

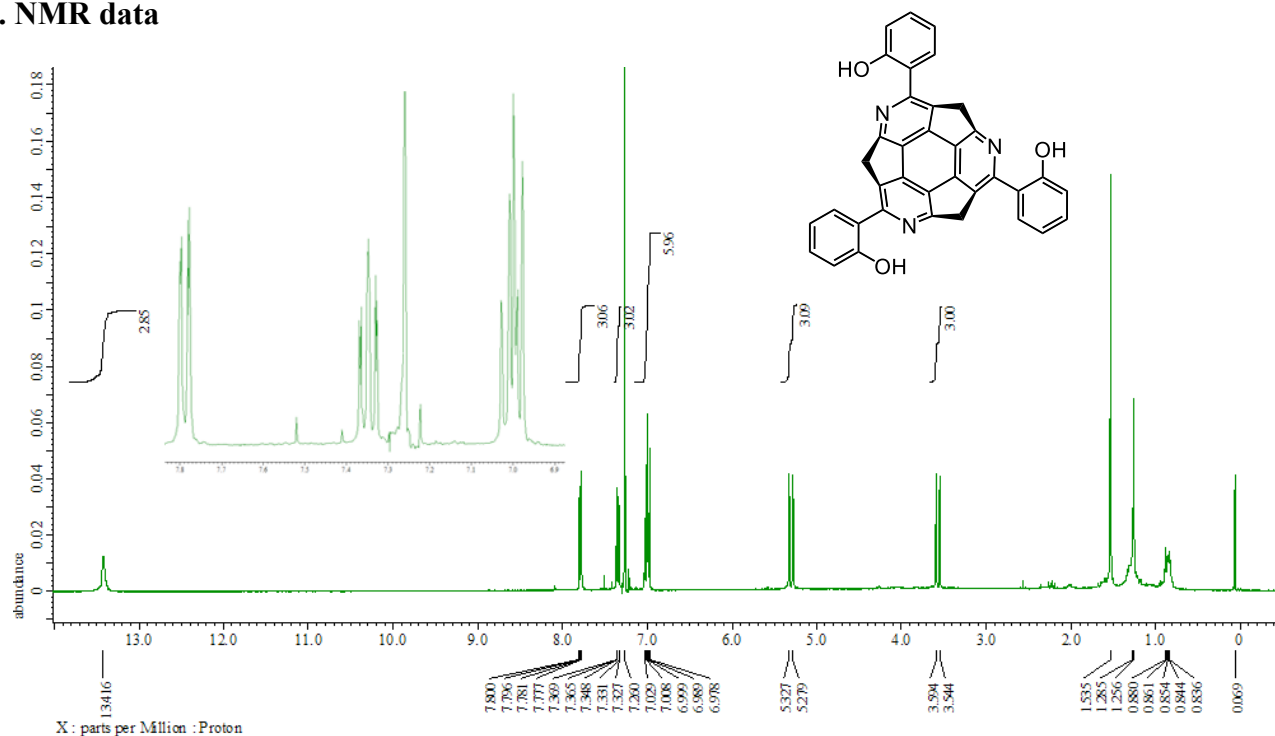
Supporting Information

Tris(2-hydroxyphenyl)triazasumanene: bowl shaped Excited State Intramolecular Proton Transfer (ESIPT) fluorophore with Aggregation Induced Enhanced Emission (AIEE)

