Supplementary Information

Study on fluorescence properties both in solutions and the solid states of three *N,O*-chelated difluoroboron compounds and their application in latent fingerprint imaging and ink-free writing

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Content

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[1] The authors contribute equally to this paper.

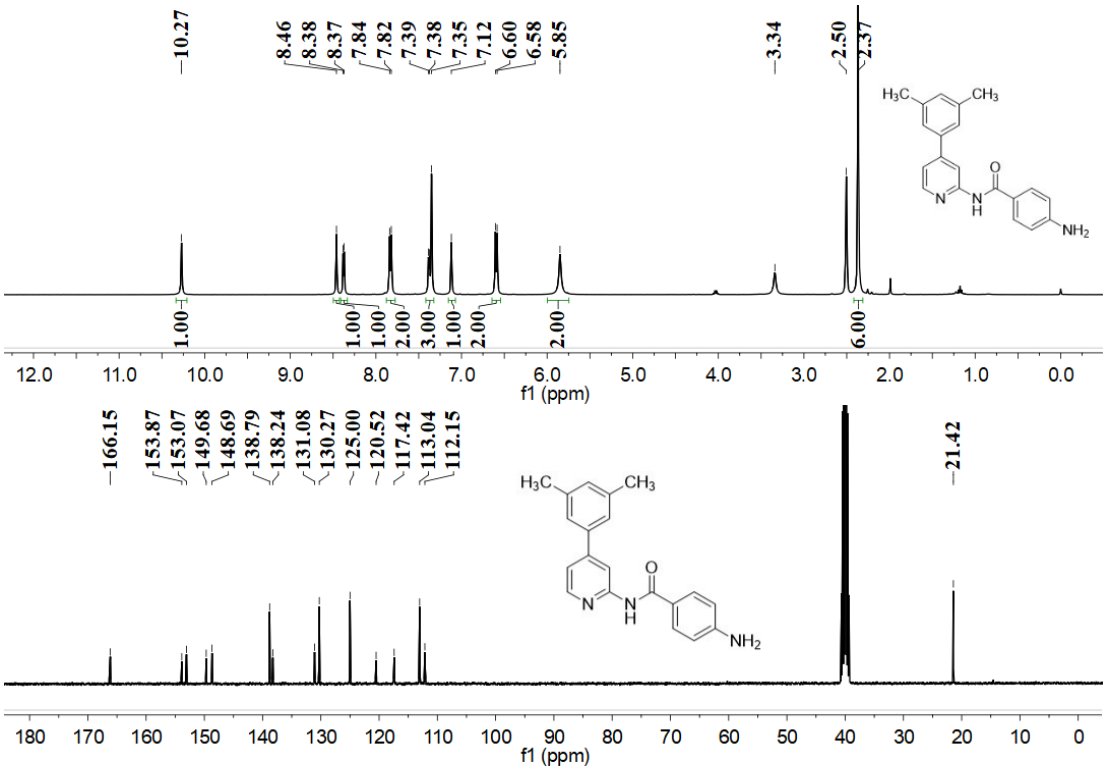


Figure S1 ^{1}H NMR and ^{13}C NMR spectra of compound **1-1** in DMSO-d_6.

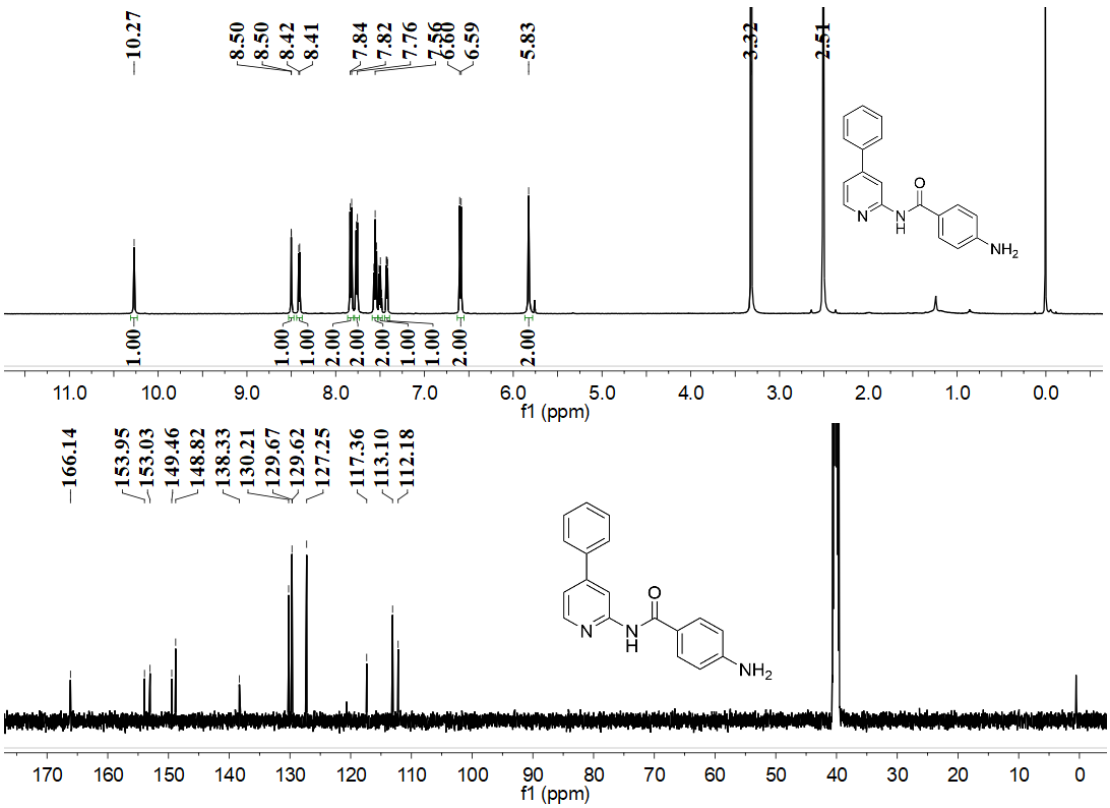


Figure S2 ^{1}H NMR and ^{13}C NMR spectra of compound **1-2** in DMSO-d_6.

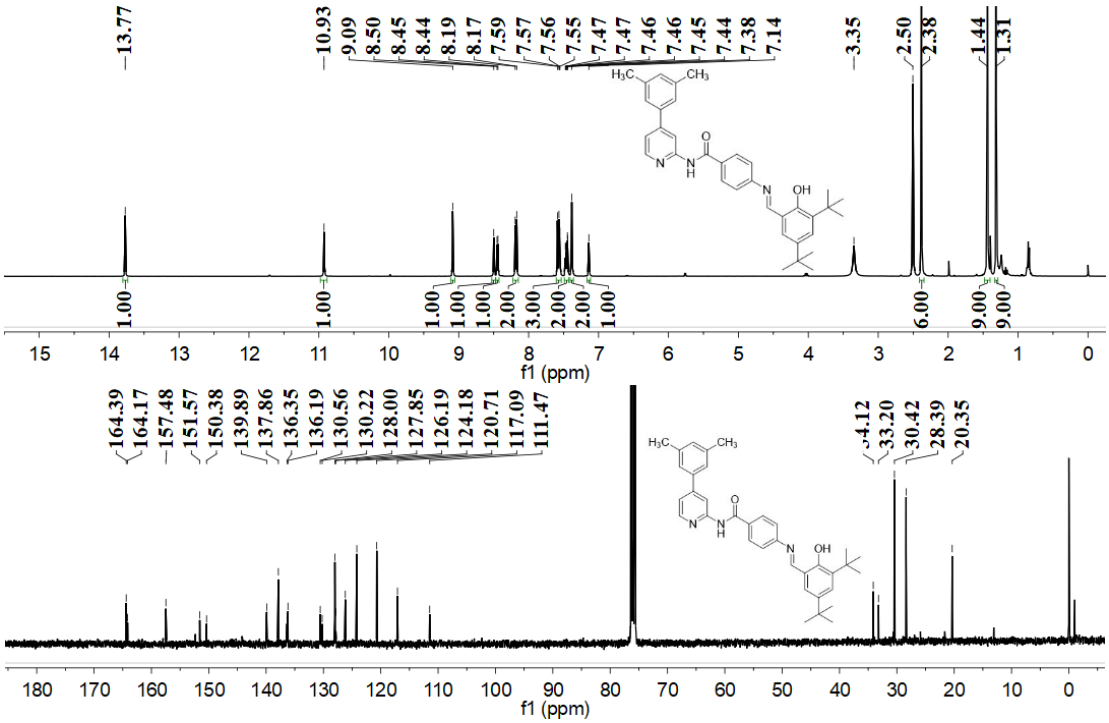


Figure S3 ^{1}H NMR and ^{13}C NMR spectra of compound **2-1** in DMSO-d_6.

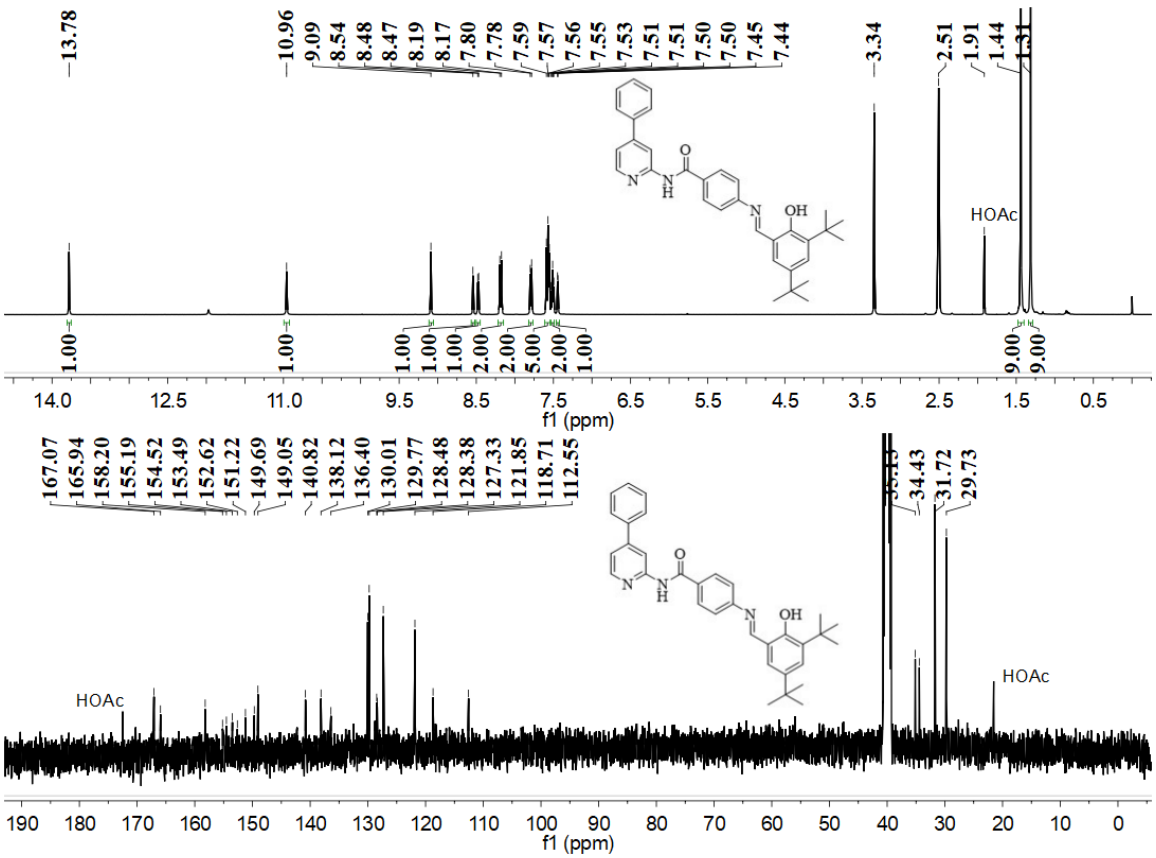


Figure S4 ^{1}H NMR and ^{13}C NMR spectra of compound **3-1** in DMSO-d_6.

