Supporting information

Novel helix-shape bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazines: synthesis, optical and charge-transfer properties

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1. General information

Synthesis of 3,6-dihydrazino-1,2,4,5-tetrazine (**1**) has been previously described.[1]

All reagents and solvents were obtained from commercial sources and used without further purification. All new compounds were characterized by standard analytic methods. ^{1}H, ^{13}C, ^{19}F NMR spectra were acquired on DRX-400 and Avance 500 instruments (Bruker BioSpin), using DMSO-d_6 as solvent. The internal standard was $SiMe_4$ (for ^{1}H and ^{13}C NMR spectra) and C_6F_6 (for ^{19}F NMR spectra). ^{15}N NMR spectra were measured on Avance II 400 instrument (Bruker BioSpin), using DMSO-d_6 as solvent, the external standard was NH_3.

The HRMS analysis was performed using a LC-MS/MS Q-TOF system (Bruker maXis impact HD Q-TOF with Agilent 1260 series LC).

Elemental analysis was performed on a PerkinElmer PE 2400 elemental analyzer.

Melting points were determined in open capillaries on a Stuart SMP3 apparatus (uncorrected).

UV–vis spectra were recorded for 10^{-6} M MeCN solutions with a Shimadzu UV-2600 spectrophotometer. UV/vis and fluorescence spectra were recorded using standard 1 cm quartz cells at room temperature. The luminescence and excitation spectra were recorded using a Varian CaryEclipse spectrometer (USA). Excitation was performed at maximun of the more energetic absorption band.

Cyclic voltammetry was carried out on a Metrohm Autolab PGSTAT302N potentiostat with a standard three-electrode configuration. Typically, a three-electrode cell equipped with a platinum disk working electrode (3 mm), a glass carbon disk counter electrode (3 mm), and an $Ag/AgNO_3$ (0.01 M) reference electrode was used. Measurements were made in dry MeCN with tetrabutylammonium tetrafluoroborate (0.1 M) as the supporting electrolyte under an argon atmosphere at a scan rate of 100 mV/s. The potential of reference electrode was calibrated by using the ferrocene/ferrocenium redox couple (Fc/Fc^+). The redox potential ($E_{1/2}$) of Fc/Fc^+ against this reference electrode was +125 mV.)

The carrier mobility was determined by the MIS-CELIV method using sandwich-type samples prepared as follows. A glassy substrate was coated with an ITO (mixture of In_2O_3 and SnO_2) conductive layer and then with a 70-nm SiO_2 layer. Then, it was successively coated with a layer of the compound under study (layer thickness d = 100 nm) and with an Al layer (d = 80 nm) as a counter electrode. The SiO_2 insulating layer played the role of the blocking layer for both types of charge carriers, i.e., it precluded injection of the charge carriers from ITO. When measuring the transient hole current, a positive potential linearly increasing at a rate of $A = 5 \cdot 10^4$ V/s was applied to ITO; this was accompanied by the extraction of holes at the Al electrode. To measure the electron mobility, the polarity of the potential applied to the electrode was reversed.

The characteristic time (t_{max}) corresponding to the maximum transient conduction current was determined using the current signal detected at the load resistor of a DL-Analog Discovery (Digilent Co.) oscilloscope. The carrier mobility was calculated using the expression $\mu = 2d^2/(At^2_{max})$.[2]

DFT calculations were performed using the Orca 5.0.3 program.[3] The ground-state geometry optimizations were performed at the B3LYP/6-311G* and PBE0/def2-TZVP level of theory in the gas phase. Frequency analyses were carried out at the same theoretical level to ensure that the optimized geometries correspond to a local minimum on the potential energy surface; all compounds were characterized by only real vibrational frequencies. The absorption spectra were calculated by TDDFT at the same theoretical level in MeCN using the SMD solvation model.[4]

X-Ray structural analyses were accomplished on an Xcalibur S four-circle automated diffractometer with CCD detector. Analysis was carried out on standard procedure (graphite monochromated MoK-irradiation, T= 295(2) K, ω-scanning with 1o steps). Solution and refinement of structure was accomplished with using SHELXL-2018/3 program package[5,6] on full-matrix least-squares method on F2, in anisotropic approximation for non-hydrogen atoms. H-atoms are placed in calculated positions and refined in isotropic approximation in "riding" model.

2. Chemistry

2.1 General procedure for the synthesis of hydrazones 2a-p.

A solution of corresponding aldehyde (2.1 mmol) in 8 ml of EtOH was added to a stirred solution of 3,6-dihydrazino-1,2,4,5-tetrazine (**1**) (1.0 mmol, 142 mg) in 8 ml of acetic acid. The reaction mixture was stirring for 24 hours at ambient temperature, the formed precipitate was filtered off and washed first with water, and then with acetonitrile (**2a-c,f,g,j,p**), ethanol (**2d,h,i,k-m**) or dimethylformamide (**2e,n,o**). An extremely low solubility of products **2** led to difficulties in recording ^{13}C NMR spectra for some of these compounds.

3,6-Bis(2-benzylidenehydrazinyl)-1,2,4,5-tetrazine (2a).

Dark violet solid, 252 mg (79%), m.p. 250-251 °C; ^1H NMR (DMSO-d_6, 400 MHz): δ/ppm 7.39 (tt, $^3J_{HH}$ = 7.2 Hz, $^4J_{HH}$ = 1.3 Hz, 2H, 2C(4)H, 2Ph), 7.45 (ddd, $^3J^1_{HH}$ = 7.6, $^3J^2_{HH}$ = 7.2 Hz, $^4J_{HH}$ = 1.4 Hz, 4H, 2C(3)H, 2C(5)H, 2Ph), 7.71 (dd, $^3J_{HH}$ = 7.6 Hz, $^4J_{HH}$ = 1.3 Hz, 4H, 2C(2)H, 2C(6)H, 2Ph), 8.23 (s, 2H, 2CH=N), 11.89 (s, 2H, 2NH). Anal. Calcd for $C_{16}H_{14}N_8$: C, 60.37; H, 4.43; N, 35.20; Found C, 59.89; H, 4.26; N, 35.25.

3,6-Bis(2-(perfuorobenzylidene)hydrazinyl)-1,2,4,5-tetrazine (2b).

Dark violet solid, 389 mg (78%), m.p. 262-263 °C; ^{1}H NMR (DMSO-d_6, 400MHz): δ/ppm 8.28 (s, 2H, 2CH=N), 12.33 (br.s, 2H, 2NH). Anal. Calcd for $C_{16}H_4F_{10}N_8$: C, 38.57; H, 0.81; N, 22.49; Found C, 38.66; H, 0.84; N, 22.61.

3,6-Bis(2-(4-fuorobenzylidene)hydrazinyl)-1,2,4,5-tetrazine (2c).

Dark violet solid, 337 mg (95%), m.p. 293-294 °C; ^{1}H NMR (DMSO-d_6, 500MHz): δ/ppm 7.29 (dd, $^{3}J_{HH} = {}^{3}J_{HF}$ = 8.8 Hz, 4H, 2Ar), 7.76 (dd, $^{3}J_{HH}$ = 8.8 Hz, $^{4}J_{HF}$ = 5.6 Hz, 4H, 2Ar), 8.22 (s, 2H, 2CH=N), 11.90 (s, 2H, 2NH). Anal. Calcd for $C_{16}H_{12}F_2N_8$: C, 54.24; H, 3.41; N, 31.63; Found C, 53.95; H, 3.49; N, 31.71.

3,6-Bis(2-(4-chlorobenzylidene)hydrazinyl)-1,2,4,5-tetrazine (2d).

Dark violet solid, 337 mg (87%), m.p. >265 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 7.51 (d, $^{3}J_{HH}$ = 8.5 Hz, 4H, 2Ar), 7.73 (d, $^{3}J_{HH}$ = 8.5 Hz, 4H, 2Ar), 8.22 (s, 2H, 2CH=N), 11.99 (s, 2H, 2NH). Anal. Calcd for $C_{16}H_{12}Cl_2N_8$: C, 49.63; H, 3.12; N, 28.94; Found C, 49.71; H, 3.18; N, 29.23.

3,6-Bis(2-(4-bromobenzylidene)hydrazinyl)-1,2,4,5-tetrazine (2e).

Dark violet solid, 429 mg (90%), m.p. 239-241 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ/ppm 7.64 (d, $^{3}J_{HH}$ = 9.0 Hz, 4H, 2Ar), 7.67 (d, $^{3}J_{HH}$ = 9.0 Hz, 4H, 2Ar), 8.20 (s, 2H, 2-CH=N), 12.00 (s, 2H, 2NH). Anal. Calcd for $C_{16}H_{12}Br_2N_8$: C, 40.36; H, 2.54; N, 23.53; Found C, 40.21; H, 2.47; N, 23.67.

3,6-Bis(2-(4-nitrobenzylidene)hydrazinyl)-1,2,4,5-tetrazine (2f).

Dark violet solid, 351 mg (86%), m.p. > 265 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 7.97 (d, $^{3}J_{HH}$ = 8.5 Hz, 4H, 2Ar), 8.30 (d, $^{3}J_{HH}$ = 8.5 Hz, 4H, 2Ar), 8.34 (s, 2H, 2CH=N), 12.38 (s, 2H, 2NH). Anal. Calcd for $C_{16}H_{12}N_{10}O_4$: C, 47.06; H, 2.96; N, 34.30; Found C, 47.06; H, 3.05; N, 34.32.

3,6-Bis(2-(but-2-en-1-ylidene)hydrazinyl)-1,2,4,5-tetrazine (2g).

Dark violet solid, 207 mg (84%), m.p. 271-272 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 1.85 (dd, $^{3}J_{HH}$ = 6.8 Hz, $^{4}J_{HH}$ = 1.4 Hz, 6H, 2CH_3), 6.10 (dq, $^{3}J^{1}_{HH}$ = 15.4 Hz, $^{3}J^{2}_{HH}$ = 6.8 Hz, 2H, 2CH_3<u>CH</u>=CH), 6.25 (ddq, $^{3}J^{1}_{HH}$ = 15.4 Hz, $^{3}J^{2}_{HH}$ = 9.3 Hz, $^{4}J_{HH}$ = 1.4 Hz, 2H, 2CH_3CH=<u>CH</u>), 7.82 (d, $^{3}J^{2}_{HH}$ = 9.3 Hz, 2H, 2CH=N), 11.46 (s, 2H, 2NH); ^{13}C NMR (DMSO-d_6, 125MHz): δ/ppm 18.3, 128.9, 135.5, 145.8, 159.7. Anal. Calcd for $C_{10}H_{14}N_8$: C, 48.77; H, 5.73; N, 45.50; Found C, 48.75; H, 5.91; N, 45.31.

3,6-Bis(2-(4-acetamidobenzylidene)hydrazinyl)-1,2,4,5-tetrazine (2h).

Dark violet solid, 368 mg (85%), m.p. 281-282 °C; ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 2.06 (s, 6H, 2CH_3), 7.62 (d, $^{3}J_{HH}$ = 8.7 Hz, 4H, 2Ar), 7.66 (d, $^{3}J_{HH}$ = 8.7 Hz, 4H, 2Ar), 8.16 (s, 2H, 2CH=N), 10.10 (s, 2H, 2NHCO), 11.76 (s, 2H, 2NH); ^{13}C NMR (DMSO-d_6, 125MHz): δ/ppm 24.1, 118.9, 127.0, 129.4, 140.3, 143.1, 159.9, 168.4. Anal. Calcd for $C_{20}H_{20}N_{10}O_2$: C, 55.55; H, 4.66; N, 32.39; Found C, 55.42; H, 4.80; N, 32.46.

3,6-Bis(2-(4-isopropylbenzylidene)hydrazinyl)-1,2,4,5-tetrazine (2i).

Dark violet solid, 290 mg (72%), m.p. 283-285 °C; ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 1.22 (d, $^{3}J_{HH}$ = 6.9 Hz, 12H, 2 CH($\underline{CH_3}$)$_2$), 2.92 (hept, $^{3}J_{HH}$ = 6.9 Hz, 2H, 2 $\underline{CH}$(CH_3)$_2$), 7.32 (d, $^{3}J_{HH}$ = 8.2 Hz, 4H, 2Ar), 7.63 (d, $^{3}J_{HH}$ = 8.2 Hz, 4H, 2Ar), 8.20 (s, 2H, 2CH=N), 11.79 (s, 2H, 2NH); ^{13}C NMR (DMSO-d_6, 125MHz): δ/ppm 23.7, 33.3, 126.5, 126.7, 132.5, 143.3, 149.8, 159.9. Anal. Calcd for $C_{22}H_{26}N_8$: C, 65.65; H, 6.51; N, 27.84; Found C, 65.44; H, 6.79; N, 28.06.

3,6-Bis(2-(4-methoxybenzylidene)hydrazinyl)-1,2,4,5-tetrazine (2j).

Dark violet solid, 330 mg (87%), m.p. 262-263 °C; ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 3.81 (s, 6H, 2OCH_3), 7.01 (d, $^{3}J_{HH}$ = 8.8 Hz, 4H, 2Ar), 7.64 (d, $^{3}J_{HH}$ = 8.8 Hz, 4H, 2Ar), 8.17 (s, 2H, 2CH=N), 11.70 (s, 2H, 2NH). Anal. Calcd for $C_{18}H_{18}N_8O_2$: C, 57.14; H, 4.79; N, 29.61; Found C, 56.79; H, 4.75; N, 29.94.

3,6-Bis(2-(3-methoxybenzylidene)hydrazinyl)-1,2,4,5-tetrazine (2k).

Dark violet solid, 247 mg (65%), m.p. 214 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 3.81 (s, 6H, 2OCH_3), 6.96 – 6.98 (m, 2H, 2Ar), 7.26-7.28 (m, 4H, 2Ar), 7.34-7.38 (m, 2H, 2Ar), 8.20 (s, 2H, 2CH=N), 11.90 (s, 2H, 2NH). Anal. Calcd for $C_{18}H_{18}N_8O_2$: C, 57.14; H, 4.79; N, 29.61; Found C, 56.84; H, 4.77; N, 30.06.

3,6-Bis(2-(2,3-dimethoxybenzylidene)hydrazinyl)-1,2,4,5-tetrazine (2l).

Dark red solid, 418 mg (95%), m.p. 226-228 °C; ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 3.79 (s, 6H, 2OCH_3), 3.84 (s, 6H, 2OCH_3), 7.06-7.08 (m, 2H, 2Ar), 7.13-7.15 (m, 2H, 2Ar), 7.47-7.49 (m, 2H, 2Ar), 8.51 (s, 2H, 2CH=N), 11.87 (s, 2H, 2NH); ^{13}C NMR (DMSO-d_6, 125MHz): δ/ppm 55.7, 61.1, 113.4, 116.7, 124.3, 128.2, 138.9, 147.3, 152.7, 159.9. Anal. Calcd for $C_{20}H_{22}N_8O_4$: C, 54.79; H, 5.06; N, 25.56; Found C, 54.71; H, 5.07; N, 25.69.

3,6-Bis(2-(4-hydroxy-3,5-dimethoxybenzylidene)hydrazinyl)-1,2,4,5-tetrazine (2m).

Brown solid, 406 mg (86%), m.p. 240 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 3.82 (s, 12H, 4OCH_3), 6.96 (s, 4H, 2Ar), 8.11 (s, 2H, 2CH=N), 8.79 (s, 2H, 2OH), 11.68 (s, 2H,

2NH); ^{13}C NMR (DMSO-d_6, 125MHz): δ/ppm 56.0, 104.0, 125.1, 137.2, 144.0, 148.1, 159.8. Anal. Calcd for $C_{20}H_{22}N_8O_6$: C, 51.06; H, 4.71; N, 23.82; Found C, 50.88; H, 4.81; N, 23.86.

3,6-Bis(2-(9H-fluoren-2-ylmethylidene)hydrazinyl)-1,2,4,5-tetrazine (2n).

Dark violet solid, 317 mg (64%), m.p. 303-305 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ/ppm 4.00 (s, 4H, 2CH_2), 7.33-7.37 (m, 2H, 2Ar), 7.40-7.44 (m, 2H, 2Ar), 7.61-7.64 (m, 2H, 2Ar), 7.71-7.74 (m, 2H, 2Ar), 7.93-7.99 (m, 6H, 2Ar), 8.32 (s, 2H, 2CH=N), 11.91 (s, 2H, 2NH). Anal. Calcd for $C_{30}H_{22}N_8$: C, 72.86; H, 4.48; N, 22.66; Found C, 72.54; H, 4.49; N, 22.58.

3,6-Bis(2-(thiophen-2-ylmethylidene)hydrazinyl)-1,2,4,5-tetrazine (2o).

Dark violet solid, 295 mg (89%), m.p. 254-255 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ/ppm 7.12 (dd, $^3J^1_{HH}$ = 5.1 Hz, $^3J^2_{HH}$ =3.7 Hz, 2H, 2C(4)H in 2 thiophen-2-yls), 7.39 (dd, $^3J_{HH}$ = 3.7 Hz, $^4J_{HH}$ = 1.2 Hz, 2H, 2CH in 2 thiophen-2-yls), 7.61 (d, $^3J_{HH}$ = 5.1 Hz, 2H, 2CH in 2 thiophen-2-yls), 8.42 (s, 2H, 2CH=N), 11.85 (s, 2H, 2NH). Anal. Calcd for $C_{12}H_{10}N_8S_2$: C, 43.62; H, 3.05; N, 33.92; S, 19.41; Found C, 43.61; H, 3.09; N, 34.04; S, 19.52.

3,6-Bis(2-(thiophen-3-ylmethylidene)hydrazinyl)-1,2,4,5-tetrazine (2p).

Dark violet solid, 298 mg (90%), m.p. 247-248 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ/ppm 7.48 (dd, $^3J_{HH}$ = 5.0 Hz, $^4J_{HH}$ = 1.2 Hz, 2H, 2C(4)H in 2 thiophen-3-yls), 7.62 (dd, $^3J_{HH}$ = 5.0 Hz, $^4J_{HH}$ = 2.9 Hz, 2H, 2C(5)H in 2 thiophen-3-yls), 7.84 (dd, $^4J^1_{HH}$ = 2.9 Hz, $^4J^2_{HH}$ = 1.2 Hz, 2H, 2C(2)H in 2 thiophen-3-yls), 8.27 (s, 2H, 2CH=N), 11.72 (s, 2H, 2NH). Anal. Calcd for $C_{12}H_{10}N_8S_2$: C, 43.62; H, 3.05; N, 33.92; S, 19.41; Found C, 43.65; H, 3.01; N, 33.93 S, 19.28.

2.2 General procedure for the synthesis of bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazines 3a-l,n-p

An oxidizing agent (**Table S1**) was added to an 80°C solution of the starting hydrazine **2** (1.0 mmol) in portions of 0.5 mmol at intervals of 15 min with constant stirring. Then the reaction mixture was heated for another 30 minutes until the initial compound completely disappeared (control by TLC) and after that cooled to room temperature. The resulting precipitate (**3c,d,f,g,h,j,l**) was filtered off and washed with $CHCl_3$; if there was no precipitate, the reaction mixture was evaporated to dryness and the residue was washed with $CHCl_3$ (**3a,e,i,k,n**). Purification of compounds **3b,o,p** is described below.

Table S1. Reaction conditions for compound **3** synthesis

Starting compound	Product	Oxidizing agent (mmol)	Solvent (ml)
2a	**3a**	PIDA* (3.0 mmol)	MeCN / DMF (3:1) (20 ml)
2b	**3b**	PIDA (3.0 mmol)	MeCN (20 ml)
2c	**3c**	PIDA (3.0 mmol)	MeCN (20 ml)
2d	**3d**	PIDA (3.0 mmol)	MeCN (20 ml)
2e	**3e**	PIDA (3.0 mmol)	MeCN / DMF (3:1) (20 ml)
2f	**3f**	PIFA** (2.0 mmol)	MeCN (15 ml)
2g	**3g**	PIDA (3.0 mmol)	MeCN (20 ml)
2h	**3h**	PIDA (3.0 mmol)	MeCN / DMF (3:1) (20 ml)
2i	**3i**	PIDA (3.0 mmol)	MeCN (20 ml)
2j	**3j**	PIDA (5.0 mmol)	MeCN (20 ml)
2k	**3k**	PIDA (3.0 mmol)	MeCN / DMF (3:1) (20 ml)
2l	**3l**	PIDA (3.0 mmol)	MeCN (20 ml)
2m	**-**	PIDA (3.0 mmol)	MeCN (20 ml)
2n	**3n**	PIDA (5.0 mmol)	MeCN / DMF (3:1) (20 ml)
2o	**3o**	PIDA (5.0 mmol)	MeCN (15 ml),NMP*** (5 ml), AcOH (5 ml)
2p	**3p**	PIDA (3.0 mmol)	MeCN / DMF (3:1) (20 ml)

* (diacetoxyiodo)benzene; ** (bis(trifluoroacetoxy)iodo)benzene; *** *N*-methyl-2-pyrrolidone

1,8-Di(phenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3a).

Yellow solid, 160 mg (51%), m.p. 250 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 7.10 (dd, $^{3}J^{1}_{HH}$ = 7.7, $^{3}J^{2}_{HH}$ = 7.2 Hz, 4H, 2C(3)H, 2C(5)H, 2Ph), 7.21 (t, $^{3}J_{HH}$ = 7.7 Hz, 2H, 2C(4)H, 2Ph), 7.47 (d, $^{3}J_{HH}$ = 7.2 Hz, 4H, 2C(2)H, 2C(6)H, 2Ph); ^{13}C NMR (DMSO-d_6, 125MHz): δ/ppm 125.2, 128.5, 129.0, 131.2, 145.7, 151.2. Anal. Calcd for $C_{16}H_{10}N_8$: C, 61.14; H, 3.21; N, 35.65; Found C, 60.80; H, 3.20; N, 35.34. HRMS (APSI): Found *m/z* = 314.1034 (M^-). $C_{16}H_{10}N_8^-$. Calculated 314.1036 (M^-).

1,8-Di(perfluorophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3b).

The reaction mixture was evaporated to dryness and the product **3b** was purified by colomn chromatography using silica gel 60 (230-400 mesh) and EtOAc : C_6H_{14} (1:1) as eluent (R_f = 0.9).

Light yellow solid, 173 mg (35%), m.p. 225 °C (decomp.); ^{19}F NMR (DMSO-d_6, 471 MHz): δ/ppm 3.55-3.68 (m, 4F, 2C_6F_5), 17.63-17.73 (m, 2F, 2C_6F_5), 27.03-27.08 (m, 4F, 2C_6F_5); ^{13}C NMR (DMSO-d_6, 125MHz): δ/ppm 101.3 (tt, $^{2}J_{CF}$ = 17 Hz, $^{3}J_{CF}$ = 4 Hz), 137.2 (dddd, $^{1}J_{CF}$ = 252 Hz, $^{2}J^{1}_{CF}$ = $^{2}J^{2}_{CF}$ = 13 Hz, $^{3}J_{CF}$ = 5 Hz), 143.4 (dtt, $^{1}J_{CF}$ = 261 Hz, $^{2}J_{CF}$ = 13 Hz, $^{3}J_{CF}$ = 4 Hz), 144.9 (dddd, $^{1}J_{CF}$ = 256 Hz, $^{2}J_{CF}$ = 13 Hz, $^{3}J^{1}_{CF}$ = $^{3}J^{2}_{CF}$ = 4 Hz), 150.7. Anal. Calcd for $C_{16}F_{10}N_8$: C, 38.88; H, 0; N, 22.67; Found C, 38.80; H, 0; N, 22.48. HRMS (APSI): Found *m/z* = 494.0096 (M^-). $C_{16}F_{10}N_8^-$. Calculated 494.0092 (M^-).

1,8-Di(4-fluorophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3c).

Yellow solid, 166 mg (47%), m.p. >300 °C (decomp.); ^{1}H NMR (DMSO-d_6, 400MHz): δ/ppm 7.02 (dd, $^{3}J_{HH} = {}^{3}J_{HF}$ = 8.8 Hz, 4H, 2Ar), 7.55 (dd, $^{3}J_{HH}$ = 8.8 Hz, $^{4}J_{HF}$ = 5.3 Hz, 4H, 2Ar); ^{13}C NMR (DMSO-d_6, 125MHz): δ/ppm 115.9 (d, $^{2}J_{CF}$ = 23 Hz), 121.6 (d, $^{4}J_{CF}$ = 3 Hz), 132.1 (d, $^{3}J_{CF}$ = 10 Hz), 144.7, 151.1, 163.5 (d, $^{1}J_{CF}$ = 250 Hz); ^{15}N NMR (DMSO-d_6, 41 MHz): δ/ppm 172.8, 320.4, 325.6 414.2. Anal. Calcd for $C_{16}H_8F_2N_8$: C, 54.86; H, 2.30; N, 31.99; Found C, 54.81; H, 2.34; N, 32.08. HRMS (APSI): Found *m/z* = 350.0847 (M^-). $C_{16}H_8F_2N_8^-$. Calculated 350.0845 (M^-).

1,8-Di(4-chlorophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3d).

Yellow solid, 200 mg (52%), m.p. >265 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500MHz): δ/ppm 7.24 (d, $^{3}J_{HH}$ = 8.5 Hz, 4H, 2Ar), 7.49 (d, $^{3}J_{HH}$ = 8.5 Hz, 4H, 2Ar); ^{13}C NMR (DMSO-d_6, 125 MHz): δ/ppm 123.8, 128.8, 131.1, 136.8, 144.7, 151.1. Anal. Calcd for $C_{16}H_8Cl_2N_8$: C, 50.15; H, 2.10; N, 29.24; Found C, 49.88; H, 2.36; N, 28.97. HRMS (APSI): Found *m/z* = 382.0259 (M^-). $C_{16}H_8Cl_2N_8^-$. Calculated 382.0254 (M^-).

1,8-Di(4-bromophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3e).

Yellow solid, 236 mg (50%), m.p. >300 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ/ppm 7.40 (d, $^{3}J_{HH}$ = 9.0 Hz, 4H, 2Ar), 7.43 (d, $^{3}J_{HH}$ = 9.0 Hz, 4H, 2Ar); ^{13}C NMR (DMSO-d_6, 125 MHz): δ/ppm 124.1, 125.8, 131.1, 131.8, 144.8, 151.1. ^{15}N NMR (DMSO-d_6, 41 MHz): δ/ppm 172.6, 321.0, 326.3, 415.1. Anal. Calcd for $C_{16}H_8Br_2N_8$: C, 40.71; H, 1.71; N, 23.74; Found C, 40.77; H, 1.66; N, 23.53. HRMS (APSI): Found *m/z* = 469.9245 (M^-). $C_{16}H_8Br_2N_8^-$. Calculated 469.9244 (M^-).

1,8-Di(4-nitrophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3f).

Yellow solid, 183 mg (45%), m.p. > 280 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 7.79 (d, $^{3}J_{HH}$ = 8.5 Hz, 4H, 2Ar), 7.95 (d, $^{3}J_{HH}$ = 8.5 Hz, 4H, 2Ar); ^{13}C NMR (DMSO-d_6, 125 MHz): δ/ppm 123.7, 130.7, 131.2, 143.8, 148.4, 151.1. Anal. Calcd for $C_{16}H_8N_{10}O_4$: C, 47.53; H, 1.99; N, 34.64; Found C, 47.30; H, 1.76; N, 34.61. HRMS (APSI): Found *m/z* = 404.0737 (M^-). $C_{16}H_8N_{10}O_4^-$. Calculated 404.0735 (M^-).

1,8-Di(propen-1-yl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3g).

Yellow solid, 119 mg (49%), m.p. 290 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 2.08 (dd, $^{3}J_{HH}$ = 6.8 Hz, $^{4}J_{HH}$ = 1.7 Hz, 6H, $2CH_3$), 6.76 (dq, $^{3}J^{1}_{HH}$ = 15.6 Hz, $^{4}J_{HH}$ = 1.7 Hz, 2H, $2CH_3CH$=<u>CH</u>), 6.99 (dq, $^{3}J^{1}_{HH}$ = 15.6 Hz, $^{3}J^{2}_{HH}$ = 6.8 Hz, 2H, $2CH_3$<u>CH</u>=CH); ^{13}C NMR (DMSO-d_6, 125MHz): δ/ppm 18.9, 115.1, 141.4, 143.4, 150.1. Anal. Calcd for $C_{10}H_{10}N_8$: C, 49.58;

H, 4.16; N, 46.26; Found C, 49.59; H, 4.25; N, 46.41. HRMS (APSI): Found *m/z* = 242.1037 (M^-). $C_{10}H_{10}N_8^-$. Calculated 242.1034 (M^-).

1,8-Di(4-acetamidophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3h).

Yellow solid, 122 mg (28%), m.p. >300 °C; ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 2.04 (s, 6H, CH_3), 7.30 (d, $^3J_{HH}$ = 8.8 Hz, 4H, 2Ar), 7.34 (d, $^3J_{HH}$ = 8.8 Hz, 4H, 2Ar), 9.98 (s, 2H, 2NH); ^{13}C NMR (DMSO-d_6, 125MHz): δ/ppm 24.1, 118.2, 118.9, 129.8, 141.8, 145.8, 151.2, 168.4. Anal. Calcd for $C_{20}H_{16}N_{10}O_2$: C, 56.07; H, 3.76; N, 32.69; Found C, 55.93; H, 3.64; N, 32.41. HRMS (APSI): Found *m/z* = 428.1460 (M^-). $C_{20}H_{16}N_{10}O_2^-$. Calculated 428.1463 (M^-).

1,8-Di(4-isopropylphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3i).

Yellow solid, 211 mg (53%), m.p. 280-285 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 1.10 (d, $^3J_{HH}$ = 7.0 Hz, 12H, 2 CH($\underline{CH_3}$)$_2$), 2.74 (hept, $^3J_{HH}$ = 7.0 Hz, 2H, 2 $\underline{CH}$(CH_3)$_2$), 7.00 (d, $^3J_{HH}$ = 8.0 Hz, 4H, 2Ar), 7.41 (d, $^3J_{HH}$ = 8.0 Hz, 4H, 2Ar). ^{13}C NMR (DMSO-d_6, 126 MHz): δ/ppm 23.1, 33.0, 122.6, 126.4, 129.0, 145.8, 151.1, 151.4. Anal. Calcd for $C_{22}H_{22}N_8$: C, 66.31; H, 5.57; N, 28.12; Found C, 65.96; H, 5.75; N, 28.27. HRMS (APSI): Found *m/z* = 398.1979 (M^-). $C_{22}H_{22}N_8^-$. Calculated 398.1973 (M^-).

1,8-Di(4-methoxyphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3j).

Yellow solid, 147 mg (39%), m.p. 252-255 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 3.73 (s, 6H, 2OCH_3), 6.62-6.67 (m, 4H, 2Ar), 7.36-7.41 (m, 4H, 2Ar). ^{13}C NMR (DMSO-d_6, 126 MHz): δ/ppm 55.2, 114.1, 117.2, 130.9, 145.8, 151.2, 161.0. Anal. Calcd for $C_{18}H_{14}N_8O_2$: C, 57.75; H, 3.77; N, 29.93; Found C, 57.36; H, 3.66; N, 29.57. HRMS (APSI): Found *m/z* = 374.1251 (M^-). $C_{18}H_{14}N_8O_2^-$. Calculated 374.1245 (M^-).

1,8-Di(3-methoxyphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3k).

