Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
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Supporting Information

Triazole-Imidazole (TA-IM) as Ultrafast Fluorescent Probes for Selective Ag^+ Detection

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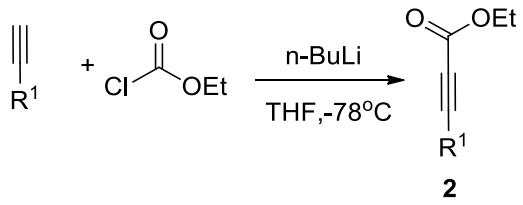
I. General Methods and Materials

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 (250μ) 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 2a-2c

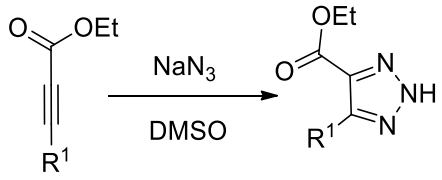


2

n-BuLi (2.5M in Hexane solution) (9.53 mL, 23.835 mmol) was slowly added to the R^1-alkynes (22 mmol) in 22 ml dry THF at -78℃. After stirred at -78℃ for 1h, cathyl chloride (27.24 mmol, 2.53 mL) was added to the system. The reaction was monitored by TLC. After reaction completion, saturated NH_4Cl (15 mL) was introduced in order to quench the reaction at room temperature. The aqueous layer was extracted with Ethyl

Acetate (EA). Organic phase was dried with anhydrous sodium sulfate and purified products **2a**-**2c** by silica gel column chromatography (Hexane and EA).

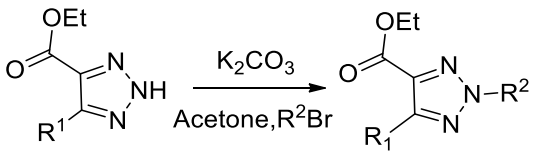
1.2 General procedure to synthesize 3a-3d



2 **3**

R^1-propiolic Acid Ethyl Ester **2** (15.4 mmol) was dissolved in 100 mL DMSO. After stirring, NaN_3 (2.8 g, 43.05 mmol) was slowly added to the mixture and refluxed for 6 h under 60 ℃. 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. Compound **3** was purified by silica gel column chromatography (Hexane and EA) to isolate the pure products **3a-3d.**

1.3 General procedure to synthesize 3Xa-3Xe

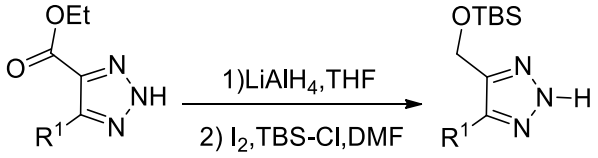


3 **3X**

Triazole **3a-3d** (1 mmol), 6 mL of acetone, the anhydrous potassium carbonate (2 mmol) and benzyl bromide (1.5 mmol) were successively join to 50 mL round bottom flask. Under the protection of nitrogen, the mixture was stirred at room temperature 12 h until raw material disappeared by TLC monitoring the reaction. The mixture was filtered to remove chloride anhydrous potassium carbonate and washed residue for three

times. We preserved the filtrate with purification by column chromatography. (Hexane and EA) to isolate the pure products **3Xa-3Xe.**

1.4 General procedure to synthesize 3Y

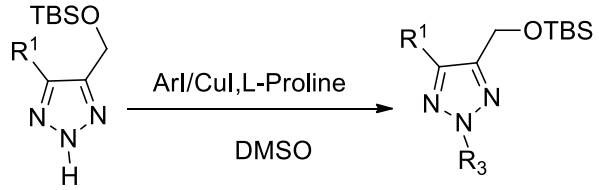


3 **3Y**

3 (3 mmol) was dissolved in 30 mL dry THF, $LiAlH_4$ (4.5 mmol) was added under 0 ^oC and the mixture was stirred for 5-6 h at room temperature until full conversion was reached (monitored by TLC). The THF was removed by vacuum distillation. Then 6 M HCl was added to the mixture until pH=2. After the aqueous layer was extracted with EA, organic layer was dried by anhydrous $NaSO_4$. The solvent was removed by rotary evaporator. Product directly be used in next step without further purification.

The alcohol (3 mmol, 1.0 equiv.) and TBS-Cl (15 mmol, 3.0 equiv, according to limiting reagent), I_2 (6 mmol, 2.0 equiv.) were dissolved in 3 mL dry DMF and the reaction was run at room temperature overnight. After reaction completion, the solvent was removed by rotary evaporator, the mixture was subjected to the silica gel column chromatography (Hexane and EA) to isolate the pure products **3Ya-3Yb.**

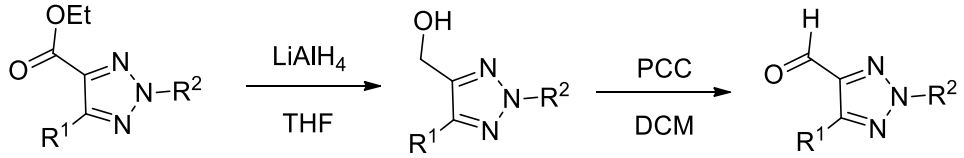
1.5 General procedure to synthesize 3Z



3Y **3Z**

3Y (4 mmol, 1.0 equiv), K_2CO_3 (8 mmol,2.0 equiv), CuI (0. 4 mmol, 0.1 equiv), L-proline (0.8 mmol,0.2 equiv), and ArI (6 mmol, 1.5 equiv) was successively added to 10 mL vial under N_2. Then anhydrous DMSO (20 mL) was added by syringes. The tube was heated to 110 ^oC for 12 h. After cooling to the room temperature. The reaction mixture was added water (15 mL) and saturated NH_4Cl solution (5 mL). Then the aqueous layer was extracted with ethyl acetate (2x15 mL). The combined organic phases were washed with brine (10 mL), dried by anhydrous Na_2SO_4 and concentrated in vacuum. The mixture was subjected to the silica gel column chromatography (Hexane: EA=8:1) to isolate the pure products **3Za-3Zc.**

1.6 General procedure to synthesize 4 (R^2=alkyl: Condition B)

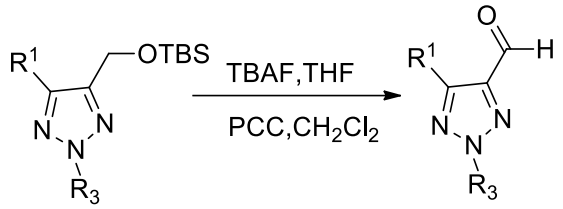


3X **4**

3X (3 mmol) was dissolved in 30 mL dry THF, $LiAlH_4$ (4.5 mmol) was added and the mixture was stirred for 5-6 h at room temperature until full conversion was reached (monitored by TLC). The THF was removed by vacuum distillation. Then 6 M HCl was added to the mixture until pH=2. After the aqueous layer was extracted with EA, organic layer was dried by anhydrous $NaSO_4$. The solvent was removed by rotary evaporator. Product directly be used in next step without further purification.

Triazole alcohol (3 mmol, 1.0 equiv) was dissolved in dry DCM (15 mL), then PCC (10 mmol) was added to the mixture, and the mixture was stirred for 4-5 h at room temperature until full conversion was reached (monitored by TLC). After reaction completion, the solvent was removed by rotary evaporator, the mixture was subjected to the silica gel column chromatography (Hexane:EA=6:1) to isolate the pure products **4a-4e**.

1.7 General procedure to synthesize 4 (R^2=aryl: Condition C)

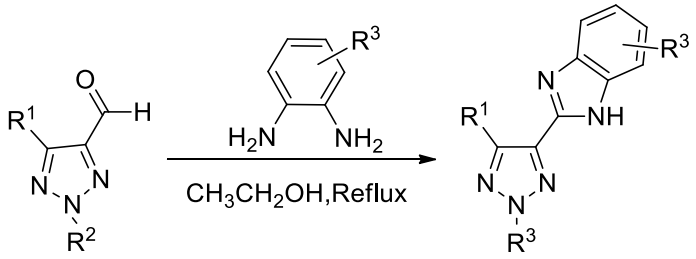


3Z **4**

3Z (3.0 mmol, 1.0 equiv) was dissolved in 30 mL dry THF, TBAF (4.5 mmol, 1.5 equiv) was added. The mixture was stirred for 0.5-1h at room temperature until full conversion was reached (monitored by TLC). The THF was removed by vacuum distillation. Then added aqueous. After the aqueous layer was extracted with EA, organic layer was dried by anhydrous $NaSO_4$. The solvent was removed by rotary evaporator. Product directly be used in next step without further purification.

The alcohol (3 mmol, 1.0 equiv) was dissolved in dry DCM (15 mL, 0.2 M), then PCC (10 mmol, 3.3 equiv) was added to the mixture, and the mixture was stirred for 4-5 h at room temperature until full conversion was reached (monitored by TLC). After reaction completion, the solvent was removed by rotary evaporator, the mixture was subjected to the silica gel column chromatography (Hexane and EA) to isolate the pure products **4f-4h.**

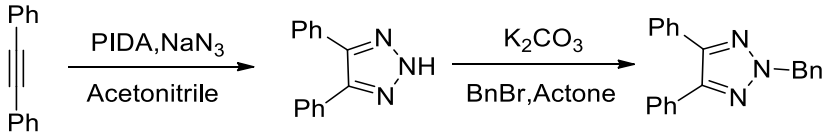
1.8 Procedure to synthesize 5



4 **5**

A 50 mL screwed vial was charged with the aldehyde **4** (2 mmol, 1.0 equiv), 1,2-diaminobenzene (2 mmol, 1.0 equiv) in 1 mL CH_3CH_2OH. The reaction was run at 60 ^oC for 4 h. Then another 15 mL CH_3CH_2OH was added to the vial and the reaction was run at 90 ^oC for 12h. After the reaction was completed, the solvent was removed under reduced pressure and the residue was purified by flash chromatography on silica gel to give desired triazole-imidazole product **5a-5k**.

1.9 Procedure to synthesize 6a



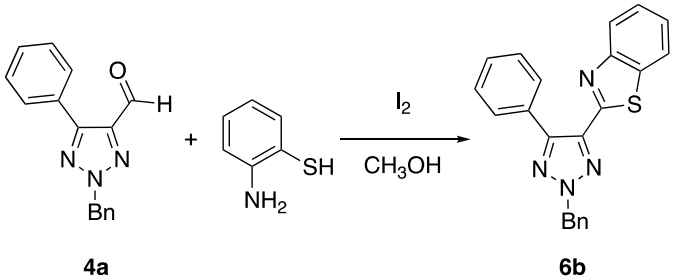
4,5-diphenyl-2*H*-1,2,3-triazole **6a**

4,5-diphenyl-2H-1,2,3-triazole was synthesized by the literature:

[1] W. M. Yan, Q. Y. Wang, Q. Lin, M. Y. Li, J. L. Petersen and X. D. Shi, *Chem. Eur. J.* 2011, ***17***, 5011-5018.

4,5-diphenyl-2H-1,2,3-triazole (2 mmol, 1.0 equiv) was dissolved in Acetone 12 mL, after that the anhydrous K_2CO_3 (4 mmol, 2.0 equiv) and R^2Br (3.0 mmol, 1.5 equiv) was added and the mixture was stirred for 12 h at 30 ^oC until full conversion was reached (monitored by TLC). After reaction completion, the solvent was removed by rotary evaporator, the mixture was subjected to the silica gel column chromatography (Hexane: EA=5:1) to isolate the pure products **6a.**

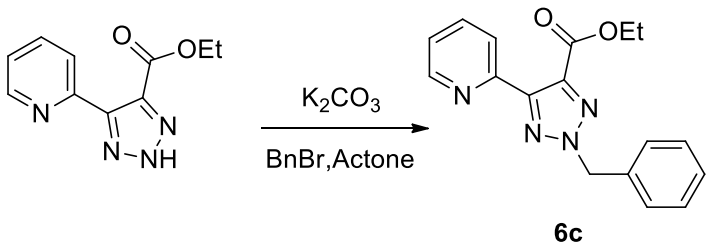
1.10 Procedure to synthesize 6b



4a **6b**

A 50 mL vial was charged with the triazole aldehyde substrate **4a** (2 mmol, 1.0 equiv), 2-aminobenzenethiol (2 mmol, 218 mg, 1.0 equiv) in anhydrous CH_3OH (20 mL, 0.1 M) and I_2 (1 mmol, 252 mg, 1.0 equiv). And the reaction was run at 30 ^oC for 3-4 h. After the reaction was completed, the solvent was removed under reduced pressure and the mixture was subjected to the silica gel column chromatography (Hexane: EA=5:1) to give desired 1,2,3-triazol-thiazole product **6b**.

1.11 Procedure to synthesize 6c



6c

Ethyl 5-(pyridin-2-yl)-2H-1,2,3-triazole-4-carboxylate was synthesized according the following literature, see:

[2] Q. Q. Hu, Y. Liu, X. C. Deng, Y. J. Li and Y. F. Chen, *Adv. Synth. Catal.* 2016, ***358***, 1689-1693.

Ethyl 5-(pyridin-2-yl)-2H-1,2,3-triazole-4-carboxylate (1 mmol, 1.0 equiv) was dissolved in Acetone 6 mL, after that the anhydrous K_2CO_3 (2 mmol, 2.0 equiv) and R^2Br (1.5 mmol, 1.5 equiv) was added and the mixture was stirred for 12 h at 30 ^oC until full conversion was reached (monitored by TLC). After reaction completion, the solvent was removed by rotary evaporator, the mixture was subjected to the silica gel column chromatography (Hexane: EA=2:1) to isolate the pure products **6c.**

II. Fluorescence property

Fluorescence detection Procedures: A series of stock solution of compound 1,2,3-triazoel **(TA)** (0.2 mmol/L) was prepared by dissolving the corresponding amount of compound powder in ethanol in a 100 mL volumetric flask, which was stored in the dark. For fluorescence detection, 200 μL stock solutions (0.2 mmol/L) were diluted with 1800 μL ethanol in the sample tubes. The fluorescence spectra of mixed solutions were recorded in the 300-600 nm emission wavelength range with the corresponding excitation wavelength at room temperature (298 K) by F-2700 spectrofluorophotometer (HITACHI Co., Ltd., Japan). The entrance slit and exit slit were set at 2.5 nm and 5 nm for the fluorescent determinations, respectively.

UV-vis absorption detection Procedures: 200 μL stock solutions (0.2 mmol/L) were diluted with 800 μL ethanol in the sample tubes. UV-vis absorption spectra of mixed solutions were obtained in the 200-800 nm wavelength by UV-3100 UV-VISNIR recording spectrophotometer (Shimadzu, Japan).

Quantum yield determination: All the quantum yields of samples were determined by EI Fluorescence Spectroscopy-FLS 980, the sample was dissolved in EtOH, concentration was 0.2 mmol/L.

2.1 The fluorescence intensity of 1b with addition of various metal ions

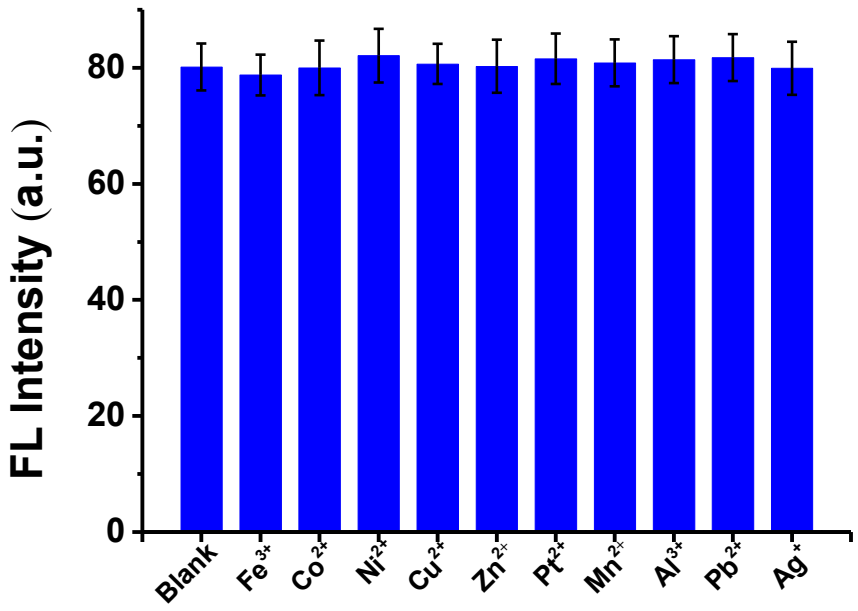


Figure S1. The fluorescence intensity of **1b** with addition of various metal ions. Concentration: **1b**, 2.0 μmol/L; metal ions, 2.0 μmol/L.

2.2 The fluorescence emission of 5a-5d

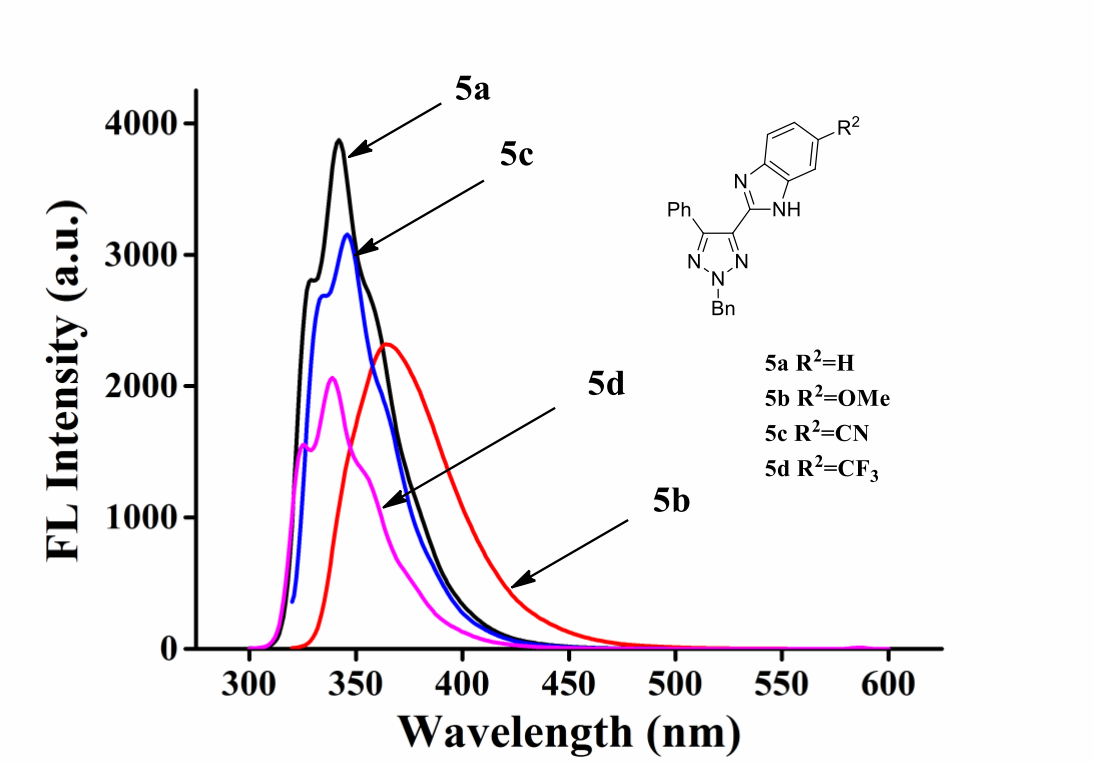


Figure S2. Fluorescence emission of compound **5a-5d**. Concentration: 20 μmol/L in EtOH.

Table S1. Comparison of optical properties of **5a-5d**.

Compound	Absorption (nm)	Excitation (λmax)	Emission (λmax)	Stokes Shift (nm)	Φ_{PL} (%)
5a	250 (0.948), 291 (0.794)	290	343	52	77
5b	250 (0.798), 310 (0.716)	310	364	54	64
5c	309 (0.774)	309	246	37	45
5d	250 (0.930), 298 (0.744)	293	329	36	41

2.3 The fluorescence emission of 5e-5h

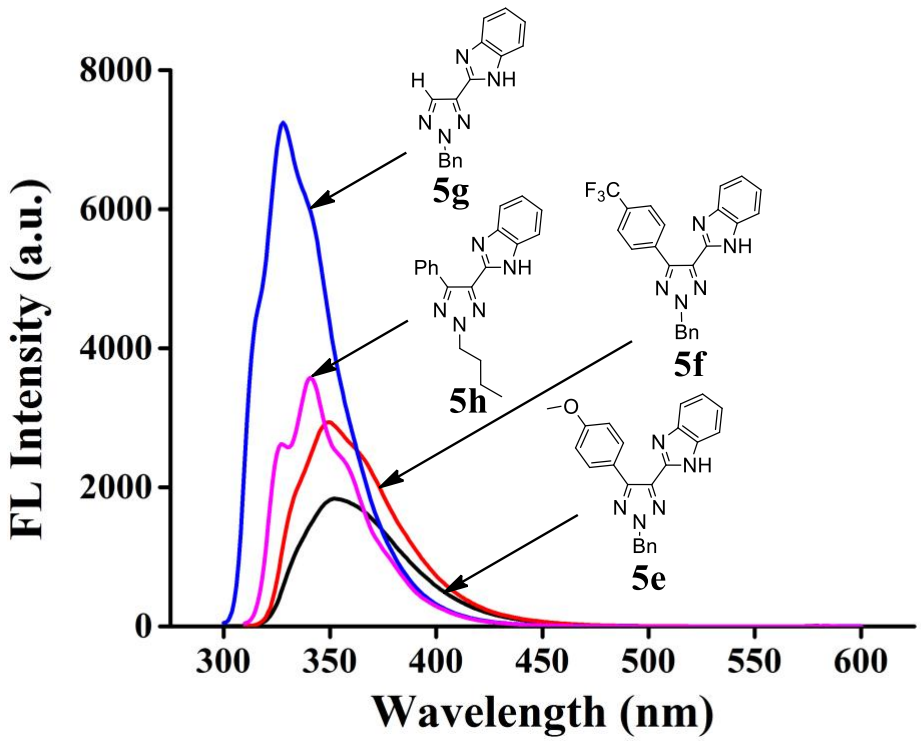


Figure S3. Fluorescence emission of compound **5e-5h.** Concentration: 20 μmol/L in EtOH.

Table S2. Comparison of optical properties of **5e-5h**.

Compound	Absorption (nm)	Excitation (λmax)	Emission (λmax)	Stokes Shift (nm)	Φ_{PL} (%)
5e	261 (0.903), 289 (0.710)	290	353	62	64
5f	252 (0.657), 294 (0.645)	293	349	56	86
5g	294 (1.046), 307 (0.828)	296	328	32	98
5h	250 (0.762), 292 (0.657)	292	341	49	72

2.4 The fluorescence emission of 5i-5k

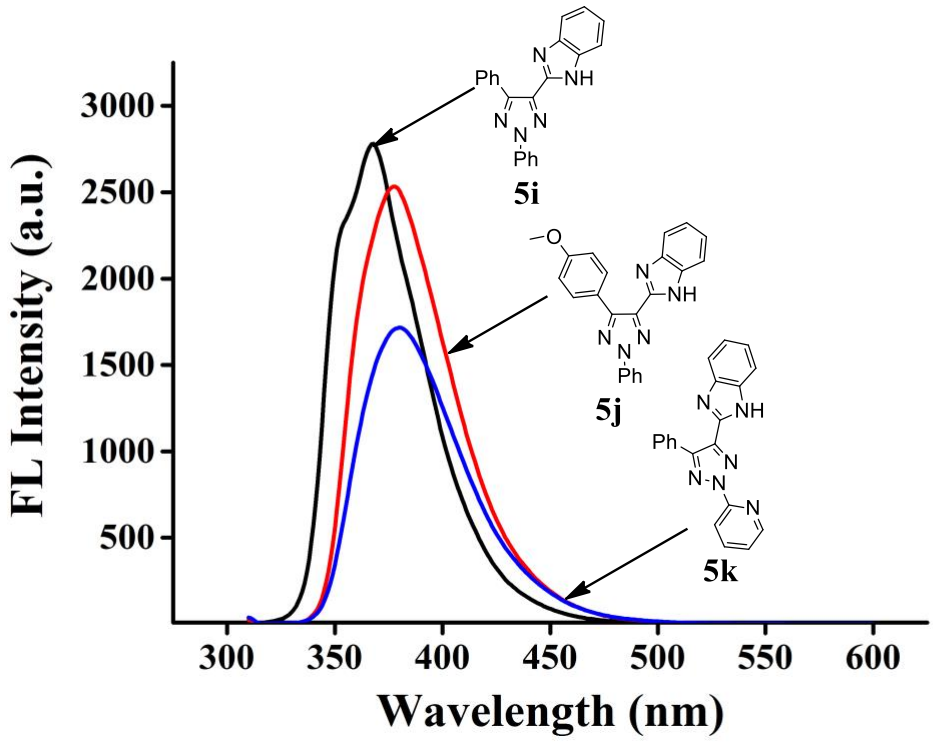


Figure S4. Fluorescence emission of compound **5i-5k**. Concentration: 20 μmol/L in EtOH.

Table S3. Comparison of optical properties of **5i-5k**.

Compound	Absorption (nm)	Excitation (λmax)	Emission (λmax)	Stokes Shift (nm)	Φ_{PL} (%)
5i	289 (0.734)	291	368	77	93
5j	250 (0.640), 307 (1.042)	309	378	69	66
5k	308 (0.903)	309	380	71	54

2.5 The fluorescence emission of 6a-6c

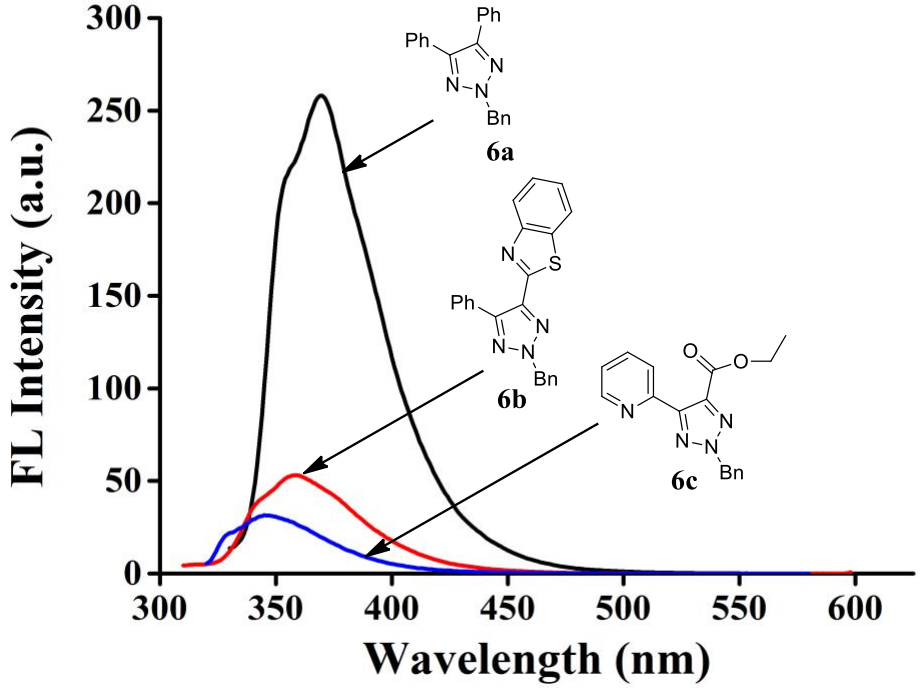


Figure S5. Fluorescence emission of compound **6a-6c**. Concentration: 20 μmol/L in EtOH.

Table S4. Comparison of optical properties of 6a-6c.

Compound	Absorption (nm)	Excitation (λmax)	Emission (λmax)	Stokes Shift (nm)	Φ_{PL} (%)
6a	257 (0.732)	317	370	53	44
6b	221 (1.273), 254 (0.785), 302 (0.666)	-	-	-	-
6c	263 (0.0215), 270 (0.0211)	-	-	-	-

III.TA-IM 5a as Ag^+ sensor

Procedures for the determination of Ag(I): For Ag(I) determination, the solutions were added to a sample tube in the following sequence with a total volume of 2 mL: 20 μL of **5a** stock solution (0.2 mmol/L), HEPES buffer solution (1.0 mmol/L, pH 7.0), 30 μL of different amounts of Ag(I). And then the mixture was mixed thoroughly and stood for 1 min before detection. The fluorescence spectra were recorded in the 300-500 nm emission wavelength range with an excitation wavelength of 290 nm. The entrance slit and exit slit were both set at 5 nm. All measurements were performed at room temperature (298 K).

3.1 The stability of 5a

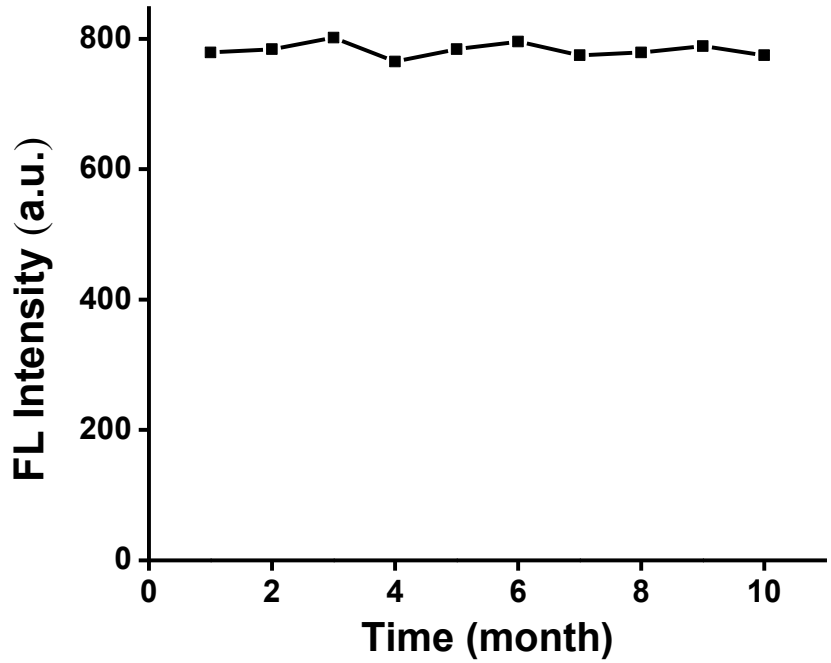


Figure S6. The stability of **5a**. Concentration: 5a, 2 μmol/L. EtOH: Hepes, v:v=1:99.

3.2 The anions selectivity and competition of 5a for Ag^+ assay.

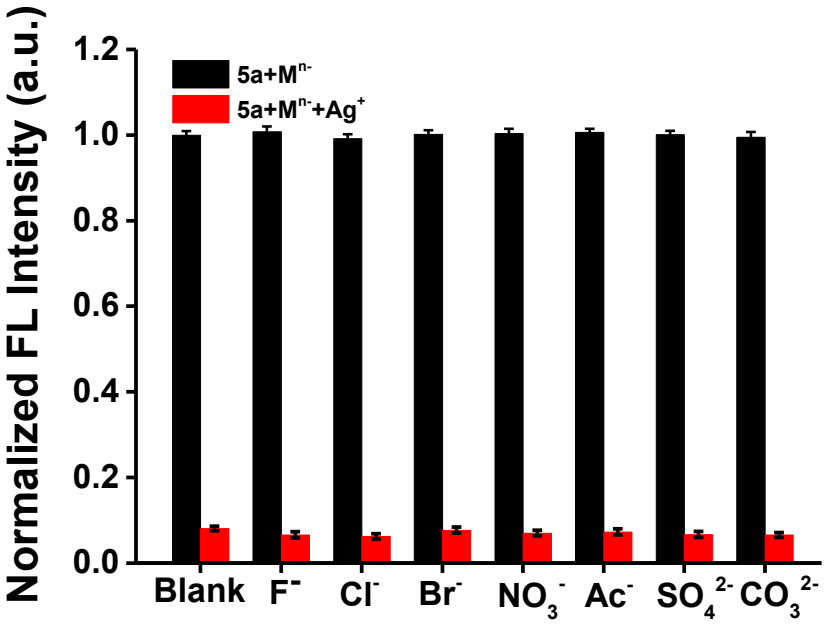


Figure S7. The fluorescence intensity of **5a** upon the addition of different anions (black bars) and the addition of Ag^+ (red bars); Concentration: **5a**, 2.0 μmol/L; Ag^+, 2.0 μmol/L; anions, 2.0 μmol/L. EtOH:Hepes, v:v=1:99

3.3 The interference of 5a for Ag^+ assay.

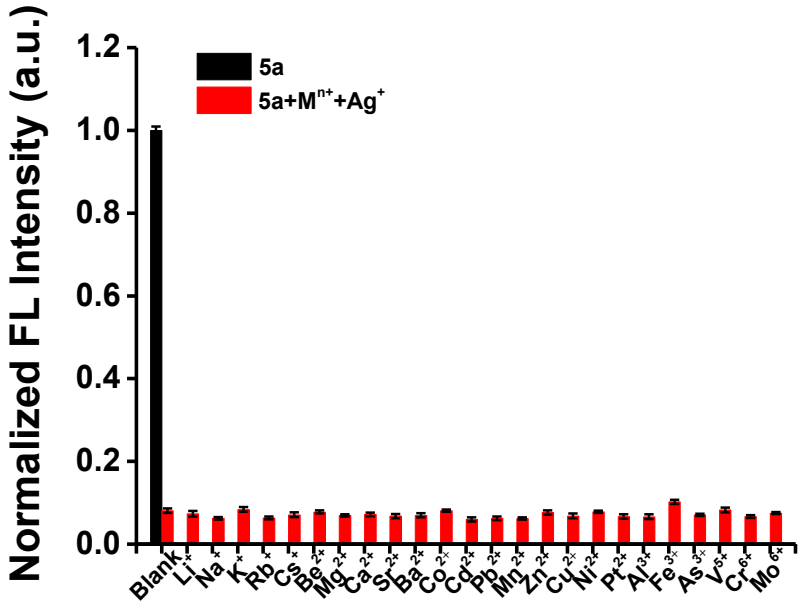


Figure S8. The fluorescence intensity of **5a**+Ag^+ system with the interfering metal ions. Concentration: **5a**, 2.0 μmol/L; Ag^+, 2.0 μmol/L; interfering metal ions, 2.0 μmol/L. EtOH:Hepes, v:v=1:99

3.4 The ESI MS of 5a and 5a+Ag^+

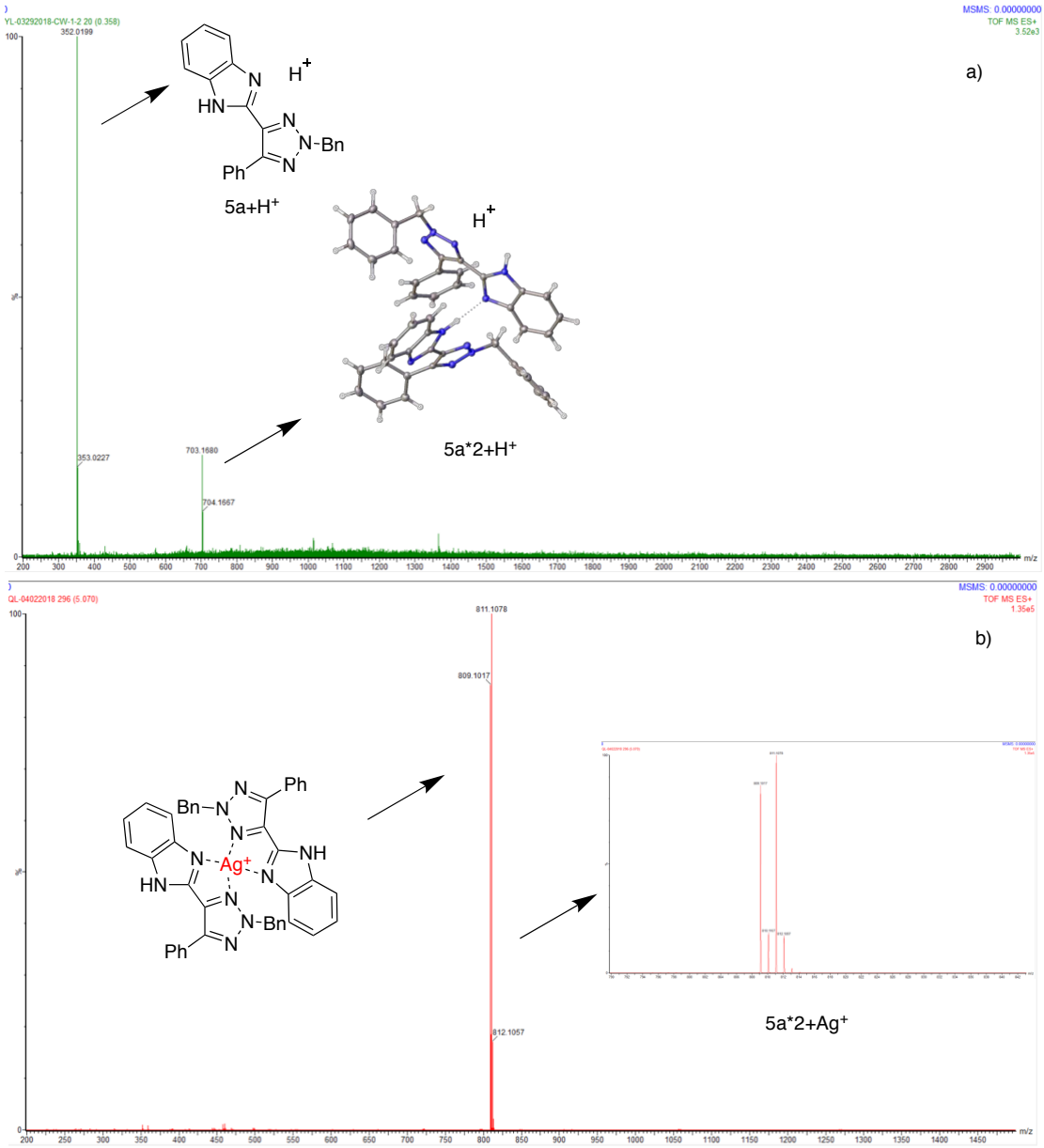


Figure S9. a) ESI Mass spectrum of complex **5a**, the sample was dissolved in MeOH.
b) ESI Mass spectrum of complex **5a**+Ag^+, the sample was dissolved in MeOH, and the $C_{\mathbf{5a}}$: C_{Ag+} = 1:1.

3.5 The Benesi-Hildebrand plot of $1/(F-F_0)$ versus $1/[Ag^+]$

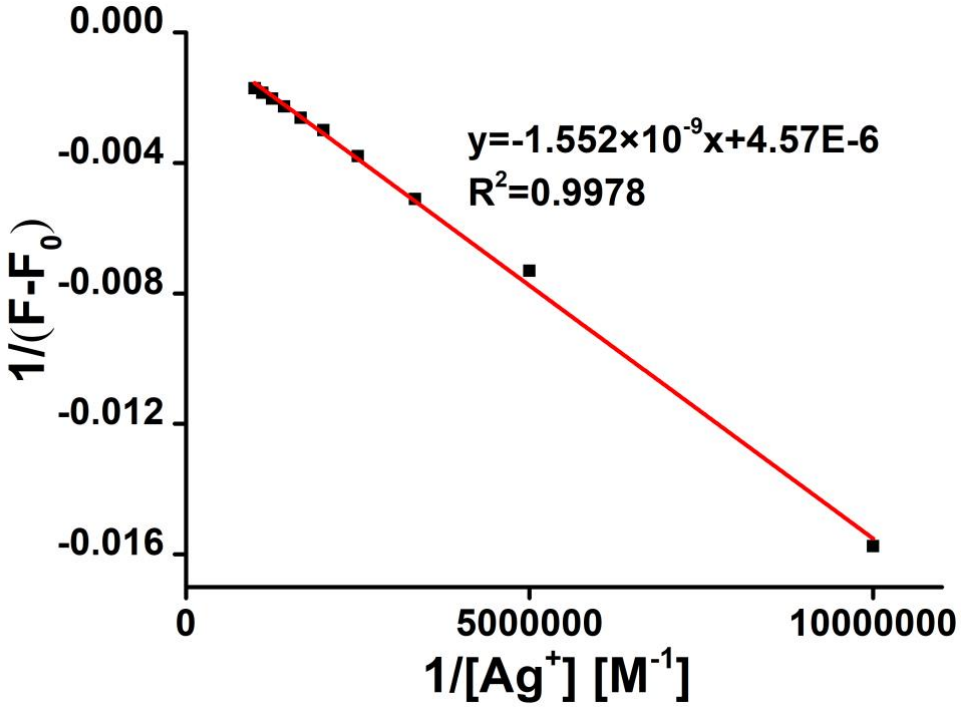


Figure S10. Benesi-Hildebrand plot of $1/(F-F_0)$ versus $1/[Ag^+]$.

3.6 The lifetime of 5a and 5a+Ag^+

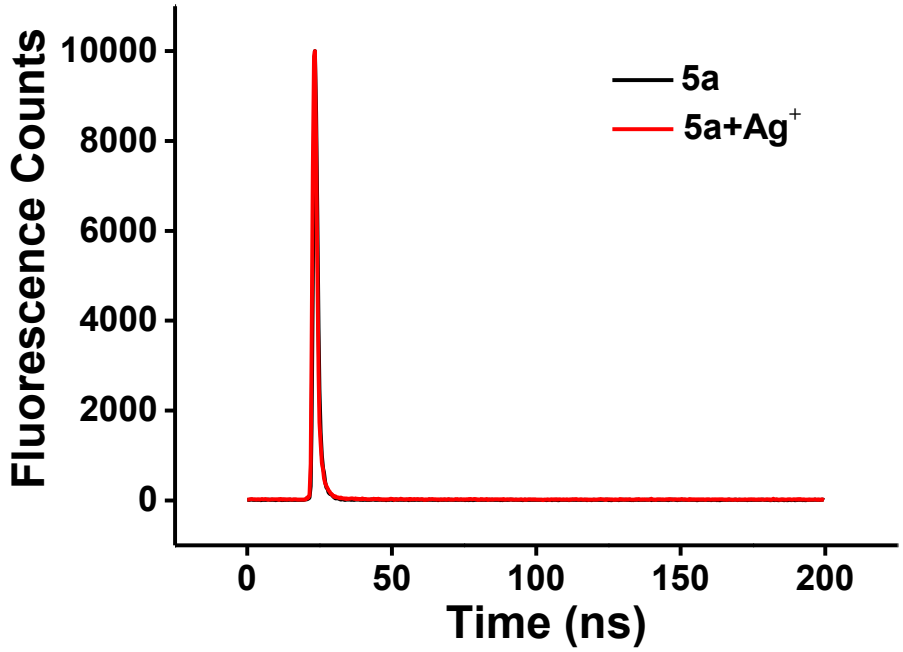


Figure S11. Fluorescence lifetime measurement: **5a** (black line) and **5a**+Ag^+ (red line). Concentration: **5a**, 2.0 μmol/L; Ag^+, 2.0 μmol/L. EtOH:Hepes, v:v=1:99

3.7 The photo-stability of 5a

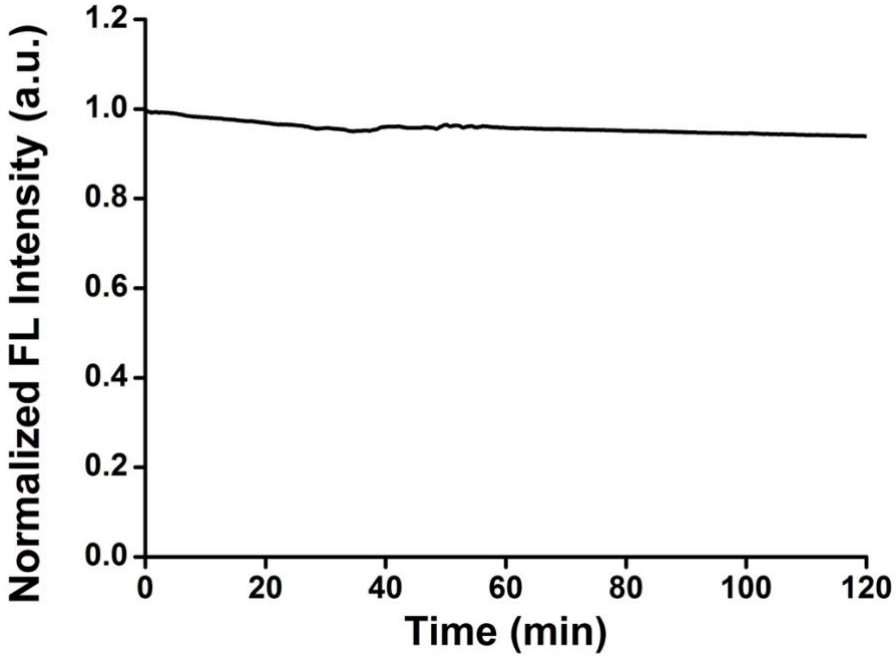


Figure S12. The effect of irradiation time on the fluorescence intensity of **5a**(2μm)

3.8 The pH range

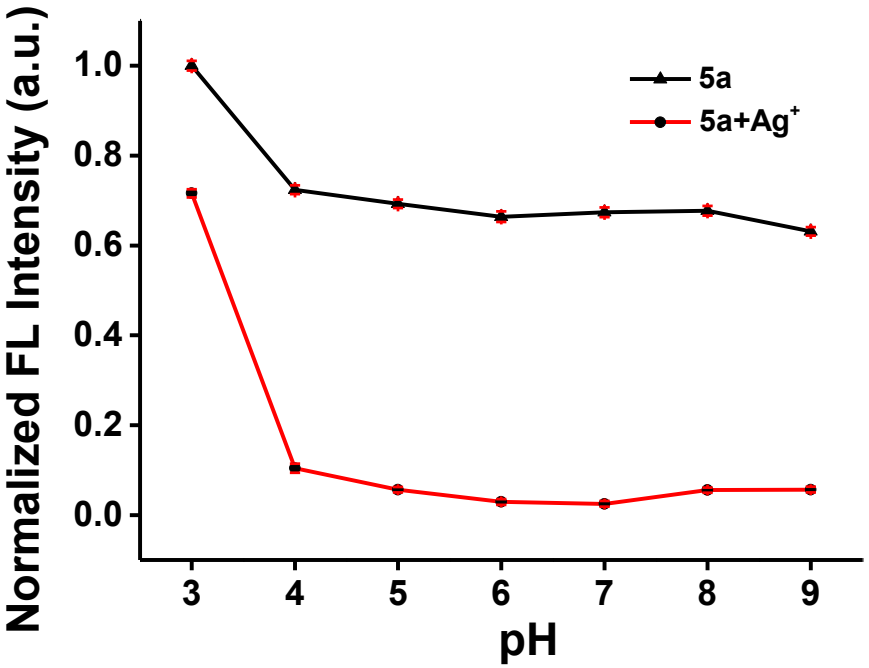


Figure S13. Effect of different pH on the fluorescence intensity of **5a** (black line) and **5a**+Ag^+ (red line); Concentration: **5a**, 2.0 μmol/L; Ag^+, 2.0 μmol/L, the solutions was mixed acids (mediated by NaOH and a mixture of acid comprising of H_3PO_4, CH_3COOH, H_3BO_3).

3.9 The different buffer

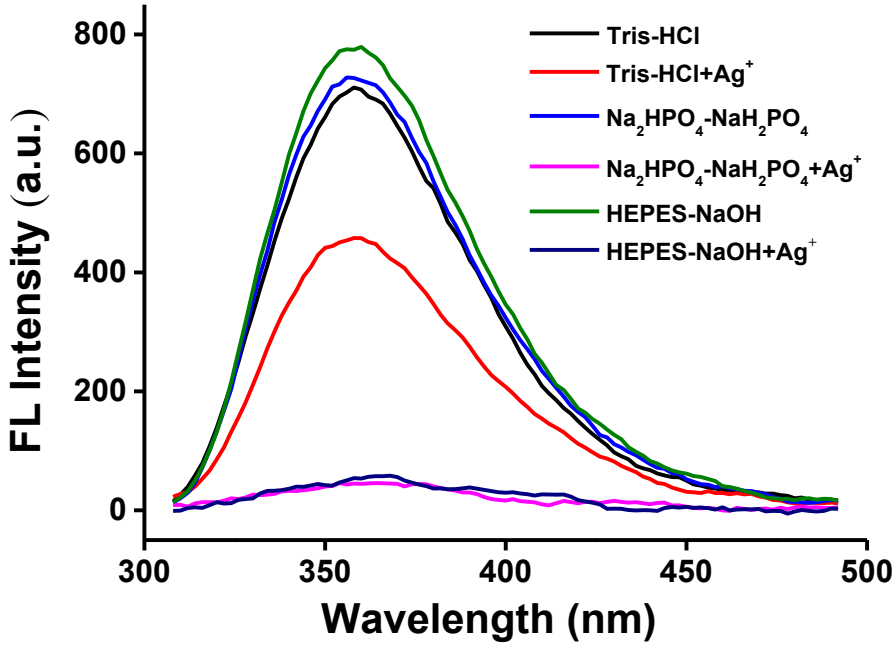


Figure S14. Effect of different buffer solution.

