

Study of two benzophenone-based difluoroboron compounds containing triphenylamine units mechanofluorochromic behaviors and latent fingerprints imaging

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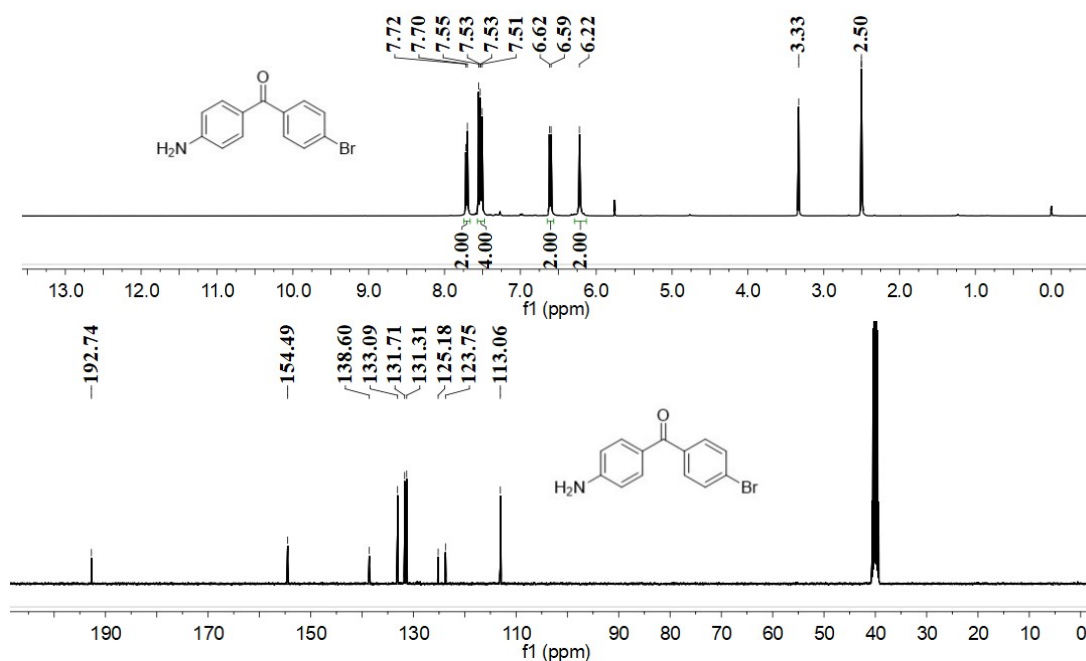


Figure S1 ¹H NMR and ¹³C NMR spectra of Br-BP-NH₂ in DMSO-*d*₆.

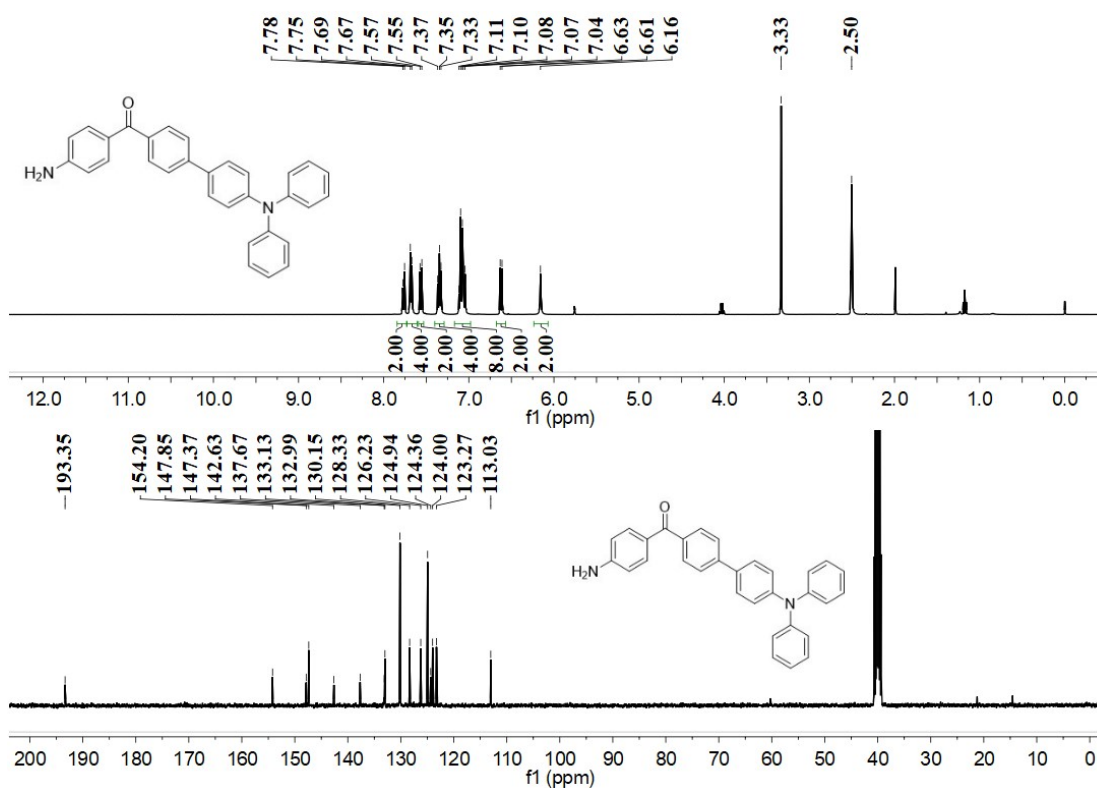


Figure S2 ¹H NMR and ¹³C NMR spectra of TPA-BP-NH₂ in DMSO-*d*₆.

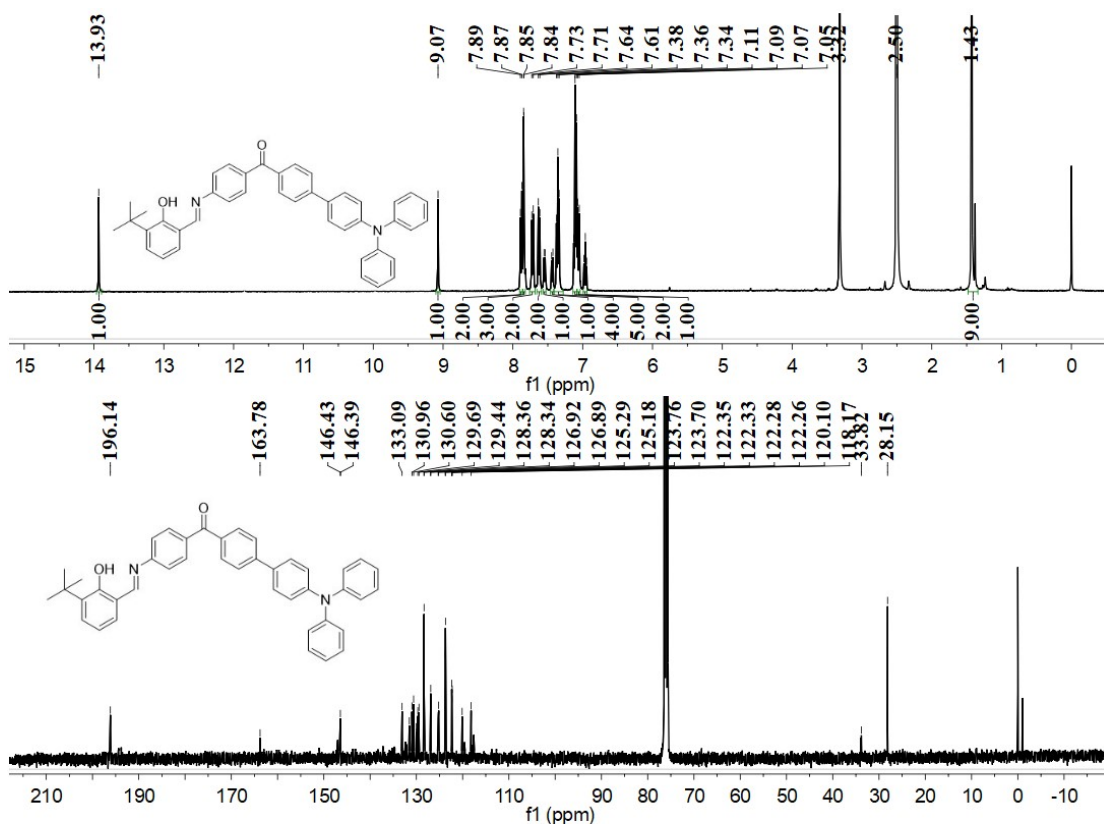


Figure S3 ¹H NMR (DMSO-*d*₆) and ¹³C NMR (CCl₃) spectra of TPA-BP-1.

