

Electronic Supplementary Information for

An investigation of the role furan versus thiophene π -bridges play in porphyrin based DSSCs

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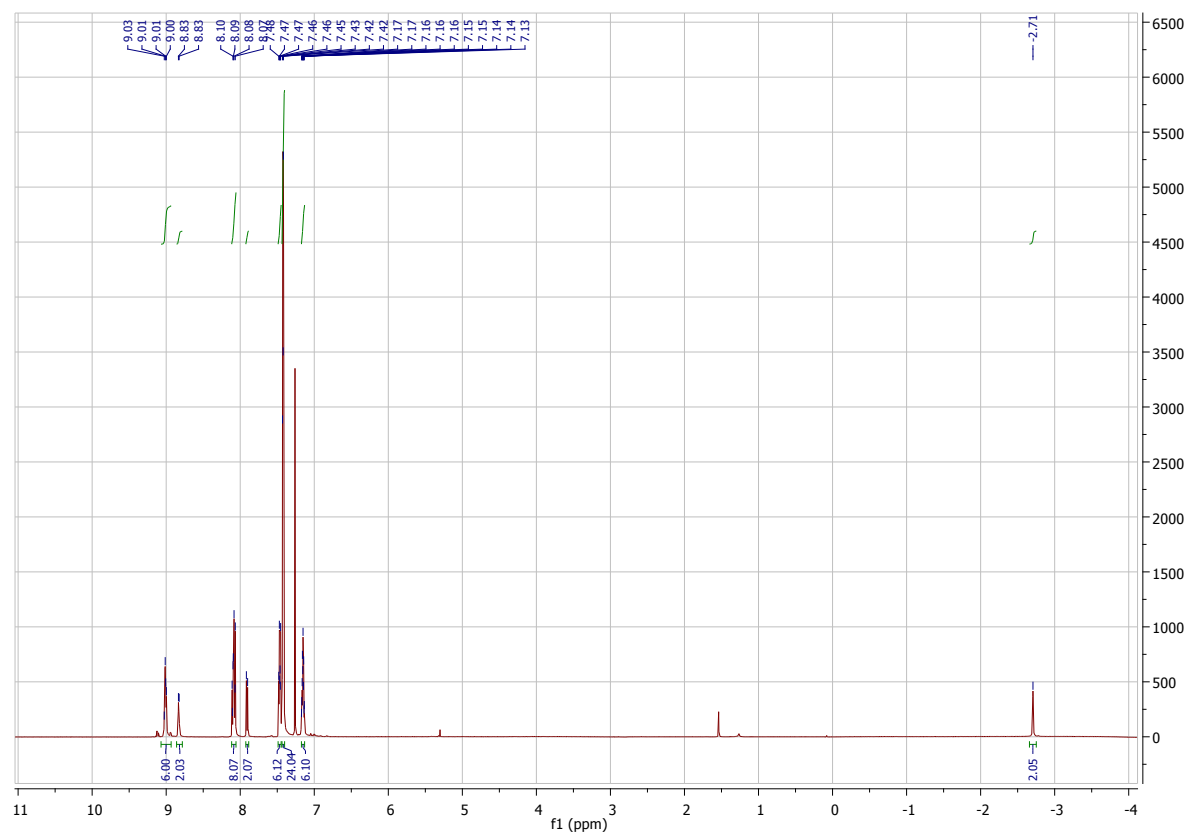
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1. NMR spectra

