Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Coumarin-tetraphenylethylene regioisomers: synthesis, photophysical properties, and aggregation–induced emission.

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Experimental:

The relative fluorescence quantum efficiency, (Φ), is evaluated by employing 9,10–diphenyl anthracene as standard (Φ =0.9) following the equation 1.

$$\Phi = \Phi_{std} \left(\frac{I_{unk}}{I_{std}}\right)\left(\frac{A_{std}}{A_{unk}}\right)\left(\frac{\eta_{unk}}{\eta_{std}}\right)^2 \text{.....} \quad 1$$

Where Φ_{unk}, Φ_{std}, I_{unk}, I_{std}, A_{std}, A_{unk}, η_{unk} and η_{std} are the fluorescence quantum efficiency, the integral of the emission intensities, the absorbance at the excitation wavelength and the refractive indexes of the corresponding solvents of the unknown samples and the standard respectively.

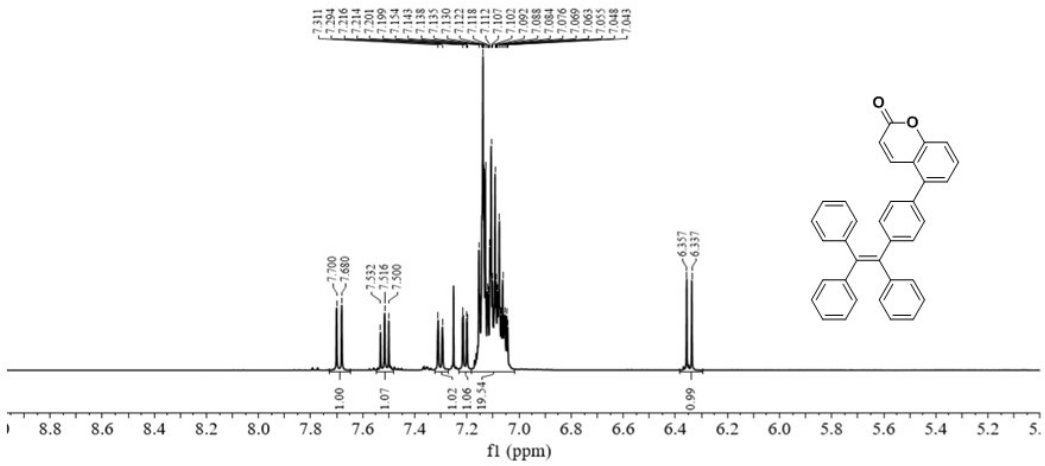


Figure S1: ^{1}H–NMR spectrum of **1** in $CDCl_3$.

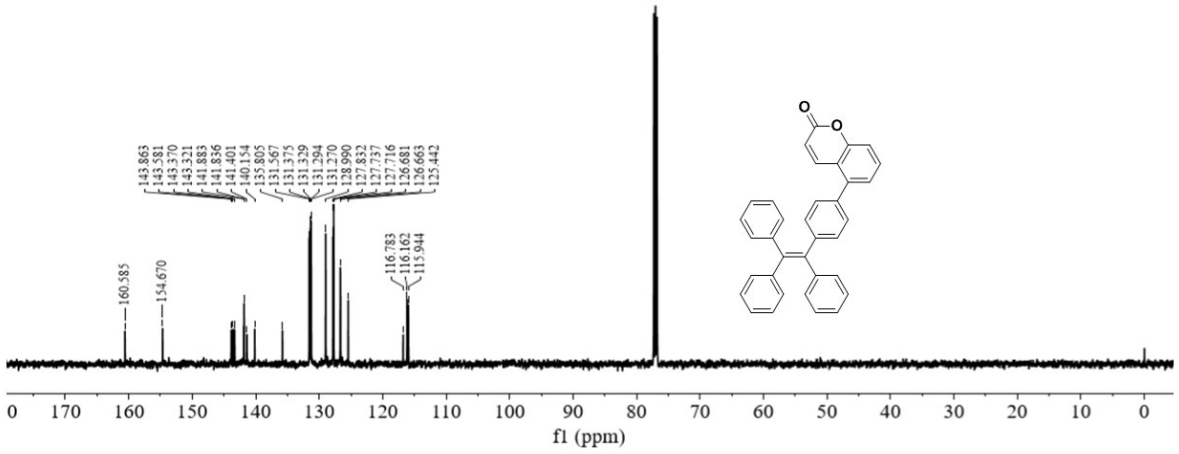


Figure S2: ^{13}C–NMR spectrum of **1** in $CDCl_3$.

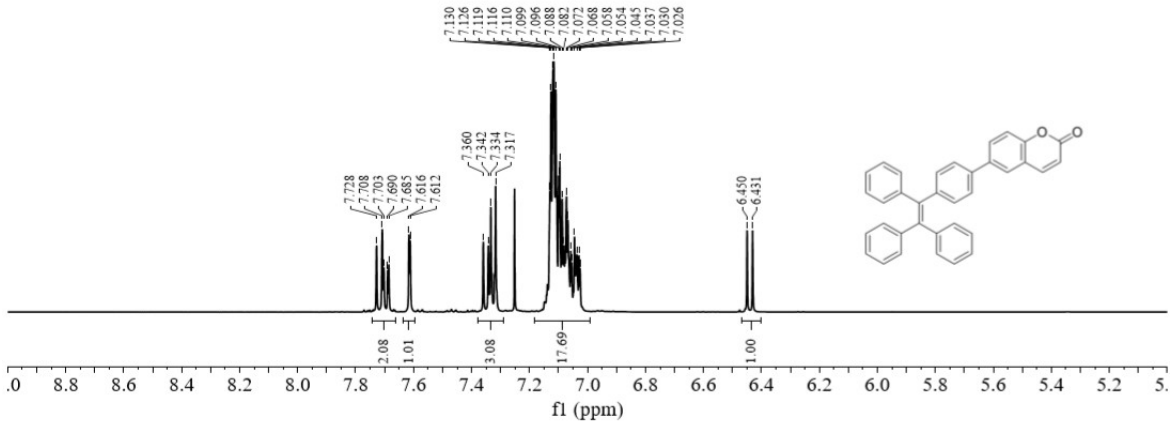
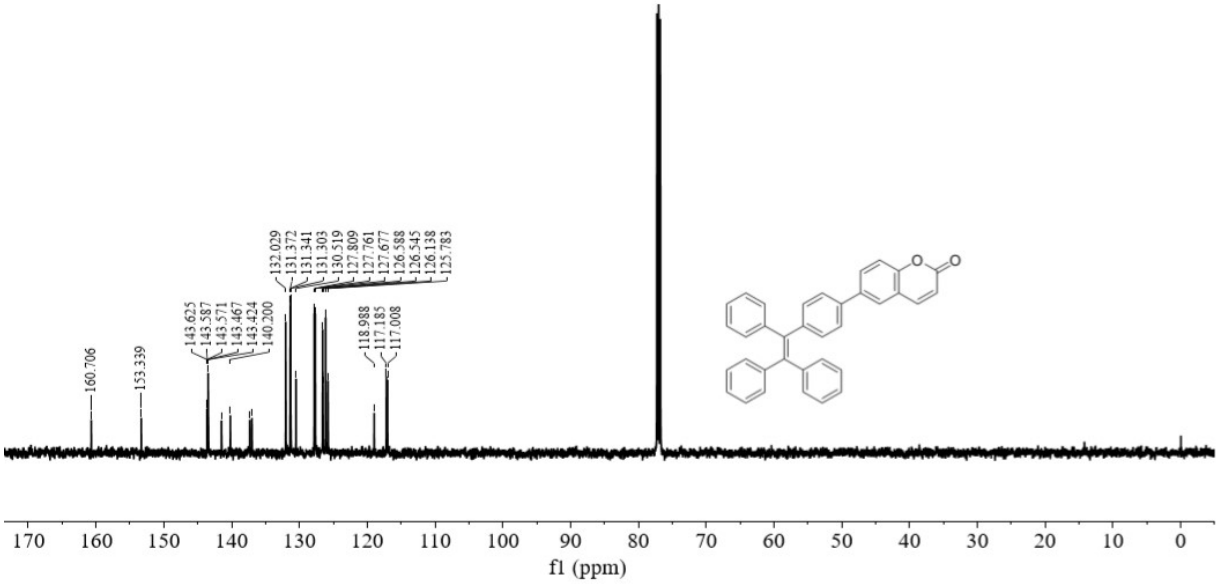


Figure S3: ^{1}H–NMR spectrum of **2** in $CDCl_3$.



f1(ppm)

Figure S4: ^{13}C–NMR spectrum of **2** in $CDCl_3$.

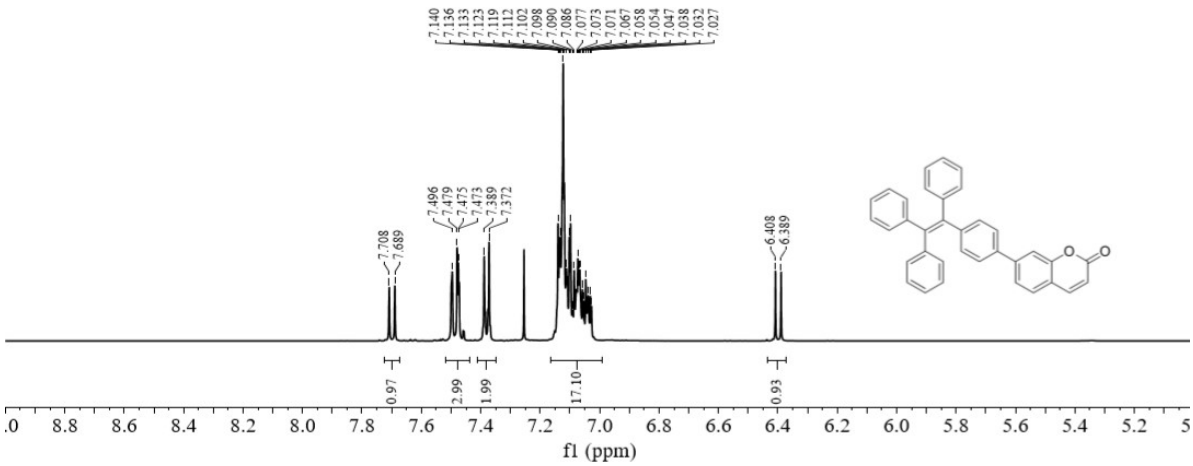


Figure S5: ^{1}H–NMR spectrum of **3** in $CDCl_3$.

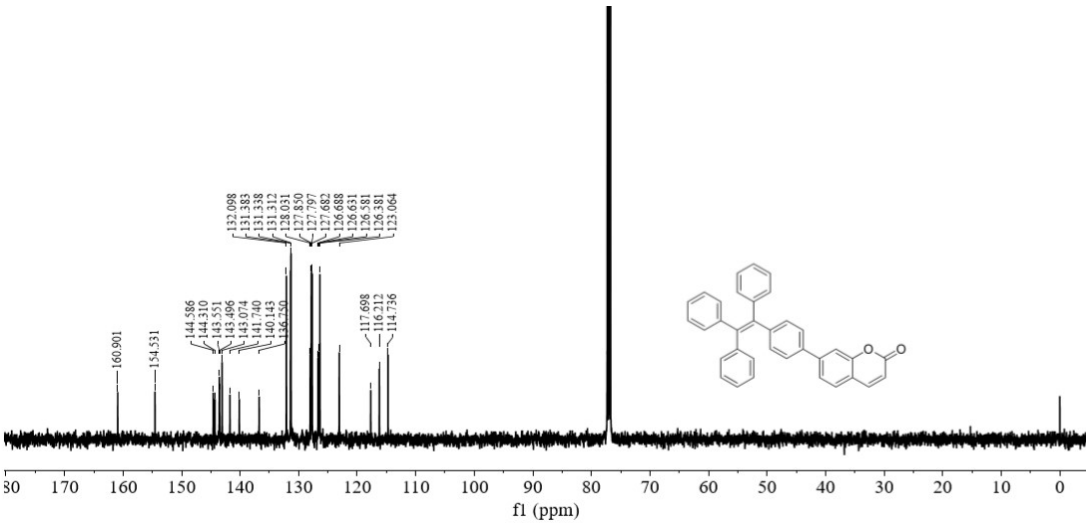


Figure S6: ^{13}C–NMR spectrum of **3** in $CDCl_3$.

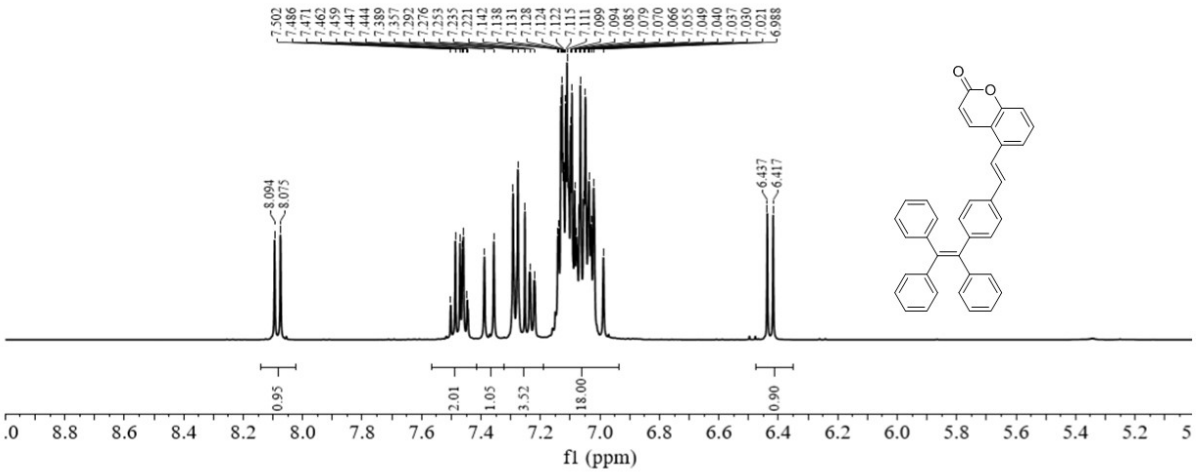


Figure S7: ^{1}H–NMR spectrum of **4** in $CDCl_3$.

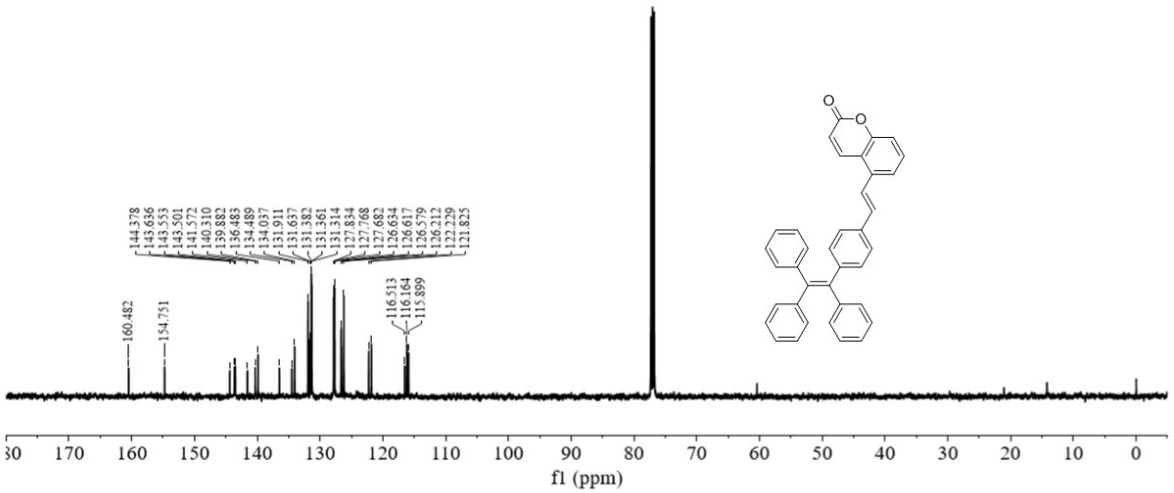


Figure S8: ^{13}C–NMR spectrum of **4** in $CDCl_3$.