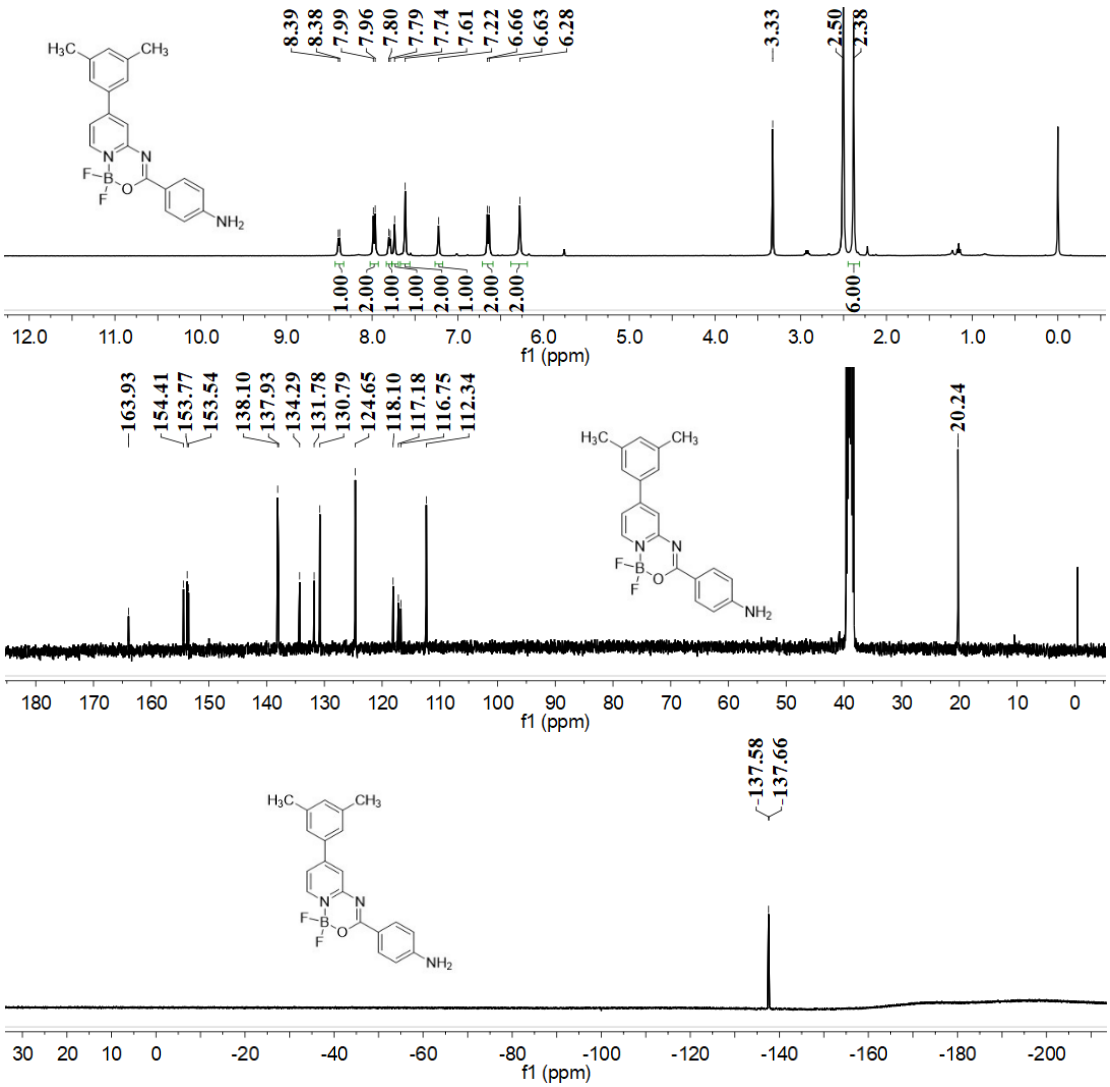


Figure S5 ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra of compound **1-BF$_2$** in DMSO-d_6.

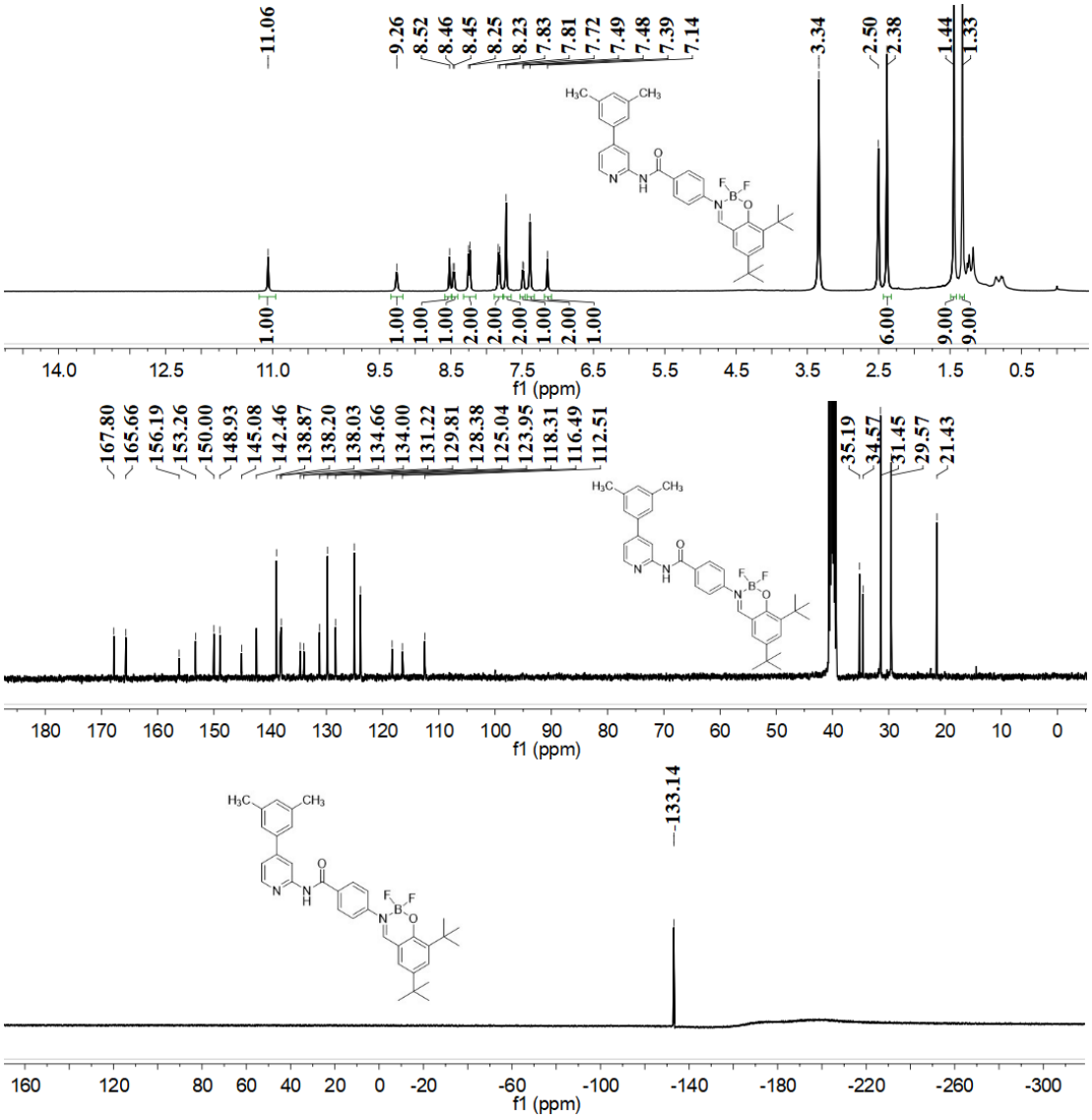


Figure S6 ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra of compound **2-BF$_2$** in DMSO-d_6.

