Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Electronic Supporting Information

Synthesis and properties of electron accepting star-shaped phosphaviologen oligomers

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UV-Vis Spectroscopy

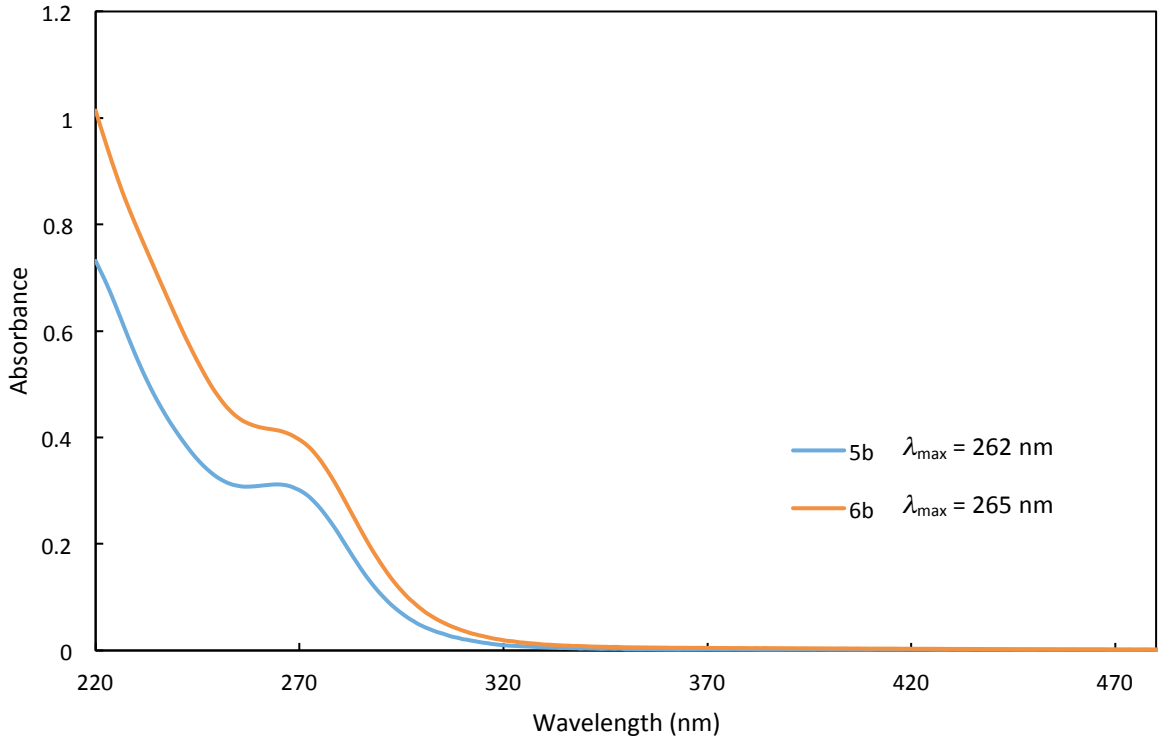


Figure S1 UV-Vis spectrum of compounds **5b** and **6b** in 5×10^{-5} M water solution.

Electrochemical Measurements

Cyclic Voltammetry

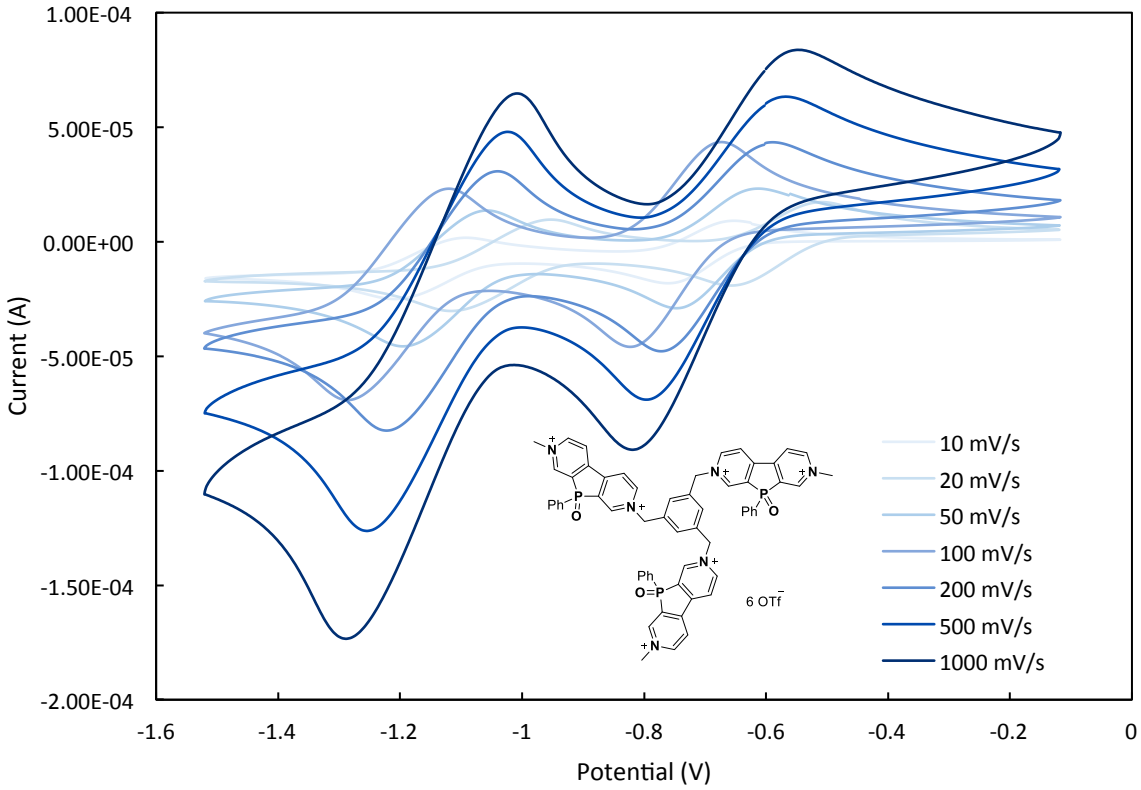


Figure S2 Cyclic voltammetry of compound **5b** at different scan rates; in DMF solution with [*n*Bu$_4$N][PF$_6$] as supporting electrolyte (0.05M), referenced to FcH/FcH$^+$.

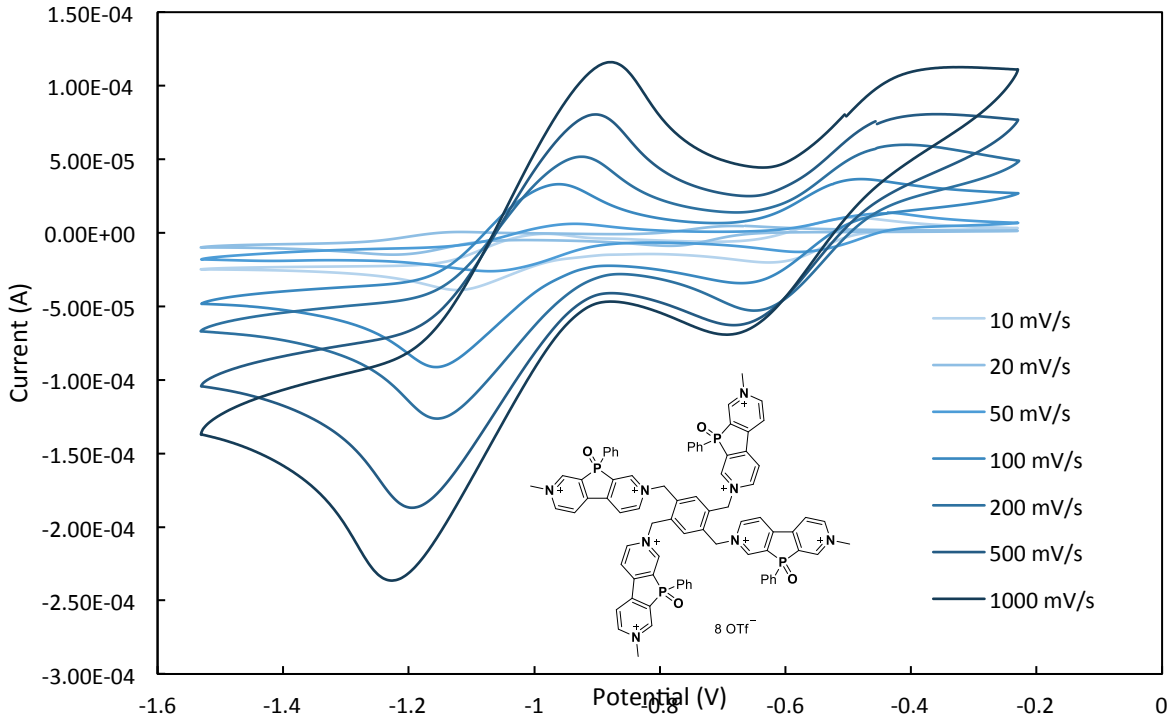


Figure S3 Cyclic voltammetry of compound **6b** at different scan rates; in DMF solution with [*n*Bu$_4$N][PF$_6$] as supporting electrolyte (0.05M), referenced to FcH/FcH$^+$.

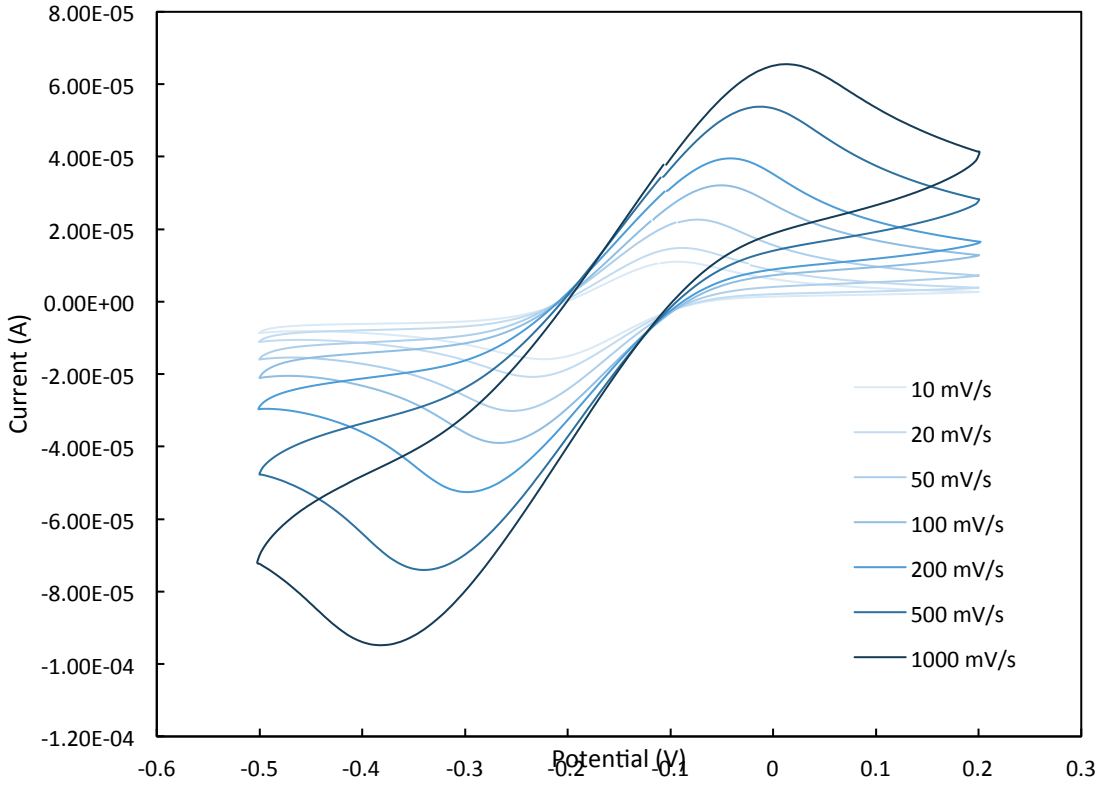


Figure S4 Cyclic voltammetry of the first reduction of compound **5b** at different scan rates; in DMF solution with [*n*Bu$_4$N][PF$_6$] as supporting electrolyte (0.05M), referenced to FcH/FcH$^+$.

