Supplementary Materials:

Near-Infrared Absorbing Molecule Based on Triphenylamine Radical Cation with Extended Homoaryl π-System

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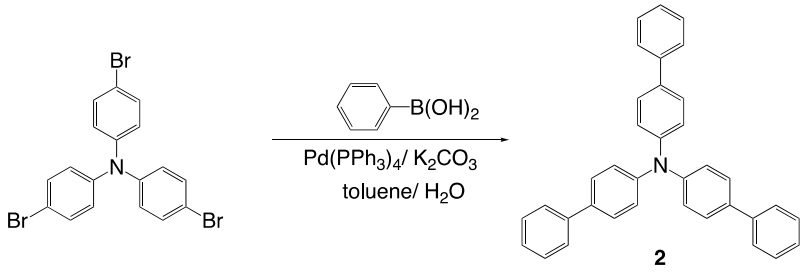
Contents

1. General

^{1}H and ^{13}C NMR spectra were recorded on JEOL JNM-ECZ600R or JEOL JNM-GSX400 spectrometers. Chemical shifts are reported in parts per million (ppm, δ scale) from residual protons in the deuterated solvent for ^{1}H NMR (δ 7.26 ppm for chloroform) and from the solvent carbon for ^{13}C NMR (δ 77.16 ppm for deuterated chloroform). Fluorescence spectra were recorded on JASCO FP-8600 Fluorescence Spectrometer. UV-vis-NIR absorption spectra were recorded on V-670 UV-Vis-NIR Spectrophotometer. Analytic thin layer chromatography (TLC) was performed on Merck, pre-coated plate silica gel 60 F_{254} (0.25 mm thickness). Unless otherwise noted, all materials were obtained from commercial suppliers and used without further purification. All reactions were performed under nitrogen atmosphere.

2. Synthesis of 2–5

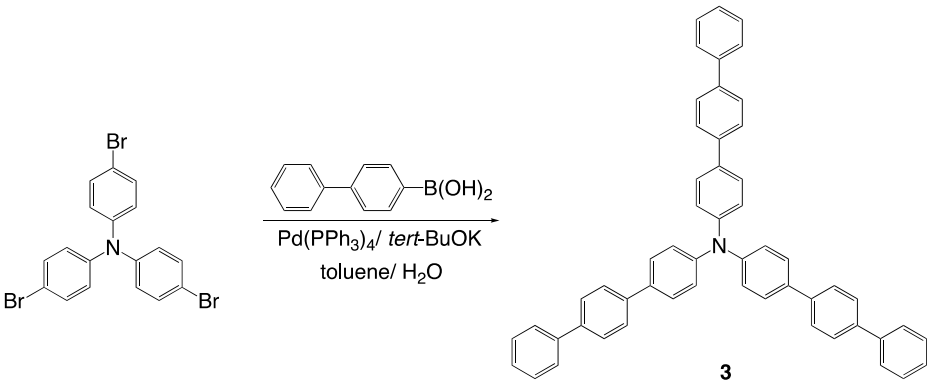


Tri([1,1'-biphenyl]-4-yl)amine (2)

A mixture of 4, 4', 4''-tribromotriphenylamine (521 mg, 1.05 mmol), pheylboronic acid (1.32 g, 10.6 mmol), tetrakis(triphenylphosphine)palladium(0) (79 mg, 0.063 mmol, K_2CO_3 (2.02 g, 5.62 mmol) in toluene (10.4 mL) and water (2.5 mL) was purged with nitrogen and stirred for 10 minutes, then heated at 90 °C under nitrogen for 24 h. After cooling to room temperature, H_2O (30 mL) was added to the resulting mixture, and the mixture was extracted with ethyl acetate (3 × 20 mL). The combined organic phase was dried over Na_2SO_4 and the solvent was evaporated in vacuo. The residue was purified by column chromatography on silica gel (eluted with *n*-hexane/ chloroform = 7/3) to give the pure product as a white solid (316 mg, 62%). The ^{1}H and ^{13}C NMR spectra were consistent with those in the literature [1].

^{1}H NMR (400MHz, $CDCl_3$): δ 7.23 (d, 6H, J = 8.8 Hz), 7.31 (t, 3H, J = 7.6 Hz), 7.42 (t, 6H, J = 7.6 Hz), 7.52 (d, 6H, J = 8.8 Hz), 7.59 (d, 6H, J = 7.6 Hz)
^{13}C NMR (100MHz, $CDCl_3$): δ 124.51, 126.77, 126.96, 127.82, 128.82, 135.79, 140.72,

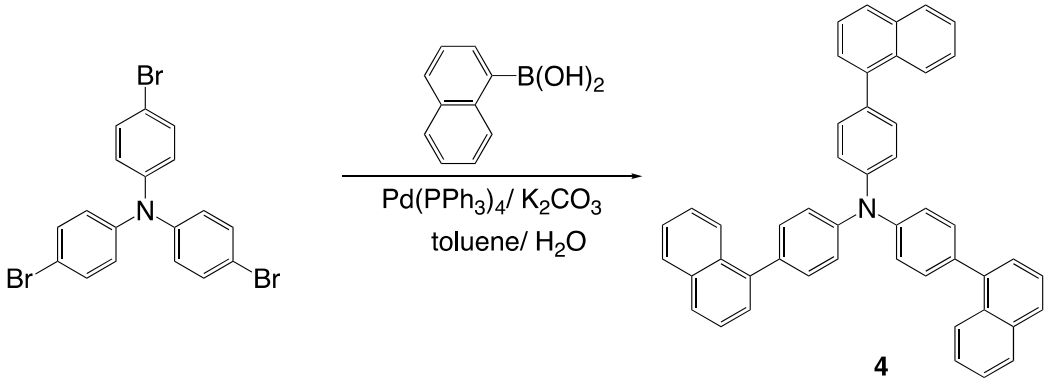
146.97
HRMS(DART): m/z: Calcd. for $C_{36}H_{27}N$ $[M]^+$: 473.2144; Found: 473.2130



Tri([1,1':4',1''-terphenyl]-4-yl)amine (3)

A mixture of 4, 4', 4''-tribromotriphenylamine (157 mg, 0.33 mmol), 4-biphenylboronic acid (241 mg, 1.22 mmol), tetrakis(triphenylphosphine)palladium(0) (17 mg, 0.014 mmol), potassium *tert*-butoxide (132 mg, 5.62 mmol) in toluene (2.1 mL) and water (1.2 mL) was purged with nitrogen and stirred for 10 minutes, then heated at 90 °C under nitrogen for 24 h. After cooling to room temperature, H_2O (30 mL) was added to the resulting mixture, and the mixture was extracted with chloroform (3 × 20 mL). The combined organic phase was dried over Na_2SO_4 and the solvent was evaporated in vacuo. The obtained solid was purified by recrystallization from ethanol to afford a white solid (108 mg, 47%). The ^1H and ^{13}C NMR spectra were consistent with those in the literature [1].

^1H NMR (400MHz, $CDCl_3$): δ 7.27 (d, J = 8.4 Hz, 6H), 7.35 (t, J = 7.6 Hz, 3H), 7.46 (t, J = 7.6 Hz, 6H), 7.58 (d, J = 8.4 Hz, 6H), 7.64 - 7.72 (m, 18H)
^{13}C NMR (100MHz, $CDCl_3$): δ 124.58, 127.05, 127.08, 127.33, 127.55, 127.89, 128.85, 135.28, 139.59, 139.85, 140.82, 146.99
HRMS(DART): m/z: Calcd. for $C_{54}H_{39}N$ $[M]^+$: 701.3083; Found: 701.3082



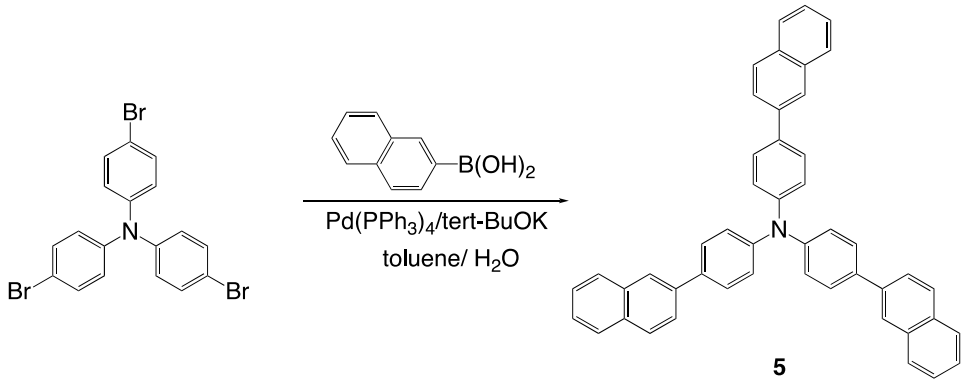
Tris(4-(naphthalen-1-yl)phenyl)amine (4)

A mixture of 4, 4', 4"-tribromotriphenylamine (2.00 g, 4.15 mmol), 1-naphthylboronic acid (3.57 g, 20.7 mmol), tetrakis(triphenylphosphine)palladium(0) (240 mg, 0.21 mmol), K_2CO_3 (2.87 g, 20.7 mmol) in toluene (42 mL) and water (10.4 mL) was purged with nitrogen and stirred for 10 minutes, then heated at 90 °C under nitrogen for 24 h. After cooling to room temperature, H_2O (30 mL) was added to the resulting mixture, and the mixture was extracted with ethyl acetate (3 × 20 mL). The combined organic phase was dried over Na_2SO_4 and the solvent was evaporated in vacuo. The residue was redissolved in small amount of ethyl acetate. Addition of large amount of methanol gave the pure product as a yellow powder (845 mg, 33%).The ^1H and ^{13}C NMR spectra were consistent with those in the literature [2].

^1H NMR (400MHz, $CDCl_3$): δ 7.40 (d, 6H, J = 8.0 Hz), 7.45 - 7.55 (m, 18H), 7.85 (d, 3H, J = 8.0 Hz), 7.91 (d, 3H, J = 8.8 Hz), 8.07 (d, 3H, J = 8.8 Hz)

^{13}C NMR (100MHz, $CDCl_3$): δ 124.11, 125.56, 125.87, 126.09, 126.19, 127.03, 127.57, 128.43, 131.14, 131.77, 133.99, 135.34, 139.99, 146.97

HRMS(DART): m/z: Calcd. for $C_{48}H_{34}N$ $[M]^+$: 623.2613; Found: 623.2613



5

Tris(4-(naphthalen-1-yl)phenyl)amine (5)

A mixture of 4, 4', 4''-tribromotriphenylamine (221 mg, 0.46 mmol), 2-naphthylboronic acid (373 mg, 20.7 mmol), tetrakis(triphenylphosphine)palladium(0) (30 mg, 0.026 mmol), potassium *tert*-butoxide (245 mg, 2.19 mmol) in toluene (4.2 mL) and water (0.9 mL) was purged with nitrogen and stirred for 10 minutes, then heated at 90 °C under nitrogen for 24 h. After cooling to room temperature, H_2O (30 mL) was added to the resulting mixture, and the mixture was extracted with ethyl acetate (3 × 20 mL). The combined organic phase was dried over Na_2SO_4 and the solvent was evaporated in vacuo. The residue was redissolved in small amount of ethyl acetate. Addition of large amount of methanol gave the pure product as a yellow powder (248 mg, 95%). The ^1H and ^{13}C NMR spectra were consistent with those in the literature [3].

^1H NMR (400MHz, $CDCl_3$): δ 7.32 (d, 6H, J = 8.8 Hz), δ7.44 - 7.52 (m, 6H), δ7.68 (d, 6H, J = 8.8 Hz), δ7.76 (dd, 3H, J = 8.8, 1.8 Hz), δ7.85 - 7.92 (m, 9H), δ8.04 (s, 3H)
^{13}C NMR (100MHz, $CDCl_3$): 124.67, 125.24, 125.36, 125.83, 126.34, 127.71, 128.19, 128.30, 128.49, 132.26, 133.89, 135.73, 138.03, 147.03
HRMS(DART): m/z: Calcd. for $C_{48}H_{34}N$ $[M]^+$: 623.2613; Found: 623.2589

3. DFT Calculations

Density functional theory (DFT) calculations were performed using Gaussian 09 program [4]. Geometries were optimized at the (U)B3LYP/6-31G(d) level of theory [5–8] with the polarizable continuum model (PCM) [9] using dichloromethane as a solvent. TD-DFT calculations were carried out at the same level of theory. The data were summarized in Figures S1-S4.

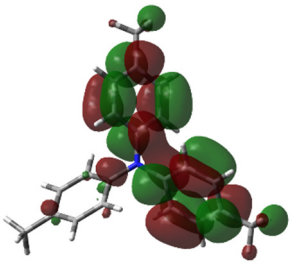
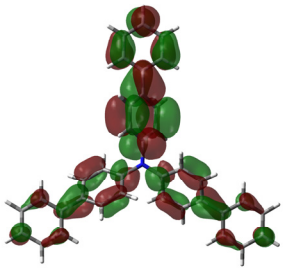
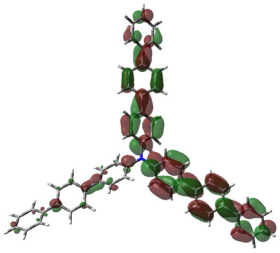
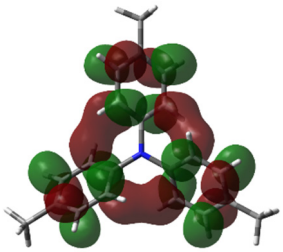
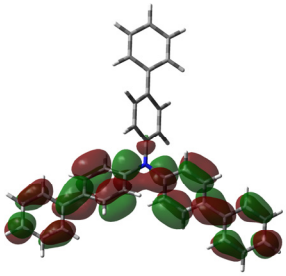
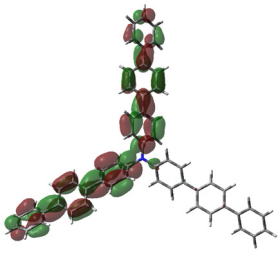
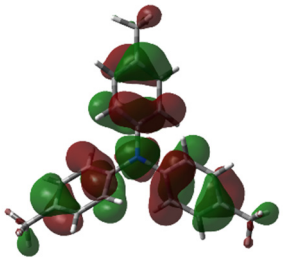
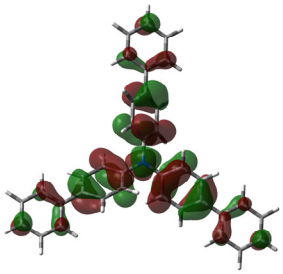
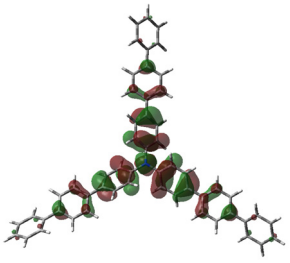
		
LUMO+1 –0.25 eV (79)	**LUMO+1** –1.03 eV (127)	**LUMO+1** –1.29 eV (187)
		
LUMO –0.36 eV (78)	**LUMO** –1.03 eV (126)	**LUMO** –1.30 eV (186)
		
HOMO –4.87 eV (77)	**HOMO** –4.97 eV (125)	**HOMO** –4.95 eV (185)
Excited State 1: 3.8056 eV (325.80 nm), f = 0.0184 77 → 78 0.69882 Excited State 2: 3.9986 eV (310.07 nm), f = 0.3940 77 → 79 0.57469 77 → 80 0.40005	Excited State 1: 3.4168 eV (362.87 nm), f = 0.7802 125 → 126 0.70281 Excited State 2: 3.4177 eV (362.77 nm), f = 0.7856 125 → 127 0.70281	Excited State 1: 3.1792 eV (389.98 nm), f = 1.1007 185 → 186 0.69857 Excited State 2: 3.1832 eV (389.50 nm), f = 1.1093 185 → 187 0.69857
1	**2**	**3**

Figure S1. HOMO, LUMO, and LUMO+1 orbitals of **1**–**3** with calculated energy levels.

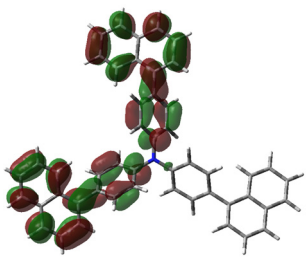
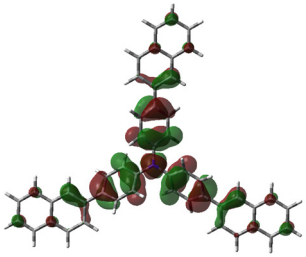
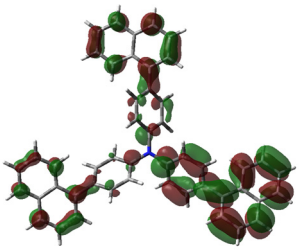
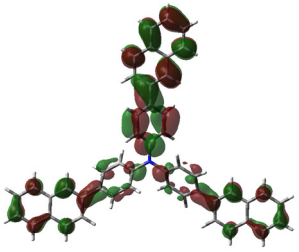
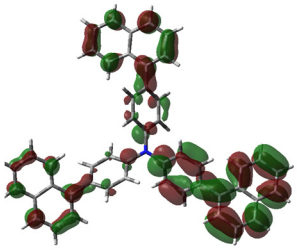
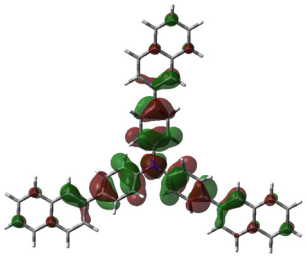
	
LUMO+1	**LUMO+1**
–1.26 eV (166)	–1.34 eV (166)
	
LUMO	**LUMO**
–1.27 eV (165)	–1.35 eV (165)
	
HOMO	**HOMO**
–5.00 eV (164)	–4.96 eV (164)
Excited State 1: 3.2674 eV (379.46 nm), f = 0.5633 164 → 165 0.68226 164 → 166 0.14462 Excited State 2: 3.2683 eV (379.35 nm), f = 0.5044 164 →165 -0.14477 164 → 166 0.68228	Excited State 1: 3.1530 eV (393.23 nm), f = 0.6550 164 → 165 0.69593 Excited State 2: 3.1642 eV 391.83 nm, f = 0.8951 164 → 166 0.69562
4	**5**

Figure S2. HOMO, LUMO, and LUMO+1 orbitals of **4** and **5** with calculated energy levels.

