†Electronic Supporting Information

for

Aggregation-induced emission compounds based on 9, 10-diheteroarylanthracene and their applications in cell imaging

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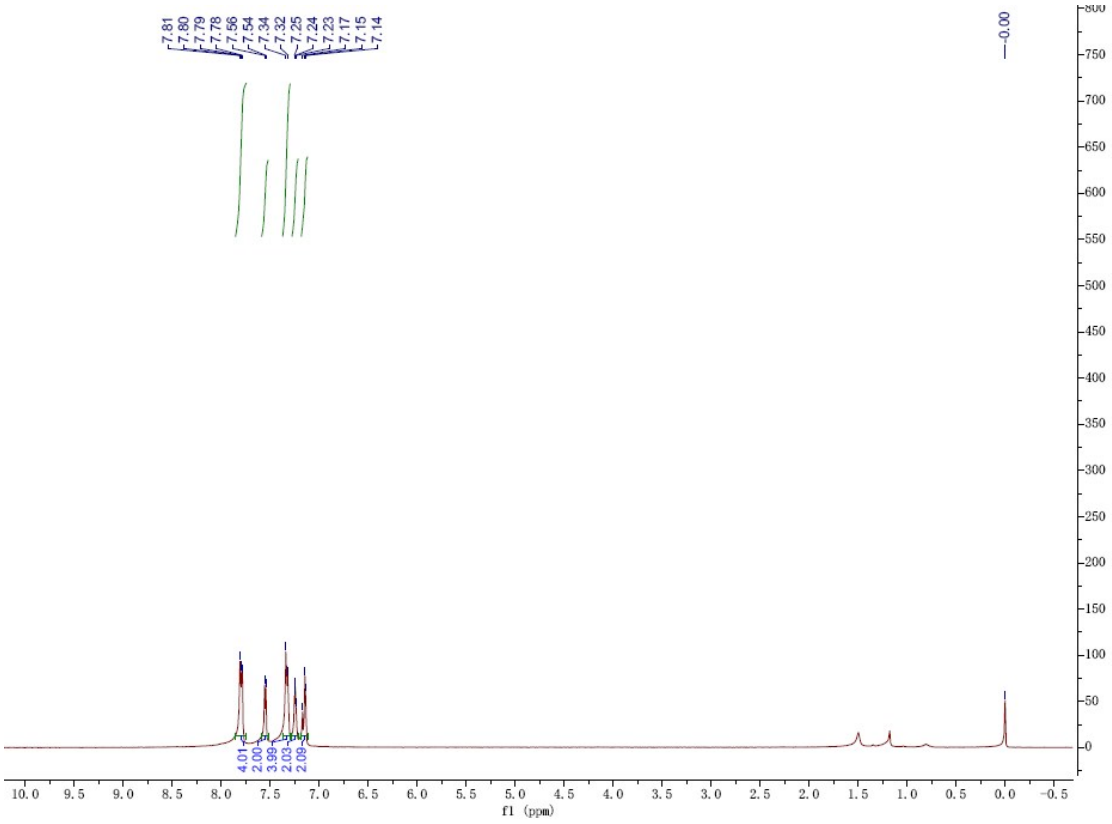
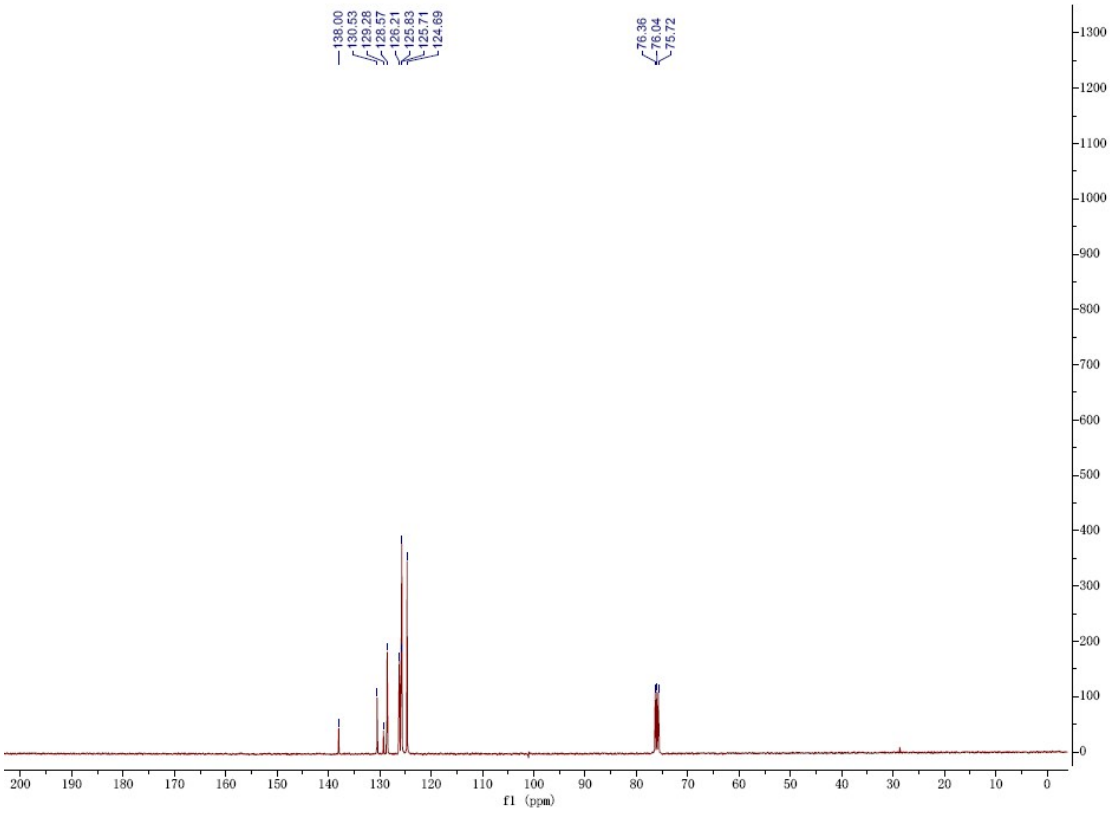
Table of Contents

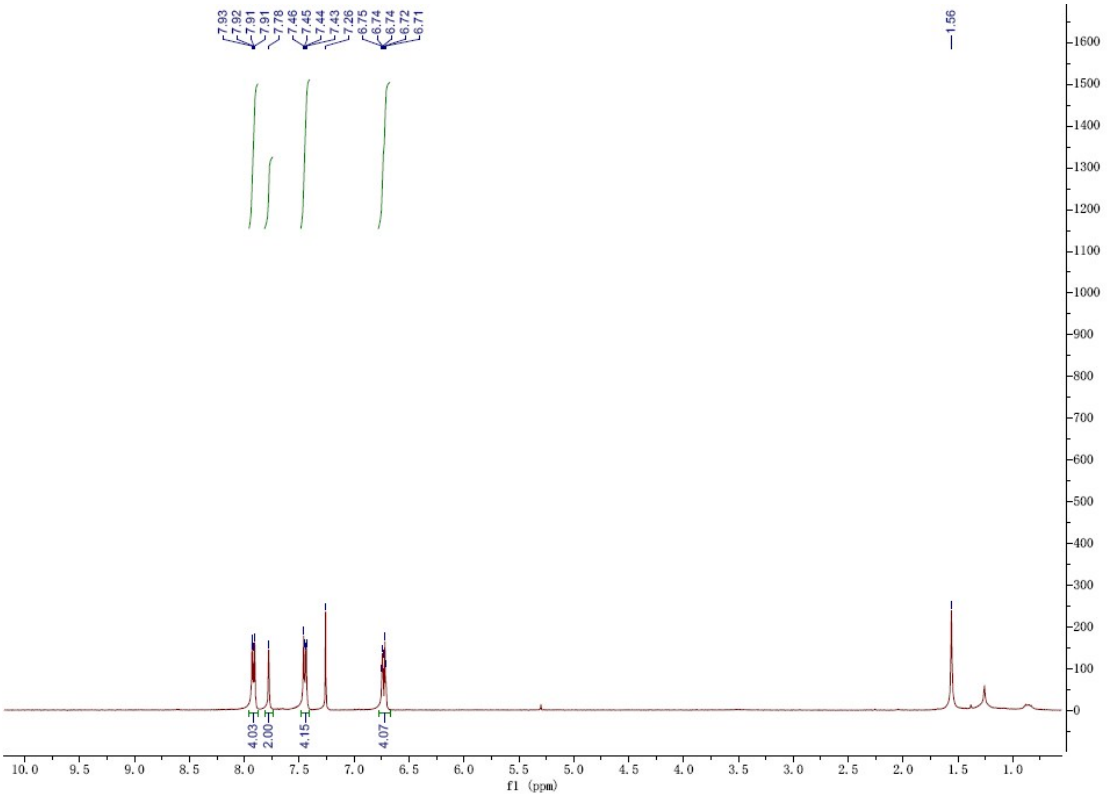


(A)



(B)

Figure S1. NMR spectra data for **DTA**: (A) ^{1}H-NMR spectra; (B) ^{13}C-NMR spectra.



