

ESI

Synthesis of mono-(*p*-dimethylamino)styryl-containing BOPHY dye for a turn-on pH sensor

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1 MO calculation	S2
2. NMR	S7

1. The geometrical coordinates of 3a and 3a-H⁺ optimized at the MP2/6-31G* level.

3a

6	0	2.108182	0.868718	-0.115875
6	0	3.367099	1.359353	-0.240888
6	0	4.612487	0.615377	-0.177189
6	0	5.836285	1.295347	-0.330969
6	0	7.059518	0.644843	-0.277642
6	0	7.128123	-0.753185	-0.068162
6	0	5.899466	-1.443420	0.095575
6	0	4.688150	-0.776640	0.039573
6	0	-1.251829	2.187642	-0.107041
7	0	-0.321340	1.162319	0.027714
5	0	-0.747696	-0.189243	0.641475
7	0	-2.300846	-0.343639	0.259485
7	0	-3.156727	0.751200	0.248156
6	0	-2.609194	1.948097	0.050534
6	0	-2.822785	-1.535423	0.011216
6	0	-4.173571	-1.782270	-0.221858
7	0	-5.110973	-0.760452	-0.094361
5	0	-4.731227	0.607449	0.509322
6	0	-0.566793	3.391741	-0.441251
6	0	0.775709	3.060141	-0.501852
6	0	0.918242	1.675652	-0.196312
6	0	-4.839561	-2.972014	-0.611253
6	0	-6.189309	-2.630217	-0.709884
6	0	-6.330535	-1.268687	-0.374760
9	0	-0.627327	-0.180534	2.013780

9	0	-0.086534	-1.264596	0.065913
9	0	-5.349617	1.655869	-0.153400
9	0	-4.975769	0.641433	1.866930
6	0	-1.194293	4.725659	-0.714821
6	0	-4.207493	-4.299908	-0.902618
6	0	-7.578964	-0.451692	-0.284224
7	0	8.337622	-1.419354	-0.027607
6	0	9.579180	-0.666162	-0.075555
6	0	8.377655	-2.832285	0.310864
1	0	1.944830	-0.190171	0.051512
1	0	3.487969	2.430020	-0.404883
1	0	5.824023	2.371052	-0.494017
1	0	7.965370	1.226771	-0.397448
1	0	5.894300	-2.512358	0.271702
1	0	3.776775	-1.352005	0.173192
1	0	-3.326721	2.757557	0.001870
1	0	-2.097434	-2.339259	-0.008052
1	0	1.586171	3.731906	-0.751490
1	0	-7.002259	-3.287689	-0.991313
1	0	-0.432552	5.509465	-0.760150
1	0	-1.913837	5.003766	0.064285
1	0	-1.732771	4.730921	-1.671115
1	0	-4.933007	-5.110005	-0.779217
1	0	-3.361574	-4.506201	-0.237415
1	0	-3.831563	-4.351645	-1.933001
1	0	-8.441213	-1.034941	-0.617632
1	0	-7.502327	0.454704	-0.892362
1	0	-7.757853	-0.128104	0.748616
1	0	10.420760	-1.360366	-0.050328
1	0	9.681594	0.028445	0.772118

1	0	9.655545	-0.083203	-1.002335
1	0	9.411386	-3.179866	0.272809
1	0	7.798615	-3.429827	-0.404626
1	0	7.984864	-3.034048	1.318935

