

Hypervalent iodine promoted ortho diversification: 2-aryl benzimidazole, quinazoline and imidazopyridine as directing templates

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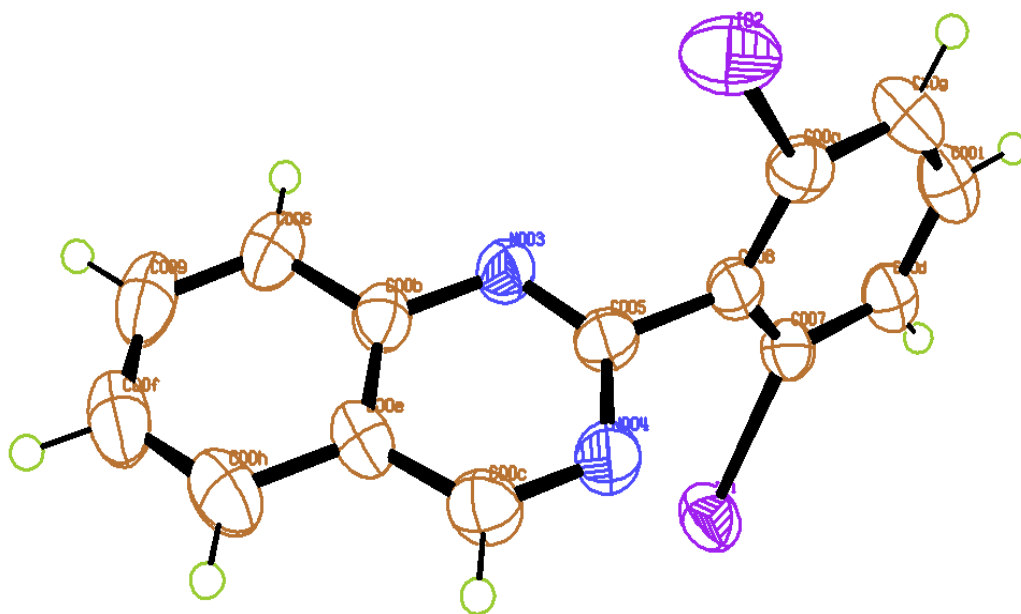
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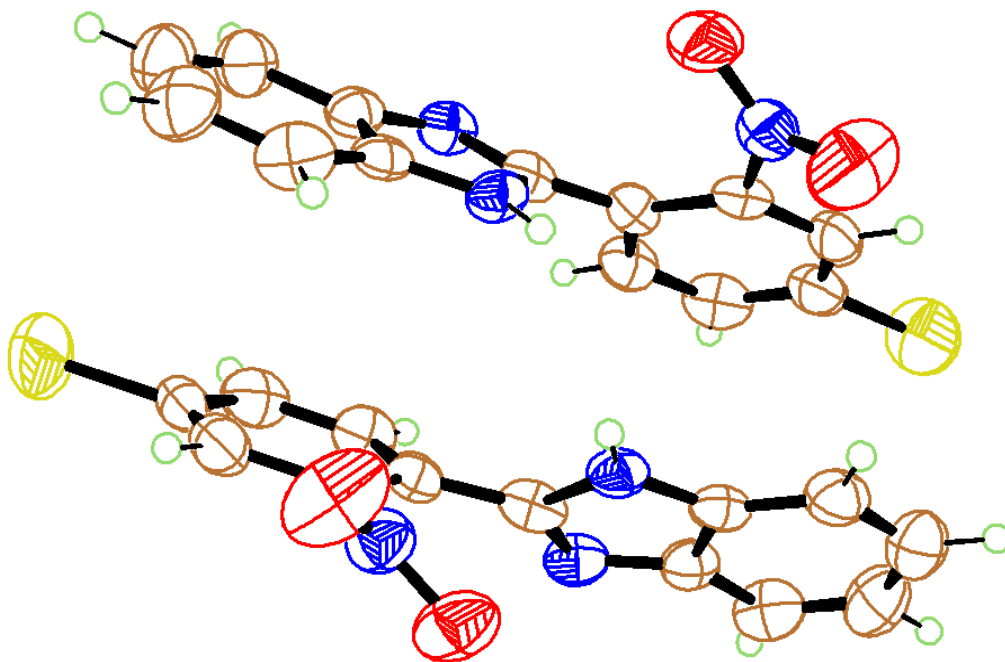
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X-ray Crystallography Analysis of Compound 4p and 5c (CCDC 1950069 and 1950441):



The X-ray structure of **4p**. The ellipsoid contour percent probability level is 50%.



The X-ray structure of **5c**. The ellipsoid contour percent probability level is 50%.

Single crystal X-ray data for compound 4p and 5c (CCDC 1950069 and 1950441):

Single crystals suitable for X-ray diffraction of **4p** and **5c** were grown from ethyl acetate and ethanol respectively. The crystals were carefully chosen using a stereo zoom microscope supported by a rotatable polarizing stage. The data were collected at 273(0) K and 296(2) K for **4p** and **5c** on a Bruker-APEX II CCD diffractometer with graphite monochromated Mo-K α radiation (0.71073 Å). The data were processed using the package SAINT.¹ Structures were solved by direct and Fourier methods and refined by full-matrix least squares based on F2 using SHELXTL² and SHELXL-97³ packages.

Table 1. Crystallographic data for the compound **4p** and **5c**

Compounds	4p	5c
empirical formula	C ₁₄ H ₈ I ₂ N ₂	C ₁₃ H ₁₀ Cl N ₃ O ₂
fw	458.02	275.69
crystal color	clear light yellow	yellow
crystal system	orthorhombic	Monoclinic
space group	P 2ac 2ab	<i>P-1</i>
<i>a</i> (Å)	7.7487(17)	7.7529(6))
<i>b</i> (Å)	8.3925(19)	7.7548(6)
<i>c</i> (Å)	21.639(5)	23.621(2)
α (°)	90.00	92.139(5)
β (°)	90.00	91.463(5)
γ (°)	90.00	118.775(3)
<i>V</i> (Å ³)	1407.2(5)	1242.40(17)

Z	4	4
T, K	273(2)	296(2)
Wavelength (Å)	0.71073	0.71073
2θ (°)	1.882-27.033	0.86-24.90
μ (mm ⁻¹)	4.453	0.308
ρ _{calcd} (g cm ⁻³)	2.162	1.474
F(000)	848	568
absorption correction	multi-scan	multi-Scan
index ranges	-9 ≤ h ≤ 9	-9 ≤ h ≤ 8
	-10 ≤ k ≤ 10	-9 ≤ k ≤ 9
	-27 ≤ l ≤ 27	-27 ≤ l ≤ 27
reflections collected	26839	15629
independent reflections (R _{int})	9980 (0.0382)	3165(0.0572)
Goodness-of-fit on F ²	1.143	2.079
R ₁ ^a /wR ₂ ^b (I > 2σ(I))	0.0611/0.1099	0.0386/0.0988
R ₁ ^a /wR ₂ ^b (for all data)	0.0200/0.0429	0.0611/0.1099
Largest diff. peak/hole / e Å ⁻³	0.399/ -0.511	0.367/ -0.329

$${}^a R_1 = [\sum ||F_o| - |F_c|| / \sum |F_o|]. \quad {}^b wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum wF_o^4]^{1/2}$$

References:

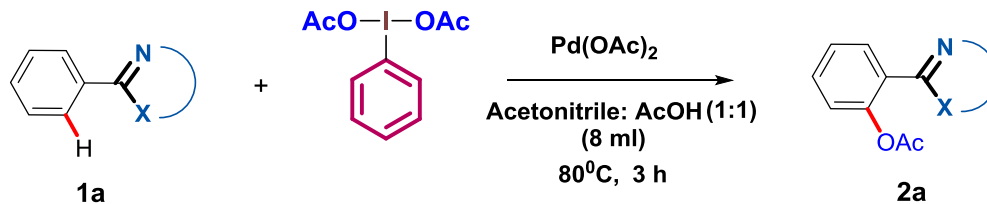
1. *APEX-II, SAINT-Plus, and TWINABS*; Bruker-NoniusAXS Inc.: Madison, WI, 2004.

2. *SHELXTL*, version 6.10; Bruker AXS Inc.: Madison, WI, 2002.
3. Sheldrick, G. M. *SHELXL-97, Crystal Structure Refinement Program*; University of Göttingen: Göttingen, Germany, 1997.
4. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), *J. Appl. Cryst.* 42, 339-341.
5. Sheldrick, G.M. (2015). *Acta Cryst.* A71, 3-8.
6. Sheldrick, G.M. (2015). *Acta Cryst.* C71, 3-8.

General Information:

Reactions were monitored by thin-layer chromatography carried out on silica plates using UV-light. Column chromatography was performed on silica gel (100-200 mesh) using hexane and ethyl acetate as eluents. Evaporation of solvents was done under reduced pressure at temperatures less than 60 °C. IR spectra were recorded as neat compounds. ¹H and ¹³C NMR spectra were recorded using DMSO-*d*₆ and CDCl₃ solvents respectively on a 300, 400, 500 and 600 and 75, 100, 150 MHz spectrometer where tetramethylsilane (TMS) was used as internal standard. Chemical shifts δ and coupling constants *J* are given in ppm (parts per million) and Hz (hertz) respectively. Proton coupling patterns are described as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), doublet of doublets (dd). HRMS data were recorded by Waters Xevo G-2 SQ TOF electrospray ionization mass spectrophotometer. Suitable single crystals of compounds **4p** and **5c** were mounted on a Bruker--APEX II CCD X-ray diffractometer with graphite monochromated Mo-K α radiation (0.71073 Å). Melting points were measured on a Köfler Block apparatus. All solvents were obtained from commercial sources and were purified and dried using standard procedure prior to use. Commercially available iodobenzene diacetate, Cs₂CO₃, Iodine, NaNO₂ were used without further purification.

Synthesis of product **2a** from 2-substituted benzimidazole (**1a**) in gram scale:

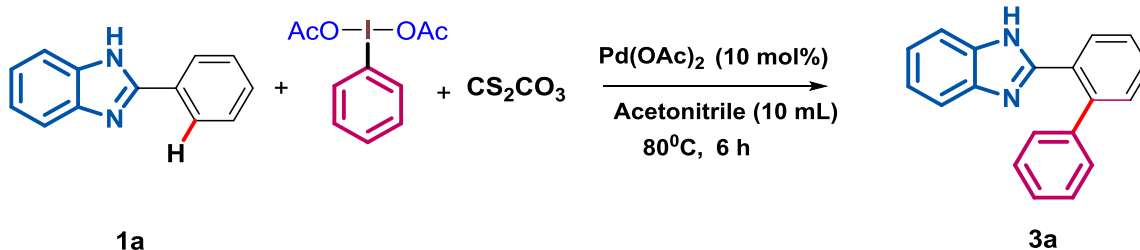


An oven-dried 25 mL round bottom flask fitted with CaCl₂ guard tube was charged with 2-phenyl benzimidazole (**1a**) (1.164 g, 6.0 mmol), Pd(OAc)₂ (135 mg, 0.6 mmol), PIDA (5.80 g, 18 mmol) in 8 mL dry acetonitrile: acetic acid (1:1 v/v). The reaction mixture was refluxed in a pre-heated oil bath to 80 °C under air for 3h. After being cooled at room temperature, the reaction mixture was neutralized with sat. NaHCO₃ solution (30 mL) and extracted with ethyl acetate (3 x 40mL). The combined organic layer was washed with brine, dried over anhydrous sodium sulphate, evaporated under reduced pressure and purified using silica gel column chromatography (100-200 mesh size) (hexane/ethyl acetate, 2:1) to give pure 2-(1H-benzo[d]imidazol-2-yl)phenyl acetate (**2a**) (1.20 g, yield 80%).

Synthesis of compound **2a** in the presence of radical inhibitor TEMPO:

An oven-dried 10 mL round bottom flask fitted with CaCl₂ guard tube was charged with 2-phenyl benzimidazole (**1a**) (97 mg, 0.5 mmol), Pd(OAc)₂ (12 mg, 0.05 mmol), PIDA (483.18 mg, 1.5 mmol), TEMPO (156 mg, 2.0 mmol) in 2 mL dry acetonitrile: acetic acid (1:1 v/v). The reaction mixture was refluxed in a pre-heated oil bath to 80 °C under air for 3h. After being cooled at room temperature, the reaction mixture was neutralized with sat. NaHCO₃ solution (5 mL) and extracted with ethyl acetate (3 x 10mL). The combined organic layer was washed with brine, dried over anhydrous sodium sulphate, evaporated under reduced pressure and then purified using silica gel column chromatography (100-200 mesh size) (hexane/ethyl acetate, 2:1) to give pure 2-(1H-benzo[d]imidazol-2-yl)phenyl acetate (**2a**) (0.102 g, yield 81%).

Synthesis of compounds (**3a**) from 2-substituted benzimidazole in gram scale:



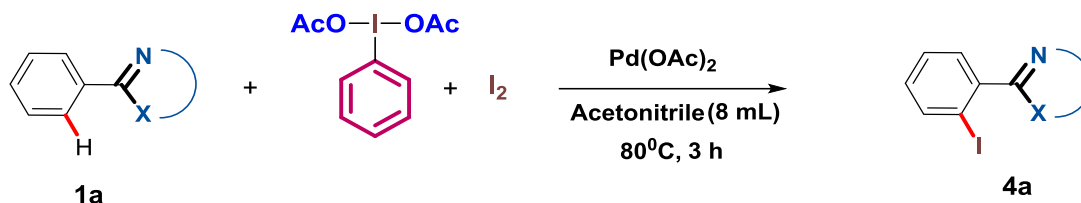
An oven dried 25 mL round bottom flask fitted CaCl_2 guard tube with was charged with 2-phenyl benzimidazole **1a** (1.164g, 6.0 mmol), $\text{Pd}(\text{OAc})_2$ (0.135 g, 0.6 mmol), PIDA (2.90 g, 9.0 mmol) and Cs_2CO_3 (3.91 g, 12 mmol) in dry acetonitrile (10 mL) under air atmosphere. The mixture was stirred at room temperature for 5 min for proper mixing of the reactants, and then heated in a preheated oil bath to 80°C for 6 h (monitored by TLC). The progress of the reaction was monitored by TLC. Upon completion, the reaction mixture was cooled to room temperature, diluted with ethyl acetate and filtered through a pad of Celite. The filtrate was then concentrated under reduced pressure and the crude residue was purified by silica gel column chromatography (100-200 mesh size) using eluent (EtOAc/petroleum ether,1:3) to afford the desired product **3a** (1.3 g, 80 %).

Synthesis of compound **3a** in the presence of radical inhibitor TEMPO

An oven dried 10 mL round bottom flask fitted CaCl_2 guard tube with was charged with 2-phenyl benzimidazole **1a** (94 mg, 0.5 mmol), $\text{Pd}(\text{OAc})_2$ (12 mg, 10 mol %), PIDA (241.6 mg, 1.5 mmol), Cs_2CO_3 (326 mg, 2.0 mmol), TEMPO (156 mg, 1.0 mmol) in dry acetonitrile (2.0 mL) under air. The mixture was stirred at room temperature for 5 min. for proper mixing of the reactants, and then heated in a preheated oil bath to 80°C for 6h. The progress of the reaction was monitored by TLC. Upon completion, the reaction mixture was cooled to room temperature, diluted with ethyl acetate and filtered through a small pad of Celite. The filtrate was concentrated under reduced

pressure and the crude residue was purified by silica gel column chromatography (100-200 mesh size) using eluent (EtOAc/petroleum ether, 1:3) to afford the desired product **3a** (107 mg, 79%).

Synthesis of compound **4a** from **1a** in gram scale:



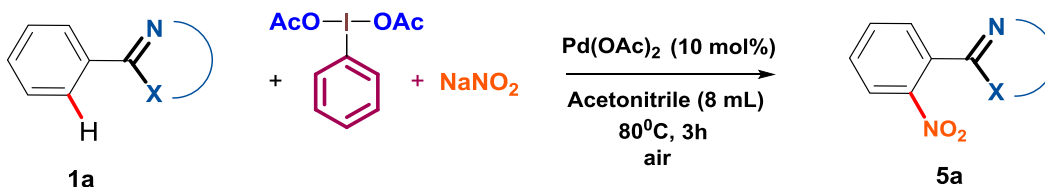
An oven-dried 25 mL round bottom flask fitted with CaCl₂ guard tube was charged with 2-phenyl benzimidazole **1a** (1.164 g, 6.0 mmol), Pd(OAc)₂ (0.135 g, 0.6 mmol), PIDA (2.90 g, 9.0 mmol) and I₂ (2.28 g, 9.0 mmol) in 8 mL dry acetonitrile. The reaction mixture was refluxed in a pre-heated oil bath to 80°C for 3h (the progress of reaction monitored by TLC). After being cooled the reaction mixture at room temperature, the excess iodine was quenched using 30% Na₂S₂O₃ solution (30 mL), washed with brine and extracted with ethyl acetate (3 x 40 ml). The combined organic part was dried over anhydrous sodium sulphate, concentrated under reduced pressure and finally purified using silica gel column chromatography (100-200 mesh size) (hexane/ethyl acetate, 3:1) to afford 2-(2-iodophenyl)-1H-benzo[d]imidazole (**4a**) (1.67 g, yield 87%). The identity and purity of the product was confirmed by spectroscopic analysis.

Synthesis of compound **4a** in the presence of radical inhibitor TEMPO

To an oven-dried 10 mL round bottom flask fitted with CaCl₂ guard tube were added 2-phenyl benzimidazole (**1a**) (97 mg, 0.5 mmol), Pd(OAc)₂ (12 mg, 0.05 mmol), PIDA (241.5 mg, 1.5 mmol), I₂ (189.75 gm, 1.5 mmol) and TEMPO (156 mg, 1.0 mmol) in 2 mL dry acetonitrile. The reaction mixture was refluxed in a pre-heated oil bath to 80°C for 3h. After completion of reaction, the reaction mixture was cooled to room temperature and excess iodine was quenched using 30% sodium thiosulfate solution (5 mL). After this the mixture was extracted with ethyl acetate (3 x 10

mL), washed with brine and the combined organic layer was dried over anhydrous sodium sulphate, concentrated under reduced pressure and purified using column chromatography (100-200 mesh size) (hexane/ethyl acetate, 3:1) and 2-(2-iodophenyl)-1*H*-benzo[*d*]imidazole (**4a**) was isolated with 88% (0.141 g).

Synthesis of compound **5a** from **1a** in gram scale.



An oven dried 25 ml round bottom flask equipped with a CaCl₂ guard tube was charged with **1a** (1.164 g, 6.0 mmol), Pd(OAc)₂ (0.135 g, 0.6 mmol), PIDA (2.90 g, 9.0 mmol) and sodium nitrite (0.621 g, 9.0 mmol) in 8 mL dry acetonitrile and refluxed in a pre-heated oil bath under air for 3h. After being stirred for appropriate time, the reaction mixture was cooled to room temperature, the solvent was distilled under vacuum. The resulting mixture was directly charged on silica gel column chromatography (100-200 mesh size) (petroleum ether/ethyl acetate=2:1) to isolate pure 2-(2-nitrophenyl)-1*H*-benzo[*d*]imidazole (**5a**) (1.32g, 92%) as a yellow solid. The identity and purity of the product was confirmed by spectroscopic analysis.

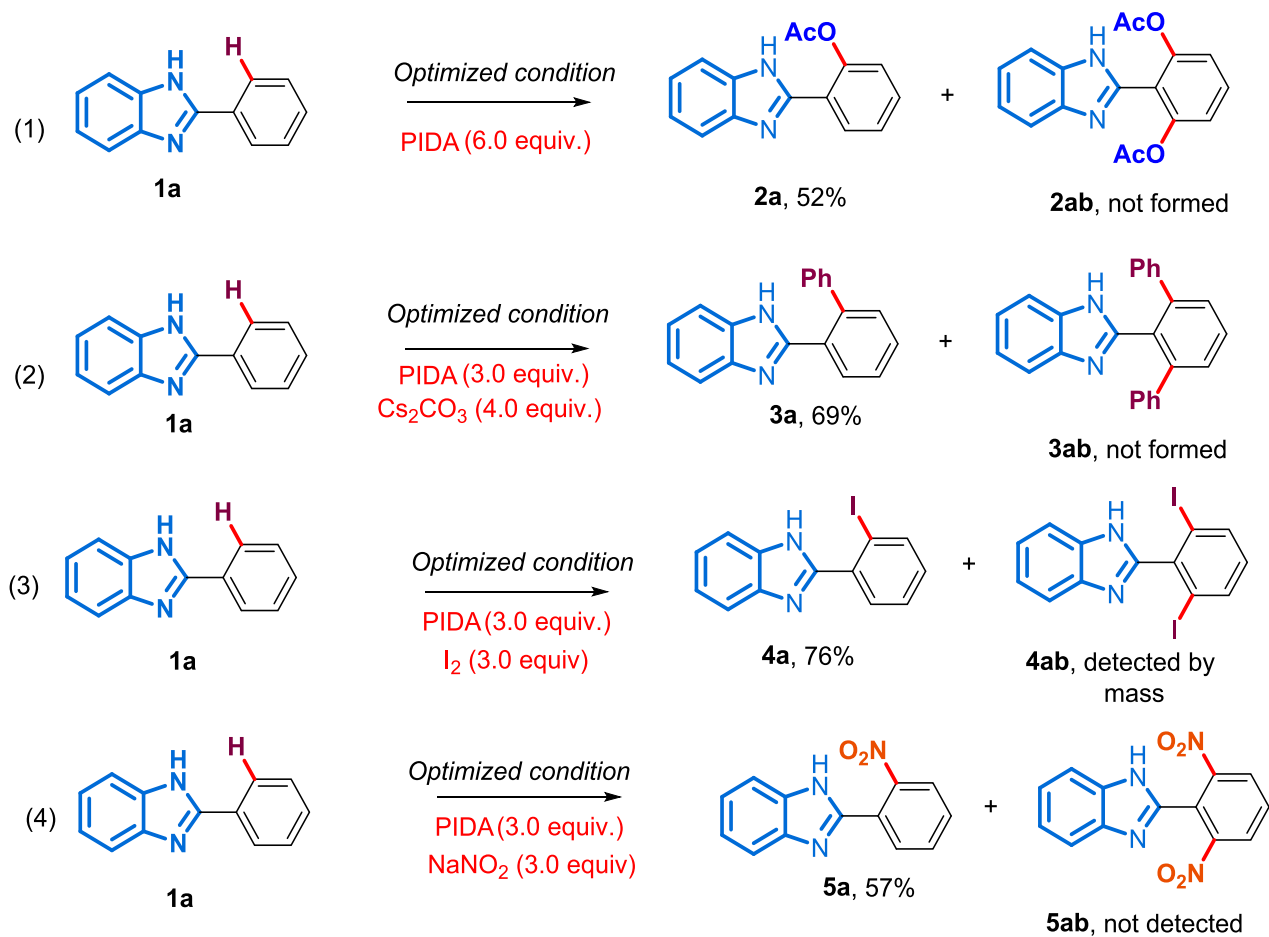
Synthesis of compound **5a** in the Presence of radical inhibitor TEMPO

To an oven-dried 10 mL round bottom flask fitted with CaCl₂ guard tube were added 2-phenyl benzimidazole (**1a**) (97 mg, 0.5 mmol), Pd(OAc)₂ (12 mg, 0.05 mmol), PIDA (241.5 mg, 1.5 mmol), NaNO₂ (51.7 mg, 1.5 mmol) and TEMPO (156 mg, 1.0 mmol) in 2 mL dry acetonitrile. The reaction mixture was refluxed in a pre-heated oil bath to 80°C for 3h. After completion of the reaction, excess solvent was evaporated under reduced pressure and the resulting mixture then

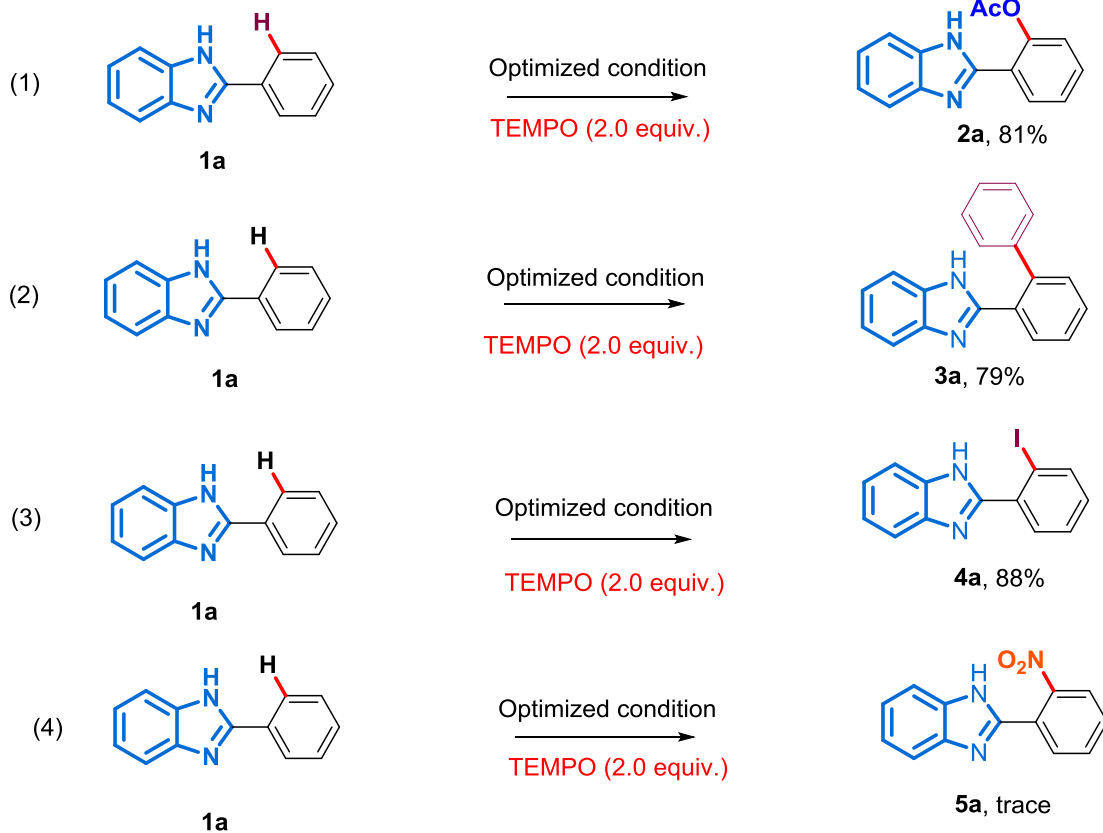
directly loaded on silica gel column chromatography (100-200 mesh size) (hexane/ethyl acetate, 3:1) and 2-(2-nitrophenyl)-1*H*-benzo[*d*]imidazole (**5a**) was isolated with 6% (7 mg).

Scheme 4: Control experiments

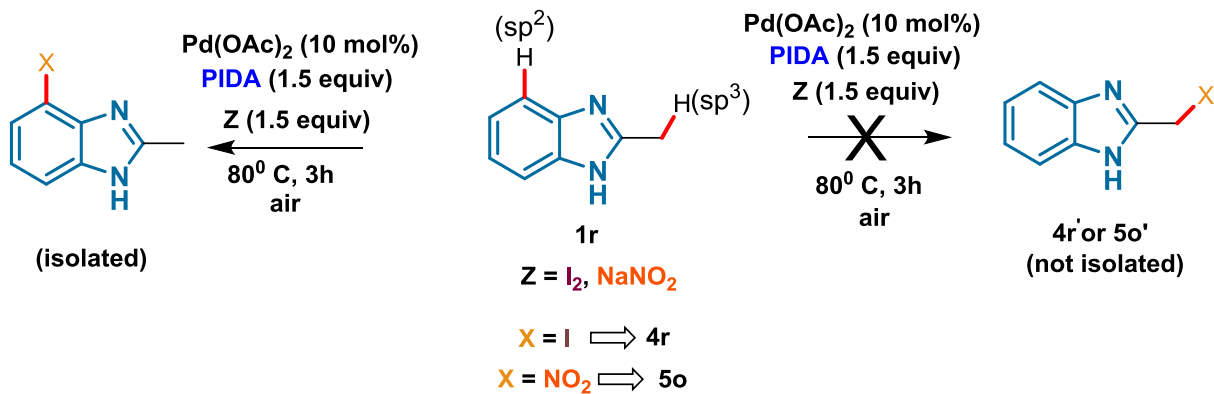
(a) Studies on selectivity of mono or di-functionalisation



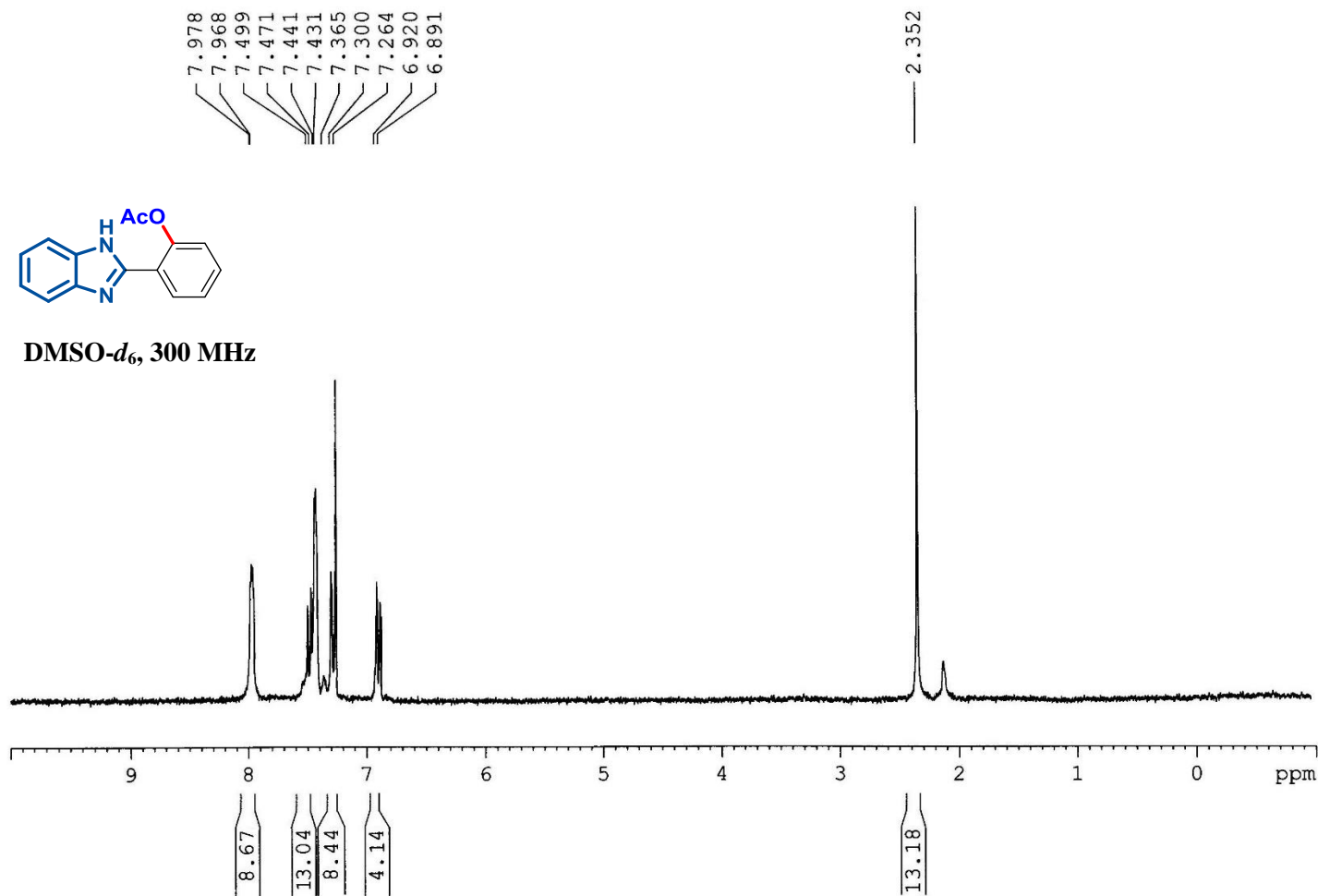
(b) Radical inhibition studies



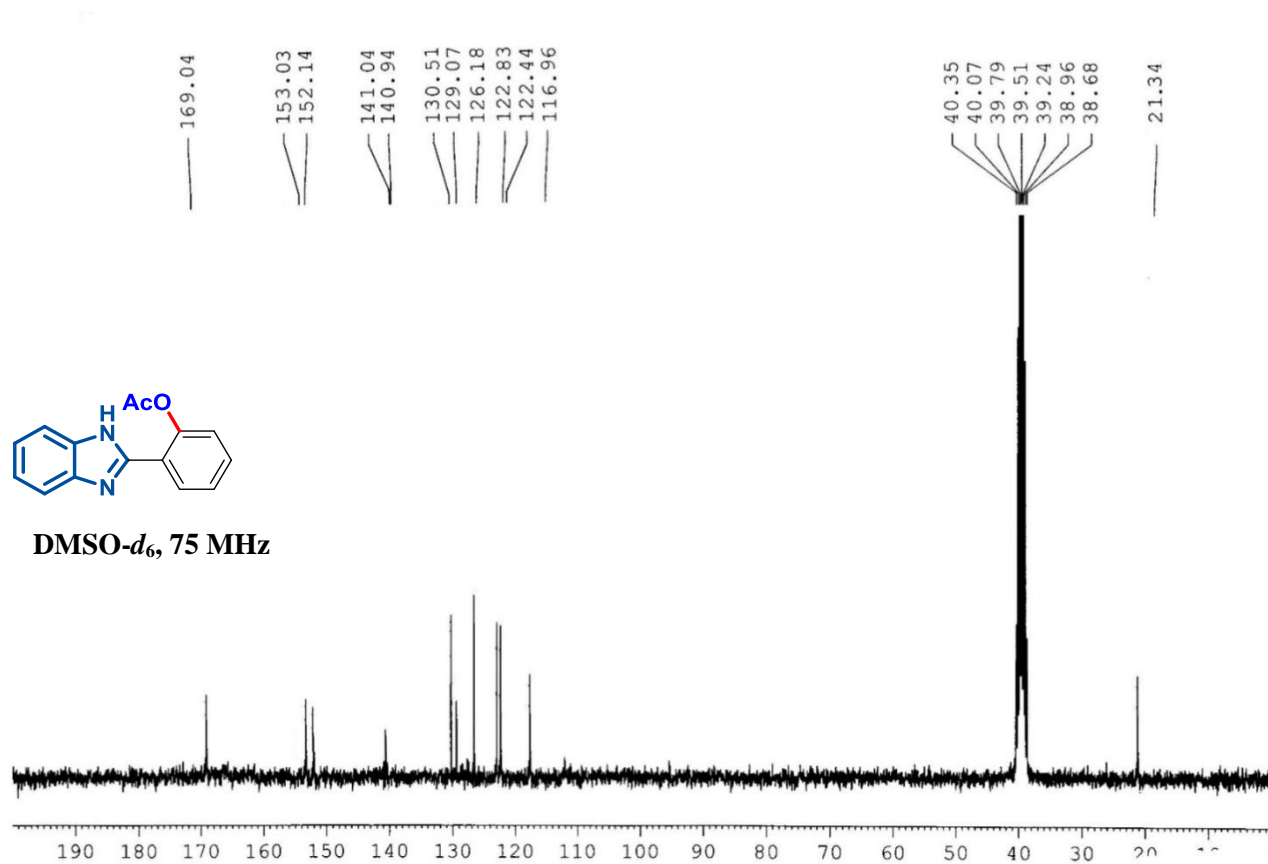
Scheme 5: Pd-catalyzed C-H activation of 2-methylbenzimidazole