Yellow solid, 244 mg (65%), m.p. 250 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 3.66 (s, 6H, 2OCH_3), 6.75 – 6.80 (m, 2H, 2Ar), 6.94 (s, 2H, 2Ar), 7.10-7.17 (m, 4H, 2Ar); ^{13}C NMR (DMSO-d_6, 126 MHz): δ/ppm 55.0, 113.9, 117.1, 121.1, 126.4, 129.9, 145.5, 151.1, 158.4; ^{15}N NMR (DMSO-d_6, 41 MHz): δ/ppm 172.5, 320.0, 325.4, 413.9. Anal. Calcd for $C_{18}H_{14}N_8O_2$: C, 57.75; H, 3.77; N, 29.93; Found C, 57.56; H, 3.76; N, 29.87. HRMS (APSI): Found *m/z* = 374.1249 (M^-). $C_{18}H_{14}N_8O_2^-$. Calculated 374.1245 (M^-).

1,8-Di(2,3-dimethoxyphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3l).

Dark yellow solid, 169 mg (39%), m.p. 310-315 °C (decomp.);

A: ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 3.37 (s, 6H, 2OCH$_3$), 3.69 (s, 6H, 2OCH$_3$), 6.87-6.89 (m, 2H, 2Ar), 6.96-7.01 (m, 4H, 2Ar); ^{13}C NMR (DMSO-d_6, 125MHz): δ/ppm 55.5, 60.9, 116.0, 120.0, 121.9, 123.7, 143.2, 146.5, 150.4, 150.9.

B: ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 3.62 (s, 6H, 2OCH$_3$), 3.75 (s, 6H, 2OCH$_3$), 6.73-6.76 (m, 2H, 2Ar), 6.83-6.85 (m, 2H, 2Ar), 6.87-6.89 (m, 2H, 2Ar); ^{13}C NMR (DMSO-d_6, 125MHz): δ/ppm 55.6, 60.8, 116.0, 119.9, 122.1, 123.4, 143.1, 146.6, 150.6, 151.4.

Anal. Calcd for $C_{20}H_{18}N_8O_4$: C, 55.30; H, 4.18; N, 25.79; Found C, 55.09; H, 4.11; N, 25.65. HRMS (APSI): Found *m/z* = 434.1463 (M^-). $C_{20}H_{18}N_8O_4^-$. Calculated 434.1456 (M^-).

1,8-Di(9H-fluoren-2-yl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3n).

Yellow solid, 173 mg (35%), m.p. 350 °C (decomp.); ^{1}H NMR (DMSO-d_6, 400 MHz): δ/ppm 3.56 (s, 4H, 2CH$_2$), 6.99-7.03 (m, 2H, 2Ar), 7.13-7.21 (m, 4H, 2Ar), 7.32-7.35 (m, 2H, 2Ar), 7.46 (d, $^{3}J_{HH}$ = 7.9 Hz, 2H, 2Ar), 7.50-7.58 (m, 4H, 2Ar); ^{13}C NMR (DMSO-d_6, 126 MHz): δ/ppm 36.0, 119.5, 119.8, 122.9, 124.3, 125.4, 126.4, 127.3, 127.9, 139.1, 142.7, 142.9, 143.7, 146.1, 151.2. Anal. Calcd for $C_{30}H_{18}N_8$: C, 73.46; H, 3.70; N, 22.84; Found C, 73.13; H, 3.85; N, 22.52. HRMS (APSI): Found *m/z* = 490.1660 (M^-). $C_{30}H_{18}N_8^-$. Calculated 490.1660 (M^-).

1,8-Di(thiophen-2-yl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3o).

The reaction mixture was evaporated and the product **3o** was purified by colomn chromatography using silica gel 60 (230-400 mesh) and C_6H_6 : MeCN (1:1) as eluent (R_f = 0.8).

Orange solid, 30 mg (9%), m.p. 237-240 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 6.79 (dd, $^{3}J^{1}_{HH}$ = 5.0 Hz, $^{3}J^{2}_{HH}$ = 3.7 Hz, 2H, 2C(4)H in 2 thiophen-2-yls), 7.27 (dd, $^{3}J_{HH}$ = 3.7 Hz, $^{4}J_{HH}$ = 1.2 Hz, 2H, 2CH in 2 thiophen-2-yls), 7.72 (dd, $^{3}J_{HH}$ = 5.0 Hz, $^{4}J_{HH}$ = 1.2 Hz, 2H, 2CH in 2 thiophen-2-yls); ^{13}C NMR (DMSO-d_6, 126 MHz): δ/ppm 124.6, 128.4, 132.0, 132.5, 141.4, 151.2. Anal. Calcd for $C_{12}H_6N_8S_2$: C, 44.16; H, 1.85; N, 34.33; Found C, 43.92; H, 1.74; N, 34.21. HRMS (APCI): Found *m/z* = 326.0161 (M^-). $C_{12}H_6N_8S_2^-$. Calculated 326.0162 (M^-).

1,8-Di(thiophen-3-yl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (3p).

The reaction mixture was evaporated and the residue was washed with $CHCl_3$ and then recrystallized from MeCN.

Yellow solid, 131 mg (40%), m.p. 285-288 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 7.11 (dd, $^{3}J_{HH}$ = 5.0 Hz, $^{4}J_{HH}$ = 1.3 Hz, 2H, 2C(4)H in 2 thiophen-3-yls), 7.40 (dd, $^{3}J_{HH}$ = 5.0 Hz, $^{4}J_{HH}$ = 2.9 Hz, 2H, 2C(5)H in 2 thiophen-3-yls), 7.98 (dd, $^{4}J^{1}_{HH}$ = 2.9 Hz, $^{4}J^{2}_{HH}$ = 1.3 Hz, 2H, 2C(2)H in 2 thiophen-3-yls); ^{13}C NMR (DMSO-d_6, 126 MHz): δ/ppm 125.1, 126.9, 127.8, 130.6, 142.2, 151.0. Anal. Calcd for $C_{12}H_6N_8S_2$: C, 44.16; H, 1.85; N, 34.33; Found C, 43.99; H,

1.80; N, 34.00. HRMS (APCI): Found *m/z* = 326.0162 (M^-). $C_{12}H_6N_8S_2^-$. Calculated 326.0162 (M^-).

2.3 Procedure for the synthesis of 1,7-diphenylimidazo[1,2-*b*][1,2,4]triazolo[3,4-*f*][1,2,4,5]tetrazine (5-*cis*) and 1,7-diphenylimidazo[1,2-b][1,2,4]triazolo[4,3-*e*][1,2,4,5]tetrazine (5-*trans*).

The starting 3-(2-benzylidenehydrazinyl)-7-phenylimidazo[1,2-*b*][1,2,4,5]tetrazine **4**[7] (1.0 mmol) was dissolved in $CHCl_3$ (15 ml) and the resulting solution was heated up to 50°C. $Pb(OAc)_4$ (1.0 mmol) was added to the stirred reaction mixture in portions of 0.5 mmol with an interval of 15 min. Then the resulting mixture was heated for another 30 minutes until the initial compound completely disappeared (control by TLC) and after that cooled to room temperature. The reaction mixture was filtered, the filtrate was evaporated to dryness and the products **5-cis** (R_f = 0.8) and **5-trans** (R_f = 0.6) were separated by colomn chromatography using silica gel 60 (230-400 mesh) and C_6H_6 : MeCN (1:1) as eluent.

5-cis: Yelow solid, 44 mg (14%), m.p. 258-260 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 7.44-7.48 (m, 1H, Ar), 7.50-7.53 (m, 2H, Ar), 7.77-7.83 (m, 3H, Ar), 7.88 (d, $^3J_{HH}$ = 7.3 Hz, 2H, Ar), 8.07 (d, $^3J_{HH}$ = 7.9 Hz, 2H, Ar), 8.30 (s, 1H, C(8)H). ^{13}C NMR (DMSO-d_6, 126 MHz): δ/ppm 109.9, 124.1, 126.7, 129.6, 129.9, 130.1, 130.7, 131.6, 132.2, 143.3, 143.8, 144.8, 150.4. Anal. Calcd for $C_{17}H_{11}N_7$: C, 65.17; H, 3.54; N, 31.29; Found C, 65.32; H, 3.68; N, 31.11. HRMS (ESI): Found *m/z* = 314.1151 ($[M+H]^+$). $C_{17}H_{12}N_7^+$. Calculated 314.1149 ($[M+H]^+$).

5-trans: Dark-green solid, 28 mg (9%), m.p. 285 °C (decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz): δ/ppm 7.62-7.73 (m, 6H, Ar), 8.41 (br.s, 2H, Ar), 8.50 (s, 2H, Ar), 9.68 (s, 1H, C(8)H). ^{13}C NMR (DMSO-d_6, 126 MHz): δ/ppm 114.0, 126.2, 126.7, 128.7, 128.8, 129.7, 130.1, 130.7, 131.5, 133.6, 143.4, 144.2, 147.9, 166.5. Anal. Calcd for $C_{17}H_{11}N_7$: C, 65.17; H, 3.54; N, 31.29; Found C, 65.04; H, 3.62; N, 31.17. HRMS (ESI): Found *m/z* = 314.1151 ($[M+H]^+$). $C_{17}H_{12}N_7^+$. Calculated 314.1149 ($[M+H]^+$).

2.4 NMR spectra of synthesized compounds

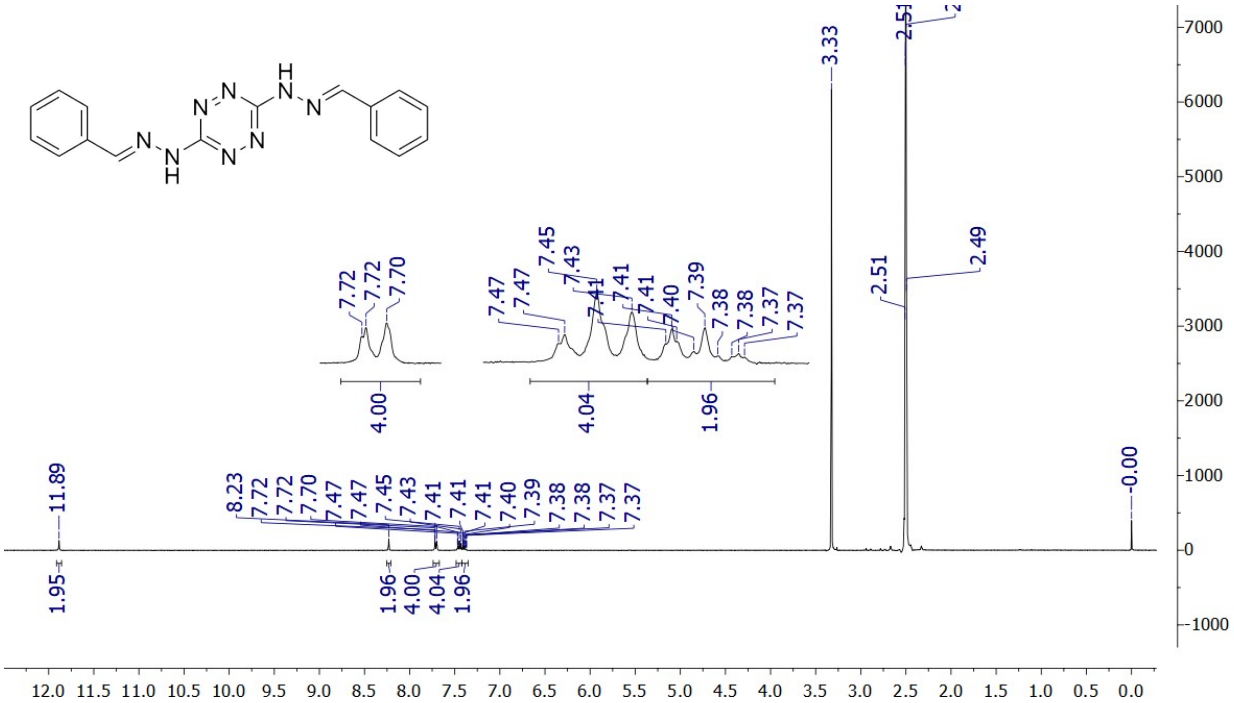


Figure S1. ^{1}H NMR spectrum of the 3,6-bis(2-benzylidenehydrazinyl)-1,2,4,5-tetrazine **(2a)**.

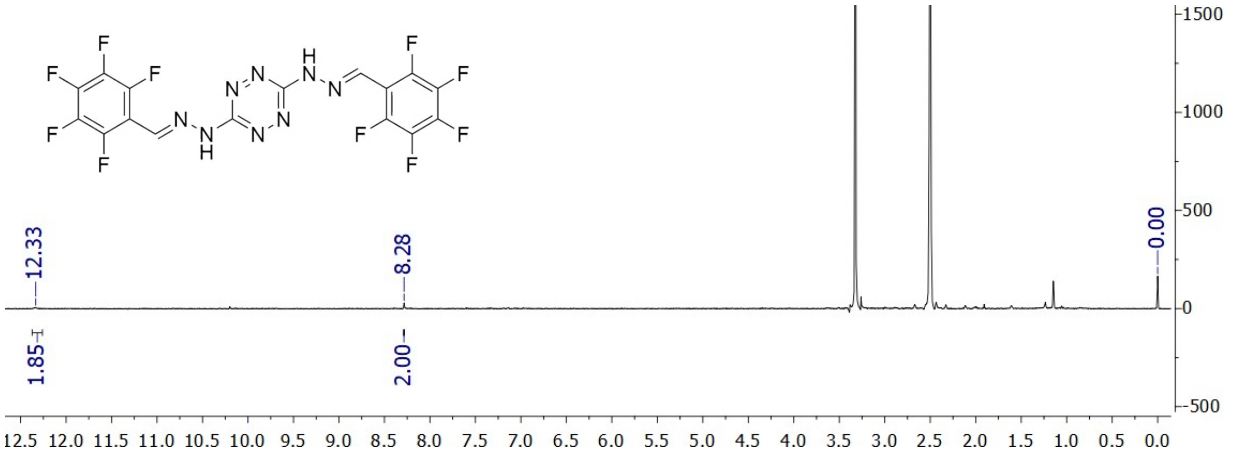


Figure S2. ^{1}H NMR spectrum of the 3,6-bis(2-(perfuorobenzylidene)hydrazinyl)-1,2,4,5-tetrazine **(2b)**.

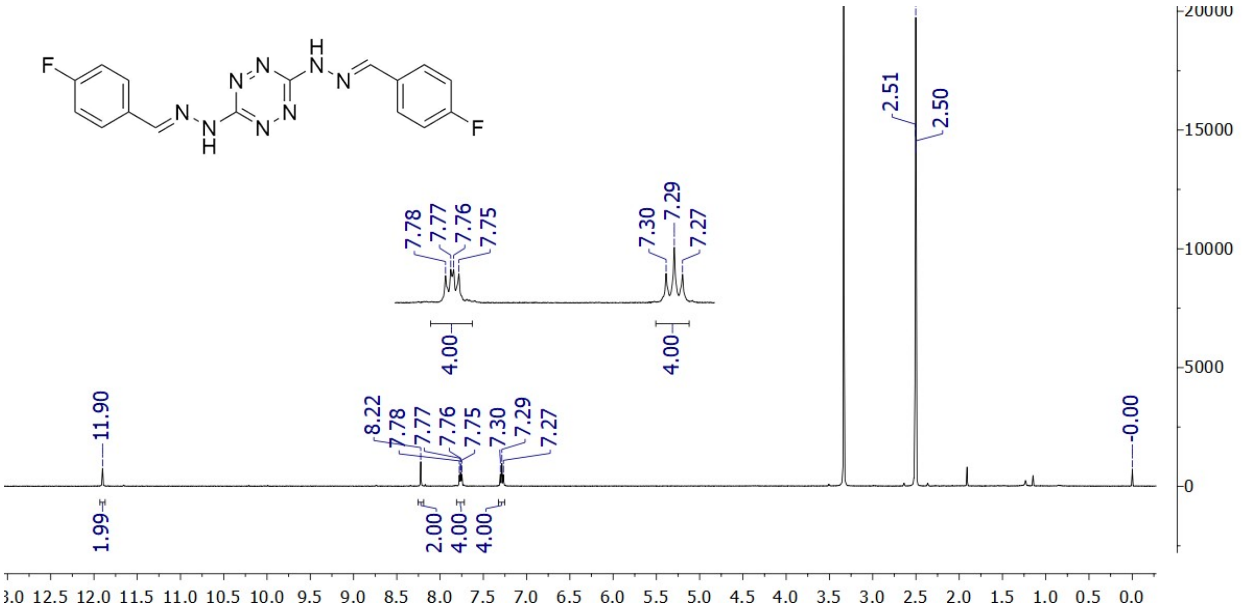


Figure S3. [1]H NMR spectrum of the 3,6-bis(2-(4-fuorobenzylidene)hydrazinyl)-1,2,4,5-tetrazine **(2c)**.

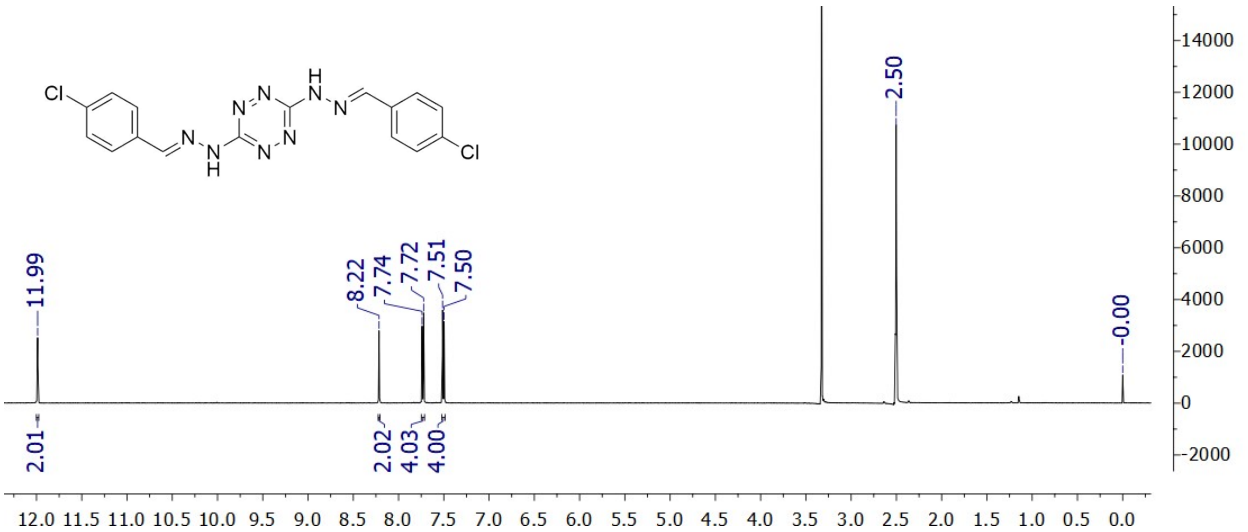


Figure S4. [1]H NMR spectrum of the 3,6-bis(2-(4-chlorobenzylidene)hydrazinyl)-1,2,4,5-tetrazine **(2d)**.

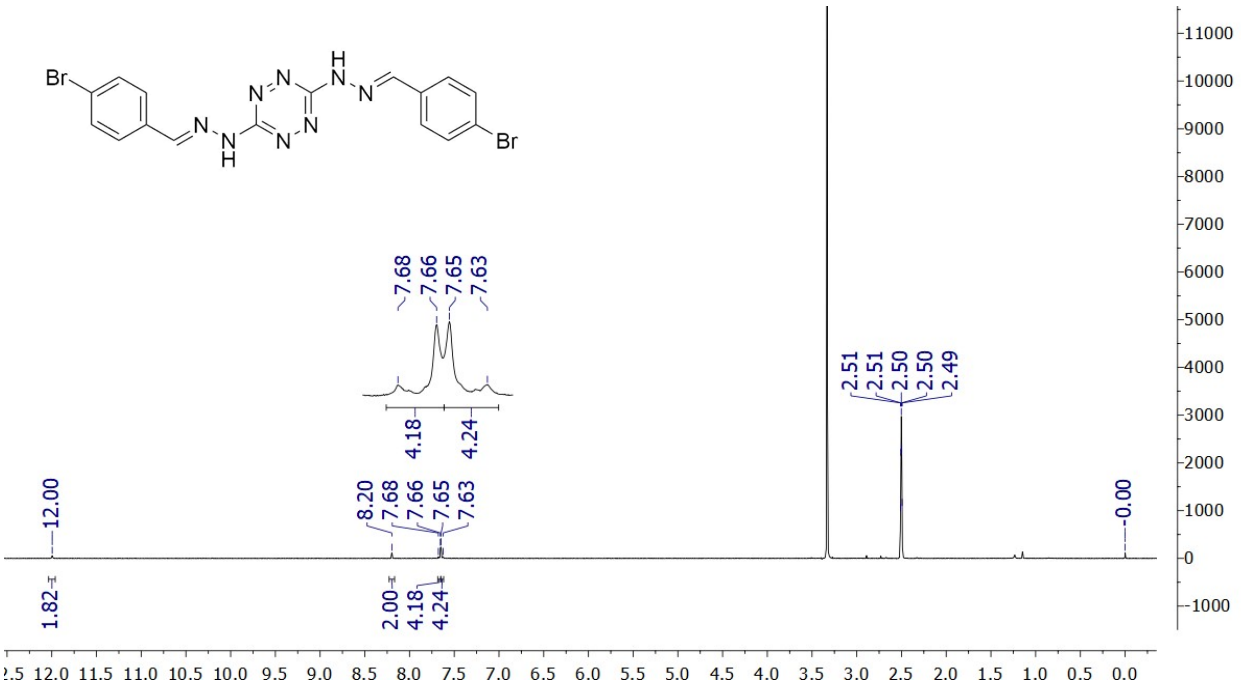


Figure S5. ^{1}H NMR spectrum of the 3,6-bis(2-(4-bromobenzylidene)hydrazinyl)-1,2,4,5-tetrazine **(2e)**.

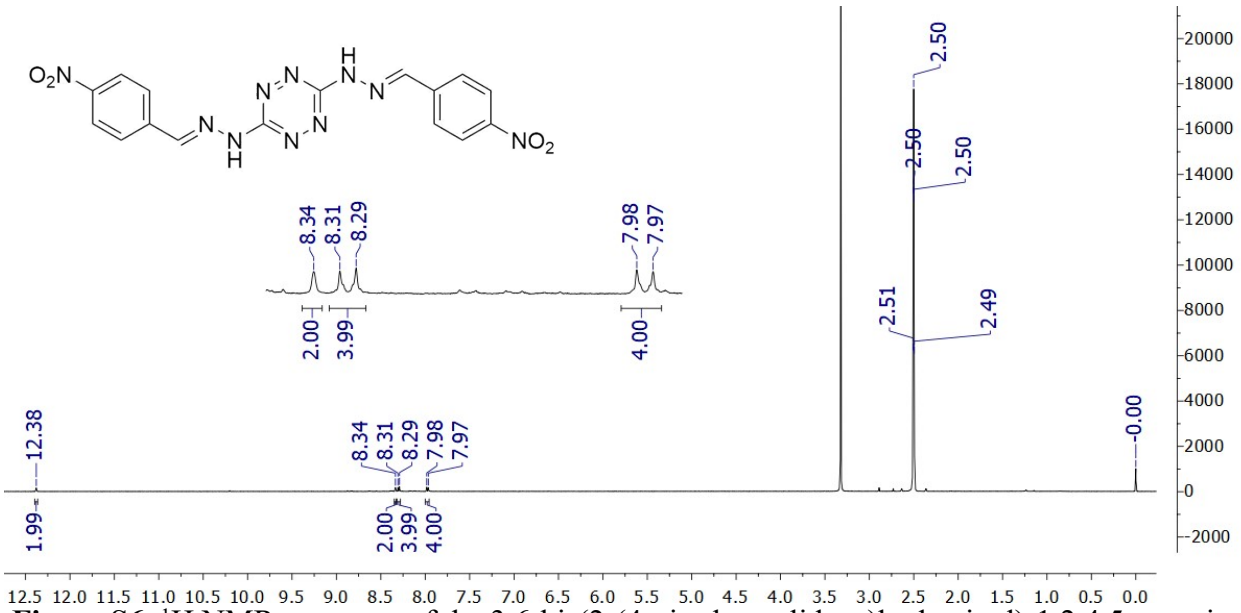


Figure S6. ^{1}H NMR spectrum of the 3,6-bis(2-(4-nitrobenzylidene)hydrazinyl)-1,2,4,5-tetrazine **(2f)**.

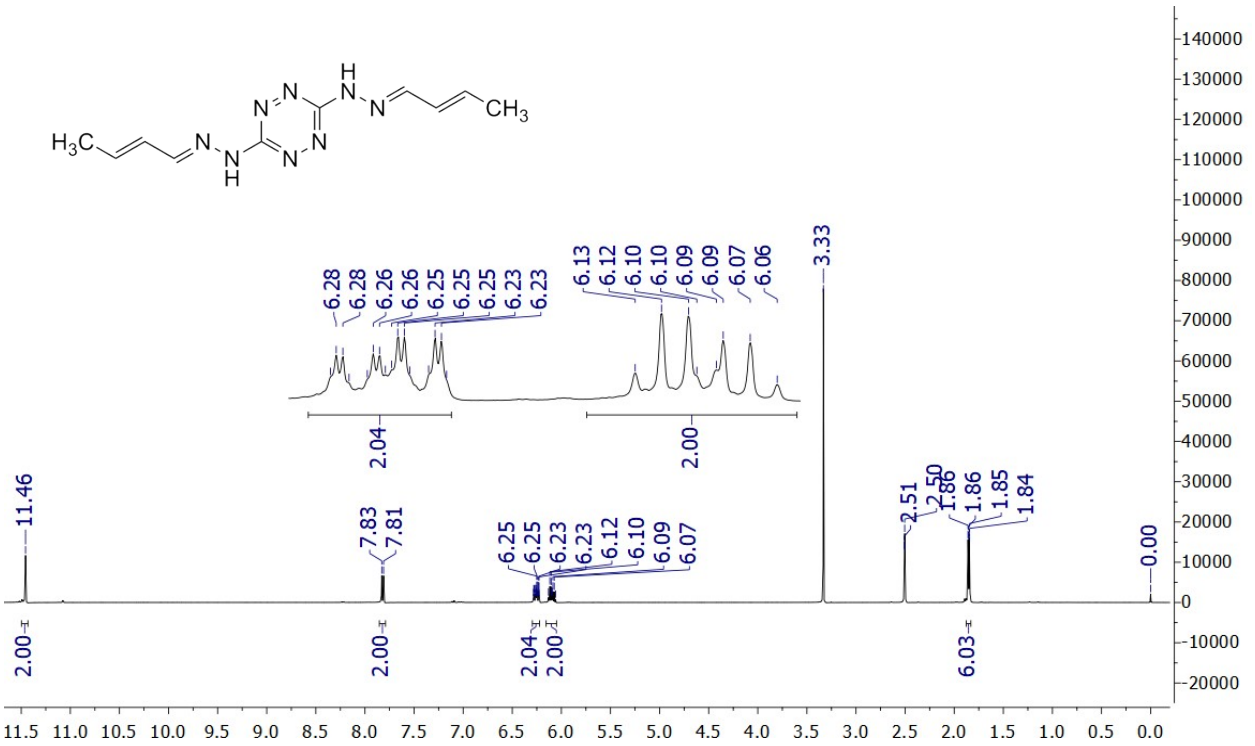


Figure S7. ^{1}H NMR spectrum of the 3,6-bis(2-(but-2-en-1-ylidene)hydrazinyl)-1,2,4,5-tetrazine (**2g**).

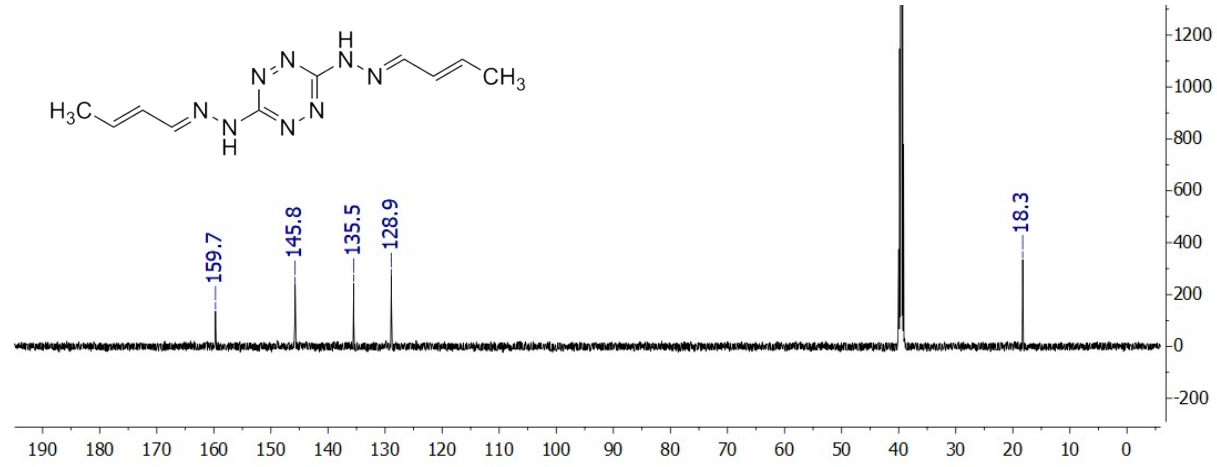


Figure S8. ^{13}C NMR spectrum of the 3,6-bis(2-(but-2-en-1-ylidene)hydrazinyl)-1,2,4,5-tetrazine (**2g**).

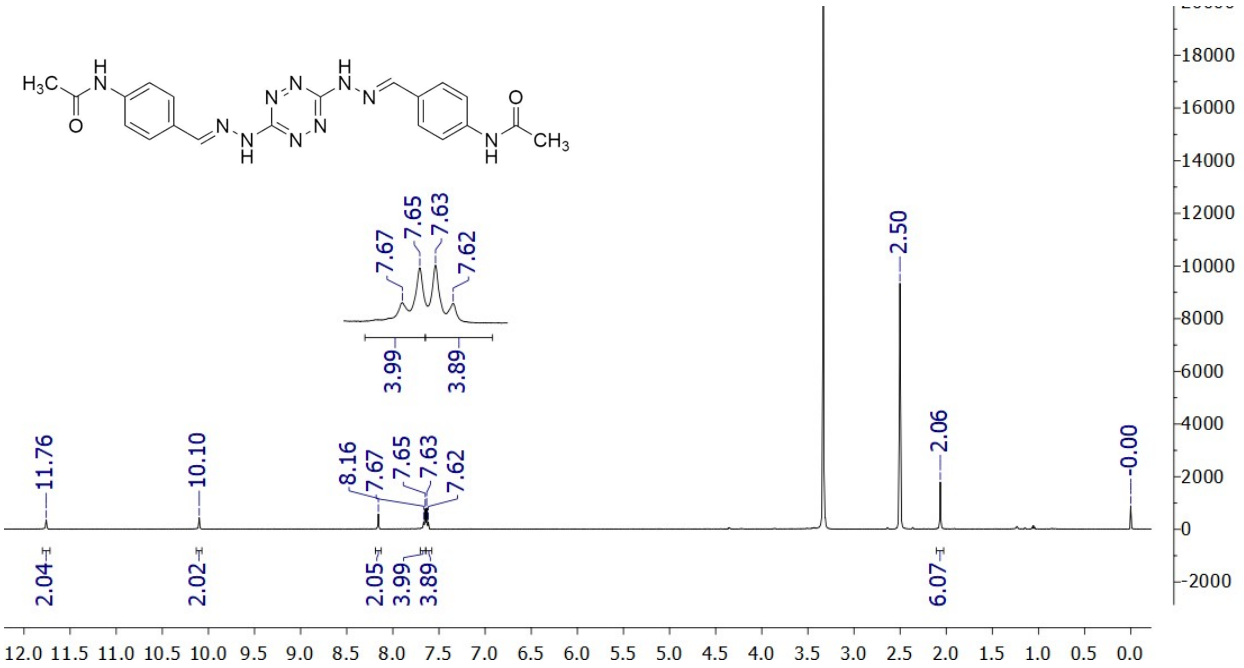


Figure S9. ^{1}H NMR spectrum of the 3,6-bis(2-(4-acetamidobenzylidene)hydrazinyl)-1,2,4,5-tetrazine **(2h)**.

