(11)	19.6(10)	-1.7(8)	1.3(8)	-1.7(8)
C34	26.9(12)	21.2(11)	38.4(13)	-3(1)	8.8(10)	-1.8(9)
C33	32.4(13)	22.2(12)	48.7(15)	-4.6(11)	11.1(11)	-8.5(10)
C32	22.0(11)	34.5(13)	36.1(13)	-1.5(10)	4.5(10)	-6.3(10)
C36	26.0(13)	45.2(16)	54.1(17)	-0.9(13)	10.5(11)	-11.7(11)
C31	19.8(11)	30.4(12)	40.8(14)	-1.1(10)	5.8(10)	2.4(9)
C30	19.6(10)	22.6(11)	29.6(12)	-1.5(9)	2.4(9)	0.9(9)
C35	25.0(12)	22.5(12)	56.9(17)	-1.6(11)	11.2(11)	4.1(9)
C37	42.4(15)	20.3(12)	88(2)	-3.9(13)	29.4(15)	0.6(11)
C38	19.9(10)	19.5(10)	15.9(10)	0.5(8)	2.1(8)	-1.1(8)
C43	36.1(12)	18.1(10)	20.4(11)	1.0(8)	0.7(9)	-5.2(9)
C42	42.5(14)	25.8(12)	20.1(11)	-4.3(9)	-2.3(10)	-10.8(10)
C41	29.0(12)	33.4(12)	13.5(10)	0.9(9)	-3.3(8)	-4.1(10)
C40	27.0(11)	22.2(11)	19.1(10)	3.3(8)	1.0(8)	3.5(9)
N7	45.0(12)	26.0(11)	23.5(10)	4.6(8)	-3.8(9)	8.5(9)
C39	24.1(11)	18.9(10)	18(1)	-1.6(8)	0.5(8)	-0.6(8)
C53	20.8(10)	17.6(10)	17.8(10)	-0.1(8)	-0.9(8)	-0.6(8)
C52	30.0(11)	17.6(11)	22.1(11)	-0.8(8)	-1.8(9)	-1.7(9)
C51	34.8(13)	16.6(11)	35.2(13)	-0.8(9)	2.9(10)	6.2(9)
C50	25.6(11)	24.7(12)	42.1(14)	-0.8(10)	7.8(10)	6.3(9)
C49	23.0(11)	19.9(11)	28.7(11)	-0.1(9)	5.9(9)	0.6(8)
C48	20.9(10)	18.6(10)	16.6(10)	1.0(8)	0.0(8)	-1.0(8)
C47	19(1)	18.1(10)	22.8(10)	4.4(8)	-1.9(8)	-1.1(8)
C46	27.5(11)	13.9(10)	29.0(11)	0.0(8)	0.3(9)	2.0(8)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C45	51.4(15)	20.3(11)	22.3(11)	-4.8(9)	-6.9(10)	4.7(10)
C44	36.7(12)	18.8(11)	19.0(11)	-0.2(8)	-5.1(9)	4.0(9)
C55	39.2(11)	46.4(11)	47.7(10)	4.0(8)	6.1(8)	-2.5(8)
C54	39.2(11)	46.4(11)	47.7(10)	4.0(8)	6.1(8)	-2.5(8)
C59	39.2(11)	46.4(11)	47.7(10)	4.0(8)	6.1(8)	-2.5(8)
C58	39.2(11)	46.4(11)	47.7(10)	4.0(8)	6.1(8)	-2.5(8)
C57	39.2(11)	46.4(11)	47.7(10)	4.0(8)	6.1(8)	-2.5(8)
C56	39.2(11)	46.4(11)	47.7(10)	4.0(8)	6.1(8)	-2.5(8)
O3	50.2(9)	64.1(10)	39.8(8)	-6.8(7)	-2.1(7)	1.6(8)
C69	50.2(9)	64.1(10)	39.8(8)	-6.8(7)	-2.1(7)	1.6(8)
C68	50.2(9)	64.1(10)	39.8(8)	-6.8(7)	-2.1(7)	1.6(8)
C67	50.2(9)	64.1(10)	39.8(8)	-6.8(7)	-2.1(7)	1.6(8)
C66	50.2(9)	64.1(10)	39.8(8)	-6.8(7)	-2.1(7)	1.6(8)

Table S3. Bond lengths in Å for **compound 1**.

Atom	Atom	Length/Å
Co1	N4	1.8960(16)
Co1	N3	1.8996(17)
Co1	N2	1.8679(17)
Co1	N1	1.8718(17)
Co1	N6	1.9972(17)
Co1	N5	1.9822(17)
O1	N7	1.216(3)
F1	C41	1.340(3)
N4	C15	1.370(3)
N4	C18	1.392(3)
N3	C13	1.367(3)
N3	C10	1.393(3)
N2	C8	1.365(3)
N2	C5	1.365(3)
N1	C4	1.365(3)
N1	C1	1.361(3)
O2	N7	1.217(3)
N6	C53	1.346(3)
N6	C49	1.344(3)
N5	C48	1.343(3)
N5	C44	1.345(3)
C15	C14	1.411(3)
C15	C16	1.442(3)
C14	C13	1.410(3)
C14	C38	1.490(3)
C13	C12	1.438(3)
C10	C11	1.431(3)
C10	C9	1.401(3)
C11	C12	1.359(3)
C9	C8	1.408(3)
C9	C29	1.497(3)
C8	C7	1.427(3)
C5	C4	1.424(3)
C5	C6	1.421(3)
C4	C3	1.423(3)
C1	C19	1.411(3)
C1	C2	1.434(3)
C19	C18	1.398(3)
C19	C20	1.496(3)
C18	C17	1.437(3)
C17	C16	1.354(3)
C20	C25	1.403(3)
C20	C21	1.400(3)
C25	C26	1.510(3)
C25	C24	1.394(3)
C24	C23	1.385(3)
C23	C27	1.507(3)
C23	C22	1.389(3)
C22	C21	1.394(3)
C21	C28	1.511(3)
C2	C3	1.382(3)
C6	C7	1.381(3)
C29	C34	1.397(3)
C29	C30	1.402(3)
C34	C33	1.397(3)
C34	C37	1.506(3)
C33	C32	1.378(4)
C32	C36	1.508(3)
C32	C31	1.387(4)
C31	C30	1.389(3)
C30	C35	1.508(3)
C38	C43	1.396(3)
C38	C39	1.390(3)
C43	C42	1.388(3)
C42	C41	1.375(3)
C41	C40	1.389(3)
C40	N7	1.465(3)
C40	C39	1.390(3)
C53	C52	1.389(3)
C52	C51	1.384(3)
C51	C50	1.383(3)
C50	C49	1.377(3)
C48	C47	1.383(3)
C47	C46	1.377(3)
C46	C45	1.377(3)
C45	C44	1.379(3)
C55	C54	1.5227
C55	C56	1.5235
C54	C59	1.5243
C59	C58	1.5250
C58	C57	1.5240
C57	C56	1.5230
O3	C69	1.4431
O3	C66	1.4434
C69	C68	1.5349
C68	C67	1.5379
C67	C66	1.5347
C70	C71	1.5239
C70	C75	1.5230
C71	C72	1.5242
C72	C73	1.5232
C73	C74	1.5246
C74	C75	1.5231
C59A	C58A	1.5236
C59A	C54A	1.5235
C58A	C57A	1.5241
C57A	C56A	1.5211
C56A	C55A	1.5229
C55A	C54A	1.5242
C65	C60	1.516(5)
C65	C64	1.525(5)
C60	C61	1.520(5)
C62	C61	1.527(5)
C62	C63	1.523(5)
C63	C64	1.522(5)
C72A	C73A	1.5251
C72A	C71A	1.5235
C73A	C74A	1.5229
C74A	C75A	1.5234
C75A	C70A	1.5251
C70A	C71A	1.5246
C70B	C75B	1.5230
C70B	C71B	1.5244
C75B	C74B	1.5234
C74B	C73B	1.5243
C73B	C72B	1.5236
C72B	C71B	1.5226

Table S4. Bond angles in ° for **compound 1.**

Atom	Atom	Atom	Angle/°
N4	Co1	N3	95.51(7)
N4	Co1	N6	90.09(7)
N4	Co1	N5	89.70(7)
N3	Co1	N6	90.79(7)
N3	Co1	N5	90.06(7)
N2	Co1	N4	172.94(7)
N2	Co1	N3	91.50(7)
N2	Co1	N1	81.36(7)
N2	Co1	N6	88.95(7)
N2	Co1	N5	91.15(7)
N1	Co1	N4	91.62(7)
N1	Co1	N3	172.84(7)
N1	Co1	N6	88.53(7)
N1	Co1	N5	90.63(7)
N5	Co1	N6	179.14(7)
C15	N4	Co1	125.63(13)
C15	N4	C18	108.51(16)
C18	N4	Co1	125.78(13)
C13	N3	Co1	125.56(14)
C13	N3	C10	108.29(16)
C10	N3	Co1	126.10(13)
C8	N2	Co1	132.60(14)
C5	N2	Co1	117.62(14)
C5	N2	C8	109.77(17)
C4	N1	Co1	117.34(14)
C1	N1	Co1	132.34(14)
C1	N1	C4	110.26(17)
C53	N6	Co1	121.30(14)
C49	N6	Co1	120.73(14)
C49	N6	C53	117.76(18)
C48	N5	Co1	120.60(14)
C48	N5	C44	117.24(18)
C44	N5	Co1	122.14(14)
N4	C15	C14	124.45(18)
N4	C15	C16	108.44(17)
C14	C15	C16	127.00(18)
C15	C14	C38	116.46(18)
C13	C14	C15	124.26(18)
C13	C14	C38	118.88(18)
N3	C13	C14	124.58(18)
N3	C13	C12	108.47(17)
C14	C13	C12	126.93(18)
N3	C10	C11	107.56(17)
N3	C10	C9	125.98(18)
C9	C10	C11	126.45(19)
C12	C11	C10	108.22(18)
C11	C12	C13	107.45(18)
C10	C9	C8	122.64(18)
C10	C9	C29	119.29(18)
C8	C9	C29	118.07(18)
N2	C8	C9	121.06(18)
N2	C8	C7	107.19(18)
C9	C8	C7	131.74(19)
N2	C5	C4	111.62(17)
N2	C5	C6	108.20(18)
C6	C5	C4	140.10(19)
N1	C4	C5	111.95(17)
N1	C4	C3	108.03(18)
C3	C4	C5	139.91(19)
N1	C1	C19	121.13(18)
N1	C1	C2	106.93(17)
C19	C1	C2	131.92(19)
C1	C19	C20	118.65(18)
C18	C19	C1	122.41(18)
C18	C19	C20	118.93(18)
N4	C18	C19	126.42(18)
N4	C18	C17	107.13(17)
C19	C18	C17	126.43(18)
C16	C17	C18	108.67(18)
C17	C16	C15	107.23(18)
C25	C20	C19	119.94(18)
C21	C20	C19	120.41(18)
C21	C20	C25	119.64(19)
C20	C25	C26	120.74(19)
C24	C25	C20	119.3(2)
C24	C25	C26	119.9(2)
C23	C24	C25	121.9(2)
C24	C23	C27	121.2(2)
C24	C23	C22	117.9(2)
C22	C23	C27	120.9(2)
C23	C22	C21	122.1(2)
C20	C21	C28	121.42(19)
C22	C21	C20	119.1(2)
C22	C21	C28	119.4(2)
C3	C2	C1	107.92(18)
C2	C3	C4	106.87(18)
C7	C6	C5	106.85(18)
C6	C7	C8	107.98(18)
C34	C29	C9	120.17(19)
C34	C29	C30	119.76(19)
C30	C29	C9	120.05(19)
C29	C34	C37	120.8(2)
C33	C34	C29	119.3(2)
C33	C34	C37	119.8(2)
C32	C33	C34	121.8(2)
C33	C32	C36	122.0(2)
C33	C32	C31	117.9(2)
C31	C32	C36	120.1(2)
C32	C31	C30	122.5(2)
C29	C30	C35	121.06(19)
C31	C30	C29	118.7(2)
C31	C30	C35	120.2(2)
C43	C38	C14	122.22(18)
C39	C38	C14	119.43(18)
C39	C38	C43	118.23(19)
C42	C43	C38	121.2(2)
C41	C42	C43	119.8(2)
F1	C41	C42	119.1(2)
F1	C41	C40	120.9(2)
C42	C41	C40	120.0(2)
C41	C40	N7	121.87(19)
C41	C40	C39	120.1(2)
C39	C40	N7	118.06(19)
O1	N7	O2	122.9(2)
O1	N7	C40	118.22(19)
O2	N7	C40	118.8(2)
C38	C39	C40	120.6(2)
N6	C53	C52	122.5(2)
C51	C52	C53	119.3(2)
C50	C51	C52	118.1(2)
C49	C50	C51	119.8(2)
N6	C49	C50	122.6(2)
N5	C48	C47	122.99(19)
C46	C47	C48	119.25(19)
C45	C46	C47	118.1(2)
C46	C45	C44	119.8(2)
N5	C44	C45	122.6(2)
C54	C55	C56	111.4
C55	C54	C59	111.4
C54	C59	C58	111.4

Atom	Atom	Atom	Angle/°
C57	C58	C59	111.3
C56	C57	C58	111.4
C57	C56	C55	111.4
C69	O3	C66	109.5
O3	C69	C68	106.4
C69	C68	C67	101.5
C66	C67	C68	101.5
O3	C66	C67	106.4
C75	C70	C71	111.3
C70	C71	C72	111.4
C73	C72	C71	111.3
C72	C73	C74	111.3
C75	C74	C73	111.4
C70	C75	C74	111.4
C54A	C59A	C58A	111.3
C59A	C58A	C57A	111.4
C56A	C57A	C58A	111.4
C57A	C56A	C55A	111.4
C56A	C55A	C54A	111.4
C59A	C54A	C55A	111.4

Atom	Atom	Atom	Angle/°
C60	C65	C64	119.9(14)
C65	C60	C61	111.9(14)
C63	C62	C61	116.5(14)
C60	C61	C62	104.1(13)
C64	C63	C62	113.0(14)
C63	C64	C65	101.0(13)
C71A	C72A	C73A	111.3
C74A	C73A	C72A	111.4
C73A	C74A	C75A	111.4
C74A	C75A	C70A	111.4
C71A	C70A	C75A	111.3
C72A	C71A	C70A	111.4
C75B	C70B	C71B	111.4
C70B	C75B	C74B	111.4
C75B	C74B	C73B	111.4
C72B	C73B	C74B	111.4
C71B	C72B	C73B	111.4
C72B	C71B	C70B	111.4

Table S5. Torsion Angles in ° for **compound 1**.