3.10 The comparison with other probes

Table S5 Comparison of different fluorescent probes for the determination of Ag^+

Fluorescent probe	Linear range (μmol/L)	Detection limit (nmol/L)	Reaction time (min)	Solvent	Reference
BODIPY	0.5-4	-	-	THF	[1]
rhodamine derivative	0.1-5	130	120	EtOH/H_2O (1:4, v/v)	[2]
Am-GQDs	3.06×10^2-9.27×10^2	3.06×10^5	-	H_2O	[3]
CdSe/ZnS Quantum Dots	1.0-40	1000	30	MOPS buffer	[4]
HACs/ssDNA	0.1-75	58	10	TE buffer	[5]
aka Au_3Pz_3	0-11 ppm (0-102 μm)	0.02 ppm (185 nm)	-	chitosan polymer media	[6]
TAIM	0.1-1	9.6	0.33	EtOH/HEPES (1:99, v/v)	This work

References

[1] A. Coskun and E. U. Akkaya, *J. Am. Chem. Soc.* 2005, **127**, 10464-10465.
[2] A. Chatterjee, M. Santra, N. Won, S. Kim, J. K. Kim, S. Bin Kim and K. H. Ahn, *J. Am. Chem. Soc.* 2009, **131**, 2040-2041.
[3] A. Suryawanshi, M. Biswal, D. Mhamane, R. Gokhale, S. Patil, D. Guin and S. Ogale and Nanoscale 2014, **6**, 11664-11670.
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[5] Z. Wang, J. Zhao, Z. Li, J. Bao, Z. Dai, *Anal. Chem.* 2017, **89,** 6815-6820.
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IV. ORTEP Drawing of the Crystal Structure

X-ray Crystallography

The X-ray diffraction data were measured on Bruker D8 Venture PHOTON 100 CMOS system equipped with a Cu K_α INCOATEC ImuS micro-focus source ($\lambda = 1.54178$ Å). Indexing was performed using Apex3 [1]. Data integration and reduction were performed using SaintPlus 6.01 [2]. Absorption correction was performed by multi-scan method implemented in SADABS [3]. Space group was determined using XPREP implemented in APEX3 [1]. Structure was solved using SHELXT [4] and refined using SHELXL-2017 [5-7] (full-matrix least-squares on F^2) within OLEX2 interface program [8]. All non-hydrogen atoms were refined anisotropically. Hydrogen atom of –NH groups were found from difference Fourier map and were freely refined. All remaining 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 1-6. **QL_TAIM_d and QL_TAIM_b:** Presence of low intensity Q-peaks (0.4el/A^3 and 0.8el/A^3 respectively) on Fourier difference map close to six-member ring fused with imidazole ring tentatively suggests that the second minor conformational isomer could be present in the crystal. In both cases the disorder was not modeled due to low intensity of q-peaks suggesting less than 10% content of second conformer for which the fused ring system is rotated approximately 180 degrees along single bond connecting it to center ring of the molecule. This would cause the $–CF_3$ or $–OCH_3$ groups to be located at positions where the observed difference electron density peaks are. Both crystals diffracted weekly and were collected at long exposure times.

[1] Bruker (2017). *APEX3* (Version 2015.9). Bruker AXS Inc., Madison, Wisconsin, USA.
[2] Bruker (2017) 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.

4.1 TA-IM-5a

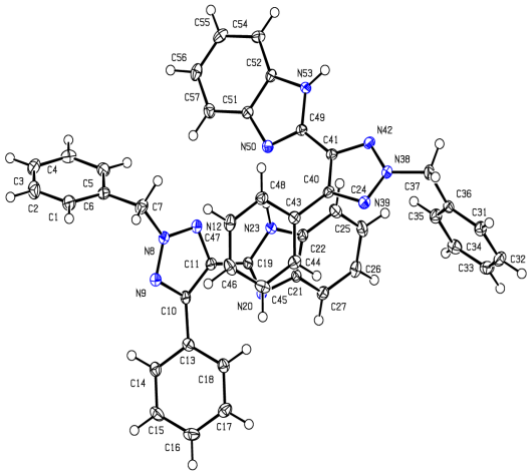


Fig.1. Asymmetric unit of **QL_TAIM_A**. Anisotropic displacement parameters were drawn at 50% probability. CCDC:1835133

Table 1 Crystal data and structure refinement for QL_TAIM_a.	
Identification code	QL_TAIM_a
Empirical formula	$C_{22}H_{17}N_5$
Formula weight	351.40
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.7774(2)
b/Å	22.0334(4)
c/Å	14.1047(3)
α/°	90
β/°	104.4370(10)
γ/°	90
Volume/Å^3	3544.54(12)
Z	8
ρ_{calc}g/cm^3	1.317
μ/mm^{-1}	0.644
F(000)	1472.0
Crystal size/mm^3	0.098 × 0.06 × 0.039
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.614 to 136.486
Index ranges	$-14 \leq h \leq 14$, $-26 \leq k \leq 26$, $-16 \leq l \leq 16$
Reflections collected	53076
Independent reflections	6450 [R_{int} = 0.0553, R_{sigma} = 0.0246]

Data/restraints/parameters	6450/0/495
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0352, wR_2 = 0.0786
Final R indexes [all data]	R_1 = 0.0469, wR_2 = 0.0844
Largest diff. peak/hole / e $Å^{-3}$	0.16/-0.27

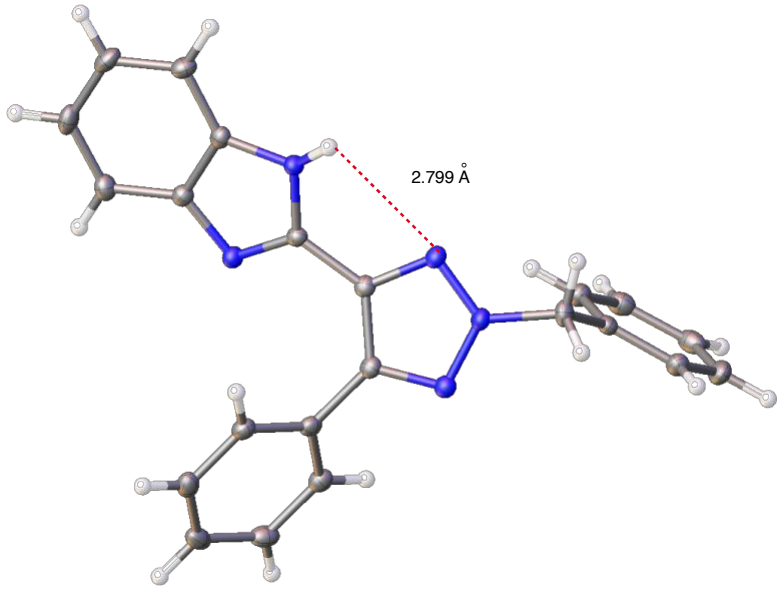


Figure S15. Intramolecular H-bond of **5a**.

4.1 TA-IM-5b

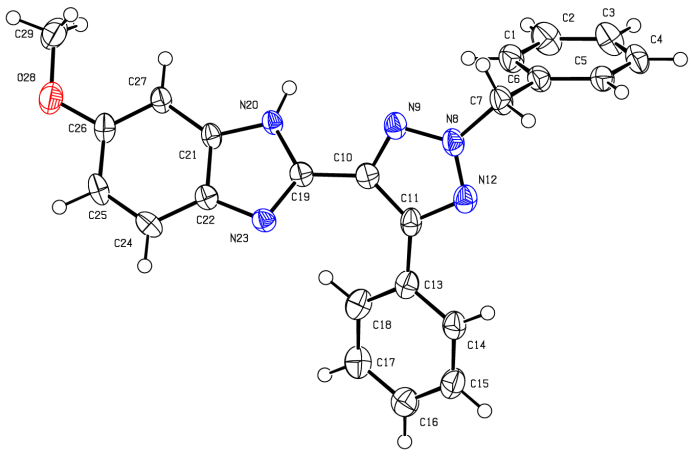


Fig.2. Asymmetric unit of **QL_TAIM_B**. Anisotropic displacement parameters were drawn at 50% probability. CCDC:1835134

Table 2 Crystal data and structure refinement for TAIM_b.	
Identification code	TAIM_b
Empirical formula	$C_{23}H_{19}N_5O$
Formula weight	381.43
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.1000(2)
b/Å	24.9541(7)
c/Å	9.6074(3)
α/°	90
β/°	97.478(2)
γ/°	90
Volume/Å^3	1925.41(9)
Z	4
ρ_{calc}g/cm^3	1.316
μ/mm^{-1}	0.675
F(000)	800.0
Crystal size/mm^3	0.171 × 0.056 × 0.014
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.084 to 148.918
Index ranges	$-9 \leq h \leq 9$, $-25 \leq k \leq 30$, $-11 \leq l \leq 11$
Reflections collected	15279
Independent reflections	3866 [R_{int} = 0.0743, R_{sigma} = 0.0505]
Data/restraints/parameters	3866/0/267
Goodness-of-fit on F^2	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0695, wR_2 = 0.1672
Final R indexes [all data]	R_1 = 0.1030, wR_2 = 0.1872
Largest diff. peak/hole / e Å^{-3}	0.79/-0.33

4.3 TA-IM-5d

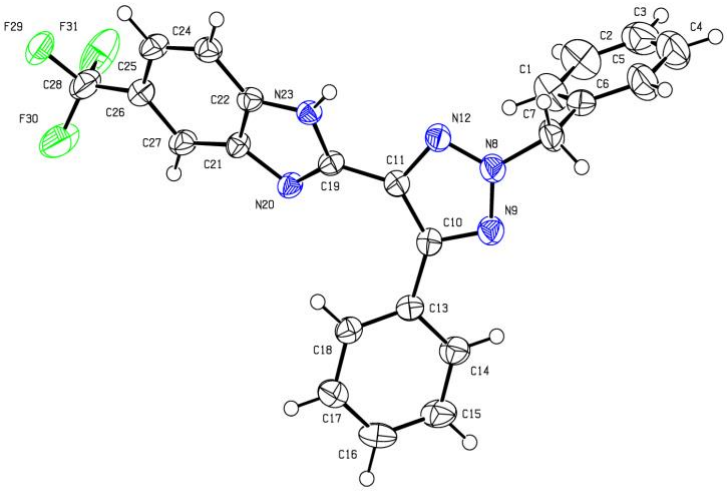


Fig.3. Asymmetric unit of **QL_TAIM_D**. Anisotropic displacement parameters were drawn at 50% probability. CCDC:1835139

Table 3 Crystal data and structure refinement for QL_TAIM_d.	
Identification code	QL_TAIM_d
Empirical formula	$C_{23}H_{16}F_3N_5$
Formula weight	419.41
Temperature/K	99.99
Crystal system	orthorhombic
Space group	Pbca
a/Å	9.8081(2)
b/Å	15.0760(3)
c/Å	26.6668(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3943.14(13)
Z	8
ρ_{calc}g/cm^3	1.413
μ/mm^{-1}	0.900
F(000)	1728.0
Crystal size/mm^3	0.116 × 0.055 × 0.02
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	6.628 to 133.188
Index ranges	-11 ≤ h ≤ 11, -17 ≤ k ≤ 15, -31 ≤ l ≤ 31
Reflections collected	36706
Independent reflections	3481 [R_{int} = 0.1259, R_{sigma} = 0.0378]

Data/restraints/parameters	3481/0/280
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0641, wR_2 = 0.1573
Final R indexes [all data]	R_1 = 0.0899, wR_2 = 0.1730
Largest diff. peak/hole / e $Å^{-3}$	0.40/-0.27

4.3 TA-IM-5i

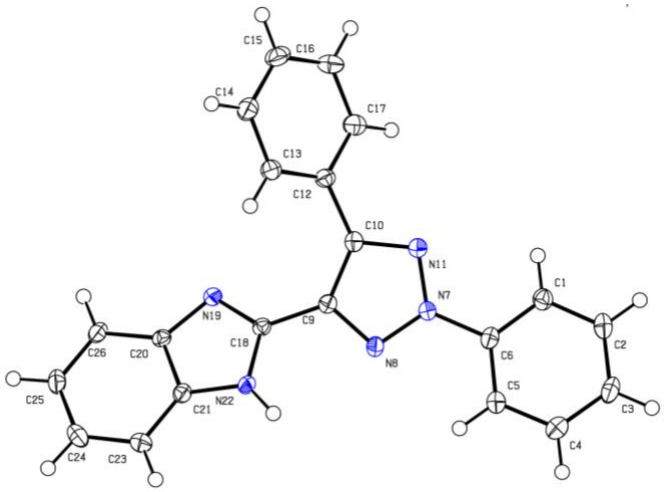


Fig.4. Asymmetric unit of **QL_TAIM_E**. Anisotropic displacement parameters were drawn at 50% probability. CCDC:1835140

Table 4 Crystal data and structure refinement for QL_TAIM_E.	
Identification code	QL_TAIM_E
Empirical formula	$C_{21}H_{15}N_5$
Formula weight	337.38
Temperature/K	100.0
Crystal system	monoclinic
Space group	Cc
a/Å	8.3507(2)
b/Å	22.0757(6)
c/Å	10.0712(3)
α/°	90

β/°	113.6909(6)
γ/°	90
Volume/Å^3	1700.14(8)
Z	4
ρ_{calc}g/cm^3	1.318
μ/mm^{-1}	0.650
F(000)	704.0
Crystal size/mm^3	0.28 × 0.15 × 0.07
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	8.01 to 154.31
Index ranges	-10 ≤ h ≤ 10, -27 ≤ k ≤ 27, -10 ≤ l ≤ 11
Reflections collected	13378
Independent reflections	3147 [R_{int} = 0.0211, R_{sigma} = 0.0187]
Data/restraints/parameters	3147/2/240
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0242, wR_2 = 0.0610
Final R indexes [all data]	R_1 = 0.0246, wR_2 = 0.0612
Largest diff. peak/hole / e Å^{-3}	0.15/-0.17
Flack parameter	0.12(9)

4.3 TA-IM-5k

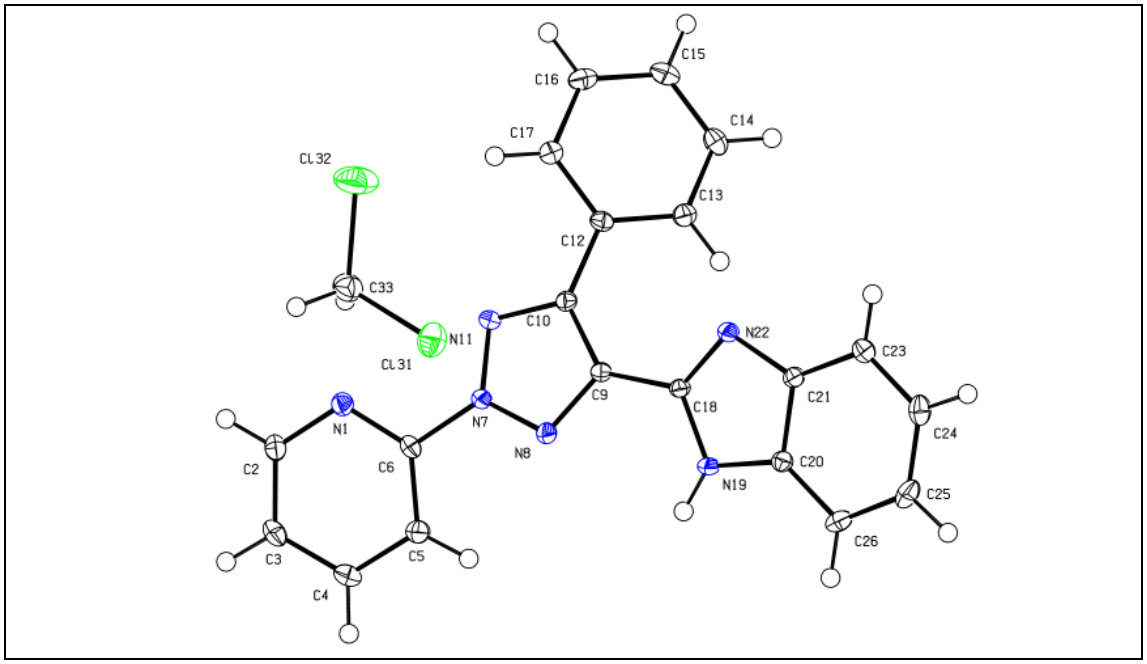
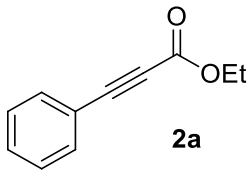


Fig.5. Asymmetric unit of **QL_TAIM_G**. Anisotropic displacement parameters were drawn at 50% probability. CCDC:1835141

Table 5 Crystal data and structure refinement for QL_TAIM_G.

Identification code	QL_TAIM_G
Empirical formula	$C_{21}H_{16}Cl_2N_6$
Formula weight	423.30
Temperature/K	100.0
Crystal system	orthorhombic
Space group	Pbca
a/Å	10.0604(2)
b/Å	14.9961(3)
c/Å	25.8051(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3893.13(14)
Z	8
ρ_{calc}g/cm^3	1.444
μ/mm^{-1}	3.168
F(000)	1744.0
Crystal size/mm^3	0.477 × 0.068 × 0.04
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	6.85 to 148.978
Index ranges	$-12 \leq h \leq 12$, $-18 \leq k \leq 18$, $-32 \leq l \leq 32$
Reflections collected	57028
Independent reflections	3989 [R_{int} = 0.0569, R_{sigma} = 0.0171]
Data/restraints/parameters	3989/0/266
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0307, wR_2 = 0.0757
Final R indexes [all data]	R_1 = 0.0362, wR_2 = 0.0790
Largest diff. peak/hole / e Å^{-3}	0.33/-0.34

V. Compounds Characterization



2a

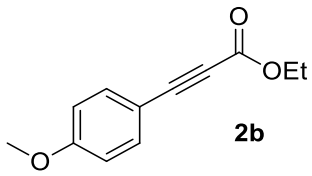
ethyl 3-phenylpropiolate

2b was prepared following the General Procedure **1.1** and purified by flash Chromatography (Hexane: EA = 20:1) as yellow oil. and 91% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 – 7.53 (m, 2H), 7.48 – 7.41 (m, 1H), 7.39 – 7.31 (m, 2H), 4.29 (q, *J* = 7.1 Hz, 2H), 1.35 (td, *J* = 7.1, 2.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.96, 132.87, 130.52, 128.48, 119.55, 85.93, 80.64, 77.00, 61.99, 14.01.

HRMS(ESI): Calculated for $C_{11}H_{12}O_2^+$ $(M+H)^+$: 175.0754ound:175.0757.



2b

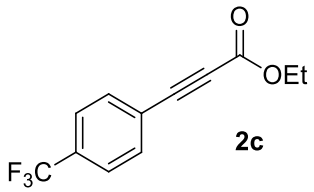
ethyl 3-(4-methoxyphenyl)propiolate

2b was prepared following the General Procedure **1.1** and purified by flash Chromatography (Hexane: EA = 20:1) as yellow oil. and 80% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 – 7.38 (m, 2H), 6.99 – 6.74 (m, 2H), 4.28 (dd, *J* = 7.8, 6.3 Hz, 2H), 3.83 (d, *J* = 1.6 Hz, 3H), 1.35 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.39, 154.19, 134.79, 114.18, 111.28, 86.77, 80.06, 61.79, 55.27, 14.02.

HRMS(ESI): Calculated for $C_{12}H_{14}O_3^+$ $(M+H)^+$: 205.0859 Found:205.0857.



2c

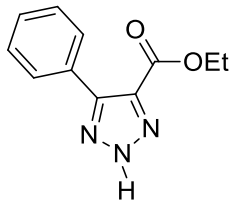
ethyl 3-(4-(trifluoromethyl)phenyl) propiolate

2c was prepared following the General Procedure **1.1** and purified by flash Chromatography (Hexane: EA = 20:1) as yellow oil. and 86% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 – 7.43 (m, 4H), 4.32 (q, *J* = 7.2 Hz, 2H), 1.37 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.55, 133.11, 131.95 (q, *J* = 32.8 Hz), 1255.52(q, *J* = 3.8 Hz), 124.84, 123.44(q, *J* = 272.5 Hz), 122.14, 83.74, 82.25, 62.37, 14.01.

HRMS(ESI): Calculated for $C_{12}H_{10}F_3O_3^+$ $(M+H)^+$: 243.0627, Found:243.0626.



3a

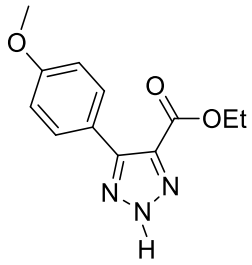
ethyl 5-phenyl-2H-1,2,3-triazole-4-carboxylate

3a was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: EA = 1:1) as white solid. and 99% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.76 (s, 2H), 7.57 – 7.39 (m, 3H), 4.28 (q, *J* = 7.1 Hz, 2H), 1.25 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 161.32, 134.84, 129.78, 129.56, 128.68, 61.18, 14.42.

HRMS(ESI): Calculated for $C_{11}H_{12}N_3O_2^+$ $(M+H)^+$: 218.0924, Found:218.0923.



3b

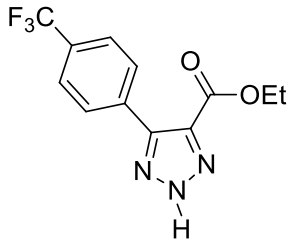
ethyl 5-(4-methoxyphenyl)-2H-1,2,3-triazole-4-carboxylate

3b was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: EA = 1:1) as white solid. and 95% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (d, *J* = 8.8 Hz, 2H), 6.97 (d, *J* = 8.9 Hz, 2H), 4.40 (d, *J* = 7.1 Hz, 2H), 3.85 (s, 3H), 1.35 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.24, 160.60, 144.71, 133.23, 130.57, 119.22, 113.65, , 61.37, 55.18, 13.91.

HRMS(ESI): Calculated for $C_{12}H_{14}N_3O_3^+$ $(M+H)^+$: 248.1030, Found:248.1027.



3c

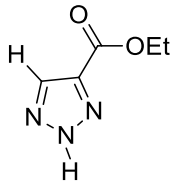
ethyl 5-(4-(trifluoromethyl) phenyl)-2H-1,2,3-triazole-4-carboxylate

3c was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: EA = 1:1) as white solid. and 99% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 16.03 (s, 1H), 8.06 (d, *J* = 8.0 Hz, 2H), 7.87 (d, *J* = 8.0 Hz, 2H), 4.34 (q, *J* = 7.1 Hz, 2H), 1.30 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 161.03, 130.34, 130.05, 129.73(q, *J* = 32.0 Hz), 128.66, 125.42(q, *J* = 3.8 Hz), 124.5(q, *J* = 272.1 Hz), 123.25, 61.45, 14.33.

HRMS(ESI): Calculated for $C_{12}H_{11}F_3N_3O_3^+$ $(M+H)^+$: 286.0798, Found:286.0770.



3d

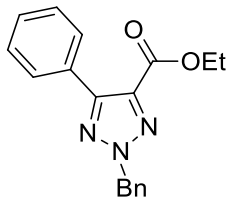
ethyl 2H-1,2,3-triazole-4-carboxylate

3d was prepared following the General Procedure **1.2** and purified by flash Chromatography (Hexane: EA = 1:1) as white solid. and 95% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 15.86 (s, 1H), 8.55 (d, 1H), 4.35 (q, J = 7.0 Hz, 2H), 1.33 (td, J = 7.1, 1.5 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 161.07, 136.46, 128.17, 61.02, 14.64, 14.58.

HRMS(ESI): Calculated for $C_5H_7N_3NaO_2$ $(M+Na)^+$: 164.0436, Found:164.0428.



3Xa

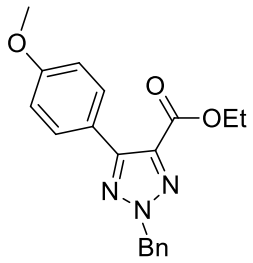
ethyl 2-benzyl-5-phenyl-2H-1,2,3-triazole-4-carboxylate

3Xa was prepared following the General Procedure **1.3** and purified by flash Chromatography (Hexane: EA = 4:1) as white solid. and 85% yield.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.39 (d, J = 2.0 Hz, 4H), 8.30 (s, 1H), 7.96 (dd, J = 8.5, 1.3 Hz, 1H), 7.87 (s, 1H), 7.80 (d, J = 8.4 Hz, 1H), 7.57 (d, J = 5.3 Hz, 6H).

^{13}C NMR ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.20, 150.26, 136.02, 134.23, 129.24, 129.10, 128.80, 128.58, 128.19, 128.03, 61.44, 59.37, 14.18.

HRMS(ESI): Calculated for $C_{18}H_{18}N_3O_2^+$ $(M+H)^+$: 308.1394, Found: 308.1401.



3Xb

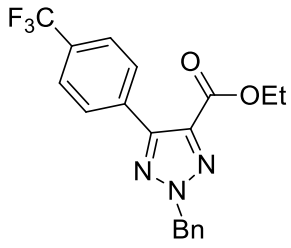
ethyl 2-benzyl-5-(4-methoxyphenyl)-2H-1,2,3-triazole-4-carboxylate

3Xb was prepared following the General Procedure **1.3** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as colorless oil. Yield = 85 %.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.68 (m, 2H), 7.44 – 7.29 (m, 5H), 7.01 – 6.90 (m, 2H), 5.65 (s, 2H), 4.40 (q, *J* = 7.1 Hz, 2H), 3.83 (s, 3H), 1.37 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.29, 160.23, 150.07, 135.51, 134.27, 130.57, 128.72, 128.47, 128.09, 121.79, 113.42, 61.31, 59.23, 55.17, 14.17.

HRMS(ESI): Calculated for $C_{19}H_{20}N_3O_3^+$ $(M+H)^+$: 338.1499, Found:338.1484.



3Xc

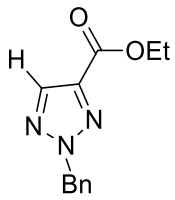
ethyl 2-benzyl-5-(4-(trifluoromethyl) phenyl)-2H-1,2,3-triazole-4-carboxylate

3Xc was prepared following the General Procedure **1.3** and purified by flash Chromatography (Hexane: Ethyl Acetate = 5:1) as white solid. Yield = 80 %.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 8.1 Hz, 2H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.48 – 7.30 (m, 5H), 5.68 (s, 2H), 4.42 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.01, 148.89, 136.32, 133.97, 133.02, 131.13, 130.82, 129.64, 128.89, 128.75, 128.28, 125.00, 61.69, 59.56, 14.19.

HRMS(ESI): Calculated for $C_{19}H_{17}F_3N_3O_2^+$ $(M+H)^+$: 376.1267, Found:376.1269.



3Xd

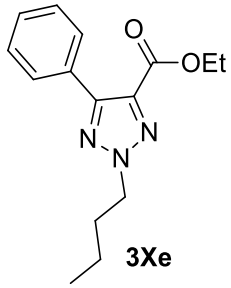
ethyl 2-benzyl-2H-1,2,3-triazole-4-carboxylate

3Xd was prepared following the General Procedure **1.3** and purified by flash Chromatography (Hexane: Ethyl Acetate = 5:1) as white solid. Yield = 81%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (s, 1H), 7.46 – 7.24 (m, 5H), 5.64 (s, 2H), 4.42 (q, *J* = 7.1 Hz, 2H), 1.40 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.52, 140.18, 137.23, 134.11, 128.76, 128.55, 128.13, 61.32, 59.30, 14.20.

HRMS(ESI): Calculated for $C_{12}H_{13}N_3NaO_2^+$ $(M+Na)^+$: 254.0900, Found:254.0892.



3Xe

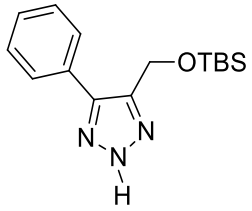
ethyl 2-butyl-5-phenyl-2H-1,2,3-triazole-4-carboxylate

3Xe was prepared following the General Procedure **1.3** and purified by flash Chromatography (Hexane: Ethyl Acetate = 6:1) as colorless oil. Yield = 90%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 – 7.75 (m, 2H), 7.43 (d, *J* = 6.6 Hz, 3H), 4.51 (t, *J* = 7.2 Hz, 2H), 4.40 (d, *J* = 7.1 Hz, 2H), 2.02 (t, J = 7.5 Hz, 2H), 1.37 (q, *J* = 8.7, 7.1 Hz, 5H), 0.96 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.23, 149.65, 135.36, 129.56, 129.13, 128.96, 127.99, 61.29, 55.51, 31.55, 19.64, 14.14, 13.41.

HRMS(ESI): Calculated for $C_{15}H_{20}N_3O_2^+$ $(M+H)^+$: 274.1550, Found:274.1552.



3Ya

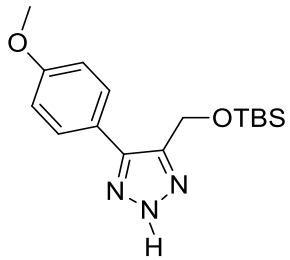
4-(((tert-butyldimethylsilyl) oxy)methyl)-5-phenyl-2H-1,2,3-triazole

3Ya was prepared following the General Procedure **1.4** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield = 74%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 – 7.81 (m, 2H), 7.51 – 7.37 (m, 3H), 4.95 (s, 2H), 0.91 (s, 9H), 0.12 (s, 6H).

^{13}C NMR (101 MHz, DMSO) δ 145.09, 143.08, 131.27, 129.11, 128.56, 127.60, 56.77, 26.10, 18.31, -4.86.

HRMS(ESI): Calculated for $C_{15}H_{24}N_3OSi^+$ $(M+H)^+$: 290.1683, Found: 290.1636.



3Yb

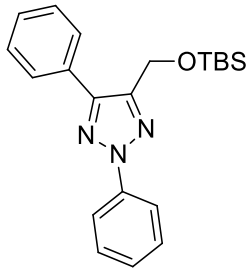
4-(((tert-butyldimethylsilyl) oxy)methyl)-5-(4-methoxyphenyl)-2H-1,2,3-triazole

3Yb was prepared following the General Procedure **1.4** and purified by flash Chromatography (Hexane: Ethyl Acetate = 3:1) as white solid. Yield = 77%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 – 7.81 (m, 2H), 7.51 – 7.37 (m, 3H), 4.95 (s, 2H), 0.91 (s, 9H), 0.12 (s, 6H).

^{13}C NMR (101 MHz, DMSO) δ 159.70, 145.01, 142.50, 128.94, 123.72, 114.55, 55.81, 55.63, 26.13, 18.32, -4.82.

HRMS(ESI): Calculated for $C_{16}H_{25}N_3O_2Si^+$ $(M+H)^+$: 320.1789, Found:320.1741.



3Za

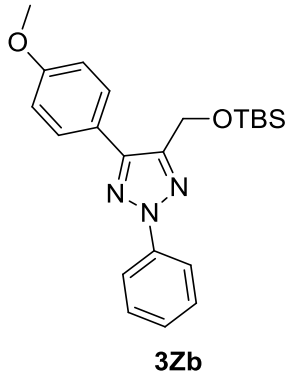
4-(((tert-butyldimethylsilyl) oxy)methyl)-2,5-diphenyl-2H-1,2,3-triazole

3Za was prepared following the General Procedure **1.5** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield = 85%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.18 – 8.07 (m, 2H), 8.04 – 7.96 (m, 2H), 7.70 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.48 (ddd, *J* = 7.9, 6.7, 4.3 Hz, 4H), 7.44 – 7.38 (m, 1H), 7.38 – 7.29 (m, 2H), 7.10 (t, *J* = 7.8 Hz, 1H), 4.95 (d, *J* = 0.8 Hz, 2H), 0.91 (d, *J* = 0.8 Hz, 9H), 0.13 (d, J = 0.9 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.52, 145.44, 139.76, 137.45, 129.20, 128.63, 128.53, 127.87, 127.21, 118.71, 56.76, 25.82, 18.28, -5.13.

HRMS(ESI): Calculated for $C_{21}H_{28}N_3OSi^+$ $(M+H)^+$: 366.1996, Found: 366.1947.



3Zb

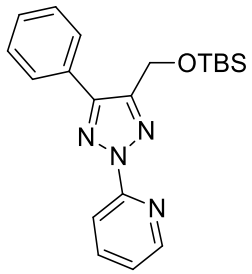
4-(((tert-butyldimethylsilyl) oxy) methyl)-5-(4-methoxyphenyl)-2-phenyl-2H-1,2,3-triazole

3Zb was prepared following the General Procedure **1.5** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield = 88%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (d, *J* = 8.1 Hz, 2H), 8.02 – 7.96 (m, 2H), 7.51 (t, *J* = 7.8 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.09 – 6.97 (m, 2H), 4.95 (s, 2H), 3.90 (s, 3H), 0.94 (s, 9H), 0.16 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.83, 147.07, 144.94, 133.63, 130.55, 128.60, 128.38, 127.81, 120.19, 114.28, 56.75, 55.56, 25.84, 18.30, -5.12.

HRMS(ESI): Calculated for $C_{22}H_{30}N_3O_2Si^+$ $(M+H)^+$: 396.2102, Found:369.2077.



3Zc

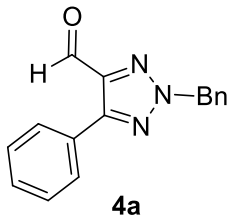
2-(4-(((tert-butyldimethylsilyl) oxy)methyl)-5-phenyl-2H-1,2,3-triazol-2-yl)pyridine

3Za was prepared following the General Procedure **1.5** and purified by flash Chromatography (Hexane: Ethyl Acetate = 3:1) as white solid. Yield = 81%.

1H NMR (400 MHz, Chloroform-*d*) δ 8.71 – 8.56 (m, 1H), 8.14 (d, *J* = 8.3 Hz, 1H), 8.10 – 8.03 (m, 2H), 7.90 (td, *J* = 7.9, 1.6 Hz, 1H), 7.46 (ddd, *J* = 13.5, 7.9, 6.2 Hz, 3H), 7.32 (dd, *J* = 7.4, 4.8 Hz, 1H), 4.99 (s, 2H), 0.90 (s, 9H), 0.13 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.79, 148.84, 148.72, 146.59, 138.70, 129.91, 128.79, 128.49, 128.06, 122.60, 113.61, 56.72, 25.73, 18.17, -5.26.

HRMS(ESI): Calculated for $C_{20}H_{27}N_4OSi^+$ (M+H)+: 367.1949, Found:367.1953.



4a

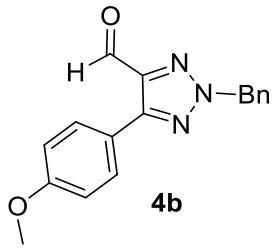
2-benzyl-5-phenyl-2H-1,2,3-triazole-4-carbaldehyde

4a was prepared following the General Procedure **1.6** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield = 90%.

^{1}H-NMR ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.20 (s, 1H), 8.03 (dd, *J* = 7.8, 1.8 Hz, 2H), 7.55 – 7.33 (m, 8H), 5.67 (s, 2H).

^{13}C-NMR (101 MHz, $CDCl_3$) δ 184.17, 149.29, 142.95, 133.88, 129.69, 128.87, 128.74, 128.60, 128.47, 128.27, 59.51.

HRMS m/z (ESI) calcd. for $C_{16}H_{14}N_3O^+$ $(M+H)^+$: 264.1131, found 264.1132.



4b

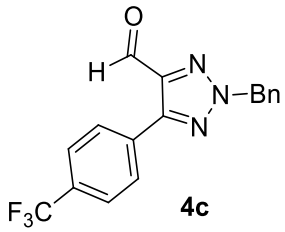
2-benzyl-5-(4-methoxyphenyl)-2H-1,2,3-triazole-4-carbaldehyde

4b was prepared following the General Procedure **1.6** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield =80%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.18 (d, *J* = 0.7 Hz, 1H), 8.16 – 7.89 (m, 2H), 7.55 – 7.30 (m, 5H), 6.97 (d, *J* = 8.8 Hz, 2H), 5.65 (s, 2H), 3.85 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.37, 160.73, 149.18, 142.65, 133.97, 130.11, 128.90, 128.75, 128.27, 121.29, 113.88, 59.49, 55.28.

HRMS m/z (ESI) calcd. for $C_{17}H_{16}N_3O_2$ $(M+H)^+$: 294.1237, found 294.1234.



4c

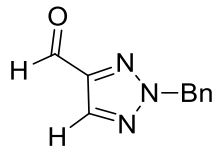
2-benzyl-5-(4-(trifluoromethyl) phenyl)-2H-1,2,3-triazole-4-carbaldehyde

4c was prepared following the General Procedure **1.6** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield = 90%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.20 (s, 1H), 8.38 – 7.97 (m, 2H), 7.70 (d, *J* = 8.2 Hz, 2H), 7.57 – 7.35 (m, 5H), 5.68 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.30, 147.54, 143.31, 133.64, 132.27, 131.54 (q, *J* = 32.6 Hz), 131.22, 129.00, 128.95, 128.37, 125.46, 125.42(q, *J* = 3.8 Hz), 125.38, 125.35, 122.57, 59.74.

HRMS m/z (ESI) calcd. for $C_{17}H_{13}F_3N_3O^+$ $(M+H)^+$: 332.1005, found 332.1000.



4d

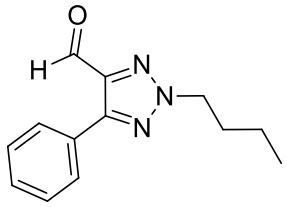
2-benzyl-2H-1,2,3-triazole-4-carbaldehyde

4d was prepared following the General Procedure **1.6** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield = 83%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.10 (s, 1H), 8.09 (s, 1H), 7.37 (s, 5H), 5.66 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.14, 147.35, 134.94, 133.88, 128.97, 128.85, 128.29, 59.50.

HRMS m/z (ESI) calcd. for $C_{10}H_{10}N_3O^+$ $(M+H)^+$: 188.0818, found 188.0810.



4e

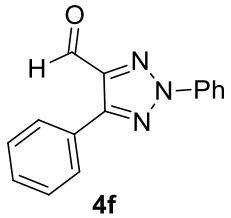
2-butyl-5-phenyl-2H-1,2,3-triazole-4-carbaldehyde

4e was prepared following the General Procedure **1.6** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield = 90%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.99 (s, 1H), 8.16 (dd, *J* = 7.1, 1.6 Hz, 1H), 7.66 (d, *J* = 6.0 Hz, 1H), 7.48 – 7.38 (m, 2H), 7.32 – 7.30 (m, 1H), 4.53 (t, *J* = 7.2 Hz, 2H), 2.14 – 1.99 (m, 2H), 1.45 (q, *J* = 7.5 Hz, 2H), 1.01 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.24, 148.95, 142.43, 129.63, 128.92, 128.55, 128.51, 55.60, 31.39, 19.63, 13.39.

HRMS m/z (ESI) calcd. for $C_{13}H_{16}N_3O^+$ $(M+H)^+$: 230.1288, found 230.1284.



4f

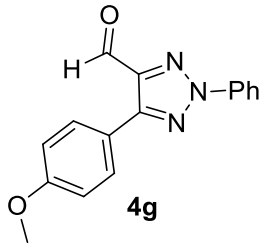
2,5-diphenyl-2H-1,2,3-triazole-4-carbaldehyde

4f was prepared following the General Procedure **1.7** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield = 88%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.34 (s, 1H), 8.26 – 8.19 (m, 2H), 8.19 – 8.12 (m, 2H), 7.60 – 7.42 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.44, 149.77, 143.61, 139.11, 130.06, 129.52, 128.93, 128.85, 128.67, 128.64, 119.49.

HRMS m/z (ESI) calcd. for $C_{15}H_{12}N_3O^+$ $(M+H)^+$: 250.0975, found 250.0968.



4g

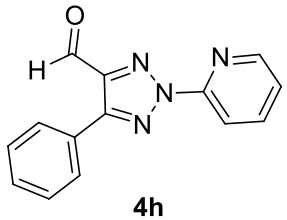
5-(4-methoxyphenyl)-2-phenyl-2H-1,2,3-triazole-4-carbaldehyde

4g was prepared following the General Procedure **1.7** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield = 83%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.32 (s, 1H), 8.23 – 8.18 (m, 2H), 8.18 – 8.14 (m, 2H), 7.55 (dd, *J* = 8.6, 7.1 Hz, 2H), 7.48 – 7.42 (m, 1H), 7.07 – 6.99 (m, 2H), 3.89 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.55, 161.01, 149.53, 143.31, 139.10, 130.32, 129.45, 128.76, 121.15, 119.39, 113.98, 55.34.

HRMS m/z (ESI) calcd. for $C_{16}H_{14}N_3O_2^+$ $(M+H)^+$: 280.1081, found 280.1082.



4h

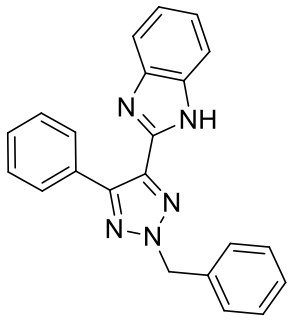
5-phenyl-2-(pyridin-2-yl)-2H-1,2,3-triazole-4-carbaldehyde

4h was prepared following the General Procedure **1.7** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield = 92%.

^{1}H NMR (400 MHz, Chloroform-*d*): δ 10.27 (s, 1H), 8.67-8.66 (m, 1H), 8.67-8.66 (m, 1H), 8.18-8.14 (m, 2H), 8.08-8.06 (m, 2H), 7.62 (ddd, *J* = 6.7, 4.9, 1.7 Hz, 1H), 7.57-7.53 (m, 3H)

^{13}C NMR (151 MHz, DMSO) δ 185.35, 150.14, 149.62, 149.53, 144.37, 140.41, 130.53, 129.48, 129.08, 129.05, 128.66, 125.39, 115.34.

HRMS m/z (ESI) calcd. for $C_{14}H_{11}N_4O^+$ $(M+H)^+$: 251.0927, found 251.0925.



5a

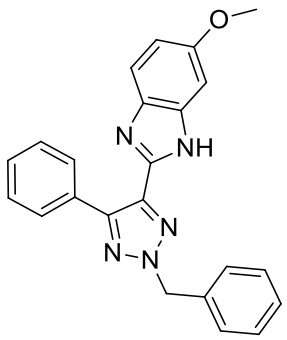
2-(2-benzyl-5-phenyl-2H-1,2,3-triazol-4-yl)-1H-benzo[d]imidazole

5a was prepared following the General Procedure **1.8** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield =72%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 13.12 (s, 1H), 8.04 (d, *J* = 6.9 Hz, 2H), 7.69 (d, *J* = 7.9 Hz, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.48 – 7.33 (m, 8H), 7.26 (dd, *J* = 12.3, 7.6 Hz, 2H), 5.83 (s, 2H).

^{13}C NMR (101 MHz, DMSO) δ 150.38, 149.37, 148.09, 143.87, 140.31, 138.79, 134.94, 129.87, 129.70, 129.56, 129.44, 128.79, 124.75, 123.89, 122.41, 119.88, 114.90, 112.28.

HRMS m/z (ESI) calcd. for $C_{22}H_{18}N_5^+$ $(M+H)^+$: 352.1557, found:352.1549.



5b

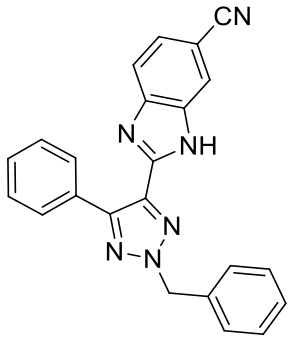
2-(2-benzyl-5-phenyl-2H-1,2,3-triazol-4-yl)-6-methoxy-1H-benzo[d]imidazole

5b was prepared following the General Procedure **1.8** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield =67%.

^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ 12.79 (d, *J* = 17.3 Hz, 1H), 8.19 (d, *J* = 7.6 Hz, 2H), 7.63 – 6.98 (m, 10H), 6.87 (dd, *J* = 33.1, 8.6 Hz, 1H), 5.82 (s, 2H), 3.80 (s, 3H).

^{13}C NMR (151 MHz, DMSO) δ 156.89, 155.93, 146.03, 145.84, 144.59, 144.42, 143.37, 138.30, 136.71, 135.77, 135.51, 130.22, 129.20, 129.15, 128.88, 128.65, 128.34, 120.16, 113.61, 112.30, 111.91, 101.81, 94.85, 58.78, 55.88.

HRMS m/z (ESI) calcd. For $C_{23}H_{20}N_5O^+$ $(M+H)^+$: 382.1662 found: 382.1663



5c

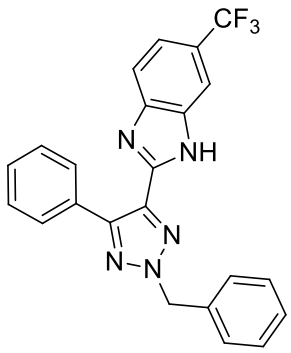
2-(2-benzyl-5-phenyl-2H-1,2,3-triazol-4-yl)-1H-benzo[d]imidazole-6-carbonitrile

5c was prepared following the General Procedure **1.8** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield =76%.

^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ 13.27 (s, 1H), 8.20 – 8.00 (m, 3H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.65 – 7.53 (m, 1H), 7.52 – 7.30 (m, 8H), 5.83 (s, 2H).

^{13}C NMR (151 MHz, DMSO) δ 146.75, 143.28, 138.07, 135.69, 135.56, 129.84, 129.41, 129.26, 129.22, 129.03, 128.73, 128.70, 128.38, 126.84, 124.60, 120.23, 116.78, 113.44, 104.57, 58.96.

HRMS m/z (ESI) calcd. For $C_{23}H_{17}N_6O^+$ $(M+H)^+$= 377.1509 found: 377.1506.



5d

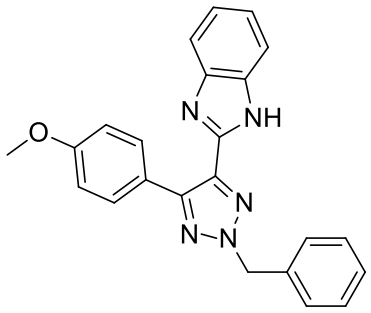
2-(2-benzyl-5-phenyl-2H-1,2,3-triazol-4-yl)-6-(trifluoromethyl)-1H benzo[d]imidazole

5d was prepared following the General Procedure **1.8** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield =81%.

^{1}H NMR (600 MHz, DMSO-d6) δ 13.39 (s, 1H), 8.16 – 8.10 (m, 2H), 7.95 (s, 1H), 7.77 (d, *J* = 8.3 Hz, 1H), 7.55 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.48 (dd, *J* = 8.2, 6.3 Hz, 2H), 7.46 – 7.39 (m, 5H), 7.38 – 7.34 (m, 1H), 5.85 (s, 2H).

^{13}C NMR (151 MHz, DMSO) δ 146.75, 146.42, 135.74, 135.22, 129.72, 128.92, 128.81, 128.65, 128.33, 128.27, 128.21, 128.04, 127.79, 125.99 (q, *J* = 271.7 Hz), 124.19, 123.63, 123.42 (q, *J* = 32.0 Hz), 123.21, 123.00, 119.12, 58.72.

HRMS m/z (ESI) calcd. For $C_{23}H_{17}F_3N_5^+$ $(M+H)^+$= 420.1431 found: 420.1431.



5e

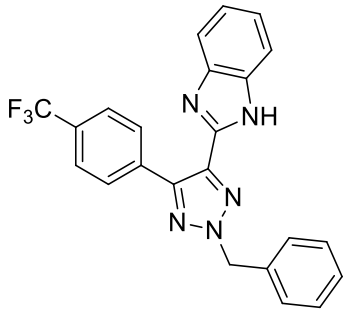
2-(2-benzyl-5-(4-methoxyphenyl)-2H-1,2,3-triazol-4-yl)-1H-benzo[d]imidazole

5e was prepared following the General Procedure **1.8** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield =83%.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 12.92 (s, 1H), 8.16 (d, *J* = 8.5 Hz, 2H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 7.7 Hz, 1H), 7.44 – 7.35 (m, 4H), 7.28 – 7.15 (m, 2H), 7.03 (dd, *J* = 8.7, 1.4 Hz, 2H), 5.80 (s, 2H), 3.81 (d, *J* = 1.3 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 160.20, 146.10, 144.60, 143.81, 136.07, 135.90, 134.82, 130.39, 129.28, 128.74, 128.40, 123.50, 122.54, 122.19, 119.63, 114.17, 112.06, 58.78, 55.67.

HRMS m/z (ESI) calcd. For $C_{23}H_{20}N_5O^+(M+H)^+$= 382.1662 found: 382.1665.



5f

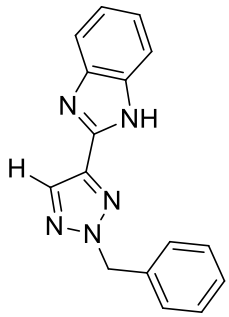
2-(2-benzyl-5-(4-(trifluoromethyl)phenyl)-2H-1,2,3-triazol-4-yl)-1H benzo[d]imidazole

5f was prepared following the General Procedure **1.8** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield =71%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 13.05 (s, 1H), 8.44 (d, J = 8.1 Hz, 2H), 7.86 (d, J = 8.1 Hz, 2H), 7.67 (d, J = 7.9 Hz, 1H), 7.53 (d, J = 7.8 Hz, 1H), 7.48 – 7.33 (m, 5H), 7.25 (dt, J = 14.1, 7.4 Hz, 2H), 5.86 (s, 2H).

^{13}C NMR (101 MHz, DMSO) δ 144.77, 144.02, 143.75, 137.16, 135.61, 134.87, 134.23, 129.77, 129.30, 128.83, 128.48, 126.05, 125.65, 123.71, 123.35, 122.33, 119.75, 112.18, 59.04.

HRMS m/z (ESI) calcd. For $C_{23}H_{16}N_5F_3^+(M+H)^+$= 420.1431 found: 420.1429.



5g

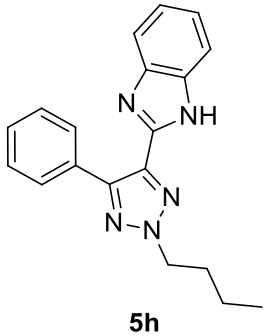
2-(2-benzyl-2H-1,2,3-triazol-4-yl)-1H-benzo[d]imidazole

5g was prepared following the General Procedure **1.8** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield =79%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 13.06 (s, 1H), 8.40 (s, 1H), 7.66 (d, J = 7.6 Hz, 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.44 – 7.30 (m, 5H), 7.28 – 7.13 (m, 2H), 5.79 (s, 2H).

^{13}C NMR (101 MHz, DMSO) δ 144.06, 140.77, 135.98, 134.21, 129.21, 128.67, 128.33, 122.98, 118.98, 112.11, 58.69.

HRMS m/z (ESI) calcd. For $C_{16}H_{14}N_5^+$ $(M+H)^+$= 276.1244 found: 276.1244.



5h

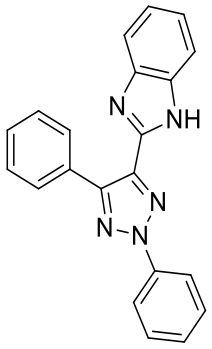
2-(2-butyl-5-phenyl-2H-1,2,3-triazol-4-yl)-1H-benzo[d]imidazole

5h was prepared following the General Procedure **1.8** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield =85%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.93 (s, 1H), 8.24 – 8.11 (m, 2H), 7.67 (d, J = 7.9 Hz, 1H), 7.53 (d, J = 7.8 Hz, 1H), 7.46 (dt, J = 13.2, 6.7 Hz, 3H), 7.23 (dd, J = 13.9, 7.7 Hz, 2H), 4.58 (t, J = 7.0 Hz, 2H), 1.98 (q, J = 7.3 Hz, 2H), 1.38 (q, J = 7.4 Hz, 2H), 0.94 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 145.64, 144.59, 143.82, 135.93, 134.82, 130.38, 129.17, 128.91, 128.72, 123.46, 122.18, 119.64, 112.04, 55.10, 31.59, 19.72, 13.87.