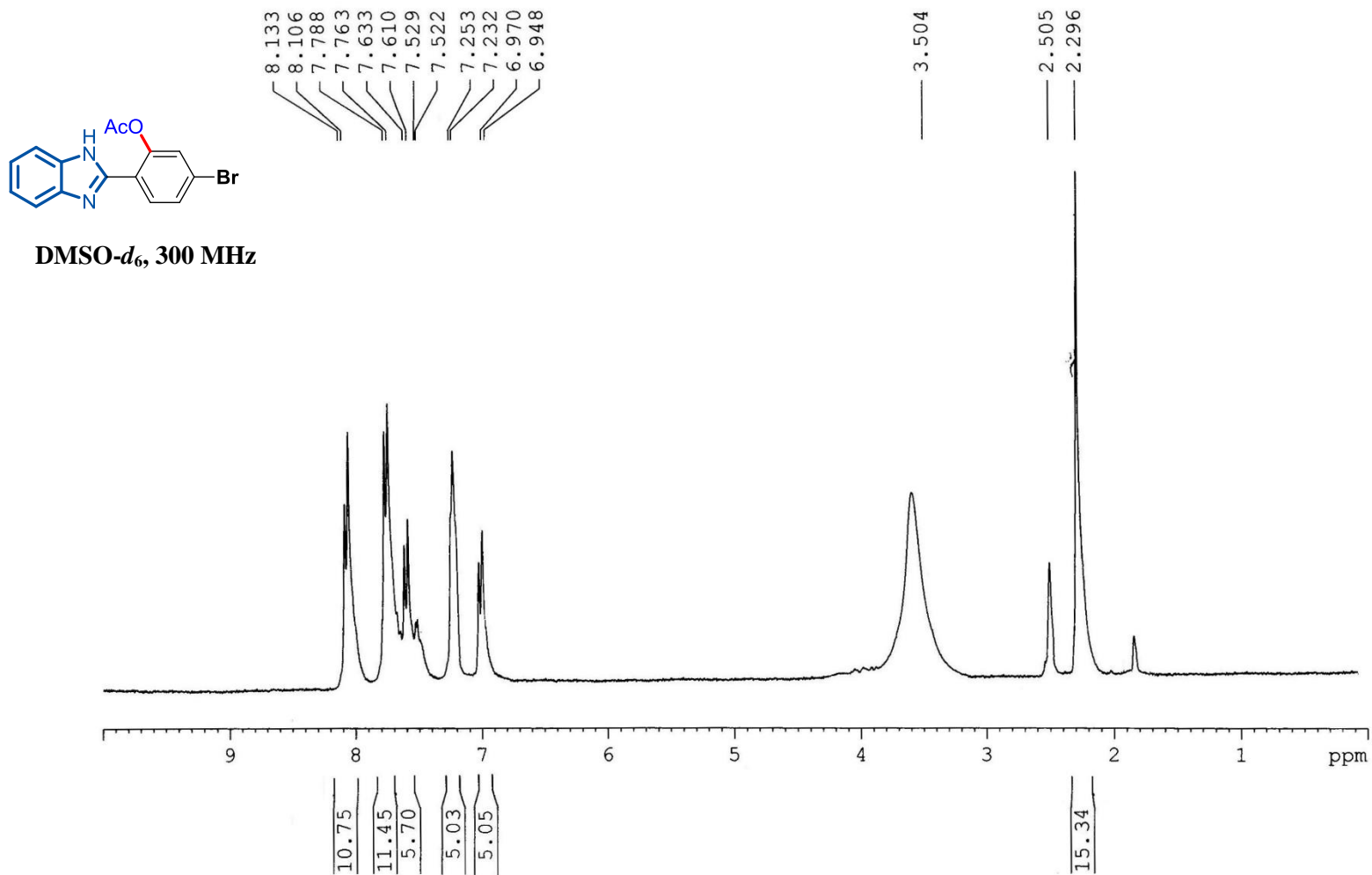
^1H NMR of Compound 2a



^{13}C NMR of Compound 2a



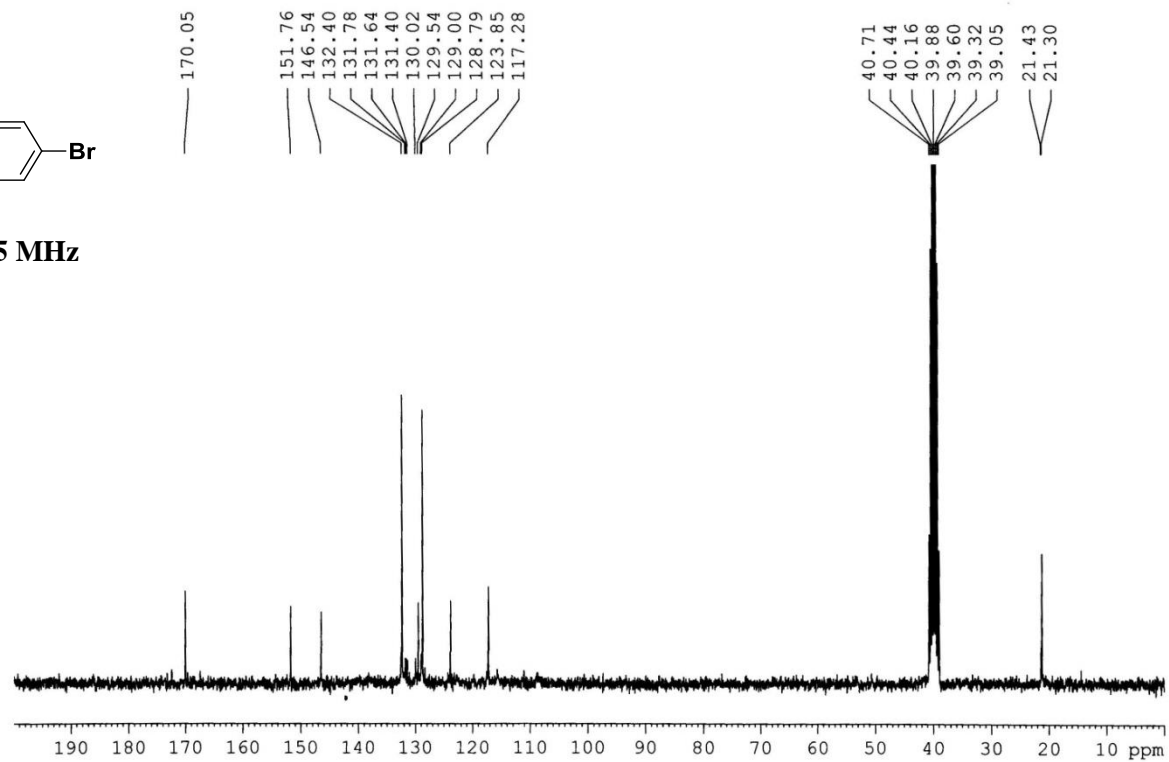
¹H NMR of Compound 2b



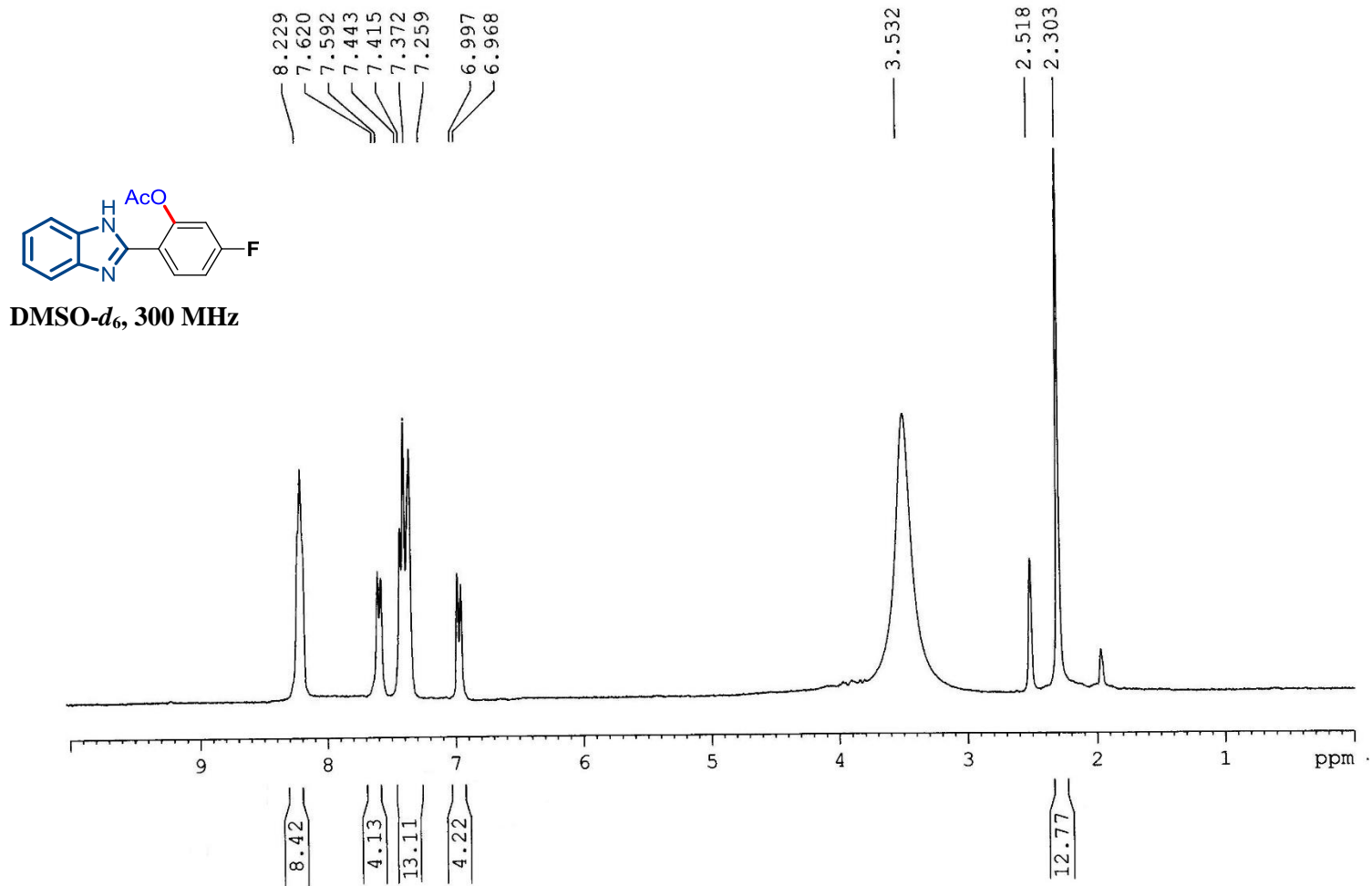
^{13}C NMR of Compound 2b



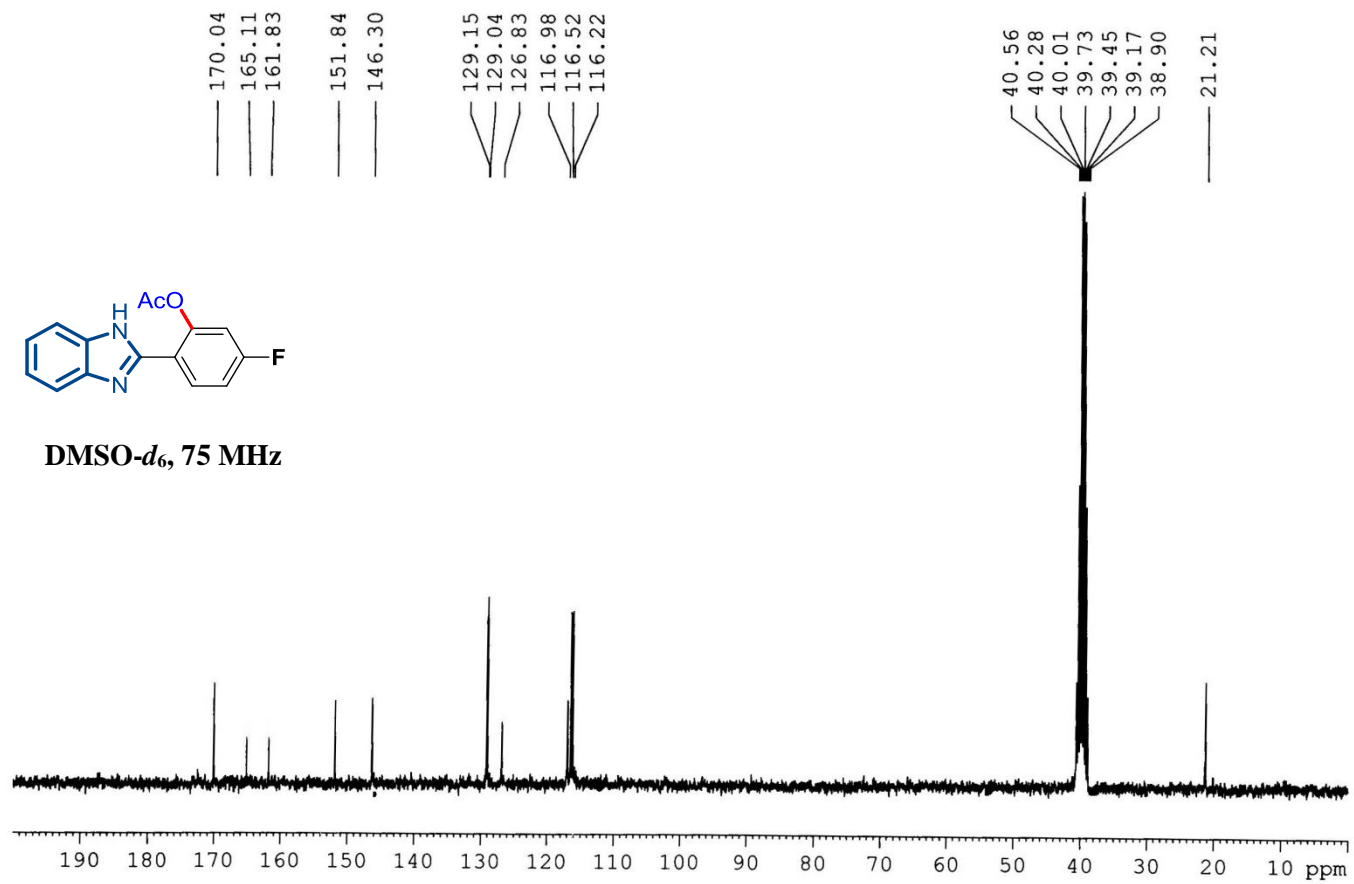
DMSO- d_6 , 75 MHz



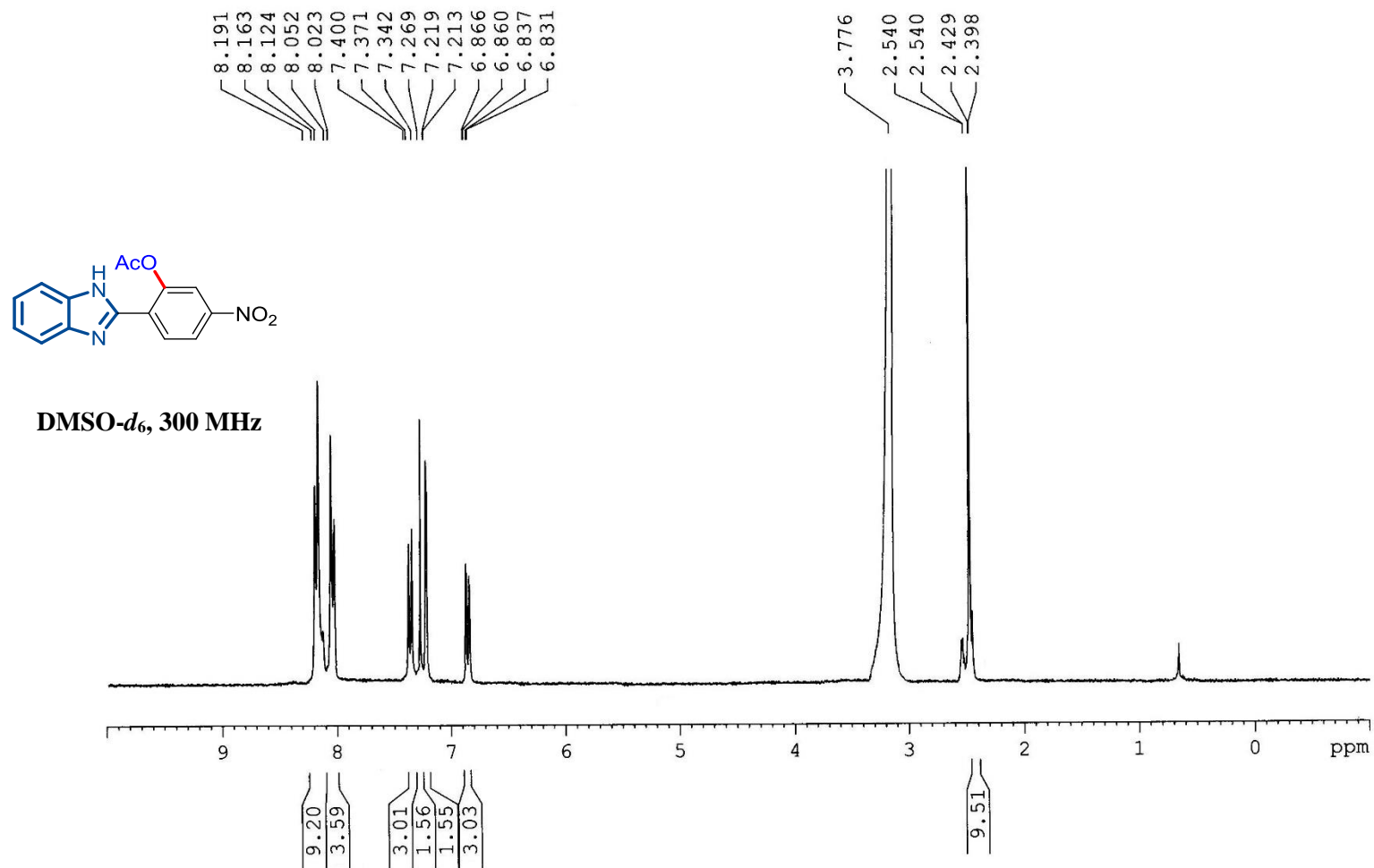
¹H NMR of Compound 2c



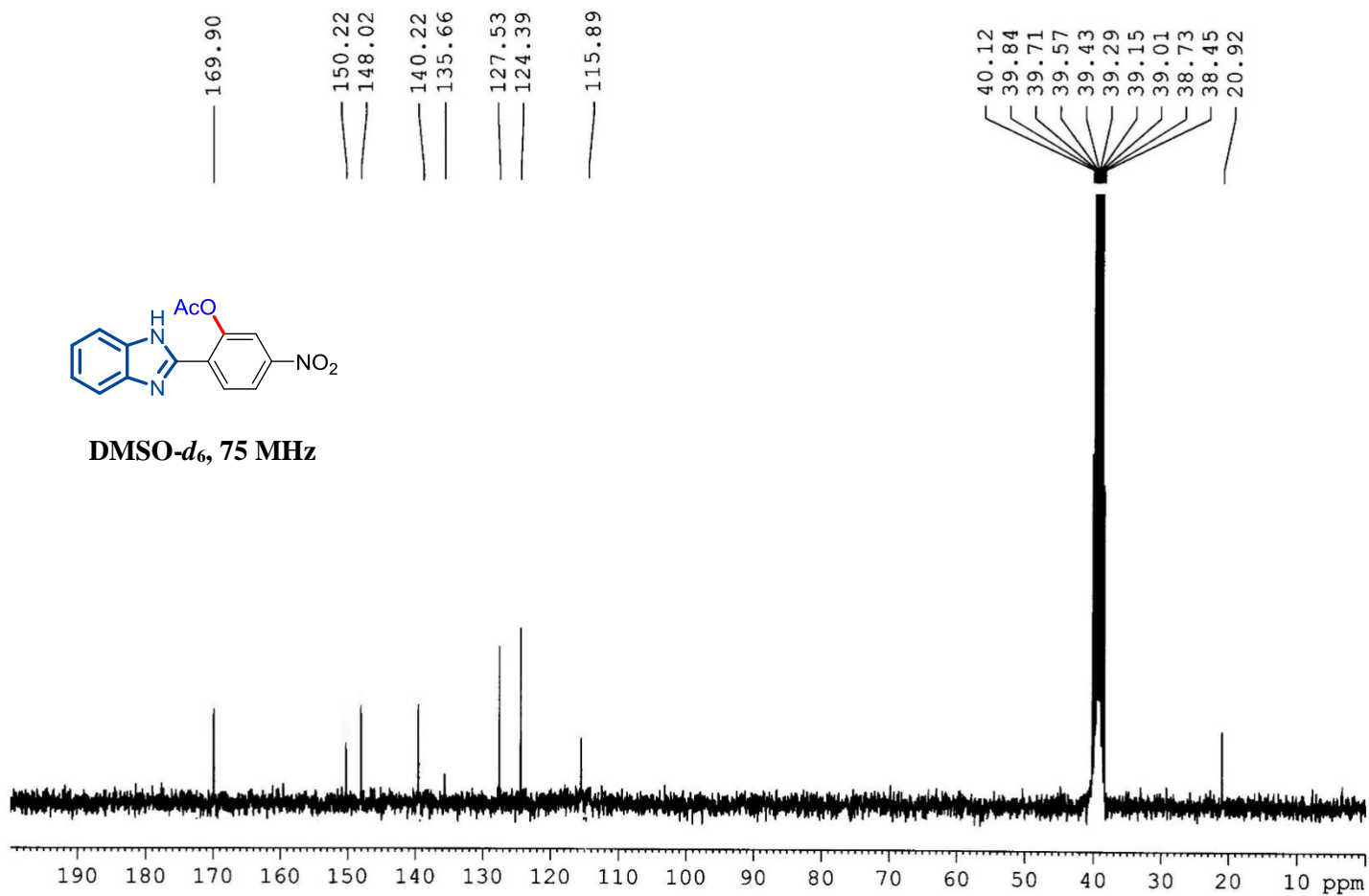
^{13}C NMR of Compound 2c



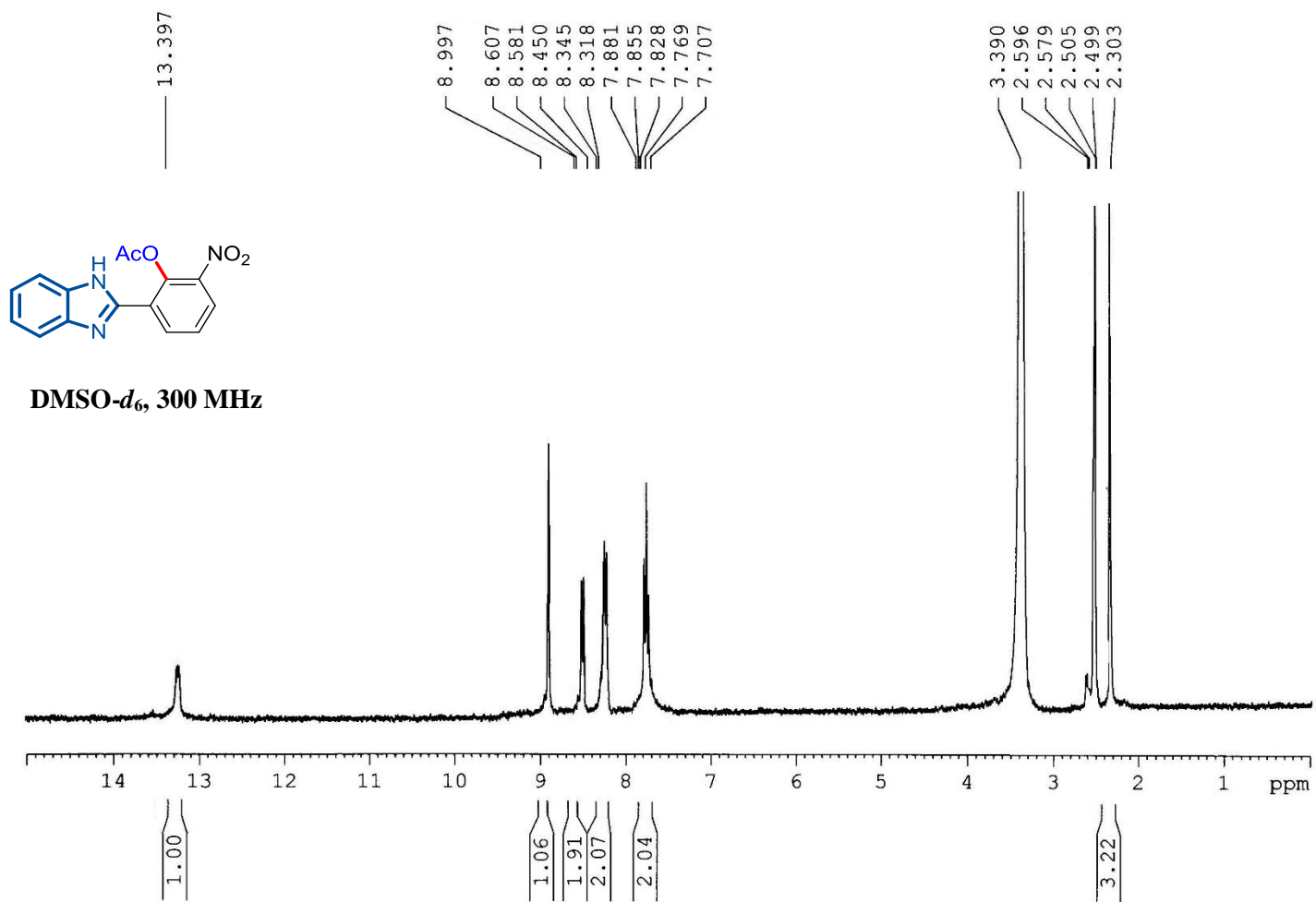
¹H NMR of Compound 2d



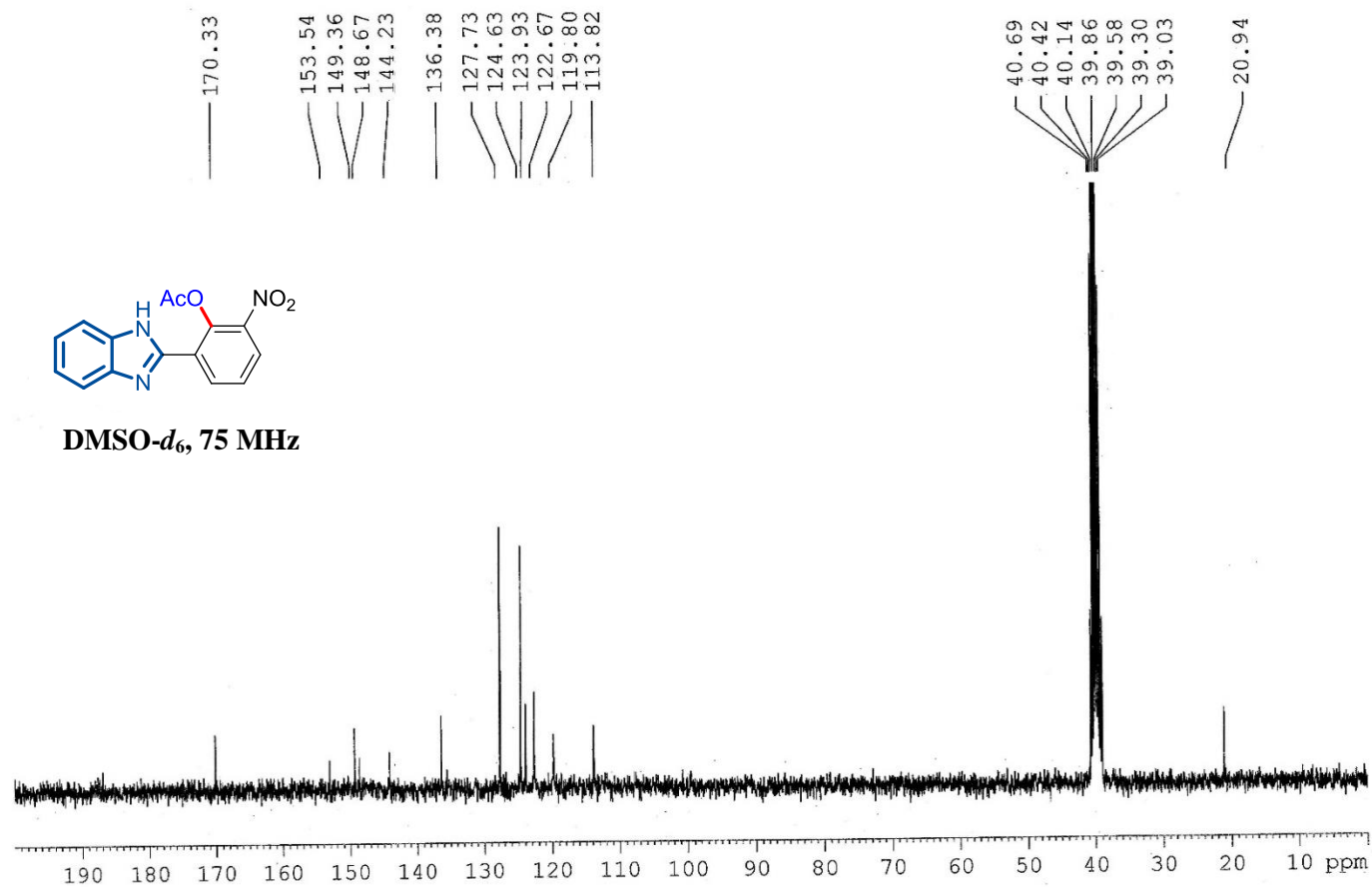
^{13}C NMR of Compound 2d



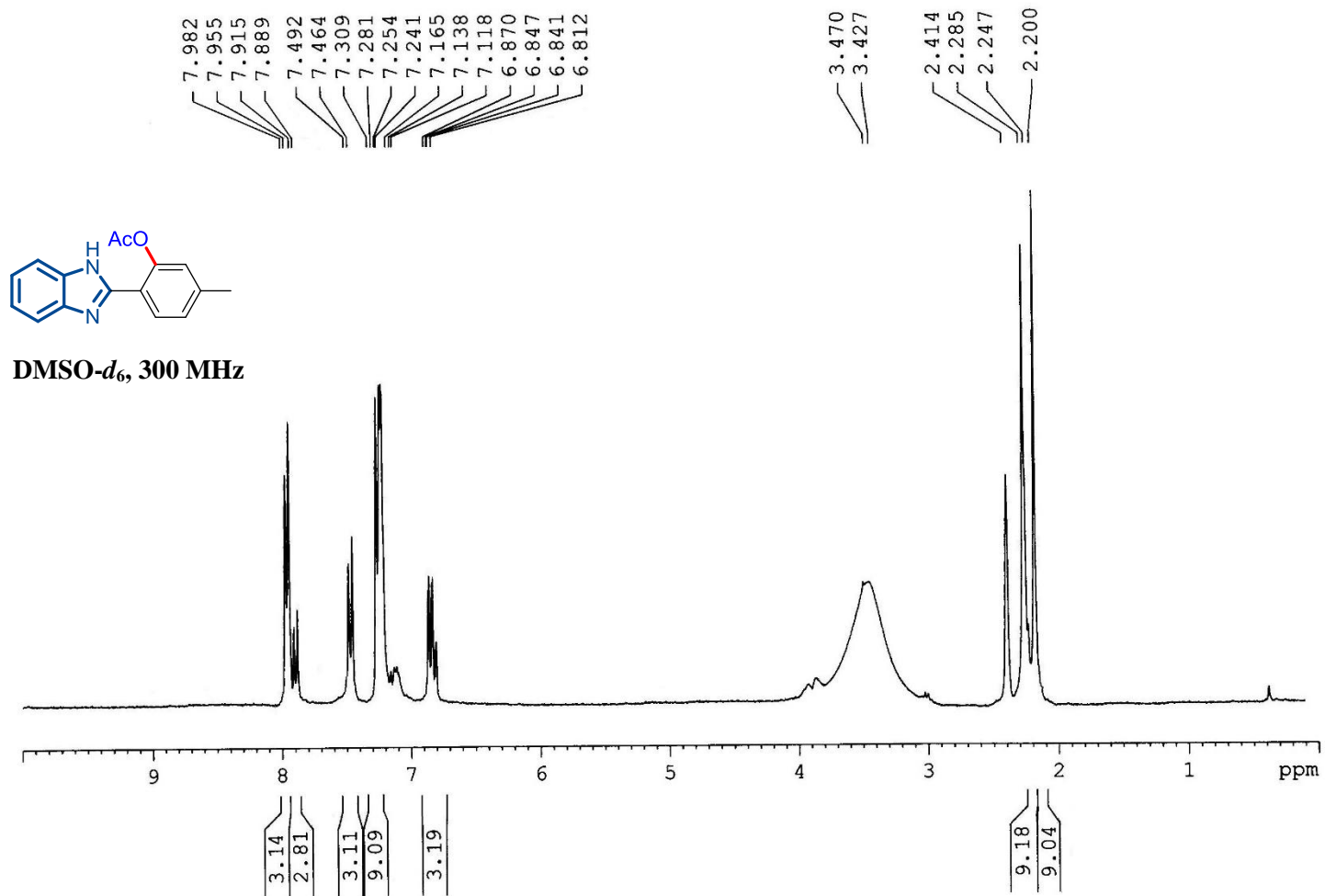
¹H NMR of Compound 2e



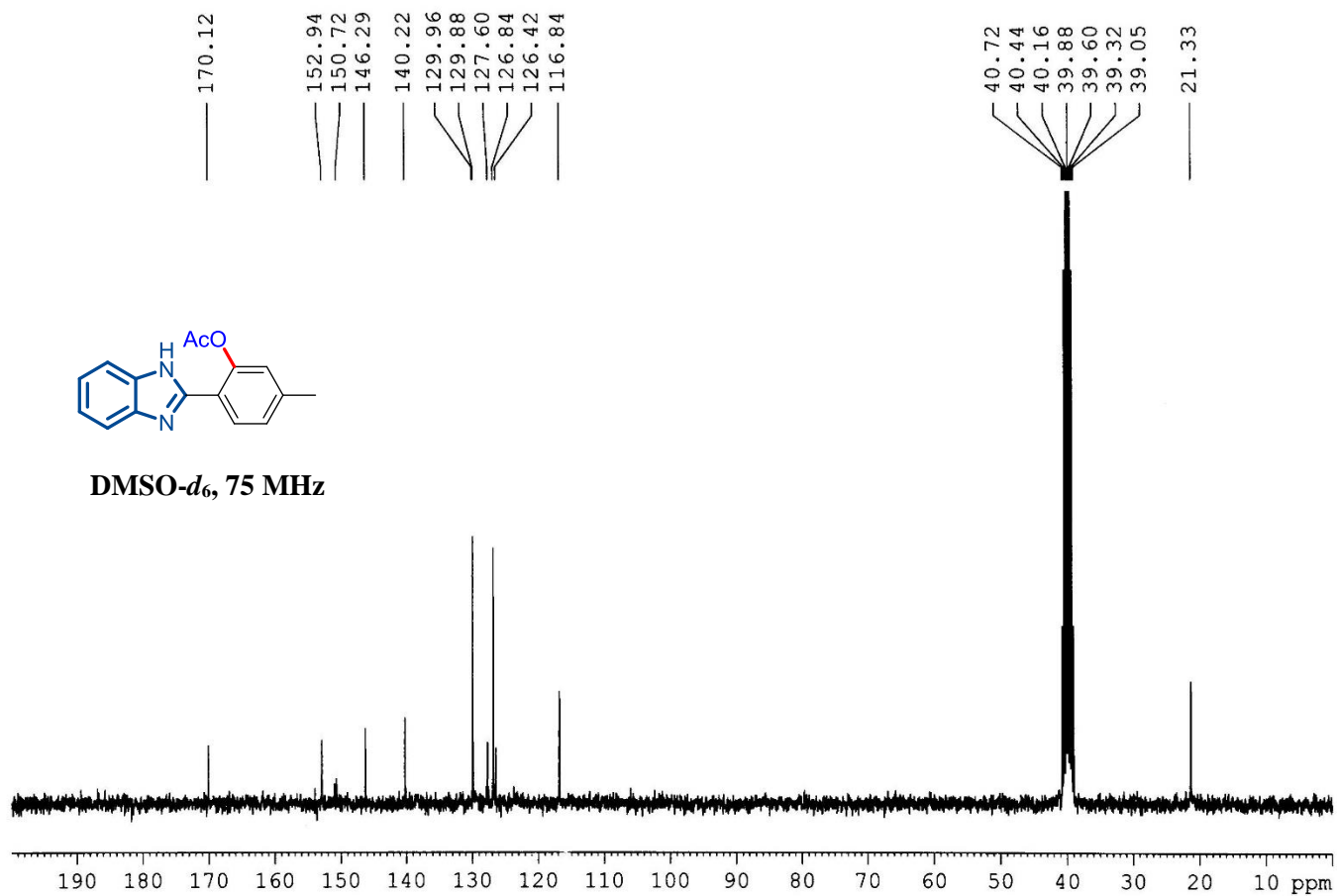
¹³C NMR of Compound 2e



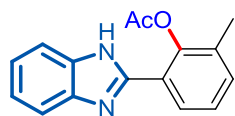
¹H NMR of Compound 2f



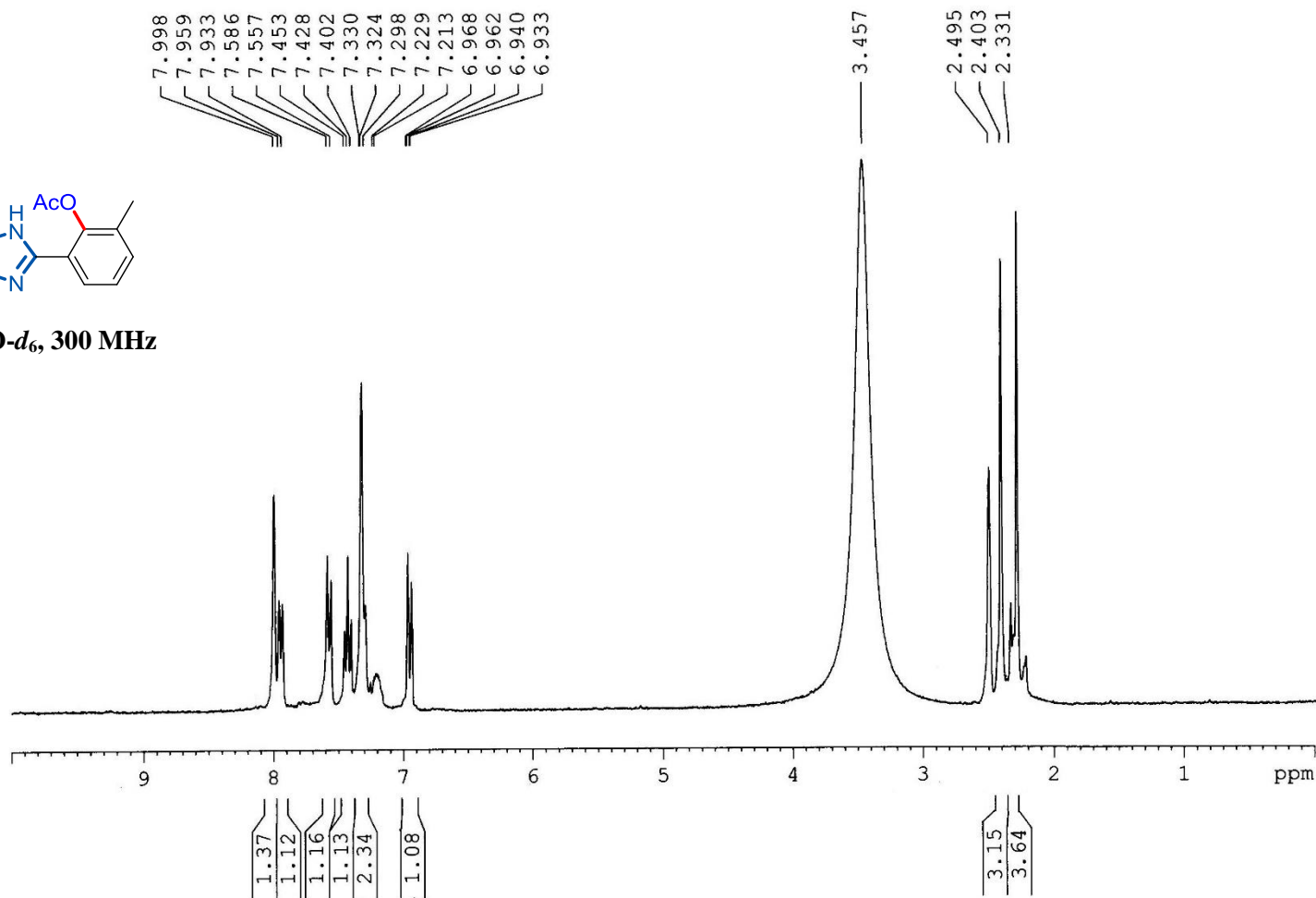
¹³C NMR of Compound 2f



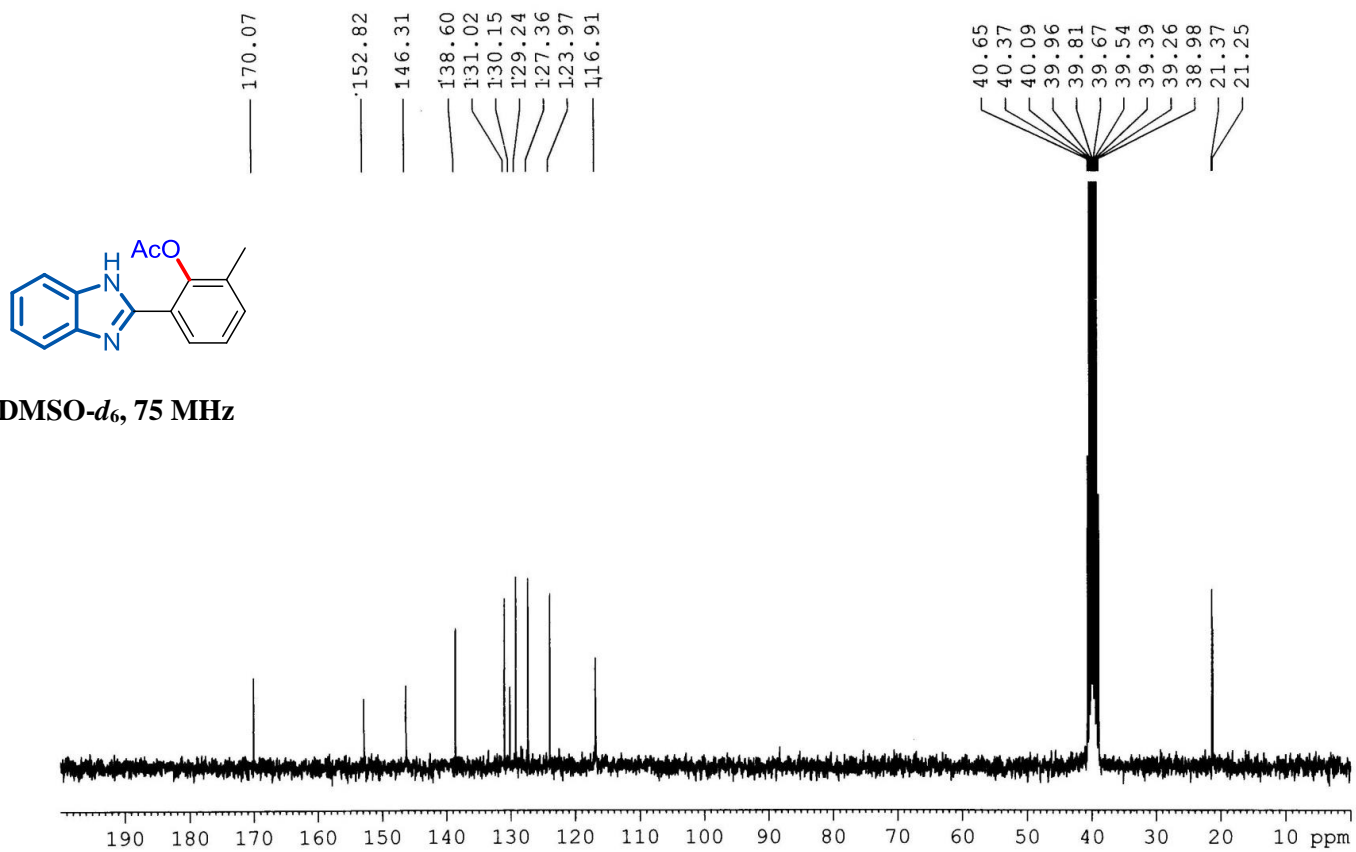
¹H NMR of Compound 2g



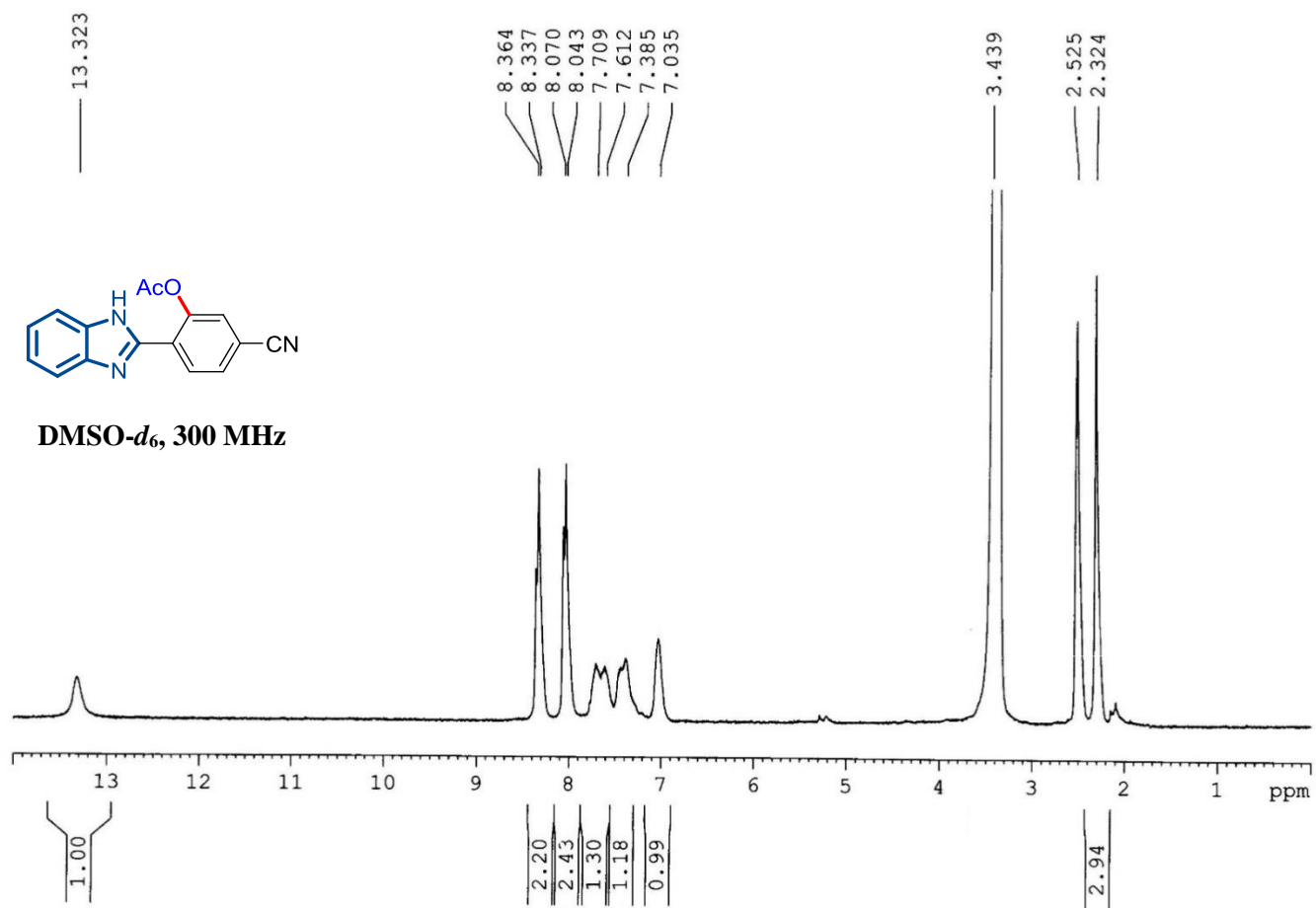
DMSO-*d*₆, 300 MHz



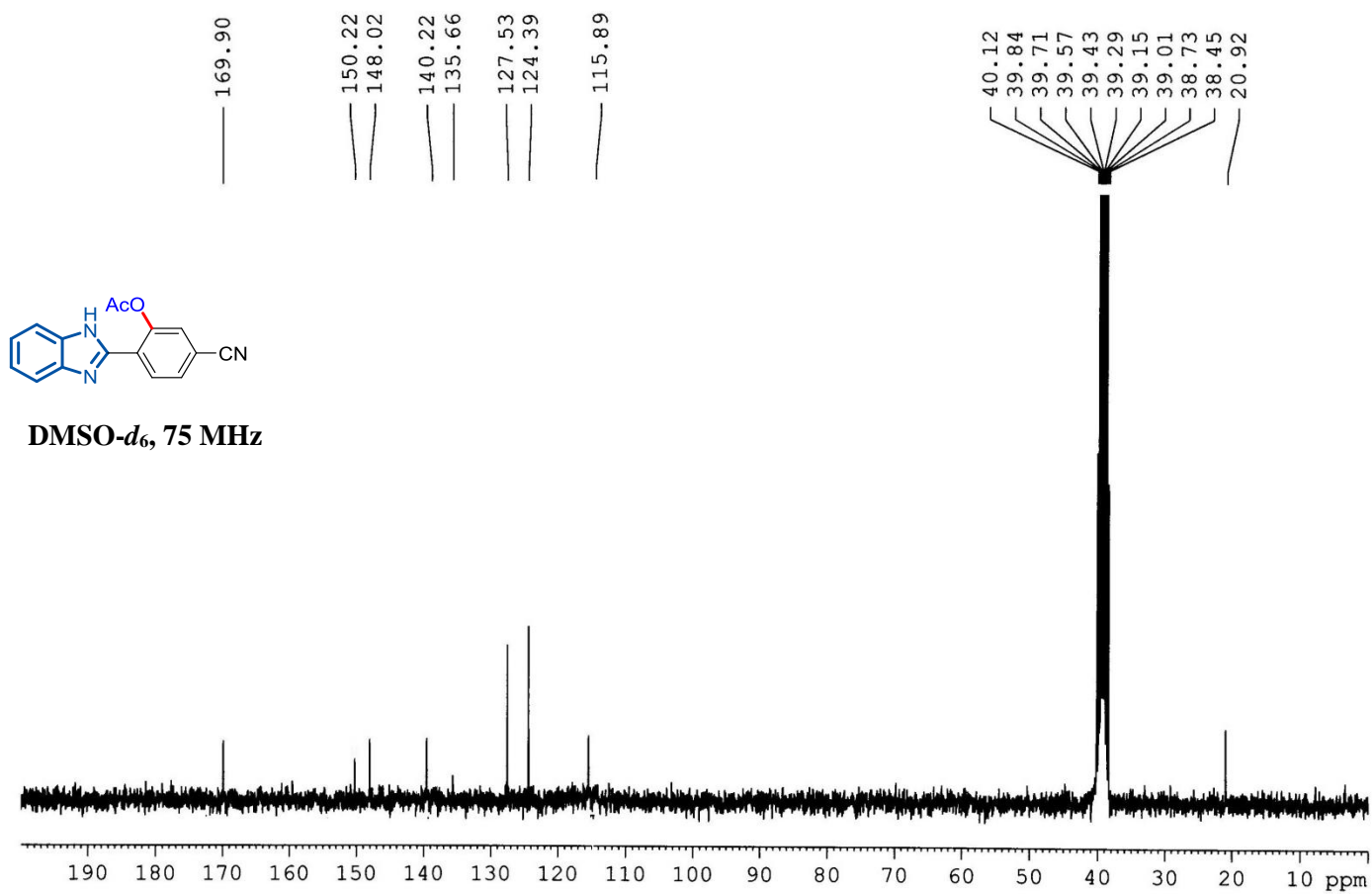
¹³C NMR of Compound 2g



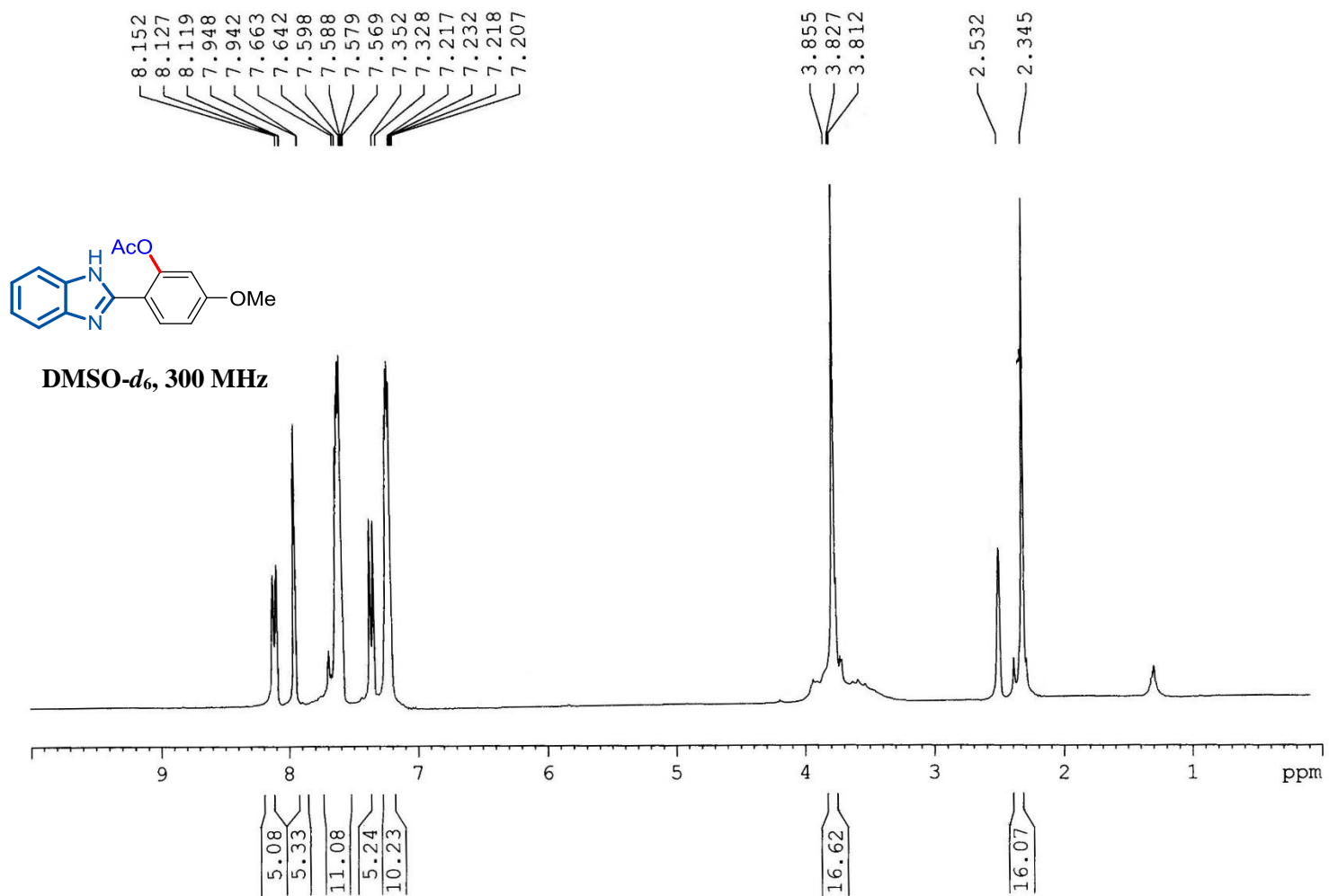
¹H NMR of Compound 2h



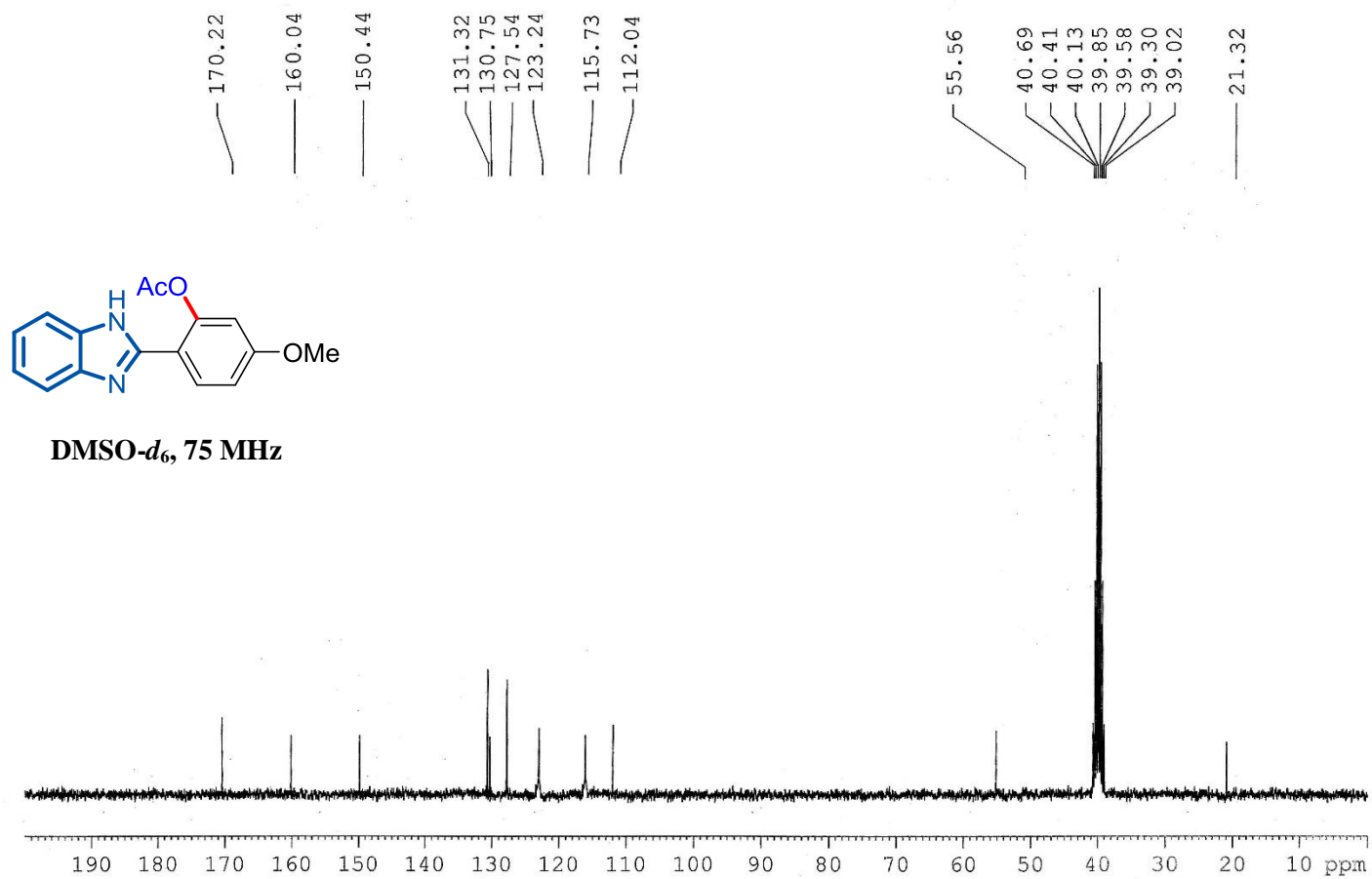
¹³C NMR of Compound 2h



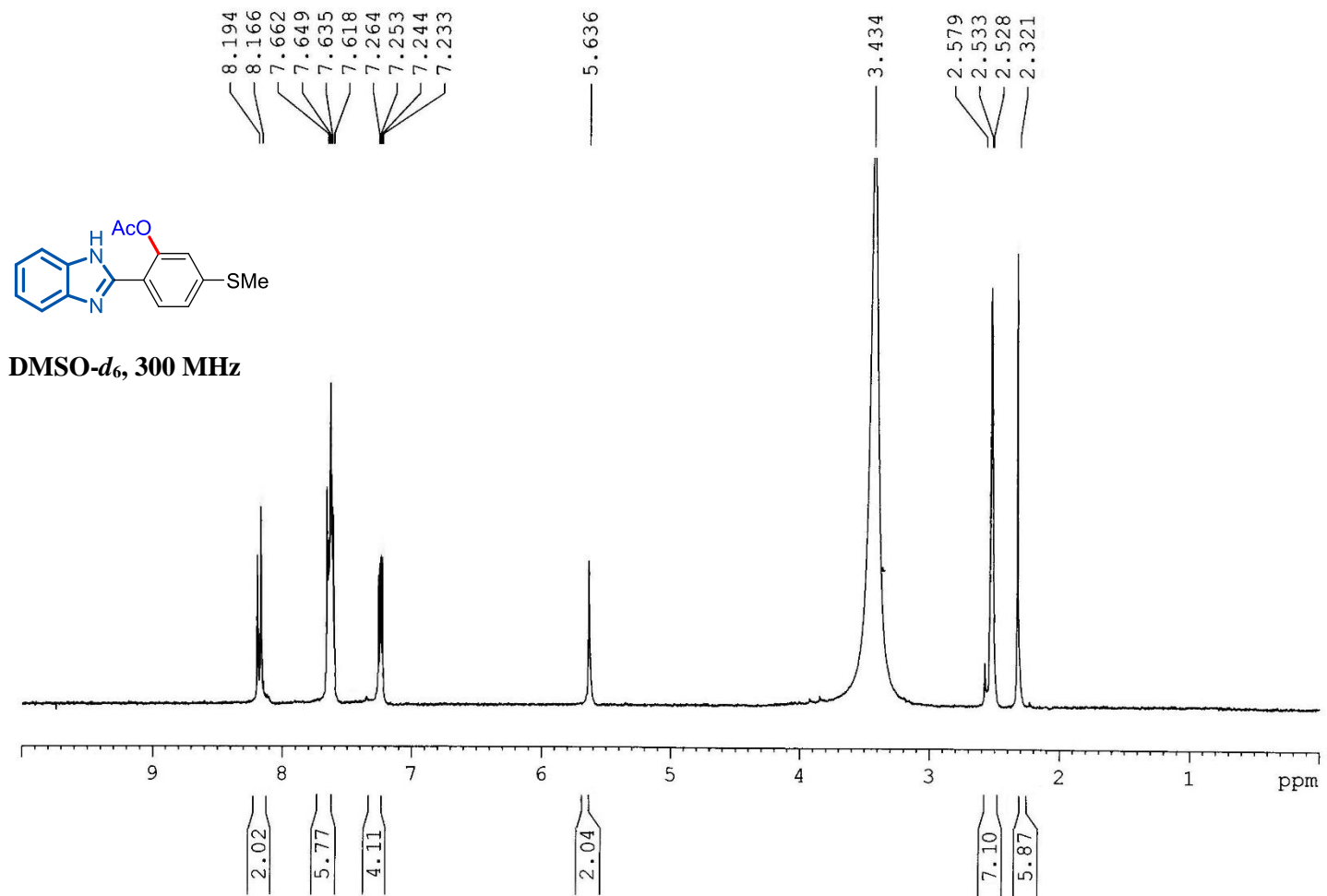
¹H NMR of Compound 2i



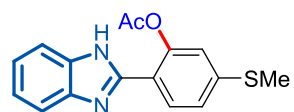
¹³C NMR of Compound 2i



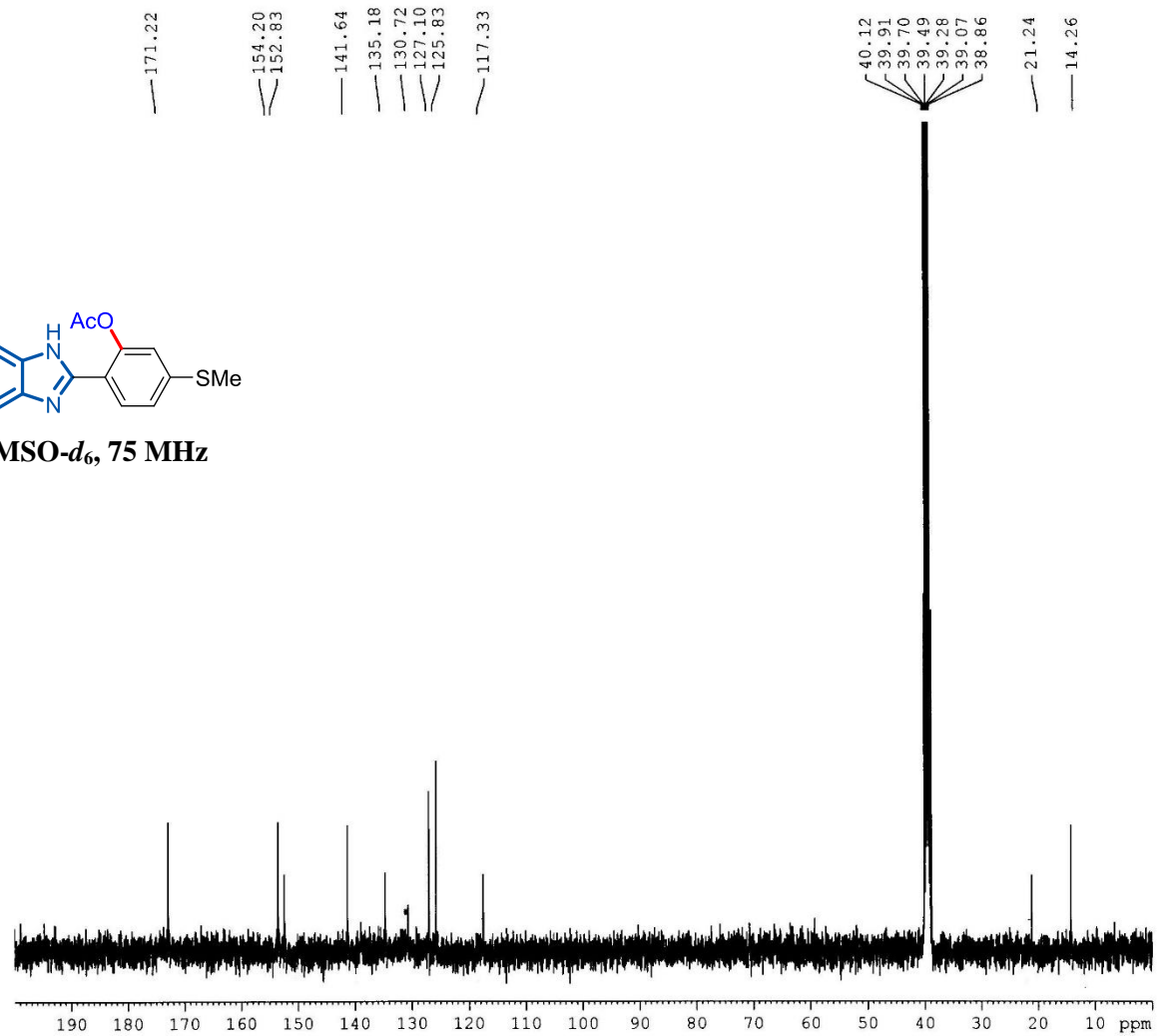
¹H NMR of Compound 2j



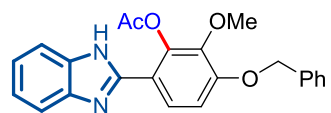
¹³C NMR of Compound 2j



