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Photoinduced synthesis of benzo[*c*]isoxazoles from 2-azidobenzaldehydes

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S1. Reagents and methods.

NMR spectra were recorded on a Bruker Fourier 300 at 303°K. Chemical shifts are reported relative to residue peaks of $CDCl_3$ (7.26 ppm for ^1H and 77.0 ppm for ^{13}C), DMSO-d_6 (2.50 ppm for ^1H and 39.5 ppm for ^{13}C). High-resolution mass spectra (HRMS) spectra were recorded on mass spectrometer Orbitrap LTQ XL with an ESI ion source; needle voltage 3.5 kV/5 kV for negative/positive ions; capillary temperature 350 °C; gas flows — Sheath: 50, Aux: 10; mass range: 100-2000. Samples were introduced via an Agilent 1100 chromatograph without a column. The eluent was water/acetonitrile (1/1 v/v) with 0.1% formic acid additive, flow rate 0.35 mL/min, injection volume 1-10 µL. Macherey-Nagel Silicagel 60 was used for flash chromatography. Thin layer chromatography (TLC) was performed on silica gel 60 F_{254} aluminium sheets (MERCK). Visualization was effected by UV light (254 nm). IUPAC compound names were generated using ChemDraw Software 16.0. Commercially available reagents were used without additional purification. Photocyclization processes were performed on Evoluchem™ PhotoRedOx box (https://hepatochem.com/photoreactors-leds-accessories/photoredox-box/, US10906022). 365 nm (LG, HCK1012-01-006, 25 mW/cm^2) light-emitting diode (LED) lamp from Evoluchem™ was used (Figure S1).

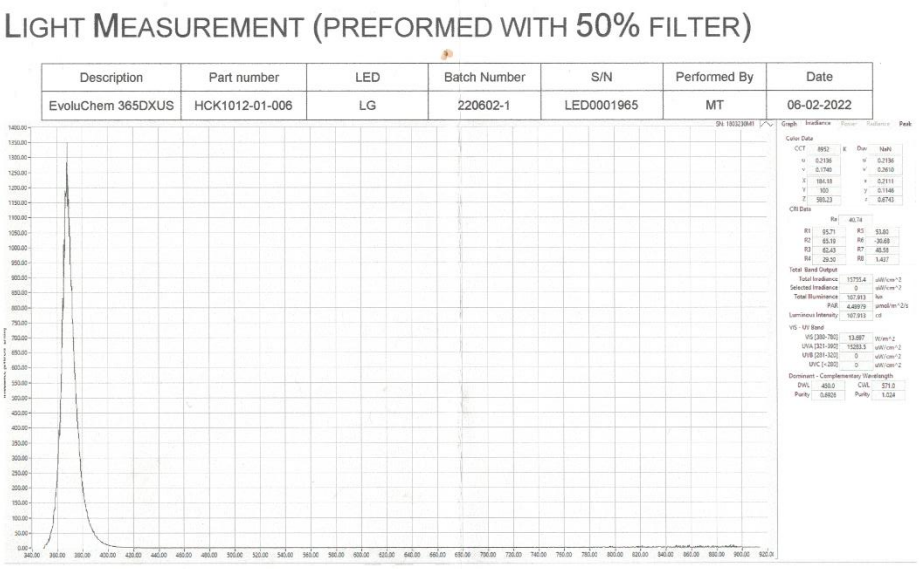


Figure S1. The emission profile of 365 nm LED lamp

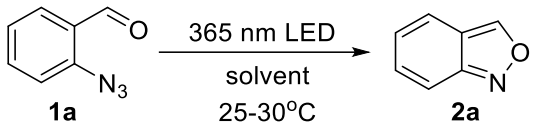
S2. Solvent optimization

Compound **1a** (12 mg) was dissolved in freshly distilled solvent (2 ml) in a glass vial. The resulting solutions were irradiated with 365 nm LED lamp in Evoluchem™ PhotoRedOx box with stirring for 2 h. Then the reaction mixture was evaporated under vacuum or (for DMSO, DMF, DMAC, NMP solutions) dissolved in EtOAc (20 ml), washed with saturated aqueous KCl solution (5x10 mL), dried over anhydrous Na_2SO_4 and evaporated under vacuum. Finally, all residues were analyzed by ^{1}H NMR in DMSO-*d*$_6$. The overall aromatic signal from 6.88 ppm to 7.86 ppm (4H) was used as a standard (400%) as a conditional evaluation method.

The quantity of components was evaluated using the following signals:

- doublet signal on 10.25 ppm (1H) for starting aldehyde **1a**
- doublet signal on 9.80 ppm (1H) for product **2a**

The results are presented in Table S1.



1a **2a**

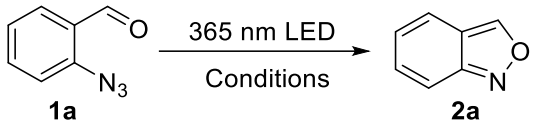
Table S1. Solvents screening results (365 nm, 2h).

Entry	Solvent	**2a**, %	**1a**, %
1	DMSO	71	6
2	DMF	75	7
3	DMAC	70	9
4	NMP	76	9
5	Toluene	0	24
6	$CHCl_3$	0	17
7	CF_3CH_2OH	21	0
8	**1,4-Dioxane**	**78**	**3**
9	MeOH	55	7
10	Pyridine	27	46
11	CH_3CN	66	15

S3. Conditions screening for 1a to 2a conversion

Compound **1a** (72 mg) was dissolved in freshly distilled 1,4-dioxane (12 ml). Next, the 2 mL portions of the resulting solution were irradiated with 365 nm LED lamp in Evoluchem™ PhotoRedOx box with stirring for 2 h or heated at the corresponding temperatures or under reflux for 2 h. Then the reaction mixtures were evaporated under vacuum. Finally, all residues were analyzed by ^{1}H NMR in DMSO-d_6 (see above in Part S2).

The results are presented in Table S2.

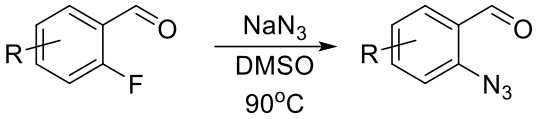


1a **2a**

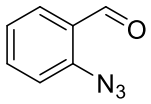
Table S2. Conditions screening for **1a** to **2a** conversion.

Entry	Conditions	**2a**, %	**1a**, %
1	**r.t (with 365 nm)**	**78**	**3**
2	r.t	0	90
3	40°C	0	90
4	60°C	0	90
5	80°C	2	88
6	101.5°C (reflux)	6	83

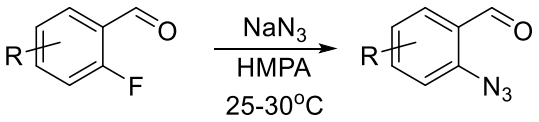
S4. Synthesis of 2-azidobenzaldehydes 1a-i



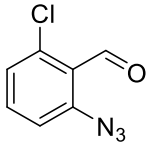
2-Azidobenzaldehyde **1a** was previously obtained by the described method.[1] To a solution of 2-fluorobenzaldehyde (1 eq) in anhydrous DMSO (2 mL/mmol) was added sodium azide (3 eq). The resulted mixture was stirred at 90°C for 6 h. After the completion of the reaction, reaction mixtures were dissolved in EtOAc (4 mL/mmol), washed with saturated KCl solution (5 × 2 mL/mmol), and dried over anhydrous Na_2SO_4. All volatiles were removed in vacuo. Product was purified with flash chromatography (eluent: mixture of hexane and EtOAc, v/v 19:1).



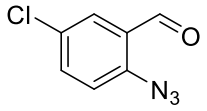
2-azidobenzaldehyde **1a**: beige solid. M.p. 35-37°C. Yield 53% (475 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.36 (d, *J* = 0.8 Hz, 1H), 7.89 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.63 (ddd, *J* = 8.1, 7.3, 1.7 Hz, 1H), 7.33 – 7.18 (m, 2H).



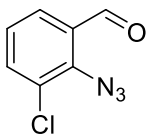
Derivatives of 2-azidobenzaldehyde **1b-i** were previously obtained by the described method.[2] To a solution of corresponding 2-fluorobenzaldehyde (1 eq) in anhydrous HMPA (1.1 mL/mmol) was added sodium azide (1 eq). The resulted mixture was stirred at room temperature for 72-120 h. After the completion of the reaction, reaction mixtures were dissolved in Et_2O (12.5 mL/mmol), washed with water (2 × 12.5 mL/mmol) and saturated KCl solution (2 × 12.5 mL/mmol), and dried over anhydrous Na_2SO_4. All volatiles were removed in vacuo. Product was used in the next step without additional purification.



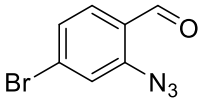
2-azido-6-chlorobenzaldehyde **1b**: white solid. M.p. 83-85°C. Yield 90% (669 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.46 (s, 1H), 7.48 (t, *J* = 8.1 Hz, 1H), 7.28 – 7.15 (m, 2H).



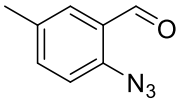
2-azido-5-chlorobenzaldehyde **1c**: white solid. M.p. 90-92°C. Yield 96% (660 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.29 (s, 1H), 7.85 (d, *J* = 2.6 Hz, 1H), 7.57 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.23 (d, *J* = 8.5 Hz, 1H).



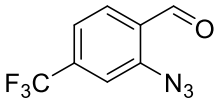
2-azido-3-chlorobenzaldehyde **1d**: beige solid. M.p. 52-54°C. Yield 80% (589 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.41 (s, 1H), 7.79 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.60 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.25 – 7.19 (m, 1H).



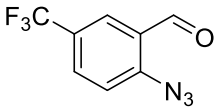
2-azido-4-bromobenzaldehyde **1e**: white solid. M.p. 90-92°C. Yield 73% (592 mg). ^{1}H NMR (300 MHz, Chloroform-d) δ 10.28 (s, 1H), 7.75 (d, *J* = 8.3 Hz, 1H), 7.43 (d, *J* = 1.7 Hz, 1H), 7.38 (dd, *J* = 8.3, 1.6 Hz, 1H).



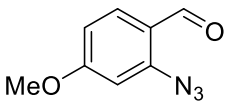
2-azido-5-methylbenzaldehyde **1f**: yellow solid. M.p. 55-57°C. Yield 60% (430 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.32 (s, 1H), 7.69 (d, *J* = 2.2 Hz, 1H), 7.42 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.17 (d, *J* = 8.2 Hz, 1H), 2.37 (s, 3H).



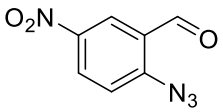
2-azido-4-(trifluoromethyl)benzaldehyde **1g**: beige solid. M.p. 74-76°C. Yield 89% (768 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.39 (s, 1H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.52 – 7.45 (m, 2H).



2-azido-5-(trifluoromethyl)benzaldehyde **1h**: yellow solid. M.p. 52-54°C. Yield 88% (755 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.36 (s, 1H), 8.15 (d, *J* = 2.2 Hz, 1H), 7.85 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.40 (d, *J* = 8.5 Hz, 1H).

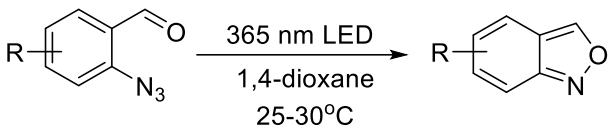


2-azido-4-methoxybenzaldehyde **1i**: beige solid. M.p. 69-71°C. Yield 84% (568 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.19 (d, *J* = 0.8 Hz, 1H), 7.86 (d, *J* = 8.7 Hz, 1H), 6.75 (ddd, *J* = 8.7, 2.3, 0.8 Hz, 1H), 6.70 (d, *J* = 2.3 Hz, 1H), 3.91 (s, 3H).



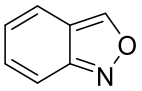
2-azido-5-nitrobenzaldehyde **1j**: orange solid. M.p. 95-97°C. Yield 81% (613 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.36 (s, 1H), 8.73 (d, *J* = 2.7 Hz, 1H), 8.46 (dd, *J* = 8.9, 2.7 Hz, 1H), 7.43 (d, *J* = 8.9 Hz, 1H).

S5. Synthesis of benzo[*c*]isoxazoles 2a-j

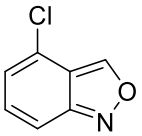


General method

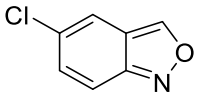
The corresponding starting compound **1** (0.5 mmol) was dissolved in 1,4-dioxane (6.3 mL) in a Schlenk vessel. The resulted mixture was stirred under 365 nm LED lamp in Evoluchem™ PhotoRedOx box. The progress of the reaction was monitored by TLC and ^{1}H NMR. After the completion of the reaction, solvent was removed in vacuum and the product **2** was purified with flash chromatography (eluent: mixture of hexane and EtOAc, v/v 19:1).



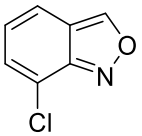
benzo[c]isoxazole **2a**: colorless liquid. Yield 73% (43 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.36 (d, *J* = 0.8 Hz, 1 H), 7.88 (dd, *J* = 1.6, 8.0 Hz, 1 H), 7.63 (ddd, *J* = 1.6, 7.6, 11.2 Hz, 1 H), 7.22–7.30 (m, 2 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.2, 154.5, 131.0, 124.5, 119.7, 118.3, 115.2. The spectral properties corresponded to the literature data.[3]



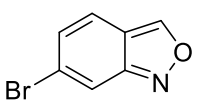
4-chlorobenzo[c]isoxazole **2b**: white solid. M.p. 47-49°C. Yield 83% (63 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.20 (d, *J* = 1.1 Hz, 1H), 7.54 (d, *J* = 9.1 Hz, 1H), 7.27 – 7.17 (m, 1H), 7.01 (d, *J* = 6.9 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.7, 155.0, 131.3, 125.5, 123.4, 119.6, 114.0. The spectral properties corresponded to the literature data.[4]



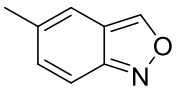
5-chlorobenzo[c]isoxazole **2c**: white solid. M.p. 81-83°C. Yield 71% (54 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.10 (d, *J* = 1.1 Hz, 1H), 7.61 (dt, *J* = 9.4, 1.0 Hz, 1H), 7.58 – 7.55 (m, 1H), 7.28 – 7.21 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.7, 154.2, 132.9, 130.4, 118.5, 117.9, 116.9. The spectral properties corresponded to the literature data.[4]



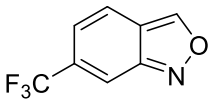
7-chlorobenzo[c]isoxazole **2d**: light yellow solid. M.p. 51-53°C. Yield 83% (63 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.22 (s, 1H), 7.51 (dd, *J* = 8.8, 0.7 Hz, 1H), 7.35 (dd, *J* = 7.0, 0.7 Hz, 1H), 6.97 (dd, *J* = 8.8, 7.0 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.2, 154.9, 130.1, 124.9, 121.4, 119.5, 118.6. The spectral properties corresponded to the literature data.[5]



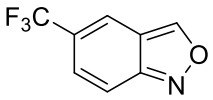
6-bromobenzo[c]isoxazole **2e**: white solid. M.p. 56-58°C. Yield 80% (79 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.12 (d, *J* = 1.1 Hz, 1H), 7.86 (q, *J* = 1.1 Hz, 1H), 7.47 (dd, *J* = 9.2, 0.9 Hz, 1H), 7.10 (dd, *J* = 9.2, 1.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.7, 155.4, 128.9, 125.9, 121.1, 117.3, 116.9. The spectral properties corresponded to the literature data.[6]



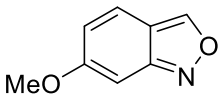
5-methylbenzo[c]isoxazole **2f**: yellow liquid. Yield 67% (44 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.99 (s, 1H), 7.53 (d, *J* = 9.2 Hz, 1H), 7.29 – 7.26 (m, 1H), 7.14 (dd, *J* = 9.2, 1.5 Hz, 1H), 2.36 (s, 3H). ^{1}H NMR (300 MHz, DMSO) δ 9.64 (s, 1H), 7.57 (d, *J* = 9.2 Hz, 1H), 7.48 – 7.37 (m, 1H), 7.25 (dd, *J* = 9.2, 1.5 Hz, 1H), 2.32 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.7, 153.2, 134.5, 134.0, 118.7, 116.7, 114.9, 21.9. The spectral properties corresponded to the literature data.[6]



6-(trifluoromethyl)benzo[c]isoxazole **2g**: white solid. M.p. 46-48°C. Yield 79% (74 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.27 (d, *J* = 1.1 Hz, 1H), 8.02 (p, *J* = 1.2 Hz, 1H), 7.74 (d, *J* = 9.2 Hz, 1H), 7.18 (dd, *J* = 9.1, 1.3 Hz, 1H). 13C NMR (75 MHz, Chloroform-d) δ 155.8, 155.0, 133.1 (q, *J* = 32.5 Hz), 123.5 (q, *J* = 272.9 Hz), 121.8, 120.4 (q, *J* = 2.8 Hz), 118.6, 114.4 (q, *J* = 5.3 Hz). The spectral properties corresponded to the literature data.[4]



5-(trifluoromethyl)benzo[c]isoxazole **2h**: yellow liquid. Yield 81% (75 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.32 (s, 1H), 7.99 (q, *J* = 1.4 Hz, 1H), 7.77 (d, *J* = 9.4 Hz, 1H), 7.45 (dd, *J* = 9.4, 1.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.3, 155.9, 127.2 (q, *J* = 32.7 Hz), 126.8 (q, *J* = 2.7 Hz), 123.7 (q, *J* = 271.9 Hz), 119.4 (q, *J* = 5.4 Hz), 117.0, 116.9. HRMS (ESI) m/z $[M+H]^+$ calcd for $C_8H_5F_3NO$: 188.0318, found: 188.0317.

