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Constitutional Isomers of Dendrimer-like Pyrene Substituted Cyclotriphosphazenes: Synthesis, theoretical calculation, and fluorescence receptor for the detection of explosive nitroaromatics

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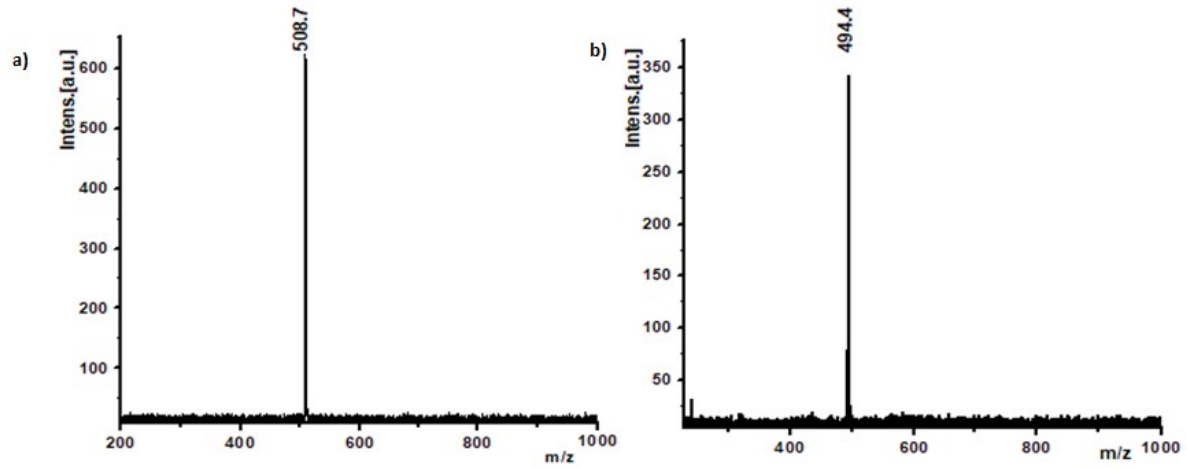

Figure S1. Positive ion and linear mode MALDI-MS spectra of compounds **3** (a) and **4** (b) were obtained in DHB (20 mg/mL THF) MALDI matrix using nitrogen laser accumulating 50 laser shots.

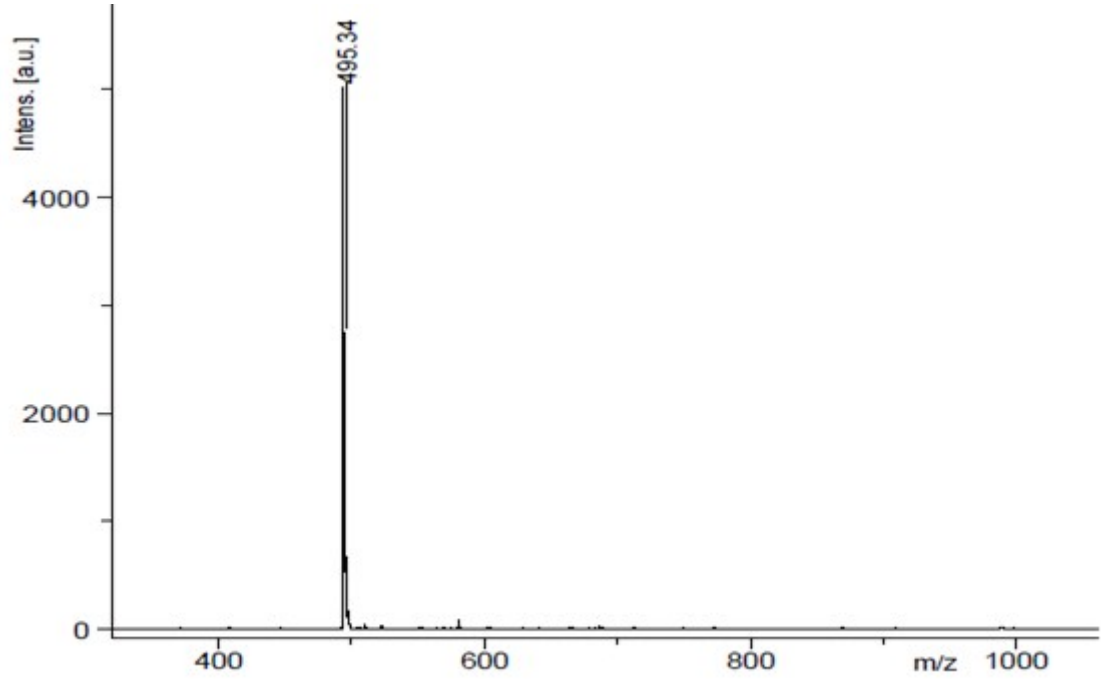

Figure S2. Positive ion and linear mode MALDI-MS spectra of compound **6** were obtained in DHB (20 mg/mL THF) MALDI matrix using nitrogen laser accumulating 50 laser shots.

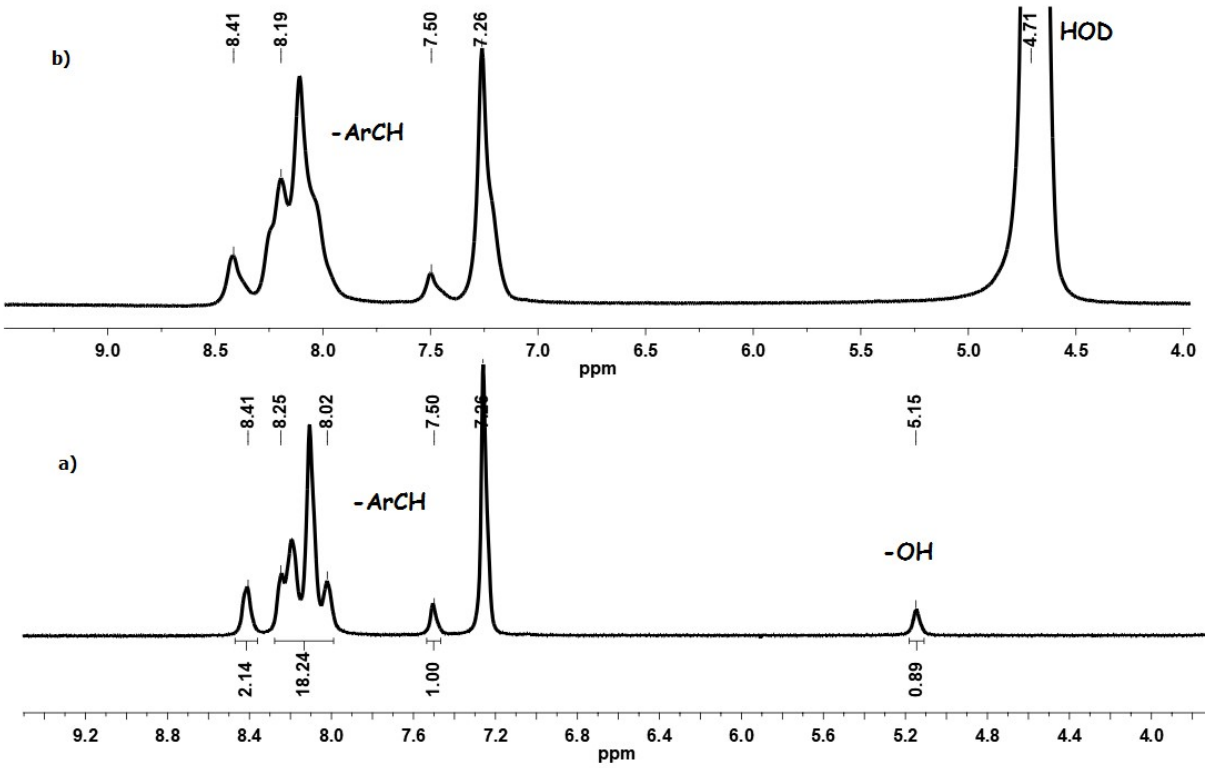

Figure S3. ^{1}H NMR spectra of compound **6** in $CDCl_3$ (a) and D_2O exchange (b).

