Supporting Information

Rational design and synthesis of yellow-light emitting triazole fluorophores with AIE and mechanochromic properties

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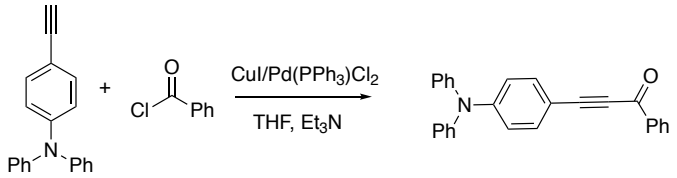
I. General Methods and Materials

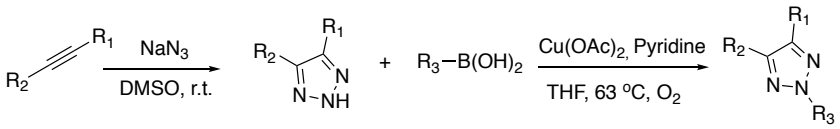
All of the reactions dealing with air and/or moisture-sensitive compounds were carried out under an atmosphere of argon using oven/flame-dried glassware and standard syringe/septa techniques. Unless otherwise noted, all commercial reagents and solvents were obtained from the commercial provider and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on Agilent 400 MHz spectrometers/Varian 600 MHz spectrometers. Chemical shifts were reported relative to internal tetramethylsilane (δ 0.00 ppm) or $CDCl_3$ (δ 7.26 ppm) or DMSO (2.50 ppm) for ^{1}H and $CDCl_3$ (δ 77.00 ppm), DMSO (40.00 ppm) for ^{13}C. Flash column chromatography was performed on 230-430 mesh silica gel. Analytical thin layer chromatography was performed with precoated glass baked plates (250 μ) and visualized by fluorescence and by charring after treatment with potassium permanganate stain. HRMS were recorded on Agilent 6540 LC/QTOF spectrometer.

1.1 General procedure to synthesize 3-(4-(diphenylamino)phenyl)-1-phenylprop-2-yn-1-one (DPPO)



Benzoyl chloride (1 mmol, 1.0 equiv), $Pd(PPh_3)Cl_2$ (34 mg, 0.05 mmol, 0.05 equiv), CuI (20 mg, 0.05 mmol, 0.05 equiv) and Et_3N (0.14 mL, 1 mmol, 1.0 equiv) was dissolved in THF(4 ml). 4-ethynyl-N, N-diphenylaniline (1 mmol, 1.0 equiv) was slowly added to the mixtures at room temperature. The reaction was monitored by TLC. After reaction completion, the solvent was removed under vacuum and **DPPO** was purified by silica gel column chromatography (Hexane and EA).

1.2 General procedure to synthesize 1a-3n



Alkynes (1.5 mmol) was dissolved in 10 mL DMSO. After stirring, NaN_3 (0.28 g, 4.3 mmol) was slowly added to the mixture and refluxed for 6 h under room temperature. In order to quench the reaction, water was introduced to the system. After extraction by using ethyl acetate as extractant, organic phase was washed with saturated salt water to remove excess DMSO and dried with anhydrous sodium sulfate. The solvent was removed by rotary evaporator. Product directly be used in next step without further purification.

Triazole (4 mmol, 1.0 equiv), Pyridine (8 mmol,2.0 equiv), $Cu(OAc)_2$ (4 mmol, 1 equiv) and $ArB(OH)_2$ (6 mmol, 1.5 equiv) was successively added to 50 mL vial, then anhydrous THF (20 mL) was added by syringes. The tube was heated to 63 ^oC for 12 h under O_2. After cooling to the room temperature, solvent was removed under vacuum. The mixture was subjected to the silica gel column chromatography (Hexane: DCM=2:1) to isolate the pure products **1a-3n.**

II. Optical properties

Fluorescence detection Procedures: A series of stock solution of compound 1,2,3-triazoel **(1a-3n)** (1.0 mmol/L) was prepared by dissolving the corresponding amount of compound powder in THF, which was stored in the dark. For fluorescence detection, 20 μL stock solutions (1.0 mmol/L) were diluted with 1980 μL THF in the sample tubes. The fluorescence spectra of mixed solutions were recorded with the corresponding excitation wavelength at room temperature (298 K). For AIE properties detection, appropriate amounts of water were added to obtain 10 μM (**1a-3n**) THF solution with different water fractions (0 vol%, 30 vol%, 50 vol%, 70 vol%,80 vol%, 90 vol%, 99 vol%). After that, the FL measurements of the resulting solutions were performed immediately.

UV-vis absorption detection Procedures: 200 μL stock solutions (1.0 mmol/L) were diluted with 1800 μL THF in the sample tubes. UV-vis absorption spectra of mixed solutions were obtained.

Quantum yield determination: All the quantum yields of samples were determined by EI Fluorescence Spectroscopy-FLS 980, the sample was dissolved in THF, concentration was 10 mmol/L.

2.1 The UV-vis absorption spectra of 1a-3n

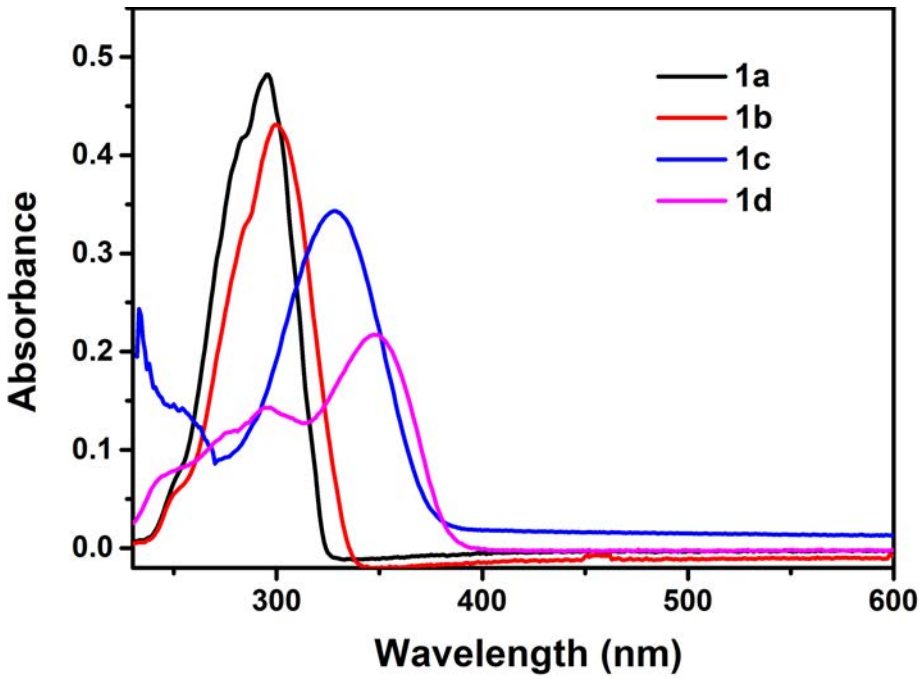


Fig. S1. UV-vis absorption spectra of compound **1a-1d**. Concentration: 100 μmol/L in THF.

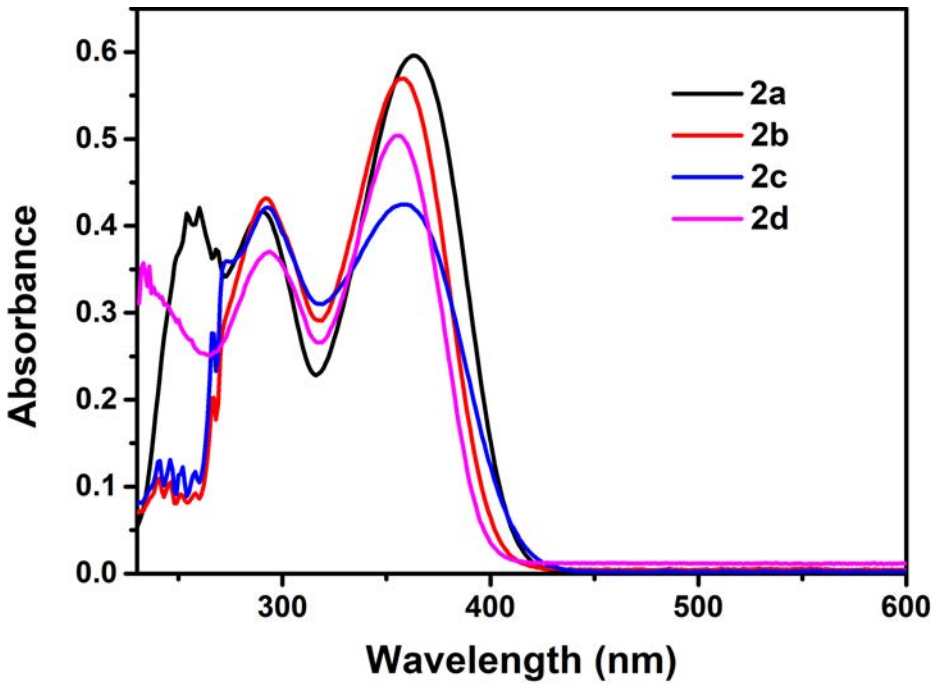


Fig. S2. UV-vis spectra of compound **2a-2d**. Concentration: 100 μmol/L in THF.

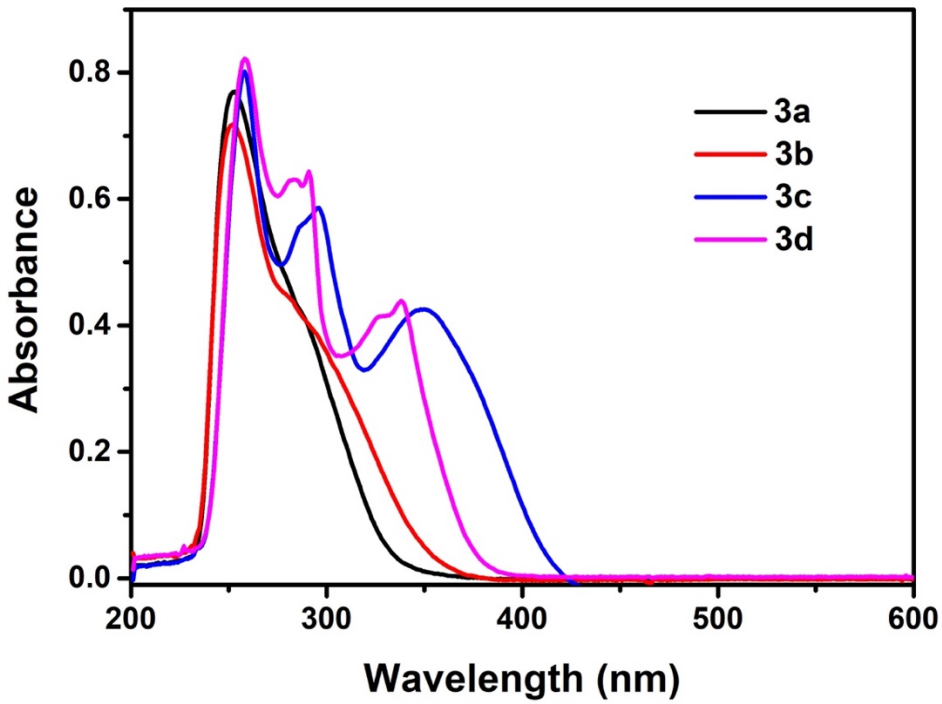


Fig. S3. UV-vis spectra of compound **3a-3d**. Concentration: 100 μmol/L in THF.

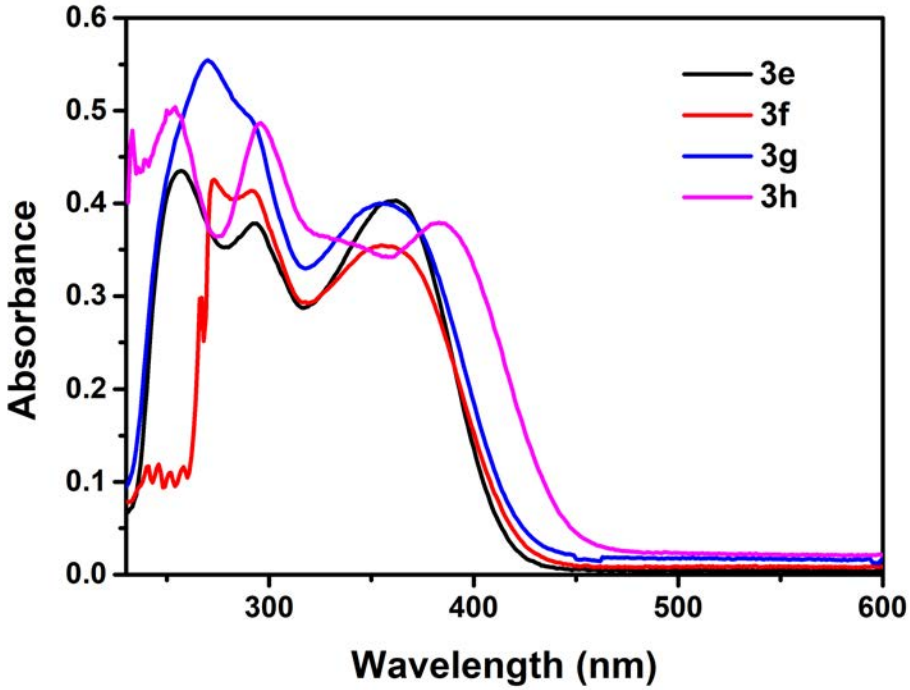


Fig. S4. UV-vis spectra of compound **3e-3h**. Concentration: 100 μmol/L in THF.

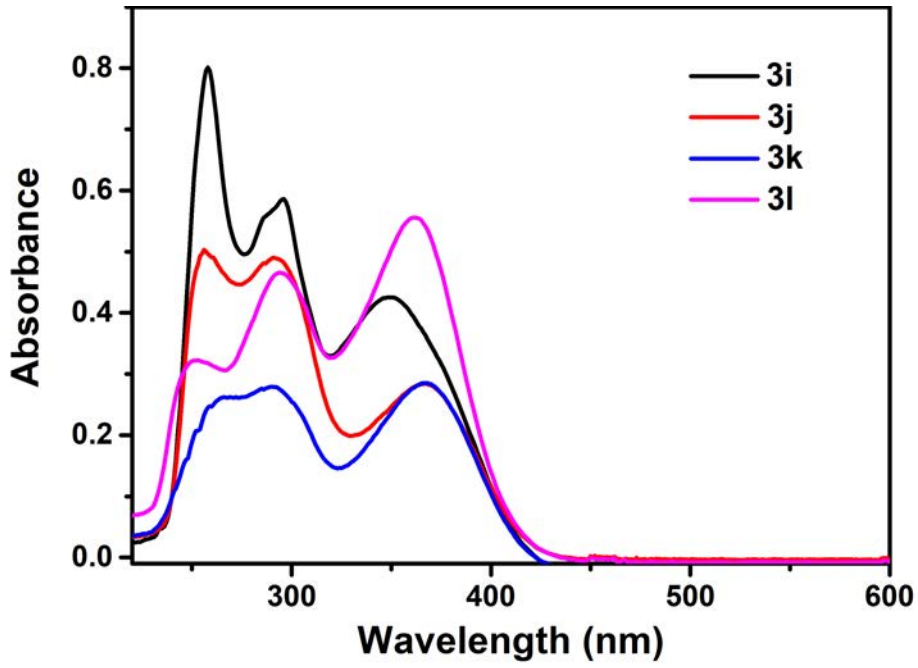


Fig. S5. UV-vis spectra of compound **3i-3l**. Concentration: 100 μmol/L in THF.

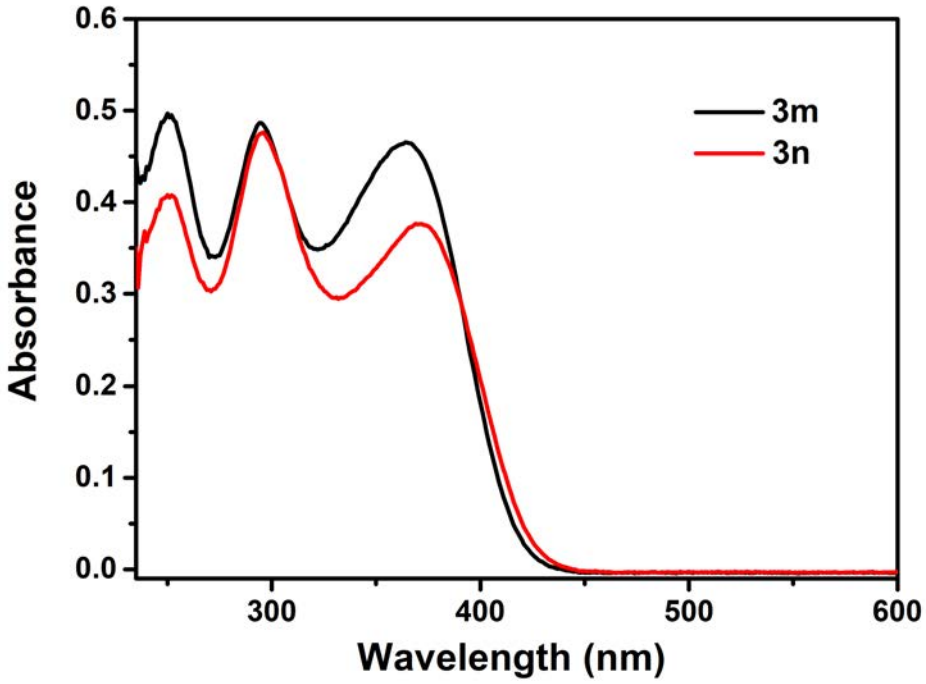


Fig. S6. UV-vis spectra of compound **3m-3n**. Concentration: 100 μmol/L in THF.

2.2 The fluorescence emission of 1a-3n in THF solution.

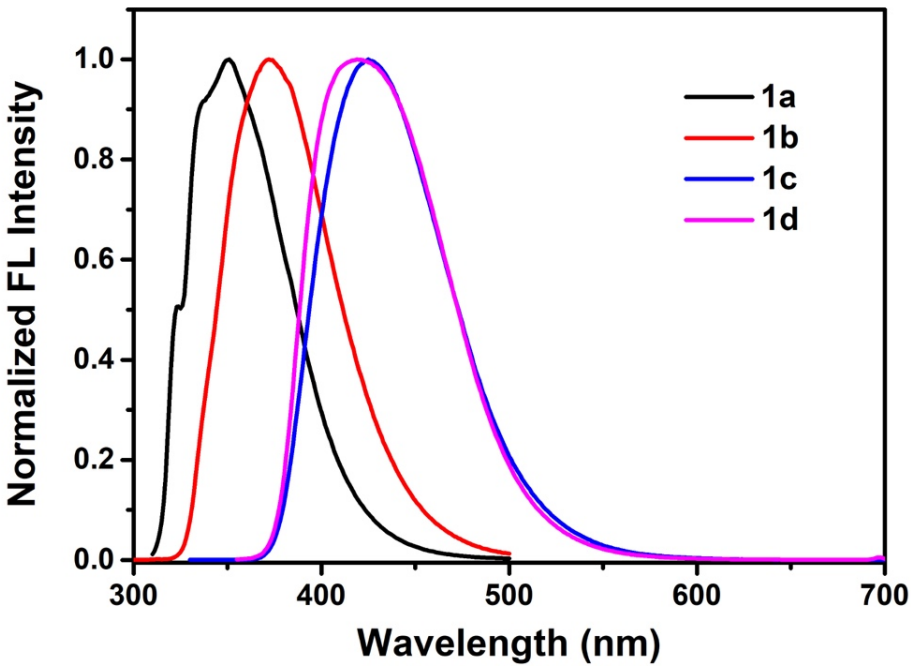


Fig. S7. Fluorescence emission of compound **1a-1d**. Concentration: 10 μmol/L in THF.

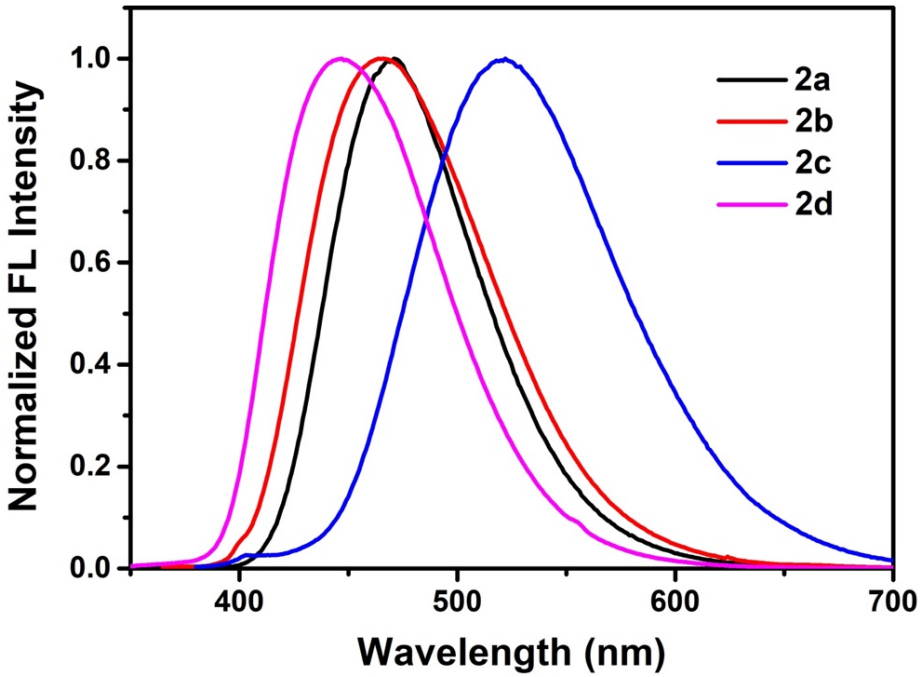


Fig. S8. Fluorescence emission of compound **2a-2d**. Concentration: 10 μmol/L in THF.

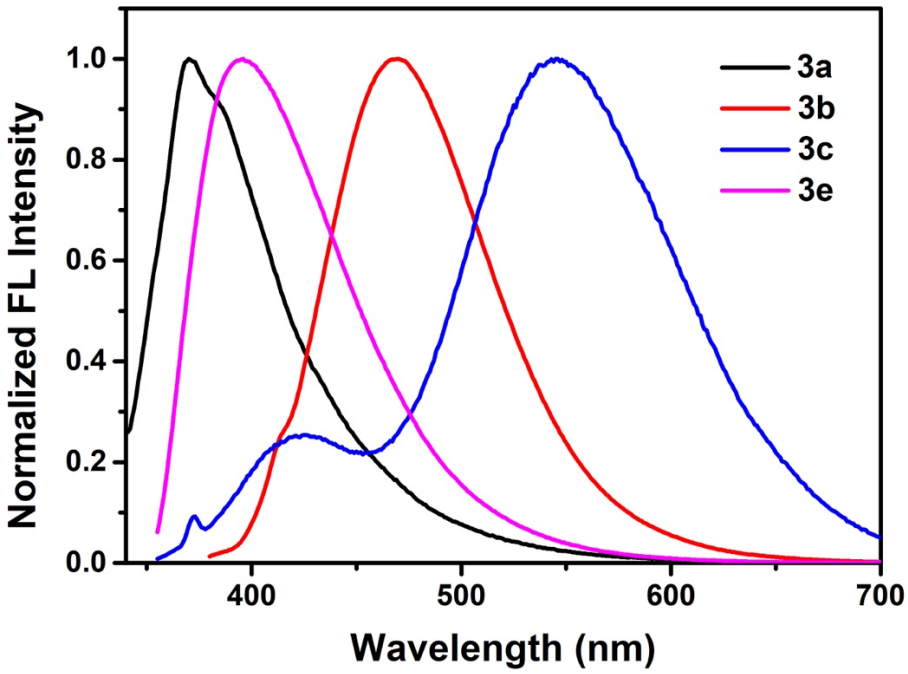


Fig. S9. Fluorescence emission of compound **3a-3d**. Concentration: 10 μmol/L in THF.

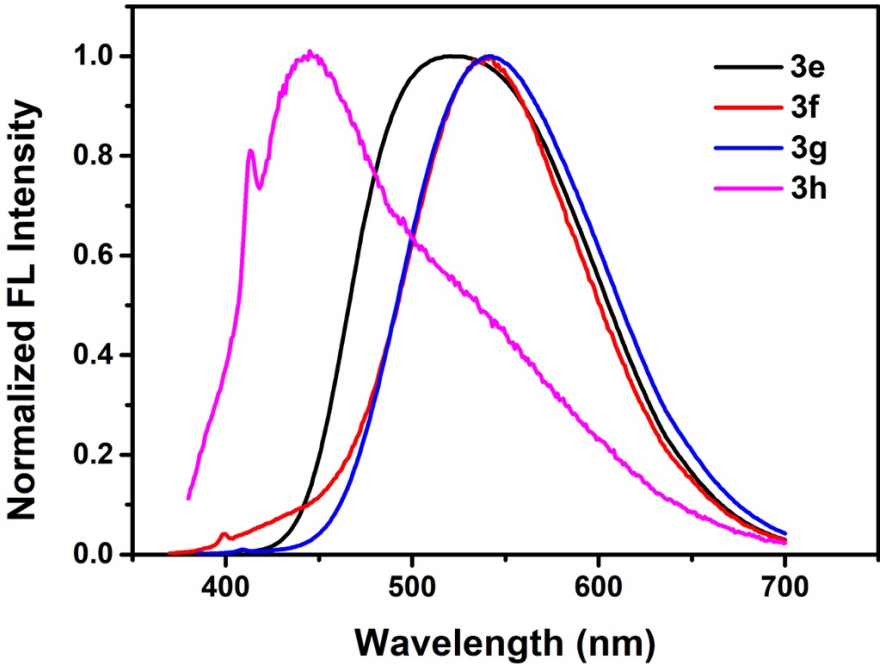


Fig. S10. Fluorescence emission of compound **3e-3h**. Concentration: 10 μmol/L in THF.

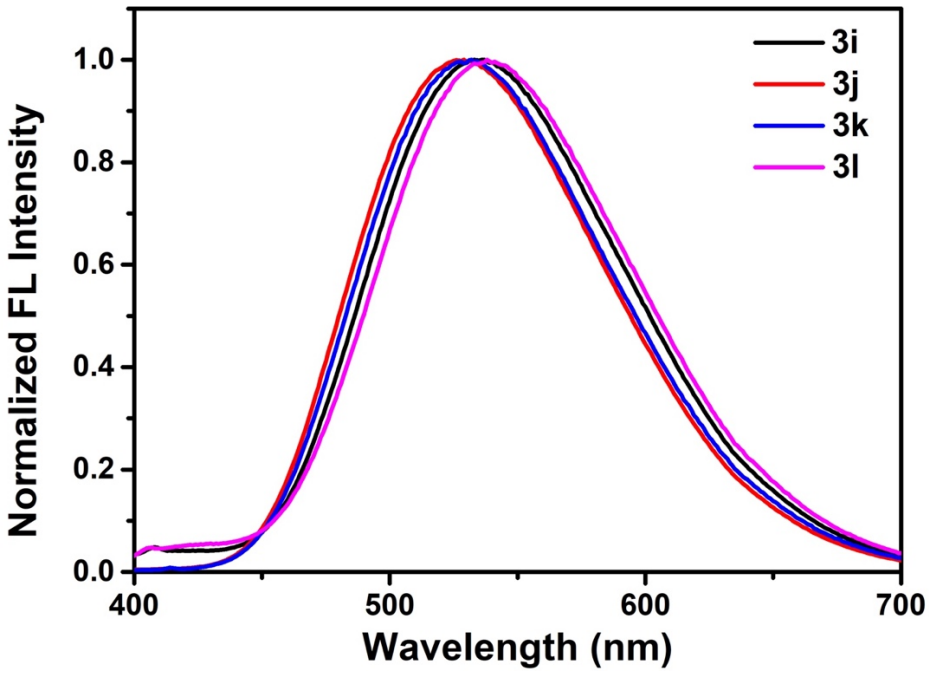


Fig. S11. Fluorescence emission of compound **3i-3l**. Concentration: 10 μmol/L in THF.

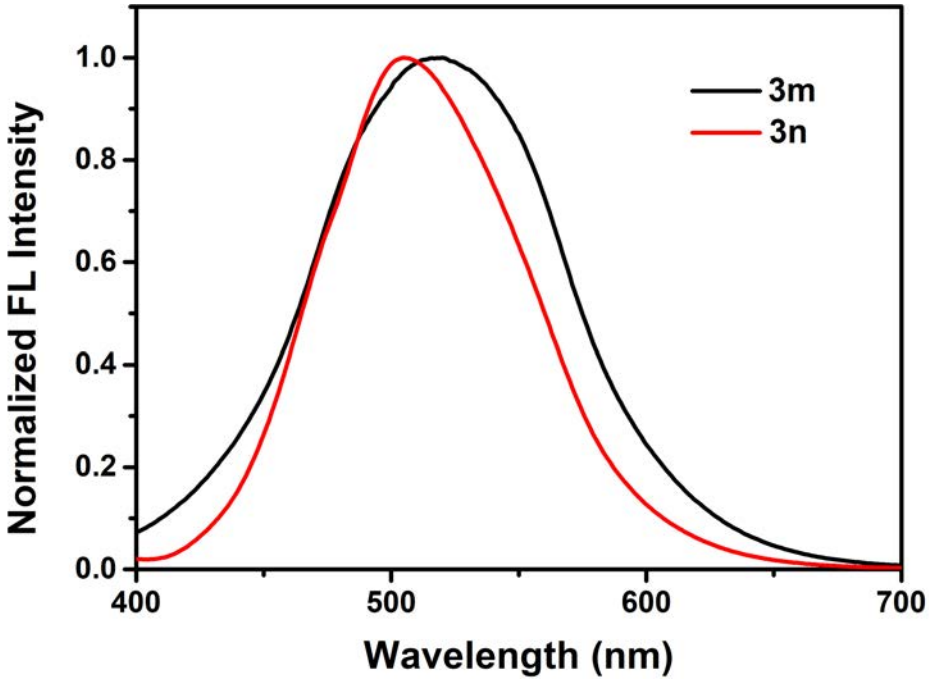


Fig. S12. Fluorescence emission of compound **3m-3n**. Concentration: 10 μmol/L in THF.

2.3 The Normalized fluorescence emission of 1a-3n in THF solution at different temperature.

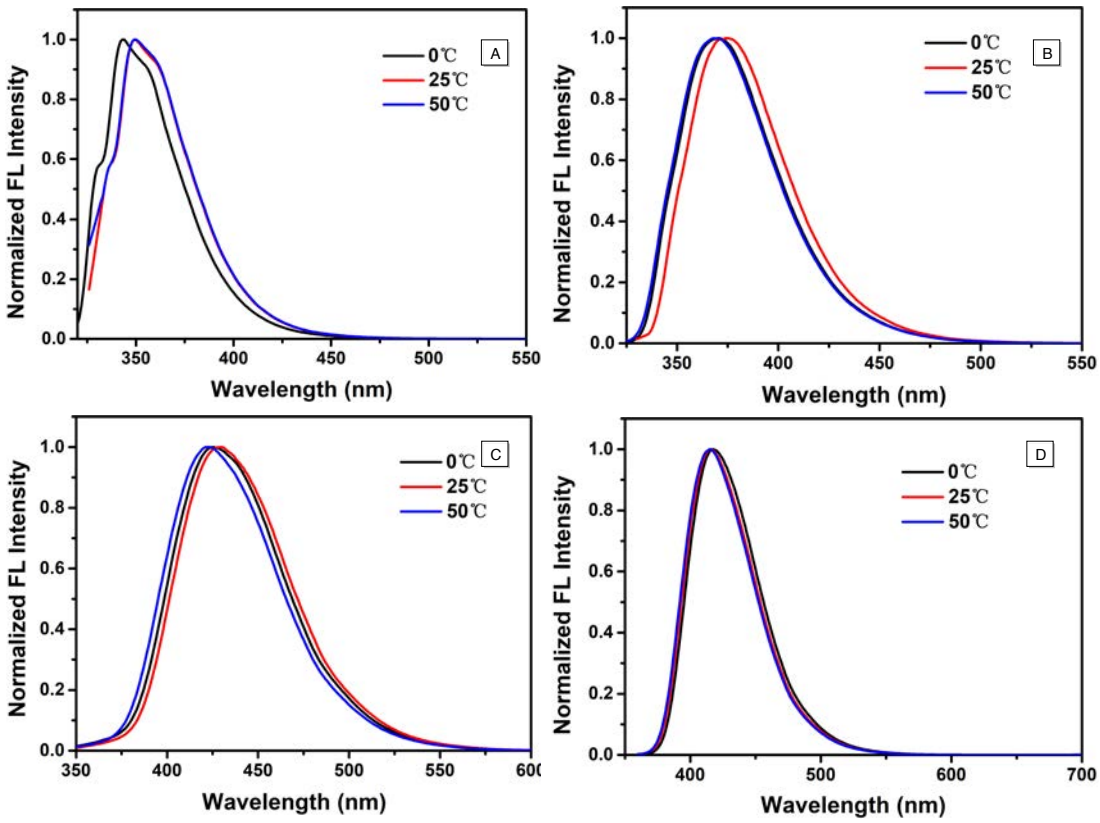


Fig. S13. Normalized fluorescence emission of compound **1a**(A), **1b**(B), **1c**(C) and **1d**(D) at different tempetature. Concentration: 10 μmol/L in THF.

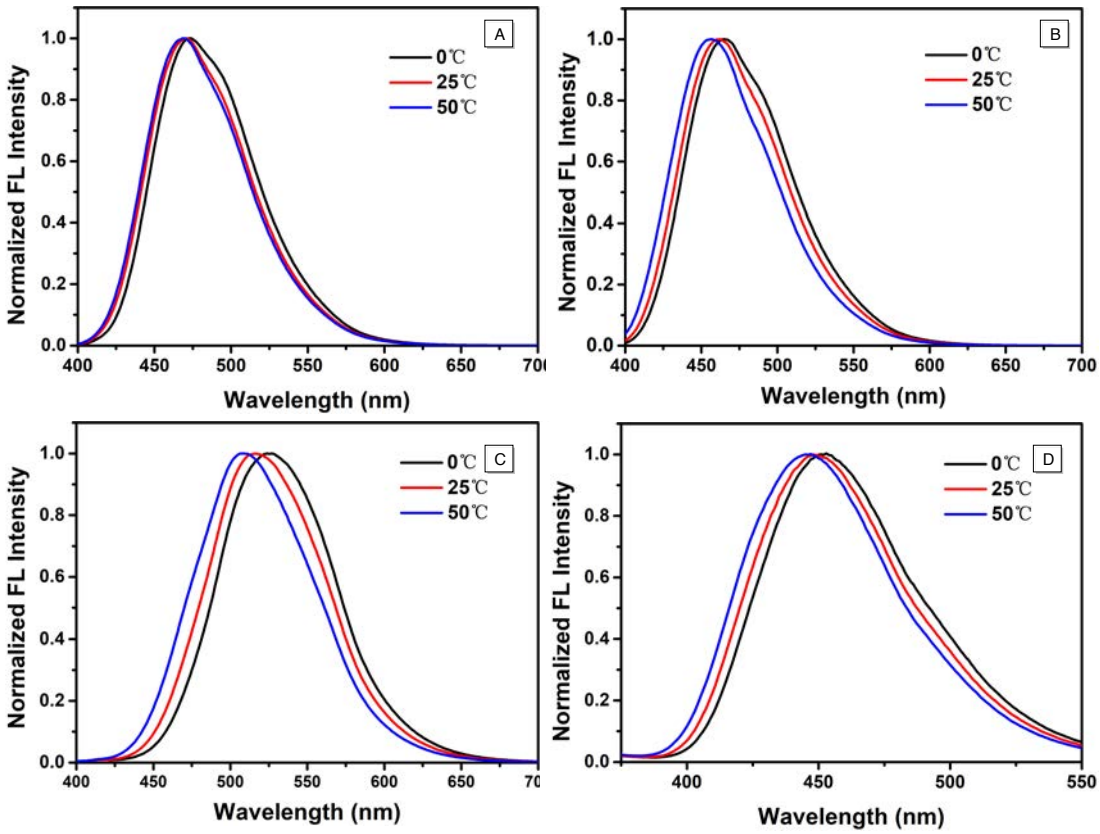


Fig. S14. Normalized fluorescence emission of compound **2a**(A), **2b**(B), **2c**(C) and **2d**(D) at different tempetature. Concentration: 10 μmol/L in THF.

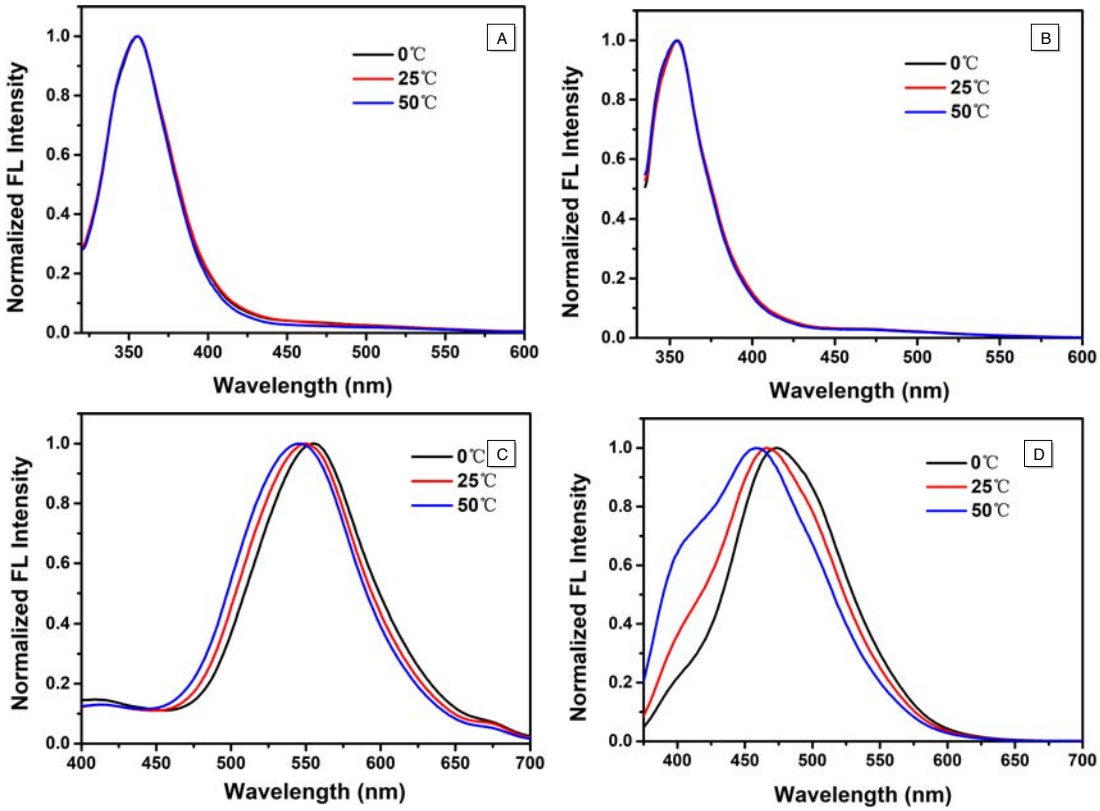


Fig. S15. Normalized fluorescence emission of compound **3a** (A), **3b** (B), **3c** (C) and **3d** (D) at different tempetature. Concentration: 10 μmol/L in THF.

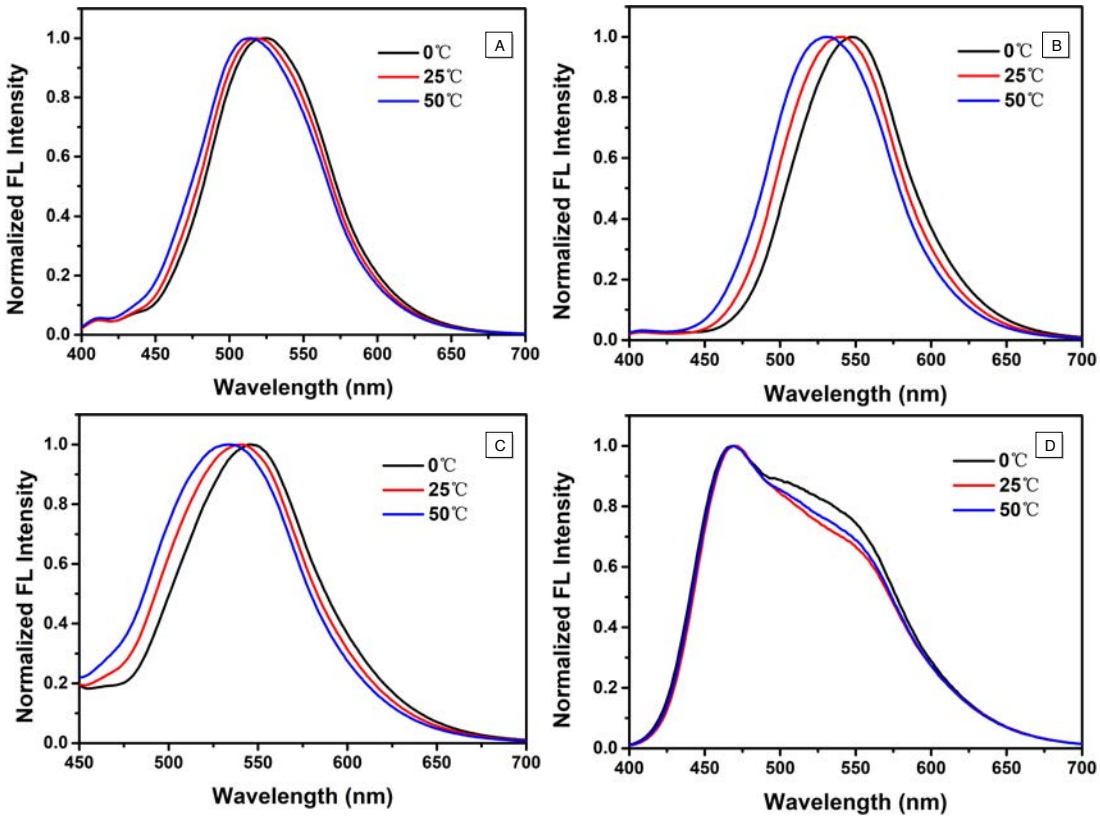


Fig. S16. Normalized fluorescence emission of compound **3e** (A), **3f** (B), **3g** (C) and **3h** (D) at different tempetature. Concentration: 10 μmol/L in THF.

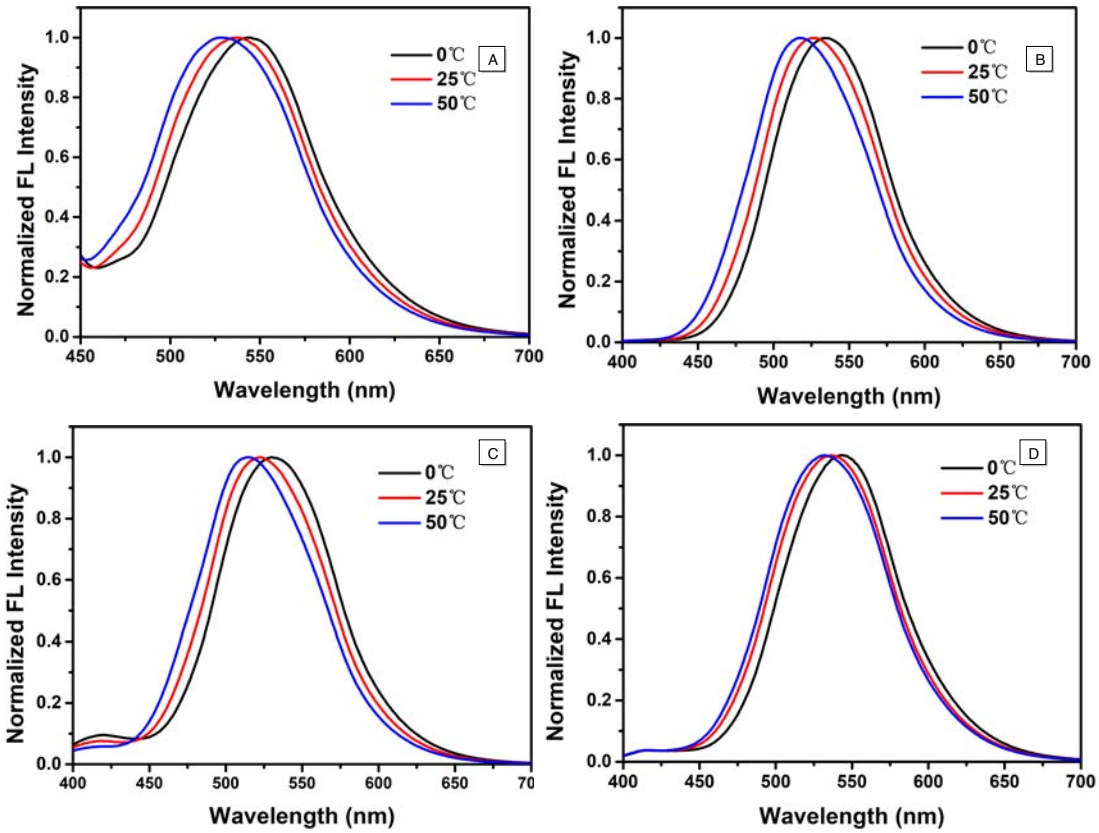


Fig. S17. Normalized fluorescence emission of compound **3i** (A), **3j** (B), **3k** (C) and **3l** (D) at different tempetature. Concentration: 10 μmol/L in THF.

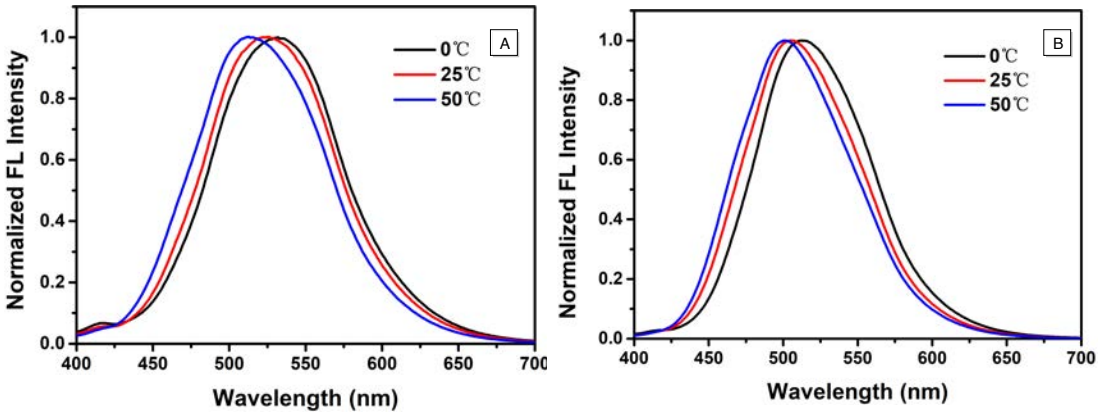


Fig. S18. Normalized fluorescence emission of compound **3m**(A) and **3n**(B) at different tempetature. Concentration: 10 μmol/L in THF.

