Supporting Information

Synthesis, characterization and photophysical studies of self-assembled azo biphenyl urea derivatives

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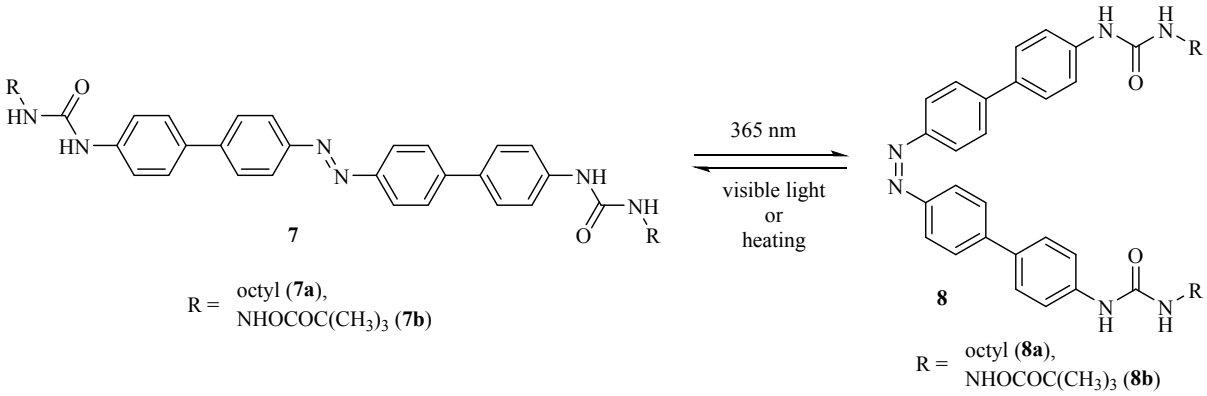
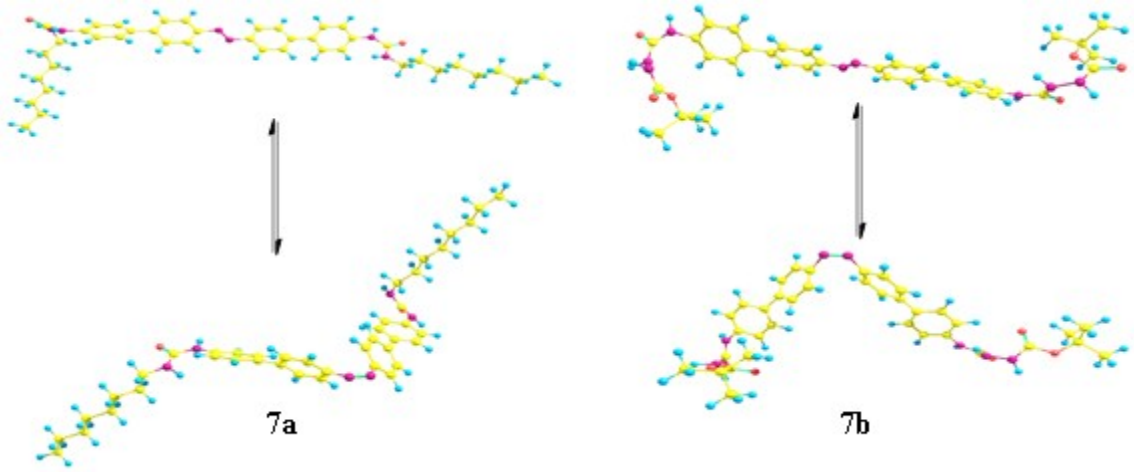
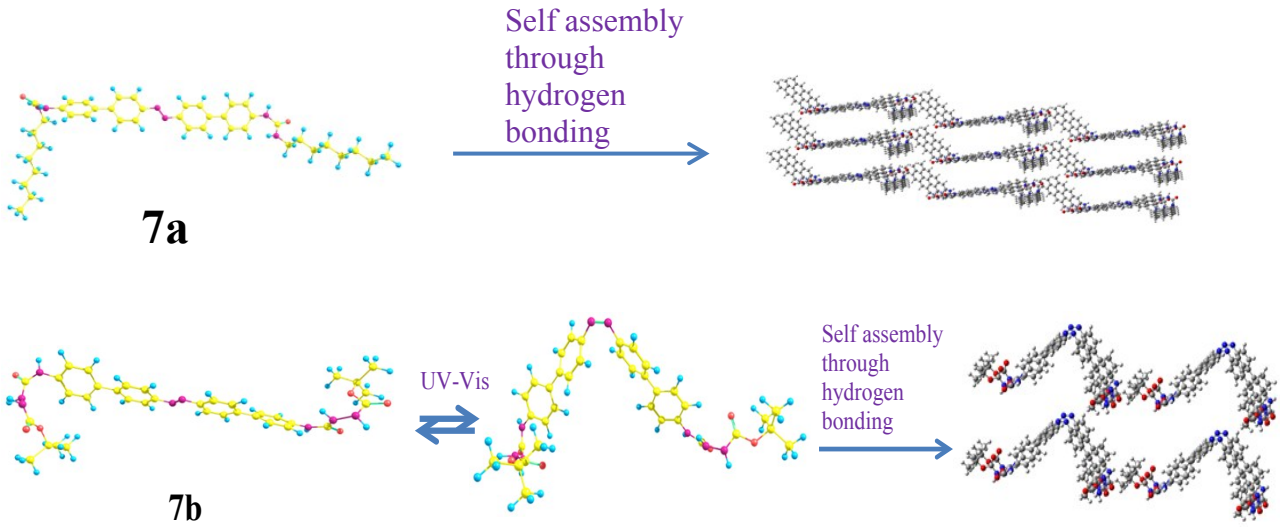


Scheme 1. Schematic representation for photo-isomerization reaction of **7**(**7a**/**7b**) upon UV and visible light irradiation.



Scheme 2. Optimized structure for *trans-cis* isomerization **7**(**7a**/**7b**).



Scheme 3. Possible sheet like self-assembly structure of **7a** and **7b** through hydrogen bonding.

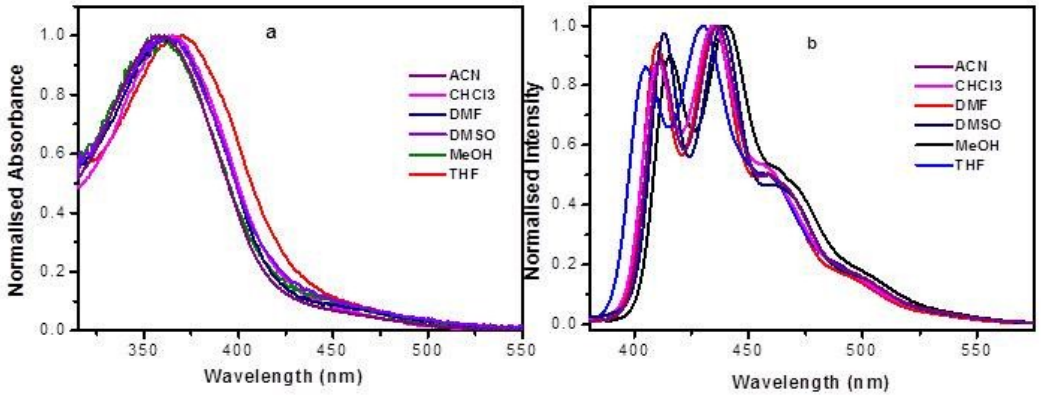


Fig. S1 Normalized absorption (a) and emission (b) spectra of DPOU (**7a**) in different solvents.

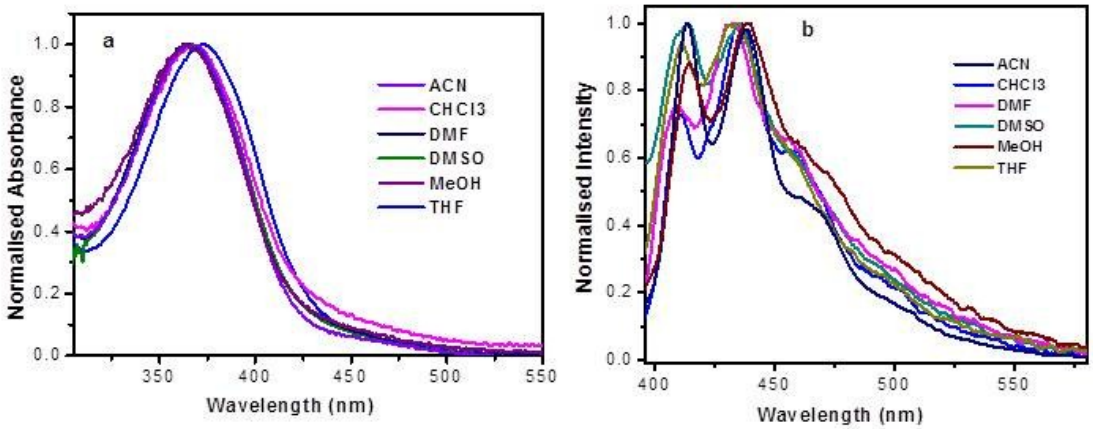


Fig. S2 Normalized absorption (a) and emission (b) spectra of DPBHU (**7b**) in different solvents.

Table 1. Absorption and emission values of **7a** (DPOU) in different solvents.

Solvents	λ_{abs} (nm)	λ_{ex} (nm)	λ_{emi} (nm)	**Stoke's shift (cm^{-1})**
THF	368	368	406, 431	3972
$CHCl_3$	365	365	410, 434	4355
DMF	358	358	409, 434	4891
DMSO	360	360	413, 438	4947
ACN	354	354	411, 436	5313
MeOH	356	356	415, 440	5363

Table 2. Absorption and emission values of **7b** (DPBHU) in different solvents.