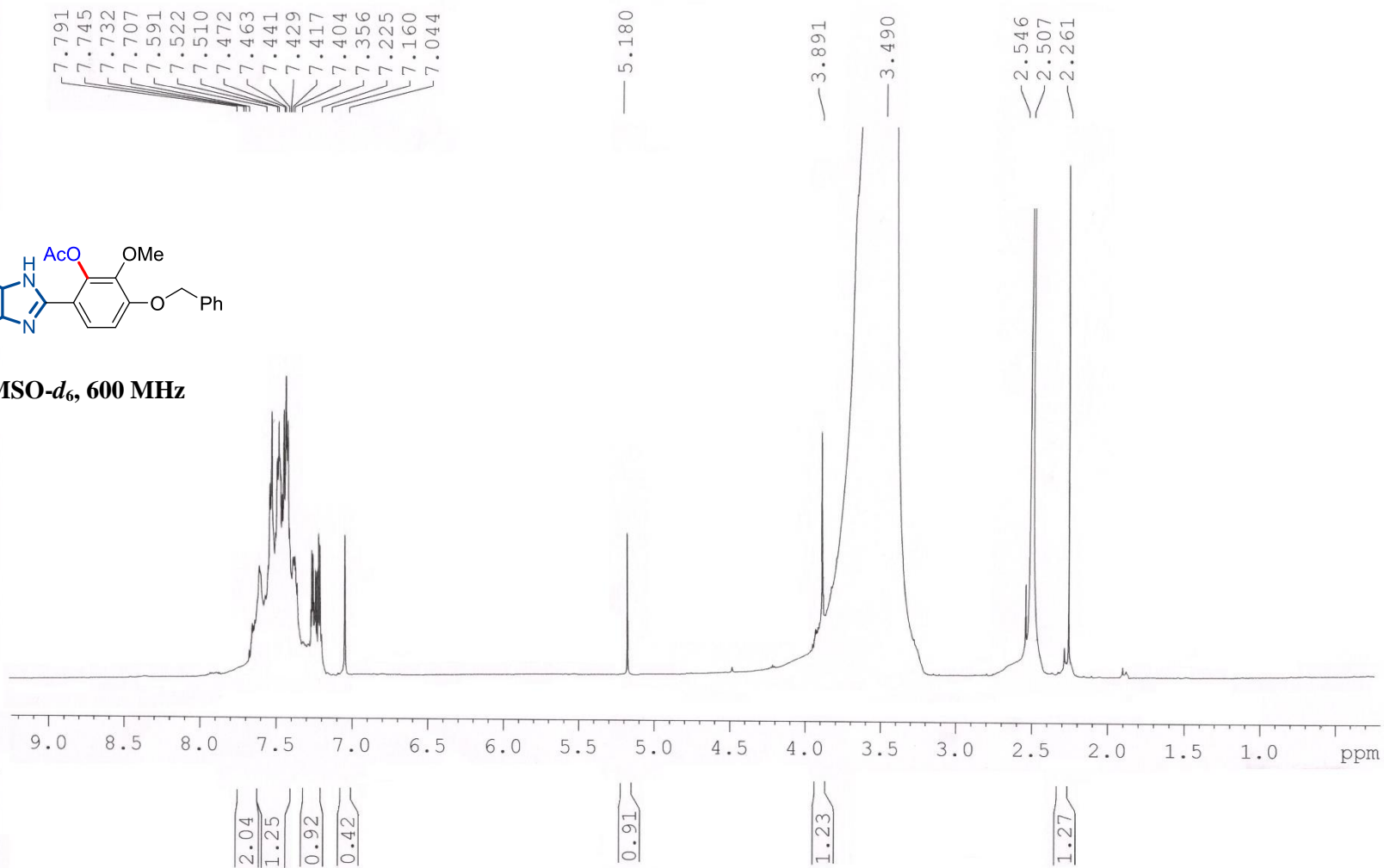
DMSO-*d*₆, 75 MHz



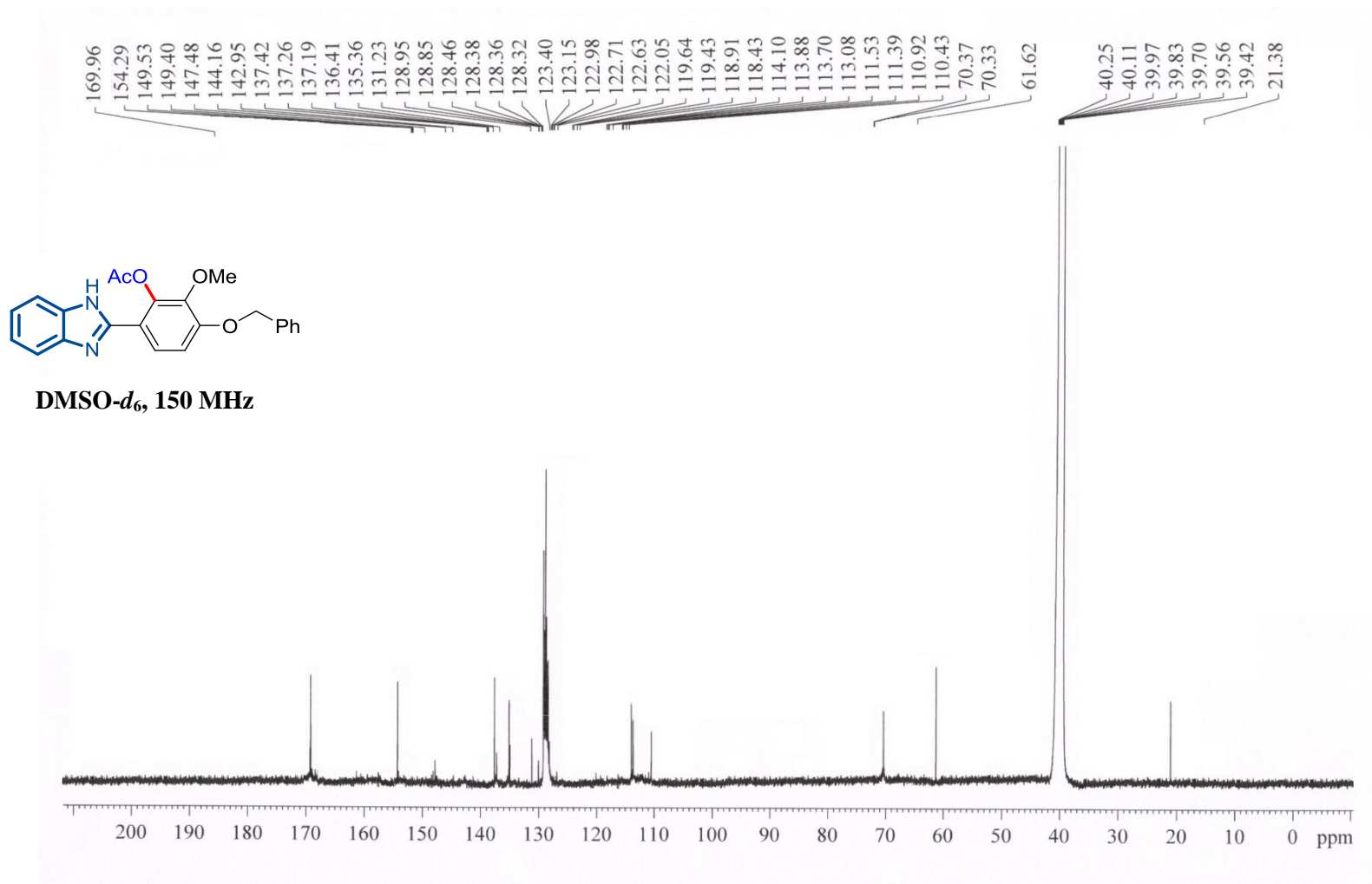
¹H NMR of Compound 2k



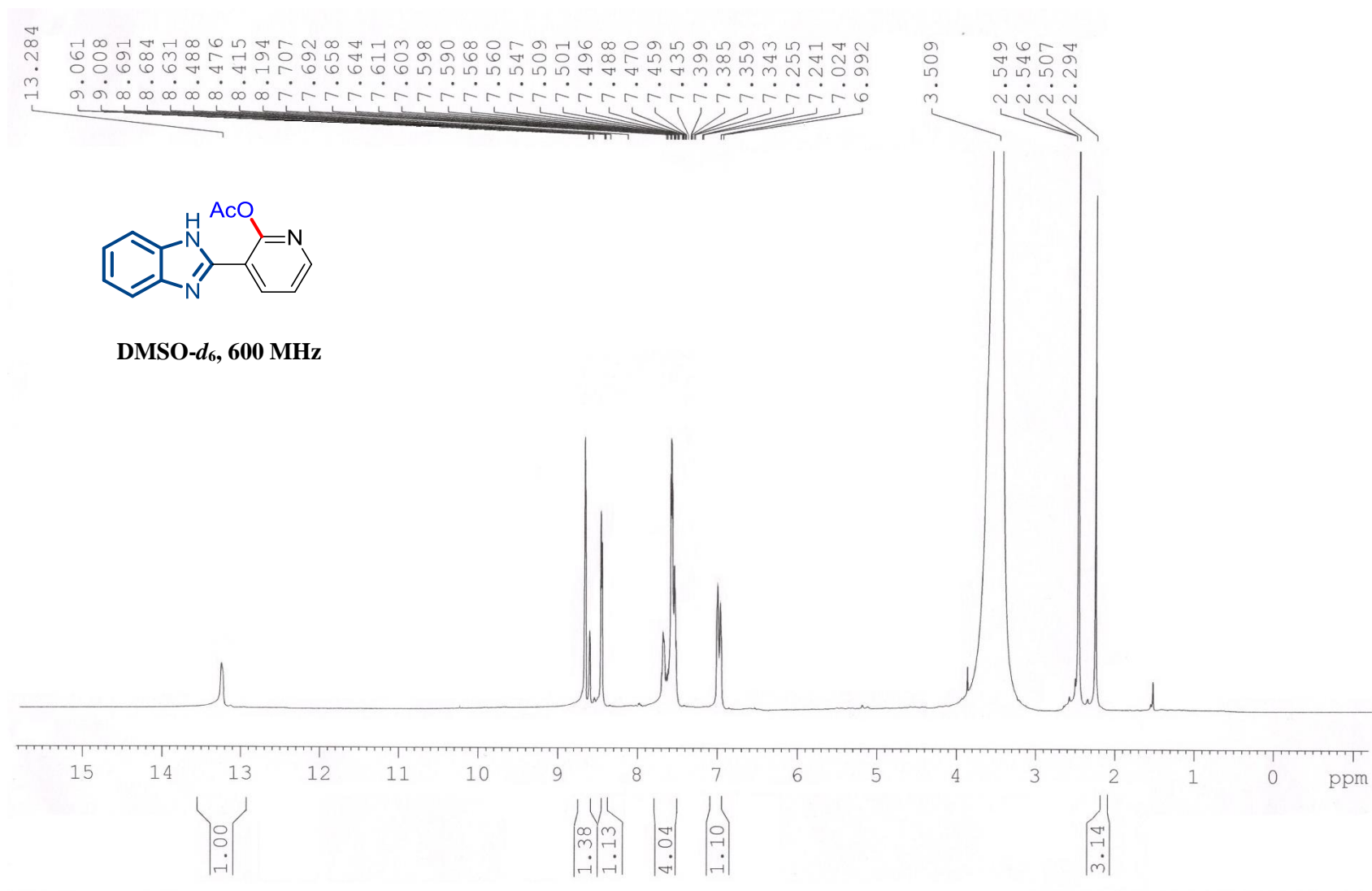
DMSO-*d*₆, 600 MHz



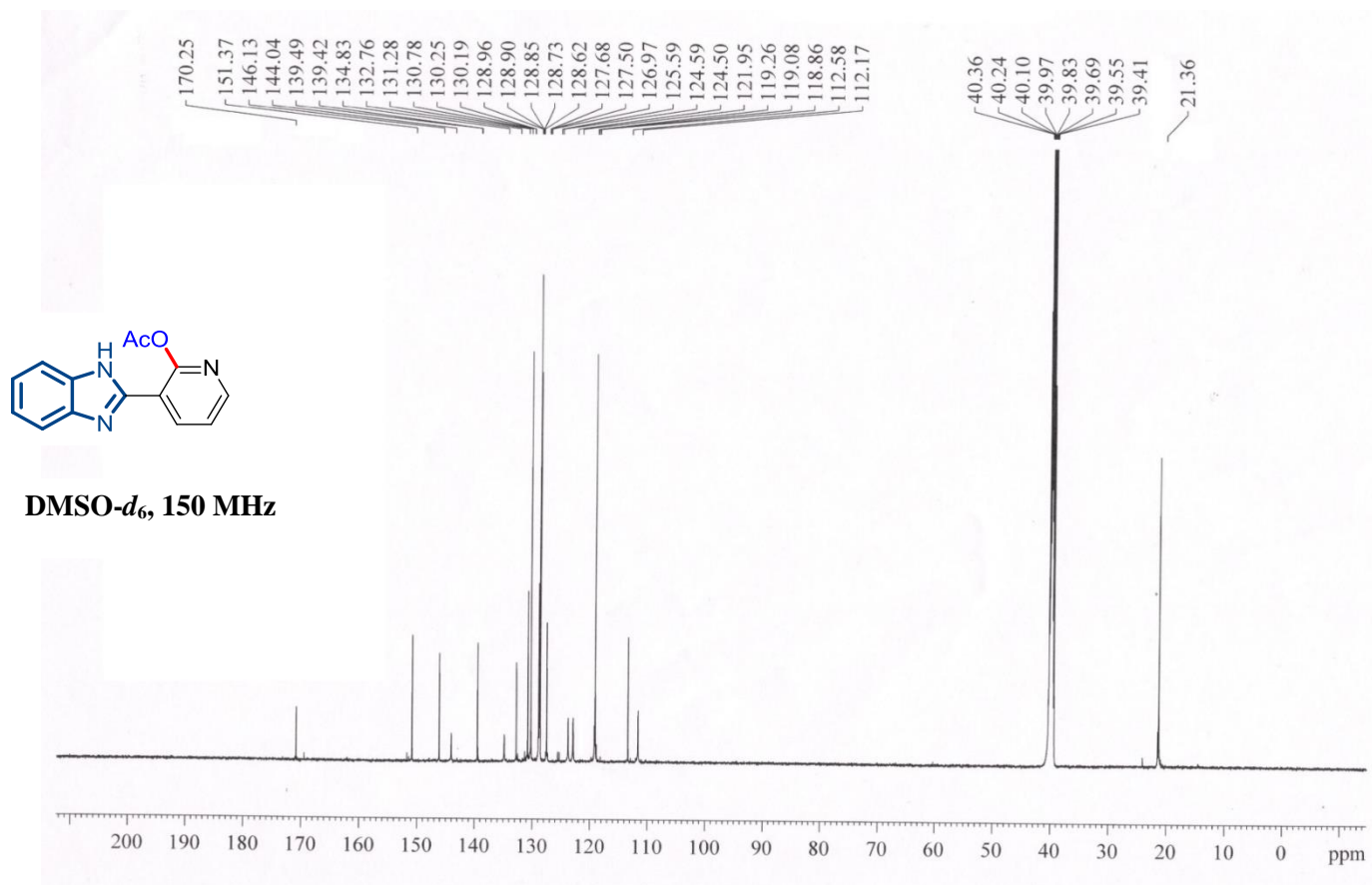
¹³C NMR of Compound 2k



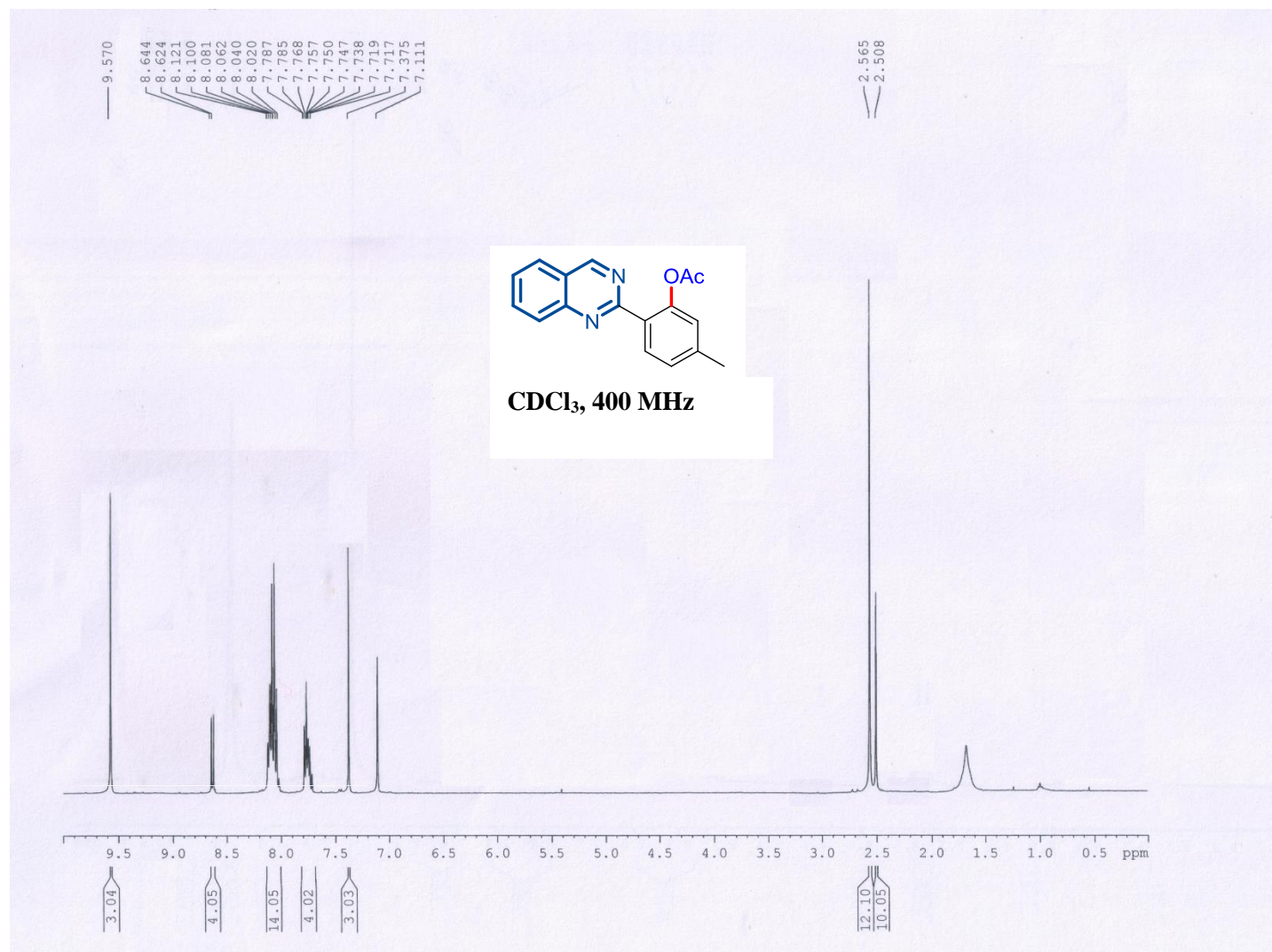
¹H NMR of Compound 2l



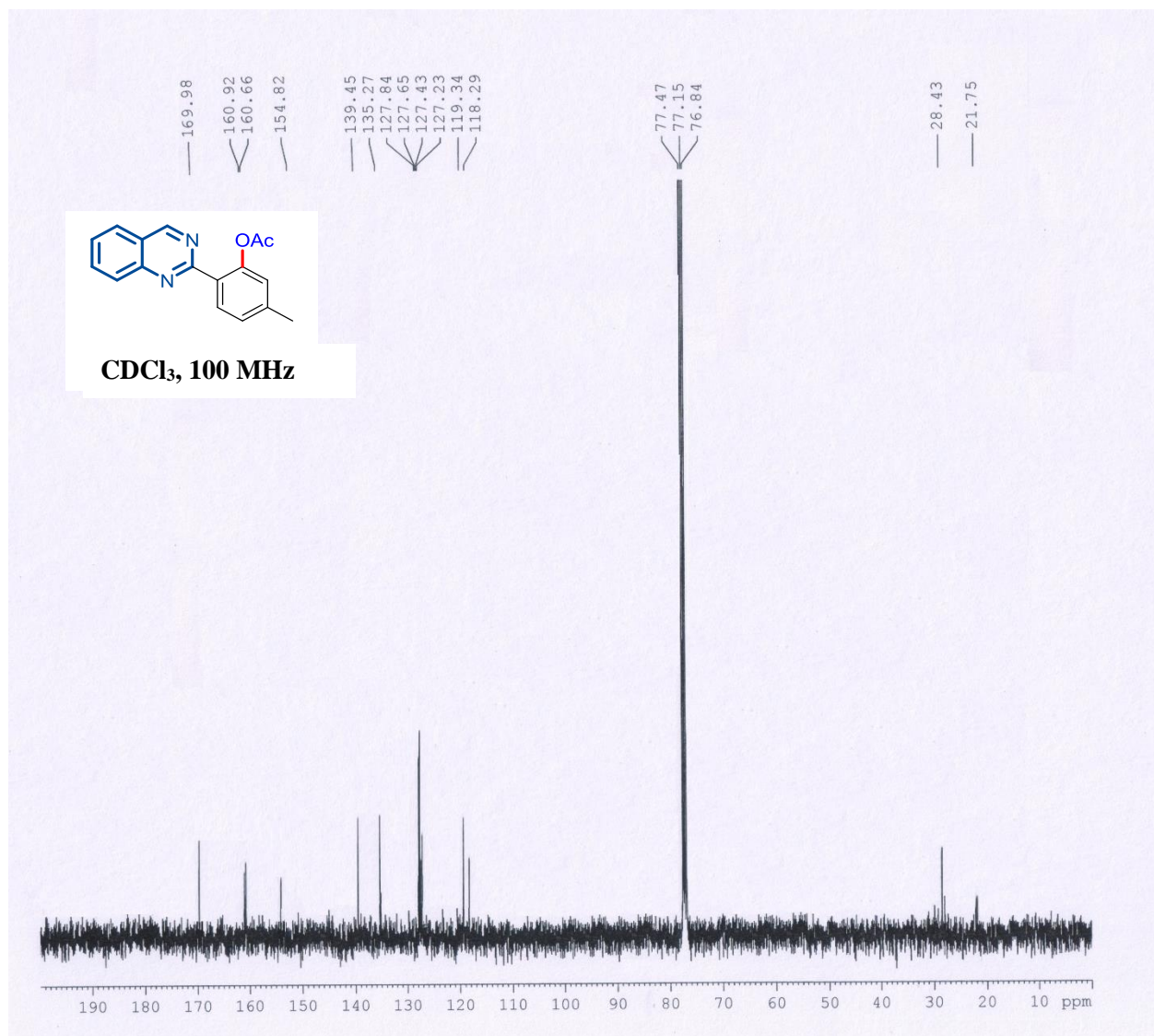
¹³C NMR of Compound 2l



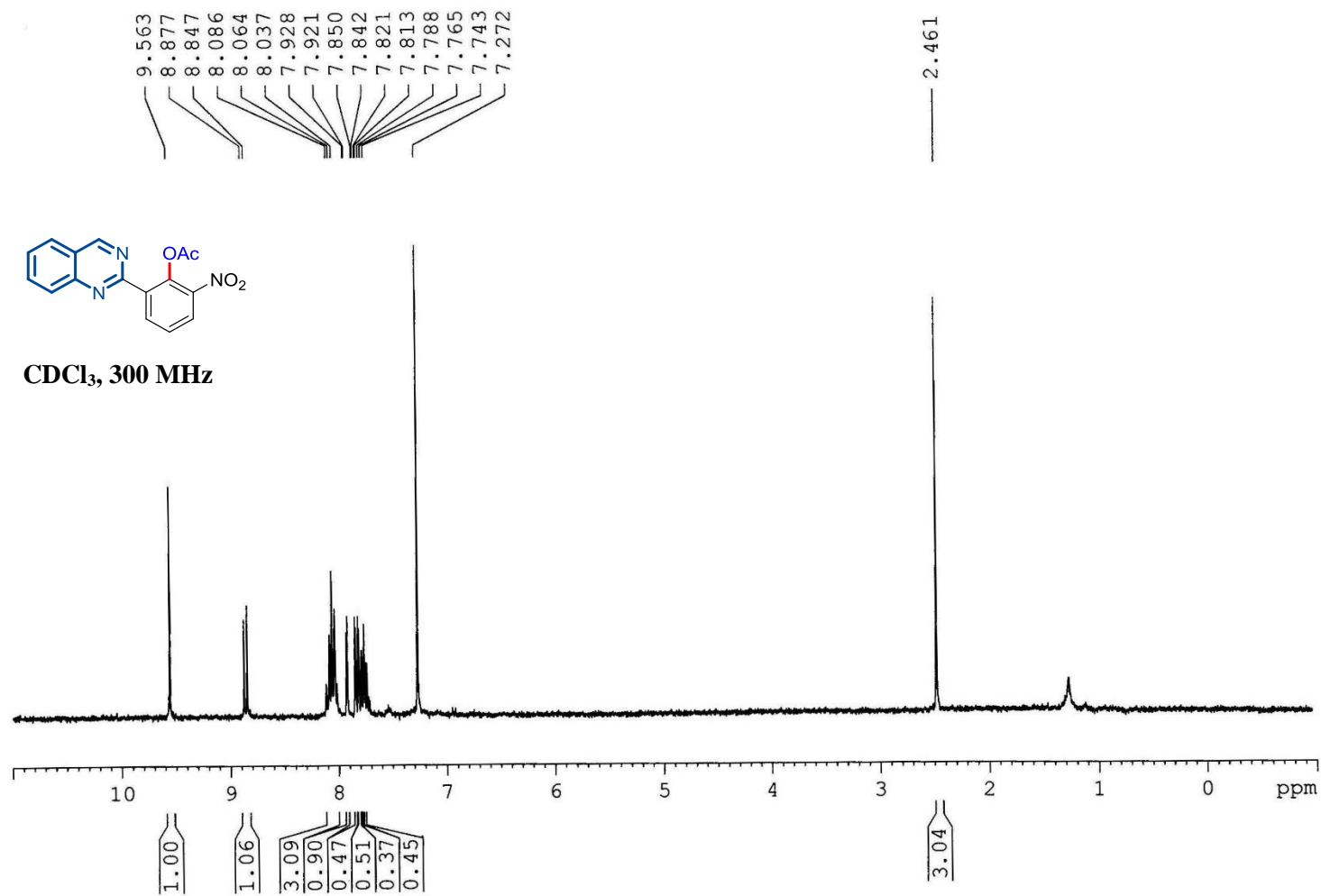
^1H NMR of Compound 2m



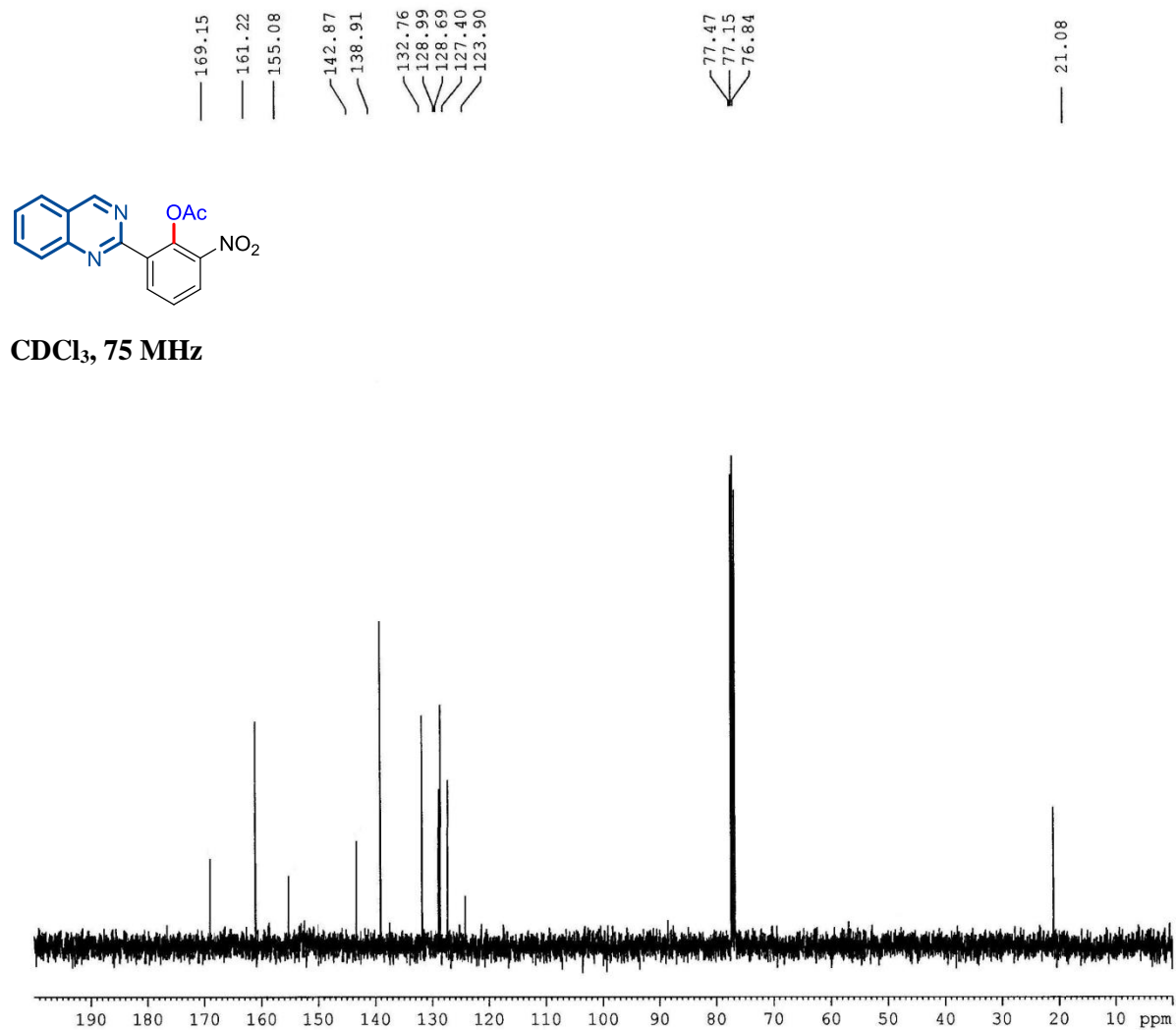
^{13}C NMR of Compound 2m



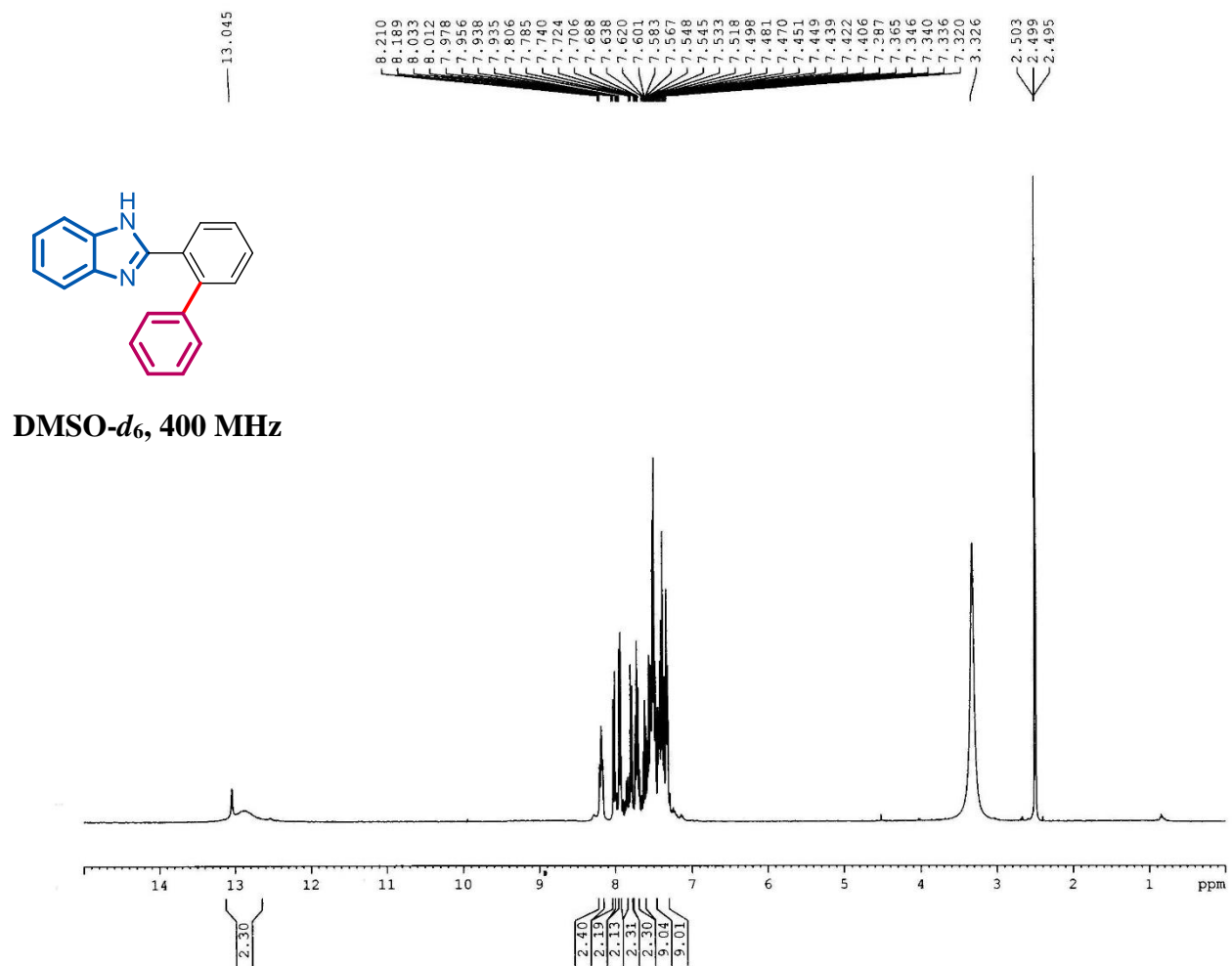
¹H NMR of Compound 2n



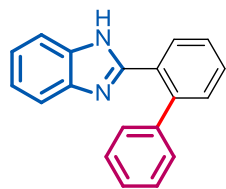
¹³C NMR of Compound 2n



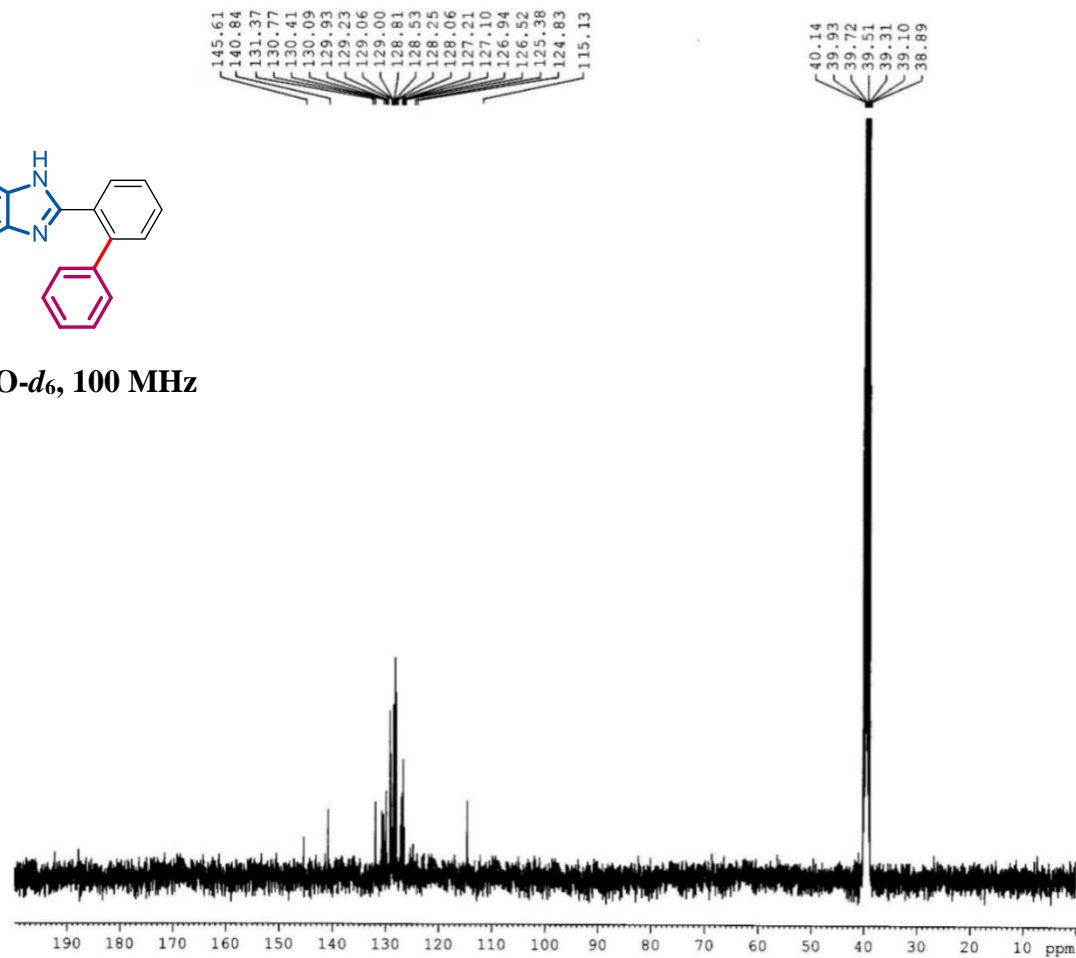
¹H NMR of Compound 3a



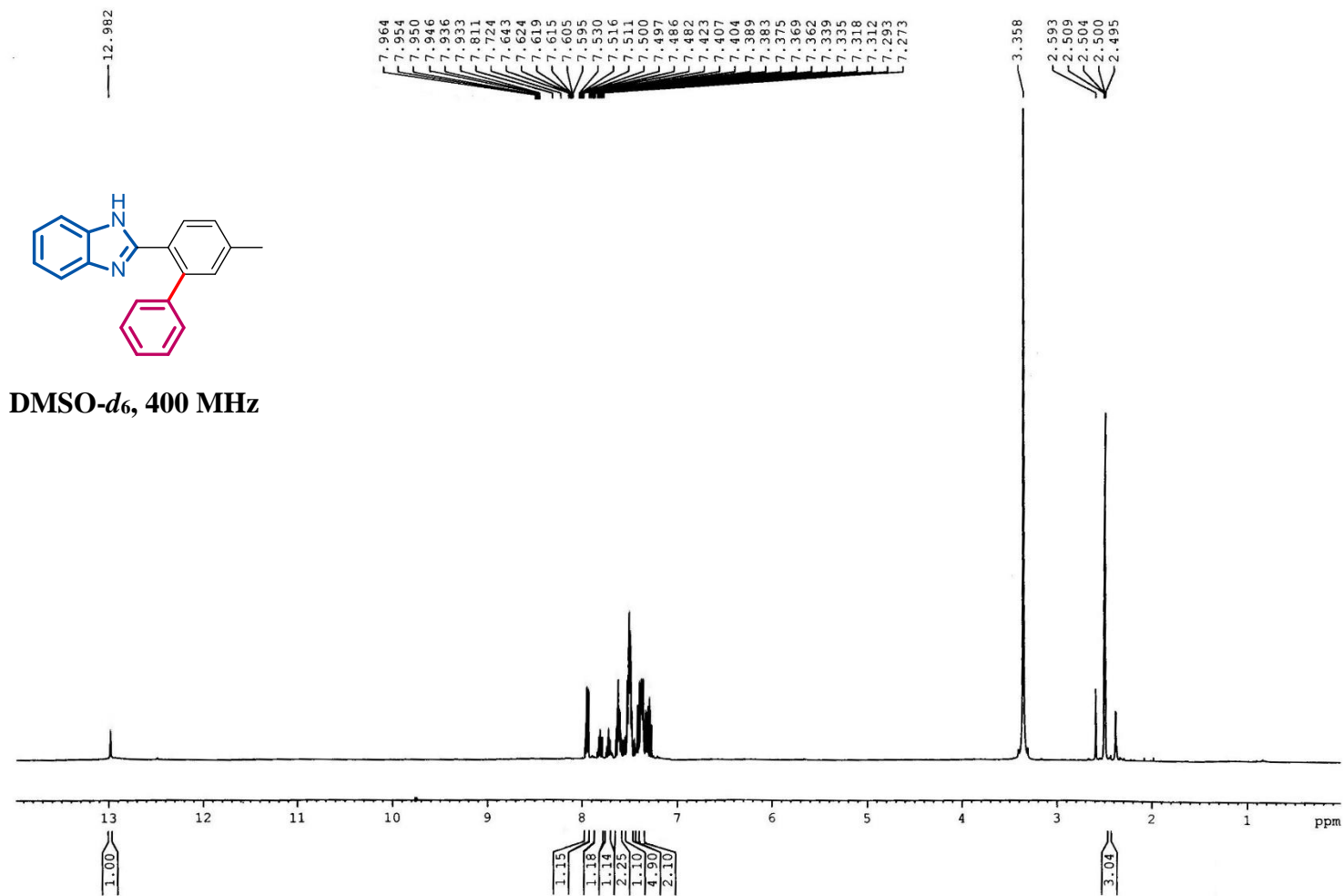
¹³C NMR of Compound 3a



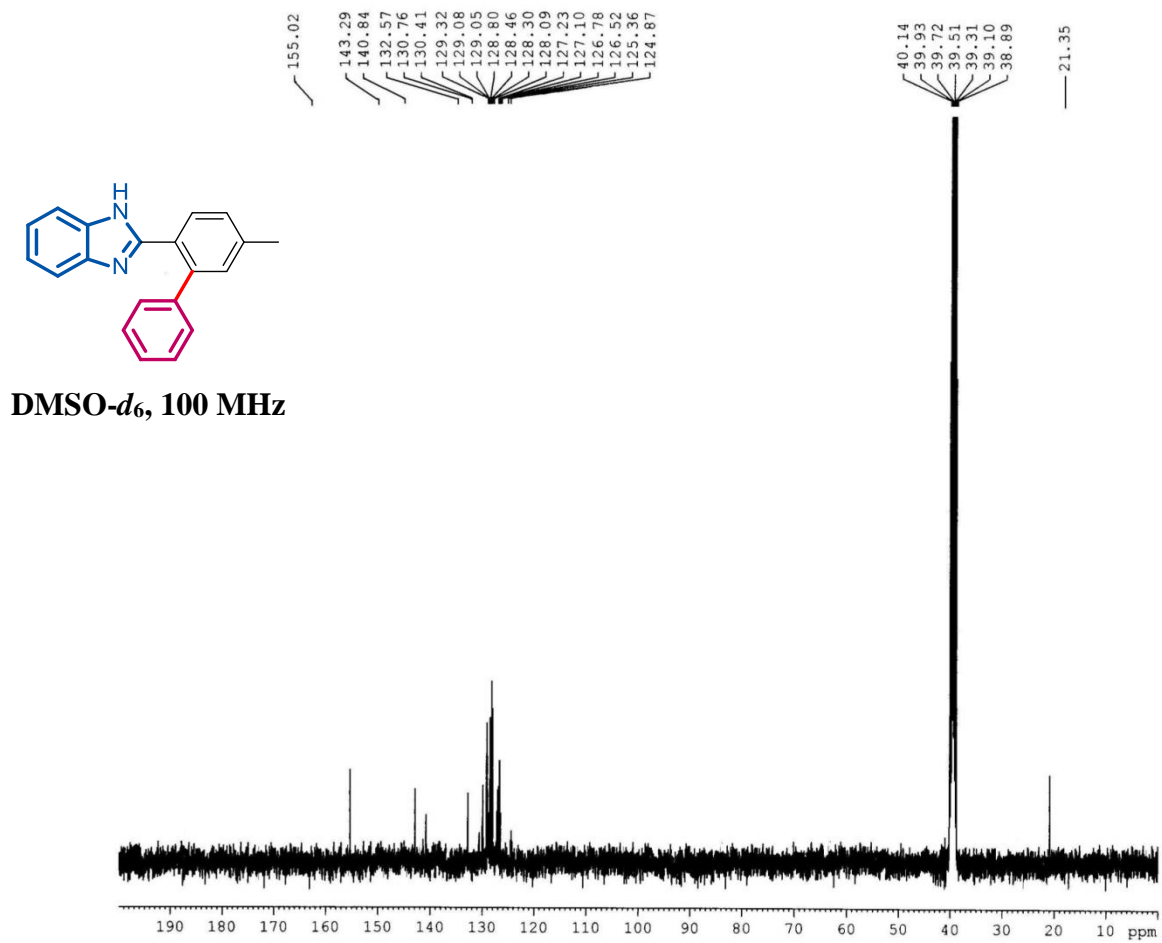
DMSO-*d*₆, 100 MHz



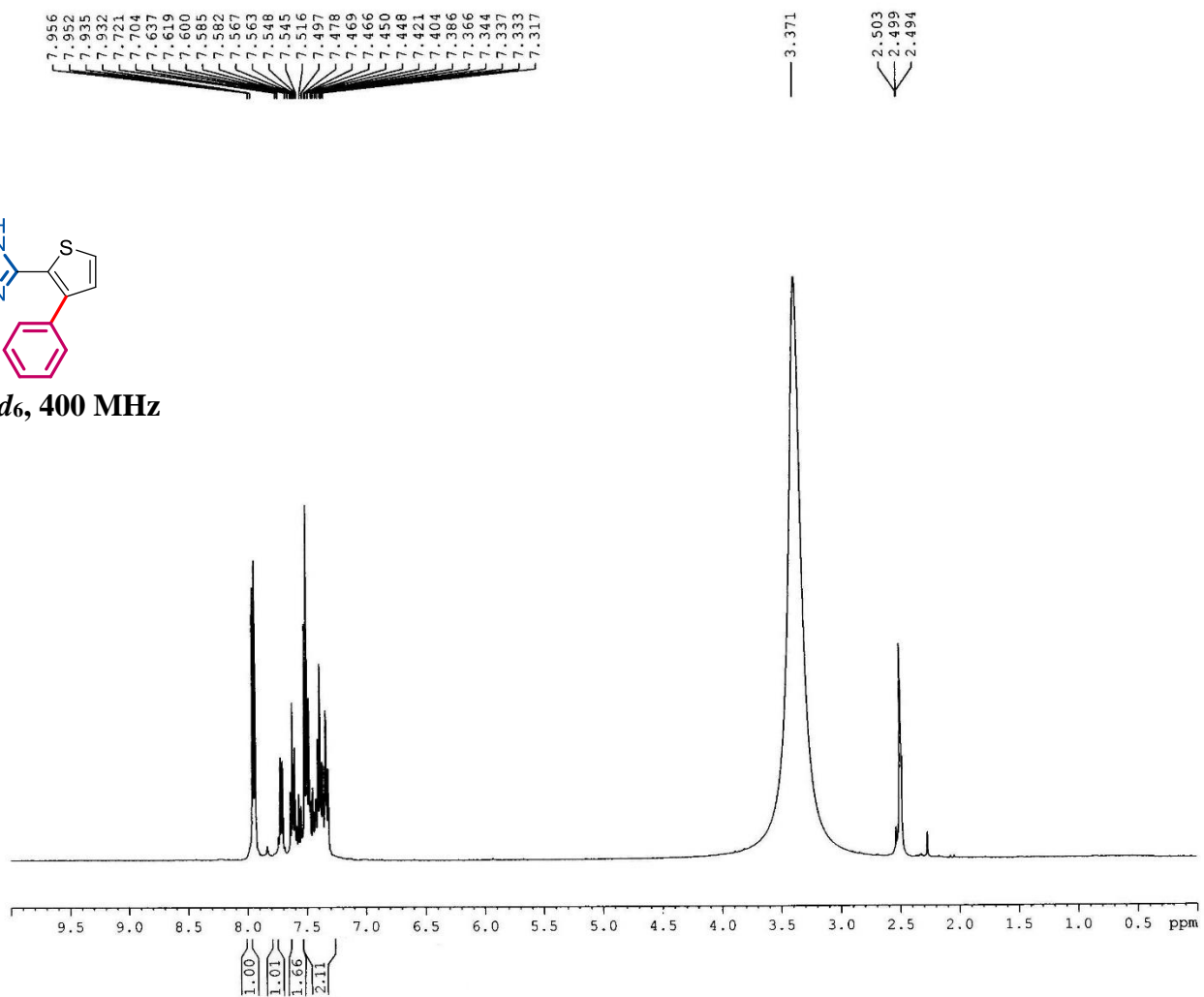
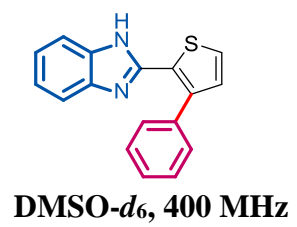
¹H NMR of Compound 3b



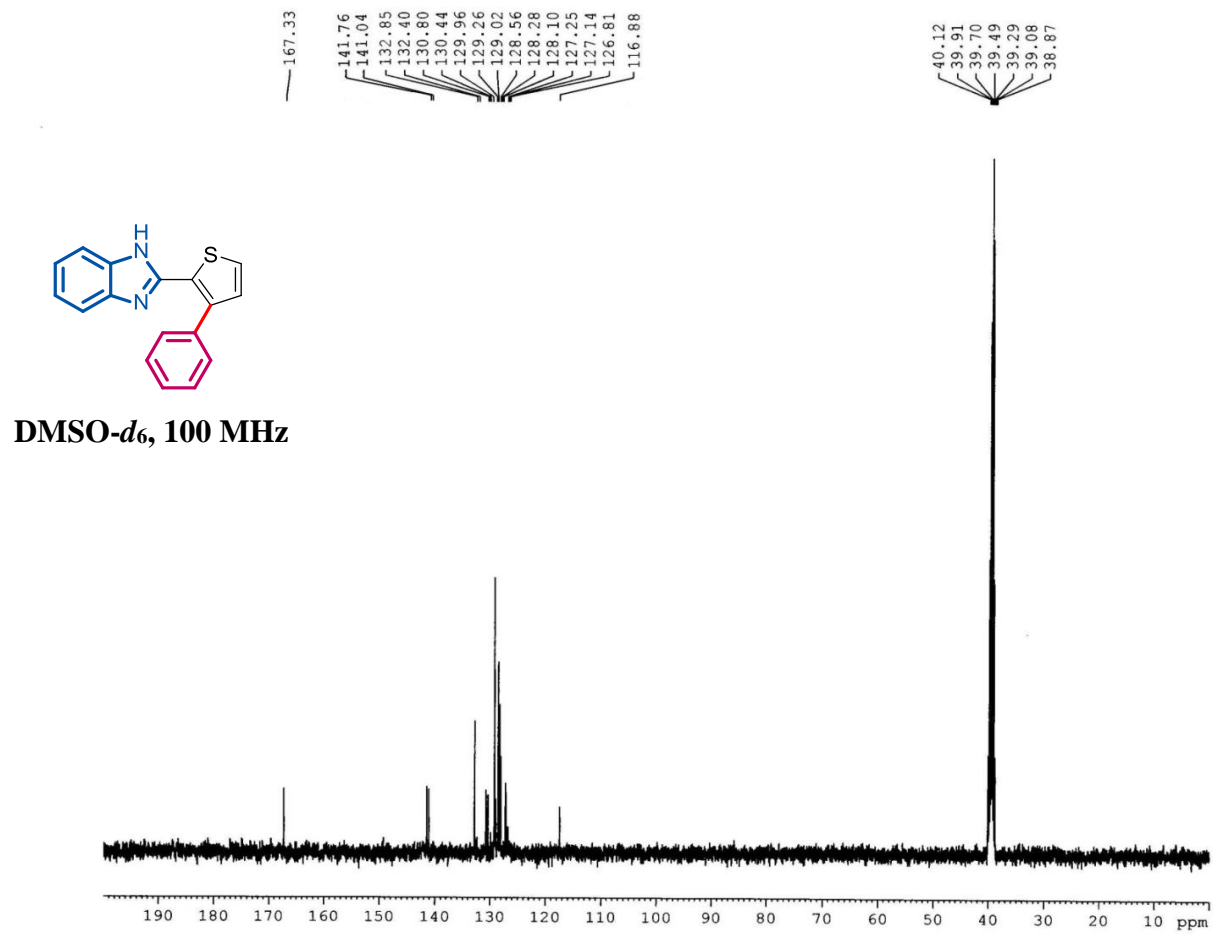
¹³C NMR of Compound 3b



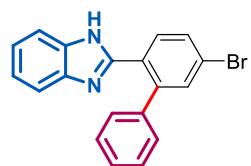
¹H NMR of Compound 3c



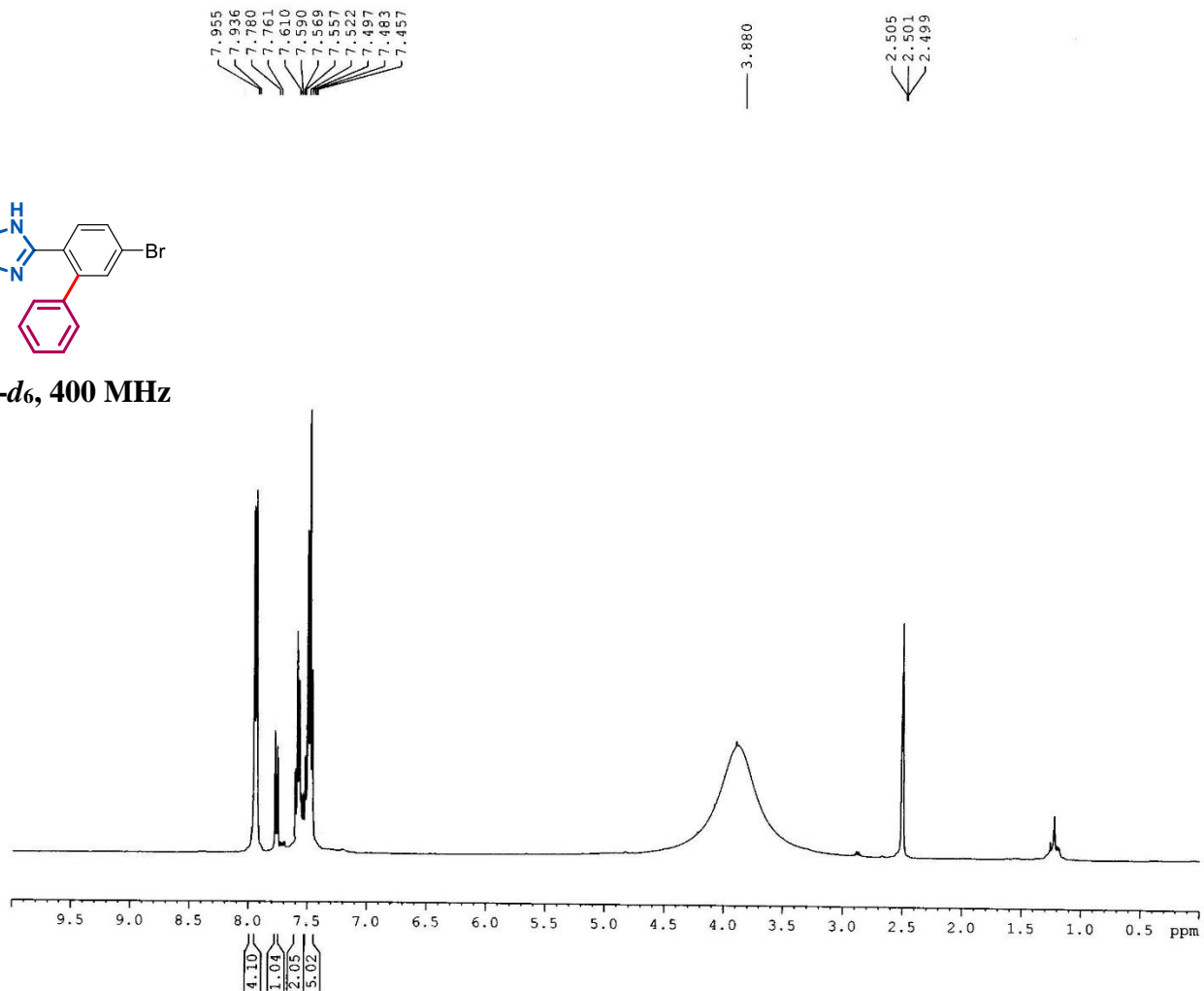
¹³C NMR of Compound 3c



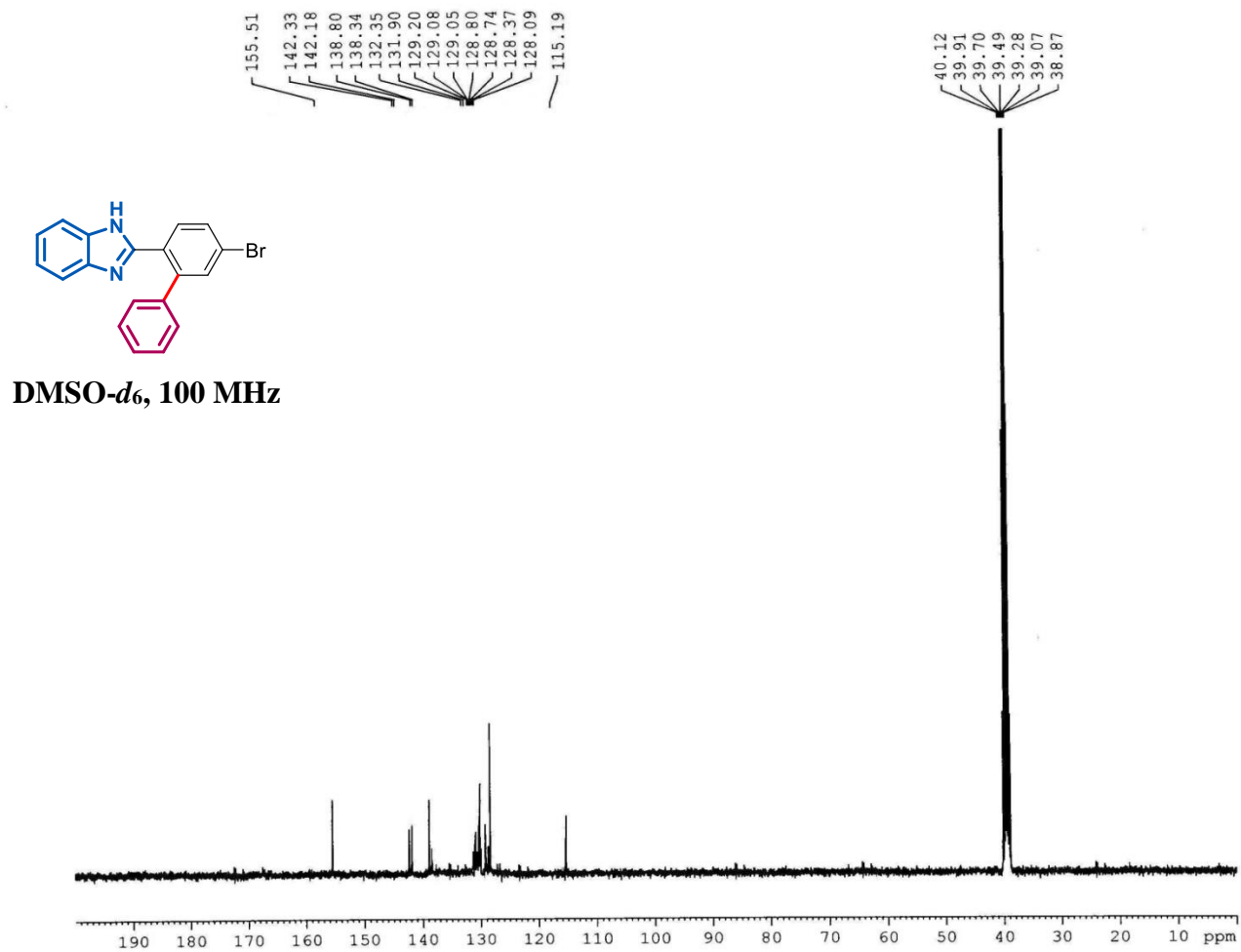
¹H NMR of Compound 3d



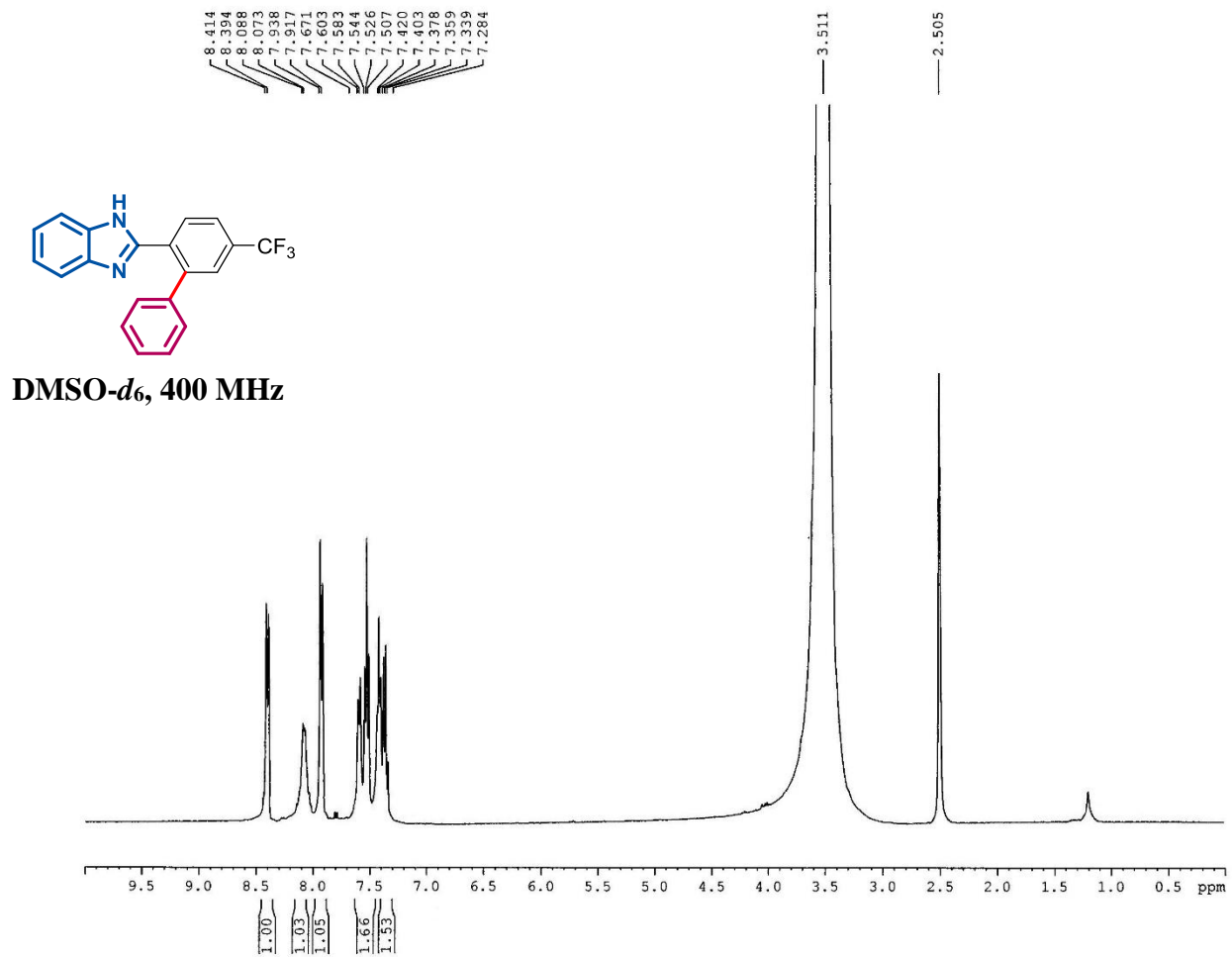
DMSO-*d*₆, 400 MHz



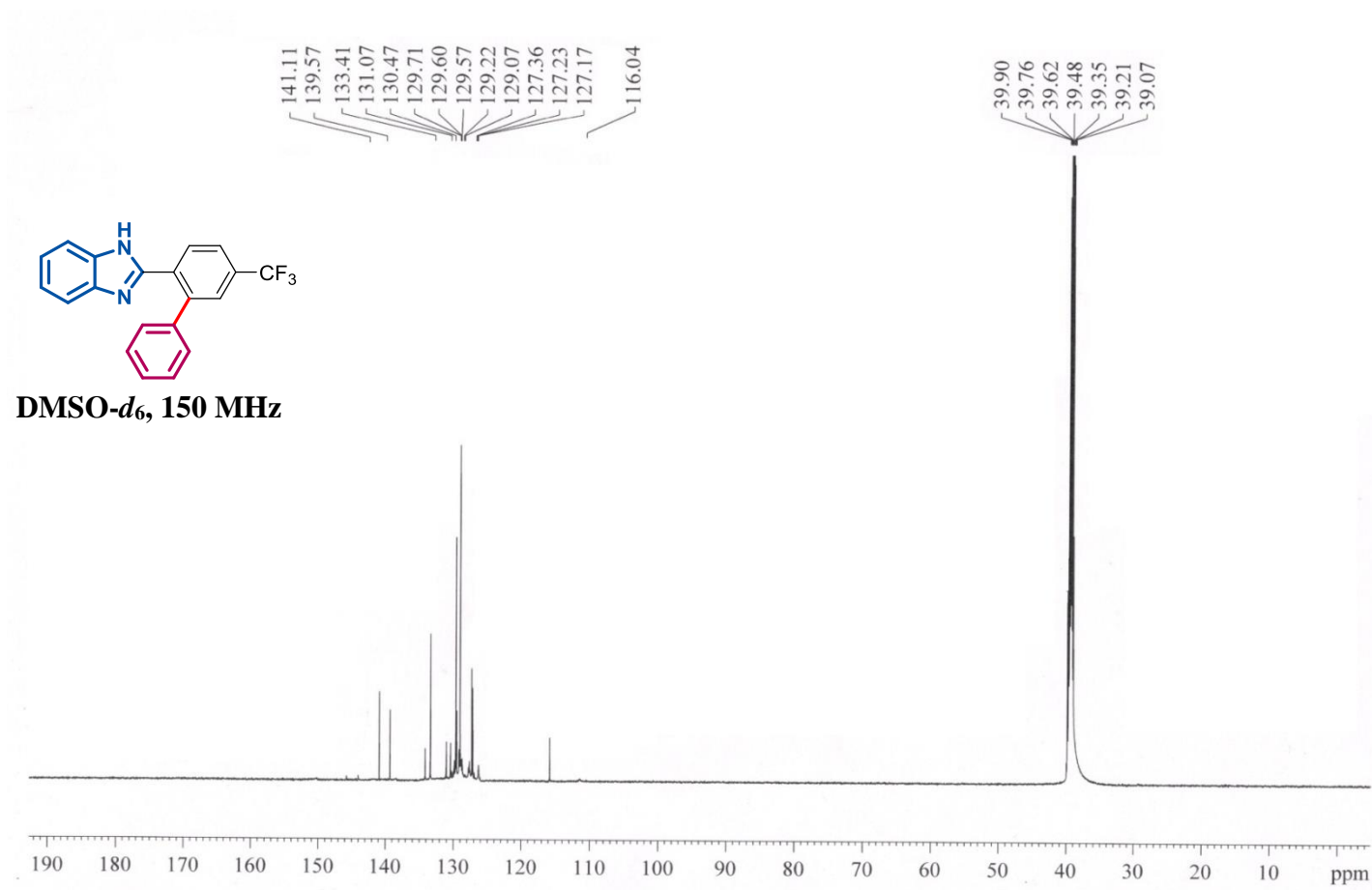
¹³C NMR of Compound 3d



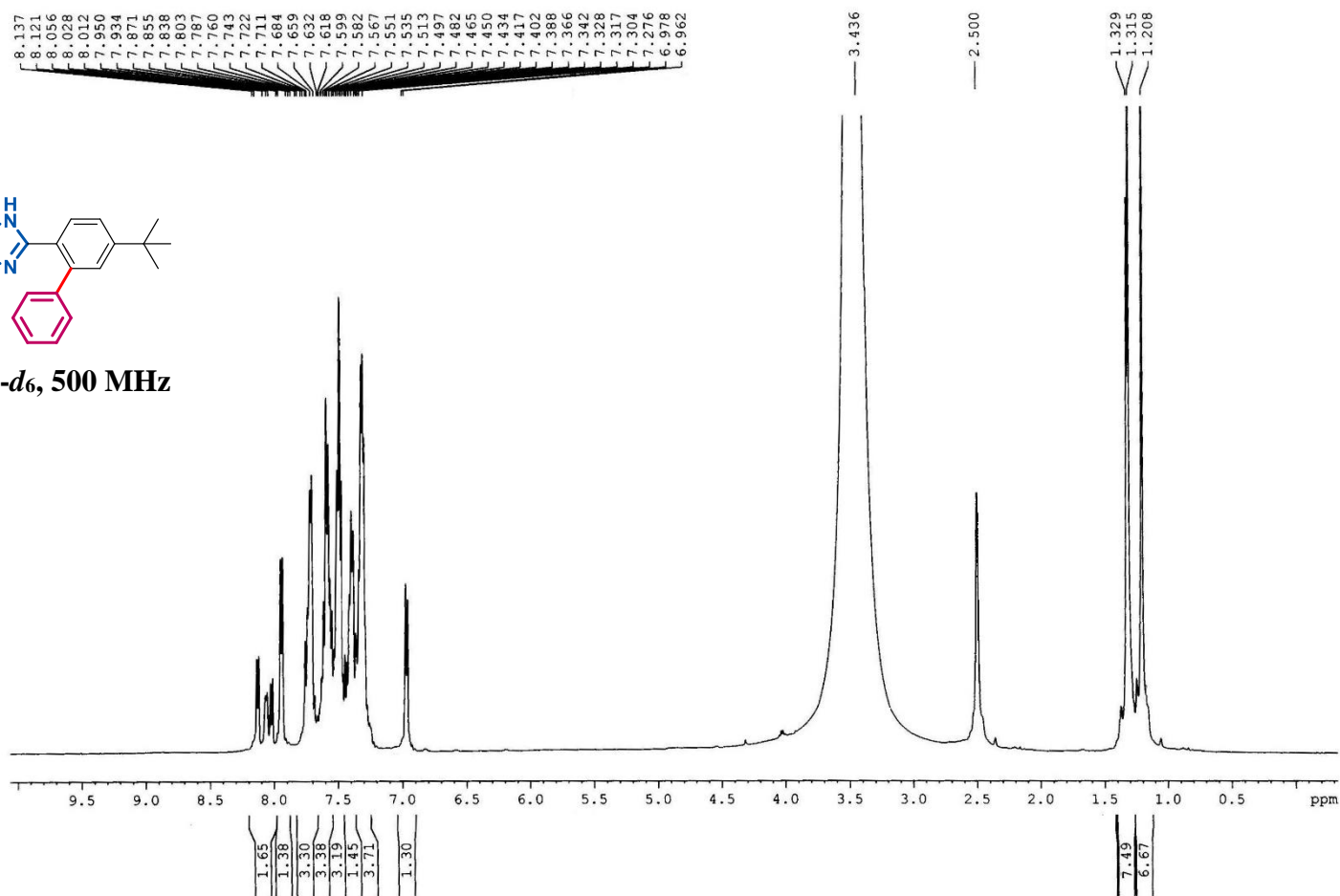
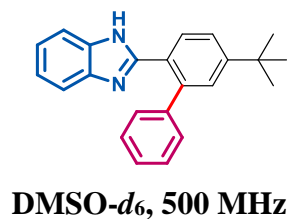
¹H NMR of Compound 3e