Atom	Atom	Atom	Atom	Angle/°
Co1	N4	C15	C14	-1.2(3)
Co1	N4	C15	C16	-177.62(13)
Co1	N4	C18	C19	-3.1(3)
Co1	N4	C18	C17	178.20(13)
Co1	N3	C13	C14	-0.6(3)
Co1	N3	C13	C12	178.04(13)
Co1	N3	C10	C11	-177.96(13)
Co1	N3	C10	C9	2.8(3)
Co1	N2	C8	C9	-0.4(3)
Co1	N2	C8	C7	-179.13(15)
Co1	N2	C5	C4	-3.3(2)
Co1	N2	C5	C6	179.24(13)
Co1	N1	C4	C5	0.7(2)
Co1	N1	C4	C3	177.61(13)
Co1	N1	C1	C19	4.0(3)
Co1	N1	C1	C2	-177.22(14)
Co1	N6	C53	C52	-174.66(15)
Co1	N6	C49	C50	173.64(18)
Co1	N5	C48	C47	176.83(15)
Co1	N5	C44	C45	-176.94(19)
F1	C41	C40	N7	-3.5(3)
F1	C41	C40	C39	176.7(2)
N4	Co1	N3	C13	-0.04(17)
N4	Co1	N3	C10	177.25(16)
N4	Co1	N1	C4	177.25(14)
N4	Co1	N1	C1	-5.91(18)
N4	C15	C14	C13	0.5(3)
N4	C15	C14	C38	-172.19(18)
N4	C15	C16	C17	-0.2(2)
N4	C18	C17	C16	-1.4(2)
N3	Co1	N4	C15	0.92(16)
N3	Co1	N4	C18	-175.54(15)
N3	Co1	N2	C8	2.62(19)
N3	Co1	N2	C5	-176.50(15)
N3	C13	C12	C11	-0.3(2)
N3	C10	C11	C12	0.1(2)
N3	C10	C9	C8	0.5(3)
N3	C10	C9	C29	179.92(18)
N2	Co1	N3	C13	179.10(16)
N2	Co1	N3	C10	-3.61(17)
N2	Co1	N1	C4	-1.96(14)
N2	Co1	N1	C1	174.88(19)
N2	C8	C7	C6	0.0(2)
N2	C5	C4	N1	1.6(2)
N2	C5	C4	C3	-173.8(2)
N2	C5	C6	C7	0.1(2)
N1	Co1	N4	C15	-178.42(16)
N1	Co1	N4	C18	5.11(16)
N1	Co1	N2	C8	-177.94(19)
N1	Co1	N2	C5	2.94(14)
N1	C4	C3	C2	0.1(2)
N1	C1	C19	C18	0.6(3)
N1	C1	C19	C20	179.46(17)
N1	C1	C2	C3	0.2(2)
N6	Co1	N4	C15	-89.88(16)
N6	Co1	N4	C18	93.65(16)
N6	Co1	N3	C13	90.13(17)
N6	Co1	N3	C10	-92.58(16)
N6	Co1	N2	C8	93.39(19)
N6	Co1	N2	C5	-85.74(15)
N6	Co1	N1	C4	87.20(15)
N6	Co1	N1	C1	-95.96(18)
N6	C53	C52	C51	0.8(3)
N5	Co1	N4	C15	90.96(16)
N5	Co1	N4	C18	-85.51(16)
N5	Co1	N3	C13	-89.75(16)

Atom	Atom	Atom	Atom	Angle/°
N5	Co1	N3	C10	87.54(16)
N5	Co1	N2	C8	-87.47(19)
N5	Co1	N2	C5	93.41(15)
N5	Co1	N1	C4	-93.03(14)
N5	Co1	N1	C1	83.81(18)
N5	C48	C47	C46	0.6(3)
C15	N4	C18	C19	179.98(19)
C15	N4	C18	C17	1.2(2)
C15	C14	C13	N3	0.5(3)
C15	C14	C13	C12	-177.88(19)
C15	C14	C38	C43	-68.7(3)
C15	C14	C38	C39	107.2(2)
C14	C15	C16	C17	-176.51(19)
C14	C13	C12	C11	178.3(2)
C14	C38	C43	C42	173.7(2)
C14	C38	C39	C40	-175.54(19)
C13	N3	C10	C11	-0.3(2)
C13	N3	C10	C9	-179.51(19)
C13	C14	C38	C43	118.2(2)
C13	C14	C38	C39	-65.9(3)
C10	N3	C13	C14	-178.31(18)
C10	N3	C13	C12	0.3(2)
C10	C11	C12	C13	0.1(2)
C10	C9	C8	N2	-1.8(3)
C10	C9	C8	C7	176.5(2)
C10	C9	C29	C34	90.9(3)
C10	C9	C29	C30	-90.6(2)
C11	C10	C9	C8	-178.53(19)
C11	C10	C9	C29	0.8(3)
C9	C10	C11	C12	179.3(2)
C9	C8	C7	C6	-178.5(2)
C9	C29	C34	C33	-179.5(2)
C9	C29	C34	C37	1.8(4)
C9	C29	C30	C31	179.6(2)
C9	C29	C30	C35	-0.8(3)
C8	N2	C5	C4	177.40(16)
C8	N2	C5	C6	-0.1(2)
C8	C9	C29	C34	-89.7(3)
C8	C9	C29	C30	88.8(2)
C5	N2	C8	C9	178.77(18)
C5	N2	C8	C7	0.0(2)
C5	C4	C3	C2	175.6(2)
C5	C6	C7	C8	0.0(2)
C4	N1	C1	C19	-179.03(17)
C4	N1	C1	C2	-0.2(2)
C4	C5	C6	C7	-176.3(2)
C1	N1	C4	C5	-176.80(16)
C1	N1	C4	C3	0.1(2)
C1	C19	C18	N4	-0.9(3)
C1	C19	C18	C17	177.65(19)
C1	C19	C20	C25	-100.8(2)
C1	C19	C20	C21	78.5(2)
C1	C2	C3	C4	-0.2(2)
C19	C1	C2	C3	178.9(2)
C19	C18	C17	C16	179.86(19)
C19	C20	C25	C26	-0.4(3)
C19	C20	C25	C24	178.95(19)
C19	C20	C21	C22	-178.83(19)
C19	C20	C21	C28	1.9(3)
C18	N4	C15	C14	175.74(18)
C18	N4	C15	C16	-0.6(2)
C18	C19	C20	C25	78.1(2)
C18	C19	C20	C21	-102.6(2)
C18	C17	C16	C15	1.0(2)
C16	C15	C14	C13	176.15(19)
C16	C15	C14	C38	3.5(3)
C20	C19	C18	N4	-179.73(18)
C20	C19	C18	C17	-1.2(3)

Atom	Atom	Atom	Atom	Angle/°
C20	C25	C24	C23	-0.1(3)
C25	C20	C21	C22	0.4(3)
C25	C20	C21	C28	-178.9(2)
C25	C24	C23	C27	179.8(2)
C25	C24	C23	C22	0.4(3)
C26	C25	C24	C23	179.2(2)
C24	C23	C22	C21	-0.3(3)
C23	C22	C21	C20	-0.1(3)
C23	C22	C21	C28	179.2(2)
C27	C23	C22	C21	-179.7(2)
C21	C20	C25	C26	-179.6(2)
C21	C20	C25	C24	-0.3(3)
C2	C1	C19	C18	-177.9(2)
C2	C1	C19	C20	1.0(3)
C6	C5	C4	N1	177.8(2)
C6	C5	C4	C3	2.4(5)
C29	C9	C8	N2	178.81(18)
C29	C9	C8	C7	-2.8(3)
C29	C34	C33	C32	-0.5(4)
C34	C29	C30	C31	-1.9(3)
C34	C29	C30	C35	177.7(2)
C34	C33	C32	C36	179.1(3)
C34	C33	C32	C31	-1.1(4)
C33	C32	C31	C30	1.3(4)
C32	C31	C30	C29	0.2(4)
C32	C31	C30	C35	-179.4(2)
C36	C32	C31	C30	-178.9(2)
C30	C29	C34	C33	2.0(3)
C30	C29	C34	C37	-176.7(2)
C37	C34	C33	C32	178.2(3)
C38	C14	C13	N3	173.01(18)
C38	C14	C13	C12	-5.4(3)
C38	C43	C42	C41	1.9(4)
C43	C38	C39	C40	0.5(3)
C43	C42	C41	F1	-178.5(2)
C43	C42	C41	C40	0.3(4)
C42	C41	C40	N7	177.7(2)
C42	C41	C40	C39	-2.1(3)
C41	C40	N7	O1	158.3(2)
C41	C40	N7	O2	-23.4(3)
C41	C40	C39	C38	1.6(3)
N7	C40	C39	C38	-178.2(2)
C39	C38	C43	C42	-2.3(3)
C39	C40	N7	O1	-21.9(3)
C39	C40	N7	O2	156.4(2)
C53	N6	C49	C50	-1.2(3)
C53	C52	C51	C50	-0.7(3)
C52	C51	C50	C49	-0.3(4)
C51	C50	C49	N6	1.3(4)
C49	N6	C53	C52	0.2(3)
C48	N5	C44	C45	1.5(3)
C48	C47	C46	C45	0.6(3)
C47	C46	C45	C44	-0.7(4)
C46	C45	C44	N5	-0.4(4)
C44	N5	C48	C47	-1.7(3)
C55	C54	C59	C58	54.9
C54	C55	C56	C57	54.9
C54	C59	C58	C57	-55.0
C59	C58	C57	C56	55.0
C58	C57	C56	C55	-55.0
C56	C55	C54	C59	-54.9
O3	C69	C68	C67	31.6
C69	O3	C66	C67	-12.3
C69	C68	C67	C66	-37.5
C68	C67	C66	O3	31.6
C66	O3	C69	C68	-12.4
C70	C71	C72	C73	55.0
C71	C70	C75	C74	55.0

Atom	Atom	Atom	Atom	Angle/°
C71	C72	C73	C74	-55.0
C72	C73	C74	C75	55.0
C73	C74	C75	C70	-55.0
C75	C70	C71	C72	-55.0
C59A	C58A	C57A	C56A	54.9
C58A	C59A	C54A	C55A	54.9
C58A	C57A	C56A	C55A	-55.0
C57A	C56A	C55A	C54A	55.0
C56A	C55A	C54A	C59A	-55.0
C54A	C59A	C58A	C57A	-54.9

Table S6. Hydrogen fractional atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for **compound 1**. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij}.

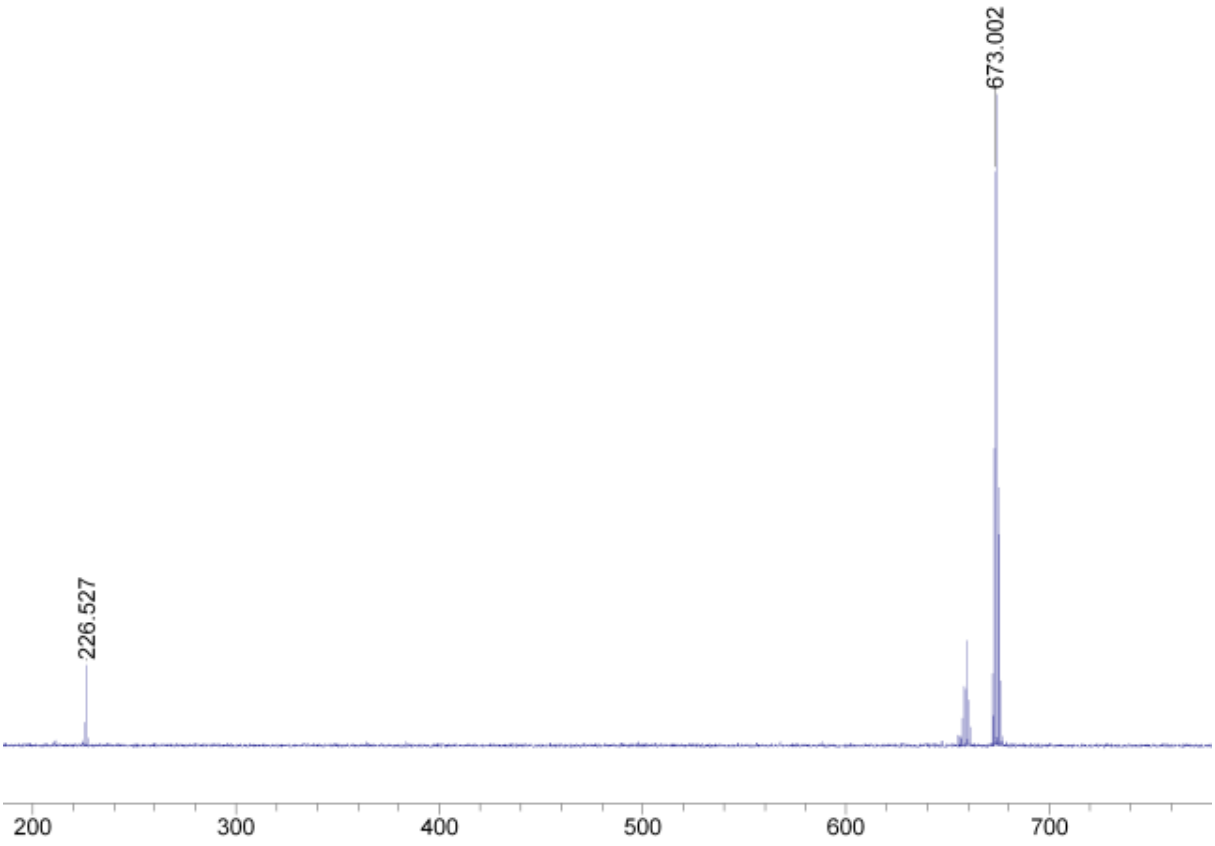
Atom	x	y	z	U_{eq}
H11	9587.16	7734.18	5527.67	25
H12	8015.26	7318.64	5059.15	25
H17	3744.04	5918.74	6249.64	22
H16	4391.76	6187.73	5506.46	23
H26A	4580.68	4459.32	6679.37	43
H26B	4132.61	3736.8	7003.25	43
H26C	5117.89	4282.98	7184.46	43
H24	2724.49	4201.79	7325.06	31
H27A	810.46	5338.51	7451.12	58
H27B	1278.62	5516.14	7967.52	58
H27C	1354.36	4542.94	7745.92	58
H22	2256	6772.47	7650.48	31
H28A	4291.39	7672.99	7679.05	43
H28B	3262.77	7933.85	7385.16	43
H28C	4221.59	7699	7131.89	43
H2	5567.75	6106.14	8043.9	24
H3	7350.37	6452.91	8320.06	24
H6	9689.01	7092.31	8028.2	25
H7	10693.09	7588.11	7405.16	26
H33	11830.73	9728.15	6332.99	41
H36A	13625.43	8672.08	5861.8	62
H36B	13998.61	8606.73	6396.91	62
H36C	13505.4	9513.37	6188.71	62
H31	12810.49	7206.76	6227.32	36
H35A	10960.94	6106.89	6652.5	51
H35B	11833.04	5962.43	6331.87	51
H35C	10707.21	6093.48	6107.5	51
H37A	9359.6	9317.32	6301.43	73
H37B	10192.92	10054.85	6450.37	73
H37C	9829.7	9386.94	6824.5	73
H43	5791.72	5468.56	4956.33	30
H42	4940.89	5625.56	4226.4	36
H39	6088.82	8157.25	5058.42	25
H53	6434.03	4962.65	6730.09	23
H52	6952.06	3475.88	6757.11	28
H51	8635.69	3136.73	6695.81	35
H50	9733.06	4322.45	6593.51	37
H49	9144.73	5775.87	6548.45	28
H48	6269.69	8124.81	6058	23
H47	5649.21	9567.93	6084.1	24
H46	5890.53	10379.63	6771.01	28
H45	6777.16	9700.66	7409.46	39
H44	7366.64	8255.42	7355.19	31
H55A	8914.8	5861.46	4068.54	53
H55B	8836.72	6289.33	3565.97	53
H54A	9963.98	7145.5	4048.51	53
H54B	9161.49	7275.9	4406.42	53
H59A	9022.51	8039.44	3505.58	53
H59B	9207.02	8592.19	3974.44	53
H58A	7589.39	8271.33	4149.26	53
H58B	7509.72	8701.35	3647.07	53
H57A	6462.27	7415.04	3664.87	53
H57B	7266.84	7285.79	3307.83	53
H56A	7219.9	5969.98	3739.49	53
H56B	7402.73	6522.83	4208.35	53
H69A	2404.22	6369.96	5486.1	62
H69B	2425.1	5293.13	5490.4	62
H68A	961.82	6420.1	4989	62
H68B	763.12	5498.96	5252.39	62
H67A	1359.37	4623.44	4681.02	62
H67B	798.69	5411.12	4376.47	62
H66A	2689.36	5160.21	4334.14	62
H66B	2256.94	6164.73	4307.2	62