Solvents	**λ_{abs} (nm)**	**λ_{ex} (nm)**	**λ_{emi} (nm)**	**Stoke's shift (cm^{-1})**
THF	372	372	412, 434	3867
$CHCl_3$	367	367	412, 434	4207
DMF	365	365	410, 432	4249
DMSO	365	365	411, 435	4409
ACN	364	364	413, 438	4641
MeOH	364	364	415, 439	4719

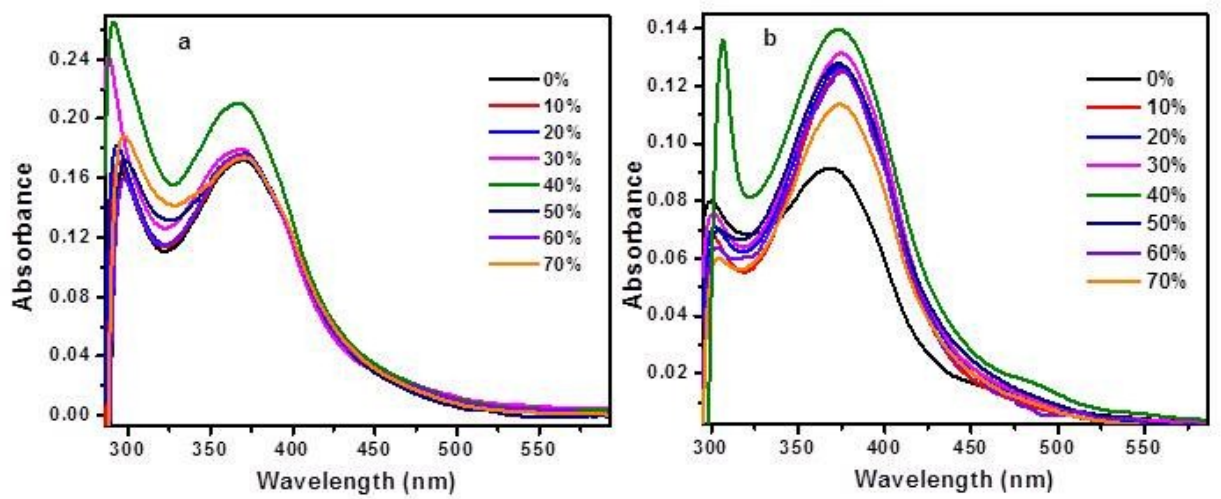


Fig. S3 Absorbance spectra of Compound **7a** (a) and **7b** (b) in different THF: H_2O fractions.

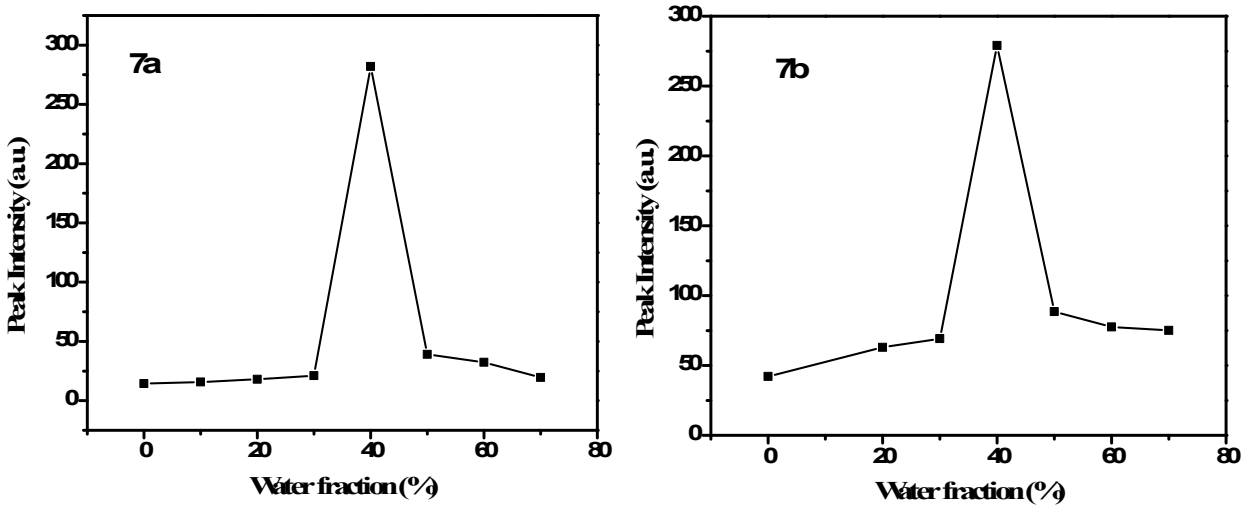


Fig. S4 Peak intensity plot of **7a** and **7b** in different THF: H_2O fractions.

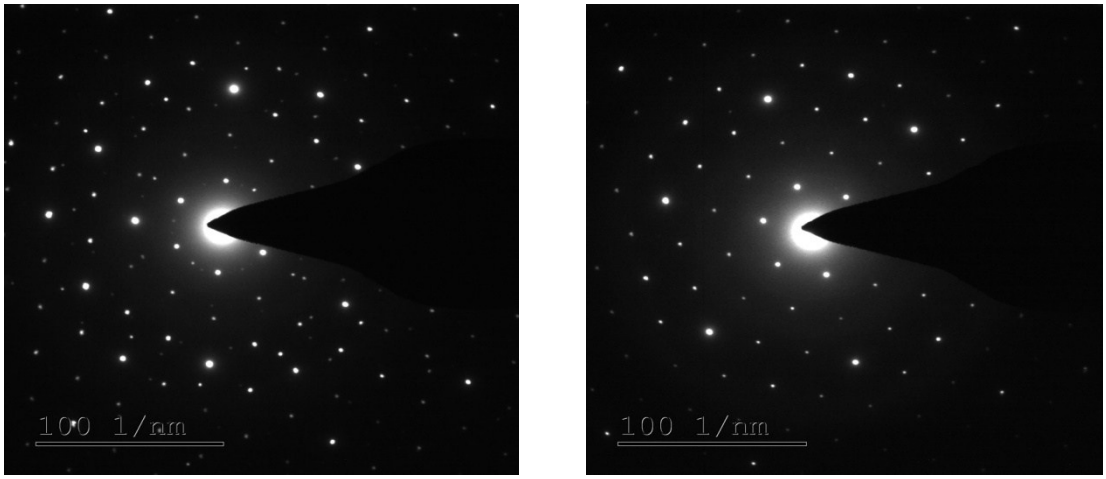


Fig. S5 Selected area electron diffraction pattern of compounds **7a** and **7b** (from left to right).

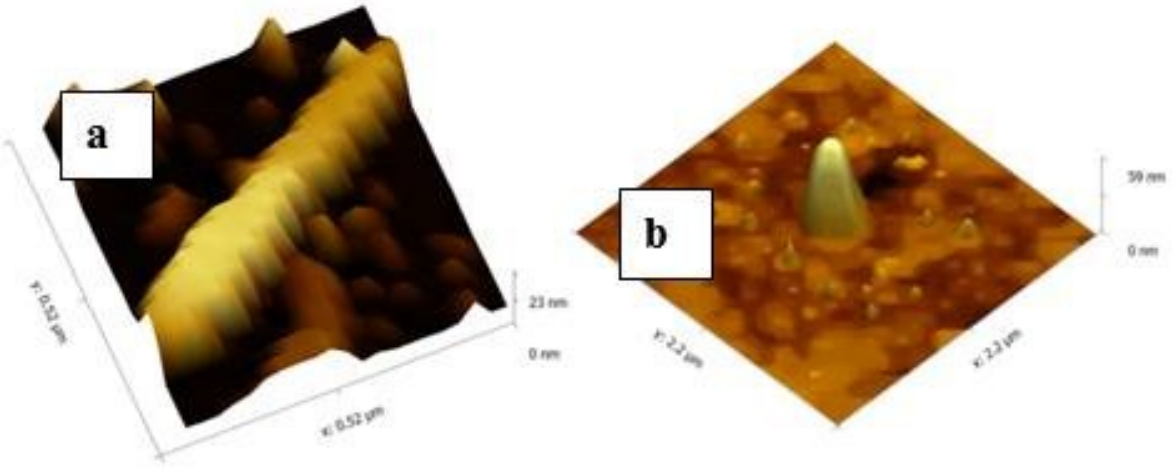


Fig. S6 AFM image of self-assembled **7a** (**a**) and **7b** (**b**) in THF-water mixture (40%) respectively, Samples were prepared by drop casting the solution (THF-water (40%)) of the compound onto a freshly cleaved, glass surface.

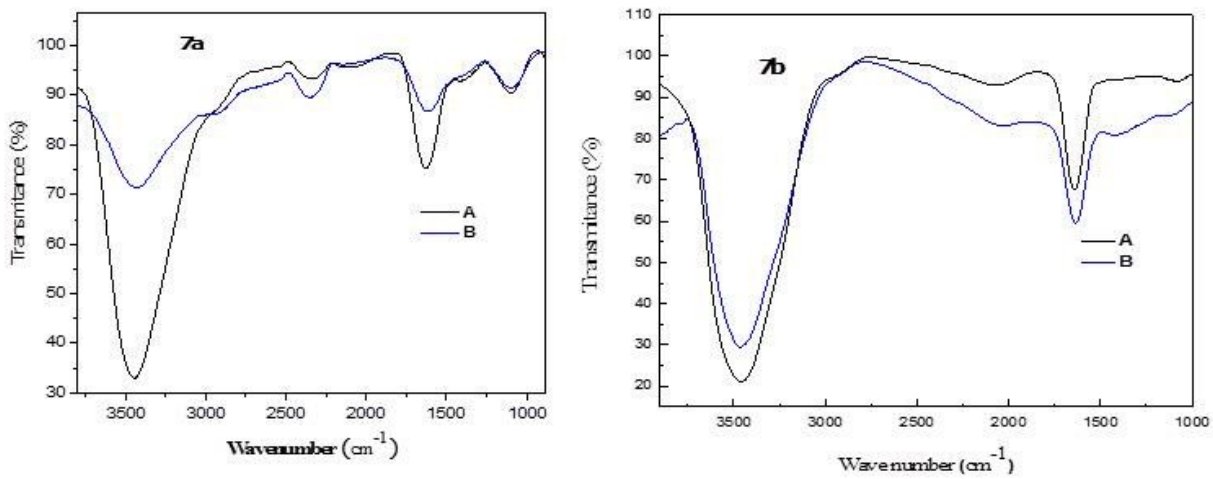


Fig. S7 FT-IR spectrum of compound **7** taken in before (A) and after (B) light irradiation at 365 nm.