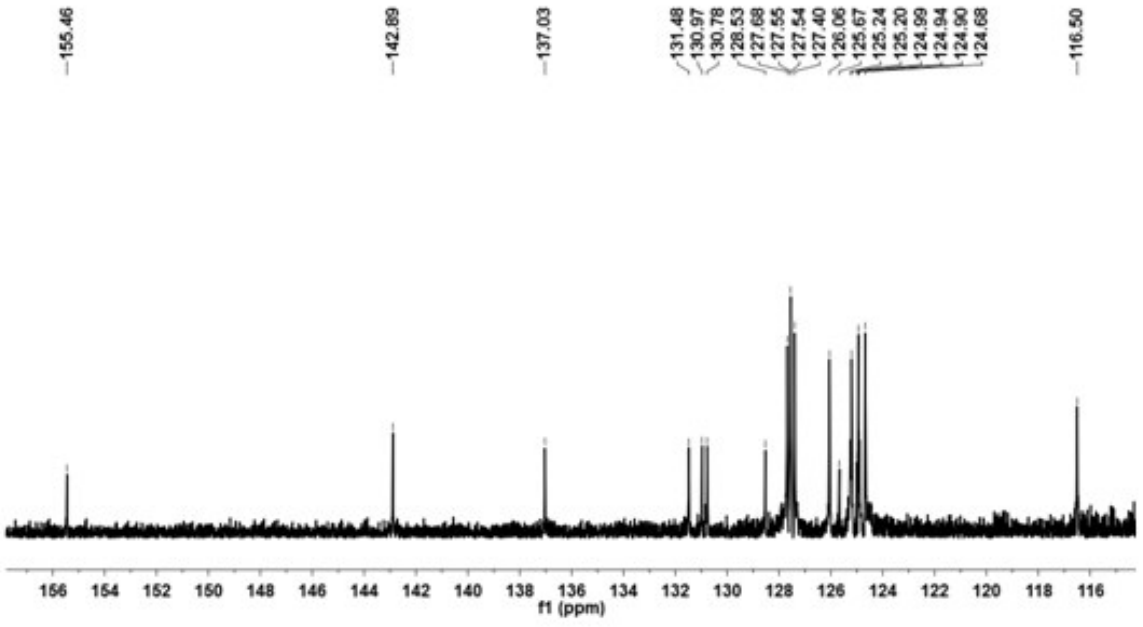

Figure S4. Proton-decoupled ^{13}C NMR spectrum of compound **6** in $CDCl_3$ solution.

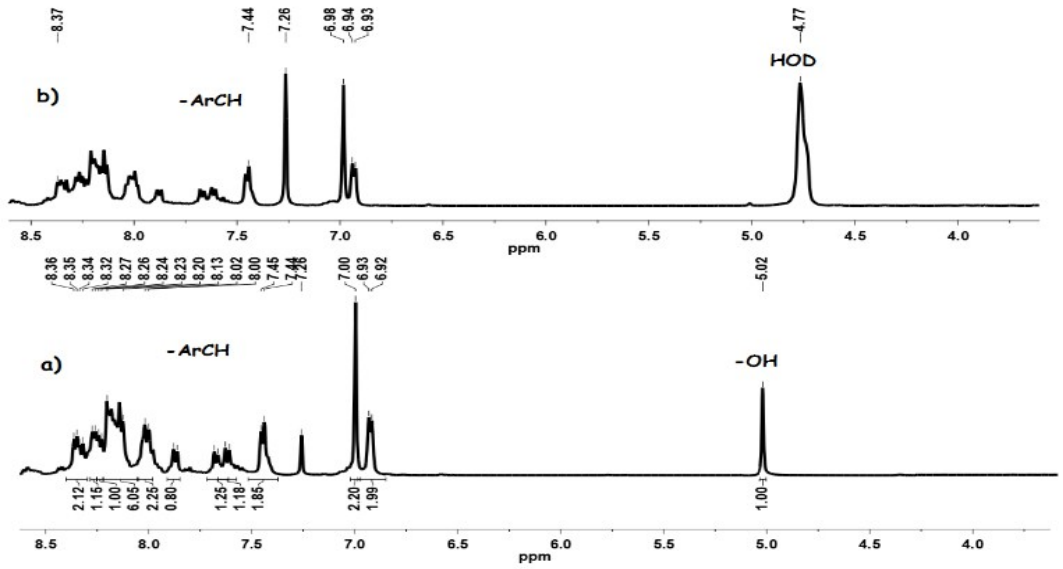

Figure S5. ^{1}H NMR spectra of compound **4** in $CDCl_3$ (a) and D_2O exchange (b).

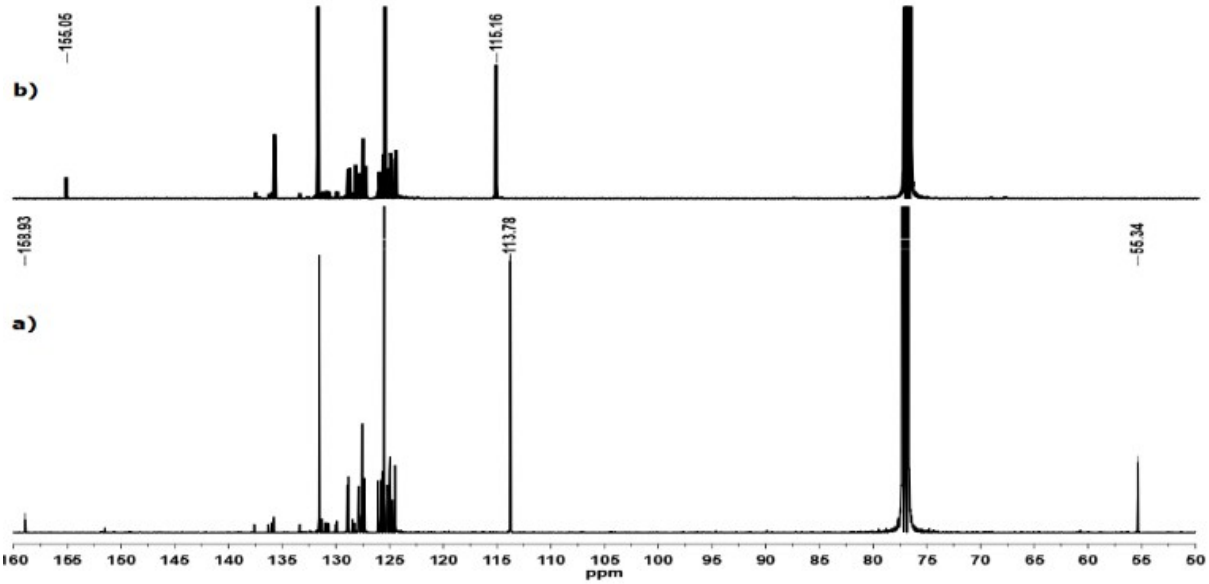

Figure S6. Proton-decoupled ^{13}C NMR spectra of compounds **3** (**a**) and **4** (**b**) in $CDCl_3$ solution.

