Electronic Supplementary Information for:

Synthesis, Electrochemistry and Electrogenerated Chemiluminesce of Two BODIPY-Appended Bipyridine Homologues

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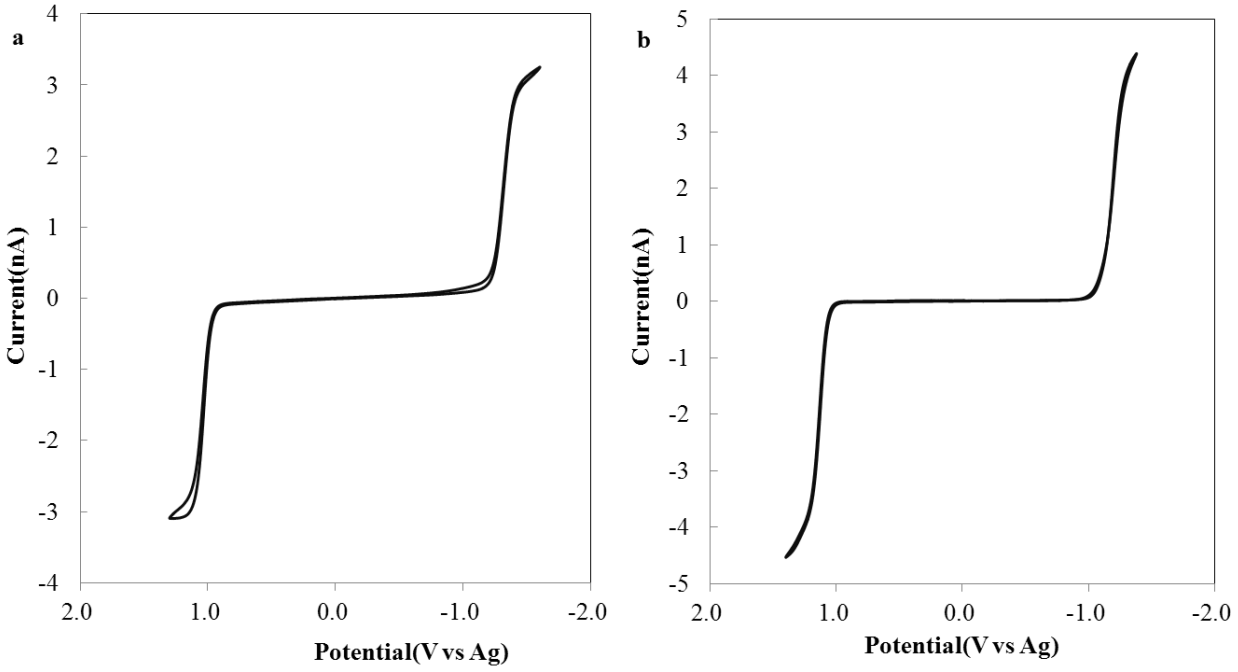

Figure S1. Cyclic voltammograms of (a) 0.59 mM **BB3** and (b) 0.68 mM **BB4** in CH_2Cl_2 containing 0.1 M $TBAPF_6$. CVs were recorded using a platinum ultramicroelectrode (r = 12.5 μm) at a scan rate (ν) of 10 mV/s.

