Supporting Information

Copper-Catalyzed Multiple Oxidation and Cycloaddition of Aryl-Alkyl Ketones (Alcohols) for Synthesis of 4-Acyl- and 4-Diketo-1,2,3-Triazoles

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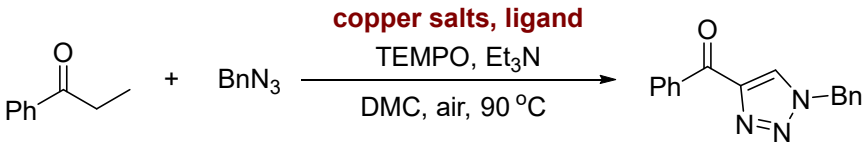
1. General information

All reactions were carried out in 10 mL or 25 mL round-bottom flasks with air condensers. Unless otherwise stated, all chemicals used in the experiments were obtained from commercial sources and used directly without further treatment. TLC was performed with the detection of compounds with UV light. Flash column chromatography purification of the products was accomplished on silica gel (200−300 mesh). petroleum ether (PE) (60−90 °C) and ethyl acetate (EA) were used as eluents for silica gel chromatography. Melting points for all solid products were measured on an X-4A melting point apparatus without correction. ^{1}H and ^{13}C NMR spectra were recorded at 22 °C on a Bruker AV 400 and 100 MHz spectrometers with tetramethylsilane (TMS) as an internal standard. 1H and ^{13}C chemical shifts in NMR spectra were referenced relative to signals of $CDCl_3$ (δ 7.26 ppm for ^{1}H and 77.0 ppm for ^{13}C). High-resolution mass spectra (HRMS) were acquired on Waters Acquity UPLC Class I/Xevo G2Q-TOF.

2. Optimization of the Reaction Conditions

2.1 synthesis of 4-acyl-1,2,3-triazoles

Table S1. Optimized copper slats and ligands

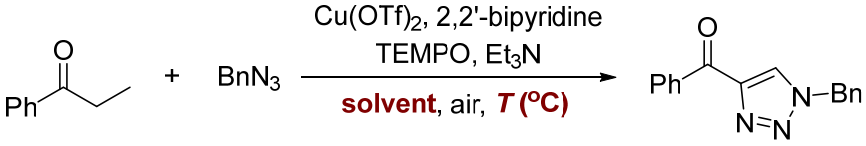


1a **2a** **3a**

entry	copper salts (10 mol %)	ligand (15 mol %)	yield
1	-	-	0
2	CuBr	-	48%
3	Cu_2O	-	15%
4	$CuBr_2$	-	50%
5	CuCl	-	45%
6	$Cu(OAc)_2·H_2O$	-	60%
7	CuI	-	17%
8	$Cu(acac)_2$	-	0%
9	$Cu(NO_3)_2$	-	0%
10	$Cu(OTf)_2$	-	64%
11	**$Cu(OTf)_2$**	**2,2'-bipyridine**	**95%**
12	$Cu(OTf)_2$	PPh_3	91%
13	$Cu(OTf)_2$	L-Proline	93%
14	$Cu(OTf)_2$	1,10-phen	89%

[a]Reaction conditions:**1a** (0.4 mmol, 1.0 equiv), **2a** (0.6 mmol, 1.5 equiv), copper salt (0.04 mmol, 10 mol%), ligand (0.06 mmol, 0.15 equiv), TEMPO (0.12 mmol, 0.3 equiv) and Et_3N (0.16 mmol, 0.4 equiv) in DMC (1 mL) under air atmosphere at 90 °C for 12 h. [b]Isolated yields based on **1a**.

Table S2. Optimized solvent

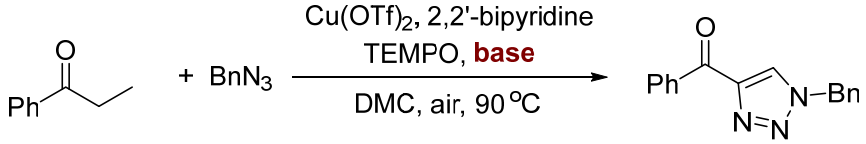


1a **2a** **3a**

entry	solvent	T (°C)	yield
1	toluene	90	89%
2	DMSO	90	0%
3	DMF	90	0%
4	**DMC**	**90**	**95%**
5	DMA	90	3%
6	CH_3CN	80	61%
7	1,4-dioxane	90	0%
8	THF	80	34%
9	H_2O	90	19%

[a]Reaction conditions: **1a** (0.4 mmol, 1.0 equiv), **2a** (0.6 mmol, 1.5 equiv), $Cu(OTf)_2$ (0.04 mmol, 10 mol%), 2,2'-bipyridine (0.06 mmol, 0.15 equiv), TEMPO (0.12 mmol, 0.3 equiv) and Et_3N (0.16 mmol, 0.4 equiv) in solvent (1 mL) under air atmosphere at 90 °C for 12 h. [b]Isolated yields based on **1a**.

Table S3. Optimized base

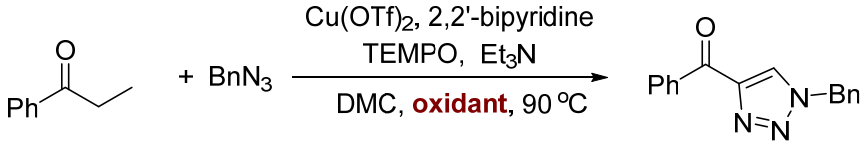


1a **2a** **3a**

entry	solvent	yield
1	**Et_3N**	**95%**
2	DBU	16%
3	TMAOH	12%
4	t-BuOK	0%
5	K_2CO_3	19%
6	$LiOH·H_2O$	0%
7	NaOH	trace
8	CS_2CO_3	0%
9	DABCO	0%

[a]Reaction conditions: **1a** (0.4 mmol, 1.0 equiv), **2a** (0.6 mmol, 1.5 equiv), $Cu(OTf)_2$ (0.04 mmol, 10 mol%), 2,2'-bipyridine (0.06 mmol, 0.15 equiv), TEMPO (0.12 mmol, 0.3 equiv) and base (0.16 mmol, 0.4 equiv) in DMC (1 mL) under air atmosphere at 90 °C for 12 h. [b]Isolated yields based on **1a**.

Table S4. Other oxidants

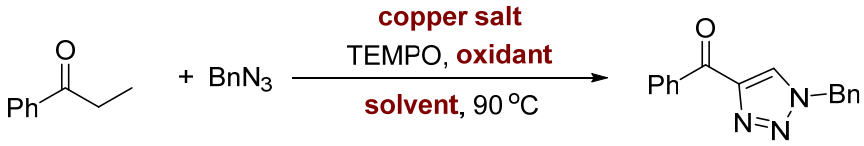


1a **2a** **3a**

entry	oxidant	yield
1	**Air**	**95%**
2	N_2	0
3	$K_2S_2O_8$	0%
4	DTBP	49%
5	Select-flour	0%
6	TBHP	51%
7	H_2O_2	71%

[a]Reaction conditions: **1a** (0.4 mmol, 1.0 equiv), **2a** (0.6 mmol, 1.5 equiv), $Cu(OTf)_2$ (0.04 mmol, 10 mol%), 2,2'-bipyridine (0.06 mmol, 0.15 equiv), oxidant (0.8 mmol, 2 equiv), TEMPO (0.12 mmol, 0.3 equiv) and Et_3N (0.16 mmol, 0.4 equiv) in DMC (1 mL) under air atmosphere at 90 °C for 12 h. [b]Isolated yields based on **1a**.

Table S5. Other catalytic systems optimization



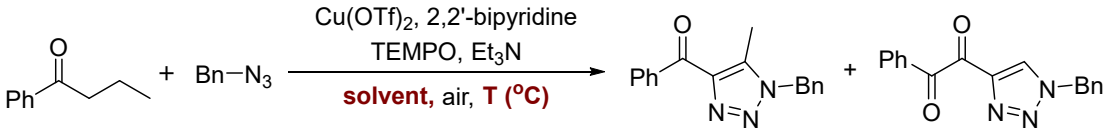
1a **2a** **3a**

entry	catalyst	oxidant	solvent	yield（%）
1	CuBr	TBHP	toluene	0
2	$Cu(OTf)_2$	TBHP	toluene	10
3	Cu_2O	TBHP	toluene	15
4	$CuBr_2$	TBHP	toluene	0
5	CuCl	TBHP	toluene	45
6	$Cu(OAc)_2·H_2O$	TBHP	toluene	60
7	CuI	TBHP	toluene	0
8	$Cu(acac)_2$	TBHP	toluene	0
9	$PdCl_2$	TBHP	toluene	trace
10	$Pd(OAc)_2$	TBHP	toluene	55
11	CH_3COOAg	TBHP	toluene	0
12	$RuCl_3$	TBHP	toluene	0
13	$Fe(NO_3)_2·9H_2O$	TBHP	toluene	15
14	CuO	TBHP	toluene	85
15	CuO	$K_2S_2O_8$	toluene	0
16	CuO	DTBP	toluene	79
17	CuO	Select-flour	toluene	0
18	**CuO**	**H_2O_2**	**toluene**	**93**
19	CuO	H_2O_2	DMSO	0
20	CuO	H_2O_2	DMF	0
21	CuO	H_2O_2	DMA	trace
22	CuO	H_2O_2	CH_3CN	61
23	CuO	H_2O_2	1,4-dioxane	0
24	CuO	H_2O_2	THF	34
25	CuO	H_2O_2	H_2O	10

[a]Reaction conditions: **1a** (0.4 mmol, 1.0 equiv), **2a** (0.6 mmol, 1.5 equiv), copper salt (0.04 mmol, 10 mol%), TEMPO (0.12 mmol, 0.3 equiv) and oxidant (1.2 mmol, 3 equiv) in toluene (1 mL) under air atmosphere at 100 °C for 12 h. [b]Isolated yields based on **1a**.

2.2 synthesis of 1,4-diketotriazole

Table S6. Optimized solvent and temperature

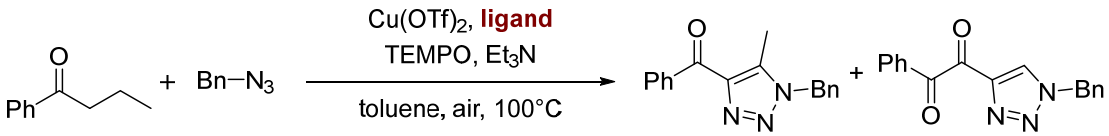


1b **2a** **5a** **6a**

entry	solvent	T (°C)	yield **5a**/**6a**
1	DMC	90	93%/<5%
2	toluene	90	80%/13%
3	DMSO	90	0%/0%
4	DMF	90	0%/0%
5	DMA	90	0%/<5%
6	CH_3CN	80	55%/<5%
7	1,4-dioxane	90	0%/0%
8	THF	80	34%/<5%
9	H_2O	90	19%/<5%
10	**toluene**	**100**	**70%/25%**
11	toluene	120	63%/15%

[a]Reaction conditions: **1b** (0.34 mmol, 1.0 equiv), **2a** (0.5 mmol, 1.5 equiv), $Cu(OTf)_2$ (0.034 mmol, 10 mol%), 2,2'-bipyridine (0.068 mmol, 0.2 equiv), TEMPO (0.14 mmol, 0.4 equiv) and Et_3N (0.16 mmol, 0.4 equiv) in toluene (1 mL) under air atmosphere at 100 °C for 24 h. [b]Isolated yields based on **1b**.

Table S7. Optimized ligands

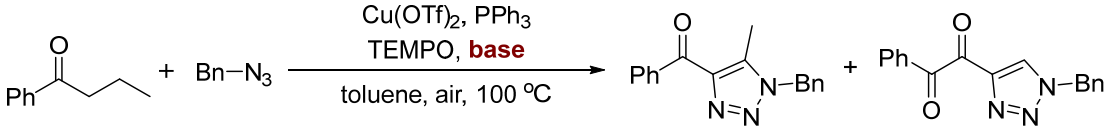


1b **2a** **5a** **6a**

entry	ligand	yield **5a**/**6a**
1	-	35%/<5%
2	2,2-bpy	70%/25%
3	**PPh_3**	**35%/52%**
4	L-proline	41%/20%
5	1,10- phenanthroline	31%/0%

[a]Reaction conditions: **1b** (0.34 mmol, 1.0 equiv), **2a** (0.5 mmol, 1.5 equiv), $Cu(OTf)_2$ (0.034 mmol, 10 mol%), ligand (0.068 mmol, 0.2 equiv), TEMPO (0.14 mmol, 0.4 equiv) and Et_3N (0.16 mmol, 0.4 equiv) in toluene (1 mL) under air atmosphere at 100 °C for 24 h. [b]Isolated yields based on **1b**.

Table S8. Optimized base

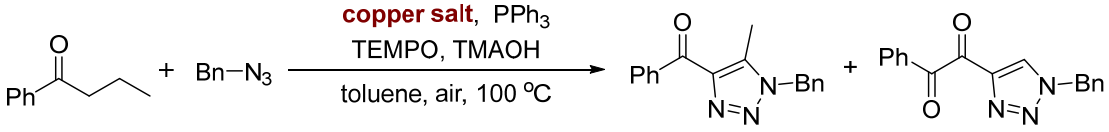


1b **2a** **5a** **6a**

entry	base	yield **5a**/**6a**
1	Et_3N	35%/52%
2	DBU	13%/<5%
3	*t*BuOK	0%/0%
4	**TMAOH**	**<5%/67%**
5	$LiOH·H_2O$	0%/0%
6	NaOH	0%/0%
7	CS_2CO_3	0%/0%
8	DABCO	<5%/11%
9	tetrahydropyrrole	<5%/<1%
10	pyridine	<5%/<1%

[a]Reaction conditions: **1b** (0.34 mmol, 1.0 equiv), **2a** (0.5 mmol, 1.5 equiv), $Cu(OTf)_2$ (0.034 mmol, 10 mol%), PPh_3 (0.068 mmol, 0.2 equiv), TEMPO (0.14 mmol, 0.4 equiv) and base (0.16 mmol, 0.4 equiv) in toluene (1 mL) under air atmosphere at 100 °C for 24 h. [b]Isolated yields based on **1b**.

Table S9. Optimized copper catalyst

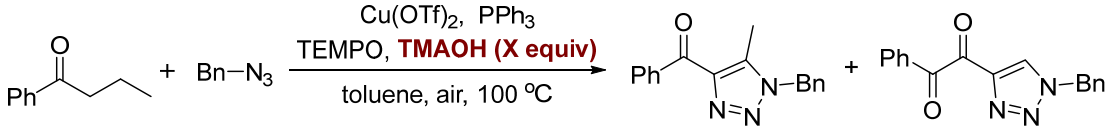


1b **2a** **5a** **6a**

entry	Cu catalyst	Yield **5a**/**6a**
1	**$Cu(OTf)_2$**	**<5%/67%**
2	$Cu(OAc)_2·H_2O$	<3%/<3%
3	CuI	<1%/<5%
4	$CuBr_2$	<5%/50%
5	CuCl	2%/41%
6	$CuSO_4$	2%/53%
7	$Cu(NO_3)_2·3H_2O$	0%/0%

[a]Reaction conditions: **1b** (0.34 mmol, 1.0 equiv), **2a** (0.5 mmol, 1.5 equiv), copper salt (0.034 mmol, 10 mol%), PPh_3 (0.068 mmol, 0.2 equiv), TEMPO (0.14 mmol, 0.4 equiv) and TMAOH (25% in methanol, 0.0425 mmol, 0.25 equiv) in toluene (1 mL) under air atmosphere at 100 °C for 24 h. [b]Isolated yields based on **1b**.

Table S10. Optimized equivalent of the base



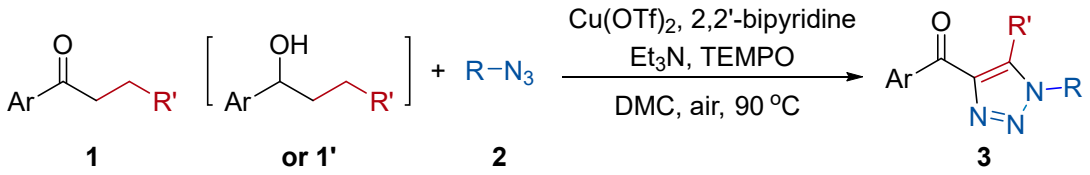
1b **2a** **5a** **6a**

entyr	Base loading	**yield of 5a/6a**
1	0.1 eq.	11%/71%
2	0.2 eq.	9%/83%
3	**0.25 eq.**	**3%/92%**
4	0.3 eq.	0%/67%
5	0.4 eq.	0%/32%
6	0.6 eq.	0%/25%
7	0.8 eq.	0%/9%
8	1 eq.	0%/<1%

[a]Reaction conditions: **1b** (0.34 mmol, 1.0 equiv), **2a** (0.5 mmol, 1.5 equiv), $Cu(OTf)_2$ (0.034 mmol, 10 mol%), PPh_3 (0.068 mmol, 0.2 equiv), TEMPO (0.14 mmol, 0.4 equiv) and TMAOH (25% in methanol, 0.1 - 1 equiv) in toluene (1 mL) under air atmosphere at 100 °C for 24 h. [b]Isolated yields based on **1b**.

3. Experimental Procedures

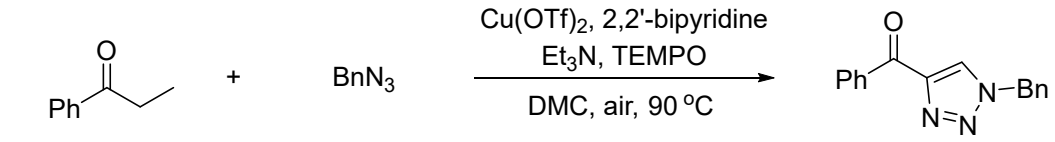
3.1 Typical procedure for synthesis of 4-acyl-1,2,3-triazoles



1 **or 1'** **2** **3**

To a solution of ketone **1** (0.4 mmol, 50 mg) and azide **2** (0.6 mmol, 74 mg) in DMC (1 mL) were added $Cu(OTf)_2$ (0.04 mmol, 10 mol%), 2,2'-bipyridine (0.06 mmol, 6 mg), TEMPO (0.12 mmol, 17.4 mg) and Et_3N (0.16 mmol, 16 mg); the mixture was stirred at 90 °C in oil bath under air atmosphere for 16 - 24 h. The reaction was checked by TLC. After completion of the reaction, the mixture was poured into water, extracted by ethyl acetate, and dried with anhydrous Na_2SO_4. The solvent was removed under reduced pressure to obtain crude product. Further purification by column chromatography on silica gel gave the 4-acyl-1,2,3-triazoles.

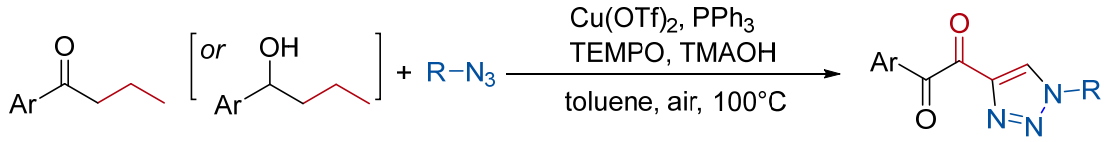
Large-scale synthesis of 3a



1a (1.0 g, 7.45 mmol) **2a** (1.5 g, 11.2 mmol) **3a** (1.39 g, 71%)

To a solution of ketone **1a** (1 g, 7.45 mmol, 1.0 equiv) and azide **2a** (1.5 g, 11.20 mmol, 1.5 equiv) in DMC (15 mL) were added $Cu(OTf)_2$ (0.27 g, 0.75 mmol, 10 mol%), 2,2'-bipyridine (0.17 g, 1.1 mmol, 15 mol%), TEMPO (0.35 g, 2.2 mmol, 0.3 equiv) and Et_3N (0.3 g, 2.98 mmol, 0.4 equiv); the mixture was stirred at 90 °C in oil bath under air atmosphere for 16 h. The reaction was checked by TLC. After completion of the reaction, the mixture was poured into water, extracted by ethyl acetate, and dried with anhydrous Na_2SO_4. The solvent was removed under reduced pressure to obtain crude product. Further purification by column chromatography on silica gel gave **3a**.

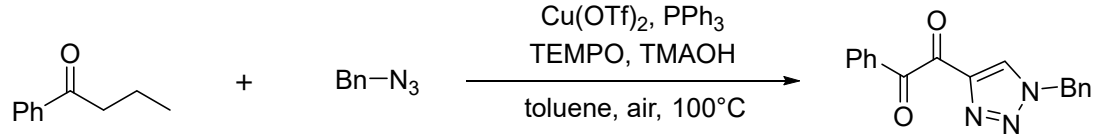
3.2 Typical procedure for synthesis of 1,4-diketotriazole



1 **or 1'** **2** **6**

To a solution of ketone **1** (0.34 mmol, 50 mg) and azide **2** (0.5 mmol, 68 mg) in toluene (1 mL) were added $Cu(OTf)_2$ (0.034mmol, 10 mol%), PPh_3 (0.068 mmol, 18 mg), TEMPO (0.14 mmol, 22 mg) and TMAOH (25% in methanol, 0.0425 mmol, 15 mg); the mixture was stirred at 100 °C in oil bath under an air atmosphere for 24 h. The reaction was checked by TLC. After completion of the reaction, the mixture was poured into water, extracted by ethyl acetate, and dried with anhydrous Na_2SO_4, and then the solvent was removed under reduced pressure to obtain crude product. Further purification by column chromatography on silica gel gave the α,β-diketotriazole.

Large-scale synthesis of 6a

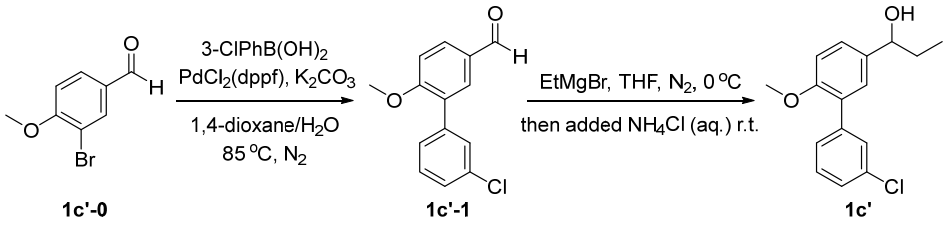


1b (1.0 g, 6.7 mmol) **2a** (1.5 g, 10.0 mmol) **6a** (1.27 g, 65%)

To a solution of ketone **1b** (1.0 g, 6.70 mmol, 1.0 equiv) and azide **2a** (1.3 g, 10.0 mmol, 1.5 equiv) in toluene (20 mL) were added $Cu(OTf)_2$ (0.24 g, 0.67 mmol, 10 mol%), PPh_3 (0.35 g, 1.34 mmol, 20 mol%), TEMPO (0.42 g, 2.68 mmol, 0.4 equiv) and TMAOH (25% in methanol, 0.6 g, 1.7 mmol, 0.25 equiv); the mixture was stirred at 100 °C in oil bath under an air atmosphere for 24 h. The reaction was checked by TLC. After completion of the reaction, the mixture was poured into water, extracted by ethyl acetate and dried with anhydrous Na_2SO_4, and then the solvent was removed under reduced pressure to obtain crude product. Further purification by column chromatography on silica gel gave the **6a**.

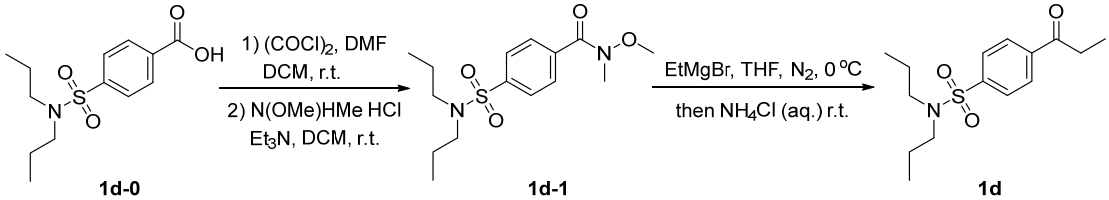
3.3 Synthesis application

1-(3'-chloro-6-methoxy-[1,1'-biphenyl]-3-yl)propan-1-ol (1c')



To a solution of 3-bromo-4-methoxybenzaldehyde (**1c'-0**, 108 mg, 0.5 mmol), (3-chlorophenyl)boronic acid (94 mg, 0.6 mmol), $PdCl_2$(dppf) (18 mg, 0.025 mmol), K_2CO_3 (138 mg, 1 mmol) in 1,4-dioxane/H_2O (v/v = 4:1, 2 mL, 0.25 M) under N_2 at 85 °C for 4 hours. After completion of the reaction, the mixture was diluted with ethyl acetate (15 mL), washed with saturated brine (5 mL for three times), and dried over Na_2SO_4. The solvent was removed under vacuum to give **1c'-1** without further purification. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 9.92 (s, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.82 (s, 1H), 7.51 (s, 1H), 7.39 – 7.31 (m, 3H), 7.09 (d, *J* = 8.0 Hz, 1H), 3.90 (s, 3H). Spectral data match those previously reported in the literature.[1] Under N_2 atmosphere, a solution of the aldehyde **1c'-1** in THF (2 mL) was added dropwise EtMgBr (1.0 M in THF, 1.05 mL, 1.05 mmol) at 0 °C. The mixture was warmed to room temperature for 2 hours. After completion of the reaction, saturated aqueous NH_4Cl solution (0.5 mL) was added. The mixture was extracted with EtOAc. The organic layer was then washed with brine and dried over Na_2SO_4. The solvent was removed under vacuum and finally purified by silica gel rapid chromatography (Petroleum ether / ethyl acetate) to give product **1c'** as colorless oil (112 mg, 81% yield for two steps). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.55 (s, 1H), 7.43 (d, *J* = 6.9 Hz, 1H), 7.34 (d, *J* = 8.5 Hz, 4H), 6.98 (d, *J* = 8.4 Hz, 1H), 4.61 (t, *J* = 6.1 Hz, 1H), 3.84 (s, 3H), 1.99 – 1.64 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H)； **^{13}C NMR (100 MHz, $CDCl_3$):** δ 155.8, 140.2, 137.0, 133.8, 129.6, 129.2, 128.5, 127.7, 127.0, 126.7, 111.2, 75.5, 55.7, 31.9, 10.2.

4-propionyl-N,N-dipropylbenzenesulfonamide (1d)

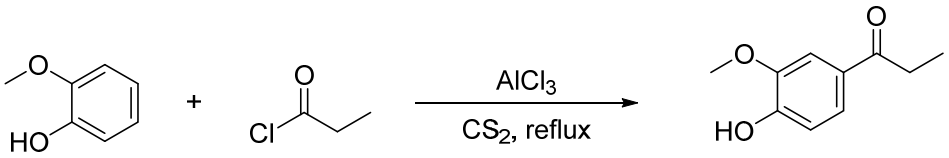


To a solution of probenecid (**1d-0**, 143 mg, 0.5 mmol) in DCM (5 mL) was added DMF (1.8 mg, 0.0025 mmol) and oxalyl chloride (2.0 M in DCM, 1 mL) at room temperature. The mixture was stirred for 1 hours and the solvent was removed under vacuum. The residue solid

was dissolved in DCM (2 mL) at 0 °C. To this solution was slowly added *N,O*-dimethylhydroxylamine hydrochloride (74 mg, 0.75 mmol), and triethylamine (126 mg, 1.25 mmol) and stirred for 2 hours at room temperature. After completion of the reaction, more DCM (25 mL) was added to the mixture. Then, the organic phase was washed with HCl solution (4.0 M in H_2O, 5 mL for three times), saturation Na_2CO_3 solution (5 mL for three times), brine (5 mL for three times), and dried with anhydrous Na_2SO_4. The solvent was removed under vacuum to give Weinreb amine **1d-1** (156 mg, 95% yield) as white solid. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.84 (d, *J* = 8.1 Hz, 2H), 7.78 (d, *J* = 8.1 Hz, 2H), 3.52 (s, 3H), 3.38 (s, 3H), 3.09 (t, *J* = 7.7 Hz, 4H), 1.77 – 1.42 (m, 4H), 0.87 (t, *J* = 7.3 Hz, 6H).

To a solution of Weinreb amine **1d-1** (120 mg, 0.36 mmol) in THF (2 mL) was added dropwise EtMgBr (1.0 M in THF, 0.4 mL, 0.4 mmol) at - 20 °C. The mixture was warmed to room temperature for 8 hours. After completion of the reaction, saturated aqueous NH_4Cl solution (1 mL) was added and the mixture was extracted with EtOAc. The organic layer was then washed with brine and dried over Na_2SO_4. The solvent was removed under vacuum and finally purified by silica gel rapid chromatography (Petroleum ether / ethyl acetate) to give product **1d** as white solid (90 mg, 83%). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.10 – 8.00 (m, 2H), 7.88 (d, *J* = 8.2 Hz, 2H), 3.09 (t, *J* = 7.5 Hz, 4H), 3.03 – 2.99 (m, 2H), 1.59 – 1.46 (m, 4H), 1.22 (d, *J* = 7.2 Hz, 3H), 0.85 (t, *J* = 7.3 Hz, 6H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 199.6, 144.0, 139.5, 128.5, 127.2, 49.9, 32.2, 21.9, 11.1, 7.9.

1-(4-hydroxy-3-methoxyphenyl)propan-1-one (1e)

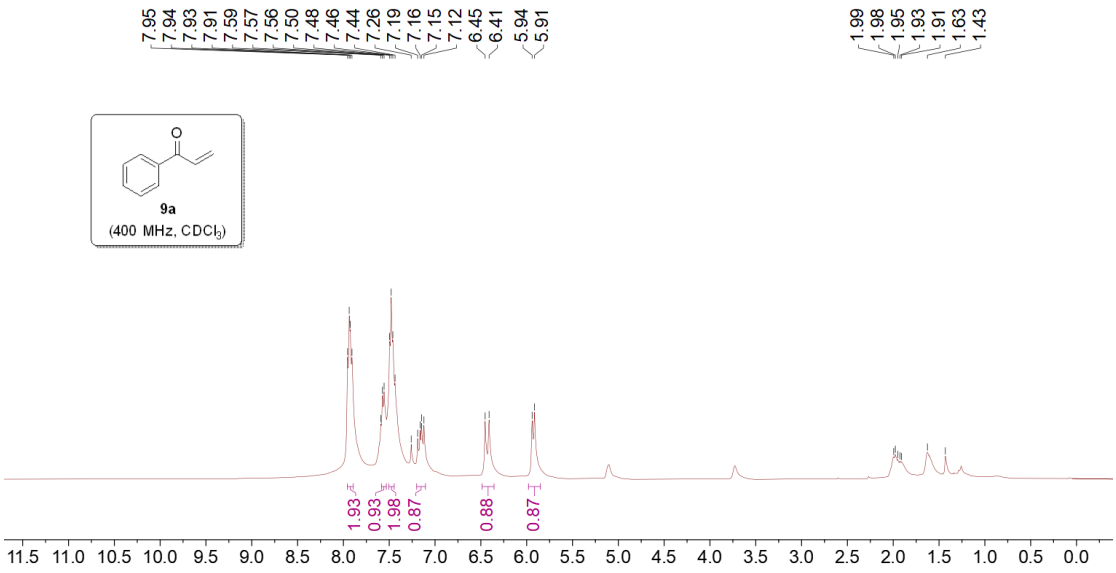


1e

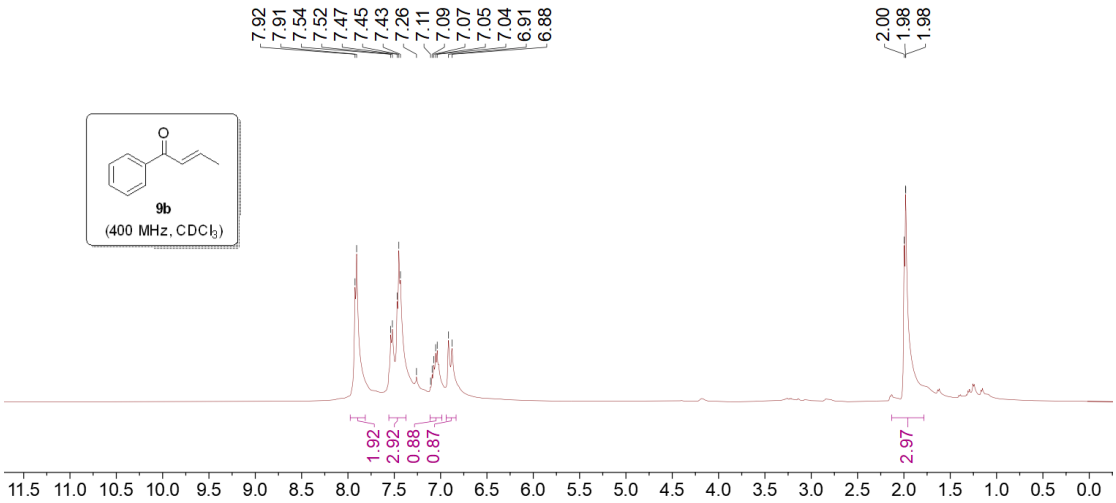
To a solution of 2-methoxyphenol (124 mg, 1 mmol) and powdered aluminum chloride ($AlCl_3$, 399 mg, 3 mmol) in CS_2 (5 mL) was added propionyl chloride (370 mg, 4 mmol). The mixture was heated to reflux for 8 hours. After completion of the reaction, The reaction mixture was poured into cold HCl solution (4.0 M in H_2O, 15 mL) and extracted with DCM. The organic phase was washed with H_2O and brine, dried with anhydrous Na_2SO_4. After evaporation of solvent, the residue was subjected to column chromatography for isolation (gradient eluent: petroleum ether/ethyl acetate/dichloromethane 40:1:1) to give product **1e** (135 mg, 75%) as colorless solid. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.64 – 7.43 (m, 2H), 6.94 (d, *J* = 8.7 Hz, 1H), 6.05 (s, 1H), 3.95 (s, 3H), 2.95 (q, *J* = 7.3 Hz, 2H), 1.21 (t, *J* = 7.3 Hz, 3H). Spectral data match those previously reported in the literature.[2]

4. Control experiment

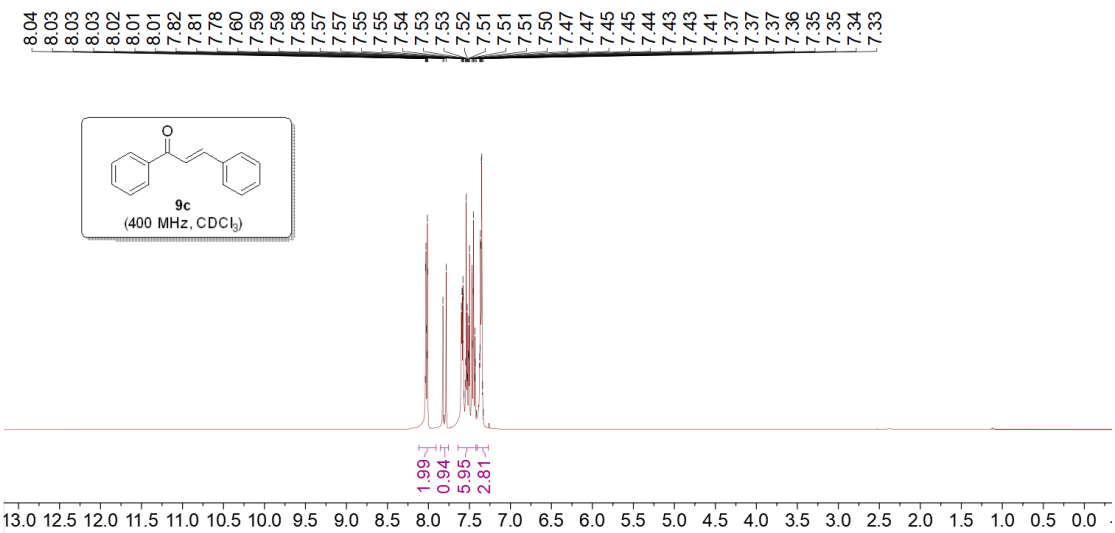
4.1 Analytical data for enone intermediate



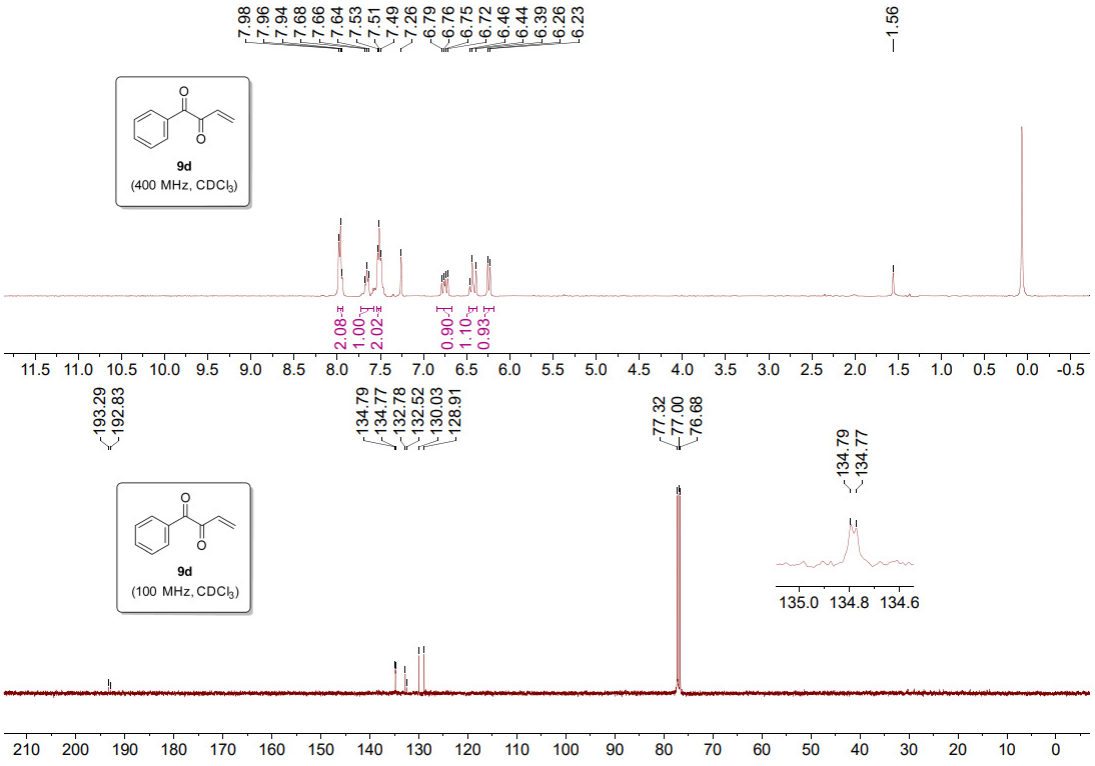
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 7.8 Hz, 2H), 7.61 – 7.53 (m, 1H), 7.49 (d, *J* = 7.3 Hz, 2H), 7.19 – 7.12 (m, 1H), 6.43 (d, *J* = 17.1 Hz, 1H), 5.93 (d, *J* = 10.5 Hz, 1H); Spectral data match those previously reported in the literature.[3]



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, *J* = 7.0 Hz, 2H), 7.63 – 7.39 (m, 3H), 7.15 – 7.02 (m, 1H), 6.90 (d, *J* = 15.2 Hz, 1H), 2.04 – 1.86 (m, 3H); Spectral data match those previously reported in the literature.[4]

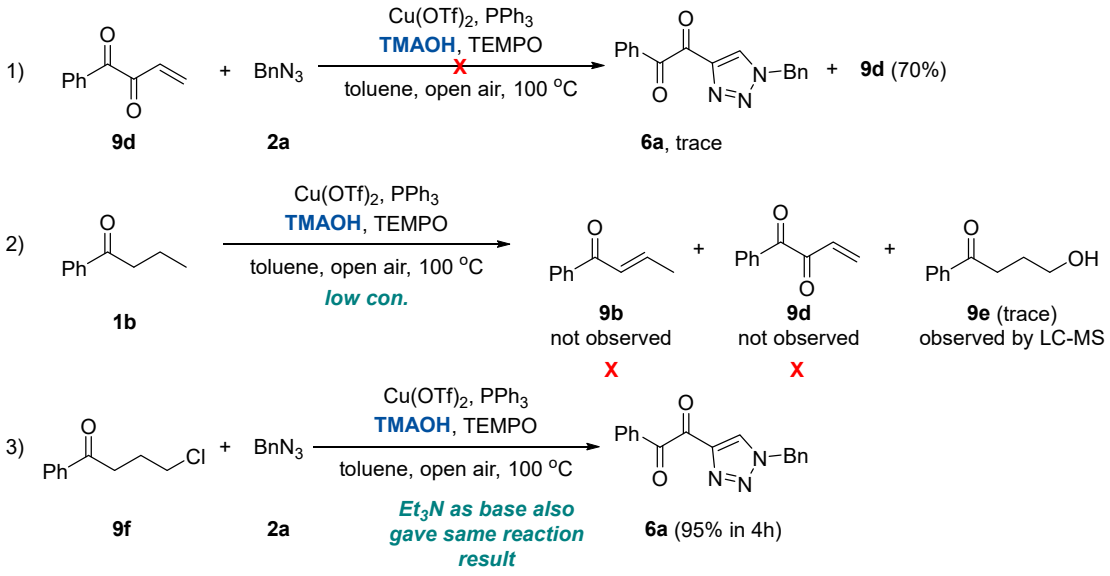


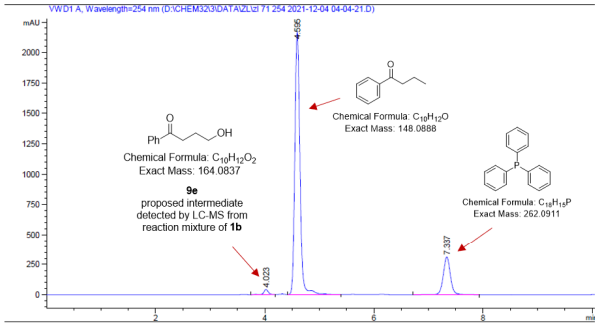
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07 – 7.97 (m, 2H), 7.91 – 7.74 (m, 1H), 7.62 – 7.41 (m, 6H), 7.38 – 7.33 (m, 3H); Spectral data match those previously reported in the literature.[3]



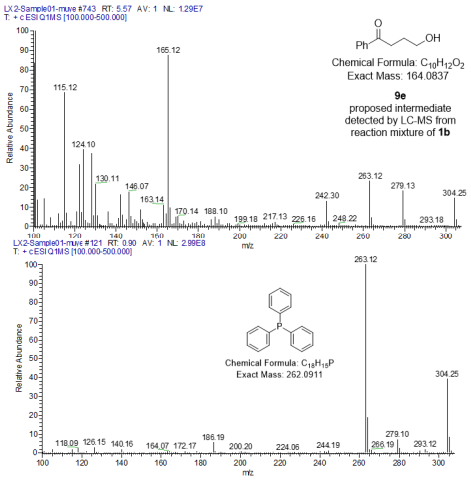
9d was prepared accrouding the reported method.[5] **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.97 (d, *J* = 8.0 Hz, 2H), 7.65 (d, *J* = 7.7 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 2H), 6.79 – 6.72 (m, 1H), 6.49 – 6.37 (m, 1H), 6.24 (d, *J* = 11.2 Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 193.3, 192.8, 134.8, 134.8, 132.8, 132.5, 130.0, 128.9. Spectral data match those previously reported in the literature.[6]

4.2 Control experiment

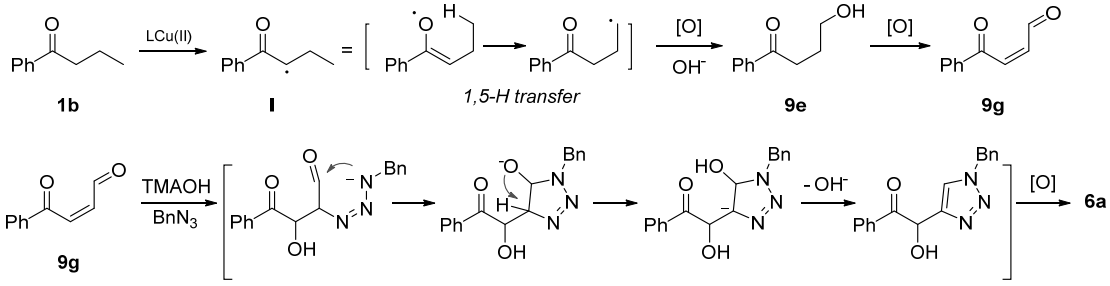




峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	4.023	VB R	0.0816	236.17630	41.72738	1.3781
2	4.595	BV R	0.0995	1.41204e4	2170.21338	82.3962
3	7.337	VB R	0.1375	2780.62646	310.58289	16.2257

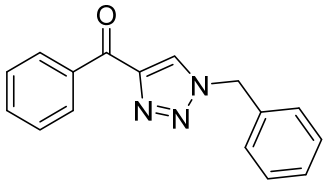


4.3 Proposed reaction pathway of the formation of 6a



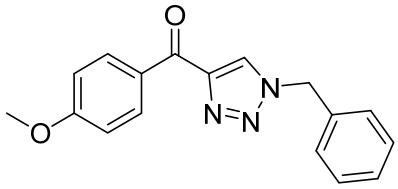
5. Analytical Data for acyl-1,2,3-triazoles

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



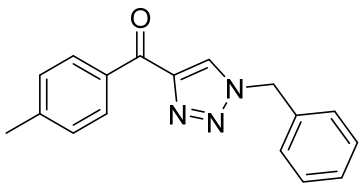
The title compound was prepared on 1.5 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 375 mg, 95% yield. White solid. Mp: 116−117 °C. R_f= 0.2 in EtOAc/petroleum ether (1:5). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.43 – 8.40 (m, 2H), 8.16 (s, 1H), 7.63 – 7.57 (m, 1H), 7.54 – 7.48 (m, 2H), 7.42 – 7.38 (m, 3H), 7.35 – 7.31 (m, 2H), 5.61 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 185.6, 148.4, 136.5, 133.7, 133.3, 130.6, 129.3, 129.2, 128.4, 128.2, 54.5; Spectral data match those previously reported in the literature.[7]

(1-Benzyl-1H-1,2,3-triazol-4-yl)(4-methoxyphenyl)methanone (3b)



The title compound was prepared on 1.2 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 249 mg, 71% yield. White solid. Mp: 129−131°C. R_f= 0.2 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.43 – 8.40 (m, 2H), 8.16 (s, 1H), 7.63 – 7.57 (m, 3H), 7.54 – 7.48 (m, 2H), 7.42 – 7.38 (m, 2H), 7.35 – 7.31 (m, 2H), 5.61 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 183.9, 163.8, 148.8, 133.7, 133.1, 129.3, 129.1, 128.4, 128.1, 113.6, 55.5, 54.4; Spectral data match those previously reported in the literature.[8]

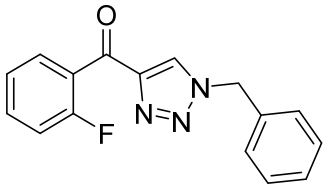
(1-Benzyl-1H-1,2,3-triazol-4-yl)(p-tolyl)methanone (3c)



The title compound was prepared on 1.3 mmol scale following General Procedure 3.1. The

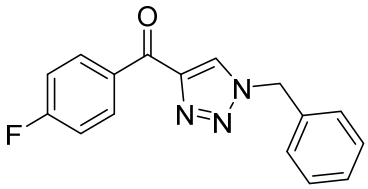
crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 263 mg, 73% yield. White solid. Mp: 130−132 °C. R_f = 0.1 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.31 (d, *J* = 8.2 Hz, 2H), 8.13 (s, 1H), 7.35 (d, *J* = 6.9 Hz, 3H), 7.30 – 7.25 (m, 4H), 5.56 (s, 2H), 2.39 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 185.1, 148.5, 144.1, 133.8(d, *J* = 23.6 Hz), 133.7, 130.6, 129.2, 129.02, 128.3, 128.1, 54.3, 21.6; Spectral data match those previously reported in the literature.[9]

(1-Benzyl-1H-1,2,3-triazol-4-yl)(2-flfluorophenyl)methanone (3d)



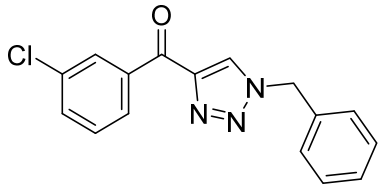
The title compound was prepared on 1.3 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 311 mg, 85% yield. White solid. Mp: 101-102 °C. R_f = 0.2 in EtOAc/petroleum ether (1:3). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.10 (s, 1H), 7.91 – 7.77 (m, 1H), 7.56 – 7.47 (m, 1H), 7.44 – 7.39 (m, 3H), 7.35 – 7.31 (m, 2H), 7.28 (d, *J* = 6.5 Hz, 1H), 7.21 – 7.15 (m, 1H), 5.60 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 184.8, 159.5, 148.0, 133.8 (d, *J* = 8.7 Hz), 133.5, 131.3, 129.4, 129.2, 128.4, 127.4, 124.1, 116.5 (d, *J* = 21.8 Hz), 54.5; Spectral data match those previously reported in the literature.[10]

(1-Benzyl-1H-1,2,3-triazol-4-yl)(4-flfluorophenyl)methanone (3e)



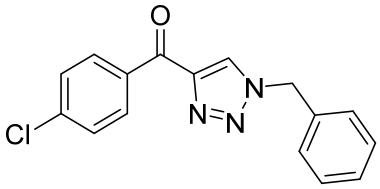
The title compound was prepared on 1.3 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 296 mg, 81% yield. White solid. Mp: 145-147 °C. R_f = 0.2 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.55 – 8.52 (m, 2H), 8.17 (s, 1H), 7.43 – 7.39 (m, 3H), 7.35 – 7.32 (m, 2H), 7.21 – 7.16 (m, 2H), 5.61 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 183.8, 166.8, 165.8, 148.3, 133.6, 133.4, 133.4, 132.7 (d, *J* = 2.9 Hz), 129.3, 129.2, 128.3, 115.5 (d, *J* = 21.7 Hz), 54.5; Spectral data match those previously reported in the literature.[8]

(1-Benzyl-1H-1,2,3-triazol-4-yl)(3-chlorophenyl)methanone (3f)



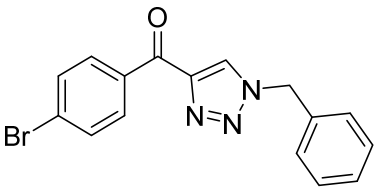
The title compound was prepared on 1.2 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 296 mg, 83% yield. White solid. Mp: 93-97 °C. R_f = 0.3 in EtOAc/petroleum ether (1:3).**^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.41 – 8.36 (m, 2H), 8.17 (s, 1H), 7.59 – 7.57 (m, 1H), 7.48 – 7.40 (m, 4H), 7.36 – 7.33 (m, 2H), 5.61 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 184.2, 148.0, 137.9, 134.6, 133.5, 133.2, 130.5, 129.7, 129.4, 129.3, 128.9, 128.4, 54.6; **HRMS (ESI) m/z** $[M+H]^+$: calcd for $C_{16}H_{13}ClN_3O$, 298.0742; found, 298.0721.

(1-Benzyl-1H-1,2,3-triazol-4-yl)(4-chlorophenyl)methanone (3g)



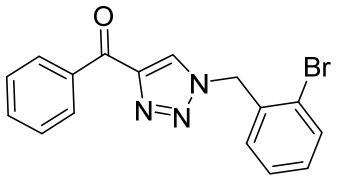
The title compound was prepared on 1.2 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 307 mg, 86% yield. White solid. Mp: 158-160 °C. R_f = 0.3 in EtOAc/ petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.43 (d, *J* = 8.7 Hz, 2H), 8.17 (s, 1H), 7.48 (d, *J* = 8.7 Hz, 2H), 7.42 – 7.38 (m, 3H), 7.36 – 7.32 (m, 2H), 5.61 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 184.2, 148.2, 139.8, 134.7, 133.5, 132.1, 129.4, 129.2, 128.7, 128.4, 54.5; Spectral data match those previously reported in the literature.[10]

(1-Benzyl-1H-1,2,3-triazol-4-yl)(4-bromophenyl)methanone (3h)



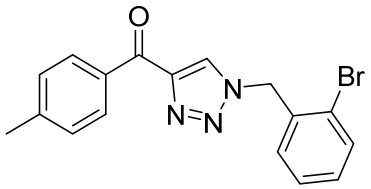
The title compound was prepared on 0.9 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 240 mg, 78% yield. White solid. Mp: 149−151 °C. R_f = 0.2 in EtOAc/ petroleum ether (1:3). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.38 – 8.31 (m, 2H), 8.18 (s, 1H), 7.67 – 7.63 (m, 2H), 7.42 – 7.39 (m, 3H), 7.35 – 7.32 (m, 2H), 5.60 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 184.3, 148.1, 135.1, 133.5, 132.2, 131.7, 129.3, 129.2, 128.6, 128.4, 54.5; Spectral data match those previously reported in the literature.[8]

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



The title compound was prepared on 1.5 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 10% EtOAc in petroleum ether) to afford the title compound 336 mg, 82% yield. White solid. Mp: 103−106 °C. R_f = 0.2 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.45 – 8.41 (m, 2H), 8.16 (s, 1H), 7.64 – 7.58 (m, 2H), 7.54 – 7.48 (m, 2H), 7.44 – 7.37 (m, 1H), 7.35 – 7.31 (m, 2H), 5.61 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 185.5, 148.1, 136.4, 133.4, 133.2, 133.2, 130.8, 130.8, 130.5, 128.5, 128.3, 123.8, 54.1; **HRMS (ESI) m/z** $[M+H]^+$: calcd for $C_{16}H_{13}BrN_3O$, 342.0237; found, 342.0213.

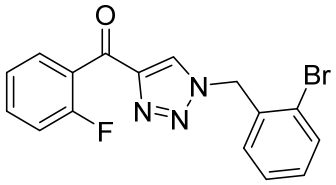
(1-(2- Bromophenyl) -1H-1,2,3-triazol-4-yl)(p-toyl)methanone (3j)



The title compound was prepared on 1.3 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 10% EtOAc in petroleum ether) to afford the title compound 333 mg, 72% yield. White solid. Mp: 97−100 °C. R_f = 0.3 in EtOAc/petroleum ether (1:3). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.35 – 8.30 (m, 2H), 8.22 (s, 1H), 7.63 – 7.61 (m, 1H), 7.35 – 7.26 (m, 4H), 7.24 (d, *J* = 4.4 Hz, 1H), 5.72 (s, 2H), 2.41 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 185.1, 148.4, 144.2, 133.9, 133.4, 133.3, 130.8, 130.8, 130.7, 129.1, 128.4, 128.3, 123.9, 54.1, 21.7; **HRMS (ESI) m/z** $[M + H]^+$: calcd for

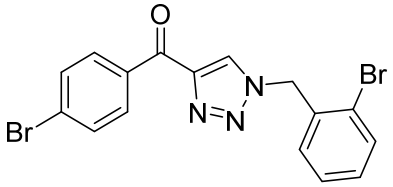
$C_{17}H_{15}BrN_3O$, 356.0393; found, 356.0368.

(1-(2- Bromophenyl) -1H-1,2,3-triazol-4-yl)(2-fluorophenyl)methanone(3k)



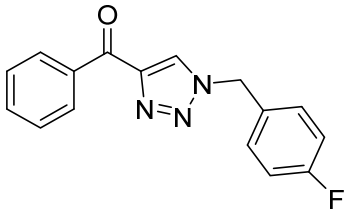
The title compound was prepared on 1.3 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 10% EtOAc in petroleum ether) to afford the title compound 395 mg, 84% yield. White solid. Mp: 60-62 °C. R_f = 0.2 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.21 (s, 1H), 7.88 – 7.83 (m, 1H), 7.67 – 7.64 (m, 1H), 7.57 – 7.52 (m, 1H), 7.38 – 7.34 (m, 1H), 7.31 – 7.27 (m, 3H), 7.20 – 7.15 (m, 1H), 5.74 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 184.8, 147.9, 133.8 (d, *J* = 8.9 Hz), 133.5, 133.1, 131.3, 131.0, 130.9, 128.4, 127.6, 124.1, 116.5 (d, *J* = 21.8 Hz), 54.2; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{16}H_{12}BrFN_3O$, 360.0142; found, 360.0145.

(1-(2- Bromophenyl) -1H-1,2,3-triazol-4-yl)(4-bromophenyl)methanone (3l)



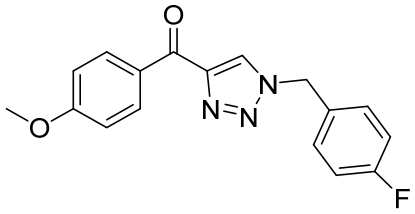
The title compound was prepared on 0.9 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 10% EtOAc in petroleum ether) to afford the title compound 326 mg, 86% yield. White solid. Mp: 106-108 °C. R_f = 0.2 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.37 – 8.32 (m, 2H), 8.27 (s, 1H), 8.27 (s, 3H), 7.65 – 7.62 (m, 1H), 7.37 – 7.25 (m, 2H), 5.73 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 184.2, 147.9, 135.0, 133.4, 133.1, 132.1, 131.6, 130.9, 130.9, 128.7, 128.6, 128.3, 123.9, 54.2; Spectral data match those previously reported in the literature.[11]

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



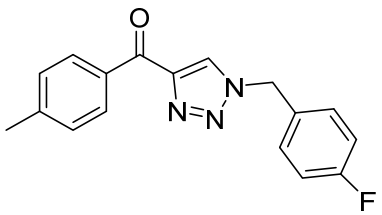
The title compound was prepared on 1.5 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 363 mg, 86% yield. White solid. Mp: 140−145 °C. R_f = 0.2 in EtOAc/ petroleum ether (1:3). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.42 – 8.39 (m, 2H), 8.18 (s, 1H), 7.64 – 7.57 (m, 1H), 7.54 – 7.47 (m, 2H), 7.37 – 7.30 (m, 2H), 7.15 – 7.04 (m, 2H), 5.58 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 185.6, 164.3, 161.8, 148.4, 136.4, 133.3, 130.6, 130.3 (d, *J* = 8.5 Hz), 129.6 (d, *J* = 3.4 Hz), 128.4, 128.1, 116.4 (d, *J* = 21.8 Hz), 53.7; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{16}H_{13}FN_3O$, 282.1037; found, 282.1014.

(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)(4-methoxyphenyl)-methanone (3n)



The title compound was prepared on 1.2 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 269 mg, 72% yield. White solid. Mp: 131−132 °C. R_f = 0.2 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.54 – 8.47 (m, 2H), 8.14 (s, 1H), 7.36 – 7.30 (m, 2H), 7.12 – 7.07 (m, 2H), 7.01 – 6.96 (m, 2H), 5.58 (s, 2H), 3.90 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 183.8, 163.9, 163.8， 162.2, 148.9, 133.1, 130.3 (d, *J* = 8.4 Hz), 129.6 (d, *J* = 3.4 Hz), 129.3, 128.0, 116.35 (d, *J* = 21.9 Hz), 113.7, 55.5, 53.6; Spectral data match those previously reported in the literature.[11]

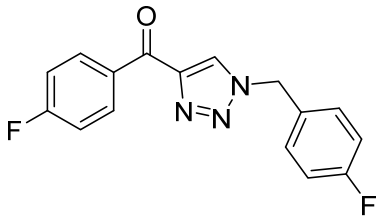
(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)(p-tolyl)methanone (3o)



The title compound was prepared on 1.3 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 288 mg, 75% yield. White solid. Mp: 145−147 °C.