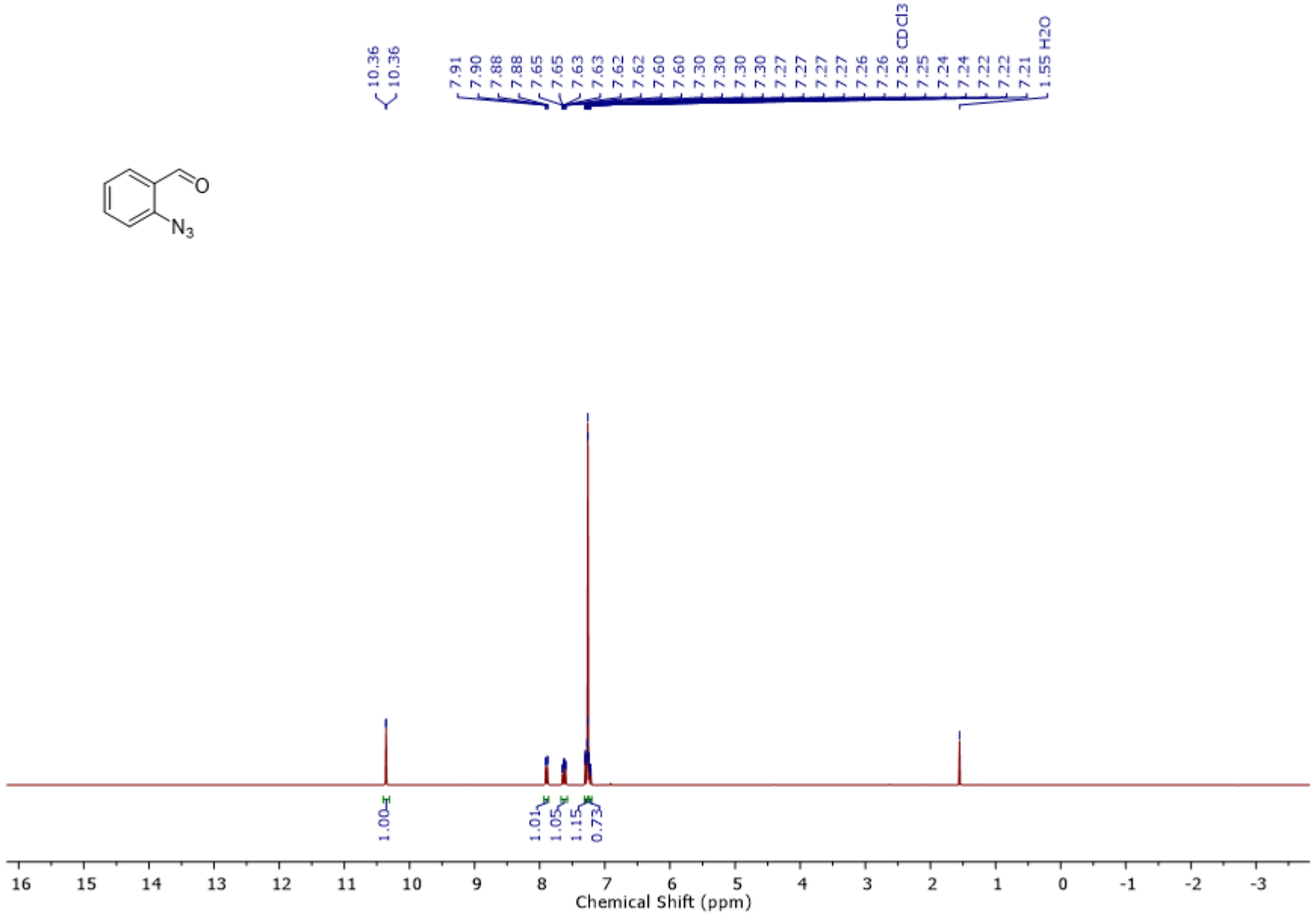


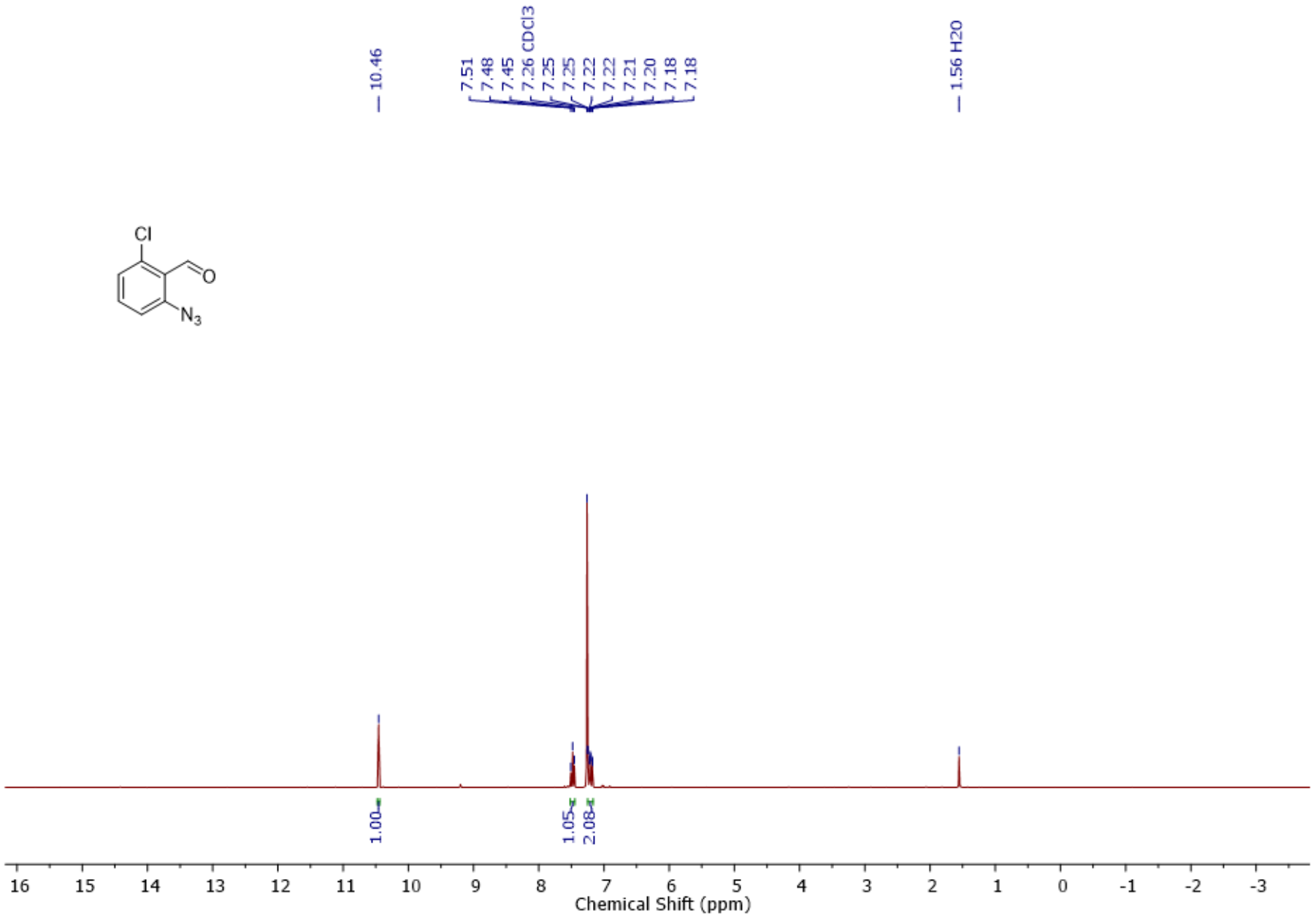
6-methoxybenzo[c]isoxazole **2i**: yellow liquid. Yield 79% (24 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.94 (d, *J* = 0.9 Hz, 1H), 7.46 – 7.40 (m, 1H), 6.77 – 6.65 (m, 2H), 3.88 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.7, 157.6, 153.7, 121.9, 120.5, 115.3, 89.5, 55.6.

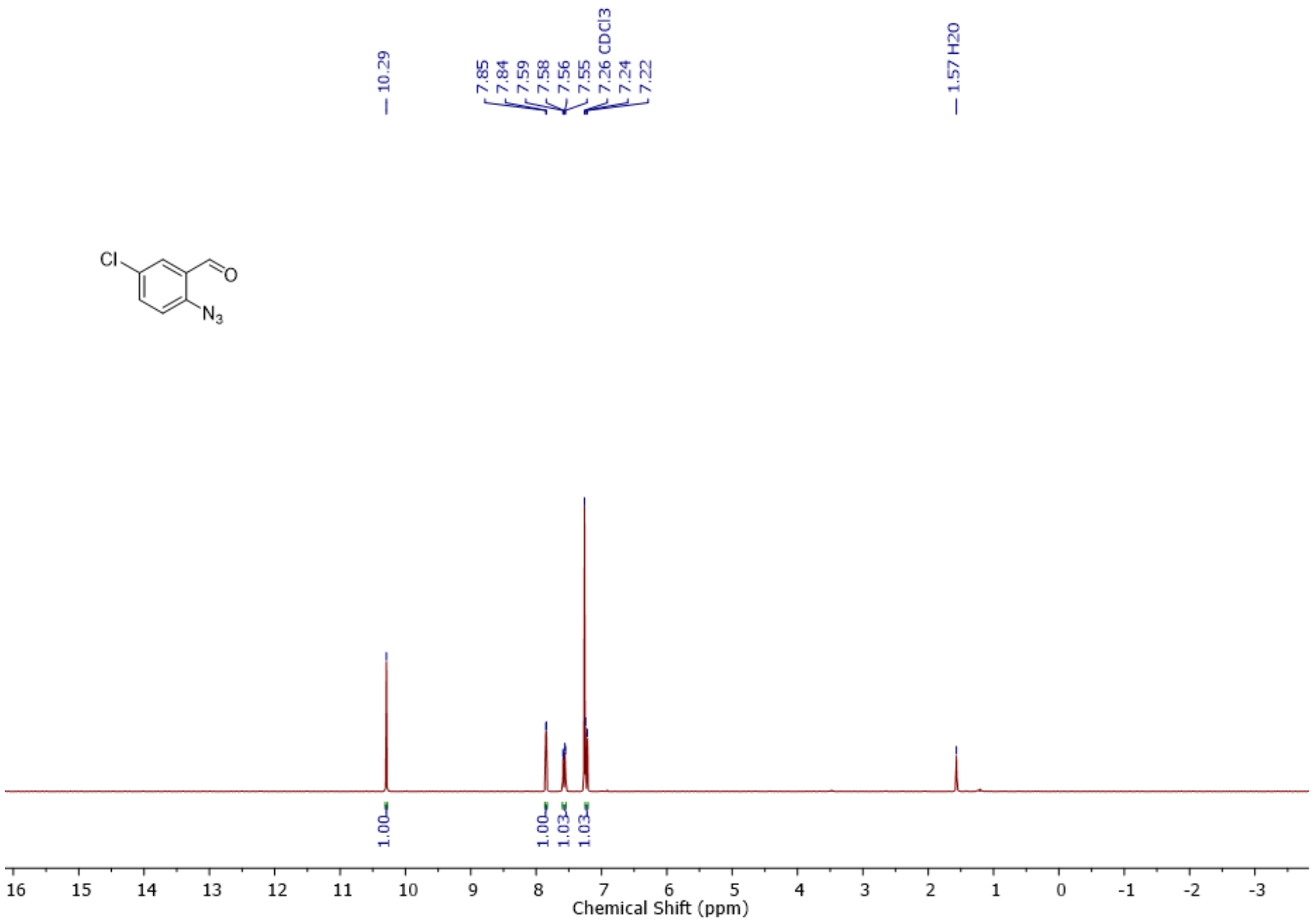
S7. References.