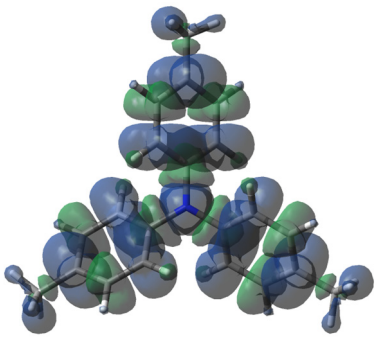
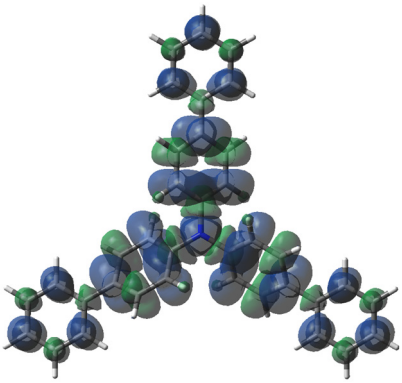
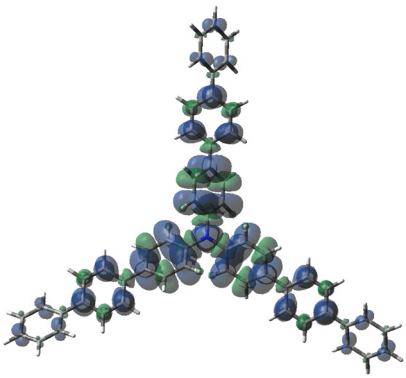
$1^{\bullet+}$	$2^{\bullet+}$	$3^{\bullet+}$
		
SOMO	**SOMO**	**SOMO**
–6.39 eV (77A)	–6.12 eV (125A)	–5.92 eV (185A)
–4.79 eV (77B)	–4.84 eV (125B)	–4.80 eV (185B)
Excited State 1: 1.9573 eV	Excited State 1: 1.4467 eV	Excited State 1: 1.1139 eV
(633.44 nm), f = 0.1138	(856.99 nm), f = 0.4062	(1113.10 nm), f = 0.5249
73B → 77B -0.40966	124B → 125B 0.99222	184B → 185B 0.99230
74B → 77B -0.12589	Excited State 2: 1.4480 eV	Excited State 2: 1.1148 eV
75B → 77B 0.22839	(856.26 nm), f = 0.4078	(1112.16 nm), f = 0.5251
76B → 77B 0.86567	123B → 125B 0.99223	183B → 185B 0.99228
Excited State 2: 1.9587 eV		
(633.00 nm), f = 0.1138		
73B → 77B 0.12414		
74B → 77B -0.41373		
75B → 77B 0.86377		
76B → 77B -0.22927		

Figure S3. Spin density plots of cation radical of **1**–**3** with their calculated energy levels.

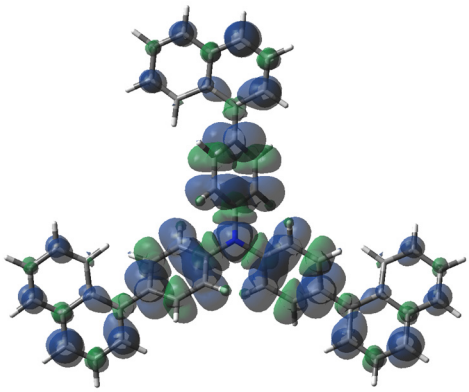
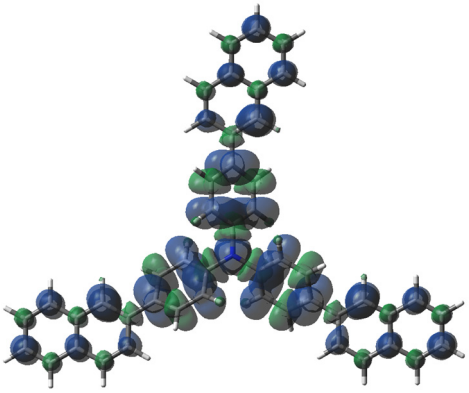
$4^{\bullet+}$	$5^{\bullet+}$
	
SOMO	**SOMO**
–5.92 eV (164A)	–5.92 eV (164A)
–4.84 eV (164B)	–4.80 eV (164B)
Excited State 1: 0.9192 eV	Excited State 1: 0.9971 eV
(1348.85 nm), f = 0.2587	(1243.50 nm), f = 0.2753
162B → 164B 0.97054	162B → 164B 0.14393
163B → 164B -0.23341	163B → 164B 0.98591
Excited State 2: 0.9207 eV	Excited State 2: 1.0038 eV
(1346.65 nm), f = 0.3431	(1235.15 nm), f = 0.3494
162B → 164B 0.23342	162B → 164B 0.98594
163B → 164B 0.97068	163B → 164B -0.14394

Figure S4. Spin density plots of cation radical of **4** and **5** with their calculated energy levels.

Computed Geometries

Tri-*p*-tolylamine (1)

N	-0.003179564332	0.000456811338	-0.002071284648
C	1.309467083054	-0.546155686887	-0.027607740154
C	-0.186621375309	1.409758417587	0.009733455123
C	-1.131764151528	-0.864575320862	0.008123851019
C	-1.172746740129	2.000091144008	0.817020327720
C	-1.353797366708	3.381408024754	0.816437141698
C	-0.552329881823	4.227315404414	0.036612120245
C	0.432078957534	3.628426846140	-0.761382210049
C	0.611343085807	2.246605290328	-0.786693207160
C	1.614317211901	-1.645229475399	-0.845738460912
C	2.899340631279	-2.184753538095	-0.855498485038
C	3.929469418993	-1.641613968089	-0.075647321293
C	3.615394652320	-0.540645215144	0.733904517118
C	2.330470262107	-0.003474278694	0.769250271777
C	-2.254582838323	-0.591291006012	-0.789257128721
C	-3.358822307562	-1.440702614027	-0.769996952699
C	-3.383728546231	-2.595146477651	0.025111571169
C	-2.252158301606	-2.865437379785	0.807120151050
C	-1.148033541007	-2.015349961177	0.812074072011
H	-1.799452049415	1.371932290816	1.442255622516
H	-2.127531515944	3.811243039630	1.449003494116
H	1.063494532632	4.252843668679	-1.389843784084
H	1.371097091129	1.810515385377	-1.427791392381
H	0.839380424269	-2.078849531055	-1.470120324544
H	3.107197195233	-3.039045150617	-1.496229270558
H	4.387281039512	-0.102234533472	1.362872323999
H	2.112178243509	0.838955386861	1.418207415399
H	-2.256510630597	0.286674519377	-1.427819201473
H	-4.214020980550	-1.207430883542	-1.400754452790
H	-2.236655031431	-3.752236052249	1.437067291913
H	-0.290368371394	-2.244022182936	1.437067929188
C	5.331083498709	-2.204493984061	-0.122560428231
H	5.942937555774	-1.694813623576	-0.879365015143
H	5.842647781802	-2.085128236476	0.838668009242

H	5.326962886666	-3.270197681498	-0.374805220091
C	-4.594239774593	-3.498942816130	0.057975536218
H	-4.315602191723	-4.533593005724	0.284621643858
H	-5.311163991643	-3.180985342102	0.827267819005
H	-5.125653229270	-3.492429157475	-0.899841425602
C	-0.726453797700	5.727669158145	0.075866557995
H	-1.770536012361	6.005390421544	0.255959946302
H	-0.128765872171	6.180075830026	0.879129453585
H	-0.408305698876	6.192283633710	-0.863573116694

Radical cation of tri-*p*-tolylamine ($1^{\bullet+}$)

N	-0.000603189451	0.001322860412	0.005814035847
C	1.162011499615	-0.800288390756	0.004791093343
C	0.112175081183	1.408870061505	0.004269861214
C	-1.276063387878	-0.604405654863	0.007433113358
C	-0.779499732150	2.191332759460	0.765777368030
C	-0.654933922513	3.572378256087	0.763115305403
C	0.340330925721	4.217202093858	0.006553907512
C	1.221125359674	3.421055663765	-0.748335517932
C	1.119462610171	2.038404745685	-0.755224893976
C	1.201881488688	-1.989079880744	-0.752119359611
C	2.348917178373	-2.767775609428	-0.747188824134
C	3.480956202986	-2.400998111170	0.003517751578
C	3.421408726065	-1.215629370253	0.758487142873
C	2.287380131601	-0.417597393804	0.762624449139
C	-2.325307971702	-0.049045797203	-0.752978345051
C	-3.572847606428	-0.654111884916	-0.745805358630
C	-3.821062626213	-1.813552597857	0.011266778189
C	-2.765275424845	-2.349111823025	0.771295460294
C	-1.507498740291	-1.765702463061	0.772497826837
H	-1.533141262094	1.710342534385	1.379221947464
H	-1.332195286626	4.165117040081	1.371069502495
H	1.990554771395	3.897383945257	-1.349034539499
H	1.789651329380	1.442798662555	-1.364847710916
H	0.349635461510	-2.273400401890	-1.359041995074

H	2.375149884150	-3.673551276849	-1.346019325759
H	4.274851227197	-0.924027746554	1.363588622061
H	2.249159401711	0.476289352094	1.375055581748
H	-2.145192434290	0.827611421611	-1.365073145753
H	-4.370121232000	-0.228255621911	-1.348055016594
H	-2.939760037592	-3.229831918009	1.382407856275
H	-0.714344170121	-2.175219804227	1.387932057710
C	4.729562373465	-3.241217396955	-0.021505511826
H	5.376108195368	-2.942002260832	-0.857462024191
H	5.310090069412	-3.123488665834	0.898229530292
H	4.495611940393	-4.301671152179	-0.155719667174
C	-5.171902757821	-2.477082561880	-0.011033796580
H	-5.219481516975	-3.221853086987	-0.817007238837
H	-5.375916854632	-3.000748295553	0.927707115913
H	-5.971787097141	-1.752405414377	-0.189982820834
C	0.445139192058	5.718571110774	-0.015105083925
H	-0.147909500147	6.132632844488	-0.841659756710
H	0.065534221620	6.159637791778	0.911300462852
H	1.479045749173	6.045520407317	-0.161455347419

Tri([1,1'-biphenyl]-4-yl)amine (2)

N	0.000000000000	0.000000000000	0.005359015073
C	0.000000000000	-0.000000000001	1.425429525109
C	0.000652501401	-1.229567476199	-0.705431782201
C	-0.000652501401	1.229567476200	-0.705431782199
C	0.798521683975	-1.397689437646	-1.848936784570
C	0.789160980935	-2.600450279969	-2.547445884787
C	0.000800572475	-3.688085845947	-2.130797995535
C	-0.787103470148	-3.509495494376	-0.979572561579
C	-0.796434508321	-2.305735583605	-0.282482660201
C	-0.795706810418	0.907117293380	2.144210052172
C	-0.785981240089	0.908222995542	3.535114076321
C	0.000000000000	-0.000000000003	4.266716439479
C	0.785981240089	-0.908222995548	3.535114076320
C	0.795706810418	-0.907117293383	2.144210052171
C	-0.798521683975	1.397689437649	-1.848936784568

C	-0.789160980935	2.600450279973	-2.547445884782
C	-0.000800572475	3.688085845950	-2.130797995529
C	0.787103470148	3.509495494377	-0.979572561574
C	0.796434508321	2.305735583605	-0.282482660197
H	1.435902974831	-0.584865214172	-2.182080771891
H	1.437973839592	-2.707806725208	-3.412063689408
H	-1.436206786061	-4.312978278805	-0.643149790051
H	-1.433579660168	-2.190998261713	0.588612434037
H	-1.431495522840	1.604173916970	1.607776269252
H	-1.432550068112	1.603950585274	4.062327757158
H	1.432550068112	-1.603950585280	4.062327757156
H	1.431495522840	-1.604173916972	1.607776269249
H	-1.435902974831	0.584865214176	-2.182080771890
H	-1.437973839592	2.707806725213	-3.412063689403
H	1.436206786061	4.312978278806	-0.643149790045
H	1.433579660168	2.190998261712	0.588612434040
C	-0.000627775714	4.971251136523	-2.876148629642
C	0.127925304235	6.200350988269	-2.203918737282
C	-0.129807494499	4.995551924181	-4.276898588696
C	0.129479898048	7.406240604941	-2.904648900836
H	0.202501523861	6.212603390873	-1.120173852539
C	-0.132425359959	6.201377968775	-4.977687513240
H	-0.204410924571	4.059923320763	-4.824017055582
C	-0.001820738635	7.413303254441	-4.295366164514
H	0.223588554070	8.342697262998	-2.361098950217
H	-0.226951581520	6.192722694677	-6.060388034362
H	-0.002311637927	8.352729020802	-4.841275474055
C	0.000000000000	-0.000000000005	5.750603753600
C	0.125980504298	-1.199228093638	6.475360297773
C	-0.125980504298	1.199228093628	6.475360297775
C	0.127883970988	-1.199251550464	7.870028246649
H	0.198577520870	-2.142445431385	5.941147895484
C	-0.127883970988	1.199251550452	7.870028246651
H	-0.198577520870	2.142445431376	5.941147895487
C	0.000000000000	-0.000000000007	8.574914840878
H	0.219875304517	-2.139895597014	8.406659881500

H	-0.219875304517	2.139895597001	8.406659881503
H	0.000000000000	-0.000000000008	9.661436249002
C	0.000627775714	-4.971251136519	-2.876148629649
C	-0.127925304235	-6.200350988266	-2.203918737292
C	0.129807494499	-4.995551924174	-4.276898588704
C	-0.129479898048	-7.406240604937	-2.904648900848
H	-0.202501523861	-6.212603390871	-1.120173852549
C	0.132425359959	-6.201377968767	-4.977687513250
H	0.204410924571	-4.059923320755	-4.824017055588
C	0.001820738635	-7.413303254434	-4.295366164525
H	-0.223588554070	-8.342697262995	-2.361098950230
H	0.226951581520	-6.192722694668	-6.060388034371
H	0.002311637927	-8.352729020794	-4.841275474068

Radical cation of tri([1,1'-biphenyl]-4-yl)amine ($2^{\bullet+}$)

N	0.007998400943	0.018820075636	0.027315649667
C	-0.009357546902	1.429733139394	0.032529375053
C	-1.204363160055	-0.702798679844	0.019679202101
C	1.237744457111	-0.672794923777	0.029729796233
C	-1.329038881528	-1.889492437427	0.770271708984
C	-2.520825910792	-2.593532097079	0.756595070404
C	-3.627895012163	-2.156549297511	-0.003355389854
C	-3.482866414987	-0.965842149596	-0.748730148699
C	-2.300408209852	-0.245598682014	-0.739727666724
C	0.937068613688	2.155066592334	-0.719497436303
C	0.910644493112	3.539245127084	-0.711824820749
C	-0.044111962412	4.255015820924	0.042969598775
C	-0.980904112261	3.510418358169	0.792367542267
C	-0.973270995697	2.125989771889	0.789809366428
C	1.391504964842	-1.850483984980	-0.729599778184
C	2.600250846755	-2.525076420987	-0.721017577624
C	3.696304970899	-2.066621218282	0.042241780938
C	3.522098548874	-0.885382182668	0.796381556103
C	2.322280505793	-0.194396349354	0.792593968100
H	-0.505898917713	-2.225051128999	1.391202588406
H	-2.610931408105	-3.477476920187	1.378557120262

H	-4.296608117401	-0.622853837326	-1.378664186922
H	-2.200189896917	0.644139217974	-1.351289310276
H	1.655105976468	1.627772767235	-1.337649058225
H	1.616400493928	4.078216685235	-1.334539329822
H	-1.699647779928	4.027250204838	1.418983545454
H	-1.678064327064	1.576639606901	1.403982482341
H	0.576811832404	-2.201591607760	-1.353068085096
H	2.712016151058	-3.401917290162	-1.349486231821
H	4.327214325496	-0.527145099652	1.428906821765
H	2.200262000245	0.688063778993	1.410704387820
C	4.979362025682	-2.798548879688	0.051101974481
C	6.200285726040	-2.114770457442	0.209976728206
C	5.012477984580	-4.198620855777	-0.099461457780
C	7.409556218377	-2.806003822205	0.214830357414
H	6.205508266695	-1.032723155058	0.298978417510
C	6.222371856124	-4.888629837375	-0.087886948052
H	4.084342026970	-4.753944911660	-0.195442169331
C	7.425853361985	-4.195561569682	0.067554976990
H	8.340831585197	-2.258338110749	0.326966122845
H	6.225268696380	-5.969626190983	-0.193757988524
H	8.369083860079	-4.734117519342	0.073956216098
C	-0.062281015735	5.732028480696	0.048427580982
C	-1.272311630139	6.438501173746	0.191397862016
C	1.129992378905	6.469089356929	-0.089208432612
C	-1.288649301939	7.831289459036	0.192970609929
H	-2.209051652538	5.895073302298	0.270694406527
C	1.112064634209	7.861831669111	-0.080487852070
H	2.079809188386	5.949468993227	-0.172433242948
C	-0.096929796158	8.548723793435	0.058836071932
H	-2.233677336090	8.357409786606	0.292532666924
H	2.043855956735	8.411760285658	-0.176073601919
H	-0.110289841275	9.634798858640	0.062849428448
C	-4.892560400318	-2.919731147900	-0.017740438624
C	-6.129948941544	-2.265037060267	-0.171669155431
C	-4.891213155859	-4.321268410986	0.122470250022
C	-7.321850743748	-2.985752615186	-0.181740337807

