

†Electronic Supporting Information

for

AIEE compounds based on 9, 10-dithienylanthracene-substituted triphenylamine: design, synthesis, and applications in cell imaging

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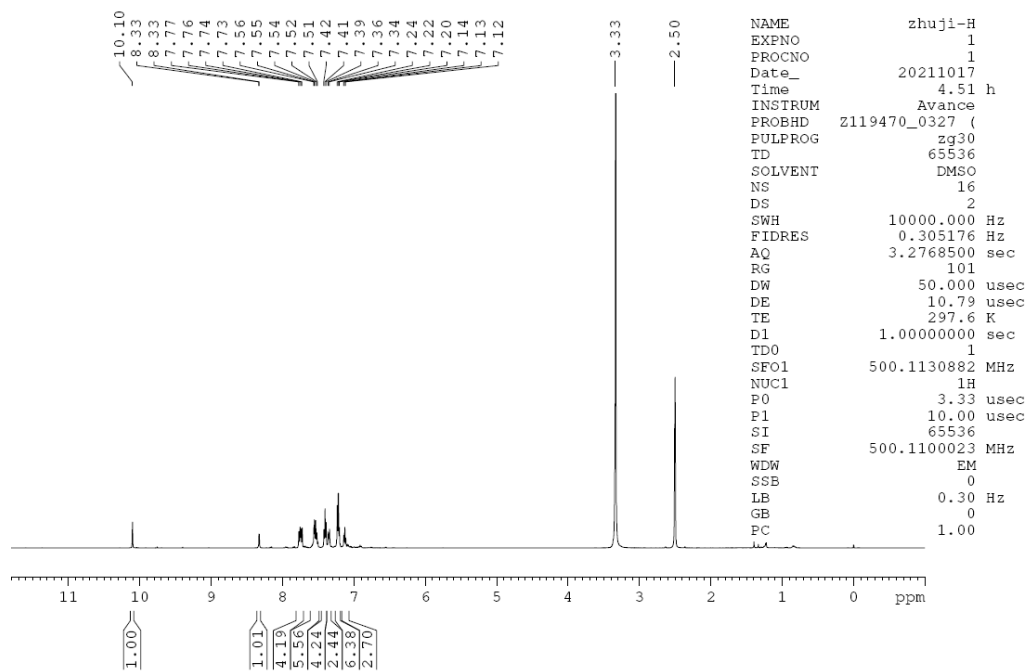
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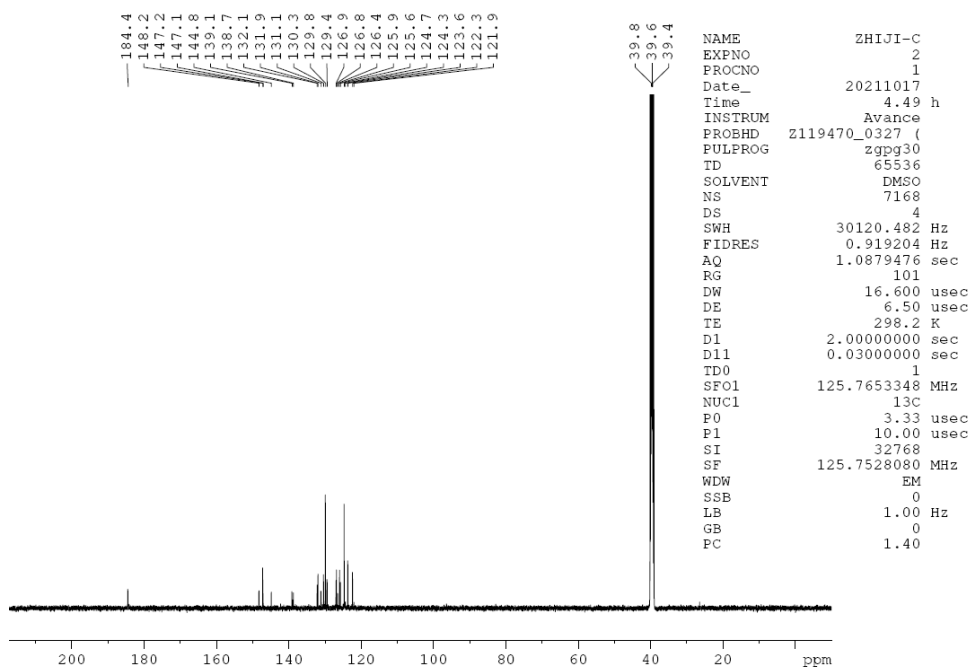
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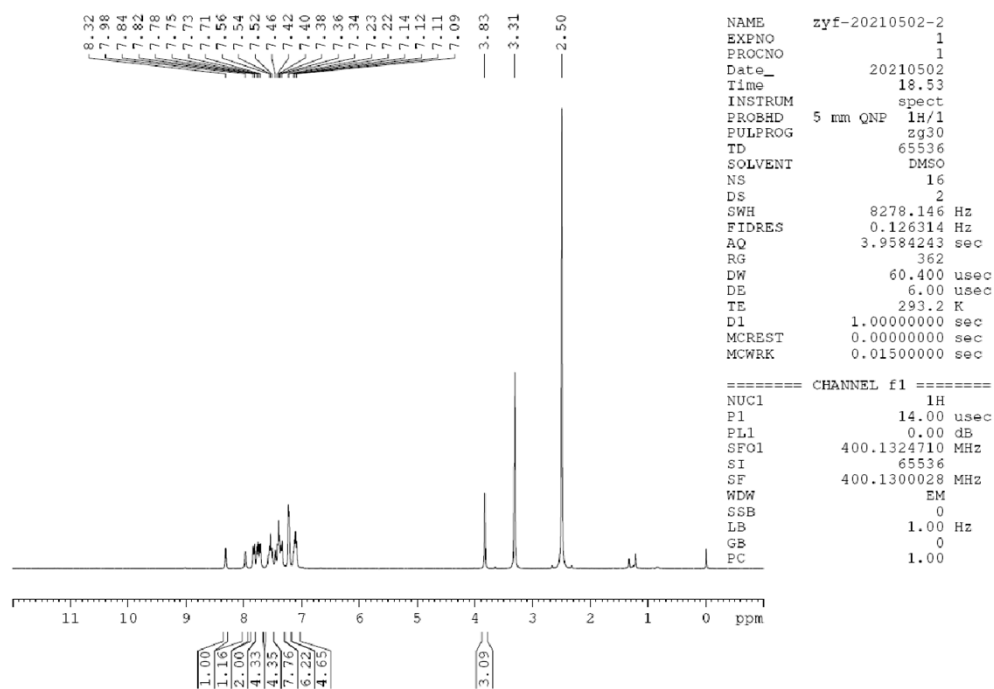


