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

Supplementary Informations

Designing inorganic-organic hybrid molecules based on carbazole/indole appended cyclotriphosphazenes and the investigation of their photophysical properties

*Duygu Palabıyık, Ceylan Mutlu Balcı, Süreyya Oğuz Tümay, Serap Beşli**

Department of Chemistry, Gebze Technical University, Gebze, Kocaeli, Turkey

Author for correspondence:

Dr. Serap Beşli, Department of Chemistry, Gebze Technical University, Gebze, Kocaeli 41400, Turkey

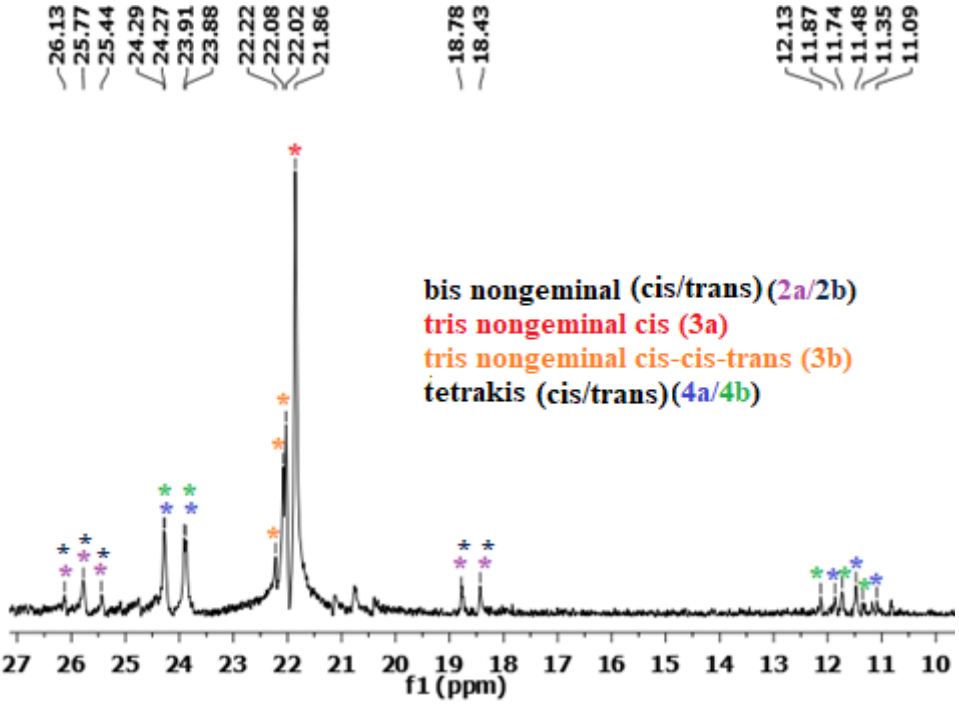

Figure S1: ^{31}P-decoupled NMR spectrum of the mixture of **1** and **I** at 1:3 mole ratio in THF solution; the reaction mixture was filtered and the solvent removed prior to dissolving in $CDCl_3$ solution.

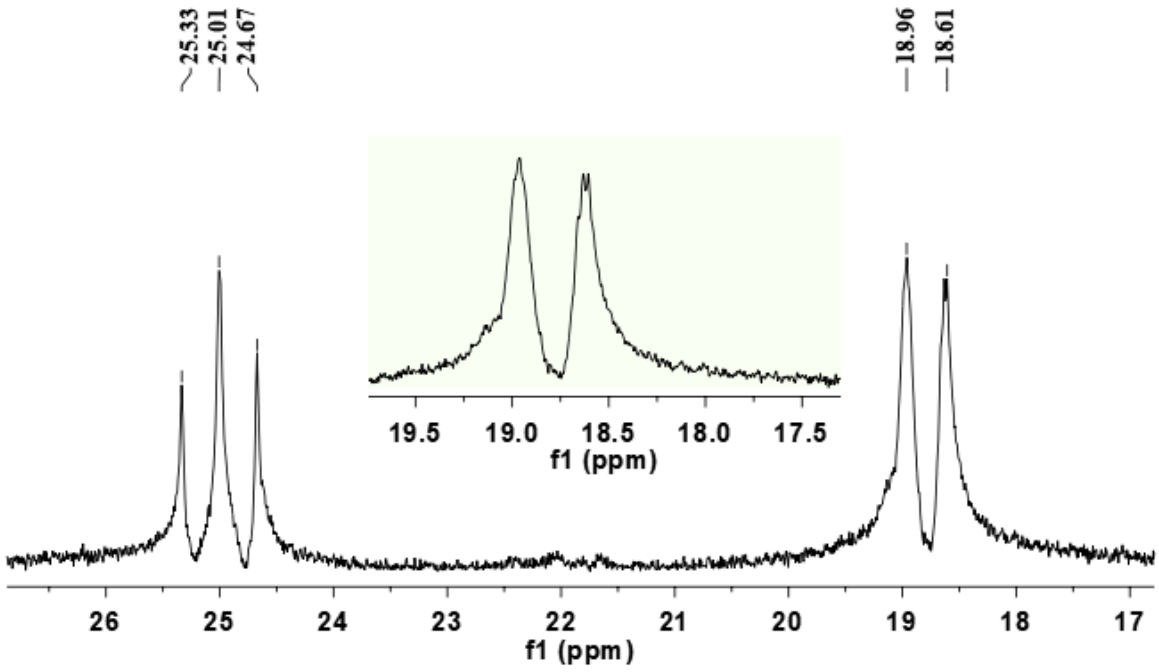

Figure S2: ^{31}P-decoupled NMR spectrum of bis nongeminal (*cis/trans*) products (**2a**/**2b**).

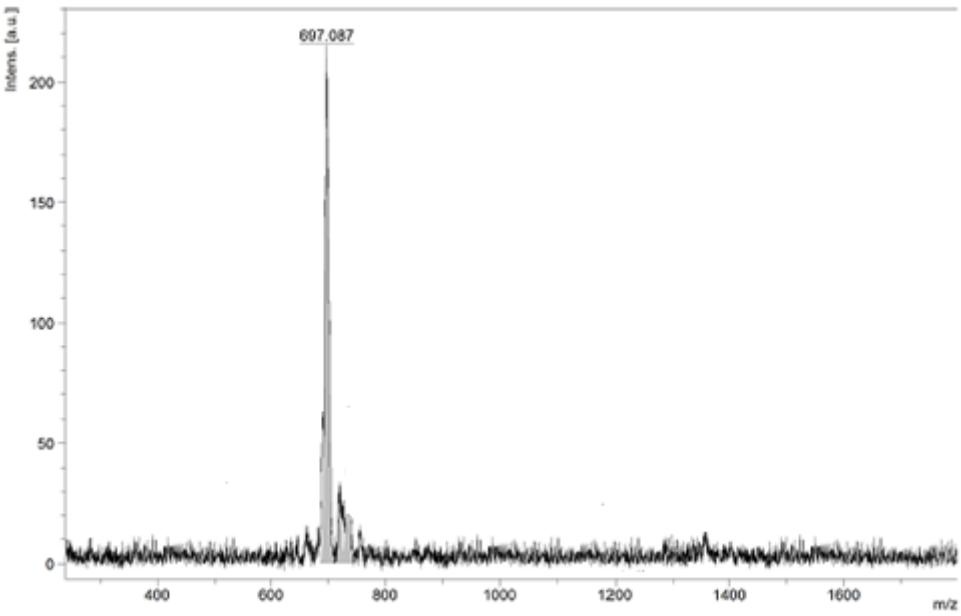

Figure S3: The mass spectrum of compounds **2a/2b**.