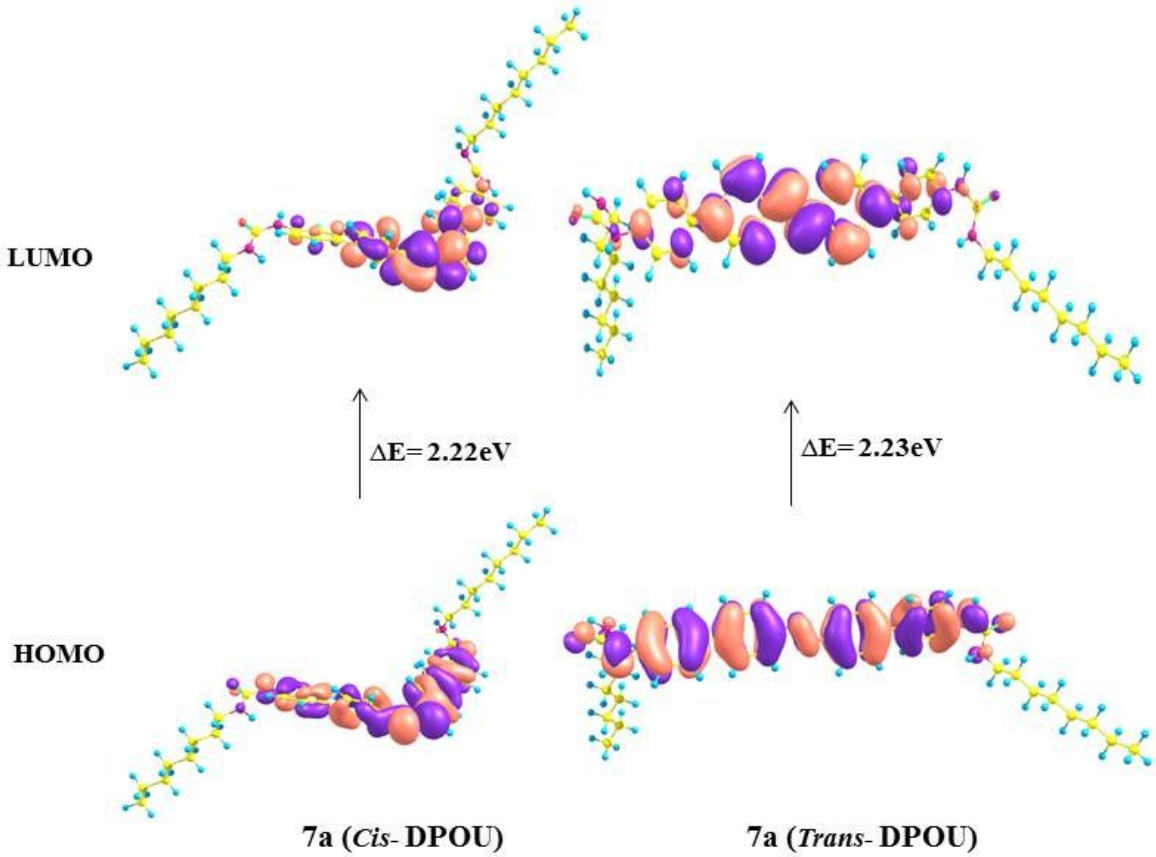


Fig. S8 DFT-computed molecular frontiers orbitals of **7a**.

Table 3. TD-DFT electronic transitions of all the compounds.

Compounds	wavelength (nm)	Oscillator strength (f)	Electronic transitions
Trans (**7a**)	443.17 nm	0.0014	HOMO-1 - LUMO
	374.57 nm	1.6996	HOMO - LUMO
	274.39 nm	0.0053	HOMO - LUMO
Cis (**7a**)	466.28 nm	0.1449	HOMO-1 - LUMO
	355.40 nm	0.3474	HOMO - LUMO
	260.60 nm	0.1014	HOMO - LUMO
Trans (**7b**)	454.00 nm	0.0011	HOMO-1 - LUMO
	367.99 nm	1.6999	HOMO - LUMO
	261.00 nm	0.0406	HOMO - LUMO
Cis (**7b**)	474.35 nm	0.1306	HOMO-1 - LUMO
	363.17 nm	0.2631	HOMO - LUMO
	257.11 nm	0.1852	HOMO - LUMO

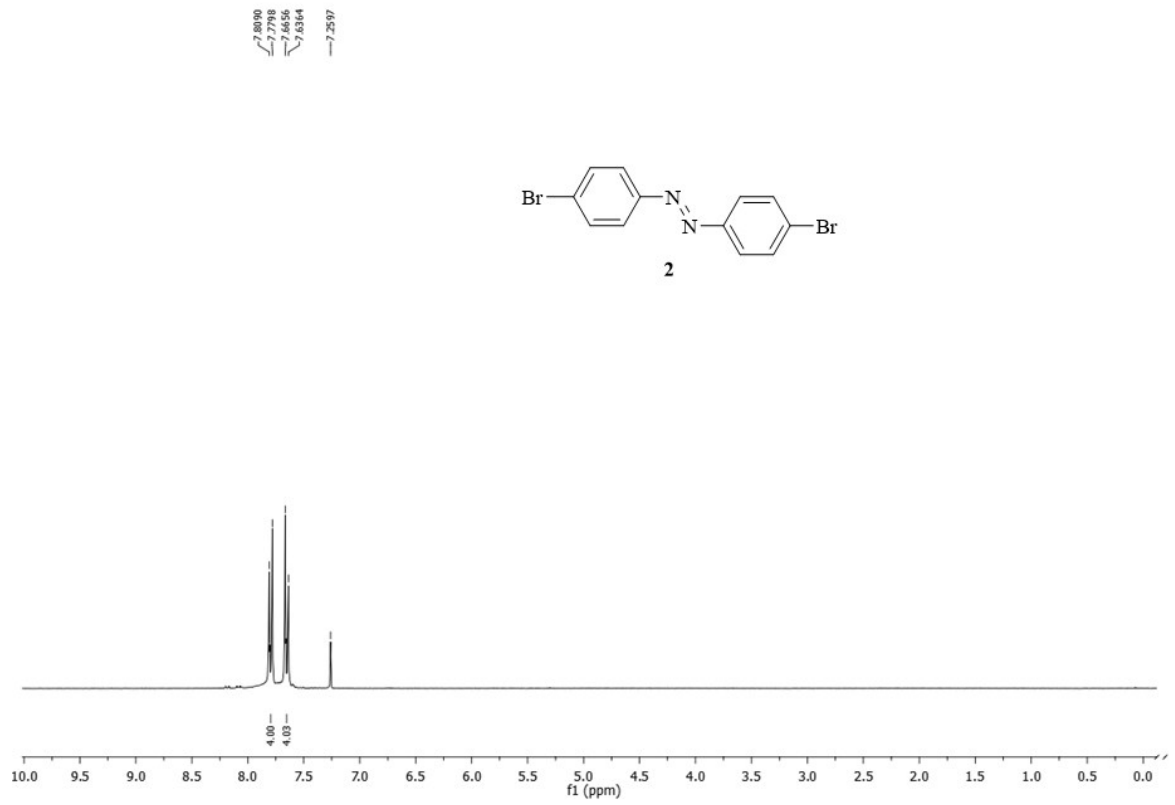


Fig. S9 ^{1}H NMR Spectrum of Compound **2**.

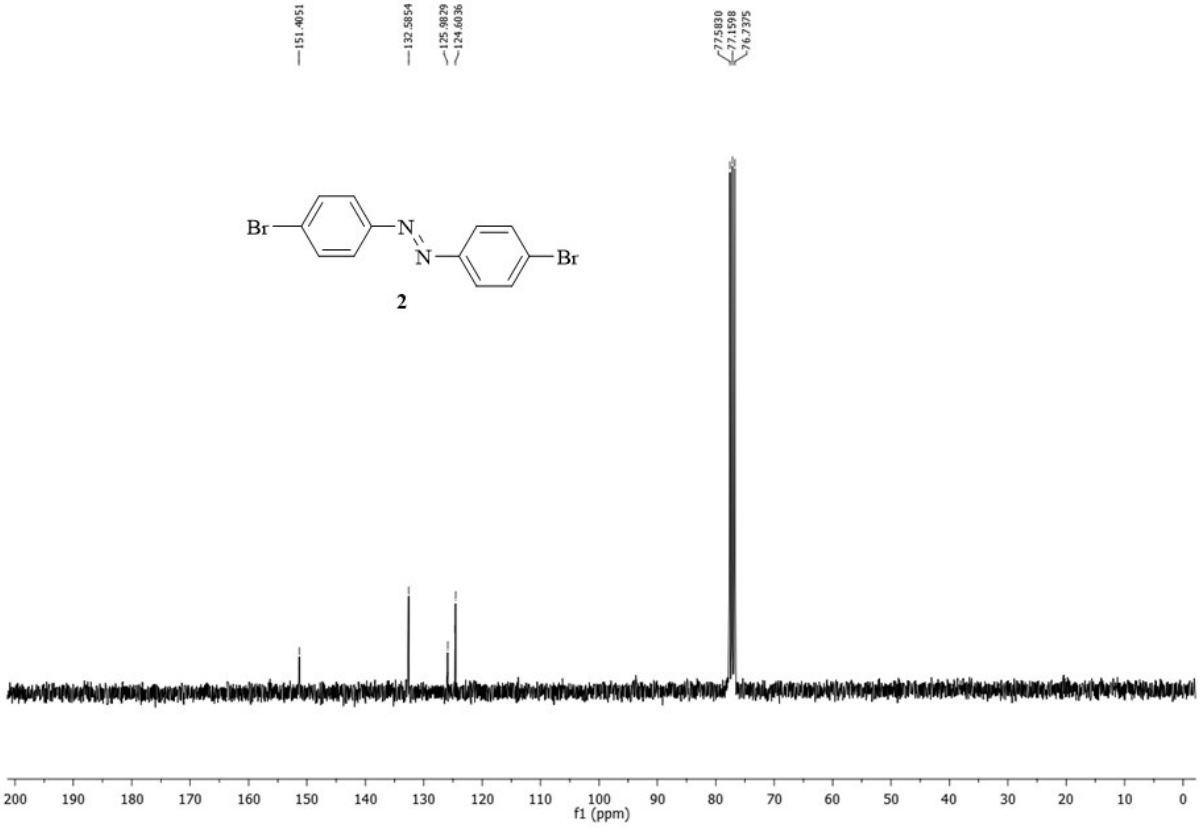


Fig. S10 ^{13}C NMR Spectrum of Compound **2**.