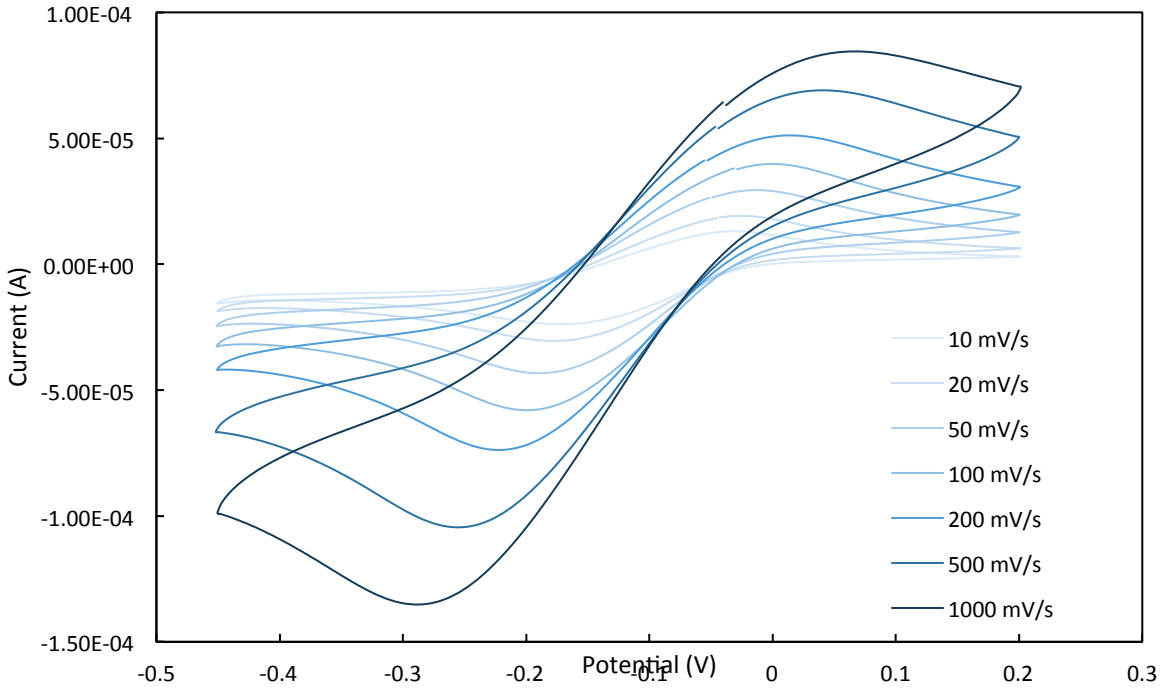


Figure S5 Cyclic voltammetry of the first reduction of compound **6b** at different scan rates; in DMF solution with [*n*Bu$_4$N][PF$_6$] as supporting electrolyte (0.05M), referenced to FcH/FcH$^+$.

Compound (scan rate)[a]	Peak Area (A·V)[b]	Trial 1[c]	Trial 2[c]	Trial 3[c]	Trial 4[c]	Trial 5[c]	Trial Ave[c]	Concentration Correction[d]	# e^- Per Event[e]
Monomer (100 mV/s)	Red 1	1.68E-04	1.52E-04	1.59E-04	1.61E-04	1.63E-04	**1.61E-04**	1.91E-05	**1.00**
	Red 2	1.62E-04	1.50E-04	1.53E-04	1.42E-04	1.38E-04	**1.49E-04**	1.77E-05	**1.00**
	Ox 1	1.55E-04	1.61E-04	1.55E-04	1.55E-04	1.64E-04	**1.58E-04**	1.88E-05	**1.00**
	Ox 2	1.68E-04	1.61E-04	1.58E-04	1.68E-04	1.52E-04	**1.61E-04**	1.92E-05	**1.00**
5b (100 mV/s)	Red 1	7.15E-05	6.64E-05	7.14E-05	6.52E-05	6.80E-05	**6.85E-05**	5.91E-05	**3.09**
	Red 2	5.65E-05	6.92E-05	7.22E-05	6.24E-05	6.22E-05	**6.45E-05**	5.56E-05	**3.13**
	Ox 1	7.01E-05	7.00E-05	6.74E-05	6.19E-05	6.45E-05	**6.68E-05**	5.76E-05	**3.06**
	Ox 2	7.48E-05	7.09E-05	7.17E-05	6.86E-05	7.02E-05	**7.12E-05**	6.14E-05	**3.20**
Monomer (20 mV/s)	Red 1	2.49E-04	2.10E-04	2.54E-04	2.20E-04	2.02E-04	**2.27E-04**	2.70E-05	**1.00**
	Red 2	2.54E-04	2.40E-04	2.35E-04	2.38E-04	2.20E-04	**2.37E-04**	2.82E-05	**1.00**
	Ox 1	2.07E-04	2.46E-04	2.46E-04	2.54E-04	2.27E-04	**2.36E-04**	2.80E-05	**1.00**
	Ox 2	2.05E-04	2.19E-04	2.26E-04	2.16E-04	2.32E-04	**2.20E-04**	2.61E-05	**1.00**
6b (20 mV/s)	Red 1	1.34E-04	1.25E-04	1.37E-04	1.39E-04	1.38E-04	**1.35E-04**	1.04E-04	**3.83**
	Red 2	1.42E-04	1.39E-04	1.49E-04	1.45E-04	1.40E-04	**1.43E-04**	1.10E-04	**3.90**
	Ox 1	1.33E-04	1.51E-04	1.48E-04	1.43E-04	1.49E-04	**1.45E-04**	1.11E-04	**3.96**
	Ox 2	1.36E-04	1.49E-04	1.24E-04	1.38E-04	1.33E-04	**1.36E-04**	1.05E-04	**4.00**

Table S1 Electron count comparison of the monomer and compounds **5b** and **6b** using peak area obtained from cyclic voltammetry. [a]A lower scan rate was necessary for **6b** due to irreversibility at higher scan rates. [b]Peak areas were manually obtained from the collected CV data. [c]Five trials of manually collecting each peak area were carried out and averaged to increase confidence in the average. [d]Peak areas were corrected by dividing each average by the respective solution concentration used in each analysis. [e]Electron counts for each reduction/oxidation event was determined by dividing the corrected concentration of the benzyl-methyl phosphaviologen monomer with the respective corrected concentration of **5b** and **6b**.

Spectroelectrochemistry

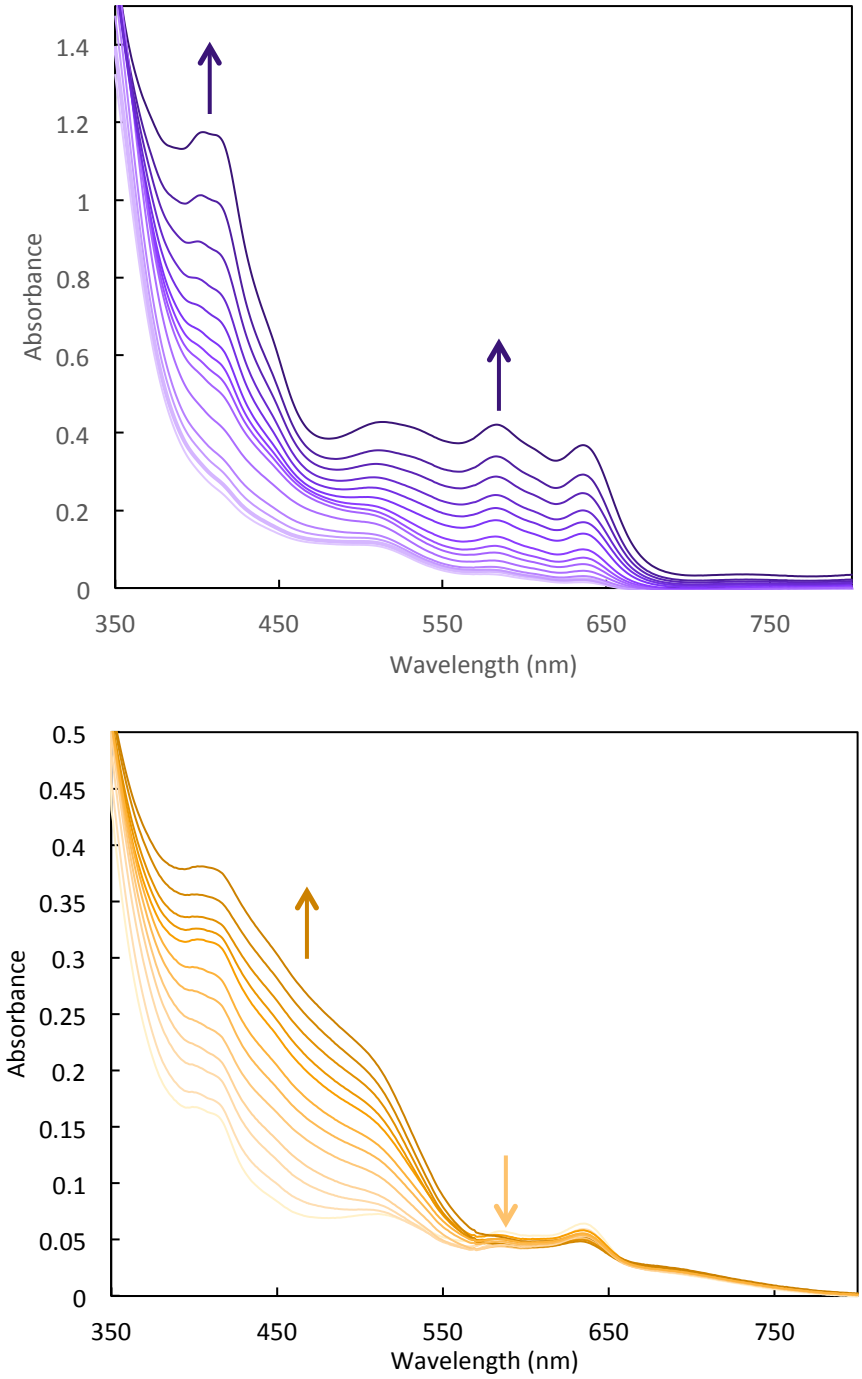


Figure S6 Spectroelectrochemistry of isolated first reduction (top) and isolated second reduction (bottom) of **5b**. UV-vis referenced to Ag/Ag^{+}, in DMF solution with $[n\mathrm{Bu_4N}][PF_6]$ (0.05 M) as supporting electrolyte.

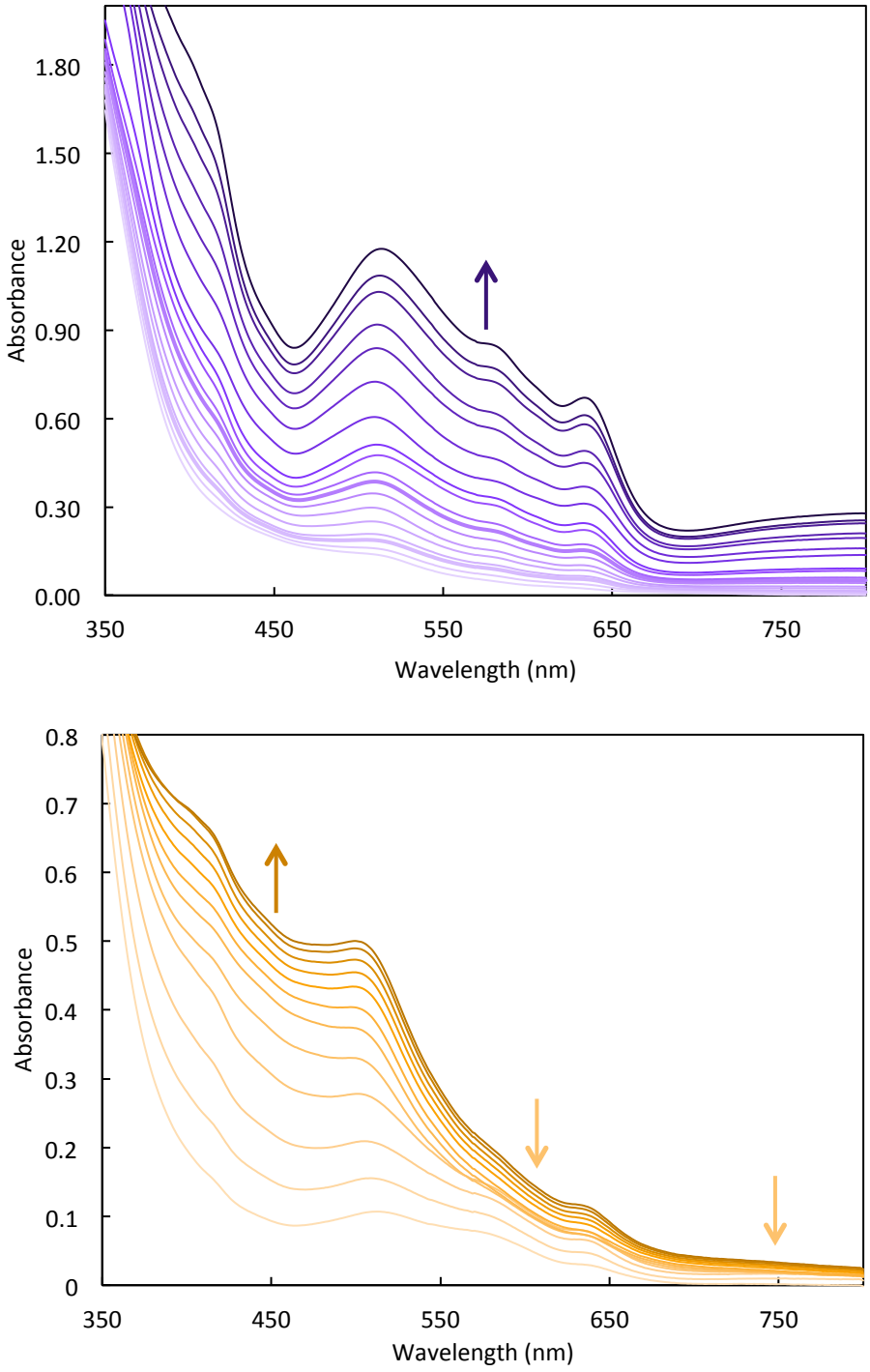


Figure S7 Spectroelectrochemistry of isolated first reduction (top) and isolated second reduction (bottom) of **6b**. UV-vis referenced to Ag/Ag^{+}, in DMF solution with $[n\mathrm{Bu_4N}][PF_6]$ (0.05 M) as supporting electrolyte.