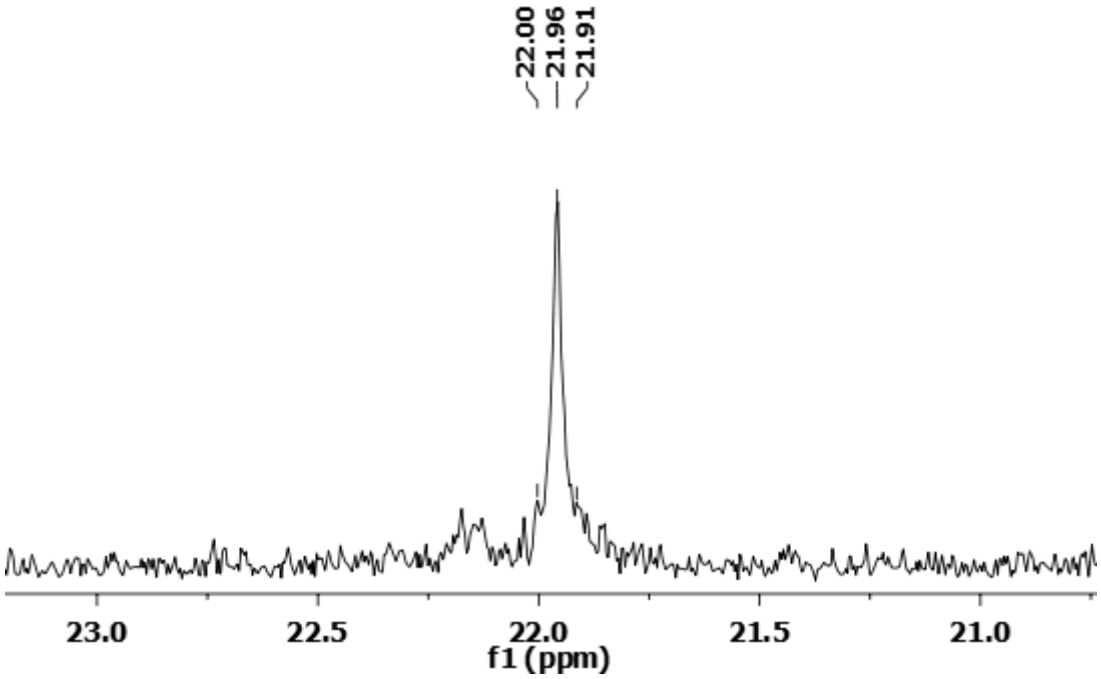

Figure S4: ^{31}P-decoupled NMR spectrum of tris nongeminal products (**3a, b)**.

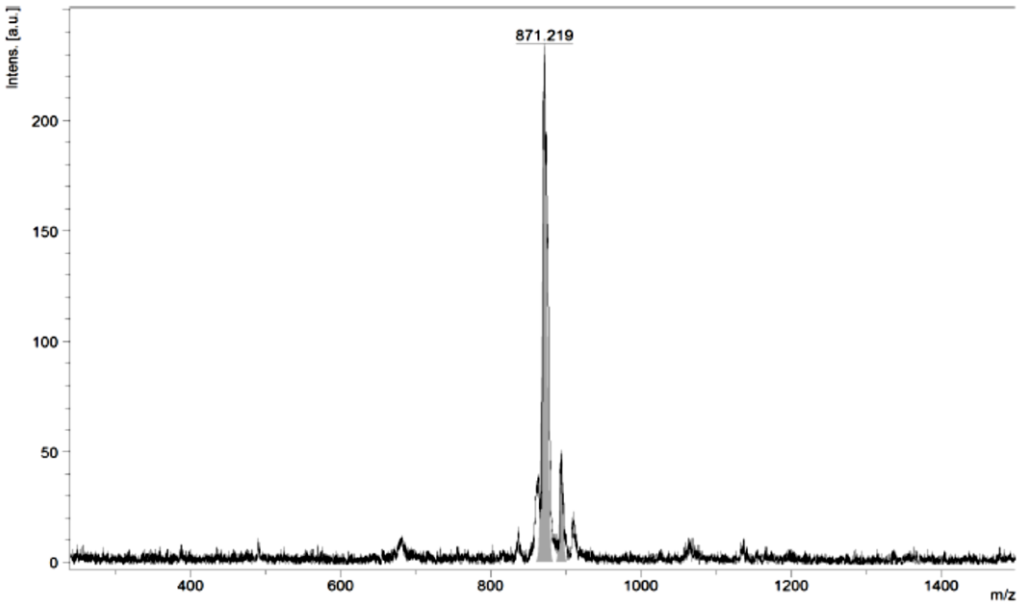

Figure S5: The mass spectrum of compounds **3a, b**.

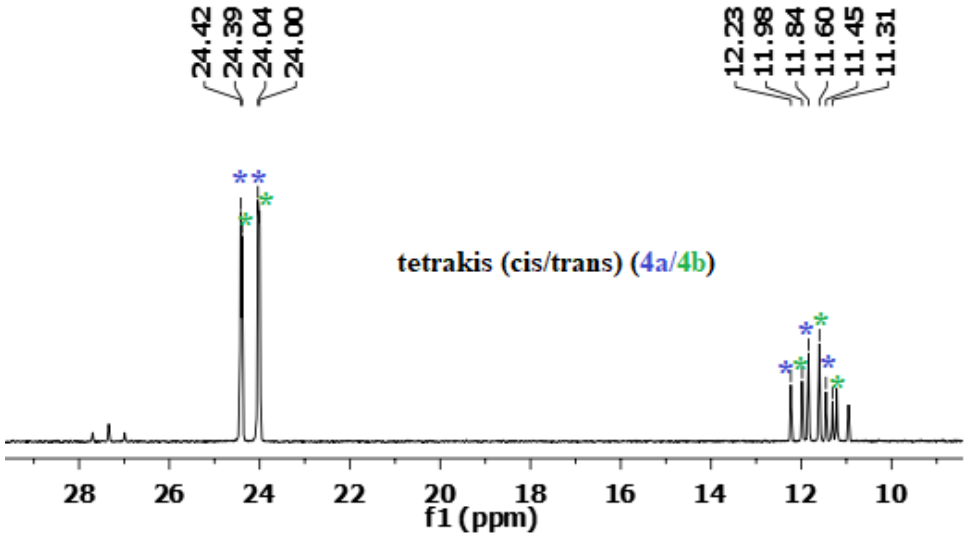

Figure S6: ^{31}P-decoupled NMR spectrum of tetrakis (*cis/trans*) products (**4a**/**4b**).

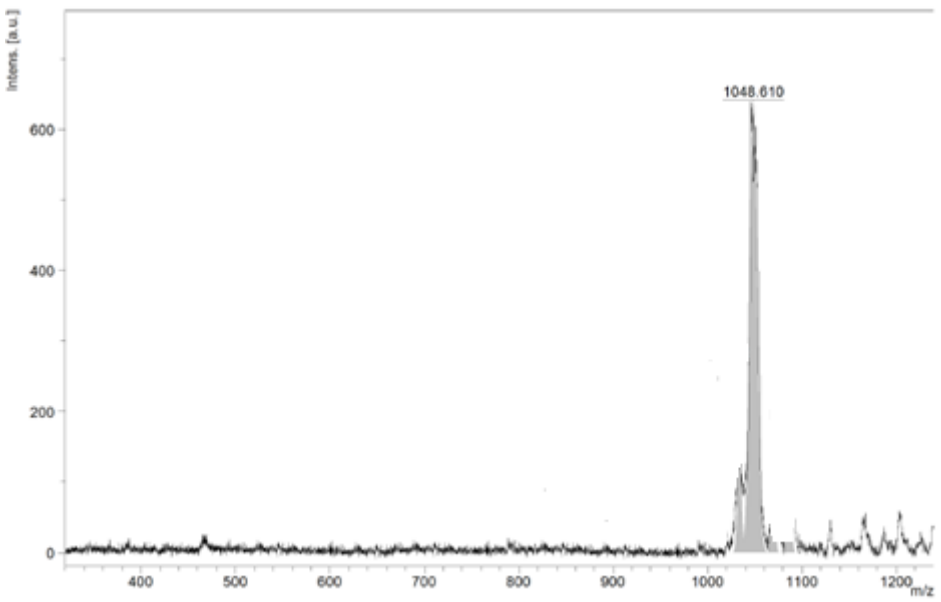

Figure S7: The mass spectrum of compounds **4a/4b**.