HRMS m/z (ESI) calcd. For $C_{19}H_{20}N_5^+$ $(M+H)^+$= 318.1713 found: 318.1714.



5i

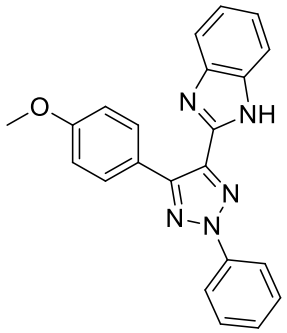
2-(2,5-diphenyl-2H-1,2,3-triazol-4-yl)-1H-benzo[d]imidazole

5i was prepared following the General Procedure **1.8** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield =89%.

^{1}H NMR (600 MHz, DMSO-*d6*) δ 13.13 (s, 1H), 8.35 – 8.28 (m, 2H), 8.26 – 8.19 (m, 2H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.70 – 7.65 (m, 2H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.56 – 7.48 (m, 4H), 7.33 – 7.28 (m, 1H), 7.27 – 7.22 (m, 1H).

^{13}C NMR (151 MHz, DMSO) δ 147.46, 143.99, 143.86, 139.17, 137.95, 134.82, 130.33, 129.75, 129.26, 128.97, 128.82, 123.84, 122.37, 119.84, 119.24, 112.14.

HRMS m/z (ESI) calcd. For $C_{21}H_{16}N_5^+$ $(M+H)^+$= 338.1400 found: 338.1401.



5j

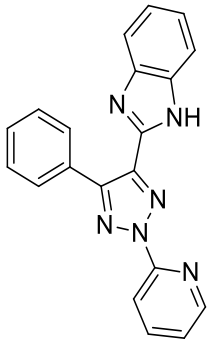
2-(5-(4-methoxyphenyl)-2-phenyl-2H-1,2,3-triazol-4-yl)-1H-benzo[d]imidazole

5j was prepared following the General Procedure **1.8** and purified by flash Chromatography (Hexane: Ethyl Acetate = 4:1) as white solid. Yield =77%.

^{1}H NMR (600 MHz, DMSO-*d6*) δ 13.10 (s, 1H), 8.35 – 8.28 (m, 2H), 8.26 – 8.13 (m, 2H), 7.73 (s, 1H), 7.69 – 7.63 (m, 2H), 7.60 (s, 1H), 7.54 – 7.48 (m, 1H), 7.27 (d, *J* = 22.9 Hz, 2H), 7.13 – 7.06 (m, 2H), 3.84 (s, 3H).

^{13}C NMR (151 MHz, DMSO) δ 160.56, 147.32, 144.22, 143.88, 139.19, 137.48, 134.79, 130.71, 130.28, 128.80, 123.66, 122.41, 122.05, 119.75, 119.13, 114.25, 112.05, 55.71.

HRMS m/z (ESI) calcd. For $C_{22}H_{17}N_5O^+$$(M+H)^+$= 368.1506 found: 368.1504.



5k

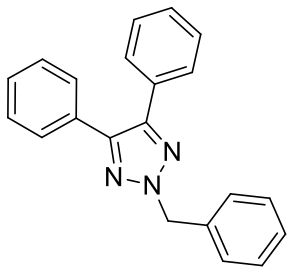
2-(5-phenyl-2-(pyridin-2-yl)-2H-1,2,3-triazol-4-yl)-1H-benzo[d]imidazole

5i was prepared following the General Procedure **1.8** and purified by flash Chromatography (Hexane: Ethyl Acetate = 3:1) as white solid. Yield =82%.

^{1}H NMR (600 MHz, DMSO-d_6) δ 13.23 (s, 1H), 8.67 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.37 – 8.27 (m, 2H), 8.23 (d, *J* = 8.1 Hz, 1H), 8.17 (td, *J* = 7.8, 1.9 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.59 (dd, *J* = 7.4, 4.8 Hz, 2H), 7.57 – 7.45 (m, 3H), 7.27 (dt, *J* = 36.1, 7.5 Hz, 2H).

^{13}C NMR (151 MHz, DMSO) δ 150.36, 149.32, 148.05, 143.81, 140.24, 138.75, 134.88, 129.80, 129.65, 129.37, 128.73, 124.70, 123.81, 122.33, 119.81, 114.88, 112.20.

HRMS m/z (ESI) calcd. For $C_{20}H_{15}N_6^+$ $(M+H)^+$= 339.1353 found: 339.1352.



6a

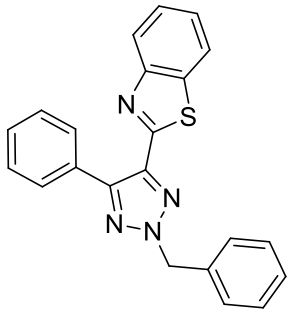
2-benzyl-4,5-diphenyl-2H-1,2,3-triazole

6a was prepared following the General Procedure **1.9** and purified by flash Chromatography (Hexane: Ethyl Acetate = 5:1) as white solid. Yield =87%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (dd, *J* = 6.7, 3.0 Hz, 4H), 7.46 – 7.40 (m, 2H), 7.39 – 7.28 (m, 9H), 5.64 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.76, 135.27, 130.99, 128.71, 128.53, 128.48, 128.37, 128.25, 128.09, 58.70.

HRMS m/z (ESI) calcd. For $C_{21}H_{18}N_3^+$ $(M+H)^+$= 312.1495 found: 312.1493.



6b

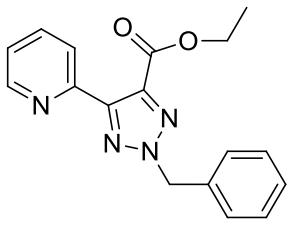
2-(2-benzyl-5-phenyl-2H-1,2,3-triazol-4-yl) benzo[d]triazole

6b was prepared following the General Procedure **1.10** and purified by flash Chromatography (Hexane: Ethyl Acetate = 5:1) as yellow solid. Yield =72%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 – 7.98 (m, 3H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.52 – 7.42 (m, 6H), 7.37 (td, *J* = 10.7, 9.2, 7.0 Hz, 4H), 5.69 (s, 2H).

^{13}C NMR (101 MHz, DMSO) δ 158.91, 153.52, 146.02, 138.85, 135.54, 134.90, 134.90, 129.74, 129.37, 129.33, 128.88, 128.81, 128.66, 127.11, 126.49, 123.64, 122.70, 58.95.

HRMS m/z (ESI) calcd. For $C_{22}H_{17}N_4S^+$ $(M+H)^+$= 369.1168 found: 369.1165.



6c

ethyl 2-benzyl-5-(pyridin-2-yl)-2H-1,2,3-triazole-4-carboxylate

6a was prepared following the General Procedure **1.9** and purified by flash Chromatography (Hexane: Ethyl Acetate = 2:1) as pale yellow solid. Yield =80%.

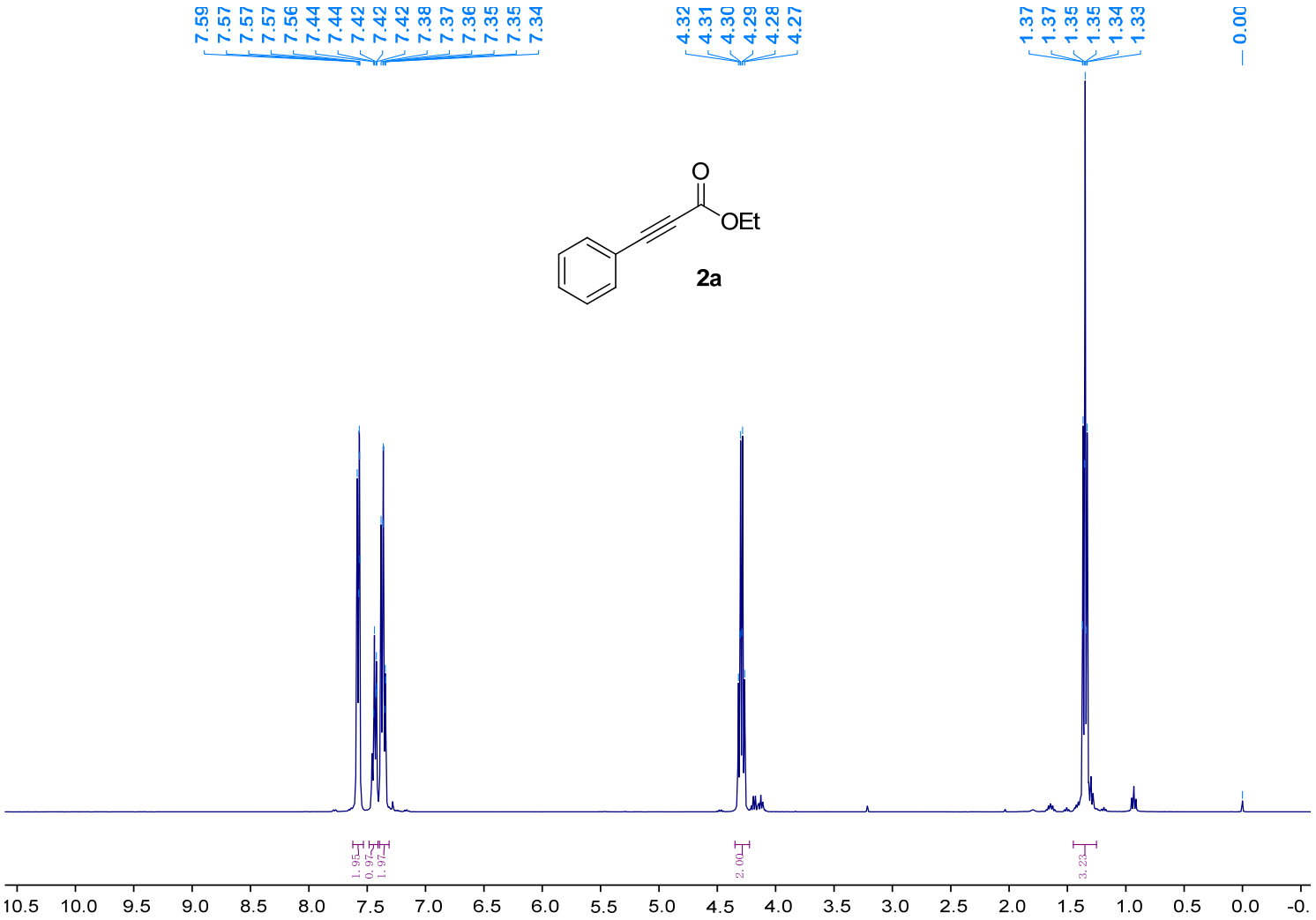
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.77 (d, *J* = 4.9 Hz, 1H), 7.73 (td, *J* = 7.8, 1.7 Hz, 1H), 7.53 (d, *J* = 7.9 Hz, 1H), 7.43 – 7.34 (m, 1H), 7.22 – 7.10 (m, 3H), 7.00 – 6.90 (m, 2H), 5.82 (s, 2H), 4.36 (q, *J* = 7.1 Hz, 2H), 1.33 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.94, 149.30, 145.84, 138.81, 136.98, 136.30, 134.57, 128.48, 128.11, 127.61, 127.04, 124.25, 77.32, 77.24, 76.93, 76.68, 76.61, 61.17, 52.72, 14.08.

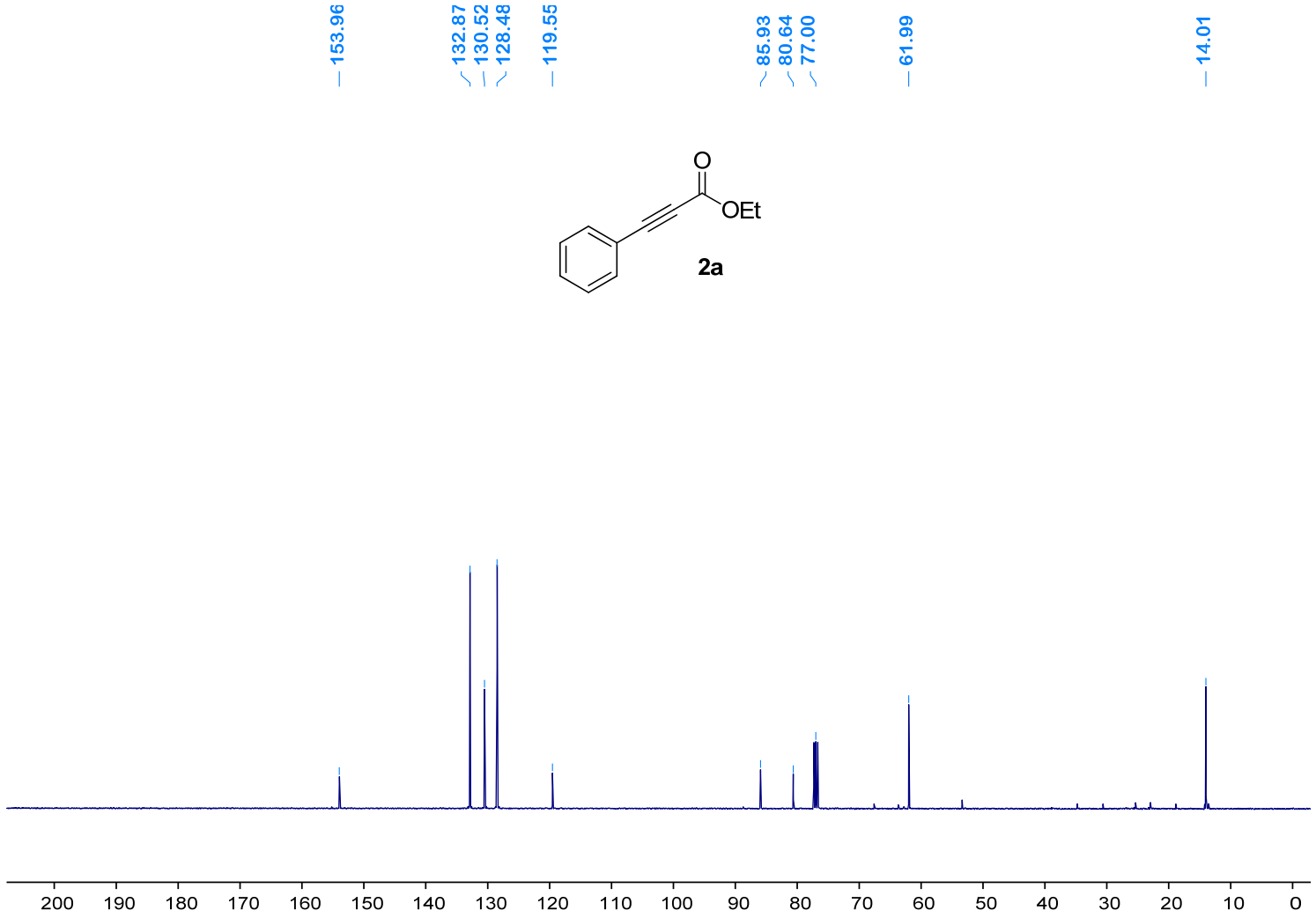
HRMS m/z (ESI) calcd. For $C_{17}H_{17}N_4O_2^+$ $(M+H)^+$= 309.1346 found: 309.1327.

III. NMR Spectra Data

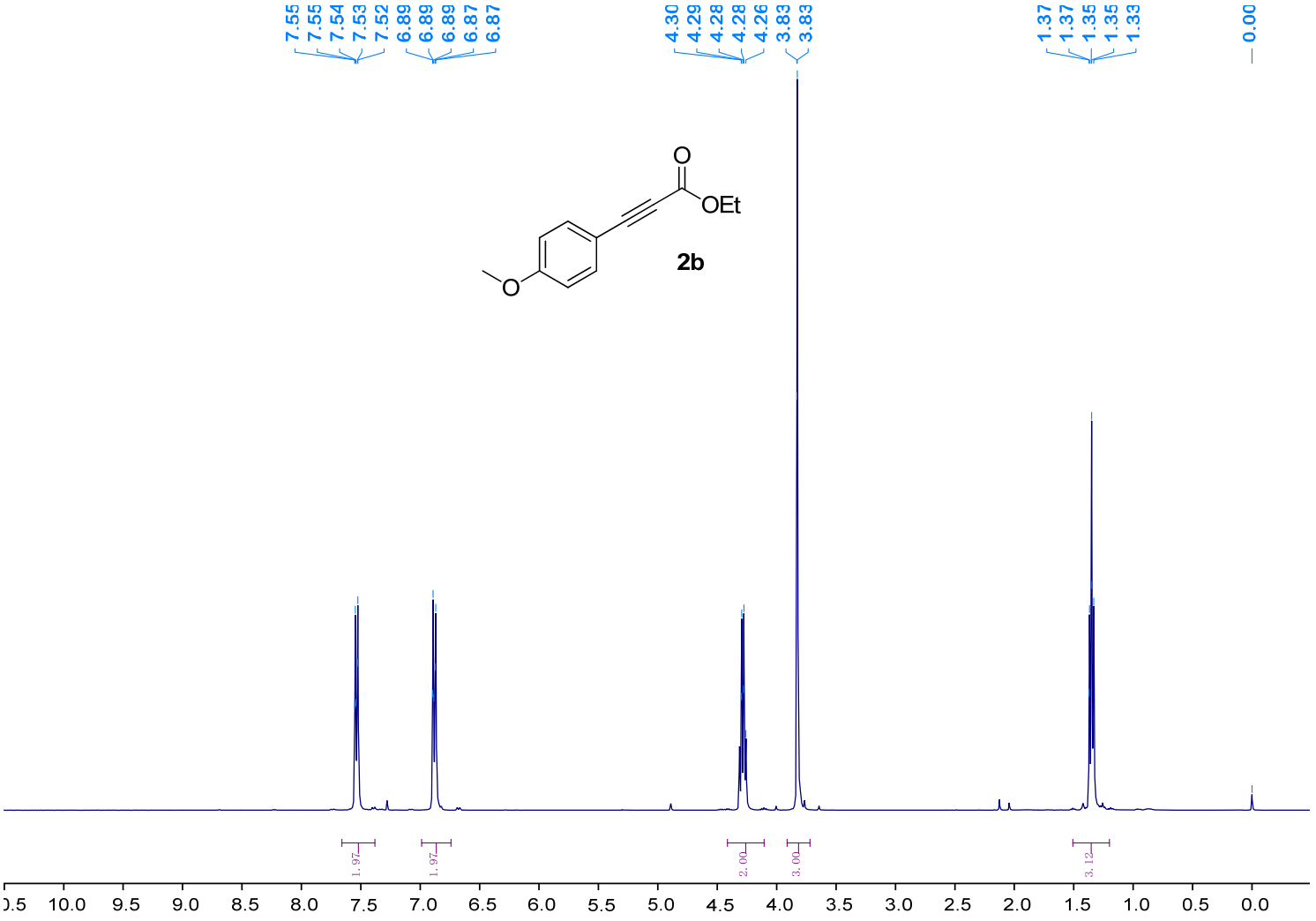
^{1}H NMR of compound 2a



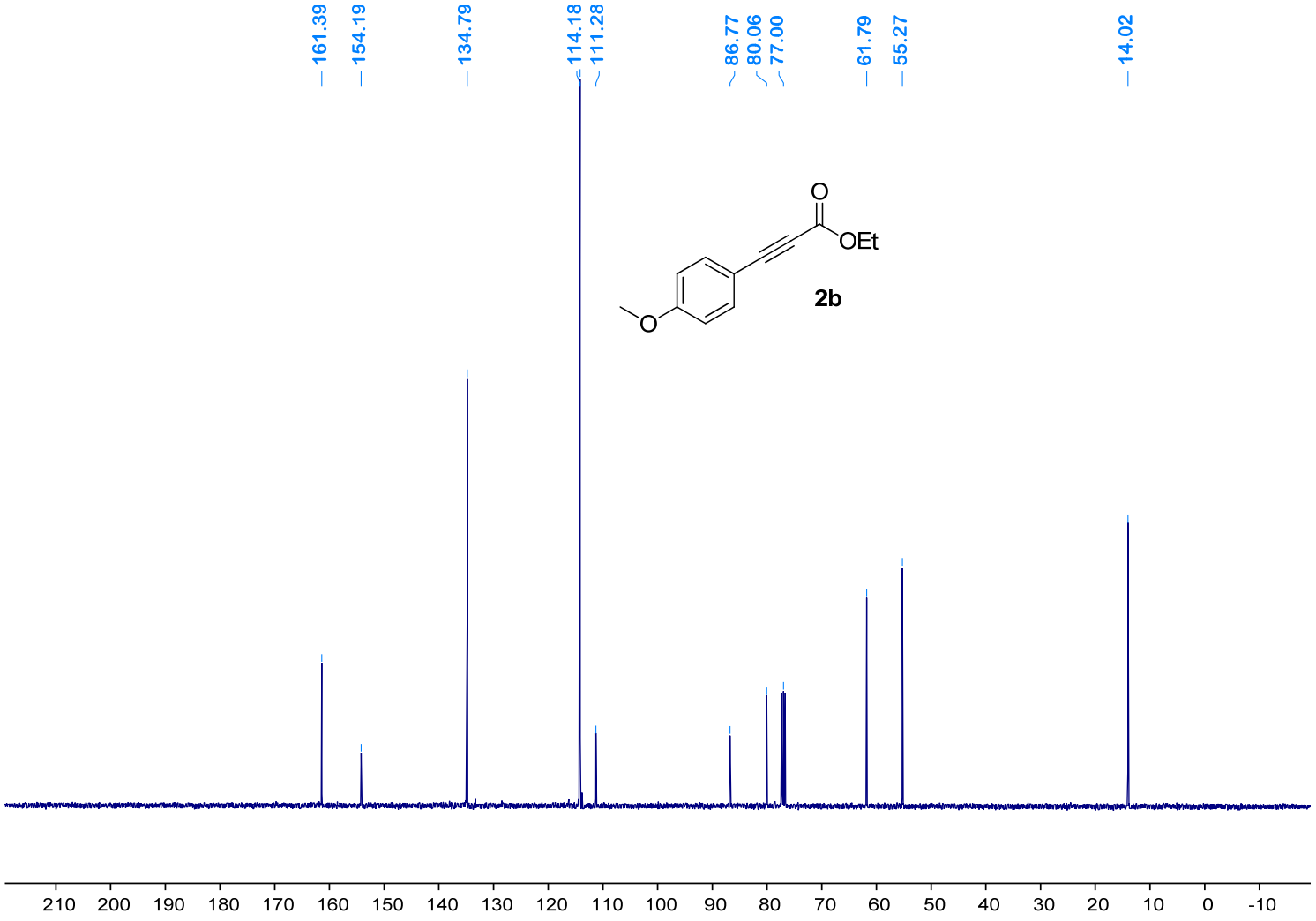
^{13}C NMR of compound 2a



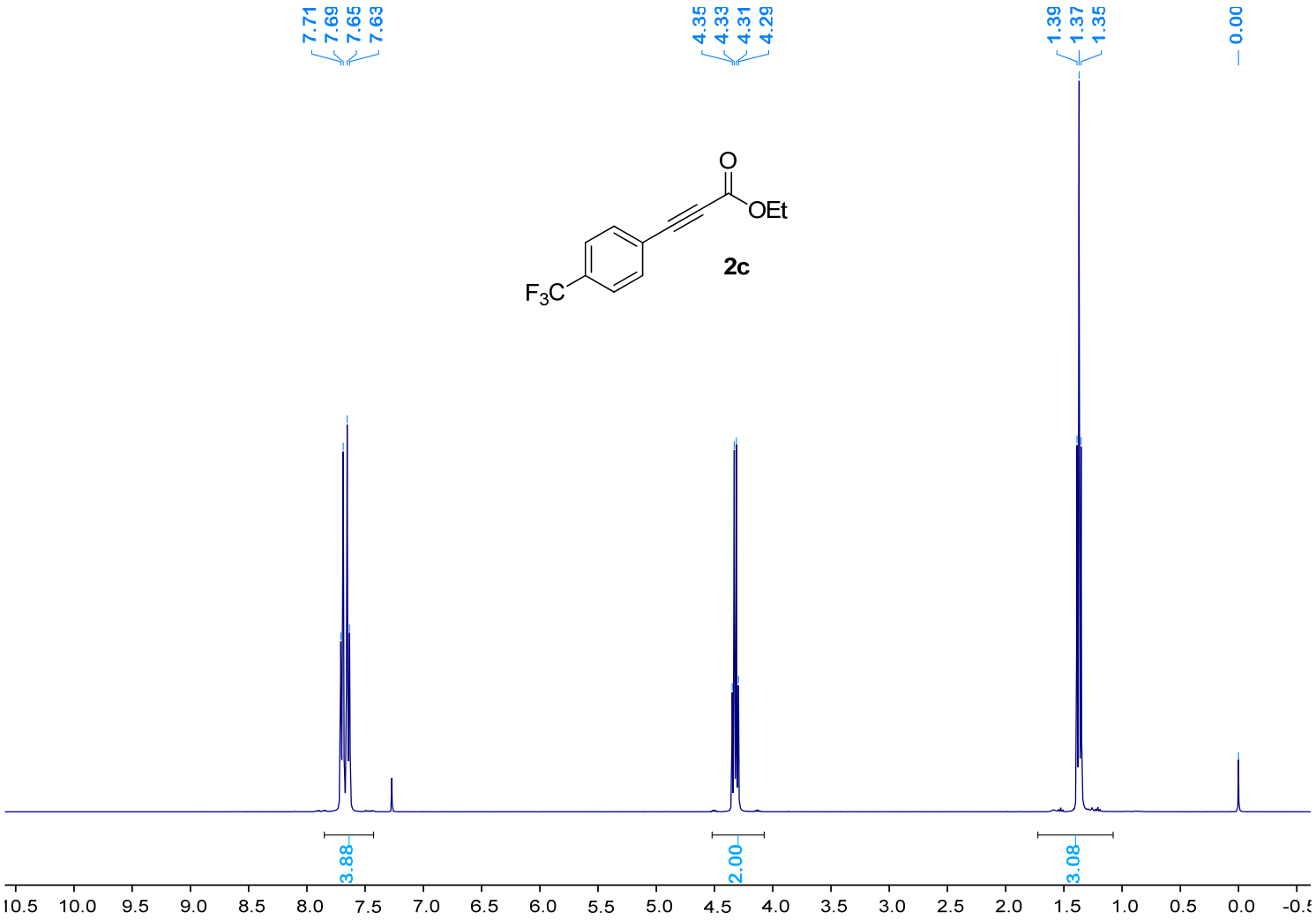
^{1}H NMR of compound 2b



^{13}C NMR of compound 2b



^{1}H NMR of compound 2c



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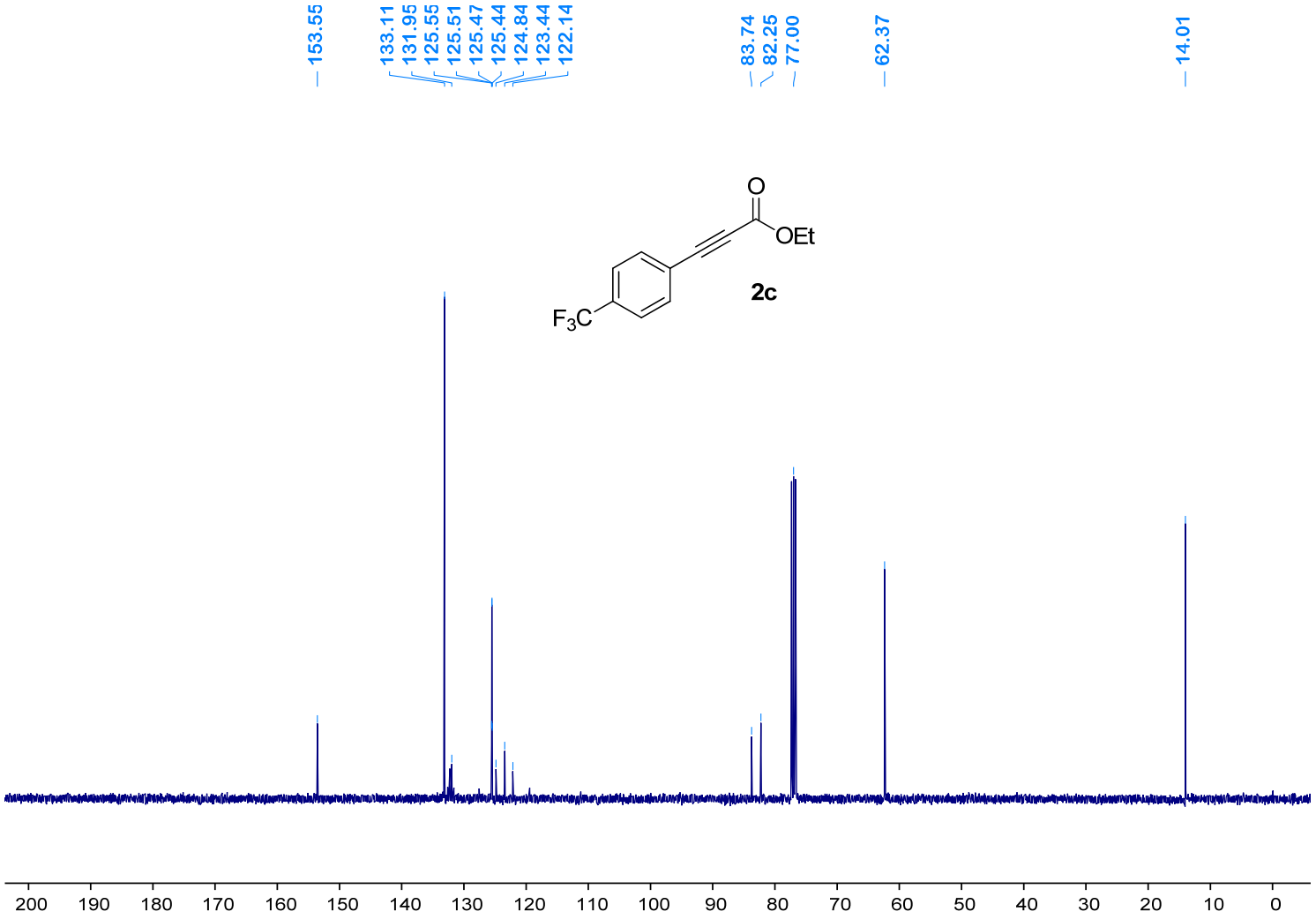
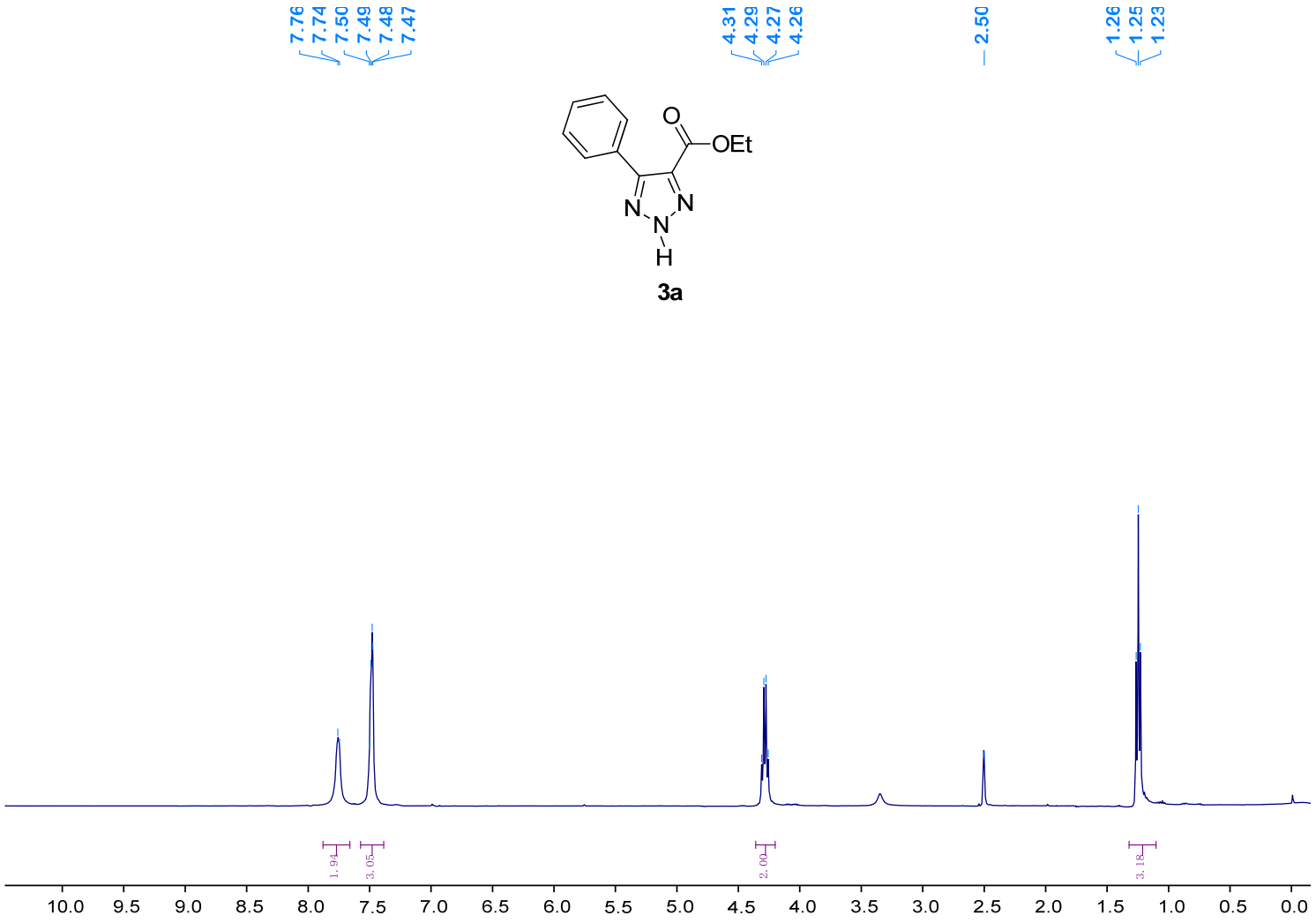
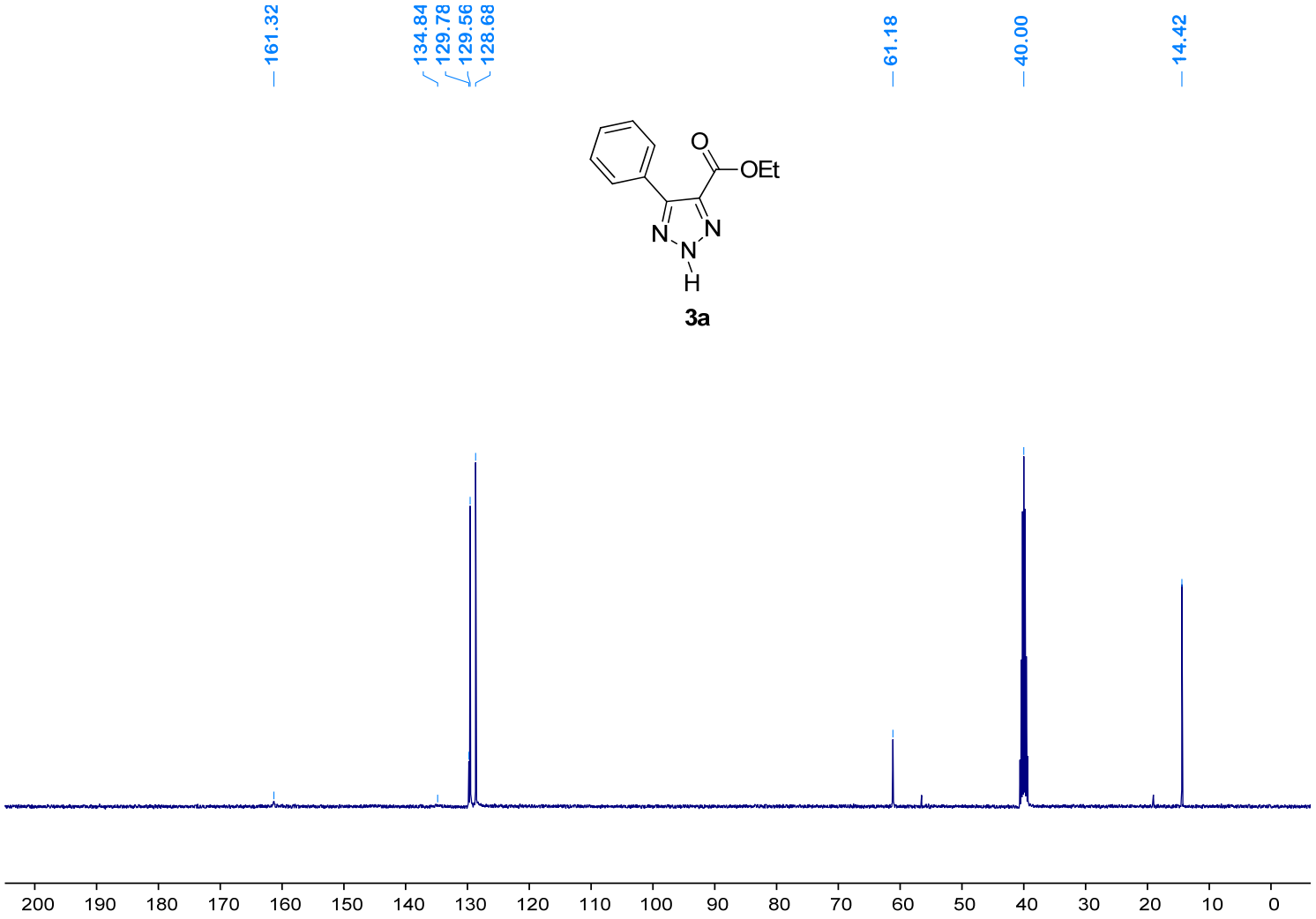


