Supporting Information

Visible-Light-Driven Copper (II) Catalysis for 2,3-Disubstituted Quinazolinone Synthesis *via* Ullmann *N*-Arylation and C-H Oxidative Amidation

Ahmed Th. Abdulghaffar,[‡a,d] Pei Hu,[‡a] Yifan Hu,[a] Chenxu Liu,[a] Yanrong Ren,[a] Zhongyan Cao,[a] Yuanqing Xu,*[a] Min Jiang,*[c] and Hao Xu*[a,b]

[a.] *College of Chemistry and Molecular Sciences, Henan University, Kaifeng 475004, China.*

[b.] *Key Laboratory of Bioorganic Phosphorus Chemistry and Chemical Biology (Ministry of Education), Department of Chemistry, Tsinghua University, Beijing 100084, China.*

[c.] *College of Material, Chemistry and Chemical Engineering, Hangzhou Normal University, Hangzhou 311121, P. R. China.*

[d.] *Chemistry Department, Faculty of Science, Fayoum University, Fayoum, 63514, Egypt.*

E-mail: xuyuanqing@henu.edu.cn; jiang-m18@hznu.edu.cn; xuhao@henu.edu.cn

‡The authors contributed equally to this work.

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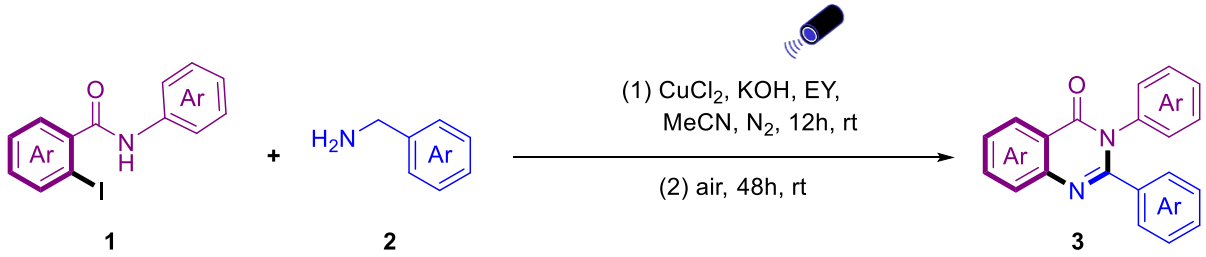
1. Supporting Figures

General Experimental Procedure for Synthesis of 2,3-Disubstituted Quinazolin-4(3*H*)-ones



1 2 3

In a 25 mL quartz reaction vial, the following components were added: ***N*-aryl-2-iodobenzamide 1** (0.3 mmol), **aryl methanamine 2** (0.45 mmol), $CuCl_2$ (0.03 mmol), Eosin Y (EY) (0.009 mmol), KOH (0.6 mmol), and anhydrous acetonitrile (3.0 mL). The mixture was stirred for 12 hours at 25 °C under nitrogen (from a balloon) and illuminated with blue LED light. A cooling thermostat maintained the reaction temperature, as shown in Figure S1, followed by an additional 48 hours of stirring under air. After the reaction, the crude products were purified by flash chromatography using petroleum ether/ethyl acetate as the eluent to yield the desired products (**3a-3f'**).

Figure S1. Reaction equipment and light source (λ_{peak} = 454 nm).

We utilize the Kessil TUNA BLUE (KSA160WE-TB) light source from DiCon Fiberoptics, Inc. in Taiwan. An energy spectrometer measured the irradiance of the 40W KSA160WE-TB at 10.9 mW/cm², with a peak wavelength of 454 nm (Figure S2). The irradiation occurs within a borosilicate glass test tube, placed 10 cm from the light source, without any light filter in between.

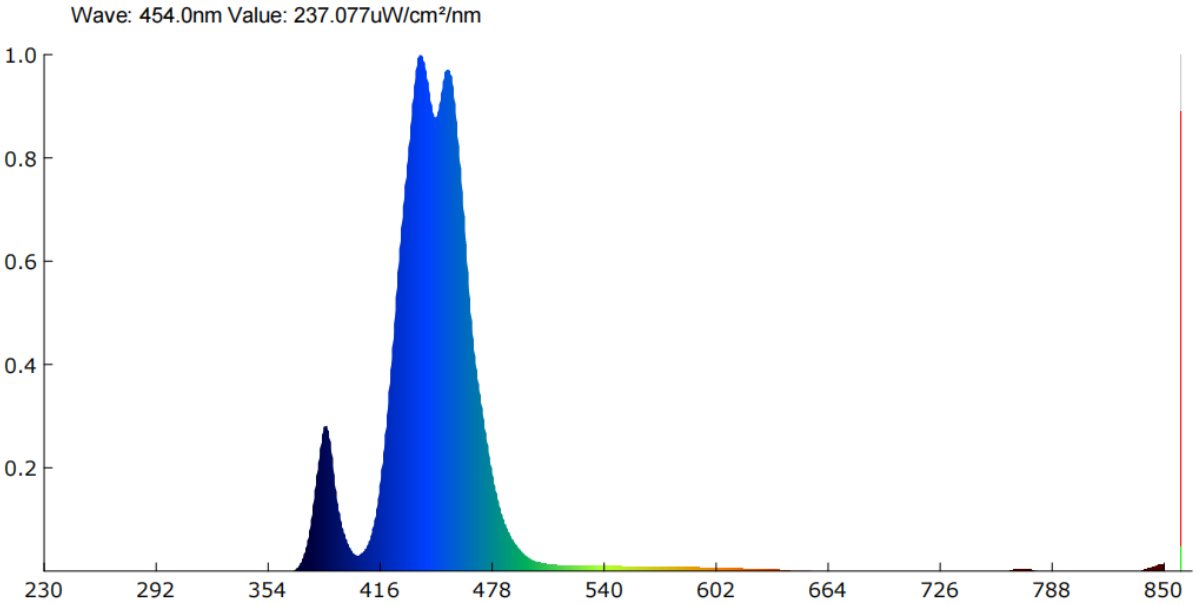


Figure S2. The emission spectrum of the 40W KSA160WE-TB, with a peak wavelength of 454 nm.

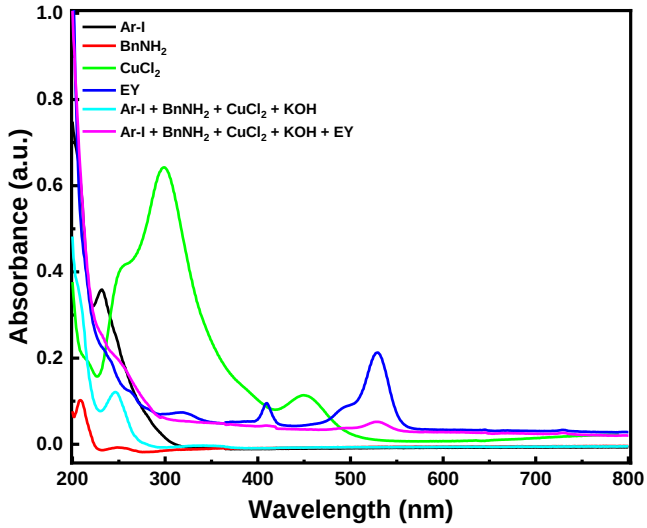


Figure S3. UV-visible absorption spectra of reaction components and their mixtures.

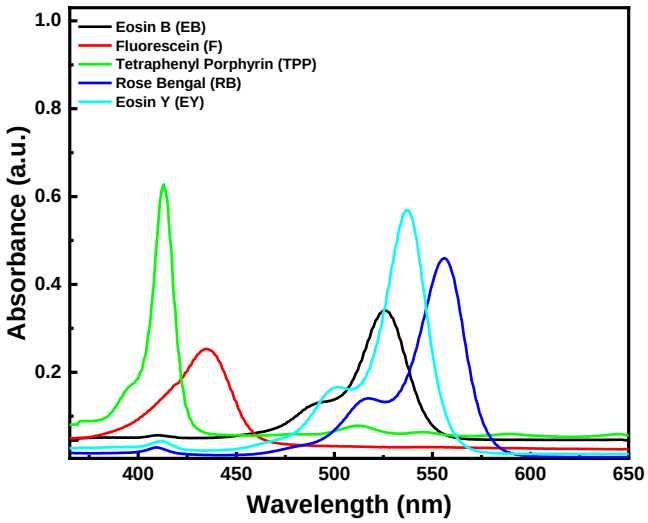


Figure S4. UV-visible absorption spectra of the screened photosensitizers.

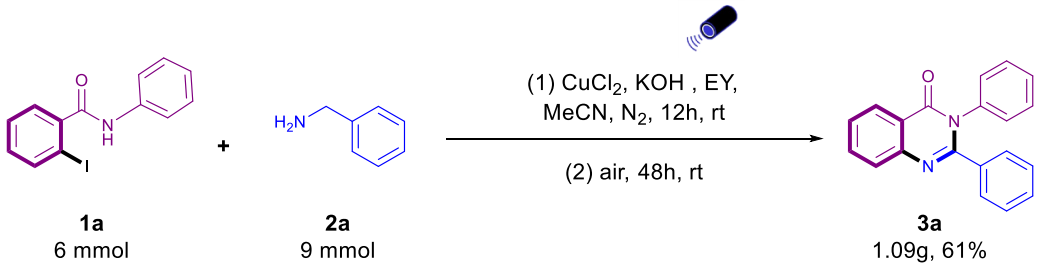


Figure S5. Gram-scale experiment.

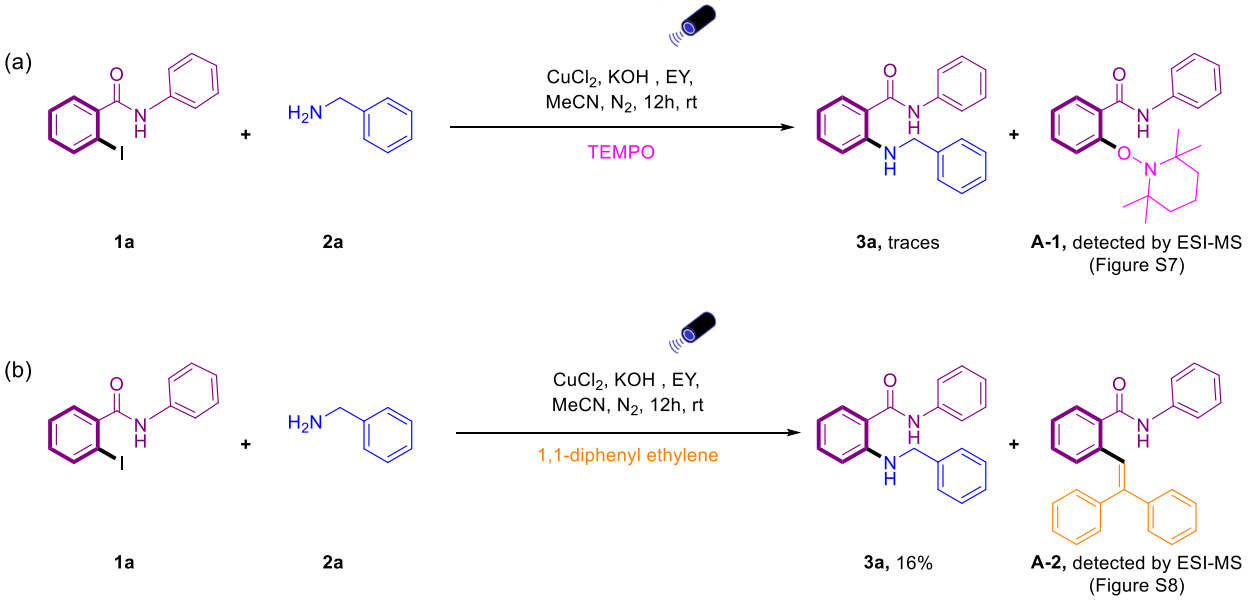


Figure S6. Radical trapping experiments.

Conditions: **1a** (0.3 mmol), **2a** (0.45 mmol), $CuCl_2$ (0.03 mmol), Eosin Y (EY) (0.009 mmol), KOH (0.6 mmol), TEMPO or 1,1-diphenylethylene (0.6 mmol), anhydrous acetonitrile (3.0 mL), stirred for 12 h at 25 ℃ under N_2 and Blue LED irradiation.

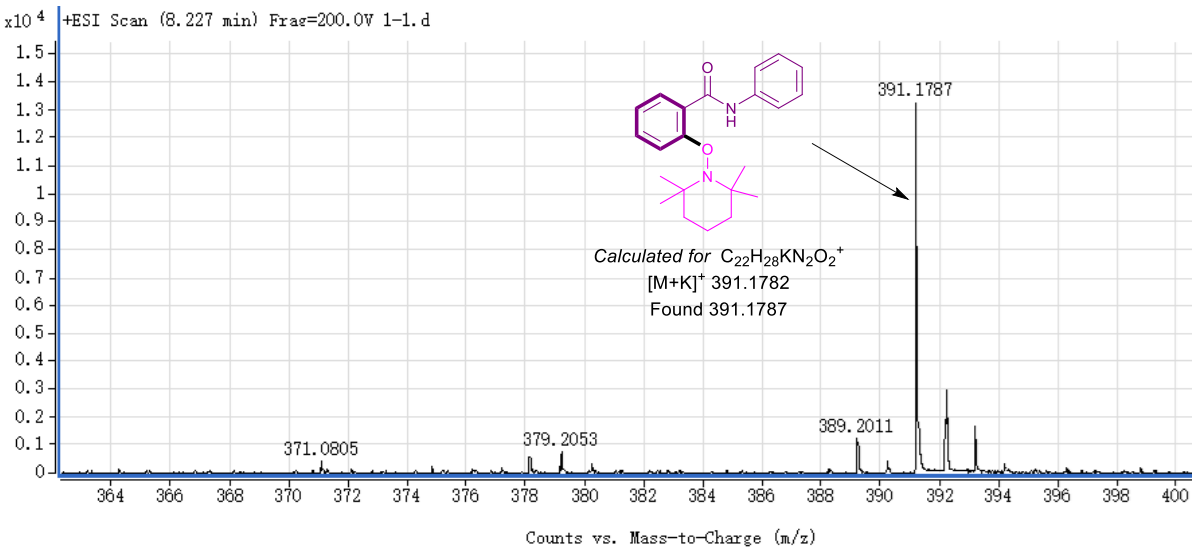


Figure S7. ESI-HRMS spectrum for radical adduct **A-1** with TEMPO.

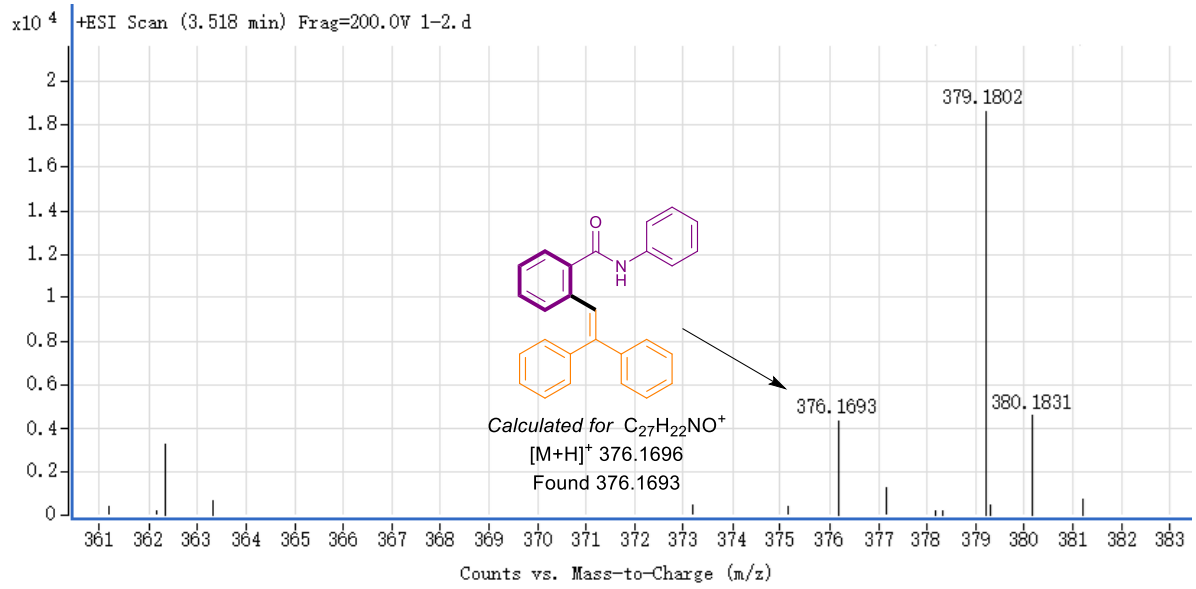


Figure S8. ESI-HRMS spectrum for radical adduct **A-2** with 1,1-diphenylethylene.

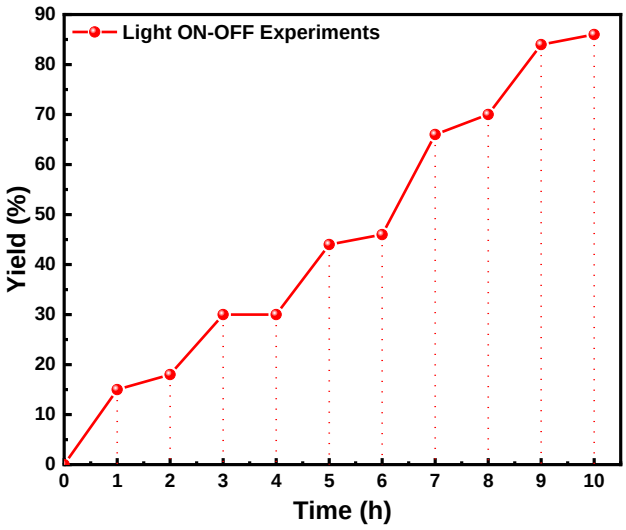


Figure S9. Light ON-OFF experiments.

Stern-Volmer Fluorescence Quenching Experiments

Firstly, the emission and excitation spectra of EY were investigated. EY (0.05 mM) solution in MeCN was chosen as the model. The fluorescence excitation wavelength of EY was measured at 562 nm emission (Figure S10), while the fluorescence emission wavelength was measured at 450 nm excitation (Figure S11). Next, we conducted the fluorescence quenching experiments. In a typical experiment, 2.0 mL of EY solution (0.05 mM) in MeCN was added to the appropriate amount of quencher in a quartz cuvette, 50 mM solution of the quencher (*Cu(II)-benzylamine complex*) was added into the cuvette by 1 μL, and the emission of the sample was collected (Figure S12). The solution was excited at 450 nm (excitation wavelength of EY) and the emission intensity was determined at 562 nm (emission wavelength of EY). By fitting the above measurements, a linear relationship was observed between the relative change in the EY emission intensity (I_o/I) and the concentration of benzylamine (Figure S13).

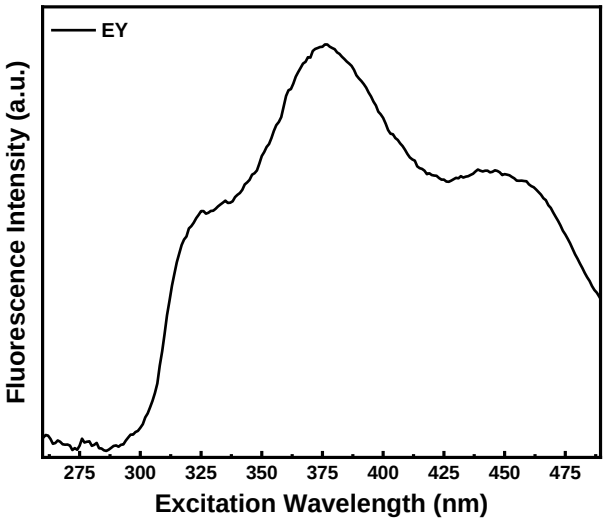


Figure S10. Fluorescence excitation spectra of EY, emitted at 562 nm.

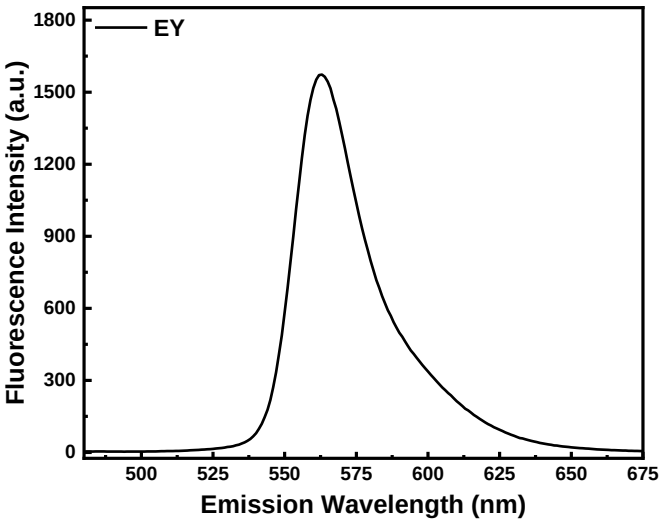


Figure S11. Fluorescence emission spectra of EY, excited at 450 nm.

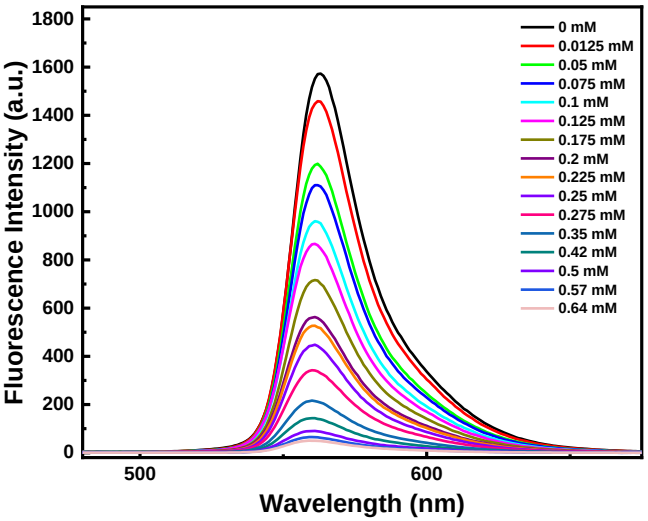


Figure S12. Fluorescence emission spectra of EY with different quencher concentrations (*Cu(II)-benzylamine complex*).

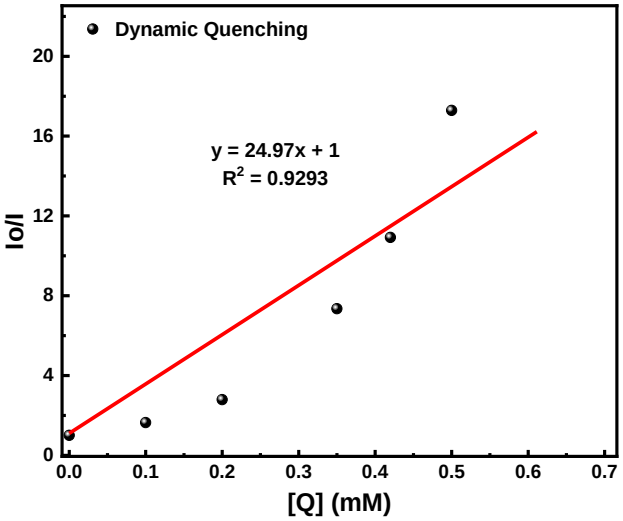


Figure S13. Dynamic emission quenching of EY by Cu(II)-benzylamine complex.

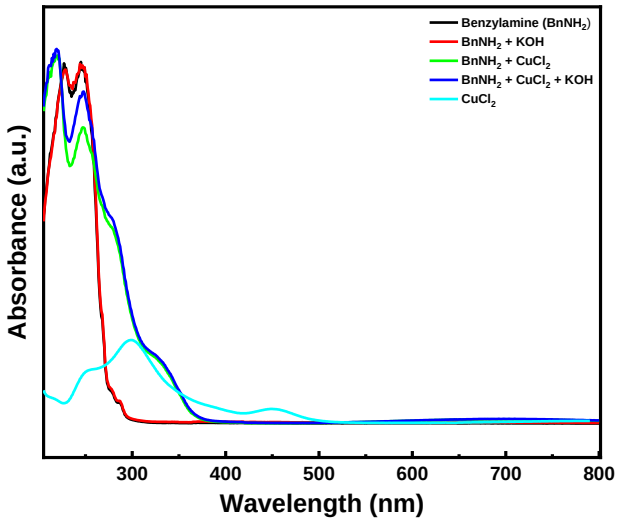


Figure S14. Coordination precedes deprotonation (UV-visible spectra evidence).

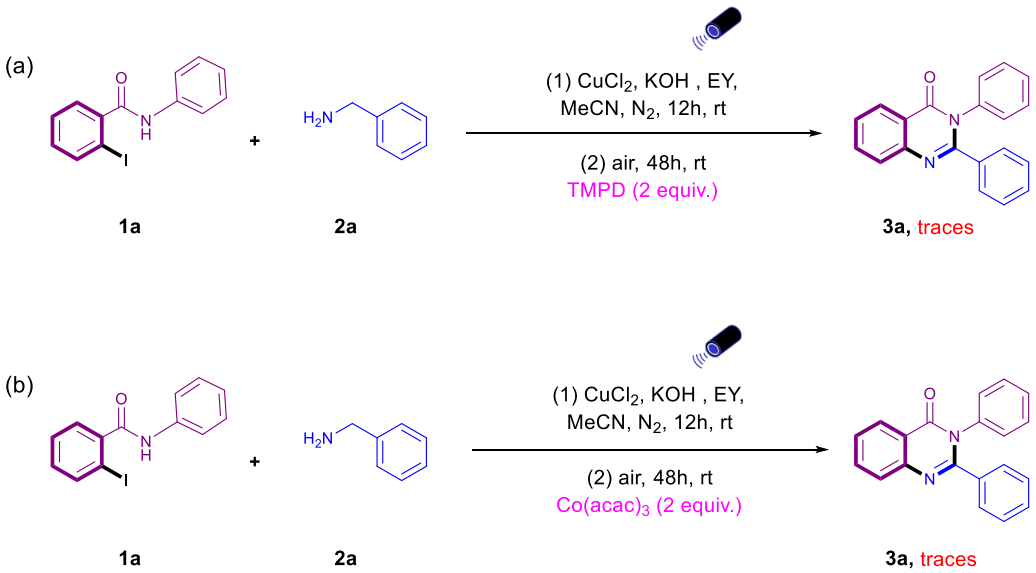
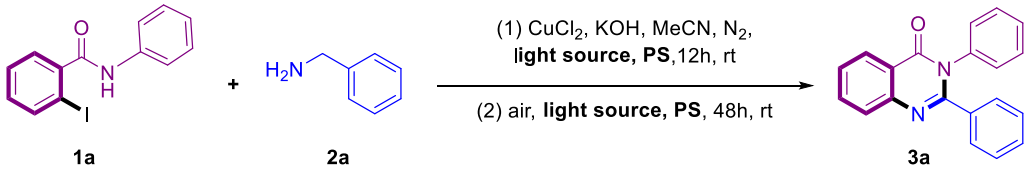


Figure S15. Singlet oxygen quenching experiments.