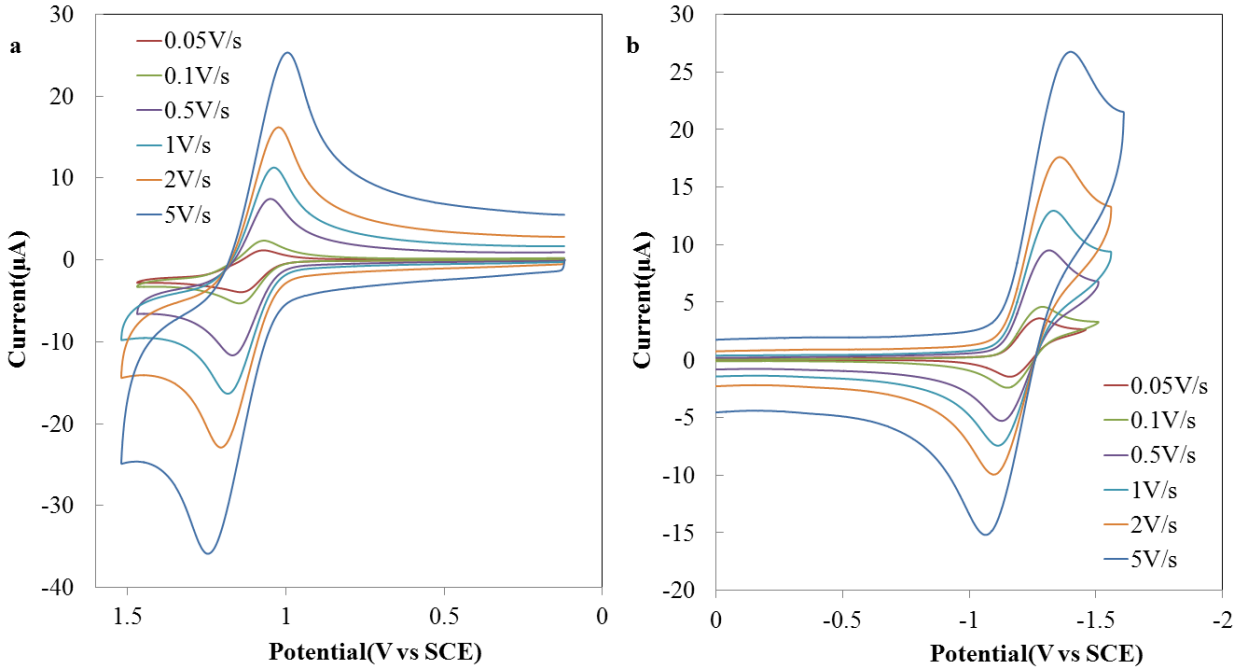

Figure S2. Scan rate dependence for (a) oxidation and (b) reduction of 0.59 mM **BB3** in CH_2Cl_2 containing 0.1 M $TBAPF_6$. CVs were recorded using a platinum disk working electrode (A = 0.043 cm^2).

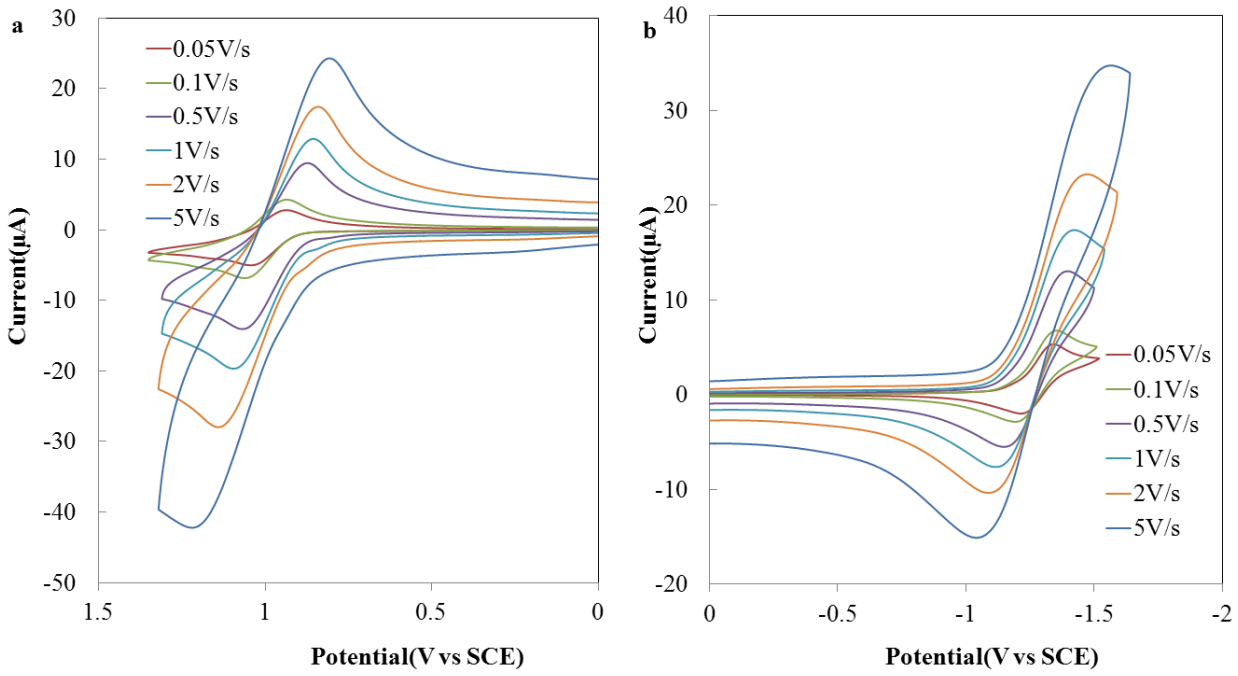

Figure S3. Scan rate dependence for (a) oxidation and (b) reduction of 0.59 mM **BB4** in CH_2Cl_2 containing 0.1 M $TBAPF_6$. CVs were recorded using a platinum disk working electrode (A = 0.043 cm^2).