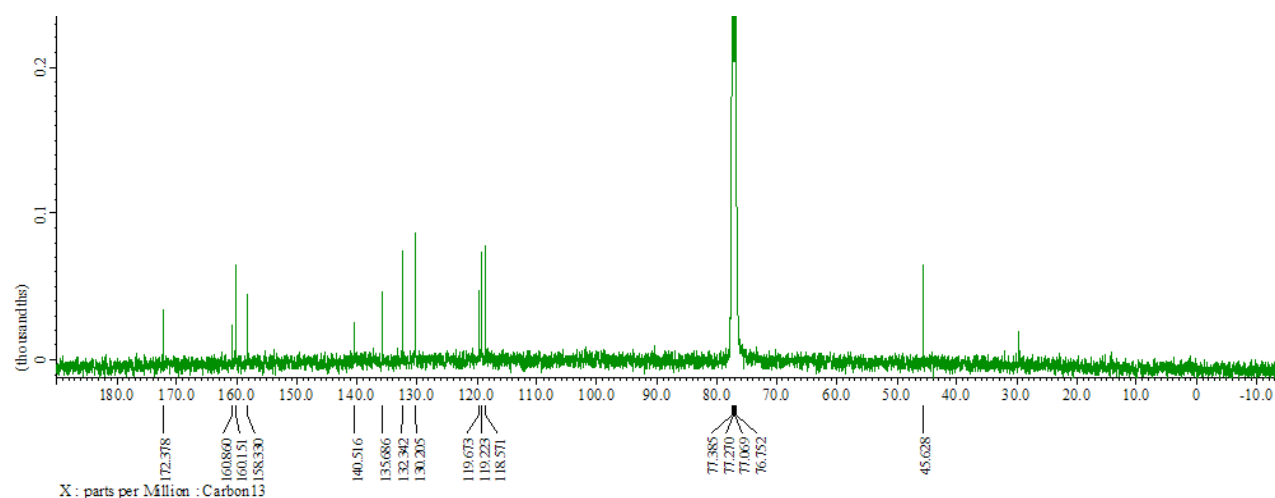
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Shuhe Higashibayashi, Hidehiro Sakurai*