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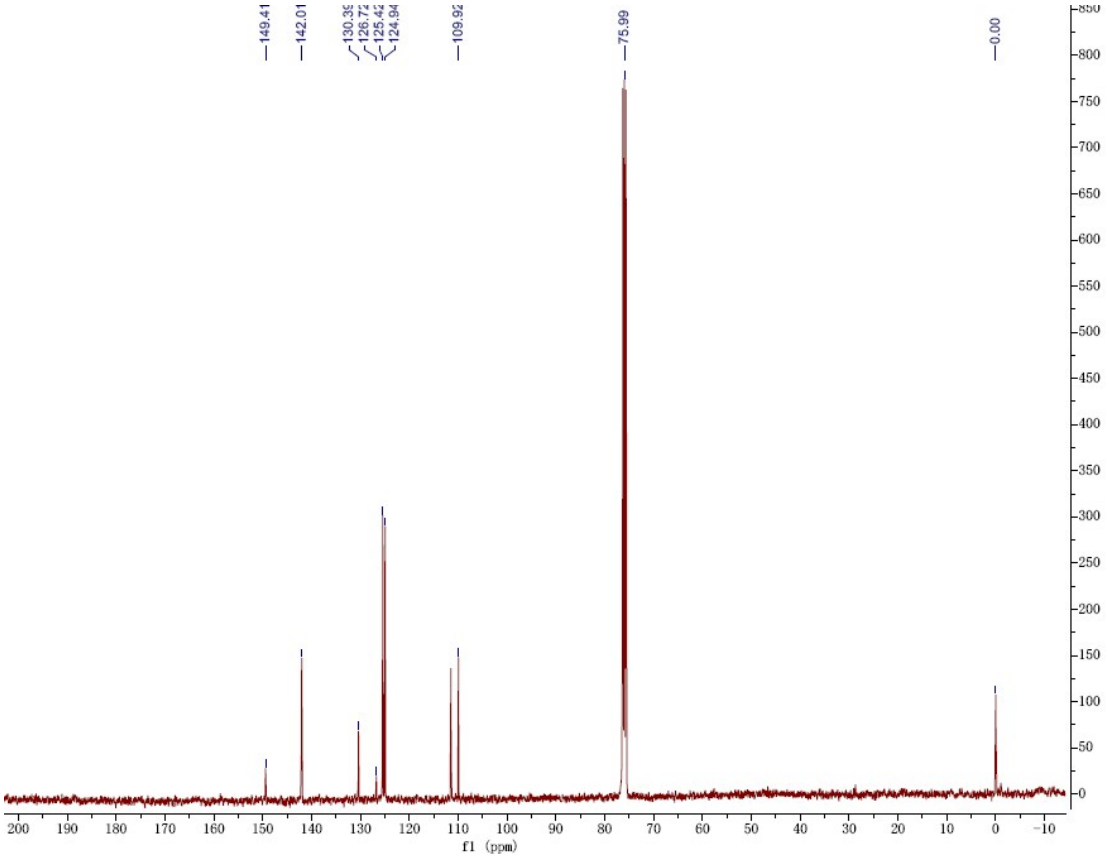
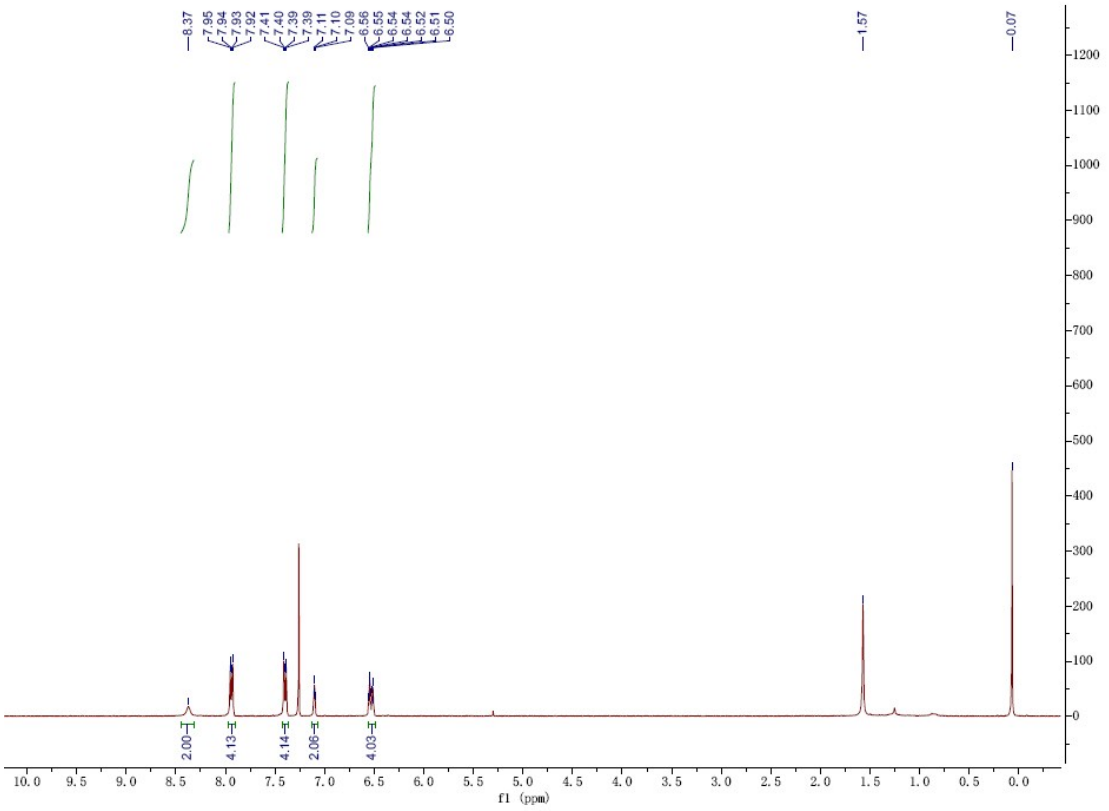


(B)

Figure S2. NMR spectra data for **DFA**: (A) ^{1}H-NMR spectra; (B) ^{13}C-NMR spectra.



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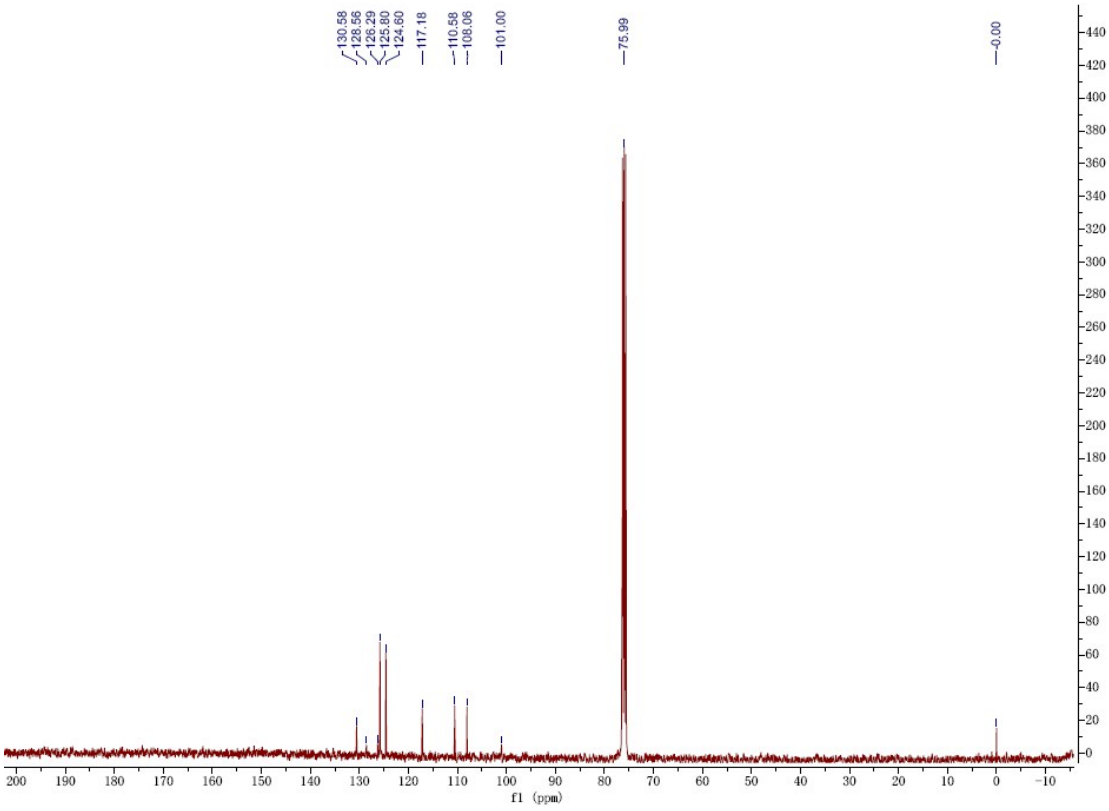
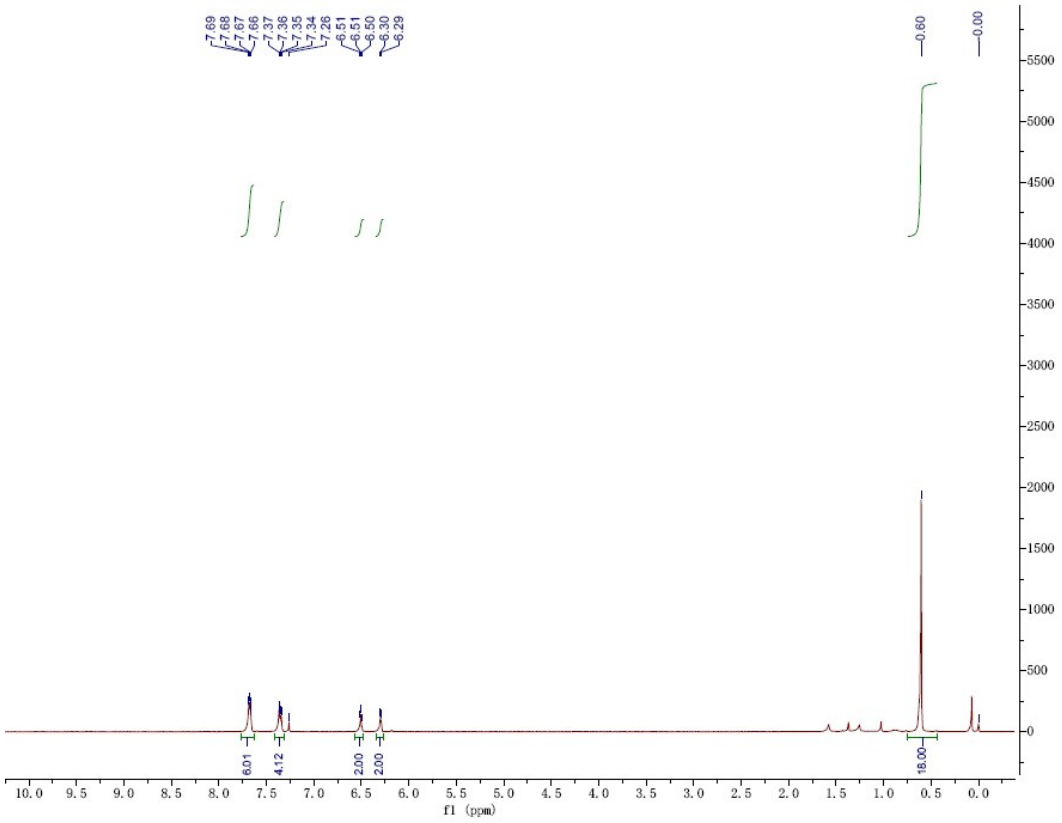
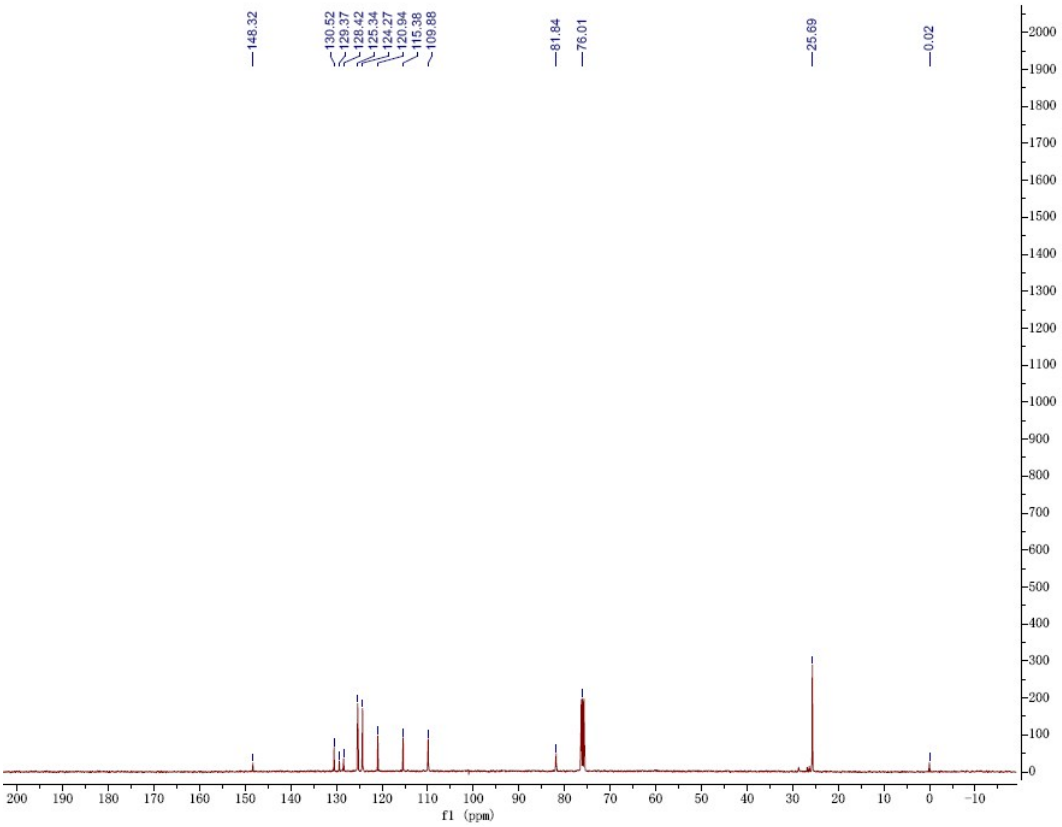