Atom	x	y	z	U_{eq}
H70A	2477.3	10551.76	4388.1	98
H70B	3511.97	10297.98	4679.94	98
H71A	2381.87	10967.1	5151.64	98
H71B	2696.59	9980.69	5326.05	98
H72A	966.28	10124.92	5326.17	98
H72B	846.74	10440.46	4801.92	98
H73A	381.13	8930.48	4826.53	98
H73B	1416.34	8677.67	5118.18	98
H74A	1511.07	8262.36	4354.21	98
H74B	1196.25	9248.93	4180.03	98
H75A	3045.09	8788.72	4704.24	98
H75B	2925.94	9104.5	4180.06	98
H59C	9510.95	7650.37	3544.25	62
H59D	9710.46	8403.64	3931.59	62
H58C	8123.92	8604.28	3496.48	62
H58D	8010.63	8463.14	4028.75	62
H57C	6817.68	7570.44	3602.52	62
H57D	7657.91	7116.5	3333.55	62
H56C	7251.98	6118.12	3899.08	62
H56D	7452.17	6871.32	4286.37	62
H55C	8951.43	6058.27	3801.7	62
H55D	8837.51	5916.06	4333.85	62
H54C	9303.94	7403.9	4497.57	62
H54D	10144.64	6949.83	4228.89	62
H65A	928.9	7087.5	4890.65	72
H65B	1094.64	6925.86	5428.82	72
H60A	2672.8	6369.91	5387.79	72
H60B	2582.04	7308.3	5122.99	72
H62A	1774.67	5192.62	4396.87	72
H62B	2717.26	4850.27	4725.9	72
H61A	3373.6	6187.48	4694.68	72
H61B	2372.48	6559.71	4407.22	72
H63A	1226.69	4511.69	5035.69	72
H63B	1914.88	5152.03	5373.31	72
H64A	247.03	5682.01	5325	72
H64B	215.86	5775.51	4775.68	72
H72C	2232.31	9649.02	5414.59	98
H72D	1046.84	9523.18	5372.21	98
H73C	892.18	10001.4	4607.04	98
H73D	1502.24	10746.59	4913.74	98
H74C	3014.62	10230.34	4688.08	98
H74D	2269.97	10431.38	4236.81	98
H75C	3098.16	9029.16	4179.79	98
H75D	1912.82	8902.82	4137.73	98
H70C	2643.93	7805.07	4638.17	98
H70D	3254	8550.24	4944.94	98
H71C	1130.37	8321.75	4864.03	98
H71D	1874.67	8120.46	5315.38	98
H70E	3200.54	8879.89	4227.39	98
H70F	3327.81	8664.41	4764.73	98
H75E	1994.85	7811.74	4417.48	98
H75F	1468.96	8688.6	4188.68	98
H74E	1707.16	8296.99	5150.28	98
H74F	666.93	8307.31	4830.24	98
H73E	760.39	9863.09	4737.94	98
H73F	891.25	9646.17	5275.11	98
H72E	2094.68	10715.99	5083.11	98
H72F	2621.73	9840.01	5312.24	98
H71E	3422.06	10220.65	4670.4	98
H71F	2381.42	10229.39	4350.6	98

Table S7. Atomic occupancies for all atoms that are not fully occupied in **compound 1**.

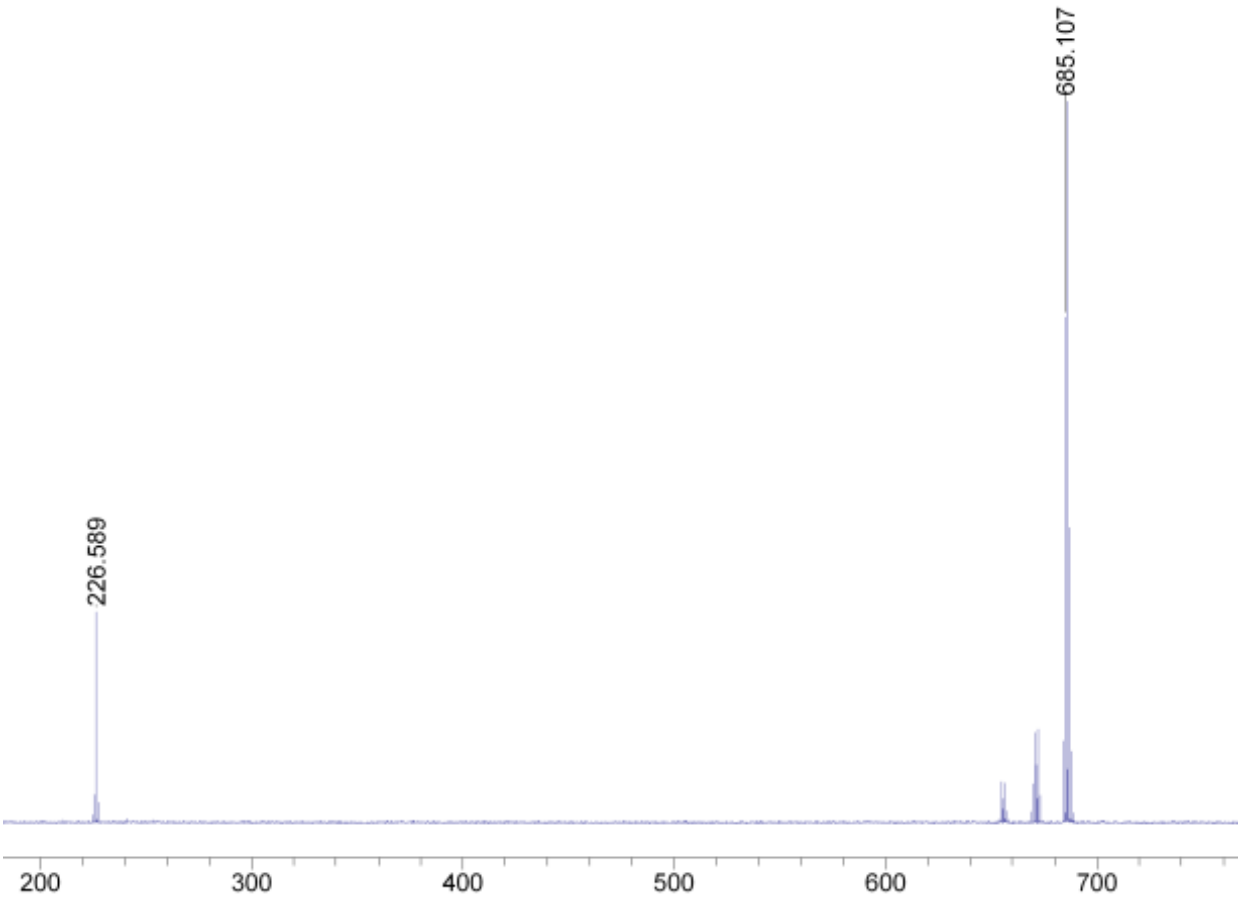
Atom	Occupancy
C55	0.69
H55A	0.69
H55B	0.69
C54	0.69
H54A	0.69
H54B	0.69
C59	0.69
H59A	0.69
H59B	0.69
C58	0.69
H58A	0.69
H58B	0.69
C57	0.69
H57A	0.69
H57B	0.69
C56	0.69
H56A	0.69
H56B	0.69
O3	0.81
C69	0.81
H69A	0.81
H69B	0.81
C68	0.81
H68A	0.81
H68B	0.81
C67	0.81
H67A	0.81
H67B	0.81
C66	0.81
H66A	0.81
H66B	0.81
C70	0.37
H70A	0.37
H70B	0.37
C71	0.37
H71A	0.37
H71B	0.37
C72	0.37
H72A	0.37
H72B	0.37
C73	0.37
H73A	0.37
H73B	0.37
C74	0.37
H74A	0.37
H74B	0.37
C75	0.37
H75A	0.37
H75B	0.37
C59A	0.31
H59C	0.31
H59D	0.31
C58A	0.31
H58C	0.31
H58D	0.31
C57A	0.31
H57C	0.31
H57D	0.31
C56A	0.31
H56C	0.31
H56D	0.31
C55A	0.31
H55C	0.31
H55D	0.31
C54A	0.31

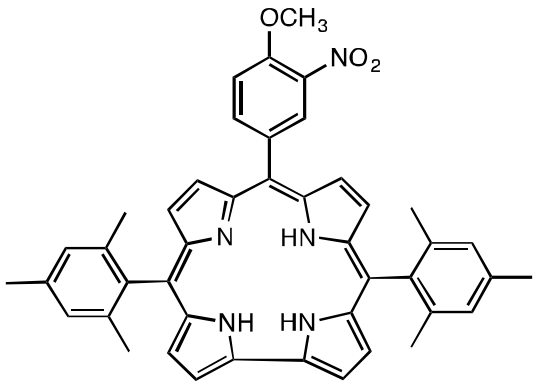
Atom	Occupancy
H54C	0.31
H54D	0.31
C65	0.19
H65A	0.19
H65B	0.19
C60	0.19
H60A	0.19
H60B	0.19
C62	0.19
H62A	0.19
H62B	0.19
C61	0.19
H61A	0.19
H61B	0.19
C63	0.19
H63A	0.19
H63B	0.19
C64	0.19
H64A	0.19
H64B	0.19
C72A	0.31
H72C	0.31
H72D	0.31
C73A	0.31
H73C	0.31
H73D	0.31
C74A	0.31
H74C	0.31
H74D	0.31
C75A	0.31
H75C	0.31
H75D	0.31
C70A	0.31
H70C	0.31
H70D	0.31
C71A	0.31
H71C	0.31
H71D	0.31
C70B	0.32
H70E	0.32
H70F	0.32
C75B	0.32
H75E	0.32
H75F	0.32
C74B	0.32
H74E	0.32
H74F	0.32
C73B	0.32
H73E	0.32
H73F	0.32
C72B	0.32
H72E	0.32
H72F	0.32
C71B	0.32
H71E	0.32
H71F	0.32



Chemical Formula: $C_{43}H_{36}FN_5O_2$
Exact Mass: 673.29
Molecular Weight: 673.79

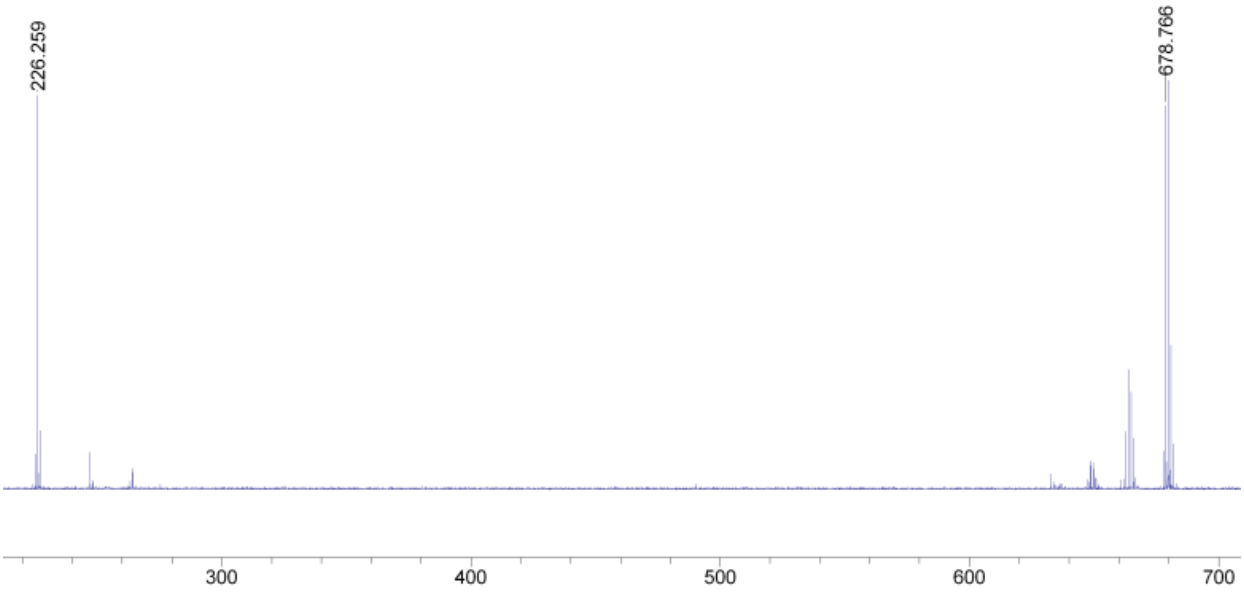
Figure S2a. MALDI/TOF MS spectrum of **1H$_3$**.