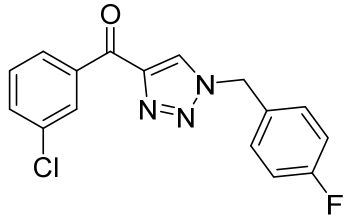
R_f = 0.3 in EtOAc/petroleum ether (1:3). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.34 (d, *J* = 8.2 Hz, 2H), 8.15 (s, 1H), 7.36 – 7.30 (m, 4H), 7.12 – 7.06 (m, 2H), 5.58 (s, 2H), 2.43 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 185.1, 164.3, 161.8, 148.7, 144.3, 133.8, 130.7, 130.3 (d, *J* = 8.5 Hz), 129.6, 129.1, 128.0, 116.4 (d, *J* = 21.9 Hz), 53.6, 21.7; Spectral data match those previously reported in the literature.[11]

(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)(4-fluorophenyl)methanone (3p)



The title compound was prepared on 1.3 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 315 mg, 81% yield. White solid. Mp: 165−168 °C. R_f = 0.1 in EtOAc/ petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.56 – 8.49 (m, 2H), 8.18 (s, 1H), 7.35 – 7.31 (m, 2H), 7.20 – 7.15 (m, 2H), 7.12 – 7.07 (m, 2H), 5.58 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 183.7, 167.2, 164.7, 164.3, 161.8, 148.4, 133.4 (d, *J* = 9.3 Hz), 132.6, 130.3 (d, *J* = 8.5 Hz), 129.5 (d, *J* = 3.4 Hz), 128.2, 116.4 (d, *J* = 21.9 Hz), 115.5 (d, *J* = 21.8 Hz), 53.7; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{16}H_{12}F_2N_3O$, 300.0943; found, 316.0920.

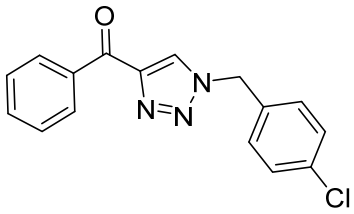
(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)(3-chlorophenyl)methanone (3q)



The title compound was prepared on 1.2 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 314 mg, 83% yield. White solid. Mp: 123−125 °C. R_f = 0.2 in EtOAc/ petroleum ether (1:5). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.40 – 8.34 (m, 2H), 8.19 (s, 1H), 7.58 – 7.56 (m, 1H), 7.45 (t, *J* = 7.9 Hz, 1H), 7.37 – 7.30 (m, 2H), 7.16 – 7.02 (m, 2H), 5.58 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 184.0, 164.3, 161.8, 148.0, 137.8, 134.6,

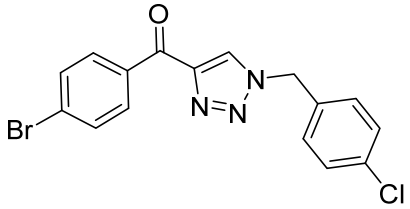
133.2, 130.4, 130.4, 130.3, 129.7, 129.4 (d, J = 3.4 Hz), 128.8, 128.3, 116.4 (d, J = 21.9 Hz), 53.7; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{16}H_{11}ClFN_3O$, 316.0647; found, 316.0640.

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



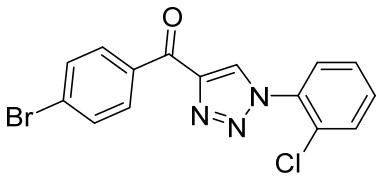
The title compound was prepared on 1.5 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 310 mg, 87% yield. White solid. Mp: 150-152 °C. R_f= 0.3 in EtOAc/petroleum ether (1:3). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.43 – 8.39 (m, 2H), 8.18 (s, 1H), 7.65 – 7.58 (m, 1H), 7.54 – 7.47 (m, 2H), 7.41 – 7.36 (m, 2H), 7.29 – 7.27 (m, 2H), 5.58 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 185.5, 148.5, 136.4, 135.3, 133.3, 132.2, 130.6, 129.6, 129.5, 128.4, 128.2, 53.7; Spectral data match those previously reported in the literature.[8]

((4-Bromophenyl)(1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methanone (3s)



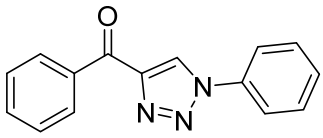
The title compound was prepared on 0.9 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 285 mg, 84% yield. White solid. Mp: 175−177 °C. R_f= 0.2 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.37 – 8.33 (m, 2H), 8.18 (s, 1H), 7.68 – 7.64 (m, 2H), 7.40 – 7.37 (m, 2H), 7.30 – 7.23 (m, 2H), 5.58 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 184.2, 148.3, 135.4, 135.0, 132.2, 132.0, 131.7, 129.7, 129.6, 128.8, 128.3, 53.8; Spectral data match those previously reported in the literature.[11]

(4-Bromophenyl)(1-(2-chlorophenyl)-1H-1,2,3-triazol-4-yl)methanone (3t)



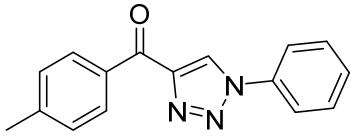
The title compound was prepared on 0.9 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 235 mg, 72% yield. White solid. Mp: 120−123 °C. R_f = 0.2 in EtOAc/petroleum ether (1:5). **^{1}H NMR (400 MHz, CDCl$_3$)**: δ 8.74 (s, 1H), 8.49 – 8.41 (m, 2H), 7.75 – 7.63 (m, 4H), 7.57 – 7.49 (m, 2H); **^{13}C NMR (100 MHz, CDCl$_3$)**: δ 184.2, 147.6, 135.1, 134.1, 132.2, 131.8, 131.4, 130.9, 130.5, 128.8, 128.7, 128.1, 127.6; Spectral data match those previously reported in the literature.[11]

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



The title compound was prepared on 1.5 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 10% EtOAc in petroleum ether) to afford the title compound 299 mg, 80% yield. White solid. Mp: 126−127 °C. R_f = 0.2 in EtOAc/petroleum ether (1:6). **^{1}H NMR (400 MHz, CDCl$_3$)**: δ 8.71 (s, 1H), 8.49 (d, *J* = 7.6 Hz, 2H), 7.82 (d, *J* = 7.5 Hz, 2H), 7.66 – 7.50 (m, 6H); **^{13}C NMR (100 MHz, CDCl$_3$)**: δ 185.6, 136.4, 133.4, 130.7, 130.0, 129.6, 128.5, 126.4, 120.8; Spectral data match those previously reported in the literature.[7]

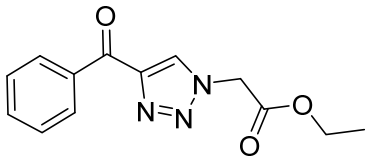
(1-Phenyl-1H-1,2,3-triazol-4-yl)(p-tolyl)methanone (3v)



The title compound was prepared on 1.3 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 10% EtOAc in petroleum ether) to afford the title compound 243 mg, 71% yield. White solid. Mp: 152−154 °C. R_f = 0.1 in EtOAc/petroleum ether (1:5). **^{1}H NMR (400 MHz, CDCl$_3$)**: δ 8.68 (s, 1H), 8.42 (d, *J* = 8.2 Hz, 2H), 7.87 – 7.73 (m, 2H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.54 – 7.49 (m, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 2.46 (s, 3H); **^{13}C NMR (100 MHz, CDCl$_3$)**: δ 185.0, 148.8, 144.4, 136.4, 133.9,

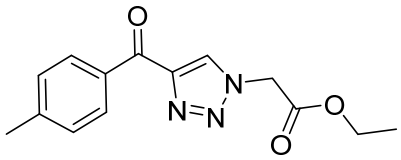
130.8, 129.9, 129.4, 129.2 126.2, 120.8, 21.7; Spectral data match those previously reported in the literature.[9]

Ethyl 2-(4-benzoyl-1H-1,2,3-triazol-1-yl)acetate (3w)



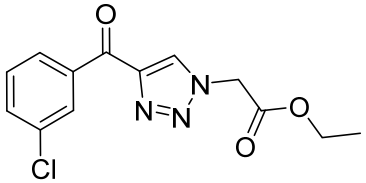
The title compound was prepared on 1.5 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 338 mg, 87% yield. White solid. Mp: 125–126 °C. R_f = 0.2 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.44 – 8.41 (m, 3H), 7.66 – 7.61 (m, 1H), 7.57 – 7.51 (m, 2H), 5.27 (s, 2H), 4.32 (q, *J* = 7.1 Hz, 2H), 1.50 – 1.01 (m, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 185.5, 165.6, 148.4, 136.4, 133.3, 130.6, 129.8, 128.4, 62.8, 51.0, 14.0; Spectral data match those previously reported in the literature.[12]

Ethyl 2-(4-(4-methylbenzoyl)-1H-1,2,3-triazol-1-yl)acetate (3x)



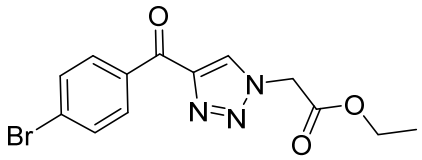
The title compound was prepared on 1.3 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 270 mg, 76% yield. White solid. Mp: 148−150 °C. R_f = 0.3 in EtOAc/petroleum ether (1:3). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.43 – 8.29 (m, 3H), 7.32 (d, *J* = 8.0 Hz, 2H), 5.25 (s, 2H), 4.30 (q, *J* = 7.1 Hz, 2H), 2.44 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 185.0, 165.6, 148.6, 144.2, 133.9, 130.7, 129.7, 129.1, 62.7, 51.0, 21.7, 14.0; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{14}H_{16}N_3O_3$, 274.1186; found, 274.1172.

Ethyl 2-(4-(3-chlorobenzoyl)-1H-1,2,3-triazol-1-yl)acetate (3y)



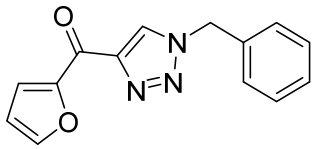
The title compound was prepared on 1.2 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 299 mg, 85% yield. White solid. Mp: 84−88 °C. R_f = 0.3 in EtOAc/petroleum ether (1:3). **^{1}H NMR (400 MHz, CDCl$_3$)**: δ 8.43 (s, 1H), 8.41 – 8.36 (m, 2H), 7.60 – 7.57 (m, 1H), 7.47 (t, *J* = 7.9 Hz, 1H), 5.26 (s, 2H), 4.31 (q, *J* = 7.1 Hz, 2H), 1.71 – 1.08 (m, 3H); **^{13}C NMR (100 MHz, CDCl$_3$)**: δ 184.0, 165.5, 148.0, 137.8, 134.6, 133.3, 130.4, 130.0, 129.7, 128.8, 62.8, 51.0, 14.0; **HRMS (ESI) m/z** [M + H]$^+$: calcd for $C_{13}H_{13}ClN_3O_3$, 294.0640; found, 294.0626.

Ethyl 2-(4-(4-bromobenzoyl)-1H-1,2,3-triazol-1-yl)acetate (3z)



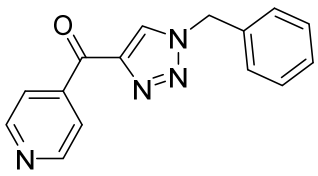
The title compound was prepared on 0.9 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 247 mg, 82% yield. White solid. Mp: 162−164 °C. R_f = 0.2 in EtOAc/petroleum ether (1:3). **^{1}H NMR (400 MHz, CDCl$_3$)**: δ 8.42 (s, 1H), 8.38 – 8.29 (m, 2H), 7.71 – 7.63 (m, 2H), 5.26 (s, 2H), 4.31 (q, *J* = 7.1 Hz, 2H), 1.32 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, CDCl$_3$)**: δ 184.2, 165.6, 148.2, 135.1, 132.2, 131.7, 130.0, 128.7, 62.8, 51.0, 14.0; Spectral data match those previously reported in the literature.[11]

(1-benzyl-1H-1,2,3-triazol-4-yl)(furan-2-yl)methanone (3aa)



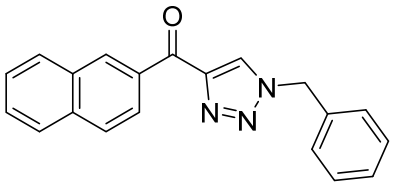
The title compound was prepared on 1.6 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 30% EtOAc in petroleum ether) to afford the title compound 357 mg, 88% yield. White solid. Mp: 142−145 °C. R_f = 0.3 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, CDCl$_3$)**: δ 8.30 – 8.01 (m, 2H), 7.69 (s, 1H), 7.36 – 7.30 (m, 5H), 6.90 – 6.31 (m, 1H), 5.58 (s, 2H); **^{13}C NMR (100 MHz, CDCl$_3$)**: δ 172.1, 150.7, 147.6, 146.9, 133.6, 129.2, 129.0, 128.2, 127.6, 122.7, 112.5, 54.3; **HRMS (ESI) m/z** [M + H]$^+$: calcd for $C_{14}H_{11}N_3O_2Na$, 276.0743; found, 276.0742.

(1-benzyl-1H-1,2,3-triazol-4-yl)(pyridin-4-yl)methanone (3ab)



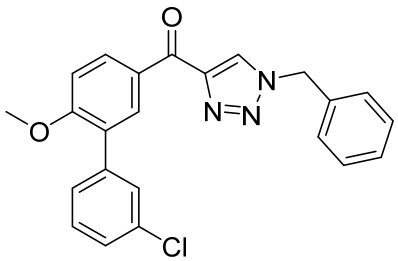
The title compound was prepared on 1.5 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 30% EtOAc in petroleum ether) to afford the title compound 337 mg, 85% yield. White solid. Mp: 120−123 °C. R_f = 0.1 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.79 (d, *J* = 4.7 Hz, 2H), 8.31 – 7.99 (m, 3H), 7.40 – 7.27 (m, 5H), 5.58 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 184.4, 150.4, 147.4, 142.3, 133.4, 129.2, 129.1, 128.5, 128.2, 123.2, 54.4; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{15}H_{12}N_4O$, 265.1084; found, 265.1083.

(1-benzyl-1H-1,2,3-triazol-4-yl)(naphthalen-2-yl)methanone (3ac)



The title compound was prepared on 1.1 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 259 mg, 75% yield. White solid. Mp: 155−157 °C. R_f = 0.2 in EtOAc/ petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 9.24 (s, 1H), 8.32 (t, *J* = 10.2 Hz, 1H), 8.20 (d, *J* = 22.5 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.95 – 7.88 (m, 2H), 7.63 – 7.53 (m, 2H), 7.44 – 7.35 (m, 5H), 5.63 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 185.3, 148.6, 135.7, 133.7, 133.4, 132.5, 131.9, 130.0, 129.3, 129.1, 128.6, 128.4, 128.1, 127.6, 126.5, 125.4, 54.4. Spectral data match those previously reported in the literature.[13]

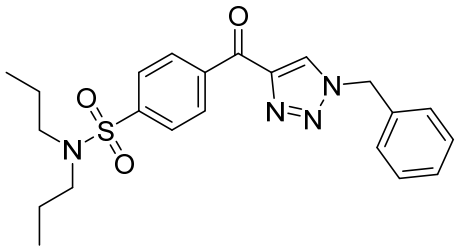
(1-benzyl-1H-1,2,3-triazol-4-yl)(3'-chloro-6-methoxy-[1,1'-biphenyl]-3-yl)methanone(3ad)



The title compound was prepared on 0.4 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in

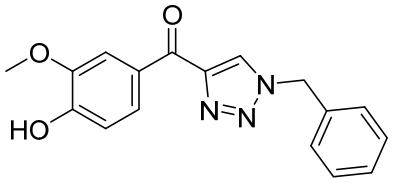
petroleum ether) to afford the title compound 139 mg, 85% yield. Light yellow solid. Mp: 182−185 °C. R_f= 0.4 in EtOAc/petroleum ether (1:3). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.62 (d, J = 8.6 Hz, 1H), 8.42 (s, 1H), 8.16 (s, 1H), 7.56 (s, 2H), 7.45 – 7.38 (m, 4H), 7.36 – 7.30 (m, 4H), 7.08 (d, J = 8.8 Hz, 1H), 5.60 (s, 2H), 3.92 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 183.8, 160.5, 148.7, 139.3, 133.8, 133.7, 133.4, 133.0, 129.6, 129.4, 129.3, 129.3, 129.2, 129.2, 128.4, 128.1, 127.8, 127.4, 110.6, 55.9, 54.5. **MS (ESI)** $[M + H]^+$: calcd for $C_{24}H_{18}ClN_3O_2$, 404.1160; found, 404.2.

4-(1-benzyl-1H-1,2,3-triazole-4-carbonyl)-N,N-dipropylbenzenesulfonamide(3ae)



The title compound was prepared on 0.3 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (10% to 40% EtOAc in petroleum ether) to afford the title compound 113 mg, 95% yield. White solid. R_f = 0.2 in EtOAc/petroleum ether (1:5). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.55 (d, J = 8.0 Hz, 2H), 8.20 (s, 1H), 7.93 (d, J = 8.0 Hz, 2H), 7.45 – 7.38 (m, 3H), 7.34 (d, J = 6.6 Hz, 2H), 5.62 (s, 2H), 3.11 (t, J = 7.5 Hz, 4H), 1.77 – 1.37 (m, 4H), 0.88 (t, J = 7.2 Hz, 6H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 184.3, 147.9, 144.0, 139.2, 133.4, 131.2, 129.4, 129.3, 128.5, 128.4, 126.9, 54.6, 50.1, 22.0, 11.1. **MS (ESI)** $[M + H]^+$: calcd for $C_{23}H_{26}N_4O_3S$, 427.1798; found, 427.2.

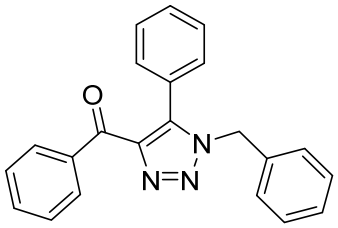
(1-benzyl-1H-1,2,3-triazol-4-yl)(4-hydroxy-3-methoxyphenyl)methanone(3af)



The title compound was prepared on 0.5 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (10% to 40% EtOAc in petroleum ether) to afford the title compound 96 mg, 62% yield. White solid. R_f = 0.2 in EtOAc/petroleum ether (1:2). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.27 (d, J = 8.4 Hz, 1H), 8.14 (s, 1H), 8.03 (s, 1H), 7.46 – 7.28 (m, 5H), 7.01 (d, J = 8.4 Hz, 1H), 6.25 (br, 1H), 5.59 (s, 2H), 3.97 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 183.6, 150.8, 148.8, 146.4, 133.7, 129.3, 129.1, 129.0,

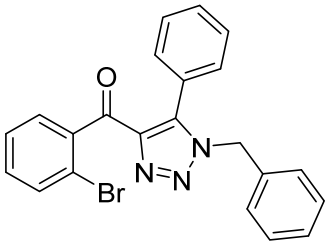
128.4, 128.2, 126.6, 114.0, 112.4, 56.1, 54.4. **MS (ESI)** $[M + H]^+$: calcd for $C_{18}H_{15}N_3O_3$, 310.1186; found, 310.2.

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



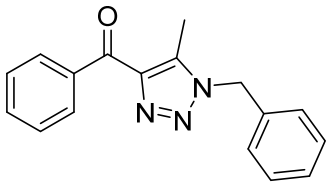
The title compound was prepared on 0.9 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 30% EtOAc in petroleum ether) to afford the title compound 263 mg, 86% yield. Colorless liquid. R_f = 0.2 in EtOAc/petroleum ether (1:6). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.36 – 8.24 (m, 2H), 7.63 – 7.54 (m, 1H), 7.50 – 7.43 (m, 5H), 7.31 – 7.24 (m, 5H), 7.12 – 7.01 (m, 2H), 5.47 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 186.2, 143.7, 141.7, 137.0, 134.6, 132.9, 130.6, 129.9, 129.7, 128.7, 128.6, 128.3, 128.1, 127.5, 126.2, 51.9; Spectral data match those previously reported in the literature.[12]

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



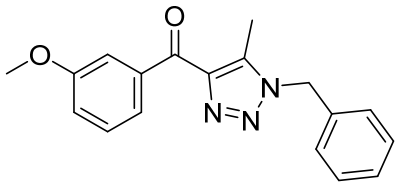
The title compound was prepared on 0.7 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 40% EtOAc in petroleum ether) to afford the title compound 231 mg, 79% yield. Light yellow liquid. R_f = 0.3 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.57 – 7.53 (m, 1H), 7.51 – 7.43 (m, 2H), 7.43 – 7.38 (m, 2H), 7.37 – 7.32 (m, 1H), 7.30 – 7.26 (m, 5H), 7.26 – 7.25 (m, 1H), 7.11 – 6.97 (m, 2H), 5.47 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 187.9, 143.1, 141.2, 140.0, 134.4, 133.0, 131.4, 130.0, 129.7, 129.5, 128.6 (d, J = 19.9 Hz), 128.5, 128.3, 127.3, 126.9, 125.4, 119.8, 51.9; Spectral data match those previously reported in the literature.[14]

(1-benzyl-5-methyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (5a)



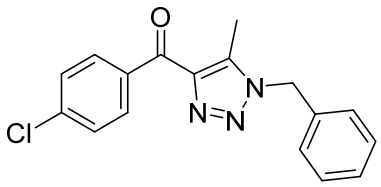
The title compound was prepared on 1.3 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 335 mg, 93% yield. Colorless liquid. R_f= 0.2 in EtOAc/petroleum ether (1:5). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.59 – 8.12 (m,2H), 7.63 – 7.54 (m, 1H), 7.54 – 7.44 (m, 2H), 7.39 – 7.30 (m, 3H), 7.24 – 7.15 (m, 2H), 5.56 (s, 2H), 2.55 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 187.5, 143.7, 139.3, 137.3, 133.9, 132.8, 130.5, 129.1, 128.5, 128.1, 127.2, 51.7, 9.5; Spectral data match those previously reported in the literature.[15]

(1-benzyl-5-methyl-1H-1,2,3-triazol-4-yl)(3-methoxyphenyl)methanone (5b)



The title compound was prepared on 1.1 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 247 mg, 73% yield. Light yellow liquid. R_f= 0.3 in EtOAc/petroleum ether (v/v = 1:5). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.99 (t, *J* = 13.1 Hz, 1H), 7.85 (t, *J* = 8.8 Hz, 1H), 7.45 – 7.34 (m, 4H), 7.24 – 7.19 (m, 2H), 7.16 – 7.12 (m, 1H), 5.57 (s, 2H), 3.88 (s, 3H), 2.55 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 187.2, 159.5, 143.8, 139.4, 138.6, 134.0, 129.2, 129.2, 128.6, 127.3, 123.6, 119.6, 114.5, 55.4, 51.8, 9.6; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{18}H_{18}N_3O_2$, 308.1394; found, 308.1321.

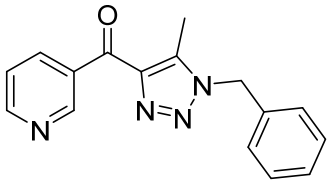
(1-benzyl-5-methyl-1H-1,2,3-triazol-4-yl)(4-chlorophenyl)methanone (5c)



The title compound was prepared on 1.1 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 298 mg, 87% yield. Yellow liquid. R_f= 0.3 in

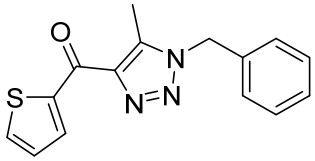
EtOAc/petroleum ether (1:6). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.42 – 8.23 (m, 2H), 7.51 – 7.44 (m, 2H), 7.41 – 7.32 (m, 3H), 7.24 – 7.18 (m, 2H), 5.57 (s, 2H), 2.56 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 186.0, 143.6, 139.6, 139.3, 135.6, 133.9, 132.1, 129.2, 128.7, 128.5, 127.3, 51.8, 9.6; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{17}H_{15}ClN_3O$, 312.0898; found, 312.0901.

(1-benzyl-5-methyl-1H-1,2,3-triazol-4-yl)(pyridin-2-yl)methanone (5d)



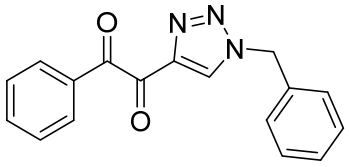
The title compound was prepared on 1.3 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 40% EtOAc in petroleum ether) to afford the title compound 314 mg, 87% yield. Yellow liquid. R_f = 0.3 in EtOAc/petroleum ether (1:5). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 9.51 (s, 1H), 8.98 – 8.57 (m, 2H), 7.49 – 7.34 (m, 4H), 7.22 (d, *J* = 6.7 Hz, 2H), 5.60 (d, *J* = 15.5 Hz, 2H), 2.58 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 185.8, 152.7, 151.5, 143.4, 139.8, 138.2, 133.7, 129.2, 128.7, 127.3, 123.3, 51.8, 9.6; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{16}H_{14}N_4O$, 279.1240; found, 279.1238.

(1-benzyl-5-methyl-1H-1,2,3-triazol-4-yl)(thiophen-2-yl)methanone (5e)



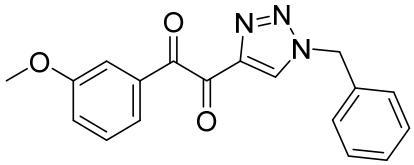
The title compound was prepared on 1.4 mmol scale following General Procedure 3.1. The crude product was purified by silica gel column chromatography (0% to 40% EtOAc in petroleum ether) to afford the title compound 329 mg, 83% yield. Yellow liquid. R_f = 0.4 in EtOAc/ petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.67 (d, *J* = 3.8 Hz, 1H), 7.71 (d, *J* = 4.9 Hz, 1H), 7.34 (t, *J* = 6.7 Hz, 3H), 7.21 – 7.20 (m, 3H), 5.56 (s, 2H), 2.56 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 178.8, 143.1, 139.0, 135.9, 134.6, 133.9, 129.2, 128.6, 128.2, 127.3, 51.8, 9.5; **HRMS (ESI) m/z** $[M + Na]^+$: calcd for $C_{15}H_{13}N_3OSNa$, 306.0672; found, 306.0671.

1-(1-benzyl-1H-1,2,3-triazol-4-yl)-2-phenylethane-1,2-dione (6a)



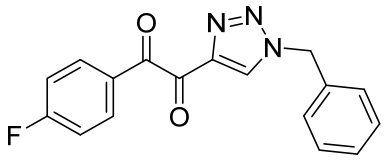
The title compound was prepared on 1.3 mmol scale following General Procedure 3.2. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 348 mg, 92% yield. Yellow solid. Mp: 114-116 °C. R_f = 0.2 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, CDCl$_3$)**: δ 8.21 (s, 1H), 8.03 – 7.97 (m, 2H), 7.67 – 7.61 (m, 1H), 7.52 – 7.46 (m, 2H), 7.42 – 7.37 (m, 3H), 7.35 – 7.30 (m, 2H), 5.60 (s, 2H); **^{13}C NMR (100 MHz, CDCl$_3$)**: δ 191.9, 185.5, 144.4, 134.9, 133.3, 132.3, 130.2, 129.4, 129.3, 128.9, 128.4, 128.2, 54.5; Spectral data match those previously reported in the literature.[16]

1-(1-benzyl-1H-1,2,3-triazol-4-yl)-2-(3-methoxyphenyl)ethane-1,2-dione (6b)



The title compound was prepared on 1.1 mmol scale following General Procedure 3.2. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 258 mg, 73% yield. Yellow solid. Mp: 109-111 °C. R_f = 0.3 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, CDCl$_3$)**: δ 8.18 (d, *J* = 2.6 Hz, 1H), 7.55 (d, *J* = 10.1 Hz, 2H), 7.44 – 7.31 (m, 6H), 7.20 (d, *J* = 8.2 Hz, 1H), 5.61 (s, 2H), 3.84 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (100 MHz, CDCl$_3$)**: δ 191.9, 185.6, 160.0, 144.6, 133.6, 133.3, 130.0, 129.5, 129.4, 128.5, 128.1, 123.5, 122.1, 113.2, 55.5, 54.6; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{18}H_{16}N_3O_3$, 322.1186; found, 322.1175.

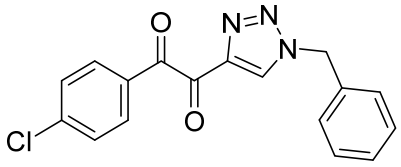
1-(1-benzyl-1H-1,2,3-triazol-4-yl)-2-(4-fluorophenyl)ethane-1,2-dione (6c)



The title compound was prepared on 1.2 mmol scale following General Procedure 3.2. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 307 mg, 83% yield. Yellow solid. R_f = 0.2

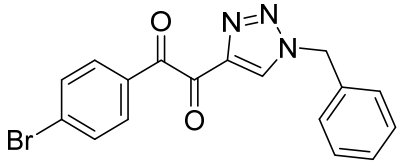
EtOAc/petroleum ether (1:2). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.31 (s, 1H), 8.05 (d, *J* = 4.7 Hz, 2H), 7.36 (d, *J* = 19.3 Hz, 5H), 7.17 (t, *J* = 7.5 Hz, 2H), 5.63 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 190.1, 185.1, 167.9, 165.4, 144.1, 133.3, 132.9 (d, *J* = 9.8 Hz), 129.2 (d, *J* = 9.7 Hz), 128.6, 128.5, 128.3, 116.3, 116.1, 54.4. **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{17}H_{13}FN_3O_2$, 310.0992; found, 310.0979.

1-(1-benzyl-1H-1,2,3-triazol-4-yl)-2-(4-chlorophenyl)ethane-1,2-dione (6d)



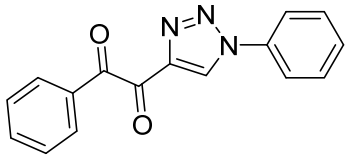
The title compound was prepared on 1.1 mmol scale following General Procedure 3.2. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 308 mg, 86% yield. Yellow solid. Mp: 115-117 °C. R_f = 0.3 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.20 (s, 1H), 7.99 – 7.96 (m, 2H), 7.52 – 7.45 (m, 2H), 7.44 – 7.37 (m, 3H), 7.33 – 7.31 (m, 2H), 5.61 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 190.5, 184.9, 144.3, 141.7, 133.2, 131.6, 130.7, 129.4, 129.4, 129.4, 128.4, 128.3, 54.6; Spectral data match those previously reported in the literature.[7]

1-(1-benzyl-1H-1,2,3-triazol-4-yl)-2-(4-bromophenyl)ethane-1,2-dione (6e)



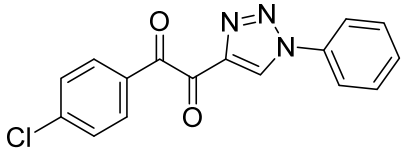
The title compound was prepared on 0.8 mmol scale following General Procedure 3.2. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 248 mg, 84% yield. Yellow solid. Mp: 104-107 °C. R_f = 0.2 in EtOAc/petroleum ether (1:3). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.20 (s, 1H), 7.89 (d, *J* = 8.6 Hz, 2H), 7.65 (d, *J* = 8.6 Hz, 2H), 7.44 – 7.39 (m, 3H), 7.34 – 7.32 (m, 2H), 5.61 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 190.7, 184.9, 144.3, 133.2, 132.3, 131.6, 131.1, 130.6, 129.4, 129.4, 128.4, 128.3, 54.6; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{17}H_{13}BrN_3O_2$, 370.0186; found, 370.0177.

1-phenyl-2-(1-phenyl-1H-1,2,3-triazol-4-yl)ethane-1,2-dione (6f)



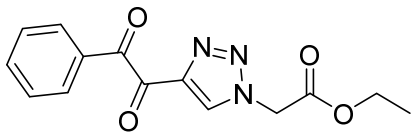
The title compound was prepared on 1.3 mmol scale following General Procedure 3.2. The crude product was purified by silica gel column chromatography (0% to 30% EtOAc in petroleum ether) to afford the title compound 299 mg, 83% yield. off-White solid. Mp: 131-132 °C. R_f= 0.3 in EtOAc/petroleum ether (1:5). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.74 (s, 1H), 8.13 – 8.03 (m, 2H), 7.79 – 7.76 (m, 2H), 7.70 – 7.66 (m, 1H), 7.60 – 7.50 (m, 5H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 191.8, 185.3, 144.6, 136.0, 135.0, 132.3, 130.3, 130.0, 129.9, 129.0, 126.4, 121.0; **HRMS (ESI) m/z** $[M+H]^+$: calcd for $C_{16}H_{12}N_3O_2$, 278.0924; found, 278.0921.

1-(4-chlorophenyl)-2-(1-phenyl-1H-1,2,3-triazol-4-yl)ethane-1,2-dione (6g)



The title compound was prepared on 1.1 mmol scale following General Procedure 3.2. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 277 mg, 81% yield. Yellow solid. Mp: 121-123 °C. R_f= 0.3 in EtOAc/petroleum ether (1:6). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.75 (s, 1H), 8.12 – 7.97 (m, 2H), 7.83 – 7.71 (m, 2H), 7.64 – 7.46 (m, 5H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 190.3, 184.7, 144.4, 141.8, 131.6, 130.7, 130.1, 129.9, 129.4, 126.6, 121.0; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{16}H_{11}ClN_3O_2$, 312.0534； found, 312.0529.

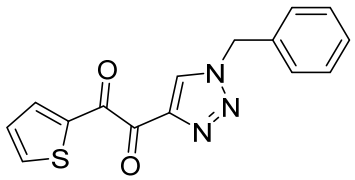
ethyl 2-(4-(2-oxo-2-phenylacetyl)-1H-1,2,3-triazol-1-yl)acetate (6h)



The title compound was prepared on 1.3 mmol scale following General Procedure 3.2. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 295 mg, 79% yield. Yellow liquid. R_f= 0.3 in EtOAc/petroleum ether (1:5). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.50 (s, 1H), 8.11 – 7.98 (m, 2H), 7.71 – 7.58 (m, 1H), 7.58 – 7.47 (m, 2H), 5.24 (d, *J* = 12.0 Hz, 2H), 4.54 – 4.17 (m, 2H), 1.57 – 1.04 (m, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 191.7, 185.4, 165.4, 144.5, 135.0, 132.3, 130.3, 130.0, 128.9, 62.9, 51.0, 14.0; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{14}H_{14}N_3O_4$, 288.0979；

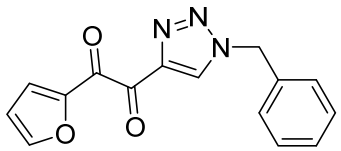
found, 288.0978.

1-(1-benyl-1H-1,2,3-triazol-4-yl)-2-(thiophen-2-yl)ethane-1,2-dione (6i)



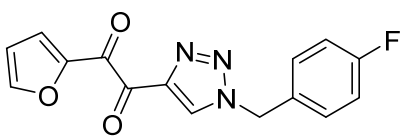
The title compound was prepared on 1.3 mmol scale following General Procedure 3.2. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 235 mg, 61% yield. Yellow solid. R_f = 0.3 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.38 (s, 1H), 8.10 (s, 1H), 7.85 (s, 1H), 7.36 (d, *J* = 27.9 Hz, 5H), 7.20 (d, *J* = 3.3 Hz, 1H), 5.62 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 194.23, 181.49, 142.95, 138.19, 137.9, 137.6, 133.4, 129.7, 129.4 (, 129.3, 128.8, 128.4, 54.5; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{15}H_{12}N_3O_2S$, 298.0650；found, 298.0645.

1-(1-benyl-1H-1,2,3-triazol-4-yl)-2-(furan-2-yl)ethane-1,2-dione (6j)



The title compound was prepared on 1.4 mmol scale following General Procedure 3.2. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 263 mg, 67% yield. Yellow solid. R_f = 0.3 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.40 (s, 1H), 7.73 (d, *J* = 21.2 Hz, 2H), 7.35 (d, *J* = 24.9 Hz, 5H), 6.63 (s, 1H), 5.61 (s, 2H);**^{13}C NMR (101 MHz, $CDCl_3$):** δ 181.0, 176.7, 149.6, 149.1, 142.8, 133.4, 129.7, 129.3, 129.2, 128.3, 125.2, 113.2, 54.5; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{15}H_{12}N_3O_3$, 282.0879；found, 282.0873.

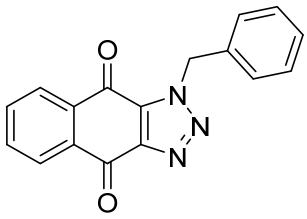
1-(1-(4-fluorobenzyl)-1H-1,2,3-triazol-4-yl)-2-(furan-2-yl)ethane-1,2-dione (6k)



The title compound was prepared on 1.4 mmol scale following General Procedure 3.2. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in

petroleum ether) to afford the title compound 259 mg, 62% yield. Yellow solid. R_f = 0.3 in EtOAc/petroleum ether (1:3). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.42 (s, 1H), 7.76 (d, *J* = 14.9 Hz, 2H), 7.33 (s, 2H), 7.10 (t, *J* = 7.7 Hz, 2H), 6.64 (s, 1H), 5.60 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 180.9, 176.6, 149.7, 149.1, 142.9, 130.3 (d, *J* = 8.4 Hz), 129.6, 125.4, 116.6, 116.3, 113.3, 53.7; **HRMS (ESI) m/z** $[M + H]^+$: calcd for $C_{15}H_{11}FN_3O_3$, 300.0784；found, 300.0779.

1-benzyl-1H-naphtho[2,3-d][1,2,3]triazole-4,9-dione (8)



The title compound was prepared on 1.2 mmol scale following General Procedure 3.2. The crude product was purified by silica gel column chromatography (0% to 20% EtOAc in petroleum ether) to afford the title compound 271 mg, 78% yield. Brown solid. Mp: 194−196 °C. R_f = 0.2 in EtOAc/petroleum ether (1:4). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.37 – 8.26 (m, 1H), 8.26 – 8.18 (m, 1H), 7.87 – 7.76 (m, 2H), 7.54 – 7.46 (m, 2H), 7.39 – 7.31 (m, 3H), 6.01 (s, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 176.7, 175.3, 145.6, 135.2, 134.2, 133.8, 133.4, 133.1, 132.8, 129.0, 128.6, 127.8, 127.4, 53.8; Spectral data match those previously reported in the literature.[17]