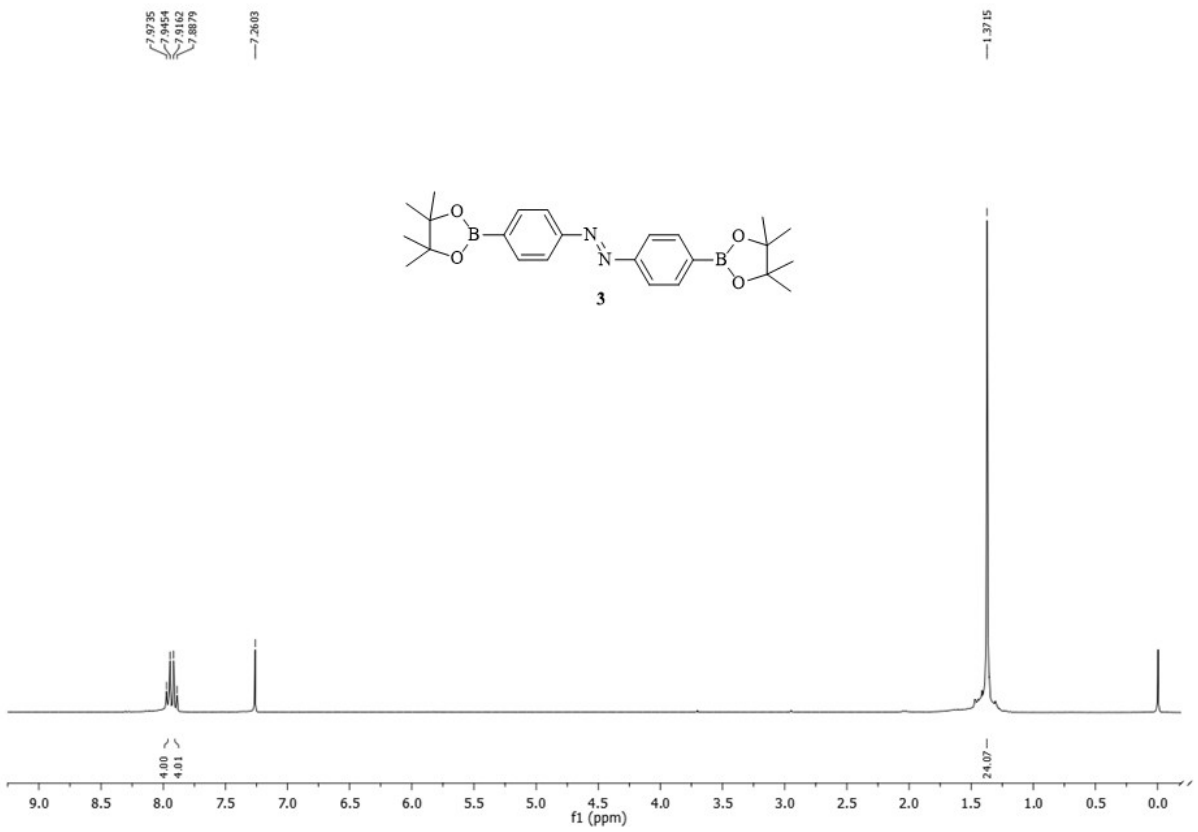


Fig. S11 ^{1}H NMR Spectrum of Compound **3**.

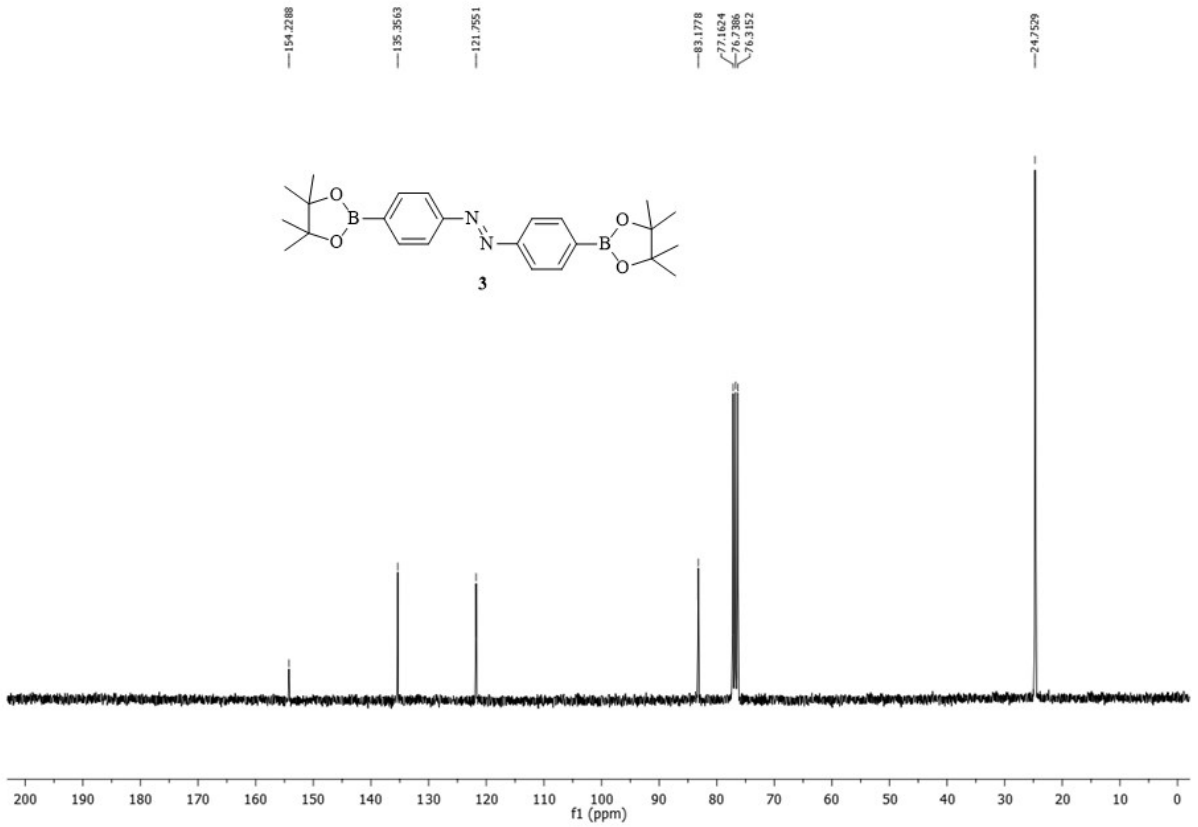


Fig. S12 ^{13}C NMR Spectrum of Compound **3**.

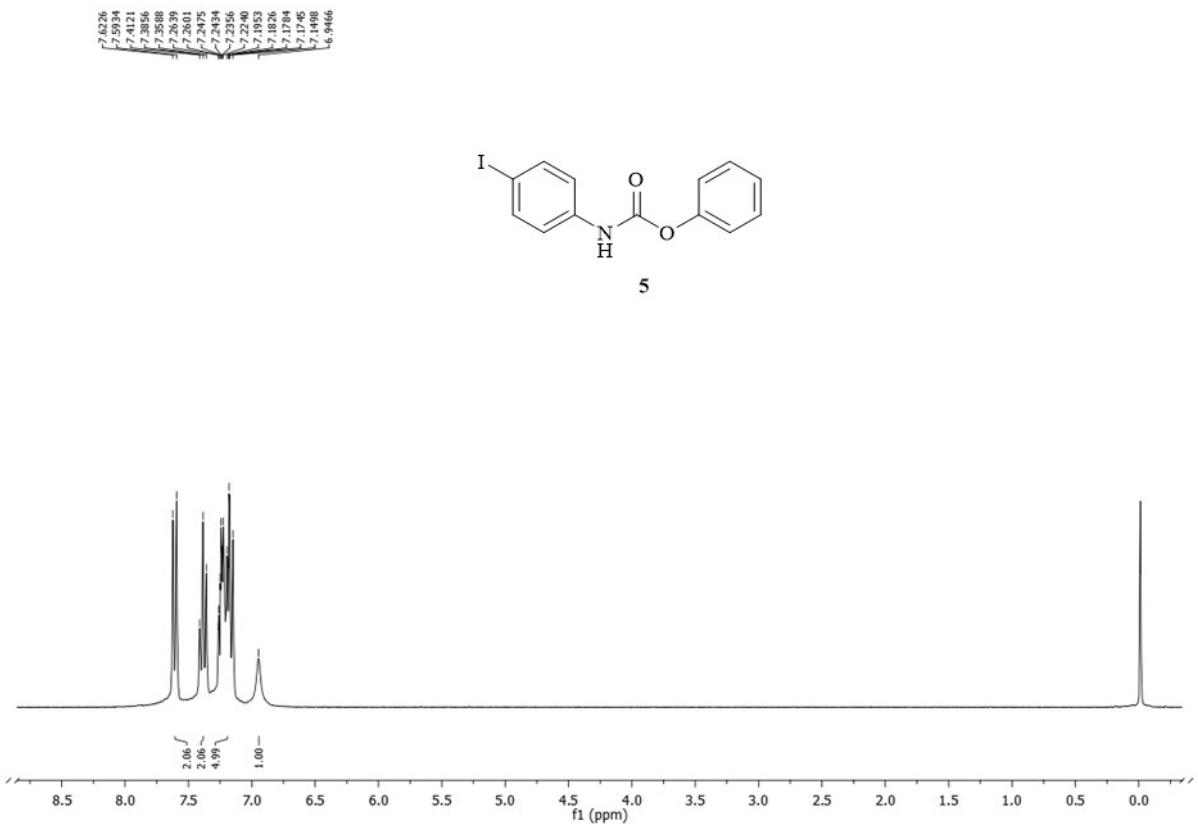


Fig. S13 ^{1}H NMR Spectrum of Compound **5**.

