Two novel indolo[3,2-b]carbazole derivatives containing dimesitylboron moieties: synthesis, photoluminescent and electroluminescent properties

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Electronic Supplementary Information (ESI)

Table S1 Coordinates of **DDBICZ** from DFT calculations

%chk=Yuan2
%mem=700MW
%nproc=4
opt rb3lyp/6-31g(d,p) scrf=(solvent=thf) geom=connectivity

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.370411	4.753350	-2.020351
2	6	0	1.774787	4.765508	-2.045342
3	6	0	2.520366	3.681131	-1.586884
4	6	0	1.825415	2.574594	-1.090662
5	6	0	0.408000	2.539258	-1.076502
6	6	0	-0.317051	3.641908	-1.541981
7	7	0	2.317569	1.358092	-0.599896
8	6	0	1.223281	0.538082	-0.269302
9	6	0	0.019543	1.247984	-0.550023
10	6	0	1.215007	-0.739502	0.283105
11	6	0	-0.034115	-1.312851	0.539539
12	6	0	-1.237564	-0.602258	0.259785
13	6	0	-1.229411	0.675051	-0.292966
14	6	0	-0.423633	-2.604880	1.063791
15	6	0	-1.841263	-2.639208	1.078062
16	7	0	-2.332405	-1.421533	0.589742
17	6	0	0.300378	-3.709263	1.526740
18	6	0	-0.388080	-4.821293	2.002438
19	6	0	-1.792441	-4.832485	2.027261
20	6	0	-2.537116	-3.746362	1.571385
21	1	0	2.295060	5.636464	-2.432893
22	1	0	3.603551	3.696726	-1.622821
23	1	0	-1.403256	3.626569	-1.534813
24	1	0	2.132010	-1.272538	0.506174
25	1	0	-2.146540	1.207903	-0.515900
26	1	0	1.386600	-3.694961	1.519786
27	1	0	-2.313354	-5.704038	2.412611

28	1	0	-3.620343	-3.760838	1.607352
29	6	0	3.683133	1.013498	-0.459211
30	6	0	4.565268	1.877085	0.207101
31	6	0	4.168333	-0.193911	-0.984120
32	6	0	5.905746	1.531496	0.341864
33	1	0	4.187204	2.799864	0.634425
34	6	0	5.513854	-0.518566	-0.846810
35	1	0	3.491695	-0.854294	-1.516231
36	6	0	6.426573	0.328712	-0.182058
37	1	0	6.570015	2.203933	0.876742
38	1	0	5.875591	-1.450246	-1.272636
39	6	0	-3.696783	-1.068989	0.457913
40	6	0	-4.170276	0.140272	0.988637
41	6	0	-4.588753	-1.923696	-0.207559
42	6	0	-5.507297	0.489954	0.833708
43	1	0	-3.487690	0.789381	1.526946
44	6	0	-5.930890	-1.575681	-0.317583
45	1	0	-4.218667	-2.845290	-0.644394
46	6	0	-6.433788	-0.357131	0.187735
47	1	0	-5.853249	1.436180	1.239119
48	1	0	-6.609460	-2.252111	-0.829578
49	5	0	7.944463	-0.048968	-0.031676
50	5	0	-7.945355	0.041724	0.032269
51	6	0	8.575601	-1.092425	-1.044373
52	6	0	8.511270	-0.891894	-2.448460
53	6	0	9.219291	-2.270553	-0.573715
54	6	0	9.076621	-1.829419	-3.321412
55	6	0	9.744685	-3.195347	-1.479249
56	6	0	9.687386	-2.995473	-2.861373
57	1	0	9.038046	-1.638734	-4.392321
58	1	0	10.221790	-4.094351	-1.094181
59	6	0	8.791254	0.642478	1.116964
60	6	0	9.936675	1.430385	0.801896
61	6	0	8.422025	0.537815	2.482122
62	6	0	10.638215	2.086873	1.813489
63	6	0	9.163489	1.201997	3.469675
64	6	0	10.269876	1.987950	3.160153
65	1	0	11.499813	2.694734	1.544228
66	1	0	8.863141	1.094153	4.510400
67	6	0	-9.018160	-1.100300	-0.206672
68	6	0	-9.153632	-2.186056	0.698497
69	6	0	-9.874813	-1.075607	-1.341943
70	6	0	-10.114093	-3.178863	0.470049
71	6	0	-10.799676	-2.101860	-1.548795