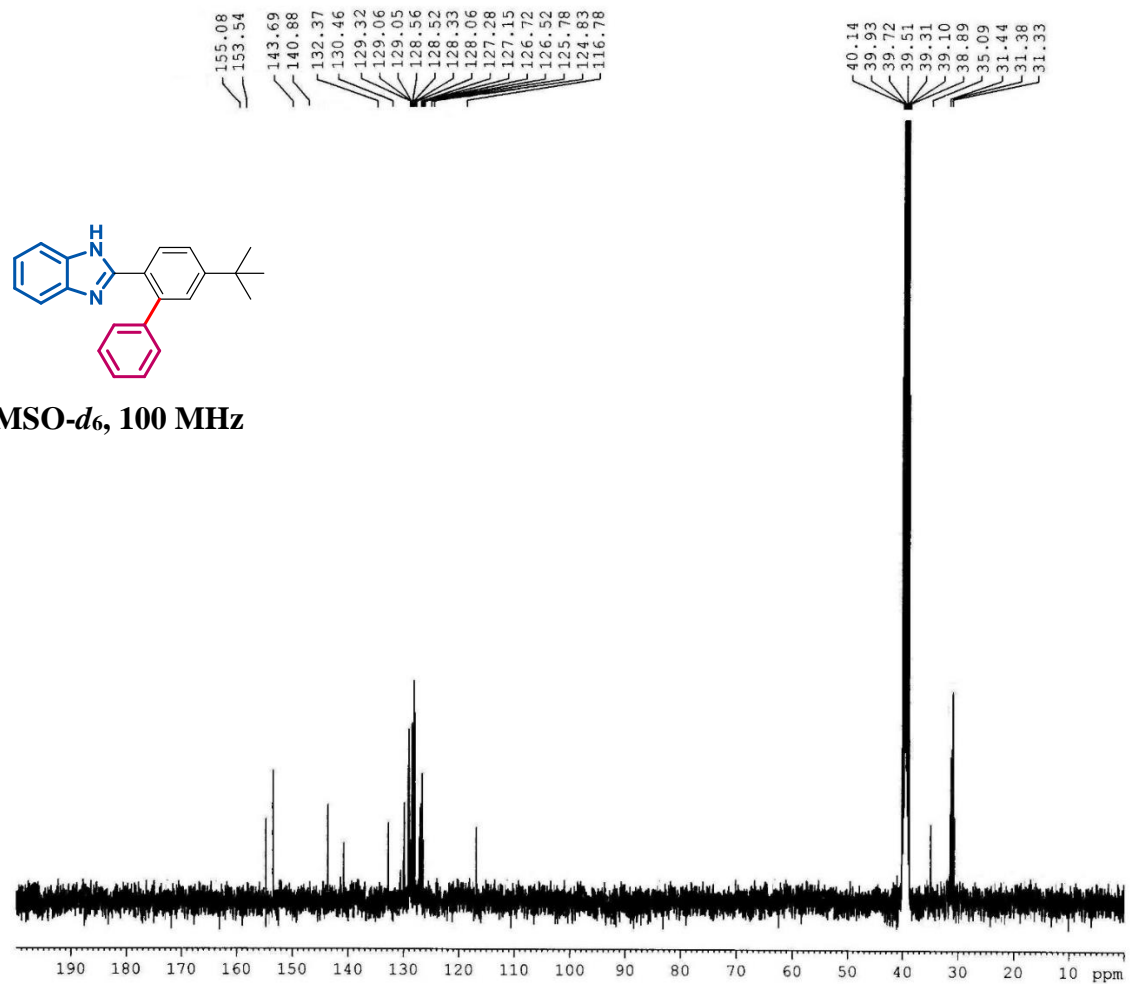
¹³C NMR of Compound 3e



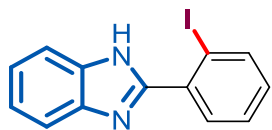
¹H NMR of Compound 3f



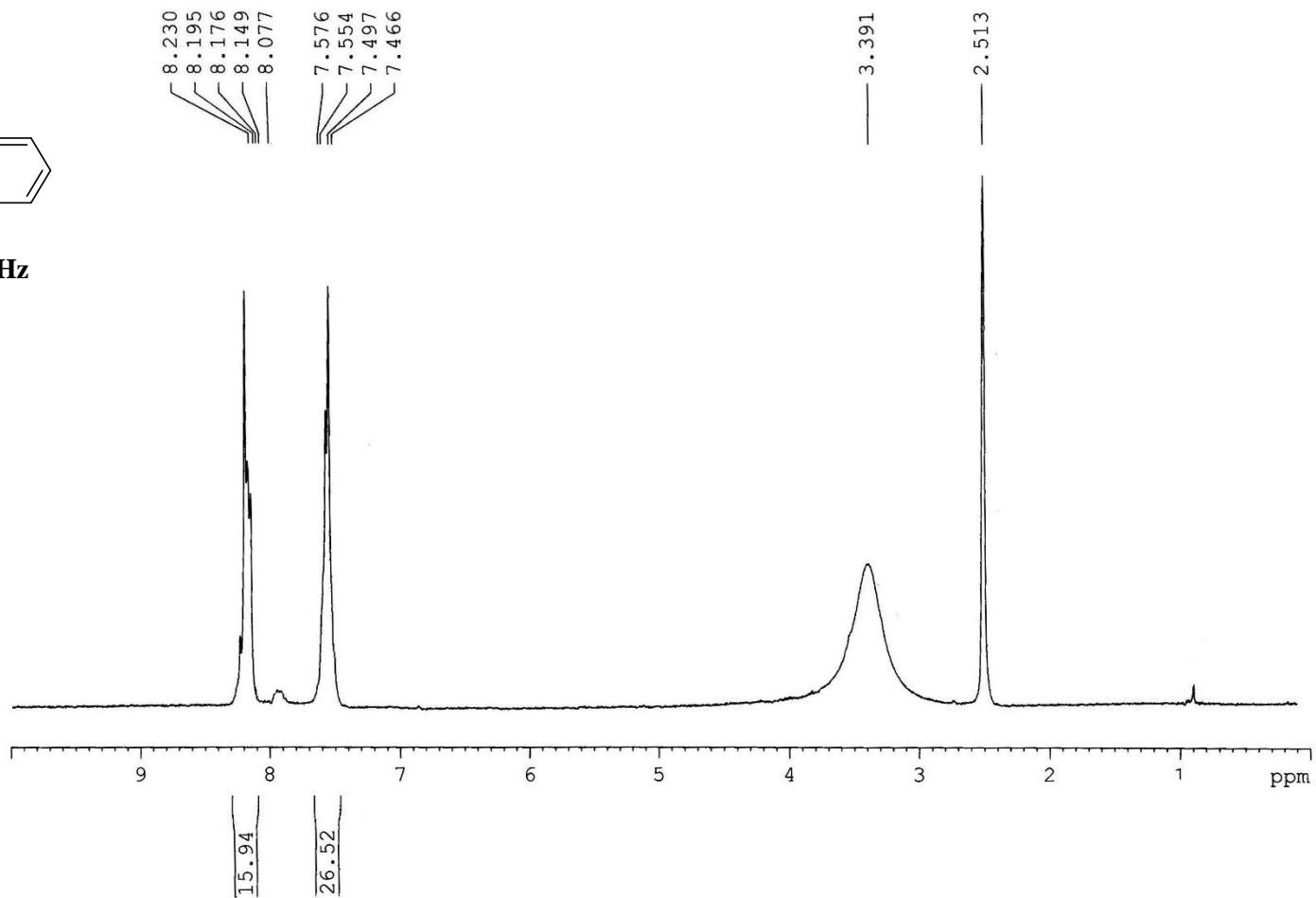
¹³C NMR of Compound 3f



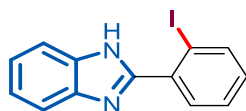
¹H NMR of Compound 4a



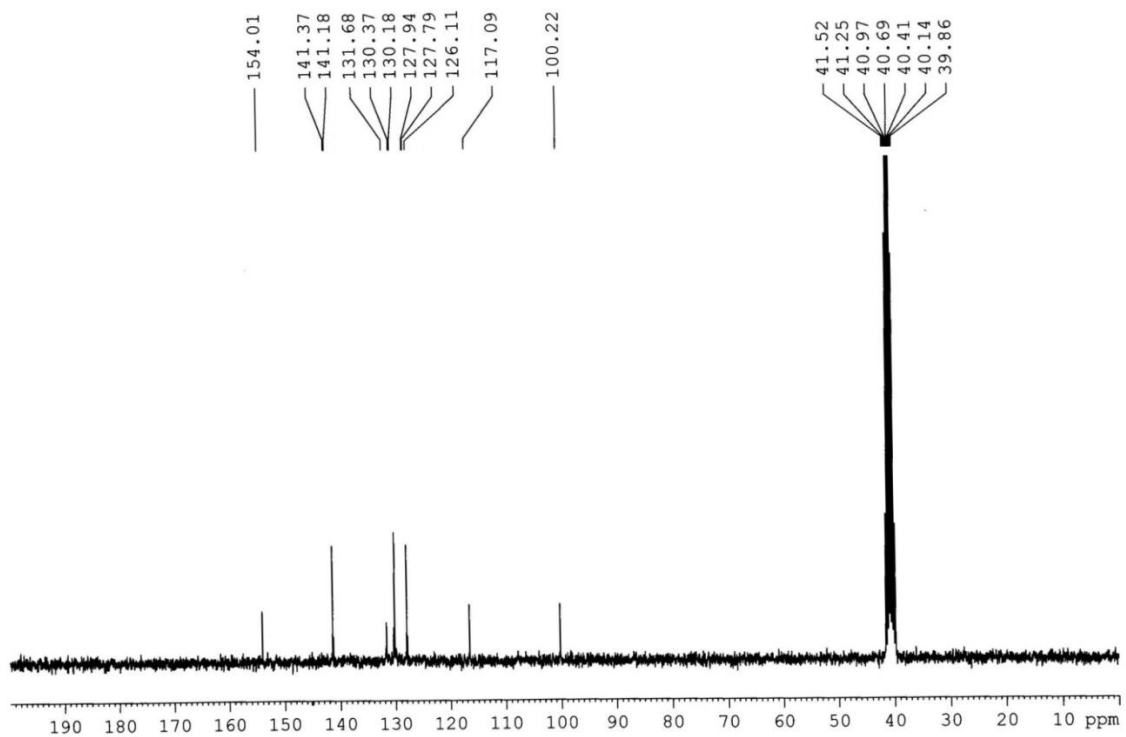
DMSO-*d*₆, 300 MHz



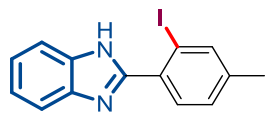
¹³C NMR of Compound 4a



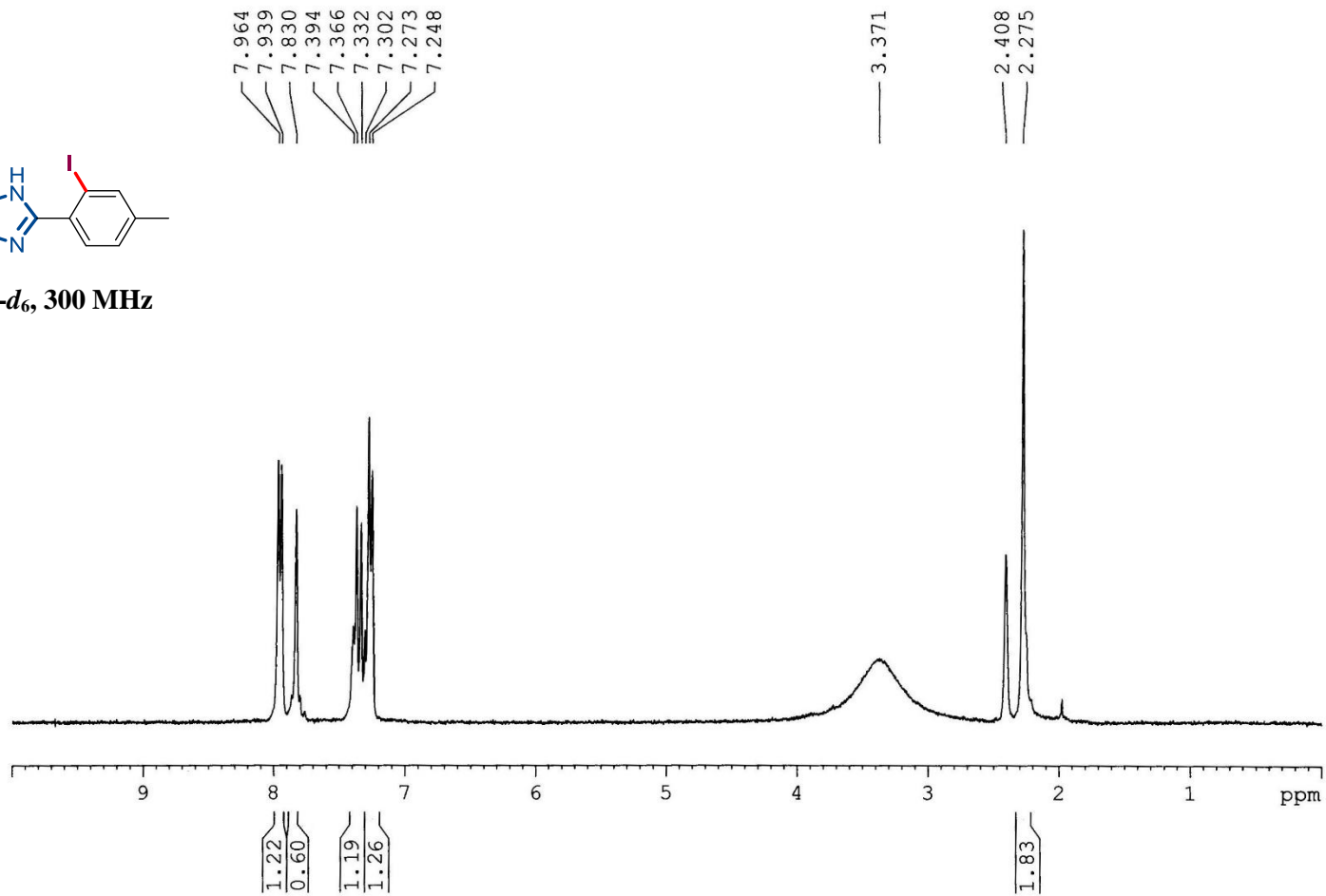
DMSO-*d*₆, 75 MHz



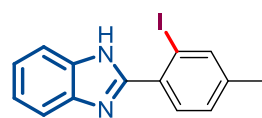
¹H NMR of Compound 4b



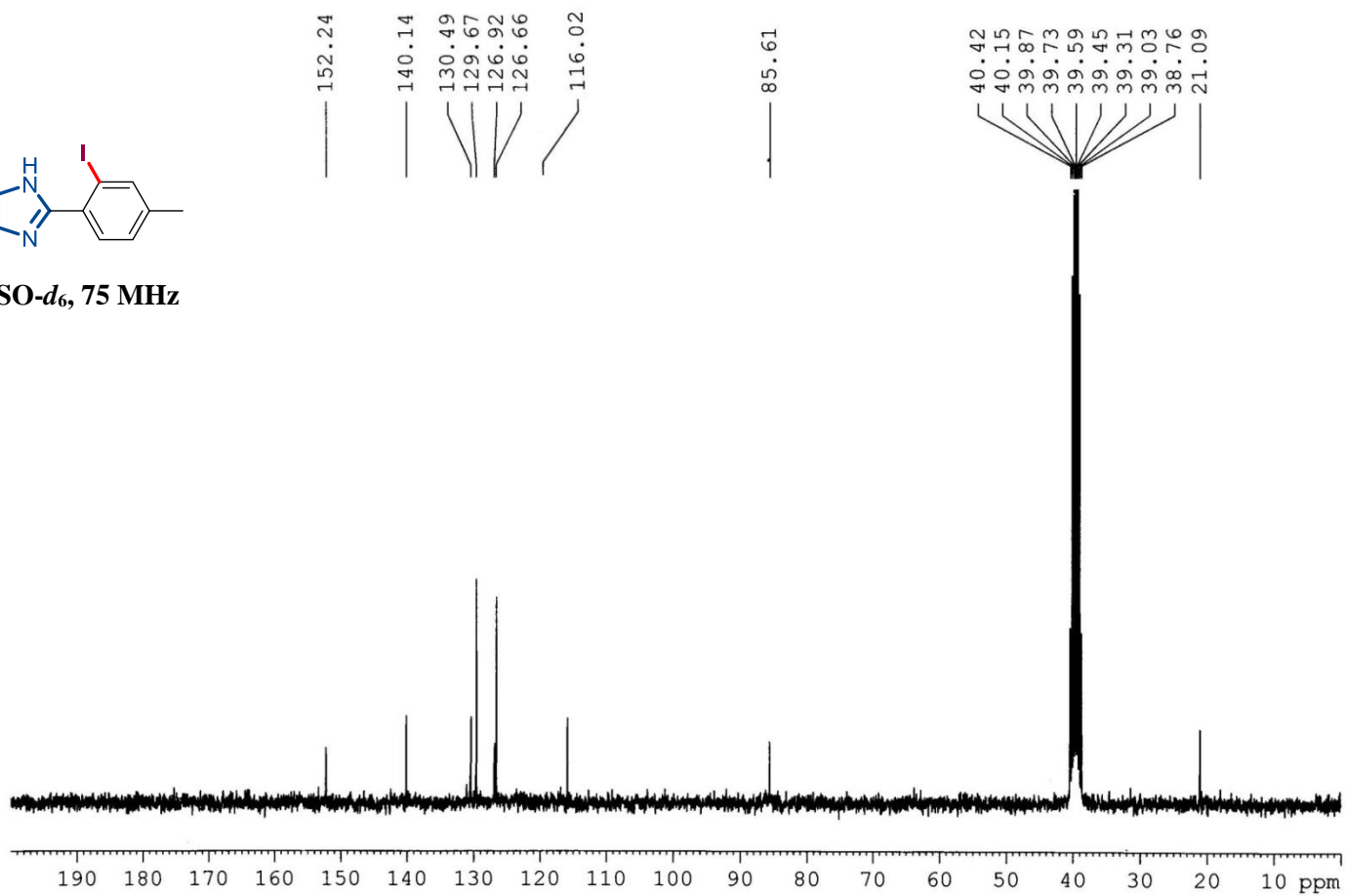
DMSO-*d*₆, 300 MHz



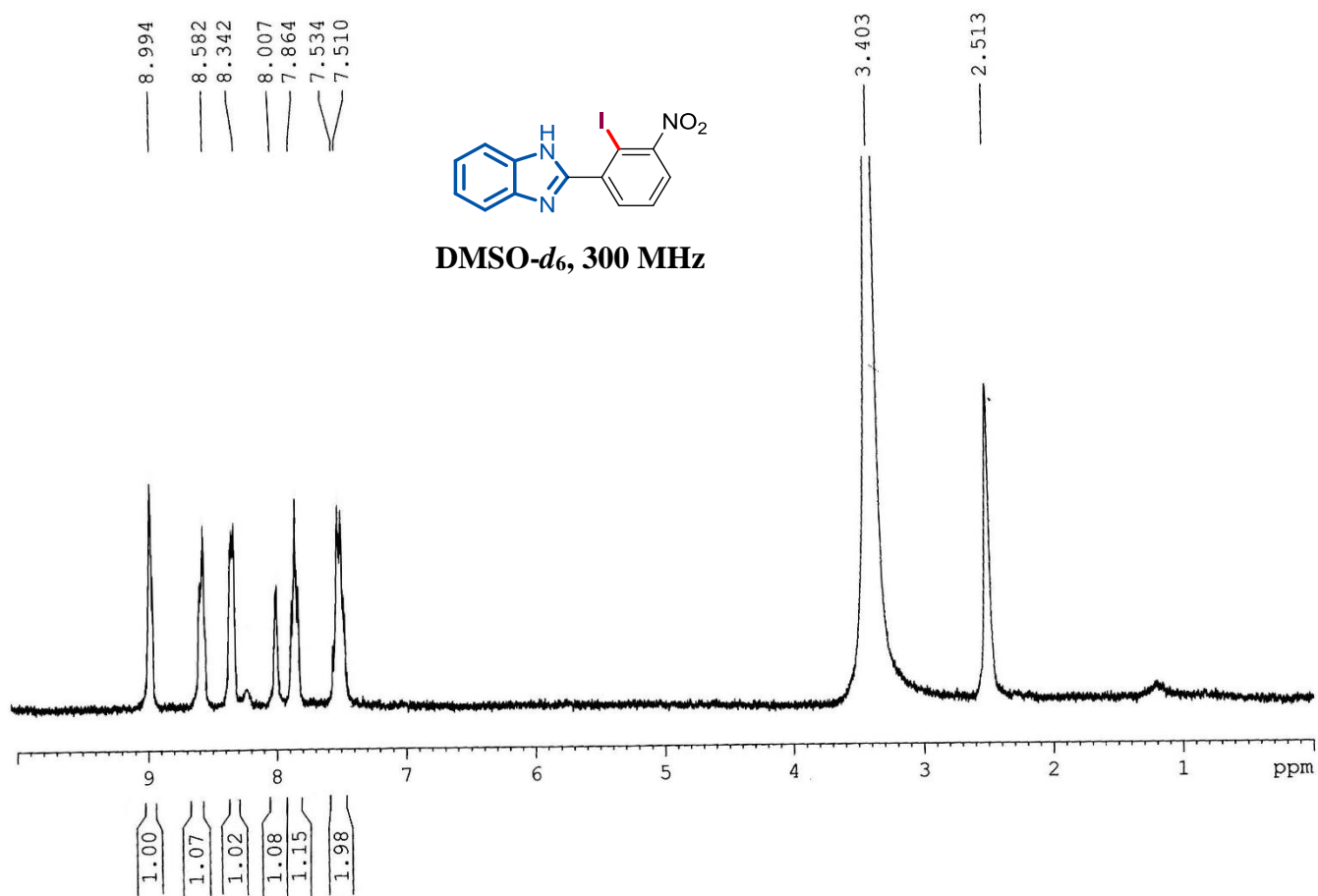
¹³C NMR of Compound 4b



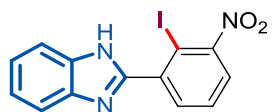
DMSO-*d*₆, 75 MHz



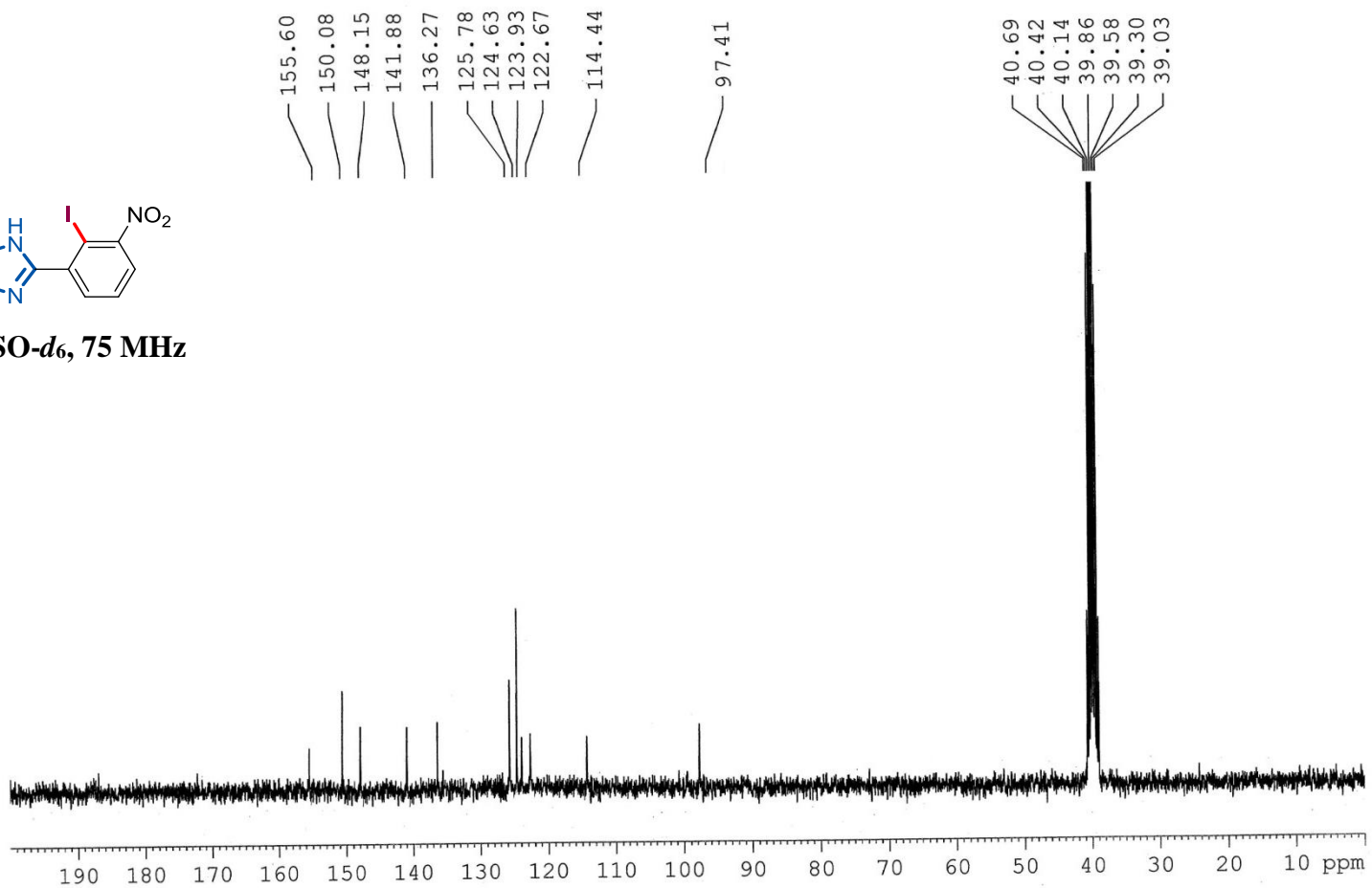
¹H NMR of Compound 4c



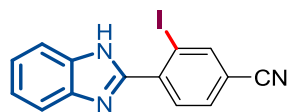
¹³C NMR of Compound 4c



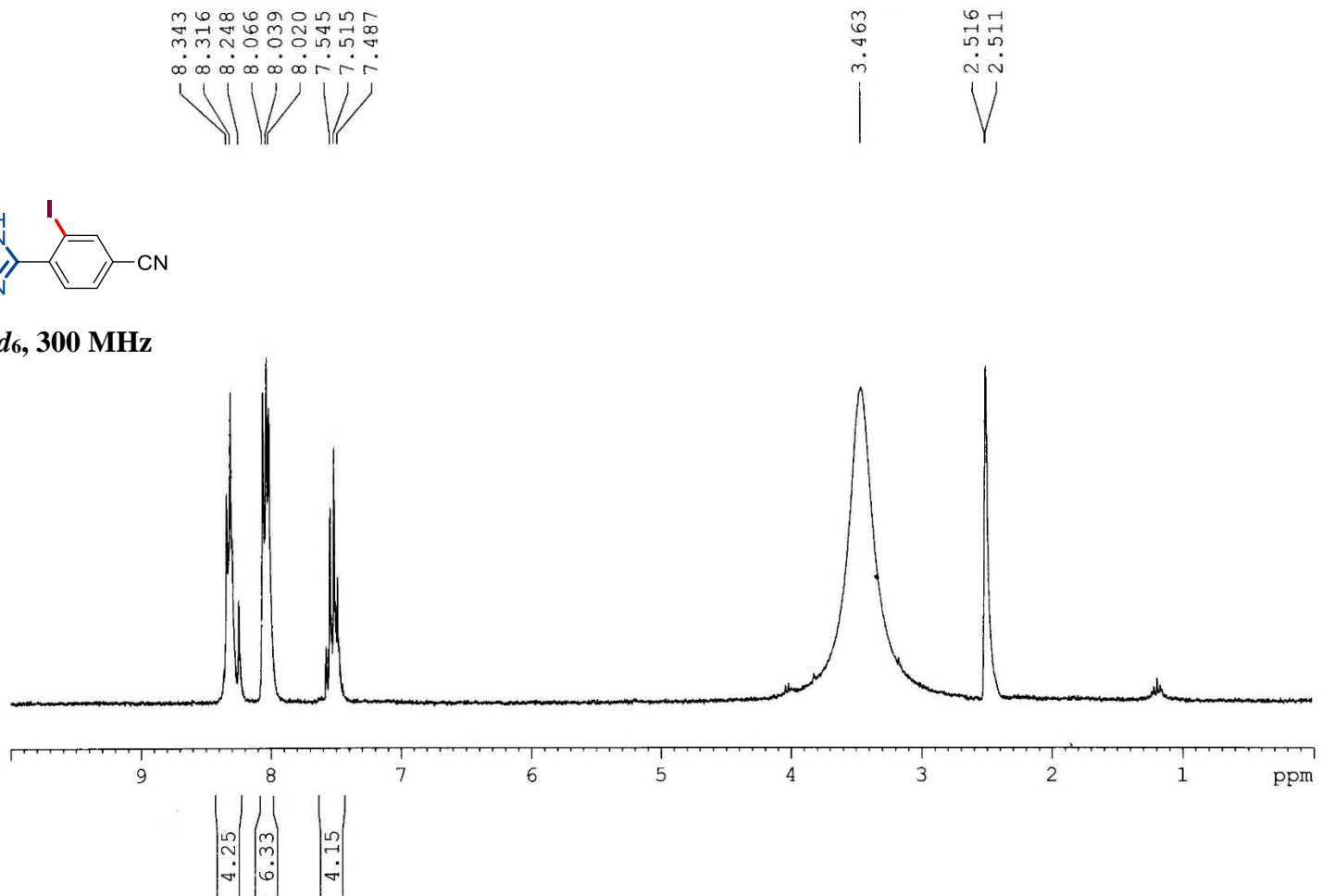
DMSO-*d*₆, 75 MHz



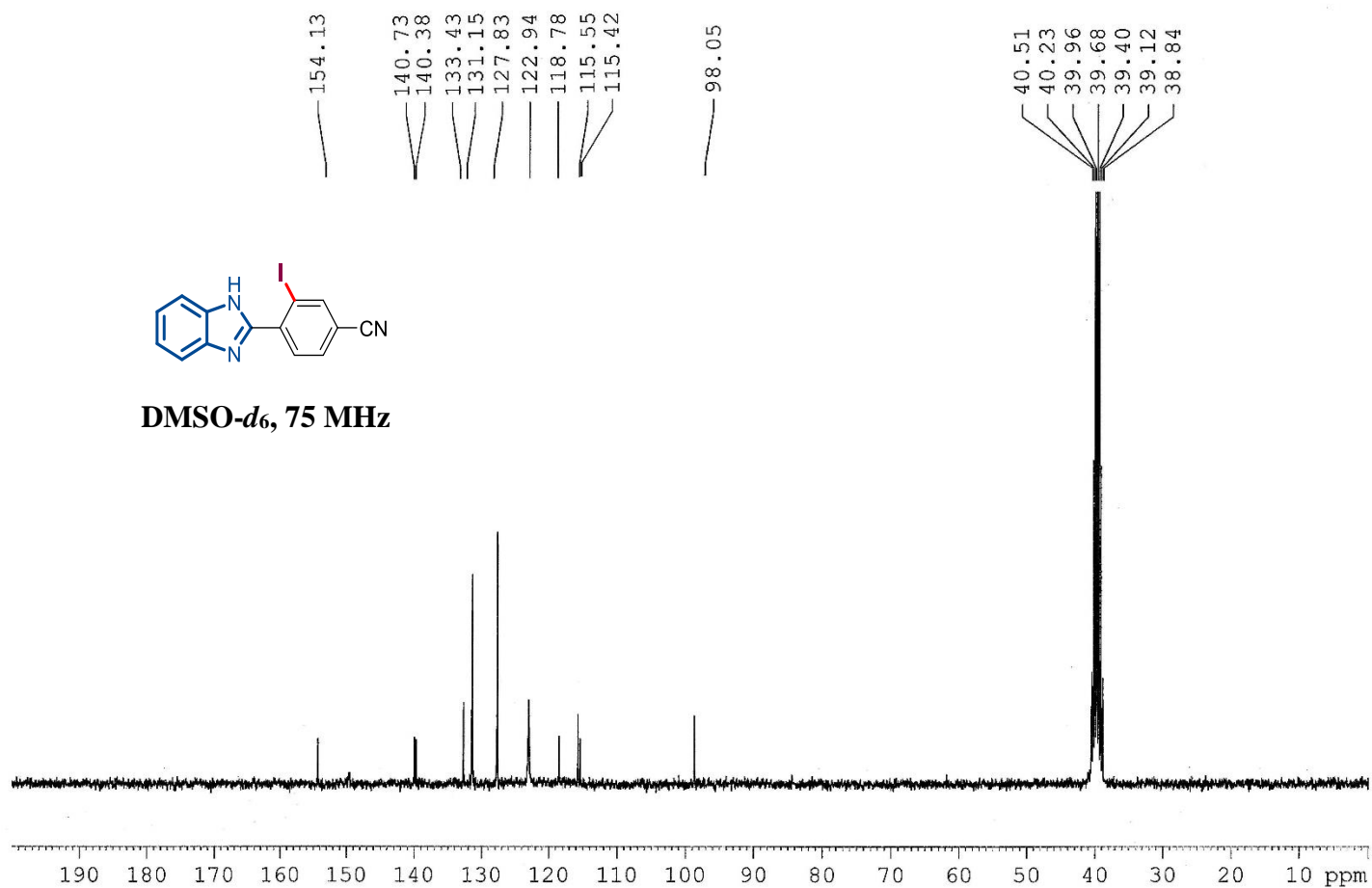
¹H NMR of Compound 4d



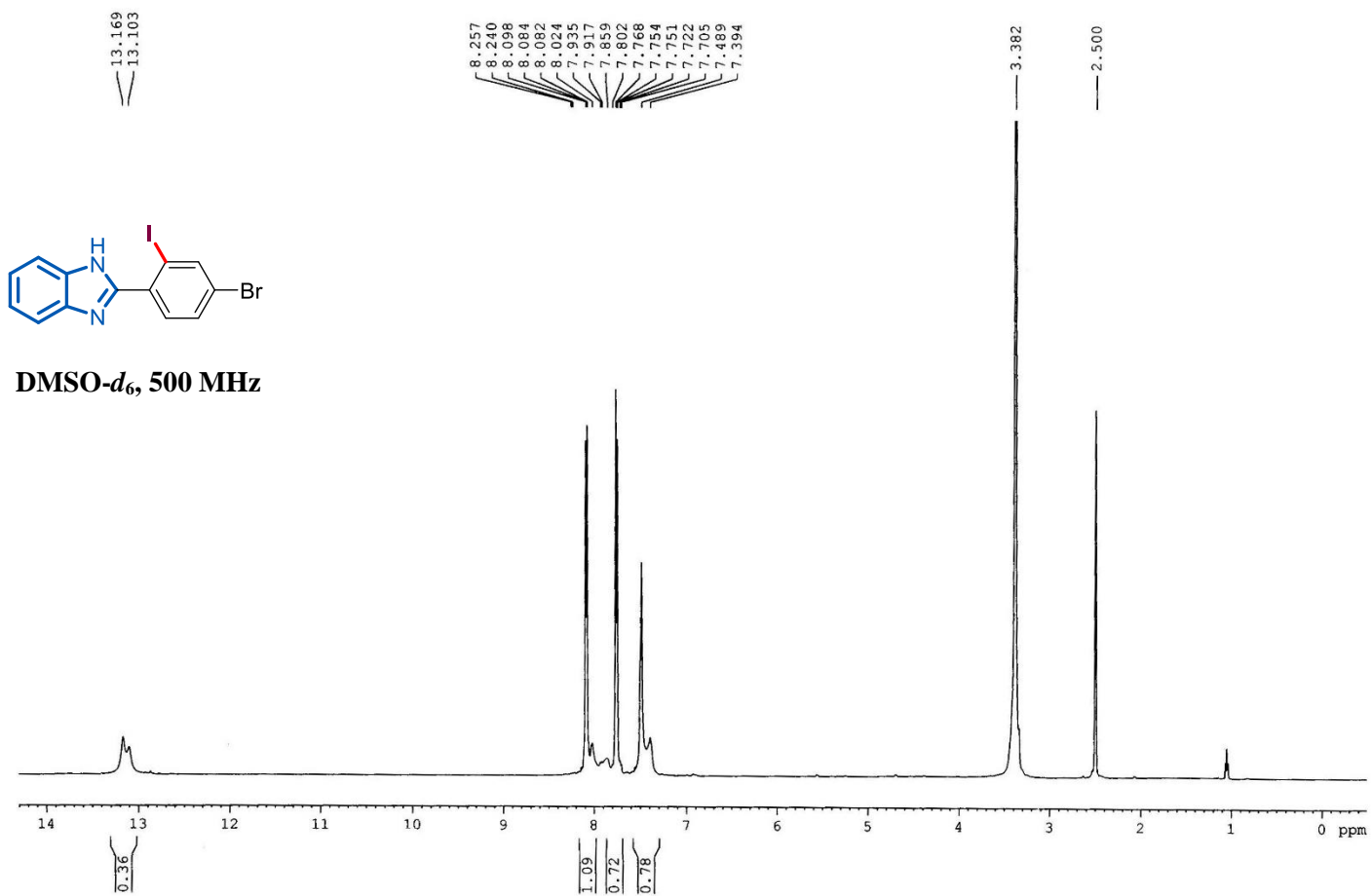
DMSO-*d*₆, 300 MHz



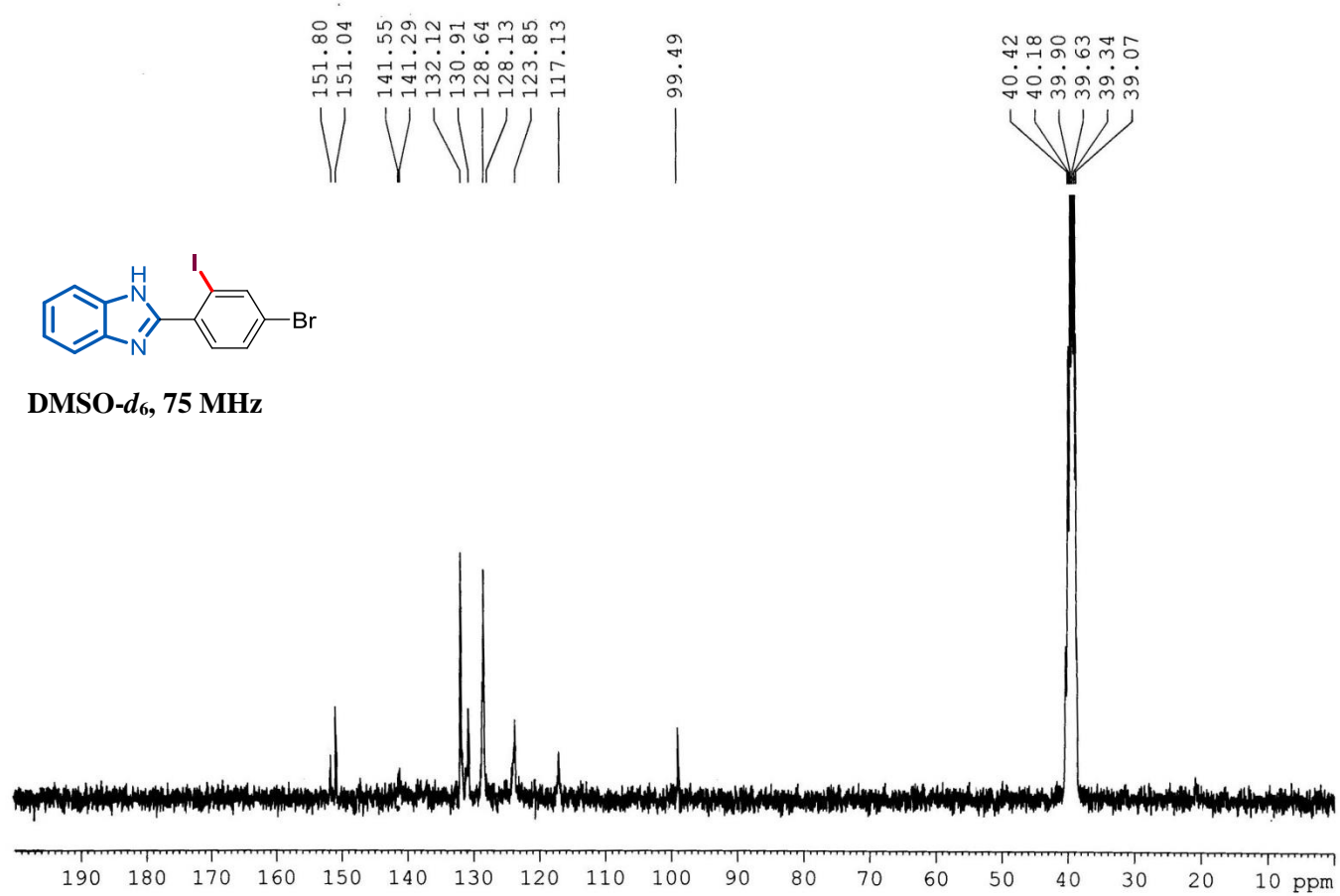
¹³C NMR of Compound 4d



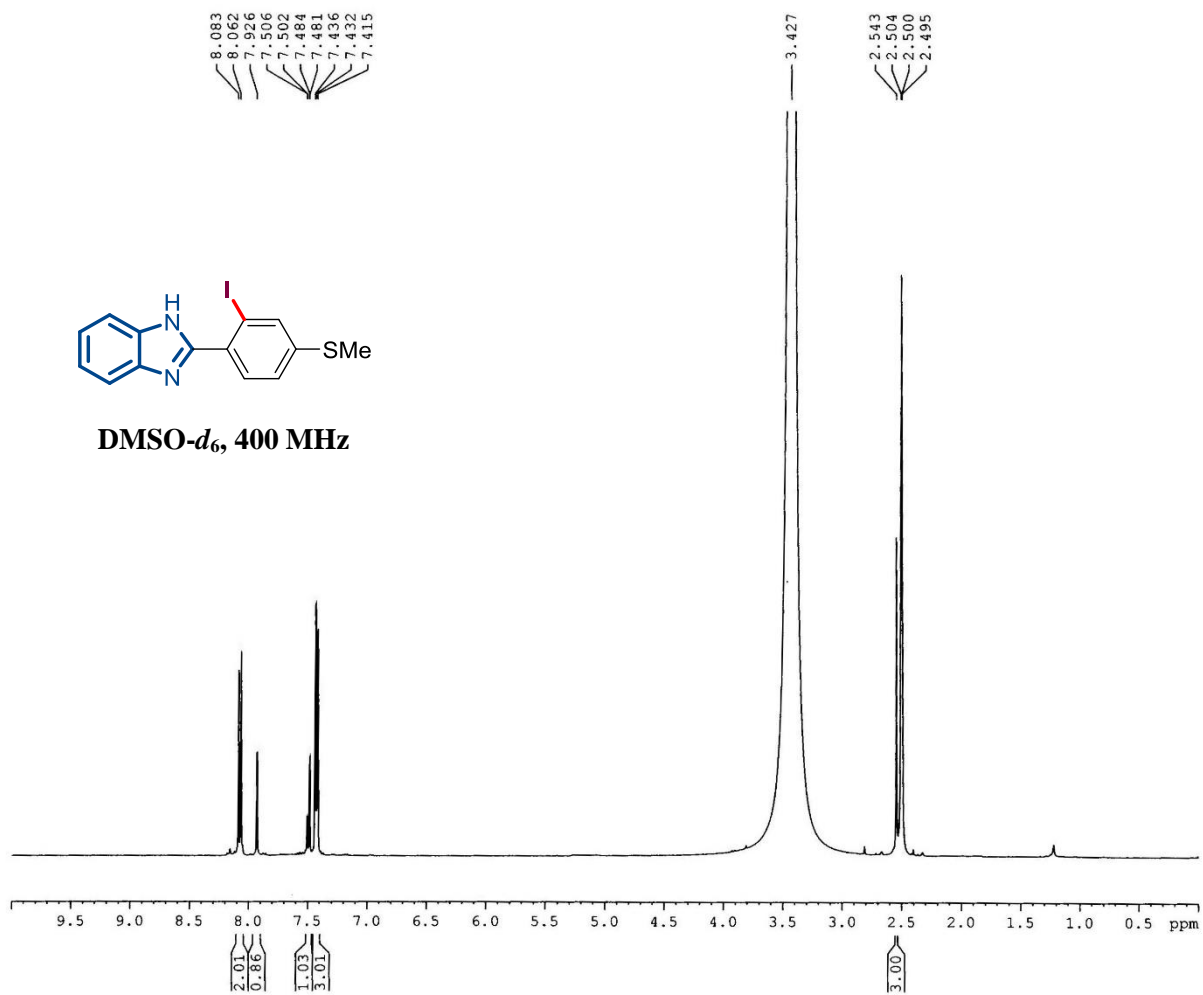
¹H NMR of Compound 4e



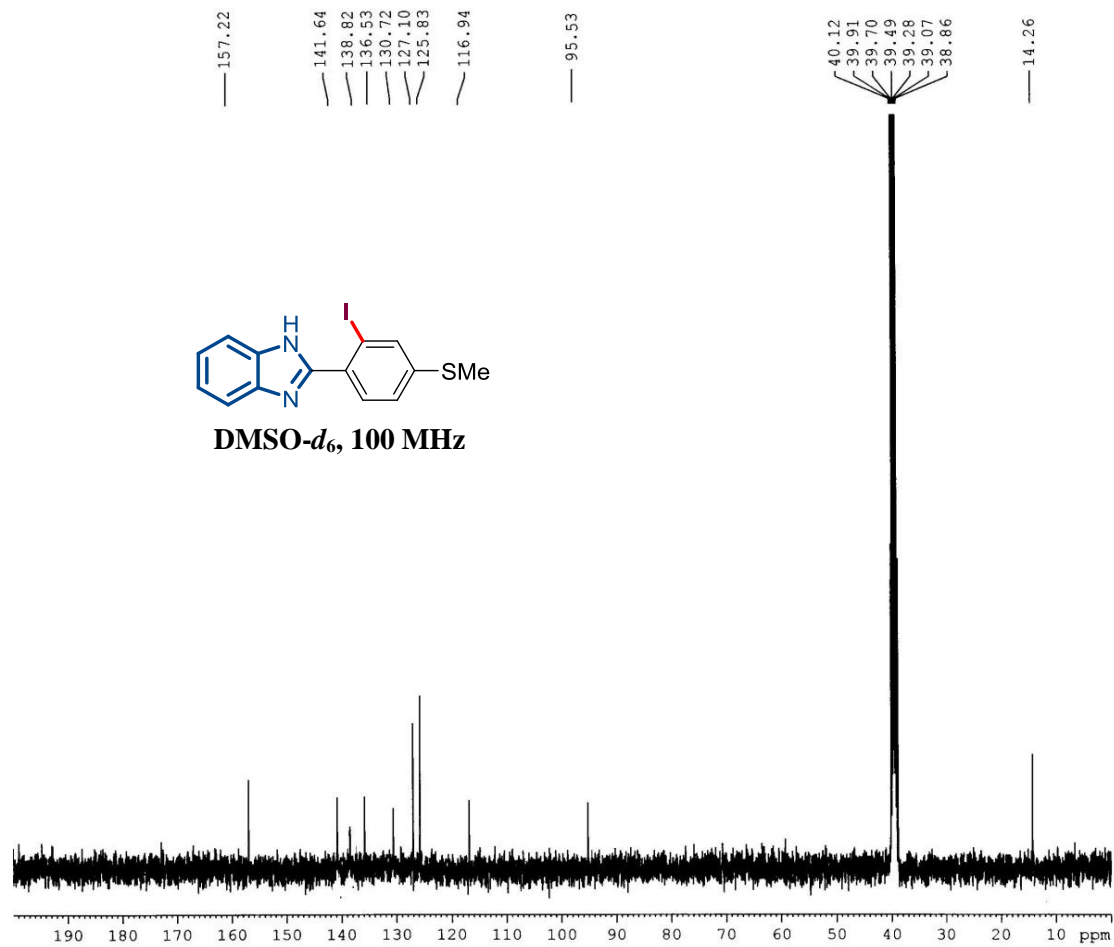
¹³C NMR of Compound 4e



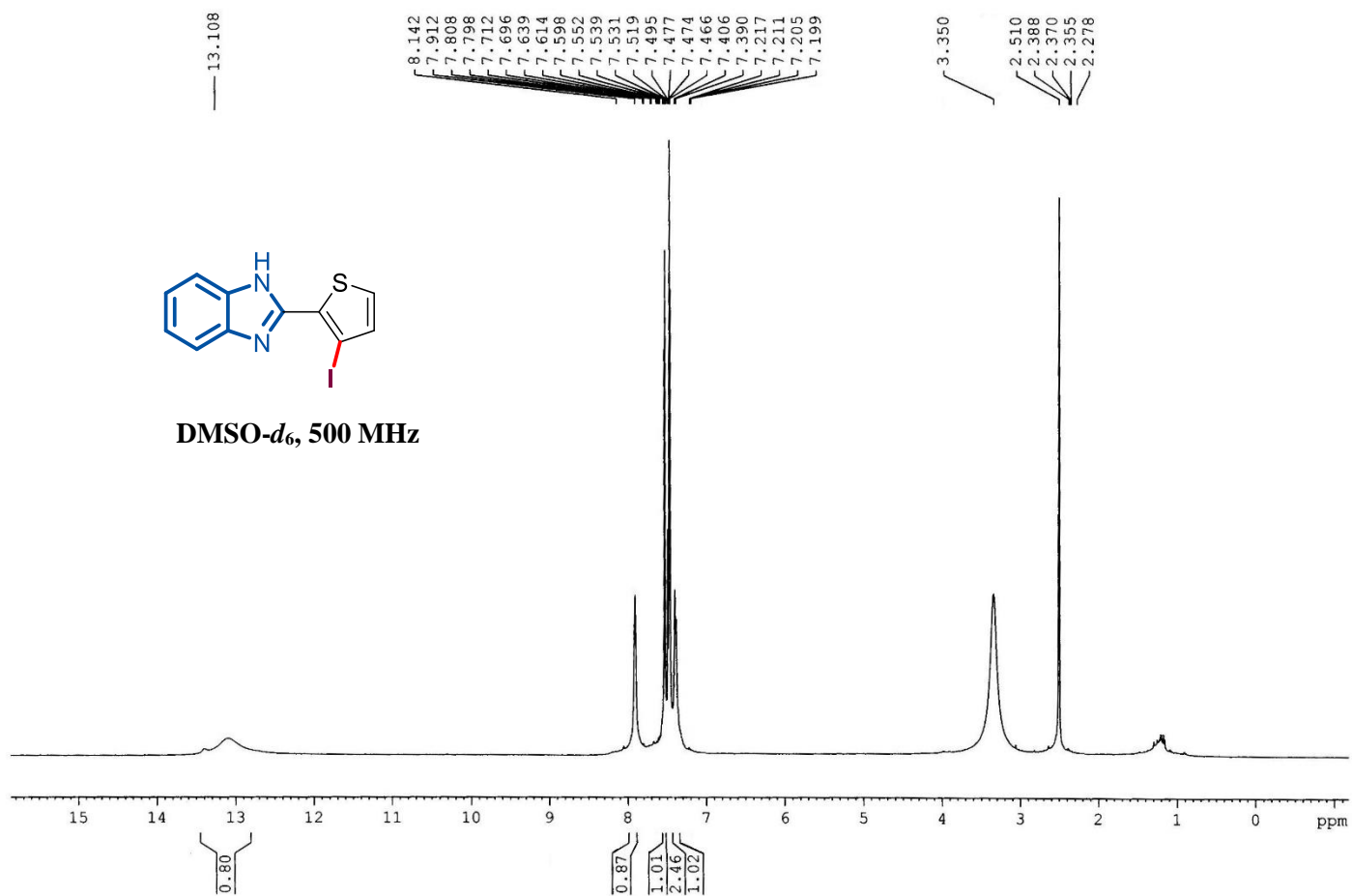
¹H NMR of Compound 4f



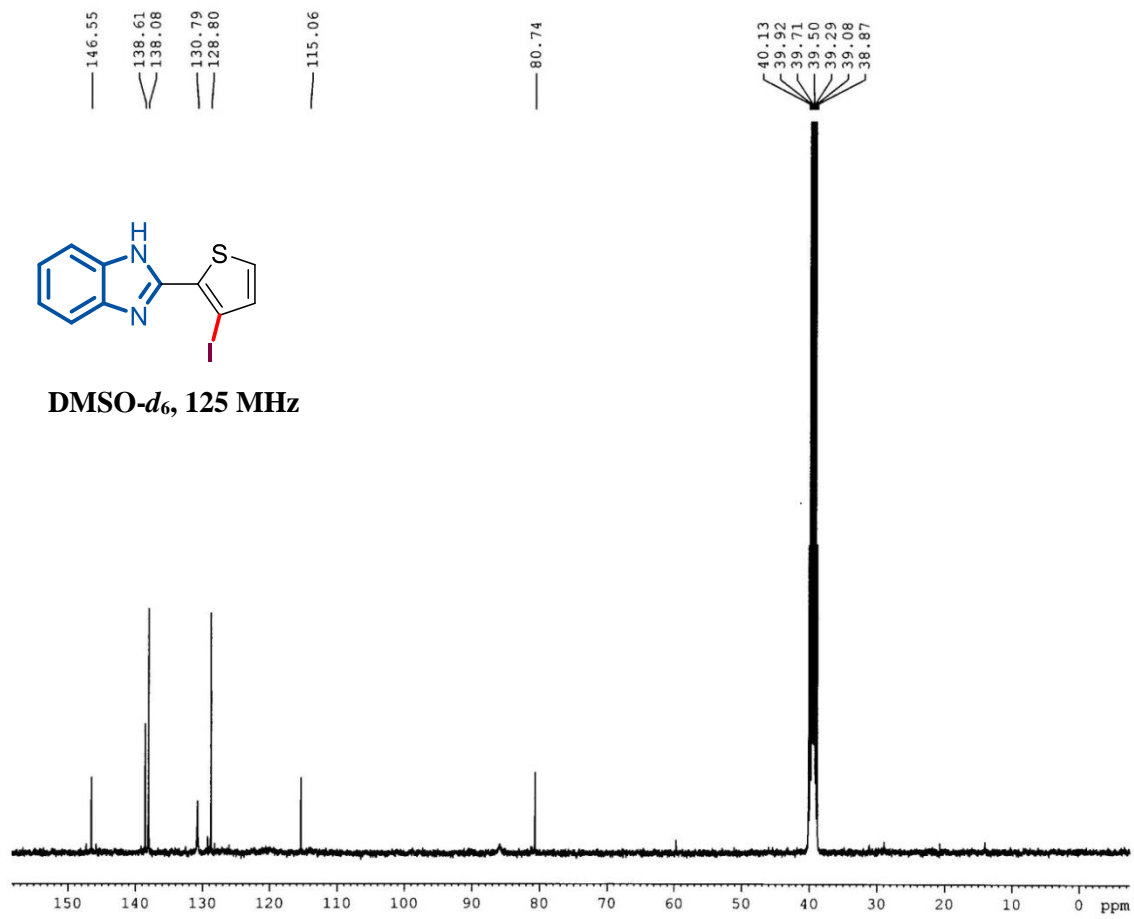
¹³C NMR of Compound 4f



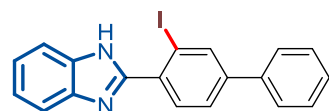
¹H NMR of Compound 4g



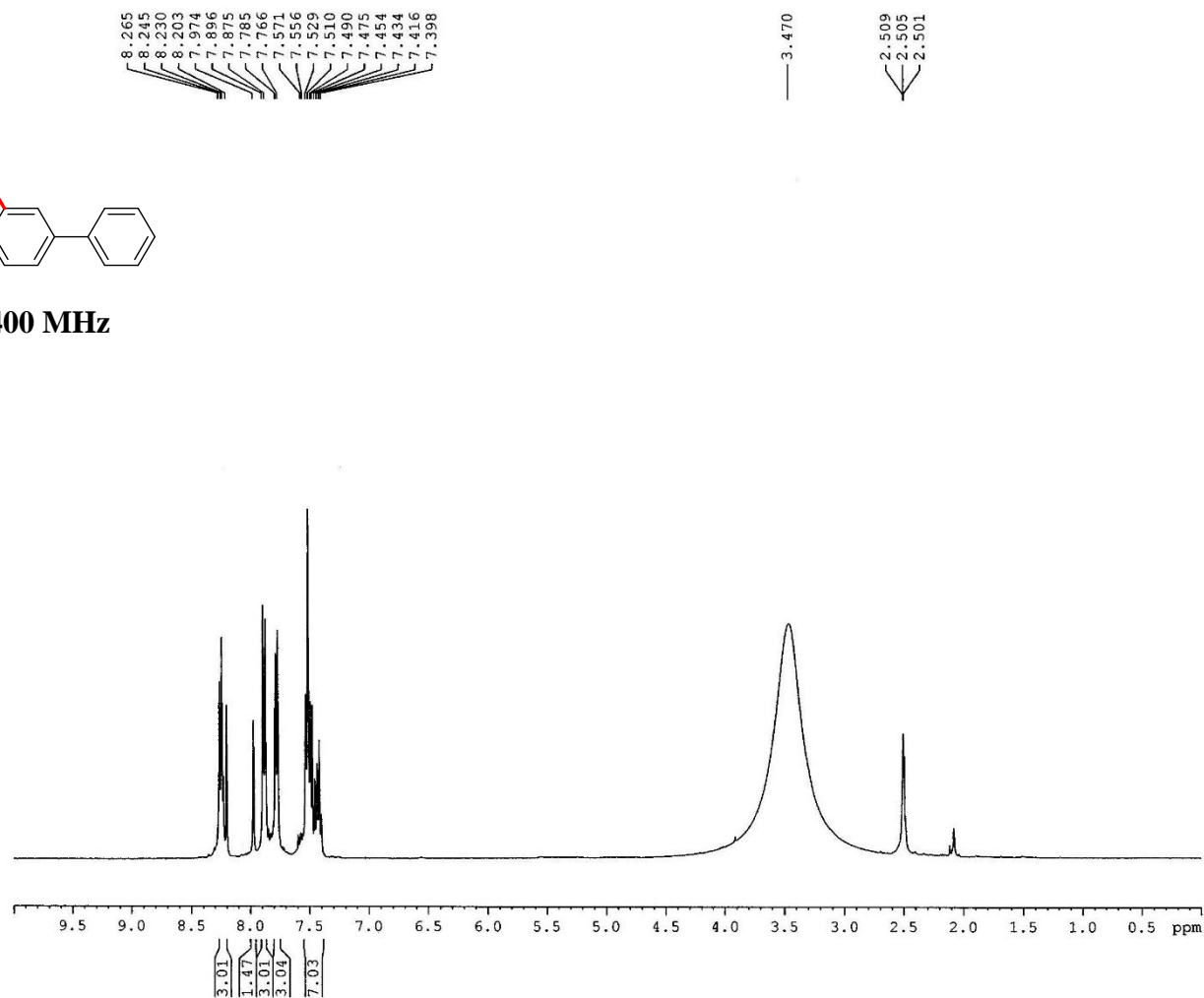
¹³C NMR of Compound 4g



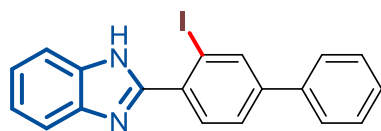
¹H NMR of Compound 4h



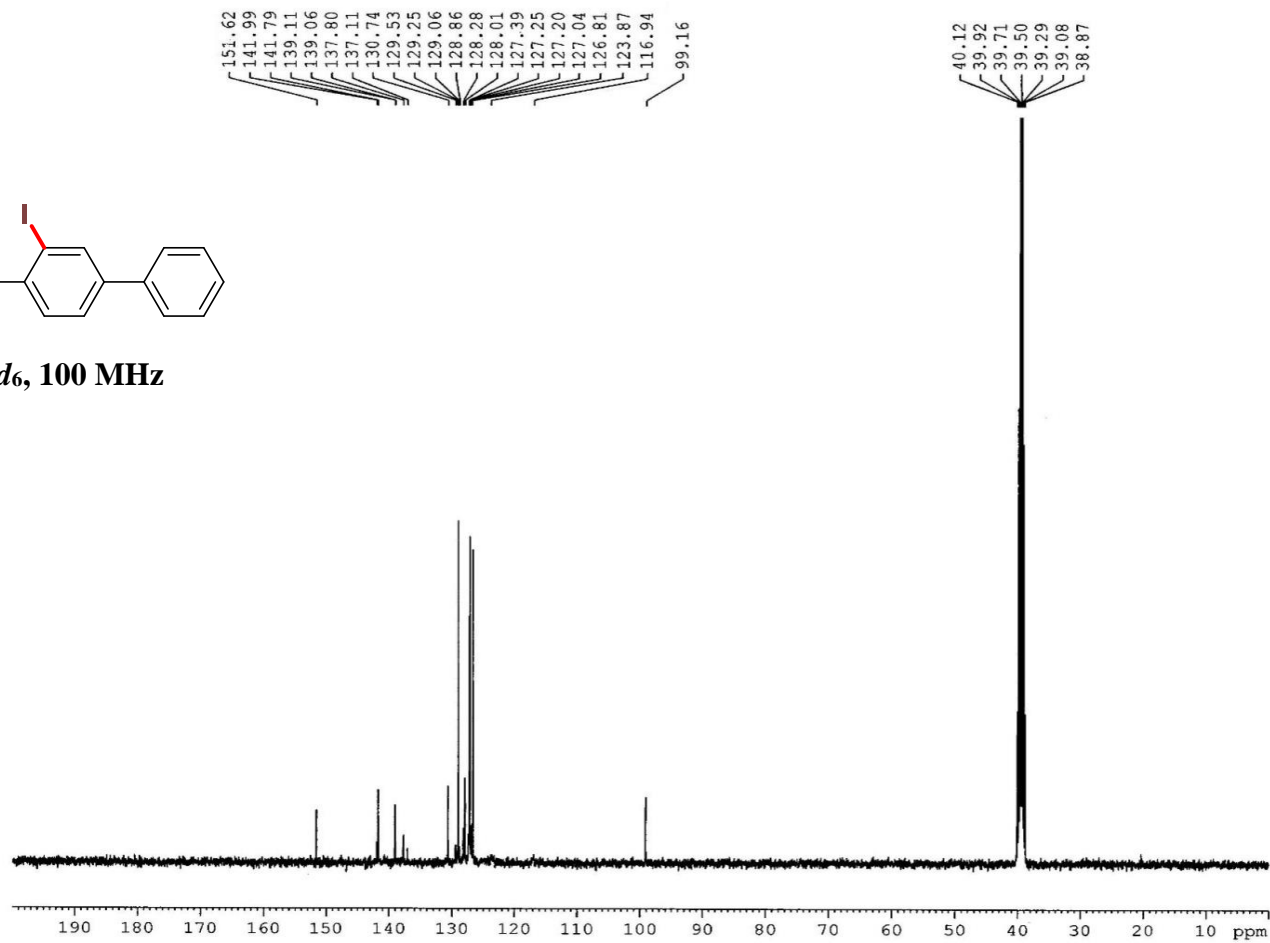
DMSO-*d*₆, 400 MHz



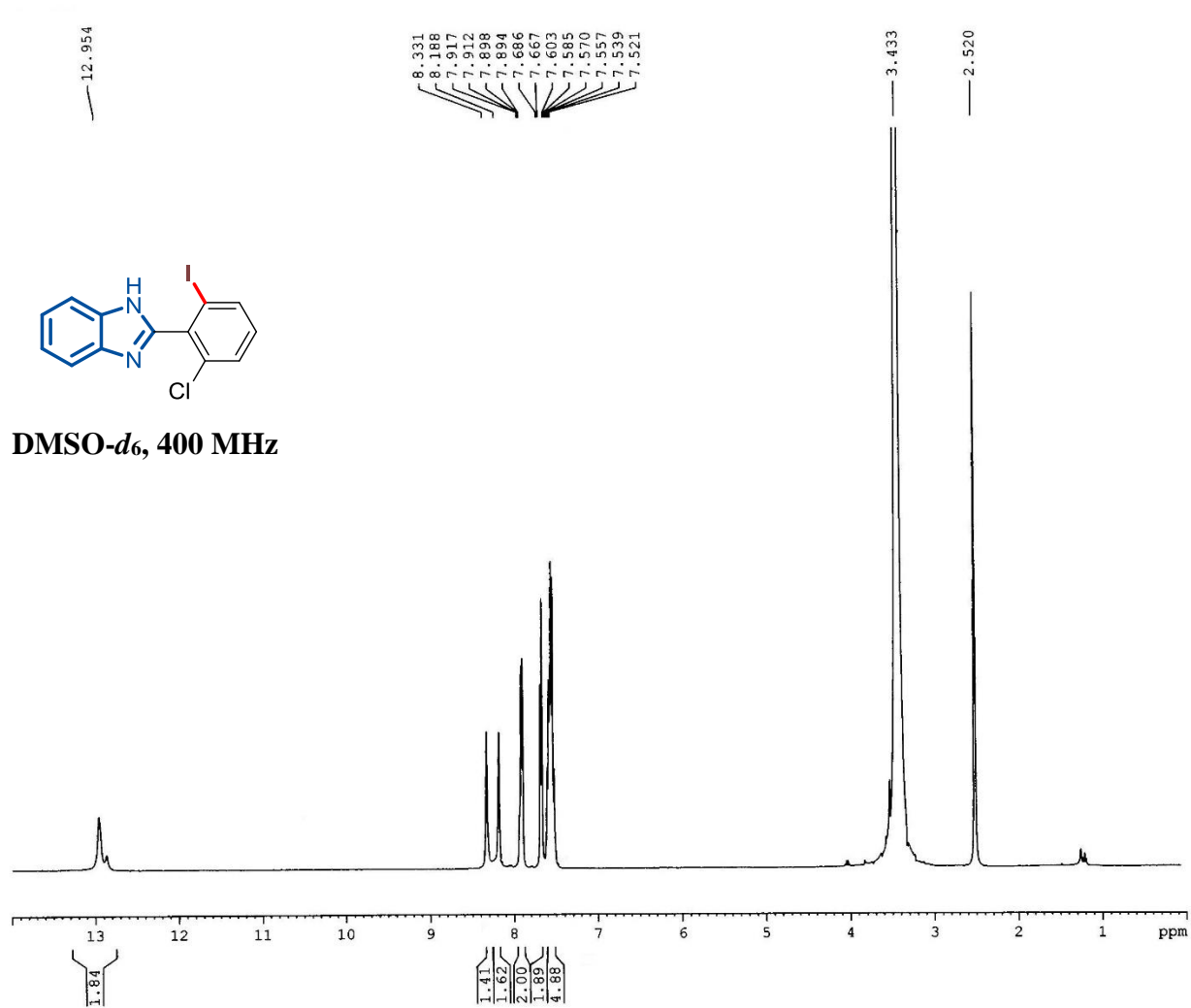
¹³C NMR of Compound 4h