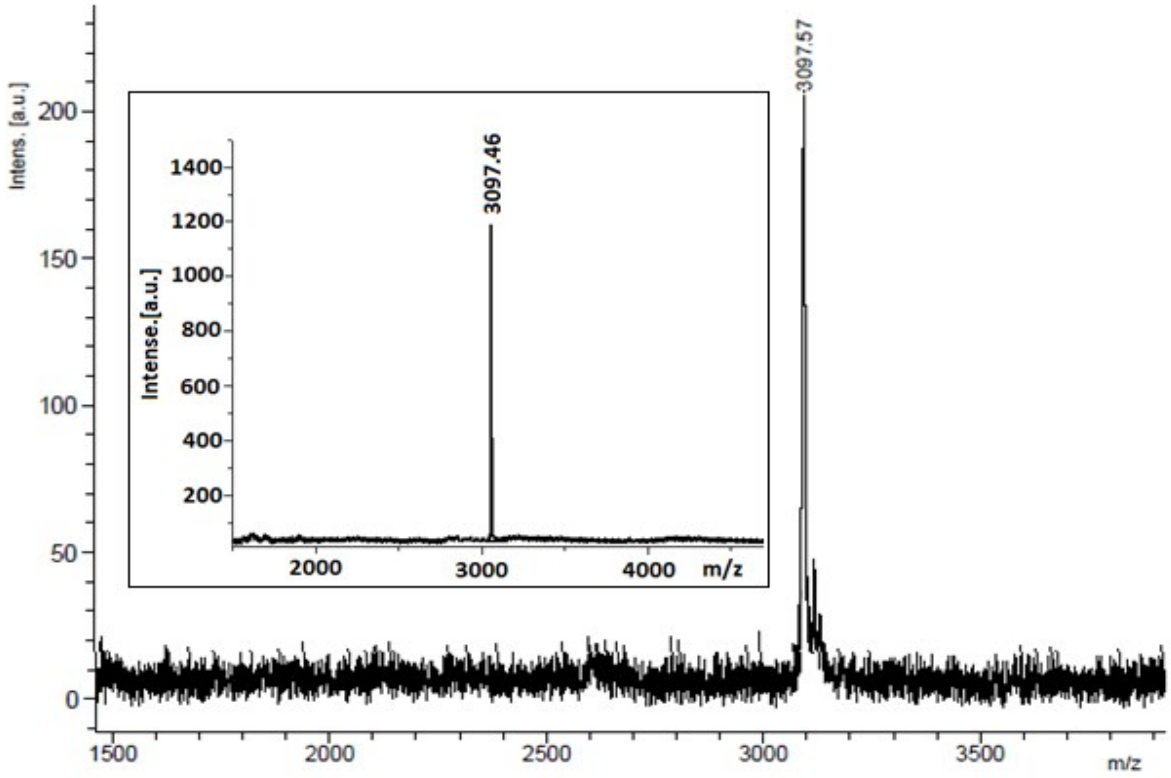

Figure S7. Positive ion and linear mode MALDI-MS spectra of compounds **5** (inset) and **7** were obtained in DHB (20 mg/mL THF) MALDI matrix using nitrogen laser accumulating 50 laser shots.

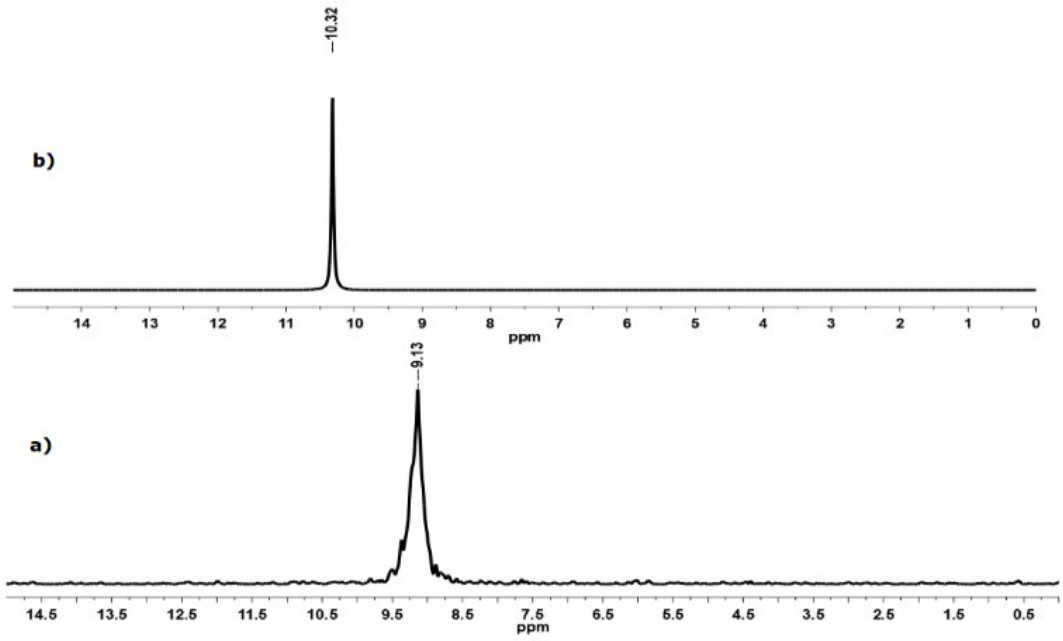

Figure S8. Proton-decoupled ^{31}P NMR spectra of compounds **5** (a) and **7** (b) in $CDCl_3$ solution.

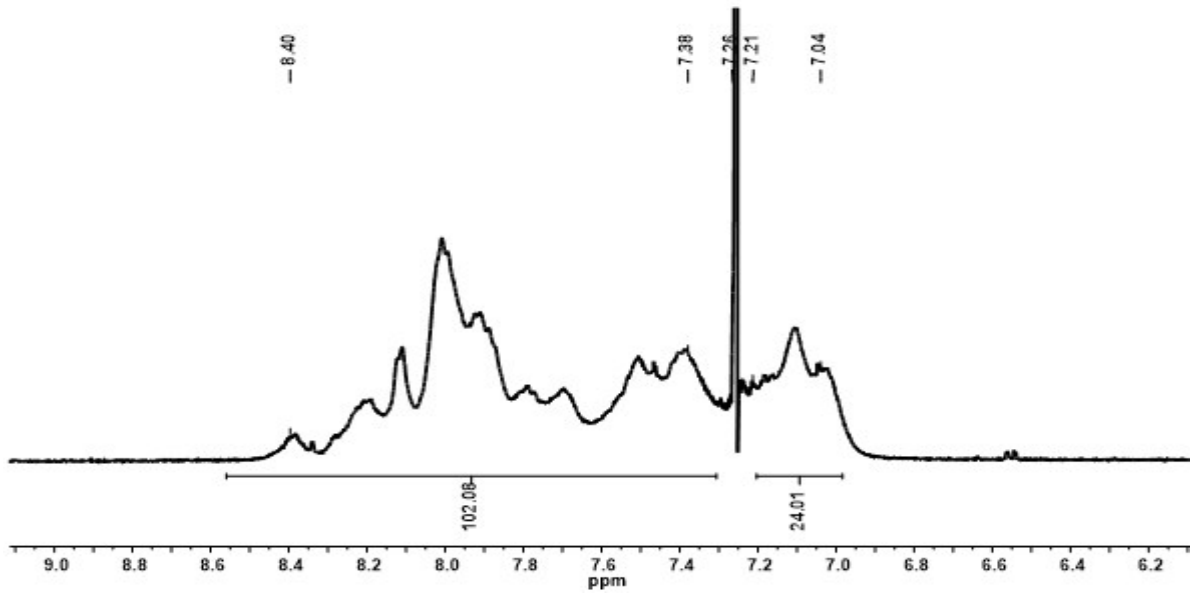

Figure S9. ^{1}H NMR spectrum of compound **5** in $CDCl_3$.