(B)

Figure S3. NMR spectra data for **DPA**: (A) ^{1}H-NMR spectra; (B) ^{13}C-NMR spectra.



(A)



(B)

Figure S4. NMR spectra data for **DBPA**: (A) ^{1}H-NMR spectra; (B) ^{13}C-NMR spectra.

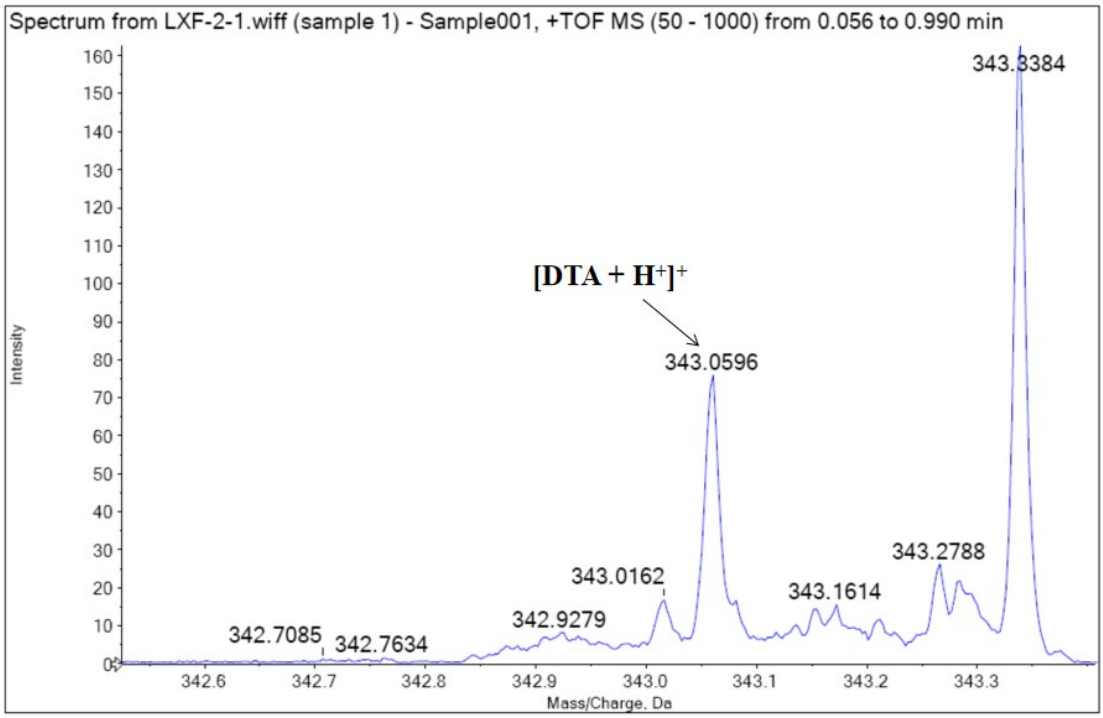


Figure S5. HRMS-ESI spectra of **DTA**.

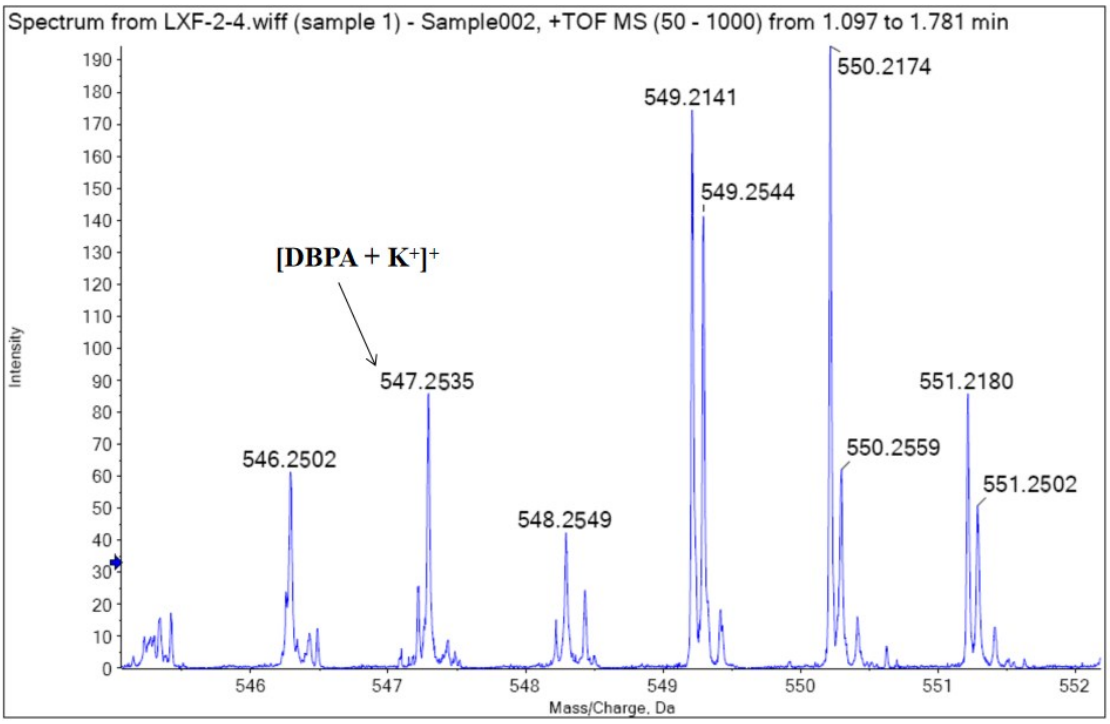


Figure S6. HRMS-ESI spectra of **DBPA**.