6. References

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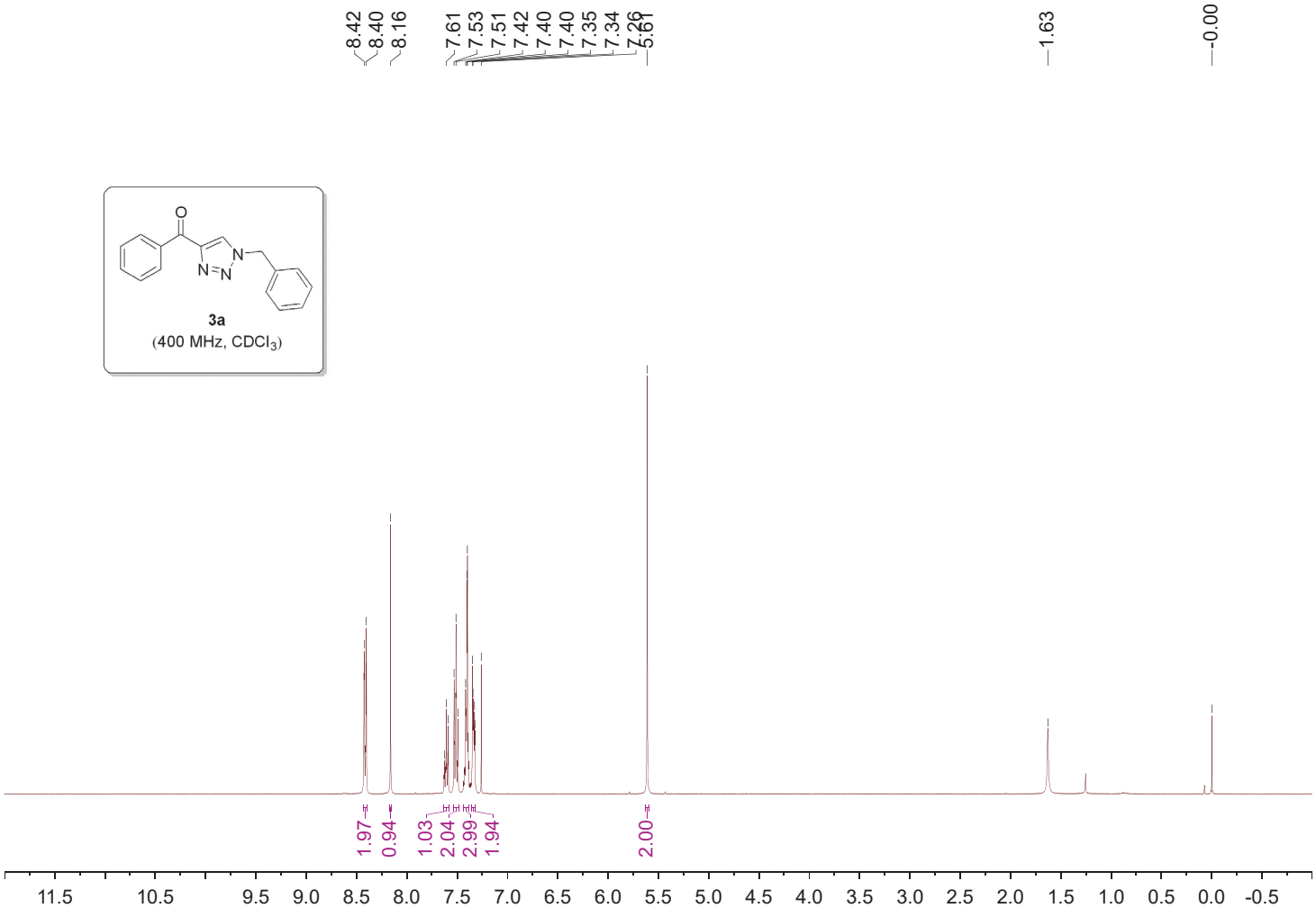
7. ^{1}H and ^{13}C NMR spectra of products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8.16
7.61
7.53
7.51
7.42
7.40
7.40
7.35
7.34
7.26
5.61
1.63
0.00
3a
(400 MHz, CDCl3)
1.97
0.94
1.03
2.04
2.99
1.94
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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1.5
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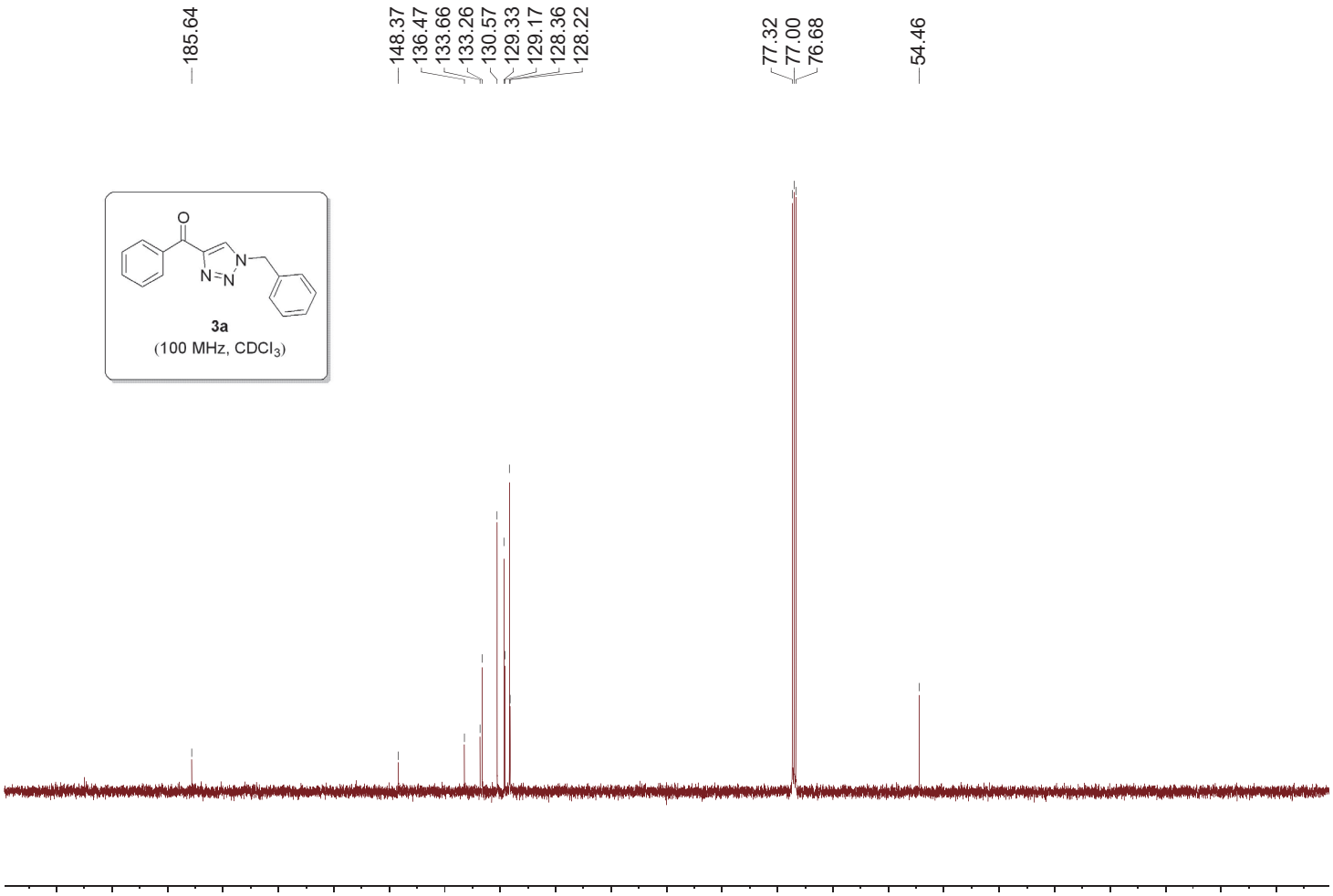
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136.47
133.66
133.26
130.57
129.33
129.17
128.36
128.22
77.32
77.00
76.68
54.46
3a
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
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60
50
40
30
20
10
0
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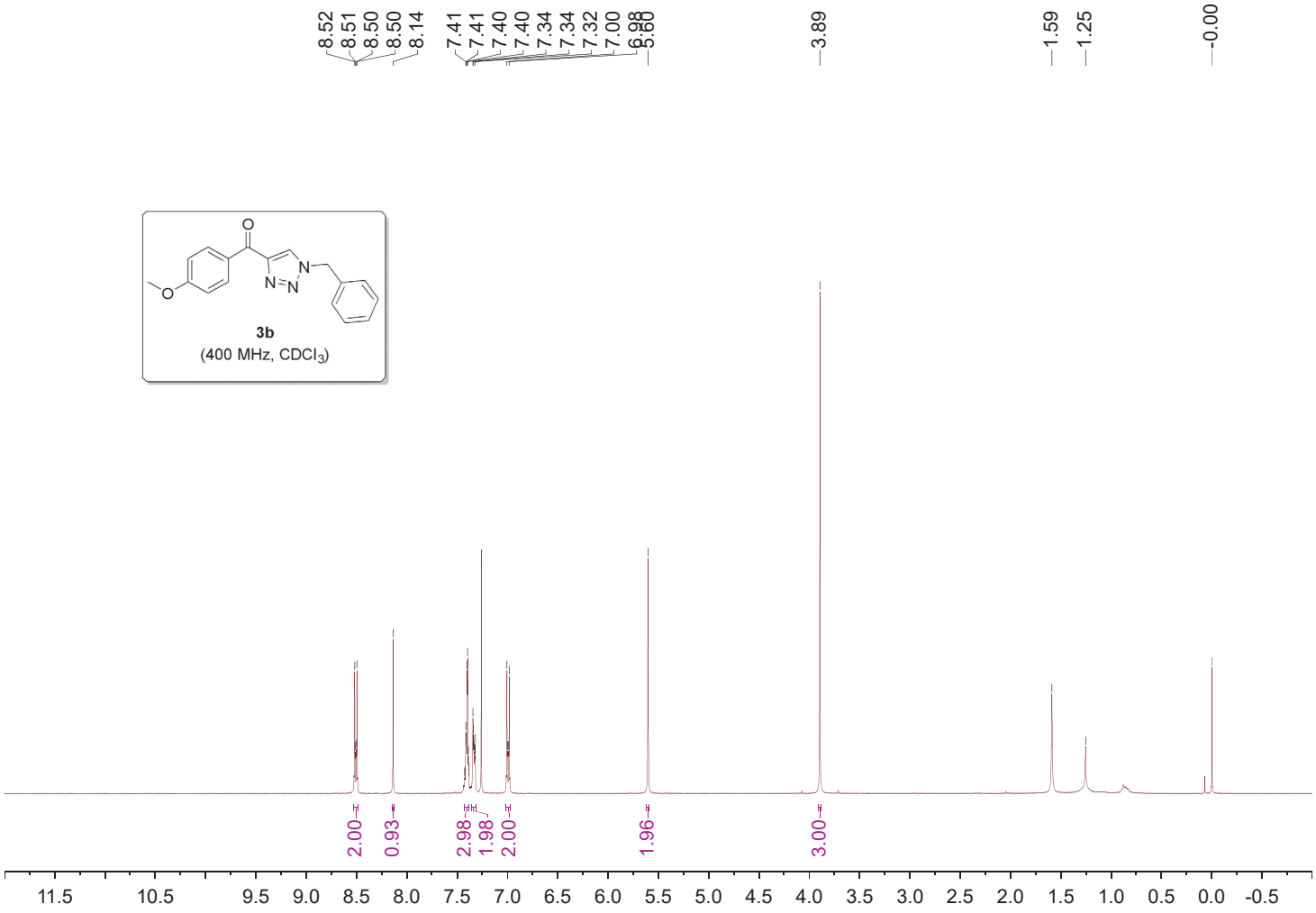
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7.41
7.40
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7.34
7.34
7.32
7.00
6.98
6.80
3.89
1.59
1.25
-0.00
3b
(400 MHz, CDCl3)
2.00
0.93
2.98
1.98
2.00
1.96
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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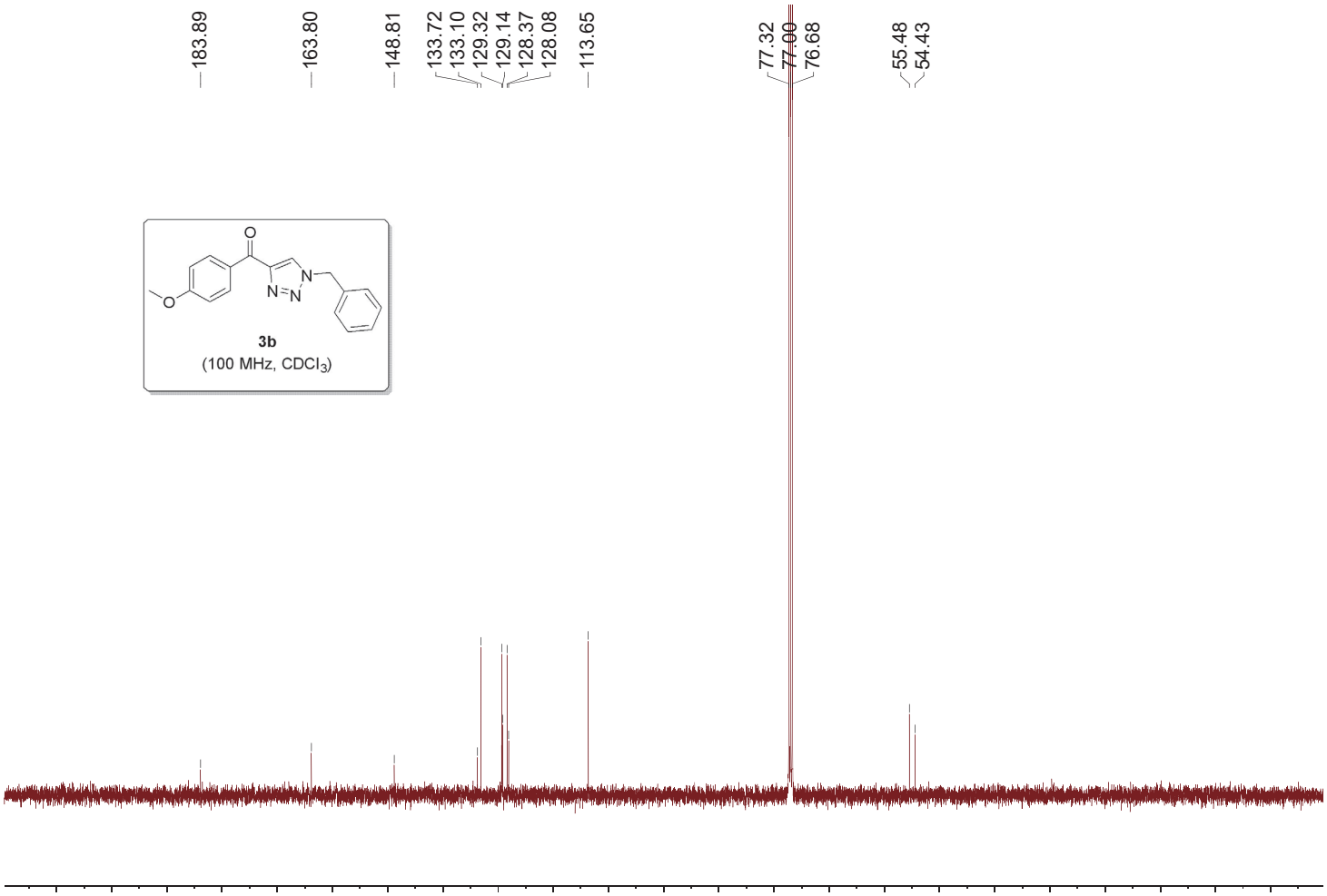
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129.14
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76.68
55.48
54.43
3b
(100 MHz, CDCl3)
210
200
190
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130
120
110
100
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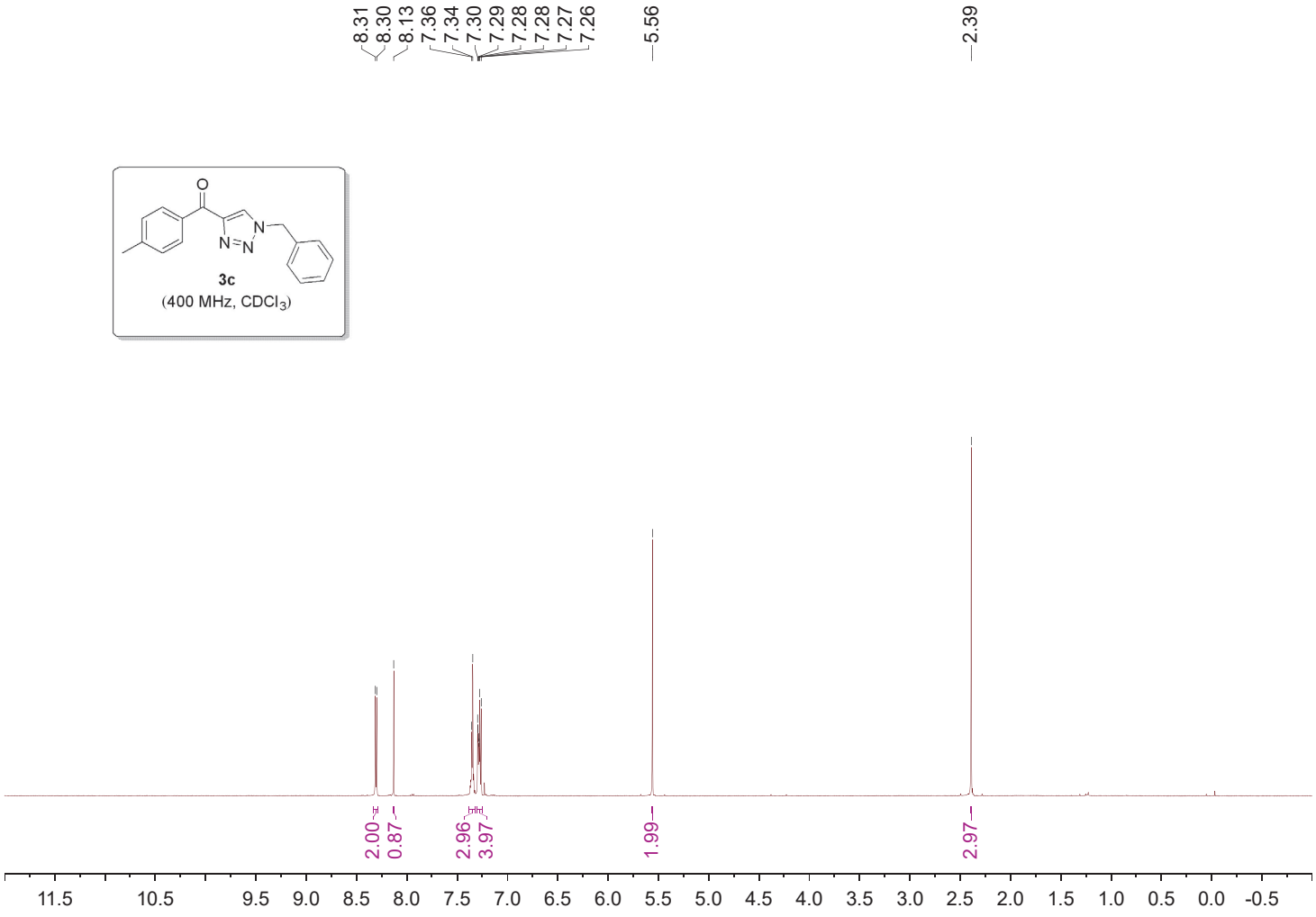
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7.28
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2.39
3c
(400 MHz, CDCl3)
2.00
0.87
2.96
3.97
1.99
2.97
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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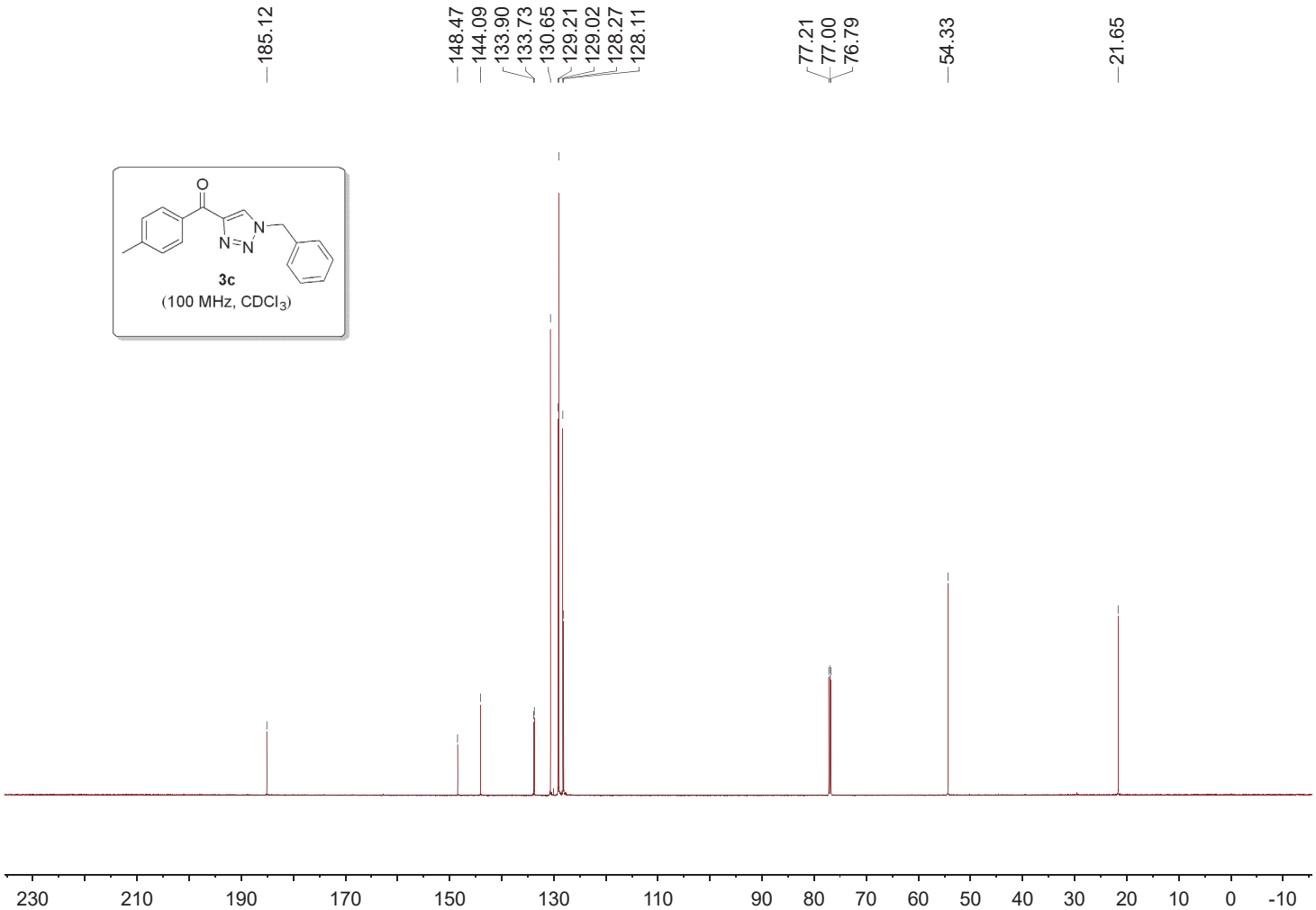
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77.00
76.79
54.33
21.65
3c
(100 MHz, CDCl3)
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90
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70
60
50
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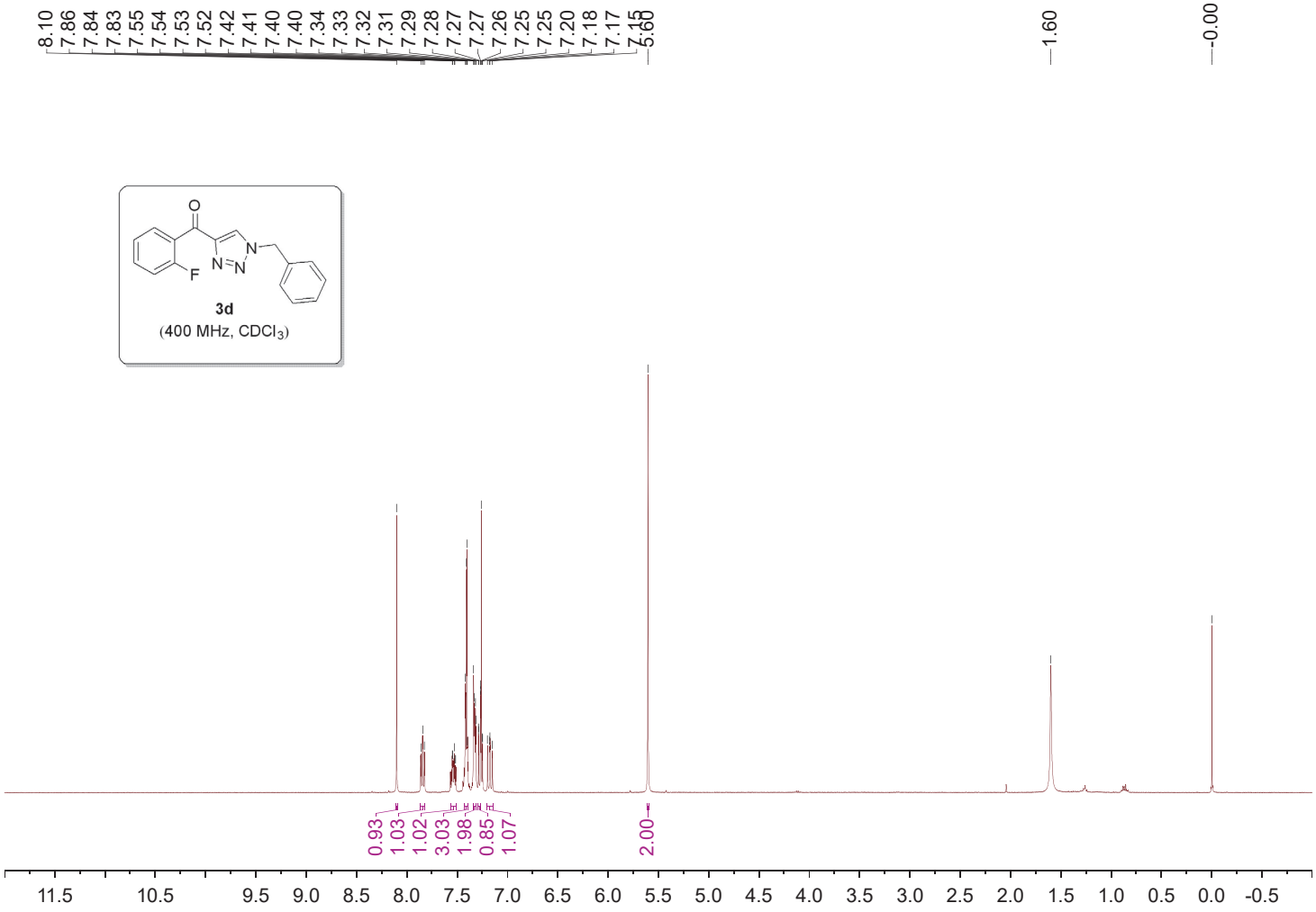
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7.17
7.15
5.60
1.60
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3d
(400 MHz, CDCl3)
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1.03
1.02
3.03
1.98
0.85
1.07
2.00
11.5
10.5
9.5
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6.0
5.5
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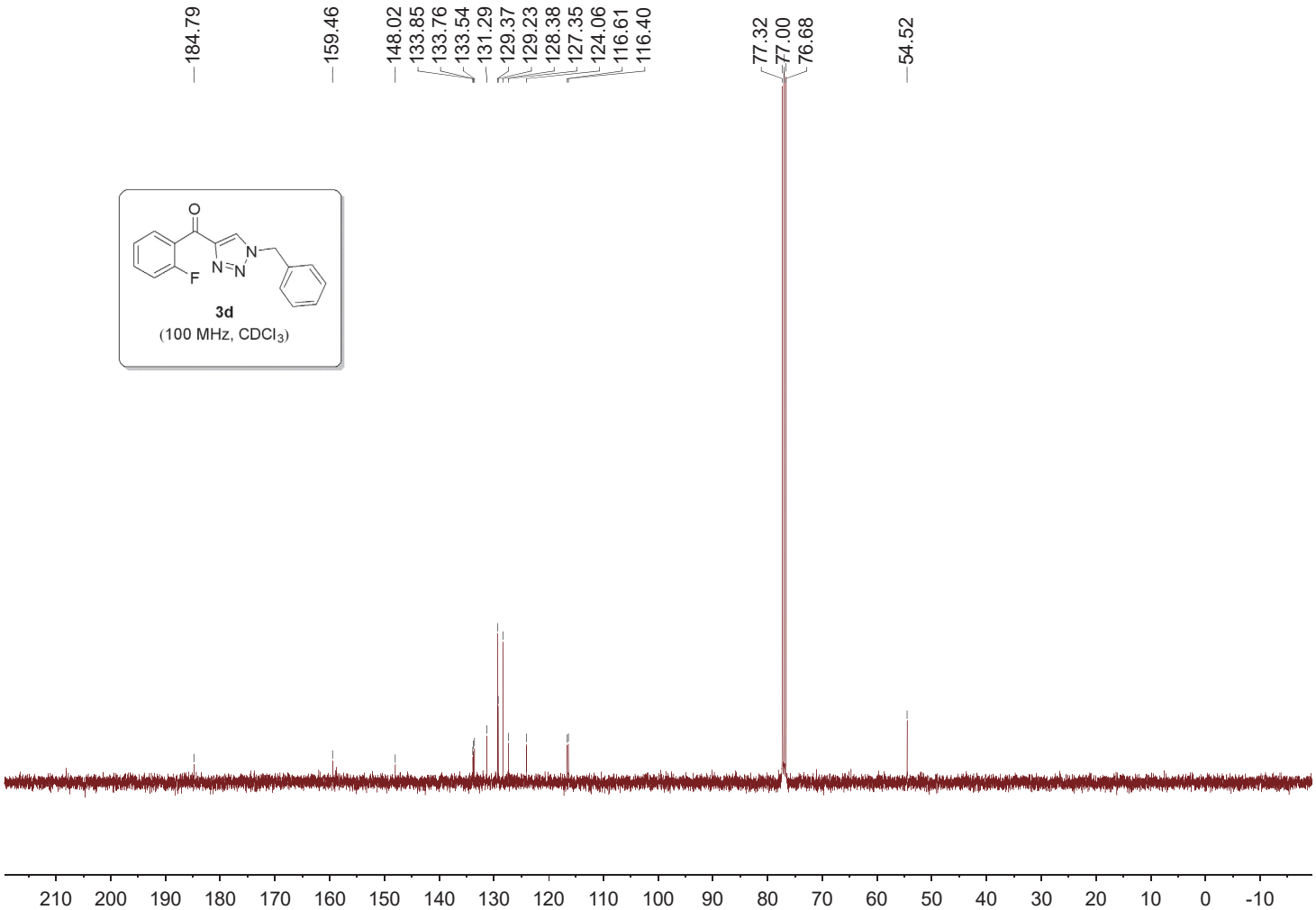
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116.61
116.40
77.32
77.00
76.68
54.52
3d
(100 MHz, CDCl3)
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200
190
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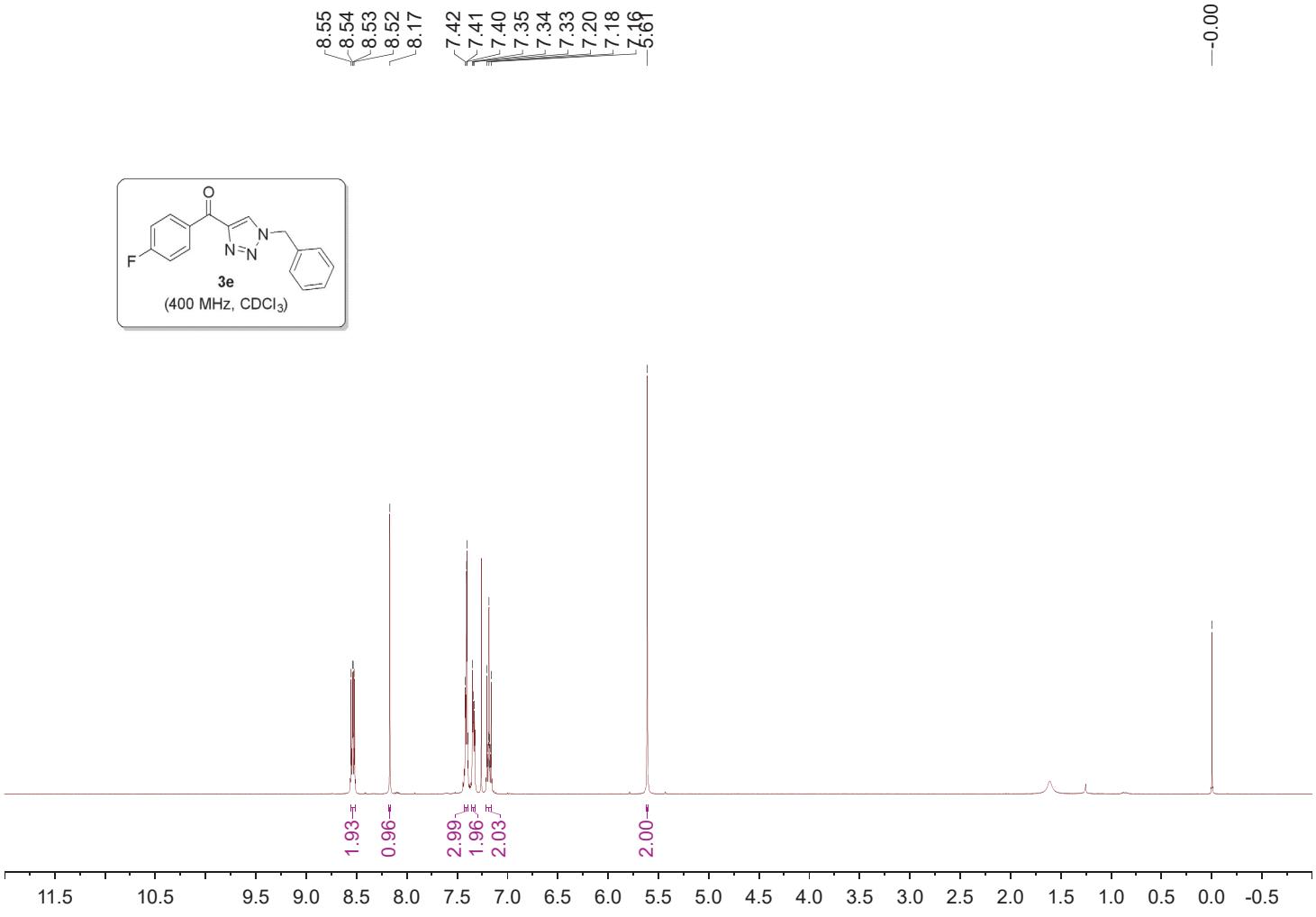
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7.18
7.16
5.61
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3e
(400 MHz, CDCl3)
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2.99
1.96
2.03
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11.5
10.5
9.5
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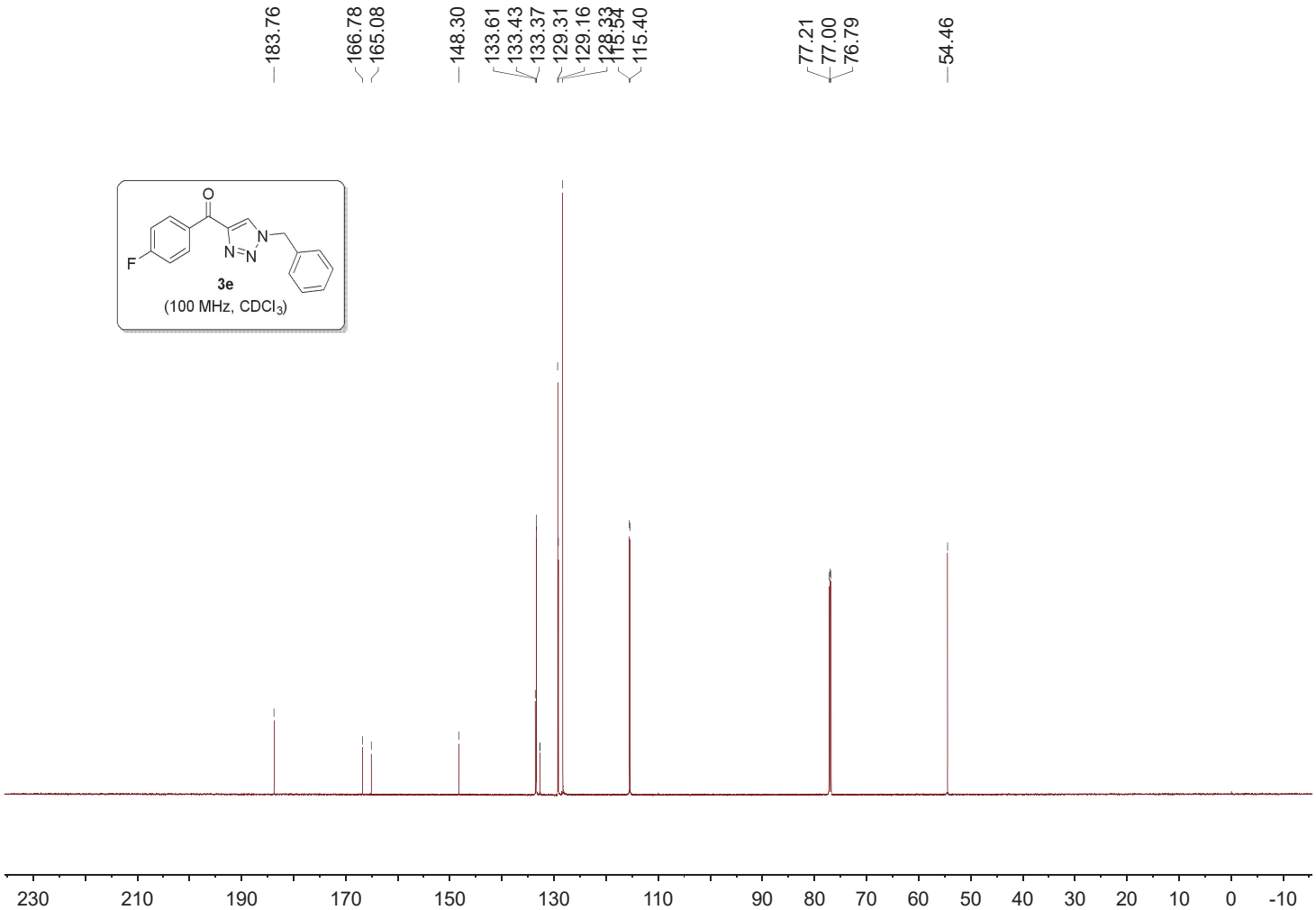
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3e
(100 MHz, CDCl3)
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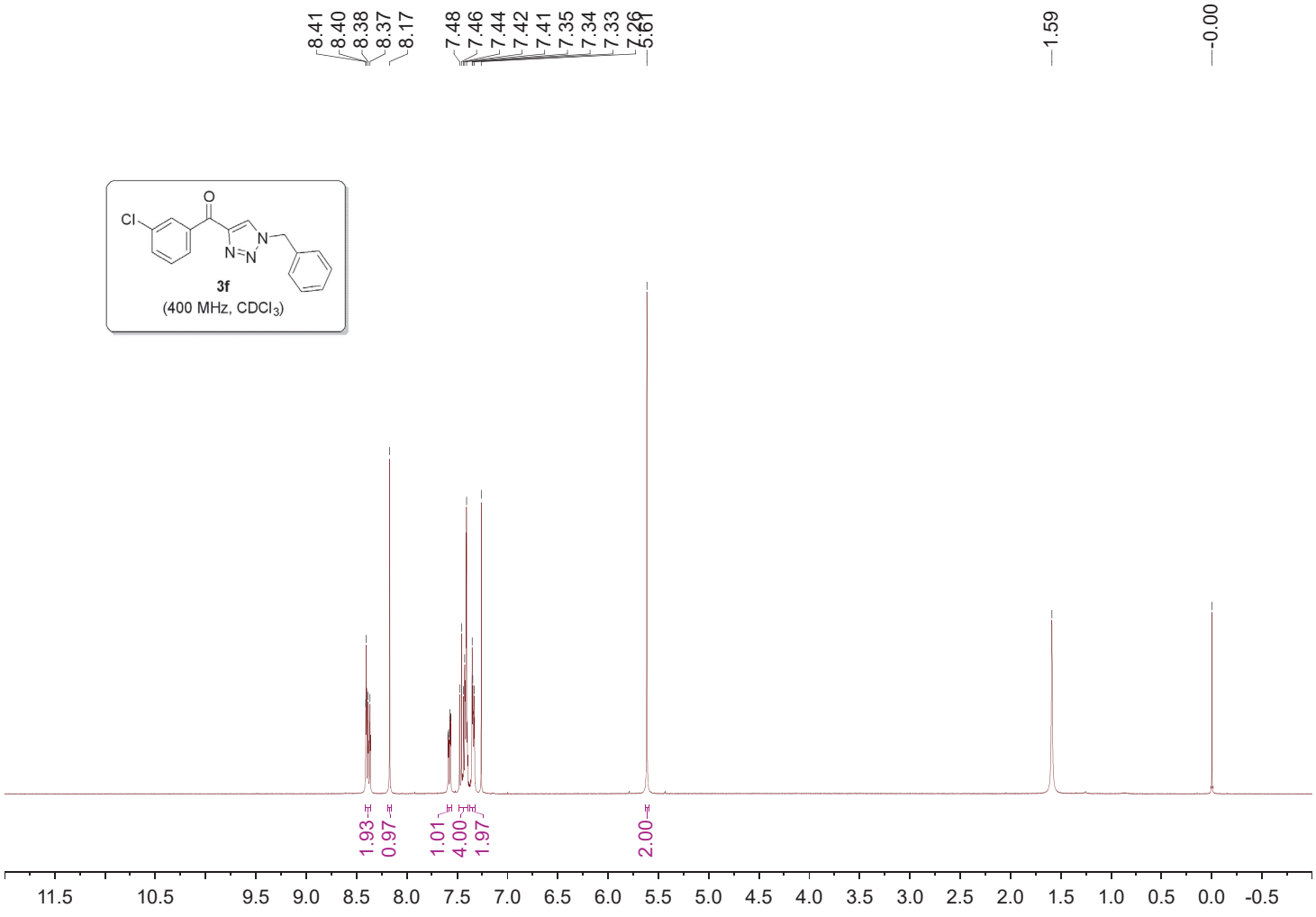
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1.59
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Cl
O
N
N
N
3f
(400 MHz, CDCl3)
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10.5
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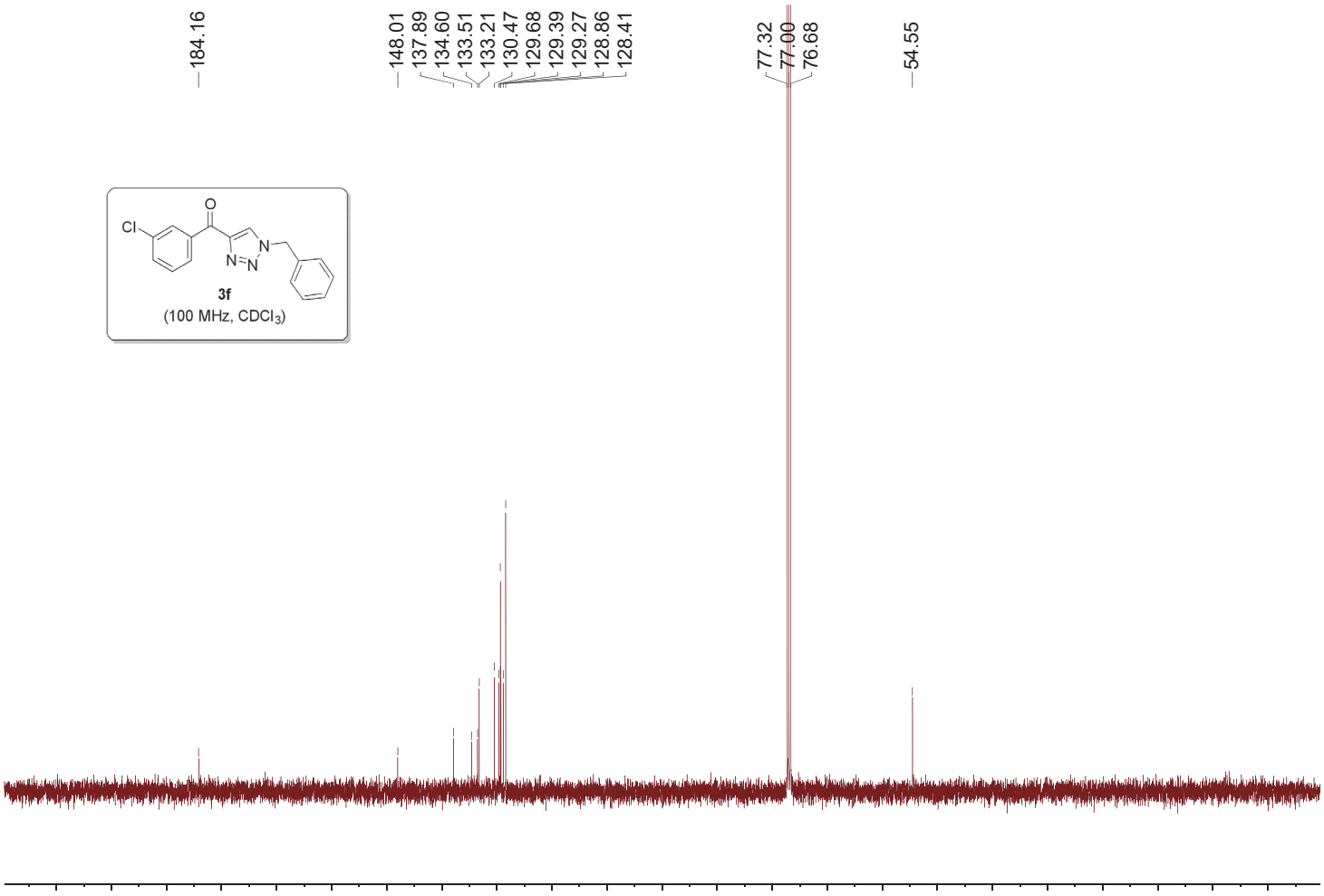
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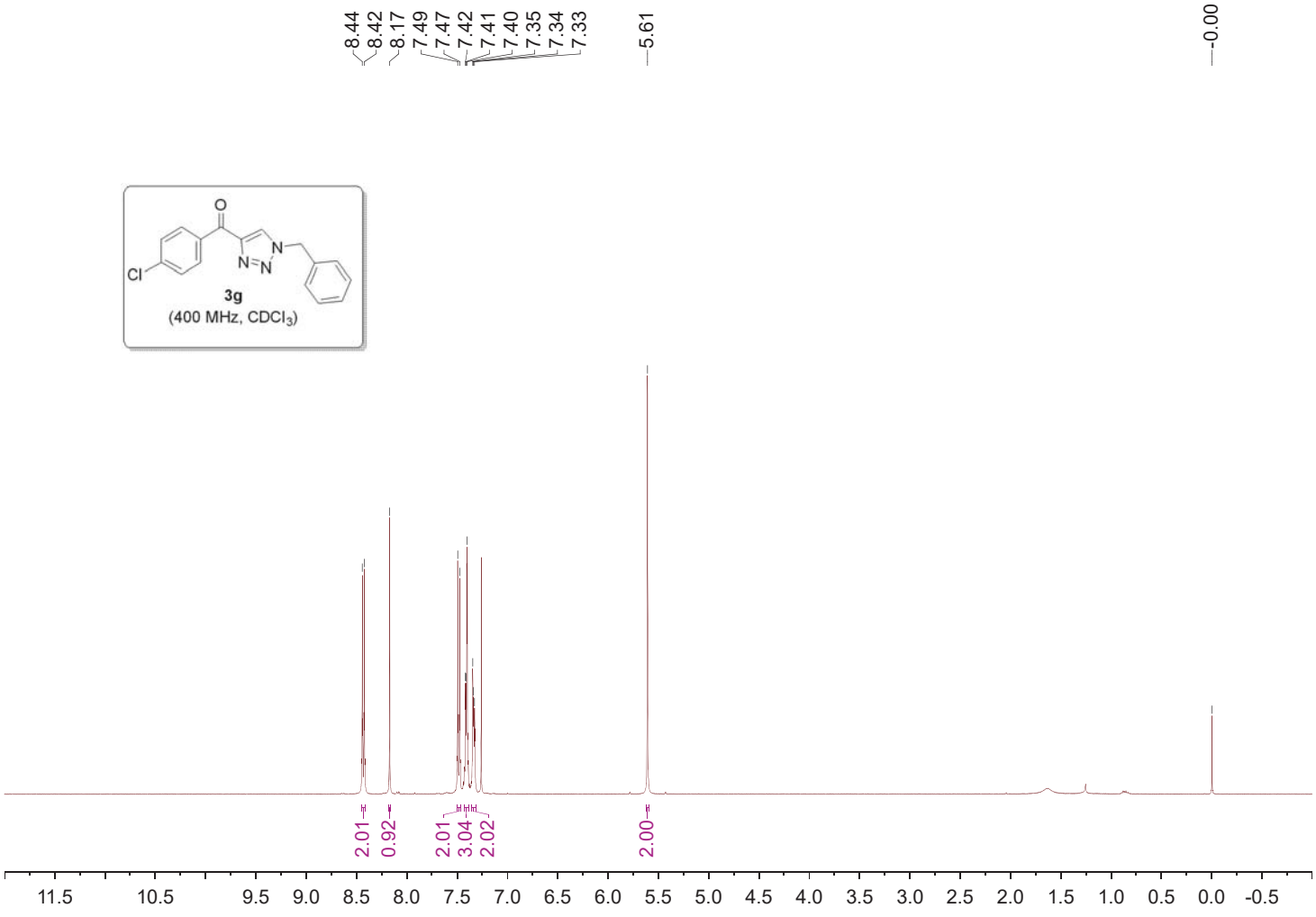
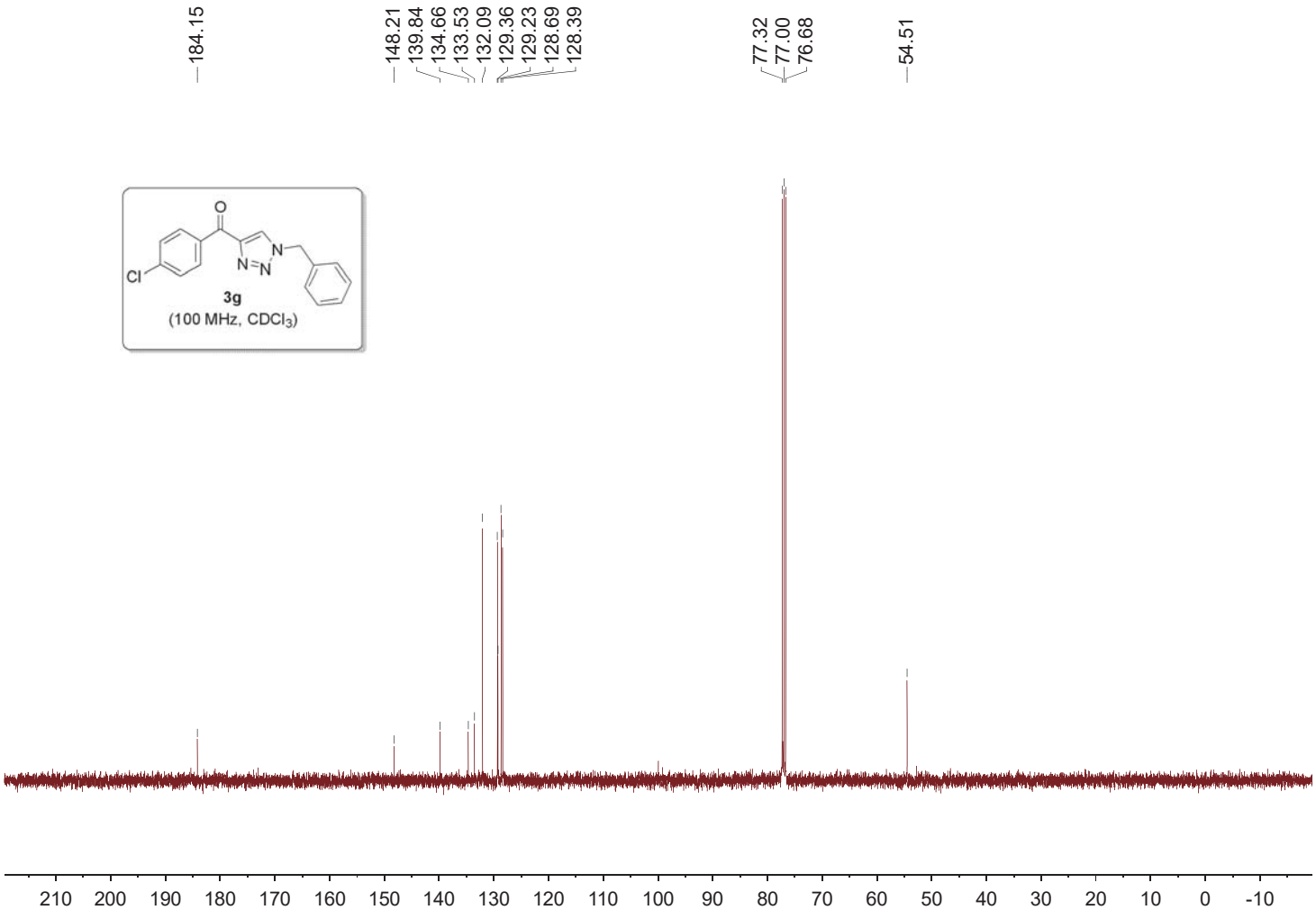
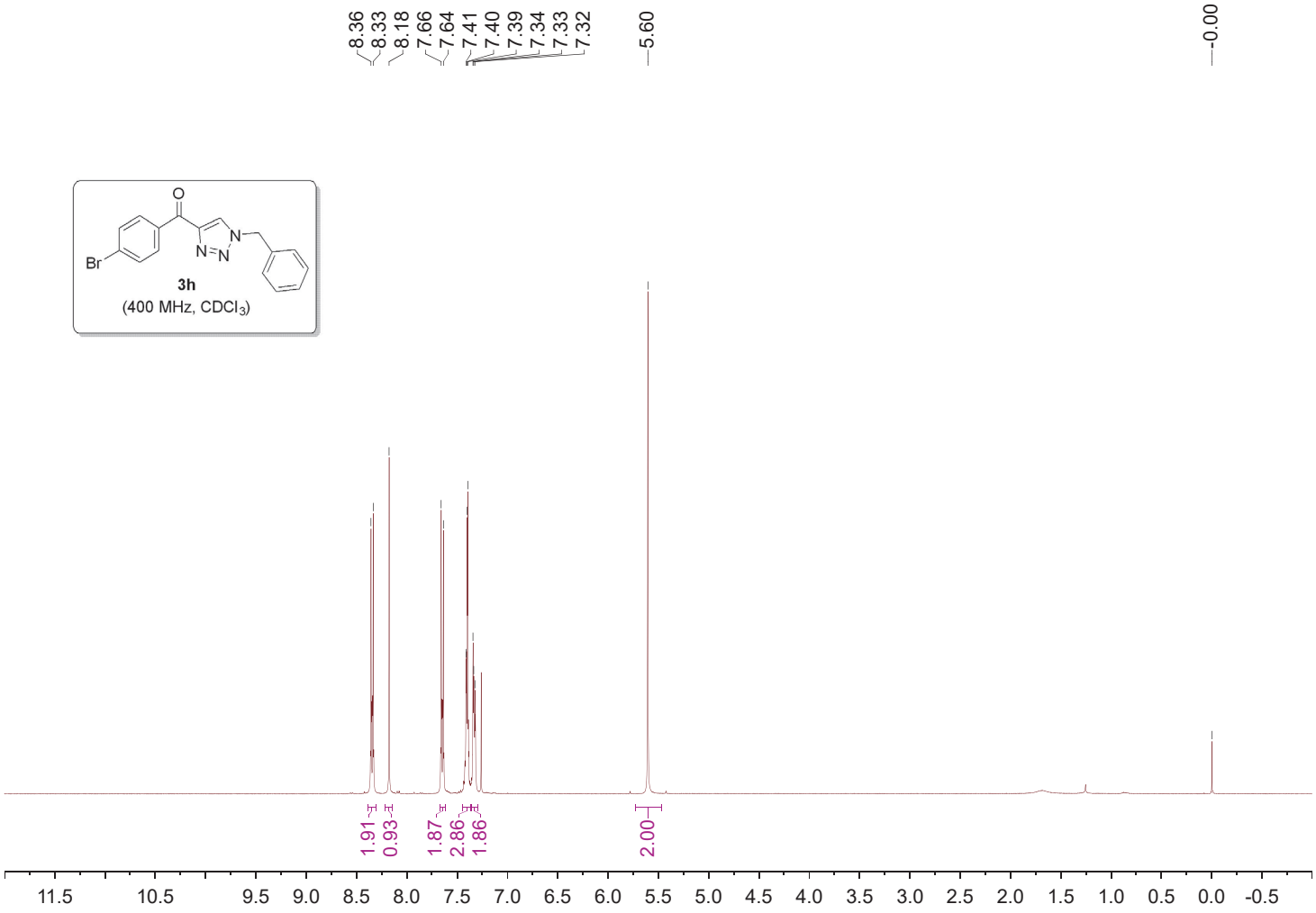
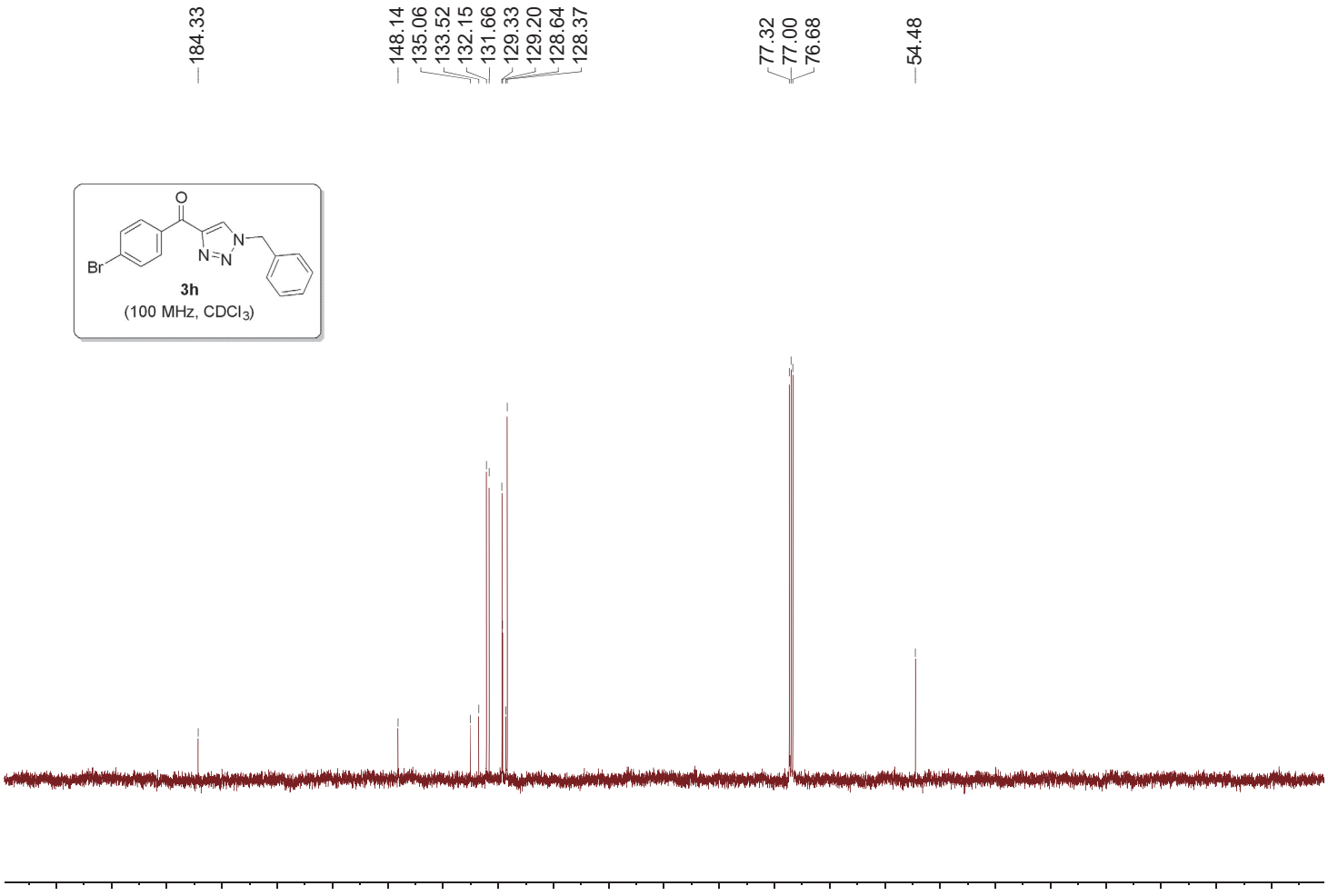
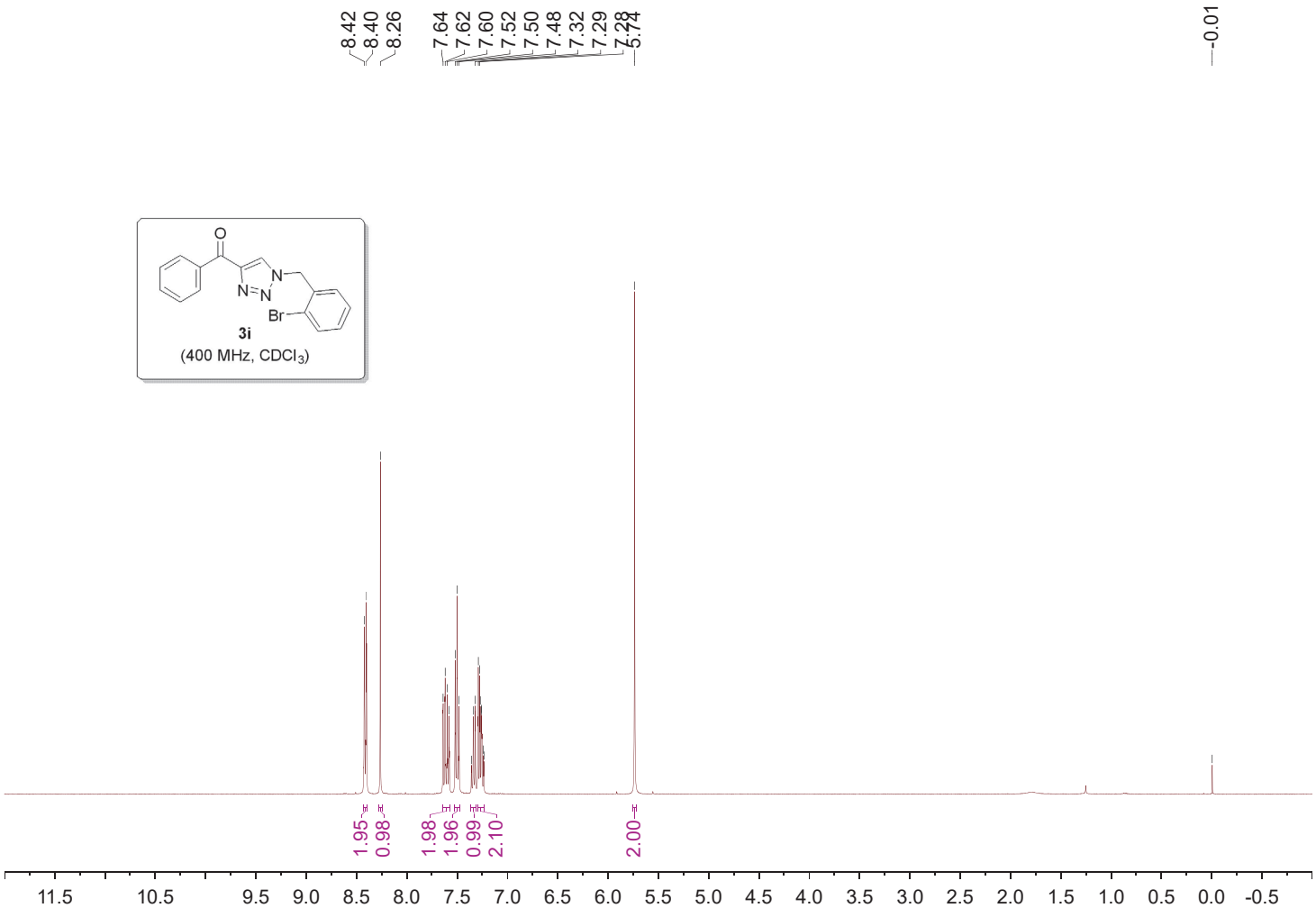
Cl
O
N
N
N
3f
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

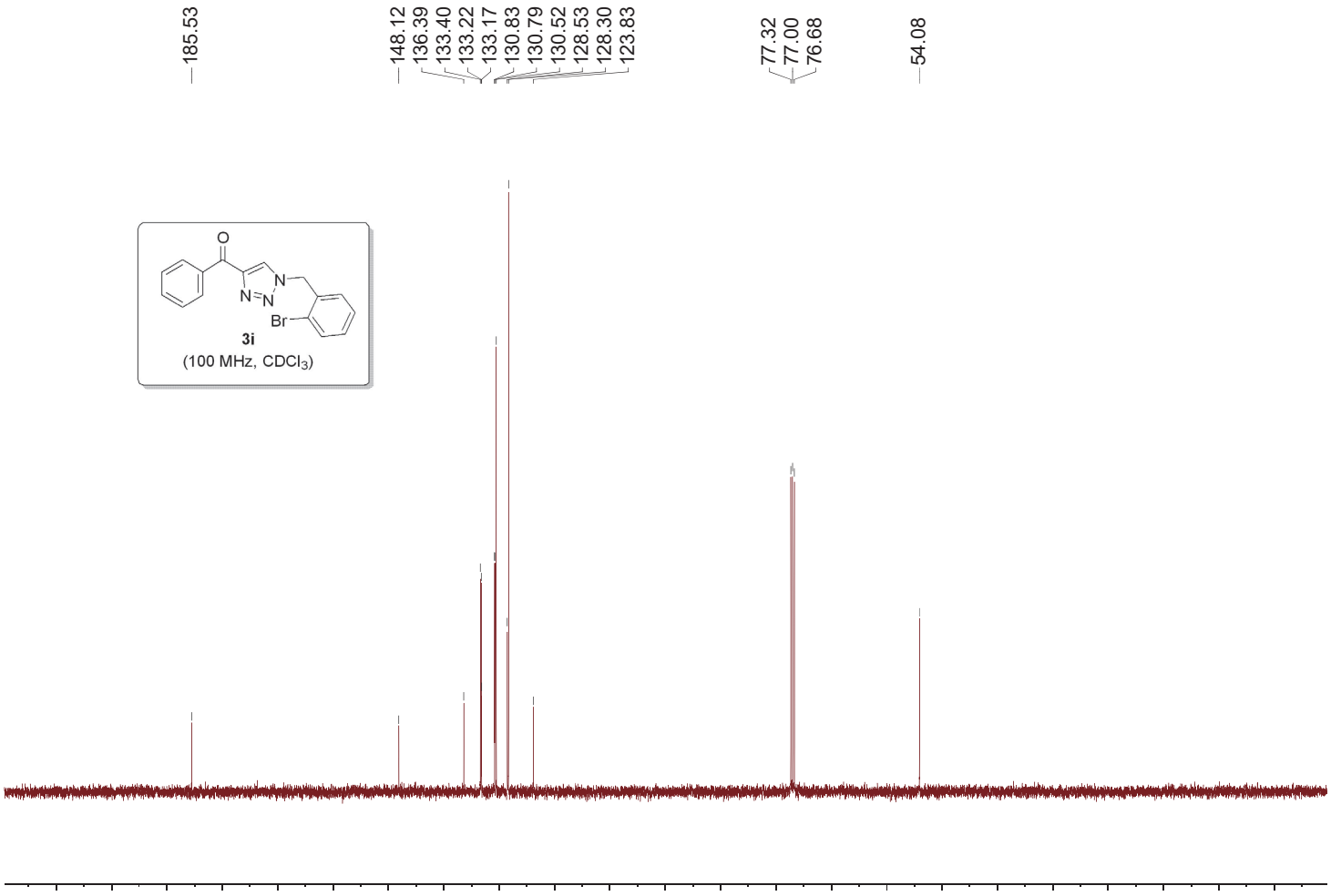

8.44
8.42
8.17
7.49
7.47
7.42
7.41
7.40
7.35
7.34
7.33
5.61
-0.00
3g
(400 MHz, CDCl3)
2.01
0.92
2.01
3.04
2.02
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

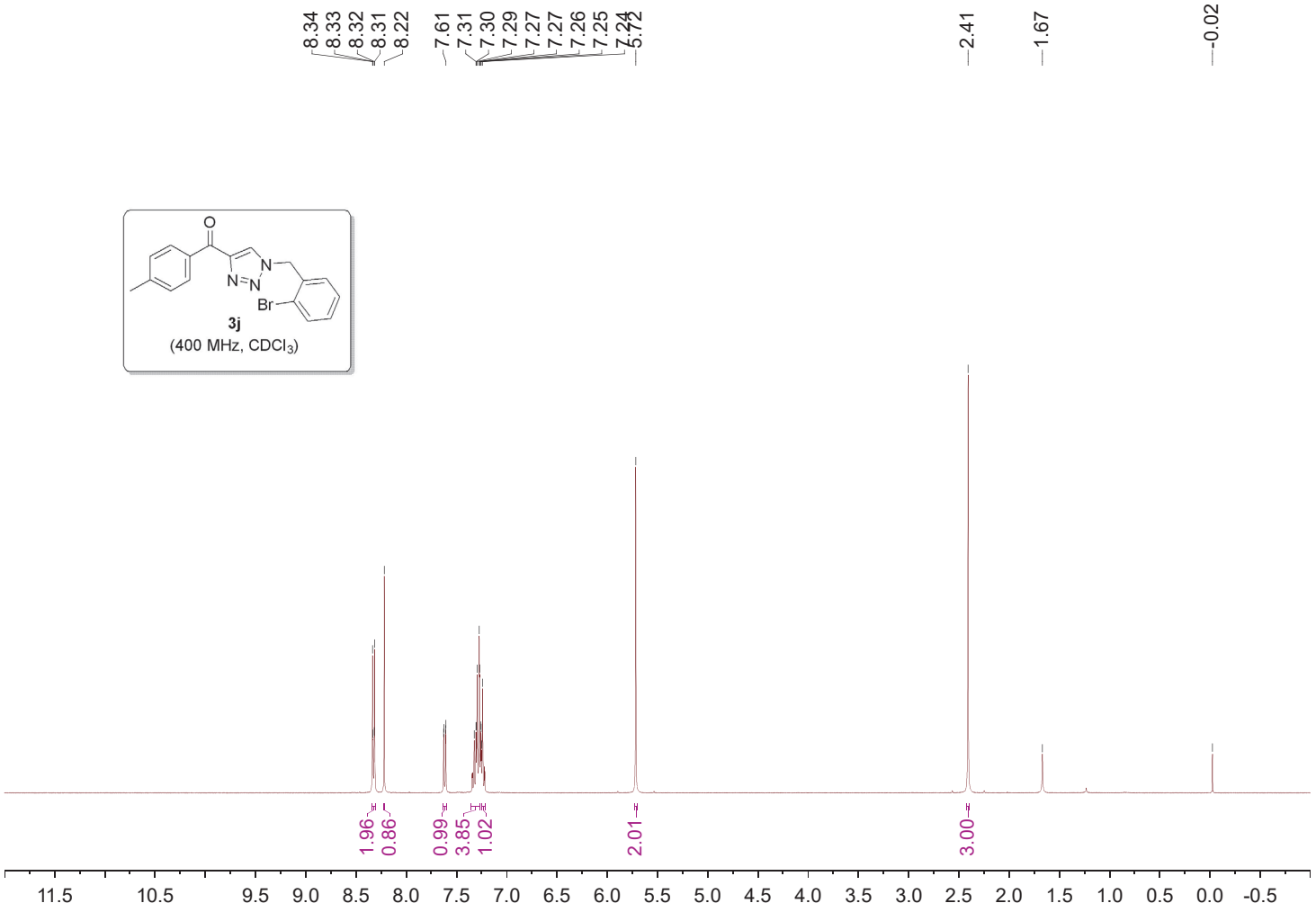

184.15
148.21
139.84
134.66
133.53
132.09
129.36
129.23
128.69
128.39
77.32
77.00
76.68
54.51
3g
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

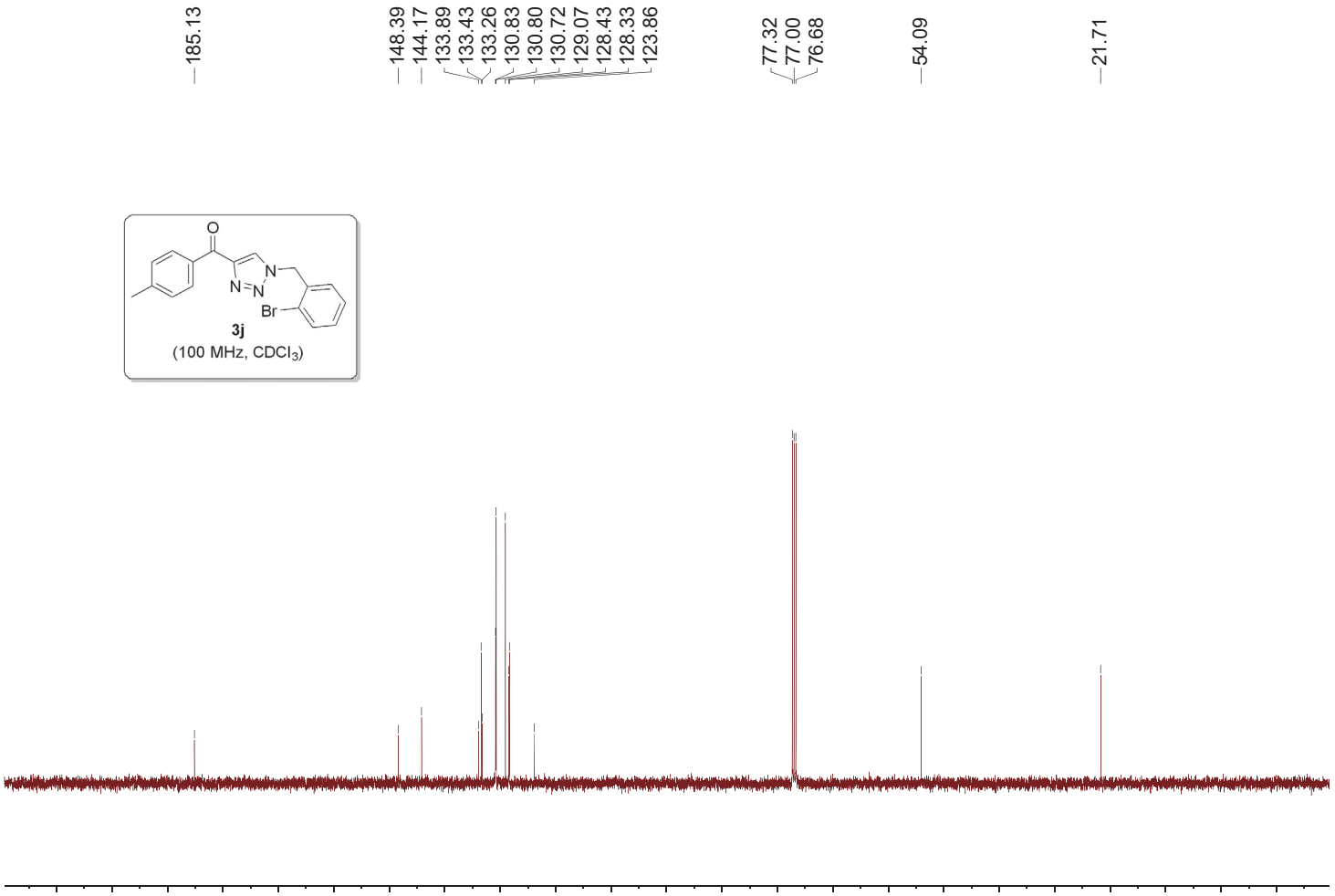

8.36
8.33
8.18
7.66
7.64
7.41
7.40
7.39
7.34
7.33
7.32
5.60
0.00
Br
3h
(400 MHz, CDCl3)
1.91
0.93
1.87
2.86
1.86
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

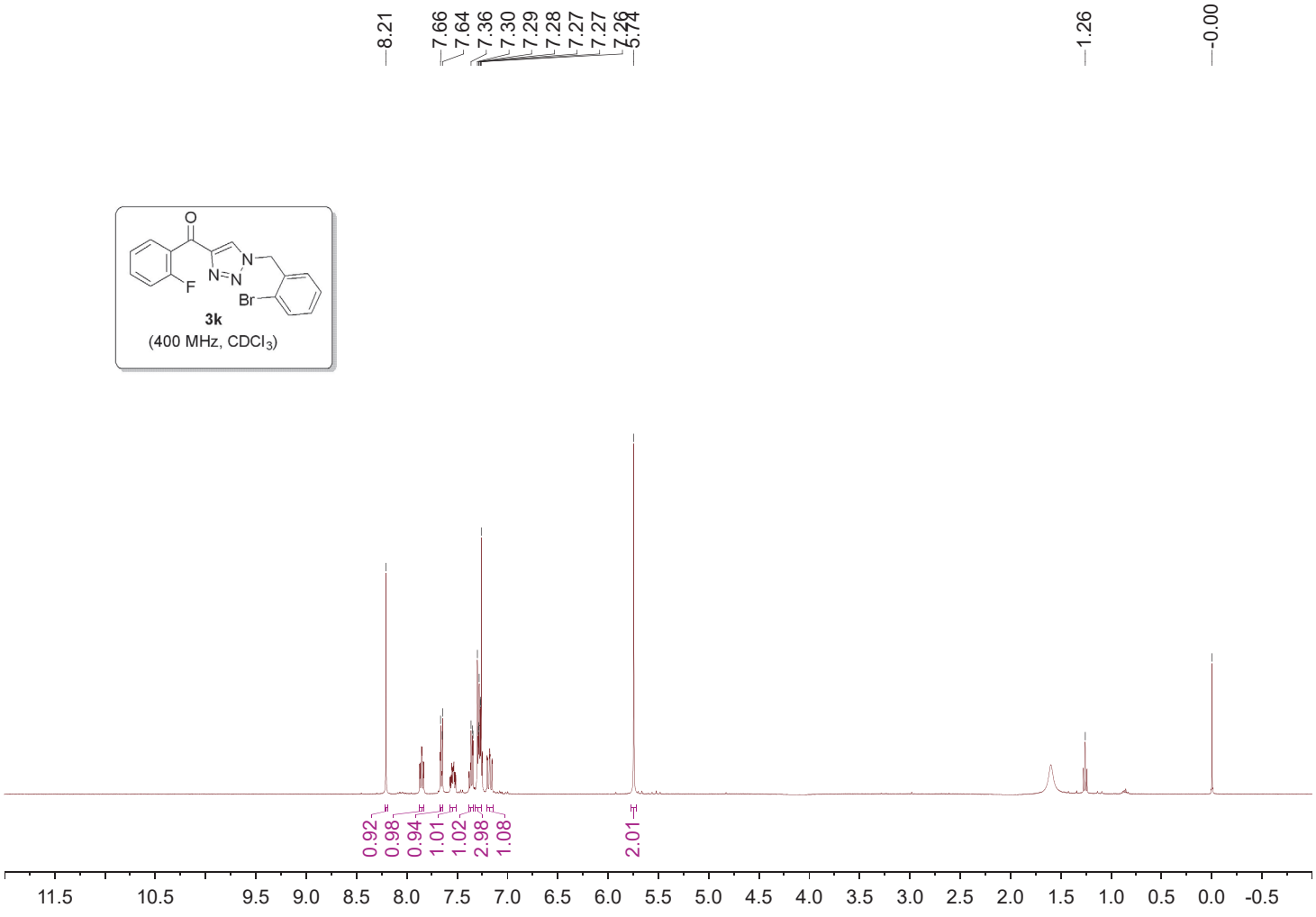

184.33
148.14
135.06
133.52
132.15
131.66
129.33
129.20
128.64
128.37
77.32
77.00
76.68
54.48
Br
3h
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