2.3 The fluorescence emission of 1a-3n in solid state.

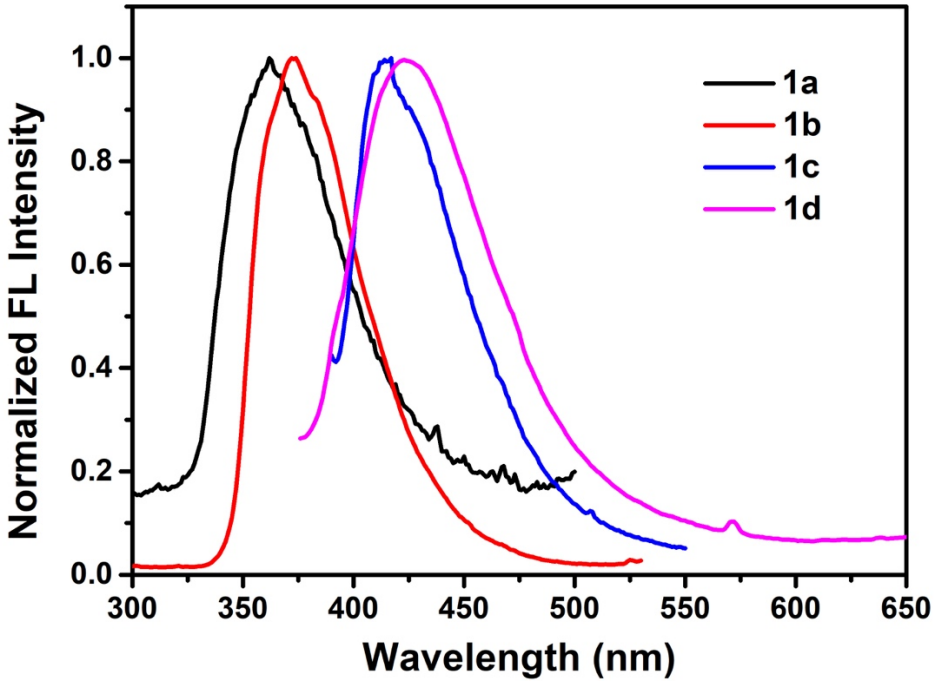


Fig. S19. Fluorescence emission of compound **1a-1d** in solid state.

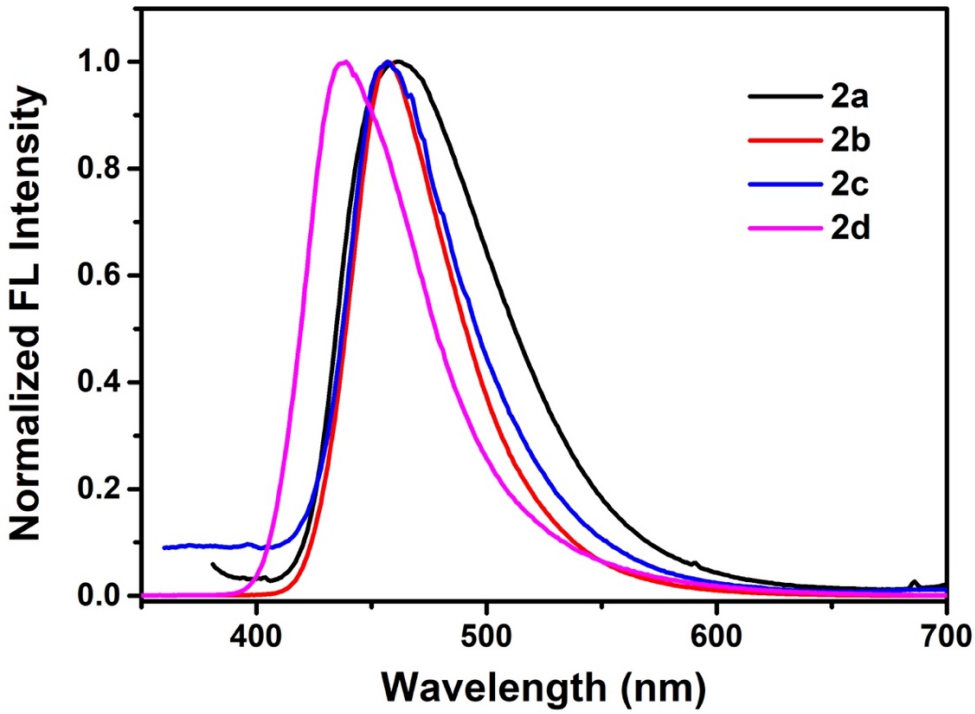


Fig. S20. Fluorescence emission of compound **2a-2d** in solid state.

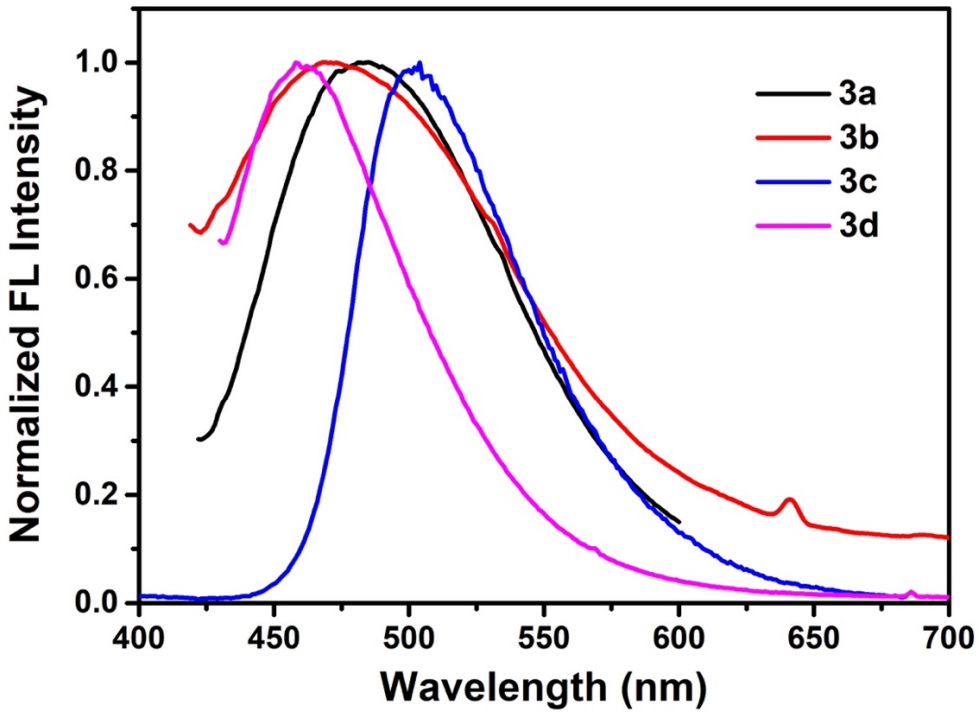


Fig. S21. Fluorescence emission of compound **3a-3d** in solid state.

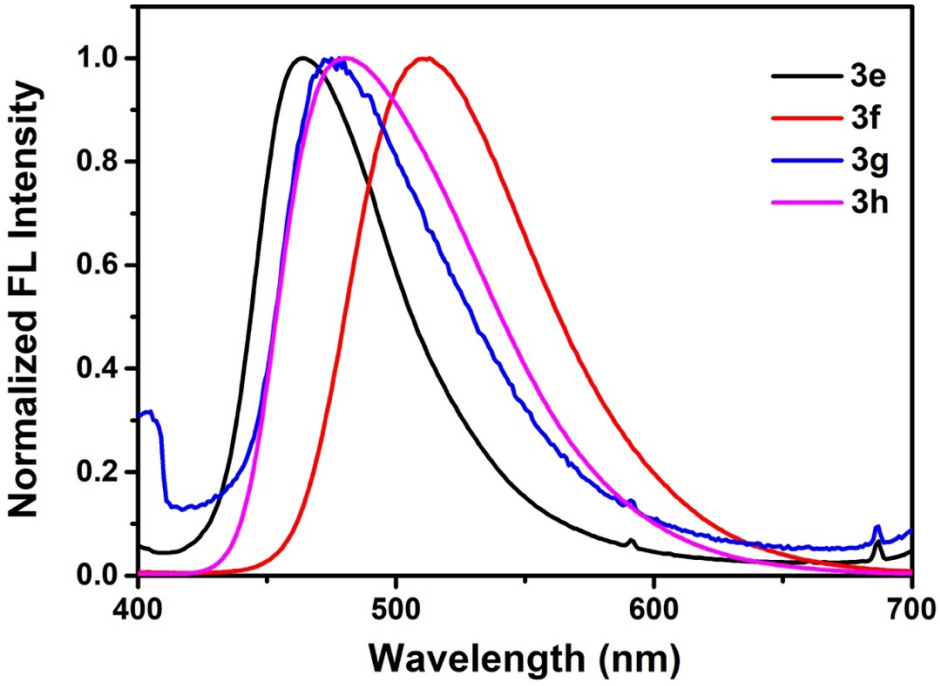


Fig. S22. Fluorescence emission of compound **3e-3h** in solid state.

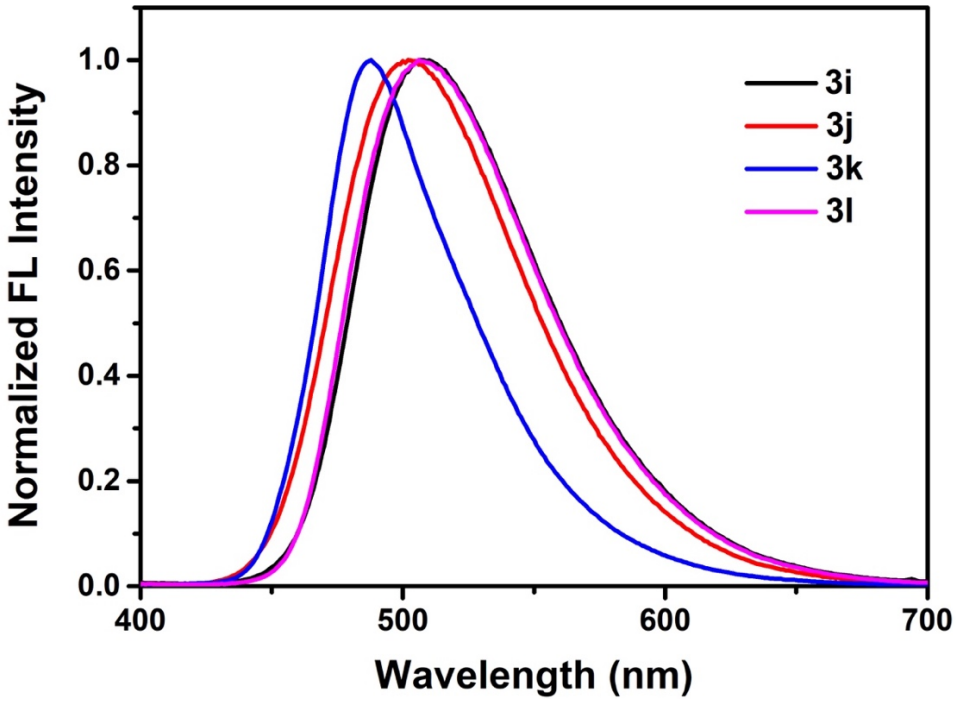


Fig. S23. Fluorescence emission of compound **3i-3l** in solid state.

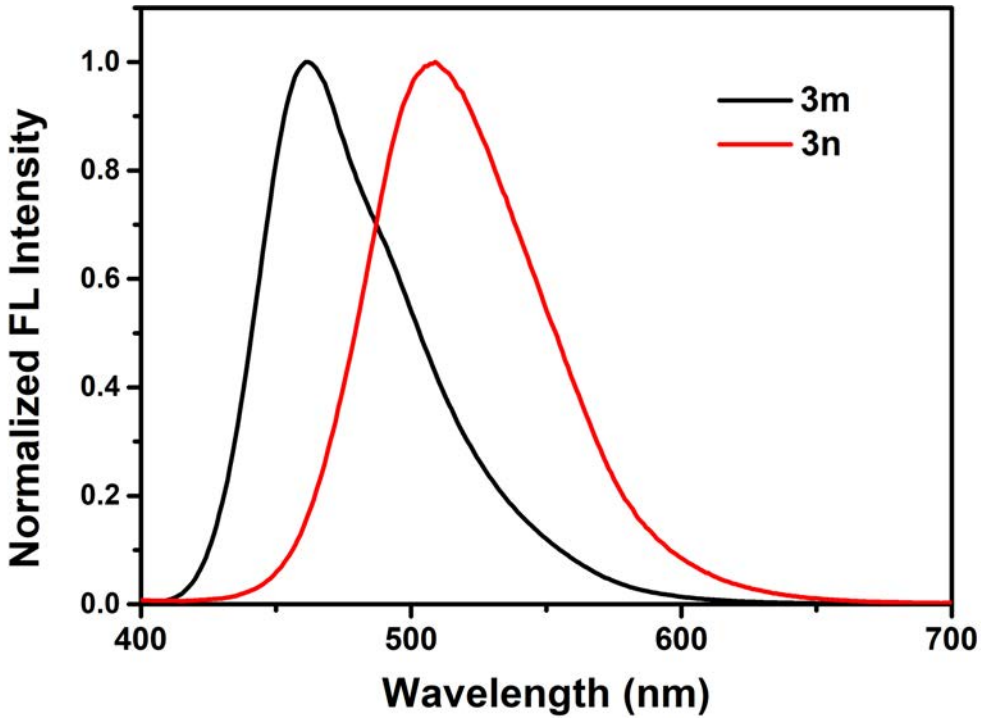


Fig. S24. Fluorescence emission of compound **3m-3n** in solid state.

2.4 The fluorescence emission of 1a-3n in solid state on a CIE chromaticity diagram.

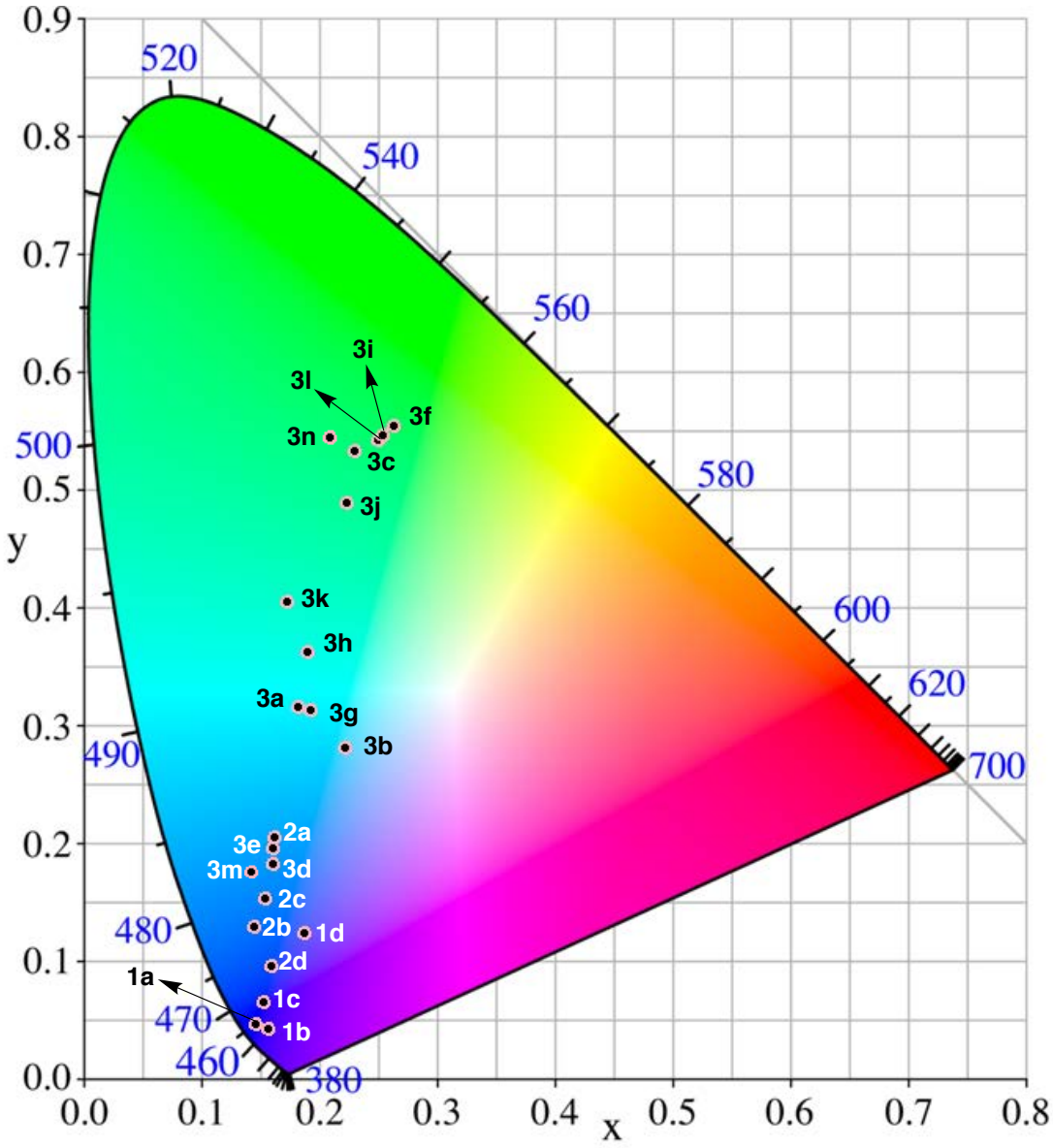


Fig. S25 Fluorescence spectra of compounds **1a-3n** plotted on a CIE chromaticity diagram.

Table S1. Coordinates of compounds **1a**-**3n** on CIE diagram.

	Compound	Coordinate (X)	Coordinate (Y)	Peak
1	**1a**	0.1459	0.0469	362
2	**1b**	0.1566	0.0427	372
3	**1c**	0.1523	0.0649	417
4	**1d**	0.187	0.1234	423
5	**2a**	0.1595	0.1964	461
6	**2b**	0.144	0.1287	457
7	**2c**	0.1527	0.1531	457
8	**2d**	0.1581	0.0956	439
9	**3a**	0.1818	0.316	485
10	**3b**	0.2209	0.2812	468
11	**3c**	0.2296	0.5329	504
12	**3d**	0.1594	0.1826	458
13	**3e**	0.1609	0.2055	464
14	**3f**	0.2622	0.5552	513
15	**3g**	0.1923	0.3131	478
16	**3h**	0.1889	0.3624	481
17	**3i**	0.253	0.5463	506
18	**3j**	0.2229	0.489	502
19	**3k**	0.1716	0.4048	488
20	**3l**	0.249	0.542	506
21	**3m**	0.1444	0.1758	461
22	**3n**	0.2109	0.5435	509

2.5 Lifetime and rate constants for radiative (kr) and nonradiative decay (knr) of each NATs.

Table S2. The fluorescence lifetime of NATs.

Compound	Lifetime in solution (ns)	Lifetime in solid state (ns)
1a	τ1 = 1.991	τ1 = 1.304(65.84%) τ2 = 4.277(34.16%)
1b	τ1 = 2.106	τ1 = 9.133(46.27%) τ2 = 2.234(53.73%)
1c	τ1 = 3.108	τ1 = 8.521(78.19%) τ2 = 2.133(21.81%)
1d	τ1 = 3.099	τ1 = 1.412(94.65%) τ2 = 6.934(5.35%)
2a	τ1 = 4.917	τ1 = 1.759(28.54%) τ2 = 3.828(71.46%)
2b	τ1 = 5.187	τ1 = 1.666(57.37%) τ2 = 2.976(42.63%)
2c	τ1 = 1.797	τ1 = 1.174(88.37%) τ2 = 4.632(11.63%)
2d	τ1 = 4.363	τ1 = 1.549(86.52%) τ2 = 4.879(13.48%)
3a	τ1 = 3.099	τ1 = 1.358(68.11%) τ2 = 4.488(31.89%)
3b	n.d	τ1 = 1.265(68.97%) τ2 = 4.006(31.03%)
3c	τ1 = 6.411(96.07%) τ2 = 3.808(3.93%)	τ1 = 1.051(85.71%) τ2 = 3.941(14.29%)

3d	τ1 = 4.283(75.36%) τ2 = 2.089(24.64%)	τ1 = 1.120(67.00%) τ2 = 4.056(33.00%)
3e	τ1 = 2.241	τ1 = 1.251(76.37%) τ2 = 4.074(23.63%)
3f	τ1 = 1.419	τ1 = 2.333(67.48%) τ2 = 8.966(32.52%)
3g	τ1 = 1.395	τ1 = 1.123(64.65%) τ2 = 4.174(35.35%)
3h	τ1 = 3.313(60.30%) τ2 = 3.027(39.70%)	τ1 = 1.707(57.36%) τ2 = 9.400(34.59%) τ3 = 3.431(8.05%)
3i	τ1 = 1.781(59.84%) τ2 = 6.407(40.16%)	τ1 = 2.129(49.65%) τ2 = 8.227(43.15%) τ3 = 6.453(7.21%)
3j	τ1 = 5.132	τ1 = 1.748(60.52%) τ2 = 4.064(39.48%)
3k	τ1 = 2.556	τ1 = 2.798(67.56%) τ2 = 5.567(32.44%)
3l	τ1 = 1.293	τ1 = 1.780(72.73%) τ2 = 5.695(27.27%)
3m	τ1 = 1.692(59.84%) τ2 = 6.179(40.16%)	τ1 = 1.771(84.18%) τ2 = 10.35(15.82%)
3n	τ1 = 1.467	τ1 = 2.067(56.84%) τ2 = 8.875(43.16%)

Table S3. The rate constants for radiative (kr) and nonradiative decay (knr) were calculated from the Φ and τ values according to the formulae kr = ΦF/τ and knr = (1–ΦF)/τ.

Compound	solution		solid state	
	kr (s^{-1})	knr (s^{-1})	kr (s^{-1})	knr (s^{-1})
1a	4.918×10^{8}	1.040×10^{7}	3.232×10^{7}	3.987×10^{8}
1b	1.982×10^{8}	2.127×10^{8}	n.d	n.d
1c	1.797×10^{8}	2.185×10^{7}	1.083×10^{7}	1.295×10^{8}
1d	2.501×10^{8}	7.173×10^{7}	1.772×10^{8}	4.086×10^{8}
2a	1.779×10^{8}	2.544×10^{7}	1.379×10^{8}	1.764×10^{8}
2b	1.794×10^{8}	1.336×10^{7}	1.722×10^{8}	2.775×10^{8}
2c	9.721×10^{7}	4.593×10^{8}	1.351×10^{8}	4.994×10^{8}
2d	2.200×10^{8}	9.168×10^{6}	2.550×10^{8}	2.450×10^{8}
3a	1.194×10^{6}	3.215×10^{8}	3.353×10^{6}	4.211×10^{8}
3b	n.d	n.d	4.310×10^{7}	4.295×10^{8}
3c	6.515×10^{7}	1.520×10^{8}	3.394×10^{7}	6.491×10^{8}
3d	3.420×10^{6}	2.638×10^{8}	3.494×10^{6}	4.752×10^{8}
3e	1.117×10^{8}	3.345×10^{8}	2.254×10^{8}	2.959×10^{8}
3f	8.534×10^{7}	6.194×10^{8}	2.910×10^{7}	2.910×10^{7}
3g	7.792×10^{7}	6.389×10^{8}	9.792×10^{7}	3.638×10^{8}
3h	5.627×10^{5}	3.120×10^{8}	6.392×10^{7}	1.579×10^{8}
3i	5.051×10^{7}	2.243×10^{8}	2.190×10^{7}	1.952×10^{8}
3j	1.011×10^{8}	9.370×10^{7}	6.589×10^{7}	3.098×10^{8}
3k	1.408×10^{8}	2.504×10^{8}	4.058×10^{7}	2.300×10^{8}
3l	3.295×10^{7}	7.404×10^{8}	2.974×10^{7}	3.214×10^{8}
3m	1.631×10^{7}	2.700×10^{8}	9.271×10^{7}	2.270×10^{8}
3n	5.317×10^{7}	6.285×10^{8}	1.479×10^{7}	1.850×10^{8}

2.6 Aggregation-induced emission properties of NATs

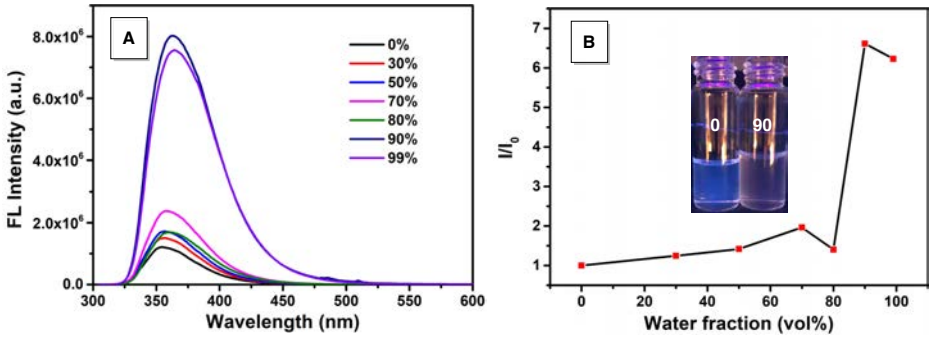


Fig. S26 (A) FL spectra of **1a** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **1a**. Inset: photograph of **1a** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

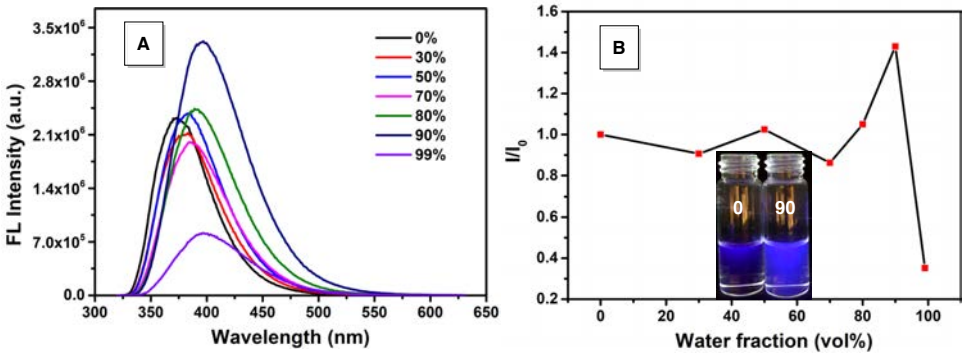


Fig. S27 (A) FL spectra of **1b** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **1b**. Inset: photograph of **1b** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

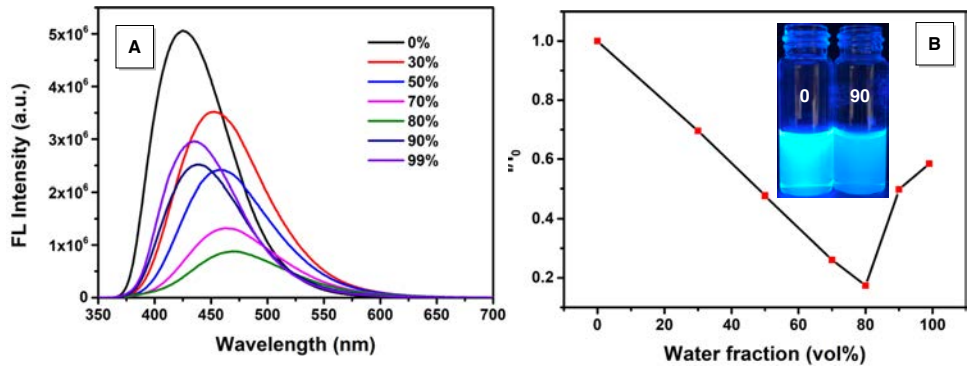


Fig. S28 (A) FL spectra of **1c** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **1c.** Inset: photograph of **1c** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

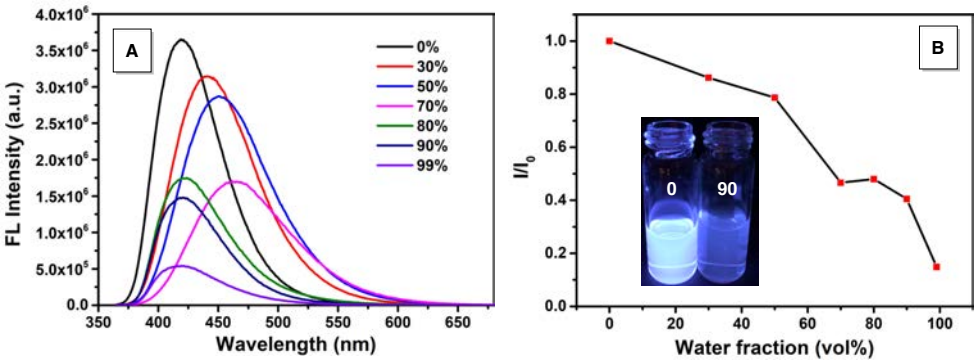


Fig. S29 (A) FL spectra of **1d** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **1d**. Inset: photograph of **1d** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

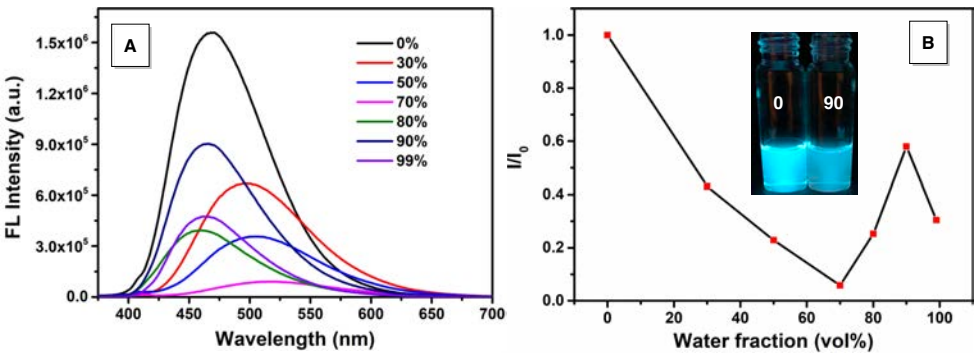


Fig. S30 (A) FL spectra of **2a** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **2a**. Inset: photograph of **2a** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

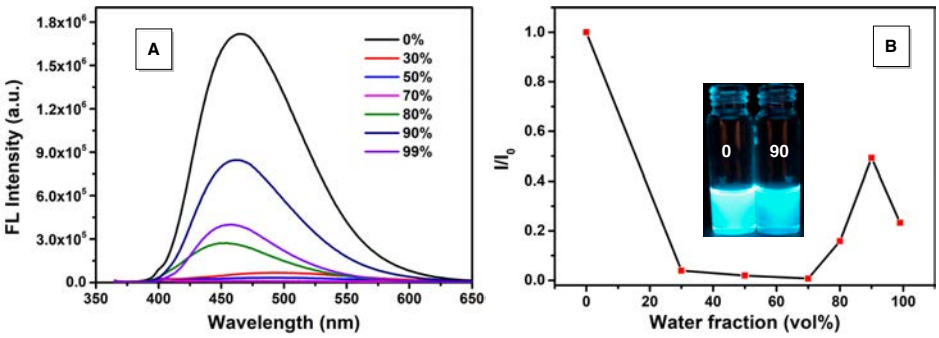


Fig. S31 (A) FL spectra of **2b** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **2b**. Inset: photograph of **2b** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

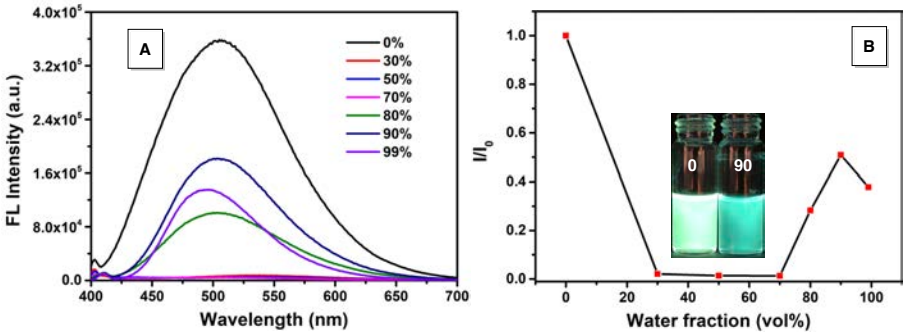


Fig. S32 (A) FL spectra of **2c** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **2c**. Inset: photograph of **2c** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

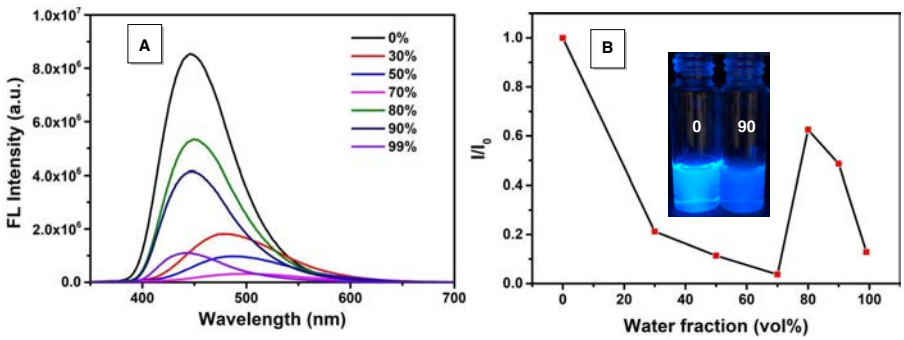


Fig. S33 (A) FL spectra of **2d** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **2d.** Inset: photograph of **2d** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

(Due to the emission intensity of compound **3a** in each condition was very low, its AIE properties cannot be measured.)

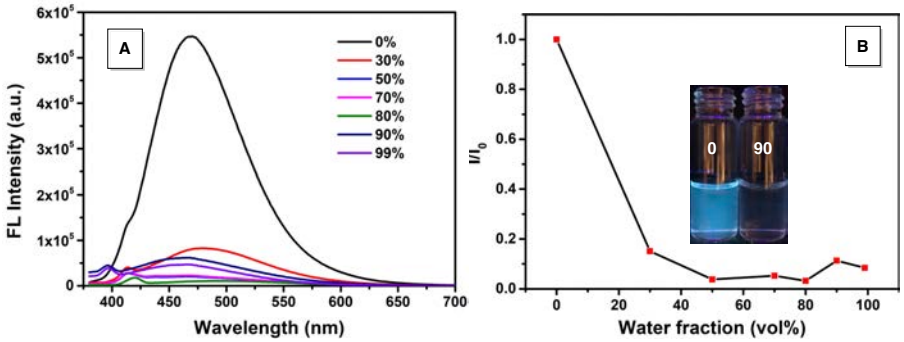


Fig. S34 (A) FL spectra of **3b** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3b**. Inset: photograph of **3b** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

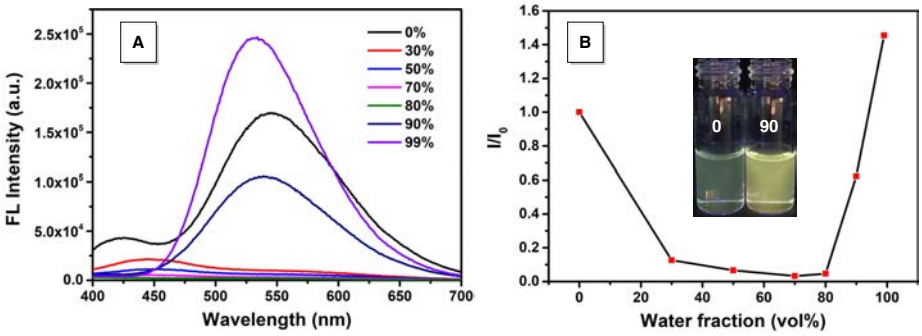


Fig. S35 (A) FL spectra of **3c** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3c**. Inset: photograph of **3c** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

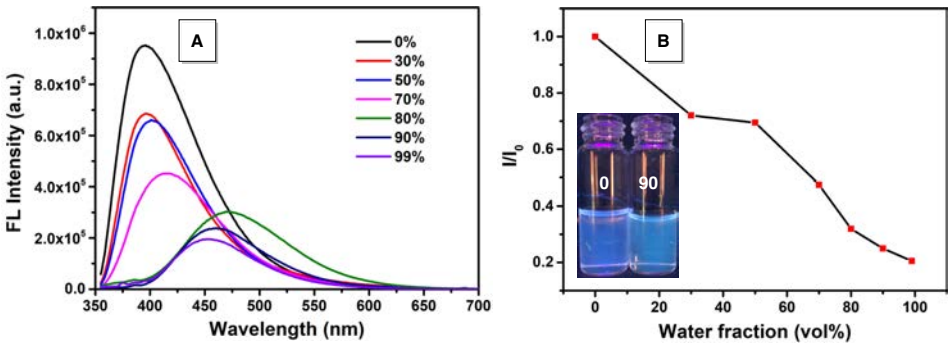


Fig. S36 (A) FL spectra of **3d** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3d**. Inset: photograph of **3d** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

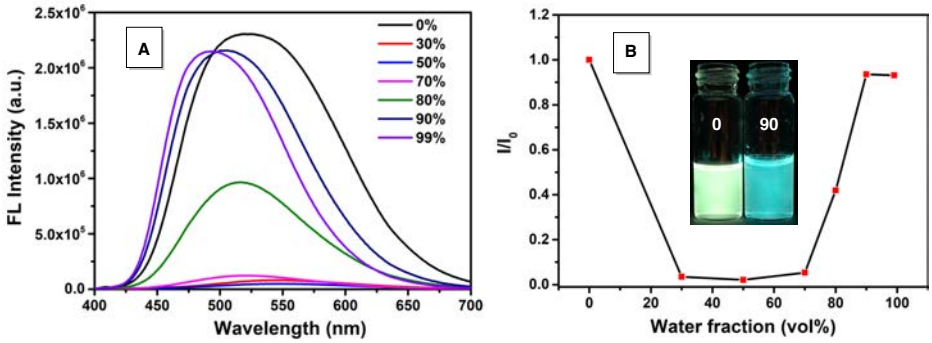


Fig. S37 (A) FL spectra of **3e** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3e.** Inset: photograph of **3e** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

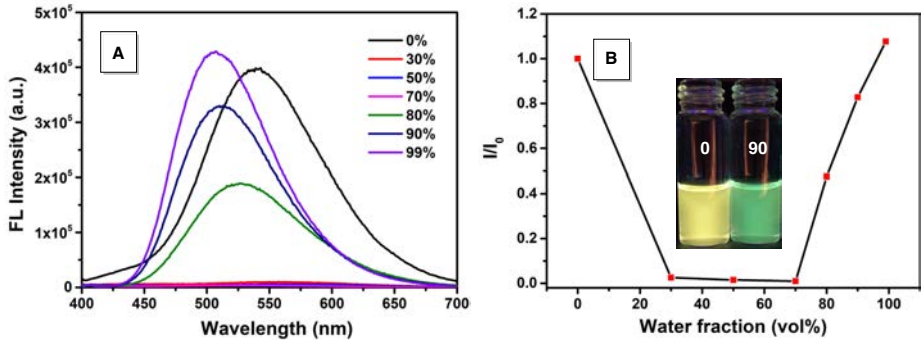


Fig. S38 (A) FL spectra of **3f** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3f.** Inset: photograph of **3f** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

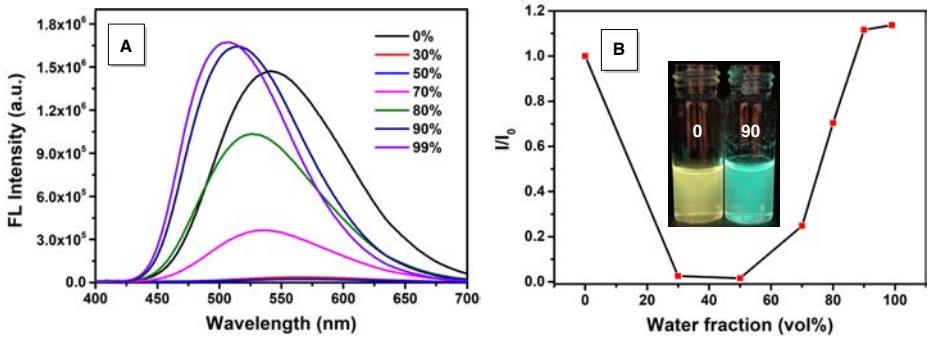


Fig. S39 (A) FL spectra of **3g** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3g.** Inset: photograph of **3g** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

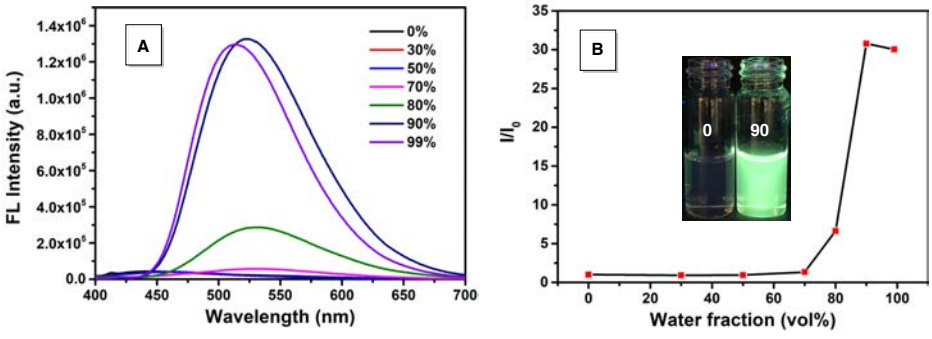


Fig. S40 (A) FL spectra of **3h** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3h**.

Inset: photograph of **3h** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

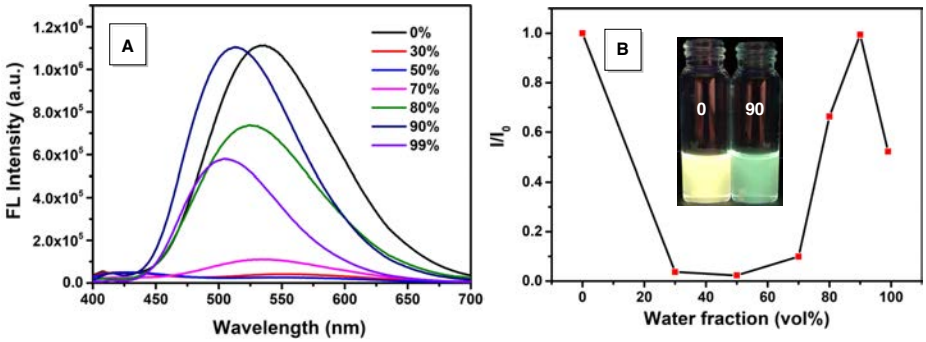


Fig. S41 (A) FL spectra of **3i** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3i.** Inset: photograph of **3i** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

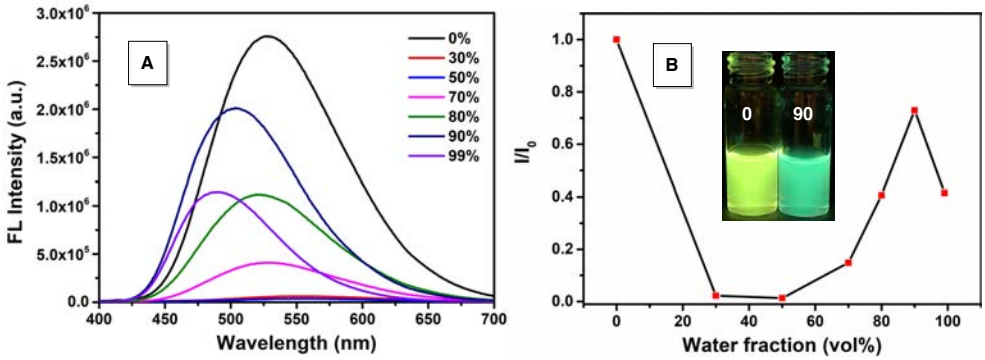


Fig. S42 (A) FL spectra of **3j** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3j**. Inset: photograph of **3j** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

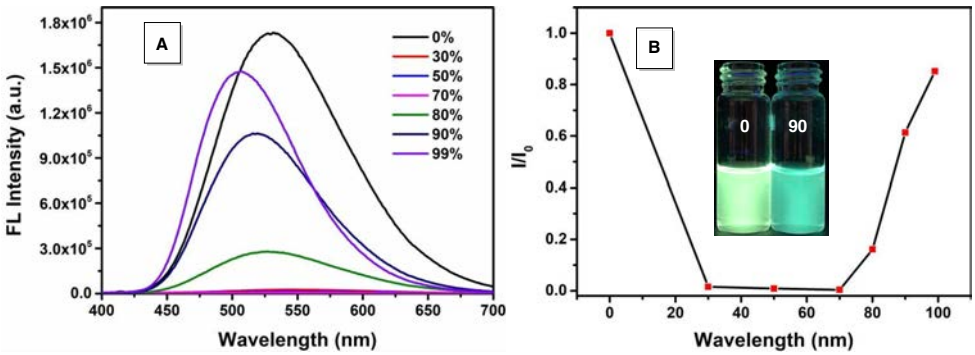


Fig. S43 (A) FL spectra of **3k** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3k**. Inset: photograph of **3k** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

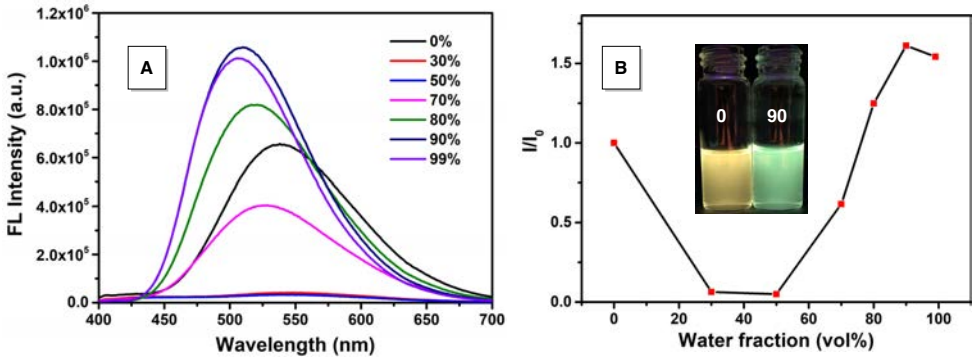


Fig. S44 (A) FL spectra of **3l** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3l.** Inset: photograph of **3l** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

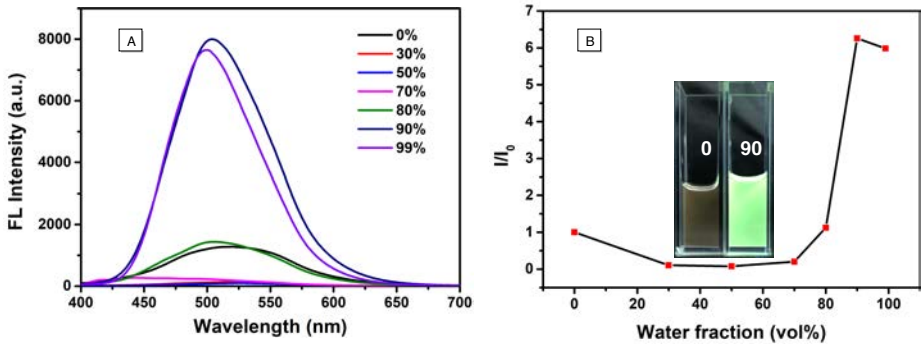


Fig. S45 (A) FL spectra of **3m** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3m.** Inset: photograph of **3m** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

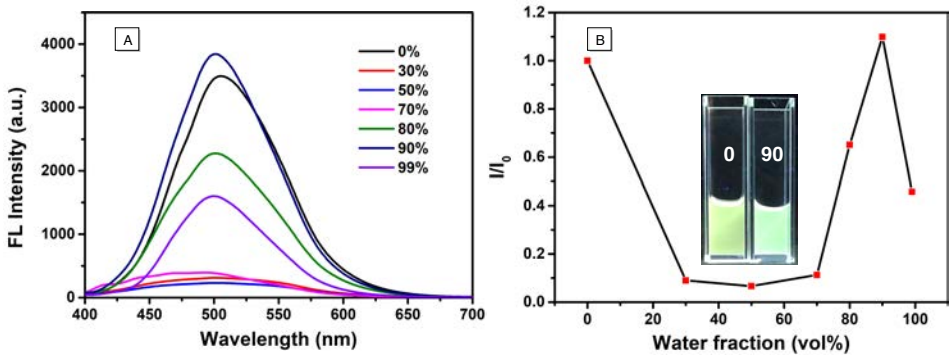


Fig. S46 (A) FL spectra of **3n** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) Plots of emission intensity versus the composition of the water mixtures of **3n.** Inset: photograph of **3n** in THF/water mixtures with fw values of 0, and 90% under irradiation of 365 nm UV light.