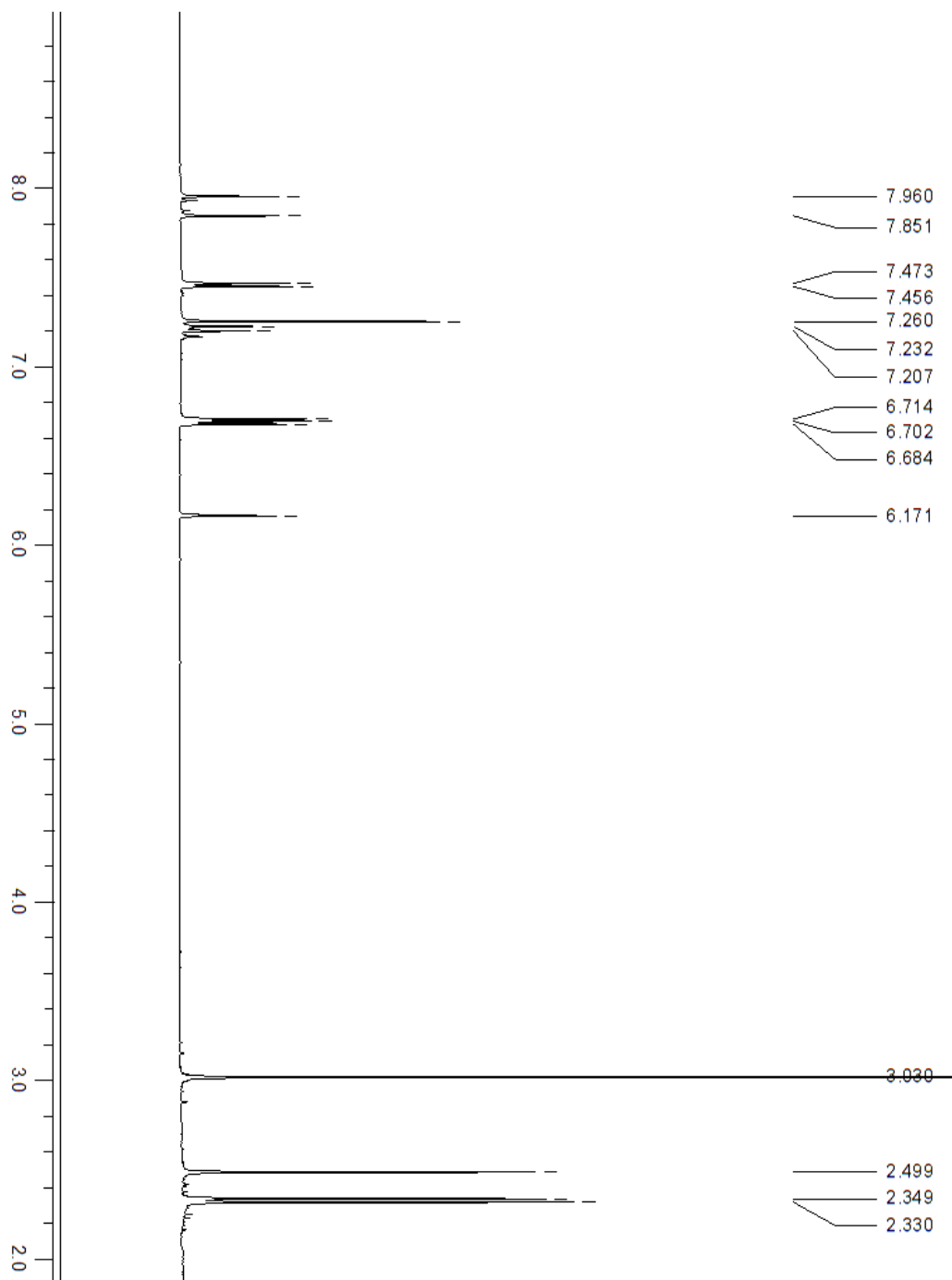
3a-H⁺

6	0	2.065164	0.932000	-0.189110
6	0	3.334207	1.398513	-0.292462
6	0	4.542749	0.595054	-0.192121
6	0	5.800729	1.229505	-0.307269
6	0	6.993728	0.524449	-0.205597
6	0	6.939933	-0.850585	0.015425
6	0	5.721165	-1.518824	0.131727
6	0	4.537495	-0.801577	0.027849
6	0	-1.288300	2.212828	-0.156089
7	0	-0.356922	1.202595	-0.038937
5	0	-0.751920	-0.175546	0.551778
7	0	-2.301590	-0.335763	0.213624
7	0	-3.164850	0.750503	0.227847
6	0	-2.653149	1.948970	0.034972
6	0	-2.834193	-1.536225	-0.024637
6	0	-4.180724	-1.789817	-0.212902
7	0	-5.127193	-0.775755	-0.059178
5	0	-4.746122	0.583488	0.556840
6	0	-0.632991	3.429183	-0.490149
6	0	0.719251	3.116020	-0.564307
6	0	0.876995	1.738871	-0.271021
6	0	-4.852018	-2.991808	-0.583083
6	0	-6.200929	-2.662887	-0.640803
6	0	-6.346449	-1.297427	-0.300138