^{1}H NMR of compound 3a

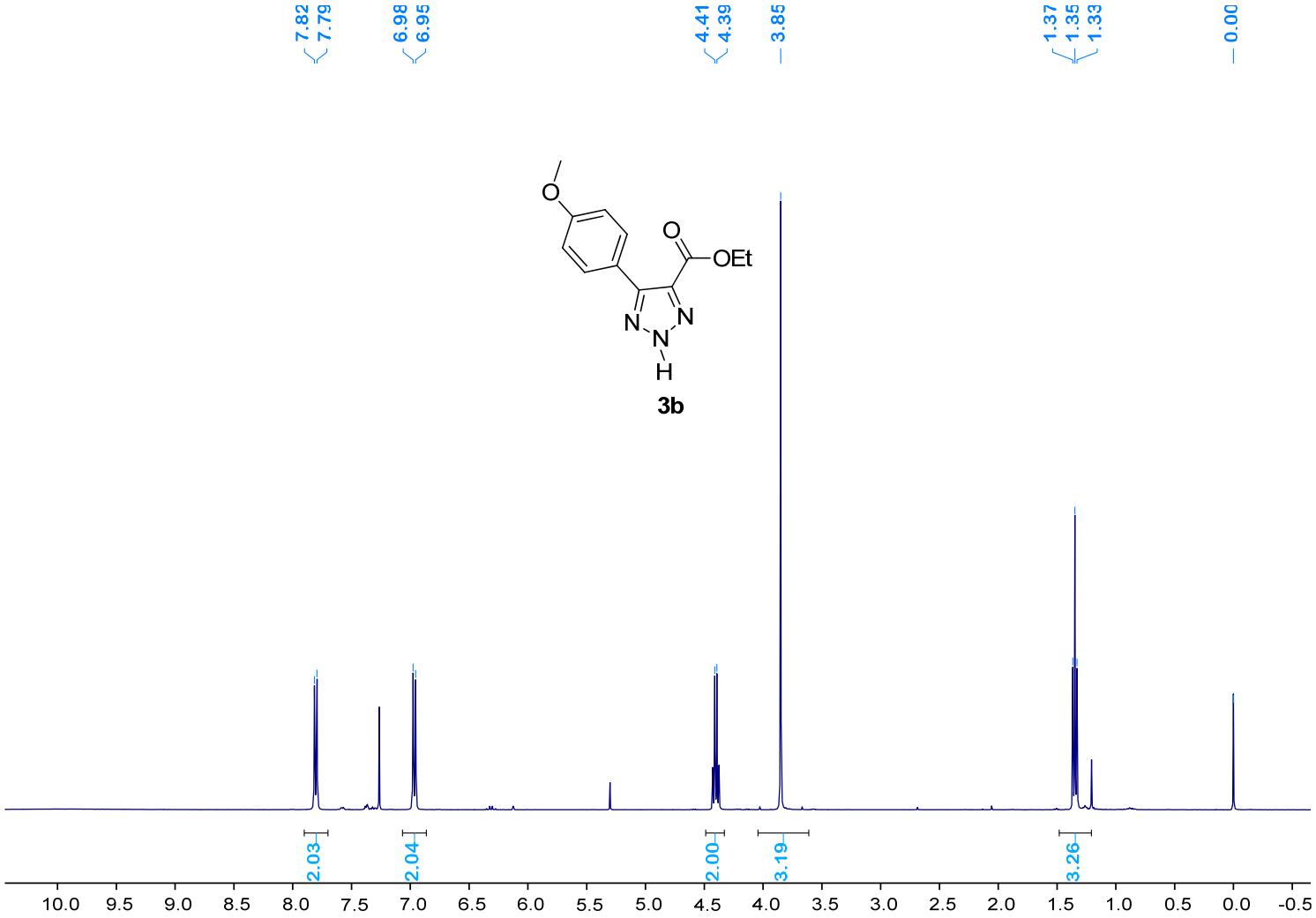


3a

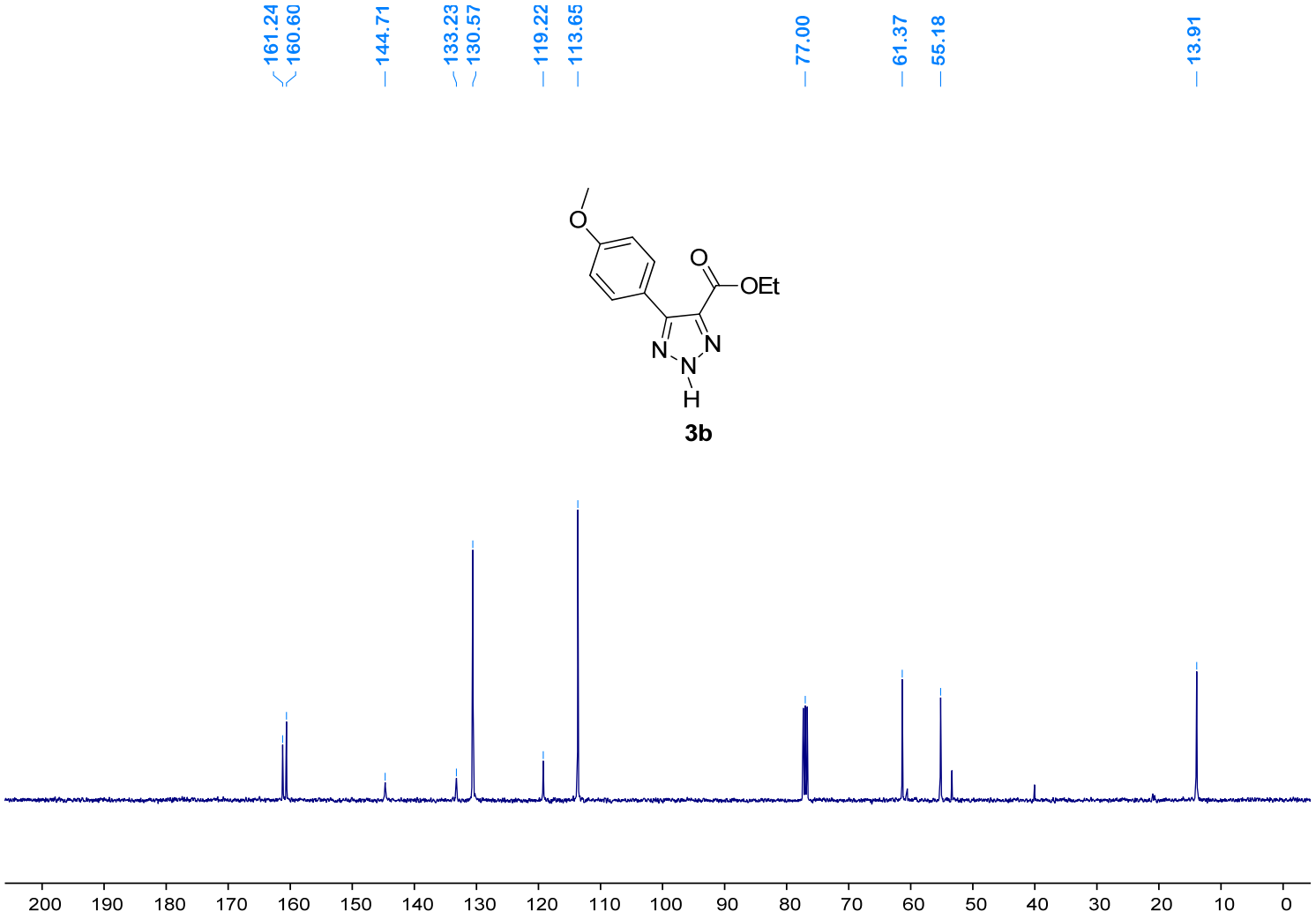
^{13}C NMR of compound 3a



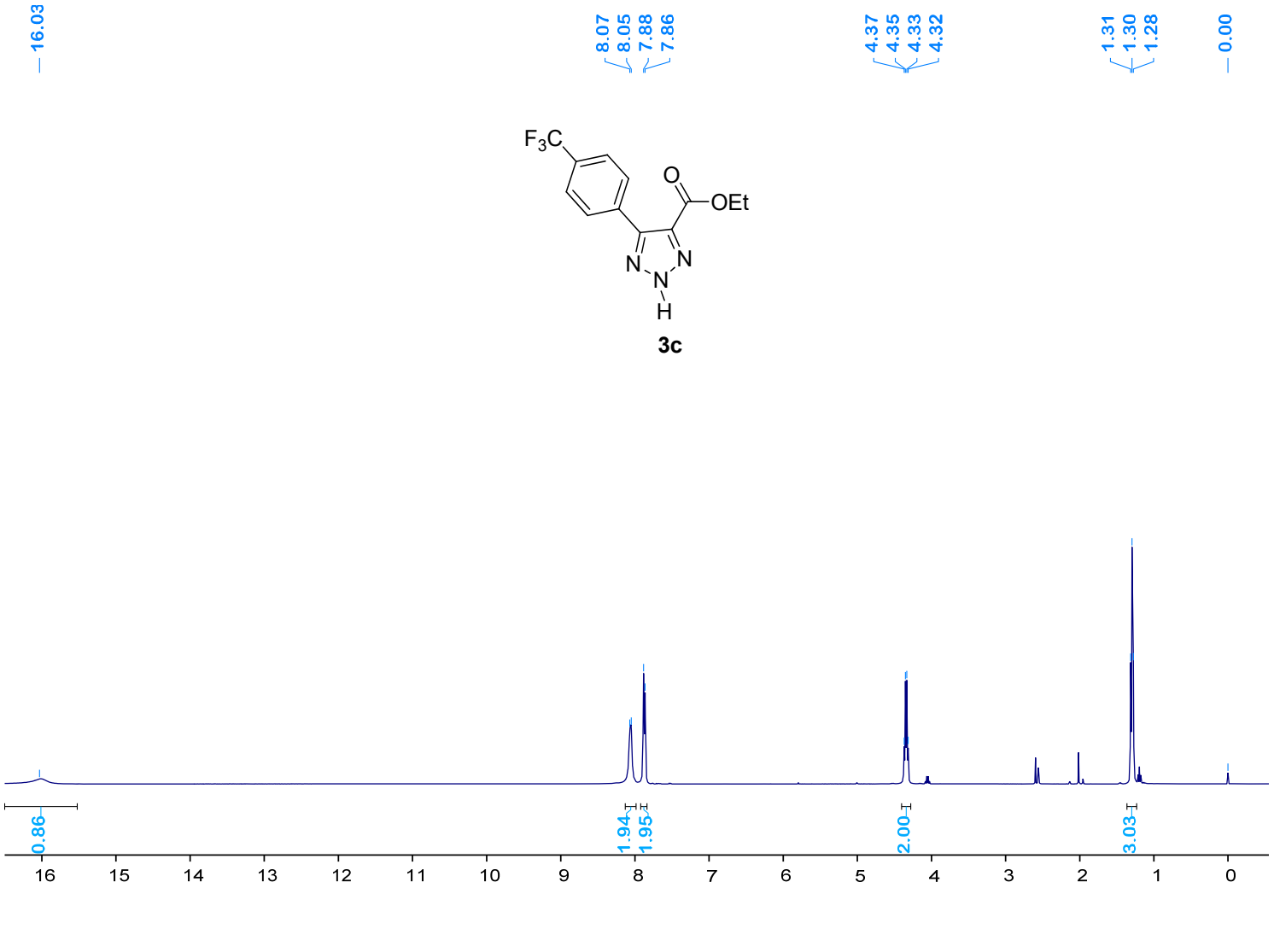
[1]H NMR of compound 3b



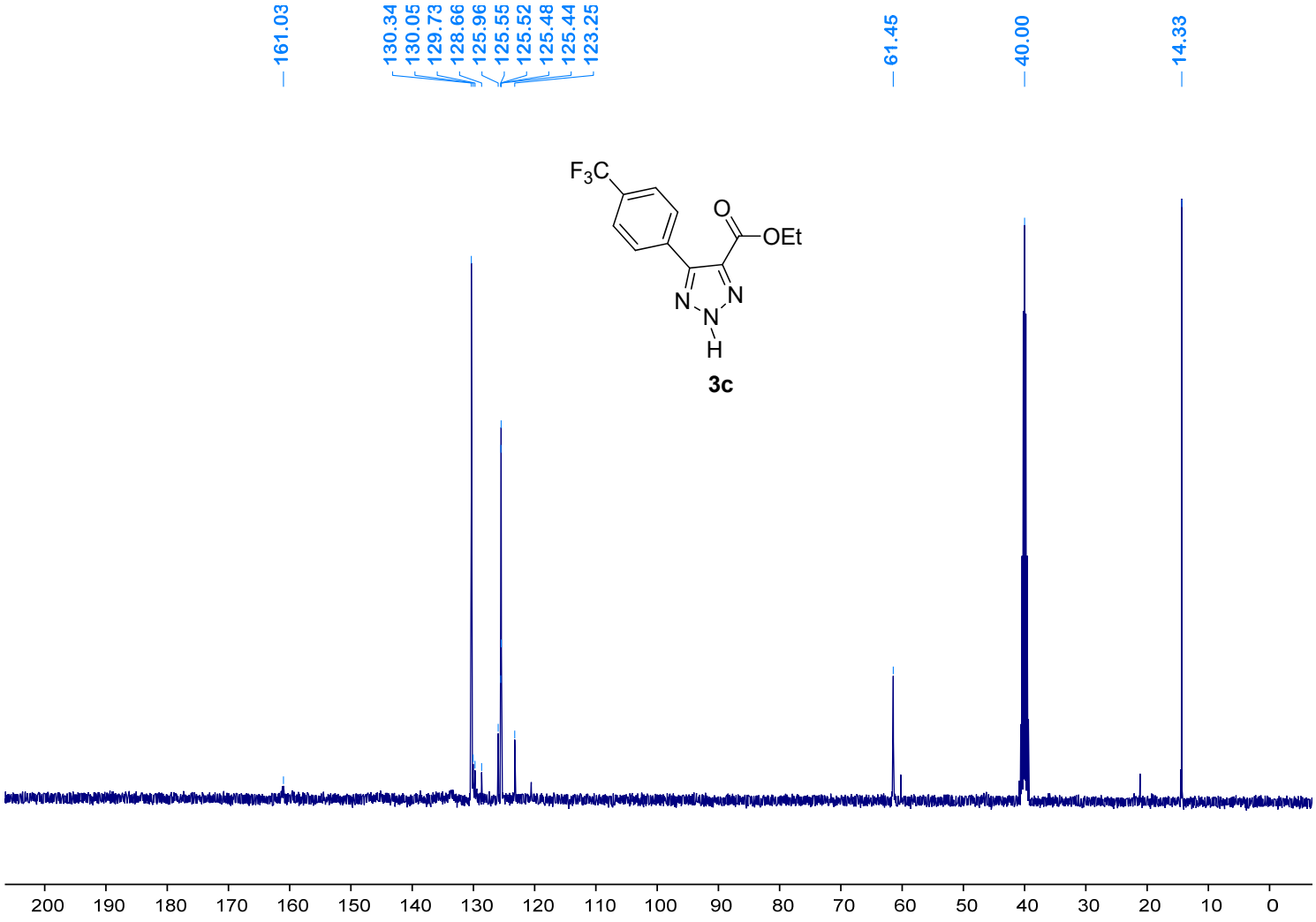
^{13}C NMR of compound 3b



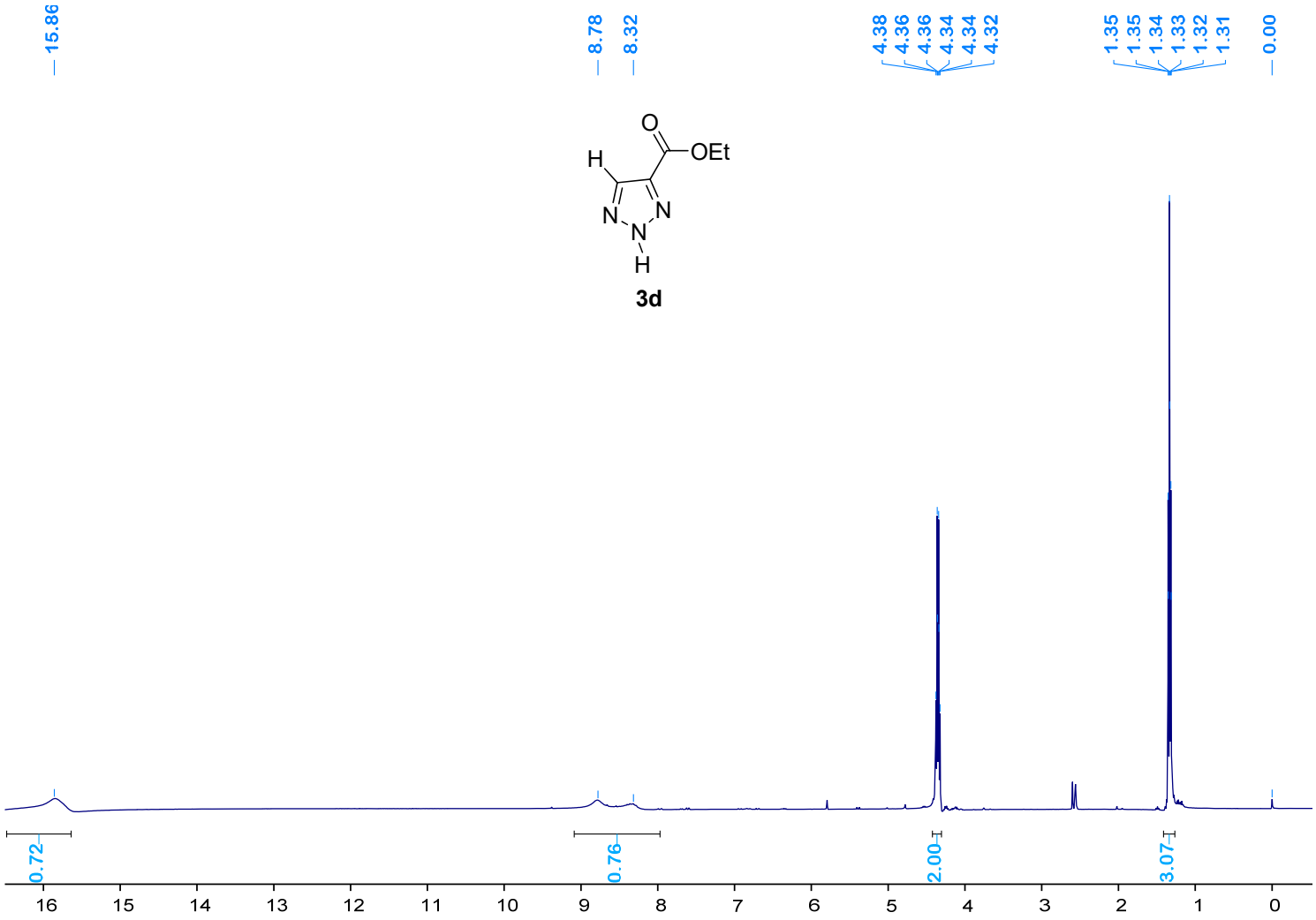
^{1}H NMR of compound 3c



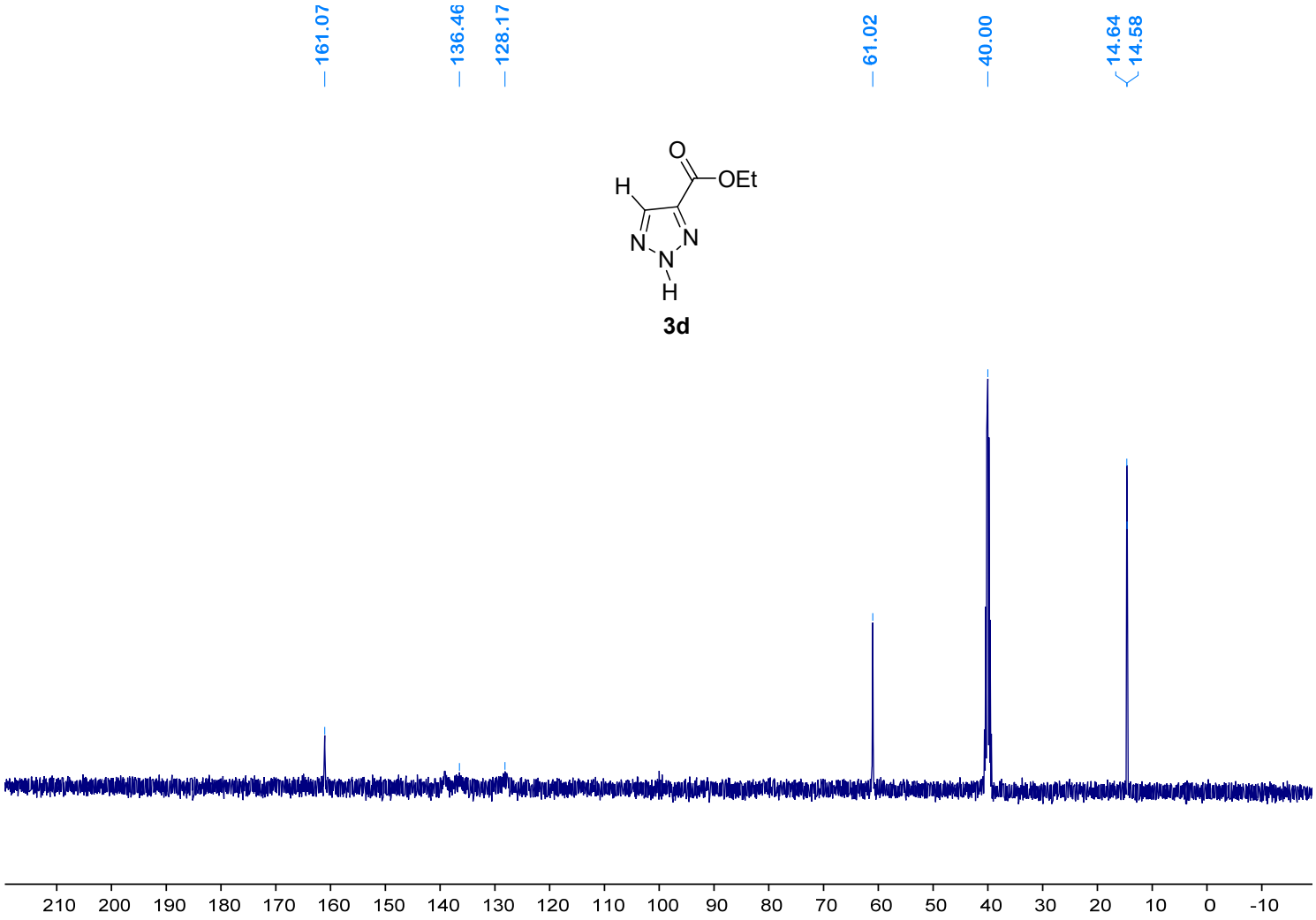
^{13}C NMR of compound 3c



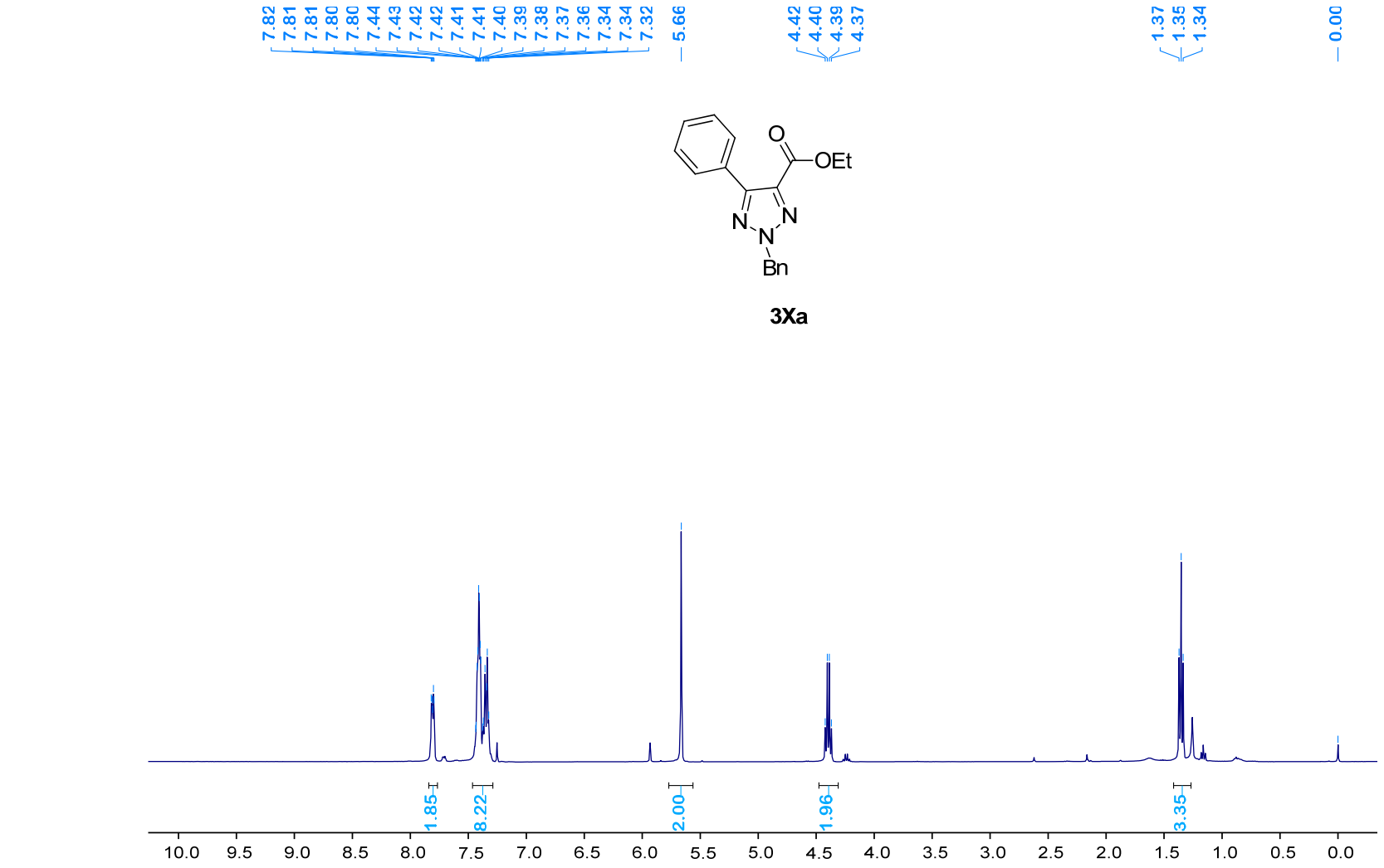
^{1}H NMR of compound 3d



^{13}C NMR of compound 3d

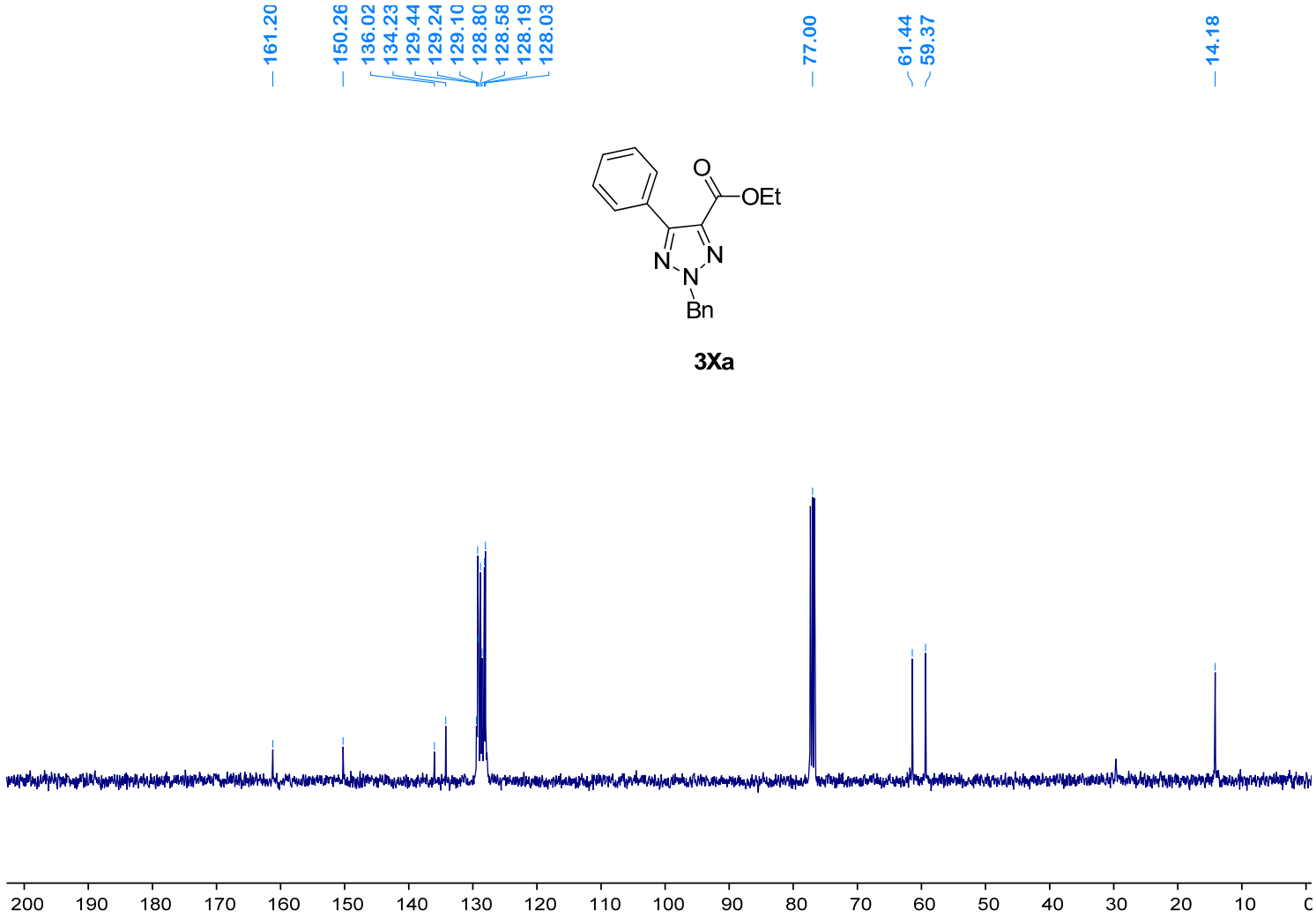


^{1}H NMR of compound 3Xa



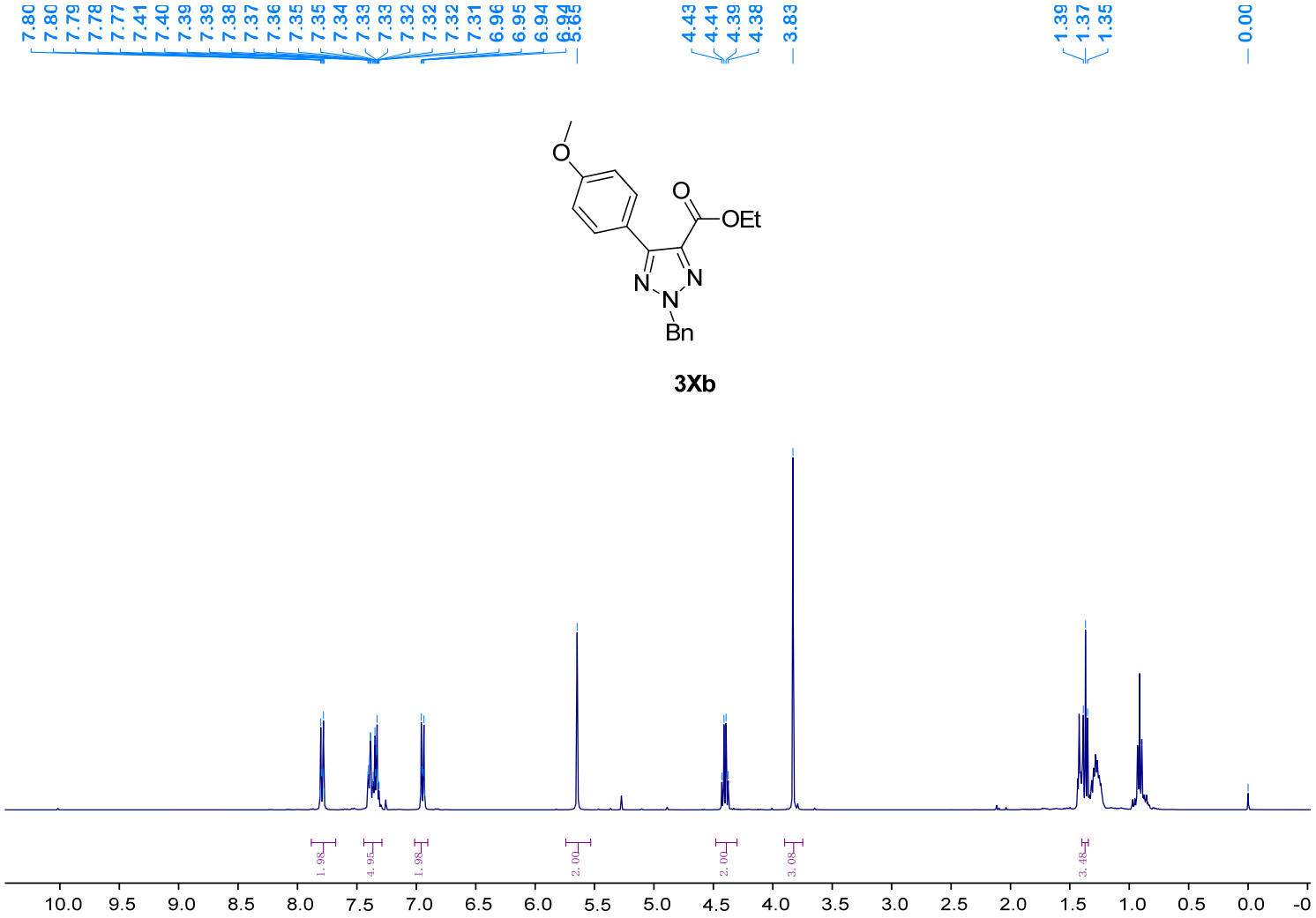
3Xa

^{13}C NMR of compound 3Xa



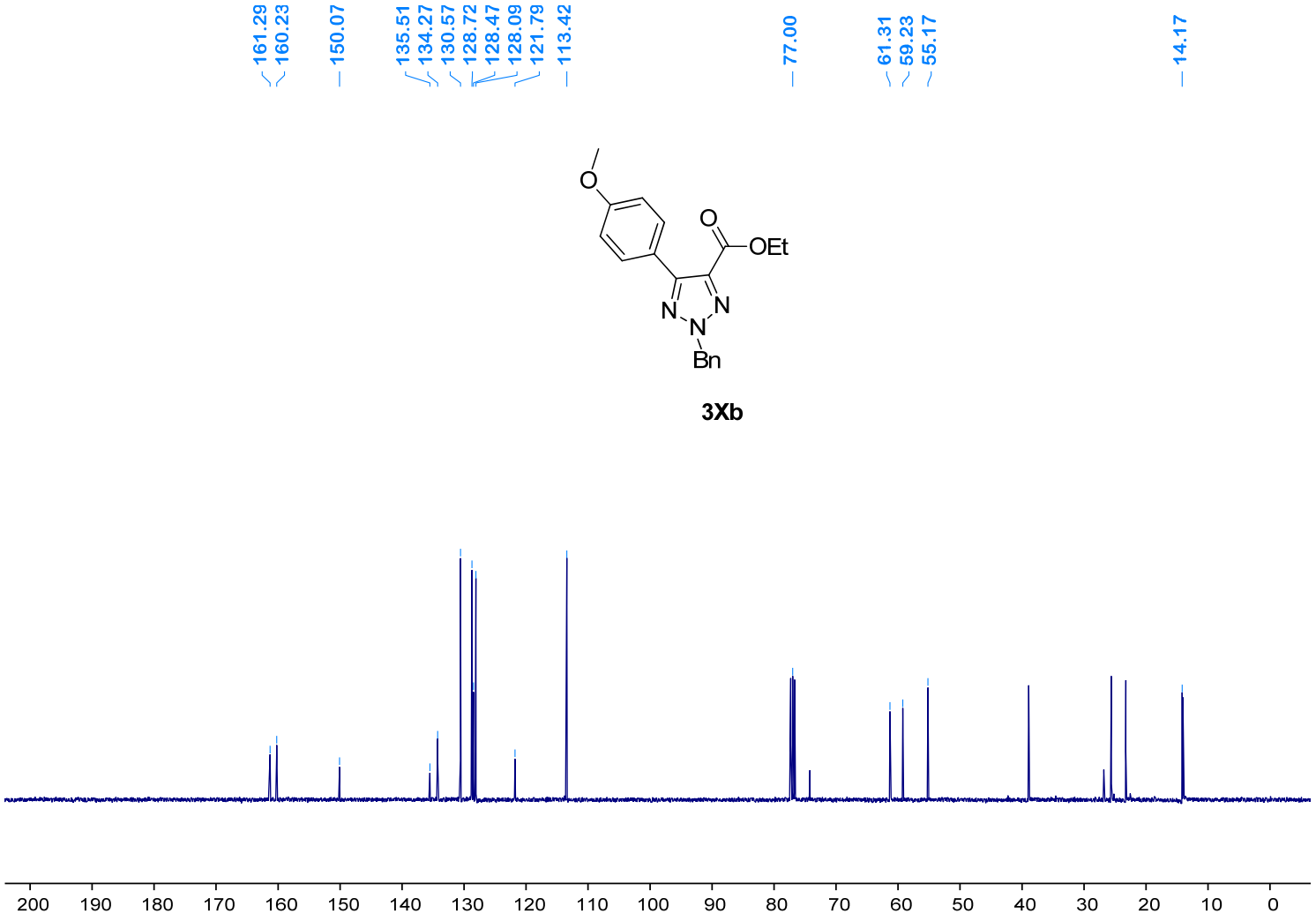
3Xa

^{1}H NMR of compound 3Xb



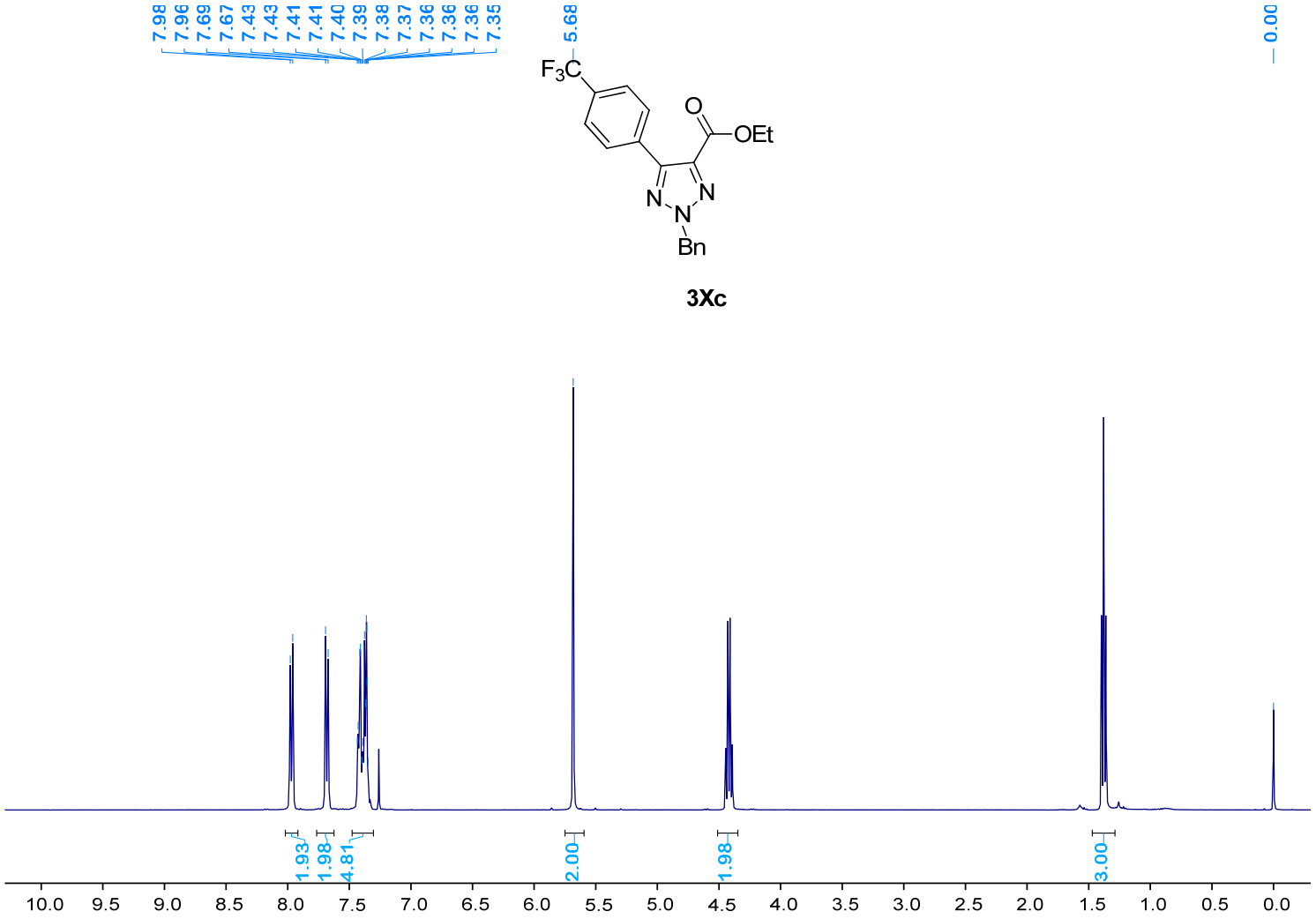
3Xb

^{13}C NMR of compound 3Xb



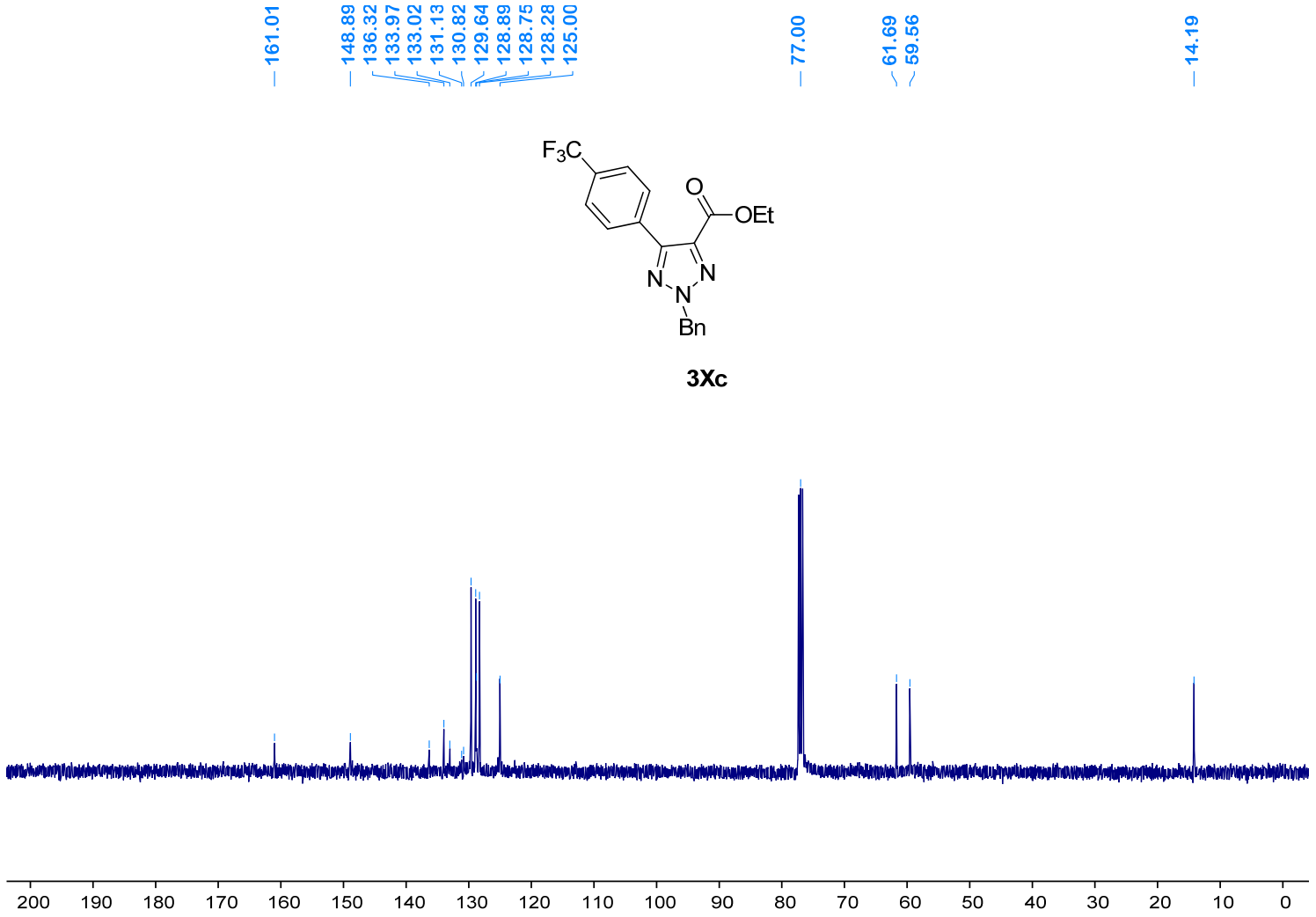
3Xb