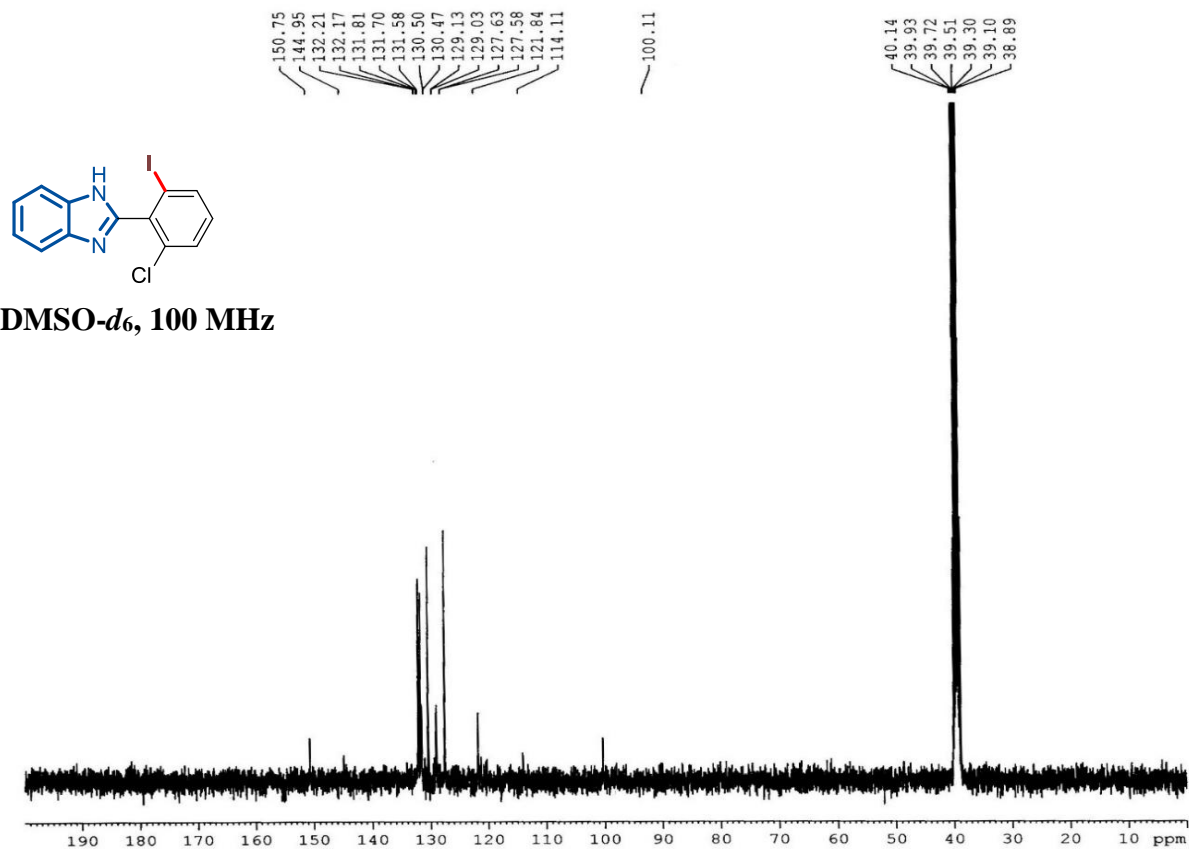
DMSO-*d*₆, 100 MHz



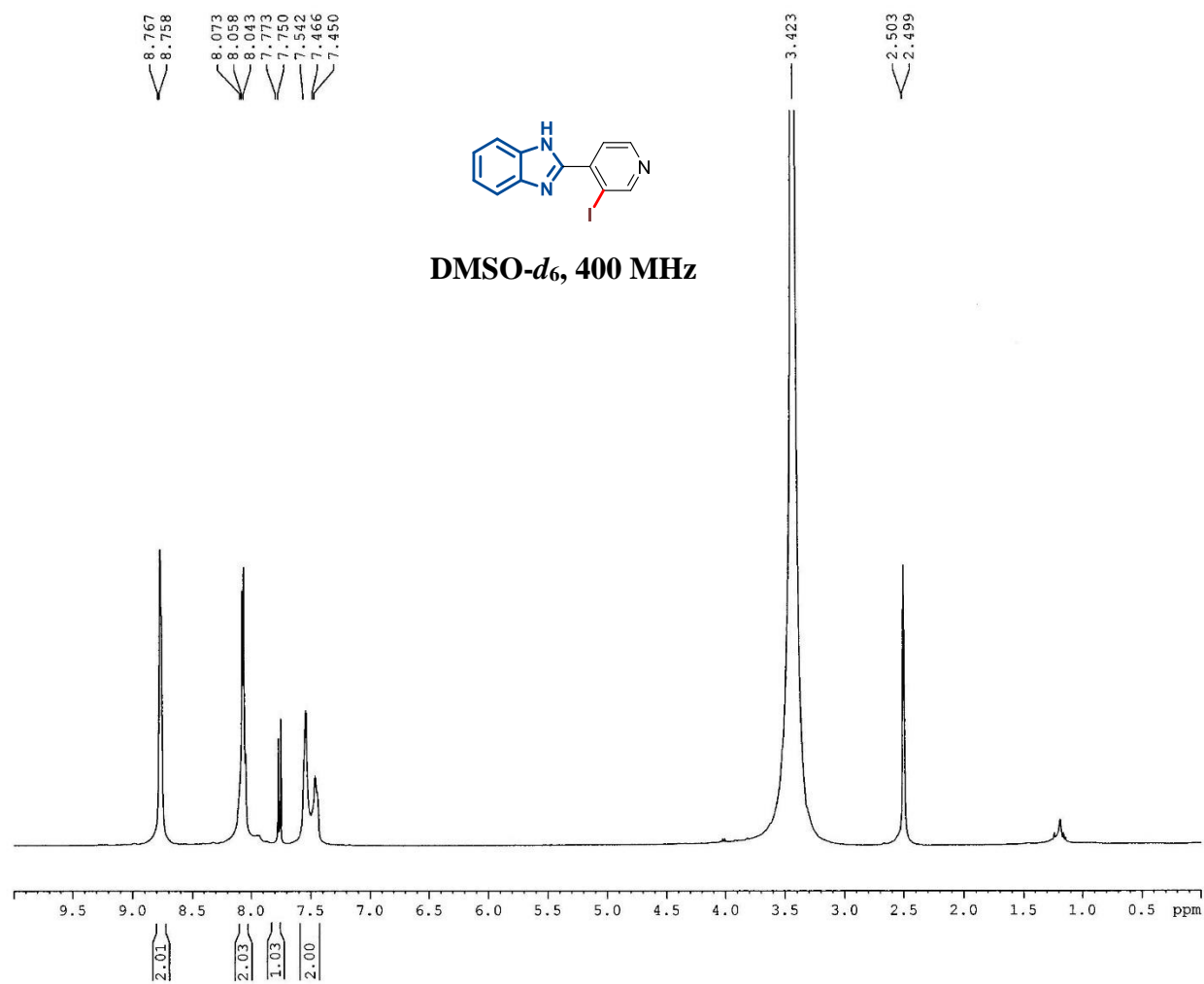
¹H NMR of Compound 4i



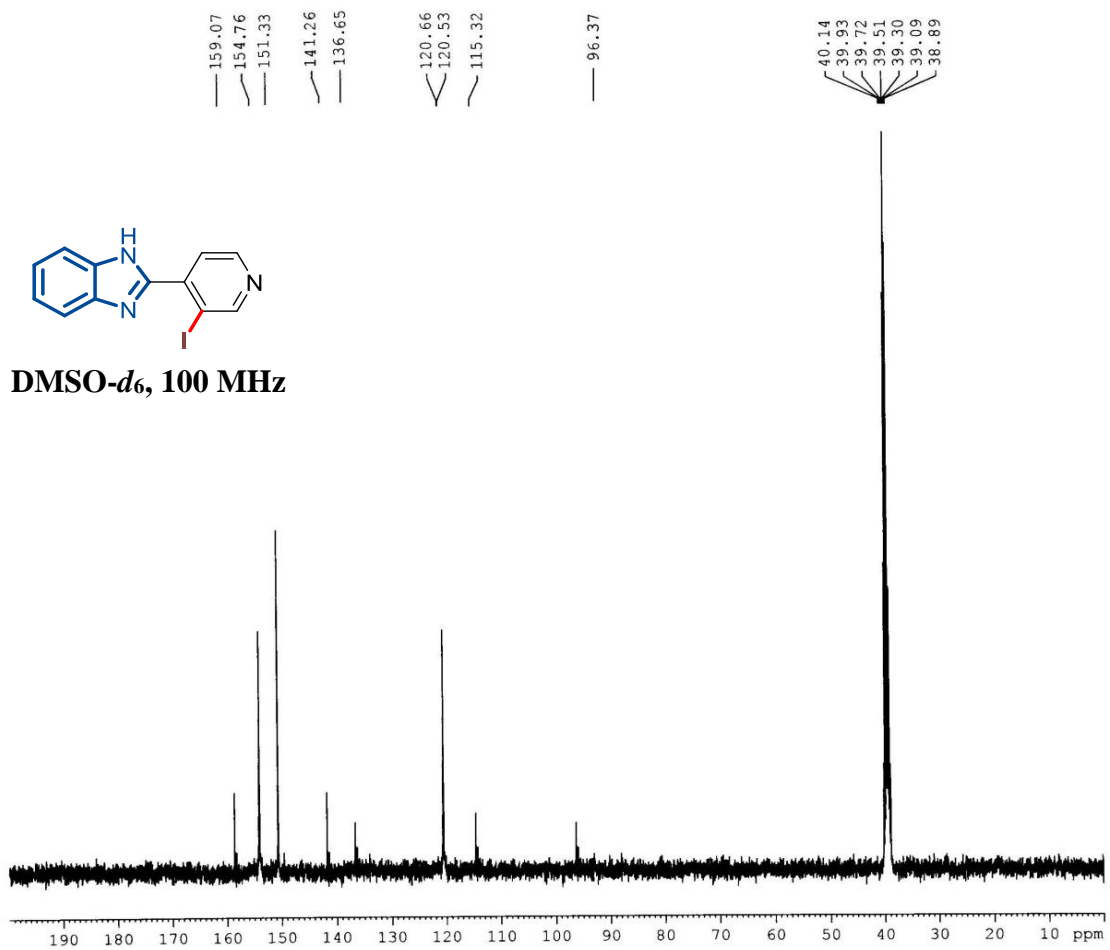
¹³C NMR of Compound 4i



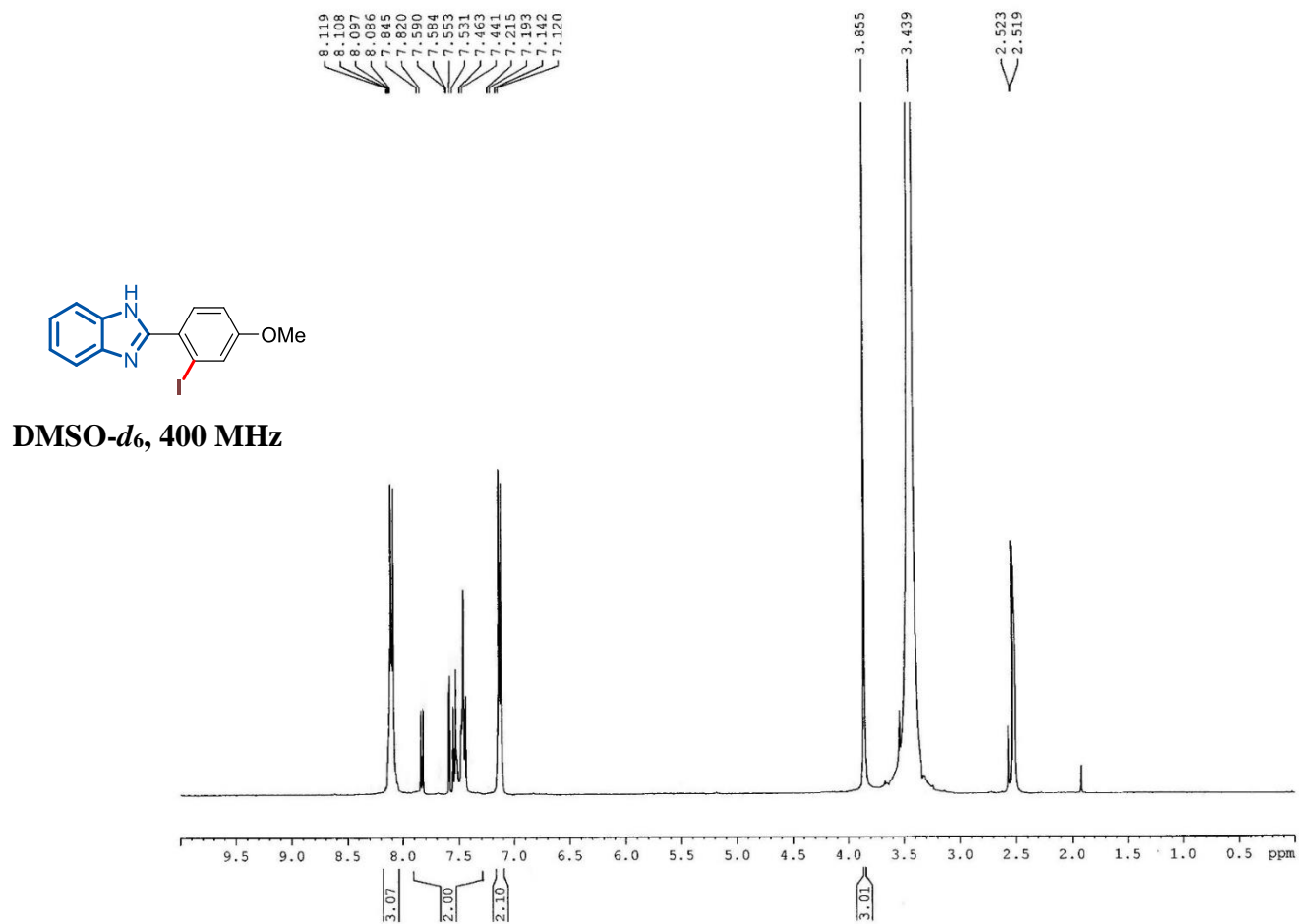
¹H NMR of Compound 4j



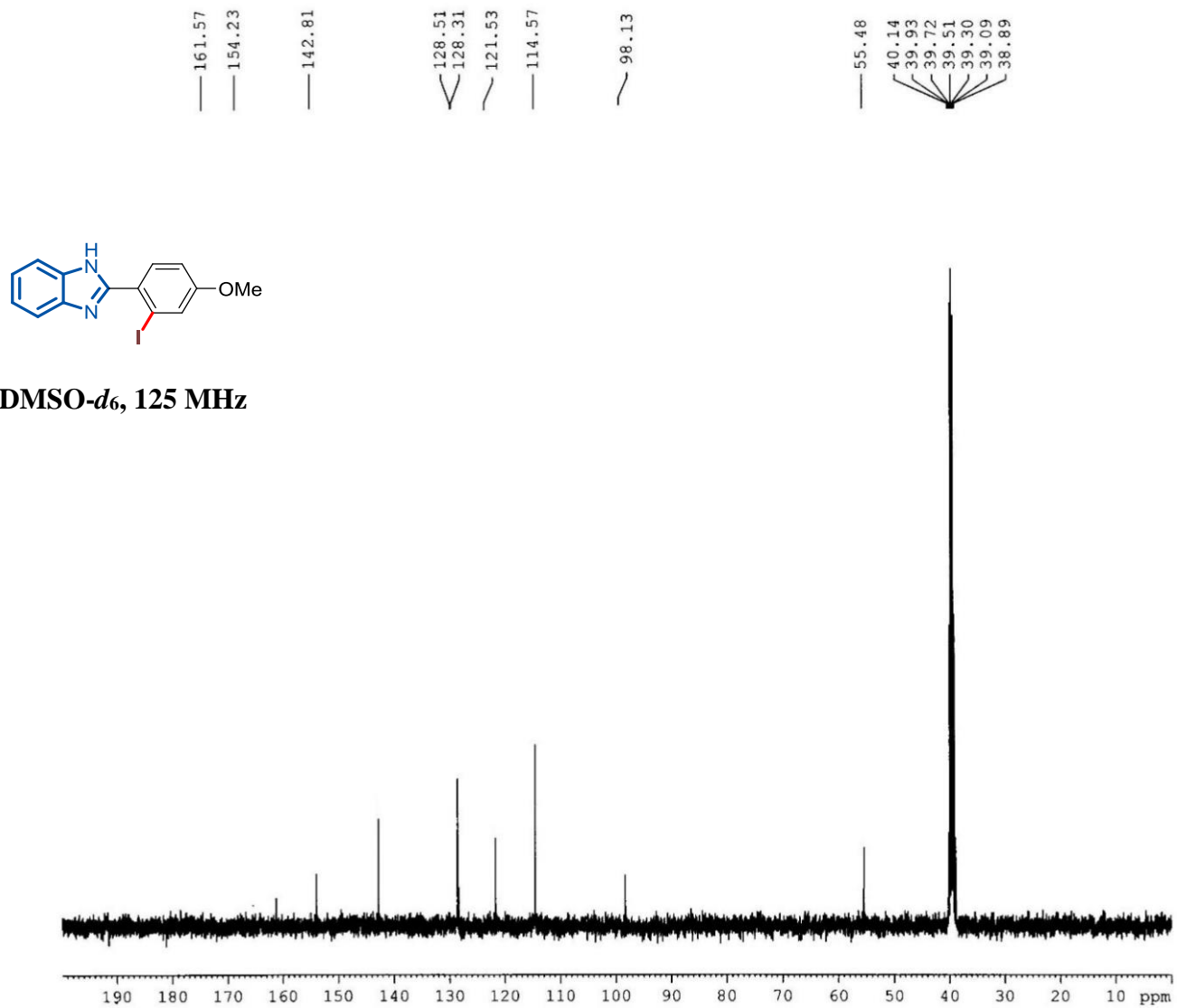
¹³C NMR of Compound 4j



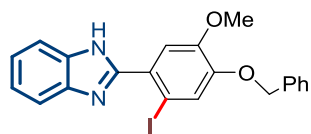
¹H NMR of Compound 4k



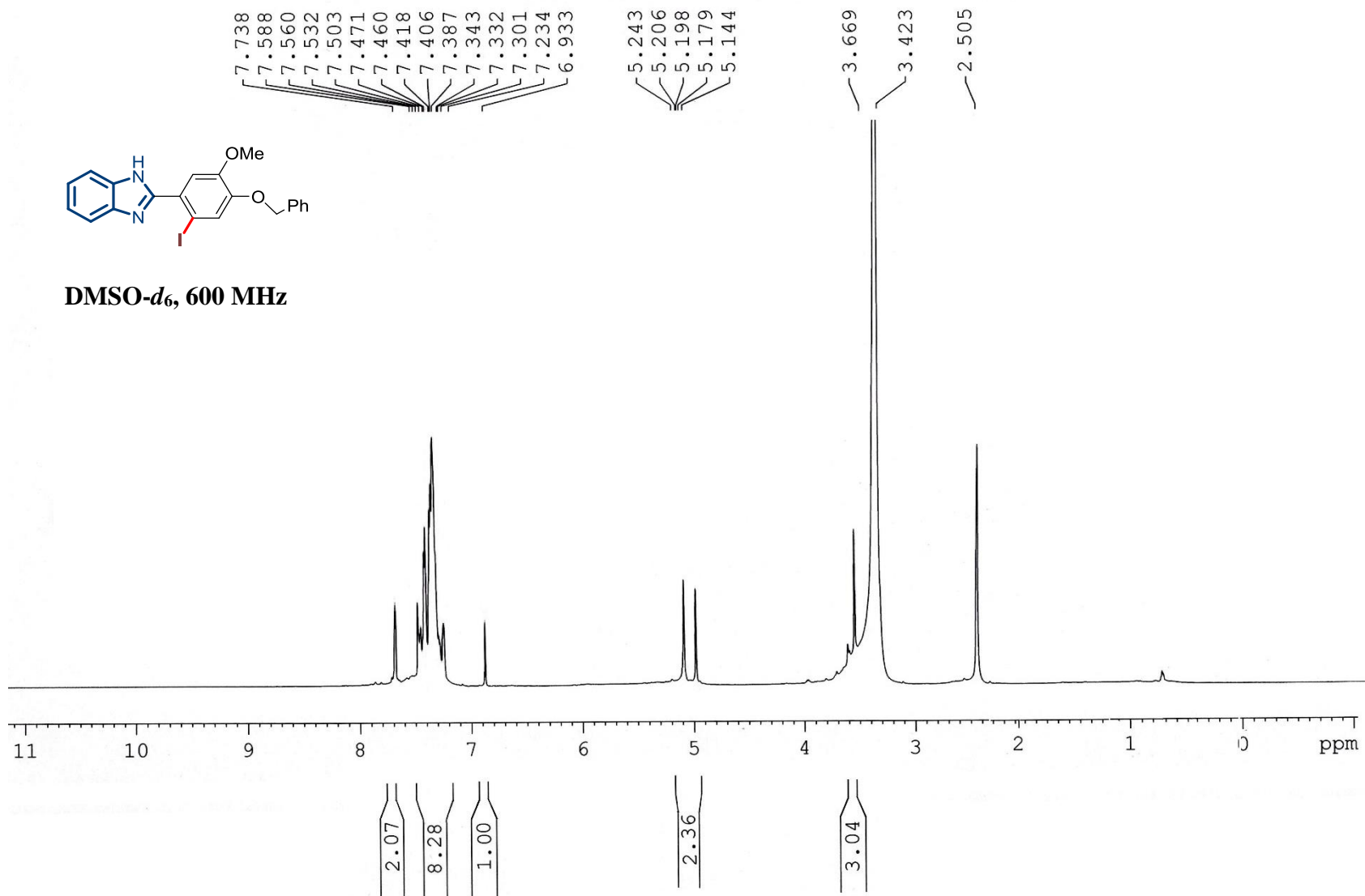
¹³C NMR of Compound 4k



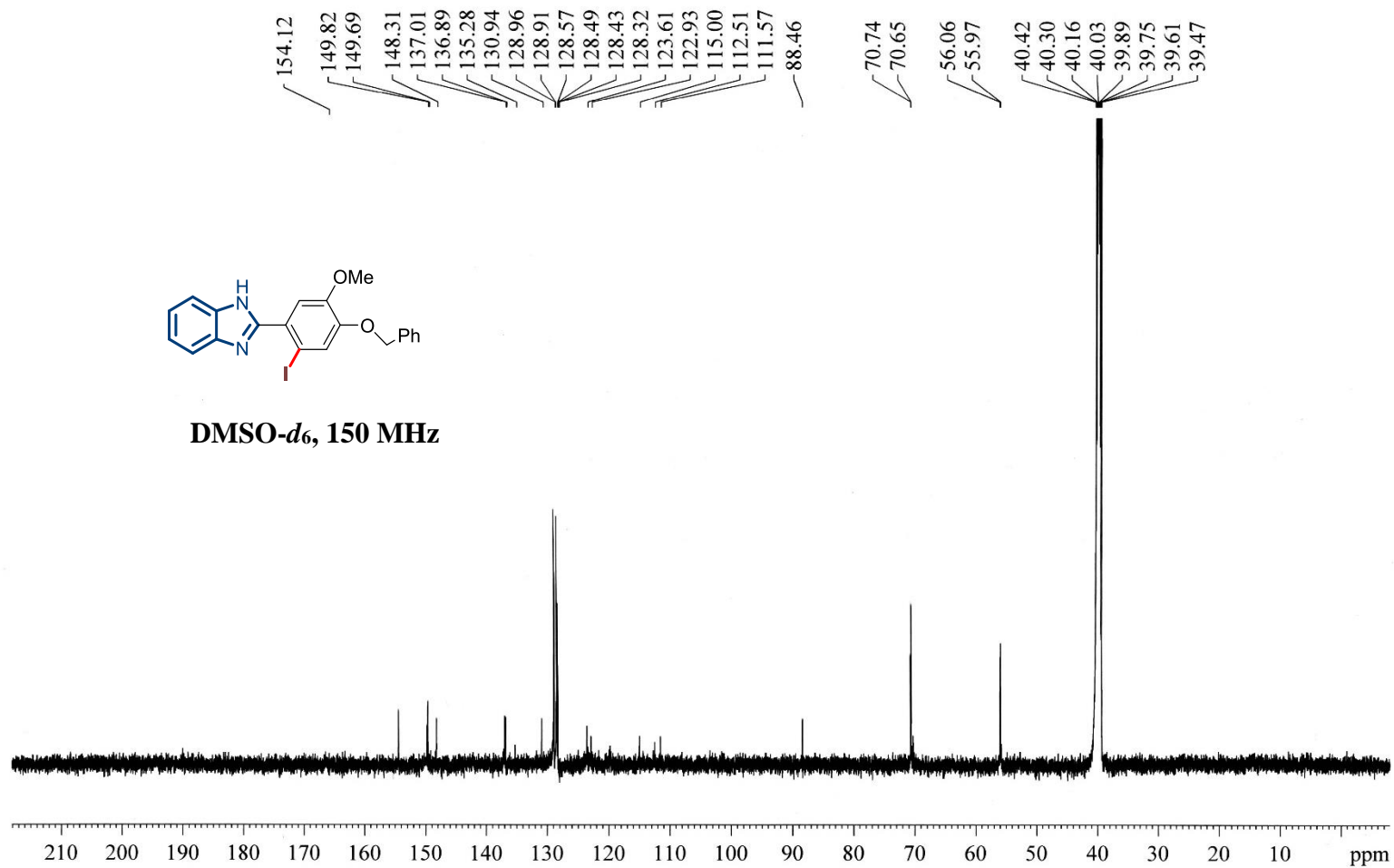
¹H NMR of Compound 4l



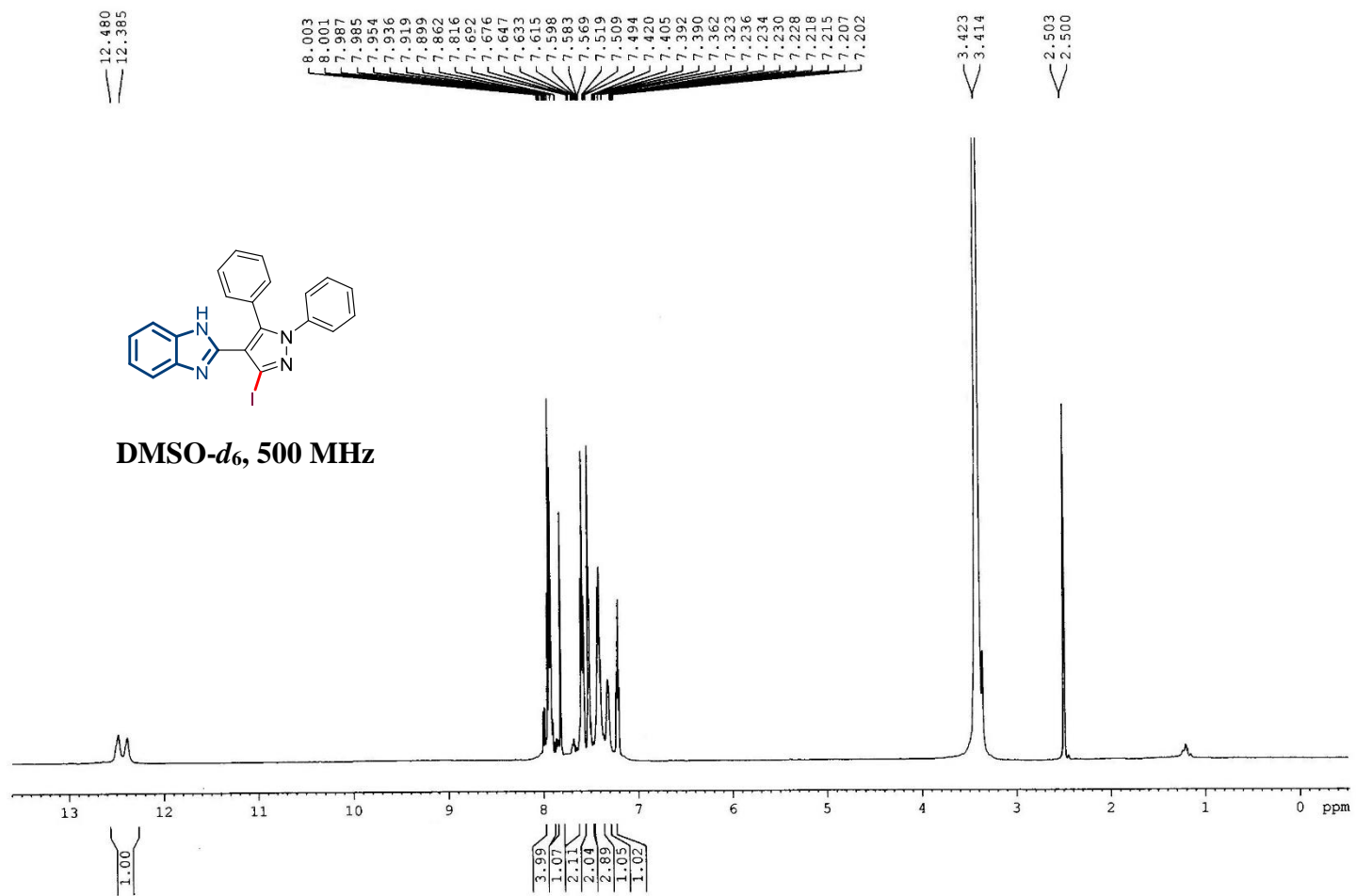
DMSO-*d*₆, 600 MHz



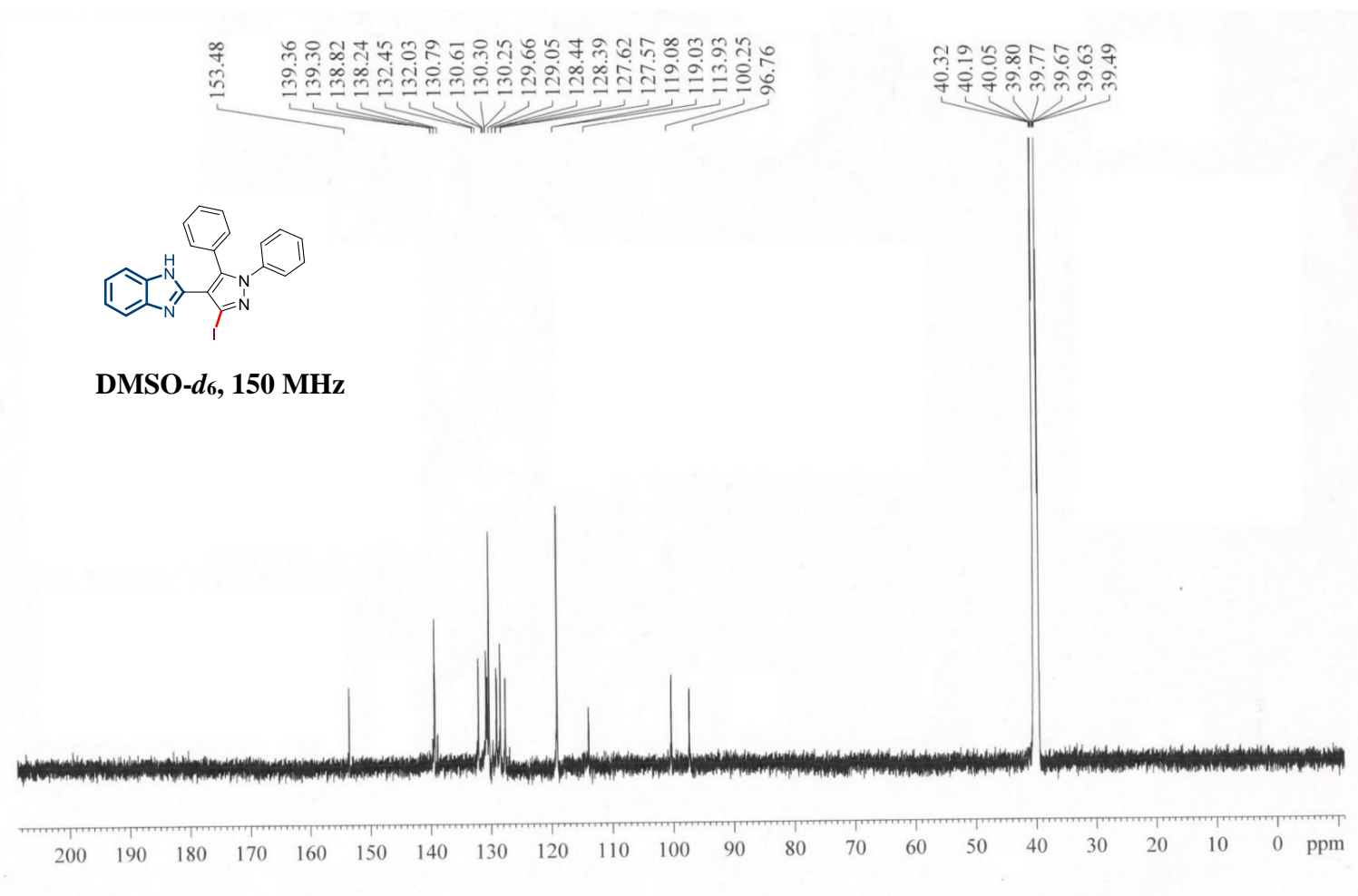
¹³C NMR of Compound 4l



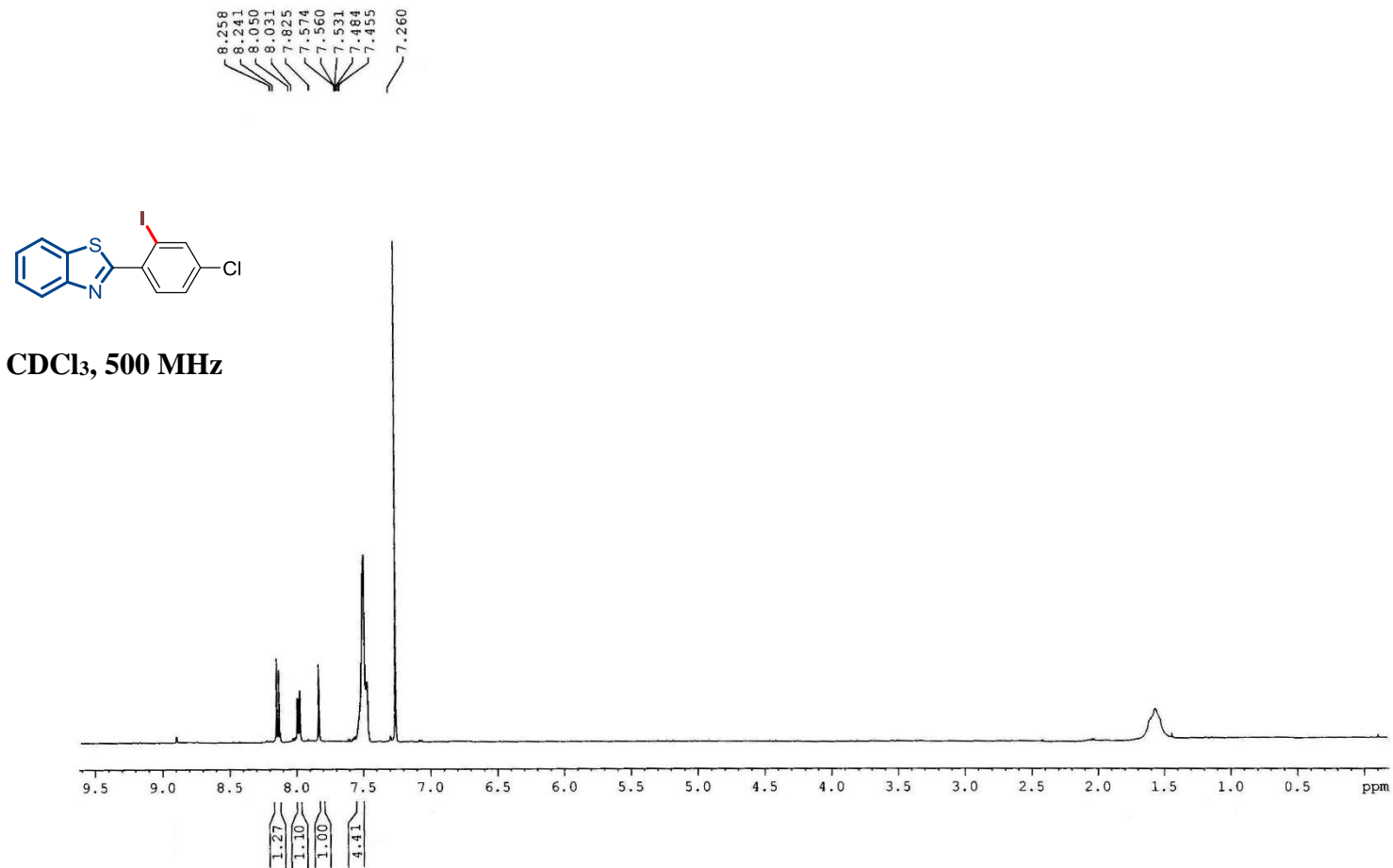
^1H NMR of Compound 4m



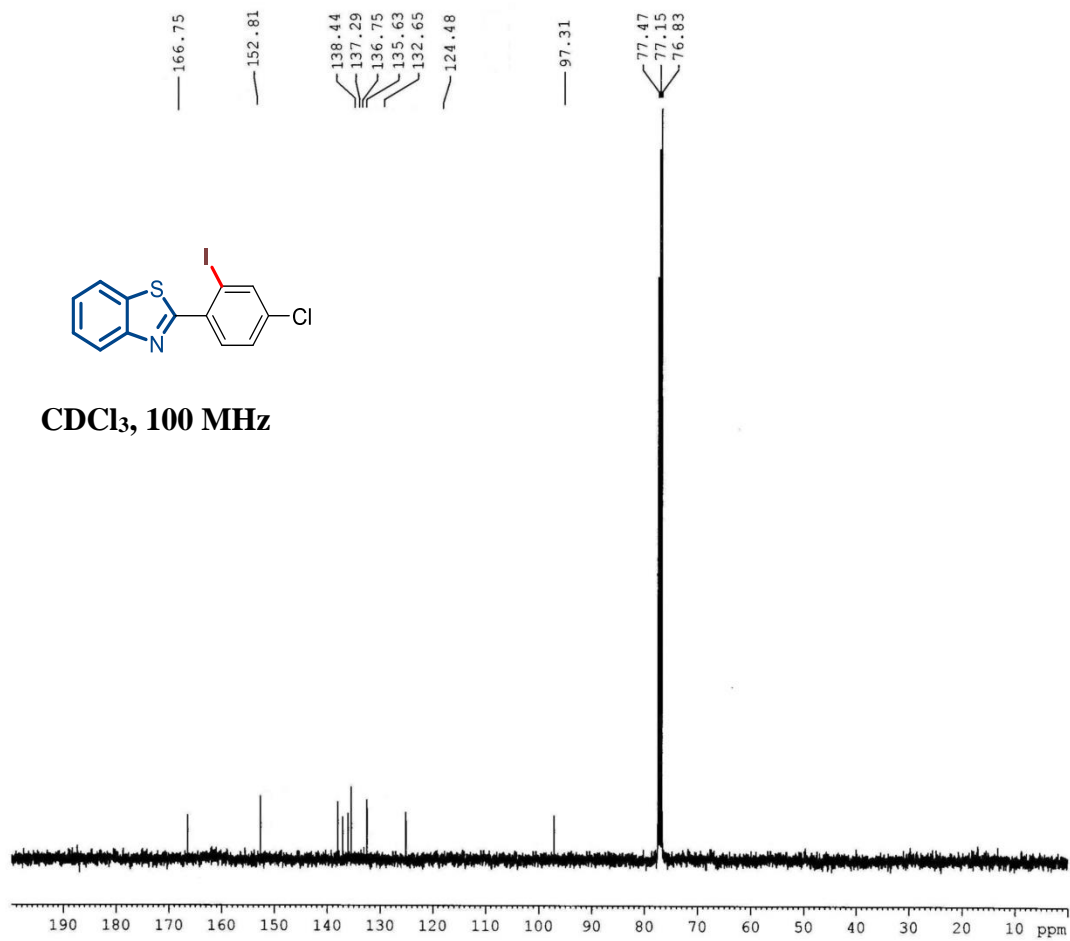
¹³C NMR of Compound 4m



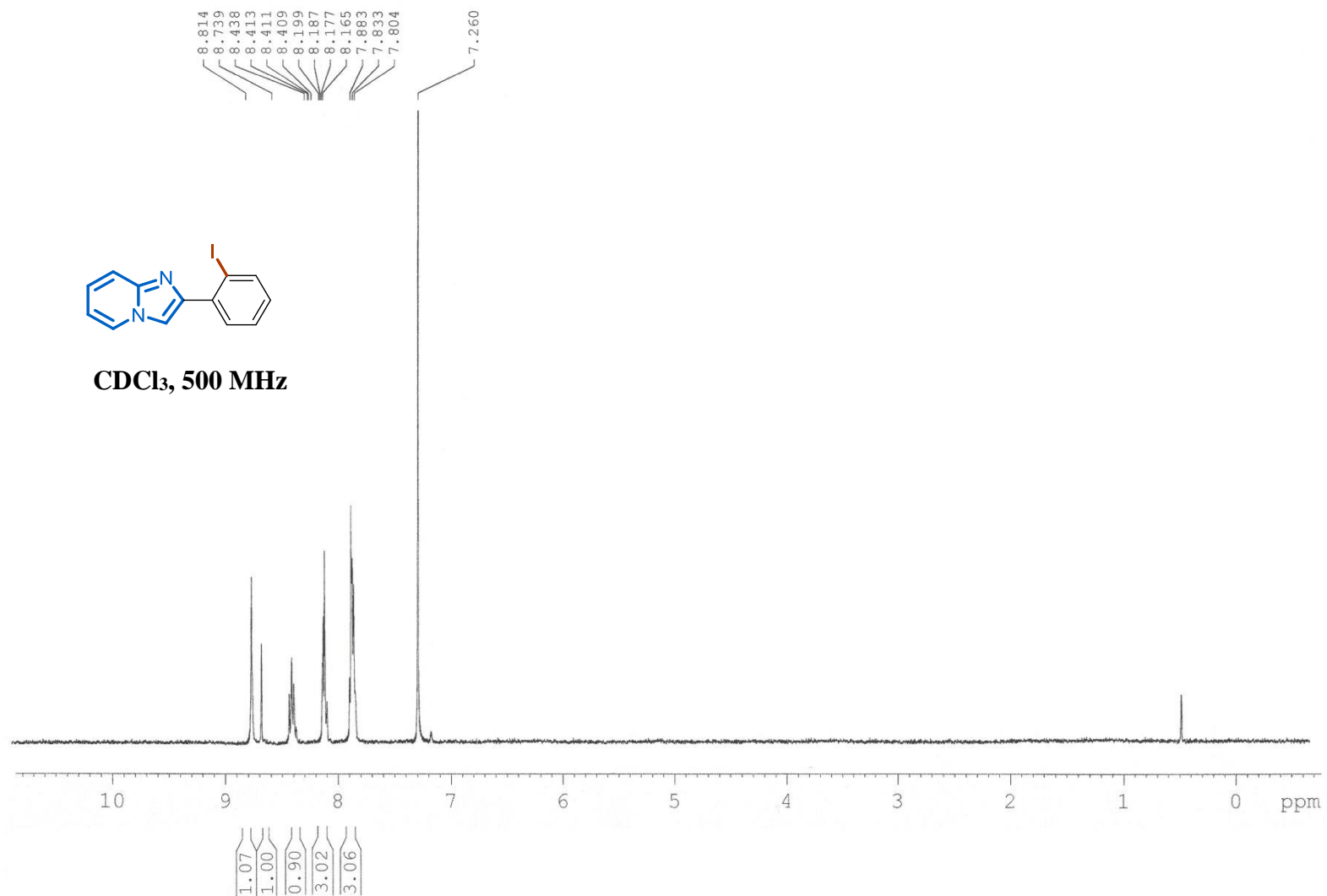
¹H NMR of Compound 4n



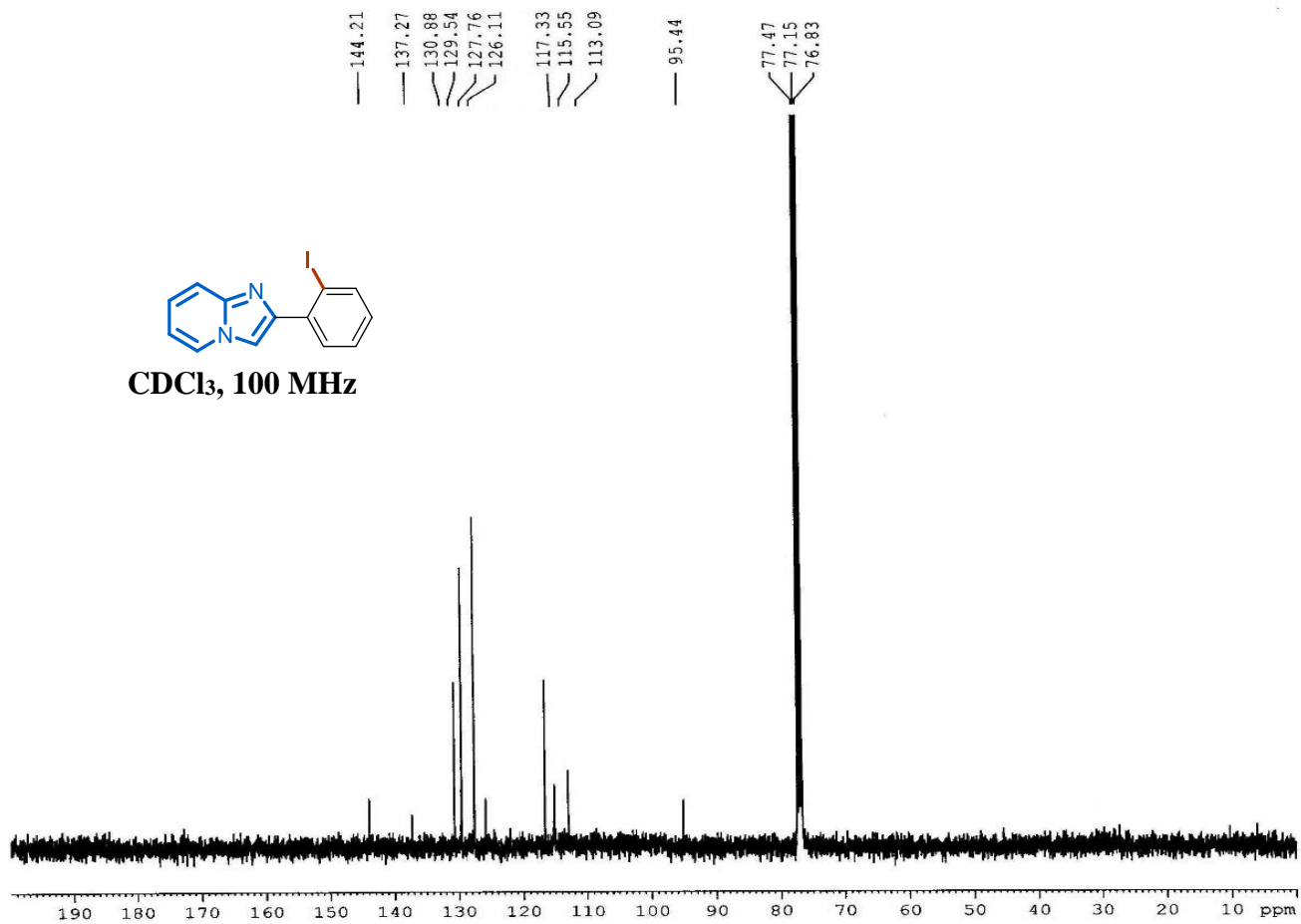
¹³C NMR of Compound 4n



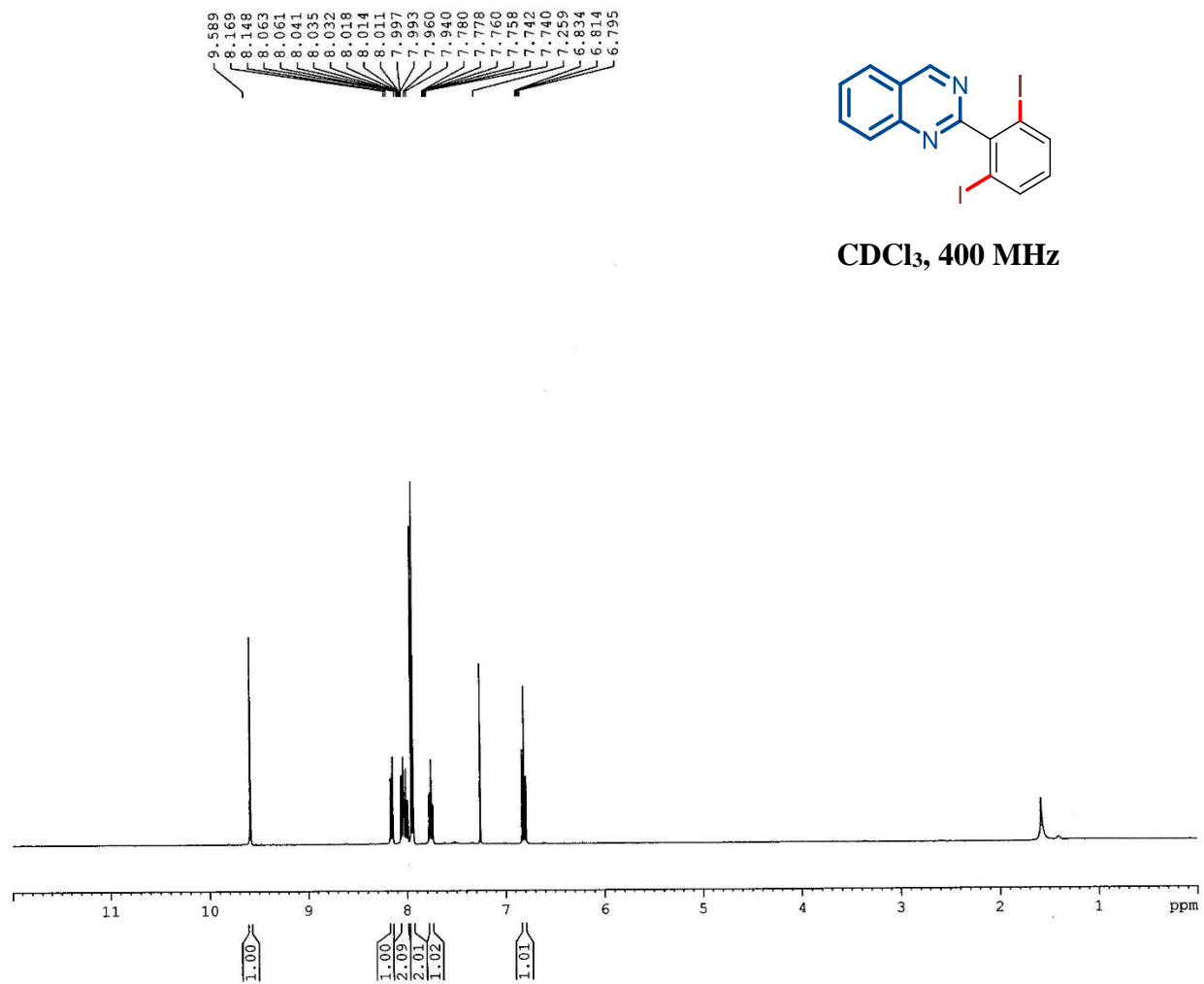
¹H NMR of Compound 4o



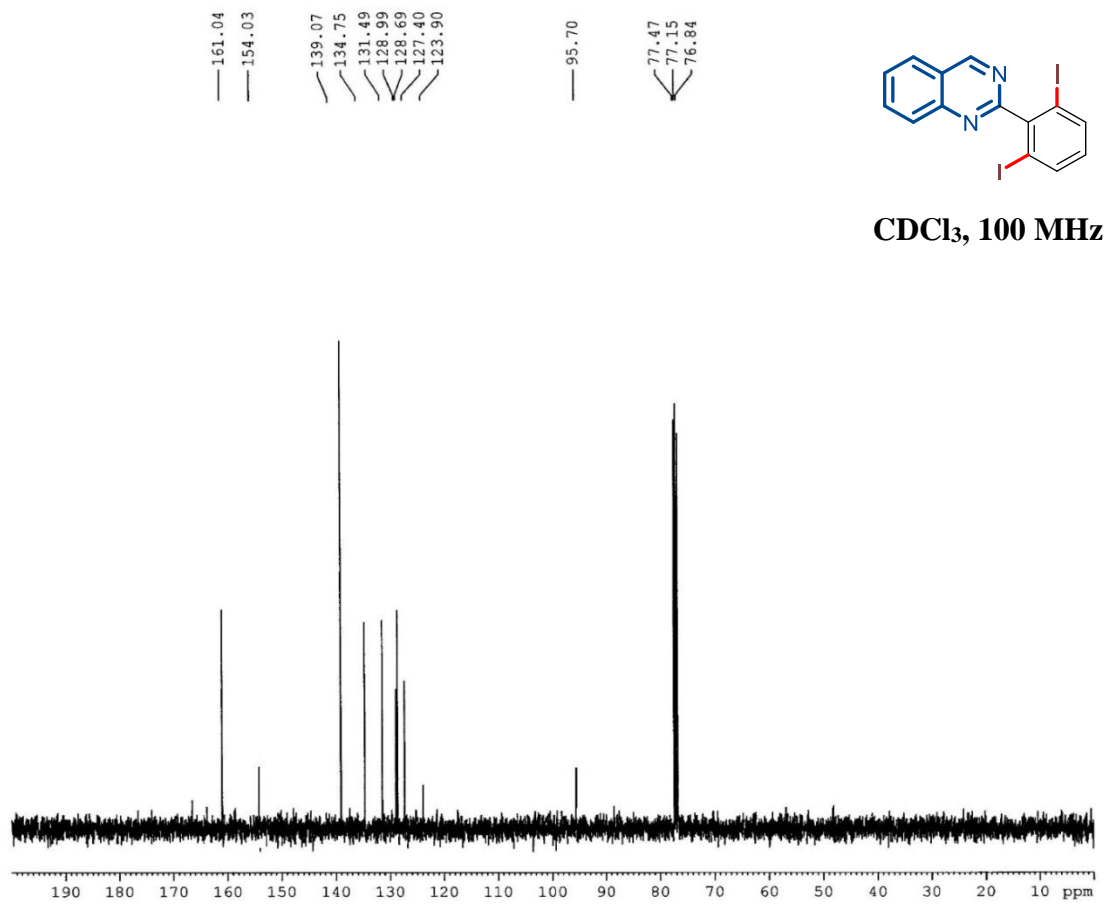
³C NMR of Compound 4o



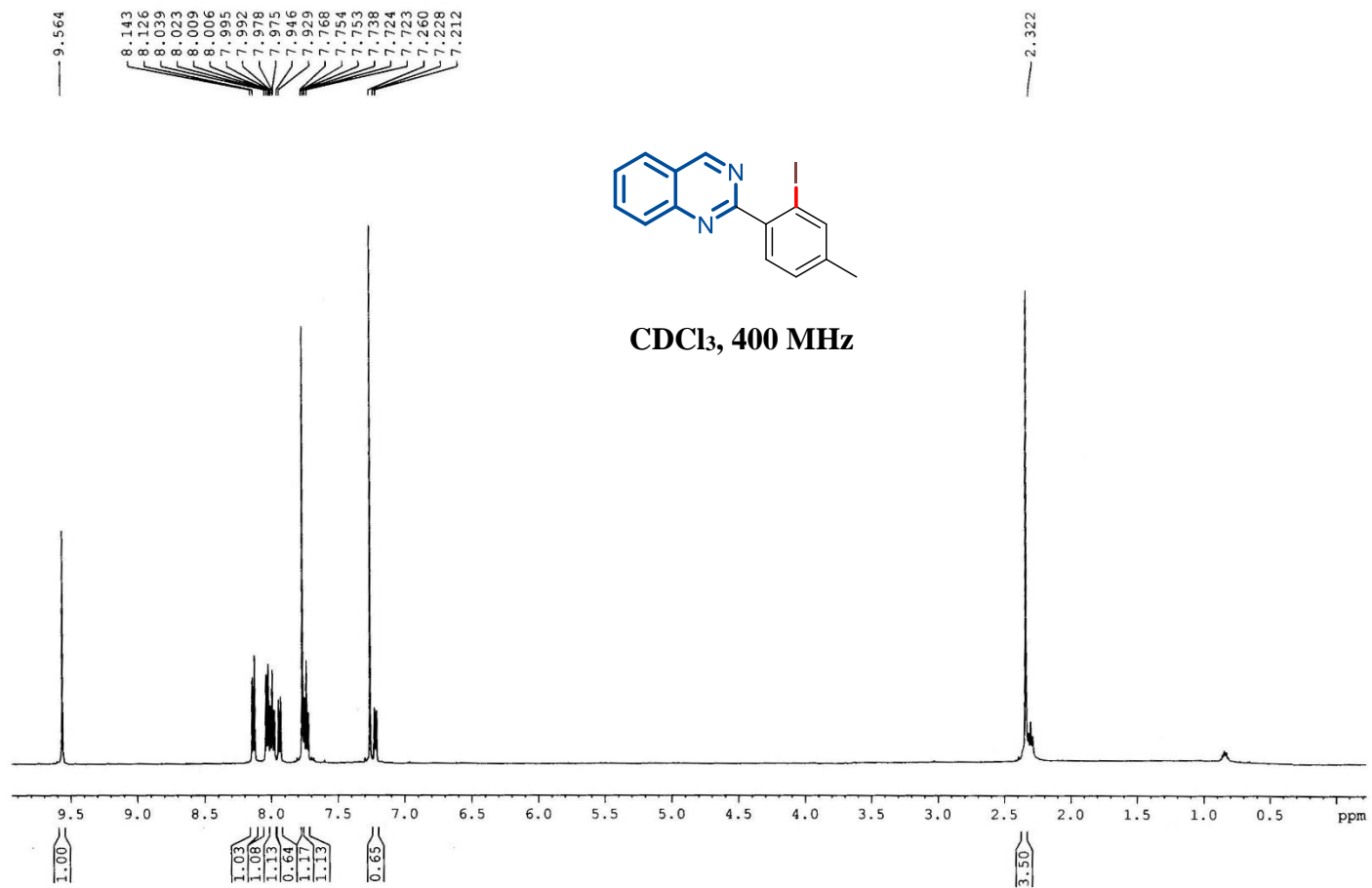
¹H NMR of Compound 4p



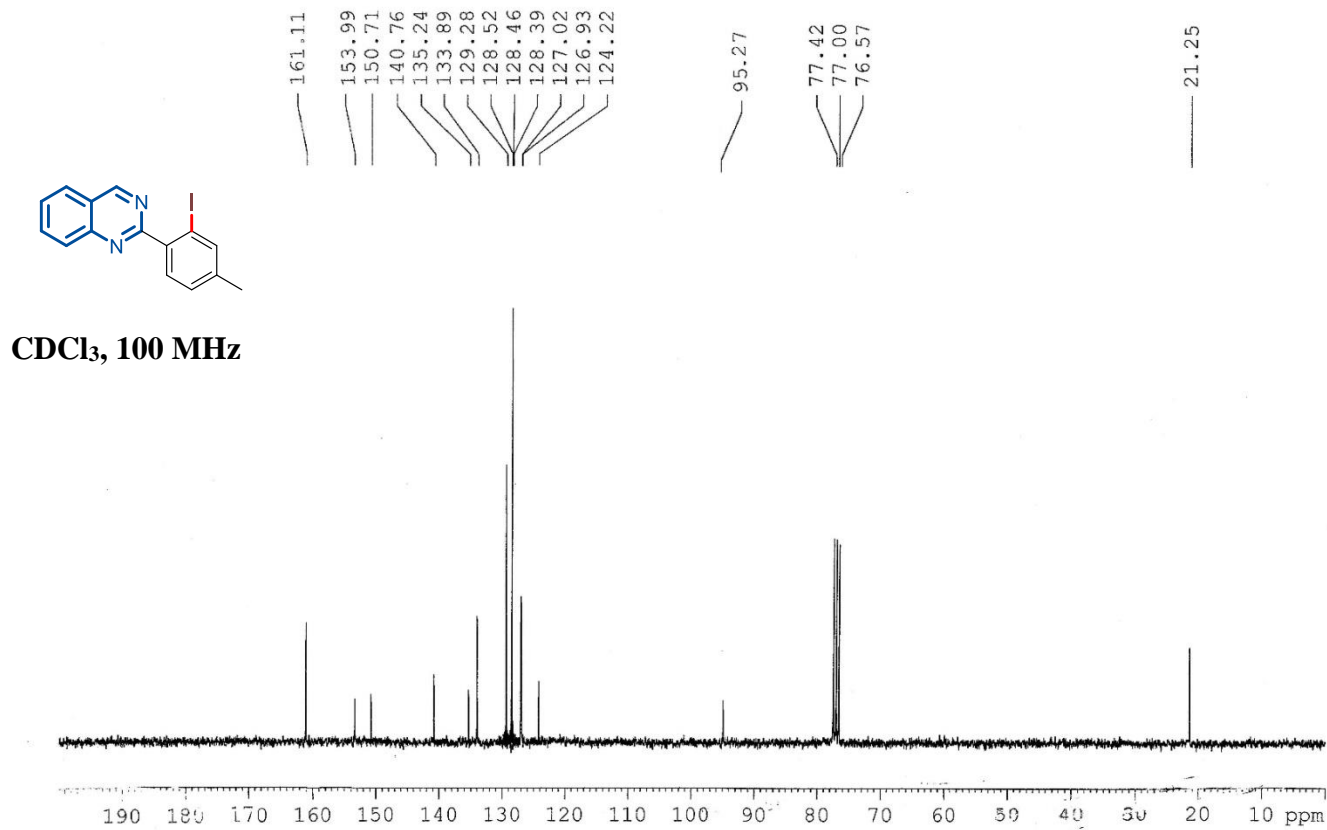
¹³C NMR of Compound 4p



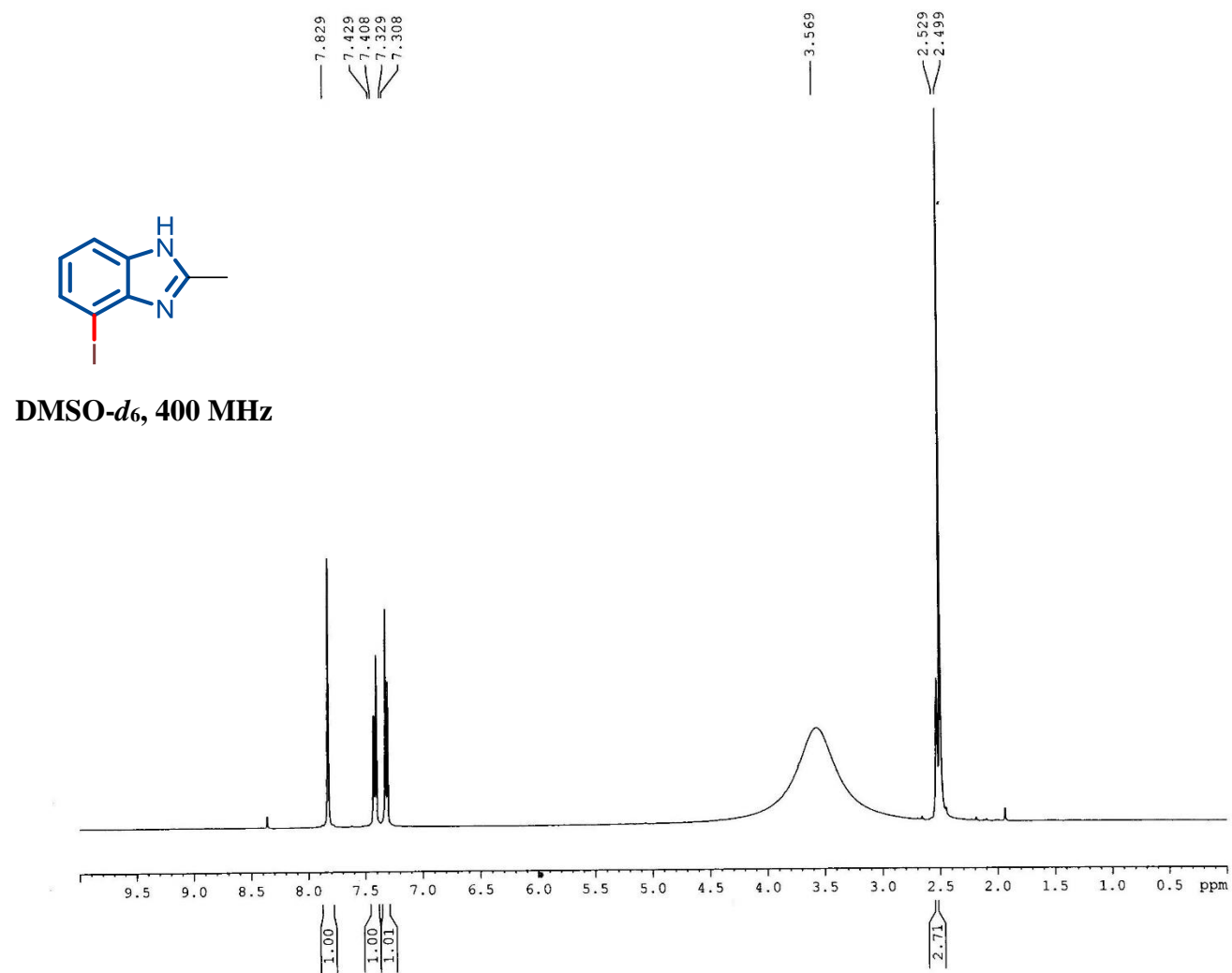
¹H NMR of Compound 4q



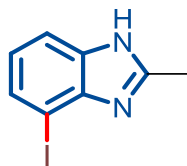
¹³C NMR of Compound 4q



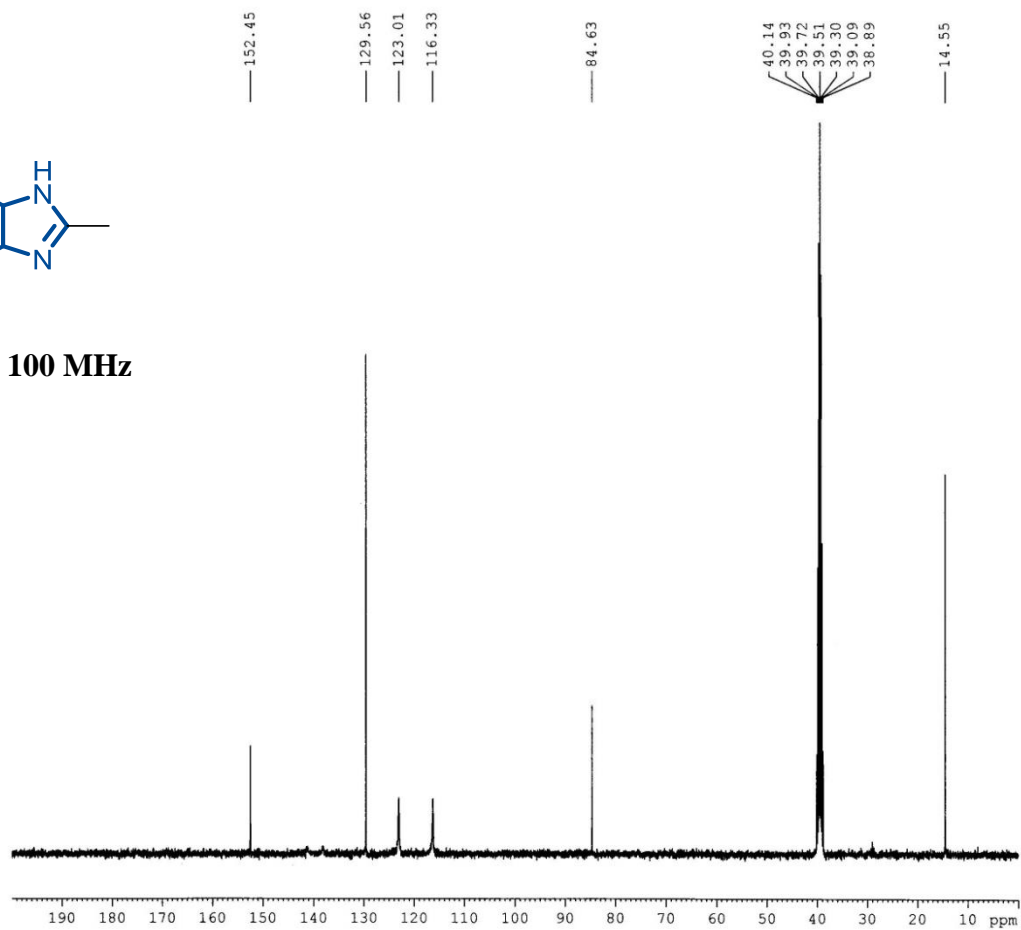
¹H NMR of Compound 4r



^{13}C NMR of Compound 4r

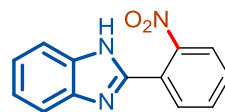


DMSO-*d*₆, 100 MHz

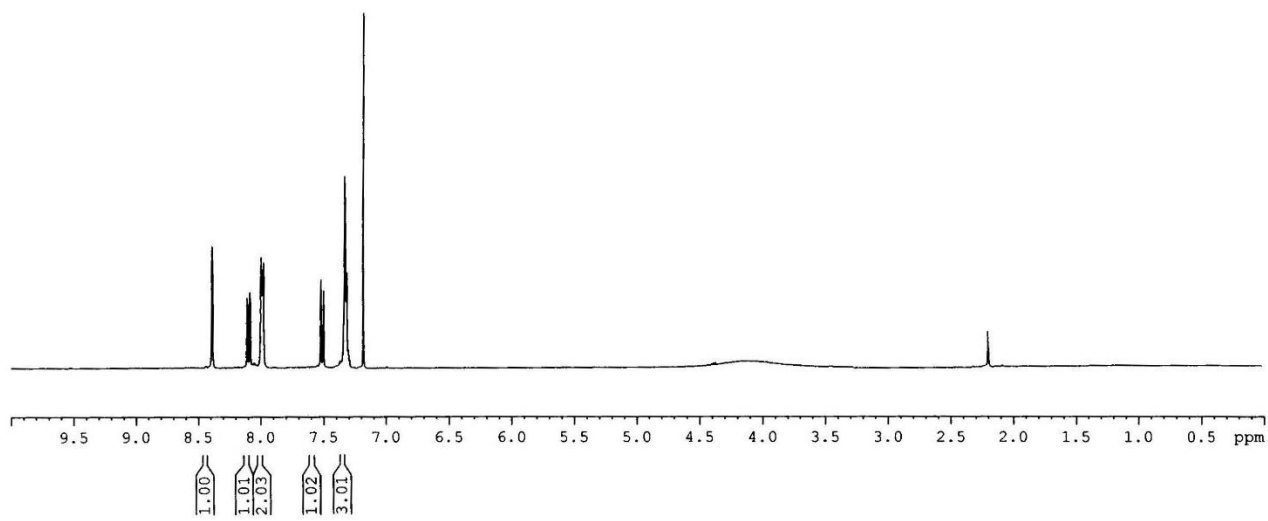


¹H NMR of Compound 5a

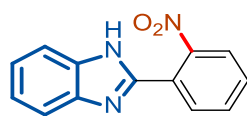
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8.160
8.149
8.142
8.064
8.058
8.043
8.039
7.536
7.511
7.363
7.359
7.353
7.347
7.233



