Supporting Information

for

Pyridyl vs bipyridyl anchoring groups of porphyrin sensitizers for dye sensitized solar cells

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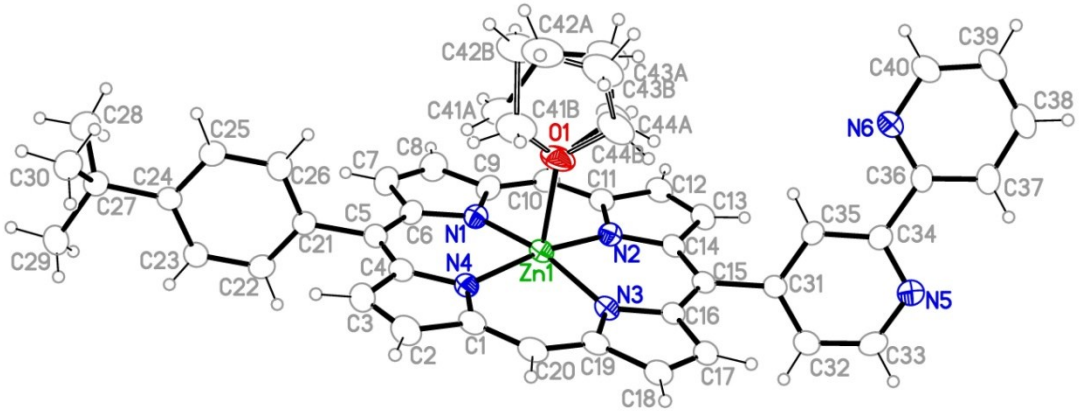

Figure S1. ORTEP representation of X-ray crystal structure of **2b**(THF) with all atoms represented by thermal ellipsoids at the 35% probability level.

Table S1. Crystal data and structure refinement for **2b**(THF).

Empirical formula	C44 H38 N6 O Zn	
Formula weight	732.17	
Temperature	292(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 21.201(7) Å	α= 90°
	b = 10.863(2) Å	β= 98.94(4)°
	c = 32.160(6) Å	γ = 90°
Volume	7317(3) $Å^3$	
Z	8	
Density (calculated)	1.329 g/cm^3	
Absorption coefficient	0.715 mm^{-1}	
F(000)	3056	
Crystal size	0.40 x 0.40 x 0.30 mm^3	
Theta range for data collection	1.94 to 29.37°	
Index ranges	-27<=h<=28, -14<=k<=14, -43<=l<=43	
Reflections collected	47595	
Independent reflections	9536 [R(int) = 0.1188]	
Completeness to theta = 25.00°	99 %	
Absorption correction	Numerical	
Max. and min. transmission	0.6868 and 0.6203	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9536 / 0 / 509	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0680, wR2 = 0.0981	
R indices (all data)	R1 = 0.1568, wR2 = 0.1178	
Largest diff. peak and hole	0.391 and -0.661 $e.Å^{-3}$	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$)for **2b**(THF)

	x	y	z	U(eq)
Zn(1)	558(1)	2758(1)	3862(1)	35(1)
N(1)	-346(1)	3491(3)	3788(1)	36(1)
N(2)	206(1)	1195(3)	3544(1)	36(1)
N(3)	1391(1)	1817(3)	4062(1)	36(1)
N(4)	859(1)	4158(3)	4281(1)	36(1)
N(5)	2148(2)	-3182(3)	3176(1)	53(1)
N(6)	1979(2)	-1206(3)	2262(1)	55(1)
C(1)	1467(2)	4296(4)	4499(1)	38(1)
C(2)	1514(2)	5469(4)	4711(1)	51(1)
C(3)	935(2)	6029(4)	4622(1)	47(1)
C(4)	519(2)	5202(3)	4351(1)	39(1)
C(5)	-122(2)	5430(3)	4195(1)	39(1)
C(6)	-527(2)	4618(4)	3936(1)	40(1)
C(7)	-1190(2)	4832(4)	3779(1)	52(1)
C(8)	-1407(2)	3855(4)	3539(1)	54(1)
C(9)	-879(2)	3021(4)	3541(1)	41(1)
C(10)	-896(2)	1905(3)	3320(1)	40(1)
C(11)	-397(2)	1077(4)	3314(1)	38(1)
C(12)	-429(2)	-48(4)	3072(1)	43(1)
C(13)	148(2)	-598(4)	3157(1)	44(1)
C(14)	550(2)	171(3)	3453(1)	36(1)
C(15)	1185(2)	-74(3)	3630(1)	36(1)
C(16)	1573(2)	678(3)	3922(1)	35(1)
C(17)	2233(2)	439(4)	4099(1)	40(1)
C(18)	2447(2)	1416(4)	4343(1)	42(1)
C(19)	1922(2)	2285(4)	4316(1)	38(1)
C(20)	1948(2)	3421(4)	4515(1)	41(1)
C(21)	-398(2)	6647(3)	4301(1)	41(1)
C(22)	-649(2)	6832(4)	4668(1)	45(1)
C(23)	-890(2)	7977(4)	4764(1)	43(1)
C(24)	-879(2)	8977(3)	4500(1)	39(1)
C(25)	-633(2)	8777(4)	4129(1)	70(2)
C(26)	-400(3)	7629(4)	4033(1)	75(2)

C(27)	-1120(2)	10262(4)	4597(1)	42(1)
C(28)	-1697(2)	10613(4)	4266(1)	58(1)
C(29)	-1323(2)	10345(4)	5035(1)	55(1)
C(30)	-595(2)	11217(4)	4575(1)	52(1)
C(31)	1494(2)	-1185(4)	3476(1)	38(1)
C(32)	1679(2)	-2196(4)	3730(1)	51(1)
C(33)	1996(2)	-3160(4)	3568(1)	56(1)
C(34)	1958(2)	-2220(4)	2929(1)	41(1)
C(35)	1637(2)	-1213(3)	3068(1)	38(1)
C(36)	2106(2)	-2249(4)	2486(1)	43(1)
C(37)	2339(2)	-3299(4)	2319(1)	52(1)
C(38)	2430(2)	-3278(4)	1900(1)	66(1)
C(39)	2308(2)	-2220(5)	1668(1)	74(2)
C(40)	2088(2)	-1212(4)	1861(1)	73(2)
O(1)	828(1)	3623(3)	3301(1)	61(1)
C(41A)	596(7)	4897(10)	3175(3)	72(3)
C(42A)	930(7)	4999(12)	2760(3)	81(3)
C(43A)	1018(7)	3848(10)	2603(3)	85(3)
C(44A)	834(7)	2951(15)	2913(3)	76(3)
C(41B)	881(16)	4740(30)	3251(7)	79(4)
C(42B)	703(14)	5300(30)	2782(8)	78(4)
C(43B)	1311(15)	4100(30)	2732(8)	83(3)
C(44B)	1071(16)	3060(40)	2987(9)	81(4)

Table S3. Bond lengths (Å) and angles (°)for **2b**(THF)

Zn(1)-N(1)	2.053(3)
Zn(1)-N(3)	2.056(3)
Zn(1)-N(2)	2.062(3)
Zn(1)-N(4)	2.065(3)
Zn(1)-O(1)	2.189(2)
N(1)-C(9)	1.375(4)
N(1)-C(6)	1.390(4)
N(2)-C(11)	1.379(4)
N(2)-C(14)	1.387(4)
N(3)-C(19)	1.381(4)
N(3)-C(16)	1.391(4)
N(4)-C(1)	1.378(4)
N(4)-C(4)	1.380(4)
N(5)-C(34)	1.337(5)
N(5)-C(33)	1.349(4)
N(6)-C(36)	1.347(5)
N(6)-C(40)	1.344(4)
C(1)-C(20)	1.389(5)
C(1)-C(2)	1.442(5)
C(2)-C(3)	1.358(5)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.452(5)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.398(5)
C(5)-C(6)	1.410(5)
C(5)-C(21)	1.506(5)
C(6)-C(7)	1.437(5)
C(7)-C(8)	1.350(5)
C(7)-H(7A)	0.9300
C(8)-C(9)	1.439(5)
C(8)-H(8A)	0.9300
C(9)-C(10)	1.403(5)
C(10)-C(11)	1.391(5)
C(10)-H(10A)	0.9300
C(11)-C(12)	1.444(5)
C(12)-C(13)	1.351(5)

C(12)-H(12A)	0.9300
C(13)-C(14)	1.443(5)
C(13)-H(13A)	0.9300
C(14)-C(15)	1.403(5)
C(15)-C(16)	1.410(5)
C(15)-C(31)	1.494(5)
C(16)-C(17)	1.448(5)
C(17)-C(18)	1.356(5)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.452(5)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.387(5)
C(20)-H(20A)	0.9300
C(21)-C(26)	1.371(5)
C(21)-C(22)	1.383(4)
C(22)-C(23)	1.397(5)
C(22)-H(22A)	0.9300
C(23)-C(24)	1.381(5)
C(23)-H(23A)	0.9300
C(24)-C(25)	1.394(5)
C(24)-C(27)	1.534(5)
C(25)-C(26)	1.393(5)
C(25)-H(25A)	0.9300
C(26)-H(26A)	0.9300
C(27)-C(30)	1.531(5)
C(27)-C(28)	1.538(5)
C(27)-C(29)	1.539(4)
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(31)-C(32)	1.387(5)
C(31)-C(35)	1.392(4)

C(32)-C(33)	1.388(5)
C(32)-H(32A)	0.9300
C(33)-H(33A)	0.9300
C(34)-C(35)	1.398(5)
C(34)-C(36)	1.504(4)
C(35)-H(35A)	0.9300
C(36)-C(37)	1.385(5)
C(37)-C(38)	1.393(5)
C(37)-H(37A)	0.9300
C(38)-C(39)	1.371(6)
C(38)-H(38A)	0.9300
C(39)-C(40)	1.376(6)
C(39)-H(39A)	0.9300
C(40)-H(40A)	0.9300
O(1)-C(41B)	1.23(3)
O(1)-C(44B)	1.35(3)
O(1)-C(44A)	1.447(12)
O(1)-C(41A)	1.503(12)
C(41A)-C(42A)	1.606(16)
C(41A)-H(41A)	0.9700
C(41A)-H(41B)	0.9700
C(42A)-C(43A)	1.372(14)
C(42A)-H(42A)	0.9700
C(42A)-H(42B)	0.9700
C(43A)-C(44A)	1.487(14)
C(43A)-H(43A)	0.9700
C(43A)-H(43B)	0.9700
C(44A)-H(44A)	0.9700
C(44A)-H(44B)	0.9700
C(41B)-C(42B)	1.62(4)
C(41B)-H(41C)	0.9700
C(41B)-H(41D)	0.9700
C(42B)-C(43B)	1.85(4)
C(42B)-H(42C)	0.9700
C(42B)-H(42D)	0.9700
C(43B)-C(44B)	1.53(3)
C(43B)-H(43C)	0.9700
C(43B)-H(43D)	0.9700

C(44B)-H(44C)	0.9700
C(44B)-H(44D)	0.9700
N(1)-Zn(1)-N(3)	165.86(10)
N(1)-Zn(1)-N(2)	90.12(12)
N(3)-Zn(1)-N(2)	88.44(12)
N(1)-Zn(1)-N(4)	88.77(12)
N(3)-Zn(1)-N(4)	89.93(12)
N(2)-Zn(1)-N(4)	168.89(9)
N(1)-Zn(1)-O(1)	95.53(11)
N(3)-Zn(1)-O(1)	98.61(11)
N(2)-Zn(1)-O(1)	93.76(11)
N(4)-Zn(1)-O(1)	97.36(11)
C(9)-N(1)-C(6)	106.1(3)
C(9)-N(1)-Zn(1)	126.3(3)
C(6)-N(1)-Zn(1)	127.2(3)
C(11)-N(2)-C(14)	106.7(3)
C(11)-N(2)-Zn(1)	125.2(3)
C(14)-N(2)-Zn(1)	127.1(2)
C(19)-N(3)-C(16)	106.1(3)
C(19)-N(3)-Zn(1)	125.7(3)
C(16)-N(3)-Zn(1)	127.5(2)
C(1)-N(4)-C(4)	107.3(3)
C(1)-N(4)-Zn(1)	125.6(2)
C(4)-N(4)-Zn(1)	126.6(2)
C(34)-N(5)-C(33)	116.6(3)
C(36)-N(6)-C(40)	117.4(3)
N(4)-C(1)-C(20)	124.6(3)
N(4)-C(1)-C(2)	109.1(4)
C(20)-C(1)-C(2)	126.3(4)
C(3)-C(2)-C(1)	107.6(4)
C(3)-C(2)-H(2A)	126.2
C(1)-C(2)-H(2A)	126.2
C(2)-C(3)-C(4)	107.1(4)
C(2)-C(3)-H(3A)	126.5
C(4)-C(3)-H(3A)	126.5
N(4)-C(4)-C(5)	126.2(3)
N(4)-C(4)-C(3)	108.9(3)