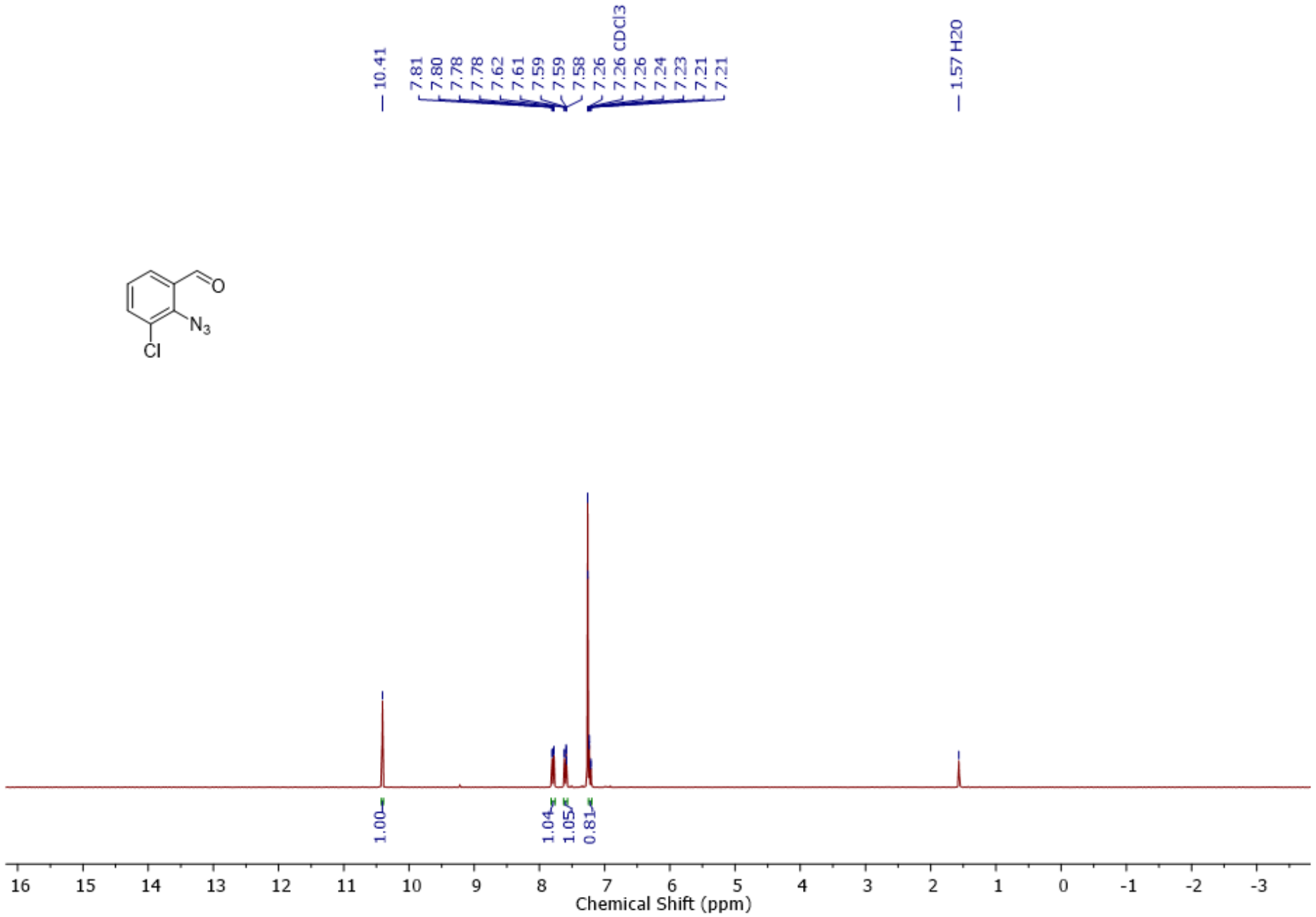
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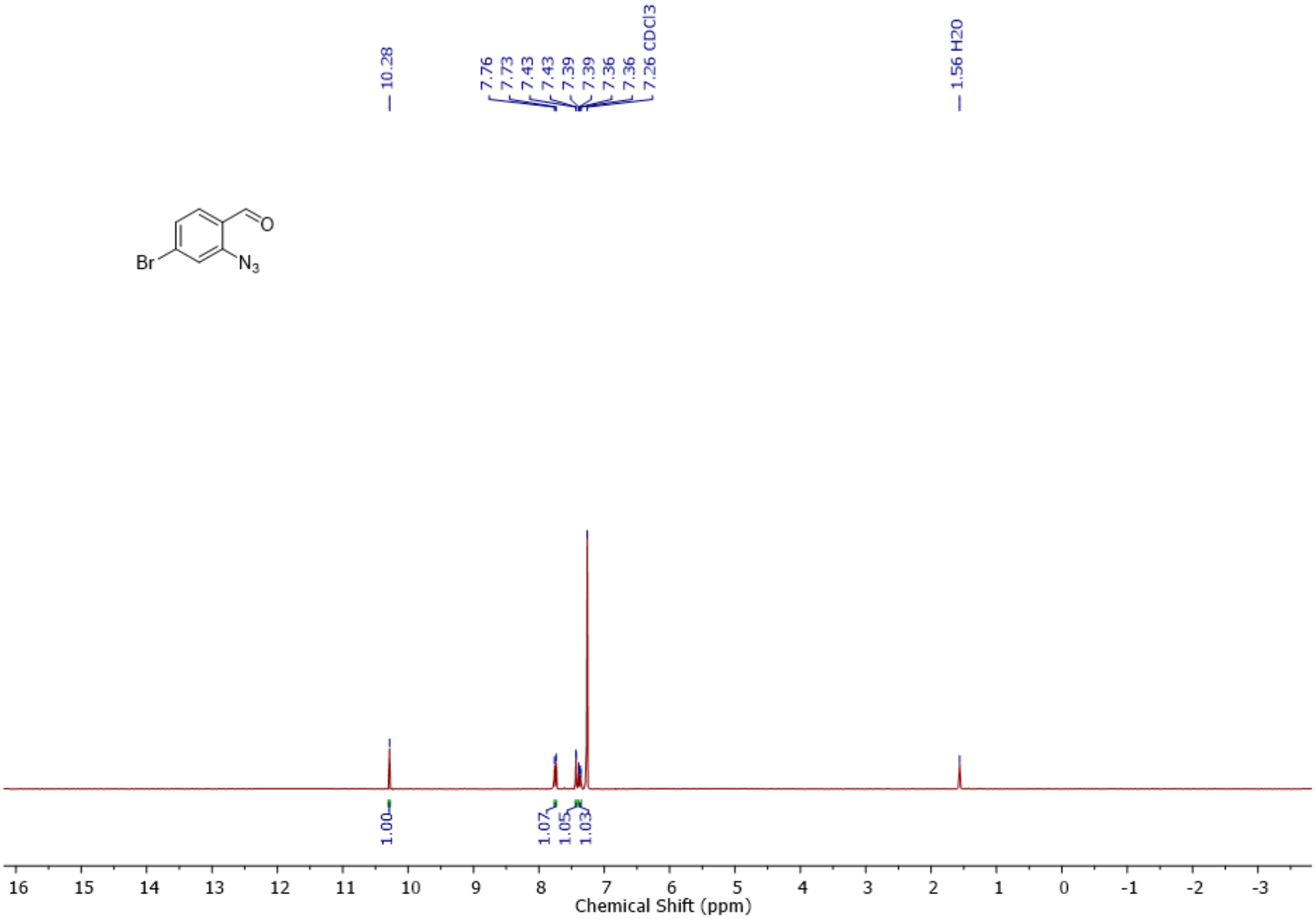
S8. Copies of ^{1}H and ^{13}C spectra

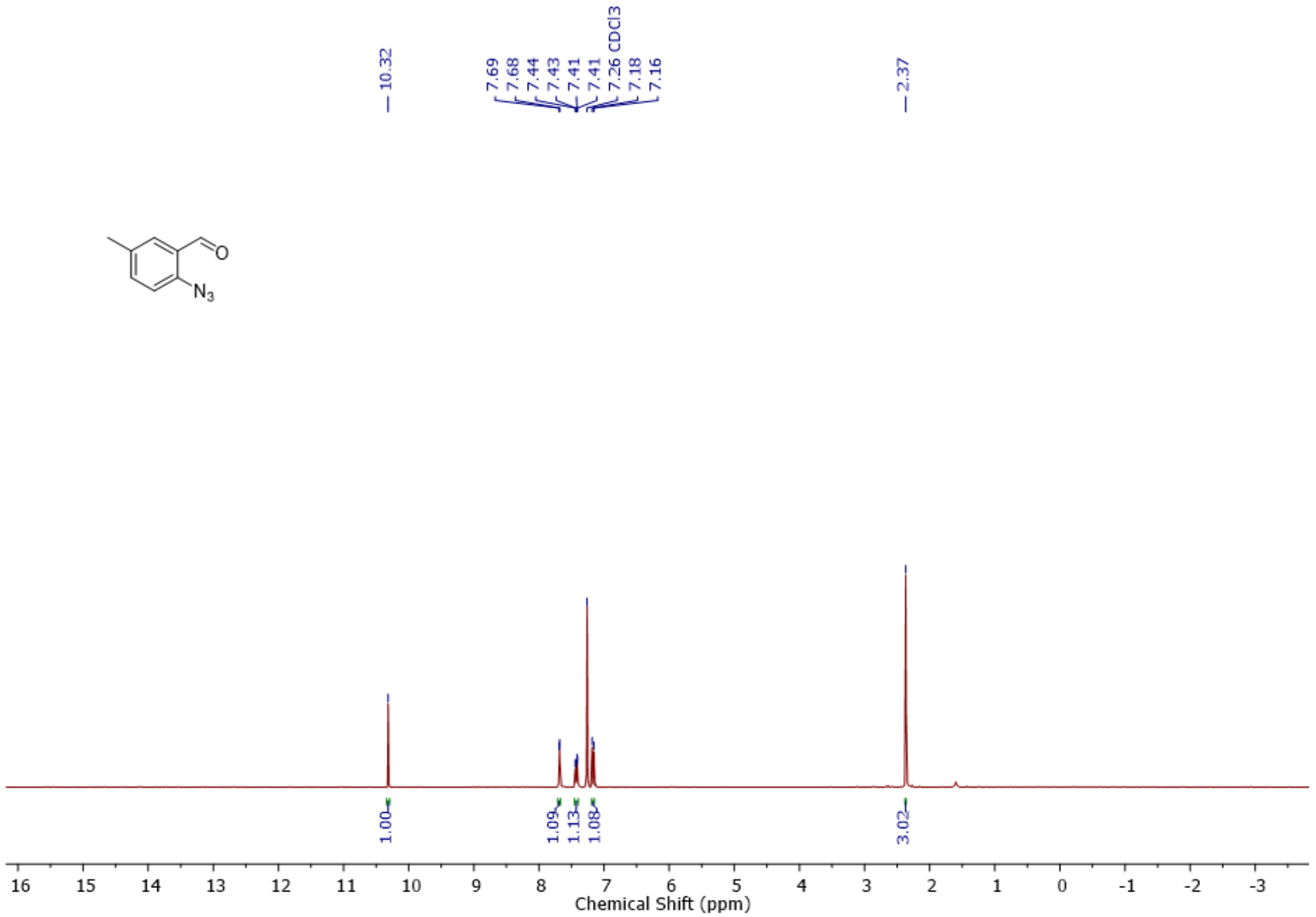


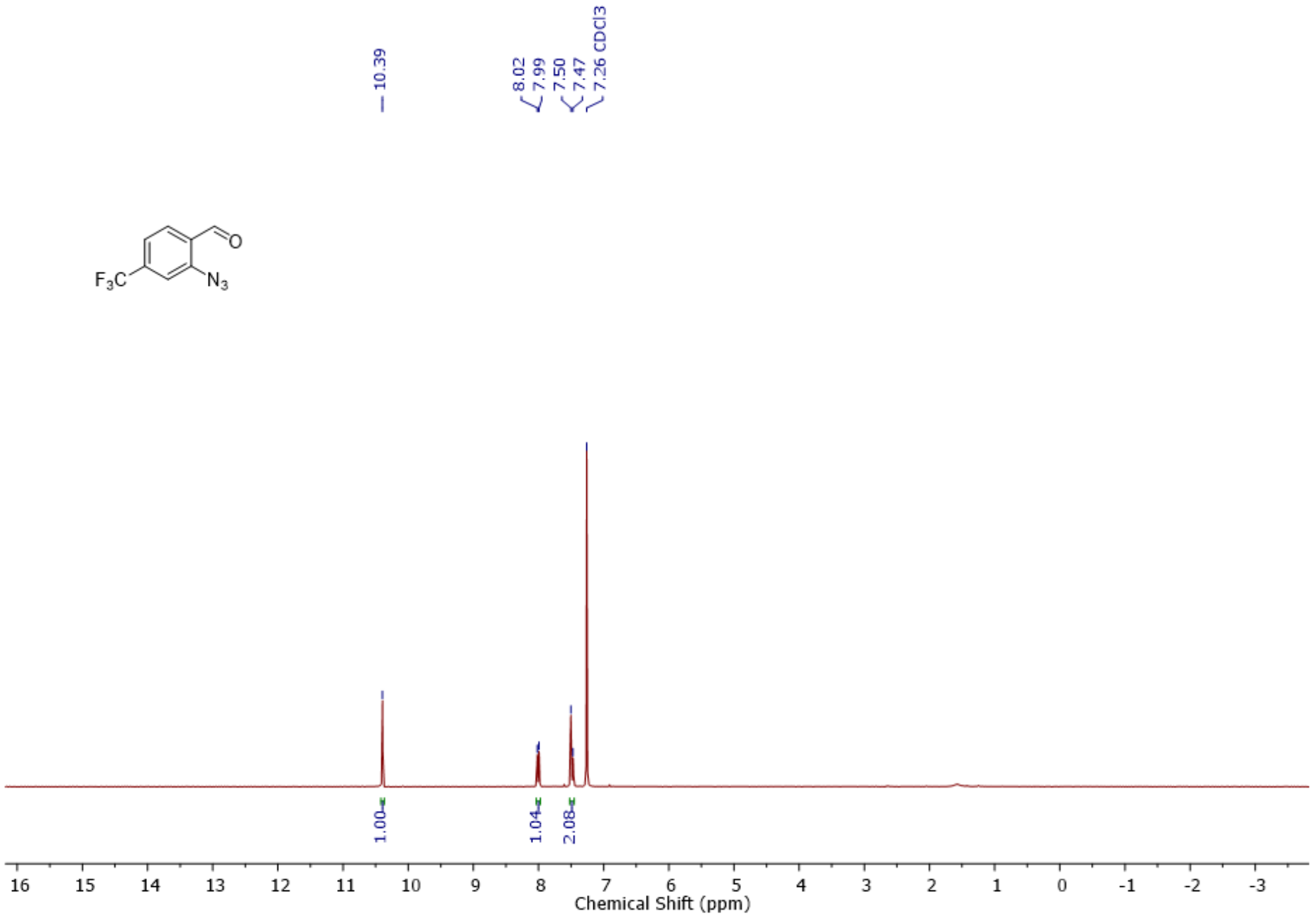

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7.51
7.48
7.45
7.26 CDCl3
7.25
7.25
7.22
7.22
7.21
7.20
7.18
7.18
1.56 H2O
Cl
O
N3
1.00
1.05
2.08
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
Chemical Shift (ppm)

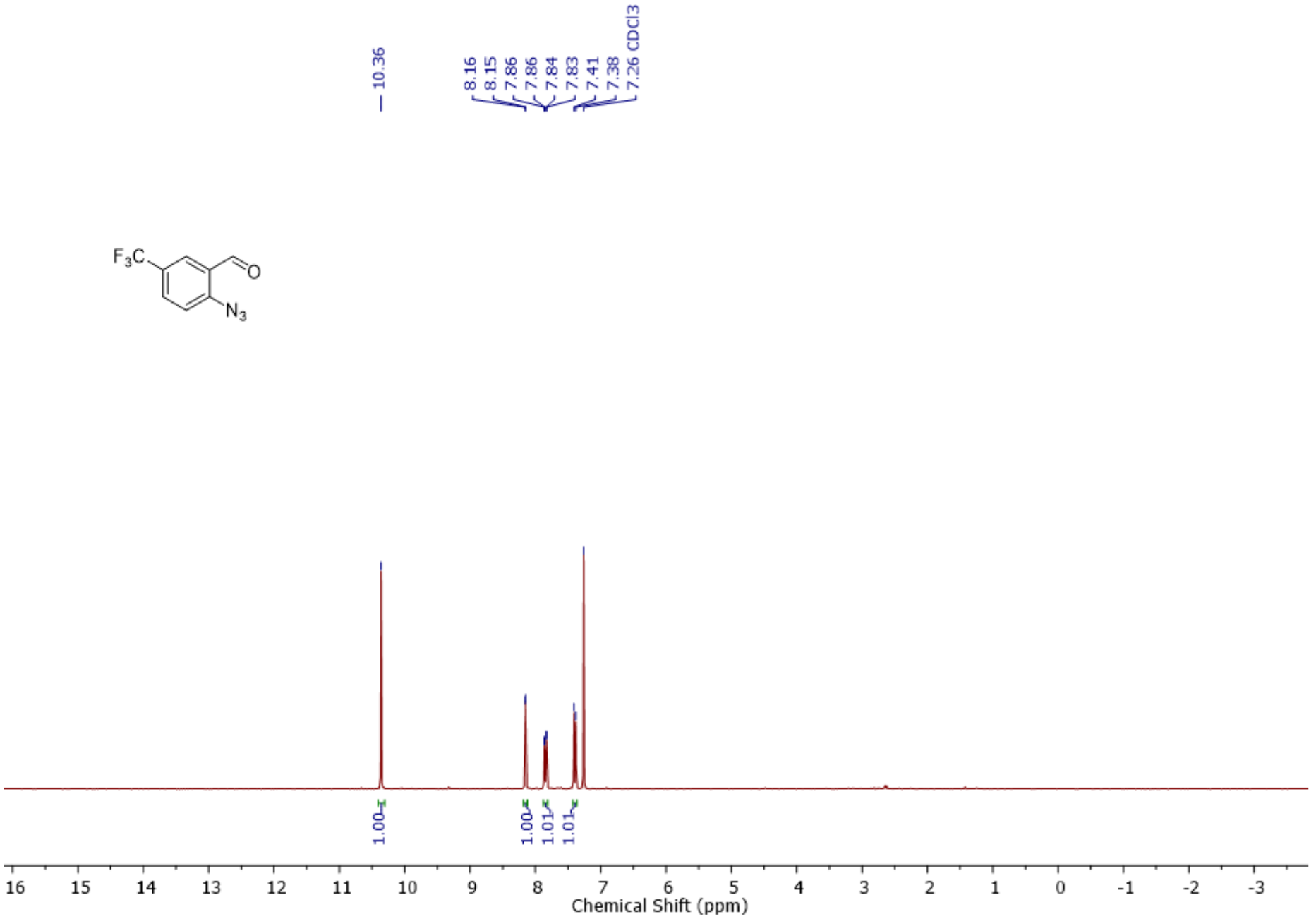

10.29
7.85
7.84
7.59
7.58
7.56
7.55
7.26 CDCl3
7.24
7.22
1.57 H20
Cl
O
N3
1.00
1.00
1.03
1.03
16
15
14
13
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7
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5
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3
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1
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-2
-3
Chemical Shift (ppm)