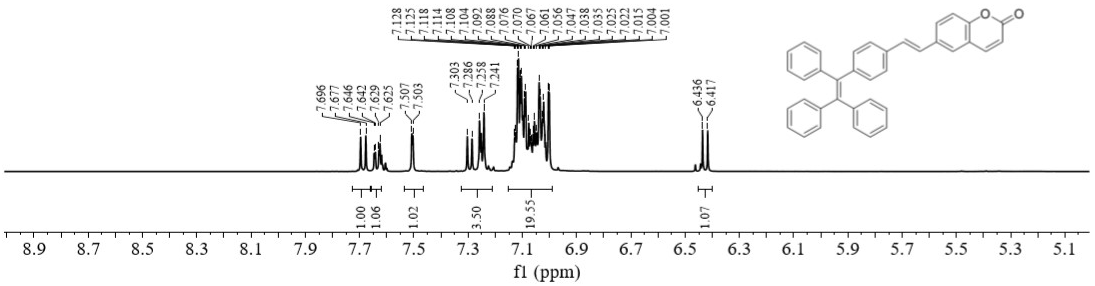


Figure S9: ^{1}H–NMR spectrum of **5** in $CDCl_3$.

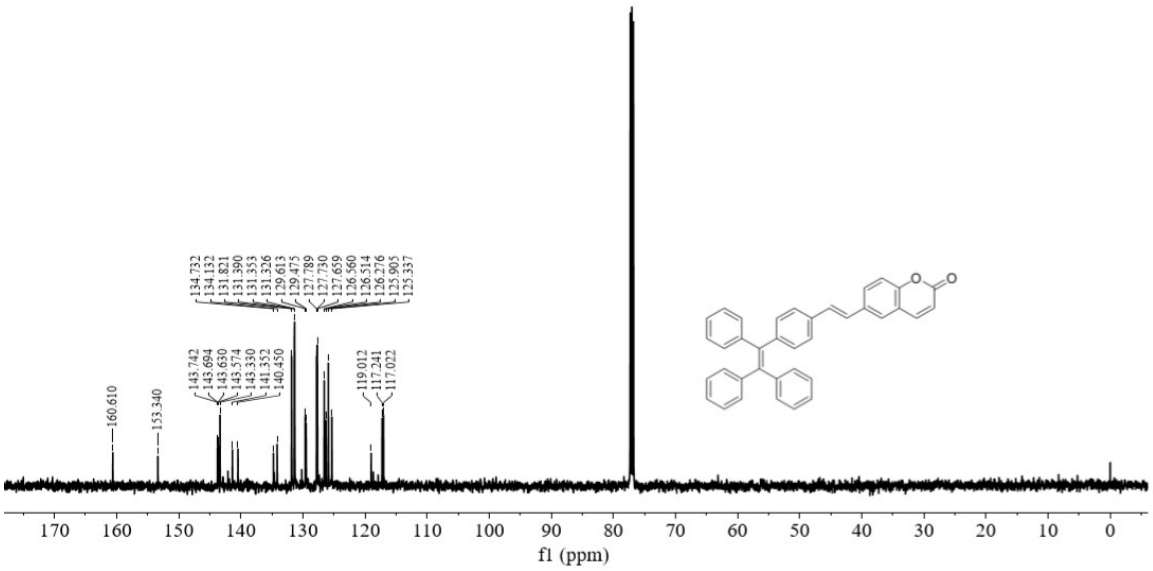


Figure S10: ^{1}H–NMR spectrum of **5** in $CDCl_3$.

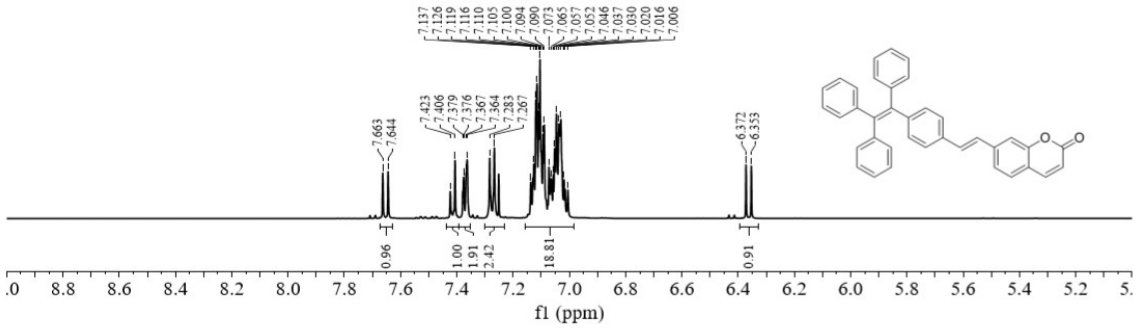


Figure S11: ^{1}H–NMR spectrum of **6** in $CDCl_3$.

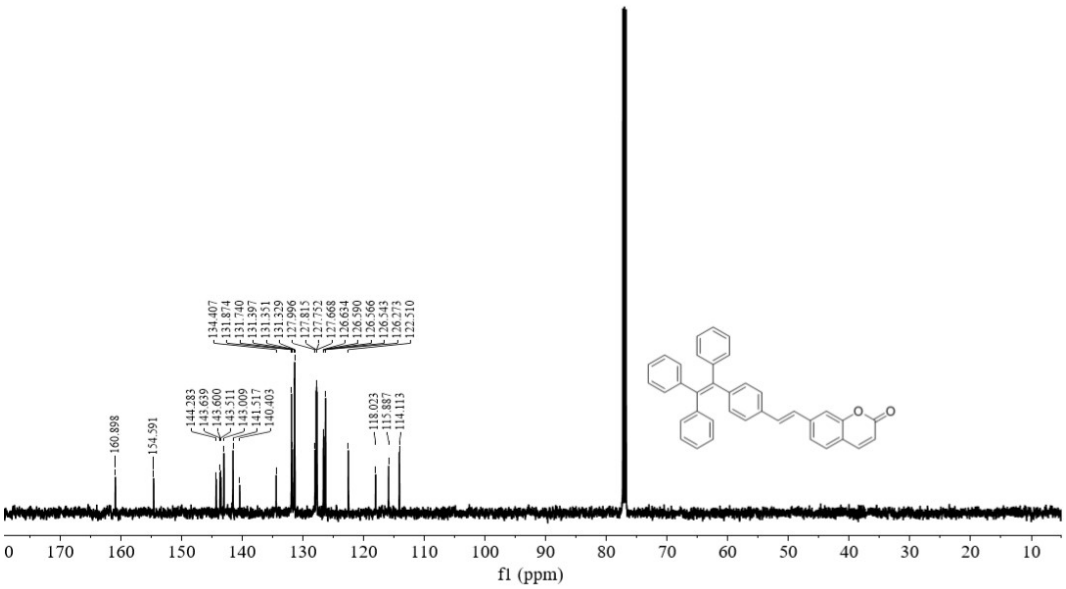


Figure S12: ^{13}C–NMR spectrum of **6** in $CDCl_3$.

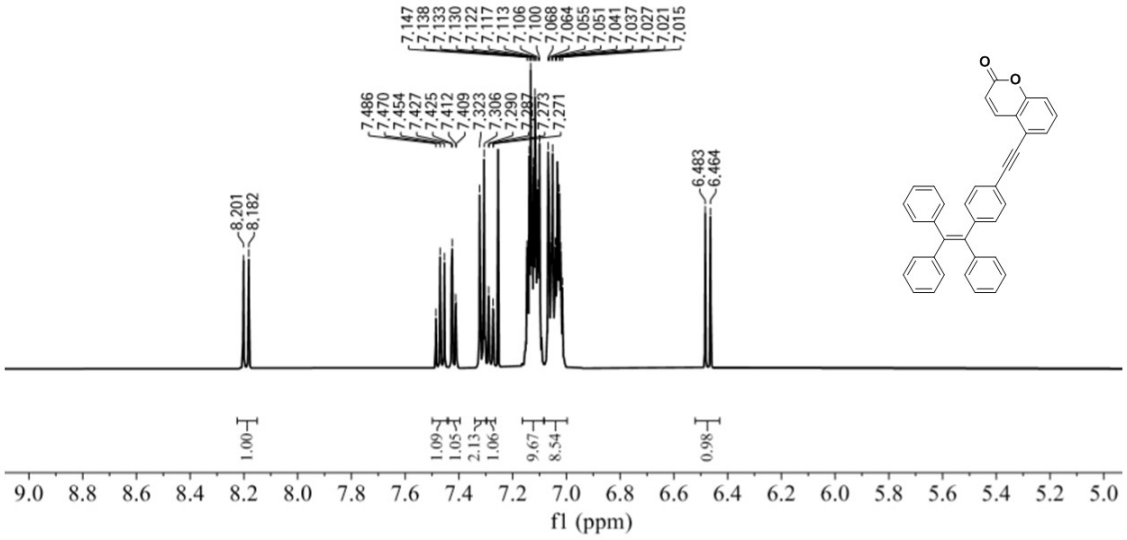


Figure S13: ^{1}H–NMR spectrum of **7** in $CDCl_3$.

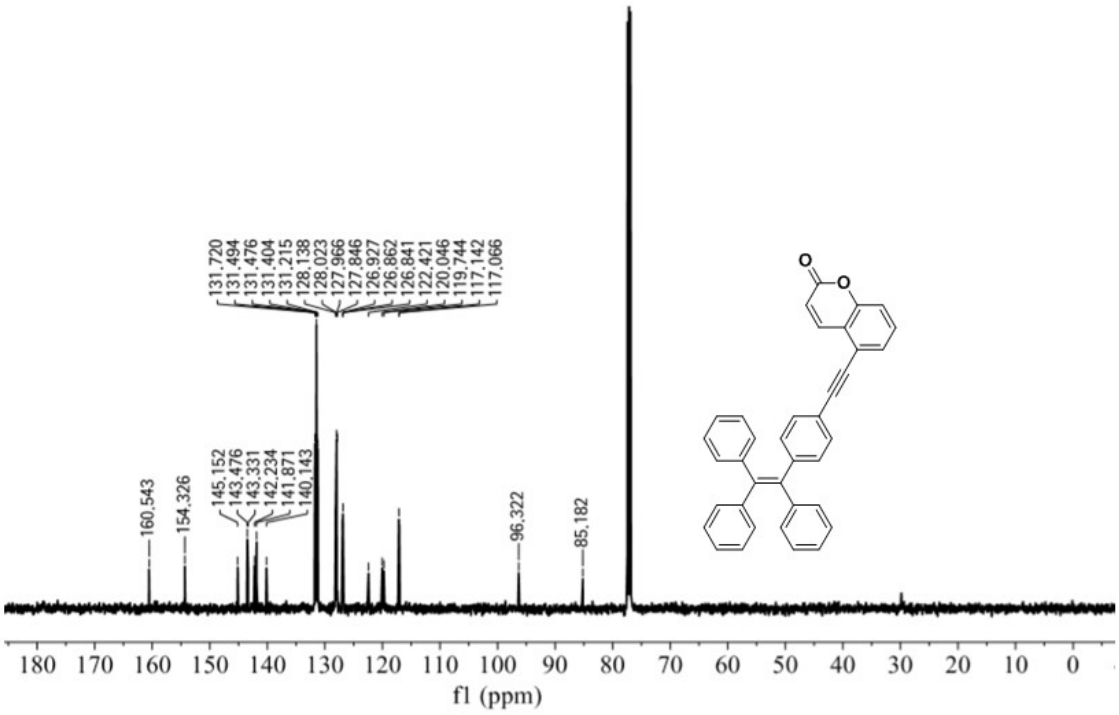


Figure S14: ^{13}C–NMR spectrum of **7** in $CDCl_3$.

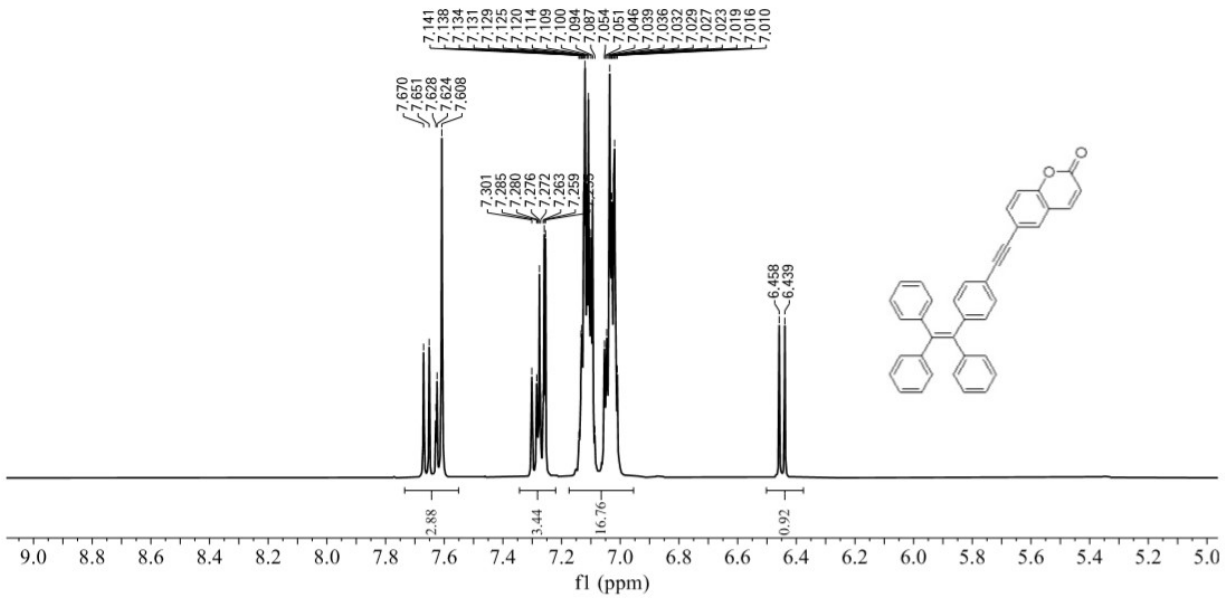


Figure S15: ^{1}H–NMR spectrum of **8** in $CDCl_3$.