H	-6.161794598373	-1.182817522016	-0.252673262703
C	-6.083768877393	-5.040725657836	0.105687361377
H	-3.949689248493	-4.854287865678	0.214429222507
C	-7.303948705028	-4.376341106151	-0.044738389099
H	-8.266326195996	-2.460346827483	-0.289910798599
H	-6.060064462875	-6.122218971144	0.203567386980
H	-8.233646771158	-4.937874025954	-0.055204769719

Tri([1,1':4',1''-terphenyl]-4-yl)amine (3)

N	-0.009653739937	-0.021182386137	0.011054839677
C	-0.006236582125	-0.013514760822	-1.410092131317
C	0.395236206777	1.144893755346	0.717219454465
C	-0.408397574753	-1.185246603190	0.723592496048
C	1.253260001189	1.055002916868	1.825353170272
C	1.640955744447	2.200440622594	2.513775731532
C	1.205054024980	3.479378109480	2.119755010165
C	0.352952534171	3.555746875220	1.002744158883
C	-0.052305882935	2.414629641212	0.317229914545
C	-1.061127002311	-0.590396531335	-2.137343066370
C	-1.049655514047	-0.581044728675	-3.528827888199
C	-0.000342217585	0.014093227056	-4.253787807867
C	1.045364995972	0.596389227214	-3.513512891873
C	1.050652242408	0.579254707399	-2.121542279275
C	-1.155814775968	-1.083126832106	1.916696787641
C	-1.540536140333	-2.233735758792	2.620569109478
C	-1.213206352523	-3.528131576760	2.161000161080
C	-0.471367618627	-3.617513103662	0.962967558147
C	-0.067559107347	-2.473676039121	0.259166747765
H	1.624096754105	0.084170945987	2.138570534952
H	2.327526184621	2.100986836538	3.349714381808
H	-0.032937153975	4.520622271609	0.686422079896
H	-0.728787102063	2.502264330316	-0.527084843803
H	-1.896825353201	-1.036118092870	-1.607381516058
H	-1.894154073690	-1.009970631768	-4.060602490039
H	1.891472950406	1.036545667384	-4.033414925862
H	1.883022545381	1.016201739846	-1.579088540449

H	-1.446887257643	-0.104269411091	2.284626397270
H	-2.139927586908	-2.119295053291	3.519958373685
H	-0.167916869566	-4.592743260778	0.591660422248
H	0.524038819001	-2.578744541085	-0.644865761915
C	-1.631334033300	-4.742012787550	2.904220790266
C	-1.961916602993	-5.934625433149	2.231970625262
C	-1.714309300329	-4.748496802553	4.309879427653
C	-2.354681803142	-7.075985371409	2.930470251019
H	-1.945267924018	-5.960678716298	1.145955062762
C	-2.109493165464	-5.889504515409	5.007742539207
H	-1.433599112892	-3.859744671796	4.868047948543
C	-2.438740935738	-7.080687653425	4.334739305289
H	-2.632538158642	-7.966813974385	2.373849060614
H	-2.130597789376	-5.863997722470	6.093804680888
C	0.003117899661	0.026710759614	-5.736119859885
C	0.561582133846	1.097623845656	-6.457622737481
C	-0.551318765560	-1.032472159822	-6.477502079794
C	0.566873564551	1.107588630711	-7.849542254325
H	0.967610323263	1.951620183423	-5.923168167753
C	-0.548710009327	-1.020684370208	-7.869305525773
H	-0.960196353841	-1.894844867481	-5.958809677833
C	0.011260416791	0.049023199172	-8.589461303980
H	0.979235594086	1.967334811734	-8.370092612198
H	-0.958188406364	-1.872109770484	-8.405533100291
C	1.625884731819	4.697459170138	2.852436051948
C	1.831113549376	5.918083474155	2.183951323172
C	1.834376316770	4.678282442883	4.243351917539
C	2.223465099100	7.062494899208	2.872339290687
H	1.714727264804	5.965491745316	1.104981193101
C	2.229206232004	5.822302601294	4.931112746114
H	1.652335930879	3.763994217758	4.800956750937
C	2.432583272382	7.042326129416	4.262407130302
H	2.402256836312	7.978599806578	2.316464318407
H	2.349644678757	5.775537557834	6.009811736701
C	-2.859420737402	-8.295743730183	5.077949495412
C	-3.645421076406	-8.197221364156	6.240766640720

C	-2.483817142686	-9.578929837431	4.639686072833
C	-4.040393170338	-9.338701989436	6.939786326590
H	-3.969129671147	-7.219491267343	6.586443107017
C	-2.880271241534	-10.720826641741	5.337183332377
H	-1.856518368187	-9.681196458683	3.758423986482
C	-3.660144490546	-10.606317759956	6.491042114425
H	-4.653654132739	-9.237234937323	7.831350732784
H	-2.571424485915	-11.700844920820	4.982960685489
H	-3.968172038876	-11.495271373800	7.034668279565
C	0.015758997862	0.060354615142	-10.074238396298
C	1.100990159687	0.596570877797	-10.790513820548
C	-1.065021625486	-0.464927373270	-10.805076827804
C	1.105042234106	0.608001820194	-12.185347427625
H	1.958916234261	0.986219605891	-10.249757596744
C	-1.060760937894	-0.455166094884	-12.199877061636
H	-1.926214002747	-0.862670707789	-10.275498310947
C	0.024267748144	0.081721474634	-12.897033422124
H	1.958416859418	1.021129964870	-12.716614429710
H	-1.910925619051	-0.860144783253	-12.742437828088
H	0.027547286093	0.089938534908	-13.983530710010
C	2.852446655379	8.263092062969	4.996259943781
C	2.364189126543	9.530952806878	4.630818253724
C	3.749899432831	8.185240392797	6.076748842234
C	2.759168893306	10.678317783477	5.319494214377
H	1.651496987810	9.615176002310	3.815081602089
C	4.143966770771	9.332270390950	6.766726617649
H	4.160018142052	7.220838371232	6.363364008845
C	3.650701725378	10.584632787909	6.391087931092
H	2.362553539588	11.645863856244	5.023260303415
H	4.844349441265	9.247766717959	7.593500939012
H	3.957872485122	11.477996622869	6.927889183993

Radical cation of tri([1,1':4',1''-terphenyl]-4-yl)amine ($3^{\bullet+}$)

N	-0.014854825477	0.002800264366	-0.001234827513
C	-0.018823680637	0.006547287337	-1.411922726861
C	0.388920822488	1.156076679081	0.705365897248

C	-0.411286355123	-1.152846897415	0.705427855545
C	1.162989919542	1.038823906013	1.877549933410
C	1.556964438126	2.175010865234	2.563288690884
C	1.195998652392	3.467612795493	2.121968715510
C	0.417489848745	3.563173491161	0.947203700677
C	0.021423173899	2.437119982048	0.246400411863
C	-1.040435739148	-0.653751171427	-2.124910207363
C	-1.034709991544	-0.646059936024	-3.509189903066
C	-0.019004616114	0.008892639814	-4.240711764701
C	0.994962200670	0.664730284810	-3.508018269605
C	1.001096169930	0.669972105658	-2.124161363244
C	-1.163907967851	-1.038142267860	1.892021742939
C	-1.551238644847	-2.175726533965	2.578849711798
C	-1.206333606965	-3.467575437035	2.123729007453
C	-0.449213130685	-3.561261270552	0.934880898820
C	-0.058410060667	-2.433515646783	0.233827461125
H	1.485002849538	0.060624789408	2.216900233982
H	2.192669454088	2.061555682442	3.434722835534
H	0.080980172074	4.534773147958	0.602181296836
H	-0.607630193689	2.536640281681	-0.631254609302
H	-1.852541246062	-1.131227743461	-1.588007944291
H	-1.855563542451	-1.120851390751	-4.035630000359
H	1.815957165031	1.140632420696	-4.033147919881
H	1.813402925820	1.146406663161	-1.586782152489
H	-1.475097191138	-0.060229560329	2.242115267209
H	-2.169915590525	-2.064417522148	3.462726444992
H	-0.124950155954	-4.533047135888	0.578594923994
H	0.555182663485	-2.532456859537	-0.654635967118
C	-1.621415427785	-4.673533108609	2.862529987290
C	-1.855916555984	-5.892866607570	2.197082519159
C	-1.799002949928	-4.648302089744	4.259818999778
C	-2.251743049800	-7.027348010570	2.893982137102
H	-1.767536917751	-5.945338276313	1.116230335007
C	-2.186781042704	-5.786381009822	4.955508573414
H	-1.591464677424	-3.739074462079	4.815849015939
C	-2.425236835413	-7.003880324555	4.290580175284

H	-2.460819050108	-7.938611523290	2.342001867859
H	-2.275309941716	-5.738694075667	6.036517520618
C	-0.014533470423	0.007072910256	-5.714628620525
C	0.539862483760	1.077540504310	-6.443489045147
C	-0.561715964133	-1.065824838298	-6.445608211570
C	0.543110058670	1.075642172516	-7.832452007429
H	0.936753335169	1.941400185533	-5.919149806808
C	-0.549524781529	-1.069118431924	-7.834751189107
H	-0.964692156070	-1.927630058993	-5.922455173911
C	0.001425655129	0.001651673484	-8.563351501743
H	0.944042180940	1.935897112324	-8.359672044442
H	-0.944381472082	-1.931332129685	-8.363328737046
C	1.615888141035	4.672562681541	2.860129574272
C	1.820681880346	5.899604818933	2.198884783813
C	1.827247818417	4.639622628589	4.252559488572
C	2.220306113576	7.033451806007	2.894844505564
H	1.706170796541	5.959799288629	1.120855239802
C	2.220081211625	5.776443630846	4.947304917172
H	1.643151199937	3.724608526187	4.806876969746
C	2.428628235508	7.001567795204	4.286506611923
H	2.405108190606	7.951241617640	2.345022510025
H	2.335990689581	5.721297145922	6.025425702557
C	-2.842769344247	-8.217081657080	5.033558512239
C	-3.673609969782	-8.121812896552	6.164748564792
C	-2.417924777622	-9.494720360023	4.625946823444
C	-4.065713863143	-9.263179945264	6.862646006162
H	-4.037198187210	-7.149400872005	6.484071638258
C	-2.808749633885	-10.635632923407	5.325185813922
H	-1.754641853653	-9.593072182012	3.771381300527
C	-3.634616710088	-10.525171701627	6.446483411388
H	-4.715352944211	-9.166829744645	7.728304052143
H	-2.461019218759	-11.611700595428	4.997980065342
H	-3.939634240011	-11.414453097847	6.990964145082
C	0.011707918949	-0.001436204988	-10.045854576234
C	1.077232075158	0.574218314758	-10.761576673523
C	-1.043199592917	-0.580114428235	-10.774696483146

C	1.087693926338	0.570541439140	-12.155621574888
H	1.916578981770	1.003824859847	-10.222250373929
C	-1.033377784168	-0.581636550257	-12.168736252229
H	-1.890455532986	-1.008093550722	-10.246511192991
C	0.032222895056	-0.006881495307	-12.865673312717
H	1.925606656761	1.012804182991	-12.687606911082
H	-1.863385261851	-1.026060276587	-12.711179714030
H	0.040077906523	-0.009004057227	-13.952051283983
C	2.852160076640	8.212929015118	5.029079220621
C	2.401541219802	9.489506017784	4.646544043200
C	3.715648464763	8.116578473634	6.135517286057
C	2.799248075932	10.627993927008	5.345917984475
H	1.713448912236	9.588639469155	3.811934664546
C	4.114935640328	9.255541721964	6.833130513043
H	4.098868242958	7.145395934109	6.435275756576
C	3.658069258682	10.516438914519	6.442028918905
H	2.431317345360	11.603052619830	5.038366449469
H	4.789950255961	9.158236970491	7.679051453321
H	3.968534006374	11.403948884880	6.986304054046

Tris(4-(5-(naphthalen-1-yl)thiophen-2-yl)phenyl)amine (4)

N	0.087202068552	0.012825395964	-0.084497720426
C	0.133987146347	0.013750763329	-1.504360856081
C	0.415611141318	1.190305854314	0.638738284628
C	-0.296266472247	-1.164857841260	0.611786901987
C	1.171256832291	1.120614529204	1.820224204409
C	1.479375926163	2.276931241126	2.530956302568
C	1.070753996958	3.545363003423	2.084886991741
C	0.321216151950	3.603591052719	0.896561417740
C	-0.010282746503	2.451408457447	0.190035246837
C	-0.867298558198	-0.620803936238	-2.256715383141
C	-0.812720004056	-0.620887847969	-3.647563818116
C	0.222993258321	0.026335214053	-4.342672743441
C	1.218669020608	0.660651855397	-3.578733350552
C	1.184050045810	0.648789531763	-2.187657547205
C	-1.151466642048	-1.096746645278	1.723169855065

C	-1.513149587183	-2.253239316537	2.407837644990
C	-1.059147749796	-3.520064242937	2.002909321515
C	-0.209178359058	-3.576601683652	0.884038307018
C	0.174166643283	-2.424000183554	0.204815900613
H	1.521570612180	0.157519152466	2.177316359995
H	2.074123215616	2.198437748838	3.436915124336
H	-0.040036031205	4.562874572841	0.537174067291
H	-0.612191077647	2.525456529911	-0.709965180693
H	-1.693297875745	-1.107833070833	-1.748422564445
H	-1.605492686823	-1.108387160011	-4.208415806096
H	2.053426163104	1.142329410544	-4.079798895010
H	1.979230481127	1.126235720866	-1.624082898066
H	-1.536696819912	-0.134876646297	2.045991913799
H	-2.184211295802	-2.176450299967	3.258937350795
H	0.189098392980	-4.533997758326	0.560601657744
H	0.851574903810	-2.495772483193	-0.640095788457
C	0.280008436575	-0.022666376419	-5.829866200010
C	0.401449641258	1.163966576644	-6.635324365277
C	0.212762895224	-1.256266637237	-6.459479484306
C	0.494221276100	1.027917152941	-8.063311683783
C	0.395173842698	2.479374426510	-6.090390905021
C	0.290360081232	-1.382178053466	-7.864931903407
H	0.126540147884	-2.152915291603	-5.851980010750
C	0.621172295214	2.194579114436	-8.866625546469
C	0.440786601034	-0.264145603303	-8.651505383073
C	0.510690558904	3.589945408494	-6.898311006530
H	0.284078523011	2.606695293321	-5.019381271041
H	0.245091399588	-2.369716634095	-8.315756136115
C	0.635805712206	3.449115299455	-8.300981318331
H	0.699159356158	2.075031732107	-9.944689390574
H	0.514554383353	-0.351334219557	-9.732754510883
H	0.498984540616	4.582389426672	-6.455897901307
H	0.731158240082	4.331758737235	-8.927426071383
C	1.372002814551	4.761884683269	2.889079691306
C	2.013256061306	5.920177678943	2.324566436300
C	1.018817646312	4.778173696606	4.229930773672

C	2.224028572158	7.072781816465	3.157177052576
C	2.488755945327	5.970908084324	0.983487358422
C	1.242560009854	5.909187417849	5.047157871415
H	0.529539618070	3.906534601541	4.655795028012
C	2.849671755746	8.224565036534	2.605340016836
C	1.821483725890	7.039455677172	4.519198203512
C	3.099782713866	7.100114672646	0.482409302345
H	2.377825072472	5.097469951456	0.350675071825
H	0.939165365122	5.882555035248	6.090125464282
C	3.274246439519	8.244669456399	1.296372411407
H	2.994078929008	9.092020071927	3.245089324332
H	1.985014159747	7.919833951884	5.135941171626
H	3.456751191871	7.109988621388	-0.543890123280
H	3.753099002775	9.130862809748	0.889017509664
C	-1.419959295263	-4.735584853798	2.783878145279
C	-1.996588061469	-5.903681516562	2.171877862493
C	-1.189167905405	-4.740048494499	4.151287696856
C	-2.271286123089	-7.052965555058	2.990437663067
C	-2.348436167673	-5.967898652783	0.793768214349
C	-1.475211229689	-5.868039484645	4.953010341255
H	-0.748731906940	-3.860811023285	4.613264249175
C	-2.834246142206	-8.214220349156	2.392911736307
C	-1.993655971090	-7.007138220081	4.382938027578
C	-2.901250101801	-7.106270721076	0.247863600958
H	-2.189323407292	-5.097563844767	0.167031174311
H	-1.267592687190	-5.831999131914	6.018895760386
C	-3.138383168731	-8.247128320107	1.051092887750
H	-3.028320306123	-9.078714988890	3.023472998538
H	-2.204402496661	-7.885047121516	4.988747317197
H	-3.163856236122	-7.126176724386	-0.806387739237
H	-3.570621012183	-9.140467161167	0.608747886403

Radical cation of tris(4-(5-(naphthalen-1-yl)thiophen-2-yl)phenyl)amine ($4^{\bullet+}$)

N	-0.302309656524	-0.311620894228	-0.020138014633
C	0.041902649601	1.058028932563	-0.031189812884
C	0.710863887182	-1.293705626208	-0.002075963872