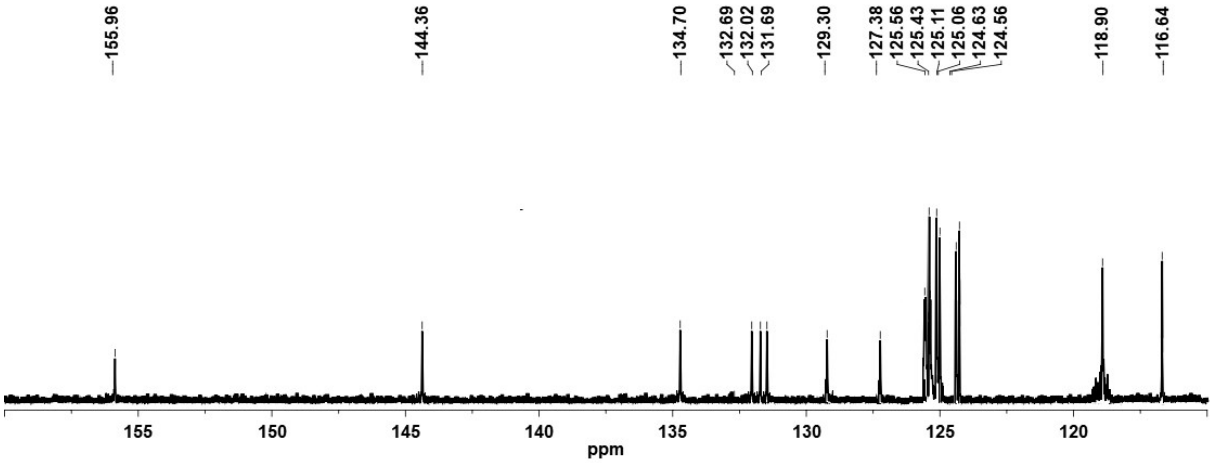

Figure S10. Proton-decoupled ^{13}C NMR spectrum of compound **5** in $CDCl_3$ solution.

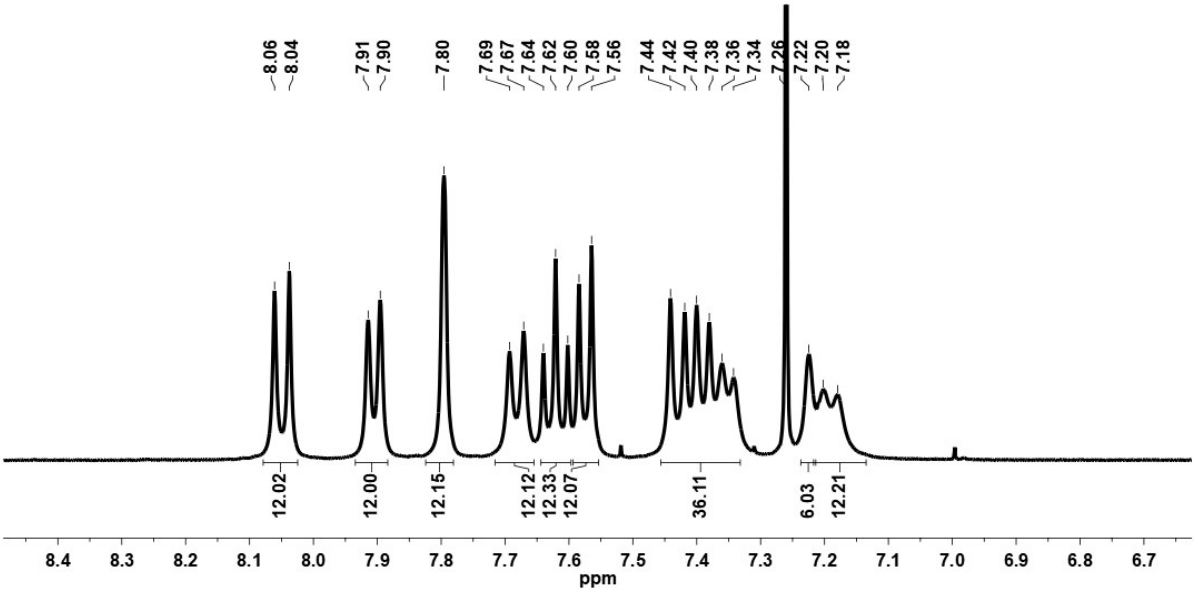

Figure S11. ^{1}H NMR spectrum of compound **7** in $CDCl_3$.