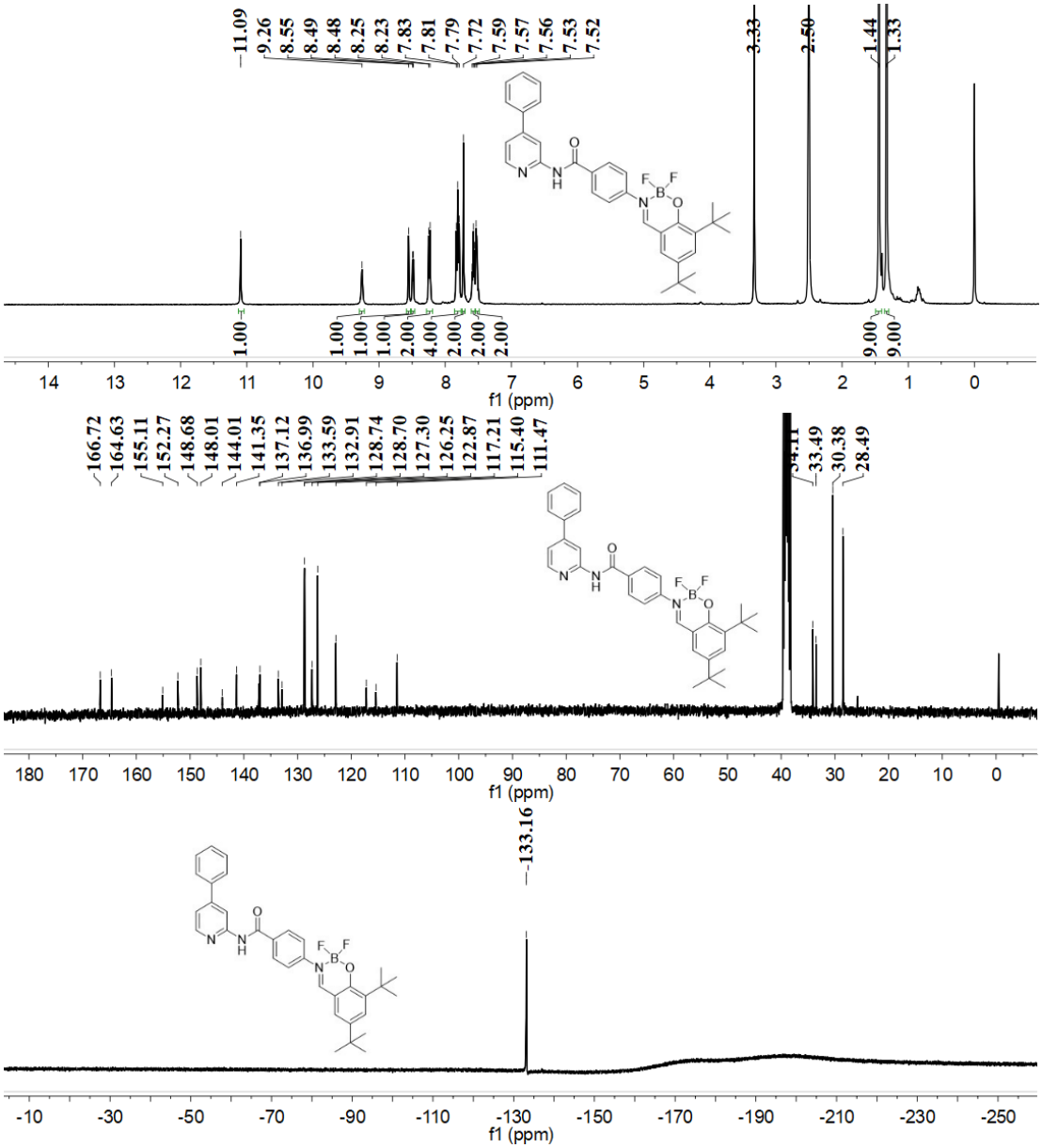
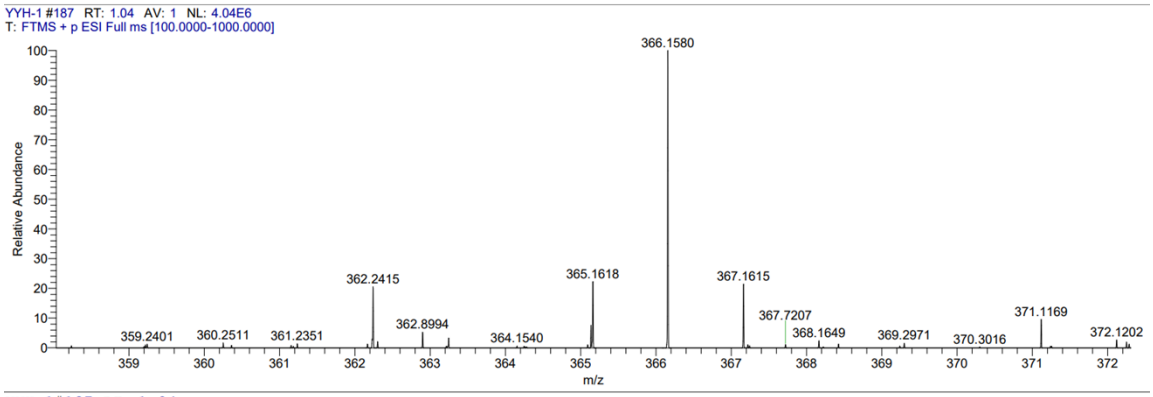


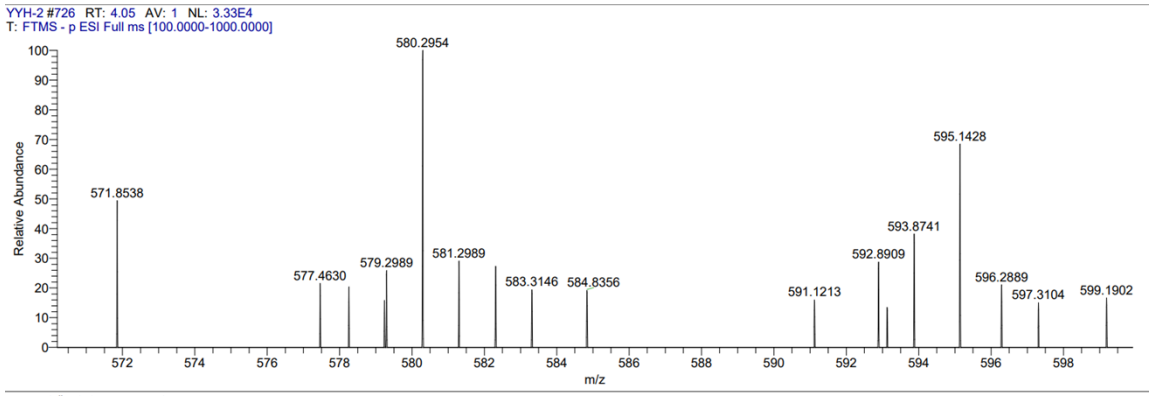
Figure S7 ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra of compound **3-BF$_2$** in DMSO-d_6.



YYH-1#187 RT: 1.04
T: FTMS + p ESI Full ms [100.0000-1000.0000]
m/z= 358.0309-372.3081

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
366.1580	4201097.5	100.00	366.1584	-0.42	$C_{20}H_{19}ON_3BF_2$

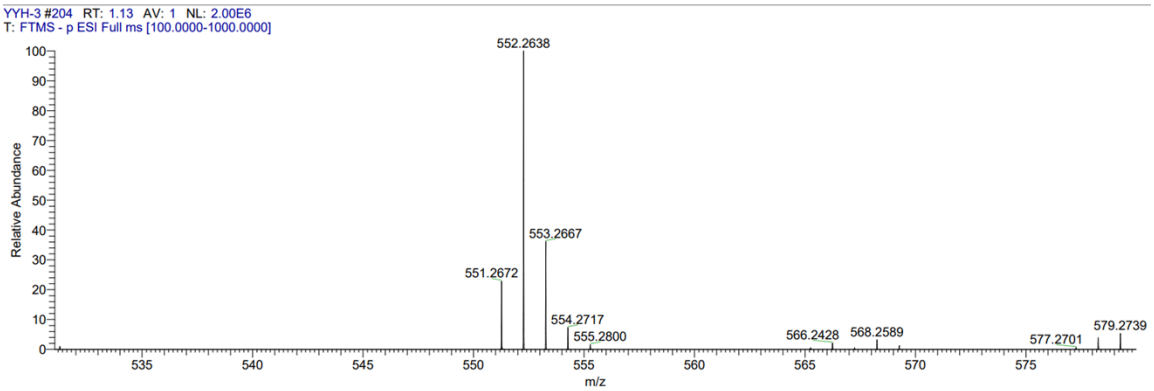
Figure S8 HRMS of compound **1-BF$_2$**.



YYH-2#726 RT: 4.05
T: FTMS - p ESI Full ms [100.0000-1000.0000]
m/z= 570.1965-599.9125

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
580.2954	35041.9	100.00	580.2941	1.27	$C_{35}H_{37}O_2N_3BF_2$

Figure S9 HRMS of compound **2-BF$_2$**.



YYH-3#204 RT: 1.13
T: FTMS - p ESI Full ms [100.0000-1000.0000]
m/z= 531.0430-579.9822

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
552.2638	2059863.0	100.00	552.2628	0.95	$C_{33}H_{33}O_2N_3BF_2$

Figure S10 HRMS of compound **3-BF$_2$**.

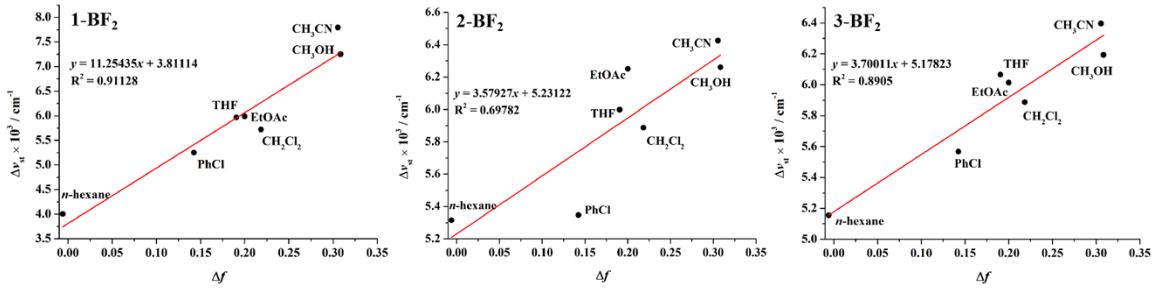


Figure S11 Lippert-Mataga plots of three compounds in different solvents.

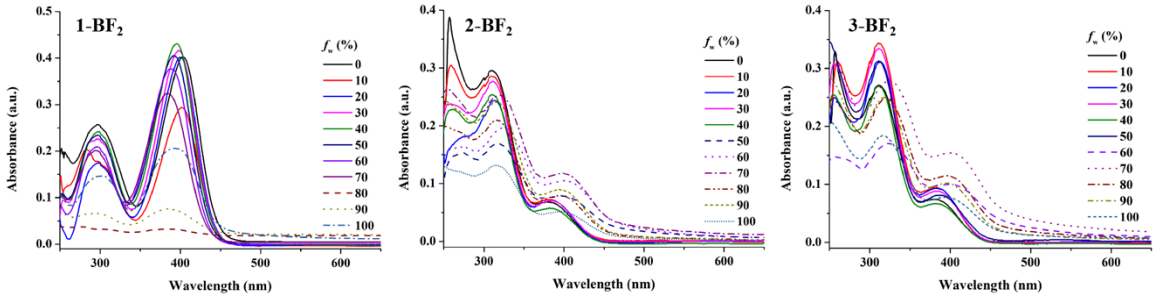


Figure S12 Absorption spectra of three compounds in DMSO/H_2O mixtures with different f_w (c = 1 × 10^{-5} mol/L), respectively.