C	-1.660664631959	-0.696503393610	-0.026719289069
C	0.558449338338	-2.488507103593	-0.734271484067
C	1.557084495756	-3.448022109276	-0.706455052057
C	2.741066533411	-3.259671488592	0.038429787015
C	2.874508273812	-2.058283227839	0.768339157709
C	1.883572034927	-1.090700039402	0.753516182354
C	-0.708395172700	1.984935506628	0.719318741504
C	-0.362322240945	3.326274968717	0.705664518361
C	0.735655214952	3.797172533380	-0.045575962162
C	1.470486783113	2.854797659973	-0.797530141266
C	1.136757984038	1.510269954940	-0.794559503616
C	-2.091542003410	-1.801233833273	0.734847543312
C	-3.426260063872	-2.171678527337	0.720427196847
C	-4.380585360214	-1.463020876566	-0.040367979703
C	-3.929647732724	-0.361999416419	-0.800467646421
C	-2.597869762862	0.019287585609	-0.798717291893
H	-0.322739438932	-2.638071549541	-1.348091064152
H	1.440729233265	-4.348061319009	-1.301300812122
H	3.749032644030	-1.904702887116	1.391232605490
H	1.988942631942	-0.196135783170	1.357031732837
H	-1.530525135296	1.641430379904	1.337218782117
H	-0.926823064567	4.023345941746	1.316231704521
H	2.288107707241	3.191333641417	-1.425720791074
H	1.690232401519	0.811520481892	-1.412050313571
H	-1.385552013516	-2.335226760881	1.361055098509
H	-3.749720565700	-3.003511948030	1.337524932269
H	-4.628130066937	0.173086405325	-1.434775504405
H	-2.267491285389	0.841350907385	-1.423849608417
C	1.049243097973	5.243618088471	-0.083570389869
C	2.387456495499	5.754195103042	0.071627530778
C	0.005480823617	6.134837773682	-0.305719584399
C	2.604865770915	7.167149249297	-0.073369310134
C	3.503739196251	4.942108223015	0.414144307547
C	0.227728714182	7.521068809217	-0.435479044229
H	-1.002511771175	5.749507527674	-0.428507121579
C	3.918655204220	7.689878803104	0.070306186221

C	1.504571918077	8.025889326615	-0.335987293408
C	4.765209657142	5.482265560317	0.554919874569
H	3.359919798019	3.881984429709	0.589702622125
H	-0.612079217057	8.181199785134	-0.630534128191
C	4.981065514767	6.867168070183	0.369830701281
H	4.066507014954	8.759930561931	-0.050982747175
H	1.688024536036	9.091377349416	-0.447700544653
H	5.599056901972	4.838305638057	0.819851877845
H	5.979965478837	7.279227738044	0.479743227875
C	3.765199517295	-4.326862962306	0.095524285279
C	5.172781071910	-4.065603993736	-0.065784929587
C	3.341456550849	-5.627470025580	0.344979188414
C	6.096820910738	-5.153079697691	0.101709276122
C	5.698985270363	-2.797037168325	-0.435232221525
C	4.255610003638	-6.689878150163	0.496853505592
H	2.280830522594	-5.823161433656	0.472549587907
C	7.489864325444	-4.914549545219	-0.047867479192
C	5.607982046984	-6.454655296855	0.391786743632
C	7.056663695535	-2.600661387800	-0.580932705492
H	5.021671895352	-1.972697045113	-0.627932367199
H	3.884965390823	-7.687329760178	0.713153940055
C	7.964871658251	-3.664139668407	-0.373946294841
H	8.175762961591	-5.746396106254	0.090452056179
H	6.321348718301	-7.264618128145	0.520354163795
H	7.430628238729	-1.621538908110	-0.866626071060
H	9.031718642191	-3.495371899349	-0.488057936619
C	-5.789506004342	-1.916317066867	-0.079748743349
C	-6.902257541549	-1.013468735278	0.068150956928
C	-6.036791454519	-3.267302902378	-0.295701111306
C	-8.233589243696	-1.534426749190	-0.076074631792
C	-6.759148511022	0.361235092962	0.403215397676
C	-7.347337629185	-3.770504583529	-0.426057203767
H	-5.197598436770	-3.946688299362	-0.412671760306
C	-9.344528924181	-0.658773534212	0.062038838180
C	-8.424409657477	-2.918227318225	-0.332478198537
C	-7.858903969987	1.183001912363	0.538070892855

H	-5.769967894119	0.768822335242	0.578557444405
H	-7.497291426556	-4.828949741584	-0.616501114041
C	-9.165261945616	0.674541503730	0.354556629457
H	-10.344631930011	-1.067601732680	-0.057726669777
H	-9.437937404516	-3.294488510221	-0.444427475251
H	-7.719868693337	2.228730206502	0.797430935298
H	-10.022642505514	1.332829147320	0.460478159808

Tris(4-(5-(naphthalen-2-yl)thiophen-2-yl)phenyl)amine (5)

N	-0.010888266257	-0.003225569635	0.019564277355
C	-0.004026579316	-0.009072507746	-1.400801680093
C	0.383767061123	1.162310450459	0.727800975298
C	-0.409942829970	-1.166941917859	0.729975829339
C	1.159057313764	1.067256185783	1.895238943418
C	1.534128869292	2.211902880756	2.590901998653
C	1.175200170434	3.496012652191	2.143577559104
C	0.404122107305	3.578209864527	0.970156030037
C	0.006620386673	2.439123915551	0.278709993456
C	-1.042128794380	-0.621571265819	-2.121582314233
C	-1.026649378416	-0.633829076871	-3.512478923930
C	0.007371244963	-0.020463071407	-4.242410093479
C	1.038535975325	0.593558469366	-3.508886562013
C	1.042019774892	0.594626267620	-2.118321424950
C	-1.223545619286	-1.070566010509	1.870524785862
C	-1.600571833279	-2.212815703811	2.569212174006
C	-1.203711720134	-3.495775410620	2.151392983053
C	-0.395230127461	-3.579194395247	1.003314418751
C	0.002376728622	-2.441997725514	0.308776848342
H	1.475791275616	0.092271658546	2.251144857569
H	2.153645541755	2.104792126406	3.476826707089
H	0.075066278338	4.549924900469	0.612919525455
H	-0.610271942589	2.534968484367	-0.608914351840
H	-1.868098163847	-1.080034424775	-1.587467498563
H	-1.857461729884	-1.094442091950	-4.039462992314
H	1.874568713243	1.045160289501	-4.035273908362
H	1.865207698617	1.054800430282	-1.581382349204

H	-1.567609201842	-0.096615105365	2.203375181728
H	-2.249617814501	-2.105132713627	3.433583860504
H	-0.037048905507	-4.548971321873	0.669685047216
H	0.647656432623	-2.537538474362	-0.558550295405
C	0.007738044740	-0.017478499242	-5.725341496006
C	0.483035427077	1.069080467093	-6.443759903278
C	-0.488703240110	-1.142183736961	-6.451269979587
C	0.488594243466	1.085566338720	-7.862606903669
H	0.840387231187	1.951427834096	-5.918760493664
C	-0.497635399391	-1.157857452934	-7.825715931217
H	-0.841705186205	-2.010748347165	-5.903074506321
C	-0.013120074173	-0.051909339186	-8.575628389882
C	0.968545560099	2.201226652880	-8.603592370528
H	-0.870819934225	-2.029467128280	-8.358269676536
C	-0.008824743154	-0.033495587839	-9.996080534321
C	0.957603104675	2.189950711641	-9.980882518995
H	1.346476067125	3.065450710527	-8.062429657950
C	0.465304576097	1.061850126494	-10.684679459296
H	-0.388036386877	-0.900339123265	-10.532231889836
H	1.327911615919	3.048097387592	-10.535102478912
H	0.462850615335	1.065927760842	-11.771201763363
C	-1.620905326436	-4.711937451812	2.890396297552
C	-1.900182933554	-5.897491634787	2.227787746763
C	-1.743465923866	-4.688024569184	4.312680694587
C	-2.294453261598	-7.070326195816	2.922393458070
H	-1.842772350903	-5.937747834613	1.142925184589
C	-2.123458222759	-5.806527668323	5.015463799855
H	-1.504762773029	-3.774214893667	4.848816287524
C	-2.410386417295	-7.029462433199	4.350353707035
C	-2.586789483301	-8.287460013607	2.246137169577
H	-2.199465714946	-5.768751281554	6.099605797605
C	-2.804538861157	-8.204360638992	5.044866848319
C	-2.968321040286	-9.409691091285	2.947664850837
H	-2.501794914327	-8.317553103869	1.162436292980
C	-3.077441864848	-9.368905815531	4.360681095333
H	-2.888578853103	-8.168966865987	6.128559449798

H	-3.187433316010	-10.333476066529	2.419190080684
H	-3.378986095390	-10.261423354110	4.902010788342
C	1.595981761325	4.713949812598	2.877314695219
C	1.931740636814	5.879712350046	2.205962314313
C	1.666717817966	4.711384134055	4.303239792080
C	2.335269730135	7.052592762798	2.895212712806
H	1.914508773953	5.902614921090	1.119184848754
C	2.053178643040	5.830773783295	5.001123073655
H	1.383771736731	3.813394612409	4.844713386335
C	2.399394524844	7.033277461601	4.326912854712
C	2.688292445937	8.248613928539	2.210239010667
H	2.089353676326	5.809486763152	6.087814949050
C	2.804311542246	8.207782754112	5.015915655419
C	3.079433850666	9.370720303795	2.906676335397
H	2.642781576343	8.262620238415	1.123788329001
C	3.137194945937	9.351463508968	4.323170460009
H	2.848722031284	8.188658847584	6.102346137764
H	3.345448599859	10.278093376386	2.371299167075
H	3.446798391900	10.243758260180	4.860264239809

Radical cation of tris(4-(5-(naphthalen-2-yl)thiophen-2-yl)phenyl)amine ($5^{\bullet+}$)

N	-0.175426205841	-0.172212599977	0.031608262000
C	0.179781209989	1.194115186939	0.028878736582
C	0.828688398967	-1.163180986960	0.023565659551
C	-1.536921231020	-0.545333559015	0.039418837941
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C	1.639517081426	-3.320643896646	-0.715000825319
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C	-0.558120563054	2.121958273364	0.791018399173
C	-0.202855718207	3.460277644807	0.786197060842
C	0.892641076022	3.930793955010	0.029339237381
C	1.615633352827	2.986363779873	-0.732484422533
C	1.274832437497	1.644862451041	-0.735904580559
C	-1.968625800746	-1.651959442596	0.797930484752

C	-3.304800740447	-2.014954264384	0.793864811854
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C	-3.810077274078	-0.193594180641	-0.711344551943
C	-2.478288022664	0.183503855374	-0.715505111962
H	-0.245957072200	-2.490207670137	-1.307125583430
H	1.498306731740	-4.208018435164	-1.322677666974
H	3.891519209057	-1.807861127166	1.341701741341
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H	2.431540079474	3.318359988338	-1.365299234048
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H	-1.260466911613	-2.193860634930	1.414838743614
H	-3.620493146860	-2.843749220800	1.418202542857
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C	1.268151509258	5.357632424609	0.036438252055
C	2.593531224584	5.748721841681	-0.112793462422
C	0.274766867164	6.369738309452	0.208989371070
C	2.975316141165	7.112514979031	-0.093623934198
H	3.375100829410	5.000837390680	-0.214012505680
C	0.613954860255	7.700000652539	0.222700823933
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H	-0.157414926353	8.456773372027	0.340090671206
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C	4.673439977831	8.850046677457	-0.212523598124
H	5.096263910813	6.752668870430	-0.360204973668
C	3.673717753992	9.841461833233	-0.049363598713
H	1.582557992817	10.241981943114	0.216629561212
H	5.712053769984	9.148780452582	-0.321395194103
H	3.956700671306	10.890137775398	-0.034877166124
C	-5.683347358531	-1.696836317562	0.040921873250
C	-6.689933862736	-0.749738132191	-0.105174346743
C	-6.055111575809	-3.067500036120	0.196843406263

C	-8.059713443640	-1.109978930954	-0.100409438429
H	-6.438048673071	0.303242199837	-0.195762894562
C	-7.374357133241	-3.447548475285	0.195477390117
H	-5.282069807914	-3.824516556605	0.282697995112
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H	-11.814875212210	-2.175686192786	-0.090880552543
C	3.894553733159	-4.182513214950	-0.012231076541
C	5.237757236382	-3.835458240243	0.070873941317
C	3.553309849083	-5.564981445887	-0.126633372666
C	6.263389629368	-4.811838265175	0.038865946561
H	5.527583901266	-2.789830116082	0.128156023810
C	4.525342886312	-6.534296223980	-0.148226769562
H	2.508085168580	-5.855452566633	-0.162830515064
C	5.904941961375	-6.195607154615	-0.070501442532
C	7.640403045413	-4.459980161762	0.107822990498
H	4.246307474319	-7.582465211745	-0.218876416847
C	6.933047635224	-7.172825084126	-0.097994601536
C	8.615290934133	-5.432060437073	0.076355089511
H	7.910263439799	-3.409916273751	0.187376860458
C	8.258747729180	-6.799947677634	-0.026349796767
H	6.659117787855	-8.221737098856	-0.178061087929
H	9.663858789302	-5.153880451262	0.130539796182
H	9.037992733654	-7.556388707168	-0.049592858338

4. Solubility test

To a sample of 5.0 mg, 100 μL of solvent was added repeatedly. The resulting suspension was shaken and sonicated at room temperature (20-25°C). The solution was sealed during the dissolution process to prevent volatilization of the solvent. The total amount of solvent was converted to solubility (wt%). The results are summarized in Table S1.

Table S1. Solubility test of compounds **2**-**5** in dichloromethane, anisole, toluene and ethyl acetate at room temperature.

Compound	dichloromethane	anisole	toluene	ethyl acetate
2	0.42	0.44	0.33	< 0.01
3	0.065	0.064	0.017	< 0.01
4	5.23	5.05	4.41	0.21
5	0.48	0.53	0.23	< 0.01

5. Cyclic voltammetry

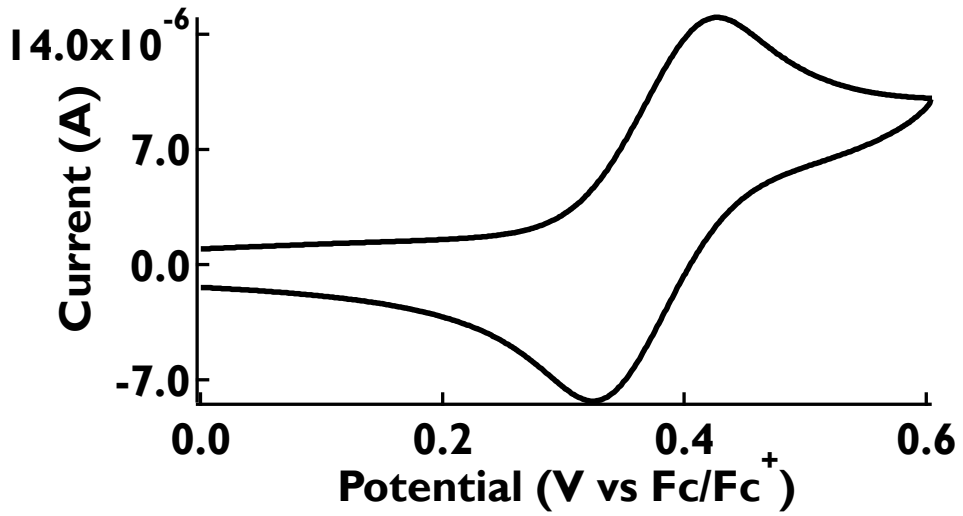


Figure S5. Cyclic voltammograms of **3** in dichloromethane (1×10^{-3} M) with Bu_4NPF_6 as a supporting electrolyte.

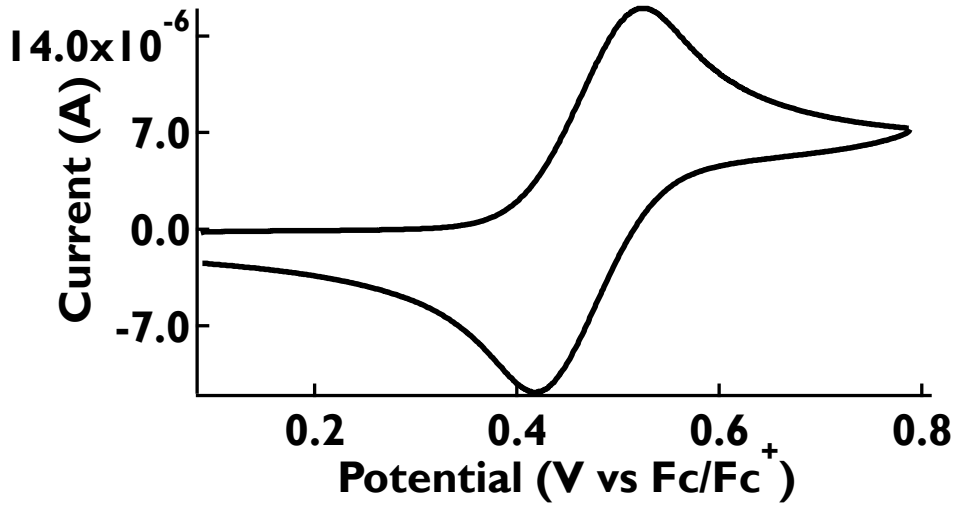


Figure S6. Cyclic voltammograms of **4** in dichloromethane (1×10^{-3} M) with Bu_4NPF_6 as a supporting electrolyte.

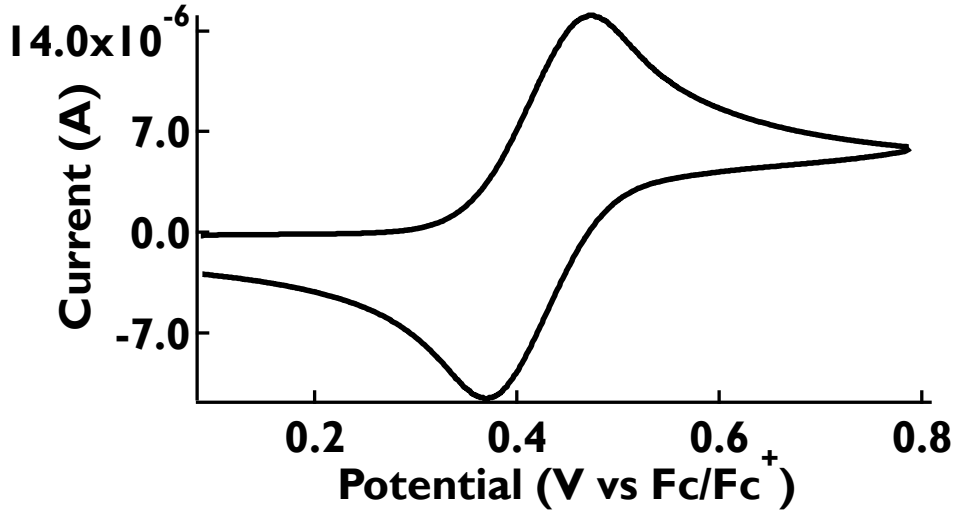


Figure S7. Cyclic voltammograms of **5** in dichloromethane (1×10^{-3} M) with Bu_4NPF_6 as a supporting electrolyte.

