

Electronic Supporting Information (ESI)

Aggregation Tailored Emission of HBT Derivative: A Photostable *turn on* Bioimaging

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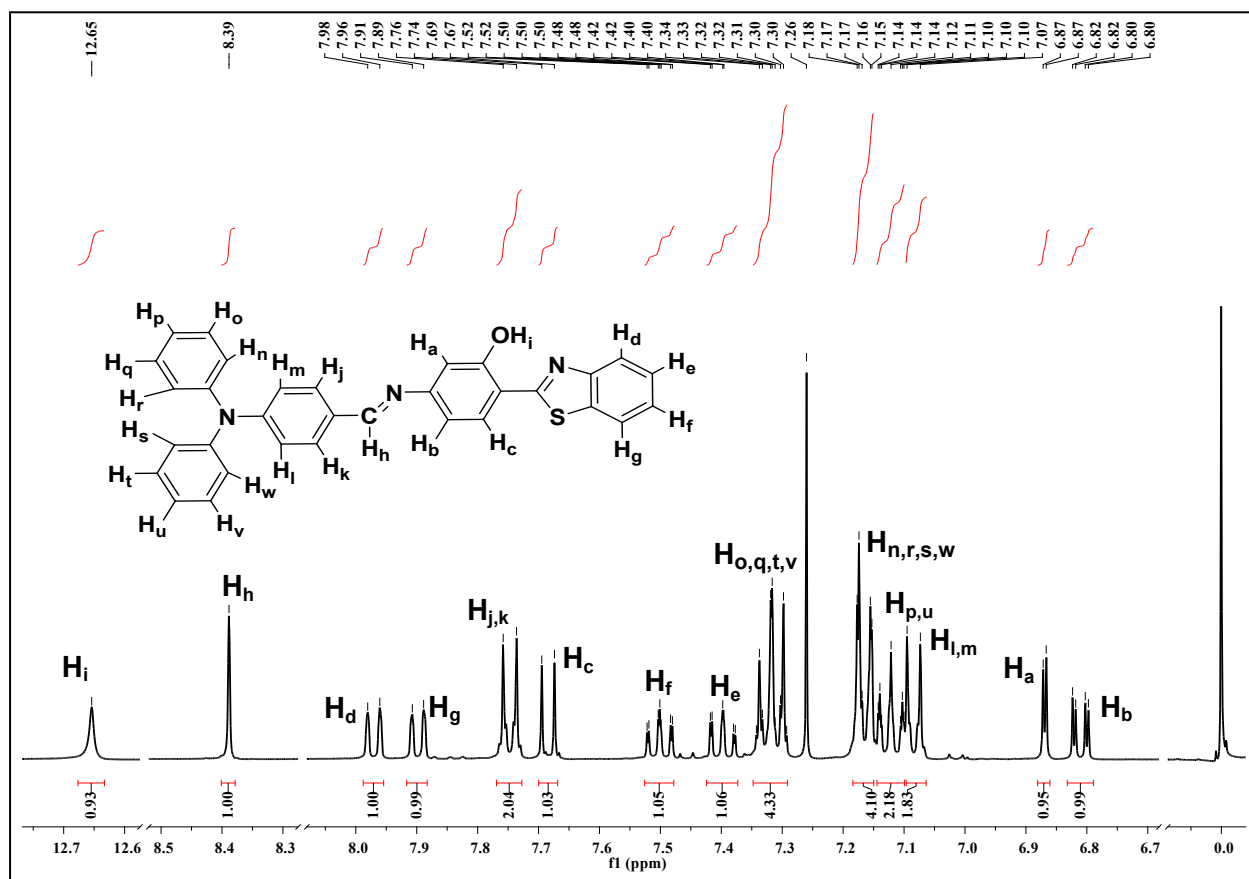


Fig.S1: ^1H NMR (CDCl_3) spectrum of **3**.