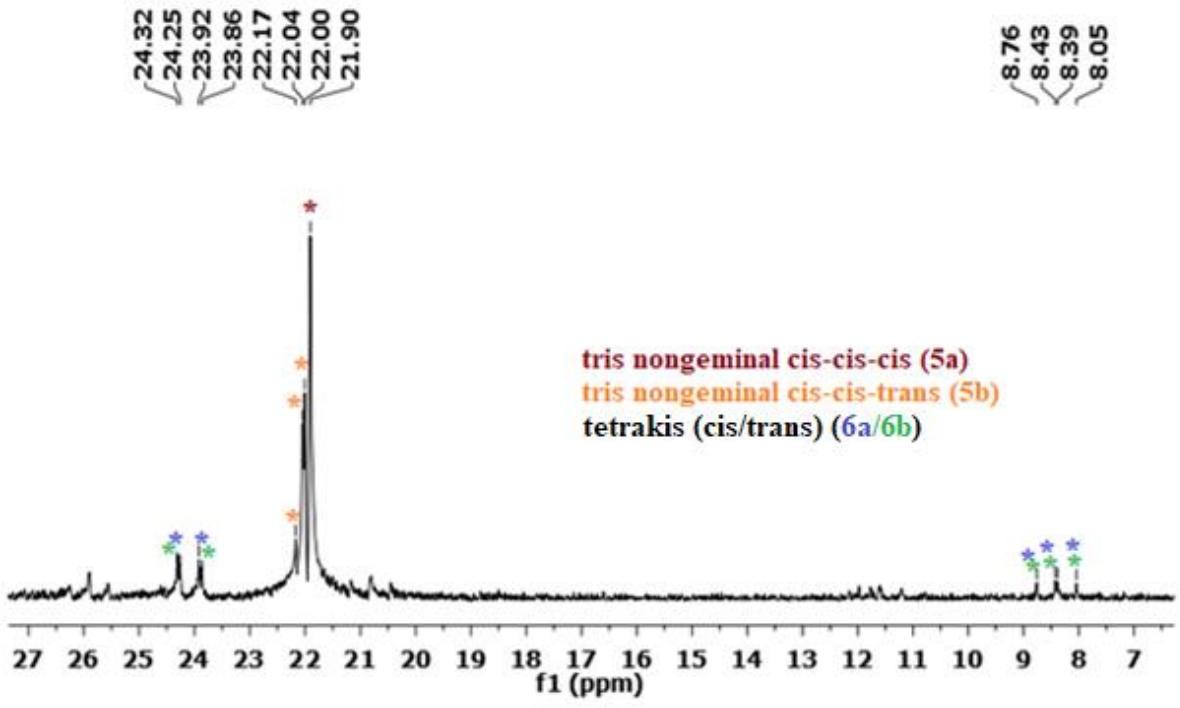

Figure S8: ^{31}P-decoupled NMR spectrum of the mixture of **1** and **II** at 1:3.1 mole ratio in THF solution; the reaction mixture was filtered and the solvent removed prior to dissolving in $CDCl_3$ solution.

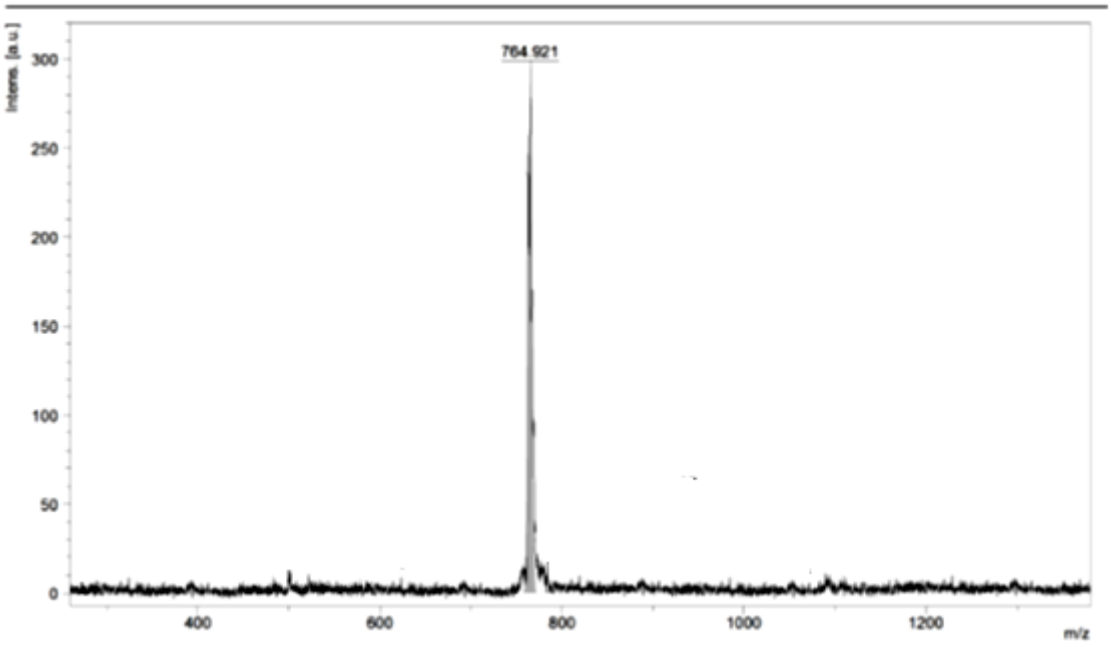

Figure S9: The mass spectrum of compounds **5a, b**.

