Journal Name

ARTICLE

Supporting Information

Meso-aryl substituted free-base tripyrrins: preparation and electrochemically induced protonation/deprotonation reactions. Single crystal X-ray analysis of (2,6-diFPh)$_2$TriPyH

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Table S1. Selected crystallographic data of (2,6-diFPh)$_2$TriPyH **1**.

chemical formula	$C_{34}H_{21}F_4N_5$
formula weight	575.56
T, K	153(2)
cryst. system	monoclinic
space group	*P*2(1)/*n*
a, Å	11.144(2)
b, Å	13.300(3)
c, Å	19.616(4)
α, deg	90.00
β, deg	106.05(3)
γ, deg	90.00
V, Å3	2794.1(11)
Z	4
λ, Å	0.71073
d_{calcd}, g.cm^{-3}	1.368
μ(mm^{-1})	0.101
F(000)	1184
reflections collected	12880
unique reflections	5520
GOF (F^2)	1.021
R_1^a,wR_2^b (I>2σ(I))	0.0448, 0.0949
R_1^a,wR_2^b (all data)	0.0544, 0.1013

$R_1^a = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2^b = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)]^{1/2}$

Table S2. Selected bond lengths (Å) and angles (^{o}) of (2,6-diFPh)$_2$TriPyH **1**.

bond lengths (Å)		angles (^{o})	
N1-H1B	0.91(4)	C4-N1-C1	107.4(8)
N3-H3A	0.90(2)	C5-N2-C8	105.2(1)
N5-H5A	0.86(2)	C10-N3-C13	110.2(1)
C4-C5	1.433(3)	C15-N4-C18	105.3(1)
C8-C9	1.374(3)	C19-N5-C22	109.6(2)
C9-C10	1.431(2)	C3-C4-C5	115.9(5)
C9-C23	1.490(3)	C4-C5-C6	124.6(2)
C13-C14	1.430(2)	C7-C8-C9	125.8(2)
C14-C15	1.374(3)	C8-C9-C23	118.7(2)
C14-C29	1.488(3)	C10-C9-C23	116.3(1)
C18-C19	1.426(3)	C9-C10-C11	129.6(2)
F1-C24	1.357(2)	C12-C13-C14	130.1(2)
F2-C28	1.354(3)	C13-C14-C29	117.6(1)
F3-C30	1.364(2)	C14-C15-C16	125.3(2)
F4-C34	1.359(2)	C17-C18-C19	124.4(2)
--	--	C18-C19-C10	131.7(2)

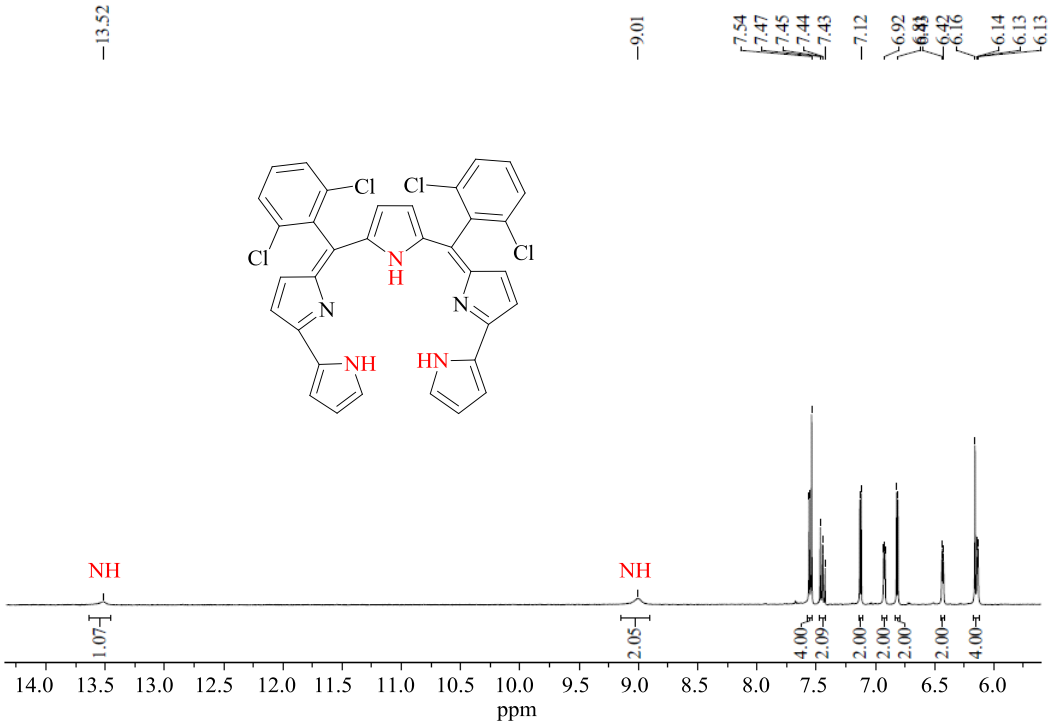

Fig S1. ^{1}H NMR spectra of (2,6-diClPh)$_2$TriPyH **2** in CD_2Cl_2 at 298 K.