2. Supporting Tables

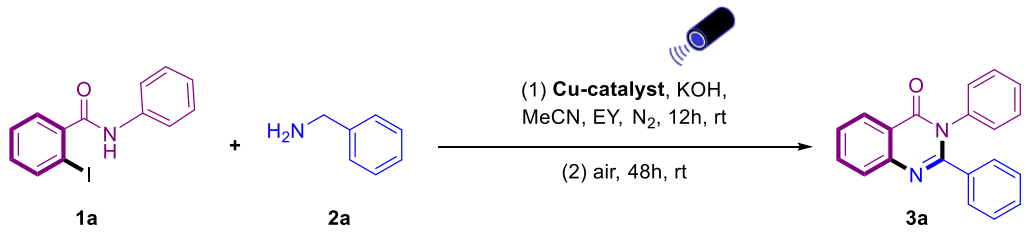
Table S1. Screening of photosensitizers and light sources according to UV-visible absorption spectra[a]



Entry	Photosensitizer (PS)	Light source	Yield (%)[b]
1	**Eosin Y (EY)**	**Blue LED (454 nm)**	**84**
2	EY	Xe lamp (400-700 nm)	62
3	Eosin B (EB)	Blue LED (454 nm)	54
4	Fluorescein (F)	Purple LED (395 nm)	10
5	Tetraphenyl Porphyrin (TPP)	Purple LED (395 nm)	8
6	Rose Bengal (RB)	Green LED (517 nm)	14
7	Tetraphenyl porphyrin (TPP)	Xe lamp (400-700 nm)	52
8	Fluorescein (F)	Xe lamp (400-700 nm)	15
9	Eosin B (EB)	Xe lamp (400-700 nm)	58
10	Rose Bengal (RB)	Xe lamp (400-700 nm)	52
11	EY	--	Trace

[a]Reaction conditions: **1a** (0.3 mmol), **2a** (0.45 mmol), $CuCl_2$ (0.03 mmol), KOH (0.6 mmol), Photosensitizer (0.009 mmol), and anhydrous acetonitrile (3.0 mL) were stirred for 12 h at 25 °C under N_2 and irradiation of visible light, followed by an additional 48 h of stirring under air. [b]Isolated yield.

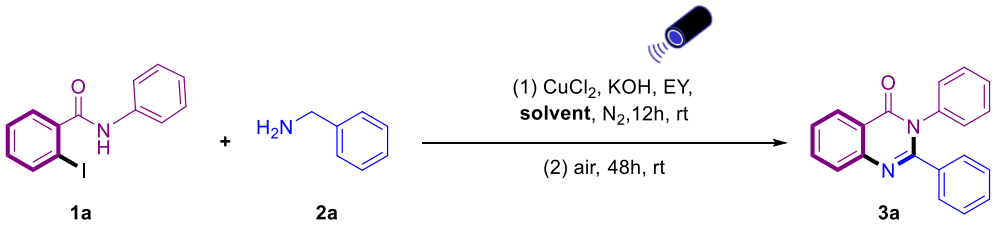
Table S2. Screening of the Cu-catalyst[a]



Entry	Cu-catalyst	Yield (%)[b]
1	**$CuCl_2$**	**84**
2	CuI	49
3	CuCl	17
4	CuBr	48
5	Cu_2O	40
6	$CuSO_4.5H_2O$	50
7	$Cu(NO_3)_2$	50
8	$Cu(OAC)_2$	54
9	Cu^0	12
10	--	0

[a]Reaction conditions: **1a** (0.3 mmol), **2a** (0.45 mmol), Cu-catalyst (0.03 mmol), KOH (0.6 mmol), EY (0.009 mmol), and anhydrous acetonitrile (3.0 mL) were stirred for 12 h at 25 °C under N_2 and irradiation of Blue LED, followed by an additional 48 h of stirring under air. [b]Isolated yield.

Table S3. Screening of Solvent[a]

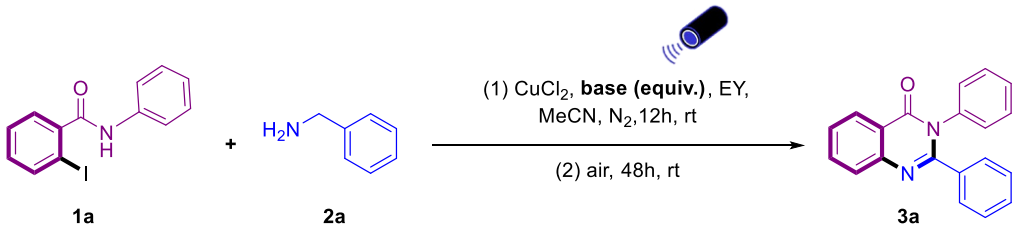


Entry	Solvent	Yield (%)[b]
1	**MeCN**	**84**
2	DMSO	35
3	DMF	10
4	DMF/MeCN (1:1)	<5
5	DMF/MeCN (1:2)	7
6	DMF/MeCN (2:1)	<5

[a]Reaction conditions: **1a** (0.3 mmol), **2a** (0.45 mmol), $CuCl_2$ (0.03 mmol), KOH (0.6 mmol), EY (0.009 mmol), and anhydrous solvent (3.0 mL) were stirred for 12 h at 25 °C under N_2 and irradiation of Blue LED, followed by an additional 48 h of stirring

under air. [b]Isolated yield.

Table S4. Screening of Base[a]

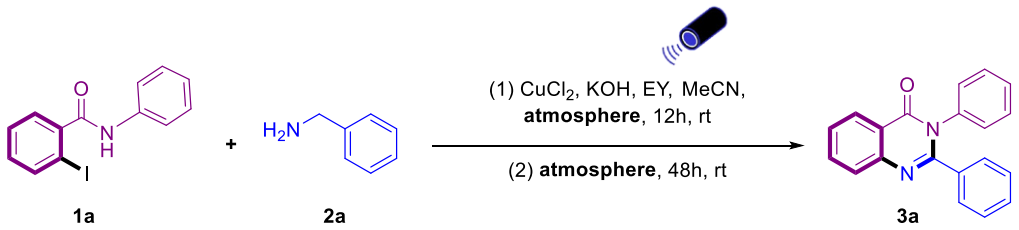


1a 2a 3a

Entry	Base (equiv.)	Yield (%)[b]
1	**KOH (2 equiv.)**	**84**
2	K_2CO_3 (2 equiv.)	34
3	Cs_2CO_3 (2 equiv.)	15
4	NaO-*t*Bu	15
5	K_3PO_4	24
6	Pyridine	10
7	Et_3N	10
8	KOH (3 equiv.)	46
9	KOH (1.5 equiv.)	22
10	KOH (1 equiv.)	12
11	--	0

[a]Reaction conditions: **1a** (0.3 mmol), **2a** (0.45 mmol), $CuCl_2$ (0.03 mmol), base (equiv.), EY (0.009 mmol), and anhydrous acetonitrile (3.0 mL) were stirred for 12 h at 25 °C under N_2 and irradiation of Blue LED, followed by an additional 48 h of stirring under air. [b]Isolated yield.

Table S5. Screening of 1st and 2nd step atmospheres[a]



1a 2a 3a

Entry	Atmosphere of 1st & 2nd steps	Yield (%)[b]
1	**N_2 & air**	**84**
2	N_2 & N_2	10
3	N_2 & O_2	47
4	air & air	19

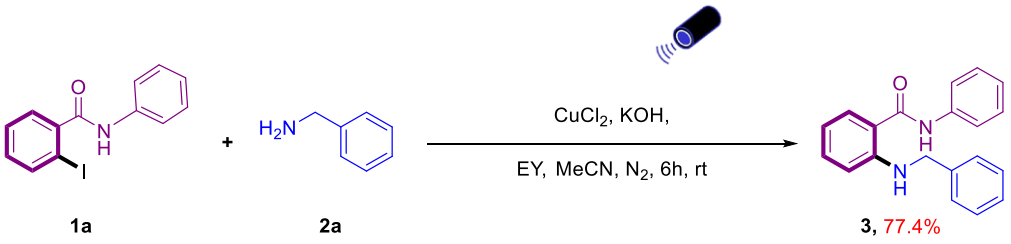
[a]Reaction conditions: **1a** (0.3 mmol), **2a** (0.45 mmol), $CuCl_2$ (0.03 mmol), KOH (0.6 mmol), EY (0.009 mmol), and anhydrous acetonitrile (3.0 mL) were stirred for 12 h at 25 °C under a certain atmosphere and irradiation of Blue LED, followed by an additional 48 h of stirring under a certain atmosphere. [b]Isolated yield.

3. Supporting Methods

Instruments and reagents

^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker 400 MHz or 300 MHz spectrometers. Proton and carbon magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded using tetramethylsilane (TMS) in the solvent of $CDCl_3$ or DMSO-d_6 as the internal standard (^{1}H NMR: TMS at 0.00 ppm, $CDCl_3$ at 7.26 ppm, and DMSO at 2.50 ppm; ^{13}C NMR: TMS at 0.00 ppm, $CDCl_3$ at 77.16 ppm, and DMSO at 39.51 ppm). Melting points were recorded on WRS-1B. Mass spectra were recorded with a Bruker Esquire 6000 using Atmospheric pressure chemical ionization (APCI) and Electrospray ionization (ESI) techniques. The UV−visible absorption spectra were obtained using a Hitachi U-3010 spectrometer. Solvents and substrates were obtained from TCI, Aldrich, Bidepharm, and Macklin. Unless otherwise noted, all the materials and reagents were commercial without further purifications.

Calculation of Apparent Quantum Efficiency (A.Q.E.)



1a **2a** **3**, 77.4%

The apparent quantum efficiency (A.Q.E.) was calculated from the ratio of the number of reacted electrons during the reaction to the number of incident photons as follows:

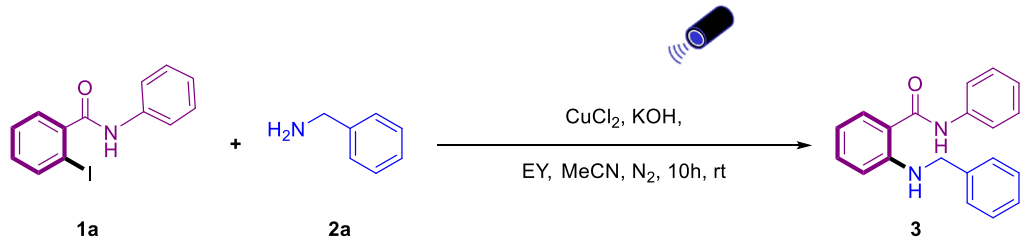
$$E_{photon} = \frac{hc}{\lambda_{inc}} = \frac{6.63 \times 10^{-34} J.s \times 3 \times 10^{8}\, ms^{-1}}{454 \times 10^{-9}\, m} = 4.38 \times 10^{-19} J$$

$$E_{total} = Pst = 15.852 \times 10^{-3}\, w/cm^2 \times 3.14\, cm^2 \times 6 \times 3600 s = 1075.146\, J$$

$$Number\ of\ incident\ photons = \frac{E_{total}}{E_{photon}} = \frac{1075.146\, J}{4.38 \times 10^{-19} J} = 24.54 \times 10^{20} = 4.076\, mmol$$

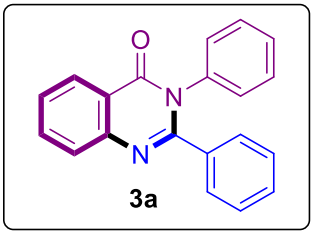
$$A.Q.E\ (\%) = \frac{Number\ of\ product}{Number\ of\ incident\ photons} \times 100 = \frac{0.2322}{4.076} \times 100 = 5.70\%$$

Procedure for the ON-OFF Experiment



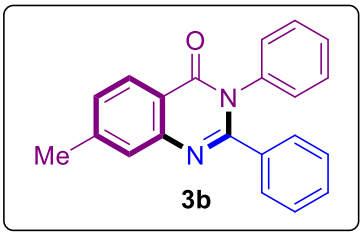
In a 25 mL quartz reaction vial, the following components were added: **1a** (0.3 mmol), **2a** (0.45 mmol), $CuCl_2$ (0.03 mmol), Eosin Y (EY) (0.009 mmol), KOH (0.6 mmol), and anhydrous acetonitrile (3.0 mL). The mixture was stirred for 1 hour at 25 °C under nitrogen (from a balloon) and illuminated with blue LED light. Subsequently, upon cessation of the light source, a 20 μL aliquot of the reaction mixture was extracted for HPLC analysis to evaluate the yield of **3**. The mixture was then stirred for an additional 1 hour at 25 °C under the same nitrogen conditions in a dark environment, followed by another 20 μL sample collection for HPLC analysis. The remaining reaction mixture was stirred alternately under blue LED light and in the dark, with HPLC analyses performed every hour until a total reaction time of 10 hours was achieved, as shown in Figure S9.

4. Characterization Data for Products 3a-3i'



2,3-Diphenyl-4(*3H*)-quinazolinone (3a)[1]

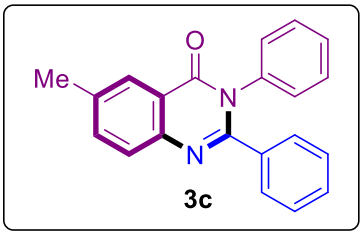
Physical properties: White solid (75.18 mg, 84% yield). Melting Point 155.7-157.5 °C, (lit.[1] mp 156-158 °C). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.75 – 7.67 (m, 2H), 7.42 (m, *J* = 8.2, 6.4, 1.9 Hz, 1H), 7.28 – 7.05 (m, 10H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.27, 155.23, 147.52, 137.71, 135.49, 134.76, 129.32, 129.17, 129.02, 129.00, 128.43, 128.01, 127.76, 127.31, 127.22, 120.99. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{15}N_2O^+$ 299.11; Found 299.14.



7-Methyl-2,3-diphenyl-4(3*H*)-quinazolinone (3b)

Physical properties: White solid (63.72 mg, 68% yield). Melting Point 138.8-140.1 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 (d, *J* = 8.1 Hz, 1H), 7.55 (s, 1H), 7.28 – 7.06 (m, 11H), 2.46 (s, 3H). ^{13}C NMR (101

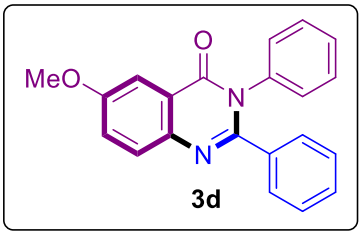
MHz, Chloroform-*d*) δ 162.19, 155.30, 147.53, 145.82, 137.74, 135.50, 129.26, 129.17, 129.00, 128.95, 128.89, 128.36, 127.98, 127.47, 127.07, 118.52, 22.02. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}N_2O^+$ 313.13; Found 313.15.



3c

6-Methyl-2,3-diphenyl-4(3*H*)-quinazolinone (3c)[2]

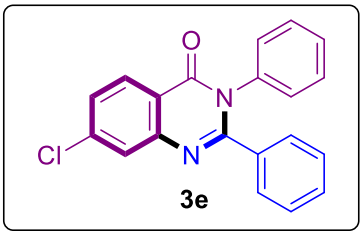
Physical properties: White solid (61.85 mg, 66% yield). Melting Point 174.9-178.1 ℃, (lit.[2] mp 175-179 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 – 7.99 (m, 1H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.52 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.27 – 7.04 (m, 10H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.27, 154.40, 145.50, 137.82, 137.55, 136.20, 135.57, 129.19, 129.02, 128.97, 128.36, 127.97, 127.56, 126.58, 120.68, 21.46. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}N_2O^+$ 313.13; Found 313.16.



3d

6-Methoxy-2,3-diphenyl-4(3*H*)-quinazolinone (3d)[3]

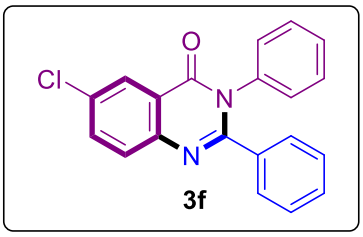
Physical properties: White solid (48.27 mg, 49% yield). Melting Point 202.9-203.7 ℃, (lit.[3] mp 202-204 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 – 7.63 (m, 2H), 7.39 (dd, *J* = 8.9, 3.0 Hz, 1H), 7.34 – 7.08 (m, 10H), 3.91 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.08, 157.73, 151.97, 141.03, 136.77, 134.43, 128.27, 128.08, 128.06, 127.97, 127.90, 127.32, 126.90, 123.83, 120.67, 105.53, 54.81. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}N_2O_2^+$ 329.12; Found 329.17.



3e

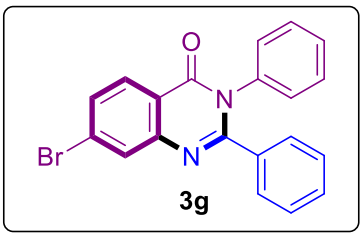
7-Chloro-2,3-diphenyl-4(3*H*)-quinazolinone (3e)[3]

Physical properties: White solid (62.9 mg, 63% yield). Melting Point 184.1-186.7 ℃, (lit.[3] mp 188-189 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.72 (d, *J* = 2.0 Hz, 1H), 7.38 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.27 – 7.06 (m, 10H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.70, 156.48, 148.45, 140.93, 137.40, 135.12, 129.58, 129.07, 129.06, 128.99, 128.70, 128.60, 128.05, 127.88, 127.30, 119.41. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}ClN_2O^+$ 333.07; Found 333.11.



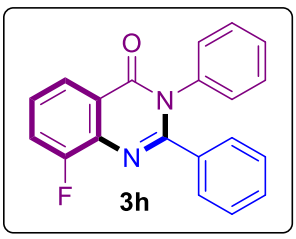
6-Chloro-2,3-diphenyl-4(3*H*)-quinazolinone (3f)

Physical properties: White solid (70.88 mg, 71% yield). Melting Point 178.3-180.1 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.31 (d, *J* = 2.2 Hz, 1H), 7.83 – 7.72 (m, 2H), 7.38 – 7.15 (m, 10H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.30, 155.47, 146.03, 137.42, 135.16, 133.08, 129.50, 129.44, 129.08, 129.02, 128.97, 128.61, 128.04, 127.00, 126.53, 122.05. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}ClN_2O^+$ 333.07; Found 333.11.



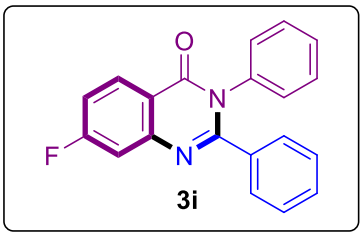
7-Bromo-2,3-diphenyl-4(3*H*)-quinazolinone (3g)

Physical properties: White solid (61.1 mg, 54% yield). Melting Point 138.4-139.3 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 (d, *J* = 8.5 Hz, 1H), 7.91 (d, *J* = 1.9 Hz, 1H), 7.53 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.29 – 7.06 (m, 10H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.85, 156.43, 148.49, 137.40, 135.10, 130.64, 130.50, 129.58, 129.47, 129.06, 129.04, 129.00, 128.68, 128.60, 128.04, 119.77. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}BrN_2O^+$ 377.02; Found 377.05.



8-Fluoro-2,3-diphenyl-4(3*H*)-quinazolinone (3h)

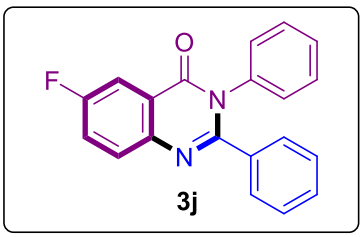
Physical properties: White solid (60.74 mg, 64% yield). Melting Point 185.1-188.2 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 (d, *J* = 7.9 Hz, 1H), 7.58 – 7.45 (m, 2H), 7.38 – 7.15 (m, 10H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.45 (d), 158.58, 156.02, 155.78, 137.49, 137.06 (d), 135.17, 129.52, 129.23, 129.05, 128.59, 127.97, 127.29 (d), 122.89 (d), 122.69 (d), 120.16 (d). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -124.71. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}FN_2O^+$ 317.10; Found 317.15.



3i

7-Fluoro-2,3-diphenyl-4(3*H*)-quinazolinone (3i)[4]

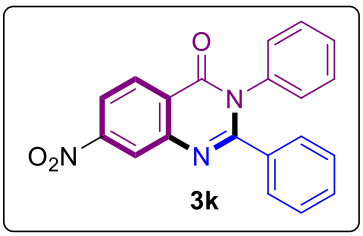
Physical properties: White solid (49.35 mg, 52% yield). Melting Point 206.4-208.7 °C, (lit.[4] mp 207-209 °C). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.28 (dd, *J* = 8.8, 6.0 Hz, 1H), 7.51 – 7.26 (m, 2H), 7.27 – 7.07 (m, 10H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.79 (d), 161.57, 156.54, 149.62 (d), 137.43, 135.13, 130.03 (d), 129.57, 129.10, 129.06, 128.98, 128.58, 128.06, 117.71, 116.07 (d), 113.08 (d). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -102.60. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}FN_2O^+$ 317.10; Found 317.15.



3j

6-Fluoro-2,3-diphenyl-4(3*H*)-quinazolinone (3j)[5]

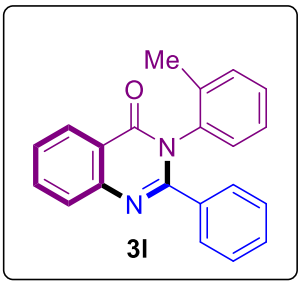
Physical properties: White solid (69.28 mg, 73% yield). Melting Point 158.2-158.5 °C, (lit.[5] mp 153-155 °C). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (dd, *J* = 8.4, 3.0 Hz, 1H), 7.76 (dd, *J* = 8.9, 4.8 Hz, 1H), 7.45 (td, *J* = 8.5, 3.0 Hz, 1H), 7.29 – 7.06 (m, 10H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.44, 161.21 (d), 159.57 (d), 154.56, 144.23 (d), 137.49, 135.23, 130.22 (d), 129.40, 129.06, 128.99, 128.56, 128.03, 123.29 (d), 122.29 (d), 112.07 (d). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -111.88. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}FN_2O^+$ 317.10; Found 317.15.



3k

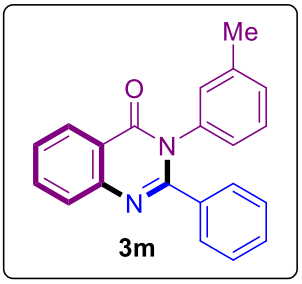
7-Nitro-2,3-diphenyl-4(3*H*)-quinazolinone (3k)

Physical properties: Yellow solid (52.53 mg, 51% yield). Melting Point 168.7-169.4 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.60 (d, *J* = 2.2 Hz, 1H), 8.44 (d, *J* = 8.7 Hz, 1H), 8.21 (dd, *J* = 8.8, 2.2 Hz, 1H), 7.38 – 7.10 (m, 10H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.18, 157.37, 151.89, 148.08, 137.05, 134.65, 129.96, 129.24, 129.20, 129.01, 128.92, 128.85, 128.15, 125.10, 123.39, 120.84. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}N_3O_3^+$ 344.10; Found 344.13.



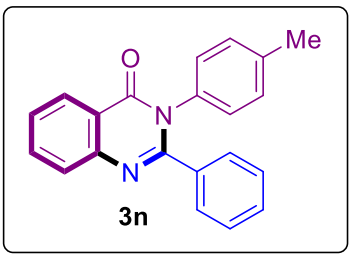
3-(2-Methylphenyl)-2-phenyl-4(3*H*)-quinazolinone (3l)[4]

Physical properties: White solid (69.35 mg, 74% yield). Melting Point 145.4-146.6 °C, (lit.[4] mp 142-143 °C). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.86 – 7.79 (m, 2H), 7.53 (m, *J* = 8.1, 6.7, 1.7 Hz, 1H), 7.34 (dt, *J* = 6.7, 1.6 Hz, 2H), 7.27 – 7.13 (m, 6H), 7.06 (dd, *J* = 7.6, 1.2 Hz, 1H), 2.13 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.84, 155.42, 147.73, 136.88, 135.68, 135.18, 134.77, 131.01, 129.52, 129.06, 128.66, 127.91, 127.79, 127.29, 127.25, 126.70, 120.93, 17.98. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}N_2O^+$ 313.13; Found 313.15.



3-(3-Methylphenyl)-2-phenyl-4(3*H*)-quinazolinone (3m)[6]

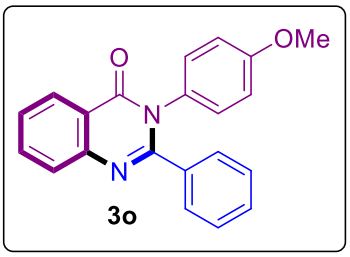
Physical properties: White solid (64.66 mg, 69% yield). Melting Point 141.3-142.5 °C, (lit.[6] mp 145 °C). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.34 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.83 – 7.76 (m, 2H), 7.51 (m, *J* = 8.1, 6.4, 1.9 Hz, 1H), 7.36 – 7.31 (m, 2H), 7.26 – 7.16 (m, 4H), 7.05 (d, *J* = 7.6 Hz, 1H), 6.98 (d, *J* = 2.0 Hz, 1H), 6.92 (dd, *J* = 7.7, 2.1 Hz, 1H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.35, 155.31, 147.51, 138.98, 137.53, 135.53, 134.72, 129.68, 129.29, 129.24, 128.96, 128.78, 127.95, 127.72, 127.27, 127.21, 126.14, 120.99, 21.23. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}N_2O^+$ 313.13; Found 313.15.



3-(4-Methylphenyl)-2-phenyl-4(3*H*)-quinazolinone (3n)[7]

Physical properties: Yellow solid (72.16 mg, 77% yield). Melting Point 166.7-168.9 °C, (lit.[7] mp 168-170 °C). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 – 8.32 (m, 1H), 7.83 – 7.76 (m, 2H), 7.53 – 7.49 (m, 1H), 7.36 – 7.33 (m, 2H), 7.27 – 7.20 (m, 3H), 7.09 (d, *J* = 8.1 Hz, 2H), 7.04 – 7.00 (m, 2H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.43, 155.40, 147.52, 138.36, 135.59, 135.00, 134.69, 129.68,

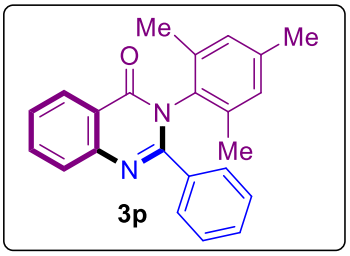
129.26, 129.02, 128.79, 128.00, 127.71, 127.23, 120.98, 21.19. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}N_2O^+$ 313.13; Found 313.15.