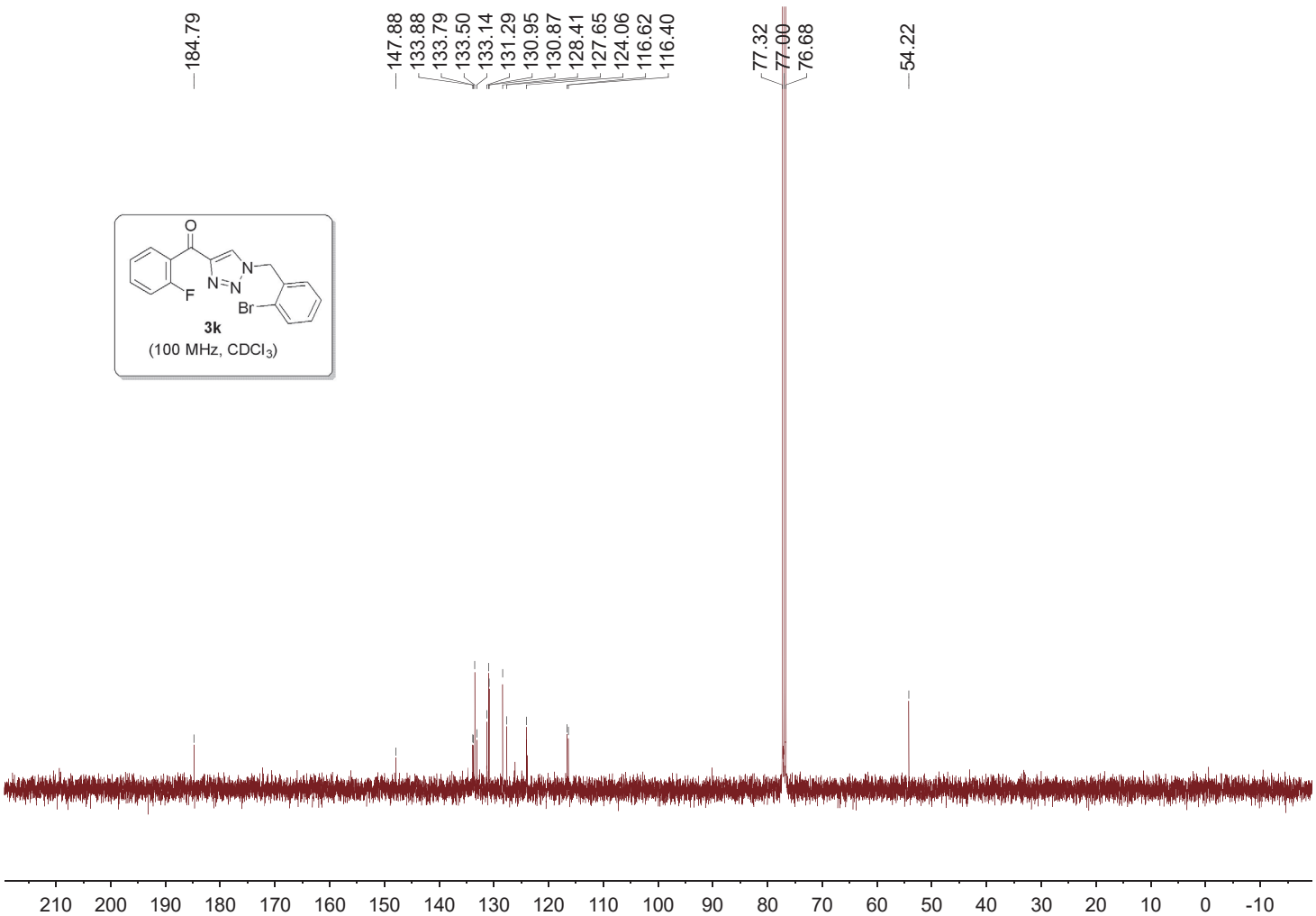

8.42
8.40
8.26
7.64
7.62
7.60
7.52
7.50
7.48
7.32
7.29
7.28
5.14
-0.01
O
N
N
N
Br
3i
(400 MHz, CDCl3)
1.95
0.98
1.98
1.96
0.99
2.10
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

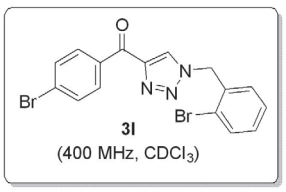

185.53
148.12
136.39
133.40
133.22
133.17
130.83
130.79
130.52
128.53
128.30
123.83
77.32
77.00
76.68
54.08
O
N
N
N
Br
3i
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


8.34
8.33
8.32
8.31
8.22
7.61
7.31
7.30
7.29
7.27
7.27
7.26
7.25
5.12
2.41
1.67
-0.02
O
N
N
Br
3j
(400 MHz, CDCl3)
1.96
0.86
0.99
3.85
1.02
2.01
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


185.13
148.39
144.17
133.89
133.43
133.26
130.83
130.80
130.72
129.07
128.43
128.33
123.86
77.32
77.00
76.68
54.09
21.71
O
N
N
Br
3j
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


8.21
7.66
7.64
7.36
7.30
7.29
7.28
7.27
7.27
7.26
5.74
1.26
-0.00
3k
(400 MHz, CDCl3)
0.92
0.98
0.94
1.01
1.02
2.98
1.08
2.01
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


184.79
147.88
133.88
133.79
133.50
133.14
131.29
130.95
130.87
128.41
127.65
124.06
116.62
116.40
77.32
77.00
76.68
54.22
3k
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10



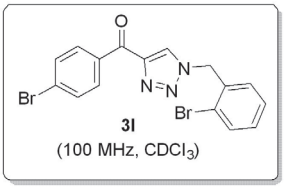
3l
(400 MHz, $CDCl_3$)

8.35 8.35 8.34 8.33 8.27 7.65 7.64 7.63 7.62 7.62 7.33 7.30 7.28 7.26 5.73

2.01 0.94 2.99 1.02 1.99 2.00

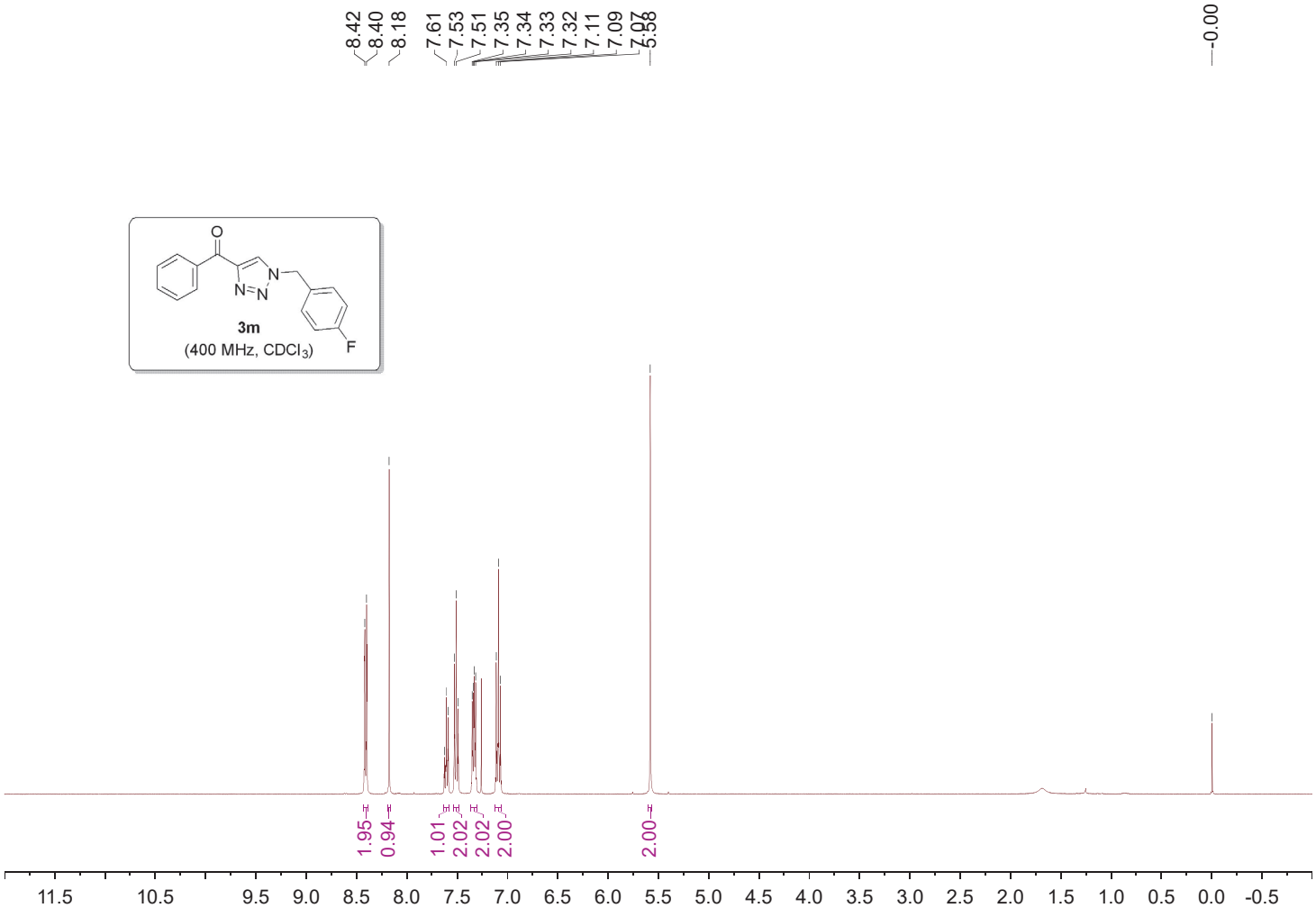
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

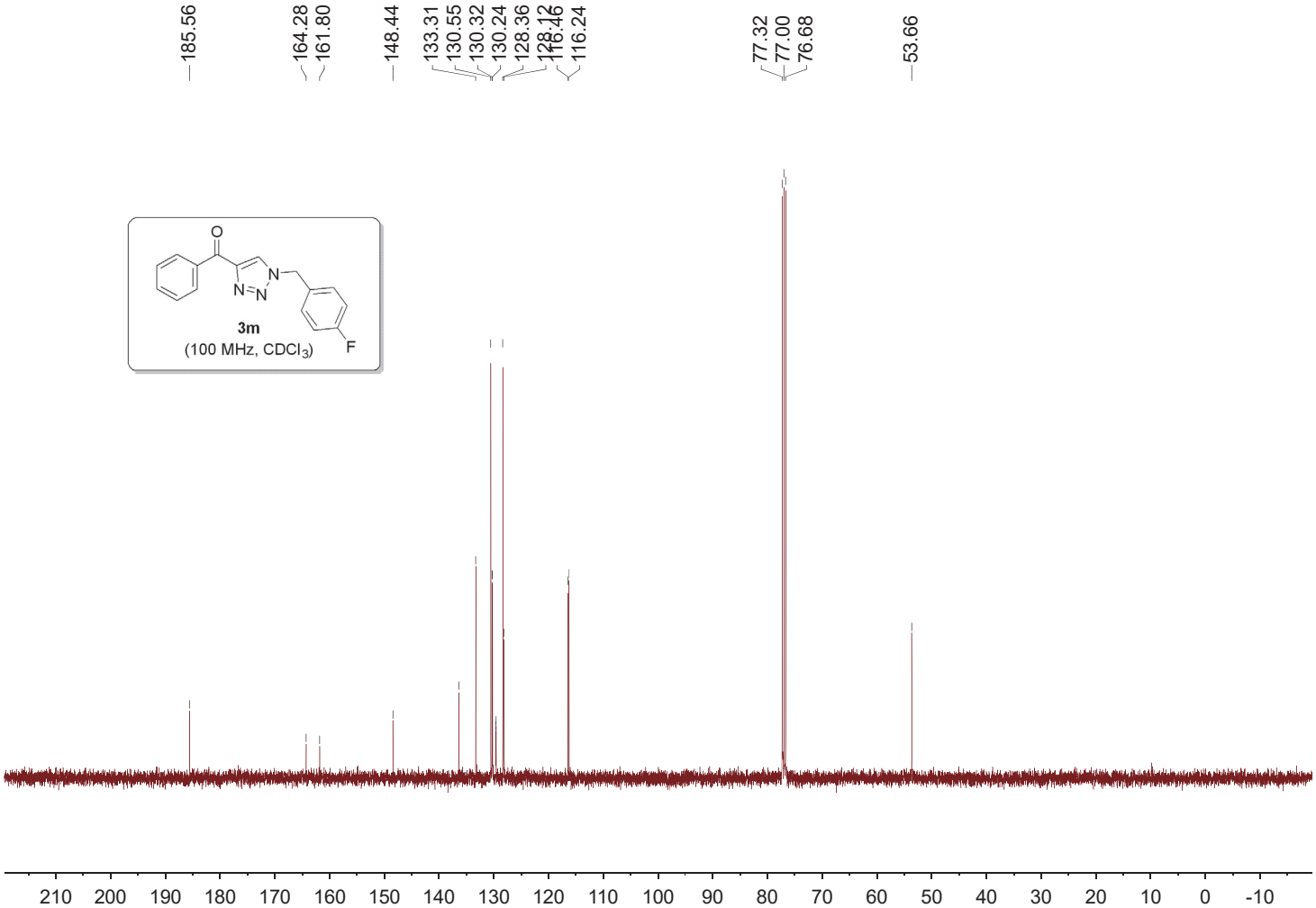
184.22 147.94 135.02 133.44 133.06 132.13 131.62 130.90 130.86 128.67 128.62 128.33 123.89 77.32 77.00 76.68 54.15

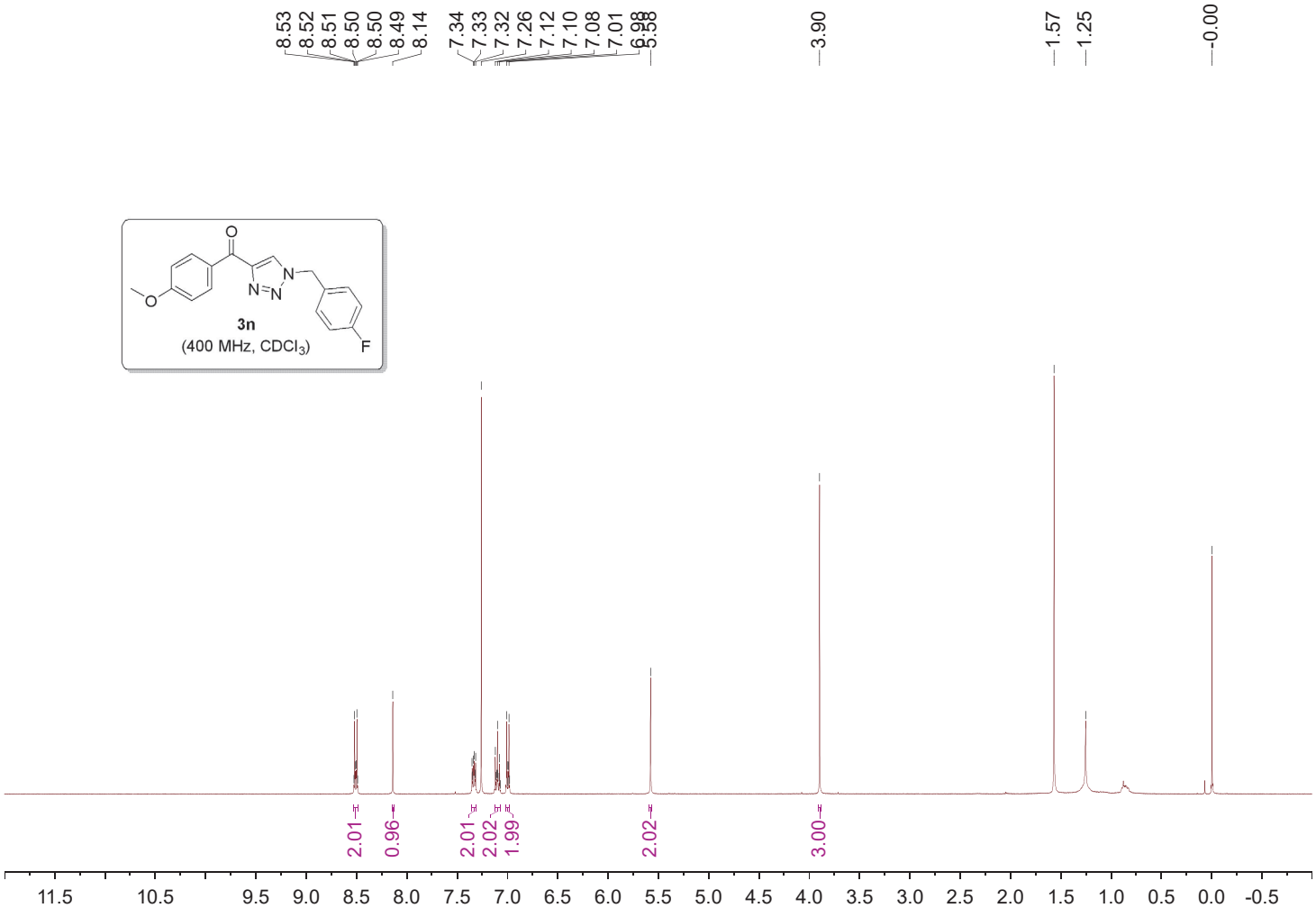


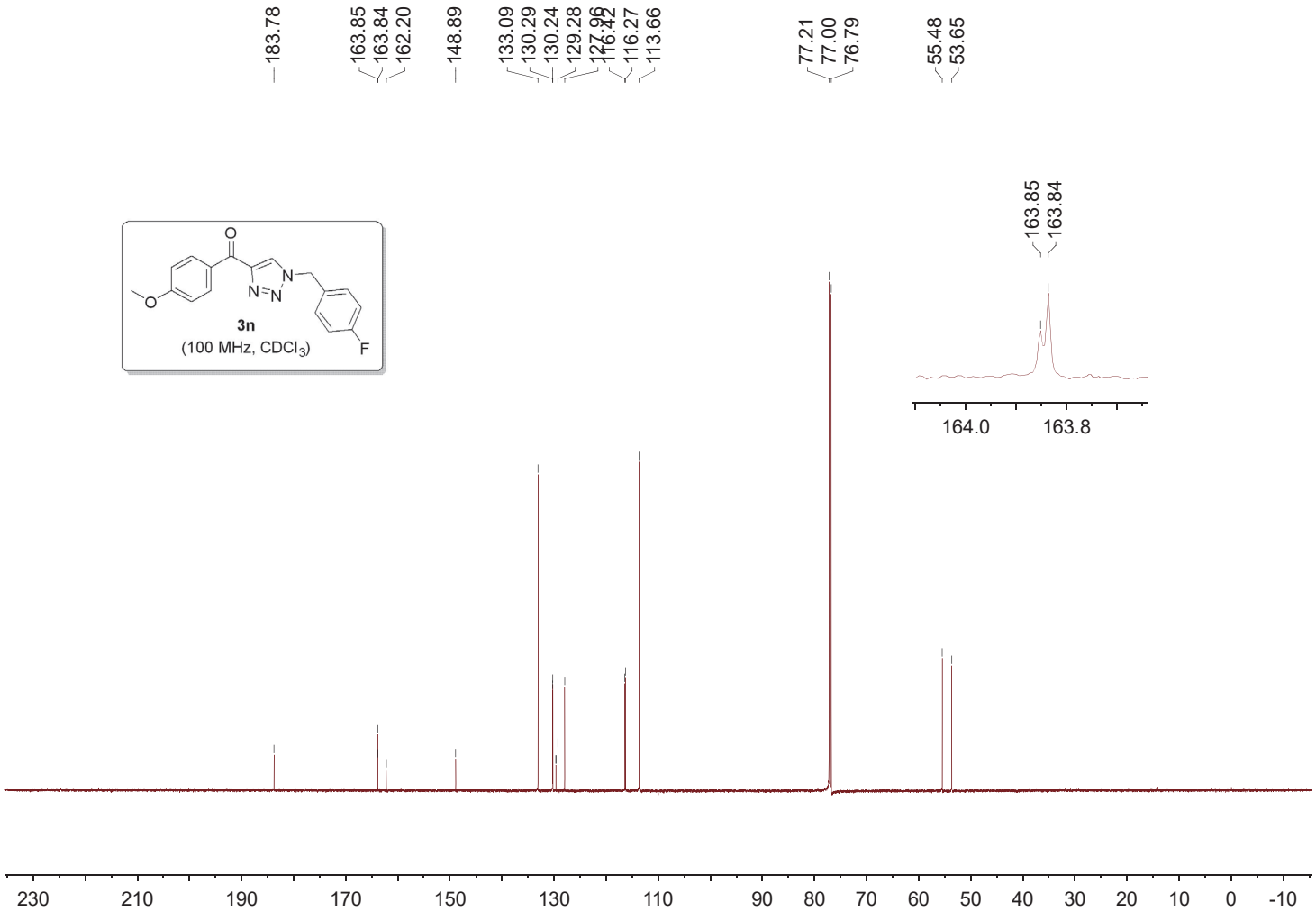
3l
(100 MHz, $CDCl_3$)

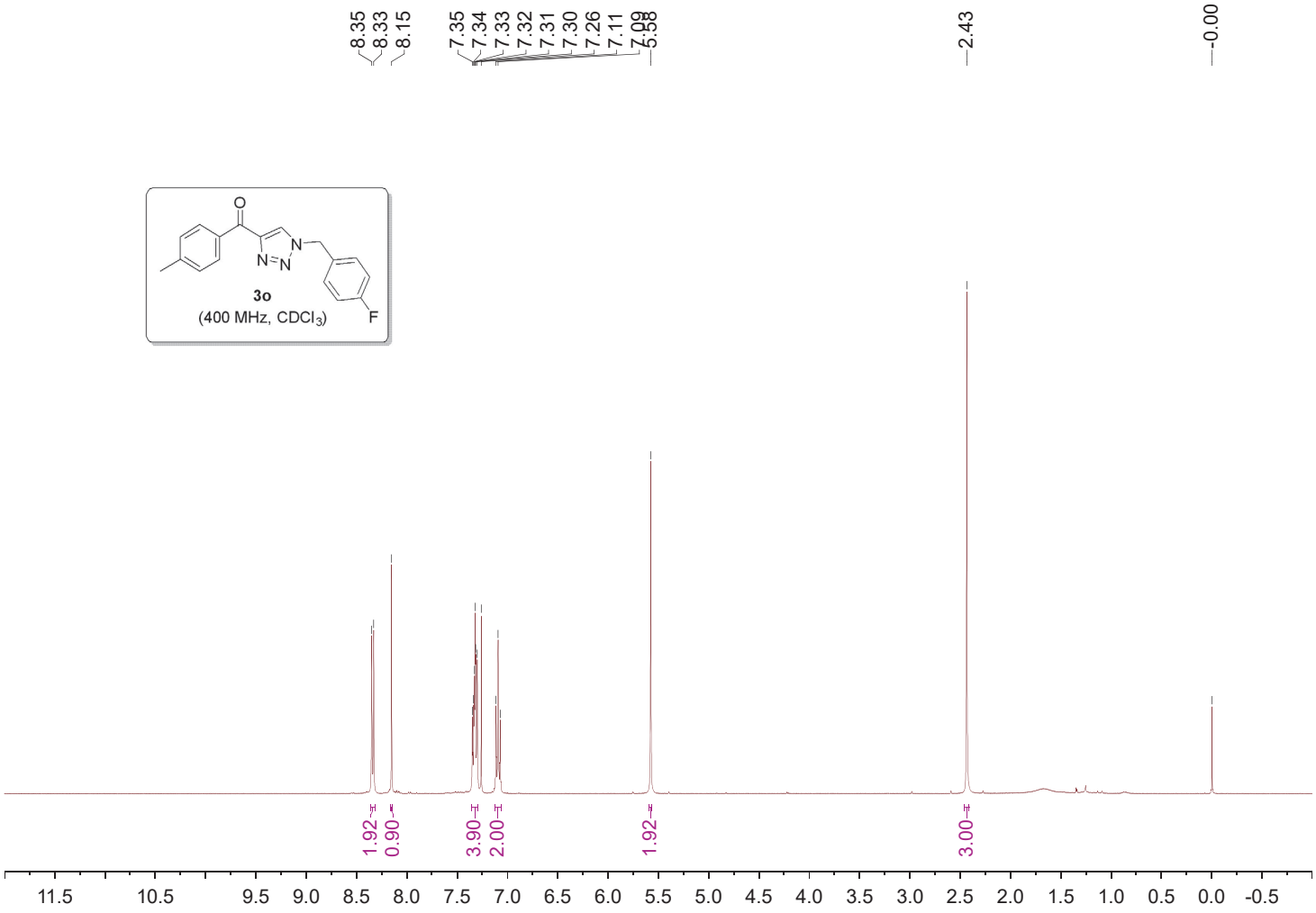
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

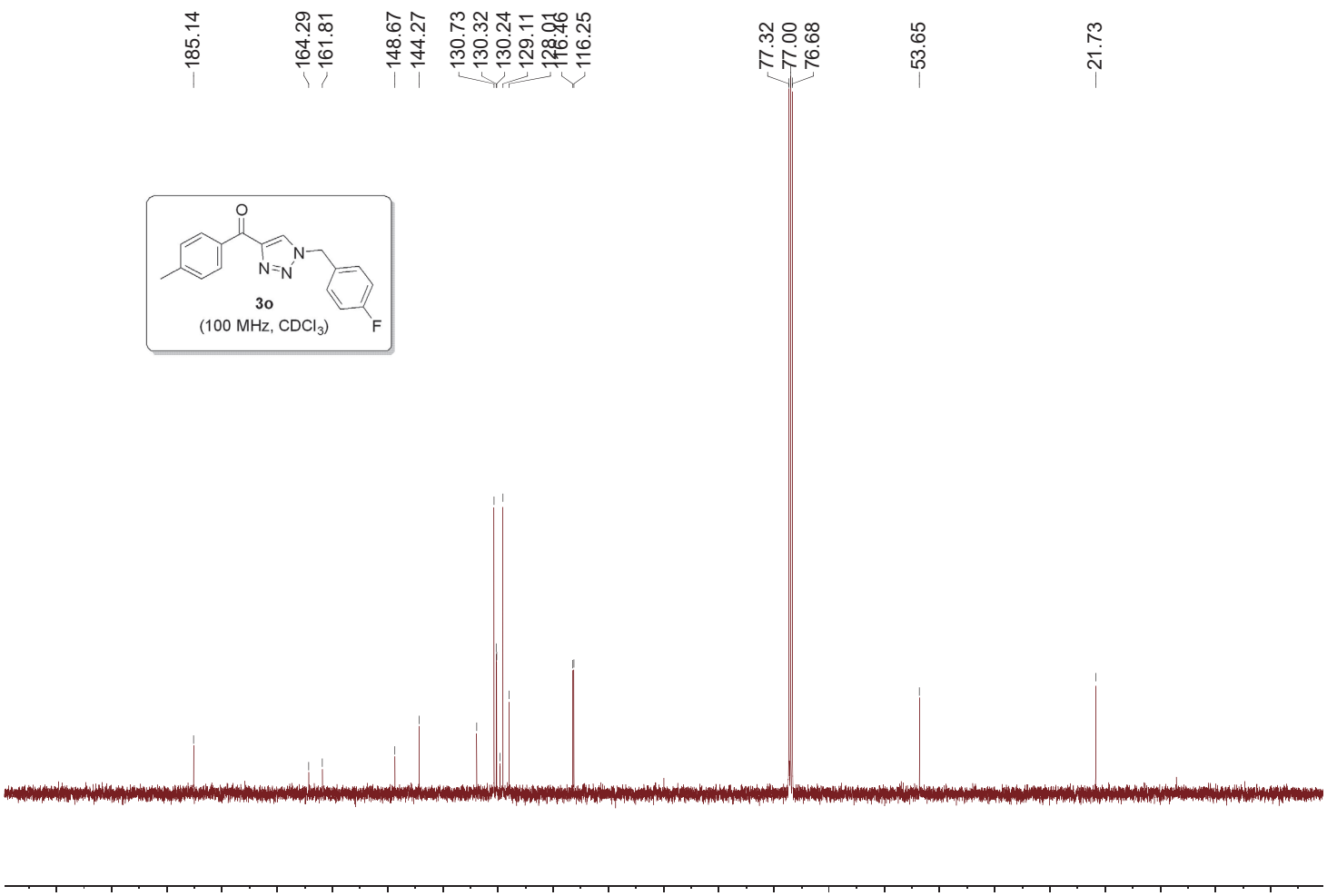

8.42
8.40
8.18
7.61
7.53
7.51
7.35
7.34
7.33
7.32
7.11
7.09
5.38
-0.00
3m
(400 MHz, CDCl3)
1.95
0.94
1.01
2.02
2.02
2.00
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

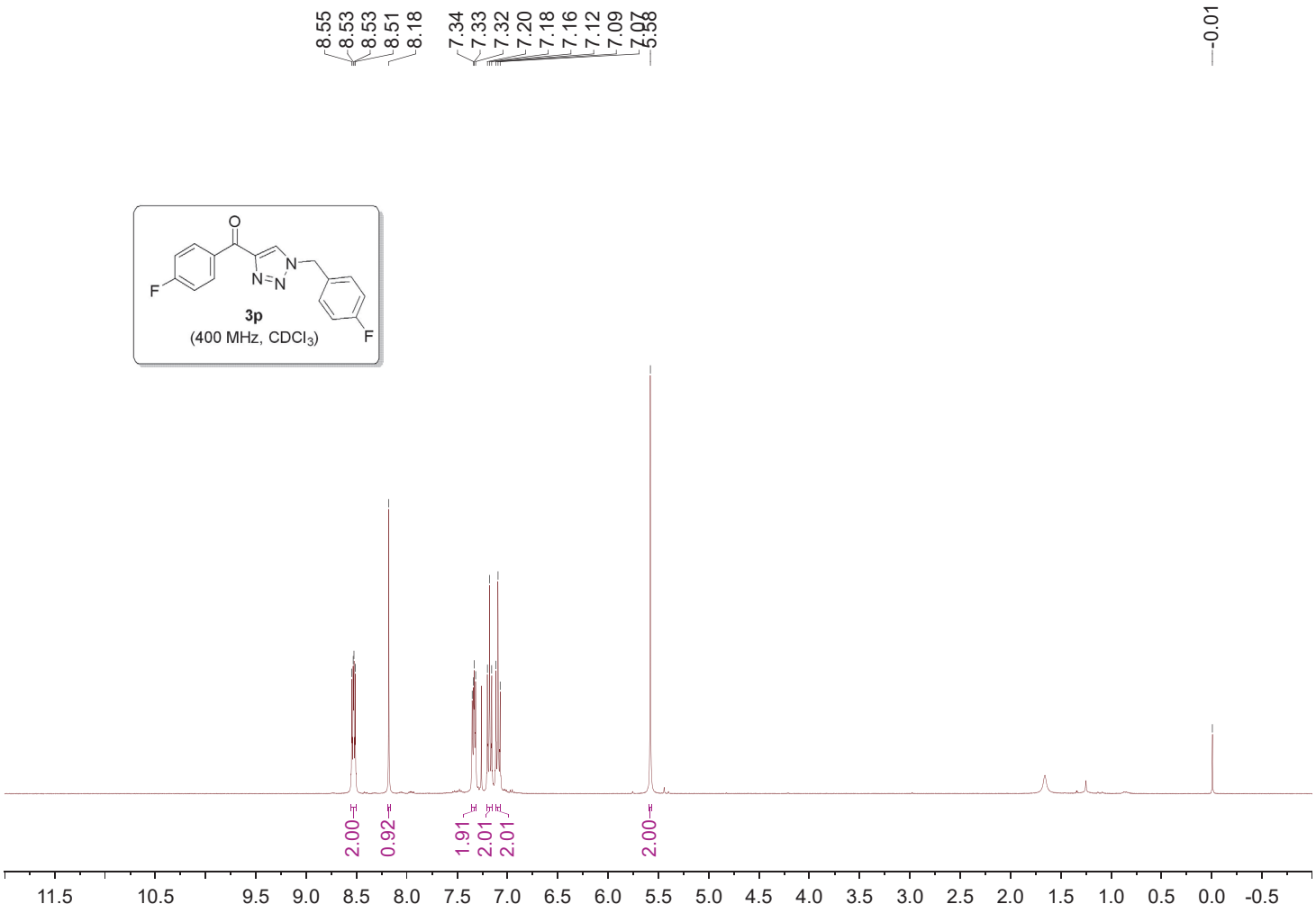

185.56
164.28
161.80
148.44
133.31
130.55
130.32
130.24
128.36
116.24
77.32
77.00
76.68
53.66
3m
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

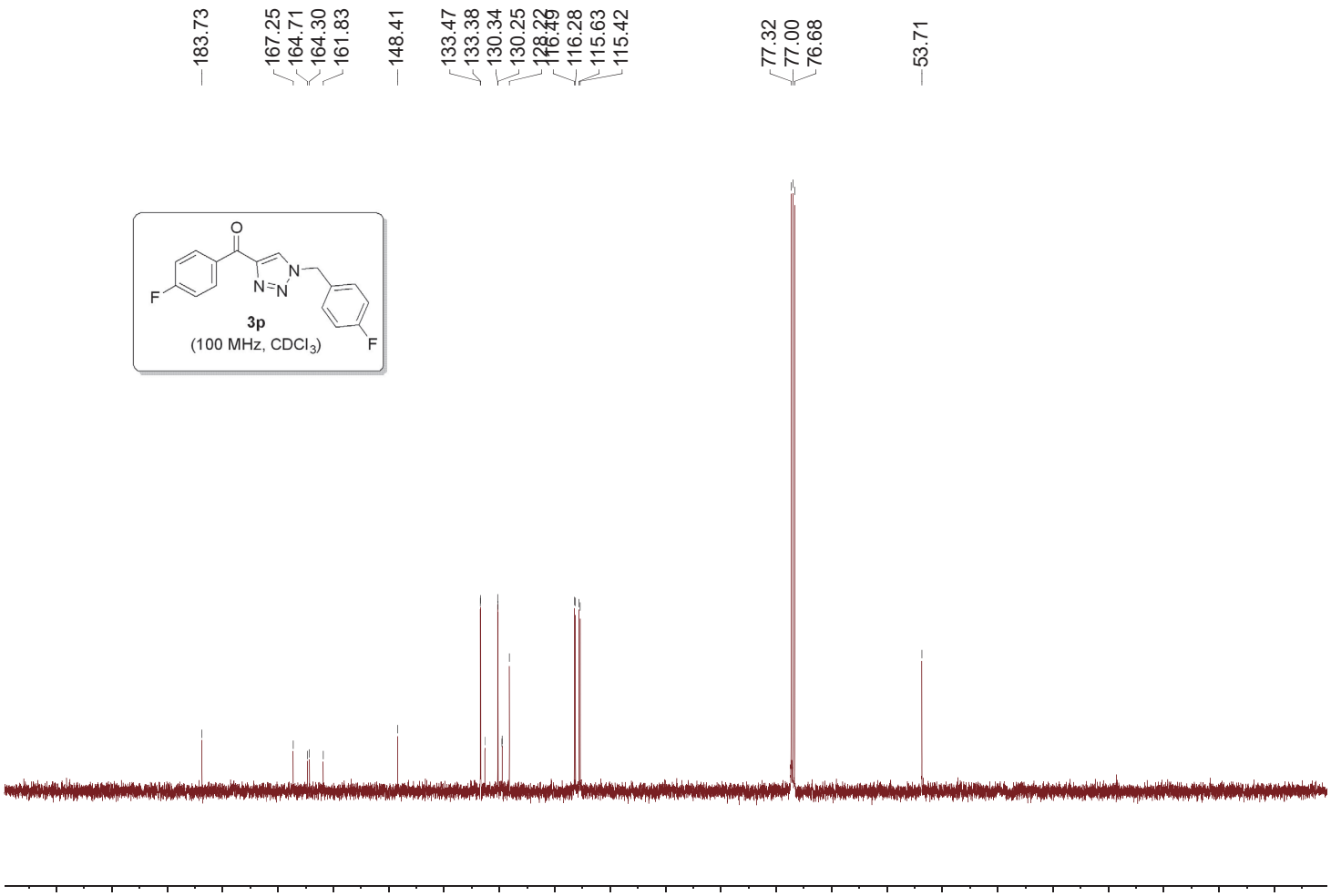

8.53
8.52
8.51
8.50
8.50
8.49
8.14
7.34
7.33
7.32
7.26
7.12
7.10
7.08
7.01
6.98
6.98
5.58
3.90
1.57
1.25
0.00
3n
(400 MHz, CDCl3)
F
2.01
0.96
2.01
2.02
1.99
2.02
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

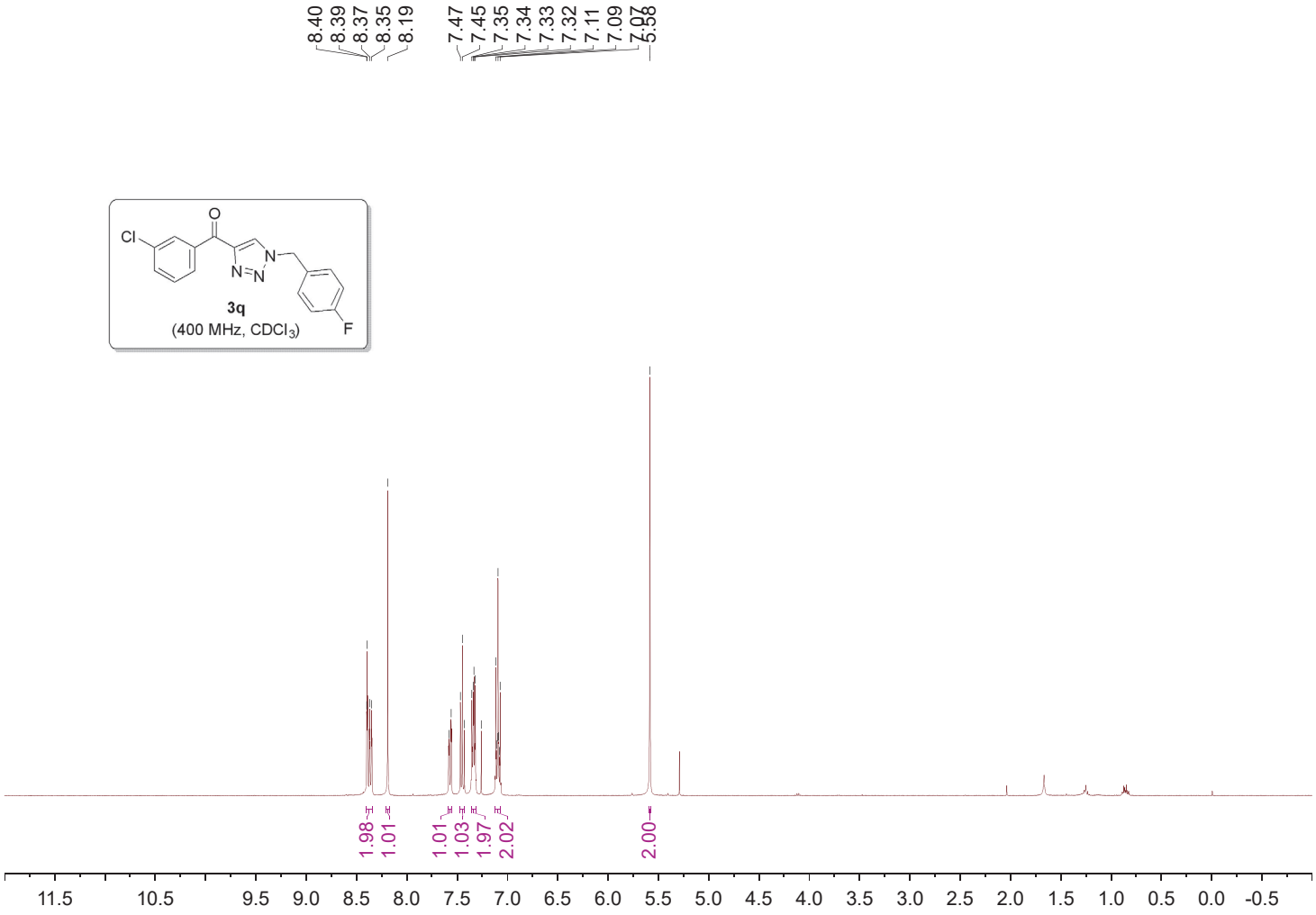

183.78
163.85
163.84
162.20
148.89
133.09
130.29
130.24
129.28
127.96
116.42
116.27
113.66
77.21
77.00
76.79
55.48
53.65
3n
(100 MHz, CDCl3)
F
163.85
163.84
164.0
163.8
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10

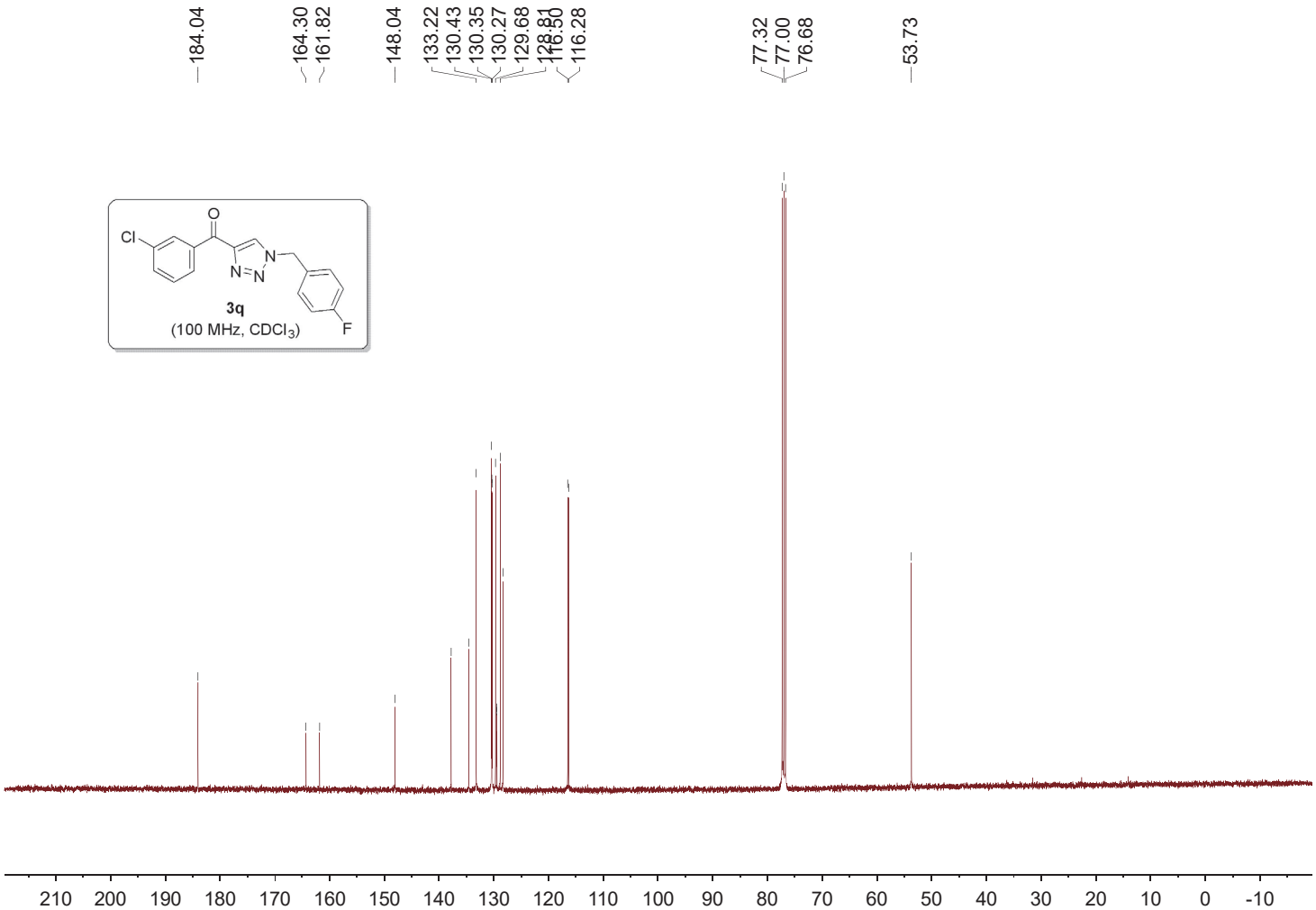

8.35
8.33
8.15
7.35
7.34
7.33
7.32
7.31
7.30
7.26
7.11
7.09
5.58
2.43
-0.00
3o
(400 MHz, CDCl3)
F
1.92
0.90
3.90
2.00
1.92
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

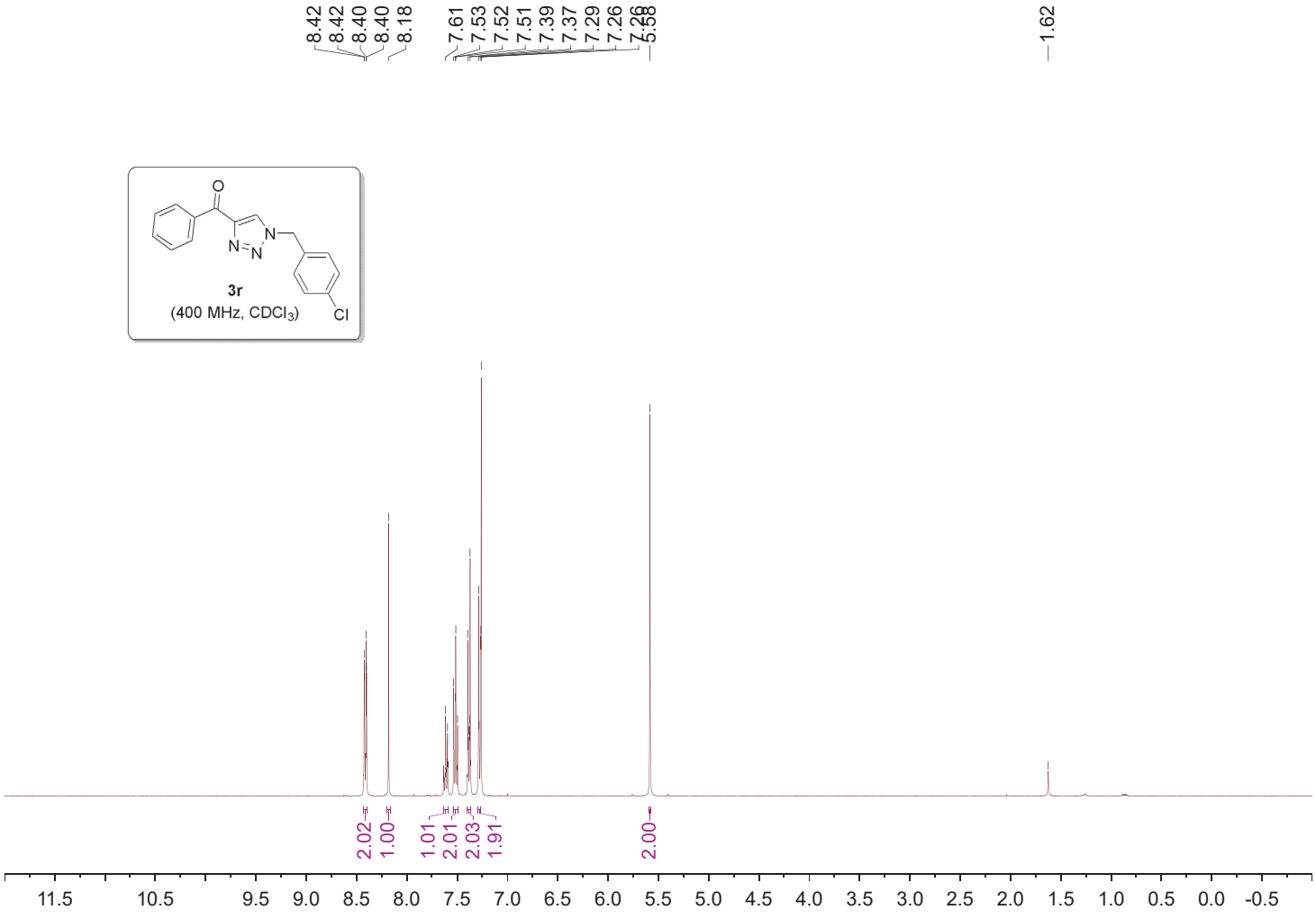

185.14
164.29
161.81
148.67
144.27
130.73
130.32
130.24
129.11
128.01
116.46
116.25
77.32
77.00
76.68
53.65
21.73
3o
(100 MHz, CDCl3)
F
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

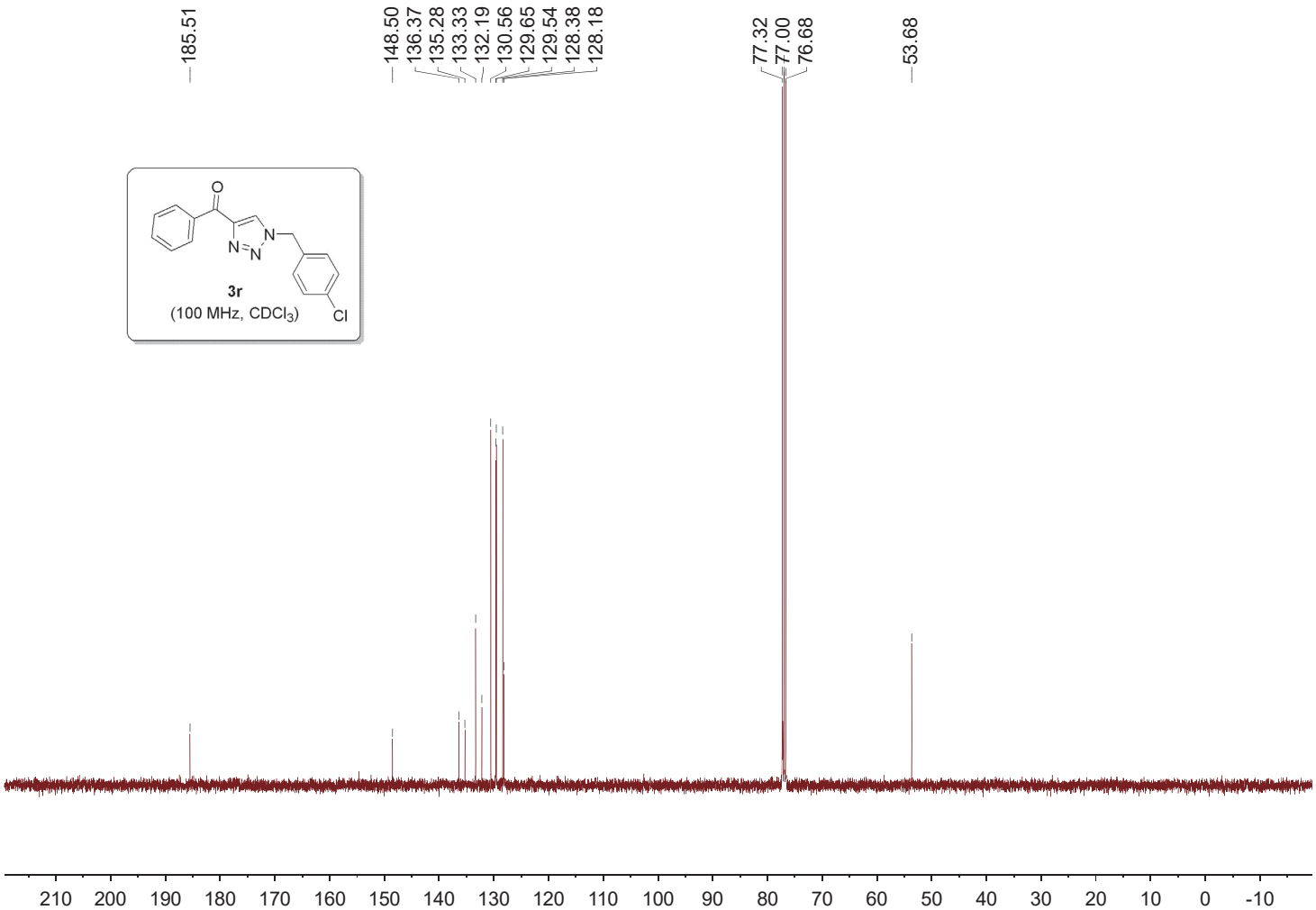

8.55
8.53
8.53
8.51
8.18
7.34
7.33
7.32
7.20
7.18
7.16
7.12
7.09
5.38
-0.01
3p
(400 MHz, CDCl3)
2.00
0.92
1.91
2.01
2.01
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

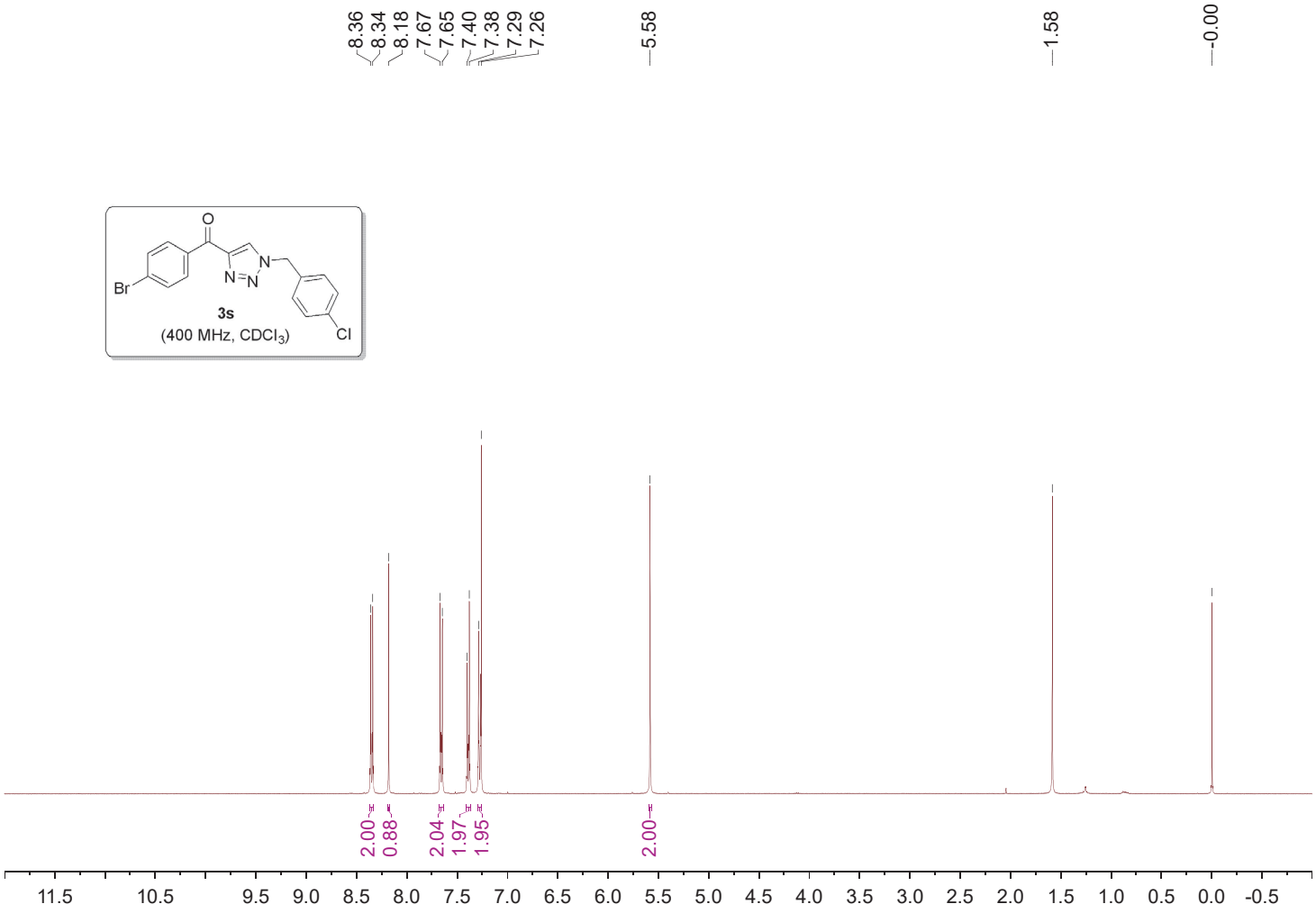

183.73
167.25
164.71
164.30
161.83
148.41
133.47
133.38
130.34
130.25
116.28
115.63
115.42
77.32
77.00
76.68
53.71
3p
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

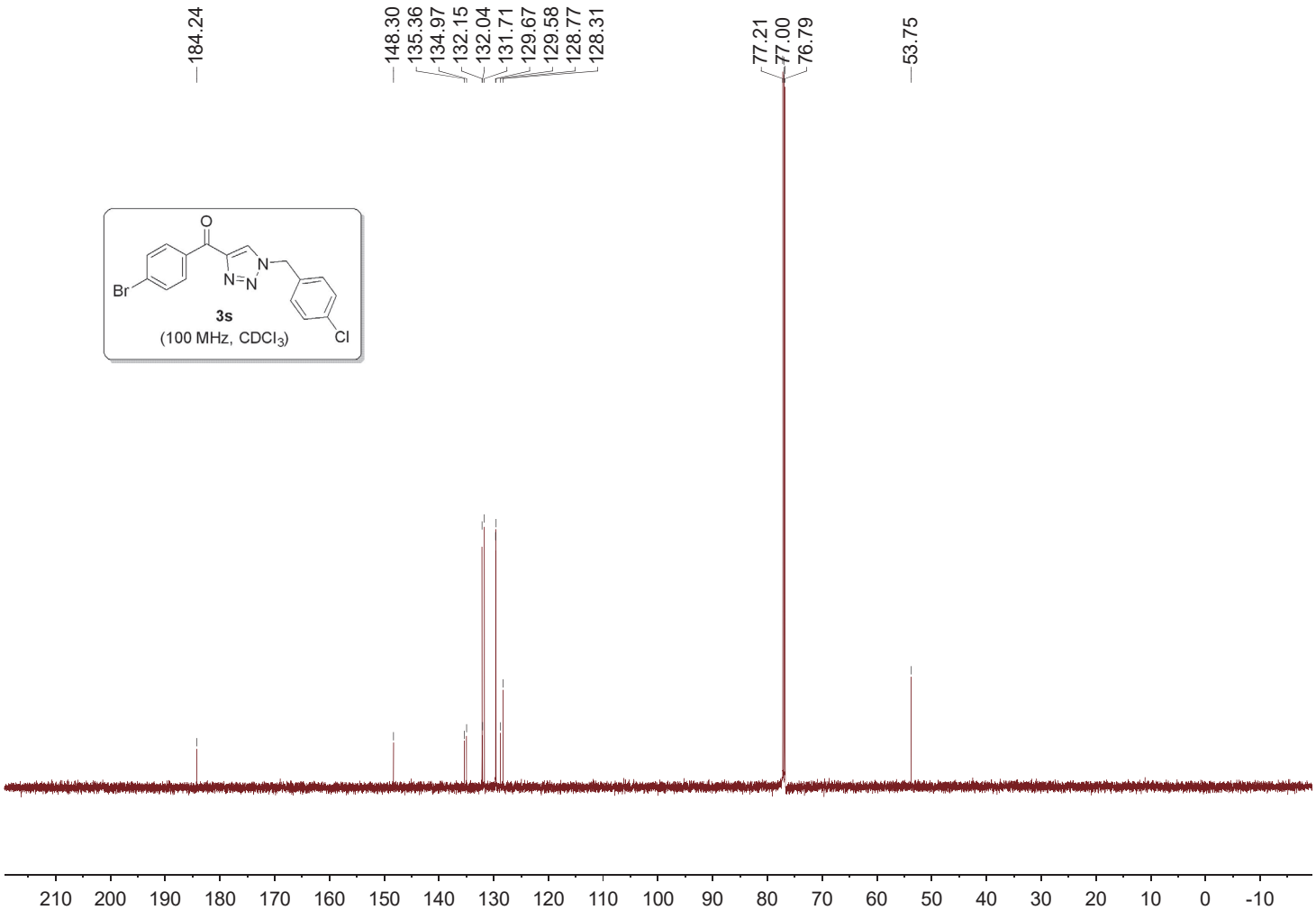

8.40
8.39
8.37
8.35
8.19
7.47
7.45
7.35
7.34
7.33
7.32
7.11
7.09
7.07
5.58
Cl
O
N
N=N
F
3q
(400 MHz, CDCl3)
1.98
1.01
1.01
1.03
1.97
2.02
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