72	6	0	-10.940943	-3.165189	-0.652922
73	1	0	-10.217182	-3.985048	1.193968
74	1	0	-11.435591	-2.064485	-2.431040
75	6	0	-8.339895	1.574384	0.132428
76	6	0	-9.240117	2.032678	1.137420
77	6	0	-7.787348	2.542788	-0.744779
78	6	0	-9.536127	3.391833	1.249547
79	6	0	-8.121309	3.897150	-0.606057
80	6	0	-8.987074	4.347183	0.387182
81	1	0	-10.216617	3.716958	2.034151
82	1	0	-7.692170	4.615798	-1.302079
83	6	0	9.337845	-2.582929	0.904224
84	1	0	9.916362	-1.820559	1.433666
85	1	0	8.357956	-2.636620	1.391050
86	1	0	9.830306	-3.547240	1.056640
87	6	0	10.252058	-4.016337	-3.819610
88	1	0	9.525707	-4.813694	-4.021880
89	1	0	10.513188	-3.563004	-4.780321
90	1	0	11.149255	-4.493772	-3.413341
91	6	0	7.869659	0.331326	-3.079189
92	1	0	6.822115	0.142594	-3.340743
93	1	0	7.876816	1.204212	-2.424386
94	1	0	8.391079	0.601971	-4.002628
95	6	0	10.411437	1.620601	-0.624009
96	1	0	10.599938	0.665723	-1.121087
97	1	0	9.673497	2.157974	-1.231166
98	1	0	11.335619	2.204499	-0.648974
99	6	0	7.287367	-0.344969	2.965425
100	1	0	6.621529	-0.663239	2.163376
101	1	0	7.683707	-1.249004	3.444593
102	1	0	6.680792	0.172174	3.716514
103	6	0	11.045223	2.717978	4.230324
104	1	0	10.908380	3.803241	4.150033
105	1	0	10.725485	2.417255	5.231831
106	1	0	12.120429	2.524901	4.146752
107	6	0	-9.802306	0.029469	-2.375848
108	1	0	-10.527155	-0.141632	-3.176503
109	1	0	-10.008854	1.009522	-1.936871
110	1	0	-8.812006	0.088385	-2.840798
111	6	0	-11.942071	-4.266808	-0.904784
112	1	0	-12.864080	-3.876672	-1.347390
113	1	0	-11.541598	-5.014239	-1.601309
114	1	0	-12.203610	-4.789743	0.019628
115	6	0	-8.307287	-2.322569	1.951681

116	1	0	-7.390456	-2.889656	1.754518
117	1	0	-7.997534	-1.360879	2.365219
118	1	0	-8.860232	-2.857392	2.729962
119	6	0	-9.867341	1.089428	2.143105
120	1	0	-10.610126	1.611734	2.752337
121	1	0	-10.360085	0.242985	1.658896
122	1	0	-9.119809	0.676623	2.831375
123	6	0	-9.314772	5.812494	0.544825
124	1	0	-10.386867	5.967062	0.706555
125	1	0	-8.794804	6.244844	1.408711
126	1	0	-9.019274	6.386442	-0.337860
127	6	0	-6.895414	2.180894	-1.916929
128	1	0	-6.499443	1.167350	-1.855809
129	1	0	-7.450306	2.262648	-2.859899
130	1	0	-6.045072	2.867507	-1.989251
131	1	0	0.162238	-5.684831	2.362841
132	1	0	-0.180572	5.615627	-2.382771

Table S2 Coordinates of **DDBICZ** from DFT calculations

%chk=Yuan4
%mem=700MW
%nproc=4
opt rb3lyp/6-31g(d,p) scrf=(solvent=thf) geom=connectivity

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.762997	-5.170955	0.381632
2	6	0	0.631140	-5.455661	0.383123
3	6	0	1.608023	-4.469282	0.346747
4	6	0	1.185303	-3.137009	0.267485
5	6	0	-0.195443	-2.803273	0.255937
6	6	0	-1.149961	-3.816184	0.328279
7	7	0	1.937896	-1.966080	0.228384
8	6	0	1.056492	-0.867764	0.180320
9	6	0	-0.280919	-1.357738	0.187500
10	6	0	1.351870	0.489410	0.094336
11	6	0	0.267170	1.367448	0.020604
12	6	0	-1.069809	0.876975	0.017291
13	6	0	-1.365579	-0.479548	0.111155