C(5)-C(4)-C(3)	124.9(4)
C(4)-C(5)-C(6)	124.8(4)
C(4)-C(5)-C(21)	117.7(3)
C(6)-C(5)-C(21)	117.5(4)
N(1)-C(6)-C(5)	125.3(4)
N(1)-C(6)-C(7)	109.3(3)
C(5)-C(6)-C(7)	125.4(4)
C(8)-C(7)-C(6)	107.5(4)
C(8)-C(7)-H(7A)	126.2
C(6)-C(7)-H(7A)	126.2
C(7)-C(8)-C(9)	107.3(4)
C(7)-C(8)-H(8A)	126.4
C(9)-C(8)-H(8A)	126.4
N(1)-C(9)-C(10)	124.5(4)
N(1)-C(9)-C(8)	109.8(3)
C(10)-C(9)-C(8)	125.6(4)
C(11)-C(10)-C(9)	127.3(4)
C(11)-C(10)-H(10A)	116.3
C(9)-C(10)-H(10A)	116.3
N(2)-C(11)-C(10)	125.1(3)
N(2)-C(11)-C(12)	109.2(3)
C(10)-C(11)-C(12)	125.6(4)
C(13)-C(12)-C(11)	107.5(3)
C(13)-C(12)-H(12A)	126.2
C(11)-C(12)-H(12A)	126.2
C(12)-C(13)-C(14)	107.5(3)
C(12)-C(13)-H(13A)	126.3
C(14)-C(13)-H(13A)	126.3
N(2)-C(14)-C(15)	124.8(3)
N(2)-C(14)-C(13)	109.1(3)
C(15)-C(14)-C(13)	126.1(3)
C(14)-C(15)-C(16)	125.7(3)
C(14)-C(15)-C(31)	117.5(3)
C(16)-C(15)-C(31)	116.6(3)
N(3)-C(16)-C(15)	124.6(3)
N(3)-C(16)-C(17)	109.4(3)
C(15)-C(16)-C(17)	125.8(3)
C(18)-C(17)-C(16)	107.6(3)

C(18)-C(17)-H(17A)	126.2
C(16)-C(17)-H(17A)	126.2
C(17)-C(18)-C(19)	106.9(3)
C(17)-C(18)-H(18A)	126.6
C(19)-C(18)-H(18A)	126.6
N(3)-C(19)-C(20)	124.8(4)
N(3)-C(19)-C(18)	110.0(3)
C(20)-C(19)-C(18)	125.2(3)
C(19)-C(20)-C(1)	128.0(4)
C(19)-C(20)-H(20A)	116.0
C(1)-C(20)-H(20A)	116.0
C(26)-C(21)-C(22)	117.3(4)
C(26)-C(21)-C(5)	120.2(3)
C(22)-C(21)-C(5)	122.4(3)
C(21)-C(22)-C(23)	121.4(3)
C(21)-C(22)-H(22A)	119.3
C(23)-C(22)-H(22A)	119.3
C(24)-C(23)-C(22)	121.5(3)
C(24)-C(23)-H(23A)	119.3
C(22)-C(23)-H(23A)	119.3
C(23)-C(24)-C(25)	116.6(4)
C(23)-C(24)-C(27)	123.6(3)
C(25)-C(24)-C(27)	119.7(3)
C(24)-C(25)-C(26)	121.4(3)
C(24)-C(25)-H(25A)	119.3
C(26)-C(25)-H(25A)	119.3
C(21)-C(26)-C(25)	121.6(3)
C(21)-C(26)-H(26A)	119.2
C(25)-C(26)-H(26A)	119.2
C(30)-C(27)-C(24)	109.9(3)
C(30)-C(27)-C(28)	107.8(3)
C(24)-C(27)-C(28)	109.9(3)
C(30)-C(27)-C(29)	108.1(3)
C(24)-C(27)-C(29)	112.8(3)
C(28)-C(27)-C(29)	108.2(3)
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5

C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(27)-C(30)-H(30A)	109.5
C(27)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(27)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(35)	117.0(3)
C(32)-C(31)-C(15)	122.9(3)
C(35)-C(31)-C(15)	120.1(3)
C(33)-C(32)-C(31)	119.0(3)
C(33)-C(32)-H(32A)	120.5
C(31)-C(32)-H(32A)	120.5
N(5)-C(33)-C(32)	124.3(3)
N(5)-C(33)-H(33A)	117.8
C(32)-C(33)-H(33A)	117.8
N(5)-C(34)-C(35)	122.5(3)
N(5)-C(34)-C(36)	117.3(3)
C(35)-C(34)-C(36)	120.2(3)
C(31)-C(35)-C(34)	120.6(3)
C(31)-C(35)-H(35A)	119.7
C(34)-C(35)-H(35A)	119.7
N(6)-C(36)-C(37)	122.6(3)
N(6)-C(36)-C(34)	115.8(3)
C(37)-C(36)-C(34)	121.6(4)
C(38)-C(37)-C(36)	118.3(4)
C(38)-C(37)-H(37A)	120.9
C(36)-C(37)-H(37A)	120.9
C(39)-C(38)-C(37)	119.8(4)
C(39)-C(38)-H(38A)	120.1

C(37)-C(38)-H(38A)	120.1
C(38)-C(39)-C(40)	118.0(3)
C(38)-C(39)-H(39A)	121.0
C(40)-C(39)-H(39A)	121.0
N(6)-C(40)-C(39)	123.9(4)
N(6)-C(40)-H(40A)	118.1
C(39)-C(40)-H(40A)	118.1
C(41B)-O(1)-C(44B)	107.2(19)
C(41B)-O(1)-C(44A)	111.8(13)
C(44B)-O(1)-C(44A)	21.7(15)
C(41B)-O(1)-C(41A)	24.6(15)
C(44B)-O(1)-C(41A)	111.2(17)
C(44A)-O(1)-C(41A)	106.1(7)
C(41B)-O(1)-Zn(1)	124.8(11)
C(44B)-O(1)-Zn(1)	127.1(16)
C(44A)-O(1)-Zn(1)	122.3(6)
C(41A)-O(1)-Zn(1)	120.1(4)
O(1)-C(41A)-C(42A)	96.9(10)
O(1)-C(41A)-H(41A)	112.4
C(42A)-C(41A)-H(41A)	112.4
O(1)-C(41A)-H(41B)	112.4
C(42A)-C(41A)-H(41B)	112.4
H(41A)-C(41A)-H(41B)	109.9
C(43A)-C(42A)-C(41A)	110.2(10)
C(43A)-C(42A)-H(42A)	109.6
C(41A)-C(42A)-H(42A)	109.6
C(43A)-C(42A)-H(42B)	109.6
C(41A)-C(42A)-H(42B)	109.6
H(42A)-C(42A)-H(42B)	108.1
C(42A)-C(43A)-C(44A)	106.6(8)
C(42A)-C(43A)-H(43A)	110.4
C(44A)-C(43A)-H(43A)	110.4
C(42A)-C(43A)-H(43B)	110.4
C(44A)-C(43A)-H(43B)	110.4
H(43A)-C(43A)-H(43B)	108.6
O(1)-C(44A)-C(43A)	106.6(9)
O(1)-C(44A)-H(44A)	110.4
C(43A)-C(44A)-H(44A)	110.4

O(1)-C(44A)-H(44B)	110.4
C(43A)-C(44A)-H(44B)	110.4
H(44A)-C(44A)-H(44B)	108.6
O(1)-C(41B)-C(42B)	119(2)
O(1)-C(41B)-H(41C)	107.7
C(42B)-C(41B)-H(41C)	107.7
O(1)-C(41B)-H(41D)	107.7
C(42B)-C(41B)-H(41D)	107.7
H(41C)-C(41B)-H(41D)	107.1
C(41B)-C(42B)-C(43B)	76(2)
C(41B)-C(42B)-H(42C)	115.9
C(43B)-C(42B)-H(42C)	115.9
C(41B)-C(42B)-H(42D)	115.9
C(43B)-C(42B)-H(42D)	115.9
H(42C)-C(42B)-H(42D)	112.9
C(44B)-C(43B)-C(42B)	100.2(18)
C(44B)-C(43B)-H(43C)	111.7
C(42B)-C(43B)-H(43C)	111.7
C(44B)-C(43B)-H(43D)	111.7
C(42B)-C(43B)-H(43D)	111.7
H(43C)-C(43B)-H(43D)	109.5
O(1)-C(44B)-C(43B)	105(2)
O(1)-C(44B)-H(44C)	110.7
C(43B)-C(44B)-H(44C)	110.7
O(1)-C(44B)-H(44D)	110.7
C(43B)-C(44B)-H(44D)	110.7
H(44C)-C(44B)-H(44D)	108.8

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2b**(THF).

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	36(1)	40(1)	30(1)	-1(1)	7(1)	-3(1)
N(1)	35(2)	35(2)	39(1)	2(1)	8(1)	-2(2)
N(2)	33(2)	39(2)	35(1)	0(1)	6(1)	-1(2)
N(3)	38(2)	40(2)	29(1)	-3(1)	7(1)	-3(2)
N(4)	37(2)	38(2)	32(1)	0(1)	7(1)	0(2)
N(5)	61(3)	54(3)	42(2)	2(1)	5(1)	13(2)
N(6)	77(3)	54(3)	36(1)	-1(1)	15(2)	16(2)
C(1)	40(3)	44(3)	30(2)	-3(1)	6(1)	-9(2)
C(2)	57(3)	51(3)	45(2)	-7(2)	7(2)	-12(2)
C(3)	60(3)	34(3)	46(2)	-5(2)	10(2)	-6(2)
C(4)	50(3)	36(3)	31(2)	1(1)	10(2)	-2(2)
C(5)	49(3)	36(3)	36(2)	3(1)	15(2)	2(2)
C(6)	42(3)	36(3)	44(2)	4(2)	12(2)	3(2)
C(7)	44(3)	53(3)	61(2)	1(2)	11(2)	12(2)
C(8)	37(3)	59(3)	63(2)	0(2)	5(2)	2(2)
C(9)	34(3)	40(3)	48(2)	3(2)	5(2)	-1(2)
C(10)	33(3)	44(3)	43(2)	4(2)	1(2)	-5(2)
C(11)	35(3)	44(3)	35(2)	1(1)	3(1)	-5(2)
C(12)	43(3)	46(3)	39(2)	-6(2)	1(2)	-12(2)
C(13)	49(3)	45(3)	38(2)	-9(2)	7(2)	-5(2)
C(14)	38(3)	39(3)	31(2)	-2(1)	9(1)	-2(2)
C(15)	40(3)	41(3)	28(1)	2(1)	10(1)	3(2)
C(16)	37(2)	39(2)	29(1)	2(1)	8(1)	4(2)
C(17)	37(3)	51(3)	32(2)	1(1)	9(1)	8(2)
C(18)	32(3)	58(3)	34(2)	0(2)	4(1)	1(2)
C(19)	37(2)	49(3)	28(1)	-1(2)	6(1)	-6(2)
C(20)	36(3)	56(3)	31(2)	-1(2)	3(1)	-7(2)
C(21)	49(3)	37(3)	37(2)	3(1)	10(2)	4(2)
C(22)	56(3)	41(3)	41(2)	9(2)	15(2)	1(2)
C(23)	52(3)	41(3)	39(2)	2(2)	17(2)	1(2)
C(24)	45(3)	39(3)	33(2)	1(1)	7(1)	0(2)
C(25)	125(5)	47(3)	46(2)	15(2)	37(2)	20(3)
C(26)	136(5)	45(3)	56(2)	12(2)	55(3)	21(3)
C(27)	45(3)	40(3)	41(2)	1(2)	8(2)	2(2)