2.7 UV-vis spectra of 1a-3m (10 μM) in THF and THF/water mixtures with different water fractions

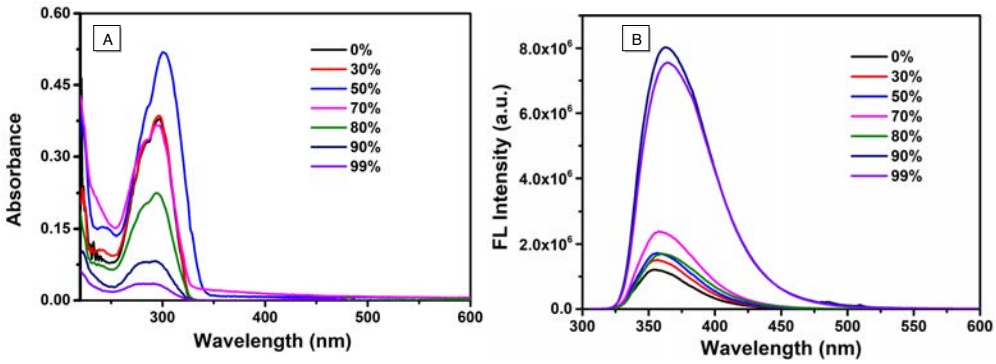


Fig. S47 (A) UV-vis spectra of **1a** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **1a** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

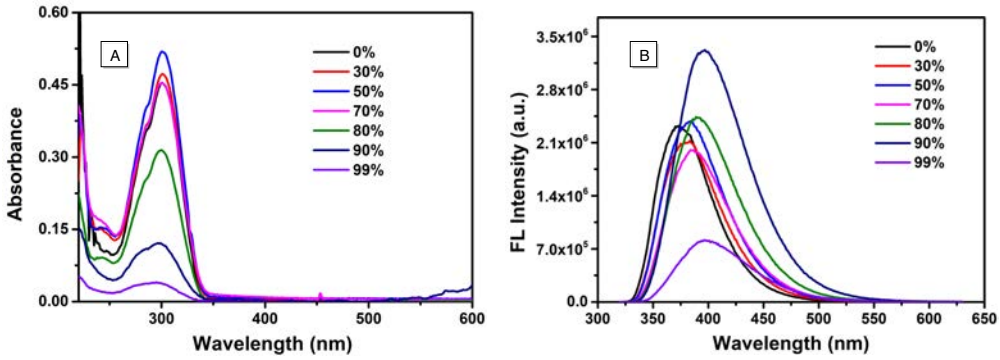


Fig. S48 (A) UV-vis spectra of **1b** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **1b** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

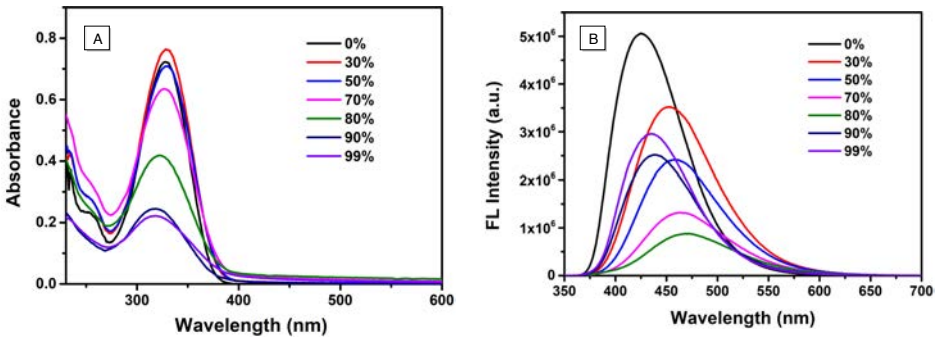


Fig. S49 (A) UV-vis spectra of **1c** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **1c** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

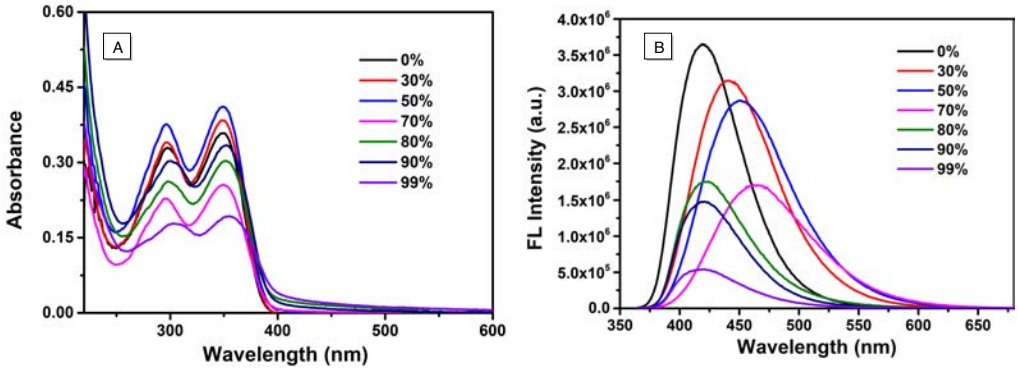


Fig. S50 (A) UV-vis spectra of **1d** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **1d** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

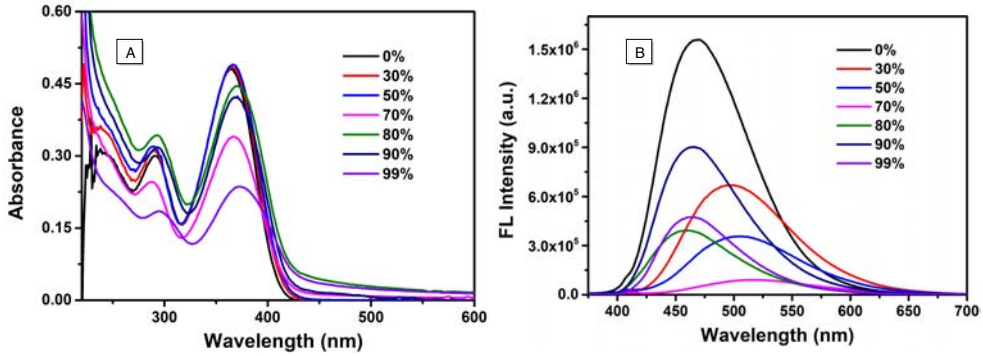


Fig. S51 (A) UV-vis spectra of 2a (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of 2a (10 μM) in THF and THF/water mixtures with different water fractions (fw).

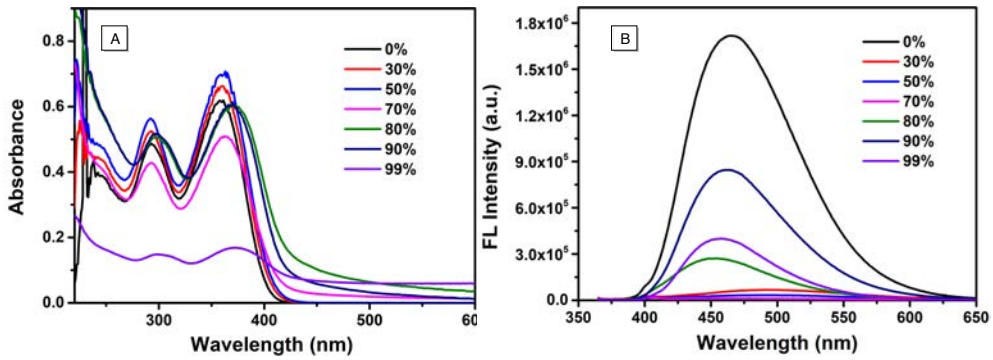


Fig. S52 (A) UV-vis spectra of **2b** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **2b** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

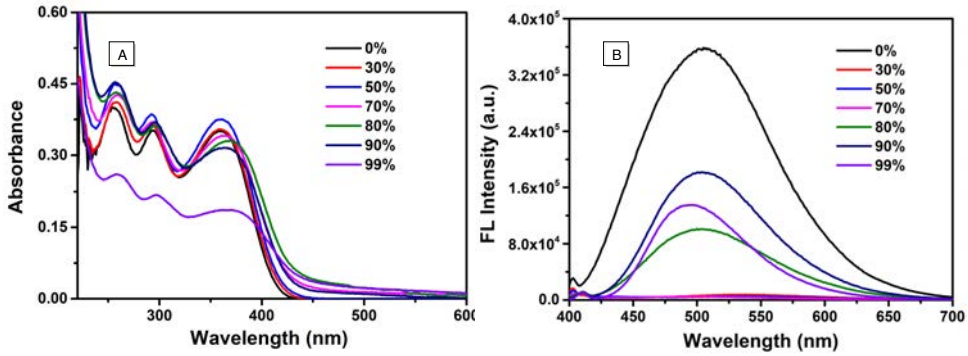


Fig. S52 (A) UV-vis spectra of **2c** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **2c** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

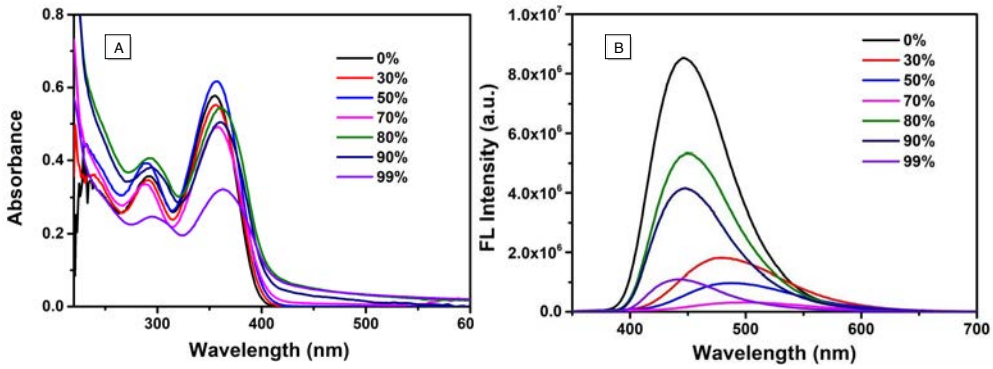


Fig. S54 (A) UV-vis spectra of **2d** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **2d** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

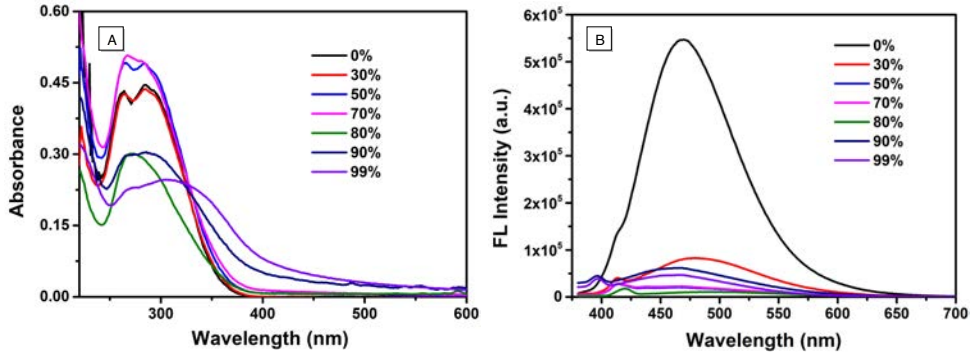


Fig. S55 (A) UV-vis spectra of **3b** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3b** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

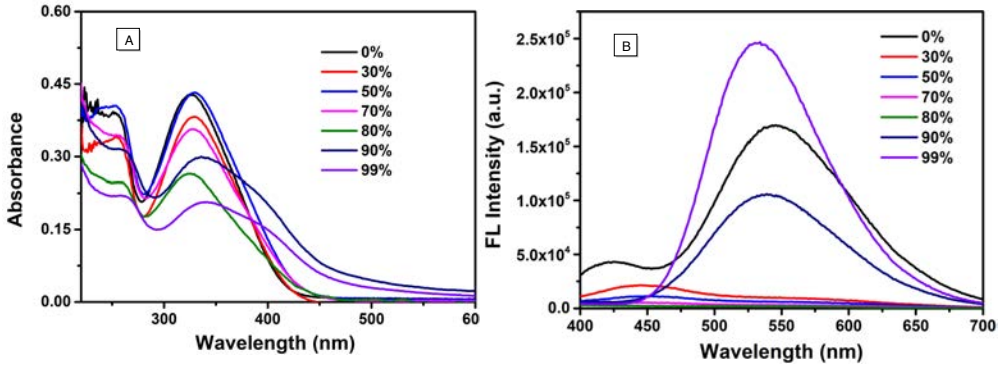


Fig. S56 (A) UV-vis spectra of **3c** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3c** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

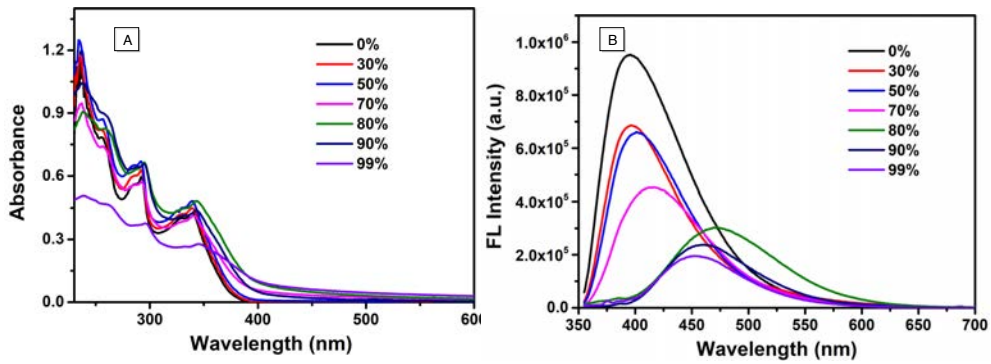


Fig. S57 (A) UV-vis spectra of **3d** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3d** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

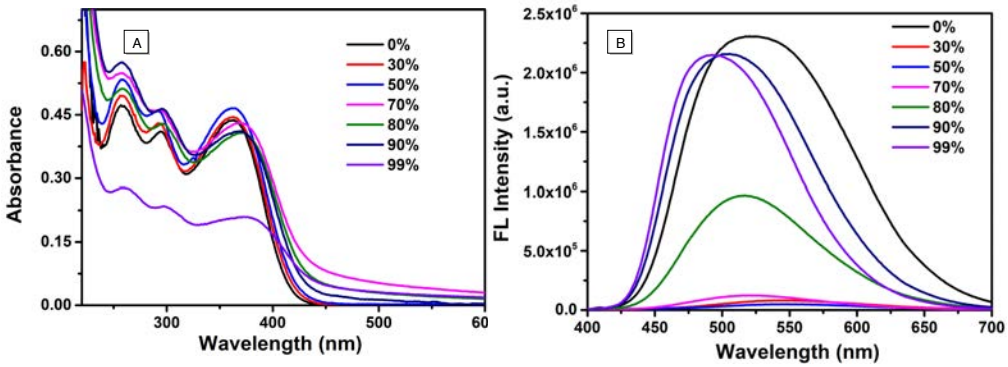


Fig. S58 (A) UV-vis spectra of **3e** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3e** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

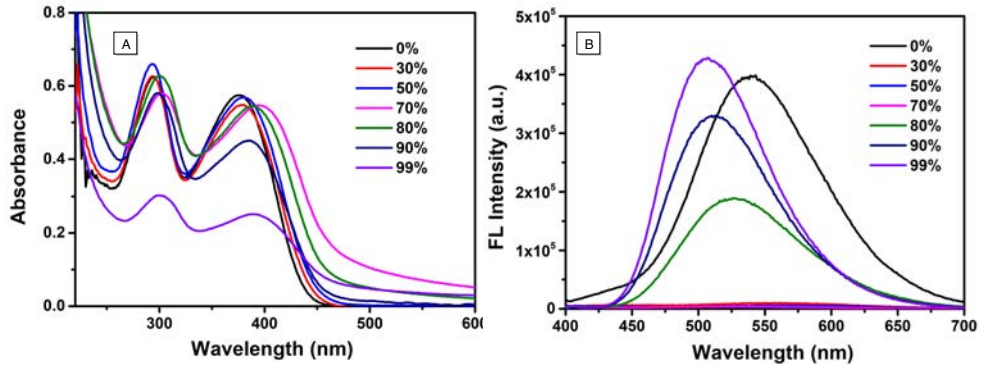


Fig. S59 (A) UV-vis spectra of **3f** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3f** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

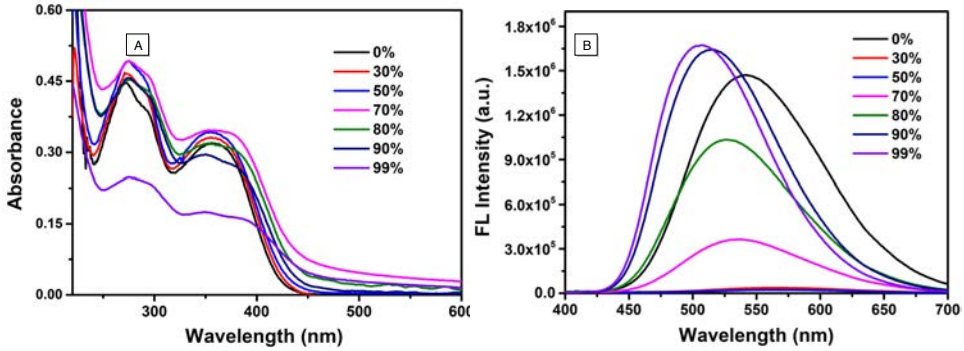


Fig. S60 (A) UV-vis spectra of **3g** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3g** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

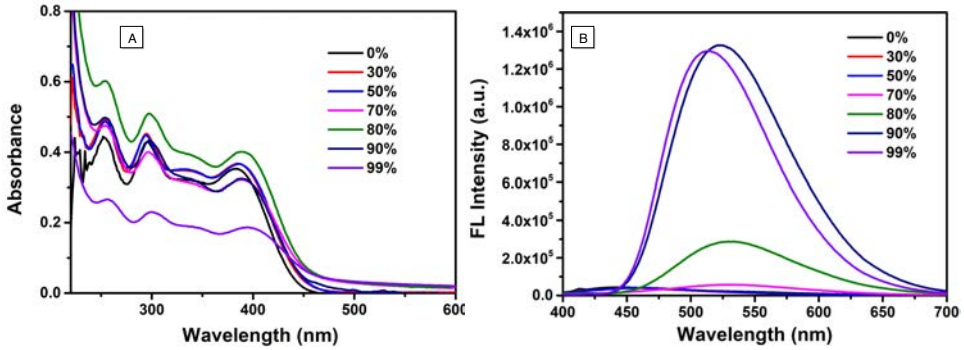


Fig. S61 (A) UV-vis spectra of **3h** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3h** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

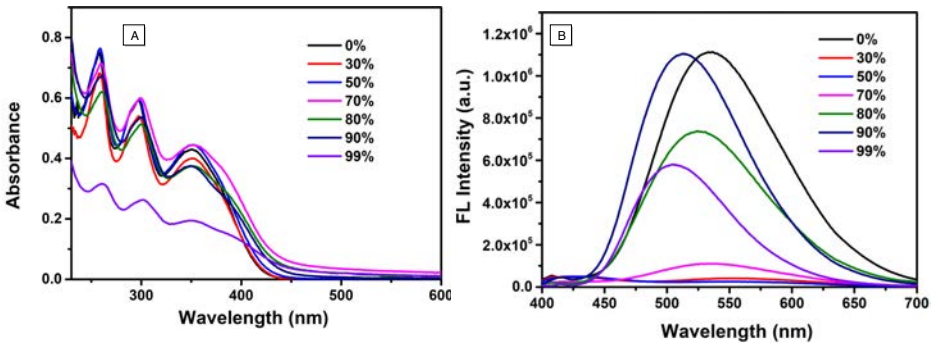


Fig. S62 (A) UV-vis spectra of **3i** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3i** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

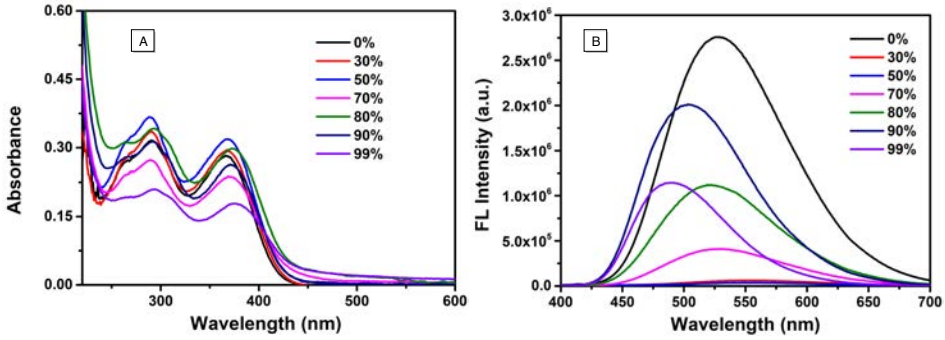


Fig. S63 (A) UV-vis spectra of **3j** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3j** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

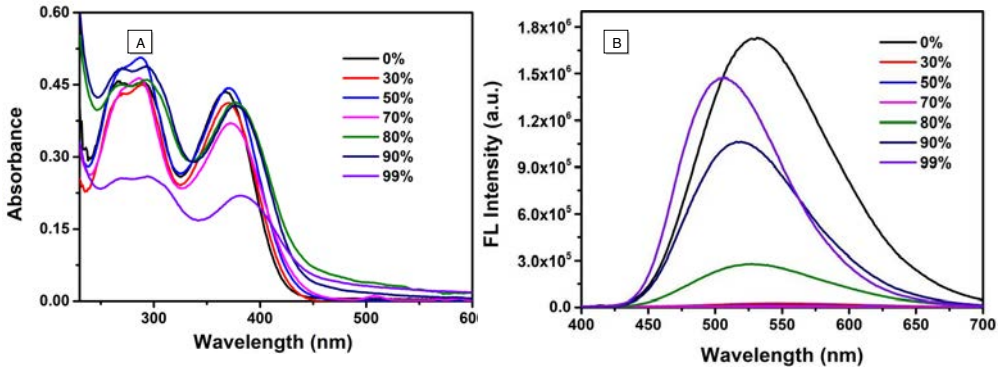


Fig. S64 (A) UV-vis spectra of **3k** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3k** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

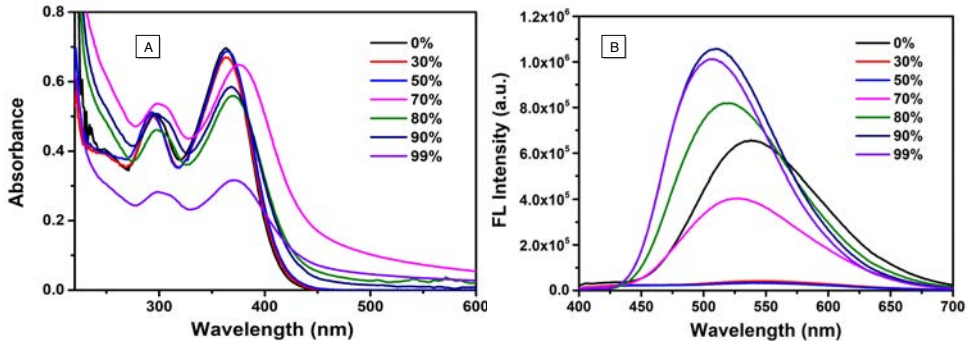


Fig. S65 (A) UV-vis spectra of **3l** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3l** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

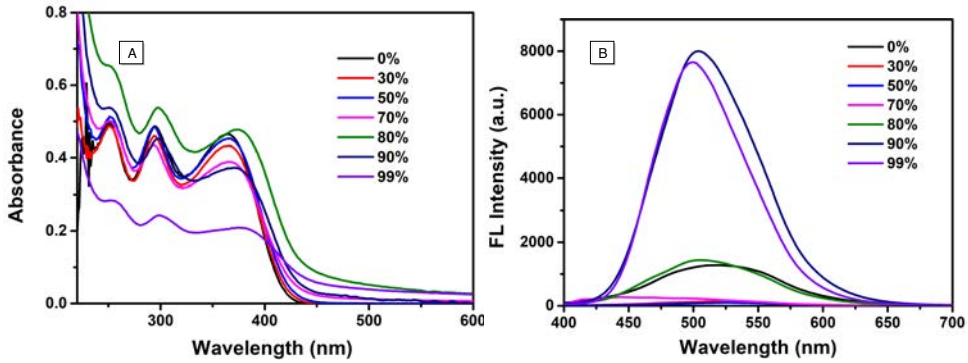


Fig. S66 (A) UV-vis spectra of **3m** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3m** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

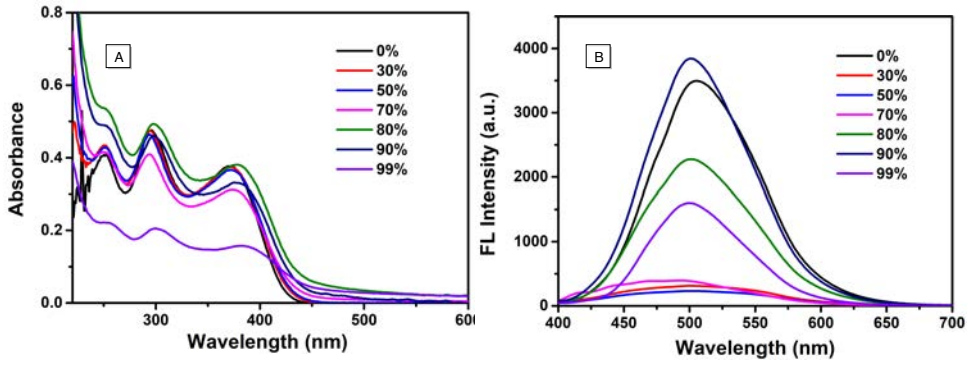


Fig. S67 (A) UV-vis spectra of **3n** (10 μM) in THF and THF/water mixtures with different water fractions (fw). (B) FL spectra of **3n** (10 μM) in THF and THF/water mixtures with different water fractions (fw).

III. Mechanochromic Luminescence Properties

3.1 FL spectra of unground[a] and ground NATs

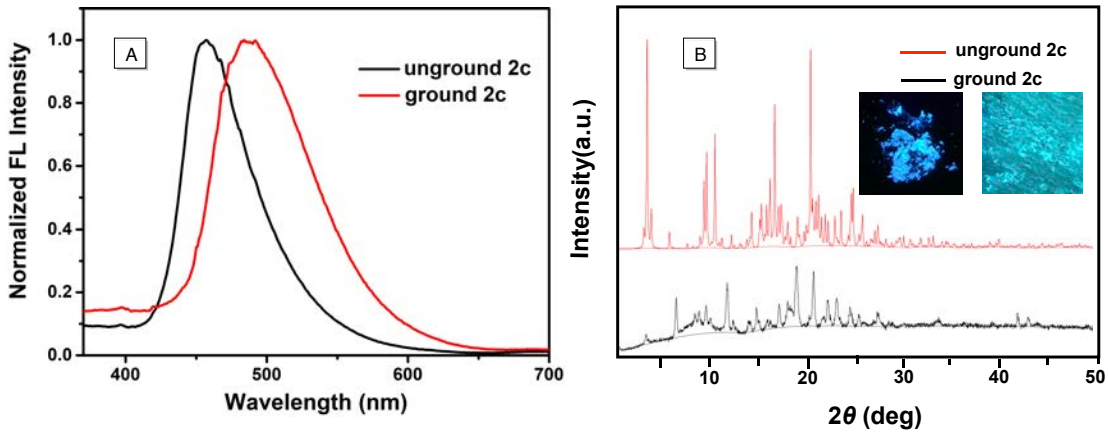


Fig. S68 (A) Normalized FL spectra of unground **2c** (black line) and ground **2c** (red line). (B) Powder XRD diffractions of unground **2c** (black line) and ground **2c** (red line). Inset: photograph of unground **2c** (left) and ground **2c** (right) taken under illumination with UV light (365 nm).

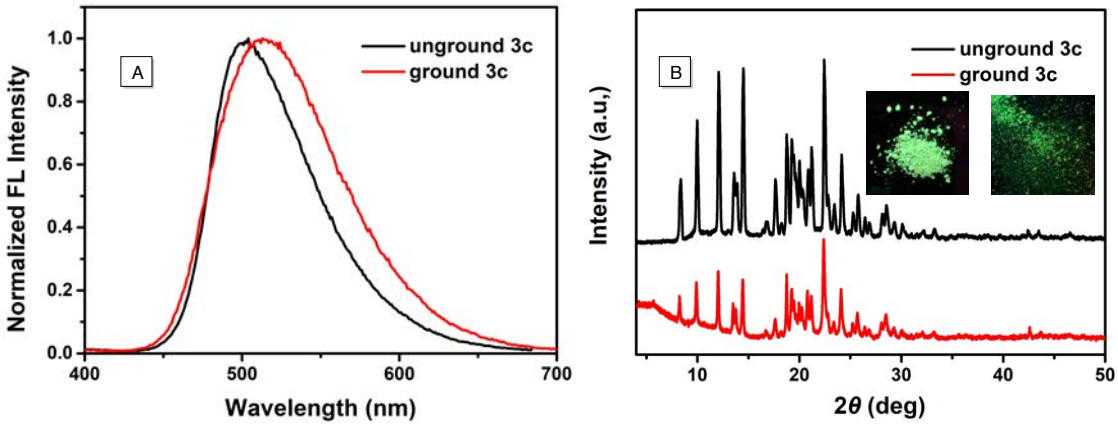


Fig. S69 (A) Normalized FL spectra of unground **3c** (black line) and ground **3c** (red line). (B) Powder XRD diffractions of unground **3c** (black line) and ground **3c** (red line). Inset: photograph of unground **3c** (left) and ground **3c** (right) taken under illumination with UV light (365 nm).

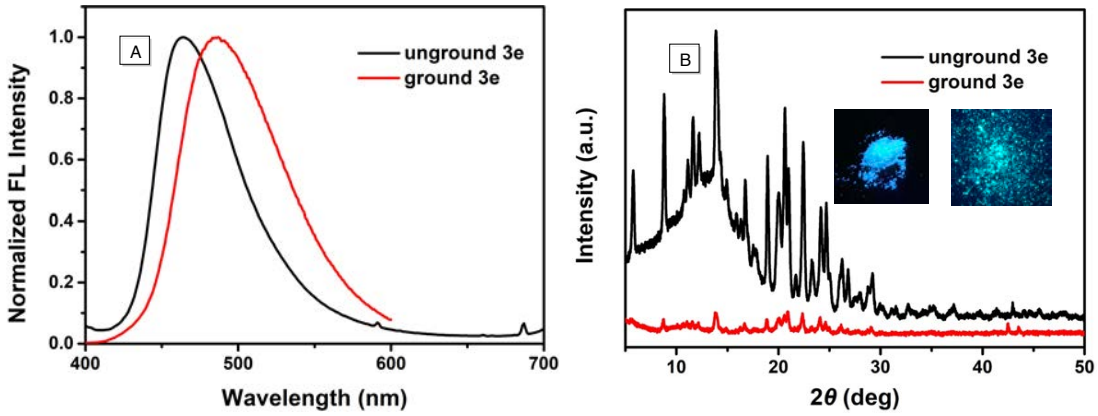


Fig. S70 (A) Normalized FL spectra of unground **3e** (black line) and ground **3e** (red line). (B) Powder XRD diffractions of unground **3e** (black line) and ground **3e** (red line). Inset: photograph of unground **3e** (left) and ground **3e** (right) taken under illumination with UV light (365 nm).

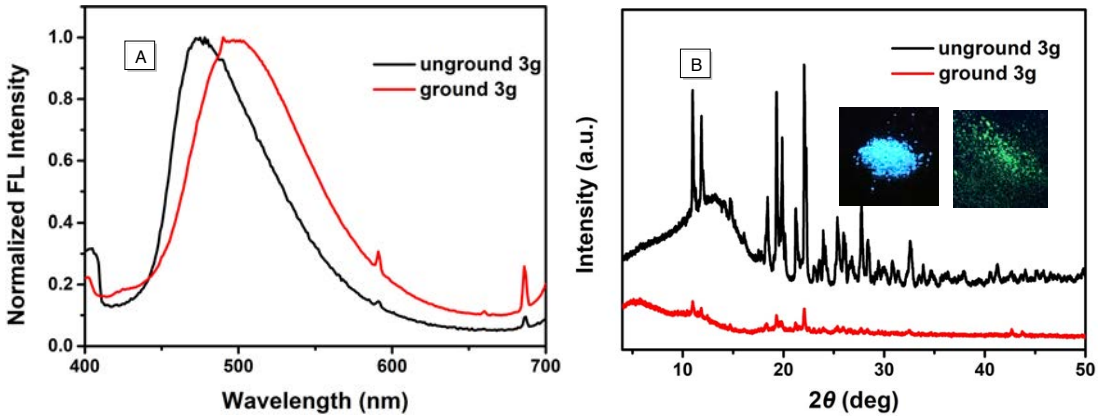


Fig. S71 (A) Normalized FL spectra of unground **3g** (black line) and ground **3g** (red line). (B) Powder XRD diffractions of unground **3g** (black line) and ground **3g** (red line). Inset: photograph of unground **3g** (left) and ground **3g** (right) taken under illumination with UV light (365 nm).

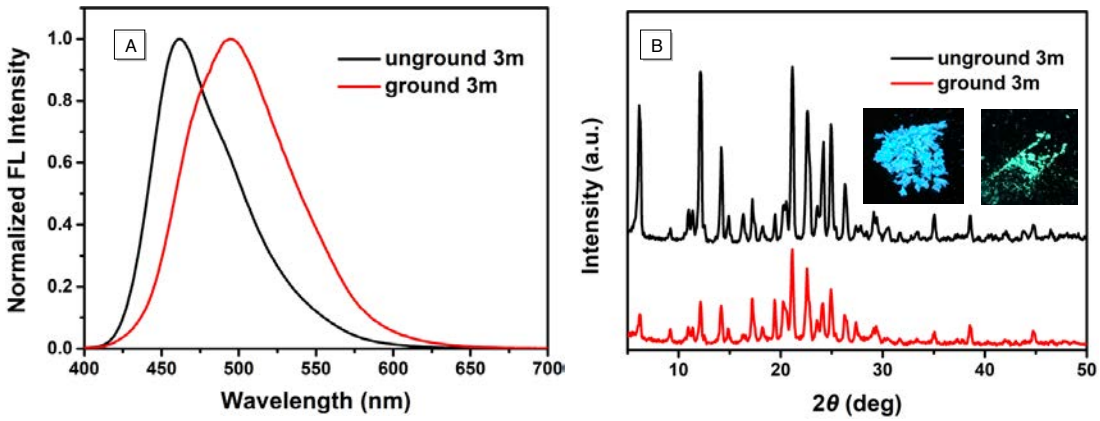


Fig. S72 (A) Normalized FL spectra of unground **3m** (black line) and ground **3m** (red line). (B) Powder XRD diffractions of unground **3m** (black line) and ground **3m** (red line). Inset: photograph of unground **3m** (left) and ground **3m** (right) taken under illumination with UV light (365 nm).

3.2 The absorption spectra of unground[a] and ground NATs

a. The unground sample was obtained by heating those NATs to 170 °C and then cooling down to the room temperature.

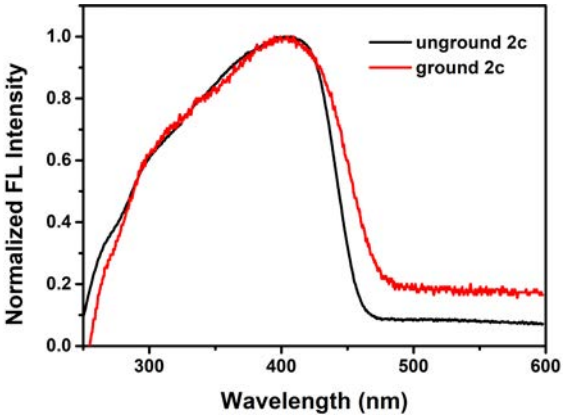
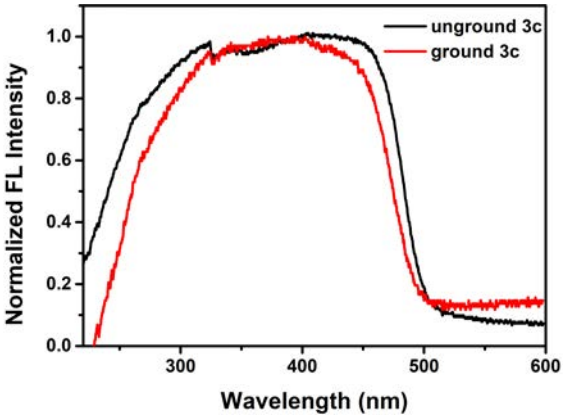


Fig.73 The absorption spectra of unground **2c** (black line) and ground **2c** (red line).



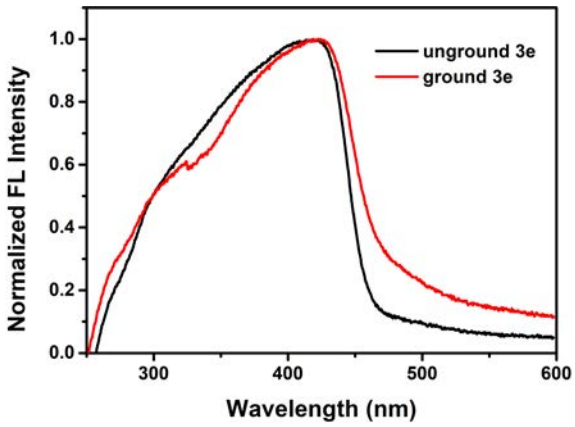


Fig.75 The absorption spectra of unground **3e** (black line) and ground **3e** (red line).

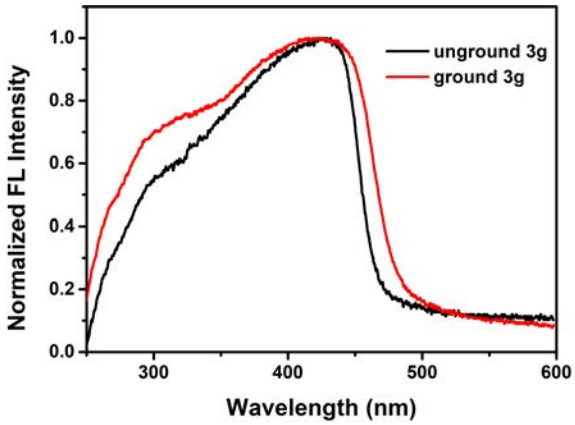


Fig.76 The absorption spectra of unground **3g** (black line) and ground **3g** (red line).

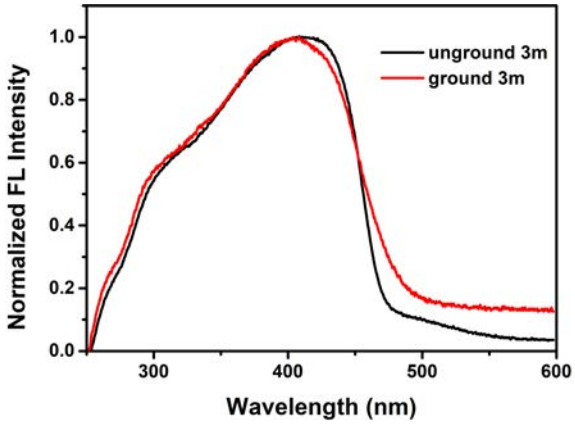


Fig.77 The absorption spectra of unground **3m** (black line) and ground **3m** (red line).

IV. ORTEP Drawing of the Crystal Structure

X-ray Crystallography

The X-ray diffraction data were measured on Bruker D8 Venture PHOTON II CPAD diffractometer equipped with a Cu K_α INCOATEC ImuS micro-focus source (λ = 1.54178 Å). Indexing was performed using Apex3 [1]. Data integration and reduction were performed using Saint [2]. Absorption correction was performed by multi-scan method implemented in SADABS [3]. Space groups were determined using XPREP implemented in APEX3 [1]. Structure was solved using SHELXT [4] and refined using SHELXL-2018 [5-7] (full-matrix least-squares on F^2) within OLEX2 interface program [8]. Graphics were done with Platon [9]. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in geometrically calculated positions and were included in the refinement process using riding model with isotropic thermal parameters**.** Crystal data and refinement conditions are shown in **Tables S4 – S13**.

[1] Bruker (2018). *APEX3* (Version 2017.3). Bruker AXS Inc., Madison, Wisconsin, USA.

[2] Bruker (2018) SAINT V8.35A. Data Reduction Software.

[3] Sheldrick, G. M. (1996). *SADABS. Program for Empirical Absorption Correction.* University of Gottingen, Germany.

[4] Sheldrick, G. M. (2015) "SHELXT - Integrated space-group and crystal structure determination" Acta Cryst. A71, 3-8

[5] Sheldrick, G.M. (1990) Acta Cryst. A46, 467-473

[6] Sheldrick, G. M. (2008) Acta Cryst. A64, 112-122.

[7] G.M. Sheldrick (2015) "Crystal structure refinement with SHELXL", Acta Cryst., C71, 3-8

[8] Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H., OLEX2: A complete structure solution, refinement and analysis program (2009). J. Appl. Cryst., 42, 339-341.

[9] A.L.Spek, Acta Cryst. 2009, D65, 148-155.