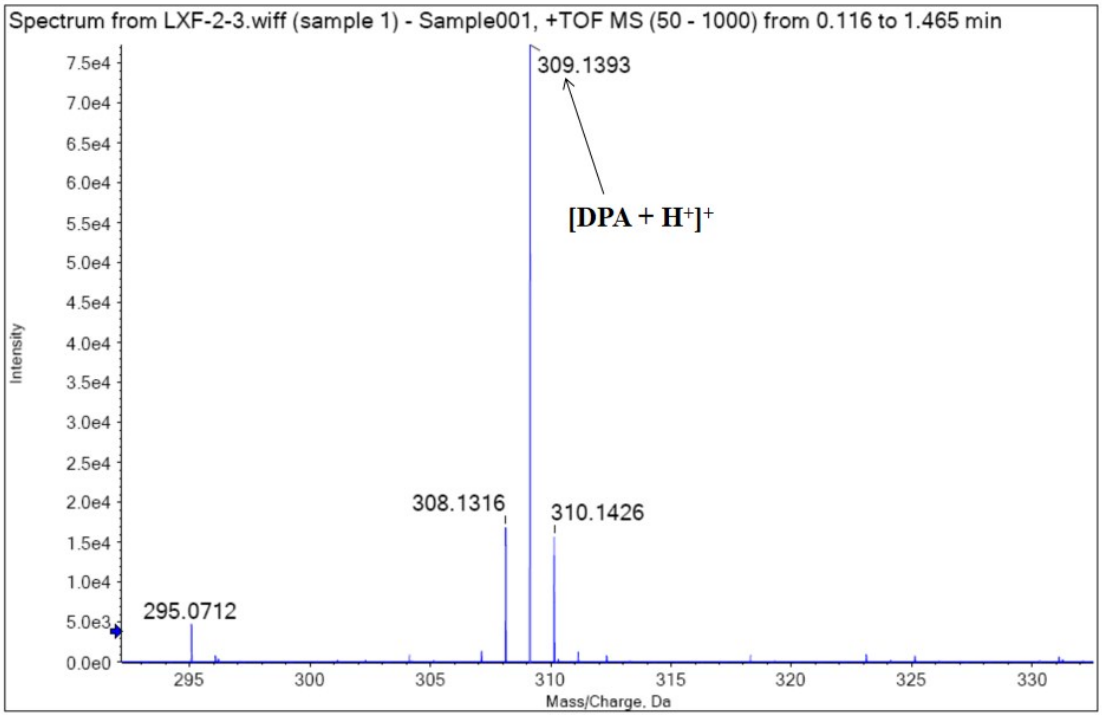


Figure S7. HRMS-ESI spectra of **DPA**.

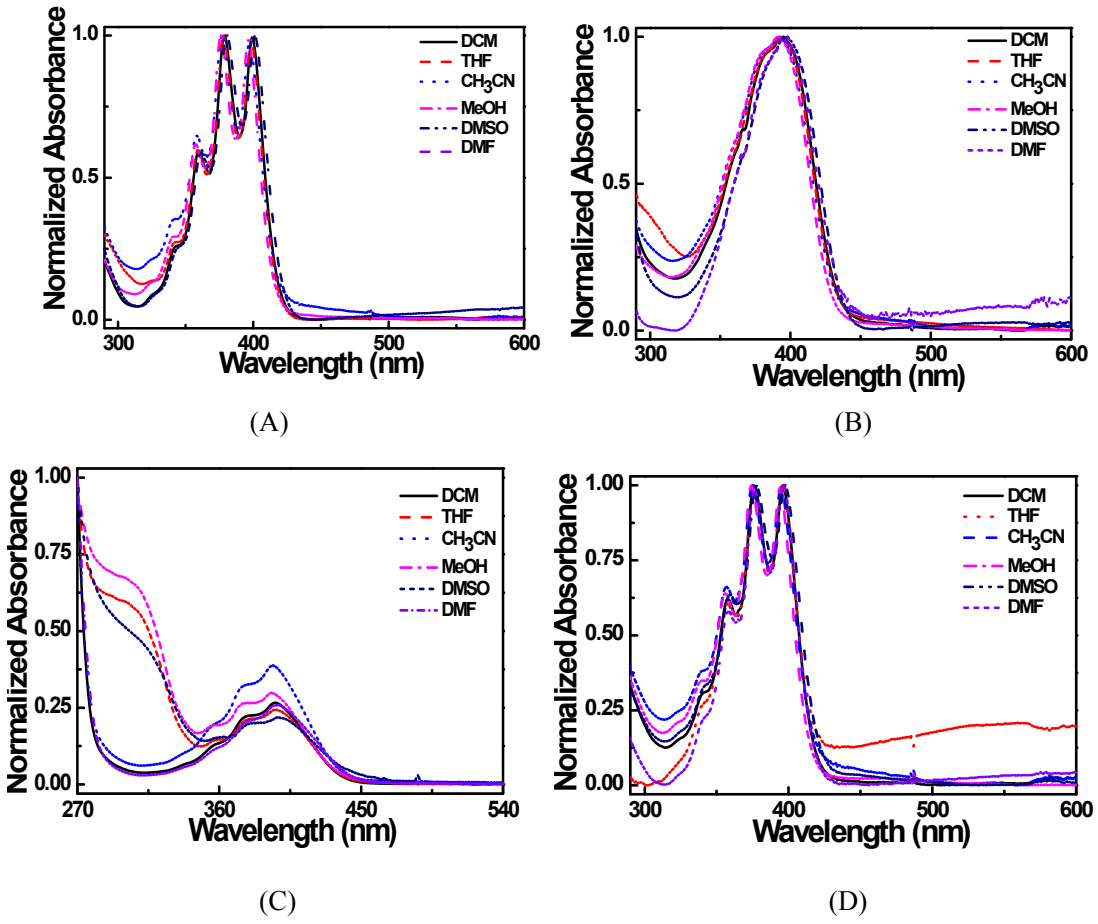


Figure S8. (A) Normalized absorption spectra of **DTA** (A), **DFA** (B), **DPA** (C) and **DBPA** (D) (*C* =2.0 × 10^{-5} mol/L) in different solvents.

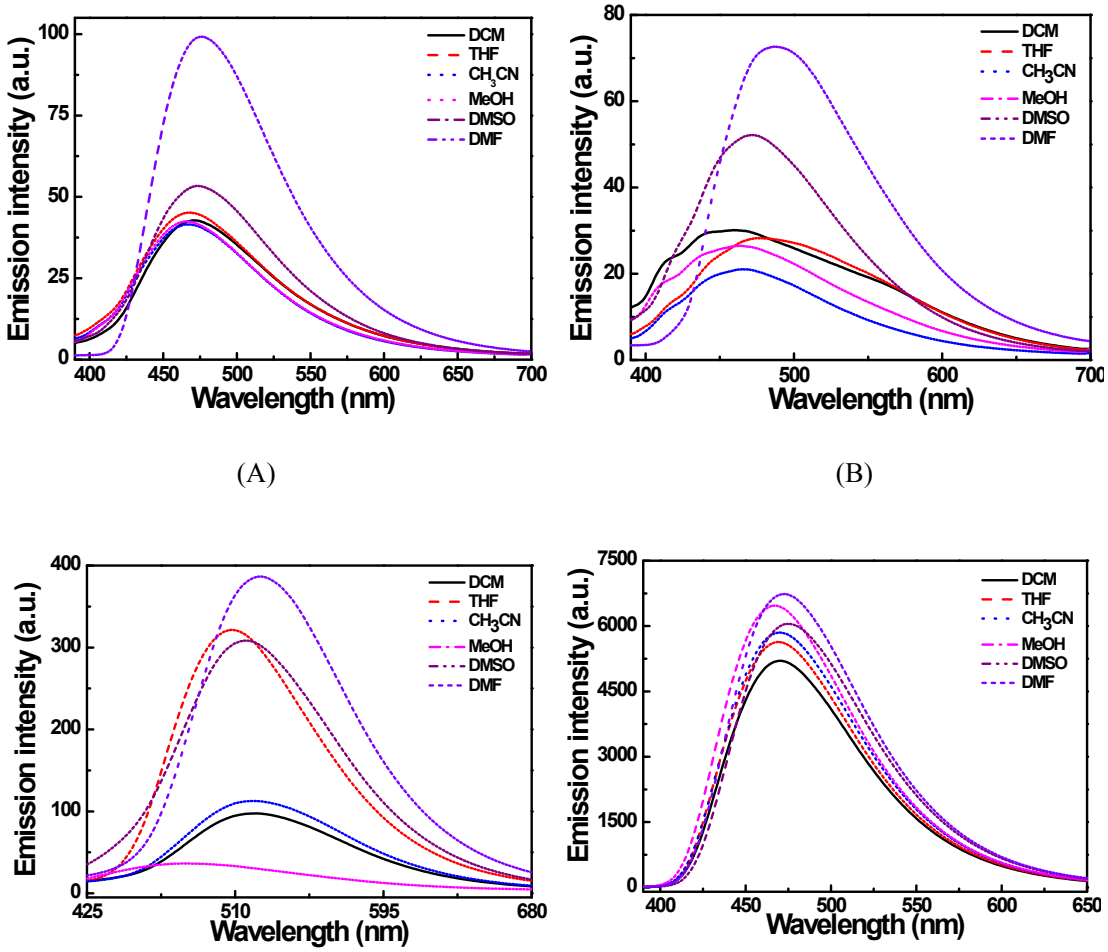
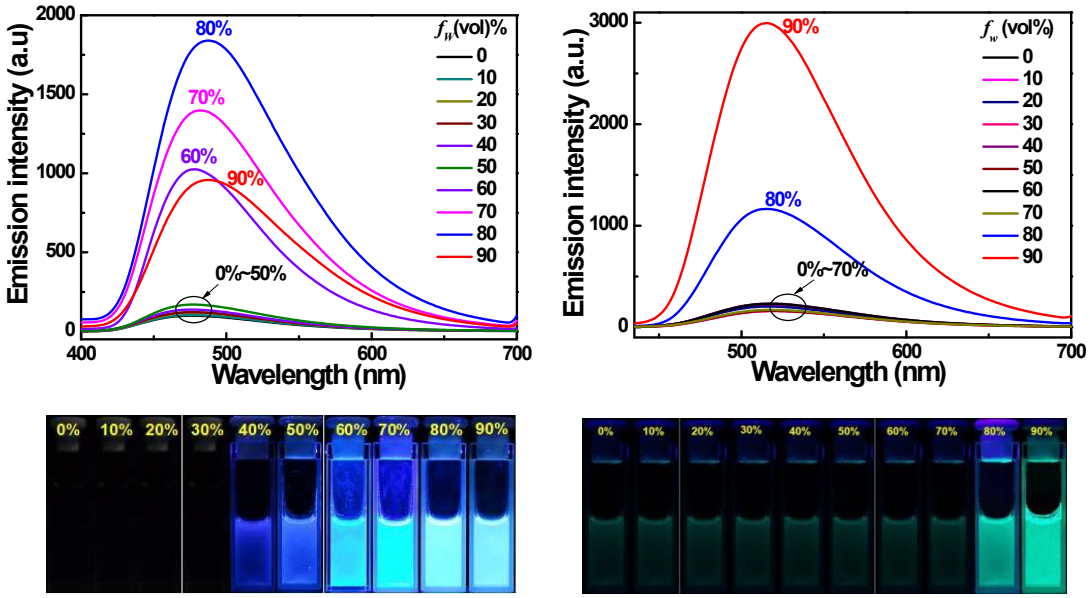
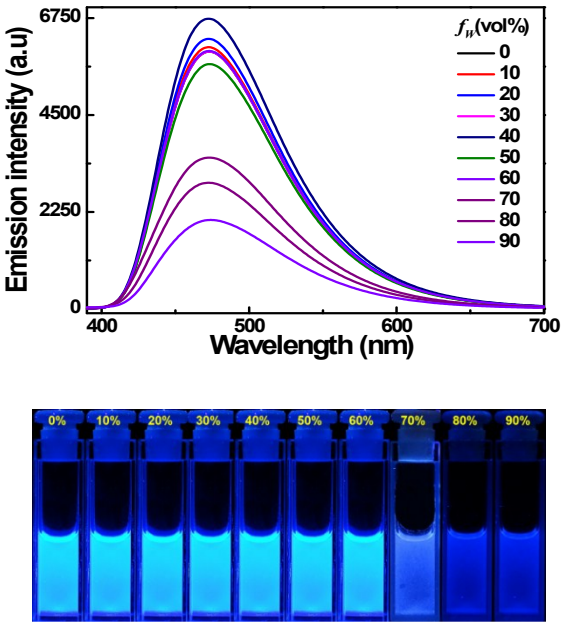