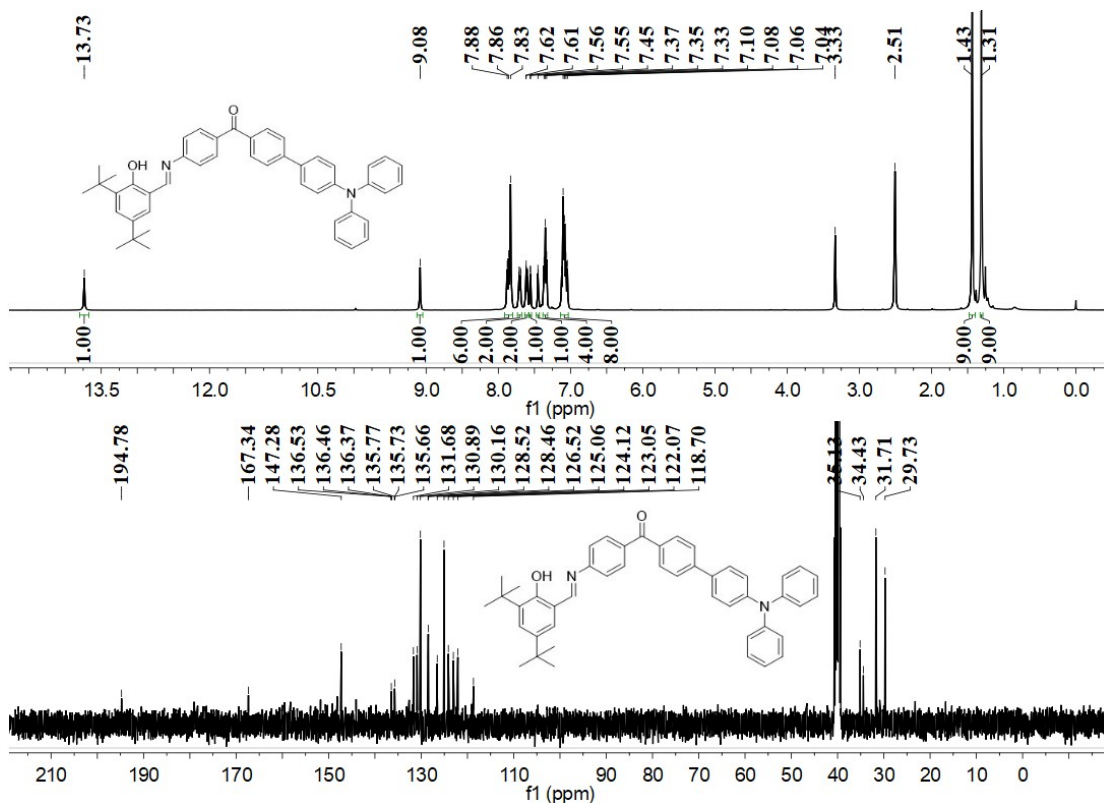


Figure S4 ¹H NMR and ¹³C NMR spectra of TPA-BP-2 in DMSO-*d*₆.

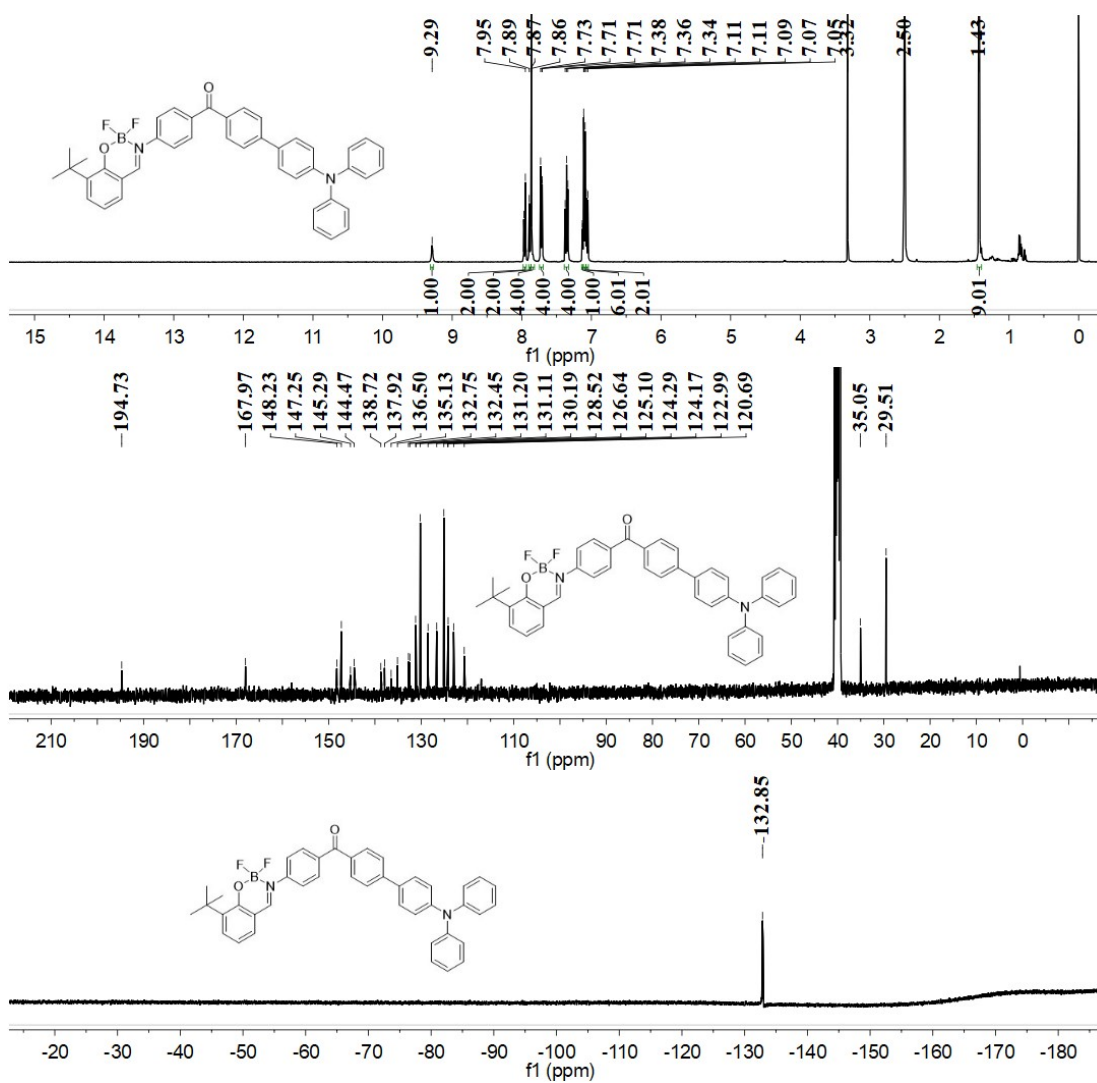


Figure S5 ¹H NMR, ¹³C NMR, and ¹⁹F NMR spectra of TPA-BP-BF₂-1 in DMSO-*d*₆.

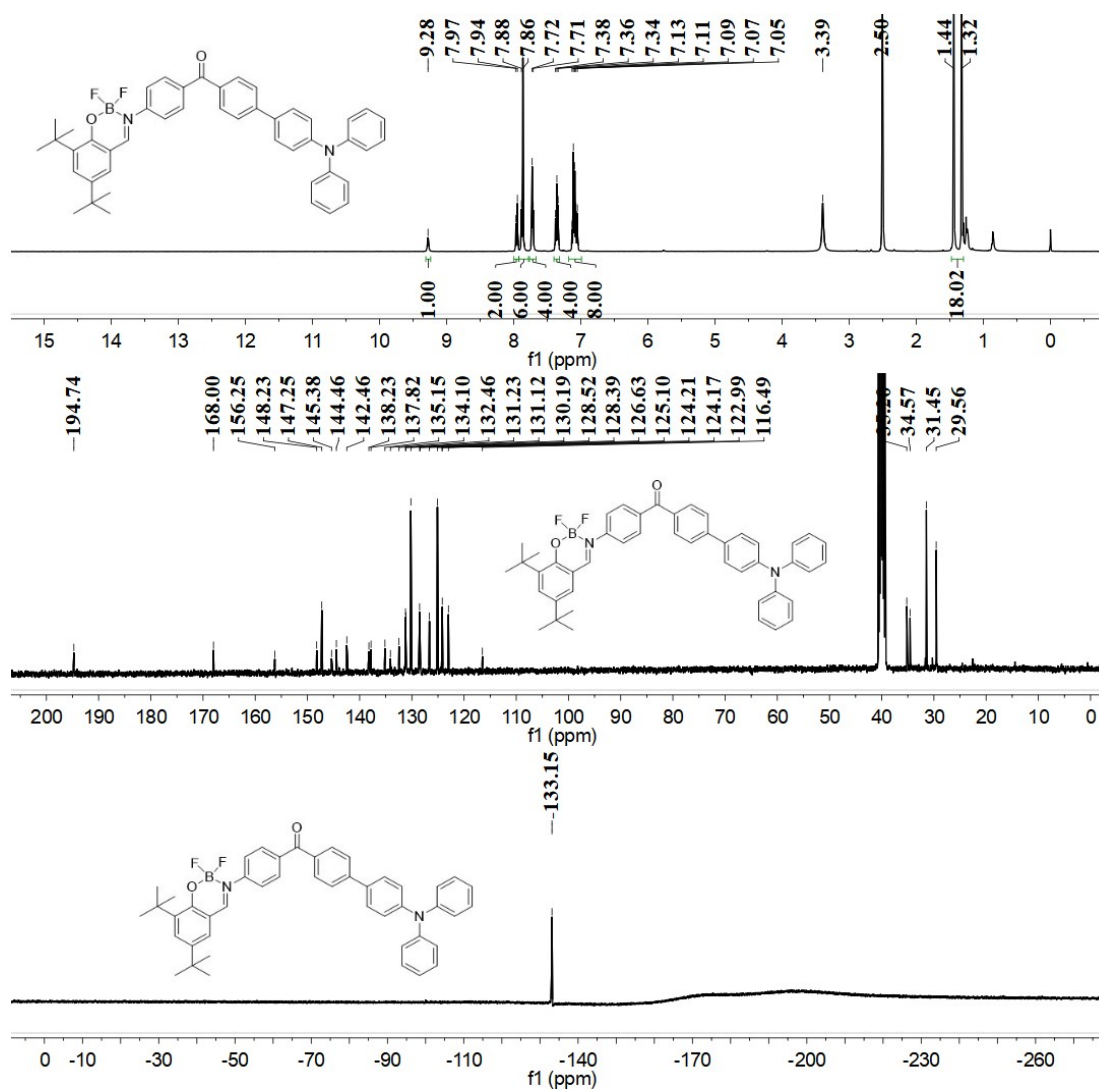


Figure S6 ¹H NMR, ¹³C NMR, and ¹⁹F NMR spectra of TPA-BP-BF₂-2 in DMSO-*d*₆.