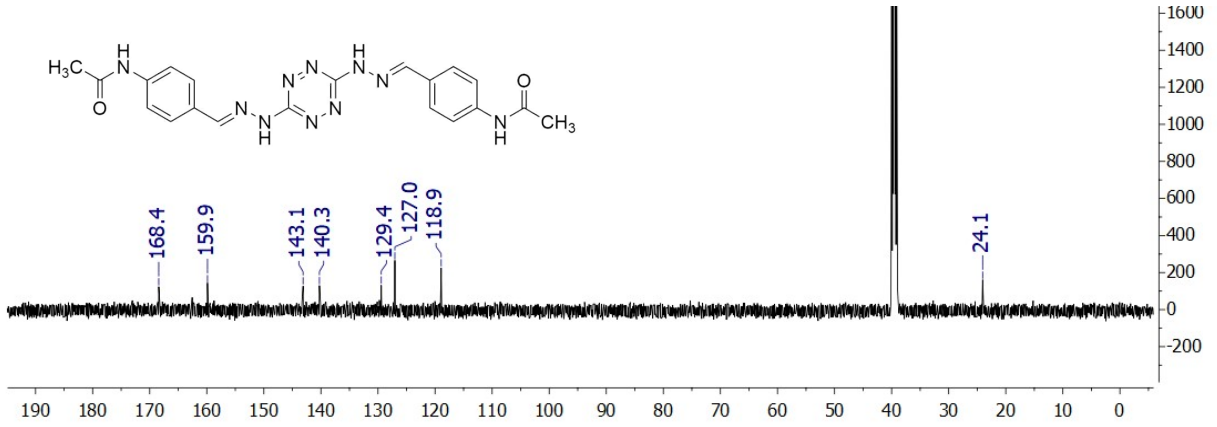


Figure S10. ^{13}C NMR spectrum of the 3,6-bis(2-(4-acetamidobenzylidene)hydrazinyl)-1,2,4,5-tetrazine **(2h)**.

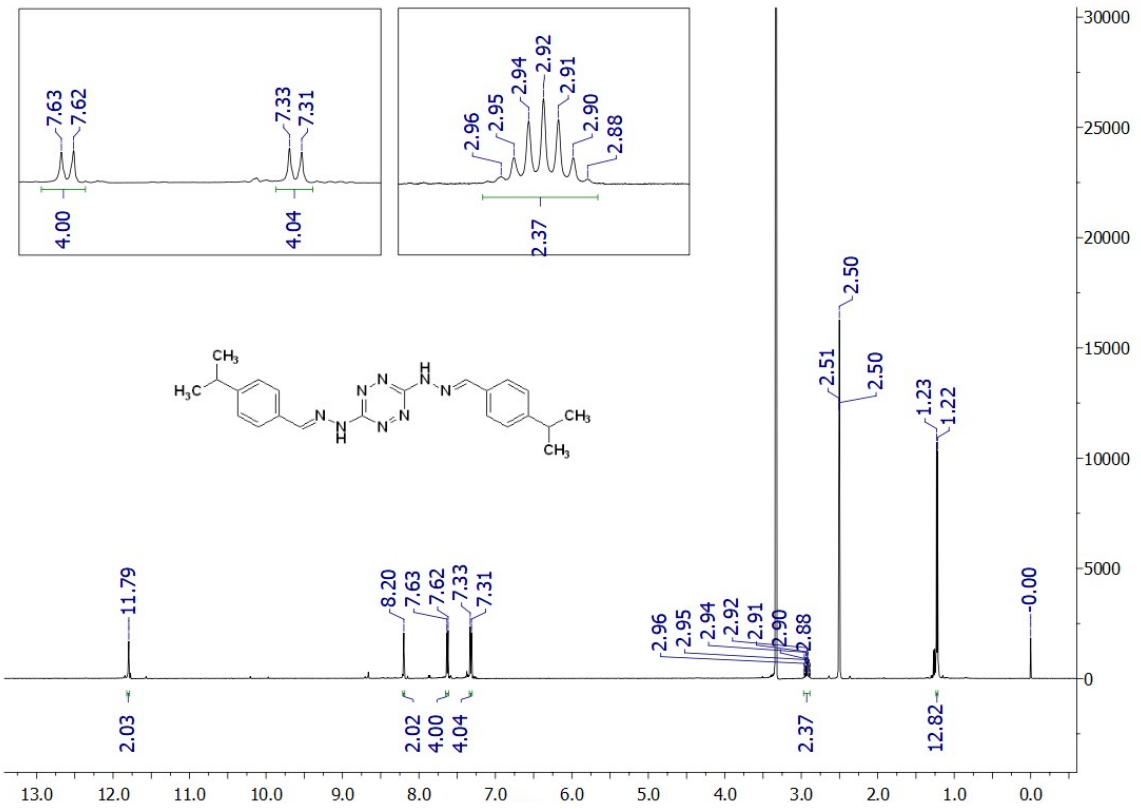


Figure S11. [1]H NMR spectrum of the 3,6-bis(2-(4-isopropylbenzylidene)hydrazinyl)-1,2,4,5-tetrazine (**2i**).

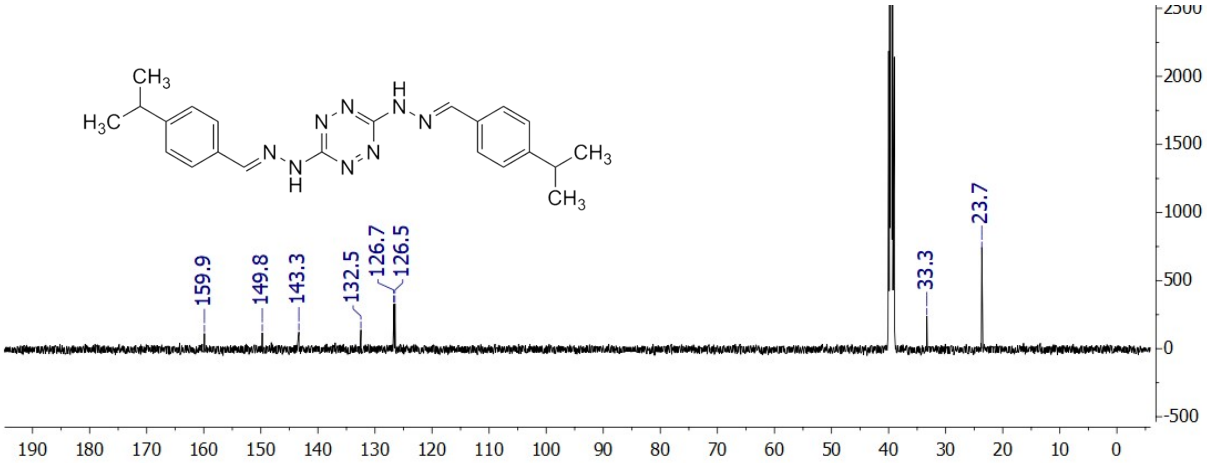


Figure S12. [13]C NMR spectrum of the 3,6-bis(2-(4-isopropylbenzylidene)hydrazinyl)-1,2,4,5-tetrazine (**2i**).

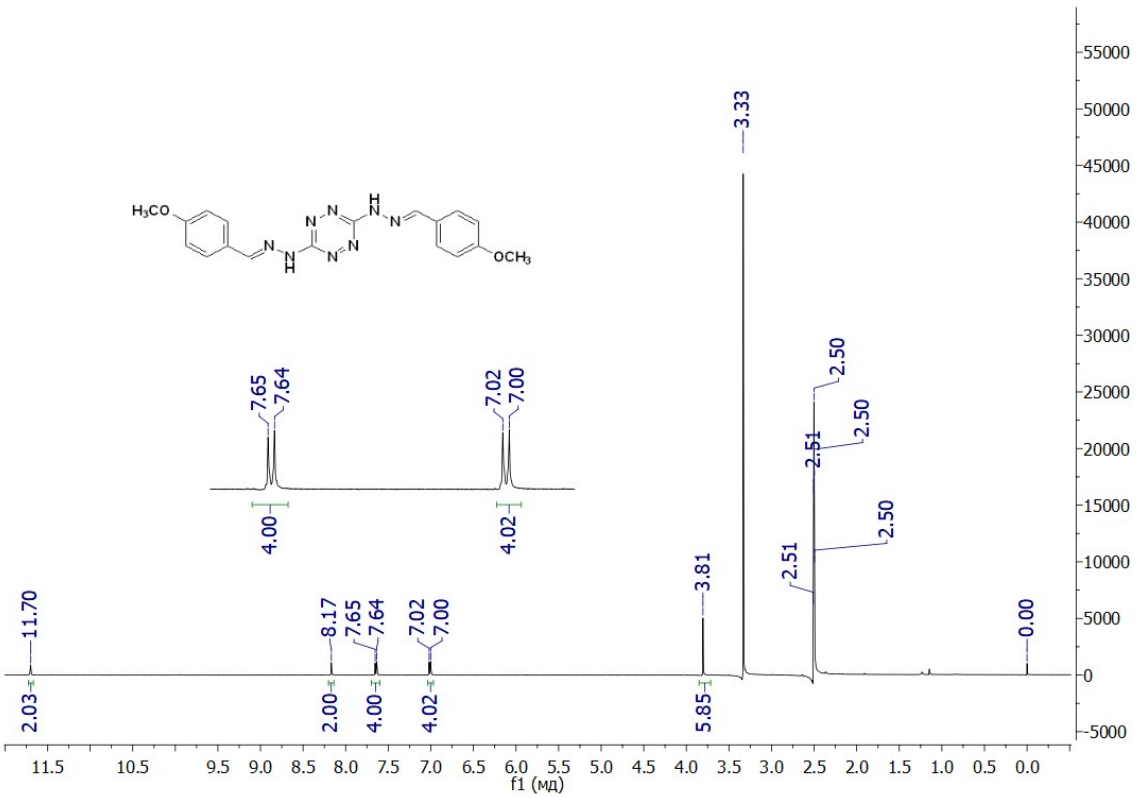


Figure S13. ^{1}H NMR spectrum of the 3,6-bis(2-(4-methoxybenzylidene)hydrazinyl)-1,2,4,5-tetrazine (**2j**).

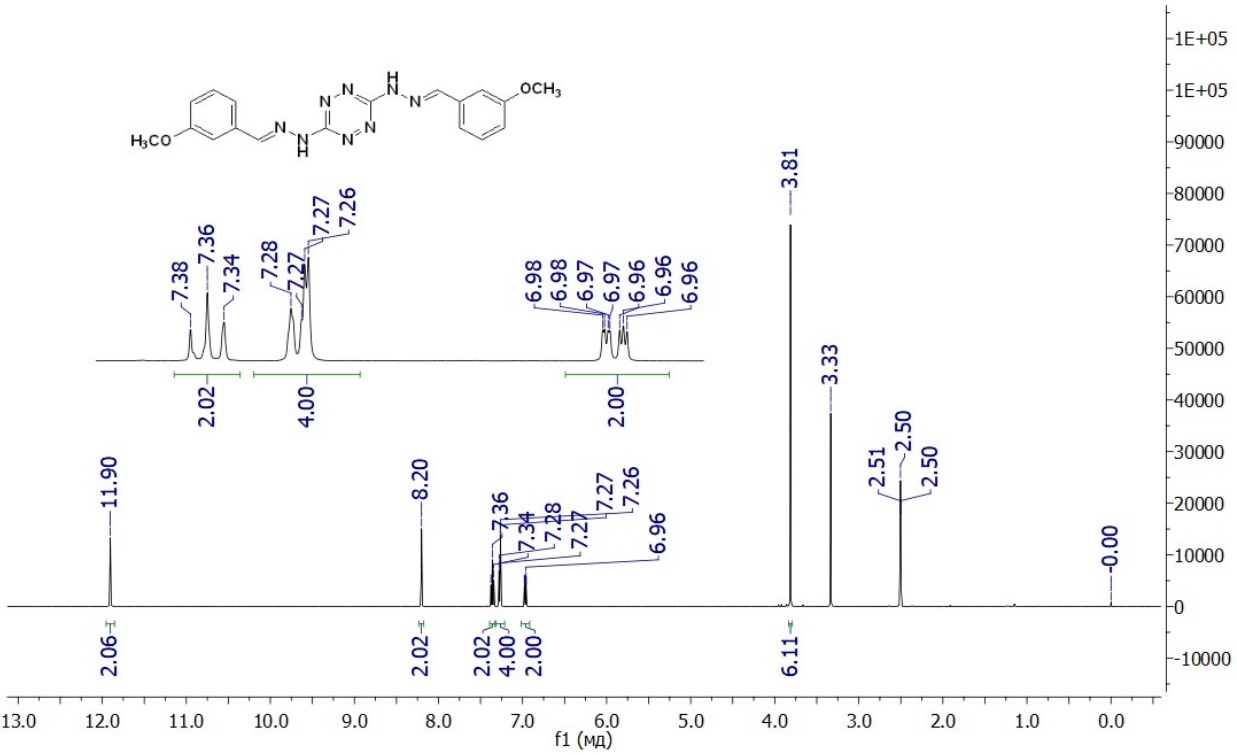


Figure S14. ^{1}H NMR spectrum of the 3,6-bis(2-(3-methoxybenzylidene)hydrazinyl)-1,2,4,5-tetrazine (**2k**).

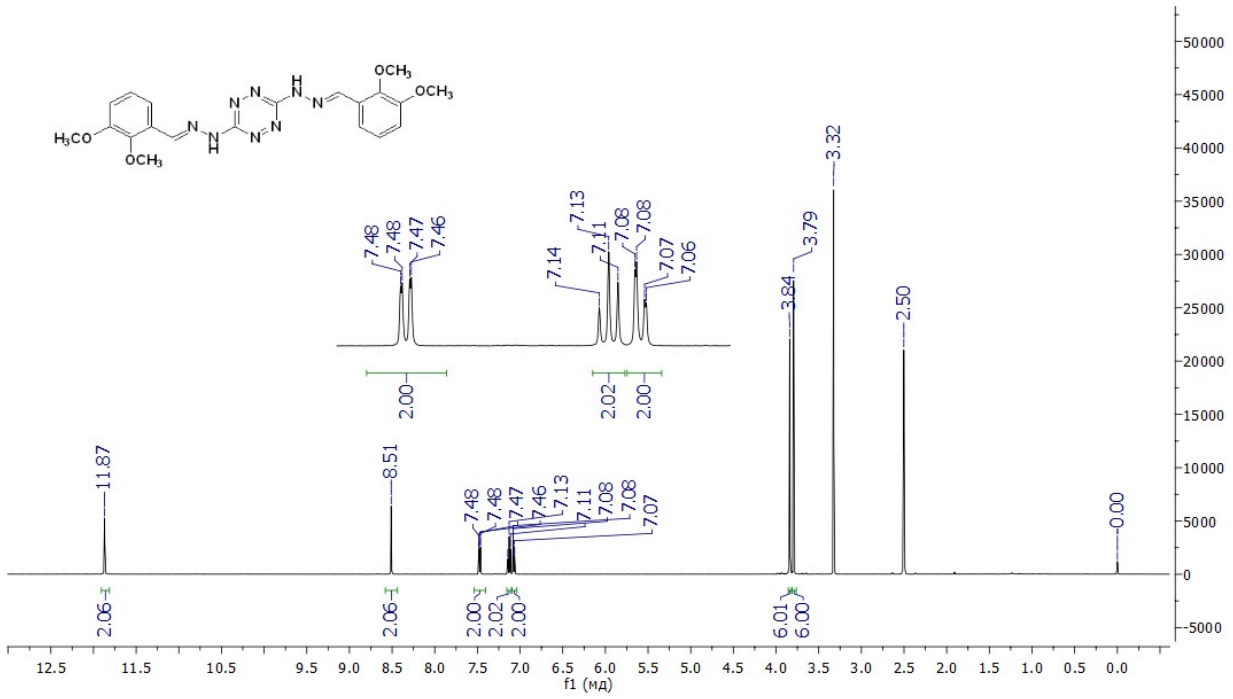


Figure S15. [1]H NMR spectrum of the 3,6-bis(2-(2,3-dimethoxybenzylidene)hydrazinyl)-1,2,4,5-tetrazine (**2l**)

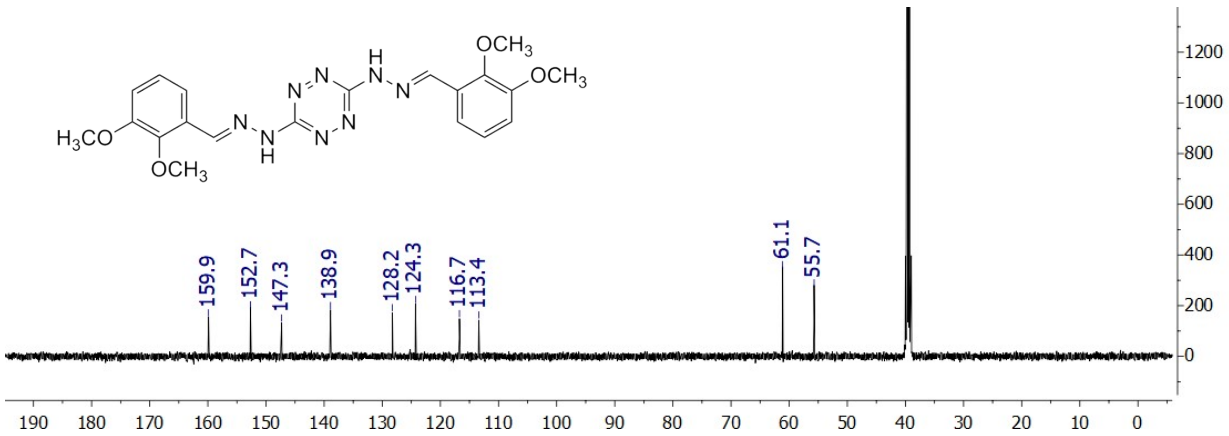


Figure S16. [13]C NMR spectrum of the 3,6-bis(2-(2,3-dimethoxybenzylidene)hydrazinyl)-1,2,4,5-tetrazine (**2l**)

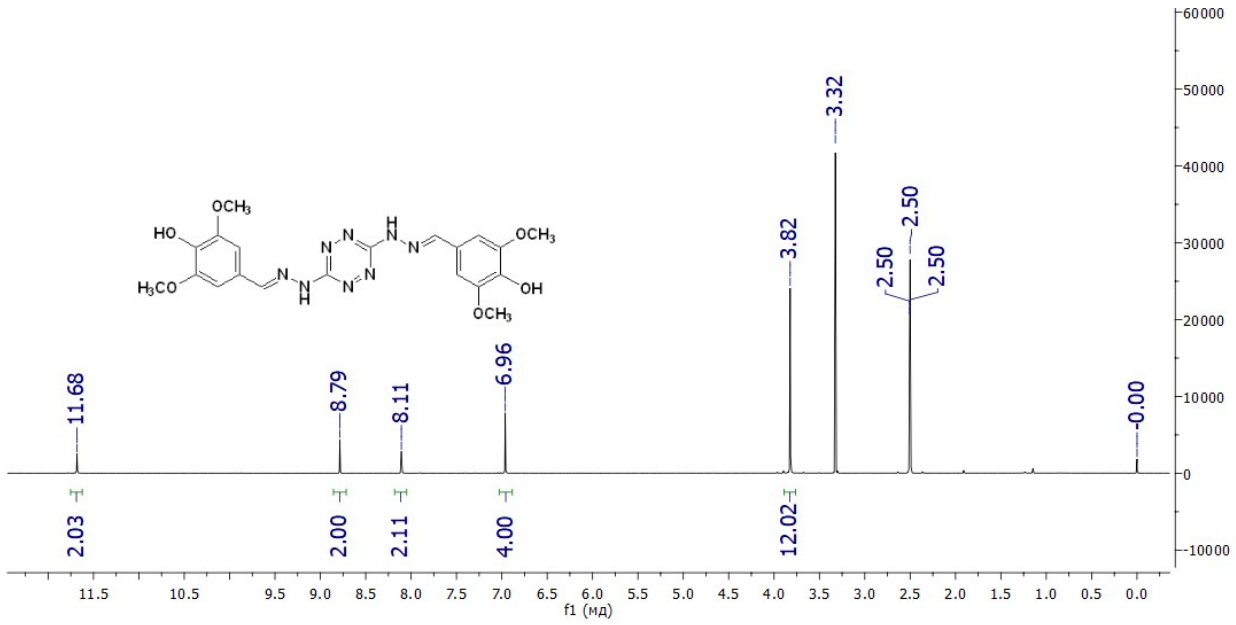


Figure S17. ^{1}H NMR spectrum of the 3,6-bis(2-(4-hydroxy-3,5-dimethoxybenzylidene)hydrazinyl)-1,2,4,5-tetrazine (**2m**)

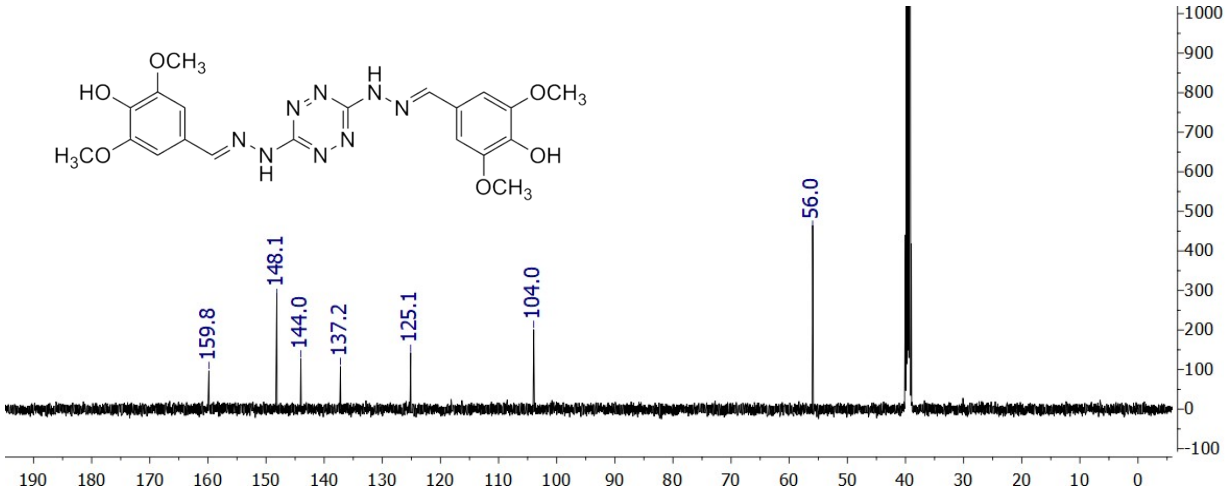


Figure S18. ^{13}C NMR spectrum of the 3,6-bis(2-(4-hydroxy-3,5-dimethoxybenzylidene)hydrazinyl)-1,2,4,5-tetrazine (**2m**)

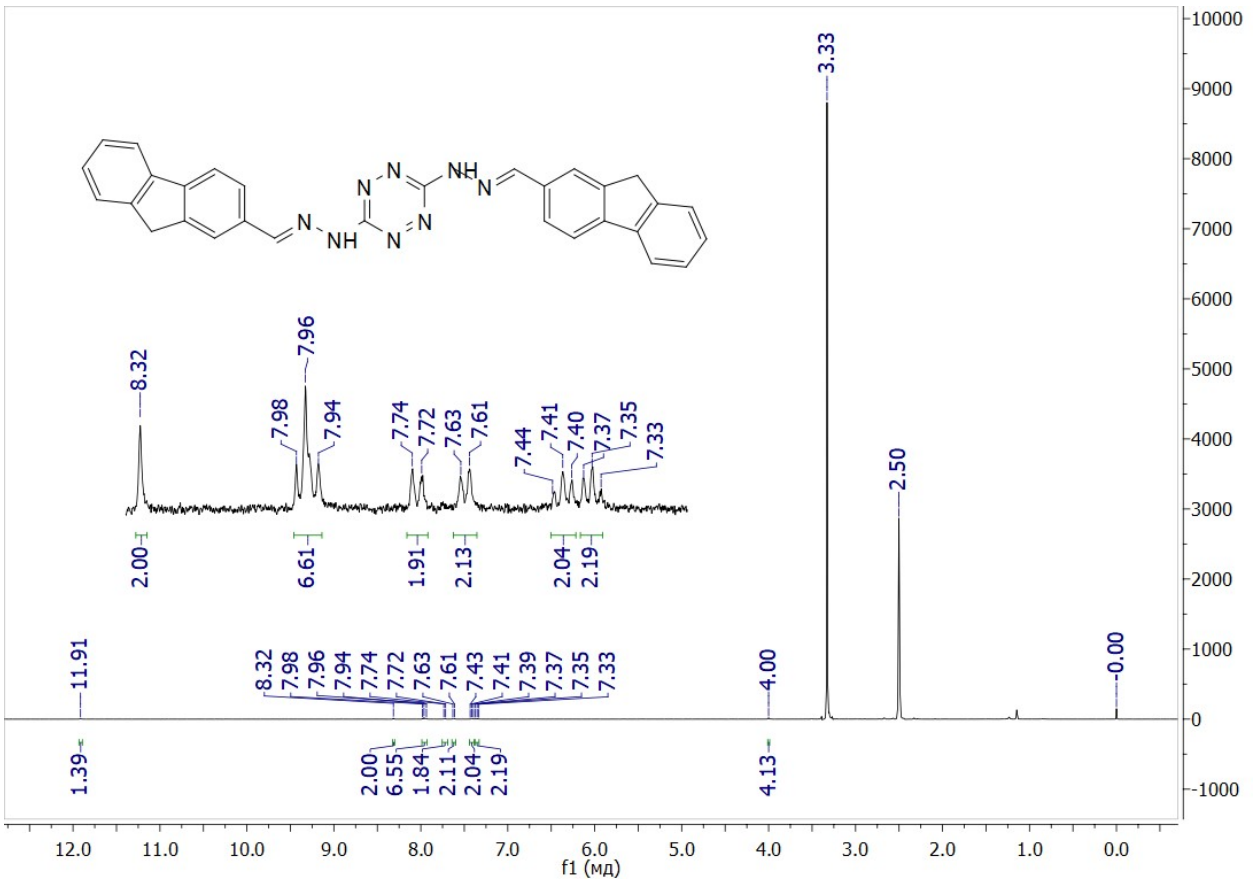


Figure S19. ^{1}H NMR spectrum of the 3,6-bis(2-(9H-fluoren-2-ylmethylidene)hydrazinyl)-1,2,4,5-tetrazine (**2n**)

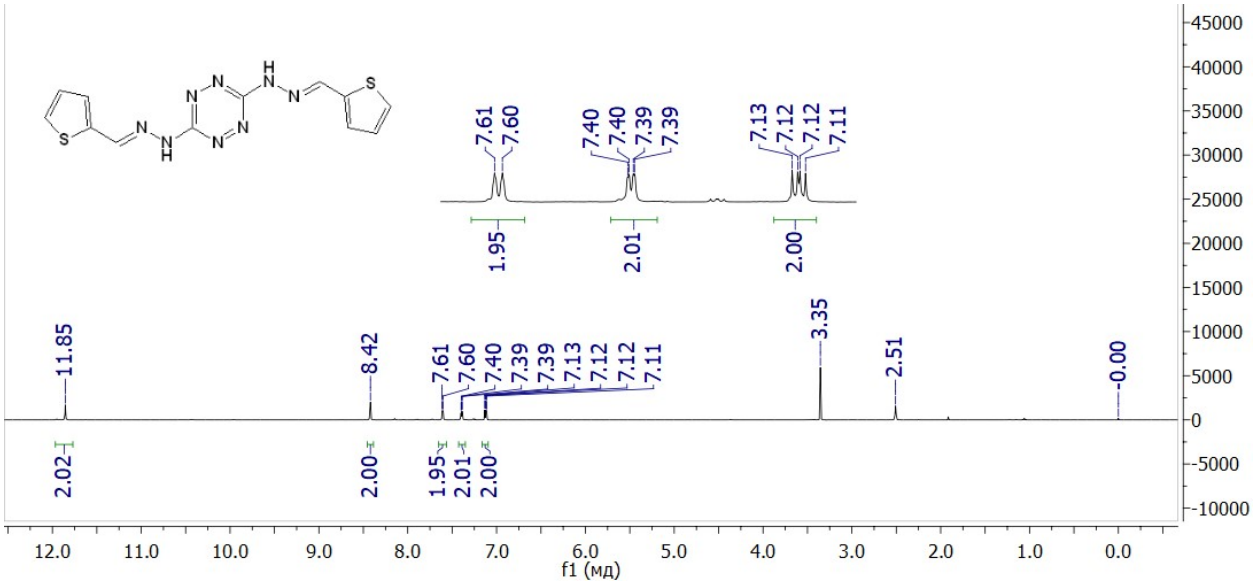


Figure S20. ^{1}H NMR spectrum of the 3,6-bis(2-(thiophen-2-ylmethylidene)hydrazinyl)-1,2,4,5-tetrazine (**2o**)

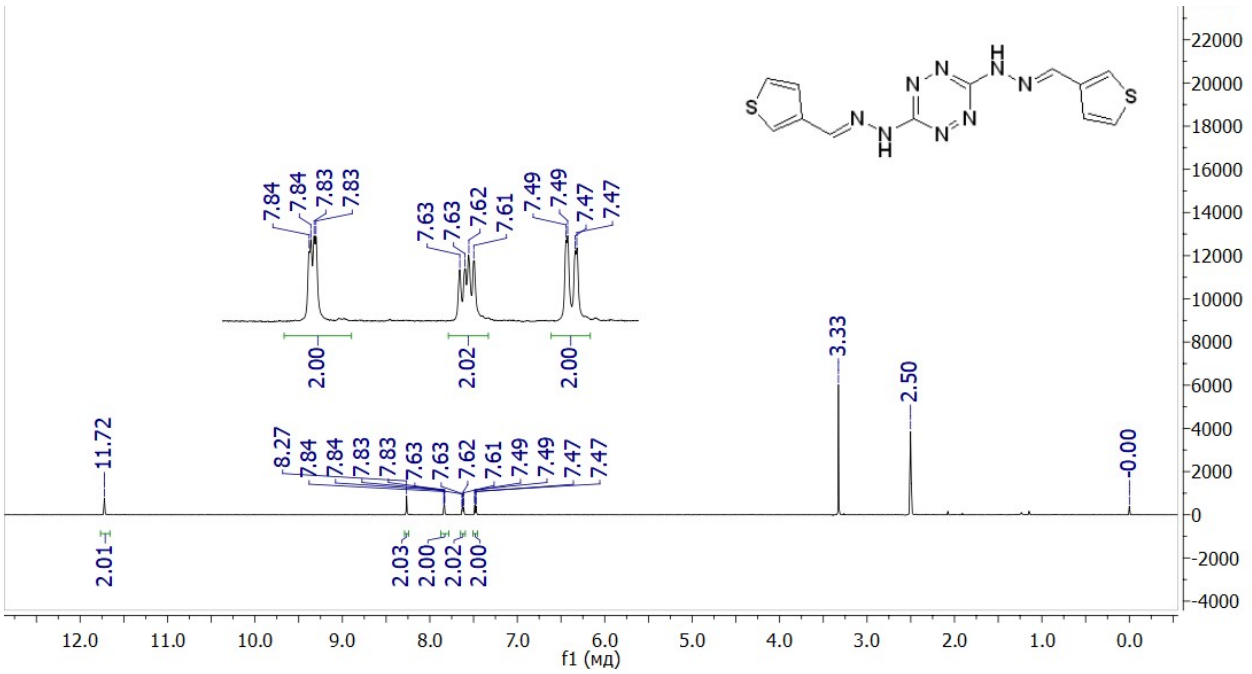


Figure S21. [1]H NMR spectrum of the 3,6-bis(2-(thiophen-3-ylmethylidene)hydrazinyl)-1,2,4,5-tetrazine (**2p**)

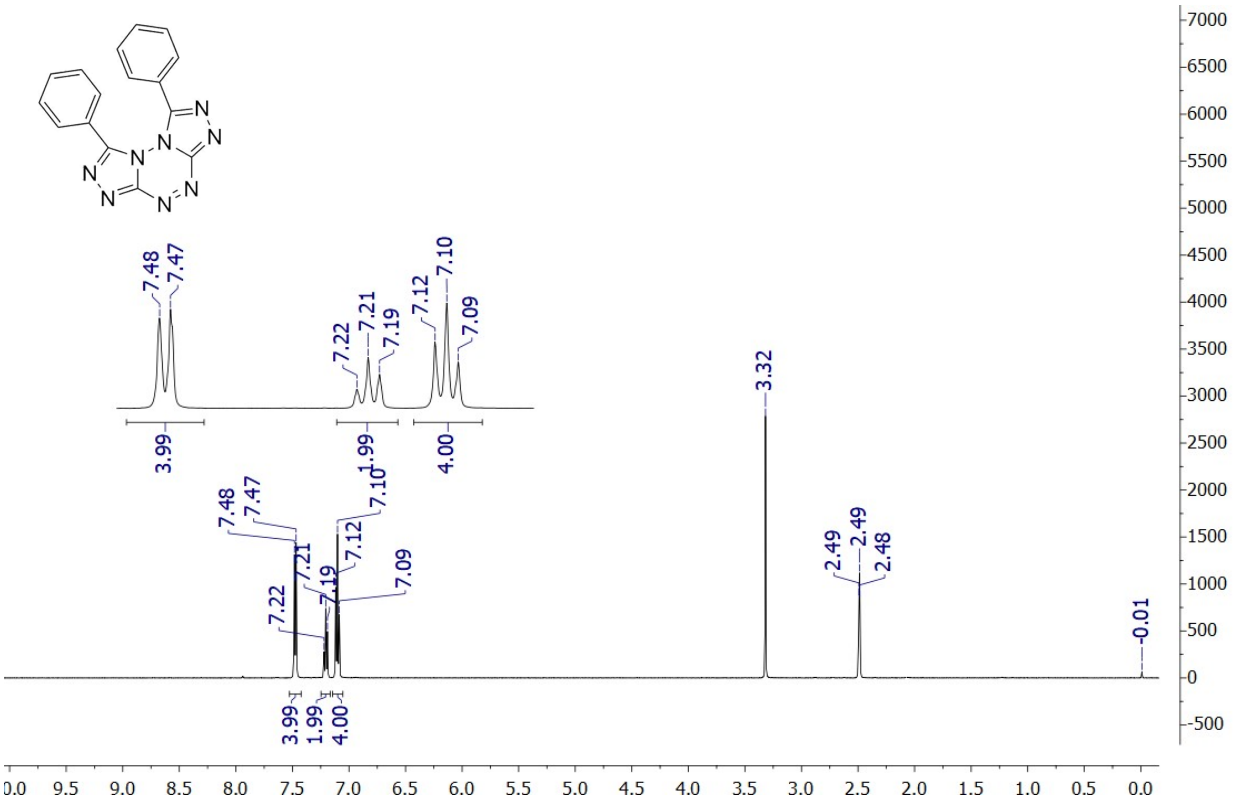


Figure S22. [1]H NMR spectrum of the 1,8-di(phenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3a)**.