C(28)	55(3)	58(3)	59(2)	7(2)	7(2)	5(2)
C(29)	69(3)	48(3)	51(2)	-4(2)	23(2)	3(2)
C(30)	59(3)	43(3)	55(2)	2(2)	11(2)	-3(2)
C(31)	38(3)	44(3)	32(2)	0(1)	5(1)	5(2)
C(32)	62(3)	55(3)	36(2)	0(2)	7(2)	10(3)
C(33)	71(3)	51(3)	46(2)	14(2)	4(2)	14(2)
C(34)	43(3)	40(2)	39(2)	1(2)	3(1)	6(2)
C(35)	41(3)	34(2)	37(2)	0(1)	3(1)	7(2)
C(36)	43(3)	44(3)	42(2)	-7(2)	7(1)	11(2)
C(37)	61(3)	44(3)	54(2)	-7(2)	13(2)	11(2)
C(38)	89(4)	55(3)	58(2)	-18(2)	27(2)	9(3)
C(39)	112(4)	68(4)	49(2)	-8(2)	35(2)	16(3)
C(40)	113(5)	70(4)	43(2)	7(2)	30(2)	25(3)
O(1)	80(2)	68(2)	38(1)	10(1)	23(1)	-11(2)
C(41A)	84(8)	76(5)	56(4)	20(3)	10(4)	-16(5)
C(42A)	96(7)	91(5)	60(3)	21(3)	24(4)	-18(5)
C(43A)	101(7)	106(5)	55(4)	10(3)	36(4)	-14(5)
C(44A)	99(8)	89(5)	45(4)	-3(3)	27(4)	-3(6)
C(41B)	93(9)	84(6)	62(5)	15(5)	23(6)	-18(7)
C(42B)	91(9)	88(6)	59(5)	18(5)	21(6)	-21(6)
C(43B)	96(9)	103(7)	59(6)	10(6)	38(6)	-18(6)
C(44B)	98(9)	96(6)	57(6)	4(6)	43(6)	-8(7)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$)for **2b**(THF).

	x	y	z	U(eq)
H(2A)	1874	5785	4879	61
H(3A)	827	6798	4717	56
H(7A)	-1427	5517	3833	63
H(8A)	-1820	3743	3398	64
H(10A)	-1285	1694	3160	49
H(12A)	-783	-340	2892	52
H(13A)	265	-1338	3044	53
H(17A)	2466	-259	4053	47
H(18A)	2853	1512	4497	50
H(20A)	2335	3621	4679	50
H(22A)	-658	6181	4855	54
H(23A)	-1061	8067	5012	51
H(25A)	-623	9424	3940	84
H(26A)	-243	7525	3781	90
H(28A)	-1568	10656	3994	87
H(28B)	-1859	11399	4336	87
H(28C)	-2025	10002	4263	87
H(29A)	-1492	11149	5073	82
H(29B)	-959	10200	5247	82
H(29C)	-1644	9736	5058	82
H(30A)	-450	11159	4307	79
H(30B)	-245	11065	4796	79
H(30C)	-762	12027	4607	79
H(32A)	1592	-2227	4004	61
H(33A)	2110	-3835	3741	68
H(35A)	1519	-557	2887	45
H(37A)	2432	-4001	2483	63
H(38A)	2573	-3978	1777	79
H(39A)	2372	-2186	1389	89
H(40A)	2009	-492	1705	88
H(41A)	754	5509	3385	87
H(41B)	134	4943	3111	87

H(42A)	664	5485	2549	97
H(42B)	1339	5410	2829	97
H(43A)	1461	3732	2570	102
H(43B)	753	3740	2331	102
H(44A)	415	2611	2812	91
H(44B)	1140	2282	2956	91
H(41C)	1320	4958	3356	94
H(41D)	616	5147	3429	94
H(42C)	832	6141	2746	94
H(42D)	274	5123	2639	94
H(43C)	1309	3868	2441	100
H(43D)	1736	4372	2854	100
H(44C)	746	2582	2813	97
H(44D)	1420	2519	3100	97

Table S6. Torsion angles (°) for **2b**(THF).

N(3)-Zn(1)-N(1)-C(9)	-93.4(5)
N(2)-Zn(1)-N(1)-C(9)	-9.3(3)
N(4)-Zn(1)-N(1)-C(9)	-178.2(3)
O(1)-Zn(1)-N(1)-C(9)	84.5(3)
N(3)-Zn(1)-N(1)-C(6)	94.4(5)
N(2)-Zn(1)-N(1)-C(6)	178.5(3)
N(4)-Zn(1)-N(1)-C(6)	9.6(2)
O(1)-Zn(1)-N(1)-C(6)	-87.7(3)
N(1)-Zn(1)-N(2)-C(11)	12.8(2)
N(3)-Zn(1)-N(2)-C(11)	178.7(2)
N(4)-Zn(1)-N(2)-C(11)	97.0(7)
O(1)-Zn(1)-N(2)-C(11)	-82.8(2)
N(1)-Zn(1)-N(2)-C(14)	179.5(2)
N(3)-Zn(1)-N(2)-C(14)	-14.5(2)
N(4)-Zn(1)-N(2)-C(14)	-96.2(7)
O(1)-Zn(1)-N(2)-C(14)	84.0(3)
N(1)-Zn(1)-N(3)-C(19)	-95.7(5)
N(2)-Zn(1)-N(3)-C(19)	180.0(2)
N(4)-Zn(1)-N(3)-C(19)	-11.0(2)
O(1)-Zn(1)-N(3)-C(19)	86.4(2)
N(1)-Zn(1)-N(3)-C(16)	95.1(5)
N(2)-Zn(1)-N(3)-C(16)	10.8(3)
N(4)-Zn(1)-N(3)-C(16)	179.8(3)
O(1)-Zn(1)-N(3)-C(16)	-82.8(3)
N(1)-Zn(1)-N(4)-C(1)	177.8(3)
N(3)-Zn(1)-N(4)-C(1)	11.9(3)
N(2)-Zn(1)-N(4)-C(1)	93.4(7)
O(1)-Zn(1)-N(4)-C(1)	-86.8(3)
N(1)-Zn(1)-N(4)-C(4)	-11.5(3)
N(3)-Zn(1)-N(4)-C(4)	-177.4(3)
N(2)-Zn(1)-N(4)-C(4)	-95.9(7)
O(1)-Zn(1)-N(4)-C(4)	83.9(3)
C(4)-N(4)-C(1)-C(20)	178.3(3)
Zn(1)-N(4)-C(1)-C(20)	-9.6(4)
C(4)-N(4)-C(1)-C(2)	-0.3(3)
Zn(1)-N(4)-C(1)-C(2)	171.9(2)

N(4)-C(1)-C(2)-C(3)	0.1(4)
C(20)-C(1)-C(2)-C(3)	-178.4(3)
C(1)-C(2)-C(3)-C(4)	0.1(4)
C(1)-N(4)-C(4)-C(5)	-178.7(3)
Zn(1)-N(4)-C(4)-C(5)	9.3(4)
C(1)-N(4)-C(4)-C(3)	0.4(3)
Zn(1)-N(4)-C(4)-C(3)	-171.7(2)
C(2)-C(3)-C(4)-N(4)	-0.3(4)
C(2)-C(3)-C(4)-C(5)	178.8(3)
N(4)-C(4)-C(5)-C(6)	-0.3(5)
C(3)-C(4)-C(5)-C(6)	-179.2(3)
N(4)-C(4)-C(5)-C(21)	-178.6(3)
C(3)-C(4)-C(5)-C(21)	2.6(5)
C(9)-N(1)-C(6)-C(5)	-178.6(3)
Zn(1)-N(1)-C(6)-C(5)	-5.2(4)
C(9)-N(1)-C(6)-C(7)	0.7(3)
Zn(1)-N(1)-C(6)-C(7)	174.2(2)
C(4)-C(5)-C(6)-N(1)	-1.9(5)
C(21)-C(5)-C(6)-N(1)	176.4(3)
C(4)-C(5)-C(6)-C(7)	178.8(3)
C(21)-C(5)-C(6)-C(7)	-2.9(5)
N(1)-C(6)-C(7)-C(8)	-0.3(4)
C(5)-C(6)-C(7)-C(8)	179.0(3)
C(6)-C(7)-C(8)-C(9)	-0.2(4)
C(6)-N(1)-C(9)-C(10)	178.0(3)
Zn(1)-N(1)-C(9)-C(10)	4.5(4)
C(6)-N(1)-C(9)-C(8)	-0.8(4)
Zn(1)-N(1)-C(9)-C(8)	-174.4(2)
C(7)-C(8)-C(9)-N(1)	0.7(4)
C(7)-C(8)-C(9)-C(10)	-178.2(3)
N(1)-C(9)-C(10)-C(11)	1.1(5)
C(8)-C(9)-C(10)-C(11)	179.8(3)
C(14)-N(2)-C(11)-C(10)	178.9(3)
Zn(1)-N(2)-C(11)-C(10)	-12.1(4)
C(14)-N(2)-C(11)-C(12)	-0.1(3)
Zn(1)-N(2)-C(11)-C(12)	168.9(2)
C(9)-C(10)-C(11)-N(2)	3.1(5)
C(9)-C(10)-C(11)-C(12)	-178.1(3)

N(2)-C(11)-C(12)-C(13)	0.0(4)
C(10)-C(11)-C(12)-C(13)	-179.0(3)
C(11)-C(12)-C(13)-C(14)	0.2(4)
C(11)-N(2)-C(14)-C(15)	-178.8(3)
Zn(1)-N(2)-C(14)-C(15)	12.4(4)
C(11)-N(2)-C(14)-C(13)	0.2(3)
Zn(1)-N(2)-C(14)-C(13)	-168.6(2)
C(12)-C(13)-C(14)-N(2)	-0.2(4)
C(12)-C(13)-C(14)-C(15)	178.7(3)
N(2)-C(14)-C(15)-C(16)	-0.7(5)
C(13)-C(14)-C(15)-C(16)	-179.5(3)
N(2)-C(14)-C(15)-C(31)	-176.4(3)
C(13)-C(14)-C(15)-C(31)	4.8(5)
C(19)-N(3)-C(16)-C(15)	-175.4(3)
Zn(1)-N(3)-C(16)-C(15)	-4.5(4)
C(19)-N(3)-C(16)-C(17)	0.5(3)
Zn(1)-N(3)-C(16)-C(17)	171.4(2)
C(14)-C(15)-C(16)-N(3)	-3.5(5)
C(31)-C(15)-C(16)-N(3)	172.3(3)
C(14)-C(15)-C(16)-C(17)	-178.8(3)
C(31)-C(15)-C(16)-C(17)	-3.0(5)
N(3)-C(16)-C(17)-C(18)	0.0(4)
C(15)-C(16)-C(17)-C(18)	175.9(3)
C(16)-C(17)-C(18)-C(19)	-0.6(4)
C(16)-N(3)-C(19)-C(20)	178.8(3)
Zn(1)-N(3)-C(19)-C(20)	7.7(4)
C(16)-N(3)-C(19)-C(18)	-0.9(3)
Zn(1)-N(3)-C(19)-C(18)	-172.0(2)
C(17)-C(18)-C(19)-N(3)	0.9(4)
C(17)-C(18)-C(19)-C(20)	-178.8(3)
N(3)-C(19)-C(20)-C(1)	-0.5(5)
C(18)-C(19)-C(20)-C(1)	179.2(3)
N(4)-C(1)-C(20)-C(19)	1.5(5)
C(2)-C(1)-C(20)-C(19)	179.8(3)
C(4)-C(5)-C(21)-C(26)	92.8(5)
C(6)-C(5)-C(21)-C(26)	-85.6(5)
C(4)-C(5)-C(21)-C(22)	-86.4(5)
C(6)-C(5)-C(21)-C(22)	95.2(4)