3o

3-(4-Methoxyphenyl)-2-phenyl-4(3*H*)-quinazolinone (3o)[4]

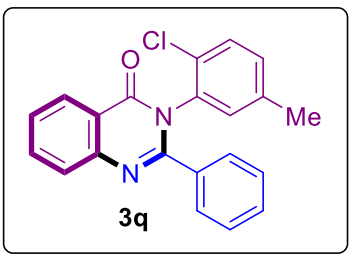
Physical properties: White solid (74.87 mg, 76% yield). Melting Point 194.1-195.4 ℃, (lit.[4] mp 195-197 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 – 8.20 (m, 1H), 7.70 (dd, *J* = 7.0, 1.8 Hz, 2H), 7.47 – 7.40 (m, 1H), 7.35 – 7.24 (m, 2H), 7.13 (d, *J* = 6.9 Hz, 3H), 7.00 – 6.94 (m, 2H), 6.81 – 6.70 (m, 2H), 3.64 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.56, 159.18, 155.55, 147.50, 135.62, 134.69, 130.28, 130.07, 129.25, 129.00, 128.05, 127.70, 127.22, 120.96, 114.25, 55.40. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}N_2O_2^+$ 329.12; Found 329.17.



3p

2-Phenyl-3-(2,4,6-trimethylphenyl)-4(3*H*)-quinazolinone (3p)

Physical properties: Yellow solid (64.34 mg, 63% yield). Melting Point 156.2-159.3 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.37 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.87 – 7.79 (m, 2H), 7.56 – 7.51 (m, 1H), 7.40 – 7.35 (m, 2H), 7.31 – 7.19 (m, 3H), 6.83 (s, 2H), 2.23 (s, 3H), 2.05 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.53, 155.53, 147.95, 138.77, 135.04, 135.02, 134.68, 133.62, 129.70, 129.39, 128.43, 127.77, 127.32, 127.12, 120.86, 21.07, 18.22. ESI m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_2O^+$ 341.16; Found 341.19.

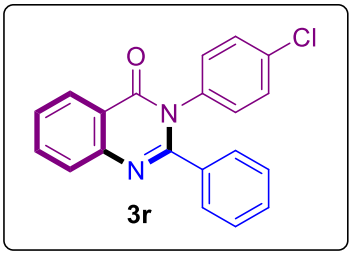


3q

3-(2-Chloro-5-methylphenyl)-2-phenyl-4(3*H*)-quinazolinone (3q)

Physical properties: White solid (58.26 mg, 56% yield). Melting Point 44.3-46.9 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.40 – 8.33 (m, 1H), 7.88 – 7.80 (m, 2H), 7.54 (m, *J* = 8.2, 6.0, 2.3 Hz, 1H), 7.46 – 7.40

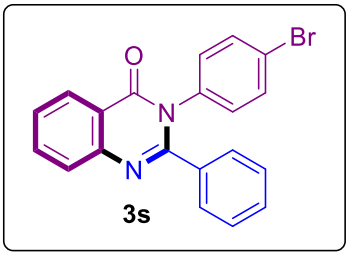
(m, 2H), 7.26 (td, *J* = 7.2, 4.1 Hz, 4H), 7.08 – 7.01 (m, 2H), 2.24 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.57, 155.14, 147.55, 137.76, 135.29, 134.89, 131.49, 131.03, 129.76, 129.69, 129.63, 128.47, 127.92, 127.81, 127.36, 127.29, 120.82, 20.73. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{16}ClN_2O^+$ 347.09; Found 347.13.



3r

3-(4-Chlorophenyl)-2-phenyl-4(3*H*)-quinazolinone (3r)[8]

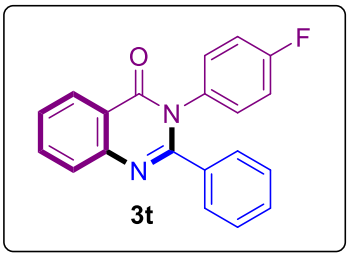
Physical properties: White solid (52.9 mg, 53% yield). Melting Point 188.5-191.2 ℃, (lit.[8] mp 189-191 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.31 (d, *J* = 8.0 Hz, 1H), 7.80 (q, *J* = 3.6, 2.2 Hz, 2H), 7.52 (td, *J* = 5.2, 2.8 Hz, 1H), 7.36 – 7.23 (m, 7H), 7.08 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.15, 154.81, 147.37, 136.19, 135.15, 134.94, 134.36, 130.45, 129.59, 129.24, 128.98, 128.24, 127.80, 127.48, 127.20, 120.75. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}ClN_2O^+$ 333.07; Found 333.11.



3s

3-(4-Bromophenyl)-2-phenyl-4(3*H*)-quinazolinone (3s)[9]

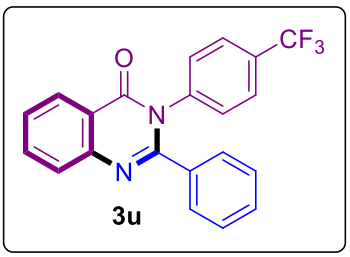
Physical properties: White solid (63.38 mg, 56% yield). Melting Point 229.8-231.1 ℃, (lit.[9] mp 228-230 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.30 (d, *J* = 7.9 Hz, 1H), 7.81 – 7.75 (m, 2H), 7.56 – 7.48 (m, 1H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 7.5 Hz, 2H), 7.28 – 7.21 (m, 3H), 7.02 (d, *J* = 8.2 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.05, 154.73, 147.34, 136.73, 135.13, 134.93, 132.22, 130.79, 129.61, 129.00, 128.26, 127.79, 127.48, 127.20, 122.47, 120.74. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}BrN_2O^+$ 377.02; Found 377.07.



3t

3-(4-Fluorophenyl)-2-phenyl-4(3*H*)-quinazolinone (3t)

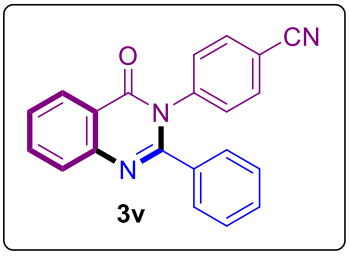
Physical properties: Yellow solid (45.55 mg, 48% yield). Melting Point 121.6-122.8 ℃, (lit.[10] mp 119.4-120 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.35 – 8.30 (m, 1H), 7.83 – 7.78 (m, 2H), 7.52 (m, *J* = 8.2, 5.2, 3.2 Hz, 1H), 7.33 – 7.30 (m, 2H), 7.24 (td, *J* = 9.1, 8.6, 5.7 Hz, 3H), 7.15 – 7.10 (m, 2H), 7.02 – 6.96 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.30, 162.01 (d), 155.06, 147.41, 135.29, 134.88, 133.59 (d), 130.86 (d), 129.47, 128.97, 128.18, 127.79, 127.43, 127.19, 120.83, 116.06 (d). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -112.32. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}FN_2O^+$ 317.10; Found 317.15.



3u

2-Phenyl-3-[(4-trifluoromethyl) phenyl]-4(3*H*)-quinazolinone (3u)[8]

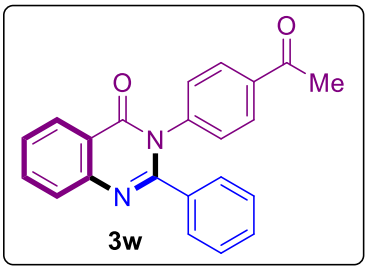
Physical properties: White solid (75.83 mg, 69% yield). Melting Point 162.2-163.8 ℃, (lit.[8] mp 161-163 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.26 (d, *J* = 7.9 Hz, 1H), 7.75 (d, *J* = 4.0 Hz, 2H), 7.51 (s, 1H), 7.49 – 7.44 (m, 2H), 7.30 – 7.15 (m, 7H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.99, 154.47, 147.33, 140.90, 135.07, 134.90, 130.52 (d), 129.78, 128.98, 128.28, 127.87, 127.61, 127.23, 126.10 (q), 123.56 (q), 120.70. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.67. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{14}F_3N_2O^+$ 367.10; Found 367.15.



3v

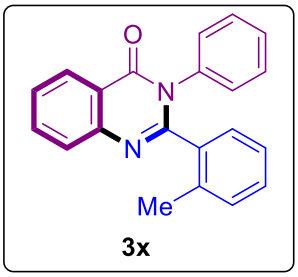
4-(4-Oxo-2-phenylquinazolin-3(4*H*)-yl) benzonitrile (3v)

Physical properties: White solid (56.26 mg, 58% yield). Melting Point 225.6-227.1 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 – 8.20 (m, 1H), 7.80 – 7.72 (m, 2H), 7.51 (d, *J* = 8.2 Hz, 2H), 7.47 (m, *J* = 8.3, 5.3, 3.0 Hz, 1H), 7.27 – 7.16 (m, 7H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.80, 154.06, 147.24, 141.79, 135.23, 134.71, 132.79, 130.28, 129.92, 128.95, 128.41, 127.93, 127.76, 127.22, 120.56, 117.87, 112.37. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{14}N_3O^+$ 324.11; Found 324.15.



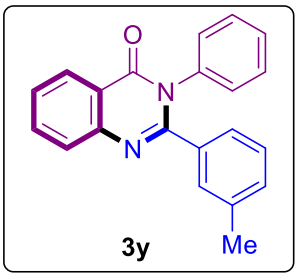
3-(4-Acetylphenyl)-2-phenylquinazolin-4(3*H*)-one (3w)[11]

Physical properties: White solid (44.94 mg, 44% yield). Melting Point 221.6-223.1 ℃, (lit.[11] mp 220-223 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 (d, *J* = 7.9 Hz, 1H), 7.84 – 7.81 (m, 2H), 7.77 (s, 1H), 7.50 – 7.46 (m, 1H), 7.26 (d, *J* = 7.4 Hz, 2H), 7.21 – 7.13 (m, 6H), 2.50 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.03, 160.02, 152.50, 145.32, 139.84, 134.54, 133.05, 132.97, 127.70, 127.51, 127.02, 126.94, 126.27, 125.84, 125.57, 125.22, 118.69, 24.71. ESI m/z: $[M+H]^+$ Calcd for $C_{22}H_{17}N_2O_2^+$ 341.12; Found 341.15.



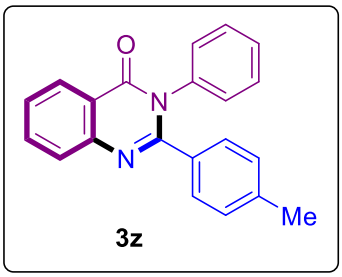
2-(2-Methylphenyl)-3-phenyl-4(3*H*)-quinazolinone (3x)[12]

Physical properties: White solid (44.05 mg, 47% yield). Melting Point 177.1-177.9 ℃, (lit.[12] mp 179-180 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (dt, *J* = 8.1, 1.2 Hz, 1H), 7.87 – 7.80 (m, 2H), 7.56 (dq, *J* = 8.2, 4.4 Hz, 1H), 7.33 – 7.22 (m, 3H), 7.17 – 7.01 (m, 6H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.28, 155.29, 147.32, 137.07, 135.27, 134.88, 134.78, 130.28, 129.21, 128.89, 128.61, 127.68, 127.38, 127.19, 125.28, 121.18, 19.82. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}N_2O^+$ 313.13; Found 313.15.



2-(3-Methylphenyl)-3-phenyl-4(3*H*)-quinazolinone (3y)

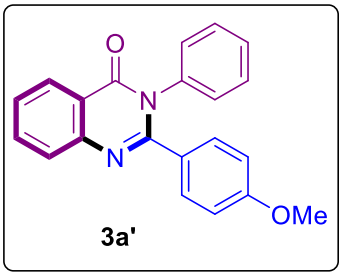
Physical properties: White solid (60.91 mg, 65% yield). Melting Point 159.3-161.5 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.88 – 7.79 (m, 2H), 7.58 – 7.51 (m, 1H), 7.37 – 7.27 (m, 3H), 7.22 (s, 1H), 7.18 – 7.14 (m, 2H), 7.05 (d, *J* = 1.5 Hz, 3H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.31, 155.46, 147.45, 137.87, 137.71, 135.21, 134.76, 130.12, 129.67, 129.11, 128.94, 128.42, 127.78, 127.69, 127.26, 127.23, 126.11, 120.94, 21.26. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}N_2O^+$ 313.13; Found 313.15.



3z

2-(4-Methylphenyl)-3-phenyl-4(3*H*)-quinazolinone (3z)[9]

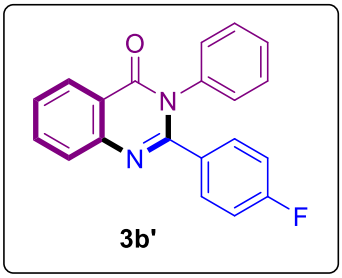
Physical properties: White solid (52.48 mg, 56% yield). Melting Point 175.4-177.3 ℃, (lit.[9] mp 174-176 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 – 8.31 (m, 1H), 7.86 – 7.77 (m, 2H), 7.52 (m, *J* = 8.1, 6.4, 1.9 Hz, 1H), 7.38 – 7.22 (m, 5H), 7.19 – 7.14 (m, 2H), 7.01 (d, *J* = 7.8 Hz, 2H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.39, 155.34, 147.52, 139.53, 137.82, 134.73, 132.53, 129.14, 129.02, 129.00, 128.68, 128.37, 127.67, 127.21, 127.17, 120.87, 21.33. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}N_2O^+$ 313.13; Found 313.15.



3a'

2-(4-Methoxyphenyl)-3-phenyl-4(3*H*)-quinazolinone (3a')[8]

Physical properties: White solid (70.93 mg, 72% yield). Melting Point 152.8-153 ℃, (lit.[8] mp 152-153 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 – 8.30 (m, 1H), 7.79 (dd, *J* = 6.3, 1.6 Hz, 2H), 7.50 (m, *J* = 8.1, 6.2, 2.1 Hz, 1H), 7.38 – 7.27 (m, 5H), 7.20 – 7.14 (m, 2H), 6.75 – 6.69 (m, 2H), 3.73 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.44, 160.29, 154.97, 147.58, 137.95, 134.70, 130.80, 129.13, 129.03, 128.36, 127.79, 127.61, 127.20, 127.04, 120.78, 113.40, 55.27. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}N_2O_2^+$ 329.12; Found 329.17.

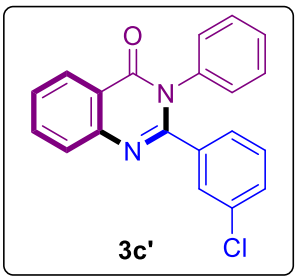


3b'

2-(4-Fluorophenyl)-3-phenyl-4(3*H*)-quinazolinone (3b')[4]

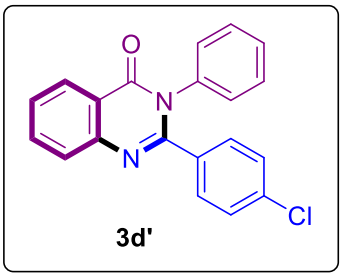
Physical properties: White solid (56 mg, 59% yield). Melting Point 163.1-163.5 ℃, (lit.[4] mp 163-165 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.30 – 8.23 (m, 1H), 7.78 – 7.71 (m, 2H), 7.46 (dd, *J* = 8.3, 4.0 Hz, 1H), 7.30 – 7.21 (m, 5H), 7.10 – 7.05 (m, 2H), 6.82 (t, *J* = 8.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.90 (d), 162.21, 154.20, 147.35, 137.60, 134.84, 131.60 (d), 131.22 (d), 129.16, 129.09, 128.60,

127.70, 127.44, 127.26, 120.93, 115.20 (d). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -110.30. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}FN_2O^+$ 317.10; Found 317.15.



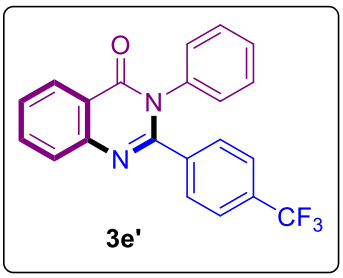
2-(3-Chlorophenyl)-3-phenyl-4(3*H*)-quinazolinone (3c')[8]

Physical properties: White solid (65.9 mg, 66% yield). Melting Point 189.9-192.1 ℃, (lit.[8] mp 184-187 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.26 (d, *J* = 7.9 Hz, 1H), 7.74 (d, *J* = 4.0 Hz, 2H), 7.47 (dd, *J* = 8.1, 4.1 Hz, 1H), 7.34 (t, *J* = 1.8 Hz, 1H), 7.32 – 7.14 (m, 4H), 7.11 – 7.01 (m, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.06, 153.72, 147.25, 137.32, 137.00, 134.90, 134.15, 129.53, 129.28, 129.21, 129.05, 128.76, 127.78, 127.64, 127.28, 127.18, 121.02. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}ClN_2O^+$ 333.07; Found 333.11.



2-(4-Chlorophenyl)-3-phenyl-4(3*H*)-quinazolinone (3d')[7]

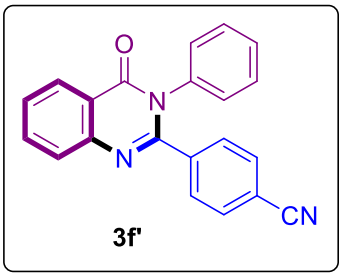
Physical properties: White solid (58.9 mg, 59% yield). Melting Point 176.2-176.8 ℃, (lit.[7] mp 175-177 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.26 (d, *J* = 7.9 Hz, 1H), 7.73 (d, *J* = 4.1 Hz, 2H), 7.46 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.31 – 7.19 (m, 5H), 7.14 – 7.05 (m, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.14, 154.09, 147.29, 137.44, 135.60, 134.88, 133.84, 130.48, 129.22, 129.07, 128.70, 128.31, 127.71, 127.54, 127.27, 120.94. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}ClN_2O^+$ 333.07; Found 333.11.



3-Phenyl-2-[(4-trifluoromethyl) phenyl)-4(3*H*)-quinazolinone (3e')[13]

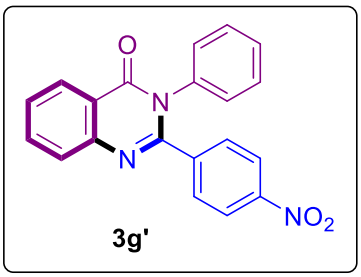
Physical properties: White solid (81.33 mg, 74% yield). Melting Point 150.3-152.7 ℃, (lit.[13] mp 150-151 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.78 – 7.72 (m, 2H), 7.48 (td, *J* = 5.5,

2.6 Hz, 1H), 7.40 (s, 4H), 7.27 – 7.19 (m, 3H), 7.11 – 7.05 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.01, 153.75, 147.22, 138.85, 137.19, 134.95, 131.19 (q), 129.49, 129.29, 129.04, 128.88, 127.82, 127.78, 127.46, 127.29, 125.02 (q), 121.04, 120.90 (q). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.93. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{14}F_3N_2O^+$ 367.10; Found 367.15.



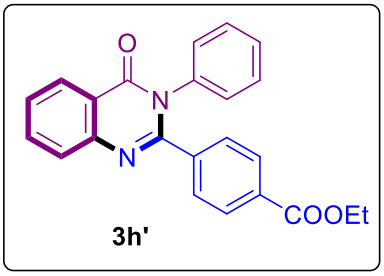
4-(4-Oxo-3-phenyl-3,4-dihydroquinazolin-2-yl) benzonitrile (3f')

Physical properties: White solid (48.5 mg, 50% yield). Melting Point 209.8-212.1 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.37 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.89 – 7.80 (m, 2H), 7.58 (m, *J* = 8.1, 6.6, 1.6 Hz, 1H), 7.54 – 7.44 (m, 4H), 7.35 (d, *J* = 7.1 Hz, 3H), 7.15 (dd, *J* = 7.6, 2.0 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.86, 153.20, 147.13, 139.63, 137.03, 135.05, 131.80, 129.76, 129.39, 129.02, 128.82, 128.00, 127.88, 127.36, 121.08, 118.01, 113.10. ESI m/z: $[M+H]^+$ Calcd for $C_{21}H_{14}N_3O^+$ 324.11; Found 324.15.



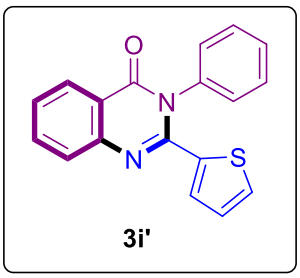
3-Phenyl-2-[(4-nito phenyl)-4(3*H*)-quinazolinone (3g')[8]

Physical properties: White solid (30.9 mg, 30% yield). Melting Point 219.8-222.1 ℃, (lit.[8] mp 221-223 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.37 (dd, *J* = 7.9, 1.5 Hz, 1H), 8.09 – 8.06 (m, 2H), 7.86 – 7.81 (m, 2H), 7.60 – 7.52 (m, 3H), 7.36 – 7.26 (m, 3H), 7.18 – 7.15 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.82, 152.92, 147.81, 147.09, 141.39, 136.99, 135.08, 130.18, 129.45, 129.10, 129.00, 128.09, 127.92, 127.37, 123.23, 121.10. ESI m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}N_3O_3^+$ 344.10; Found 344.15.



Ethyl 4-(4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl) benzoate(3h')

Physical properties: Yellow liquid (64.45 mg, 58% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (d, *J* = 8.0 Hz, 1H), 7.81 – 7.71 (m, 4H), 7.45 (dt, *J* = 8.4, 3.9 Hz, 1H), 7.33 (d, *J* = 8.2 Hz, 2H), 7.25 – 7.15 (m, 4H), 7.08 – 7.04 (m, 2H), 4.24 (q, *J* = 7.1 Hz, 2H), 1.27 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.78, 162.03, 154.26, 147.30, 139.50, 137.32, 134.87, 130.95, 129.17, 129.08, 129.07, 128.72, 127.81, 127.64, 127.26, 121.03, 61.27, 14.27. ESI m/z: $[M+H]^+$ Calcd for $C_{23}H_{19}N_2O_3^+$ 371.14; Found 371.17.



3i'

3-Phenyl-2-(thiophen-2-yl) quinazolin-4(3*H*)-one (3i')[8]

Physical properties: White solid (52.05 mg, 57% yield). Melting Point 175.1-175.9 ℃, (lit.[8] mp 173-175 ℃). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.29 (d, *J* = 7.9 Hz, 1H), 7.78 (d, *J* = 4.0 Hz, 2H), 7.56 – 7.51 (m, 3H), 7.48 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.39 – 7.31 (m, 3H), 6.77 (dd, *J* = 5.1, 3.9 Hz, 1H), 6.37 (d, *J* = 3.9 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.50, 148.69, 147.66, 138.09, 137.76, 134.78, 131.28, 130.80, 129.80, 129.62, 129.22, 127.49, 127.46, 127.18, 126.96, 120.43. ESI m/z: $[M+H]^+$ Calcd for $C_{18}H_{13}N_2OS^+$ 304.07; Found 304.11.