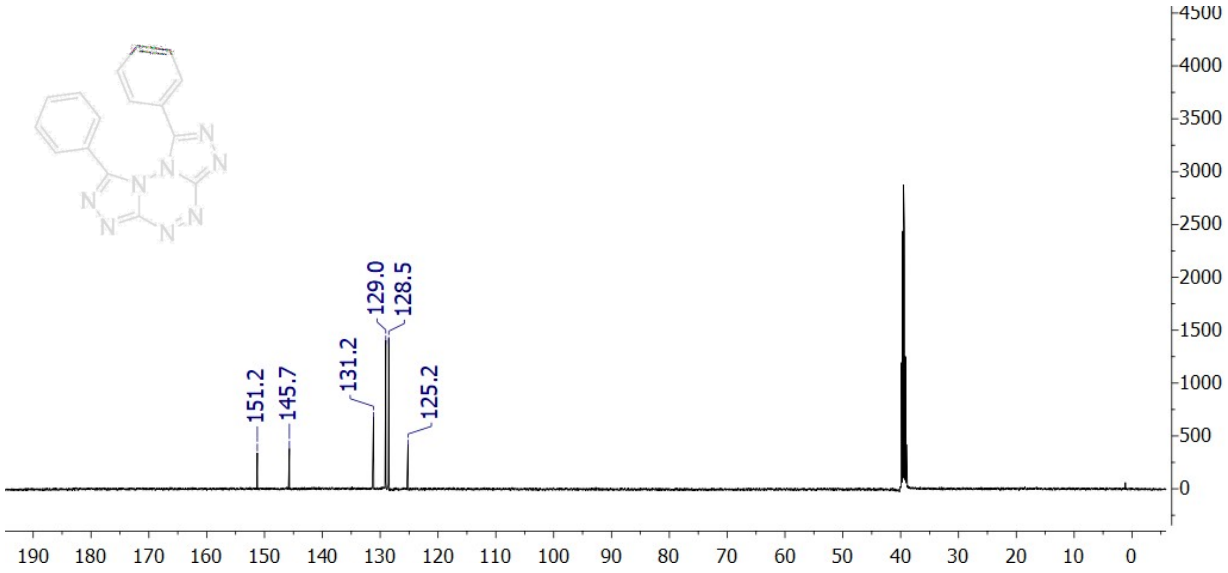


Figure S23. ^{13}C NMR spectrum of the 1,8-di(phenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3a)**.

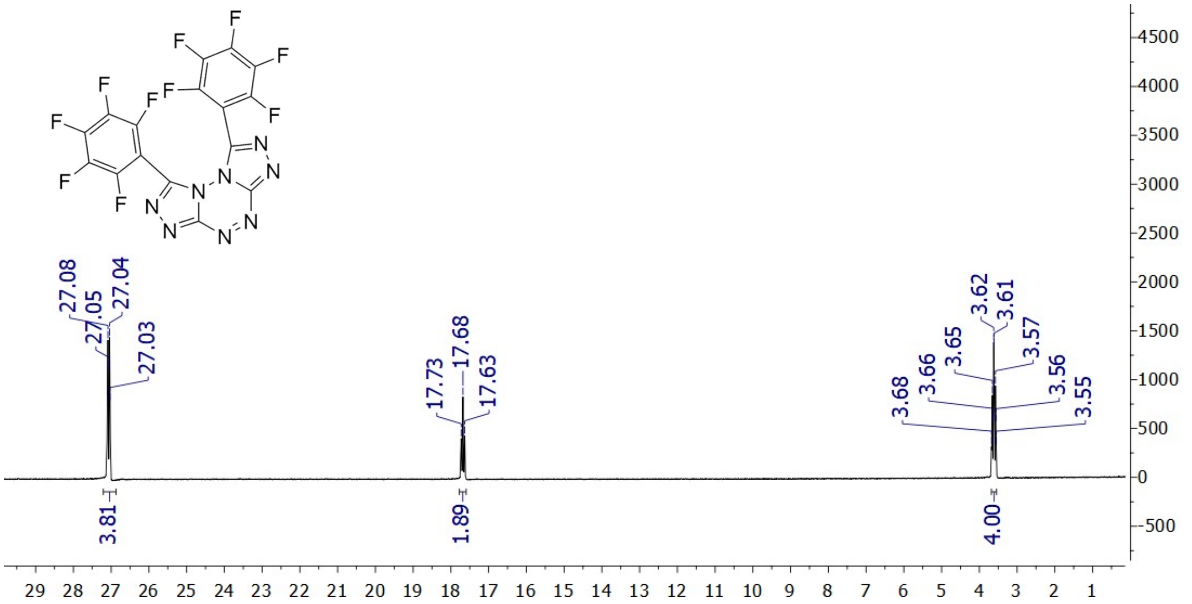


Figure S24. ^{19}F NMR spectrum of the 1,8-di(perfluorophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3b)**.

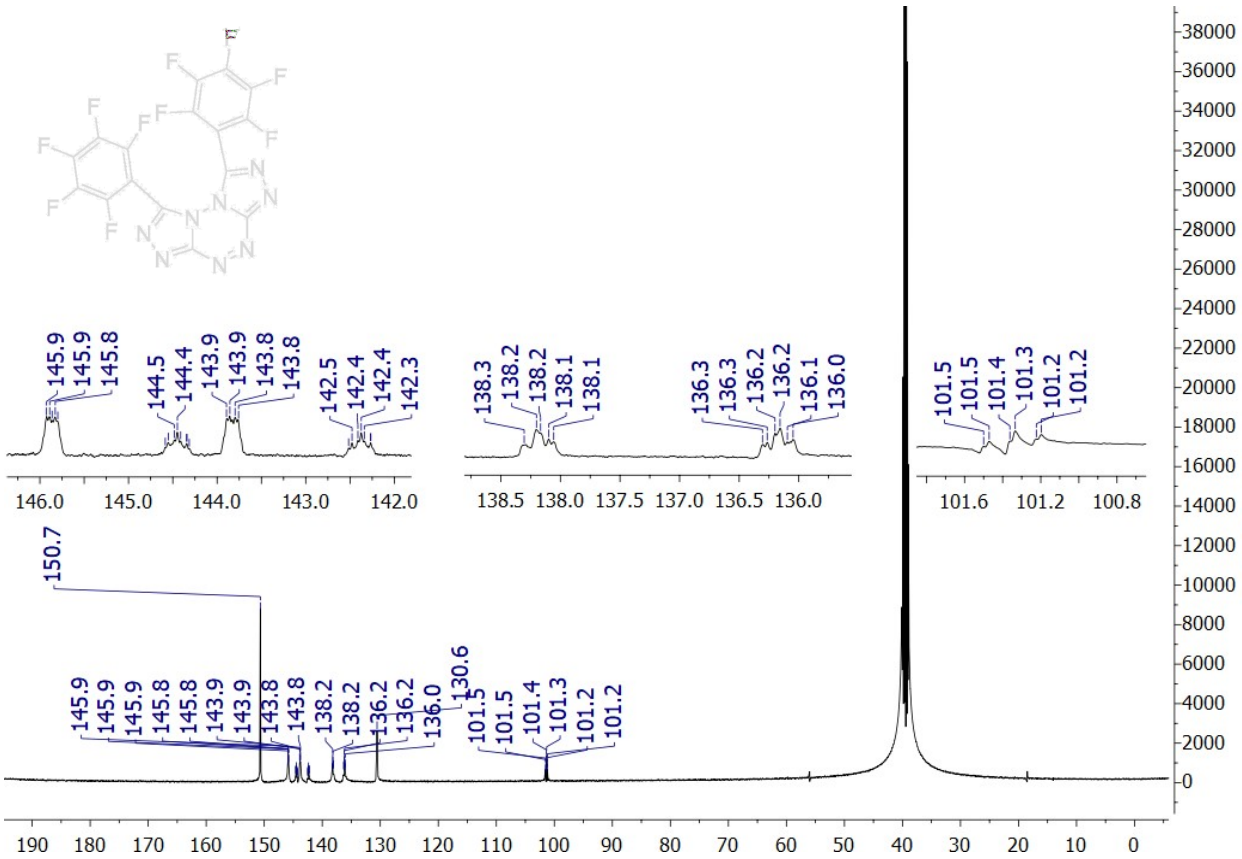


Figure S25. ^{13}C NMR spectrum of the 1,8-di(perfluorophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3b**).

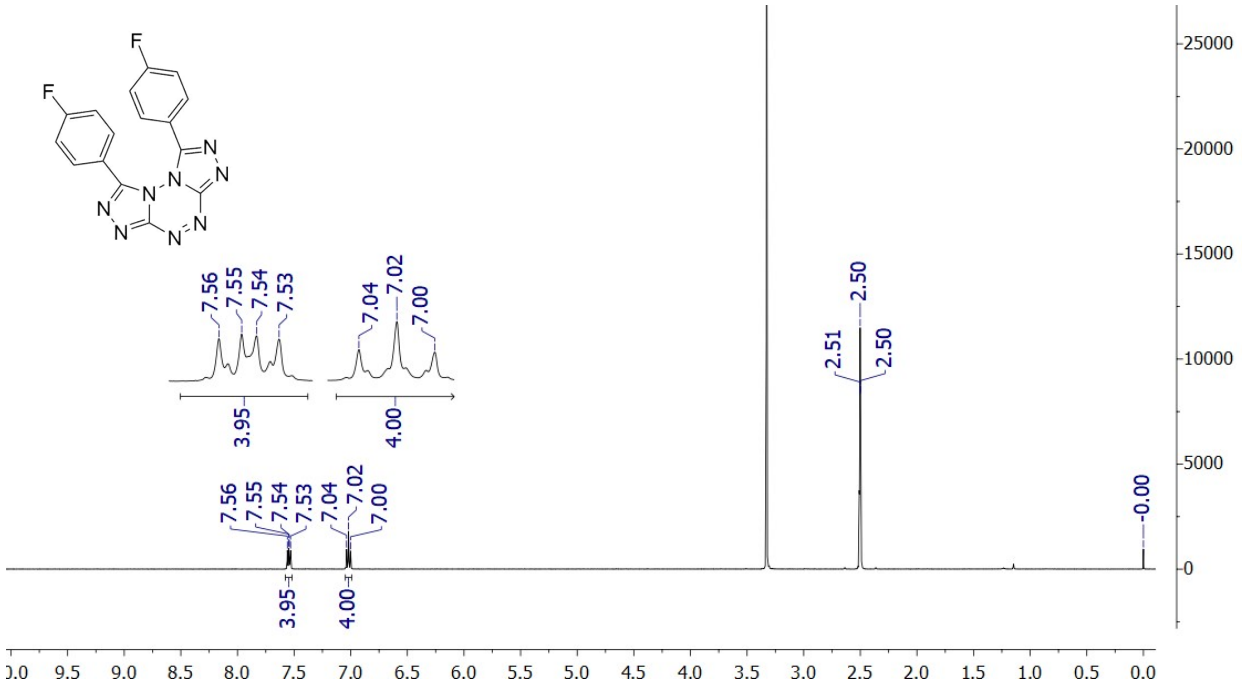


Figure S26. ^{1}H NMR spectrum of the 1,8-di(4-fluorophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3c)**.

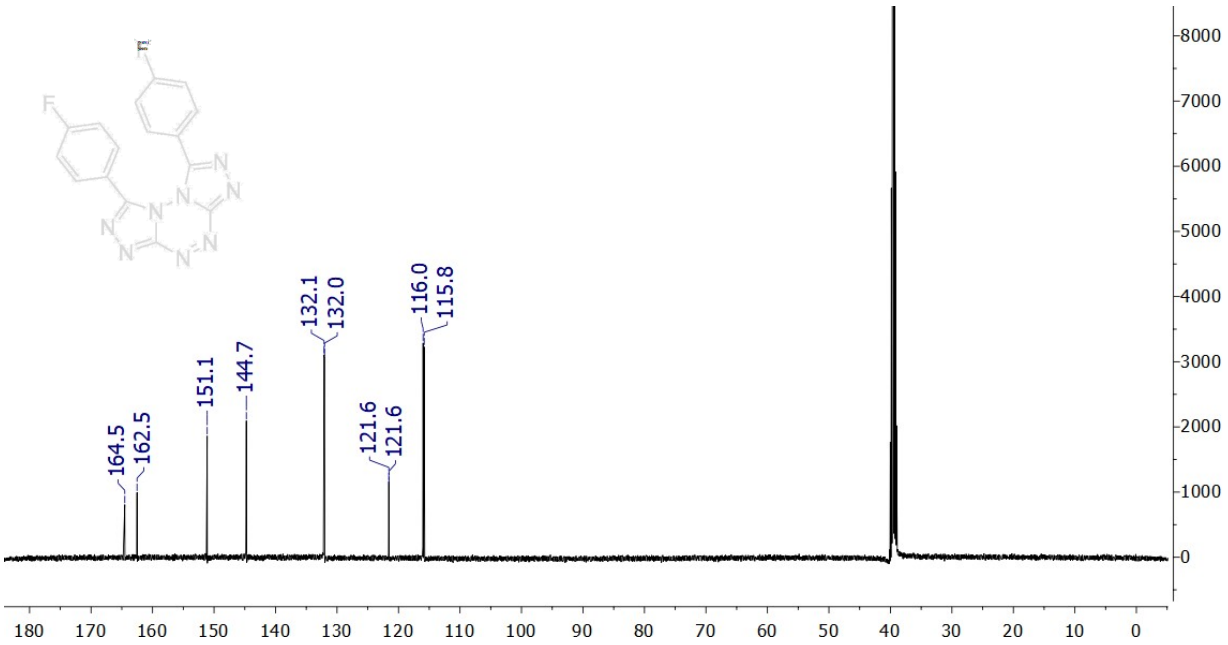


Figure S27. ^{13}C NMR spectrum of the 1,8-di(4-fluorophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3c)**.

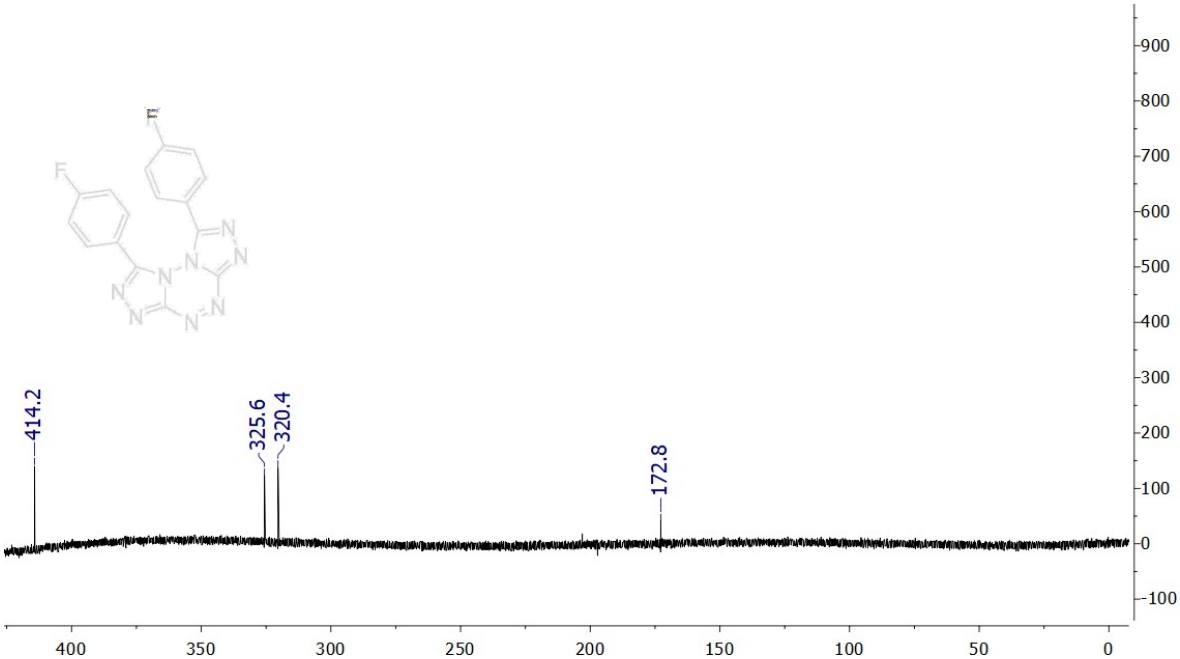


Figure S28. ^{15}N NMR spectrum of the 1,8-di(4-fluorophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3c)**.

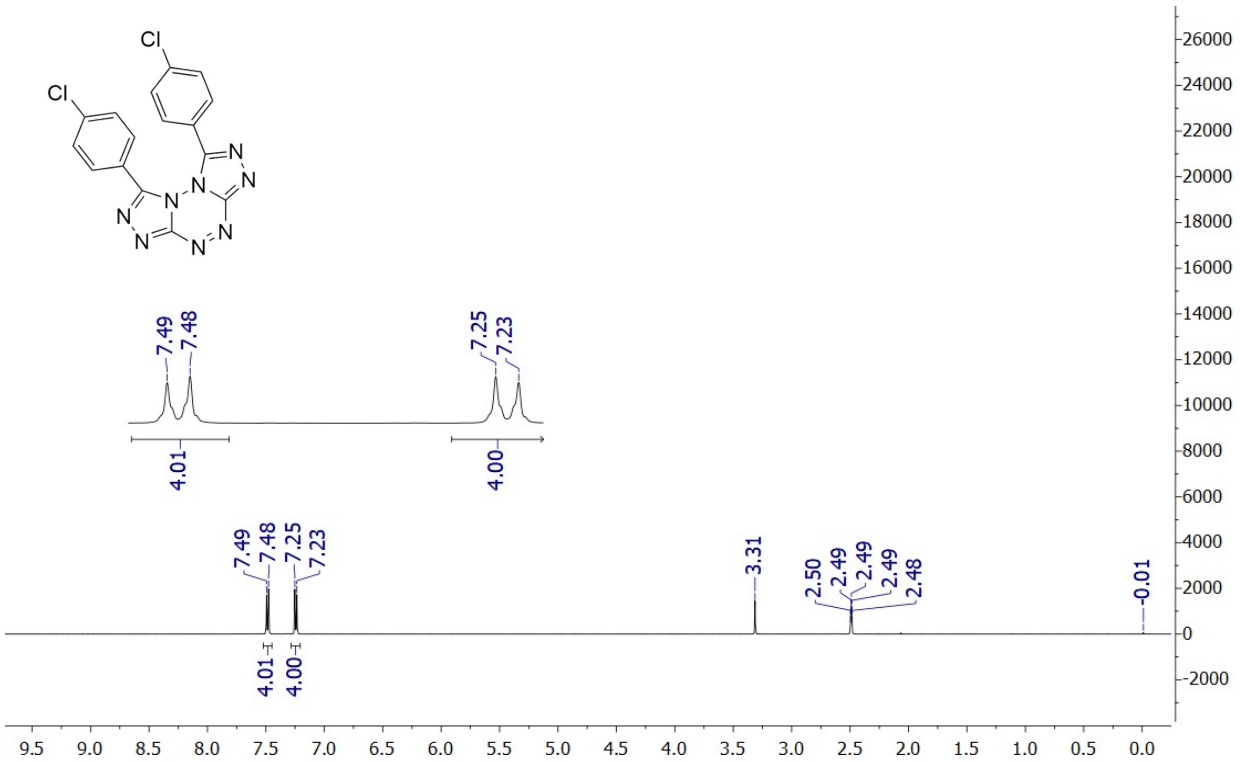


Figure S29. ^{1}H NMR spectrum of the 1,8-di(4-chlorophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3d)**.

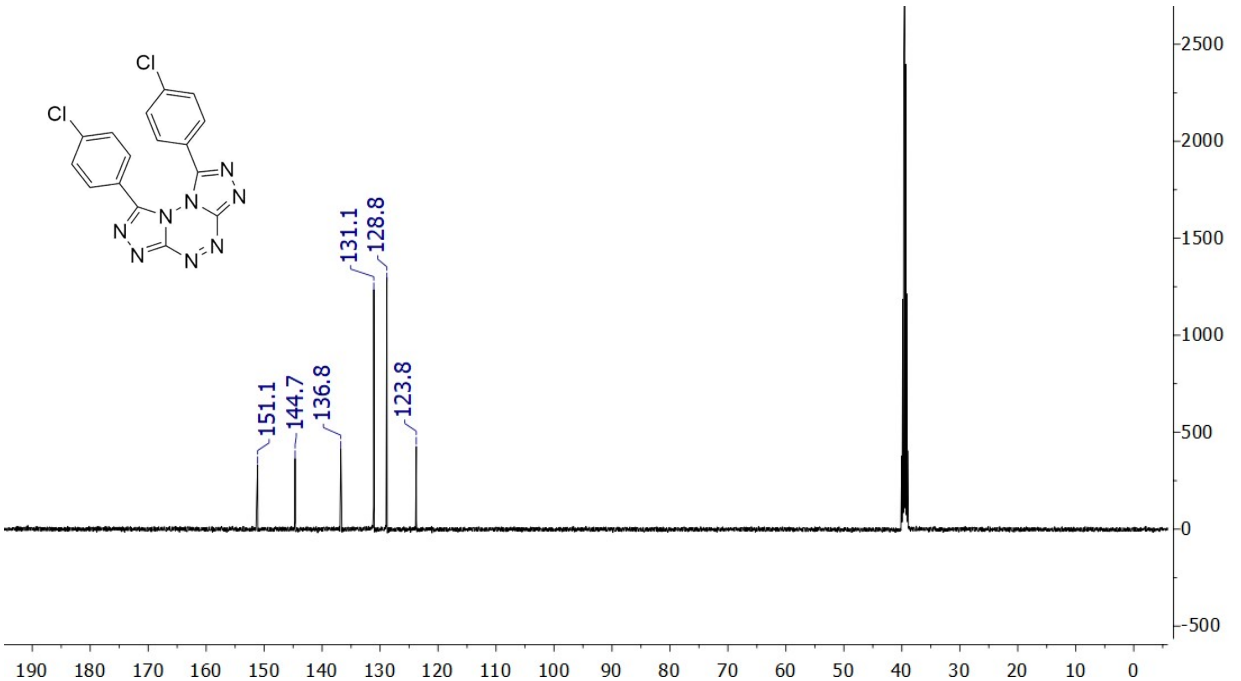


Figure S30. ^{13}C NMR spectrum of the 1,8-di(4-chlorophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3d)**.

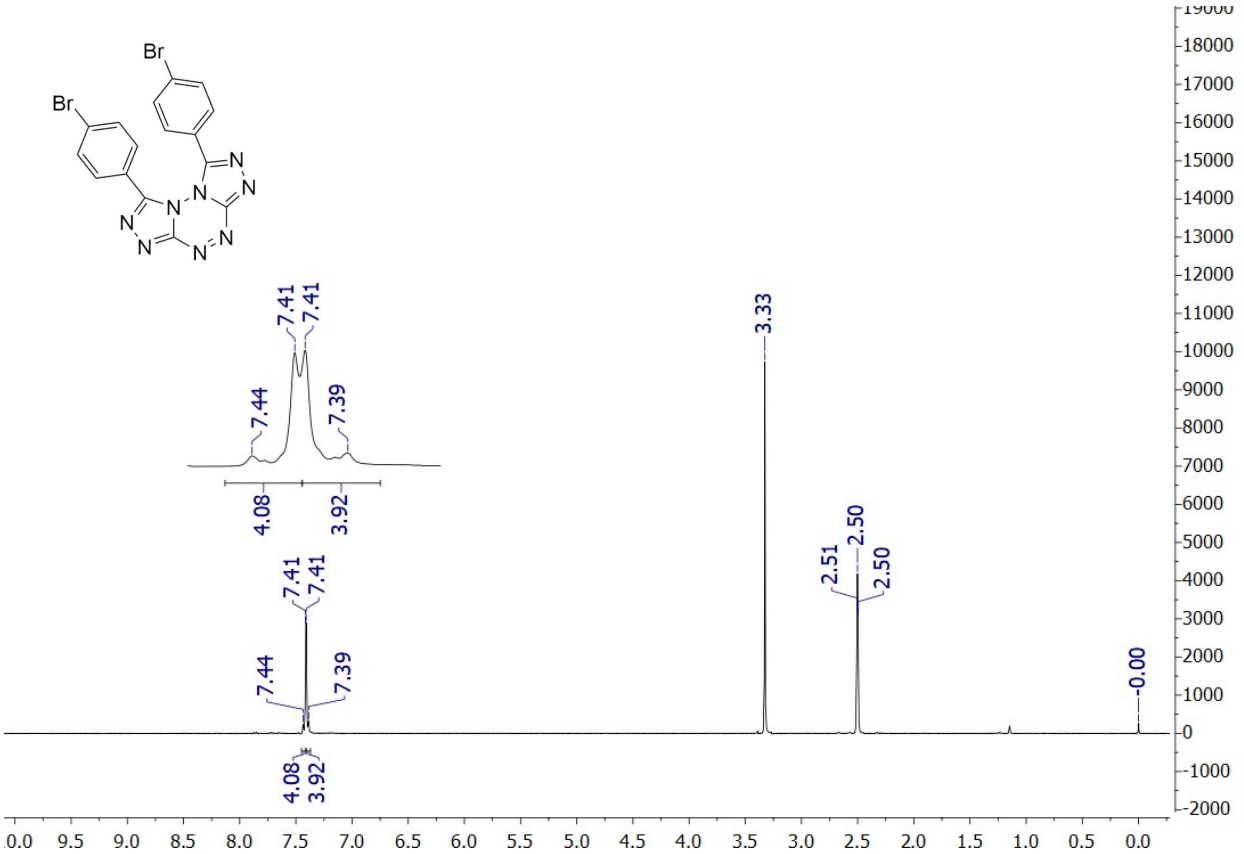


Figure S31. [1]H NMR spectrum of the 1,8-di(4-bromophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3e)**.

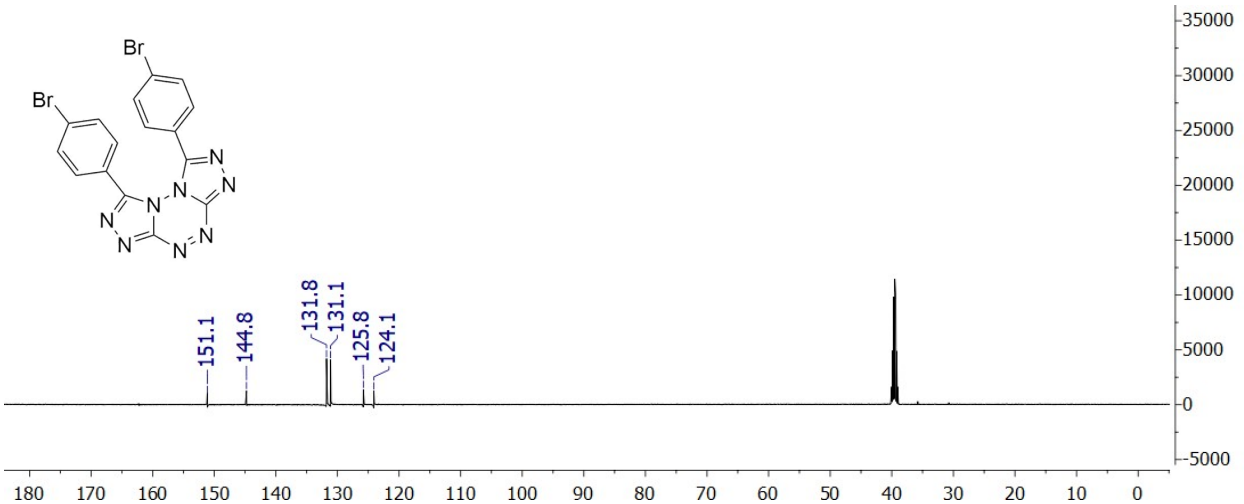


Figure S32. [13]C NMR spectrum of the 1,8-di(4-bromophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3e)**.