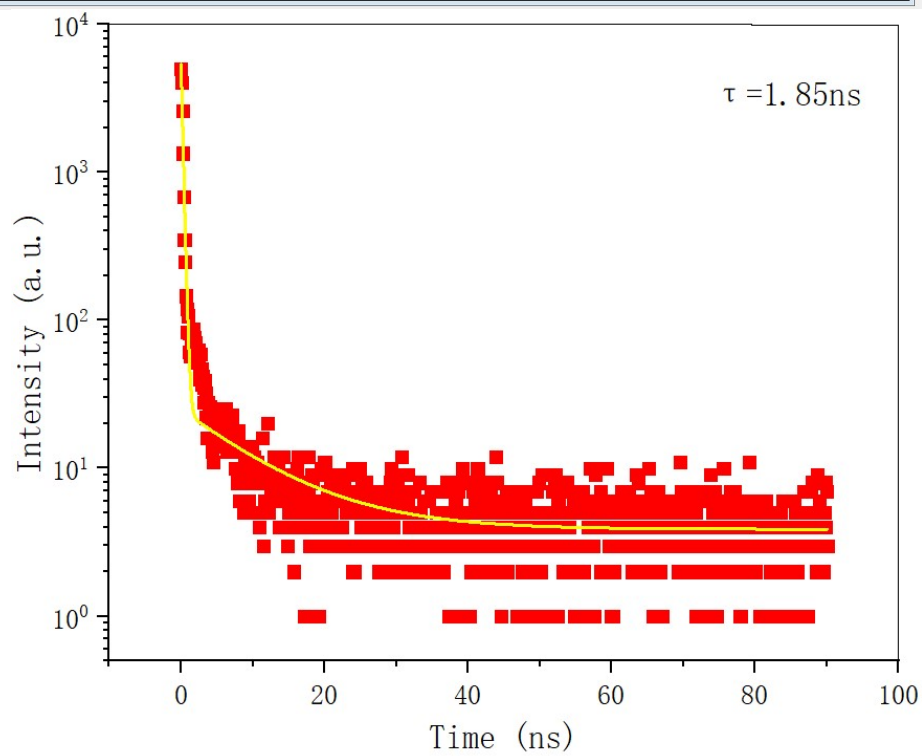
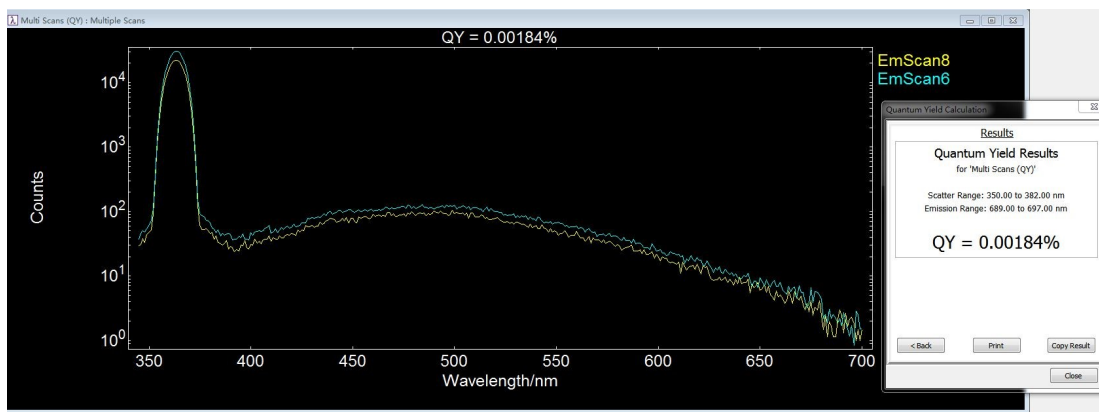


Figure S9 The Φ_f and τ of compound **TPA-BP-BF₂-1** in THF/water mixture of $f_w = 0\%$.

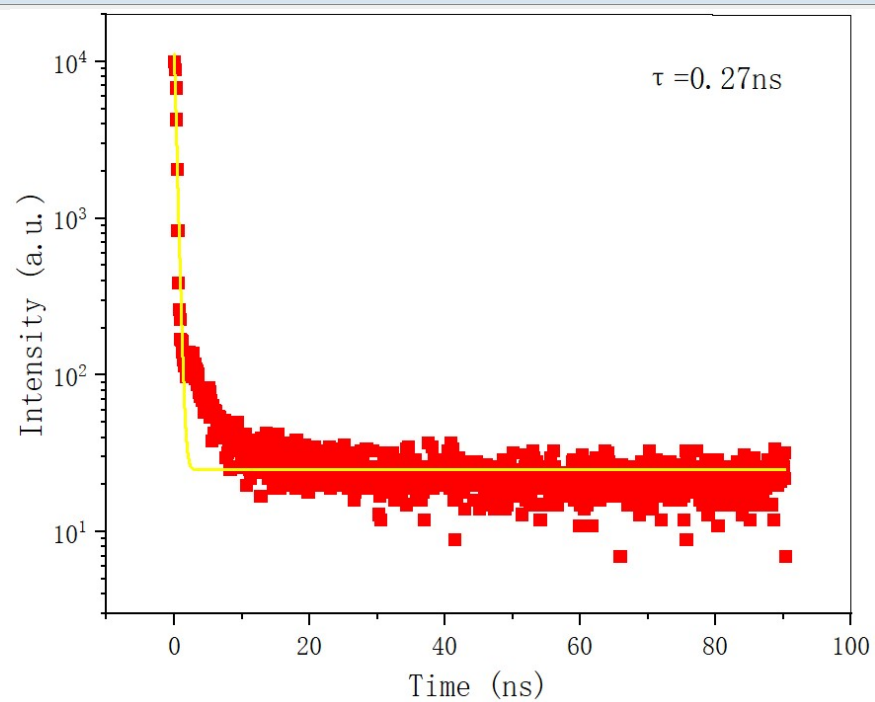
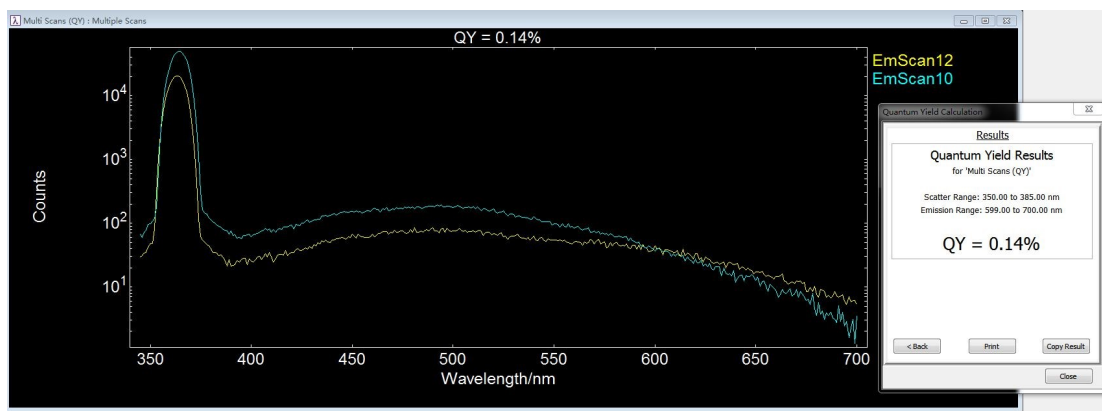


Figure S10 The Φ_f and τ of compound **TPA-BP-BF₂-1** in THF/water mixture of $f_w = 80\%$.

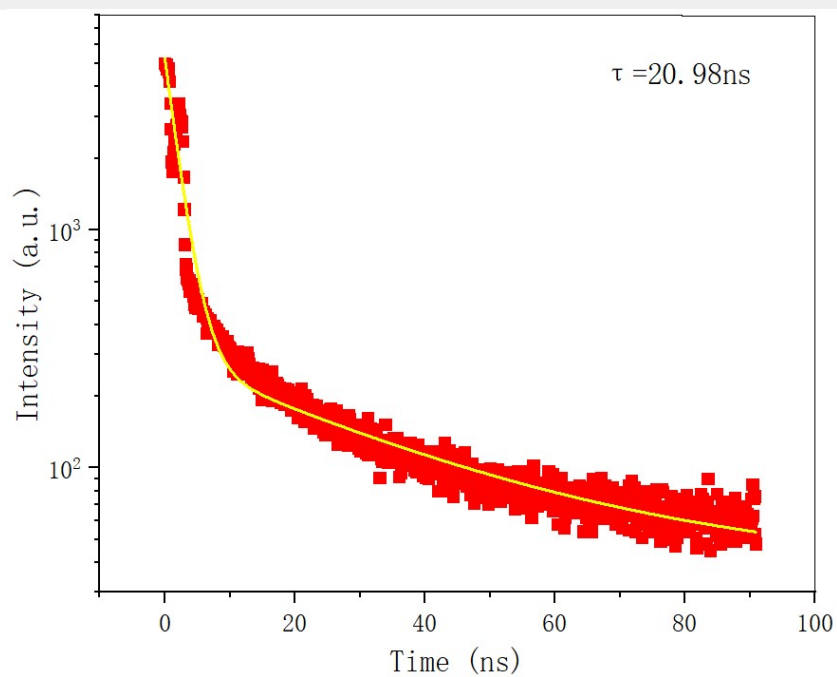
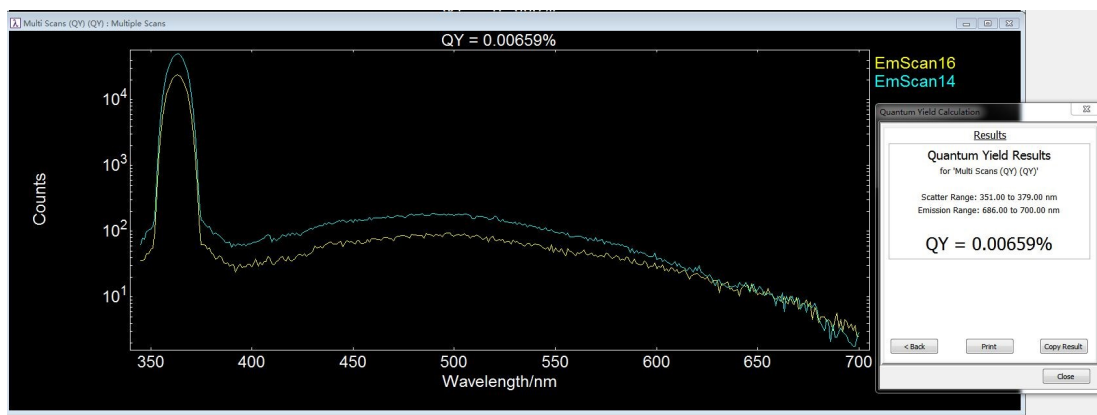


Figure S11 The Φ_f and τ of compound **TPA-BP-BF₂-1** in THF/water mixture of $f_w = 100\%$.