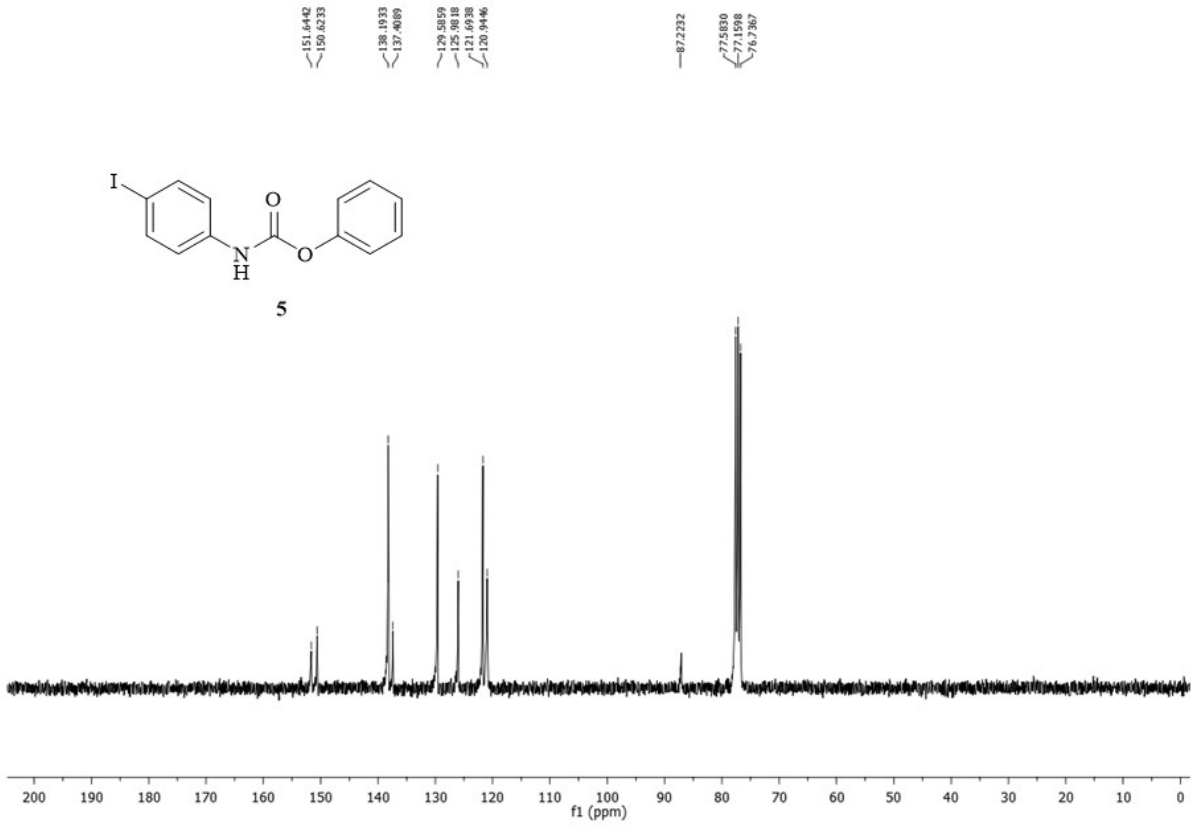


Fig. S14 ^{13}C NMR Spectrum of Compound **5**.

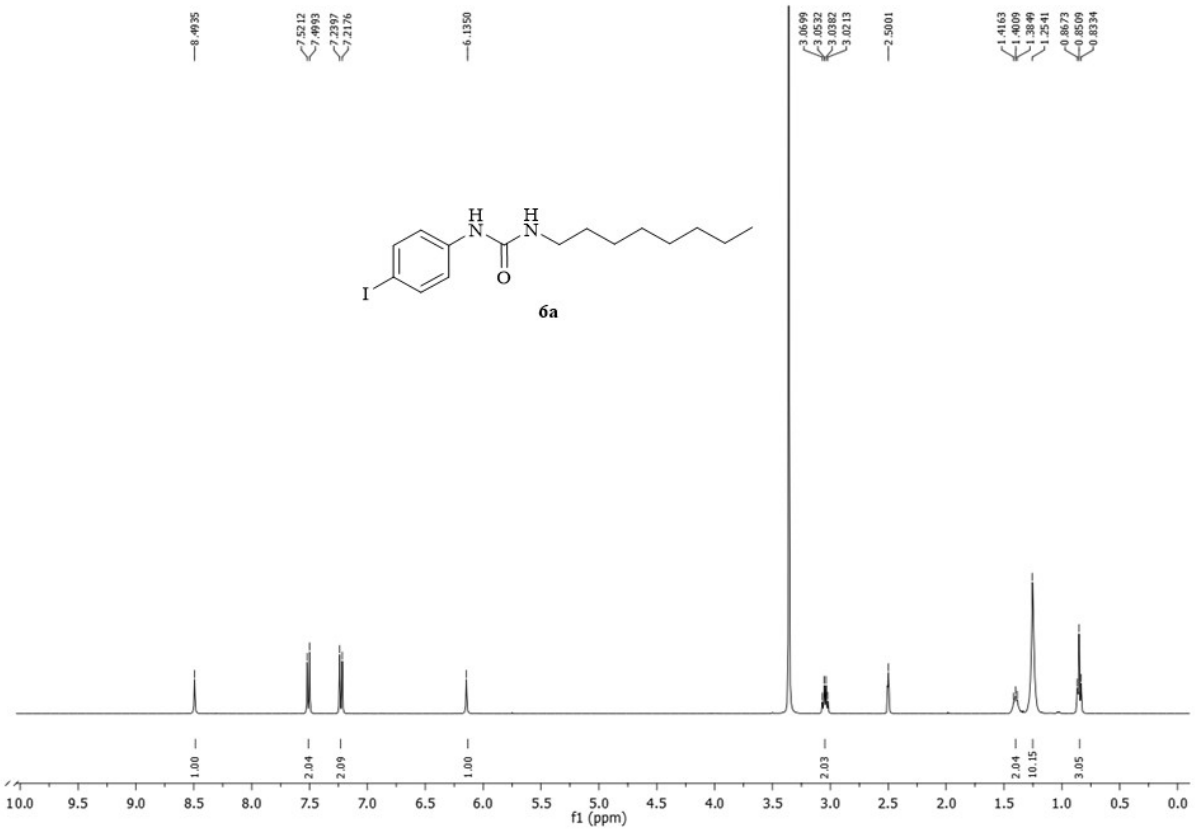


Fig. S15 [1]H NMR Spectrum of Compound **6a**.

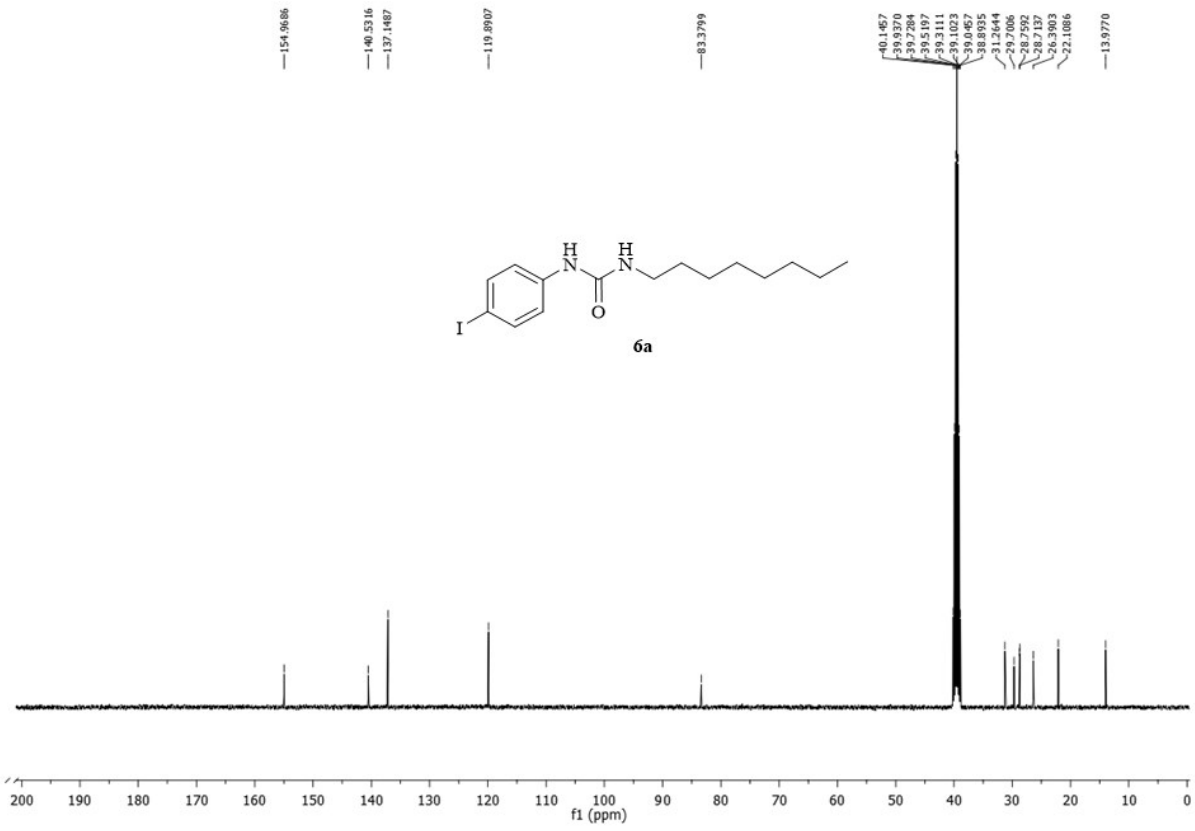


Fig. S16 [13]C NMR Spectrum of Compound **6a**.