[1]H NMR of compound 3Xc



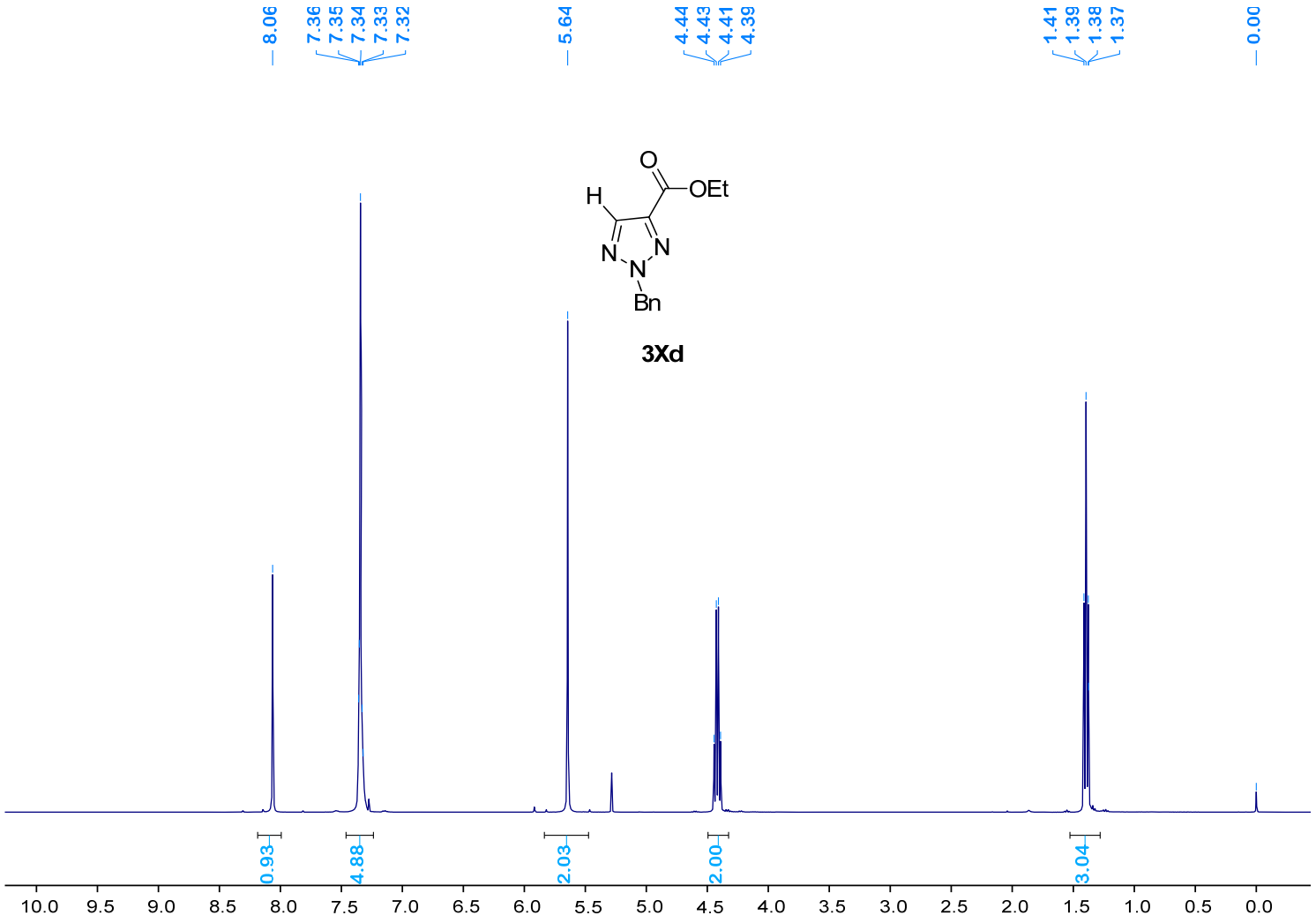
3Xc

^{13}C NMR of compound 3Xc

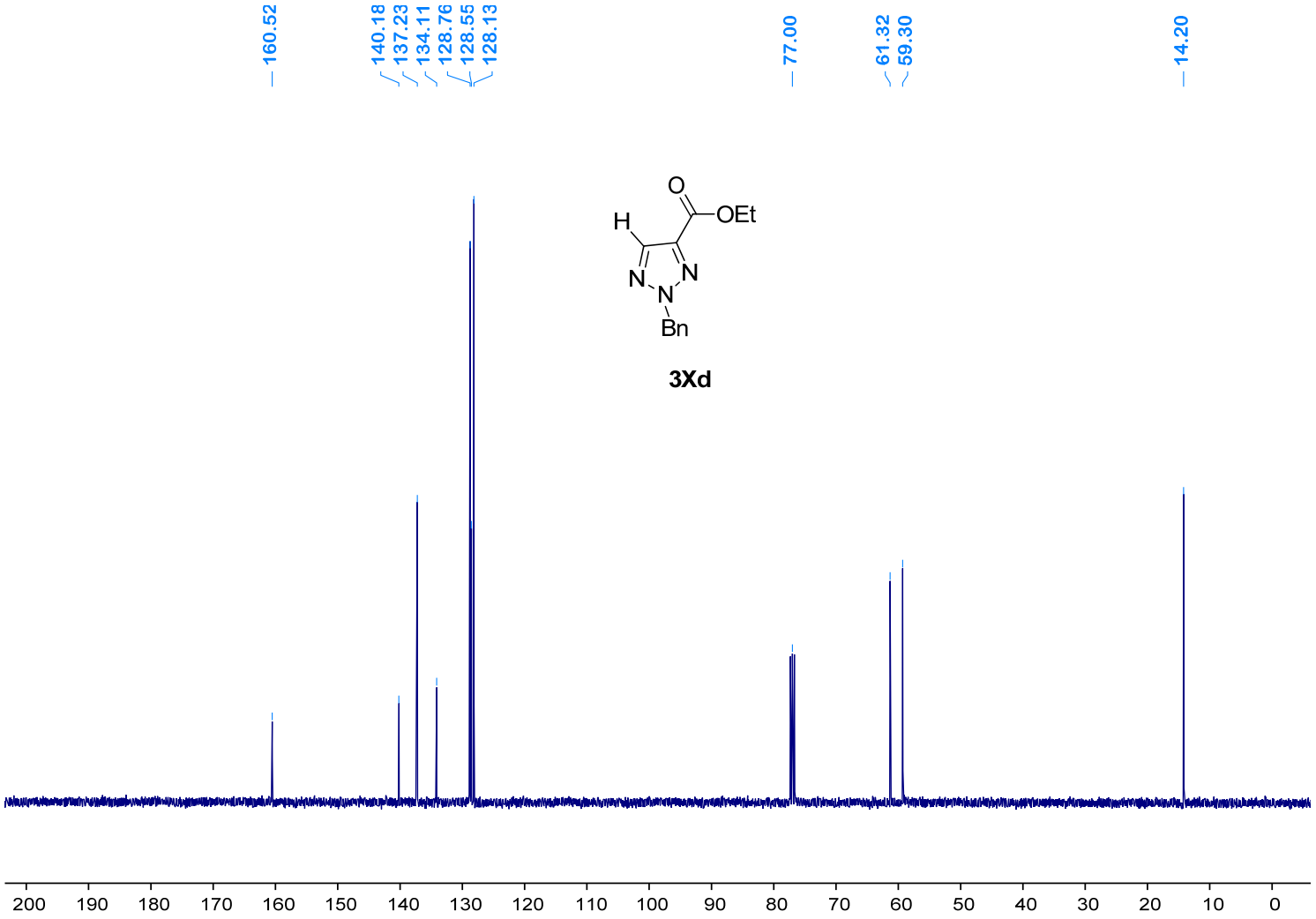


3Xc

^{1}H NMR of compound 3Xd

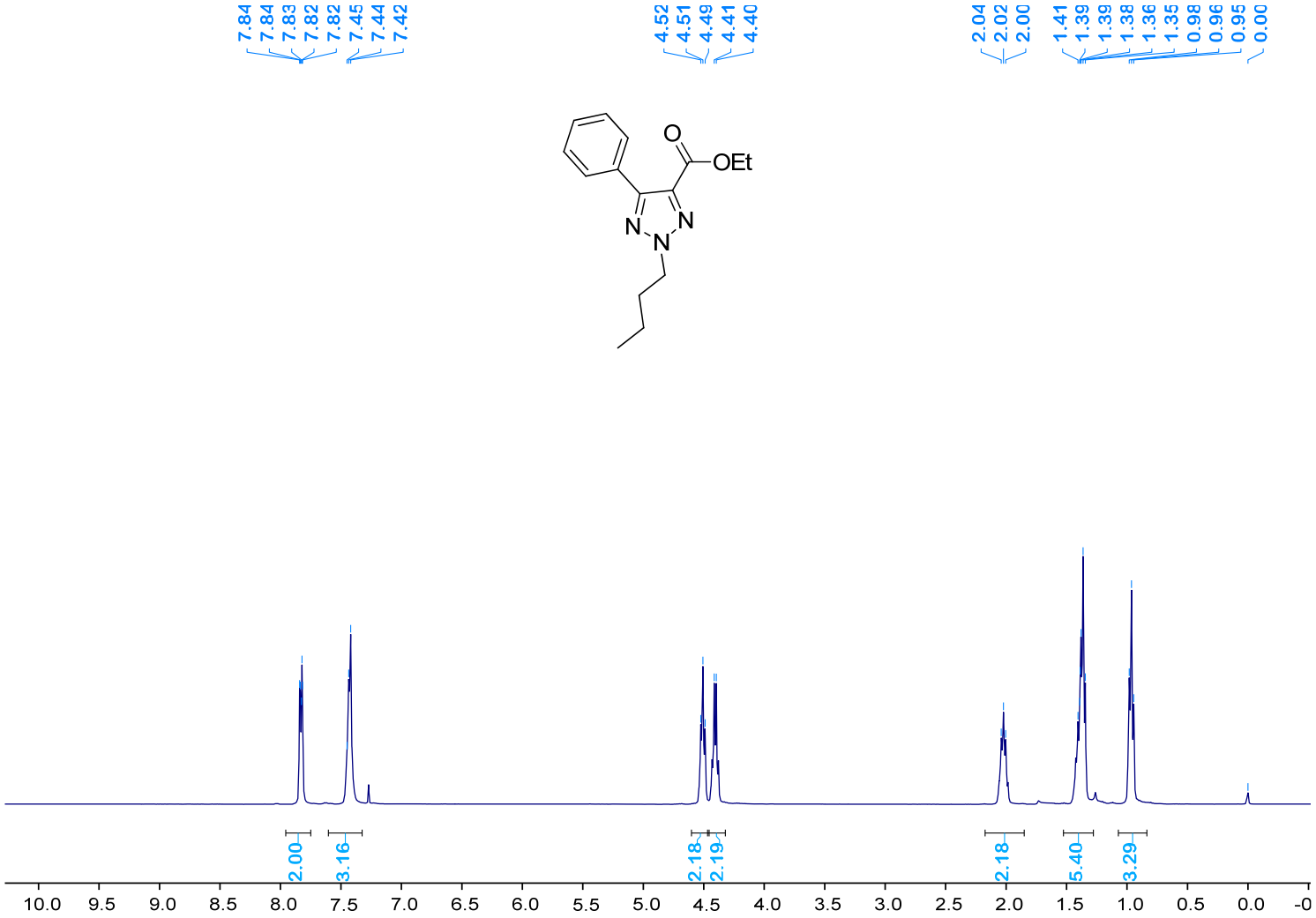


^{13}C NMR of compound 3Xd

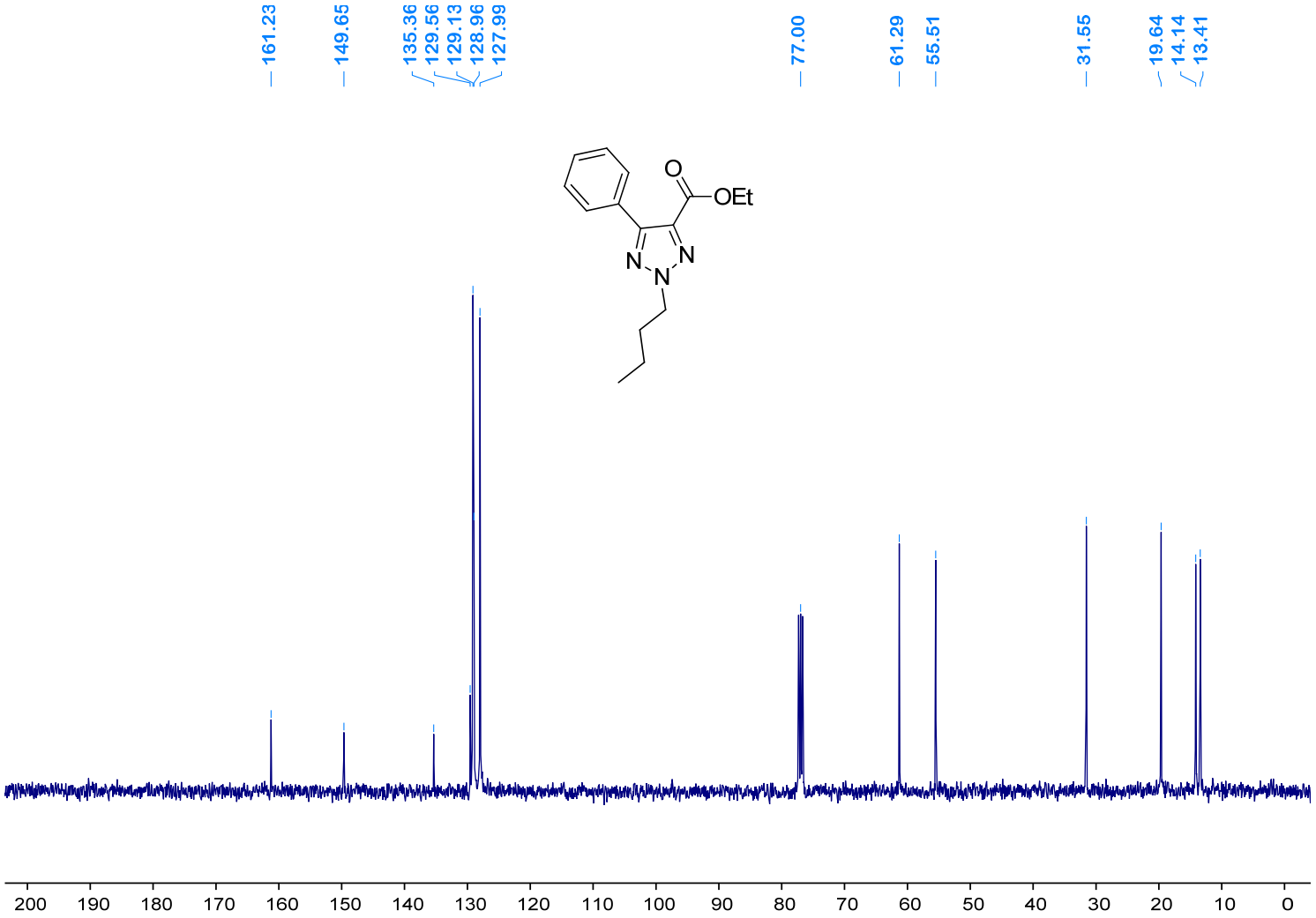


3Xd

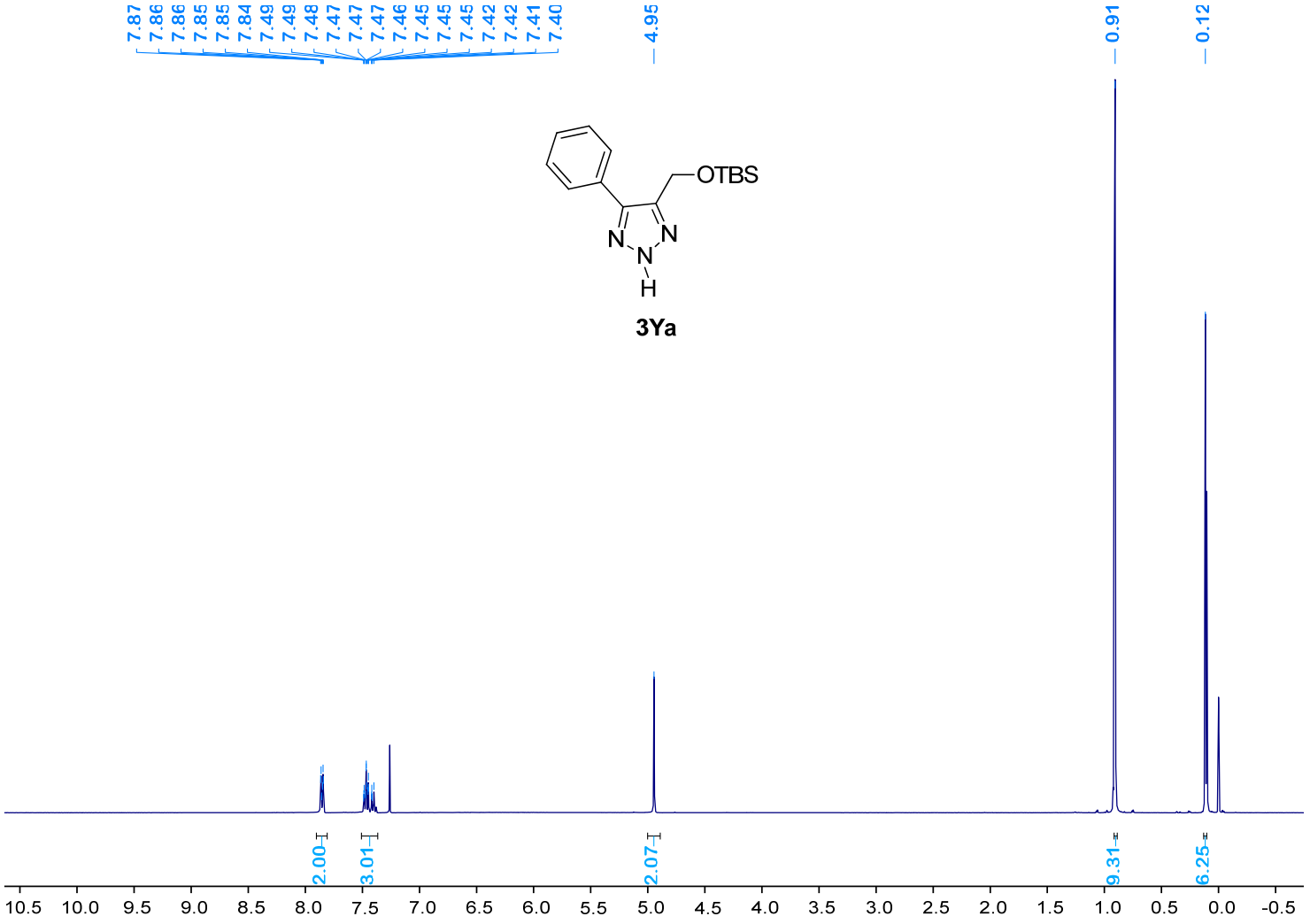
^{1}H NMR of compound 3Xe



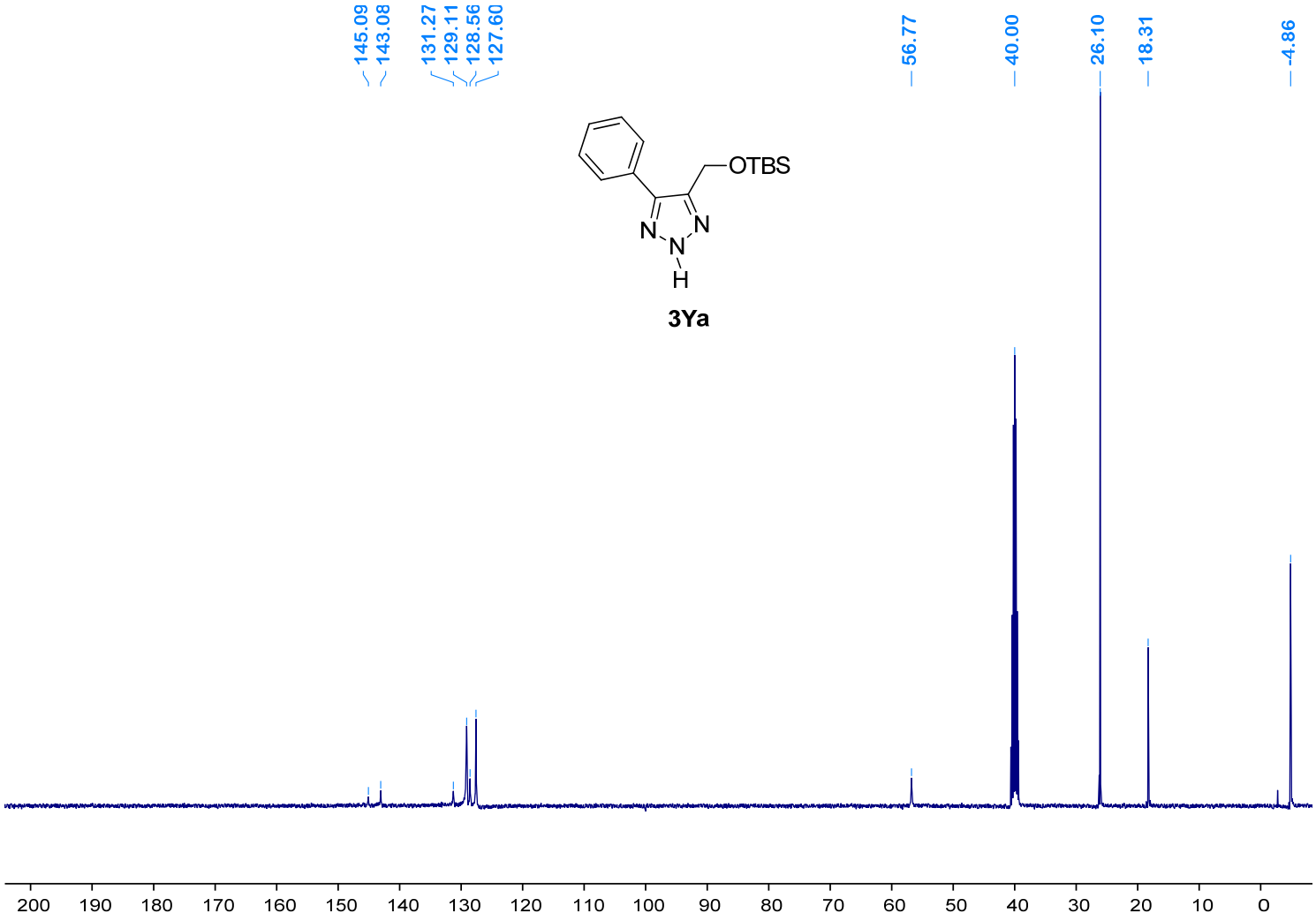
^{13}C NMR of compound 3Xe



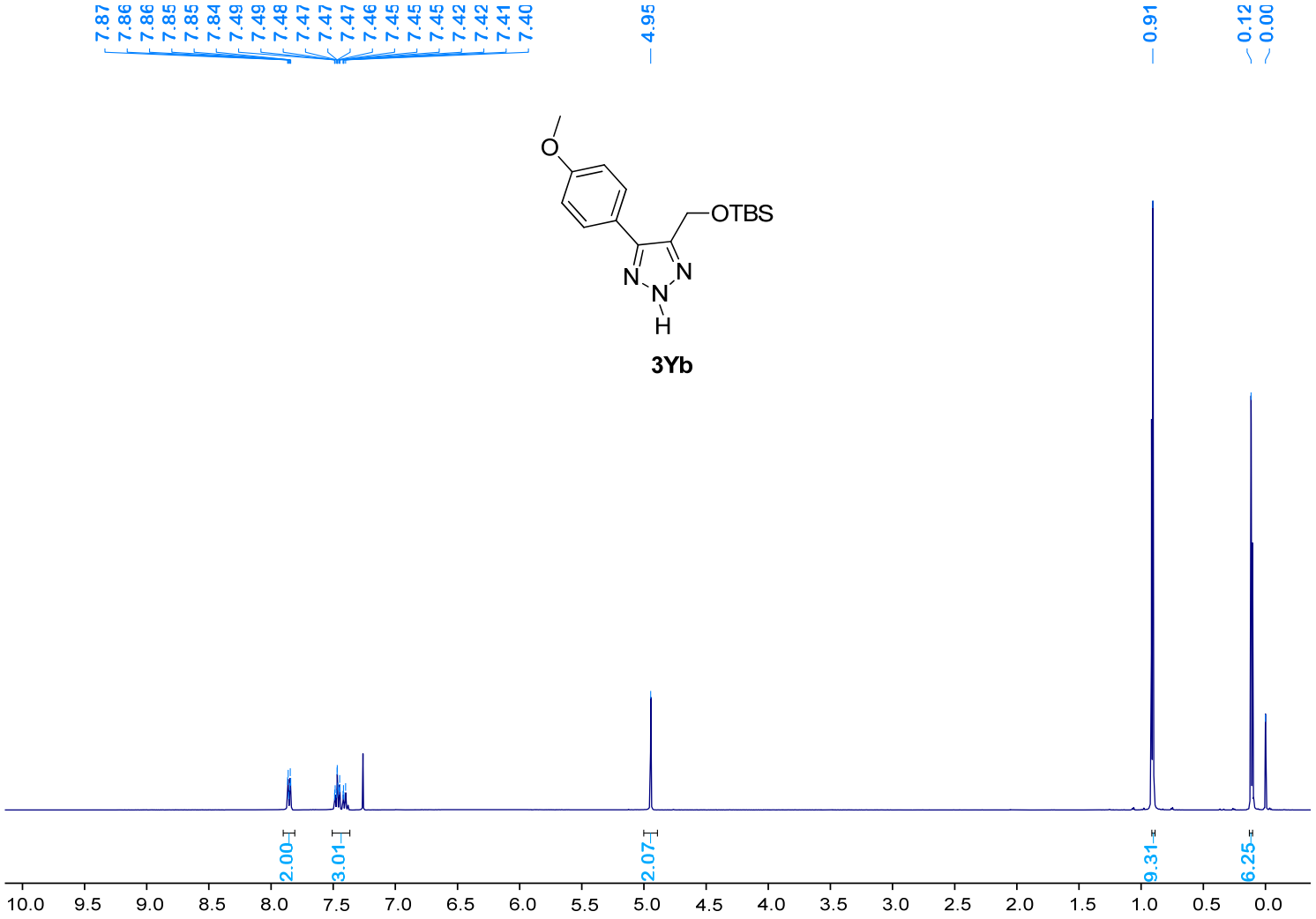
[1]H NMR of compound 3Ya



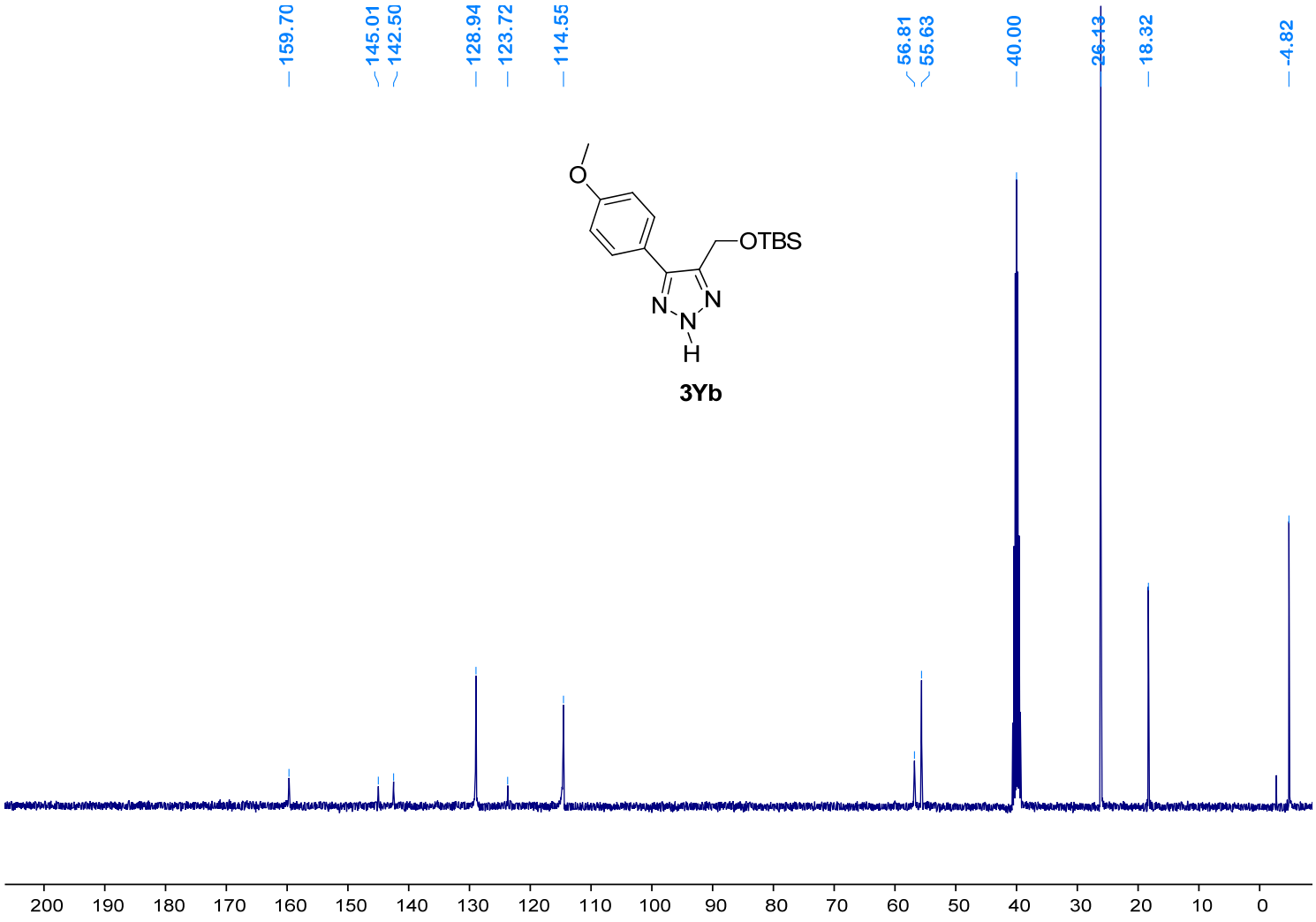
^{13}C NMR of compound 3Ya



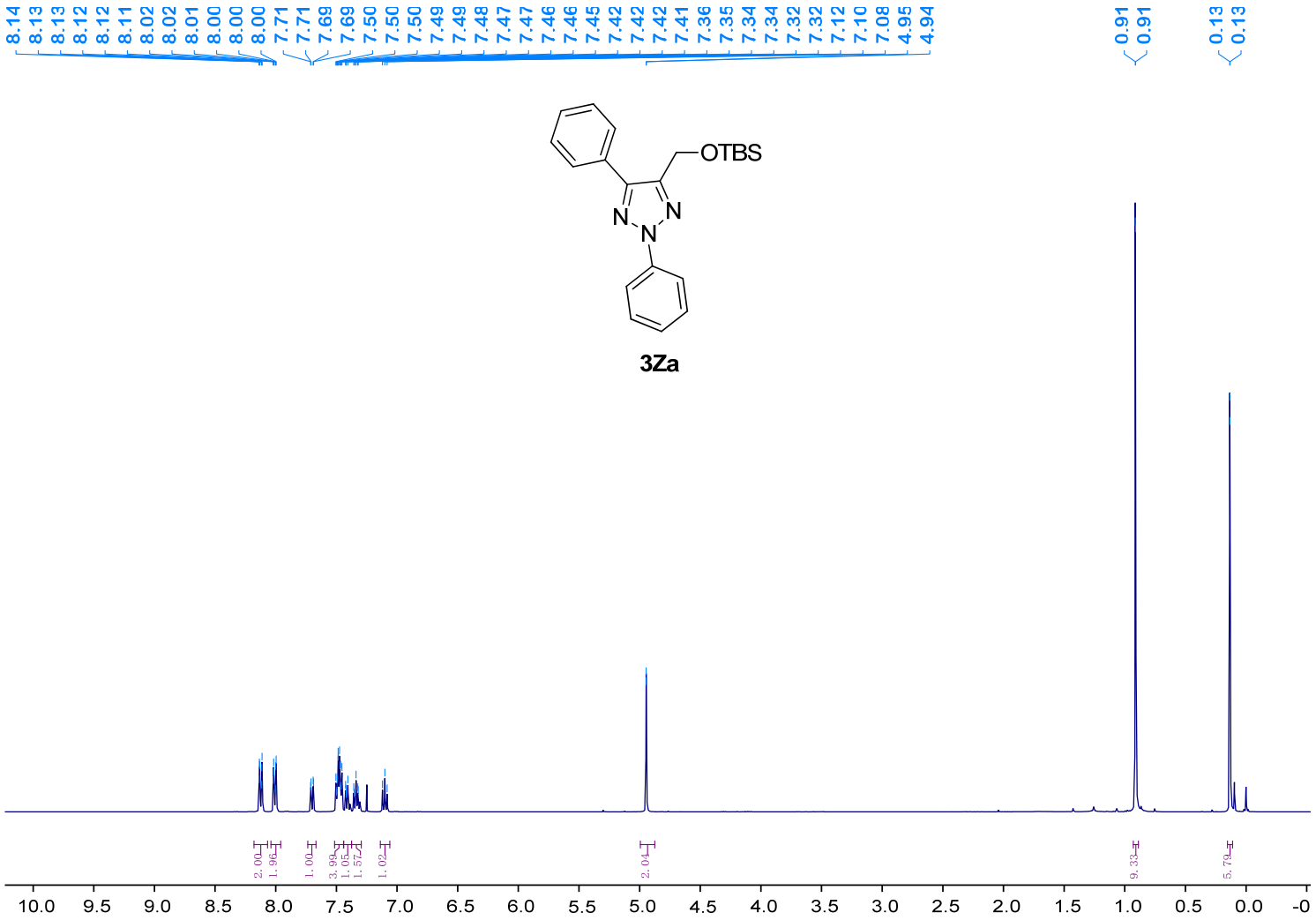
^{1}H NMR of compound 3Yb



^{13}C NMR of compound 3Yb



^{1}H NMR of compound 3Za



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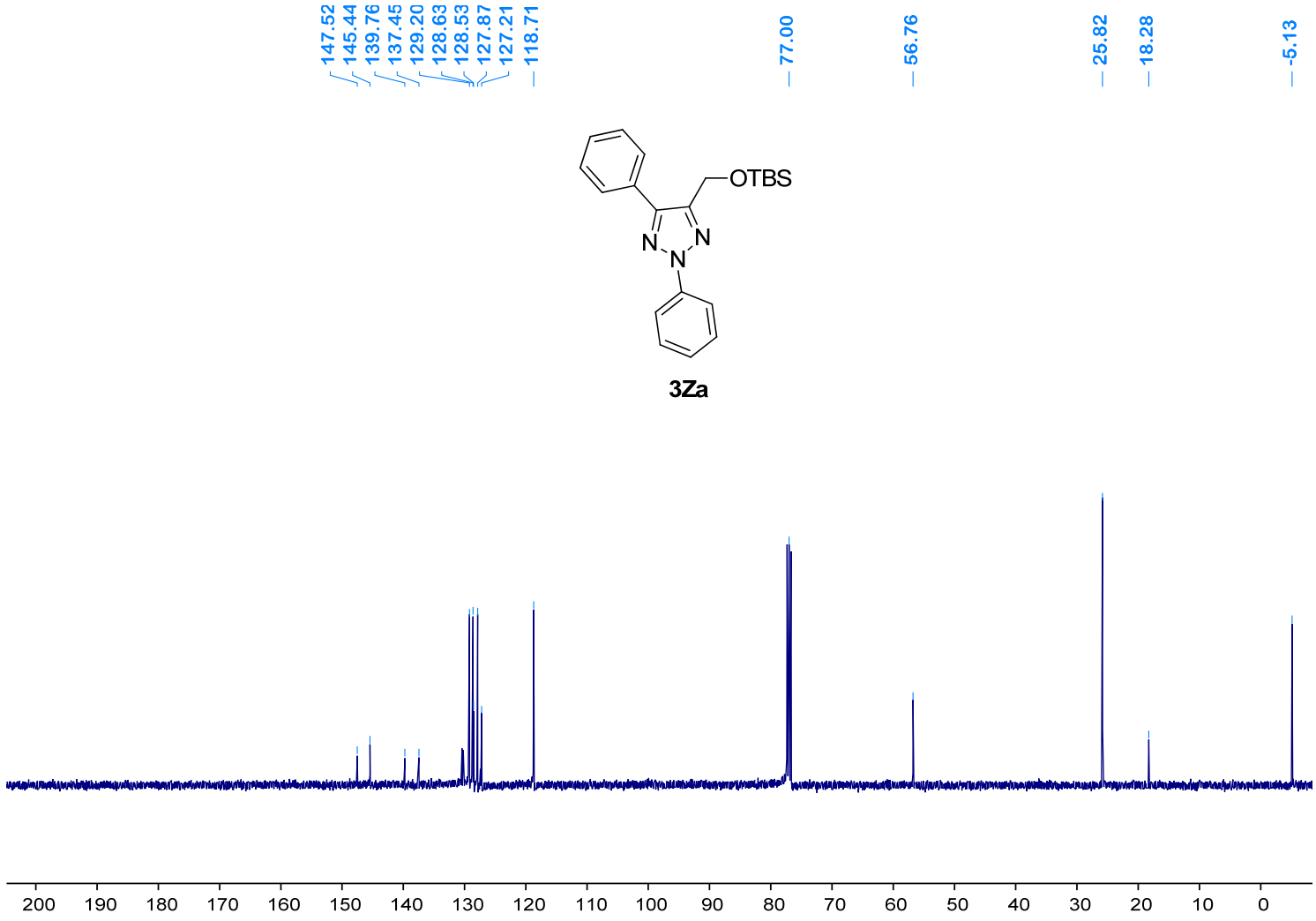
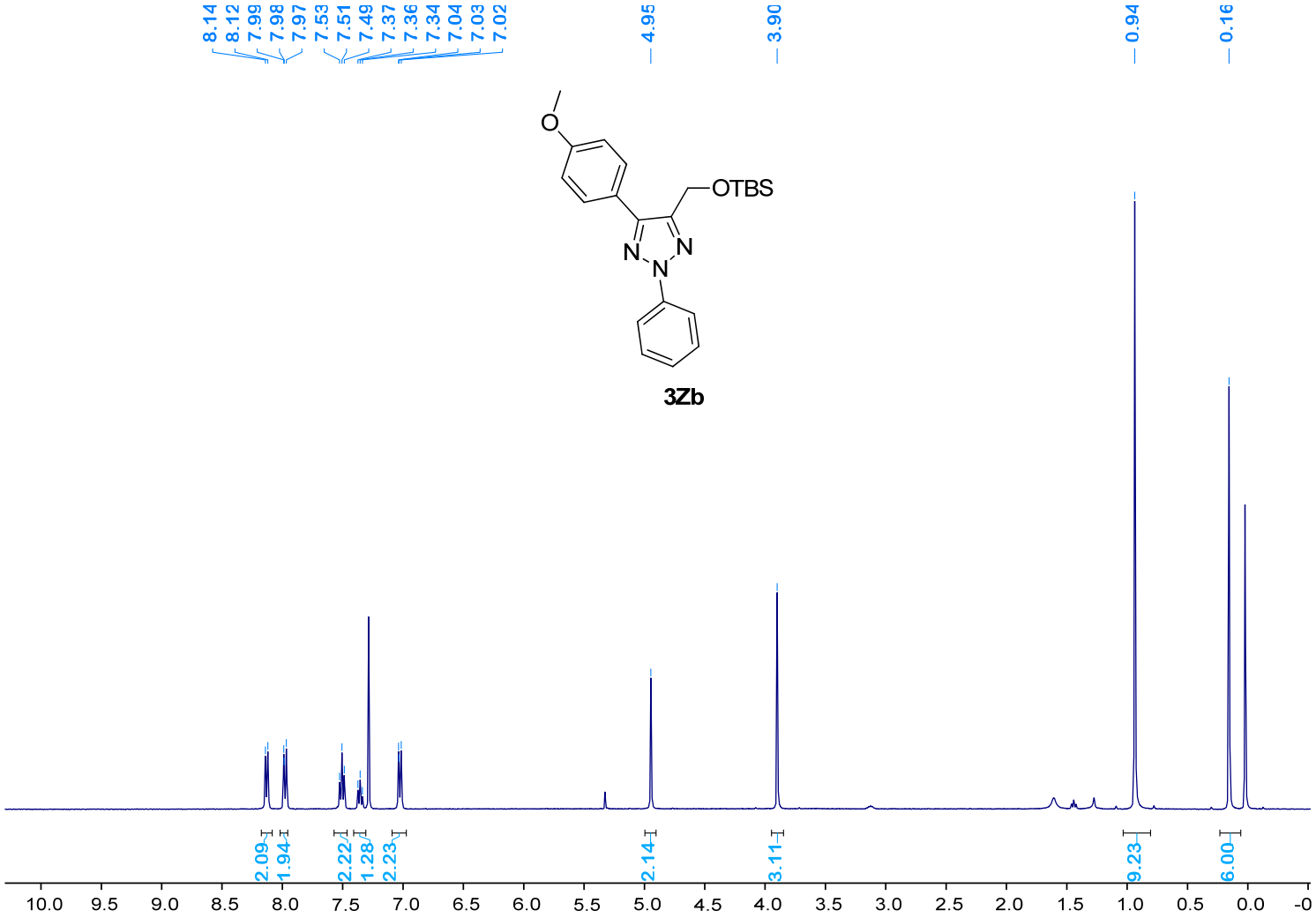
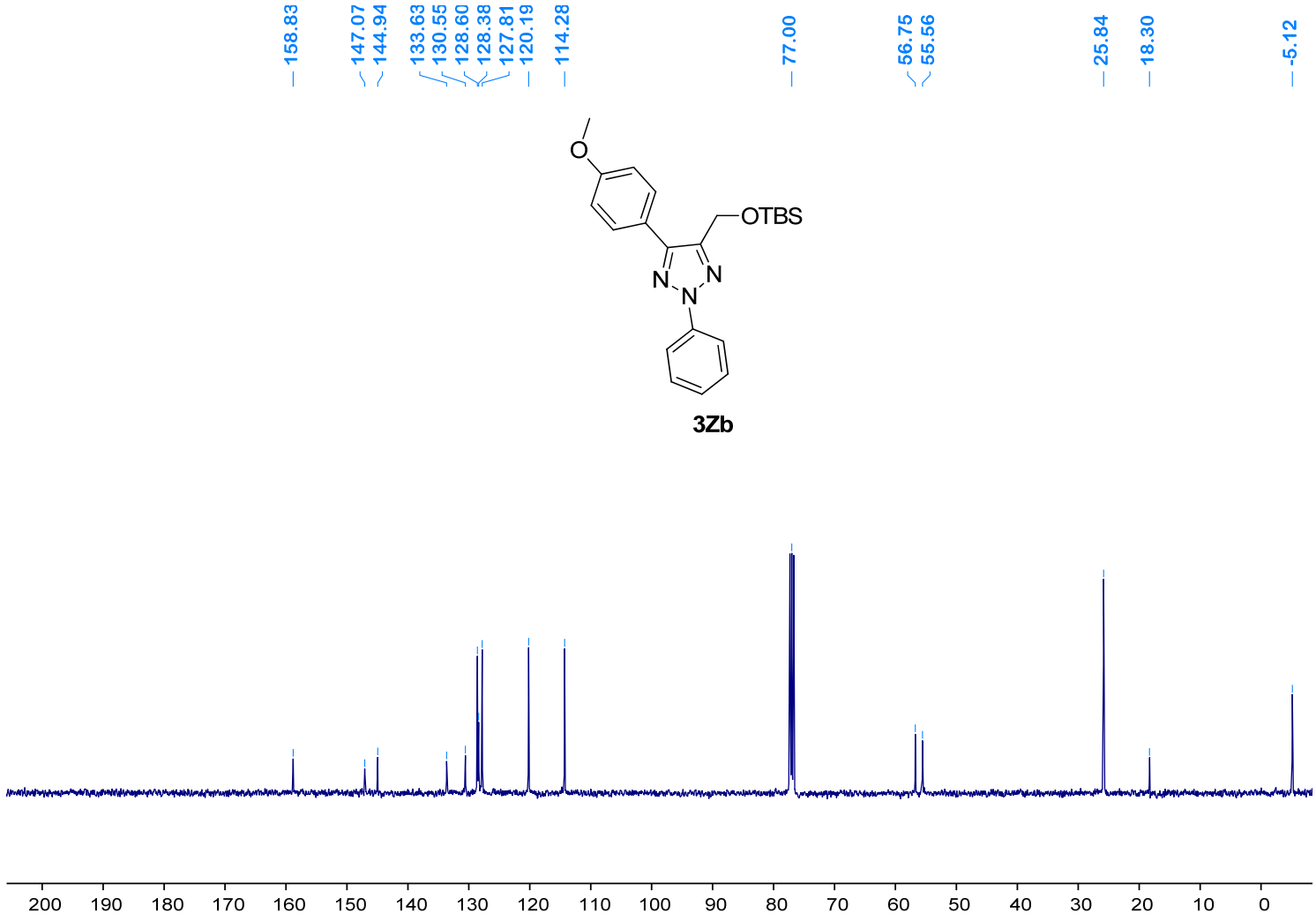