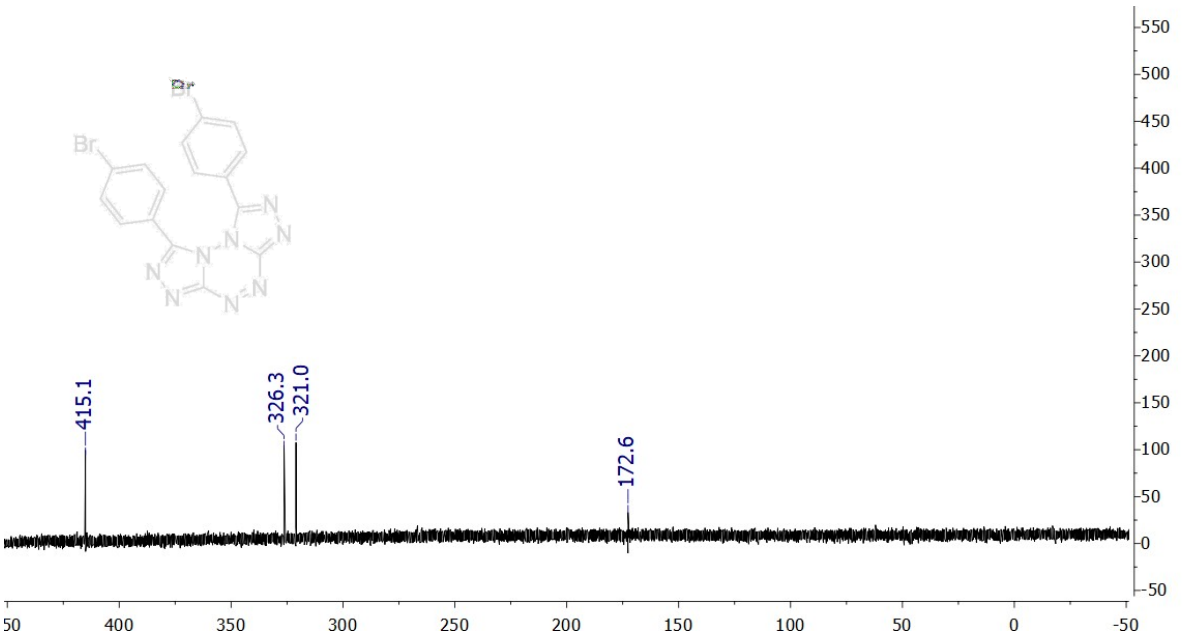


Figure S33. ^{15}N NMR spectrum of the 1,8-di(4-bromophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3e)**.

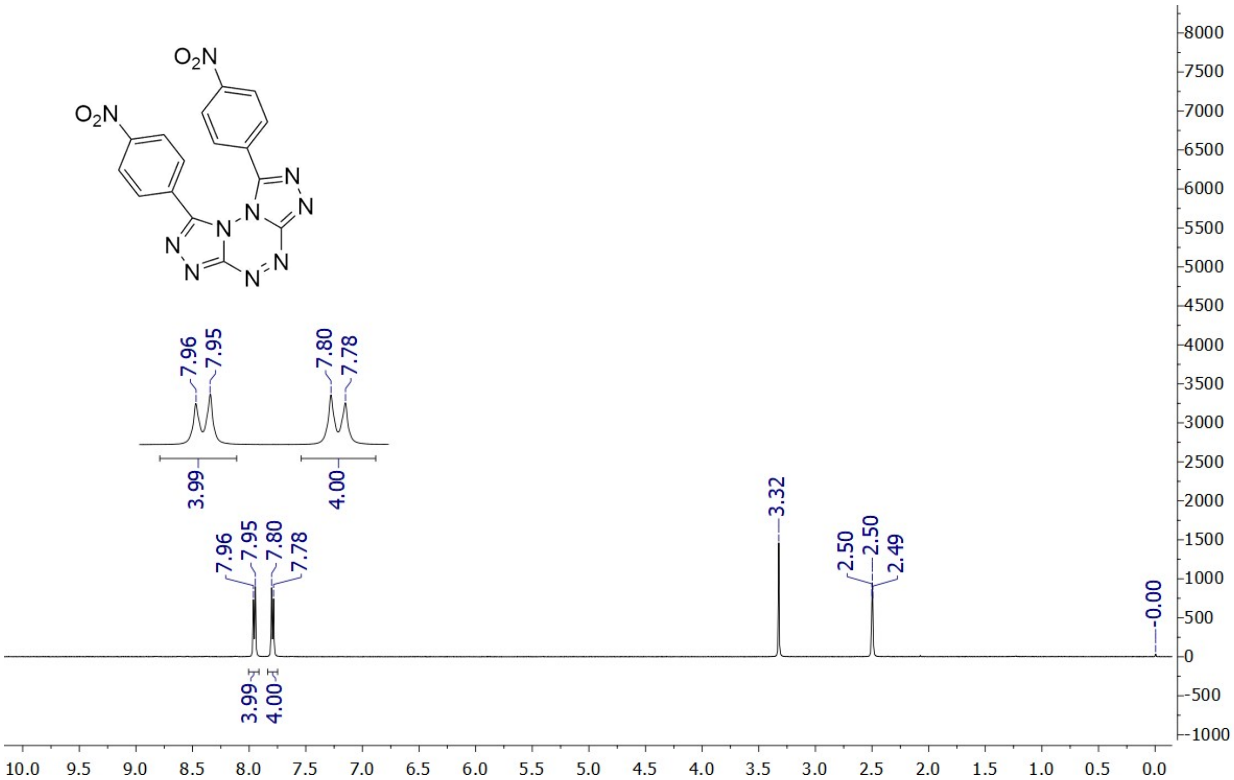


Figure S34. ^{1}H NMR spectrum of the 1,8-di(4-nitrophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3f)**.

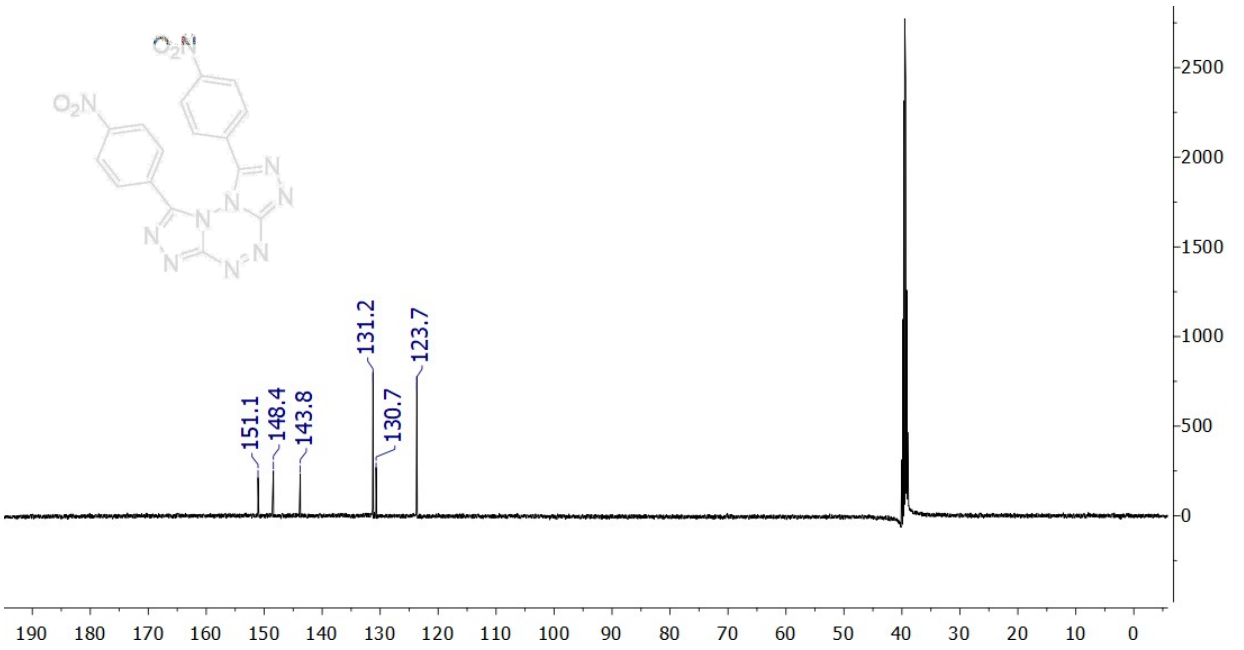


Figure S35. ^{13}C NMR spectrum of the 1,8-di(4-nitrophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3f)**.

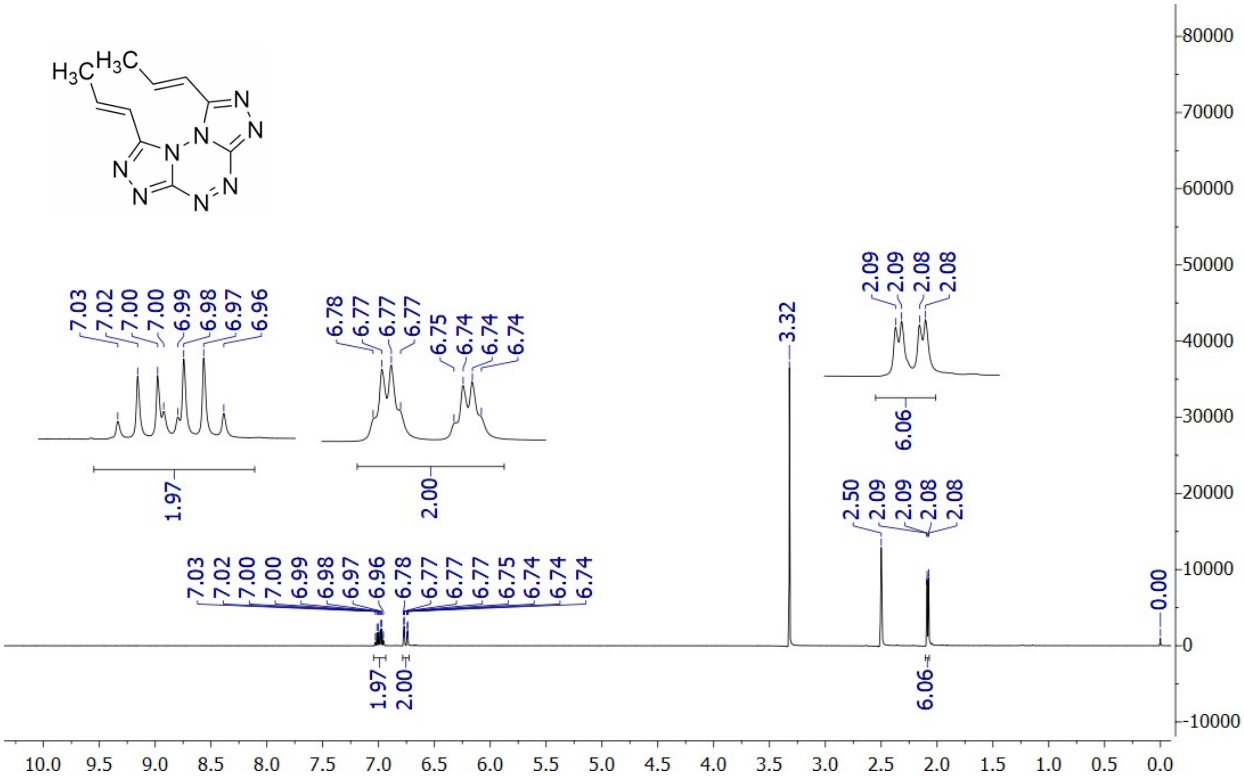


Figure S36. ^{1}H NMR spectrum of the 1,8-di(propen-1-yl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3g**).

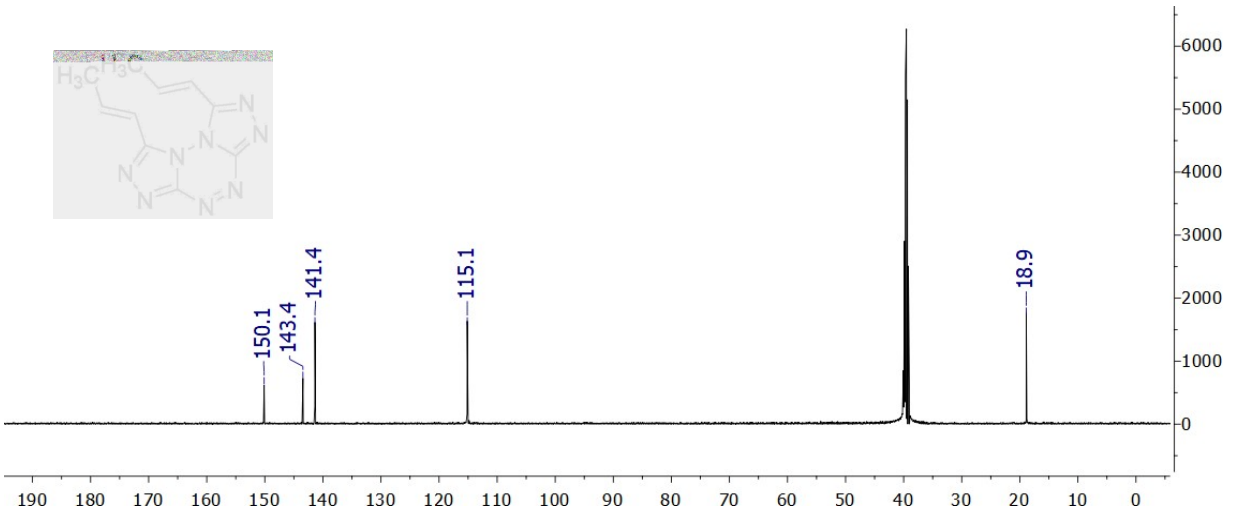


Figure S37. ^{13}C NMR spectrum of the 1,8-di(propen-1-yl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3g**).

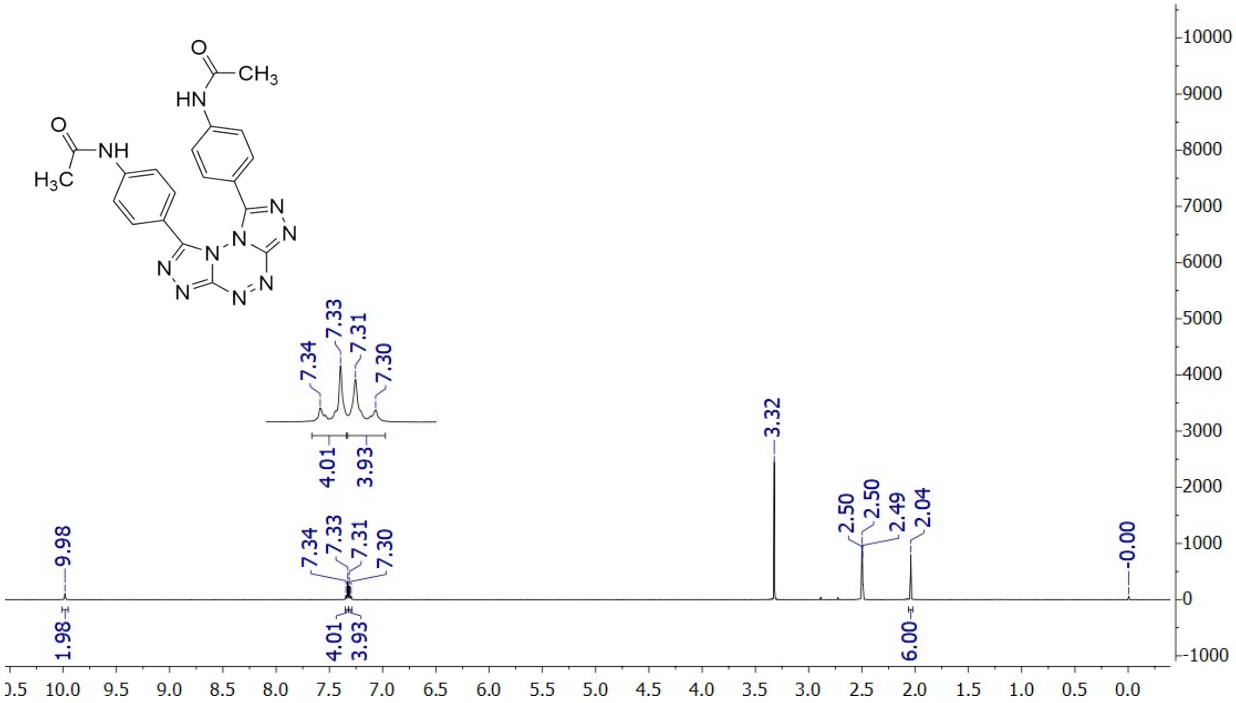


Figure S38. ^{1}H NMR spectrum of the 1,8-di(4-acetamidophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3h)**.

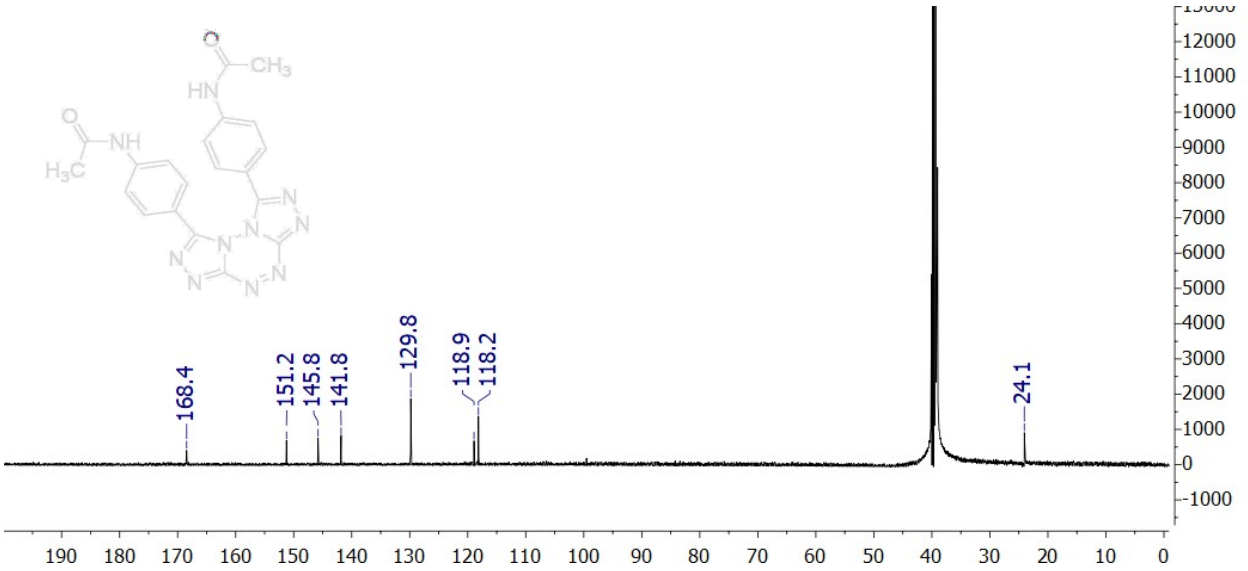


Figure S39. ^{13}C NMR spectrum of the 1,8-di(4-acetamidophenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine **(3h)**.

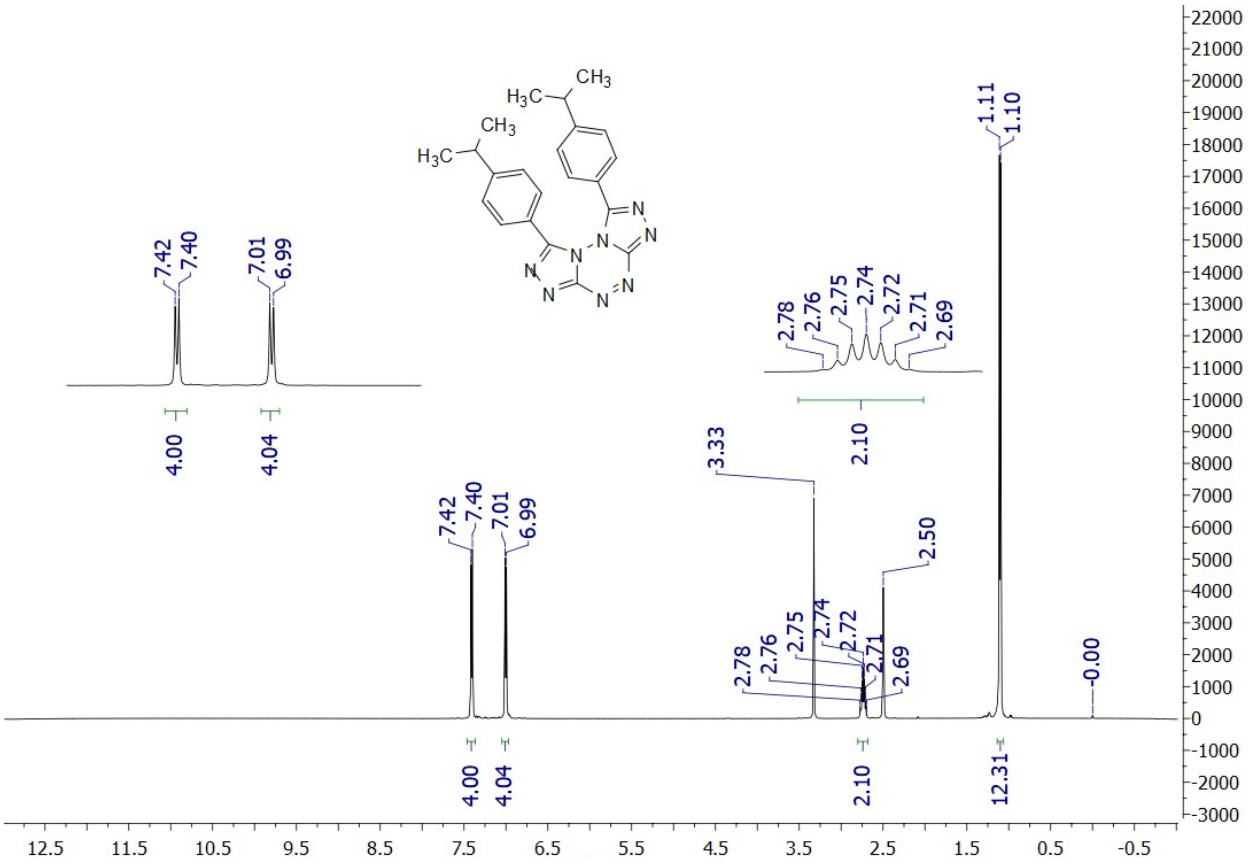


Figure S40. ^{1}H NMR spectrum of the 1,8-di(4-isopropylphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3i**).

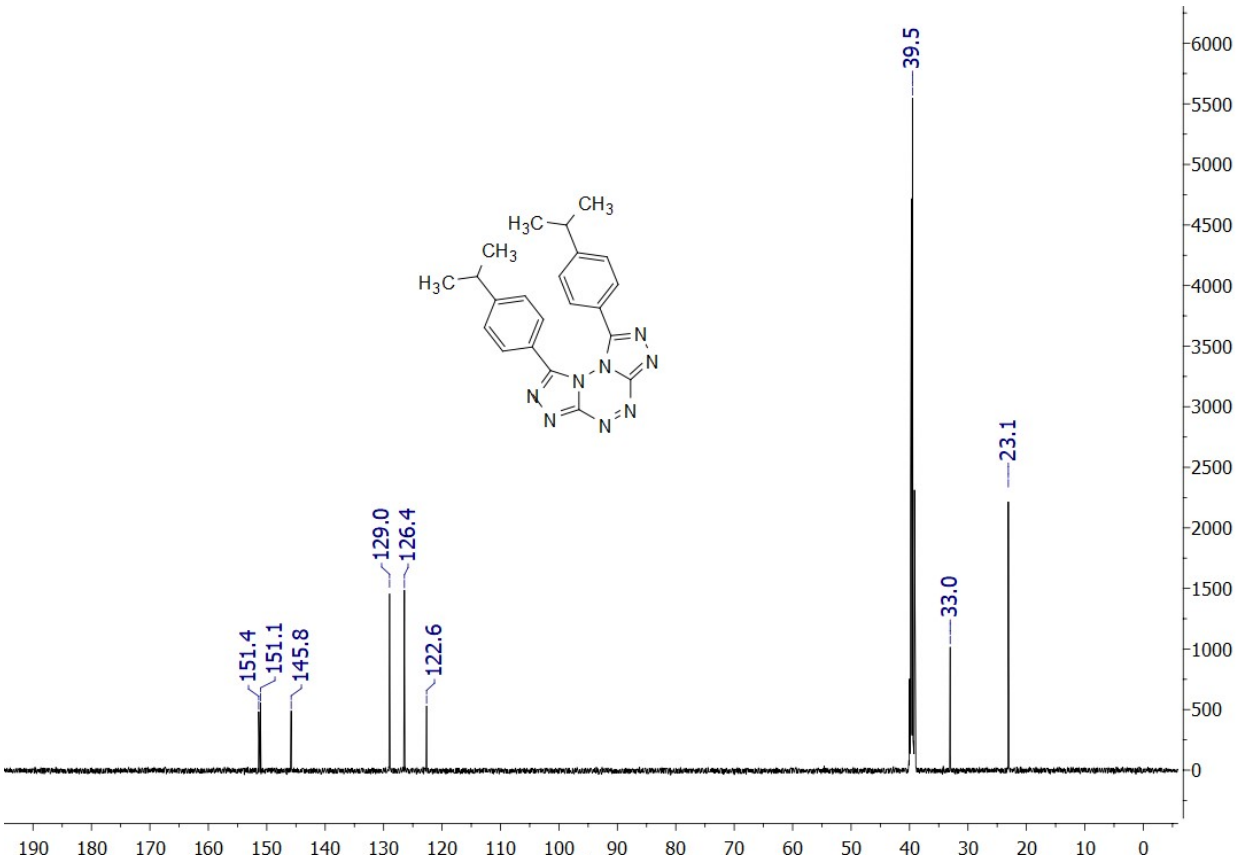


Figure S41. ^{13}C NMR spectrum of the 1,8-di(4-isopropylphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3i**).

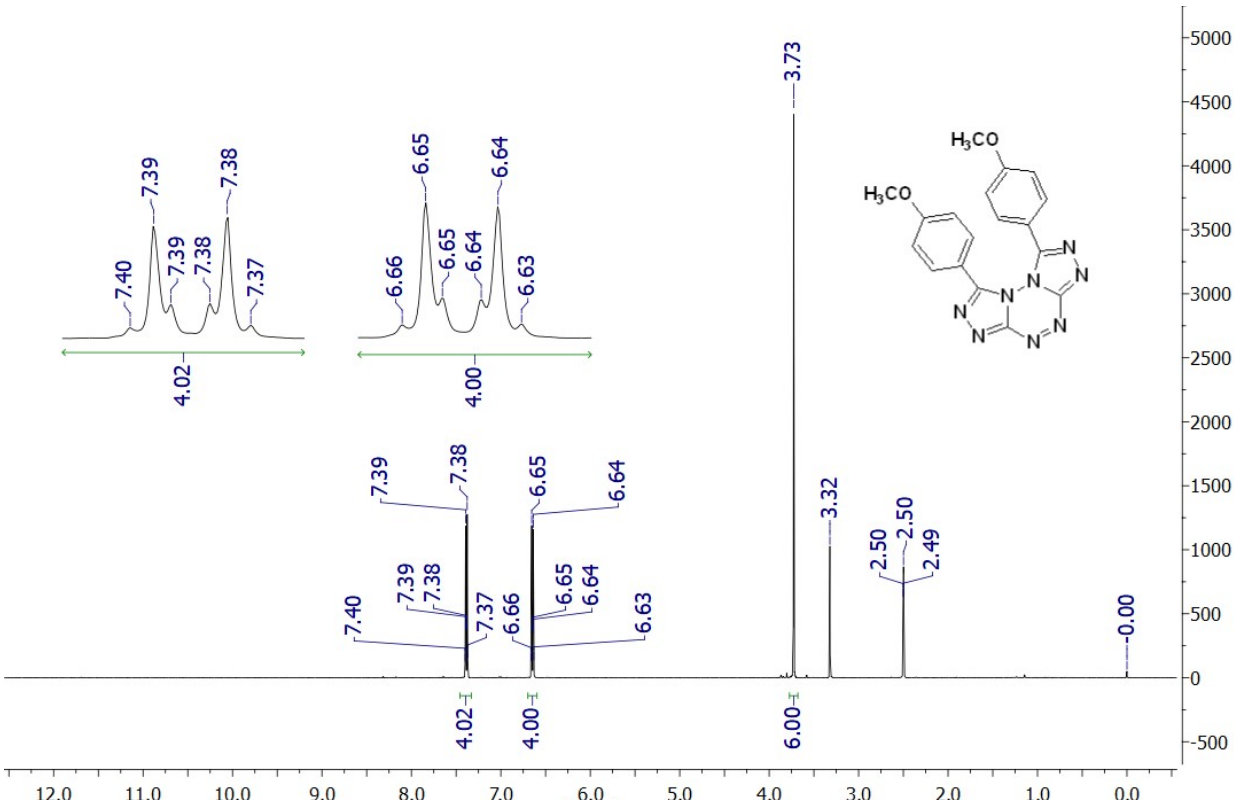


Figure S42. ^{1}H NMR spectrum of the 1,8-di(4-methoxyphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3j**).

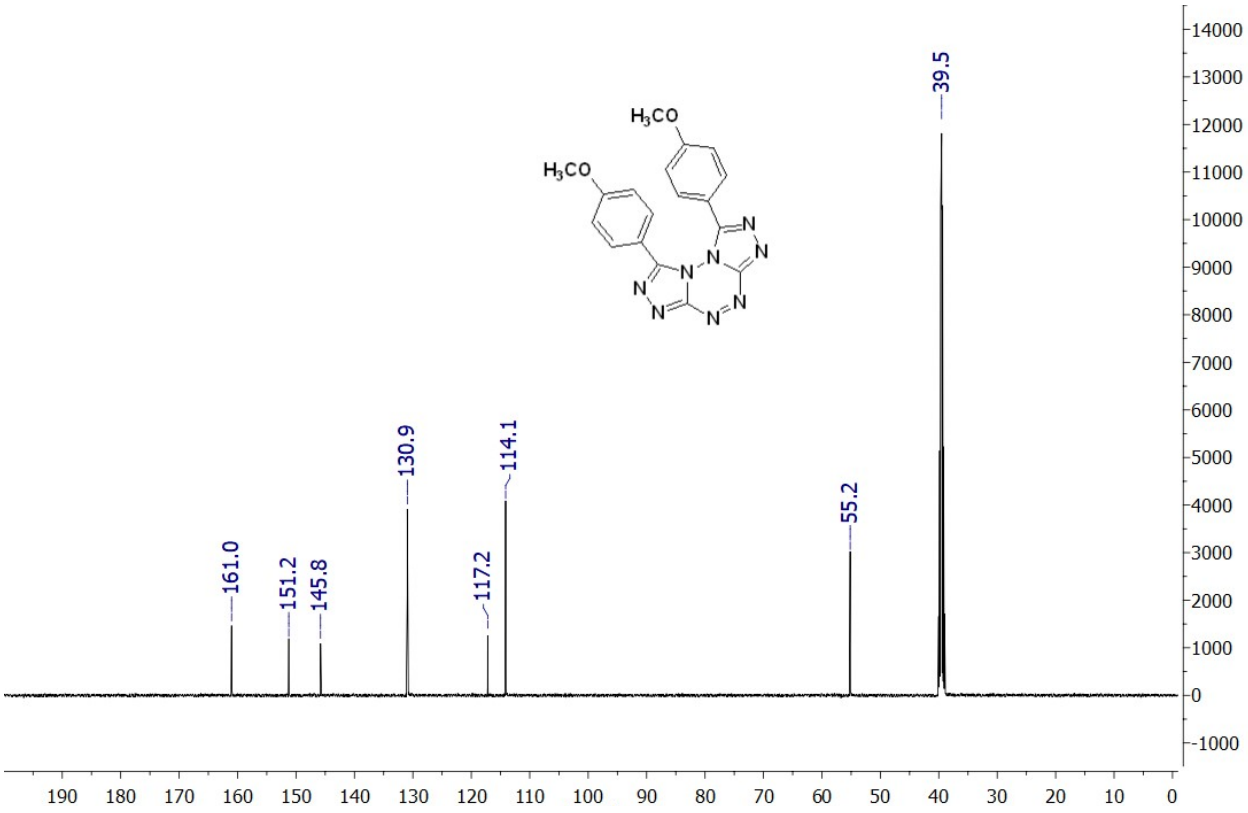


Figure S43. ^{13}C NMR spectrum of the 1,8-di(4-methoxyphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3j**).