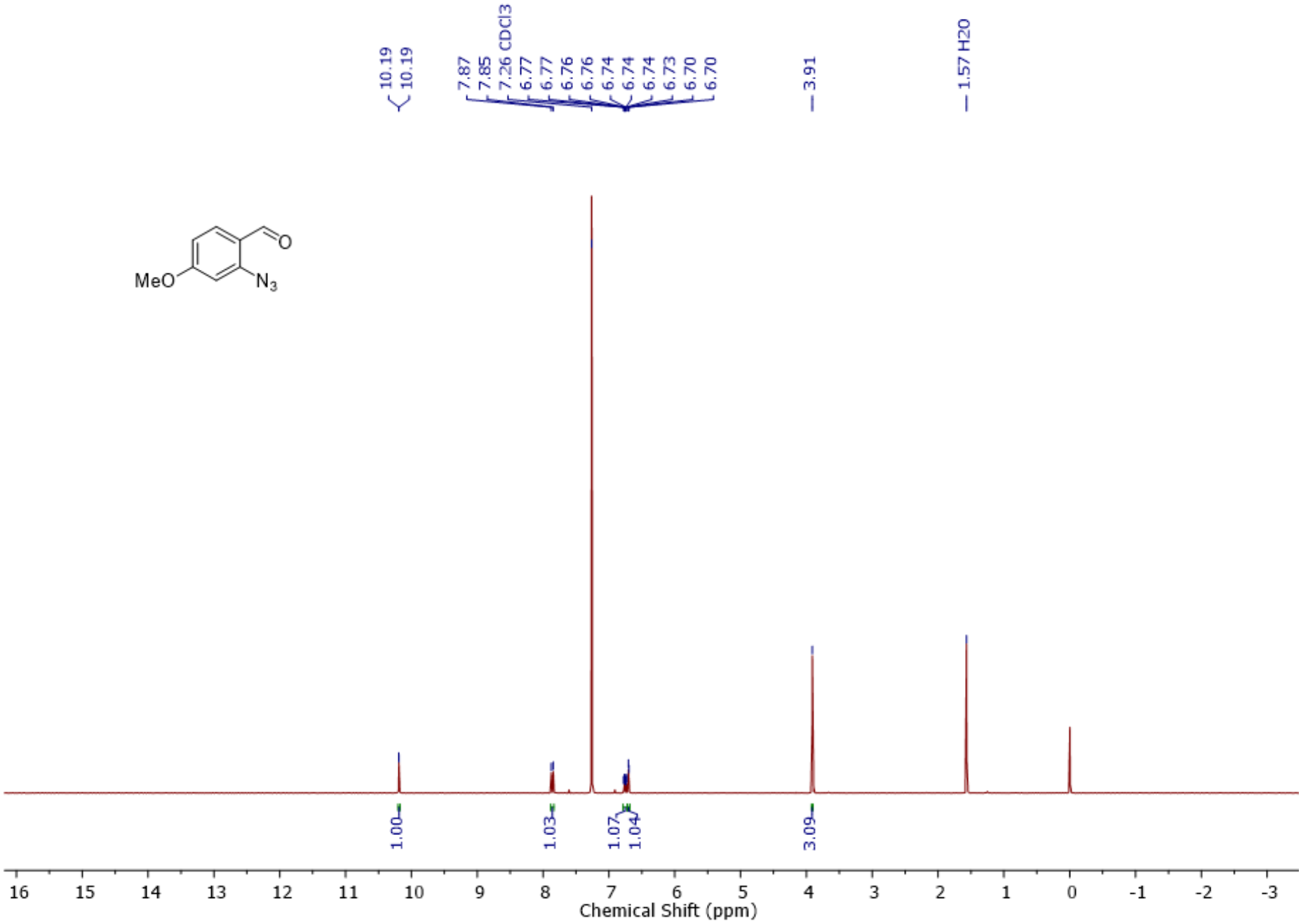

10.41
7.81
7.80
7.78
7.78
7.62
7.61
7.59
7.59
7.58
7.26 CDCl3
7.26
7.24
7.23
7.21
7.21
1.57 H20
O
N3
Cl
1.00
1.04
1.05
0.81
16
15
14
13
12
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8
7
6
5
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-2
-3
Chemical Shift (ppm)

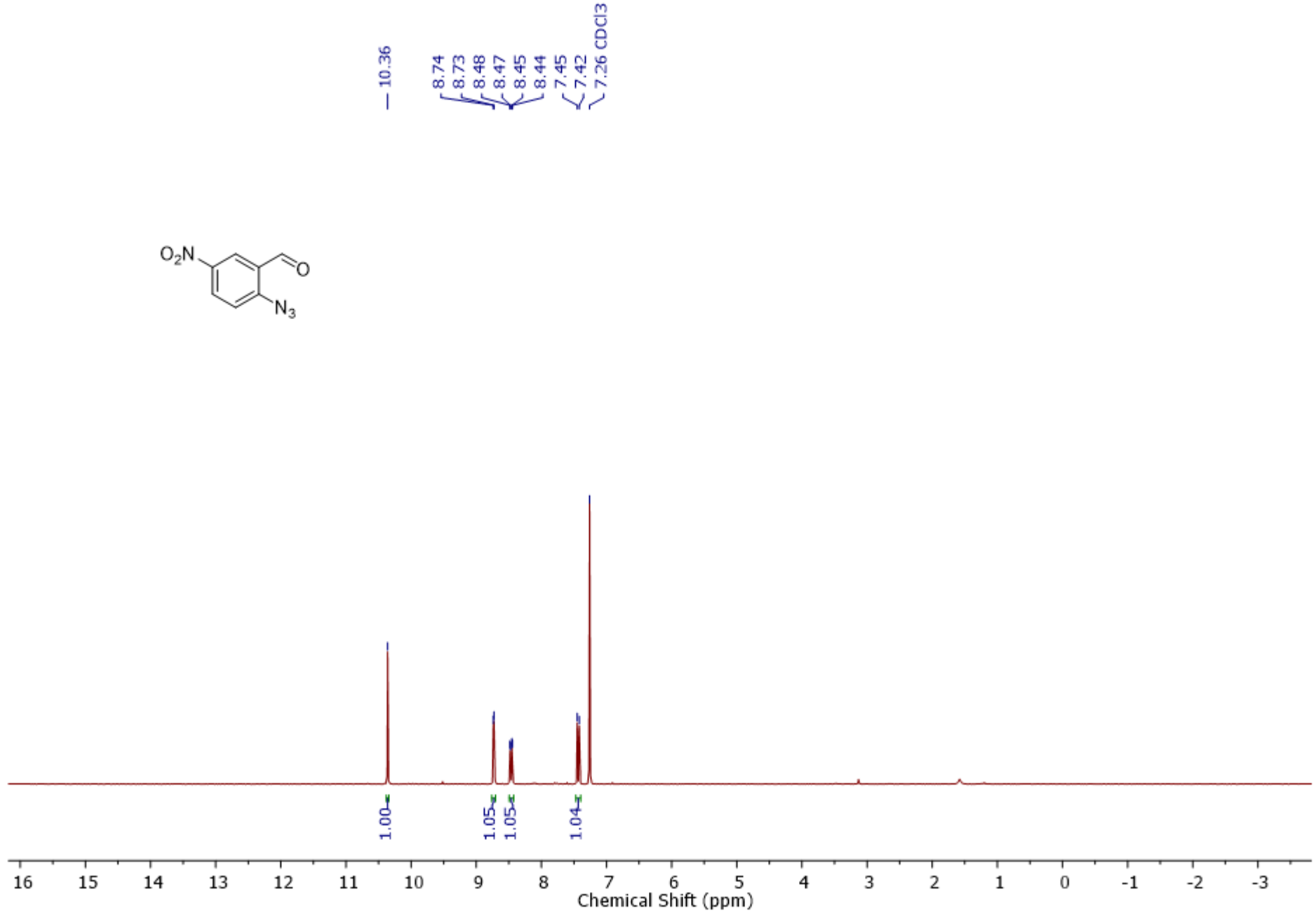

10.28
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7.73
7.43
7.43
7.39
7.39
7.36
7.36
7.26 CDCl3
1.56 H2O
Br
N3
O
1.00
1.07
1.05
1.03
16
15
14
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8
7
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Chemical Shift (ppm)

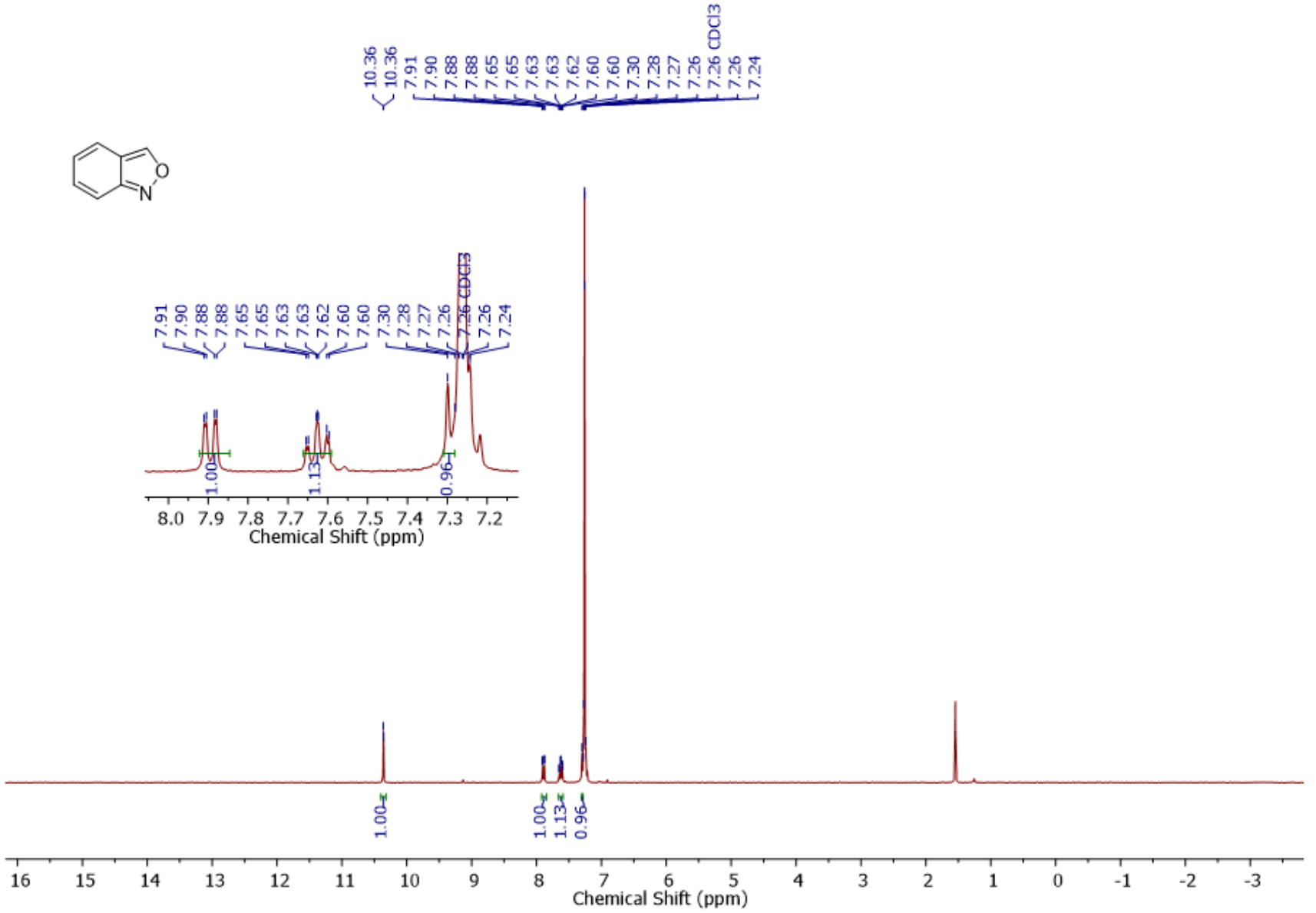

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O
N3
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1.09
1.13
1.08
3.02
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-3
Chemical Shift (ppm)

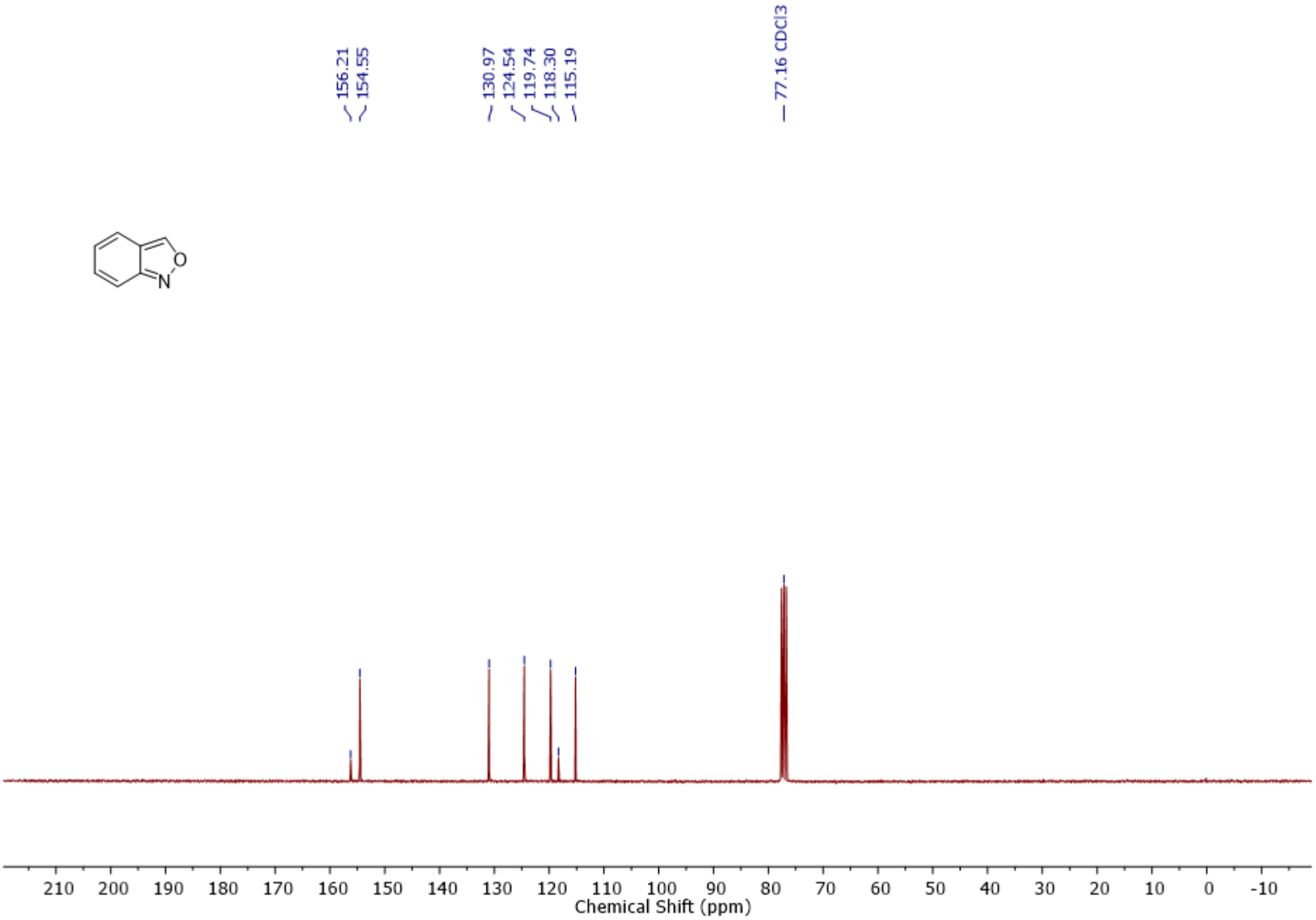

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O
F3C
N3
1.00
1.04
2.08
16
15
14
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-2
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Chemical Shift (ppm)