C(26)-C(21)-C(22)-C(23)	-0.6(6)
C(5)-C(21)-C(22)-C(23)	178.6(4)
C(21)-C(22)-C(23)-C(24)	-0.9(6)
C(22)-C(23)-C(24)-C(25)	1.7(6)
C(22)-C(23)-C(24)-C(27)	-178.3(4)
C(23)-C(24)-C(25)-C(26)	-1.0(7)
C(27)-C(24)-C(25)-C(26)	179.0(5)
C(22)-C(21)-C(26)-C(25)	1.4(7)
C(5)-C(21)-C(26)-C(25)	-177.9(5)
C(24)-C(25)-C(26)-C(21)	-0.6(8)
C(23)-C(24)-C(27)-C(30)	125.5(4)
C(25)-C(24)-C(27)-C(30)	-54.5(5)
C(23)-C(24)-C(27)-C(28)	-116.0(4)
C(25)-C(24)-C(27)-C(28)	64.0(5)
C(23)-C(24)-C(27)-C(29)	4.8(5)
C(25)-C(24)-C(27)-C(29)	-175.2(4)
C(14)-C(15)-C(31)-C(32)	-114.0(4)
C(16)-C(15)-C(31)-C(32)	69.9(5)
C(14)-C(15)-C(31)-C(35)	69.2(5)
C(16)-C(15)-C(31)-C(35)	-107.0(4)
C(35)-C(31)-C(32)-C(33)	0.5(6)
C(15)-C(31)-C(32)-C(33)	-176.4(4)
C(34)-N(5)-C(33)-C(32)	-2.2(6)
C(31)-C(32)-C(33)-N(5)	0.9(7)
C(33)-N(5)-C(34)-C(35)	2.1(6)
C(33)-N(5)-C(34)-C(36)	-178.1(3)
C(32)-C(31)-C(35)-C(34)	-0.6(6)
C(15)-C(31)-C(35)-C(34)	176.5(4)
N(5)-C(34)-C(35)-C(31)	-0.8(6)
C(36)-C(34)-C(35)-C(31)	179.4(3)
C(40)-N(6)-C(36)-C(37)	0.1(6)
C(40)-N(6)-C(36)-C(34)	-178.1(4)
N(5)-C(34)-C(36)-N(6)	-172.2(4)
C(35)-C(34)-C(36)-N(6)	7.6(5)
N(5)-C(34)-C(36)-C(37)	9.6(6)
C(35)-C(34)-C(36)-C(37)	-170.6(4)
N(6)-C(36)-C(37)-C(38)	-1.6(6)
C(34)-C(36)-C(37)-C(38)	176.5(4)

C(36)-C(37)-C(38)-C(39)	2.0(7)
C(37)-C(38)-C(39)-C(40)	-0.9(8)
C(36)-N(6)-C(40)-C(39)	1.1(7)
C(38)-C(39)-C(40)-N(6)	-0.7(8)
N(1)-Zn(1)-O(1)-C(41B)	64.8(19)
N(3)-Zn(1)-O(1)-C(41B)	-115.7(19)
N(2)-Zn(1)-O(1)-C(41B)	155.3(19)
N(4)-Zn(1)-O(1)-C(41B)	-24.7(19)
N(1)-Zn(1)-O(1)-C(44B)	-128.0(17)
N(3)-Zn(1)-O(1)-C(44B)	51.4(17)
N(2)-Zn(1)-O(1)-C(44B)	-37.5(17)
N(4)-Zn(1)-O(1)-C(44B)	142.5(17)
N(1)-Zn(1)-O(1)-C(44A)	-102.2(8)
N(3)-Zn(1)-O(1)-C(44A)	77.3(8)
N(2)-Zn(1)-O(1)-C(44A)	-11.7(8)
N(4)-Zn(1)-O(1)-C(44A)	168.4(8)
N(1)-Zn(1)-O(1)-C(41A)	36.1(6)
N(3)-Zn(1)-O(1)-C(41A)	-144.5(6)
N(2)-Zn(1)-O(1)-C(41A)	126.6(6)
N(4)-Zn(1)-O(1)-C(41A)	-53.4(6)
C(41B)-O(1)-C(41A)-C(42A)	72(3)
C(44B)-O(1)-C(41A)-C(42A)	-13.0(19)
C(44A)-O(1)-C(41A)-C(42A)	-35.3(14)
Zn(1)-O(1)-C(41A)-C(42A)	-179.4(7)
O(1)-C(41A)-C(42A)-C(43A)	25.8(19)
C(41A)-C(42A)-C(43A)-C(44A)	-6.4(19)
C(41B)-O(1)-C(44A)-C(43A)	10(2)
C(44B)-O(1)-C(44A)-C(43A)	-72(6)
C(41A)-O(1)-C(44A)-C(43A)	35.0(10)
Zn(1)-O(1)-C(44A)-C(43A)	178.1(5)
C(42A)-C(43A)-C(44A)-O(1)	-17.0(13)
C(44B)-O(1)-C(41B)-C(42B)	44(4)
C(44A)-O(1)-C(41B)-C(42B)	21(4)
C(41A)-O(1)-C(41B)-C(42B)	-60(3)
Zn(1)-O(1)-C(41B)-C(42B)	-147(2)
O(1)-C(41B)-C(42B)-C(43B)	-56(3)
C(41B)-C(42B)-C(43B)-C(44B)	44(2)
C(41B)-O(1)-C(44B)-C(43B)	1(3)

C(44A)-O(1)-C(44B)-C(43B)	107(6)
C(41A)-O(1)-C(44B)-C(43B)	27(2)
Zn(1)-O(1)-C(44B)-C(43B)	-167.5(12)
C(42B)-C(43B)-C(44B)-O(1)	-35(2)

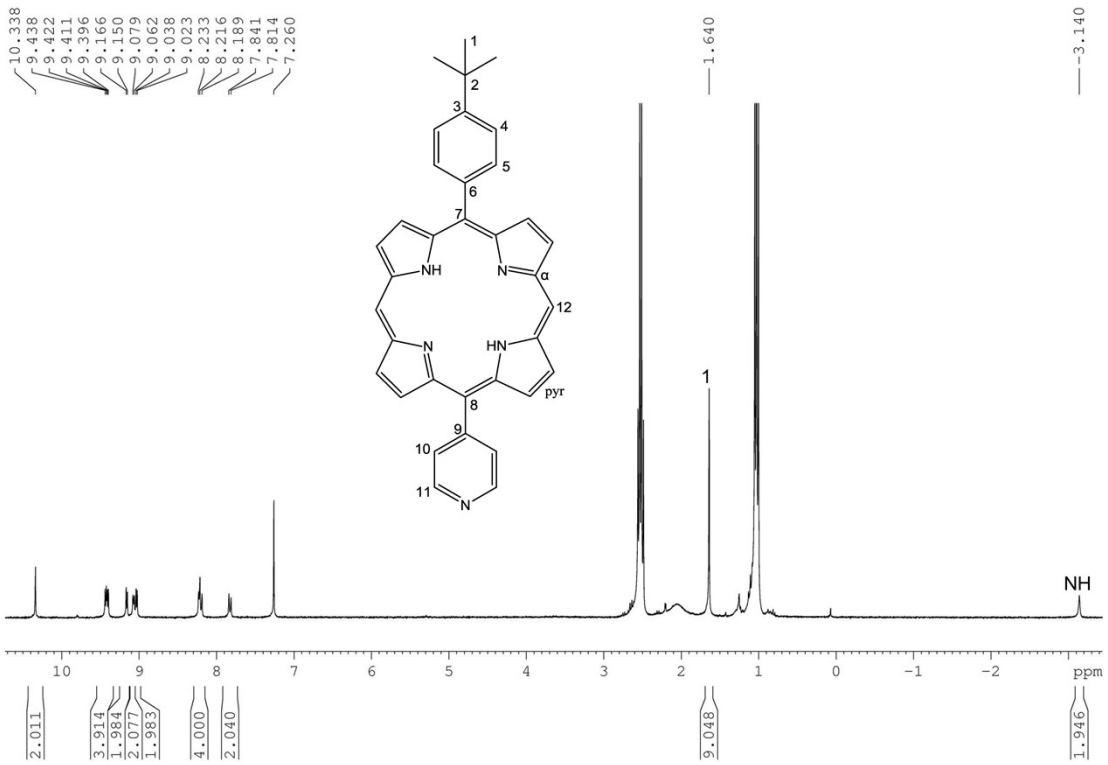

Figure S2. ^{1}H NMR spectrum of **1a** (300 MHz, $CDCl_3$ + 1% Et_3N).

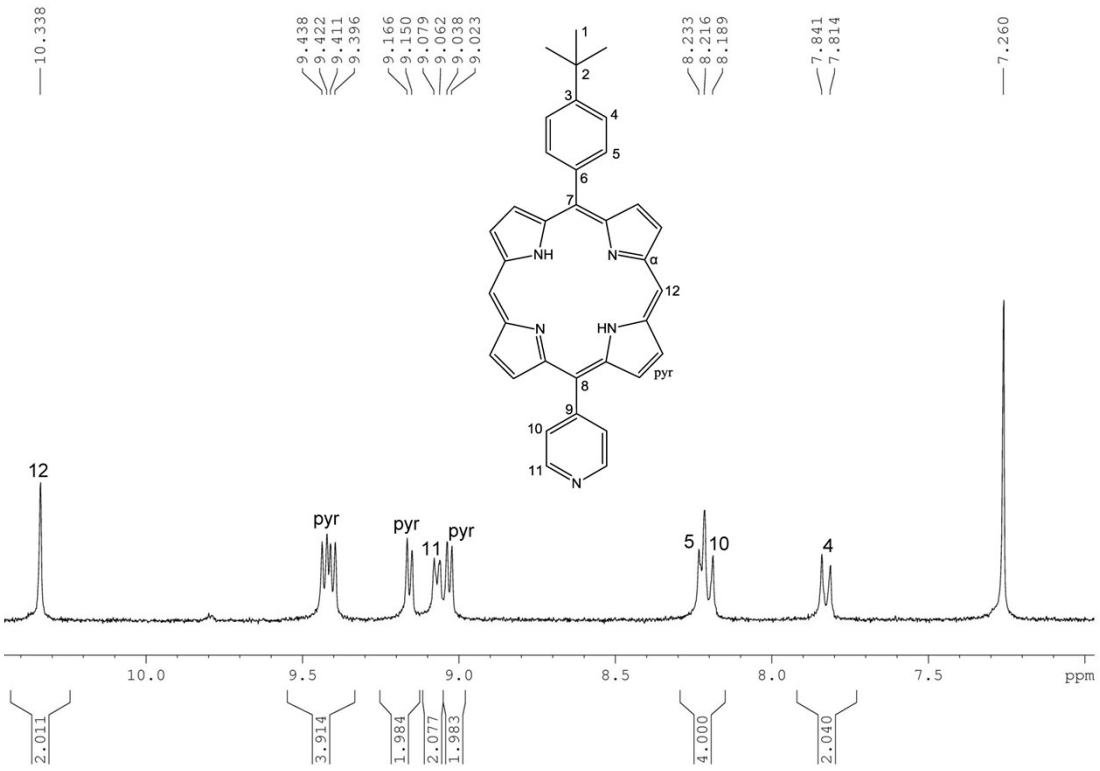

Figure S3. Aromatic region of the ^{1}H NMR spectrum of **1a** (300 MHz, $CDCl_3$ + 1% Et_3N).