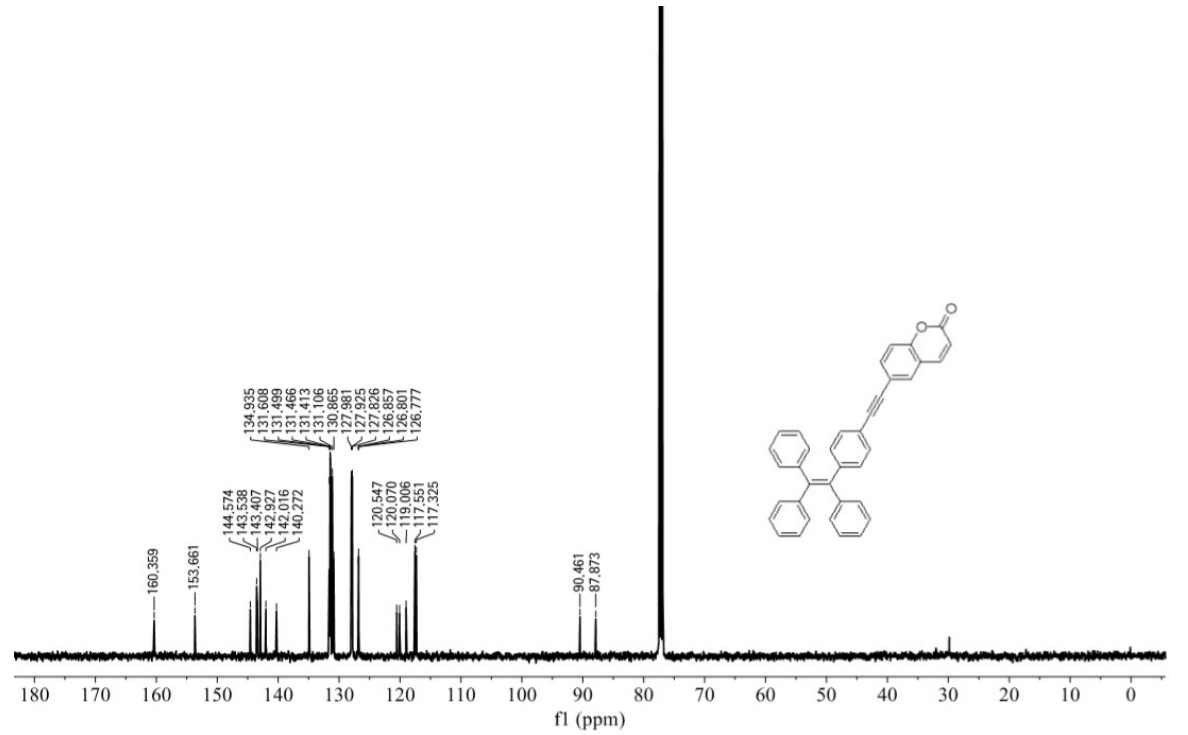


Figure S16: ^{13}C–NMR spectrum of **8** in $CDCl_3$.

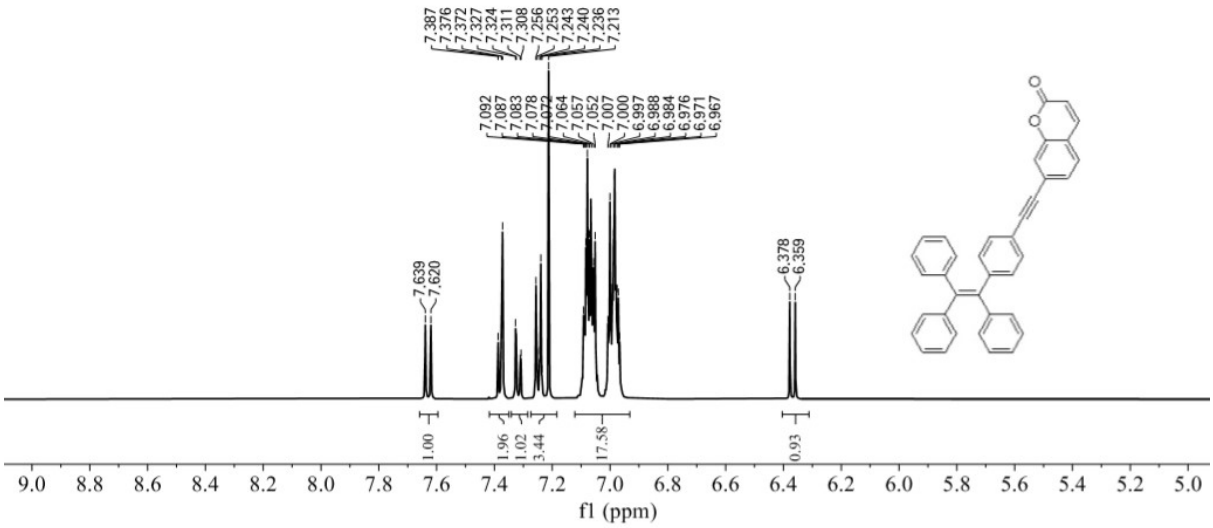


Figure S17: ^{1}H–NMR spectrum of **9** in $CDCl_3$.

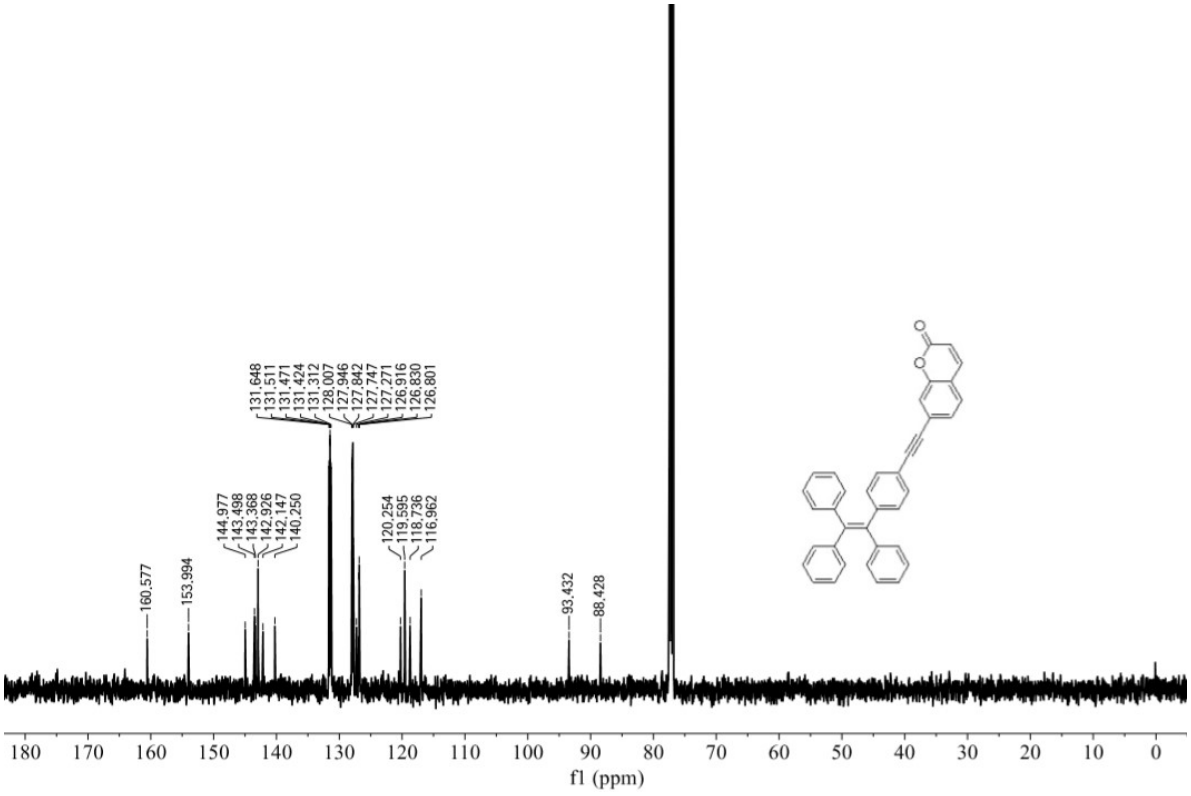


Figure S18: ^{13}C–NMR spectrum of **9** in $CDCl_3$.

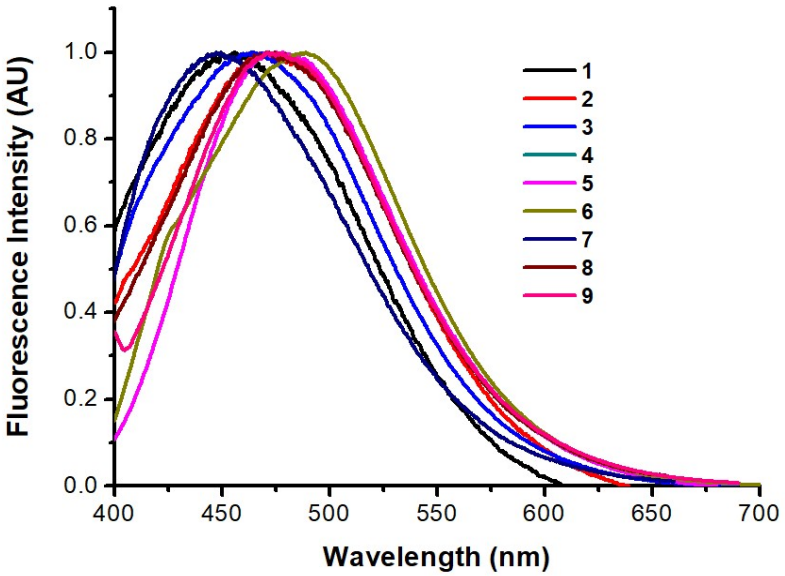


Figure S19: Normalized fluorescence spectra of CTPEs **1-9** in THF solvent at 25 °C.

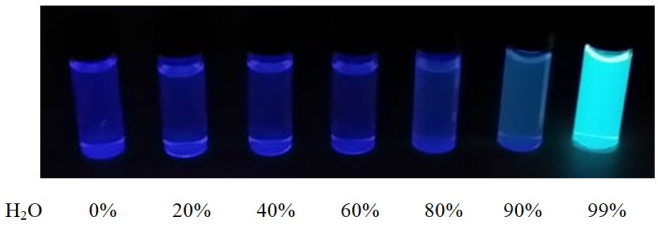


Figure S20: Photographs of **1** taken under 365 nm UV–light in different THF/H_2O mixtures (32 μM) (bottom).

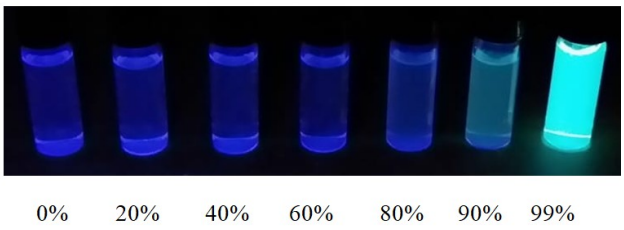


Figure S21: Photographs of **2** taken under 365 nm UV–light in different THF/H_2O mixtures (32 μM) (bottom).

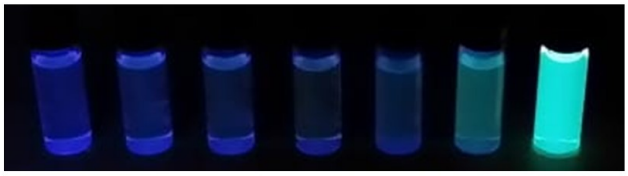


Figure S22: Photographs of **3** taken under 365 nm UV–light in different THF/H_2O mixtures (32 μM) (bottom).

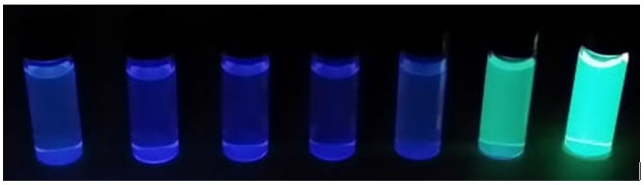


Figure S23: Photographs of **4** taken under 365 nm UV–light in different THF/H_2O mixtures (30 μM) (bottom).

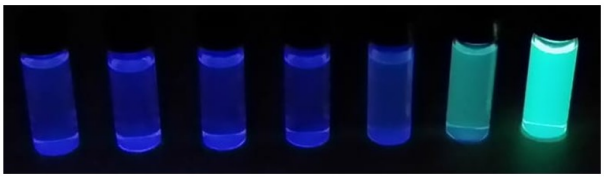


Figure S24: Photographs of **5** taken under 365 nm UV–light in different THF/H_2O mixtures (30 μM) (bottom).

Figure S25: Photographs of **6** taken under 365 nm UV–light in different THF/H_2O mixtures (30 μM) (bottom).

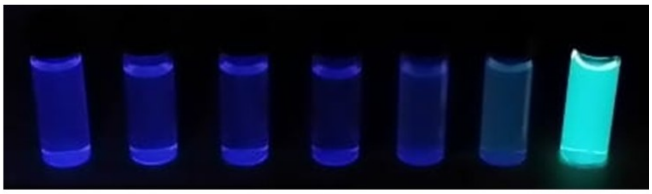


Figure S26: Photographs of **7** taken under 365 nm UV–light in different THF/H_2O mixtures (30 μM) (bottom).

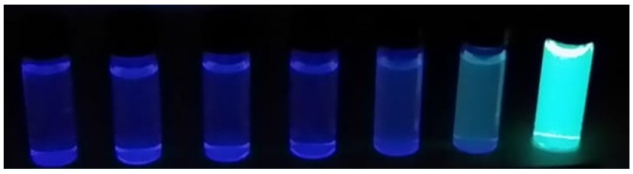


Figure S27: Photographs of **8** taken under 365 nm UV–light in different THF/H_2O mixtures (30 μM) (bottom).

Figure S28: Photographs of **9** taken under 365 nm UV–light in different THF/H_2O mixtures (30 μM) (bottom).

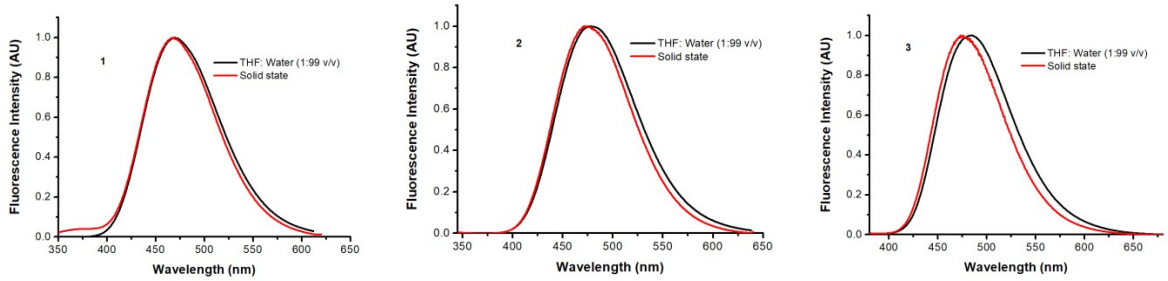


Figure S29: Solid film and AIE state normalized fluorescence spectra of CTPEs **1** (λ_{ex}=312 nm), **2** (λ_{ex}=325 nm) and **3** (λ_{ex}=348 nm).

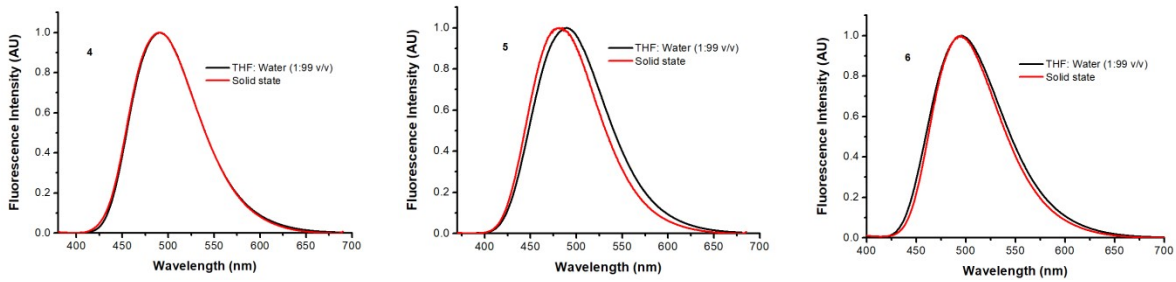


Figure S30: Solid film and AIE state normalized fluorescence spectra of CTPEs **4** (λ_{ex}=350 nm), **5** (λ_{ex}=346 nm) and **6** (λ_{ex}=376 nm).