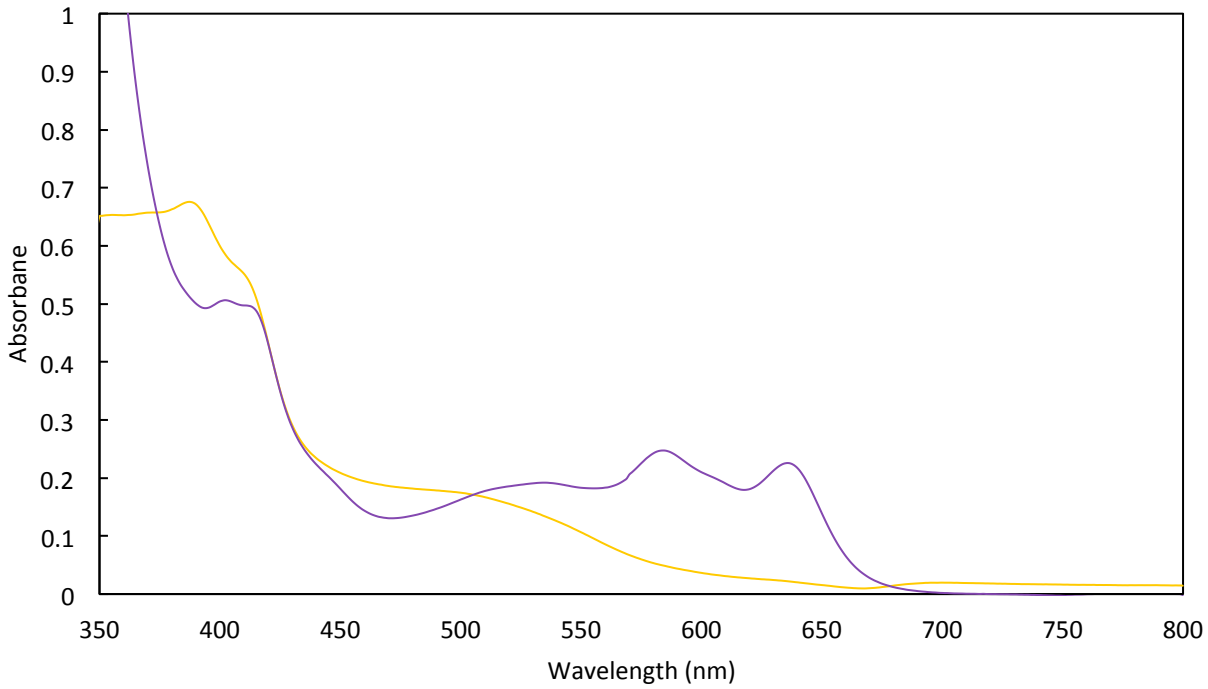


Figure S8 UV-vis of isolated first (purple) and second (yellow) reduction of **5b** in DMF using zinc and sodium, respectively.

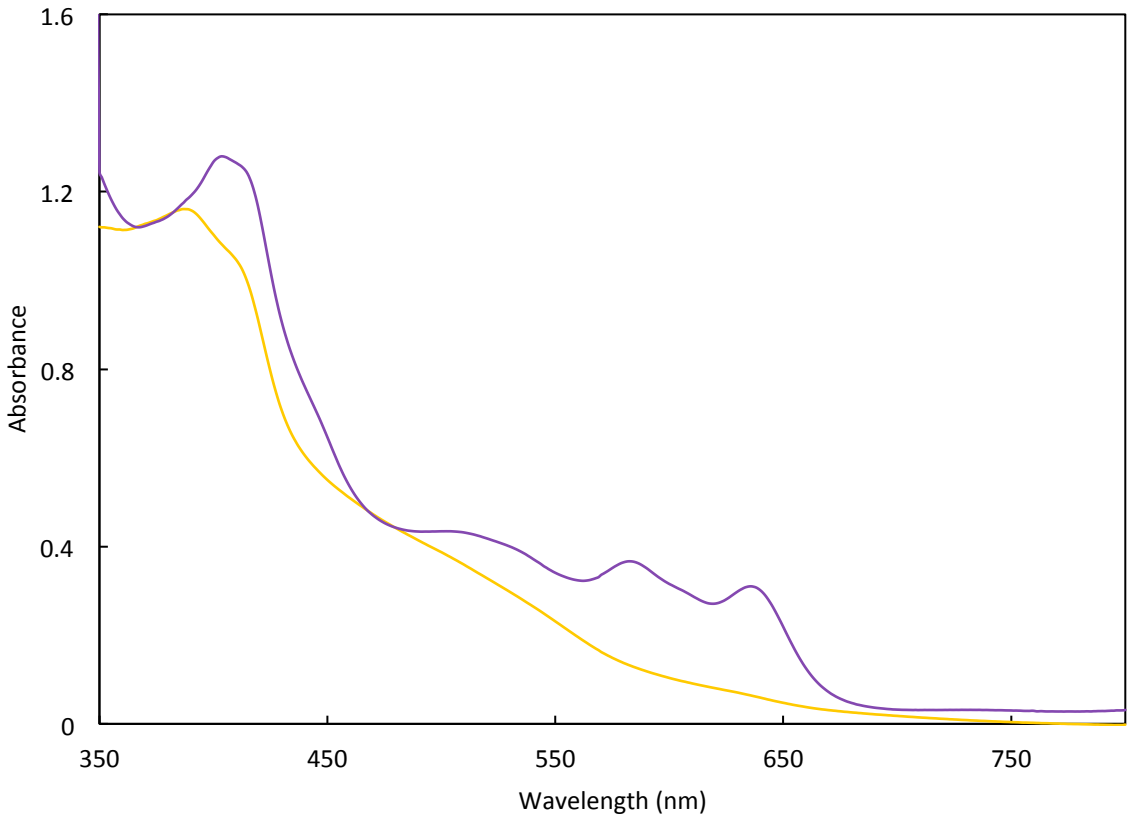


Figure S9 UV-vis of isolated first (purple) and second (yellow) reduction of **6b** in DMF using zinc and sodium, respectively.

NMR spectroscopy

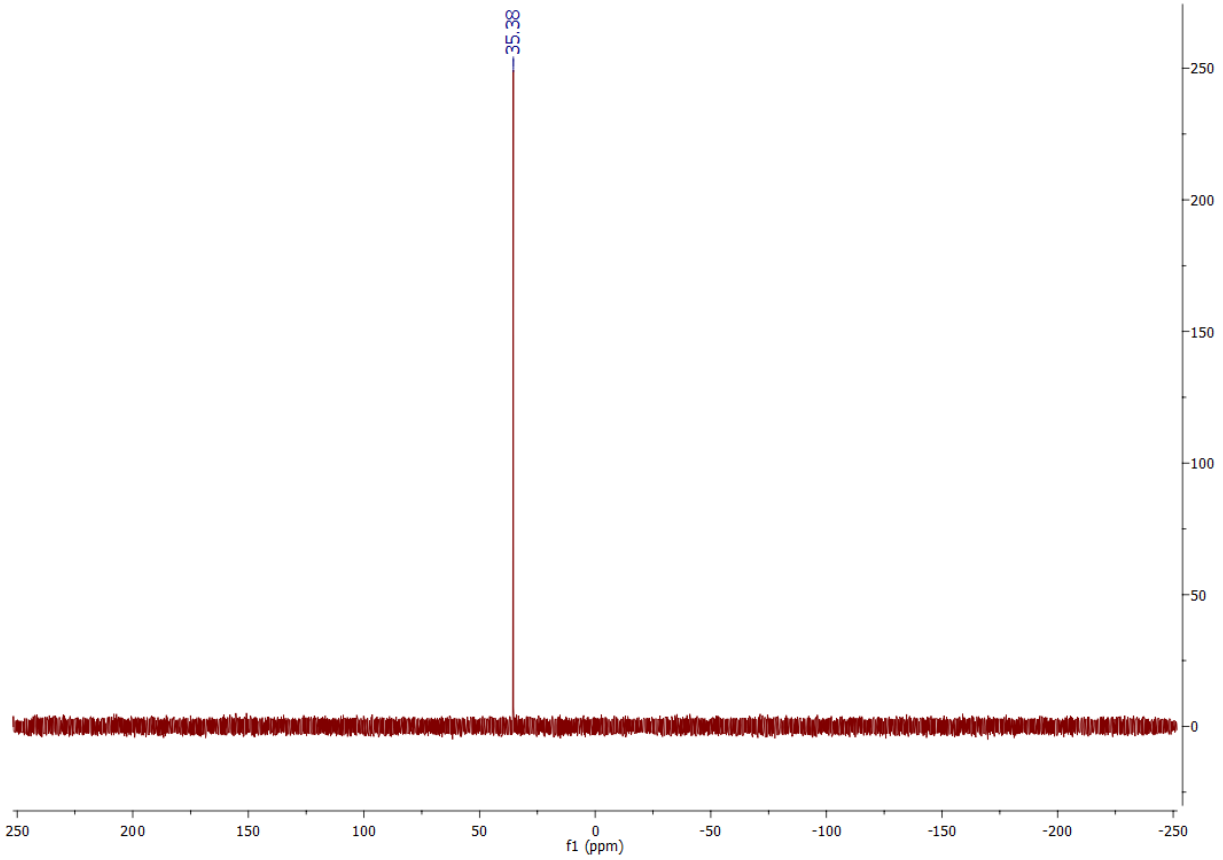


Figure S10 $^{31}P\{^{1}H\}$-NMR of **1** in methanol-d_4.

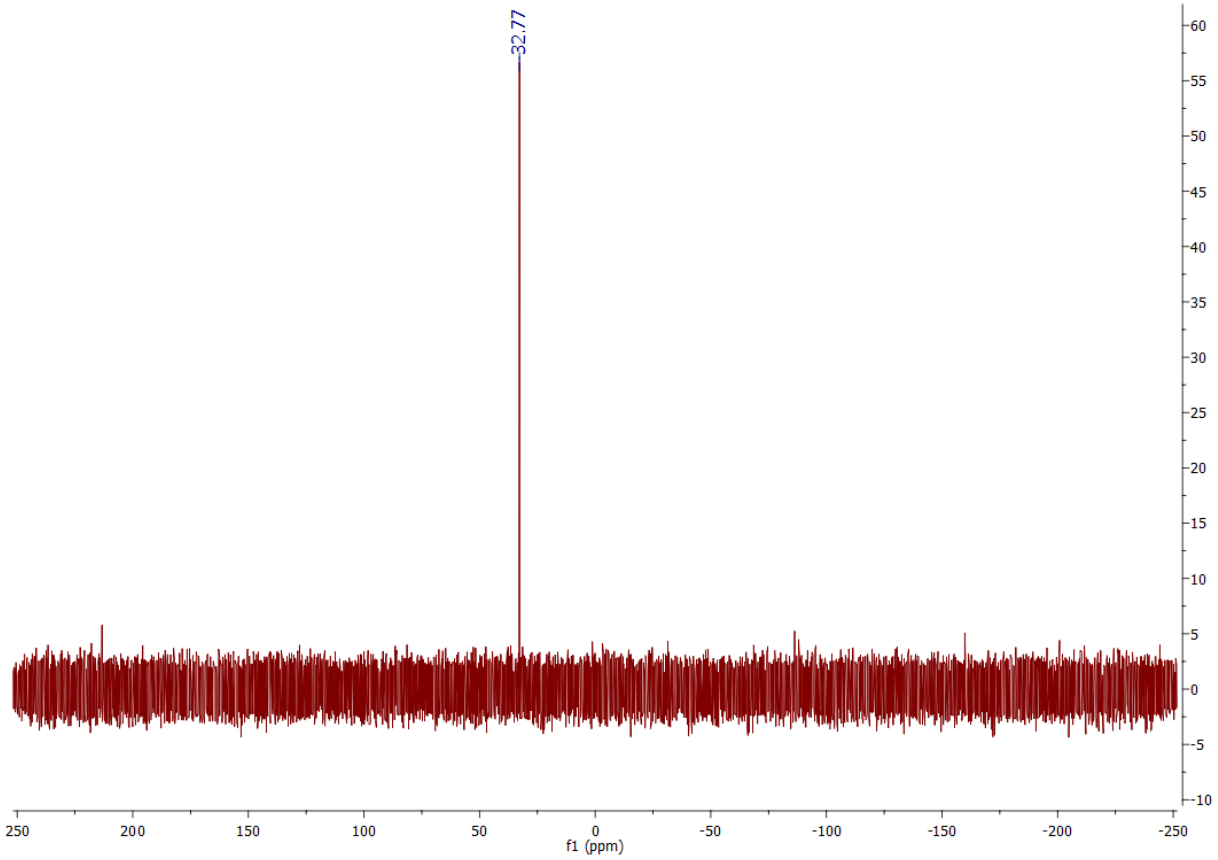


Figure S11 $^{31}P\{^{1}H\}$-NMR of **4** in methanol-d_4.