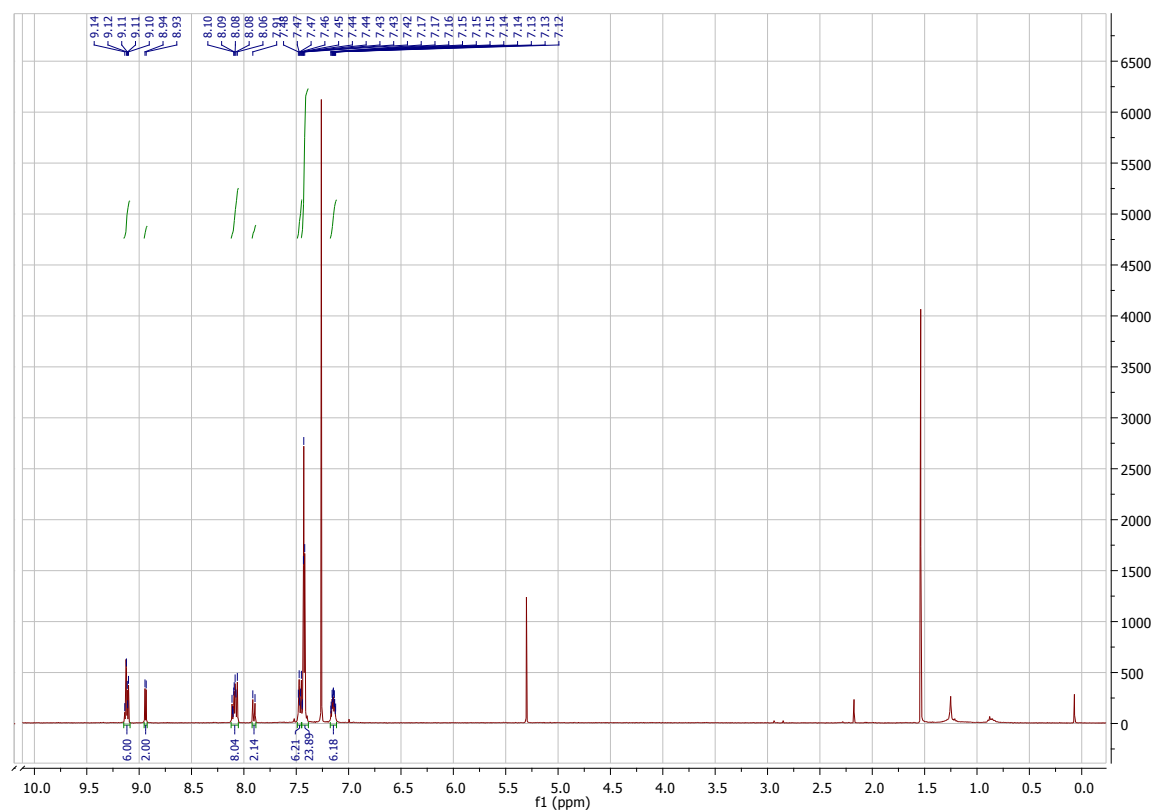
Compound 3

^1H (500 MHz, CDCl_3 , TMS)

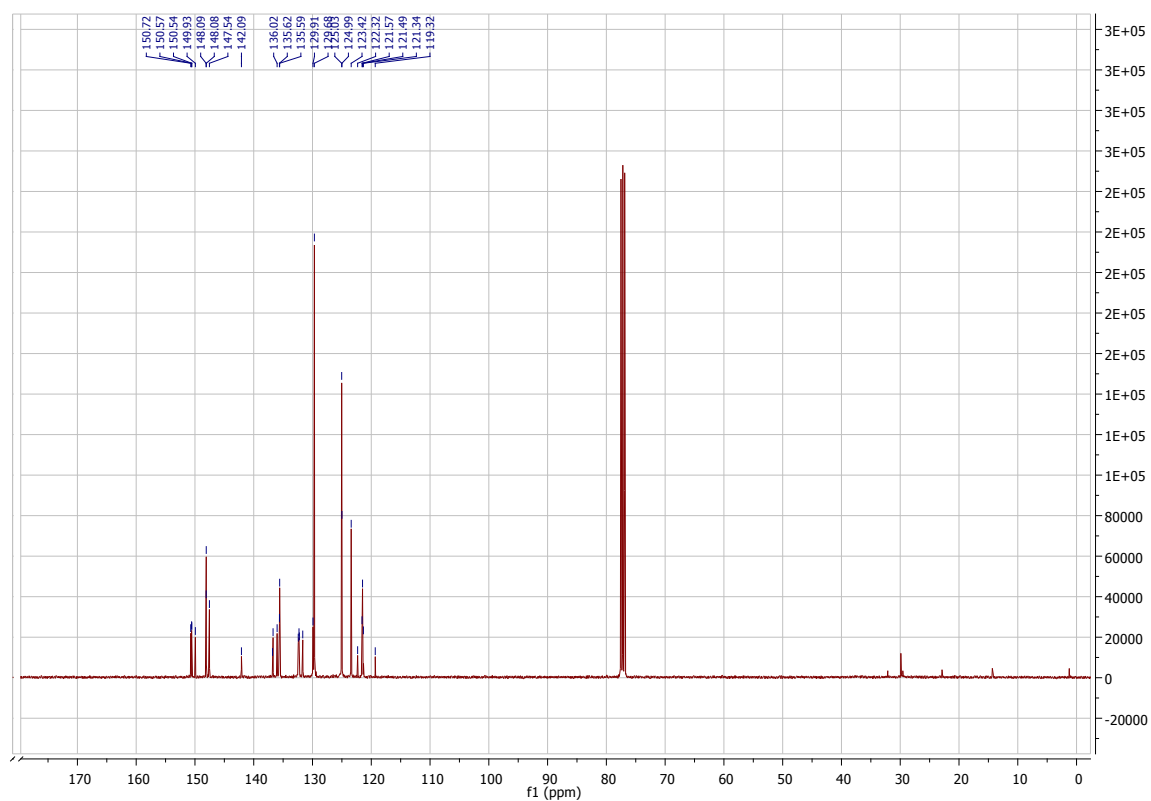


Compound 4

^1H (400 MHz, CDCl_3 , TMS)