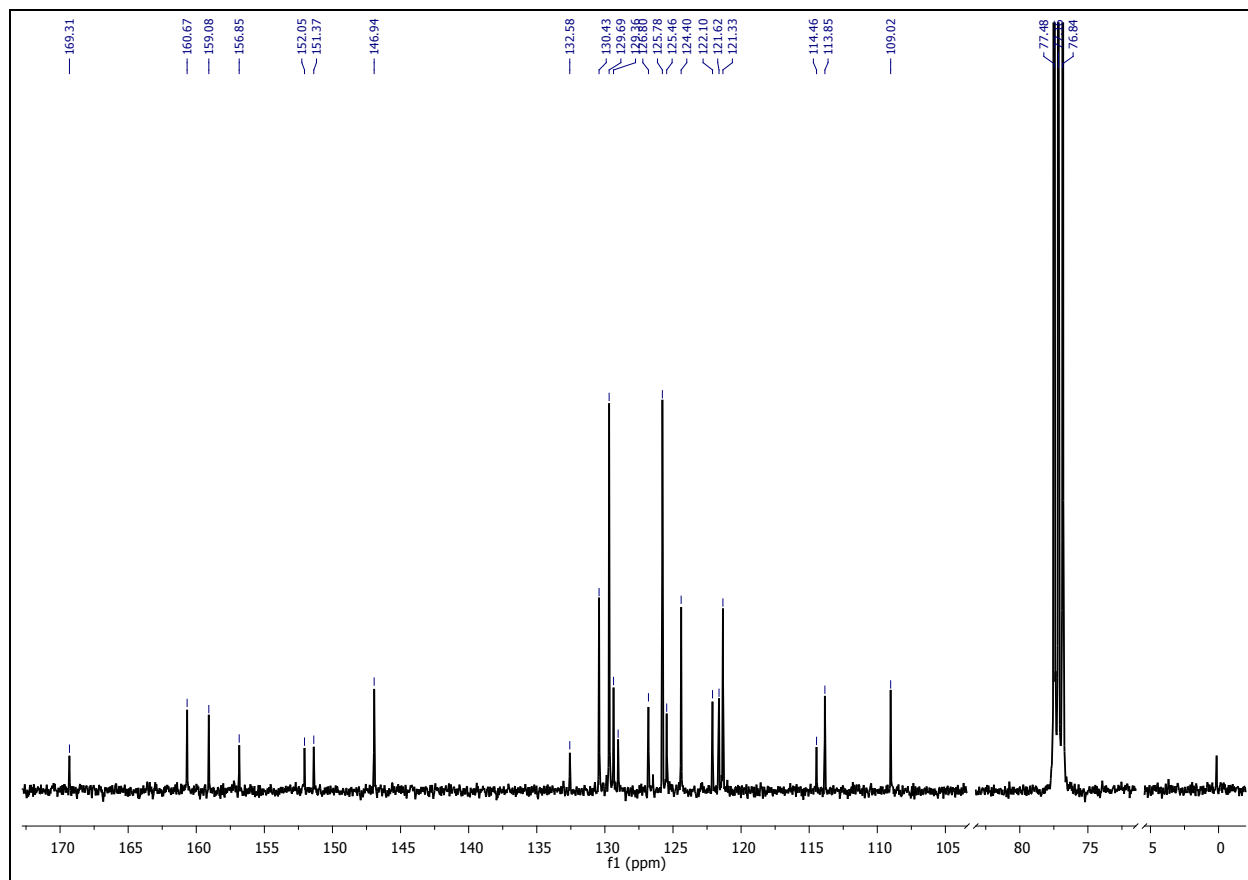


Fig.S2: ^{13}C NMR (CDCl_3) spectrum of **3**.

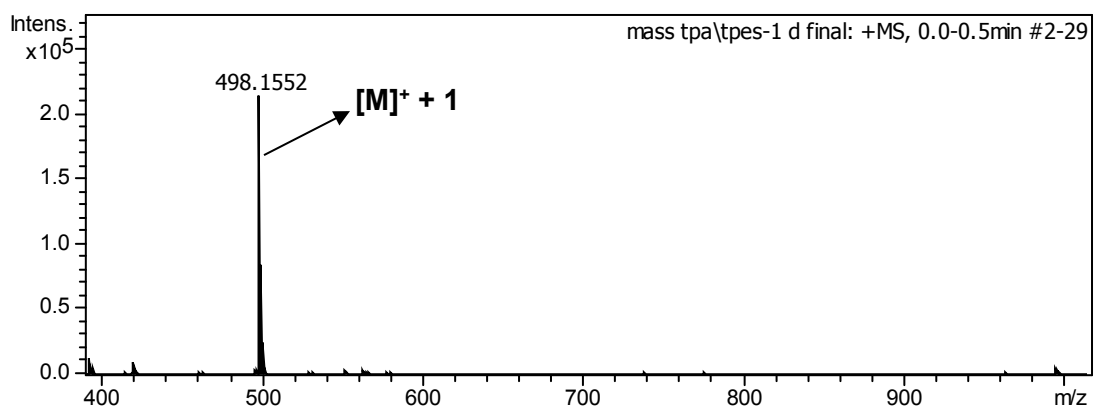


Fig.S3: EI Mass Spectrum of **3**.

