Supporting Information

Why Does *para*-amino group make green fluorescent protein chromophore non-fluorescent: coherent intramolecular charge transfer reduces *Z*/*E*-photoisomerization barrier

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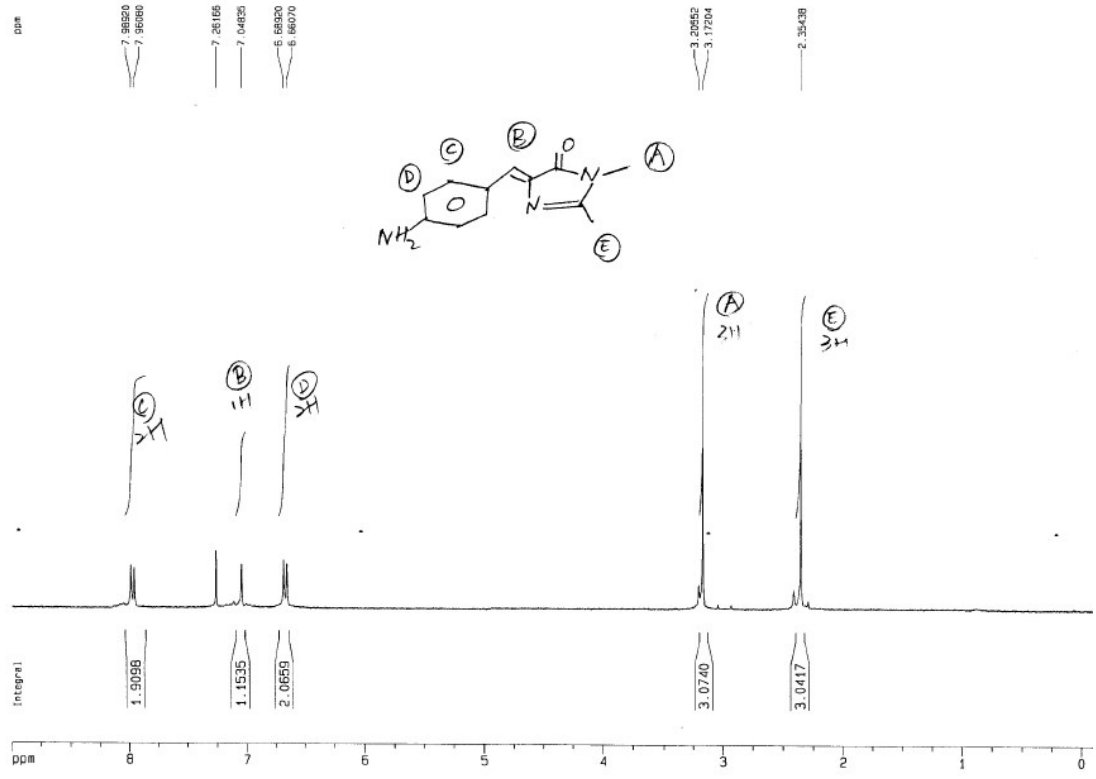