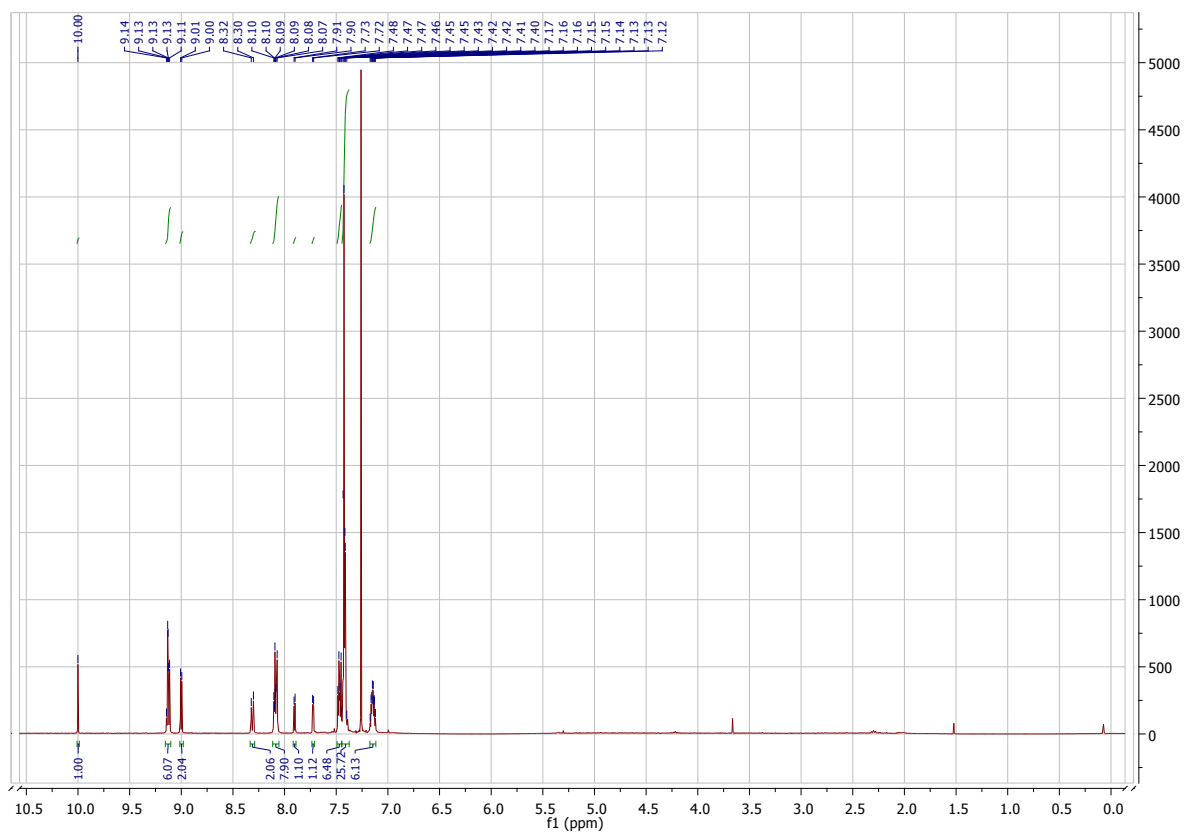


^{13}C (100 MHz, CDCl_3 , TMS)

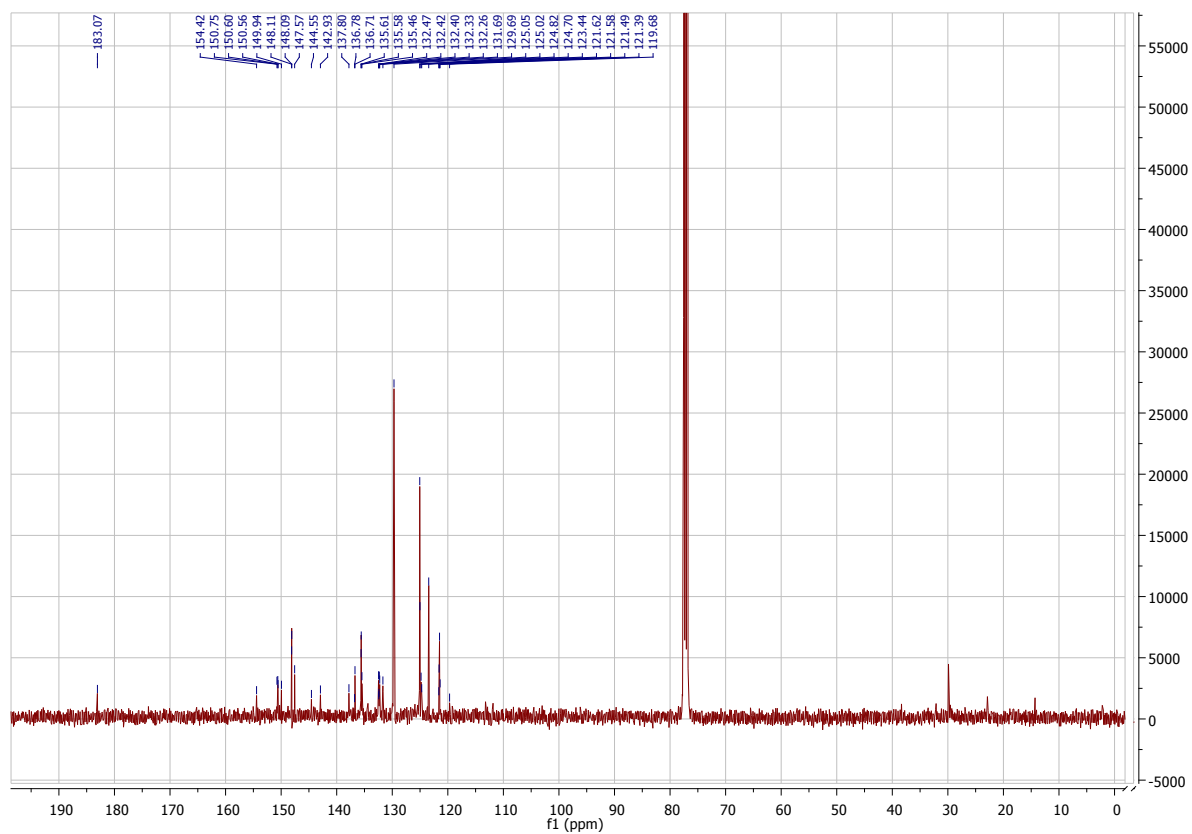


Compound 6a

^1H (400 MHz, CDCl_3 , TMS)