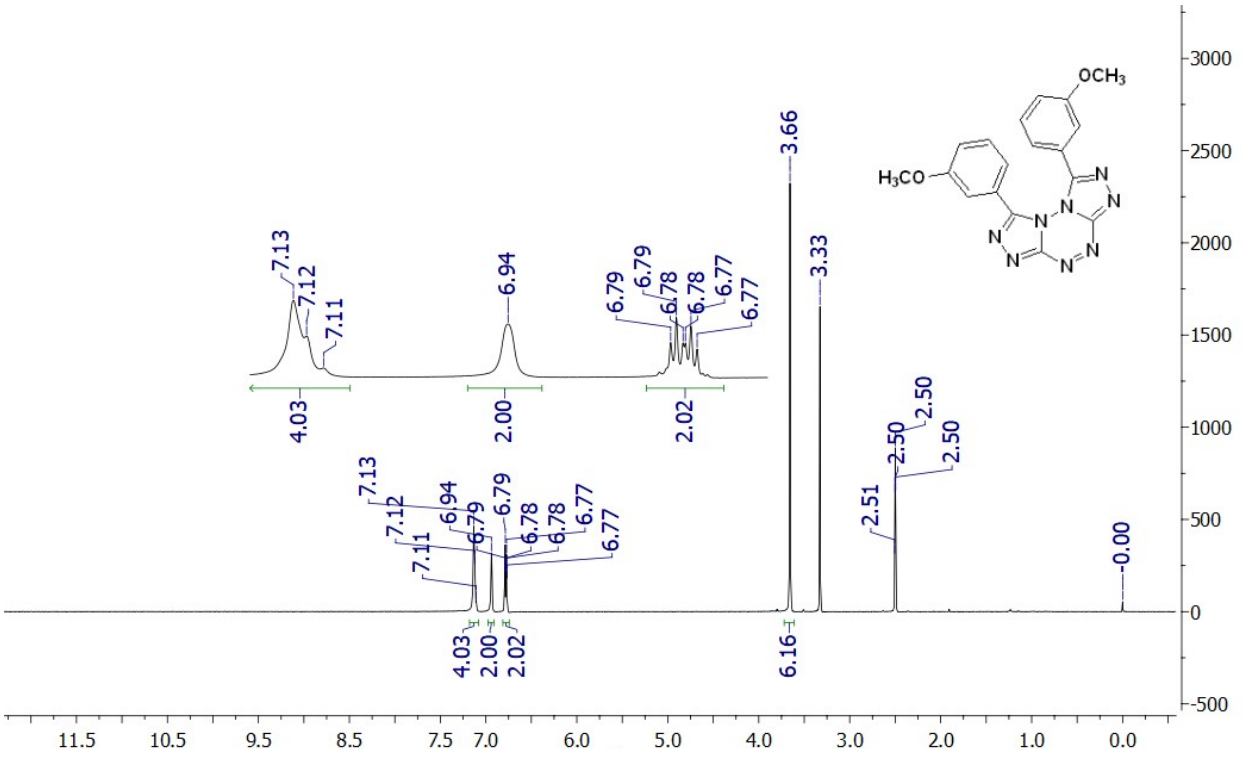


Figure S44. ^{1}H NMR spectrum of the 1,8-di(3-methoxyphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3k**).

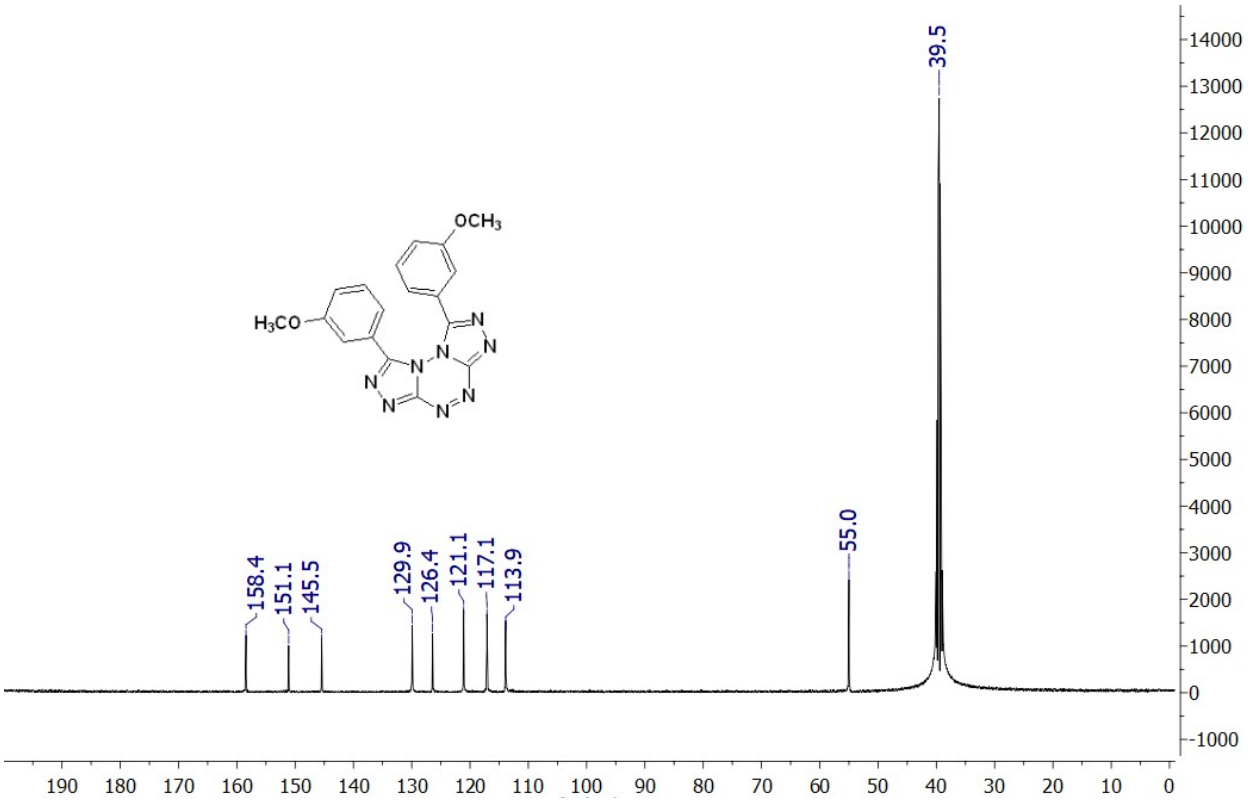


Figure S45. ^{13}C NMR spectrum of the 1,8-di(3-methoxyphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3k**).

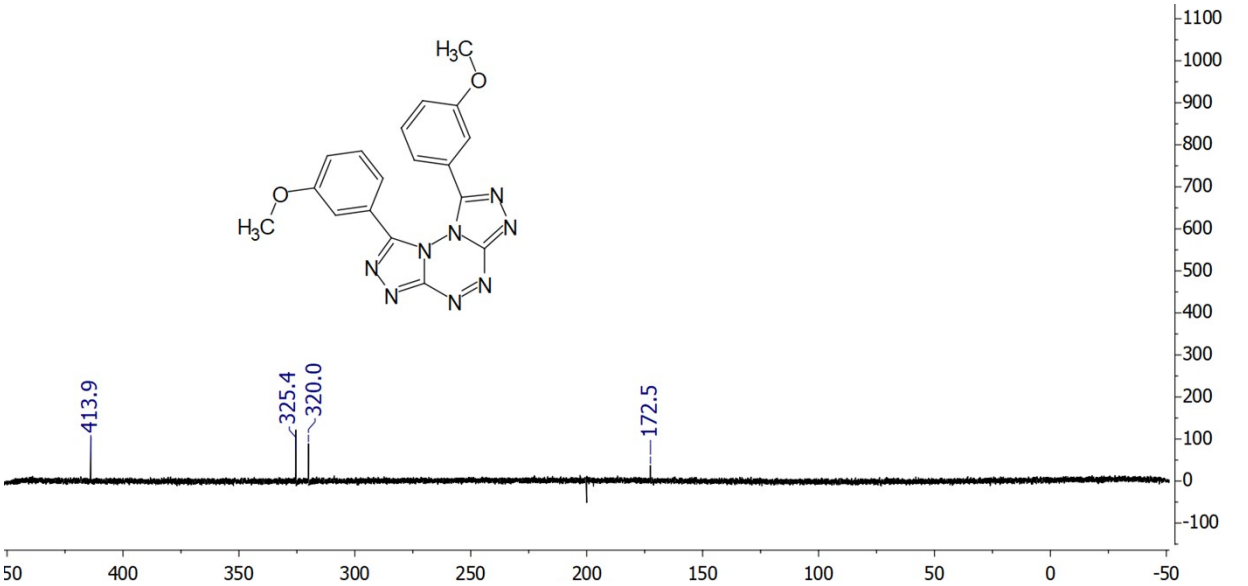


Figure S46. ^{15}N NMR spectrum of the 1,8-di(3-methoxyphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3k**).

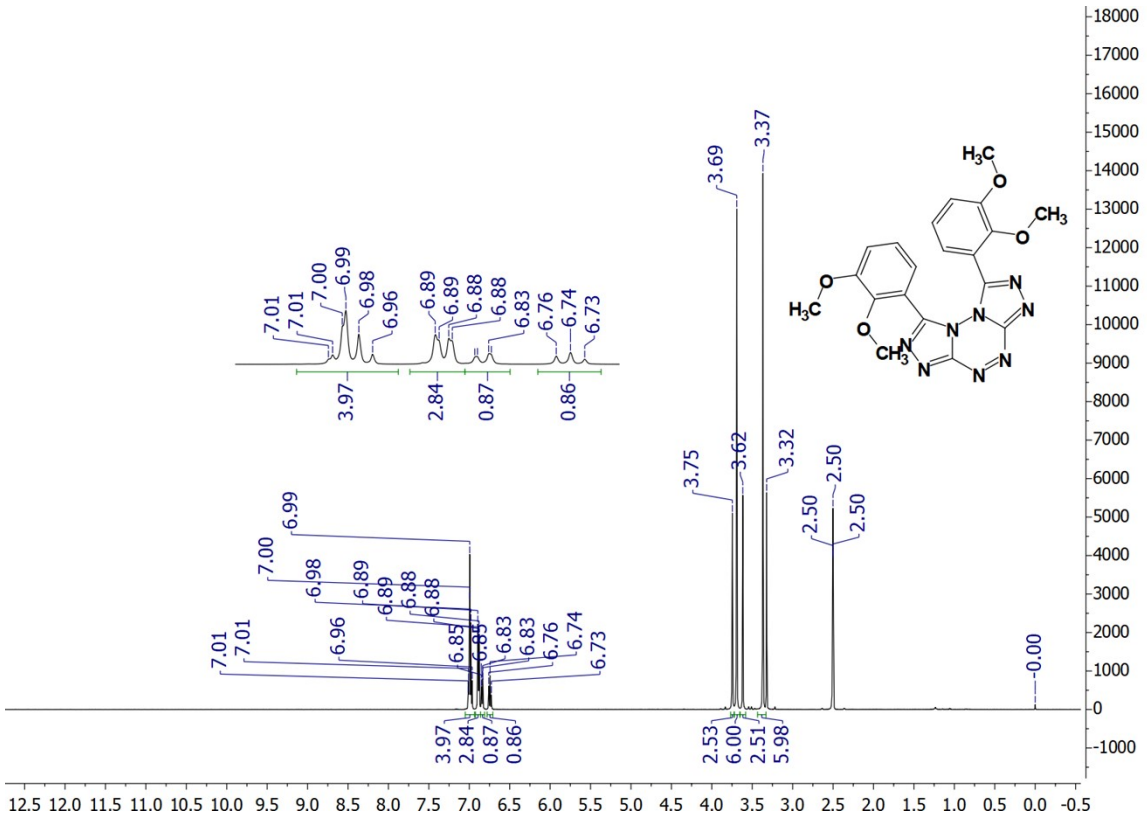


Figure S47. ^{1}H NMR spectrum of the 1,8-di(2,3-dimethoxyphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3l**).

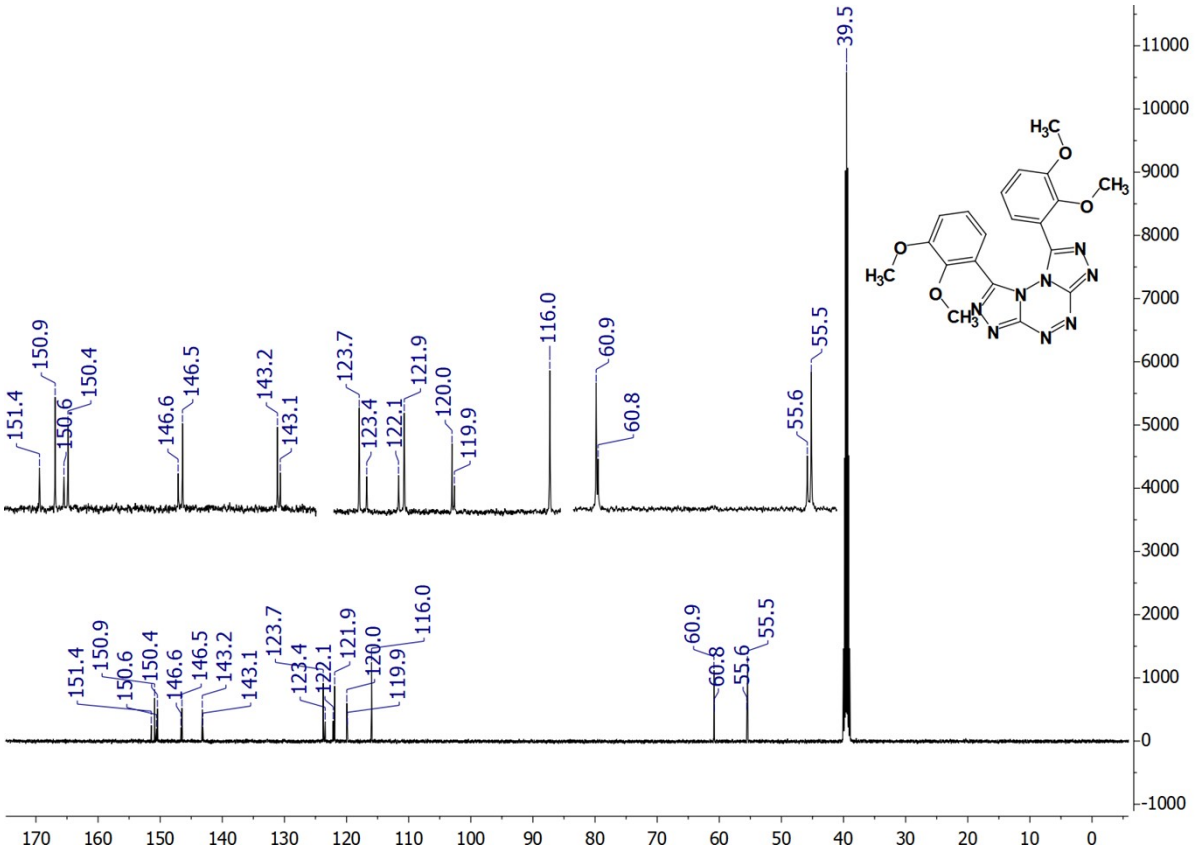


Figure S48. ^{13}C NMR spectrum of the 1,8-di(2,3-dimethoxyphenyl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3l**).

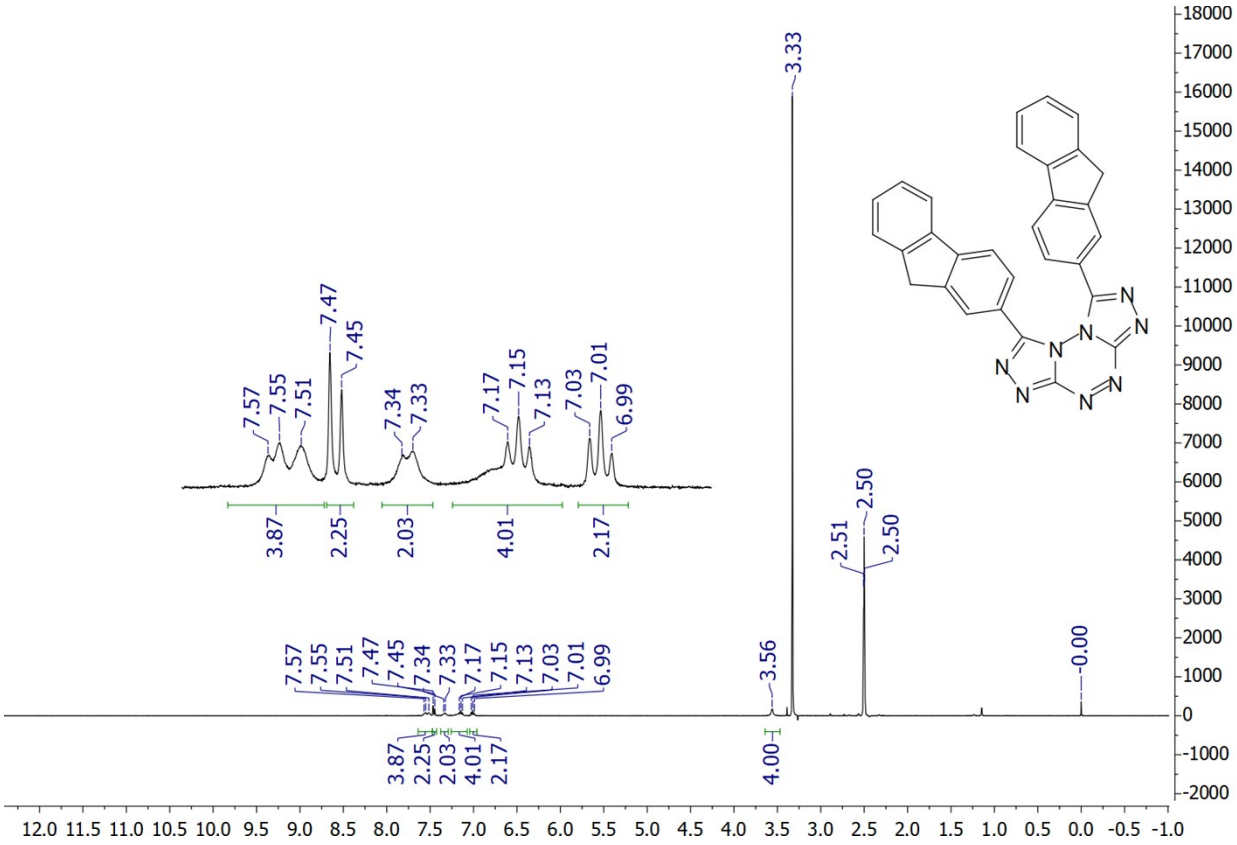


Figure S49. ^{1}H NMR spectrum of the 1,8-di(9H-fluoren-2-yl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3n**).

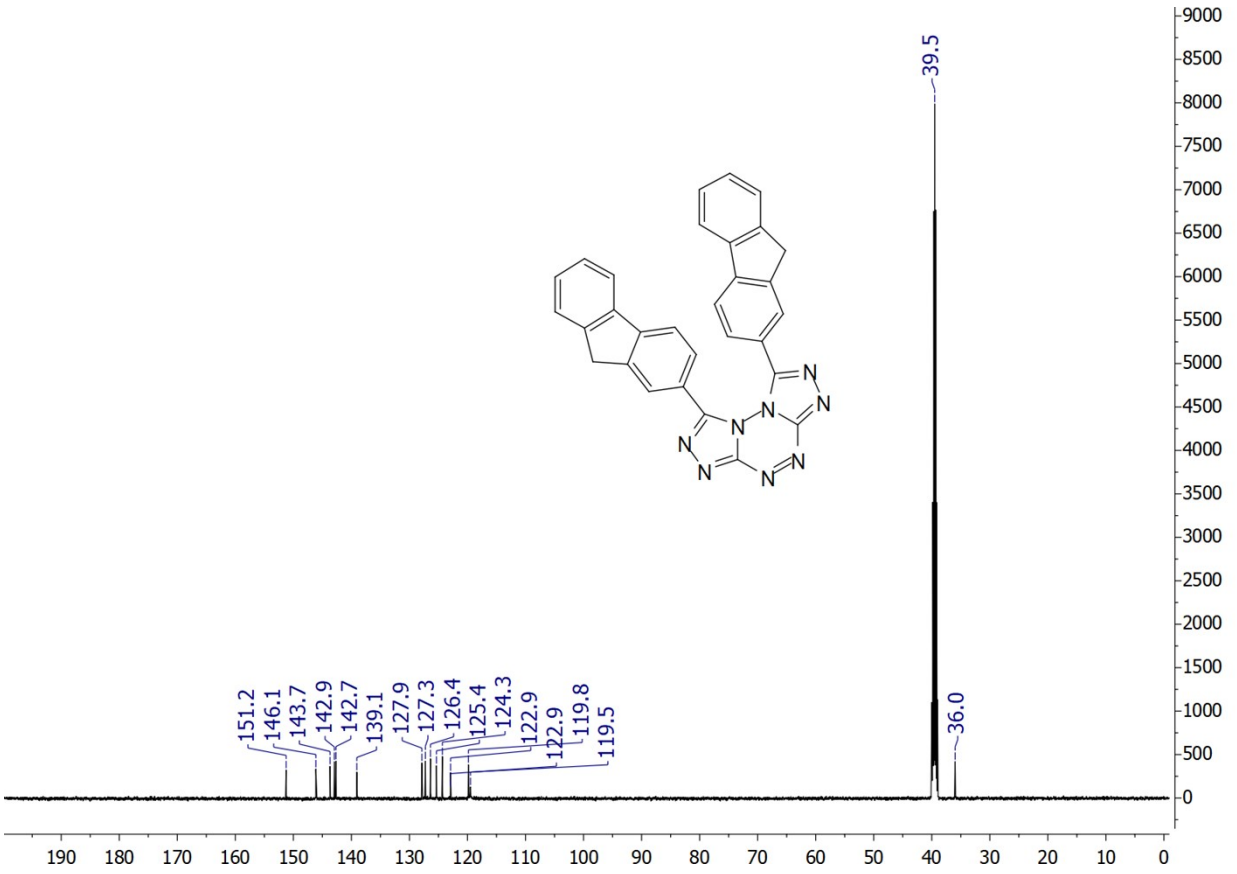


Figure S50. ^{13}C NMR spectrum of the 1,8-di(9H-fluoren-2-yl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3n**).

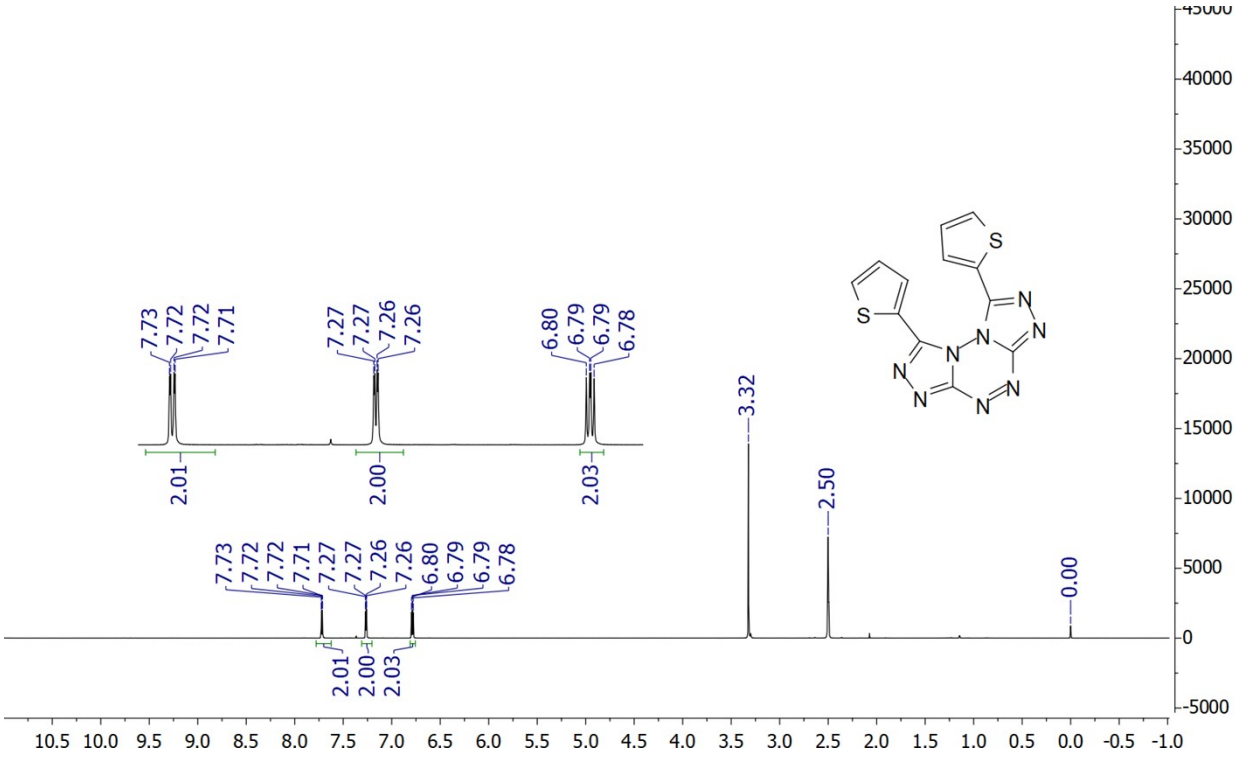


Figure S51. [1]H NMR spectrum of the 1,8-di(thiophen-2-yl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3o**)

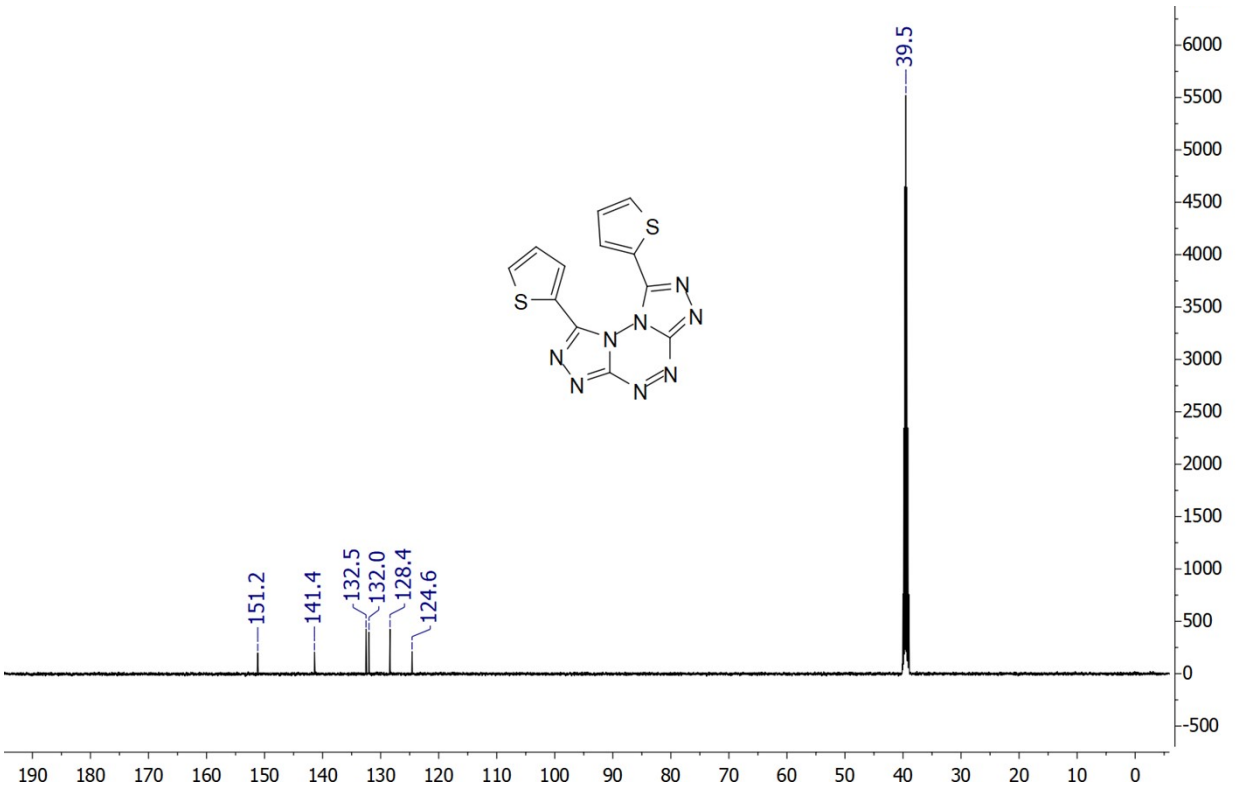


Figure S52. [13]C NMR spectrum of the 1,8-di(thiophen-2-yl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3o**)

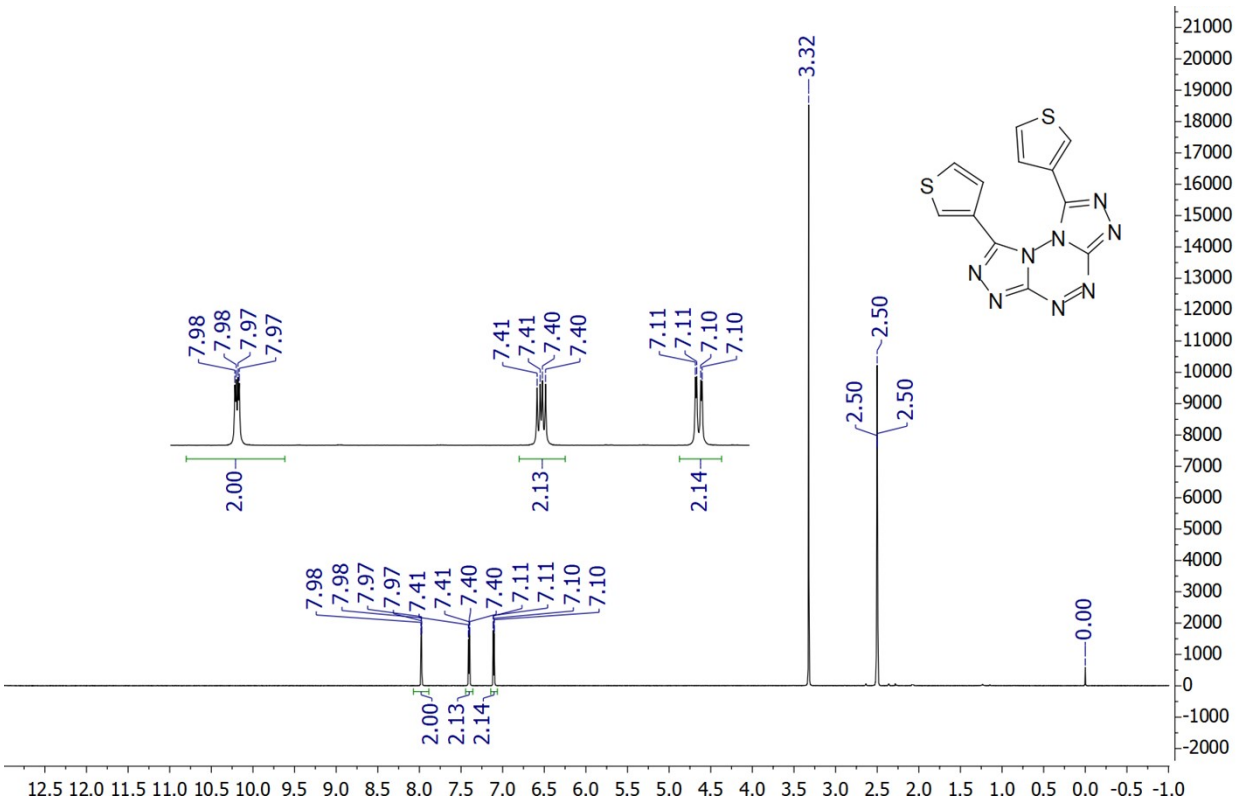


Figure S53. ^{1}H NMR spectrum of the 1,8-di(thiophen-3-yl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3p**)