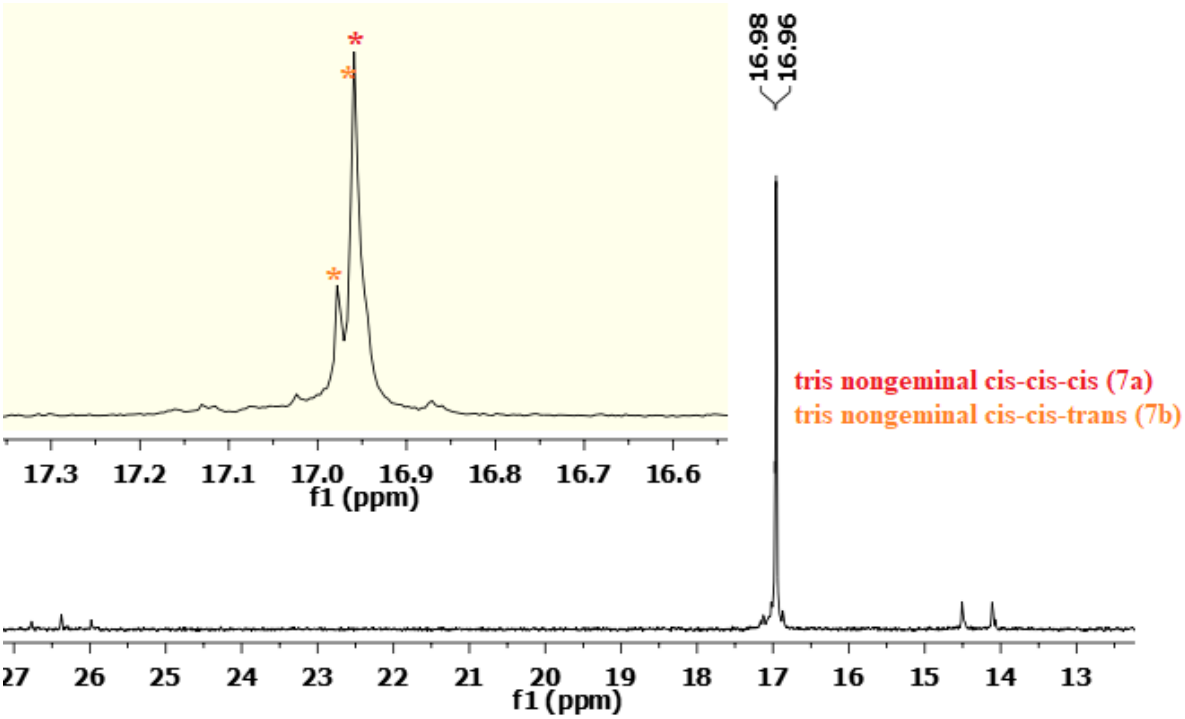

Figure S10: ^{31}P-decoupled NMR spectrum of the reaction mixture of **5a** and **5b** with **I** in THF solution; the reaction mixture was filtered and the solvent removed prior to dissolving in $CDCl_3$ solution.

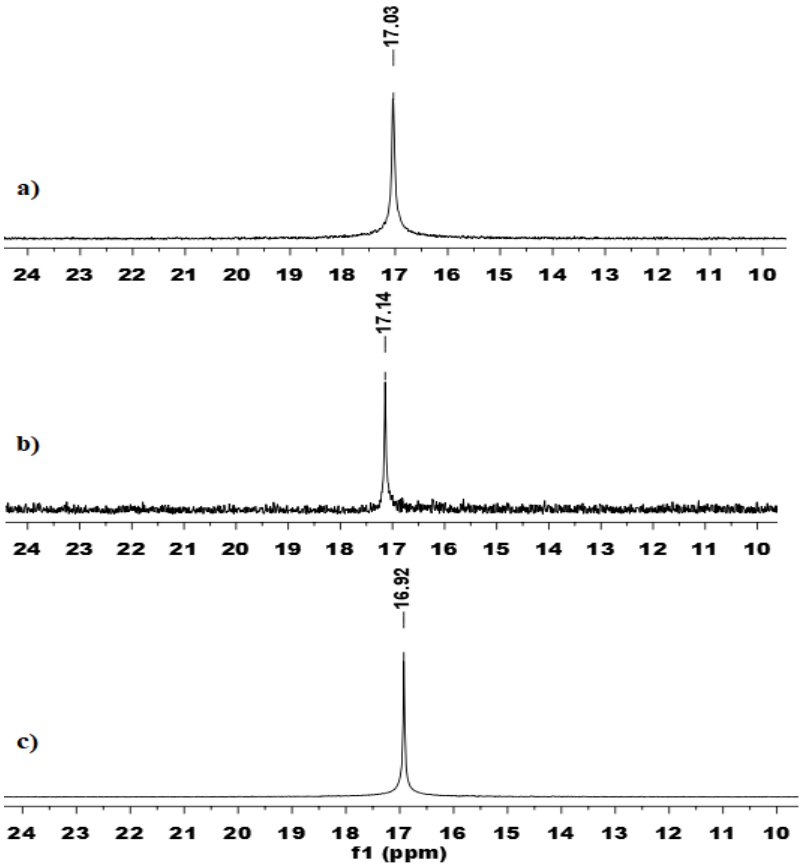

Figure S11: ^{31}P-decoupled NMR spectra of compounds a) **7a** b) **8** c) **9**.

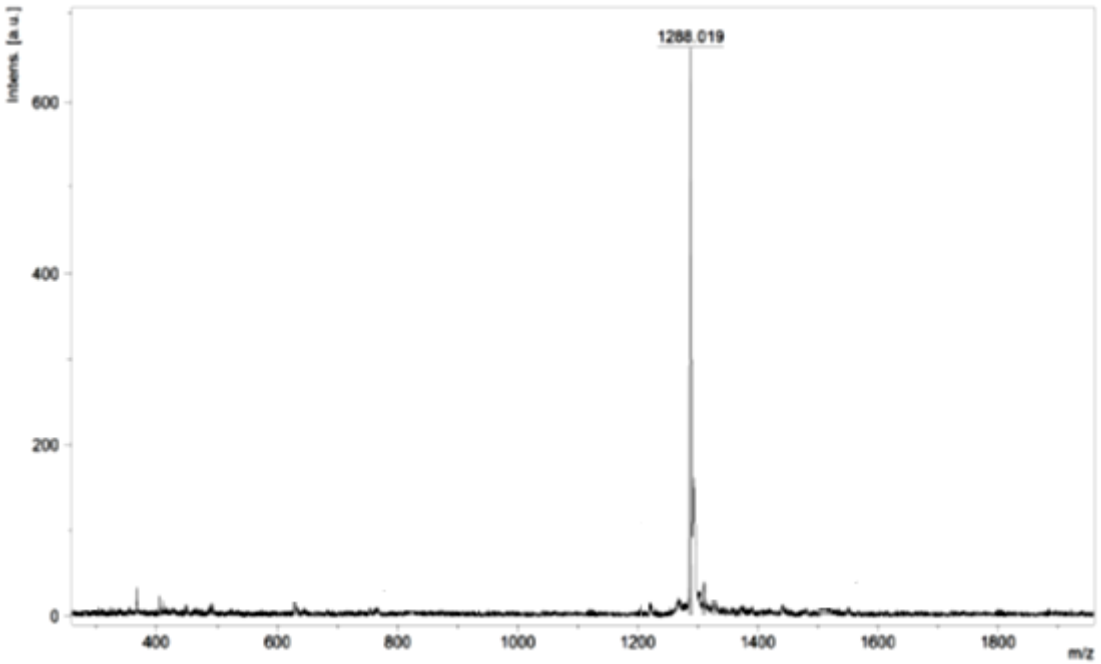

Figure S12: The mass spectrum of compound **7a**.

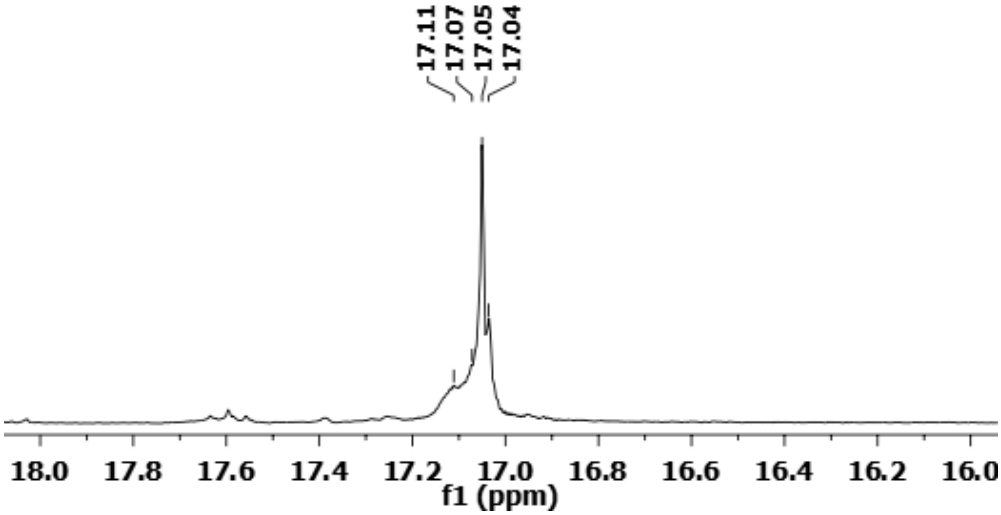

Figure S13: ^{31}P-decoupled NMR spectrum of compounds **7a**, **b**.