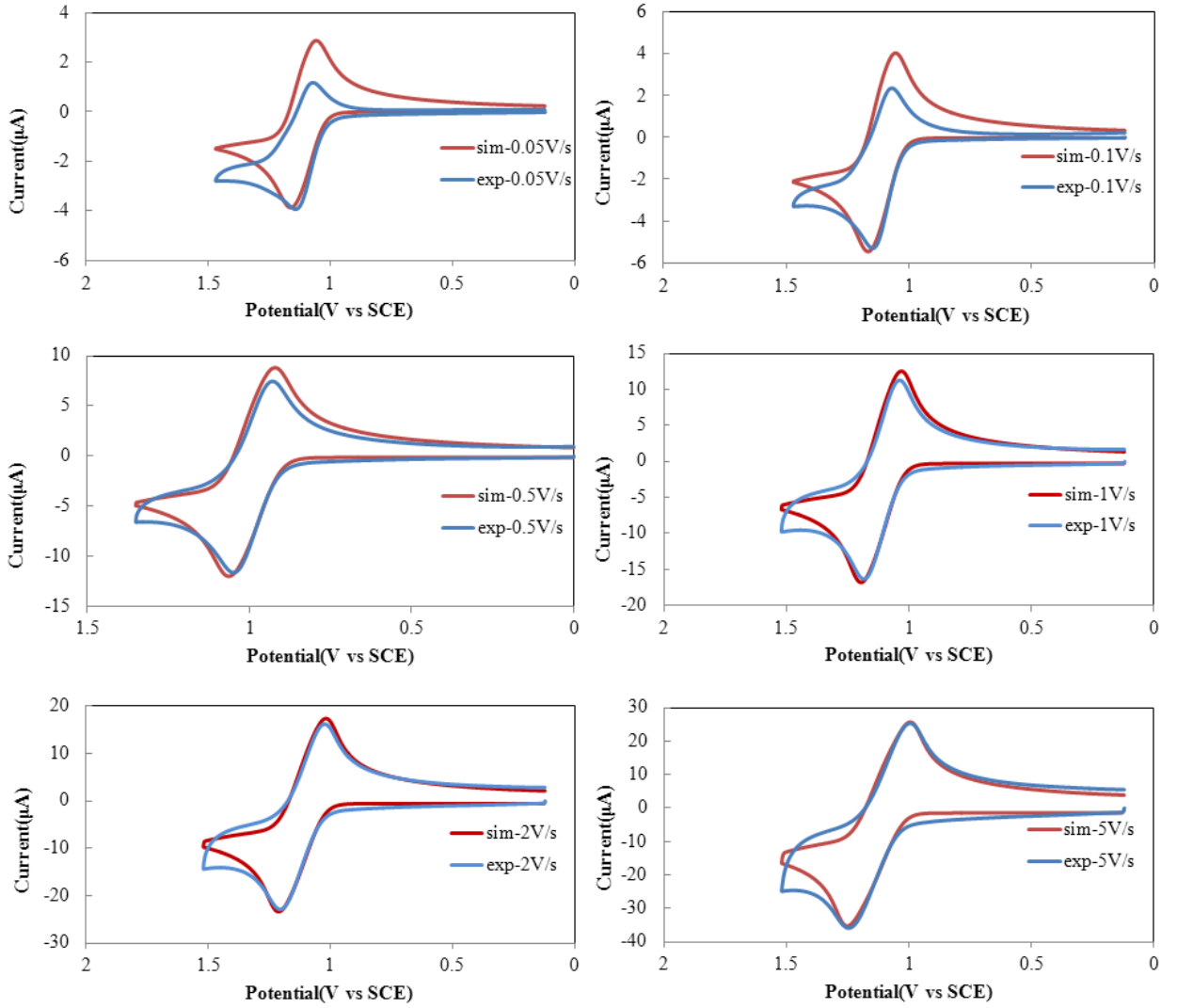

Figure S4. Comparison between simulated and experimental polarization curves for oxidation of a 0.59 mM solution of **BB3** at various scan rates. Simulations were prepared for an EE mechanism ($E_{1/2}(A/A^{+})$ = 1.14 V; $E_{1/2}(A^{+}/A^{2+})$ = 1.19 V) with a heterogeneous ET rate constant of $k°$ > 0.01 cm/s, diffusion coefficient of D = 4.0 × 10^{-6} cm^2/s, uncompensated resistance of 2032 Ω, and capacitance of 3.0 × 10^{-7} F. Experimental polarization curves were recorded in CH_2Cl_2 containing 0.1 M $TBAPF_6$ with a platinum disk working electrode (A = 0.043 cm^2).