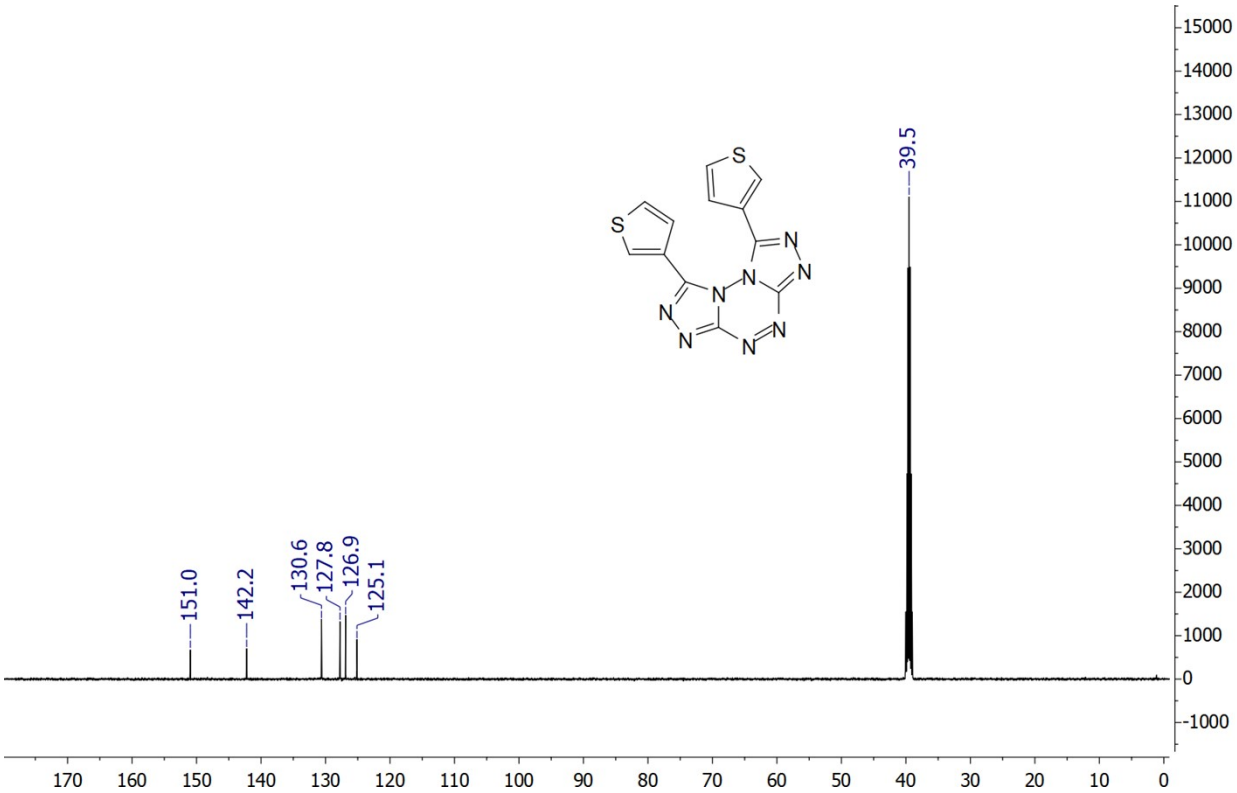


Figure S54. ^{13}C NMR spectrum of the 1,8-di(thiophen-3-yl)bis[1,2,4]triazolo[4,3-*b*:3',4'-*f*][1,2,4,5]tetrazine (**3p**)

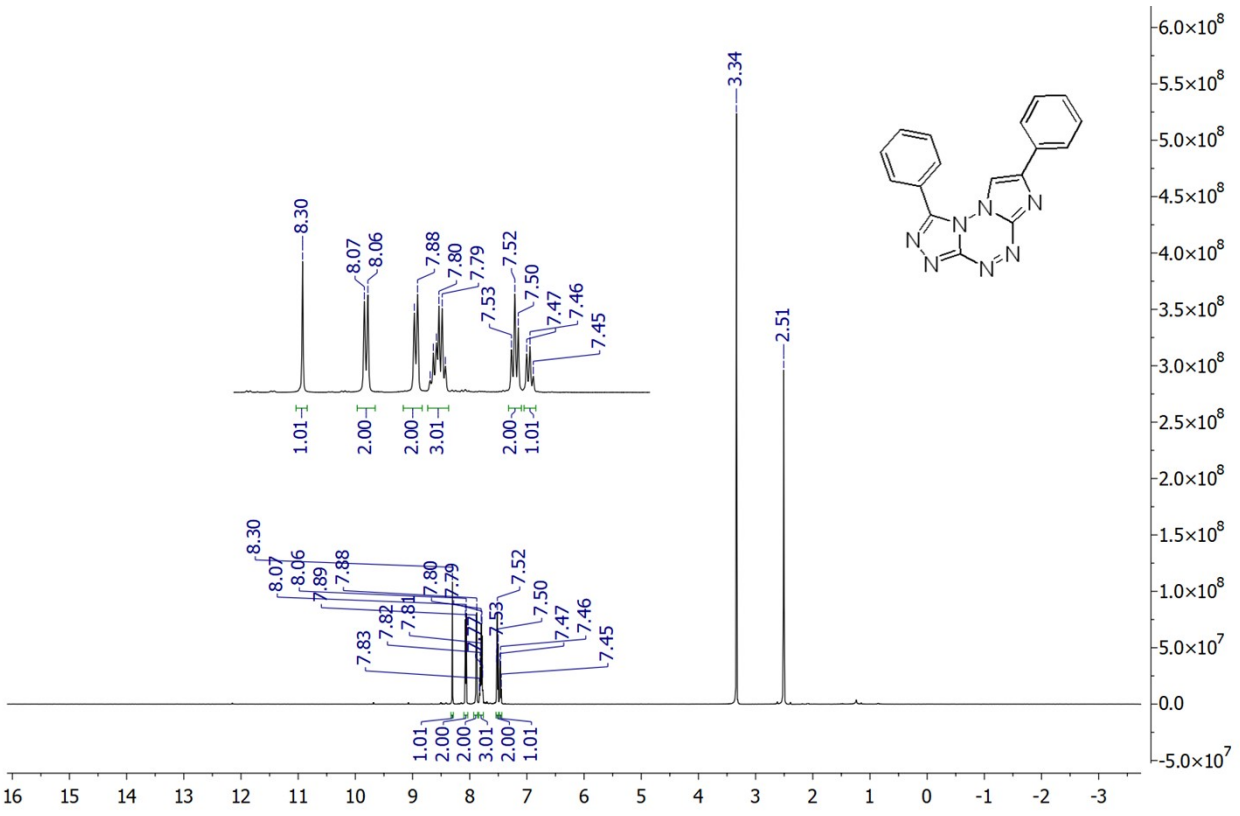


Figure S55. ^{1}H NMR spectrum of the 1,7-diphenylimidazo[1,2-*b*][1,2,4]triazolo[3,4-*f*][1,2,4,5]tetrazine (**5-*cis***)

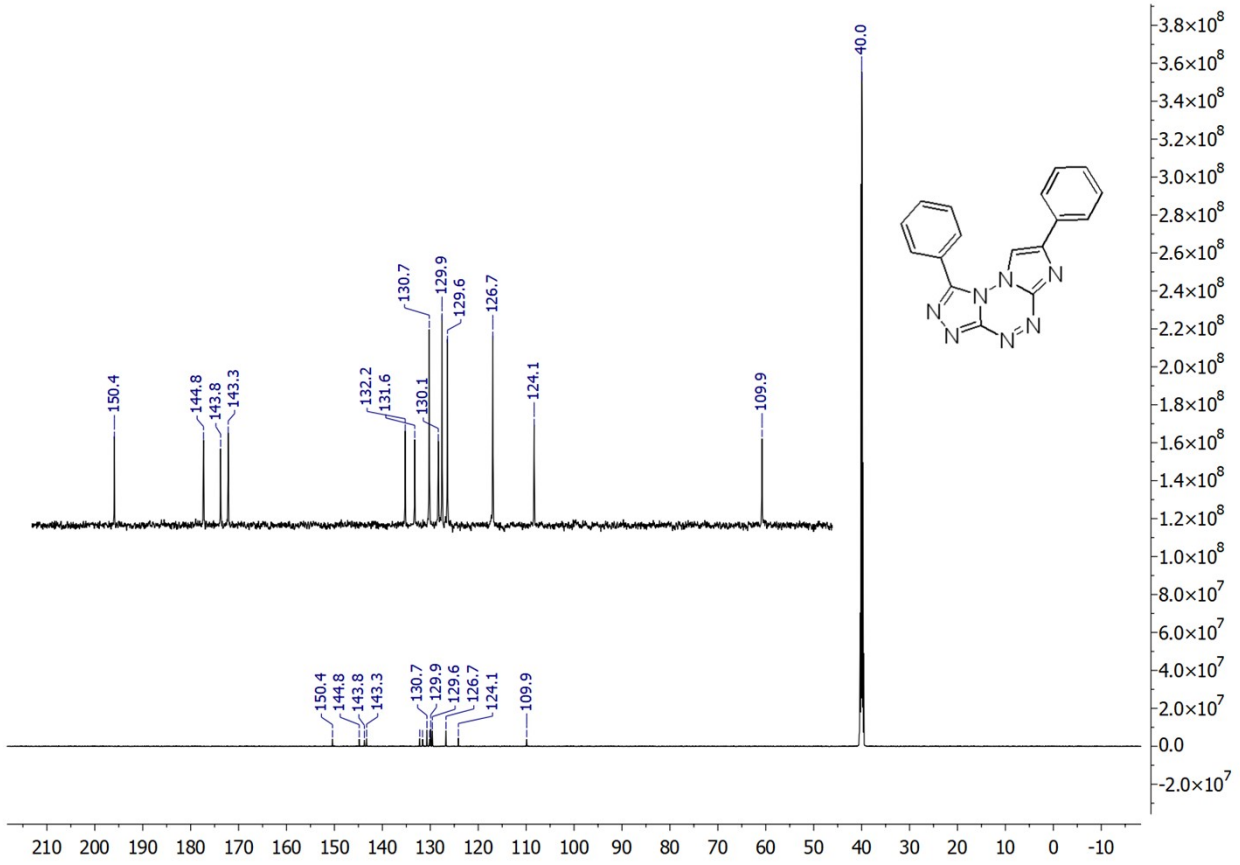


Figure S56. ^{13}C NMR spectrum of the 1,7-diphenylimidazo[1,2-*b*][1,2,4]triazolo[3,4-*f*][1,2,4,5]tetrazine (**5-*cis***)

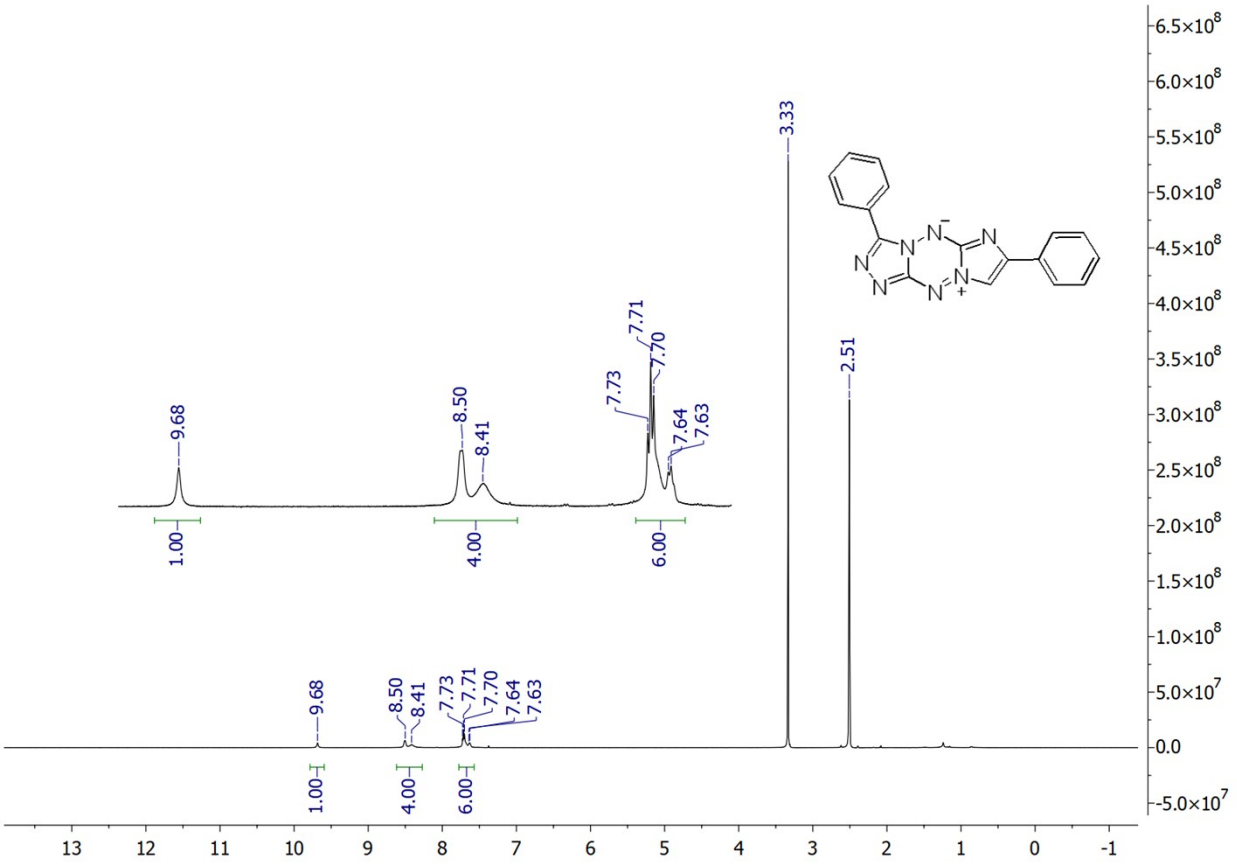


Figure S57. ^{1}H NMR spectrum of the 1,7-diphenylimidazo[1,2-*b*][1,2,4]triazolo[4,3-*e*][1,2,4,5]tetrazine (**5-*trans***)

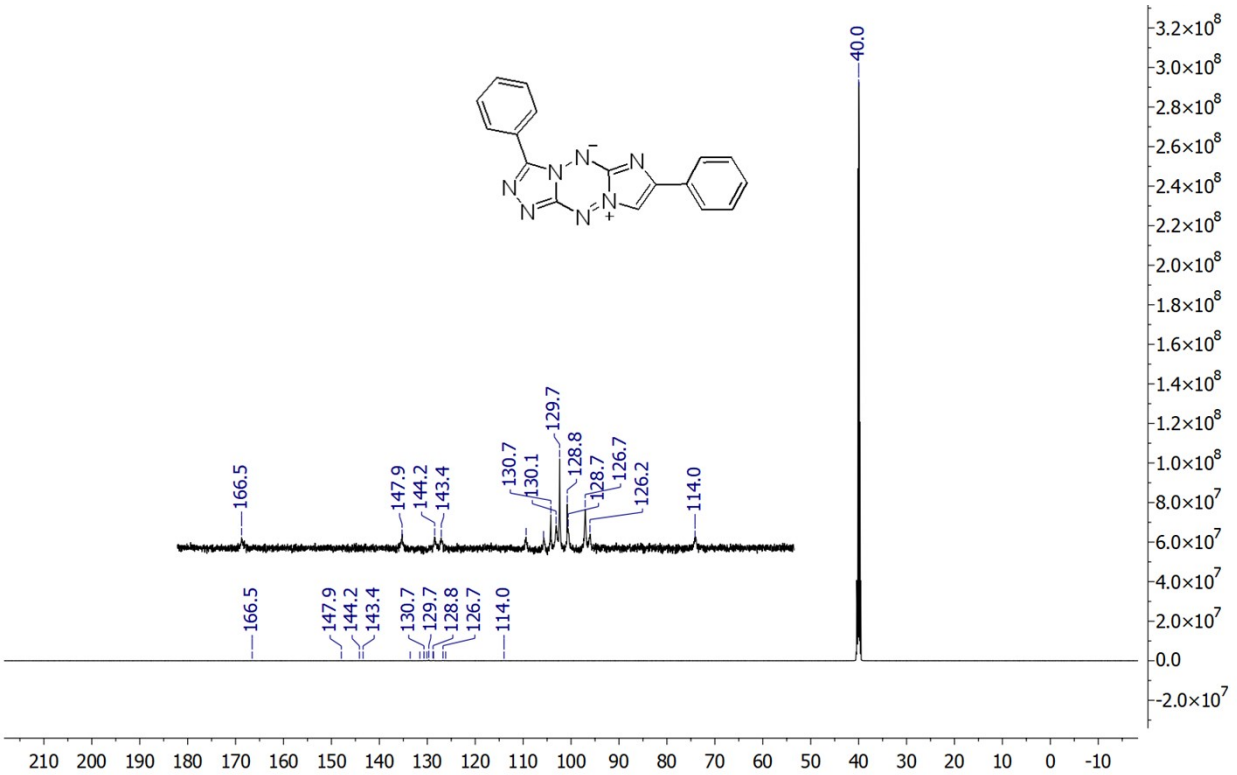


Figure S58. ^{13}C NMR spectrum of the 1,7-diphenylimidazo[1,2-*b*][1,2,4]triazolo[4,3-*e*][1,2,4,5]tetrazine (**5-*trans***)

3. X-ray data

The X-ray crystallography data for the structures was deposited with Cambridge Crystallography Data Centre as supplementary publication CCDC 2301657 (compound **3a**) and CCDC 2301658 (compound **3l**). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via *www.ccdc.cam.ac.uk/data_request/cif*.

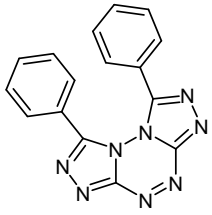
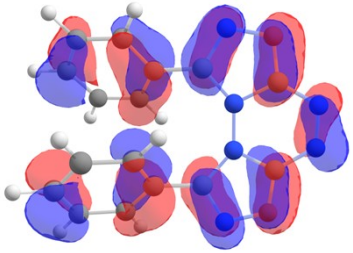
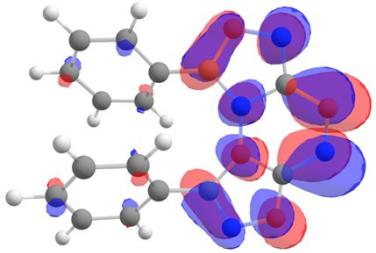
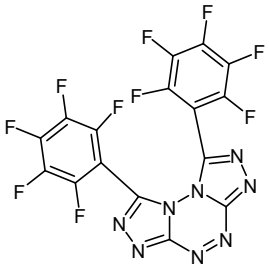
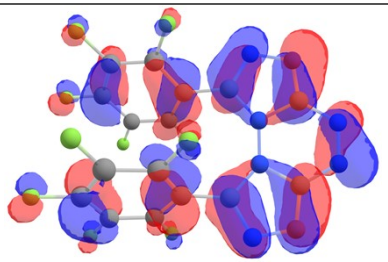
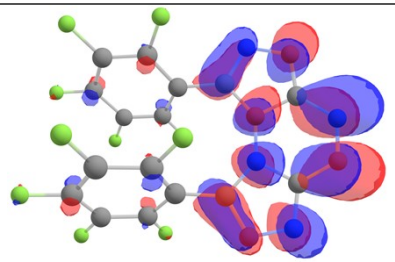
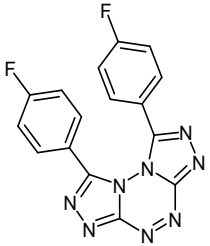
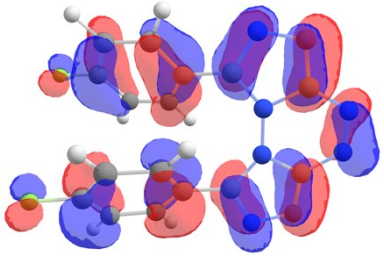
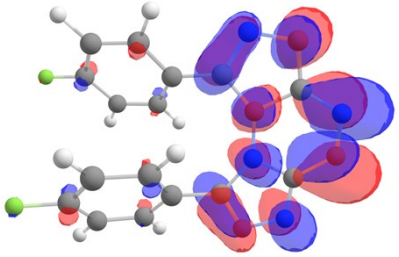
3a: Yellow needle crystal 0.51x0.26x0.05 mm. On the angles $5.40 < 2\theta < 52.78°$ 6837 reflections was collected, 4592 independent reflections (R_{int}= 0.0471), 1720 reflections with I>2σ(I). Completeness 98.2 %. Absorption correction not applied (μ= 0.093 mm^{-1}). Crystal system is orthorhombic, space group $P2_12_12$, a = 21.273(4) Å, b= 7.2489(12) Å, c= 15.064(3) Å, V=2322.9(7) $Å^3$, formula $C_{50}H_{33}N_{25}$ (for Z= 2). Final refinement parameters: R_1= 0.1546, wR_2= 0.0579 (all data), R_1= 0.0407, wR_2= 0.0456 (I>2σ(I)), GooF= 0.717. Maximum/minimum of residual electronic density Δρē= 0.146/-0.160 ē$Å^{-3}$.

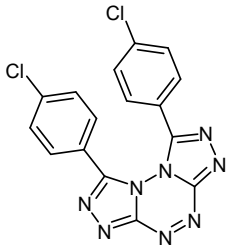
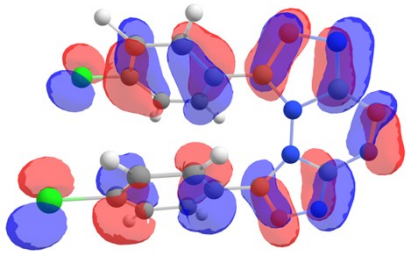
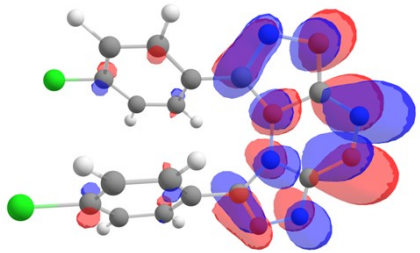
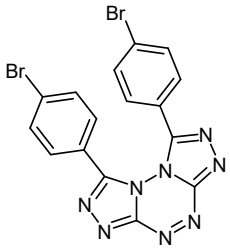
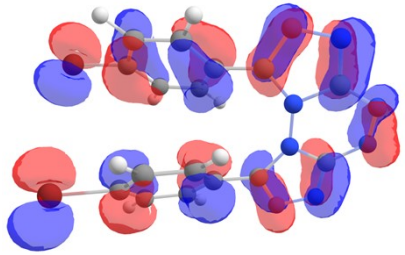
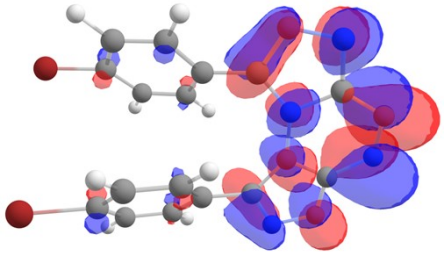
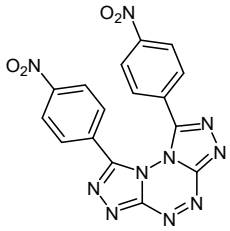
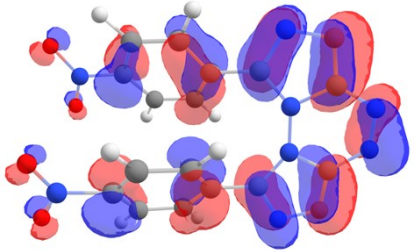
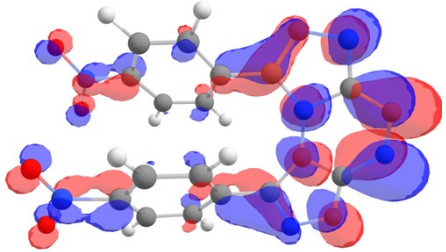
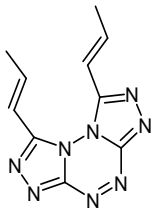
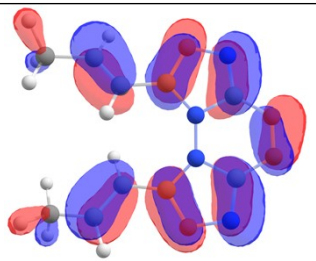
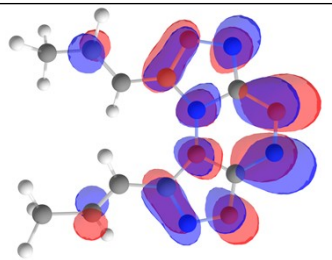
3l: Brown prismatic crystal 0.35x0.30x0.25 mm. On the angles $5.42 < 2\theta < 52.74°$ 17062 reflections were collected, 5705 independent reflections (R_{int}= 0.0688), 1913 reflections with I>2σ(I). Completeness 99.0 %. Empirical absorption correction was applied (μ= 0.100 mm^{-1}). Crystal system is monoclinic, space group P2/c, a = 14.290(3) Å, b= 7.870(3) Å, c= 25.420(9) Å, β= 100.45(2)°, V= 2811.2(17) $Å^3$, formula $C_{29}H_{27}N_8O_6$ (for Z= 4). Final refinement parameters: R_1= 0.1729, wR_2= 0.0505 (all data), R_1= 0.0436, wR_2= 0.0453 (I>2σ(I)), GooF= 0.886. Maximum/minimum of residual electronic density Δρē= 0.174/-0.147 ē$Å^{-3}$.

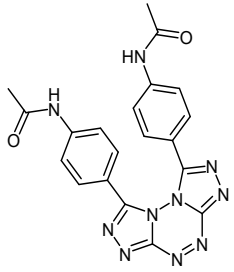
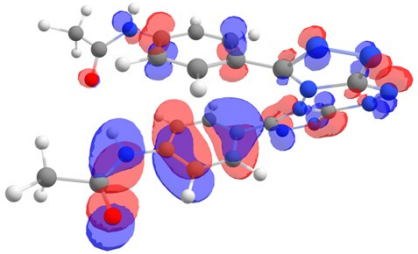
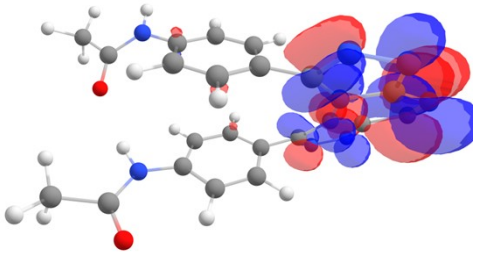
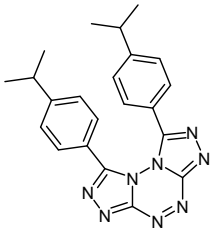
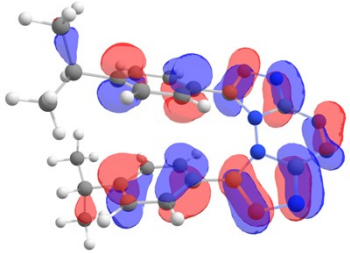
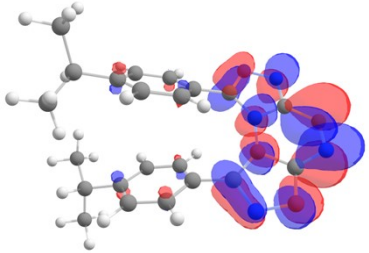
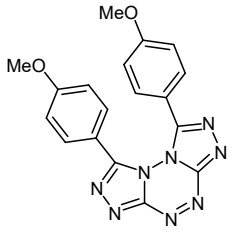
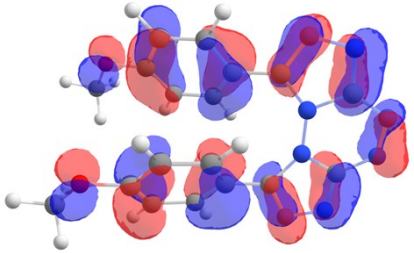
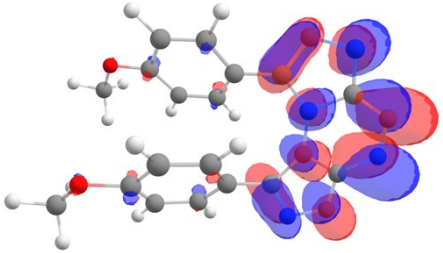
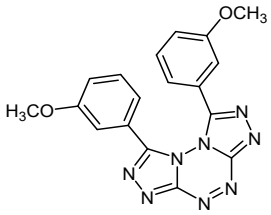
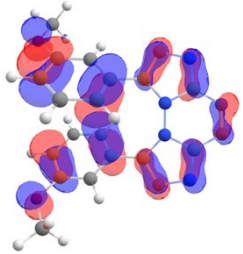
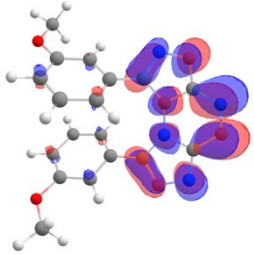
4. Quantum chemical calculations

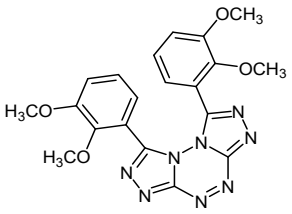
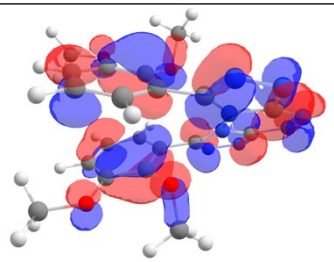
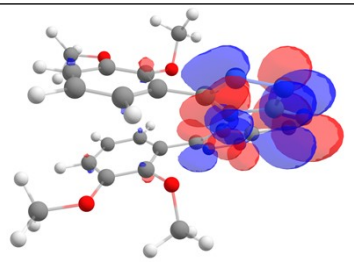
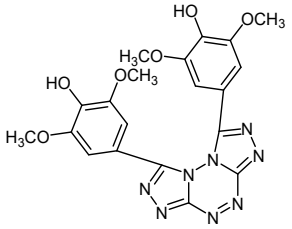
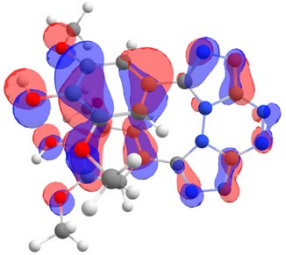
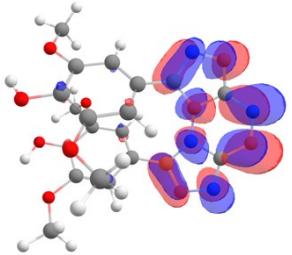
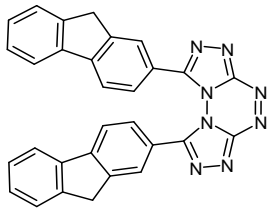
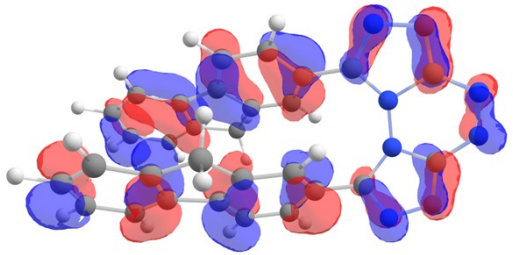
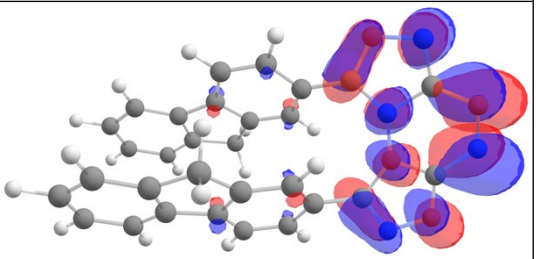
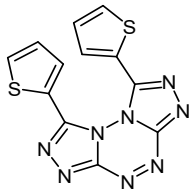
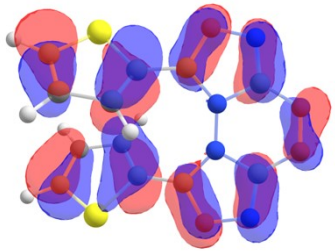
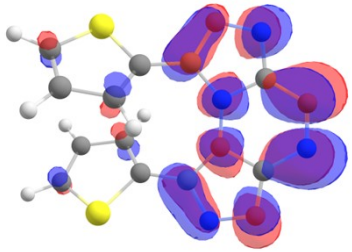
4.1 DFT calculations

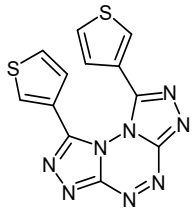
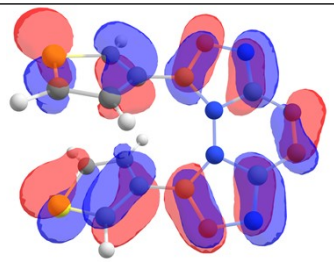
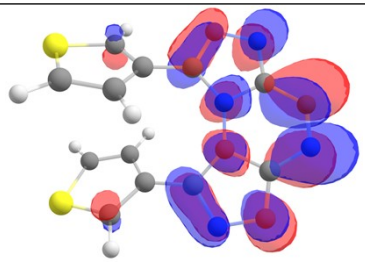
Table S2. Visualization of the electron density distribution of HOMO and LUMO in series of compounds **3** (PBE0/def2-TZVP).