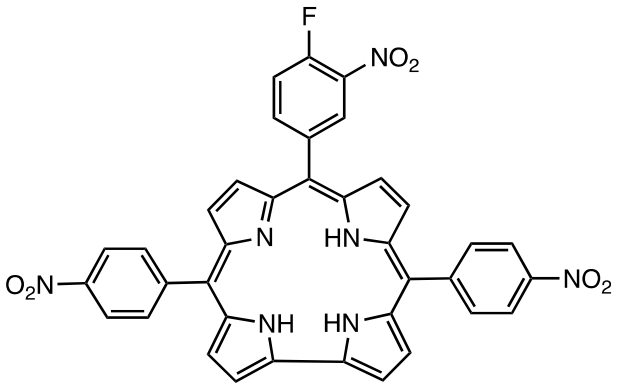




Chemical Formula: $C_{44}H_{39}N_5O_3$
Exact Mass: 685.31
Molecular Weight: 685.83

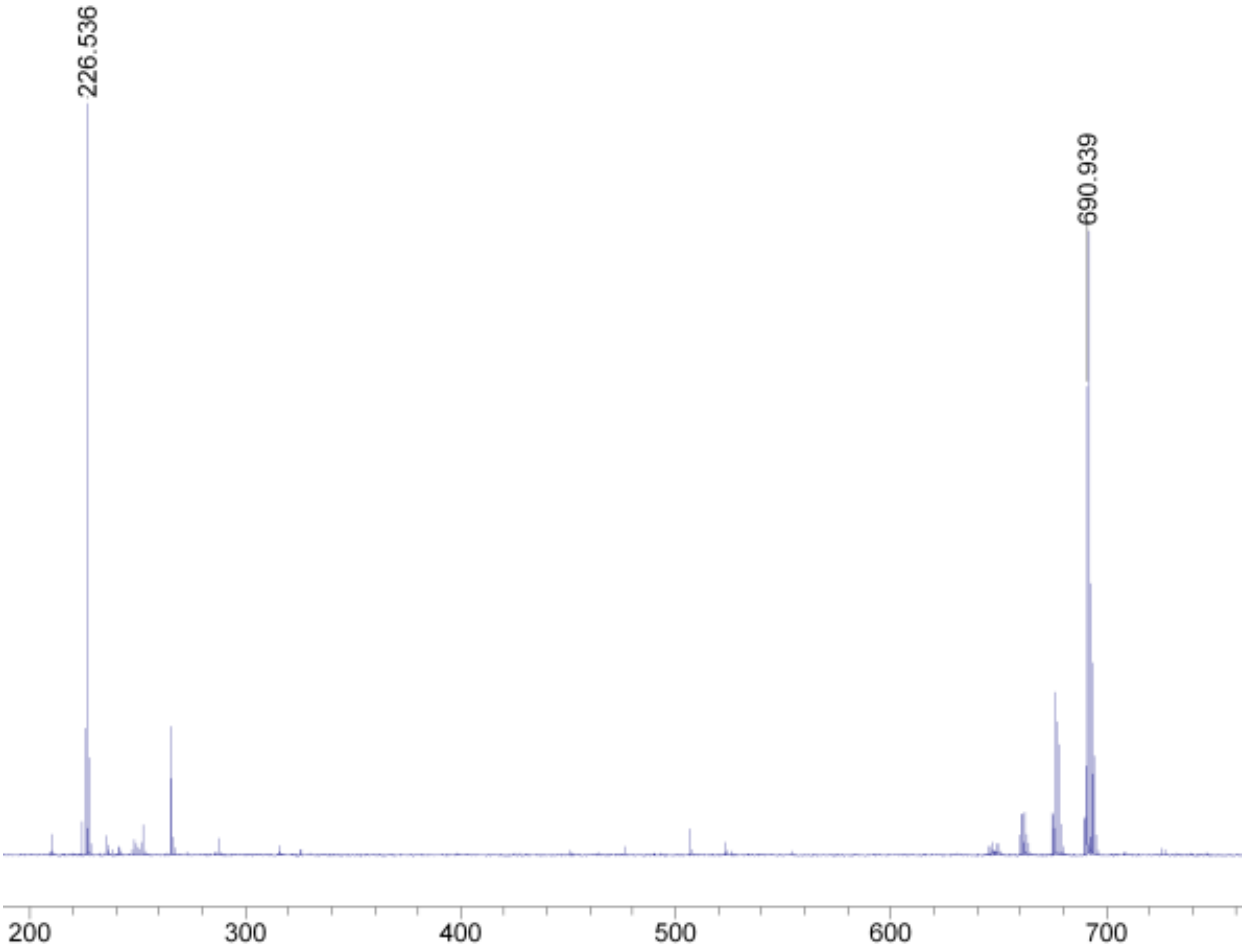
Figure S2b. MALDI/TOF MS spectrum of **2H$_3$**.

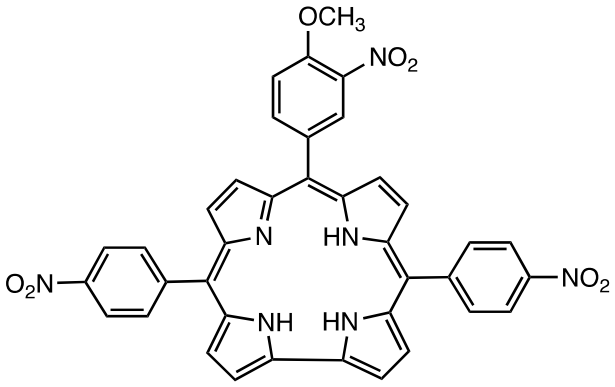




Chemical Formula: $C_{37}H_{22}FN_7O_6$
Exact Mass: 679.16
Molecular Weight: 679.62

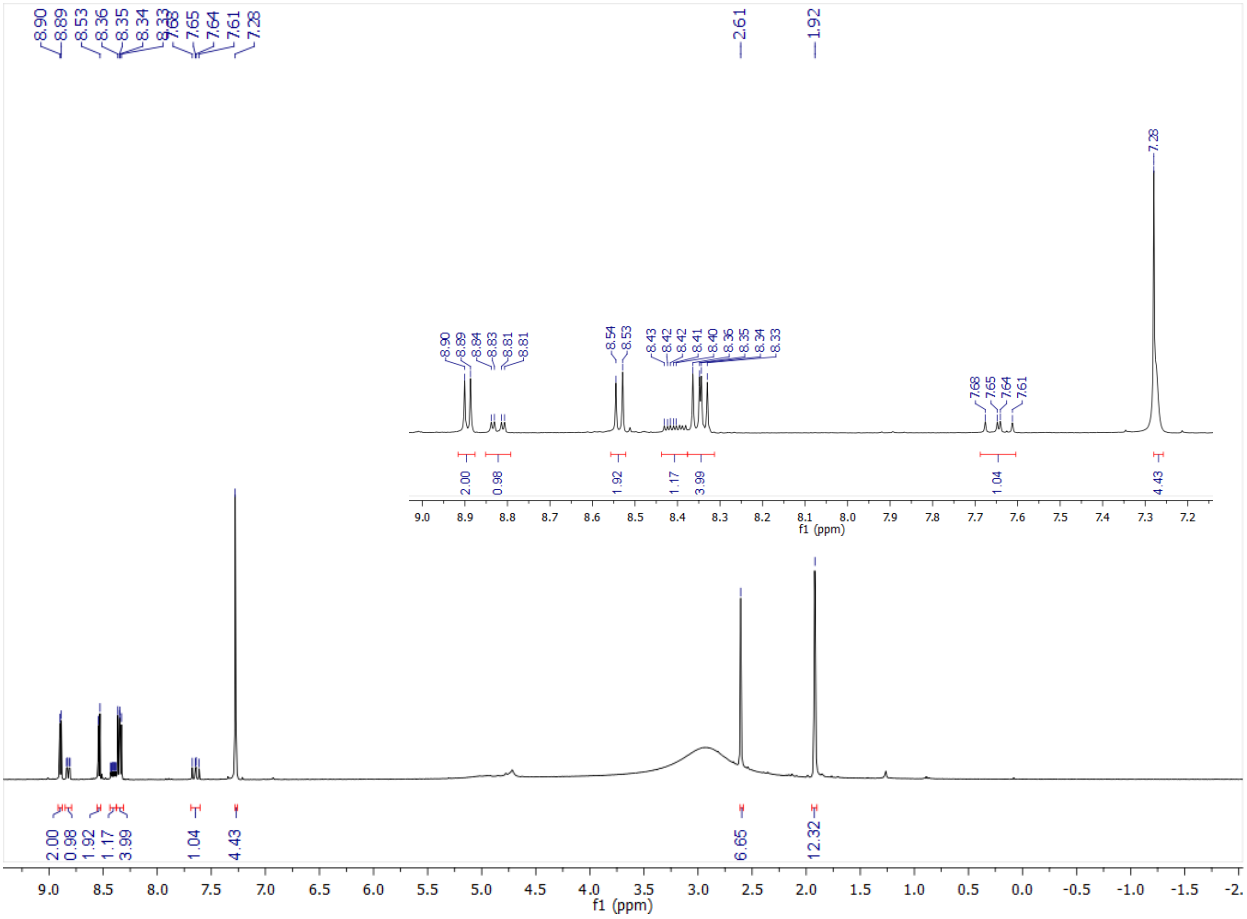
Figure S2c. MALDI/TOF MS spectrum of **3H$_3$**.

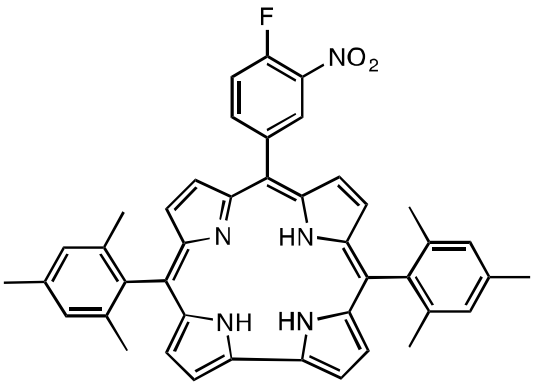




Chemical Formula: $C_{38}H_{25}N_7O_7$
Exact Mass: 691.18
Molecular Weight: 691.66

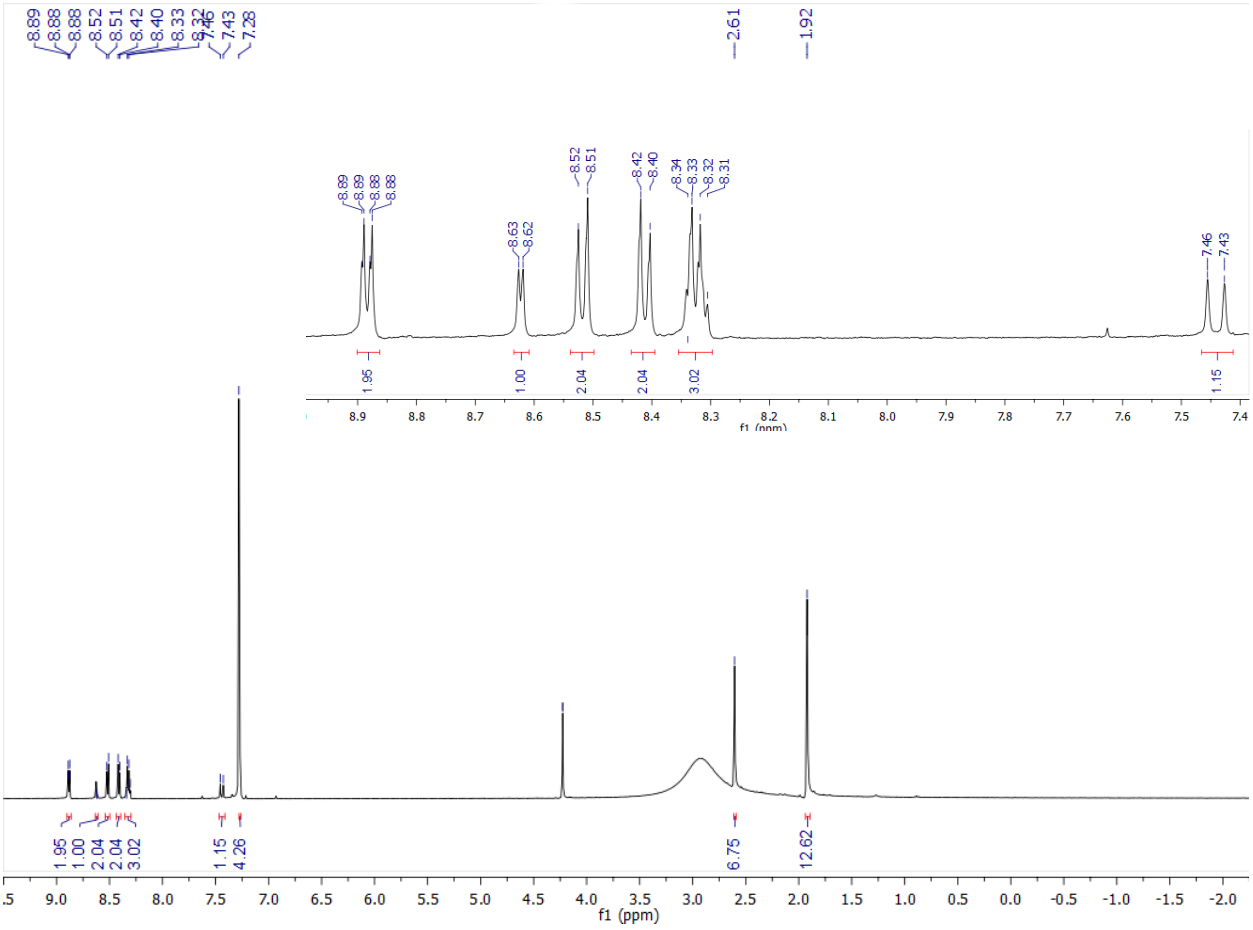
Figure S2d. MALDI/TOF MS spectrum of **4H$_3$**.