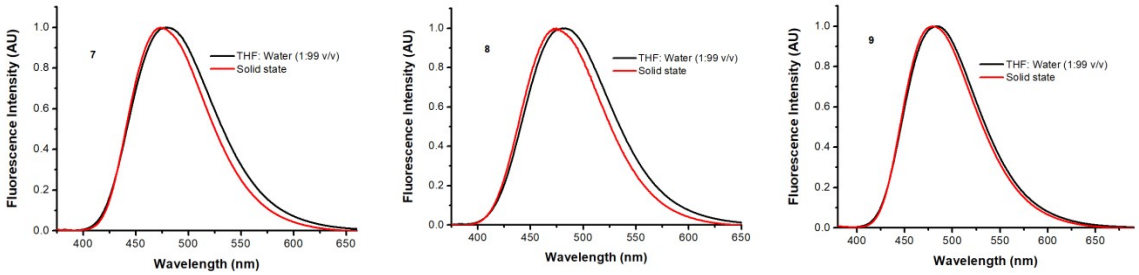


Figure S31: Solid film and AIE state normalized fluorescence spectra of CTPEs**7** (λ_{ex}=338 nm), **8**(λ_{ex}=333 nm) and **9** (λ_{ex}=354 nm).

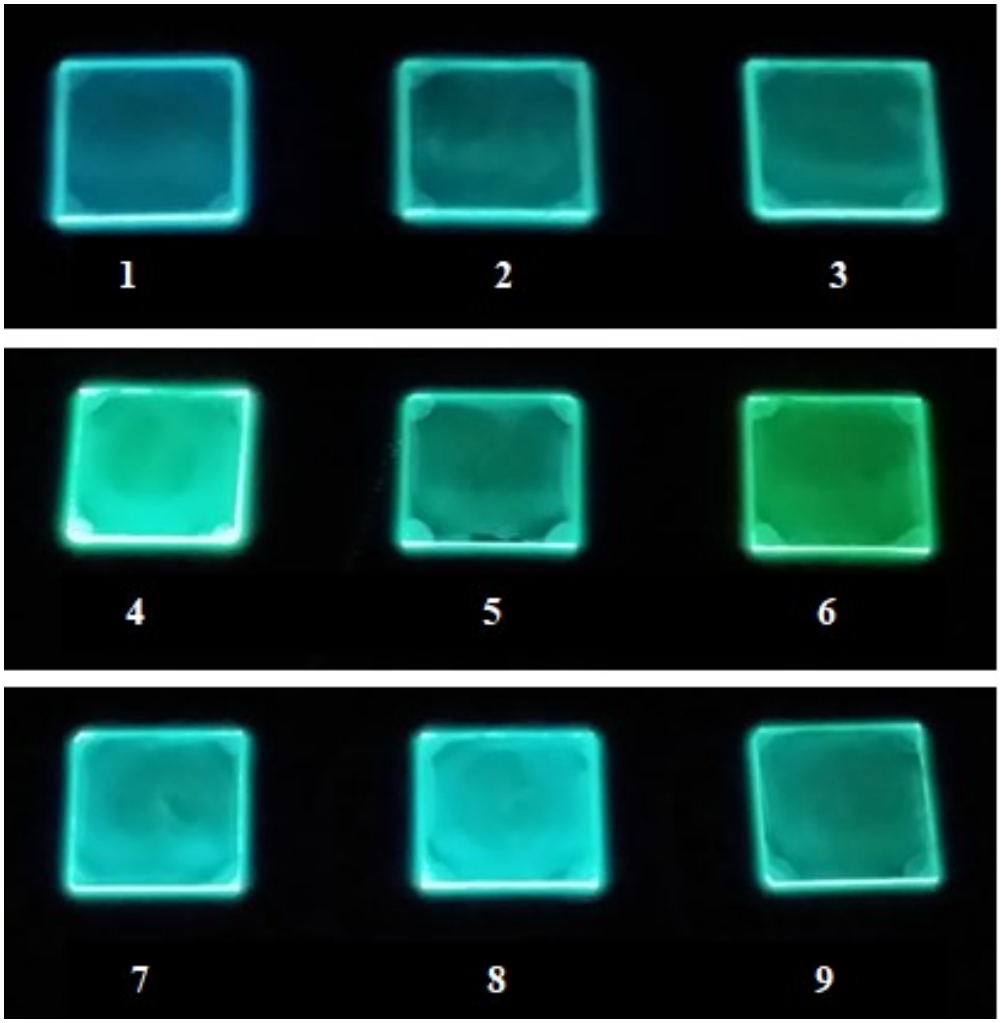


Figure S32: Photographs of solid films of **1-9** (top to bottom) taken under 365 nm UV–light.

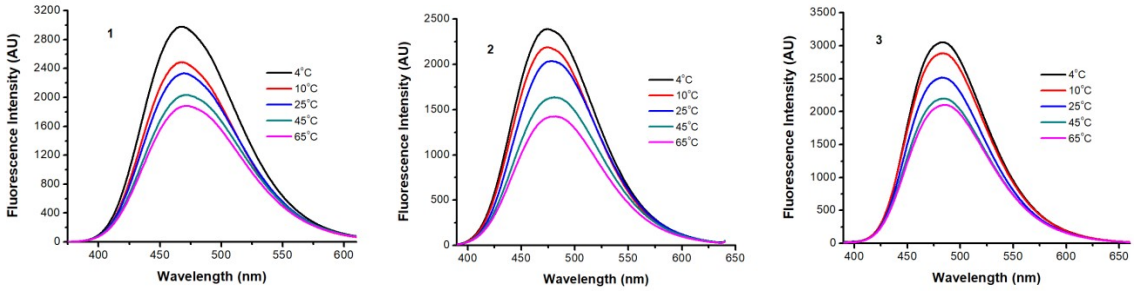


Figure S33: Effect of temperature on AIE of CTPEs **1**(λ_{ex}=312 nm), **2** (λ_{ex}=325 nm) and **3** (λ_{ex}=348 nm) (15.75 μM) left to right in THF–H_2O (1:99 v/v).

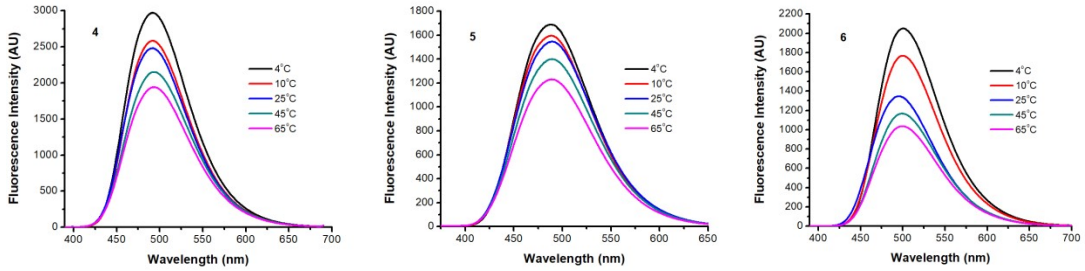


Figure S34: Effect of temperature on AIE of CTPEs **4** (λ_{ex}=350 nm), **5** (λ_{ex}=346 nm) and **6** (λ_{ex}=376 nm) (14.92 μM) left to right in THF–H_2O (1:99 v/v).

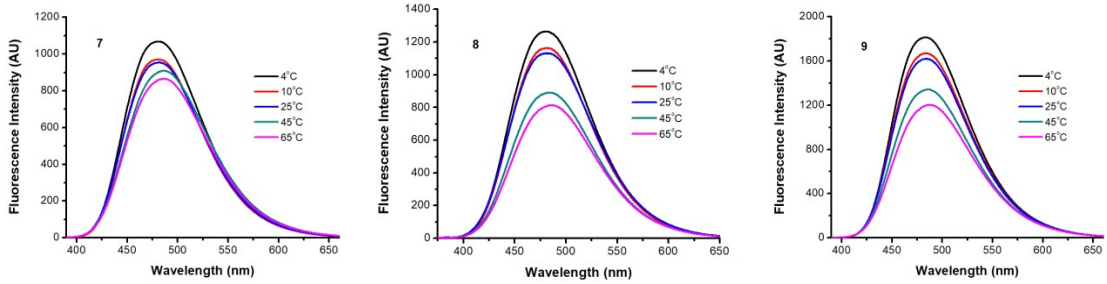


Figure S35: Effect of temperature on AIE of CTPEs **7** (λ_{ex}=338 nm), **8** (λ_{ex}=333 nm) and **9** (λ_{ex}=354 nm) (15 μM) left to right in THF–H_2O (1:99 v/v).

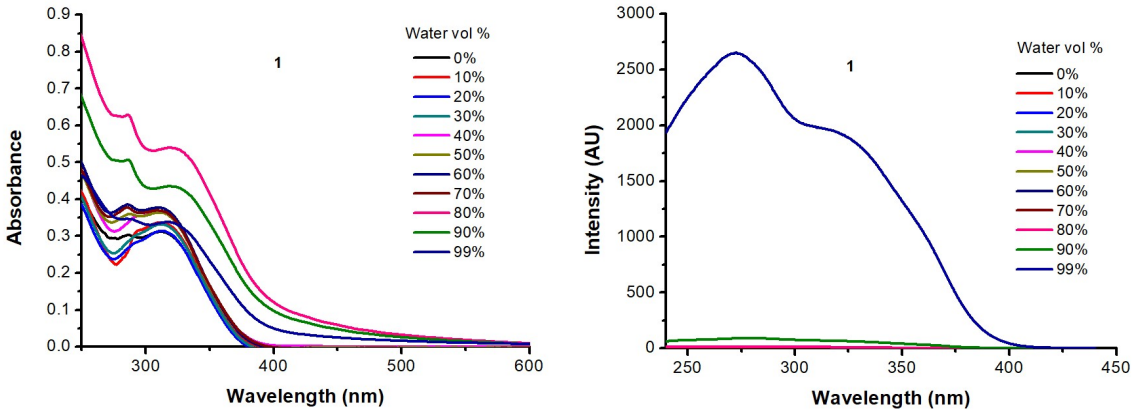


Figure S36: UV–visible and excitation spectra of **1** (15.75 μM) in THF–H_2O mixtures with different volume fractions of water (λ_{em}=469 nm) at 25 °C.

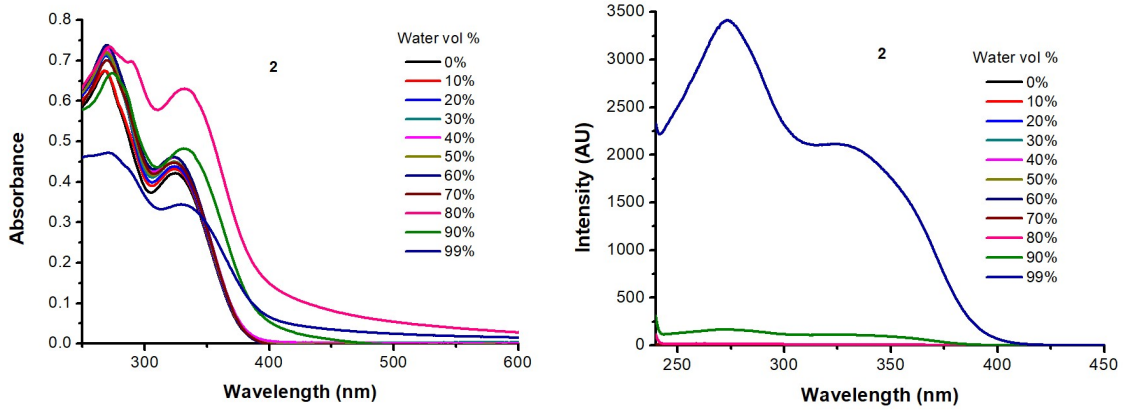


Figure S37: UV–visible and excitation spectra of **2** (15.75 μM) in THF–H_2O mixtures with different volume fractions of water (λ_{em}=478 nm) at 25 °C.

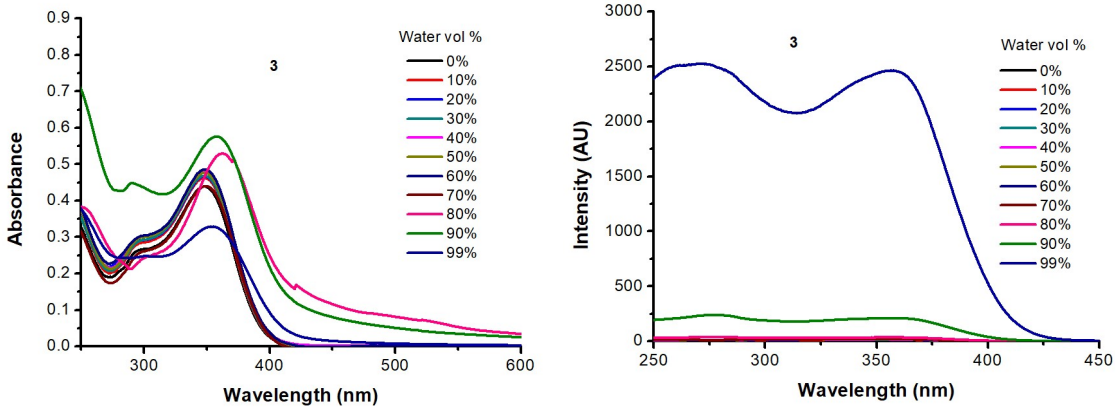


Figure S38: UV–visible and excitation spectra of **3** (15.75 μM) in THF–H_2O mixtures with different volume fractions of water (λ_{em}=484 nm) at 25 °C.

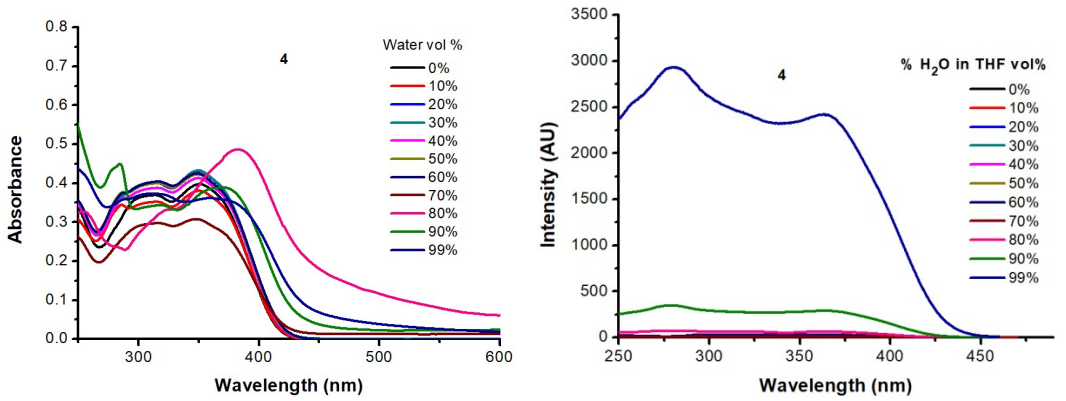


Figure S39: UV–visible and excitation spectra of **4** (14.92 μM) in THF–H_2O mixtures with different volume fractions of water (λ_{em}=490 nm) at 25 °C.