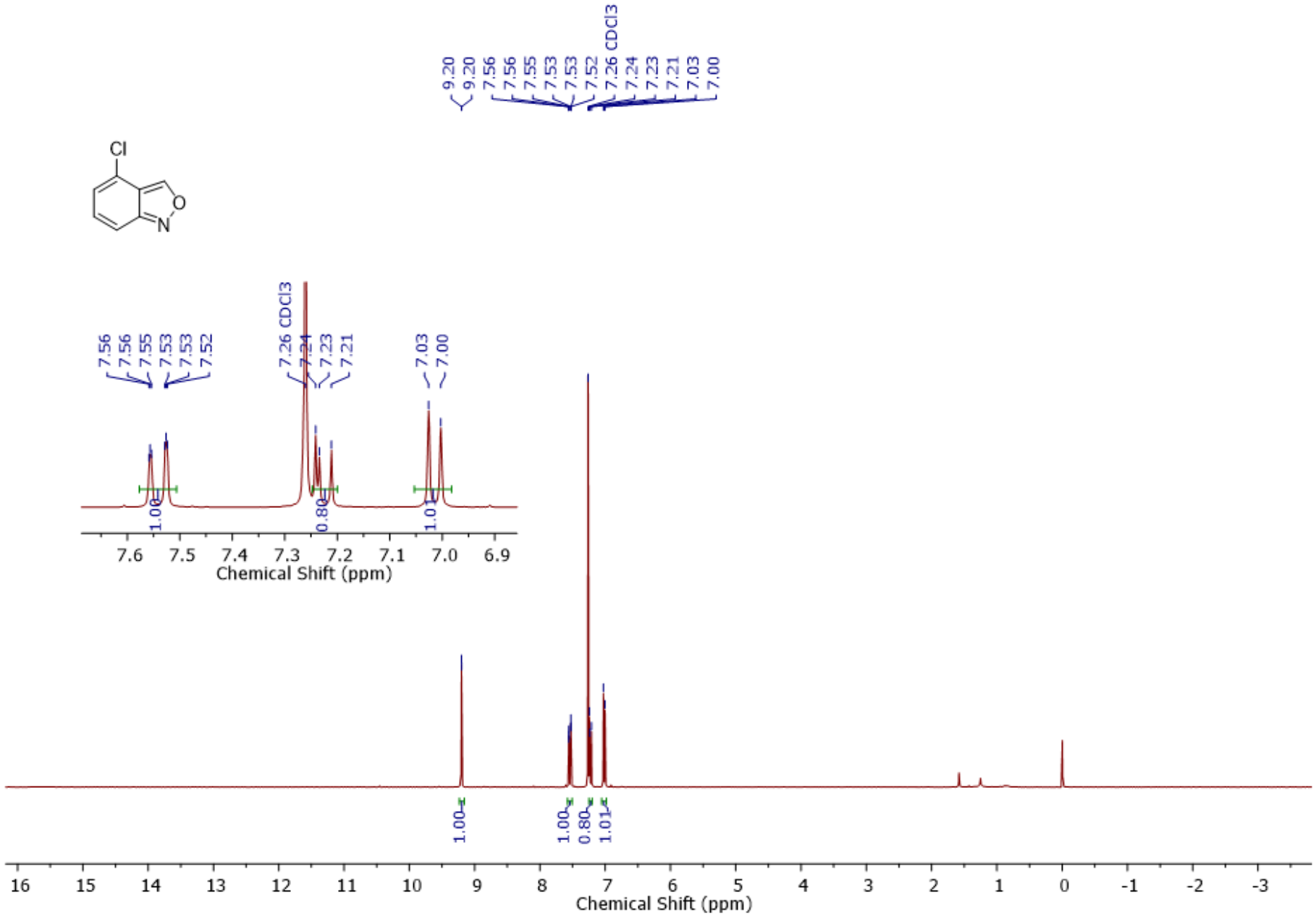

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7.83
7.41
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F3C
O
N3
1.00
1.00
1.01
1.01
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Chemical Shift (ppm)

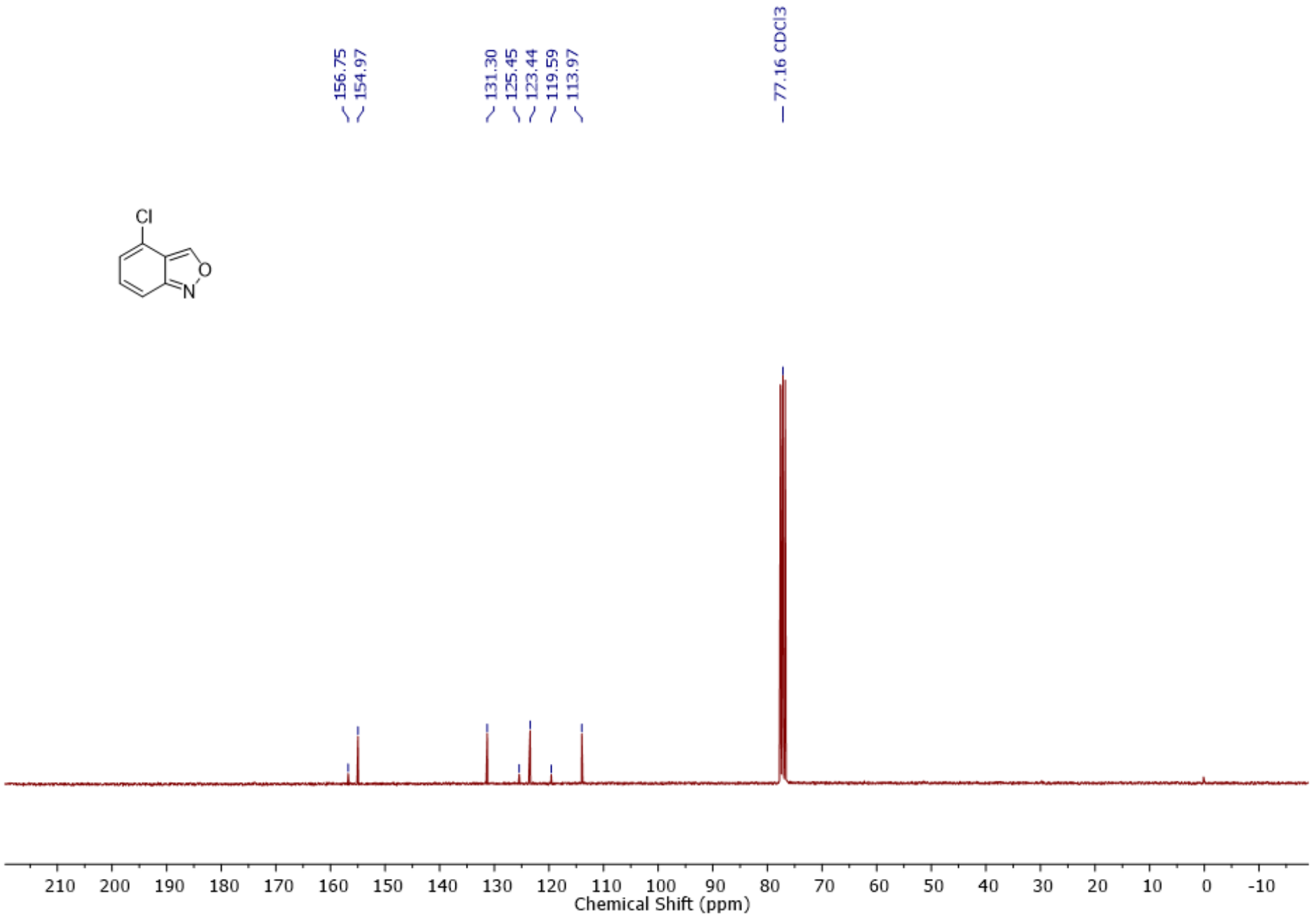

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6.76
6.74
6.74
6.74
6.73
6.70
6.70
3.91
1.57 H20
MeO
N3
O
1.00
1.03
1.07
1.04
3.09
16
15
14
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Chemical Shift (ppm)

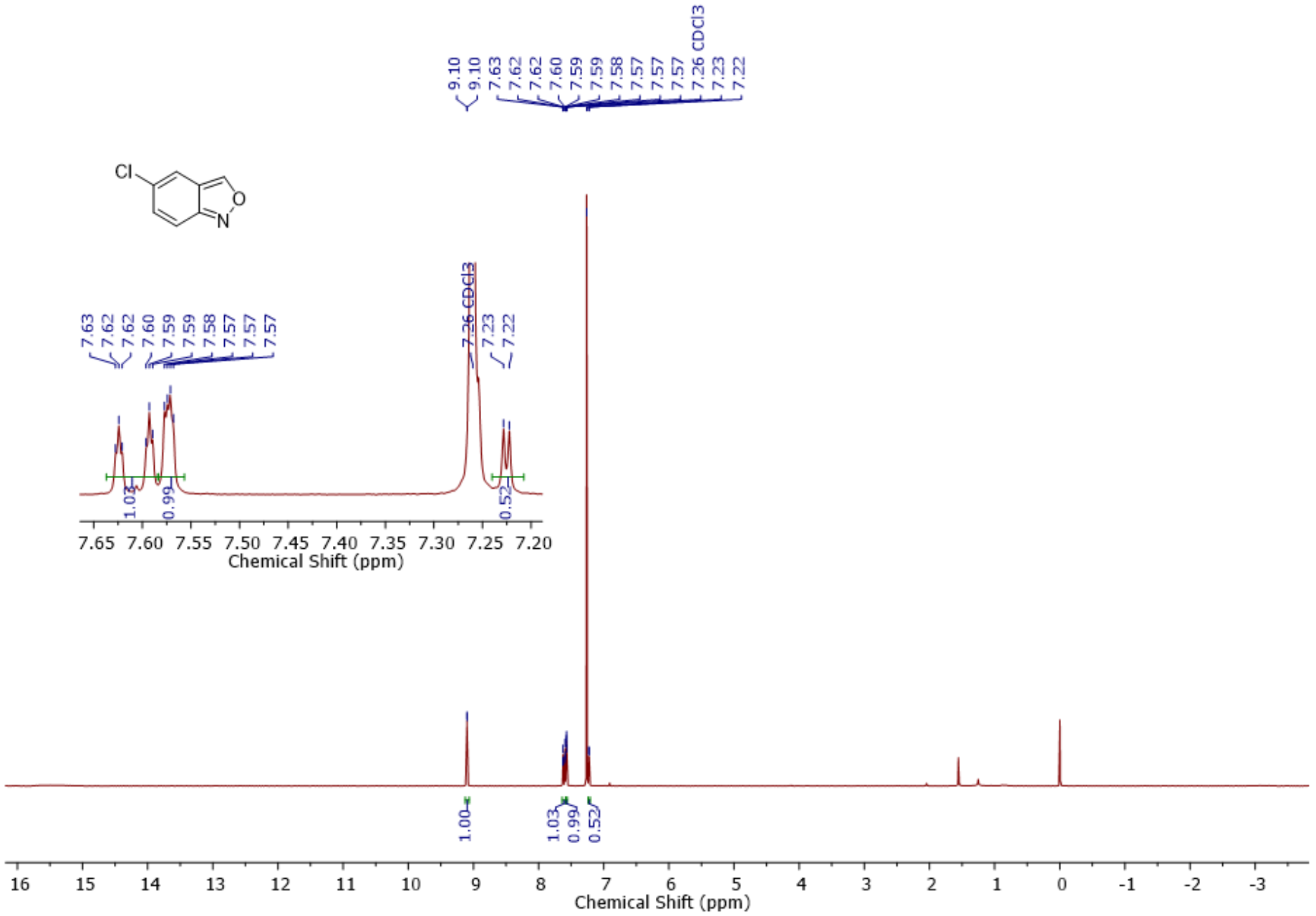

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7.45
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O2N
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N3
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1.05
1.04
16
15
14
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-3
Chemical Shift (ppm)

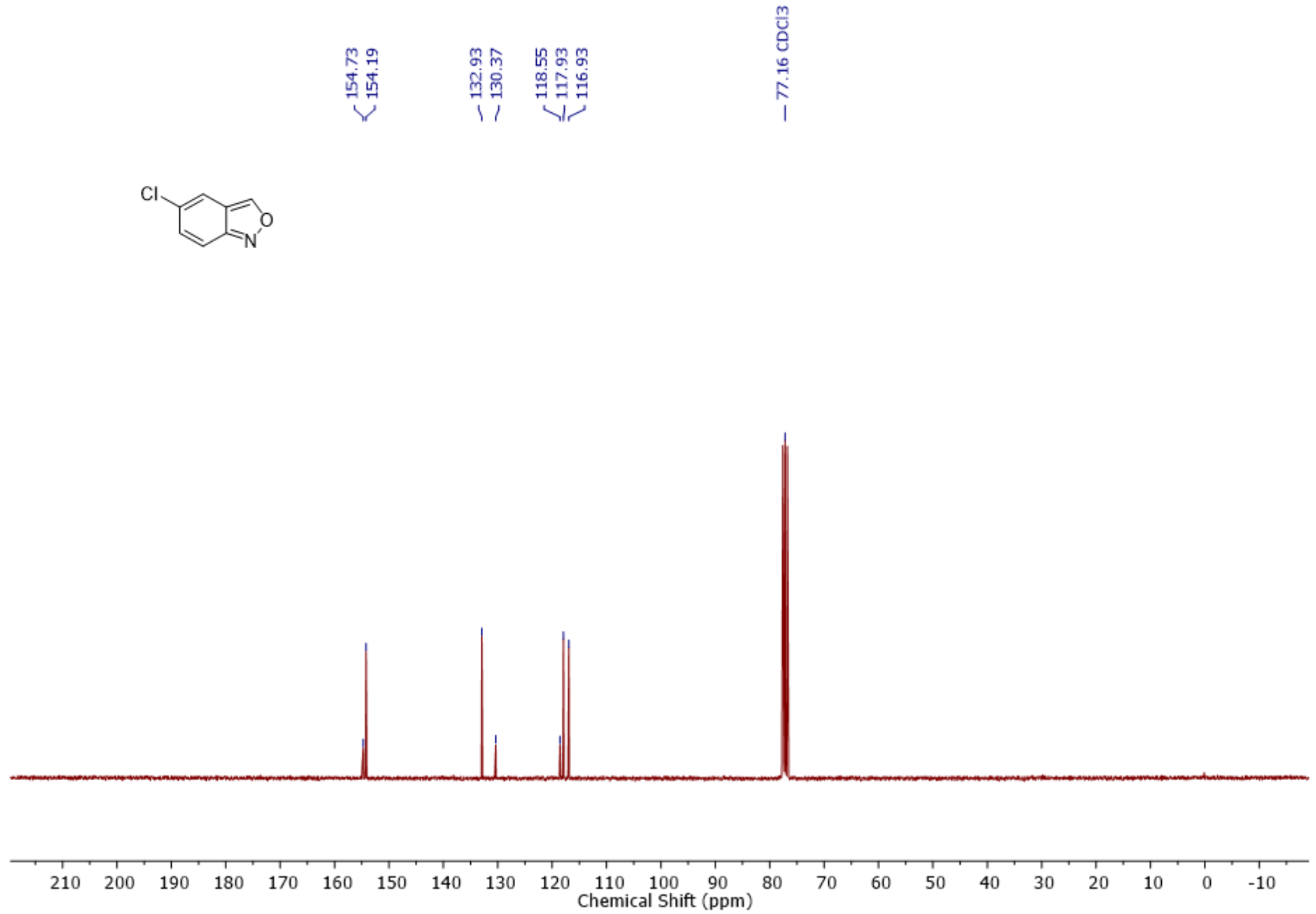

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7.30
7.28
7.27
7.26
7.26 CDCl3
7.26
7.24
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1.13
0.96
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
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Chemical Shift (ppm)