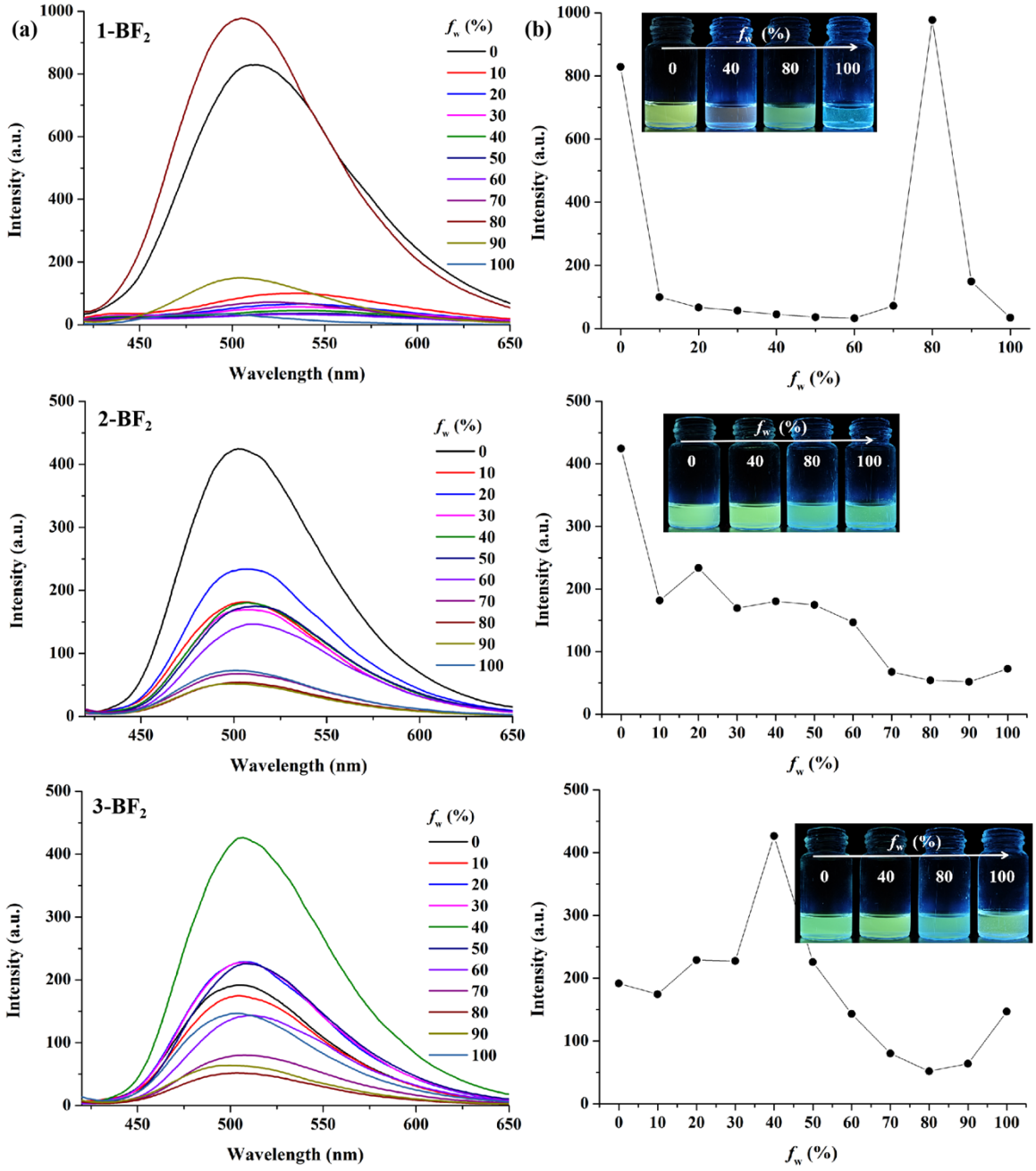


Figure S13 (a) Emission spectra of three compounds in THF/H_2O mixtures with different f_w (c = 1 × 10^{-5} mol/L, excited at 390 nm), and (b) plots of emission peak intensity versus f_w. Inset: photos in different f_w under 365 nm irradiation.

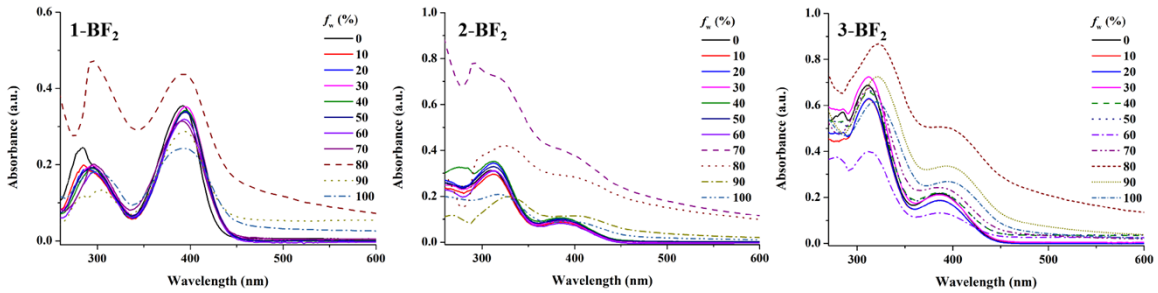


Figure S14 Absorption spectra of three compounds in THF/H_2O mixtures with different f_w (c = 1 × 10^{-5} mol/L), respectively.

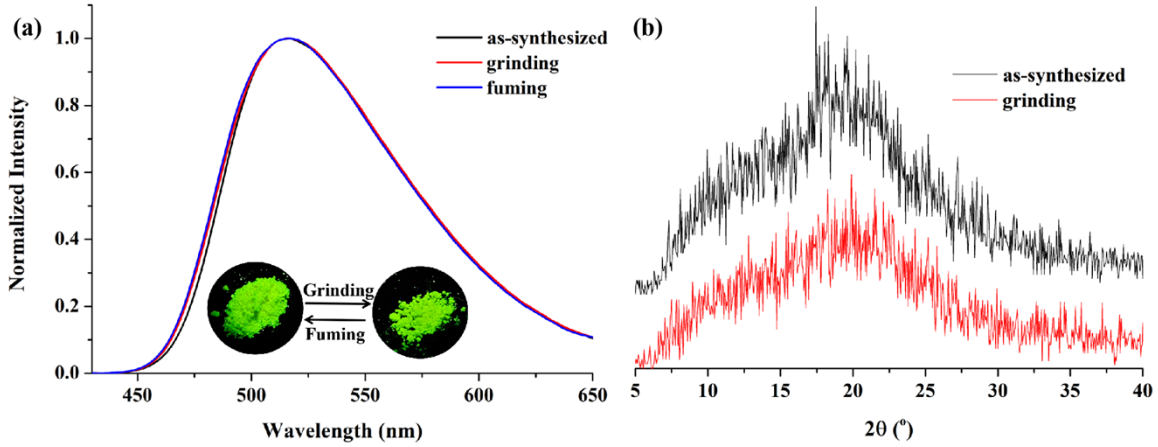


Figure S15 (a) Normalized emission spectra (λ_{ex} = 390 nm) and (b) XRD patterns of compound **2-BF_2** in different solid states. Inset: photos of luminescence colors change under a 365 nm UV lamp irradiation.

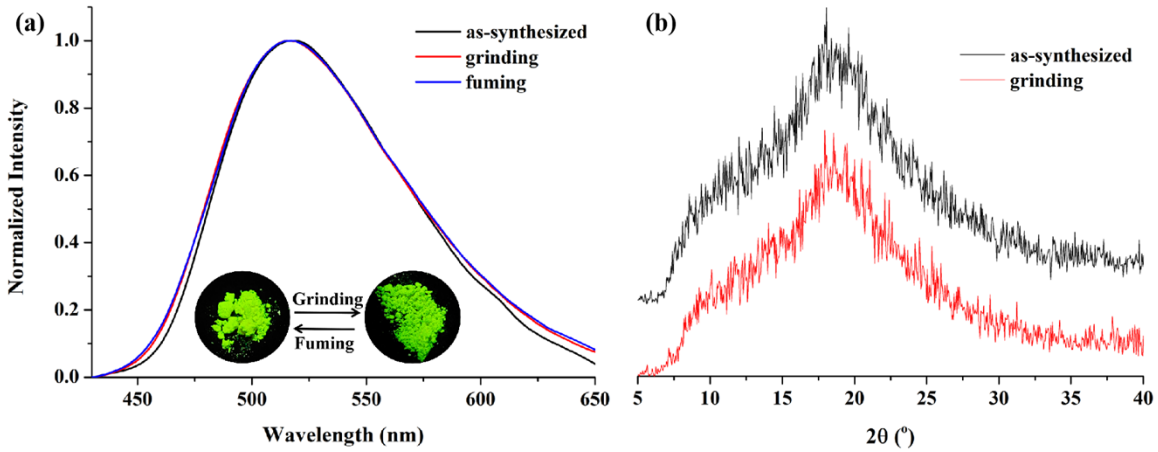


Figure S16 (a) Normalized emission spectra (λ_{ex} = 390 nm) and (b) XRD patterns of compound **3-BF_2** in different solid states. Inset: photos of luminescence colors change under a 365 nm UV lamp irradiation.

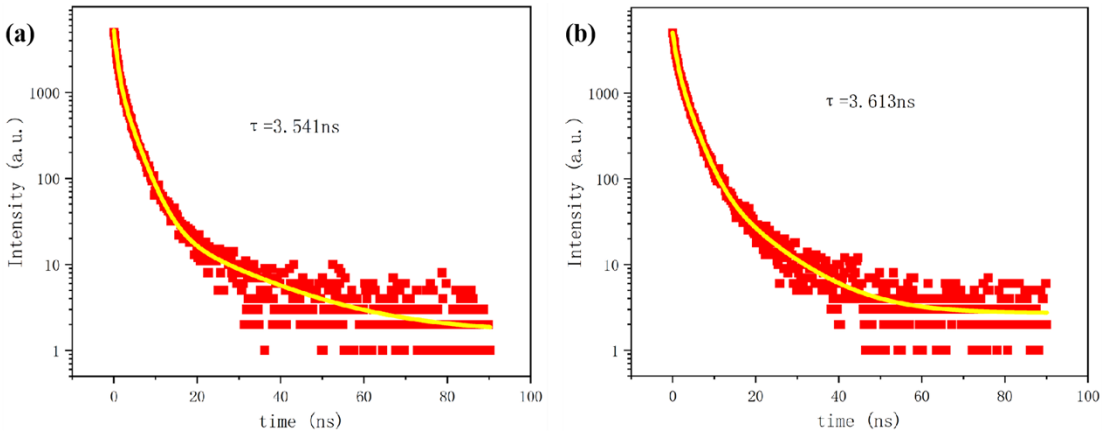


Figure S17 The τ of compound **1-BF$_2$** in (a) as-synthesized and (b) grinding states.