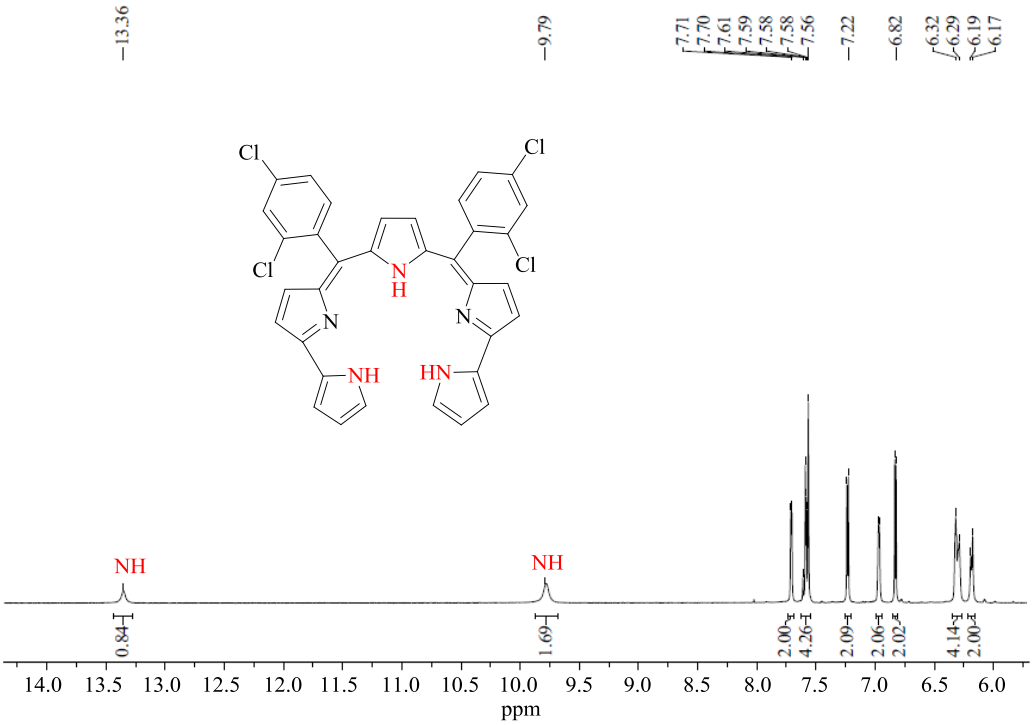

Fig S2. ^{1}H NMR spectra of (2,4-diClPh)$_2$ TriPyH **3** in CD_3COCD_3 at 298 K.