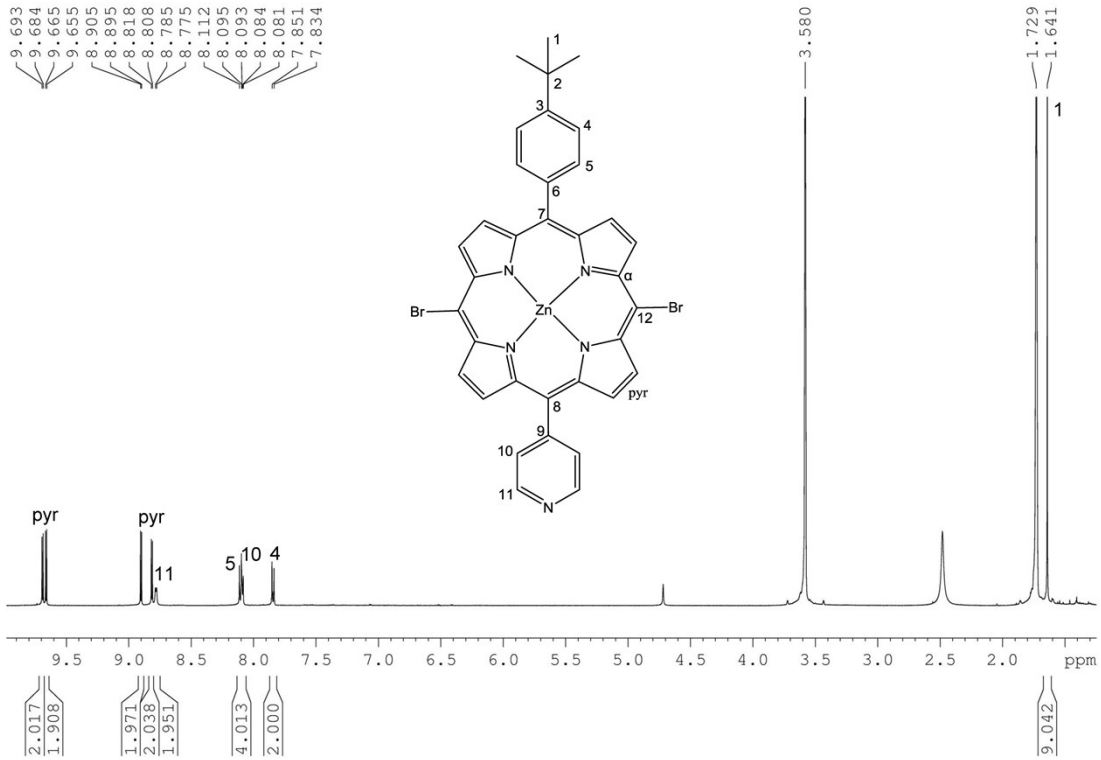

Figure S4. ^{1}H NMR spectrum of **3a** (500 MHz, THF-d_8).

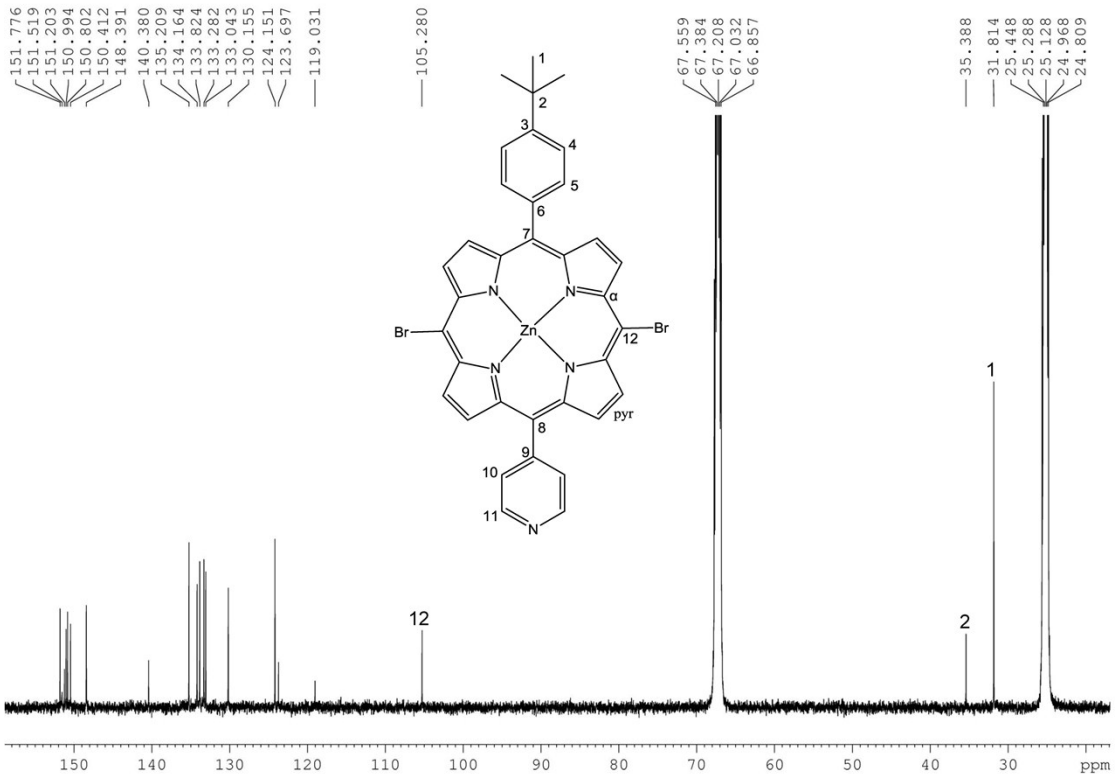

Figure S5. ^{13}C NMR spectrum of **3a** (125 MHz, THF-d_8).

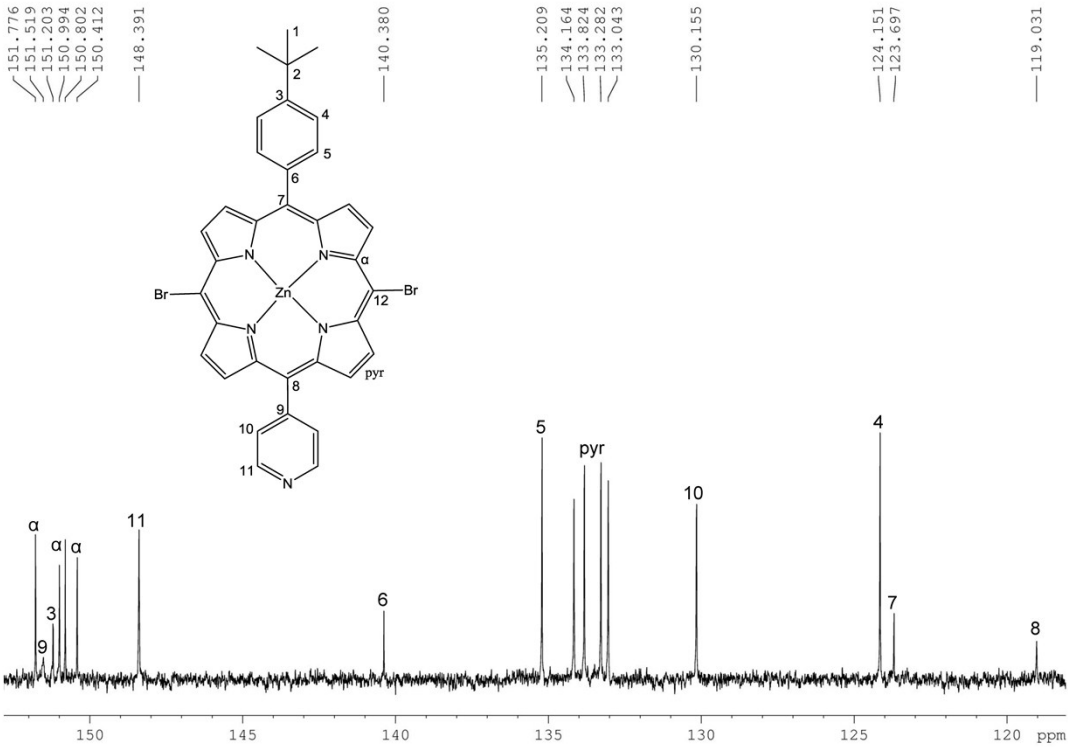

Figure S6. Aromatic region of the ^{13}C NMR spectrum of **3a** (125 MHz, THF-d_8).

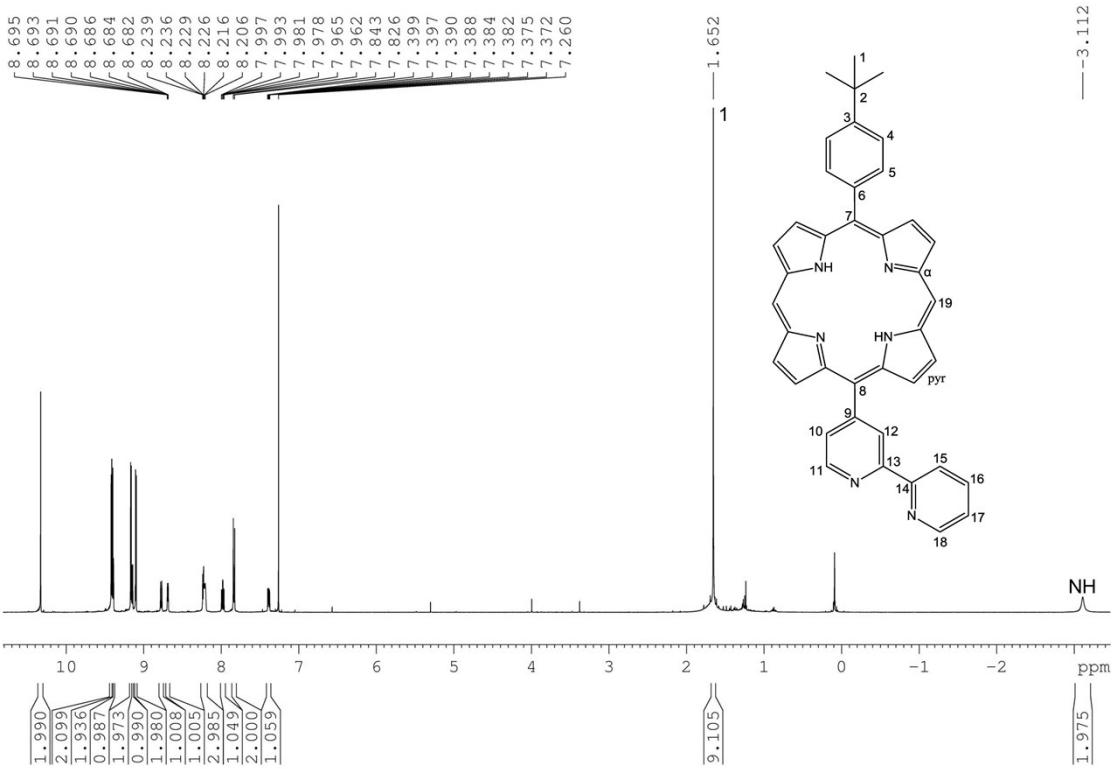

Figure S7. ^{1}H NMR spectrum of **1b** (500 MHz, $CDCl_3$).