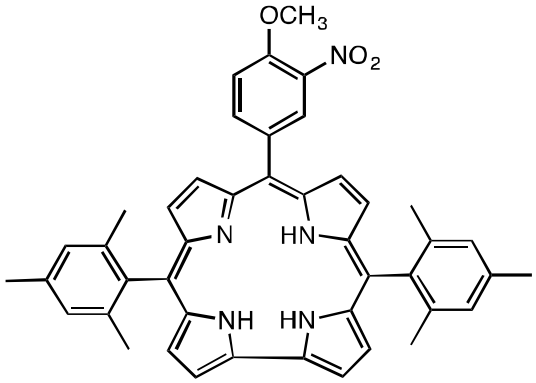




Chemical Formula: $C_{43}H_{36}FN_5O_2$
Exact Mass: 673.29
Molecular Weight: 673.79

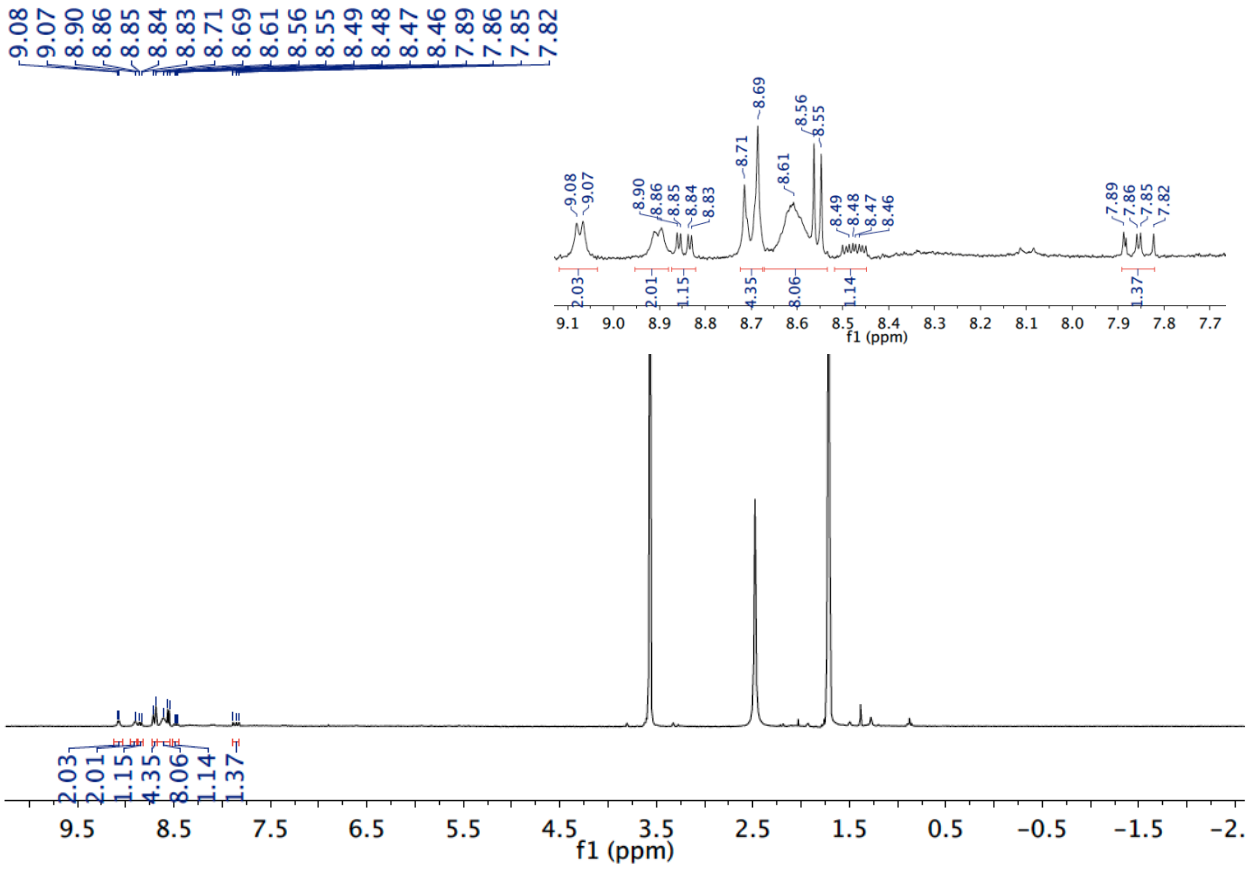
Figure S3a. ^{1}H NMR spectrum of **1H$_3$** in $CDCl_3$ with 50 μL of hydrate NH_2NH_2.

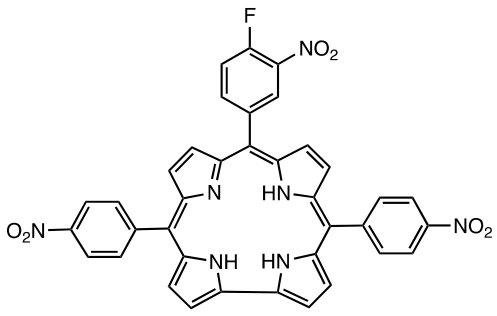




Chemical Formula: $C_{44}H_{39}N_5O_3$
Exact Mass: 685.31
Molecular Weight: 685.83

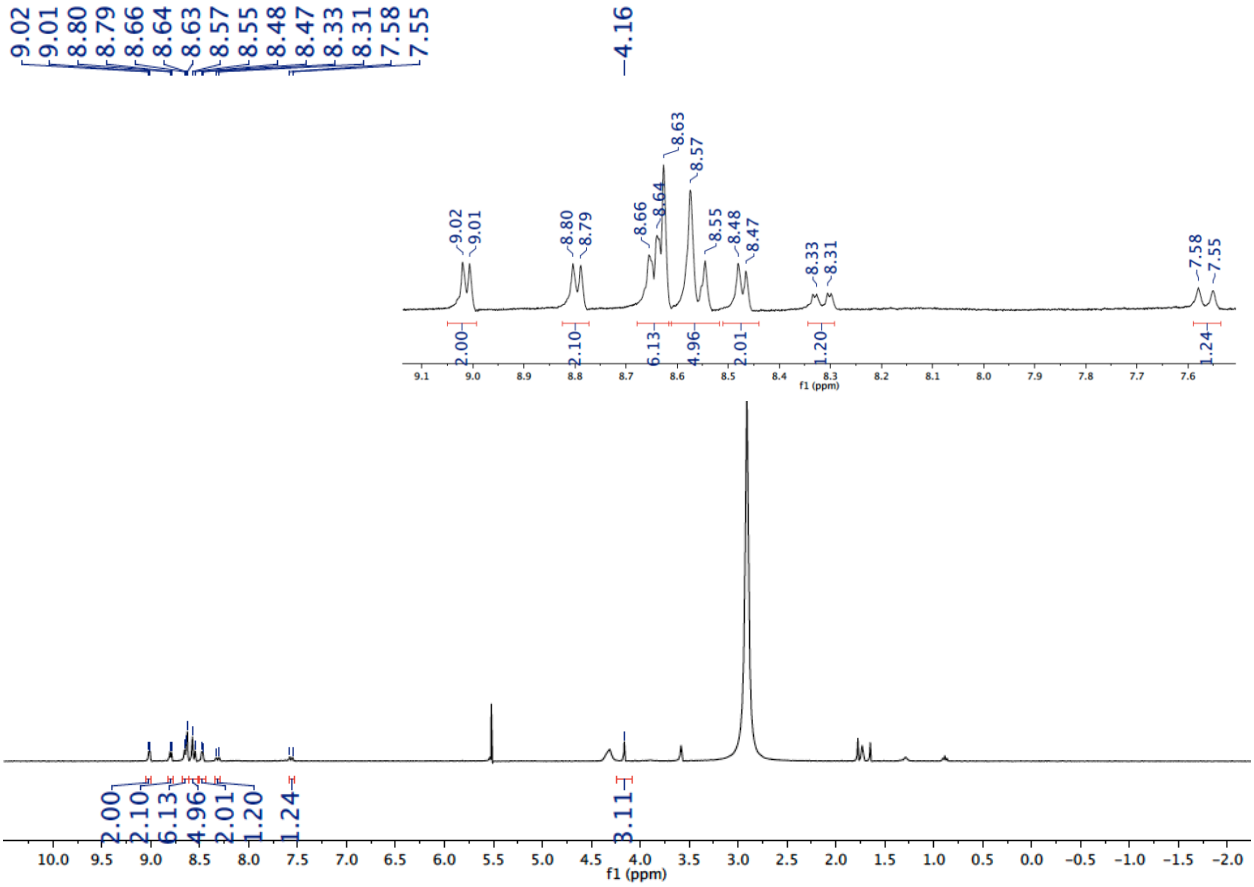
Figure S3b. ^{1}H NMR spectrum of **2H$_3$** in $CDCl_3$ with 50 μL of hydrate NH_2NH_2.

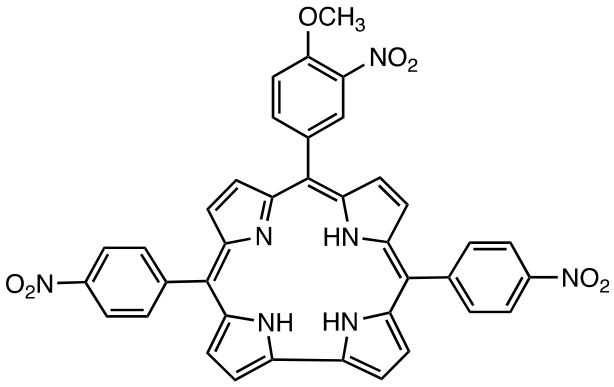




Chemical Formula: $C_{37}H_{22}FN_7O_6$
Exact Mass: 679.16
Molecular Weight: 679.62

Figure S3c. ^{1}H NMR spectrum of **3H$_3$** in THF-d$_8$.





Chemical Formula: $C_{38}H_{25}N_7O_7$
Exact Mass: 691.18
Molecular Weight: 691.66

Figure S3d. ^{1}H NMR spectrum of **4H$_3$** in THF-d$_8$ with 50 μL of hydrate NH_2NH_2.

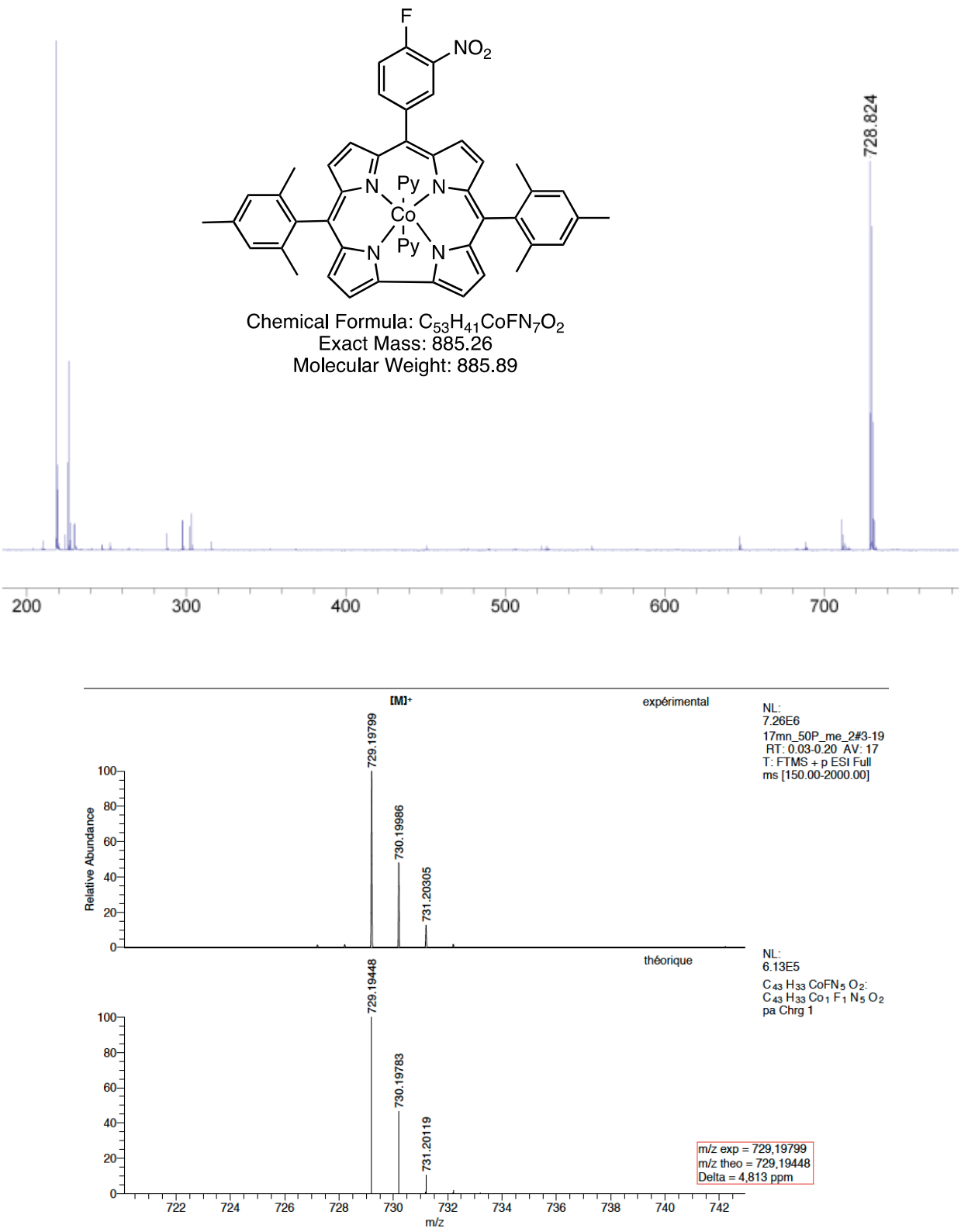


Figure S4a. MALDI/TOF MS (top) and ESI HRMS (bottom) spectra of **1**. The molecular peak for [M-2py] is observed in both ionization modes.