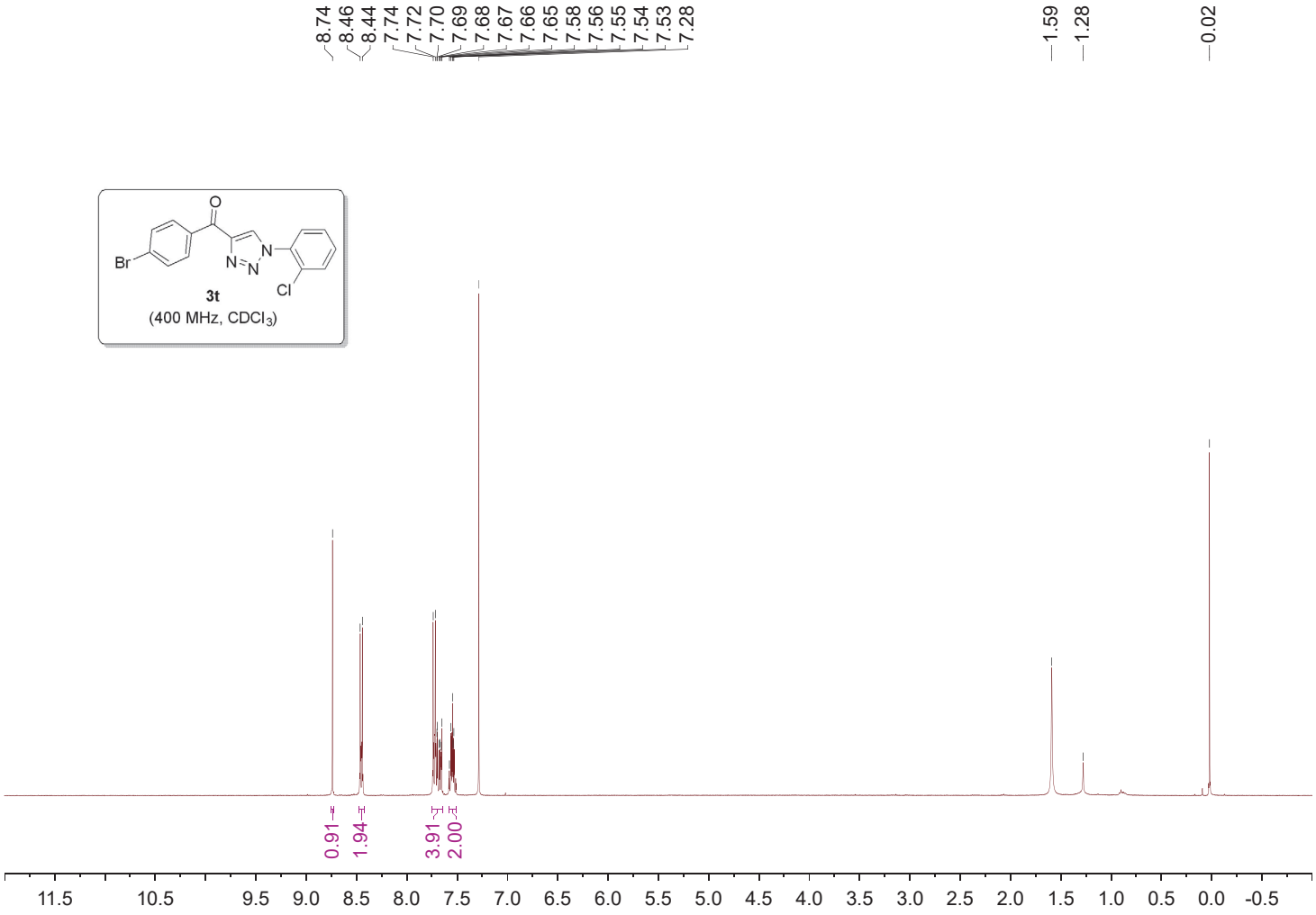

184.04
164.30
161.82
148.04
133.22
130.43
130.35
130.27
129.68
128.81
116.50
116.28
77.32
77.00
76.68
53.73
Cl
O
N
N=N
F
3q
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

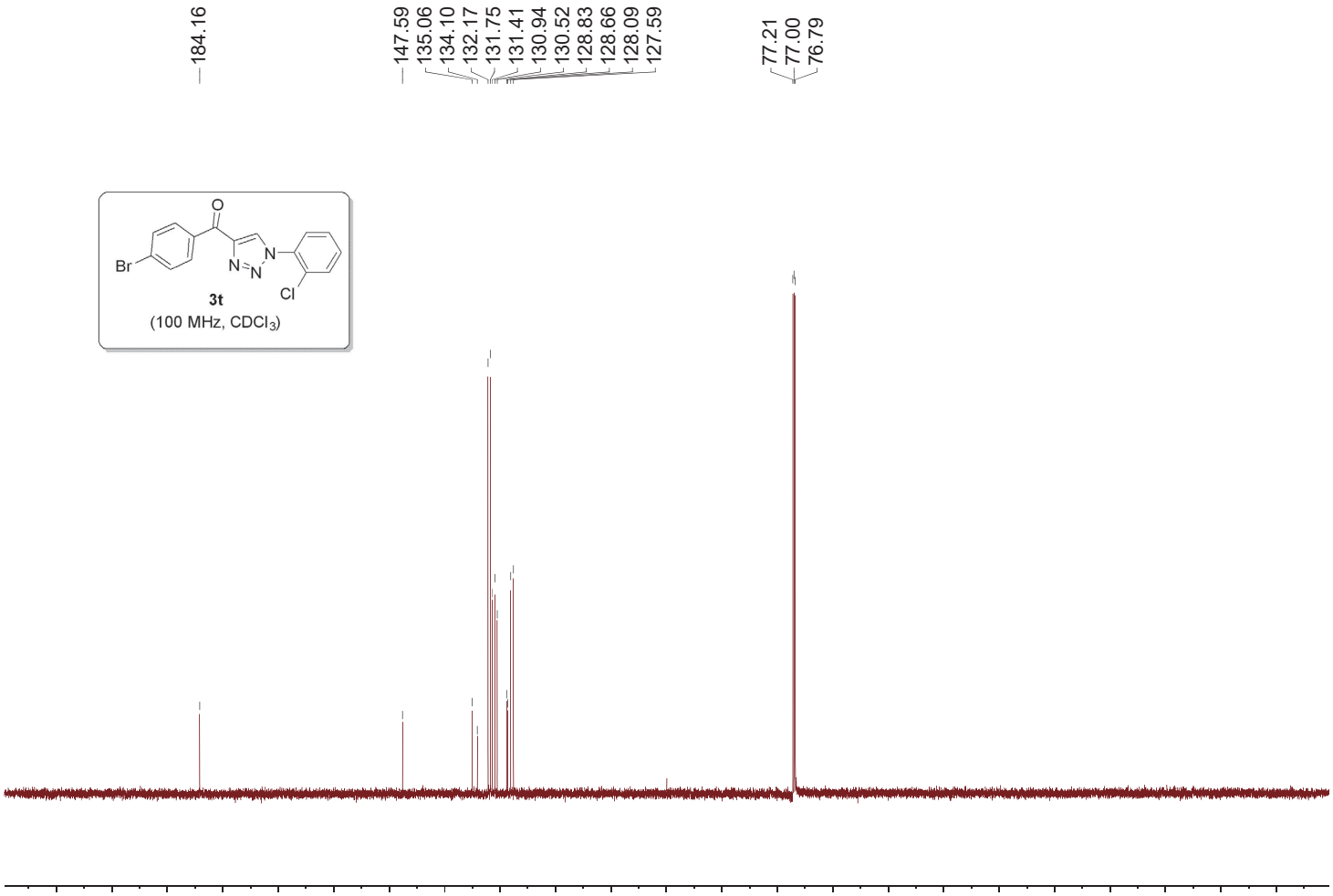

8.42
8.42
8.40
8.40
8.18
7.61
7.53
7.52
7.51
7.39
7.37
7.29
7.26
5.58
1.62
3r
(400 MHz, CDCl3)
Cl
2.02
1.00
1.01
2.01
2.03
1.91
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

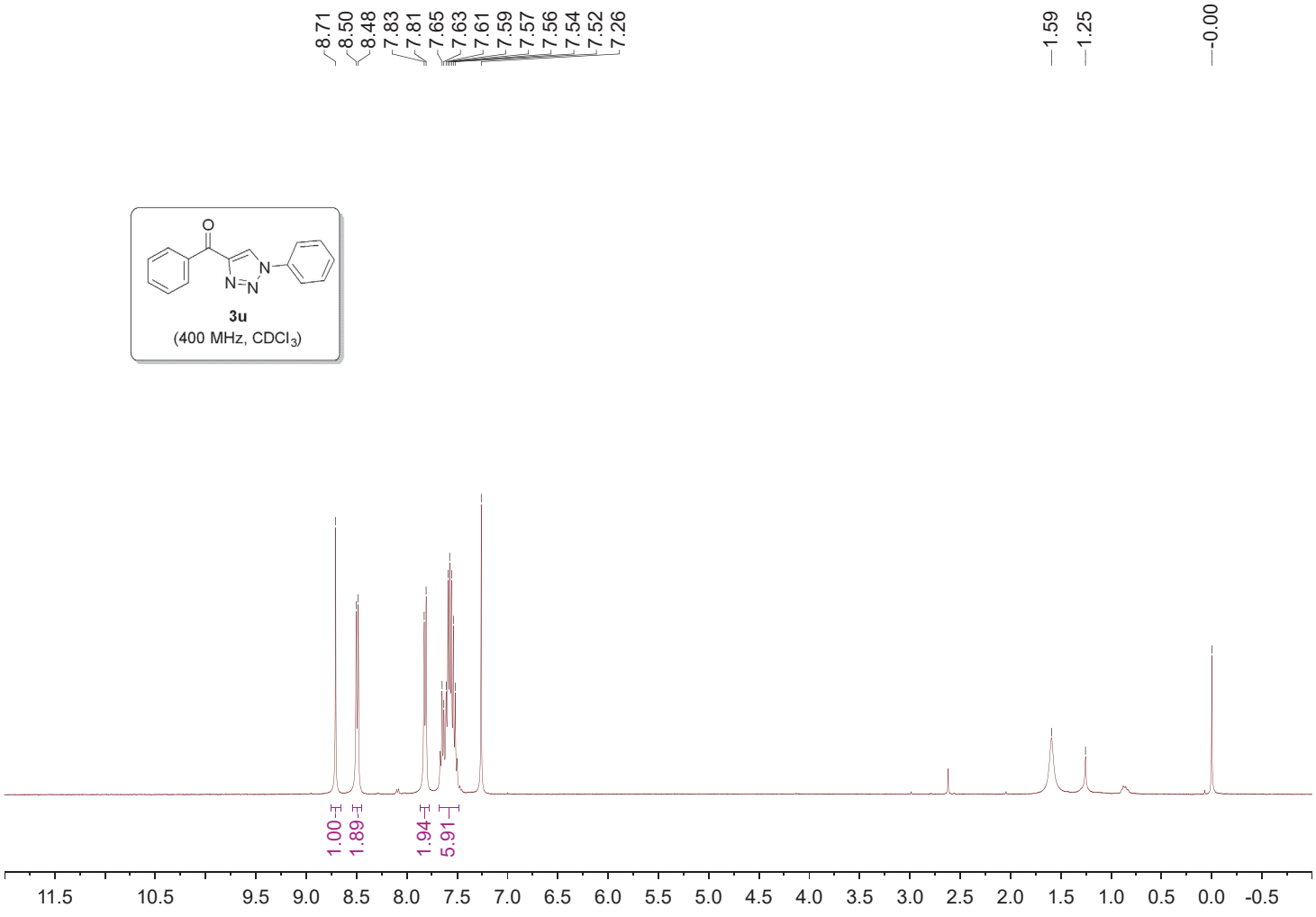

185.51
148.50
136.37
135.28
133.33
132.19
130.56
129.65
129.54
128.38
128.18
77.32
77.00
76.68
53.68
3r
(100 MHz, CDCl3)
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

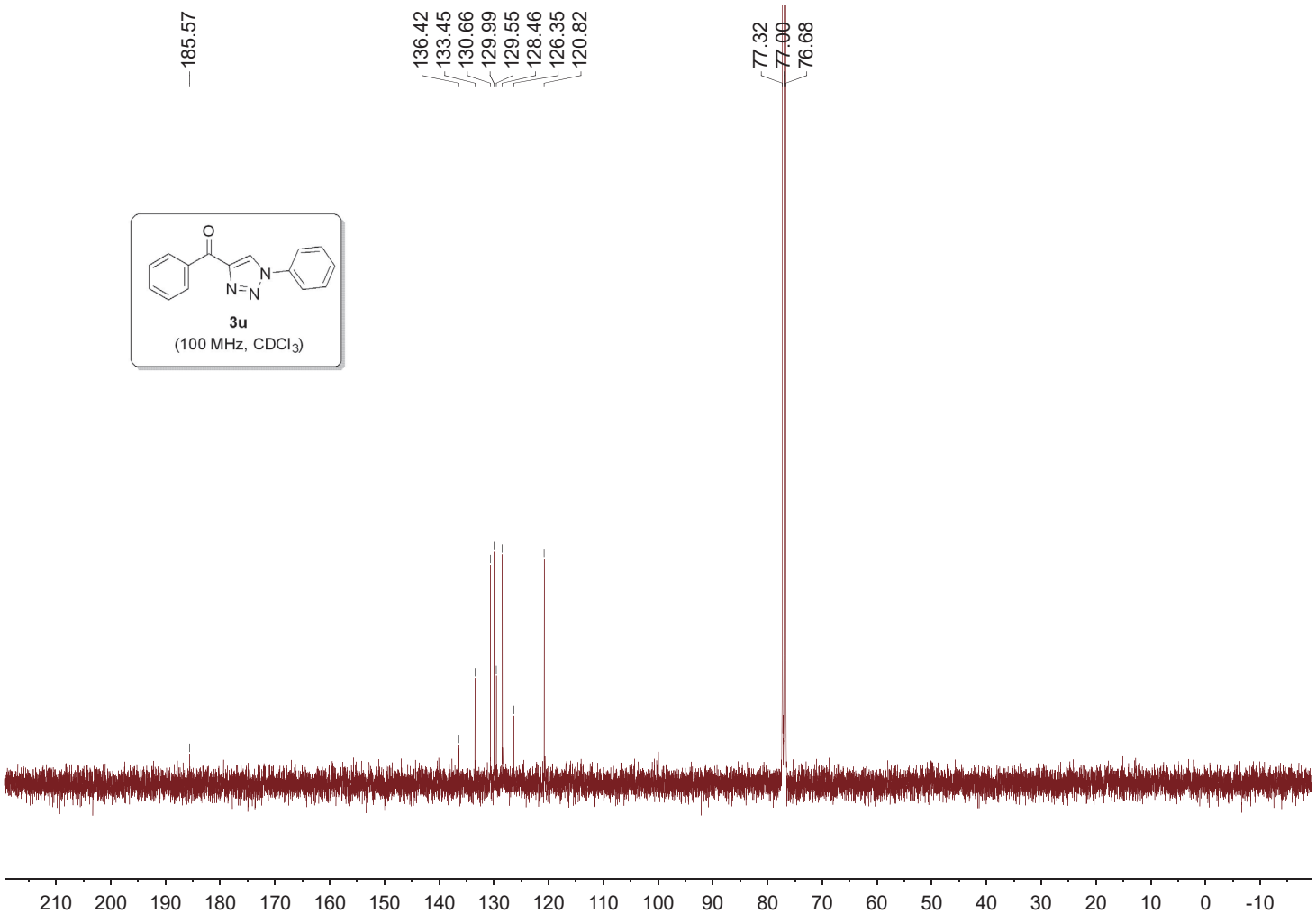

8.36
8.34
8.18
7.67
7.65
7.40
7.38
7.29
7.26
5.58
1.58
-0.00
O
N
N
Br
Cl
3s
(400 MHz, CDCl3)
2.00
0.88
2.04
1.97
1.95
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

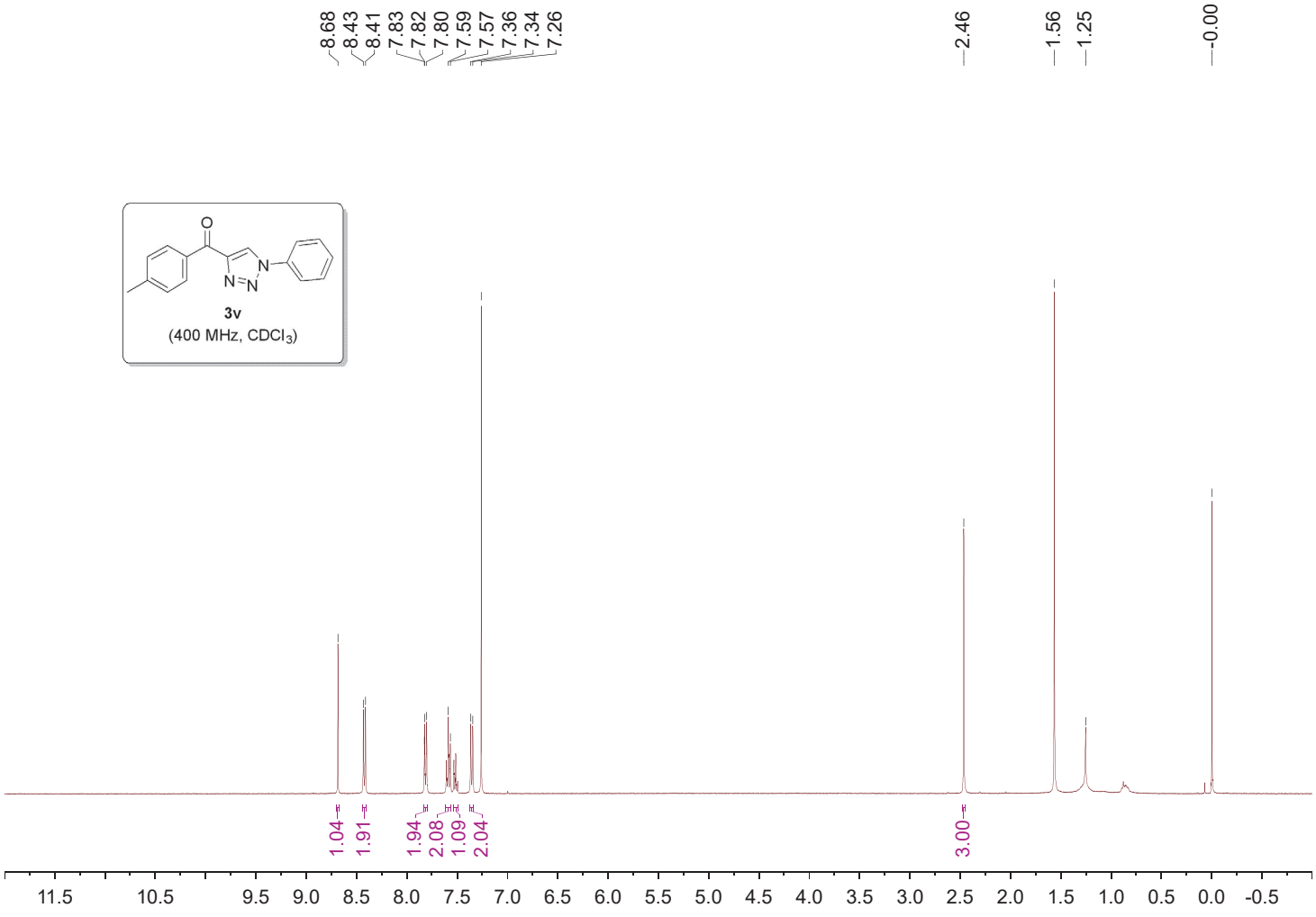

184.24
148.30
135.36
134.97
132.15
132.04
131.71
129.67
129.58
128.77
128.31
77.21
77.00
76.79
53.75
O
N
N
Br
Cl
3s
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

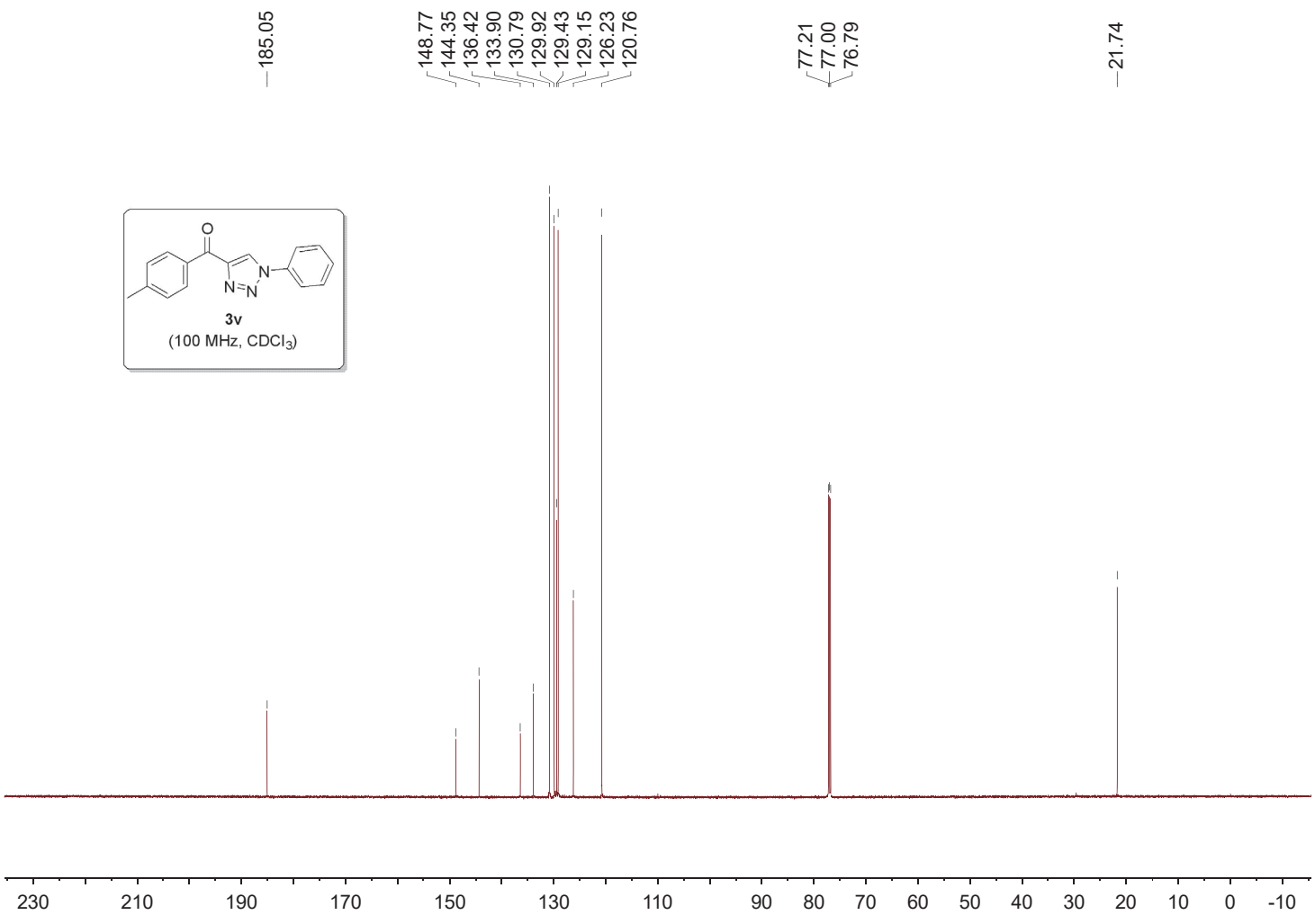

8.74
8.46
8.44
7.74
7.72
7.70
7.69
7.68
7.67
7.66
7.65
7.58
7.56
7.55
7.54
7.53
7.28
1.59
1.28
0.02
Br
O
N
N
N
Cl
3t
(400 MHz, CDCl3)
0.91
1.94
3.91
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

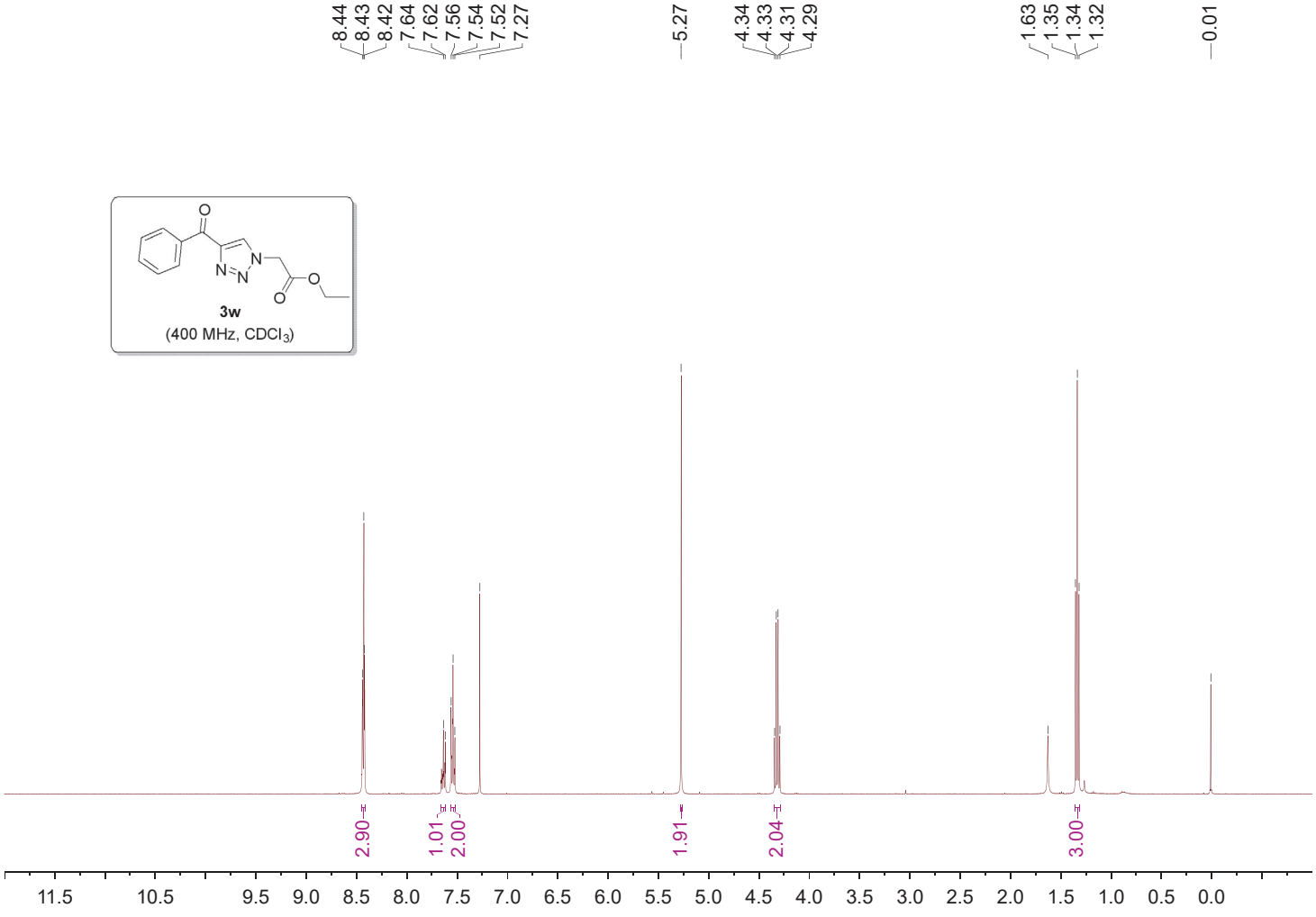

184.16
147.59
135.06
134.10
132.17
131.75
131.41
130.94
130.52
128.83
128.66
128.09
127.59
77.21
77.00
76.79
Br
O
N
N
N
Cl
3t
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

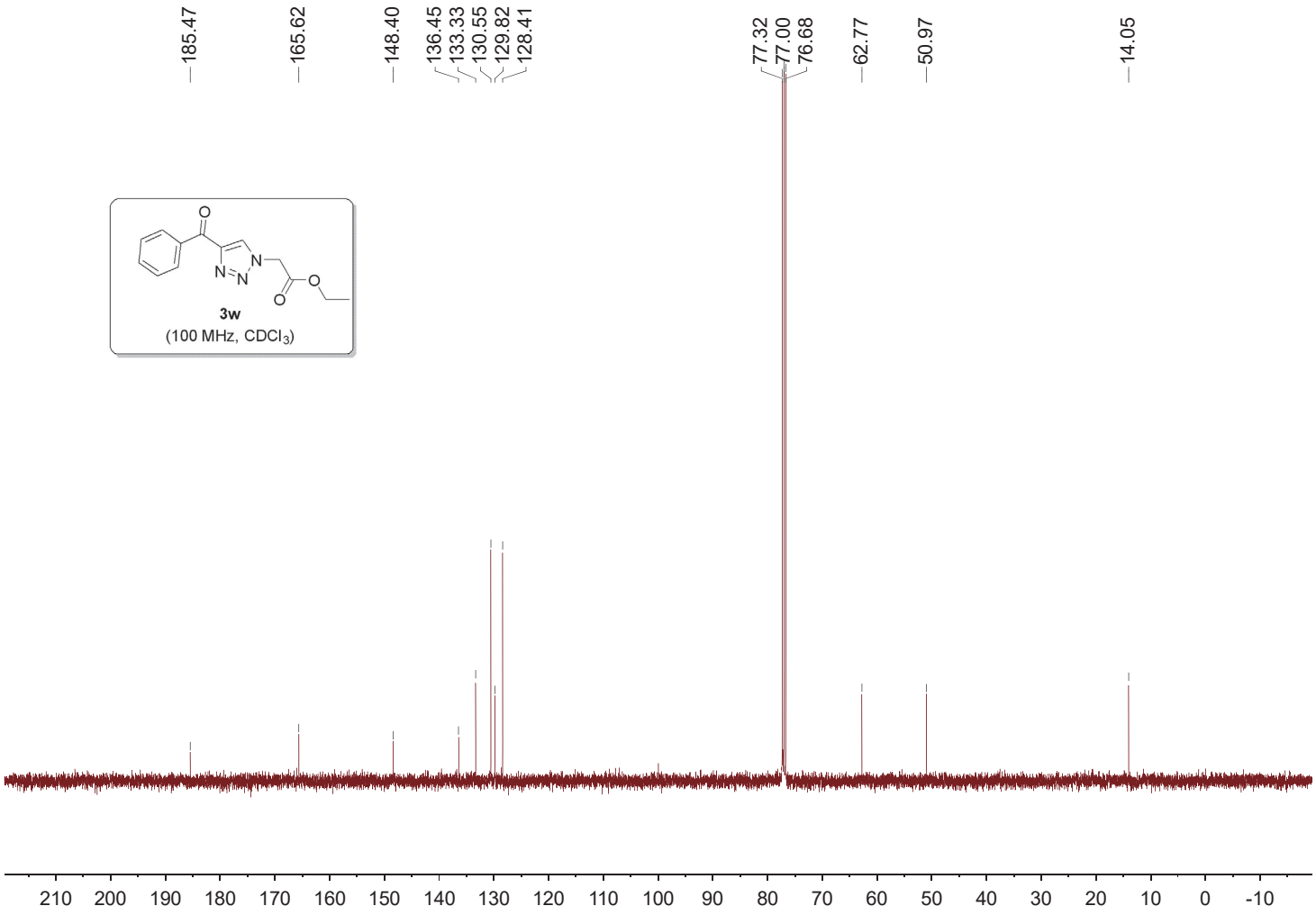

8.71
8.50
8.48
7.83
7.81
7.65
7.63
7.61
7.59
7.57
7.56
7.54
7.52
7.26
1.59
1.25
0.00
3u
(400 MHz, CDCl3)
1.00
1.89
1.94
5.91
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

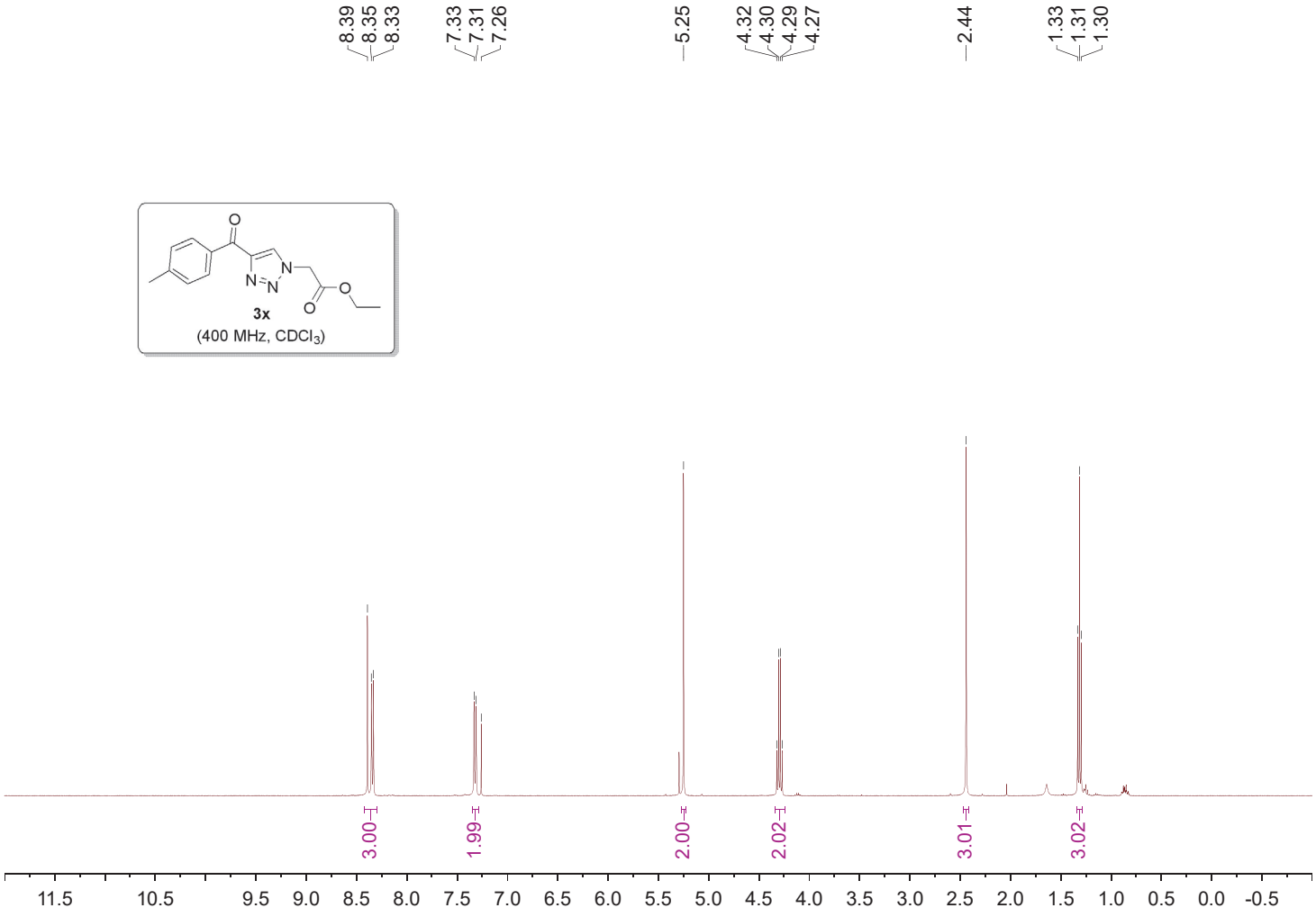

185.57
136.42
133.45
130.66
129.99
129.55
128.46
126.35
120.82
77.32
77.00
76.68
3u
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

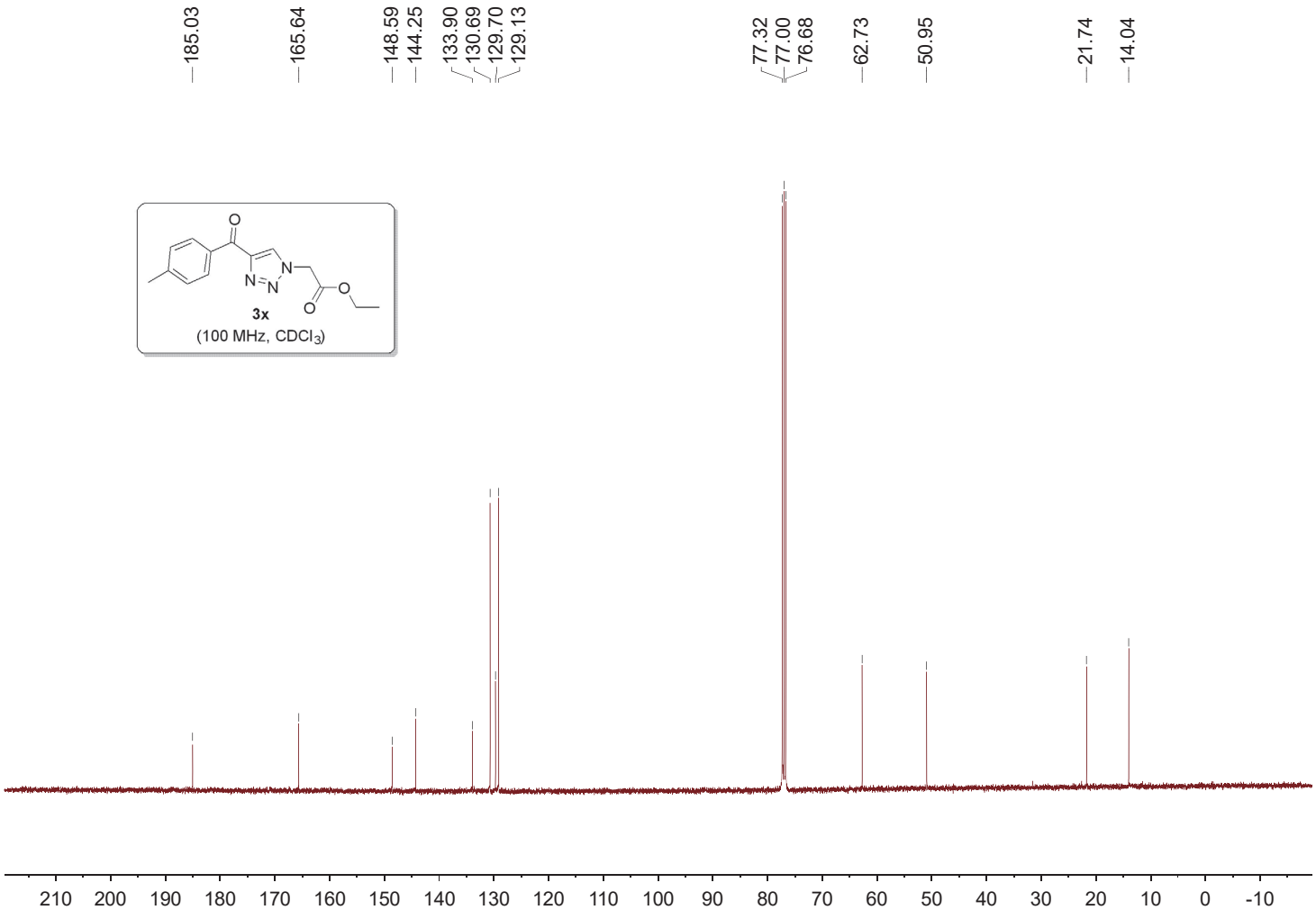

8.68
8.43
8.41
7.83
7.82
7.80
7.59
7.57
7.36
7.34
7.26
2.46
1.56
1.25
0.00
3v
(400 MHz, CDCl3)
1.04
1.91
1.94
2.08
1.09
2.04
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

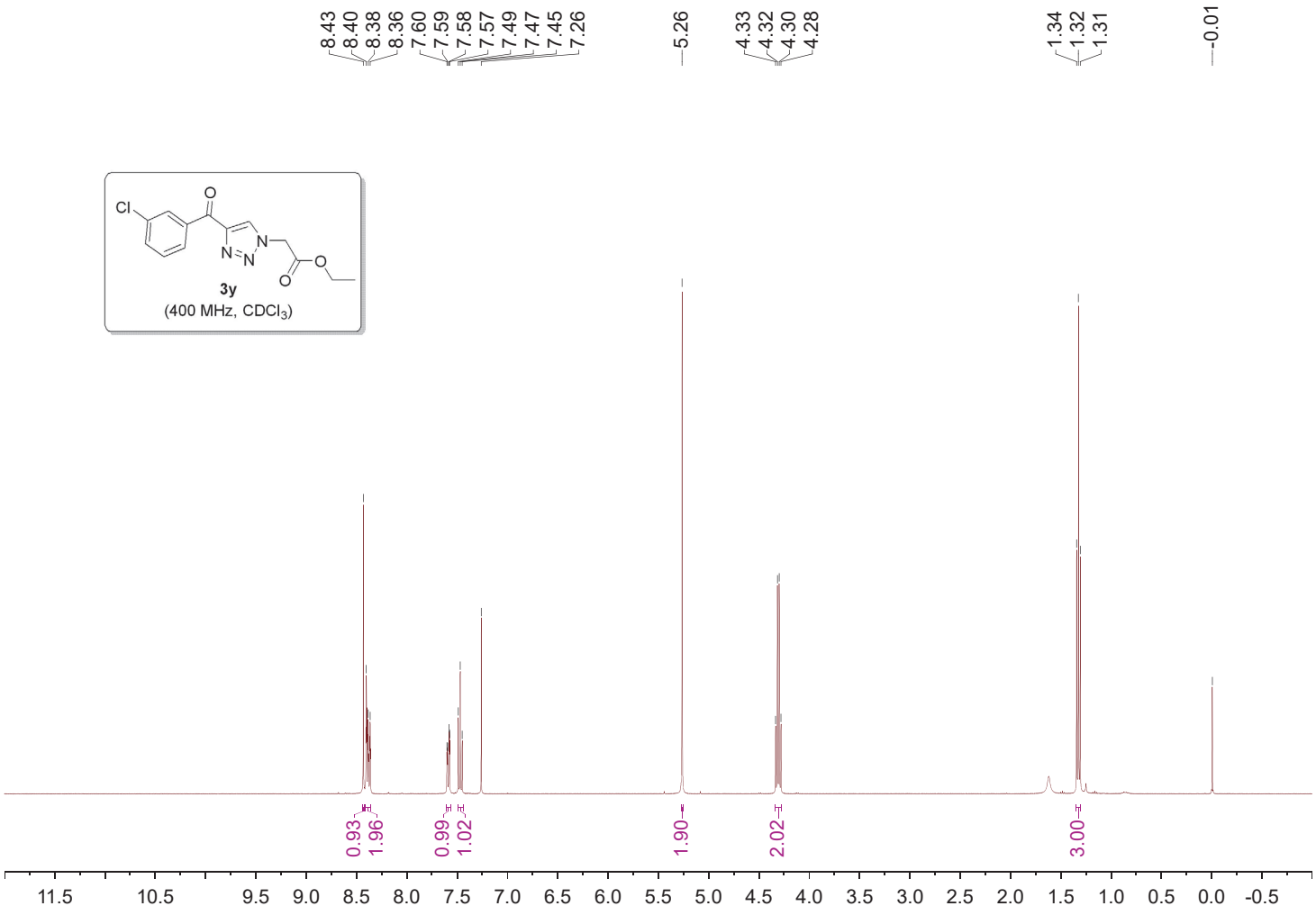

185.05
148.77
144.35
136.42
133.90
130.79
129.92
129.43
129.15
126.23
120.76
77.21
77.00
76.79
21.74
3v
(100 MHz, CDCl3)
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10

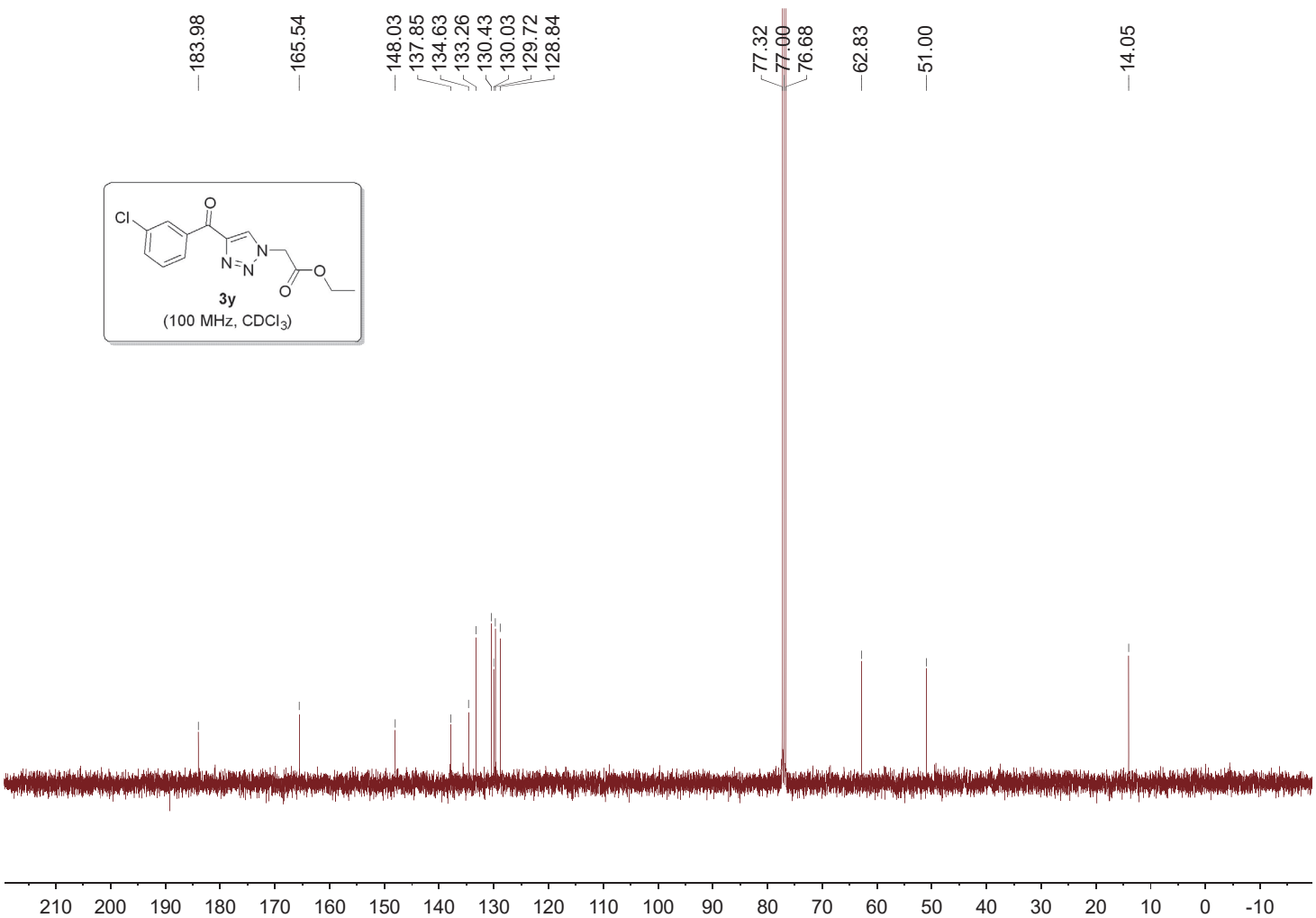

8.44
8.43
8.42
7.64
7.62
7.56
7.54
7.52
7.27
5.27
4.34
4.33
4.31
4.29
1.63
1.35
1.34
1.32
0.01
3w
(400 MHz, CDCl3)
2.90
1.01
2.00
1.91
2.04
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

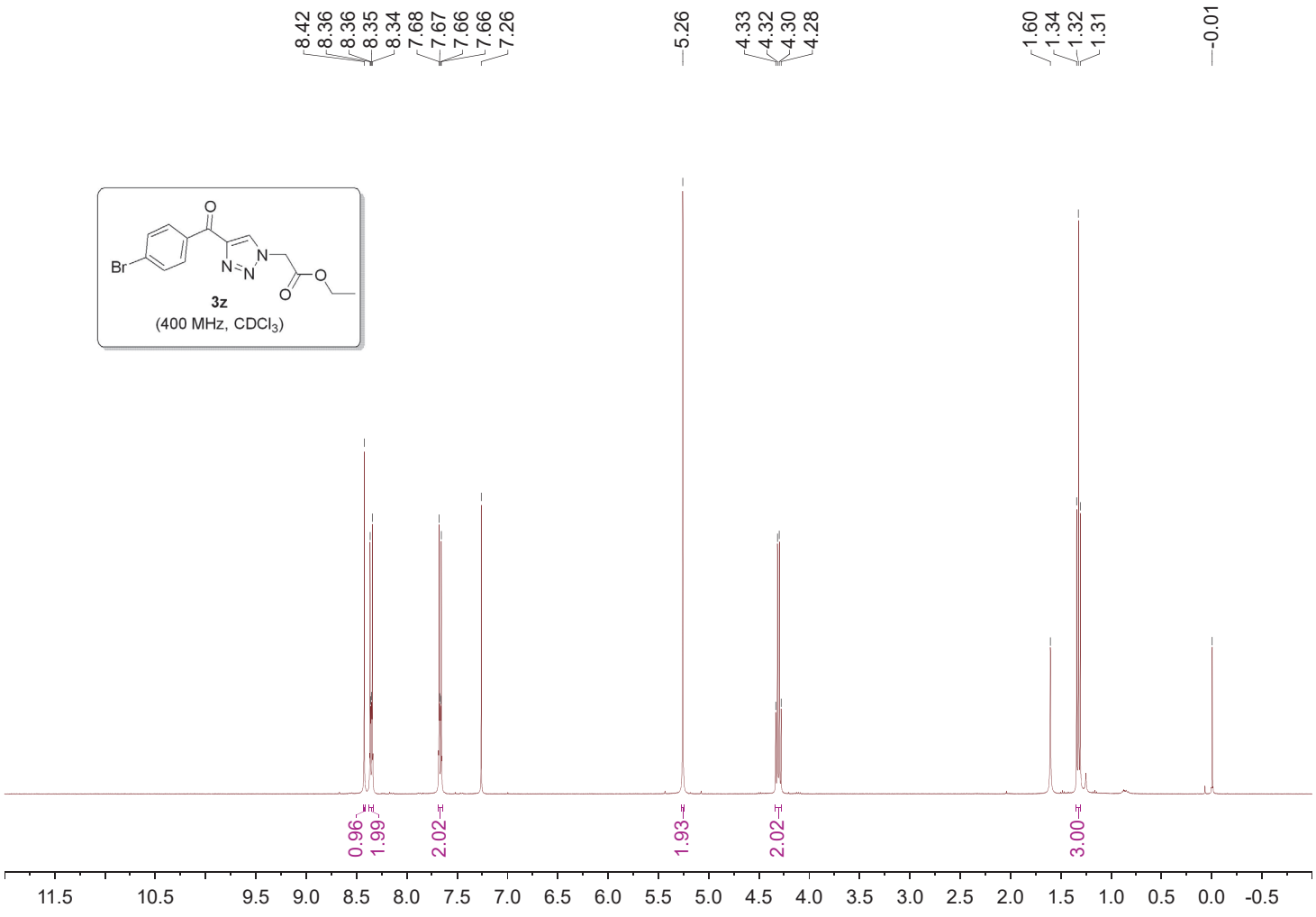

185.47
165.62
148.40
136.45
133.33
130.55
129.82
128.41
77.32
77.00
76.68
62.77
50.97
14.05
3w
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

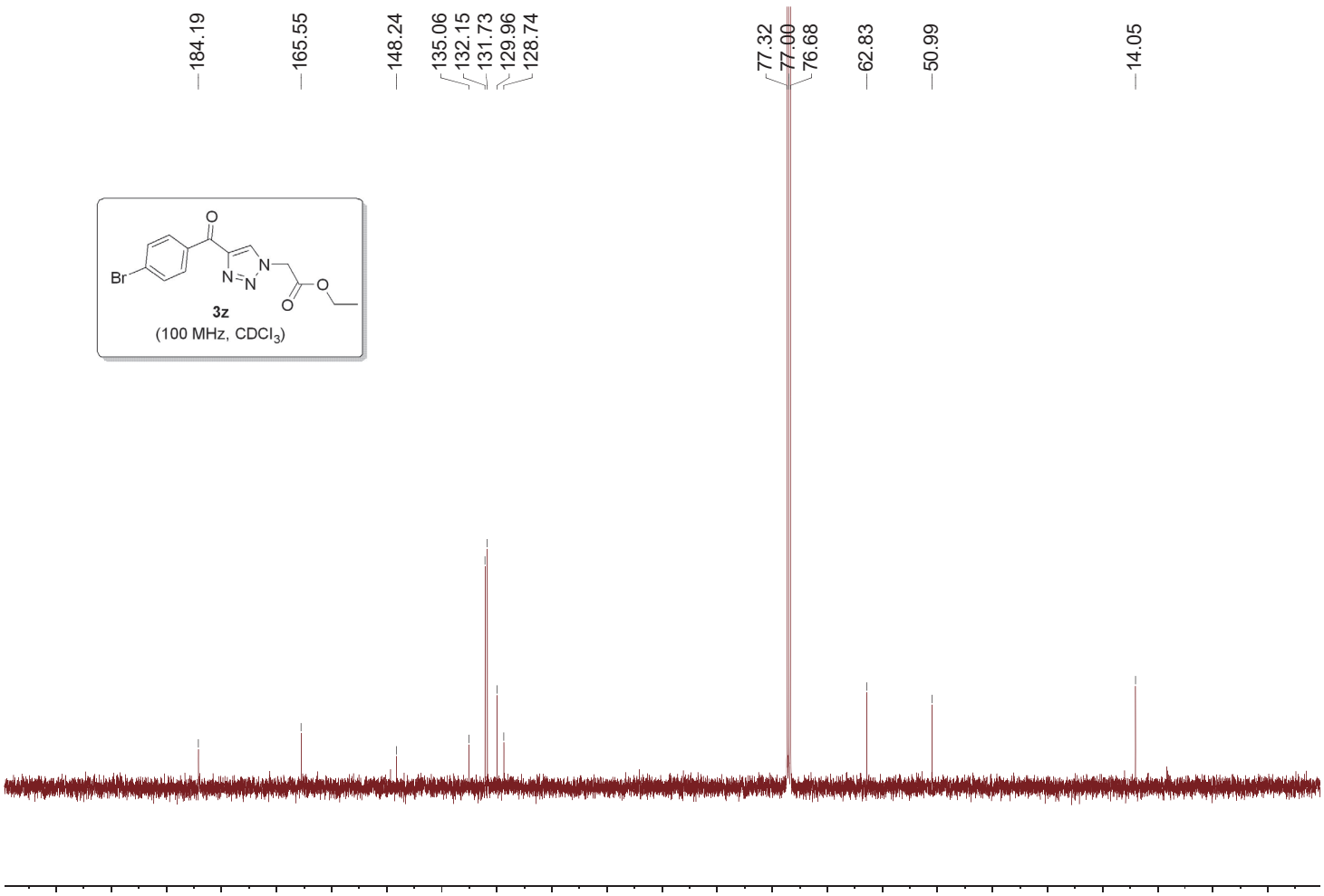

8.39
8.35
8.33
7.33
7.31
7.26
5.25
4.32
4.30
4.29
4.27
2.44
1.33
1.31
1.30
3x
(400 MHz, CDCl3)
3.00
1.99
2.00
2.02
3.01
3.02
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

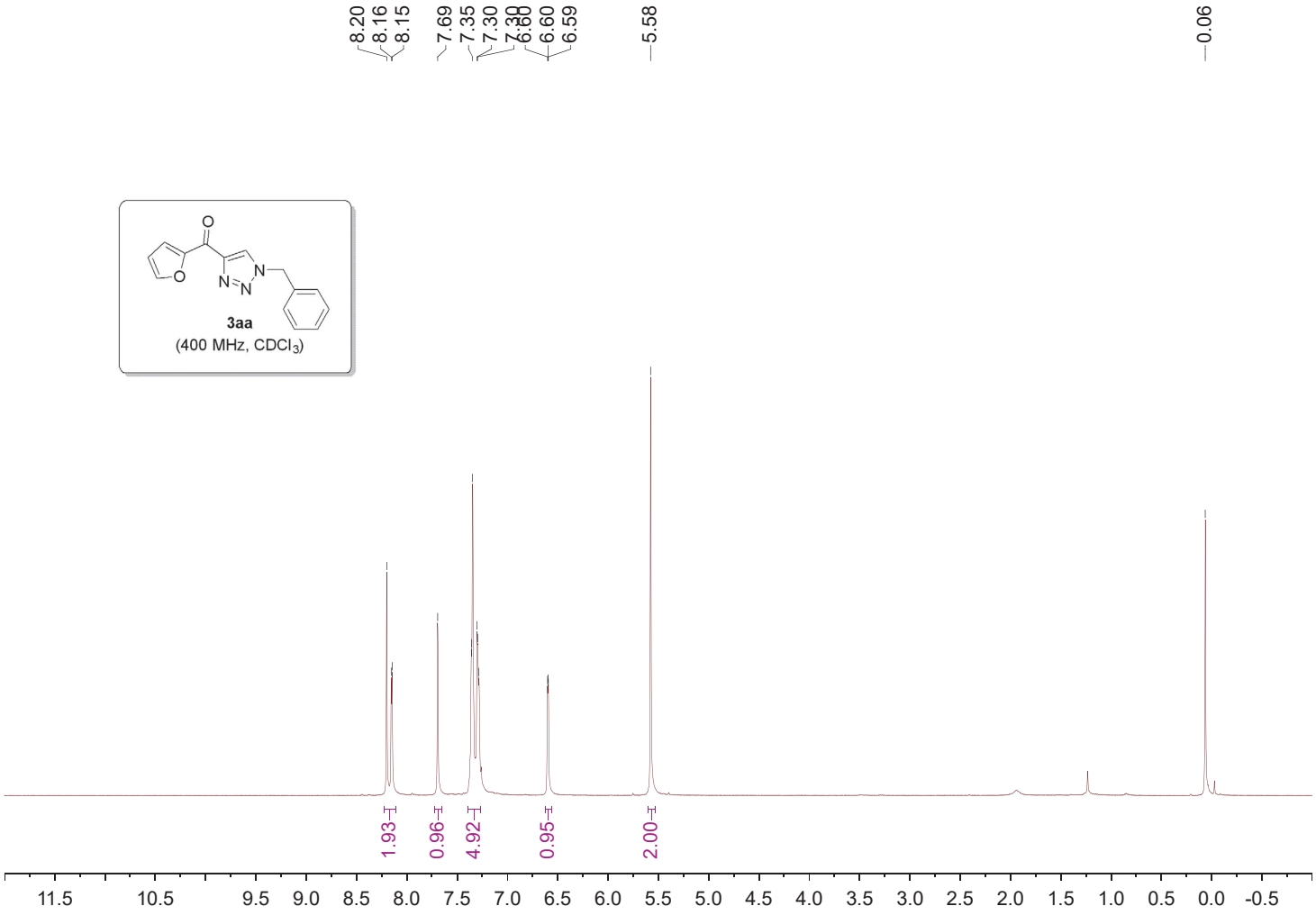

185.03
165.64
148.59
144.25
133.90
130.69
129.70
129.13
77.32
77.00
76.68
62.73
50.95
21.74
14.04
3x
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