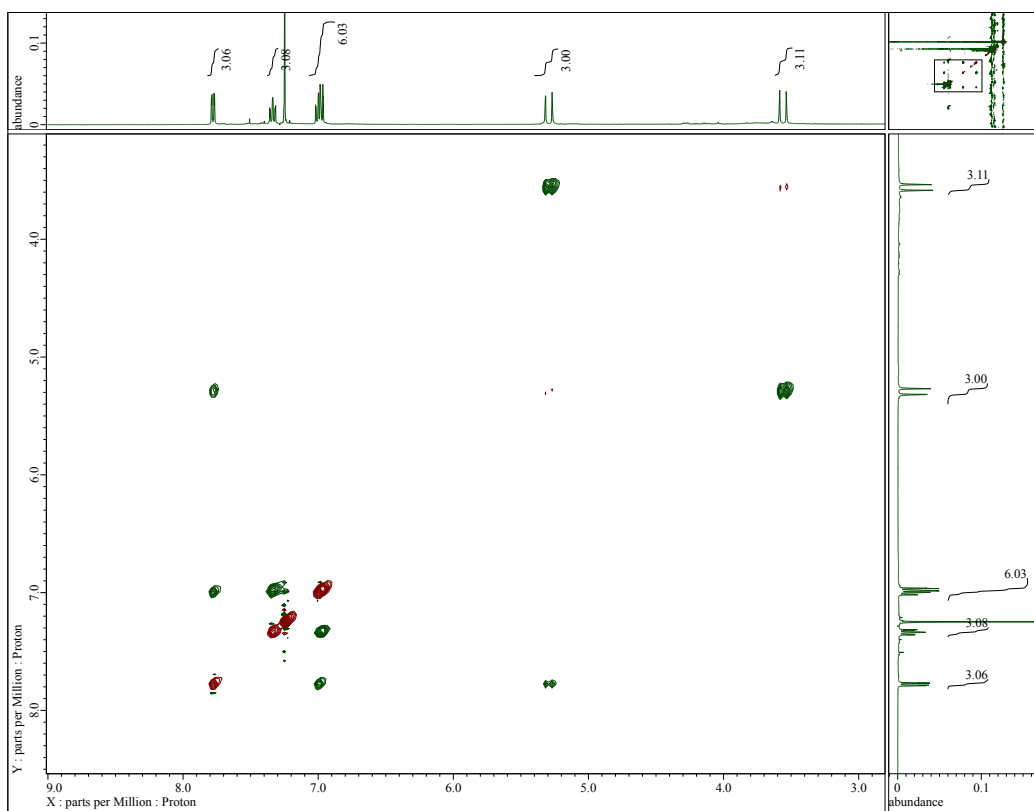
1. NMR data



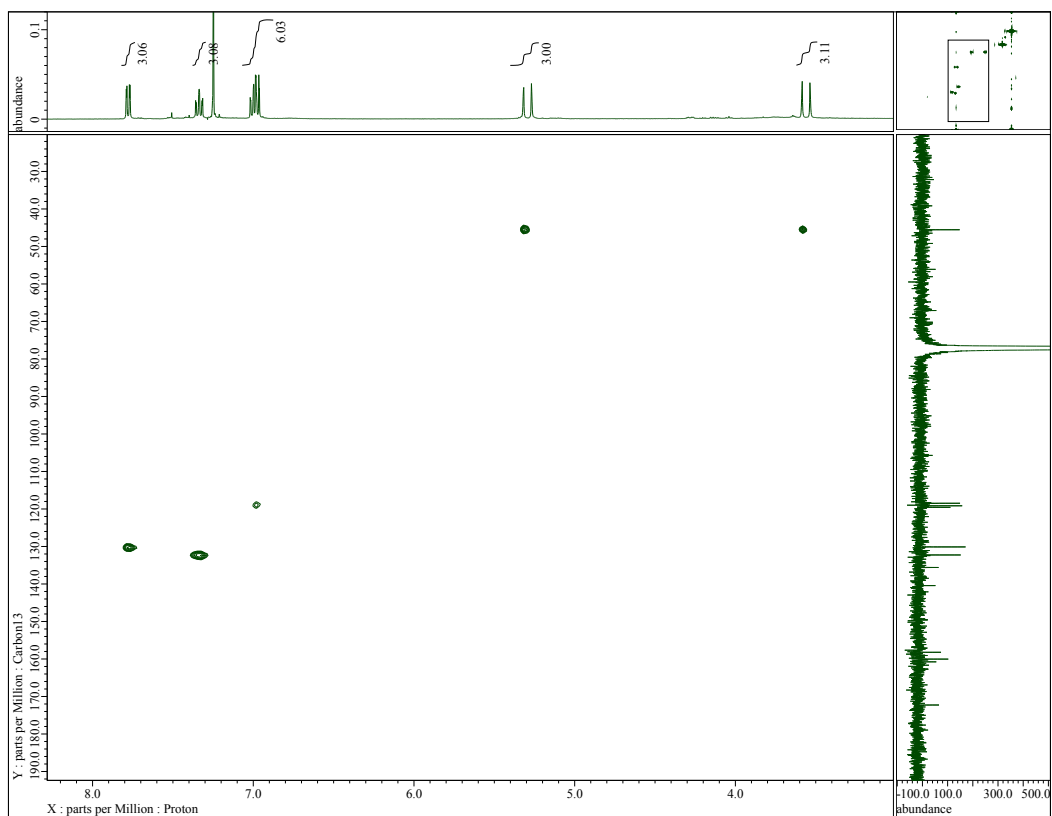
¹H-NMR spectrum of (A)-(+)-1 in CDCl₃.



¹³C-NMR spectrum of (A)-(+)-1 in CDCl₃.