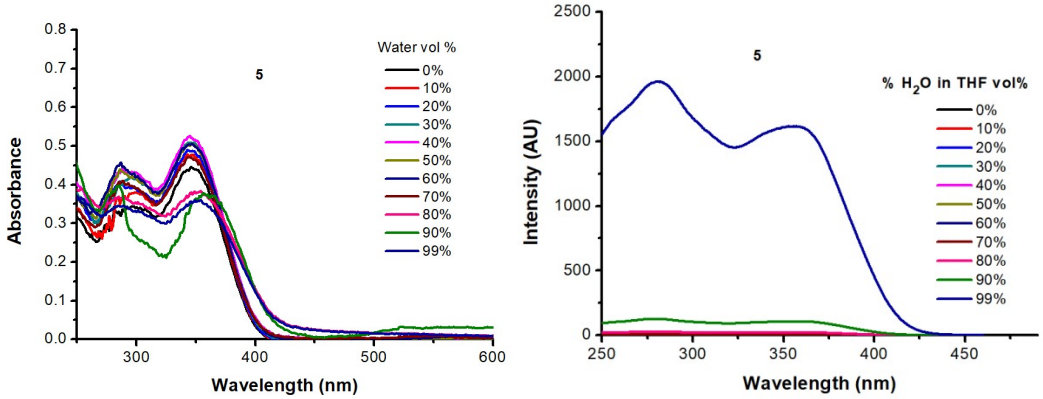


Figure S40: UV–visible and excitation spectra of **5** (14.92 μM) in THF–H_2O mixtures with different volume fractions of water (λ_{em}=489 nm) at 25 °C.

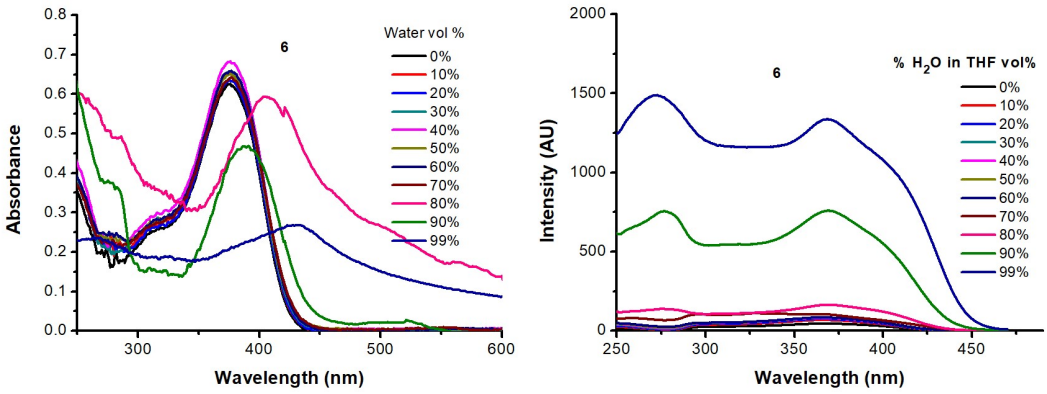


Figure S41: UV–visible and excitation spectra of **6** (14.92 μM) in THF–H_2O mixtures with different volume fractions of water (λ_{em}=495 nm) at 25 °C.

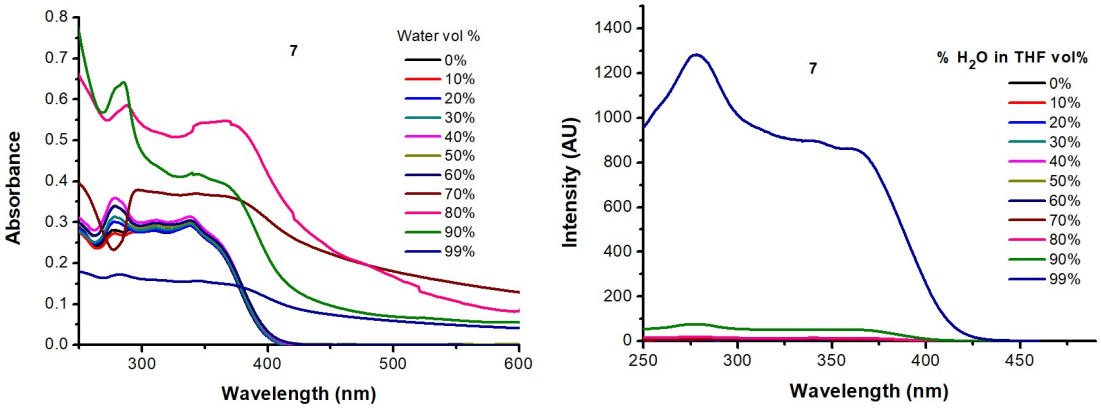


Figure S42: UV–visible and excitation spectra of **7** (15 μM) in THF–H_2O mixtures with different volume fractions of water (λ_{em}=479 nm) at 25 °C.

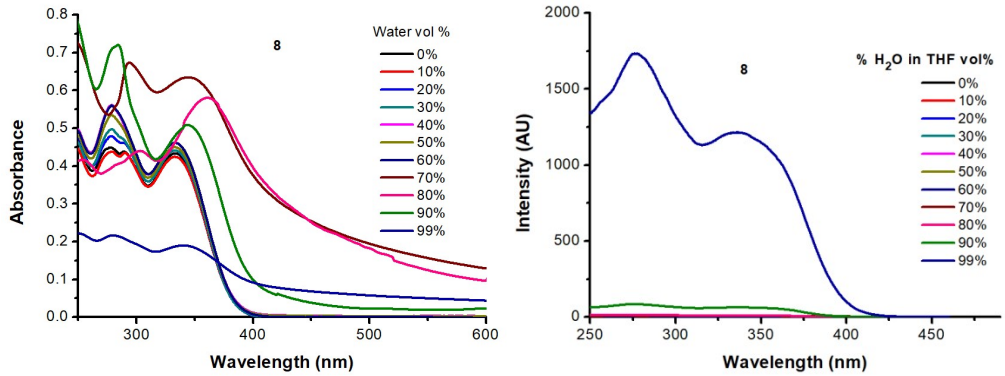


Figure S43: UV–visible and excitation spectra of **8** (15 μM) in THF–H_2O mixtures with different volume fractions of water (λ_{em}=480 nm) at 25 °C.

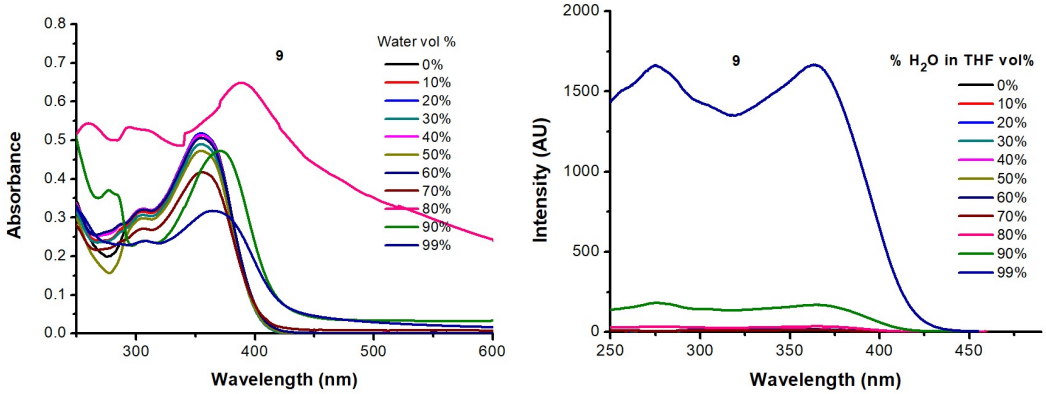


Figure S44: UV–visible and excitation spectra of **9** (15 μM) in THF–H_2O mixtures with different volume fractions of water (λ_{em}=483 nm) at 25 °C.

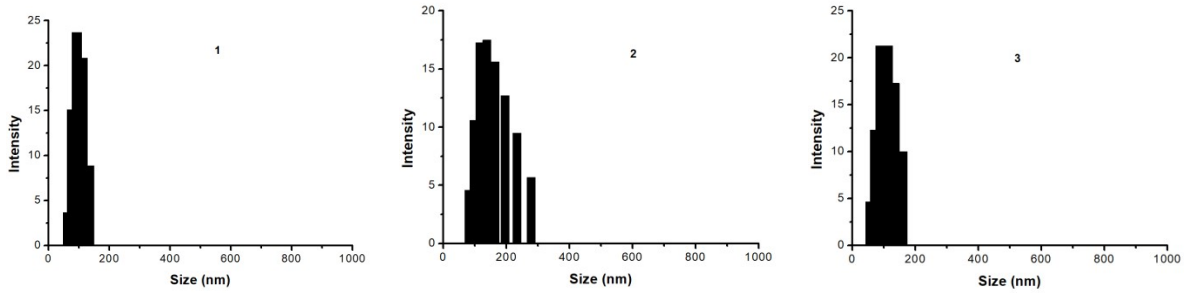


Figure S45: DLS–size distribution profile of the fluorescent organic nanoaggregates of **1–3** (32 μM) (left to right) in THF/H_2O (1:99).

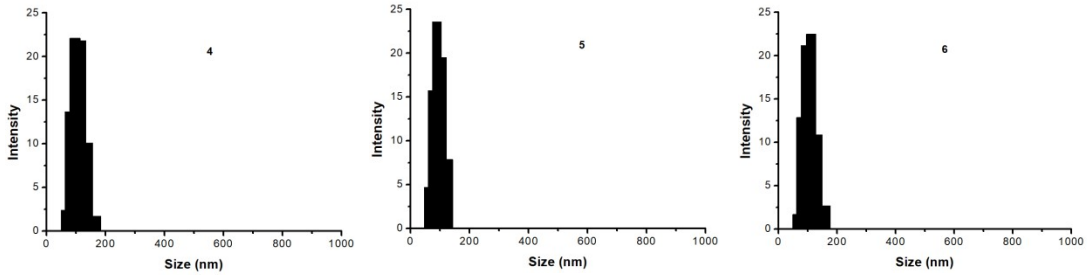


Figure S46: DLS–size distribution profile of the fluorescent organic nanoaggregates of **4-6** (left to right) in THF/H_2O (1:99; 30 μM).

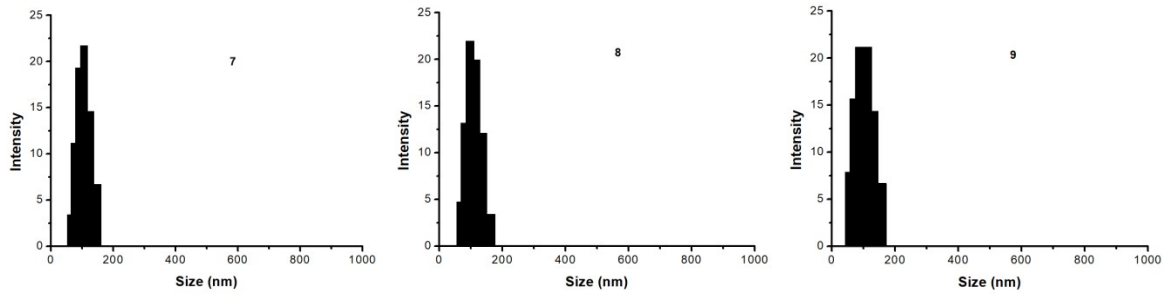


Figure S47: DLS–size distribution profile of the fluorescent organic nanoaggregates of **7-9** (left to right) in THF/H_2O (1:99; 30 μM).

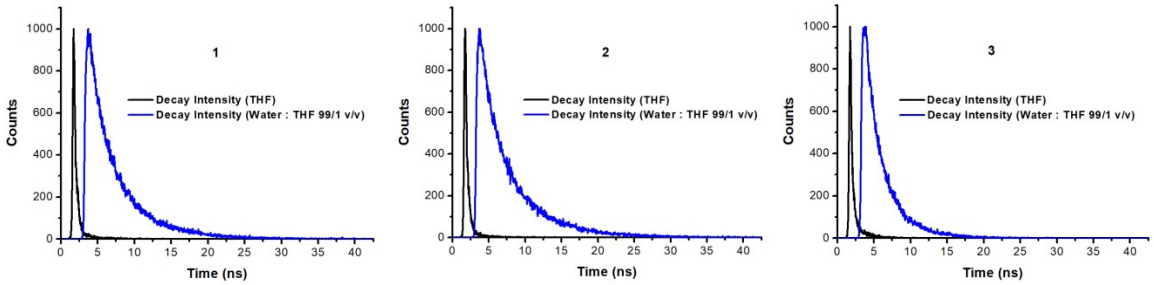


Figure 48: Time–resolved fluorescence decay curves **1**–**3** (32 μM) in THF and THF:H_2O (1/99 v/v) at 25 °C.

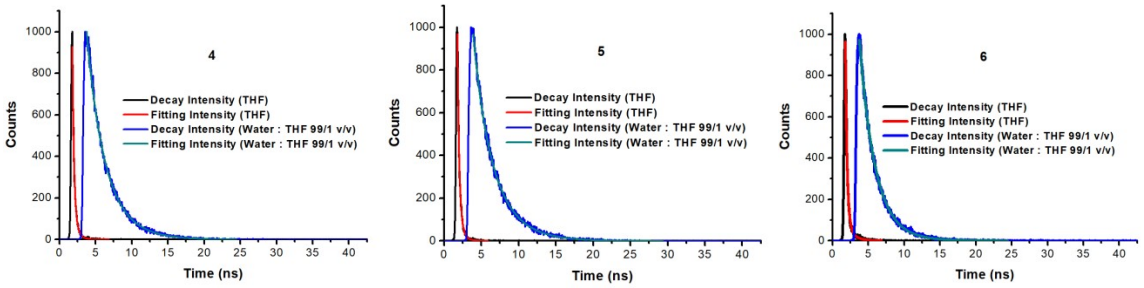


Figure 49: Time–resolved fluorescence decay curves **4-6** in THF and THF:H_2O (1/99 v/v) at 25 °C.

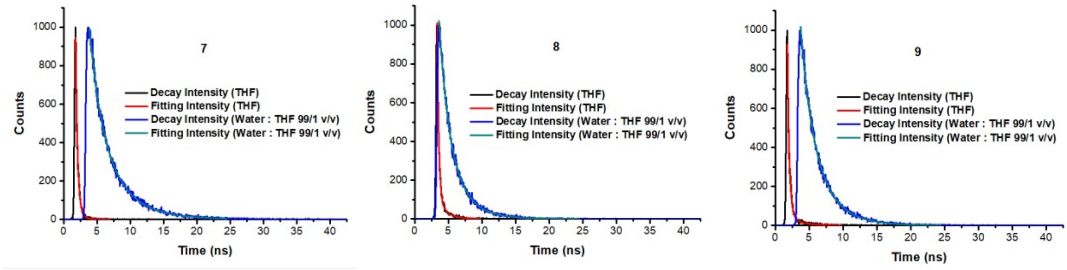


Figure 50: Time–resolved fluorescence decay curves **7-9** in THF and THF:H_2O (1/99 v/v) at 25 °C.

Figure S51: The frontier molecular orbitals (HOMO and LUMO) of the CTPEs **1-6** calculated using B3LYP level of TD–DFT theory.