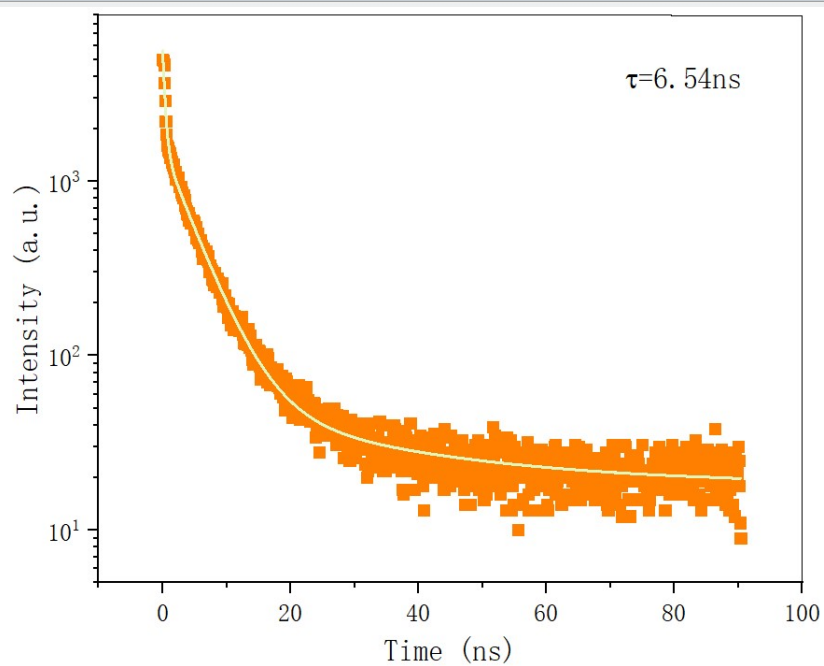
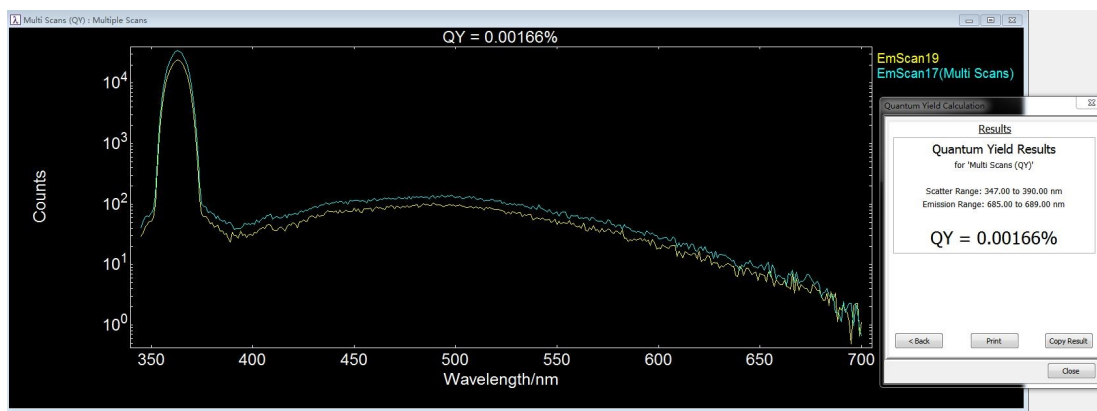


Figure S12 The Φ_f and τ of compound **TPA-BP-BF₂-2** in THF/water mixture of $f_w = 0\%$.

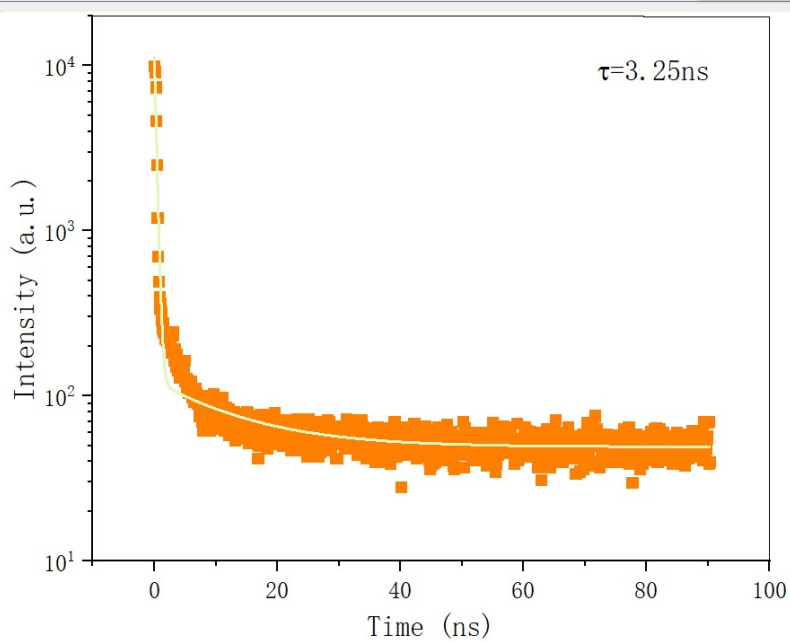
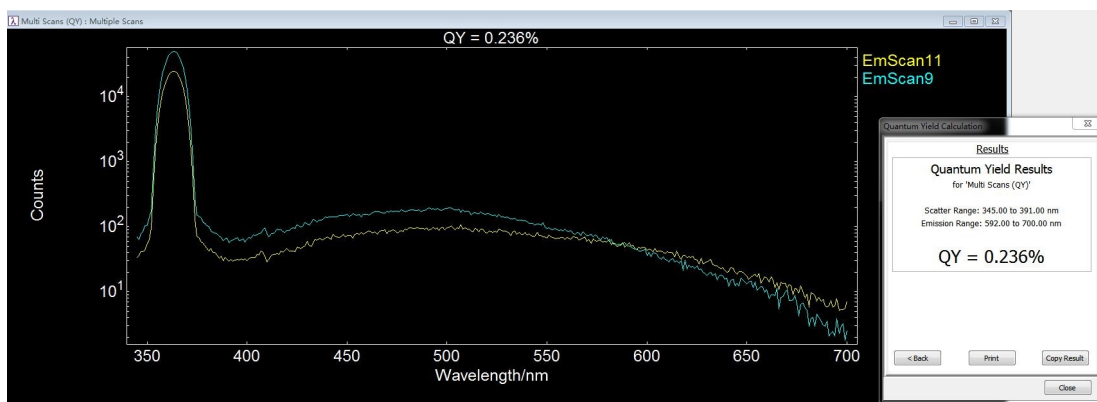


Figure S13 The Φ_f and τ of compound **TPA-BP-BF₂-2** in THF/water mixture of $f_w = 80\%$.

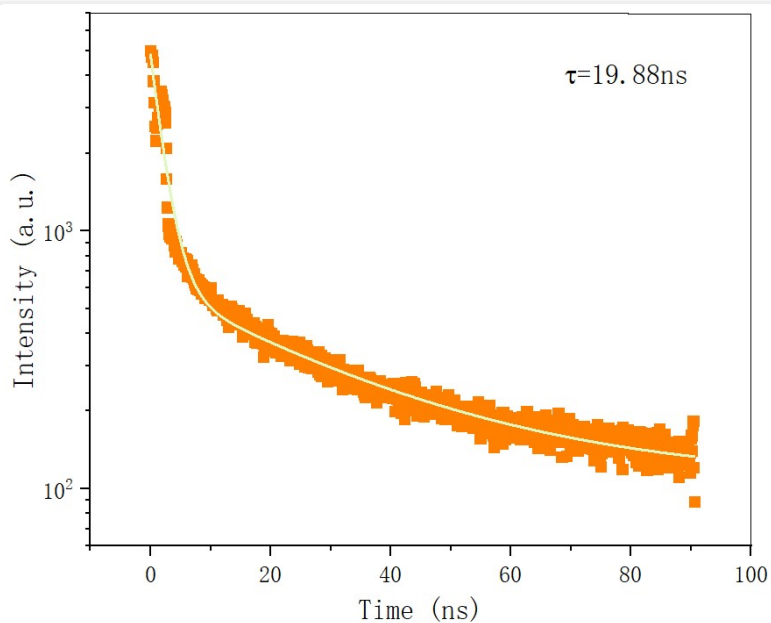
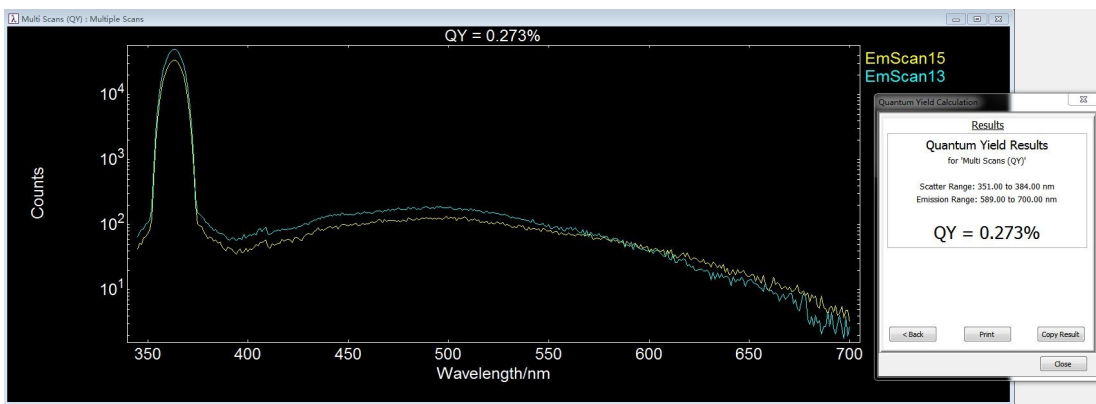


Figure S14 The Φ_f and τ of compound **TPA-BP-BF₂-2** in THF/water mixture of $f_w = 100\%$.