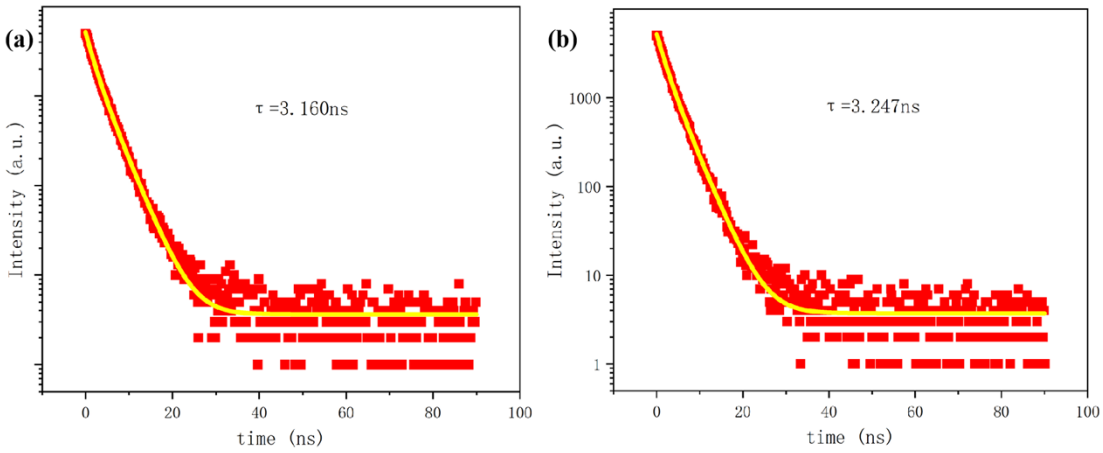


Figure S18 The τ of compound **2-BF$_2$** in (a) as-synthesized and (b) grinding states.

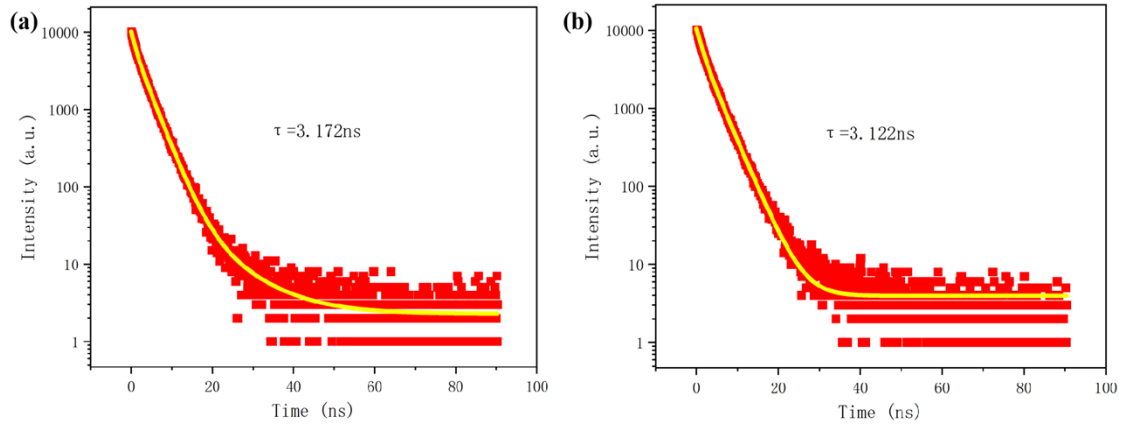


Figure S19 The τ of compound **3-BF$_2$** in (a) as-synthesized and (b) grinding states.

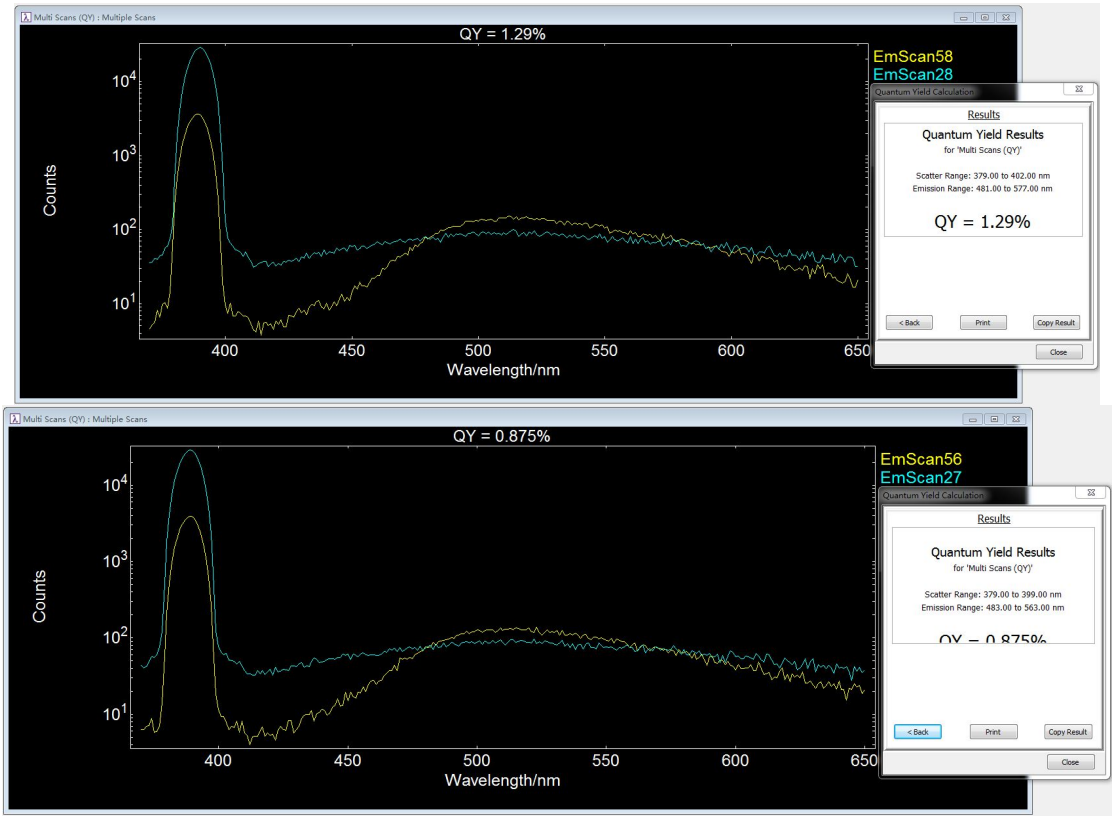


Figure S20 The Φ_f of compound **1-BF$_2$** in as-synthesized (up) and grinding (down) states.

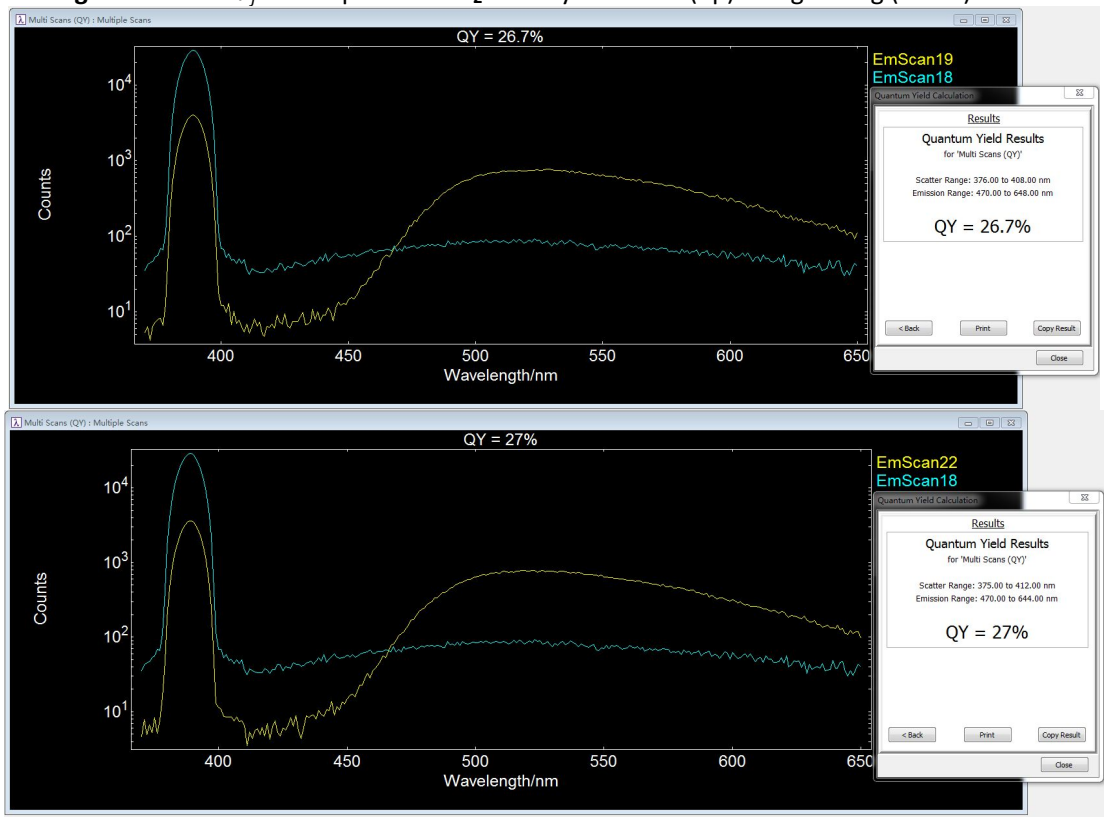


Figure S21 The Φ_f of compound **2-BF$_2$** in as-synthesized (up) and grinding (down) states.

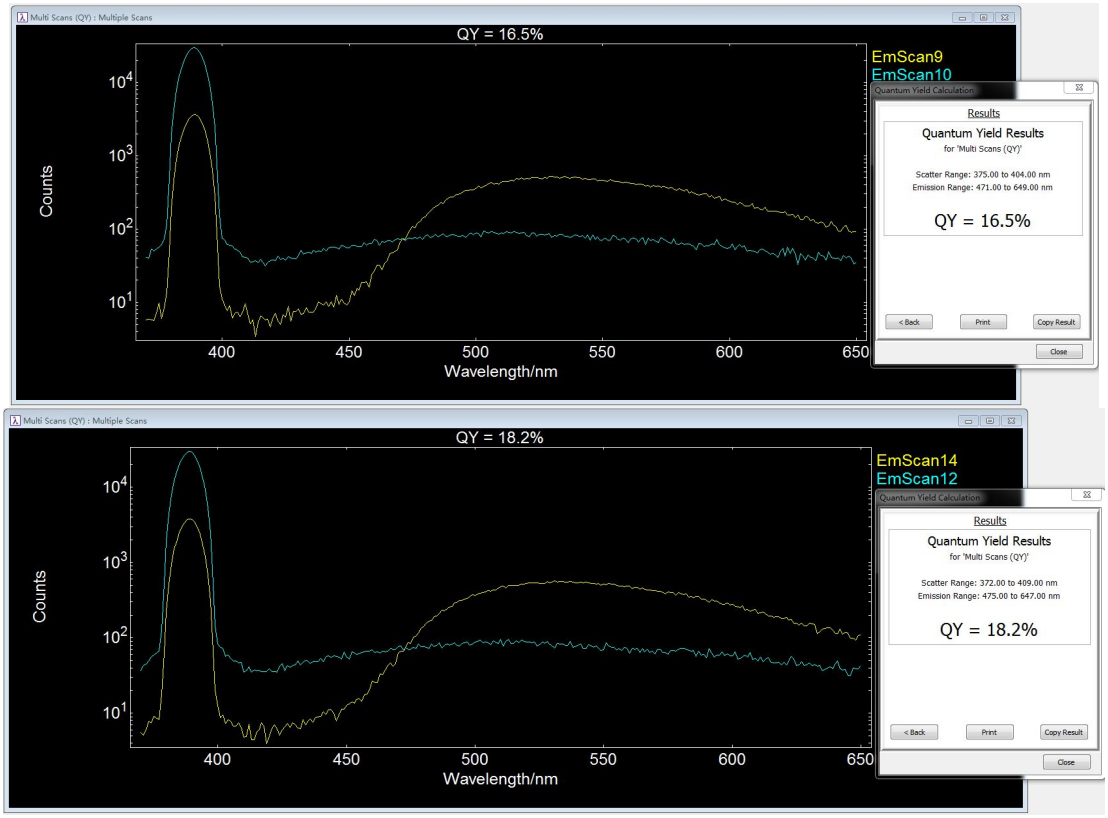


Figure S22 The Φ_f of compound **3-BF_2** in as-synthesized (up) and grinding (down) states.

