Electronic Supplementary Information

Submillisecond-lived photoinduced charge separation in a fully conjugated phthalocyanine-perylenebenzimidazole dyad

Vicente M. Blas-Ferrando,[a] Javier Ortiz[a], Kei Ohkubo,[b] Shunichi Fukuzumi,*[,b,c] Fernando Fernández-Lázaro[a] and Ángela Sastre-Santos.*[,a]

(a)División de Química Orgánica Instituto de Bioingeniería, Universidad Miguel Hernández, Elche, Spain

(b) Department of Material and Life Science, Graduate School of Engineering, Osaka University, ALCA, Japan Science and Technology Agency (JST), Suita, Osaka 565-0871, Japan.

(c) Department of Bioinspired Science, Ewha Womans University, Seoul, 120-750, Korea

** To whom correspondence should be addressed.*
E-mail: asastre@umh.es, fukuzumi@chem.eng.osaka-u.ac.jp

2,3,9,10,16,17-hexakis-*p*-(*tert*-octyl)phenoxyl-22,23-thiadiazolo[4,5-b]-phthalocyaninate zinc (II) (ZnPc 5)

Fig. S1 ^{1}H NMR (THF-d_8) of **ZnPc 5**

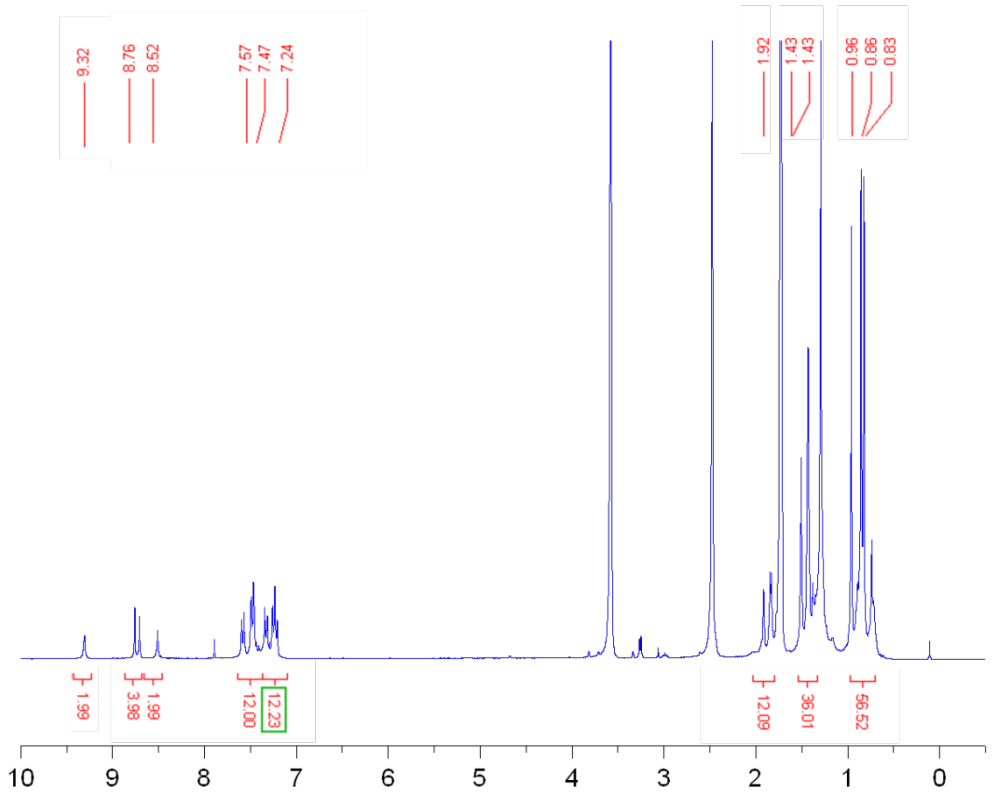


Fig. S2 MS of **ZnPc 5**

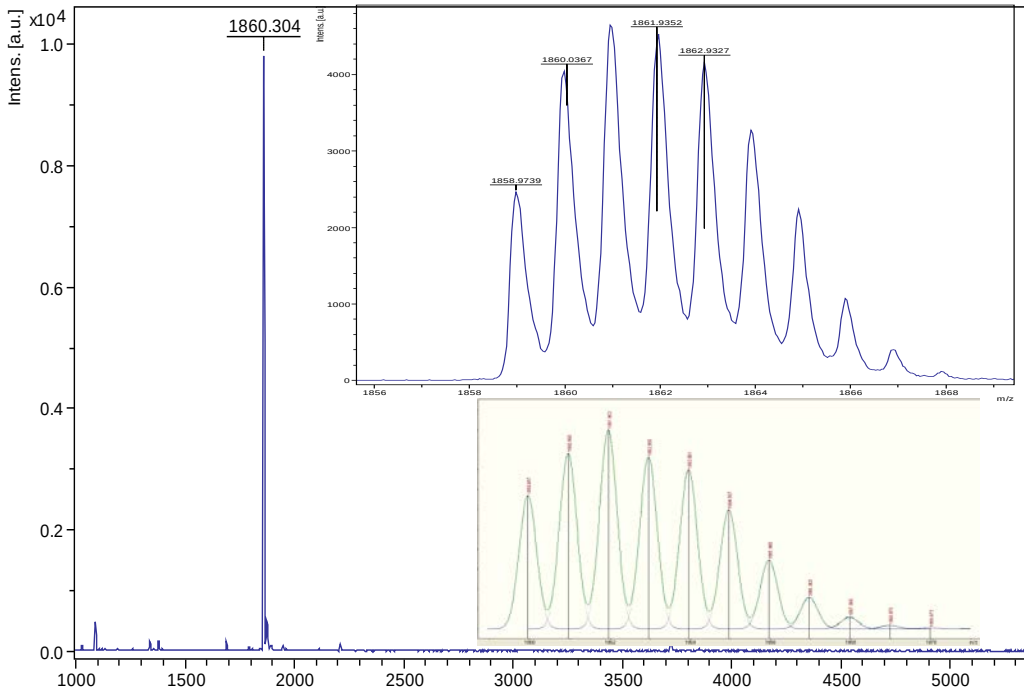
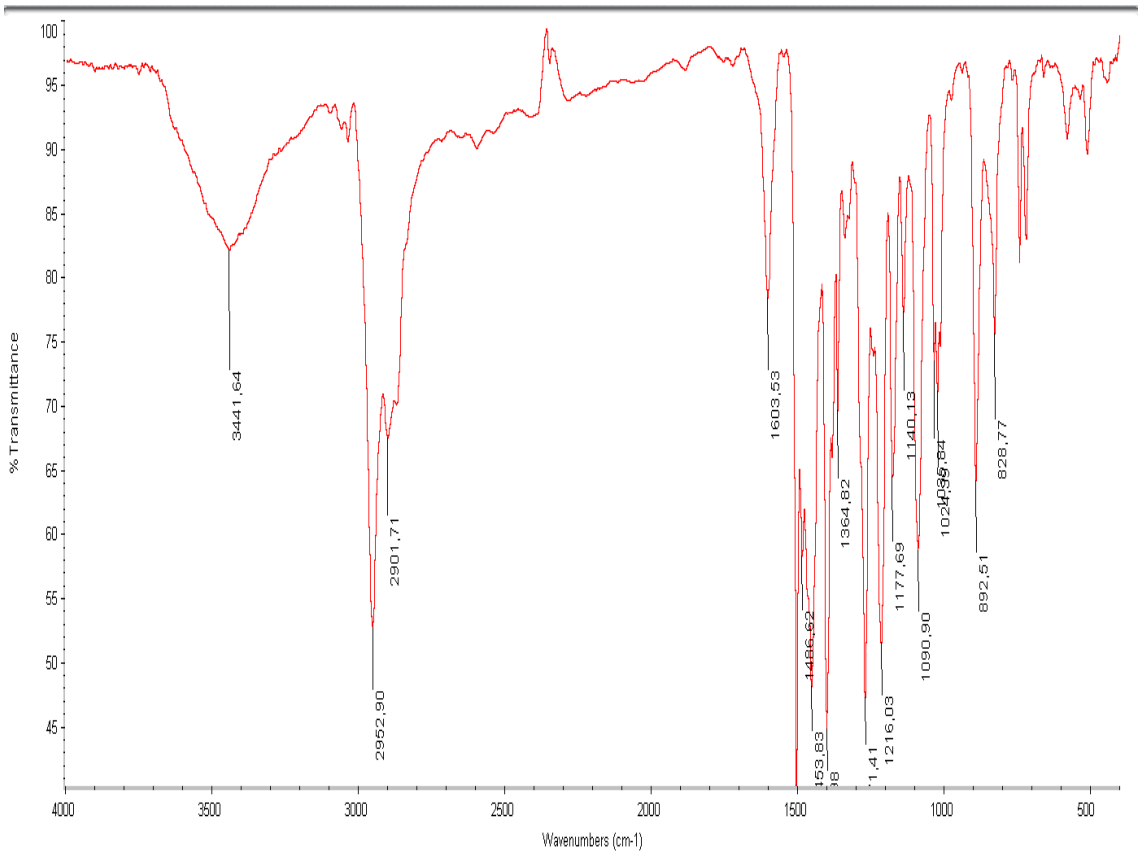


Fig. S3 IR spectrum (KBr) of **ZnPc 5**



2,3,9,10,16,17-hexakis-*p*-(*tert*-octyl)phenoxyl-22,23-diamino-phthalocyaninate zinc (II) (ZnPc 4)