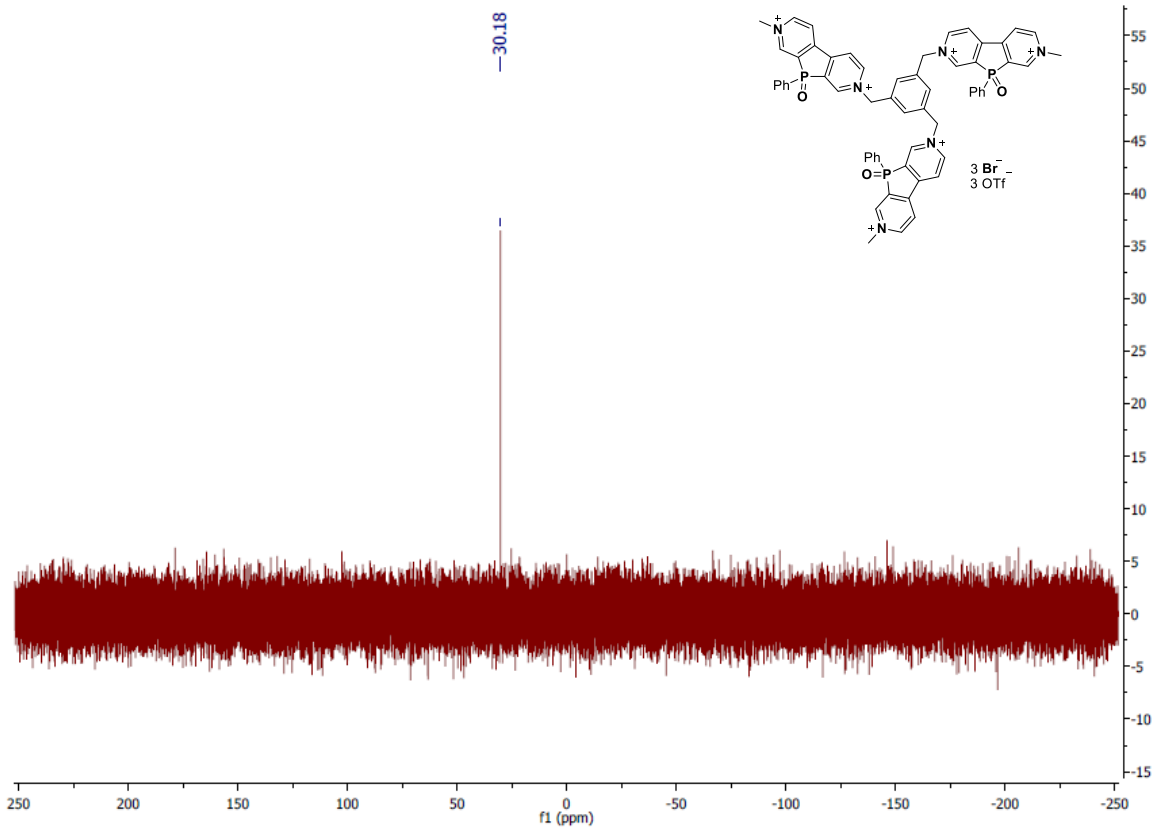


Figure S12 $^{31}P\{^{1}H\}$-NMR of **5a** in methanol-d_4.

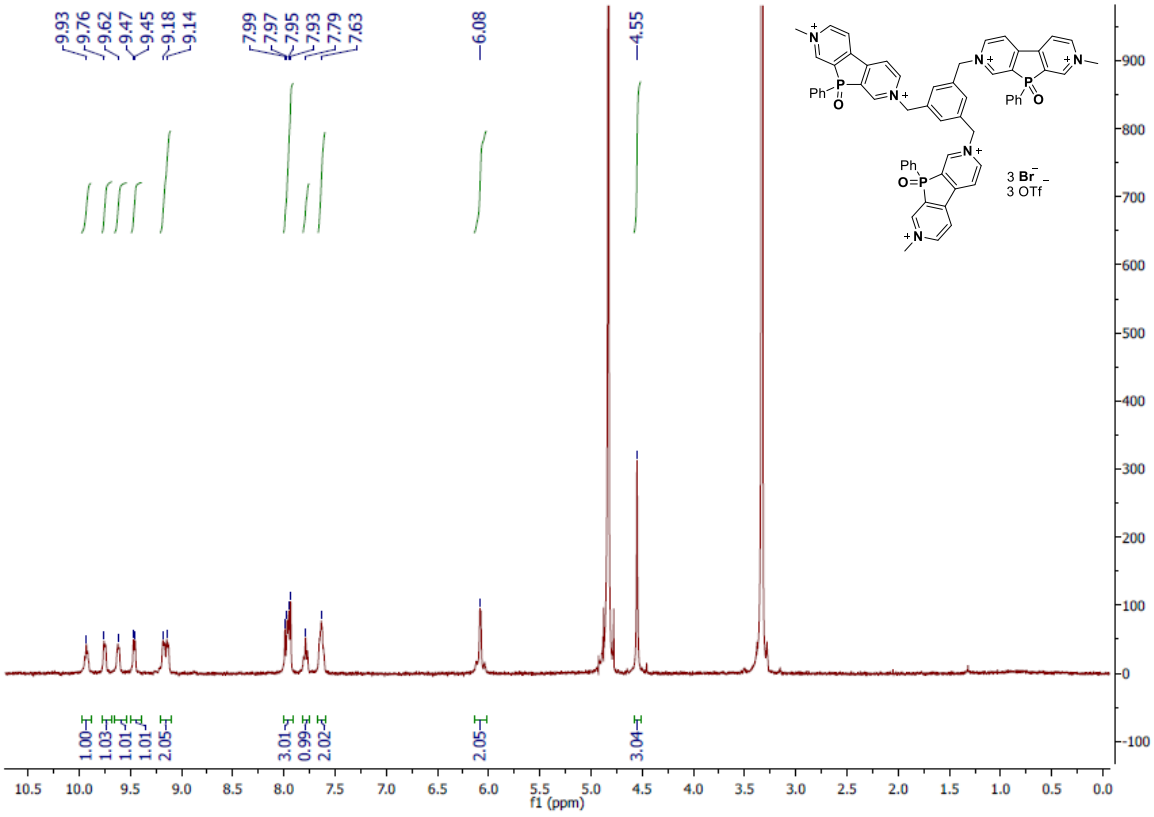


Figure S13 ^{1}H-NMR of **5a** in methanol-d_4.

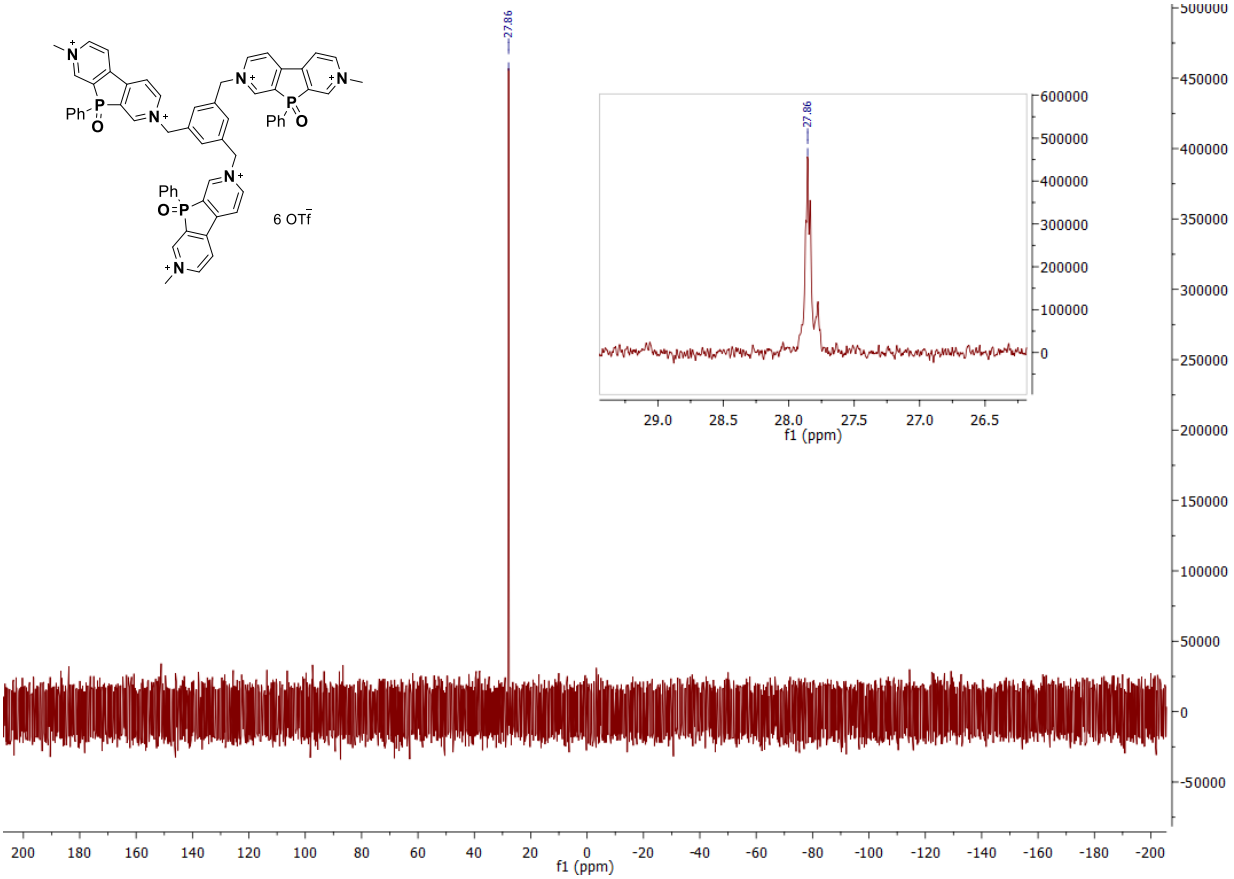


Figure S14 $^{31}P\{^{1}H\}$-NMR of **5b** in methanol-d_4.

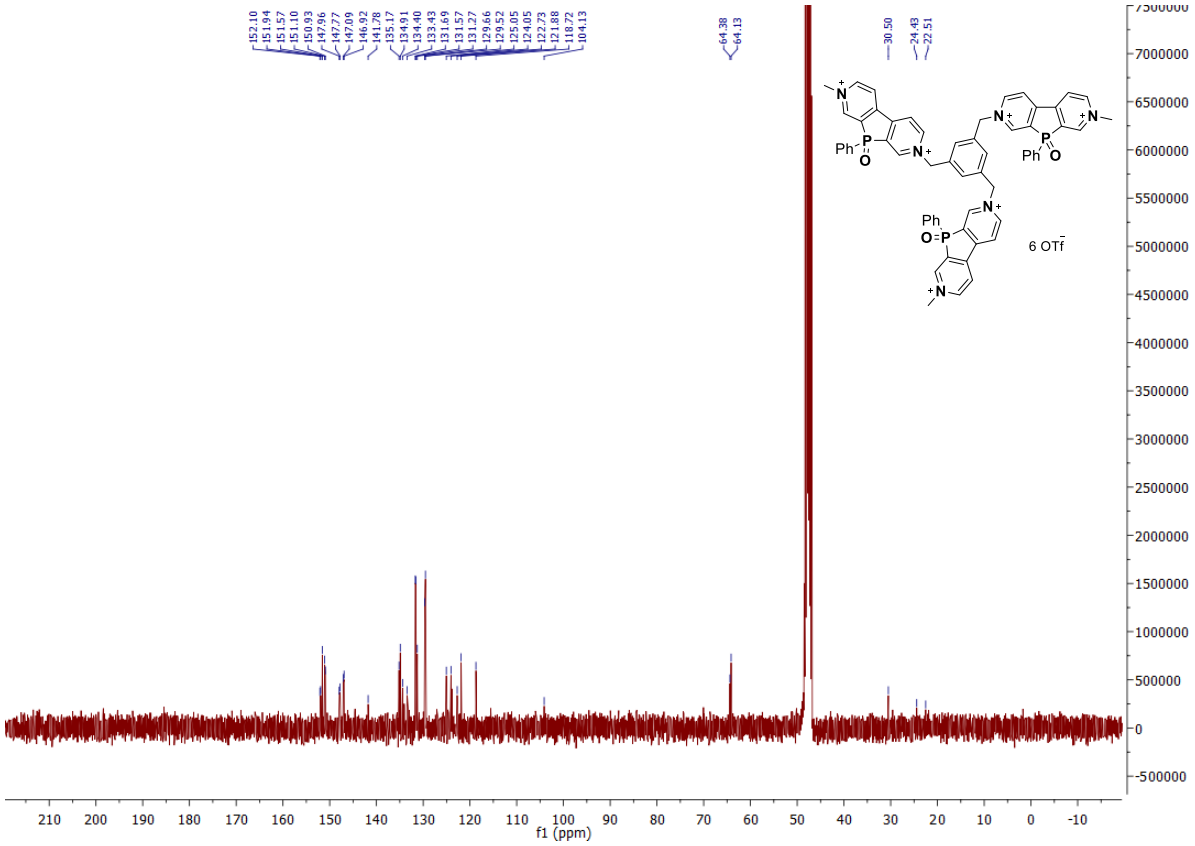


Figure S15 $^{13}C\{^{1}H\}$-NMR of **5b** in methanol-d_4.