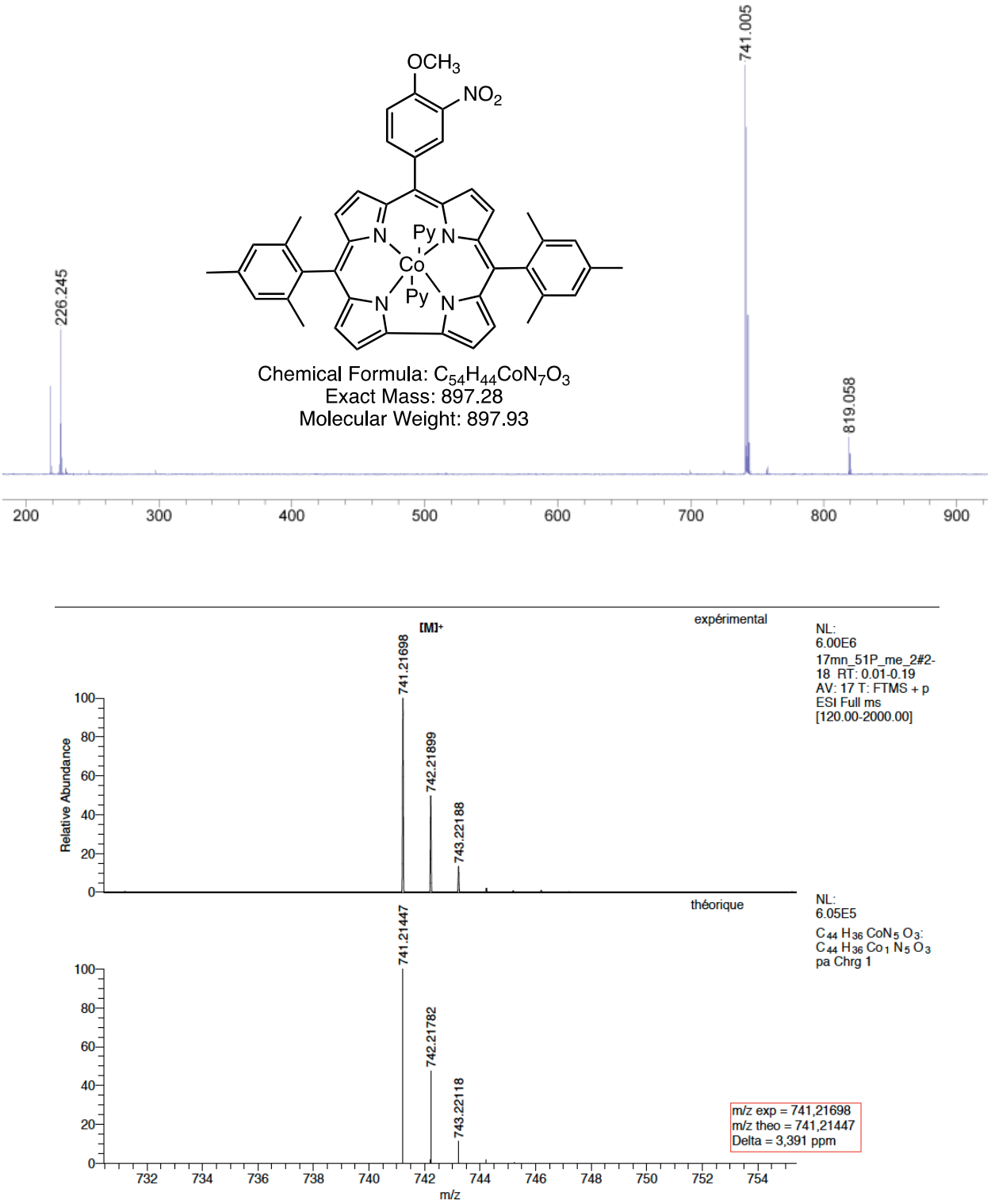


Figure S4b. MALDI/TOF MS (top) and ESI HRMS (bottom) spectra of **2**. The molecular peak for [M-2py] is observed in both ionization modes.

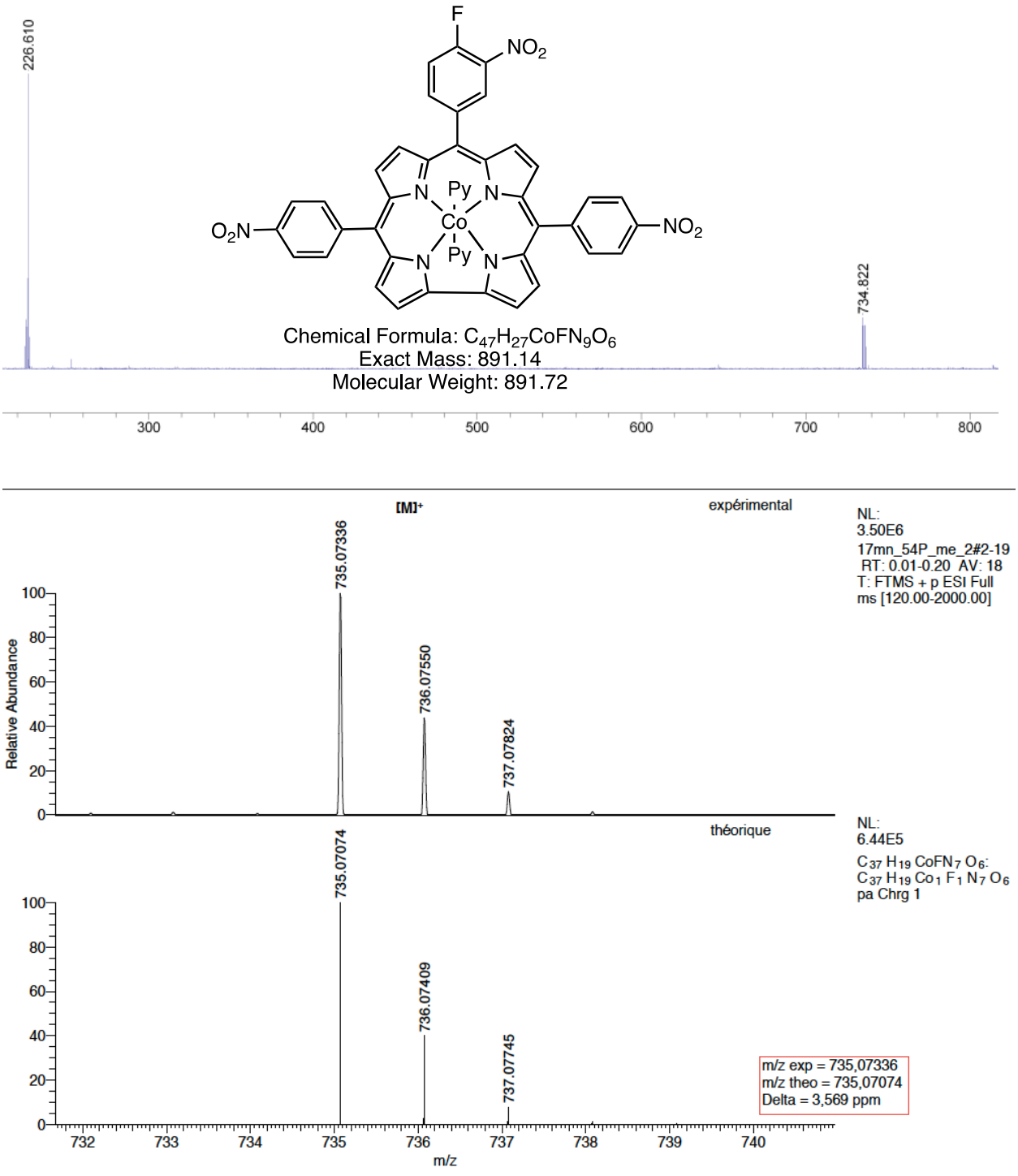


Figure S4c. MALDI/TOF MS (top) and ESI HRMS (bottom) spectra of **3**. The molecular peak for [M-2py] is observed in both ionization modes.

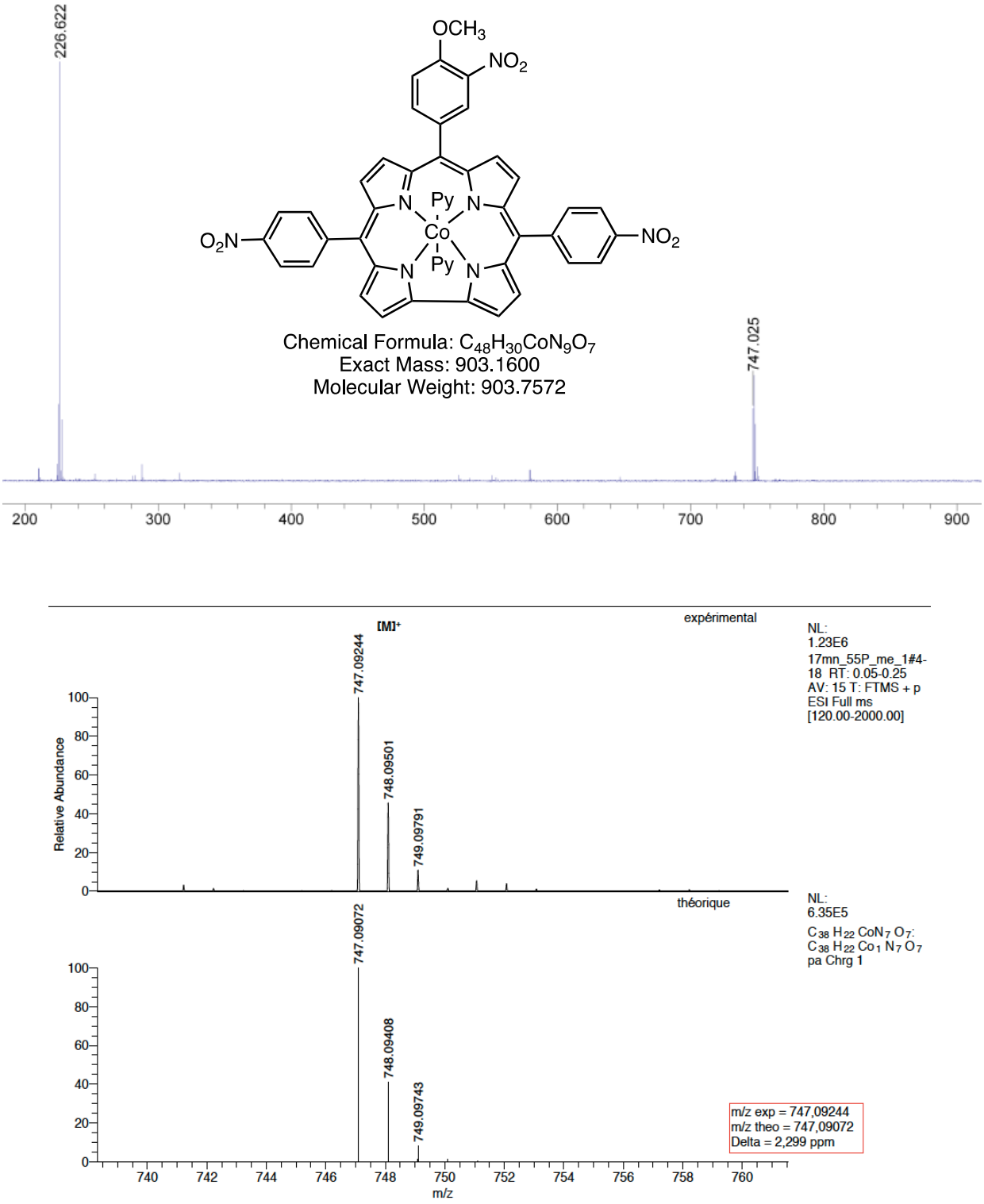
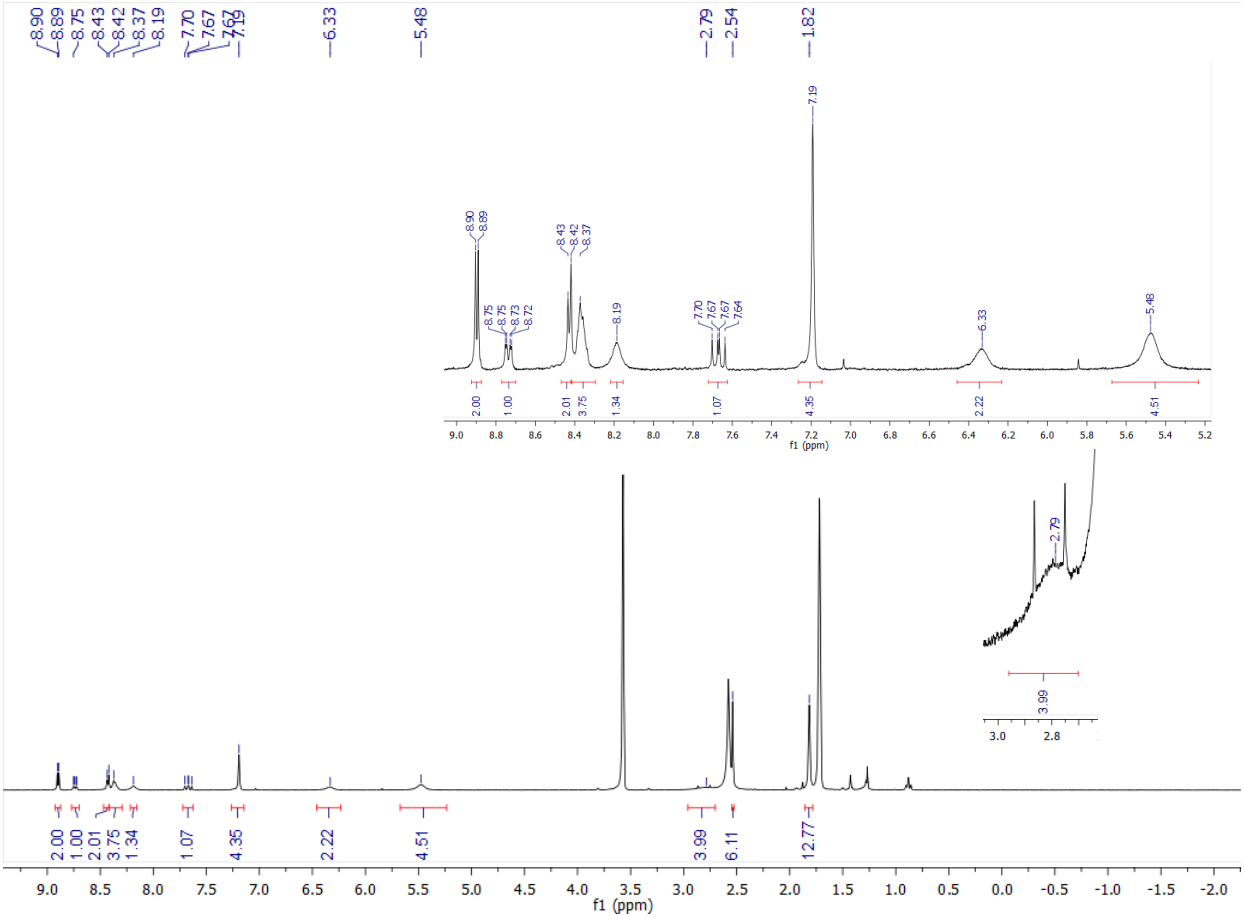
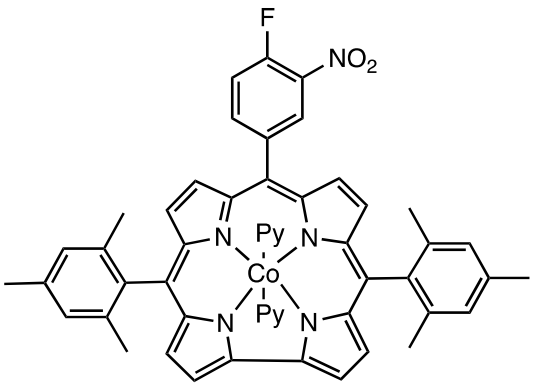