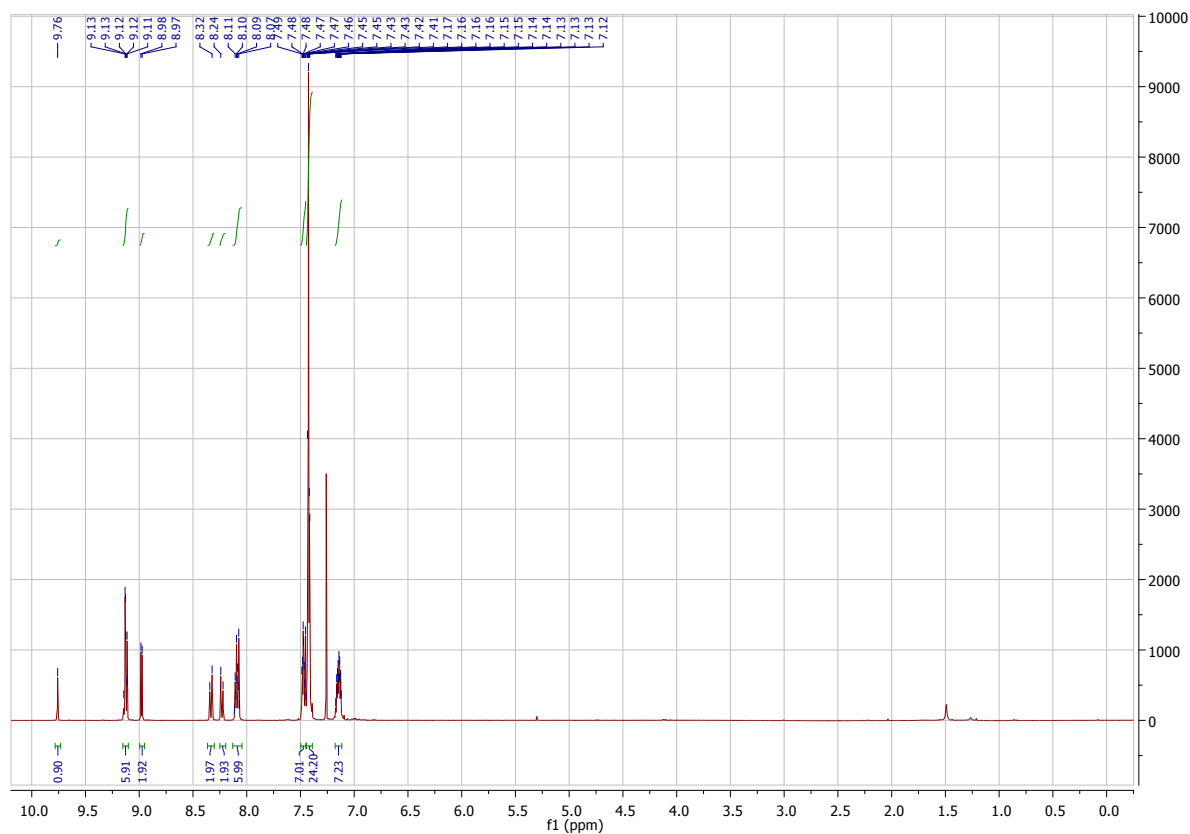


^{13}C (100 MHz, CDCl_3 , TMS)