14	6	0	0.181413	2.812420	-0.056612
15	6	0	-1.198923	3.144780	-0.099022
16	7	0	-1.950966	1.973951	-0.054358
17	6	0	1.136321	3.825043	-0.114947
18	6	0	0.751592	5.178879	-0.205050
19	6	0	-0.642667	5.461000	-0.250856
20	6	0	-1.619969	4.475229	-0.212403
21	1	0	0.944766	-6.494237	0.427084
22	1	0	2.661462	-4.724253	0.378192
23	1	0	-2.206659	-3.563922	0.342171
24	1	0	2.372108	0.855146	0.081969
25	1	0	-2.386124	-0.844704	0.118780
26	1	0	2.192701	3.573032	-0.093084
27	1	0	-0.955871	6.497705	-0.328151
28	1	0	-2.672575	4.728508	-0.272213
29	5	0	-1.824916	-6.317731	0.439893
30	5	0	1.817872	6.321849	-0.259348
31	6	0	-1.397993	-7.787171	0.011602
32	6	0	-1.480059	-8.866829	0.937588
33	6	0	-0.889438	-8.070978	-1.281198
34	6	0	-1.055856	-10.144223	0.571384
35	6	0	-0.488950	-9.373248	-1.615306
36	6	0	-0.558970	-10.424911	-0.706687
37	1	0	-1.112424	-10.946277	1.304921
38	1	0	-0.111363	-9.562848	-2.618645
39	6	0	-3.300919	-5.985432	0.927515
40	6	0	-3.560536	-5.443526	2.212782
41	6	0	-4.415721	-6.206237	0.069429
42	6	0	-4.874507	-5.152278	2.606237
43	6	0	-5.707113	-5.888002	0.493248
44	6	0	-5.964463	-5.369094	1.767160
45	1	0	-5.044238	-4.748081	3.602797
46	1	0	-6.538891	-6.054228	-0.188725
47	6	0	1.369774	7.818243	0.034428
48	6	0	1.527782	8.828431	-0.958300
49	6	0	0.771038	8.195733	1.262502
50	6	0	1.085363	10.129136	-0.717651
51	6	0	0.353643	9.518827	1.470947
52	6	0	0.495894	10.501629	0.496131
53	1	0	1.202578	10.876422	-1.500210
54	1	0	-0.094592	9.781112	2.427812
55	6	0	3.324431	5.952864	-0.608672
56	6	0	3.679415	5.318684	-1.825470
57	6	0	4.369222	6.219403	0.323193

58	6	0	5.014544	4.970953	-2.080946
59	6	0	5.682212	5.845516	0.037341
60	6	0	6.031964	5.219327	-1.164864
61	1	0	5.258174	4.493434	-3.028530
62	1	0	6.457356	6.046906	0.774358
63	6	0	-1.986287	-8.668699	2.351700
64	1	0	-1.372236	-7.951441	2.907777
65	1	0	-3.012351	-8.290147	2.365219
66	1	0	-1.966386	-9.611652	2.905089
67	6	0	-0.126378	-11.822676	-1.079340
68	1	0	0.590506	-12.225894	-0.355286
69	1	0	-0.979737	-12.511280	-1.100850
70	1	0	0.343390	-11.846329	-2.066579
71	6	0	-0.813059	-7.035594	-2.387024
72	1	0	-1.591751	-7.217141	-3.138457
73	1	0	-0.935694	-6.015523	-2.024197
74	1	0	0.149079	-7.091335	-2.907591
75	6	0	-2.478940	-5.220198	3.252792
76	1	0	-2.542671	-5.980102	4.041583
77	1	0	-1.473010	-5.259026	2.836271
78	1	0	-2.601280	-4.246481	3.739203
79	6	0	-4.246261	-6.753254	-1.333004
80	1	0	-3.610441	-6.107590	-1.948980
81	1	0	-3.784674	-7.744865	-1.326743
82	1	0	-5.213534	-6.834040	-1.836670
83	6	0	-7.376220	-5.089186	2.224404
84	1	0	-7.394514	-4.376668	3.054279
85	1	0	-7.989773	-4.681762	1.414416
86	1	0	-7.869020	-6.006670	2.570179
87	6	0	0.609932	7.243578	2.432648
88	1	0	1.307033	7.505156	3.238427
89	1	0	-0.399657	7.307930	2.853142
90	1	0	0.790932	6.203166	2.164098
91	6	0	0.044354	11.922718	0.734020
92	1	0	0.897015	12.611770	0.766068
93	1	0	-0.617557	12.271570	-0.066590
94	1	0	-0.494365	12.017954	1.680938
95	6	0	2.139877	8.527613	-2.310611
96	1	0	3.161177	8.148010	-2.215816
97	1	0	1.566795	7.771797	-2.859017
98	1	0	2.169730	9.427399	-2.931474
99	6	0	4.094974	6.875228	1.660662
100	1	0	3.638502	7.861757	1.541447
101	1	0	3.411290	6.277976	2.274356