Fig. S4 ^{1}H NMR (THF-d_8) of **ZnPc 4**

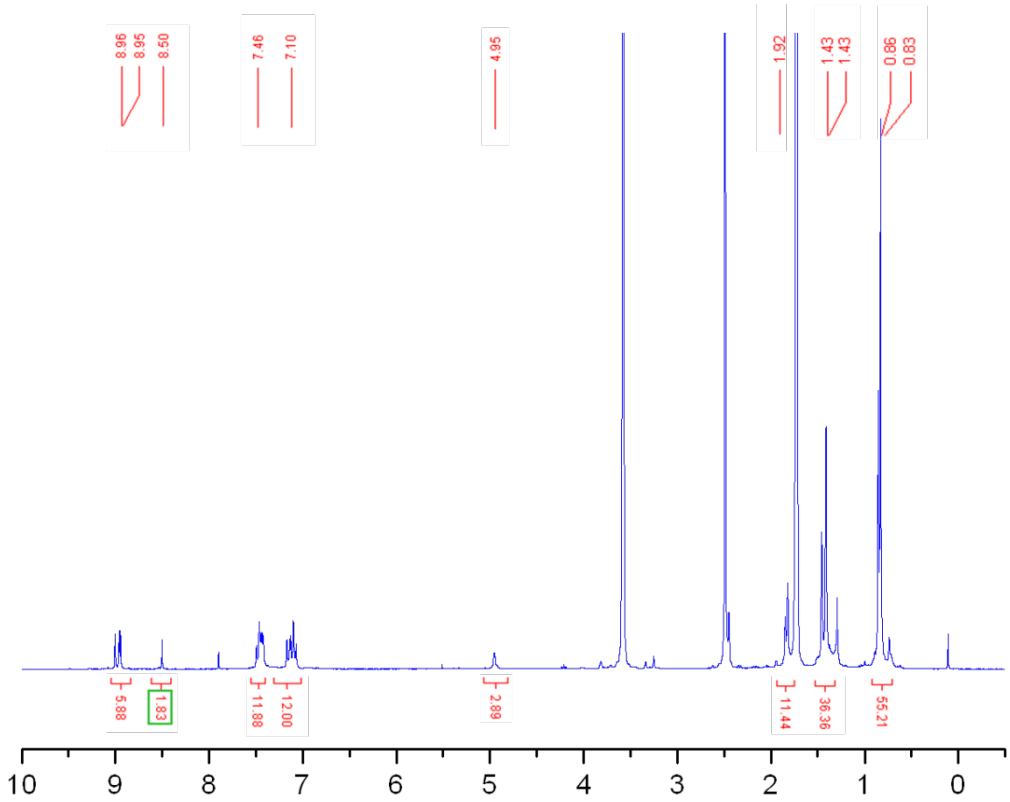


Fig. S5 MS of **ZnPc 4**

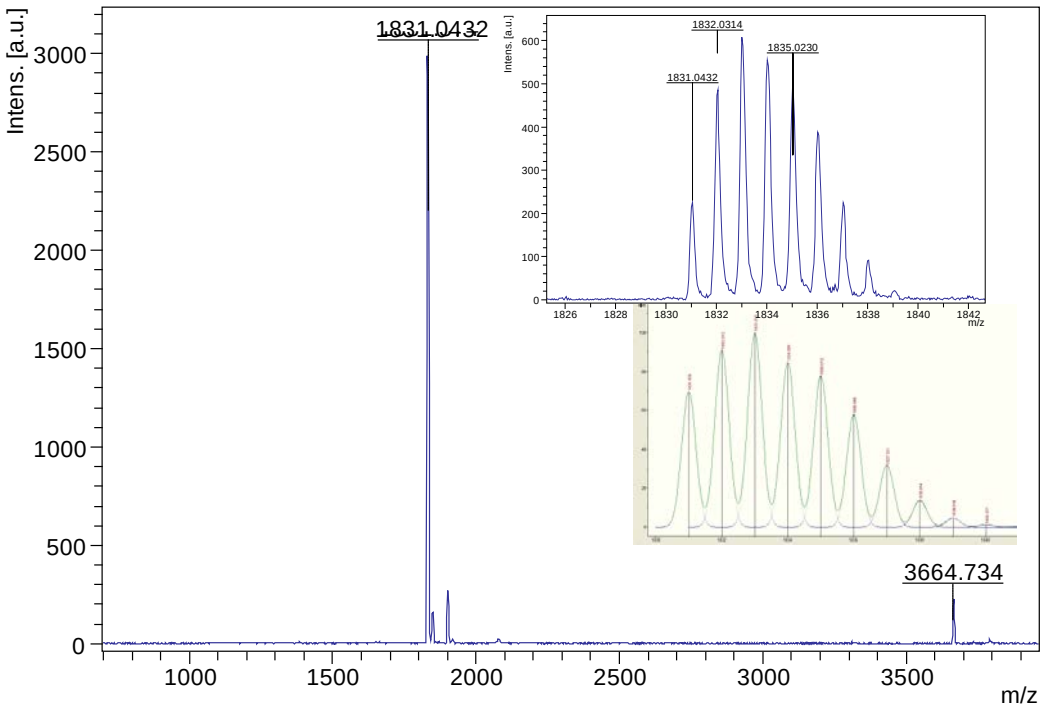
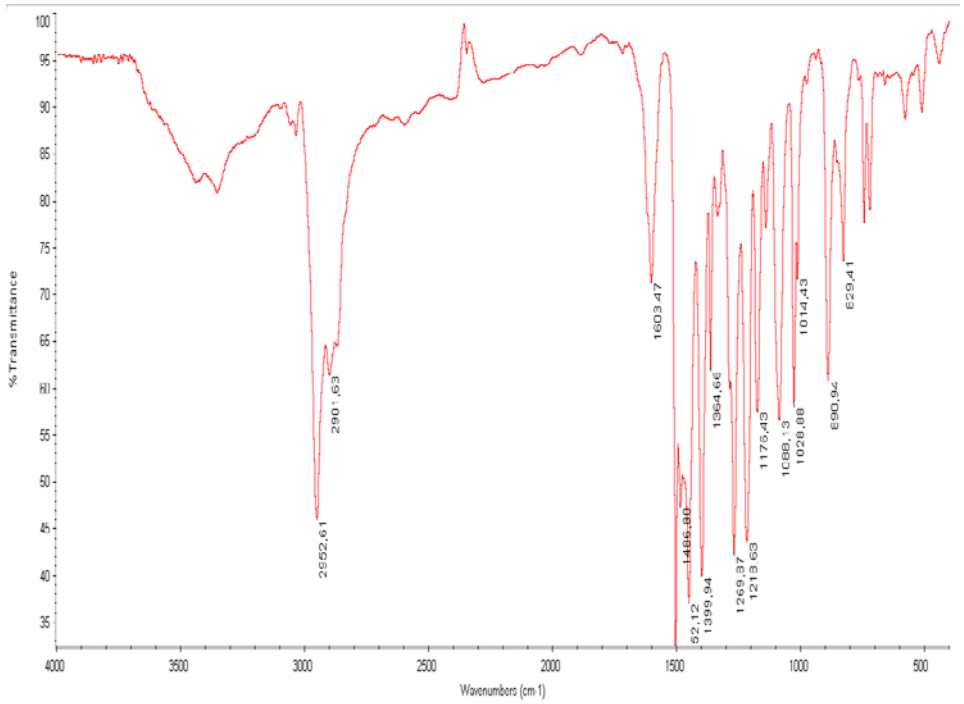