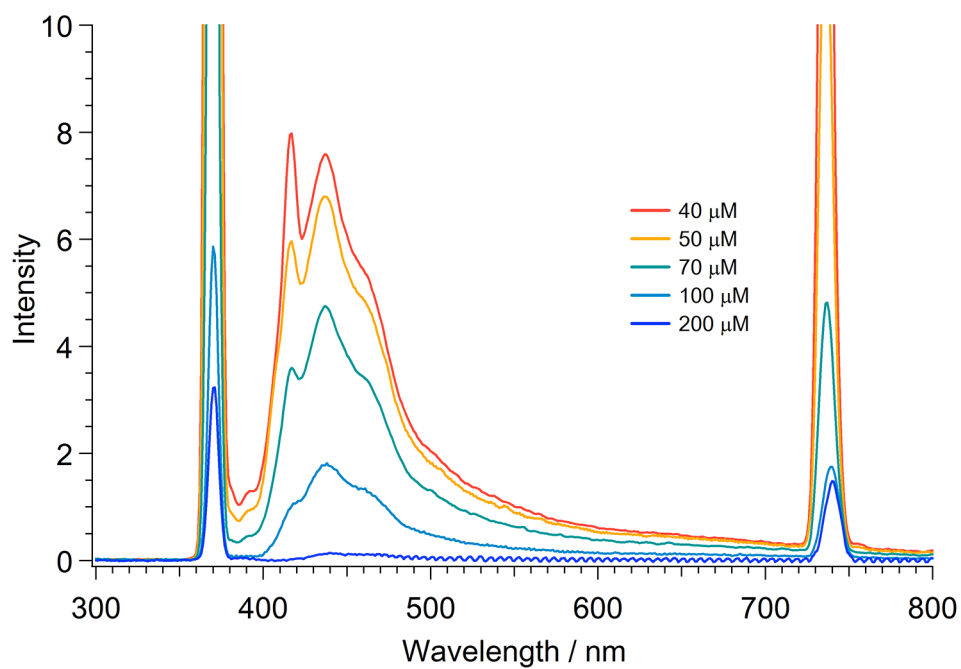
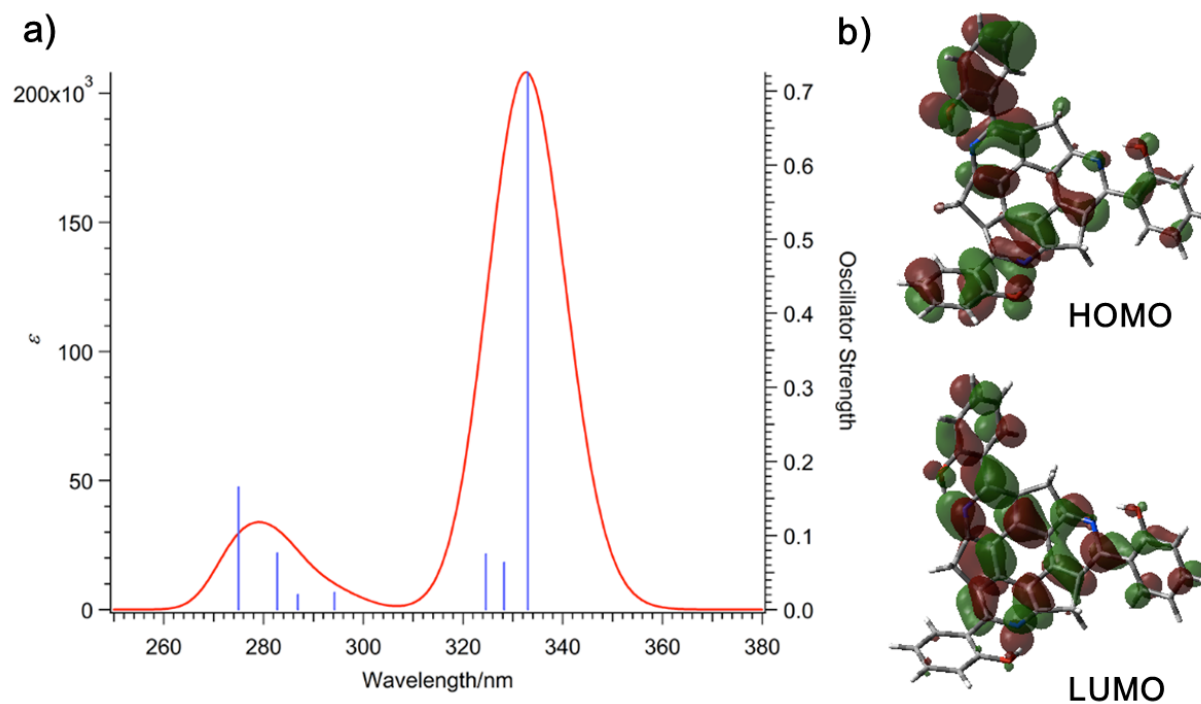


NOESY spectrum of (*A*)-(+)-**1** in CDCl₃.