Figure S9. PL spectra of **DTA** (A), **DFA** (B), **DPA** (C) and **DBPA** (D) (C =2.0 × 10^{-5} mol/L) in different solvents (λ_{ex} = 355 nm).



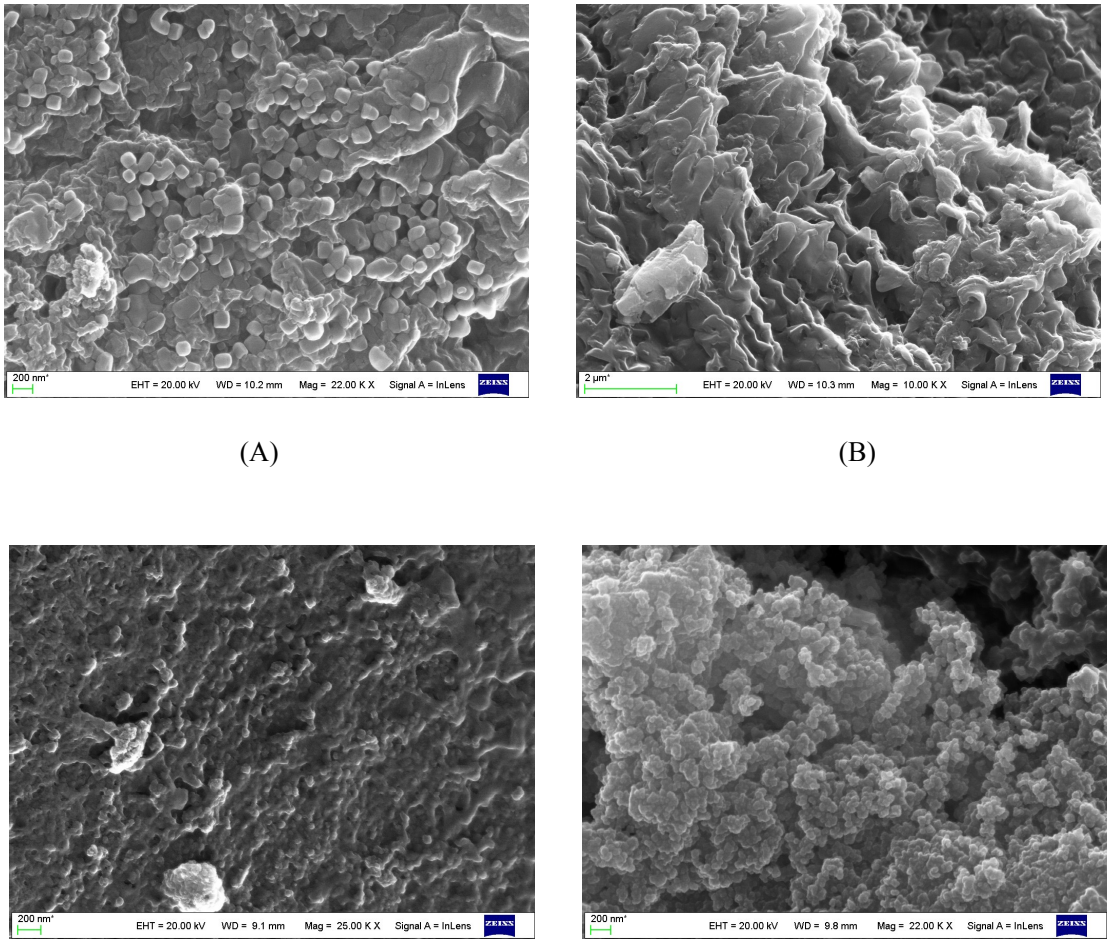
(A)

(B)



(C)

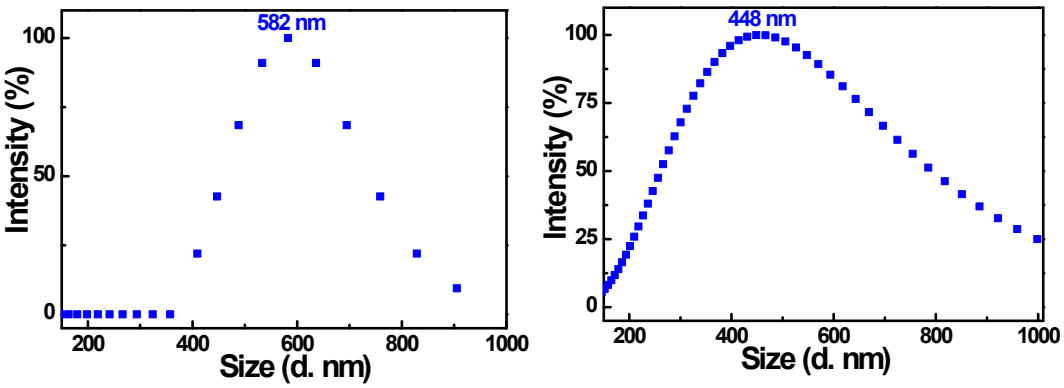
Figure S10. Changes of fluorescence spectra and color of **DTA** (A), **DPA** (B) and **DBPA** (C) (20 μM) in the different DMF/H_2O fraction solutions (λ_{ex} = 355 nm).



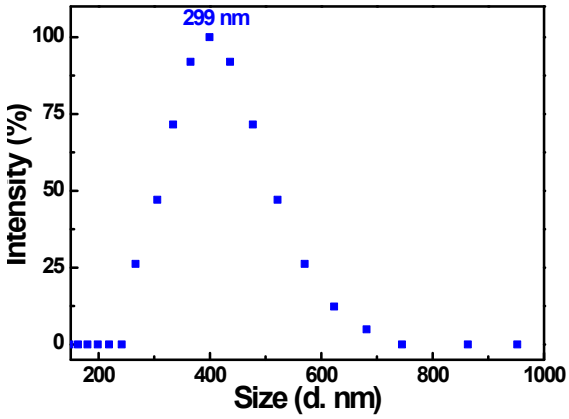
(A) (B)

(C) (D)

Figure S11. SEM images of **DHA** compound: (A) **DTA**; (B) **DFA**; (C) **DPA** and (D) **DBPA** (20 μM) formed from DMF/water mixture (f_w=90%).



(A) (B)



(C)

Figure S12. Size distribution curve of **DHA** compounds: (A) **DTA**, (B) **DFA** and (C) **DPA** (20 μM) in DMF/water mixtures with 90% volume fraction of water.