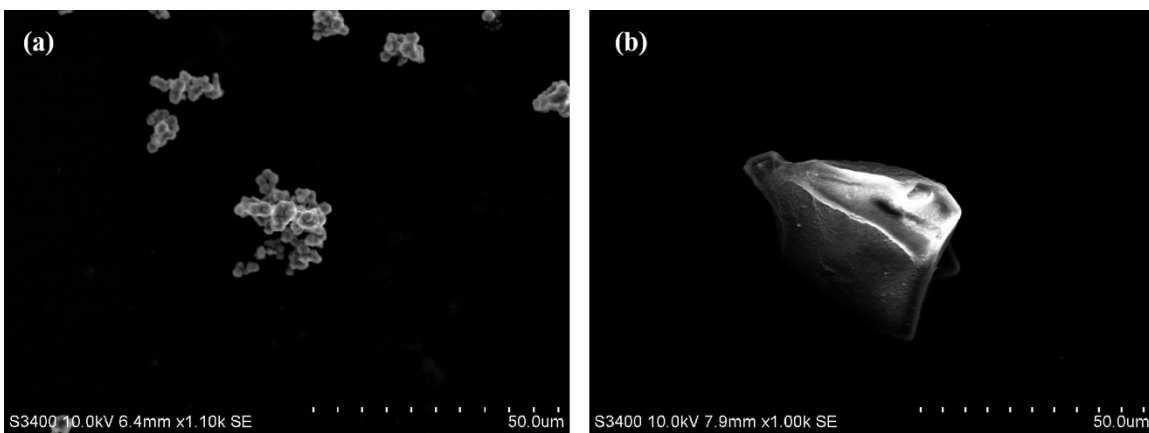


Figure S15 SEM images of compounds (a) **TPA-BP-BF₂-1** and (b) **TPA-BP-BF₂-2** in pure water ($c = 1 \times 10^{-5}$ mol/L), respectively.

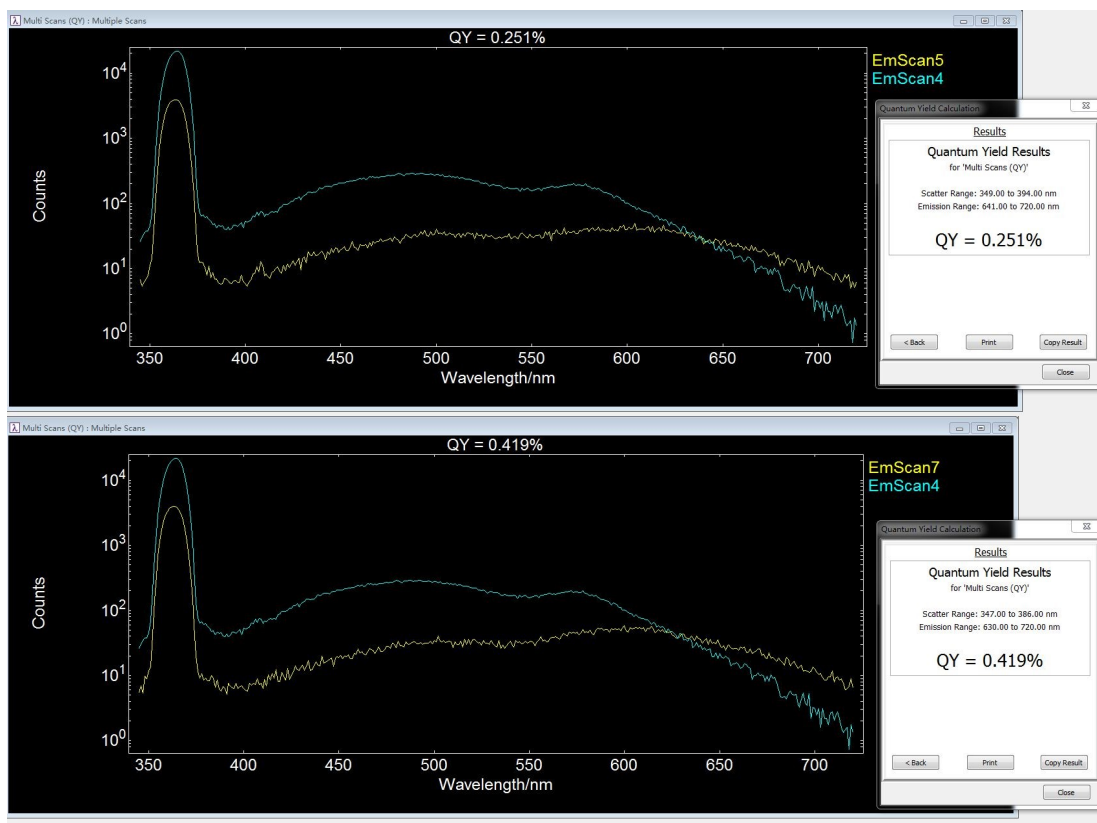


Figure S16 The Φ_f of solid of compound TPA-BP-BF₂-1 before (up) and after grinding (down).

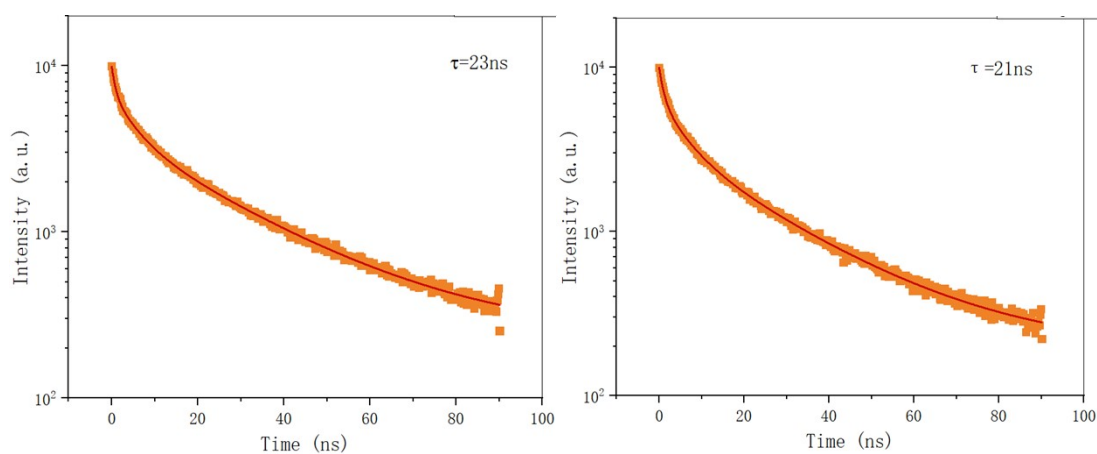


Figure S17 The τ of solid of compound TPA-BP-BF₂-1 before (left) and after grinding (right).

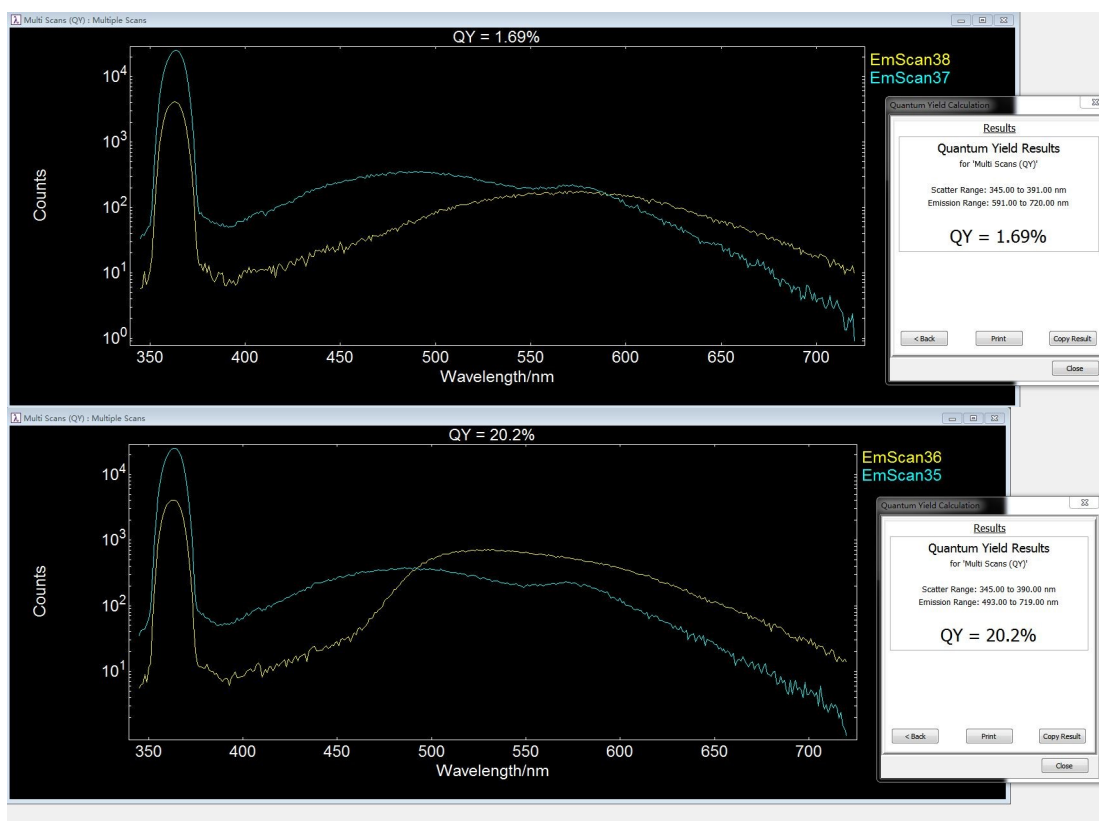


Figure S18 The Φ_f of solid of compound TPA-BP-BF₂-2 before (up) and after grinding (down).