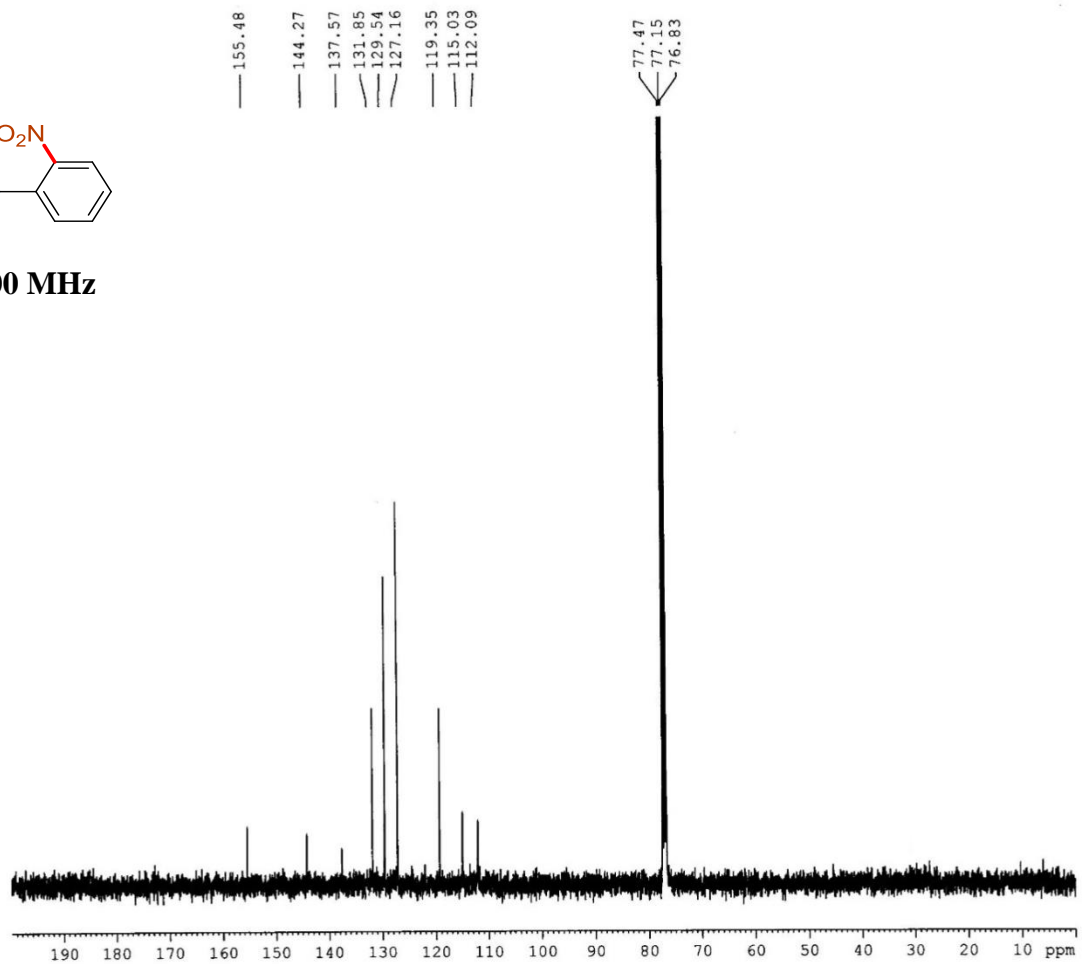
CDCl₃, 400 MHz



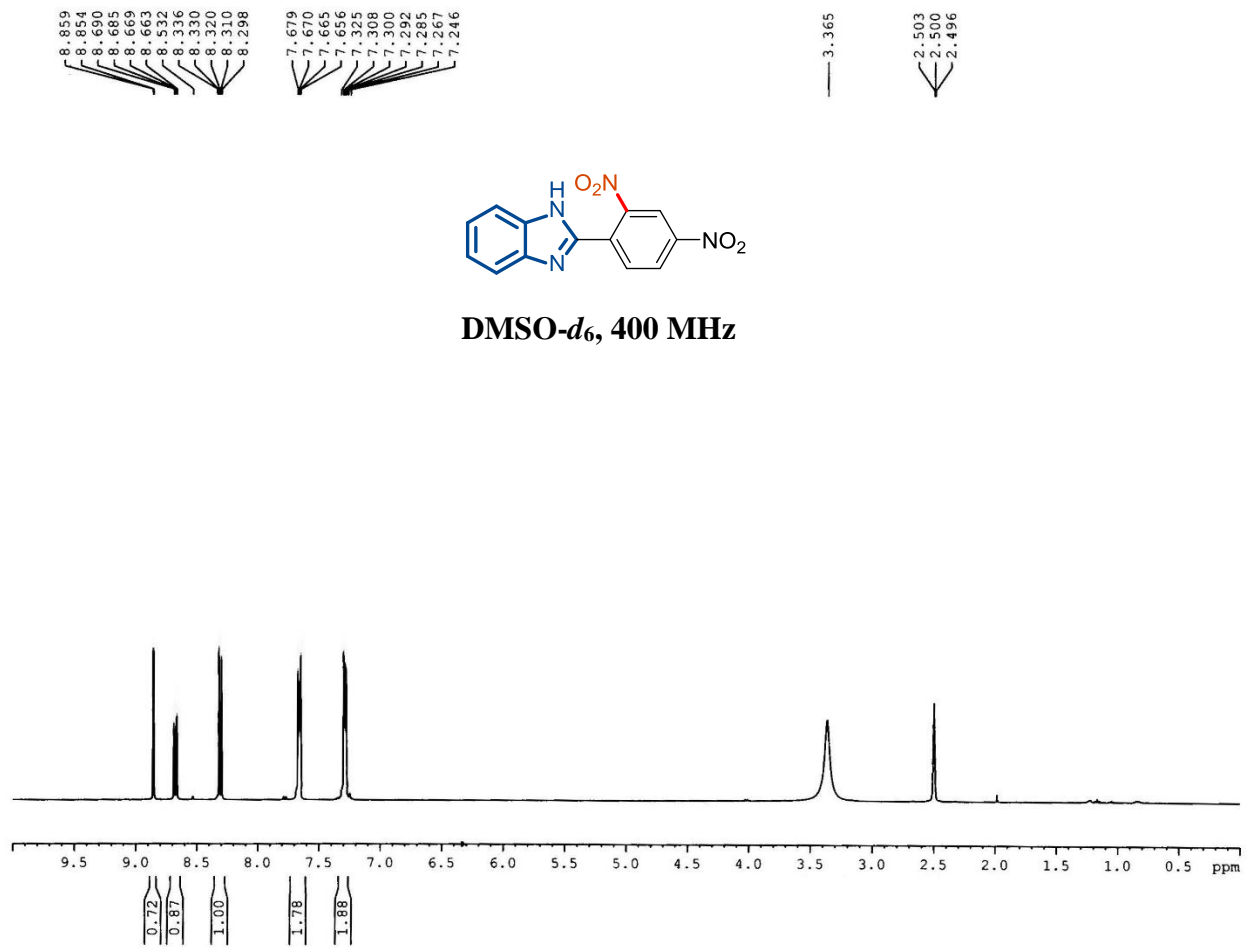
¹³C NMR of Compound 5a



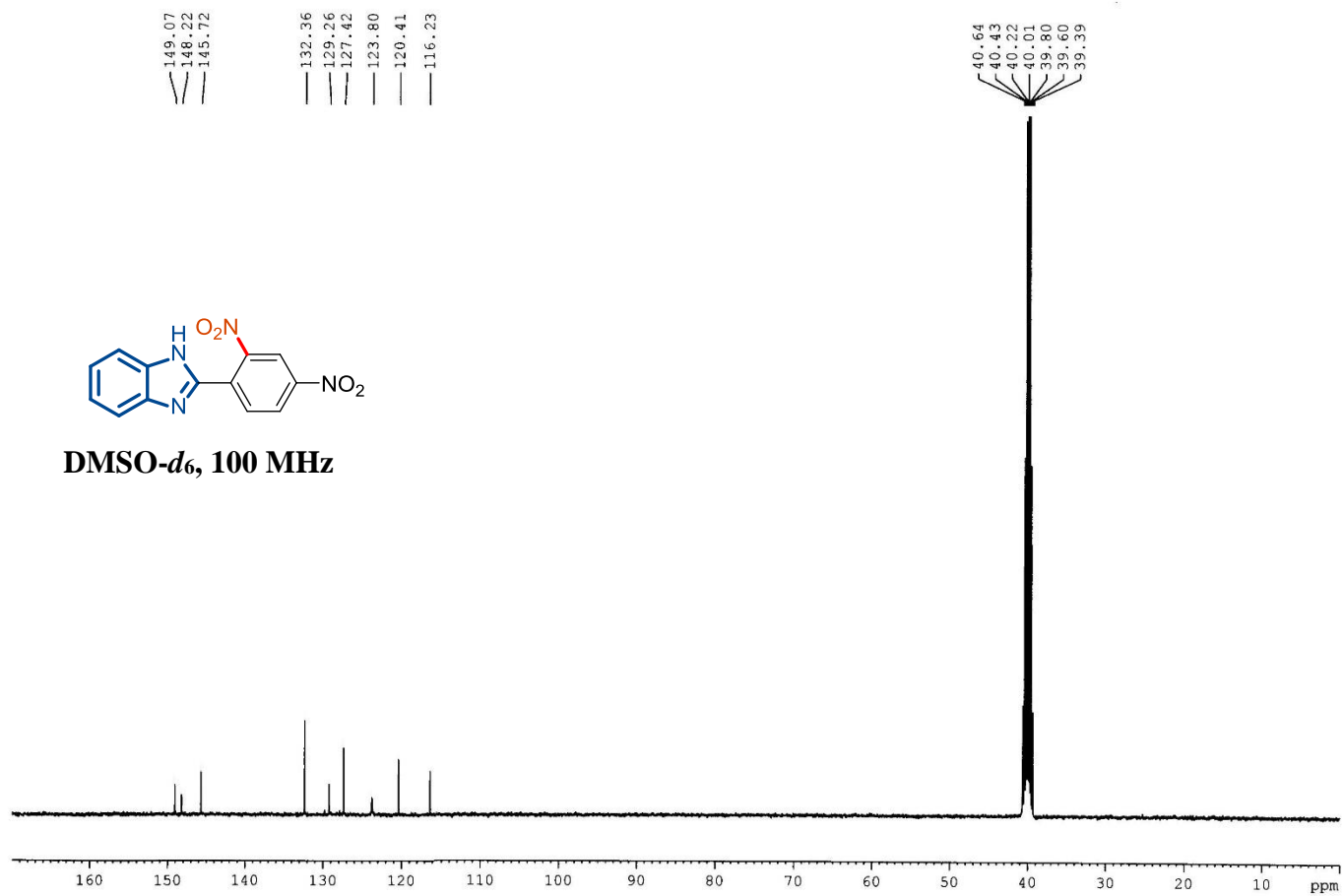
CDCl₃, 100 MHz



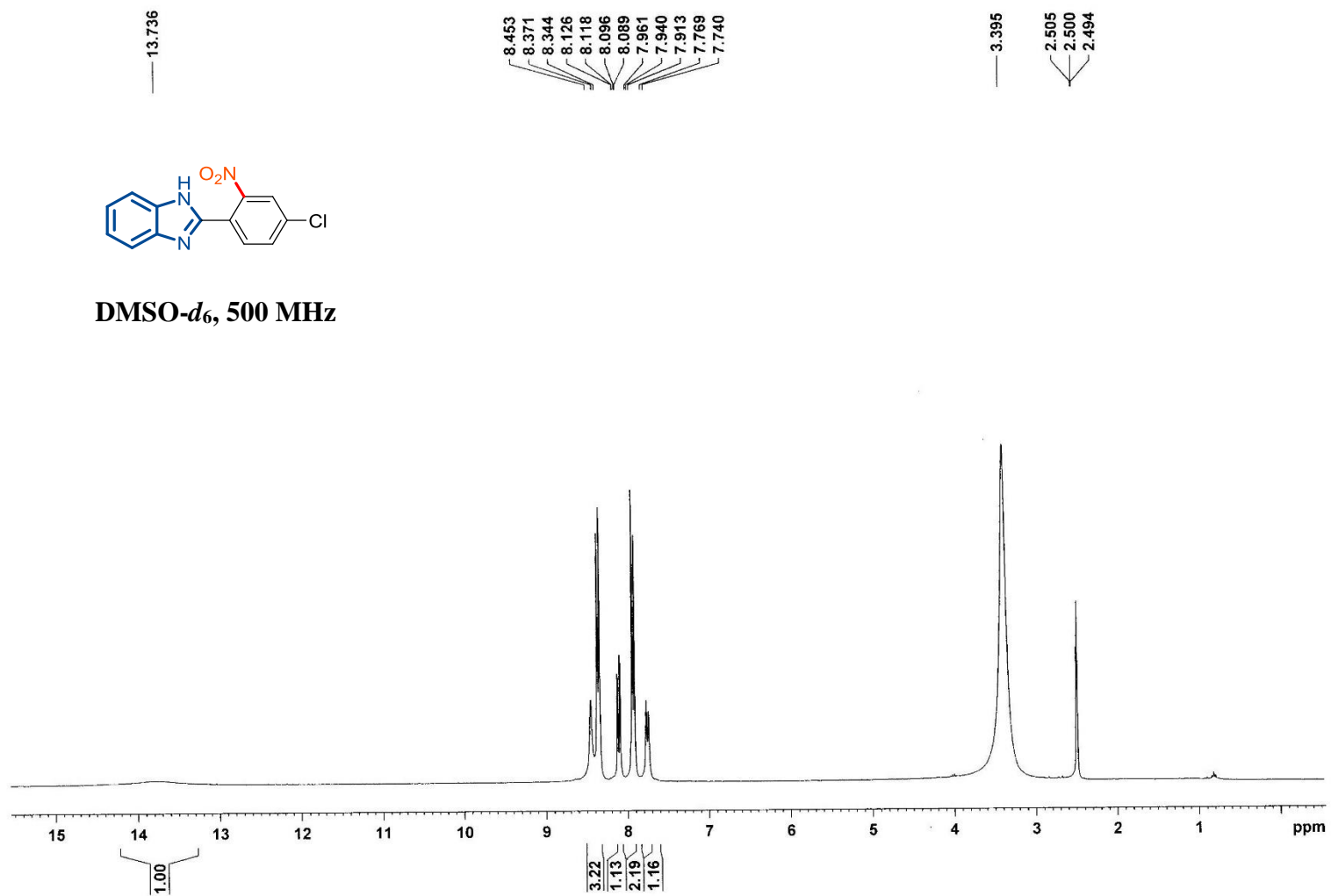
^1H NMR of Compound 5b



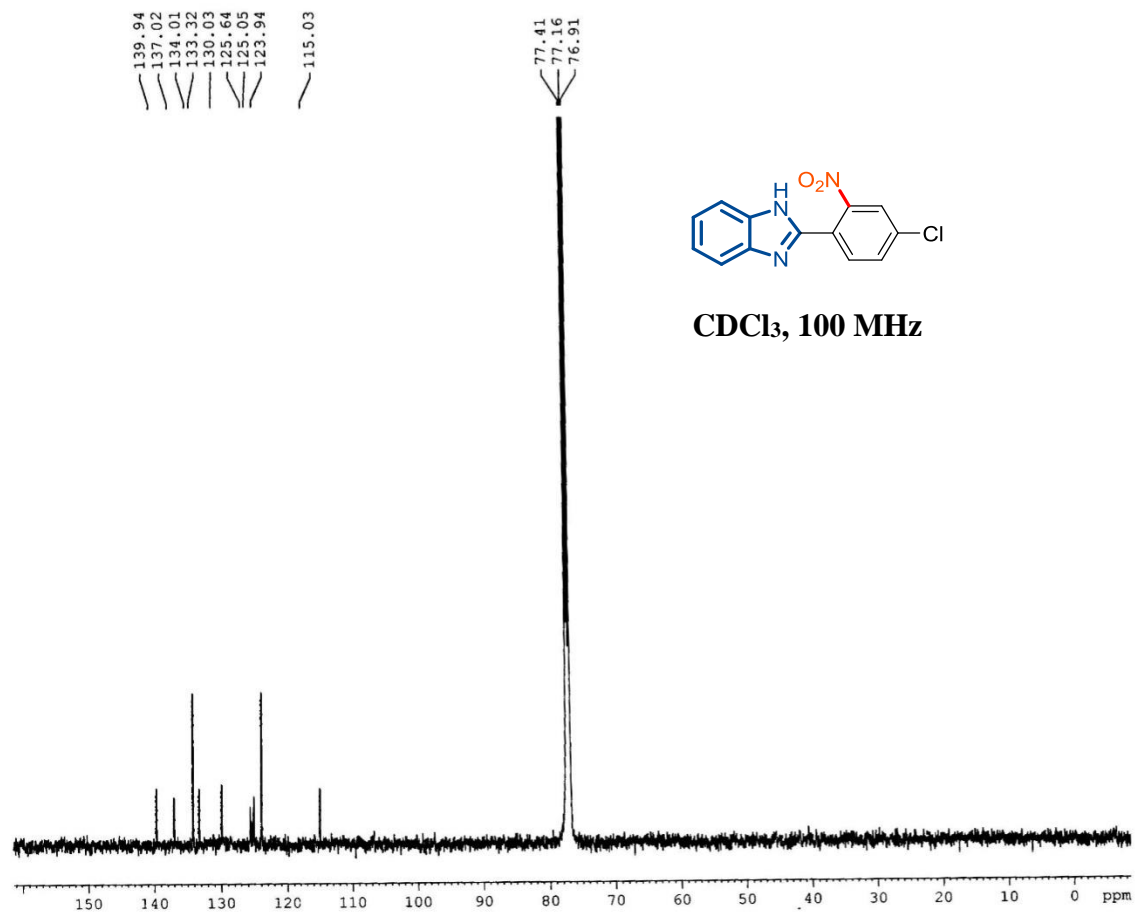
¹³C NMR of Compound 5b



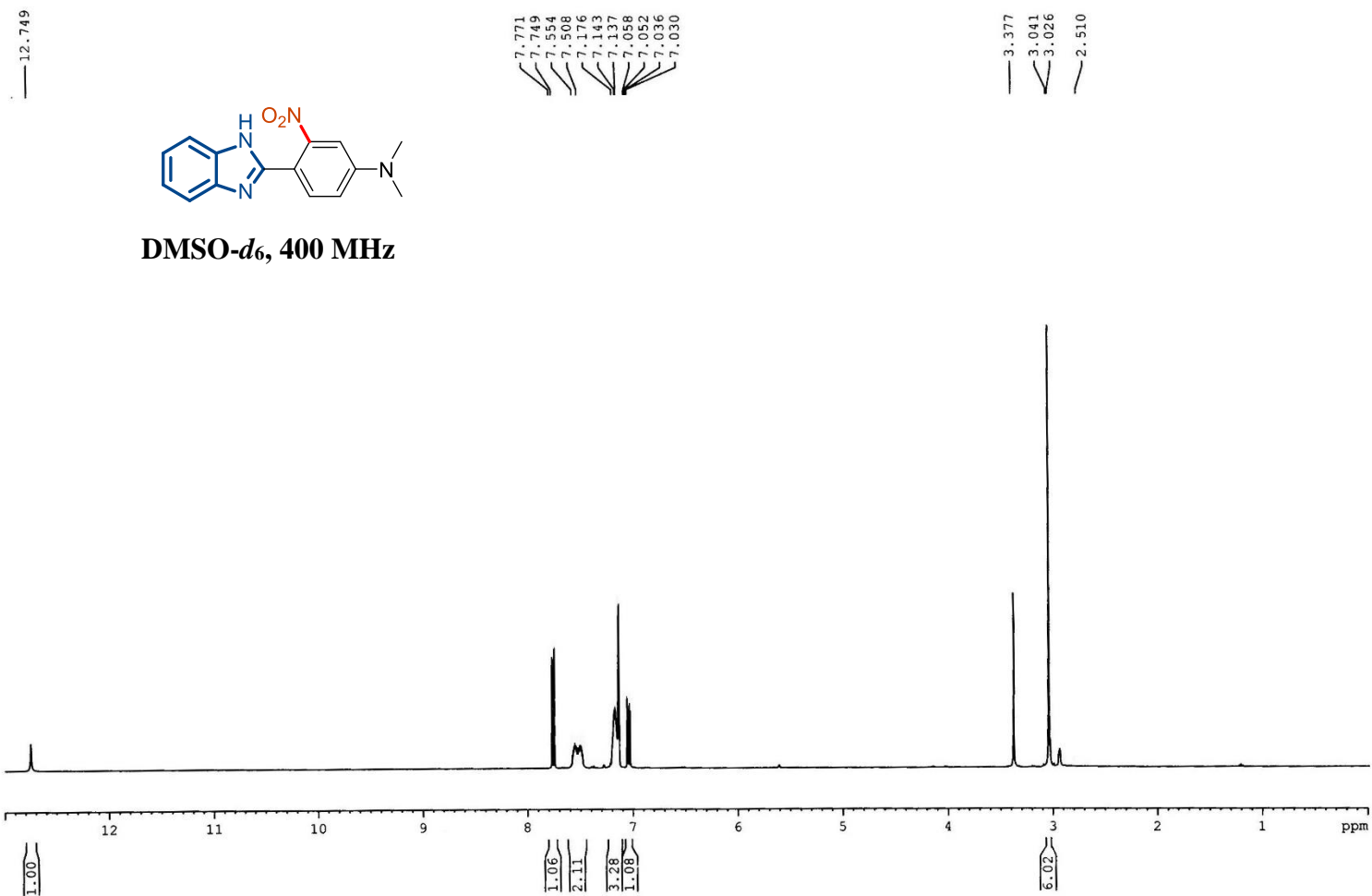
^1H NMR of Compound 5c



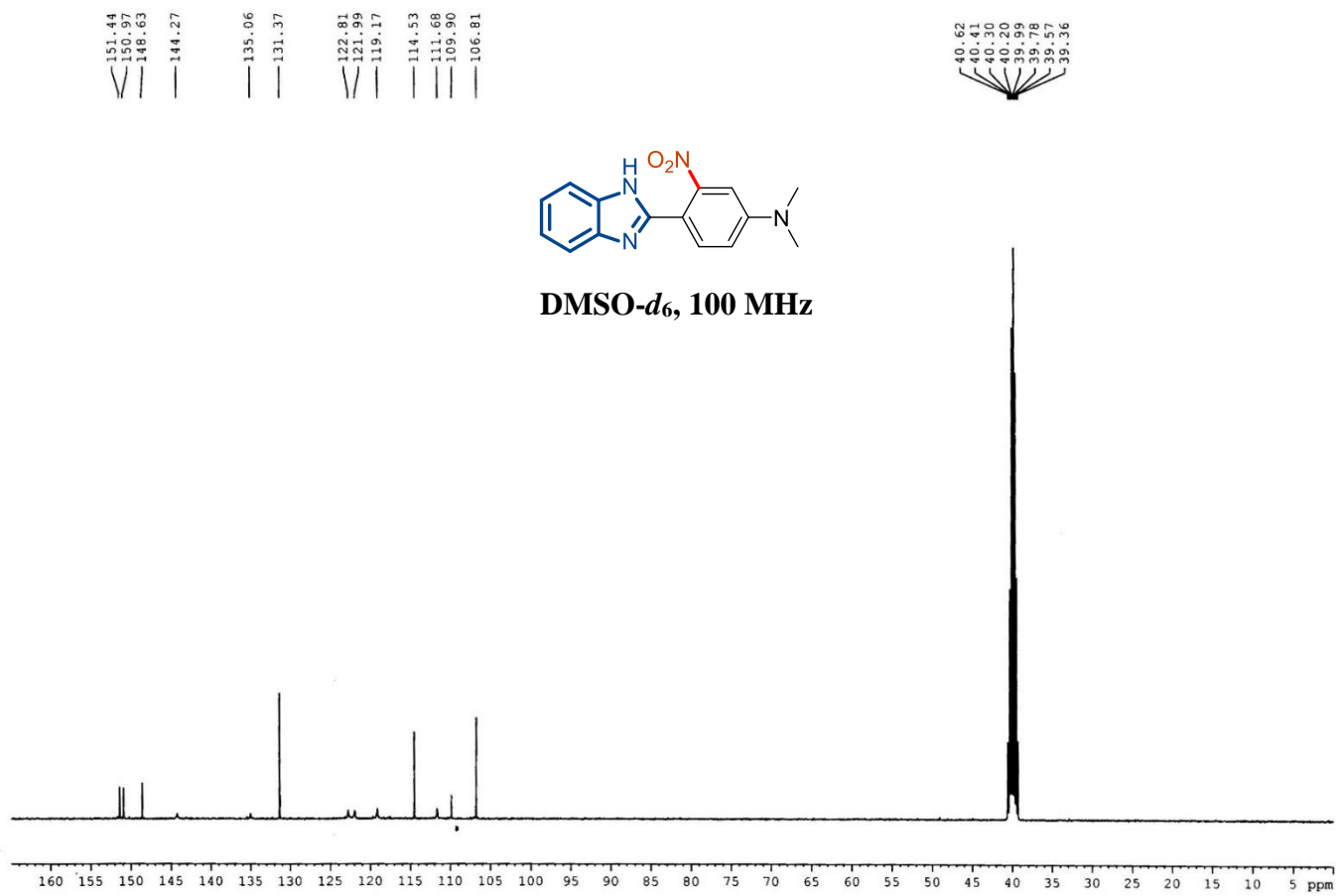
^{13}C NMR of Compound 5c



^1H NMR of compound 5d

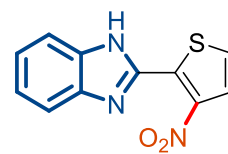


^{13}C NMR of compound 5d

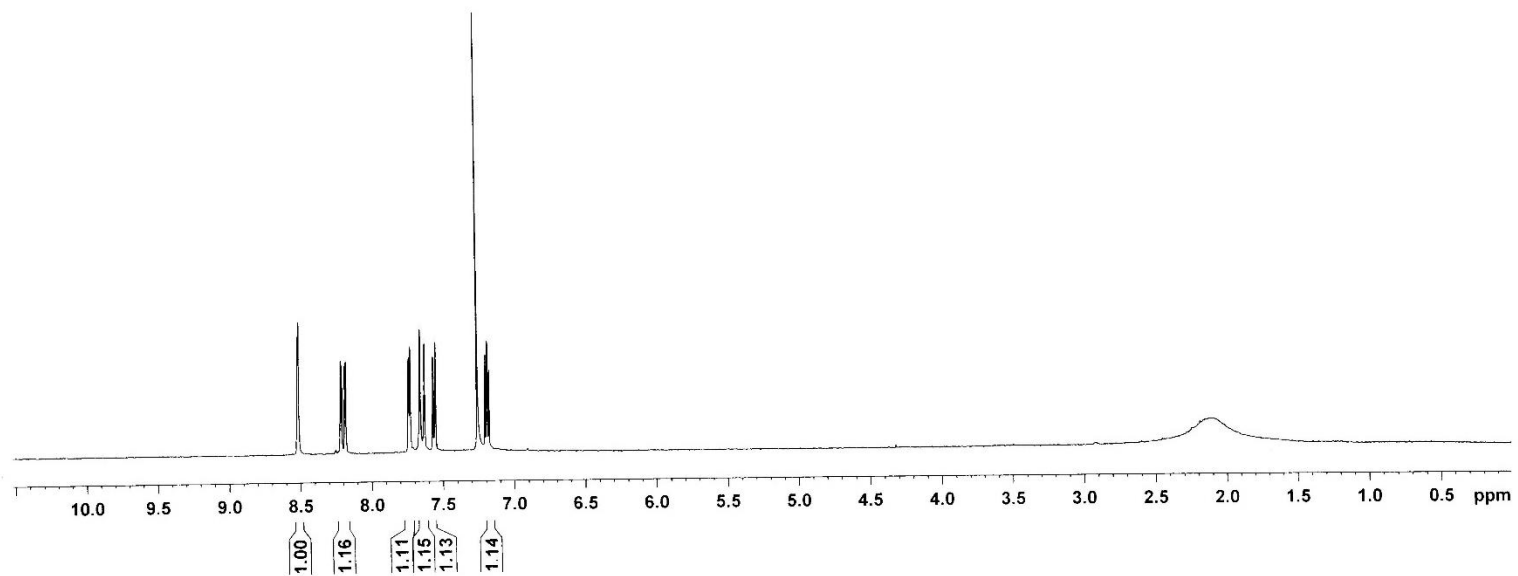


¹H NMR of compound 5e

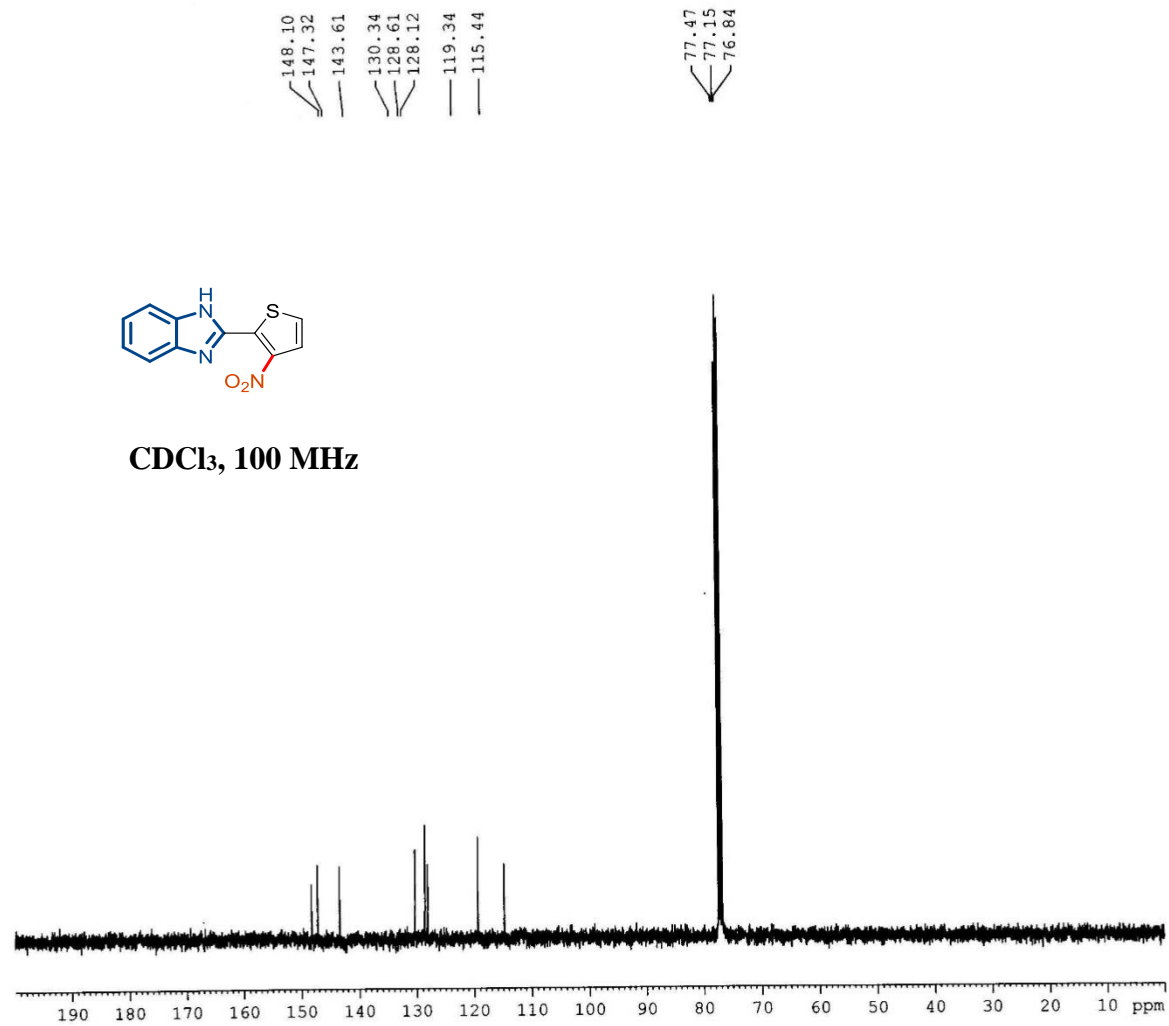
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8.183
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7.557
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7.259
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7.194
7.190
7.177