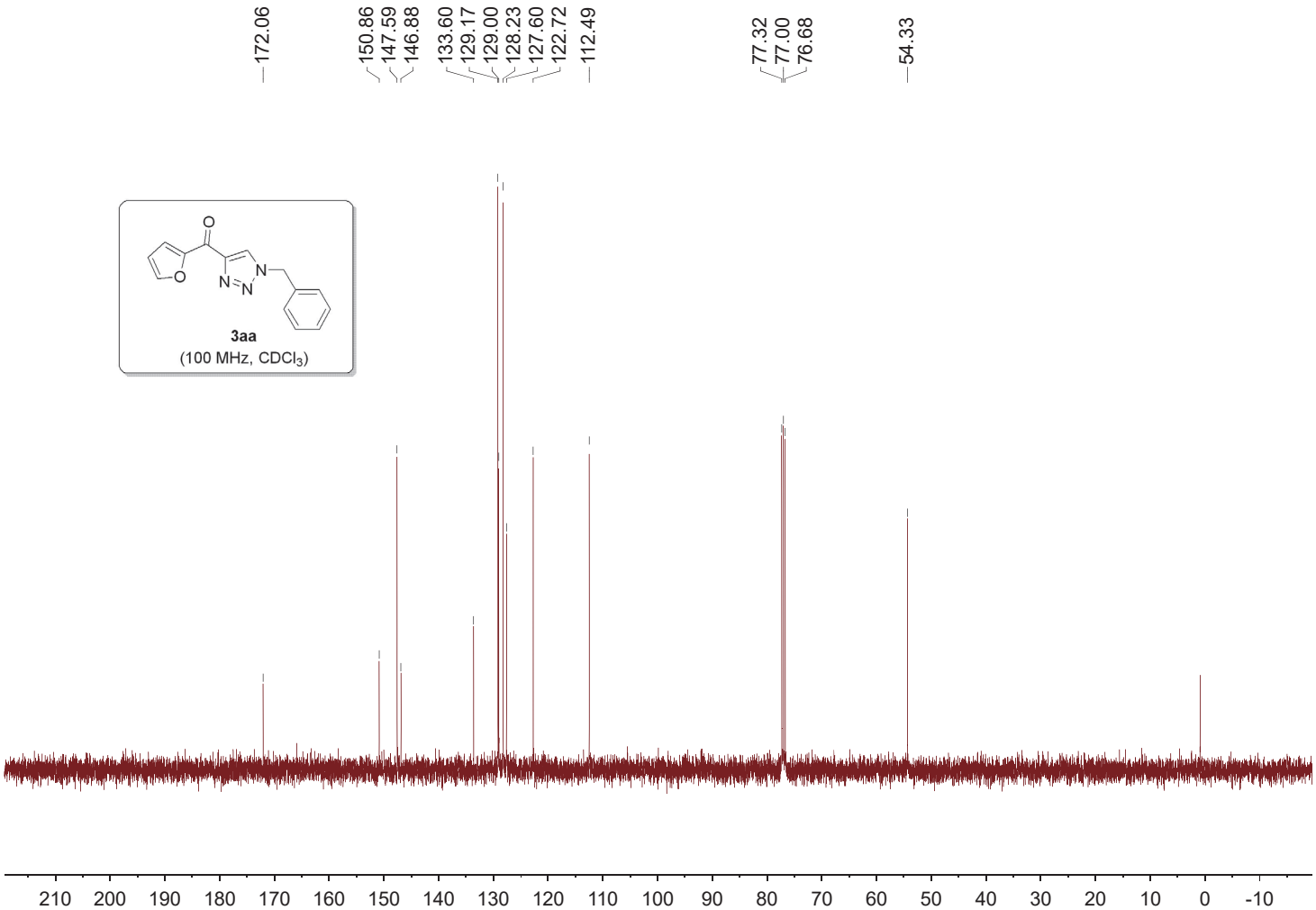

8.43
8.40
8.38
8.36
7.60
7.59
7.58
7.57
7.49
7.47
7.45
7.26
5.26
4.33
4.32
4.30
4.28
1.34
1.32
1.31
-0.01
Cl
O
N
N
O
O
3y
(400 MHz, CDCl3)
0.93
1.96
0.99
1.02
1.90
2.02
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

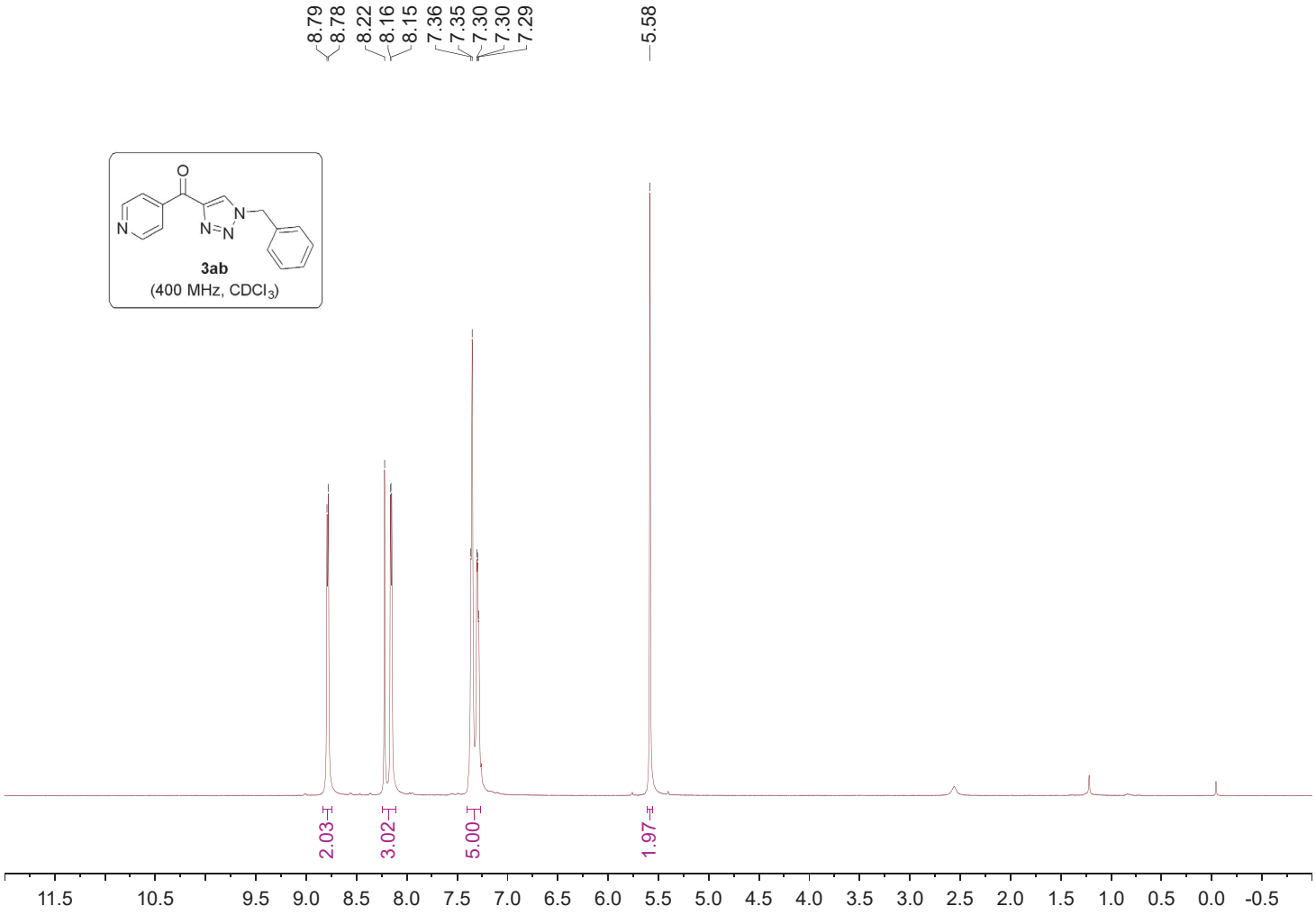

183.98
165.54
148.03
137.85
134.63
133.26
130.43
130.03
129.72
128.84
77.32
77.00
76.68
62.83
51.00
14.05
Cl
O
N
N
O
O
3y
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

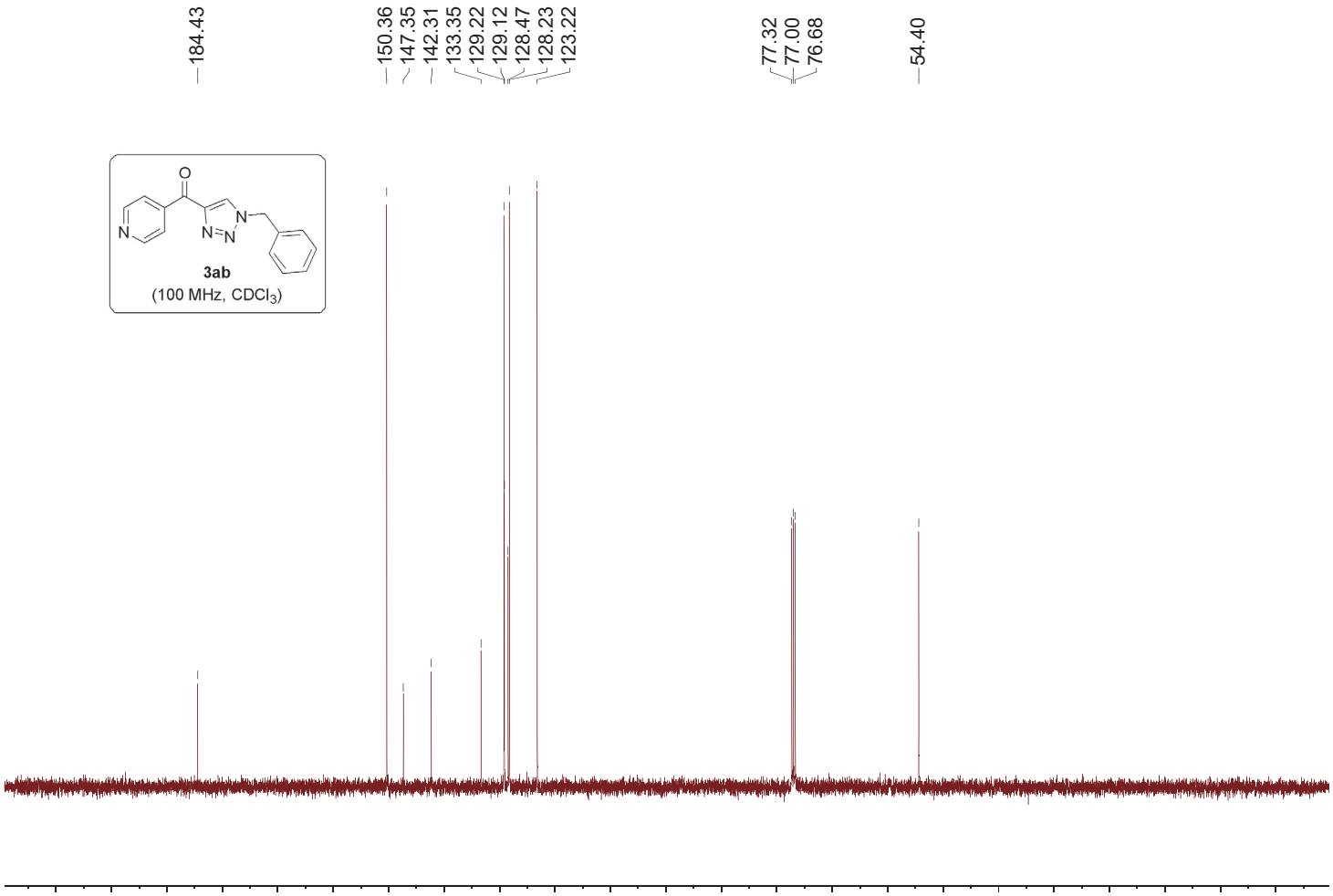

8.42
8.36
8.36
8.35
8.34
7.68
7.67
7.66
7.66
7.26
5.26
4.33
4.32
4.30
4.28
1.60
1.34
1.32
1.31
-0.01
Br
3z
(400 MHz, CDCl3)
0.96
1.99
2.02
1.93
2.02
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

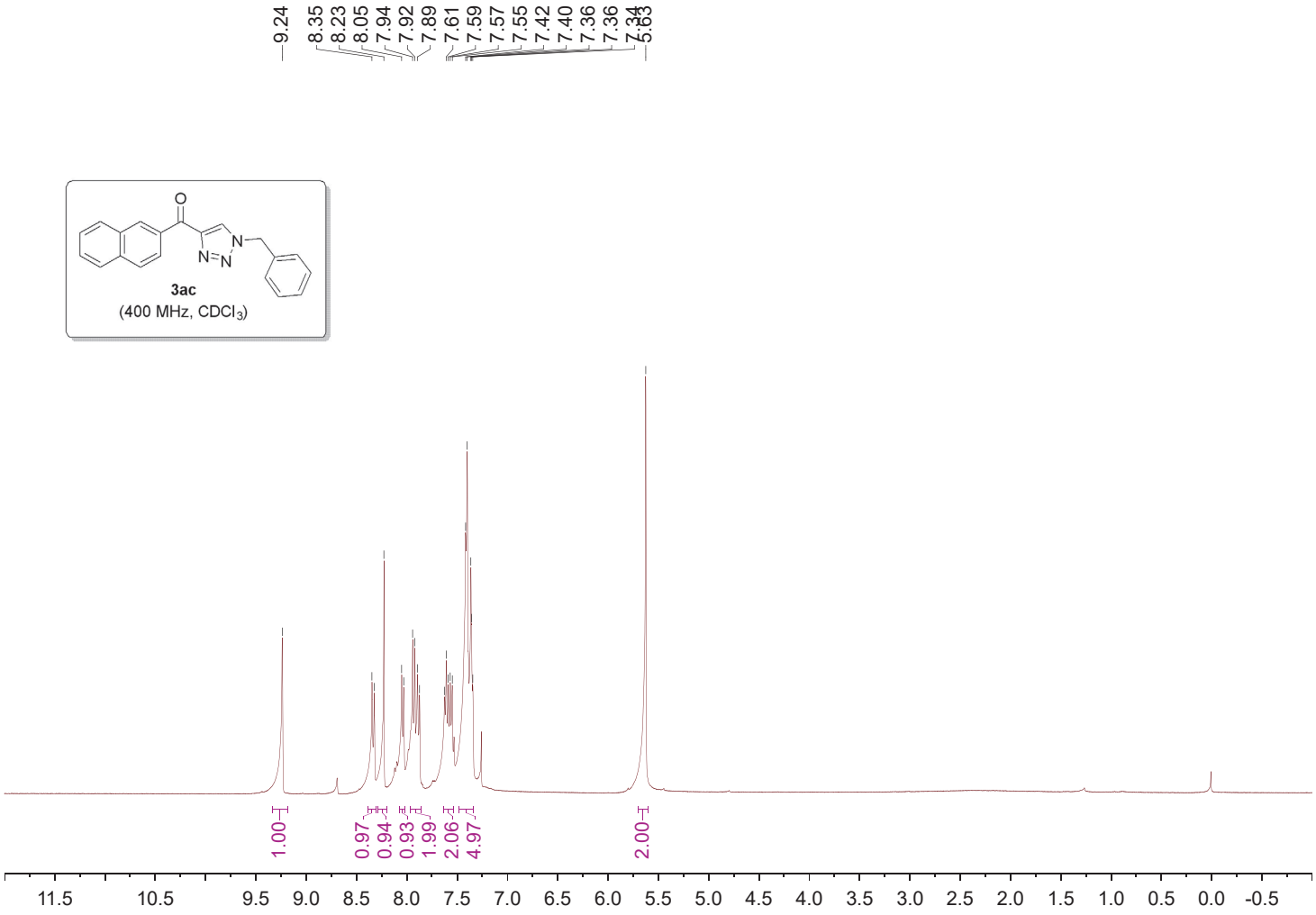

184.19
165.55
148.24
135.06
132.15
131.73
129.96
128.74
77.32
77.00
76.68
62.83
50.99
14.05
Br
3z
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

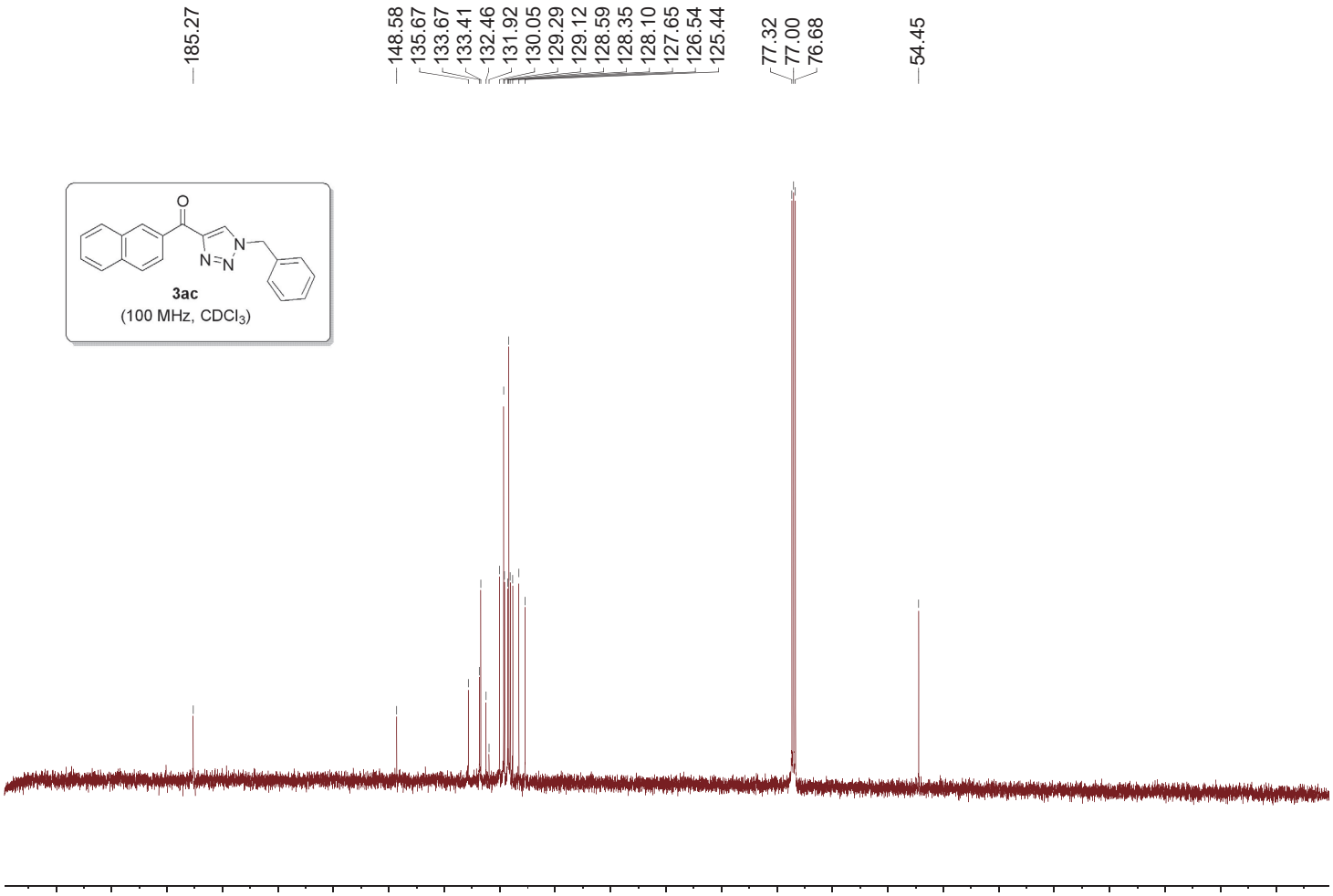

8.20
8.16
8.15
7.69
7.35
7.30
6.60
6.59
5.58
0.06
3aa
(400 MHz, CDCl3)
1.93
0.96
4.92
0.95
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

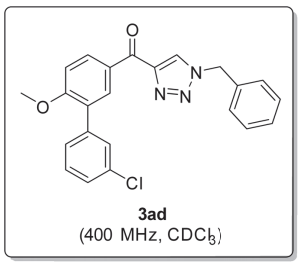

172.06
150.86
147.59
146.88
133.60
129.17
129.00
128.23
127.60
122.72
112.49
77.32
77.00
76.68
54.33
3aa
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


8.79
8.78
8.22
8.16
8.15
7.36
7.35
7.30
7.30
7.29
5.58
3ab
(400 MHz, CDCl3)
2.03
3.02
5.00
1.97
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

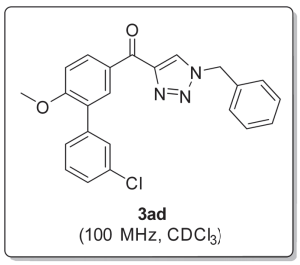

184.43
150.36
147.35
142.31
133.35
129.22
129.12
128.47
128.23
123.22
77.32
77.00
76.68
54.40
3ab
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


9.24
8.35
8.23
8.05
7.94
7.92
7.89
7.61
7.59
7.57
7.55
7.42
7.40
7.36
7.36
7.34
5.63
3ac
(400 MHz, CDCl3)
1.00
0.97
0.94
0.93
1.99
2.06
4.97
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

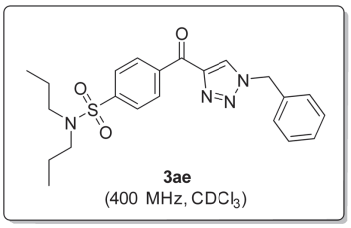

185.27
148.58
135.67
133.67
133.41
132.46
131.92
130.05
129.29
129.12
128.59
128.35
128.10
127.65
126.54
125.44
77.32
77.00
76.68
54.45
3ac
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10



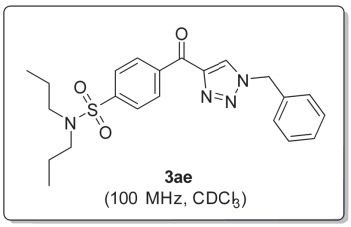
3ad
(400 MHz, $CDCl_3$)



3ad
(100 MHz, $CDCl_3$)


3ae
(400 MHz, CDCl3)

8.56
8.54
8.20
7.94
7.92
7.42
7.40
7.40
7.35
7.33
7.26
5.62
3.13
3.11
3.09
1.63
1.59
1.57
1.56
1.54
1.52
0.89
0.88
0.86
2.01
1.00
2.04
3.00
2.01
2.01
4.03
4.03
6.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


3ae
(100 MHz, CDCl3)