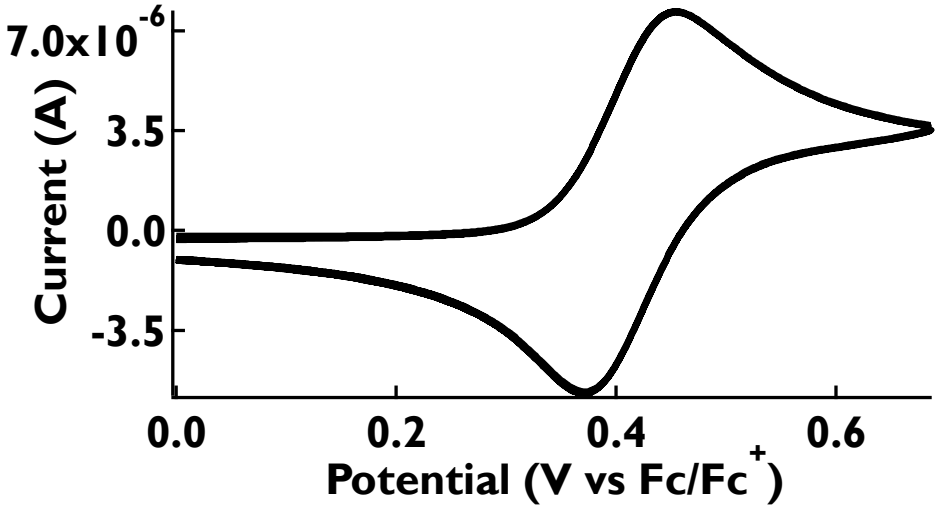


Figure S8. Cyclic voltammogram of **2** in dichloromethane (1×10^{-3} M) after repeating sweep ten cycles in the range of -0.03 and 0.69 V (vs Fc/Fc^+). The scan rate is 25 mV/s. Bu_4NPF_6 (1×10^{-1} M) was employed as a supporting electrolyte.

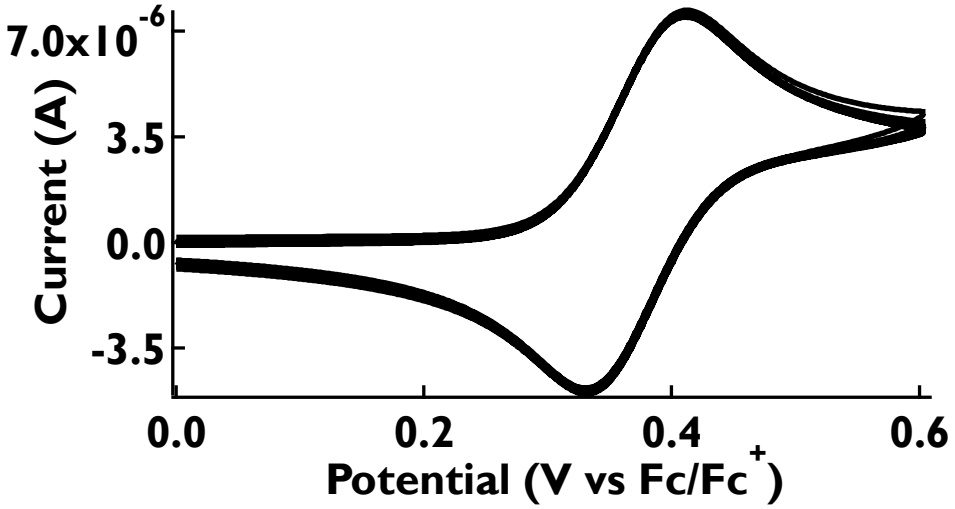


Figure S9. Cyclic voltammogram of **3** in dichloromethane (1×10^{-3} M) after repeating sweep ten cycles in the range of -0.03 and 0.60 V (vs Fc/Fc^{+}). The scan rate is 25 mV/s. Bu_4NPF_6 (1×10^{-1} M) was employed as a supporting electrolyte.

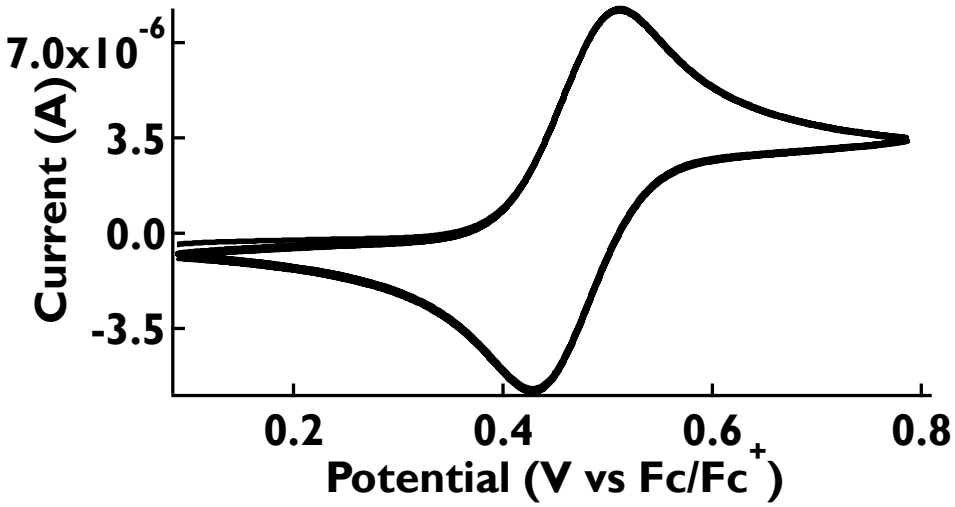


Figure S10. Cyclic voltammogram of **4** in dichloromethane (1×10^{-3} M) after repeating sweep ten cycles in the range of 0.09 and 0.79 V (vs Fc/Fc^{+}). The scan rate is 25 mV/s. Bu_4NPF_6 (1×10^{-1} M) was employed as a supporting electrolyte.

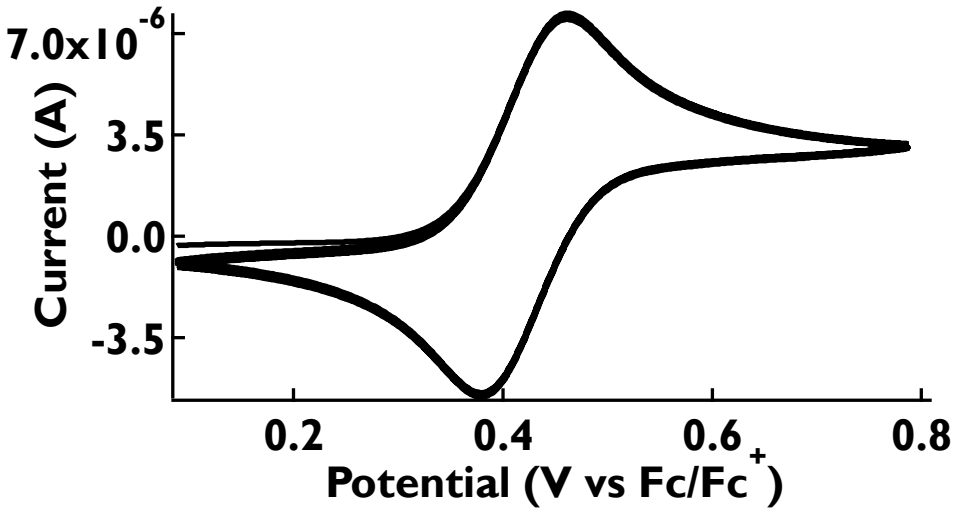


Figure S11. Cyclic voltammogram of **5** in dichloromethane (1×10^{-3} M) after repeating sweep ten cycles in the range of 0.09 and 0.79 V (vs Fc/Fc^{+}). The scan rate is 25 mV/s. Bu_4NPF_6 (1×0^{-1} M) was employed as a supporting electrolyte.

6. Absorption and fluorescence spectra of the neutral or oxidized species

Typical procedure for the preparation of radical cationic species for UV measurements is as follows. To a solution of Ar_3-TPA in dry dichloromethane (5.0×10^{-4} M, 100μL) was added a solution of $SbCl_5$ in dry dichloromethane (5.0×10^{-3} M, 100μL). The obtained solution was diluted to 5 mL with dry dichloromethane.

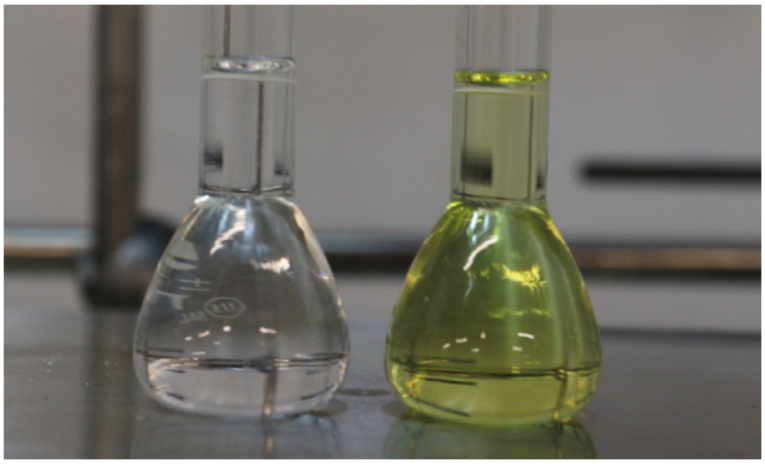


Figure S12. Dichloromethane solution of **3** in the absence (left) and presence of ten equivalents of $SbCl_5$ (right). [**3**] = 1×10^{-5} M.

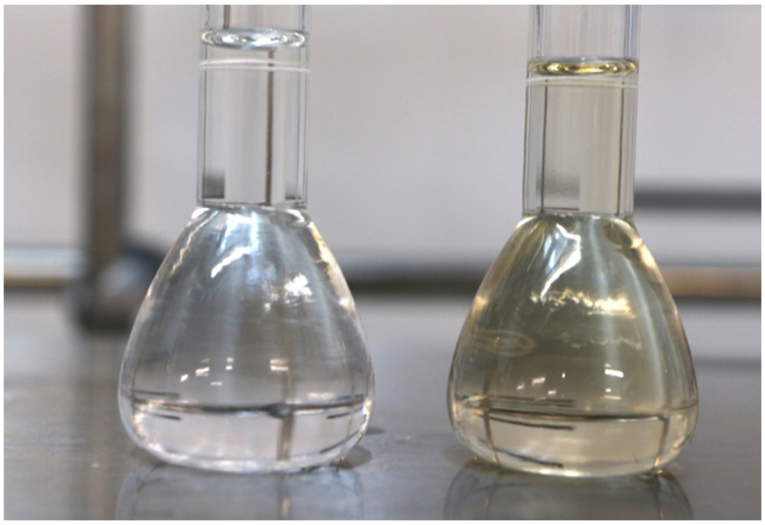


Figure S13. Dichloromethane solution of **4** in the absence (left) and presence of ten equivalents of $SbCl_5$ (right). [**4**] = 1×10^{-5} M.

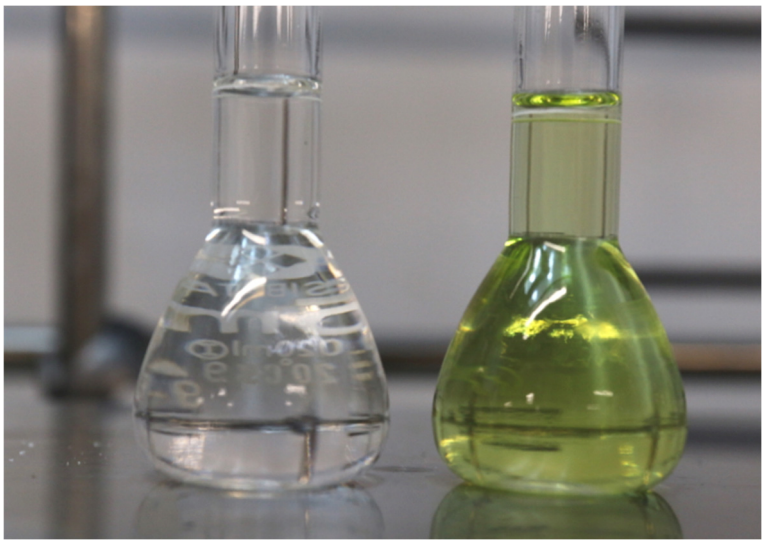


Figure S14. Dichloromethane solution of **5** in the absence (left) and presence of ten equivalents of $SbCl_5$ (right). [**5**] = 1×10^{-5} M.

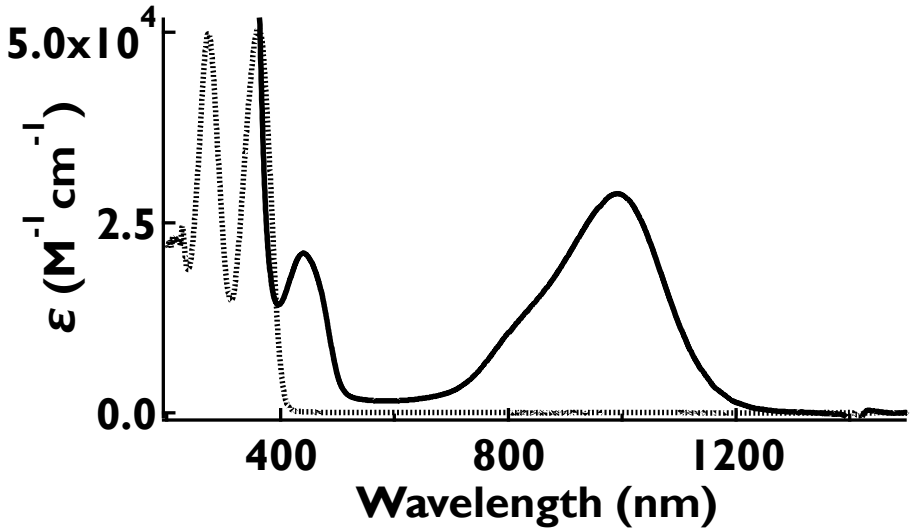


Figure S15. Absorption spectra of **3** before (dotted line) and after oxidation with 10 equivalents of $SbCl_5$ (solid line) in dichloromethane at room temperature. [**3**] = 1×10^{-5} M.

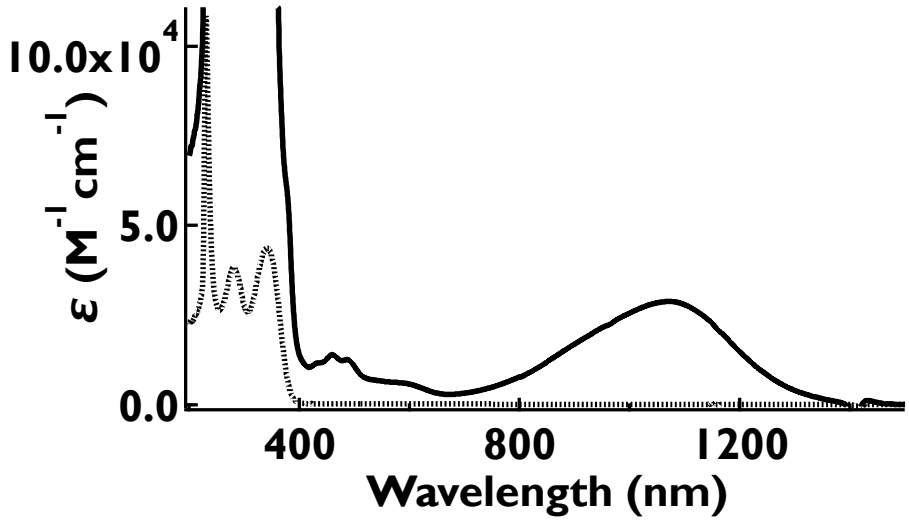


Figure S16. Absorption spectra of **4** before (dotted line) and after oxidation with 10 equivalents of $SbCl_5$ (solid line) in dichloromethane at room temperature. [**4**] = 1×10^{-5} M.

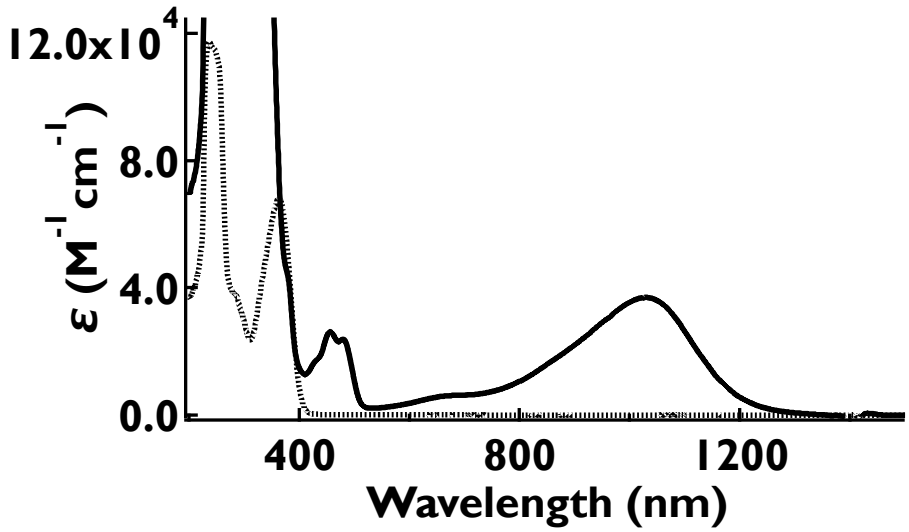


Figure S17. Absorption spectra of **5** before (dotted line) and after oxidation with 10 equivalents of $SbCl_5$ (solid line) in dichloromethane at room temperature. [**5**] = 1×10^{-5} M.