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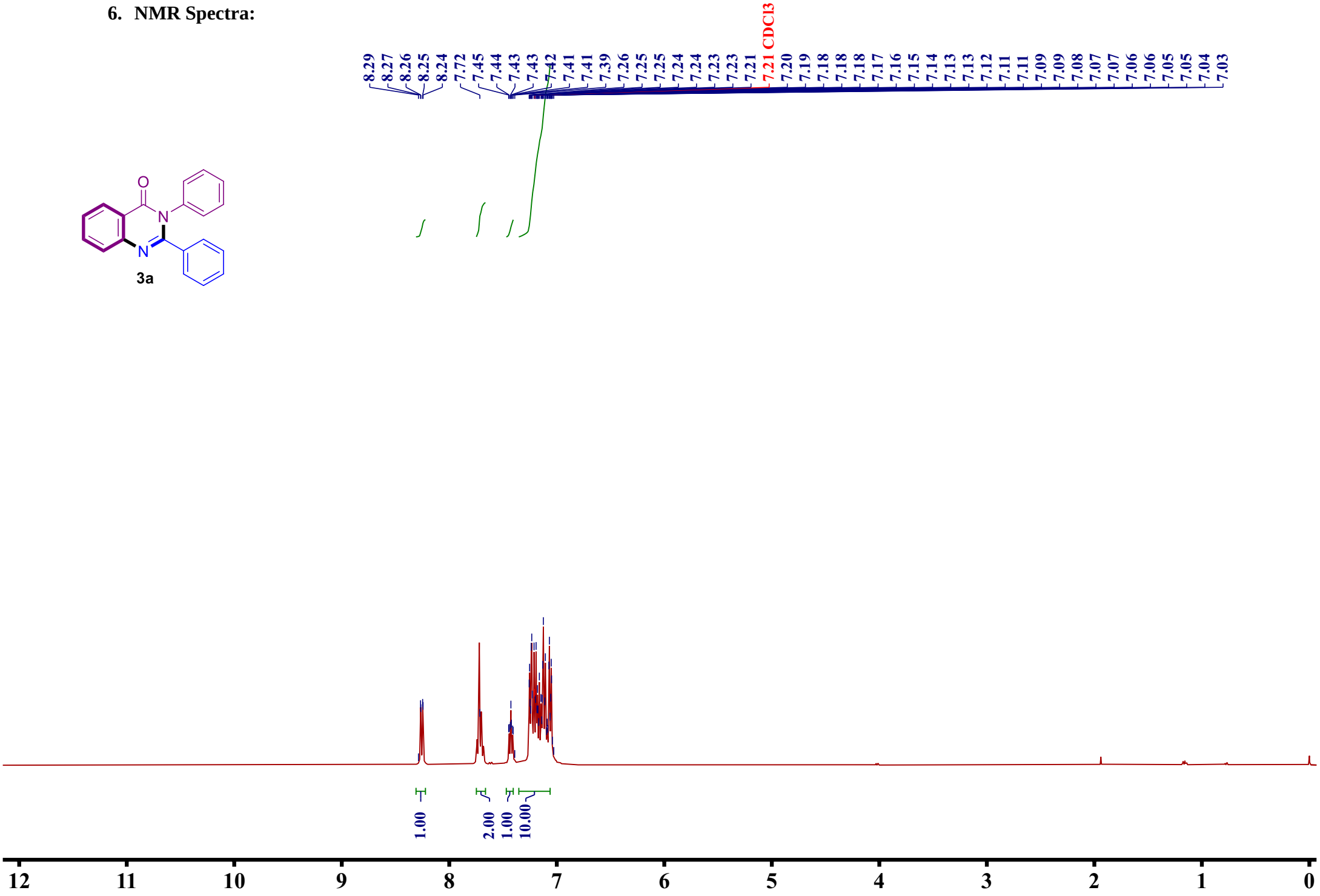
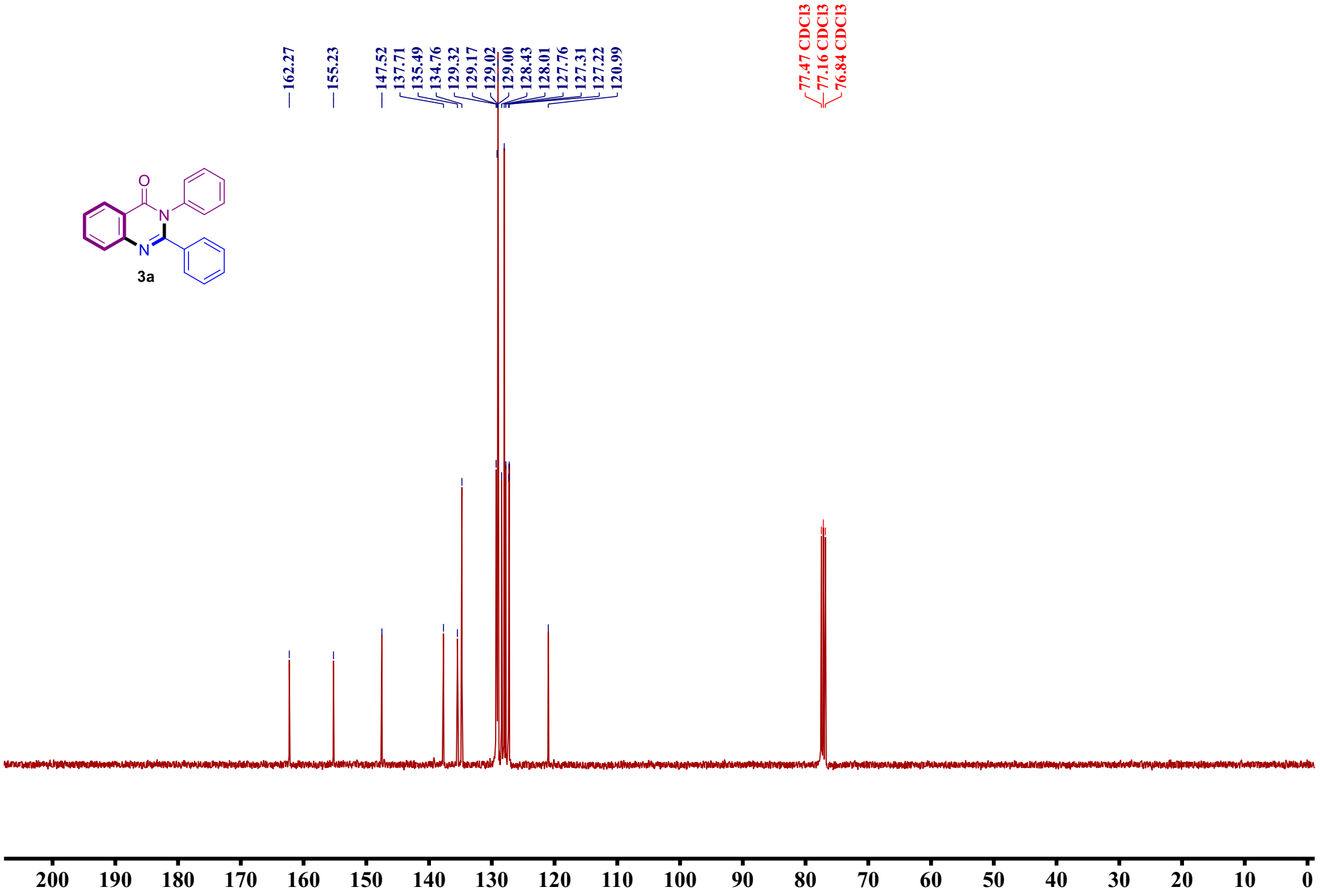
6. NMR Spectra:

3a

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N
N
3a
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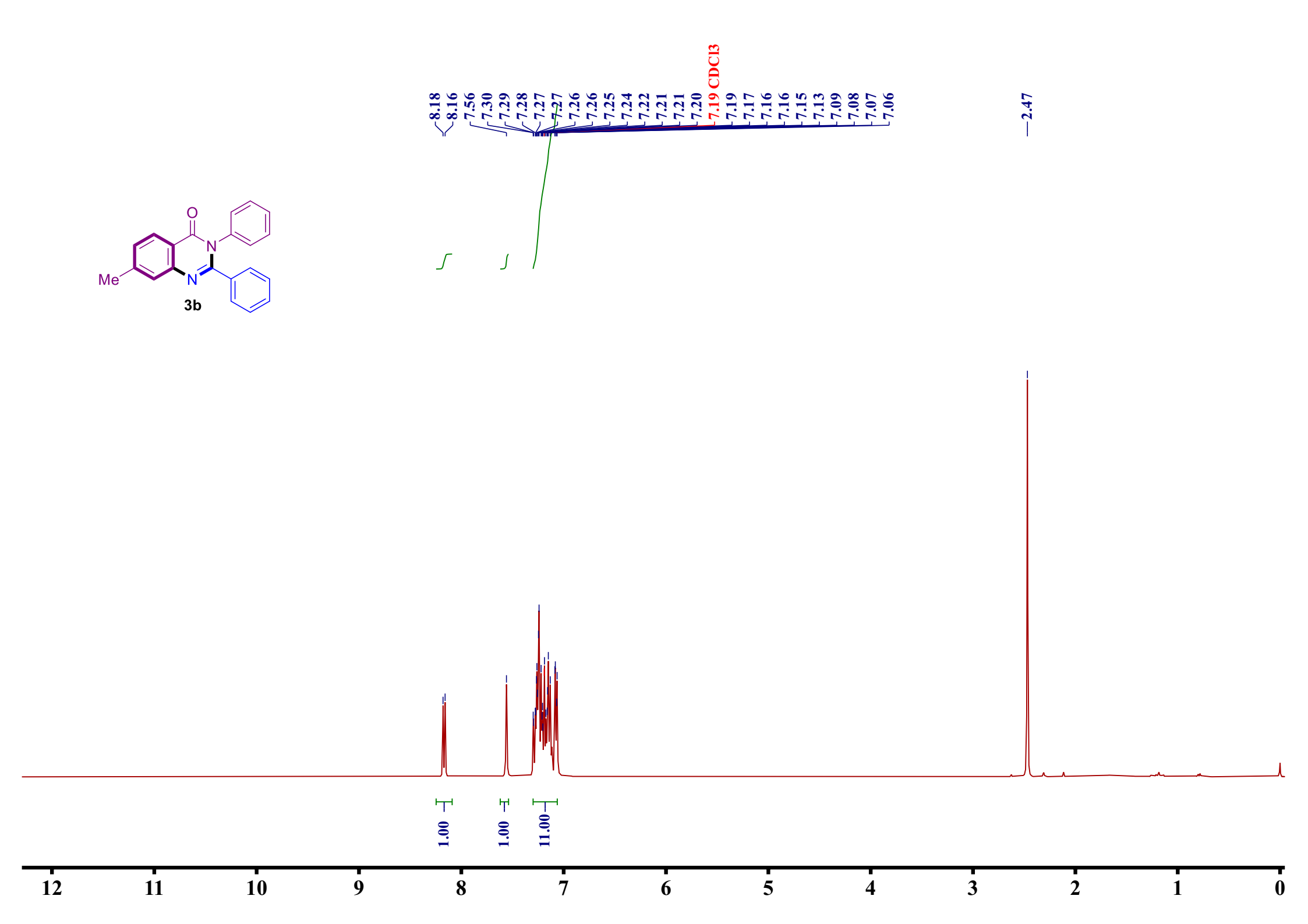
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7.20
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N
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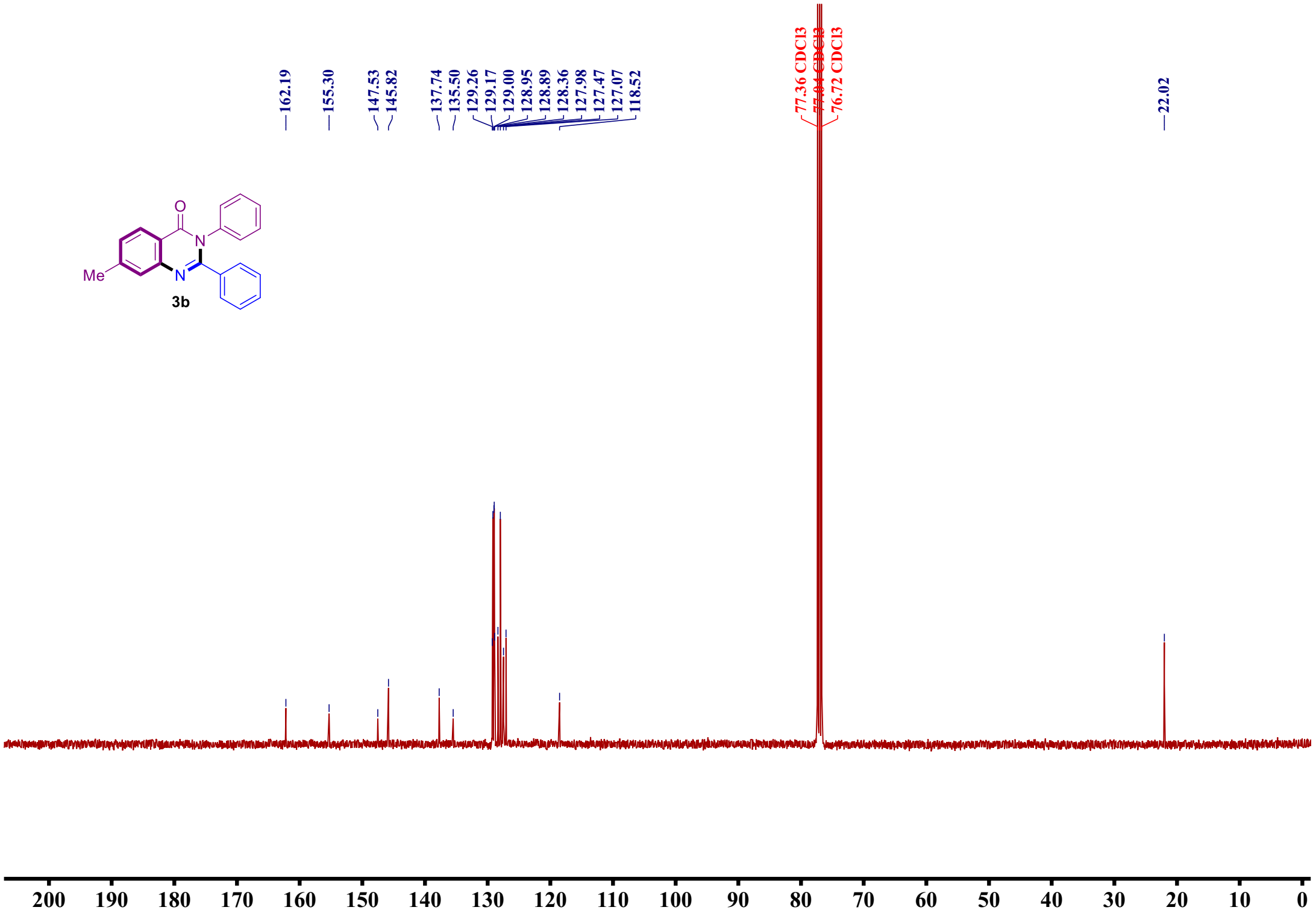
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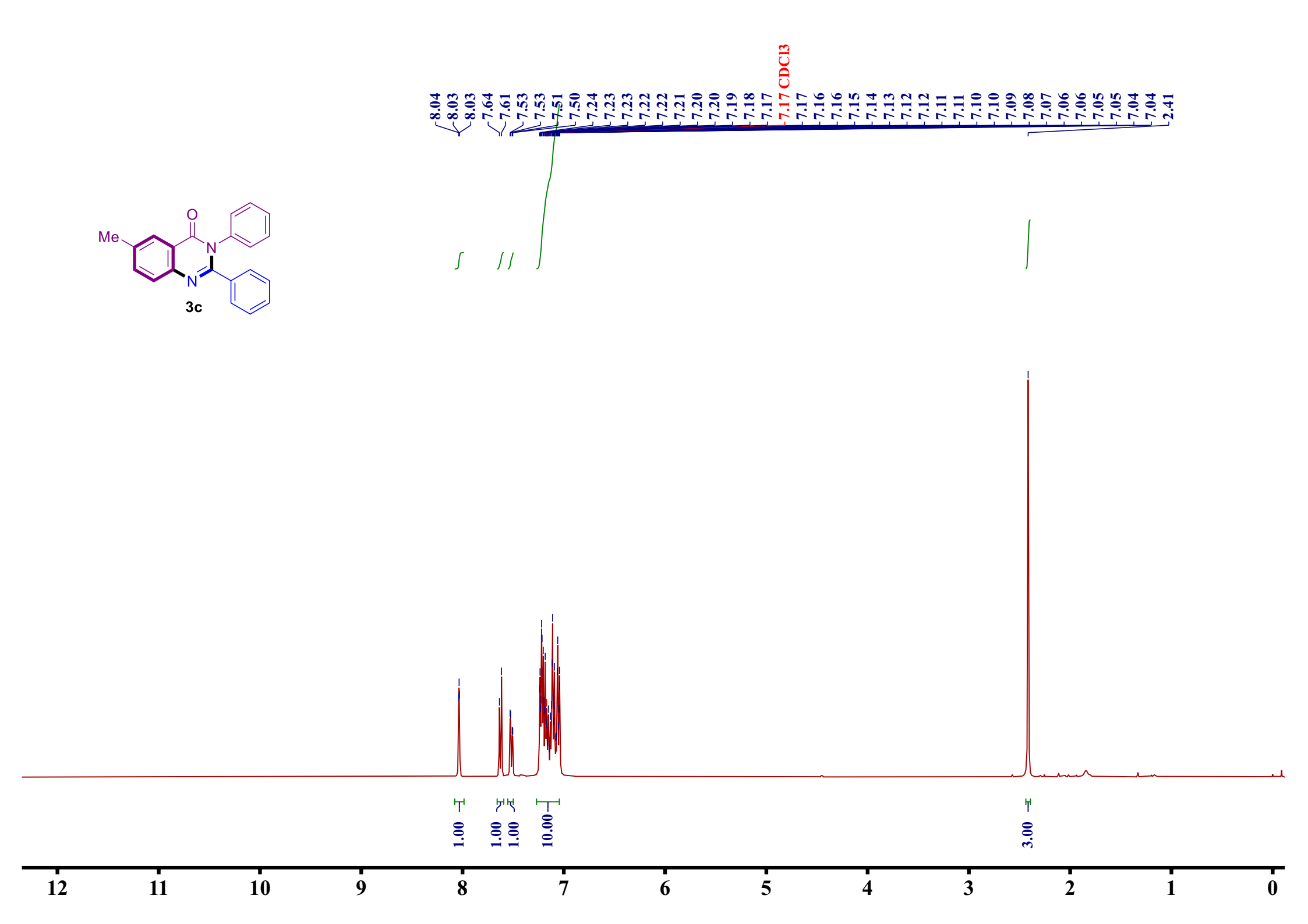
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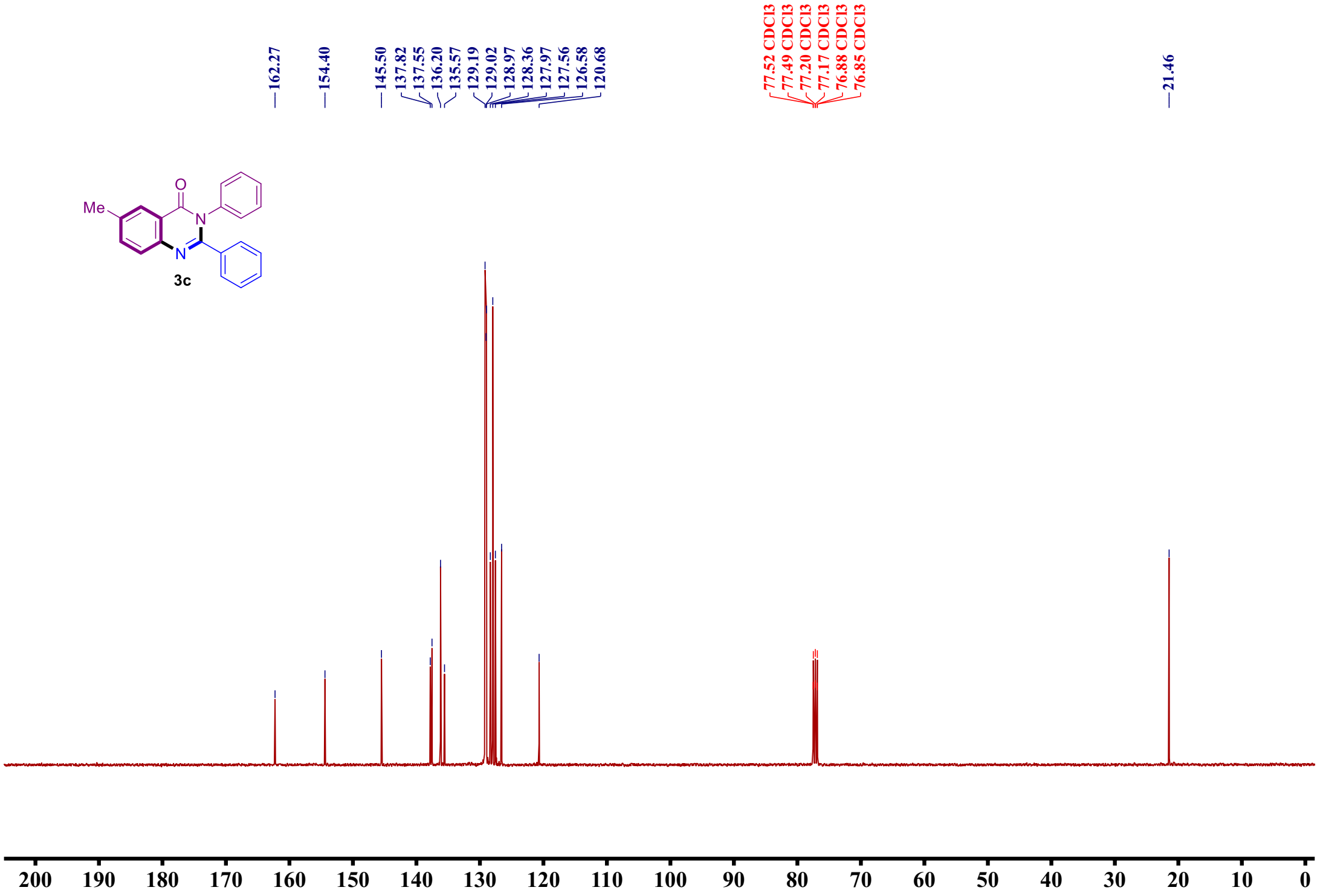
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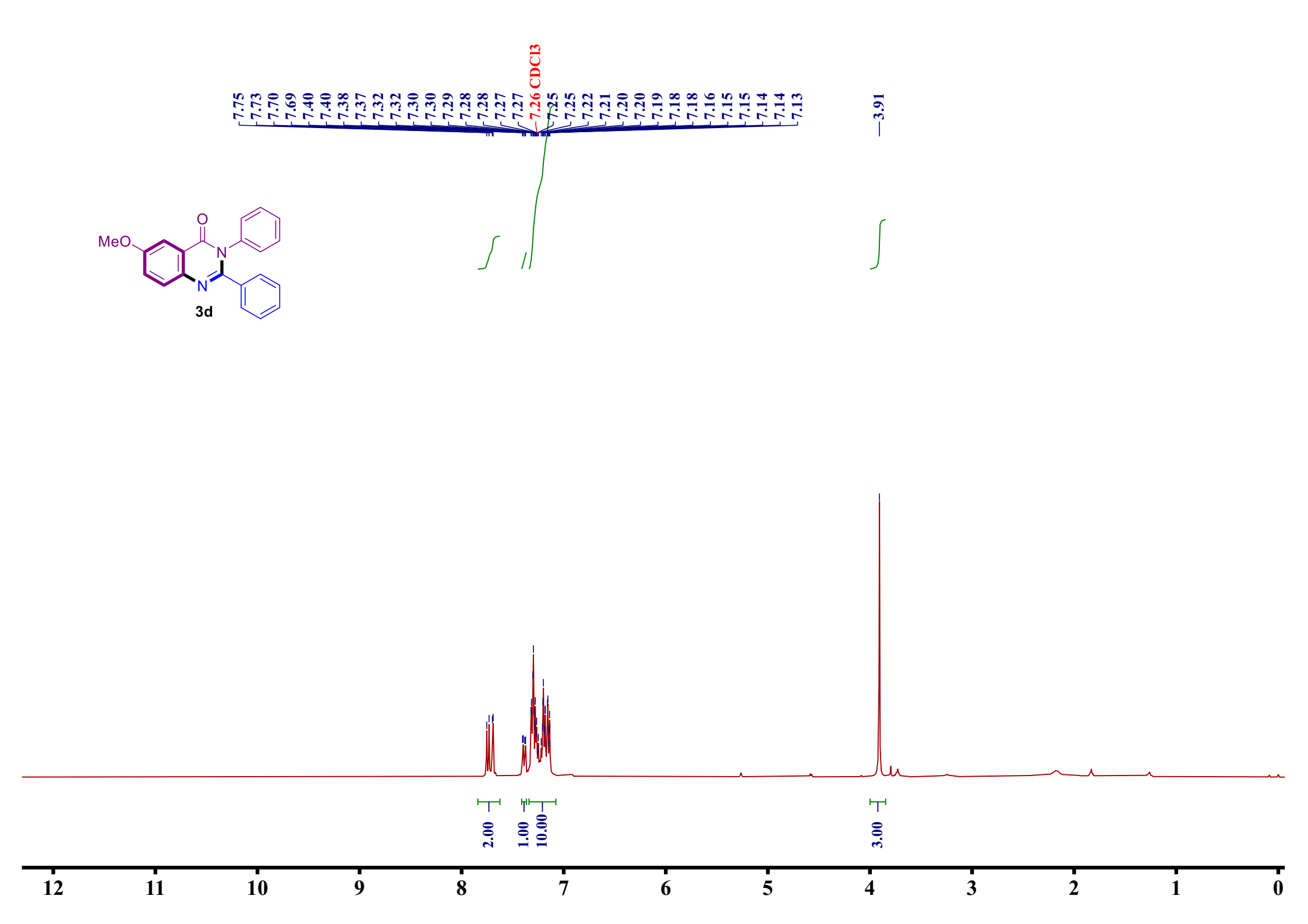
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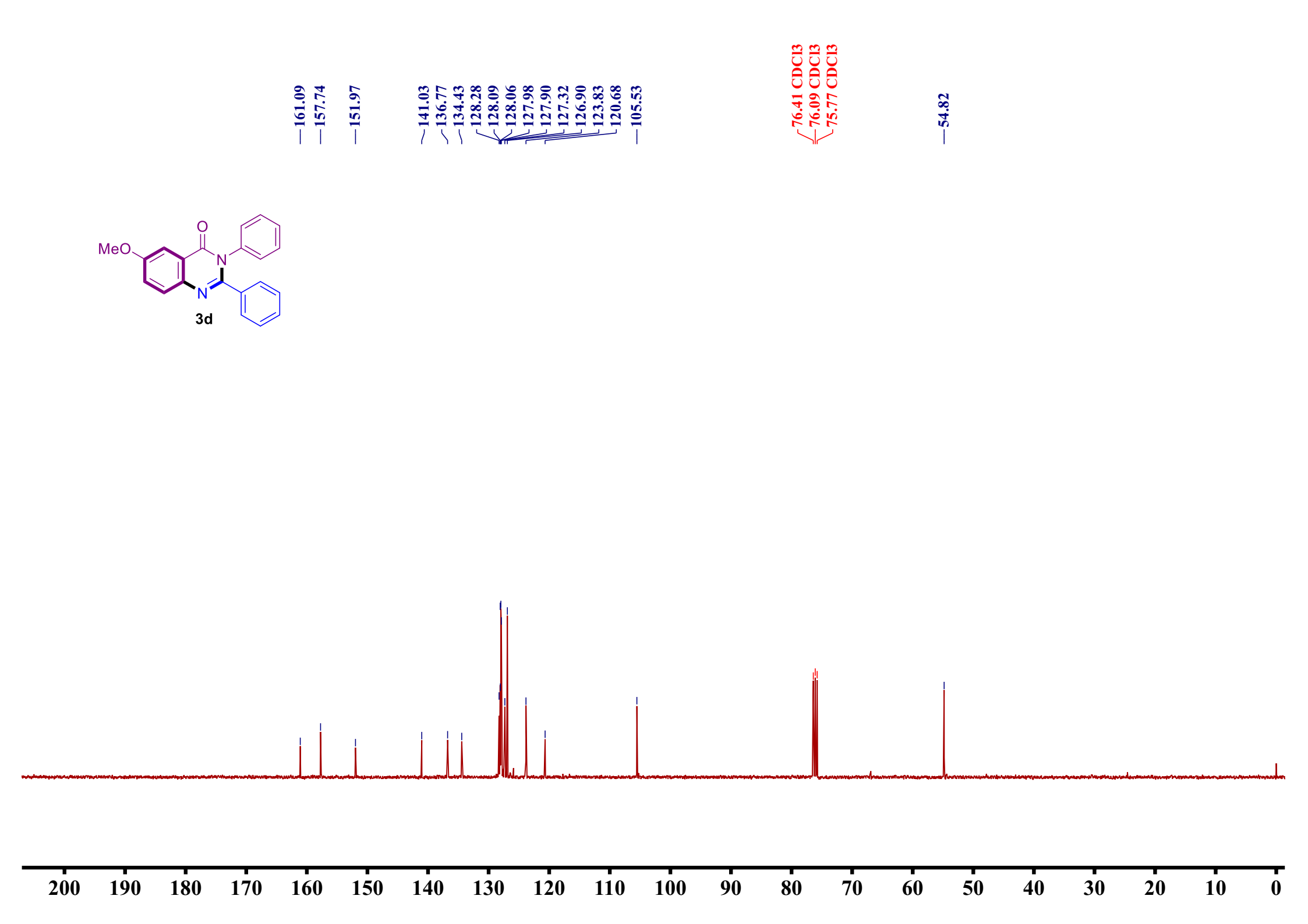
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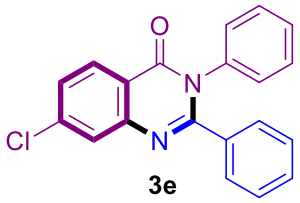