3Za

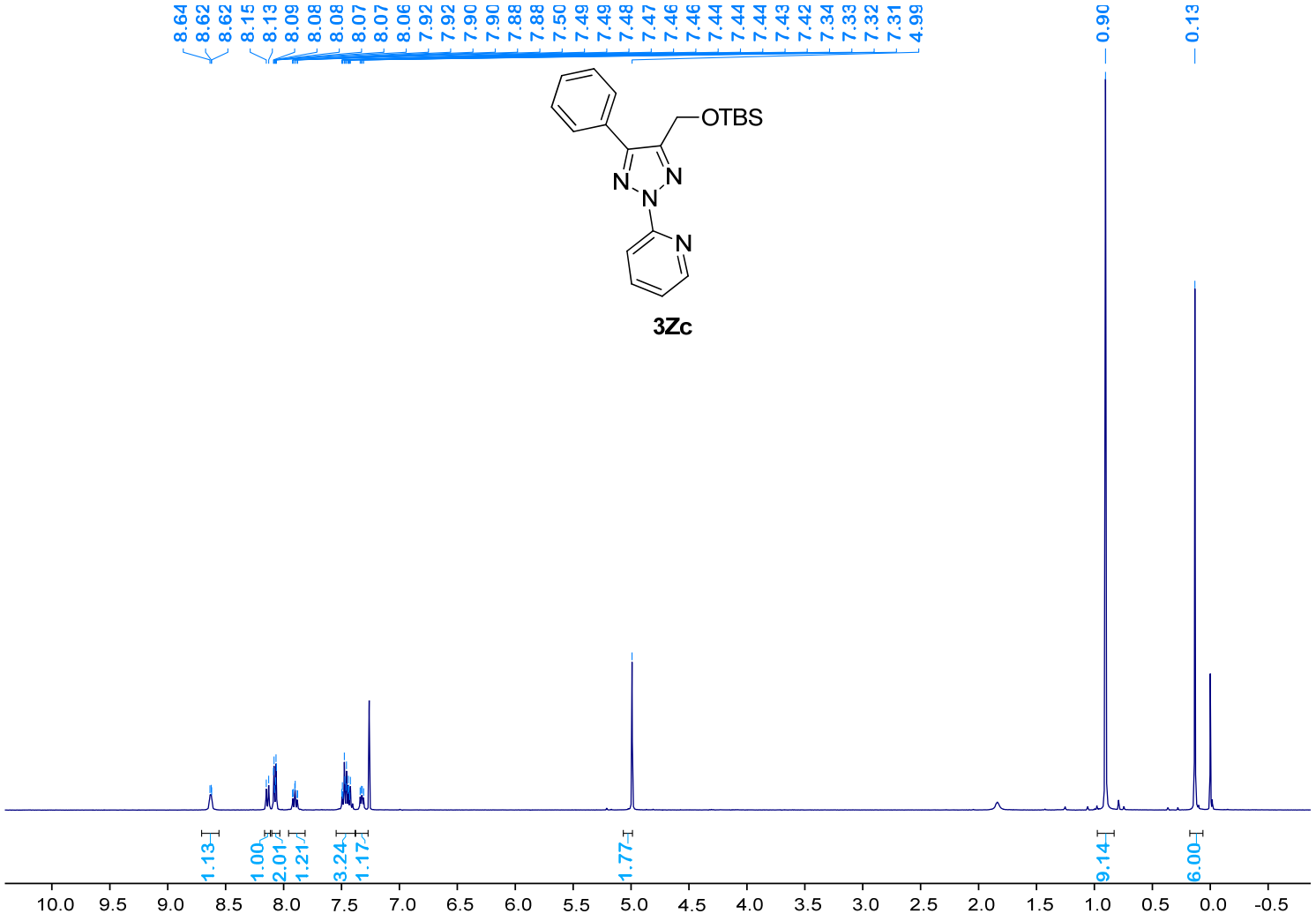
^{1}H NMR of compound 3Zb



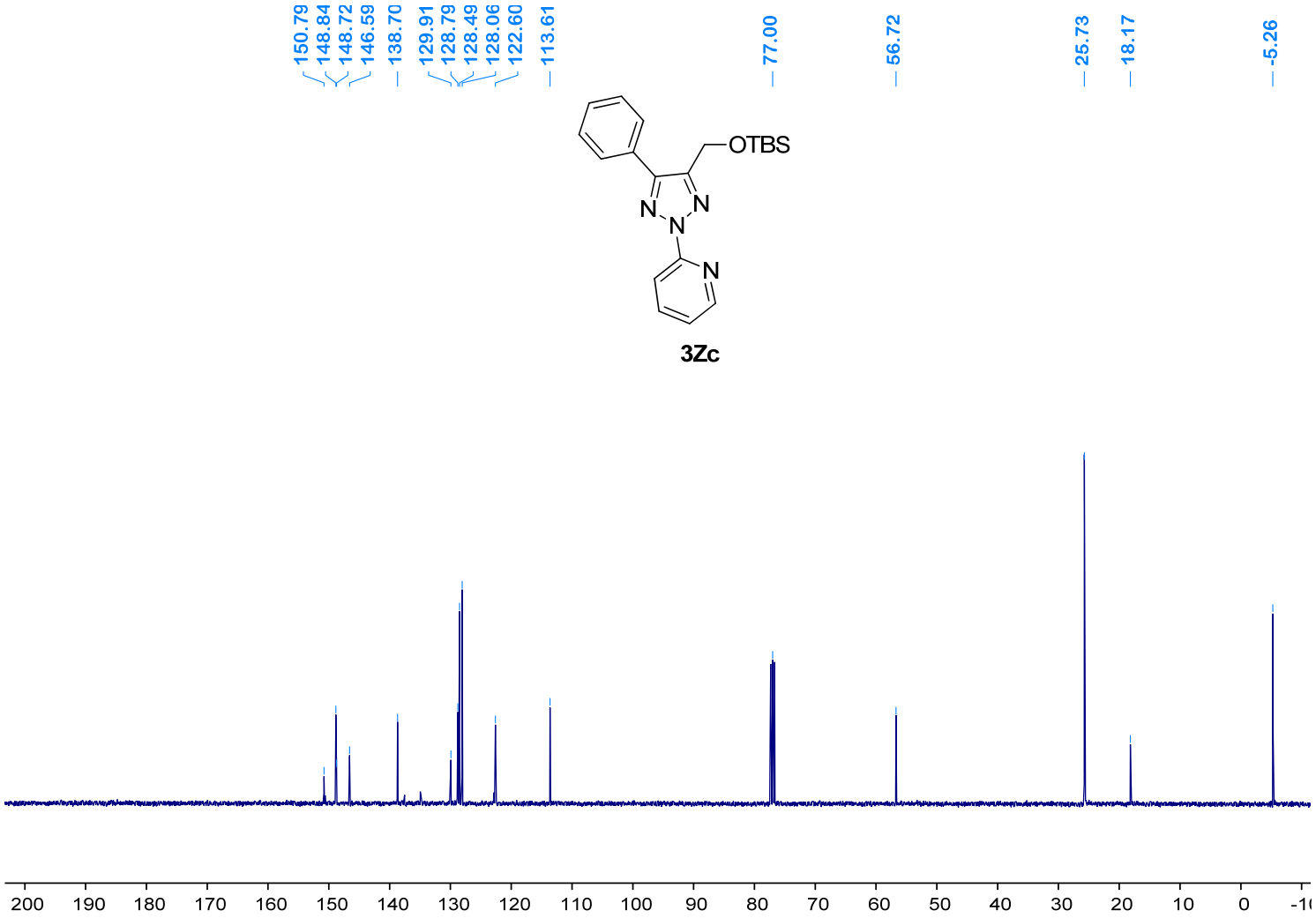
^{13}C NMR of compound 3Zb



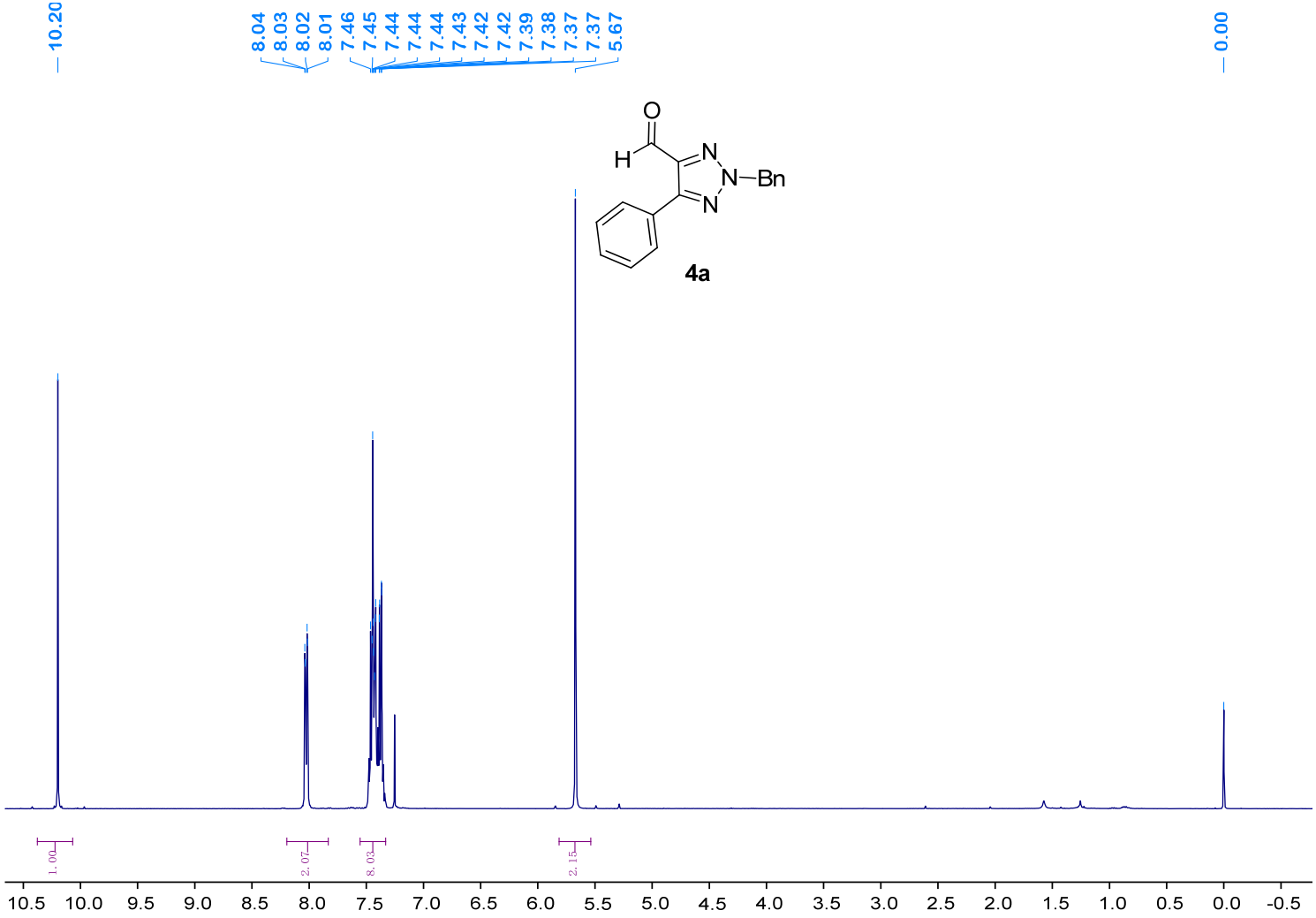
[1]H NMR of compound 3Zc



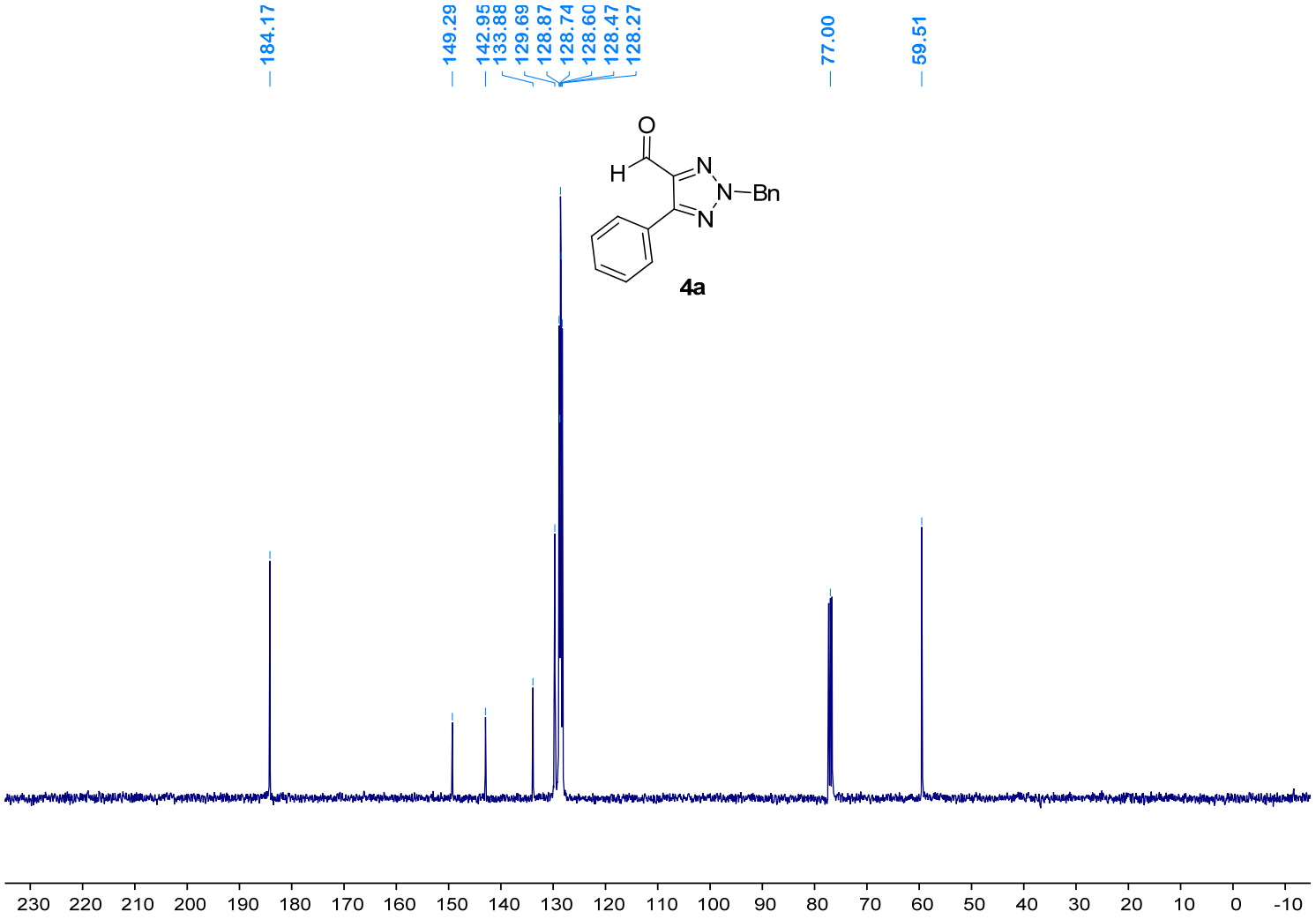
^{13}C NMR of compound 3Zc



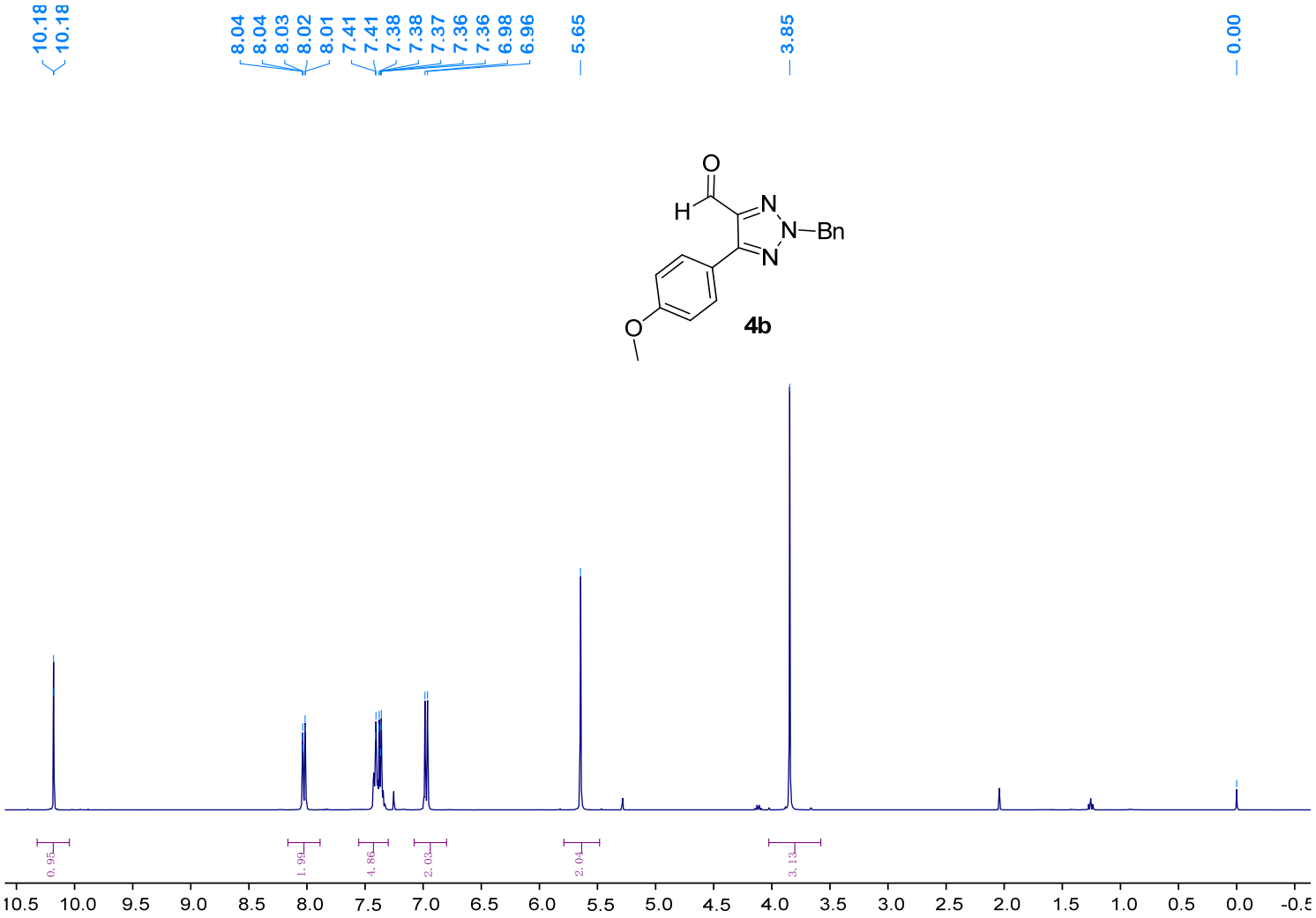
^{1}H NMR of compound 4a



^{13}C NMR of compound 4a



^{1}H NMR of compound 4b



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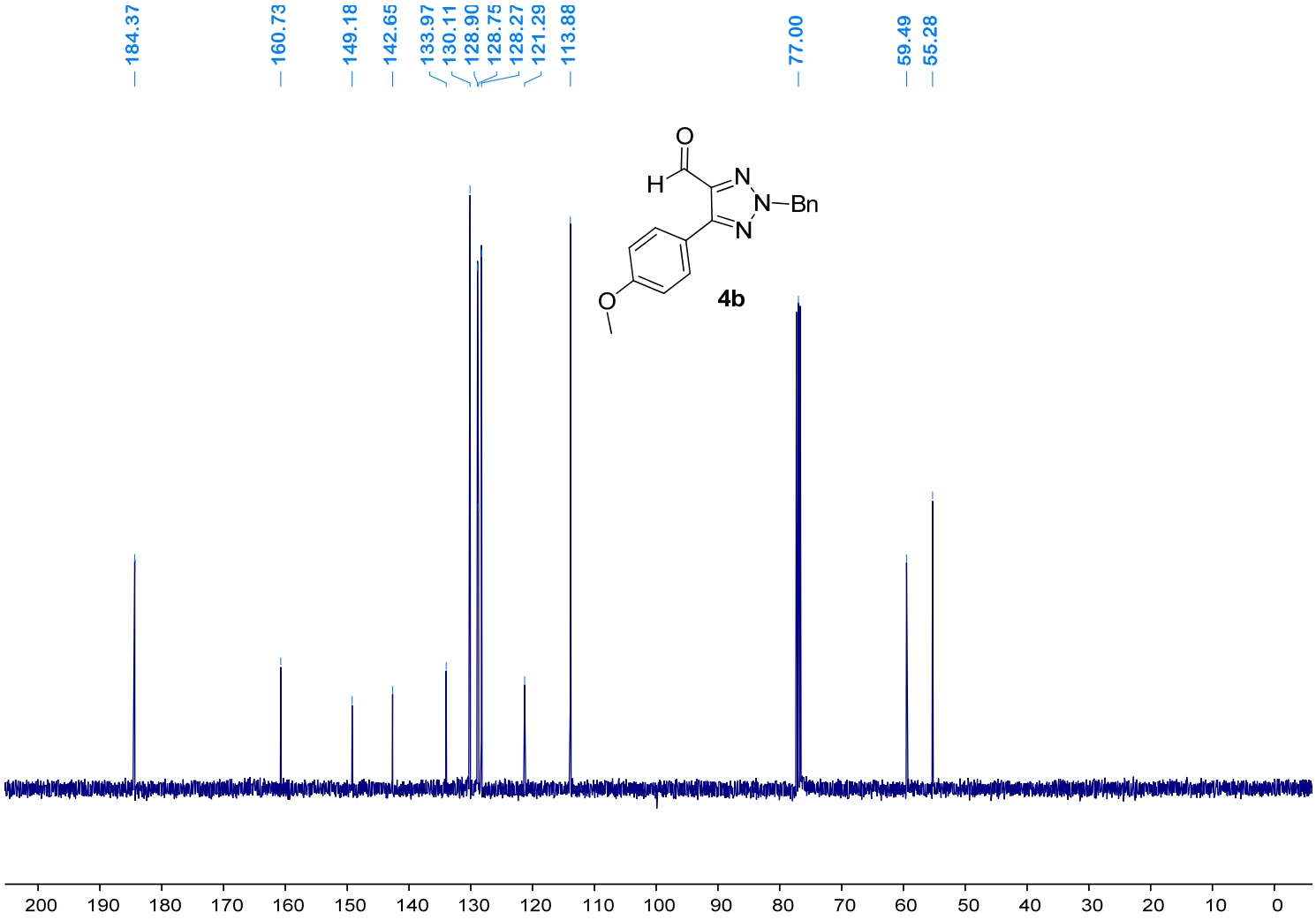
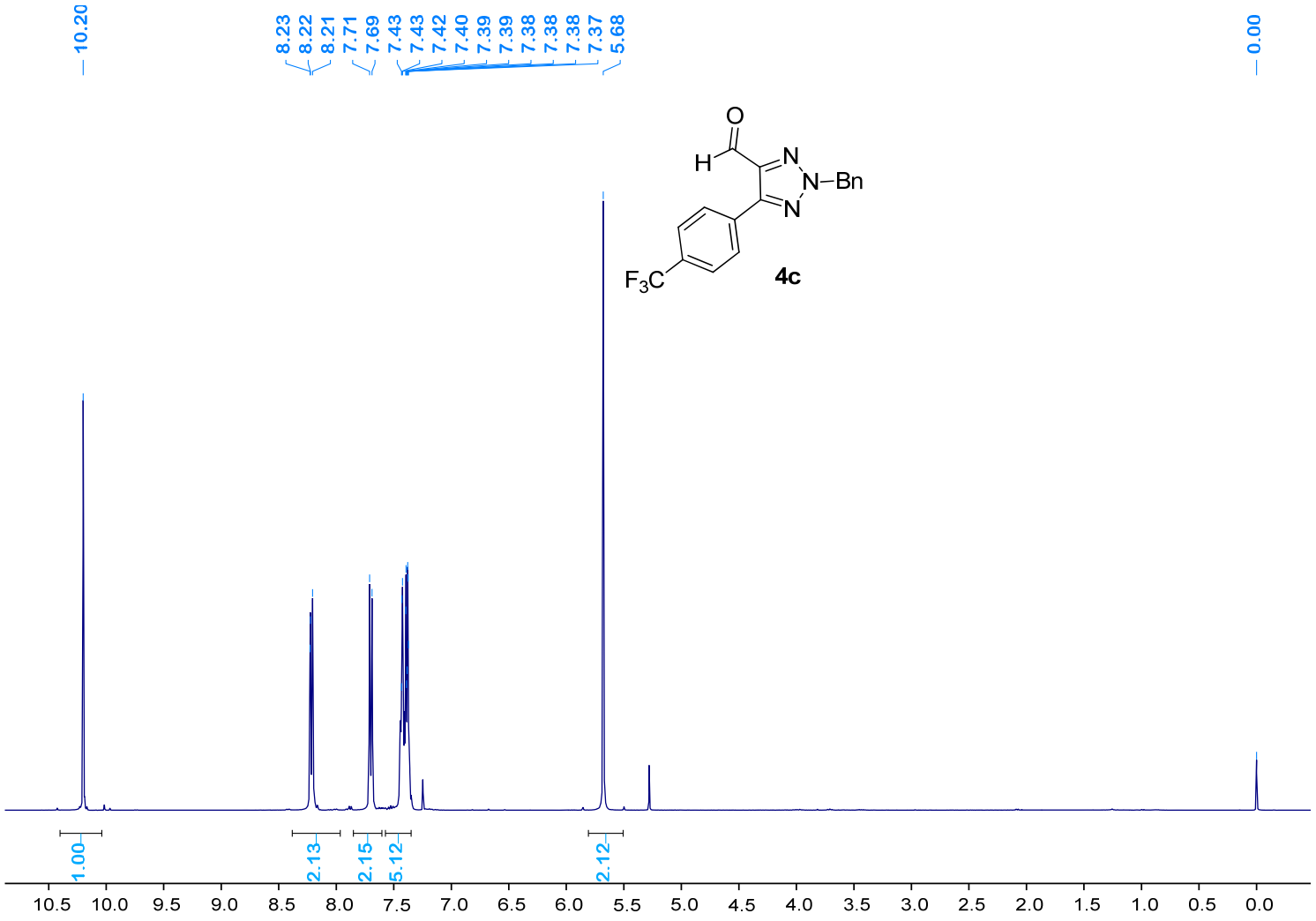
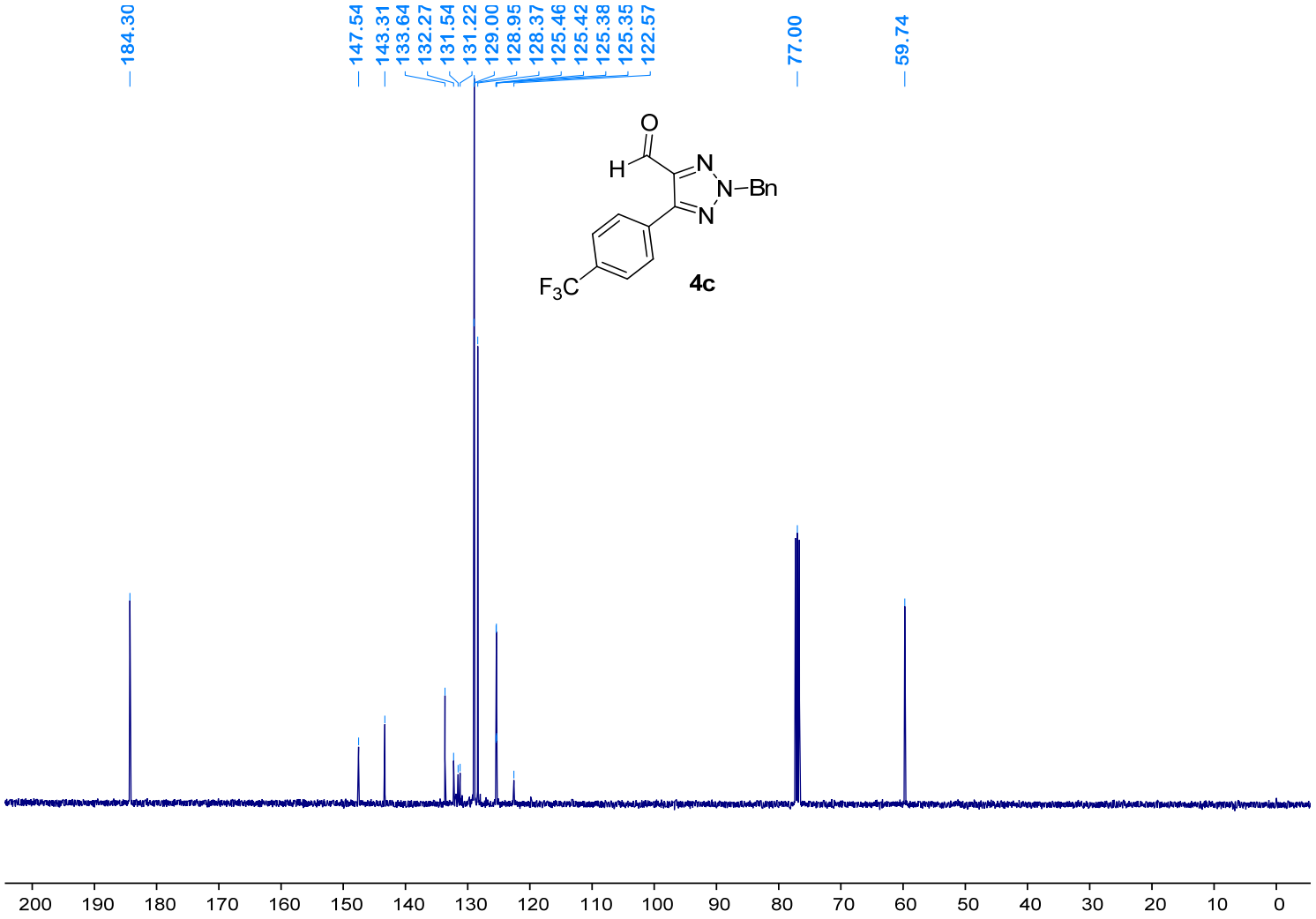