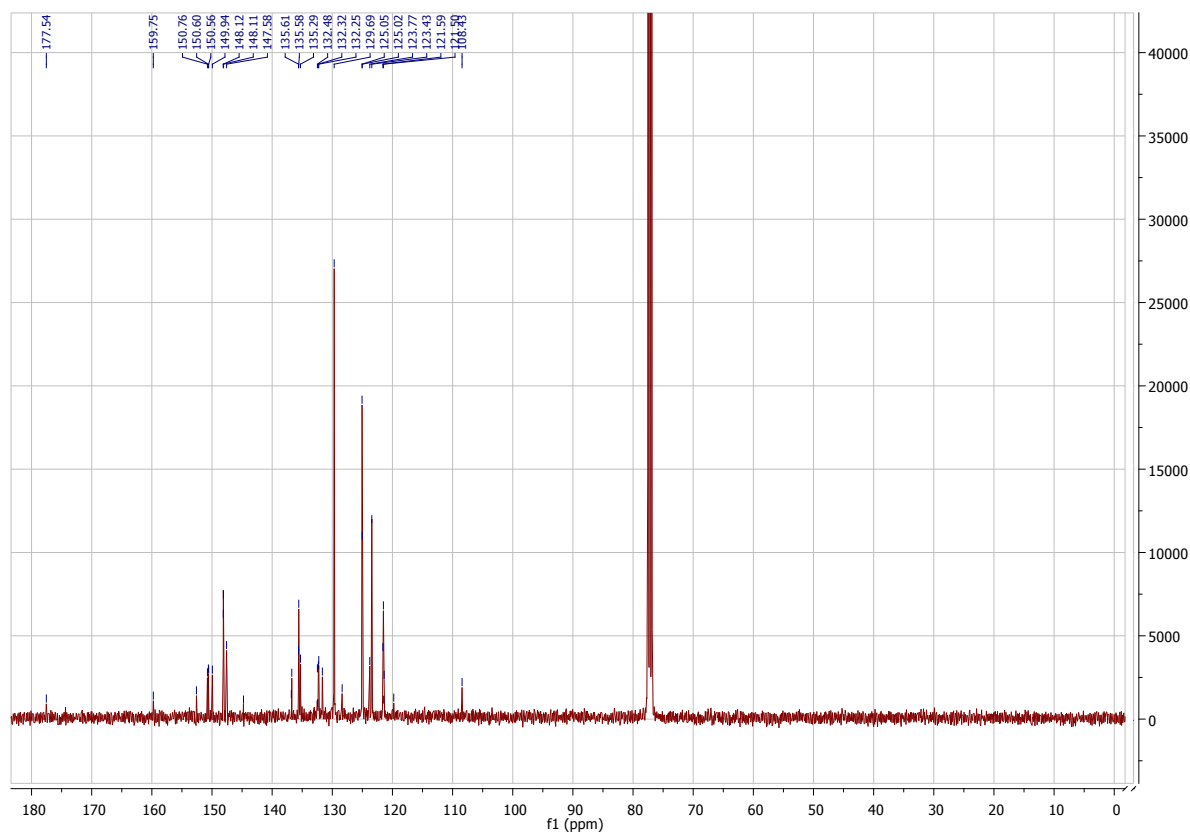


Compound 6b

^1H (400 MHz, CDCl_3 , TMS)

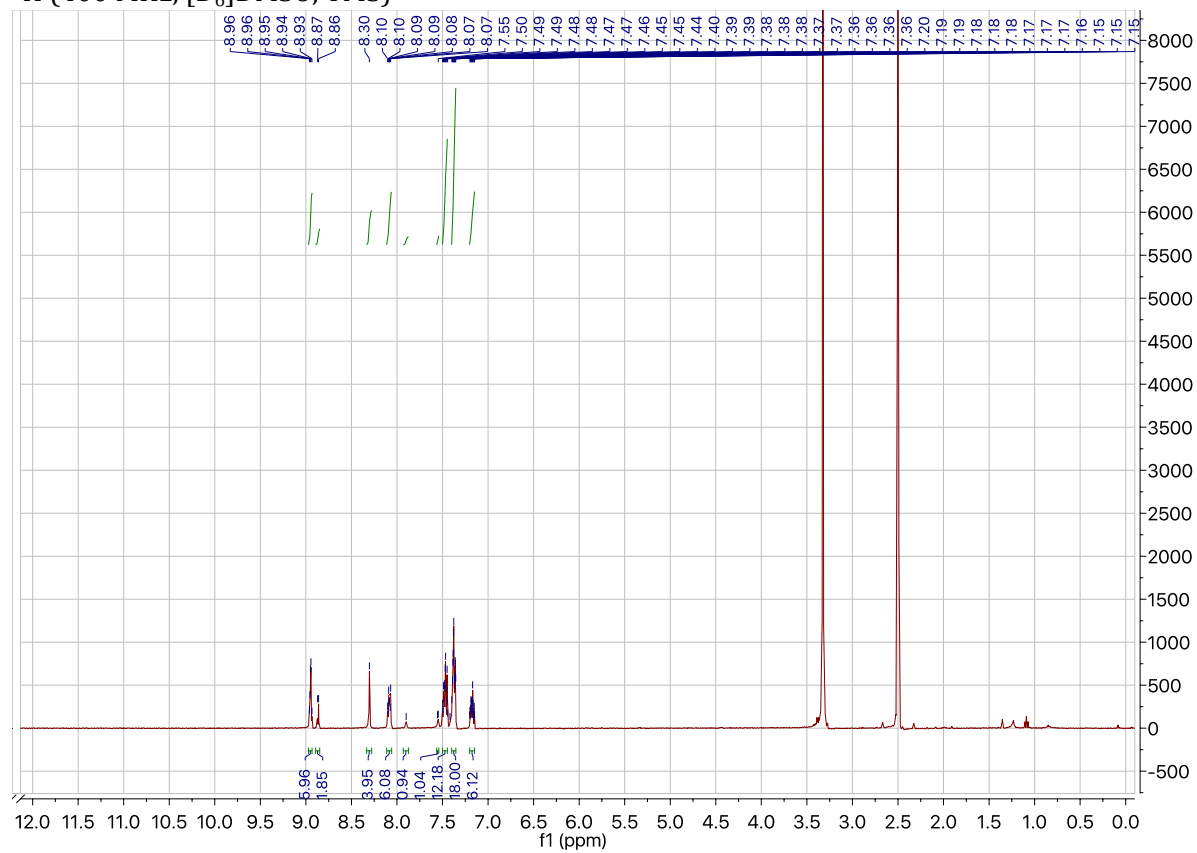


^{13}C (100 MHz, CDCl_3 , TMS)