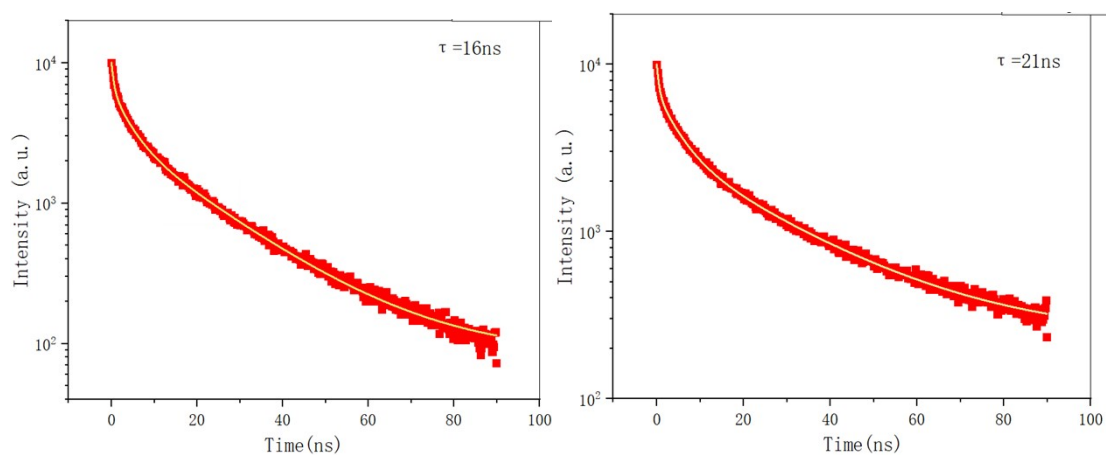


Figure S19 The τ of solid of compound TPA-BP-BF₂-2 before (left) and after grinding (right).

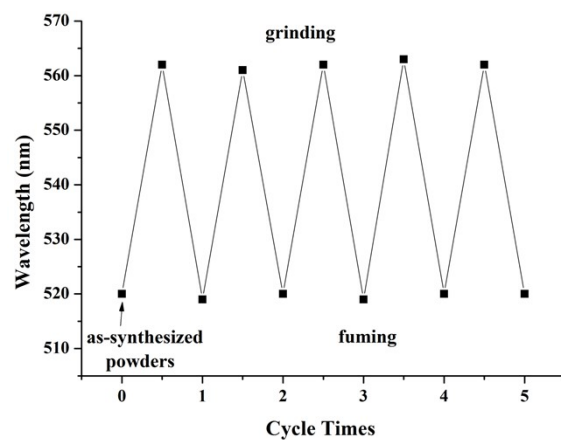


Figure S20 The emission wavelength of **TPA-BP-BF₂-2** upon treated by grinding and fuming with CH₂Cl₂ repeatedly.

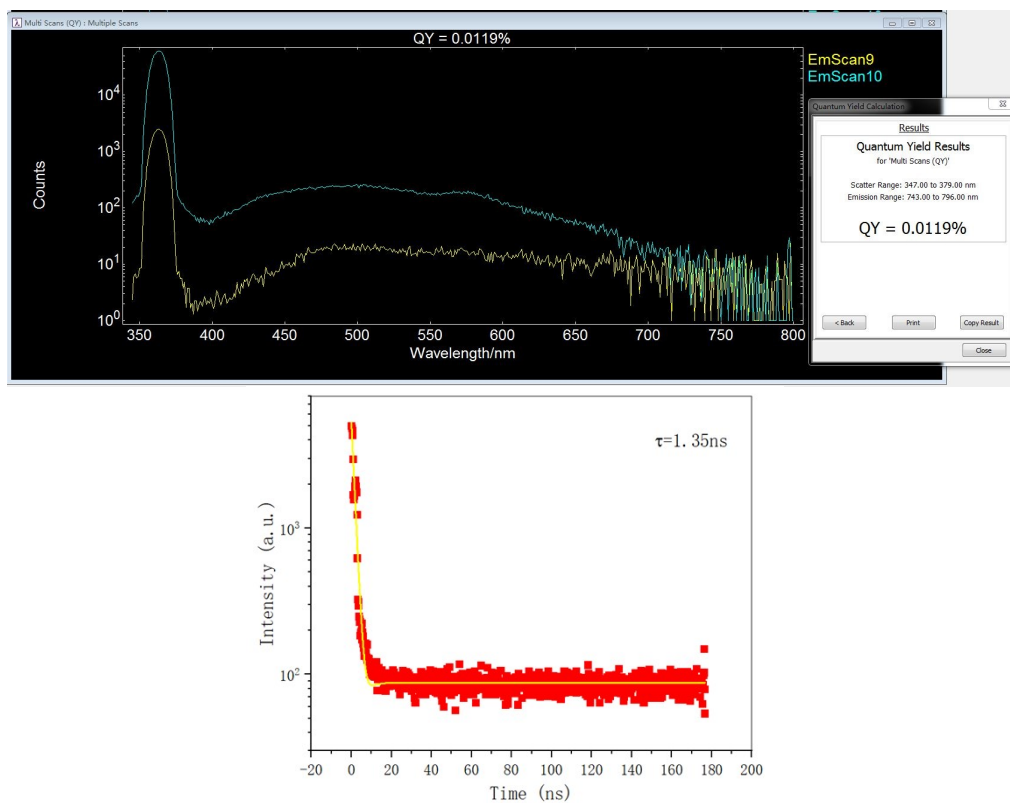


Figure S21 The Φ_f (up) and τ (down) of the developer with compound TPA-BP-BF₂-1.

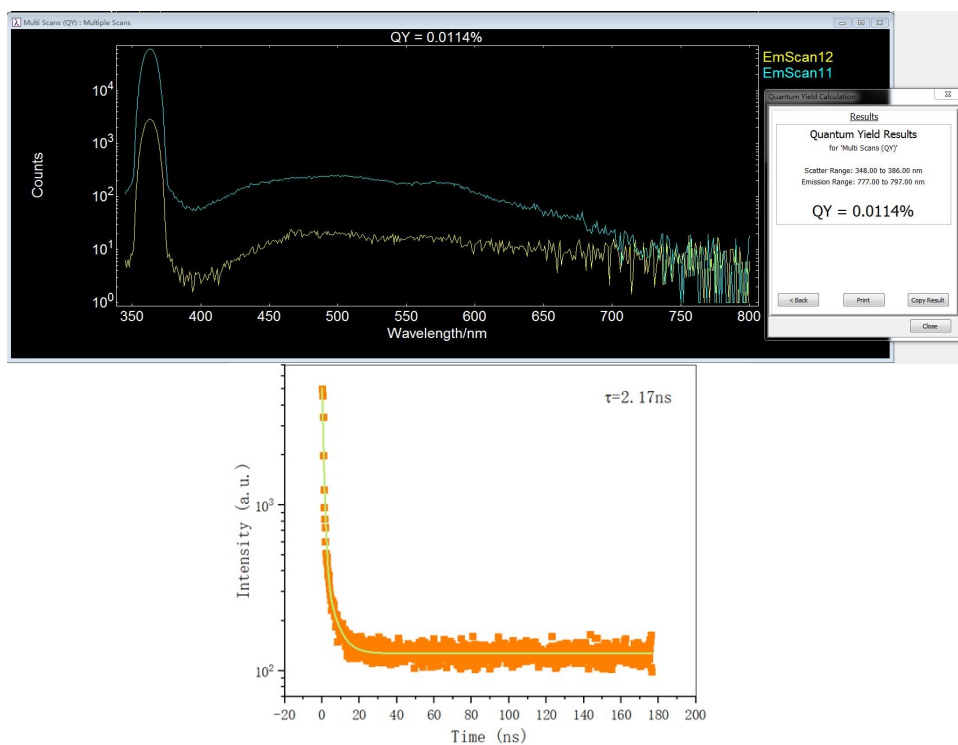


Figure S22 The Φ_f (up) and τ (down) of the developer with compound TPA-BP-BF₂-2.

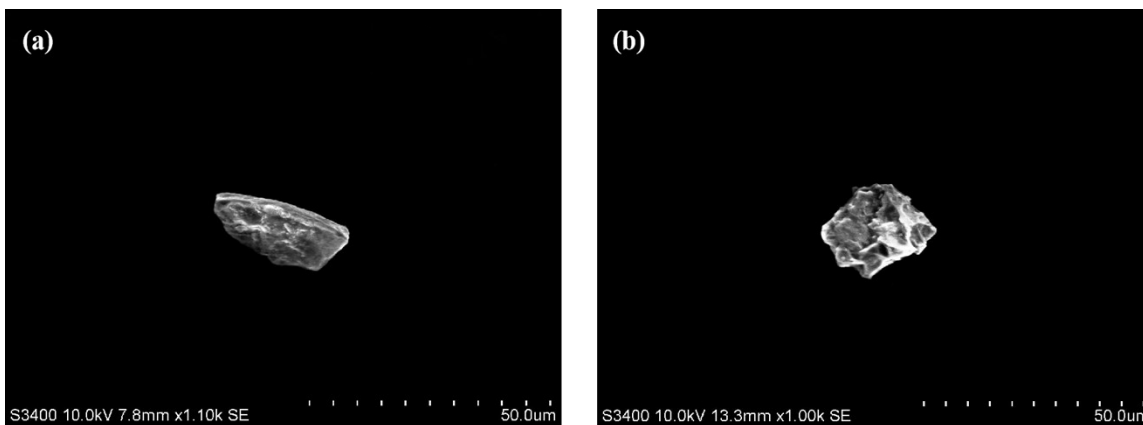


Figure S23 SEM images of developers with (a) **TPA-BP-BF₂-1** and (b) **TPA-BP-BF₂-2**, respectively.