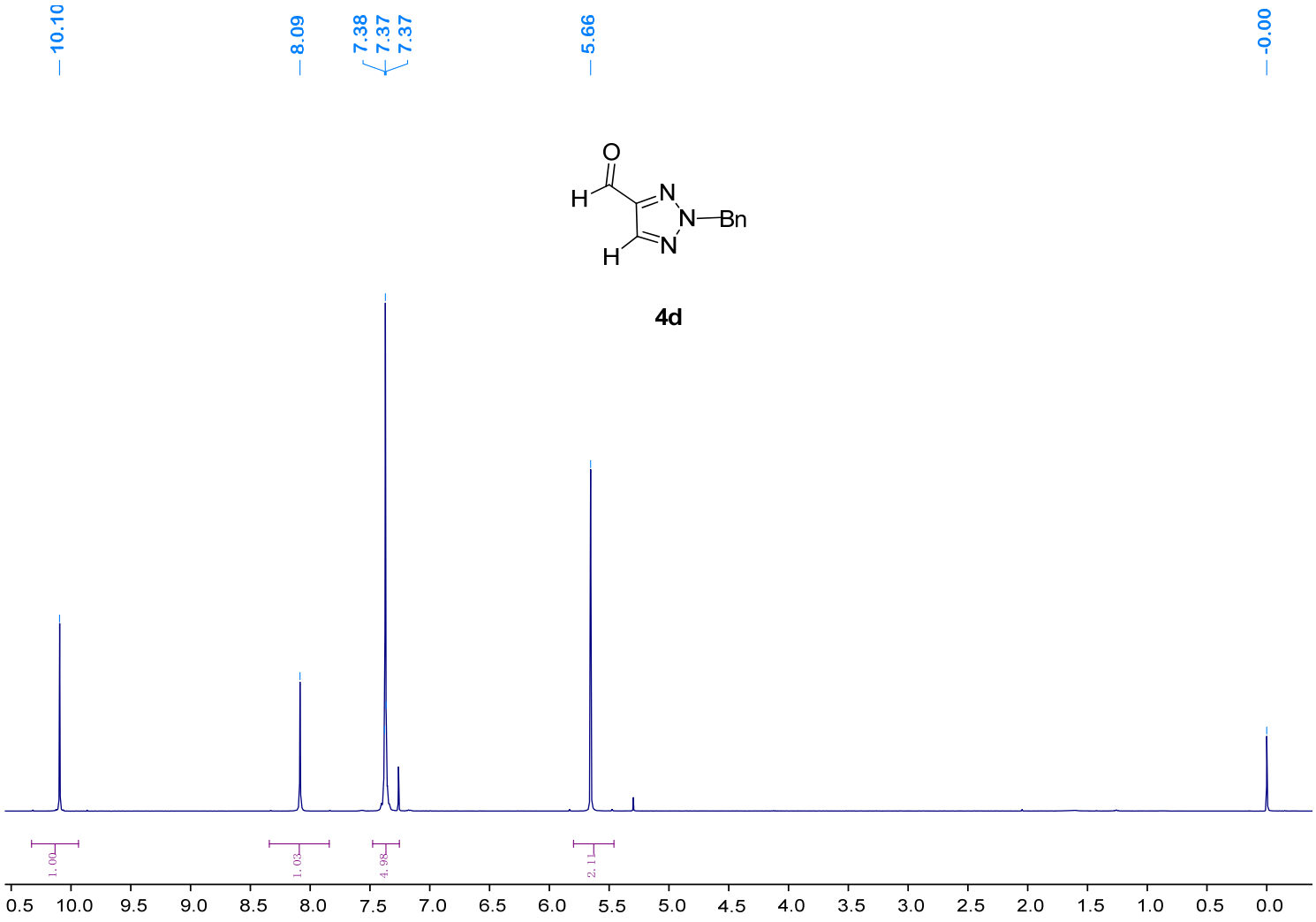
^{1}H NMR of compound 4c



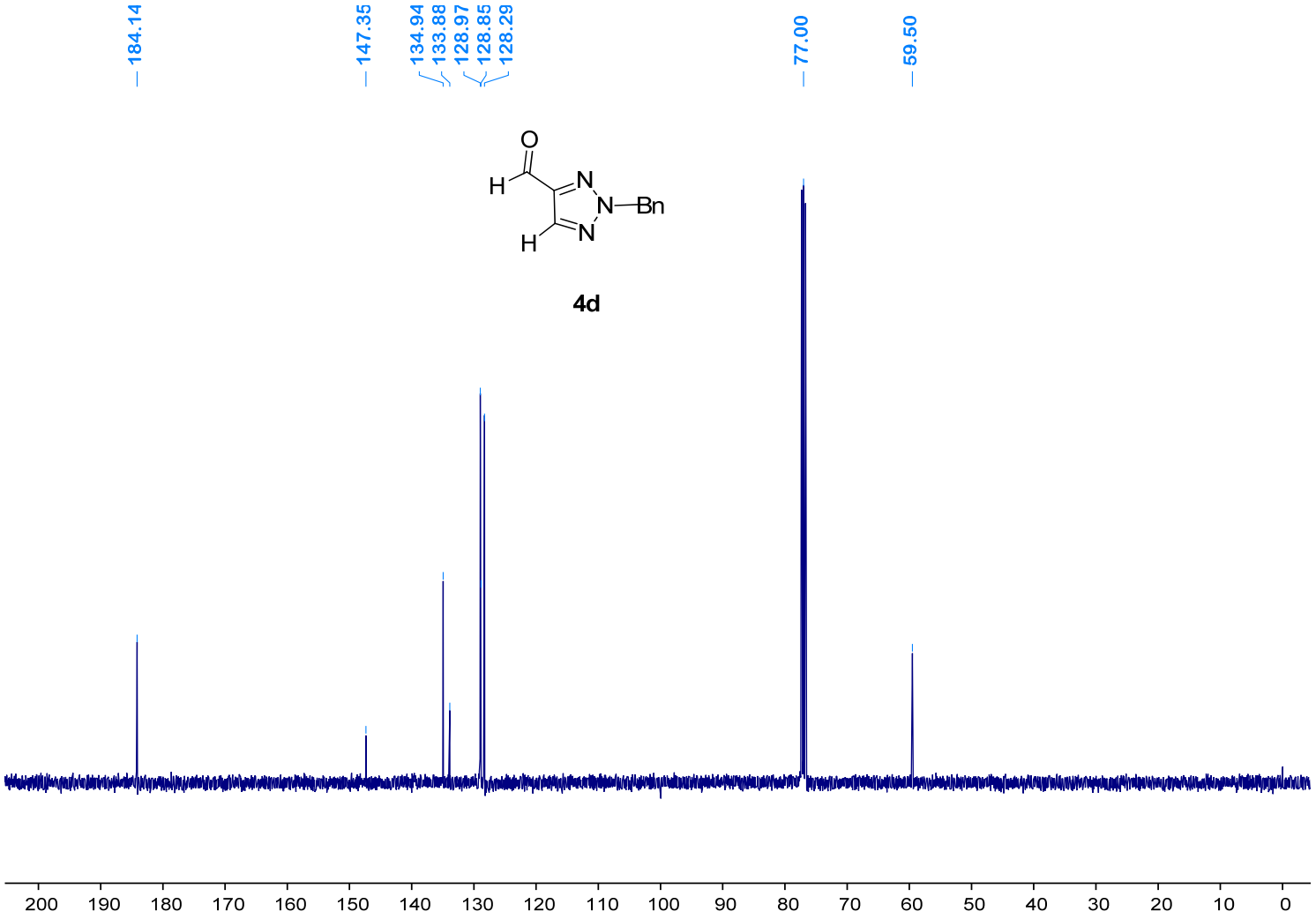
^{13}C NMR of compound 4c



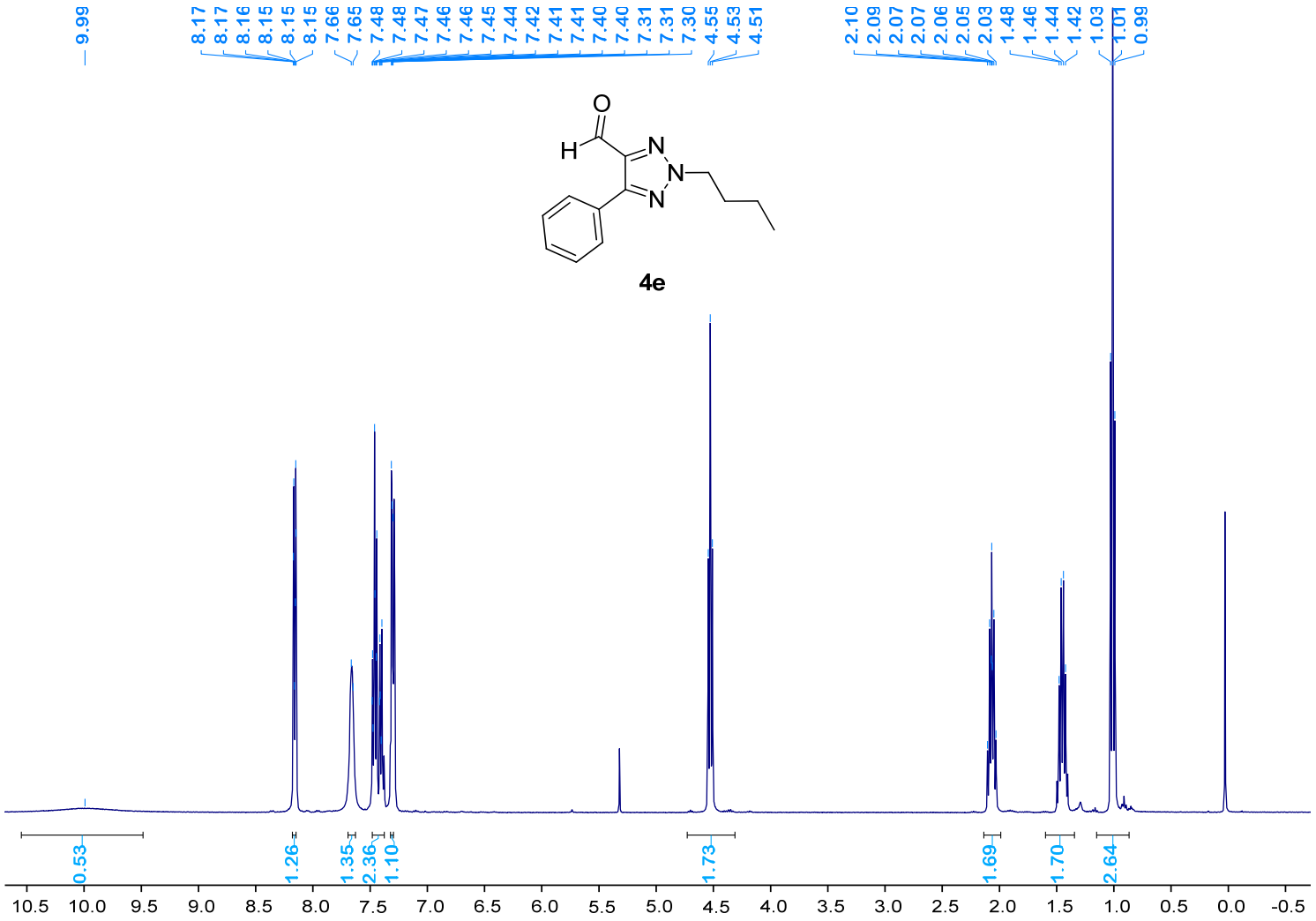
^{1}H NMR of compound 4d



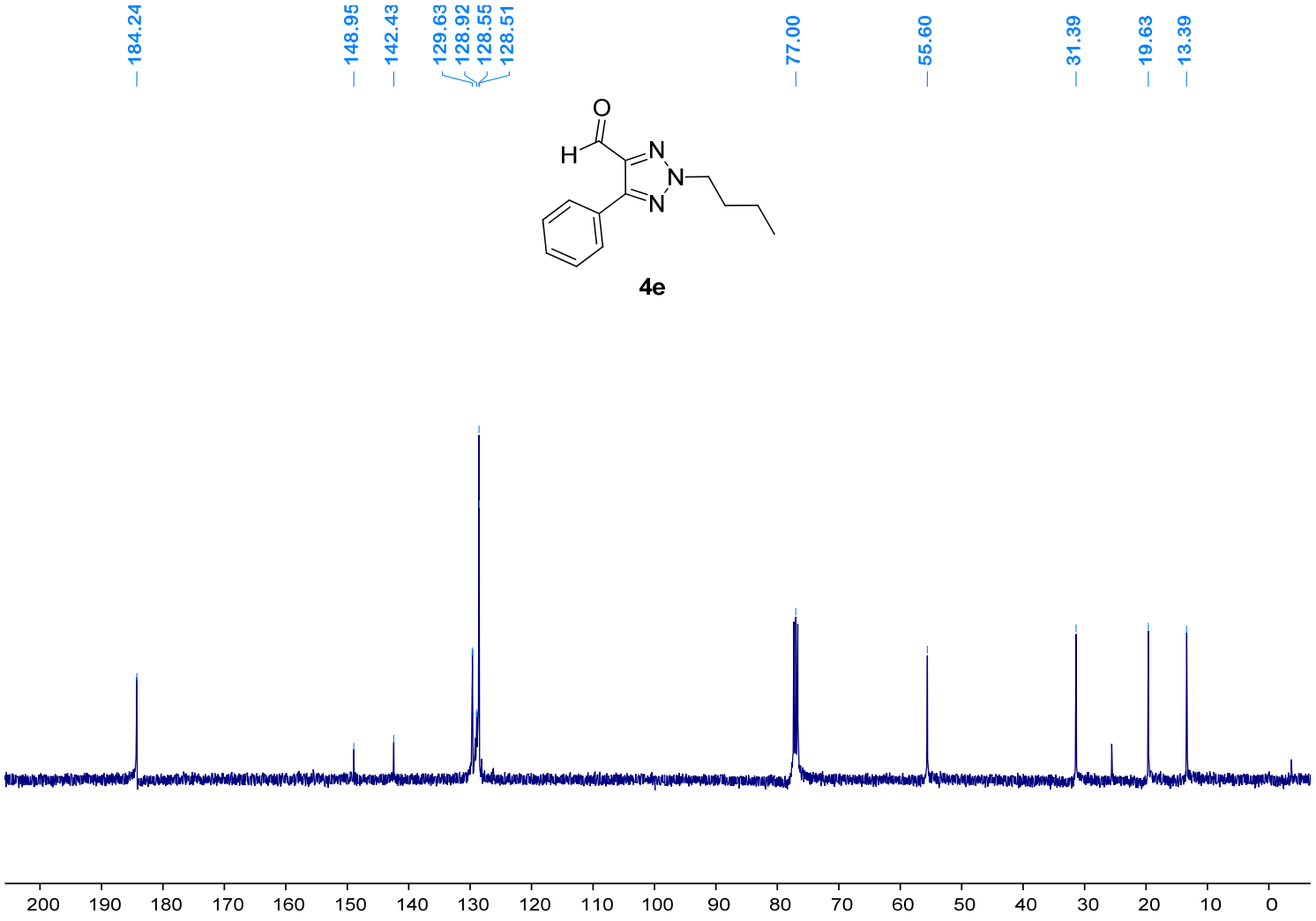
^{13}C NMR of compound 4d



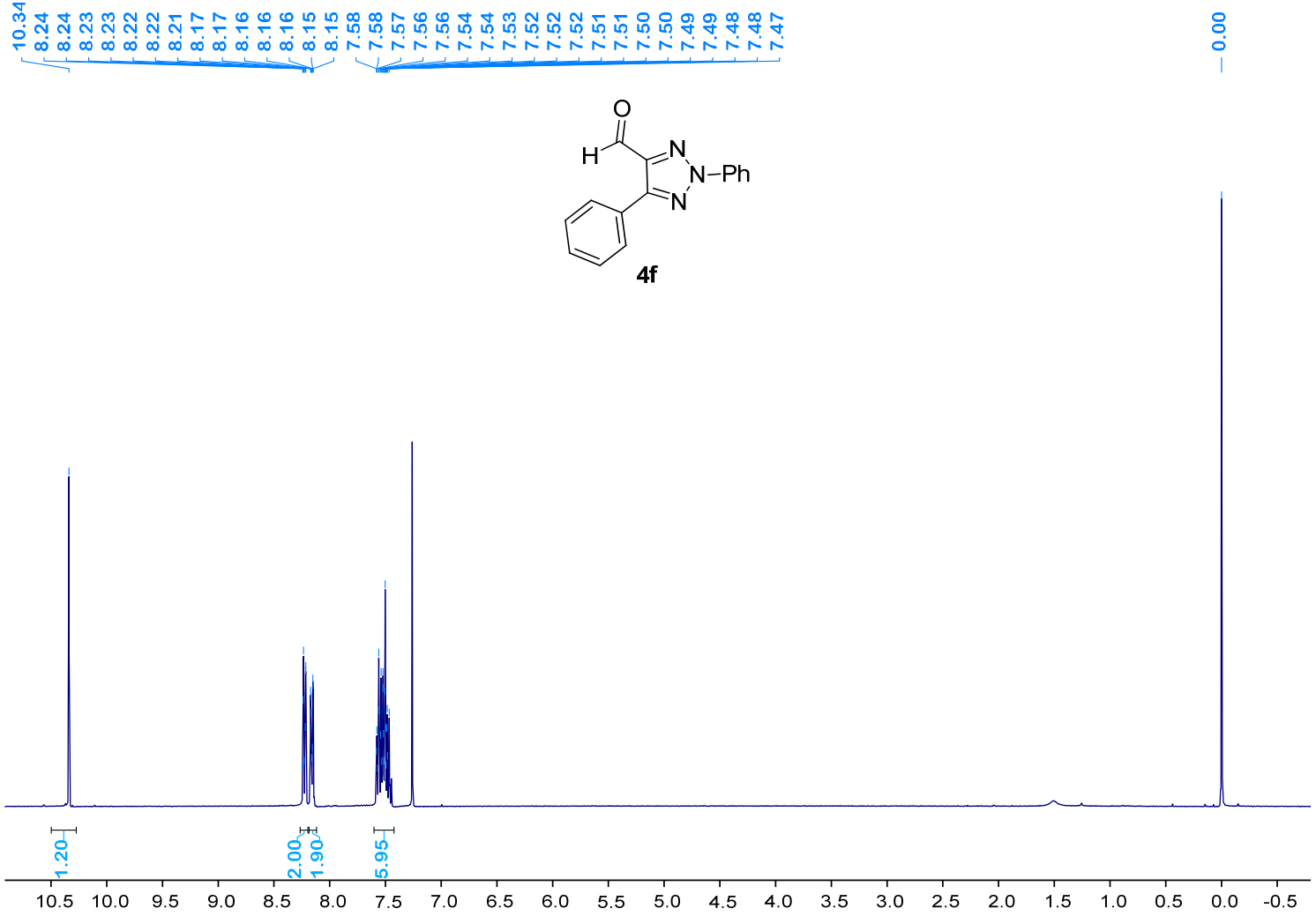
[1]H NMR of compound 4e



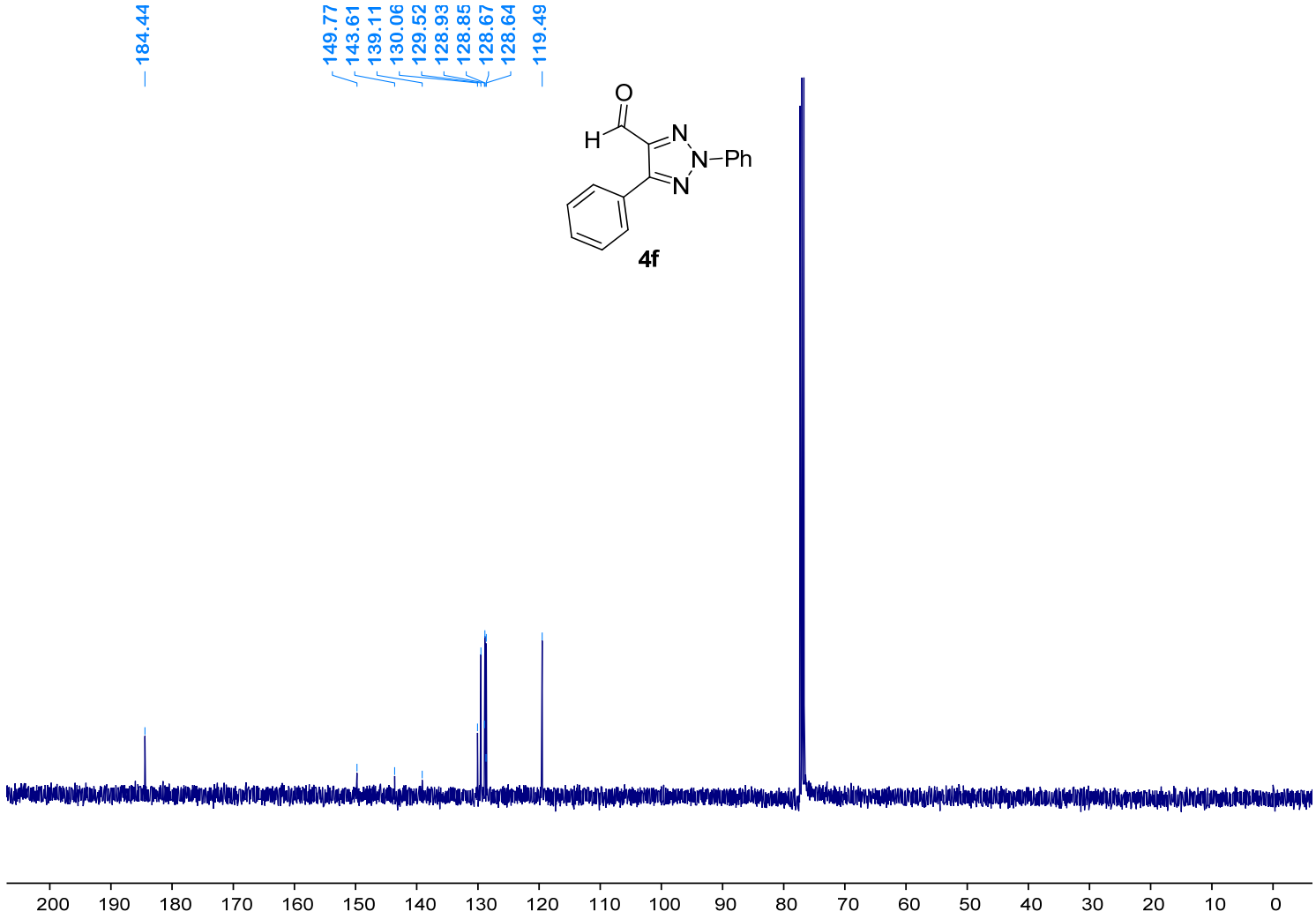
^{13}C NMR of compound 4e



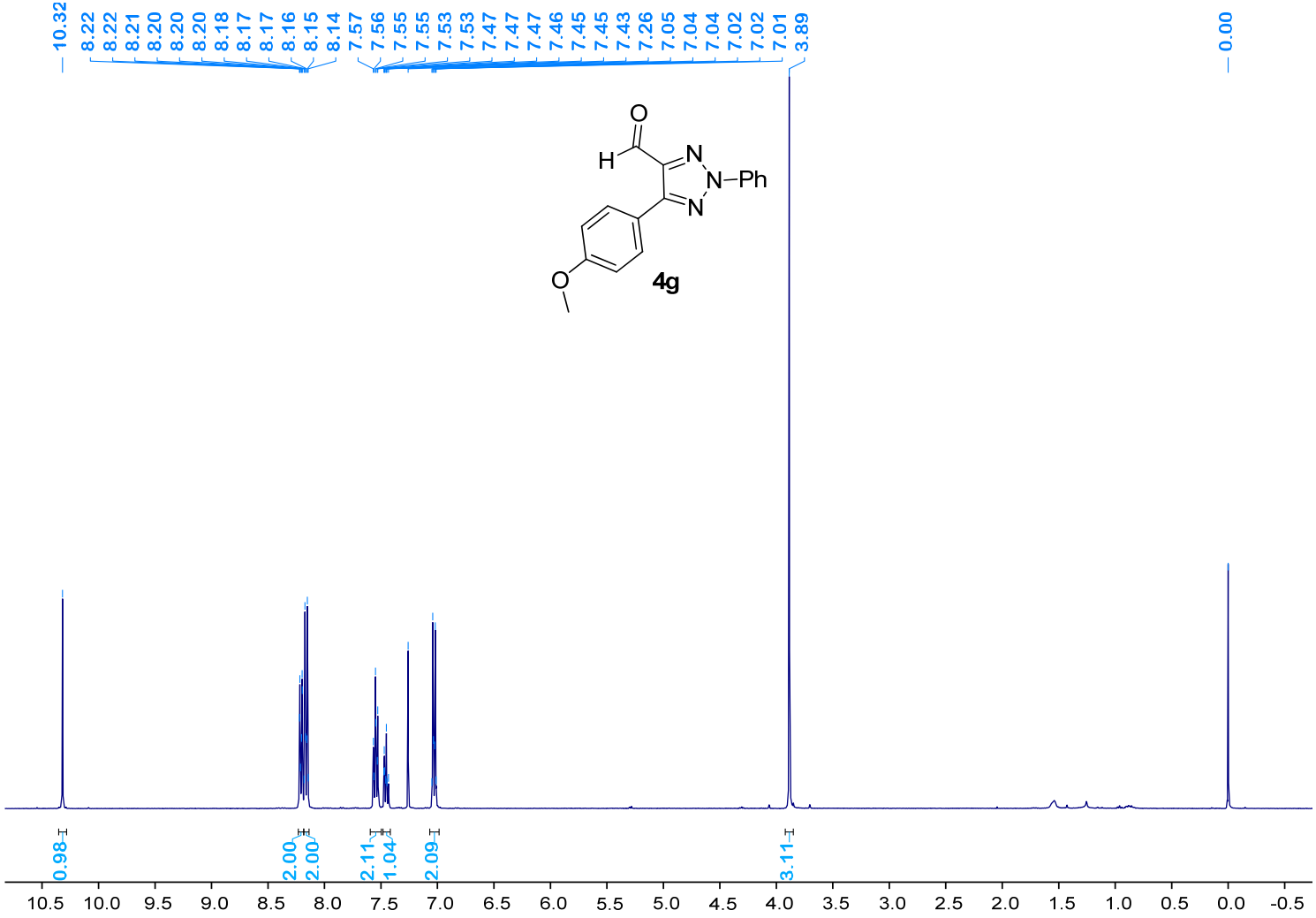
^{1}H NMR of compound 4f



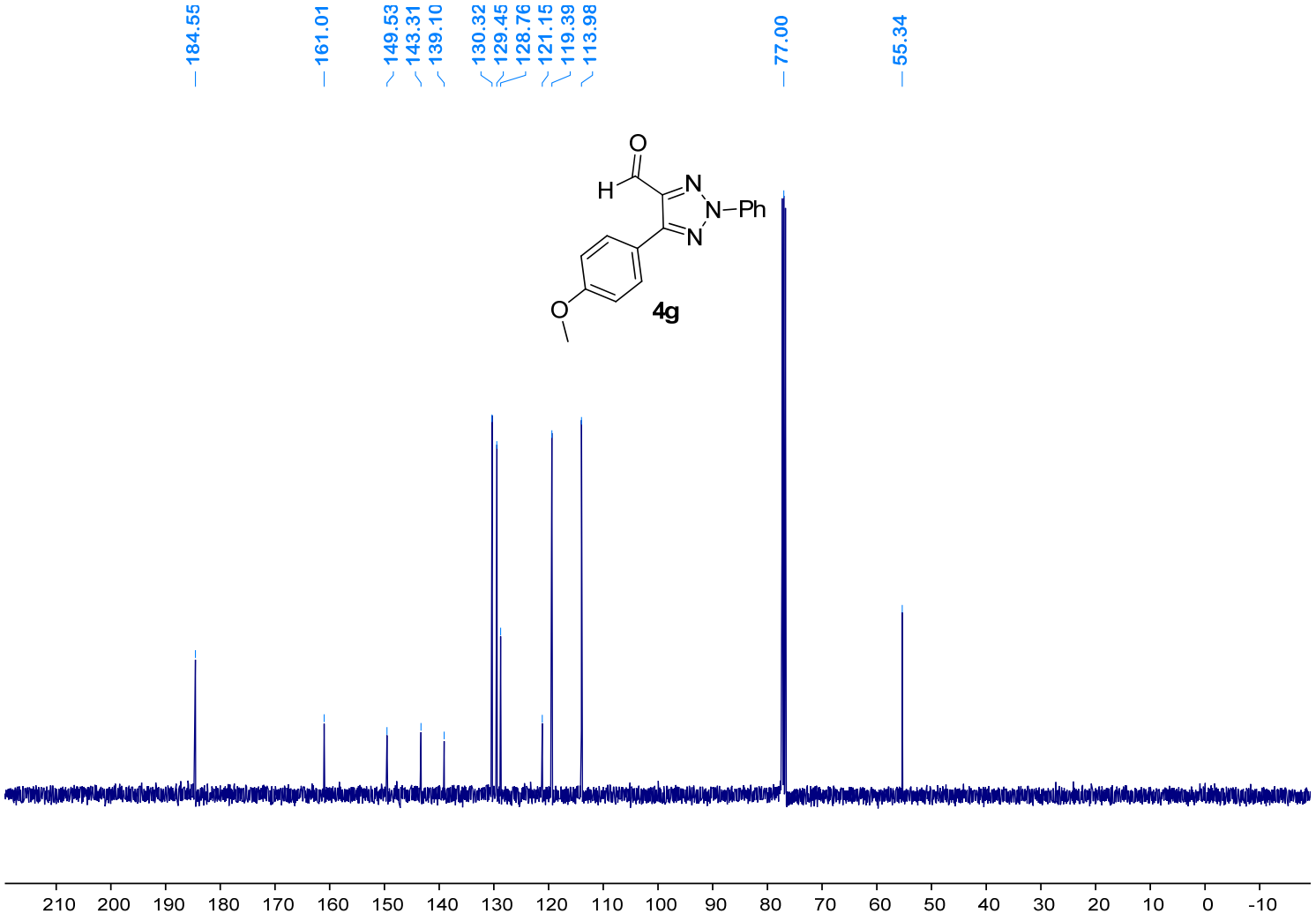
^{13}C NMR of compound 4f



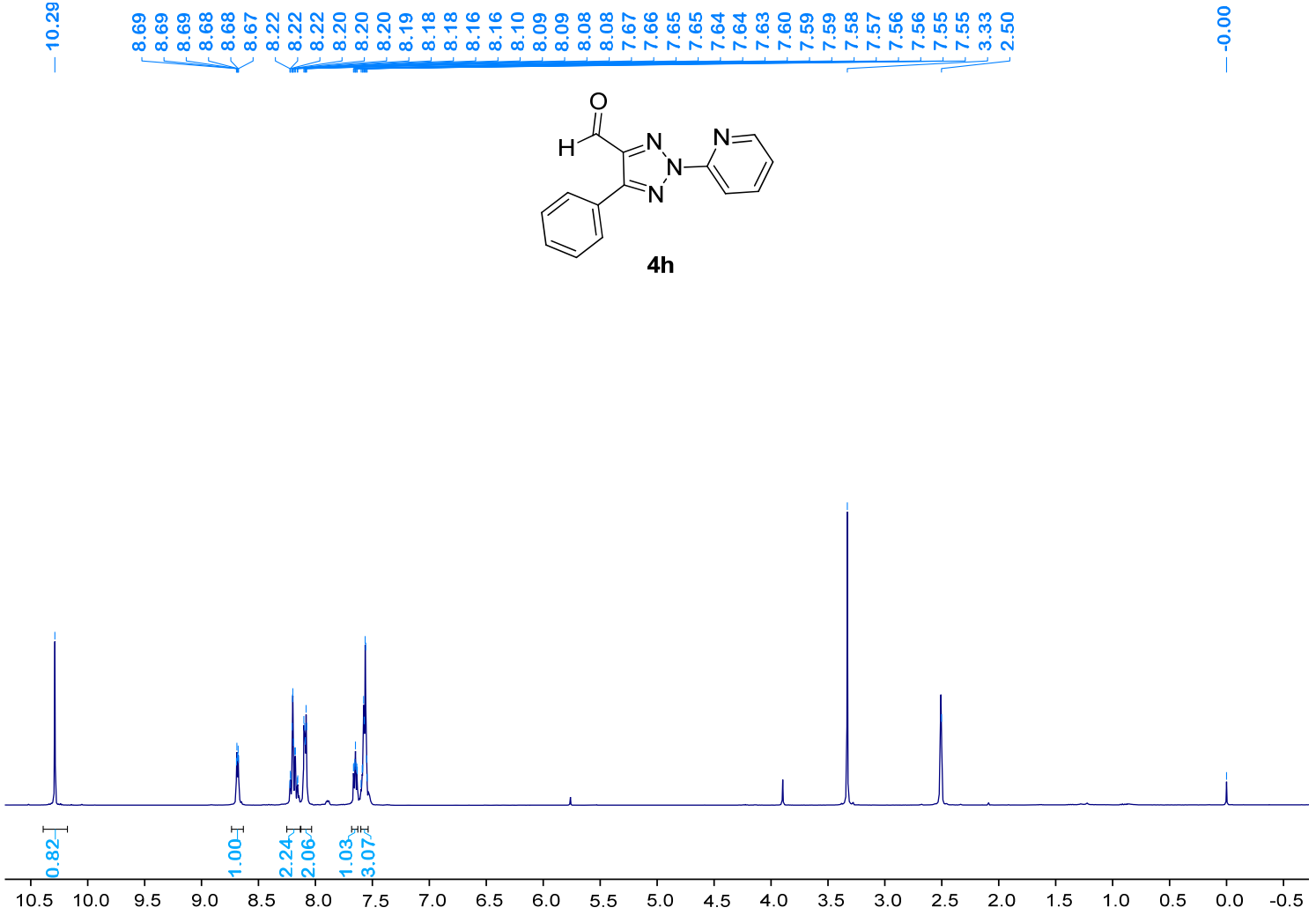
^{1}H NMR of compound 4g



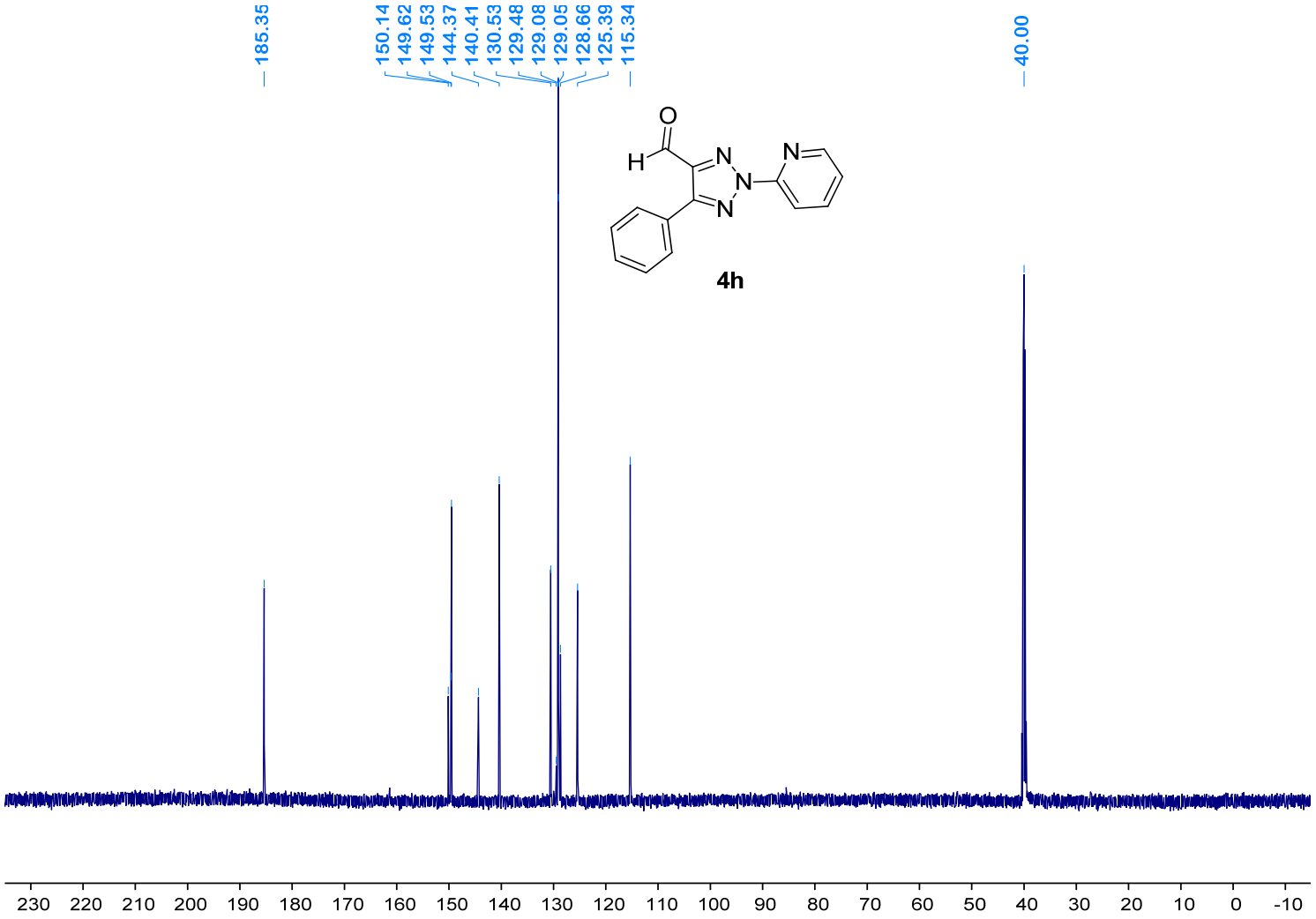
^{13}C NMR of compound 4g



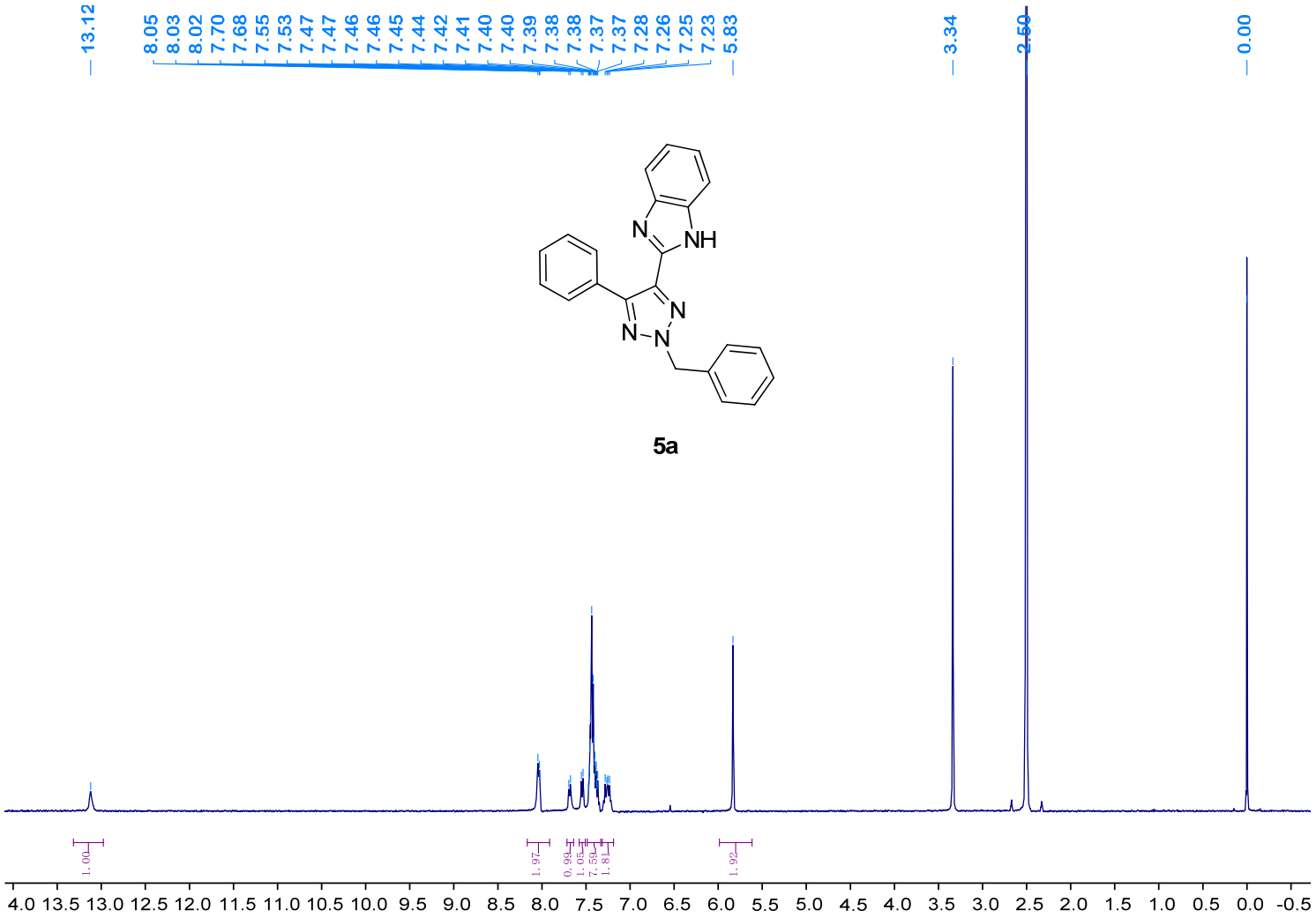
^{1}H NMR of compound 4h



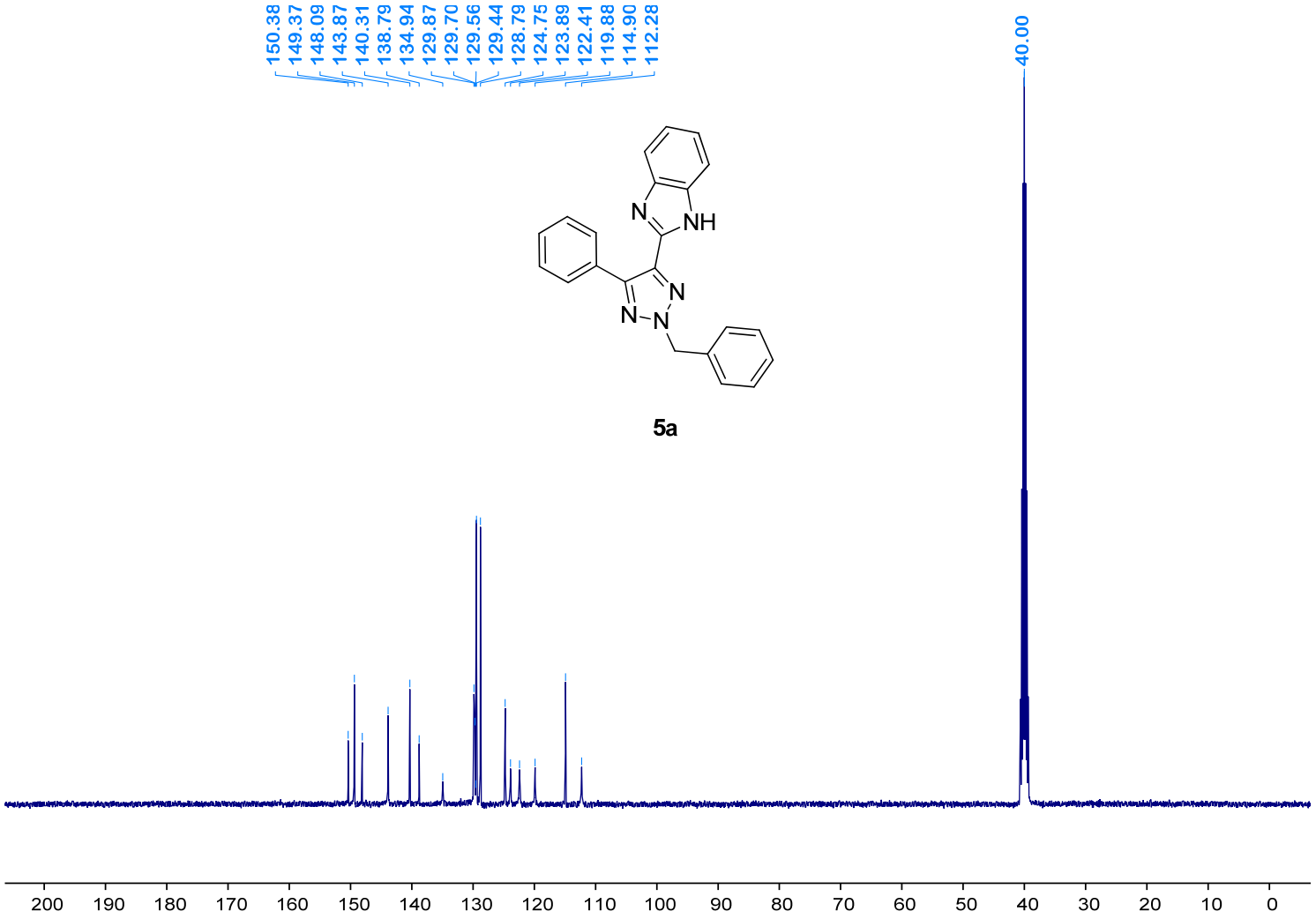
^{13}C NMR of compound 4h



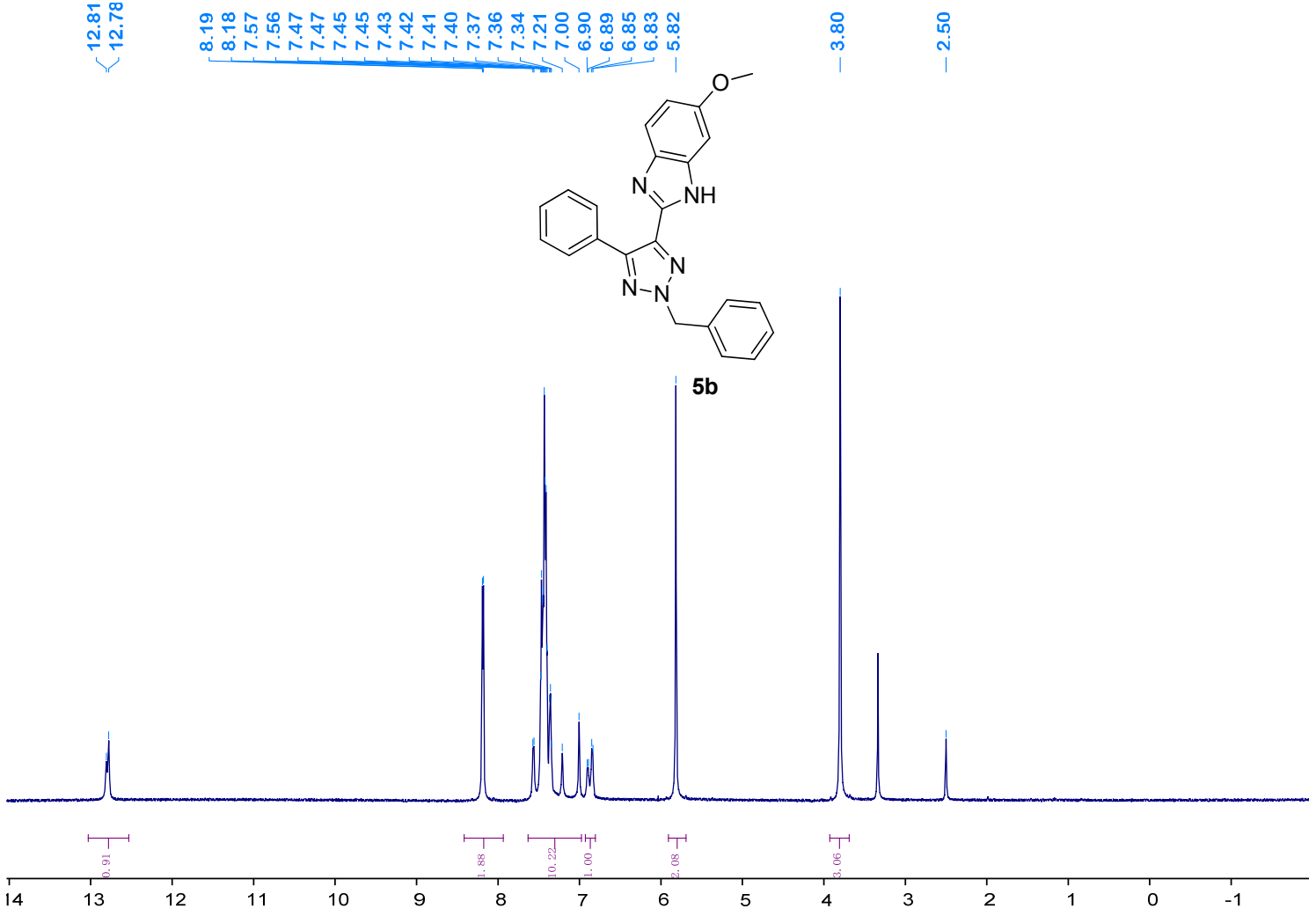
[1]H NMR of compound 5a



^{13}C NMR of compound 5a



^{1}H NMR of compound 5b



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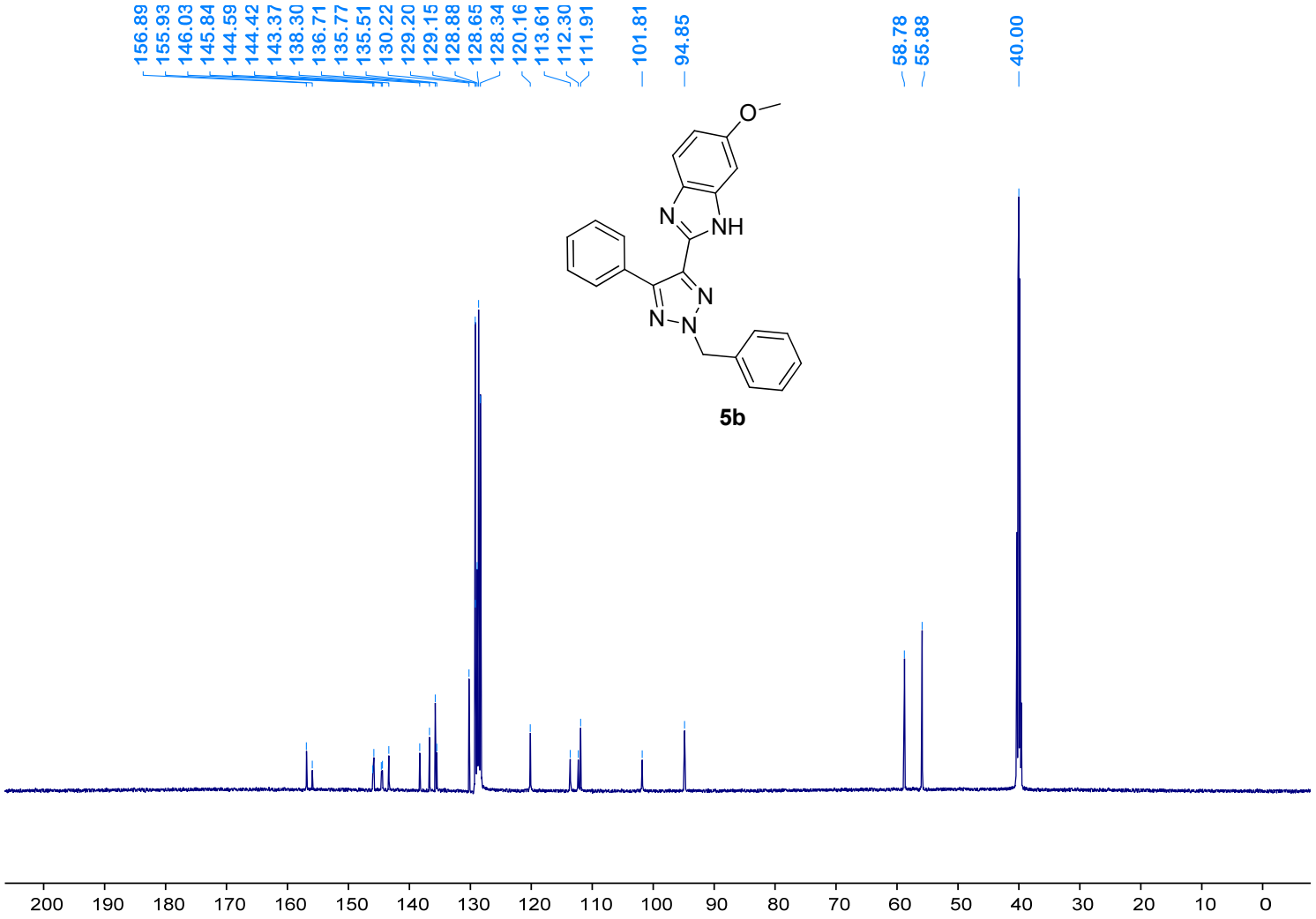
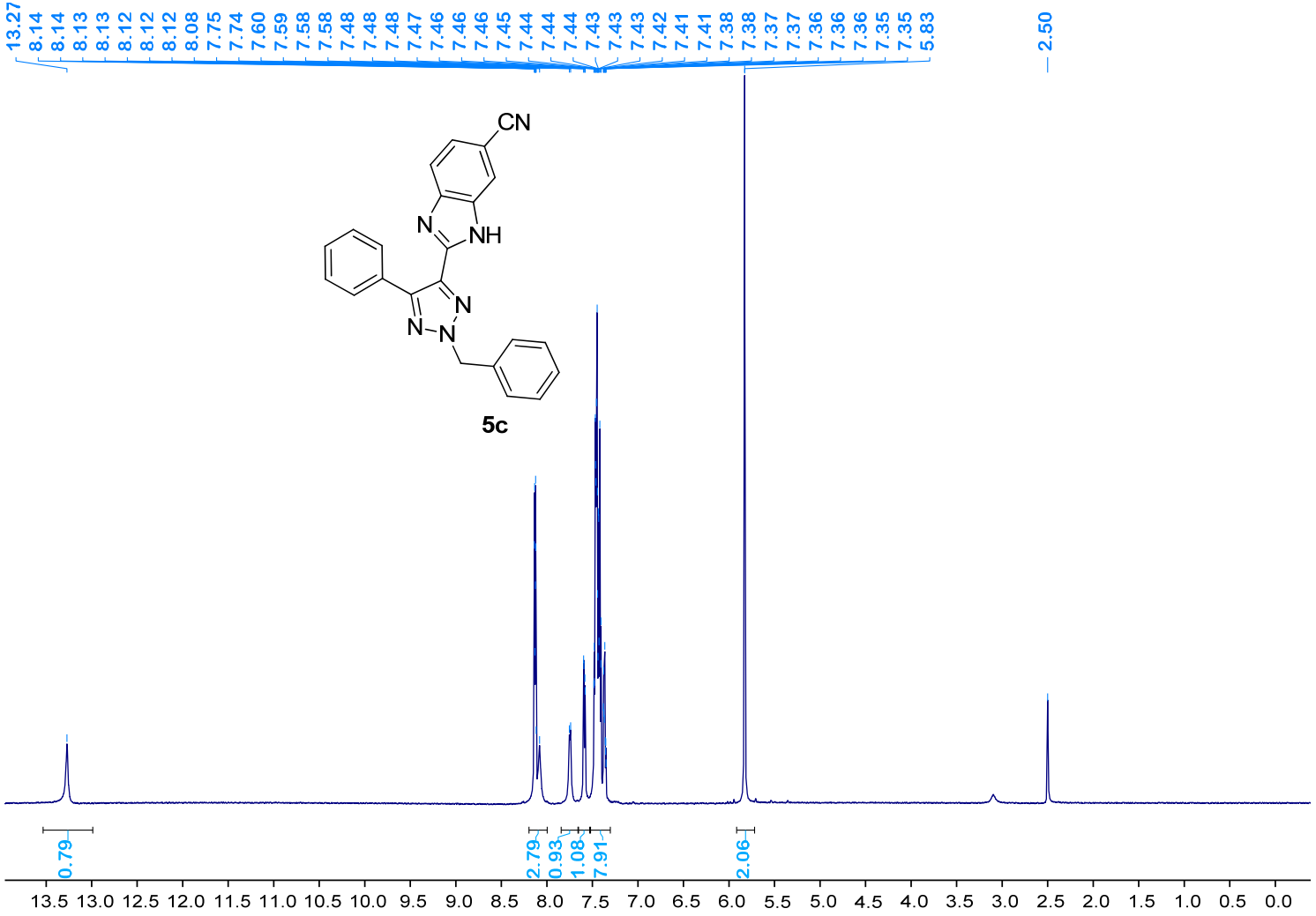
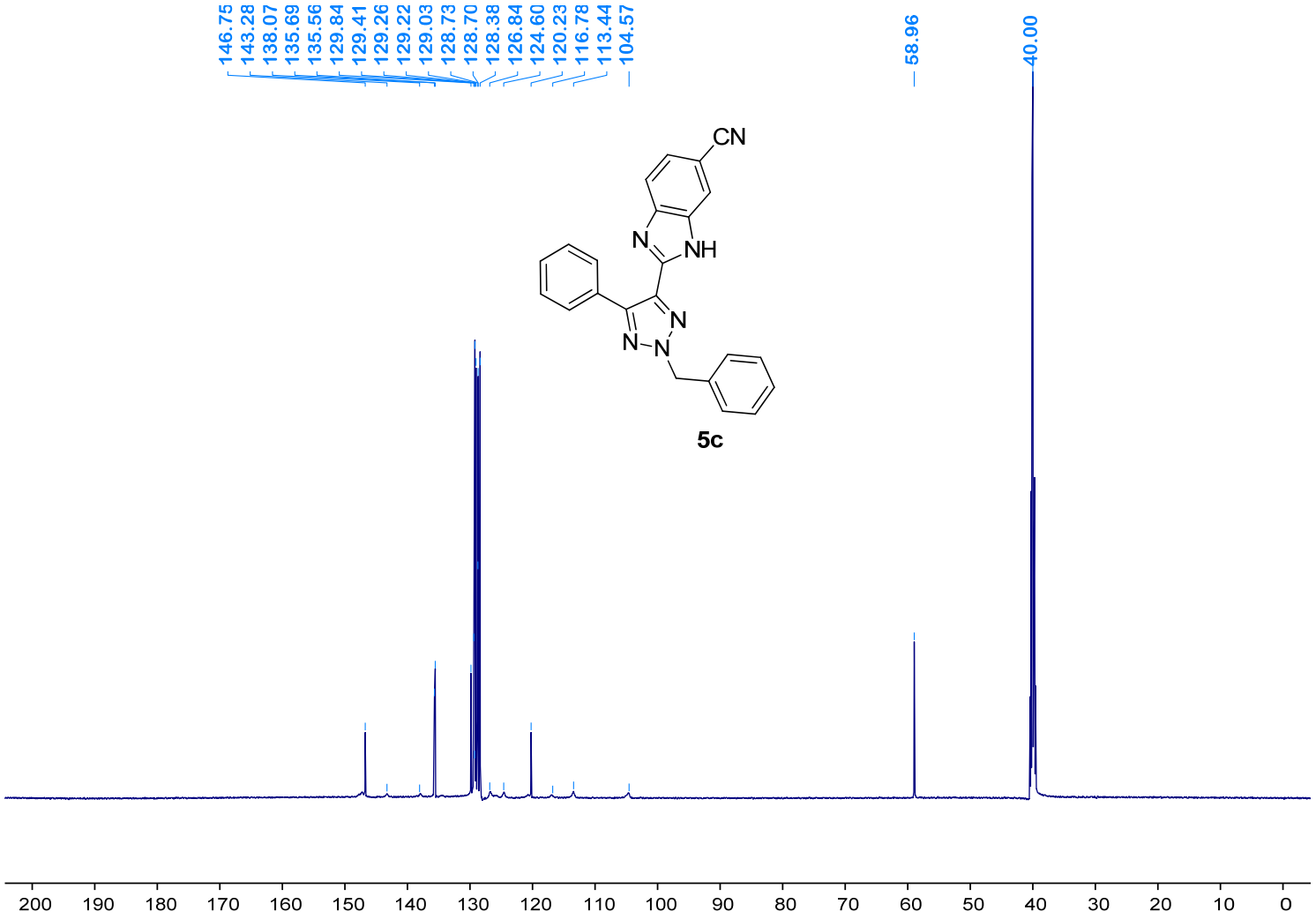


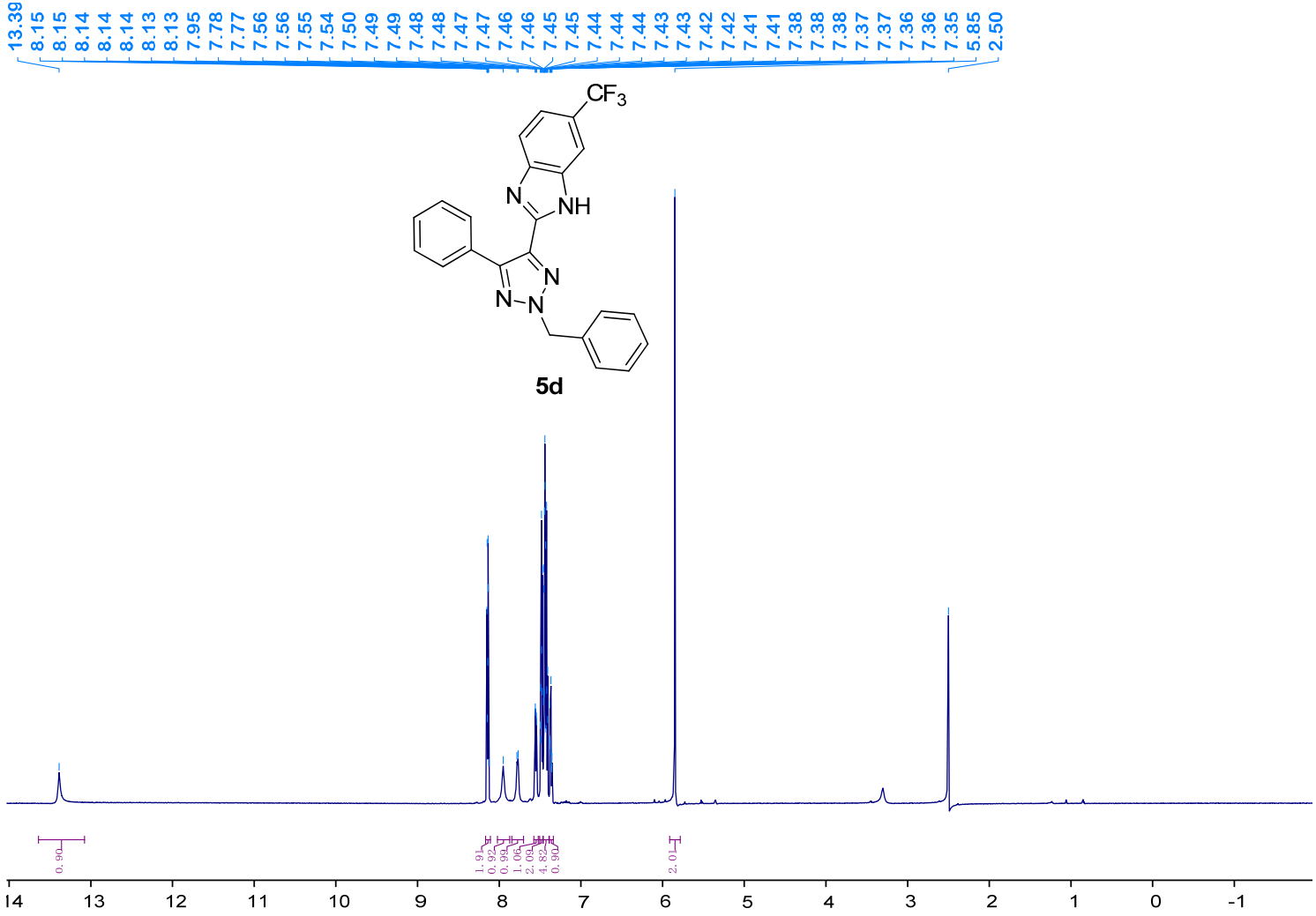
[1]H NMR of compound 5c



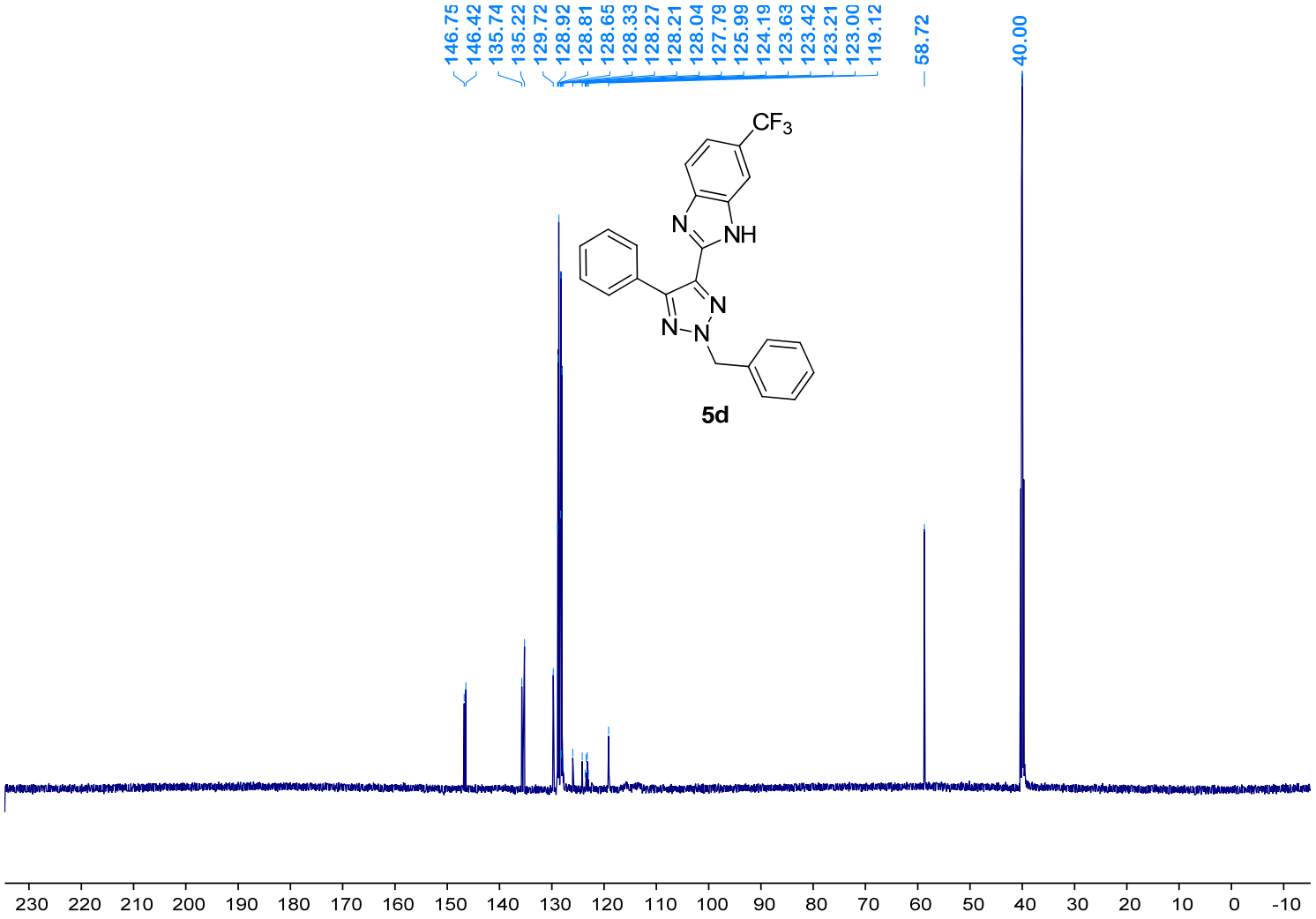
^{13}C NMR of compound 5c



^{1}H NMR of compound 5d



^{13}C NMR of compound 5d



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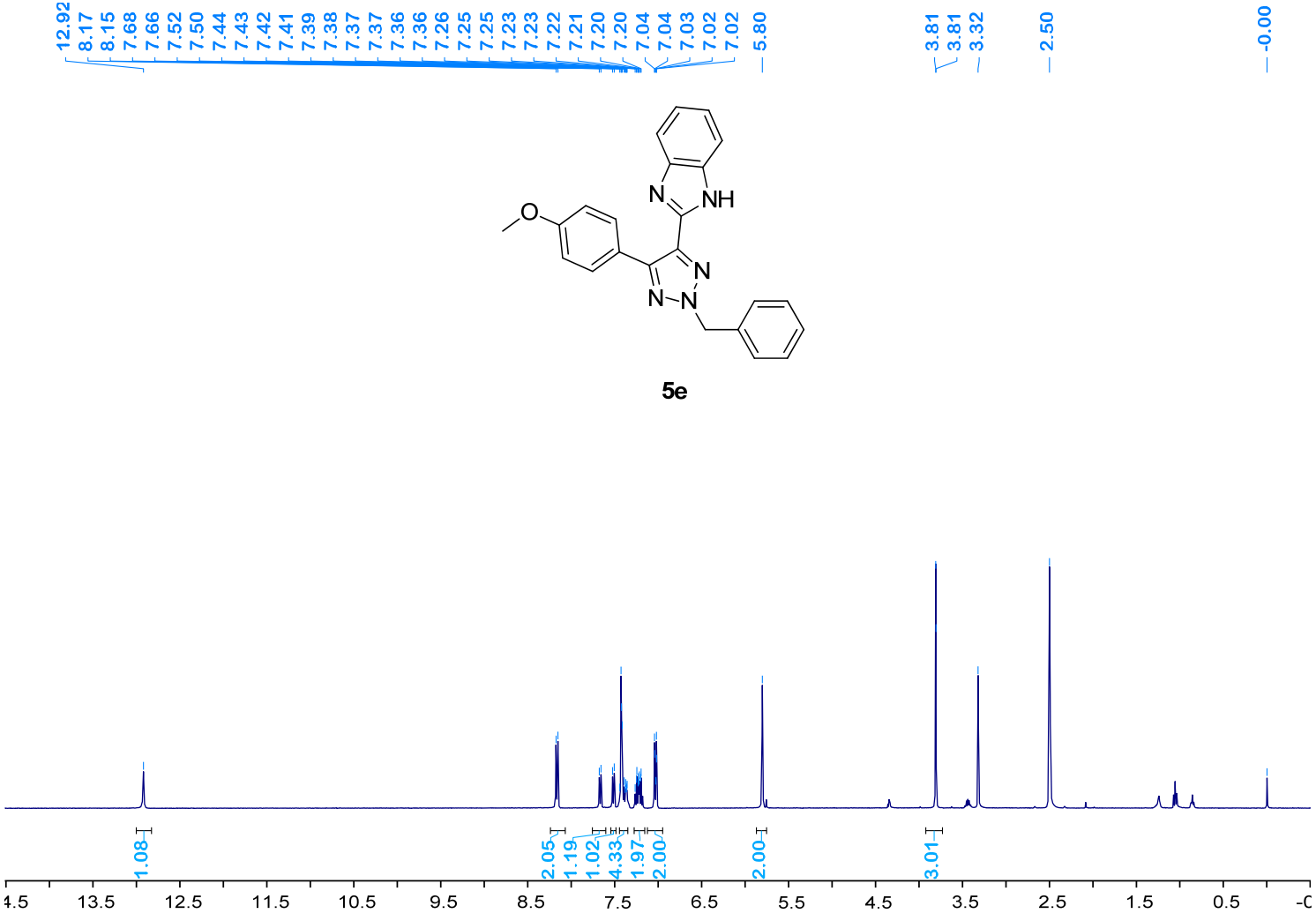
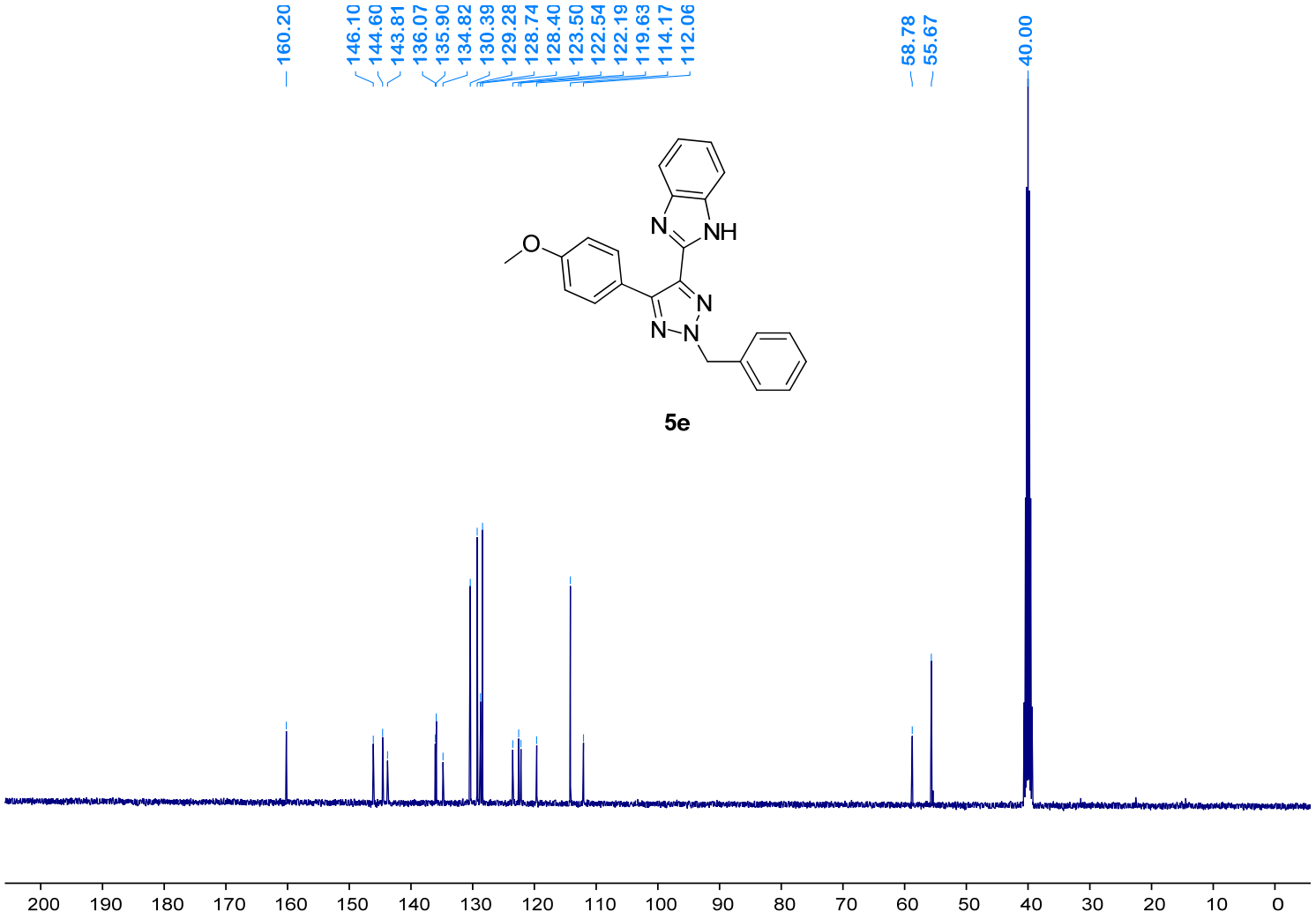
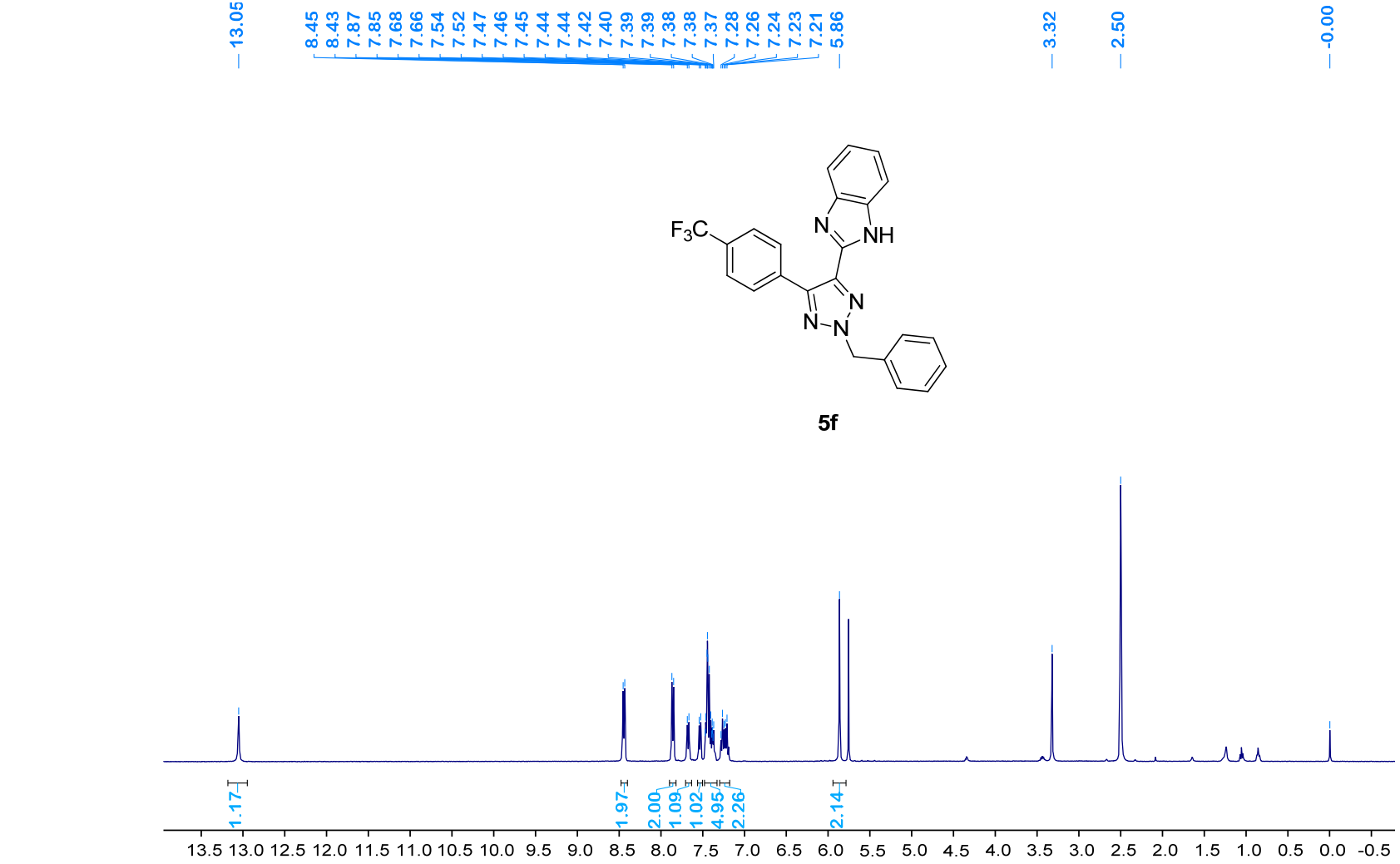