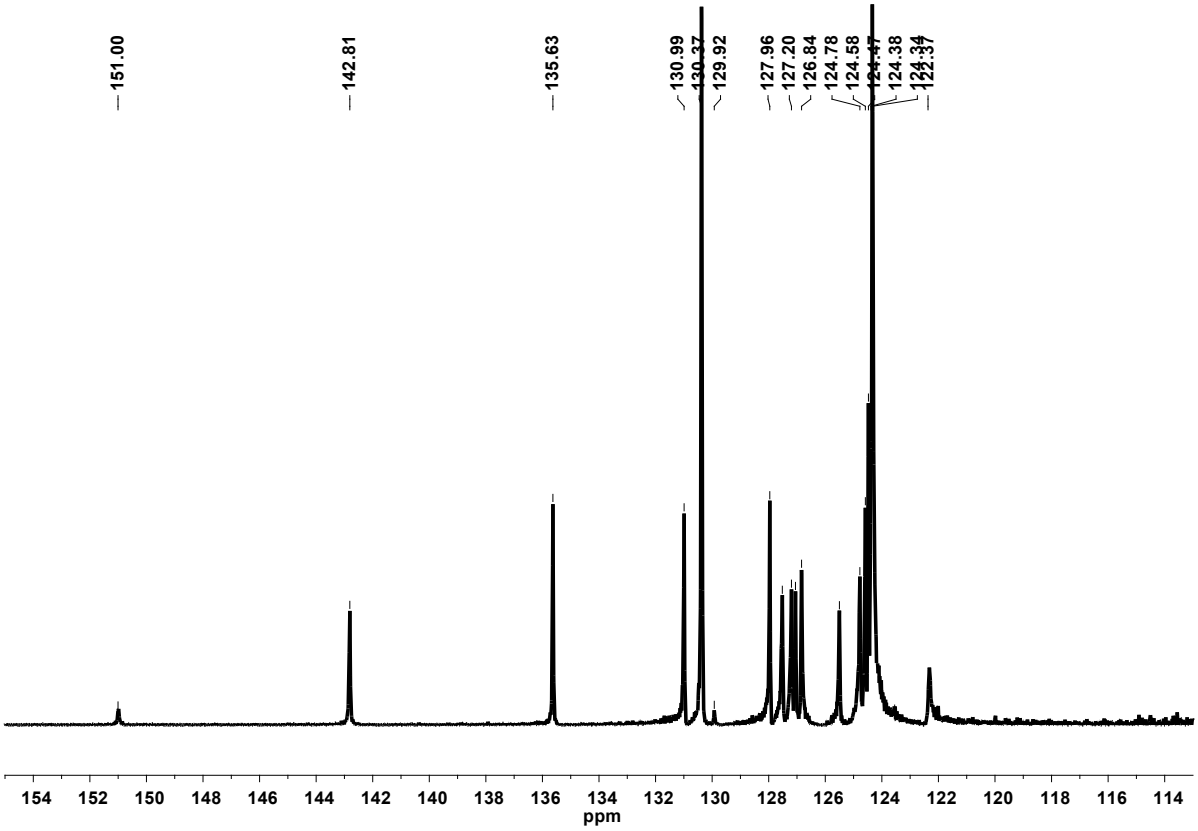

Figure S12. Proton-decoupled ^{13}C NMR spectrum of compound **7** in $CDCl_3$ solution.

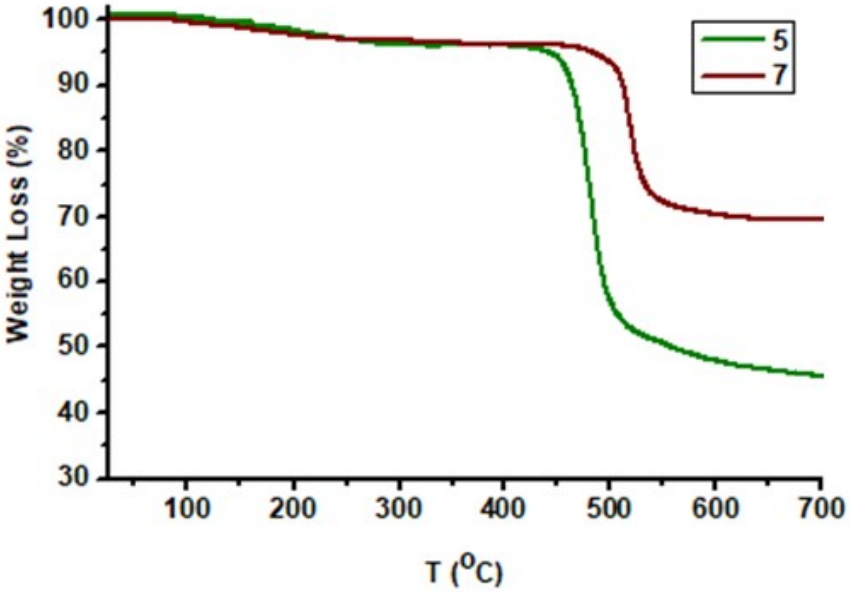

Figure S13. TGA thermograms of **5** and **7** from 25 to 700°C at a heating rate of 10°C/min under N_2 flow of 50mL/min.

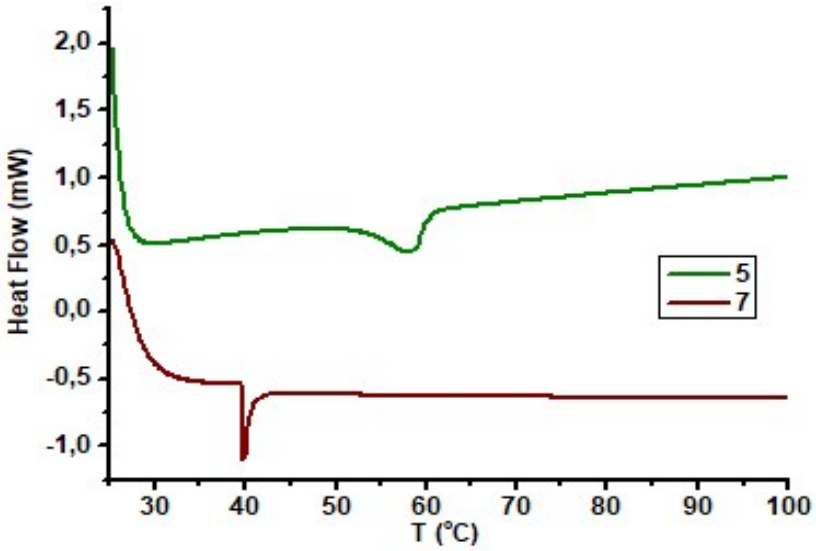

Figure S14. DSC thermograms in N_2 atmosphere of compounds **(5** and **7)** from 25 to 180°C at a heating rate of 10°C/min.

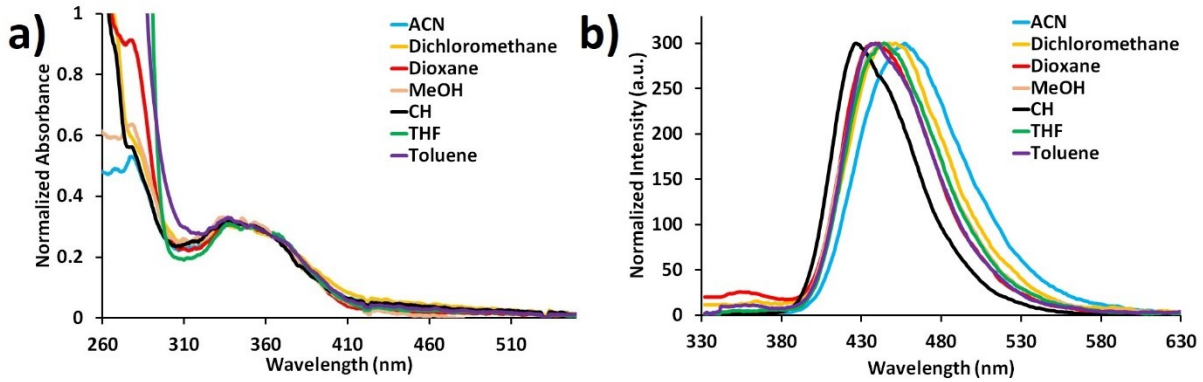

Figure S15. a) UV (normalized) and **b)** fluorescence spectra (normalized) of **4** in different solvents (λ_{ex}= 325 nm).