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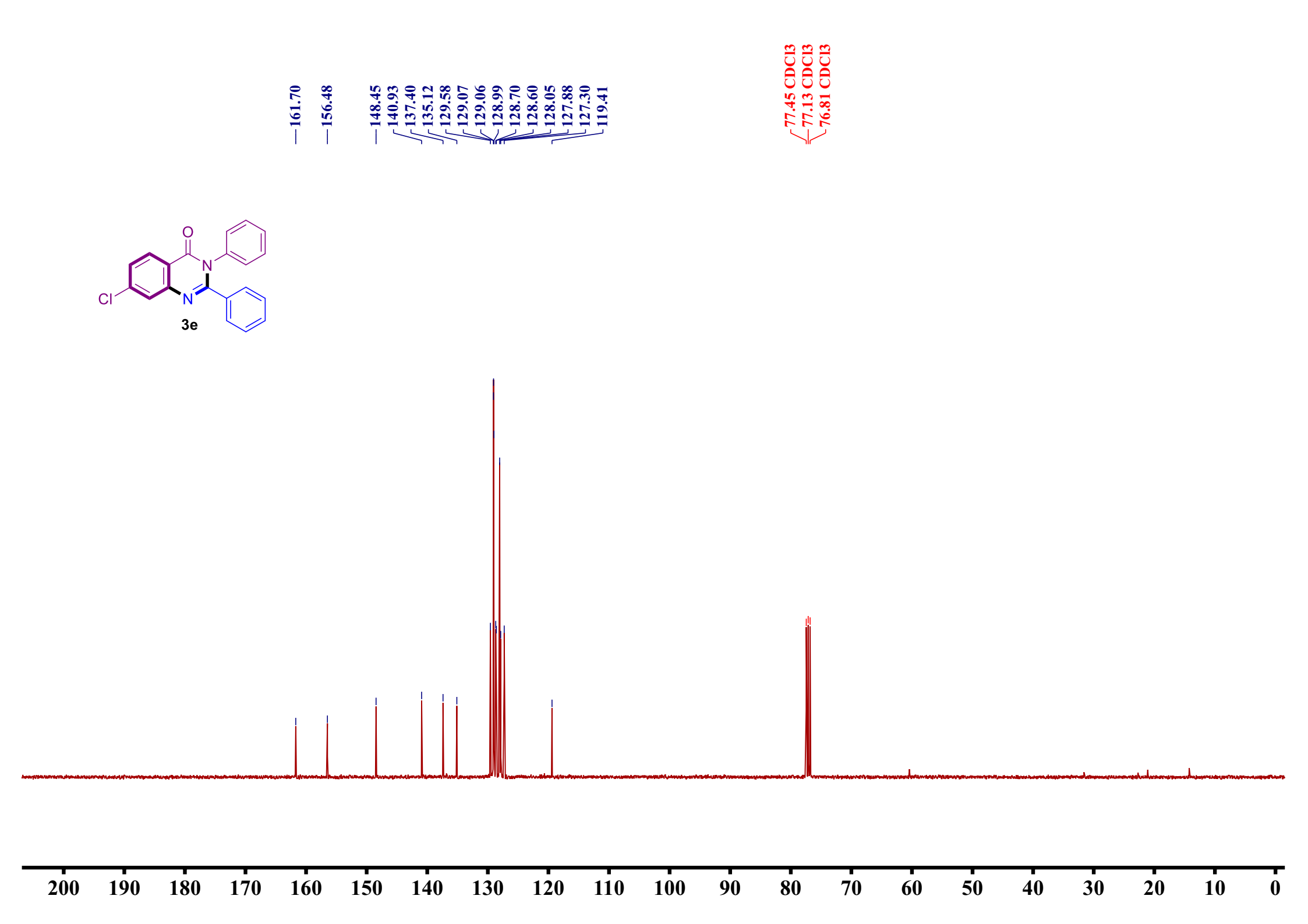
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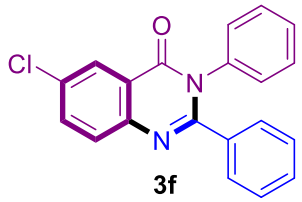

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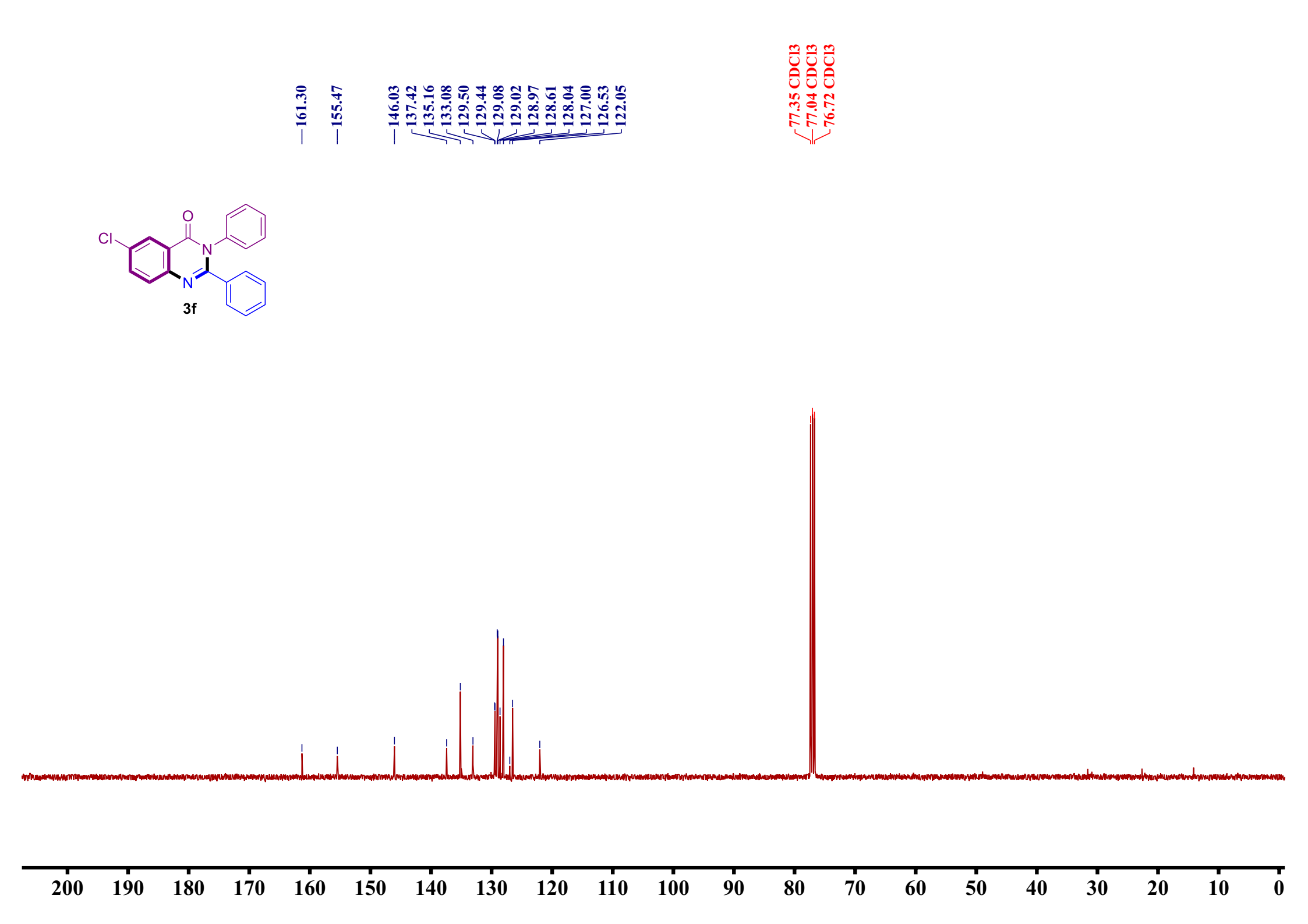
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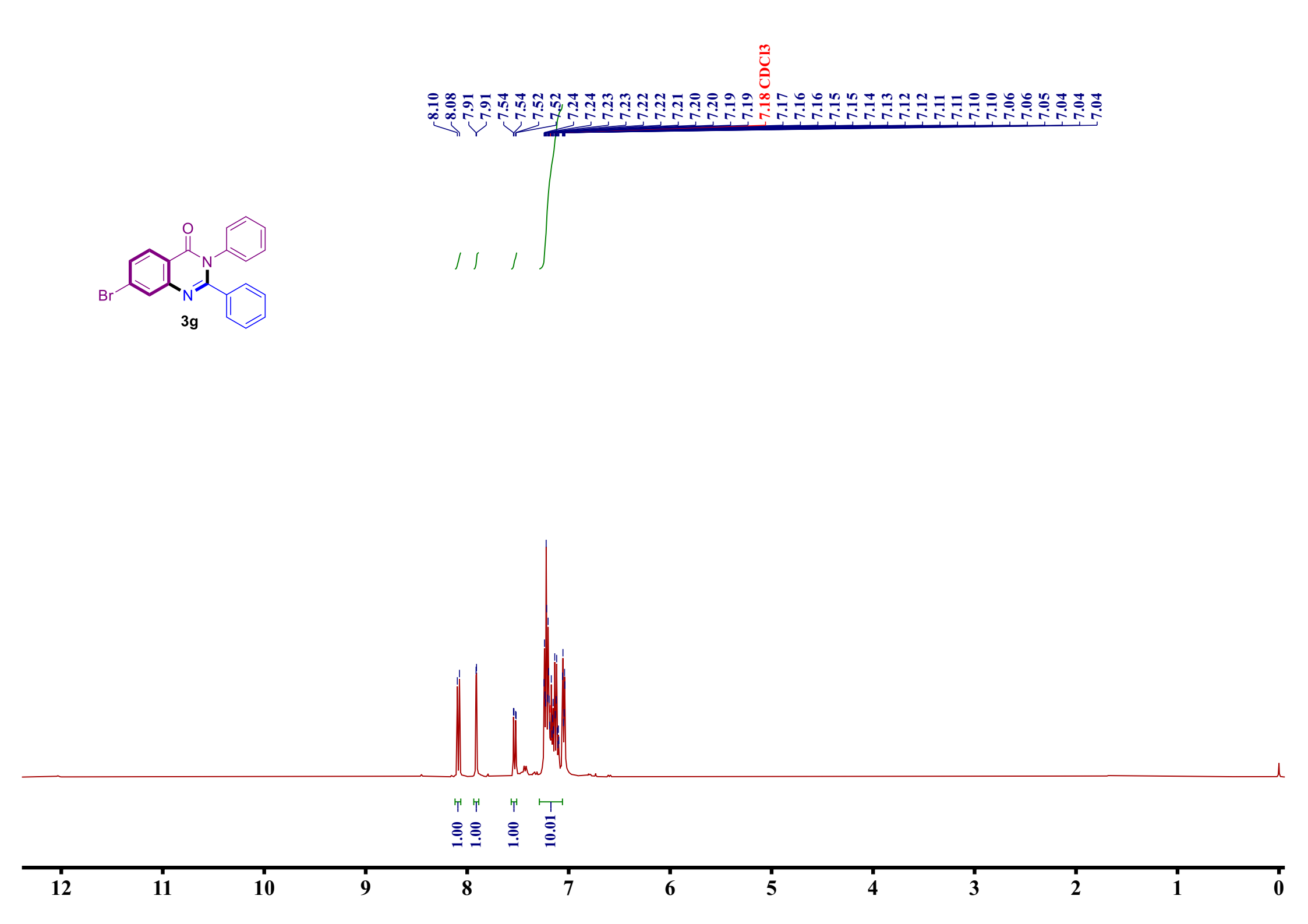
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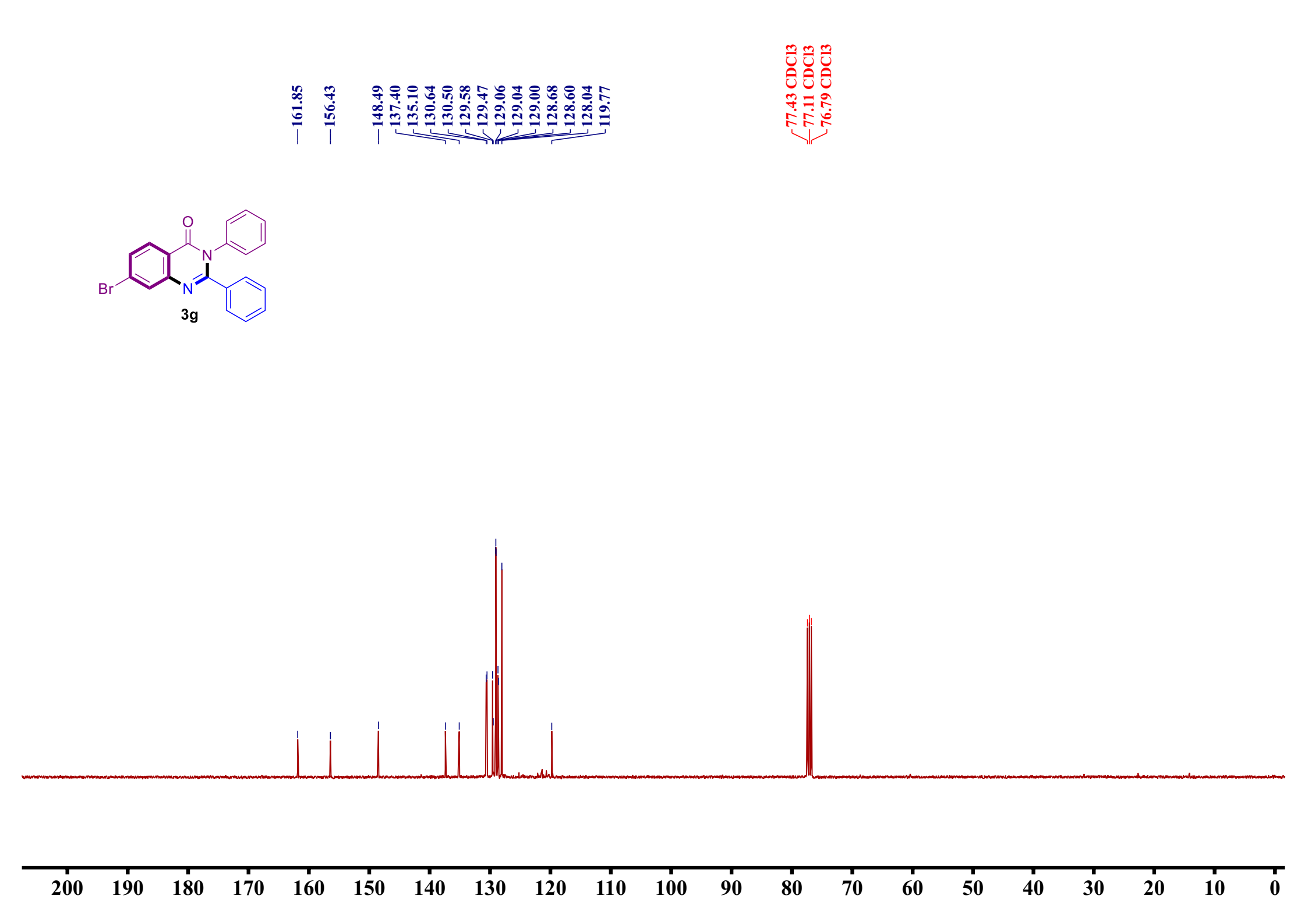
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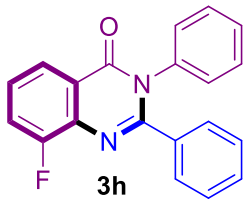

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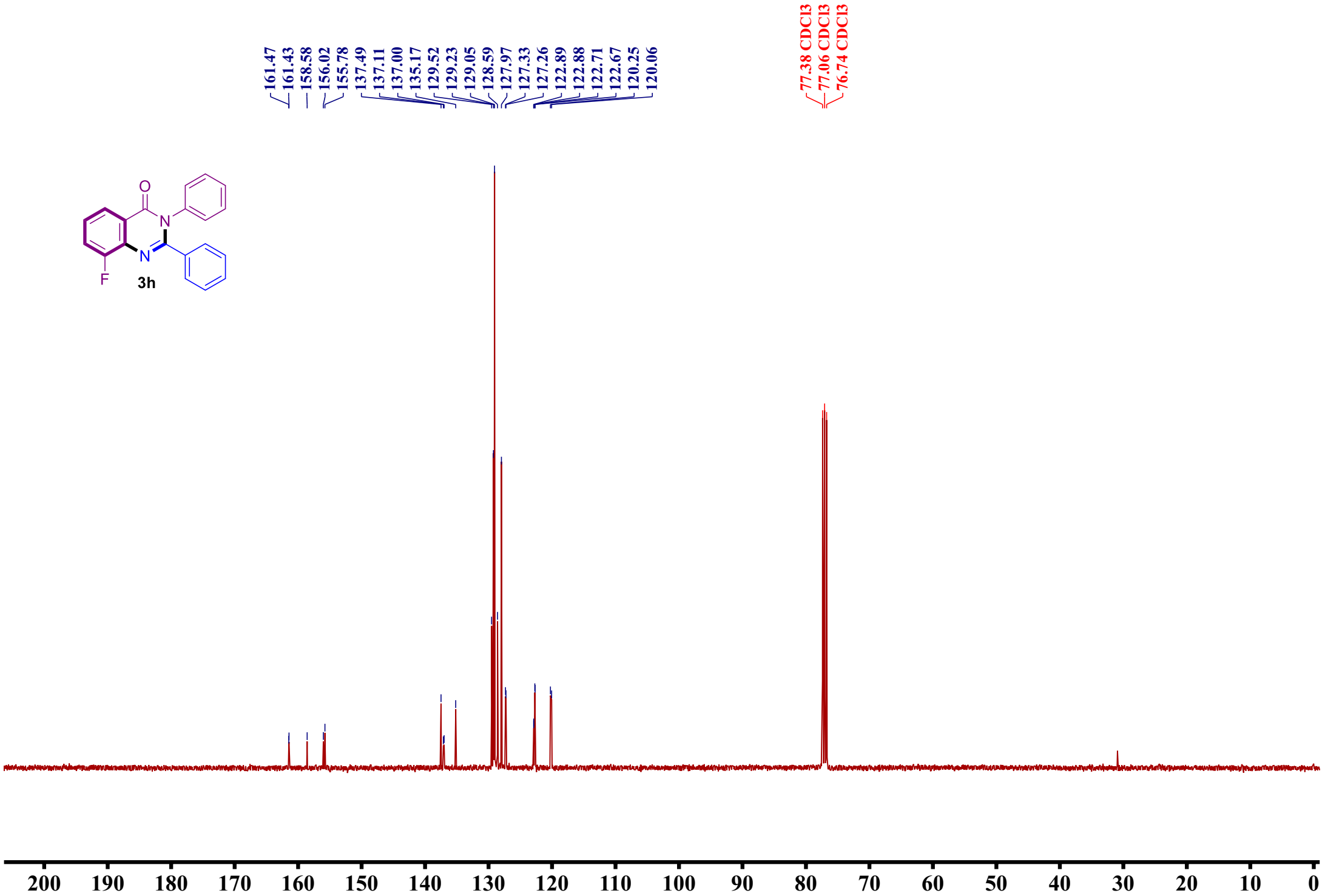
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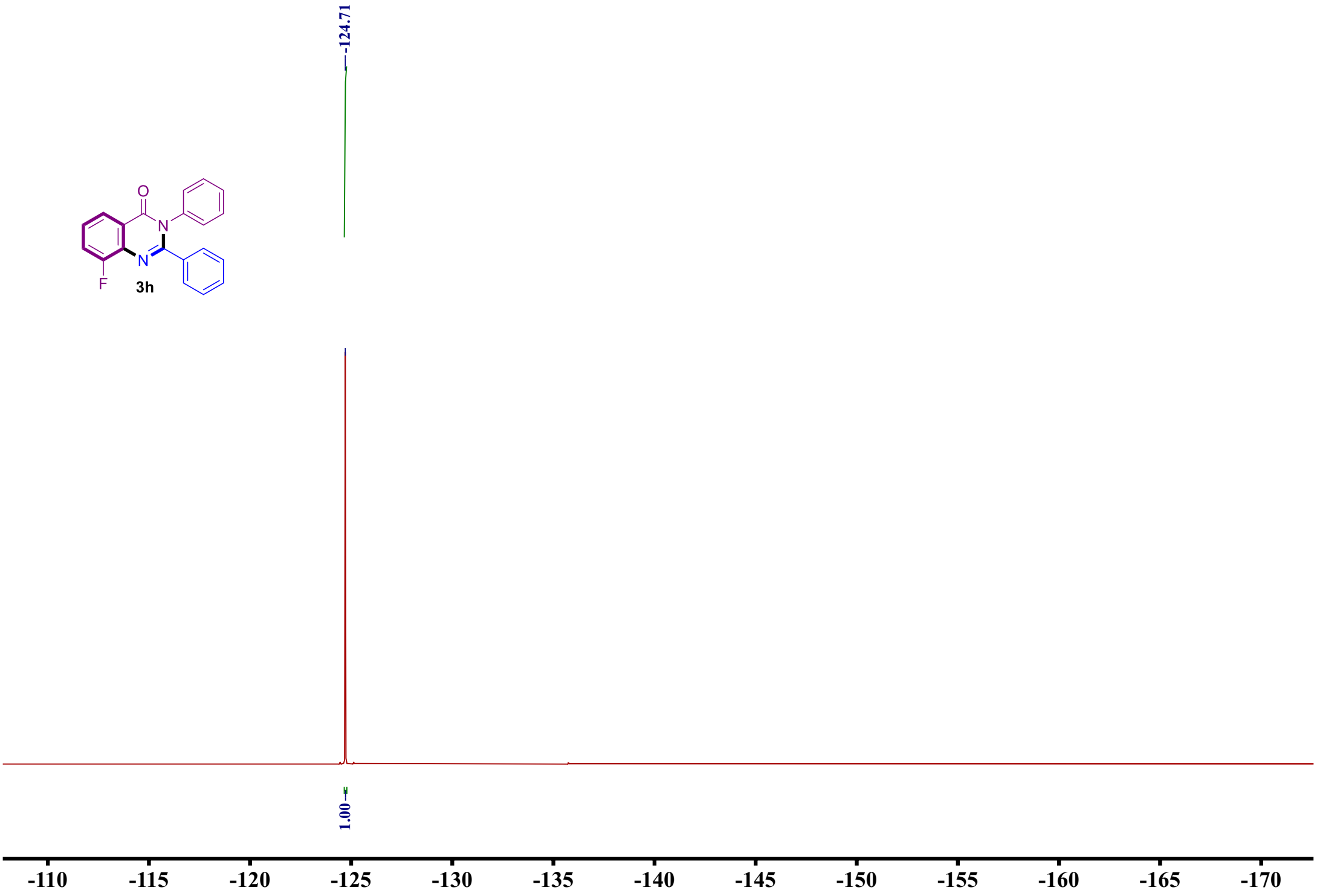
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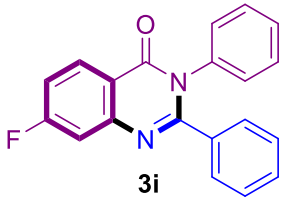