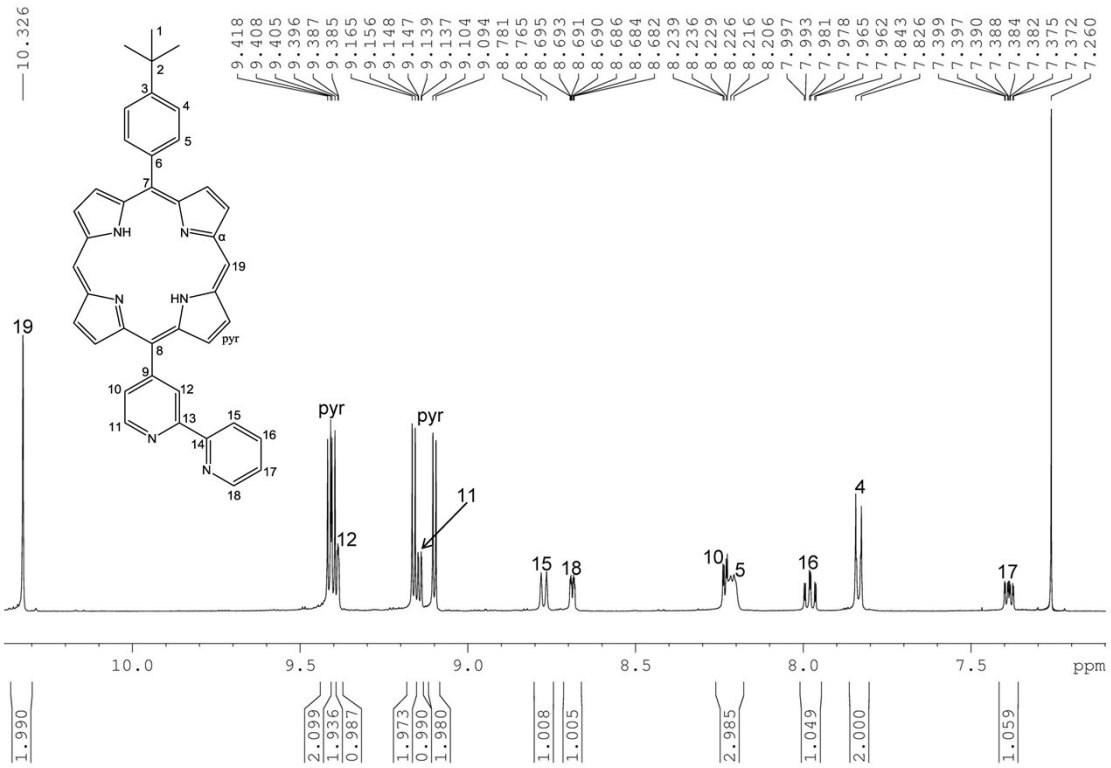

Figure S8. Aromatic region of the ^{1}H NMR spectrum of **1b** (500 MHz, $CDCl_3$).

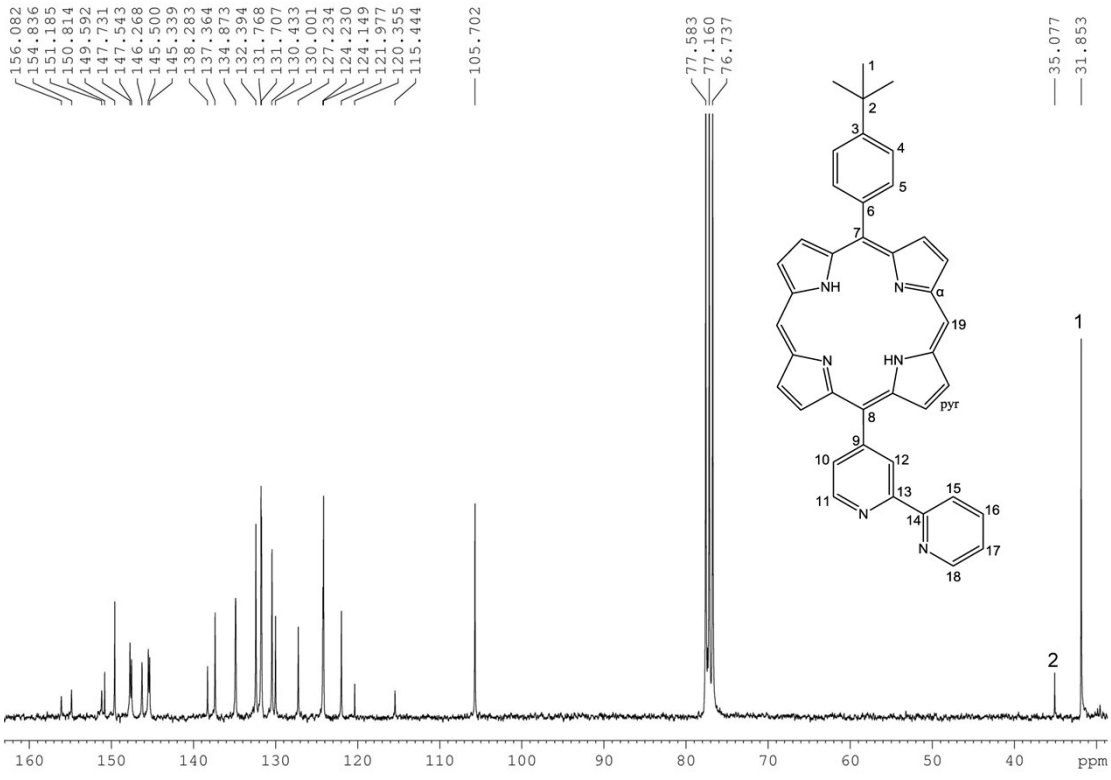

Figure S9. ^{13}C NMR spectrum of **1b** (75 MHz, $CDCl_3$).

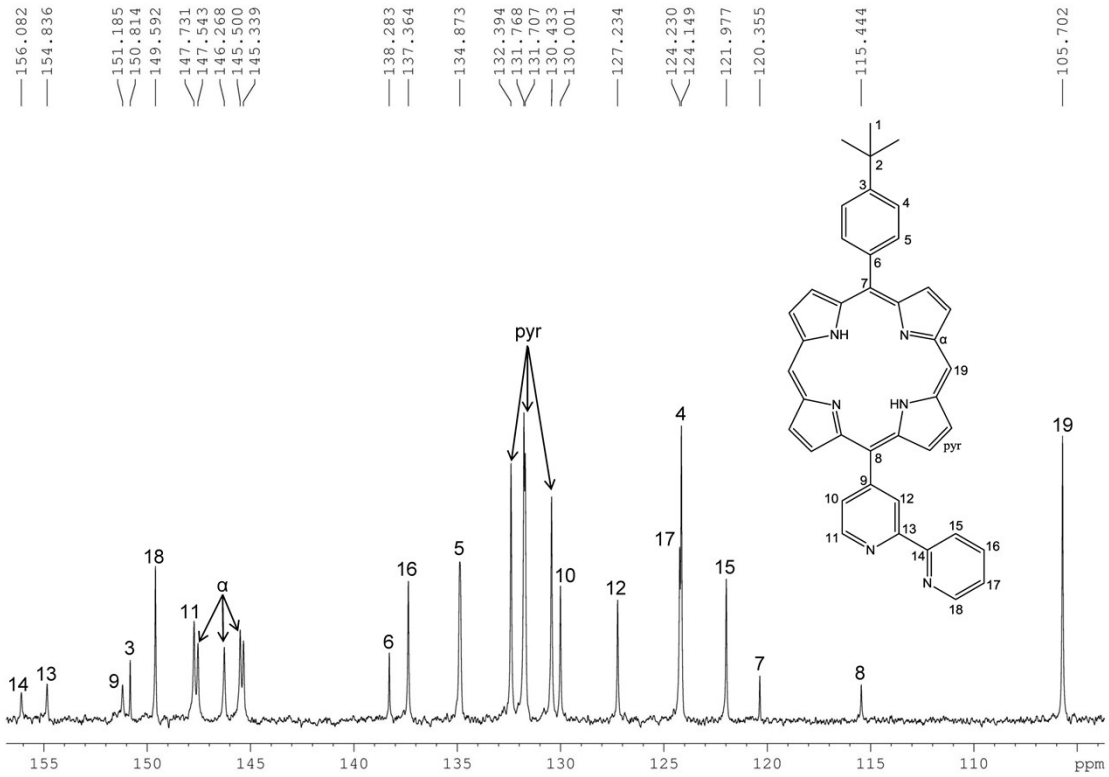

Figure S10. Aromatic region of the ^{13}C NMR spectrum of **1b** (75 MHz, $CDCl_3$).

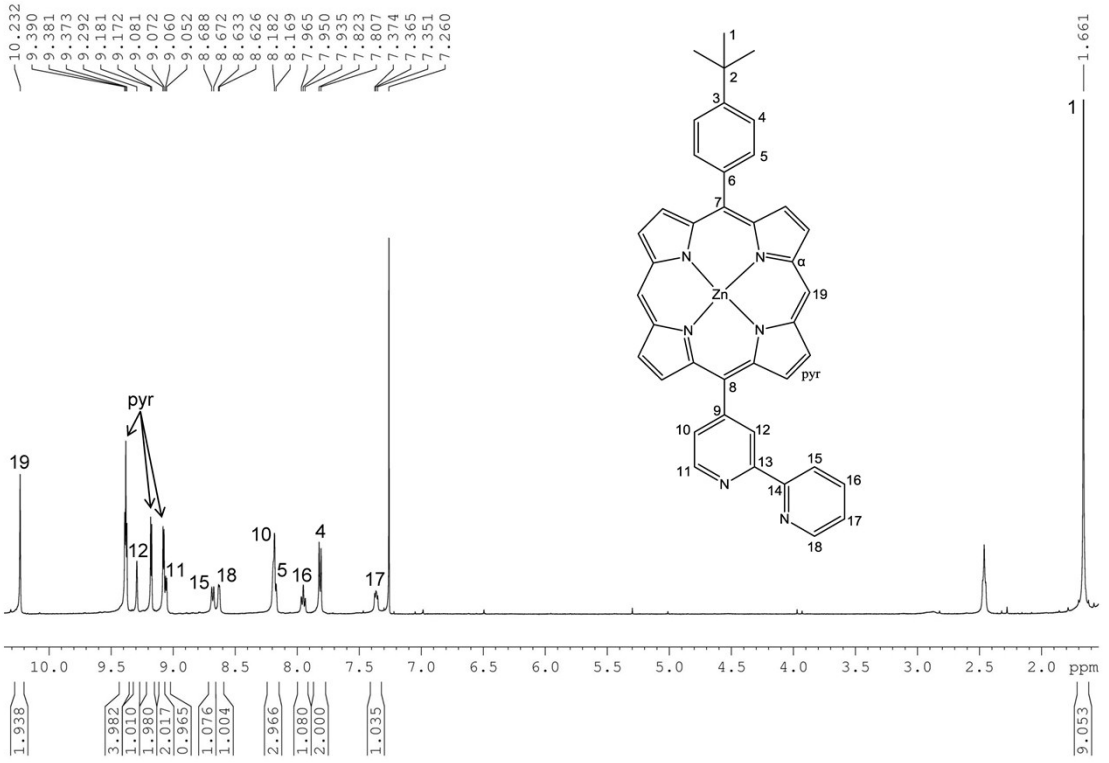

Figure S11. ^{1}H NMR spectrum of **2b** (500 MHz, $CDCl_3$).

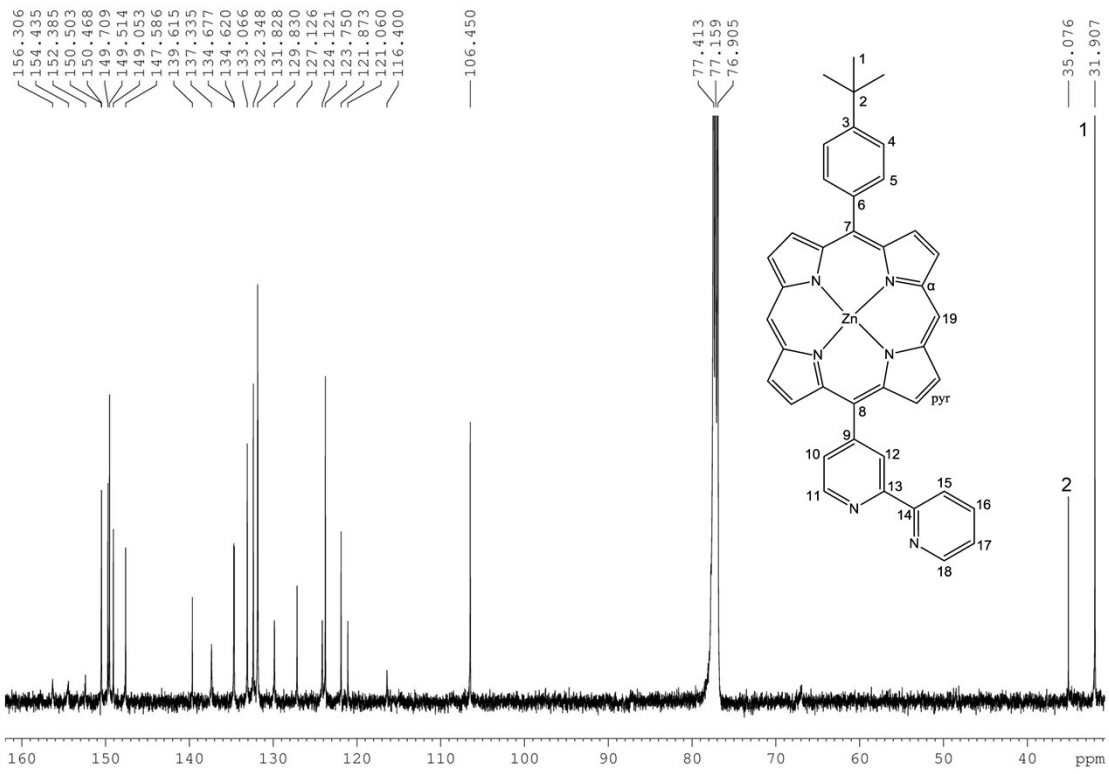

Figure S12. ^{13}C NMR spectrum of **2b** (125 MHz, $CDCl_3$).