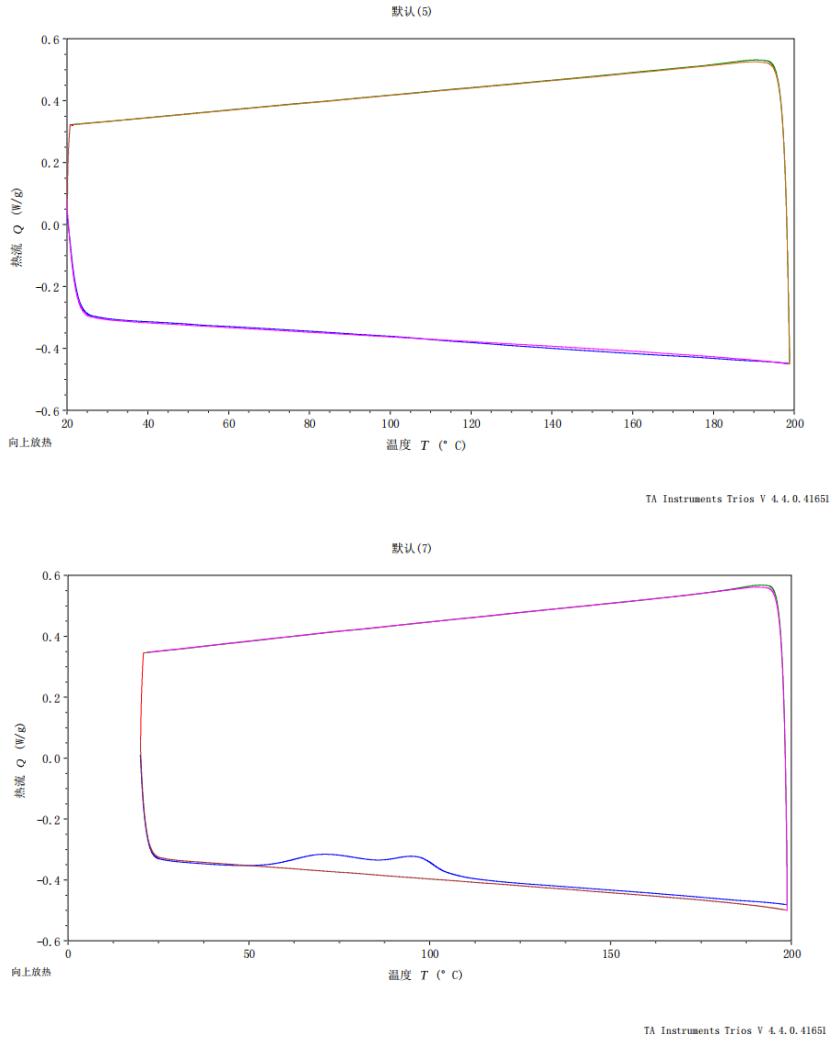


Figure S23 The DSC of compound **1-BF_2** in as-synthesized (up) and grinding (down) states.

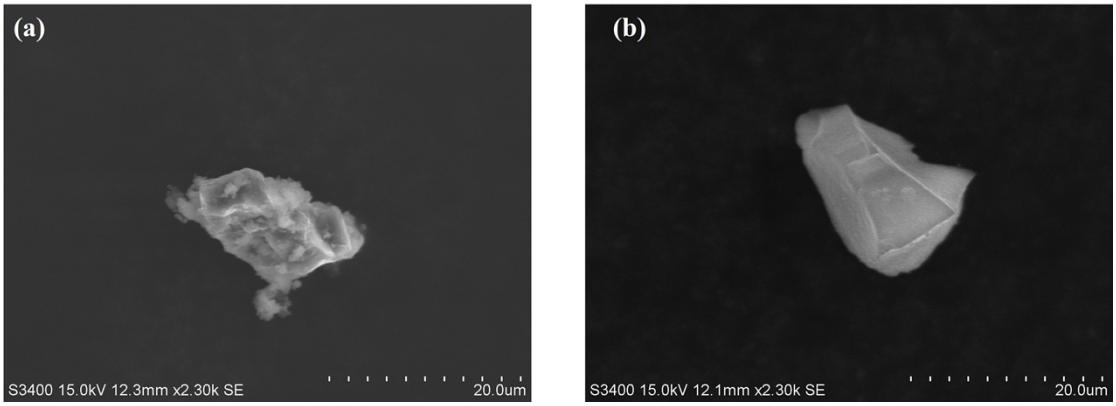


Figure S24 SEM images of developers based on compounds (a) **1-BF_2** and (b) **3-BF_2**, respectively.

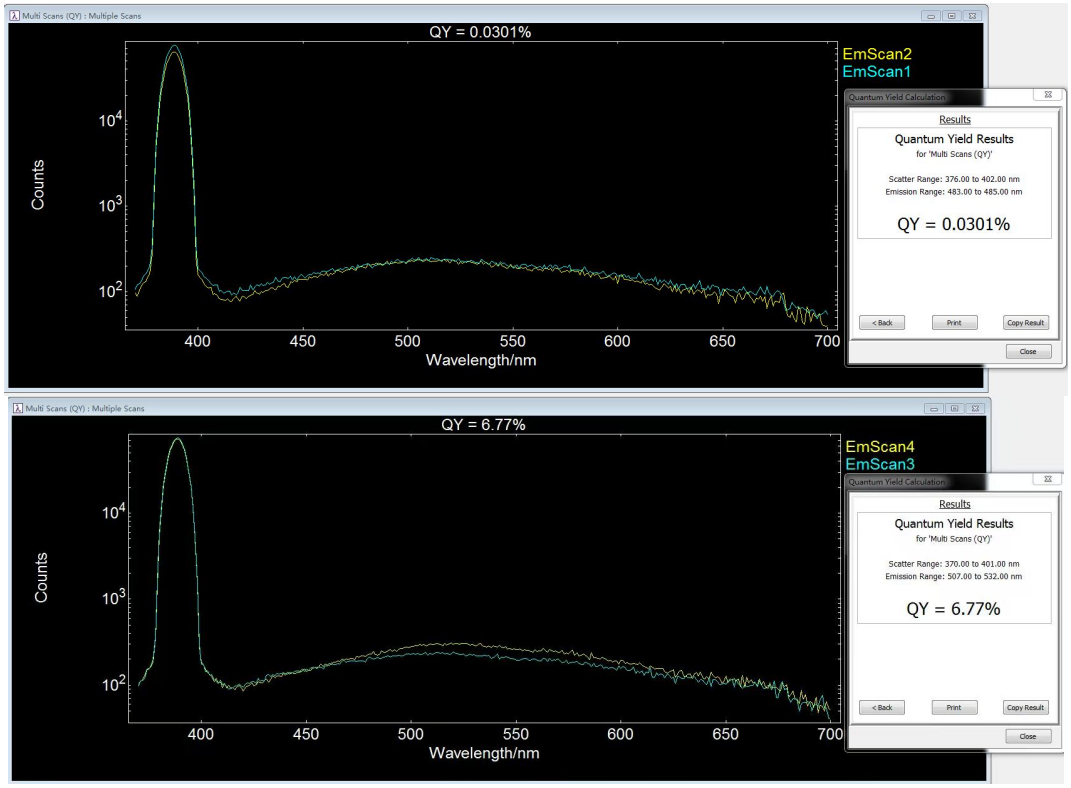


Figure S25 The Φ_f of developers based on compounds **1-BF$_2$** (up) and **3-BF$_2$** (down).

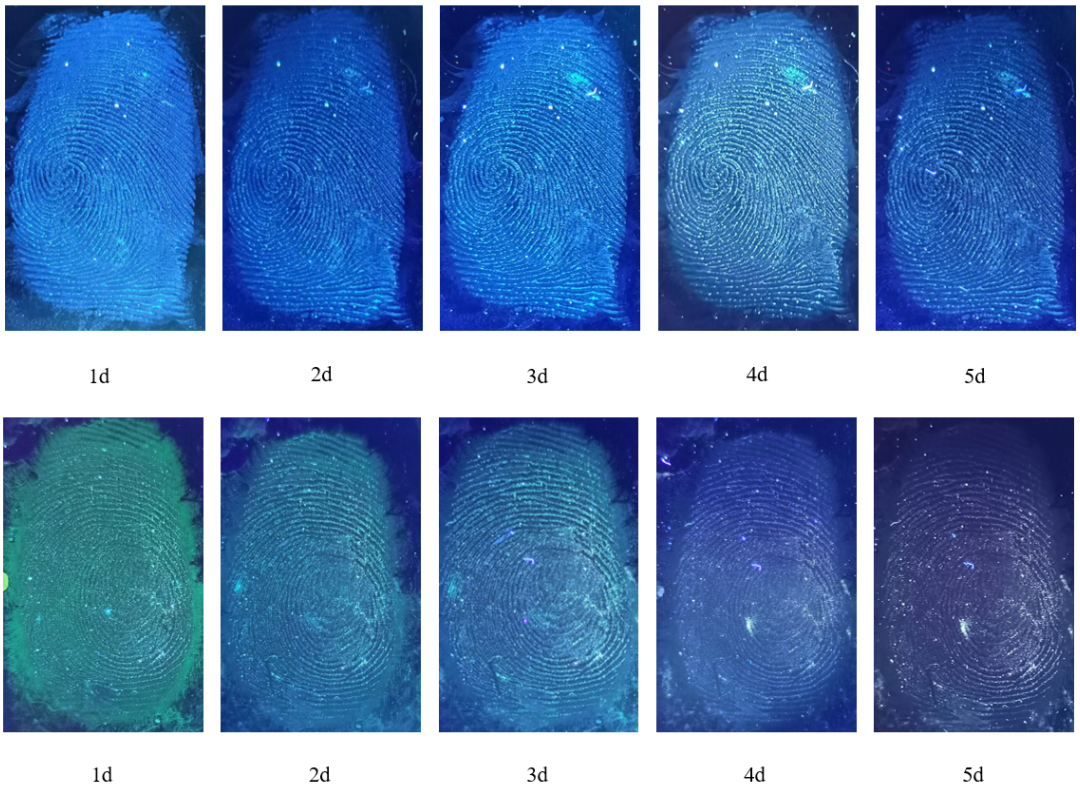


Figure S26 Photographs of LFPs undergoing different aging times with **1-BF$_2$** and **3-BF$_2$** contrast agents on tinfoil (365 nm UV light)