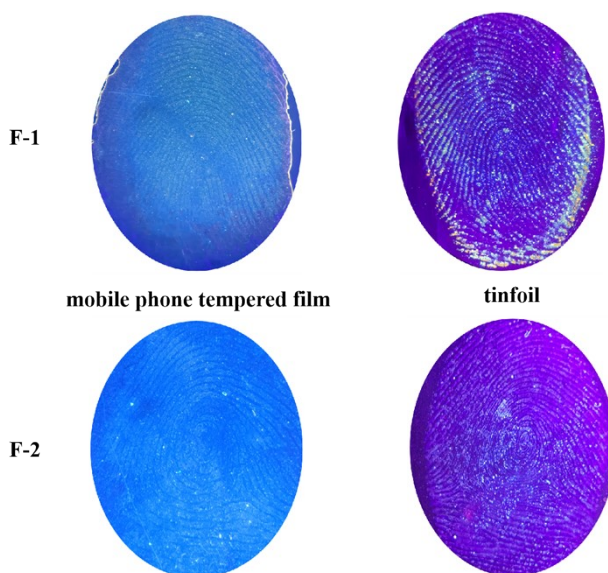


Figure S24 Photograph of the LFPs imaging on mobile phone tempered film and tinfoil substrates after being processed with compounds **F-1** and **F-2** under 365 nm UV light.

Table S1 Photophysical data of compounds **TPA-BP-BF₂-1** and **TPA-BP-BF₂-2** in solvents.

			TPA-BP-BF₂-1	TPA-BP-BF₂-2
solvents	UV (λ_{abs} , nm)	<i>n</i> -hexane	303, 381	305, 382
		CH ₂ Cl ₂	304, 384	305, 389
		CH ₃ CN	301, 376	279, 380
		DMF	304, 379	305, 384
		CH ₃ OH	301, 380	304, 384
	PL (λ_{nm} , nm)	<i>n</i> -hexane	481	499
		CH ₂ Cl ₂	518	517
		CH ₃ CN	529	519
		DMF	523	510
		CH ₃ OH	486	512

Table S2 The emission wavelengths of compounds **TPA-BP-BF₂-1** and **TPA-BP-BF₂-2** in mixtures of THF/water.

f_w (%)	0	10	20	30	40	50	60	70	80	90	100
TPA-BP-BF₂-1	471	493	488	481	480	485	490	472	488	600	603
TPA-BP-BF₂-2	488	502	506	504	504	509	512	499	494	497	586

Computational details

Kohn-Sham density functional theory (DFT) has been employed to optimize the ground state geometries of the investigated complexes at the B3LYP/6-31G(d, p) level. All the optimized geometries were tested to be local minima by frequency calculations at the same level. To get insight into the photophysical properties of the investigated complexes, time-dependent density functional theory (TD-DFT) calculations at the CAM-B3LYP¹/6-31G(d, p) have been performed. The effect of the solvent was considered in all DFT and TD-DFT calculations utilizing the integral equation formalism polarized continuum model (IEF-PCM) with the dichloromethane as solvent which has been employed in the experiment. All the DFT and TD-DFT calculations were performed using the Gaussian 16 software suit.²

According to the hole-electron analysis method, the “hole” and “electron” denote where the excited electron leaves and goes, respectively. In many cases, any excitation can be identified as a definitive distribution of hole and electron. The theory proved to be a useful and powerful method in unraveling nature of electron excitations.³ The wavefunction analysis was calculated by means of the Multiwfn version 3.8(dev) code⁴ and plotted using VMD⁵ and GaussView 6.0⁶ software.

References

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- [5] Humphrey, W.; Dalke, A.; Schulten, K. VMD: visual molecular dynamics. *Journal of molecular graphics* **1996**, *14* (1), 33-38.
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Cartesian coordinates at the IEF-PCM-B3LYP/6-31G(d, p) level.

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TPA-BP-BF2-1

C	-4.507295	-2.404407	0.862761
C	-4.616982	-1.309553	-0.006526
C	-3.494246	-0.848579	-0.702469
C	-2.265202	-1.482638	-0.534157
C	-2.142217	-2.582488	0.327001
C	-3.281698	-3.038782	1.010064
C	-0.865085	-3.353174	0.490522
C	0.456335	-2.669765	0.375736
O	-0.919593	-4.561277	0.719655
N	-5.885787	-0.669560	-0.170185
C	0.649686	-1.310328	0.672126
C	1.919911	-0.745762	0.612996
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C	2.838666	-2.873416	-0.053681
C	1.576783	-3.444089	0.028256
C	4.388360	-0.901323	0.160023
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C	6.811531	-1.073118	0.400692
C	6.977119	0.268449	0.011219
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N	8.262833	0.850030	-0.062165
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C	10.380698	-1.519181	-2.017909
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C	8.854242	4.909911	0.990076
C	8.062565	4.082737	1.790534
C	7.870284	2.743911	1.452893
C	-6.296490	-0.322029	-1.363958
C	-7.505163	0.388518	-1.600652
C	-8.273034	0.845414	-0.487006
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C	-9.797628	1.839545	-2.037501

C	-9.053721	1.392691	-3.141883
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C	-9.993883	1.849360	1.849149
C	-10.436477	3.711468	0.254294
C	-11.818679	1.596566	0.176974
B	-6.798927	-0.381098	1.108643
F	-7.368142	-1.588021	1.509876
H	-5.384672	-2.753081	1.392651
H	-3.571610	0.017829	-1.350915
H	-1.405245	-1.122373	-1.087068
H	-3.190062	-3.903262	1.658241
H	-0.186809	-0.697434	0.989601
H	2.047720	0.295648	0.889634
H	3.678211	-3.484452	-0.369016
H	1.433886	-4.496643	-0.191875
H	5.453918	-2.671303	0.795655
H	7.680124	-1.665024	0.666872
H	5.929226	2.045959	-0.624926
H	3.702286	1.039626	-0.497983
H	10.682093	0.801042	1.069990
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H	12.451336	-2.016107	-1.660925
H	10.288234	-2.165616	-2.885773
H	8.345570	-0.823075	-2.152034
H	9.696723	2.651281	-1.417359
H	10.060202	5.017805	-0.795323
H	9.007965	5.949993	1.260164
H	7.602721	4.475397	2.692734
H	7.267902	2.101358	2.086375
H	-5.681377	-0.597972	-2.218411
H	-10.697941	2.409408	-2.242743
H	-9.387748	1.622757	-4.147557
H	-7.294626	0.308307	-3.750535
H	-10.739489	2.298835	2.514405
H	-9.969641	0.775534	2.044022
H	-9.016729	2.259853	2.108292
H	-11.114556	4.135878	1.002592
H	-10.788215	4.031066	-0.730954
H	-9.443338	4.143932	0.414072
H	-12.225091	1.844246	-0.807689
H	-11.819103	0.506293	0.277199
H	-12.502137	2.005610	0.928803

F	-6.004573	0.158567	2.100985	C	-7.220640	1.040357	-1.774971
				O	-6.953585	-0.351173	1.612667
96				C	-9.468648	1.056782	2.002228
TPA-BP-BF2-2				C	-9.897346	-0.384995	2.372625
C	-3.526252	-3.016715	0.537747	C	-8.613259	1.664551	3.141495
C	-3.718980	-1.695310	0.109291	C	-10.749550	1.905979	1.880287
C	-2.653279	-0.971840	-0.437354	B	-5.848199	-1.311552	1.582349
C	-1.400451	-1.568133	-0.561524	F	-6.345766	-2.612948	1.582684
C	-1.195268	-2.890789	-0.143291	H	-4.359252	-3.566956	0.956434
C	-2.277712	-3.605969	0.395169	H	-2.792149	0.060901	-0.739397
C	0.108470	-3.611241	-0.322804	H	-0.586504	-1.000061	-0.997137
C	1.401823	-2.868794	-0.267803	H	-2.123460	-4.635691	0.698045
O	0.100015	-4.826167	-0.520176	H	0.755265	-1.262805	1.029525
N	-5.011969	-1.096831	0.239273	H	2.951947	-0.190590	1.151637
C	1.582120	-1.687704	0.470974	H	4.581696	-3.221201	-1.435128
C	2.830632	-1.077375	0.538204	H	2.381721	-4.338674	-1.490272
C	3.941246	-1.609567	-0.142781	H	6.415893	-2.774569	-0.167680
C	3.751996	-2.797576	-0.878546	H	8.601260	-1.678693	-0.074973
C	2.513637	-3.421241	-0.926744	H	6.669641	2.160664	0.108548
C	5.263394	-0.947732	-0.085102	H	4.483385	1.065394	0.014249
C	6.457550	-1.690484	-0.128011	H	11.563083	0.630369	0.971395
C	7.701138	-1.074241	-0.066181	H	13.485006	-0.255251	-0.309648
C	7.804728	0.325802	0.023610	H	13.188209	-0.985347	-2.671860
C	6.617003	1.078802	0.058717	H	10.945596	-0.798811	-3.738304
C	5.378463	0.450975	0.014123	H	9.033371	0.117877	-2.465995
N	9.067229	0.958228	0.076559	H	10.359931	3.177669	-0.657929
C	9.254990	2.128946	0.866942	H	10.715407	5.201808	0.718731
C	10.168147	0.432233	-0.659765	H	9.793284	5.325294	3.028719
C	11.432876	0.322901	-0.060839	H	8.526833	3.387425	3.946408
C	12.512736	-0.176863	-0.787277	H	8.201301	1.352065	2.580262
C	12.346774	-0.590320	-2.111247	H	-4.923427	-0.303104	-1.660086
C	11.087159	-0.489207	-2.706938	H	-10.014232	2.273108	-0.387552
C	10.005904	0.026429	-1.993926	H	-6.635946	1.013322	-2.687579
C	9.965573	3.224335	0.351682	H	-10.468300	-0.372487	3.307673
C	10.163202	4.362727	1.131794	H	-10.539474	-0.809175	1.593092
C	9.643234	4.434830	2.426301	H	-9.037610	-1.042665	2.505500
C	8.929183	3.348693	2.938330	H	-9.195457	1.685365	4.069405
C	8.742387	2.199192	2.172072	H	-8.326205	2.694388	2.902630
C	-5.497931	-0.370152	-0.738271	H	-7.706397	1.086052	3.320191
C	-6.734377	0.323480	-0.655323	H	-11.431081	1.519280	1.115365
C	-7.444596	0.315396	0.572408	H	-11.283391	1.884832	2.835261
C	-8.661556	1.040377	0.687576	H	-10.530419	2.953968	1.650054
C	-9.085811	1.720138	-0.451934	F	-5.013378	-1.089147	2.660008
C	-8.403385	1.747833	-1.696364	C	-8.994742	2.546049	-2.871232