4.1 NAT-2a

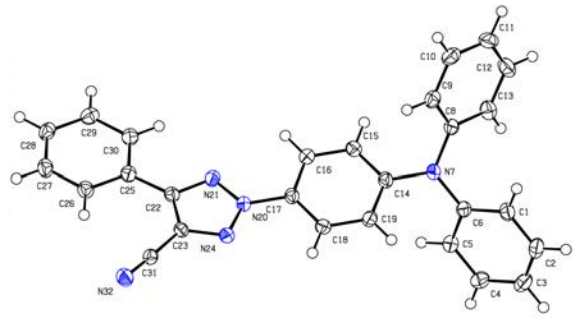


Fig.S78. Asymmetric unit of QL_160_1. Anisotropic displacement parameters were drawn at 50% probability. CCDC: 1888248

Table S4 Crystal data and structure refinement for QL_160_1.	
Identification code	QL_160_1
Empirical formula	$C_{27}H_{19}N_5$
Formula weight	413.47
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.7931(3)
b/Å	10.0013(4)
c/Å	10.8744(4)
α/°	95.079(2)
β/°	90.2830(10)
γ/°	100.4010(10)
Volume/Å^3	1043.23(7)
Z	2
ρ_{calc}g/cm^3	1.316
μ/mm^{-1}	0.634

F(000)	432.0
Crystal size/mm^3	0.14 × 0.1 × 0.08
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	8.164 to 133.164
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -12 ≤ l ≤ 12
Reflections collected	34077
Independent reflections	3655 [R_{int} = 0.0438, R_{sigma} = 0.0202]
Data/restraints/parameters	3655/0/289
Goodness-of-fit on F^2	1.020
Final R indexes [I>=2σ (I)]	R_1 = 0.0340, wR_2 = 0.0788
Final R indexes [all data]	R_1 = 0.0408, wR_2 = 0.0834
Largest diff. peak/hole / e Å^{-3}	0.15/-0.23

4.2 NAT-2b

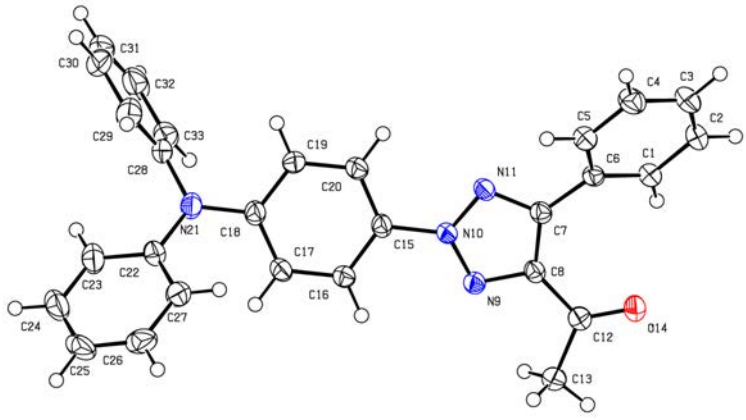


Fig. S79. Asymmetric unit of **QL_1_133_1.** Anisotropic displacement parameters were drawn at 50% probability. CCDC: 1888246

Table S5 Crystal data and structure refinement for QL_1_133_1.	
Identification code	QL_1_133_1

Empirical formula	$C_{28}H_{22}N_4O$
Formula weight	430.49
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.2269(2)
b/Å	27.1036(8)
c/Å	11.1290(3)
α/°	90
β/°	90.4517(14)
γ/°	90
Volume/Å^3	2179.83(11)
Z	4
ρ_{calc}g/cm^3	1.312
μ/mm^{-1}	0.647
F(000)	904.0
Crystal size/mm^3	0.2 × 0.04 × 0.03
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	6.522 to 155.99
Index ranges	$-8 \leq h \leq 8$, $-34 \leq k \leq 32$, $-13 \leq l \leq 14$
Reflections collected	23216
Independent reflections	4566 [R_{int} = 0.0465, R_{sigma} = 0.0295]
Data/restraints/parameters	4566/0/299
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0440, wR_2 = 0.0988
Final R indexes [all data]	R_1 = 0.0543, wR_2 = 0.1055

Largest diff. peak/hole / e Å^{-3} 0.22/-0.23

4.3 NAT-2c

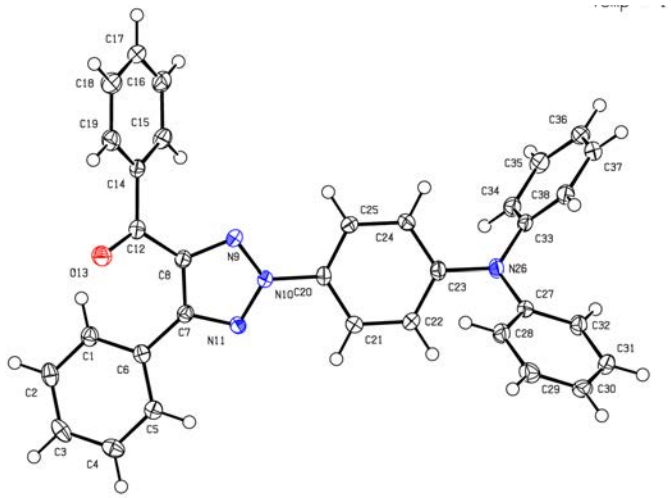


Fig. S80. Asymmetric unit of **ql_151_1.** Anisotropic displacement parameters were drawn at 50% probability. CCDC: 1888249

Table S6 Crystal data and structure refinement for ql_151_1.	
Identification code	ql_151_1
Empirical formula	$C_{33}H_{24}N_4O$
Formula weight	492.56
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.0532(2)
b/Å	29.8500(8)
c/Å	10.4081(3)
α/°	90

β/°	90.3969(9)
γ/°	90
Volume/Å^3	2501.92(12)
Z	4
ρ_{calc}g/cm^3	1.308
μ/mm^{-1}	0.636
F(000)	1032.0
Crystal size/mm^3	0.2 × 0.15 × 0.14
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	5.922 to 159.844
Index ranges	$-9 \leq h \leq 9$, $-37 \leq k \leq 35$, $-13 \leq l \leq 13$
Reflections collected	34122
Independent reflections	5299 [R_{int} = 0.0342, R_{sigma} = 0.0190]
Data/restraints/parameters	5299/0/343
Goodness-of-fit on F^2	1.019
Final R indexes [I>=2σ (I)]	R_1 = 0.0368, wR_2 = 0.0860
Final R indexes [all data]	R_1 = 0.0408, wR_2 = 0.0891
Largest diff. peak/hole / e Å^{-3}	0.17/-0.29

4.4 NAT-3c

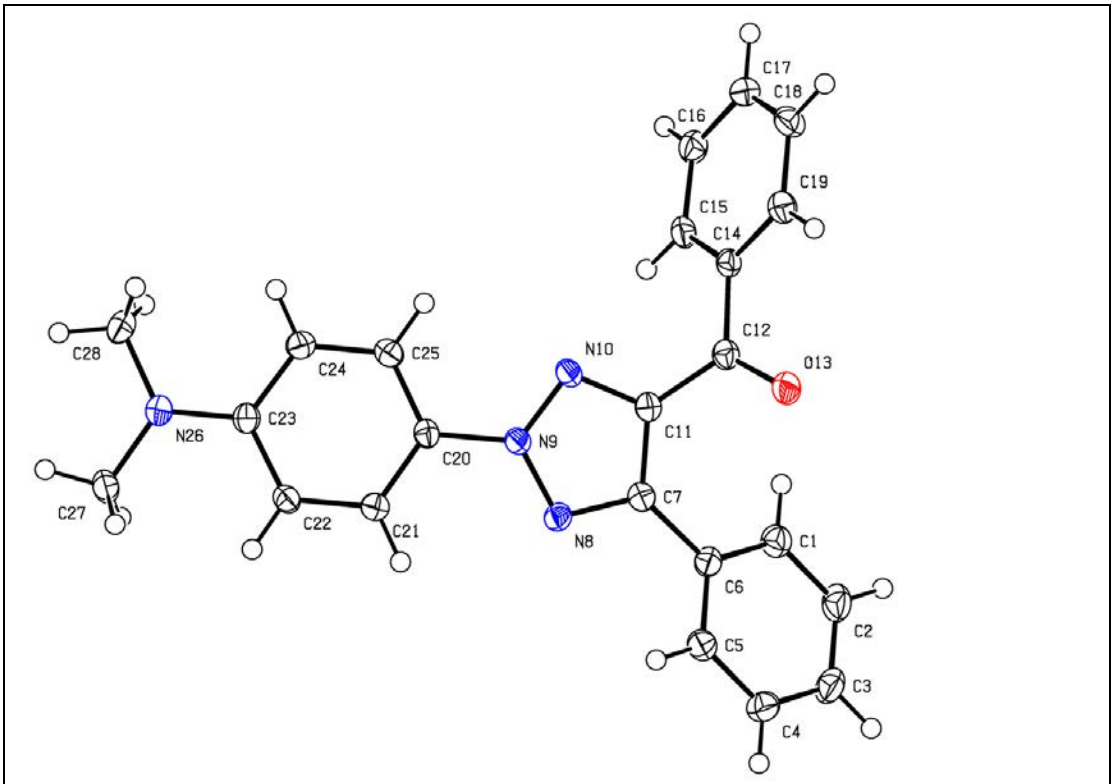


Fig. S81. Asymmetric unit of **QL_1023_D7**. Anisotropic displacement parameters were drawn at 50% probability. CCDC:1888252

Table S7 Crystal data and structure refinement for QL_1023_D7.	
Identification code	QL_1023_D7
Empirical formula	$C_{23}H_{20}N_4O$
Formula weight	368.43
Temperature/K	99.98
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.5248(5)

b/Å	9.9507(5)
c/Å	18.3419(9)
α/°	90
β/°	99.599(2)
γ/°	90
Volume/$Å^3$	1894.04(16)
Z	4
$\rho_{calc}g/cm^3$	1.292
μ/mm^{-1}	0.650
F(000)	776.0
Crystal size/mm^3	0.09 × 0.09 × 0.03
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	8.52 to 159.606
Index ranges	$-12 \leq h \leq 11$, $-11 \leq k \leq 10$, $-22 \leq l \leq 21$
Reflections collected	26941
Independent reflections	3950 [R_{int} = 0.0474, R_{sigma} = 0.0246]
Data/restraints/parameters	3950/0/255
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0372, wR_2 = 0.0857
Final R indexes [all data]	R_1 = 0.0447, wR_2 = 0.0917
Largest diff. peak/hole / e $Å^{-3}$	0.20/-0.25

4.4 NAT-3e

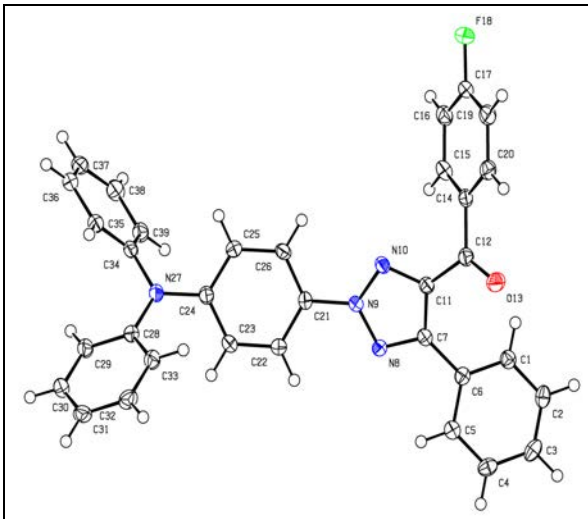


Fig. S82. Asymmetric unit of **QL_1020I**. Anisotropic displacement parameters were drawn at 50% probability. CCDC:1888251

Table S8 Crystal data and structure refinement for QL_1020I.

Identification code	QL_1020I
Empirical formula	$C_{33}H_{23}FN_4O$
Formula weight	510.55
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.0102(3)
b/Å	30.2706(10)
c/Å	10.4005(3)
α/°	90
β/°	92.3798(17)
γ/°	90
Volume/Å^3	2519.67(15)
Z	4
ρ_{calc}g/cm^3	1.346

μ/mm^{-1}	0.711
F(000)	1064.0
Crystal size/mm^3	0.14 × 0.09 × 0.07
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	5.84 to 160.014
Index ranges	$-10 \leq h \leq 10$, $-38 \leq k \leq 38$, $-13 \leq l \leq 13$
Reflections collected	61906
Independent reflections	5445 [R_{int} = 0.0604, R_{sigma} = 0.0234]
Data/restraints/parameters	5445/0/353
Goodness-of-fit on F^2	1.052
Final R indexes [I>=2σ (I)]	R_1 = 0.0393, wR_2 = 0.0818
Final R indexes [all data]	R_1 = 0.0485, wR_2 = 0.0871
Largest diff. peak/hole / e $Å^{-3}$	0.26/-0.19

4.5 NAT-3f

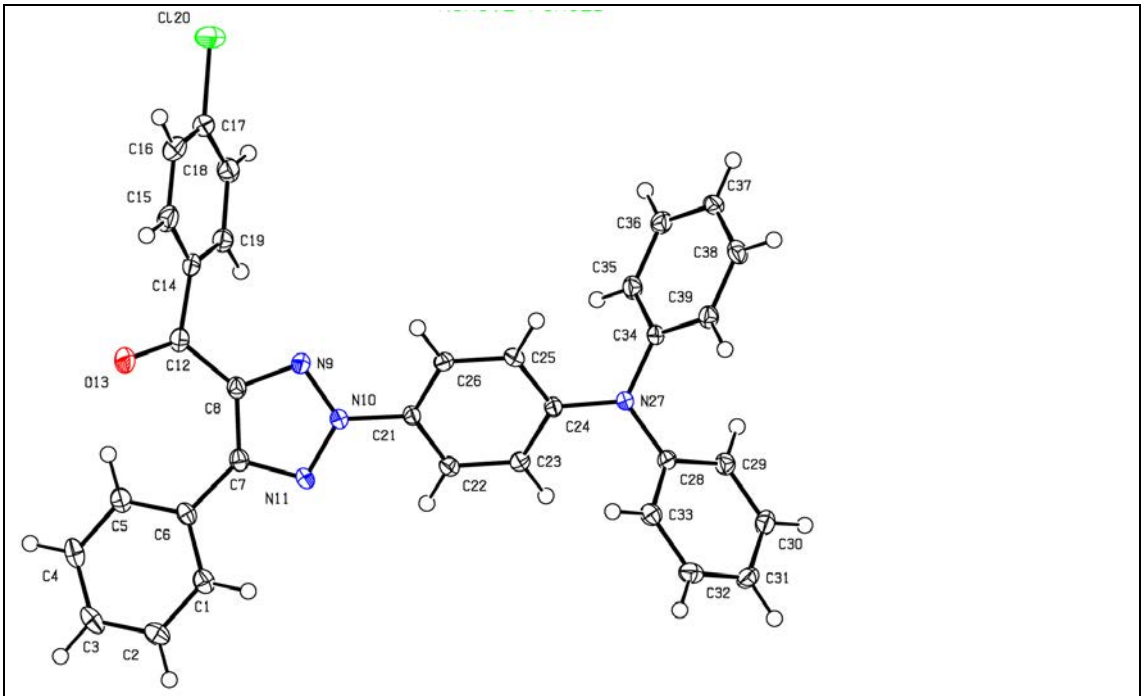


Fig. S83. Asymmetric unit of **ql_151_2.** Anisotropic displacement parameters were drawn at 50% probability. CCDC: 1888247

Table S9 Crystal data and structure refinement for ql_151_2.	
Identification code	ql_151_2
Empirical formula	$C_{33}H_{23}ClN_4O$
Formula weight	527.00
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.7632(3)
b/Å	9.9216(2)
c/Å	17.6080(4)
α/°	90

β/°	94.7020(10)
γ/°	90
Volume/Å^3	2570.44(9)
Z	4
ρ_{calc}g/cm^3	1.362
μ/mm^{-1}	1.590
F(000)	1096.0
Crystal size/mm^3	0.2 × 0.1 × 0.08
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	6.006 to 159.732
Index ranges	-18 ≤ h ≤ 18, -12 ≤ k ≤ 12, -21 ≤ l ≤ 22
Reflections collected	35770
Independent reflections	5515 [R_{int} = 0.0338, R_{sigma} = 0.0205]
Data/restraints/parameters	5515/0/353
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0343, wR_2 = 0.0780
Final R indexes [all data]	R_1 = 0.0385, wR_2 = 0.0810
Largest diff. peak/hole / e Å^{-3}	0.28/-0.41

4.6 NAT-3g

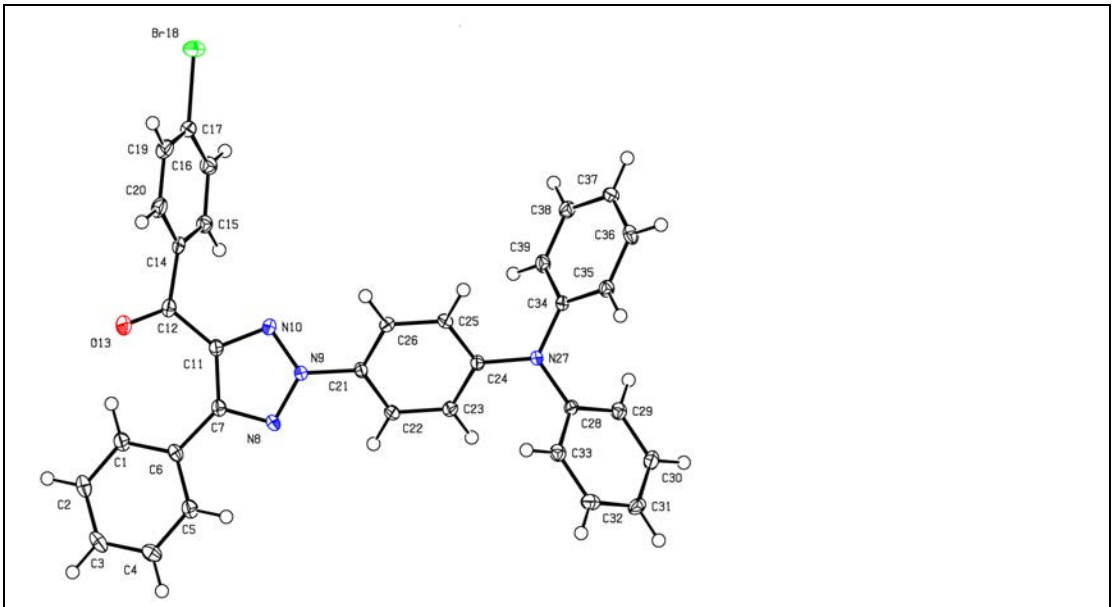


Fig. S84. Asymmetric unit of **QL_1020_H**. Anisotropic displacement parameters were drawn at 50% probability. CCDC:1888250

Table S10 Crystal data and structure refinement for QL_1020_H.	
Identification code	QL_1020_H
Empirical formula	$C_{33}H_{23}BrN_4O$
Formula weight	571.46
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.7956(4)
b/Å	9.9124(3)
c/Å	17.6965(4)
α/°	90
β/°	95.2860(10)
γ/°	90

Volume/$Å^3$	2584.33(12)
Z	4
$\rho_{calc}g/cm^3$	1.469
μ/mm^{-1}	2.442
F(000)	1168.0
Crystal size/mm^3	0.187 × 0.123 × 0.061
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	5.998 to 159.886
Index ranges	$-18 \leq h \leq 18$, $-11 \leq k \leq 12$, $-22 \leq l \leq 22$
Reflections collected	33190
Independent reflections	5503 [R_{int} = 0.0316, R_{sigma} = 0.0187]
Data/restraints/parameters	5503/0/352
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0266, wR_2 = 0.0644
Final R indexes [all data]	R_1 = 0.0287, wR_2 = 0.0660
Largest diff. peak/hole / e $Å^{-3}$	0.41/-0.61

4.6 NAT-3h

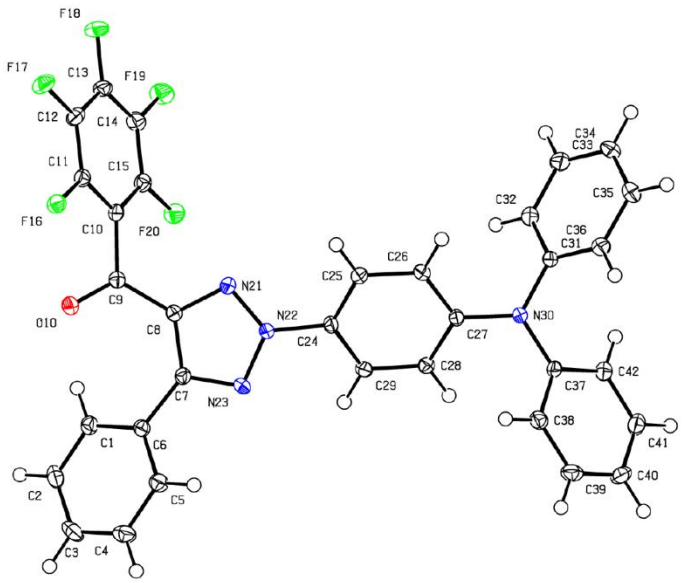


Fig. S85. Asymmetric unit of QL_1105_Q**.** Anisotropic displacement parameters were drawn at 50% probability. CCDC: 1888253

Table 11 Crystal data and structure refinement for QL_1105_Q.	
Identification code	QL_1105_Q
Empirical formula	$C_{33}H_{19}F_5N_4O$
Formula weight	582.52
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1$
a/Å	9.4579(2)
b/Å	8.3826(2)
c/Å	16.9770(4)
α/°	90
β/°	105.2450(10)
γ/°	90
Volume/Å^3	1298.60(5)
Z	2
ρ_{calc}g/cm^3	1.490
μ/mm^{-1}	0.996
F(000)	596.0

Crystal size/mm^3	0.18 × 0.13 × 0.1
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	5.396 to 159.894
Index ranges	-12 ≤ h ≤ 12, -10 ≤ k ≤ 10, -21 ≤ l ≤ 21
Reflections collected	32608
Independent reflections	5496 [R_{int} = 0.0269, R_{sigma} = 0.0186]
Data/restraints/parameters	5496/1/389
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0234, wR_2 = 0.0604
Final R indexes [all data]	R_1 = 0.0236, wR_2 = 0.0607
Largest diff. peak/hole / e Å^{-3}	0.22/-0.16
Flack parameter	0.045(19)

4.7 NAT-3j

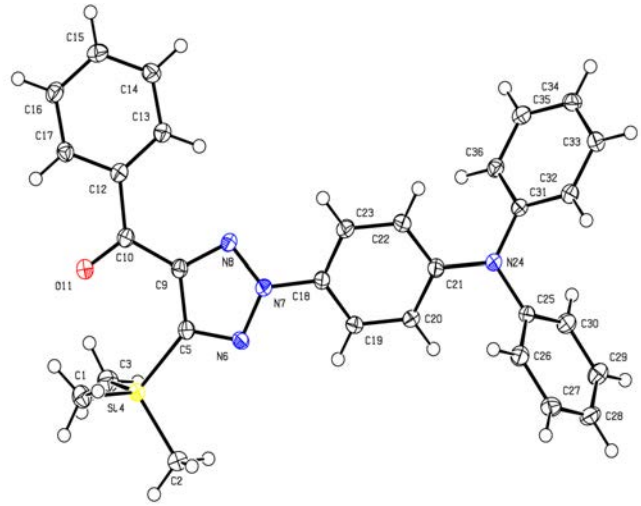


Fig. S86. Asymmetric unit of ql_1023_d5. Anisotropic displacement parameters were drawn at 50% probability. CCDC:1888254

Table S12 Crystal data and structure refinement for ql_1023_d5.	
Identification code	ql_1023_d5
Empirical formula	$C_{30}H_{28}N_4OSi$
Formula weight	488.65
Temperature/K	100

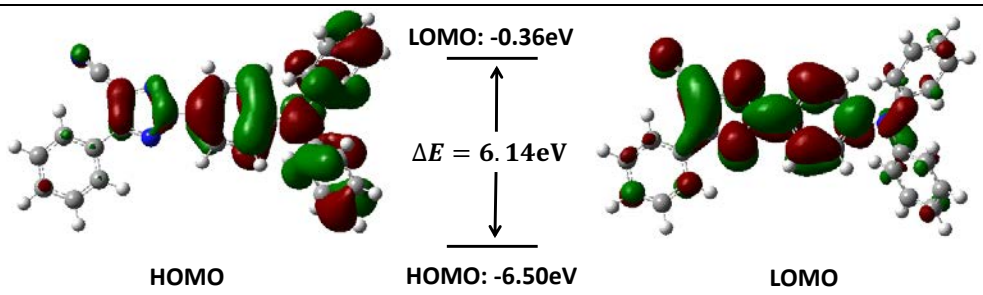
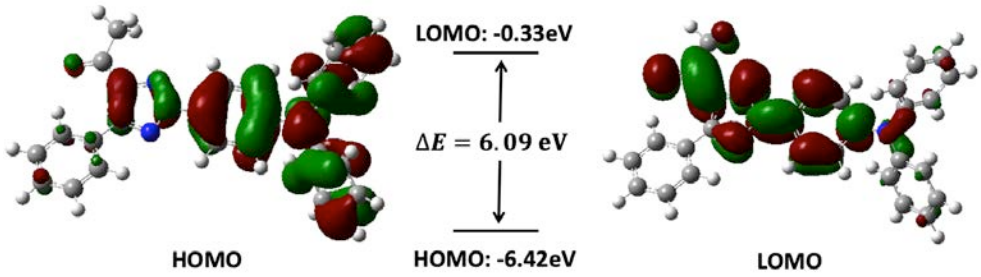
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.8270(5)
b/Å	19.5256(9)
c/Å	14.1862(6)
α/°	90
β/°	109.903(2)
γ/°	90
Volume/Å^3	2559.4(2)
Z	4
ρ_{calc}g/cm^3	1.268
μ/mm^{-1}	1.044
F(000)	1032.0
Crystal size/mm^3	0.15 × 0.11 × 0.05
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	8.026 to 159.722
Index ranges	$-11 \leq h \leq 11$, $-24 \leq k \leq 24$, $-18 \leq l \leq 18$
Reflections collected	55930
Independent reflections	5457 [R_{int} = 0.0549, R_{sigma} = 0.0237]
Data/restraints/parameters	5457/0/328
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0355, wR_2 = 0.0850
Final R indexes [all data]	R_1 = 0.0412, wR_2 = 0.0906
Largest diff. peak/hole / e Å^{-3}	0.32/-0.29

V. Theoretical Calculation Based on the Single Crystal

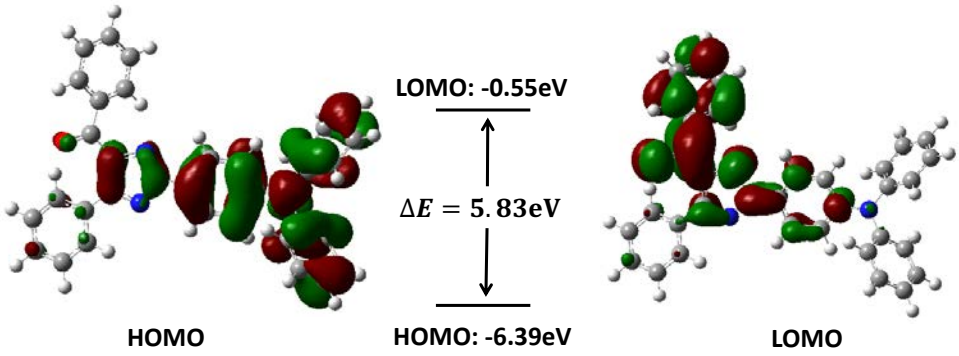
Table S13. HOMO and LUMO Energy of NATs.

NATs	HOMO energy (ev)	LUMO energy (ev)	Gap energy (ev)
2a	-6.500514	-0.357391	6.143122
2b	-6.422735	-0.328033	6.094702
2c	-6.387965	-0.553086	5.834879
3c	-6.506541	-0.425888	6.080653
3e	-6.419937	-0.624138	5.795799
3f	-6.442792	-0.763573	5.679220
3g	-6.441079	-0.761317	5.679762
3h	-6.497685	-0.876746	5.620940
3j	-6.384952	-0.6503798	5.734574

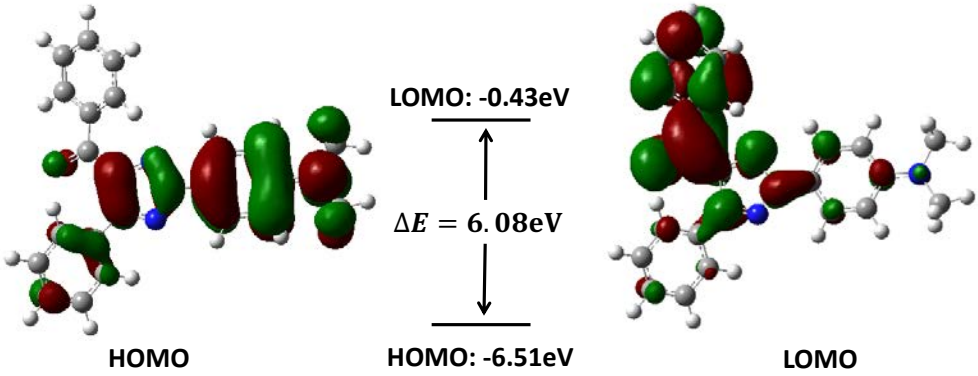
Table S14. Molecular orbital amplitude plots of both HOMO and LUMO [a]

NATs	Cmpd
2a	
2b	

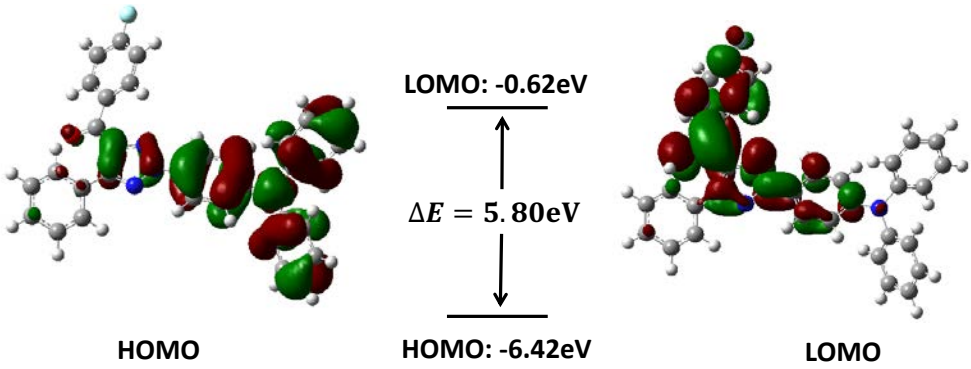
2c


LOMO: -0.55eV
$\Delta E = 5.83$eV
HOMO: -6.39eV
HOMO
LOMO

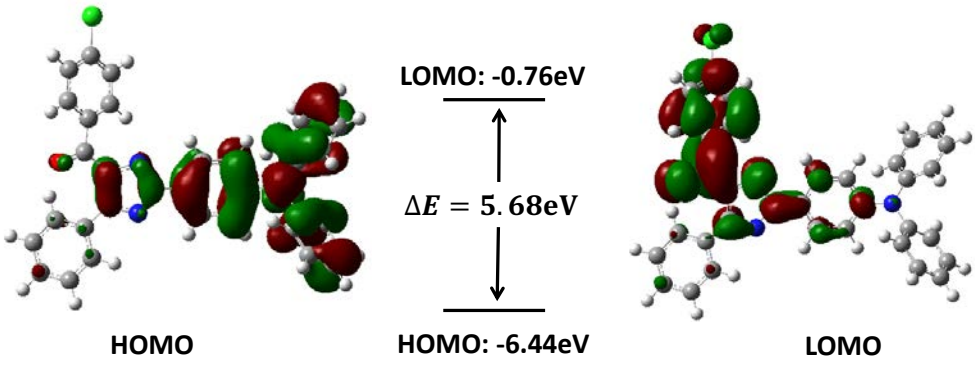
3c

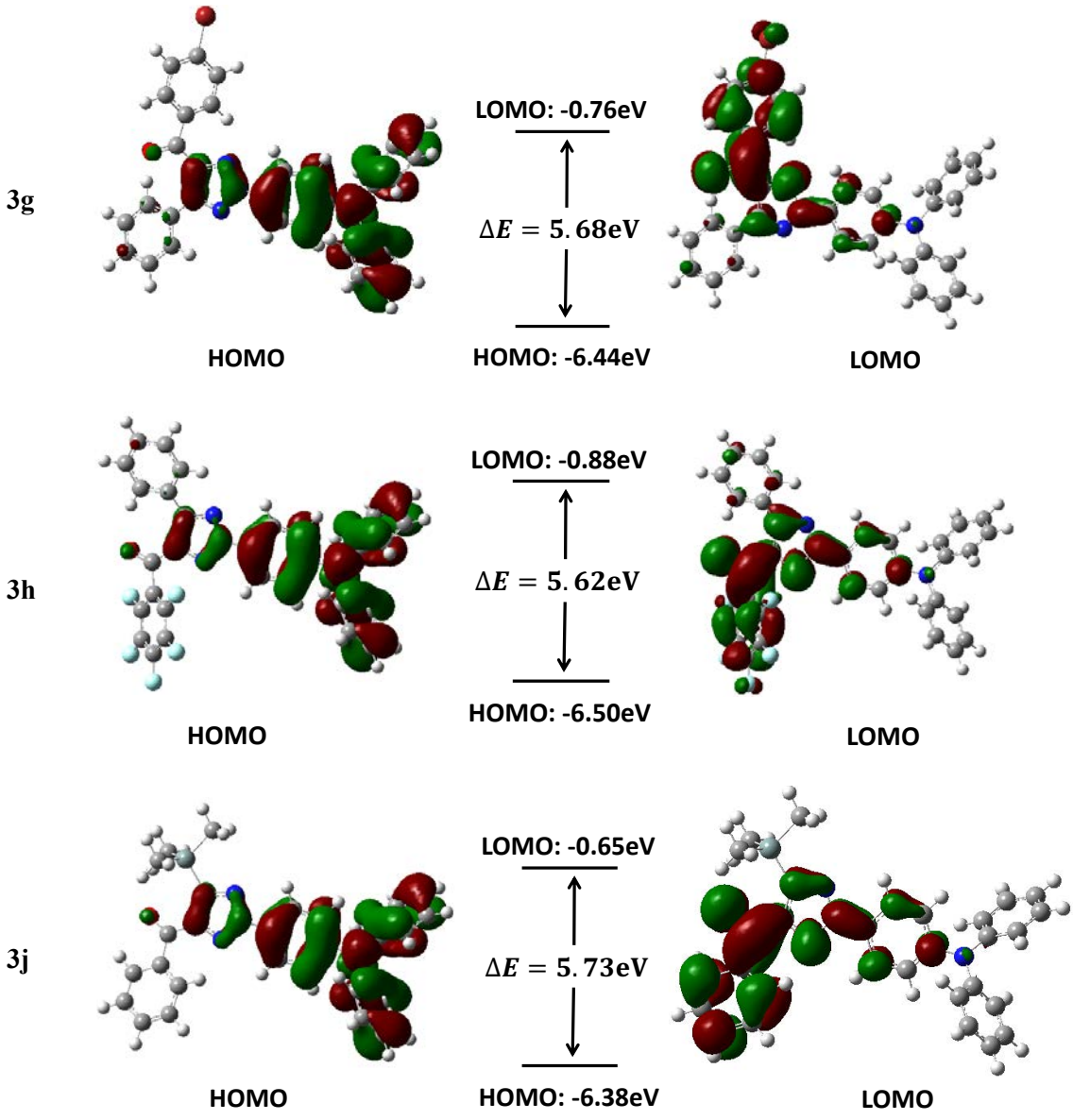

LOMO: -0.43eV
$\Delta E = 6.08$eV
HOMO: -6.51eV
HOMO
LOMO

3e


LOMO: -0.62eV
$\Delta E = 5.80$eV
HOMO: -6.42eV
HOMO
LOMO

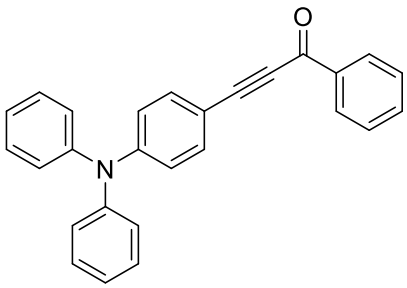
3f


LOMO: -0.76eV
$\Delta E = 5.68$eV
HOMO: -6.44eV
HOMO
LOMO



[a]The energy gap between HOMO and LUMO of corresponding single crystal structure were calculated at the CAM-B3LYP/6-31G (d, p) level of theory.

VI. Compounds Characterization



DPPO

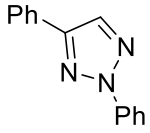
3-(4-(diphenylamino)phenyl)-1-phenylprop-2-yn-1-one

m was prepared following the General Procedure **1.1** and purified by flash Chromatography (Hexane: EA= 20:1) as yellow oil. 91% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 – 8.17 (m, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.54 – 7.48 (m, 4H), 7.32 (t, *J* = 7.8 Hz, 4H), 7.15 (dd, *J* = 8.1, 3.1 Hz, 6H), 6.99 (d, *J* = 8.7 Hz, 2H).

^{13}C NMR (101 MHz, cdcl$_3$) δ 177.95, 150.33, 146.42, 137.19, 134.54, 133.76, 129.62, 129.45, 128.52, 125.83, 124.59, 120.55, 111.27, 95.18, 87.40,

HRMS(ESI): Calculated for $C_{27}H_{20}NO^+$ $(M+H)^+$: 374.1539，found: 374.1521.



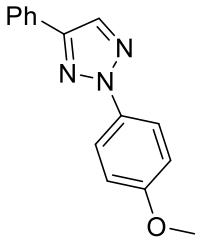
1a

2,4-diphenyl-2H-1,2,3-triazole

1a was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as white solid. 81% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.18 – 8.10 (m, 2H), 8.06 (s, 1H), 7.94 – 7.87 (m, 2H), 7.55 – 7.44 (m, 4H), 7.43 – 7.33 (m, 2H).

HRMS (ESI): Calculated for $C_{14}H_{12}N_3^+$ $(M+H)^+$: 222.1026，found:222.1017.



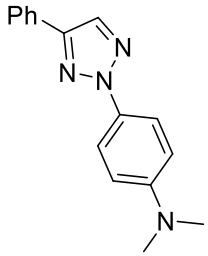
1b

2-(4-methoxyphenyl)-4-phenyl-2H-1,2,3-triazole

1b was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as white solid. 85% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 – 7.98 (m, 3H), 7.96 – 7.84 (m, 2H), 7.50 – 7.43 (m, 2H), 7.39 (d, *J* = 7.3 Hz, 1H), 7.01 (d, *J* = 9.1 Hz, 2H), 3.87 (s, 3H).

HRMS (ESI): Calculated for $C_{15}H_{14}N_3O^+$ $(M+H)^+$: 252.1131，found:252.1123.



1c

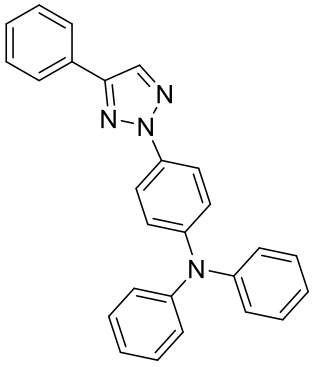
N,N-dimethyl-4-(4-phenyl-2H-1,2,3-triazol-2-yl)aniline

1c was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as white solid. 62% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 (s, 1H), 7.97 (d, *J* = 8.5 Hz, 2H), 7.88 (d, *J* = 7.5 Hz, 2H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.38 (d, *J* = 7.3 Hz, 1H), 7.27 (d, *J* = 15.6 Hz, 4H), 7.15 (dd, *J* = 19.2, 8.2 Hz, 5H), 7.05 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.85, 147.94, 131.53, 131.43, 130.44, 128.85, 128.41, 125.99, 120.07, 112.35, 40.65.

HRMS (ESI): Calculated for $C_{16}H_{17}N_6^+$ $(M+H)^+$: 265.1448，found: 265.1448.



1d

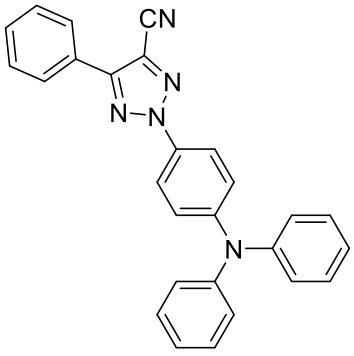
N,N-diphenyl-4-(4-phenyl-2H-1,2,3-triazol-2-yl)aniline

1d was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as white solid. 45% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 (s, 1H), 7.97 (d, *J* = 8.5 Hz, 2H), 7.88 (d, *J* = 7.5 Hz, 2H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.38 (d, *J* = 7.3 Hz, 1H), 7.27 (d, *J* = 15.6 Hz, 4H), 7.15 (dd, *J* = 19.2, 8.2 Hz, 5H), 7.05 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.51, 147.42, 147.26, 134.57, 132.21, 132.14, 130.11, 129.35, 128.90, 126.03, 124.49, 123.81, 123.24, 119.87.

HRMS (ESI): Calculated for $C_{26}H_{21}N_4^+$ $(M+H)^+$: 389.1761，found:389.1739.



2a

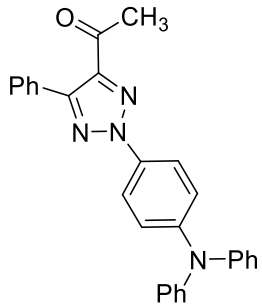
2-(4-(diphenylamino)phenyl)-5-phenyl-2H-1,2,3-triazole-4-carbonitrile

2a was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as yellow solid. 55% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.07 (d, *J* = 7.1 Hz, 2H), 7.96 (d, *J* = 8.3 Hz, 2H), 7.51 (p, *J* = 7.1 Hz, 3H), 7.31 (t, *J* = 7.6 Hz, 4H), 7.22 – 6.99 (m, 8H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.30, 148.88, 146.95, 132.75, 130.31, 129.53, 129.17, 127.47, 126.82, 125.11, 123.96, 122.50, 120.53, 118.32, 112.78.

HRMS (ESI): Calculated for $C_{27}H_{20}N_5^+$ $(M+H)^+$: 414.1713，found: 414.1681.



2b

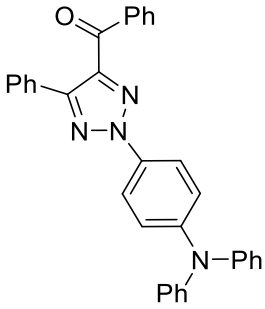
1-(2-(4-(diphenylamino)phenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)ethan-1-one

2b was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as yellow solid. 52% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 – 7.92 (m, 4H), 7.45 (d, *J* = 7.2 Hz, 3H), 7.34 – 7.25 (m, 4H), 7.20 – 7.12 (m, 6H), 7.09 (d, *J* = 7.3 Hz, 2H), 2.74 (s, 3H).

^{13}C NMR (101 MHz, $cdcl_3$) δ 192.73, 149.17, 148.28, 147.16, 143.05, 133.38, 129.46, 129.42, 129.23, 128.19, 124.84, 123.66, 123.10, 120.40, 28.74.

HRMS (ESI): Calculated for $C_{28}H_{23}N_4O^+$ $(M+H)^+$: 431.1866，found: 431.1843.



2c

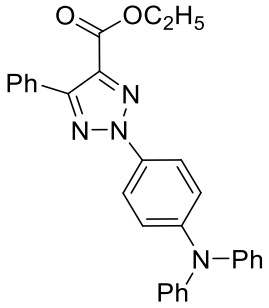
(2-(4-(diphenylamino)phenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone

2c was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as yellow solid. 63% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15 (d, *J* = 7.9 Hz, 2H), 8.00 (d, *J* = 9.0 Hz, 2H), 7.91 (d, *J* = 6.3 Hz, 2H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.53 – 7.40 (m, 5H), 7.29 (t, *J* = 7.8 Hz, 4H), 7.20 – 7.05 (m, 8H).

^{13}C NMR (101 MHz, cdcl$_3$) δ 188.06, 150.60, 148.48, 147.51, 142.88, 137.59, 133.83, 133.69, 130.86, 129.85, 129.77, 129.58, 129.13, 128.71, 128.63, 125.12, 123.94, 123.49, 120.73.

HRMS (ESI): Calculated for $C_{33}H_{25}N_4O^+$ $(M+H)^+$: 493.2030，found: 493.2014.



2d

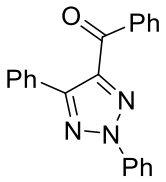
ethyl 2-(4-(diphenylamino)phenyl)-5-phenyl-2H-1,2,3-triazole-4-carboxylate

2d was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as white solid. 49% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 (d, *J* = 8.5 Hz, 2H), 7.89 (d, *J* = 6.7 Hz, 2H), 7.46 (d, *J* = 6.0 Hz, 3H), 7.29 (t, *J* = 7.8 Hz, 4H), 7.12 (dt, *J* = 17.6, 7.8 Hz, 8H), 4.43 (q, *J* = 6.3, 5.3 Hz, 2H), 1.38 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, cdcl$_3$) δ 161.37, 150.34, 148.30, 147.19, 136.66, 133.45, 129.45, 129.33, 129.27, 128.13, 124.83, 124.10, 123.62, 123.02, 120.67, 61.54, 14.18.

HRMS(ESI): Calculated for $C_{29}H_{25}N_4O_2^+$ $(M+H)^+$: 461.1972，found: 461.1956.



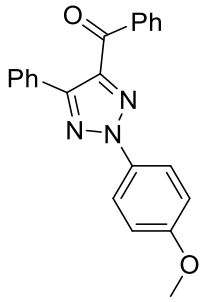
3a

(2,5-diphenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone

3a was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as white solid. 83% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 – 8.05 (m, 4H), 7.99 – 7.87 (m, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.55 – 7.41 (m, 8H).

HRMS(ESI): Calculated for $C_{21}H_{16}N_3O^+$ $(M+H)^+$: 326.1288，found: 326.1273.



3b

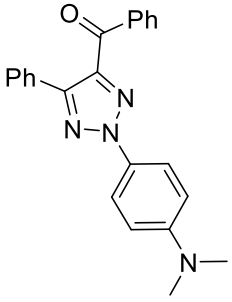
(2-(4-methoxyphenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone

3b was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane:DCM = 2:1) as white solid. 72% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.11 (dd, *J* = 28.1, 8.1 Hz, 4H), 7.91 (dd, *J* = 7.1, 3.9 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.46 (dd, *J* = 27.1, 7.3 Hz, 5H), 6.99 (d, *J* = 8.5 Hz, 2H), 3.84 (d, *J* = 4.7 Hz, 3H).

^{13}C NMR (101 MHz, cdcl$_3$) δ 187.70, 159.61, 150.17, 142.49, 137.24, 133.31, 132.91, 130.49, 129.53, 129.20, 128.77, 128.47, 128.34, 128.27, 120.73, 114.39, 55.53.

HRMS(ESI): Calculated for $C_{22}H_{18}N_3O_2^+$ $(M+H)^+$: 356.1394，found: 356.1387.



3c

(2-(4-(dimethylamino)phenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone

3c was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as yellow solid. 67% yield.

^{1}H NMR

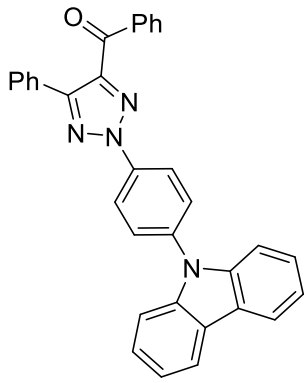
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 (d, *J* = 7.6 Hz, 2H), 7.96 (dd, *J* = 40.1, 7.7 Hz, 4H), 7.60 (s, 1H), 7.46 (dd, *J* = 29.0, 7.3 Hz, 5H), 6.78 (d, *J* = 8.6 Hz, 2H), 3.03 (s, 6H).

d-7 ^{13}C NMR

^{13}C NMR

^{13}C NMR (101 MHz, cdcl$_3$) δ 187.80, 150.42, 149.98, 142.03, 137.50, 133.19, 130.59, 129.86, 129.45, 129.07, 128.86, 128.33, 128.25, 120.59, 112.06, 40.49.

HRMS(ESI): Calculated for $C_{23}H_{21}N_4^+$ $(M+H)^+$: 369.1710，found: 369.1705.



3d

(2-(4-(9H-carbazol-9-yl)phenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone

3d was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as white solid. 72% yield.

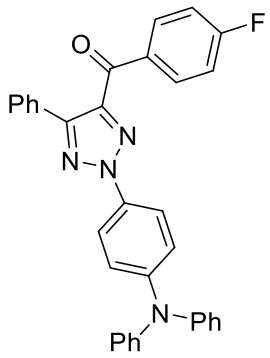
^{1}H NMR

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.41 (d, *J* = 8.3 Hz, 2H), 8.17 (dd, *J* = 14.2, 7.8 Hz, 4H), 7.95 (d, *J* = 6.8 Hz, 2H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 7.5 Hz, 1H), 7.57 – 7.37 (m, 9H), 7.32 (d, *J* = 7.1 Hz, 2H).

^{13}C NMR

^{13}C NMR (101 MHz, cdcl$_3$) δ 187.72, 150.73, 143.31, 140.58, 137.87, 137.72, 137.10, 133.60, 130.55, 129.51, 129.24, 128.81, 128.49, 128.42, 127.89, 126.13, 123.58, 120.79, 120.43, 120.33, 109.58.