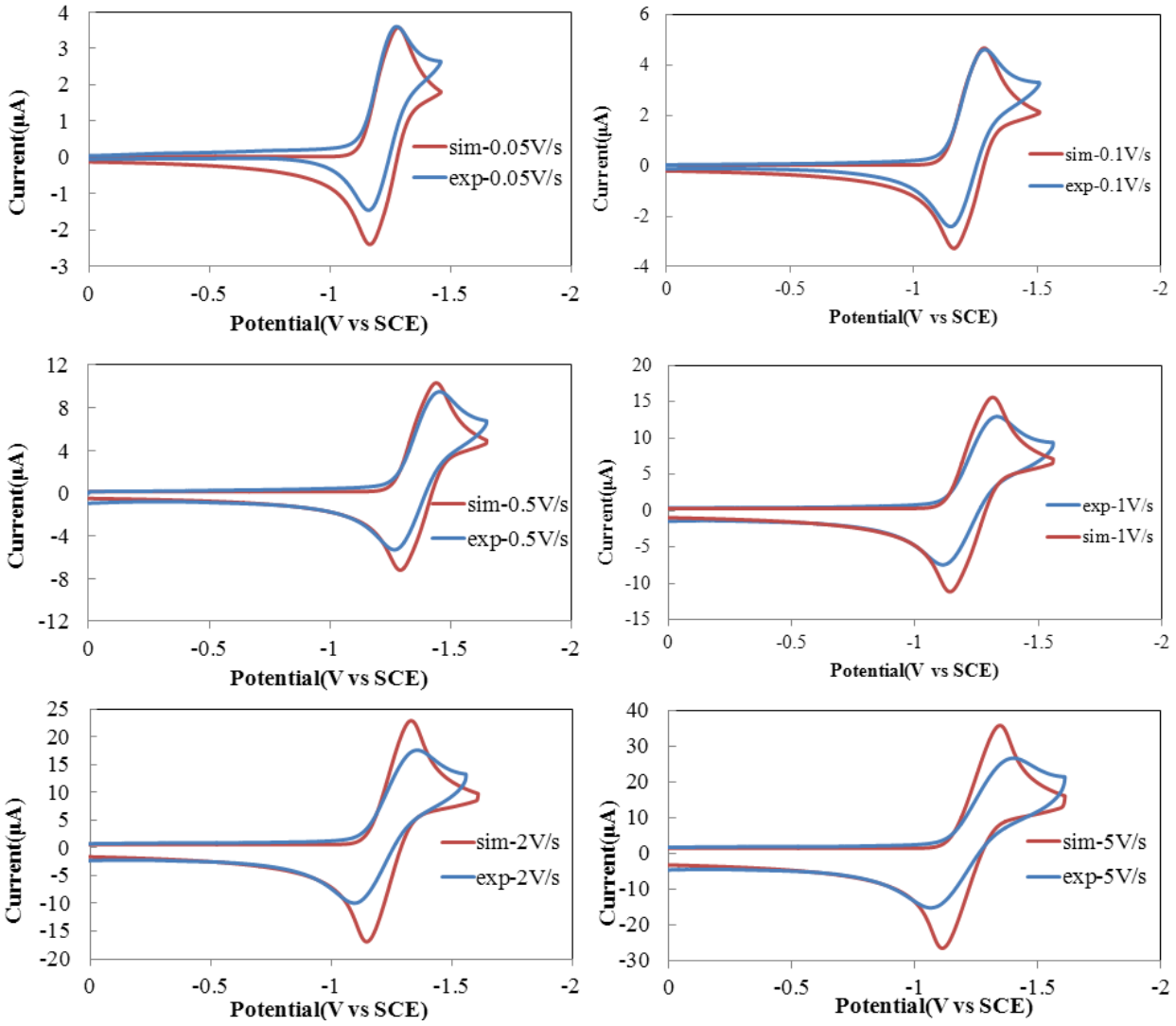

Figure S5. Comparison between simulated and experimental polarization curves for reduction of a 0.59 mM solution of **BB3** at various scan rates. Simulations were prepared for an EE mechanism ($E_{1/2}(A/A^{-})$ = –1.17 V; $E_{1/2}(A^{-}/A^{2-})$ = –1.24 V) with a heterogeneous ET rate constant of $k°$ > 0.01 cm/s, diffusion coefficient of D = 4.0 × 10^{-6} cm^2/s, uncompensated resistance of 2032 Ω, and capacitance of 3.0 × 10^{-7} F. Experimental polarization curves were recorded in CH_2Cl_2 containing 0.1 M $TBAPF_6$ with a platinum disk working electrode (A = 0.043 cm^2).