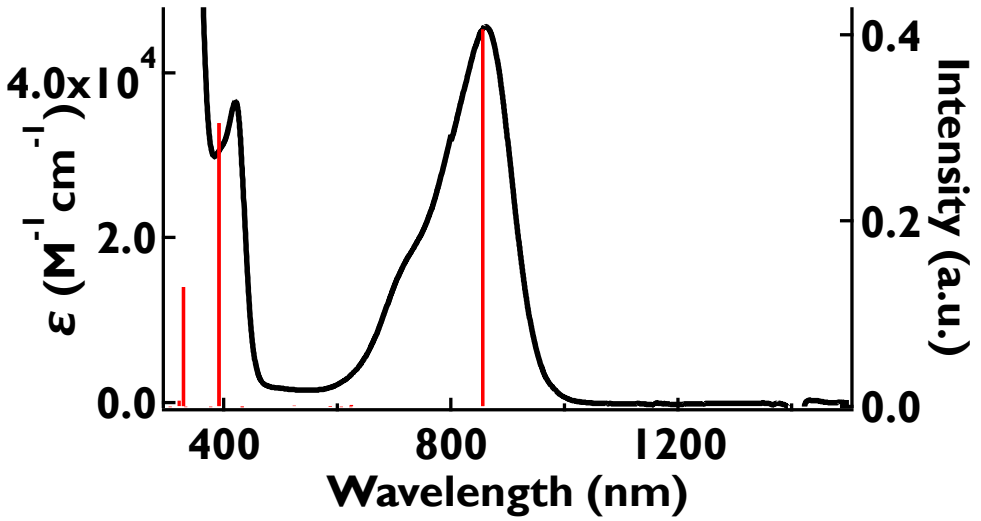


Figure S18. Experimental UV-vis absorption spectra of **2** after oxidation with ten equivalents of $SbCl_5$ and TD-DFT calculated energy transition with oscillator strength shown as a vertical red line. See also Figure S3.

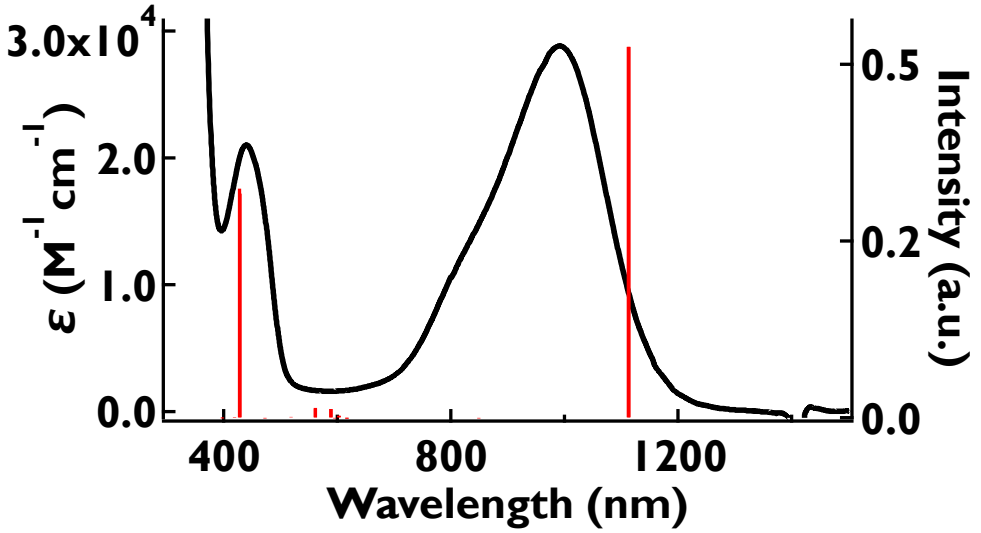


Figure S19. Experimental UV-vis absorption spectra of **3** after oxidation with ten equivalents of $SbCl_5$ and TD-DFT calculated energy transition with oscillator strength shown as a vertical red line. See also Figure S3.

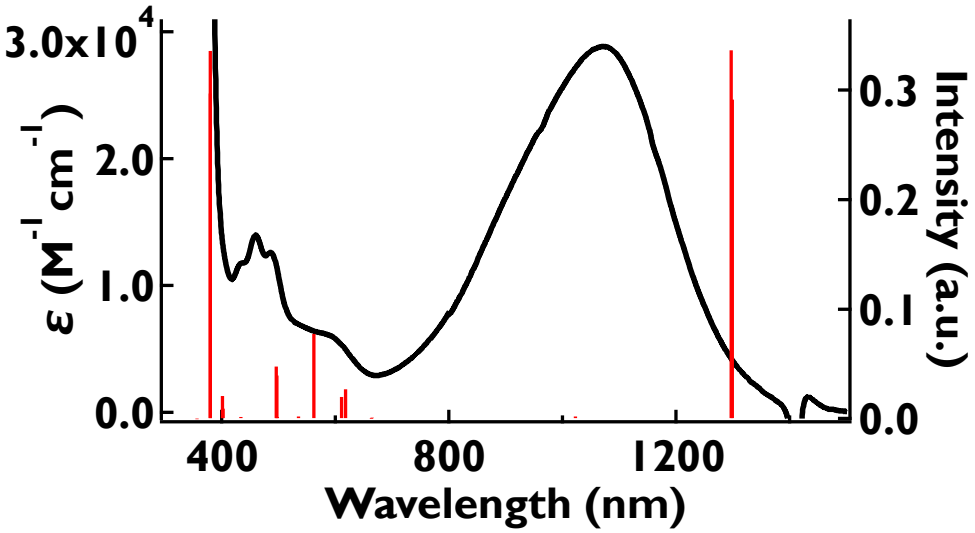


Figure S20. Experimental UV-vis absorption spectra of **4** after oxidation with ten equivalents of $SbCl_5$ and TD-DFT calculated energy transition with oscillator strength shown as a vertical red line. See also Figure S4.

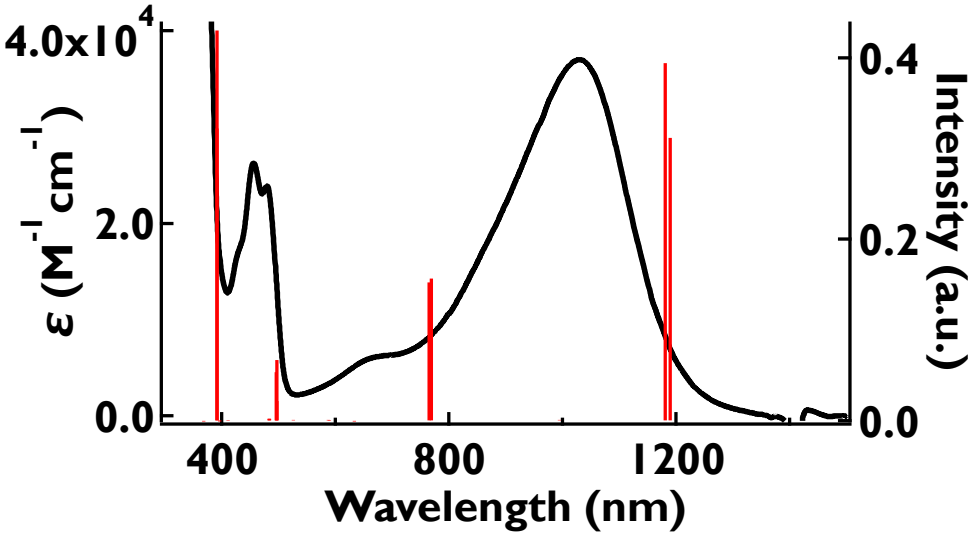


Figure S21. Experimental UV-vis absorption spectra of **5** after oxidation with ten equivalents of $SbCl_5$ and TD-DFT calculated energy transition with oscillator strength shown as a vertical red line. See also Figure S4.

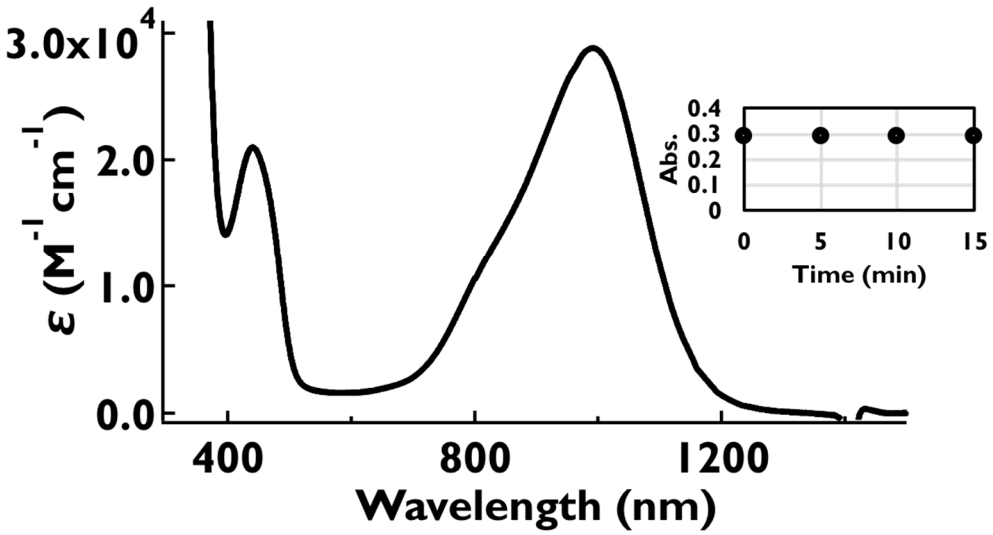


Figure S22. Time course of UV-vis absorption spectra of **3** with ten equivalents of $SbCl_5$ in dichloromethane at room temperature recorded every 5 minutes. The initial concentration of **3** is 1×10^{-5} M. Inset: time-course of the peak intensity at 991 nm.

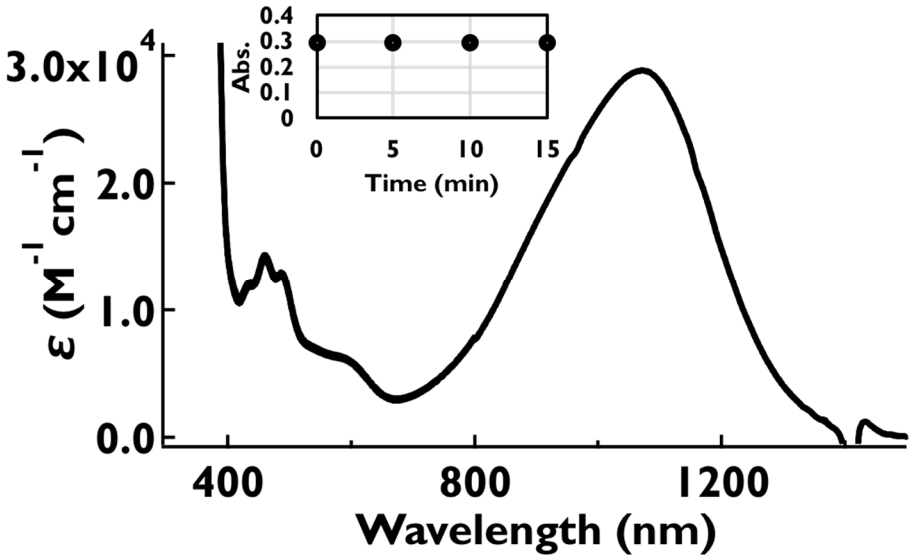


Figure S23. Time course of UV-vis absorption spectra of **4** with ten equivalents of $SbCl_5$ in dichloromethane at room temperature recorded every 5 minutes. The initial concentration of **4** is 1×10^{-5} M. Inset: time-course of the peak intensity at 1071 nm.

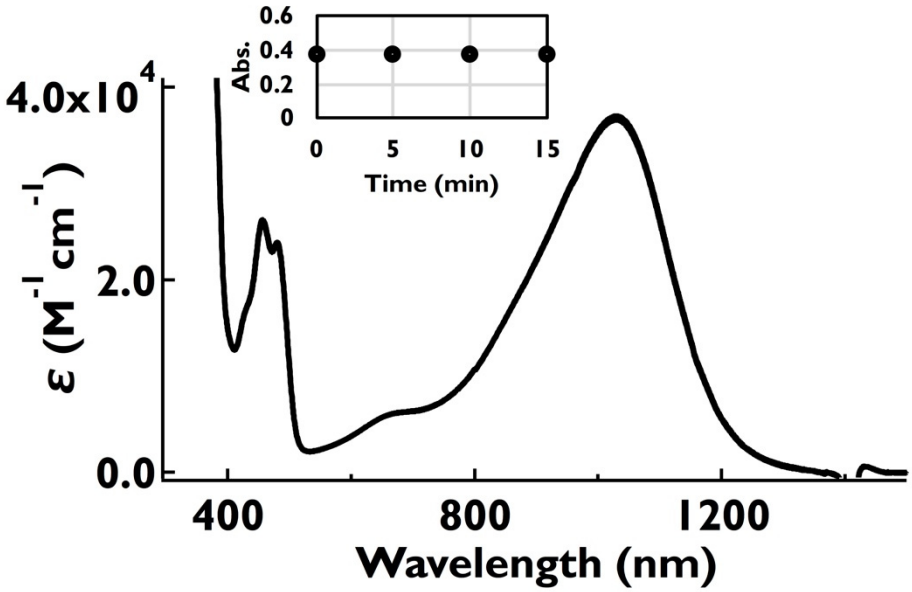


Figure S24. Time course of UV-vis absorption spectra of **5** with ten equivalents of $SbCl_5$ in dichloromethane at room temperature recorded every 5 minutes. The initial concentration of **5** is 1×10^{-5} M. Inset: time-course of the peak intensity at 1028 nm.

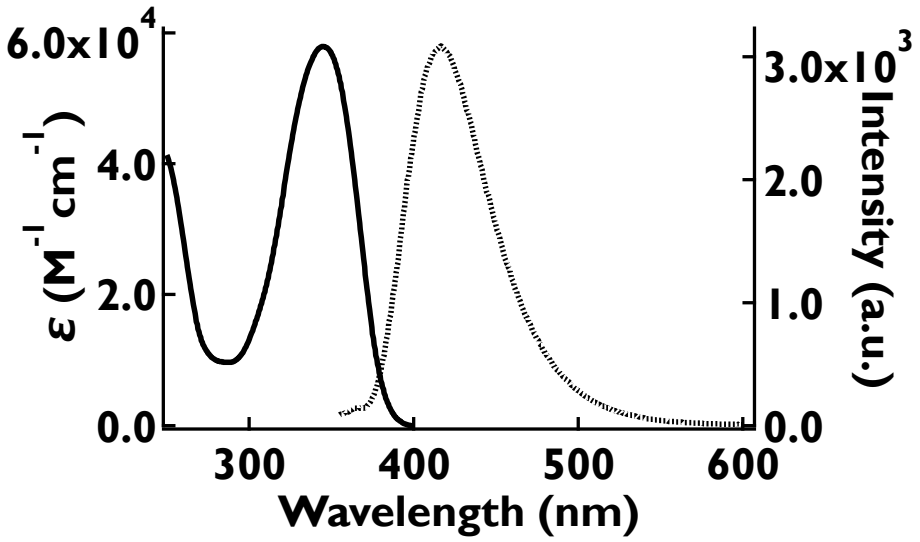


Figure S25. UV-vis (solid line) and fluorescence (dotted line) spectra of **2** in dichloromethane. The concentration is 1×10^{-5} M for UV-vis and 1×10^{-6} M for fluorescence spectra.

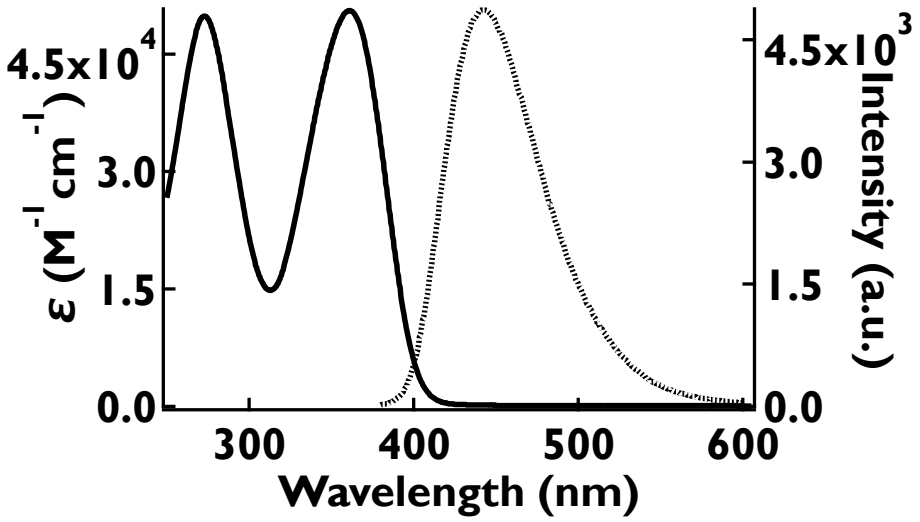


Figure S26. UV-vis (solid line) and fluorescence emission (dotted line) spectra of **3** in dichloromethane. The concentration is 1×10^{-5} M for UV-vis and 1×10^{-6} M for fluorescence spectrum.