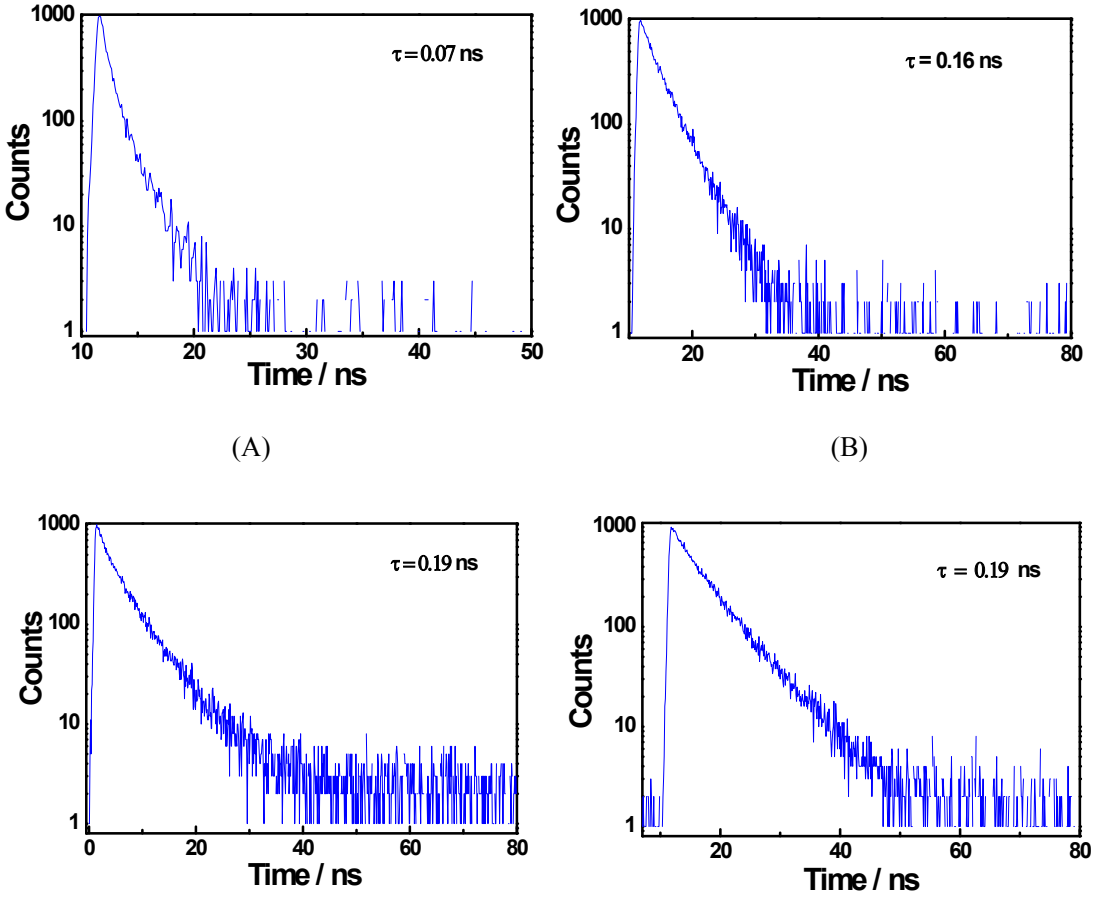


Figure S13. Decay curve of **DHA** compounds: (A) **DTA**, (B) **DFA** and (C) **DPA**, and **DBPA** (D) in solid state (λ_{ex} = 355 nm).

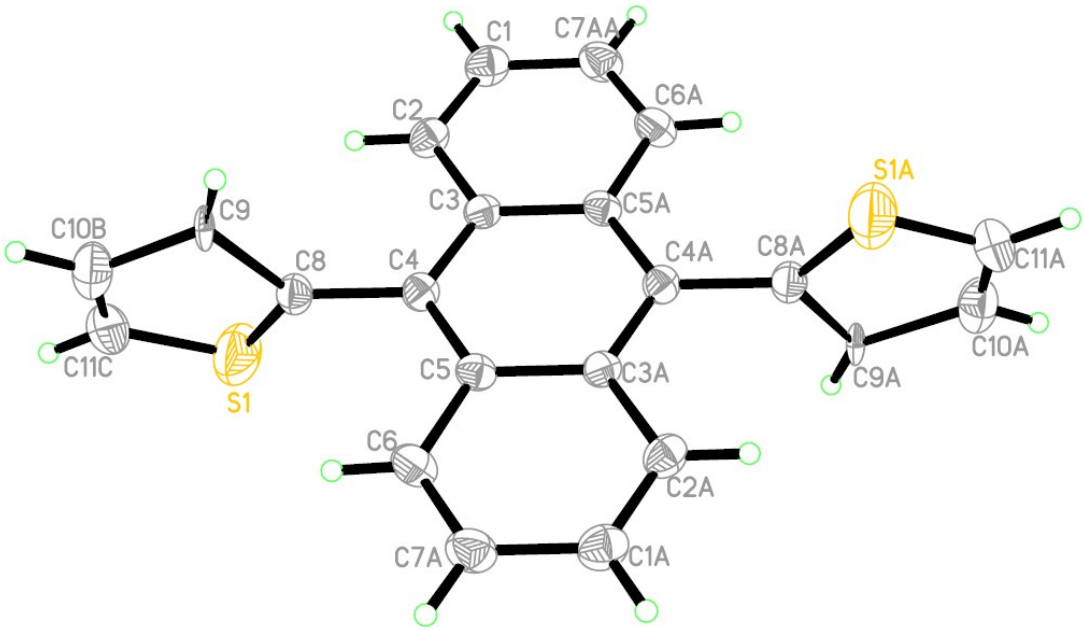


Figure S14. ORTEP drawings of crystal of **DTA** showing about 30% probability displacement ellipsoids.

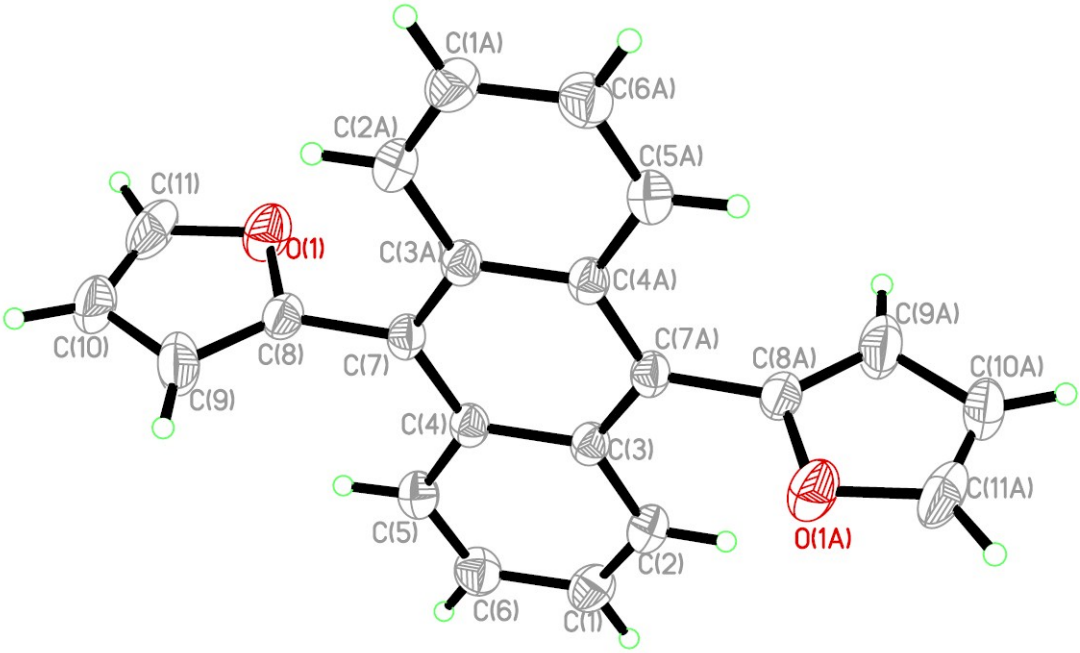


Figure S15. ORTEP drawings of crystal of **DFA** showing about 30% probability displacement ellipsoids.

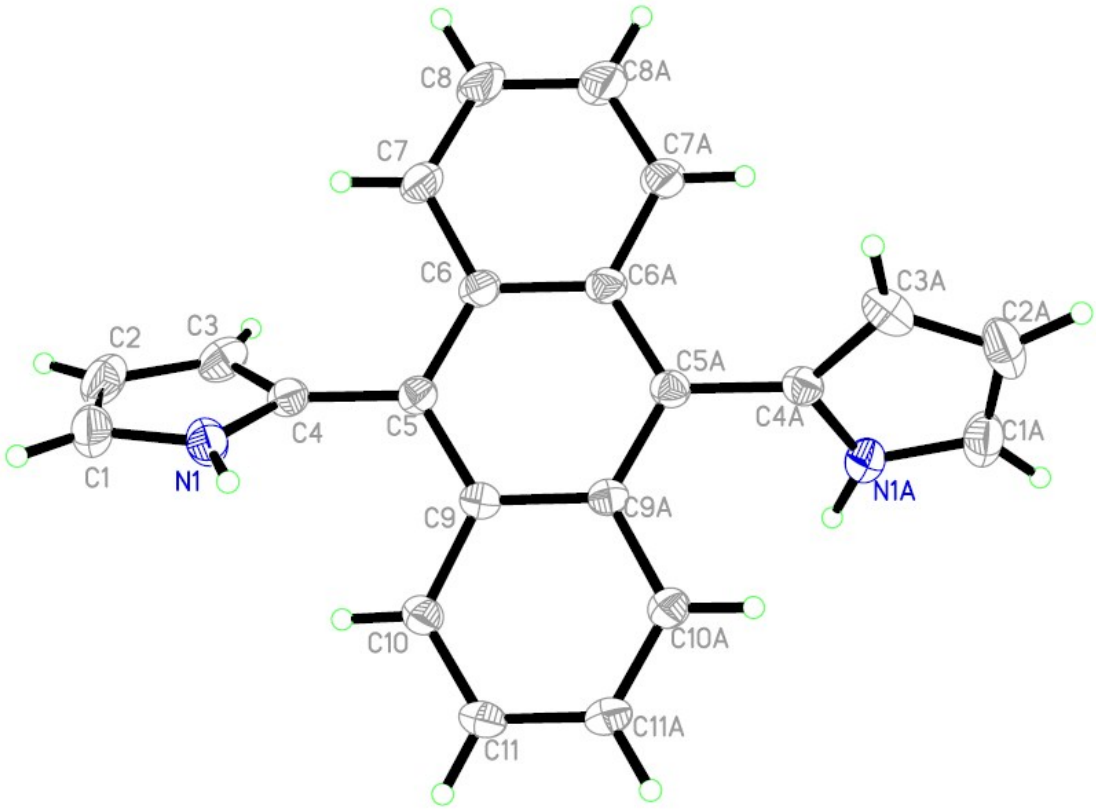


Figure S16. ORTEP drawings of crystal of **DPA** showing about 30% probability displacement ellipsoids.