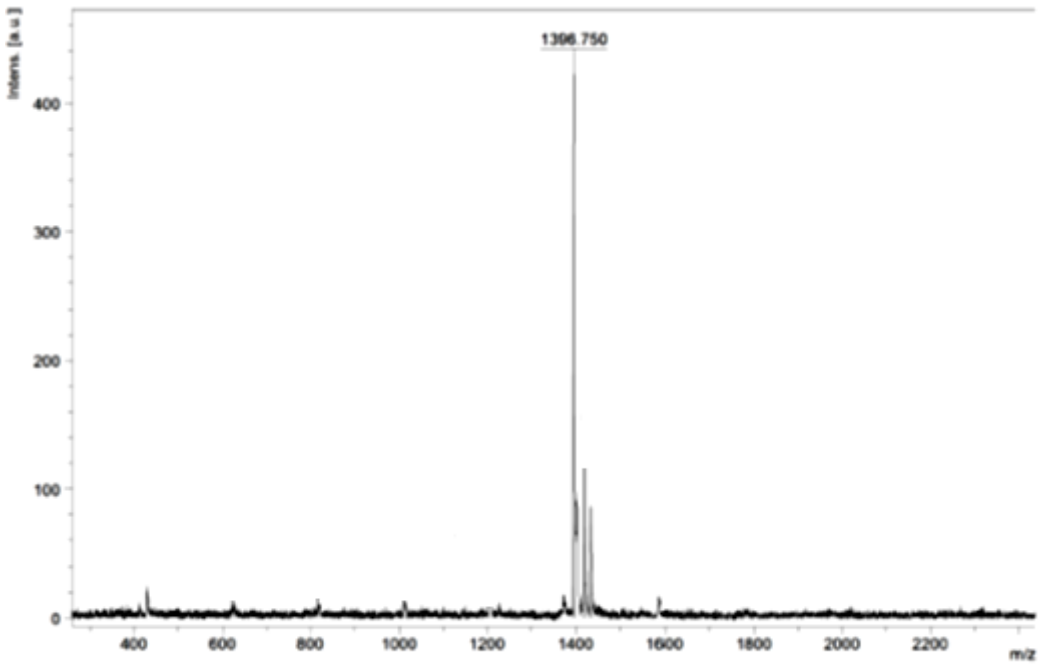

Figure S14: The mass spectrum of compound **8**.

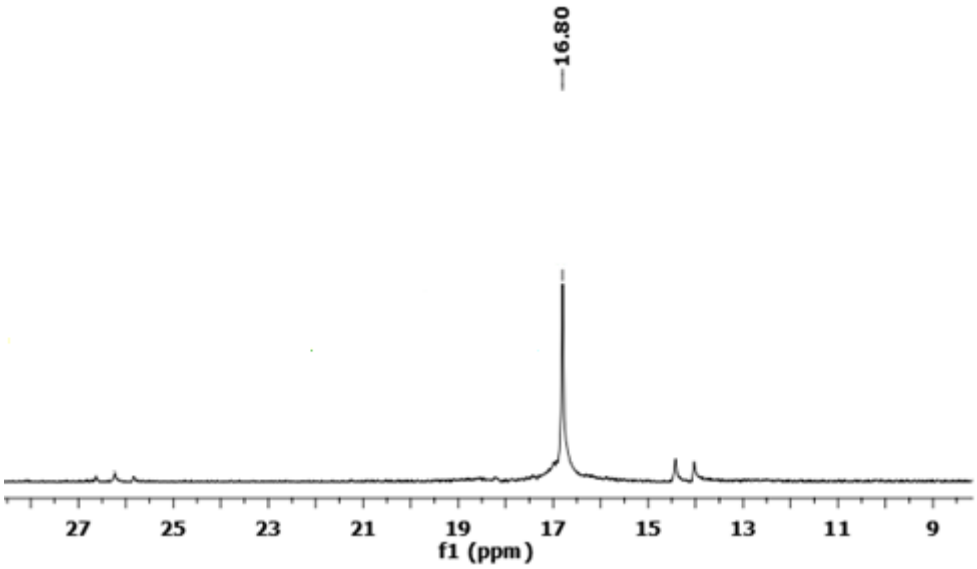

Figure S15: ^{31}P-decoupled NMR spectrum of the reaction mixture of **1** with **II** at 1:8 mole ratio.

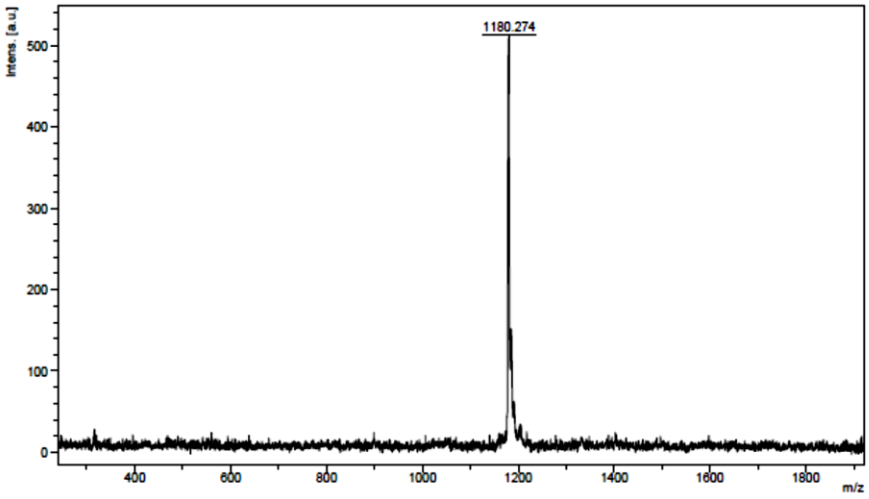

Figure S16: The mass spectrum of compound **9**.