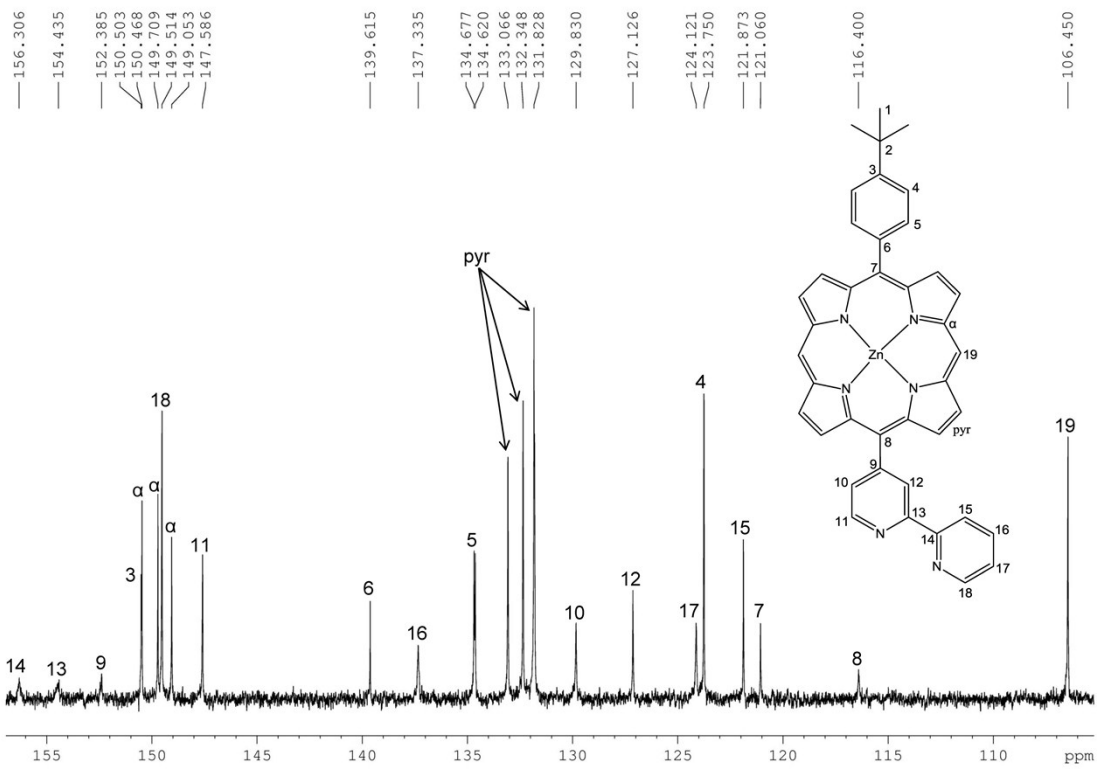

Figure S13. Aromatic region of the ^{13}C NMR spectrum of **2b** (125 MHz, $CDCl_3$).

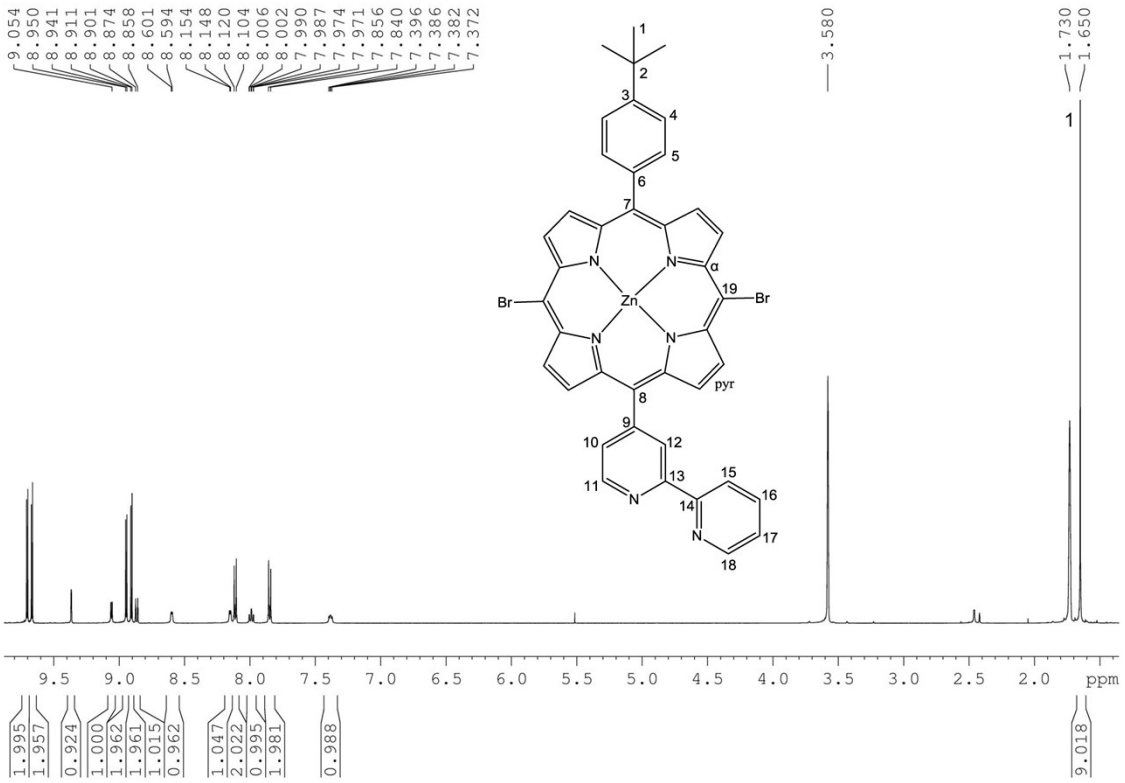

Figure S14. ^{1}H NMR spectrum of **3b** (500 MHz, THF-d_8).

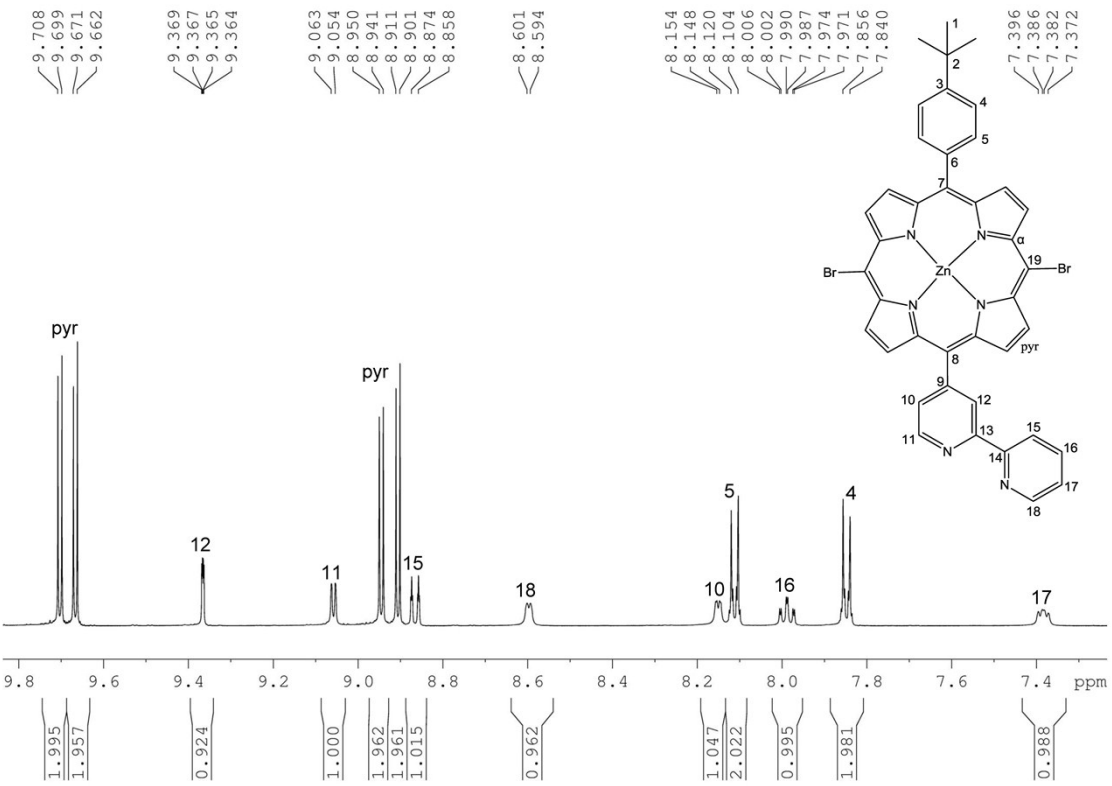

Figure S15. Aromatic region of the ^{1}H NMR spectrum of **3b** (500 MHz, THF-d_8).

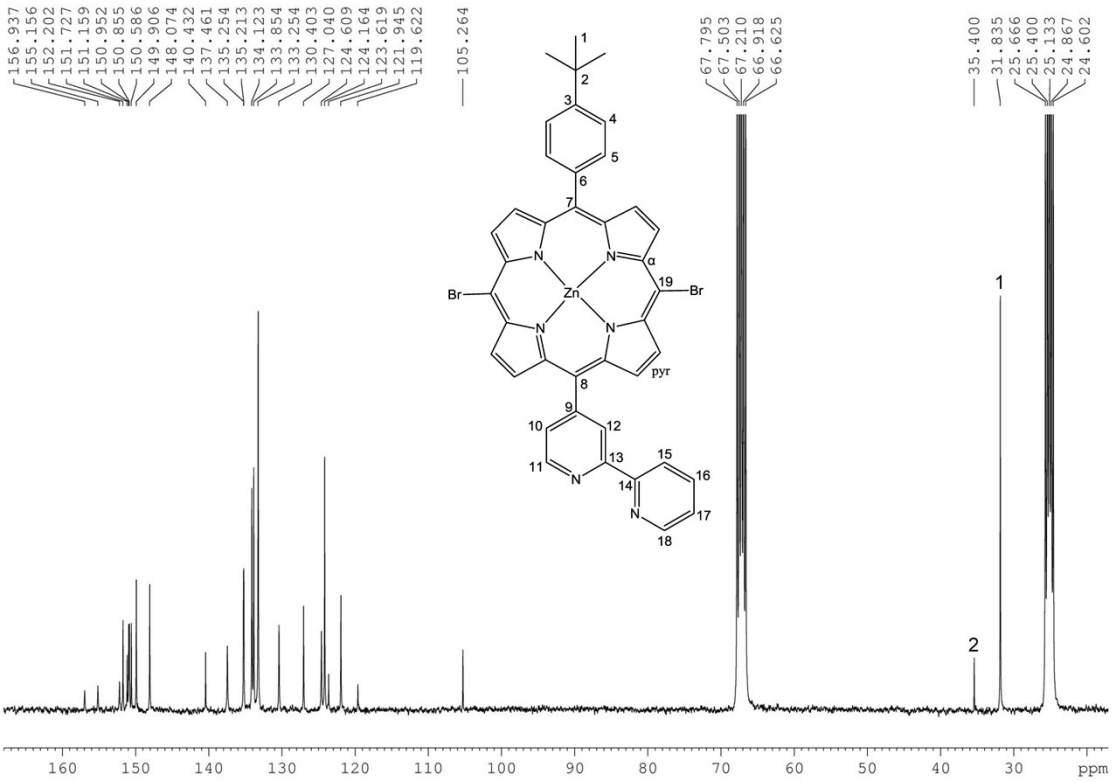

Figure S16. ^{13}C NMR spectrum of **3b** (75 MHz, THF-d_8).