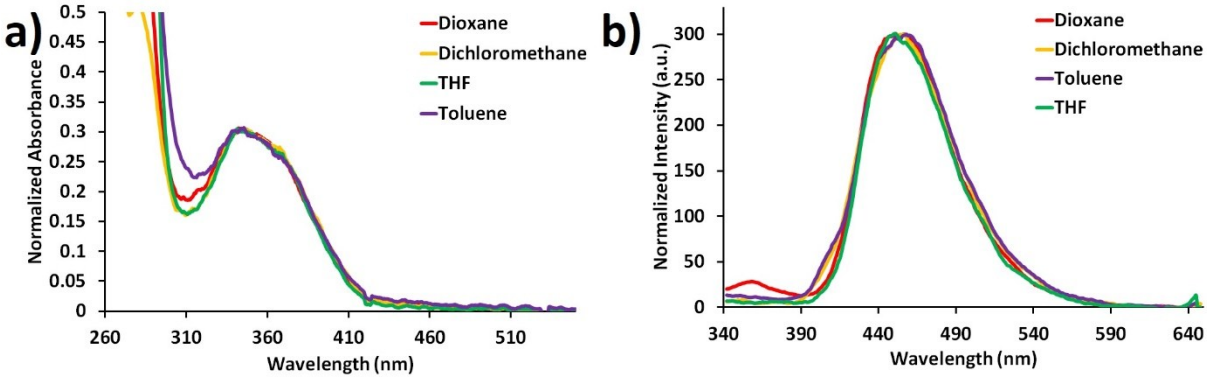

Figure S16. a) UV (normalized) and **b)** fluorescence spectra (normalized) of **5** in different solvents (λ_{ex}= 325 nm).

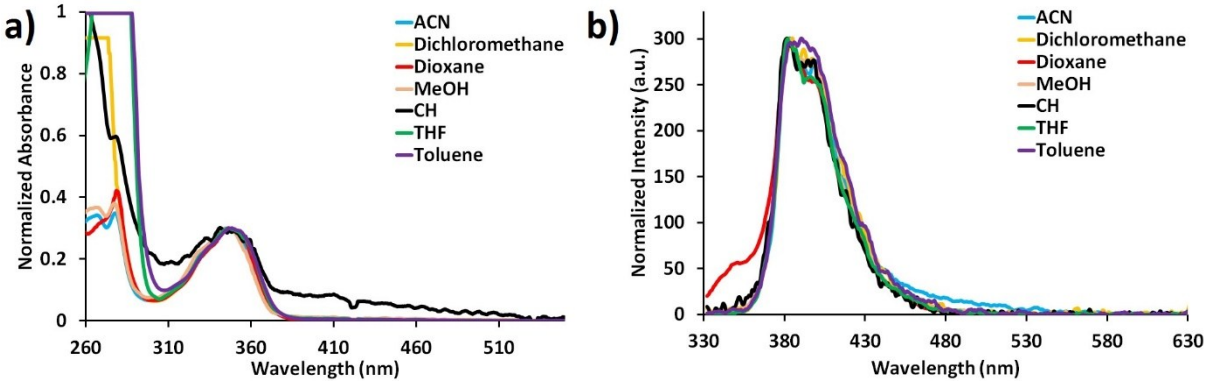

Figure S17. a) UV (normalized) and **b)** fluorescence spectra (normalized) of **6** in different solvents (λ_{ex}= 325 nm).

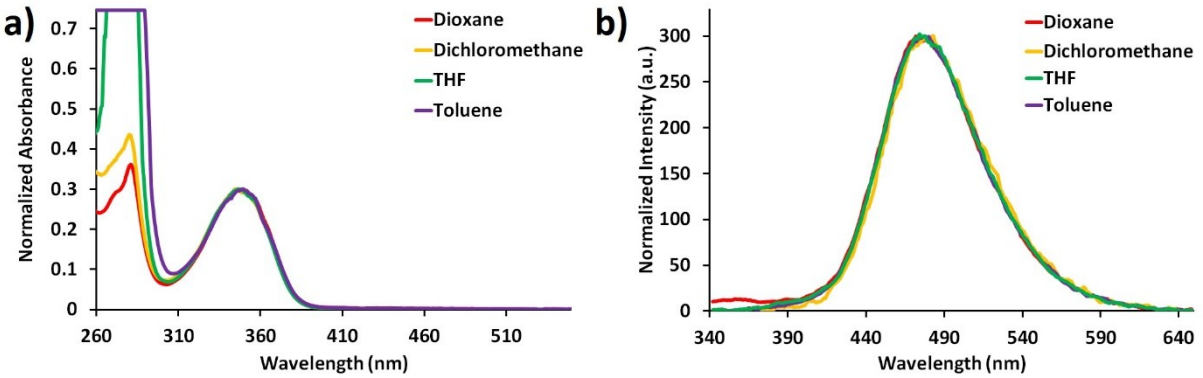

Figure S18. a) UV (normalized) and **b)** fluorescence spectra (normalized) of **7** in different solvents (λ_{ex}= 325 nm).

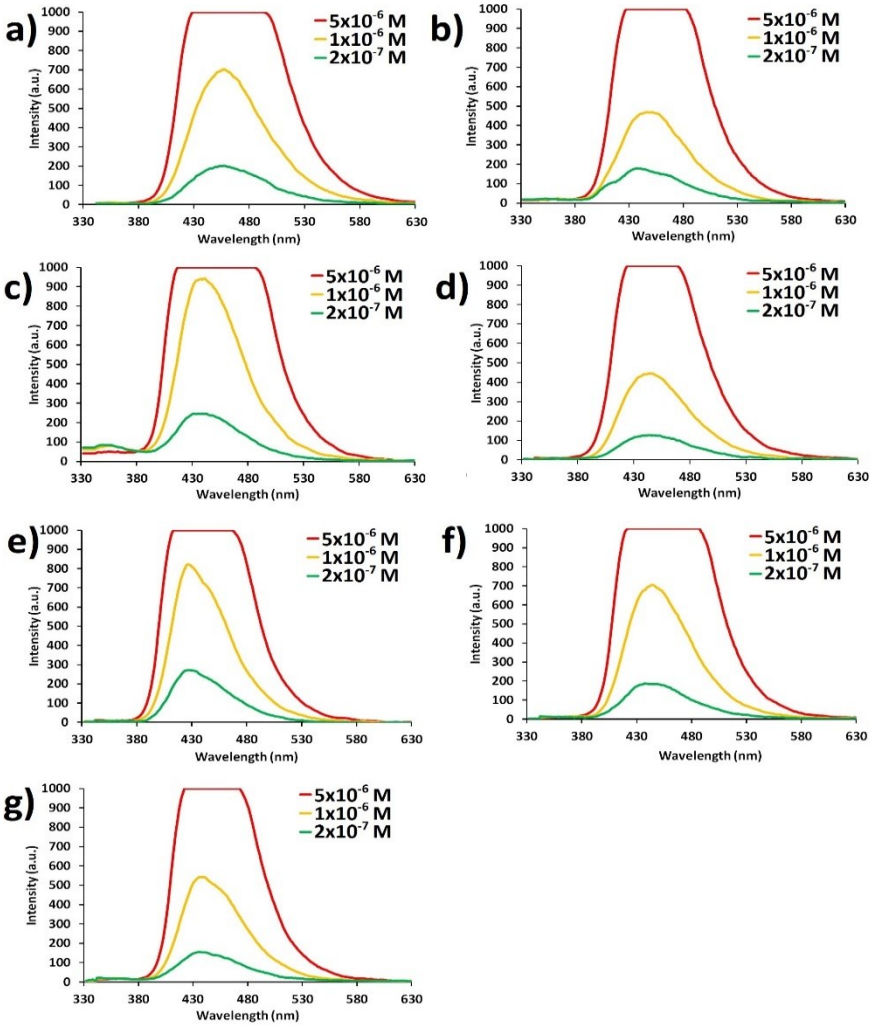

Figure S19. Fluorescence spectra of **4** at different concentration in **a)** ACN, **b)** dichloromethane, **c)** dioxane, **d)** MeOH, **e)** CH, **f)** THF and **g)** toluene (λ_{ex}= 325 nm).