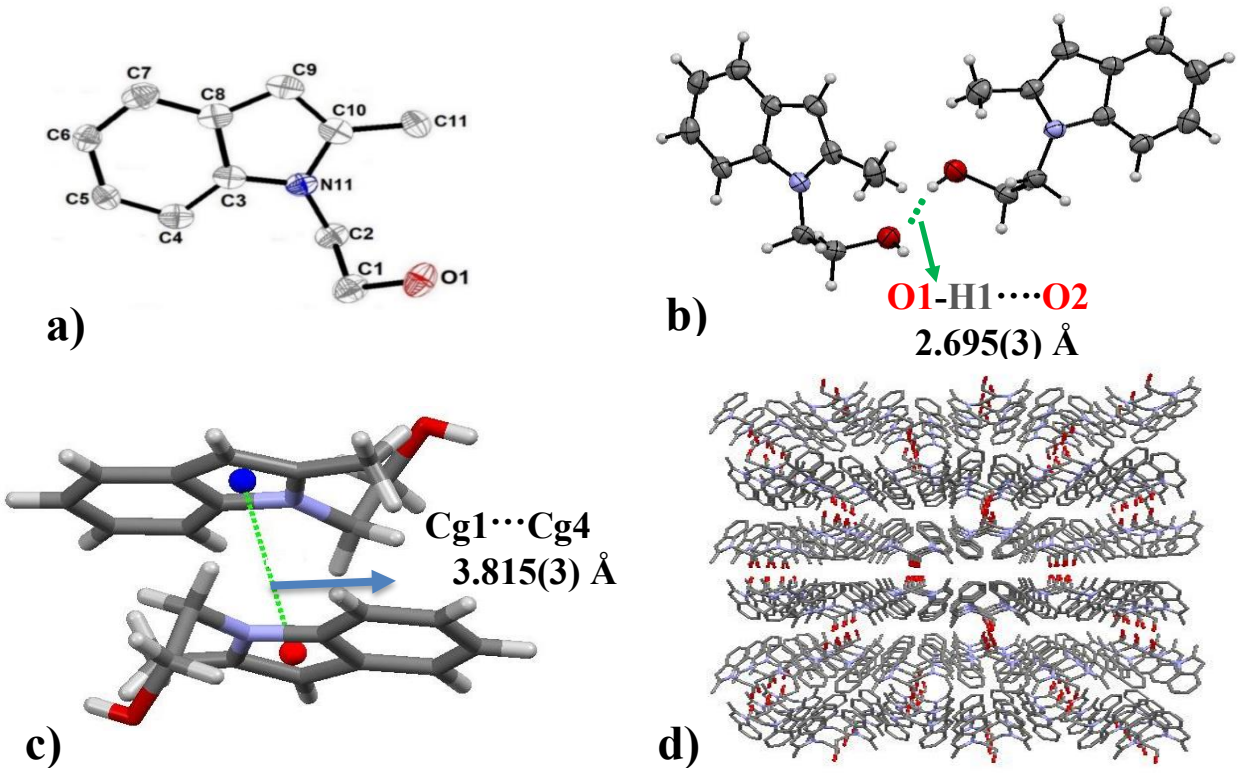

Figure S17: a) Crystal structure of **II** with atom numbering scheme, displacement ellipsoids are drawn at the 30% probability level and H atoms are omitted for clarity. **b)** A view of classical intermolecular O-H/O (green dotted lines along the a-axis) hydrogen bonding. **c)** Perspective view of intermolecular π-π stacking interactions. **d)** Crystal packing illustration of **II.**

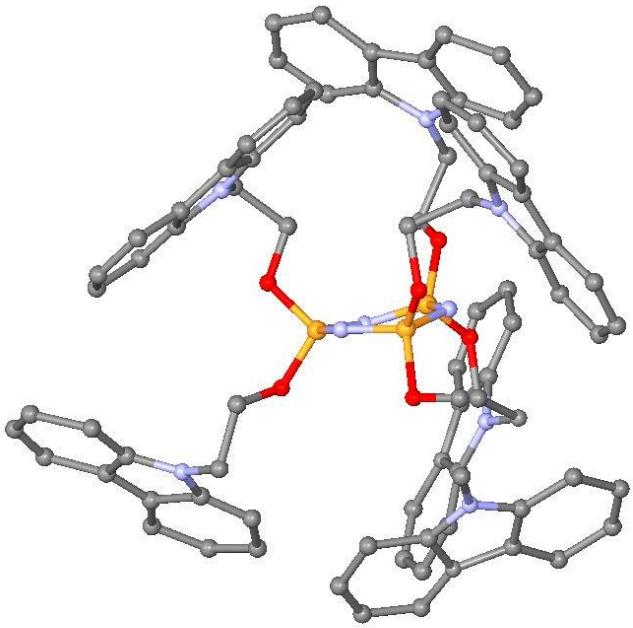

Figure S18: Crystal structure of compound **8**. Displacement ellipsoids are drawn at the 30% probability level and H atoms are omitted for clarity. The grey, blue-, red- and orange-coloured atoms represent C, N, O and P atoms, respectively.

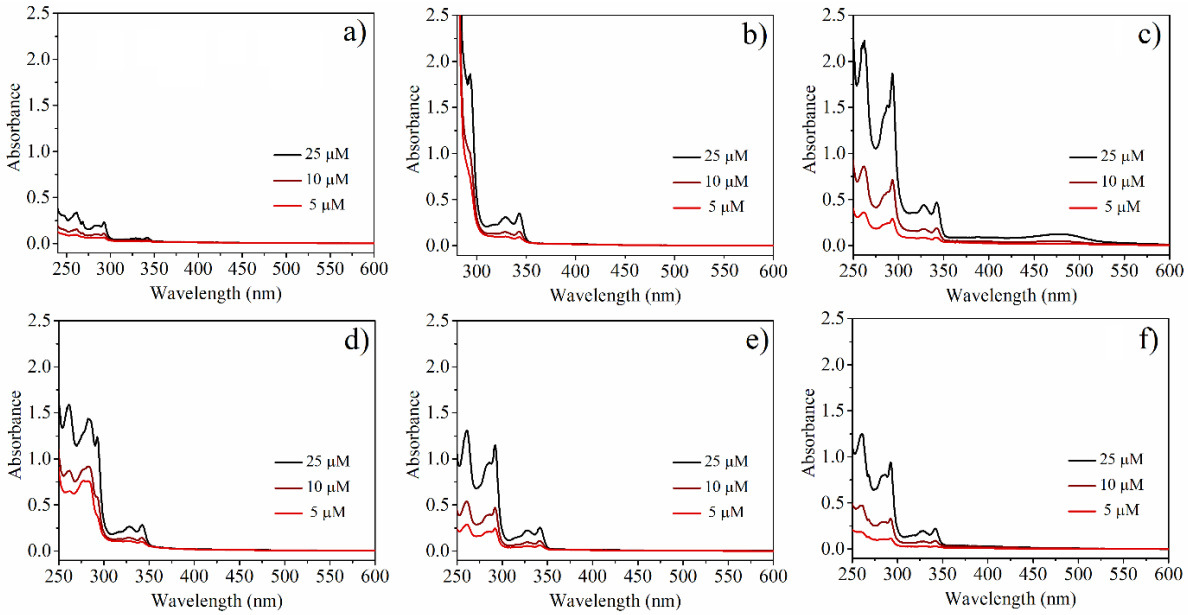

Figure S19: UV-Vis absorption spectra for **7a** in various solvents (**a**: n-hexane; **b**: toluene; **c**: dichloromethane; **d**: 1,4-dioxane; **e**: ACN; **f**: EtOH).

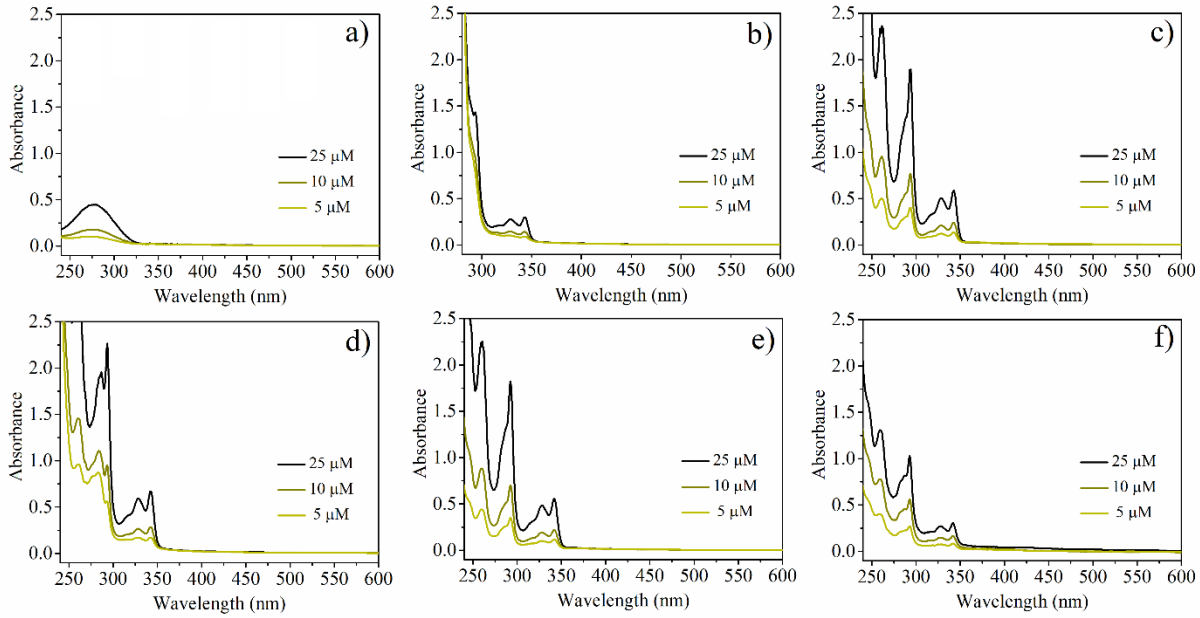

Figure S20: UV-Vis absorption spectra for **8** in various solvents (**a**: n-hexane; **b**: toluene; **c**: dichloromethane; **d**: 1,4-dioxane; **e**: ACN; **f**: EtOH).