184.26
147.90
144.04
139.17
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131.18
129.39
129.29
128.54
128.40
126.90
77.32
77.00
76.68
54.58
50.08
22.03
11.14
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128.40
126.90
131 130 129 128 127
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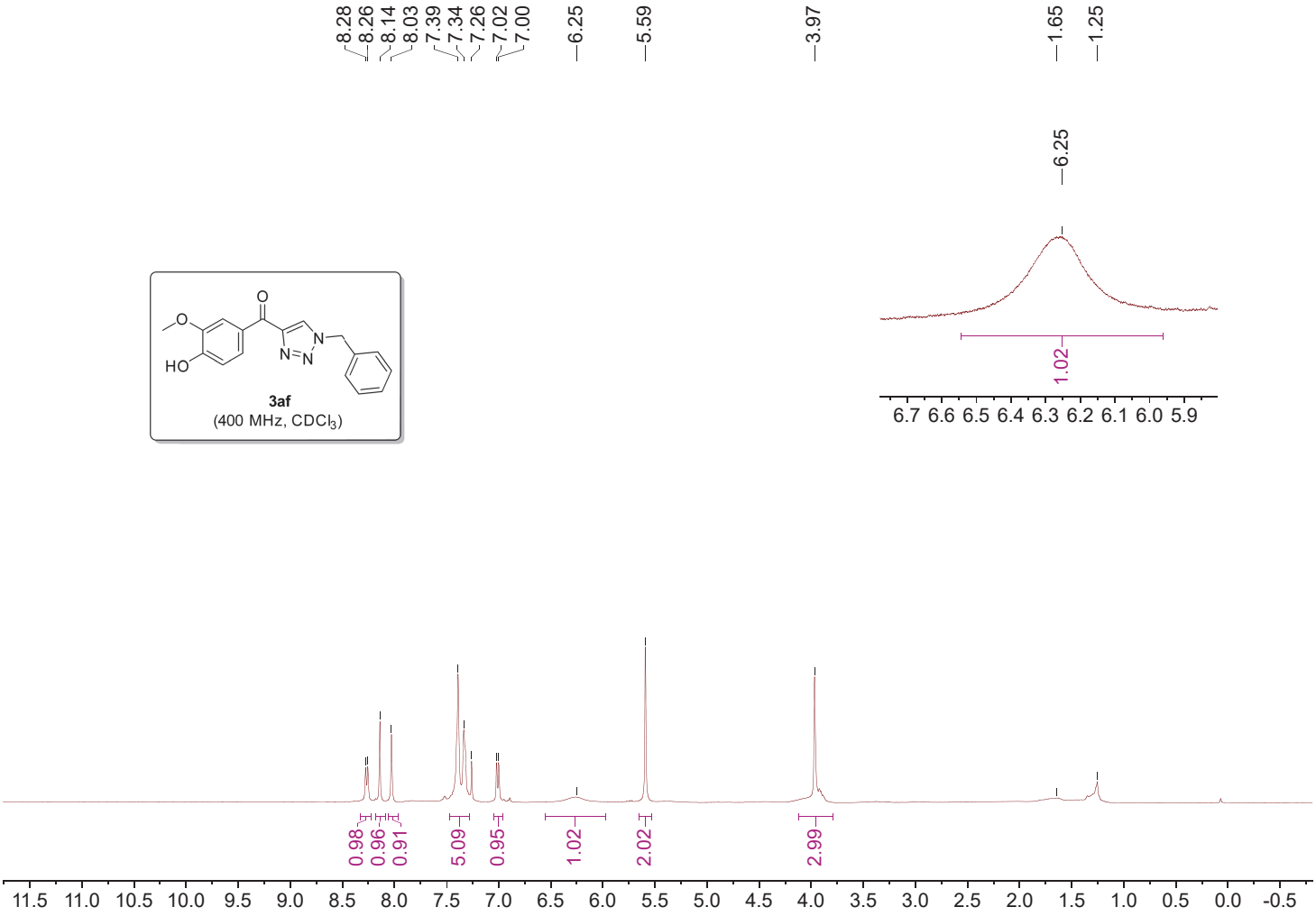
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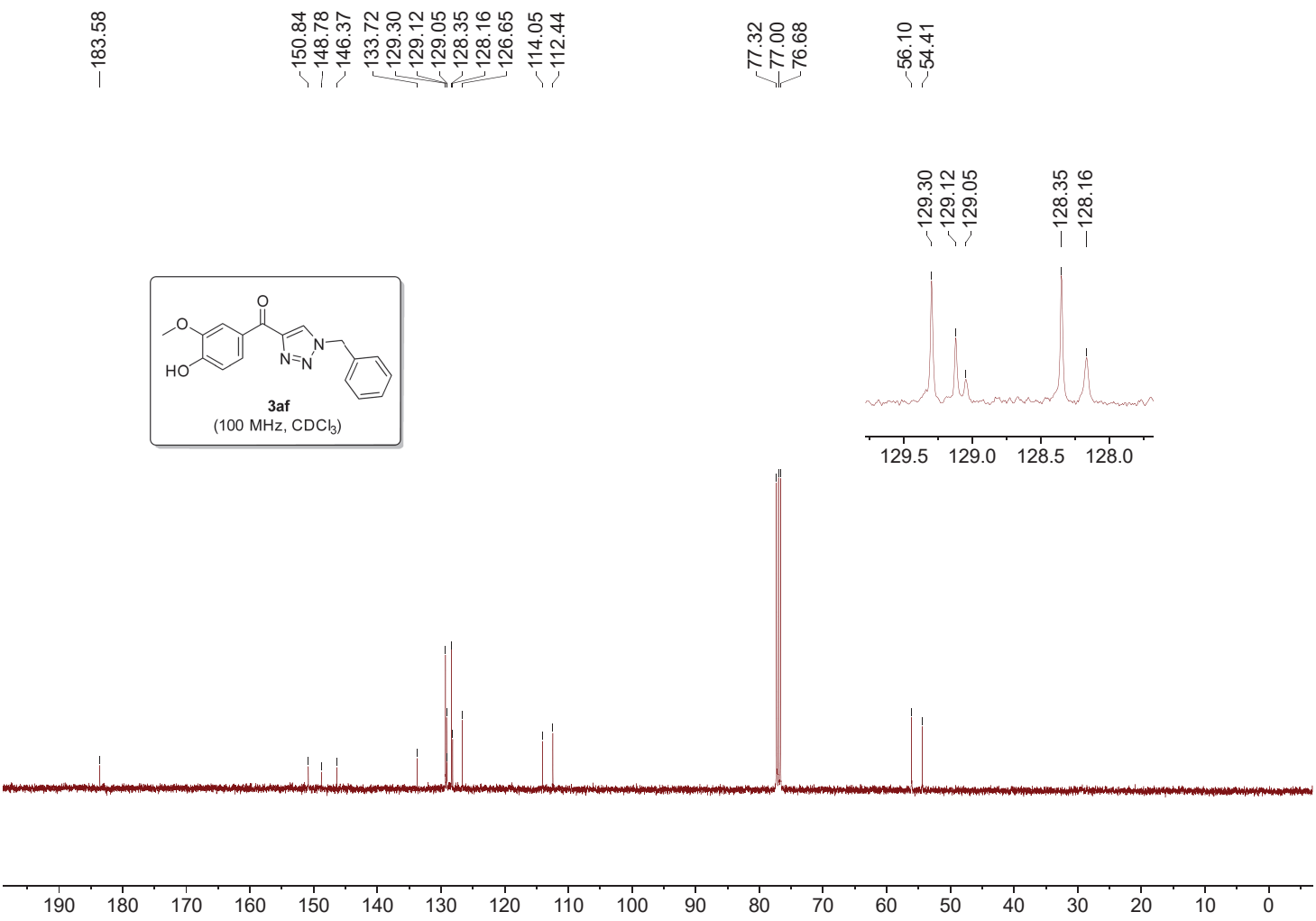
7.34
7.26
7.02
7.00
6.25
5.59
3.97
1.65
1.25
3af
(400 MHz, CDCl3)
6.25
1.02
6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 5.9
0.98
0.96
0.91
5.09
0.95
1.02
2.02
2.99
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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129.30
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129.05
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128.16
126.65
114.05
112.44
77.32
77.00
76.68
56.10
54.41
129.30
129.12
129.05
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3af
(100 MHz, CDCl3)
129.5 129.0 128.5 128.0
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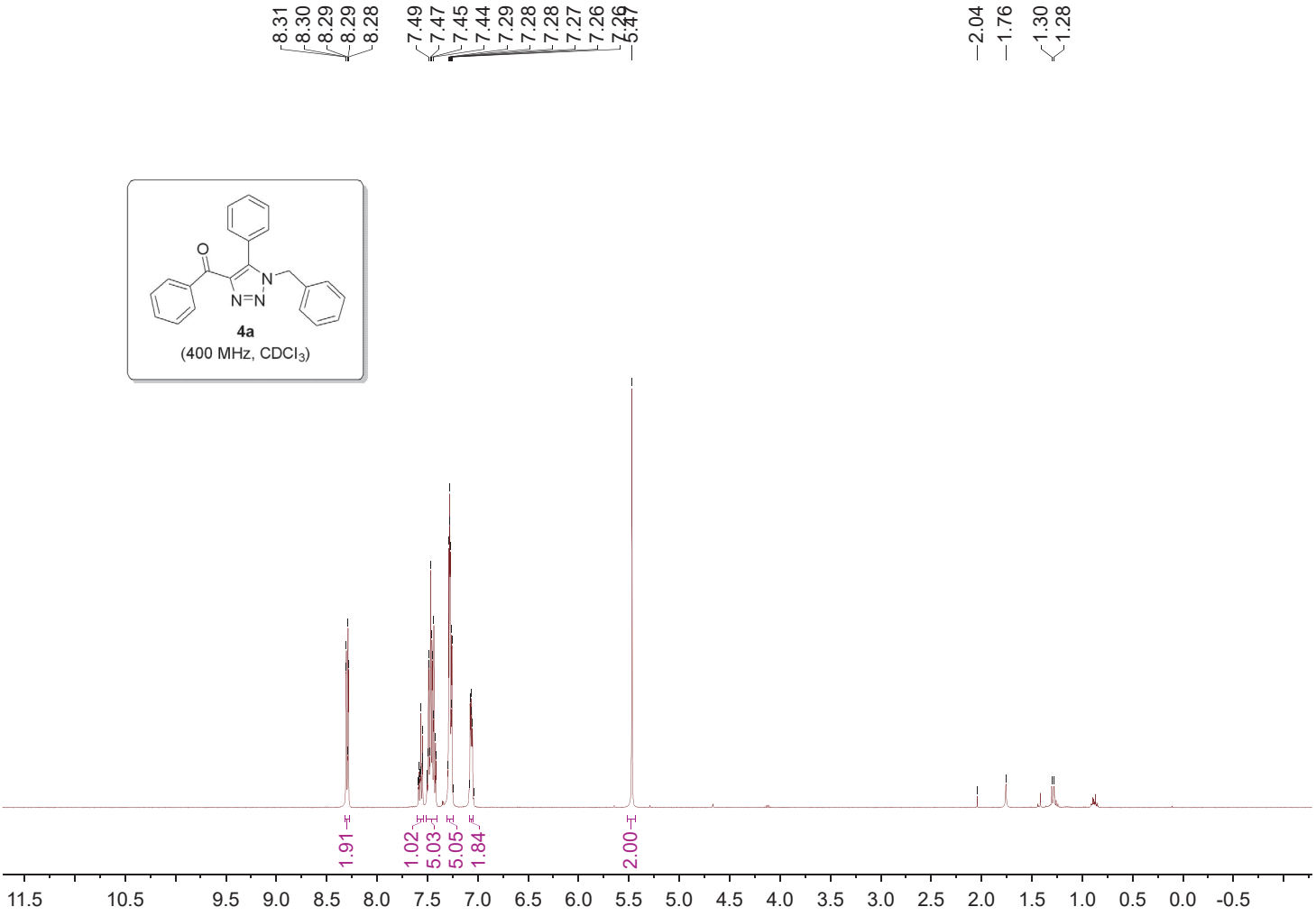
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7.27
7.26
7.26
5.47
2.04
1.76
1.30
1.28
4a
(400 MHz, CDCl3)
1.91
1.02
5.03
5.05
1.84
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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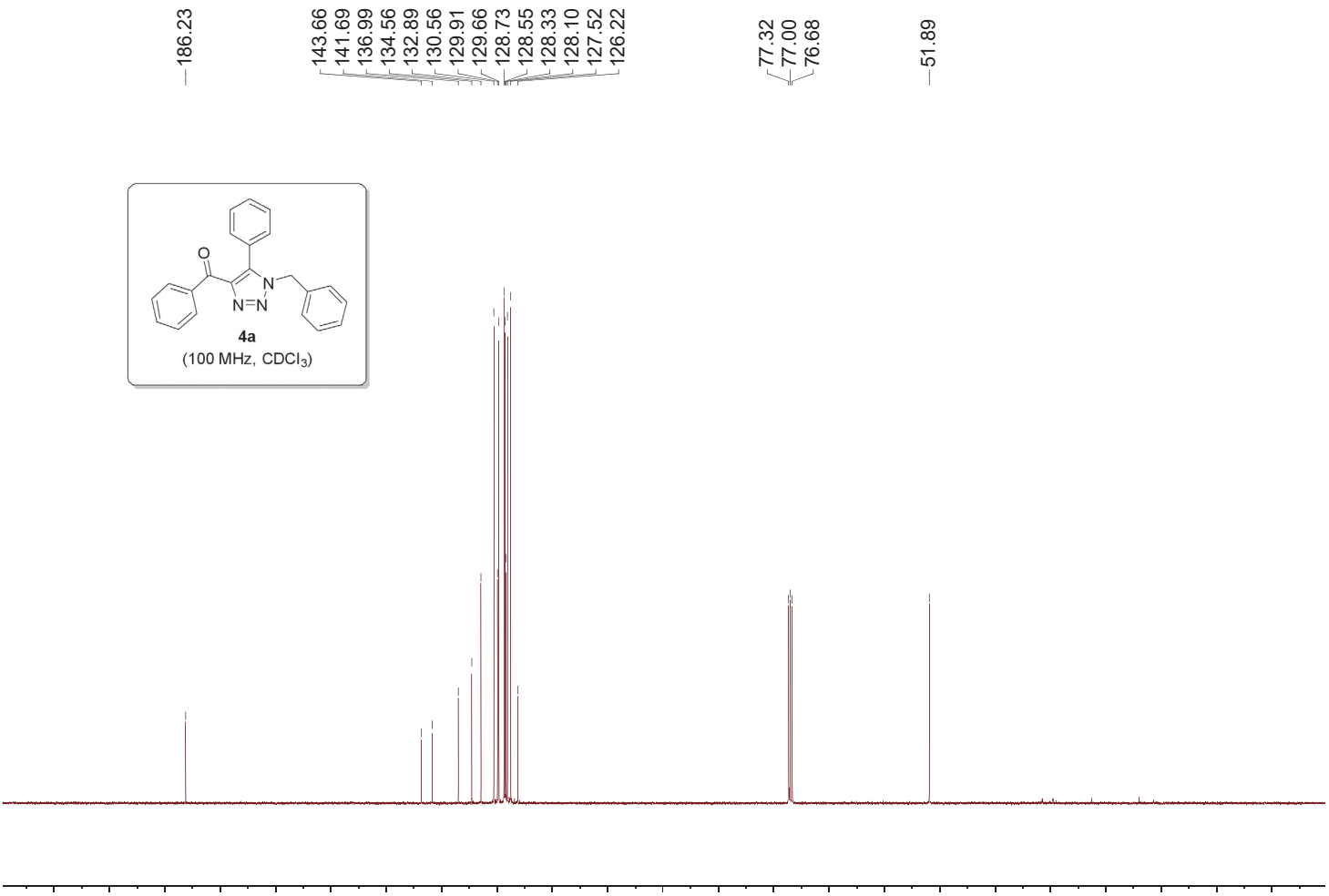
0.0
-0.5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143.66
141.69
136.99
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132.89
130.56
129.91
129.66
128.73
128.55
128.33
128.10
127.52
126.22
77.32
77.00
76.68
51.89
4a
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
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100
90
80
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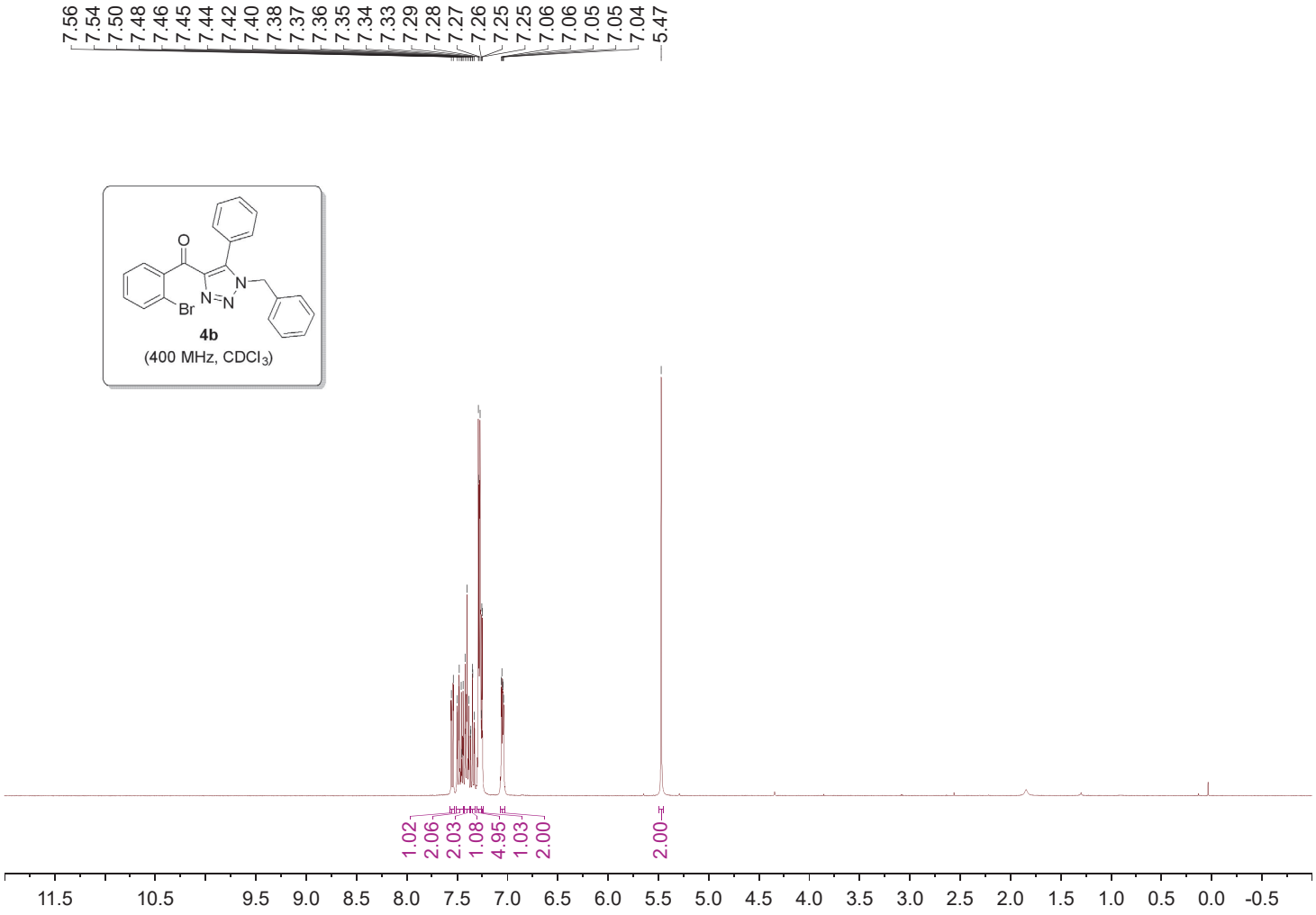
0
-10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7.35
7.34
7.33
7.29
7.28
7.27
7.26
7.25
7.25
7.06
7.06
7.05
7.05
7.04
5.47
4b
(400 MHz, CDCl3)
1.02
2.06
2.03
1.08
4.95
1.03
2.00
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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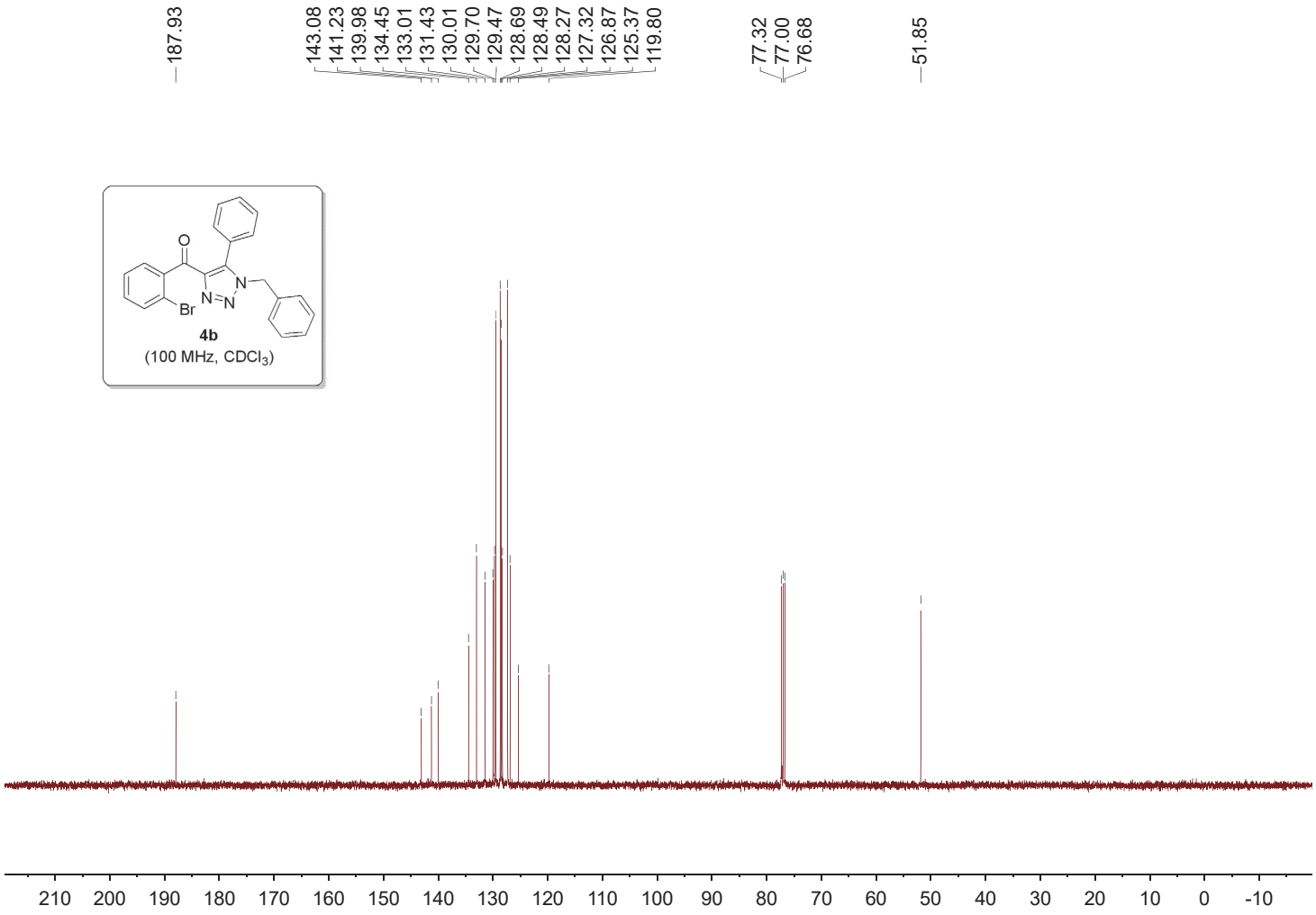
-0.5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139.98
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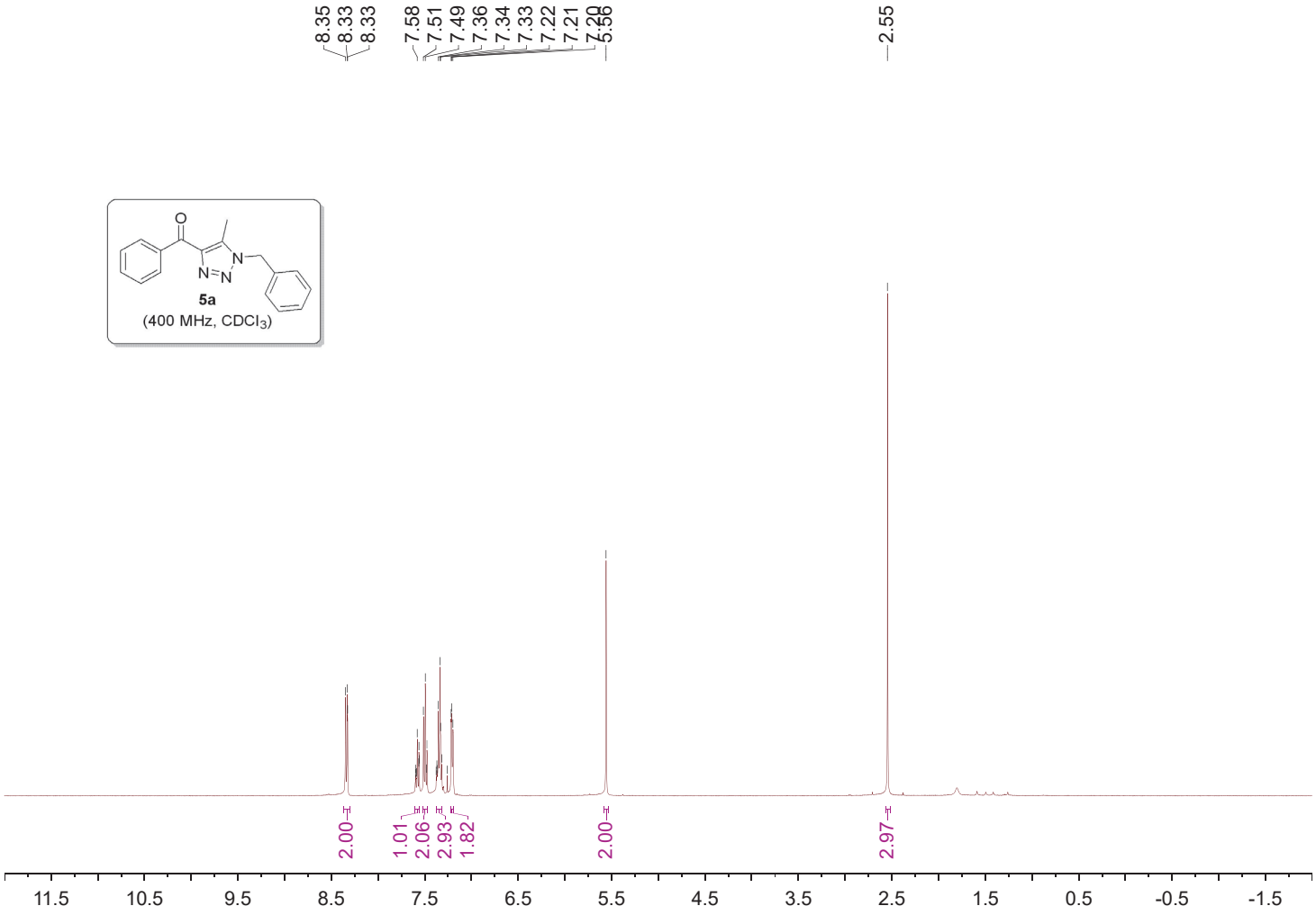
133.01
131.43
130.01
129.70
129.47
128.69
128.49
128.27
127.32
126.87
125.37
119.80
77.32
77.00
76.68
51.85
4b
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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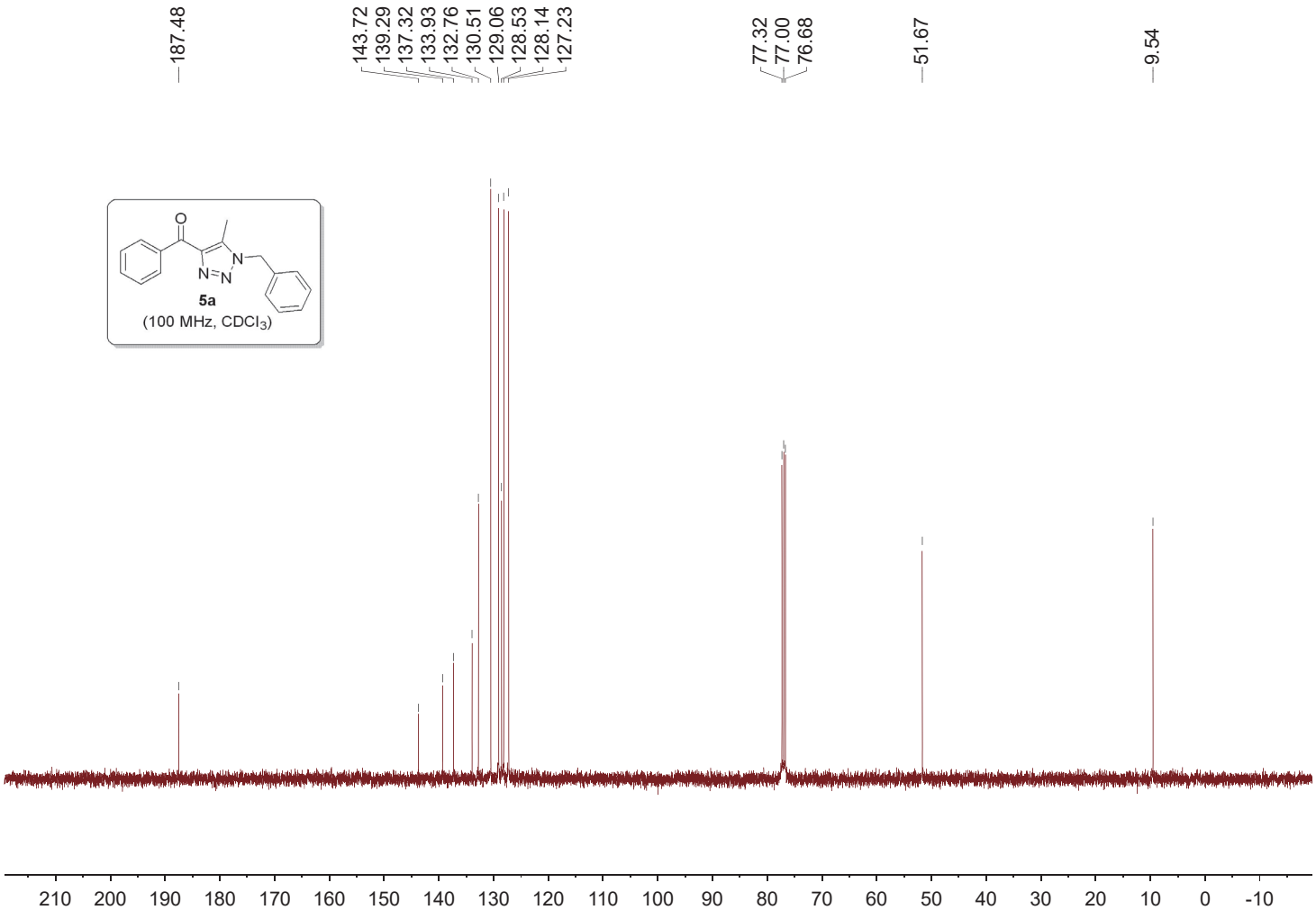
8.33
8.33
7.58
7.51
7.49
7.36
7.34
7.33
7.22
7.21
7.20
5.56
2.55
5a
(400 MHz, CDCl3)
2.00
1.01
2.06
2.93
1.82
2.00
2.97
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5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143.72
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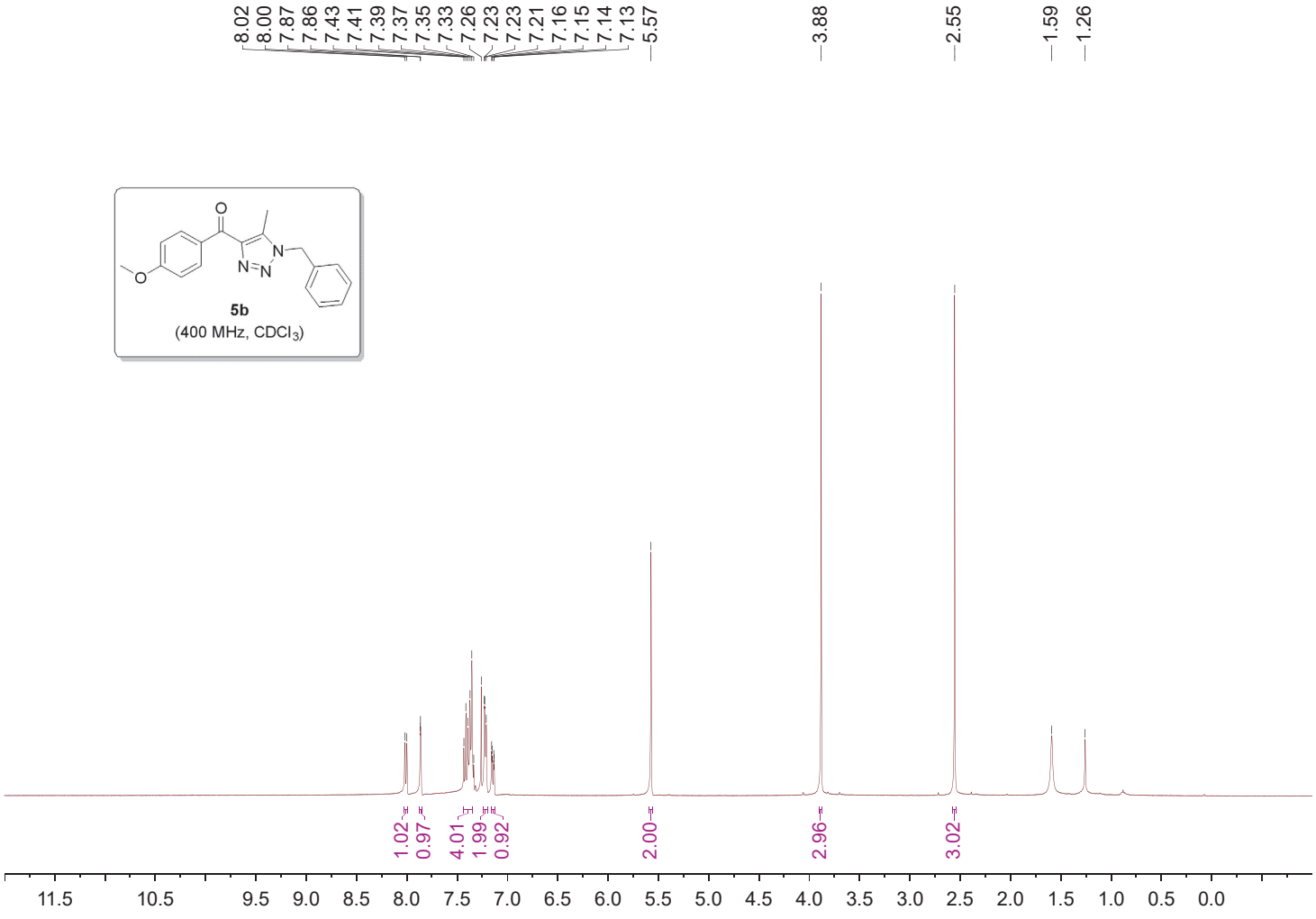
132.76
130.51
129.06
128.53
128.14
127.23
77.32
77.00
76.68
51.67
9.54
5a
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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8.00
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7.86
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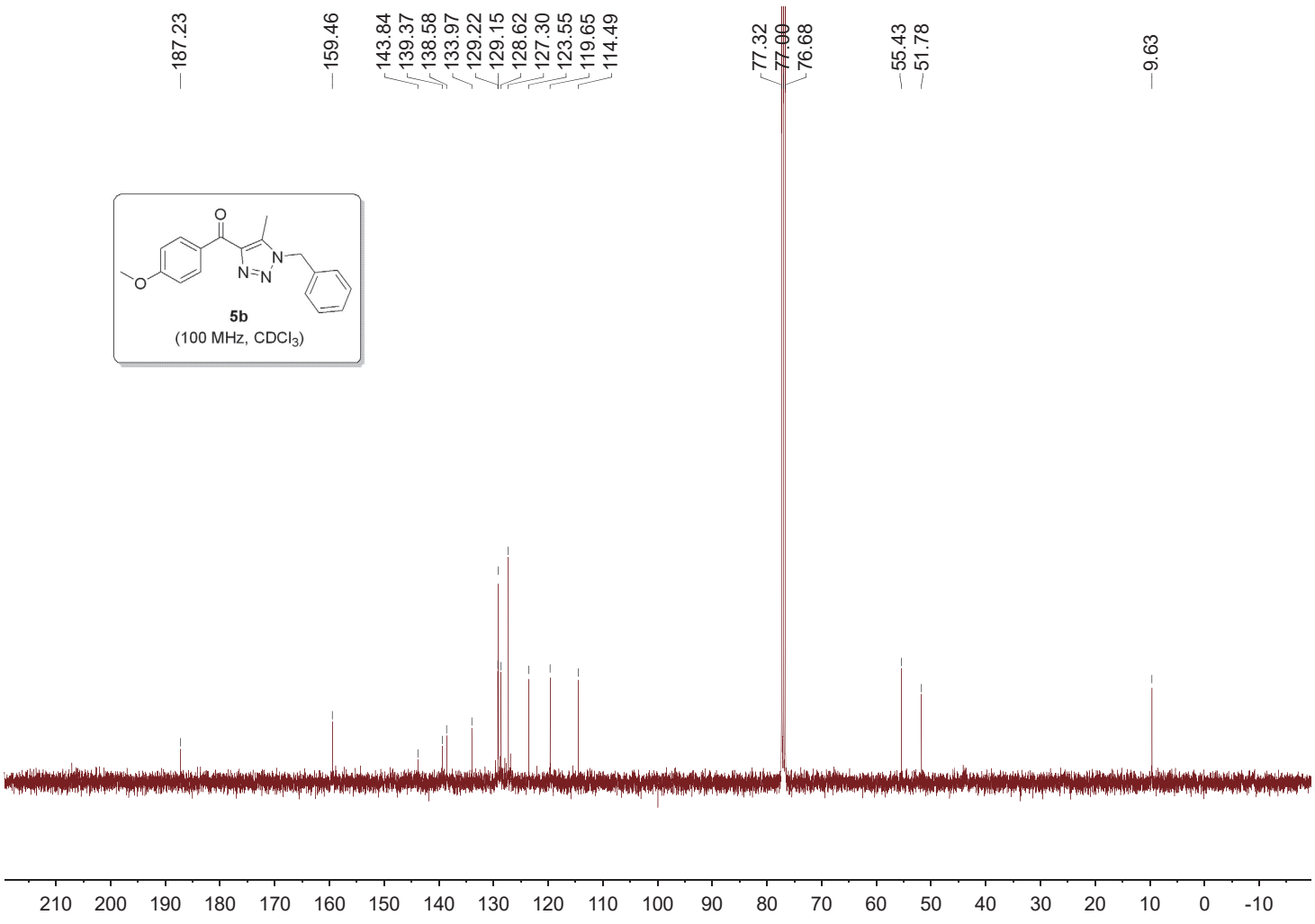
7.41
7.39
7.37
7.35
7.33
7.26
7.23
7.23
7.21
7.16
7.15
7.14
7.13
5.57
3.88
2.55
1.59
1.26
5b
(400 MHz, CDCl3)
1.02
0.97
4.01
1.99
0.92
2.00
2.96
3.02
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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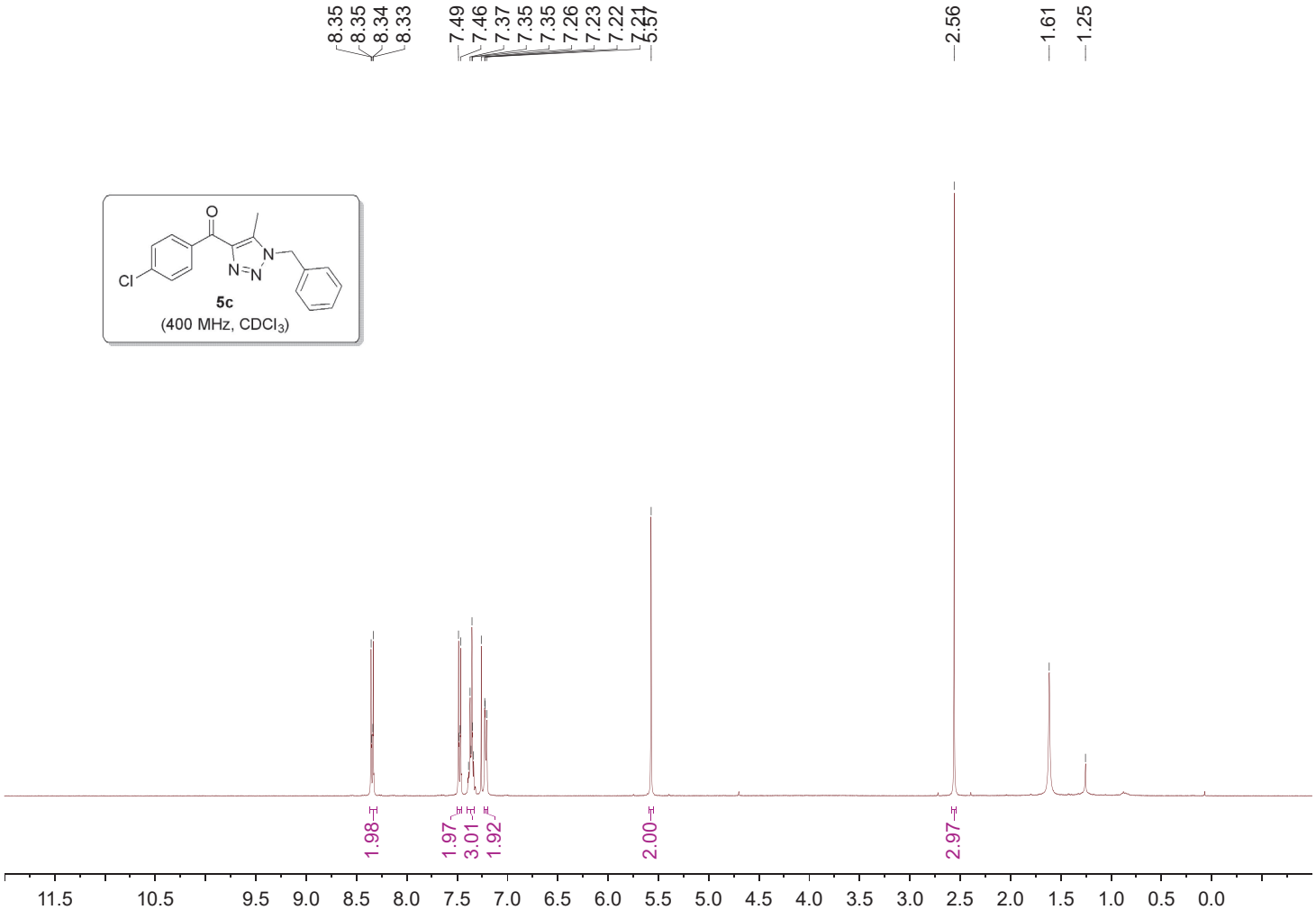
138.58
133.97
129.22
129.15
128.62
127.30
123.55
119.65
114.49
77.32
77.00
76.68
55.43
51.78
9.63
5b
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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8.34
8.33
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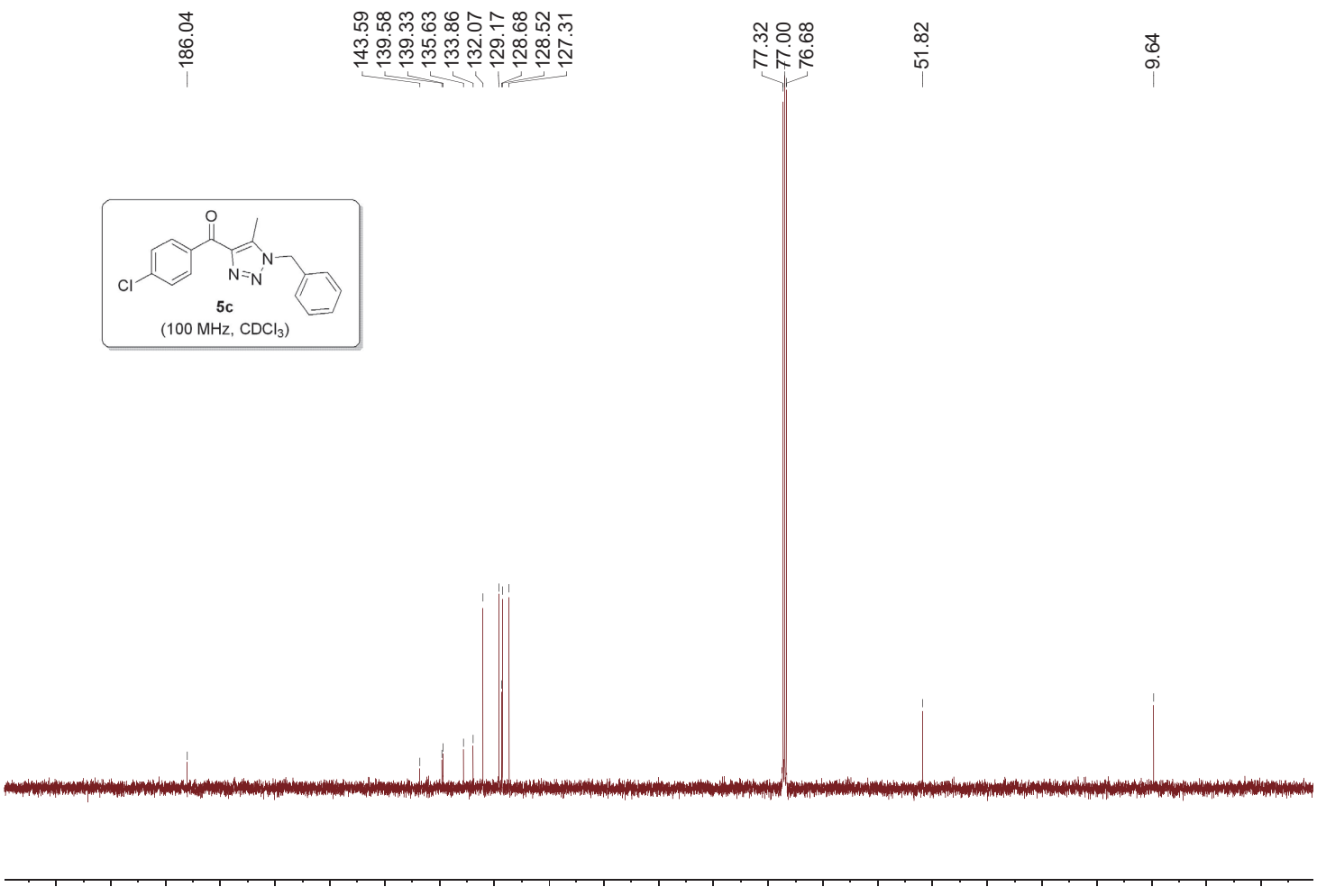
7.46
7.37
7.35
7.35
7.26
7.23
7.22
7.21
5.57
2.56
1.61
1.25
5c
(400 MHz, CDCl3)
1.98
1.97
3.01
1.92
2.00
2.97
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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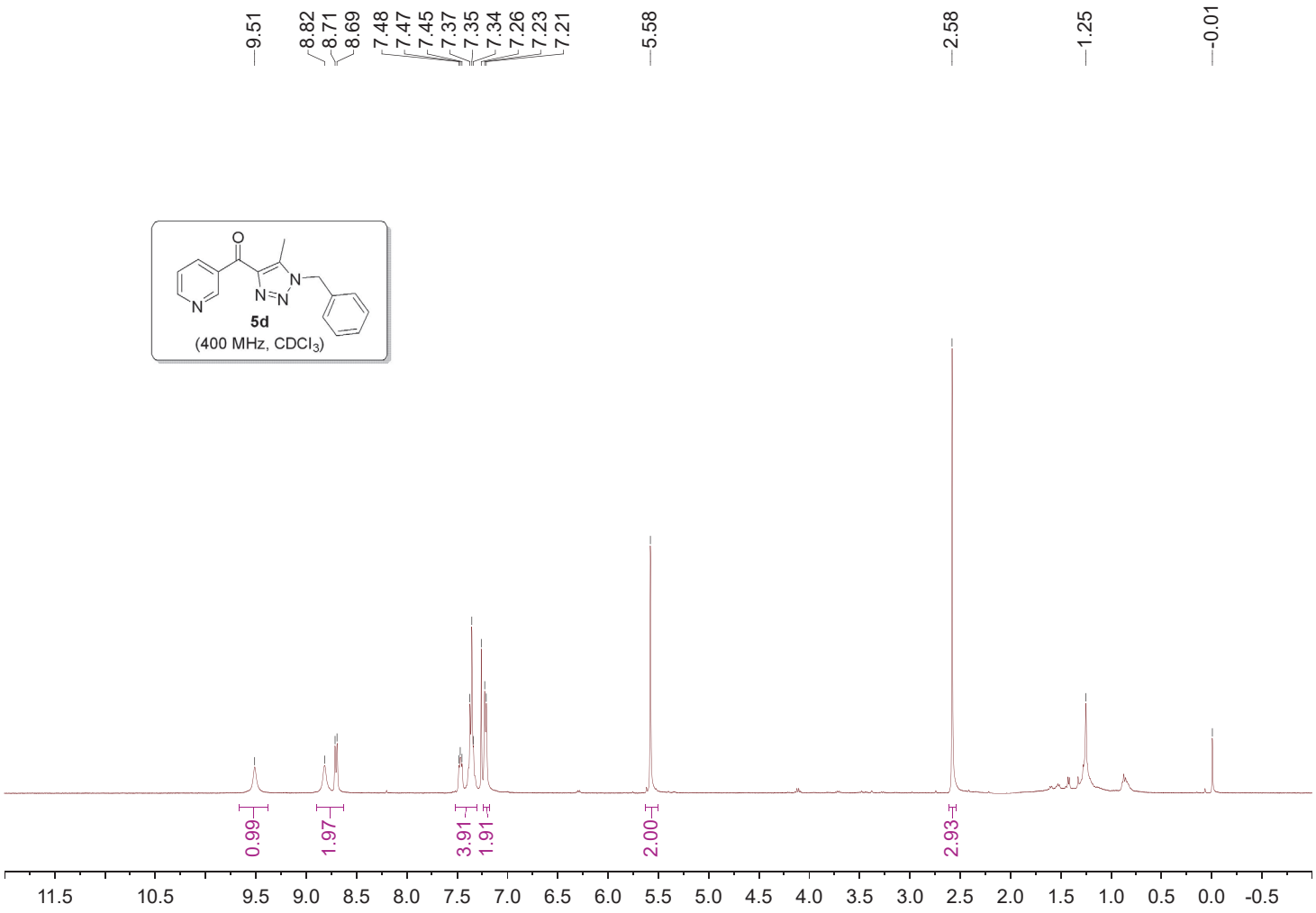
143.59
139.58
139.33
135.63
133.86
132.07
129.17
128.68
128.52
127.31
77.32
77.00
76.68
51.82
9.64
5c
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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8.82
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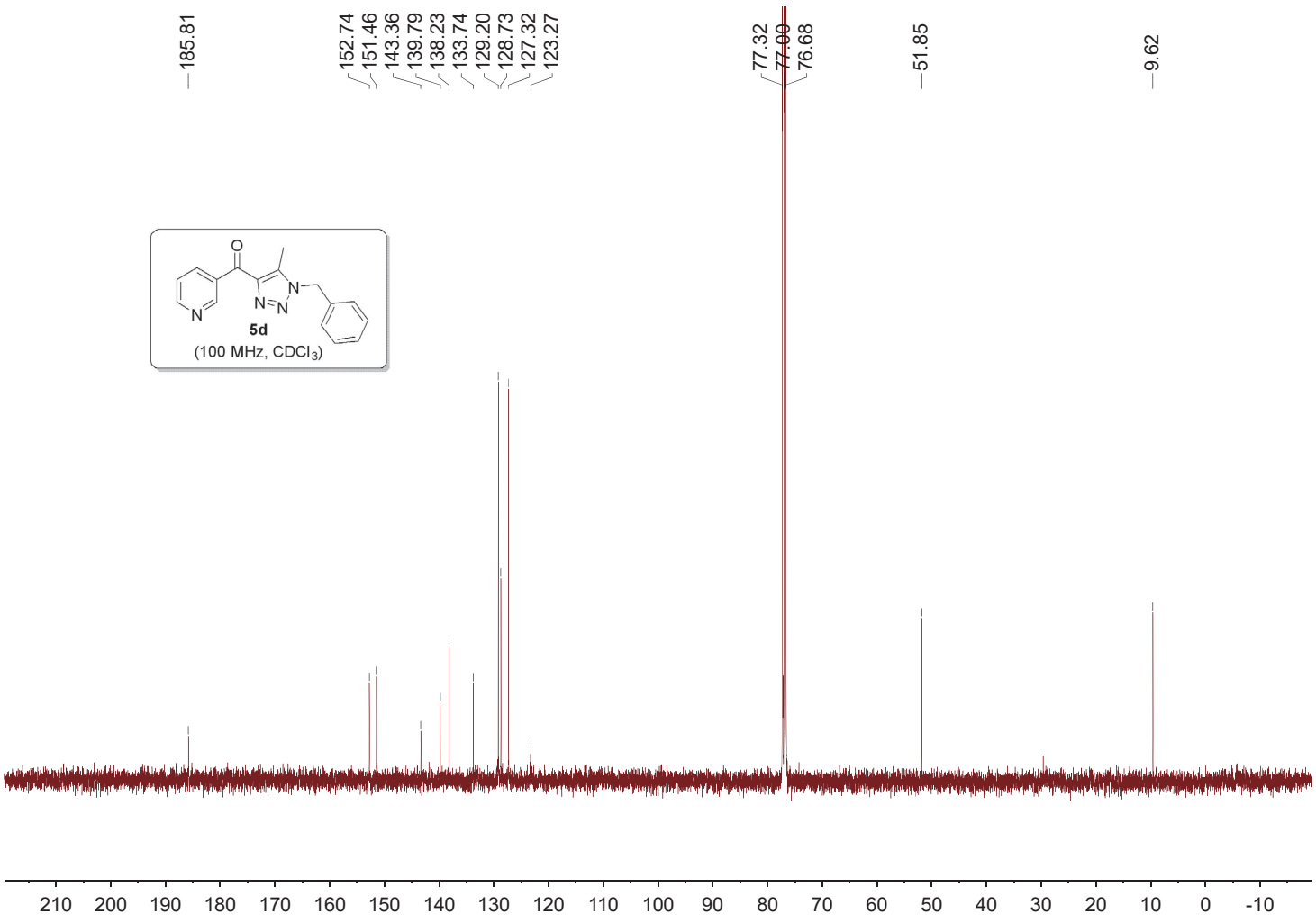
7.47
7.45
7.37
7.35
7.34
7.26
7.23
7.21
5.58
2.58
1.25
-0.01
5d
(400 MHz, CDCl3)
0.99
1.97
3.91
1.91
2.00
2.93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138.23
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129.20
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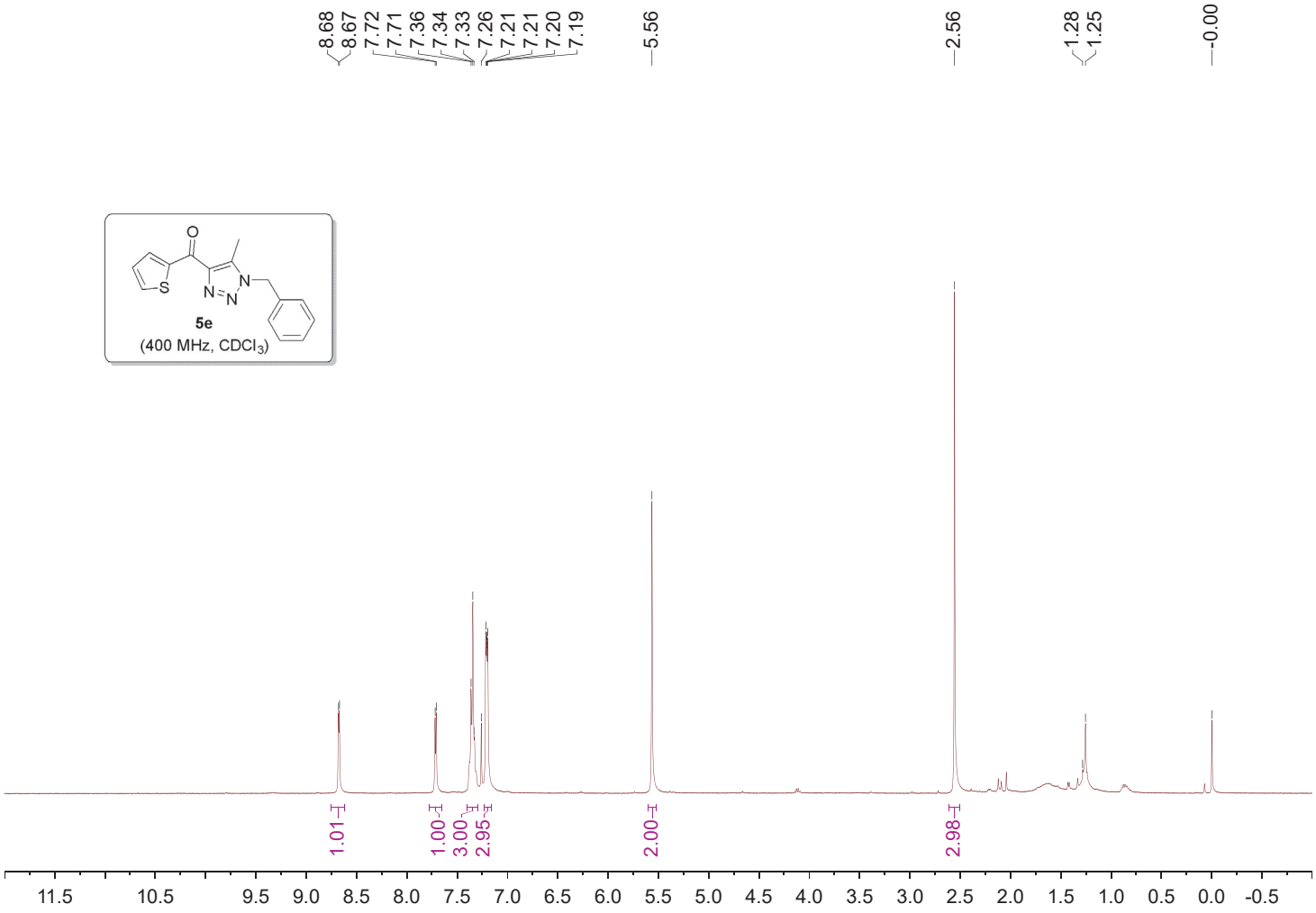
127.32
123.27
77.32
77.00
76.68
51.85
9.62
5d
(100 MHz, CDCl3)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7.33
7.26
7.21
7.21
7.20
7.19
5.56
2.56
1.28
1.25
0.00
5e
(400 MHz, CDCl3)
1.01
1.00
3.00
2.95
2.00
2.98
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
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2.5
2.0
1.5
1.0
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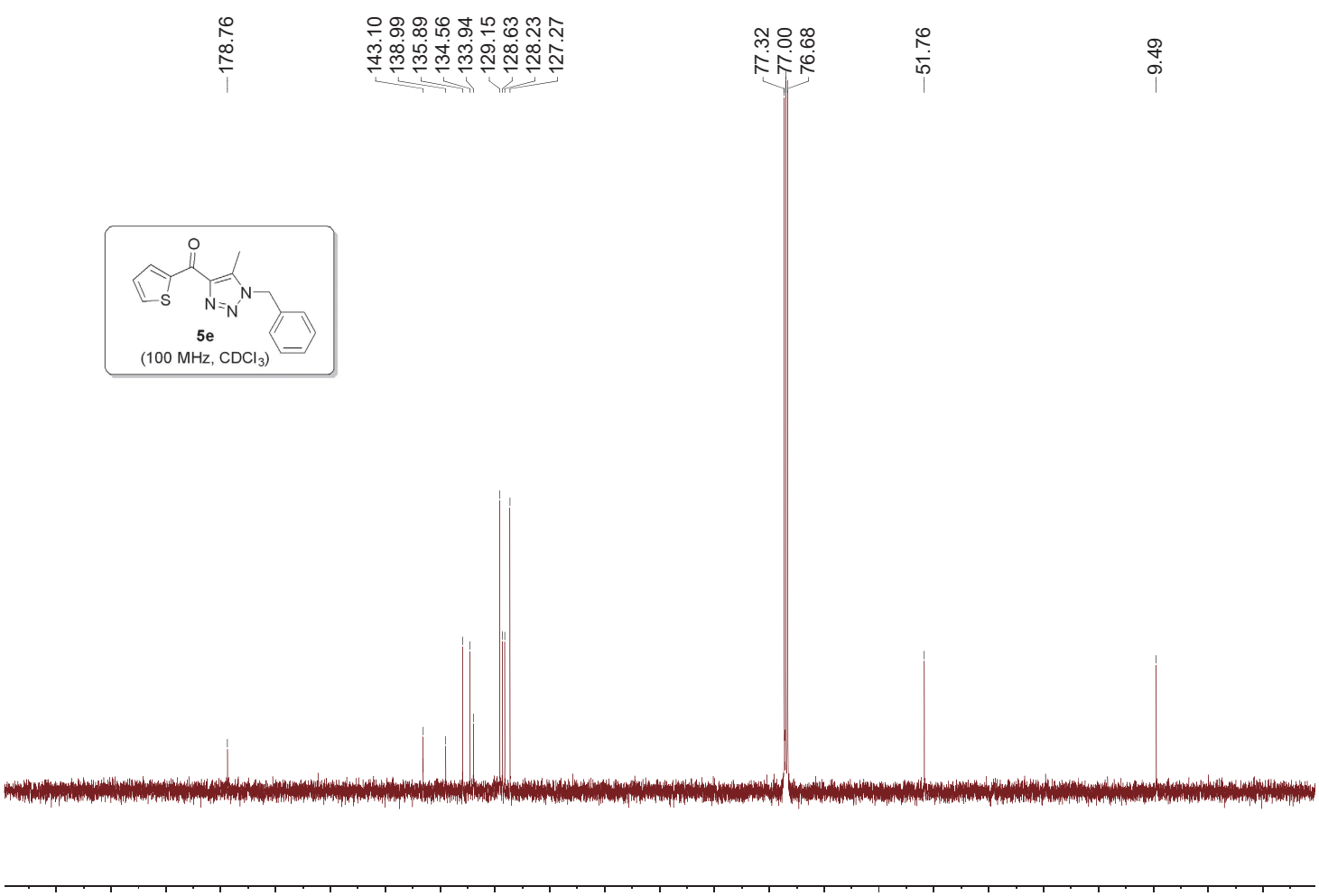
0.0
-0.5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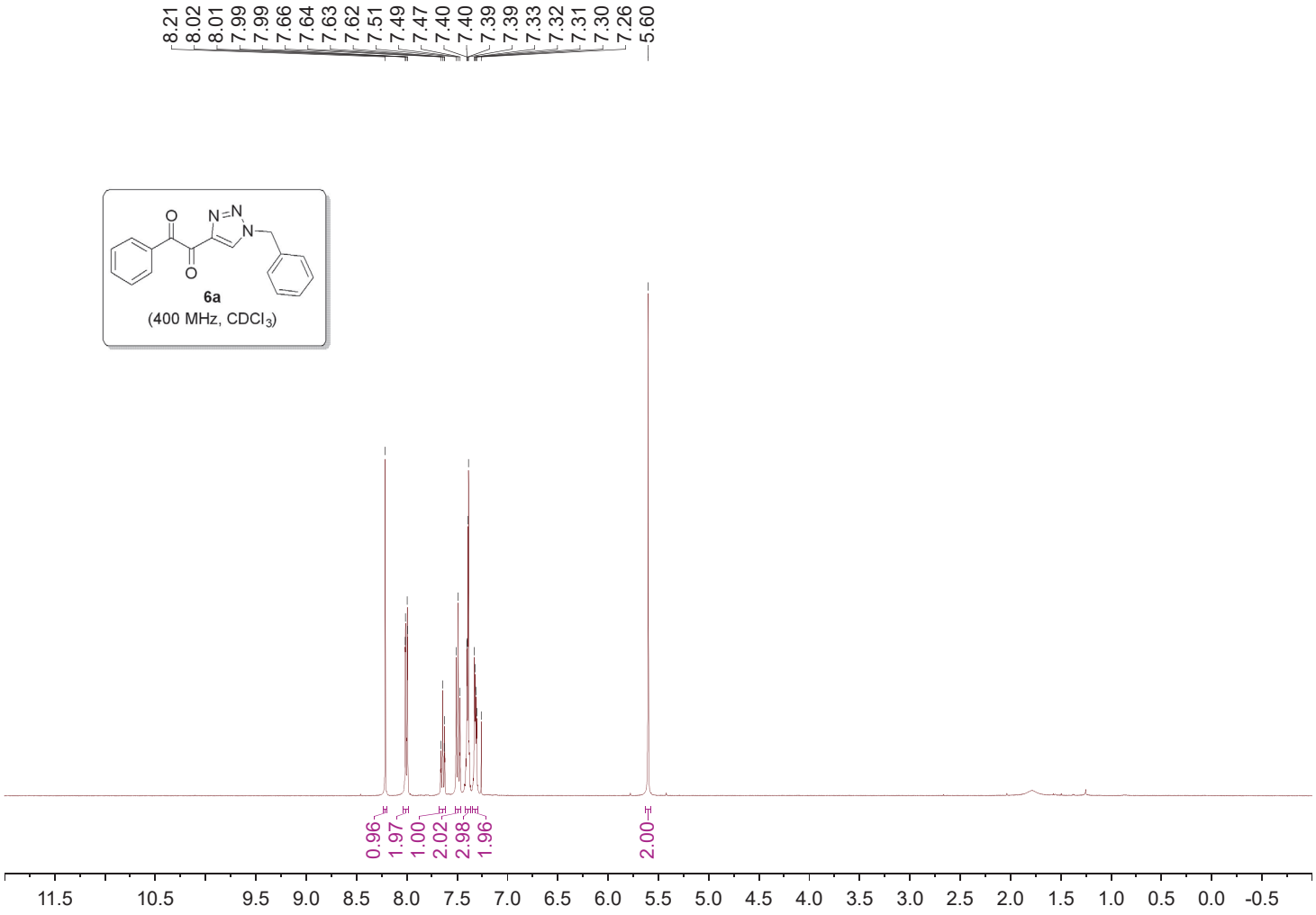
129.15
128.63
128.23
127.27
77.32
77.00
76.68
51.76
9.49
5e
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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7.99
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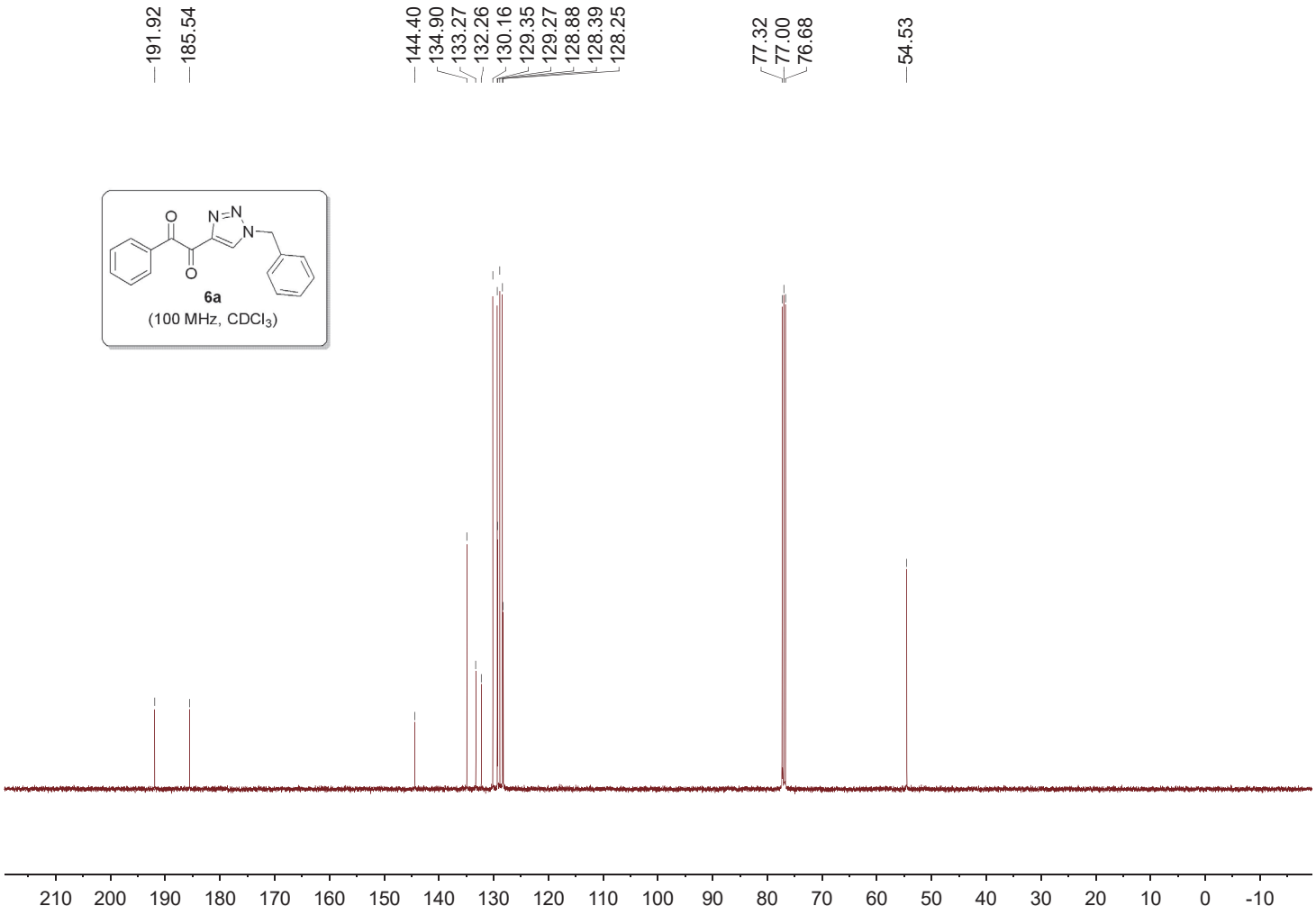
7.64
7.63
7.62
7.51
7.49
7.47
7.40
7.40
7.39
7.39
7.33
7.32
7.31
7.30
7.26
5.60
6a
(400 MHz, CDCl3)
0.96
1.97
1.00
2.02
2.98
1.96
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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132.26
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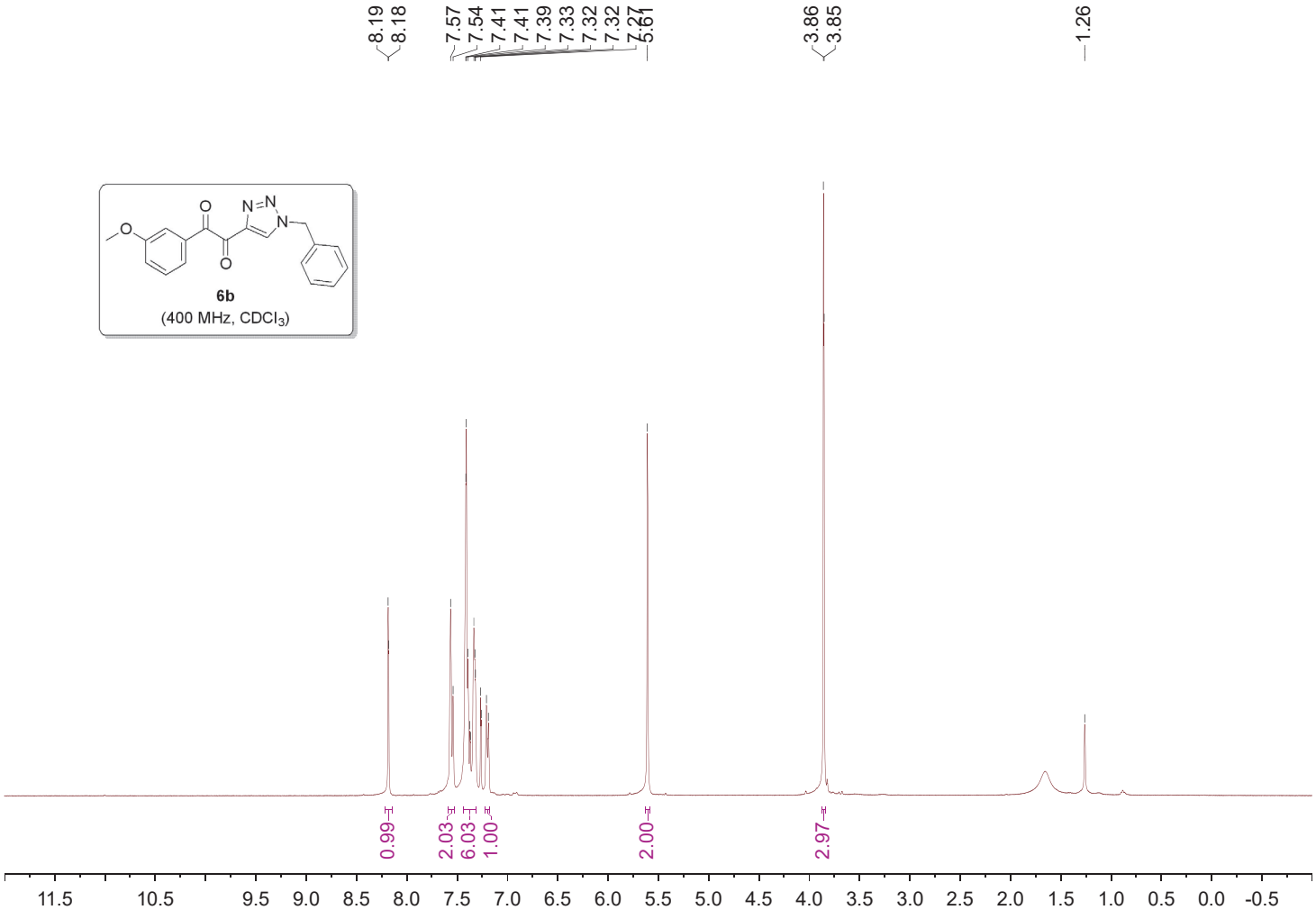
129.35
129.27
128.88
128.39
128.25
77.32
77.00
76.68
54.53
6a
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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7.54
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7.41
7.39
7.33
7.32
7.32
7.27
5.61
3.86
3.85
1.26
6b
(400 MHz, CDCl3)
0.99
2.03
6.03
1.00
2.00
2.97
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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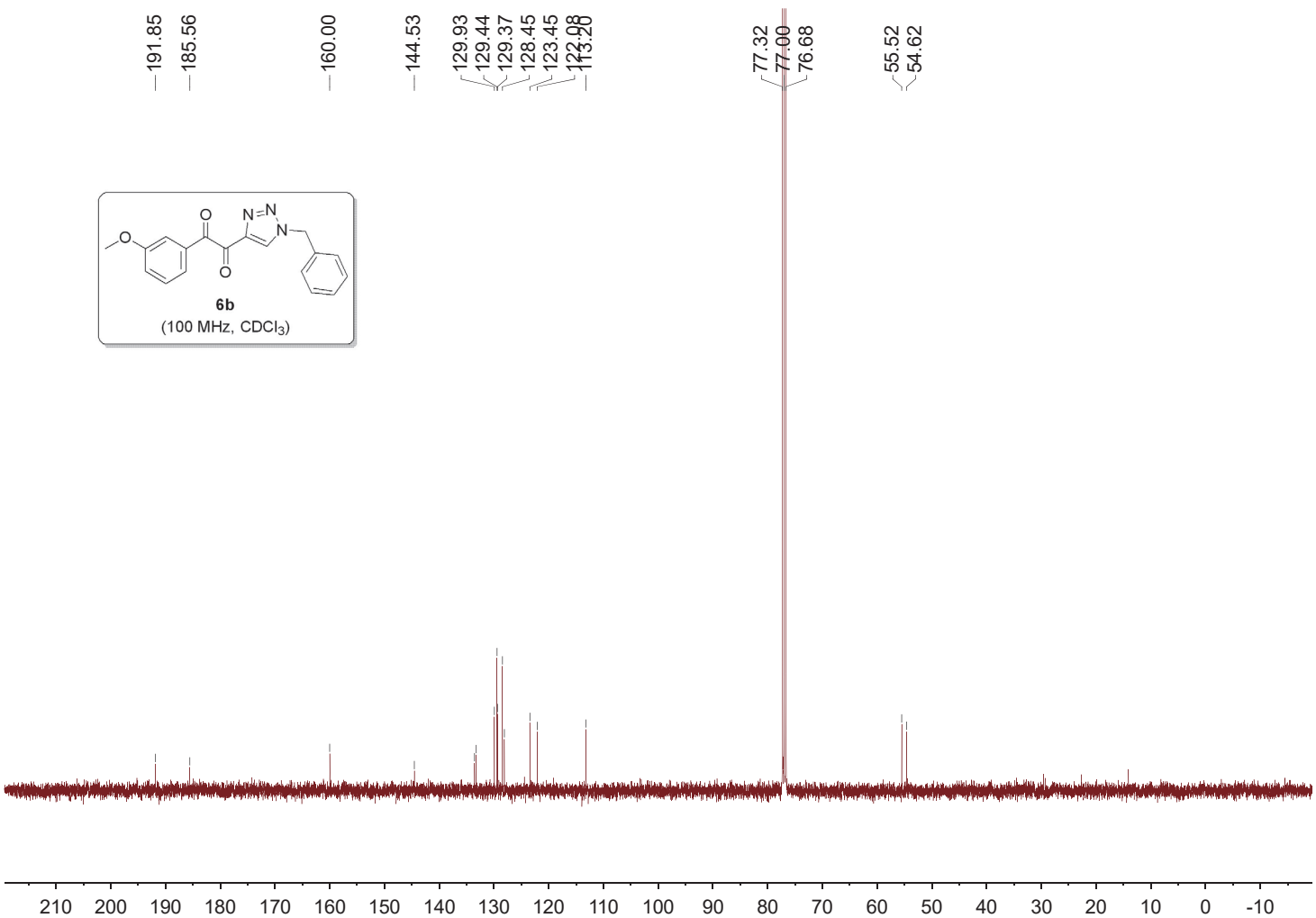
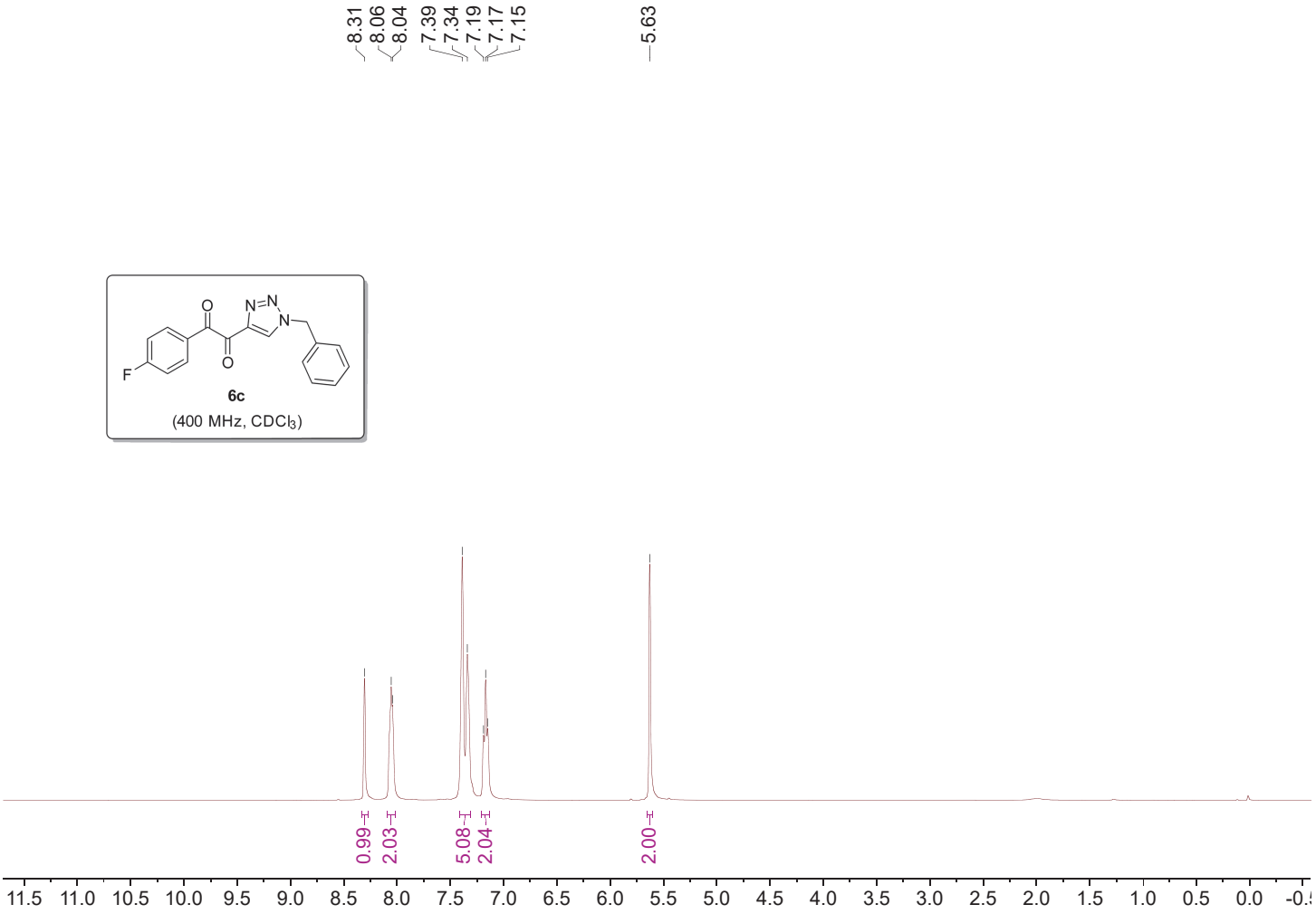
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


191.85
185.56
160.00
144.53
129.93
129.44
129.37
128.45
123.45
77.32
77.00
76.68
55.52
54.62
6b
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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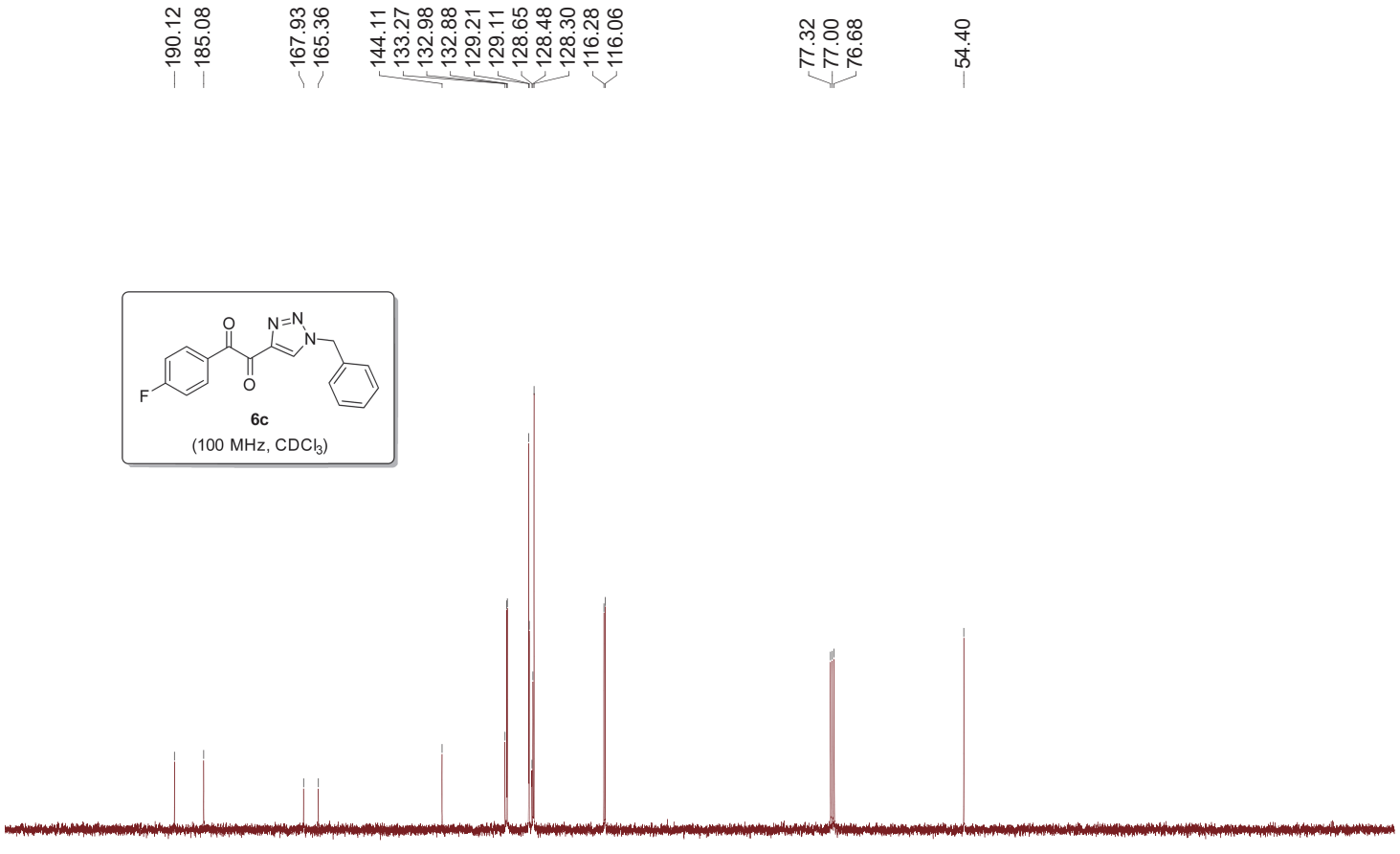
8.06
8.04
7.39
7.34
7.19
7.17
7.15
5.63
6c
(400 MHz, CDCl3)
0.99
2.03
5.08
2.04
2.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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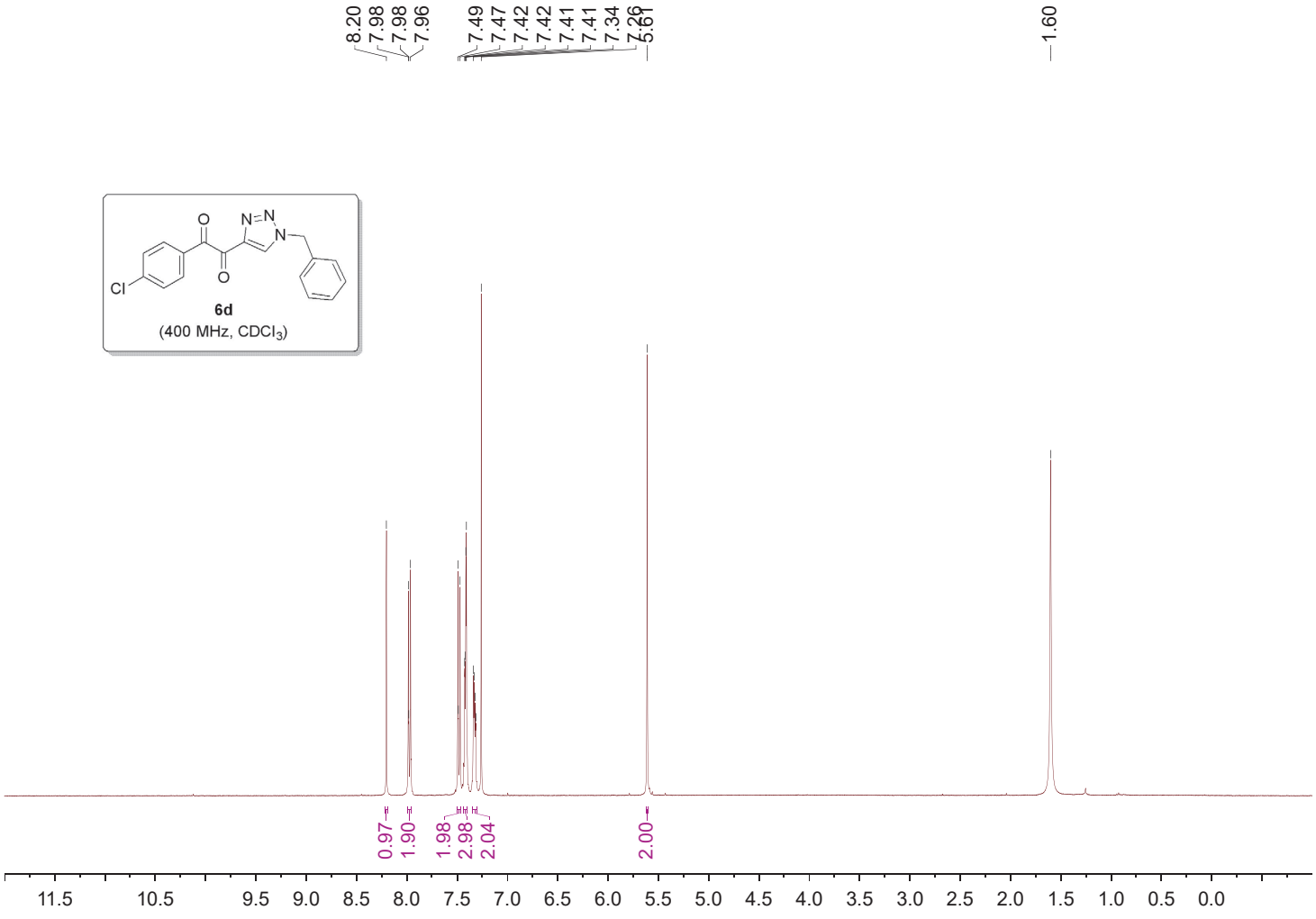
185.08
167.93
165.36
144.11
133.27
132.98
132.88
129.21
129.11
128.65
128.48
128.30
116.28
116.06
77.32
77.00
76.68
54.40
6c
(100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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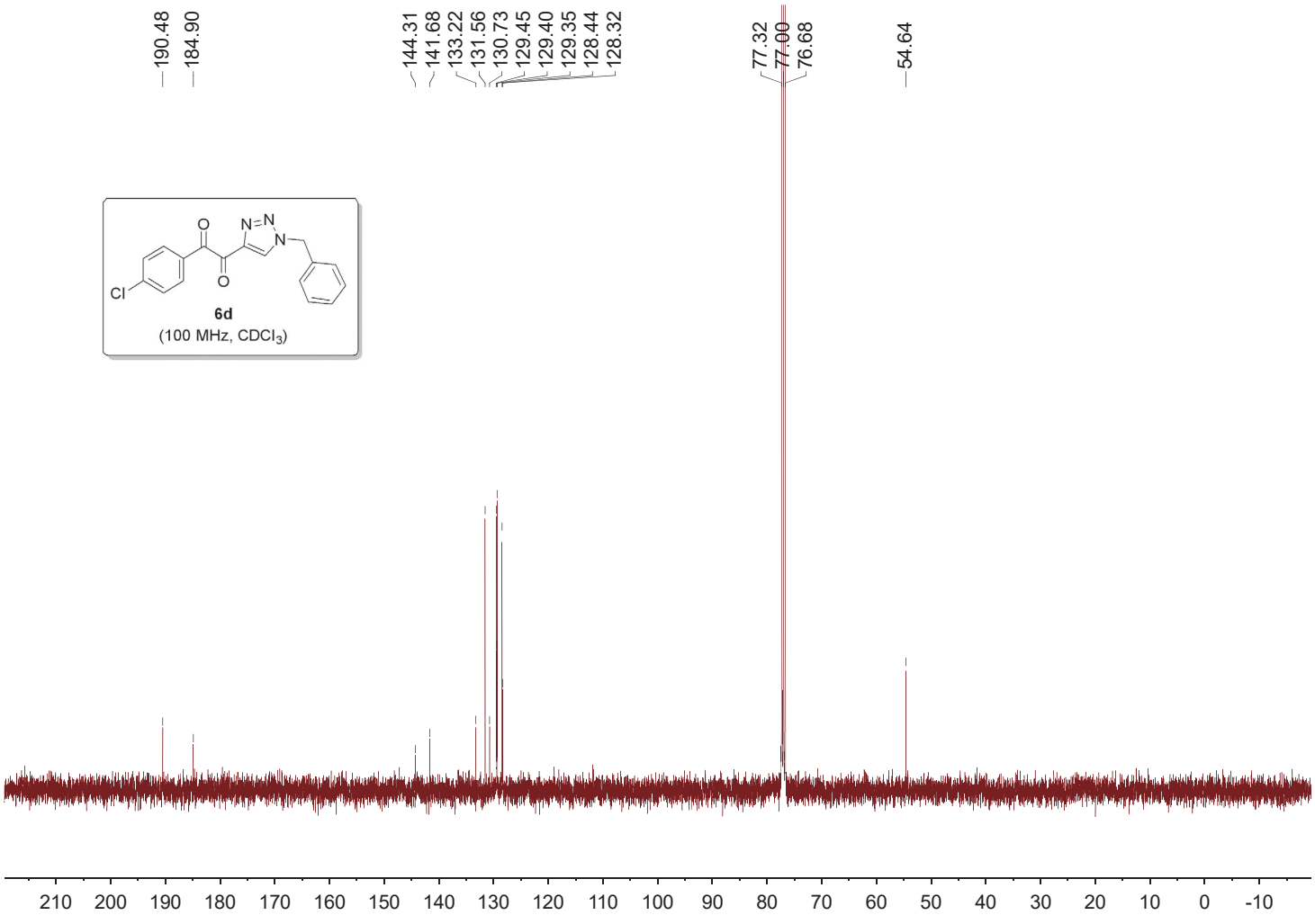
7.98
7.98
7.96
7.49
7.47
7.42
7.42
7.41
7.41
7.34
7.26
5.61
1.60
6d
(400 MHz, CDCl3)
0.97
1.90
1.98
2.98
2.04
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