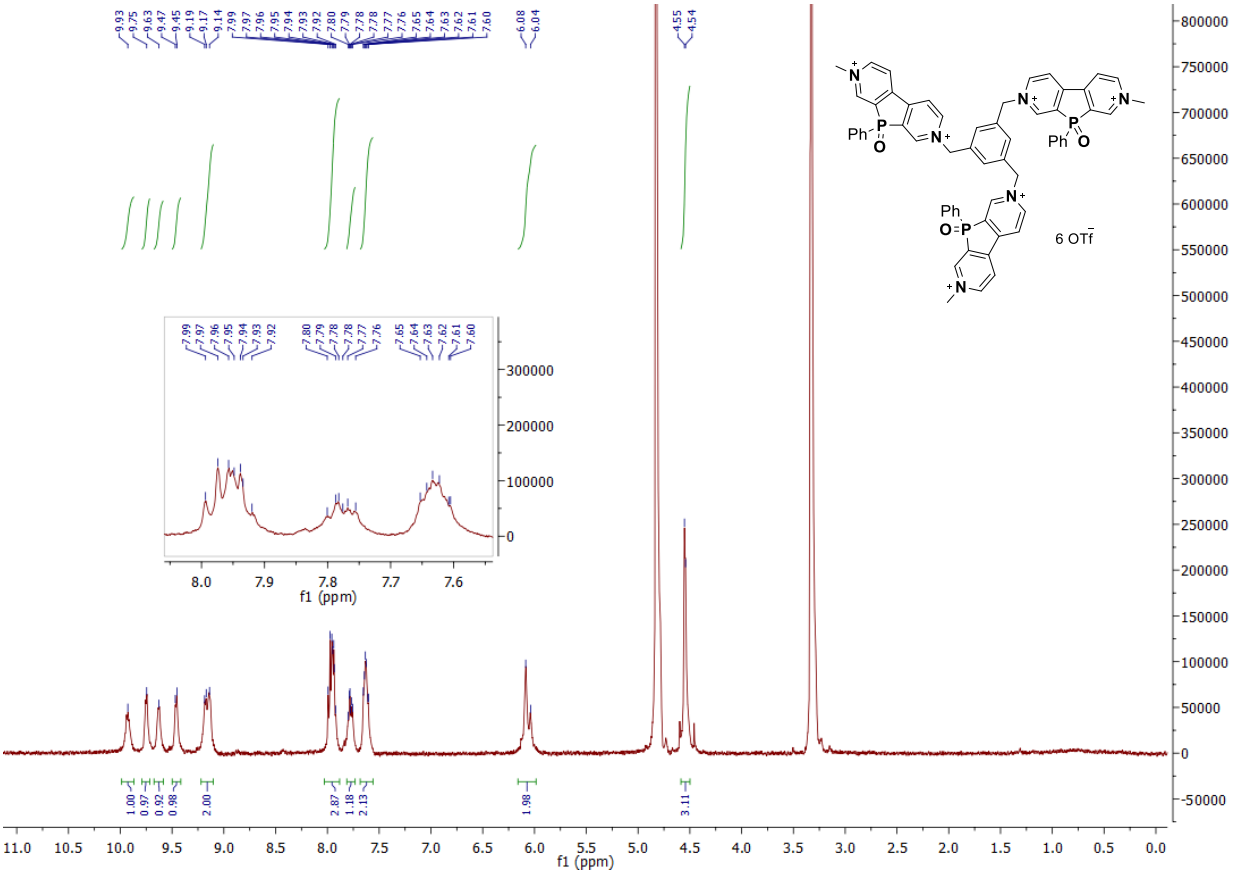


Figure S16 ^{1}H-NMR of **5b** in methanol-d_4.

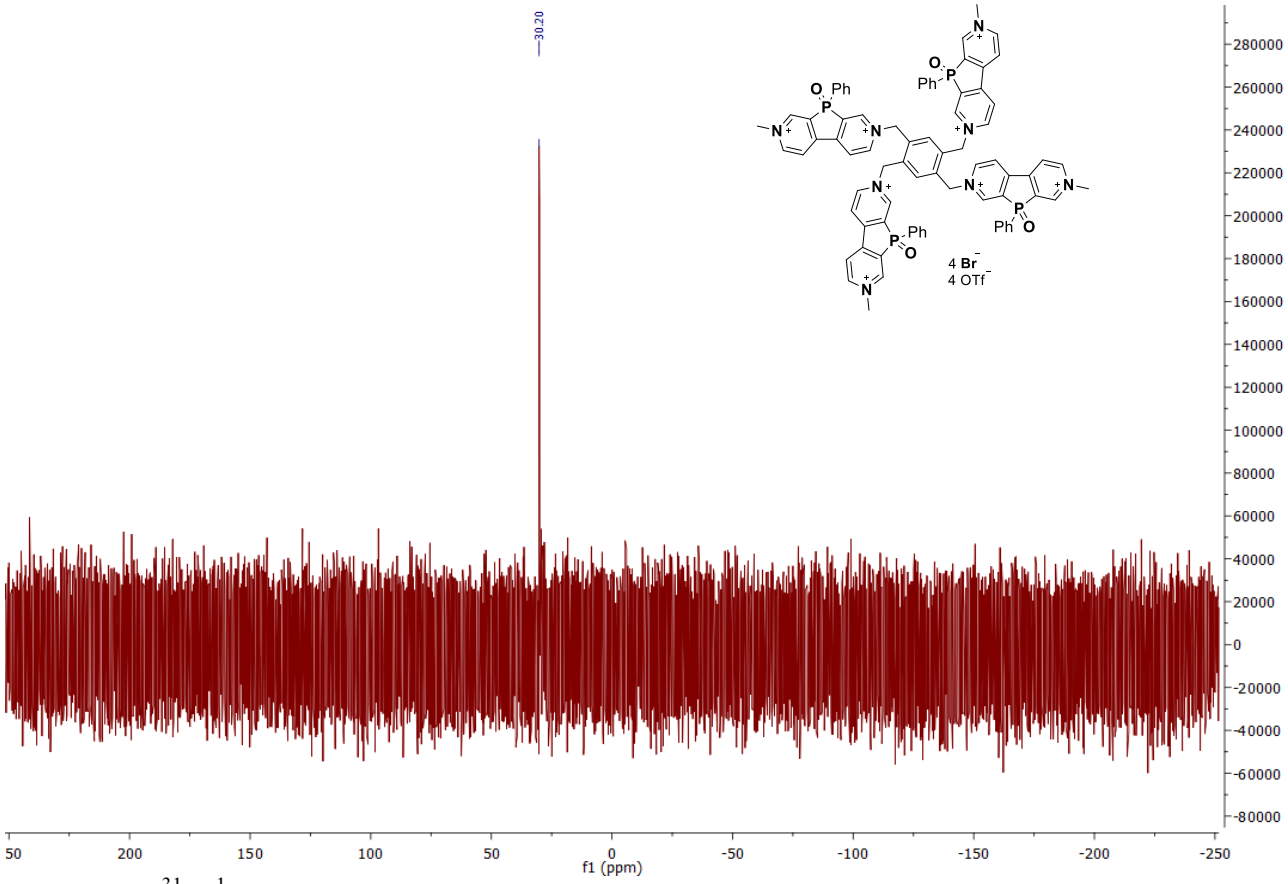


Figure S17 $^{31}P\{^{1}H\}$-NMR of **6a** in methanol-d_4.

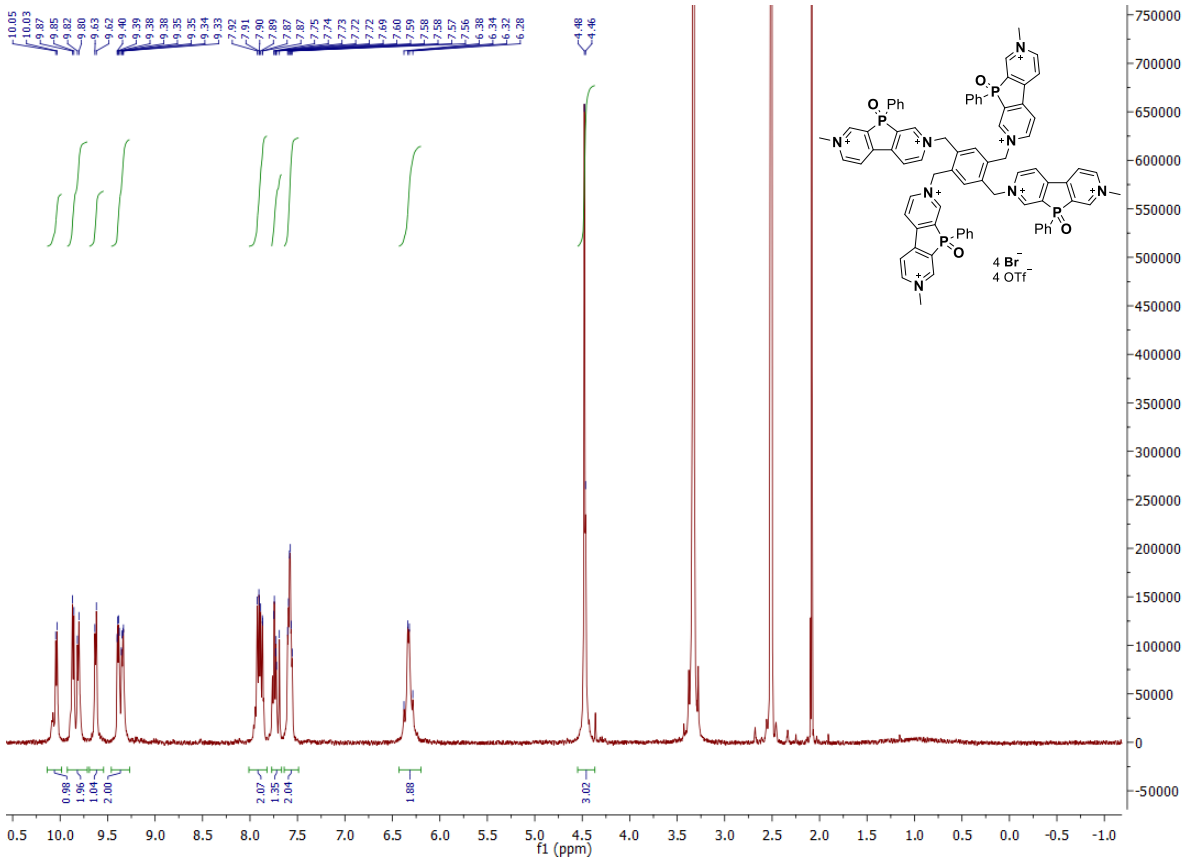


Figure S18 ^{1}H-NMR of **6a** in methanol-d_4.

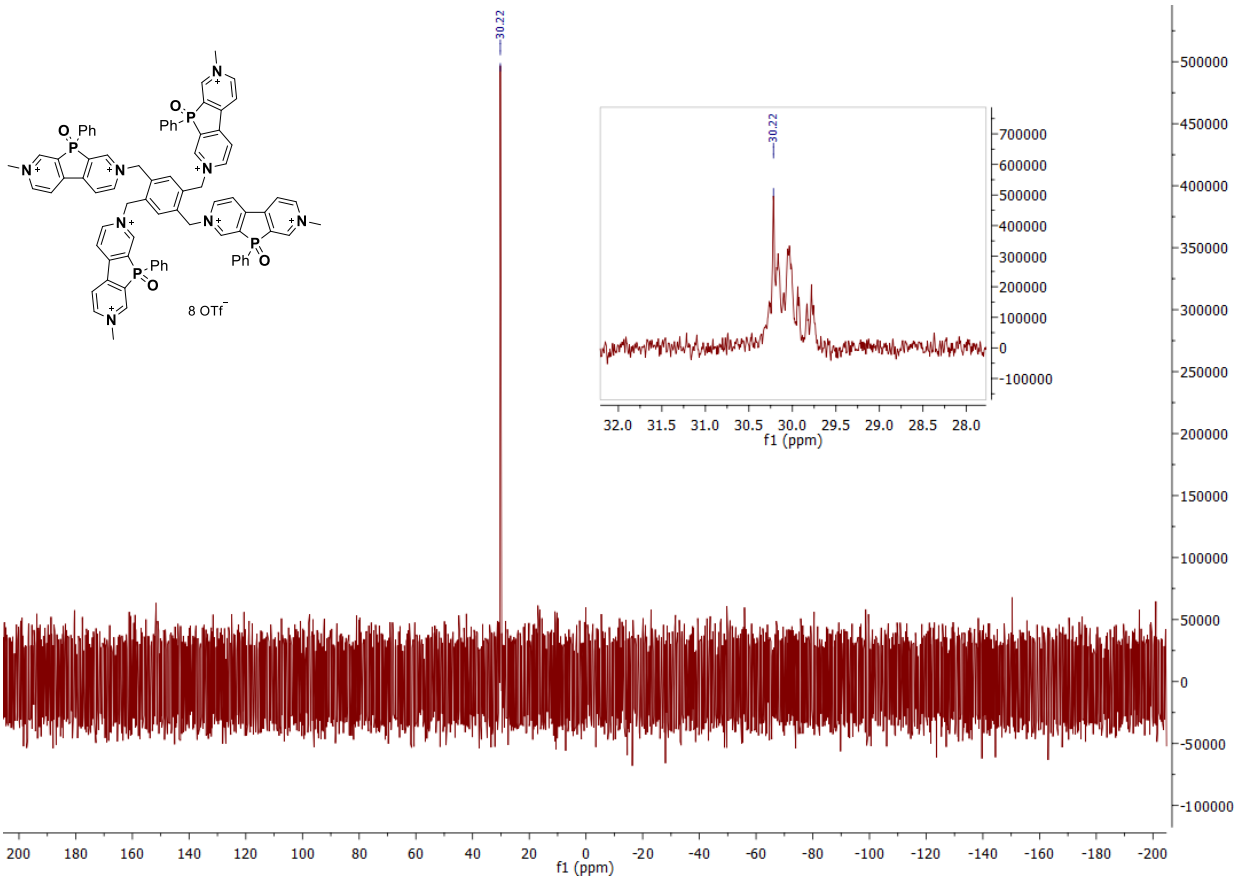


Figure S19 $^{31}P\{^{1}H\}$-NMR of **6b** in methanol-d_4.