Table S1 Photophysical data of compounds **1-BF_2**, **2-BF_2** and **3-BF_2** in various organic solvents.

		n-hexane	PhCl	CH_2Cl_2	THF	EtOAc	CH_3CN	CH_3OH
1-BF_2	UV (λ_{abs}, nm)	282, 377	285, 384	287, 379	289, 391	286, 386	286, 383	288, 387
	PL (λ_{em}, nm)	444	481	484	510	502	546	538
	$\Delta\nu_{st}$ (10^3, cm^{-1})[a]	4.0027	502516	5.7241	5.9676	5.9864	7.7946	7.2524
2-BF_2	UV (λ_{abs}, nm)	312, 395	315, 397	313, 394	311, 387	309, 385	308, 383	310, 386
	PL (λ_{em}, nm)	500	504	513	504	507	508	509
	$\Delta\nu_{st}$ (10^3, cm^{-1})[a]	5.3161	5.3476	5.8875	5.9985	6.2502	6.4246	6.2604
3-BF_2	UV (λ_{abs}, nm)	312, 396	315, 396	314, 394	311, 386	309, 385	309, 384	310, 387
	PL (λ_{em}, nm)	496	508	513	504	501	509	509
	$\Delta\nu_{st}$ (10^3, cm^{-1})[a]	501552	505675	508875	6.0655	6.0139	6.3953	6.1934
	Δf [b]	-0.006	0.1425	0.2185	0.1906	0.2	0.3055	0.3085

[a] $\Delta\nu_{st} = \Delta\nu_{ICT,\,abs} - \Delta\nu_{em}$

[b] Δf referred to solvent polarity parameters, it was calculated as follows:

$$\Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}$$

where ε was the static dielectric constant, *n* was the optical refractive index of the solvent.

Table S2 The emission wavelengths and intensities of compounds **1-BF_2**, **2-BF_2** and **3-BF_2** in mixtures of DMSO/water.

f_w (%)		0	10	20	30	40	50	60	70	80	90	100
1-BF_2	Wavelength (nm)	557	542	547	541	536	534	522	485	464	464	497
	Intensity (a.u.)	18	13	18	19	17	16	13	15	82	275	782
2-BF_2	Wavelength (nm)	511	512	513	515	516	506	502	502	502	502	504
	Intensity (a.u.)	149	153	155	146	106	92	114	135	84	119	60
3-BF_2	Wavelength (nm)	509	512	514	517	516	490	489	504	498	504	504
	Intensity (a.u.)	707	914	872	811	492	78	157	658	546	478	337

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-B3LYP[1]/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]

References

1. Yanai, T.; Tew, D. P.; Handy, N. C. A new hybrid exchange-correlation functional using the Coulomb-attenuating method (CAM-B3LYP). *Chemical Physics Letters* **2004,** *393* (1-3), 51-57.
2. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 16 Rev. A.03*, Gaussian, Inc.: Wallingford, CT, 2016.

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

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1-BF_2

C	2.220847	1.875485	-0.370272
C	0.996746	2.495362	-0.410978
N	-0.161313	1.821034	-0.203705
C	-0.146662	0.473821	0.026344
C	1.091874	-0.193889	0.087232
C	2.291058	0.483905	-0.106466
C	3.594822	-0.217296	-0.044966
N	-1.298013	-0.237998	0.188297
C	-2.456409	0.345873	-0.027263
C	-3.690573	-0.434609	0.045202
O	-2.606823	1.623972	-0.339816
B	-1.529140	2.608995	-0.144187
C	4.731061	0.438534	0.452986
C	5.966388	-0.212999	0.529550
C	6.052278	-1.535795	0.079925
C	4.939060	-2.216362	-0.431389
C	3.713901	-1.546699	-0.482235
C	-4.946641	0.179069	-0.124976
C	-6.117243	-0.556284	-0.050842
C	-6.078445	-1.946218	0.198696
C	-4.818082	-2.564248	0.368459
C	-3.653986	-1.821425	0.291730
C	5.072042	-3.632509	-0.940456
C	7.172763	0.484356	1.113255
N	-7.234723	-2.689363	0.226745
H	3.114760	2.453583	-0.566153
H	0.887536	3.552650	-0.618397
H	1.066260	-1.254157	0.304097
H	4.648945	1.458894	0.815914
H	7.010350	-2.049233	0.127006
H	2.849168	-2.055615	-0.897547
H	-4.993115	1.245938	-0.310761
H	-7.077119	-0.064984	-0.182653
H	-4.770569	-3.633008	0.557816
H	-2.691539	-2.302269	0.424026
H	5.648625	-4.251659	-0.245876
H	4.094128	-4.099735	-1.082273
H	5.594758	-3.657674	-1.903990
H	7.084635	1.571186	1.031777
H	7.289534	0.243817	2.176965
H	8.093346	0.176322	0.608947
H	-7.197690	-3.595329	0.671152
H	-8.104336	-2.196783	0.371248
F	-1.553089	3.543997	-1.161401
F	-1.646670	3.209021	1.101135

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2-BF_2

C	7.839646	-0.589895	-1.915389
C	6.919916	-1.216672	-2.747968
N	5.603796	-1.291272	-2.502523
C	5.176190	-0.741541	-1.362952
C	6.017900	-0.090842	-0.449536
C	7.386163	0.003487	-0.724085
C	8.314809	0.688286	0.209693
N	3.794497	-0.779910	-1.083809
C	2.901597	-1.788894	-1.402589
C	1.471980	-1.492382	-1.041661
O	3.221476	-2.851196	-1.919417
C	7.904824	1.830806	0.917190
C	8.770484	2.488695	1.794138
C	10.066475	1.980643	1.961753
C	10.504580	0.842210	1.277145
C	9.618270	0.208233	0.398158
C	0.619553	-2.582081	-0.812542
C	-0.717641	-2.387712	-0.492095
C	-1.227883	-1.084348	-0.417250
C	-0.389697	0.012163	-0.647222
C	0.951442	-0.193883	-0.962131
C	11.892146	0.288225	1.502851
C	8.330615	3.725845	2.541915
N	-2.610103	-0.888047	-0.103705
C	-3.314293	-0.007333	-0.772628
C	-4.666200	0.304006	-0.468311
C	-5.266097	-0.287165	0.673008
C	-6.601781	0.051047	1.021471
C	-7.248555	0.956515	0.183282
C	-6.682083	1.562547	-0.968528
C	-5.379753	1.222494	-1.275119
O	-4.565064	-1.133536	1.421673
C	-7.294036	-0.564368	2.255199
C	-7.364847	-2.104444	2.104639
C	-6.512742	-0.192924	3.539938

C	-8.736490	-0.046811	2.423457	H	-8.556634	3.416740	-0.060927
C	-7.521348	2.546487	-1.801992	F	-3.477308	-3.039705	0.599631
C	-6.732492	3.100488	-3.002983				
C	-8.779334	1.824173	-2.340279	75			
C	-7.954020	3.738585	-0.915575	**3-BF_2**			
B	-3.280831	-1.741810	1.066474	C	8.472439	0.659289	-1.382480
F	-2.440542	-1.720817	2.162533	C	7.605732	0.620513	-2.468452
H	8.884137	-0.540190	-2.201305	N	6.282817	0.423529	-2.374977
H	7.253317	-1.671507	-3.678580	C	5.791853	0.228641	-1.148421
H	5.611778	0.305873	0.475067	C	6.576877	0.240122	0.013718
H	3.472678	-0.097738	-0.411840	C	7.952302	0.470172	-0.090097
H	6.907177	2.230081	0.758042	C	8.822126	0.500994	1.112175
H	10.750111	2.486368	2.640537	N	4.401491	0.042886	-1.007425
H	9.941551	-0.686342	-0.126603	C	3.543190	-0.590111	-1.890690
H	1.022549	-3.585236	-0.894756	C	2.096039	-0.562101	-1.482410
H	-1.376834	-3.227995	-0.314827	O	3.904232	-1.151516	-2.916440
H	-0.775385	1.022423	-0.559985	C	8.354202	1.032052	2.326195
H	1.578329	0.668729	-1.163941	C	9.173468	1.061965	3.453850
H	12.591839	1.074276	1.800599	C	10.474772	0.559006	3.390396
H	11.890376	-0.465862	2.299435	C	10.951557	0.027535	2.190106
H	12.281815	-0.193679	0.601466	C	10.134240	0.000405	1.060983
H	7.306824	4.007144	2.282254	C	1.266855	-1.585413	-1.963946
H	8.371432	3.568676	3.625681	C	-0.083941	-1.620167	-1.643982
H	8.981605	4.578133	2.317855	C	-0.631120	-0.606253	-0.845666
H	-2.835500	0.504820	-1.604951	C	0.183601	0.423170	-0.361628
H	-8.269644	1.220951	0.426660	C	1.538723	0.445287	-0.683826
H	-4.870895	1.644021	-2.134725	N	-2.026700	-0.636620	-0.530964
H	-7.857036	-2.539498	2.981530	C	-2.735920	0.464554	-0.590467
H	-7.950108	-2.379553	1.220509	C	-4.104413	0.531878	-0.216053
H	-6.373465	-2.549436	2.013020	C	-4.720223	-0.617714	0.341763
H	-7.013994	-0.622602	4.414307	C	-6.076201	-0.556571	0.762720
H	-6.480383	0.894014	3.672454	C	-6.724704	0.662994	0.582190
H	-5.489209	-0.568106	3.514262	C	-6.142025	1.831232	0.024980
H	-9.369889	-0.301113	1.567132	C	-4.821063	1.743370	-0.366400
H	-9.180902	-0.511590	3.308838	O	-4.016413	-1.736281	0.488968
H	-8.772103	1.037944	2.569662	C	-6.787088	-1.782561	1.372173
H	-7.363267	3.793570	-3.568054	C	-6.803013	-2.943514	0.346664
H	-5.840308	3.650492	-2.685734	C	-6.059887	-2.227337	2.665335
H	-6.420890	2.304920	-3.687783	C	-8.250322	-1.472463	1.745827
H	-9.388830	2.516391	-2.931260	C	-6.985859	3.110235	-0.113983
H	-9.407195	1.437898	-1.531751	C	-6.180178	4.265506	-0.736630
H	-8.502140	0.981874	-2.982543	C	-8.206739	2.827156	-1.021543
H	-7.081871	4.275948	-0.528873	C	-7.477794	3.560129	1.282339
H	-8.556649	4.443529	-1.498519	B	-2.705223	-2.015923	-0.100280