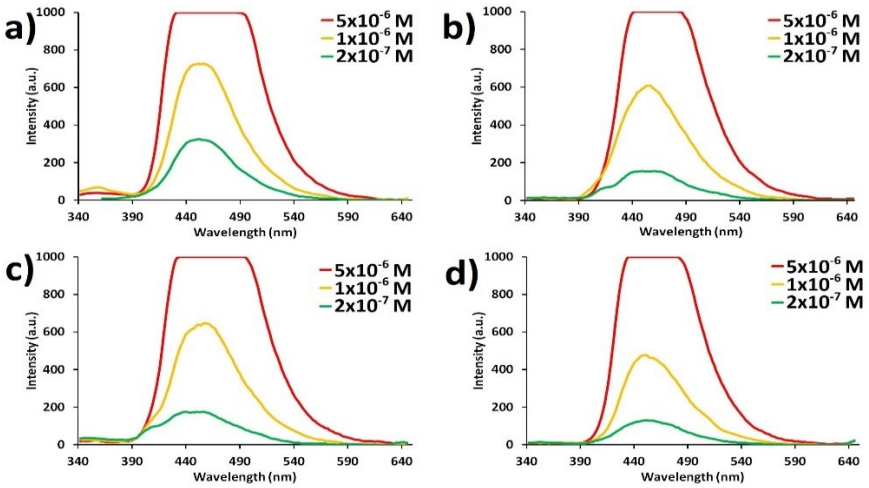

Figure S20. Fluorescence spectra of **5** at different concentration in **a)** dioxane, **b)** dichloromethane, **c)** THF and **d)** toluene (λ_{ex}= 325 nm).

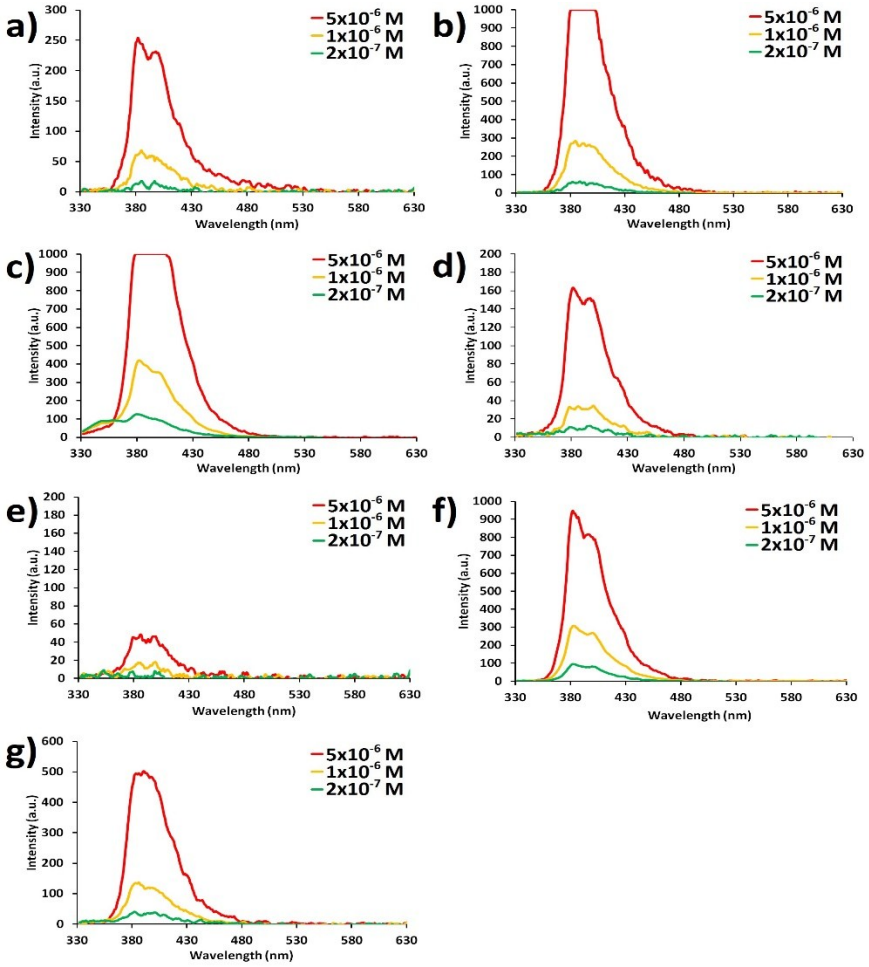

Figure S21. Fluorescence spectra of **6** at different concentration in **a)** ACN, **b)** dichloromethane, **c)** dioxane, **d)** MeOH, **e)** CH, **f)** THF and **g)** toluene (λ_{ex}= 325 nm).

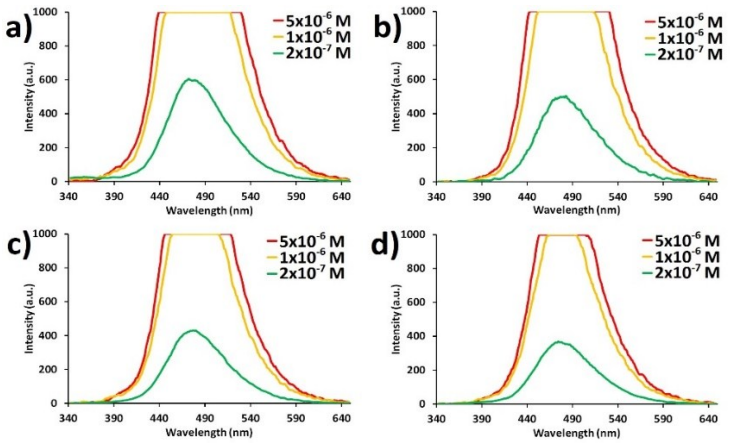

Figure S22. Fluorescence spectra of **7** at different concentration in **a)** dioxane, **b)** dichloromethane, **c)** THF and **d)** toluene (λ_{ex}= 325 nm).

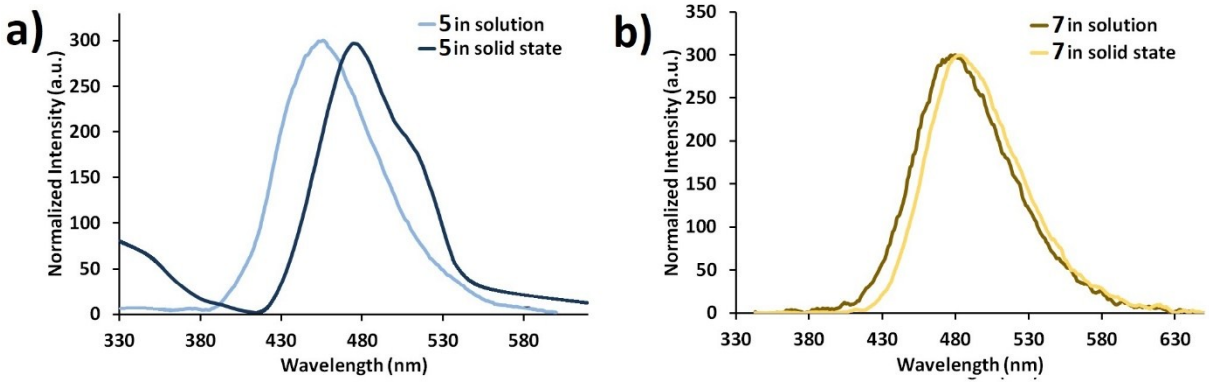

Figure S23. Fluorescence spectra (normalized) of **a) 5** and **b) 7** in CH_2Cl_2 and solid state (λ_{ex}= 325 nm).