102	1	0	5.020812	6.997330	2.229800
103	6	0	7.464361	4.836185	-1.450311
104	1	0	7.555893	4.317681	-2.408937
105	1	0	8.114544	5.718435	-1.485444
106	1	0	7.865115	4.176627	-0.671687
107	6	0	2.685496	5.042581	-2.938322
108	1	0	1.650933	5.203634	-2.637022
109	1	0	2.886573	5.690139	-3.800708
110	1	0	2.770142	4.008776	-3.291277
111	6	0	3.354445	-1.884082	0.223271
112	6	0	4.099751	-2.593630	-0.728353
113	6	0	4.016966	-1.085206	1.165763
114	6	0	5.487264	-2.489923	-0.737797
115	1	0	3.584334	-3.197122	-1.468321
116	6	0	5.405911	-1.004649	1.149784
117	1	0	3.439752	-0.550567	1.912967
118	6	0	6.184619	-1.697049	0.198341
119	1	0	6.049436	-3.024939	-1.497493
120	1	0	5.906059	-0.390840	1.893473
121	6	0	-3.365797	1.889063	-0.124031
122	6	0	-3.974659	1.087336	-1.099420
123	6	0	-4.162658	2.602504	0.781763
124	6	0	-5.361155	0.990549	-1.148366
125	1	0	-3.356392	0.553450	-1.813578
126	6	0	-5.549180	2.521154	0.695080
127	1	0	-3.688756	3.202564	1.551758
128	6	0	-6.193179	1.708109	-0.262050
129	1	0	-5.817609	0.353456	-1.899869
130	1	0	-6.154141	3.083026	1.400866
131	5	0	7.752718	-1.574157	0.170597
132	5	0	-7.761175	1.595225	-0.331405
133	6	0	8.511869	-1.173451	1.501832
134	6	0	8.345200	-1.918953	2.698549
135	6	0	9.380468	-0.046883	1.539460
136	6	0	9.033224	-1.549607	3.860732
137	6	0	10.025142	0.304761	2.727549
138	6	0	9.869883	-0.435003	3.903329
139	1	0	8.909985	-2.153787	4.757496
140	1	0	10.675779	1.176916	2.733570
141	6	0	8.510229	-1.867489	-1.190111
142	6	0	9.489479	-2.899599	-1.271577
143	6	0	8.218899	-1.143250	-2.374794
144	6	0	10.108037	-3.186977	-2.488914
145	6	0	8.874033	-1.454766	-3.574347