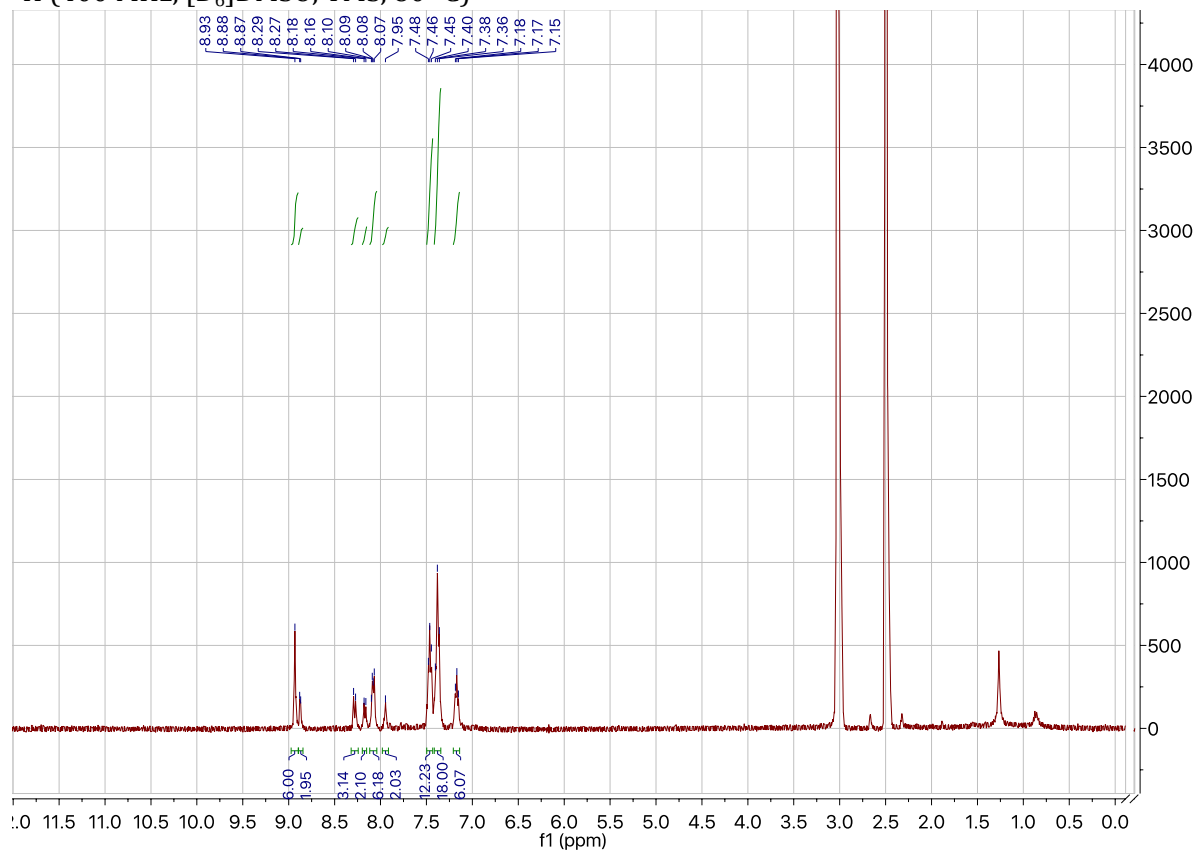
Compound **PorF**

^1H (400 MHz, $[\text{D}_6]\text{DMSO}$, TMS)



Compound **PorT**

^1H (400 MHz, $[\text{D}_6]\text{DMSO}$, TMS, 80 °C)



2. Square wave voltammetry

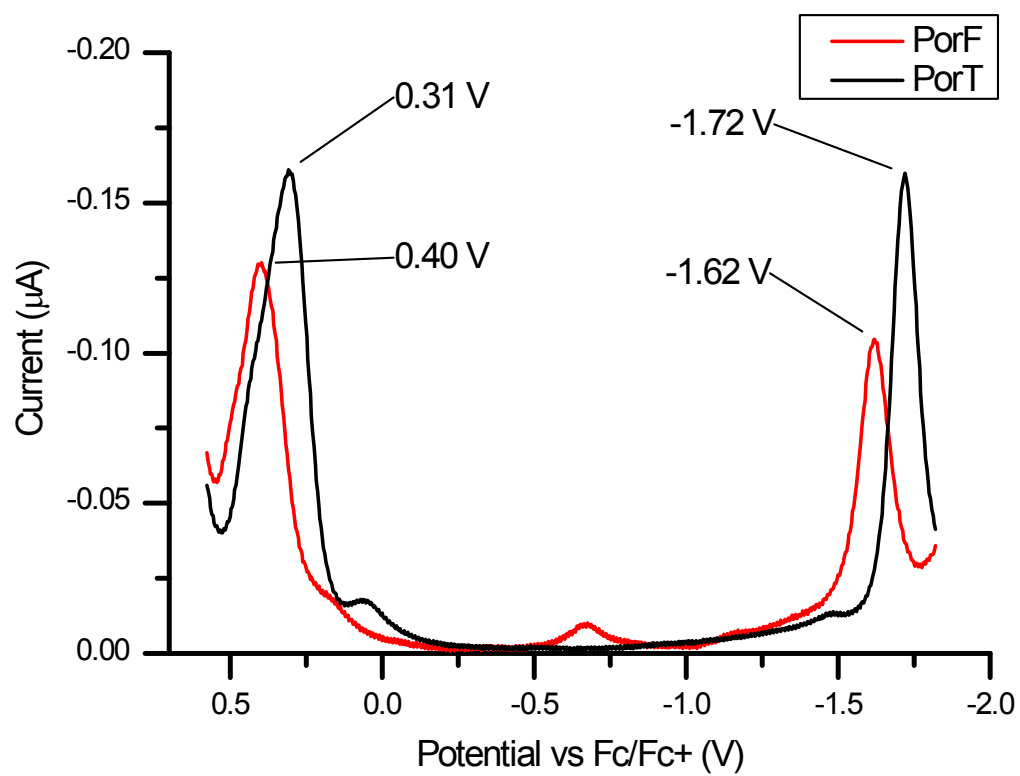


Figure S1 – Square wave voltammetry plots of dyes **PorT** and **PorF** in solution of DMF ($C = 10^{-3}$ M).