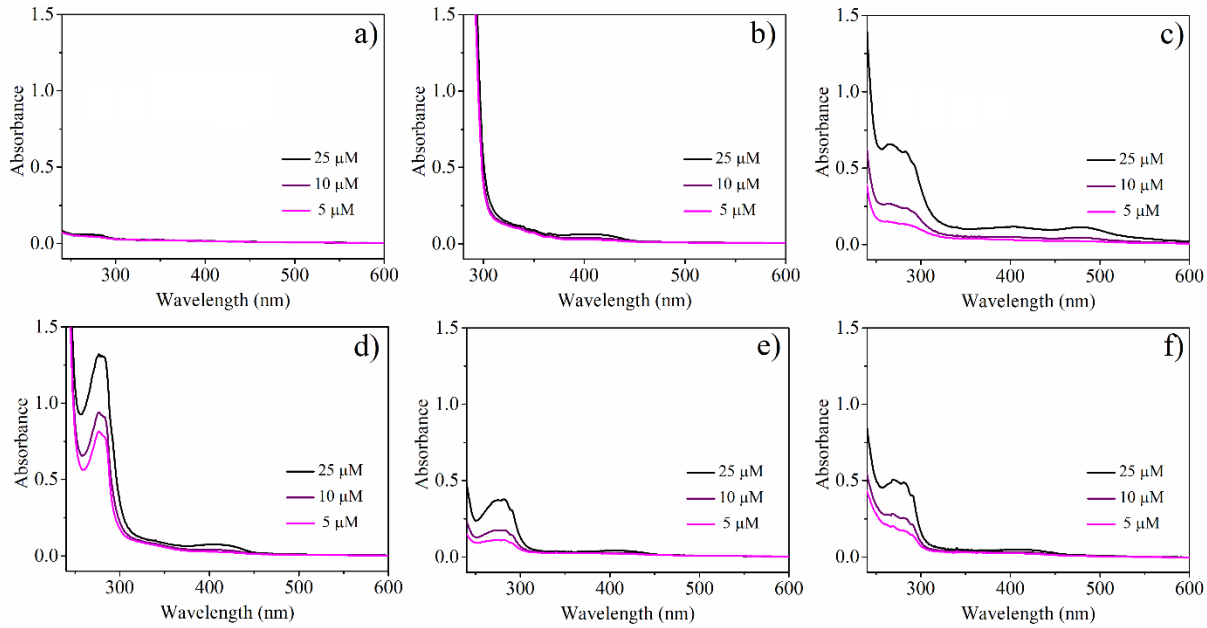

Figure S21: UV-Vis absorption spectra for **9** in various solvents (**a**: n-hexane; **b**: toluene; **c**: dichloromethane; **d**: 1,4-dioxane; **e**: ACN; **f**: EtOH).

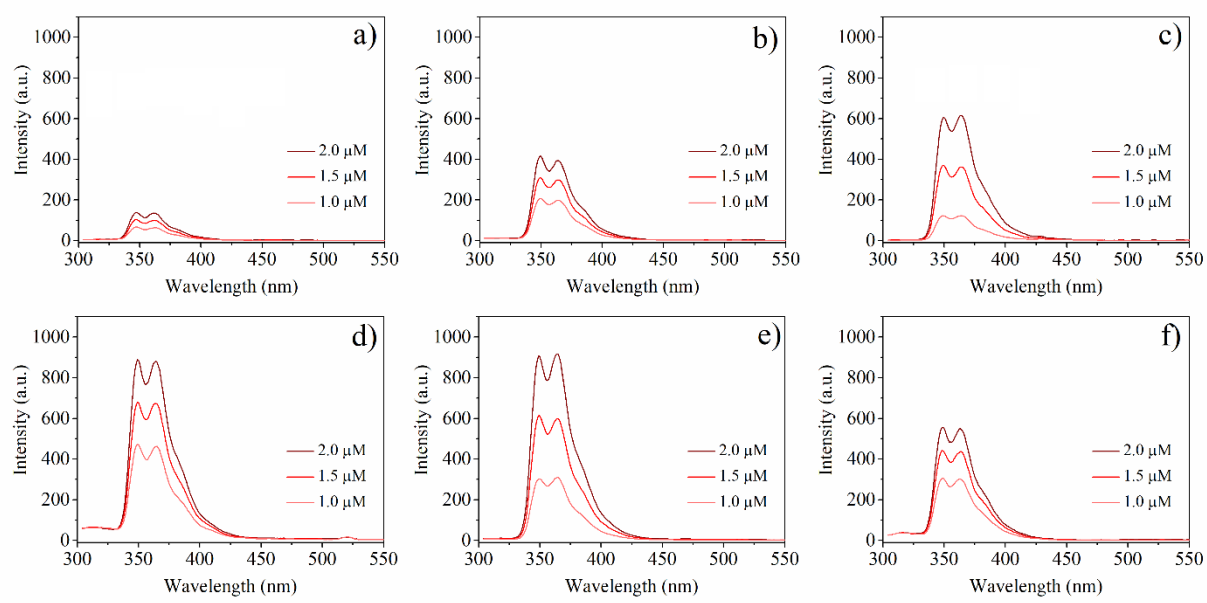

Figure S22: Fluorescence spectra for **7a** in various solvents (**a**: n-hexane; **b**: toluene; **c**: dichloromethane; **d**: 1,4-dioxane; **e**: ACN; **f**: EtOH).

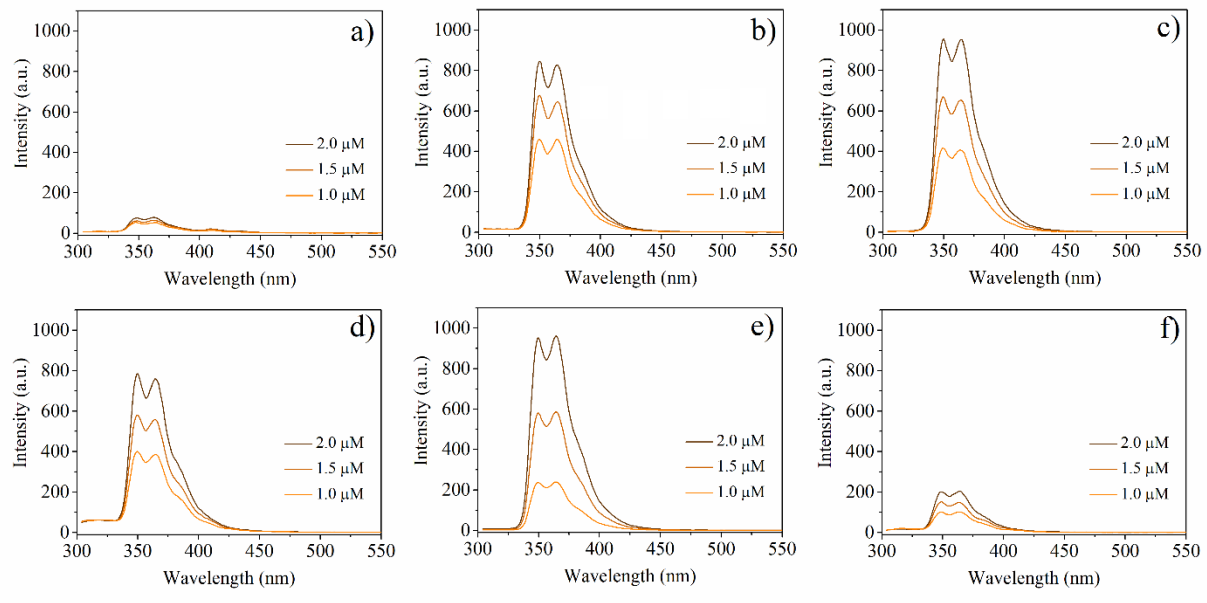

Figure S23: Fluorescence spectra for **8** in various solvents (**a**: n-hexane; **b**: toluene; **c**: dichloromethane; **d**: 1,4-dioxane; **e**: ACN; **f**: EtOH).