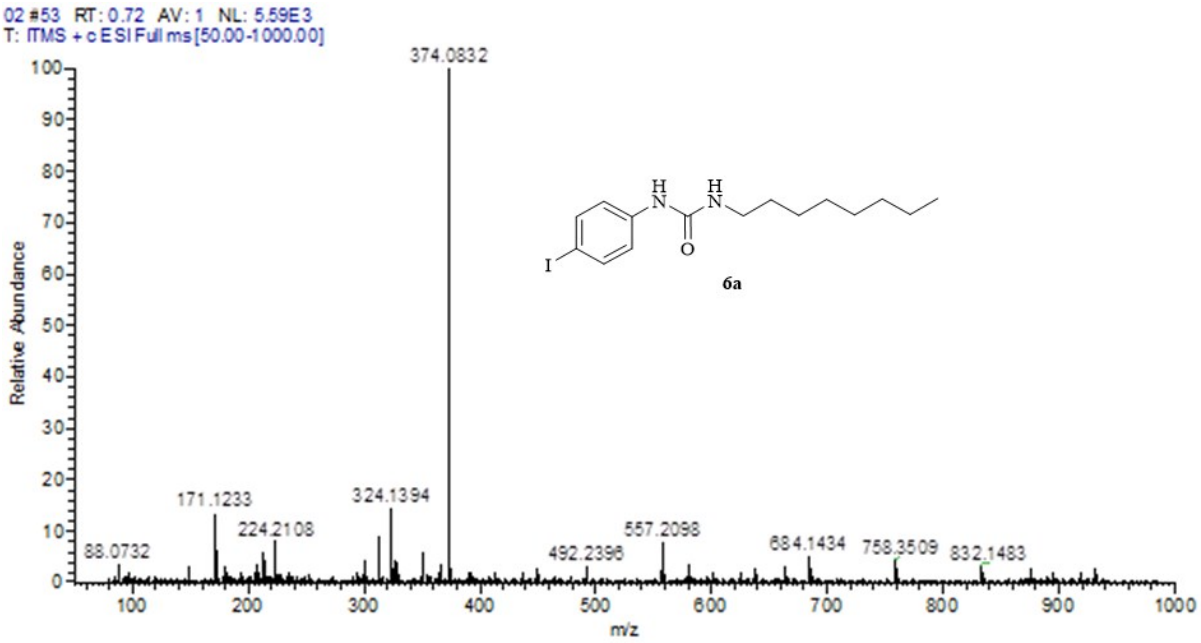


Fig. S17 ESI - Mass Spectrum of Compound **6a**.

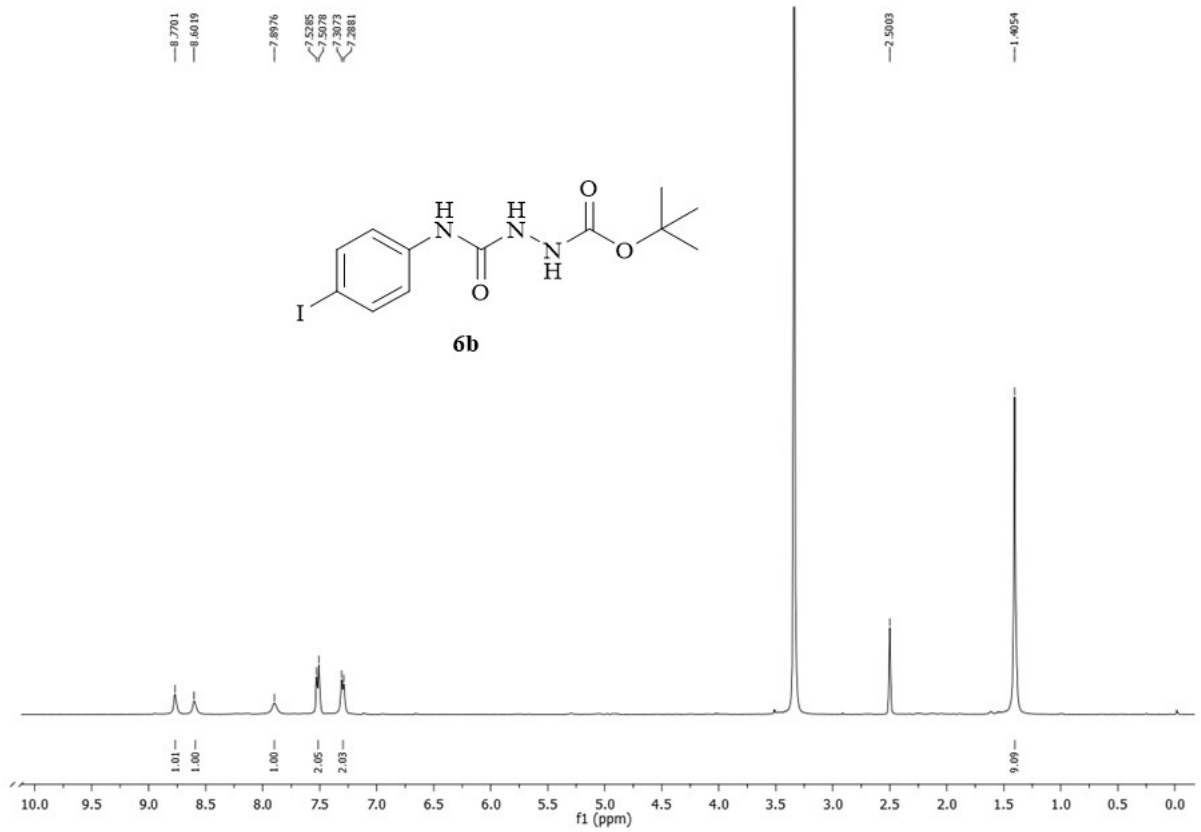


Fig. S18 [1]H NMR Spectrum of Compound **6b**.

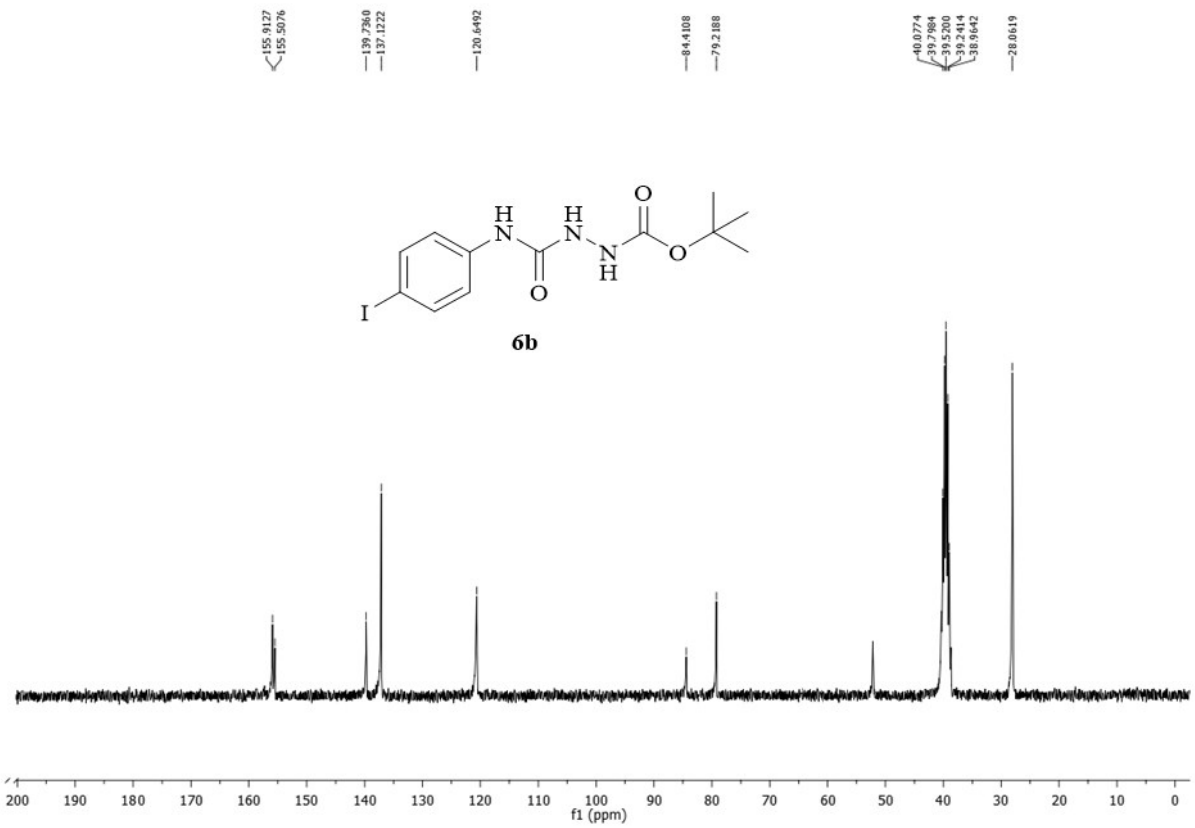


Fig. S19 ^{13}C NMR Spectrum of Compound **6b**.