HRMS(ESI): Calculated for $C_{33}H_{24}N_4O^+$ $(M+H)^+$: 491.1866，found: 491.1855.



3e

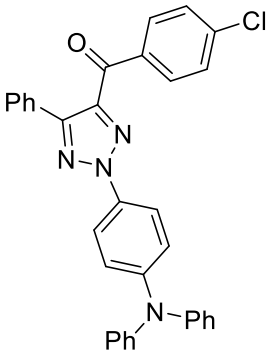
(2-(4-(diphenylamino)phenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(4-fluorophenyl)methanone

3e was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as yellow solid. 56% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.22 (td, *J* = 5.5, 2.5 Hz, 2H), 8.04 – 7.97 (m, 2H), 7.90 (tt, *J* = 4.9, 2.1 Hz, 2H), 7.48 – 7.40 (m, 3H), 7.30 (tt, *J* = 8.0, 4.2 Hz, 5H), 7.16 (ddd, *J* = 11.9, 8.4, 4.1 Hz, 8H), 7.09 (d, *J* = 6.2 Hz, 2H).

^{13}C NMR (101 MHz, cdcl$_3$) δ 185.97, 150.42, 148.26, 147.15, 142.33, 133.61, 133.38, 133.30, 133.20, 129.47, 129.34, 128.83, 128.41, 124.85, 123.68, 123.09, 120.40, 115.59, 115.38.

HRMS(ESI): Calculated for $C_{33}H_{24}FN_4O^+$ $(M+H)^+$: 511.1929，found: 511.1905.



3f

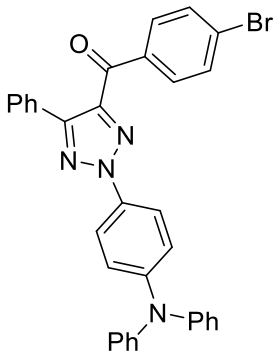
(4-chlorophenyl)(2-(4-(diphenylamino)phenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)methanone

3f was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as yellow solid. 62% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 (d, *J* = 8.5 Hz, 2H), 7.99 (d, *J* = 8.9 Hz, 2H), 7.90 (dd, *J* = 7.2, 2.4 Hz, 2H), 7.51 – 7.40 (m, 5H), 7.30 (t, *J* = 7.7 Hz, 4H), 7.15 (dd, *J* = 10.6, 8.4 Hz, 6H), 7.09 (d, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, cdcl$_3$) δ 186.25, 150.54, 148.30, 147.14, 142.19, 139.84, 135.65, 133.33, 131.93, 129.48, 129.40, 128.87, 128.64, 128.41, 124.86, 123.70, 123.06, 120.40.

HRMS(ESI): Calculated for $C_{33}H_{24}ClN_4O^+$ $(M+H)^+$: 527.1633，found: 527.1603.



3g

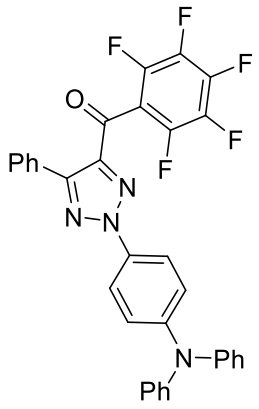
(4-bromophenyl)(2-(4-(diphenylamino)phenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)methanone

3g was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as yellow solid. 69% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.07 – 8.02 (m, 2H), 8.02 – 7.96 (m, 2H), 7.94 – 7.87 (m, 2H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.44 (d, *J* = 6.1 Hz, 3H), 7.29 (t, *J* = 7.7 Hz, 4H), 7.15 (t, *J* = 9.2 Hz, 6H), 7.08 (t, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, cdcl$_3$) δ 186.41, 150.56, 148.30, 147.13, 142.14, 136.08, 133.31, 132.01, 131.62, 129.47, 129.40, 128.87, 128.62, 128.40, 124.86, 123.69, 123.04, 120.40.

HRMS(ESI): Calculated for $C_{33}H_{24}BrN_4O^+$ $(M+H)^+$: 570.1128，found: 571.1088.



3h

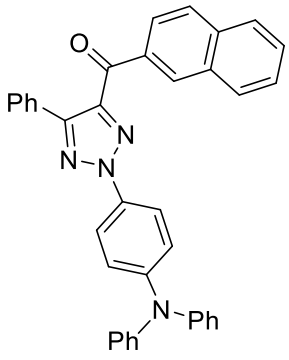
(2-(4-(diphenylamino)phenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(perfluorophenyl)methanone

3h was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as yellow solid. 42% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 (d, *J* = 6.6 Hz, 2H), 7.89 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 5.6 Hz, 3H), 7.29 (t, *J* = 7.8 Hz, 4H), 7.21 – 7.01 (m, 8H).

^{13}C NMR (101 MHz, cdcl$_3$) δ 177.82, 150.78, 148.87, 146.96, 145.46, 143.85, 142.82, 142.12, 138.72, 132.66, 130.10, 129.52, 129.15, 128.57, 128.45, 125.07, 123.93, 122.53, 120.69.

HRMS(ESI): Calculated for $C_{33}H_{20}F_5N_4O^+$ $(M+H)^+$: 583.1552，found: 583.1530.



3i

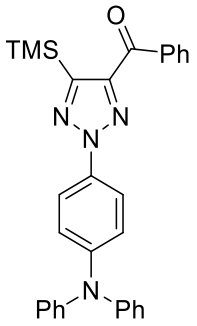
(2-(4-(diphenylamino)phenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(naphthalen-2-yl)methanone

3i was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as yellow solid. 39% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.71 (s, 1H), 8.20 (d, *J* = 8.6 Hz, 1H), 8.03 (d, *J* = 8.5 Hz, 2H), 7.92 (dt, *J* = 15.8, 7.7 Hz, 5H), 7.60 (d, *J* = 7.7 Hz, 1H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.43 (q, *J* = 7.2 Hz, 3H), 7.30 (d, *J* = 7.8 Hz, 3H), 7.21 – 7.03 (m, 9H).

^{13}C NMR (101 MHz, cdcl$_3$) δ 187.73, 150.23, 148.16, 147.20, 142.79, 135.76, 134.57, 133.57, 133.29, 132.38, 129.88, 129.46, 129.26, 128.78, 128.43, 128.19, 127.76, 126.68, 125.44, 124.82, 124.10, 123.62, 123.20, 122.79, 120.40.

HRMS(ESI): Calculated for $C_{37}H_{27}N_4O^+$ $(M+H)^+$: 543.2179，found: 543.2152.



3j

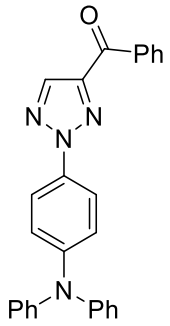
(2-(4-(diphenylamino)phenyl)-5-(trimethylsilyl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone

3j was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: DCM= 2:1) as yellow solid. 61% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.33 (d, *J* = 7.6 Hz, 2H), 7.99 (d, *J* = 8.4 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 7.29 (d, *J* = 7.8 Hz, 3H), 7.20 – 7.03 (m, 9H), 0.44 (s, 9H).

^{13}C NMR (101 MHz, cdcl$_3$) δ 186.95, 153.09, 152.05, 147.96, 147.24, 137.15, 133.85, 132.98, 130.50, 129.41, 128.24, 124.69, 123.51, 123.34, 120.68, -1.56.

HRMS(ESI): Calculated for $C_{30}H_{29}N_4OSi^+$ $(M+H)^+$: 489.2105，found: 489.2085.



3k

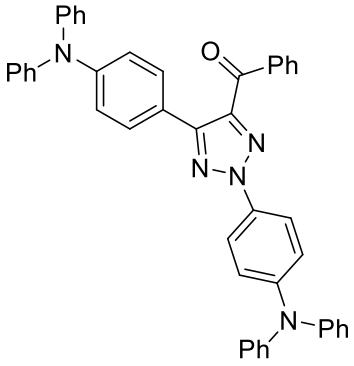
(2-(4-(diphenylamino)phenyl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone

3k was prepared following the General Procedure **1.1** and purified by flash Chromatography (Hexane: DCM= 2:1) as yellow solid. 46% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (d, *J* = 9.6 Hz, 3H), 7.99 (d, *J* = 8.5 Hz, 2H), 7.63 (d, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.7 Hz, 4H), 7.13 (dt, *J* = 18.8, 9.4 Hz, 8H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.35, 147.15, 138.44, 136.64, 133.58, 130.35, 129.59, 129.39, 128.55, 128.33, 124.98, 123.75, 123.12, 122.95, 120.61, 120.48.

HRMS(ESI): Calculated for $C_{27}H_{21}N_4O^+$ $(M+H)^+$: 417.1710，found: 417.1694.



3l

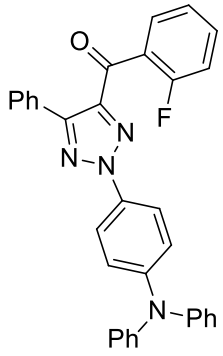
(2,5-bis(4-(diphenylamino)phenyl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone

3l was prepared following the General Procedure **1.1** and purified by flash Chromatography (Hexane: DCM= 2:1) as yellow solid. 43% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 – 8.11 (m, 2H), 8.02 – 7.96 (m, 2H), 7.83 – 7.77 (m, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.31 – 7.26 (m, 7H), 7.16 – 7.04 (m, 17H).

^{13}C NMR (101 MHz, cdcl$_3$) δ 187.93, 150.16, 148.78, 148.08, 147.31, 147.21, 142.26, 137.46, 133.56, 133.26, 130.55, 129.72, 129.45, 129.31, 128.27, 124.90, 124.78, 123.59, 123.35, 123.21, 122.81, 122.41, 120.35.

HRMS(ESI): Calculated for $C_{45}H_{34}N_5O^+$ $(M+H)^+$: 660.2758，found: 660.2720.



3m

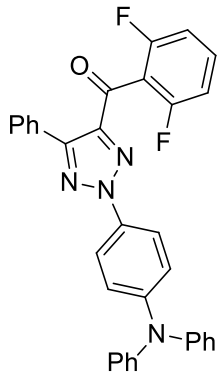
(2-(4-(diphenylamino)phenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(2-fluorophenyl)methanone

3m was prepared following the General Procedure **1.1** and purified by flash Chromatography (Hexane: EA = 20:1) as white solid. 75% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 – 7.99 (m, 2H), 8.00 – 7.94 (m, 2H), 7.78 (td, *J* = 7.4, 1.8 Hz, 1H), 7.59 – 7.52 (m, 1H), 7.52 – 7.43 (m, 3H), 7.35 – 7.27 (m, 5H), 7.20 – 7.05 (m, 9H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 185.79, 162.20, 159.66, 149.97, 148.28, 147.16, 143.20, 133.89, 133.40, 131.11, 129.45, 129.31, 128.99, 128.34, 127.43, 124.82, 124.02, 123.64, 123.06, 120.54, 116.28 (d, *J* = 22.0 Hz).

HRMS(ESI): Calculated for $C_{33}H_{24}FN_4O^+$ $(M+H)^+$: 511.1934，found: 511.1942.



3n

(2,6-difluorophenyl)(2-(4-(diphenylamino)phenyl)-5-phenyl-2H-1,2,3-triazol-4-yl)methanone

3n was prepared following the General Procedure **1.1** and purified by flash Chromatography (Hexane: EA = 20:1) as yellow solid. 64% yield.

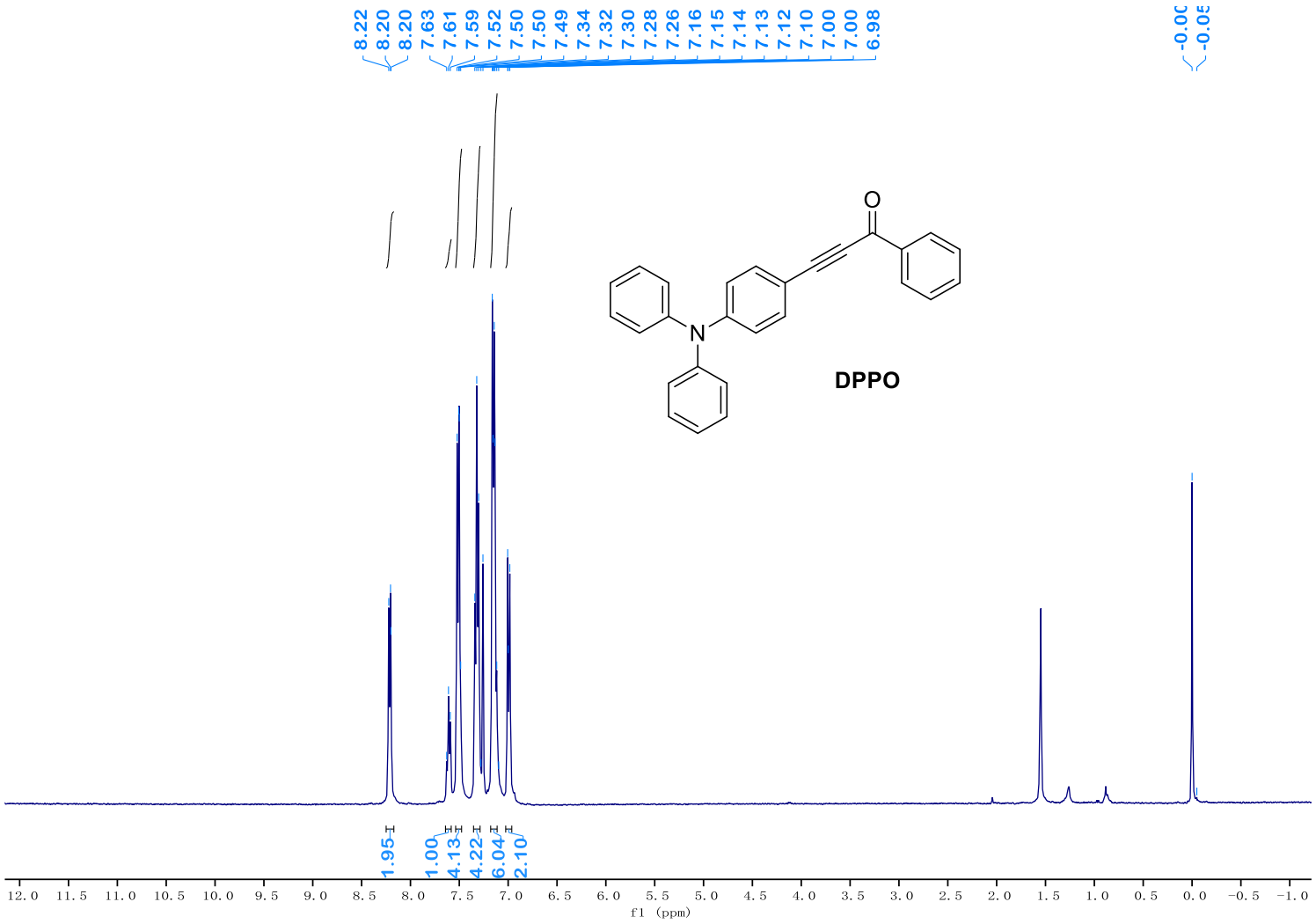
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 – 8.03 (m, 2H), 7.93 – 7.86 (m, 2H), 7.53 – 7.45 (m, 3H), 7.45 – 7.37 (m, 1H), 7.28 (dd, *J* = 8.5, 7.3 Hz, 4H), 7.14 – 7.04 (m, 8H), 6.96 (t, *J* = 7.9 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.68, 160.11 (dd, *J* = 252.8, 6.8 Hz), 150.35, 148.54, 147.13, 143.12, 133.17, 132.16 (t, *J* = 10.5 Hz), 129.79, 129.54, 129.51, 129.12, 128.40, 124.96, 123.80, 122.89, 120.66, 111.72 (d, *J* = 22.8 Hz).

HRMS(ESI): Calculated for $C_{33}H_{23}F_2N_4O^+$ $(M+H)^+$: 529.1840, found: 529.1849.

VII. NMR Spectra Data

DPPO ^{1}H NMR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8.20
8.20
7.63
7.61
7.59
7.52
7.50
7.50
7.49
7.34
7.32
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7.28
7.26
7.16
7.15
7.14
7.13
7.12
7.10
7.00
7.00
6.98
-0.00
-0.03
O
N
DPPO
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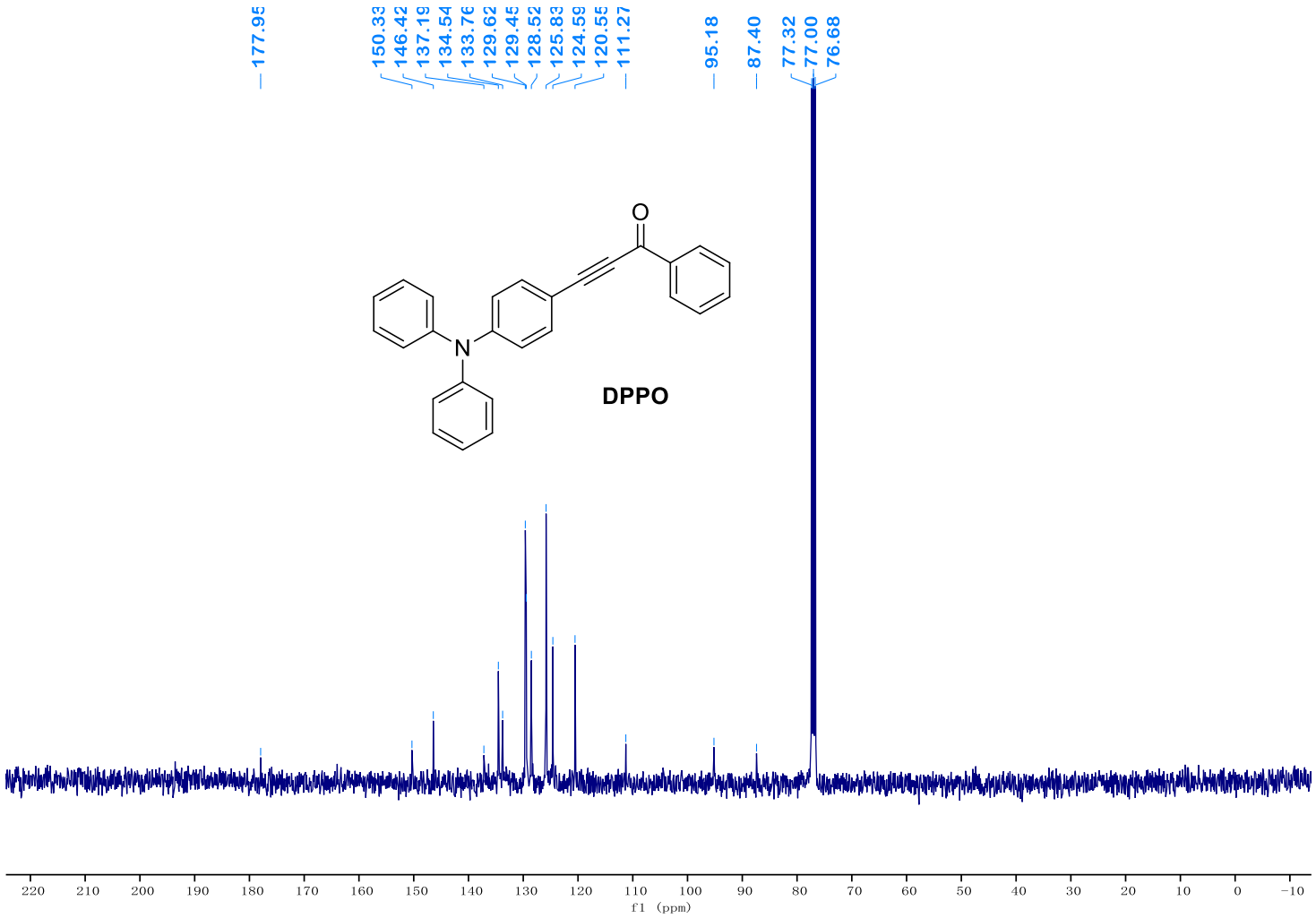
1.00
4.13
4.22
6.04
2.10
f1 (ppm)

DPPO ^{13}C NMR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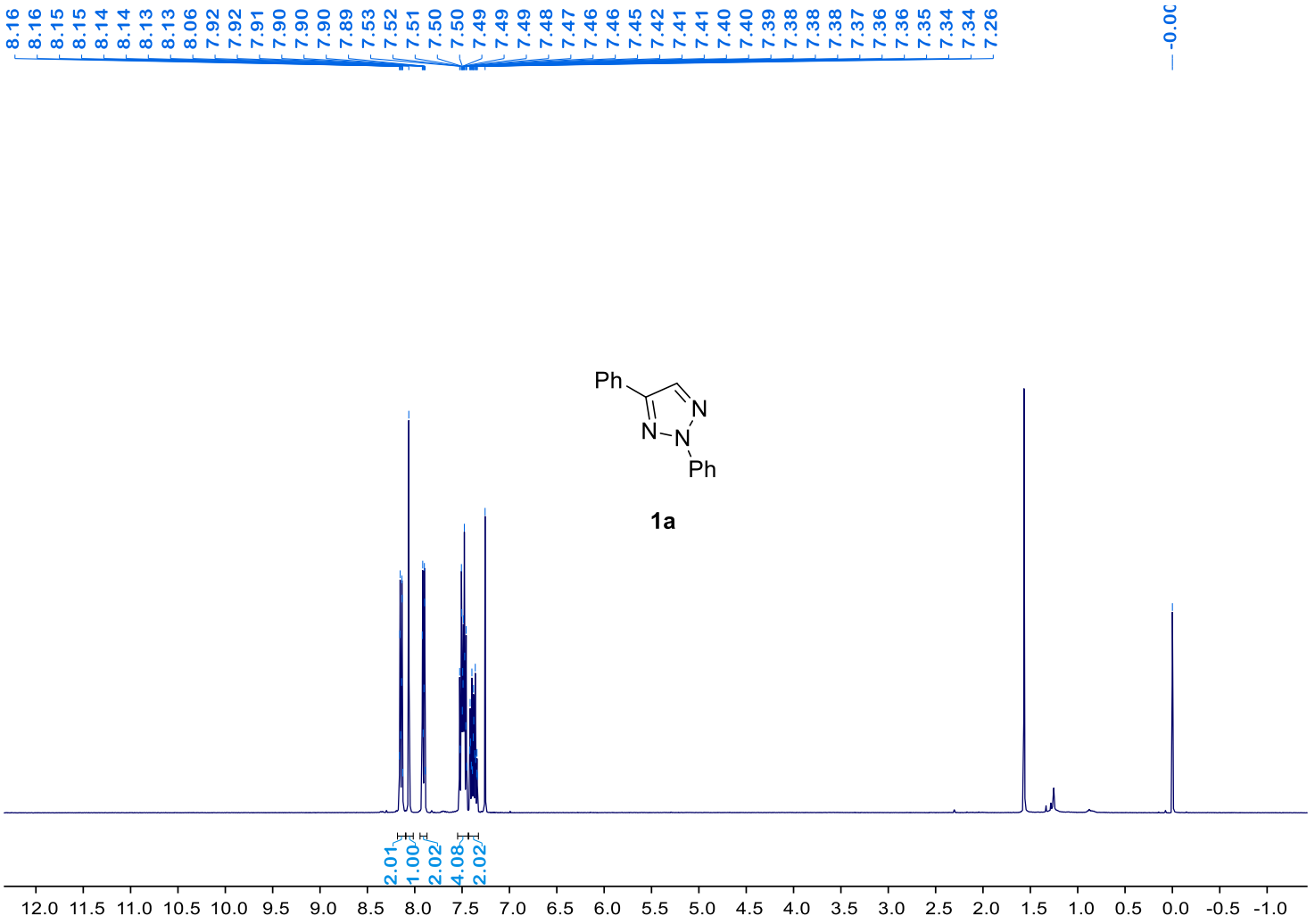
129.62
129.45
128.52
125.83
124.59
120.55
111.27
95.18
87.40
77.32
77.00
76.68
O
N
DPPO
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

1a ^{1}H NMR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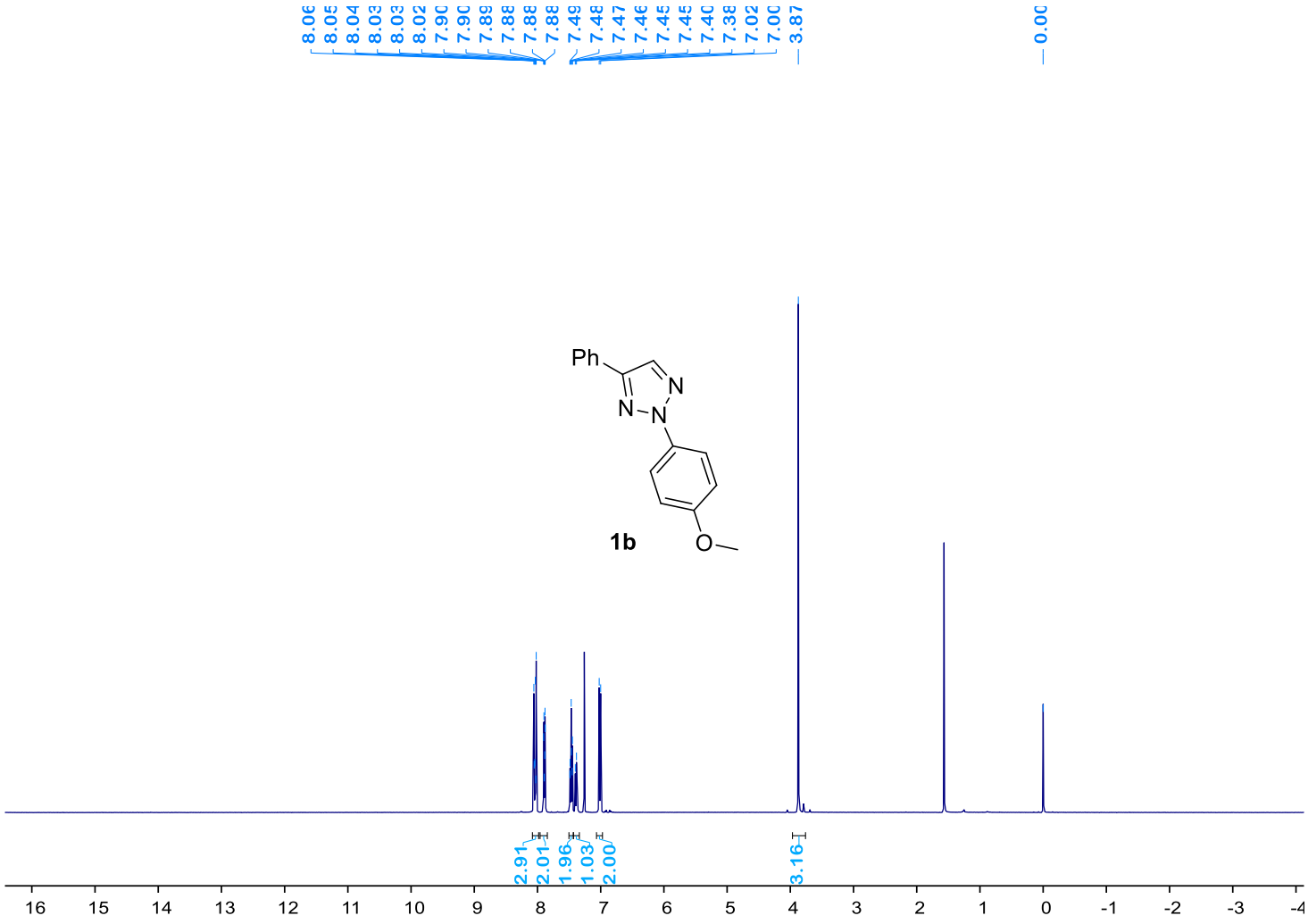
7.38
7.38
7.37
7.36
7.36
7.35
7.34
7.34
7.26
-0.00
Ph
N
N
N
Ph
1a
2.01
1.00
2.02
4.08
2.02
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

1b ^{1}H NMR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8.05
8.04
8.03
8.03
8.02
7.90
7.90
7.89
7.88
7.88
7.88
7.49
7.48
7.47
7.46
7.45
7.45
7.40
7.38
7.02
7.00
3.87
0.00
Ph
N
N
N
1b
O
2.91
2.01
1.96
1.03
2.00
3.16
16
15
14
13
12
11
10
9
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7
6
5
4
3
2
1
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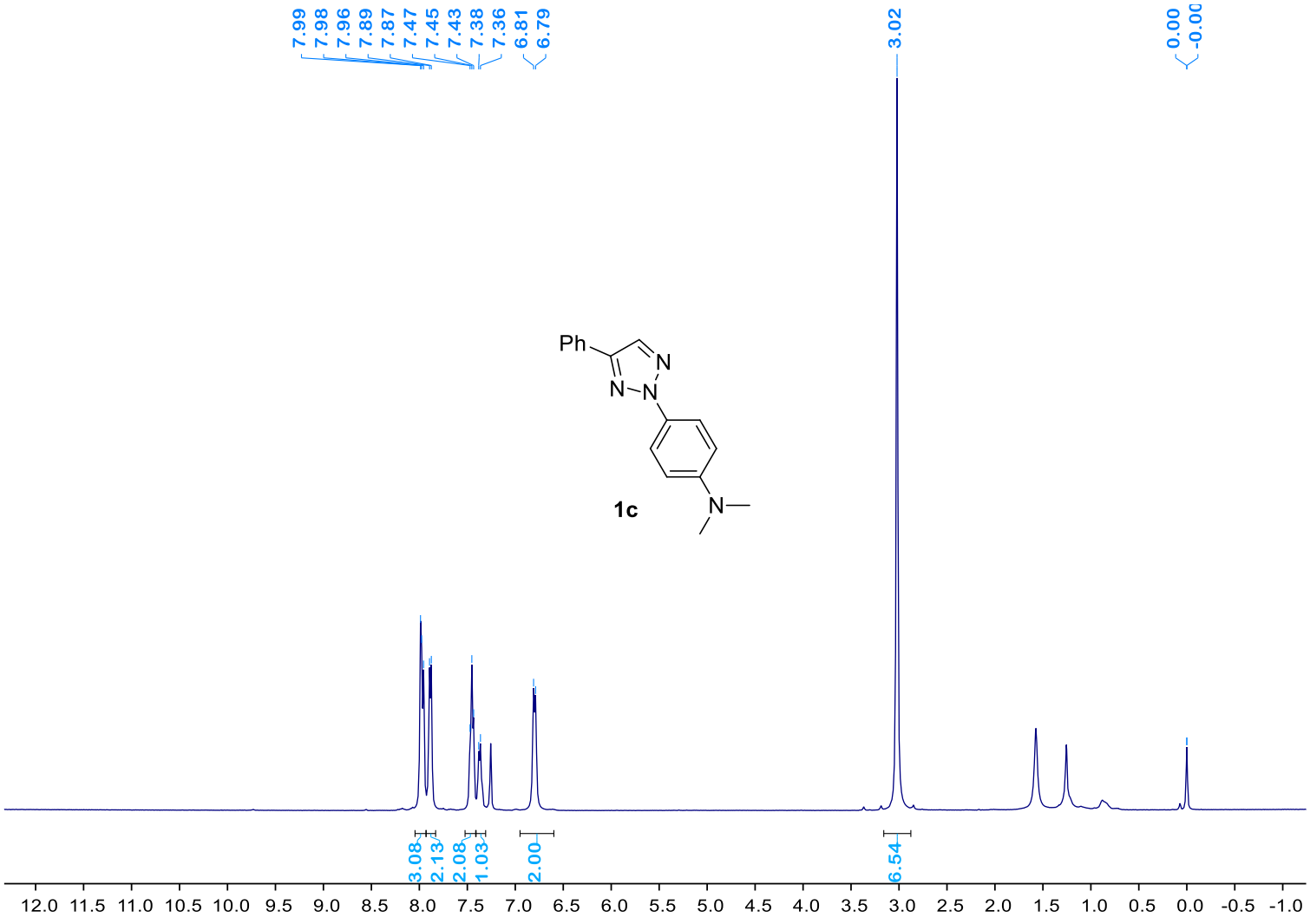
-1
-2
-3
-4

1c ^{1}H NMR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7.89
7.87
7.47
7.45
7.43
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7.36
6.81
6.79
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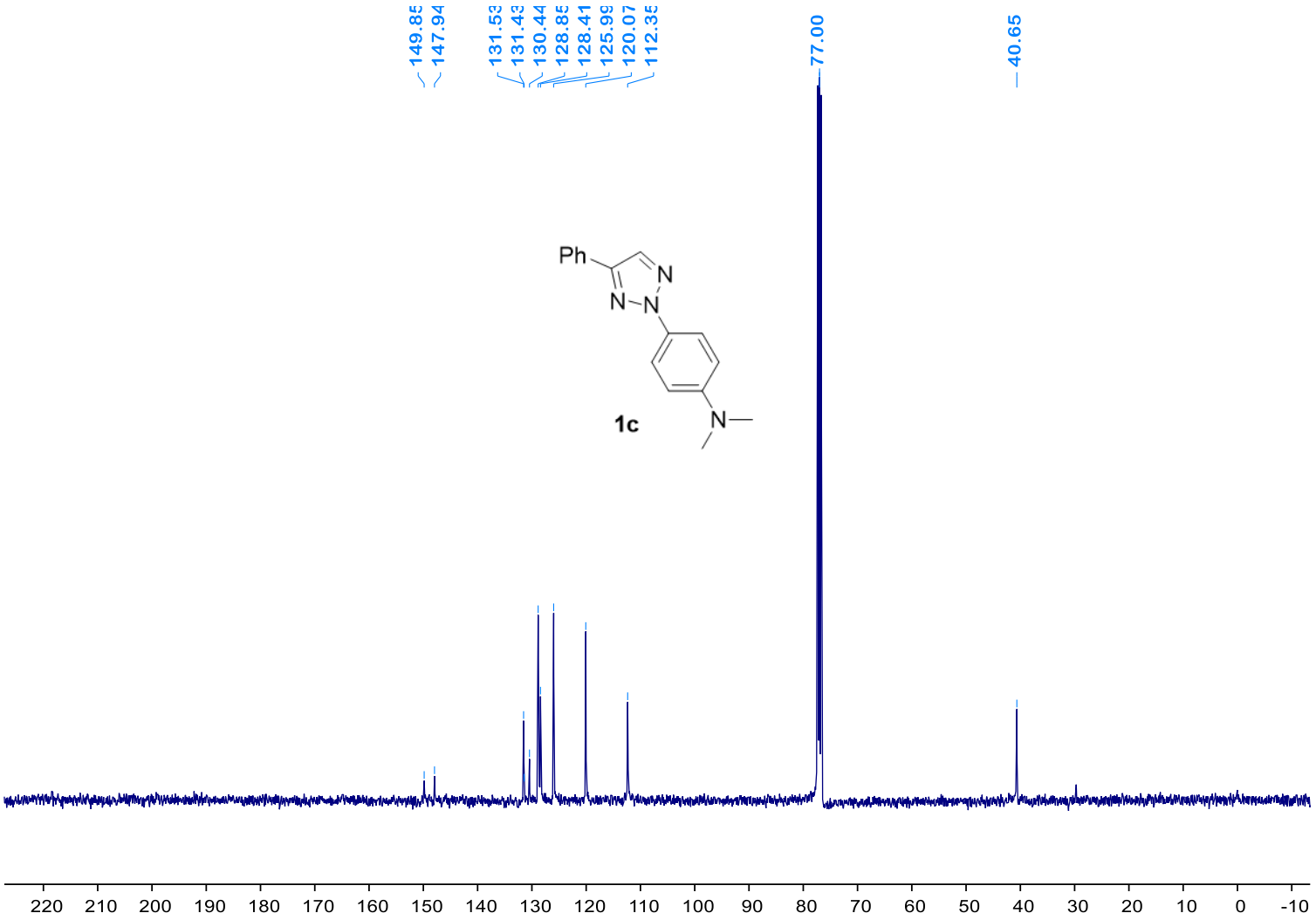
0.00
-0.00
Ph
N
N
N
N—
1c
3.08
2.13
2.08
1.03
2.00
6.54
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

1c ^{13}C NMR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128.85
128.41
125.99
120.07
112.35
77.00
40.65
Ph
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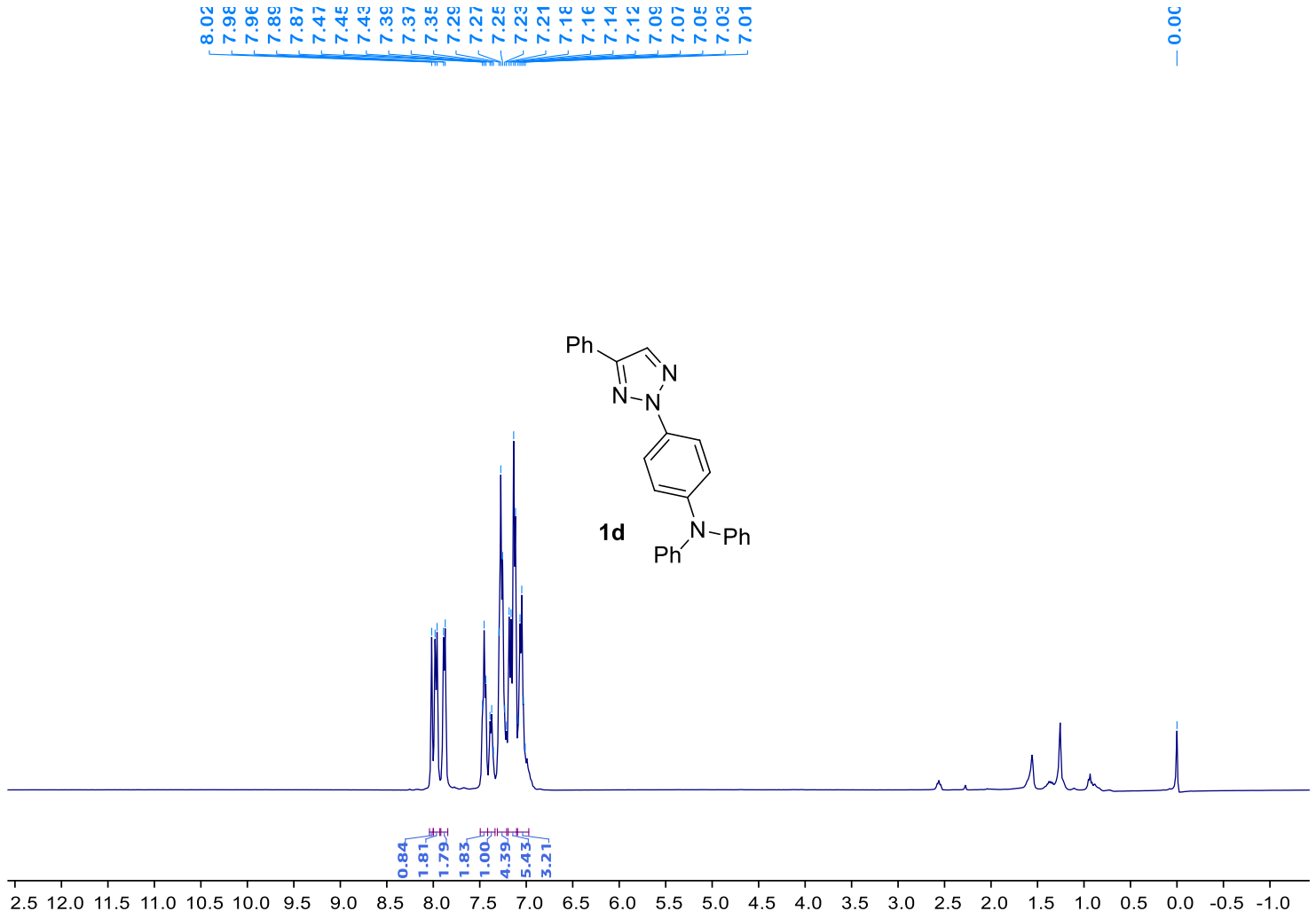
N
N
N
1c
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

1d ^{1}H NMR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7.47
7.45
7.43
7.39
7.37
7.35
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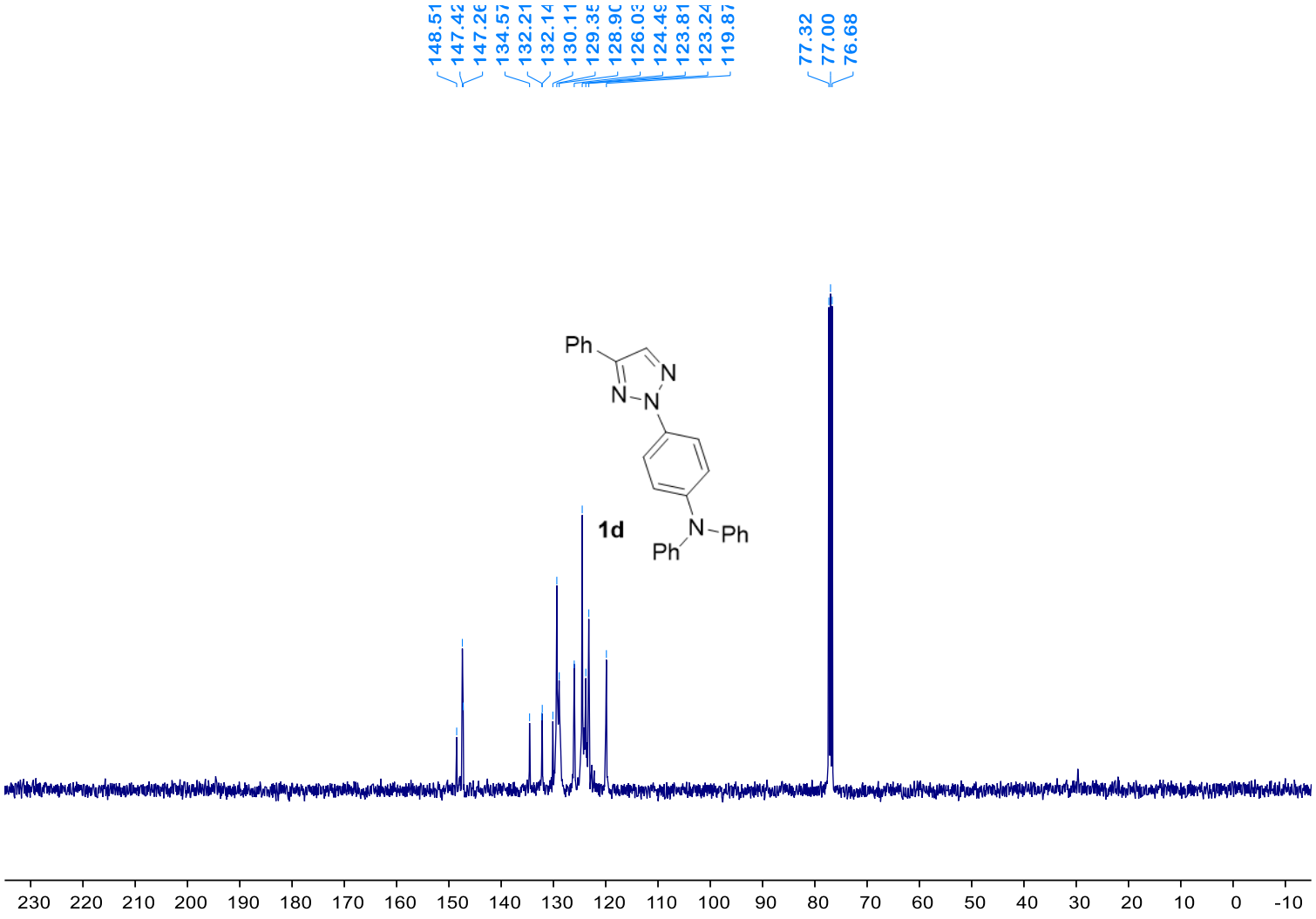
7.14
7.12
7.09
7.07
7.05
7.03
7.01
0.00
Ph
N
N
N
1d
N
Ph
Ph
0.84
1.81
1.79
1.83
1.00
4.39
5.43
3.21
2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

1d ^{13}C NMR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132.14
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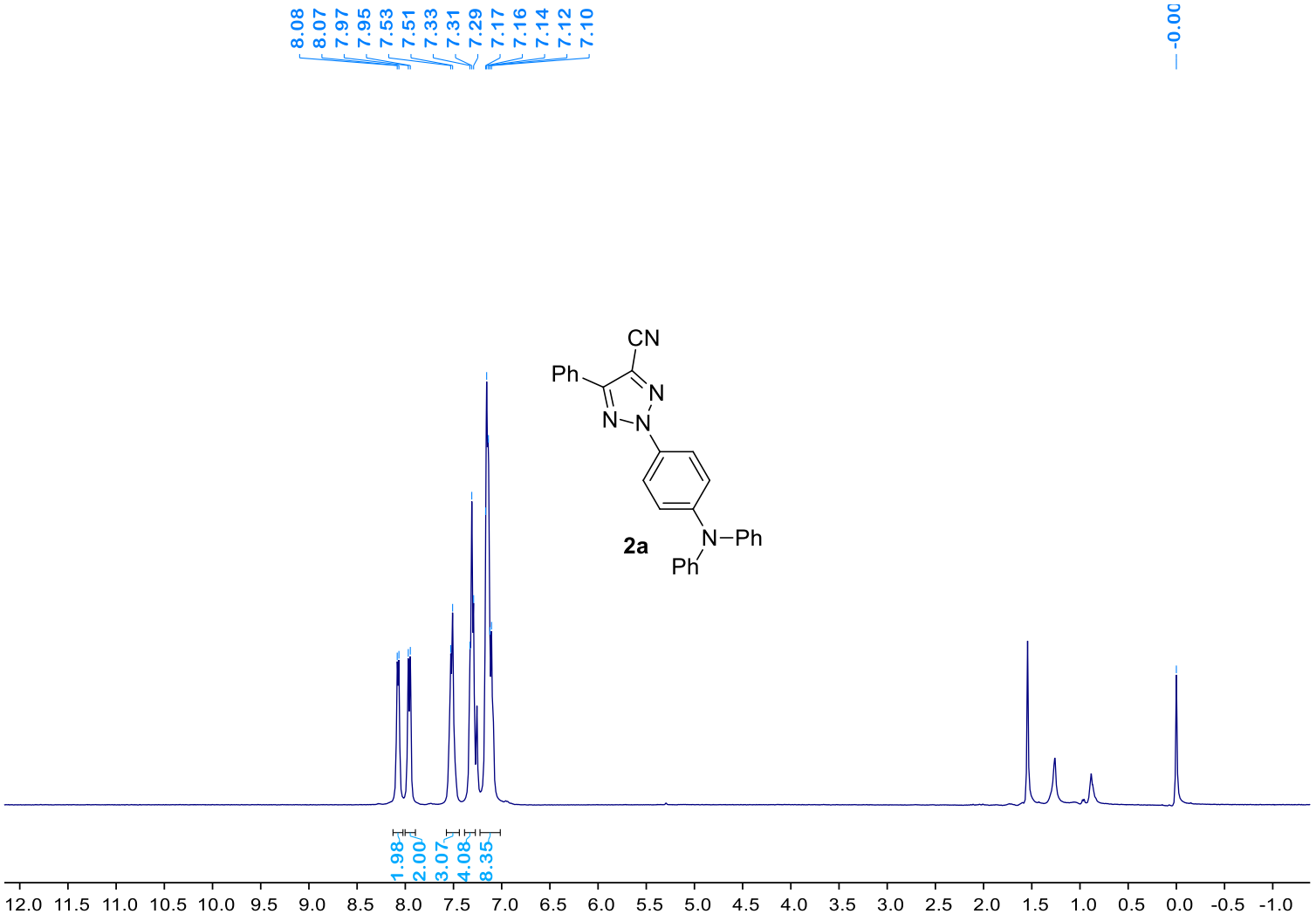
129.35
128.90
126.03
124.49
123.81
123.24
119.87
77.32
77.00
76.68
Ph
N
N
N
1d
N
Ph
Ph
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