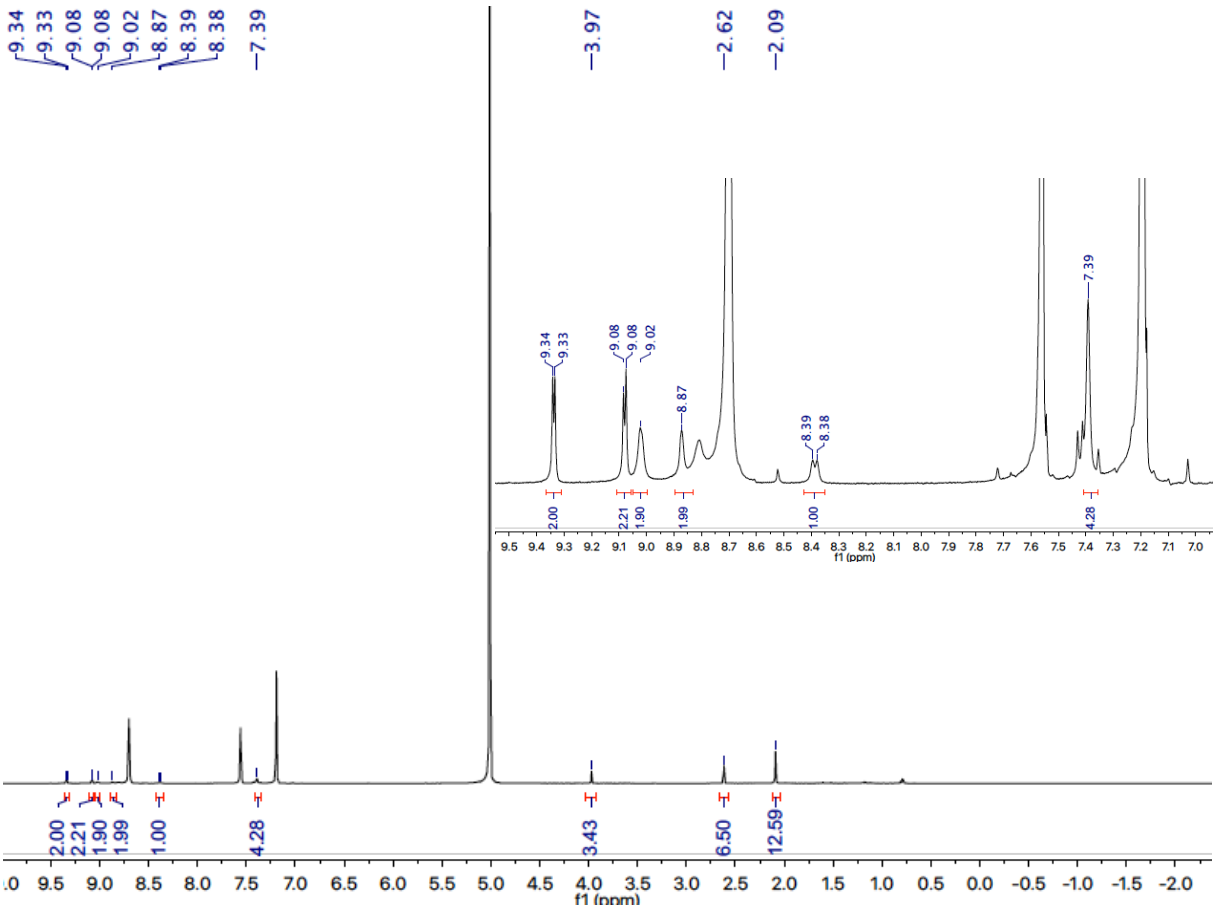
Figure S4d. MALDI/TOF MS (top) and ESI HRMS (bottom) spectra of **4**. The molecular peak for [M-2py] is observed in both ionization modes.

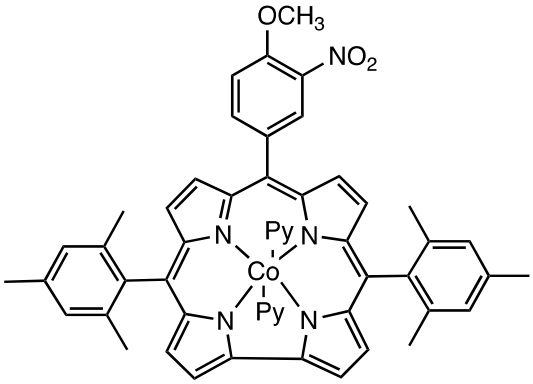




Chemical Formula: $C_{53}H_{41}CoFN_7O_2$
Exact Mass: 885.26
Molecular Weight: 885.89

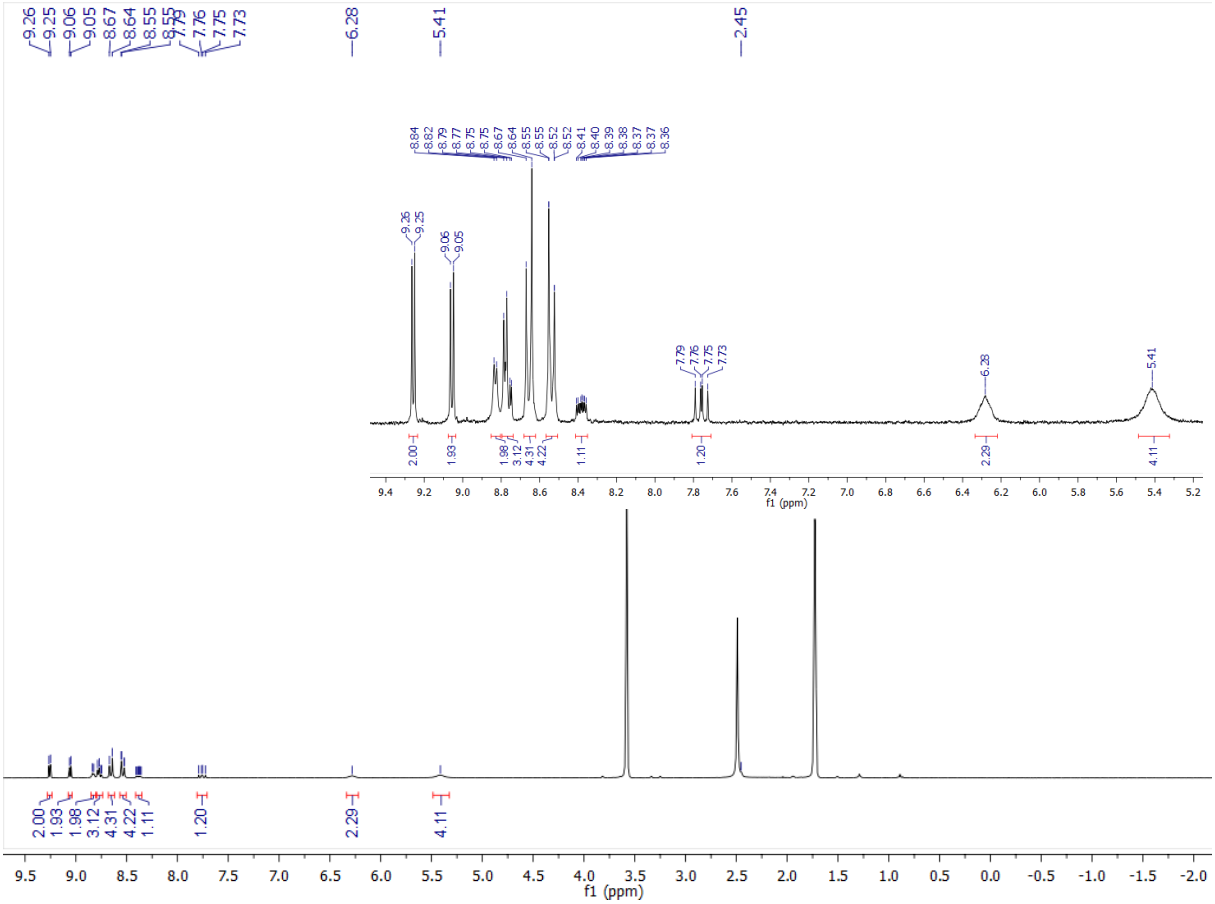
Figure S5a. ^{1}H NMR spectrum of **1** in THF-d_8.

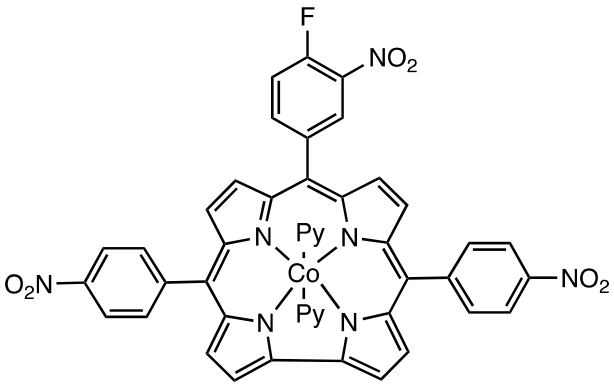




Chemical Formula: $C_{54}H_{44}CoN_7O_3$
Exact Mass: 897.28
Molecular Weight: 897.93

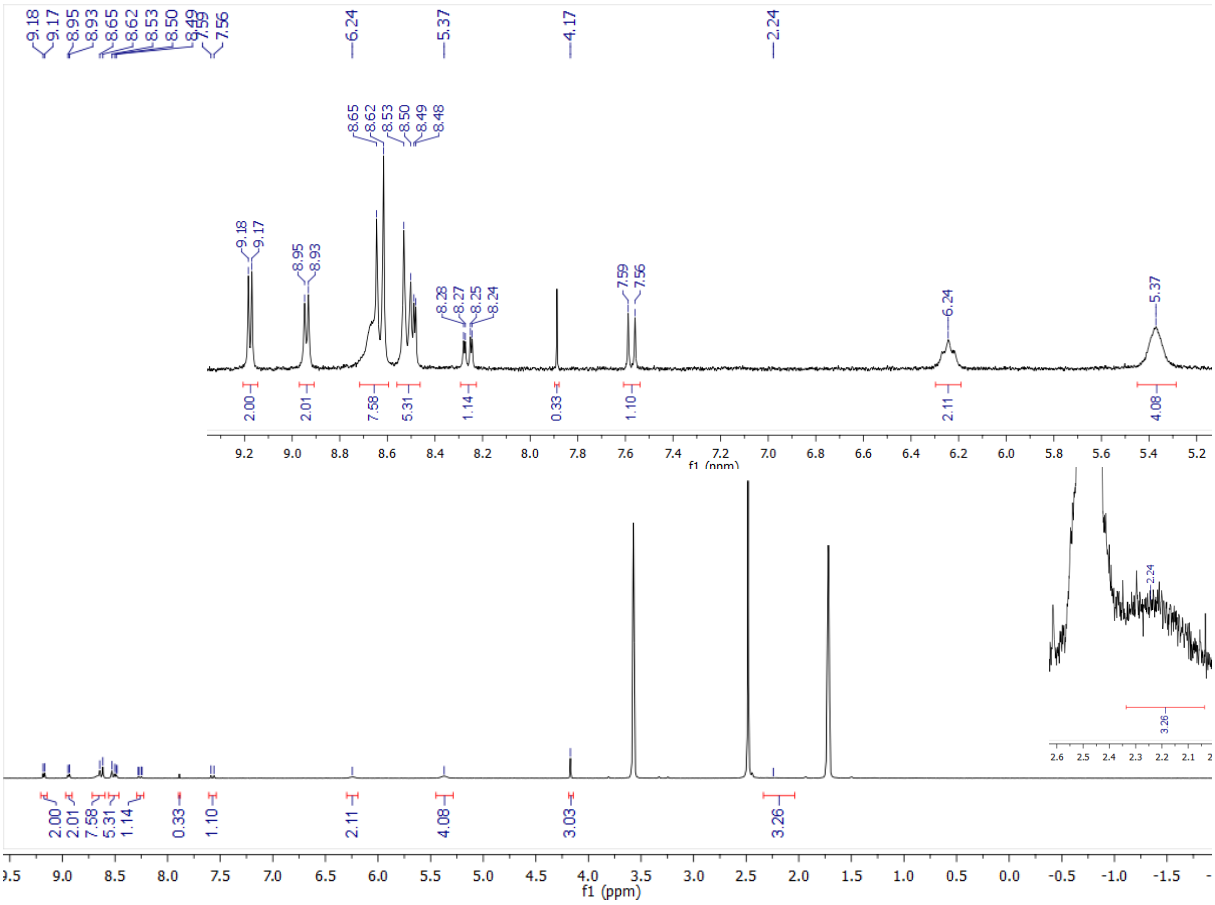
Figure S5b. ^{1}H NMR spectrum of **2** in pyridine-d_5.

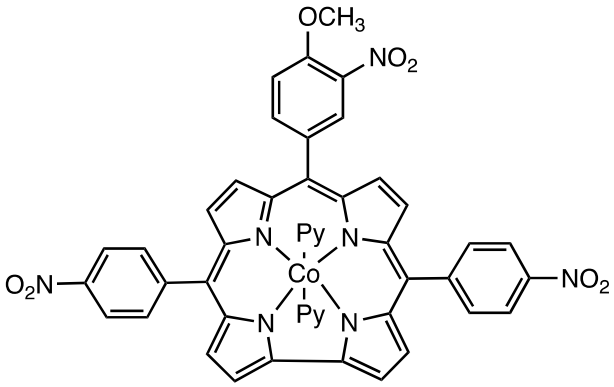




Chemical Formula: $C_{47}H_{27}CoFN_9O_6$
Exact Mass: 891.14
Molecular Weight: 891.72

Figure S5c. ^{1}H NMR spectrum of **3** in THF-d$_8$.





Chemical Formula: $C_{48}H_{30}CoN_9O_7$
Exact Mass: 903.1600
Molecular Weight: 903.7572

Figure S5d. ^{1}H NMR spectrum of **4** in THF-d_8.