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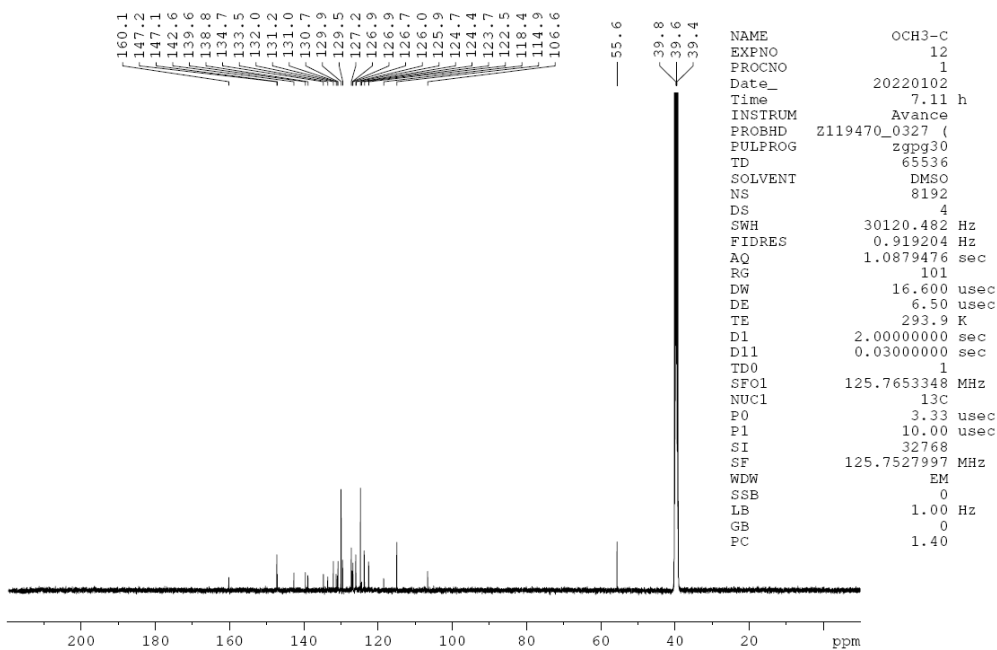


(B)

Figure S1. NMR spectra data for TPA-DTA-C in DMSO- d_6 : (A) ^1H -NMR spectra; (B) ^{13}C -NMR spectra.

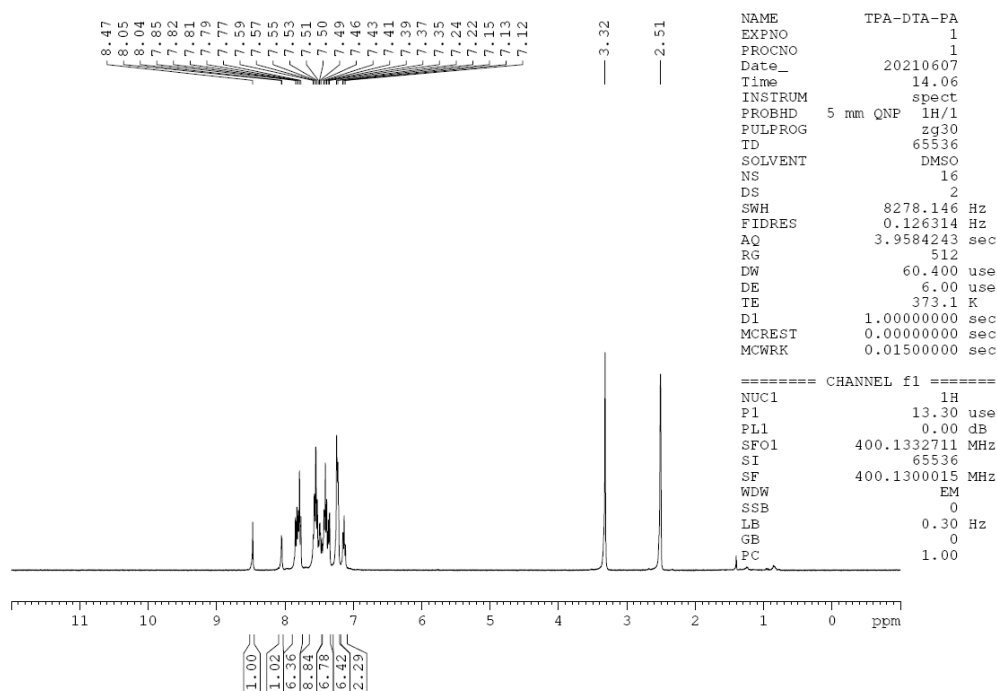


(A)

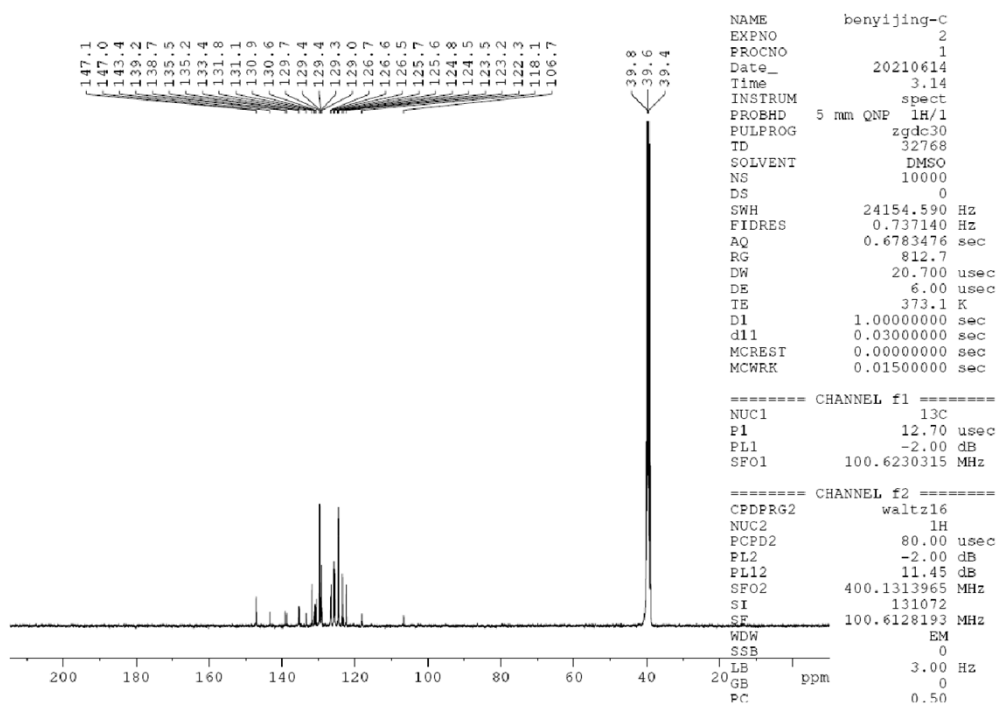


(B)

Figure S2. NMR spectra data for TPA-DTA-PAM in DMSO- d_6 : (A) ^1H -NMR spectra; (B) ^{13}C -NMR spectra.