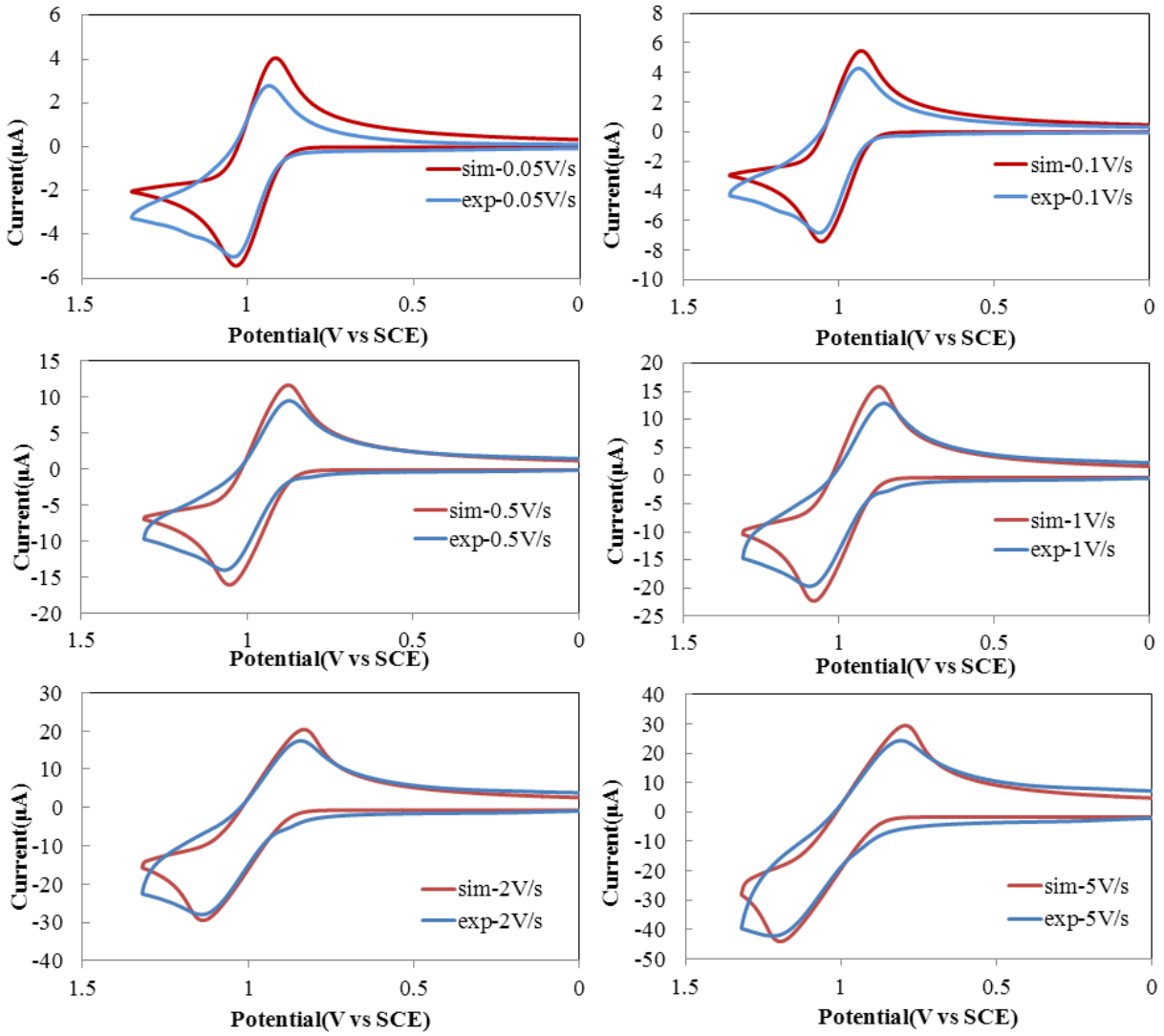

Figure S6. Comparison between simulated and experimental polarization curves for oxidation of a 0.68 mM solution of **BB4** at various scan rates. Simulations were prepared for an EE mechanism ($E_{1/2}(A/A^+)$ = 1.12 V; $E_{1/2}(A^+/A^{2+})$ = 1.17 V) with a heterogeneous ET rate constant of $k°$ > 0.01 cm/s, diffusion coefficient of D = 4.0 × 10^{-6} cm^2/s, uncompensated resistance of 3500 Ω, and capacitance of 3.5 × 10^{-7} F. Experimental polarization curves were recorded in CH_2Cl_2 containing 0.1 M $TBAPF_6$ with a platinum disk working electrode (A = 0.043 cm^2).