Figure S1. ^{1}H-NMR spectrum of *p*-ABDI

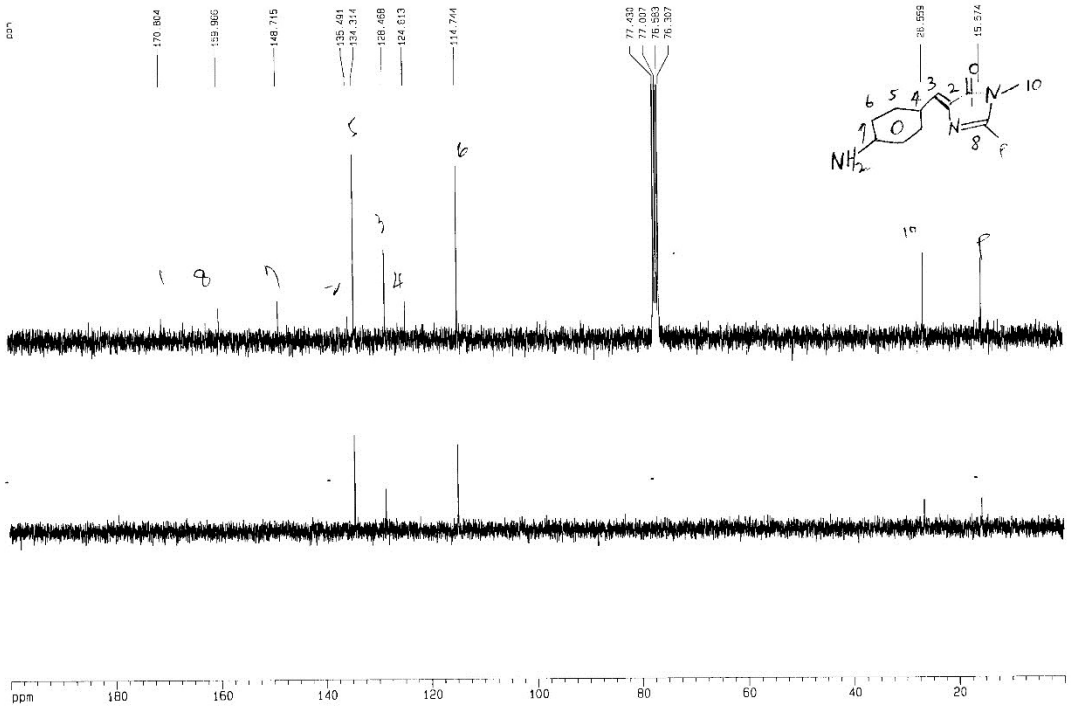

Figure S2. ^{13}C-NMR spectrum of *p*-ABDI

Compound: ground-state *Z*-*p*-AbDI

Method/basis set: CASSCF(8, 8)/6-31G*

Energy of the optimized structure: -622.2345011 Hartree

Cartesian coordinate of the optimized structure:

6	-3.517915	-0.156421	-0.015386
6	-2.575097	-1.192196	-0.020873
6	-1.215758	-0.919220	-0.017080
6	-0.752507	0.406308	-0.008844
6	-1.707356	1.428787	-0.007373
6	-3.057480	1.159887	-0.010795
1	-2.911926	-2.214425	-0.034396
1	-1.381902	2.454406	-0.002590
1	-3.764691	1.971315	-0.015775
6	0.661772	0.784651	-0.001920
1	0.855170	1.844018	0.000287
6	1.762154	0.035916	0.002158
7	1.869350	-1.379452	0.000704
6	3.127969	0.627983	0.008540
7	3.938803	-0.482522	0.009383
6	3.142609	-1.618015	0.004499
8	3.476867	1.770716	0.012236
1	-0.513322	-1.727929	-0.019874
7	-4.883223	-0.437712	-0.069558
1	-5.469074	0.280076	0.299464
1	-5.137069	-1.328280	0.300595
1	4.932007	-0.448965	0.012140
1	3.576214	-2.597616	0.004358

Compound: ground-state *E*-*p*-AbDI

Method/basis set: CASSCF(8, 8)/6-31G*

Energy of the optimized structure: -622.202649 Hartree

Cartesian coordinate of the optimized structure:

6	2.63568	0.43433	-0.06239
6	1.56598	1.34394	-0.07397
6	0.25533	0.90545	-0.05706
6	-0.03908	-0.4713	-0.03031
6	1.02806	-1.36018	-0.02444
6	2.34884	-0.92855	-0.03917
1	1.7711	2.40011	-0.10209
1	0.83566	-2.41859	-0.0064
1	3.1492	-1.64769	-0.03948
6	-1.37973	-1.0551	-0.01026
1	-1.3753	-2.13175	-0.00575
6	-2.62319	-0.56165	0.00443
7	-3.72471	-1.46535	0.02178
6	-3.16767	0.82785	0.00933
7	-4.52177	0.61945	0.02831
6	-4.77643	-0.74693	0.03465
8	-2.63411	1.90103	0.00051
1	-5.77977	-1.12247	0.04899
1	-5.18847	1.35645	0.03525
7	3.95086	0.89098	-0.12833
1	4.08971	1.81244	0.2265
1	-0.5397	1.62118	-0.0634
1	4.63068	0.26	0.23769

Compound: ES1 (The first S_1 excited-state minimum of *p*-AbDI)

Method/basis set: CASSCF(8, 8)/6-31G*

Energy of the optimized structure: -622.0563606 Hartree

Cartesian coordinate of the optimized structure:

6	-3.382176	-0.190232	0.013711
6	-2.386733	0.524360	0.791559
6	-1.083632	0.295863	0.656306
6	-0.583184	-0.733207	-0.297510
6	-1.595731	-1.494545	-1.022990
6	-2.929696	-1.247631	-0.871511
1	-2.730246	1.265825	1.493615
1	-1.266877	-2.269317	-1.692083
1	-3.656909	-1.828663	-1.410449
6	0.759342	-1.012419	-0.524568
1	0.994338	-1.782182	-1.236821
6	1.942971	-0.408470	0.066248
7	2.011801	0.554992	0.972838
6	3.310332	-0.852452	-0.322304
7	4.114112	-0.052604	0.446291
6	3.331595	0.782138	1.213083
8	3.647891	-1.691792	-1.104697
1	-0.368592	0.844765	1.233076
7	-4.740171	-0.019565	0.275609
1	-5.339054	-0.270817	-0.483063
1	-4.980728	0.886780	0.619130
1	3.713750	1.499352	1.902215
1	5.107278	-0.090649	0.429805