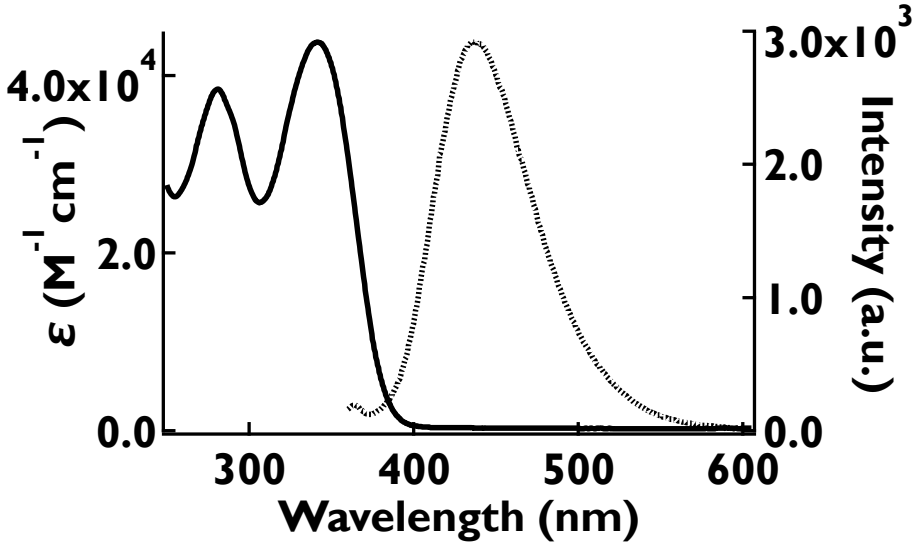


Figure S27. UV-vis (solid line) and fluorescence emission (dotted line) spectra of **4** in dichloromethane. The concentration is 1×10^{-5} M for UV-vis and 1×10^{-6} M for fluorescence spectrum.

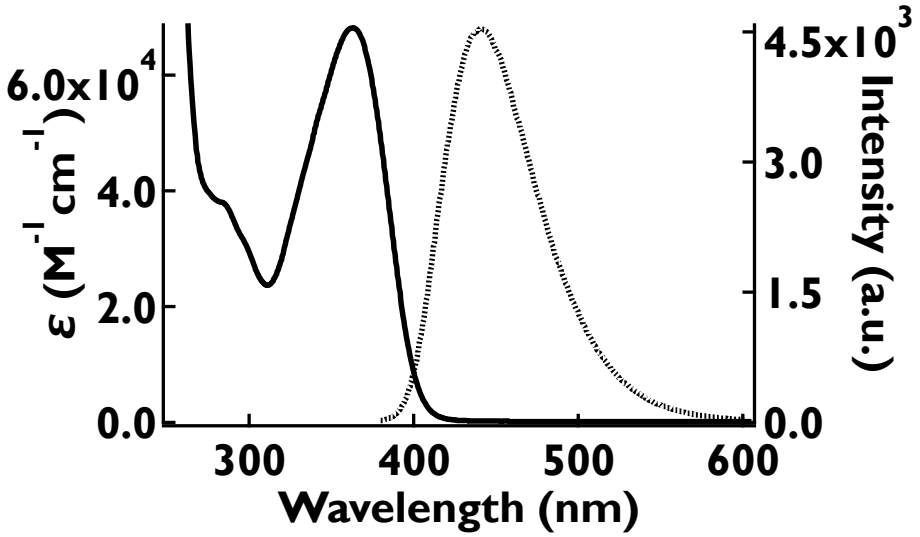


Figure S28. UV-vis (solid line) and fluorescence emission (dotted line) spectra of **5** in dichloromethane. The concentration is 1×10^{-5} M for UV-vis and 1×10^{-6} M for fluorescence spectrum.

7. Reduction of the radical cation $4^{\bullet+}$ with ascorbic acid.

To the solution of **4** (34.8 mg, 5.56×10^{-2} mmol) in dichloromethane (20 mL), 10 eq. of $SbCl_5$ in dichloromethane was slowly dropped at room temperature under nitrogen atmosphere. The solution was stirred for 5 min. The obtained solution was mixed with aqueous ascorbic acid solution, extracted with ethyl acetate, dried over sodium sulfate, and evaporated under reduced pressure to give white powder (34.4 mg).

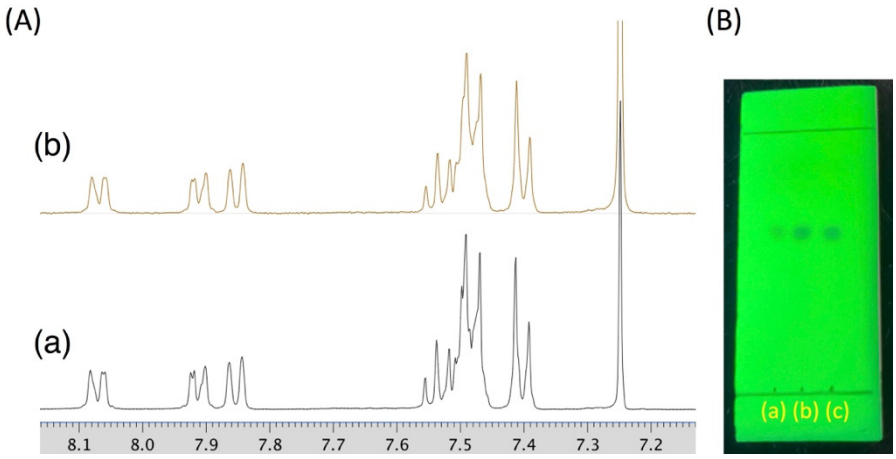


Figure S29. (A) ^{1}H NMR spectra of (a) **4** and (b) the resulting mixture after treatment of **4** with $SbCl_5$, followed by reduction with excess ascorbic acid. (B) TLC plate of (a) **4**, (b) overstrike of **4** and the mixture obtained after oxidation of **4** followed by reduction and (c) the mixture obtained after oxidation of **4** followed by reduction (irradiation at 365 nm with a 4W UV lamp).

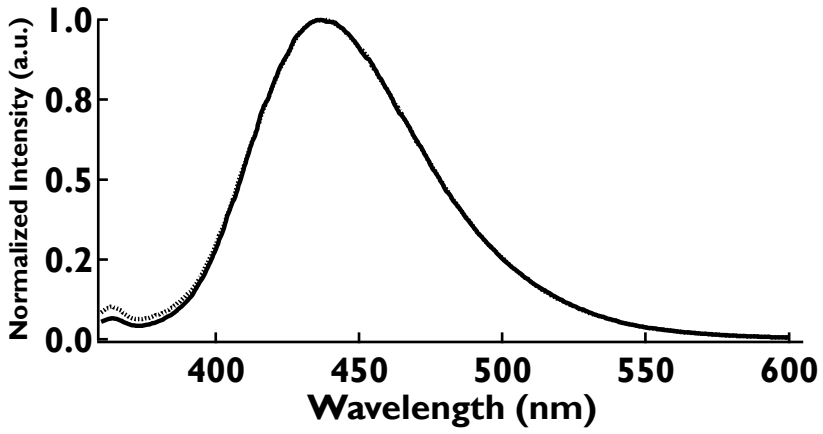


Figure S30. Normalized fluorescence spectra of **4** (solid line), and after addition of ten equivalents of $SbCl_5$ followed by reduction with excess ascorbic acid (dotted line).

8. Fluorescence spectra

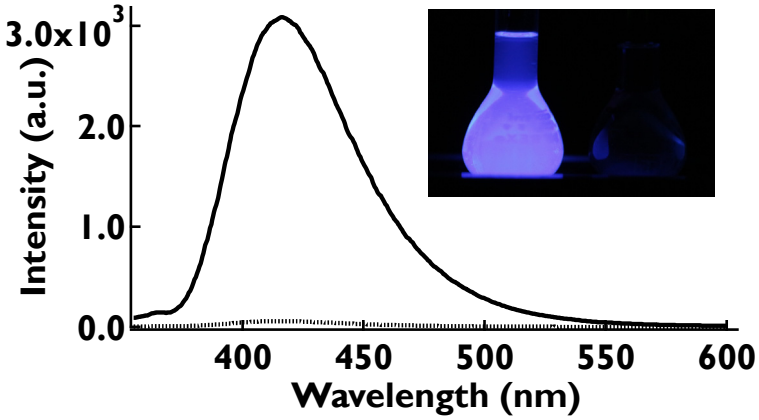


Figure S31. Fluorescence spectra of **2** before (solid line) and after oxidation with 10 equivalents of $SbCl_5$ (dotted line) in dichloromethane at room temperature. Excitation at 344 nm. [**2**] = 1×10^{-6} M. Inset: Luminescence arising from a dichloromethane solution of **2** in the absence (left) and presence of 10 equivalents of $SbCl_5$ (right), (irradiation with a 4W UV lamp). [**2**] = 1×10^{-5} M.

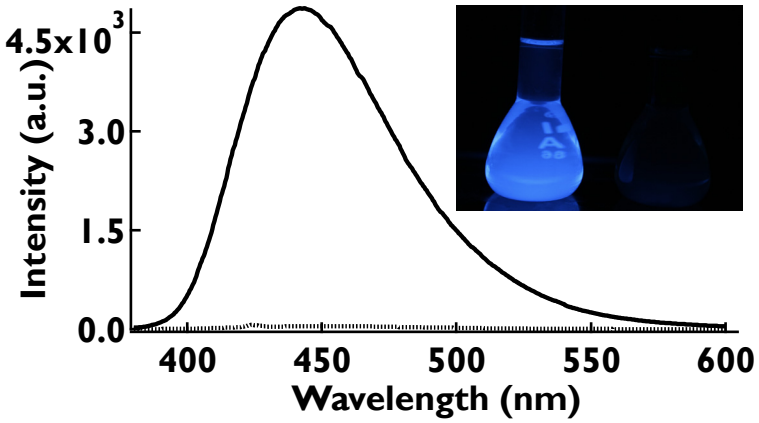


Figure S32. Fluorescence spectra of **3** before (solid line) and after oxidation with 10 equivalents of $SbCl_5$ (dotted line) in dichloromethane at room temperature. Excitation at 361 nm. [**3**] = 1×10^{-6} M. Inset: Luminescence arising from a dichloromethane solution of **3** in the absence (left) and presence of 10 equivalents of $SbCl_5$ (right), (irradiation with a 4W UV lamp). [**3**] = 1×10^{-5} M.

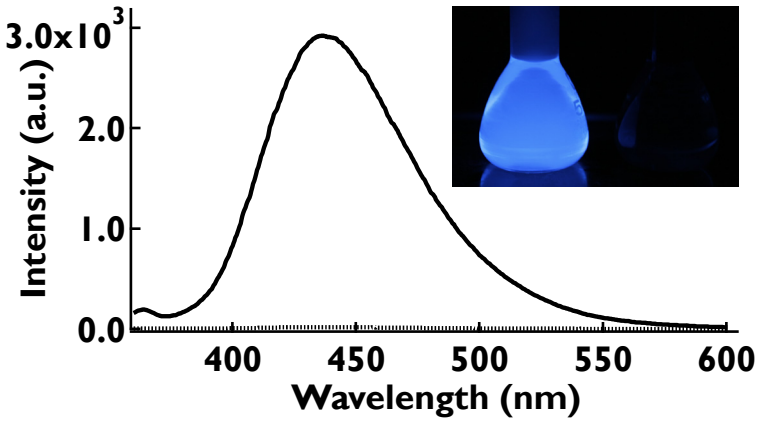


Figure S33. Fluorescence spectra of **4** before (solid line) and after oxidation with 10 equivalents of $SbCl_5$ (dotted line) in dichloromethane at room temperature. Excitation at 341 nm. [**4**] = 1×10^{-6} M. Inset: Luminescence arising from a dichloromethane solution of **4** in the absence (left) and presence of 10 equivalents of $SbCl_5$ (right), (irradiation with a 4W UV lamp). [**4**] = 1×10^{-5} M.

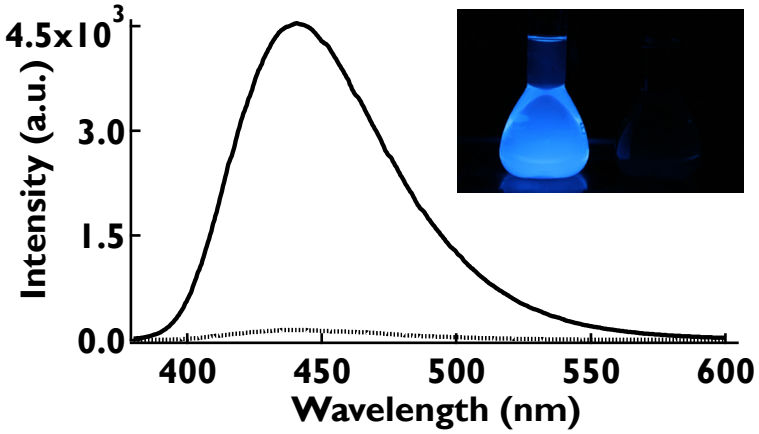


Figure S34. Fluorescence spectra of **5** before (solid line) and after oxidation with 10 equivalents of $SbCl_5$ (dotted line) in dichloromethane at room temperature. Excitation at 363 nm. [**5**] = 1×10^{-6} M. Inset: Luminescence arising from a dichloromethane solution of **5** in the absence (left) and presence of 10 equivalents of $SbCl_5$ (right), (irradiation with a 4W UV lamp). [**5**] = 1×10^{-5} M.

9. ^{1}H and ^{13}C spectra

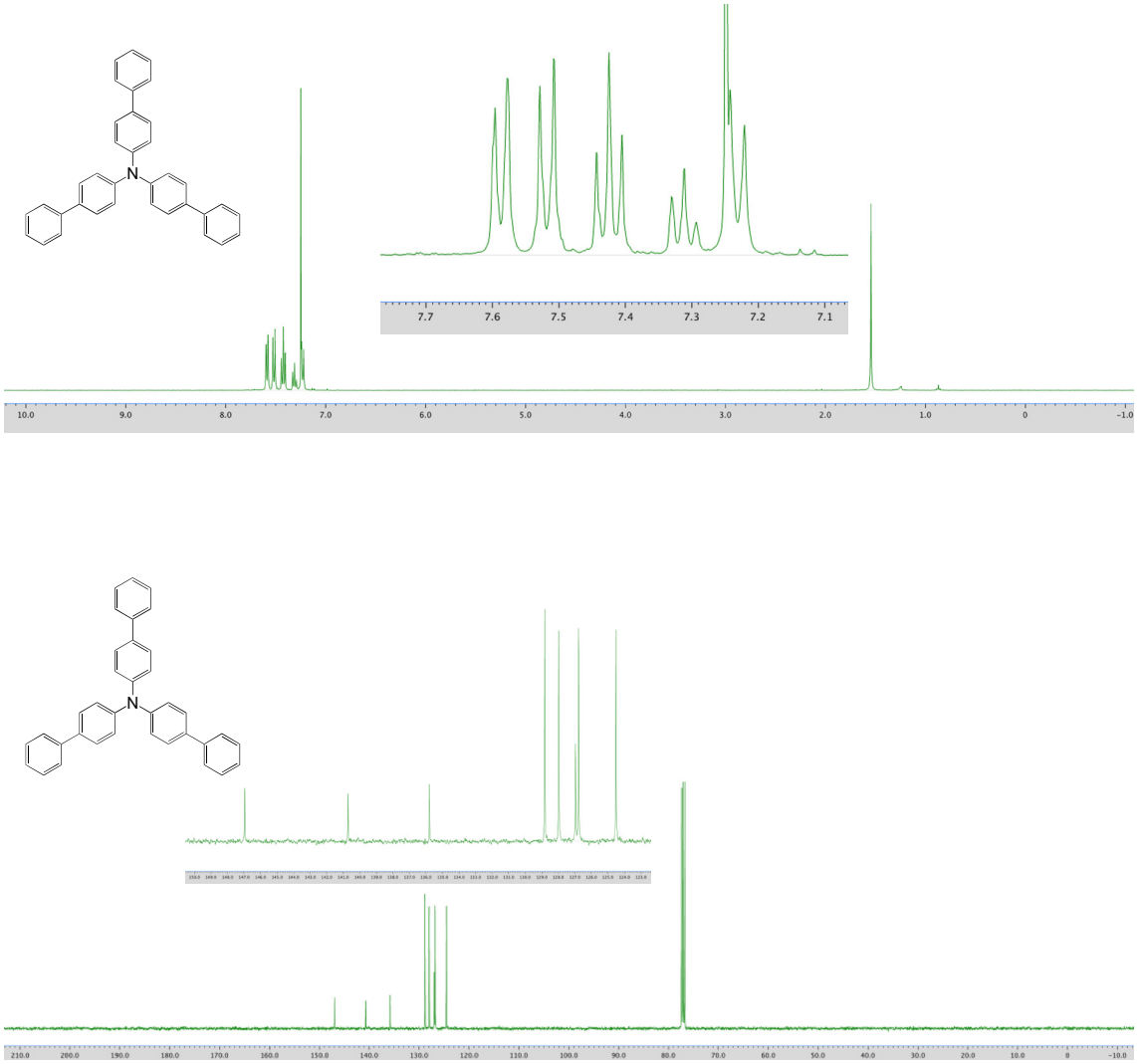
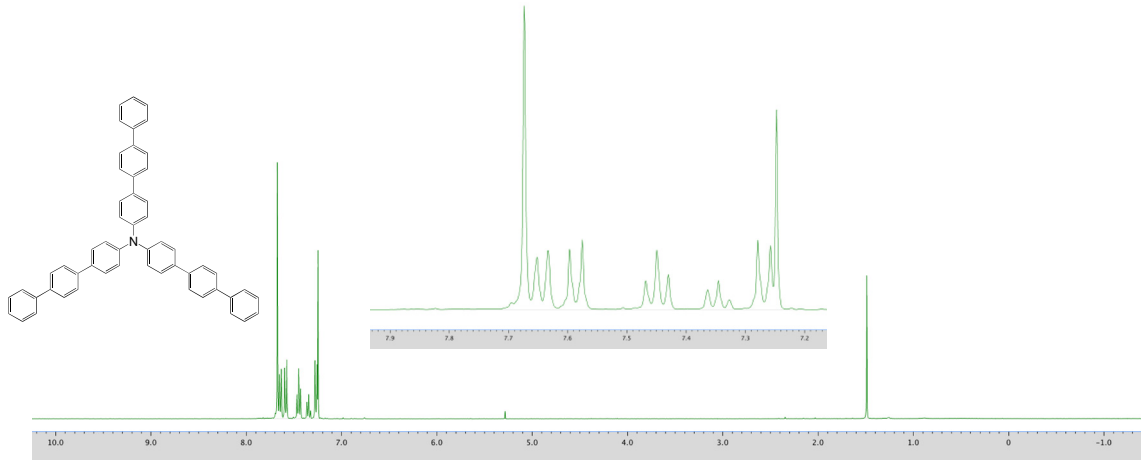


Figure S35. ^{1}H and ^{13}C spectra of **2**.