3i

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1.70 H2O

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2.00
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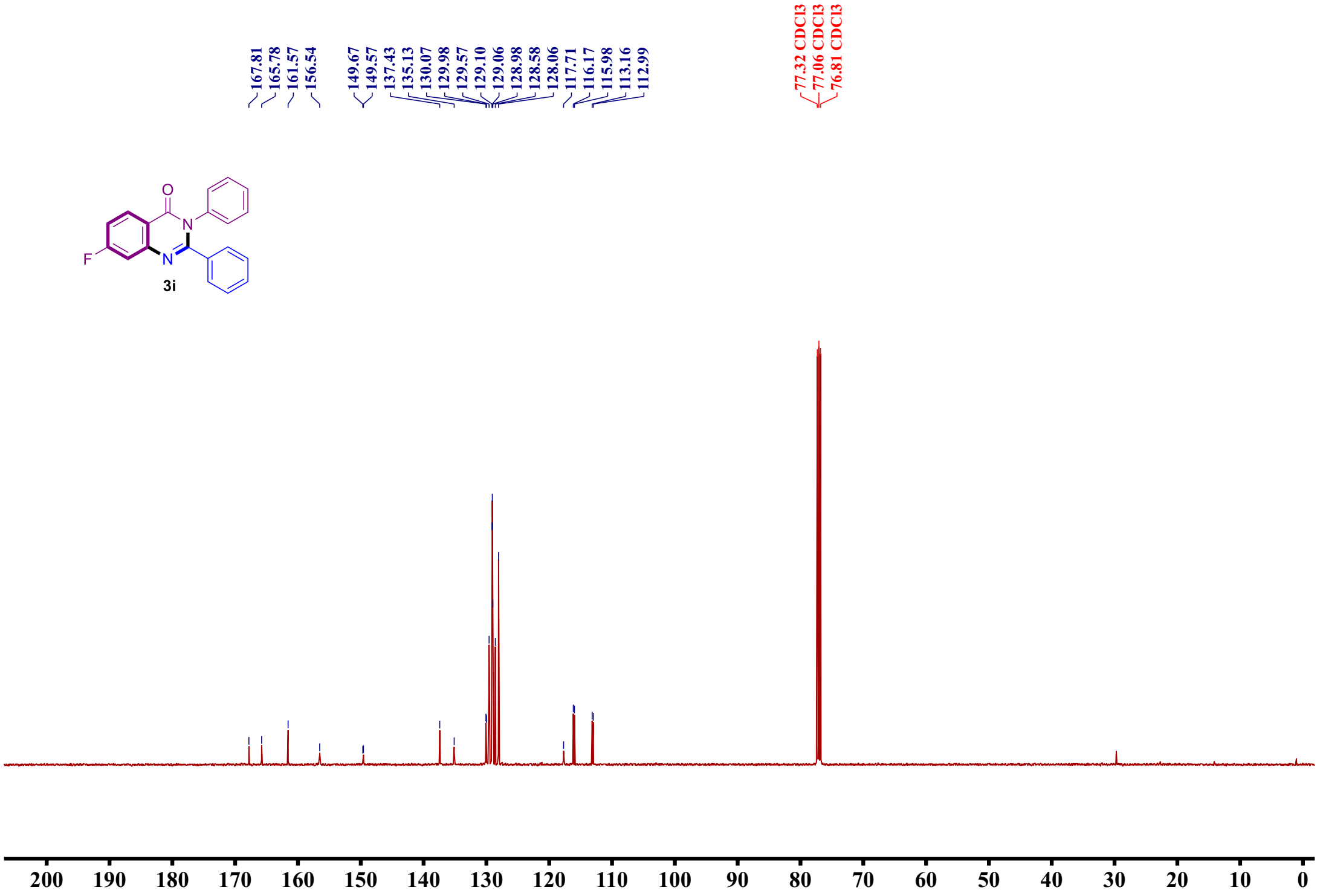
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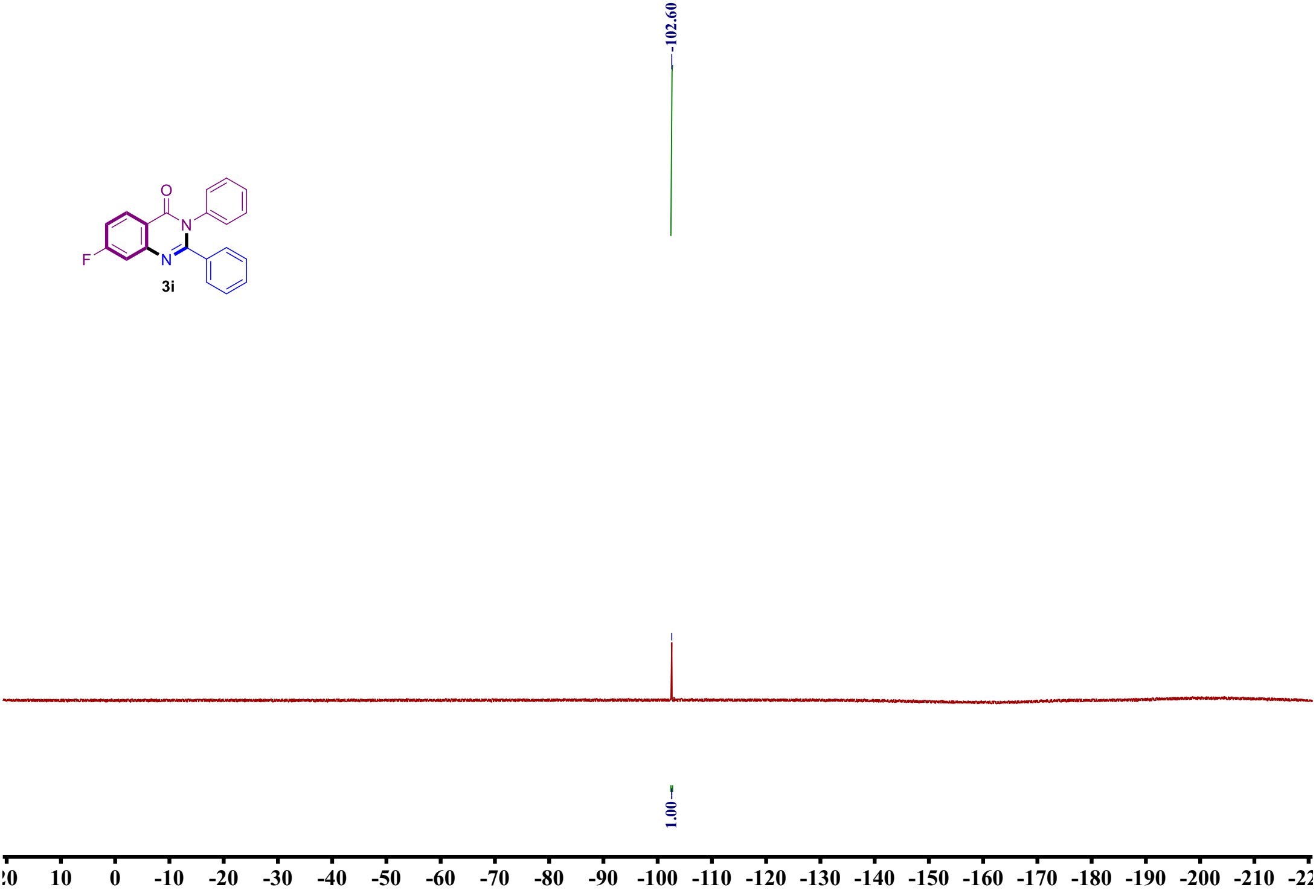
3i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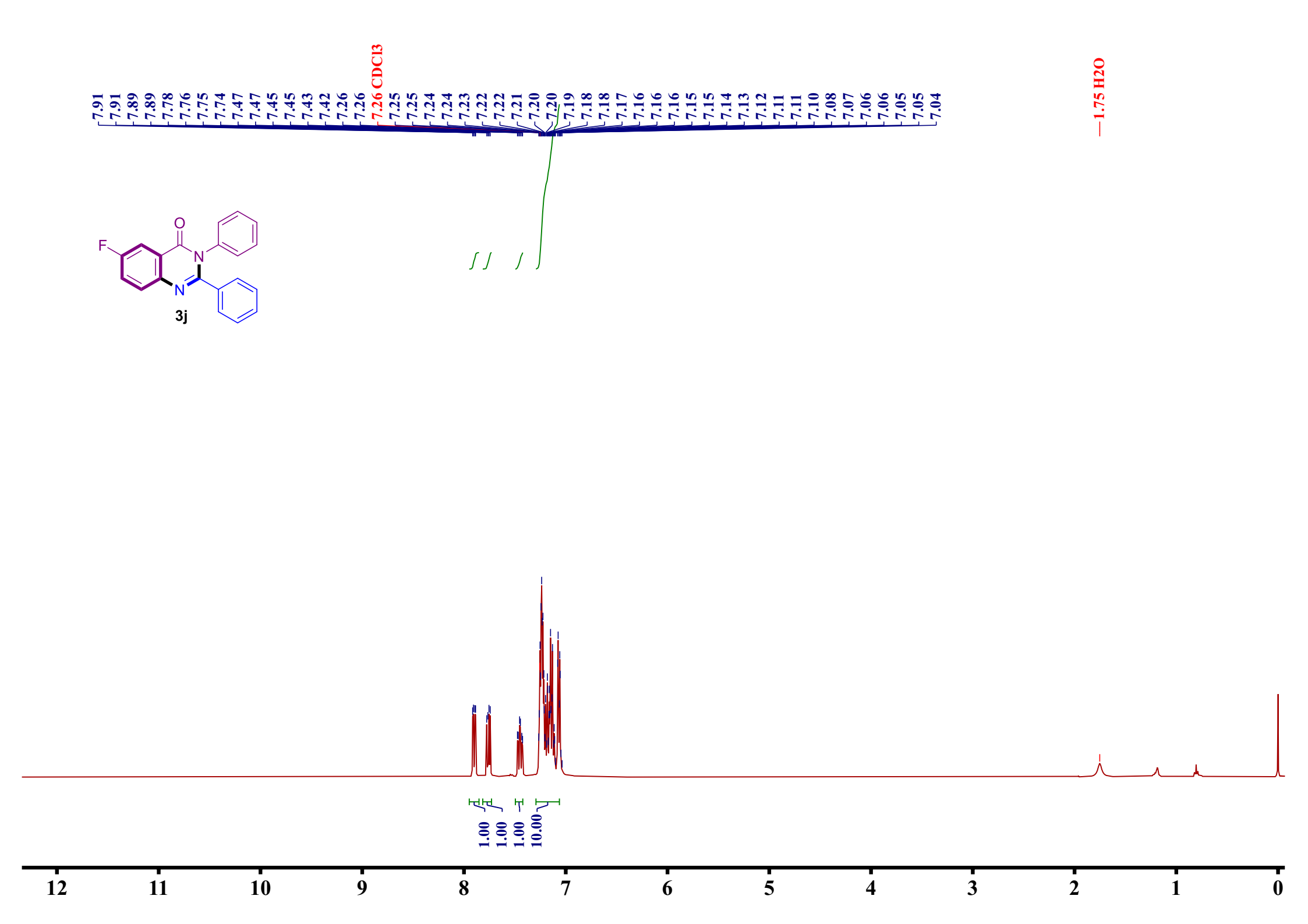
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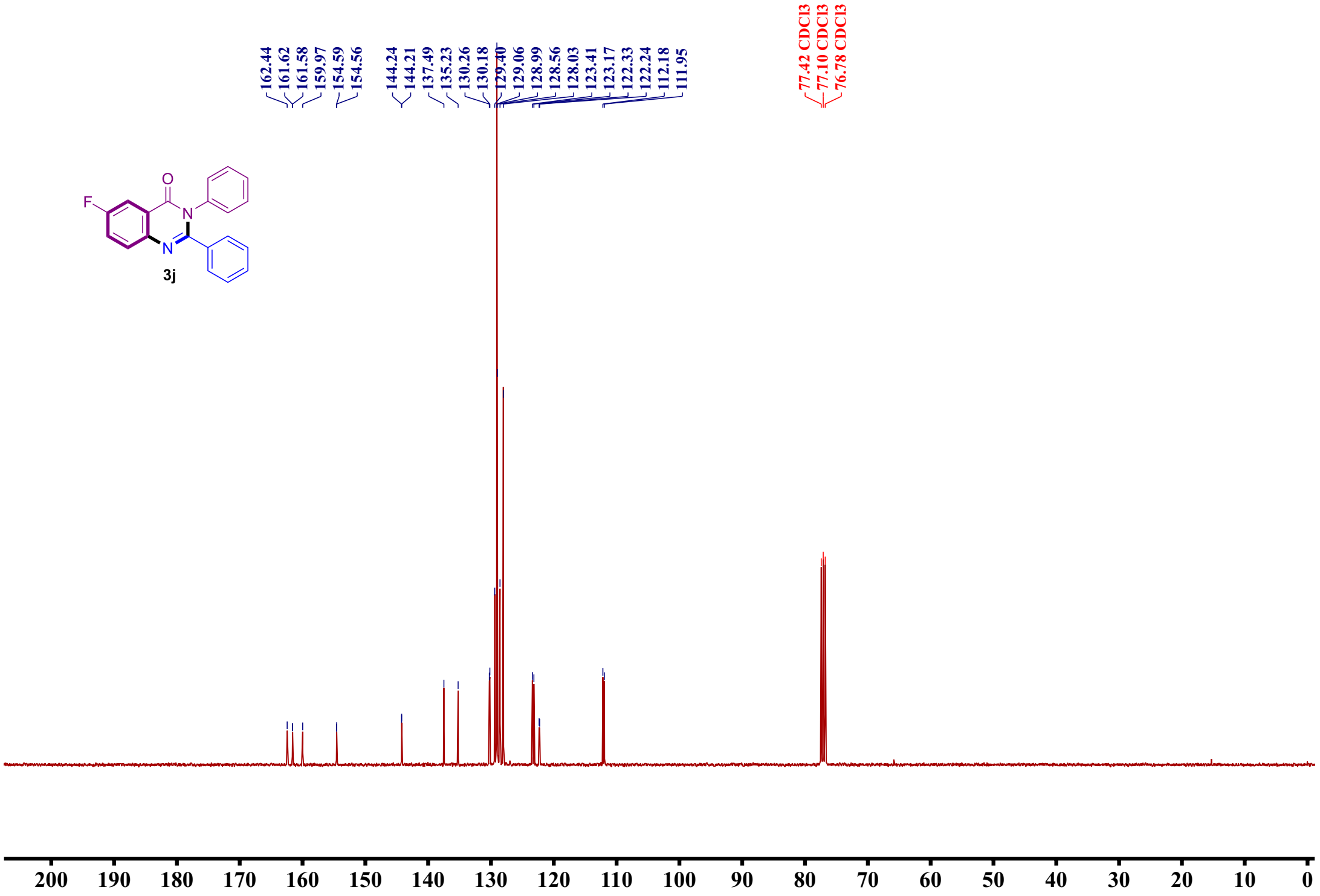
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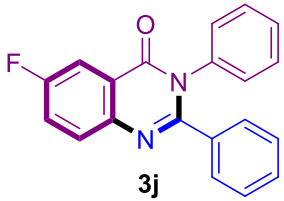