Fig. S6 IR spectrum (KBr) of **ZnPc 4**



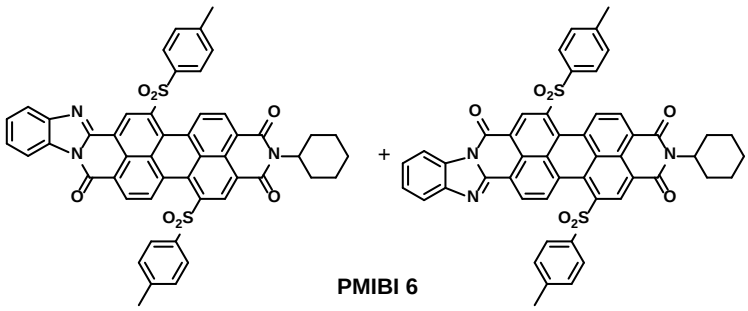


Fig. S7 ^{1}H NMR ($CDCl_3$) of **1,7-(TolSO$_2$)-PMABI 6**

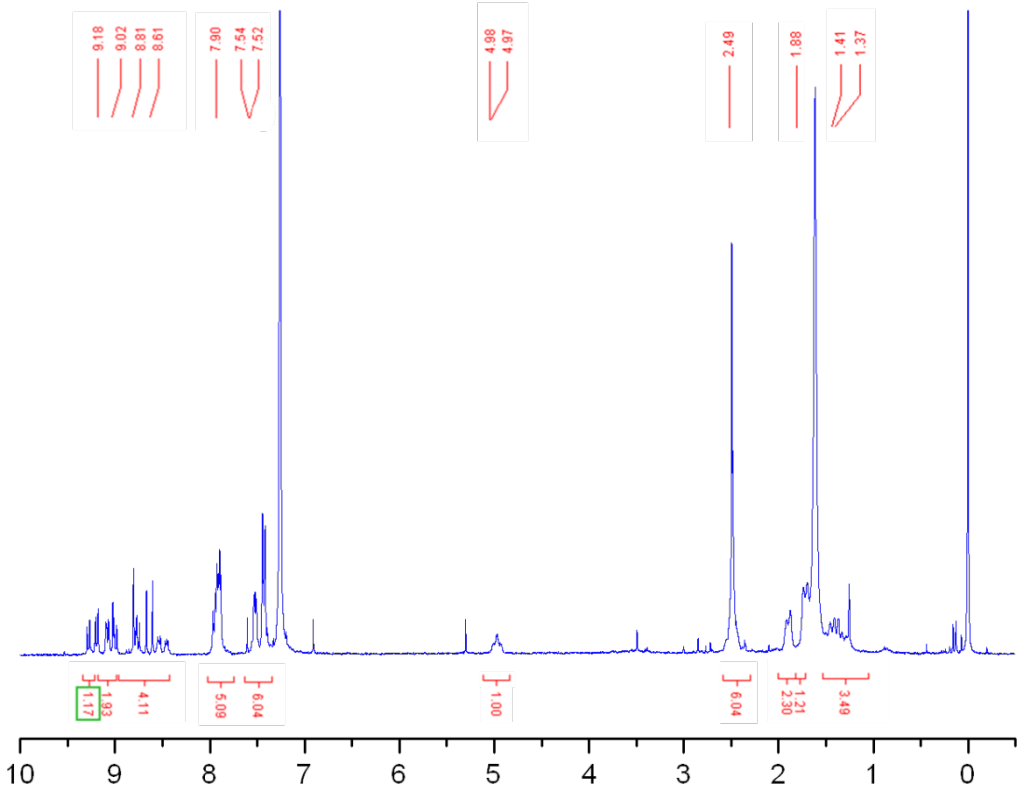


Fig. S8 ^{13}C NMR ($CDCl_3$) of **1,7-(TolSO$_2$)-PMABI 6**

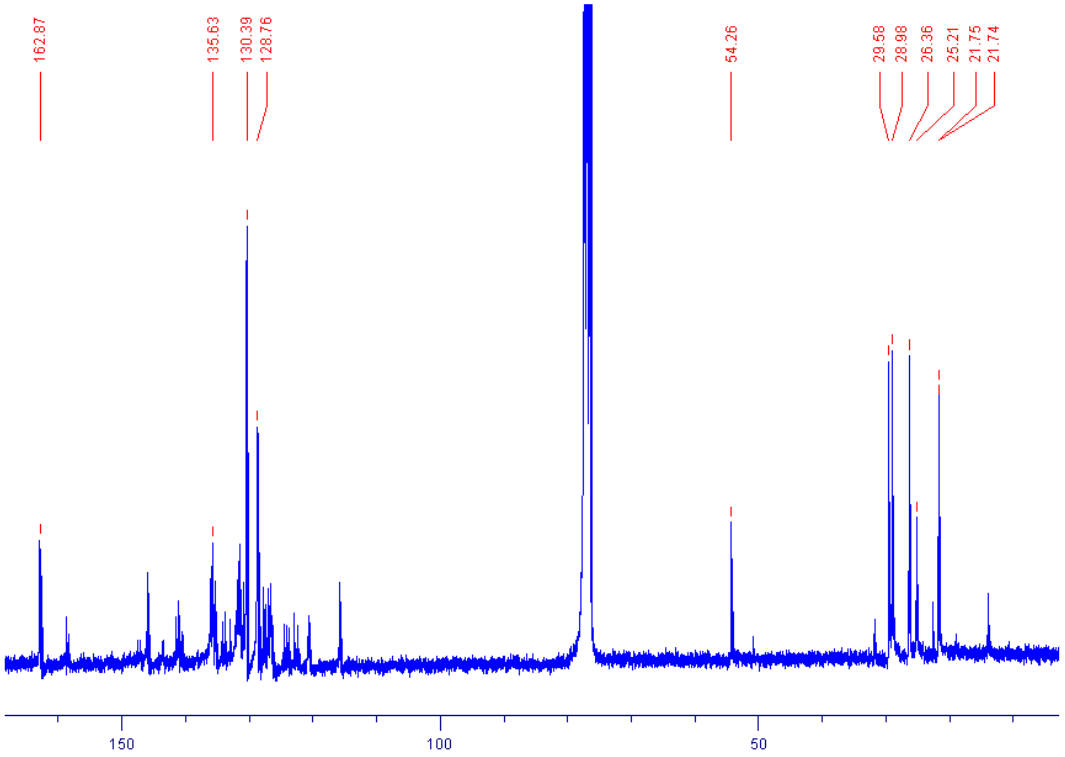


Fig. S9 MS of **1,7-(TolSO$_2$)-PMABI 6**

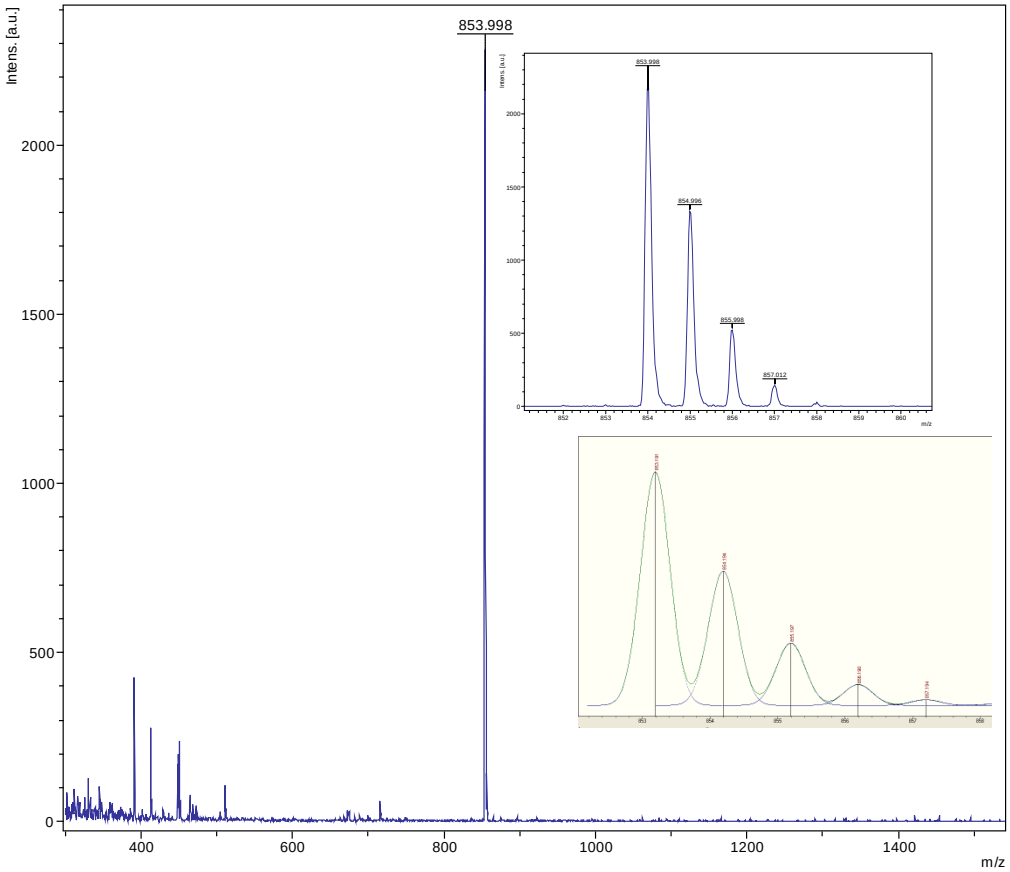
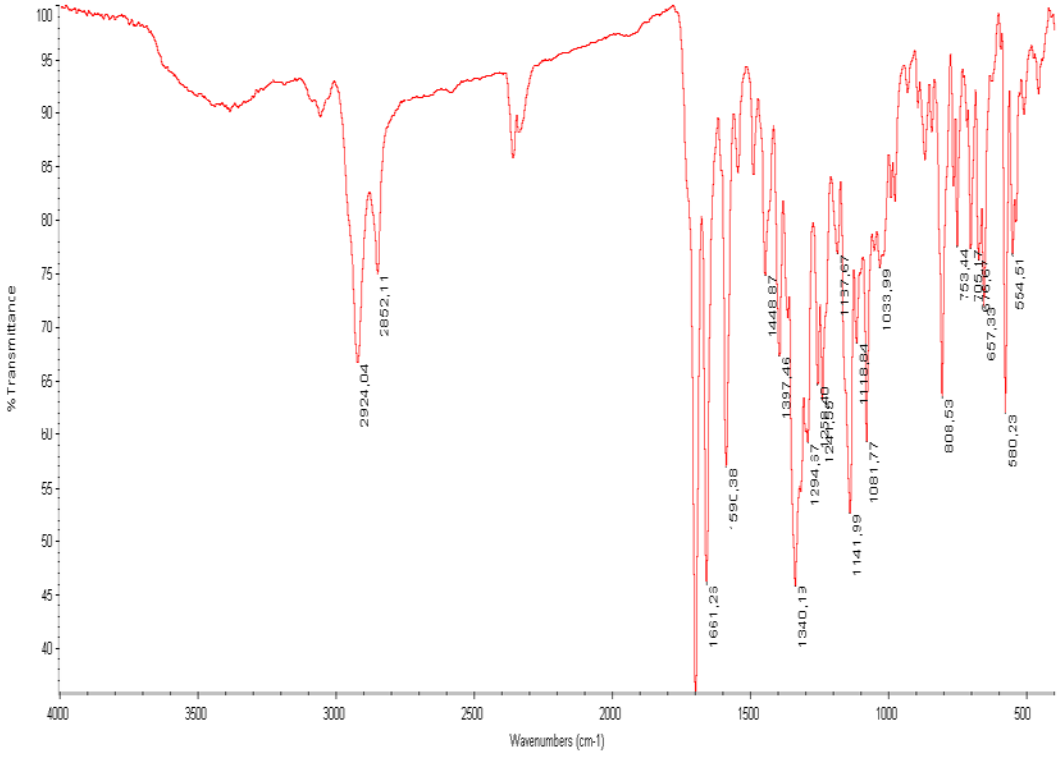