HMQC spectrum of (*A*)-(+)-**1** in CDCl₃.

2. Supporting figures



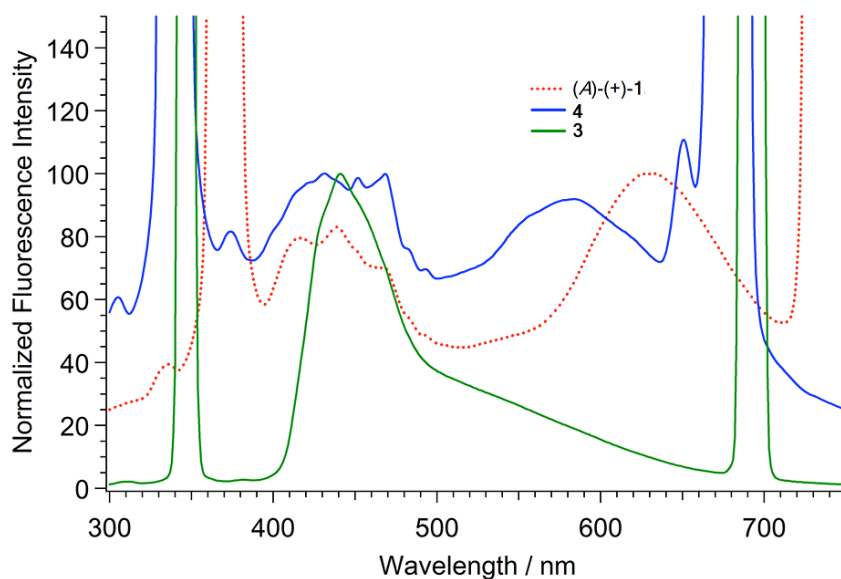


Figure S3 Solid state emission spectra of triphenyltriazasumanene **4** and Tris(trifluoromethylphenyl)triazasumanene **3** with (*A*)-(+)-**1**.

Hexane (%)	Fluorescence intensity	
	$\lambda_{max} = 436 \text{ nm}$	$\lambda_{max} = 628 \text{ nm}$
0	40.0327	1.58396
10	41.2264	1.67634
20	41.4778	1.77174
30	42.0225	1.79973
40	42.1193	1.94502
50	41.1466	1.78331
60	42.2179	1.74152
70	41.8891	1.54623
80	42.6611	1.26089
90	50.5892	6.27589
92	65.1788	12.1428
94	66.799	12.8405
96	70.582	13.9267
98	72.9734	16.9494

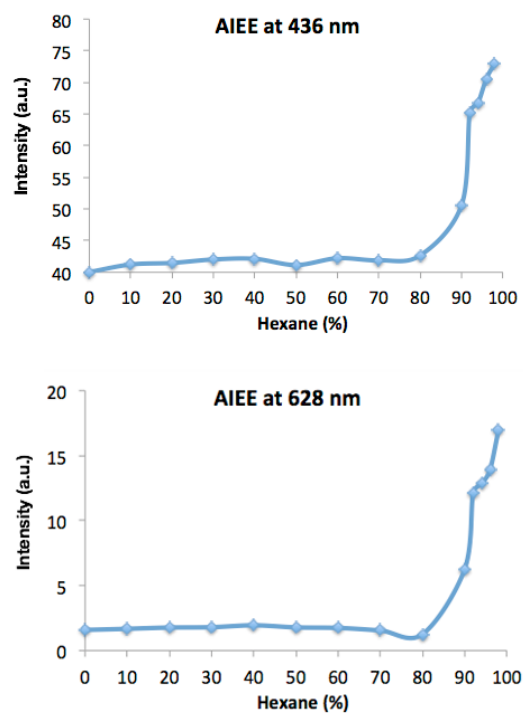


Figure S4. Fluorescence intensity change at the specific wavelength of aggregated (*A*)-(+)-**1** at various ratio of hexane and CH₂Cl₂.