2a ^{1}H NMR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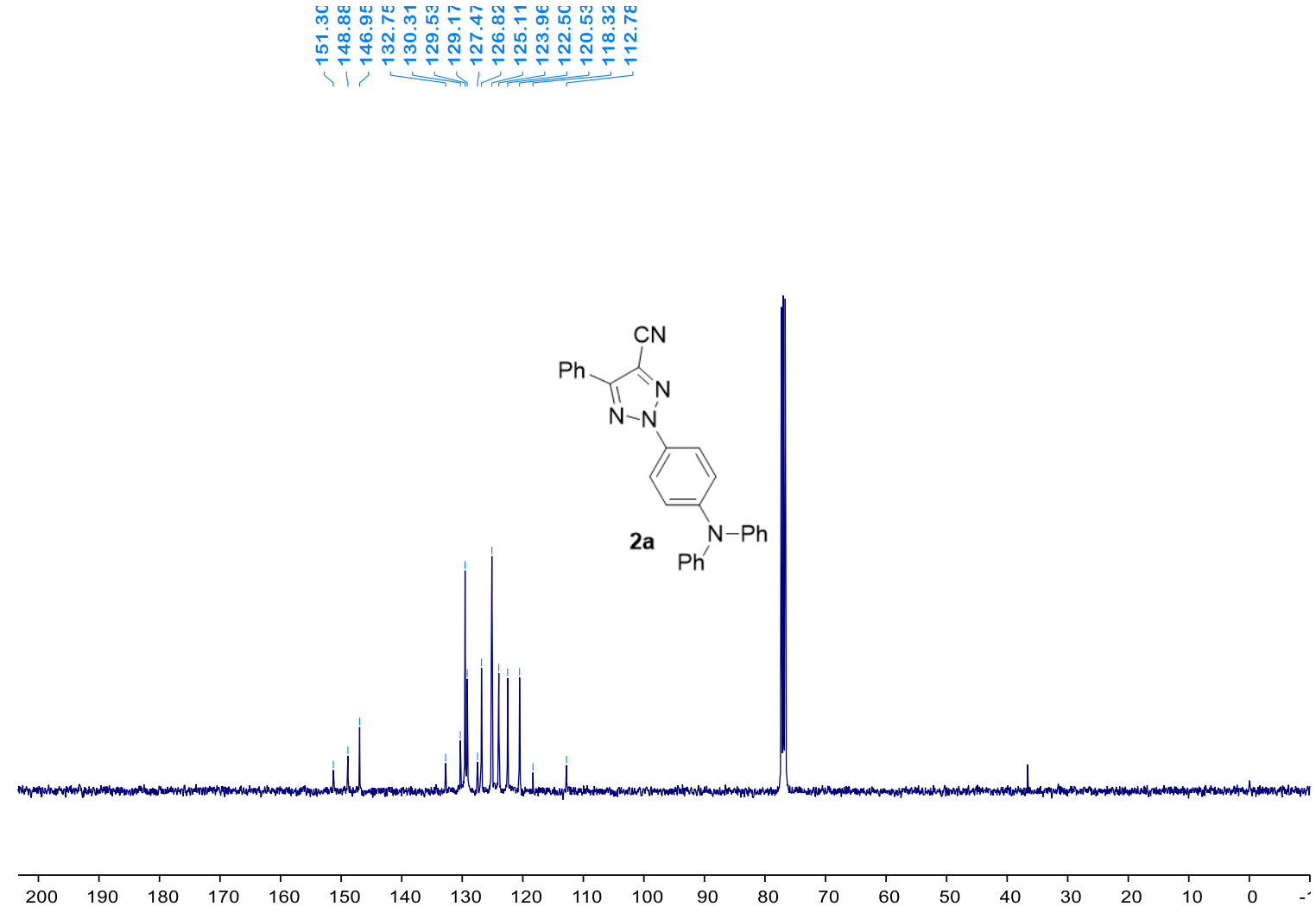
7.53
7.51
7.33
7.31
7.29
7.17
7.16
7.14
7.12
7.10
-0.00
CN
Ph
N
N
N
N–Ph
Ph
2a
1.98
2.00
3.07
4.08
8.35
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

2a ^{13}C NMR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123.96
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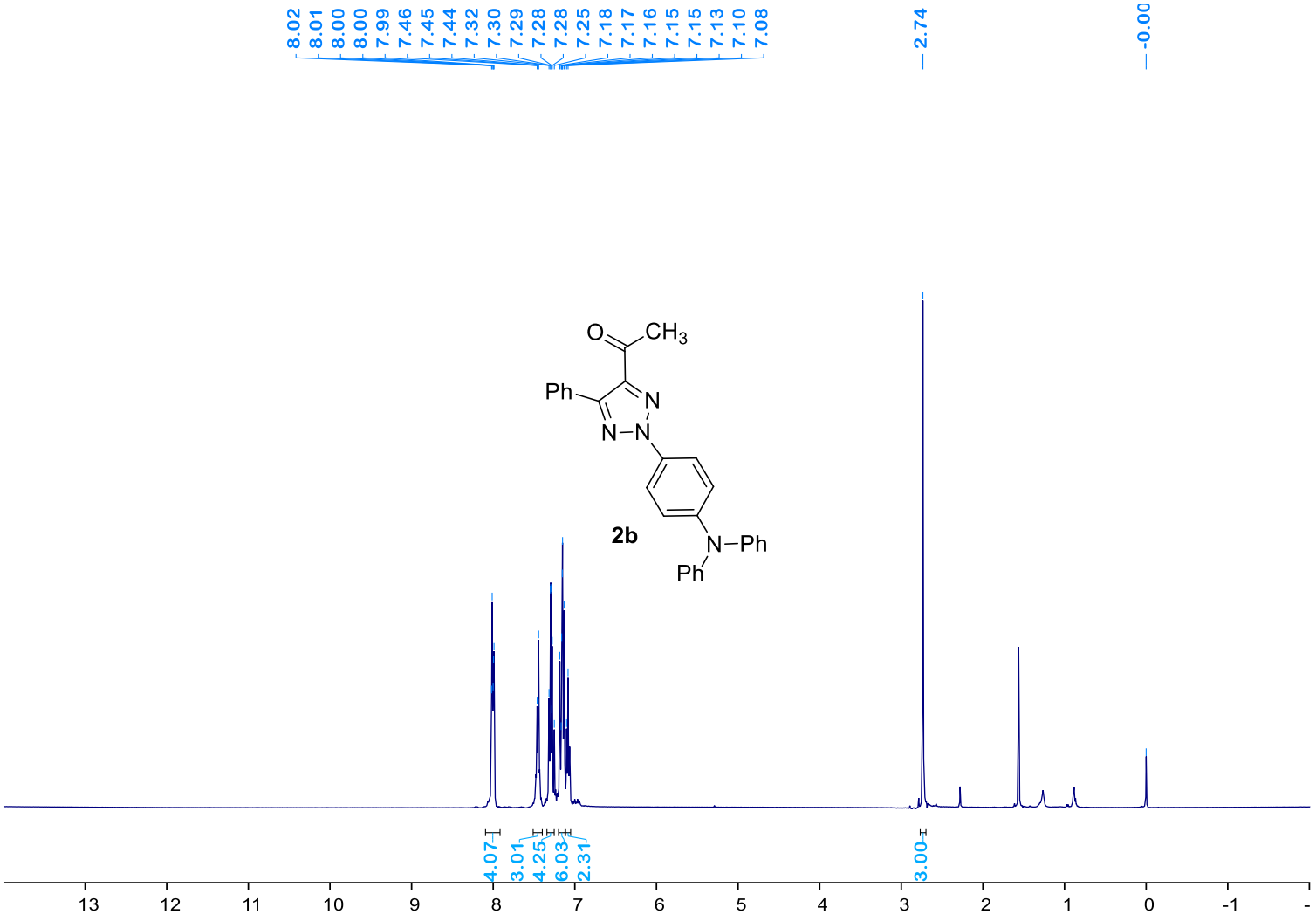
N
N
2a
N–Ph
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

2b ^{1}H NMR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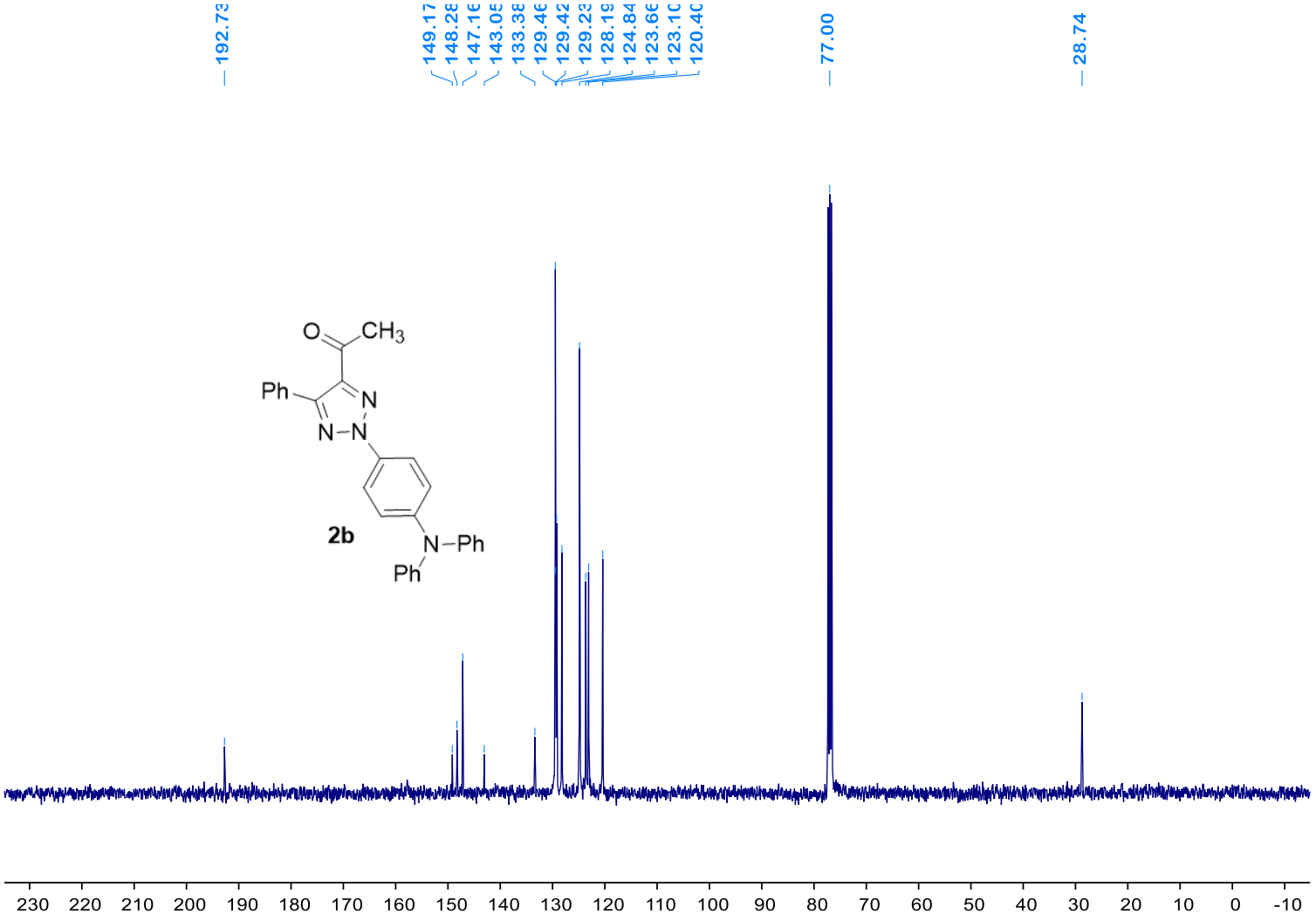
8.01
8.00
8.00
7.99
7.46
7.45
7.44
7.32
7.30
7.29
7.28
7.28
7.25
7.18
7.17
7.16
7.15
7.15
7.13
7.10
7.08
2.74
-0.00
O
CH3
Ph
N
N–N
2b
N–Ph
Ph
4.07
3.01
4.25
6.03
2.31
3.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1

2b ^{13}C NMR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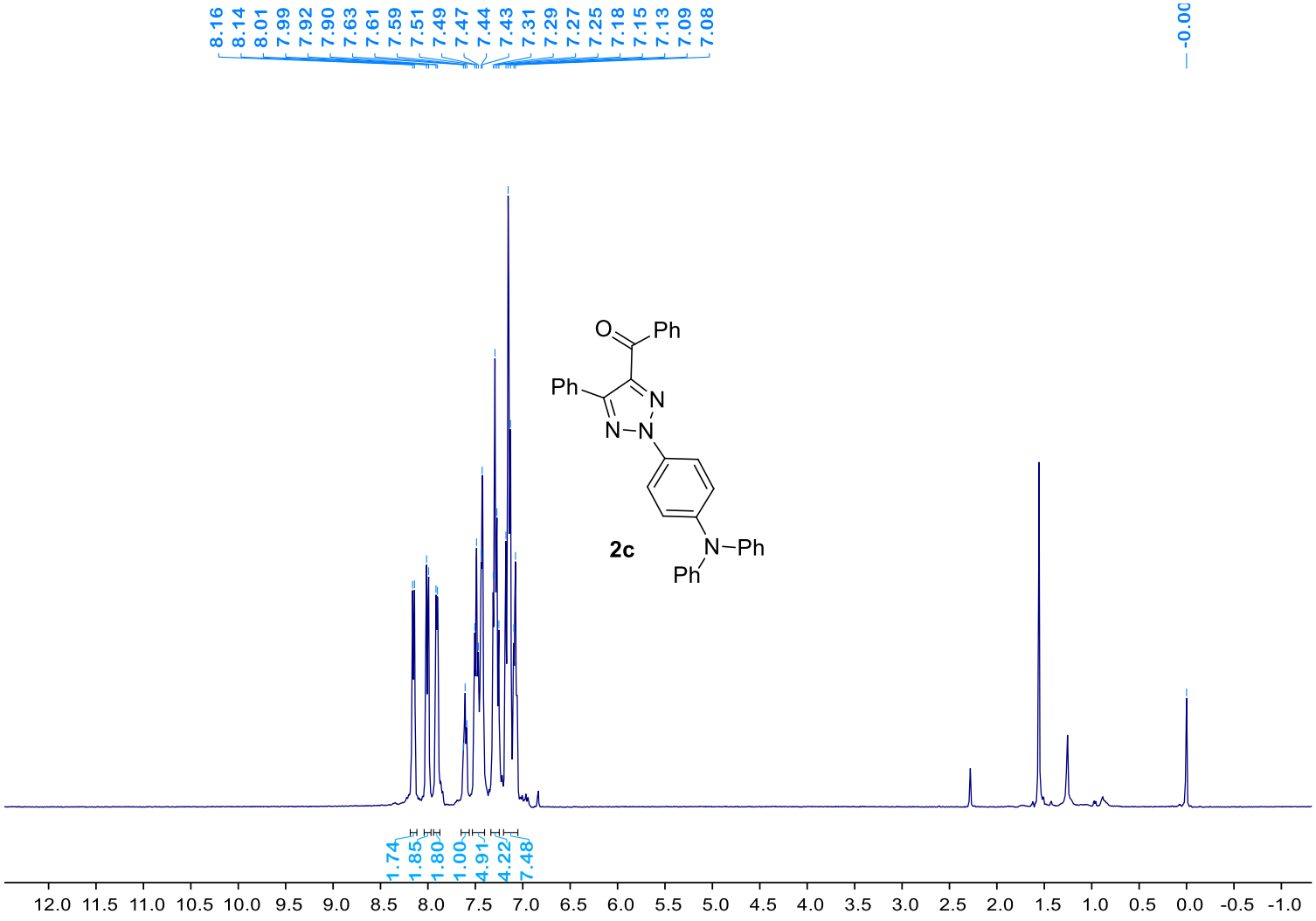
149.17
148.28
147.16
143.05
133.38
129.46
129.42
129.23
128.19
124.84
123.66
123.10
120.40
77.00
28.74
O
CH3
Ph
N
N–N
2b
N–Ph
Ph
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

2c ^{1}H NMR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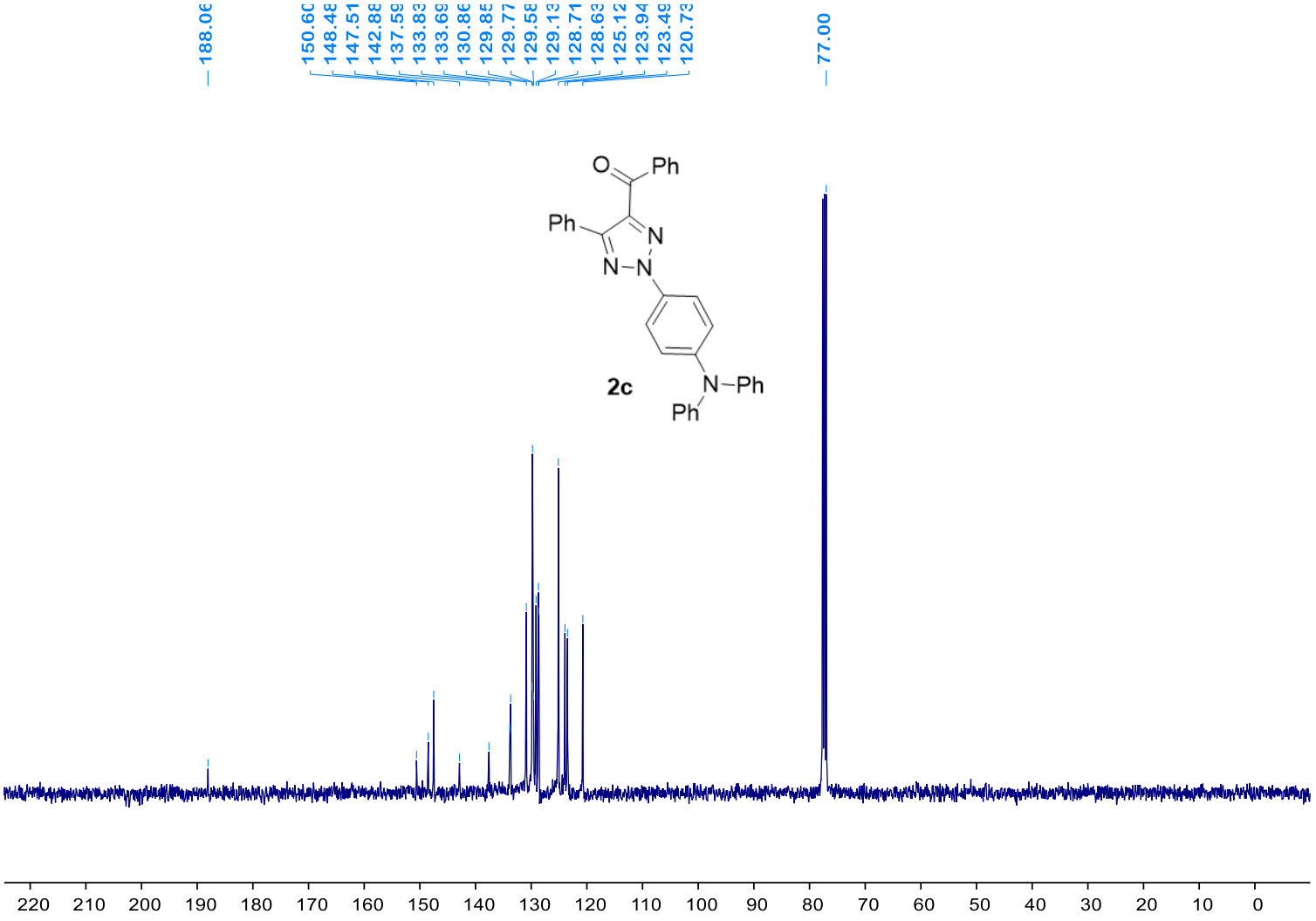
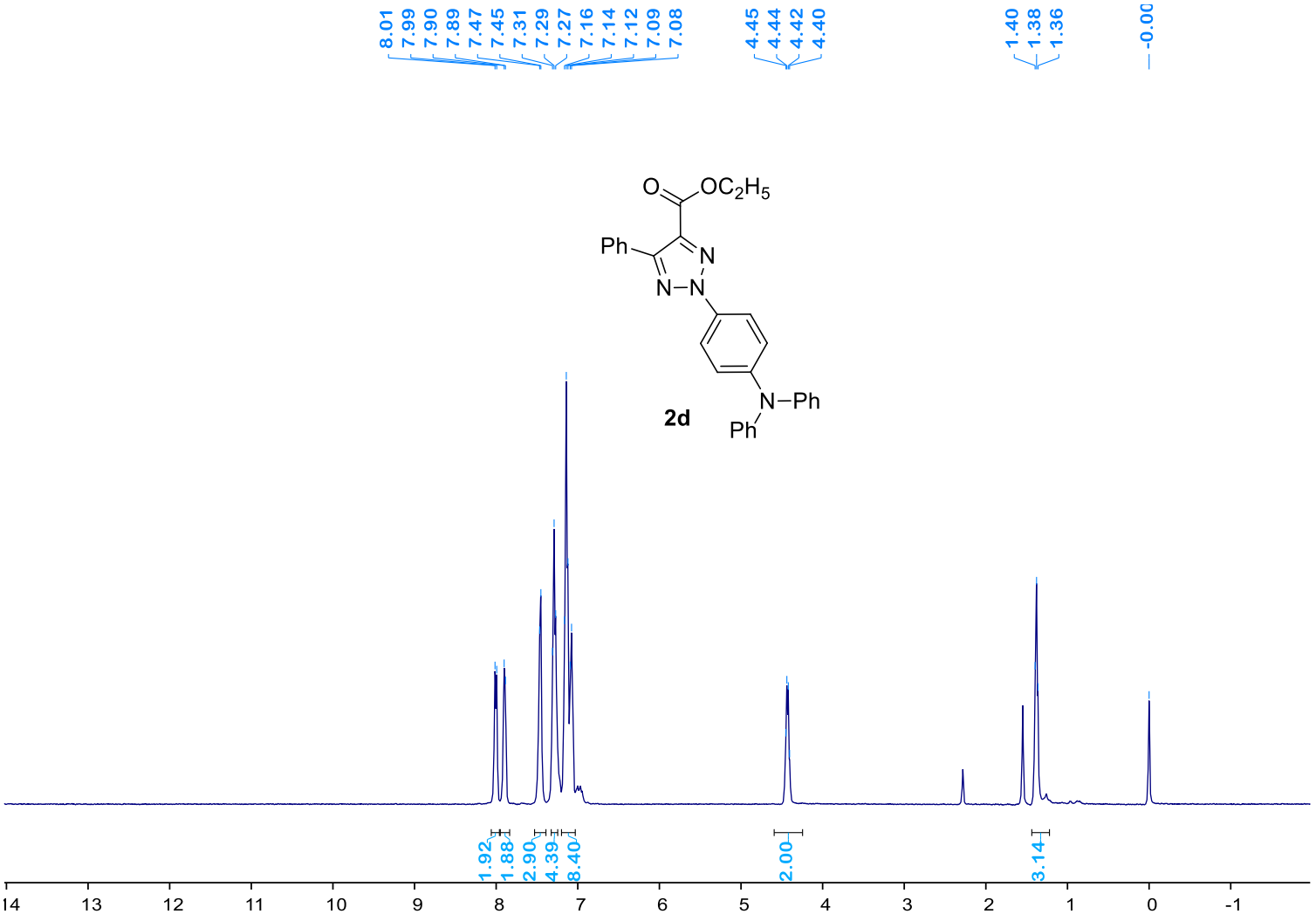
8.14
8.01
7.99
7.92
7.90
7.63
7.61
7.59
7.51
7.49
7.47
7.44
7.43
7.31
7.29
7.27
7.25
7.18
7.15
7.13
7.09
7.08
-0.00
O
Ph
Ph
N
N–N
2c
N–Ph
Ph
1.74
1.85
1.80
1.00
4.91
4.22
7.48
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

2c ^{13}C NMR


188.06
150.60
148.48
147.51
142.88
137.59
133.83
133.69
130.86
129.85
129.77
129.58
129.13
128.71
128.63
125.12
123.94
123.49
120.73
77.00
O
Ph
Ph
N
N–N
2c
N–Ph
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

2d ^{1}H NMR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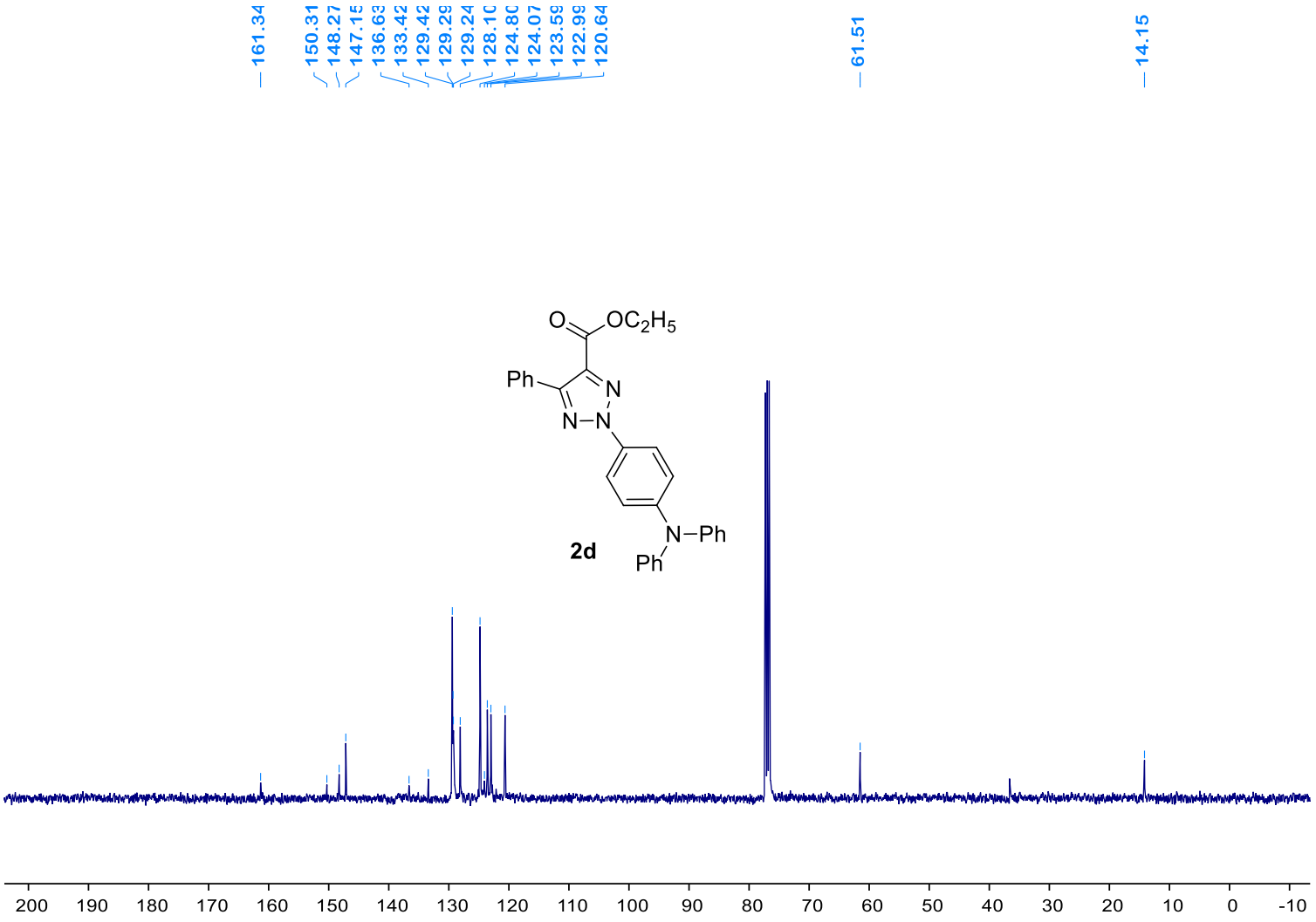
7.99
7.90
7.89
7.47
7.45
7.31
7.29
7.27
7.16
7.14
7.12
7.09
7.08
4.45
4.44
4.42
4.40
1.40
1.38
1.36
-0.00
O
OC2H5
Ph
N
N–N
N–Ph
Ph
2d
1.92
1.88
2.90
4.39
8.40
2.00
3.14
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1

2d ^{13}C NMR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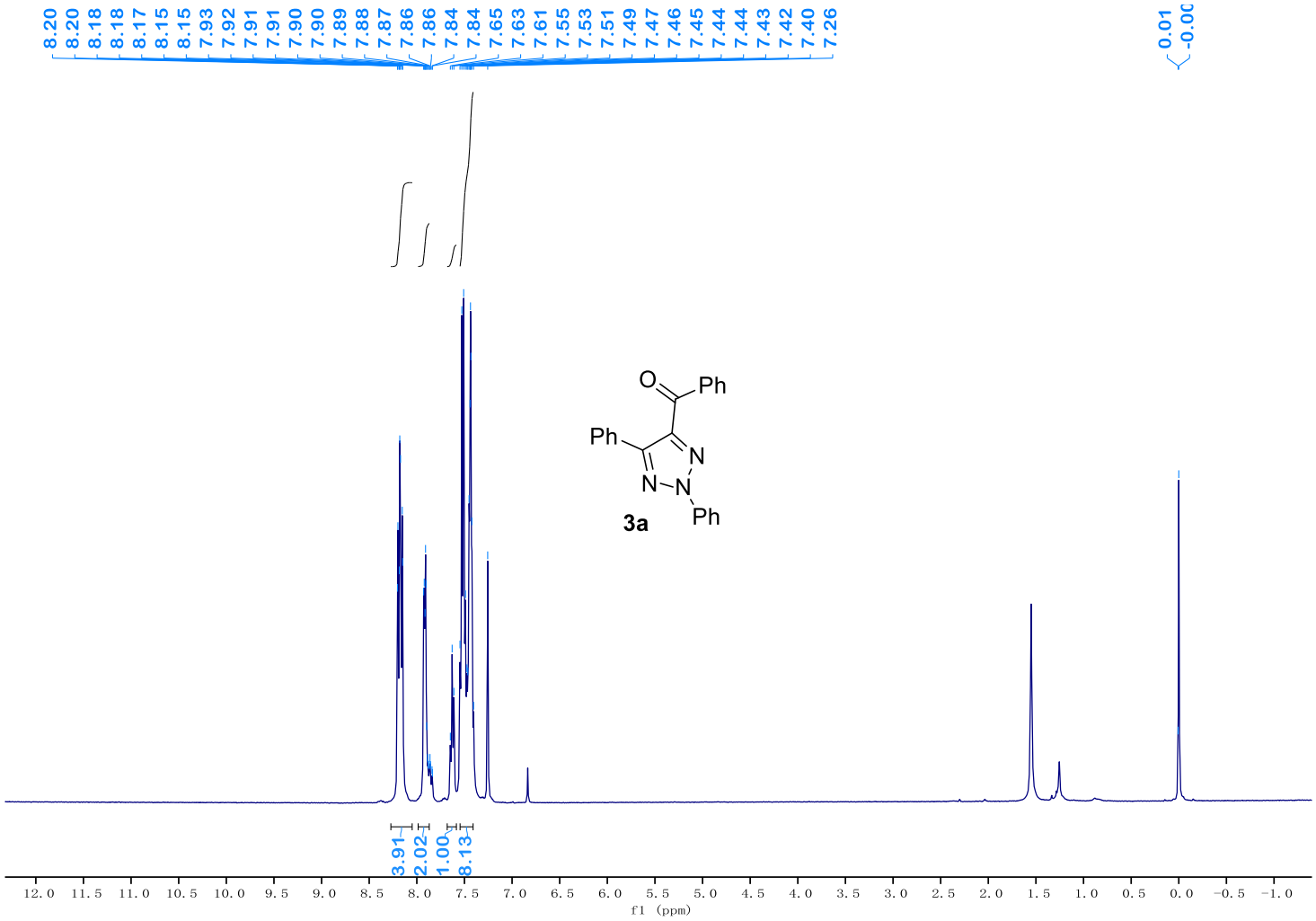
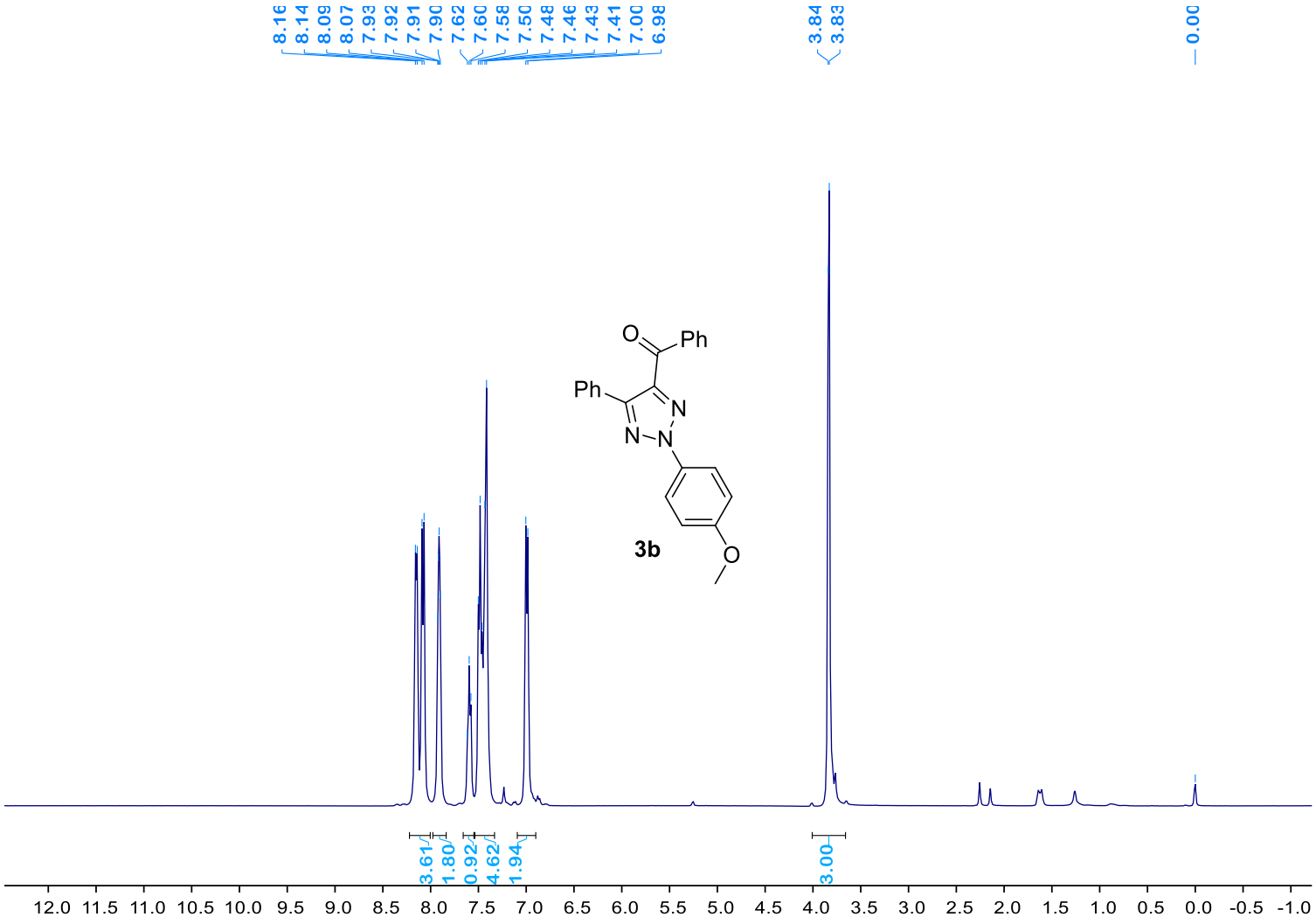
150.31
148.27
147.15
136.63
133.42
129.42
129.29
129.24
128.10
124.80
124.07
123.59
122.99
120.64
61.51
14.15
O
OC2H5
Ph
N
N–N
N–Ph
Ph
2d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

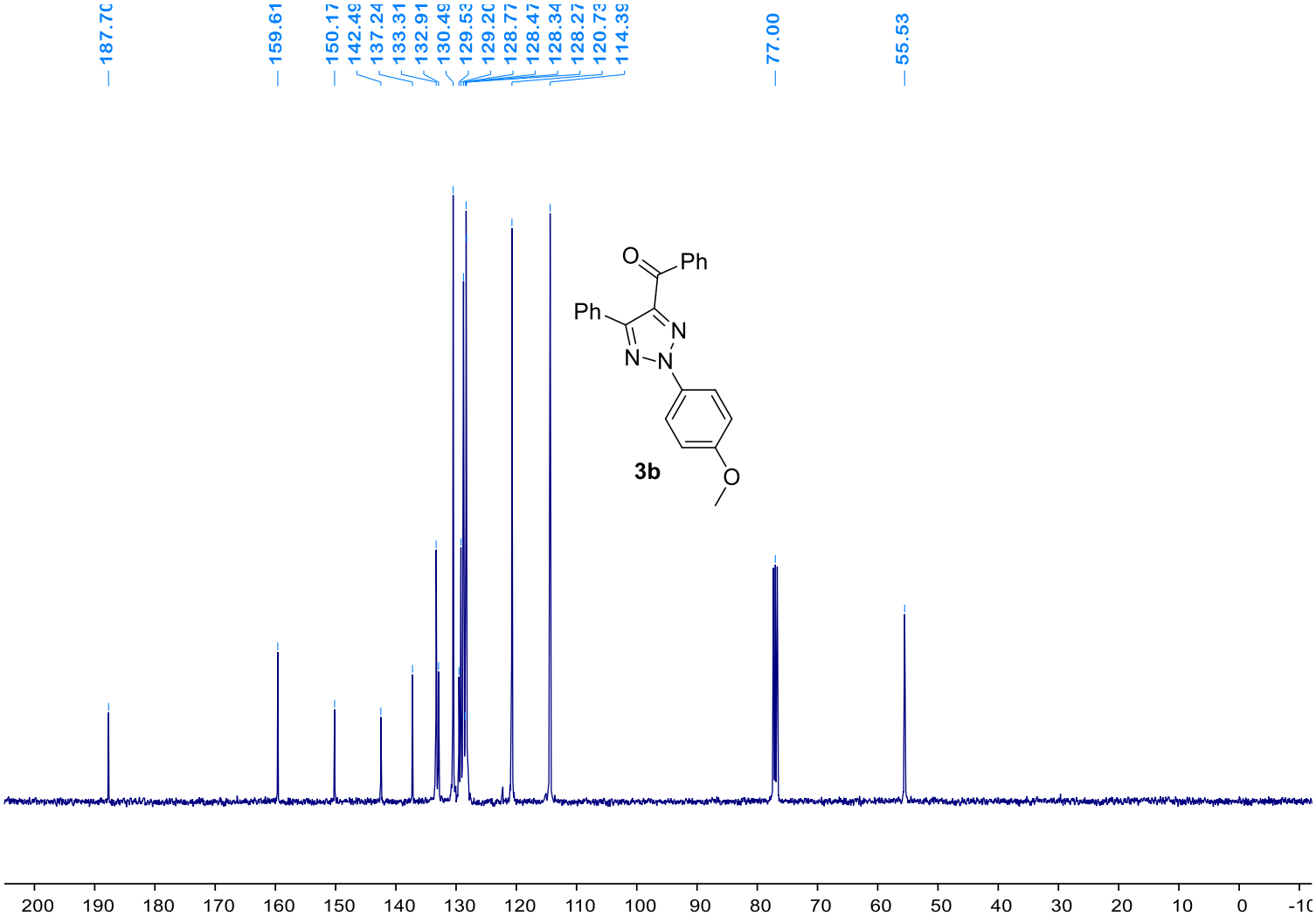
3a ^{1}H NMR


8.20
8.20
8.18
8.18
8.17
8.15
8.15
7.93
7.92
7.91
7.91
7.90
7.90
7.89
7.88
7.87
7.86
7.86
7.84
7.84
7.65
7.63
7.61
7.55
7.53
7.51
7.49
7.47
7.46
7.45
7.44
7.44
7.43
7.42
7.40
7.26
0.01
-0.00
O
Ph
Ph
N
N
N
Ph
3a
3.91
2.02
1.00
8.13
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

3b ^{1}H NMR


8.16
8.14
8.09
8.07
7.93
7.92
7.91
7.90
7.62
7.60
7.58
7.50
7.48
7.46
7.43
7.41
7.00
6.98
3.84
3.83
0.00
O
Ph
Ph
N
N
N
3b
O
3.61
1.80
0.92
4.62
1.94
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

3b ^{13}C NMR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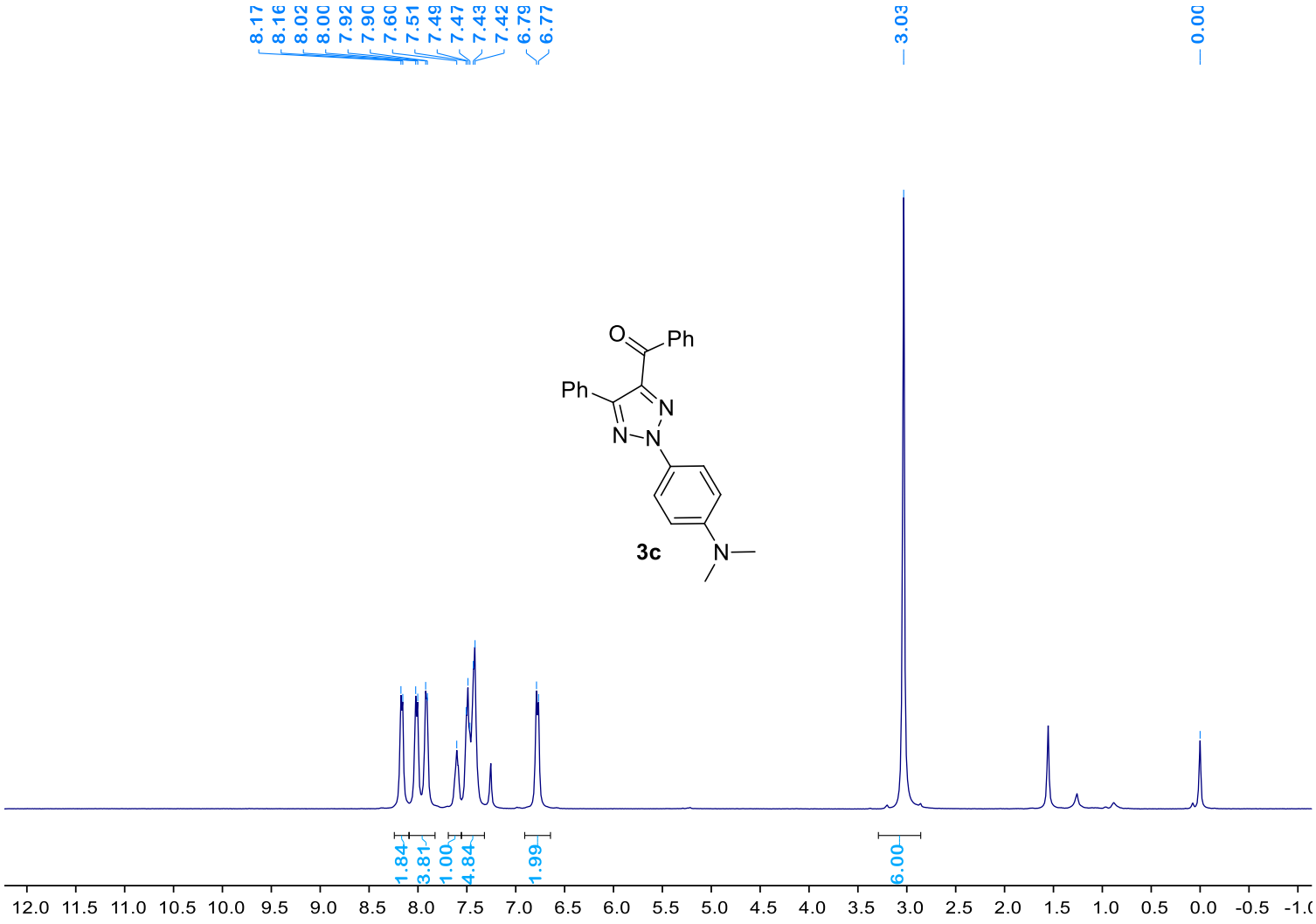
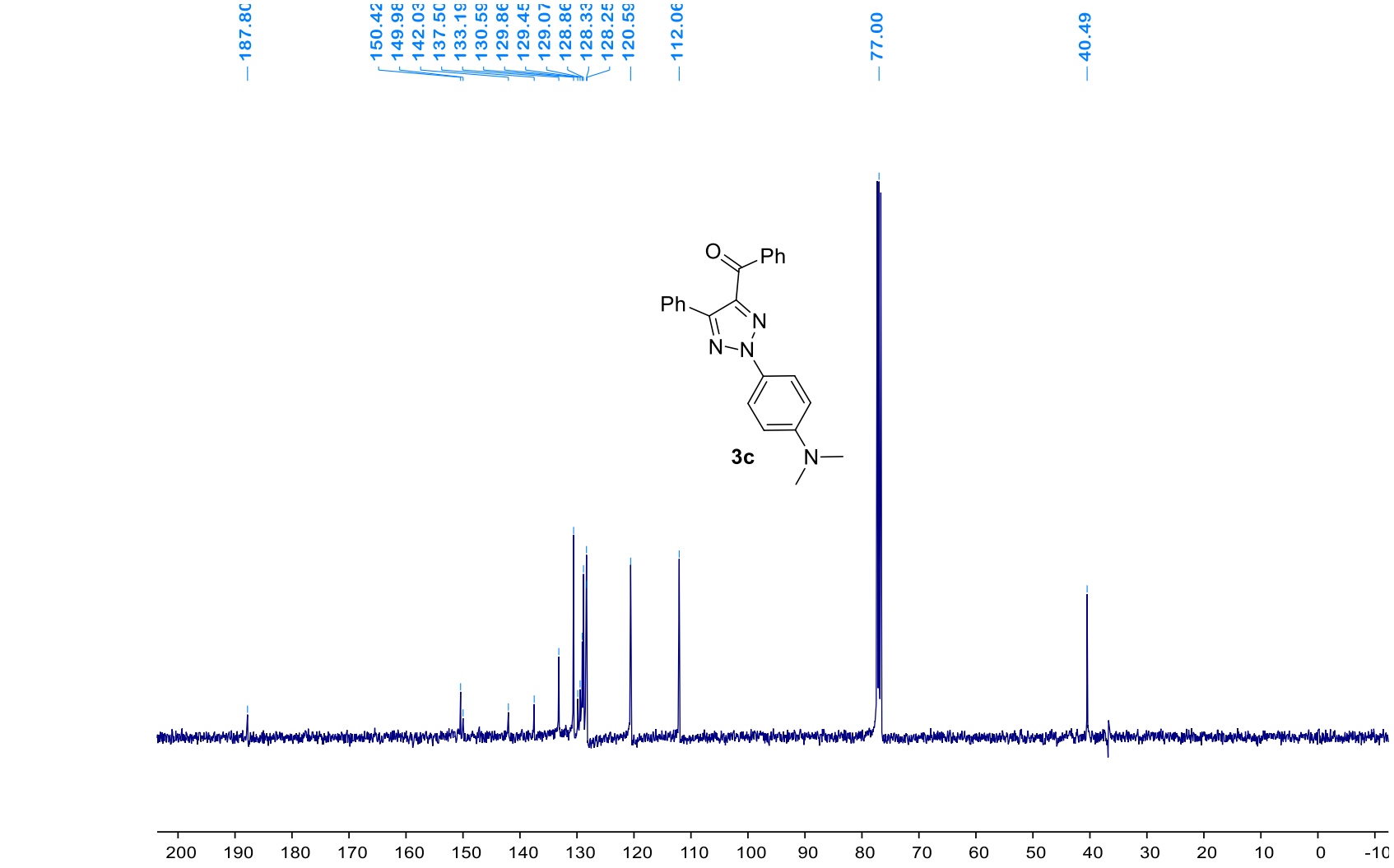
159.61
150.17
142.49
137.24
133.31
132.91
130.49
129.53
129.20
128.77
128.47
128.34
128.27
120.73
114.39
77.00
55.53
O
Ph
Ph
N
N
N
3b
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