C	-8.111468	2.455816	-4.129493	C	11.547470	-1.435323	-1.464103
H	-8.566014	3.034713	-4.939300	C	10.323265	-1.460817	-2.124471
H	-7.110297	2.863430	-3.954489	C	9.250264	-0.718000	-1.649572
H	-8.006261	1.423896	-4.480335	C	9.314010	3.004415	-0.298001
C	-10.395202	1.989140	-3.221488	C	9.540898	4.301533	0.143380
H	-10.334930	0.937314	-3.519578	C	8.957146	4.759411	1.320116
H	-11.087301	2.059921	-2.377018	C	8.149542	3.900642	2.058863
H	-10.829207	2.554119	-4.053587	C	7.933260	2.596193	1.634270
C	-9.119813	4.036048	-2.473269	C	-6.026401	0.337987	-1.309230
H	-8.139682	4.460397	-2.232050	C	-7.206891	1.108941	-1.428001
H	-9.546090	4.613584	-3.300715	C	-8.263548	0.987177	-0.434024
H	-9.769304	4.175120	-1.603811	C	-9.457816	1.760212	-0.505880

Cartesian coordinates at the TD-IEF-PCM-CAM-B3LYP/6-31G(d, p) level.

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C	-4.513585	-2.385474	0.575672
C	-4.593415	-1.176526	-0.152005
C	-3.409139	-0.646848	-0.704720
C	-2.201196	-1.292586	-0.526124
C	-2.121458	-2.489577	0.196155
C	-3.304845	-3.024854	0.727393
C	-0.865755	-3.267191	0.359615
C	0.465204	-2.595440	0.282244
O	-0.920178	-4.476728	0.555967
N	-5.820513	-0.549831	-0.310081
C	0.686131	-1.283289	0.707445
C	1.961246	-0.737948	0.675080
C	3.051678	-1.476857	0.203287
C	2.822853	-2.794758	-0.215248
C	1.555752	-3.348122	-0.161929
C	4.407864	-0.885731	0.152947
C	5.546530	-1.658674	0.403404
C	6.816975	-1.107931	0.365800
C	6.998225	0.244077	0.054649
C	5.865861	1.023355	-0.206126
C	4.598603	0.467005	-0.147622
N	8.290435	0.807232	0.004609
C	8.510042	2.138067	0.446891
C	9.384067	0.048573	-0.489059
C	10.611722	0.066406	0.177447
C	11.685507	-0.664058	-0.314662

C	11.547470	-1.435323	-1.464103
C	10.323265	-1.460817	-2.124471
C	9.250264	-0.718000	-1.649572
C	9.314010	3.004415	-0.298001
C	9.540898	4.301533	0.143380
C	8.957146	4.759411	1.320116
C	8.149542	3.900642	2.058863
C	7.933260	2.596193	1.634270
C	-6.026401	0.337987	-1.309230
C	-7.206891	1.108941	-1.428001
C	-8.263548	0.987177	-0.434024
C	-9.457816	1.760212	-0.505880
C	-9.564581	2.645168	-1.589064
C	-8.565429	2.759517	-2.551635
C	-7.391511	1.995757	-2.476029
O	-8.081450	0.137496	0.533122
C	-10.621739	1.703902	0.493107
C	-10.470839	0.709403	1.653538
C	-10.798685	3.108811	1.108719
C	-11.905119	1.321852	-0.275614
B	-6.962800	-0.831614	0.716624
F	-7.489441	-2.094710	0.521902
H	-5.416011	-2.826002	0.975744
H	-3.426075	0.294851	-1.238021
H	-1.309393	-0.863131	-0.966695
H	-3.250529	-3.966538	1.261214
H	-0.133634	-0.693145	1.100950
H	2.116706	0.269249	1.046126
H	3.646501	-3.384345	-0.603172
H	1.387888	-4.371810	-0.477010
H	5.437875	-2.704702	0.670465
H	7.678873	-1.726330	0.587636
H	5.983734	2.069143	-0.464905
H	3.741840	1.091842	-0.377767
H	10.718959	0.656419	1.080815
H	12.633133	-0.638969	0.213657
H	12.385848	-2.010564	-1.841927
H	10.203344	-2.052461	-3.026323
H	8.302090	-0.728963	-2.175453
H	9.760440	2.654708	-1.222174
H	10.169048	4.961984	-0.445677
H	9.130437	5.775246	1.658625
H	7.693708	4.242003	2.982690
H	7.315315	1.925490	2.220776

H	-5.274206	0.431125	-2.080349	C	11.027127	-0.385147	-2.653463
H	-10.450491	3.258100	-1.691085	C	9.948850	0.090691	-1.918972
H	-8.694818	3.452495	-3.375449	C	9.909369	3.171765	0.576713
H	-6.623028	2.101296	-3.233724	C	10.095265	4.266507	1.410840
H	-11.369449	0.777830	2.273688	C	9.556446	4.276928	2.693285
H	-10.376465	-0.320095	1.306576	C	8.835784	3.173255	3.138268
H	-9.608303	0.933638	2.281743	C	8.661649	2.066877	2.317174
H	-11.644583	3.098952	1.801959	C	-5.305601	-0.048458	-0.741839
H	-10.995140	3.872563	0.353346	C	-6.534580	0.637049	-0.578035
H	-9.906099	3.404180	1.666824	C	-7.517456	0.149470	0.361322
H	-12.139859	2.028561	-1.074156	C	-8.757263	0.823388	0.558244
H	-11.811033	0.326857	-0.718932	C	-8.976355	1.972680	-0.194246
H	-12.752383	1.306607	0.415744	C	-8.042872	2.473530	-1.125867
F	-6.488296	-0.661553	1.995353	C	-6.827917	1.783878	-1.299854
				O	-7.249065	-0.933215	1.034777
96				C	-9.791989	0.287201	1.550192
TPA-BP-BF2-2				C	-10.235354	-1.129667	1.129486
C	-3.558029	-3.109019	0.173436	C	-9.192211	0.252910	2.971132
C	-3.739284	-1.744226	-0.146089	C	-11.044527	1.172189	1.595164
C	-2.614776	-0.996167	-0.551756	B	-6.071053	-1.831945	0.875851
C	-1.367320	-1.585333	-0.622212	F	-6.538158	-3.015187	0.332128
C	-1.187459	-2.937394	-0.305645	H	-4.413750	-3.707979	0.451797
C	-2.311857	-3.684242	0.078243	H	-2.708531	0.059808	-0.770186
C	0.112959	-3.643422	-0.434219	H	-0.523531	-0.984932	-0.940800
C	1.401208	-2.893192	-0.349263	H	-2.180941	-4.737954	0.295815
O	0.133399	-4.856421	-0.616222	H	0.751056	-1.381956	1.043580
N	-5.003866	-1.179796	-0.063388	H	2.942505	-0.304262	1.212293
C	1.577433	-1.765652	0.456180	H	4.564687	-3.155816	-1.553212
C	2.819166	-1.154333	0.550111	H	2.371310	-4.281748	-1.658760
C	3.918565	-1.636693	-0.168389	H	6.386719	-2.788918	-0.207689
C	3.734724	-2.771446	-0.970191	H	8.567138	-1.688693	-0.057723
C	2.502770	-3.397002	-1.046134	H	6.625344	2.123925	0.221349
C	5.238206	-0.971748	-0.079057	H	4.444089	1.023826	0.073666
C	6.426904	-1.707363	-0.130956	H	11.510182	0.609361	1.046598
C	7.663680	-1.090394	-0.038107	H	13.430820	-0.204991	-0.272897
C	7.758122	0.299255	0.092874	H	13.128404	-0.855402	-2.650588
C	6.575056	1.044636	0.136457	H	10.882430	-0.661674	-3.692869
C	5.342920	0.416128	0.060667	H	8.972121	0.185322	-2.380208
N	9.015418	0.933391	0.178833	H	10.320047	3.172230	-0.426792
C	9.193055	2.059133	1.024864	H	10.655302	5.122620	1.048618
C	10.114155	0.450346	-0.578896	H	9.697332	5.136299	3.339949
C	11.377840	0.335795	0.005775	H	8.416152	3.164456	4.139066
C	12.455193	-0.122844	-0.741039	H	8.112136	1.202628	2.673263
C	12.286560	-0.490646	-2.071989	H	-4.601626	0.318785	-1.475496

H	-9.905734	2.507527	-0.067866	C	-7.260284	4.143777	-2.878782
H	-6.093025	2.146896	-2.006573	H	-7.556722	5.051901	-3.409247
H	-10.985223	-1.499551	1.835187	H	-6.323928	4.358312	-2.356439
H	-10.690229	-1.112158	0.134748	H	-7.070347	3.371214	-3.628905
H	-9.401543	-1.830624	1.117047	C	-9.664295	3.500608	-2.723344
H	-9.947410	-0.109494	3.674964	H	-9.532188	2.681597	-3.435451
H	-8.891538	1.255790	3.288279	H	-10.516597	3.260786	-2.084104
H	-8.325736	-0.404542	3.030459	H	-9.912389	4.404927	-3.286338
H	-11.549941	1.218959	0.626466	C	-8.604037	4.896978	-0.917849
H	-11.750786	0.750008	2.314297	H	-7.704755	5.088608	-0.326252
H	-10.816331	2.191959	1.917824	H	-8.848571	5.808364	-1.470952
F	-5.533020	-2.018911	2.127574	H	-9.426661	4.693202	-0.229111
C	-8.376112	3.737736	-1.909221				