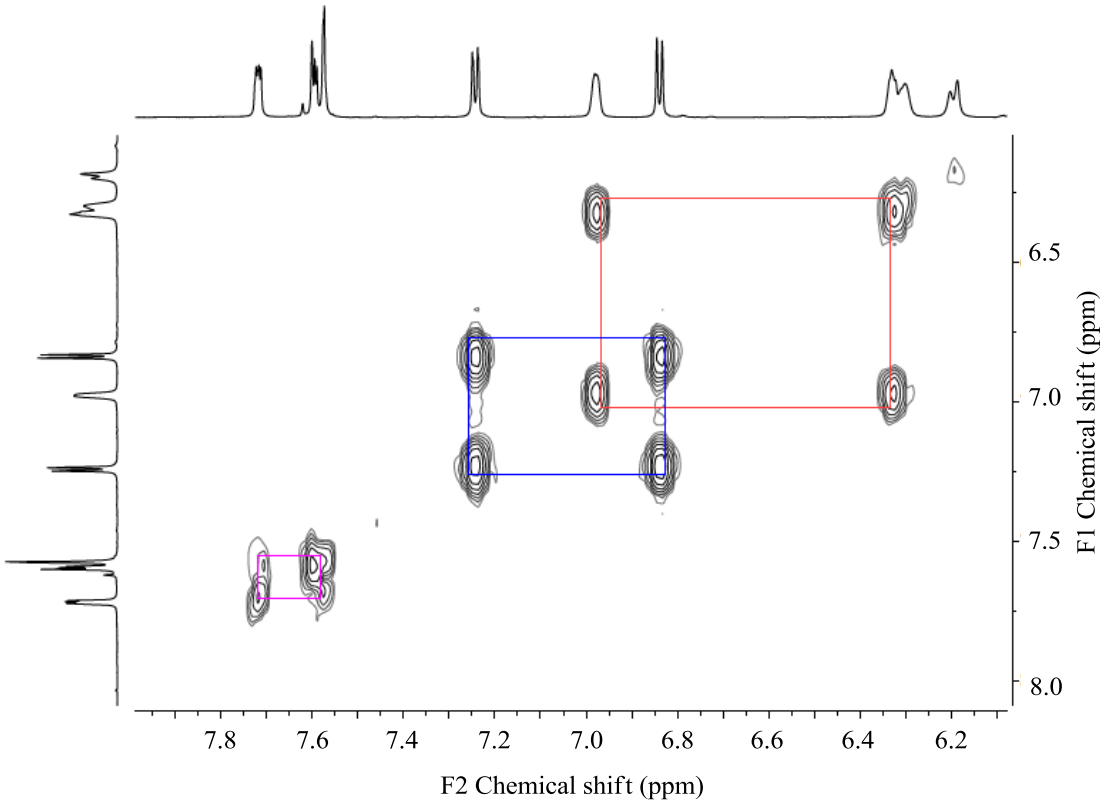

Figure S3. H-H COSY NMR spectrum of (2,4-diClPh)$_2$TriPyH **3** in CD_3COCD_3.

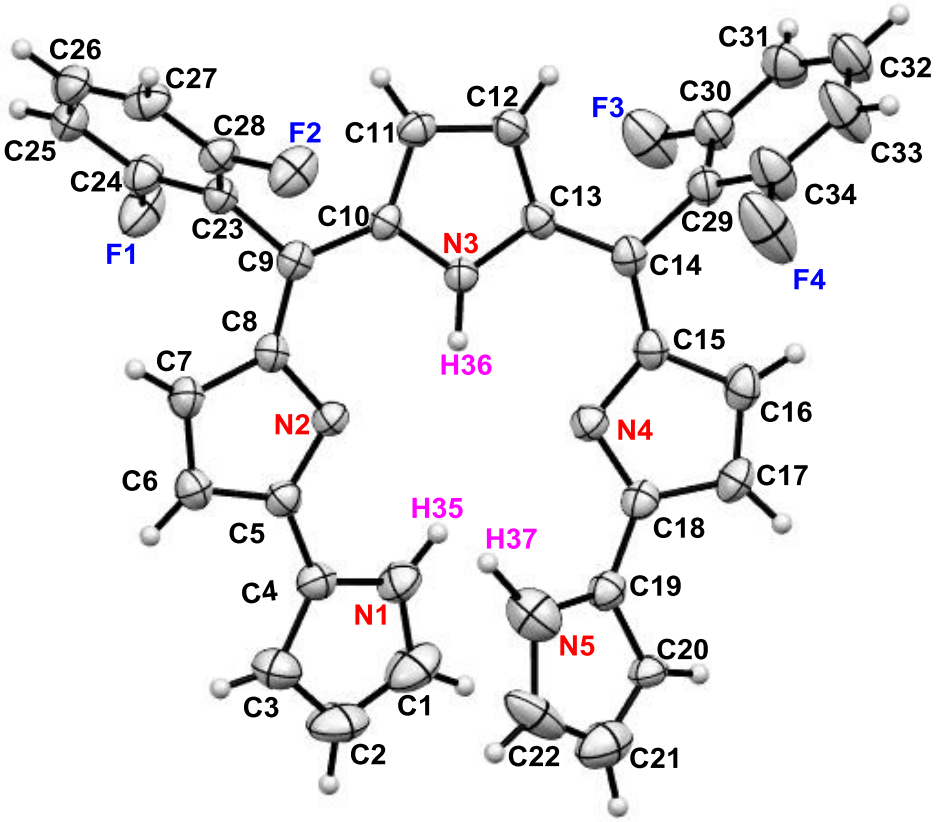

Figure S4. The crystal structures of (2,6-diFPh)$_2$TriPyH **1** with thermal ellipsoids set at 50 % probability.