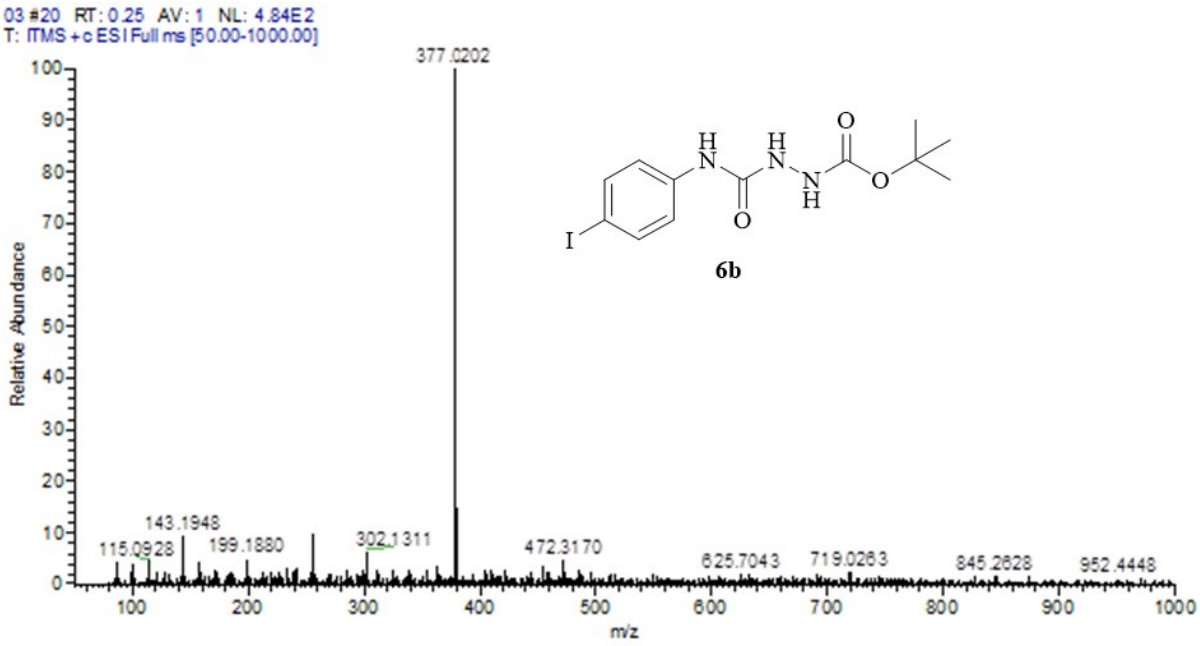


Fig. S20 ESI - Mass Spectrum of Compound **6b**.

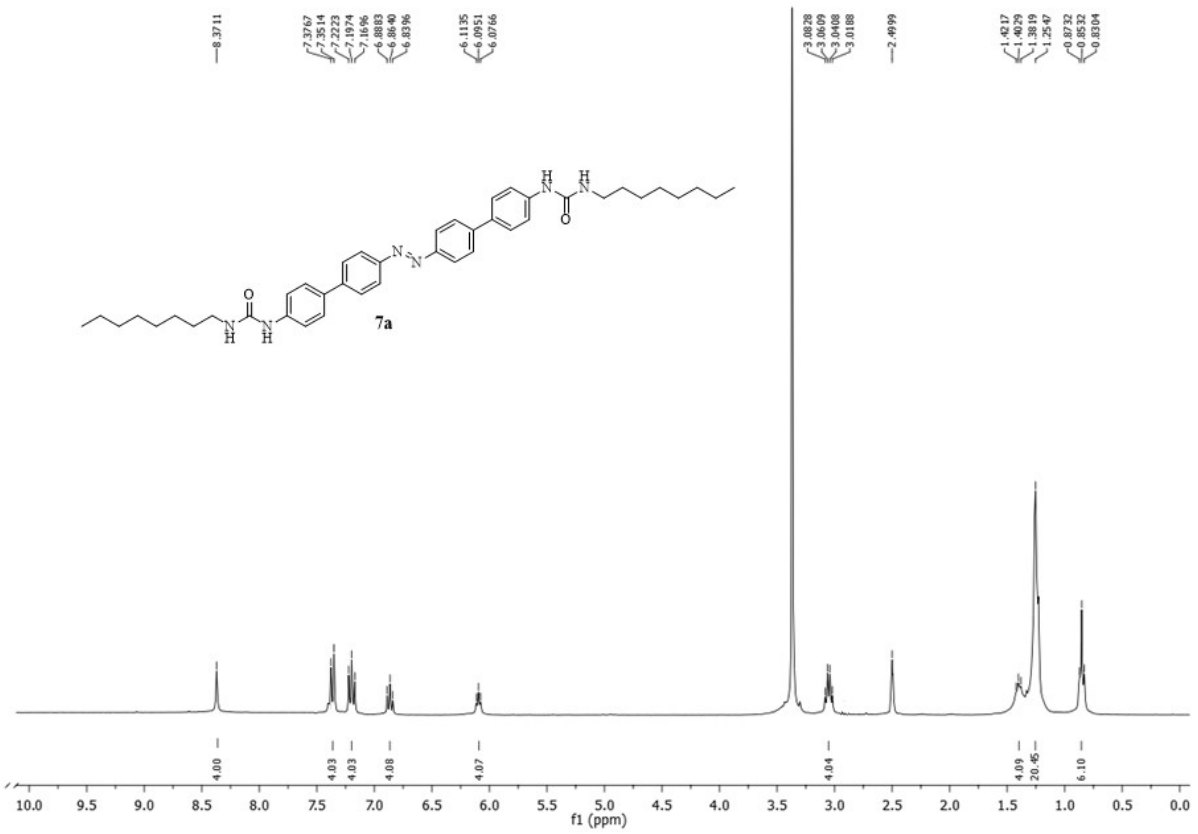


Fig. S21 ^{1}H NMR Spectrum of Compound **7a**.

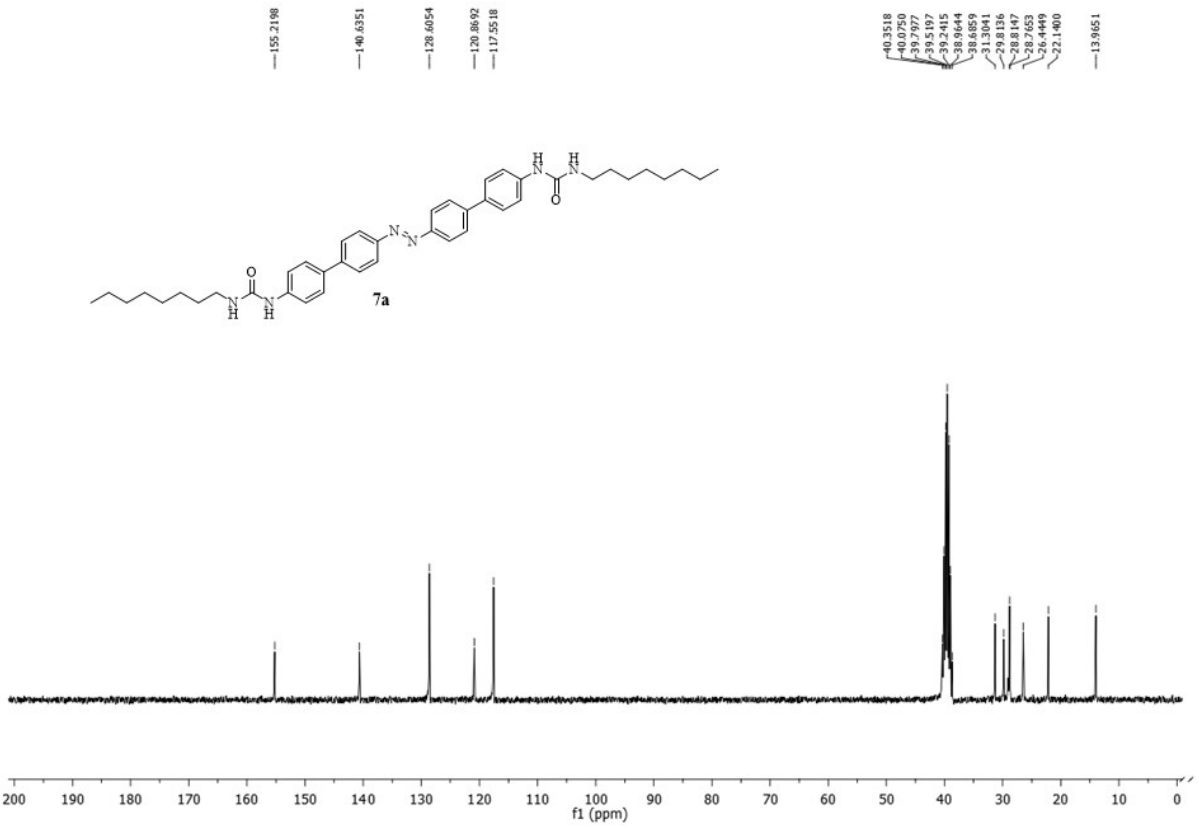


Fig. S22 ^{13}C NMR Spectrum of Compound **7a**.

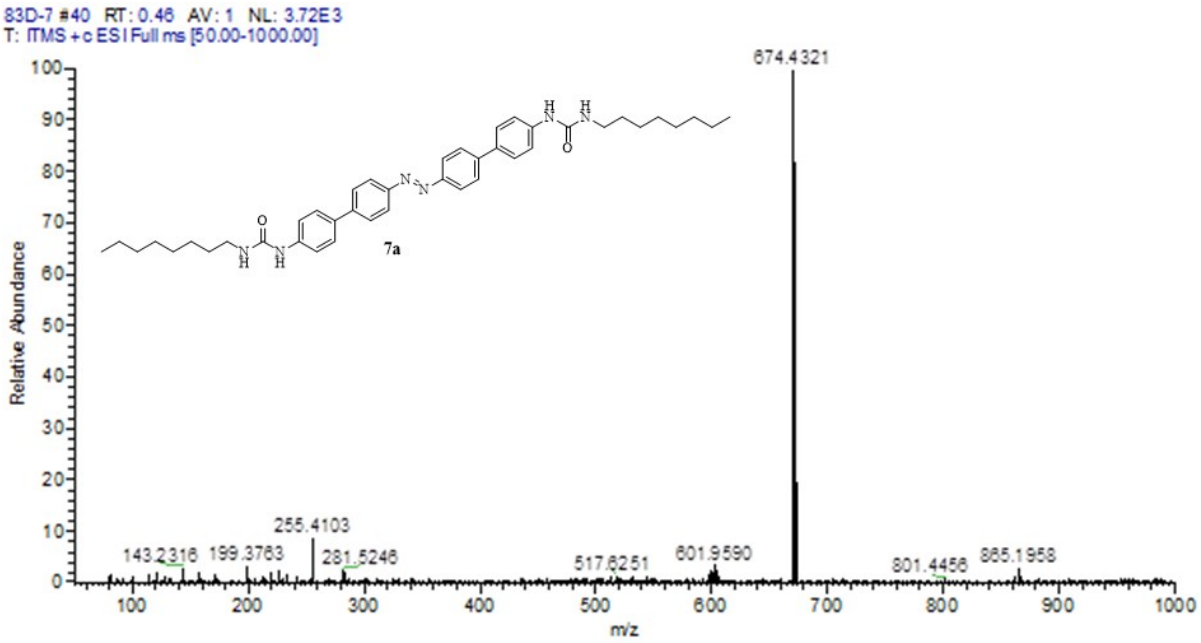


Fig. S23 ESI - Mass Spectrum of Compound **7a**.