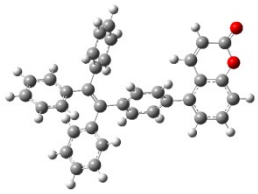
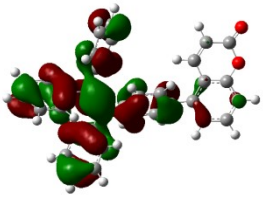
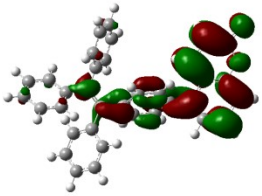
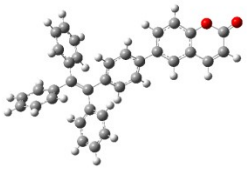
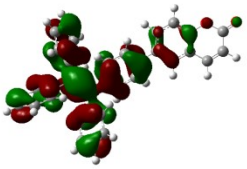
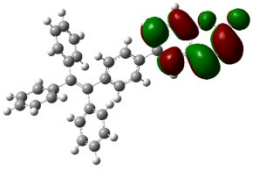
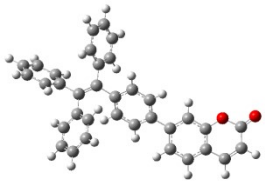
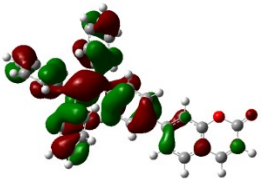
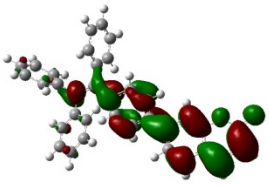
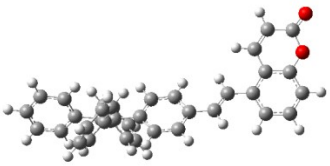
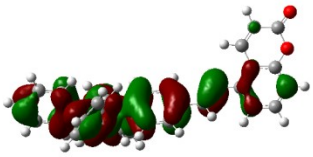
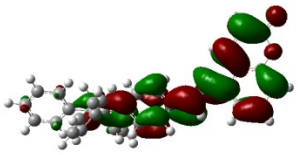
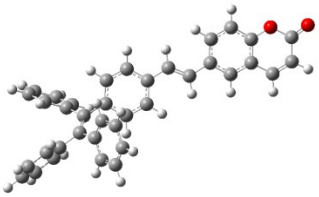
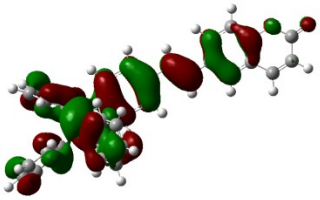
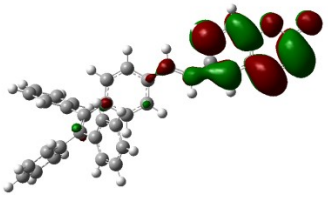
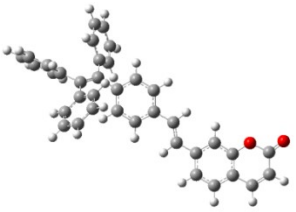
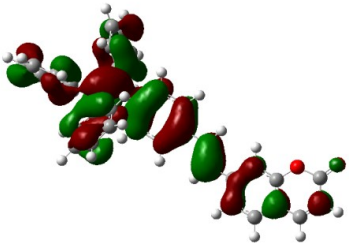
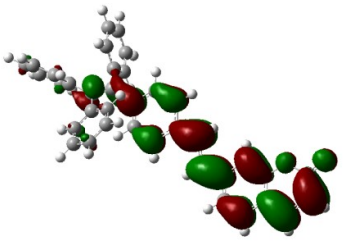
CTPEs	Optimized structure	HOMO	LUMO
1			
2			
3			
4			
5			
6			

Figure S52: The frontier molecular orbitals (HOMO and LUMO) of the CTPEs **7-9** calculated using B3LYP level of TD–DFT theory.

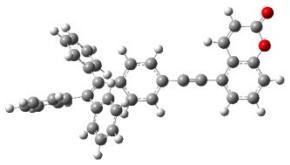
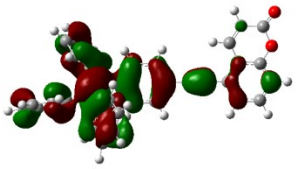
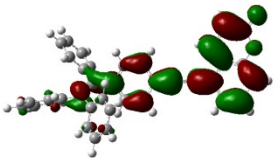
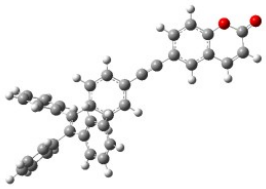
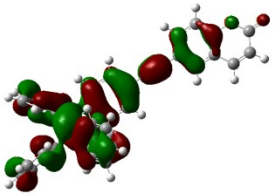
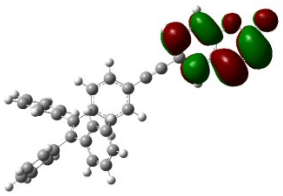
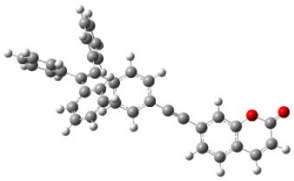
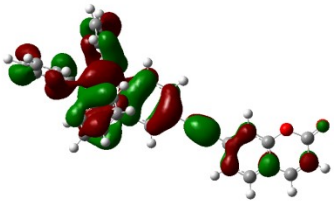
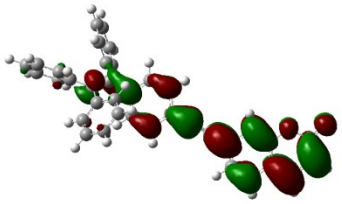
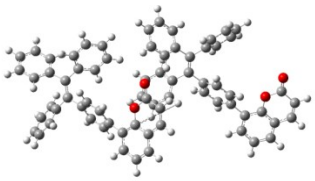
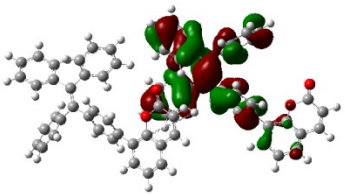
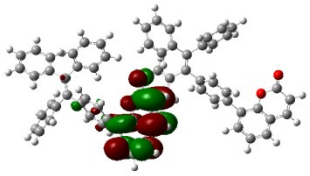
CTPEs	Optimized structure	HOMO	LUMO
7			
8			
9			

Figure S53: The frontier molecular orbitals (HOMO and LUMO) of the CTPEs **1-dimer** calculated using B3LYP level of TD–DFT theory.

CTPEs	Optimized structure	HOMO	LUMO
1-dimer			

DFT data of **1:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.029007	3.030865	-0.715369
2	6	0	1.310053	4.213624	-0.552323
3	6	0	1.869390	1.959021	0.180458
4	6	0	0.433176	4.360238	0.524314
5	6	0	0.992400	2.126162	1.265620
6	6	0	0.282661	3.313782	1.436203
7	1	0	0.874158	1.317894	1.979792
8	1	0	2.719599	2.928828	-1.547062
9	6	0	2.660895	0.702012	0.009131
10	6	0	2.089806	-0.538395	0.060468
11	6	0	4.123292	0.909569	-0.218452
12	6	0	4.849284	1.807379	0.583928
13	6	0	4.797696	0.263496	-1.268357
14	6	0	6.208356	2.025346	0.365590
15	1	0	4.340820	2.332401	1.386897
16	6	0	6.154030	0.490509	-1.494355
17	1	0	4.249745	-0.417711	-1.910762
18	6	0	6.866868	1.367713	-0.675141
19	1	0	6.752433	2.713553	1.006174
20	1	0	6.653568	-0.015843	-2.315320
21	1	0	7.924194	1.543100	-0.850798
22	6	0	2.890334	-1.797255	0.159460
23	6	0	2.609921	-2.889447	-0.680251
24	6	0	3.898793	-1.945480	1.126559
25	6	0	3.333536	-4.076229	-0.578048
26	1	0	1.821765	-2.800643	-1.422043
27	6	0	4.614458	-3.136335	1.236875
28	1	0	4.117969	-1.119053	1.794514
29	6	0	4.338983	-4.205050	0.382027
30	1	0	3.108894	-4.902639	-1.246360
31	1	0	5.386371	-3.230424	1.995306
32	1	0	4.898334	-5.132069	0.467385
33	6	0	0.610192	-0.740716	0.028963
34	6	0	-0.016283	-1.606417	0.942076
35	6	0	-0.195056	-0.120409	-0.940764
36	6	0	-1.392786	-1.807293	0.915637
37	1	0	0.584596	-2.115245	1.689504
38	6	0	-1.570397	-0.328846	-0.975173
39	1	0	0.266588	0.526799	-1.678806
40	6	0	-2.199658	-1.165618	-0.038124
41	1	0	-1.855645	-2.456947	1.652650
42	1	0	-2.161516	0.141386	-1.755506
43	1	0	-0.382916	3.424434	2.287661
44	1	0	-0.120202	5.285313	0.656881
45	1	0	1.438857	5.024018	-1.264087
46	6	0	-3.665351	-1.416876	-0.074761
47	6	0	-4.612182	-0.354798	-0.077385
48	6	0	-4.132174	-2.733314	-0.109784
49	6	0	-4.278568	1.044660	0.052198
50	6	0	-5.984853	-0.671248	-0.152453
51	6	0	-5.501085	-3.016529	-0.171553
52	1	0	-3.412845	-3.545541	-0.118183
53	6	0	-5.239773	1.996112	0.044354
54	1	0	-3.237971	1.325945	0.171952

55	6	0	-6.436557	-1.990524	-0.200853
56	1	0	-5.835235	-4.048840	-0.209487
57	6	0	-6.651328	1.663834	-0.093825
58	1	0	-5.013699	3.050447	0.148249
59	1	0	-7.502495	-2.179926	-0.256811
60	8	0	-6.943776	0.300578	-0.169155
61	8	0	-7.573453	2.443110	-0.136229

HF= −1498.67

DFT data of **2:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.216039	-2.956331	-0.656780
2	6	0	-2.853914	-4.288812	-0.467899
3	6	0	-2.760348	-1.953074	0.216571
4	6	0	-2.047590	-4.651329	0.612917
5	6	0	-1.958157	-2.335091	1.305200
6	6	0	-1.606504	-3.669405	1.501709
7	1	0	-1.613951	-1.577030	2.001005
8	1	0	-3.855271	-2.682938	-1.490813
9	6	0	-3.175425	-0.530154	0.021311
10	6	0	-2.285915	0.506992	0.051410
11	6	0	-4.639607	-0.332225	-0.204788
12	6	0	-5.581255	-0.976756	0.616706
13	6	0	-5.114681	0.451170	-1.270259
14	6	0	-6.948714	-0.817017	0.400604
15	1	0	-5.233315	-1.602571	1.432942
16	6	0	-6.482129	0.600849	-1.494107
17	1	0	-4.402840	0.942009	-1.925569
18	6	0	-7.405342	-0.027624	-0.656542
19	1	0	-7.658526	-1.313955	1.055805
20	1	0	-6.826516	1.206633	-2.327401
21	1	0	-8.470876	0.090712	-0.830403
22	6	0	-2.711868	1.938114	0.128299
23	6	0	-2.140435	2.899441	-0.723833
24	6	0	-3.644083	2.371513	1.086128
25	6	0	-2.511874	4.240328	-0.642944
26	1	0	-1.403758	2.587201	-1.458073
27	6	0	-4.006814	3.714263	1.175243
28	1	0	-4.083059	1.646867	1.763899
29	6	0	-3.446866	4.653886	0.307836
30	1	0	-2.067389	4.963563	-1.320810
31	1	0	-4.725791	4.027297	1.926936
32	1	0	-3.731440	5.699773	0.376505
33	6	0	-0.807446	0.298563	0.013634
34	6	0	0.038390	0.981156	0.905166
35	6	0	-0.206464	-0.535391	-0.944010
36	6	0	1.417858	0.808442	0.865112
37	1	0	-0.396385	1.642133	1.648704
38	6	0	1.173999	-0.696497	-0.994237
39	1	0	-0.831840	-1.052689	-1.663702
40	6	0	2.017235	-0.033472	-0.086906
41	1	0	2.038520	1.315808	1.597881
42	1	0	1.606362	-1.322246	-1.769339
43	1	0	-0.990759	-3.942708	2.353887

44	1	0	-1.772383	-5.690831	0.765569
45	1	0	-3.206686	-5.045864	-1.162508
46	6	0	3.489300	-0.209430	-0.139082
47	6	0	4.059597	-1.462601	-0.455954
48	6	0	4.356128	0.854101	0.122385
49	6	0	5.434205	-1.647412	-0.511343
50	6	0	5.751084	0.695443	0.076087
51	1	0	3.953319	1.838251	0.343686
52	6	0	6.279044	-0.568901	-0.245016
53	6	0	6.691316	1.759431	0.327894
54	6	0	8.022420	1.534268	0.262721
55	1	0	6.308656	2.747178	0.572647
56	6	0	8.564497	0.218112	-0.063886
57	1	0	8.757070	2.308609	0.447226
58	8	0	7.624442	-0.786783	-0.307913
59	1	0	5.869403	-2.612495	-0.746069
60	1	0	3.406508	-2.310099	-0.637637
61	8	0	9.734226	-0.071954	-0.140894

HF= −1498.67

DFT data of **3:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.327102	-2.908998	-0.617343
2	6	0	-3.029785	-4.255837	-0.417819
3	6	0	-2.812110	-1.920677	0.240050
4	6	0	-2.230249	-4.646956	0.658035
5	6	0	-2.017777	-2.331042	1.324155
6	6	0	-1.730653	-3.679190	1.531255
7	1	0	-1.629163	-1.584042	2.008448
8	1	0	-3.961097	-2.612838	-1.447561
9	6	0	-3.157717	-0.480992	0.033174
10	6	0	-2.217417	0.510751	0.043266
11	6	0	-4.612496	-0.211897	-0.179964
12	6	0	-5.576752	-0.803286	0.655198
13	6	0	-5.058795	0.586233	-1.247019
14	6	0	-6.936737	-0.578000	0.450600
15	1	0	-5.252246	-1.439320	1.473137
16	6	0	-6.419296	0.801560	-1.459163
17	1	0	-4.330173	1.036468	-1.912900
18	6	0	-7.364143	0.225302	-0.608239
19	1	0	-7.663749	-1.034501	1.116271
20	1	0	-6.741528	1.417649	-2.293750
21	1	0	-8.424188	0.394874	-0.773008
22	6	0	-2.571960	1.961811	0.109278
23	6	0	-1.971307	2.884164	-0.765373
24	6	0	-3.464042	2.450280	1.078688
25	6	0	-2.276568	4.242204	-0.694442
26	1	0	-1.264160	2.528482	-1.508846
27	6	0	-3.760220	3.809907	1.157633
28	1	0	-3.924087	1.755335	1.773464
29	6	0	-3.172369	4.711162	0.268285
30	1	0	-1.810255	4.935382	-1.388749
31	1	0	-4.448698	4.166083	1.918602
32	1	0	-3.404625	5.770333	0.329363

33	6	0	-0.751679	0.230000	-0.007302
34	6	0	0.136788	0.888012	0.861331
35	6	0	-0.203000	-0.648112	-0.957436
36	6	0	1.505987	0.652902	0.805767
37	1	0	-0.256536	1.582021	1.597660
38	6	0	1.167087	-0.875777	-1.020720
39	1	0	-0.861082	-1.147563	-1.660355
40	6	0	2.052327	-0.234584	-0.137237
41	1	0	2.159104	1.146798	1.518725
42	1	0	1.559453	-1.534602	-1.789393
43	1	0	-1.119943	-3.974023	2.379864
44	1	0	-2.005815	-5.697336	0.819220
45	1	0	-3.427936	-5.001502	-1.100121
46	6	0	3.512342	-0.479431	-0.204641
47	6	0	4.016284	-1.758470	-0.534988
48	6	0	4.422405	0.551973	0.059284
49	6	0	5.379466	-1.990776	-0.598411
50	6	0	5.792709	0.310144	-0.004136
51	1	0	4.085607	1.556581	0.287990
52	6	0	6.300976	-0.960691	-0.334962
53	6	0	7.731159	-1.114121	-0.381033
54	6	0	8.018323	1.250809	0.217913
55	6	0	8.546792	-0.067197	-0.119463
56	1	0	3.323507	-2.573801	-0.712716
57	1	0	5.754077	-2.980669	-0.844293
58	1	0	8.144677	-2.088039	-0.631334
59	1	0	9.626847	-0.144837	-0.145552
60	8	0	8.668546	2.238589	0.463751
61	8	0	6.625103	1.360909	0.256312