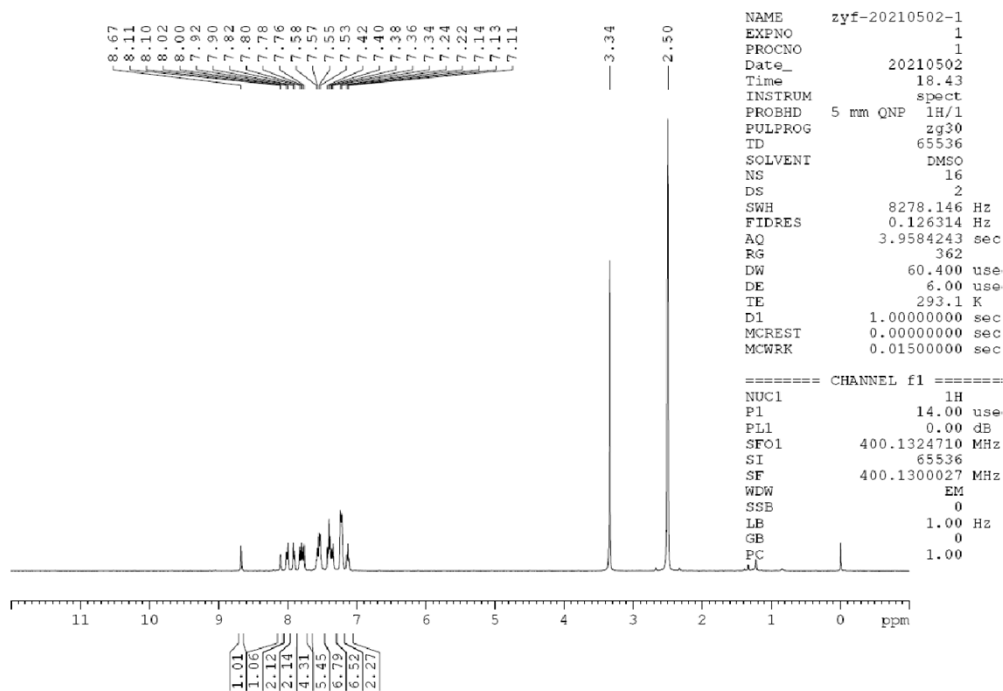


(A)

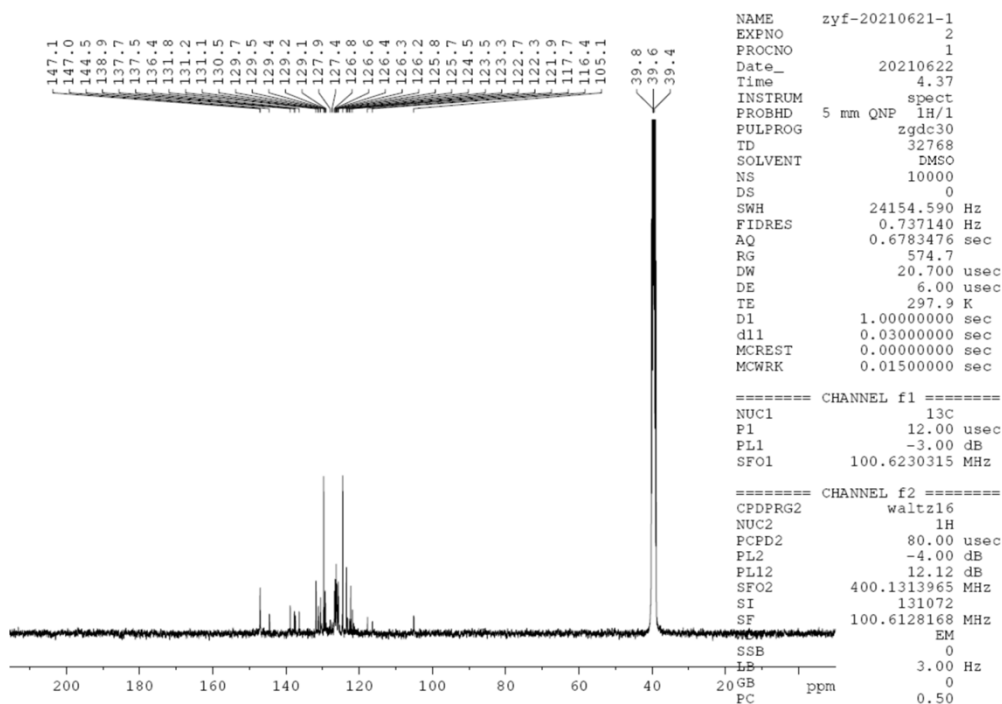


(B)

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(A)



(B)

Figure S4. NMR spectra data for TPA-DTA-PATF in DMSO- d_6 : (A) ^1H -NMR spectra; (B) ^{13}C -NMR spectra.

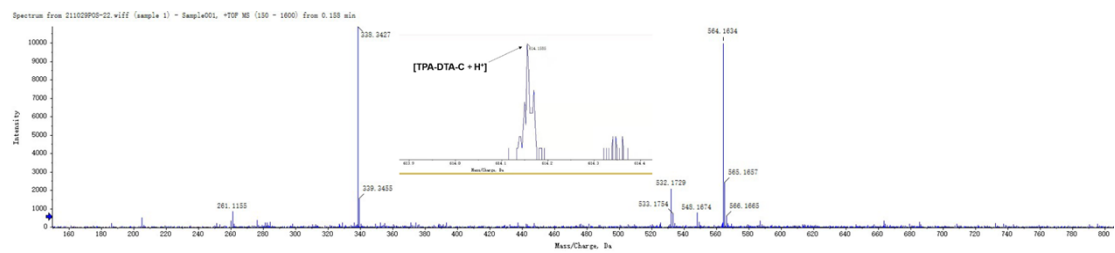


Figure S5. HRMS-ESI spectra of TPA-DTA-C.

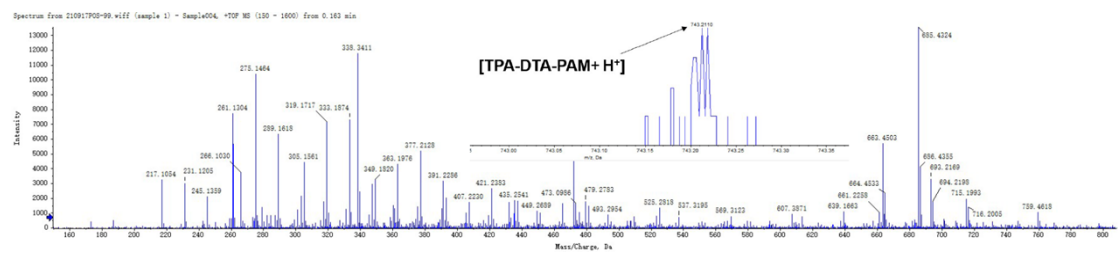


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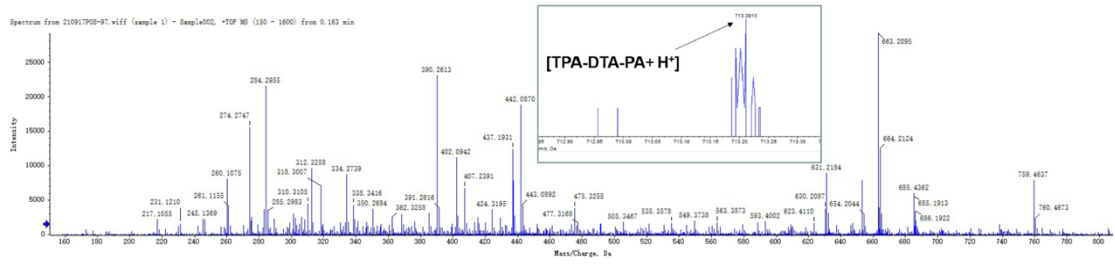


Figure S7. HRMS-ESI spectra of TPA-DTA-PA.

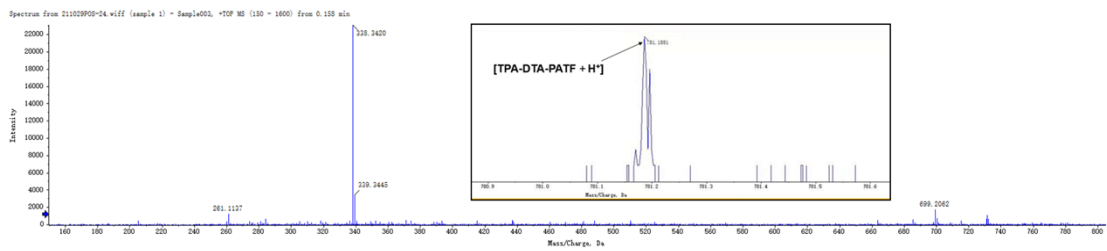


Figure S8. HRMS-ESI spectra of TPA-DTA-PATF.