Compound: ES2 (The second S_1 excited-state minimum of *p*-AbDI)

Method/basis set: CASSCF(8, 8)/6-31G*

Energy of the optimized structure: -622.087084 Hartree

Cartesian coordinate of the optimized structure:

6	-1.585200	-2.401787	-3.242379
6	-0.441171	-1.578167	-3.475818
6	0.278751	-1.100793	-2.423493
6	-0.098459	-1.408528	-1.073098
6	-1.246568	-2.233965	-0.874737
6	-1.971453	-2.715422	-1.917121
1	-0.160305	-1.354553	-4.488776
1	-1.536347	-2.476455	0.131236
1	-2.832892	-3.337136	-1.754811
6	0.628901	-0.945224	0.005411
1	0.249841	-1.266858	0.971596
6	1.813727	-0.114324	-0.072752
7	1.755872	1.280872	0.009294
6	3.134282	-0.589802	-0.059568
7	3.861547	0.597667	-0.016950
6	2.988820	1.661869	0.037089
8	3.626474	-1.716764	-0.093118
1	1.146557	-0.490048	-2.569504
7	-2.281507	-2.870044	-4.275653
1	-3.073006	-3.457626	-4.143709
1	-2.013805	-2.670194	-5.212400
1	4.852751	0.626430	0.028919
1	3.321749	2.678616	0.084860

Compound: The conical intersection CI of *p*-AbDI
Method/basis set: CASSCF(8,8)/6-31G*
Energy of the optimized structure: -622.076625 Hartree

Cartesian coordinate of the optimized structure:

6	-1.585667	-2.511249	-3.271155
6	-0.447799	-1.699777	-3.636210
6	0.313125	-1.162598	-2.660496
6	-0.011726	-1.383325	-1.273092
6	-1.146329	-2.189620	-0.948359
6	-1.926739	-2.742266	-1.903696
1	-0.229600	-1.562843	-4.678675
1	-1.373360	-2.354956	0.088209
1	-2.778221	-3.352379	-1.670319
6	0.782671	-0.867815	-0.291404
1	0.437952	-1.143667	0.709996
6	1.968025	-0.057336	-0.510217
7	1.841860	1.332511	-0.157843
6	3.172916	-0.561255	-0.082509
7	3.895592	0.602939	0.213854
6	3.020532	1.669855	0.220903
8	3.635468	-1.717162	0.040456
1	1.186116	-0.568011	-2.837279
7	-2.305875	-3.042154	-4.214613
1	-3.095411	-3.615983	-4.009275
1	-2.086239	-2.901446	-5.177310
1	4.808974	0.579256	0.601488
1	3.336774	2.668490	0.452987

Compound: ground-state *Z*-*p*-ABDI

Method/basis set: CASSCF(8, 8)/6-31G*

Energy of the optimized structure: -700.2855465 Hartree

Cartesian coordinate of the optimized structure:

6	-3.513402	-0.154953	-0.014123
6	-2.555211	-1.192825	-0.018675
6	-1.210636	-0.911082	-0.013263
6	-0.749841	0.426285	-0.006336
6	-1.701089	1.425449	-0.005950
6	-3.068982	1.149034	-0.007628
1	-2.889044	-2.216110	-0.034710
1	-1.387039	2.454916	-0.000993
1	-3.776822	1.959759	-0.009837
6	0.666408	0.807278	0.000072
1	0.861165	1.865802	0.002226
6	1.776702	0.043258	0.003486
7	1.884406	-1.362820	0.001488
6	3.150640	0.618127	0.008896
7	3.956998	-0.492304	0.008634
6	3.137198	-1.626923	0.004178
8	3.508261	1.759718	0.012850
1	-0.501019	-1.713895	-0.015766
7	-4.867162	-0.467722	-0.067376
1	-5.477380	0.255073	0.247570
1	-5.111243	-1.348166	0.331645
6	5.400290	-0.445105	0.012037
1	5.811346	-0.921365	-0.870464
1	5.687628	0.594968	0.014721
1	5.807360	-0.924830	0.894526
6	3.718579	-3.002241	0.002821
1	4.339016	-3.161995	-0.873206
1	4.334989	-3.165559	0.881047
1	2.913301	-3.722638	-0.000611