Fig. S10 IR spectrum (KBr) of **1,7-(TolSO$_2$)-PMABI 6**



Dyad ZnPc-PMIBI 2

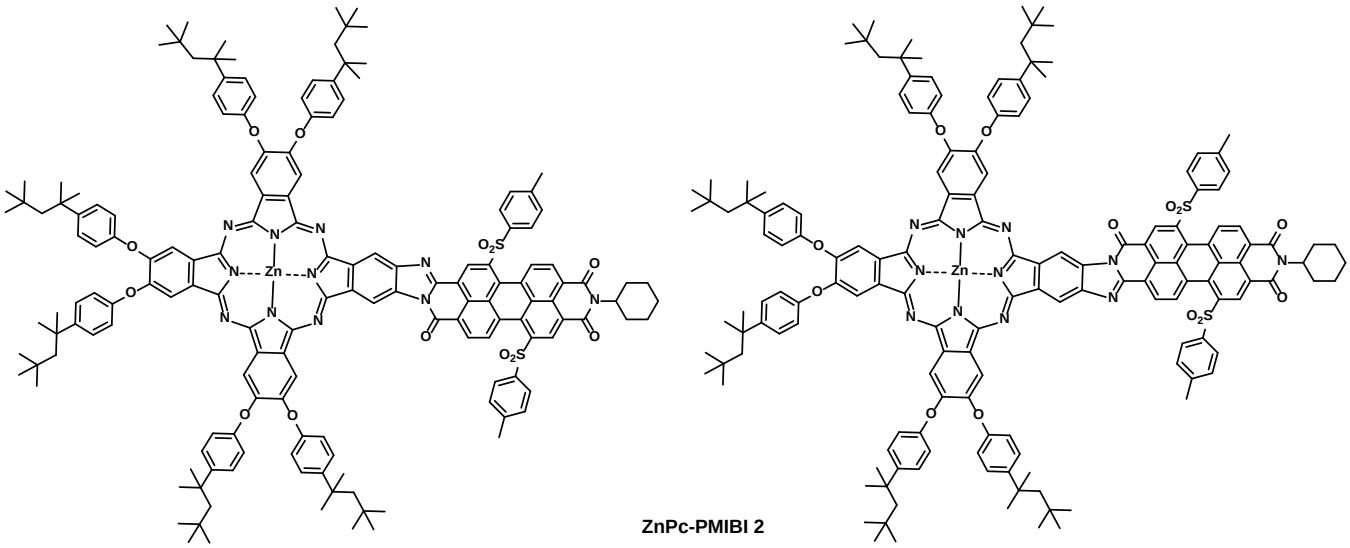


Fig. S11 ^{1}H NMR (THF-*d*8) of **Dyad ZnPc-PMIBI 2**

Parameters: Quantity: 1.5 mg, Ns= 3024 scans, D1= 3 seg and RGA= 1024

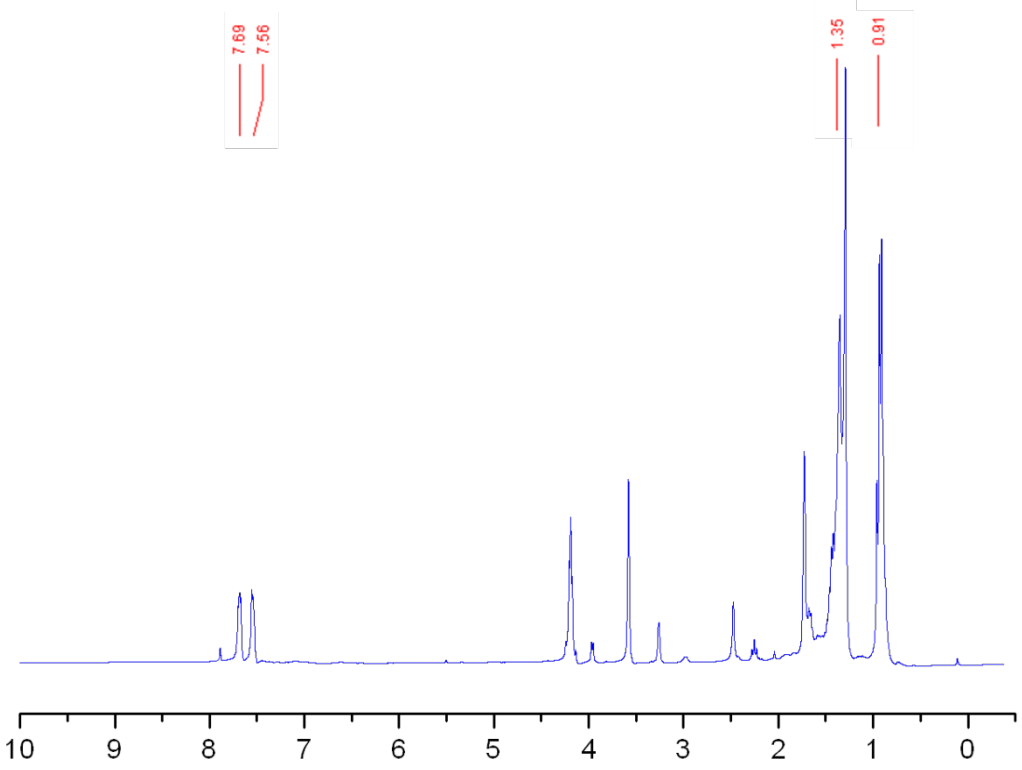


Fig. S12 MS of **Dyad ZnPc-PMIBI 2**

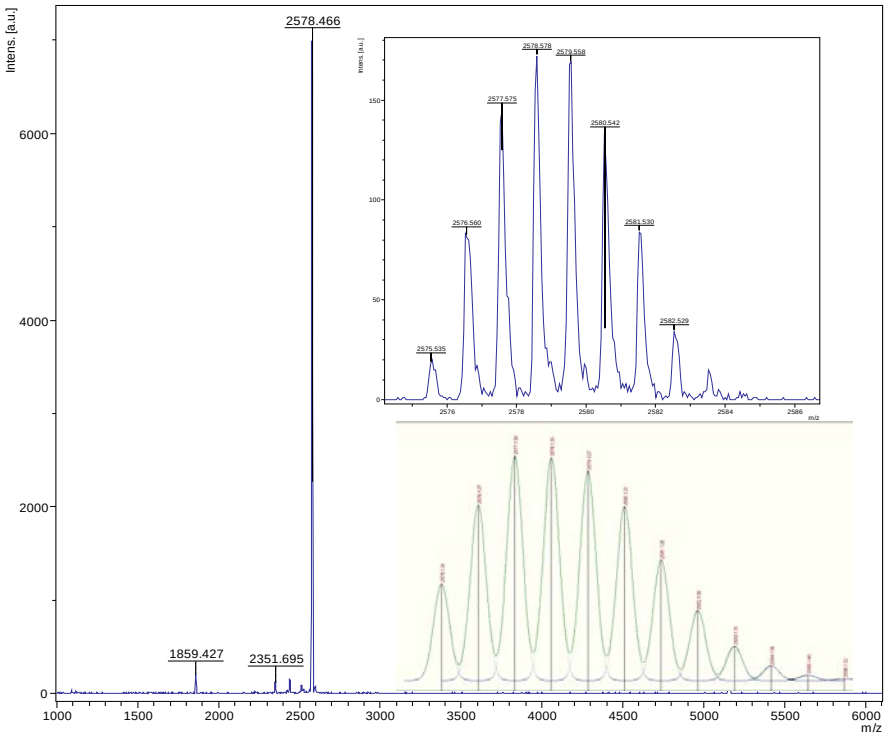
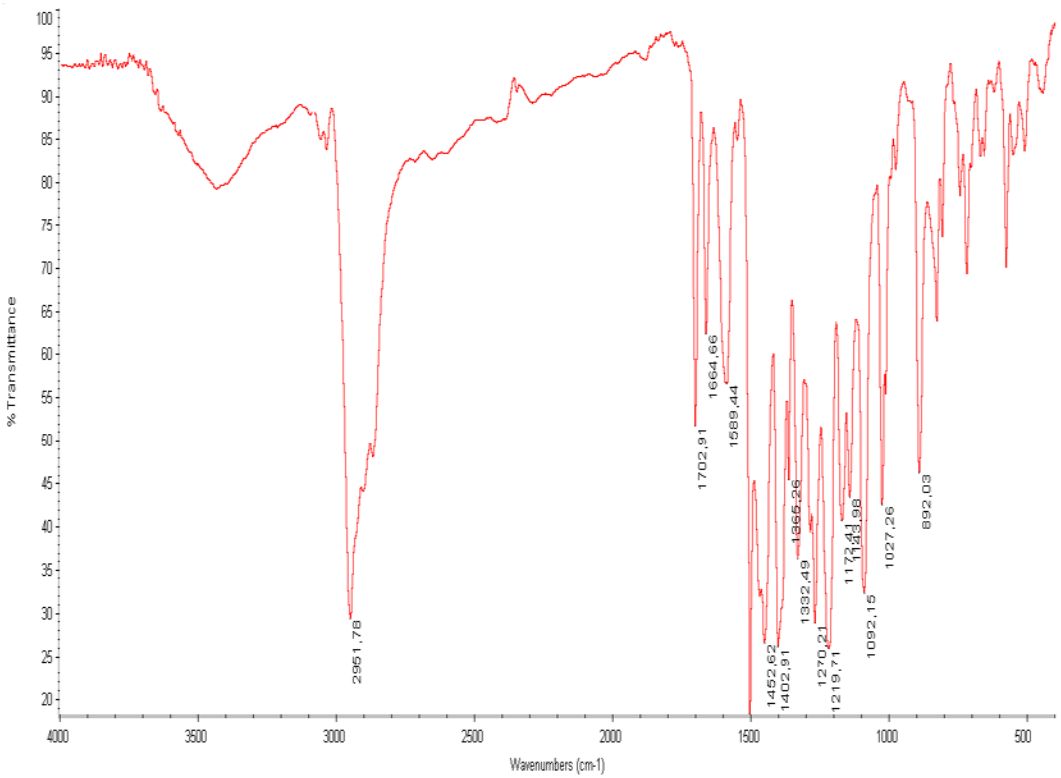


Fig. S13 IR spectrum (KBr) of **Dyad ZnPc-PMIBI 2**



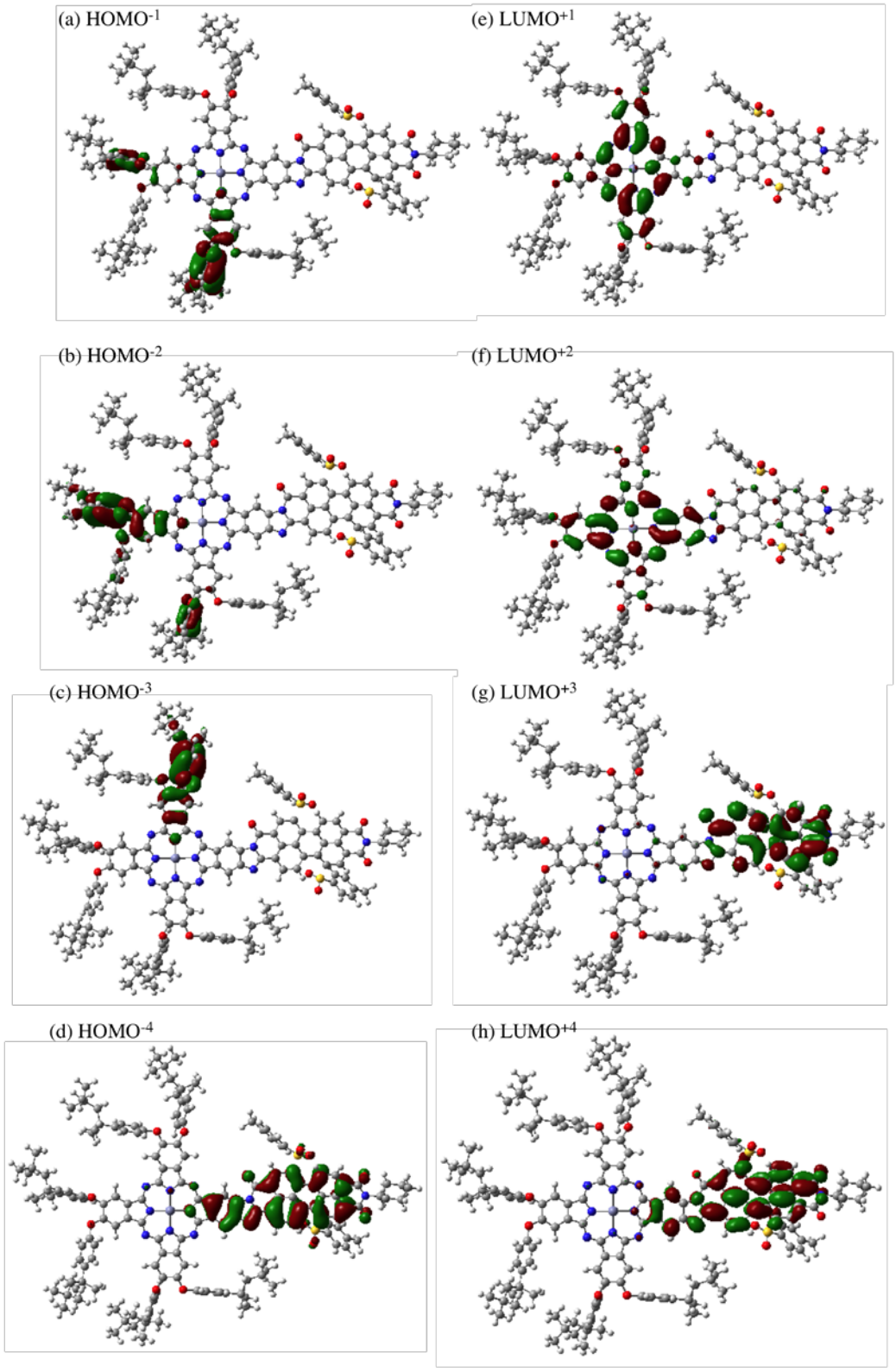


Fig. S14 Optimized structure with (a-d) $HOMO^{-1}$ ~ $HOMO^{-4}$ and (e-h) $LUMO^{+1}$ ~ $LUMO^{+4}$ of ZnPc-PMIBI **2** calculated by DFT at the B3LYP/6-31G(d) level of theory.

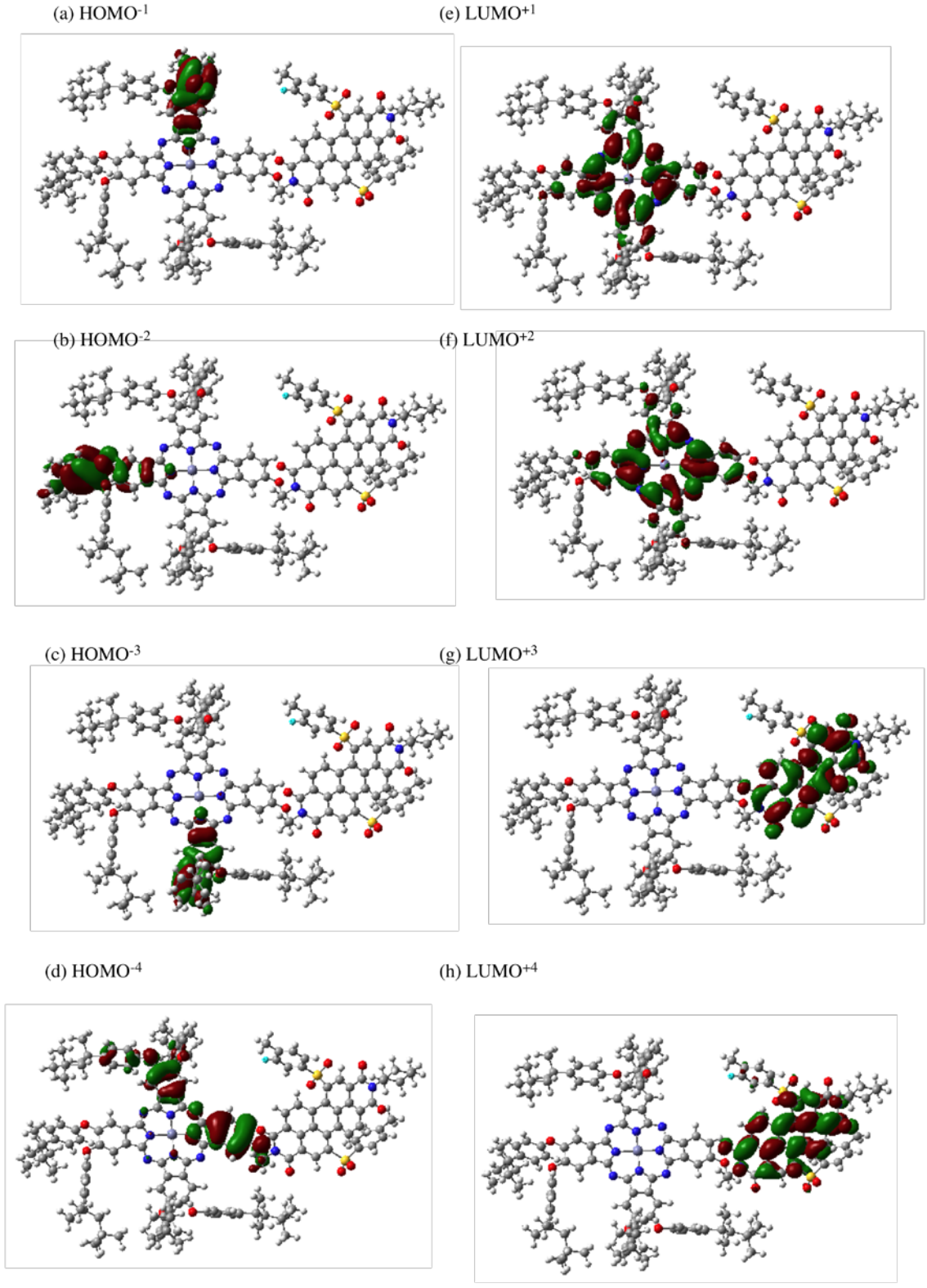


Fig. S15 Optimized structure with (a-d) $HOMO^{-1}$ ~ $HOMO^{-4}$ and (e-h) $LUMO^{+1}$ ~ $LUMO^{+4}$ of ZnPc-PDI **1** calculated by DFT at the B3LYP/6-31G(d) level of theory.