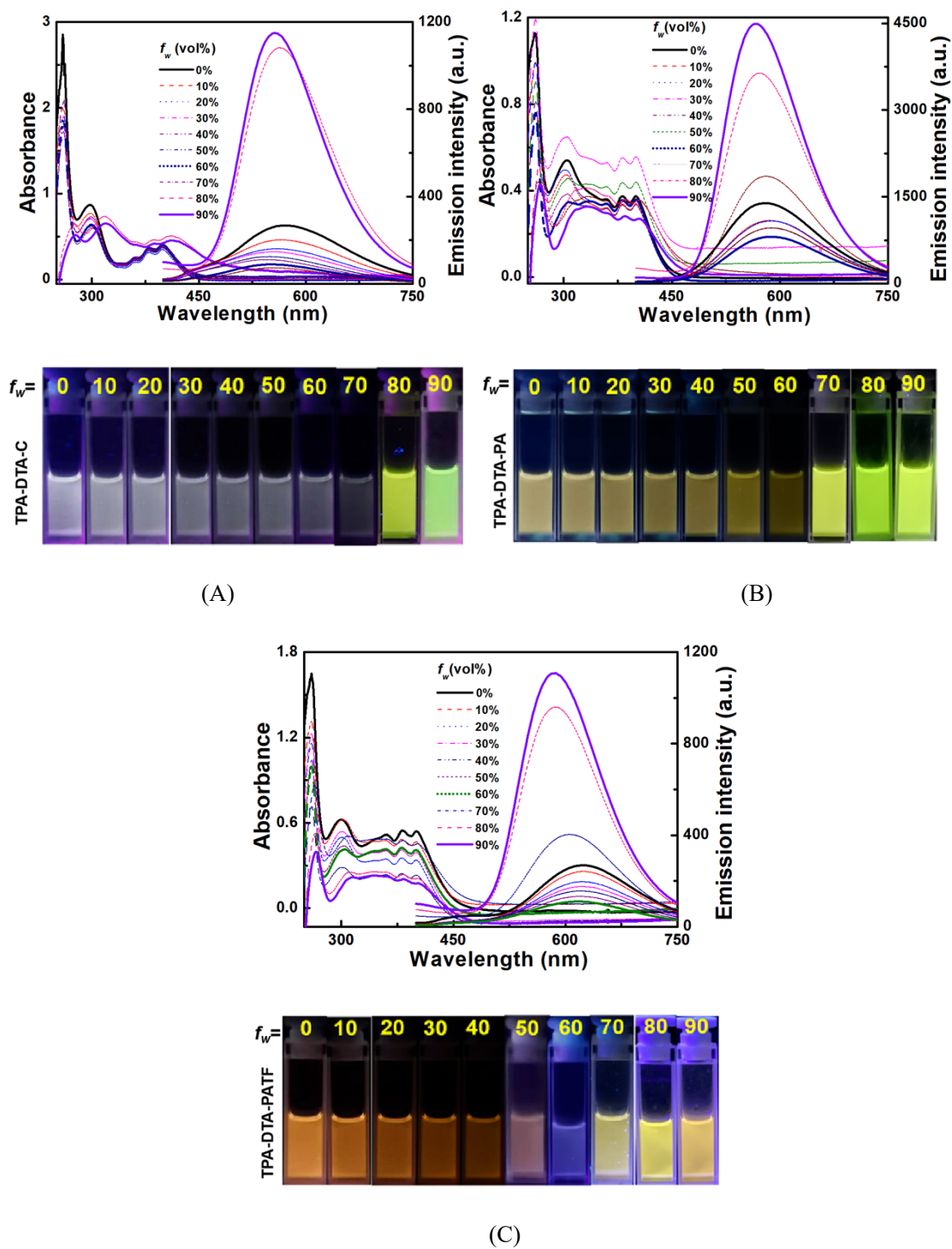


Figure S9. The changes of absorption, fluorescence spectra and photos in THF/H₂O with different fraction for TPA-DTA-C (A), TPA-DTA-PA (B), and TPA-DTA-PATF ($\lambda_{\text{ex}} = 400 \text{ nm}$, $C = 2.0 \times 10^{-5} \text{ mol/L}$).

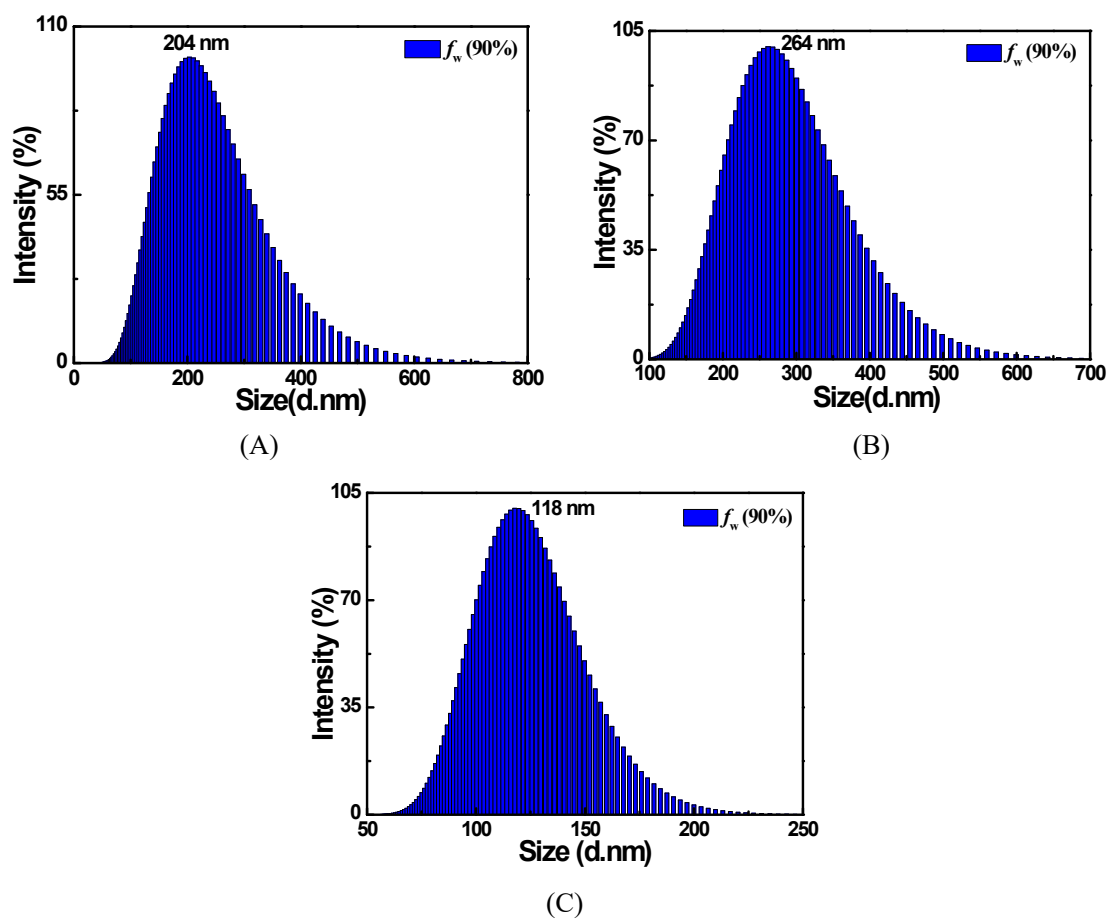
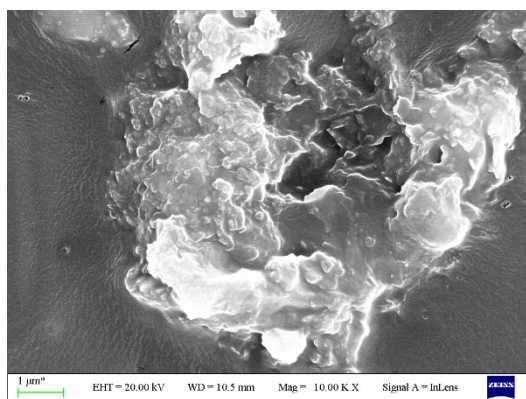
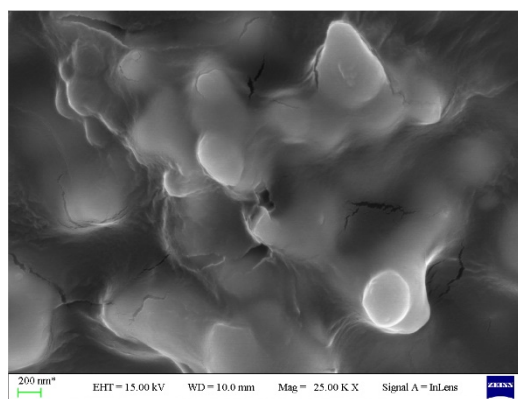