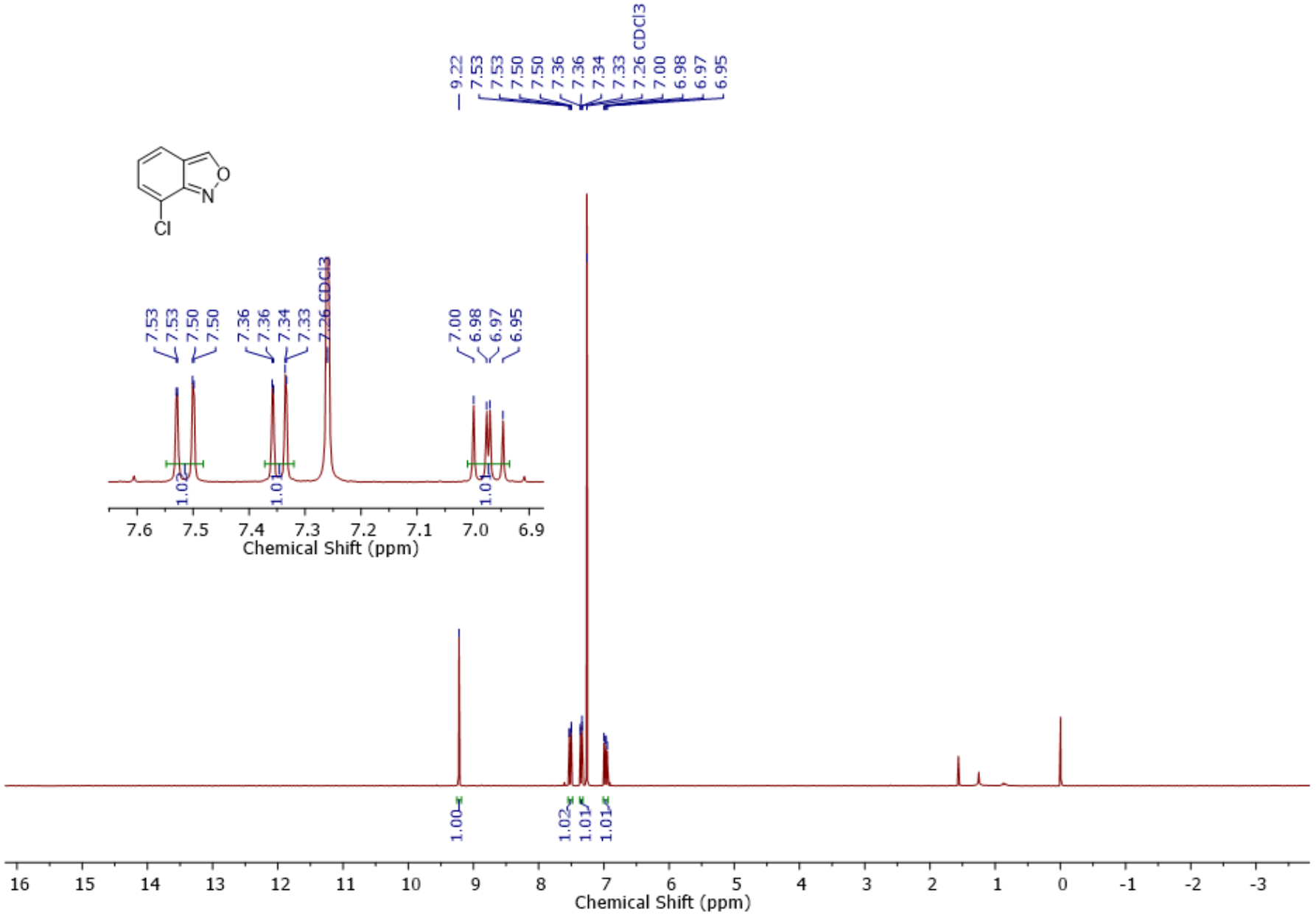

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154.55
130.97
124.54
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115.19
77.16 CDCl3
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical Shift (ppm)

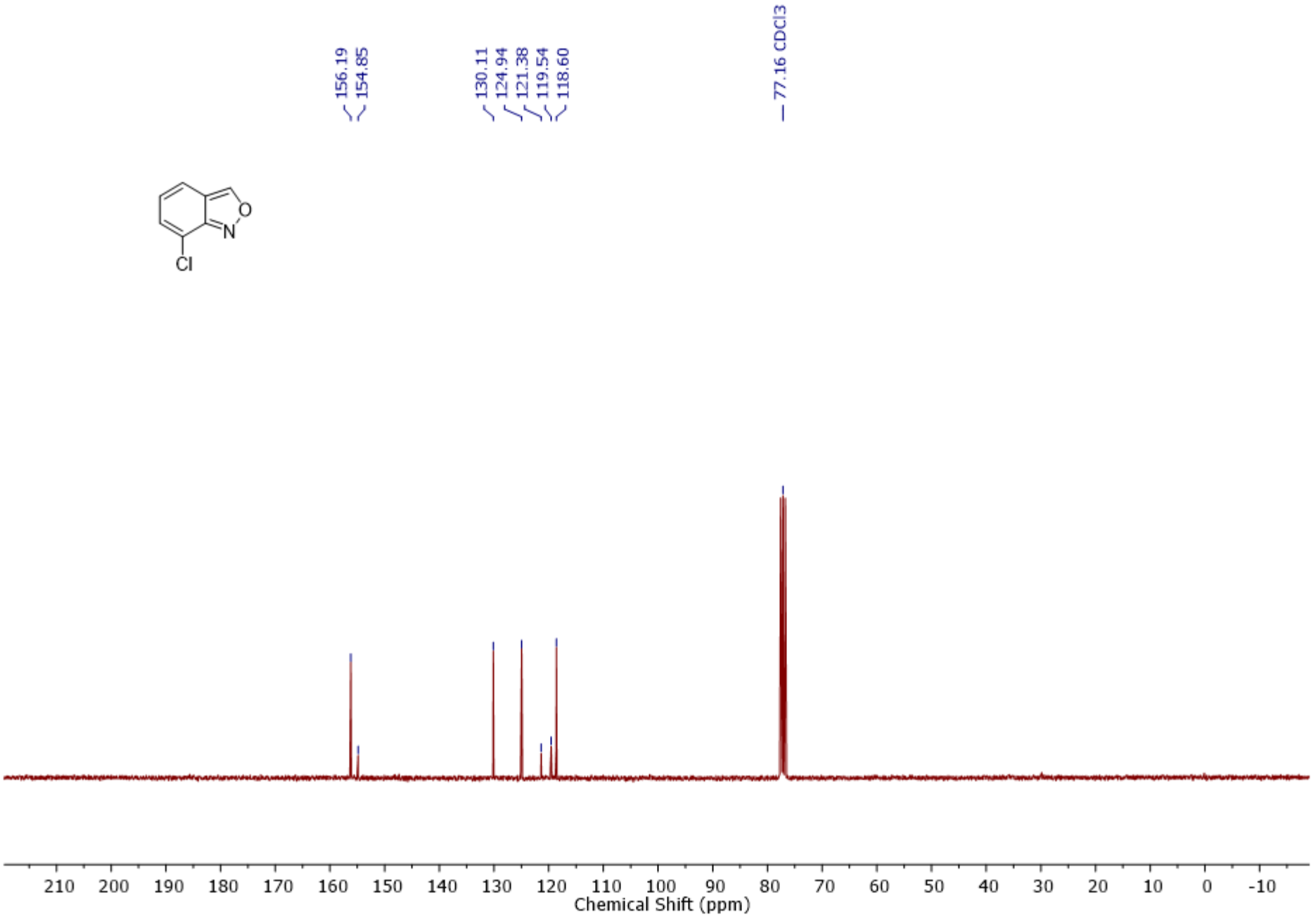

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7.56
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7.53
7.52
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7.21
7.03
7.00
Cl
O
N
7.56
7.56
7.55
7.53
7.53
7.52
7.26 CDCl3
7.24
7.23
7.21
7.03
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0.80
1.01
7.6
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7.4
7.3
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7.0
6.9
Chemical Shift (ppm)
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-3
Chemical Shift (ppm)

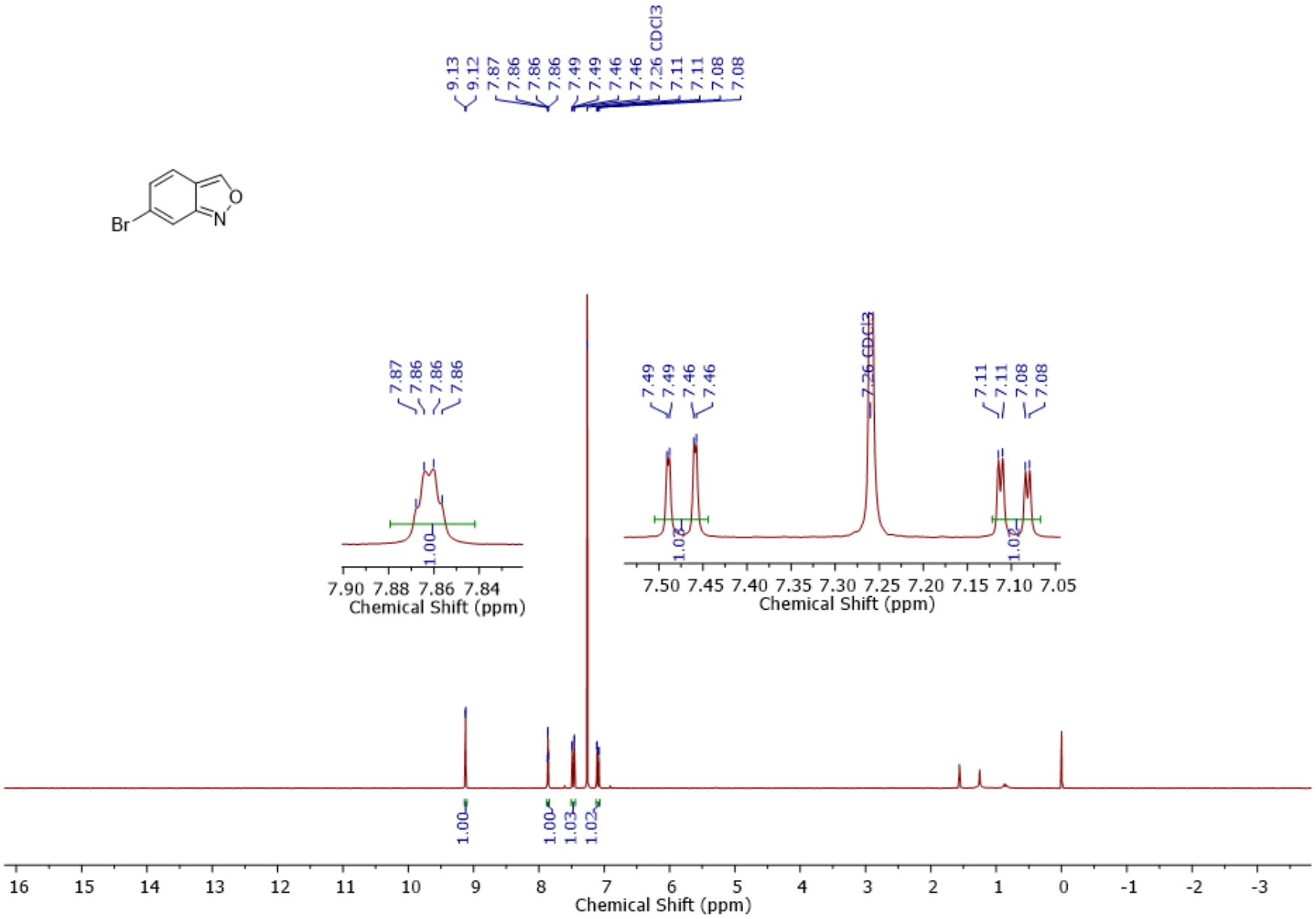

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Cl
O
N
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Chemical Shift (ppm)

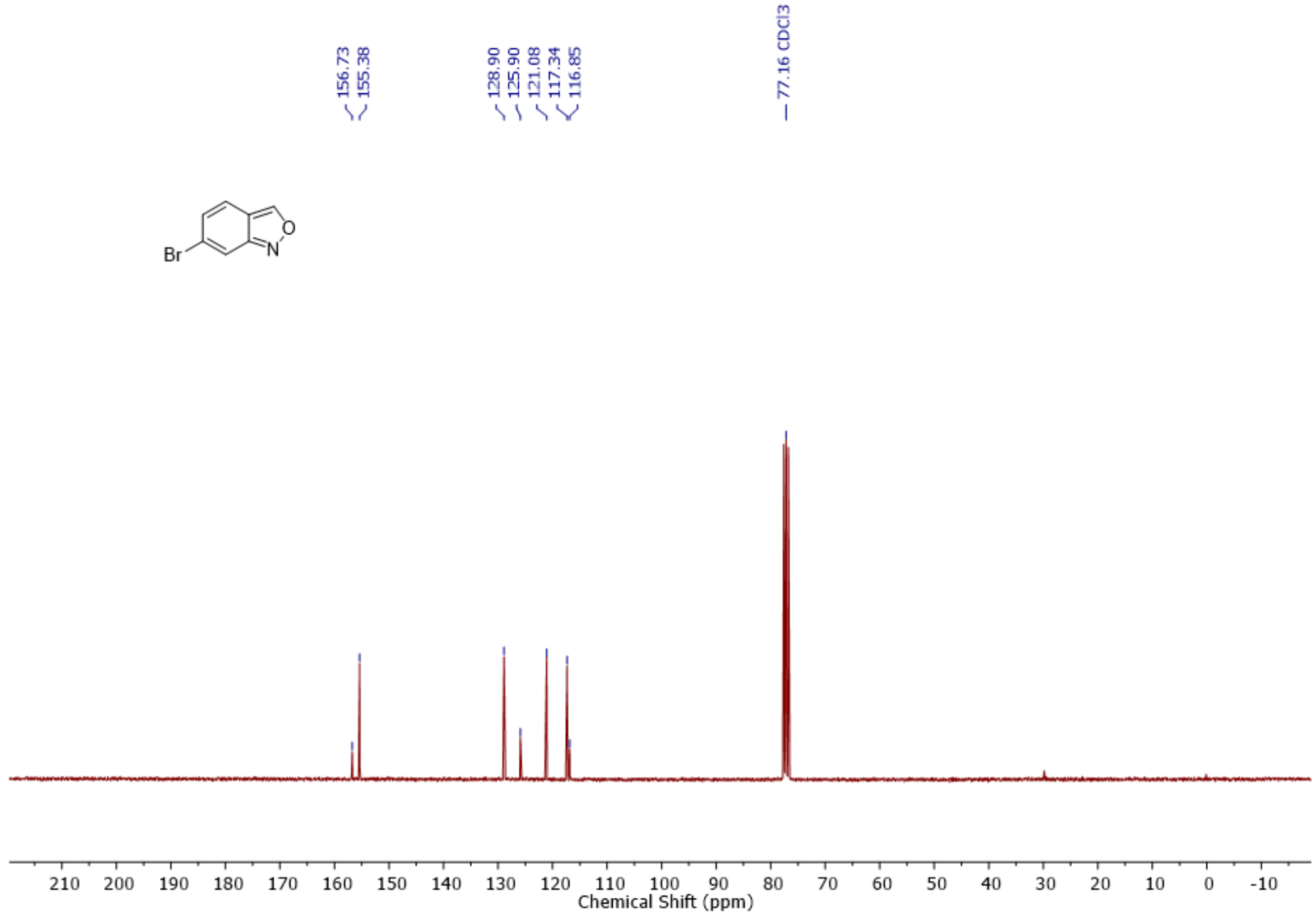

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7.22
Cl
O
N
7.63
7.62
7.62
7.60
7.59
7.59
7.58
7.57
7.57
7.57
7.26 CDCl3
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7.22
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0.99
0.52
7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20
Chemical Shift (ppm)
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1.03
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0.52
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Chemical Shift (ppm)