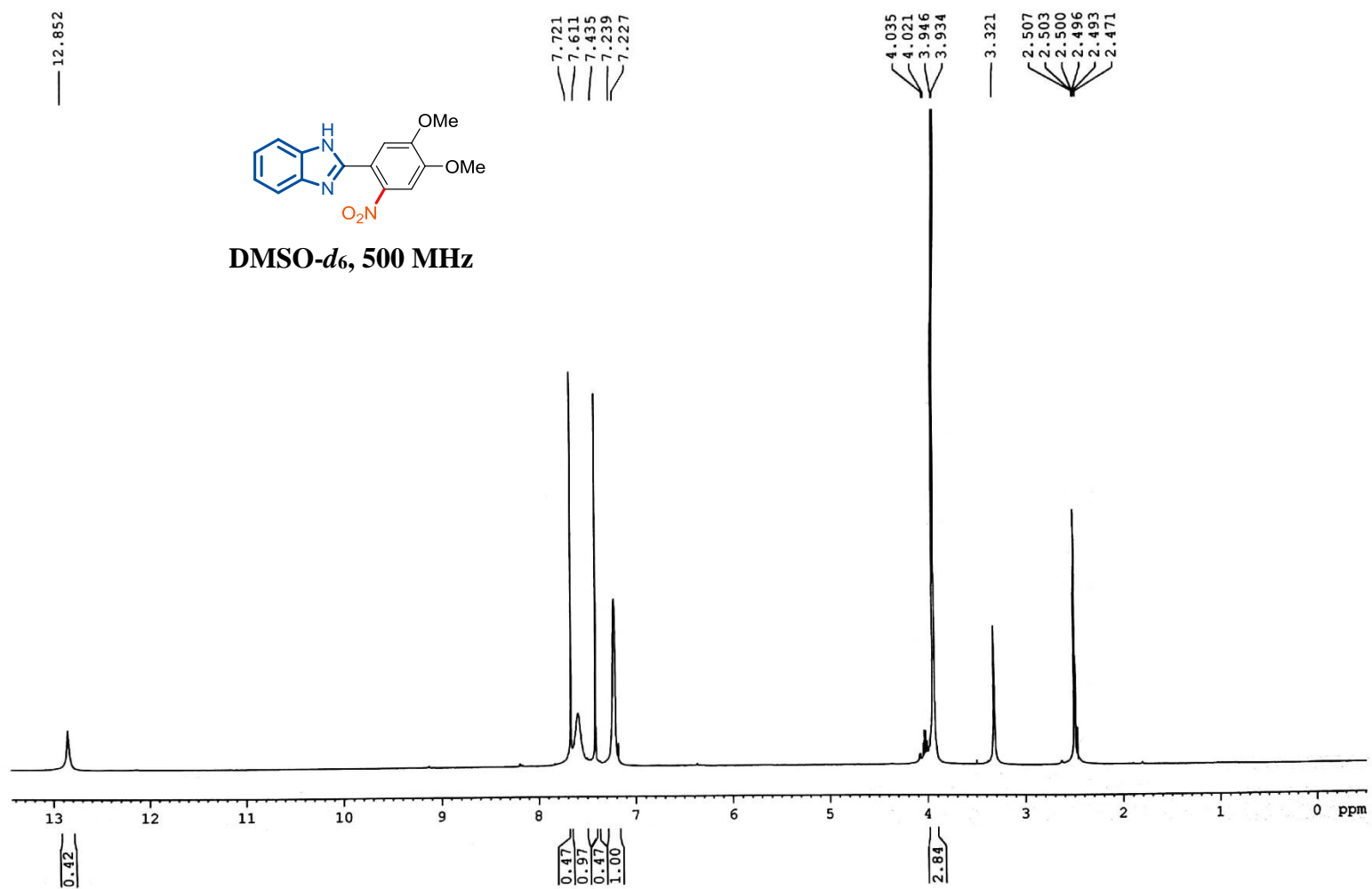
CDCl₃, 300 MHz



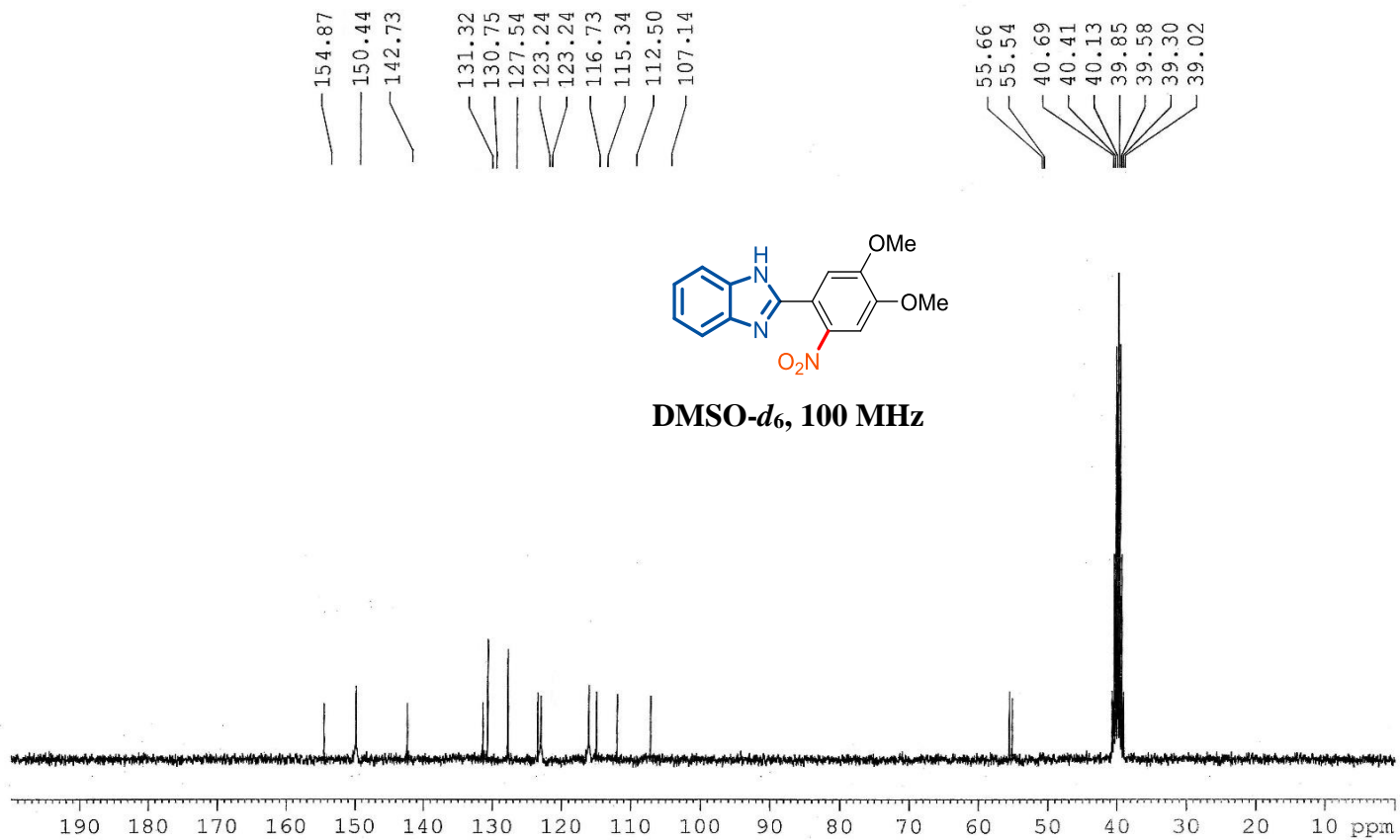
¹³C NMR of compound 5e



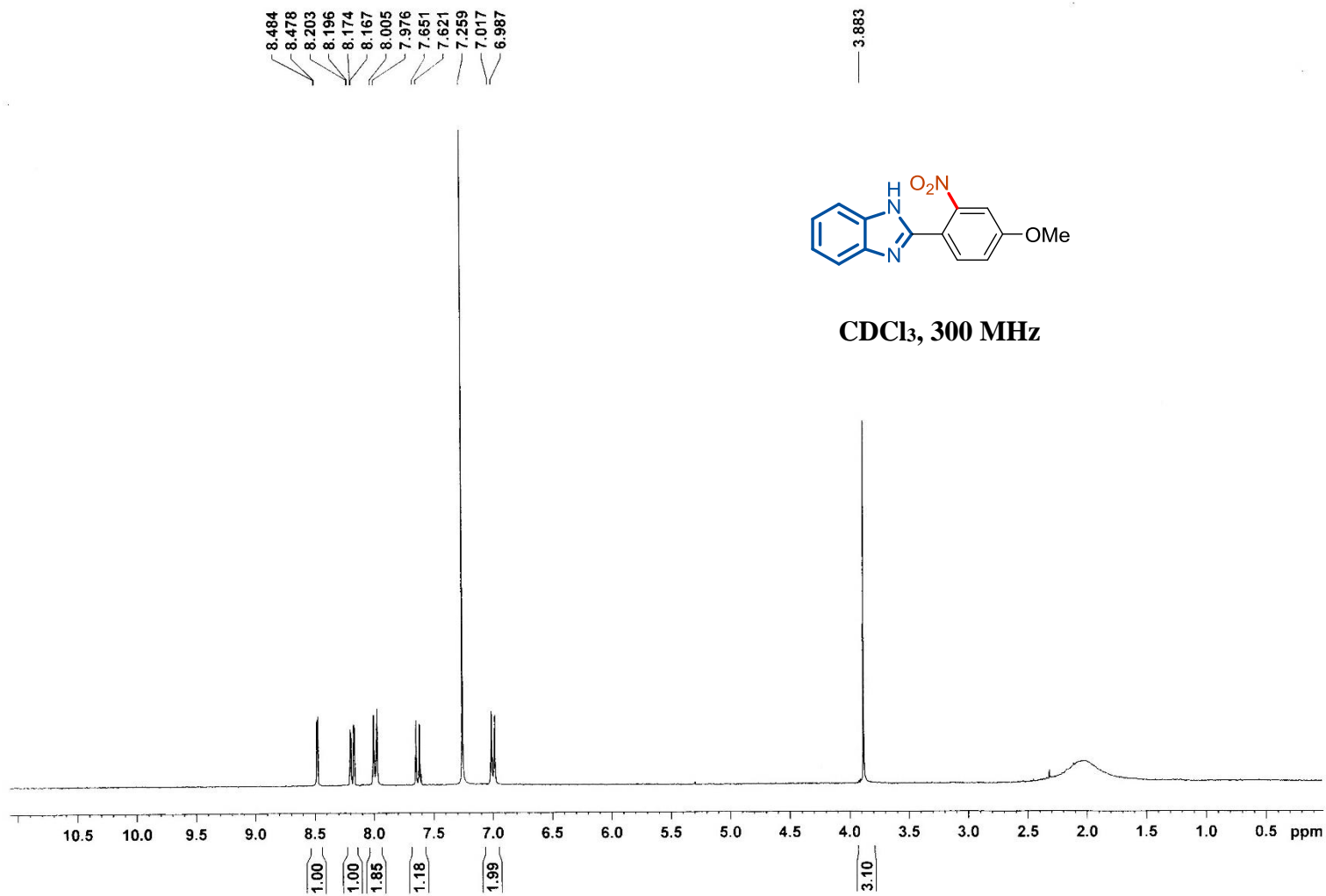
¹H NMR of compound 5f



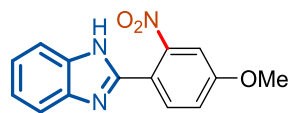
¹³C NMR of compound 5f



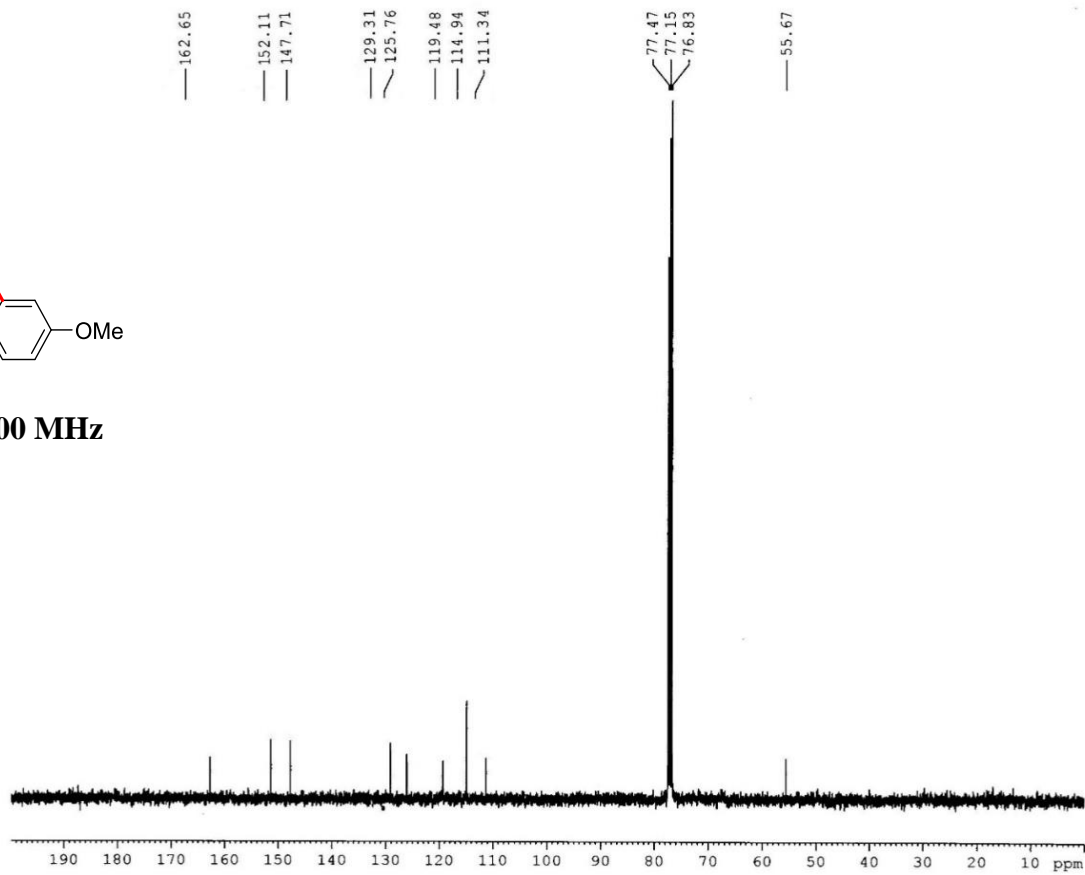
^1H NMR of compound 5g



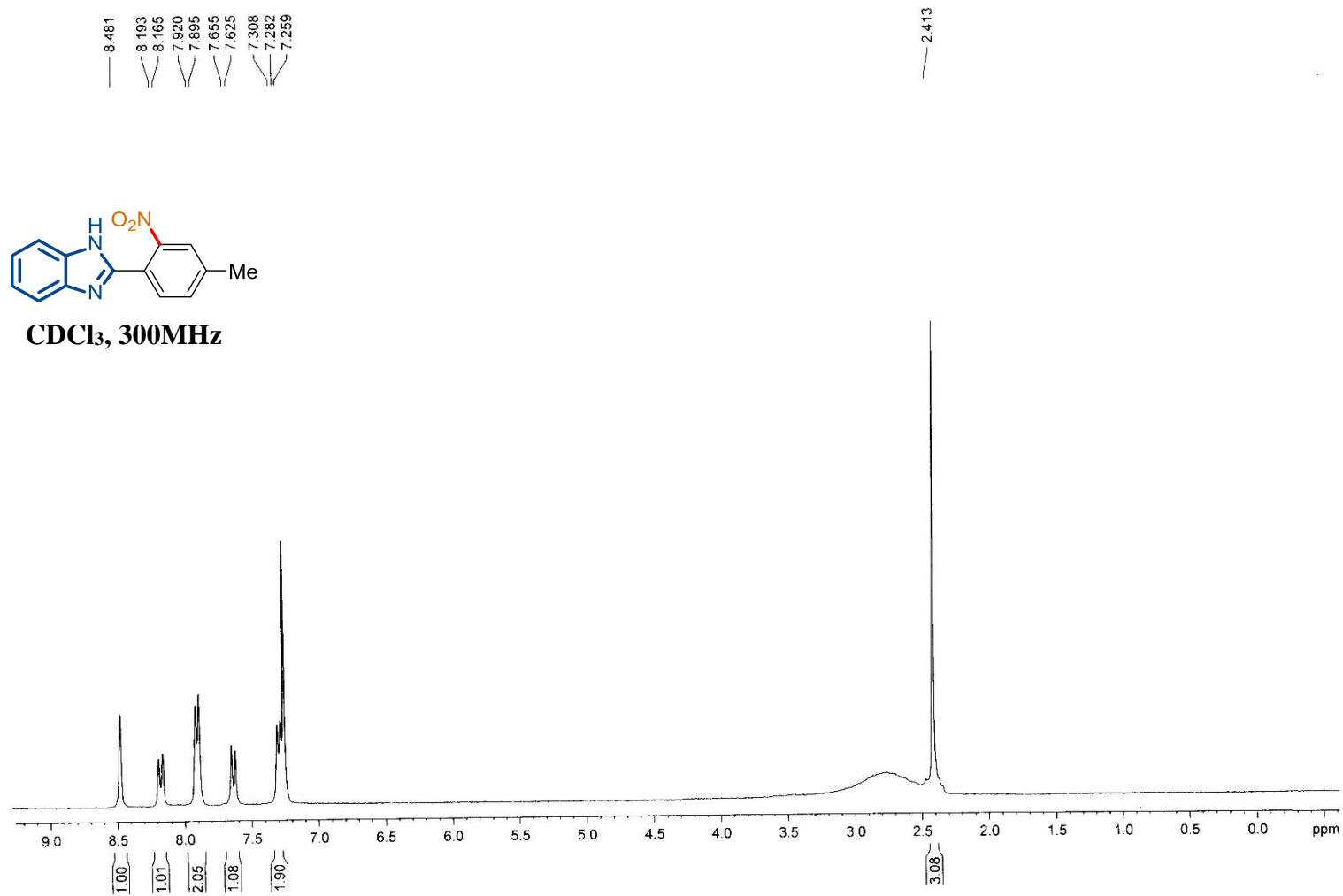
^{13}C NMR of compound 5g



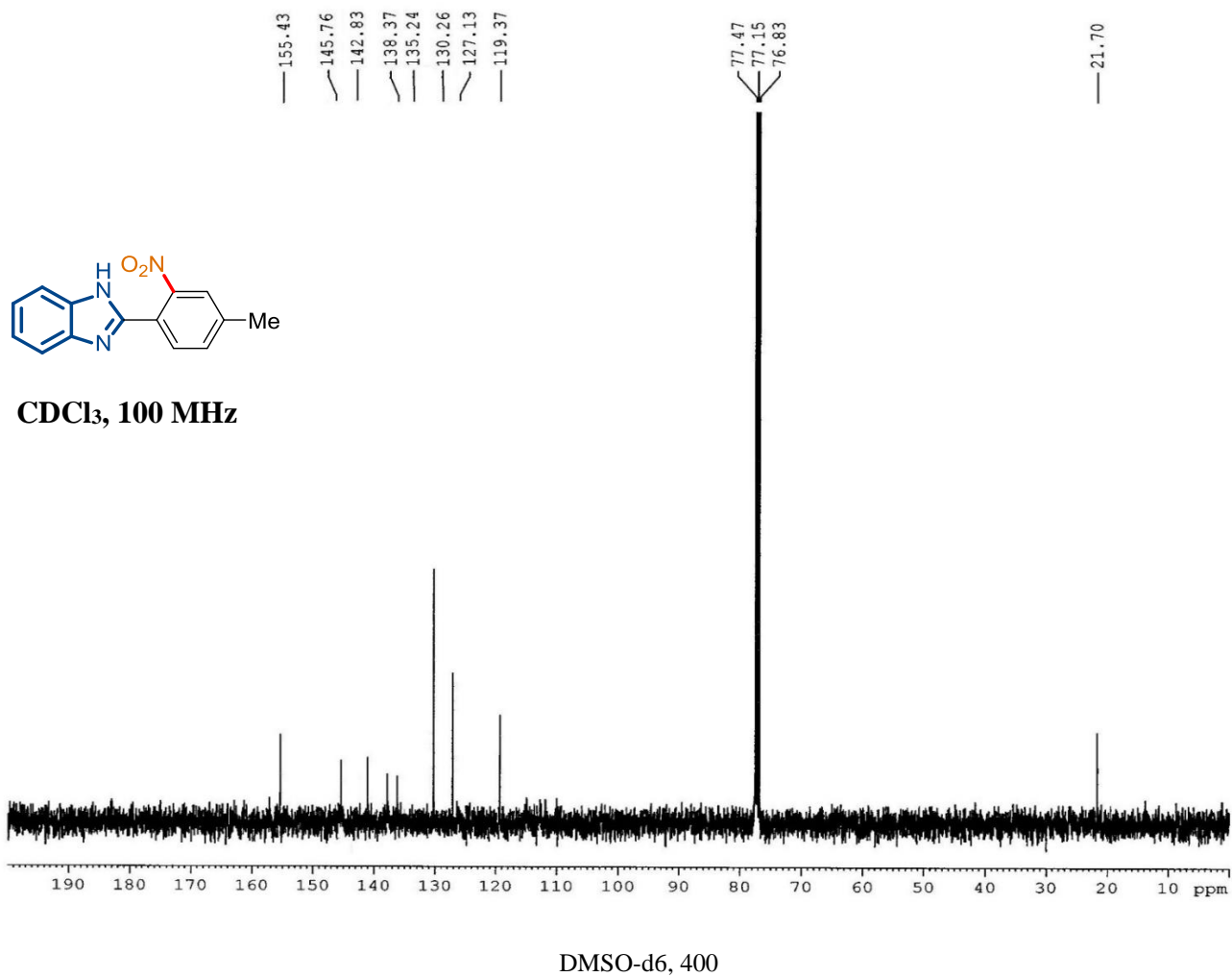
CDCl_3 , 100 MHz



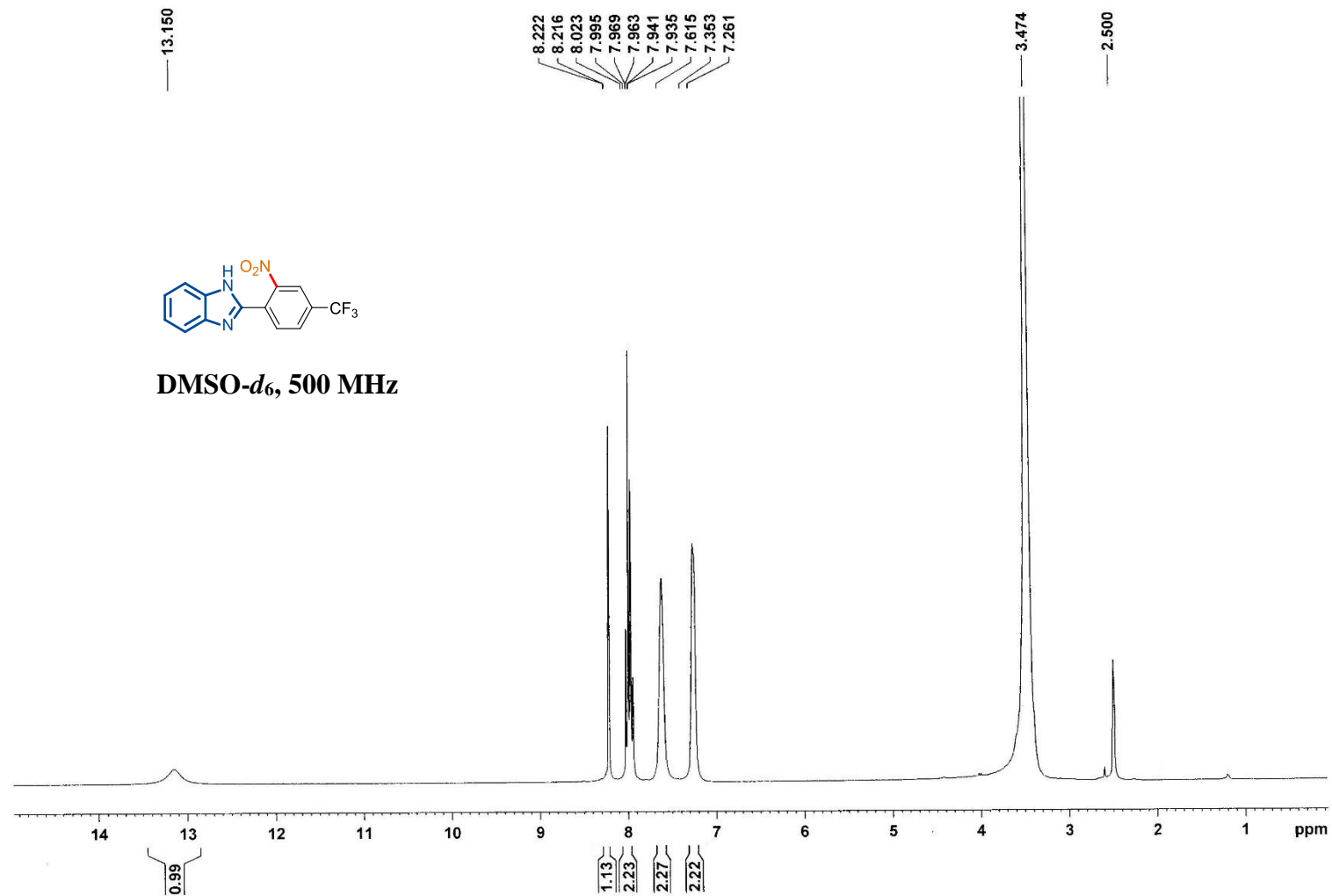
¹H NMR of compound 5h



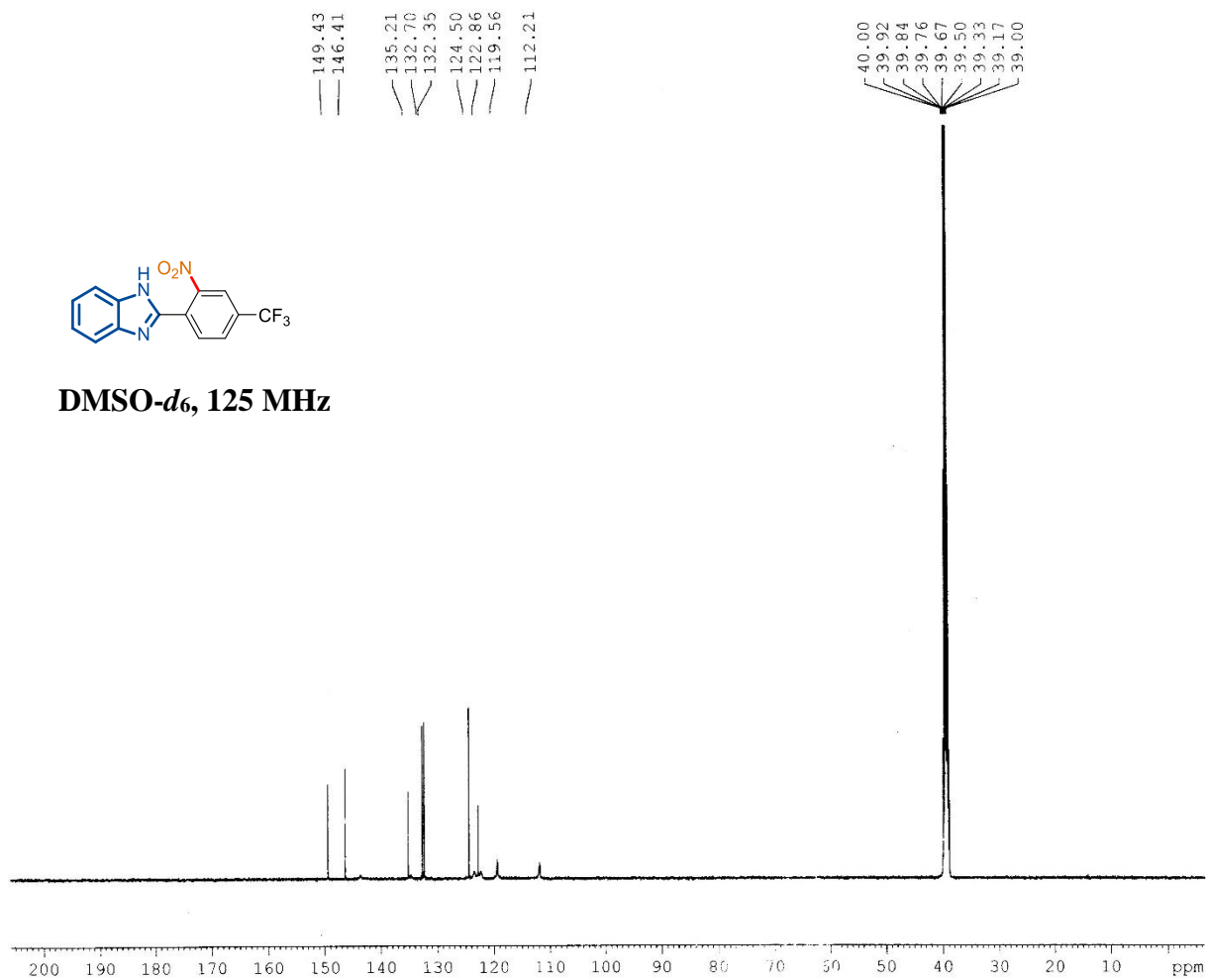
^{13}C NMR of compound 5h



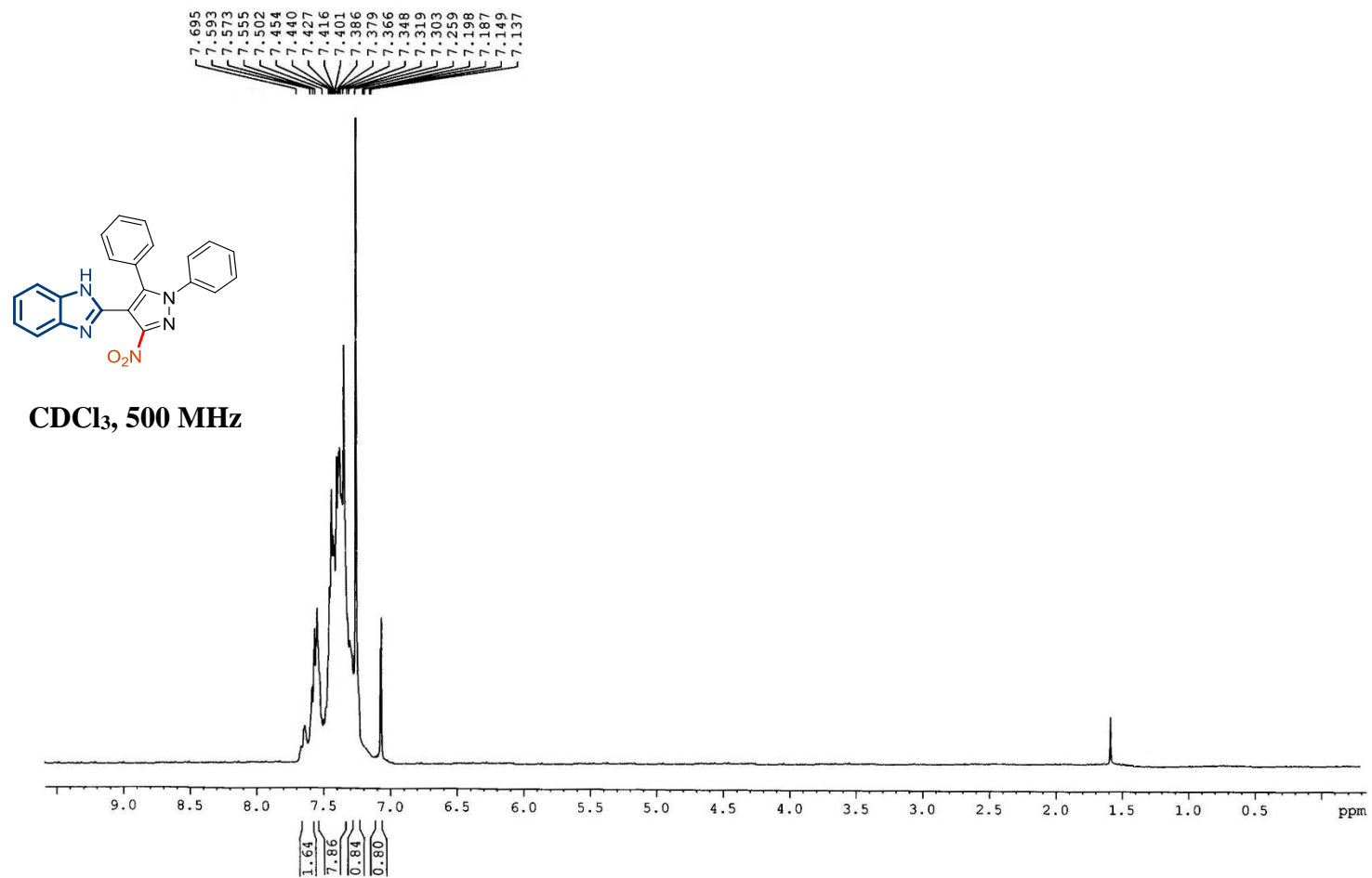
¹H NMR of compound 5i



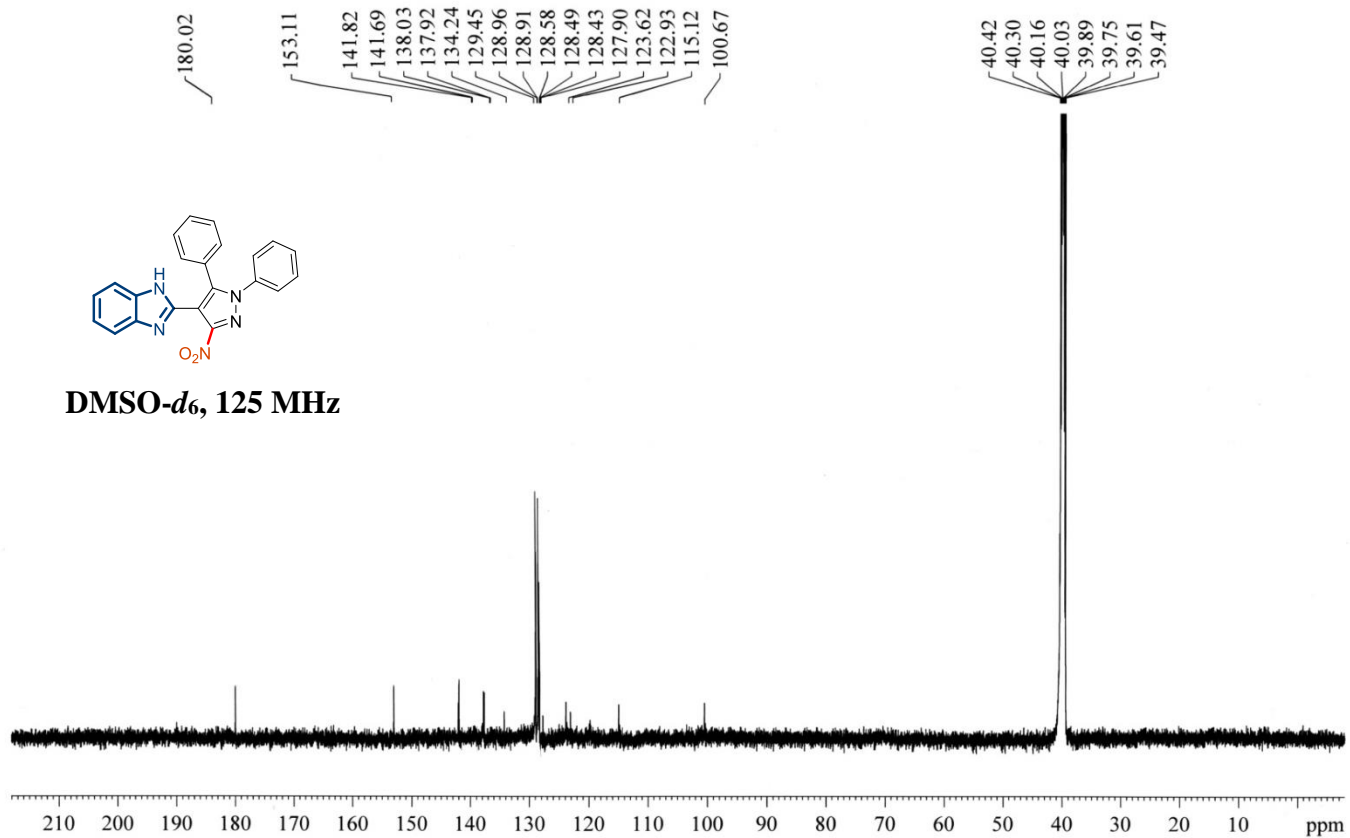
¹³C NMR of compound 5i



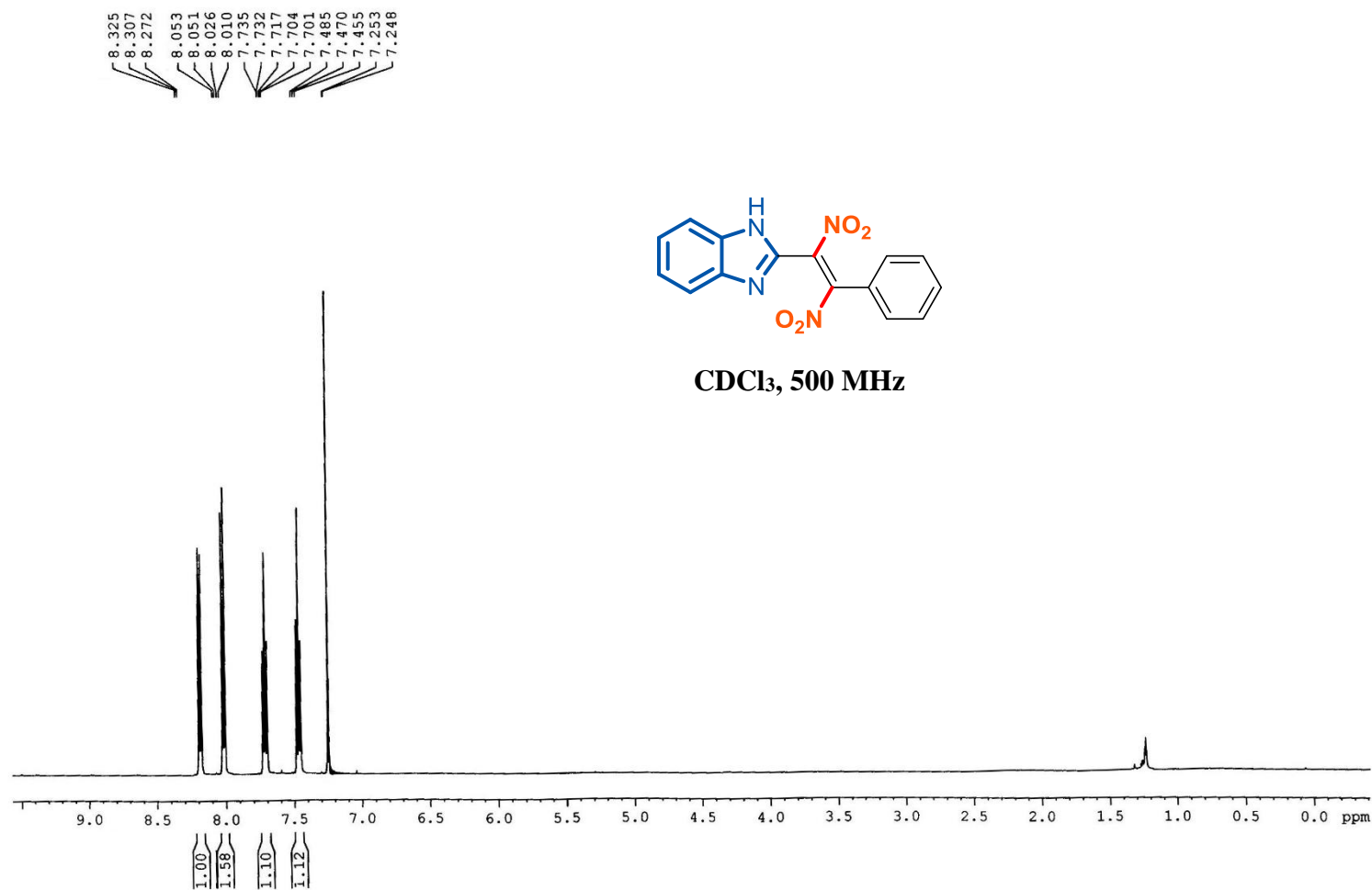
¹H NMR of compound 5j



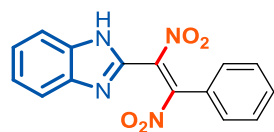
¹³C NMR of compound 5j



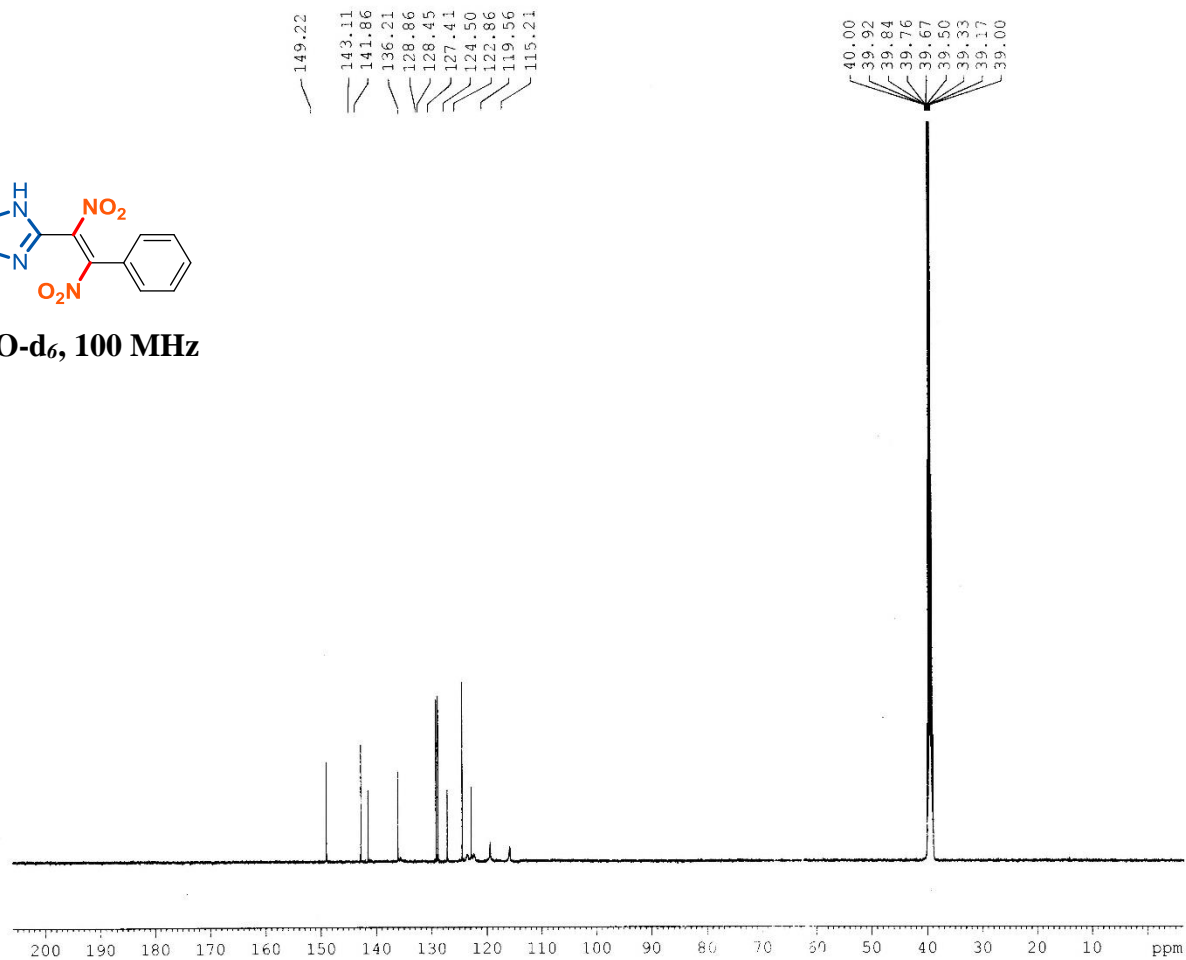
¹H NMR of compound 5k



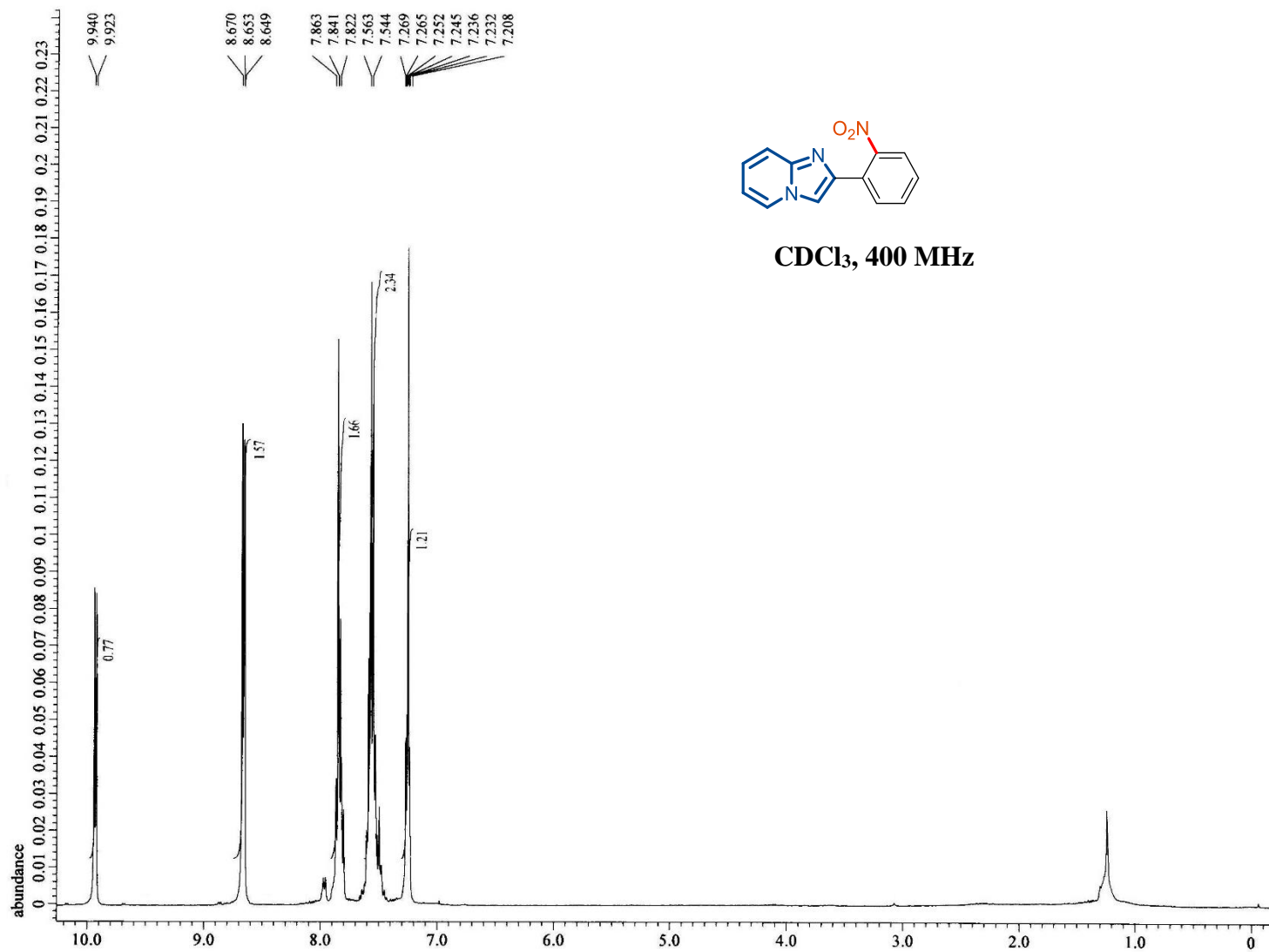
¹³C NMR of compound 5k



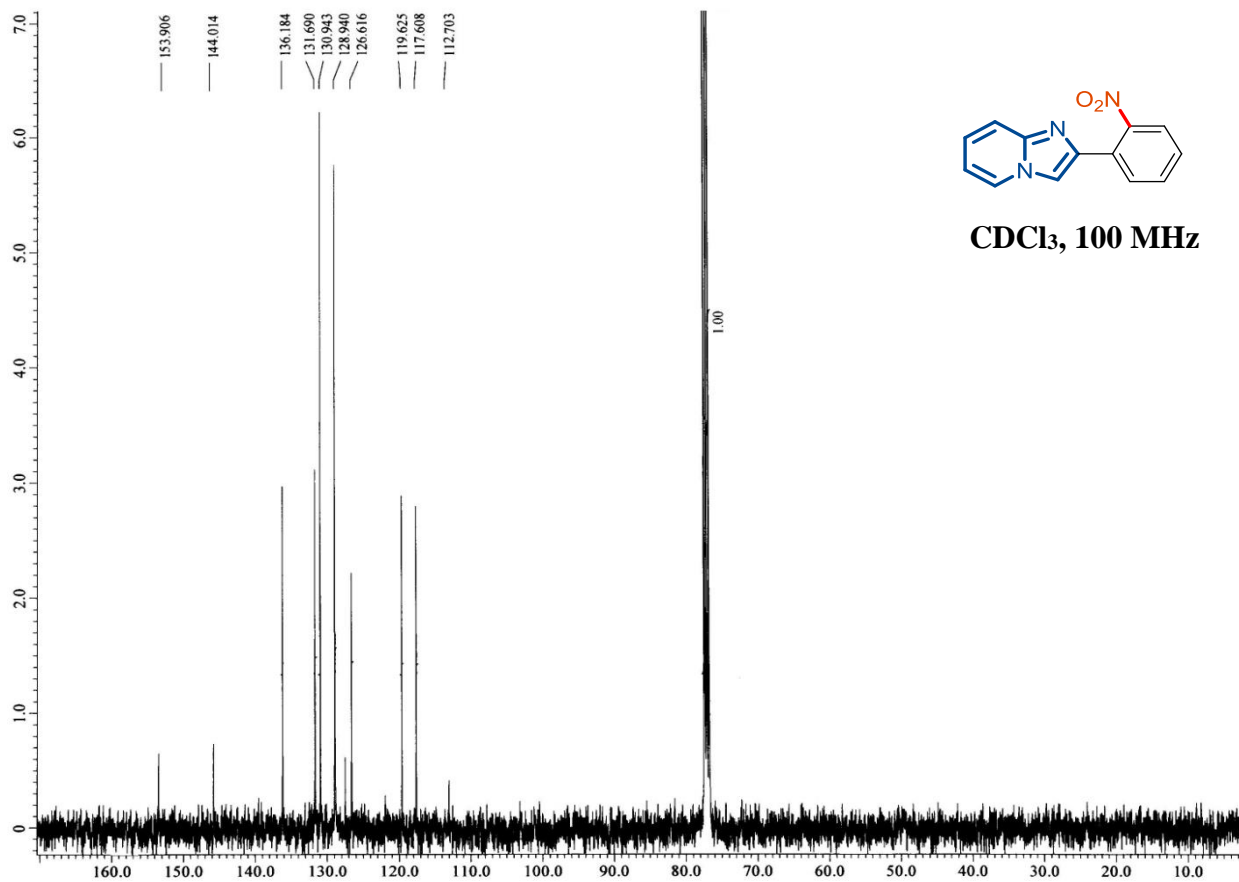
DMSO-d₆, 100 MHz



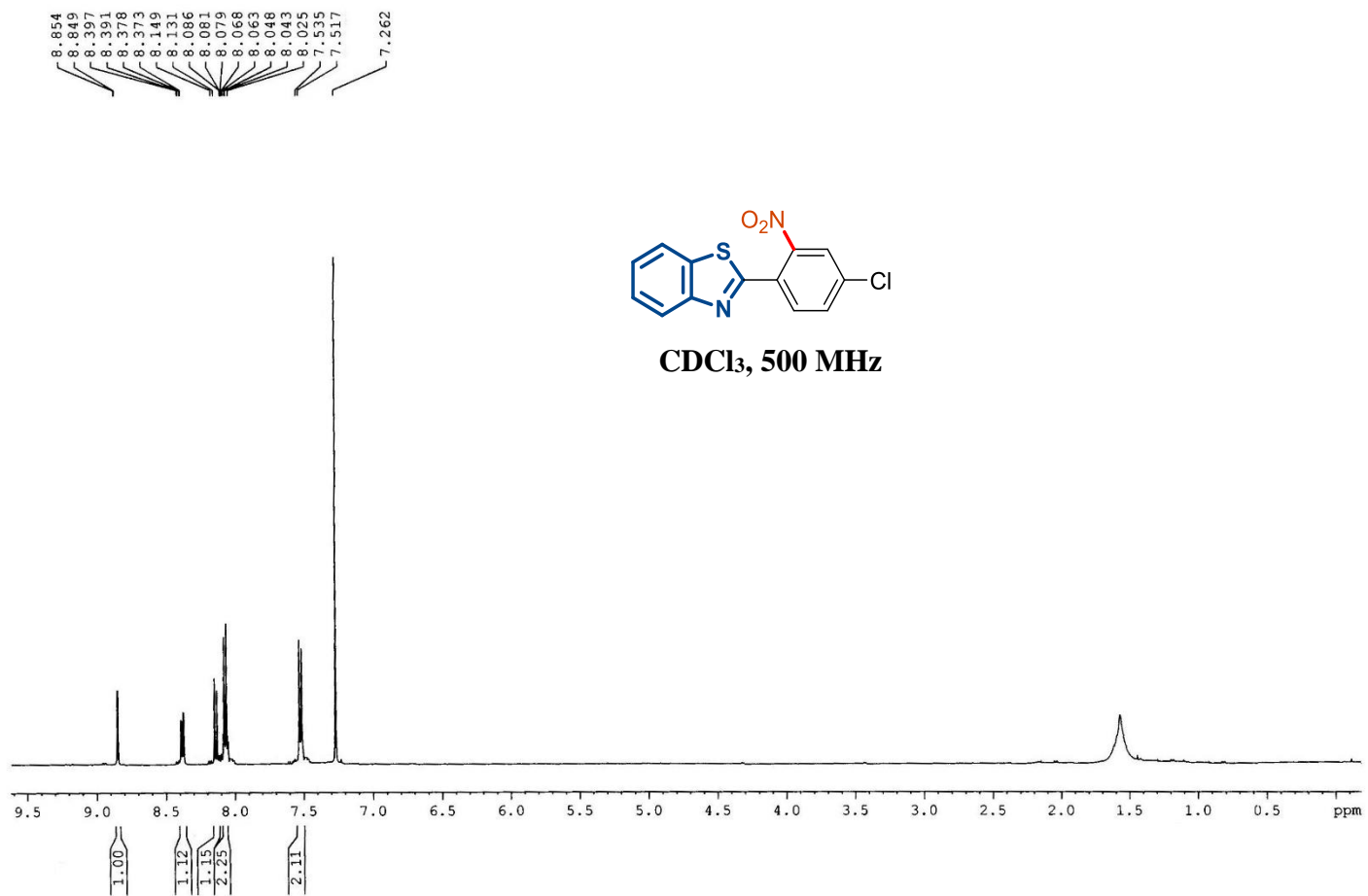
^1H NMR of compound 5l



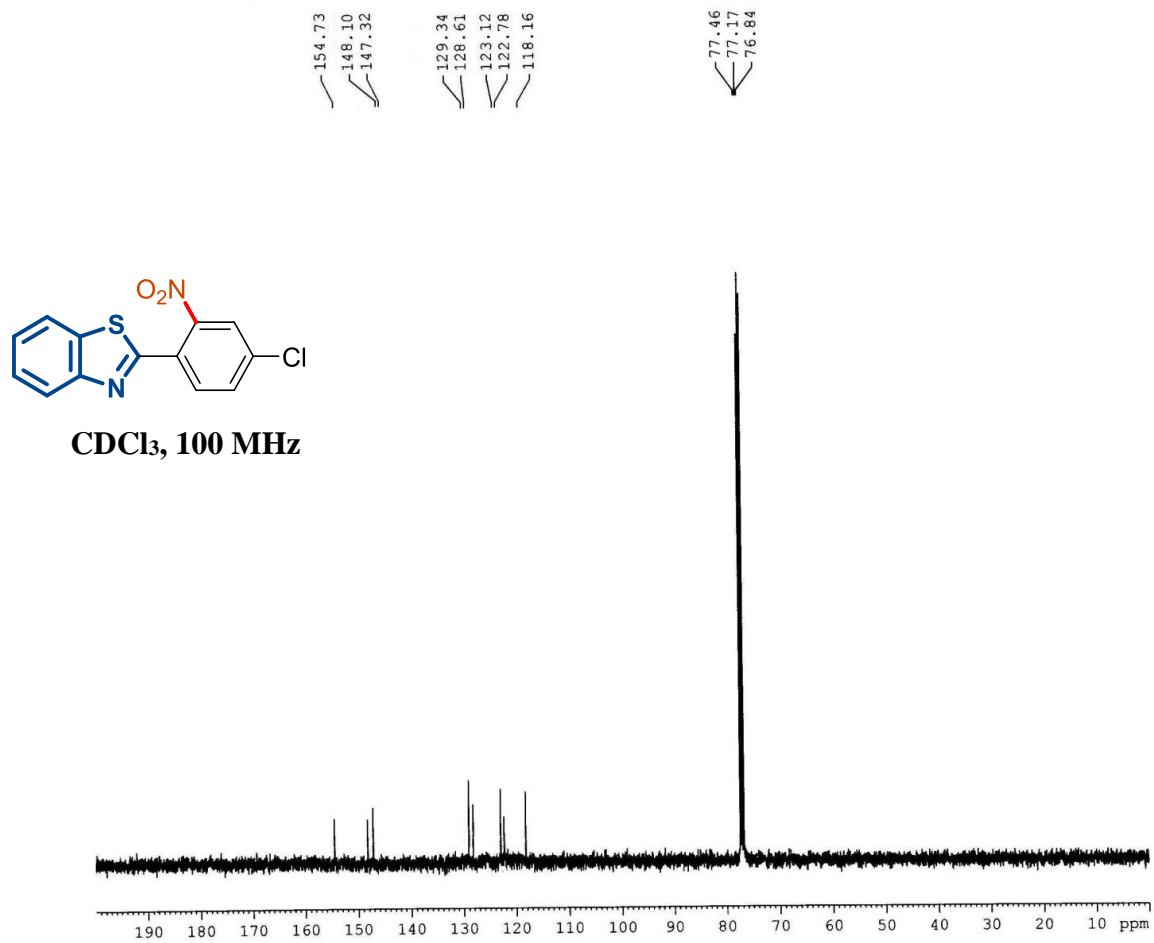
^{13}C NMR of compound 5l



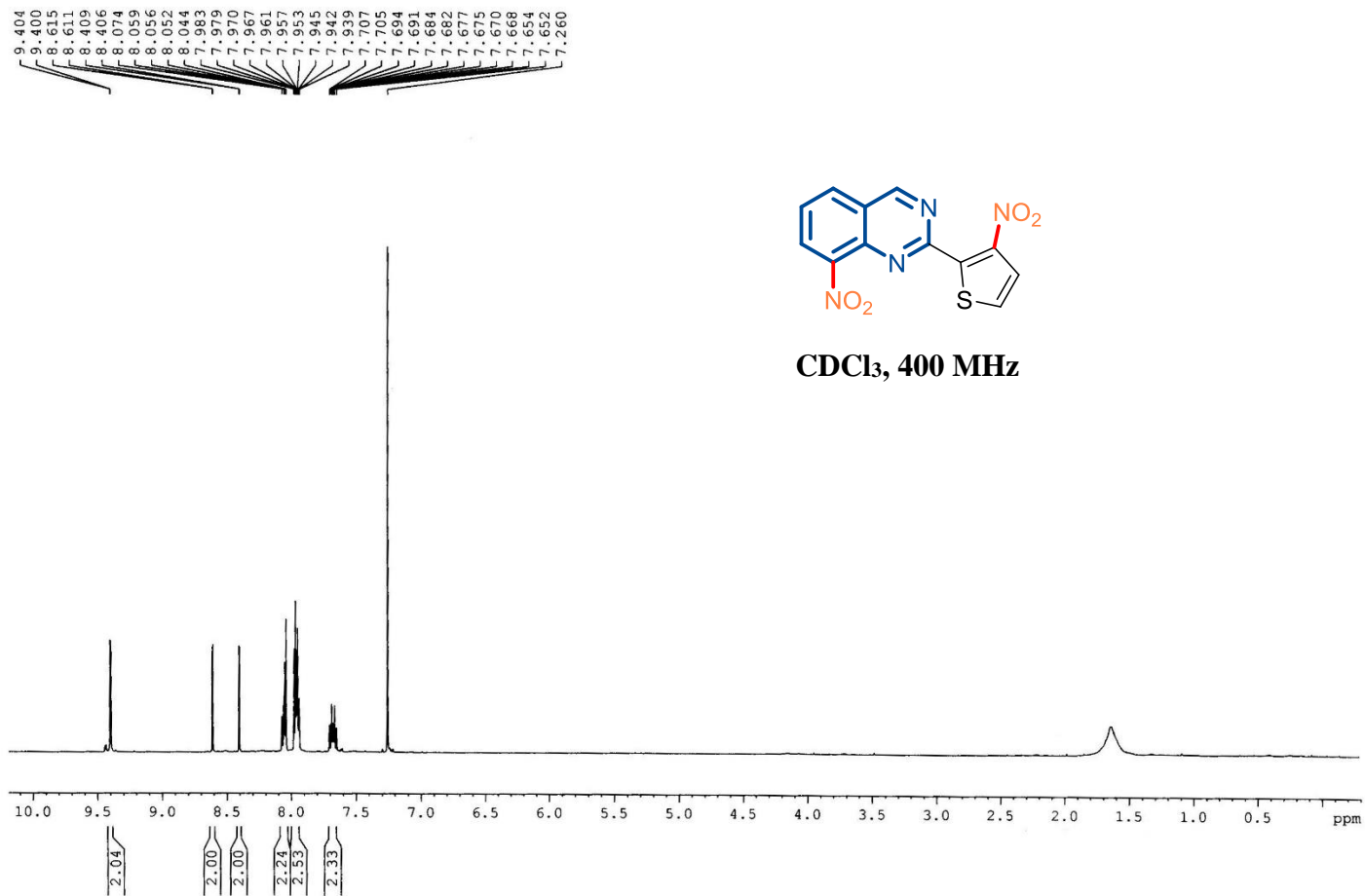
^1H NMR of compound 5m



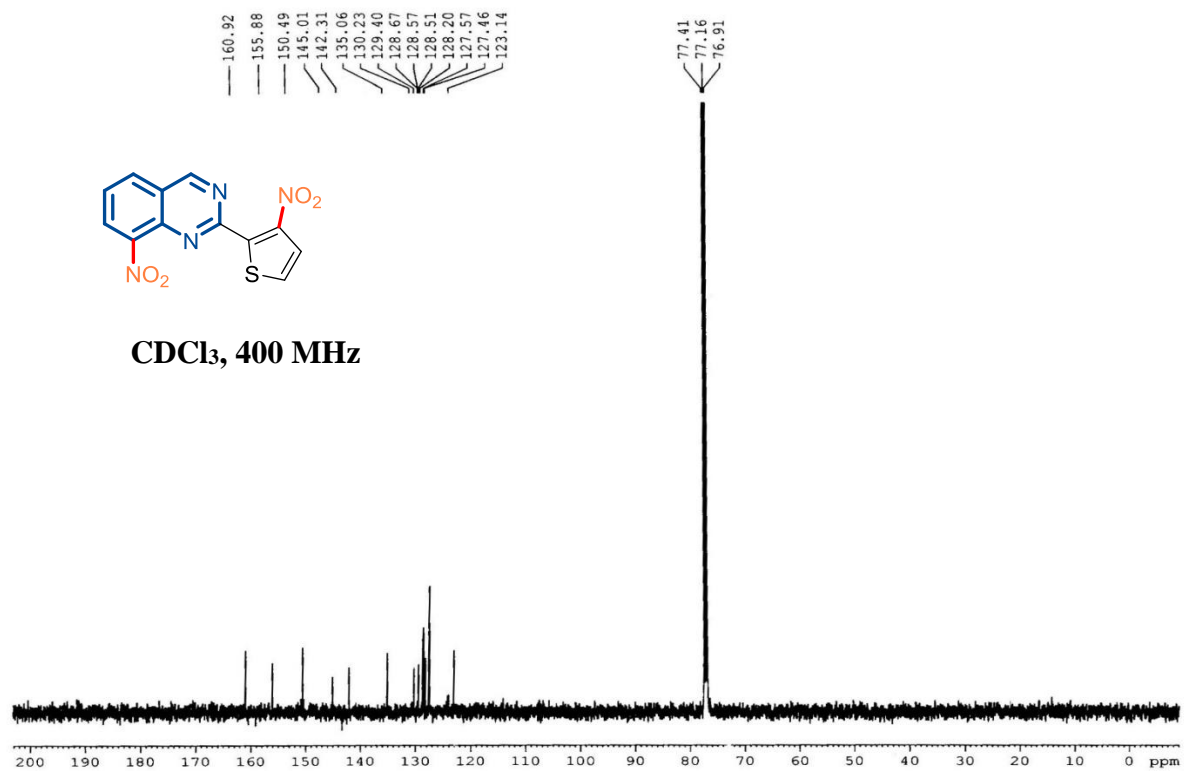
^{13}C NMR of compound 5m



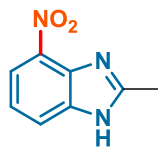
¹H NMR of compound 5n



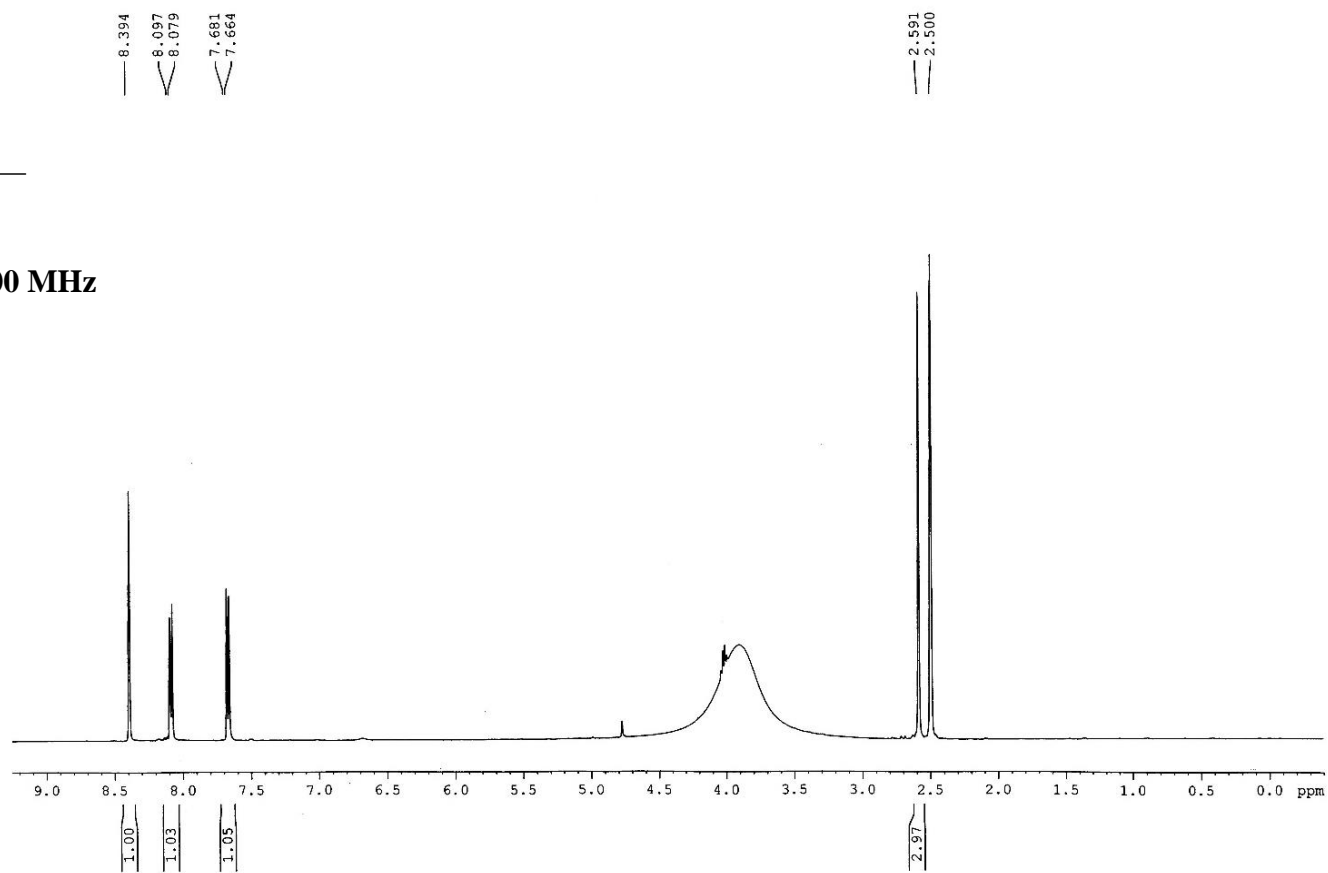
^{13}C NMR of compound 5n



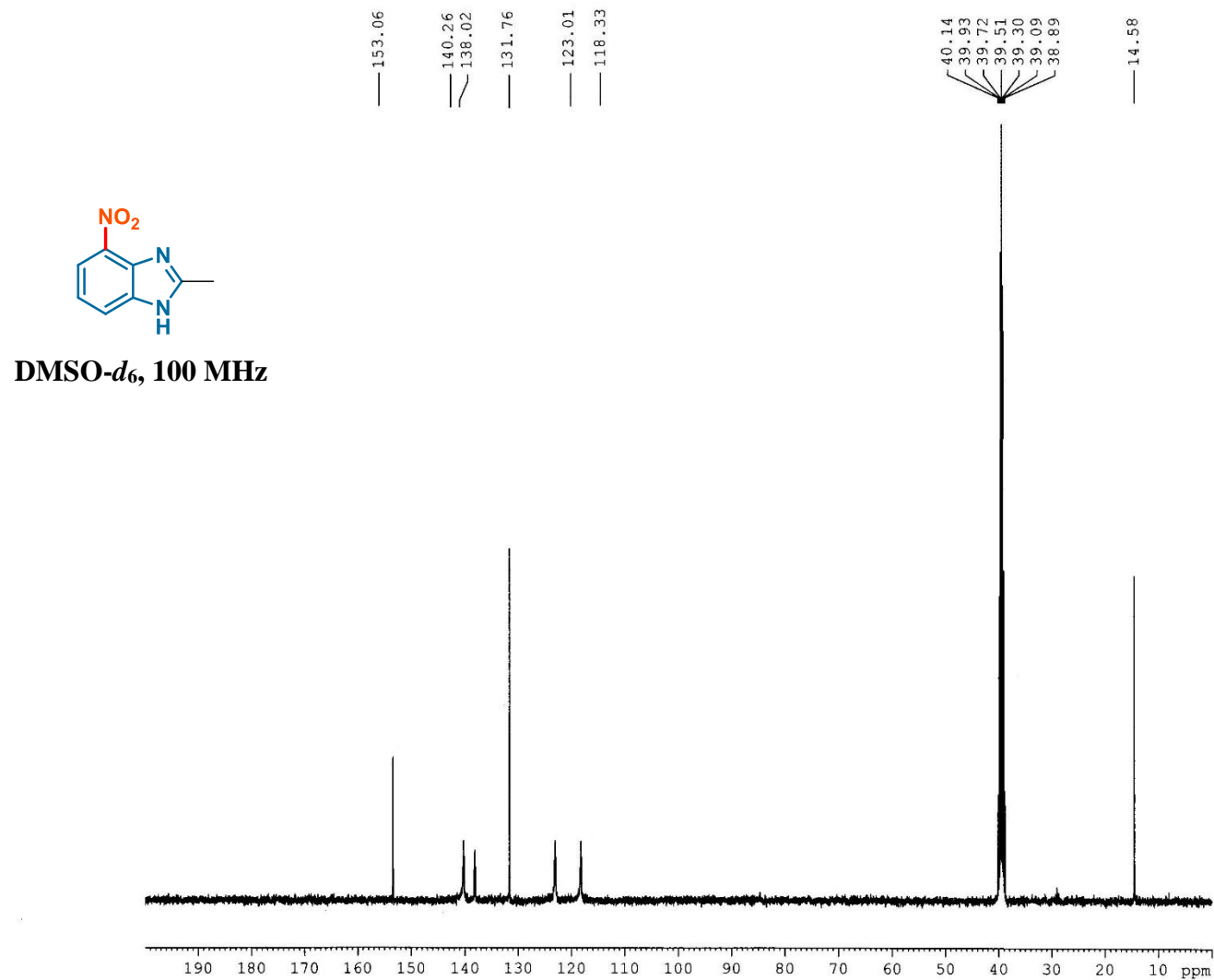
^1H NMR of compound 5o



DMSO- d_6 , 400 MHz

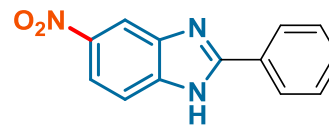


^{13}C NMR of compound 5o

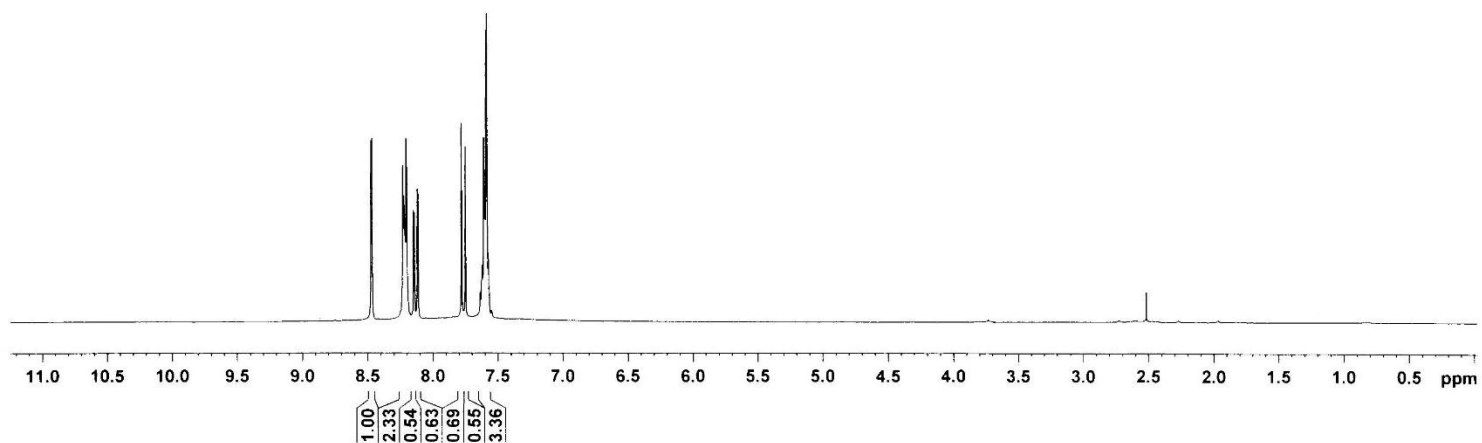


¹H NMR of compound 5p

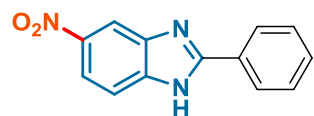
8.472
8.465
8.228
8.220
8.212
8.209
8.202
8.196
8.147
8.140
8.118
8.110
7.779
7.749
7.623
7.618
7.607
7.596
7.588
7.582
7.573
7.566