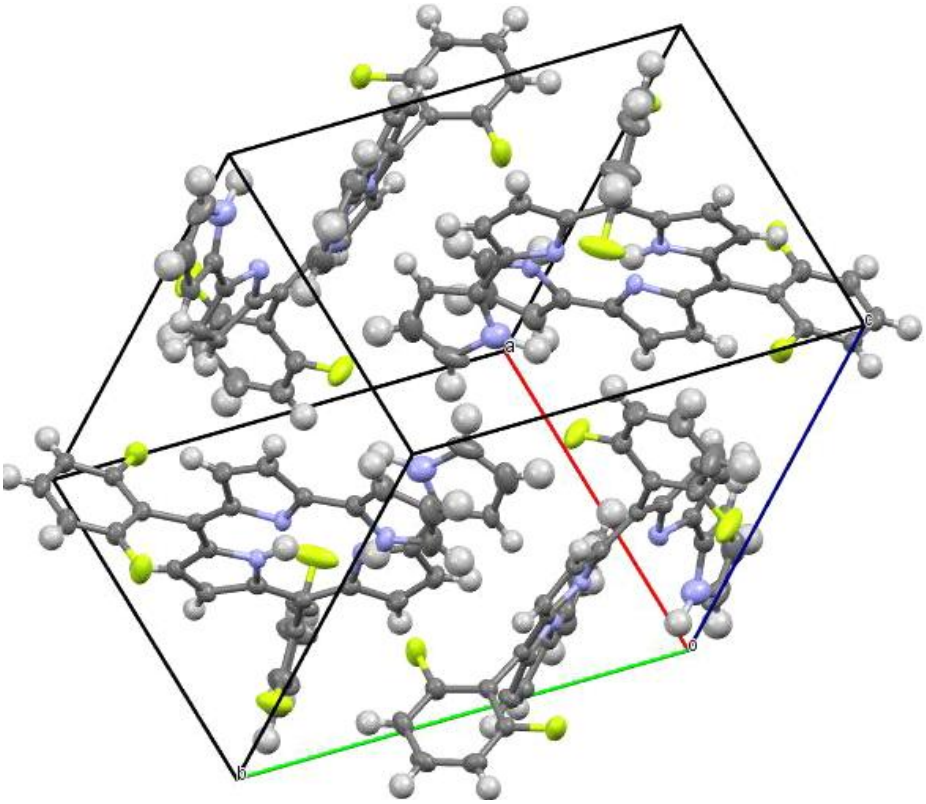

Figure S5. Packing diagram of (2,6-diFPh)$_2$TriPyH **1**. The solvent molecules and protons are omitted for clarity.

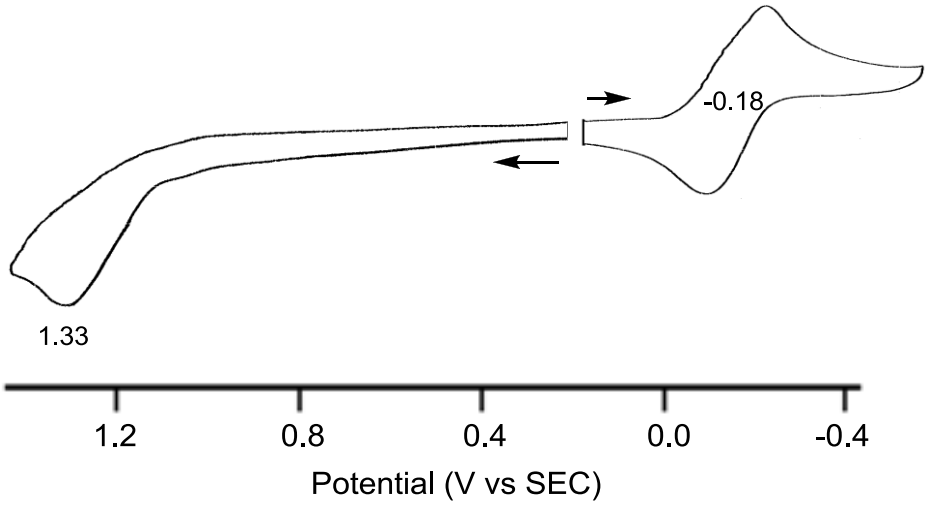

Figure S6. Cyclic voltammograms of **3** obtained in CH_2Cl_2 containing 0.1 M TBAP after addition of 2. 0 eq TFA. Scan rate = 0.10 V/s.