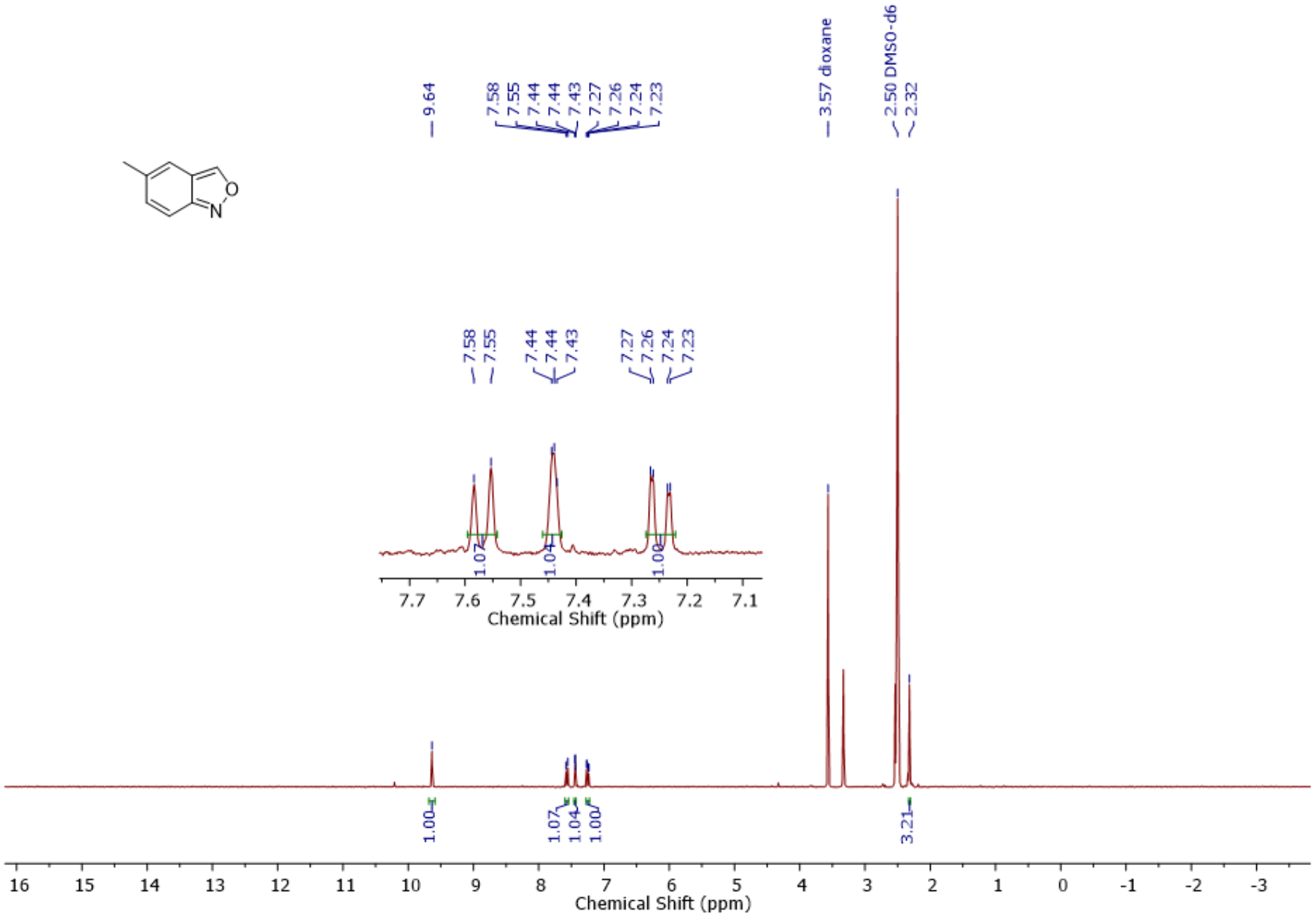

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116.93
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Cl
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N
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Chemical Shift (ppm)

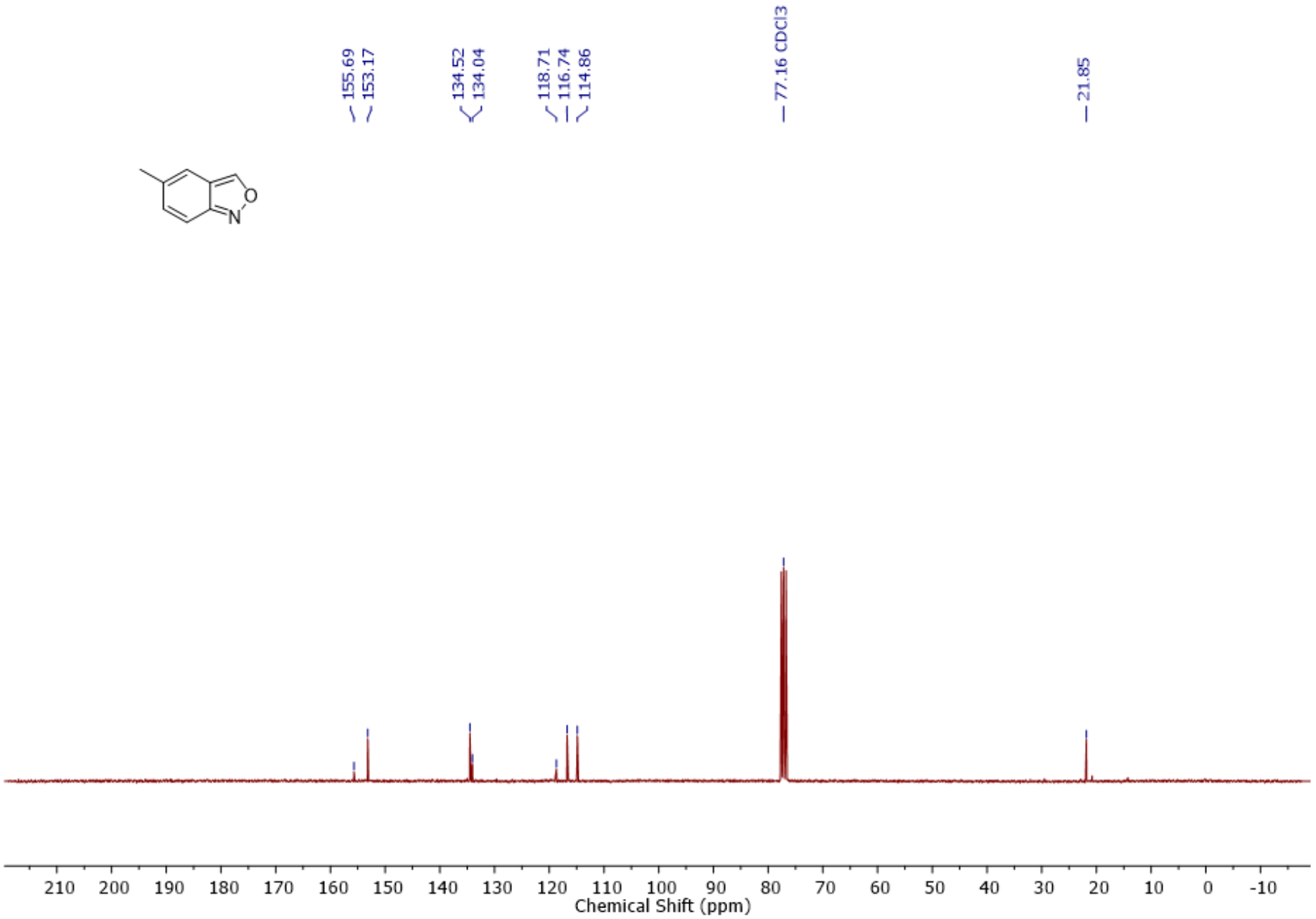

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7.50
7.36
7.36
7.34
7.33
7.26 CDCl3
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6.97
6.95
Cl
O
N
1.00
1.02
1.01
1.01
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
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Chemical Shift (ppm)

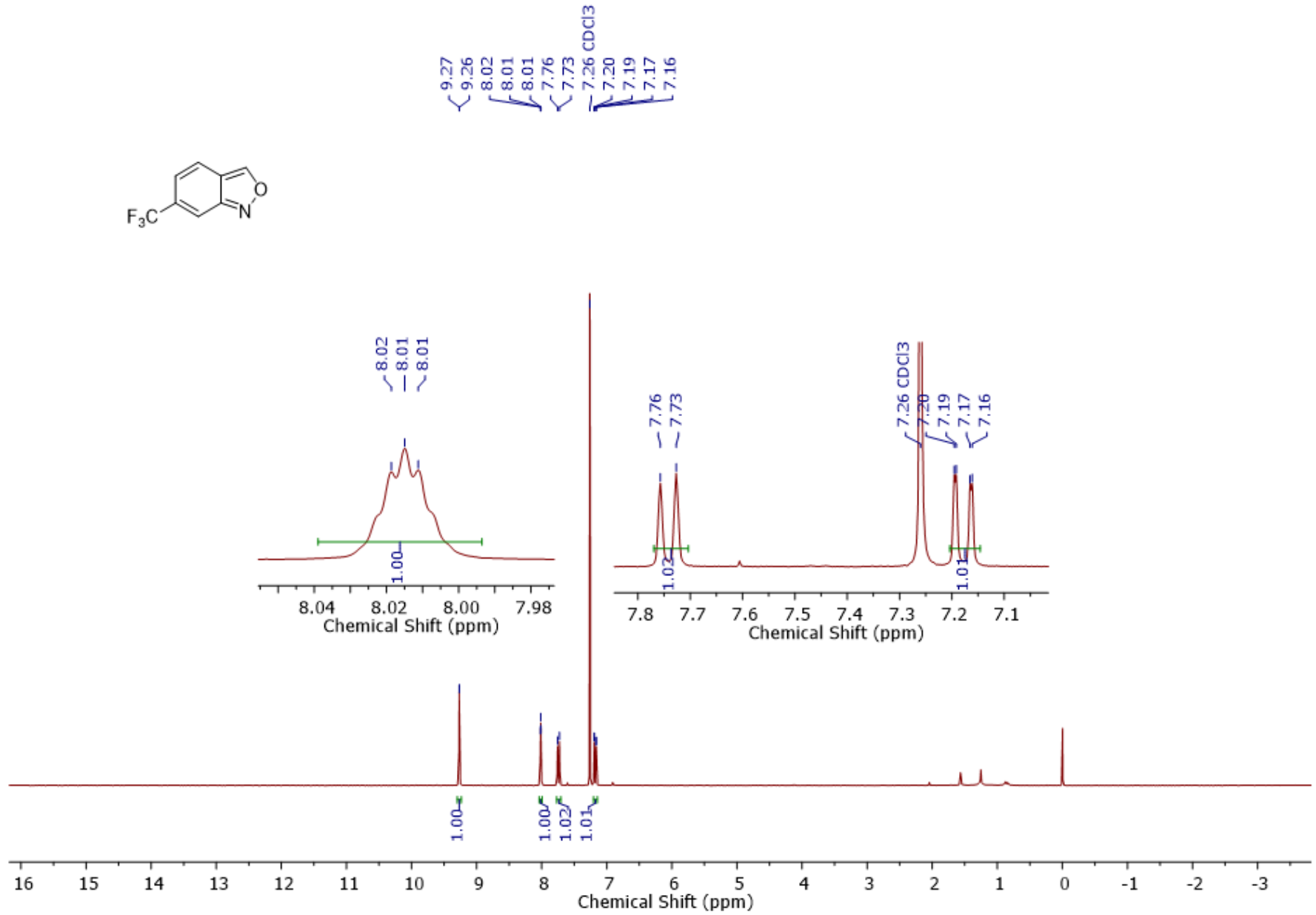

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124.94
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77.16 CDCl3
O
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical Shift (ppm)

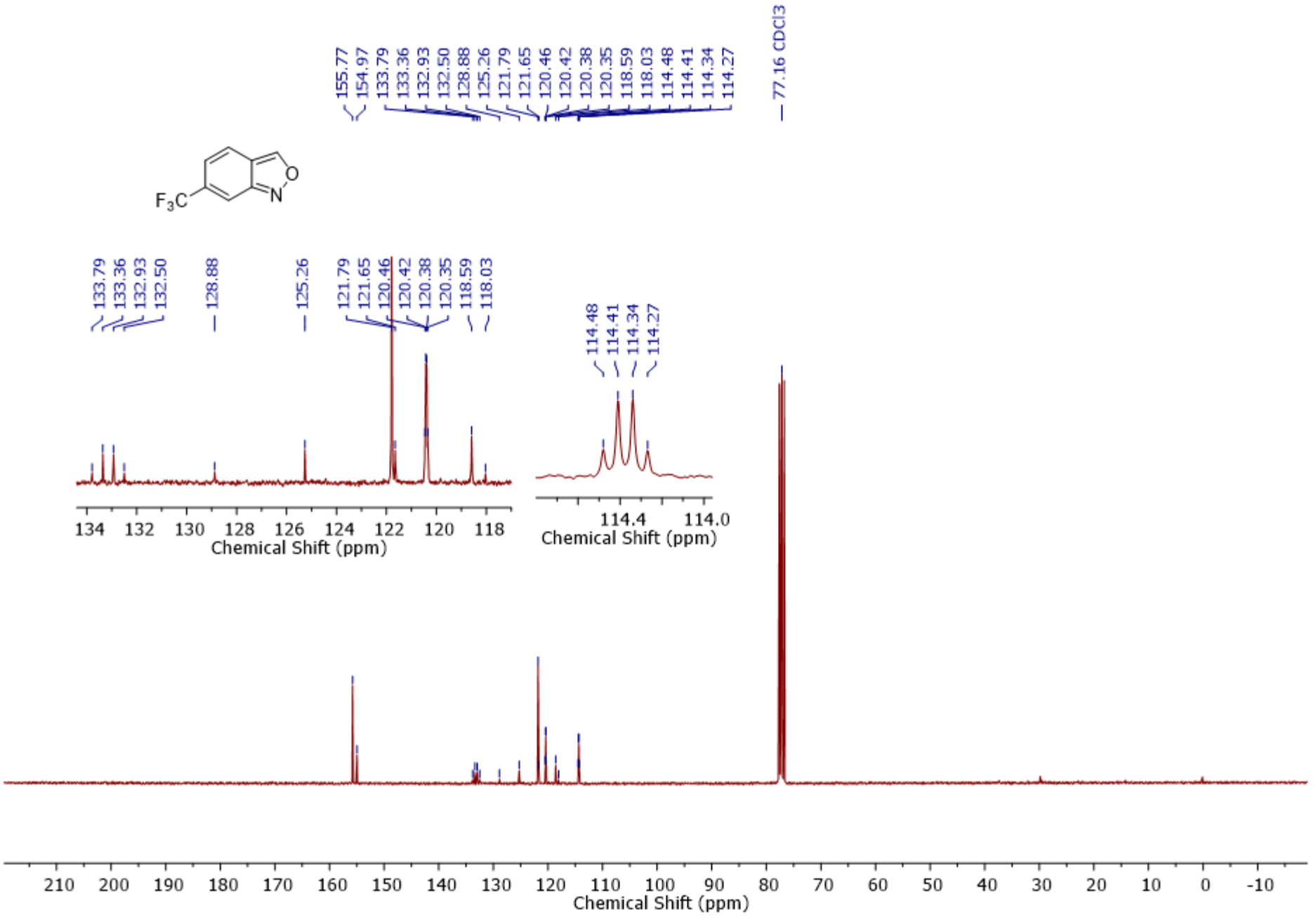

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7.49
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7.08
Br
O
N
7.87
7.86
7.86
7.86
1.00
7.90 7.88 7.86 7.84
Chemical Shift (ppm)
7.49
7.49
7.46
7.46
7.26 CDCl3
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7.11
7.08
7.08
1.02
1.02
7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05
Chemical Shift (ppm)
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1.00
1.03
1.02
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Chemical Shift (ppm)