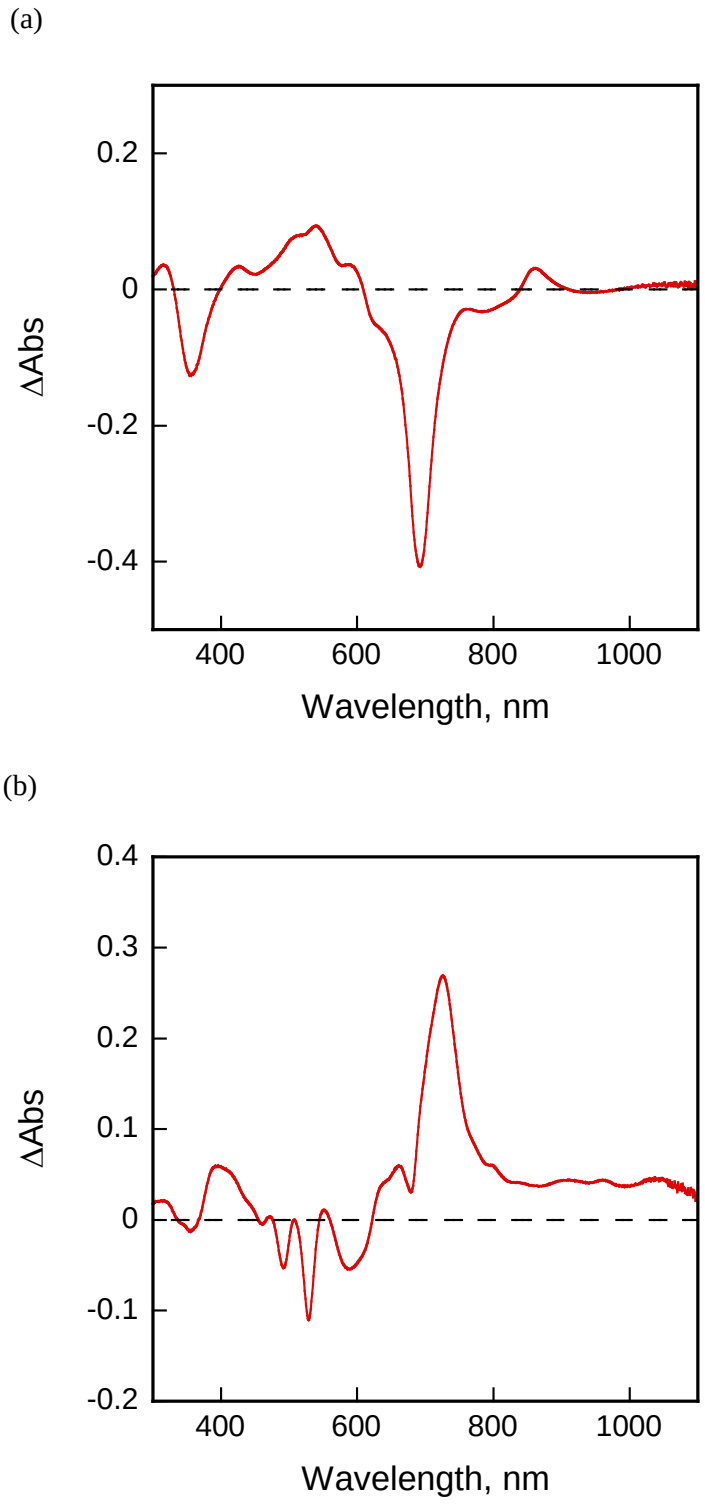


Fig. S16 Difference absorption spectra before and after electrolysis at an applied potential of (a) +0.70 V *vs.* SCE for the oxidation and (b) –0.45 V *vs.* SCE for the reduction of **ZnPc-PDI 2** in deaerated PhCN containing Bu_4ClO_4 (0.20 M).

Table S1 Report of the optimized geometry of ZnPc-PDI **1** calculated by DFT at the B3LYP/6-31G(d) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.296315	-0.655667	-0.780141
2	6	0	0.395996	0.278941	-1.228892
3	7	0	0.559803	1.595430	-1.304295
4	6	0	1.677843	2.231038	-0.961712
5	7	0	2.839806	1.680541	-0.482524
6	6	0	3.767080	2.675888	-0.285838
7	6	0	3.170478	3.951273	-0.661585
8	6	0	1.854936	3.674518	-1.077844
9	6	0	0.993273	4.683228	-1.511393
10	6	0	1.480949	5.987824	-1.536140
11	6	0	2.808606	6.270479	-1.103115
12	6	0	3.656549	5.260830	-0.670120
13	1	0	4.665156	5.503278	-0.353274
14	1	0	-0.016367	4.453321	-1.829086
15	7	0	5.012720	2.542382	0.162471
16	6	0	5.566697	1.381808	0.498088
17	7	0	4.991447	0.134258	0.457694
18	6	0	5.905845	-0.801325	0.874135
19	7	0	5.733331	-2.118436	0.964474
20	6	0	4.610201	-2.748846	0.637575
21	7	0	3.447227	-2.198091	0.158057
22	6	0	2.532234	-3.196718	-0.075029
23	7	0	1.296834	-3.069459	-0.550325
24	6	0	0.736334	-1.907121	-0.878328
25	6	0	-0.608213	-1.778973	-1.426055
26	6	0	-0.823182	-0.407033	-1.648560
27	6	0	-2.013691	0.081616	-2.185325
28	6	0	-3.004834	-0.851558	-2.502860
29	6	0	-2.797292	-2.233256	-2.274527
30	6	0	-1.607759	-2.705871	-1.740205
31	1	0	-1.453003	-3.767185	-1.572876
32	1	0	-3.602115	-2.911830	-2.538519
33	8	0	-4.212647	-0.545648	-3.064851
34	1	0	-2.133005	1.147271	-2.336223
35	6	0	3.137610	-4.476350	0.277170
36	6	0	4.440859	-4.196806	0.727435
37	6	0	5.301782	-5.206850	1.156948
38	6	0	4.830810	-6.518275	1.123367
39	6	0	3.518913	-6.804726	0.649337
40	6	0	2.667747	-5.790443	0.231817
41	1	0	1.668578	-6.033624	-0.113000
42	1	0	6.297803	-4.977084	1.516347
43	6	0	7.152327	-0.123625	1.205261
44	6	0	6.942094	1.247908	0.970104
45	6	0	7.947295	2.191978	1.184552
46	6	0	9.181943	1.731619	1.638868
47	6	0	9.400004	0.342021	1.860827
48	6	0	8.391184	-0.587436	1.653606
49	1	0	7.769938	3.246389	1.009616
50	6	0	-4.534992	0.813290	-3.346556
51	6	0	-5.035751	1.576432	-2.117179
52	7	0	-6.323420	1.060656	-1.627637
53	6	0	-7.474527	1.480763	-2.305086
54	6	0	-8.772809	0.975379	-1.797300
55	6	0	-8.823808	0.070405	-0.714031
56	6	0	-7.625095	-0.347503	-0.088216
57	6	0	-6.311239	0.185383	-0.526197
58	8	0	-5.269050	-0.104790	0.040102
59	6	0	-7.680765	-1.240802	0.965546
60	6	0	-8.906680	-1.792054	1.356670

61	6	0	-10.103291	-1.445856	0.734317
62	6	0	-10.084907	-0.411048	-0.256264
63	6	0	-11.298556	0.153592	-0.775070
64	6	0	-12.513866	-0.112732	0.010609
65	6	0	-12.548460	-1.263210	0.867730
66	6	0	-11.383441	-2.063554	1.098865
67	6	0	-11.569452	-3.323900	1.707045
68	6	0	-12.812827	-3.683509	2.256252
69	6	0	-13.880702	-2.807221	2.234197
70	6	0	-15.141882	-3.182754	2.923300
71	8	0	-15.233321	-4.231044	3.547203
72	7	0	-16.219954	-2.279357	2.835065
73	6	0	-16.164296	-1.069332	2.128210
74	8	0	-17.123843	-0.310689	2.077718
75	6	0	-14.890437	-0.736951	1.435721
76	6	0	-13.773744	-1.600775	1.512054
77	6	0	-14.787341	0.440029	0.719504
78	6	0	-13.618080	0.739329	0.002745
79	1	0	-13.583929	1.659455	-0.565020
80	1	0	-15.633847	1.118062	0.698860
81	1	0	-12.952096	-4.664511	2.693977
82	6	0	-11.194071	0.939933	-1.942828
83	6	0	-9.940238	1.342177	-2.436114
84	1	0	-9.884451	1.947956	-3.333109
85	1	0	-8.913511	-2.491622	2.179718
86	1	0	-6.759954	-1.522737	1.464533
87	8	0	-7.391720	2.233862	-3.268266
88	1	0	-4.329094	1.499927	-1.291747
89	1	0	-5.178223	2.625137	-2.387077
90	1	0	-3.676582	1.337311	-3.784531
91	1	0	-5.322906	0.771012	-4.100976
92	30	0	3.117927	-0.251394	-0.091395
93	8	0	0.770913	7.078063	-1.963396
94	8	0	3.296986	7.557312	-1.196003
95	8	0	10.609401	-0.079250	2.374017
96	8	0	5.542713	-7.603816	1.556333
97	8	0	3.041734	-8.096980	0.697702
98	16	0	-12.553859	1.463689	-3.076342
99	8	0	-13.381469	2.514511	-2.454330
100	8	0	-11.884683	1.749094	-4.354555
101	16	0	-10.408215	-4.747832	1.603065
102	8	0	-11.276200	-5.932542	1.683941
103	8	0	-9.530529	-4.549877	0.441244
104	8	0	10.254659	2.536135	1.911573
105	1	0	8.579384	-1.639310	1.839714
106	6	0	3.560040	-9.055038	-0.155823
107	6	0	3.290559	-10.384369	0.172884
108	6	0	4.272902	-8.763434	-1.314537
109	6	0	3.740504	-11.404026	-0.657141
110	1	0	2.734810	-10.601014	1.079899
111	6	0	4.720432	-9.806062	-2.132402
112	1	0	4.476752	-7.733434	-1.589155
113	6	0	4.467253	-11.152357	-1.836821
114	1	0	3.521481	-12.426091	-0.362952
115	1	0	5.278967	-9.531764	-3.019067
116	6	0	6.896853	-7.467384	1.846622
117	6	0	7.304994	-7.495775	3.177913
118	6	0	7.837574	-7.383883	0.825308
119	6	0	8.664375	-7.436130	3.476565
120	1	0	6.559117	-7.570323	3.963153
121	6	0	9.195729	-7.320938	1.144870
122	1	0	7.509209	-7.378025	-0.209486
123	6	0	9.645658	-7.347024	2.473160
124	1	0	8.959998	-7.455990	4.521389
125	1	0	9.904895	-7.257251	0.328008
126	6	0	11.722040	-0.113726	1.553601
127	6	0	12.952074	-0.296395	2.188984
128	6	0	11.673238	-0.016783	0.166264
129	6	0	14.114140	-0.380662	1.430751
130	1	0	12.981057	-0.363055	3.272121

131	6	0	12.855732	-0.101184	-0.575802
132	1	0	10.723961	0.116999	-0.341795 z
133	6	0	14.107170	-0.292157	0.025140
134	1	0	15.052711	-0.510089	1.961491
135	1	0	12.768548	-0.013272	-1.652004
136	6	0	10.171928	3.899434	1.641774
137	6	0	9.793866	4.780369	2.647769
138	6	0	10.543601	4.379275	0.387076
139	6	0	9.785995	6.154378	2.392396
140	1	0	9.515970	4.392468	3.623022
141	6	0	10.526801	5.751152	0.150519
142	1	0	10.851463	3.678920	-0.383259
143	6	0	10.150771	6.675247	1.142766
144	1	0	9.489775	6.817534	3.196762
145	1	0	10.816859	6.104875	-0.834437
146	6	0	2.820985	8.535334	-0.342304
147	6	0	3.117872	9.854934	-0.688597
148	6	0	2.118592	8.273943	0.830367
149	6	0	2.704170	10.894254	0.136606
150	1	0	3.662859	10.048671	-1.607232
151	6	0	1.707353	9.336115	1.642541
152	1	0	1.892703	7.252600	1.119044
153	6	0	1.987318	10.673097	1.328387
154	1	0	2.942549	11.907617	-0.172468
155	1	0	1.156870	9.084358	2.540860
156	6	0	-0.597670	6.979810	-2.194949
157	6	0	-1.466555	7.558633	-1.272260
158	6	0	-1.097414	6.399251	-3.355138
159	6	0	-2.836029	7.541186	-1.519183
160	1	0	-1.059678	8.024612	-0.380186
161	6	0	-2.477883	6.379941	-3.578330
162	1	0	-0.415028	5.966596	-4.080554
163	6	0	-3.385622	6.950424	-2.672823
164	1	0	-3.488616	8.000955	-0.783362
165	1	0	-2.829045	5.906081	-4.486493
166	6	0	-13.555919	-0.006767	-3.305611
167	6	0	-14.922770	0.052523	-3.043975
168	6	0	-12.970366	-1.162593	-3.832371
169	6	0	-15.709188	-1.072493	-3.295700
170	1	0	-15.359133	0.966567	-2.656642
171	6	0	-13.768206	-2.276876	-4.065632
172	1	0	-11.909520	-1.188636	-4.061415
173	6	0	-15.148340	-2.251223	-3.801117
174	1	0	-16.776162	-1.030720	-3.093234
175	1	0	-13.316216	-3.180510	-4.466862
176	6	0	-9.389116	-4.739891	3.089267
177	6	0	-8.006358	-4.869434	2.946410
178	6	0	-9.980385	-4.719329	4.355095
179	6	0	-7.211679	-4.963293	4.087800
180	1	0	-7.569498	-4.899416	1.953525
181	6	0	-9.168943	-4.803933	5.483394
182	1	0	-11.057665	-4.644356	4.465163
183	6	0	-7.775519	-4.925847	5.370616
184	1	0	-6.135432	-5.070134	3.978279
185	1	0	-9.626553	-4.785066	6.469206
186	6	0	-4.929519	6.939349	-2.859539
187	6	0	-5.292735	6.254916	-4.214554
188	6	0	-5.517137	6.139643	-1.667838
189	6	0	-5.440155	8.397705	-2.797847
190	1	0	-4.639842	6.685372	-4.984377
191	1	0	-4.985598	5.203969	-4.117593
192	1	0	-5.217456	6.577904	-0.710318
193	1	0	-6.607895	6.118412	-1.692112
194	1	0	-5.155726	5.104428	-1.681464
195	1	0	-6.533213	8.432471	-2.814637
196	1	0	-5.116497	8.895471	-1.878441
197	1	0	-5.063992	8.985761	-3.641963
198	6	0	1.511190	11.886007	2.176126
199	6	0	0.483589	12.657257	1.307188
200	6	0	0.852691	11.370108	3.494911