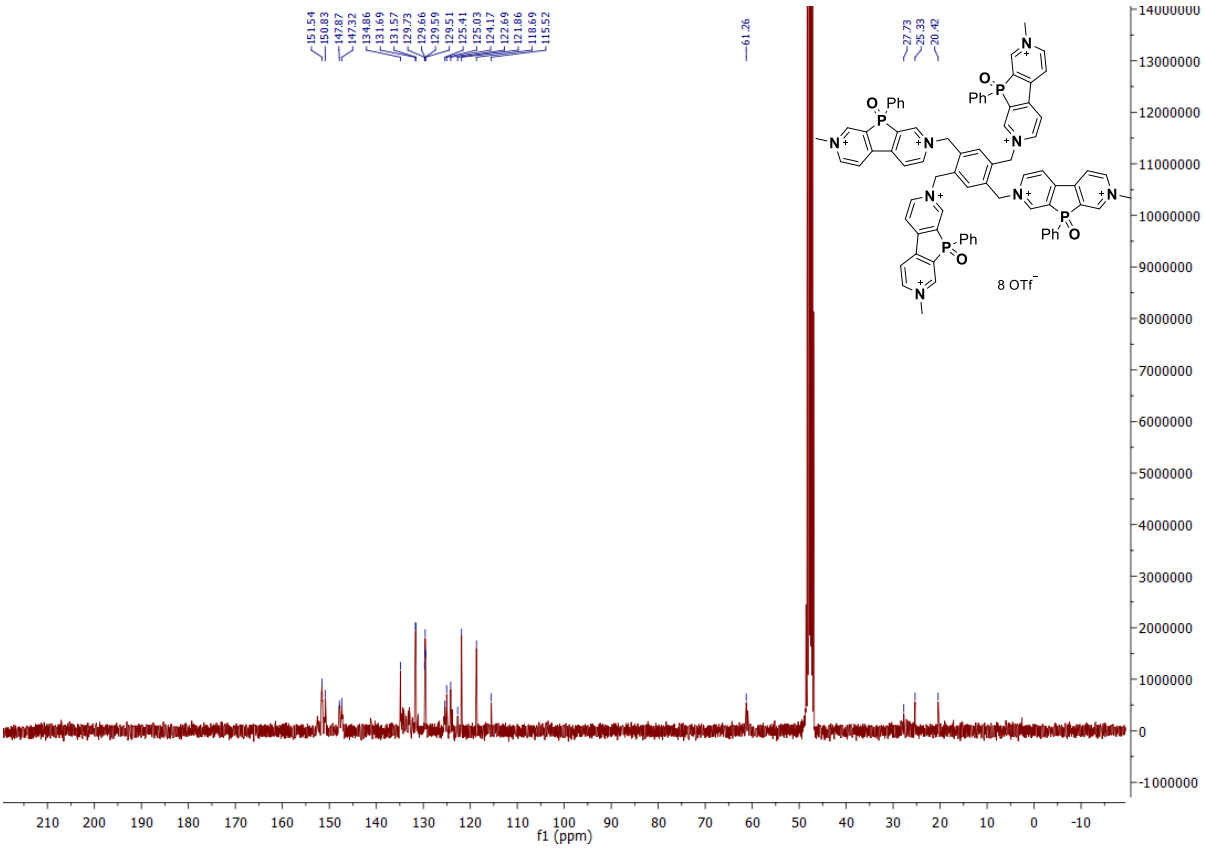


Figure S20 $^{13}C\{^{1}H\}$-NMR of **6b** in methanol-d_4.

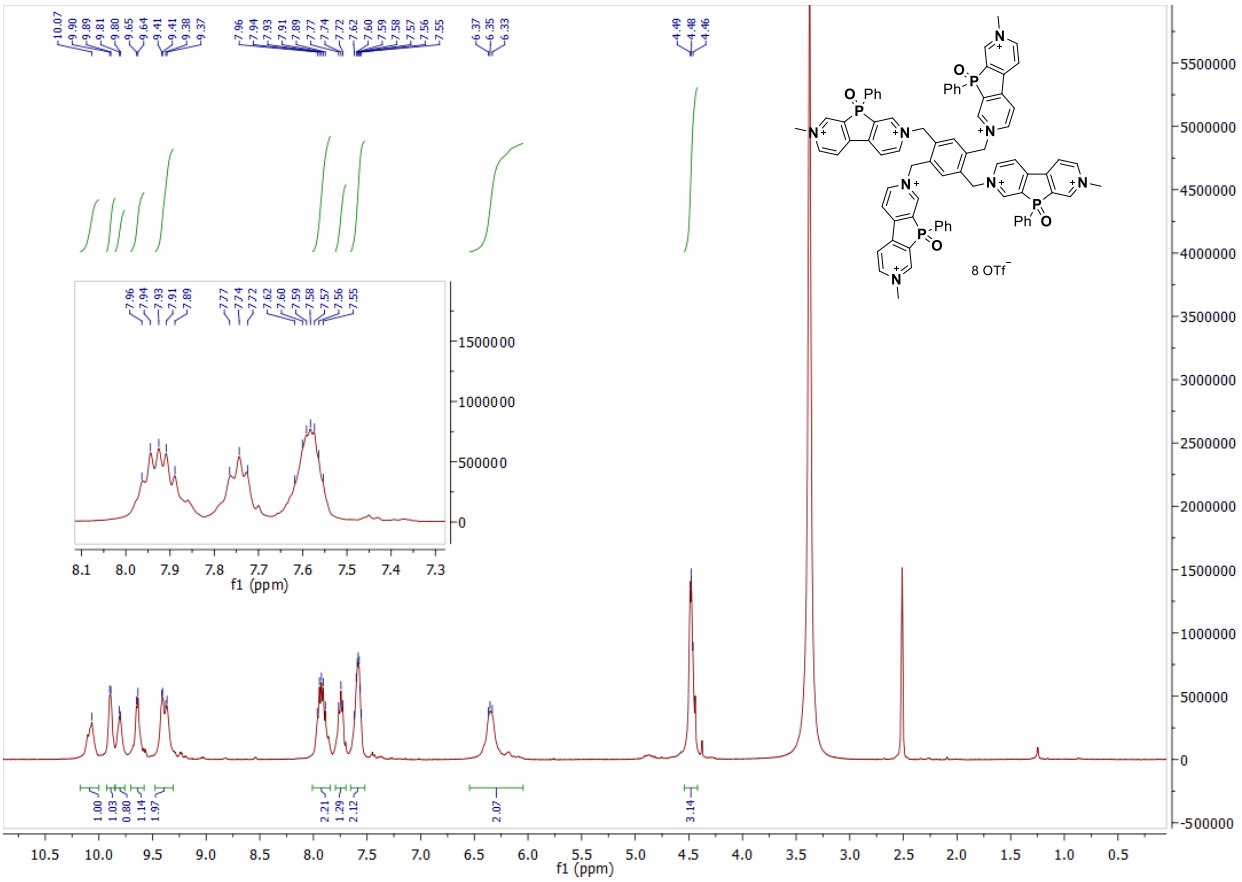
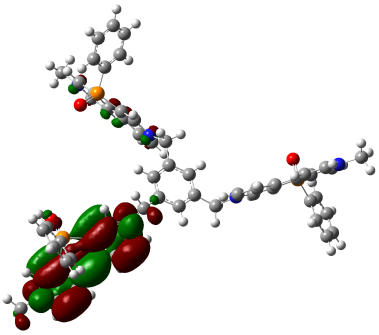


Figure S21 ^{1}H-NMR of **6b** in methanol-d_4.

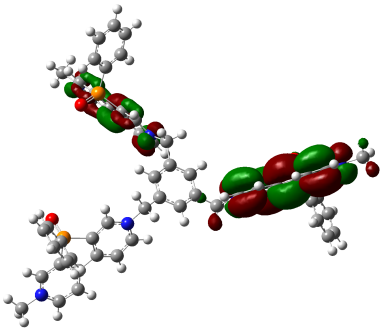
DFT Calculations

Figure S22 DFT calculations for **5b**.