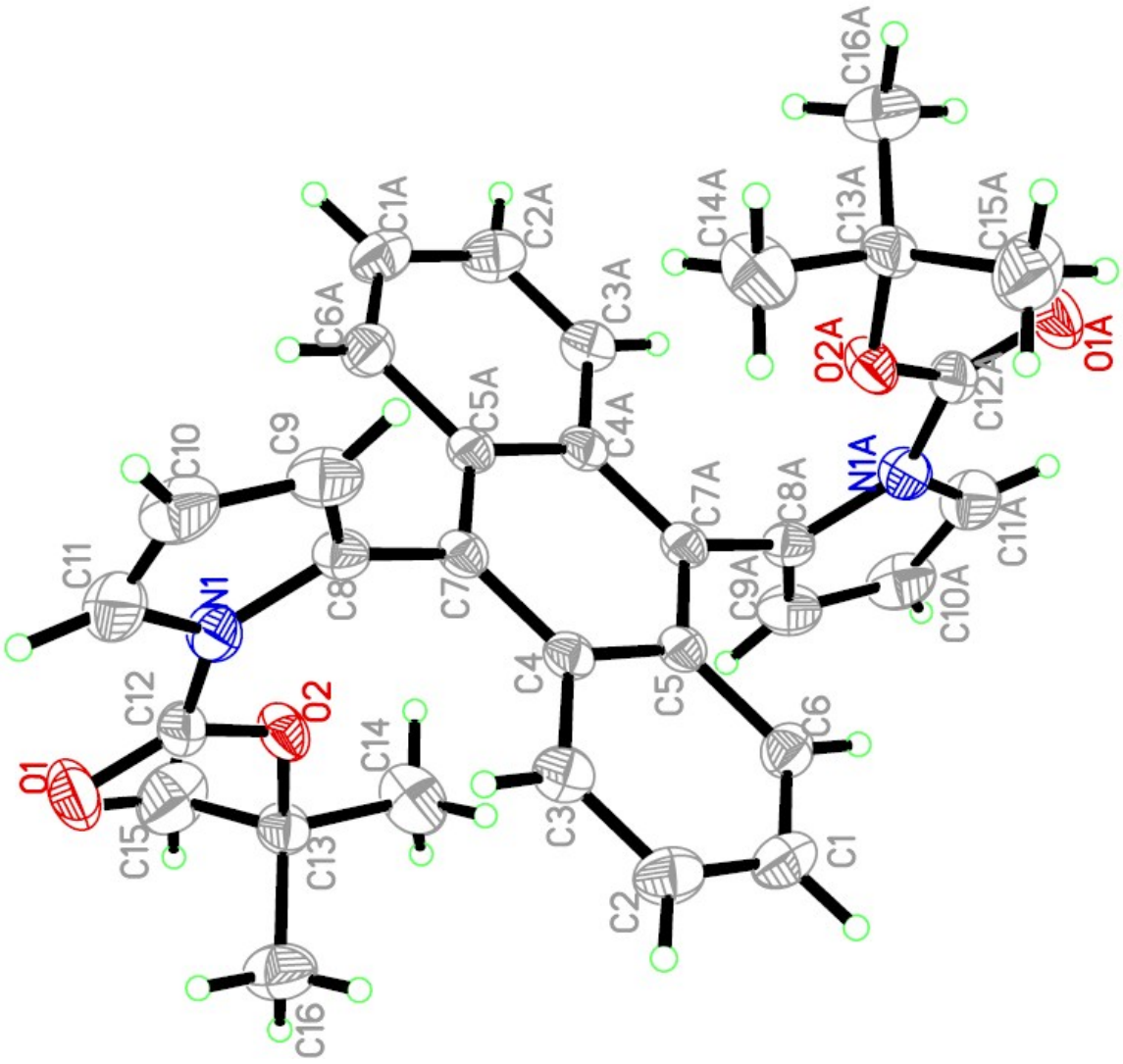


Figure S17. ORTEP drawings of crystal of **DBPA** showing about 30% probability displacement ellipsoids.

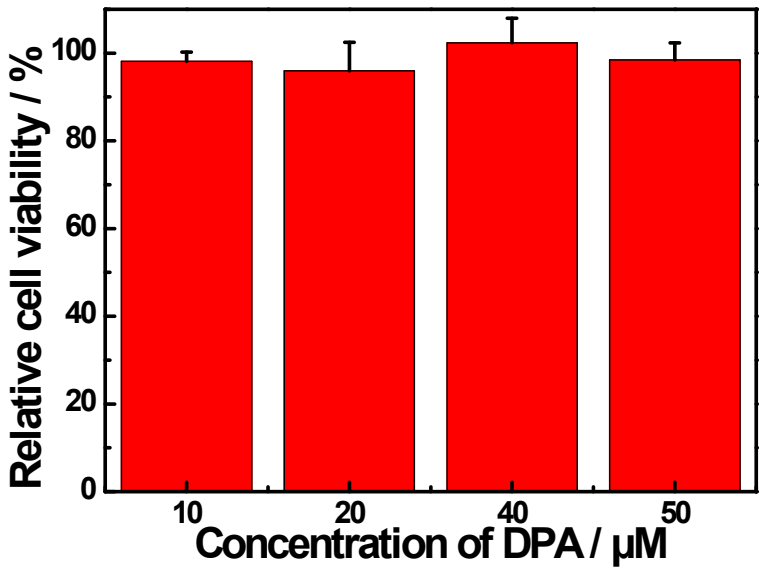


Figure S18. % cell viability of HeLa cells treated with different concentrations (10→50 μM) of **DPA** for 24 h determined by MTT assay.

Table S1. Absorption and fluorescence spectral properties of **DHA** compounds in different solvents.

Solvents	DTA		DFA		DPA		DBPA	
	λ_{em} (nm)[a] I_{max}	λ (nm)[b]	λ_{em} (nm)[a] I_{max}	λ (nm)[b]	λ_{em} (nm)[a] I_{max}	λ (nm)[b]	λ_{em} (nm)[a] I_{max}	λ (nm)[b]
n-Hexane	467, 53.59	376, 396	448, 270.9	393	512, 61.95	394	464,3835	376, 396
DCM	470, 42.76	379, 399	459, 30.09	395	522, 97.51	396	470,5202	376, 396
THF	468, 45.16	378, 398	481, 28.2	393	508, 312.4	396	469,5633	374, 394
Acetonitrile	468, 41.5	377, 397	468, 21.02	392	519, 112.6	394	470,5850	375, 395
DMSO	473, 53.36	381, 401	473, 52.14	398	516, 308.4	397	475,6050	378, 398
DMF	476, 99.21	379, 399	488, 72.62	398	525, 386.5	398	473,6734	375, 395

[a] Fluorescence emission wavelength; [b] Absorption wavelength.

Table S2. Crystal data for **DHA** compounds.

	Compounds			
	DTA	**DFA**	**DPA**	**DBPA**
Formula	$C_{22}H_{14}S_2$	$C_{22}H_{14}O_2$	$C_{22}H_{16}N_2$	$C_{32}H_{32}N_2O_4$
Formula weight	342.45	310.33	308.37	508.60
Temperature	296(2)	296(2)	296(2)	296(2)
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Monoclinic
Space group	P2(1)/c	P2(1)/n	Pbcn	P2(1)/n
Unit cell dimensions *a* (Å)	9.8461(12)	9.1632(14)	18.3966(19)	9.3335(10)
b (Å)	9.2276(11)	8.9491(14)	11.3788(12)	10.1341(12)
c (Å)	10.1454(12)	10.3448(16)	7.4311(8)	15.0800(18)
α (°)	90.00	90.00	90.00	90.00
β (°)	115.242(2)	111.284(2)	90	101.550(2)
γ (°)	90.00	90.00	90.00	90.00
Volume ($Å^3$)	833.75(17)	790.4(2)	1555.6(3)	1397.5(3)
Z	2	2	4	2
Density (calcd.) (g/cm^3)	1.364	0.083	1.317	1.209
Goodness-of-fit on F^2	2.478	1.049	0.942	1.015
Final R_1[I >2s(I)]	0.1595	0.0421	0.0449	0.0487
wR_2[I >2s(I)]	0.4885	0.1127	0.1228	0.1205
R_1 (all data)	0.1733	0.0577	0.0644	0.0803
wR_2 (all data)	0.5128	0.1248	0.1433	0.1432

Table S3. Symbolic Z-Matrix of **DTA**.