201	6	0	2.721608	12.802988	2.464913
202	1	0	0.921961	12.939092	0.344129
203	1	0	-0.393403	12.033801	1.097711
204	1	0	0.142643	13.573867	1.793345
205	1	0	1.522853	10.610278	3.917724
206	1	0	-0.054932	10.830140	3.191836
207	1	0	2.407204	13.724664	2.963721
208	1	0	3.458608	12.300685	3.101104
209	1	0	3.229668	13.099053	1.542308
210	6	0	10.139046	8.190502	0.825270
211	6	0	8.940856	8.410740	-0.168502
212	6	0	9.942016	9.010779	2.117934
213	6	0	11.517850	8.578416	0.238507
214	1	0	8.967700	7.593239	-0.899876
215	1	0	8.032947	8.231624	0.424572
216	1	0	10.695174	8.744254	2.868436
217	1	0	10.043930	10.079185	1.920906
218	1	0	8.951362	8.852619	2.558809
219	1	0	11.593800	9.661454	0.100576
220	1	0	12.316609	8.275218	0.925266
221	1	0	11.715200	8.106577	-0.728480
222	6	0	15.448364	-0.353908	-0.758299
223	6	0	16.236277	-1.605554	-0.309451
224	6	0	15.150626	-0.380715	-2.291276
225	6	0	16.248621	0.916516	-0.369682
226	1	0	16.378782	-1.622724	0.775159
227	1	0	15.713543	-2.526801	-0.588946
228	1	0	17.233030	-1.624749	-0.760070
229	1	0	14.705191	0.594175	-2.532910
230	1	0	14.355302	-1.119300	-2.455225
231	1	0	17.245629	0.925280	-0.816117
232	1	0	15.720829	1.821754	-0.691448
233	1	0	16.373647	0.979335	0.716434
234	6	0	11.143405	-7.265087	2.857143
235	6	0	12.031145	-7.435341	1.605440
236	6	0	11.341324	-5.843737	3.499924
237	6	0	11.468953	-8.436034	3.815425
238	1	0	11.781383	-8.359613	1.071475
239	1	0	11.922682	-6.598700	0.906157
240	1	0	13.085573	-7.495370	1.880131
241	1	0	10.488501	-5.665435	4.166956
242	1	0	11.211148	-5.129208	2.674974
243	1	0	12.542458	-8.485173	4.023029
244	1	0	10.949502	-8.355852	4.774628
245	1	0	11.176492	-9.387861	3.357110
246	6	0	4.979532	-12.344725	-2.692495
247	6	0	3.792258	-13.283486	-3.006538
248	6	0	5.643673	-11.800307	-3.996930
249	6	0	6.012980	-13.104461	-1.820098
250	1	0	3.278883	-13.600097	-2.093724
251	1	0	3.052743	-12.790032	-3.646664
252	1	0	4.132612	-14.192841	-3.510829
253	1	0	6.538024	-11.248481	-3.676589
254	1	0	4.965191	-11.047115	-4.418285
255	1	0	6.376497	-14.009487	-2.311664
256	1	0	6.875408	-12.466230	-1.595421
257	1	0	5.570270	-13.404455	-0.864529
258	6	0	-15.998335	-3.470180	-4.066264
259	1	0	-17.043939	-3.296989	-3.795773
260	1	0	-15.966857	-3.750631	-5.126135
261	1	0	-15.640117	-4.334711	-3.494525
262	6	0	-6.904374	-4.993647	6.601470
263	1	0	-5.989649	-5.564498	6.413589
264	1	0	-6.601688	-3.988377	6.923173
265	1	0	-7.431805	-5.458902	7.440295
266	6	0	-17.477347	-2.658644	3.548013
267	6	0	-17.824359	-1.685110	4.688013
268	6	0	-18.659335	-2.876794	2.587189
269	1	0	-17.231020	-3.622853	3.996043
270	6	0	-19.060010	-2.189832	5.452827

271	1	0	-18.022462	-0.690418	4.277968
272	1	0	-16.966818	-1.598463	5.367375
273	6	0	-19.888074	-3.372809	3.369076
274	1	0	-18.899633	-1.939502	2.076643
275	1	0	-18.375586	-3.609276	1.820861
276	6	0	-20.254045	-2.414341	4.512510
277	1	0	-19.322591	-1.472791	6.240392
278	1	0	-18.815798	-3.135404	5.959049
279	1	0	-20.736077	-3.491847	2.683403
280	1	0	-19.679809	-4.369636	3.784818
281	1	0	-21.110484	-2.806344	5.075346
282	1	0	-20.569196	-1.449354	4.089802
283	6	0	6.076072	-12.678172	-5.220692
284	6	0	6.884553	-13.940122	-4.862572
285	6	0	4.873553	-13.081588	-6.102698
286	6	0	6.985280	-11.766656	-6.079601
287	1	0	7.744994	-13.705650	-4.225169
288	1	0	6.276625	-14.692321	-4.349589
289	1	0	7.270013	-14.406736	-5.777896
290	1	0	4.282698	-12.202767	-6.388967
291	1	0	5.226421	-13.556806	-7.026542
292	1	0	4.203163	-13.788818	-5.608456
293	1	0	7.284647	-12.274001	-7.004726
294	1	0	6.469567	-10.839619	-6.359661
295	1	0	7.898233	-11.490814	-5.537694
296	6	0	16.205985	-0.675827	-3.410980
297	6	0	17.521930	0.116020	-3.287557
298	6	0	16.529303	-2.182042	-3.527825
299	6	0	15.528283	-0.252436	-4.736490
300	1	0	17.339190	1.192213	-3.188702
301	1	0	18.124914	-0.206451	-2.432640
302	1	0	18.131853	-0.033973	-4.187302
303	1	0	15.612305	-2.775915	-3.628643
304	1	0	17.142168	-2.367461	-4.418813
305	1	0	17.082580	-2.565515	-2.667310
306	1	0	16.168241	-0.490598	-5.594671
307	1	0	14.572017	-0.771072	-4.879445
308	1	0	15.329536	0.826128	-4.755760
309	6	0	12.602337	-5.393712	4.308702
310	6	0	13.944146	-5.679831	3.608484
311	6	0	12.468811	-3.860517	4.468102
312	6	0	12.629025	-6.005483	5.726312
313	1	0	14.173541	-6.749853	3.572383
314	1	0	13.955613	-5.292577	2.583214
315	1	0	14.762086	-5.193041	4.154455
316	1	0	11.518542	-3.590080	4.944734
317	1	0	13.279442	-3.464181	5.092052
318	1	0	12.512120	-3.350097	3.498498
319	1	0	13.439237	-5.558844	6.316136
320	1	0	11.689434	-5.811027	6.258741
321	1	0	12.791185	-7.086438	5.716465
322	6	0	8.699812	9.709865	-1.006185
323	6	0	7.269712	9.574788	-1.581176
324	6	0	8.759106	11.016174	-0.191533
325	6	0	9.671340	9.814241	-2.201813
326	1	0	7.156178	8.648025	-2.156707
327	1	0	6.515812	9.565688	-0.784927
328	1	0	7.040798	10.413080	-2.250773
329	1	0	9.774806	11.251514	0.143322
330	1	0	8.421210	11.857503	-0.809605
331	1	0	8.109872	10.973989	0.690693
332	1	0	9.385212	10.652275	-2.849611
333	1	0	10.706050	9.981576	-1.891500
334	1	0	9.646078	8.903138	-2.812791
335	6	0	0.448794	12.269275	4.712940
336	6	0	1.667522	12.664628	5.576091
337	6	0	-0.344709	13.538885	4.348758
338	6	0	-0.463857	11.382084	5.593400
339	1	0	2.249313	11.780468	5.864528
340	1	0	2.341686	13.357332	5.066692

341	1	0	1.332530	13.154243	6.499067
342	1	0	-1.215280	13.309768	3.723269
343	1	0	-0.713552	14.021700	5.262490
344	1	0	0.268618	14.276016	3.820564
345	1	0	-0.745395	11.905435	6.515159
346	1	0	-1.386757	11.112982	5.065126
347	1	0	0.041353	10.451101	5.879453
348	6	0	-6.718988	6.251030	-4.867437
349	6	0	-6.672344	5.142581	-5.946288
350	6	0	-7.882245	5.915307	-3.913926
351	6	0	-7.020968	7.584600	-5.586479
352	1	0	-5.838591	5.297706	-6.643125
353	1	0	-6.557168	4.153077	-5.488588
354	1	0	-7.598914	5.132355	-6.532607
355	1	0	-8.053968	6.699606	-3.168901
356	1	0	-8.810320	5.812722	-4.490070
357	1	0	-7.717368	4.965899	-3.393482
358	1	0	-7.956195	7.502556	-6.153763
359	1	0	-7.132597	8.424028	-4.895221
360	1	0	-6.225099	7.839371	-6.297723

Table S2 Report of the optimized geometry of ZnPc-PDI **2** calculated by DFT at the B3LYP/6-31G(d) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.523846	-0.373477	-1.005713
2	6	0	-0.240837	-1.509291	-0.942630
3	7	0	0.178012	-2.770562	-0.919259
4	6	0	1.455988	-3.135623	-0.955167
5	7	0	2.559113	-2.322621	-1.025758
6	6	0	3.694792	-3.098449	-1.038567
7	6	0	3.303615	-4.501485	-0.971462
8	6	0	1.897946	-4.525510	-0.918557
9	6	0	1.183152	-5.720677	-0.847345
10	6	0	1.909107	-6.910407	-0.831828
11	6	0	3.332636	-6.888508	-0.869527
12	6	0	4.033448	-5.692221	-0.944175
13	1	0	5.117361	-5.705264	-0.982034
14	1	0	0.100477	-5.720988	-0.814632
15	7	0	4.956409	-2.681119	-1.095493
16	6	0	5.320022	-1.402795	-1.147080
17	7	0	4.503825	-0.298483	-1.150663
18	6	0	5.274177	0.837381	-1.210277
19	7	0	4.853974	2.099643	-1.230249
20	6	0	3.575859	2.464533	-1.193550
21	7	0	2.472021	1.649988	-1.129878
22	6	0	1.336043	2.424042	-1.106179
23	7	0	0.074232	2.008611	-1.046142
24	6	0	-0.293324	0.730984	-1.000652
25	6	0	-1.683233	0.291294	-0.930862
26	6	0	-1.650178	-1.129973	-0.894957
27	6	0	-2.803623	-1.902609	-0.825829
28	6	0	-4.007887	-1.195035	-0.791528
29	6	0	-4.023308	0.232983	-0.826710
30	6	0	-2.876092	1.015894	-0.897410
31	1	0	-2.904574	2.096932	-0.923553
32	1	0	-2.775271	-2.986212	-0.798824
33	6	0	1.725862	3.827788	-1.155649
34	6	0	3.131432	3.855688	-1.212493
35	6	0	3.840190	5.056055	-1.276056
36	6	0	3.107015	6.241432	-1.284584
37	6	0	1.685033	6.214562	-1.204052
38	6	0	0.989962	5.014757	-1.146696
39	1	0	-0.093652	5.020681	-1.100049
40	1	0	4.922255	5.063623	-1.329257
41	6	0	6.678287	0.448939	-1.245595
42	6	0	6.709907	-0.957905	-1.207375
43	6	0	7.912923	-1.664372	-1.228609
44	6	0	9.095687	-0.929524	-1.297645
45	6	0	9.064727	0.494222	-1.316999
46	6	0	7.862217	1.187293	-1.295453
47	1	0	7.925922	-2.747573	-1.202309
48	30	0	2.515337	-0.336835	-1.106820
49	8	0	1.345943	-8.156024	-0.778558
50	8	0	4.029430	-8.076518	-0.927923
51	8	0	10.238835	1.200938	-1.463050
52	8	0	3.655705	7.491872	-1.361418
53	8	0	0.976199	7.394592	-1.280654
54	8	0	10.347845	-1.479225	-1.311273
55	1	0	7.863976	2.271497	-1.324676
56	6	0	1.007546	8.285320	-0.222334
57	6	0	0.533609	9.571618	-0.486142
58	6	0	1.431218	7.954589	1.062012
59	6	0	0.493840	10.514836	0.534610
60	1	0	0.204753	9.815582	-1.491545
61	6	0	1.388757	8.920483	2.071919
62	1	0	1.787074	6.953298	1.281860