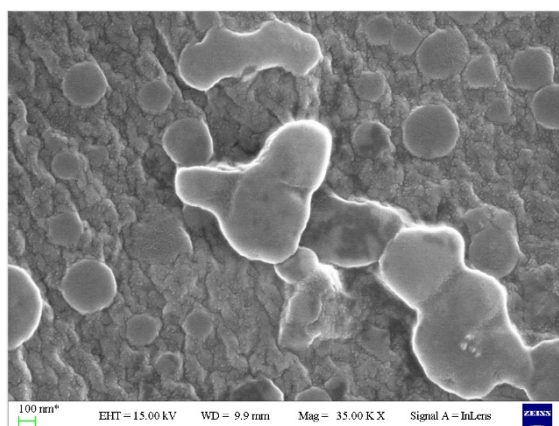
Figure S10. Size distribution curve of TPA-DTA-C (A), TPA-DTA-PA (B) TPA-DTA-PATF (C) in THF-H₂O ($f_w=90\%$) mixture.



(A)



(B)



(C)

Figure S11. SEM images of **TPA-DTA-C** (A), **TPA-DTA-PA** (B) and **TPA-DTA-PATF** (C) in THF/H₂O ($f_w = 90\%$)..

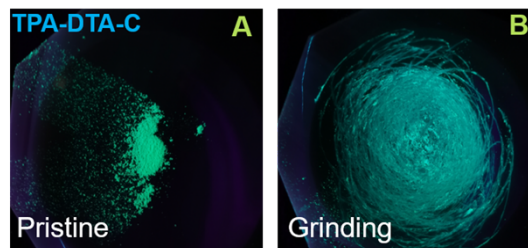


Figure S12. Photographic images of TPA-DTA-C in various states under 365 nm UV irradiation.

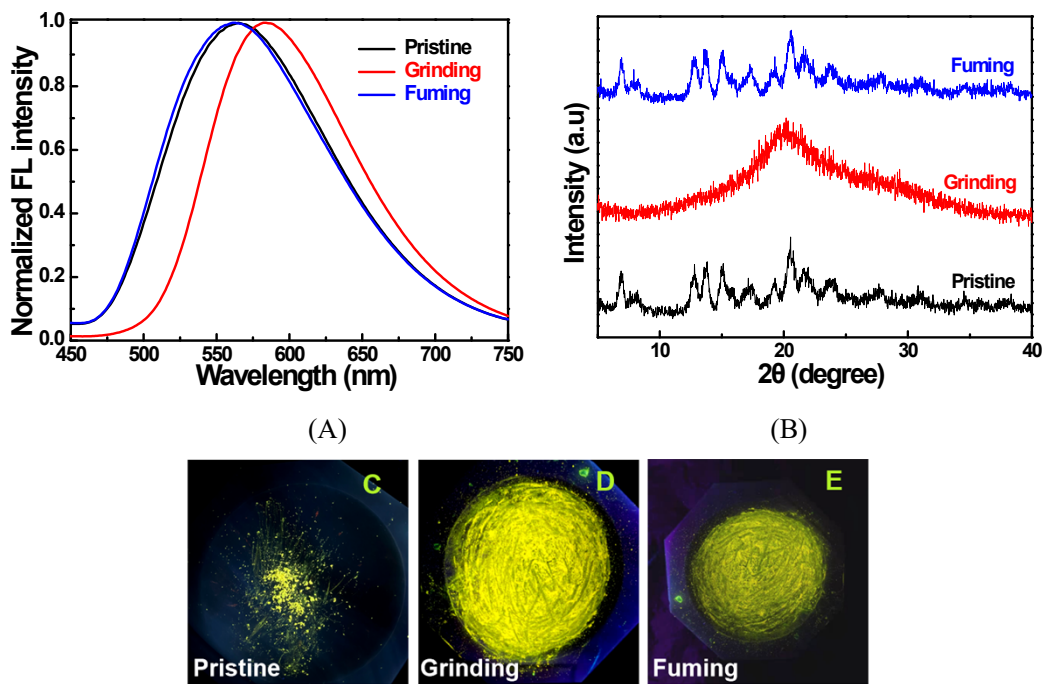


Figure S13. (A) Solid state PL spectra of TPA-DTA-PA before and after the grinding, and after treatment with DCM vapor. (B) XRD curves of TPA-DTA-PA in pristine, ground, and fumed form, (C-E) Photographic images of TPA-DTA-PA in various states under 365 nm UV irradiation.