MeOH (%)	Fluorescence intensity (a.u.)	
	$\lambda_{max} = 436 \text{ nm}$	$\lambda_{max} = 628 \text{ nm}$
0	43.3066	1.73752
10	44.0602	2.12645
20	42.471	1.73024
30	43.5295	1.84288
40	44.2622	1.84754
50	44.1891	1.83398
60	44.449	1.80838
70	44.1584	1.77274
80	44.8034	1.79751
90	51.5229	3.01561
92	54.2021	3.48754
94	59.7861	4.02055
96	65.9333	4.51872
98	65.5269	4.38881

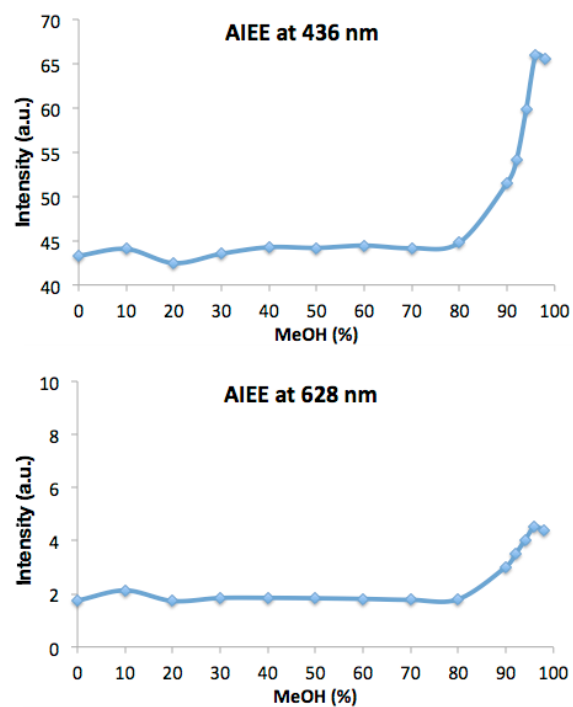


Figure S5. Fluorescence intensity change at the specific wavelength of aggregated (*A*)-(+)-**1** at various ratio of MeOH and CH₂Cl₂.

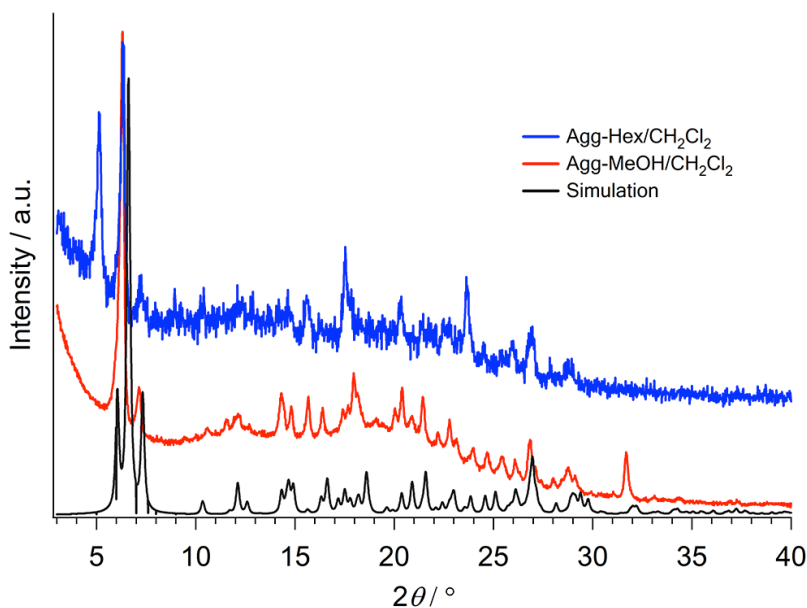


Figure. S6 PXRD patterns of aggregated (*A*)-(+)-**1** obtained from MeOH/CH₂Cl₂ (red line) and hexane/CH₂Cl₂ (blue line) and simulated one from the single crystal data of (*A*)-(+)-**1** (black line).