H	9.526344	0.860575	-1.537123
H	7.990344	0.774941	-3.474509
H	6.120520	0.040287	0.977600
H	4.039221	0.211071	-0.079406
H	7.352563	1.447284	2.380601
H	8.797114	1.484848	4.380489
H	11.112245	0.581401	4.269049
H	11.959347	-0.372733	2.133487
H	10.507548	-0.435343	0.139477
H	1.699392	-2.351387	-2.597669
H	-0.724867	-2.410201	-2.014159
H	-0.231548	1.191645	0.281806
H	2.147557	1.267479	-0.321800
H	-2.248387	1.368237	-0.951050
H	-7.760564	0.728393	0.889519
H	-4.299730	2.591033	-0.796726
H	-7.305887	-3.814397	0.781605
H	-7.353166	-2.654318	-0.555346
H	-5.795387	-3.240954	0.054218
H	-6.575244	-3.090699	3.100573
H	-6.066494	-1.423009	3.409025
H	-5.024632	-2.509467	2.471255
H	-8.847140	-1.182431	0.874707
H	-8.707469	-2.370955	2.171449
H	-8.326123	-0.678738	2.496542
H	-6.814985	5.153101	-0.818692
H	-5.314009	4.535106	-0.123301
H	-5.826024	4.019106	-1.743034
H	-8.819377	3.729550	-1.123151
H	-8.845771	2.037634	-0.614728
H	-7.887292	2.518736	-2.022371
H	-6.632785	3.779061	1.943365
H	-8.084849	4.467712	1.194645
H	-8.093658	2.795977	1.766080
F	-1.897328	-2.627771	0.838135
F	-2.850607	-2.804134	-1.239927

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

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1-BF_2

C	2.194706	1.877878	-0.374636
C	0.972733	2.497287	-0.404587
N	-0.190196	1.842512	-0.215301
C	-0.163691	0.464303	-0.015625
C	1.081794	-0.198046	0.043974
C	2.280469	0.473965	-0.130951
C	3.575729	-0.221246	-0.056964
N	-1.293179	-0.234537	0.098249
C	-2.480120	0.371532	-0.075418
C	-3.664465	-0.415538	0.018638
O	-2.620958	1.665681	-0.373562
B	-1.541178	2.608029	-0.074487
C	4.724354	0.456516	0.366335
C	5.956865	-0.186956	0.446339
C	6.035086	-1.529829	0.082502
C	4.910088	-2.235612	-0.349419
C	3.690556	-1.572555	-0.413136
C	-4.949612	0.176816	-0.158652
C	-6.089127	-0.573141	-0.080955
C	-6.018635	-1.970538	0.180754
C	-4.741919	-2.569343	0.364444
C	-3.604650	-1.817717	0.284758
C	5.028882	-3.681369	-0.756029
C	7.174520	0.545338	0.947093
N	-7.139893	-2.710340	0.252510
H	3.082989	2.464230	-0.569409
H	0.876968	3.560210	-0.593664
H	1.049321	-1.262295	0.241116
H	4.654925	1.496846	0.667734
H	6.994488	-2.039063	0.132841
H	2.820115	-2.108255	-0.778067
H	-5.004653	1.239501	-0.357476
H	-7.061436	-0.111596	-0.219121
H	-4.684748	-3.633505	0.568814
H	-2.631742	-2.271187	0.422483
H	5.459511	-4.283612	0.049267
H	4.055429	-4.105016	-1.010949
H	5.682520	-3.793862	-1.626483
H	7.086136	1.622152	0.786803
H	7.314601	0.383872	2.021153
H	8.080956	0.197731	0.445676
H	-7.101020	-3.702243	0.429637
H	-8.050183	-2.295329	0.126567
F	-1.562433	3.649557	-0.983628
F	-1.667471	3.088432	1.224186

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2-BF_2

C	7.860793	-0.925024	-1.654808
C	6.966199	-1.687591	-2.385492
N	5.648076	-1.708520	-2.174018
C	5.189221	-0.962163	-1.175310
C	6.004952	-0.160946	-0.372775
C	7.374345	-0.125378	-0.614838
C	8.279113	0.716254	0.205195
N	3.803865	-0.942371	-0.943701
C	2.927354	-2.000787	-1.079425
C	1.494026	-1.657940	-0.846379
O	3.278046	-3.138369	-1.346902
C	7.868028	1.973523	0.652589
C	8.710639	2.775446	1.418295
C	9.977873	2.292031	1.741843
C	10.415203	1.039254	1.314384
C	9.556260	0.262737	0.540069
C	0.620461	-2.698580	-0.510178
C	-0.719629	-2.465771	-0.291151
C	-1.246749	-1.162856	-0.419848
C	-0.369977	-0.117148	-0.770588
C	0.973408	-0.367251	-0.978278
C	11.773631	0.522346	1.710160
C	8.277126	4.149231	1.858783
N	-2.602550	-0.942577	-0.209897
C	-3.217658	0.142135	-0.735931
C	-4.560458	0.480159	-0.435259
C	-5.323543	-0.330533	0.484965
C	-6.674162	-0.015204	0.811908
C	-7.222685	1.114029	0.210277
C	-6.508767	1.926446	-0.693744
C	-5.176267	1.584879	-1.001421
O	-4.749095	-1.371564	1.018408
C	-7.473368	-0.896344	1.774418
C	-7.579636	-2.327554	1.207029
C	-6.788193	-0.925905	3.156415
C	-8.899877	-0.367826	1.974129
C	-7.195310	3.140054	-1.309019
C	-6.280303	3.917183	-2.262408
C	-8.433070	2.669082	-2.099593
C	-7.641276	4.091888	-0.180496
B	-3.404363	-1.929944	0.696213
F	-2.743015	-2.106419	1.889455
H	8.914350	-0.933343	-1.906655
H	7.324290	-2.307255	-3.204007
H	5.572889	0.402196	0.447035
H	3.462676	-0.143440	-0.430949
H	6.885564	2.345867	0.378390
H	10.642174	2.908274	2.342740
H	9.878472	-0.721784	0.214870
H	1.020261	-3.702909	-0.432933
H	-1.383007	-3.286694	-0.057142
H	-0.731800	0.900455	-0.843854
H	1.613320	0.460383	-1.266101
H	12.499962	1.334581	1.790180
H	11.734207	0.023369	2.684202
H	12.150112	-0.203670	0.986110
H	7.188679	4.228442	1.903606
H	8.678952	4.395292	2.844633
H	8.633839	4.915045	1.161966
H	-2.680515	0.742840	-1.456669
H	-8.243775	1.381008	0.437829
H	-4.605763	2.192539	-1.691808
H	-8.162322	-2.947782	1.894703
H	-8.093817	-2.322708	0.241470
H	-6.600851	-2.787628	1.076209
H	-7.381444	-1.538325	3.842035
H	-6.722871	0.081706	3.577384
H	-5.784735	-1.346174	3.103201
H	-9.466098	-0.348156	1.038725
H	-9.429081	-1.028987	2.664788
H	-8.909348	0.636298	2.407455
H	-6.826068	4.772295	-2.668451
H	-5.393931	4.304172	-1.752212
H	-5.954802	3.303332	-3.106666
H	-8.935265	3.534139	-2.542129
H	-9.154852	2.152700	-1.463273
H	-8.146501	1.991303	-2.908193
H	-6.782418	4.442453	0.398166
H	-8.139128	4.964207	-0.613550
H	-8.342273	3.614439	0.507390
F	-3.615967	-3.130943	0.041724

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3-BF_2

C	8.483414	-0.344088	-1.319904
C	7.654953	-1.047499	-2.176964

N	6.330003	-1.135329	-2.038248	H	11.791313	1.010556	2.241752
C	5.794288	-0.522675	-0.988424	H	10.405785	-0.279336	0.665481
C	6.539004	0.209260	-0.059922	H	1.706432	-3.466054	-0.780528
C	7.915825	0.316179	-0.224780	H	-0.719855	-3.176131	-0.429508
C	8.746083	1.089683	0.729774	H	-0.198997	1.094202	-0.680633
N	4.400465	-0.576493	-0.827286	H	2.172698	0.785237	-1.079042
C	3.569846	-1.634373	-1.141879	H	-2.130285	0.939313	-1.375086
C	2.117572	-1.370875	-0.923096	H	-7.724144	1.209742	0.521572
O	3.971710	-2.713722	-1.543737	H	-4.100974	2.344247	-1.482688
C	8.266485	2.274326	1.296214	H	-7.536935	-3.244646	1.506535
C	9.046119	2.999235	2.188413	H	-7.480532	-2.444127	-0.069677
C	10.316955	2.549879	2.531158	H	-5.978324	-2.960856	0.716617
C	10.803754	1.371852	1.974516	H	-6.790898	-2.033918	3.597567
C	10.025689	0.648598	1.079662	H	-6.170055	-0.380154	3.509771
C	1.273276	-2.473160	-0.746444	H	-5.198695	-1.727038	2.888540
C	-0.079602	-2.312136	-0.541377	H	-8.902562	-0.602395	0.931835
C	-0.648626	-1.020891	-0.523694	H	-8.848757	-1.451335	2.476244
C	0.198035	0.087831	-0.719985	H	-8.370415	0.244201	2.399054
C	1.554754	-0.091308	-0.914285	H	-6.391571	4.945896	-2.204884
N	-2.015400	-0.871477	-0.322383	H	-4.945248	4.421357	-1.343605
C	-2.658030	0.245638	-0.735272	H	-5.487643	3.550112	-2.791864
C	-4.013618	0.508460	-0.417426	H	-8.469812	3.658859	-2.199944
C	-4.759780	-0.420371	0.399345	H	-8.658287	2.170898	-1.267359
C	-6.119113	-0.177229	0.751094	H	-7.653711	2.177110	-2.724070
C	-6.695700	0.995961	0.272045	H	-6.321706	4.302590	0.812785
C	-6.000965	1.919781	-0.534568	H	-7.698006	4.894001	-0.132007
C	-4.657715	1.650003	-0.866725	H	-7.860506	3.429734	0.842797
O	-4.161687	-1.501186	0.814629	F	-2.146563	-2.283882	1.619137
C	-6.896894	-1.176590	1.610212	F	-2.968759	-3.100543	-0.350992
C	-6.967975	-2.540598	0.891909				
C	-6.211757	-1.338129	2.983164				
C	-8.336071	-0.707535	1.861346				
C	-6.716966	3.175095	-1.018700				
C	-5.824230	4.067051	-1.889065				
C	-7.949183	2.763057	-1.849603				
C	-7.176462	3.993586	0.205087				
B	-2.798756	-1.981997	0.446160				
H	9.547392	-0.289260	-1.516208				
H	8.075581	-1.558218	-3.039722				
H	6.046480	0.662147	0.793450				
H	4.006282	0.137613	-0.233580				
H	7.284517	2.643098	1.018592				
H	8.661665	3.921104	2.612203				
H	10.925590	3.115504	3.228831				