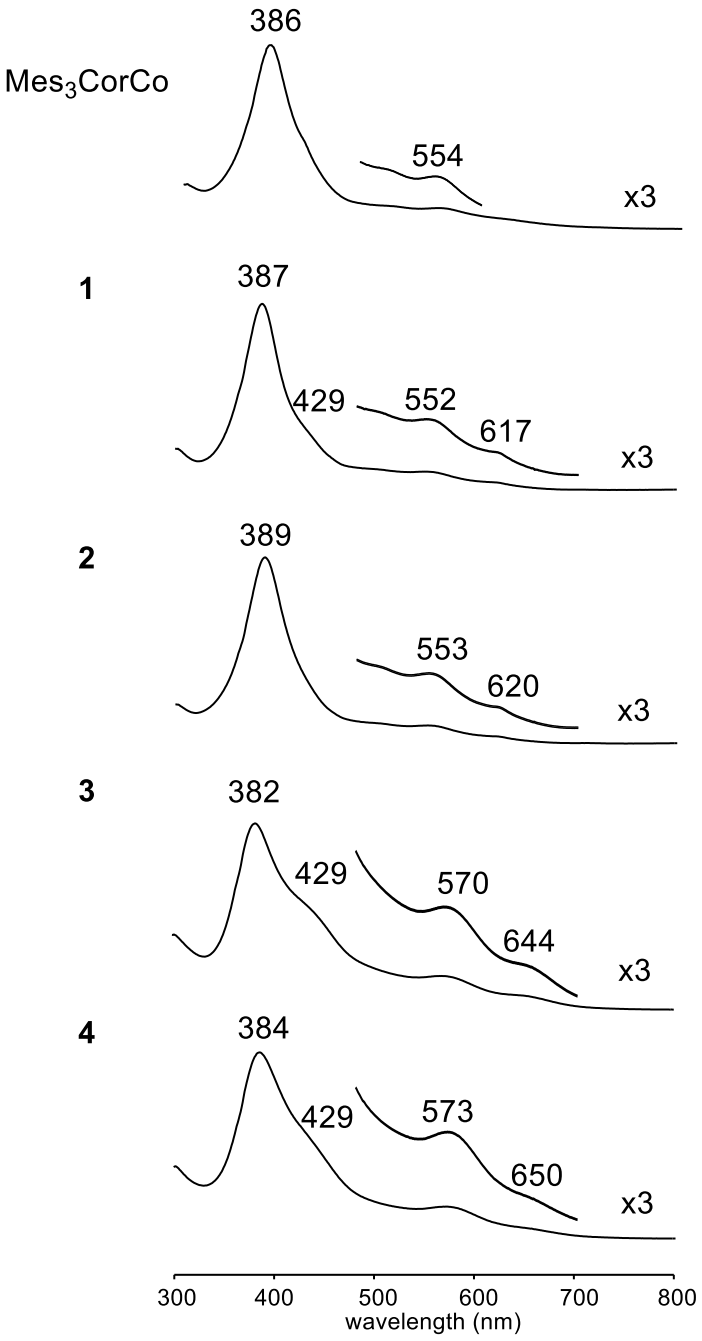


Figure S6. UV-visible spectra of **1**-**4** (10^{-5} M) in PhCN.

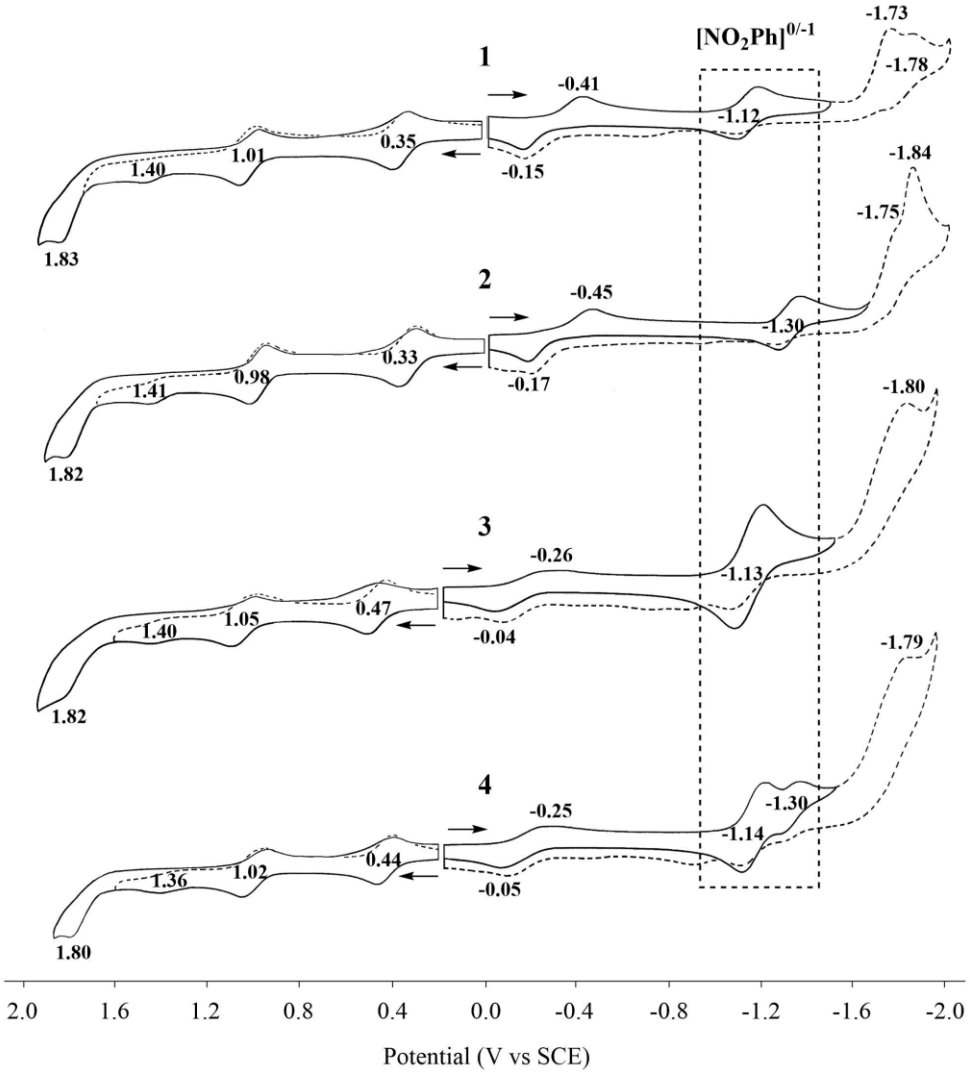


Figure S7. Cyclic voltammograms of compounds **1-4** in PhCN containing 0.1 M TBAP.

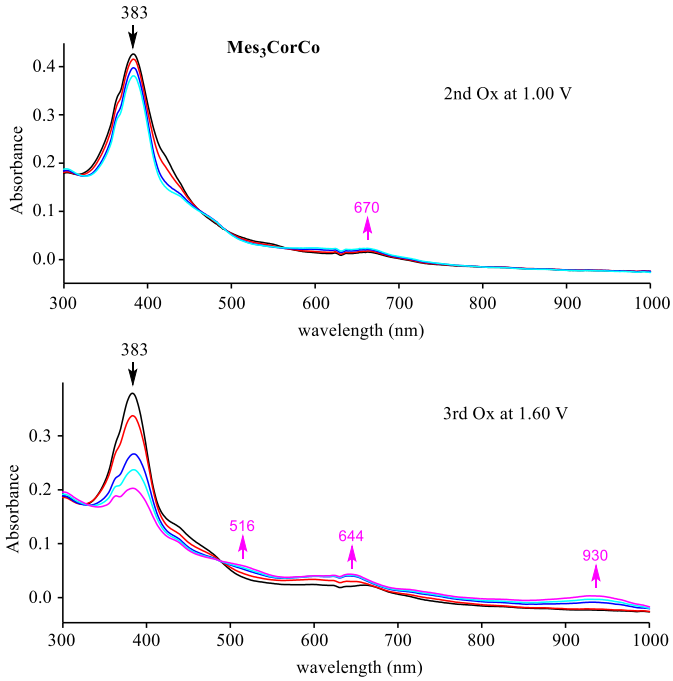


Figure S8. Spectral changes during the second and third controlled-potential oxidation of Mes_3CorCo in CH_2Cl_2 containing 0.1 M TBAP.

EPR Spectra of 1 and 3.

Continuous wave (CW) EPR spectra were recorded on a Bruker ELEXSYS 500. The instrument was equipped with a 4122 SHQE/0405 X-band resonant cavity operating at 9.43 GHz, a X-band high power dual gun-oscillator bridge, and a quartz cryostat cooled with a stream of nitrogen. The temperature was regulated with an ER 4131VT accessory. All equipment as well as the data acquisition were controlled with the Xepr software. The magnetic field was swept from 2800 to 3800 G with 2048 points. Spectra were recorded at 6 mW power, 100 kHz frequency modulation, 0.5 mT modulation amplitude, 10 ms time constant and 40 ms conversion time.

The six coordinated Co(III) corroles have previously been characterized as containing central metal ion in a low-spin ground state ($S = 0$).[5] In order to analyse the magnetism properties of theses complexes, EPR spectra were recorded at 298 K and 100 K for both corroles **1** and **3** in toluene for **1** and in a CH_2Cl_2/toluene 1/1 mixture for **3** for solubility reasons. Figure S9 shows quite broad signals at 298 K (FWHM ≈ 40 G and 50 G for **1** and **3**, respectively) and 100 K (FWHM = ≈ 60 G and 50 G for **1** and **3**, respectively) centered at $g = 2.003$ that are typical of cation radicals. The low anisotropy of the signal is assigned to the weak metallic character of the paramagnetic species, and accordingly to the delocalization of the unpaired electron on the aromatic core. Obviously, the spectra morphology is significantly different than regular Co^{2+} corrole or porphyrin complexes previously described.[6] The low intensity of the signals indicates that the compounds are mainly diamagnetic due to the presence of an antiferromagnetic coupling between the cobalt ion and the ligand, in accordance to a Co^{2+}-$L^{+\bullet}$ cation radical in the $S = 0$ ground spin state. Therefore, the existence of signals with broad lineshape can be assigned to the excited triplet state $S = 1$ for Co^{2+}-$L^{+\bullet}$ (ferromagnetic coupling).[5, 7]

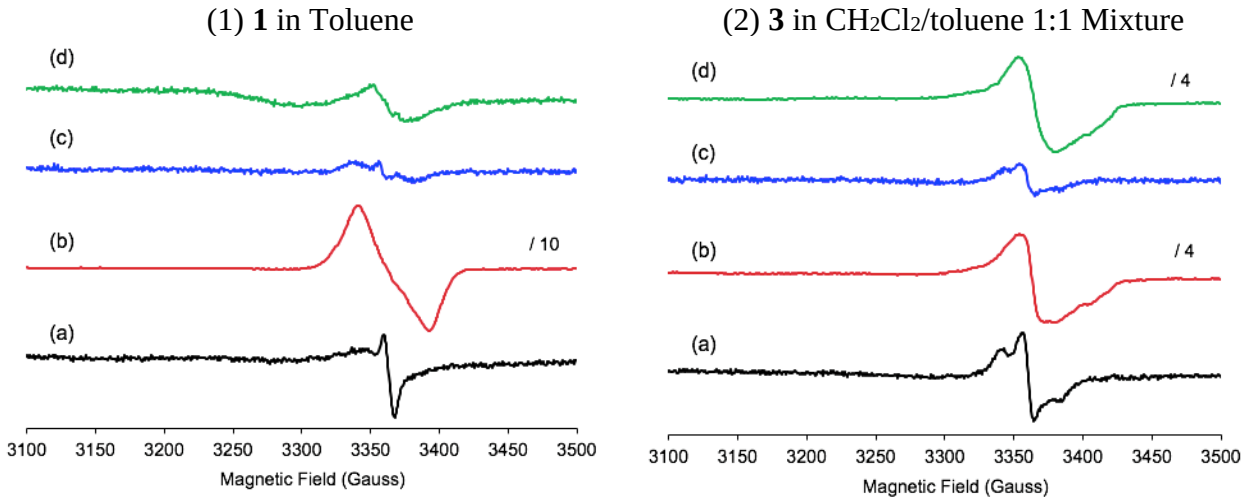


Figure S9. EPR spectra of 10^{-3} M of (1) **1** in Toluene **;** (2) **3** in CH_2Cl_2/toluene 1:1 Mixture. (a) 298 K, no pyridine; (b) 100 K, no pyridine; (c) 298 K, with an excess of pyridine and (d) 100 K, with an excess of pyridine.

The energy difference between the antiferromagnetic (singlet state) and ferromagnetic (triplet state) direct the signal intensity at low (100 K) and high temperature (298 K). A large exchange coupling constant leads obviously to a decrease of the signal intensity when the temperature decrease, while the relative population of the two states at a given temperature follows the Boltzmann distribution. As a result, the intensity of the signal depends of both phenomena. In other words, higher intensity of the signal at low temperature corresponds to a lower exchange coupling constant. Therefore, if we compare the spectral data for **1** and **3** after adding pyridine (see spectra c and d), we can anticipate a stronger exchange coupling interaction for **1** than for **3**.

EPR spectra were recorded at 10^{-3} M as for UV-vis spectra. Spectra for **3** are almost unchanged in the presence or in the absence of an excess of pyridine. This indicates that pyridine does not decoordinate when the corrole complex is dissolved in dichloromethane. However, for corrole **1**, different spectral morphologies were observed before and after addition of pyridine, especially if we compare the spectra recorded at 100 K. This must be due to the fact that the **1** corrole complex partially

release pyridine when dissolving in toluene. As seen in Table 2, pyridine association for **1-4** in DCM and PhCN followed by UV-Vis spectroscopy directly depends on the number of nitro EWG anchored to the phenyl and the concentration of the complexes (10^{-5} to 10^{-3} M). EPR results perfectly fit with the UV-visible data at 10^{-3} M concentration and correlate with the pyridine binding constants shown in Table 2, since compound **1** shows a weaker association constant than **3**. This is also consistent with the three electron-withdrawing nitrophenyl groups on **3**, which leads to the increase of the Lewis acidity of the cobalt metal center.

References

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4. Software for the Integration of CCD Detector System Bruker Analytical X-ray Systems, Bruker Axs, Madison, WI (Bruker 2016).
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7. Yadav, P.; Sankar, M.; Ke, X.; Cong, L.; Kadish, K. M., Highly Reducible π-extended Copper Corroles. *Dalton Trans.* **2017,** *46*, 10014-10022.