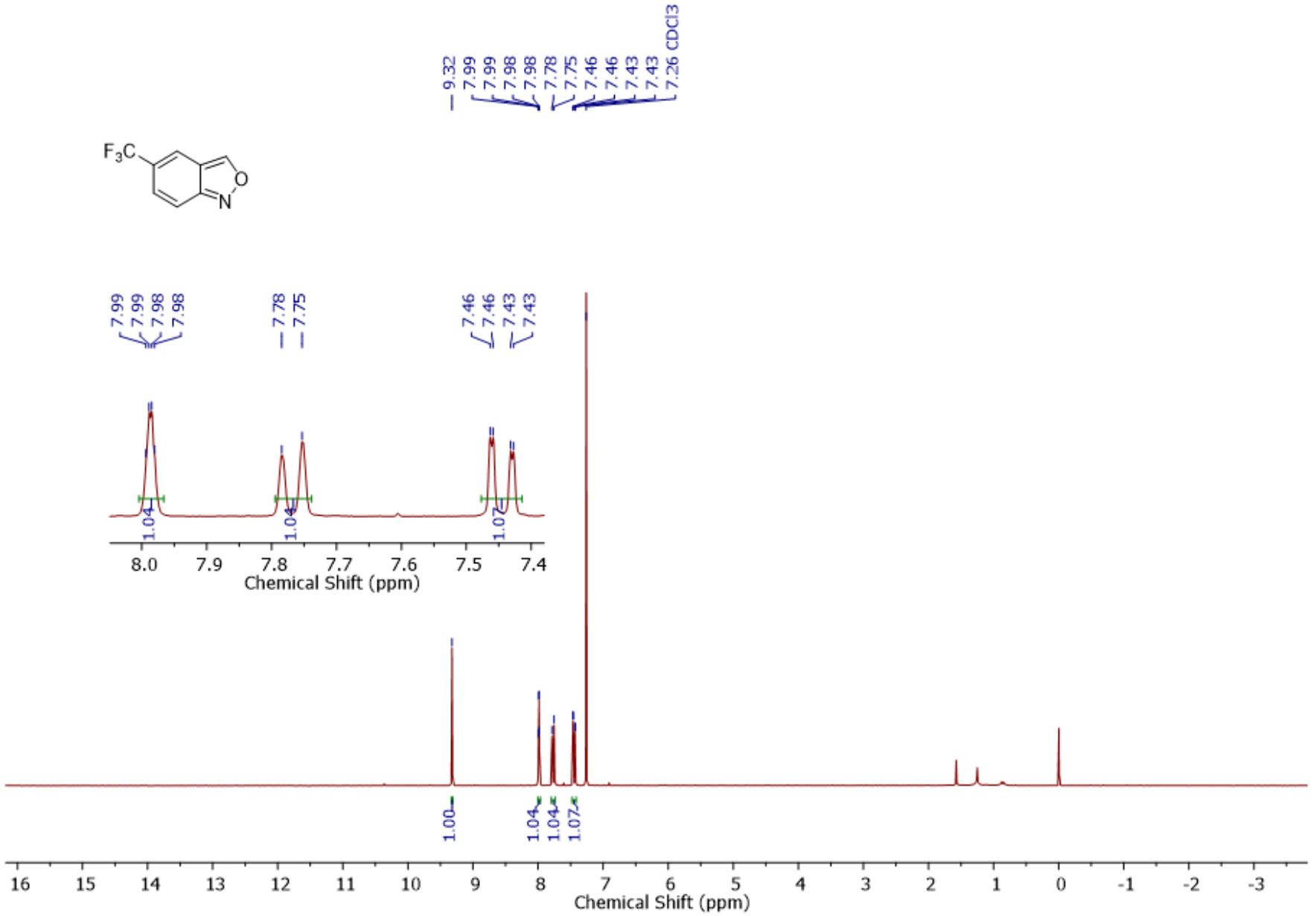

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125.90
121.08
117.34
116.85
77.16 CDCl3
Br
O
N
210
200
190
180
170
160
150
140
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40
30
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-10
Chemical Shift (ppm)

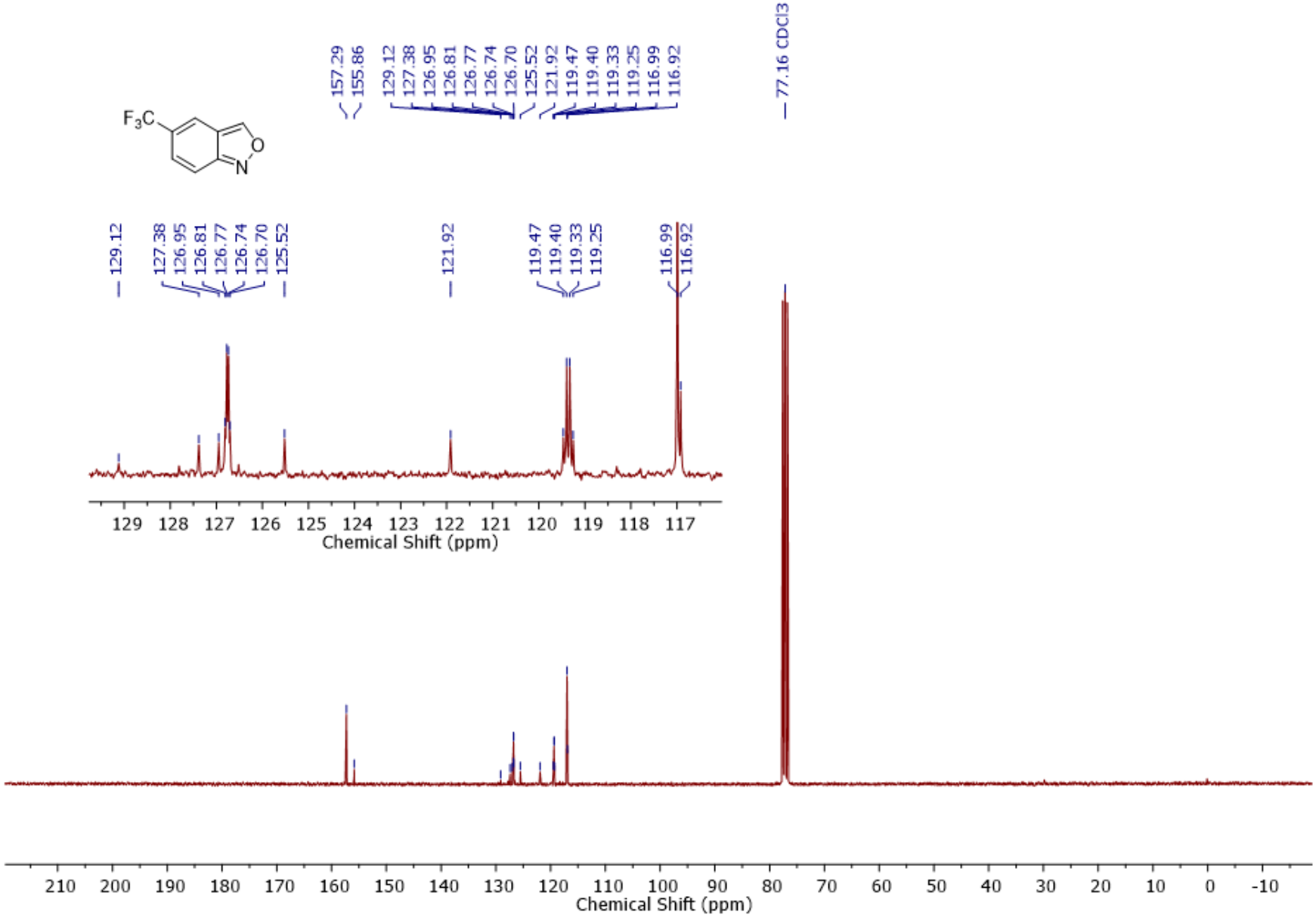

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7.44
7.43
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7.26
7.24
7.23
3.57 dioxane
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1.07
1.04
1.00
3.21
Chemical Shift (ppm)
Chemical Shift (ppm)

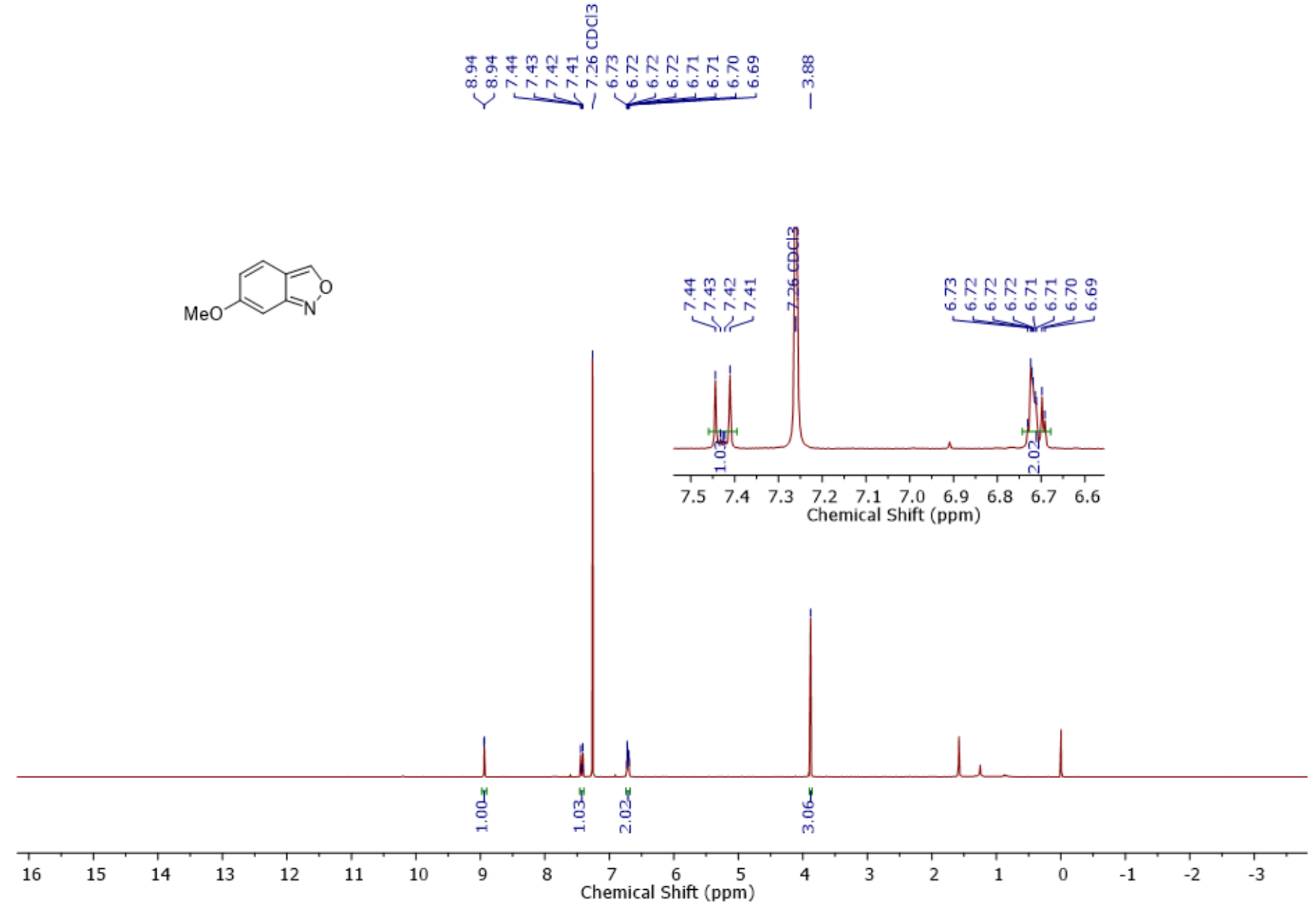

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153.17
134.52
134.04
118.71
116.74
114.86
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21.85
O
N
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Chemical Shift (ppm)

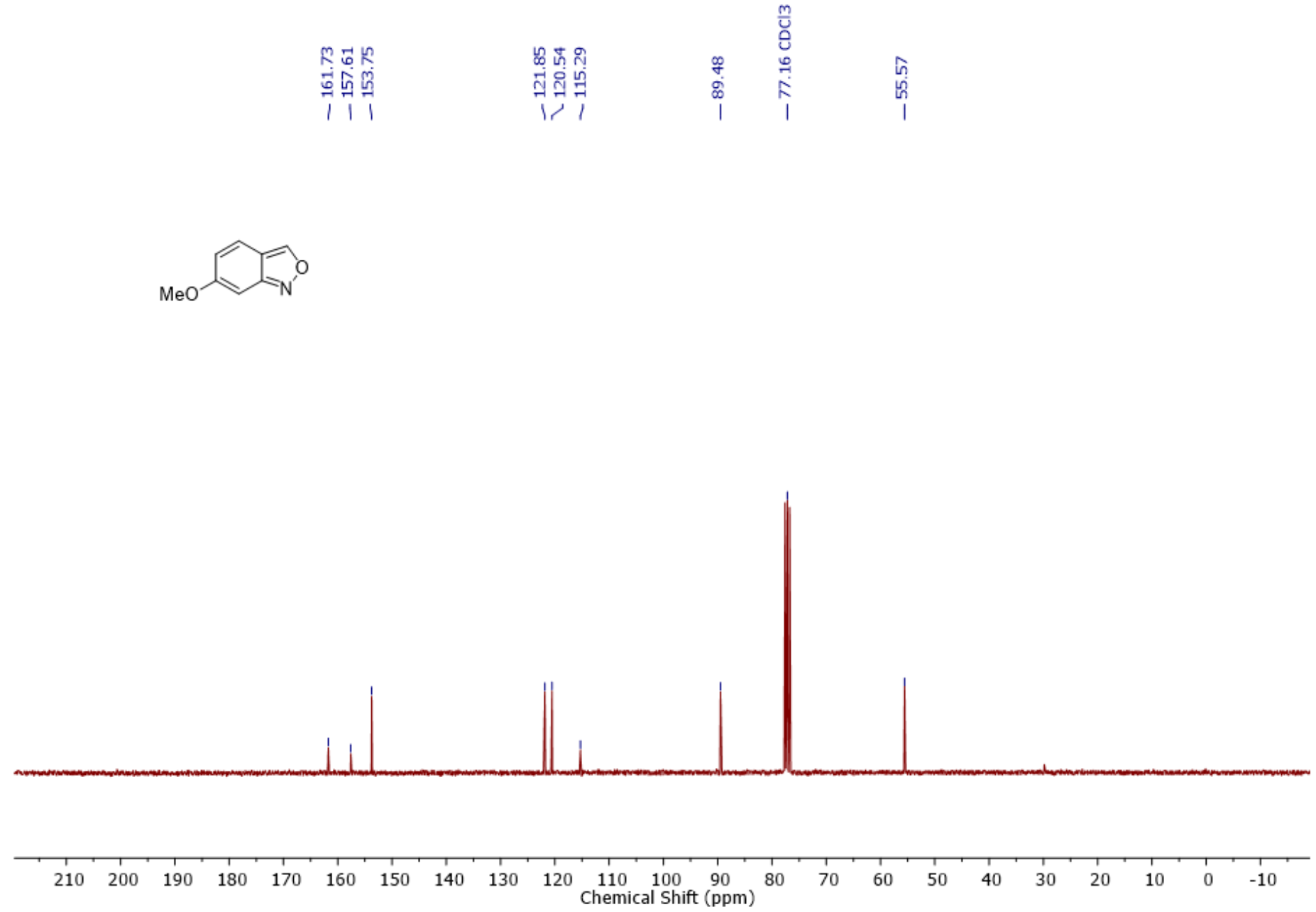

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8.01
7.76
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7.19
7.17
7.16
F3C
O
N
8.02
8.01
8.01
1.00
8.04
8.02
8.00
7.98
Chemical Shift (ppm)
7.76
7.73
7.26 CDCl3
7.20
7.19
7.17
7.16
1.02
1.01
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
Chemical Shift (ppm)
1.00
1.00
1.02
1.01
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
Chemical Shift (ppm)


155.77
154.97
133.79
133.36
132.93
132.50
128.88
125.26
121.79
121.65
120.46
120.42
120.38
120.35
118.59
118.03
114.48
114.41
114.34
114.27
77.16 CDCl3
F3C
O
N
Chemical Shift (ppm)
Chemical Shift (ppm)
Chemical Shift (ppm)


9.32
7.99
7.99
7.98
7.98
7.78
7.75
7.46
7.46
7.43
7.43
7.26 CDCl3
F3C
O
N
1.00
1.04
1.04
1.07
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
Chemical Shift (ppm)
8.0
7.9
7.8
7.7
7.6
7.5
7.4
Chemical Shift (ppm)


157.29
155.86
129.12
127.38
126.95
126.81
126.77
126.74
126.70
125.52
121.92
119.47
119.40
119.33
119.25
116.99
116.92
77.16 CDCl3
F3C
O
N
Chemical Shift (ppm)
Chemical Shift (ppm)


8.94
8.94
7.44
7.43
7.42
7.41
7.26 CDCl3
6.73
6.72
6.72
6.72
6.71
6.71
6.70
6.69
3.88
MeO
O
N
7.44
7.43
7.42
7.41
7.26 CDCl3
6.73
6.72
6.72
6.72
6.71
6.71
6.70
6.69
1.03
2.02
7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6
Chemical Shift (ppm)
1.00
1.03
2.02
3.06
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
Chemical Shift (ppm)


161.73
157.61
153.75
121.85
120.54
115.29
89.48
77.16 CDCl3
55.57
MeO
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical Shift (ppm)