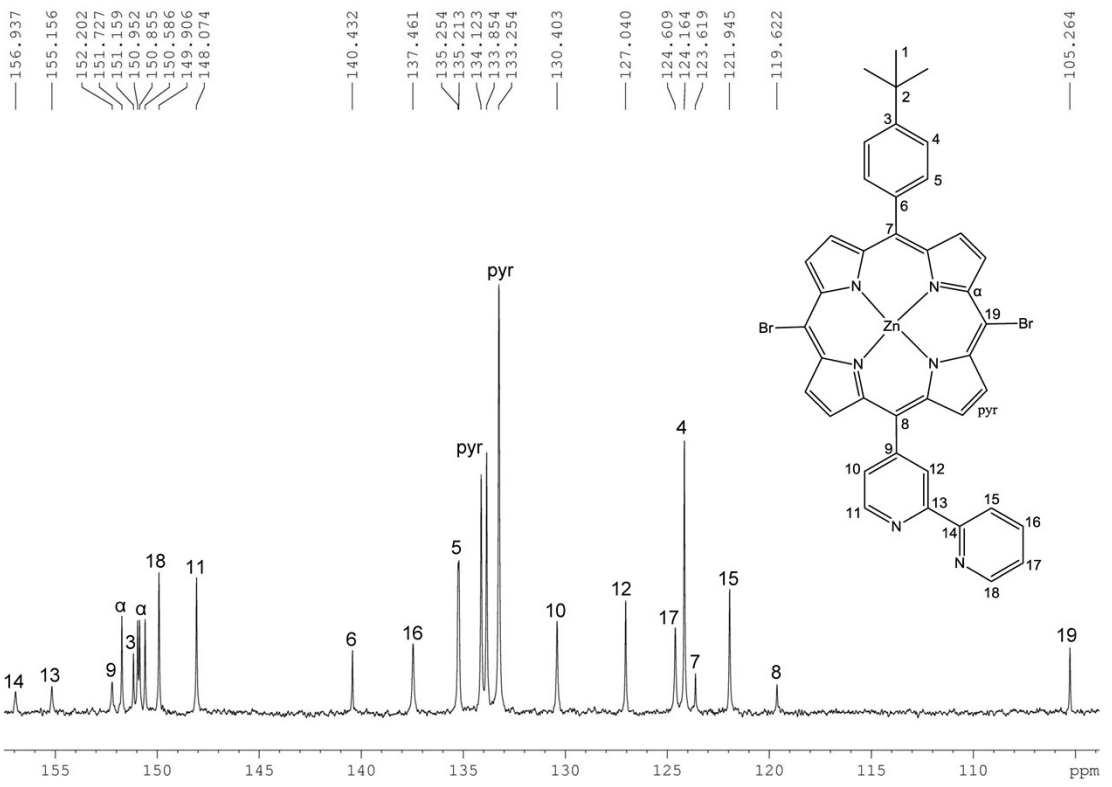

Figure S17. Aromatic region of the ^{13}C NMR spectrum of **3b** (75 MHz, THF-d_8).

Table S7. Cartesian coordinates of geometry optimized structure of **3a** in THF at the B3LYP/LANL2DG/6-31G* level with energy. E = -6830.9978981 Hartree/particle.

C	1.716452000	-3.600442000	2.453999000
C	0.805060000	-3.999410000	3.501758000
C	1.132975000	-3.279127000	4.609545000
C	2.254599000	-2.435049000	4.255862000
N	2.582563000	-2.645849000	2.937910000
C	1.743203000	-4.089659000	1.137492000
C	2.888776000	-1.525706000	5.128587000
C	3.951105000	-0.660392000	4.791620000
C	4.619956000	0.230763000	5.715833000
C	5.587234000	0.885372000	5.016338000
C	5.528299000	0.398184000	3.657471000
N	4.528871000	-0.542619000	3.550058000
C	6.346997000	0.799998000	2.589033000
C	6.348445000	0.336214000	1.261563000
C	7.183601000	0.815443000	0.184774000
C	6.850196000	0.099826000	-0.924727000
C	5.814292000	-0.833854000	-0.538679000
N	5.524721000	-0.662269000	0.795050000
C	5.196171000	-1.756452000	-1.410511000
C	4.150778000	-2.638959000	-1.061298000
C	3.567613000	-3.619727000	-1.951210000
C	2.600205000	-4.275249000	-1.252199000
C	2.585168000	-3.710375000	0.077115000
N	3.538736000	-2.722601000	0.167652000
C	5.688359000	-1.802582000	-2.824236000
Br	7.637642000	2.170695000	2.995434000
C	2.390059000	-1.474364000	6.539821000
C	6.979795000	-2.250301000	-3.129436000

C	7.434976000	-2.294112000	-4.449522000
C	6.623882000	-1.891525000	-5.519670000
C	5.329458000	-1.442164000	-5.203510000
C	4.868595000	-1.398277000	-3.890327000
C	2.570166000	-2.551259000	7.419300000
C	2.088590000	-2.452330000	8.724904000
C	1.280383000	-0.349227000	8.363155000
C	1.723813000	-0.346921000	7.040373000
C	7.091469000	-1.925294000	-6.985749000
C	7.030298000	-0.496786000	-7.578180000
C	8.535377000	-2.442930000	-7.128616000
C	6.161767000	-2.856950000	-7.799891000
Zn	4.044348000	-1.643716000	1.862180000
N	1.451294000	-1.376272000	9.207322000
Br	0.456574000	-5.463959000	0.730672000
H	0.014219000	-4.727348000	3.400458000
H	0.651274000	-3.313411000	5.575864000
H	4.387804000	0.338803000	6.765312000
H	6.281657000	1.624299000	5.386614000
H	7.919323000	1.601393000	0.265492000
H	7.263720000	0.199538000	-1.917361000
H	3.865330000	-3.790201000	-2.975253000
H	1.962173000	-5.073555000	-1.599957000
H	7.635889000	-2.577715000	-2.327121000
H	8.441315000	-2.654739000	-4.631444000
H	4.661815000	-1.114547000	-5.995600000
H	3.863802000	-1.038406000	-3.685087000
H	3.085422000	-3.450078000	7.093692000
H	2.226162000	-3.280528000	9.418686000
H	0.758388000	0.519280000	8.762385000

H	1.547128000	0.516971000	6.406446000
H	7.353179000	-0.506505000	-8.626286000
H	7.687905000	0.184986000	-7.026557000
H	6.016345000	-0.084131000	-7.546106000
H	8.821524000	-2.446029000	-8.186357000
H	8.641480000	-3.468152000	-6.755524000
H	9.251679000	-1.808039000	-6.594594000
H	5.120541000	-2.518515000	-7.774050000
H	6.192172000	-3.880424000	-7.408505000
H	6.477614000	-2.884973000	-8.849878000

Table S7. Cartesian coordinates of geometry optimized structure of **3b** in THF at the B3LYP/LANL2DG/6-31G* level with energy. E=-7078.0874628 Hartree/particle.

C	2.359163000	-6.357856000	1.836643000
C	1.333895000	-7.136770000	2.492400000
C	1.694308000	-8.444663000	2.378505000
C	2.942329000	-8.483379000	1.645745000
N	3.325782000	-7.200520000	1.335481000
C	2.394410000	-4.959259000	1.709902000
C	3.656491000	-9.657510000	1.326876000
C	4.898337000	-9.715280000	0.659892000
C	5.593808000	-10.934461000	0.305750000
C	6.741823000	-10.573522000	-0.330892000
C	6.759877000	-9.129588000	-0.382135000
N	5.627321000	-8.634581000	0.224350000
C	7.759003000	-8.325694000	-0.955642000
C	7.806882000	-6.924013000	-1.057972000
C	8.879611000	-6.139329000	-1.624435000
C	8.515849000	-4.831776000	-1.513871000
C	7.211983000	-4.799892000	-0.887351000

N	6.809179000	-6.086569000	-0.614902000
C	6.489324000	-3.623459000	-0.593095000
C	5.240434000	-3.572119000	0.063329000
C	4.488520000	-2.361070000	0.311899000
C	3.345617000	-2.720387000	0.959110000
C	3.378639000	-4.157215000	1.105451000
N	4.537195000	-4.649388000	0.550028000
C	7.097108000	-2.320202000	-1.012353000
Br	9.262999000	-9.268526000	-1.702409000
C	3.039944000	-10.961433000	1.731335000
C	7.547077000	-1.390627000	-0.061091000
C	8.107931000	-0.178648000	-0.455467000
C	8.244245000	0.168088000	-1.811494000
C	7.792950000	-0.766223000	-2.754120000
C	7.232839000	-1.985601000	-2.365424000
C	3.604811000	-11.760696000	2.732944000
C	2.972244000	-12.957651000	3.072563000
C	1.305132000	-12.647343000	1.528464000
C	1.866369000	-11.426425000	1.125275000
C	8.864998000	1.521179000	-2.202810000
C	8.020924000	2.668419000	-1.597472000
C	8.920674000	1.720202000	-3.729373000
C	10.309024000	1.602783000	-1.652037000
Zn	5.076425000	-6.641944000	0.375988000
N	1.851463000	-13.403708000	2.498116000
Br	0.893945000	-4.014471000	2.461162000
C	0.056019000	-13.159240000	0.887160000
N	-0.793417000	-13.848120000	1.671436000
C	-1.919353000	-14.310359000	1.119337000
C	-2.265190000	-14.124496000	-0.221355000

C	-1.380023000	-13.417489000	-1.032916000
C	-0.201797000	-12.927195000	-0.472959000
H	0.458359000	-6.736024000	2.980778000
H	1.163958000	-9.302876000	2.764869000
H	5.249074000	-11.937721000	0.509892000
H	7.502973000	-11.224220000	-0.734429000
H	9.793104000	-6.535779000	-2.041657000
H	9.082138000	-3.965491000	-1.822484000
H	4.792106000	-1.365943000	0.022155000
H	2.549079000	-2.074668000	1.296997000
H	7.462878000	-1.625089000	0.996846000
H	8.448105000	0.507227000	0.315515000
H	7.867951000	-0.553020000	-3.814694000
H	6.887487000	-2.681602000	-3.125478000
H	4.510606000	-11.452199000	3.246011000
H	3.393761000	-13.590851000	3.852362000
H	1.387972000	-10.829647000	0.355420000
H	7.972291000	2.607592000	-0.505121000
H	8.458392000	3.639827000	-1.858265000
H	6.994398000	2.644222000	-1.981309000
H	9.367127000	2.694719000	-3.956993000
H	7.921826000	1.701324000	-4.180358000
H	9.532776000	0.954324000	-4.219420000
H	10.762154000	2.565624000	-1.917531000
H	10.335542000	1.511222000	-0.561004000
H	10.934122000	0.805837000	-2.071147000
H	-2.585263000	-14.858367000	1.785088000
H	-3.195808000	-14.526197000	-0.610983000
H	-1.596211000	-13.256052000	-2.085528000
H	0.516814000	-12.393673000	-1.087125000