Compound: ES1 (The first S_1 excited-state minimum of *p*-ABDI)

Method/basis set: CASSCF(8, 8)/6-31G*

Energy of the optimized structure: -700.1268941916 Hartree

Cartesian coordinate of the optimized structure:

6	-3.366418	-0.211173	0.039421
6	-2.384674	0.519080	0.805190
6	-1.076461	0.295431	0.661053
6	-0.582500	-0.723249	-0.286679
6	-1.608463	-1.488816	-1.019585
6	-2.909386	-1.248843	-0.859786
1	-2.732008	1.260272	1.505285
1	-1.278754	-2.258253	-1.694801
1	-3.642684	-1.824557	-1.398414
6	0.755393	-1.001194	-0.516146
1	0.979764	-1.771721	-1.232131
6	1.958407	-0.409266	0.064103
7	2.030994	0.557438	0.977426
6	3.297189	-0.840967	-0.314978
7	4.120926	-0.044260	0.453346
6	3.339786	0.784768	1.219221
8	3.653439	-1.690806	-1.109232
1	-0.360180	0.850206	1.231388
7	-4.720930	-0.012552	0.251567
1	-5.313483	-0.272458	-0.508198
1	-4.967616	0.885173	0.610716
6	3.864321	1.792700	2.180768
1	3.027901	2.299625	2.642278
1	4.460837	1.332893	2.964661
1	4.486648	2.536326	1.689317
6	5.563247	-0.105412	0.426225
1	5.986952	0.842717	0.116448
1	5.959737	-0.367714	1.400086
1	5.846518	-0.865847	-0.284814

Compound: ES2 (The second S_1 excited-state minimum of *p*-ABDI)

Method/basis set: CASSCF(8, 8)/6-31G*

Energy of the optimized structure: -700.1612273719 Hartree

Cartesian coordinate of the optimized structure:

6	-1.583411	-2.403692	-3.241696
6	-0.437195	-1.584550	-3.478670
6	0.283840	-1.104117	-2.428240
6	-0.094527	-1.404249	-1.076958
6	-1.244486	-2.225329	-0.874783
6	-1.970570	-2.709889	-1.915304
1	-0.155469	-1.366374	-4.492596
1	-1.535154	-2.462209	0.132287
1	-2.833761	-3.328433	-1.750101
6	0.634109	-0.936612	-0.000390
1	0.252505	-1.252847	0.967018
6	1.819271	-0.107687	-0.081621
7	1.764989	1.288048	0.000175
6	3.136131	-0.578426	-0.051274
7	3.876127	0.605962	0.003397
6	2.997156	1.673983	0.040946
8	3.631020	-1.706889	-0.078975
1	1.153535	-0.496460	-2.576040
7	-2.281126	-2.874912	-4.273200
1	-3.074326	-3.459519	-4.138597
1	-2.012768	-2.680118	-5.210777
6	3.451883	3.095961	0.110582
1	4.046302	3.287890	1.000592
1	4.058537	3.372001	-0.749027
1	2.581319	3.738111	0.135647
6	5.311430	0.639506	0.045338
1	5.726643	1.182035	-0.799604
1	5.677173	1.098880	0.959335
1	5.653647	-0.383644	0.007478

Compound: The conical intersection CI of *p*-ABDI
Method/basis set: CASSCF(8,8)/6-31G*
Energy of the optimized structure: -700.150718998 Hartree

Cartesian coordinate of the optimized structure:

6	-1.552532	-2.491833	-3.291652
6	-0.399665	-1.729316	-3.614466
6	0.335273	-1.207276	-2.601303
6	-0.029822	-1.396703	-1.231548
6	-1.207951	-2.175972	-0.925878
6	-1.957348	-2.706636	-1.910630
1	-0.127203	-1.598695	-4.644300
1	-1.476873	-2.325426	0.102705
1	-2.836777	-3.292250	-1.719420
6	0.781448	-0.867772	-0.271764
1	0.439236	-1.107382	0.739914
6	1.976652	-0.076341	-0.521024
7	1.847441	1.321382	-0.181797
6	3.169203	-0.567050	-0.043668
7	3.887809	0.595406	0.280827
6	3.013815	1.669012	0.225033
8	3.633300	-1.719612	0.099575
1	1.232223	-0.636249	-2.743521
7	-2.275337	-3.024202	-4.233531
1	-3.084427	-3.569960	-4.029845
1	-2.035810	-2.910312	-5.195262
6	3.437650	3.069514	0.543814
1	3.853319	3.151621	1.545662
1	4.192433	3.438400	-0.148033
1	2.573246	3.718375	0.478232
6	5.247975	0.581910	0.727751
1	5.890438	1.195174	0.099291
1	5.348708	0.932435	1.753280
1	5.582281	-0.443978	0.679856