146	6	0	9.815996	-2.476508	-3.658633
147	1	0	10.841826	-3.989696	-2.527485
148	1	0	8.639643	-0.873756	-4.464511
149	6	0	-8.637124	2.760545	0.288360
150	6	0	-8.470643	4.109799	-0.119305
151	6	0	-9.610758	2.487254	1.289534
152	6	0	-9.255609	5.120433	0.449919
153	6	0	-10.352626	3.527896	1.852247
154	6	0	-10.194636	4.856251	1.445799
155	1	0	-9.127210	6.143267	0.100847
156	1	0	-11.082429	3.294216	2.624890
157	6	0	-8.395382	0.325314	-1.035758
158	6	0	-9.248993	0.474032	-2.167191
159	6	0	-8.100480	-0.994309	-0.603894
160	6	0	-9.741860	-0.651749	-2.828718
161	6	0	-8.626172	-2.097391	-1.290399
162	6	0	-9.441554	-1.952384	-2.409929
163	1	0	-10.379336	-0.510921	-3.699368
164	1	0	-8.387317	-3.097561	-0.933297
165	6	0	9.615590	0.825259	0.322991
166	1	0	10.038847	0.256046	-0.509208
167	1	0	8.685959	1.279073	-0.038879
168	1	0	10.304657	1.640676	0.559704
169	6	0	10.573173	-0.028834	5.175963
170	1	0	10.044971	0.792998	5.675575
171	1	0	10.629792	-0.859778	5.884912
172	1	0	11.592096	0.318737	4.977038
173	6	0	7.455058	-3.145620	2.787390
174	1	0	6.434159	-2.877284	3.082021
175	1	0	7.376534	-3.686710	1.842471
176	1	0	7.838128	-3.842298	3.539284
177	6	0	9.868739	-3.743389	-0.071615
178	1	0	10.206541	-3.130321	0.767827
179	1	0	9.024872	-4.343788	0.288253
180	1	0	10.672130	-4.439384	-0.327973
181	6	0	7.277490	0.045278	-2.405293
182	1	0	6.640131	0.109438	-1.523812
183	1	0	7.845830	0.981740	-2.469429
184	1	0	6.626620	0.007964	-3.285296
185	6	0	10.492332	-2.821420	-4.963521
186	1	0	10.099229	-3.757464	-5.379243
187	1	0	10.340485	-2.039251	-5.712493
188	1	0	11.570762	-2.958719	-4.830625
189	6	0	-9.859902	1.083369	1.802511

190	1	0	-10.625910	1.087633	2.582808
191	1	0	-10.193957	0.414085	1.004679
192	1	0	-8.956360	0.640033	2.235524
193	6	0	-11.005220	5.962771	2.076399
194	1	0	-12.048242	5.662609	2.220836
195	1	0	-10.608644	6.231039	3.063615
196	1	0	-10.994359	6.867523	1.462089
197	6	0	-7.478834	4.532646	-1.188303
198	1	0	-6.520697	4.831611	-0.747793
199	1	0	-7.259927	3.741721	-1.907833
200	1	0	-7.862065	5.393315	-1.745162
201	6	0	-9.620802	1.834628	-2.720496
202	1	0	-10.336101	1.734891	-3.541457
203	1	0	-10.067206	2.477008	-1.957416
204	1	0	-8.747713	2.366362	-3.116875
205	6	0	-9.971700	-3.150363	-3.160206
206	1	0	-11.024948	-3.019474	-3.429900
207	1	0	-9.418825	-3.309749	-4.094348
208	1	0	-9.884803	-4.065167	-2.567269
209	6	0	-7.301908	-1.292464	0.650142
210	1	0	-6.696373	-0.449141	0.982249
211	1	0	-7.974677	-1.557734	1.475569
212	1	0	-6.634542	-2.147171	0.498961

Rotational constants (GHZ): 0.0124634 0.0089038 0.0057142

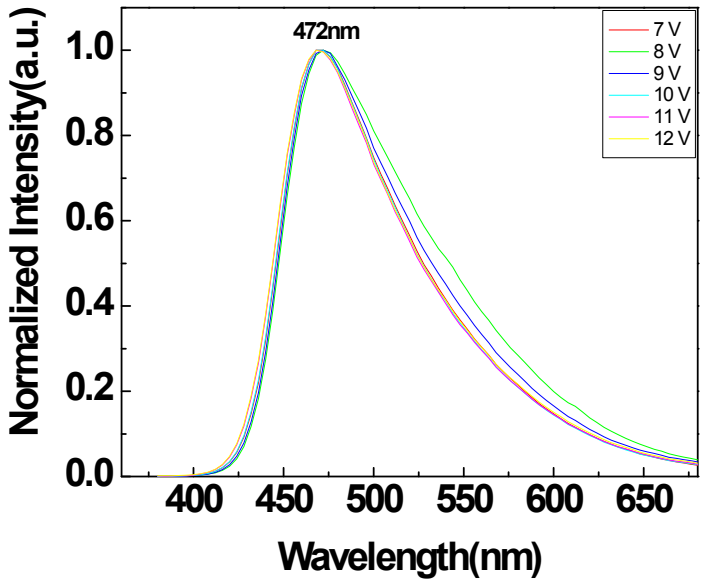

Fig. S1. Normalized electroluminescence spectrum of **Device A** taken at different

voltages. All spectra display similar spectral characteristics.