63	6	0	0.920472	10.220529	1.843181
64	1	0	0.123578	11.507426	0.295233
65	1	0	1.729696	8.627856	3.058828
66	6	0	5.037502	7.637505	-1.444918
67	6	0	5.687719	7.510381	-2.667802
68	6	0	5.748894	7.995030	-0.302338
69	6	0	7.064958	7.731748	-2.739256
70	1	0	5.119946	7.245146	-3.554490
71	6	0	7.121351	8.215926	-0.393786
72	1	0	5.221554	8.106023	0.640058
73	6	0	7.817552	8.083588	-1.608733
74	1	0	7.545693	7.625313	-3.704814
75	1	0	7.654538	8.498114	0.508771
76	6	0	11.148562	1.255644	-0.421393
77	6	0	12.427532	1.711670	-0.746415
78	6	0	10.843070	0.934348	0.897772
79	6	0	13.388722	1.833418	0.250084
80	1	0	12.651455	1.960887	-1.779014
81	6	0	11.827692	1.058195	1.882953
82	1	0	9.847891	0.593243	1.163845
83	6	0	13.122968	1.503974	1.592411
84	1	0	14.373612	2.193667	-0.033449
85	1	0	11.553982	0.796248	2.898821
86	6	0	10.530387	-2.829343	-1.583346
87	6	0	10.165581	-3.382784	-2.811699
88	6	0	11.185262	-3.603636	-0.633560
89	6	0	10.455925	-4.719756	-3.068027
90	1	0	9.667566	-2.770231	-3.556932
91	6	0	11.473660	-4.941894	-0.913188
92	1	0	11.473689	-3.152499	0.310649
93	6	0	11.113866	-5.536805	-2.130114
94	1	0	10.169812	-5.127590	-4.033063
95	1	0	11.988645	-5.518083	-0.153379
96	6	0	4.132847	-8.872582	0.199226
97	6	0	3.799952	-8.450254	1.486441
98	6	0	4.646935	-10.152622	0.002774
99	6	0	3.980037	-9.321657	2.560073
100	1	0	3.411523	-7.451021	1.653534
101	6	0	4.824623	-11.004933	1.091269
102	1	0	4.902733	-10.468442	-1.003896
103	6	0	4.493395	-10.618773	2.399479
104	1	0	3.713604	-8.963341	3.550200
105	1	0	5.229078	-11.992147	0.897807
106	6	0	-0.041720	-8.266874	-0.716495
107	6	0	-0.794361	-8.272399	-1.889009
108	6	0	-0.659650	-8.434542	0.516931
109	6	0	-2.175816	-8.434976	-1.811607
110	1	0	-0.297299	-8.152271	-2.846806
111	6	0	-2.045862	-8.598566	0.574821
112	1	0	-0.056379	-8.442922	1.419504
113	6	0	-2.839200	-8.599589	-0.582070
114	1	0	-2.501229	-8.726275	1.550157
115	7	0	-5.383283	0.563190	-0.772475
116	6	0	-6.085314	-0.653739	-0.706654
117	6	0	-5.967507	1.837236	-0.776321
118	6	0	-7.530033	-0.638594	-0.632706
119	6	0	-7.449739	1.827296	-0.717745
120	8	0	-5.289560	2.851343	-0.822479
121	6	0	-8.193062	0.621319	-0.645354
122	6	0	-8.277823	-1.804549	-0.571837
123	6	0	-8.109456	3.042396	-0.684614
124	6	0	-9.617701	0.679555	-0.598467
125	6	0	-9.668458	-1.747144	-0.442183
126	1	0	-7.771095	-2.762885	-0.605060
127	6	0	-9.509385	3.109280	-0.687417
128	1	0	-7.506459	3.942133	-0.660613
129	6	0	-10.288069	1.935572	-0.773183
130	6	0	-10.355632	-0.532376	-0.388624
131	6	0	-11.720455	1.872400	-1.089464
132	6	0	-11.805657	-0.455294	-0.183794

133	6	0	-12.459441	0.705459	-0.709993
134	6	0	-12.383245	2.879892	-1.792314
135	6	0	-12.620118	-1.440027	0.417826
136	6	0	-13.873694	0.705441	-0.881817
137	6	0	-13.764320	2.828356	-2.027058
138	6	0	-14.017186	-1.400217	0.286865
139	6	0	-14.518213	1.773119	-1.546951
140	6	0	-14.640460	-0.374390	-0.398039
141	1	0	-14.260137	3.625068	-2.570496
142	1	0	-14.642563	-2.173749	0.715643
143	6	0	-15.988311	1.758480	-1.766218
144	6	0	-16.114861	-0.406589	-0.563860
145	8	0	-16.545665	2.663311	-2.373588
146	7	0	-16.709163	0.667959	-1.252551
147	8	0	-16.782133	-1.332599	-0.119727
148	7	0	-5.296876	-1.699142	-0.718168
149	1	0	-10.211826	-2.682102	-0.397440
150	1	0	-11.832280	3.724807	-2.184957
151	6	0	0.886961	11.309967	2.940932
152	6	0	1.204041	10.708610	4.323071
153	6	0	1.941180	12.388496	2.497820
154	6	0	-0.550644	11.886566	3.002139
155	1	0	0.525589	9.877954	4.549818
156	1	0	2.231453	10.335836	4.390818
157	1	0	1.069964	11.458035	5.107764
158	1	0	1.547148	12.832257	1.573786
159	1	0	2.841387	11.839574	2.189407
160	1	0	-0.667622	12.594678	3.826305
161	1	0	-0.825644	12.406885	2.078788
162	1	0	-1.273329	11.076218	3.152880
163	6	0	9.339907	8.353981	-1.667937
164	6	0	10.022631	7.498023	-0.570496
165	6	0	9.923690	7.917650	-3.025376
166	6	0	9.502465	9.895729	-1.406580
167	1	0	9.727670	7.806238	0.437840
168	1	0	9.748504	6.443536	-0.688521
169	1	0	11.111383	7.565940	-0.628036
170	1	0	9.552406	8.524843	-3.857374
171	1	0	11.013817	7.999708	-3.016738
172	1	0	9.680925	6.869151	-3.233441
173	1	0	8.748581	10.402341	-2.024481
174	1	0	9.180755	10.060566	-0.369583
175	6	0	4.706795	-11.536665	3.626835
176	6	0	3.380189	-11.593479	4.425886
177	6	0	5.043406	-12.973701	3.185506
178	6	0	5.870070	-10.872096	4.449269
179	1	0	3.117478	-10.623138	4.859830
180	1	0	2.557662	-11.895244	3.767334
181	1	0	3.433508	-12.315532	5.244396
182	1	0	6.011669	-13.039885	2.678371
183	1	0	5.075654	-13.642792	4.049775
184	1	0	4.276232	-13.360396	2.504612
185	1	0	6.654833	-10.610884	3.726193
186	1	0	5.475853	-9.910240	4.803607
187	6	0	11.441049	-7.009546	-2.477249
188	6	0	11.918935	-7.765979	-1.219175
189	6	0	10.148110	-7.702208	-2.969016
190	6	0	12.577577	-6.944153	-3.562203
191	1	0	12.884017	-7.394923	-0.856152
192	1	0	11.189992	-7.670660	-0.406179
193	1	0	12.036561	-8.830862	-1.425973
194	1	0	9.773735	-7.283971	-3.908001
195	1	0	10.313976	-8.772611	-3.125966
196	1	0	9.355836	-7.596959	-2.218935
197	1	0	12.298795	-6.162849	-4.280383
198	1	0	13.457166	-6.545930	-3.036619
199	6	0	14.225644	1.662943	2.667175
200	6	0	15.497801	0.927743	2.181412
201	6	0	14.420419	3.211302	2.852569
202	6	0	13.787911	0.996065	3.989292

203	1	0	15.257599	-0.113587	1.937711
204	1	0	15.936485	1.383290	1.288679
205	1	0	16.267383	0.916381	2.959934
206	1	0	13.489716	3.567285	3.317055
207	1	0	14.425541	3.659491	1.850951
208	1	0	14.602821	0.990123	4.715737
209	1	0	12.940313	1.514342	4.451809
210	1	0	13.495503	-0.046560	3.819517
211	6	0	10.830065	10.699993	-1.602078
212	6	0	12.059791	10.056104	-0.933724
213	6	0	11.139670	10.966745	-3.091061
214	6	0	10.587296	12.072682	-0.930415
215	1	0	11.871461	9.824968	0.121226
216	1	0	12.365901	9.131925	-1.434282
217	1	0	12.913312	10.744443	-0.974527
218	1	0	10.280418	11.424059	-3.597202
219	1	0	11.984216	11.661126	-3.182495
220	1	0	11.405944	10.058411	-3.637289
221	1	0	11.449358	12.735048	-1.075548
222	1	0	9.707058	12.572353	-1.353309
223	1	0	10.424806	11.966080	0.149170
224	6	0	2.444138	13.573502	3.386965
225	6	0	1.318248	14.385374	4.054318
226	6	0	3.449061	13.112058	4.464723
227	6	0	3.204233	14.519297	2.426541
228	1	0	0.566452	14.708274	3.324738
229	1	0	0.807095	13.819030	4.839607
230	1	0	1.732603	15.286528	4.523872
231	1	0	4.263824	12.527538	4.019300
232	1	0	3.899232	13.981718	4.959528
233	1	0	2.985202	12.500239	5.242625
234	1	0	3.656481	15.353361	2.977018
235	1	0	4.008400	13.990210	1.900482
236	1	0	2.532618	14.942645	1.669661
237	6	0	15.606965	3.885266	3.616196
238	6	0	15.869969	3.309947	5.020968
239	6	0	16.916976	3.848754	2.799989
240	6	0	15.205585	5.370291	3.780891
241	1	0	14.955259	3.279807	5.624436
242	1	0	16.285033	2.297555	4.983106
243	1	0	16.596816	3.936685	5.553083
244	1	0	16.768106	4.265927	1.796078
245	1	0	17.689221	4.450408	3.295537
246	1	0	17.314746	2.837044	2.686924
247	1	0	16.015730	5.944441	4.246941
248	1	0	14.983232	5.832657	2.811257
249	1	0	14.314522	5.473679	4.412109
250	6	0	13.062257	-8.153449	-4.428452
251	6	0	14.370452	-7.680328	-5.105159
252	6	0	13.382067	-9.427737	-3.623713
253	6	0	12.059457	-8.500497	-5.550084
254	1	0	14.211008	-6.761821	-5.683419
255	1	0	15.151430	-7.475518	-4.362689
256	1	0	14.753015	-8.445202	-5.792006
257	1	0	12.480539	-9.902262	-3.223116
258	1	0	13.873710	-10.165340	-4.270338
259	1	0	14.058374	-9.220315	-2.786239
260	1	0	12.490075	-9.250463	-6.225335
261	1	0	11.121701	-8.909166	-5.164890
262	1	0	11.818655	-7.615384	-6.152234
263	6	0	6.606161	-11.531232	5.662443
264	6	0	5.663844	-12.113011	6.732982
265	6	0	7.606788	-12.620421	5.219164
266	6	0	7.424934	-10.394074	6.318409
267	1	0	4.911403	-11.381787	7.050850
268	1	0	5.139973	-13.007793	6.381428
269	1	0	6.238743	-12.403829	7.621363
270	1	0	8.291086	-12.239058	4.451102
271	1	0	8.216271	-12.944852	6.072086
272	1	0	7.112802	-13.508352	4.816640