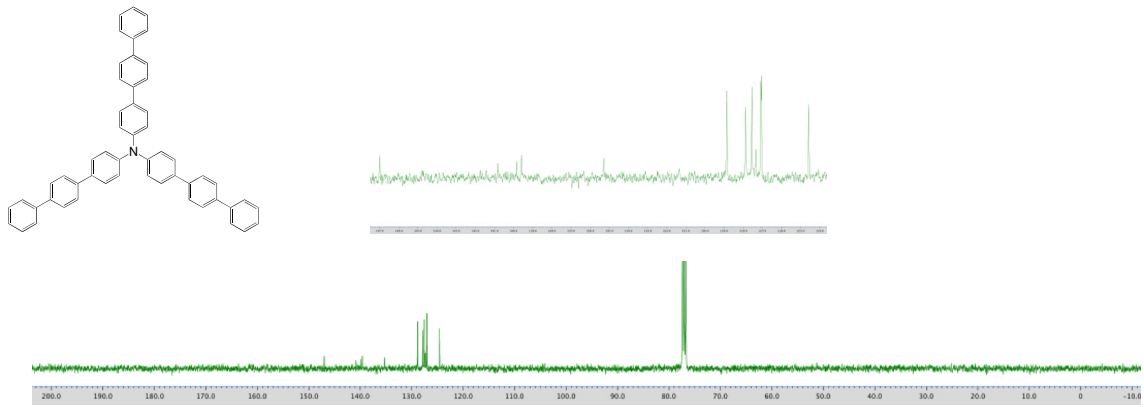


Figure S36. ^{1}H and ^{13}C spectra of **3**.

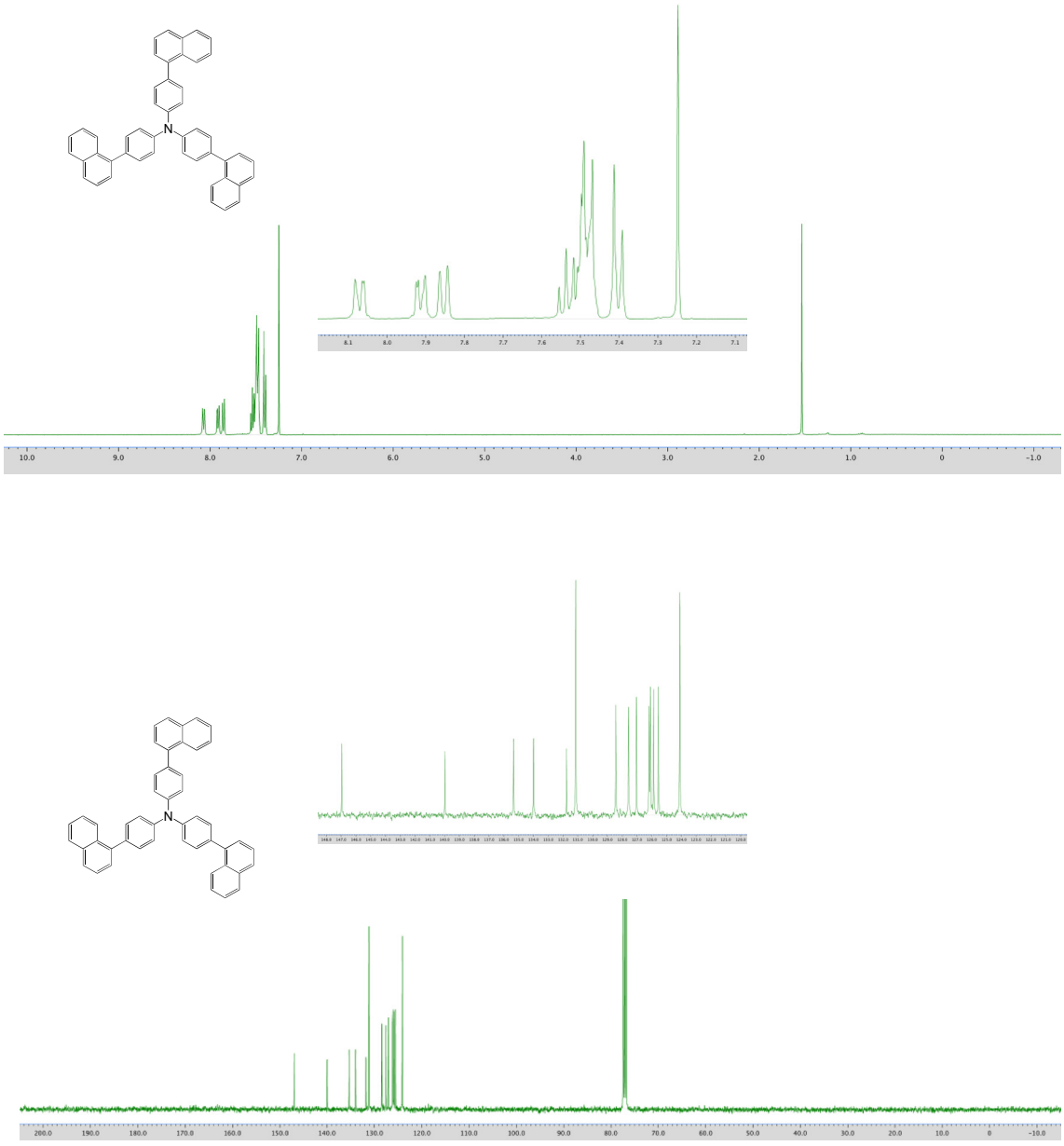
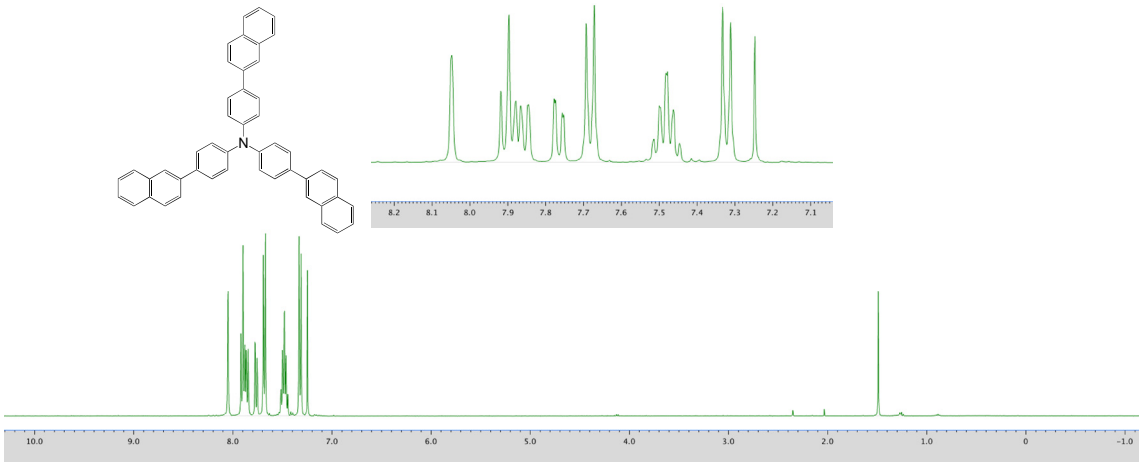


Figure S37. ^{1}H and ^{13}C spectra of **4**.



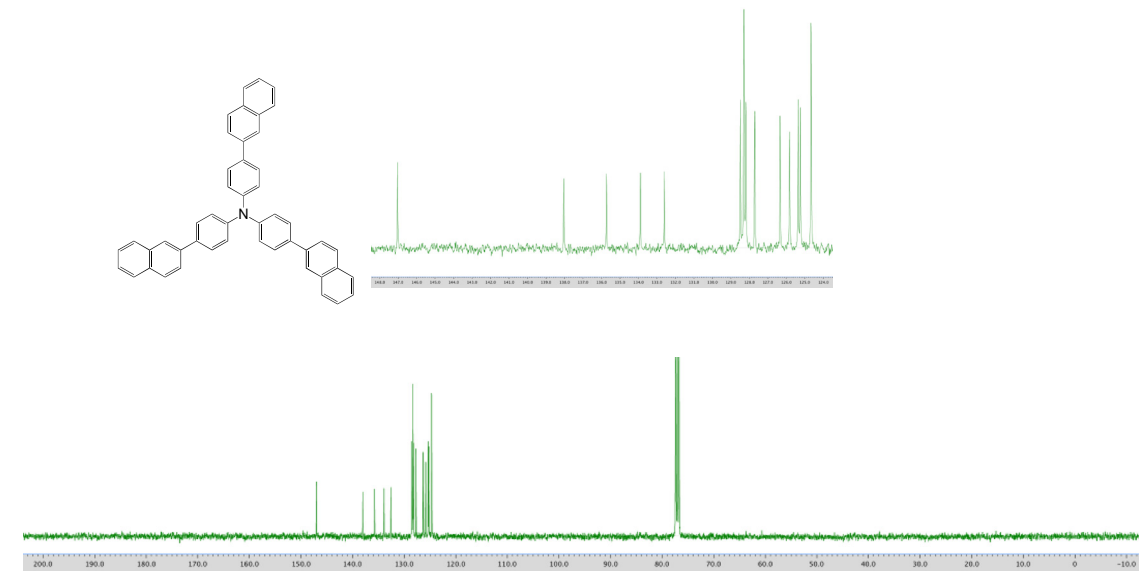


Figure S38. ^{1}H and ^{13}C spectra of **5**.

10. ESR spectra

Typical procedure for the preparation of radical cationic species for ESR measurements is as follows. To a solution of Ar_3-TPA in dry dichloromethane (5.0×10^{-4} M, 100μL) was added a solution of $SbCl_5$ in dry dichloromethane (5.0×10^{-3} M, 100μL). The obtained solution was diluted to 5 mL with dry dichloromethane.

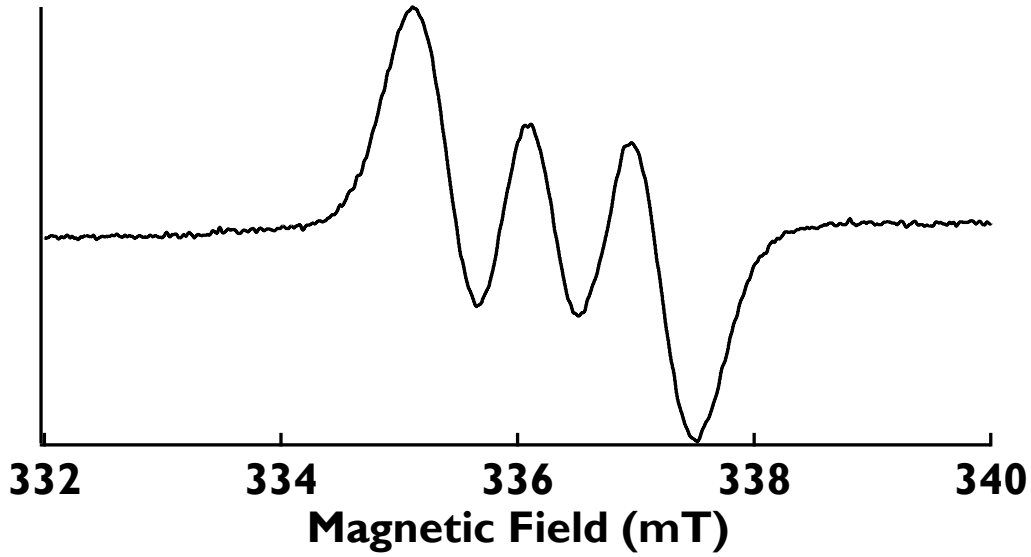


Figure S39. ESR spectrum of $\mathbf{2}^{\bullet+}$ in CH_2Cl_2.

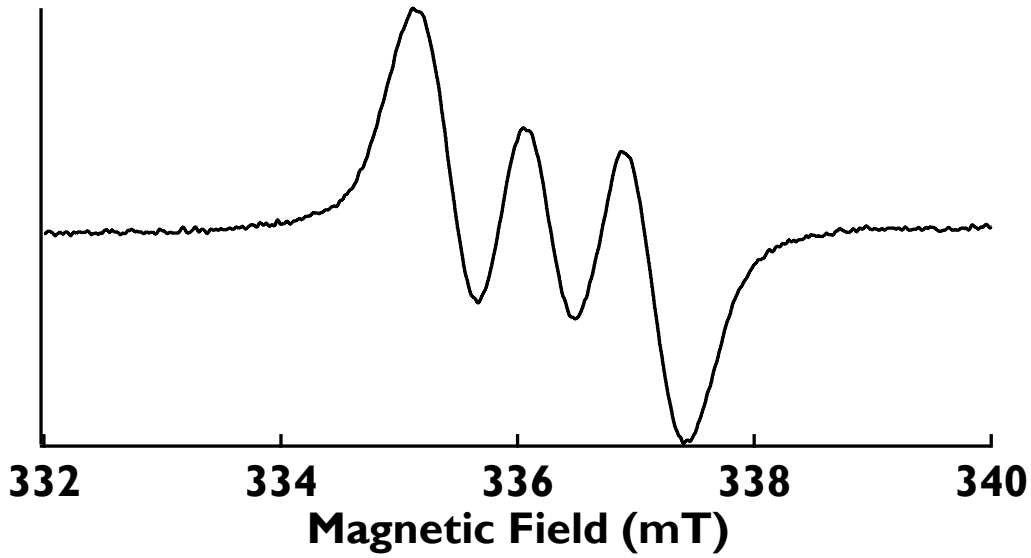


Figure S40. ESR spectrum of $\mathbf{3}^{\bullet+}$ in CH_2Cl_2.

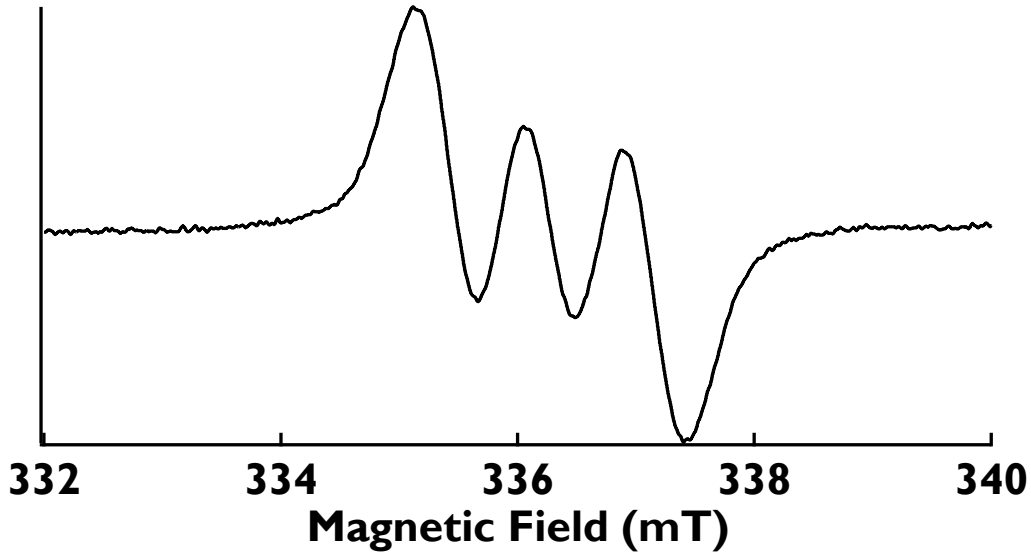


Figure S41. ESR spectrum of $\mathbf{4}^{\bullet+}$ in CH_2Cl_2.

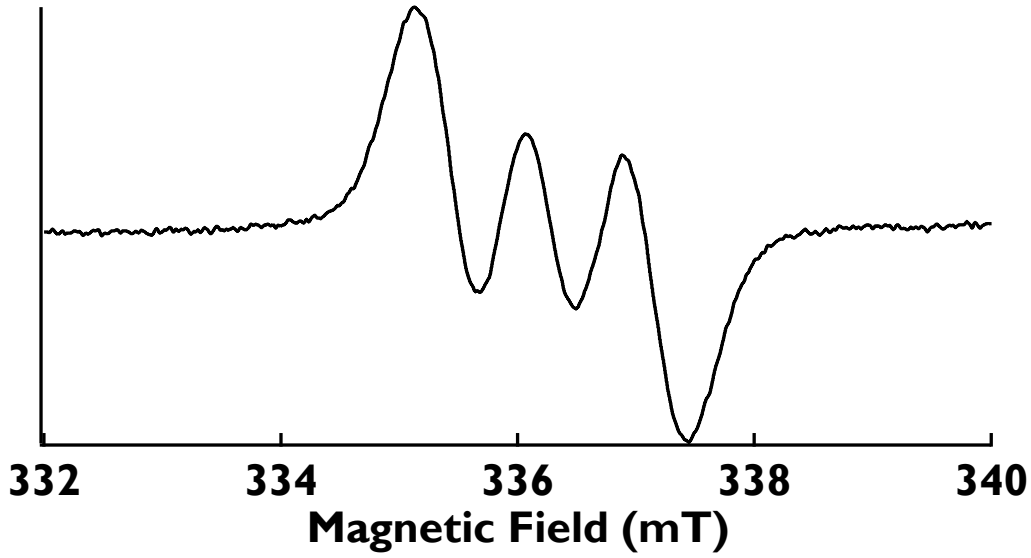


Figure S42. ESR spectrum of $\mathbf{5}^{\bullet+}$ in CH_2Cl_2.

11. References

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