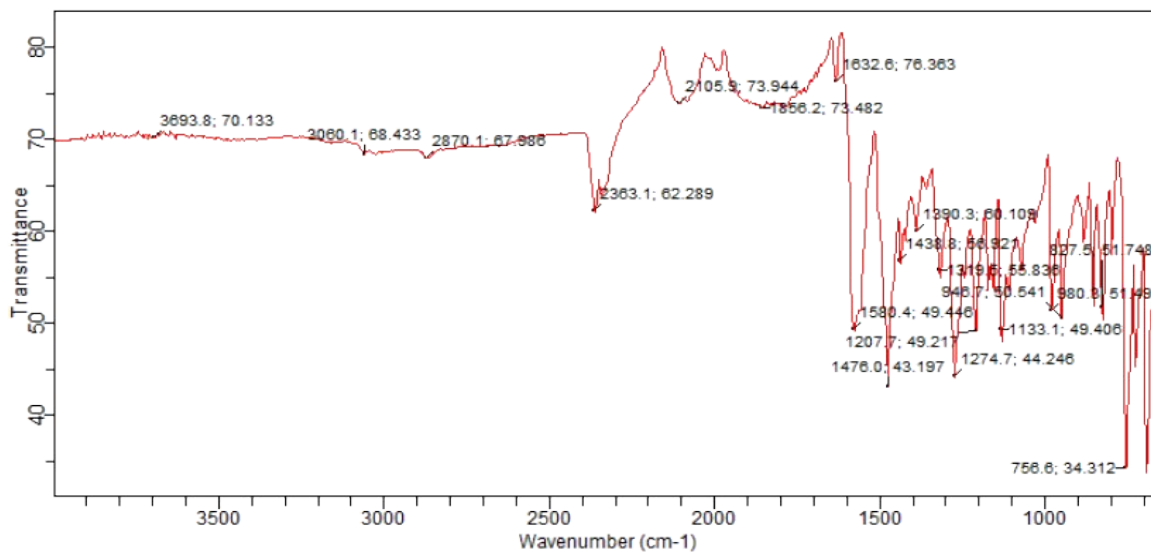


Fig.S4: FTIR spectrum of **3**.

Table S1: Cartesian coordinates of **3** (THF).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	C	0	-7.599359	1.914751	1.126541
2	C	0	-6.701392	1.271827	0.268719
3	C	0	-6.298340	1.873275	-0.905155
4	C	0	-6.787316	3.128774	-1.269173
5	C	0	-7.701237	3.785404	-0.422687
6	C	0	-8.105841	3.177631	0.775183
7	H	0	-7.892015	1.428451	2.046738
8	H	0	-5.584591	1.321864	-1.503234
9	H	0	-6.465173	3.591555	-2.192665

10	H	0	-8.085827	4.760550	-0.692052
11	H	0	-8.800866	3.682595	1.433294
12	N	0	-6.089516	-0.030708	0.538631
13	C	0	-4.623497	-0.098228	0.562304
14	C	0	-3.864940	-0.725993	-0.462573
15	C	0	-3.947723	0.504423	1.634411
16	C	0	-2.472352	-0.748482	-0.402164
17	H	0	-4.375481	-1.187210	-1.289701
18	C	0	-2.551946	0.488276	1.688694
19	H	0	-4.520674	0.976946	2.420514
20	C	0	-1.798568	-0.139857	0.680577
21	H	0	-1.895991	-1.221635	-1.185504
22	H	0	-2.033195	0.947539	2.518858
23	C	0	-6.990685	-1.054197	-0.008444
24	C	0	-6.891988	-2.336658	0.573424
25	C	0	-7.972371	-0.866126	-1.057148
26	C	0	-7.711063	-3.386238	0.151578
27	H	0	-6.179352	-2.497537	1.370138
28	C	0	-8.789287	-1.934675	-1.447498
29	H	0	-8.088507	0.098929	-1.594037
30	C	0	-8.667888	-3.194404	-0.852403
31	H	0	-7.614428	-4.354996	0.624276
32	H	0	-9.514683	-1.781762	-2.236274