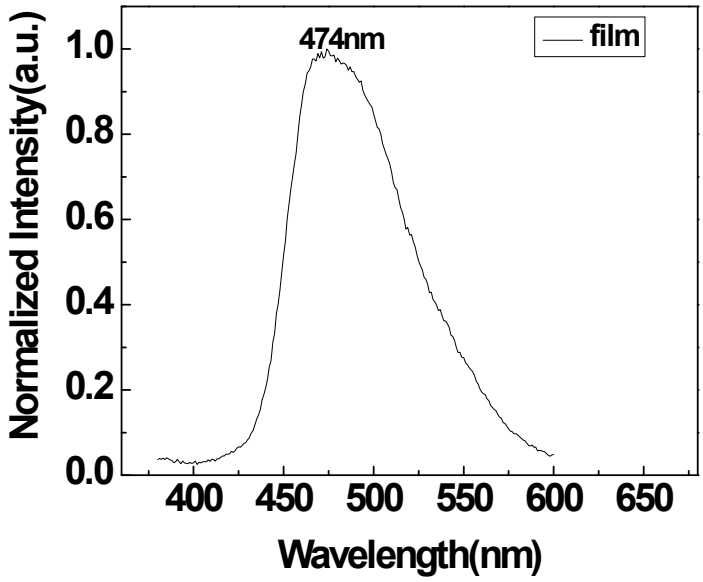

Fig. S2. normalized photoluminescence spectra of film of **DDBICZ**

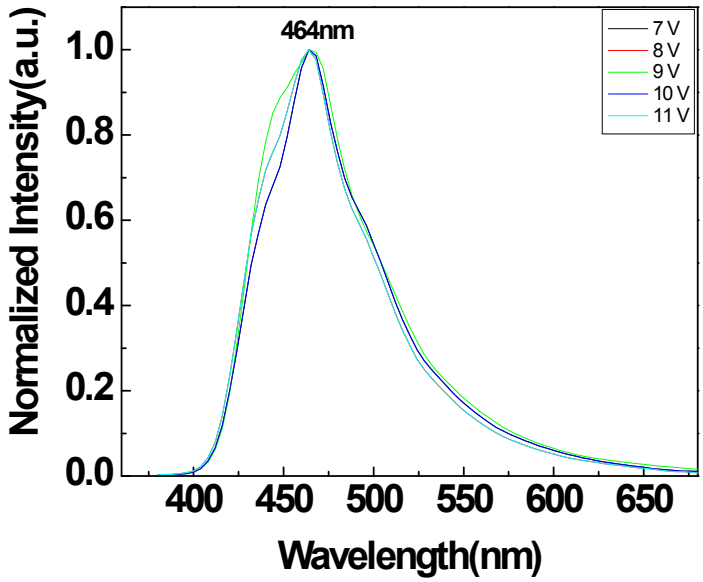

Fig. S3. Normalized electroluminescence spectrum of **Device B** taken at different voltages. All spectra display similar spectral characteristics.

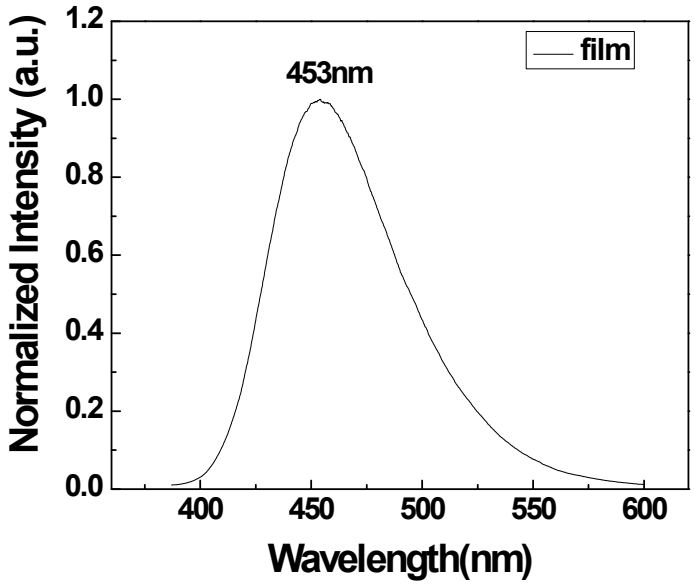

Fig. S4. normalized photoluminescence spectra of film of **DDDBICZ**