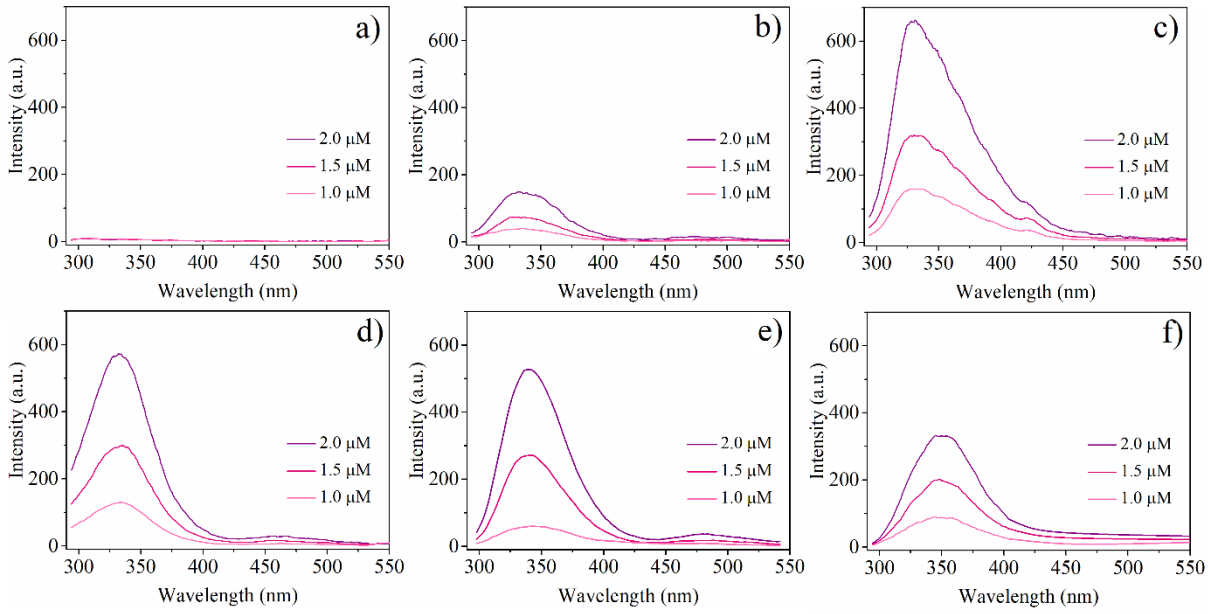

Figure S24: Fluorescence spectra for **9** in various solvents (**a**: n-hexane; **b**: toluene; **c**: dichloromethane; **d**: 1,4-dioxane; **e**: ACN; **f**: EtOH).

Table S1. Some bond and conformational parameters of compound **3a**.

Bond length	**3a**	**Bond / Torsion angles**	**3a**
P1-N1	1.593(4)	**N1-P1-N3**	117.0(2)
N1-P2	1.567(4)	**N1-P2-N2**	118.7(2)
P2-N2	1.579(4)	**N2-P3-N3**	117.4(2)
N2-P3	1.574(4)	**P1-N1-P2**	118.9(2)
P3-N3	1.592(4)	**P2-N2-P3**	122.2(2)
P1-N3	1.589(4)	**P1-N3-P3**	118.6(2)
P1-O1	1.559(3)	**P1-O1-C1**	118.0(3)
P2-O2	1.551(3)	**P2-O2-C15**	123.8(3)
P3-O3	1.557(3)	**P3-O3-C29**	119.5(3)
P1-Cl1	2.021(2)	**P1-N1-P2-N2**	-13.2(4)
P2-Cl2	2.024(17)	**P2-N2-P3-N3**	-2.7(4)
P3-Cl3	1.990(18)	**P3-N3-P1-N1**	-31.8(4)
Puckering amplitude, Q for P_3N_3 rings	0.261(3)	**Max. Deviation for P_3N_3 rings**	0.1826(18) (P1)

Table S2. Selected intermolecular interactions for **II** and **3a**.

Intermolecular interactions					
II					
I···J		**D(I···J)**			**Symmetry code**
O1…O2		2.682(3)			-1/2+x,1/2-y,z
C6…H4		2.82			1/2+x,1/2-y,z
H1…H2		2.39			-1/2+x,1/2-y,z
H1…O2		1.90			-1/2+x,1/2-y,z
3a					
I···J		**D(I···J)**			**Symmetry code**
Cl1…H11		2.94			x,-1+y,z
Cl2…H24		2.94			x,-1+y,z
Cl2…H35		2.88			x,1/2-y,1/2+z
C7…H1B		2.88			1-x,1/2+y,3/2-z
C9…H18		2.76			x,1/2-y,-1/2+z
H6…H15A		2.35			1-x,1/2+y,3/2-z
II					
I···J		**X-H(I)···Cg(J)**			**Symmetry code**
C1—H1B…Cg1		3.807(4)			-1/2+x,1/2-y,z
C11—H11C…Cg5		3.754(5)			1/2-x,-1/2+y,-1/2+z
C11—H11C…Cg6		3.730(5)			1/2-x,-1/2+y,-1/2+z
C13—H13B…Cg5		3.752(4)			-1/2+x,1/2-y,z
C22—H22C…Cg2		3.552(4)			1/2-x,1/2+y,1/2+z
C22—H22C…Cg3		3.561(4)			1/2-x,1/2+y,1/2+z
3a					
X—H(I)…Cg(J)	**H..Cg**	**H-Perp**	**X..Cg**	**X-H..Cg**	**Symmetry code**
C2—H2A…Cg7	2.88	-2.86	3.664(6)	137	x,y,z
C18—H18…Cg1	2.82	-2.72	3.506(5)	130	x,1/2-y,1/2+z
C19—H19…Cg5	2.81	-2.81	3.600(5)	141	x,1/2-y,1/2+z
C30—H30A…Cg9	2.95	-2.83	3.709(7)	135	-x,1-y,1-z

Table S3. Some selected intramolecular interactions for **II** and **3a**.

.

Intramolecular interactions	
II	
I···J	**D(I···J)**
O1…N1	3.054(4)
N1…C9	2.230(5)
C2…C4	3.074(6)
C3…C9	2.267(5)
C4…C7	2.809(6)
C2…C11	3.056(6)
C1…C3	3.307(5)
C3…C6	2.742(6)
C5…C8	2.777(5)
C8…C10	2.255(5)
3a	
I···J	**D(I···J)**
Cl1…C1	3.278(6)
Cl2…C15	3.343(5)
P1…N2	3.110(4)
P2…N3	3.149(4)
O1…N4	3.025(5)
O3…N6	2.876(5)
N4…C9	2.260(6)
C14…C8	2.290(9)
C14…C11	2.751(9)
C3…C9	2.280(7)
C4…C7	2.809(7)
C15…N1	3.177(6)
N5…C23	2.273(6)
C37…N6	2.264(6)