Comp.	Structure	HOMO	LUMO
3a		 -7.11 eV	 -3.24 eV
3b		 -7.94 eV	 -3.73eV
3c		 -7.18 eV	 -3.35 eV

3d		 -7.16 eV	 -3.40 eV
3e		 -7.13 eV	 -3.43 eV
3f		 -7.87 eV	 -3.89 eV
3g		 -7.11 eV	 -3.13 eV

3h		 -6.76 eV	 -3.14 eV
3i		 -6.86 eV	 -3.13 eV
3j		 -6.55 eV	 -3.04eV
3k		 -6.73 eV	 -3.19 eV

3l		 -6.76 eV	 -2.84 eV
3m		 -6.18 eV	 -3.01 eV
3n		 -6.51 eV	 -3.13 eV
3o		 -6.88 eV	 -3.33 eV

3p		 -7.08 eV	 -3.23 eV

Visualization of orbitals for B3LYP/6-311G* is not presented, because visually they are similar to those presented above; the values of the calculated energies are given in **Table S3** below.

Table S3. Calculated energies HOMO, LUMO; width of theoretical and optical band gaps

Comp.	HOMO (B3LYP/6-311G*), eV	LUMO (B3LYP/6-311G*), eV	HOMO (PBE0/def2-TZPV), eV	LUMO (PBE0/def2-TZPV), eV	ΔE (B3LYP/6-311G*), eV	ΔE (PBE0/def2-TZPV), eV	ΔEopt, eV
3a	-6.78	-3.33	-7.11	-3.24	3.45	3.87	2.62
3b	-7.69	-3.88	-7.94	-3.73	3.80	4.21	2.96
3c	-6.88	-3.47	-7.18	-3.35	3.41	3.82	2.63
3d	-6.91	-3.54	-7.16	-3.40	3.37	3.76	2.62
3e	-6.83	-3.54	-7.14	-3.43	3.30	3.71	2.62
3f	-7.56	-3.98	-7.87	-3.89	3.58	3.98	2.78
3g	-7.11	-3.60	-7.11	-3.13	3.52	3.98	2.68
3h	-6.39	-3.24	-6.76	-3.14	3.15	3.62	2.21
3i	-6.56	-3.23	-6.86	-3.13	3.32	3.73	2.52
3j	-6.23	-3.14	-6.55	-3.04	3.09	3.51	2.46
3k	-6.39	-3.28	-6.73	-3.19	3.10	3.55	2.60
3l	-6.36	-2.88	-6.76	-2.84	3.48	3.92	2.55
3m	-5.88	-3.13	-6.18	-3.01	2.75	3.17	-
3n	-6.18	-3.22	-6.51	-3.13	2.96	3.39	2.51
3o	-6.57	-3.44	-6.88	-3.33	3.13	3.55	2.35
3p	-6.80	-3.36	-7.08	-3.25	3.44	3.83	2.52

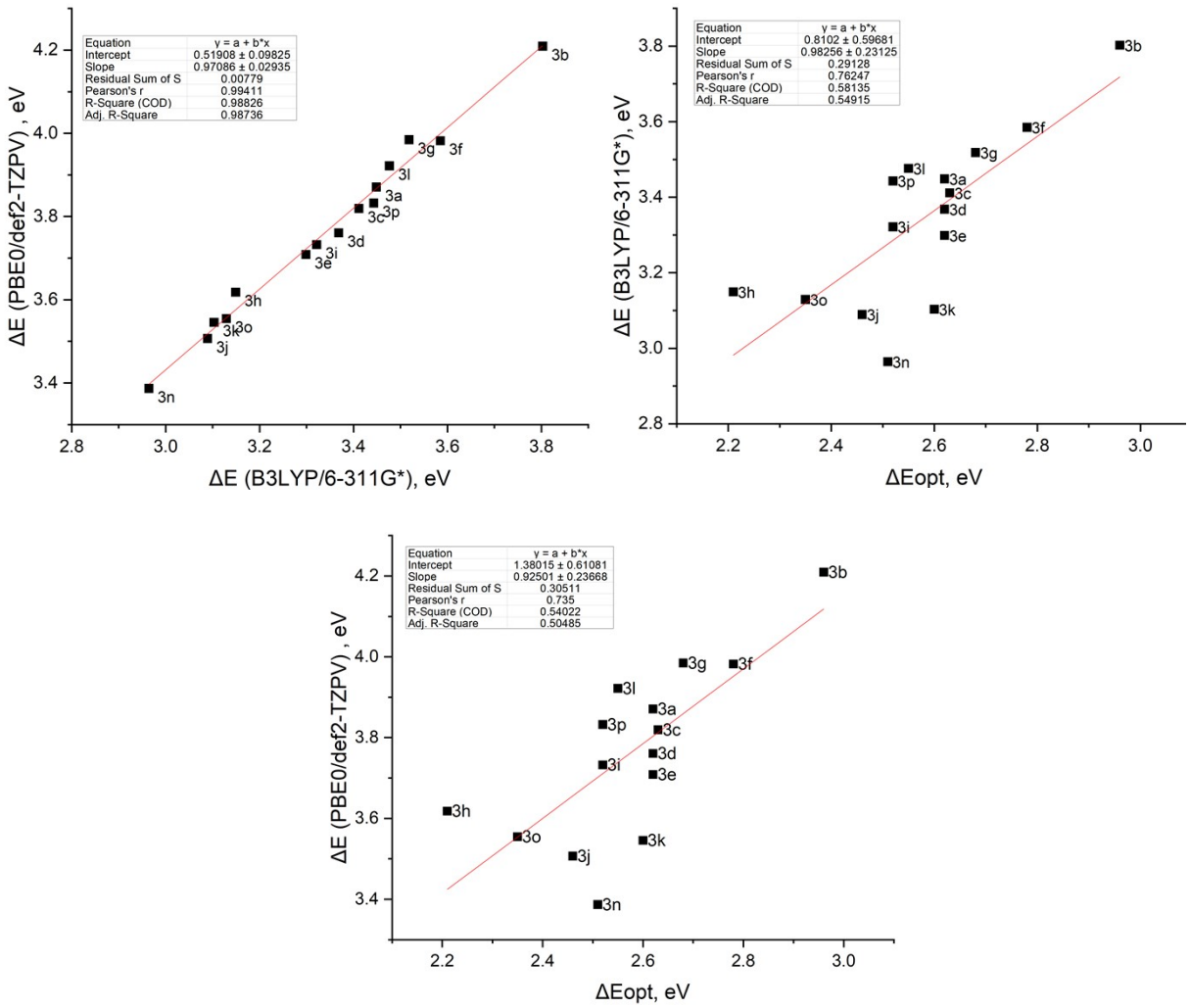


Fig S59. Linear correlation between theoretical bandgap from DFT calculations and optical bandgap from absorption-emission spectra (ΔEopt). ΔEopt is calculated as the intersection point of the reduced and normalized absorption and emission spectra.[8]

4.2 TDDFT

Table S4. Data for calculated (first ten transitions) and experimental absorption spectra

№	PBE0 def2-TZVP (MeCN)				B3LYP 6-311G* (MeCN)				CAM-B3LYP 6-311G* (MeCN)				Experimental
		ν (cm^{-1})	λ (nm)	*f*		ν (cm^{-1})	λ (nm)	*f*		ν (cm^{-1})	λ (nm)	*f*	λ (ε/*f*)*
3a	1	23343.6	428.4	0.124	1	21496.9	465.2	0.098	1	26219.5	381.4	0.088	350-440 (4.5/0.181)
	2	26631.2	375.5	0.012	2	25910.9	385.9	0.017	2	27658.5	361.6	0.120	
	3	28661.0	348.9	0.023	3	25932.1	385.6	0.007	3	35315.5	283.2	0.015	
	4	30377.4	329.2	0.030	4	27852.0	359.0	0.025	4	35632.0	280.6	0.060	
	5	31491.8	317.5	0.007	5	29584.2	338.0	0.007	5	37287.9	268.2	0.036	
	6	31867.2	313.8	0.060	6	29625.8	337.5	0.056	6	37730.1	265.0	0.004	
	7	32990.4	303.1	0.000	7	31162.9	320.9	0.000	7	38293.6	261.1	0.057	
	8	36012.9	277.7	0.138	8	34128.7	293.0	0.152	8	39945.4	250.3	0.101	
	9	36784.7	271.9	0.356	9	35401.6	282.5	0.268	9	41151.5	243.0	0.135	
	10	38827.1	257.6	0.293	10	36788.5	271.8	0.277	10	41162.4	242.9	0.779	
3b	1	25439.5	393.1	0.052	1	24371.0	410.3	0.060	1	26334.1	379.7	0.011	300-390 (5.4/0.255)
	2	27341.2	365.7	0.090	2	26275.2	380.6	0.052	2	30523.4	327.6	0.226	
	3	28410.4	352.0	0.003	3	26841.7	372.6	0.003	3	35875.6	278.7	0.0129	
	4	29846.2	335.1	0.017	4	28449.5	351.5	0.014	4	37614.7	265.9	0.000	
	5	31427.5	318.2	0.021	5	29701.7	336.7	0.015	5	37768.6	264.8	0.019	
	6	32757.4	305.3	0.040	6	31131.1	321.2	0.018	6	39311.9	254.4	0.042	
	7	34021.0	293.9	0.033	7	32378.6	308.8	0.036	7	40038.3	249.8	0.011	
	8	35966.5	278.0	0.125	8	34297.5	291.6	0.119	8	41002.5	243.9	0.044	
	9	38528.7	259.5	0.060	9	36724.8	272.3	0.008	9	42575.2	234.9	0.008	
	10	39406.2	253.8	0.048	10	37821.6	264.4	0.352	10	42627.5	234.6	0.014	
3c	1	22930.3	436.1	0.121	1	21136.5	473.1	0.093	1	26133.4	382.7	0.091	337-439 (5.1/0.244)
	2	26644.4	375.3	0.011	2	25961.2	385.2	0.007	2	27670.9	361.4	0.112	
	3	29493.4	339.1	0.072	3	27100.0	369.0	0.050	3	35407.5	282.4	0.015	
	4	30940.6	323.2	0.018	4	29183.2	342.7	0.019	4	35878.2	278.7	0.093	
	5	31697.2	315.5	0.020	5	29228.4	342.1	0.033	5	37204.4	268.8	0.019	
	6	32682.3	306.0	0.015	6	30094.5	332.3	0.005	6	38951.1	256.7	0.002	
	7	33159.0	301.6	0.000	7	31299.8	319.5	0.000	7	39649.6	252.2	0.082	
	8	35657.3	280.4	0.152	8	33728.9	296.5	0.166	8	39971.2	250.2	0.135	
	9	36543.1	273.6	0.397	9	35252.1	283.7	0.314	9	40944.8	244.2	0.043	
	10	39264.1	254.7	0.003	10	36654.7	272.8	0.213	10	41163.4	242.9	0.823	

3d	1 22801.3 438.6 0.111 2 26585.6 376.1 0.010 3 29151.3 343.0 0.086 4 30922.2 323.4 0.021 5 31299.0 319.5 0.015 6 32642.0 306.4 0.011 7 33152.0 301.6 0.000 8 34508.5 289.8 0.150 9 35660.9 280.4 0.538 10 38062.3 262.7 0.014	1 21171.4 472.3 0.088 2 25872.1 386.5 0.007 3 27053.3 369.6 0.052 4 29027.4 344.5 0.033 5 29204.8 342.4 0.019 6 30121.7 332.0 0.005 7 31283.7 319.7 0.000 8 32802.1 304.9 0.156 9 34487.8 290.0 0.454 10 36398.3 274.7 0.132	1 26222.8 381.3 0.073 2 27733.0 360.6 0.128 3 35422.3 282.3 0.015 4 36060.1 277.3 0.103 5 37241.4 268.5 0.025 6 38741.2 258.1 0.004 7 39421.1 253.7 0.097 8 39510.4 253.1 0.400 9 40460.8 247.2 0.029 10 40830.4 244.9 0.727	340-440 (4.7/0.229)
3e	1 22482.4 444.8 0.103 2 26507.2 377.3 0.007 3 28710.3 348.3 0.095 4 30858.9 324.1 0.024 5 31082.9 321.7 0.009 6 32625.6 306.5 0.004 7 33061.6 302.5 0.000 8 33513.0 298.4 0.146 9 35109.5 284.8 0.569 10 37464.5 266.9 0.013	1 20663.5 483.9 0.08 2 25802.2 387.6 0.005 3 26493.5 377.5 0.072 4 28523.0 350.6 0.017 5 29144.0 343.1 0.019 6 29929.0 334.1 0.006 7 31210.9 320.4 0.000 8 31542.8 317.0 0.143 9 33776.3 296.1 0.485 10 34567.8 289.3 0.005	1 26126.1 382.8 0.005 2 27565.5 362.8 0.013 3 35357.2 282.8 0.002 4 35654.4 280.5 0.025 5 37139.5 269.3 0.001 6 38573.0 259.2 0.000 7 39039.9 256.1 0.003 8 39140.6 255.5 0.194 9 39965.6 250.2 0.000 10 40642.7 246.0 0.054	332-441 (5.0/0.210)
3f	1 24860.3 402.2 0.133 2 26462.8 377.9 0.030 3 30585.7 327.0 0.005 4 30787.3 324.8 0.008 5 31212.8 320.4 0.347 6 31870.7 313.8 0.018 7 32644.1 306.3 0.037 8 32800.0 304.9 0.066 9 33023.2 302.8 0.000 10 33147.2 301.7 0.000	1 23457.2 426.3 0.115 2 25722.2 388.8 0.015 3 28137.8 355.4 0.003 4 29110.0 343.5 0.010 5 29365.2 340.5 0.245 6 30147.9 331.7 0.003 7 30436.5 328.6 0.030 8 31078.9 321.8 0.063 9 31292.4 319.6 0.072 10 31481.5 317.6 0.001	1 26413.5 378.6 0.027 2 28530.8 350.5 0.186 3 32843.7 304.5 0.069 4 32850.8 304.4 0.005 5 35495.4 281.7 0.008 6 36062.5 277.3 0.037 7 36229.1 276.0 0.017 8 36717.0 272.4 0.522 9 36753.3 272.1 0.019 10 37408.4 267.3 0.096	300-412 (8.4/0.322)
3g	1 25087.5 398.6 0.285 2 26938.4 371.2 0.040 3 30035.1 332.9 0.101 4 31253.1 320.0 0.006 5 33150.4 301.7 0.004 6 37975.3 263.3 0.118 7 39335.6 254.2 0.120 8 40130.0 249.2 0.679	1 23945.8 417.6 0.274 2 26187.2 381.9 0.023 3 28312.4 353.2 0.088 4 29675.1 337.0 0.006 5 31396.4 318.5 0.004 6 36422.0 274.6 0.038 7 37712.7 265.2 0.116 8 38447.5 260.1 0.604	1 26915.8 371.5 0.062 2 28148.5 355.3 0.339 3 34645.0 288.6 0.103 4 35525.1 281.5 0.009 5 37375.3 267.6 0.013 6 40354.4 247.8 0.003 7 43033.1 232.4 1.318 8 44301.2 225.7 0.205	342-434 (6.9/0.290)

	9 41224.0 242.6 0.080 10 42771.2 233.8 0.065	9 39440.6 253.5 0.082 10 41956.4 238.3 0.096	9 45379.6 220.4 0.009 10 47928.2 208.6 0.001	
3h	1 20518.7 487.4 0.036 2 24790.7 403.4 0.077 3 26398.0 378.8 0.005 4 28518.3 350.7 0.021 5 30280.0 330.3 0.077 6 30648.4 326.3 0.032 7 31851.2 314.0 0.027 8 32693.2 305.9 0.075 9 32861.8 304.3 0.001 10 33461.9 298.8 0.016	1 18088.4 552.8 0.029 2 22179.1 450.9 0.066 3 25505.7 392.1 0.010 4 25693.3 389.2 0.009 5 26934.6 371.3 0.002 6 28656.1 349.0 0.056 7 29545.8 338.5 0.010 8 29981.7 333.5 0.008 9 31014.1 322.4 0.0147 10 31103.7 321.5 0.118	1 25596.6 390.7 0.044 2 27695.8 361.1 0.062 3 31906.9 313.4 0.161 4 34060.8 293.6 0.098 5 35997.8 277.8 0.011 6 36813.8 271.6 0.021 7 37037.5 270.0 0.054 8 38309.5 261.0 0.236 9 39657.3 252.2 0.389 10 39812.6 251.2 0.052	543 (-/-)
3i	1 21880.2 457.0 0.108 2 26572.1 376.3 0.007 3 27589.7 362.5 0.061 4 29969.8 333.7 0.051 5 30257.4 330.5 0.035 6 31397.0 318.5 0.005 7 32891.6 304.0 0.000 8 34927.1 286.3 0.151 9 35478.4 281.9 0.543 10 38006.6 263.1 0.021	1 20065.1 498.4 0.043 2 24984.1 400.3 0.001 3 25865.1 386.6 0.004 4 27619.5 362.1 0.004 5 27795.0 359.8 0.006 6 29547.5 338.4 0.003 7 31089.3 321.7 0.000 8 33230.5 300.9 0.014 9 34126.0 293.0 0.133 10 36334.1 275.2 0.001	1 25582.4 390.9 0.137 2 27219.7 367.4 0.049 3 34246.5 292.0 0.127 4 35171.7 284.3 0.021 5 36686.1 272.6 0.023 6 37220.4 268.7 0.002 7 37992.5 263.2 0.070 8 38988.6 256.5 0.583 9 40171.2 248.9 0.052 10 40494.5 246.9 0.480	360-456 (4.9/0.154)
3j	1 19603.4 510.1 0.081 2 25547.7 391.4 0.118 3 26704.9 374.5 0.005 4 30233.2 330.8 0.007 5 30803.4 324.6 0.028 6 31777.7 314.7 0.004 7 33064.7 302.4 0.004 8 33355.9 299.8 0.174 9 33962.7 294.4 0.566 10 37059.6 269.8 0.009	1 17520.1 570.8 0.061 2 23348.6 428.3 0.103 3 26054.8 383.8 0.004 4 27499.9 363.6 0.003 5 28291.4 353.5 0.004 6 29561.4 338.3 0.026 7 31287.1 319.6 0.001 8 31595.5 316.5 0.171 9 32512.4 307.6 0.499 10 35660.4 280.4 0.019	1 24181.7 413.5 0.132 2 27225.6 367.3 0.017 3 32514.8 307.6 0.161 4 35142.8 284.6 0.042 5 36878.5 271.2 0.011 6 37682.1 265.4 0.112 7 37922.6 263.7 0.778 8 38435.1 260.2 0.028 9 39003.9 256.4 0.003 10 40257.6 248.4 0.230	396-487 (3.8/0.124)
3k	1 20229.3 494.3 0.046 2 23161.7 431.7 0.002 3 26359.1 379.4 0.013 4 27512.8 363.5 0.131 5 30241.0 330.7 0.065 6 31186.1 320.7 0.005	1 17910.8 558.3 0.030 2 20442.8 489.2 0.001 3 25067.8 398.9 0.080 4 26070.4 383.6 0.037 5 27973.4 357.5 0.061 6 29540.4 338.5 0.006	1 25378.4 394.0 0.004 2 27135.6 368.5 0.004 3 31306.4 319.4 0.000 4 32983.8 303.2 0.004 5 35841.4 279.0 0.004 6 36119.7 276.9 0.012	326-448 (4.3/0.241)

	7 32910.4 303.9 0.000 8 33408.5 299.3 0.248 9 34939.9 286.2 0.041 10 35406.6 282.4 0.112	7 31135.0 321.2 0.001 8 31749.0 315.0 0.198 9 32877.4 304.2 0.094 10 33451.5 298.9 0.048	7 37264.2 268.4 0.006 8 37776.1 264.7 0.062 9 38481.5 259.9 0.004 10 40120.3 249.3 0.002	
3l	1 21179.3 472.2 0.006 2 22545.6 443.5 0.0013 3 23441.0 426.6 0.096 4 26842.0 372.6 0.016 5 29812.2 335.4 0.076 6 31176.9 320.8 0.020 7 33148.0 301.7 0.000 8 33725.0 296.5 0.045 9 34886.0 286.6 0.001 10 34949.3 286.1 0.020	1 18172.7 550.3 0.002 2 20285.5 493.0 0.001 3 21432.9 466.6 0.078 4 26161.5 382.2 0.009 5 26933.8 371.3 0.064 6 29573.1 338.1 0.017 7 31302.8 319.5 0.000 8 31542.1 317.0 0.034 9 32608.8 306.7 0.000 10 32912.3 303.8 0.006	1 26128.6 382.7 0.080 2 27677.3 361.3 0.059 3 29457.9 339.5 0.058 4 31057.0 322.0 0.001 5 35567.8 281.2 0.016 6 35959.5 278.1 0.109 7 37309.4 268.0 0.004 8 38622.2 258.9 0.000 9 39506.6 253.1 0.092 10 39698.6 251.9 0.091	337-442 (4.4/0.120)
3m	1 17171.2 582.4 0.041 2 21357.8 468.2 0.039 3 23026.6 434.3 0.040 4 24912.5 401.4 0.025 5 26551.3 376.6 0.004 6 30688.7 325.9 0.109 7 31638.1 316.1 0.290 8 31897.0 313.5 0.099 9 32927.6 303.7 0.000 10 34101.0 293.2 0.037	1 14807.5 675.3 0.027 2 18655.0 536.0 0.030 3 20460.8 488.7 0.035 4 22154.6 451.4 0.021 5 25771.0 388.0 0.003 6 29134.3 343.2 0.100 7 29756.1 336.1 0.216 8 30153.0 331.6 0.080 9 31104.0 321.5 0.000 10 32064.7 311.9 0.036	1 22973.3 435.3 0.077 2 26920.5 371.5 0.008 3 28848.6 346.6 0.059 4 30863.5 324.0 0.059 5 32370.4 308.9 0.066 6 34809.7 287.3 0.072 7 36005.5 277.7 0.402 8 36405.3 274.7 0.066 9 36933.4 270.8 0.006 10 37601.6 265.9 0.016	-
3n	1 19357.7 516.6 0.051 2 23528.0 425.0 0.142 3 26573.5 376.3 0.002 4 27078.8 369.3 0.011 5 28495.7 350.9 0.003 6 29154.7 343.0 0.041 7 29896.0 334.5 0.000 8 30428.9 328.6 0.070 9 31040.2 322.2 0.735 10 31619.4 316.3 0.018	1 17036.7 587.0 0.037 2 21033.4 475.4 0.125 3 23964.3 417.3 0.008 4 25753.4 388.3 0.005 5 25787.4 387.8 0.003 6 26165.7 382.2 0.007 7 26657.1 375.1 0.000 8 28324.9 353.0 0.095 9 29456.2 339.5 0.590 10 29702.0 336.7 0.006	1 24395.5 409.9 0.100 2 27134.2 368.5 0.011 3 31042.2 322.1 0.268 4 34377.8 290.9 0.086 5 34972.7 285.9 1.200 6 35629.1 280.7 0.021 7 36106.9 277.0 0.039 8 36227.2 276.0 0.006 9 36369.5 275.0 0.153 10 37286.9 268.2 0.002	400-491 (3.6/0.101)
3o	1 20513.1 487.5 0.103 2 26445.0 378.1 0.007 3 27973.2 357.5 0.064 4 29556.8 338.3 0.010	1 18650.0 536.2 0.083 2 25745.2 388.4 0.006 3 25815.2 387.4 0.047 4 27329.2 365.9 0.013	1 24311.6 411.3 0.141 2 26966.5 370.8 0.023 3 34303.1 291.5 0.077 4 35131.9 284.6 0.029	390-490 (3.1/0.110)

	5 29822.3 335.3 0.016 6 31445.7 318.0 0.010 7 33097.5 302.1 0.010 8 33522.2 298.3 0.510 9 35101.6 284.9 0.141 10 37748.6 264.9 0.074	5 27571.9 362.7 0.008 6 29707.4 336.6 0.014 7 31323.3 319.3 0.006 8 31969.5 312.8 0.457 9 33335.9 300.0 0.130 10 35806.5 279.3 0.092	5 36251.1 275.9 0.467 6 36642.0 272.9 0.230 7 37837.9 264.3 0.003 8 38485.8 259.8 0.042 9 39702.6 251.9 0.095 10 40530.9 246.7 0.020	
3p	1 23126.3 432.4 0.150 2 25768.7 388.1 0.033 3 26724.3 374.2 0.016 4 27998.5 357.2 0.002 5 31266.3 319.8 0.011 6 31500.9 317.5 0.067 7 33105.9 302.1 0.000 8 36040.2 277.5 0.177 9 37567.8 266.2 0.275 10 38695.1 258.4 0.019	1 21610.2 462.7 0.126 2 23148.9 432.0 0.026 3 25609.7 390.5 0.001 4 26026.0 384.2 0.012 5 29516.7 338.8 0.061 6 29635.4 337.4 0.011 7 31303.7 319.5 0.000 8 34291.0 291.6 0.187 9 36175.9 276.4 0.116 10 36750.2 272.1 0.019	1 26278.8 380.5 0.089 2 27858.9 359.0 0.168 3 33021.9 302.8 0.058 4 35442.4 282.1 0.010 5 36786.4 271.8 0.005 6 37286.6 268.2 0.006 7 37806.8 264.5 0.045 8 40480.0 247.0 0.010 9 40793.3 245.1 0.093 10 41984.8 238.2 0.999	345-460 (4.3/0.161)

*****Oscillator strength (*f*) is calculated from experimental spectra using the equation $f = 4.32 \cdot 10^{-9} \int \varepsilon(\nu) d\nu$

Table S5. Cartesian coordinates for the optimized geometry of compounds **3**

№	B3LYP 6-311G*			PBE0 def2-TZVP		
3a	N 0.52758172738653	2.10257639154243	-1.08150314836982	N 0.52393218688367	2.09306188799392	-1.07146372972579
	C 0.92505403880967	3.14988339047685	-1.91928582728369	C 0.92435912353126	3.13203992742830	-1.89428906710937
	N 0.36845163260463	4.40125626543629	-1.89404237799093	N 0.37041591476820	4.37652605475990	-1.87608610048548
	N -0.57611242470466	4.64916877227251	-1.06560846063308	N -0.57342099619045	4.61929543759397	-1.06317411542544
	C -1.08068500208908	3.63089173087987	-0.30104074331899	C -1.07745793221039	3.60182781913273	-0.31039382369985
	N -2.12785215174290	3.68663896427405	0.49619433117368	N -2.12467001397784	3.65669492466438	0.47774187601316
	N -2.38444580287634	2.42865855996130	0.91959670767369	N -2.37642352680832	2.41292107501016	0.89663584926434
	C -1.51204441644747	1.57207620020220	0.39135419367015	C -1.50152555131807	1.56190834561814	0.37875554719545
	C -1.60464394429117	0.12290033139690	0.54380706948809	C -1.60299839597440	0.11844878189125	0.53468604976860
	C -1.97407213308527	-0.39757472361588	1.78930840191844	C -1.97877380462745	-0.39050650444926	1.77579461035205
	C -2.08837072944459	-1.77169351285828	1.95919532952854	C -2.11982079703866	-1.75598368777412	1.94670824577863
	C -1.84345933572720	-2.63137334704231	0.88983451348713	C -1.89420727883386	-2.61765690256521	0.88270698939614
	C -1.50577073810014	-2.11363189566603	-0.35902648738056	C -1.54679504120231	-2.11058487152923	-0.36097006685552
	C -1.39450631461912	-0.74091643379491	-0.53632016934778	C -1.40919336693840	-0.74590709197293	-0.53928893510313
	N -0.63044757304774	2.30817456313940	-0.36801671276359	N -0.62660261272684	2.29420530719517	-0.37197561729020
	N 1.98347135686896	2.77055748673403	-2.60587785028037	N 1.98329417560855	2.75736445804753	-2.57219240638726
	N 2.29924865047346	1.51775886680098	-2.20771918441086	N 2.29181358304205	1.51766721020125	-2.18013236387223
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References

1 D. E. Chavez and M. A. Hiskey, *J. Heterocycl. Chem.*, 1998, 35, 1329–1332.

2 V. V. Malov, T. Ghosh, V. C. Nair, M. M. Maslov, K. P. Katin, K. N. N. Unni and A. R. Tameev, *Mendeleev Commun.*, 2019, **29**, 218–219.

3 F. Neese, *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 2022, **12**, 1–15.

4 A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378–6396.

5 G. M. Sheldrick, *Acta Crystallogr. Sect. A Found. Crystallogr.*, 2015, **71**, 3–8.

6 G. M. Sheldrick, *Acta Crystallogr. Sect. C Struct. Chem.*, 2015, **71**, 3–8.

7 I. N. Ganebnykh, R. I. Ishmetova, S. G. Tolshchina, A. V. Korotina, D. S. Filatov, P. A. Slepukhin and G. L. Rusinov, *Russ. Chem. Bull. Vol.*, 2018, 1716–1723.

8 K. Vandewal, J. Benduhn and V. C. Nikolis, *Sustain. Energy Fuels*, 2018, **2**, 538–544.