3c ^{1}H NMR


8.17
8.16
8.02
8.00
7.92
7.90
7.60
7.51
7.49
7.47
7.43
7.42
6.79
6.77
3.03
0.00
O
Ph
Ph
N
N
N
3c
N
1.84
3.81
1.00
4.84
1.99
6.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

3c ^{13}C NMR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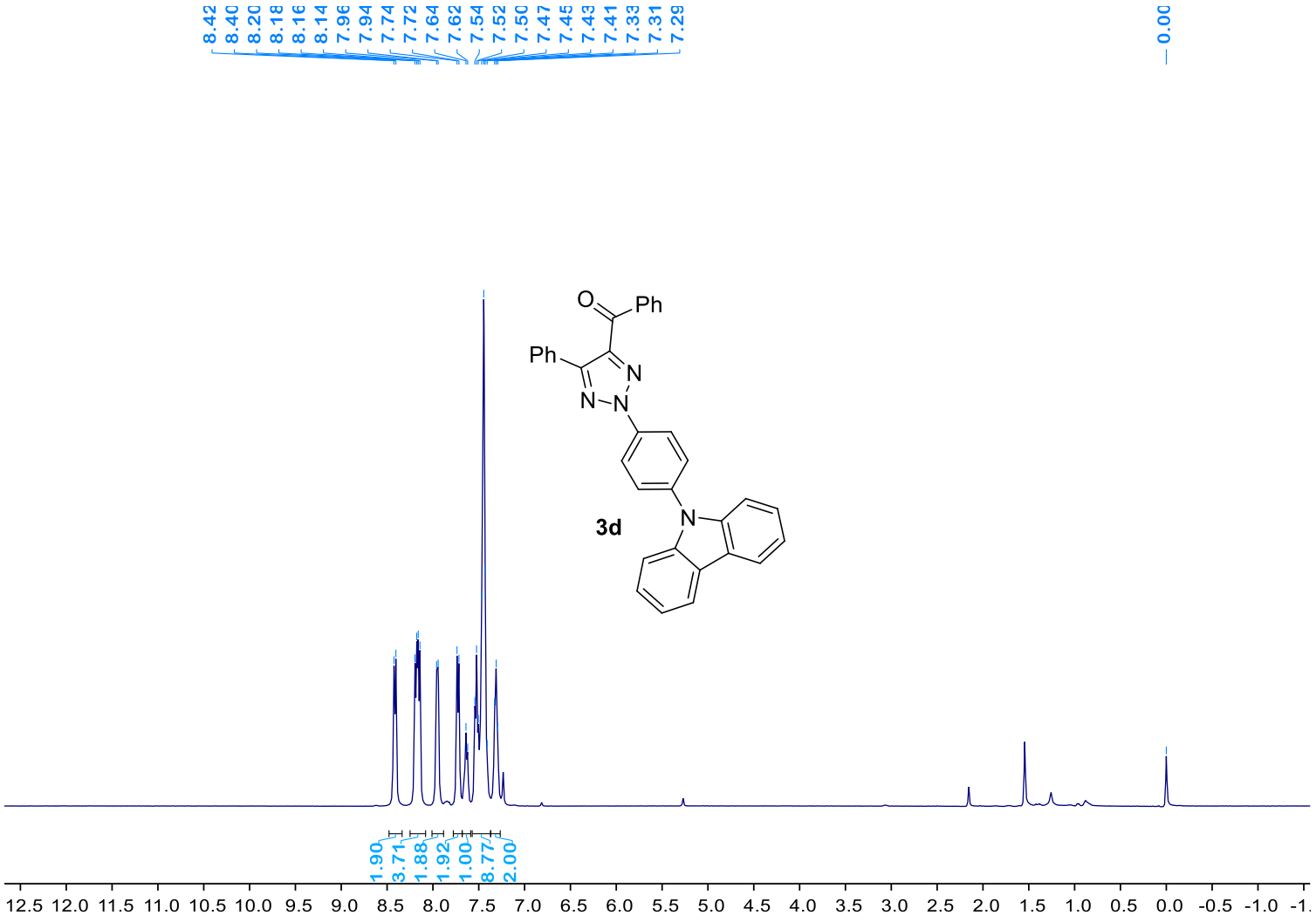
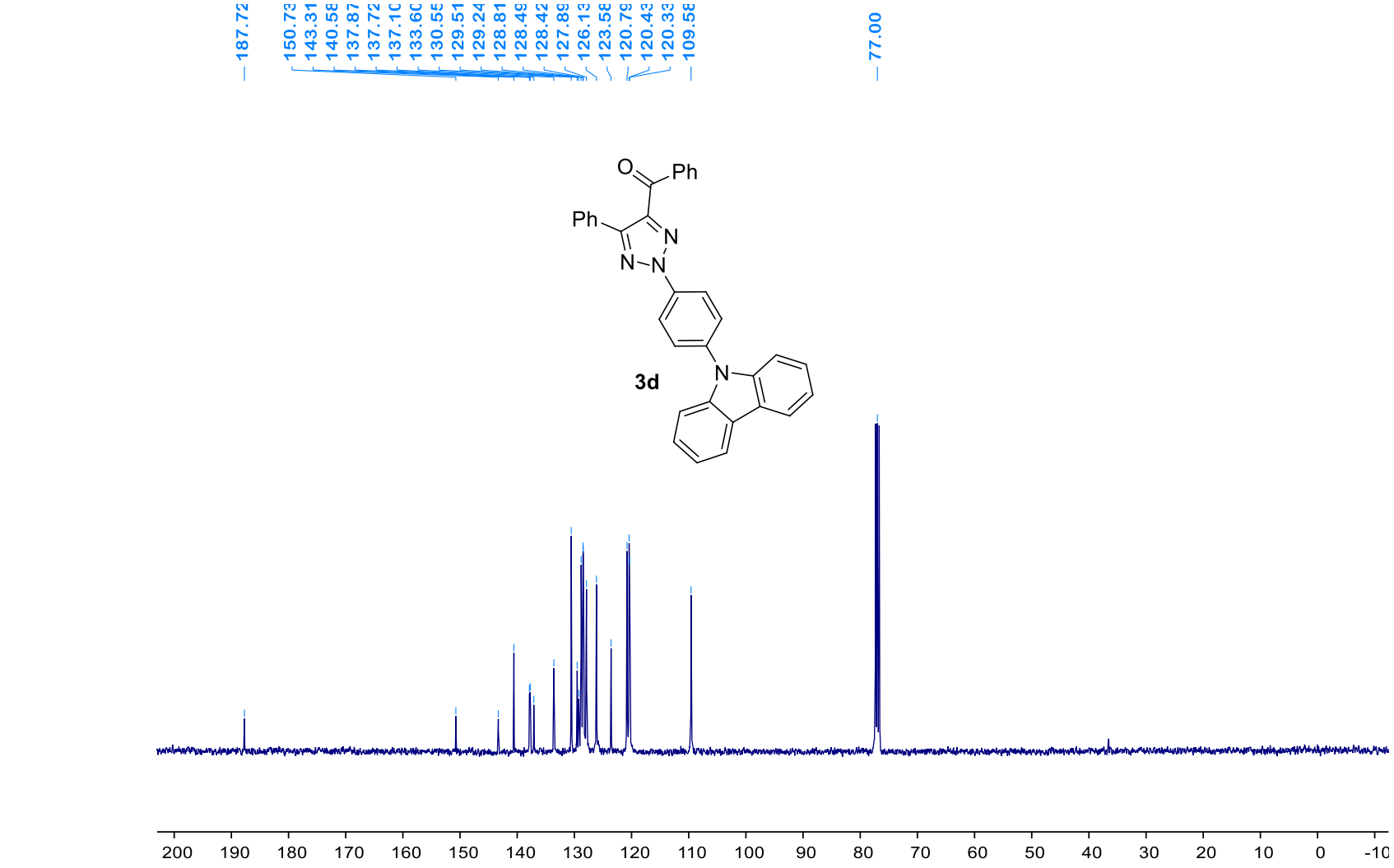
149.98
142.03
137.50
133.19
130.59
129.86
129.45
129.07
128.86
128.33
128.25
120.59
112.06
77.00
40.49
O
Ph
Ph
N
N
N
3c
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

3d ^{1}H NMR


8.42
8.40
8.20
8.18
8.16
8.14
7.96
7.94
7.74
7.72
7.64
7.62
7.54
7.52
7.50
7.47
7.45
7.43
7.41
7.33
7.31
7.29
0.00
O
Ph
Ph
N
N
N
N
3d
1.90
3.71
1.88
1.92
1.00
8.77
2.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.

3d ^{13}C NMR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150.73
143.31
140.58
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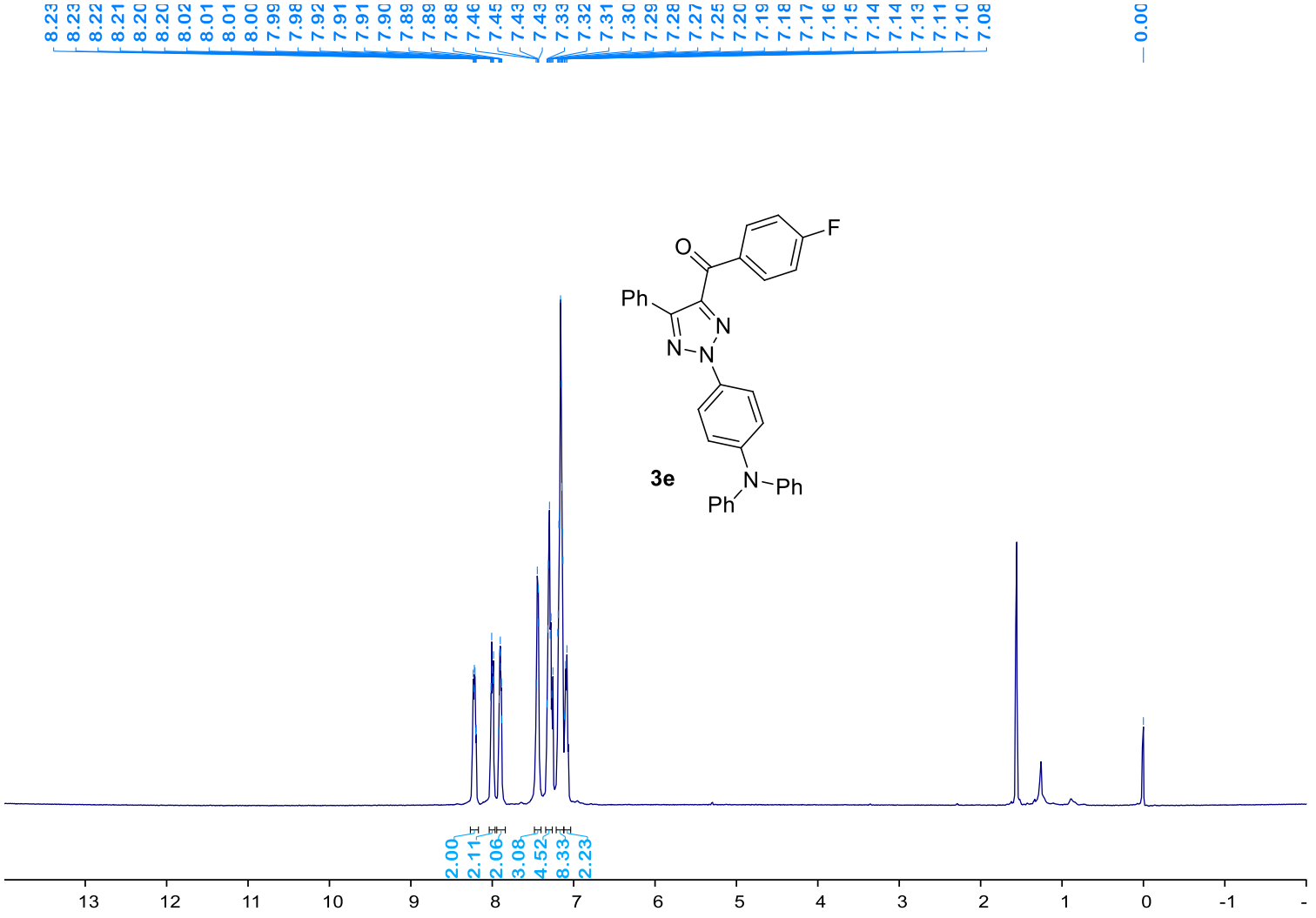
137.72
137.10
133.60
130.55
129.51
129.24
128.81
128.49
128.42
127.89
126.13
123.58
120.79
120.43
120.33
109.58
77.00
O
Ph
Ph
N
N
N
N
3d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

3e ^{1}H NMR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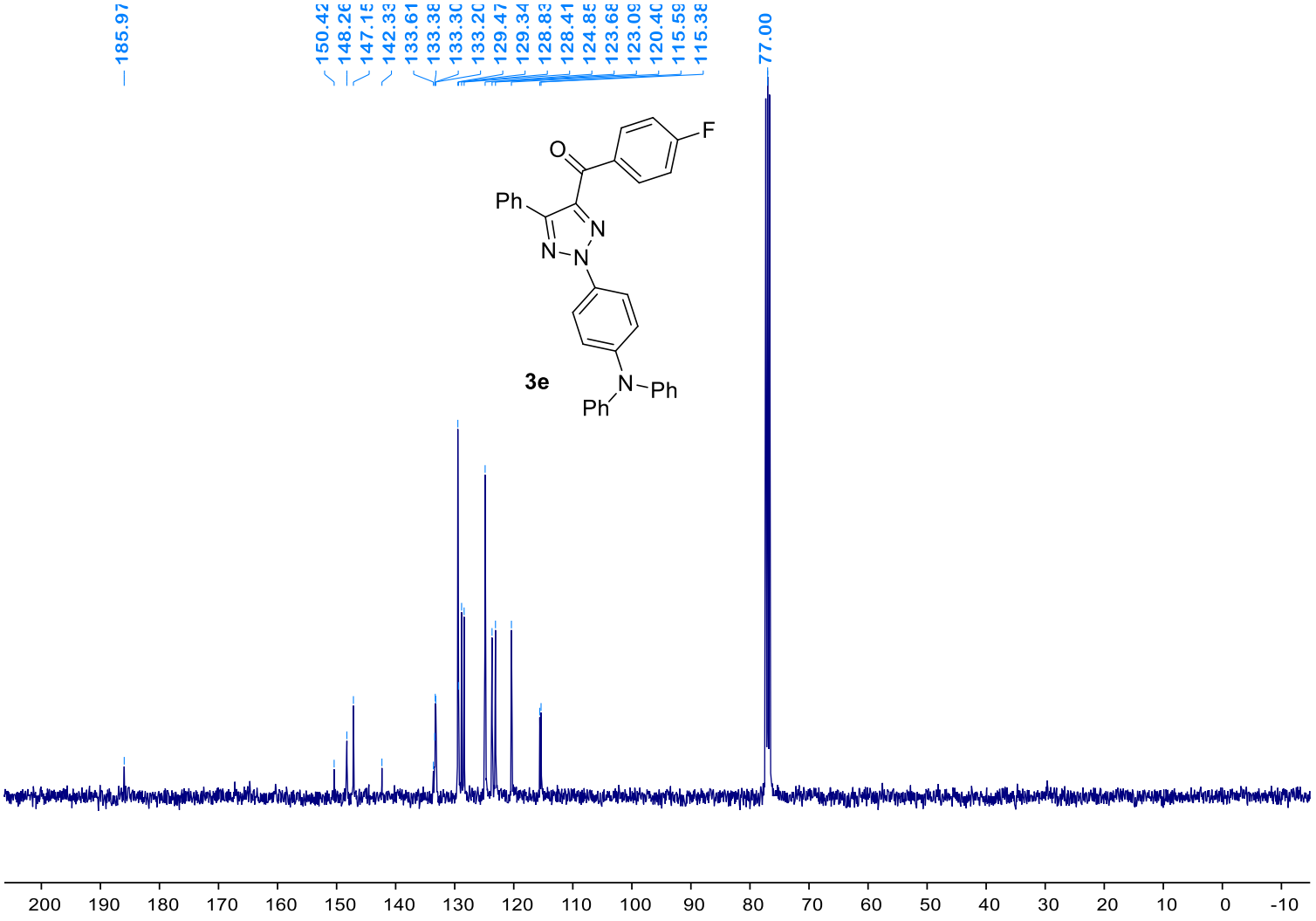
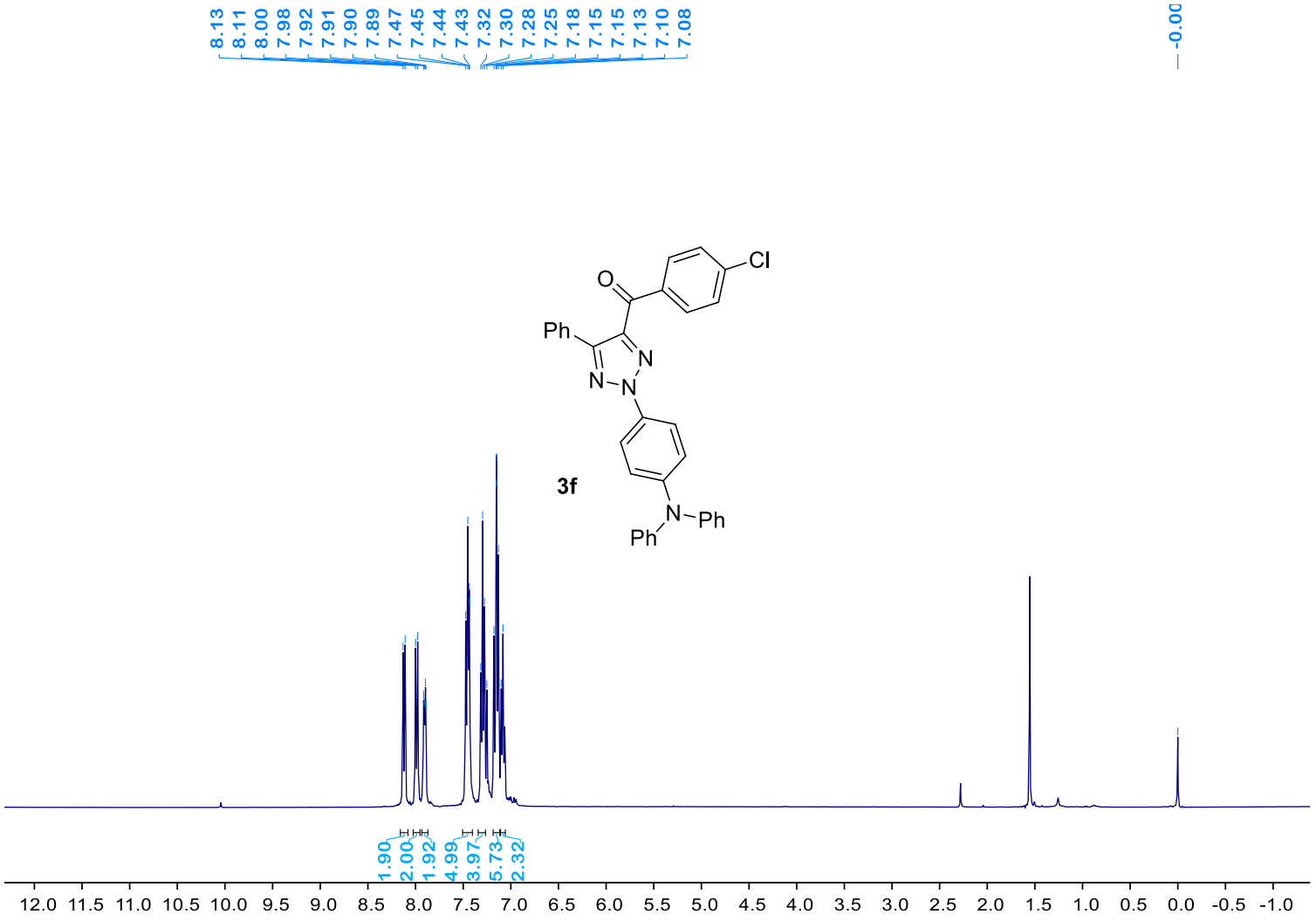
8.23
8.22
8.21
8.20
8.20
8.02
8.01
8.01
8.00
7.99
7.98
7.92
7.91
7.91
7.90
7.89
7.89
7.88
7.46
7.45
7.43
7.43
7.33
7.32
7.31
7.30
7.29
7.28
7.27
7.25
7.20
7.19
7.18
7.17
7.16
7.15
7.14
7.14
7.13
7.11
7.10
7.08
0.00
O
F
Ph
N
N
N
3e
N
Ph
Ph
2.00
2.11
2.06
3.08
4.52
8.33
2.23
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1

3e ^{13}C NMR


185.97
150.42
148.26
147.15
142.33
133.61
133.38
133.30
133.20
129.47
129.34
128.83
128.41
124.85
123.68
123.09
120.40
115.59
115.38
77.00
O
F
Ph
N
N
N
3e
N
Ph
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

3f ^{1}H NMR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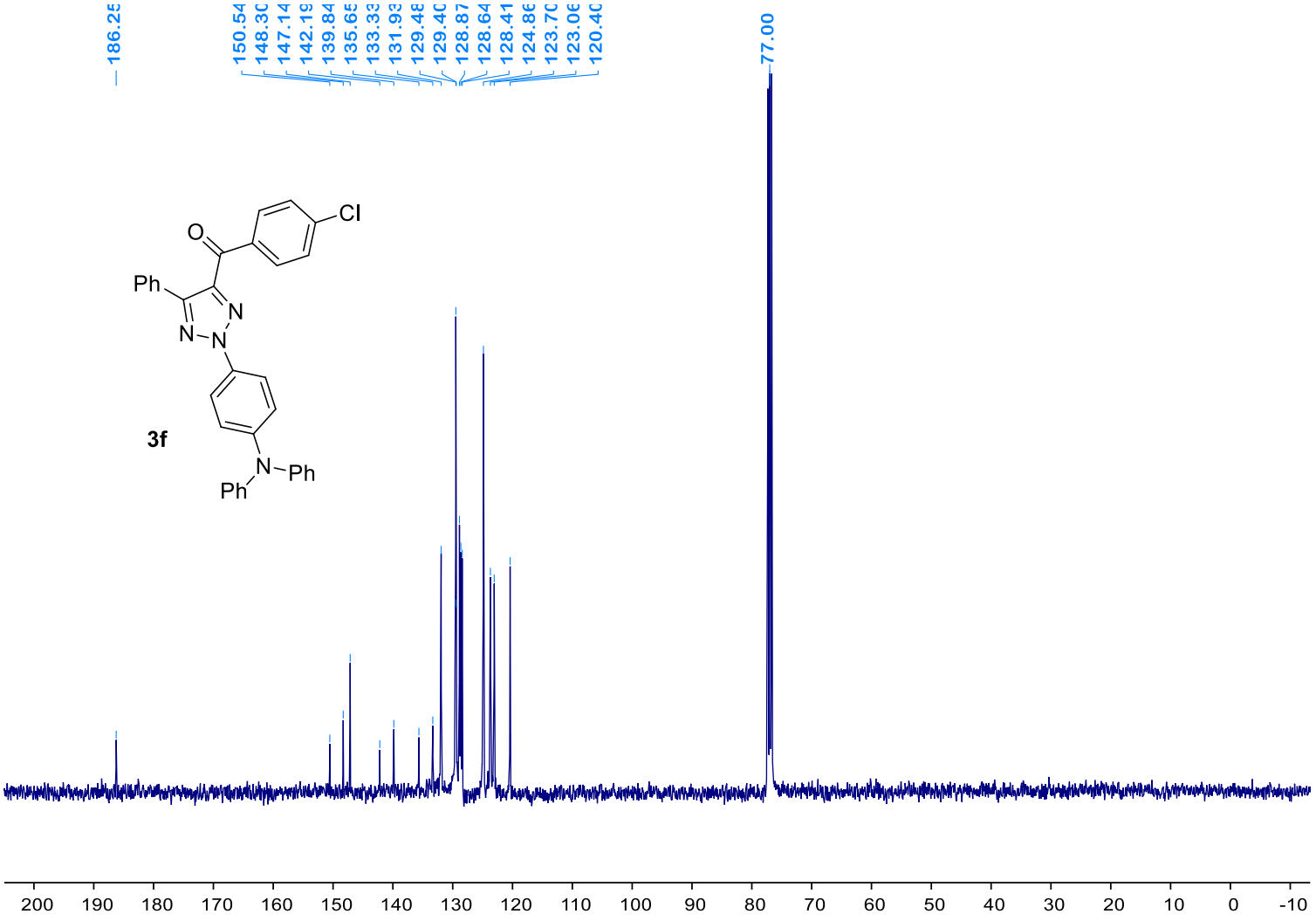
8.11
8.00
7.98
7.92
7.91
7.90
7.89
7.47
7.45
7.44
7.43
7.32
7.30
7.28
7.25
7.18
7.15
7.15
7.13
7.10
7.08
-0.00
Cl
O
Ph
N
N
N
3f
N
Ph
Ph
1.90
2.00
1.92
4.99
3.97
5.73
2.32
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

3f ^{13}C NMR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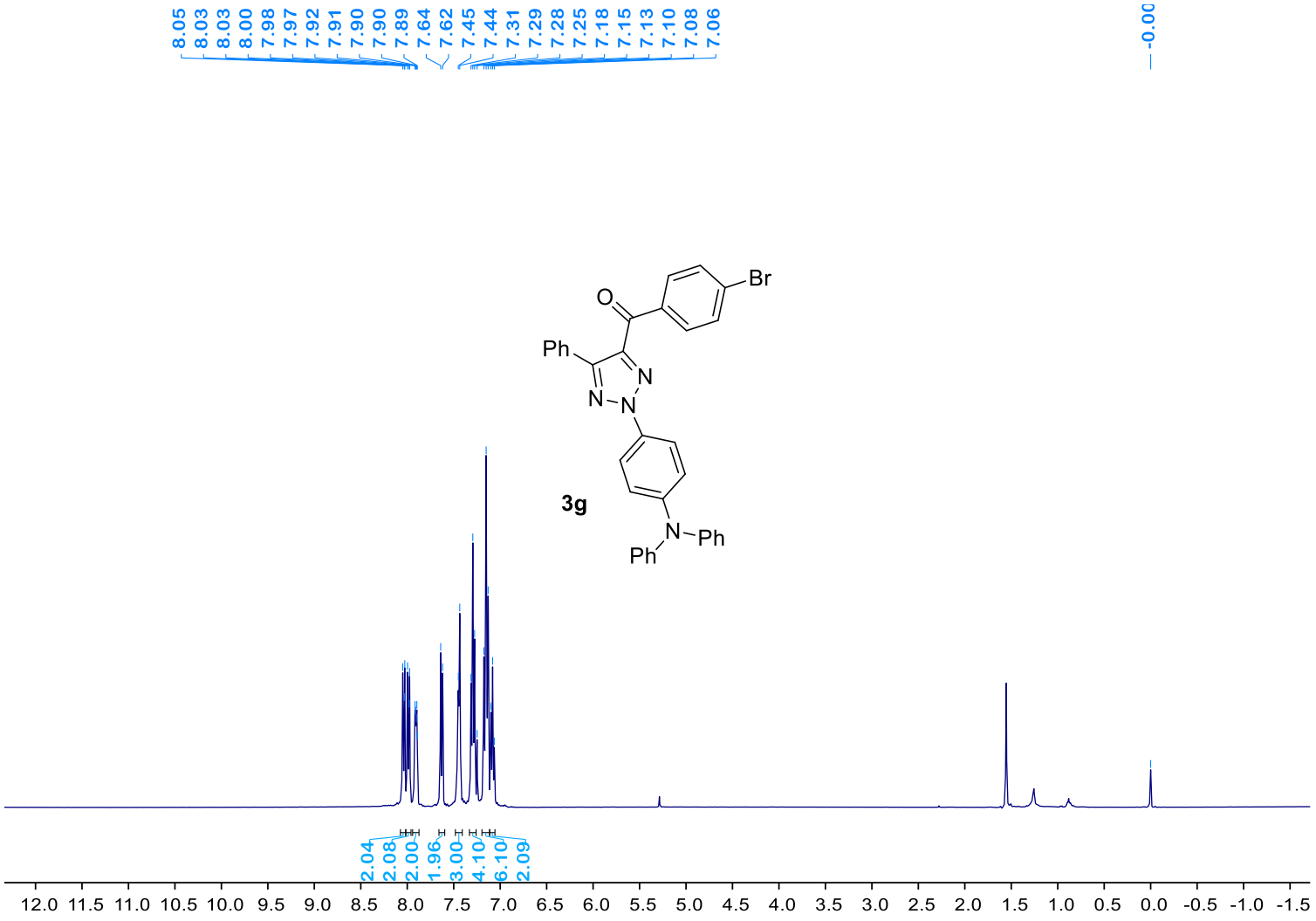
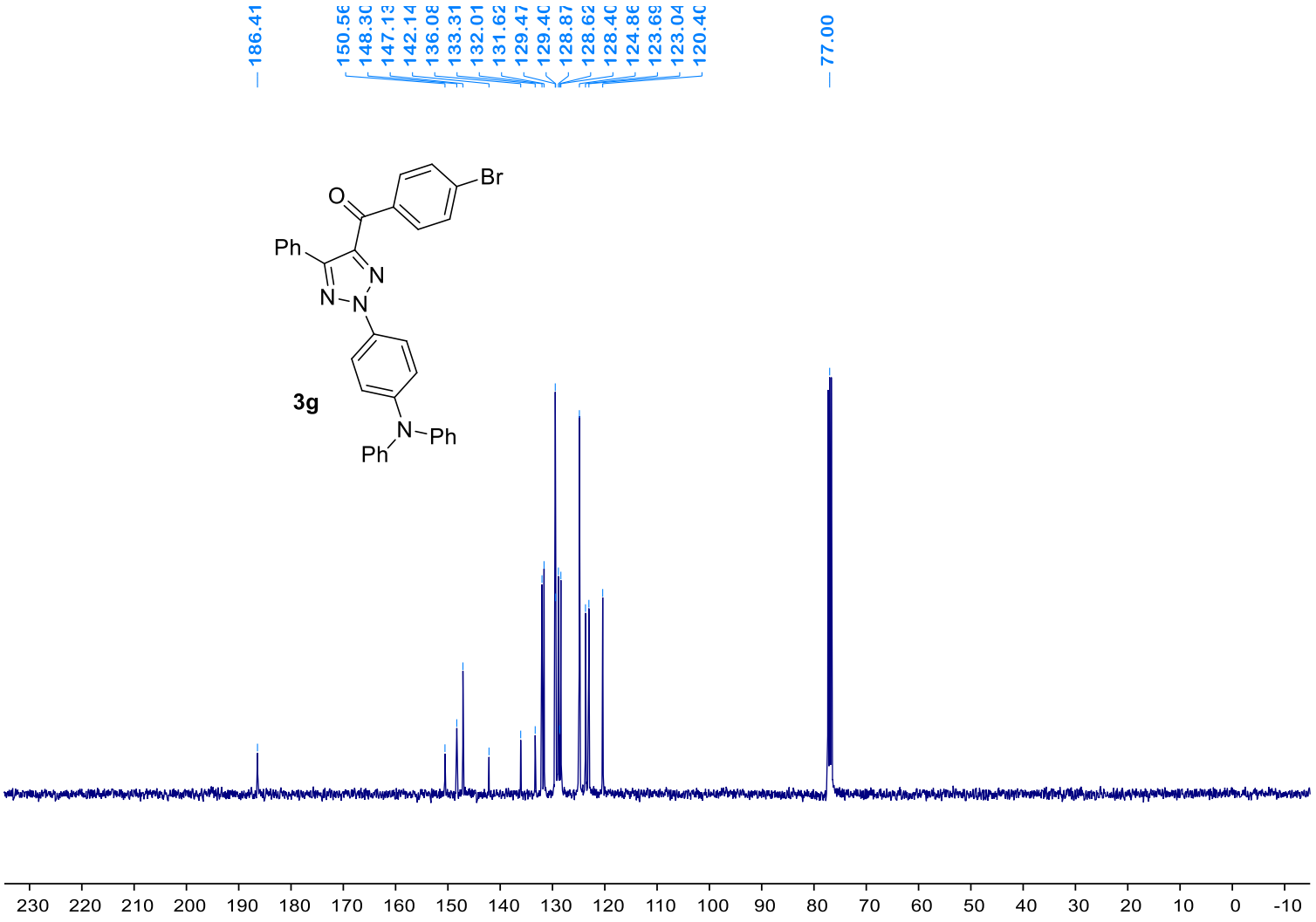
142.19
139.84
135.65
133.33
131.93
129.48
129.40
128.87
128.64
128.41
124.86
123.70
123.06
120.40
77.00
Cl
O
Ph
N
N
N
3f
N
Ph
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

3g ^{1}H NMR


8.05
8.03
8.03
8.00
7.98
7.97
7.92
7.91
7.90
7.90
7.89
7.64
7.62
7.45
7.44
7.31
7.29
7.28
7.25
7.18
7.15
7.13
7.10
7.08
7.06
-0.00
Br
O
Ph
N
N
N
3g
N
Ph
Ph
2.04
2.08
2.00
1.96
3.00
4.10
6.10
2.09
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5

3g ^{13}C NMR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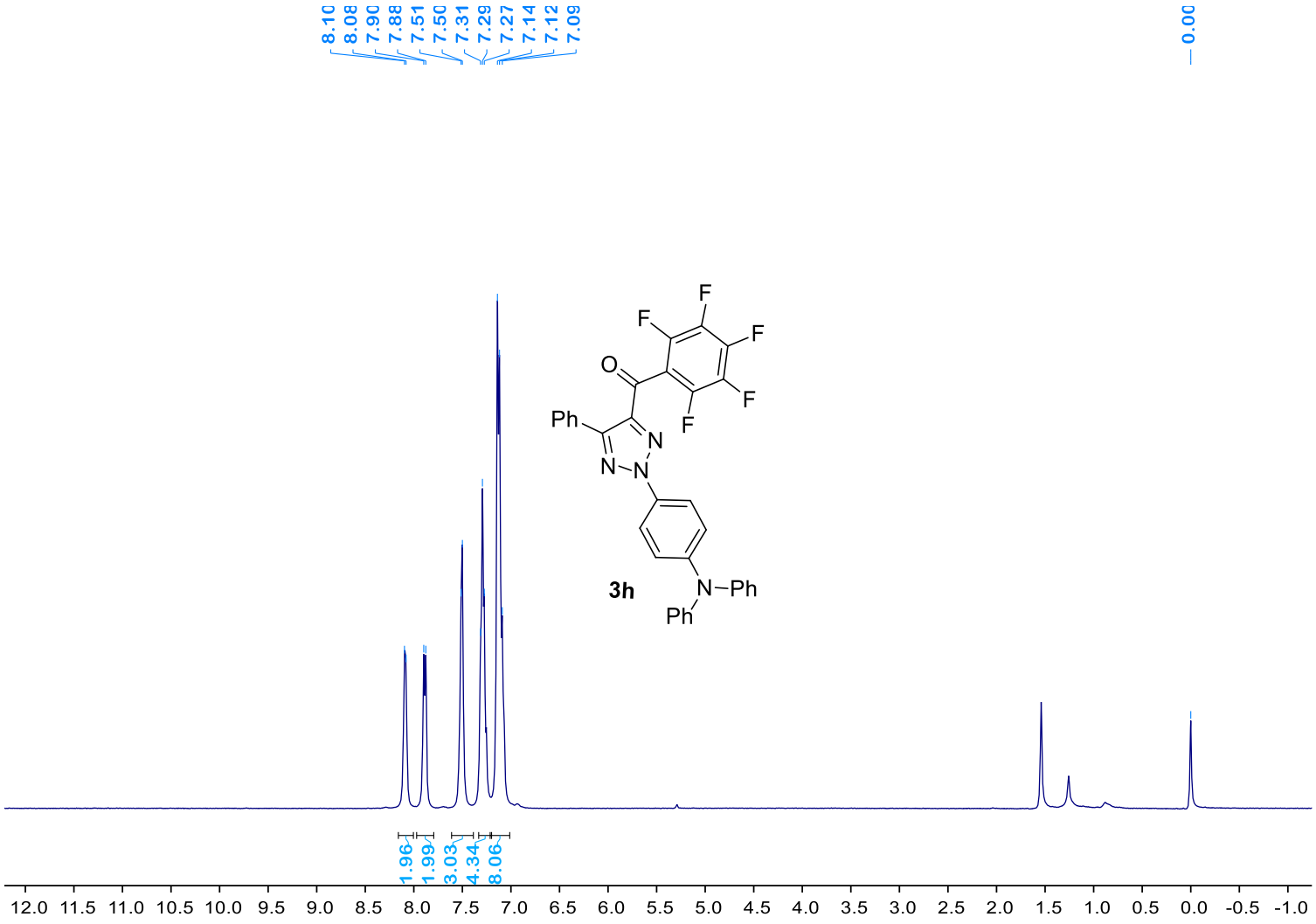
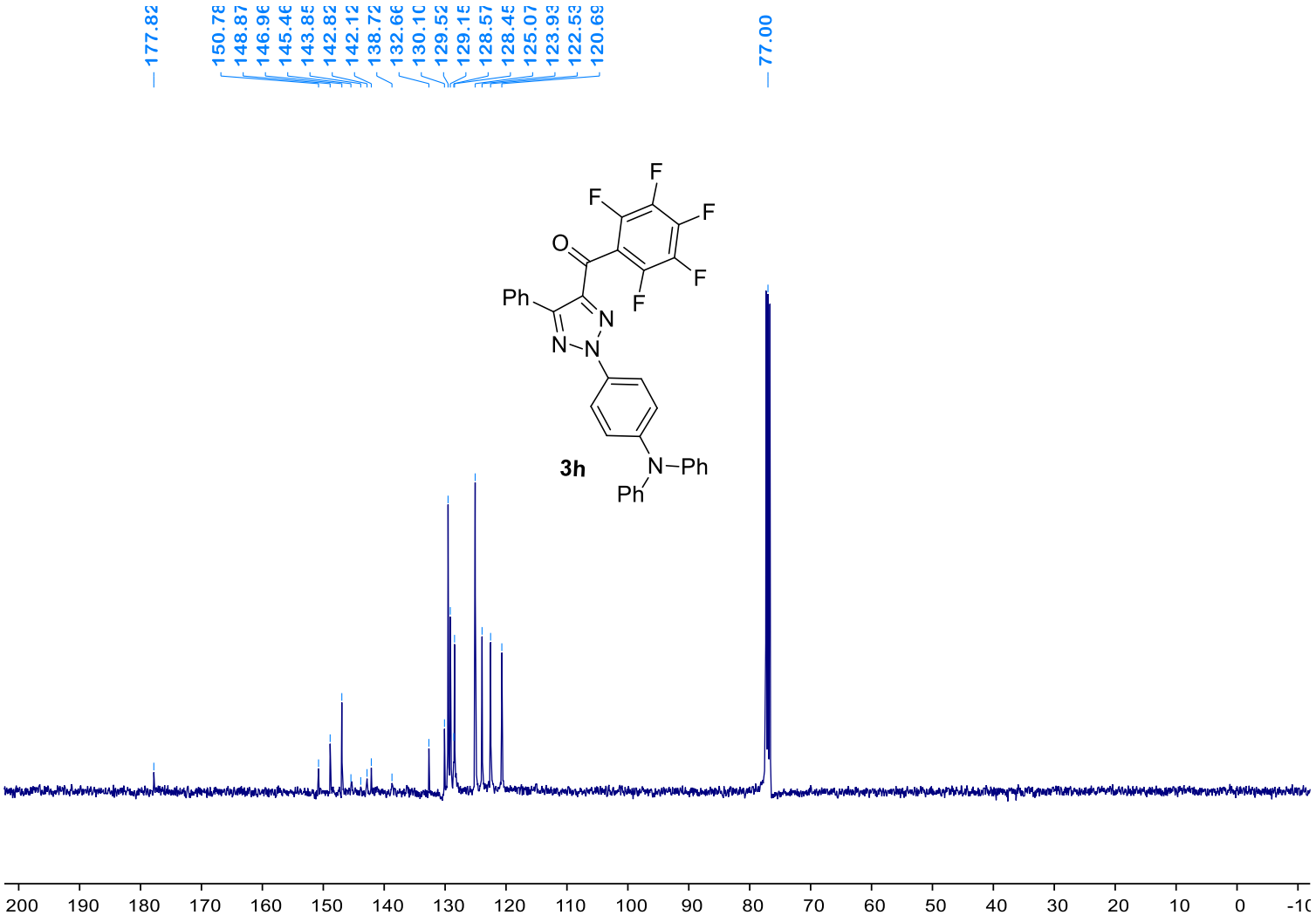
148.30
147.13
142.14
136.08
133.31
132.01
131.62
129.47
129.40
128.87
128.62
128.40
124.86
123.69
123.04
120.40
77.00
Br
O
Ph
N
N
N
3g
N
Ph
Ph
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

3h ^{1}H NMR


8.10
8.08
7.90
7.88
7.51
7.50
7.31
7.29
7.27
7.14
7.12
7.09
0.00
F
F
F
F
F
O
Ph
N
N
N
3h
N–Ph
Ph
1.96
1.99
3.03
4.34
8.06
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

3h ^{13}C NMR


177.82
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146.96
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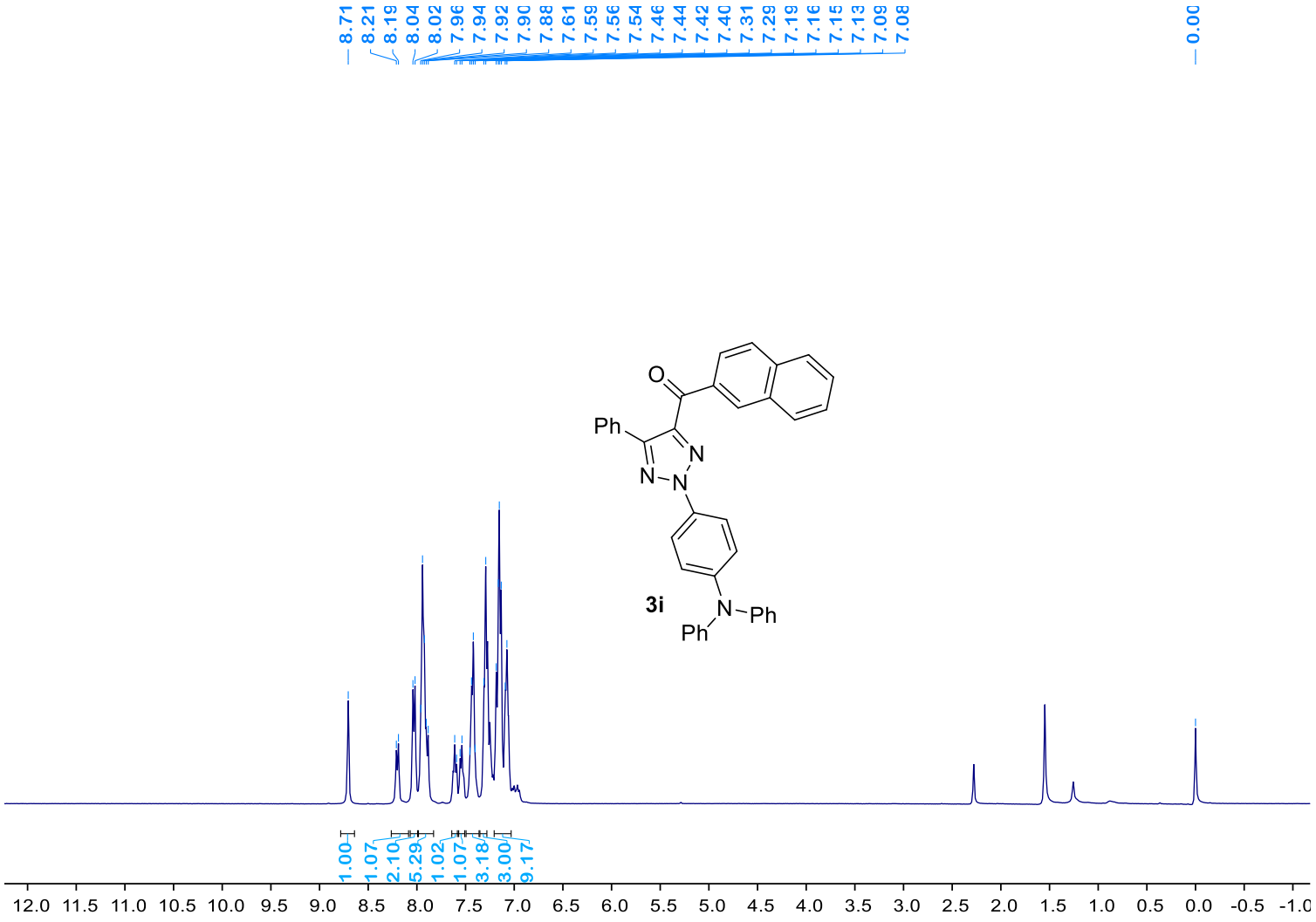
143.85
142.82
142.12
138.72
132.66
130.10
129.52
129.15
128.57
128.45
125.07
123.93
122.53
120.69
77.00
F
F
F
F
F
O
Ph
N
N
N
3h
N–Ph
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