33	H	0	-9.300819	-4.013314	-1.167881
34	C	0	-0.326948	-0.147763	0.759683
35	N	0	0.710646	-0.706350	-0.023036
36	C	0	2.129256	-0.517660	0.034132
37	C	0	2.995006	-1.602285	-0.185773
38	C	0	2.651783	0.796265	0.214795
39	C	0	4.372161	-1.403618	-0.167977
40	H	0	2.602134	-2.589170	-0.367746
41	C	0	4.027575	0.985355	0.194829
42	H	0	1.976227	1.626871	0.365854
43	C	0	4.911250	-0.109996	0.028372
44	H	0	4.441877	1.973445	0.341078
45	C	0	8.597597	-0.404808	0.250829
46	C	0	8.800530	0.919949	-0.385346
47	C	0	10.079297	1.432524	-0.614124
48	C	0	11.176263	0.668909	-0.229962
49	C	0	11.013601	-0.592911	0.375571
50	C	0	9.751589	-1.129767	0.615234
51	C	0	6.386572	0.056664	0.001205
52	H	0	10.221630	2.399815	-1.078889
53	H	0	12.172431	1.053275	-0.403072
54	H	0	11.891176	-1.158175	0.657443
55	H	0	9.636137	-2.098681	1.080676

56	N	0	7.276207	-0.788788	0.454524
57	S	0	7.153324	1.658032	-0.800677
58	O	0	5.135558	-2.512650	-0.287314
59	H	0	6.052563	-2.367919	0.016780

Table S2: Cartesian coordinates of **3** (H₂O).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	C	0	7.865866	-1.372412	0.754628
2	C	0	6.789995	-1.179858	-0.128684
3	C	0	6.562752	-2.109140	-1.159051
4	C	0	7.396492	-3.223947	-1.291645
5	C	0	8.471624	-3.414117	-0.413151
6	C	0	8.704248	-2.481727	0.606390
7	H	0	8.039859	-0.656396	1.550160
8	H	0	5.741303	-1.954388	-1.849773
9	H	0	7.213576	-3.935562	-2.090190
10	H	0	9.120519	-4.276474	-0.523253
11	H	0	9.532258	-2.621553	1.293681
12	N	0	5.948641	-0.021568	0.009842
13	C	0	4.546720	-0.138562	0.030114
14	C	0	3.725590	0.946015	-0.371961

15	C	0	3.921745	-1.336719	0.451055
16	C	0	2.343925	0.835421	-0.345953
17	H	0	4.183838	1.866193	-0.712445
18	C	0	2.536536	-1.441008	0.470937
19	H	0	4.527681	-2.174466	0.771727
20	C	0	1.713867	-0.362125	0.078030
21	H	0	1.727112	1.668900	-0.664500
22	H	0	2.070526	-2.361352	0.807098
23	C	0	6.585215	1.261712	0.143925
24	C	0	6.232840	2.125525	1.195695
25	C	0	7.584935	1.646504	-0.765408
26	C	0	6.865266	3.366101	1.323706
27	H	0	5.472011	1.823148	1.906774
28	C	0	8.223707	2.882345	-0.621935
29	H	0	7.854817	0.980041	-1.577083
30	C	0	7.864461	3.748858	0.418901
31	H	0	6.586724	4.026178	2.138704
32	H	0	8.994229	3.171153	-1.329325
33	H	0	8.358139	4.709018	0.524967
34	C	0	0.279618	-0.503692	0.121587
35	N	0	-0.639654	0.317993	-0.170593
36	C	0	-2.033702	0.143994	-0.102754
37	C	0	-2.837378	1.219769	-0.494752
38	C	0	-2.634786	-1.058909	0.343459

39	C	0	-4.231637	1.119997	-0.449322
40	H	0	-2.382946	2.140969	-0.836654
41	C	0	-4.014685	-1.158699	0.389466
42	H	0	-2.004359	-1.886809	0.644466
43	C	0	-4.849789	-0.085646	0.000268
44	H	0	-4.466860	-2.083407	0.733156
45	C	0	-8.448931	0.533646	-0.193974
46	C	0	-8.743775	-0.761576	0.292821
47	C	0	-10.057193	-1.194512	0.468589
48	C	0	-11.090297	-0.305353	0.147547
49	C	0	-10.809615	0.986414	-0.337782
50	C	0	-9.493432	1.415176	-0.512010
51	C	0	-6.291148	-0.166130	0.043696
52	H	0	-10.277900	-2.187542	0.841851
53	H	0	-12.120253	-0.619702	0.275963
54	H	0	-11.627374	1.656401	-0.579128
55	H	0	-9.264729	2.406885	-0.884720
56	N	0	-7.086309	0.820014	-0.315663
57	S	0	-7.200221	-1.671961	0.615995
58	O	0	-4.969116	2.204714	-0.845039
59	H	0	-5.954667	1.983288	-0.756796

Reference:

1. 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, D.J. Fox, Gaussian 09, Revision B.01, Gaussian, Inc., Wallingford CT, 2010.