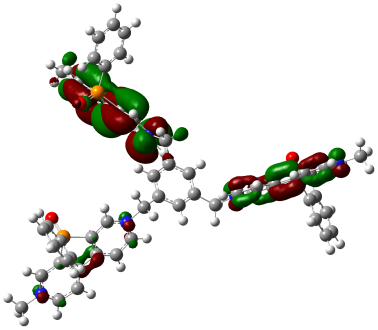
LUMO+2 -4.31 eV



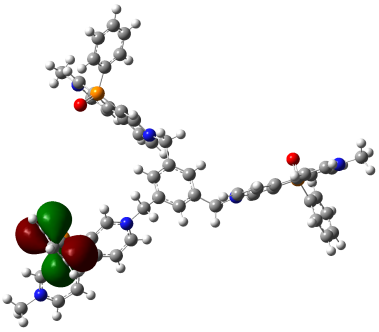
LUMO+1 -4.31 eV



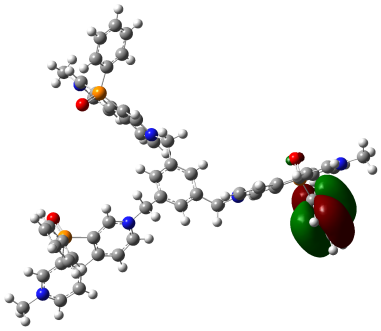
LUMO -4.32 eV



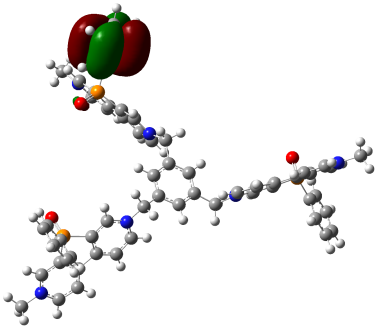
HOMO -7.69 eV



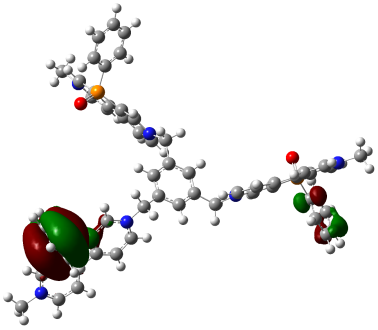
HOMO-1 -7.69 eV



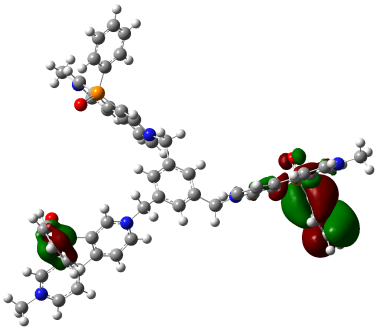
HOMO-2 -7.69 eV

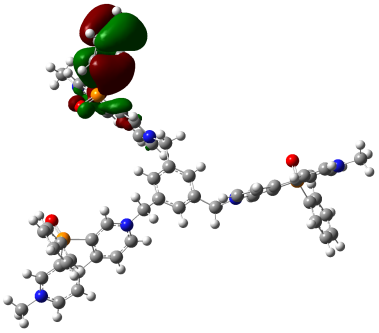


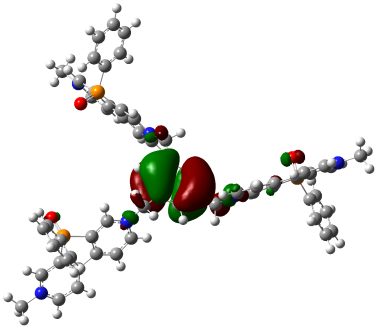
HOMO-3 -7.83 eV

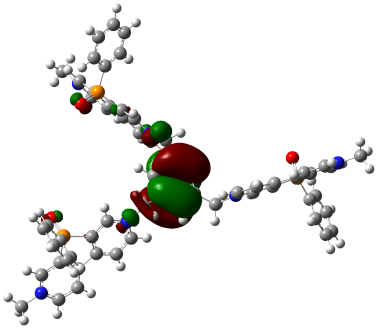


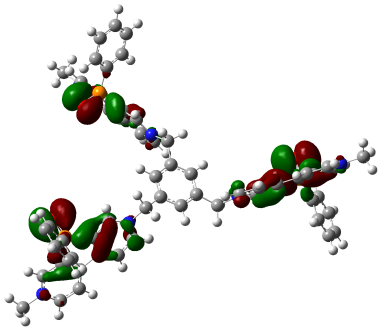
HOMO-4 -7.83 eV



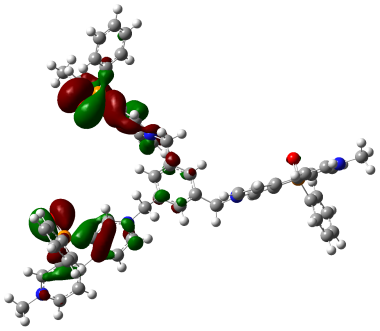
HOMO-5  -7.83 eV

HOMO-6  -8.17 eV

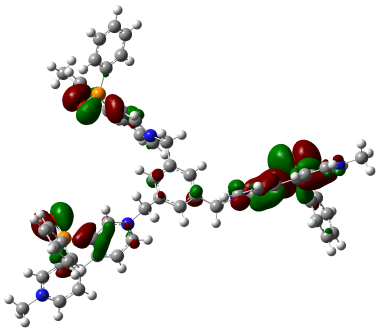
HOMO-7  -8.23 eV

HOMO-8  -8.64 eV

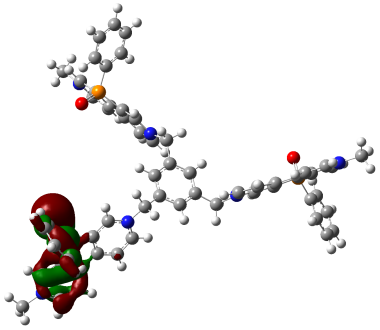
HOMO-9 -8.64 eV



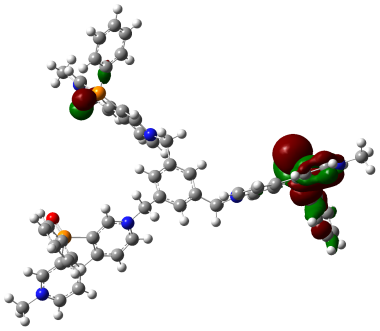
HOMO-10 -8.65 eV

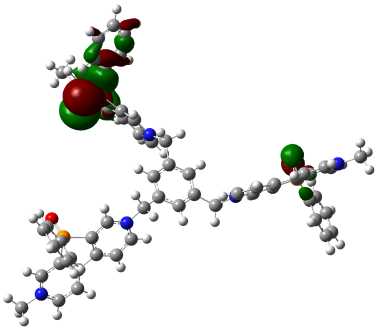


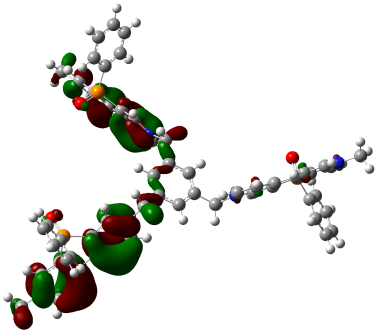
HOMO-11 -8.73 eV

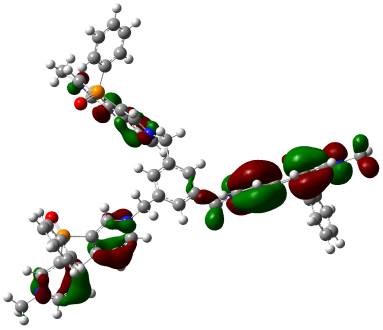


HOMO-12 -8.74 eV



HOMO-13  -8.74 eV

HOMO-14  -9.22 eV

HOMO-15  -9.23 eV

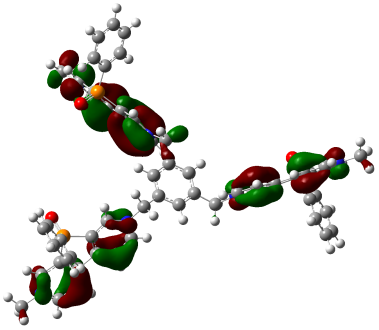
HOMO-16  -9.25 eV

Table S2 Cartesian Coordinates for optimized structure of **5b**.

C	-0.49958406	-0.16011801	0.59283007
C	0.52981104	0.74881503	0.28557005
C	1.75646812	0.25021797	-0.18021199
C	1.97677110	-1.12991914	-0.32590000
C	0.93954000	-2.01152219	0.00935103
C	-0.30723408	-1.54460412	0.46549606
H	-1.43982713	0.21231305	0.99419110
H	2.56389320	0.94529900	-0.40186901
H	1.11345098	-3.08387827	-0.05876198
C	5.67164338	-1.11369624	-0.70432603
C	4.57731528	-2.03044828	1.17438411
C	6.88173448	-1.13226927	-0.03806898
H	5.57360637	-0.75428021	-1.72316111
C	5.76150837	-2.06439431	1.89481517
H	3.64037720	-2.37722228	1.59314515
C	6.94043844	-1.60952331	1.28628912
H	5.73704636	-2.44473934	2.91077325
C	-0.29556996	3.32616725	-1.44214609
C	-1.37596703	3.91151233	0.57238107
C	-0.99145099	4.29997435	-2.14226114
H	0.43296308	2.68313819	-1.92146012
C	-2.09296306	4.90114342	-0.07192798
H	-1.47852404	3.71598231	1.63446715
C	-1.90033004	5.11442043	-1.45103608
H	-0.80140797	4.40716435	-3.20517322
C	-2.17081928	-3.59425323	-1.05499605
C	-3.67330639	-3.20356416	0.71985908
C	-3.14234137	-4.27107626	-1.77770811
H	-1.16619520	-3.45673124	-1.43508608
C	-4.67799048	-3.87431118	0.04993203
H	-3.82093538	-2.76617812	1.70160415
C	-4.41880147	-4.42817123	-1.21929007
H	-2.87943036	-4.66399529	-2.75433418
C	8.30357057	-1.52488534	1.87472917
C	8.71871959	-1.95109338	3.14102826
C	9.23768568	-0.92789131	1.00809610
C	10.04504971	-1.75759240	3.50474529
H	8.05497754	-2.42790140	3.85437432
C	10.54803676	-0.75861833	1.42785114
H	10.43204772	-2.06402343	4.47079136
H	11.31391182	-0.30087232	0.81072009
C	-2.74514907	6.21272553	-1.99168313
C	-3.61036312	6.76294261	-1.02785105
C	-2.75612806	6.72473860	-3.29356923
C	-4.46797016	7.79091773	-1.38705308
C	-3.63391710	7.75853568	-3.59326925
H	-2.10807702	6.35681854	-4.08189129
H	-5.16154620	8.25444678	-0.69344003
H	-3.69129009	8.20223069	-4.58153732

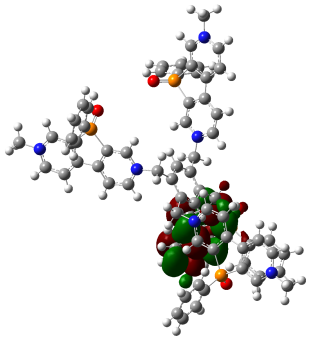
C	-5.60316060	-5.10696226	-1.80963111
C	-6.75365464	-4.99694522	-1.00649505
C	-5.67730161	-5.80491630	-3.01965021
C	-7.94209874	-5.56776822	-1.43370709
C	-6.89488570	-6.35946130	-3.39331524
H	-4.82831354	-5.93779731	-3.68172126
H	-8.86449782	-5.51363418	-0.86501804
H	-7.01997072	-6.91381437	-4.31723330
N	4.53329728	-1.56123524	-0.10108298
N	10.93027980	-1.17108338	2.66095223
N	-0.48052998	3.14013424	-0.10785898
N	-4.46833915	8.27071173	-2.65484518
N	-7.99635381	-6.23560531	-2.61224717
N	-2.43016928	-3.07528118	0.17335604
P	8.49225962	-0.35203625	-0.59653002
P	-6.49082262	-3.96506915	0.51947306
P	-3.51194714	5.90977754	0.62275307
O	-7.09907562	-2.60422903	0.47184006
O	-4.65949925	5.01278549	0.94456010
O	8.32393765	1.12433387	-0.72456903
C	9.24830367	-1.23551734	-1.94744212
C	9.67537670	-0.46392929	-3.04528821
C	9.47206966	-2.62727845	-1.91703012
C	10.32611575	-1.09199235	-4.10757129
H	9.51261771	0.60966880	-3.05499321
C	10.11795166	-3.23884651	-2.98635420
H	9.15522457	-3.23123149	-1.06884406
C	10.54622973	-2.47114147	-4.07792929
H	10.66833479	-0.50265732	-4.95244835
H	10.29965165	-4.30897860	-2.97097720
H	11.06021472	-2.95315052	-4.90419035
C	-2.98489907	7.08021760	1.85903017
C	-3.69373712	7.07474363	3.07590226
C	-1.95165297	8.01296563	1.63398615
C	-3.36364407	8.00551471	4.06123034
H	-4.49953220	6.36453458	3.23545627
C	-1.63179792	8.93138974	2.62839523
H	-1.40462492	8.03293165	0.69331008
C	-2.33893197	8.92846974	3.83848532
H	-3.91321011	8.01550769	4.99724940
H	-0.84179984	9.65740177	2.46327521
H	-2.09213494	9.65596881	4.60598638
C	-6.77235365	-4.96586021	1.96701418
C	-7.58527273	-4.40783315	2.97240525
C	-6.26365868	-6.27427033	2.09838719
C	-7.88511577	-5.16538720	4.10493834
H	-7.98483171	-3.40458907	2.85802424
C	-6.56818368	-7.01466037	3.23581627
H	-5.64339564	-6.71877440	1.32231913
C	-7.37964974	-6.46107233	4.23553035
H	-8.51967280	-4.74641815	4.87955440
H	-6.18613670	-8.02491546	3.34480628

H	-7.62268677	-7.04862736	5.11584242
C	12.34903988	-1.00211740	3.10628926
H	12.35445289	-0.54315937	4.09655834
H	12.82579392	-1.98507549	3.13933027
H	12.86891197	-0.35770836	2.39865621
C	-9.27559990	-6.87433431	-3.05389221
H	-9.41512791	-6.68442826	-4.11908929
H	-9.21466890	-7.94926640	-2.86414319
H	-10.10140497	-6.43997023	-2.49161216
C	-5.37844220	9.39685987	-3.03312421
H	-4.78256813	10.30594489	-3.14858322
H	-5.87628824	9.14730586	-3.97162628
H	-6.12070224	9.53287085	-2.24759315
C	0.43550707	2.22464815	0.67114507
H	0.10782105	2.30612217	1.70961216
H	1.42645816	2.68312416	0.61406507
C	-1.31886519	-2.52906317	1.04806311
H	-1.82520921	-2.06716312	1.89672317
H	-0.79284617	-3.41014325	1.42770114
C	3.26885319	-1.67913922	-0.92282805
H	3.48804421	-1.17351519	-1.86562212
H	3.15482415	-2.74345630	-1.14665306

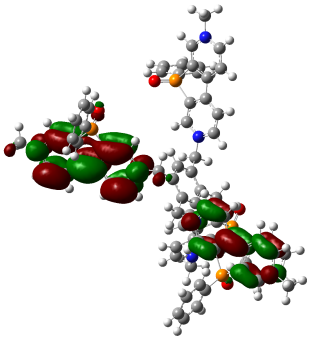
Compound 6b

Figure S23 DFT calculations for **6b**.