HF= −1498.68

DFT data of **4:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.281907	3.010939	0.693774
2	6	0	-2.801839	4.291412	0.425253
3	6	0	-3.137851	1.973908	-0.244899
4	6	0	-2.188762	4.569707	-0.798087
5	6	0	-2.528970	2.272494	-1.475603
6	6	0	-2.060524	3.556325	-1.749517
7	1	0	-2.428889	1.489791	-2.220353
8	1	0	-3.770110	2.804559	1.641443
9	6	0	-3.676856	0.609638	0.041977
10	6	0	-2.945931	-0.528406	-0.158944
11	6	0	-5.079360	0.588427	0.557516
12	6	0	-6.077438	1.361916	-0.061175
13	6	0	-5.426936	-0.152068	1.700127
14	6	0	-7.383190	1.368859	0.425620
15	1	0	-5.823324	1.956786	-0.933214
16	6	0	-6.729830	-0.135142	2.194611
17	1	0	-4.666228	-0.740727	2.201877
18	6	0	-7.715132	0.620365	1.556488
19	1	0	-8.141208	1.963598	-0.076113
20	1	0	-6.974391	-0.710659	3.082820
21	1	0	-8.730739	0.631531	1.941184
22	6	0	-3.557515	-1.893167	-0.141575
23	6	0	-2.964763	-2.932356	0.596758
24	6	0	-4.701383	-2.188089	-0.902209
25	6	0	-3.515030	-4.212858	0.600294

26	1	0	-2.068961	-2.728545	1.175730
27	6	0	-5.245444	-3.471288	-0.907783
28	1	0	-5.162389	-1.402404	-1.491639
29	6	0	-4.658152	-4.487944	-0.152655
30	1	0	-3.048033	-4.997630	1.188598
31	1	0	-6.127727	-3.677757	-1.506843
32	1	0	-5.083403	-5.487294	-0.156050
33	6	0	-1.476881	-0.506739	-0.419473
34	6	0	-0.915547	-1.293694	-1.439824
35	6	0	-0.597249	0.253462	0.375412
36	6	0	0.454343	-1.292308	-1.674754
37	1	0	-1.565350	-1.905749	-2.057450
38	6	0	0.771336	0.244615	0.149054
39	1	0	-1.001658	0.859799	1.178715
40	6	0	1.334434	-0.529020	-0.885315
41	1	0	0.858654	-1.899881	-2.480524
42	1	0	1.409780	0.853790	0.781432
43	1	0	-1.598448	3.765987	-2.709974
44	1	0	-1.821815	5.569492	-1.010991
45	1	0	-2.911410	5.074364	1.170245
46	6	0	2.767909	-0.579958	-1.172334
47	1	0	3.032366	-1.142317	-2.066557
48	6	0	3.766064	-0.038710	-0.442422
49	1	0	3.515764	0.470155	0.484360
50	6	0	5.188201	-0.079909	-0.802472
51	6	0	6.198184	-0.045812	0.204675
52	6	0	5.590769	-0.126306	-2.143983
53	6	0	5.938687	-0.037188	1.623786
54	6	0	7.553229	-0.055616	-0.185340
55	6	0	6.941579	-0.150401	-2.497768
56	1	0	4.836575	-0.106445	-2.922914
57	6	0	6.948051	-0.002926	2.523862
58	1	0	4.913518	-0.074142	1.976500
59	6	0	7.934682	-0.112336	-1.525684
60	1	0	7.220266	-0.180404	-3.546718
61	6	0	8.344552	0.021768	2.110171
62	1	0	6.774107	0.001361	3.593033
63	1	0	8.989724	-0.118119	-1.774217
64	8	0	8.563570	-0.018539	0.732665
65	8	0	9.308949	0.066203	2.836367

HF= −1576.08

DFT data of **5:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.779591	-3.018848	-0.477399
2	6	0	-3.306103	-4.302782	-0.213828
3	6	0	-3.432825	-1.936298	0.350390
4	6	0	-2.494137	-4.537896	0.897473
5	6	0	-2.623306	-2.190946	1.470479
6	6	0	-2.159969	-3.477213	1.741319
7	1	0	-2.361034	-1.371595	2.131626
8	1	0	-4.421977	-2.845968	-1.335594
9	6	0	-3.966676	-0.568048	0.072822
10	6	0	-3.176185	0.547856	0.075118
11	6	0	-5.434625	-0.515357	-0.203376
12	6	0	-6.341111	-1.199592	0.625626
13	6	0	-5.943125	0.164919	-1.322776
14	6	0	-7.709638	-1.176634	0.363480

15	1	0	-5.965113	-1.748122	1.483974
16	6	0	-7.310508	0.177669	-1.592098
17	1	0	-5.257087	0.683702	-1.984020
18	6	0	-8.200567	-0.487811	-0.747299
19	1	0	-8.392967	-1.701510	1.025032
20	1	0	-7.680525	0.705634	-2.466356
21	1	0	-9.266235	-0.475879	-0.956606
22	6	0	-3.740090	1.933175	0.069939
23	6	0	-3.247052	2.901132	-0.822695
24	6	0	-4.731932	2.320388	0.986550
25	6	0	-3.750895	4.200598	-0.820658
26	1	0	-2.466534	2.626323	-1.525960
27	6	0	-5.228058	3.622858	0.996491
28	1	0	-5.112868	1.591108	1.693783
29	6	0	-4.743978	4.567305	0.089641
30	1	0	-3.364572	4.928617	-1.528372
31	1	0	-5.991770	3.900932	1.717174
32	1	0	-5.132151	5.581640	0.096622
33	6	0	-1.685979	0.481680	0.086793
34	6	0	-0.935483	1.308121	0.940580
35	6	0	-0.976143	-0.358829	-0.792384
36	6	0	0.453783	1.266613	0.940388
37	1	0	-1.451051	1.984419	1.615371
38	6	0	0.410591	-0.389890	-0.802213
39	1	0	-1.528087	-0.990744	-1.479882
40	6	0	1.165473	0.417470	0.072371
41	1	0	1.006159	1.906469	1.624165
42	1	0	0.912239	-1.047021	-1.505656
43	1	0	-1.540181	-3.651436	2.616241
44	1	0	-2.131610	-5.539785	1.108089
45	1	0	-3.576219	-5.121790	-0.874413
46	6	0	2.627391	0.423485	0.118177
47	1	0	3.047434	1.124374	0.837916
48	6	0	3.468511	-0.333807	-0.616374
49	1	0	3.048488	-1.039239	-1.330462
50	6	0	4.932494	-0.328544	-0.567241
51	6	0	5.643684	-1.216661	-1.408126
52	6	0	5.683314	0.507813	0.268879
53	6	0	7.029797	-1.275058	-1.418581
54	6	0	7.084463	0.470384	0.279880
55	1	0	5.187625	1.210184	0.932185
56	6	0	7.751124	-0.431514	-0.573540
57	6	0	7.903347	1.308802	1.121516
58	6	0	9.251134	1.220645	1.082619
59	1	0	7.414498	2.014012	1.789159
60	6	0	9.935499	0.283013	0.196249
61	1	0	9.896172	1.833812	1.700134
62	1	0	5.083672	-1.875010	-2.066462
63	1	0	7.566511	-1.959426	-2.066122
64	8	0	9.112401	-0.512432	-0.605252
65	8	0	11.130274	0.138322	0.097662

HF=-1576.08

DFT data of **6:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.814788	-3.009791	-0.368126
2	6	0	-3.369958	-4.296636	-0.071046
3	6	0	-3.424374	-1.910763	0.417454
4	6	0	-2.543776	-4.517191	1.032810

5	6	0	-2.601331	-2.150505	1.530974
6	6	0	-2.166783	-3.439280	1.835707
7	1	0	-2.306296	-1.317675	2.160726
8	1	0	-4.468575	-2.847529	-1.219767
9	6	0	-3.927066	-0.538289	0.105080
10	6	0	-3.106502	0.554652	0.056418
11	6	0	-5.398323	-0.453597	-0.143243
12	6	0	-6.305133	-1.090355	0.722482
13	6	0	-5.911816	0.208797	-1.271103
14	6	0	-7.677675	-1.038107	0.486963
15	1	0	-5.926179	-1.624669	1.588419
16	6	0	-7.283600	0.250586	-1.513513
17	1	0	-5.226298	0.690253	-1.960464
18	6	0	-8.173144	-0.367328	-0.632768
19	1	0	-8.360738	-1.526005	1.176487
20	1	0	-7.657592	0.763839	-2.394791
21	1	0	-9.242221	-0.332695	-0.821089
22	6	0	-3.631403	1.954722	0.018762
23	6	0	-3.132390	2.879254	-0.915552
24	6	0	-4.590567	2.398823	0.944329
25	6	0	-3.599102	4.192191	-0.943849
26	1	0	-2.376652	2.560202	-1.627201
27	6	0	-5.049072	3.714892	0.923703
28	1	0	-4.975513	1.703676	1.683144
29	6	0	-4.559695	4.615955	-0.023532
30	1	0	-3.208789	4.886156	-1.682855
31	1	0	-5.787360	4.037607	1.652209
32	1	0	-4.918429	5.640937	-0.040115
33	6	0	-1.618935	0.446832	0.041133
34	6	0	-0.829409	1.279719	0.852796
35	6	0	-0.951069	-0.441323	-0.824567
36	6	0	0.557694	1.201061	0.825647
37	1	0	-1.313180	1.990287	1.515624
38	6	0	0.433538	-0.509813	-0.862066
39	1	0	-1.534911	-1.080745	-1.477903
40	6	0	1.227211	0.306223	-0.030366
41	1	0	1.141822	1.846890	1.476378
42	1	0	0.903503	-1.203569	-1.551983
43	1	0	-1.536001	-3.601613	2.705013
44	1	0	-2.203681	-5.521065	1.269741
45	1	0	-3.673648	-5.129164	-0.699357
46	6	0	2.687972	0.277120	-0.016953
47	1	0	3.142173	0.977717	0.681392
48	6	0	3.495309	-0.509622	-0.760966
49	1	0	3.046378	-1.212210	-1.459665
50	6	0	4.956876	-0.531749	-0.738203
51	6	0	5.632759	-1.430299	-1.598988
52	6	0	5.727767	0.294282	0.096613
53	6	0	7.014167	-1.499649	-1.623925
54	6	0	7.114639	0.219145	0.066476
55	1	0	5.273242	1.003138	0.778645
56	6	0	7.790901	-0.674946	-0.789985
57	6	0	9.227953	-0.678836	-0.748281
58	6	0	9.198425	1.074125	0.972170
59	6	0	9.898052	0.149454	0.086314
60	1	0	5.048972	-2.074711	-2.249457
61	1	0	7.515515	-2.195408	-2.291136
62	1	0	9.767614	-1.360839	-1.400821
63	1	0	10.979320	0.173796	0.144463
64	8	0	7.802392	1.050670	0.904837
65	8	0	9.711786	1.846190	1.746608

HF= −1576.08

DFT data of **7:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.937937	-2.989133	-0.235090
2	6	0	-3.595423	-4.296839	0.103553
3	6	0	-3.402176	-1.896922	0.470016
4	6	0	-2.728443	-4.542303	1.170361
5	6	0	-2.539955	-2.160450	1.547695
6	6	0	-2.207264	-3.468816	1.894523
7	1	0	-2.133929	-1.330245	2.116234
8	1	0	-4.623567	-2.805305	-1.056771
9	6	0	-3.792087	-0.498507	0.114350
10	6	0	-2.875215	0.502934	-0.048509
11	6	0	-5.262126	-0.279626	-0.040705
12	6	0	-6.162862	-0.790852	0.910431
13	6	0	-5.787370	0.386807	-1.160890
14	6	0	-7.537207	-0.612911	0.763527
15	1	0	-5.777360	-1.326260	1.772747
16	6	0	-7.162356	0.554040	-1.314048
17	1	0	-5.108969	0.771935	-1.914774
18	6	0	-8.043172	0.060197	-0.350080
19	1	0	-8.213963	-1.004815	1.517453
20	1	0	-7.546268	1.067446	-2.190917
21	1	0	-9.114576	0.192304	-0.469255
22	6	0	-3.261224	1.945859	-0.126373
23	6	0	-2.746749	2.769827	-1.142655
24	6	0	-4.097100	2.528254	0.841042
25	6	0	-3.081314	4.121296	-1.207143
26	1	0	-2.084105	2.342019	-1.889162
27	6	0	-4.422799	3.882200	0.783283
28	1	0	-4.490343	1.910964	1.641988
29	6	0	-3.920901	4.683540	-0.243663
30	1	0	-2.682363	4.736636	-2.008498
31	1	0	-5.066961	4.312386	1.544787
32	1	0	-4.176266	5.738156	-0.289116
33	6	0	-1.409364	0.244597	-0.156539
34	6	0	-0.488529	1.037793	0.553711
35	6	0	-0.897240	-0.747673	-1.012630
36	6	0	0.879582	0.829391	0.443717
37	1	0	-0.857297	1.824274	1.204343
38	6	0	0.469209	-0.956553	-1.138660
39	1	0	-1.585021	-1.357443	-1.587998
40	6	0	1.385676	-0.174302	-0.406711
41	1	0	1.570977	1.443296	1.011860
42	1	0	0.843770	-1.722632	-1.809595
43	1	0	-1.543391	-3.649514	2.735041
44	1	0	-2.467786	-5.561622	1.439715
45	1	0	-4.010376	-5.125569	-0.463019
46	6	0	2.786312	-0.388209	-0.533459
47	6	0	3.983052	-0.580745	-0.650111
48	6	0	5.376386	-0.820783	-0.801054
49	6	0	6.331538	-0.023071	-0.106324
50	6	0	5.827655	-1.850392	-1.640657
51	6	0	5.984773	1.057599	0.778835
52	6	0	7.699410	-0.296724	-0.287359
53	6	0	7.194240	-2.092814	-1.795707
54	1	0	5.099515	-2.456111	-2.167974
55	6	0	6.944604	1.774207	1.406721

56	1	0	4.933336	1.282145	0.928935
57	6	0	8.139474	-1.323168	-1.124825
58	1	0	7.524123	-2.894036	-2.449580
59	6	0	8.362244	1.489662	1.218287
60	1	0	6.716193	2.592712	2.078461
61	1	0	9.204337	-1.495470	-1.231906
62	8	0	8.658990	0.433637	0.351041
63	8	0	9.285790	2.072649	1.733437