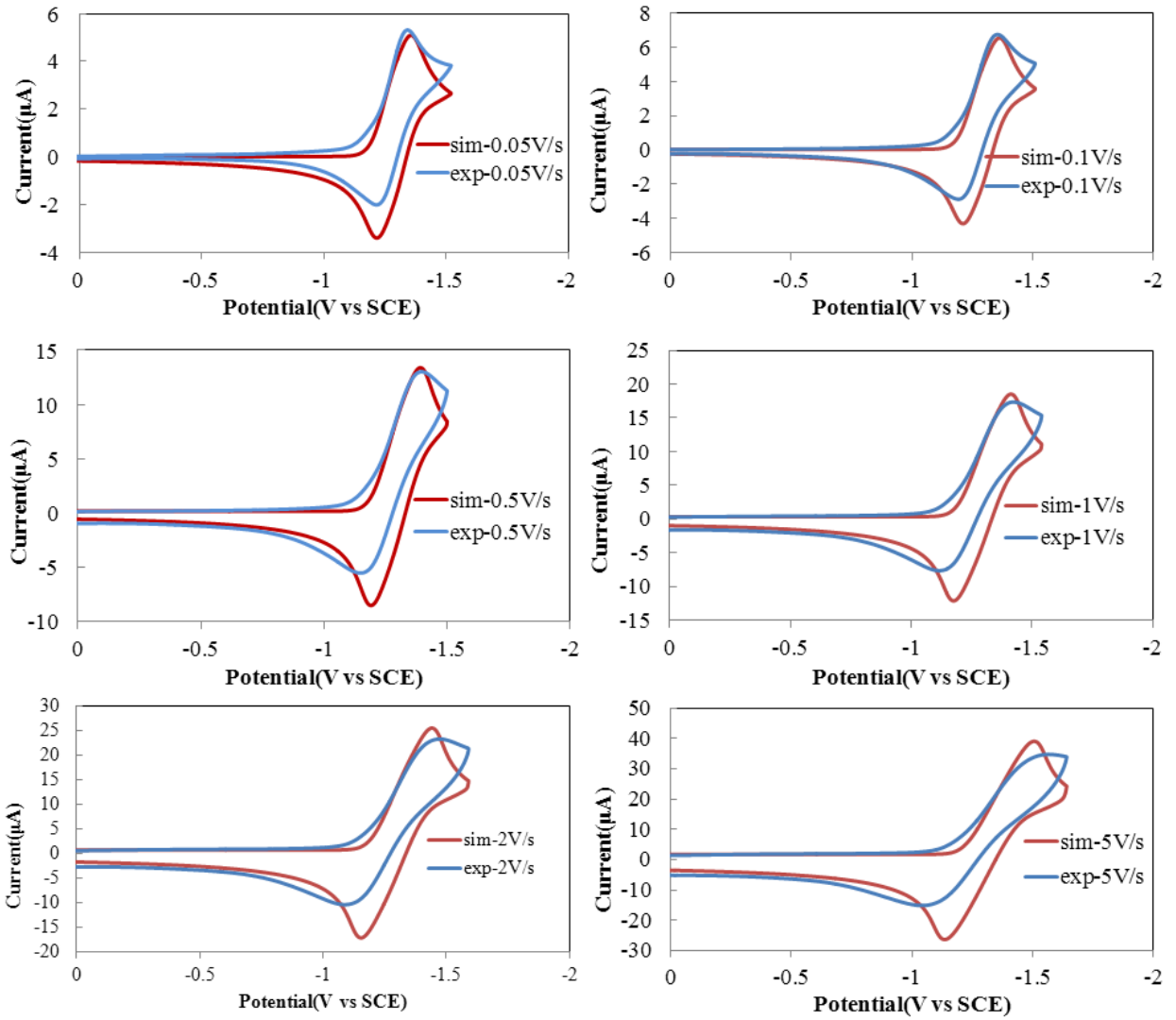

Figure S7. Comparison between simulated and experimental polarization curves for reduction of a 0.68 mM solution of **BB4** at various scan rates. Simulations were prepared for an EE mechanism ($E_{1/2}(A/A^+)$ = –1.18 V; $E_{1/2}(A^+/A^{2+})$ = –1.24 V) with a heterogeneous ET rate constant of $k°$ > 0.01 cm/s, diffusion coefficient of D = 4.0 × 10^{-6} cm^2/s, uncompensated resistance of 3500 Ω, and capacitance of 3.5 × 10^{-7} F. Experimental polarization curves were recorded in CH_2Cl_2 containing 0.1 M $TBAPF_6$ with a platinum disk working electrode (A = 0.043 cm^2).

Table S1. Cartesian coordinates for DFT optimized structure of **BB3**

Atom	X-position	Y-position	Z-position
B	12.45162308	5.97078156	18.59874221
B	4.72633538	-0.73817455	6.41639447
F	11.76743826	6.55759135	19.65301748
F	13.81690982	6.14041117	18.77716245
F	3.87999738	-1.82774463	6.30690810
F	4.87364625	-0.14156688	5.16593203
N	12.11673264	4.46433175	18.49900167
N	12.02169588	6.61769384	17.25632617
N	8.48270000	2.59410000	14.41060000
N	8.65638352	2.23059101	10.83566118
N	6.11034655	-1.16294114	6.95831950
N	4.15253279	0.29380446	7.42686052
C	12.47039987	3.49669845	19.36561456
C	12.02584901	2.23213112	18.90449304
C	11.35076341	2.44913638	17.71236654
C	11.42013746	3.85424132	17.44597670
C	13.29417676	3.77616246	20.59032018
H	13.05524765	4.65562221	20.94946825
H	14.24461978	3.76572783	20.35367062
H	13.11705155	3.08902704	21.26543652
C	12.32367580	0.93054684	19.58065972
H	11.61138669	0.28134779	19.35145475
H	12.30182429	1.06726525	20.56158526
C	13.66422789	0.34138916	19.19654816
H	13.77326244	-0.53149769	19.62787381
H	14.38127518	0.94310259	19.49039650
H	13.70667932	0.23238812	18.22315591
C	10.71874972	1.37590352	16.88907581
H	10.88062450	0.50526246	17.30705916
H	11.10506754	1.38385586	15.98900059
H	9.75338931	1.53537288	16.83144875
C	12.26630740	7.87102926	16.85816054
C	11.74735286	8.08704745	15.58321653
C	11.14442642	6.90587663	15.16665621
C	11.31578358	5.96997113	16.23617387
C	13.00949765	8.86778047	17.71141710
H	12.88396507	8.64668569	18.65772868
H	12.66430286	9.76904408	17.53780235
H	13.96353677	8.83702251	17.49252734
C	12.33660690	9.41692632	14.52054350