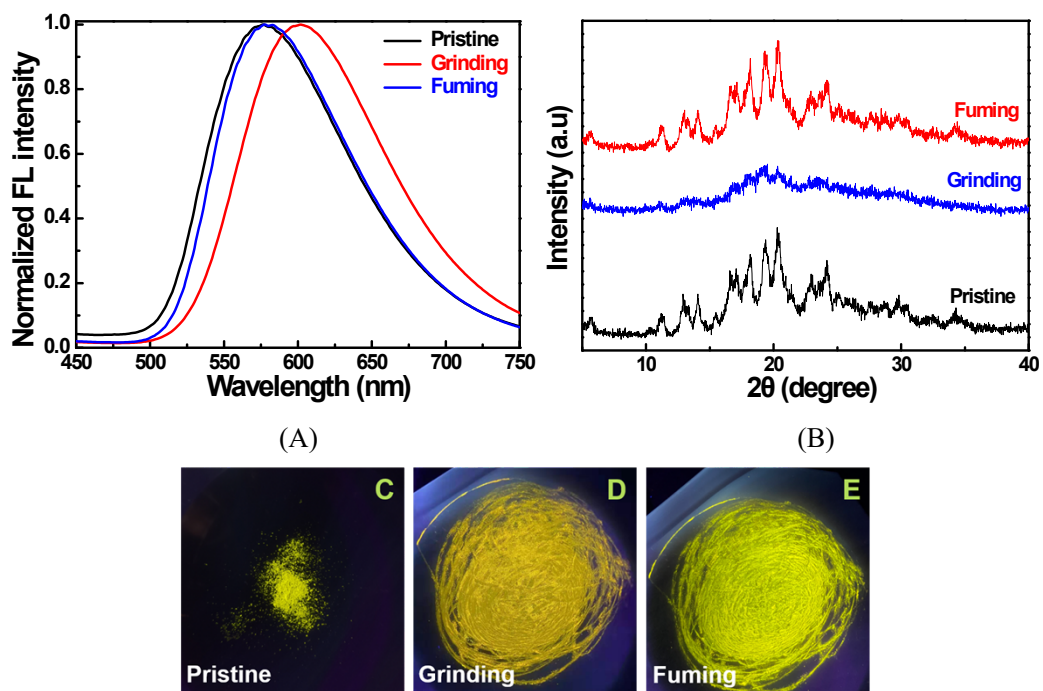


Figure S14. (A) Solid state PL spectra of **TPA-DTA-PATF** before and after the grinding, and after treatment with DCM vapor, (B) XRD curves of **TPA-DTA-PATF** in pristine, ground, and fumed form, (C-E) Photographic images of **TPA-DTA-PATF** in various states under 365 nm UV irradiation.

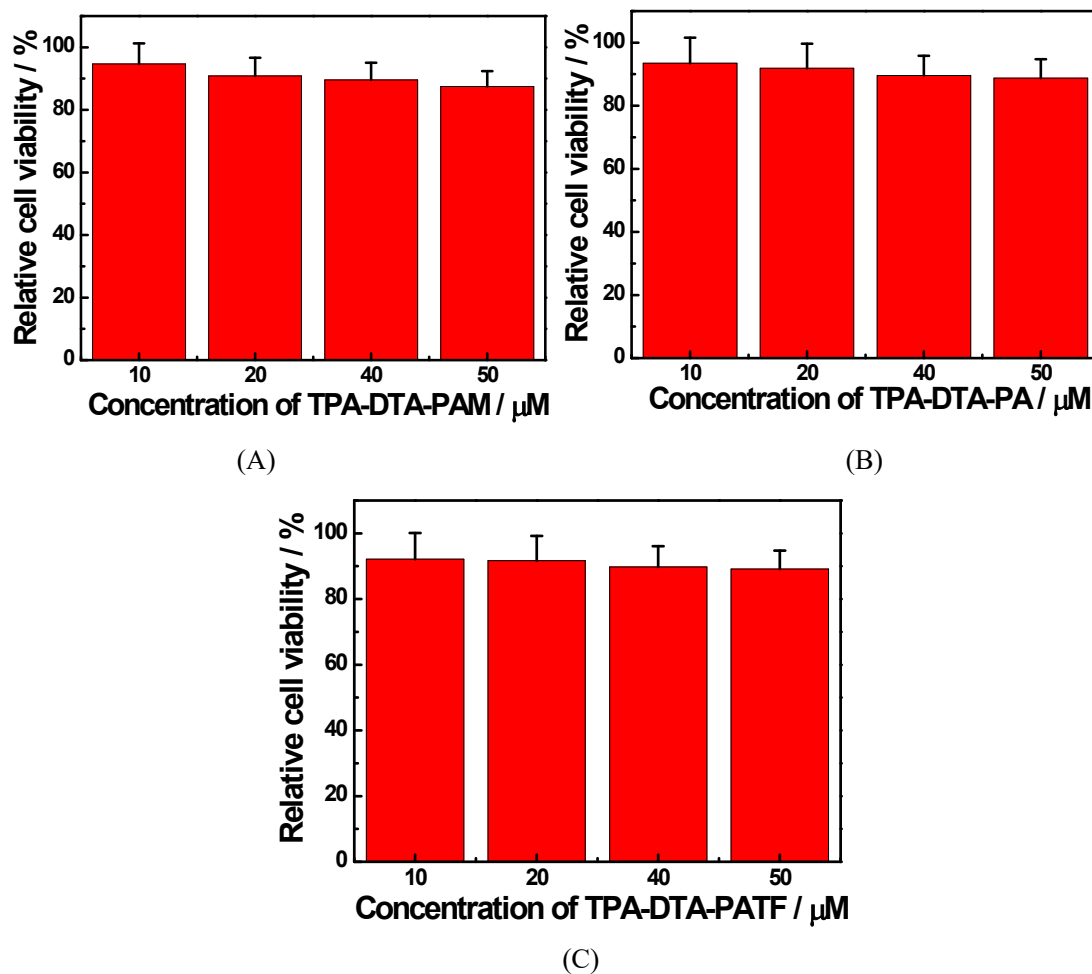


Figure S15. % cell viability of HeLa cells treated with different concentrations (10→50 μM) of

TPA-DTAs for 24 h determined by MTT assay.

Table S1. Symbolic Z-Matrix of TPA-DTA-C.

C	-0.883	0.47461	0
C	-1.917	1.29261	-0.227
C	-3.171	1.11361	0.252
C	-3.327	0.13361	1.186
C	-2.302	-0.74239	1.313
C	-1.098	-0.60639	0.746
C	-4.211	1.91261	-0.117
C	-5.391	1.70861	0.526
C	-5.497	0.84761	1.563
C	-4.487	-0.00039	1.89
C	-6.548	2.25961	0.084
C	-7.698	2.24061	0.768
C	-7.703	1.64561	1.961
C	-6.61	0.96461	2.326
C	-4.152	2.92261	-1.031
C	-4.727	-0.94539	2.844
C	-4.765	4.11061	-0.866
C	-4.519	4.96261	-1.864
C	-3.675	4.40961	-2.745
S	-3.289	3.09561	-2.212
C	-3.93485	-2.02155	3.04078
C	-4.30998	-2.76524	4.08608
C	-5.36259	-2.1788	4.66504
S	-5.67493	-0.92448	3.97597
C	-3.233	4.95261	-3.901
C	-2.364	4.34161	-4.729
C	-1.96	4.88961	-5.887
C	-2.369	6.09461	-6.343
C	-3.229	6.69761	-5.49
C	-3.643	6.16061	-4.331
N	-1.985	6.61461	-7.468
C	-1.975	7.90361	-7.618
C	-1.617	5.84461	-8.446
C	-2.125	8.51261	-8.82
C	-2.122	9.84461	-8.991
C	-1.959	10.65961	-7.943
C	-1.804	10.10861	-6.733
C	-1.816	8.77361	-6.591
C	-0.742	6.22861	-9.406
C	-0.351	5.44361	-10.423
C	-0.832	4.19961	-10.539
C	-1.701	3.77161	-9.616
C	-2.071	4.57761	-8.608

C	-5.97542	-2.68939	5.77015
O	-6.9384	-2.23526	6.353
H	0.112	0.65861	-0.442
H	-1.605	2.13761	-0.849
H	-2.351	-1.67339	1.887
H	-0.293	-1.34239	0.909
H	-6.634	2.77061	-0.888
H	-8.603	2.74161	0.386
H	-8.602	1.67461	2.6
H	-6.702	0.50661	3.324
H	-5.402	4.41561	-0.021
H	-4.975	5.96061	-1.905
H	-3.04018	-2.29748	2.46301
H	-3.81362	-3.69085	4.40782
H	-1.929	3.35761	-4.48
H	-1.195	4.30261	-6.426
H	-3.718	7.65261	-5.747
H	-4.376	6.75361	-3.76
H	-2.342	7.94261	-9.739
H	-2.277	10.27661	-9.995
H	-1.954	11.75461	-8.071
H	-1.646	10.76061	-5.857
H	-1.606	8.42861	-5.564
H	-0.228	7.20461	-9.37
H	0.384	5.81061	-11.159
H	-0.521	3.54661	-11.37
H	-2.129	2.75761	-9.704
H	-2.848	4.14861	-7.952
H	-5.5101	-3.63219	6.14763

Table S2. Total energies of TPA-DTA-C.