S	-0.78906	0.8125	0
C	-1.50956	2.2483	-2.3208
H	-1.54766	2.8618	-3.0187
C	-0.20906	4.4334	0.0853
C	0.30194	3.2901	-0.5515
C	1.67584	3.1886	-0.8635
C	2.19964	2.0268	-1.5151
H	1.63804	1.3139	-1.719
C	-0.63576	2.1938	-0.9351
C	-1.58046	4.5635	0.4588
H	-2.16476	3.8639	0.2736
C	3.52564	1.9659	-1.8381
H	3.85844	1.2184	-2.2801
C	-2.05426	5.6634	1.0691
H	-2.95906	5.7256	1.2738
C	-2.26556	0.8826	-2.0455
H	-2.91836	0.5808	-2.6346
C	-1.96156	0.185	-0.9819
H	-2.38366	-0.6212	-0.7881
S	3.14484	7.8937	-0.4331
C	3.86534	6.4579	1.8876
H	3.90334	5.8444	2.5856
C	2.56474	4.2728	-0.5185
C	2.05384	5.4161	0.1184
C	0.67984	5.5176	0.4304
C	0.15604	6.6794	1.0819
H	0.71764	7.3923	1.2858
C	2.99144	6.5124	0.502
C	3.93614	4.1427	-0.892
H	4.52044	4.8423	-0.7067
C	-1.16986	6.7403	1.4049
H	-1.50276	7.4878	1.8469
C	4.40994	3.0428	-1.5022
H	5.31484	2.9806	-1.7069
C	4.62134	7.8236	1.6123
H	5.27414	8.1254	2.2015
C	4.31734	8.5212	0.5488
H	4.73944	9.3274	0.3549

Table S4. Total energies of **DTA**.

Zero-point correction	0.287010 (Hartree/Particle)
Thermal correction to Energy	0.305716
Thermal correction to Enthalpy	0.30666
Thermal correction to Gibbs Free Energy	0.237965
Sum of electronic and zero-point Energies	-1643.074475
Sum of electronic and thermal Energies	-1643.055769
Sum of electronic and thermal Enthalpies	-1643.054825
Sum of electronic and thermal Free Energies	-1643.12352

Table S5. Symbolic Z-Matrix of **DFA**.

O	-0.66406	0.89062	0
C	0.18384	3.12212	-2.3226
C	0.70494	2.00772	-1.6363
C	1.04784	4.22072	-2.6496
C	-0.18586	0.88582	-1.2682
C	-1.18796	3.19762	-2.7205
H	-1.75626	2.48492	-2.5363
C	0.48034	5.35342	-3.3177
H	1.02234	6.08062	-3.5236
C	-0.83306	5.38512	-3.6557
H	-1.18156	6.13322	-4.0843
C	-1.67556	4.28912	-3.3612
H	-2.57166	4.31662	-3.6088
C	-1.44846	-0.23438	0.1111
H	-1.90516	-0.48278	0.8827
C	-1.46856	-0.90108	-0.9945
H	-1.92576	-1.69328	-1.1615
C	-0.65646	-0.18328	-1.9006
H	-0.48126	-0.41858	-2.7834
O	3.78114	5.28632	-3.9342
C	2.93314	3.05482	-1.6116
C	2.41214	4.16922	-2.2979
C	2.06914	1.95622	-1.2845
C	3.30284	5.29112	-2.666
C	4.30504	2.97932	-1.2137
H	4.87324	3.69202	-1.3978
C	2.63664	0.82352	-0.6164
H	2.09474	0.09632	-0.4106
C	3.95004	0.79182	-0.2785
H	4.29854	0.04372	0.1501
C	4.79254	1.88782	-0.573
H	5.68864	1.86032	-0.3254
C	4.56544	6.41132	-4.0453
H	5.02224	6.65972	-4.8169
C	4.58554	7.07802	-2.9397
H	5.04274	7.87022	-2.7727
C	3.77354	6.36022	-2.0336
H	3.59824	6.59552	-1.1508

Table S6. Total energies of **DFA**.

Zero-point correction	0.293742 (Hartree/Particle)
Thermal correction to Energy	0.311371
Thermal correction to Enthalpy	0.312315
Thermal correction to Gibbs Free Energy	0.246901
Sum of electronic and zero-point Energies	-997.097435
Sum of electronic and thermal Energies	-997.079805
Sum of electronic and thermal Enthalpies	-997.078861
Sum of electronic and thermal Free Energies	-997.144276

Table S7. Symbolic Z-Matrix of **DPA**.

C	-1.67969	1.73437	0
H	-0.92709	2.09997	0.4063
C	-1.68609	0.92397	-1.0775
H	-0.93809	0.62997	-1.5455
C	-3.03119	0.59977	-1.3711
H	-3.32679	0.05427	-2.0635
C	-3.82229	1.23827	-0.4452
C	-5.28669	1.24047	-0.2359
C	-5.98459	0.02147	-0.0981
C	-5.31779	-1.23653	-0.1479
H	-4.39249	-1.25593	-0.2406
C	-5.99569	-2.40093	-0.0647
H	-5.53519	-3.20783	-0.1054
C	-5.99159	2.46037	-0.1427
C	-5.35749	3.72347	-0.356
H	-4.46309	3.74337	-0.6099
C	-6.02239	4.89067	-0.1977
H	-5.58899	5.69647	-0.3645
N	-2.96829	1.92187	0.3871
H	-3.23859	2.47807	1.0574
C	-11.71089	1.73437	0.0193
H	-12.46349	2.09997	-0.387
C	-11.70449	0.92397	1.0968
H	-12.45249	0.62997	1.5647
C	-10.35939	0.59977	1.3903
H	-10.06379	0.05427	2.0828
C	-9.56829	1.23827	0.4644
C	-8.10389	1.24047	0.2551
C	-7.40599	0.02147	0.1174
C	-8.07279	-1.23653	0.1672
H	-8.99809	-1.25593	0.2599
C	-7.39489	-2.40093	0.0839
H	-7.85539	-3.20783	0.1247
C	-7.39899	2.46037	0.162
C	-8.03309	3.72347	0.3752
H	-8.92749	3.74337	0.6291
C	-7.36819	4.89067	0.217
H	-7.80159	5.69647	0.3838
N	-10.42229	1.92187	-0.3679
H	-10.15199	2.47807	-1.0382

Table S8. Total energies of **DPA**.

Zero-point correction	0.318959 (Hartree/Particle)
Thermal correction to Energy	0.337061
Thermal correction to Enthalpy	0.338005
Thermal correction to Gibbs Free Energy	0.271924
Sum of electronic and zero-point Energies	-957.352745
Sum of electronic and thermal Energies	-957.334642
Sum of electronic and thermal Enthalpies	-957.333698
Sum of electronic and thermal Free Energies	-957.39978

Table S9. Symbolic Z-Matrix of **DBPA**.

C	-0.5567	-0.44714	-3.6222
H	-0.97039	-0.78202	-4.56534
C	0.55398	0.4527	-3.62195
H	0.96698	0.78899	-4.5649
C	1.08616	0.88275	-2.44199
H	1.92773	1.57158	-2.4456
C	0.56183	0.45297	-1.18235
C	-0.56273	-0.45108	-1.18261
C	-1.08799	-0.87897	-2.44249
H	-1.92954	-1.56782	-2.4465
C	1.11352	0.88902	0.0387
C	2.23497	1.86208	0.03903
C	2.14808	3.22988	0.07159
H	1.21936	3.78221	0.10382
C	3.46953	3.77663	0.03987
H	3.73727	4.82301	0.0531
C	4.34199	2.73076	-0.01178
H	5.41737	2.68486	-0.04379
C	4.27696	0.29879	-0.04488
C	3.87584	-2.1219	-0.03989
C	2.56151	-2.8985	0.03001
H	2.76516	-3.97216	0.0039
H	2.01966	-2.67221	0.95296
H	1.91739	-2.64574	-0.816
C	4.74692	-2.40527	1.18776
H	4.96729	-3.47302	1.23642
H	5.69066	-1.85847	1.14855
H	4.21535	-2.12152	2.10356
C	4.60617	-2.39091	-1.35743
H	4.83922	-3.45861	-1.43305
H	3.97229	-2.13157	-2.20892
H	5.53718	-1.83142	-1.41988
N	3.60955	1.54617	-0.01227
O	5.4815	0.2303	-0.10245
O	3.41124	-0.70722	-0.00702
C	0.55673	0.43435	3.69908
H	0.98324	0.76922	4.64222
C	-0.55396	-0.43988	3.69883
H	-0.97976	-0.77617	4.64178
C	-1.09895	-0.86992	2.51887
H	-1.94052	-1.54595	2.52248
C	-0.56181	-0.45294	1.25922

C	0.56275	0.4511	1.25949
C	1.10082	0.86618	2.51937
H	1.94239	1.54222	2.52338
C	-1.1135	-0.88899	0.03818
C	-2.23494	-1.86206	0.03785
C	-2.14803	-3.22987	0.06935
H	-1.21931	-3.78219	0.10119
C	-3.46948	-3.77663	0.03701
H	-3.7372	-4.82302	0.0494
C	-4.34195	-2.73078	-0.01384
H	-5.41733	-2.68489	-0.04589
C	-4.27696	-0.2988	-0.04482
C	-3.8759	2.12189	-0.03699
C	-2.5616	2.89853	0.03406
H	-2.76528	3.97218	0.00893
H	-1.91723	2.64663	-0.81201
H	-2.01998	2.67141	0.95695
C	-4.60604	2.39243	-1.35433
H	-4.83926	3.46017	-1.42862
H	-5.53695	1.83279	-1.41764
H	-3.97195	2.13431	-2.20606
C	-4.74719	2.40369	1.19086
H	-4.96745	3.47138	1.24086
H	-4.21581	2.11874	2.10642
H	-5.69099	1.85698	1.15078
N	-3.60952	-1.54618	-0.01335
O	-5.4815	-0.23034	-0.10255
O	-3.41127	0.70722	-0.0058

Table S10. Total energies of **DBPA**.

Zero-point correction	0.571287 (Hartree/Particle)
Thermal correction to Energy	0.606308
Thermal correction to Enthalpy	0.607252
Thermal correction to Gibbs Free Energy	0.501016
Sum of electronic and zero-point Energies	-1648.917864
Sum of electronic and thermal Energies	-1648.882843
Sum of electronic and thermal Enthalpies	-1648.881899
Sum of electronic and thermal Free Energies	-1648.988135