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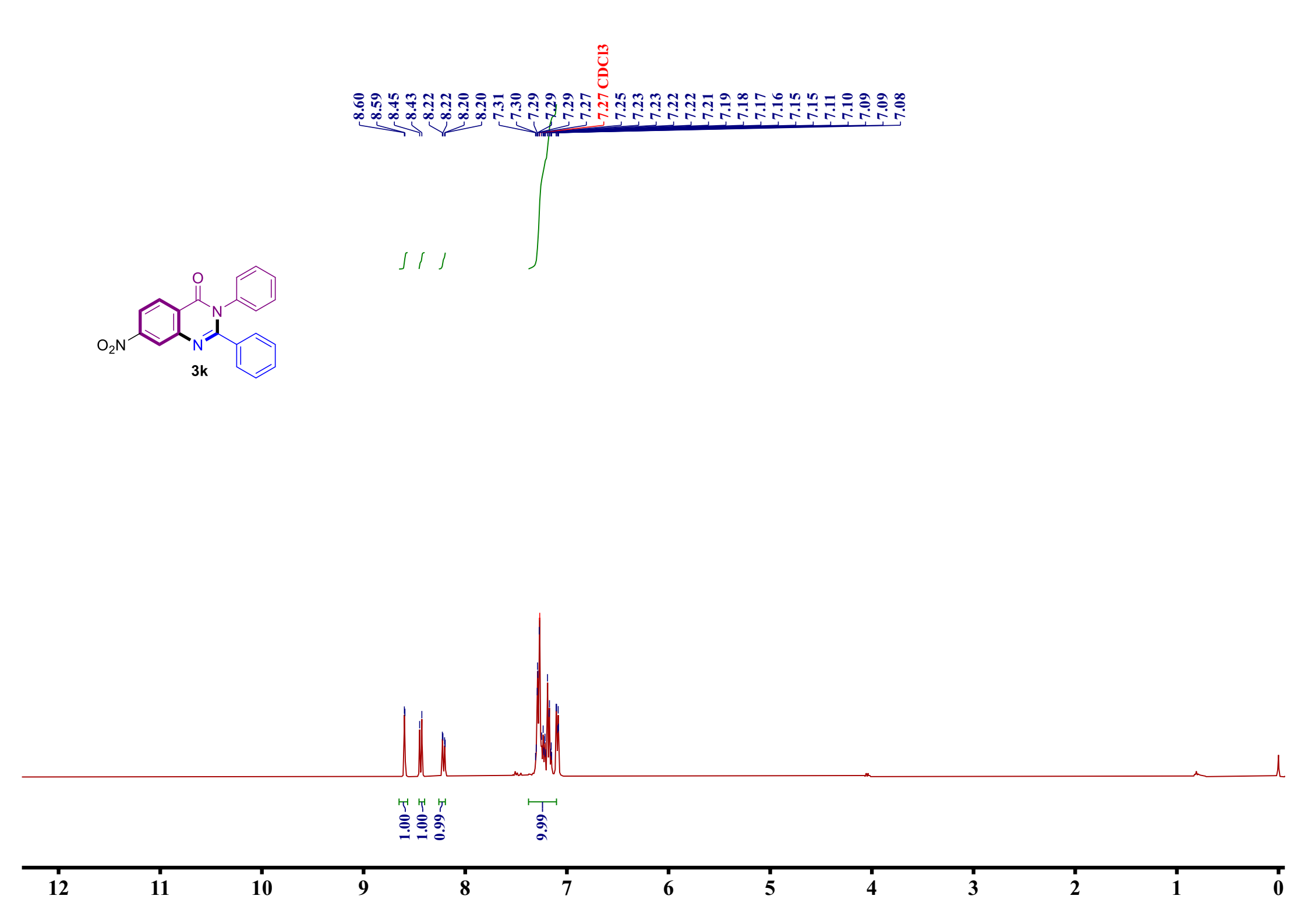
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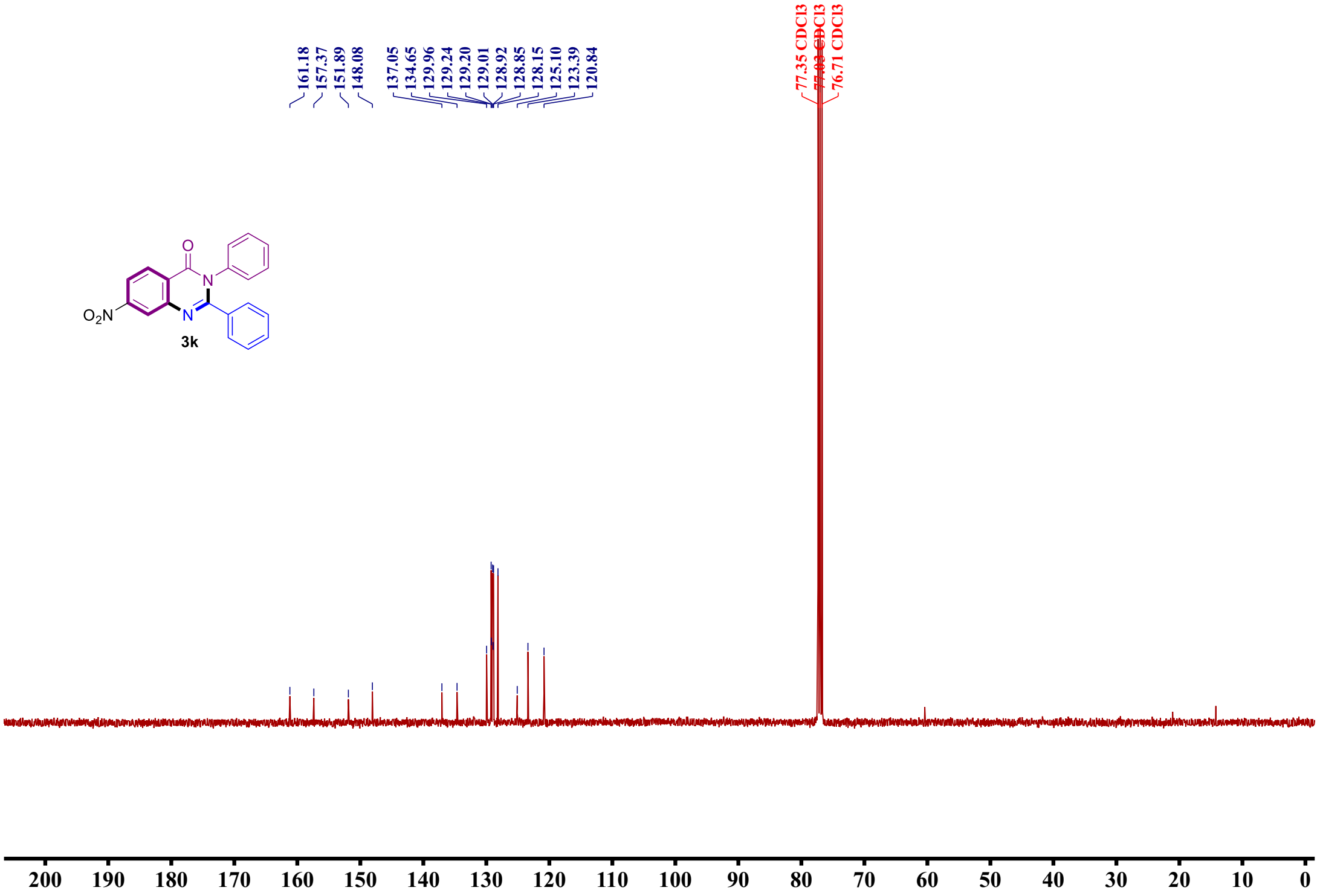
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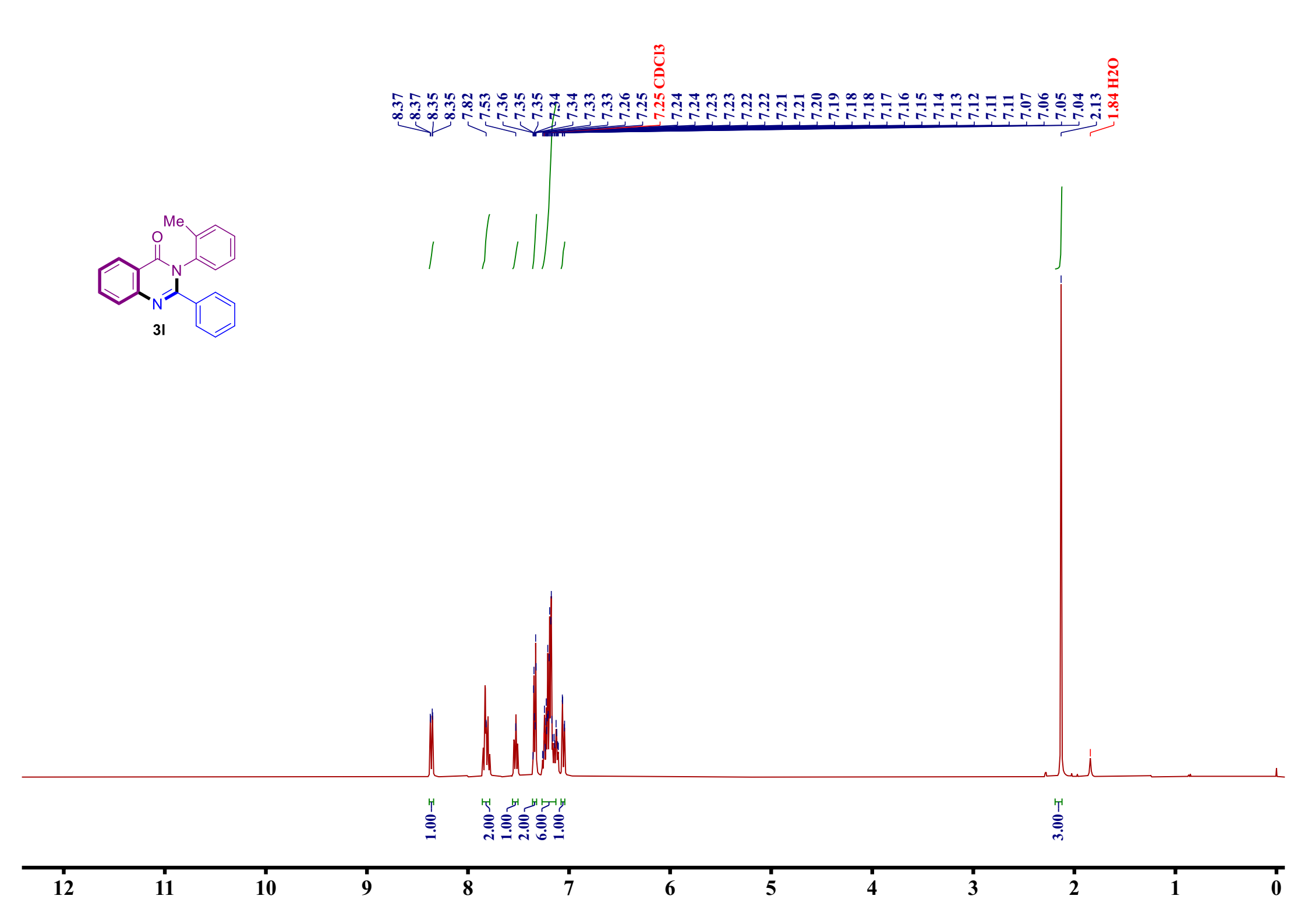
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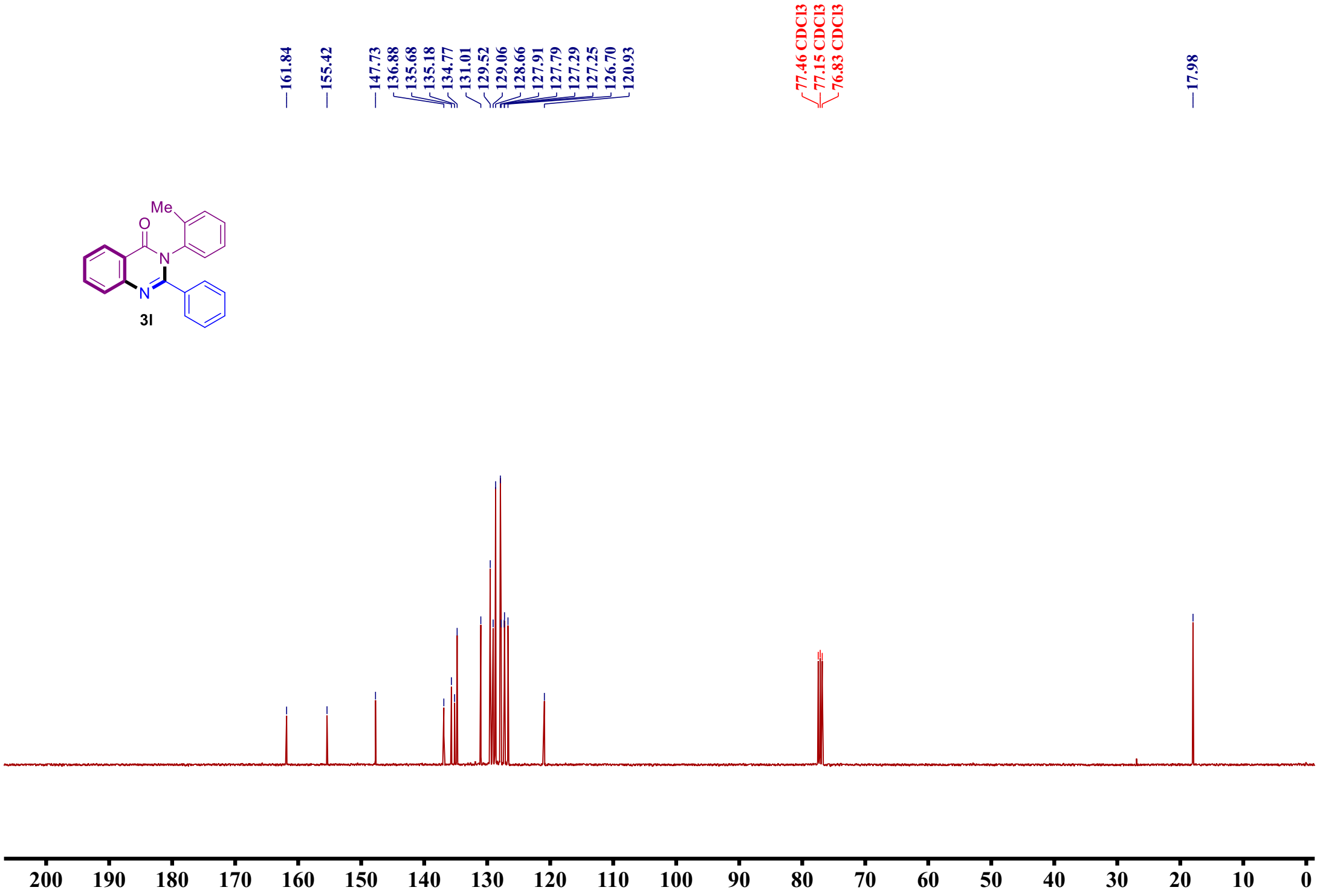
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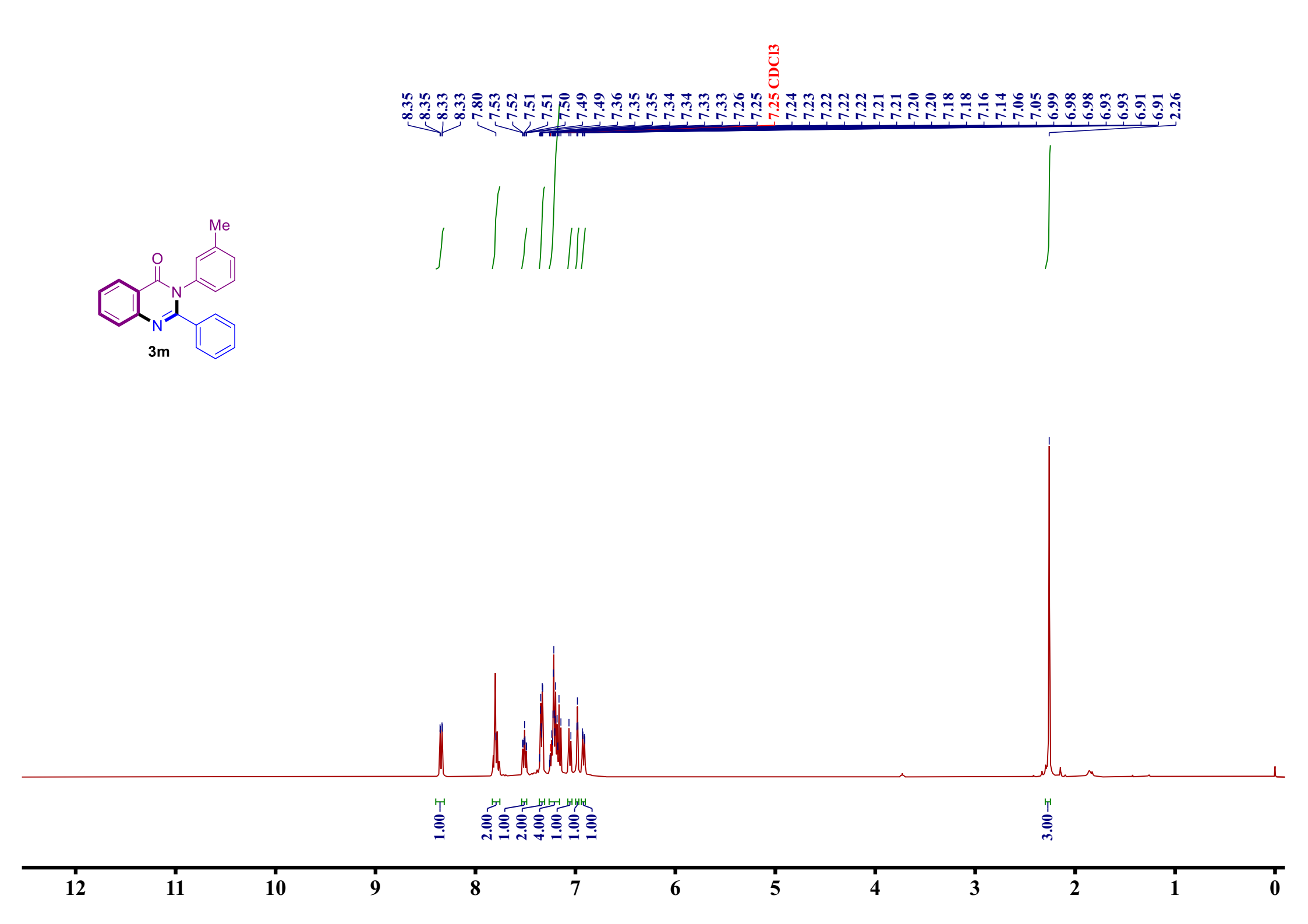
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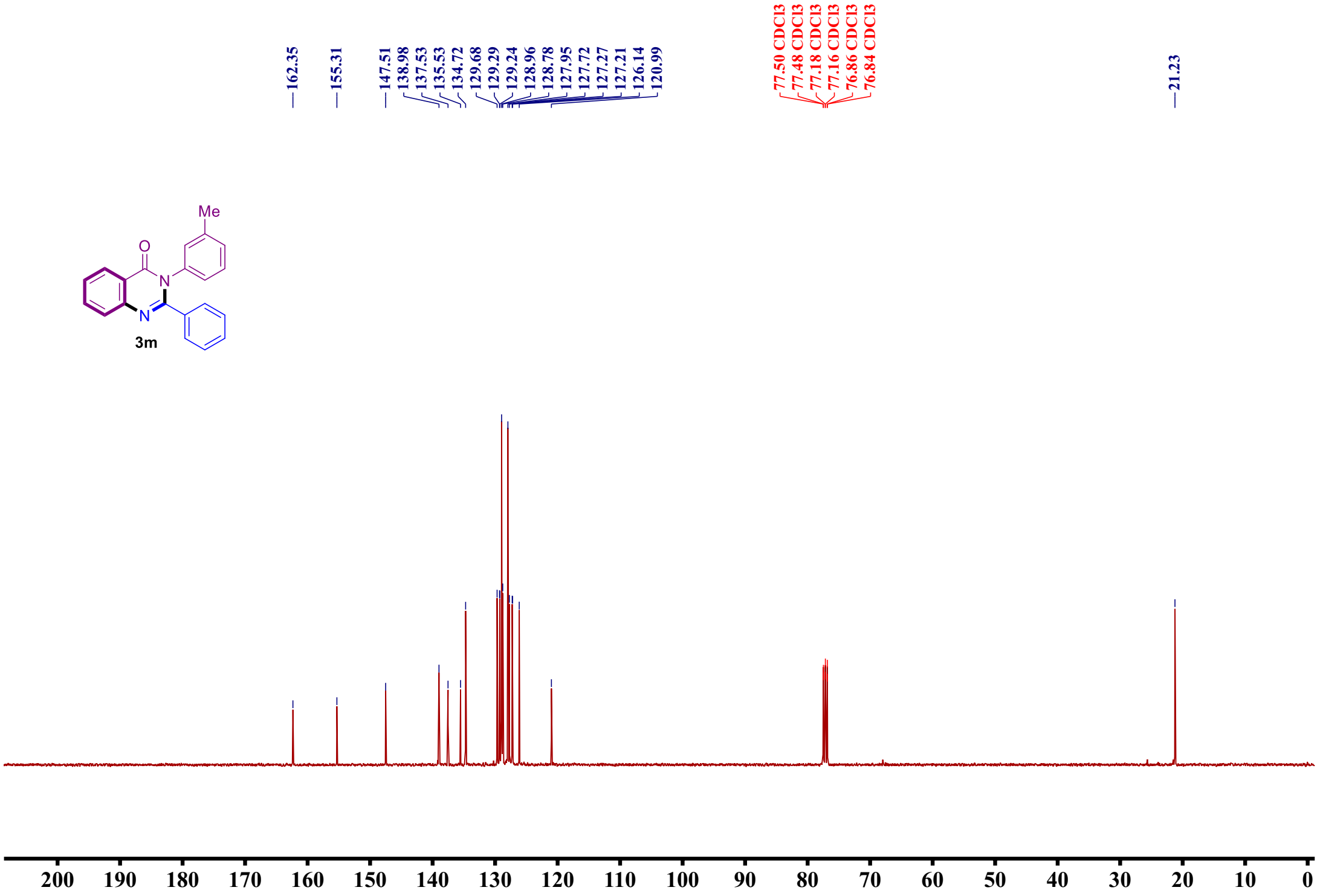
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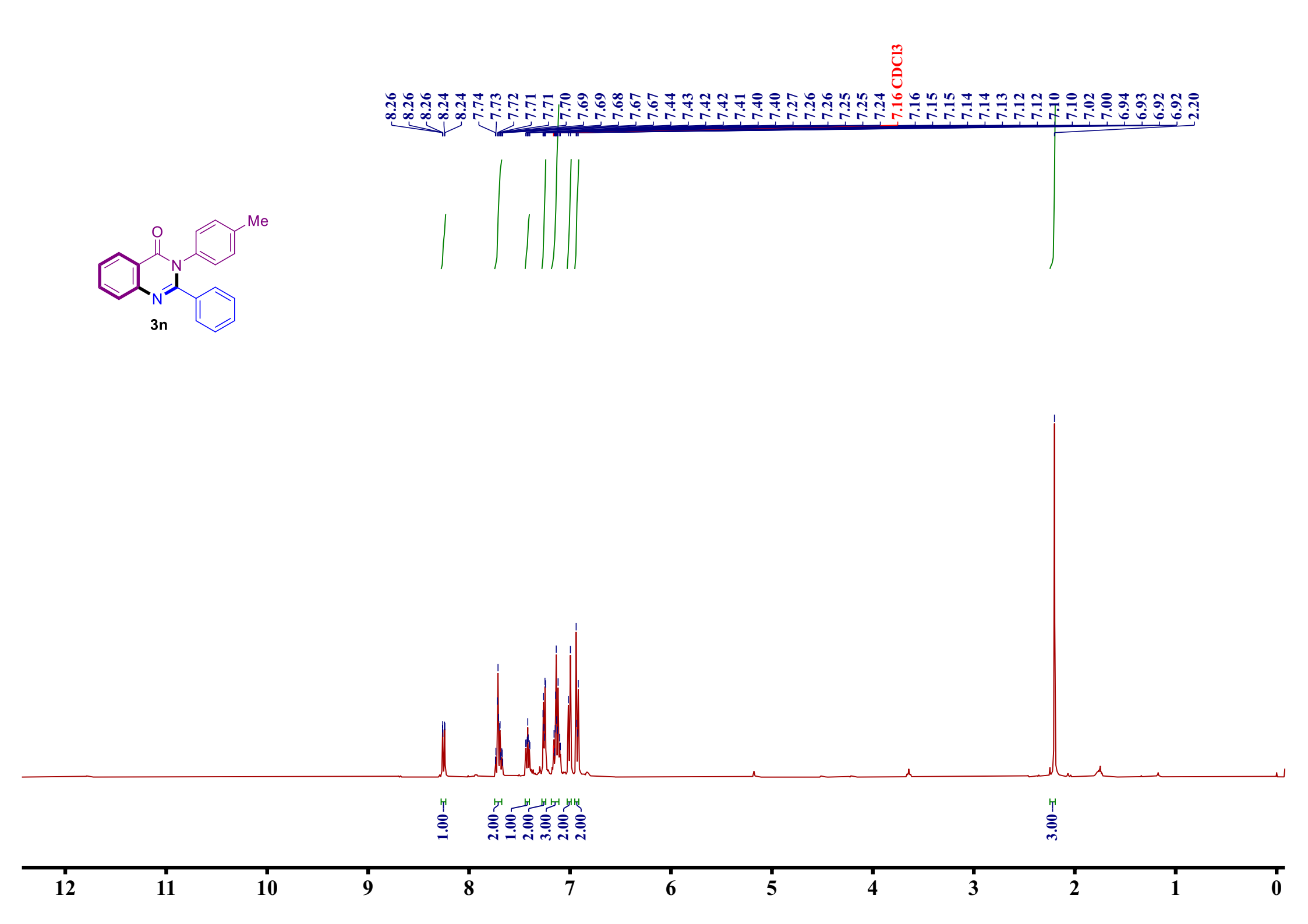
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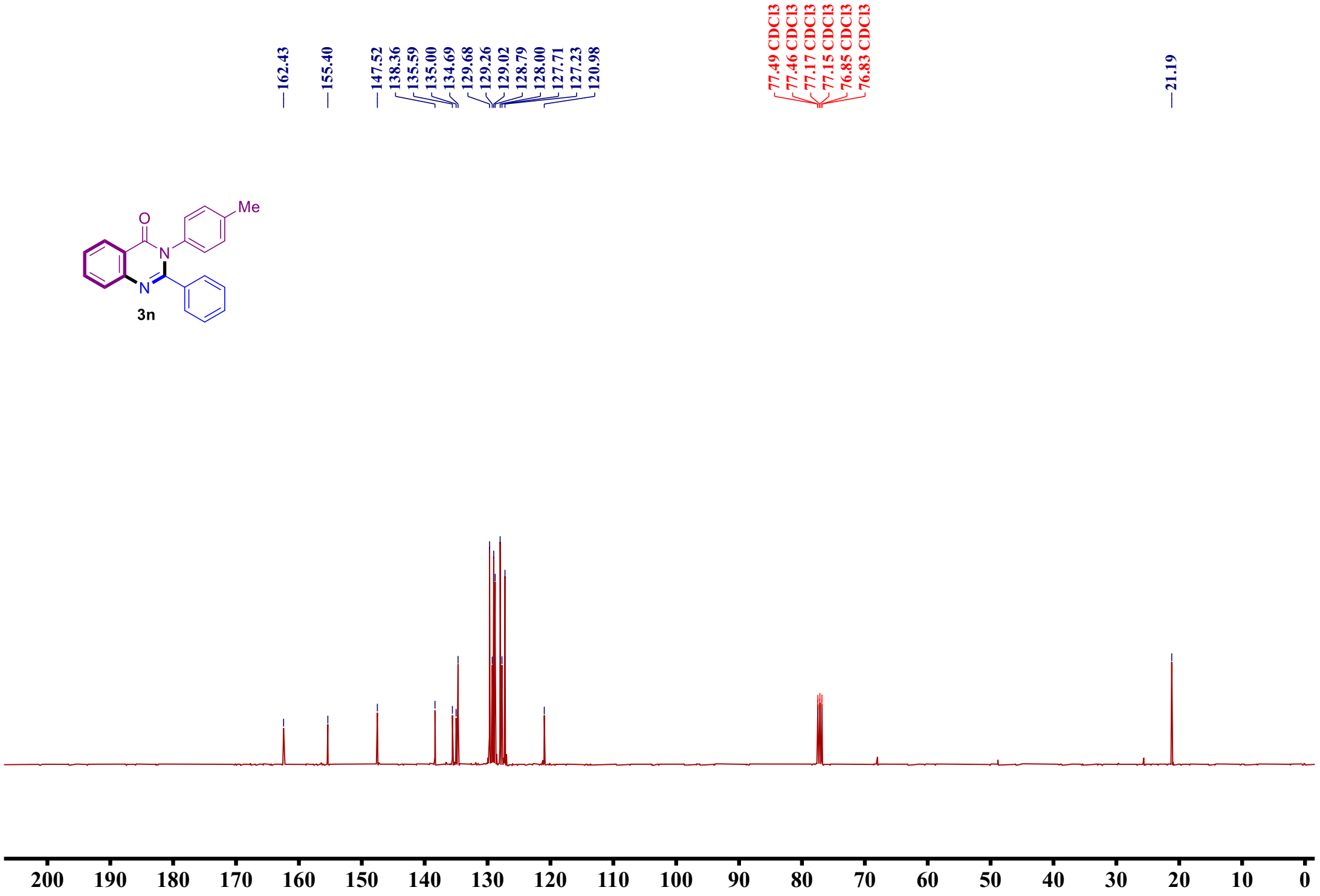
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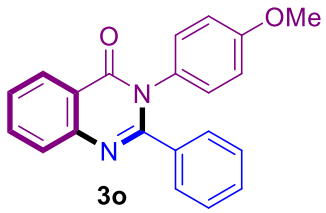
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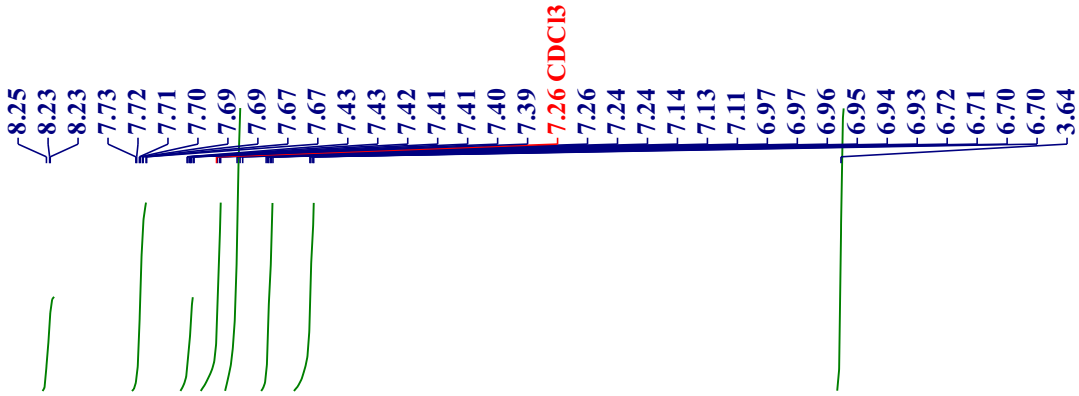
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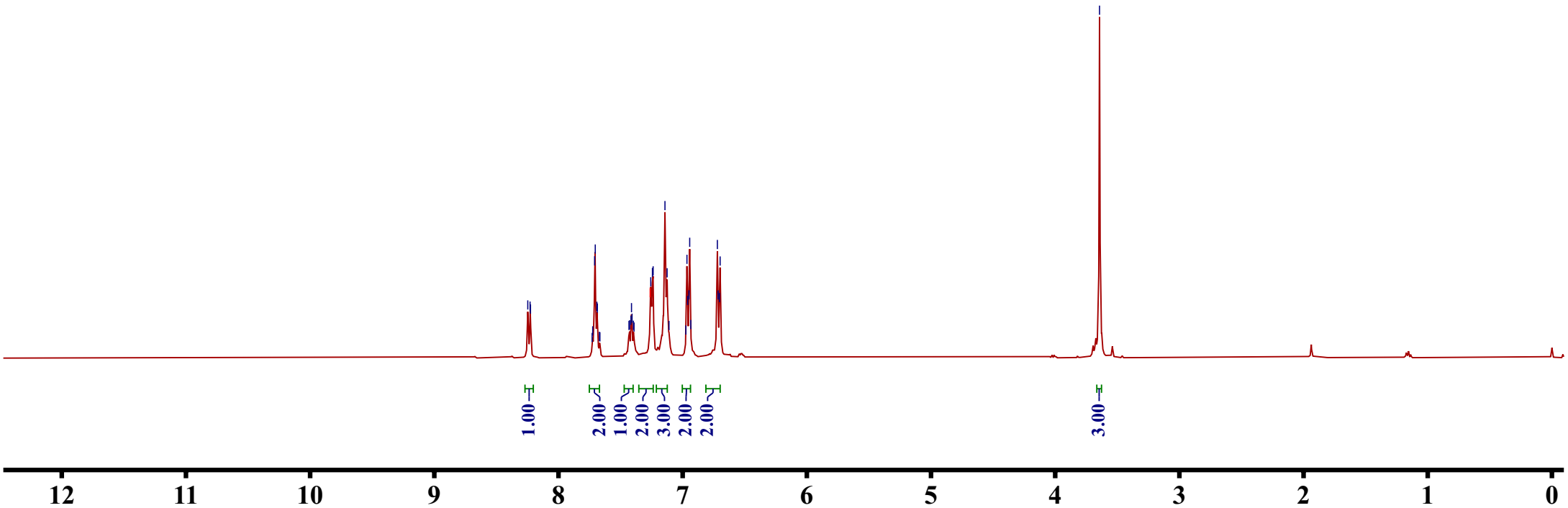
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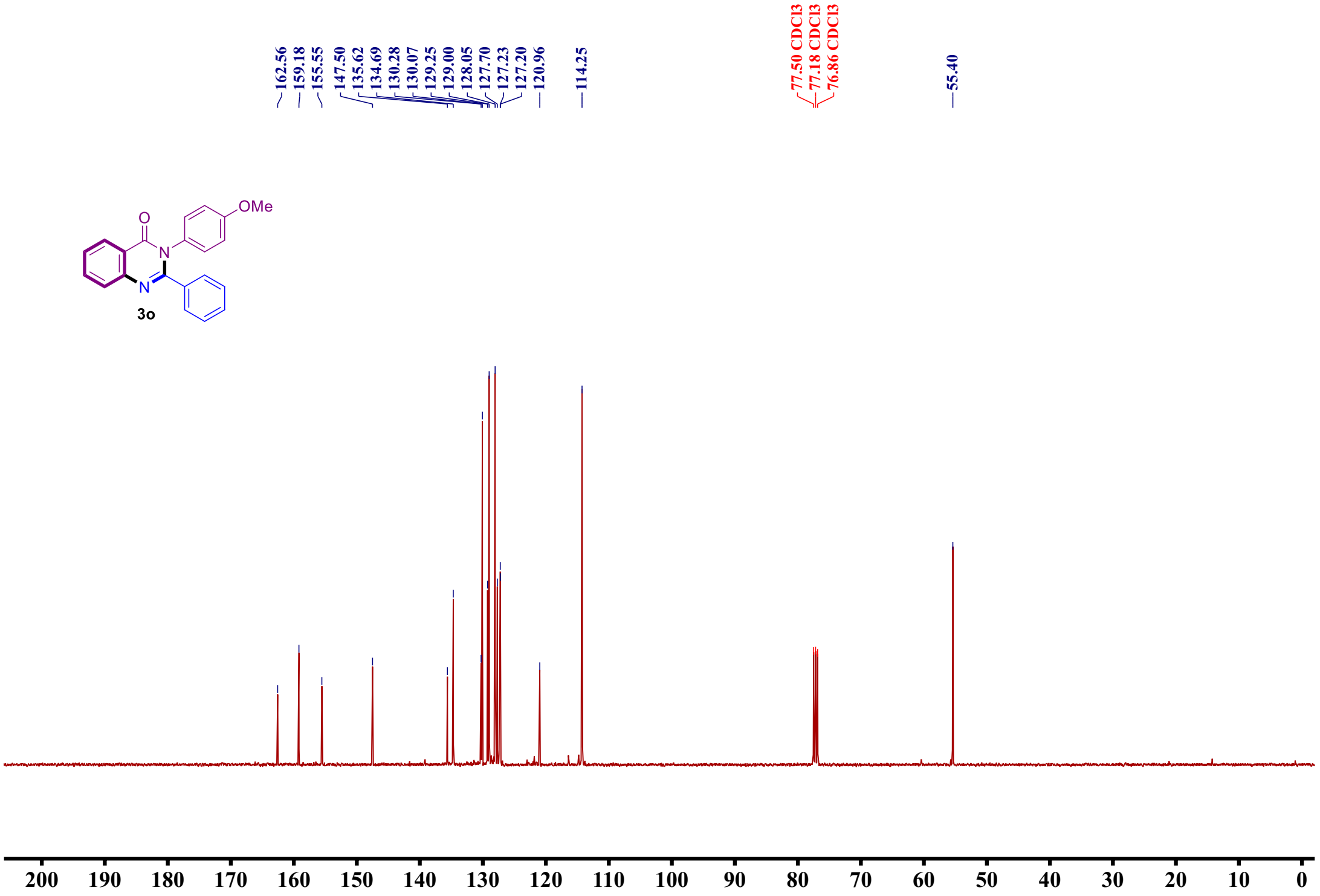
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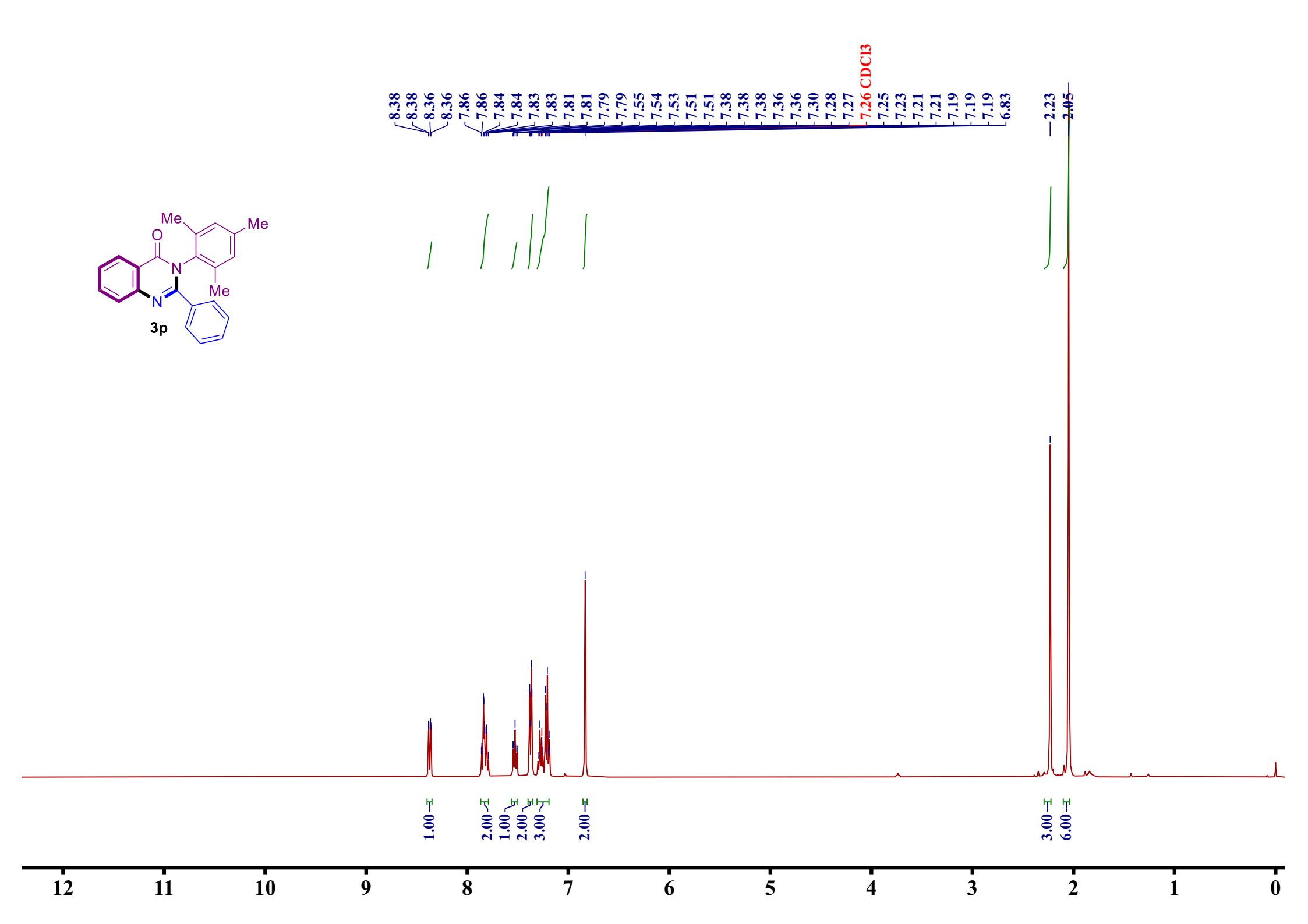
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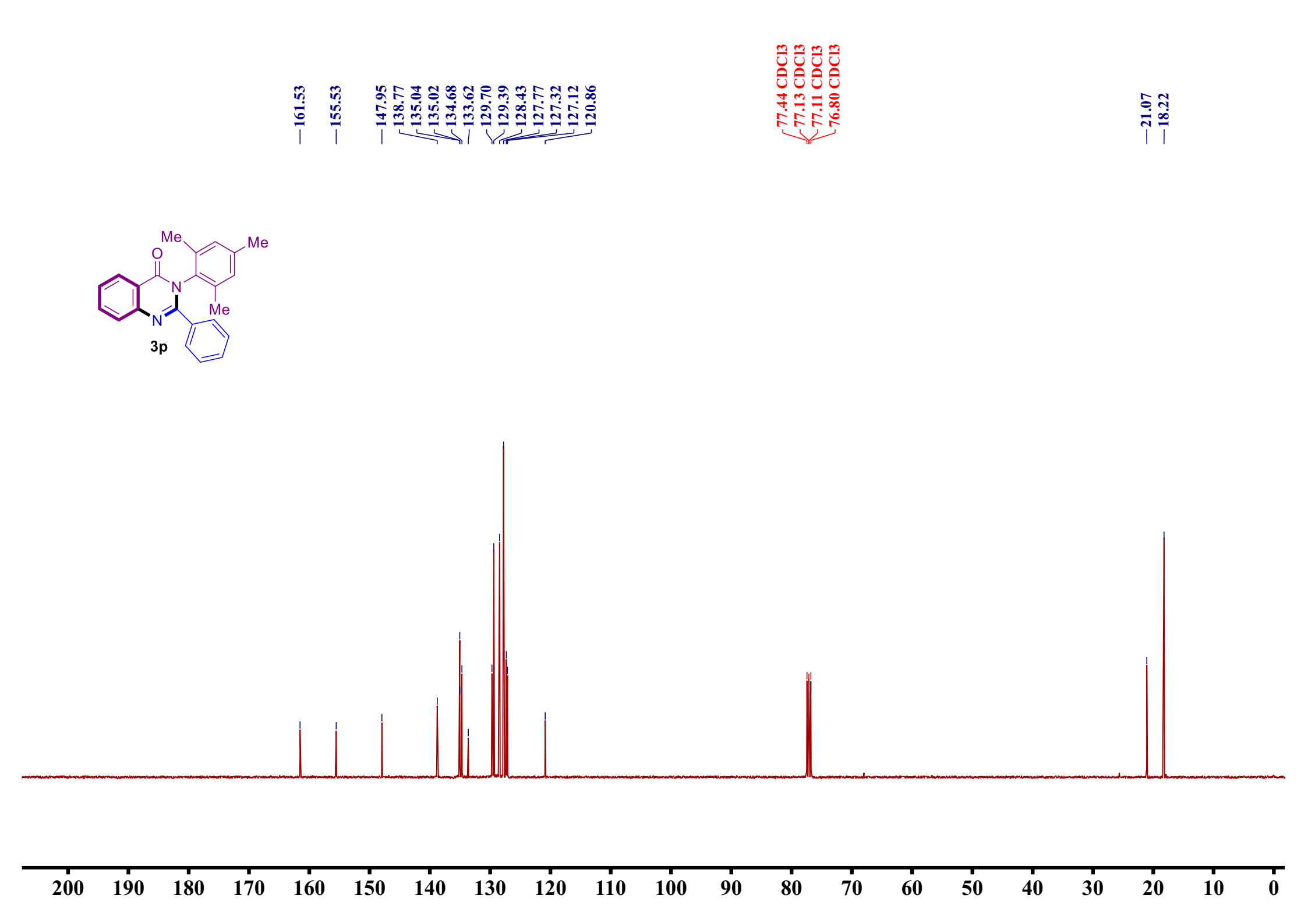
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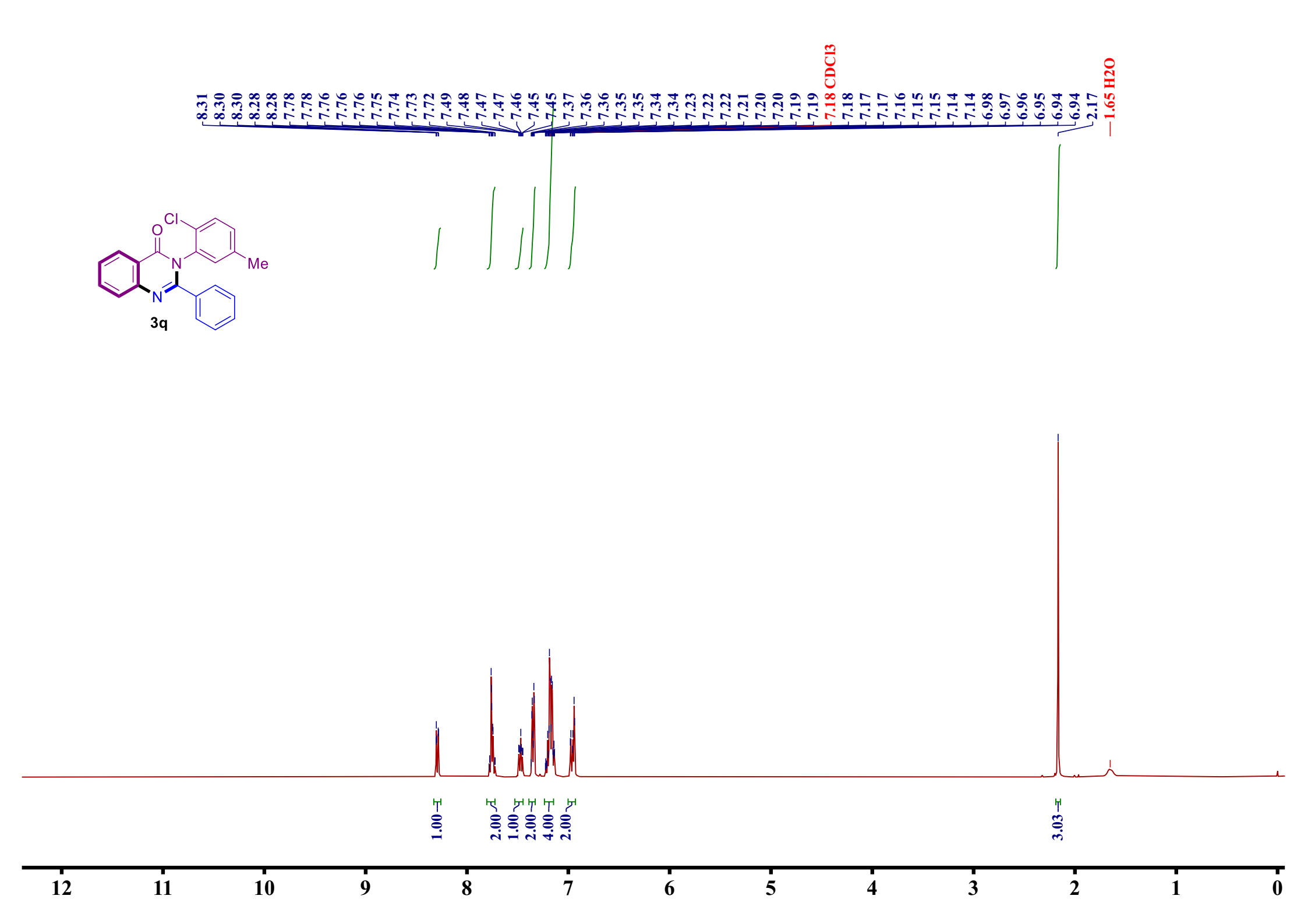
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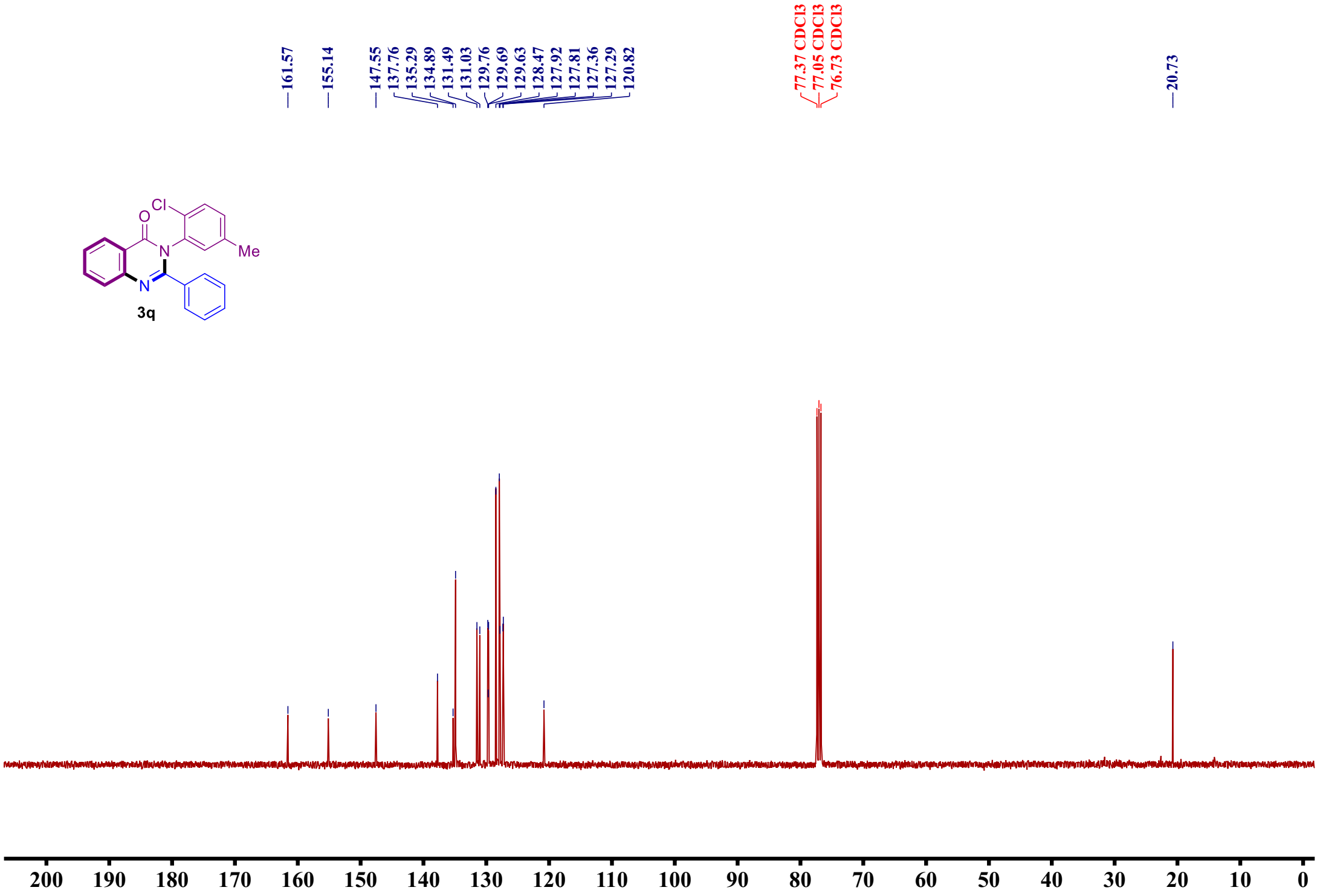
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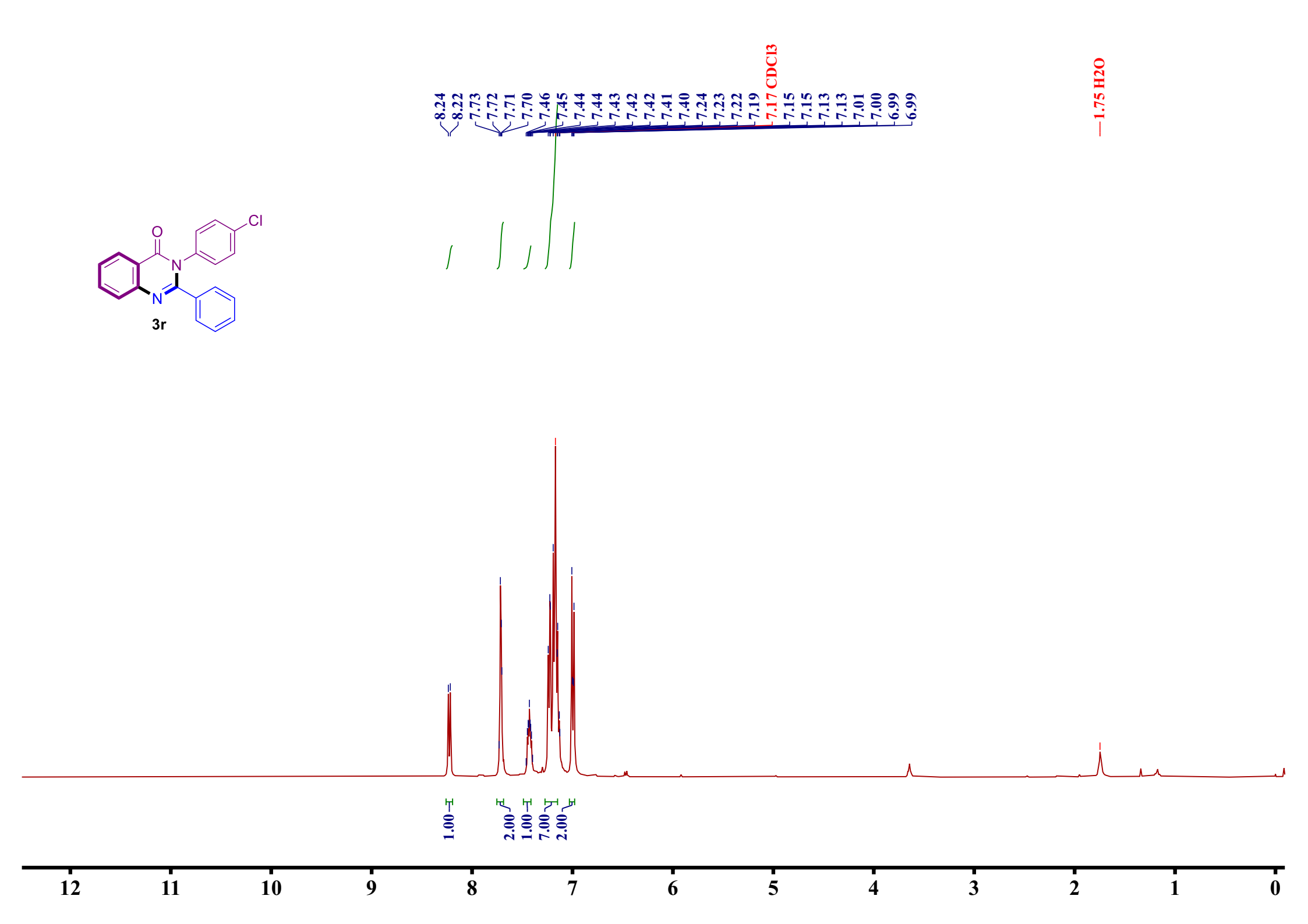
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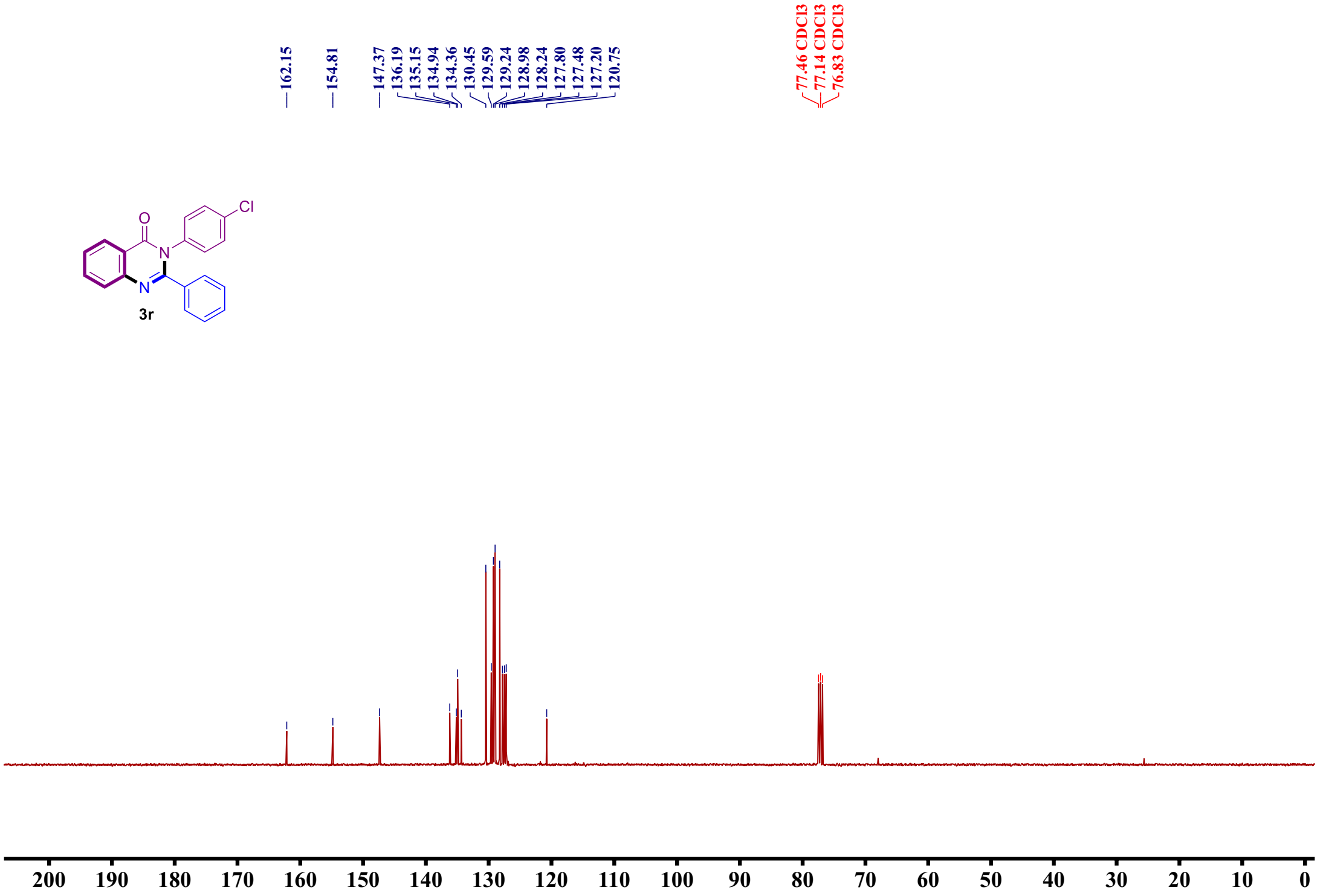
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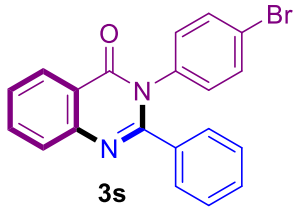