Zero-point correction	0.558239 (Hartree/Particle)
Thermal correction to Energy	0.594417
Thermal correction to Enthalpy	0.595361
Thermal correction to Gibbs Free Energy	0.482156
Sum of electronic and zero-point Energies	-2504.619982
Sum of electronic and thermal Energies	-2504.583804
Sum of electronic and thermal Enthalpies	-2504.582860
Sum of electronic and thermal Free Energies	-2504.696065

Table S3. Symbolic Z-Matrix of TPA-DTA-PAM.

C	-1.22212	-5.53657	0.45127
C	-1.92683	-4.38169	0.23902
C	-1.26613	-3.12876	0.02401
C	0.17894	-3.10685	0.07737
C	0.87362	-4.34056	0.29279
C	0.19914	-5.5188	0.46727
C	-1.97891	-1.92698	-0.21327
C	0.87311	-1.88484	-0.07044
C	0.16051	-0.68191	-0.27967
C	-1.28141	-0.70298	-0.36703
C	-1.95755	0.52915	-0.6432
H	-3.03674	0.52537	-0.73125
C	-1.26992	1.70452	-0.78928
C	0.14598	1.72942	-0.66756
C	0.83588	0.57237	-0.42417
H	-1.75142	-6.47109	0.61702
H	-3.01003	-4.40196	0.24266
H	1.95716	-4.32221	0.32534
H	0.74899	-6.44171	0.63074
H	-1.80872	2.62439	-0.99987
H	0.68046	2.6695	-0.77439
H	1.91623	0.58944	-0.33415
C	-3.44835	-1.95513	-0.32105
C	-4.30797	-2.13989	-1.37061
C	-5.63709	-2.03296	-0.84935
H	-4.01995	-2.31521	-2.39778
C	-5.49868	-1.7914	0.48274
H	-6.5654	-2.12208	-1.39634
C	2.35656	-1.86519	-0.01148
C	3.16925	-1.74081	1.087
C	4.56394	-1.76376	0.77637
H	2.77415	-1.63469	2.09187
C	4.80487	-1.90735	-0.56127
H	5.3489	-1.67683	1.52011
S	3.32839	-2.01604	-1.46593
S	-4.18103	-1.73819	0.82497
C	6.16231	-1.97626	-1.2853
H	6.19419	-2.09154	-2.34859
C	7.31662	-1.89139	-0.58036
C	8.66971	-1.9612	-1.31238
N	9.67715	-2.01318	-1.85741
C	7.27988	-1.72538	0.95023

C	7.25291	-0.44902	1.51296
C	7.27345	-2.85098	1.77396
C	7.22021	-0.29839	2.89912
H	7.25877	0.43819	0.86329
C	7.23974	-2.70048	3.16055
H	7.29452	-3.85702	1.3306
C	7.21326	-1.42446	3.72322
H	7.19959	0.70762	3.34276
H	7.23427	-3.58816	3.80976
C	-6.49583	-1.58076	1.63726
C	-6.94889	-2.67423	2.37586
C	-6.94596	-0.29684	1.94463
C	-7.8524	-2.48381	3.42115
H	-6.59442	-3.68641	2.13279
C	-7.84899	-0.10608	2.99085
H	-6.58884	0.56511	1.36272
C	-8.30235	-1.19929	3.72901
H	-8.21004	-3.34571	4.00297
H	-8.20341	0.9064	3.23323
N	-9.25457	-0.9989	4.83084
C	-10.70054	-1.04627	4.57041
C	-11.38662	0.11999	4.23038
C	-11.38668	-2.25712	4.66312
C	-12.75863	0.07543	3.9838
H	-10.84553	1.07459	4.15812
C	-12.75893	-2.30205	4.41553
H	-10.84607	-3.17644	4.93093
C	-13.44499	-1.13602	4.07604
H	-13.29958	0.99476	3.71639
H	-13.29958	-3.25697	4.4883
H	-14.52677	-1.17092	3.88151
C	-8.76082	-0.75115	6.19309
C	-8.52712	-1.82234	7.05589
C	-8.52585	0.55477	6.6231
C	-8.05919	-1.58752	8.34861
H	-8.71319	-2.85174	6.71683
C	-8.05685	0.78977	7.91585
H	-8.70983	1.39913	5.94315
C	-7.82363	-0.28108	8.77866
H	-7.87556	-2.43175	9.02894
H	-7.87129	1.81951	8.25448
H	-7.45463	-0.09618	9.79795
O	7.179	-1.27024	5.14447
C	7.19454	0.12115	5.47415

H	6.3418	0.60007	5.04014
H	7.16539	0.23607	6.53756
H	8.08806	0.56841	5.09143

Table S4. Total energies of TPA-DTA-PAM.

Zero-point correction	0.693761 (Hartree/Particle)
Thermal correction to Energy	0.739369
Thermal correction to Enthalpy	0.740313
Thermal correction to Gibbs Free Energy	0.603621
Sum of electronic and zero-point Energies	-2906.177911
Sum of electronic and thermal Energies	-2906.132303
Sum of electronic and thermal Enthalpies	-2906.131359
Sum of electronic and thermal Free Energies	-2906.268051

Table S5. Symbolic Z-Matrix of TPA-DTA-PA.

C	-1.22212	-5.53657	0.45127
C	-1.92683	-4.38169	0.23902
C	-1.26613	-3.12876	0.02401
C	0.17894	-3.10685	0.07737
C	0.87362	-4.34056	0.29279
C	0.19914	-5.5188	0.46727
C	-1.97891	-1.92698	-0.21327
C	0.87311	-1.88484	-0.07044
C	0.16051	-0.68191	-0.27967
C	-1.28141	-0.70298	-0.36703
C	-1.95755	0.52915	-0.6432
H	-3.03674	0.52537	-0.73125
C	-1.26992	1.70452	-0.78928
C	0.14598	1.72942	-0.66756
C	0.83588	0.57237	-0.42417
H	-1.75142	-6.47109	0.61702
H	-3.01003	-4.40196	0.24266
H	1.95716	-4.32221	0.32534
H	0.74899	-6.44171	0.63074
H	-1.80872	2.62439	-0.99987
H	0.68046	2.6695	-0.77439
H	1.91623	0.58944	-0.33415
C	-3.44835	-1.95513	-0.32105
C	-4.30797	-2.13989	-1.37061
C	-5.63709	-2.03296	-0.84935
H	-4.01995	-2.31521	-2.39778
C	-5.49868	-1.7914	0.48274
H	-6.5654	-2.12208	-1.39634
C	2.35656	-1.86519	-0.01148
C	3.16925	-1.74081	1.087
C	4.56394	-1.76376	0.77637
H	2.77415	-1.63469	2.09187
C	4.80487	-1.90735	-0.56127
H	5.3489	-1.67683	1.52011
S	3.32839	-2.01604	-1.46593
S	-4.18103	-1.73819	0.82497
C	6.16231	-1.97626	-1.2853
H	6.19419	-2.09154	-2.34859
C	7.31662	-1.89139	-0.58036
C	8.66971	-1.9612	-1.31238
N	9.67715	-2.01318	-1.85741
C	7.27988	-1.72538	0.95023