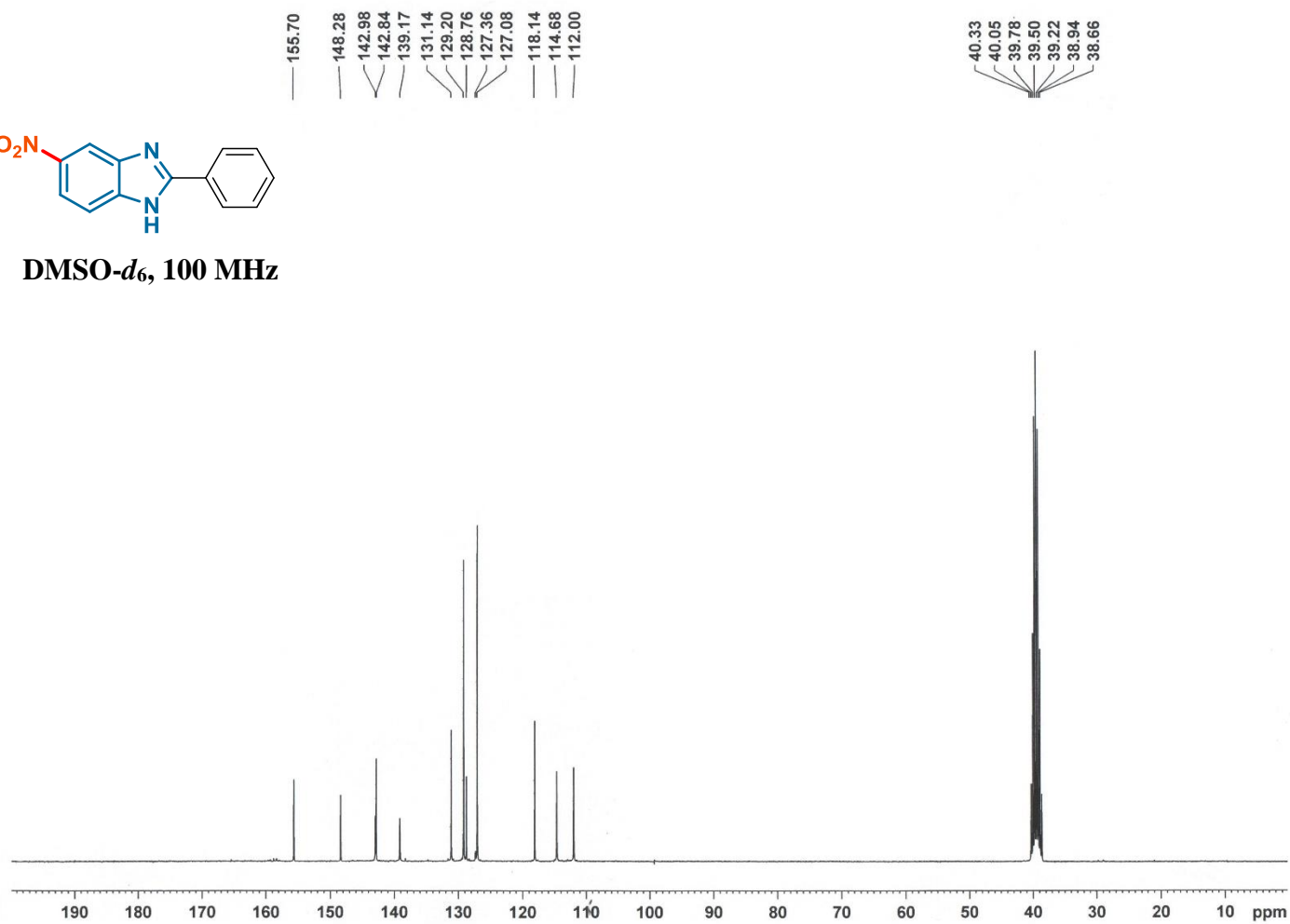
DMSO-*d*₆, 500 MHz



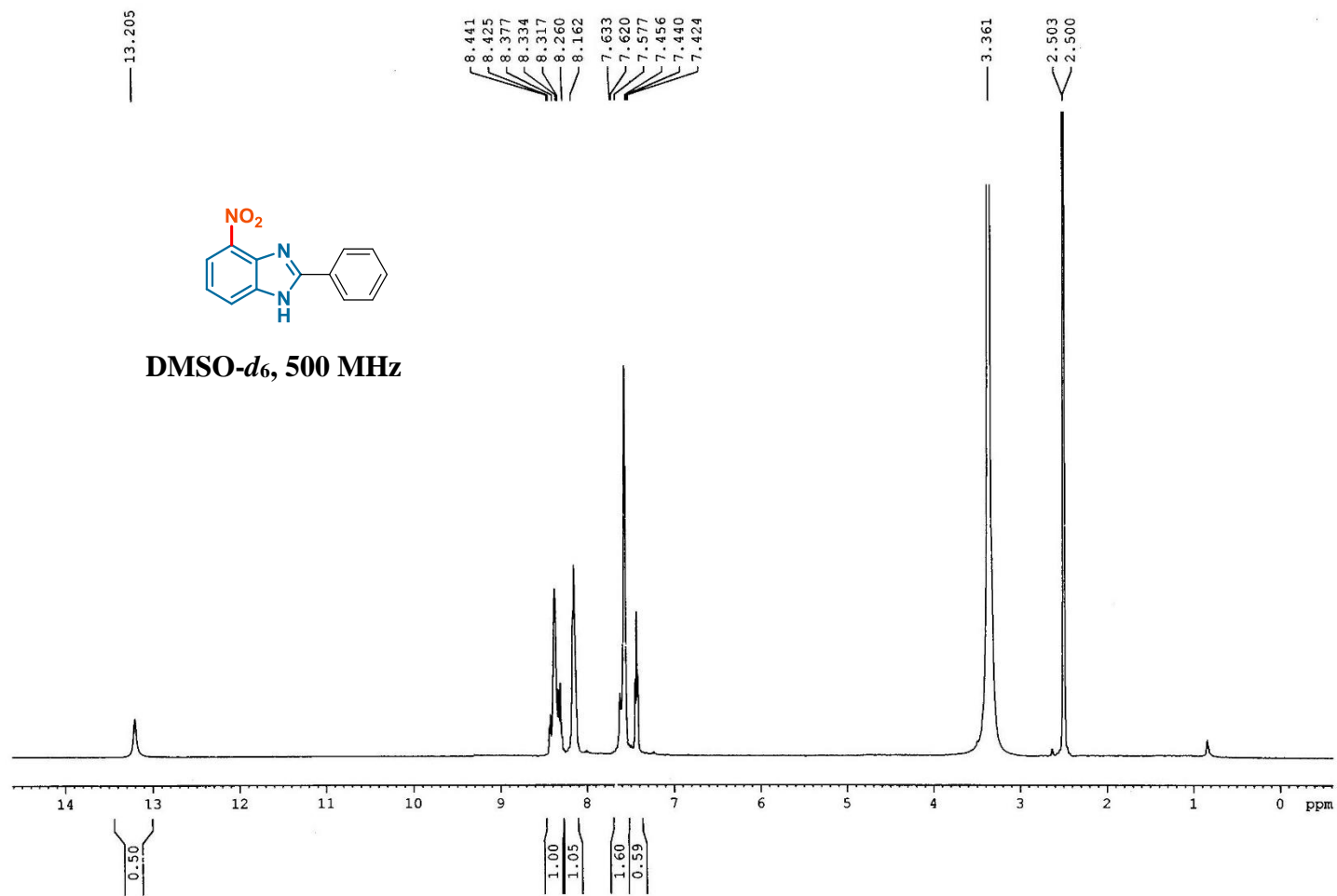
¹³C NMR of compound 5p



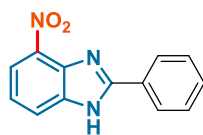
DMSO-*d*₆, 100 MHz



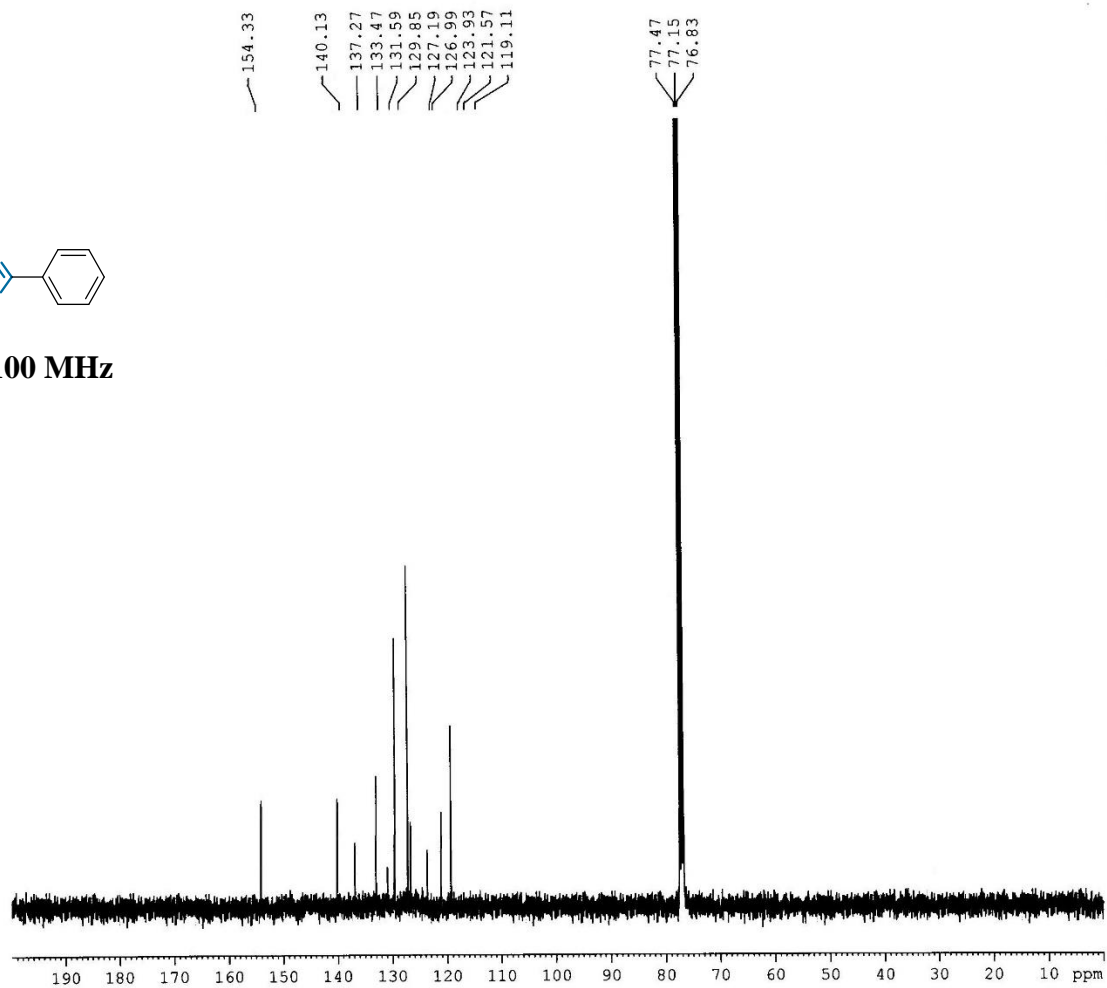
^1H NMR of compound 5q



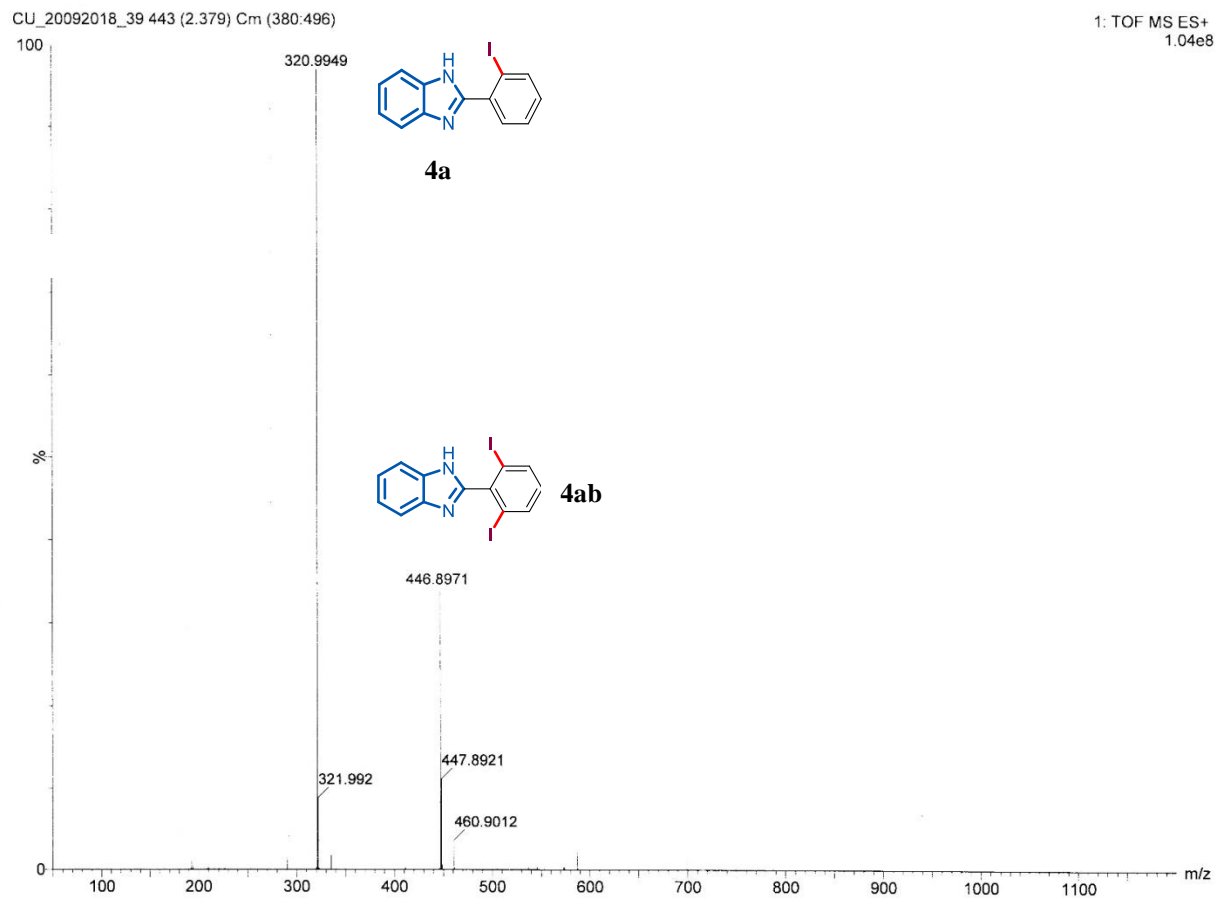
^{13}C NMR of compound 5q



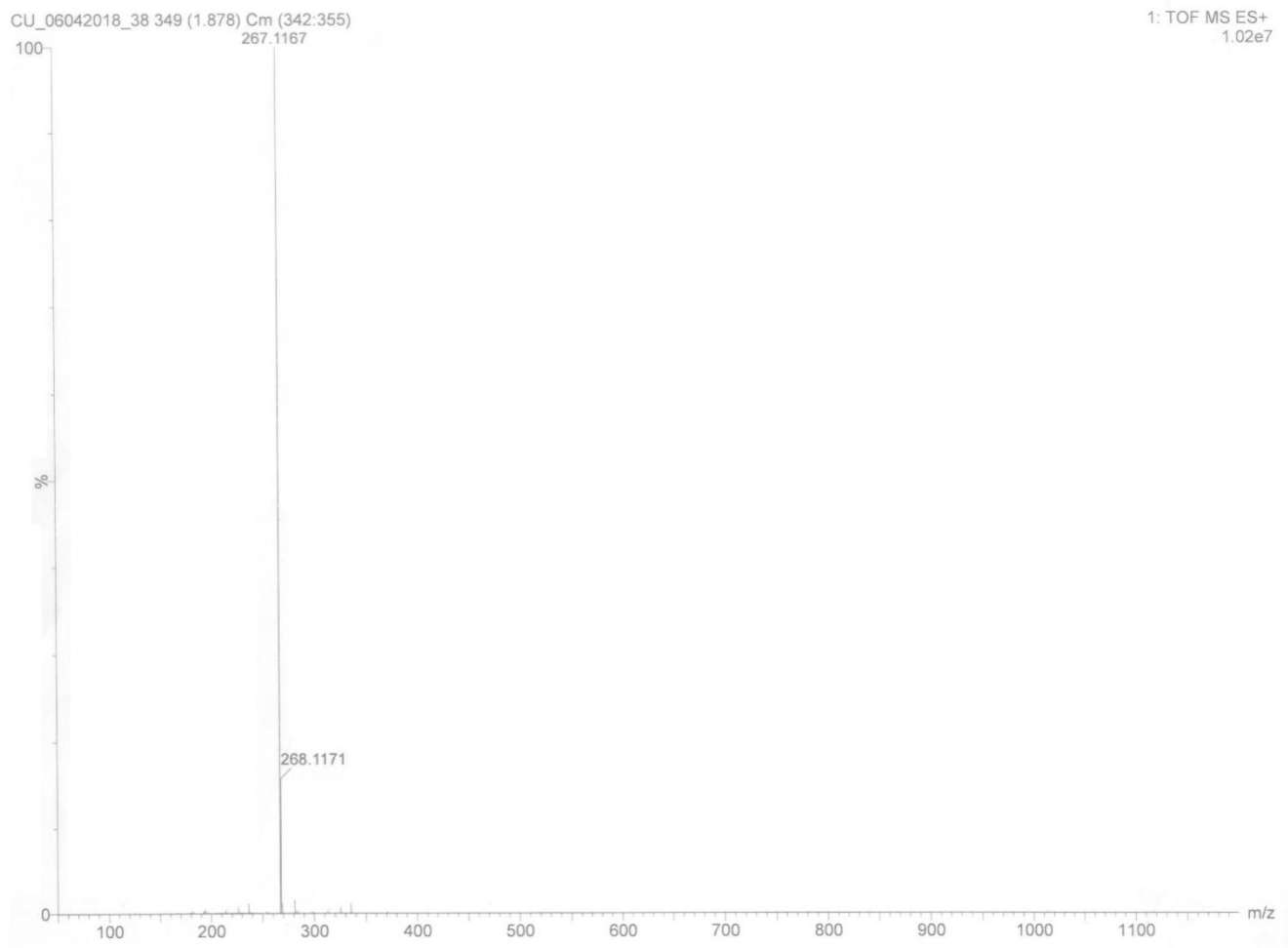
CDCl_3 , 100 MHz



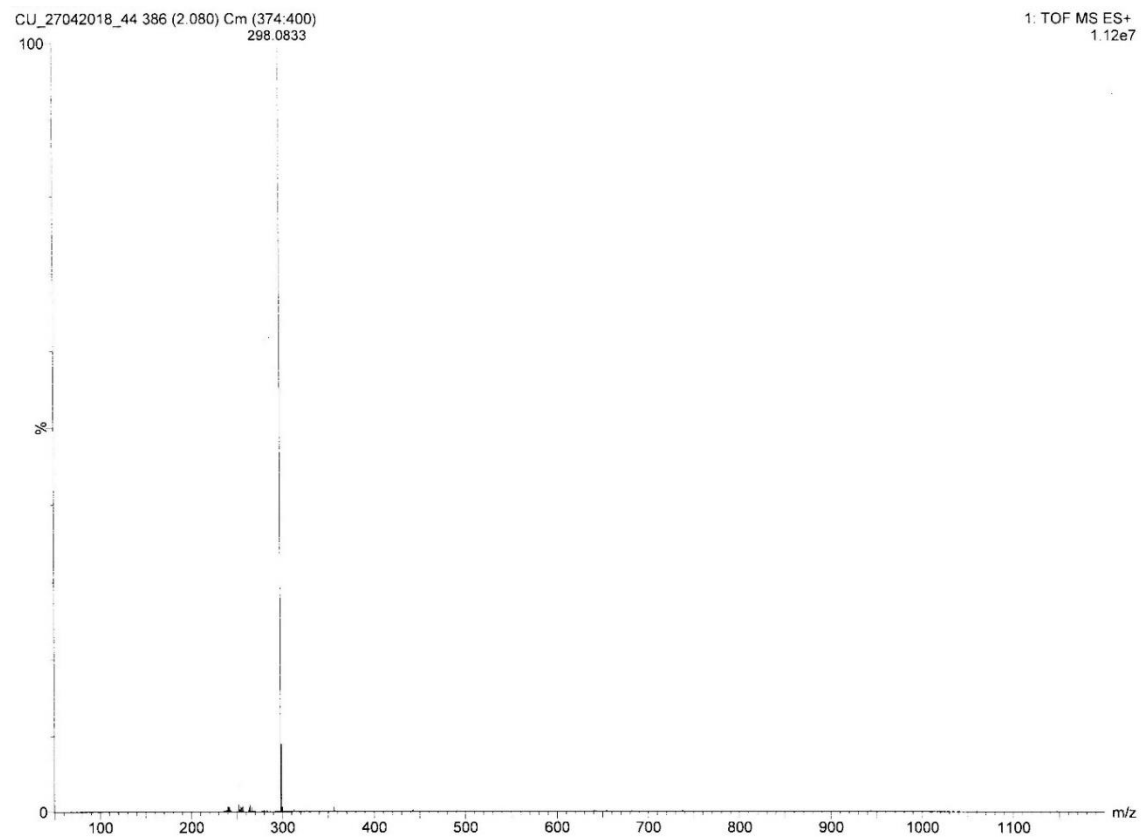
Mass spectrum of RM-1



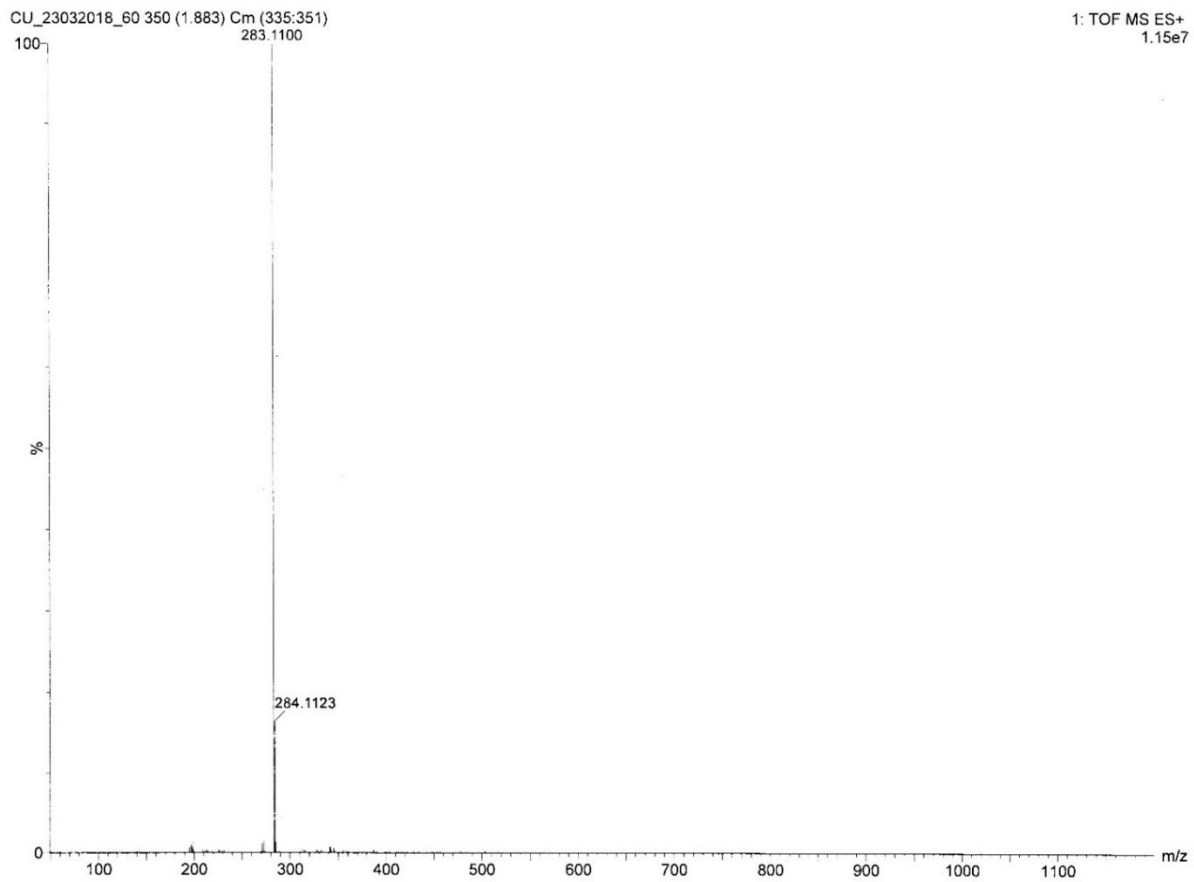
Mass spectrum of Compound 2e



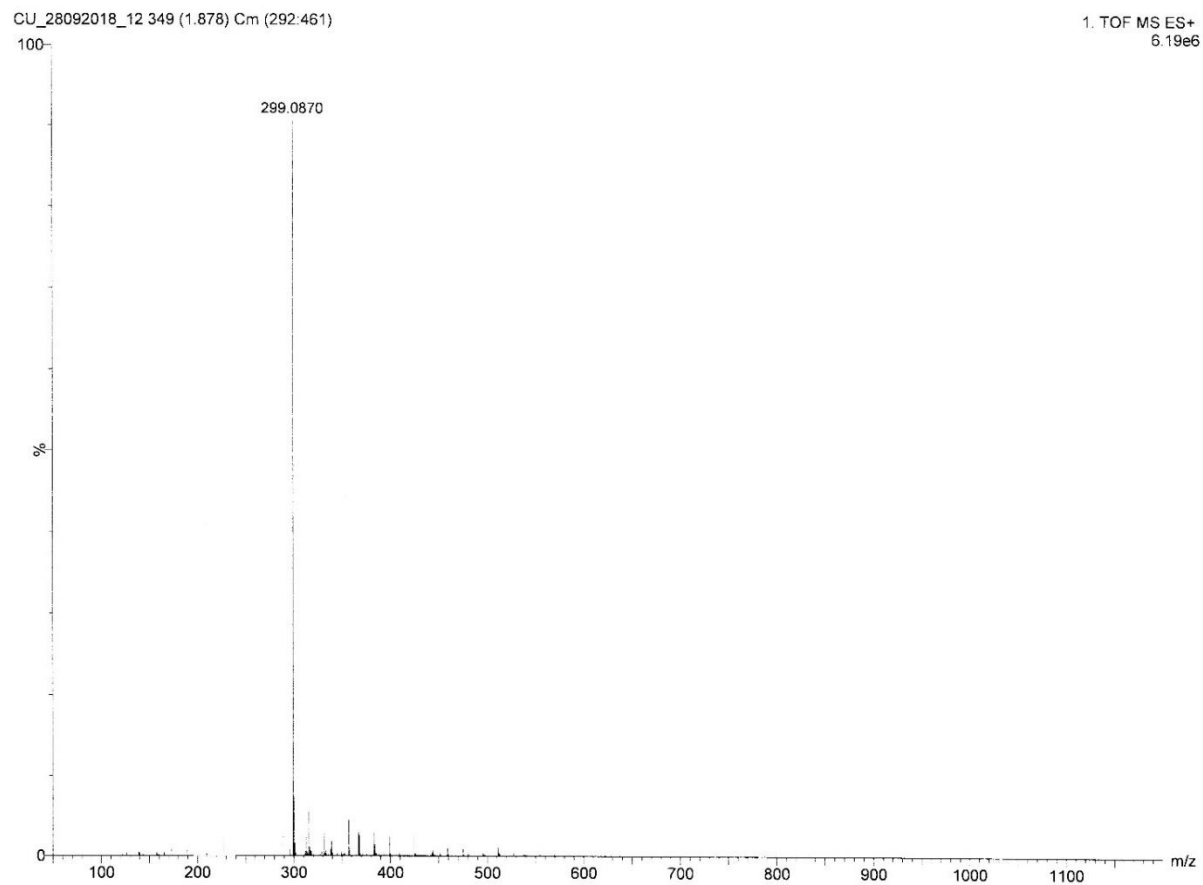
Mass spectrum of Compound 2f



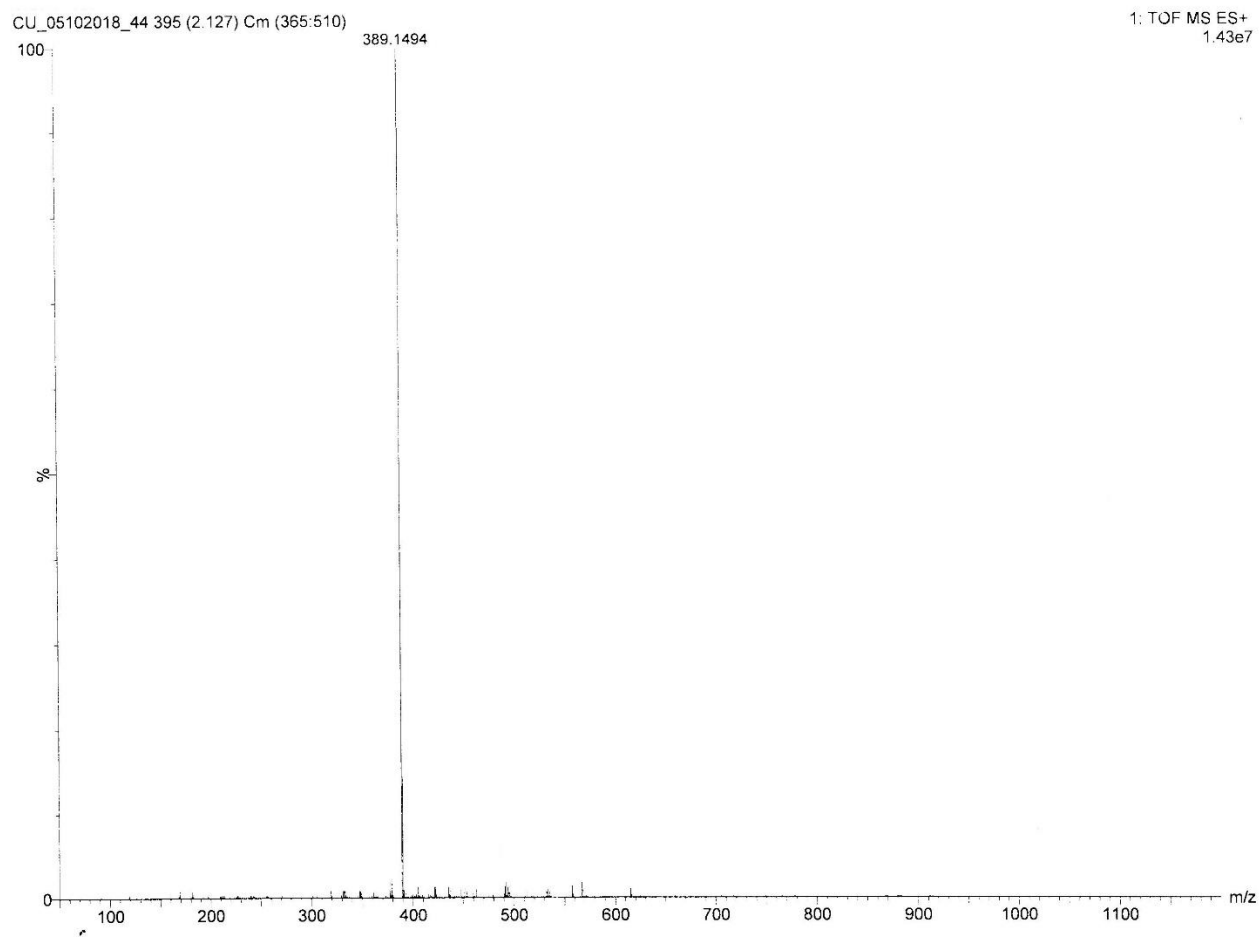
Mass spectrum of Compound 2i



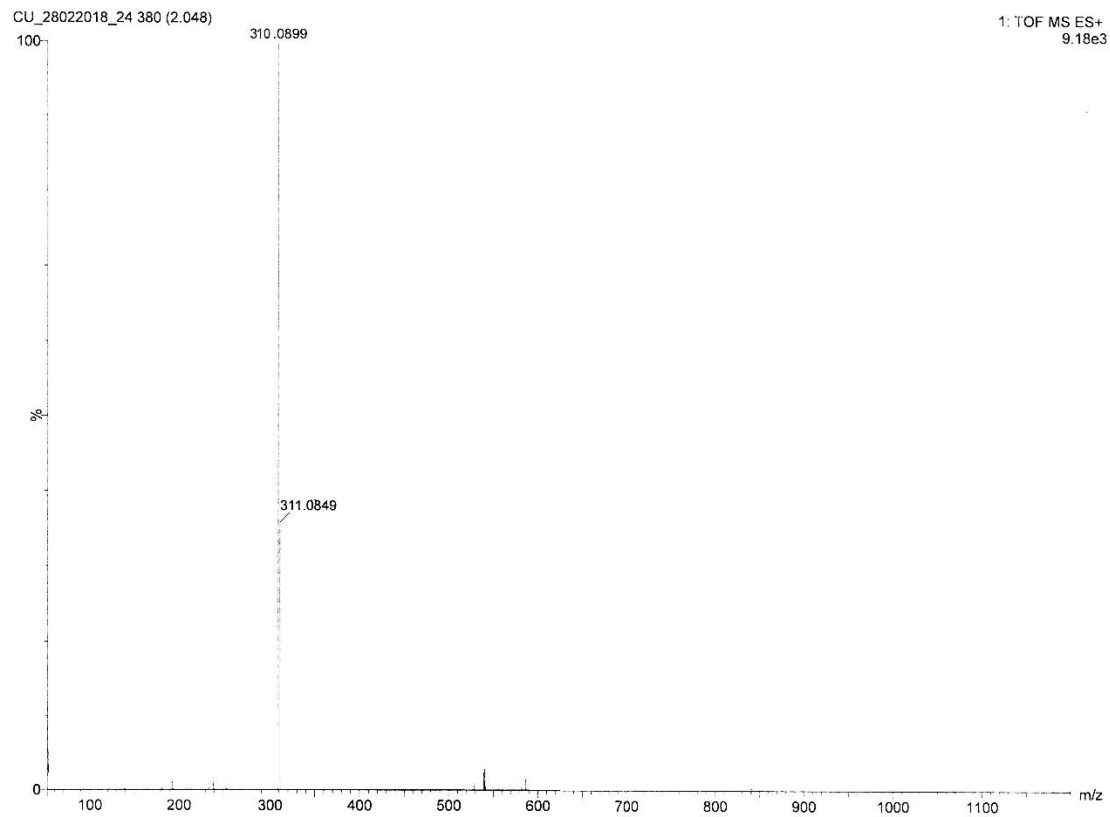
Mass spectrum of Compound 2j



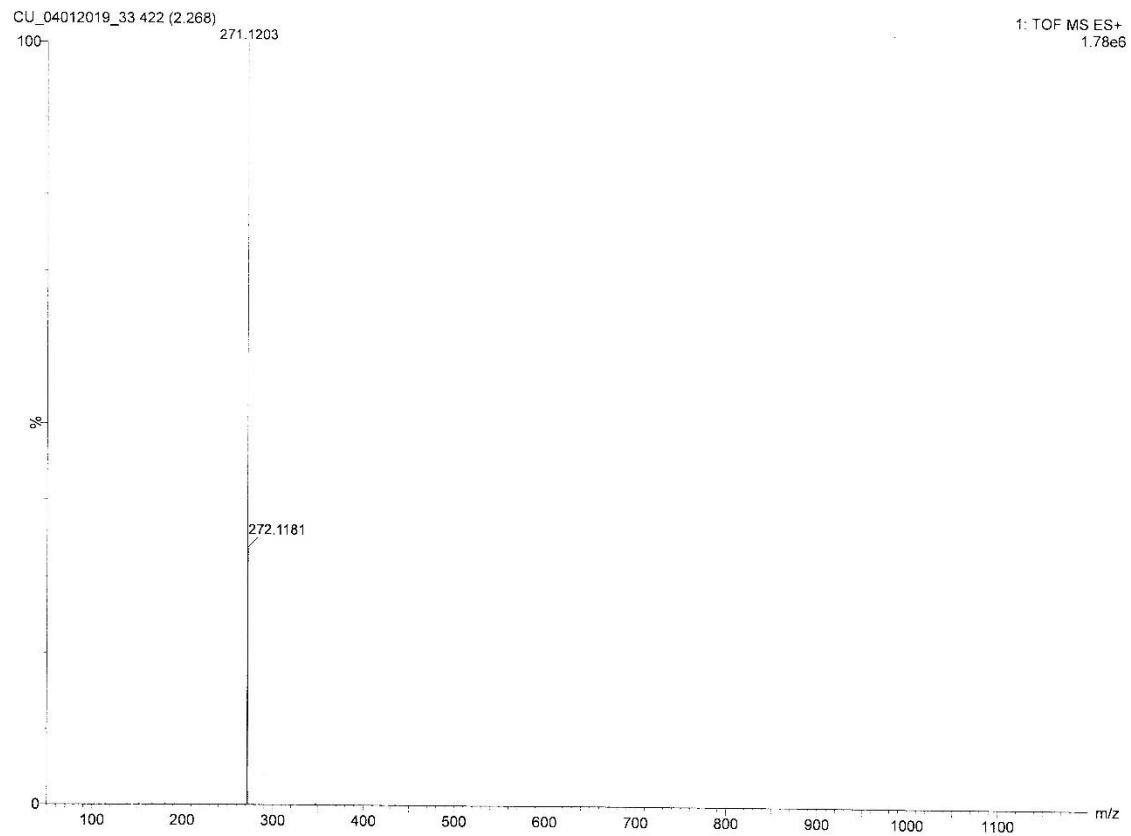
Mass spectrum of Compound 2k



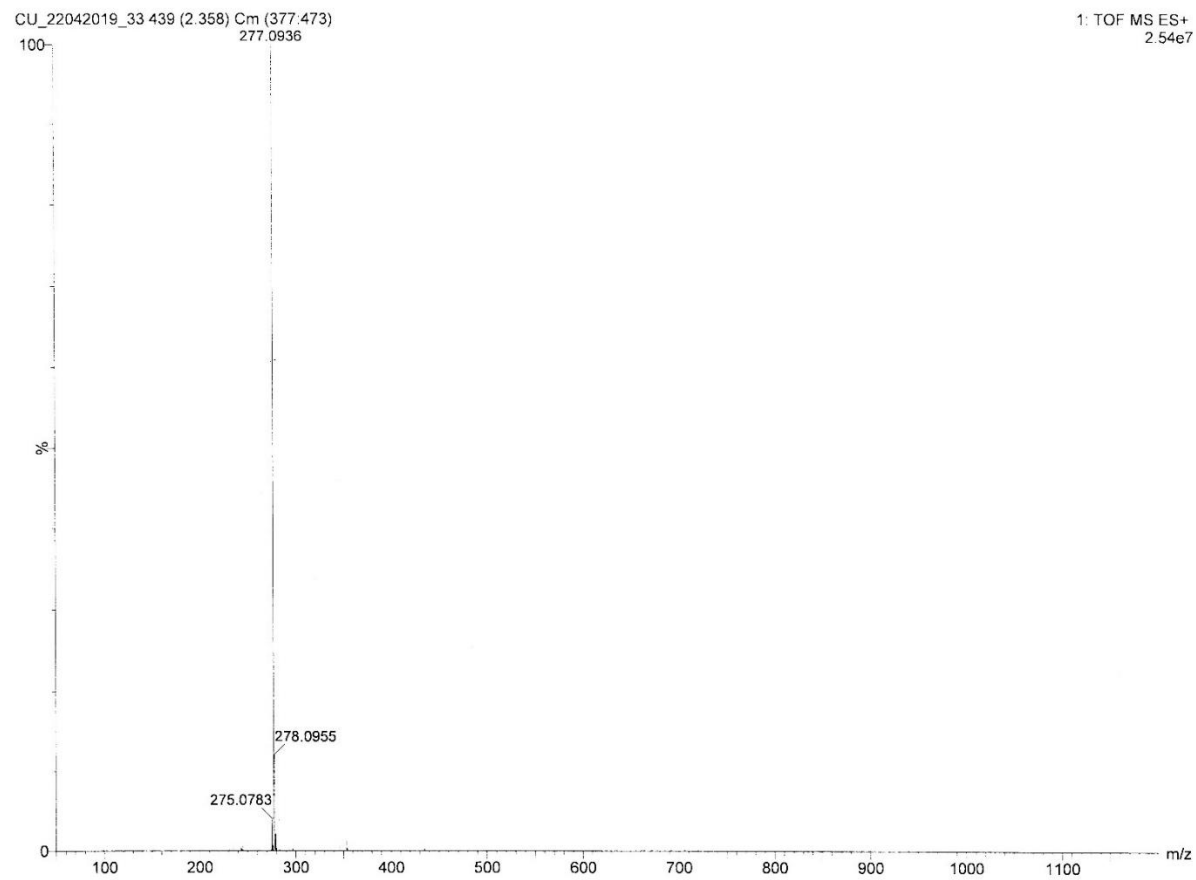
Mass spectrum of Compound 2m



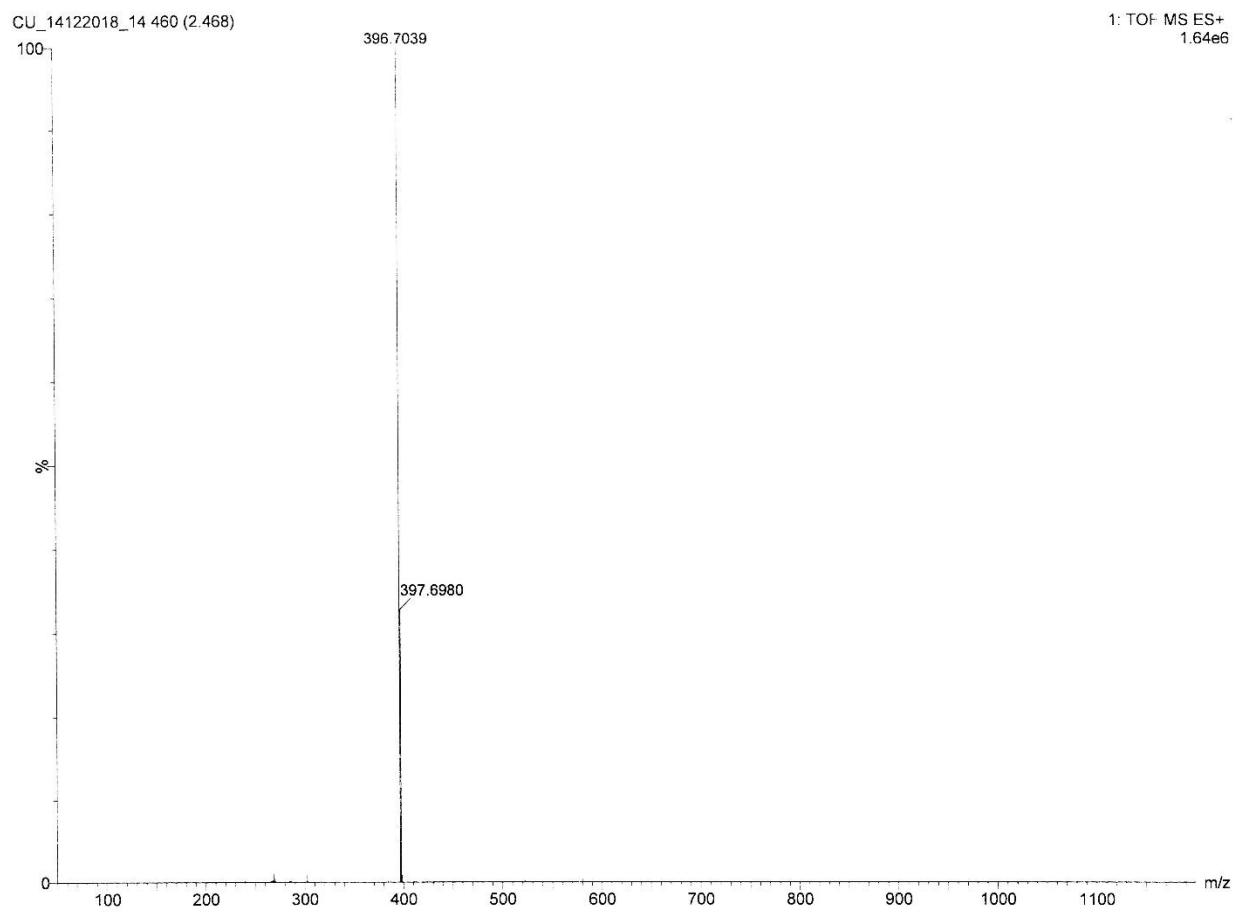
Mass spectrum of Compound 3a



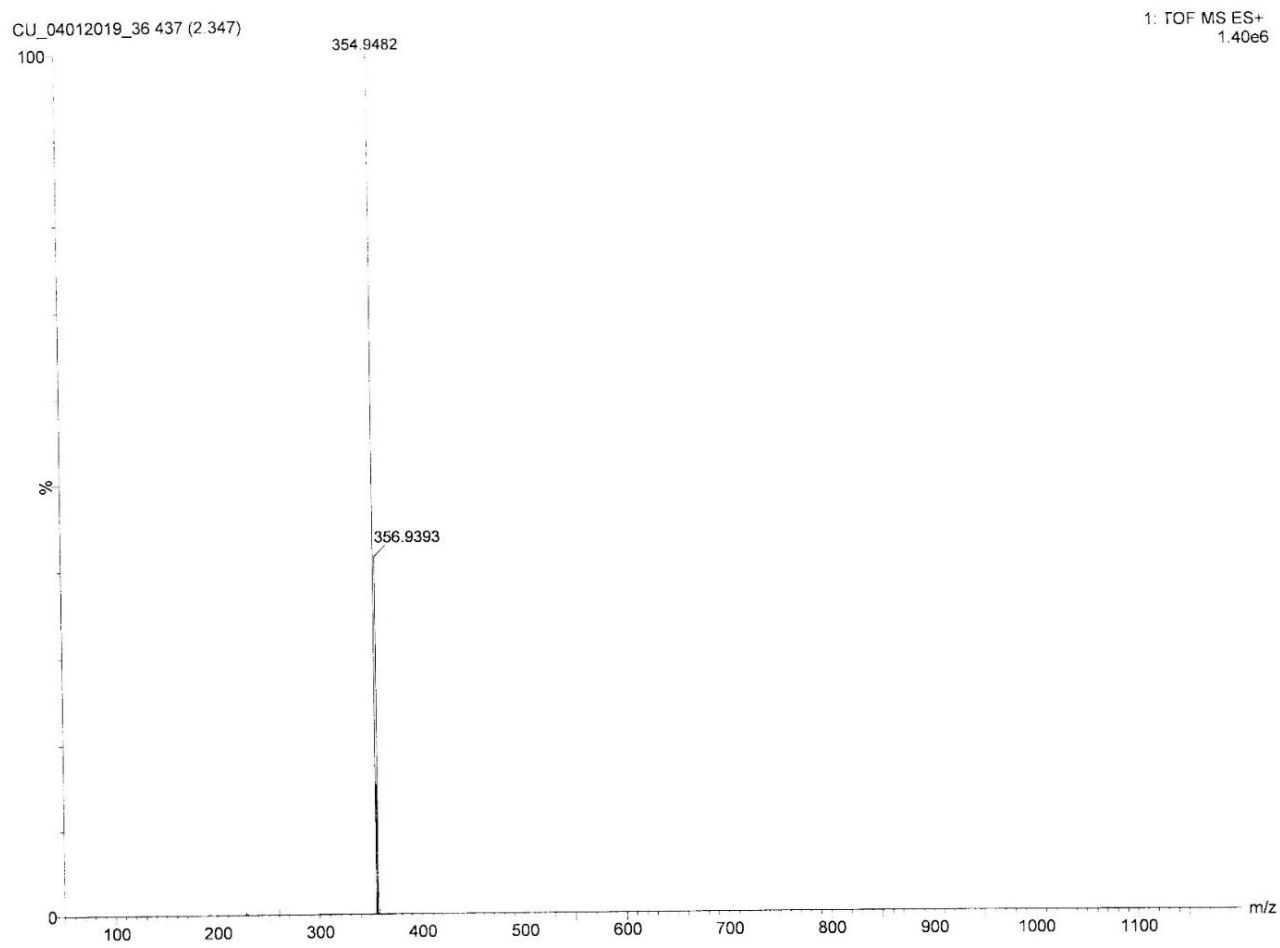
Mass spectrum of Compound 3c



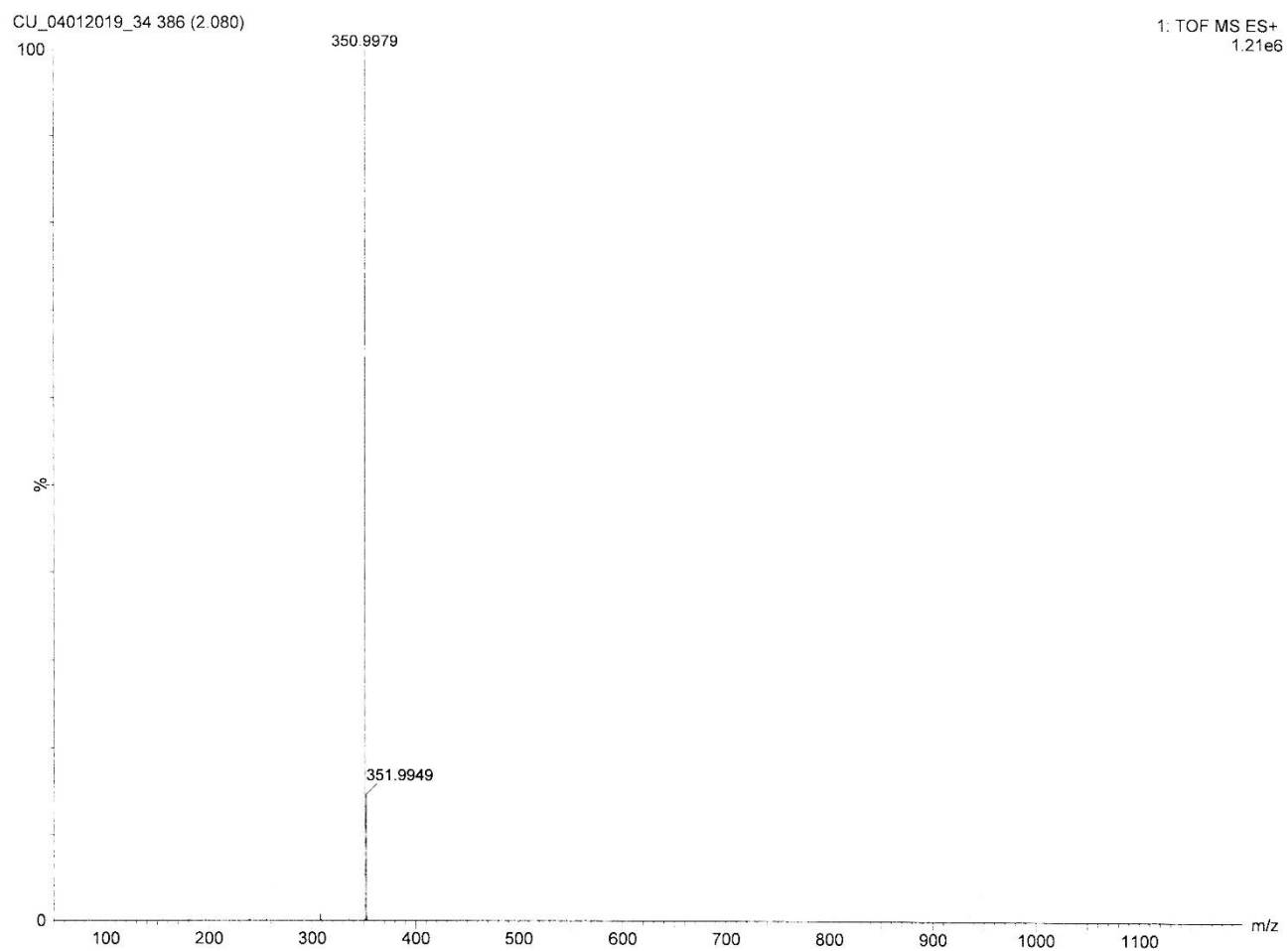
Mass spectrum of Compound 4h



Mass spectrum of Compound 4i



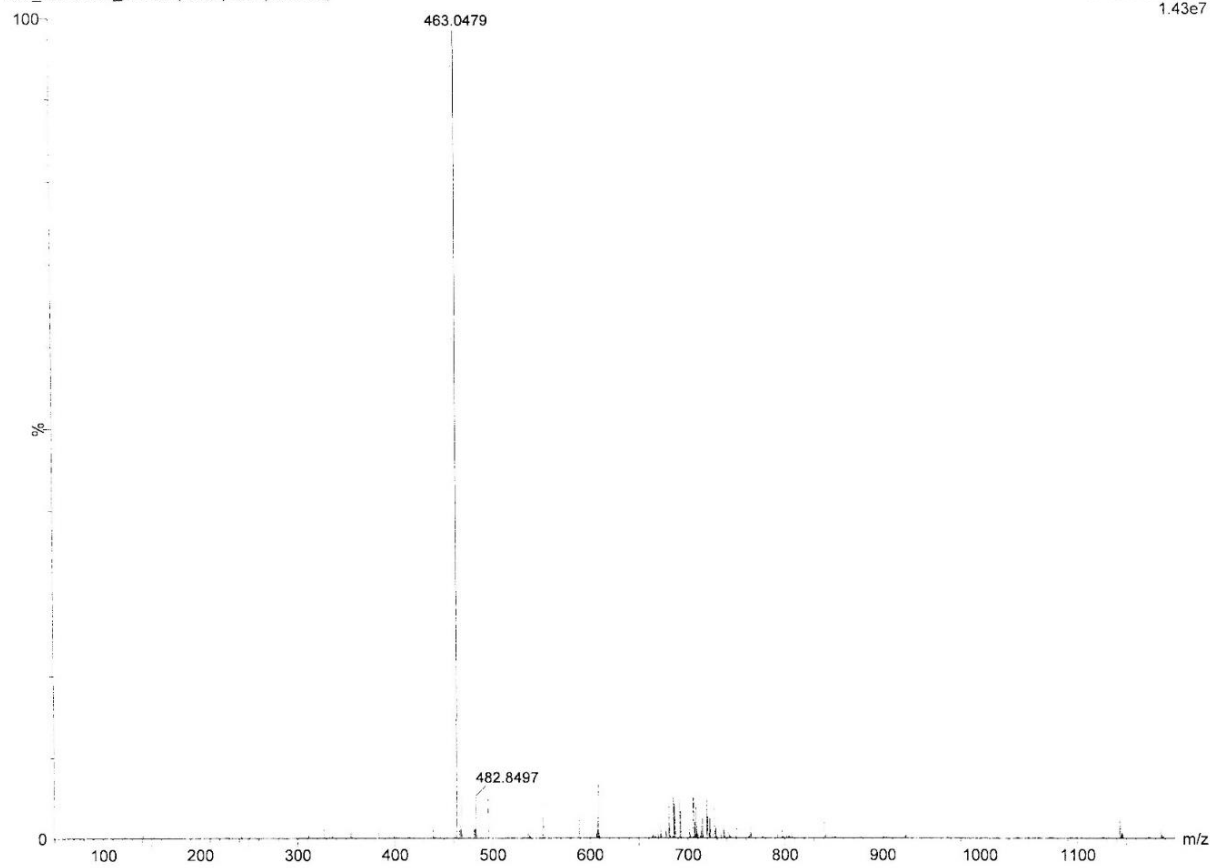
Mass spectrum of Compound 4k



Mass spectrum of Compound 4m

CU_22042019_31 651 (3.484) Cm (615-685)

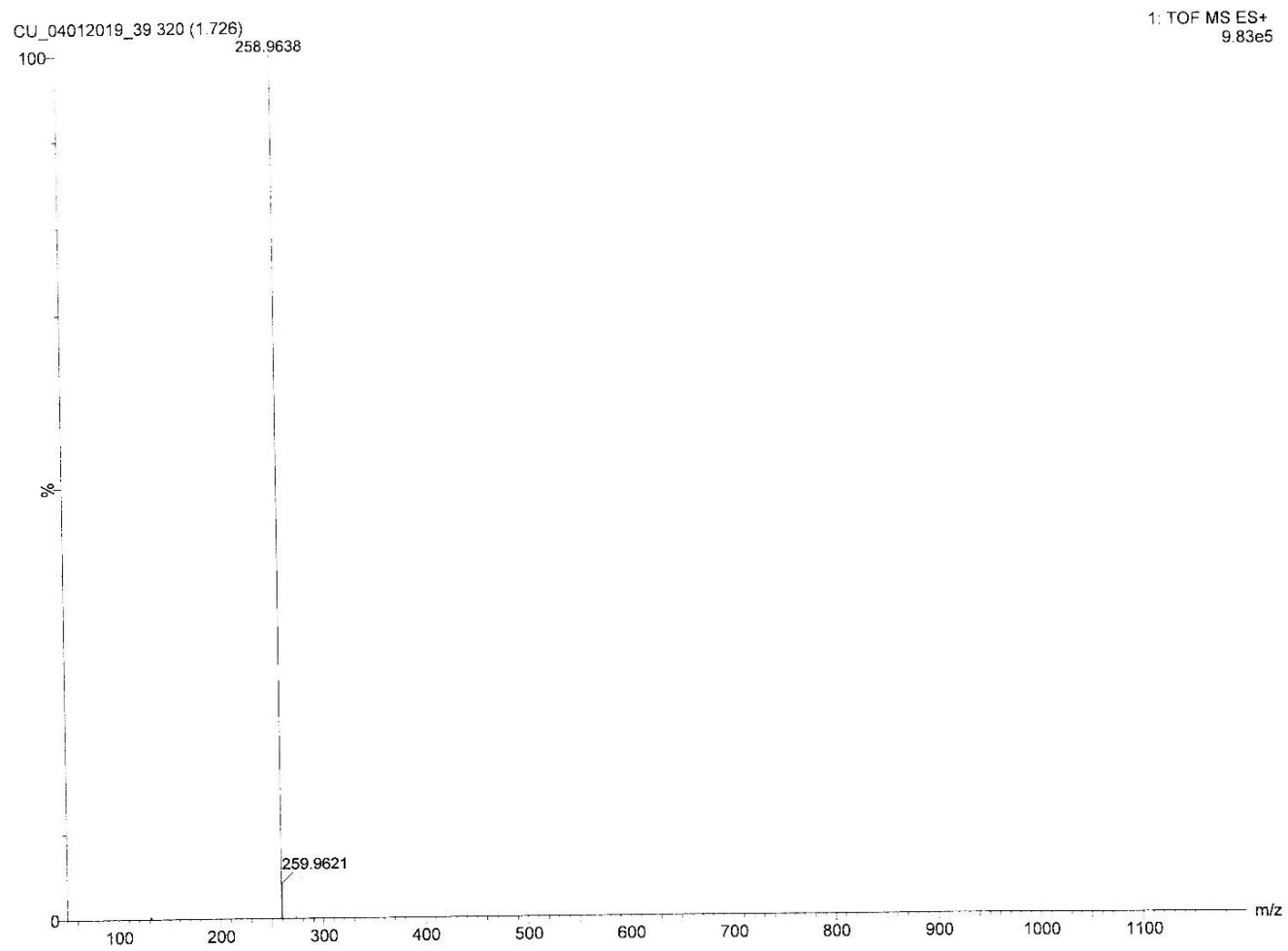
1: TOF MS ES+
1.43e7



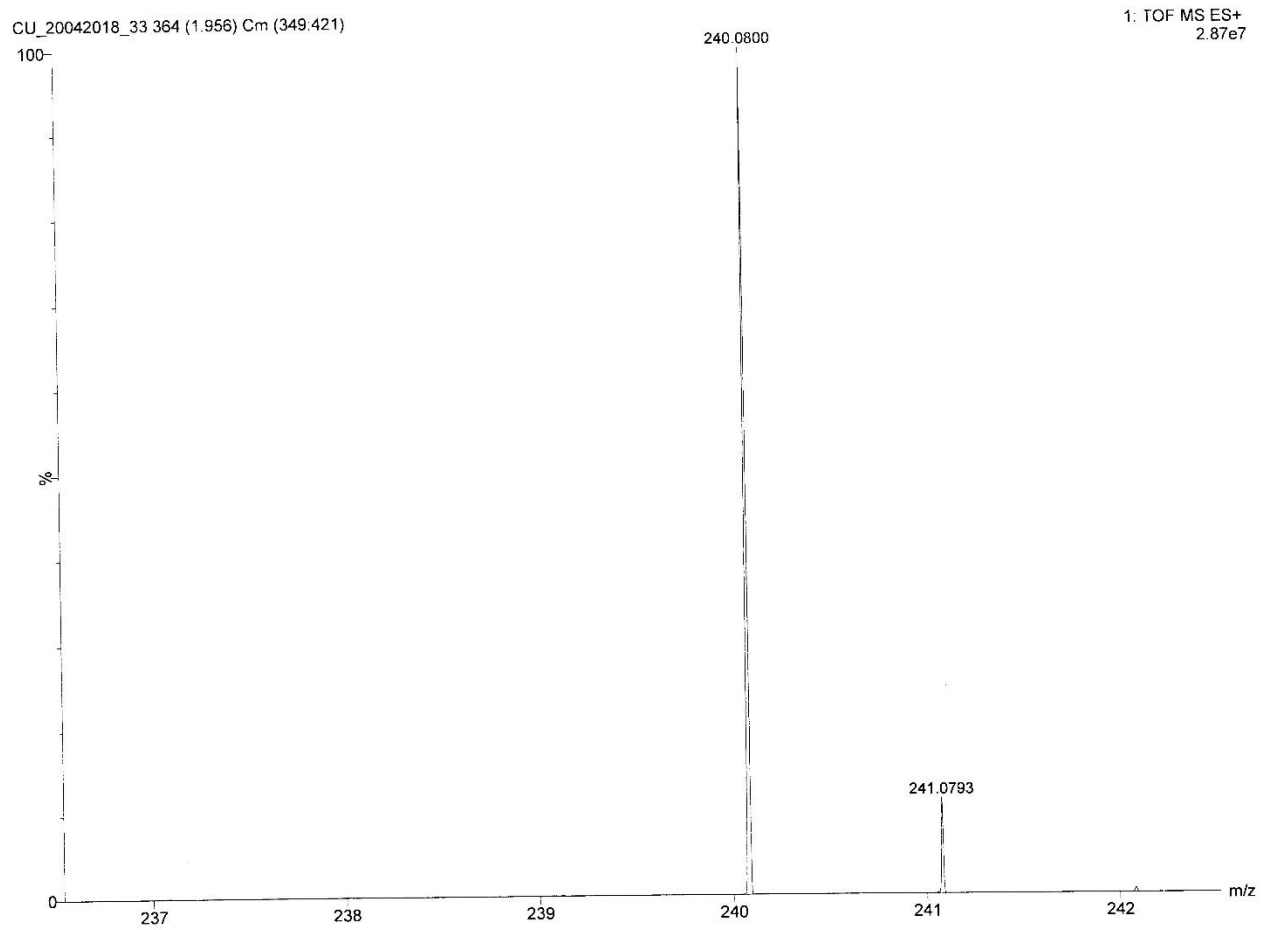
Mass spectrum of Compound 4n



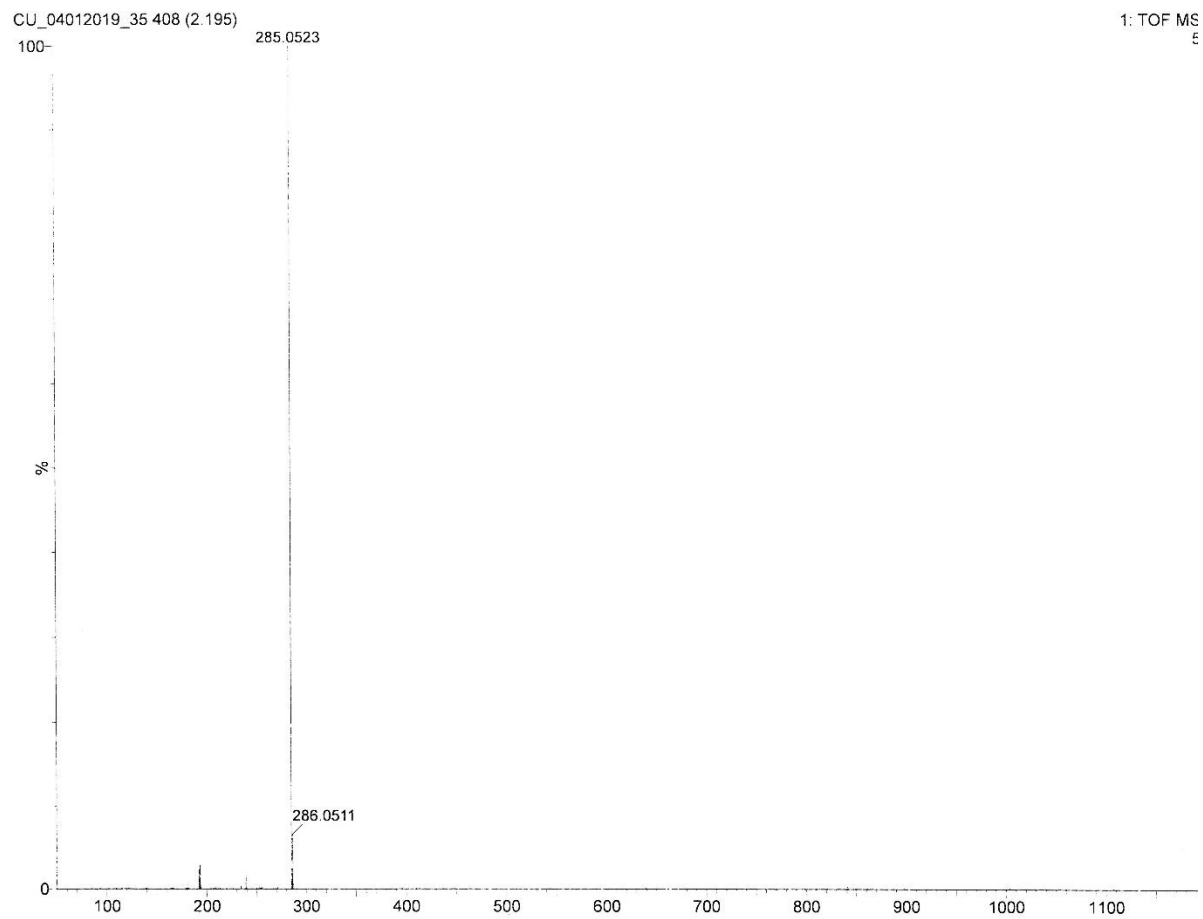
Mass spectrum of Compound 4r



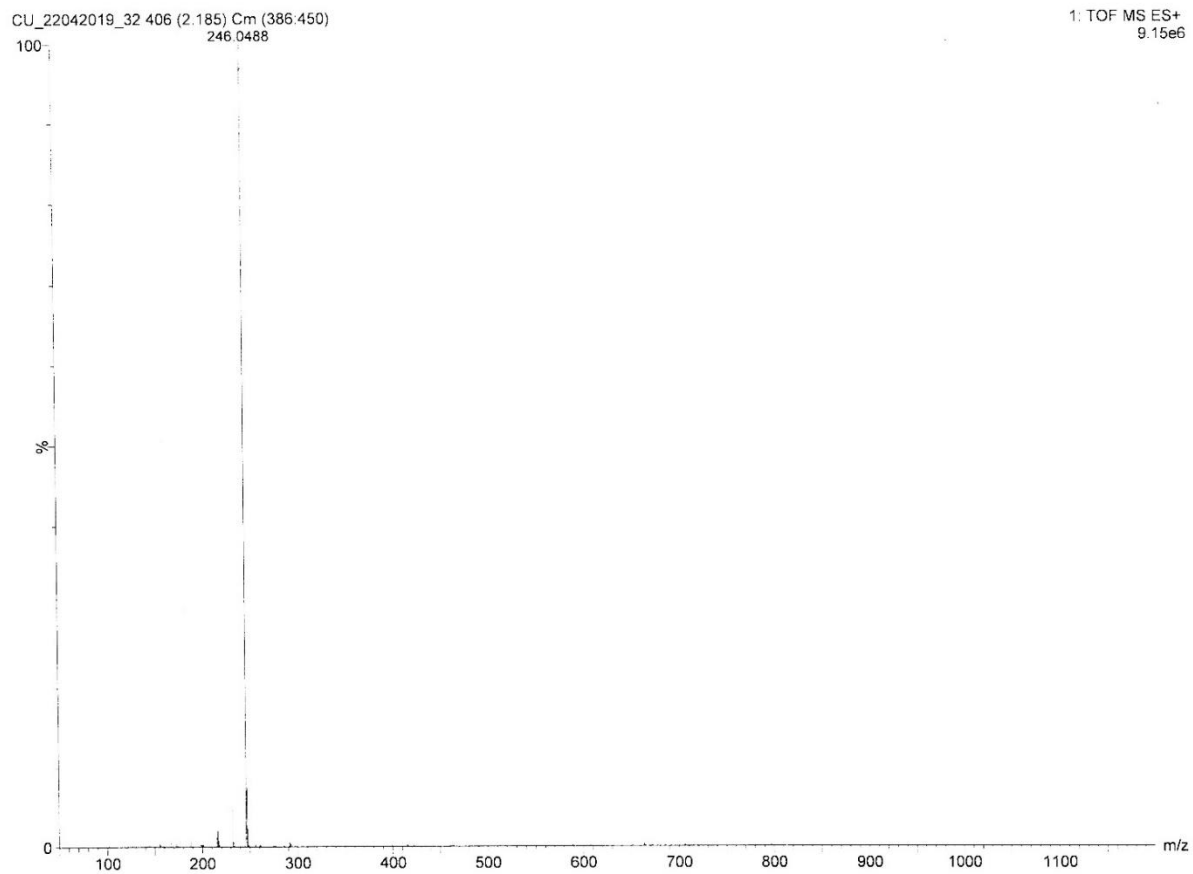
Mass spectrum of Compound 5a



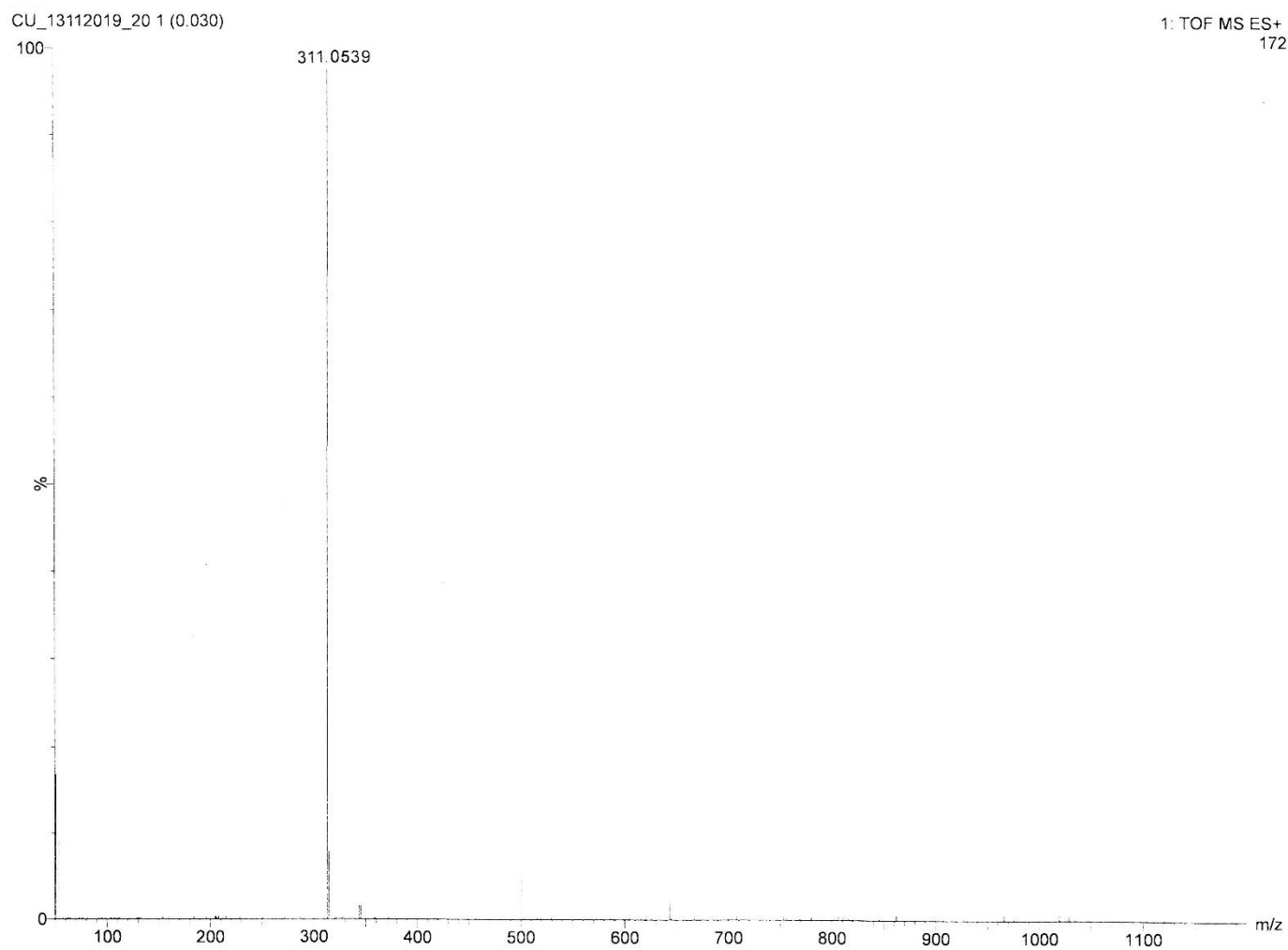
Mass spectrum of Compound 5b



Mass spectrum of Compound 5e



Mass spectrum of Compound 5k



Mass spectrum of Compound 5p