273	1	0	8.029003	-10.777980	7.149572
274	1	0	8.106721	-9.927105	5.596922
275	1	0	6.769812	-9.608738	6.715105
276	1	0	-2.742912	-8.432541	-2.737187
277	6	0	-4.379500	-8.740082	-0.541359
278	6	0	-4.787511	-9.860059	-1.532304
279	6	0	-4.855579	-9.166007	0.860861
280	6	0	-4.936792	-7.331955	-0.967051
281	1	0	-4.578917	-9.589769	-2.572490
282	1	0	-4.233887	-10.779889	-1.311048
283	1	0	-5.853305	-10.088520	-1.461453
284	1	0	-4.679288	-8.393453	1.616379
285	1	0	-5.927661	-9.380368	0.851879
286	1	0	-4.344694	-10.081083	1.182497
287	1	0	-4.367013	-6.583258	-0.399752
288	1	0	-4.632469	-7.192002	-2.013078
289	6	0	-6.436222	-6.895525	-0.870817
290	6	0	-7.425099	-7.909839	-1.476708
291	6	0	-6.861959	-6.571111	0.577205
292	6	0	-6.543017	-5.584217	-1.685555
293	1	0	-7.142084	-8.191138	-2.497955
294	1	0	-7.498032	-8.825199	-0.880077
295	1	0	-8.430419	-7.472822	-1.520189
296	1	0	-6.174576	-5.851434	1.038574
297	1	0	-7.863166	-6.122807	0.585606
298	1	0	-6.899334	-7.457282	1.215850
299	1	0	-7.567876	-5.193182	-1.648403
300	1	0	-5.874597	-4.806596	-1.295944
301	1	0	-6.289692	-5.747444	-2.740575
302	6	0	-18.190604	0.614785	-1.436016
303	6	0	-18.917843	1.769639	-0.725363
304	6	0	-18.596949	0.494194	-2.915290
305	1	0	-18.472833	-0.313524	-0.936314
306	6	0	-20.440249	1.590778	-0.854719
307	1	0	-18.618046	2.724117	-1.167592
308	1	0	-18.625932	1.788887	0.332381
309	6	0	-20.121705	0.325450	-3.029169
310	1	0	-18.279413	1.388478	-3.459518
311	1	0	-18.085305	-0.366139	-3.365200
312	6	0	-20.871883	1.465857	-2.324047
313	1	0	-20.951386	2.435533	-0.376438
314	1	0	-20.750716	0.687592	-0.308585
315	1	0	-20.408444	0.275615	-4.086944
316	1	0	-20.417319	-0.634085	-2.579447
317	1	0	-21.955174	1.302183	-2.387657
318	1	0	-20.665320	2.412109	-2.844715
319	16	0	-10.225295	4.784475	-0.475522
320	8	0	-10.375207	5.407814	-1.805208
321	8	0	-11.379250	4.657221	0.428031
322	16	0	-11.960937	-2.778130	1.480170
323	8	0	-11.739946	-3.979082	0.649530
324	8	0	-10.863537	-2.209423	2.278573
325	6	0	-8.958289	5.704498	0.403826
326	6	0	-8.142026	6.591023	-0.300538
327	6	0	-8.854852	5.570413	1.790320
328	6	0	-7.194773	7.335866	0.399219
329	1	0	-8.262955	6.700868	-1.373021
330	6	0	-7.900334	6.321846	2.470151
331	1	0	-9.523394	4.903693	2.325093
332	6	0	-7.051977	7.207767	1.788164
333	1	0	-6.557922	8.030333	-0.142523
334	1	0	-7.816448	6.225560	3.549644
335	6	0	-13.299874	-3.157923	2.615686
336	6	0	-14.096166	-4.280818	2.387089
337	6	0	-13.475958	-2.364957	3.752424
338	6	0	-15.096616	-4.596393	3.304881
339	1	0	-13.920145	-4.899922	1.513758
340	6	0	-14.481632	-2.696212	4.655712
341	1	0	-12.822755	-1.517400	3.932318
342	6	0	-15.310774	-3.808975	4.444422

343	1	0	-15.718306	-5.471490	3.134591
344	1	0	-14.621617	-2.086262	5.544609
345	6	0	-16.418490	-4.138309	5.415484
346	1	0	-17.324909	-3.564454	5.181772
347	1	0	-16.684096	-5.199287	5.376471
348	1	0	-16.135431	-3.893781	6.444613
349	6	0	-5.996829	7.991223	2.530382
350	1	0	-6.296939	8.189560	3.564256
351	1	0	-5.051245	7.434339	2.564752
352	1	0	-5.791729	8.949559	2.042864

Table S3 Results of TD-DFT calculation of dyad **2** to estimate the absorption maxima and absorption strength calculated by TD-B3LYP/6-31G(d)// B3LYP/6-31G(d)

338: LUMO, 337: HOMO

Excited State 1: Singlet-A 0.8628 eV 1437.06 nm f=0.2392 <S**2>=0.000
337 -> 338 0.70733 (Charge-transfer ZnP-->PDI)

Excited State 2: Singlet-A 1.9149 eV 647.46 nm f=1.2651 <S**2>=0.000
333 -> 338 0.45258
335 -> 338 -0.14354
337 -> 339 0.50892 (Transition ZnP--> ZnP)

Excited State 3: Singlet-A 1.9475 eV 636.62 nm f=0.0030 <S**2>=0.000
334 -> 338 0.12334
335 -> 338 -0.16799
336 -> 338 0.66965

Excited State 4: Singlet-A 1.9816 eV 625.68 nm f=0.0423 <S**2>=0.000
333 -> 338 0.10403
334 -> 338 0.24608
335 -> 338 0.61680 (Charge-transfer ZnP-->PDI)
337 -> 340 0.17840
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 5: Singlet-A 2.0144 eV 615.50 nm f=0.2328 <S**2>=0.000 **A**
334 -> 338 0.29237
334 -> 339 -0.10084
335 -> 338 -0.24309
336 -> 338 -0.18306
337 -> 340 0.54342 (Transition ZnP--> ZnP)

Excited State 6: Singlet-A 2.0531 eV 603.88 nm f=0.1353 <S**2>=0.000 **B**
334 -> 338 0.57842 (Charge-transfer ZnP-->PDI)
337 -> 340 -0.36505

Excited State 7: Singlet-A 2.0980 eV 590.95 nm f=0.0321 <S**2>=0.000 **C**
331 -> 338 0.13133
333 -> 338 0.50179 PDI-->PDI
337 -> 339 -0.44968

Excited State 8: Singlet-A 2.3172 eV 535.06 nm f=0.0058 <S**2>=0.000
331 -> 338 -0.11769
337 -> 341 0.68851

Excited State 9: Singlet-A 2.4986 eV 496.22 nm f=0.0273 <S**2>=0.000 **D**
329 -> 338 0.10164
331 -> 338 0.32045
332 -> 338 0.60189

Excited State 10: Singlet-A 2.5053 eV 494.89 nm f=0.0636 <S**2>=0.000
328 -> 338 0.12276
329 -> 338 0.12757
331 -> 338 0.54538
332 -> 338 -0.35769
333 -> 338 -0.11137
337 -> 341 0.10130

Excited State 11: Singlet-A 2.5299 eV 490.08 nm f=0.0178 <S**2>=0.000
337 -> 342 0.69553

Excited State 12: Singlet-A 2.6476 eV 468.29 nm f=0.0410 <S**2>=0.000
328 -> 338 0.29044
329 -> 338 0.43410
330 -> 338 0.43332
331 -> 338 -0.13117

Excited State 13: Singlet-A 2.7139 eV 456.84 nm f=0.0038 <S**2>=0.000
328 -> 338 -0.17174
329 -> 338 -0.37184
330 -> 338 0.54518
331 -> 338 0.16744

Excited State 14: Singlet-A 2.7620 eV 448.89 nm f=0.0018 <S**2>=0.000
335 -> 340 -0.42699
336 -> 340 0.53656

Excited State 15: Singlet-A 2.7821 eV 445.65 nm f=0.0005 <S**2>=0.000
328 -> 338 0.42645
329 -> 338 -0.24999
334 -> 339 0.18033
335 -> 339 -0.24634
335 -> 340 0.18401
336 -> 339 -0.32371

Excited State 16: Singlet-A 2.7907 eV 444.28 nm f=0.0067 <S**2>=0.000
328 -> 338 0.41323
329 -> 338 -0.25581
334 -> 339 -0.21980
335 -> 339 0.20540
336 -> 339 0.36852
336 -> 340 -0.10659

Excited State 17: Singlet-A 2.8024 eV 442.43 nm f=0.0041 <S**2>=0.000
334 -> 340 0.16852
335 -> 340 0.47915
336 -> 339 0.18335
336 -> 340 0.42013

Excited State 18: Singlet-A 2.8712 eV 431.82 nm f=0.0199 <S**2>=0.000
327 -> 338 0.40834
335 -> 339 -0.38989
336 -> 339 0.37781

Excited State 19: Singlet-A 2.8785 eV 430.72 nm f=0.0001 <S**2>=0.000
327 -> 338 0.50256
334 -> 339 0.14923
335 -> 339 0.43157
336 -> 339 -0.12040

Excited State 20: Singlet-A 2.9203 eV 424.56 nm f=0.1821 <S**2>=0.000
327 -> 338 -0.20353
333 -> 339 -0.30935
334 -> 339 0.44408
334 -> 340 -0.25036
335 -> 339 0.18319
336 -> 339 0.17871

Excited State 21: Singlet-A 2.9392 eV 421.82 nm f=0.0367 <S**2>=0.000
326 -> 338 0.63413
334 -> 339 0.11942
334 -> 340 0.22999

Excited State 22: Singlet-A 2.9416 eV 421.48 nm f=0.1872 <S**2>=0.000
326 -> 338 -0.29203
327 -> 338 -0.11165
333 -> 340 -0.14303
334 -> 339 0.24298
334 -> 340 0.50382
335 -> 340 -0.13253
336 -> 339 0.10983

Excited State 23: Singlet-A 3.0057 eV 412.50 nm f=0.0846 <S**2>=0.000
333 -> 339 0.56260
333 -> 340 -0.16569
334 -> 339 0.23572

```
   334 -> 340       -0.21251

Excited State  24:      Singlet-A      3.0238 eV  410.03 nm  f=0.0012  <S**2>=0.000
   332 -> 339       -0.28145
   332 -> 340        0.63757

Excited State  25:      Singlet-A      3.0484 eV  406.71 nm  f=0.0005  <S**2>=0.000
   322 -> 338        0.68549
   322 -> 341        0.11445

Excited State  26:      Singlet-A      3.0501 eV  406.49 nm  f=0.0073  <S**2>=0.000
   332 -> 339        0.59648
   332 -> 340        0.26899
   332 -> 341       -0.10926
   333 -> 340        0.17118

Excited State  27:      Singlet-A      3.0549 eV  405.86 nm  f=0.0113  <S**2>=0.000
   332 -> 339       -0.12393
   333 -> 340        0.14000
   337 -> 343        0.65337

Excited State  28:      Singlet-A      3.0609 eV  405.05 nm  f=0.1781  <S**2>=0.000
   332 -> 339       -0.12296
   333 -> 339        0.15963
   333 -> 340        0.60348
   334 -> 339        0.14033
   337 -> 343       -0.16446

Excited State  29:      Singlet-A      3.1382 eV  395.08 nm  f=0.0030  <S**2>=0.000
   321 -> 338        0.12070
   337 -> 343       -0.12236
   337 -> 344        0.67251

Excited State  30:      Singlet-A      3.2070 eV  386.61 nm  f=0.0013  <S**2>=0.000
   317 -> 338       -0.25542
   321 -> 338        0.30527
   325 -> 338        0.50453
   333 -> 341        0.16825
   337 -> 344       -0.11623
SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 LETran=     550.
```