Compound: ground-state *Z*-*p*-AAbDI

Method/basis set: CASSCF(8, 8)/6-31G*

Energy of the optimized structure: -734.9568018 Hartree

Cartesian coordinate of the optimized structure:

6	2.53969	-0.11386	-1.46095
6	1.53615	-1.09932	-1.5166
6	0.25909	-0.82678	-1.11717
6	-0.08222	0.45516	-0.63796
6	0.91217	1.41204	-0.58884
6	2.22444	1.15056	-0.99356
1	1.77922	-2.08335	-1.87981
1	0.68067	2.39853	-0.22777
1	2.96955	1.91493	-0.94219
6	-1.4256	0.82936	-0.19086
1	-1.53118	1.84563	0.14853
6	-2.54889	0.11835	-0.13266
7	-2.75861	-1.23677	-0.49856
6	-3.83099	0.69342	0.36148
7	-4.70052	-0.36594	0.24804
6	-4.01232	-1.45778	-0.25772
8	-4.08355	1.79003	0.76092
1	-4.50579	-2.39379	-0.42507
1	-5.66214	-0.32845	0.49626
7	3.82419	-0.4894	-1.8939
1	3.9144	-1.43021	-2.20557
6	4.95908	0.25459	-1.94576
1	5.79574	-0.32775	-2.33194
8	5.08208	1.39575	-1.62548
1	-0.48988	-1.59086	-1.16756

Compound: ES (The second S_1 excited-state minimum of *p*-AAbDI)
Method/basis set: CASSCF(8, 8)/6-31G*
Energy of the optimized structure: -734.7447974041 Hartree
Cartesian coordinate of the optimized structure:

6	2.68958	-0.40951	0.00169
6	1.65089	-1.37043	0.00477
6	0.35068	-0.99469	0.00262
6	-0.0088	0.42217	-0.00289
6	1.09458	1.37515	-0.00583
6	2.3837	0.99098	-0.00371
1	1.90818	-2.41525	0.00876
1	0.85542	2.42299	-0.0099
1	3.17877	1.70393	-0.00591
6	-1.29671	0.85539	-0.00538
1	-1.47858	1.91589	-0.00828
6	-2.5463	0.05943	-0.00312
7	-2.65856	-1.30336	-0.01657
6	-3.83561	0.67784	0.01141
7	-4.6814	-0.42716	0.00501
6	-3.92705	-1.55714	-0.01118
8	-4.1797	1.8482	0.02433
1	-4.35745	-2.53714	-0.0181
1	-5.67314	-0.36535	0.01165
7	3.97719	-0.88644	0.00397
1	4.06505	-1.87949	0.00764
6	5.17217	-0.20403	0.00194
1	6.01353	-0.89358	0.00473
8	5.31151	0.97455	-0.00237
1	-0.44016	-1.71671	0.00422

Compound: The conical intersection CI of *p*-AAbDI
Method/basis set: CASSCF(8,8)/6-31G*
Energy of the optimized structure: -734.7940202 Hartree

Cartesian coordinate of the optimized structure:

6	-2.367557	0.618350	1.626607
6	-1.355253	-0.150630	2.228090
6	-0.092222	-0.142941	1.705968
6	0.197513	0.647511	0.575611
6	-0.833429	1.406754	-0.015999
6	-2.104358	1.406752	0.490782
1	-1.584423	-0.745581	3.093124
1	-0.613469	2.003895	-0.882392
1	-2.882546	1.984934	0.044569
6	1.518144	0.708911	0.093021
1	1.621163	1.388452	-0.755678
6	2.605442	-0.095724	0.549338
7	2.585257	-0.858866	-0.710881
6	3.925461	0.444918	0.693144
7	4.680111	-0.351207	-0.189788
6	3.825340	-0.997531	-1.038441
8	4.406027	1.317238	1.388605
1	4.178569	-1.643554	-1.819190
1	5.665470	-0.272789	-0.289838
7	-3.612110	0.552141	2.206513
1	-3.682942	-0.035226	3.008681
6	-4.784112	1.182764	1.840166
1	-5.596200	0.917407	2.512689
8	-4.925907	1.920103	0.924765
1	0.714756	-0.717939	2.114531