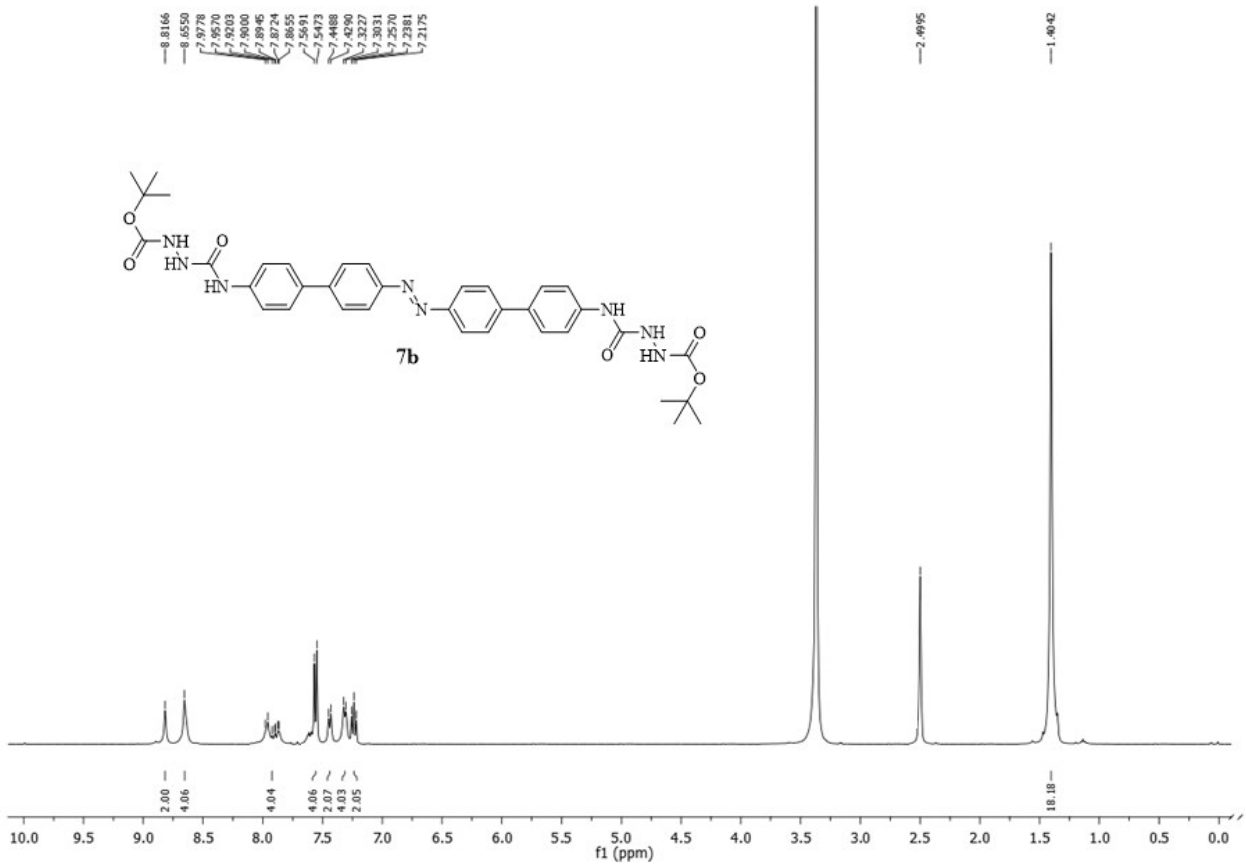


Fig. S24 ^{1}H NMR Spectrum of Compound **7b**.

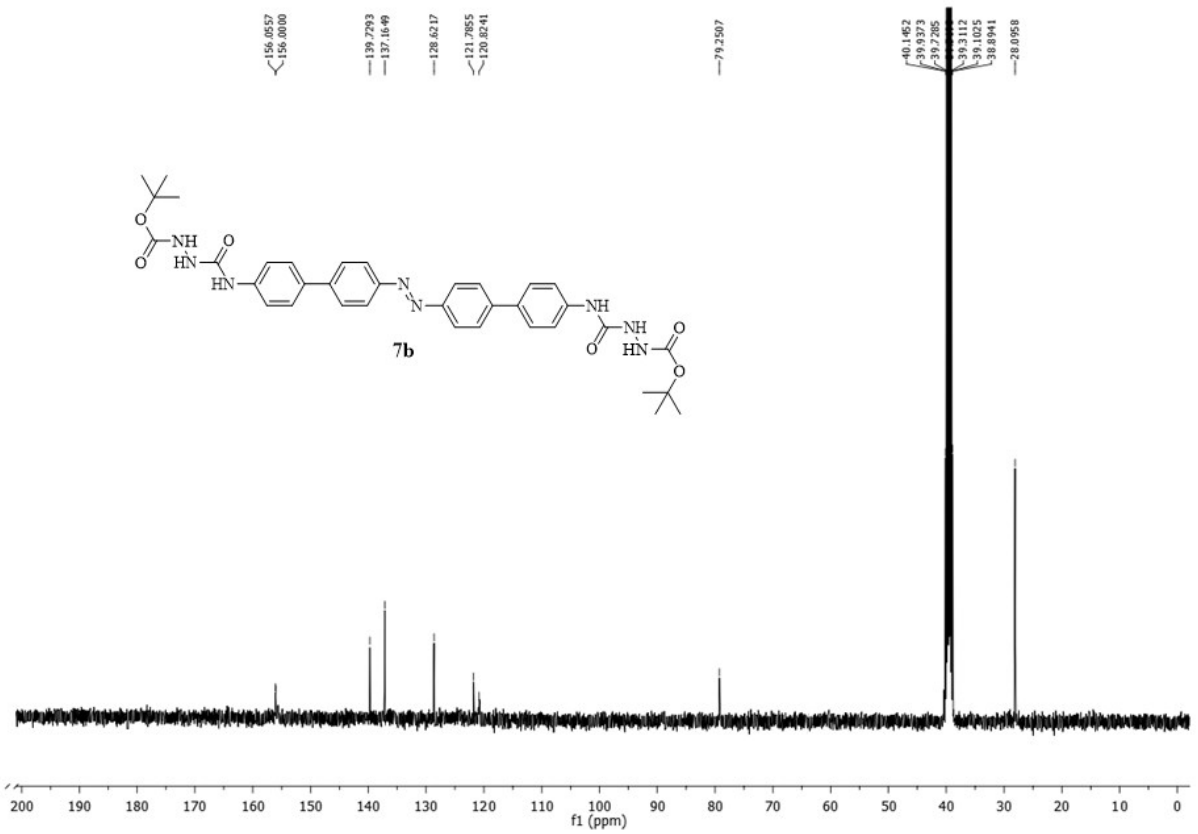


Fig. S25 ^{13}C NMR Spectrum of Compound **7b**.

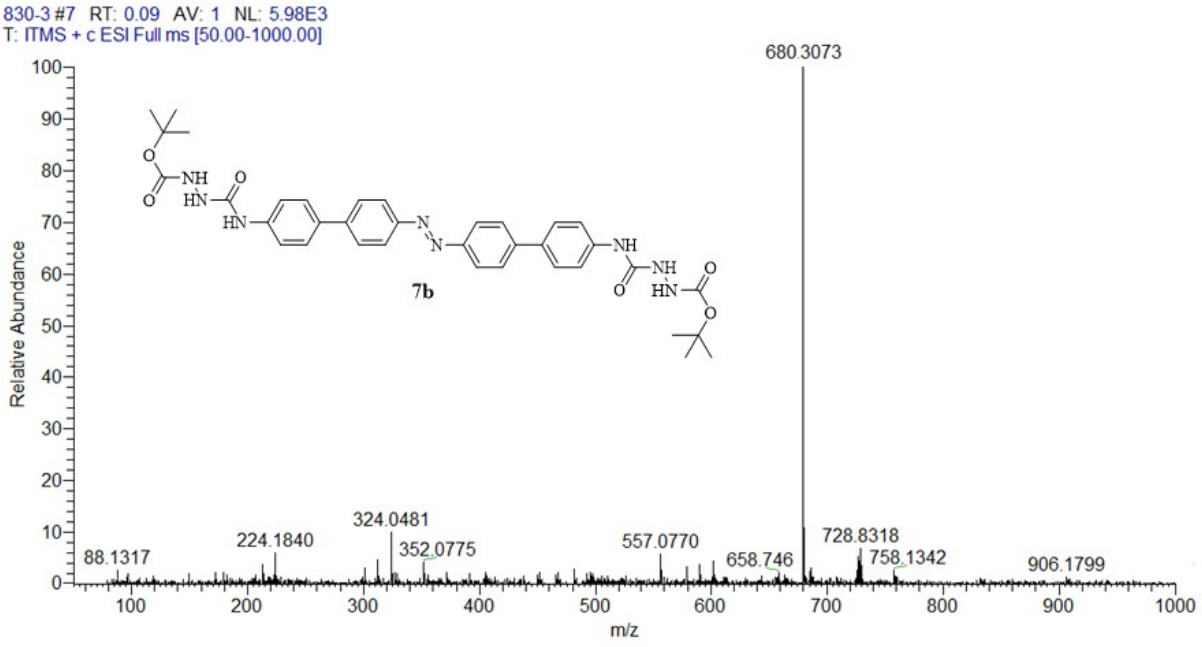


Fig. S26 ESI - Mass Spectrum of Compound **7b**.