C	7.25291	-0.44902	1.51296
C	7.27345	-2.85098	1.77396
C	7.22021	-0.29839	2.89912
H	7.25877	0.43819	0.86329
C	7.23974	-2.70048	3.16055
H	7.29452	-3.85702	1.3306
C	7.21326	-1.42446	3.72322
H	7.19959	0.70762	3.34276
H	7.23427	-3.58816	3.80976
C	-6.49583	-1.58076	1.63726
C	-6.94889	-2.67423	2.37586
C	-6.94596	-0.29684	1.94463
C	-7.8524	-2.48381	3.42115
H	-6.59442	-3.68641	2.13279
C	-7.84899	-0.10608	2.99085
H	-6.58884	0.56511	1.36272
C	-8.30235	-1.19929	3.72901
H	-8.21004	-3.34571	4.00297
H	-8.20341	0.9064	3.23323
N	-9.25457	-0.9989	4.83084
C	-10.7005	-1.0462	4.57041
C	-11.3866	0.1199	4.23038
C	-11.3866	-2.2571	4.66312
C	-12.7586	0.0754	3.9838
H	-10.8455	1.0745	4.15812
C	-12.7589	-2.302	4.41553
H	-10.846	-3.1764	4.93093
C	-13.4449	-1.136	4.07604
H	-13.2995	0.9947	3.71639
H	-13.2995	-3.2569	4.4883
H	-14.5267	-1.1709	3.88151
C	-8.76082	-0.75115	6.19309
C	-8.52712	-1.82234	7.05589
C	-8.52585	0.55477	6.6231
C	-8.05919	-1.58752	8.34861
H	-8.71319	-2.85174	6.71683
C	-8.05685	0.78977	7.91585
H	-8.70983	1.39913	5.94315
C	-7.82363	-0.28108	8.77866
H	-7.87556	-2.43175	9.02894
H	-7.87129	1.81951	8.25448
H	-7.45463	-0.09618	9.79795
H	7.18762	-1.30907	4.78667

Table S6. Total energies of TPA-DTA-PA

Zero-point correction	0.660927 (Hartree/Particle)
Thermal correction to Energy	0.703963
Thermal correction to Enthalpy	0.704907
Thermal correction to Gibbs Free Energy	0.573940
Sum of electronic and zero-point Energies	-2791.686982
Sum of electronic and thermal Energies	-2791.643946
Sum of electronic and thermal Enthalpies	-2791.643001
Sum of electronic and thermal Free Energies	-2791.773968

Table S7. Symbolic Z-Matrix of TPA-DTA-PATF.

C	-1.22212	-5.53657	0.45127
C	-1.92683	-4.38169	0.23902
C	-1.26613	-3.12876	0.02401
C	0.17894	-3.10685	0.07737
C	0.87362	-4.34056	0.29279
C	0.19914	-5.5188	0.46727
C	-1.97891	-1.92698	-0.21327
C	0.87311	-1.88484	-0.07044
C	0.16051	-0.68191	-0.27967
C	-1.28141	-0.70298	-0.36703
C	-1.95755	0.52915	-0.6432
H	-3.03674	0.52537	-0.73125
C	-1.26992	1.70452	-0.78928
C	0.14598	1.72942	-0.66756
C	0.83588	0.57237	-0.42417
H	-1.75142	-6.47109	0.61702
H	-3.01003	-4.40196	0.24266
H	1.95716	-4.32221	0.32534
H	0.74899	-6.44171	0.63074
H	-1.80872	2.62439	-0.99987
H	0.68046	2.6695	-0.77439
H	1.91623	0.58944	-0.33415
C	-3.44835	-1.95513	-0.32105
C	-4.30797	-2.13989	-1.37061
C	-5.63709	-2.03296	-0.84935
H	-4.01995	-2.31521	-2.39778
C	-5.49868	-1.7914	0.48274
H	-6.5654	-2.12208	-1.39634
C	2.35656	-1.86519	-0.01148
C	3.16925	-1.74081	1.087
C	4.56394	-1.76376	0.77637
H	2.77415	-1.63469	2.09187
C	4.80487	-1.90735	-0.56127
H	5.3489	-1.67683	1.52011
S	3.32839	-2.01604	-1.46593
S	-4.18103	-1.73819	0.82497
C	6.16231	-1.97626	-1.2853
H	6.19419	-2.09154	-2.34859
C	7.31662	-1.89139	-0.58036
C	8.66971	-1.9612	-1.31238
N	9.67715	-2.01318	-1.85741
C	7.27988	-1.72538	0.95023

C	7.25291	-0.44902	1.51296
C	7.27345	-2.85098	1.77396
C	7.22021	-0.29839	2.89912
H	7.25877	0.43819	0.86329
C	7.23974	-2.70048	3.16055
H	7.29452	-3.85702	1.3306
C	7.21326	-1.42446	3.72322
H	7.19959	0.70762	3.34276
H	7.23427	-3.58816	3.80976
C	7.17707	-1.25779	5.25375
F	6.51368	-0.12465	5.56745
F	8.43879	-1.18671	5.72863
F	6.54701	-2.3159	5.80686
C	-6.49583	-1.58076	1.63726
C	-6.94889	-2.67423	2.37586
C	-6.94596	-0.29684	1.94463
C	-7.8524	-2.48381	3.42115
H	-6.59442	-3.68641	2.13279
C	-7.84899	-0.10608	2.99085
H	-6.58884	0.56511	1.36272
C	-8.30235	-1.19929	3.72901
H	-8.21004	-3.34571	4.00297
H	-8.20341	0.9064	3.23323
N	-9.25457	-0.9989	4.83084
C	-10.7005	-1.0462	4.57041
C	-11.3866	0.1199	4.23038
C	-11.3866	-2.2571	4.66312
C	-12.7586	0.0754	3.9838
H	-10.8455	1.0745	4.15812
C	-12.7589	-2.302	4.41553
H	-10.846	-3.1764	4.93093
C	-13.4449	-1.136	4.07604
H	-13.2995	0.9947	3.71639
H	-13.2995	-3.2569	4.4883
H	-14.5267	-1.1709	3.88151
C	-8.76082	-0.75115	6.19309
C	-8.52712	-1.82234	7.05589
C	-8.52585	0.55477	6.6231
C	-8.05919	-1.58752	8.34861
H	-8.71319	-2.85174	6.71683
C	-8.05685	0.78977	7.91585
H	-8.70983	1.39913	5.94315
C	-7.82363	-0.28108	8.77866
H	-7.87556	-2.43175	9.02894

H	-7.87129	1.81951	8.25448
H	-7.45463	-0.09618	9.79795

Table S8. Total energies of TPA-DTA-PATF.

Zero-point correction	0.665673 (Hartree/Particle)
Thermal correction to Energy	0.712348
Thermal correction to Enthalpy	0.713292
Thermal correction to Gibbs Free Energy	0.573009
Sum of electronic and zero-point Energies	-3128.718801
Sum of electronic and thermal Energies	-3128.672126
Sum of electronic and thermal Enthalpies	-3128.671182
Sum of electronic and thermal Free Energies	-3128.811466