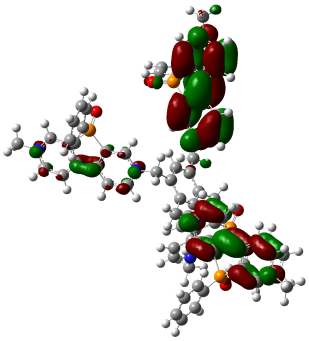
LUMO+3 -4.46 eV



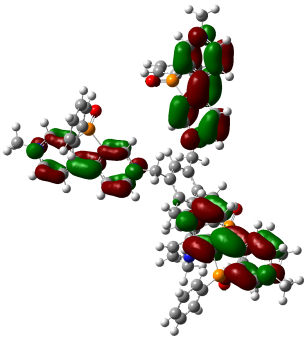
LUMO+2 -4.48 eV



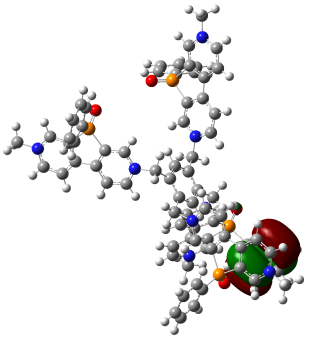
LUMO+1 -4.51 eV



LUMO -4.52 eV

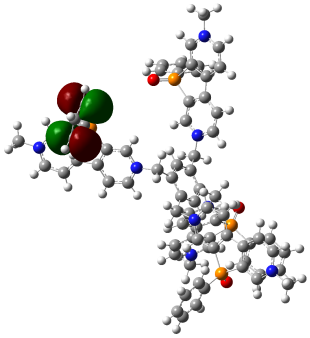


HOMO



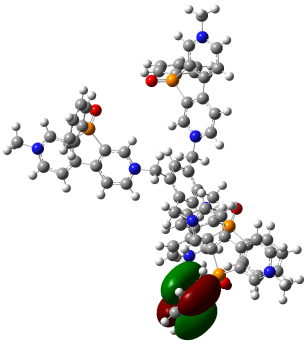
-7.69 eV

HOMO-1



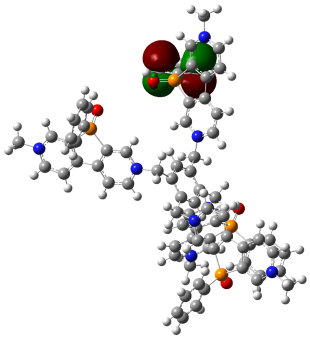
-7.69 eV

HOMO-2

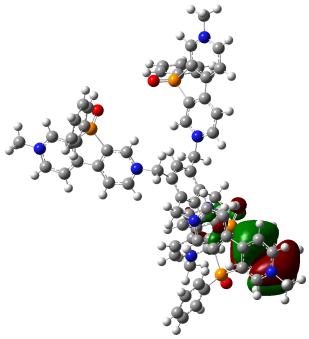


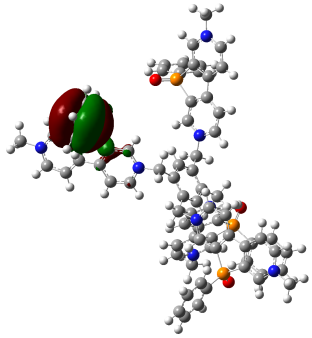
-7.69 eV

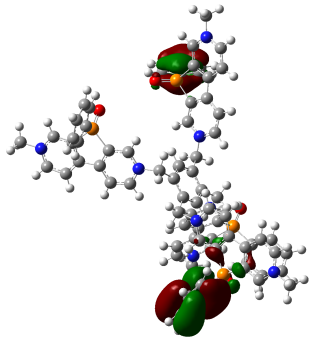
HOMO-3

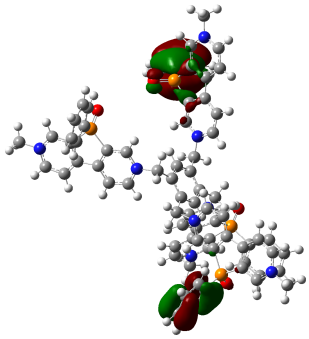


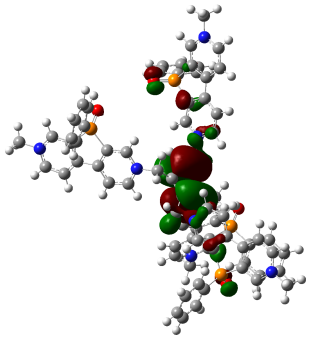
-7.70 eV

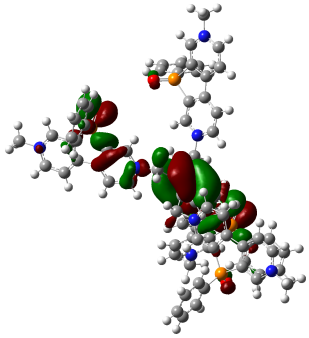
HOMO-4  -7.85 eV

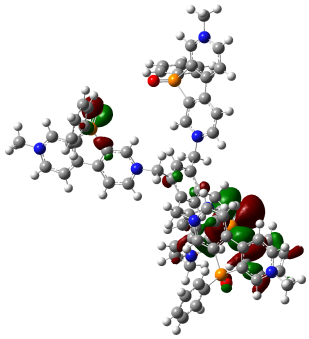
HOMO-5  -7.85 eV

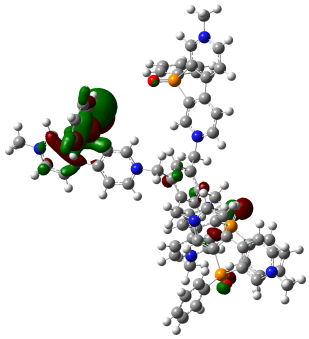
HOMO-6  -7.85 eV

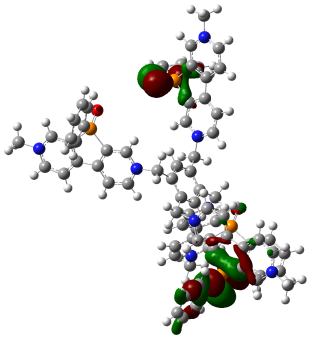
HOMO-7  -7.86 eV

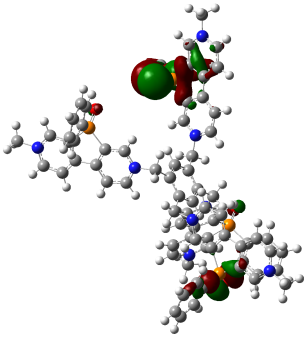
HOMO-8  -8.59 eV

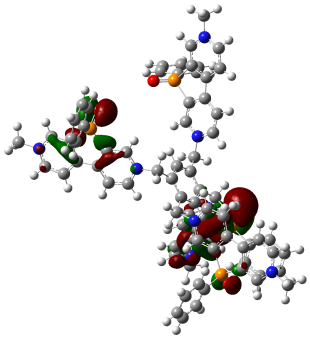
HOMO-9  -8.72 eV

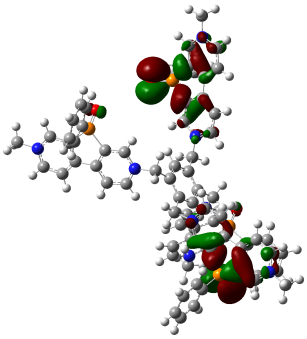
HOMO-10  -8.74 eV

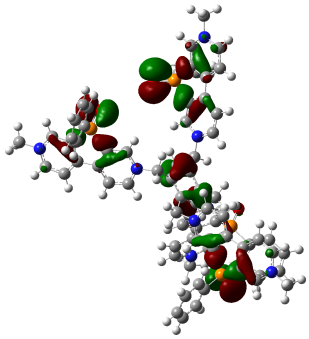
HOMO-11  -8.76 eV

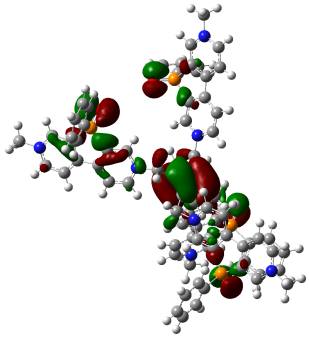
HOMO-12  -8.76 eV

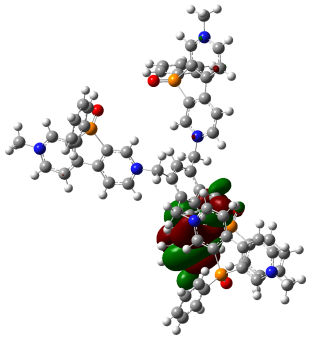
HOMO-13  -8.77 eV

HOMO-14  -8.81 eV

HOMO-15  -8.83 eV

HOMO-16  -8.85 eV

HOMO-17  -8.89 eV

HOMO-18  -9.39 eV

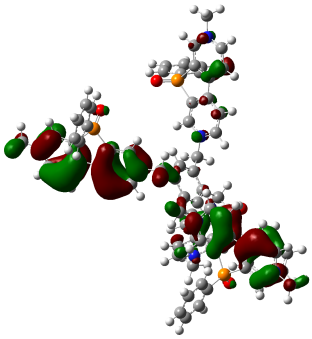
HOMO-19  -9.41 eV

Table S3 Cartesian coordinates for optimized structure of **6b**.

C	1.51309	-0.14228	0.32716
C	0.80827	-1.35634	0.22449
C	-0.61034	-1.30062	0.2022
C	-1.225	-0.034	0.30113
C	-0.51984	1.17304	0.42614
C	0.90182	1.12012	0.42883
H	2.59996	-0.18504	0.35251
H	-2.31263	0.00363	0.30264
C	-3.55717	-3.4883	-0.75163
C	-1.78457	-2.95431	-2.21567
C	-4.28391	-4.04054	-1.78783
H	-3.93473	-3.45493	0.2652
C	-2.47545	-3.48183	-3.29684
H	-0.80148	-2.5138	-2.32676
C	-3.74872	-4.039	-3.09359
H	-2.00843	-3.44229	-4.27572
C	-2.04212	2.70916	2.80926
C	-3.61139	3.0841	1.08424
C	-2.96559	3.06993	3.77686
H	-1.0325	2.41251	3.06746
C	-4.57065	3.46025	2.00545
H	-3.80645	3.07155	0.01688
C	-4.25667	3.45793	3.38095
H	-2.65921	3.04296	4.81777
C	1.5303	3.34233	-1.56725
C	3.3281	4.03668	-0.205
C	1.97722	4.13623	-2.61466
H	0.64291	2.72738	-1.65249
C	3.82629	4.8322	-1.21661
H	3.81682	3.95782	0.76082
C	3.14212	4.90273	-2.44919
H	1.40406	4.14252	-3.53624
C	3.91622	-3.31433	0.641
C	2.26674	-3.31286	2.33201
C	4.84505	-3.84992	1.51188
H	4.15593	-3.08811	-0.39275
C	3.15911	-3.84163	3.25083
H	1.23944	-3.09253	2.59667
C	4.47529	-4.12165	2.84631
H	2.80934	-4.02591	4.26164
C	-4.67676	-4.61304	-4.1044
C	-4.44	-4.82582	-5.46756
C	-5.92924	-4.95834	-3.56244
C	-5.45983	-5.36372	-6.2443
H	-3.49634	-4.59672	-5.95131
C	-6.90983	-5.4896	-4.38867
H	-5.34043	-5.55498	-7.30581
H	-7.89505	-5.77332	-4.033
C	3.76703	5.85384	-3.40707

C	4.85519	6.55326	-2.85183
C	3.3948	6.10973	-4.73223
C	5.53269	7.48898	-3.62182
C	4.11226	7.05639	-5.45404
H	2.57694	5.59968	-5.23011
H	6.37797	8.06016	-3.25215
H	3.87731	7.29996	-6.48525
C	-5.40282	3.84889	4.24345
C	-6.59159	4.04573	3.51621
C	-5.41114	4.03077	5.63155
C	-7.75228	4.40573	4.1873
C	-6.60319	4.39422	6.24732
H	-4.53044	3.91112	6.25379
H	-8.69983	4.57212	3.68549
H	-6.67742	4.55449	7.31823
C	5.59681	-4.65102	3.66637
C	5.55555	-5.0985	4.9923
C	6.81875	-4.67913	2.96817
C	6.73223	-5.54989	5.57864
H	4.64787	-5.12007	5.58624
C	7.96184	-5.13905	3.6081
H	6.76836	-5.91292	6.60089
H	8.93298	-5.18629	3.12637
C	9.13635	-6.06578	5.58347
H	9.98967	-5.94842	4.91695
H	9.29125	-5.48177	6.49345
H	8.99385	-7.12146	5.82807
C	-8.99311	4.97219	6.25612
H	-9.18588	4.24667	7.04941
H	-8.84809	5.9695	6.6794
H	-9.824	4.98193	5.55206
C	5.884	8.73868	-5.73256
H	6.29562	8.2373	-6.6118
H	5.17973	9.51812	-6.03308
H	6.68846	9.17254	-5.14032
C	-7.71919	-6.27524	-6.59254
H	-7.44284	-7.30843	-6.82038
H	-8.67577	-6.24806	-6.07207
H	-7.7799	-5.68715	-7.51005
P	-6.41138	3.71276	1.69468
N	-7.74209	4.57211	5.53212
N	-2.3549	2.71436	1.48173
N	-2.3145	-2.95294	-0.96183
N	-6.66414	-5.68155	-5.70746
N	2.18672	3.29963	-0.37618
N	5.15359	7.72704	-4.90053
N	2.63536	-3.0491	1.04576
N	7.90321	-5.56238	4.89394
O	-6.96734	2.41518	1.20914
C	-6.81526	5.19867	0.80406
C	-7.66845	5.05508	-0.30873
C	-6.39998	6.47837	1.23049

C	-8.10288	6.19466	-0.98592
H	-8.00422	4.06956	-0.61713
C	-6.83674	7.60343	0.53931
H	-5.75282	6.60279	2.09658
C	-7.69045	7.46137	-0.56387
H	-8.77454	6.09422	-1.83278
H	-6.53017	8.59317	0.86333
H	-8.04293	8.34543	-1.08704
P	5.17925	6.13373	-1.06867
O	4.72082	7.14006	-0.06559
C	6.82608	5.47838	-0.92669
C	7.61714	5.98206	0.12599
C	7.36948	4.57439	-1.86472
C	8.94853	5.57923	0.23079
H	7.20119	6.69582	0.83071
C	8.6965	4.17725	-1.74048
H	6.77264	4.1895	-2.68937
C	9.4853	4.68277	-0.69721
H	9.56977	5.97581	1.02778
H	9.12709	3.48787	-2.46009
H	10.52593	4.38243	-0.61712
P	6.70296	-4.00324	1.23873
O	7.23684	-2.62372	1.03617
C	7.18418	-5.27952	0.09785
C	8.06812	-4.90393	-0.93422
C	6.79475	-6.62718	0.255
C	8.559	-5.881	-1.8004
H	8.38431	-3.87004	-1.03529
C	7.28757	-7.58709	-0.62249
H	6.12424	-6.93168	1.05629
C	8.17174	-7.21476	-1.64512
H	9.25451	-5.60332	-2.58626
H	7.00093	-8.62772	-0.50634
H	8.56734	-7.97275	-2.31482
C	-1.28243	2.50654	0.44141
H	-1.78212	2.63935	-0.52158
H	-0.59465	3.34757	0.54898
C	1.8231	2.31446	0.71839
H	2.77668	1.92995	1.09038
H	1.40331	2.92583	1.5195
C	1.6086	-2.65328	0.014
H	2.16513	-2.56837	-0.92274
H	0.95036	-3.51615	-0.0979
C	-1.51461	-2.54204	0.25672
H	-2.26053	-2.37874	1.037
H	-0.94995	-3.42851	0.55224
P	-6.09701	-4.55365	-1.75458
C	-6.41979	-6.05832	-0.86261
C	-7.43674	-6.00757	0.11236
C	-5.77453	-7.27667	-1.16467
C	-7.80313	-7.17835	0.77646
H	-7.94716	-5.07255	0.323

C	-6.1471	-8.43296	-0.48758
H	-4.99877	-7.33101	-1.92611
C	-7.16281	-8.38401	0.47789
H	-8.59778	-7.15168	1.51551
H	-5.66368	-9.37737	-0.7177
H	-7.4615	-9.29441	0.98923
O	-6.90549	-3.34239	-1.43001

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(Note: this also doubles as the full reference 18 from the main manuscript) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.