5e

^{13}C NMR of compound 5e

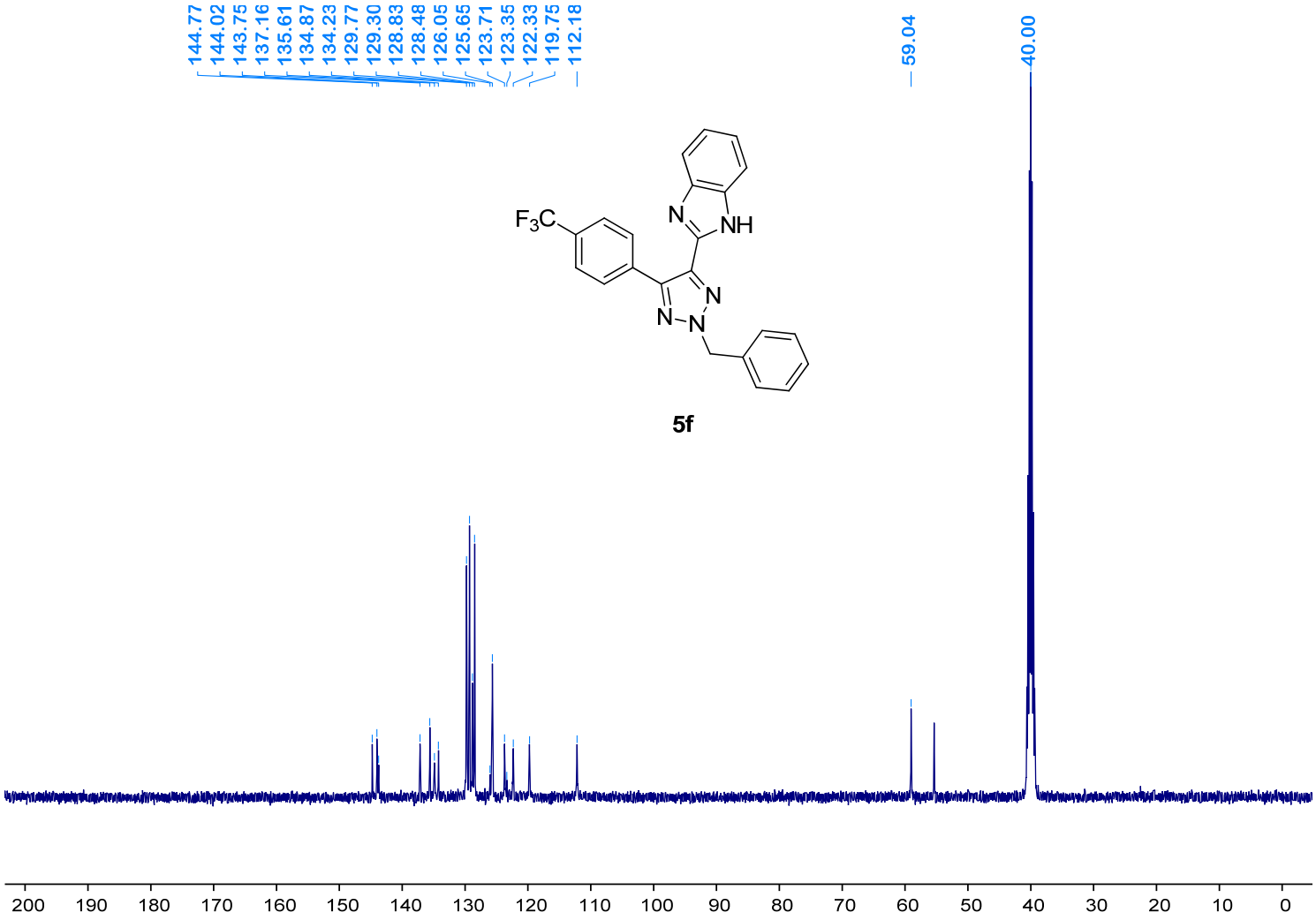


^{1}H NMR of compound 5f

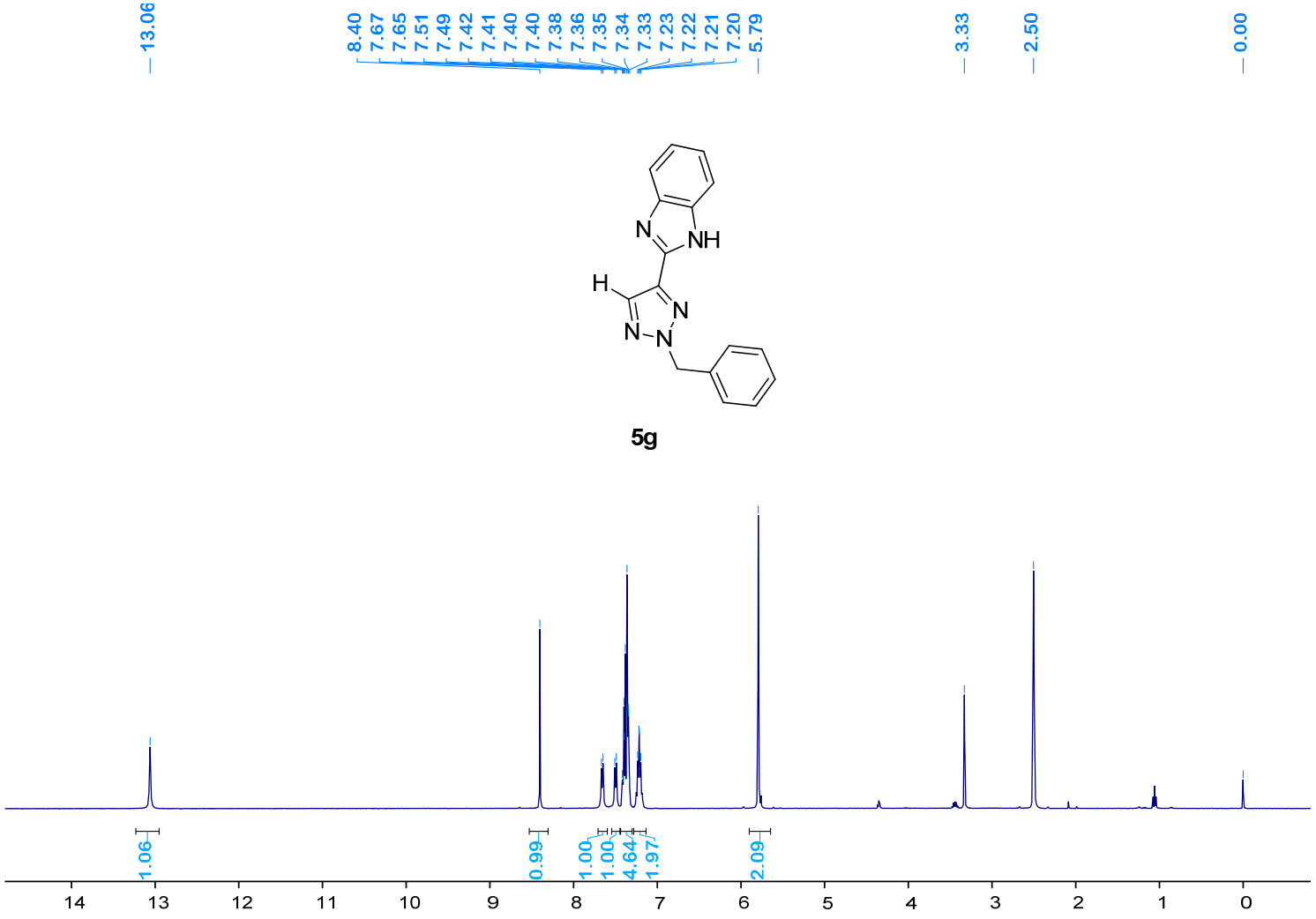


5f

^{13}C NMR of compound 5f

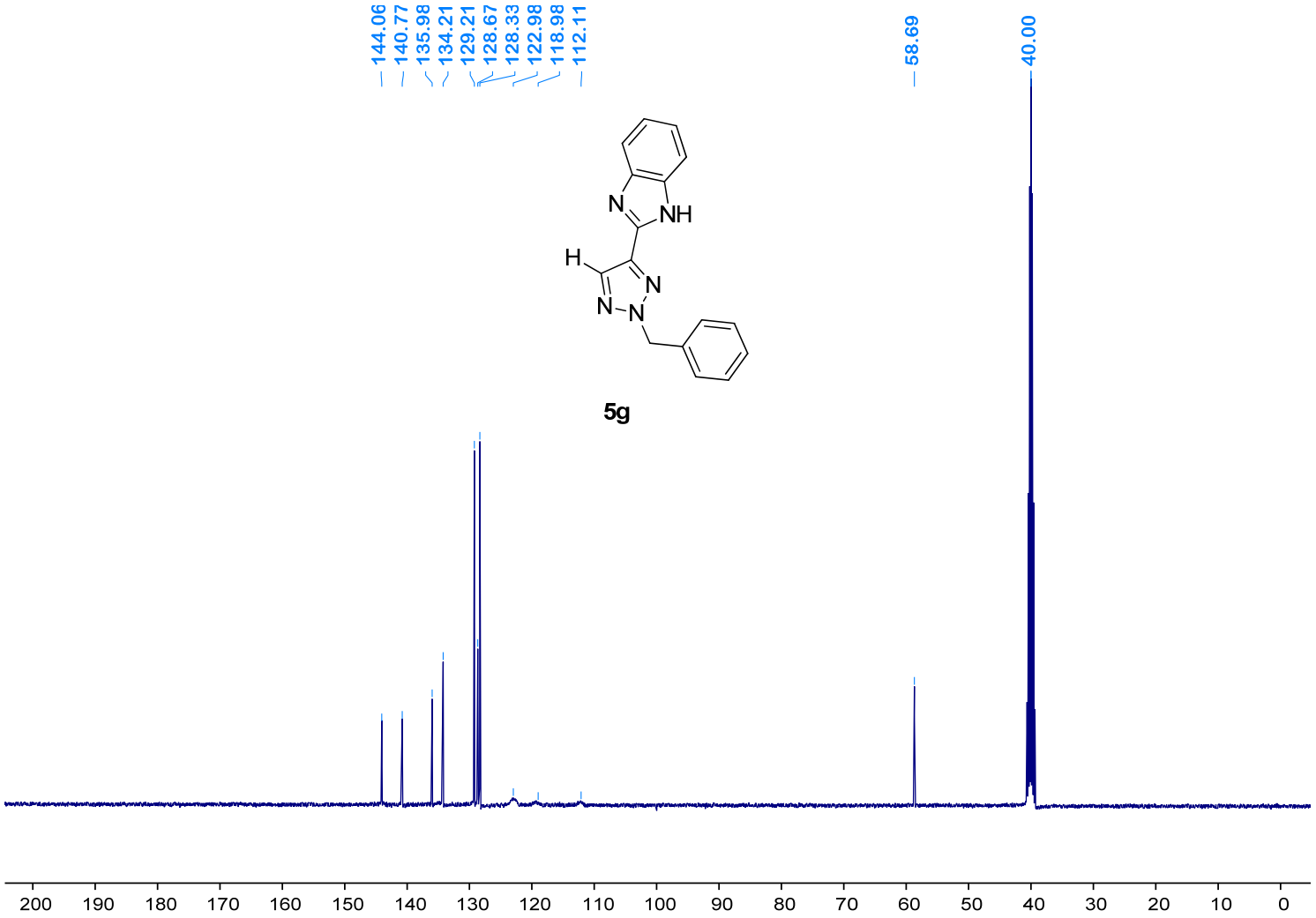


^{1}H NMR of compound 5g

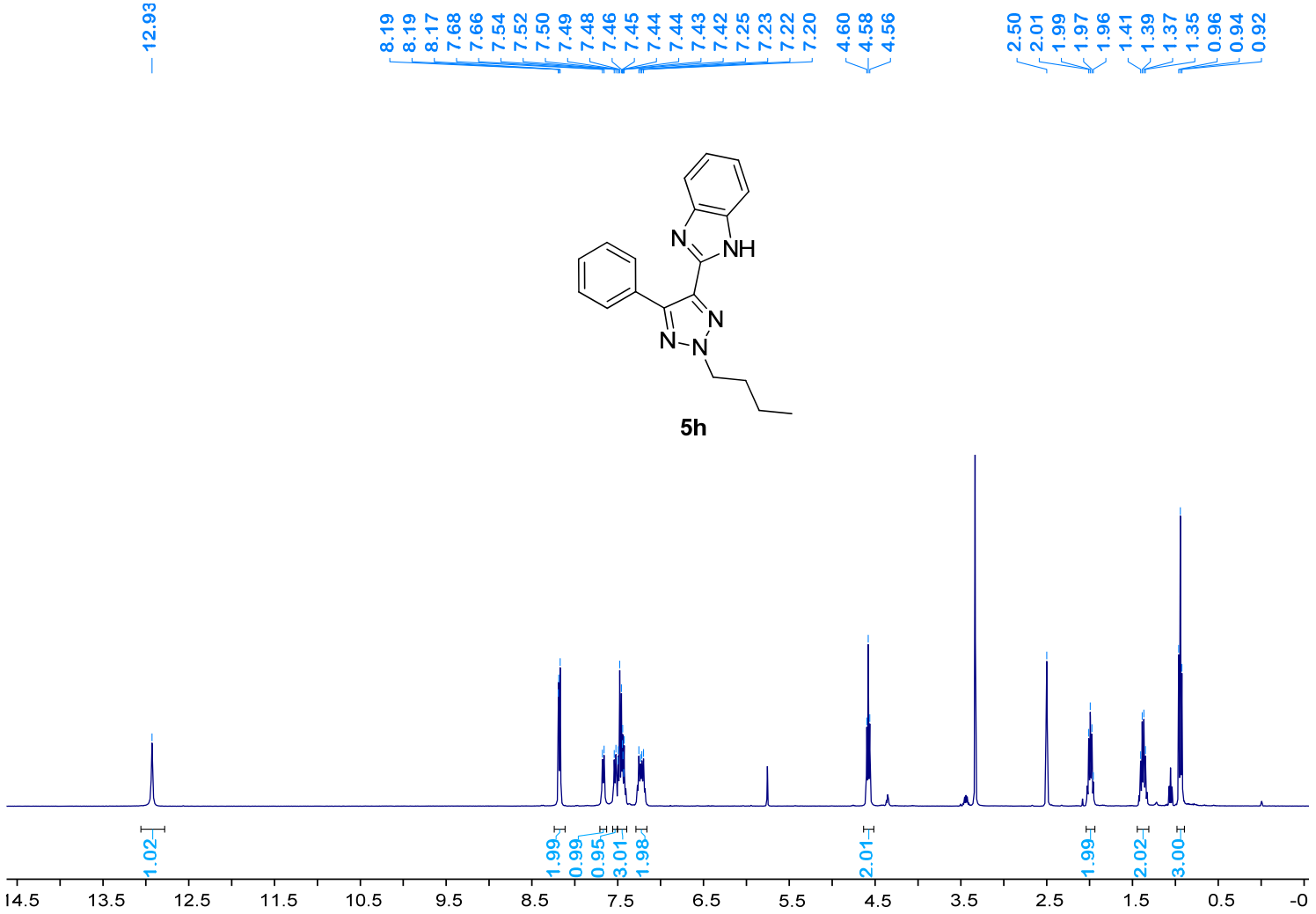


5g

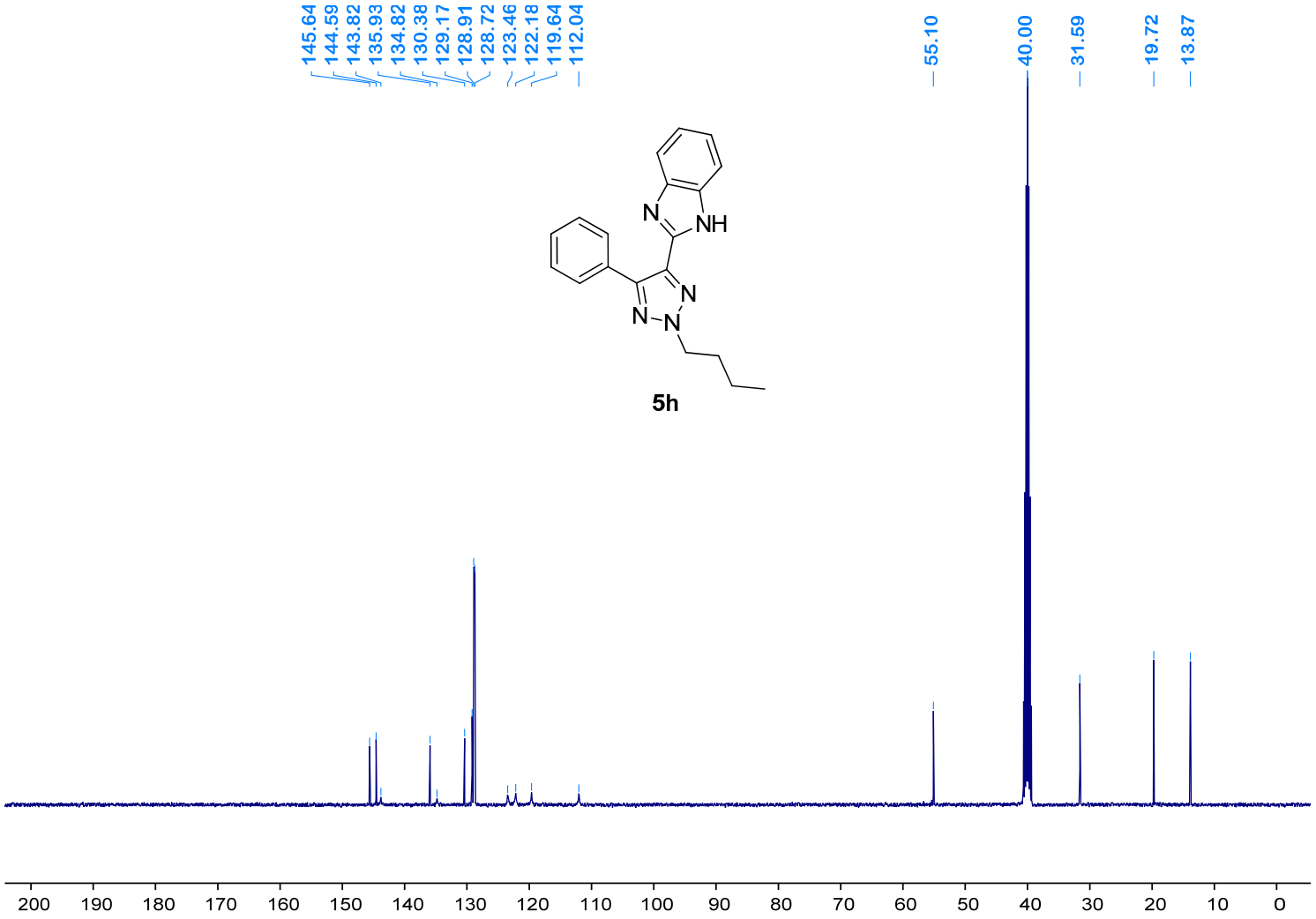
^{13}C NMR of compound 5g



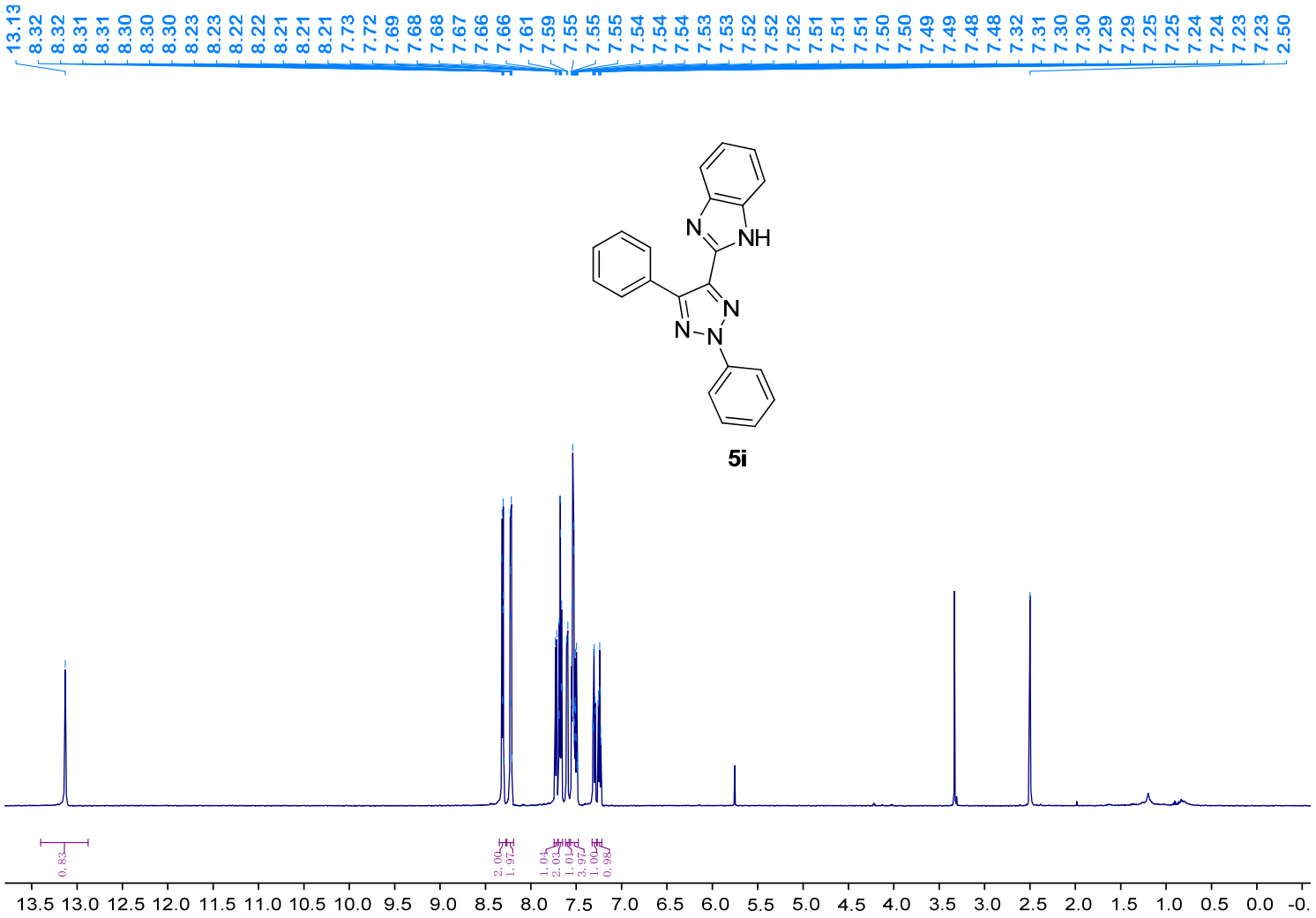
^{1}H NMR of compound 5h



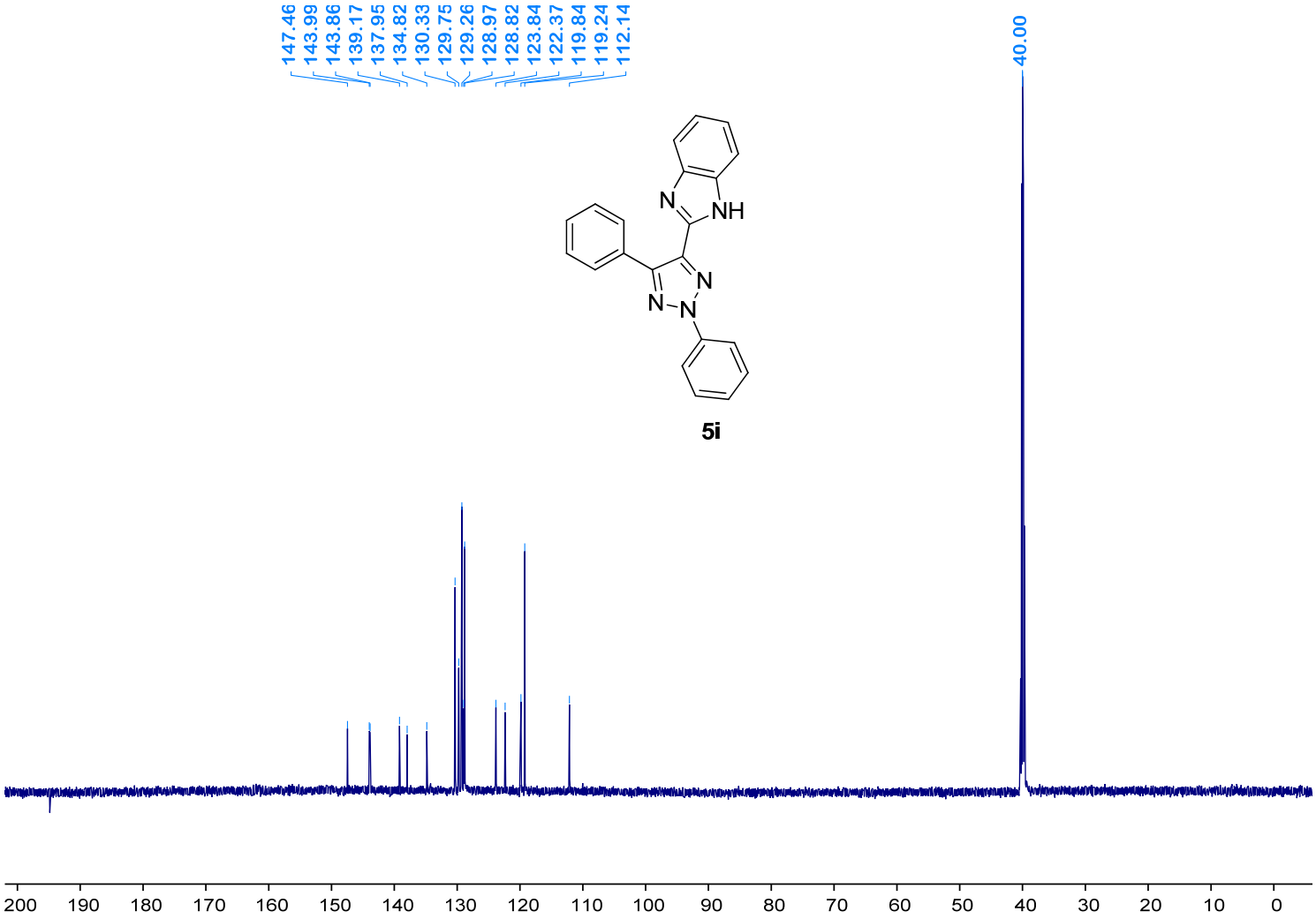
^{13}C NMR of compound 5h



^{1}H NMR of compound 5i

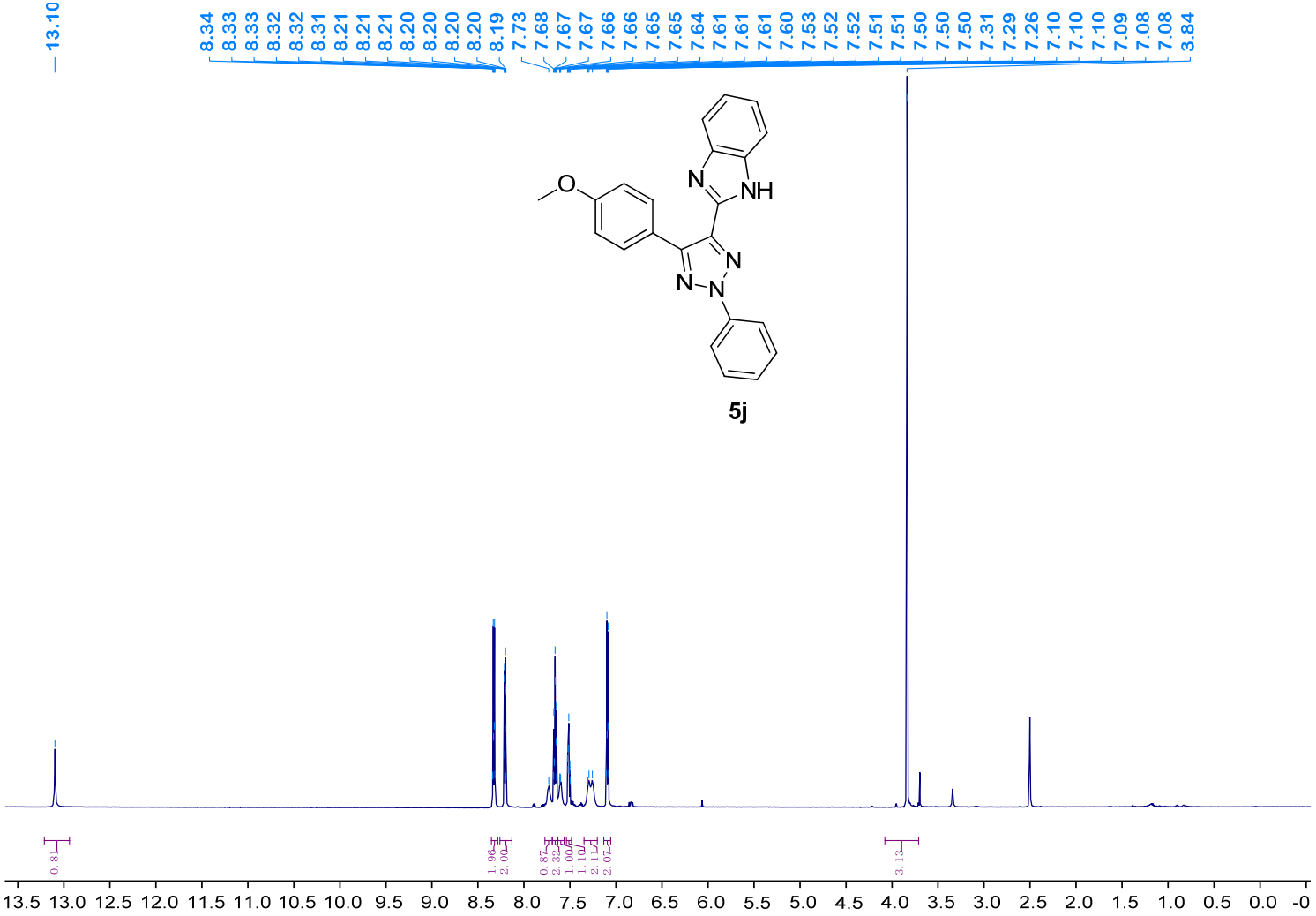


^{13}C NMR of compound 5i

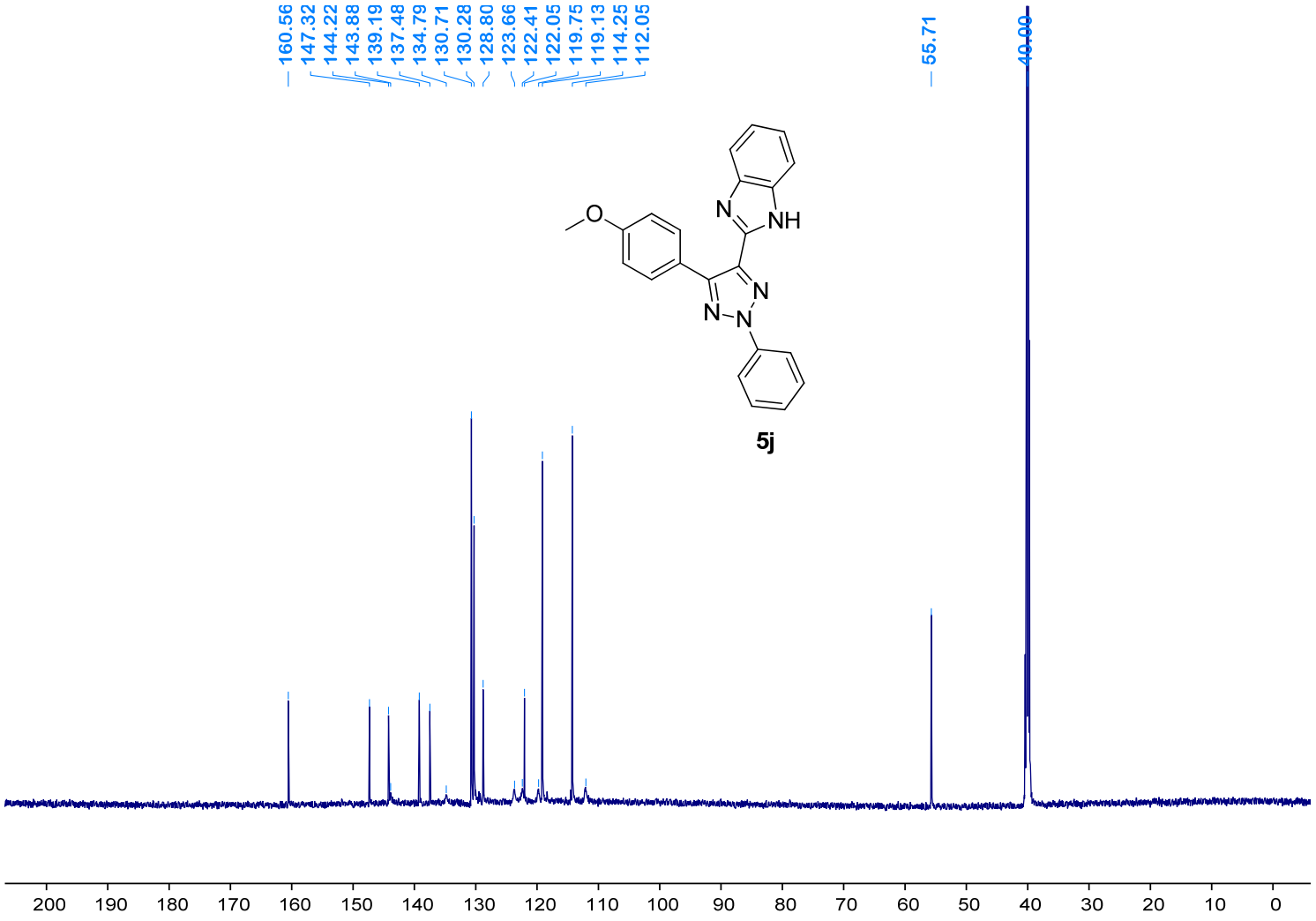


5i

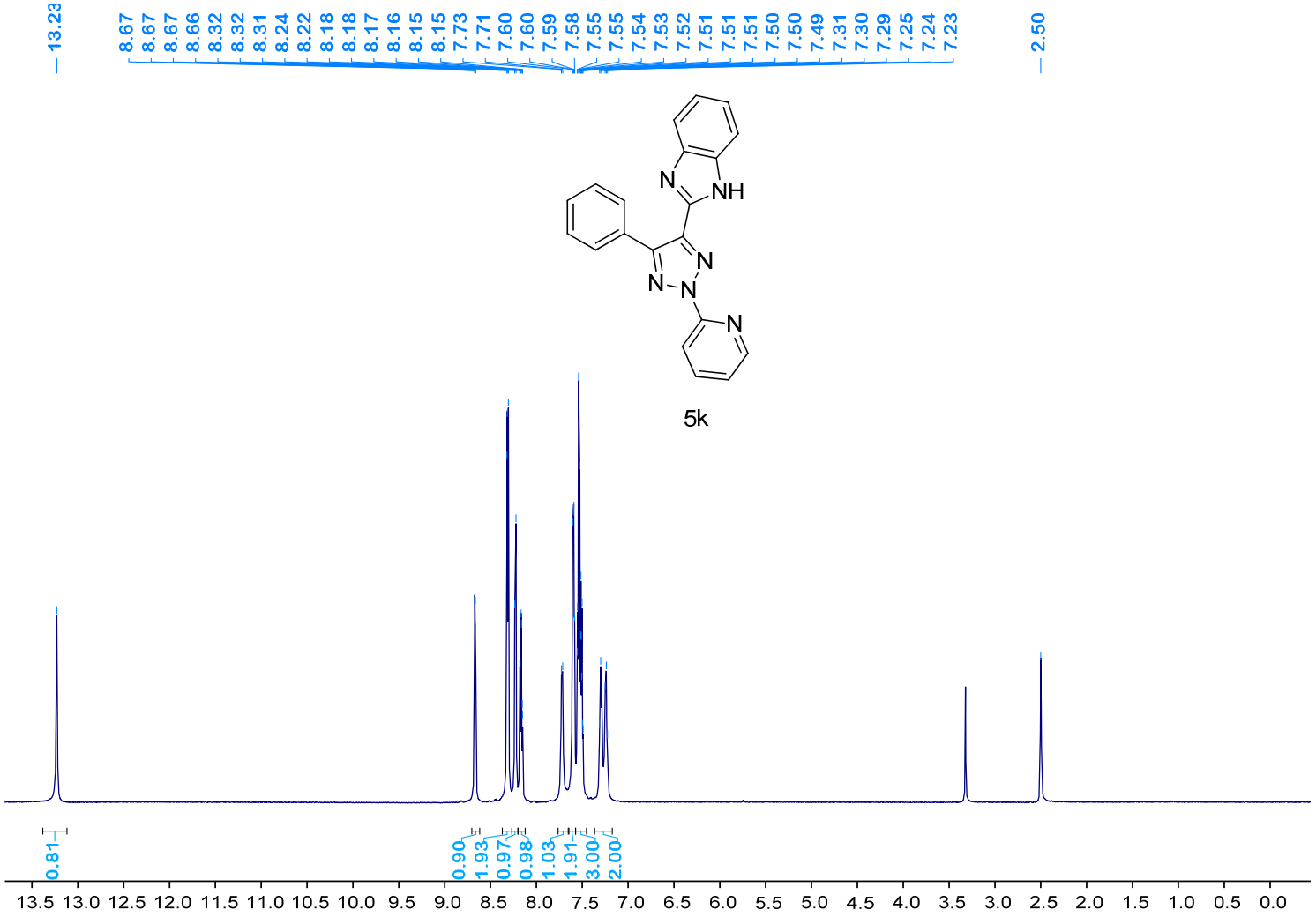
[1]H NMR of compound 5j



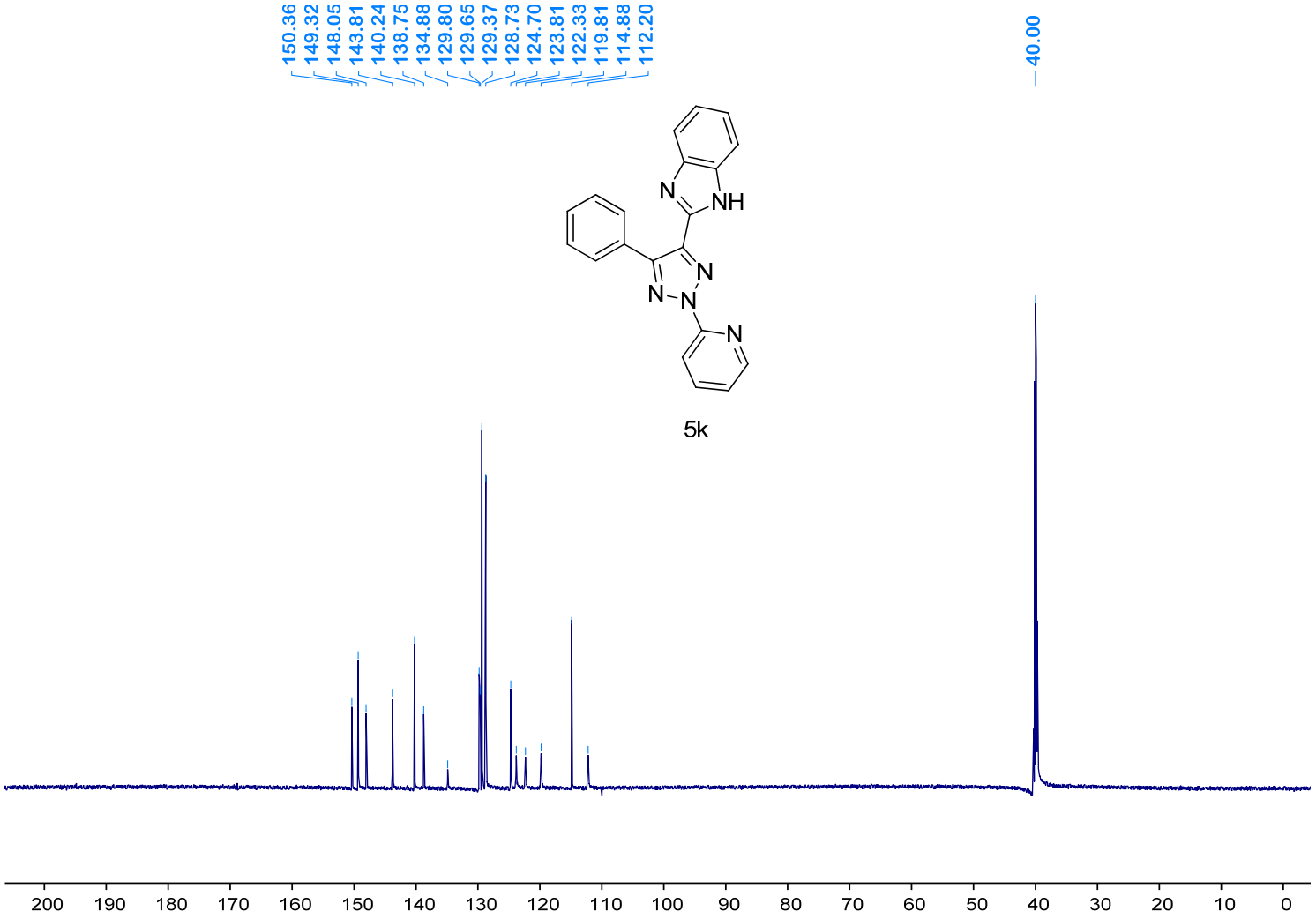
^{13}C NMR of compound 5j



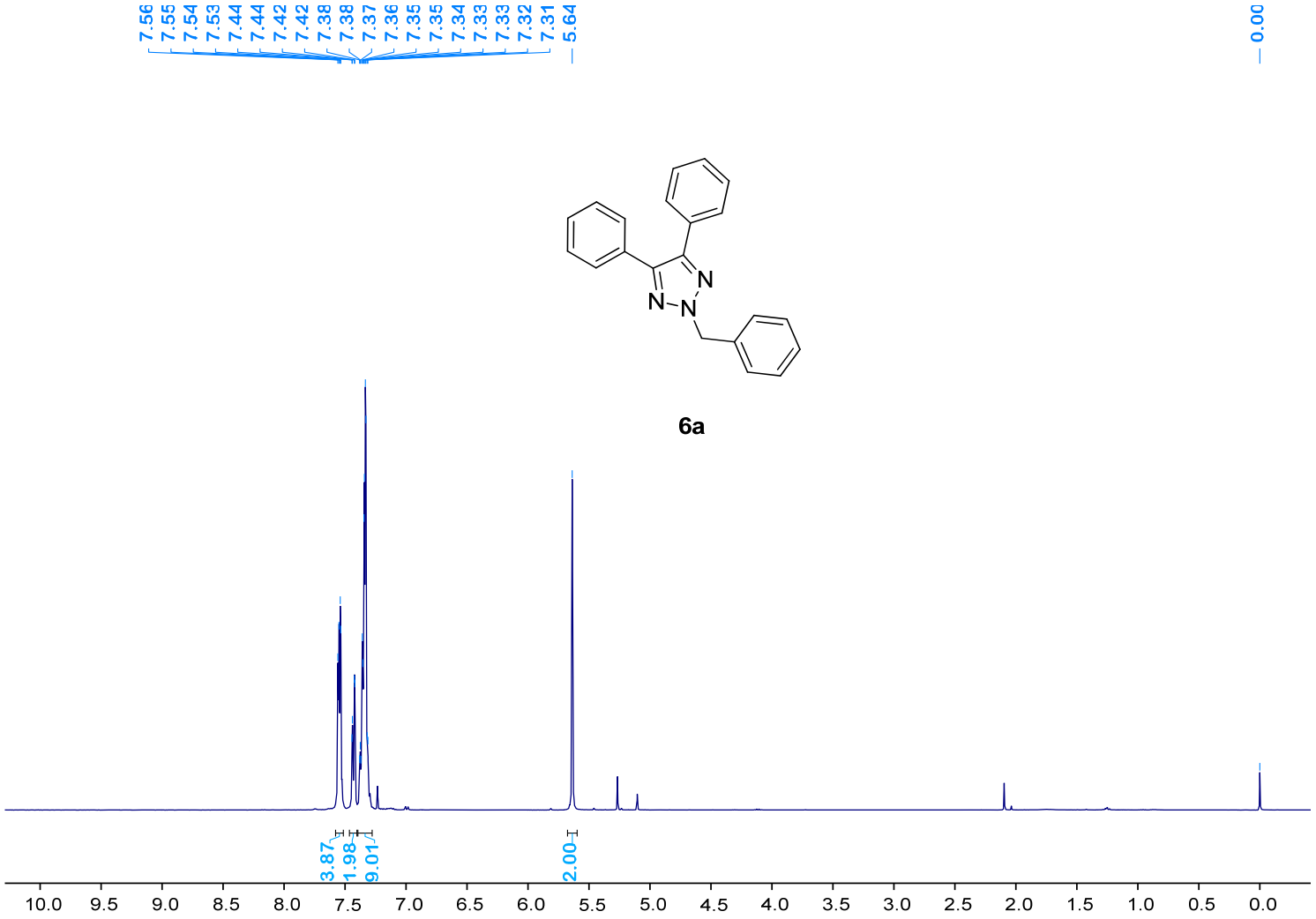
^{1}H NMR of compound 5k



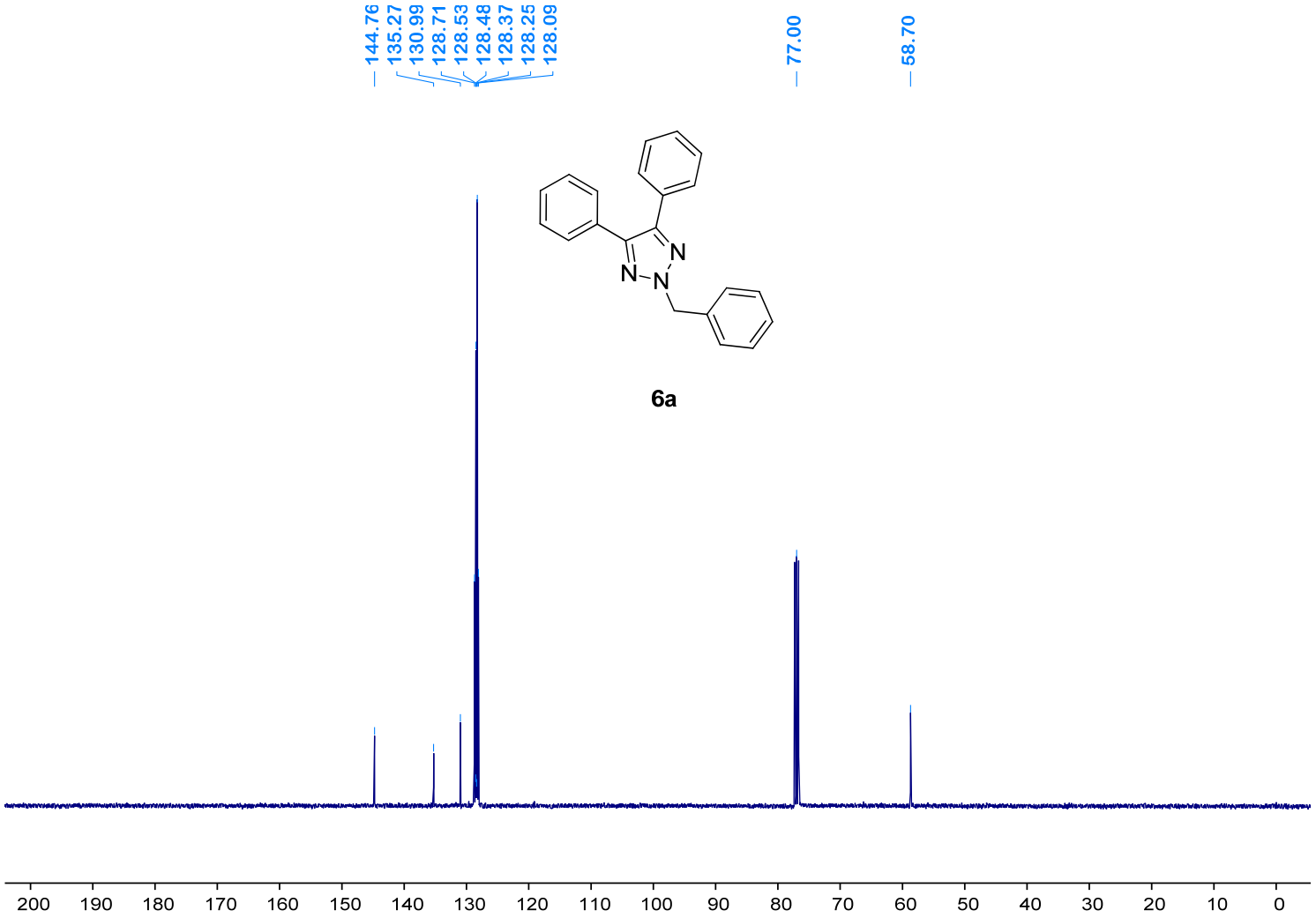
^{13}C NMR of compound 5k



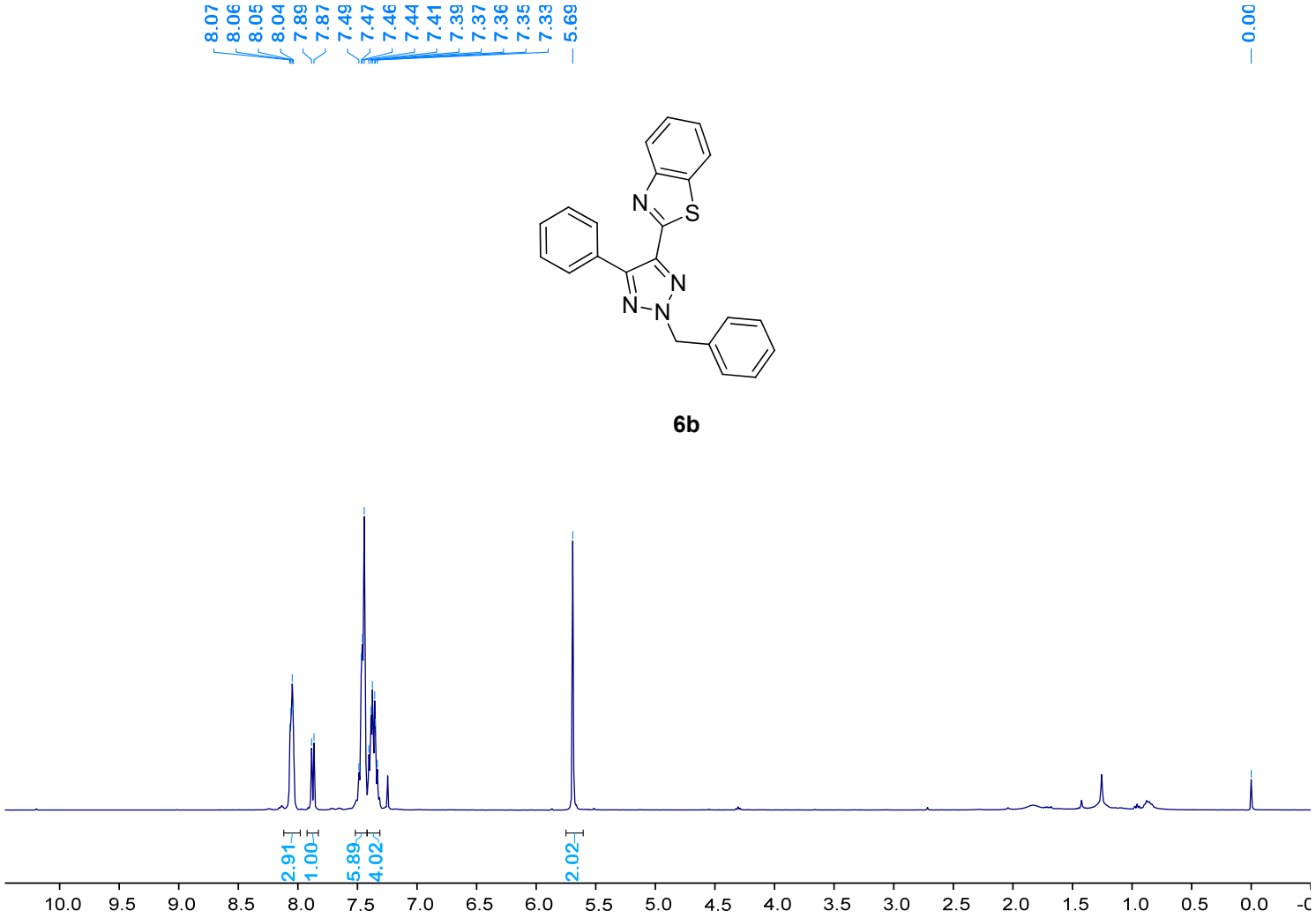
^{1}H NMR of compound 6a



^{13}C NMR of compound 6a

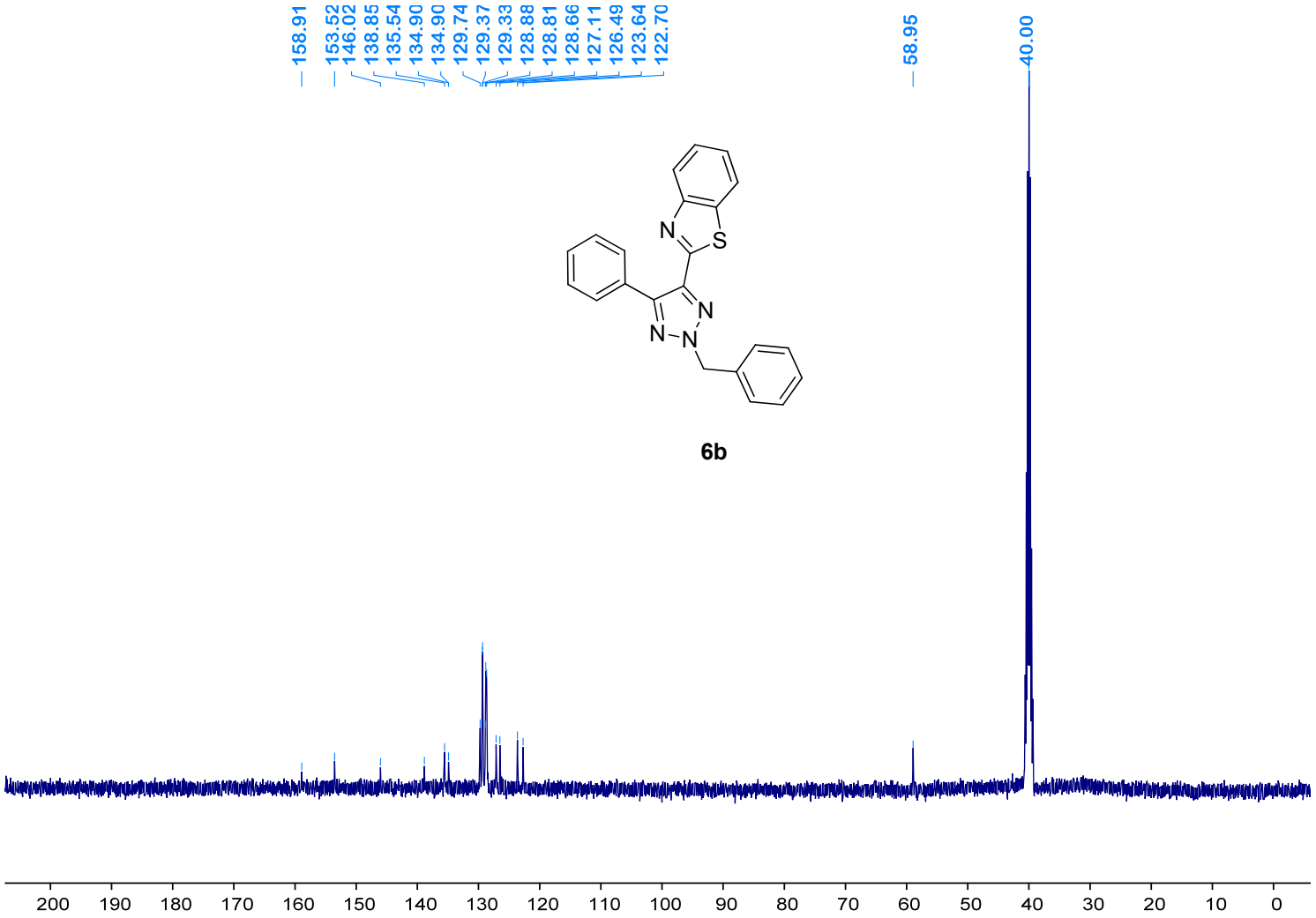


^{1}H NMR of compound 6b

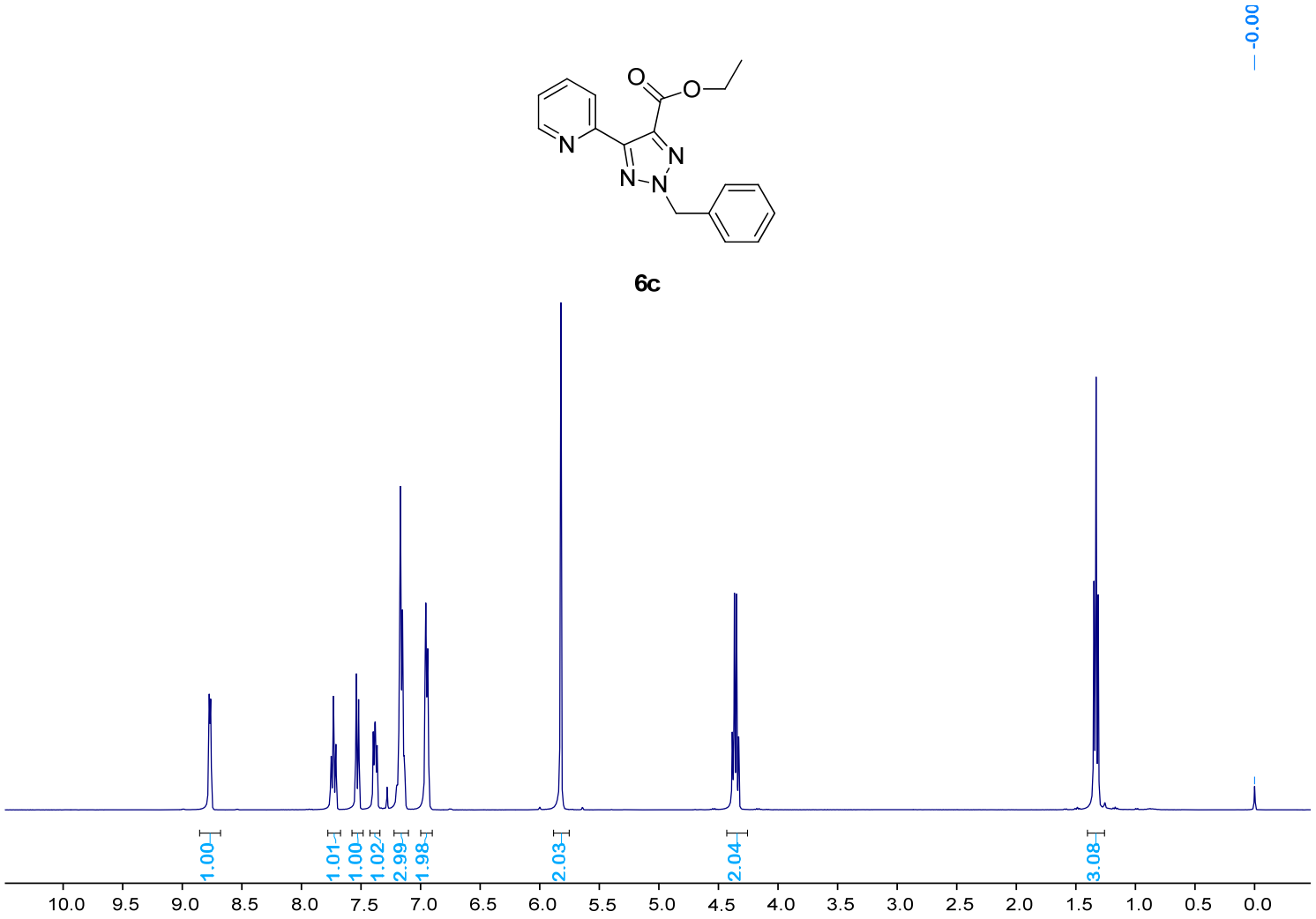


6b

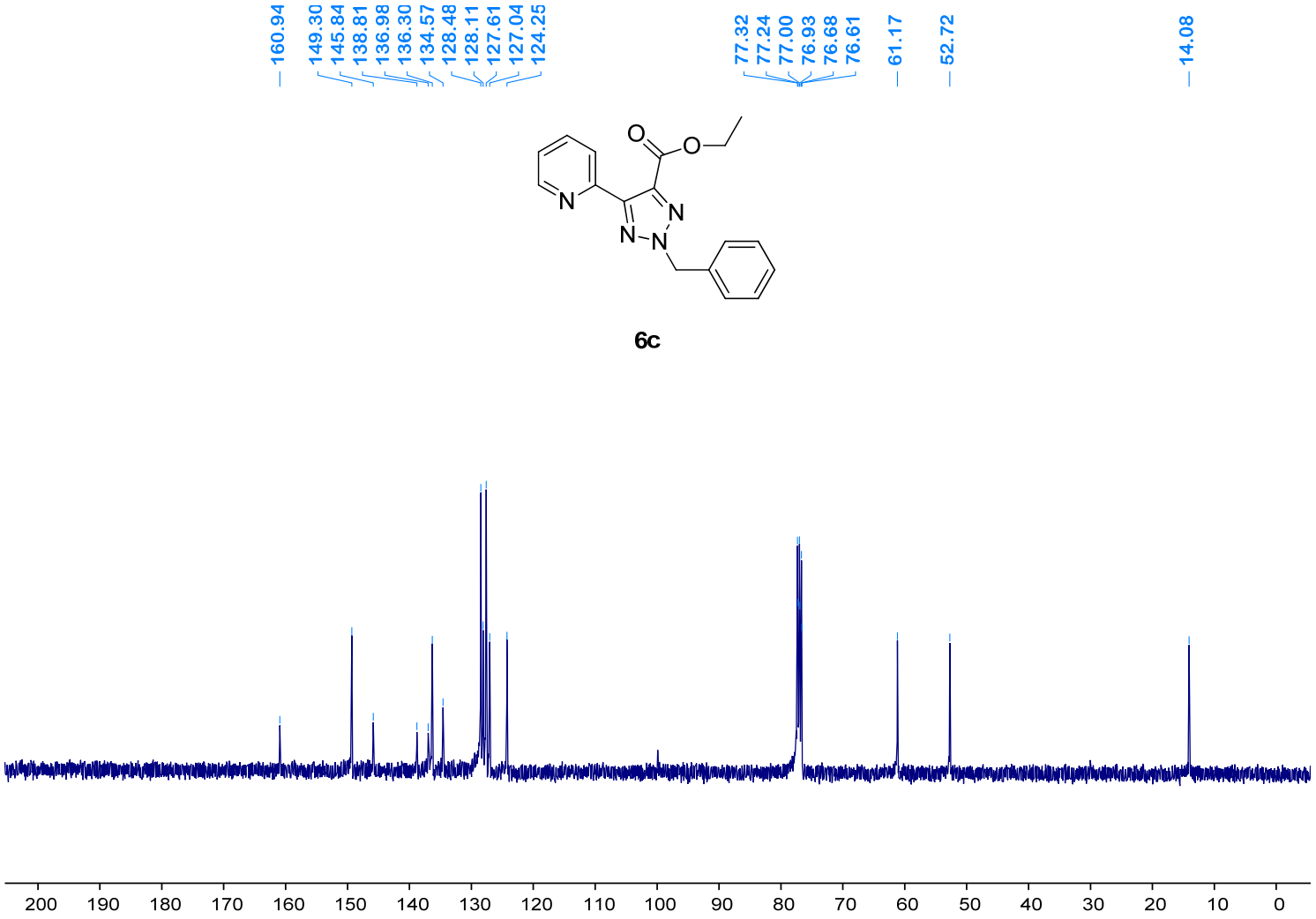
^{13}C NMR of compound 6b



[1]H NMR of compound 6c



^{13}C NMR of compound 6c



6c