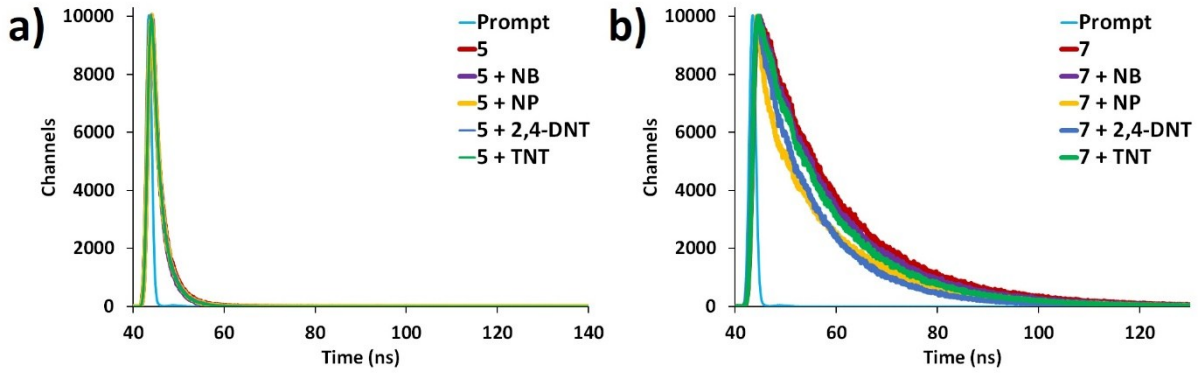

Figure S24. Fluorescence decay profile of **a) 5** and **b) 7** with nitrobenzene (NB), nitrophenol (NP), 2,4-dinitrotoulene (2,4-DNT) and 2,4,6-trinitrotoluene (TNT) using laser excitation source of 390 nm.

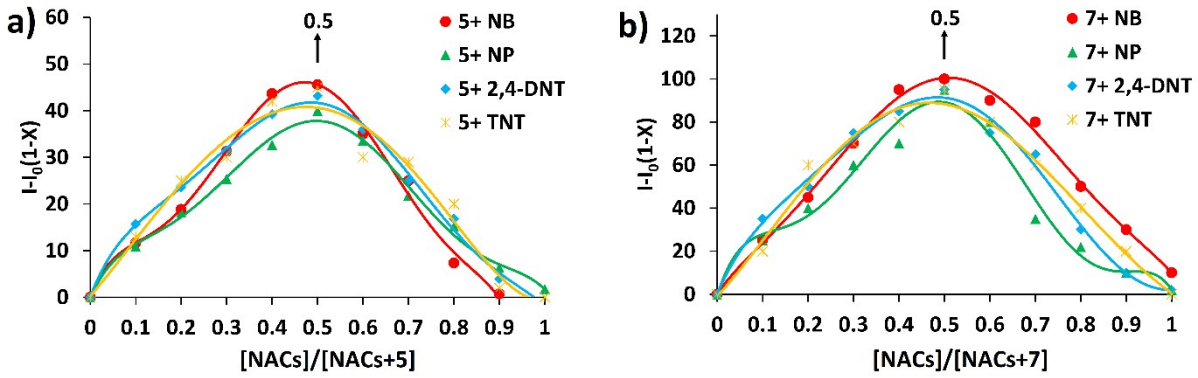

Figure S25. Job's Plots of **a)** compound **5** and **b)** compound **7** with NACs.

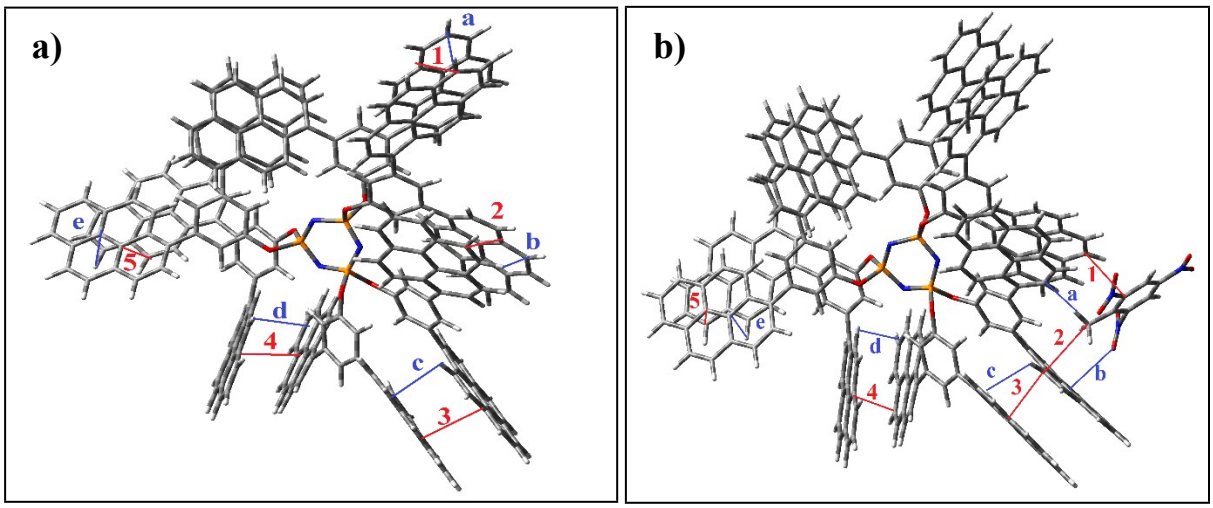

Figure S26. Intramolecular π –π and CH- π interactions in the structure of compound 7 in THF and intramolecular interactions among the pyrene units in compound **7** and intermolecular interactions between compound 7 and TNT (Å).

Table S1. Comparison of the selected intramolecular CH--π interaction distances for compounds **4**, **5, 6** and **7** (Å).

4		**5**		**6**		**7**	
a	2.654	**a**	3.638	**a**	3.260	**a**	3.263
b	2.950	**b**	2.870	**b**	3.942	**b**	3.251
c	3.052	**c**	3.541	**c**	4.744	**c**	3.126
d	2.980	**d**	3.172	**d**	5.498	**d**	3.297
e	3.567	**e**	3.148	**e**	7.33	**e**	3.42

				5			9
f	2.711	**f**	3.281		**f**	3.469	
g	2.743				**g**	3.388	
					h	3.840	

Table S2. Comparison of the selected intramolecular CH--π and π--π interactions distances for compounds 7 in THF and intramolecular interactions among the pyrene units in compound **7** and intermolecular interactions between compound 7 and TNT (Å).

π--π interactions in THF		π--π interactions in TNT + compound **7**		H--π interactions in THF		H--π interactions in TNT + compound **7**	
1	3.396	a	3.311	1	3.152	a	3.440
2	3.963	b	3.241	2	3.599	b	2.980
3	3.487	c	3.235	3	3.135	c	2.938
4	3.584	d	3.731	4	3.295	d	3.170
5	3.677	e	3.572	5	3.323	e	3.126