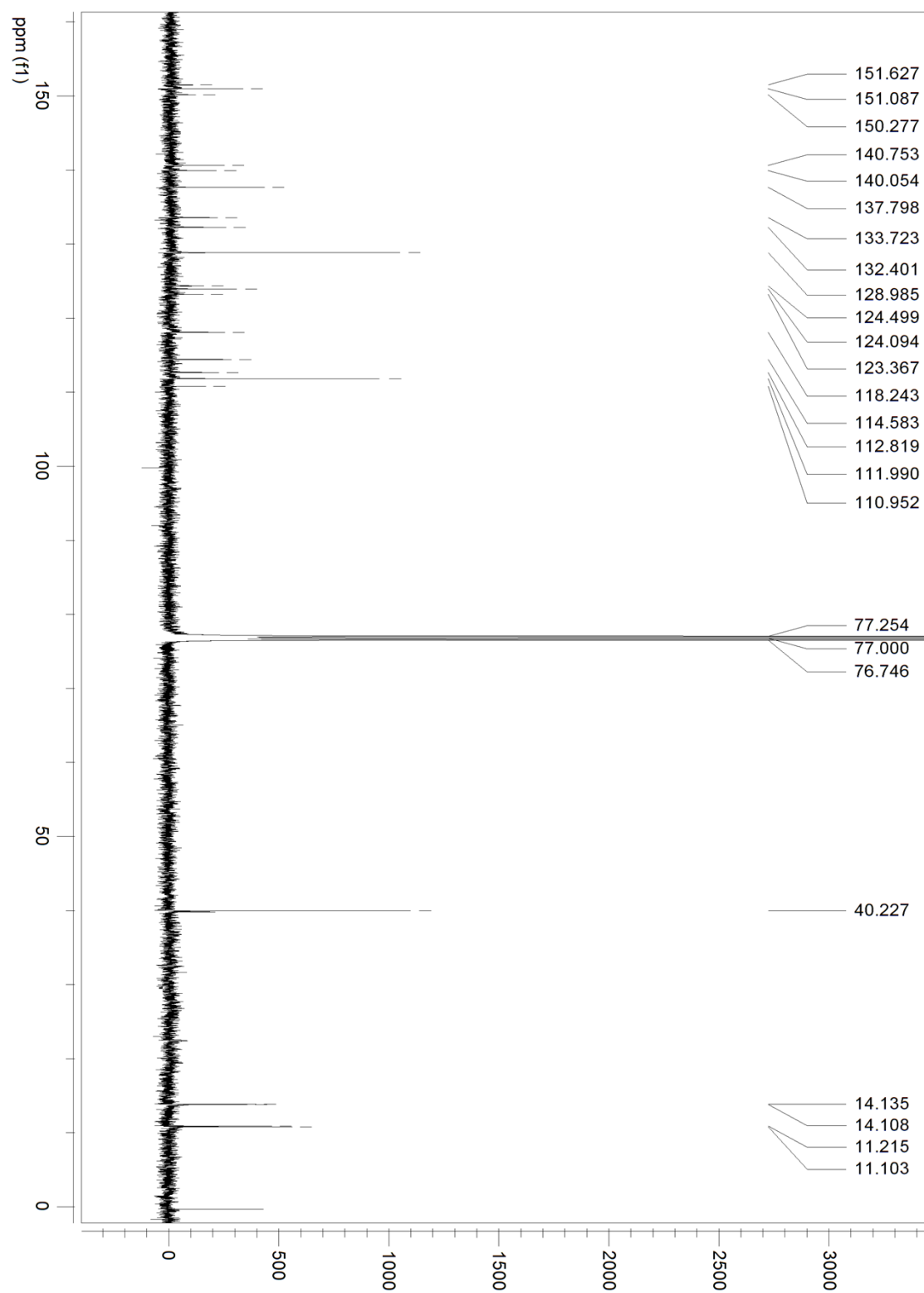
9	0	-0.568018	-0.199562	1.915248
9	0	-0.081483	-1.217253	-0.078870
9	0	-5.386861	1.639024	-0.057558
9	0	-4.899695	0.584893	1.921585
6	0	-1.283021	4.755601	-0.747007
6	0	-4.216287	-4.313316	-0.889343
6	0	-7.603046	-0.501629	-0.169509
7	0	8.195443	-1.644510	0.141630
6	0	9.020356	-1.255102	1.346928
6	0	9.021370	-1.652014	-1.123995
1	0	1.883586	-0.125871	-0.030351
1	0	3.496386	2.462701	-0.449415
1	0	5.838008	2.301410	-0.477075
1	0	7.937942	1.053619	-0.297564
1	0	5.684124	-2.593127	0.305205
1	0	3.598635	-1.335013	0.124626
1	0	-3.382647	2.749431	0.021222
1	0	-2.105769	-2.336019	-0.075933
1	0	1.517106	3.802564	-0.815039
1	0	-7.016796	-3.325747	-0.898485
1	0	-0.537590	5.555648	-0.758257
1	0	-2.023807	5.001997	0.022141
1	0	-1.799424	4.771396	-1.714947
1	0	-3.785685	-4.326727	-1.898946
1	0	-4.954537	-5.118420	-0.837120
1	0	-3.410237	-4.552052	-0.186326
1	0	-8.460371	-1.080300	-0.520831
1	0	-7.539498	0.430753	-0.737910
1	0	-7.777934	-0.226753	0.878220
1	0	7.895032	-2.612405	0.297172

1	0	9.867547	-1.938544	1.429902
1	0	8.384055	-1.315695	2.229856
1	0	9.372044	-0.233051	1.209670
1	0	9.868754	-2.326580	-0.987650
1	0	9.373333	-0.638476	-1.313851
1	0	8.386052	-1.986550	-1.944104

2. NMR of 3a



^1H NMR of 3a



¹³C NMR of 3a