H	13.21392148	9.79423305	14.78350373
H	12.30327915	9.21266696	13.55136658
C	11.27846547	10.09539176	14.97921024
H	11.35446590	11.03411210	14.71189274
H	11.25647189	10.03456393	15.95709714
H	10.45971864	9.71027763	14.60757382
C	10.47162541	6.71596692	13.82694635
H	10.34329032	7.58864584	13.40109940
H	9.60233624	6.28437062	13.95775546
H	11.03388365	6.15252638	13.25631108
C	11.00590000	4.61740000	16.35080000
C	9.15610000	3.19620000	15.41740000
H	8.82480000	3.10320000	16.30190000
C	10.30650000	3.94340000	15.21750000
C	10.78940000	4.07490000	13.94040000
H	11.58320000	4.57100000	13.77640000
C	10.10360000	3.47230000	12.88760000
H	10.42130000	3.55910000	11.99740000
C	8.95170000	2.74410000	13.15220000
C	8.18390000	2.07740000	12.08800000
C	7.02289852	1.35361687	12.35989253
H	6.70195657	1.26122157	13.24902866
C	6.34598273	0.76905772	11.29282914
H	5.55165212	0.27355741	11.45051799
C	6.82415589	0.90860659	10.01492980
C	7.97968382	1.63745692	9.82360764
H	8.31763611	1.72722238	8.94089896
C	6.08321203	0.31861973	8.86075352
C	6.94542084	-2.05851184	6.39039795
C	8.15838409	-2.11822701	7.11769342
C	8.05518848	-1.19142954	8.15110317
C	6.76971648	-0.59881039	8.06282872
C	6.60955220	-2.85340776	5.16570195
H	5.63699290	-2.90419686	5.06656800
H	6.97825206	-3.75752252	5.25087665
H	6.99516925	-2.41622715	4.37744690
C	9.30857610	-3.01513108	6.75249974
H	9.86008503	-3.18204584	7.55718490
H	8.95665782	-3.88629510	6.43732925
C	10.16453325	-2.40716746	5.68100260
H	10.92396536	-2.99806919	5.49454411
H	10.49629819	-1.53552711	5.98267583
H	9.63283032	-2.29102087	4.86468103

C	9.18637898	-0.87987425	9.10697263
H	9.90563838	-1.53494326	8.98781290
H	8.85658543	-0.92050520	10.02873633
H	9.53121657	0.02068429	8.92362583
C	2.93495410	0.87754417	7.35997216
C	2.73536654	1.70471344	8.47747178
C	3.90800036	1.64205468	9.24260680
C	4.78754011	0.75411688	8.57312158
C	2.00144532	0.68614440	6.19832230
H	2.04467882	-0.24338390	5.89290578
H	2.26456005	1.28211737	5.46642601
H	1.08580118	0.89725475	6.47669909
C	1.50222911	2.51809893	8.78089027
H	0.70946719	2.03966090	8.43316208
H	1.40316050	2.59229763	9.76373599
C	1.53353721	3.89650604	8.19219478
H	0.70678127	4.36849139	8.42210323
H	1.61449444	3.83410133	7.21787545
H	2.30135154	4.38856535	8.55318828
C	4.14147652	2.43007452	10.50609843
H	3.30334187	2.85233746	10.78835634
H	4.81563908	3.12158542	10.34014819
H	4.45878385	1.82777598	11.21275000