HF= −1574.83

DFT data of **8:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.738476	3.071561	0.534225
2	6	0	-3.235807	4.342820	0.263577
3	6	0	-3.442961	1.983553	-0.306170
4	6	0	-2.445517	4.559801	-0.866858
5	6	0	-2.654889	2.220043	-1.445244
6	6	0	-2.162211	3.493981	-1.722735
7	1	0	-2.432830	1.396696	-2.116121
8	1	0	-4.363495	2.912950	1.407843
9	6	0	-4.006866	0.629428	-0.018813
10	6	0	-3.247140	-0.507120	-0.040556
11	6	0	-5.469183	0.615286	0.290300
12	6	0	-6.374911	1.327449	-0.515605
13	6	0	-5.970542	-0.055606	1.418541
14	6	0	-7.737319	1.340642	-0.222646
15	1	0	-6.003493	1.869127	-1.380264
16	6	0	-7.331301	-0.032041	1.718748
17	1	0	-5.284296	-0.595823	2.062165
18	6	0	-8.221621	0.660942	0.896620
19	1	0	-8.420777	1.886629	-0.866709
20	1	0	-7.695835	-0.553262	2.599316
21	1	0	-9.282209	0.677178	1.130015
22	6	0	-3.845986	-1.877484	-0.022400
23	6	0	-3.359494	-2.857296	0.860789
24	6	0	-4.866126	-2.239093	-0.918128
25	6	0	-3.896517	-4.143386	0.870187
26	1	0	-2.558006	-2.602518	1.547868
27	6	0	-5.395749	-3.528323	-0.916561
28	1	0	-5.242396	-1.500387	-1.618013
29	6	0	-4.917329	-4.484550	-0.019077
30	1	0	-3.514315	-4.880984	1.570121
31	1	0	-6.181126	-3.786933	-1.620987
32	1	0	-5.331433	-5.488575	-0.017227
33	6	0	-1.755702	-0.480206	-0.087978
34	6	0	-1.051852	-1.322949	-0.968486
35	6	0	-1.006011	0.335861	0.778516
36	6	0	0.336058	-1.325979	-1.010804
37	1	0	-1.606746	-1.978739	-1.632087
38	6	0	0.382059	0.330876	0.753097
39	1	0	-1.524162	0.978727	1.481687
40	6	0	1.081317	-0.496335	-0.148841
41	1	0	0.859208	-1.972134	-1.708185
42	1	0	0.941349	0.963647	1.434469

43	1	0	-1.559487	3.654586	-2.612016
44	1	0	-2.060193	5.552002	-1.082733
45	1	0	-3.466046	5.166190	0.933741
46	6	0	2.503900	-0.498963	-0.183001
47	6	0	3.720345	-0.496531	-0.212484
48	6	0	5.143031	-0.493956	-0.250896
49	6	0	5.841798	-1.332570	-1.154397
50	6	0	5.884243	0.336563	0.600122
51	6	0	7.226741	-1.338587	-1.204152
52	6	0	7.286144	0.343836	0.563925
53	1	0	5.366748	0.985971	1.299131
54	6	0	7.947385	-0.502354	-0.347514
55	6	0	8.107412	1.173885	1.411255
56	6	0	9.455005	1.130619	1.322325
57	1	0	7.620532	1.835524	2.123196
58	6	0	10.135455	0.251782	0.375186
59	1	0	10.102533	1.739037	1.941882
60	8	0	9.307257	-0.538238	-0.429252
61	1	0	5.274435	-1.978224	-1.815905
62	1	0	7.767475	-1.977570	-1.893338
63	8	0	11.329027	0.148649	0.227722

HF= −1574.83

DFT data of **9:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.035575	-2.996931	-0.424969
2	6	0	-3.628936	-4.304791	-0.167574
3	6	0	-3.568885	-1.927920	0.360235
4	6	0	-2.765736	-4.575874	0.896077
5	6	0	-2.709668	-2.218096	1.433537
6	6	0	-2.313258	-3.527688	1.699158
7	1	0	-2.356524	-1.408137	2.063251
8	1	0	-4.718260	-2.794681	-1.244760
9	6	0	-4.027954	-0.530966	0.091551
10	6	0	-3.163801	0.525892	0.016503
11	6	0	-5.504714	-0.379740	-0.079853
12	6	0	-6.393240	-0.997865	0.817701
13	6	0	-6.045404	0.328780	-1.166276
14	6	0	-7.772382	-0.883614	0.653411
15	1	0	-5.994633	-1.566724	1.652213
16	6	0	-7.424514	0.432516	-1.337737
17	1	0	-5.375730	0.796660	-1.880066
18	6	0	-8.294341	-0.168005	-0.425792
19	1	0	-8.440134	-1.358467	1.366607
20	1	0	-7.819874	0.980273	-2.188361
21	1	0	-9.369051	-0.085323	-0.558926
22	6	0	-3.623404	1.948902	0.023916
23	6	0	-3.129327	2.863035	-0.923152
24	6	0	-4.511057	2.423043	1.004284
25	6	0	-3.532562	4.197054	-0.909273
26	1	0	-2.428231	2.519565	-1.678059
27	6	0	-4.905516	3.759716	1.025264
28	1	0	-4.889863	1.735407	1.753237
29	6	0	-4.422415	4.651353	0.065877
30	1	0	-3.147840	4.883253	-1.658348

31	1	0	-5.588648	4.105802	1.795630
32	1	0	-4.731322	5.692428	0.081982
33	6	0	-1.684504	0.351144	-0.075650
34	6	0	-0.820980	1.126311	0.721190
35	6	0	-1.106102	-0.540530	-0.997548
36	6	0	0.557926	0.993503	0.630358
37	1	0	-1.243930	1.836631	1.424447
38	6	0	0.271633	-0.670059	-1.106898
39	1	0	-1.751354	-1.134319	-1.635737
40	6	0	1.131034	0.091006	-0.288615
41	1	0	1.207419	1.588428	1.264098
42	1	0	0.699197	-1.358052	-1.828872
43	1	0	-1.652960	-3.729329	2.537729
44	1	0	-2.455109	-5.595990	1.101978
45	1	0	-3.991040	-5.114118	-0.795188
46	6	0	2.543009	-0.041855	-0.393431
47	6	0	3.752062	-0.154220	-0.479410
48	6	0	5.162286	-0.291708	-0.586472
49	6	0	5.725080	-1.122596	-1.588062
50	6	0	6.012155	0.392926	0.298160
51	6	0	7.096744	-1.257042	-1.692718
52	6	0	7.390576	0.245413	0.179512
53	1	0	5.610698	1.034371	1.073465
54	6	0	7.961221	-0.577449	-0.812669
55	6	0	9.396332	-0.667010	-0.856740
56	6	0	9.566929	0.868099	1.053702
57	6	0	10.159340	0.016998	0.026681
58	1	0	5.064813	-1.648453	-2.268265
59	1	0	7.525349	-1.894133	-2.461304
60	1	0	9.857189	-1.296108	-1.614282
61	1	0	11.241567	-0.026896	0.023154
62	8	0	8.169925	0.931529	1.065686
63	8	0	10.167070	1.511911	1.880403

HF= −1574.83

DFT data of **1-dimer:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.237765	2.699922	0.700614
2	6	0	-5.291610	3.613175	1.162226
3	6	0	-5.864329	1.635036	-0.138758
4	6	0	-3.954165	3.491497	0.781455
5	6	0	-4.516979	1.537737	-0.526484
6	6	0	-3.570922	2.452118	-0.067830
7	1	0	-4.212670	0.733587	-1.188154
8	1	0	-7.277302	2.803515	0.996509
9	6	0	-6.892397	0.668024	-0.629088
10	6	0	-6.706436	-0.686237	-0.620473
11	6	0	-8.152158	1.298080	-1.131719
12	6	0	-8.097854	2.373926	-2.035222
13	6	0	-9.412708	0.876015	-0.677479
14	6	0	-9.264162	2.982726	-2.494770
15	1	0	-7.131161	2.728816	-2.379653
16	6	0	-10.578871	1.493757	-1.126386

17	1	0	-9.473039	0.059189	0.034040
18	6	0	-10.510398	2.545233	-2.041804
19	1	0	-9.199313	3.803896	-3.203024
20	1	0	-11.542536	1.154695	-0.756984
21	1	0	-11.419359	3.024835	-2.393199
22	6	0	-7.626650	-1.628484	-1.330907
23	6	0	-8.132631	-2.762462	-0.671724
24	6	0	-7.963359	-1.442047	-2.681944
25	6	0	-8.971038	-3.660329	-1.330009
26	1	0	-7.867379	-2.933514	0.367406
27	6	0	-8.792553	-2.345997	-3.344278
28	1	0	-7.569732	-0.580903	-3.211738
29	6	0	-9.304302	-3.456175	-2.670485
30	1	0	-9.361430	-4.522439	-0.796497
31	1	0	-9.036102	-2.183830	-4.390447
32	1	0	-9.951838	-4.159008	-3.186622
33	6	0	-5.568528	-1.348938	0.084573
34	6	0	-4.842639	-2.373831	-0.546756
35	6	0	-5.212933	-1.017781	1.403402
36	6	0	-3.790891	-3.014122	0.100627
37	1	0	-5.101474	-2.662987	-1.560539
38	6	0	-4.163288	-1.657810	2.053316
39	1	0	-5.768200	-0.245514	1.924440
40	6	0	-3.427844	-2.669023	1.413377
41	1	0	-3.230828	-3.782413	-0.424889
42	1	0	-3.918525	-1.375562	3.070609
43	1	0	-2.531969	2.348980	-0.365309
44	1	0	-3.211867	4.198869	1.137576
45	1	0	-5.600580	4.420506	1.820331
46	6	0	-2.328162	-3.405819	2.088490
47	6	0	-1.320226	-2.767475	2.842308
48	6	0	-2.238161	-4.799967	1.970604
49	6	0	-0.269603	-3.491922	3.440379
50	6	0	-1.207194	-5.538798	2.561311
51	1	0	-3.012905	-5.317334	1.413893
52	6	0	0.726159	-2.746105	4.168556
53	6	0	-0.226126	-4.889557	3.293403
54	6	0	-0.431563	-0.652406	3.650839
55	6	0	0.655934	-1.400551	4.268012
56	1	0	-1.184410	-6.617885	2.449155
57	1	0	0.582601	-5.444526	3.760169
58	1	0	1.542066	-3.292490	4.635079
59	1	0	1.389211	-0.811320	4.804942
60	8	0	-1.378233	-1.407405	2.961244
61	8	0	-0.584121	0.546880	3.691934
62	6	0	4.783088	4.020741	1.332419
63	6	0	5.979243	4.732955	1.396459
64	6	0	4.396803	3.363823	0.150947
65	6	0	6.803565	4.824248	0.273284
66	6	0	5.229370	3.477280	-0.974915
67	6	0	6.419911	4.199308	-0.914255
68	1	0	4.936742	2.993089	-1.900890
69	1	0	4.140089	3.962673	2.205471
70	6	0	3.106123	2.612180	0.089247
71	6	0	3.017891	1.344907	-0.414279
72	6	0	1.923893	3.355437	0.622499
73	6	0	1.707960	4.698182	0.262124
74	6	0	1.039777	2.764571	1.540721
75	6	0	0.632433	5.414311	0.783067
76	1	0	2.391106	5.178637	-0.431855
77	6	0	-0.030987	3.482181	2.071879

78	1	0	1.192014	1.738135	1.853815
79	6	0	-0.238760	4.810176	1.693071
80	1	0	0.479667	6.447912	0.485041
81	1	0	-0.688685	2.991611	2.781952
82	1	0	-1.064383	5.376845	2.115135
83	6	0	1.707843	0.689849	-0.718320
84	6	0	1.428299	-0.603201	-0.242849
85	6	0	0.750196	1.319062	-1.530152
86	6	0	0.217815	-1.228906	-0.535222
87	1	0	2.166461	-1.113051	0.369437
88	6	0	-0.453221	0.685196	-1.839228
89	1	0	0.956352	2.310847	-1.919338
90	6	0	-0.729477	-0.587257	-1.335454
91	1	0	0.013480	-2.220213	-0.140960
92	1	0	-1.174671	1.186444	-2.478669
93	1	0	-1.672436	-1.076004	-1.561165
94	6	0	4.214054	0.501536	-0.711733
95	6	0	4.295561	-0.222444	-1.913647
96	6	0	5.266434	0.352200	0.208018
97	6	0	5.389998	-1.033529	-2.192704
98	1	0	3.495237	-0.136330	-2.642047
99	6	0	6.358445	-0.464180	-0.065434
100	1	0	5.224660	0.883580	1.152580
101	6	0	6.443748	-1.176041	-1.273805
102	1	0	5.438091	-1.550652	-3.146675
103	1	0	7.147629	-0.556639	0.671144
104	1	0	7.049427	4.273436	-1.796214
105	1	0	7.735067	5.380276	0.321869
106	1	0	6.267004	5.219243	2.324258
107	6	0	7.567144	-2.098890	-1.580829
108	6	0	8.919375	-1.787720	-1.321345
109	6	0	7.312638	-3.342453	-2.176803
110	6	0	9.962266	-2.677163	-1.649808
111	6	0	8.332520	-4.240388	-2.509526
112	1	0	6.279948	-3.617508	-2.365283
113	6	0	11.311804	-2.261065	-1.359703
114	6	0	9.652717	-3.911491	-2.247263
115	6	0	10.490828	-0.139406	-0.453327
116	6	0	11.567517	-1.060907	-0.794922
117	1	0	8.084239	-5.194250	-2.963560
118	1	0	10.459460	-4.595468	-2.494866
119	1	0	12.125149	-2.938214	-1.608766
120	1	0	12.569906	-0.720381	-0.565761
121	8	0	9.197873	-0.576395	-0.754285
122	8	0	10.613785	0.947135	0.059199

HF= -2997.34

Single Crystal X–ray Diffraction Studies:

Single crystal X–ray structural studies of **1** was performed on a Bruker D8 Venture PHOTON II 14diffractometer equipped with a graphite-monochromated Mo Kα (λ=0.71073 Å) radiation source and a nitrogen cold stream (-50 °C). Data collection and integration were performed with APEX3 (Bruker, 2016) and SAINT-Plus (Bruker, 2016) [2]. Absorption correction was performed by multi-scan method implemented in SADABS [2]. The structure was solved by direct methods and refined by full-matrix least-squares on F^2 using SHELXTL [3]. All the non-hydrogen atoms were refined anisotropically, and hydrogen atoms were added to their geometrically ideal positions. The CCDC number 1975276 contain the supplementary crystallographic data for **1** respectively. This data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data centre, 12 Union Road, Cambridge CB21 EZ, UK; Fax: (+44)1223–336–033; or deposit@ccdc.cam.ac.uk).

Table S1: Crystal structure and data refinement parameters of **1**.

Parameters	**1**
Empirical formula	$C_{35}H_{24}O_2$
Formula Weight	476.54
Temperature	223(2) K
Wavelength Å	0.71073
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit Cell Dimensions	
α/ Å	9.0695(4)
α/°	90°
β/ Å	30.7871(15)
β/°	101.2203 (17)°
γ/ Å	9.1428(4)
γ/°	90°
Volume/ $Å^3$	2504.1 (2)
Z	4
Calculated density/Mg/m^3	1.264
Absorption coefficient/mm^{-1}	0.077
F(000)	1000
Crystal size/mm^3	0.271 x 0.240 x 0.121
θ range from data collection	2.289 to 28.354°
Reflections collected	83136
Independent reflections	6230 [R(int)=0.0823]
Completeness to theta= 25.242°	99.9 %
Absorption correction	Semi –empirical from equivalents
Maximum and minimum transmission	0.7475 and 0.7010
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	6230 / 0 / 334
Goodness of fit on F^2	1.068
Final R indices [I>2 σ(I)]	R_1=0.0504, WR_2=0.1131
R indices (all data)	R_1=0.0884, WR_2=0.1407
Largest diff. Peak and hole/e $Å^{-3}$	0.180 and –0.241
CCDC number	

References:

1. Reynolads G A, Drexhage K H. New coumarin yes with rigidized structure for flash lamp–pumped dye lasers. Opt Commun 1975; 13: 222–225.
2. SMART, SAINT-Plus and XPREP, Bruker AXS Inc., Madison, Wisconsin, USA, 2016.
3. G. M. Sheldrick, SADABS v 2.03, University of Göttingen, Germany, 2002.
4. SHELXTL v 6.10; Bruker AXS, Inc: Madison, Wisconsin, USA, 2000.