3i ^{1}H NMR


8.71
8.21
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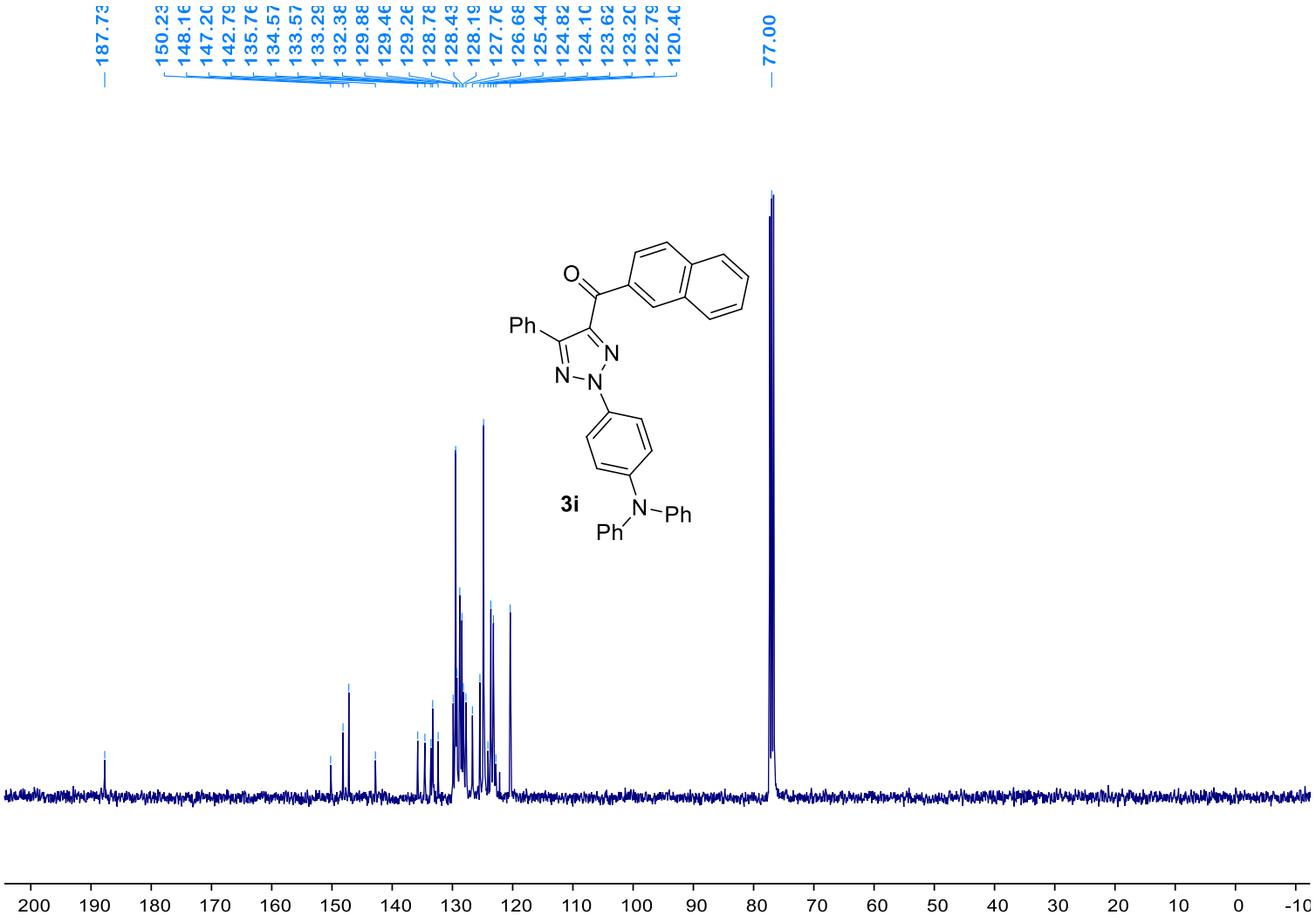
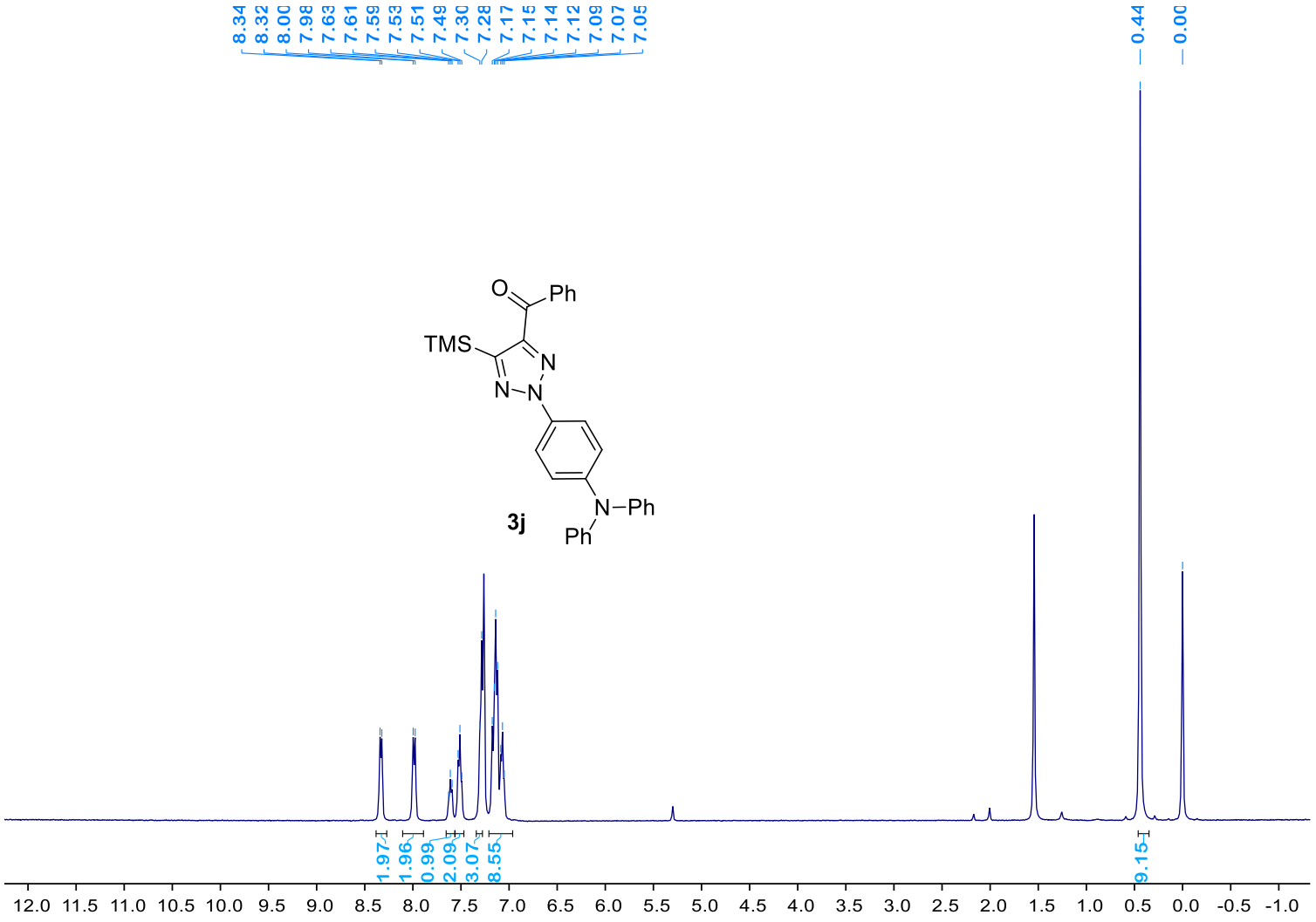
8.04
8.02
7.96
7.94
7.92
7.90
7.88
7.61
7.59
7.56
7.54
7.46
7.44
7.42
7.40
7.31
7.29
7.19
7.16
7.15
7.13
7.09
7.08
0.00
O
Ph
N
N
N
3i
N
Ph
Ph
1.00
1.07
2.10
5.29
1.02
1.07
3.18
3.00
9.17
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

3i ^{13}C NMR


187.73
150.23
148.16
147.20
142.79
135.76
134.57
133.57
133.29
132.38
129.88
129.46
129.26
128.78
128.43
128.19
127.76
126.68
125.44
124.82
124.10
123.62
123.20
122.79
120.40
77.00
O
Ph
N
N
N
3i
N
Ph
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

3j ^{1}H NMR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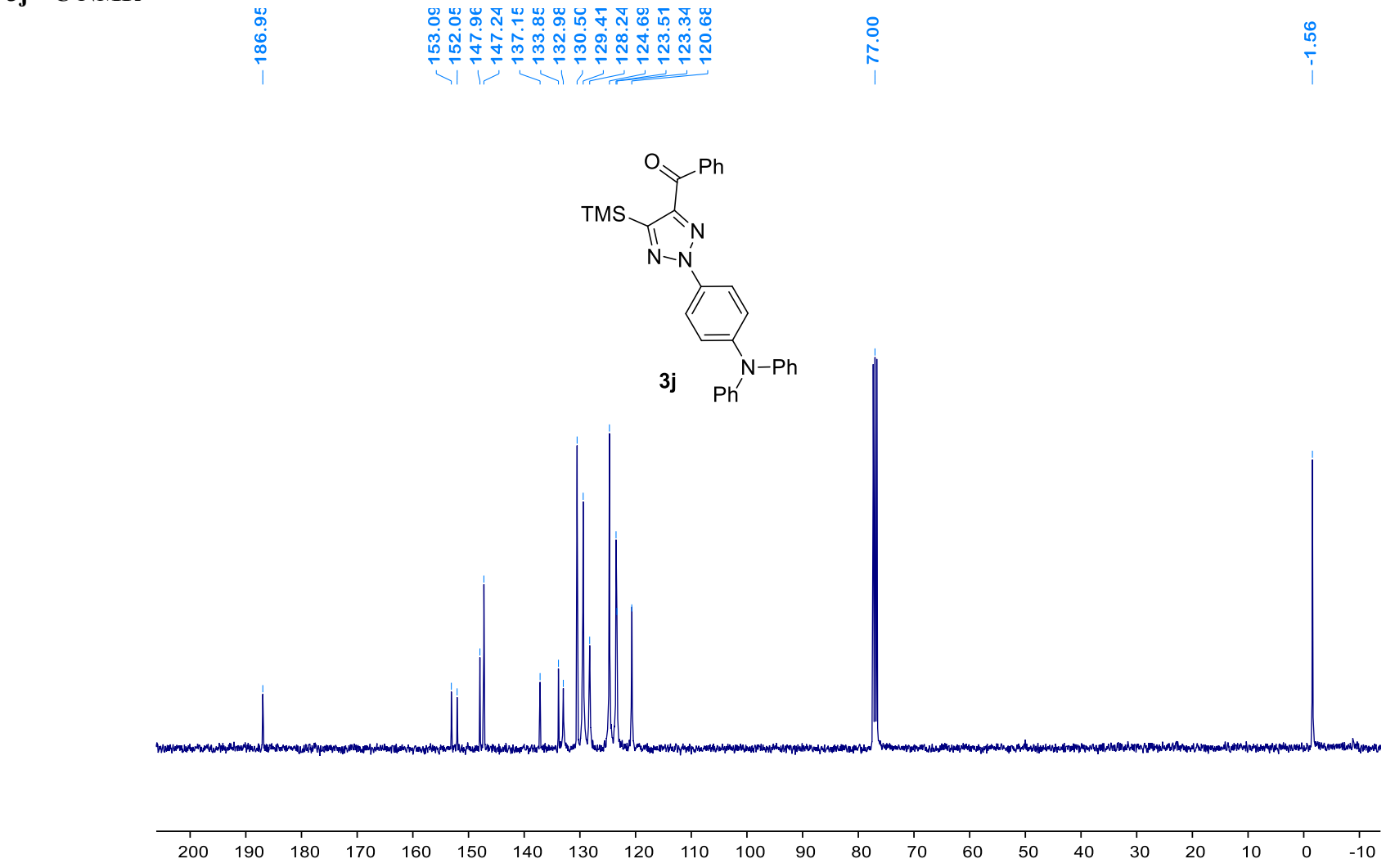
8.32
8.00
7.98
7.63
7.61
7.59
7.53
7.51
7.49
7.30
7.28
7.17
7.15
7.14
7.12
7.09
7.07
7.05
0.44
0.00
O
Ph
TMS
N
N
N
N–Ph
Ph
3j
1.97
1.96
0.99
2.09
3.07
8.55
9.15
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

3j ^{13}C NMR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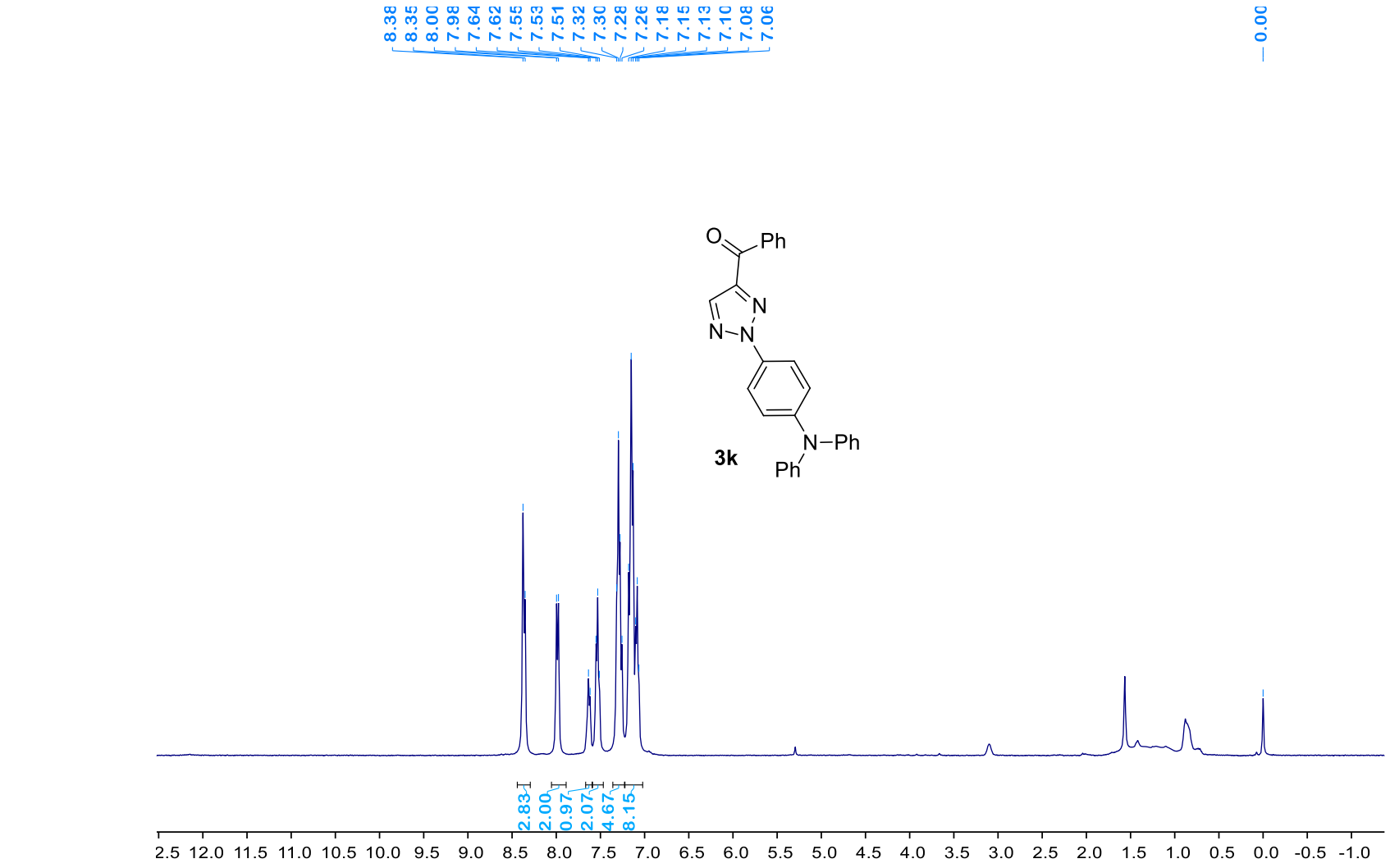
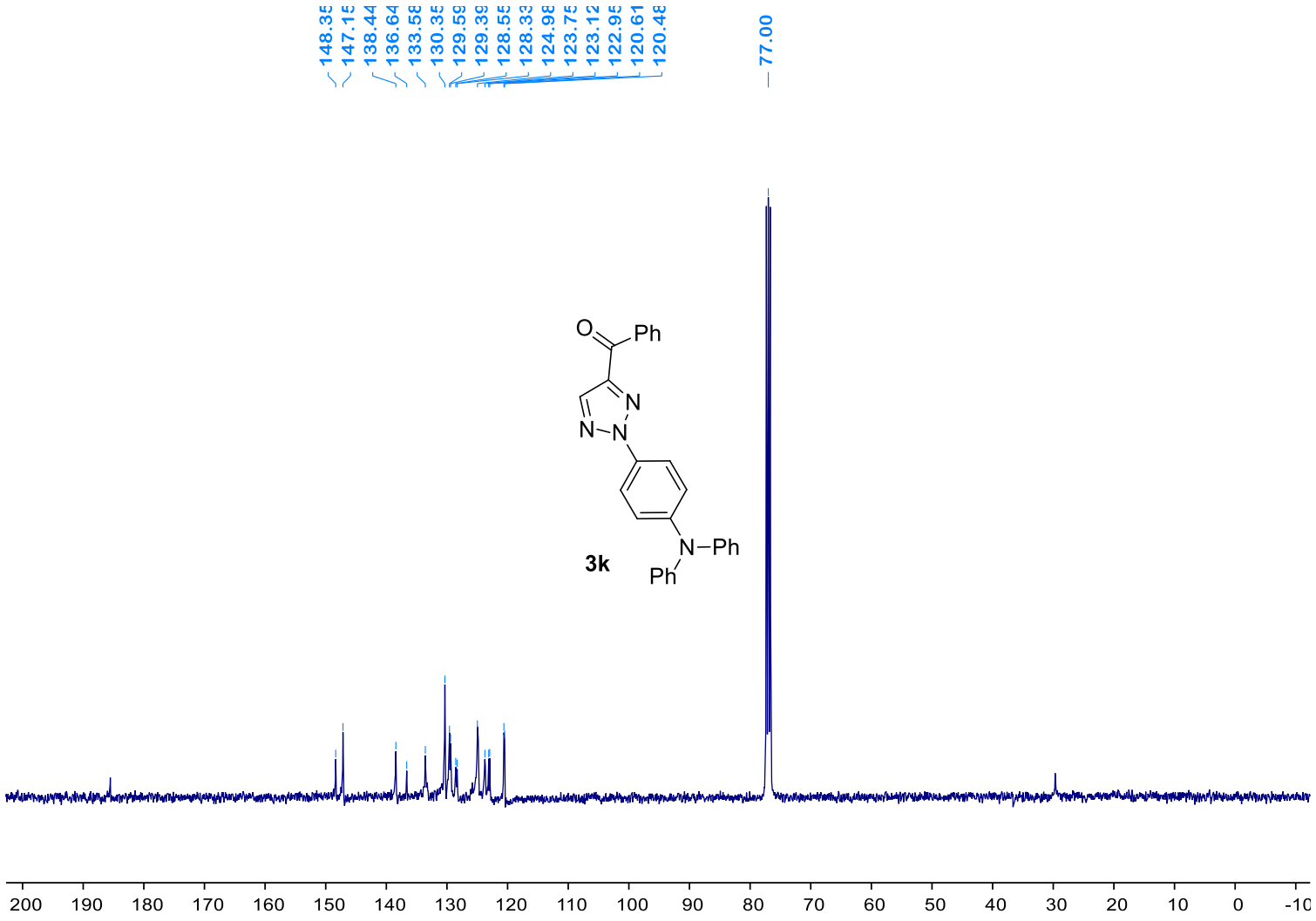
153.09
152.05
147.96
147.24
137.15
133.85
132.98
130.50
129.41
128.24
124.69
123.51
123.34
120.68
77.00
-1.56
O
Ph
TMS
N
N
N
N–Ph
Ph
3j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

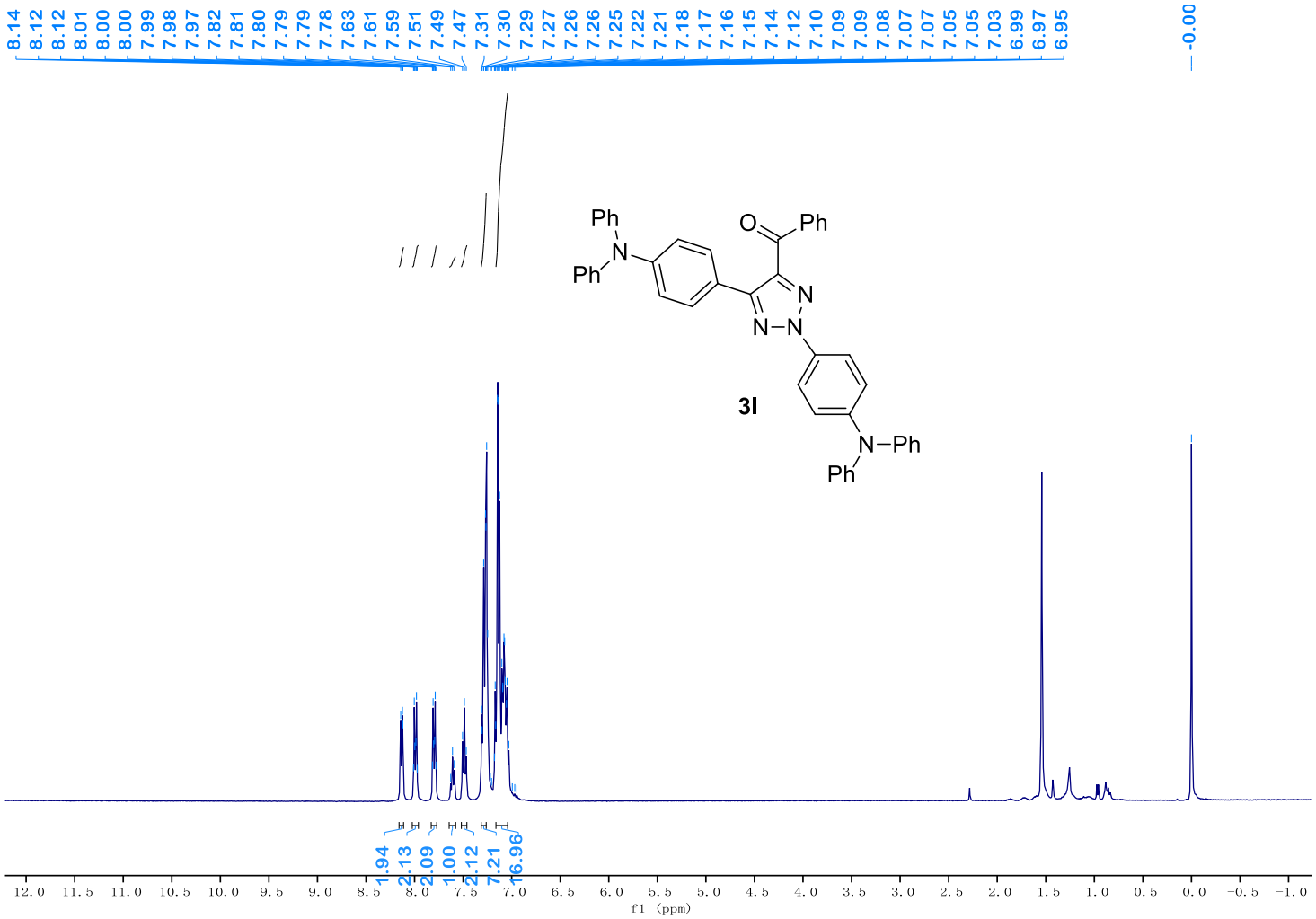
3k ^{1}H NMR


8.38
8.35
8.00
7.98
7.64
7.62
7.55
7.53
7.51
7.32
7.30
7.28
7.26
7.18
7.15
7.13
7.10
7.08
7.06
0.00
O
Ph
N
N
N
N–Ph
Ph
3k
2.83
2.00
0.97
2.07
4.67
8.15
2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

3k ^{13}C NMR


148.35
147.15
138.44
136.64
133.58
130.35
129.59
129.39
128.55
128.33
124.98
123.75
123.12
122.95
120.61
120.48
77.00
O
Ph
N
N
N
N–Ph
Ph
3k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

3l ^{1}H NMR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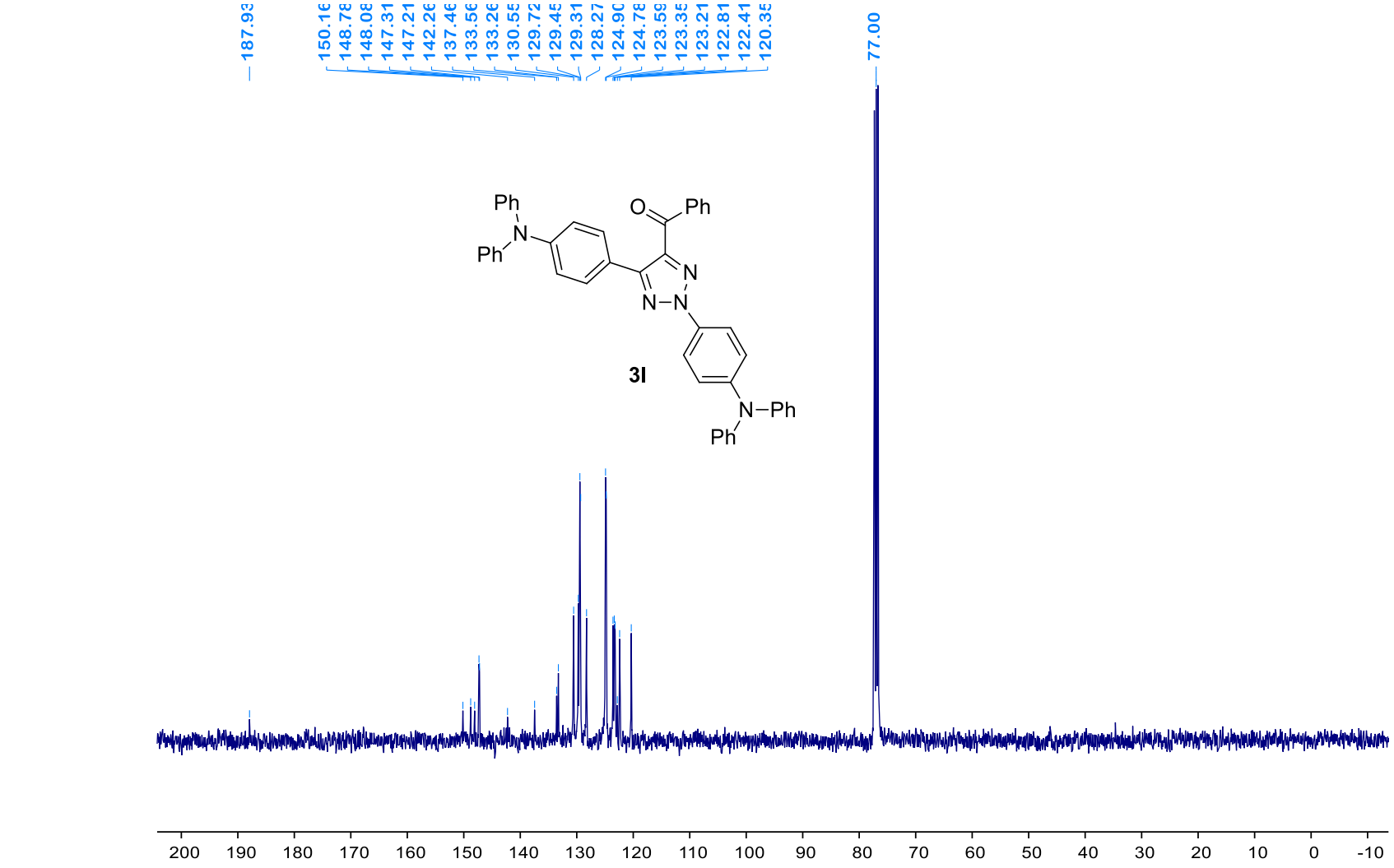
-0.00
Ph
N
Ph
O
Ph
N
N–N
3l
N–Ph
Ph
1.94 2.13 2.09 1.00 2.12 7.21 16.96
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0
f1 (ppm)

3l ^{13}C NMR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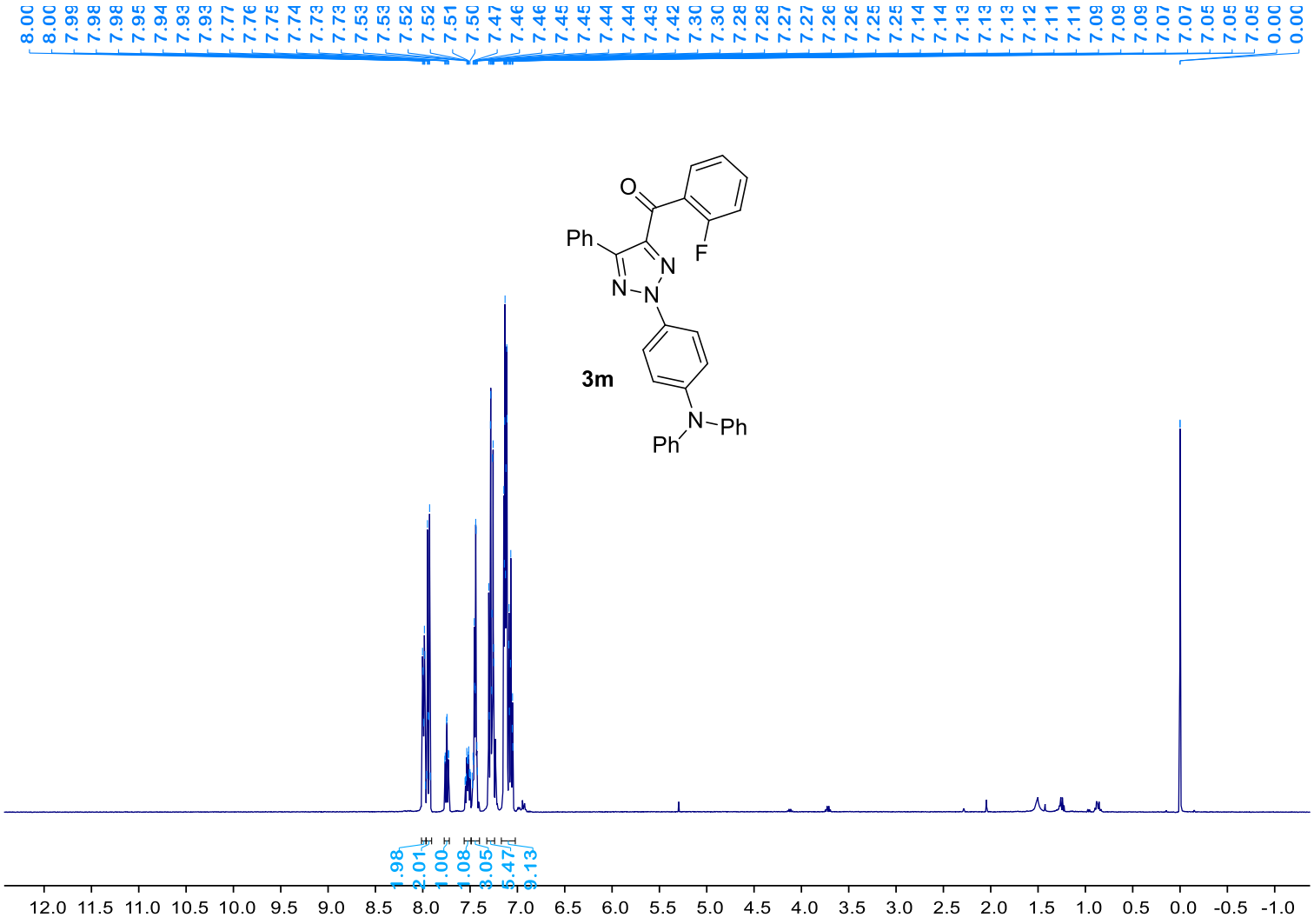
150.16
148.78
148.08
147.31
147.21
142.26
137.46
133.56
133.26
130.55
129.72
129.45
129.31
128.27
124.90
124.78
123.59
123.35
123.21
122.81
122.41
120.35
77.00
Ph
N
Ph
O
Ph
N
N–N
N–Ph
Ph
3l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

3m ^{1}H NMR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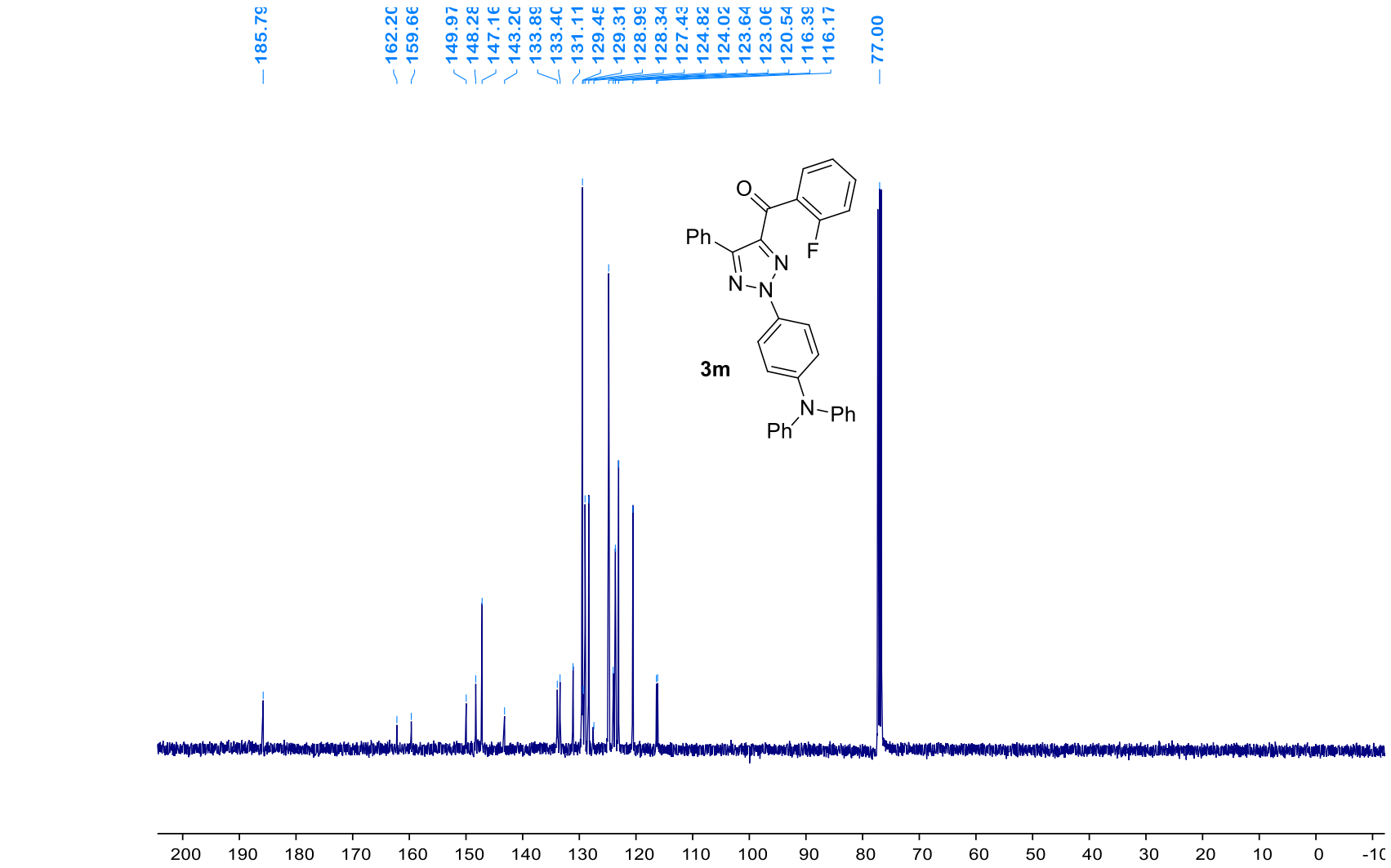
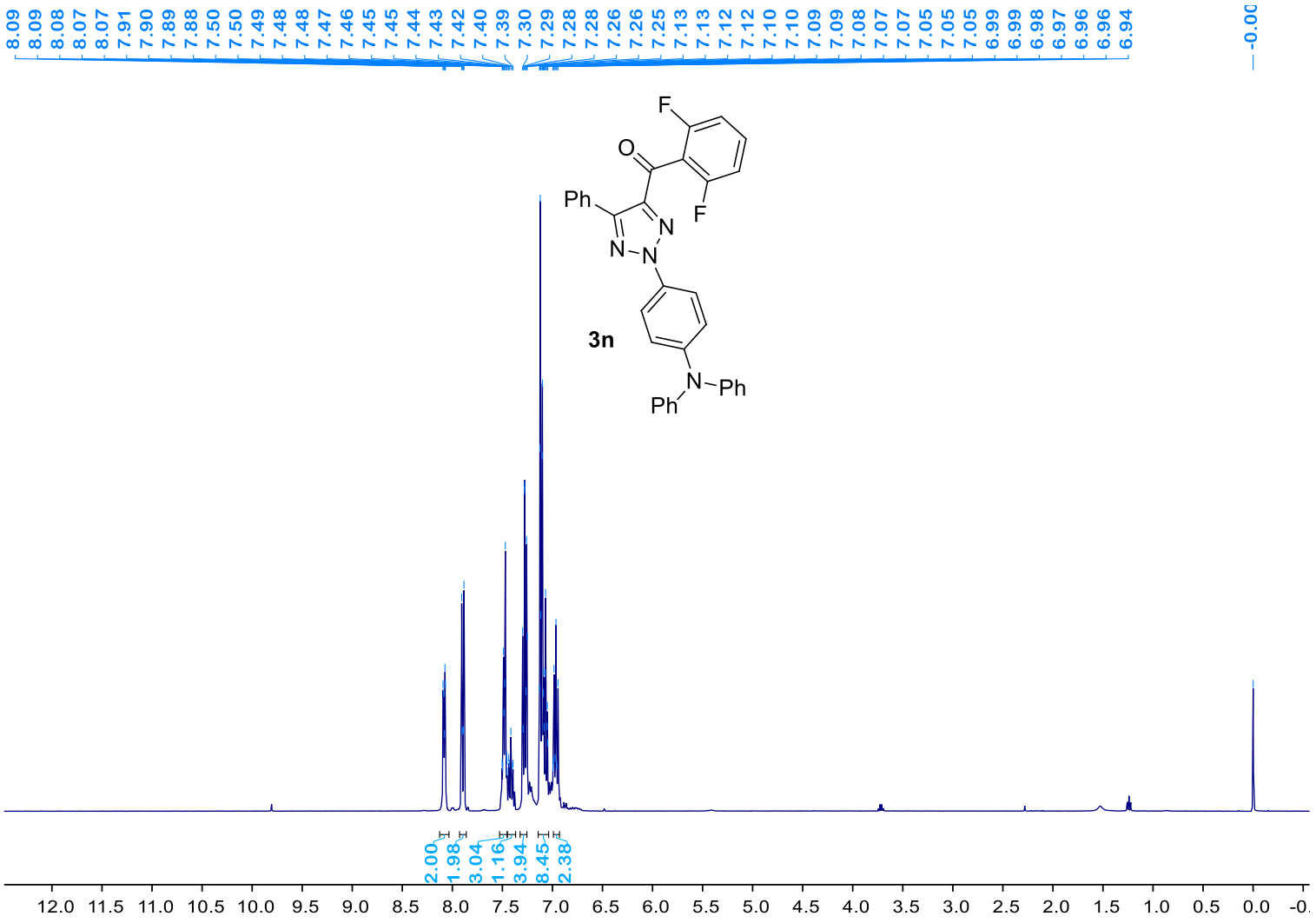
O
Ph
F
N
N
N
3m
N
Ph
Ph
1.98 2.01 1.00 1.08 3.05 5.47 9.13
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

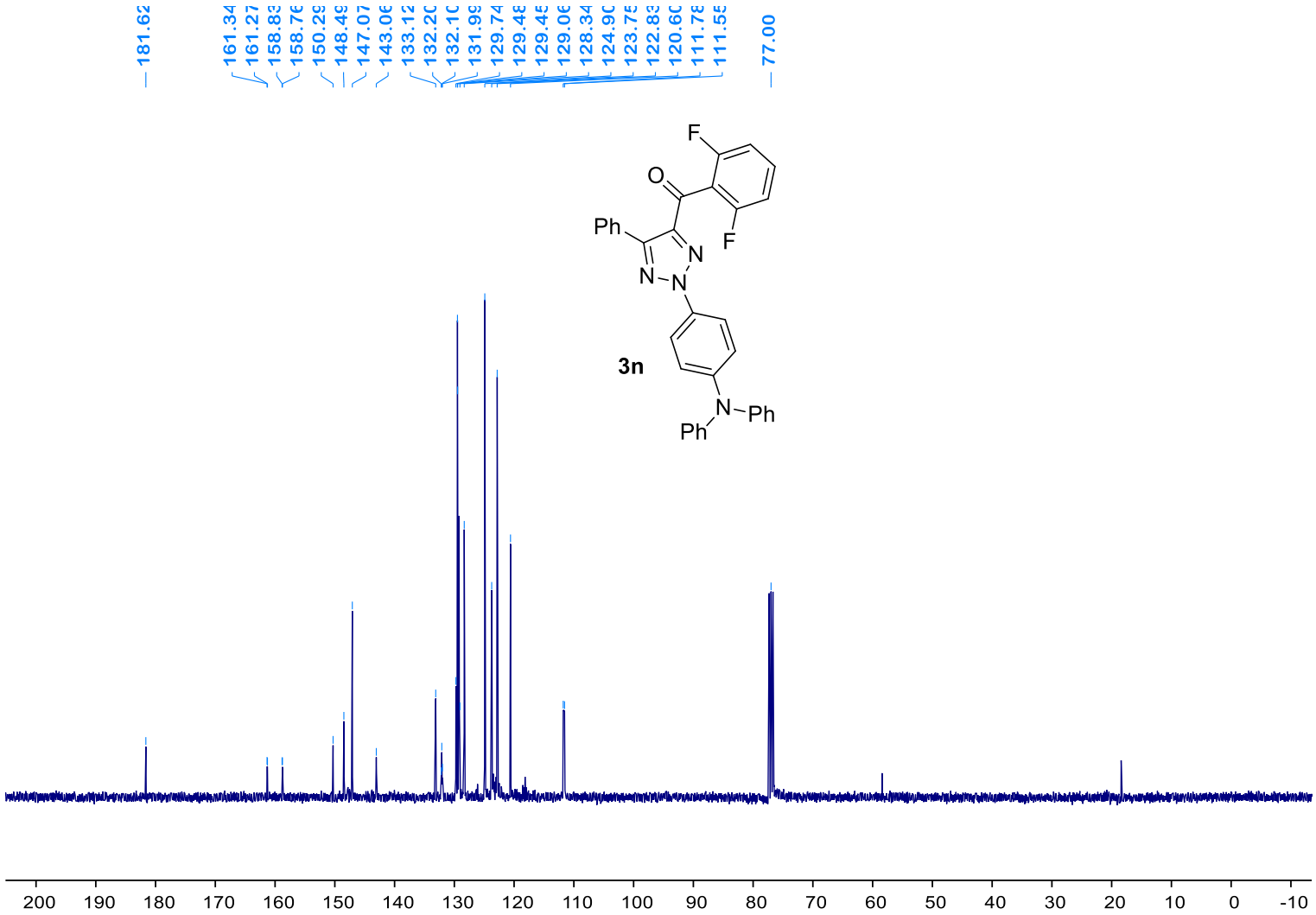
3m ^{13}C NMR


185.79
162.20
159.66
149.97
148.28
147.16
143.20
133.89
133.40
131.11
129.45
129.31
128.99
128.34
127.43
124.82
124.02
123.64
123.06
120.54
116.39
116.17
77.00
O
Ph
F
N
N
N
3m
N
Ph
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

3n ^{1}H NMR


8.09 8.09 8.08 8.07 8.07 7.91 7.90 7.89 7.88 7.50 7.50 7.49 7.48 7.48 7.47 7.46 7.45 7.45 7.44 7.43 7.42 7.40 7.39 7.30 7.29 7.28 7.28 7.26 7.26 7.25 7.13 7.13 7.12 7.12 7.10 7.10 7.09 7.09 7.08 7.07 7.07 7.05 7.05 7.05 6.99 6.99 6.98 6.97 6.96 6.96 6.94
-0.00
F
O
F
Ph
N
N
N
3n
N
Ph
Ph
2.00 1.98 3.04 1.16 3.94 8.45 2.38
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.

3n ^{13}C NMR


181.62
161.34
161.27
158.83
158.76
150.29
148.49
147.07
143.06
133.12
132.20
132.10
131.99
129.74
129.48
129.45
129.06
128.34
124.90
123.75
122.83
120.60
111.78
111.55
77.00
F
O
Ph
F
N
N
N
3n
N
Ph
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10