Table S2. Cartesian coordinates for DFT optimized structure of **BB4**

Atom	X-position	Y-position	Z-position
B	18.92561336	2.46523773	17.82702666
F	20.00315218	3.28241460	18.17884079
F	18.76784419	2.49742061	16.45353262
N	15.18480000	0.09350000	20.82760000
N	19.19120510	1.02637309	18.32948705
N	17.64597756	2.94696113	18.55106144
C	14.56820000	-0.54390000	21.85210000
C	15.27880000	-1.12700000	22.89500000
H	14.82180000	-1.57620000	23.59750000
C	16.66500000	-1.04270000	22.89500000
H	17.17320000	-1.44920000	23.58620000
C	17.28380000	-0.36610000	21.88330000
H	18.22990000	-0.27940000	21.87610000
C	16.52860000	0.18710000	20.87490000
C	17.28270000	0.92490000	19.80150000
C	18.40865748	0.31567592	19.23626344
C	19.00994100	-0.96493926	19.44340199
C	20.17623204	-0.98592175	18.66568064
C	20.24328217	0.24674374	17.99007944
C	18.56153176	-2.08949685	20.29739589
H	18.95902731	-2.92495006	19.97392773
H	17.58357094	-2.15847999	20.26038599
H	18.84220485	-1.93044849	21.22189107
C	21.19443857	-2.07072138	18.55613906
H	21.55606772	-2.07837970	17.63458459
H	20.75288608	-2.94268710	18.71321624
C	22.33696898	-1.92130002	19.52663104
H	22.93987833	-2.69010575	19.44520367
H	21.98573319	-1.87790658	20.44022815
H	22.83047289	-1.09891827	19.32632853
C	21.30849431	0.72249752	17.05597307
H	20.89432932	1.05505075	16.23195098
H	21.91191826	-0.02049216	16.84212083
H	21.81745266	1.44386141	17.48104138
C	17.10268351	4.17905857	18.44901285
C	16.02220448	4.30844989	19.35182948
C	15.90729208	3.09096462	20.03223207
C	16.92974590	2.23660383	19.51110440
C	17.62644016	5.22652071	17.52830560
H	18.56930821	5.40184889	17.73440436

H	17.10914505	6.05106205	17.64252251
H	17.54533246	4.91737390	16.60139251
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H	14.32995160	5.29203026	19.89708735
H	15.09080800	5.98054681	18.67116459
C	15.84821870	6.53351045	20.49190006
H	15.22884394	7.27769053	20.64129328
H	16.68079320	6.87439774	20.10245982
H	16.04196197	6.09404355	21.34557082
C	14.95526104	2.82990329	21.14963569
H	14.20277912	3.45440213	21.09047931
H	15.41495483	2.95374554	22.00596407
H	14.62287786	1.91036997	21.08723833
B	8.69170000	1.52065141	26.40159207
F	7.33460000	1.22498645	26.55489879
F	9.09200000	2.34192246	27.43970887
N	12.47820000	0.02464303	22.91635459
N	8.91410000	2.19924791	25.02922845
N	9.51250000	0.20944181	26.37387371
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C	12.38420000	-1.15552789	20.82567059
H	12.84120000	-1.53931074	20.08540198
C	10.99800000	-1.19767789	20.89867653
H	10.48980000	-1.59302465	20.20103720
C	10.37920000	-0.65981999	21.99047932
H	9.43310000	-0.69693461	22.06916372
C	11.13440000	-0.06311998	22.97376457
C	10.38030000	0.49757169	24.14941811
C	9.71610000	1.71980864	23.99644162
C	9.63310000	2.63393583	22.90012689
C	8.74540000	3.64529807	23.29339610
C	8.33820000	3.34824842	24.60730118
C	10.30610000	2.58708144	21.58108107
H	10.33770000	3.48844720	21.19746978
H	11.22010000	2.24825400	21.69214742
H	9.80930000	1.99375997	20.98114401
C	8.27350000	4.81931946	22.50313140
H	8.13290000	5.58292846	23.11732181
H	8.97940000	5.07751596	21.85892195
C	6.99600000	4.55981236	21.74801088
H	6.76910000	5.34502656	21.20658000
H	7.11490000	3.78342464	21.16235386
H	6.27120000	4.38276373	22.38306810

C	7.37880000	4.11016086	25.46323013
H	7.78440000	4.27416181	26.34057215
H	7.16750000	4.96688567	25.03513923
H	6.55610000	3.58976743	25.57477799
C	9.54150000	-0.71963299	27.35347846
C	10.28510000	-1.84574892	26.93136848
C	10.72850000	-1.58125543	25.63065231
C	10.24420000	-0.27782463	25.29384394
C	8.84390000	-0.54918946	28.65866161
H	7.88670000	-0.40312024	28.50166230
H	8.96560000	-1.35533949	29.20255442
H	9.22010000	0.22255013	29.13216943
C	10.48430000	-3.08047614	27.73057875
H	11.31690000	-3.52429255	27.42769132
H	10.60600000	-2.82924996	28.67964224
C	9.35010000	-4.06266599	27.63278147
H	9.58800000	-4.88419959	28.11051942
H	8.54510000	-3.67273451	28.03400035
H	9.17860000	-4.27097173	26.69117760
C	11.46630000	-2.55146128	24.77189814
H	11.91170000	-3.21573711	25.33765762
H	10.83560000	-3.00335182	24.17359551
H	12.13580000	-2.07321632	24.23995356