3. Computational data

Input parameters for PorT

opt freq b3lyp/genecp

O 1

H	14.17170800	1.25565400	2.51769900
O	14.93995100	0.66284100	2.54951500
C	15.10712500	0.04371800	1.34658600
O	16.15022200	-0.49433400	1.07293300
C	13.92541900	0.05172500	0.42188300
C	14.23707800	-0.12269500	-0.95919900
N	14.46198100	-0.24417400	-2.09513200
C	12.63821100	0.11427100	0.88527300
H	12.52998000	0.17509000	1.96715300
C	11.40145600	0.06690400	0.16455800
C	11.12008600	-0.00102200	-1.19492900
H	11.88836100	-0.02680900	-1.95698300
C	9.74212700	-0.01807900	-1.47998600
H	9.34711000	-0.03947300	-2.48916700
C	8.92793100	0.03661700	-0.35805500
S	9.90116900	0.09788400	1.08560400
C	7.46520000	0.03659500	-0.30138800
C	6.71345500	-0.51100900	-1.35813100
H	7.22257600	-0.95658100	-2.20729300
C	5.32368600	-0.51181500	-1.31998100
H	4.76494500	-0.93785300	-2.14794900
C	4.62448600	0.02784900	-0.22708600
C	5.37593900	0.57084100	0.82817600
H	4.85870500	0.99078700	1.68562900
C	6.76607900	0.57679600	0.79344500
H	7.31502600	1.02081700	1.61970000
C	3.13017000	0.02104400	-0.18660800
C	2.48546000	-1.22962500	-0.15254700
C	3.16765800	-2.49880900	-0.05155900
H	4.23742800	-2.63205900	0.01757900
C	2.21018200	-3.46500700	-0.02835300
H	2.35256200	-4.53172600	0.06168500
C	0.93229600	-2.79813000	-0.11671600
N	1.12425400	-1.43461700	-0.17830300
C	-0.31015200	-3.45896600	-0.11525700
C	-1.55949700	-2.80809500	-0.10221000
C	-2.83087600	-3.48425200	-0.20696100
H	-2.96351700	-4.55019900	-0.31852700
C	-3.79652600	-2.52644200	-0.16824600
H	-4.86510700	-2.66389800	-0.24253600
C	-3.12626300	-1.25411800	-0.03994700
N	-1.76245500	-1.44862100	-0.01450300
C	-3.78600100	-0.01161900	0.02146800
C	-3.13596600	1.23726000	0.03852900
C	-3.80875300	2.50384700	0.20531400
H	-4.87170500	2.63189600	0.34676200
C	-2.85161700	3.47062700	0.17949800
H	-2.98654300	4.53582200	0.29548700
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C	-0.34142500	3.46799600	-0.06570600
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H	2.29606800	4.56597200	-0.39487000
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H	4.19911700	2.68412000	-0.45391800

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H	-7.86220700	-1.04871700	2.06041200
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C	-11.75430100	3.28310600	-1.15085200
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H	-12.12224900	-4.29154900	2.13088200
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H	-12.84048500	-1.99058500	2.75849900
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H	0.64672900	-5.12593900	-2.05496700
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H	3.88837600	-11.85733800	-2.14655700
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H	1.56710200	-12.58753400	-2.67800200
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C	-2.26713900	-11.78632500	1.65778700
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C	-3.78336800	-10.25582900	0.57835600
H	-4.79470100	-9.93546000	0.34177600
C	-2.70323100	-9.54147500	0.06342600
H	-2.87080400	-8.67479600	-0.56820300
C	-0.34926800	4.96255800	-0.05777200
C	-0.94782000	5.69276800	-1.09775300
H	-1.39793800	5.15897600	-1.93006700
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H	-1.39825800	7.62262700	-1.92967900
C	-0.36301800	7.80232700	-0.04531900
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H	-4.90893800	9.90031500	-0.33402900
C	-3.75236200	11.35222100	-1.43345600
H	-4.61957200	11.90042200	-1.79030600
C	-2.46429800	11.76415700	-1.78175200
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C	-1.34895800	11.05875700	-1.33385100
H	-0.35022800	11.37512300	-1.61760700
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H	-0.40467200	11.36235200	1.55596600
C	1.70624000	11.76814400	1.72069500
H	1.55884700	12.63135200	2.36448300
C	2.99734500	11.36999400	1.36762200
H	3.86027800	11.92297600	1.72744900
C	3.16660100	10.25362500	0.54585800
H	4.16489200	9.93695700	0.25511600
C	2.06197200	9.54689300	0.07402100
H	2.19769100	8.68963200	-0.57780200

C 0

6-311g(d,p)

H 0

6-311g(d,p)

O 0

6-311g(d,p)

N 0

6-311g(d,p)

S 0

6-311g(d,p)