190.48
184.90
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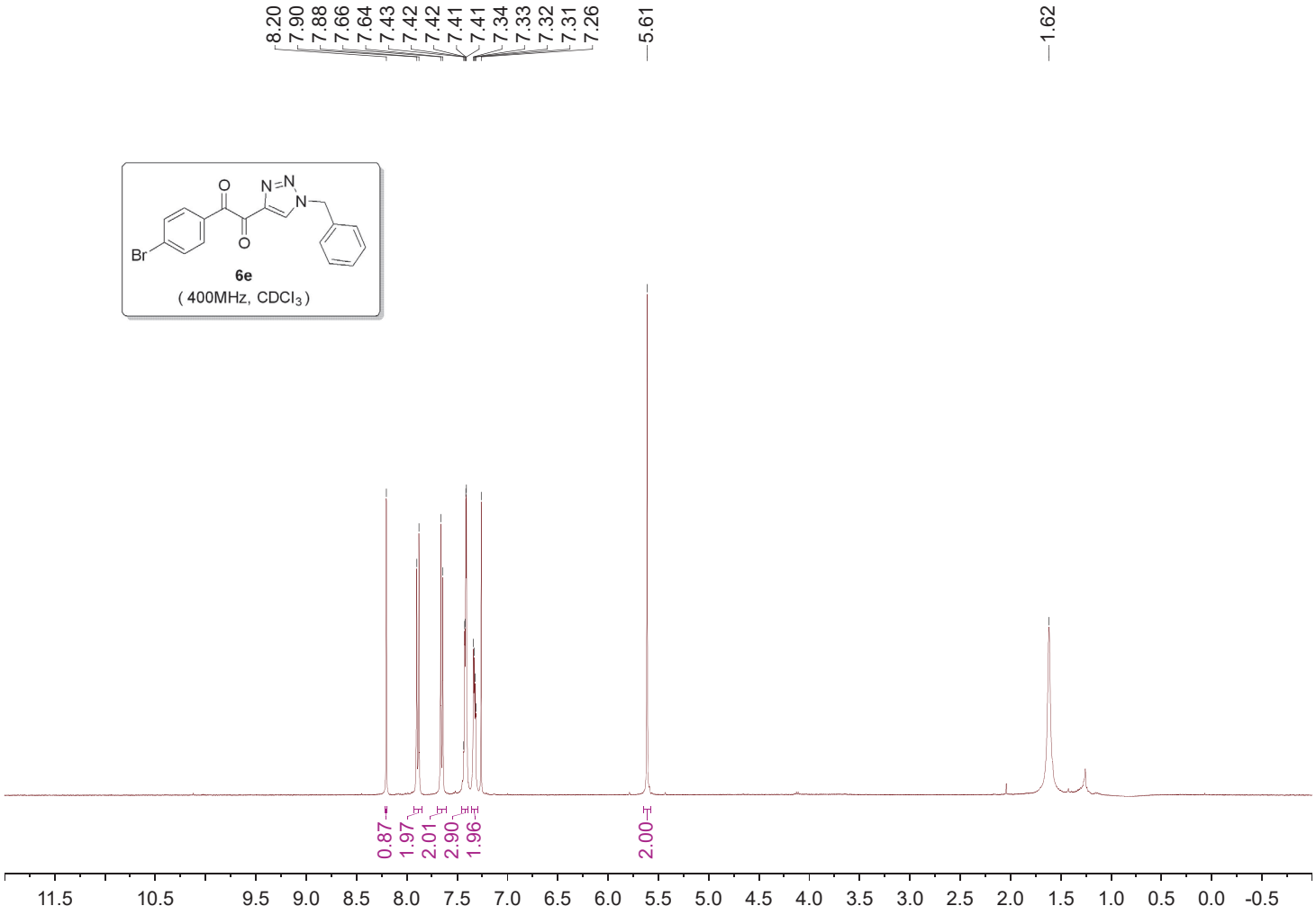
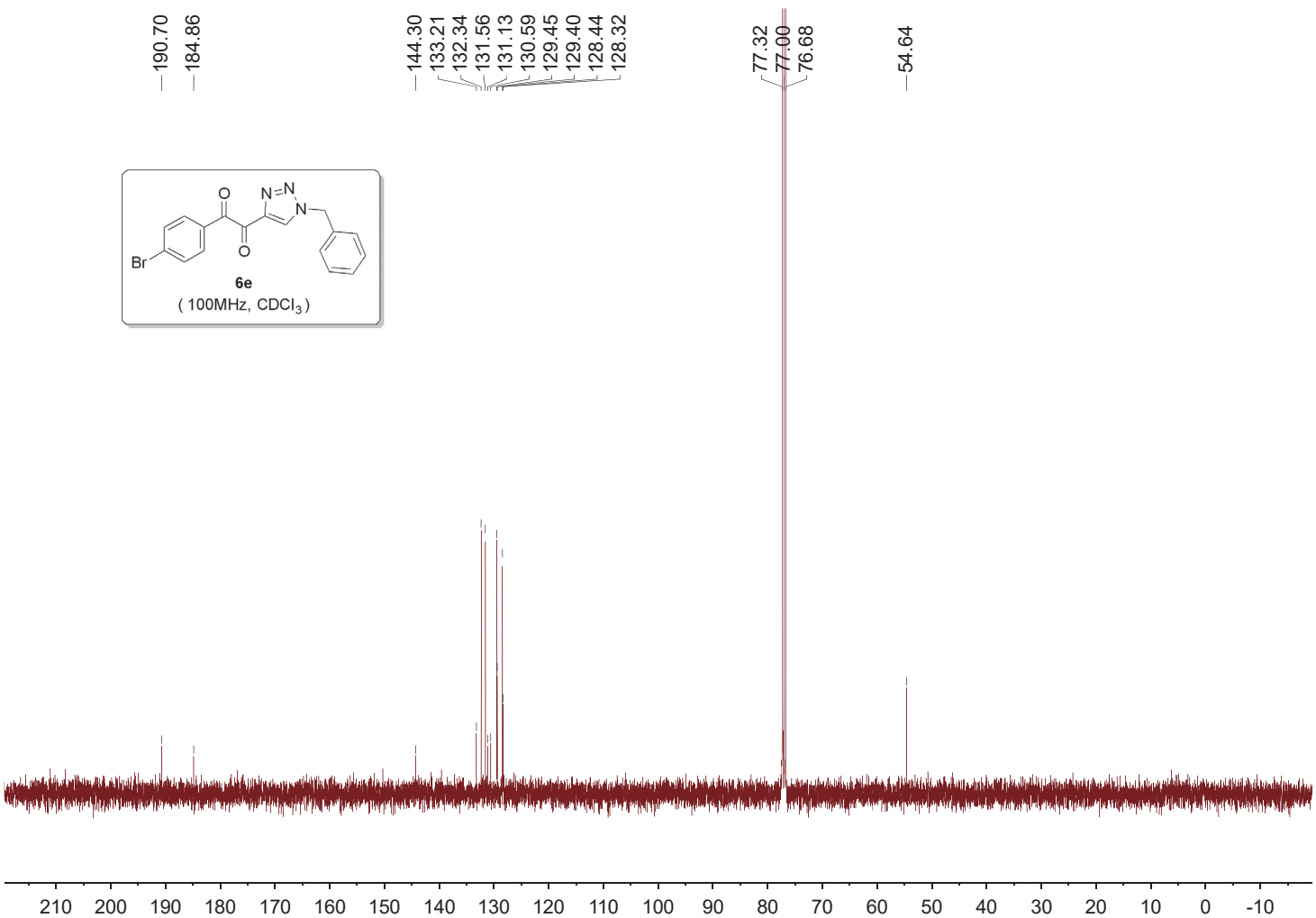
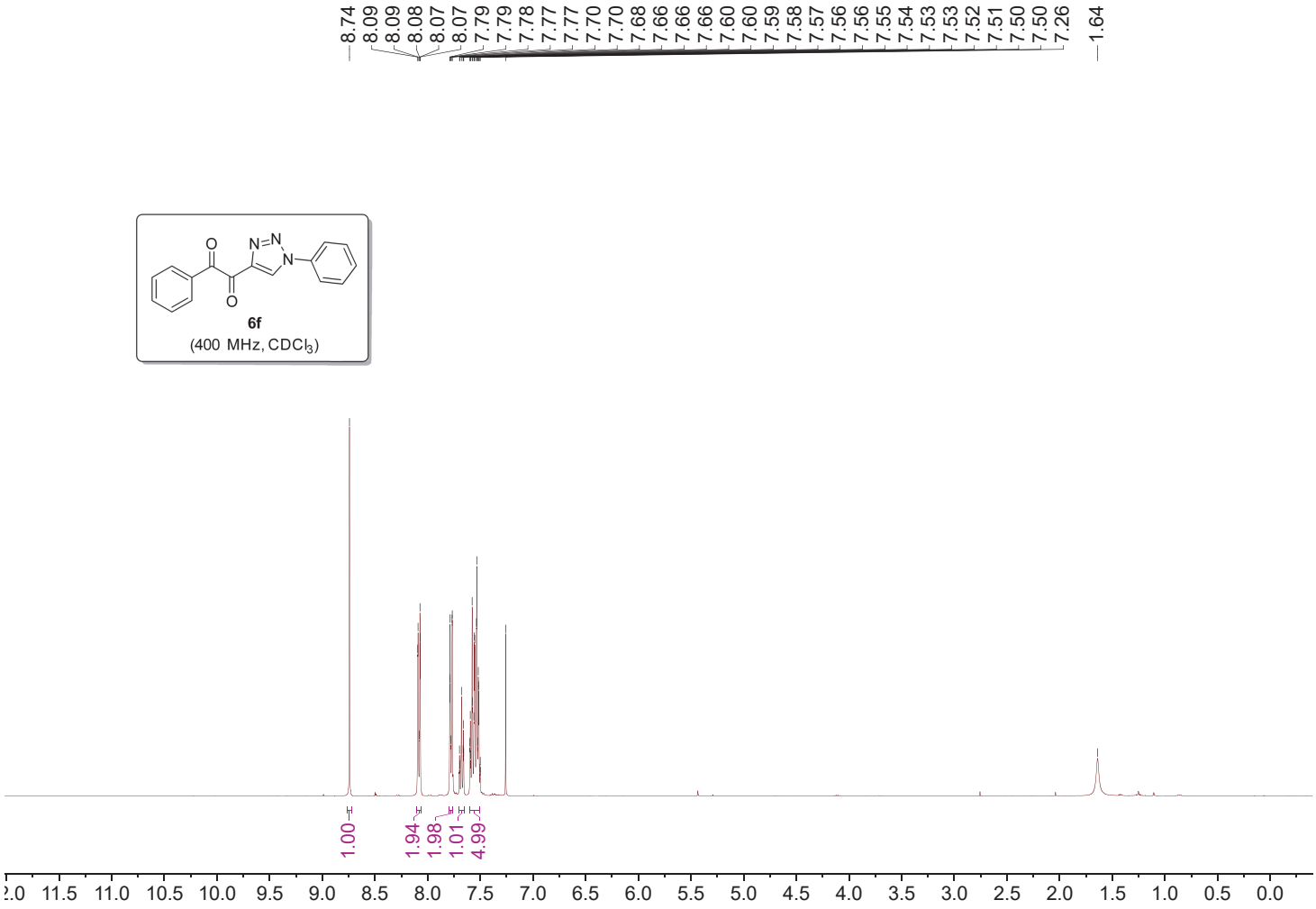
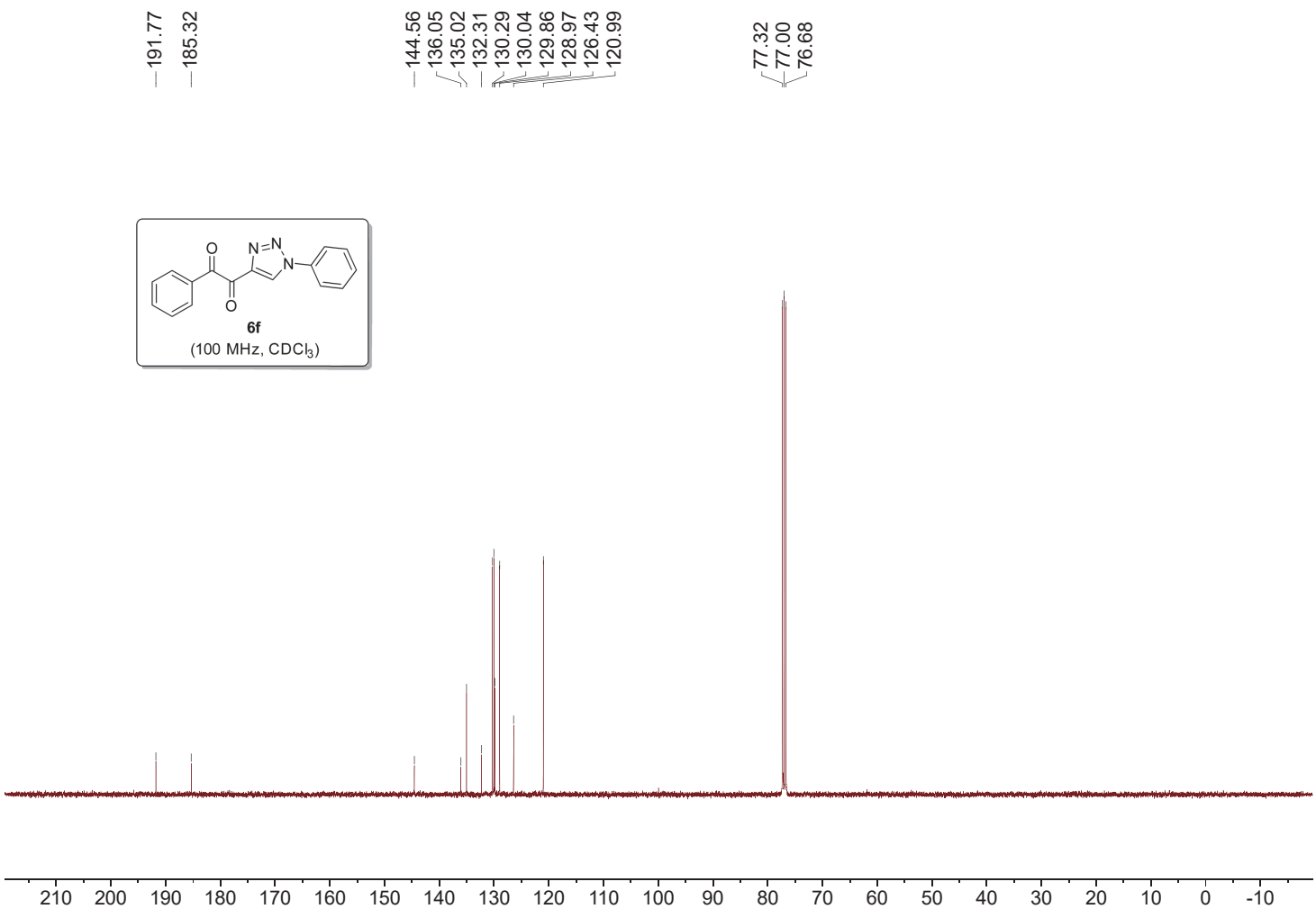
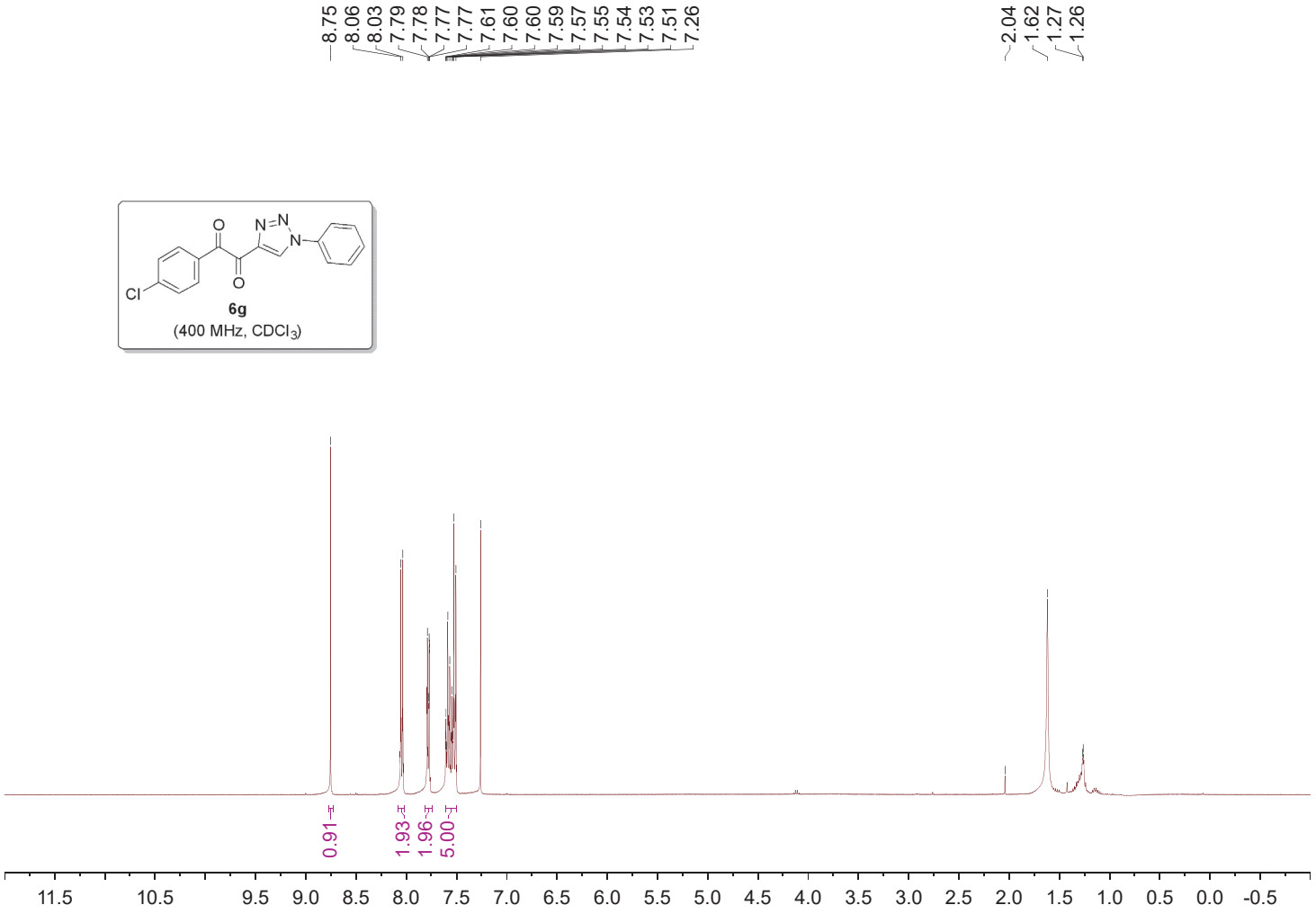
141.68
133.22
131.56
130.73
129.45
129.40
129.35
128.44
128.32
77.32
77.00
76.68
54.64
6d
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

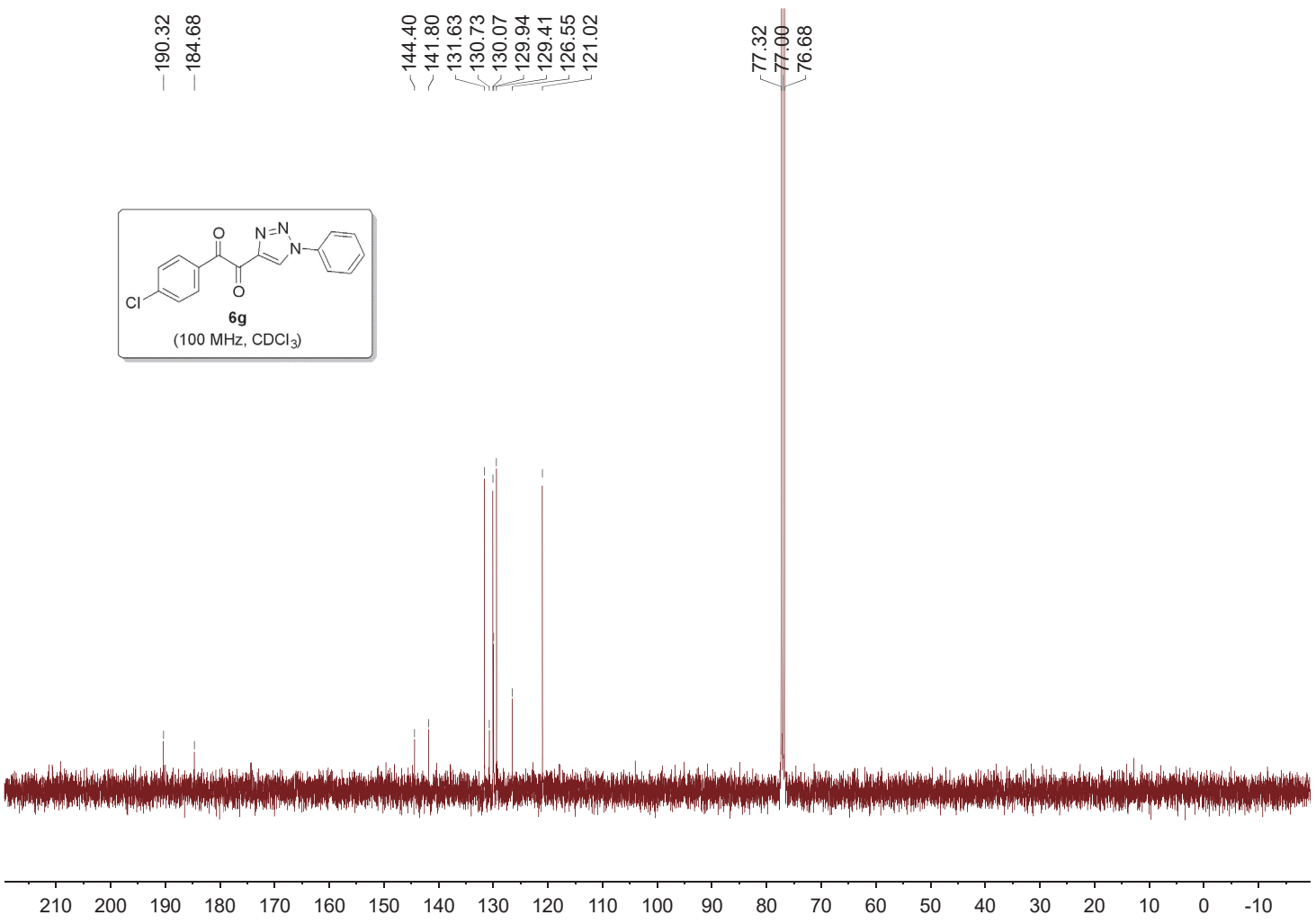

8.20
7.90
7.88
7.66
7.64
7.43
7.42
7.42
7.41
7.41
7.34
7.33
7.32
7.31
7.26
5.61
1.62
Br
6e
(400MHz, CDCl3)
0.87
1.97
2.01
2.90
1.96
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

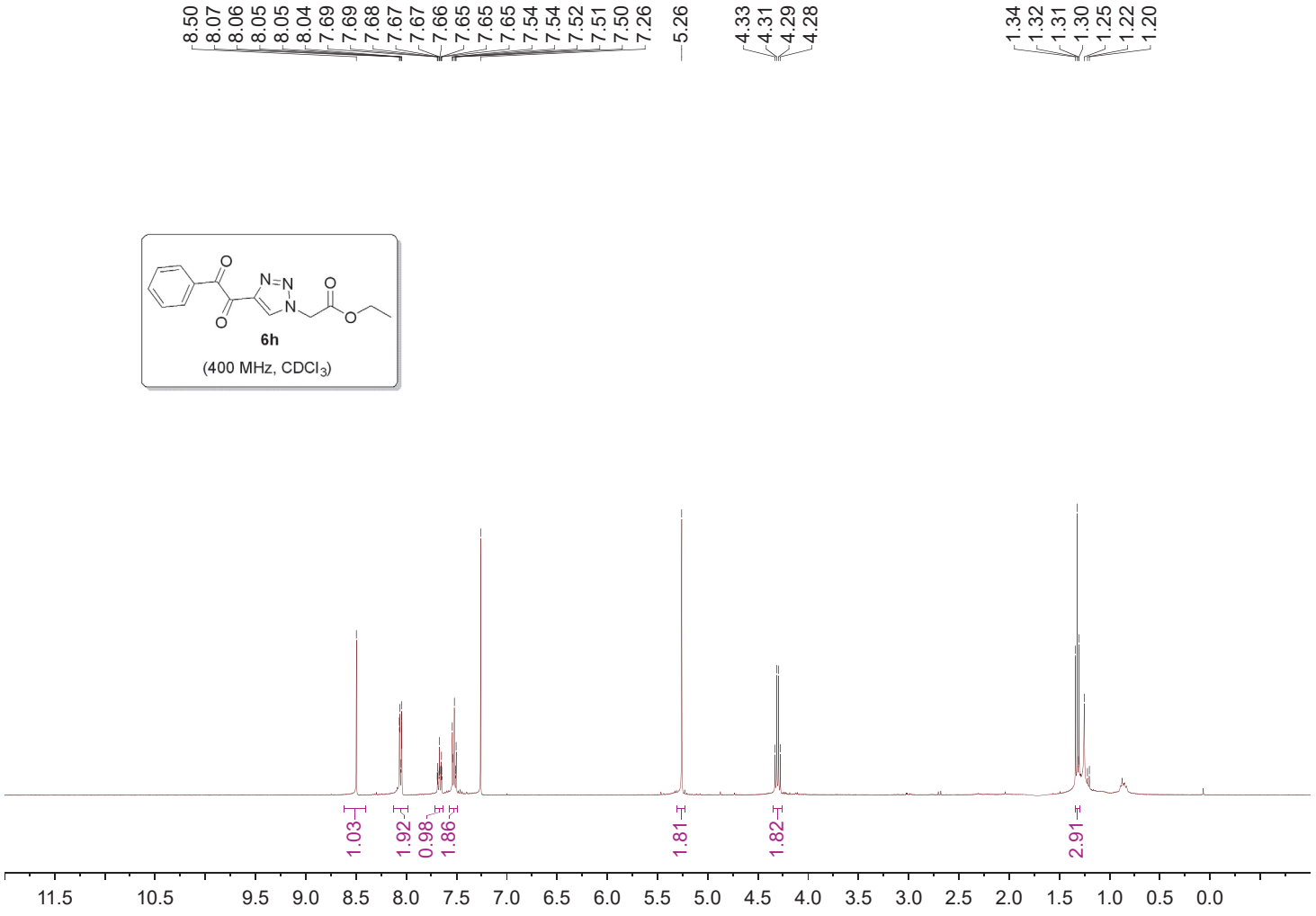

190.70
184.86
144.30
133.21
132.34
131.56
131.13
130.59
129.45
129.40
128.44
128.32
77.32
77.00
76.68
54.64
Br
6e
(100MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

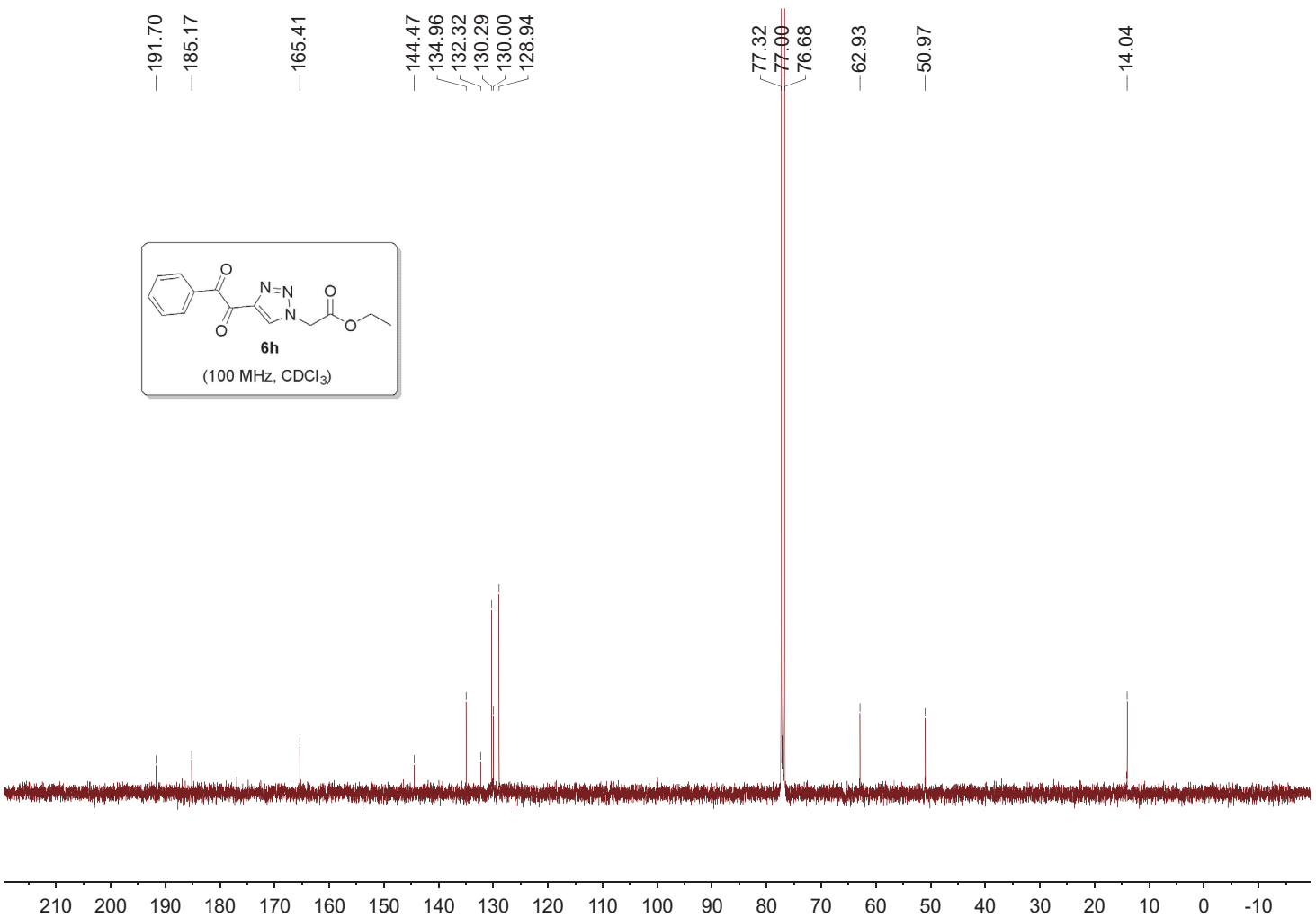

8.74
8.09
8.09
8.08
8.07
8.07
7.79
7.79
7.78
7.77
7.77
7.70
7.70
7.68
7.66
7.66
7.66
7.60
7.60
7.59
7.58
7.57
7.56
7.56
7.55
7.54
7.53
7.53
7.52
7.51
7.50
7.50
7.26
1.64
6f
(400 MHz, CDCl3)
1.00
1.94
1.98
1.01
4.99

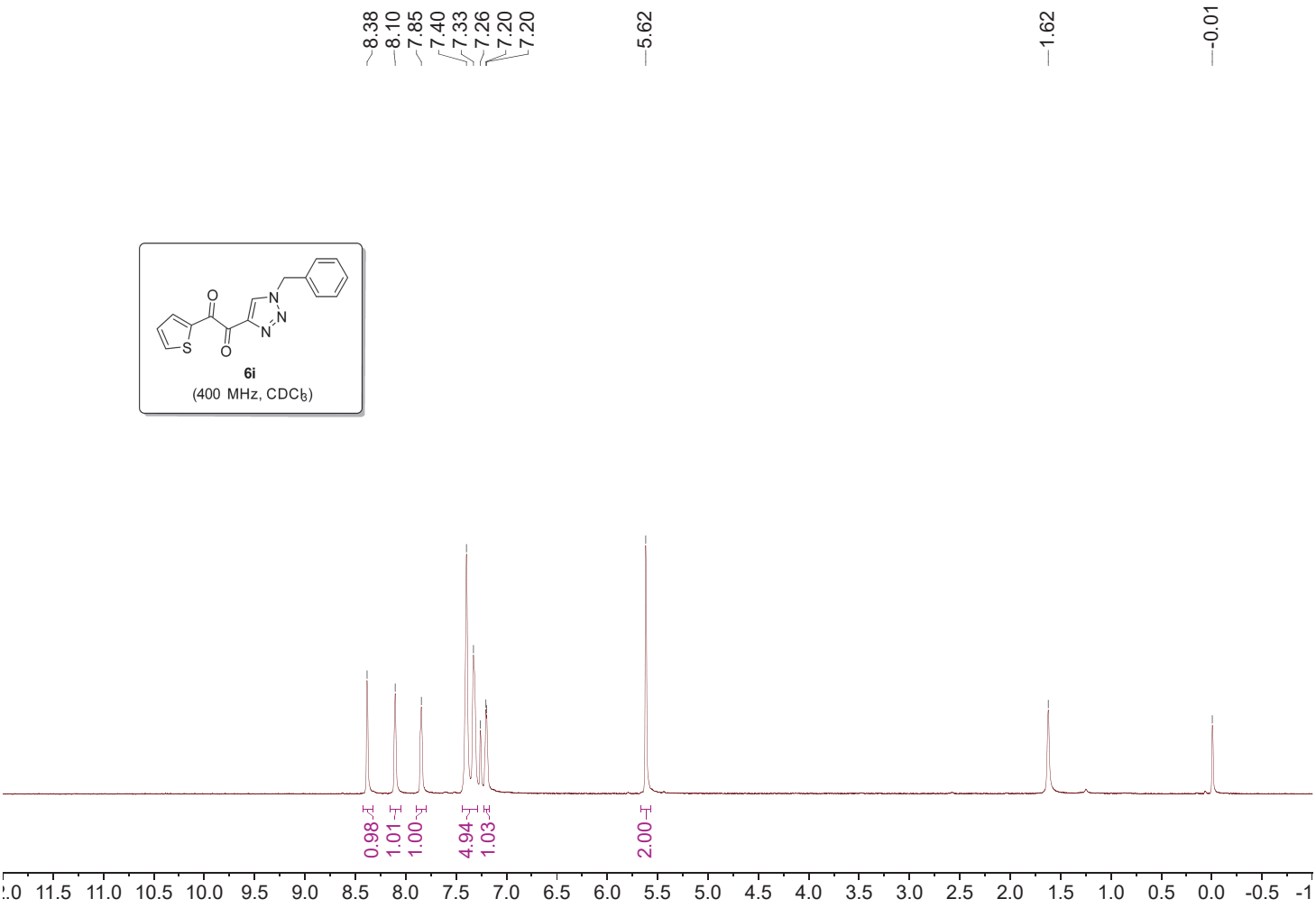

191.77
185.32
144.56
136.05
135.02
132.31
130.29
130.04
129.86
128.97
126.43
120.99
77.32
77.00
76.68
6f
(100 MHz, CDCl3)

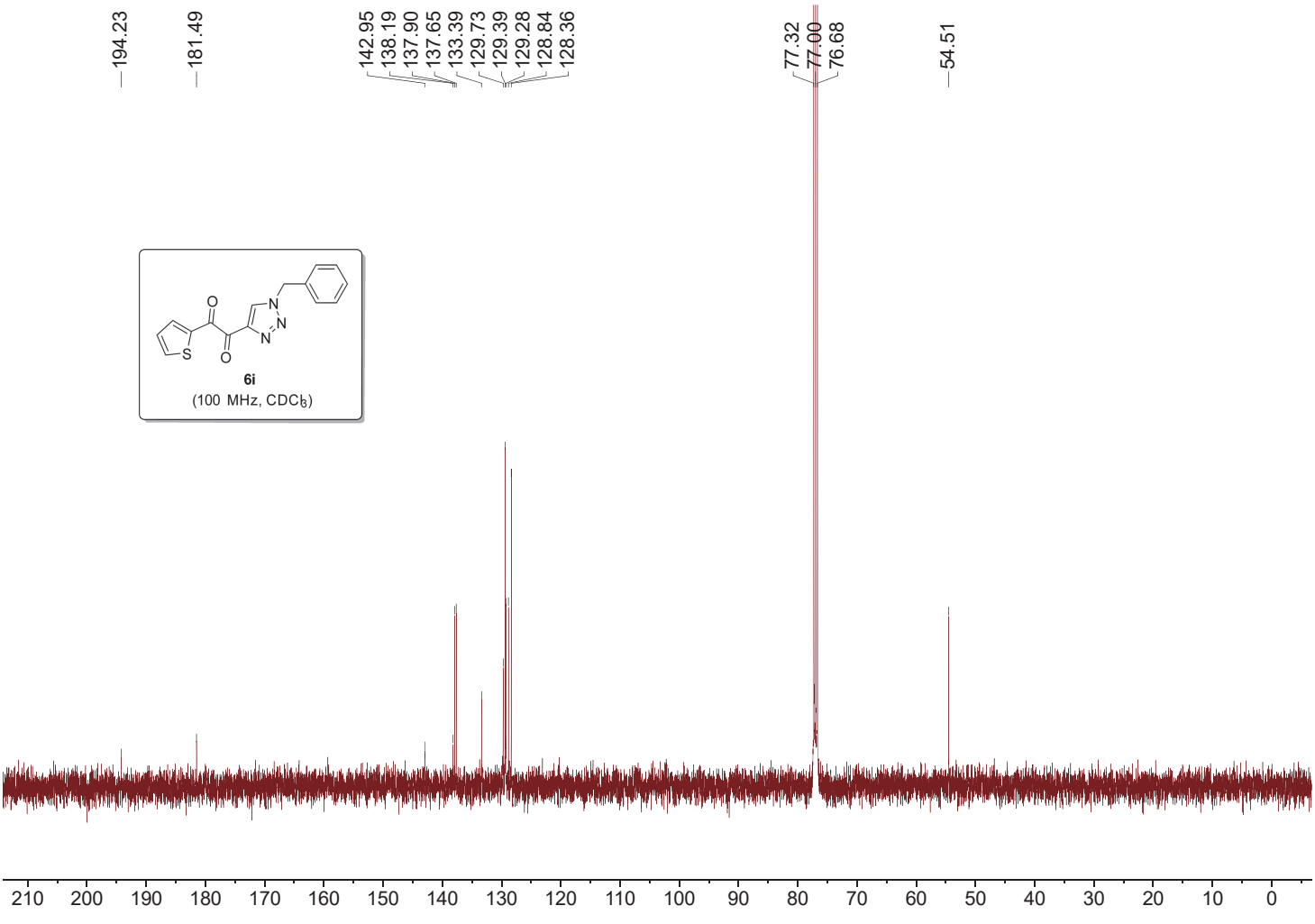

8.75
8.06
8.03
7.79
7.78
7.77
7.77
7.61
7.60
7.60
7.59
7.57
7.55
7.54
7.53
7.51
7.26
2.04
1.62
1.27
1.26
6g
(400 MHz, CDCl3)
0.91
1.93
1.96
5.00

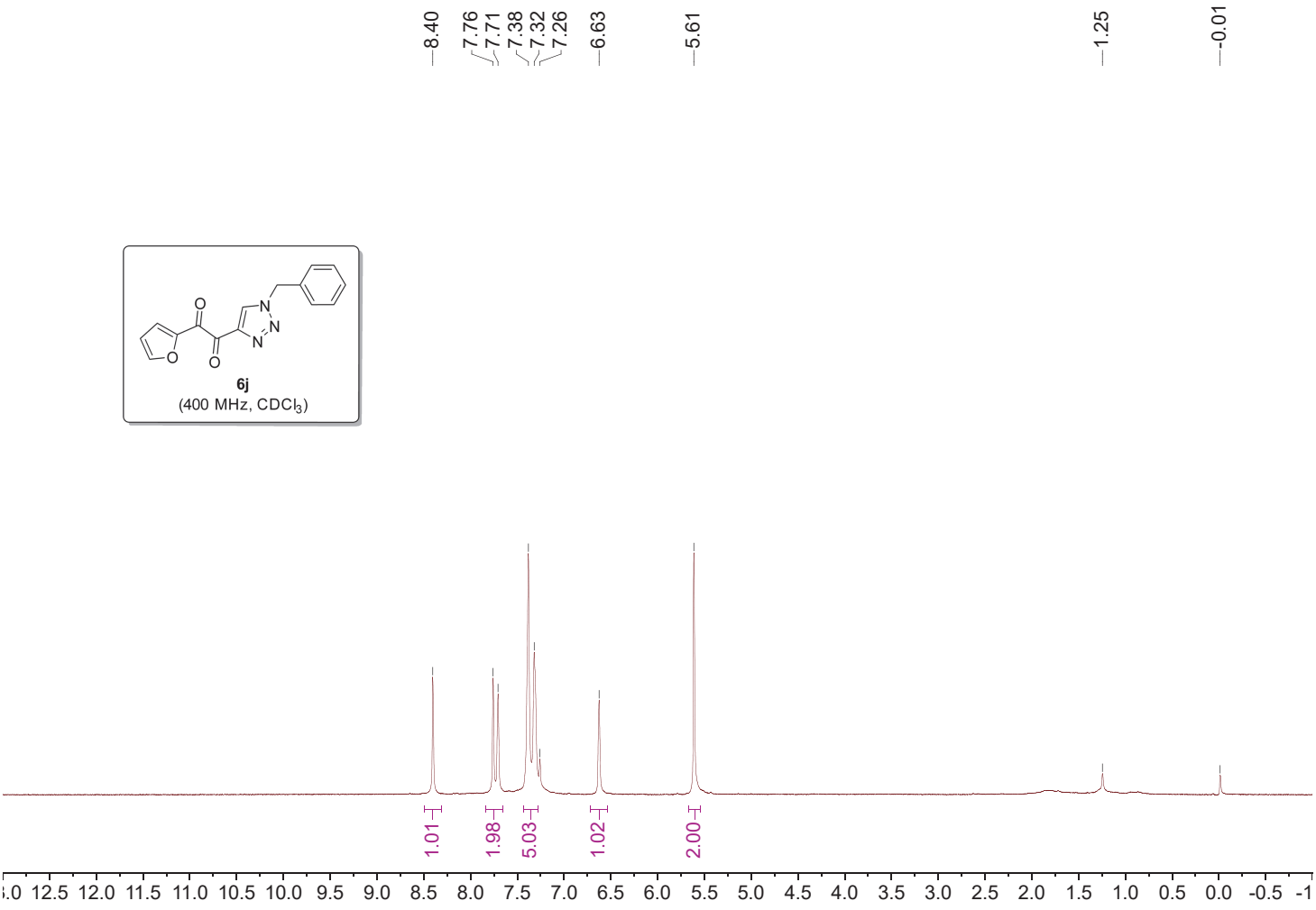

190.32
184.68
144.40
141.80
131.63
130.73
130.07
129.94
129.41
126.55
121.02
77.32
77.00
76.68
6g
(100 MHz, CDCl3)

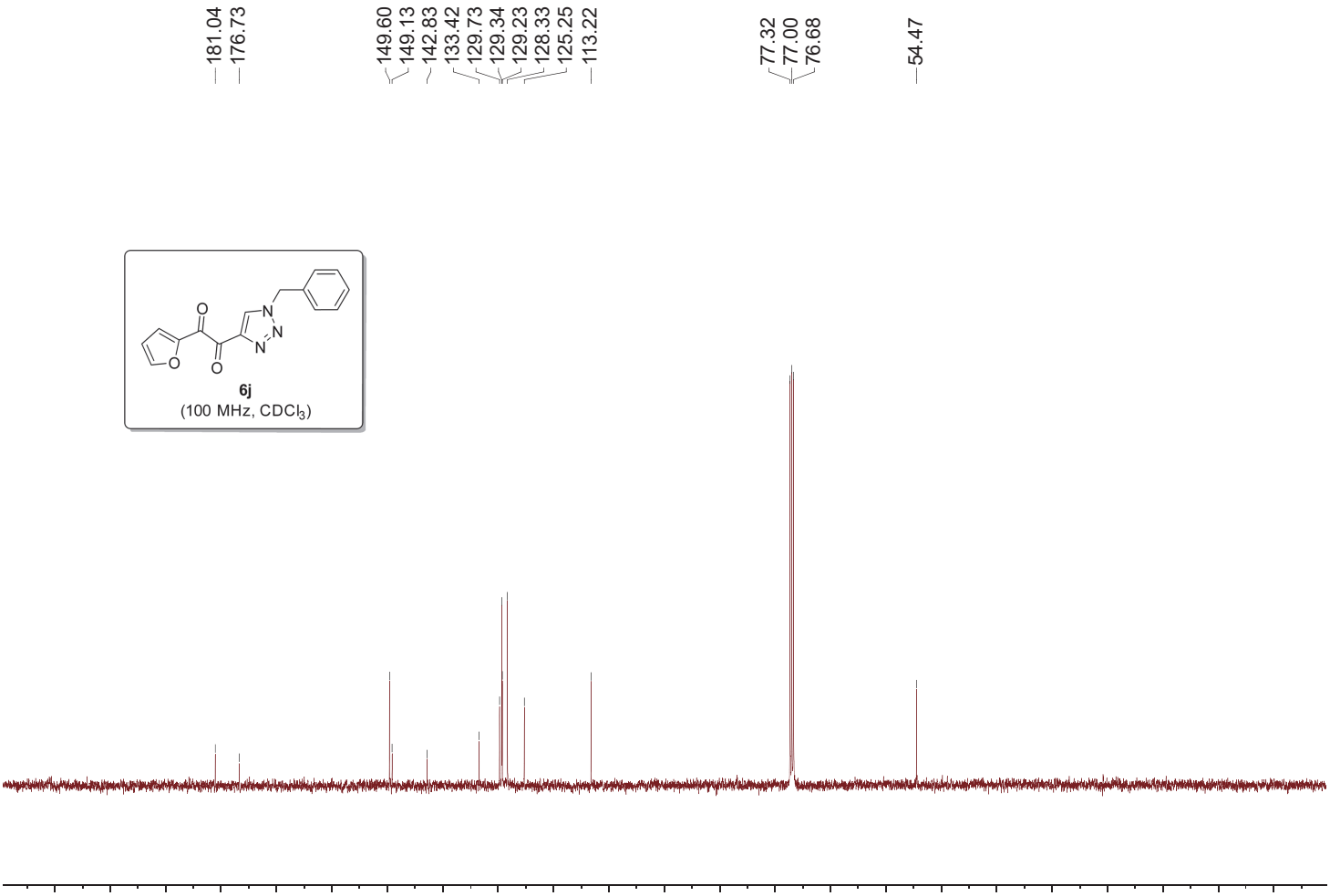

8.50
8.07
8.06
8.05
8.05
8.04
7.69
7.69
7.68
7.67
7.67
7.66
7.65
7.65
7.65
7.54
7.54
7.52
7.51
7.50
7.26
5.26
4.33
4.31
4.29
4.28
1.34
1.32
1.31
1.30
1.25
1.22
1.20
6h
(400 MHz, CDCl3)
1.03
1.92
0.98
1.86
1.81
1.82
2.91
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

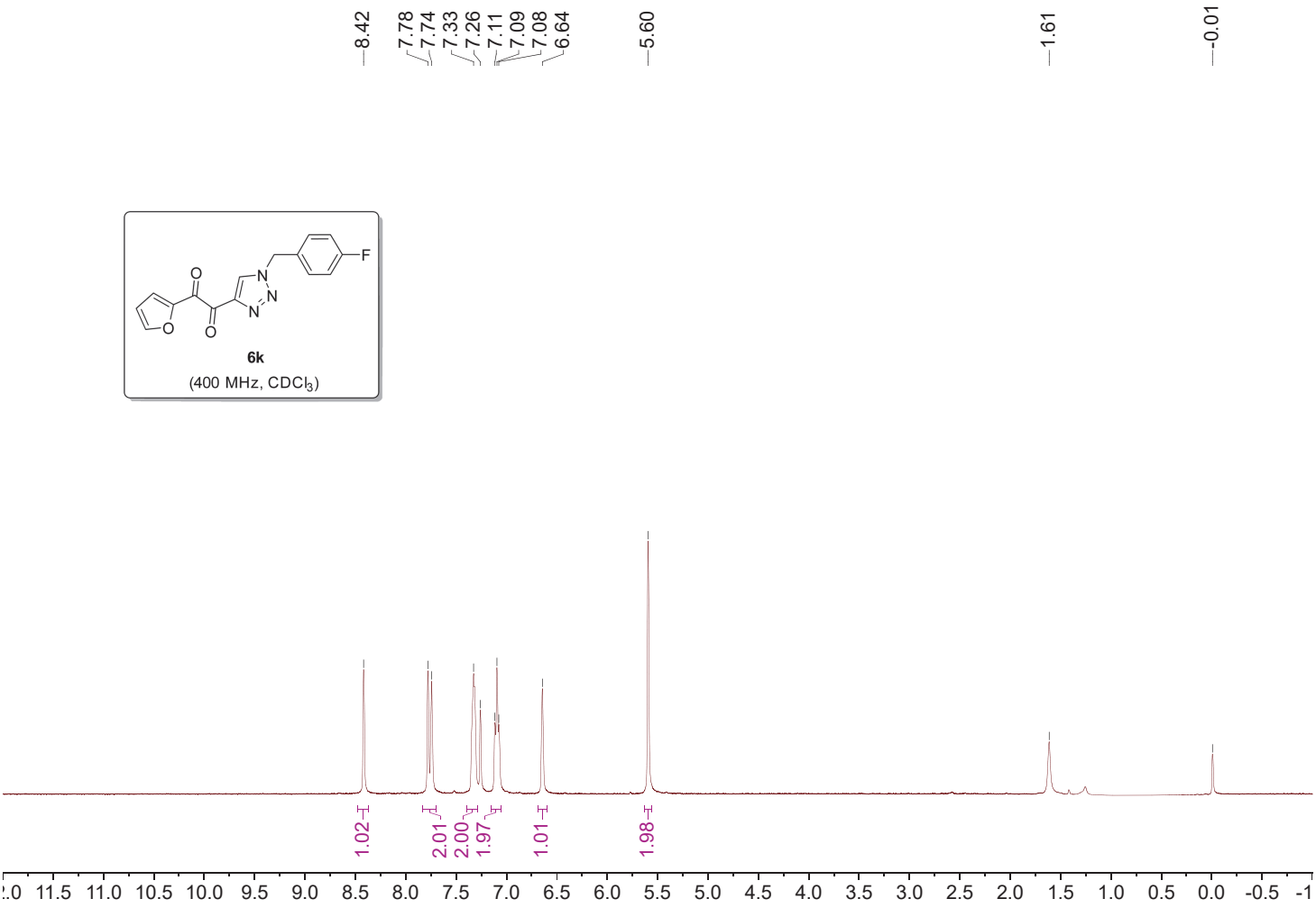

191.70
185.17
165.41
144.47
134.96
132.32
130.29
130.00
128.94
77.32
77.00
76.68
62.93
50.97
14.04
6h
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

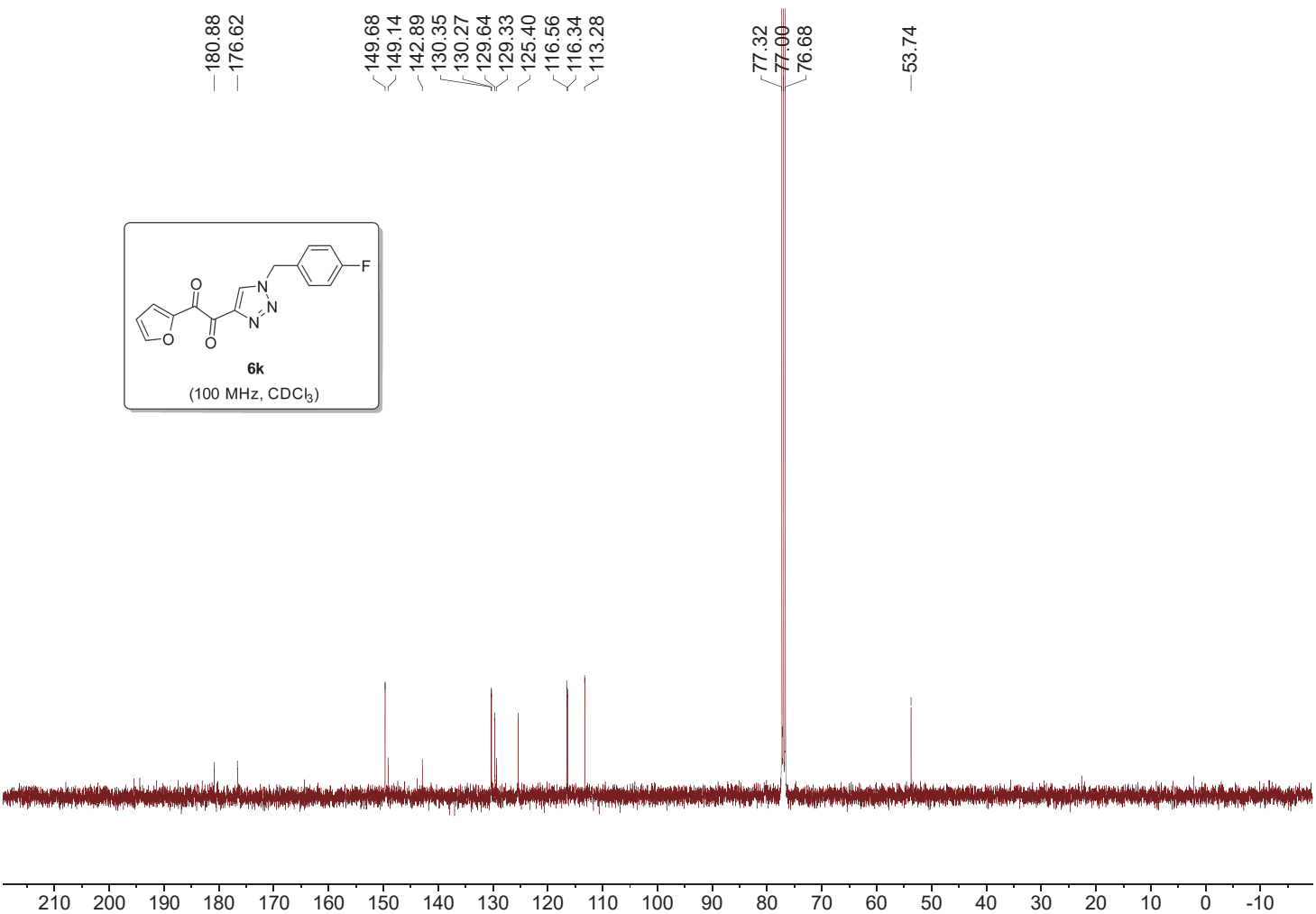

8.38
8.10
7.85
7.40
7.33
7.26
7.20
7.20
5.62
1.62
-0.01
6i
(400 MHz, CDCl3)
0.98
1.01
1.00
4.94
1.03
2.00

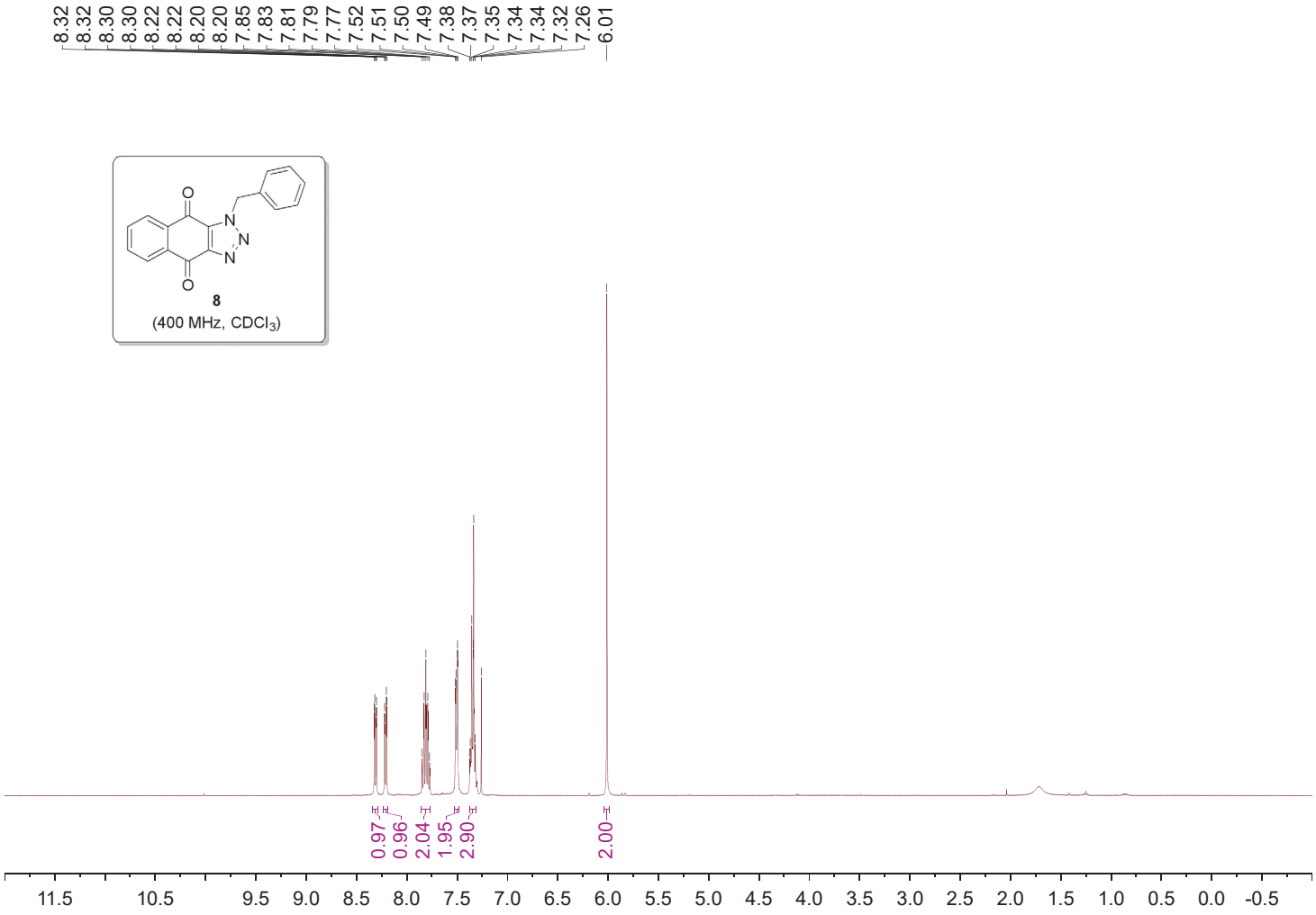

194.23
181.49
142.95
138.19
137.90
137.65
133.39
129.73
129.39
129.28
128.84
128.36
77.32
77.00
76.68
54.51
6i
(100 MHz, CDCl3)

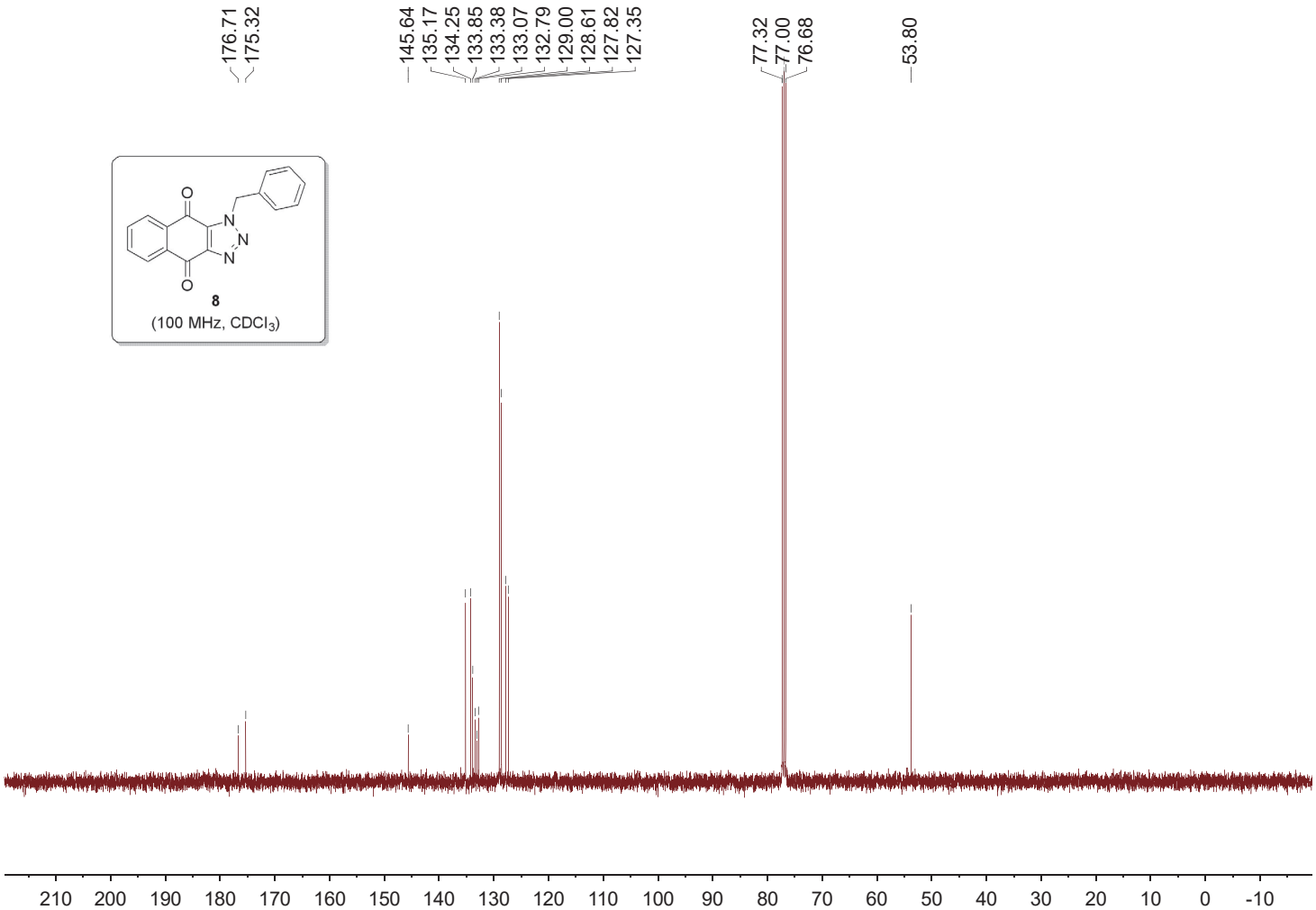

8.40
7.76
7.71
7.38
7.32
7.26
6.63
5.61
1.25
-0.01
6j
(400 MHz, CDCl3)
1.01
1.98
5.03
1.02
2.00


181.04
176.73
149.60
149.13
142.83
133.42
129.73
129.34
129.23
128.33
125.25
113.22
77.32
77.00
76.68
54.47
6j
(100 MHz, CDCl3)


8.42
7.78
7.74
7.33
7.26
7.11
7.09
7.08
6.64
5.60
1.61
-0.01
F
O
N
N
N
O
O
6k
(400 MHz, CDCl3)
1.02
2.01
2.00
1.97
1.01
1.98
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1


180.88
176.62
149.68
149.14
142.89
130.35
130.27
129.64
129.33
125.40
116.56
116.34
113.28
77.32
77.00
76.68
53.74
F
O
N
N
N
O
O
6k
(100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


8.32
8.32
8.30
8.30
8.22
8.22
8.20
8.20
7.85
7.83
7.81
7.79
7.77
7.52
7.51
7.50
7.49
7.38
7.37
7.35
7.34
7.34
7.32
7.26
6.01
8
(400 MHz, CDCl3)
0.97
0.96
2.04
1.95
2.90
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


176.71
175.32
145.64
135.17
134.25
133.85
133.38
133.07
132.79
129.00
128.61
127.82
127.35
77.32
77.00
76.68
53.80
8
(100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10