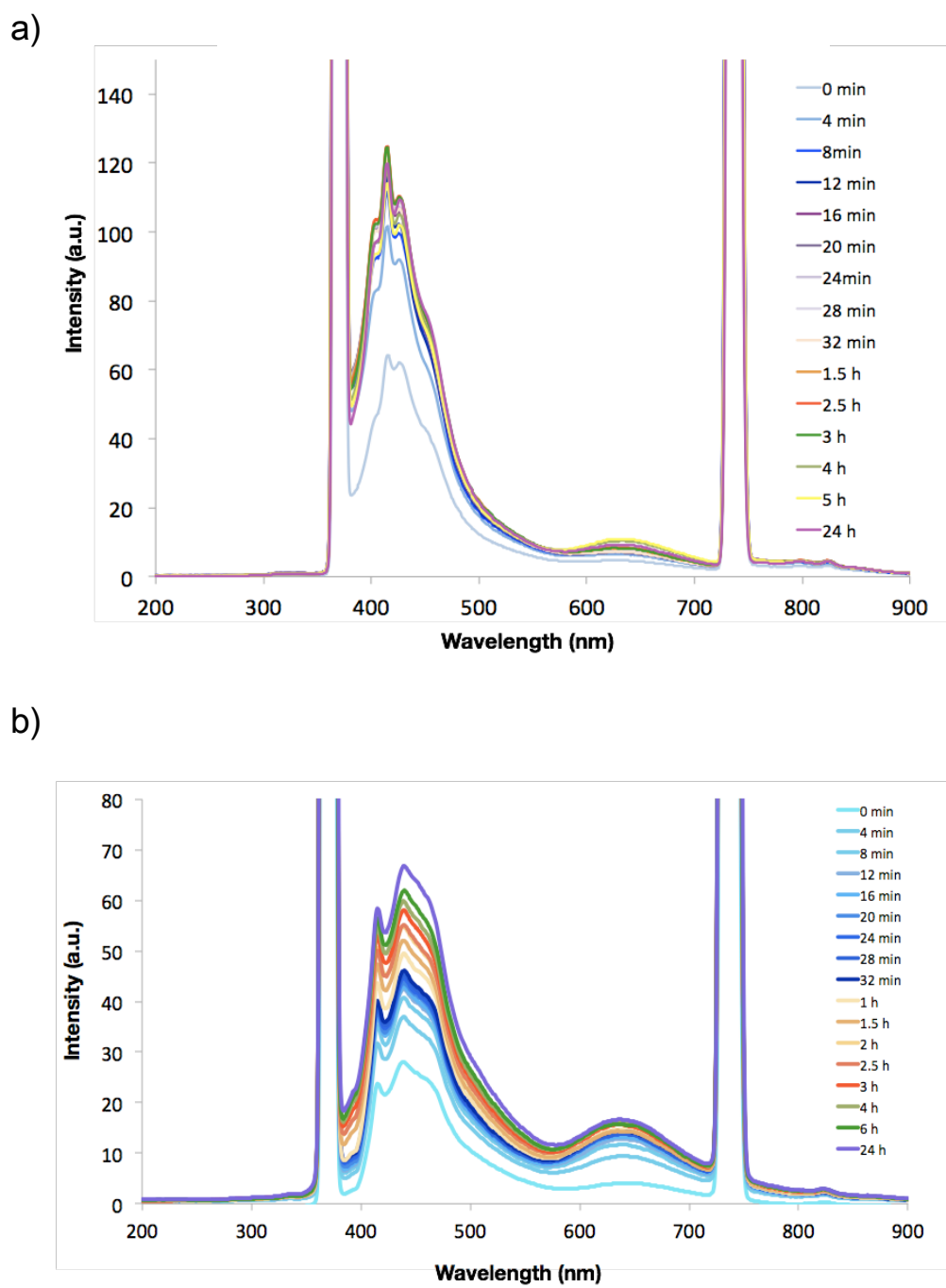


Figure. S7 Time-dependent emission intensity change of the aggregated (*A*)-(+)-**1** prepared from a) hexane/CH₂Cl₂, b) MeOH/CH₂Cl₂.