Zn 0

lanl2dz

Zn 0

LanL2DZ

Input parameters for PorF

opt freq b3lyp/genecp

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O 1
H      13.03108300  0.20982900  2.54519100
O      13.70389100 -0.29185400  3.03309000
C      14.13199100 -1.35284400  2.29206000
O      15.14986800 -1.93132700  2.58023200
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C      13.90068700 -2.52548200  0.12437900
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C      10.96296900 -1.88318900  0.12515800
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H      11.85994900 -2.98410300 -1.55416700
C      9.65998100 -2.58669900 -1.56085600
H      9.31693000 -3.03833900 -2.48038200
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C      7.45681300 -1.62949600 -0.55804700
C      6.58954200 -2.03736200 -1.58826100
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C      5.23020400 -1.75780100 -1.52244700
H      4.57748900 -2.07339500 -2.33074900
C      4.68237400 -1.05947700 -0.43180300
C      5.55406700 -0.65281300  0.59287400
H      5.15129100 -0.12011600  1.44910500
C      6.91477800 -0.93148000  0.53628500
H      7.56564300 -0.61572700  1.34458300
C      3.22021900 -0.75827400 -0.36291600
C      2.33166800 -1.84820200 -0.29997200
C      2.73768500 -3.23081000 -0.19912000
H      3.75754400 -3.58279100 -0.14634000
C      1.60133900 -3.97736200 -0.15133800
H      1.52066800 -5.04994400 -0.05492000
C      0.48822500 -3.06020500 -0.22120500
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H     -1.81398400  4.92523800  0.25588800
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H      4.80576000  1.62329400 -0.70831300
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N      1.54700100  1.06577400 -0.22751500
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C	-7.03183400	1.94852100	-0.78396700
H	-7.52423900	2.49355600	-1.58272100
C	-5.67080200	1.67247000	-0.86998400
H	-5.11567400	2.00639700	-1.74213000
N	-9.16290000	1.81064900	0.42568100
C	-9.66802400	3.06464700	-0.01916700
C	-8.98394500	4.25564000	0.27243200
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H	-8.94009800	6.39130800	0.06384900
C	-10.67694900	5.54032600	-0.89201300
H	-11.06647900	6.49654800	-1.22939100
C	-11.36496000	4.35835200	-1.17407900
H	-12.29232500	4.38912700	-1.74008600
C	-10.86418600	3.12837300	-0.75157500
H	-11.39549500	2.21117100	-0.98507800
C	-10.05677200	0.85275800	0.98248000
C	-9.96935100	-0.50048000	0.61906900
H	-9.21529400	-0.81205200	-0.09691800
C	-10.84351500	-1.43443700	1.17215700
H	-10.76222100	-2.47811700	0.87978500
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C	-11.92422500	0.31177900	2.43339400
H	-12.68162100	0.63623100	3.14218400
C	-11.04257500	1.24987800	1.89952100
H	-11.11170500	2.29382400	2.18852000
C	-1.16675900	-4.91277100	-0.19994900
C	-0.81673500	-5.72184200	-1.29344000
H	-0.33431800	-5.26938600	-2.15540300
C	-1.10309800	-7.08338500	-1.31164000
H	-0.84223600	-7.67884200	-2.18045800
C	-1.73686800	-7.69563600	-0.21684000
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H	-2.62437600	-11.12009400	-1.84557200
C	-3.22747700	-9.57434200	0.34679000
C	-3.21624400	-10.73122300	1.14210900
H	-2.27665500	-11.24267100	1.32569100
C	-4.40107400	-11.21903500	1.69018600
H	-4.37383200	-12.11603800	2.30333200
C	-5.61046400	-10.55584500	1.47221700
H	-6.53094500	-10.93482100	1.90696300
C	-5.62329600	-9.40014800	0.68834600
H	-6.55816400	-8.87768200	0.50272100
C	-4.44650100	-8.91540000	0.12053900

H	-4.46420500	-8.02558400	-0.50084100
C	0.84258500	4.79778000	-0.19457700
C	0.35200800	5.64113000	-1.20531600
H	-0.24275700	5.21603200	-2.00891700
C	0.63715600	7.00299600	-1.21793500
H	0.26303900	7.62630000	-2.02363800
C	1.41516600	7.58004800	-0.20006900
C	1.90215500	6.74676100	0.82111500
H	2.49146900	7.17499200	1.62549500
C	1.62654300	5.38294500	0.81364900
H	2.00426100	4.76077600	1.62017000
N	1.70137300	8.96811300	-0.20255000
C	0.70476300	9.90378700	-0.59819100
C	-0.62170400	9.76144200	-0.16030400
H	-0.88247800	8.93209000	0.48952700
C	-1.59465900	10.67739000	-0.55576100
H	-2.61649600	10.55193100	-0.20718900
C	-1.26164800	11.75826500	-1.37493800
H	-2.02111500	12.47451700	-1.67509200
C	0.05903000	11.90818600	-1.80320500
H	0.33246900	12.74060700	-2.44634800
C	1.03513000	10.98687300	-1.42830400
H	2.05751500	11.10051800	-1.77449900
C	2.98723000	9.43308900	0.19227400
C	3.11304300	10.55522600	1.02653300
H	2.21915300	11.06212100	1.37591200
C	4.37446900	11.01425800	1.40118600
H	4.45357300	11.88439600	2.04764600
C	5.52763200	10.35639900	0.96795400
H	6.50885100	10.71310400	1.26774400
C	5.40511600	9.23556200	0.14401700
H	6.29366100	8.71841300	-0.20875700
C	4.14862200	8.78015000	-0.25076900
H	4.05884800	7.91828900	-0.90444400
O	9.66346700	-1.49845900	0.39292000

C 0

6-311g(d,p)

H 0

6-311g(d,p)

O 0

6-311g(d,p)

N 0

6-311g(d,p)

Zn 0

lanl2dz

Zn 0

LanL2DZ