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2.02 H2O

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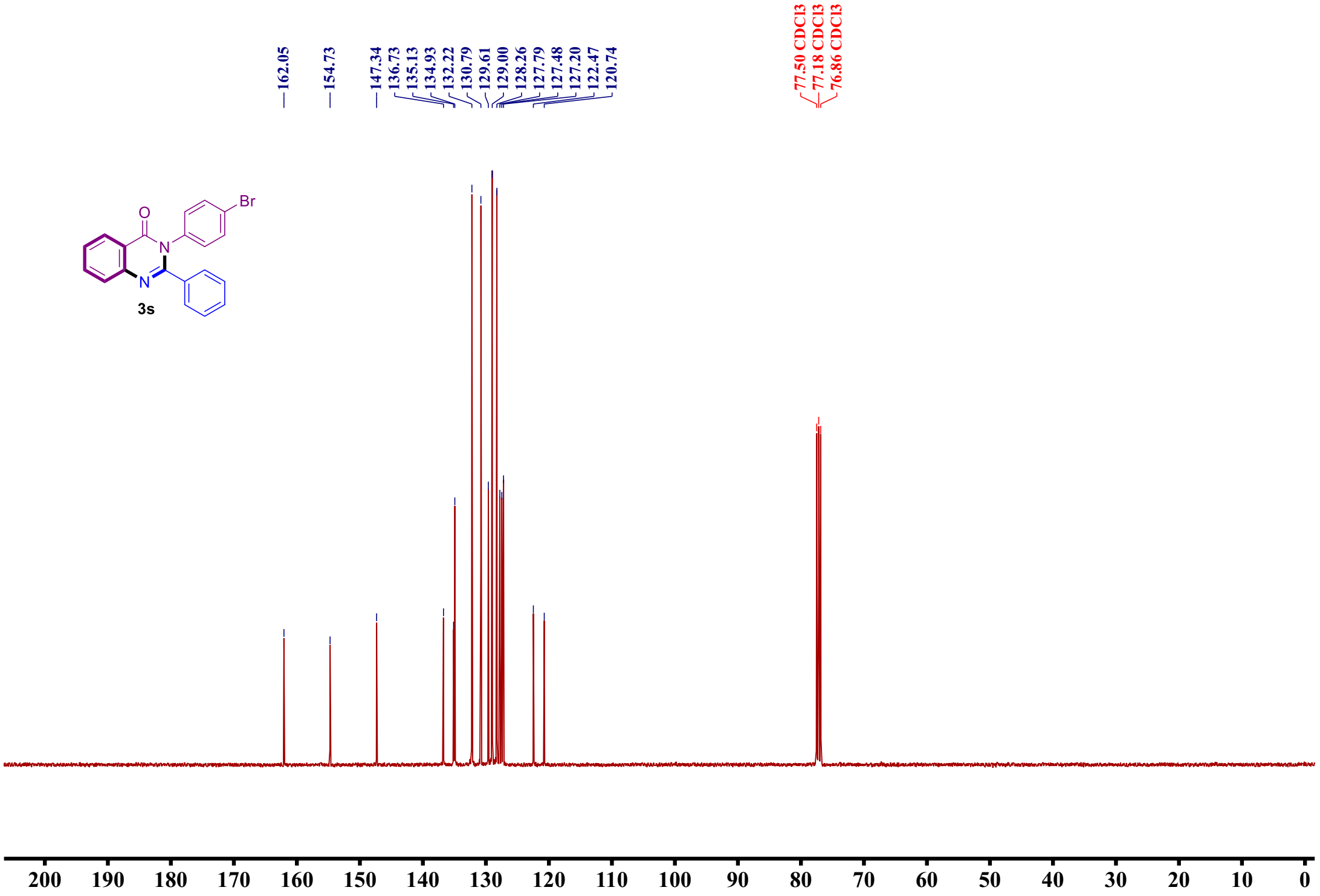
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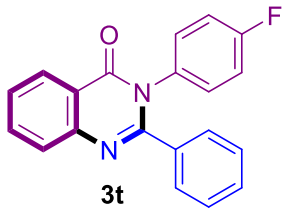

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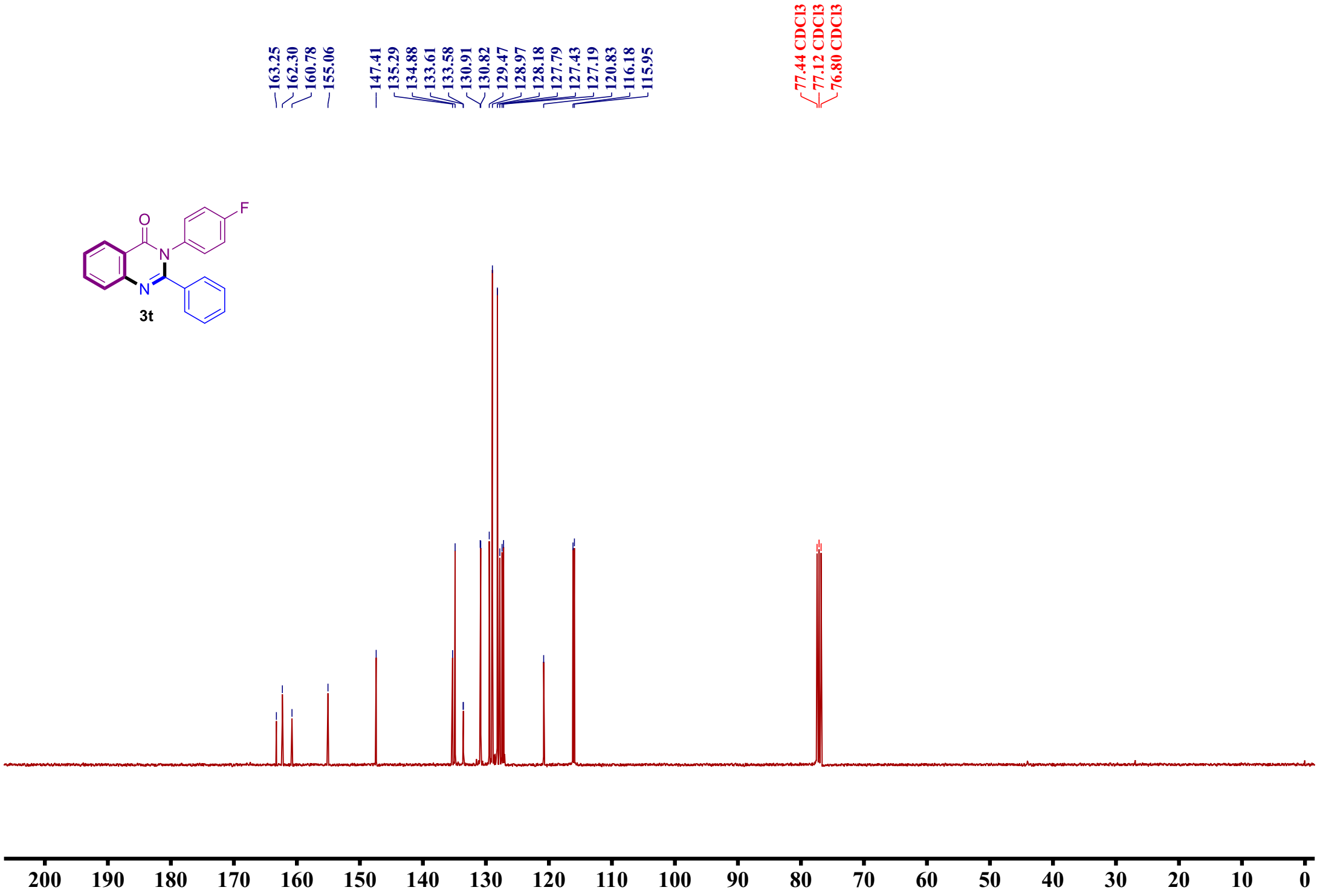
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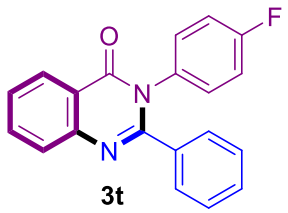

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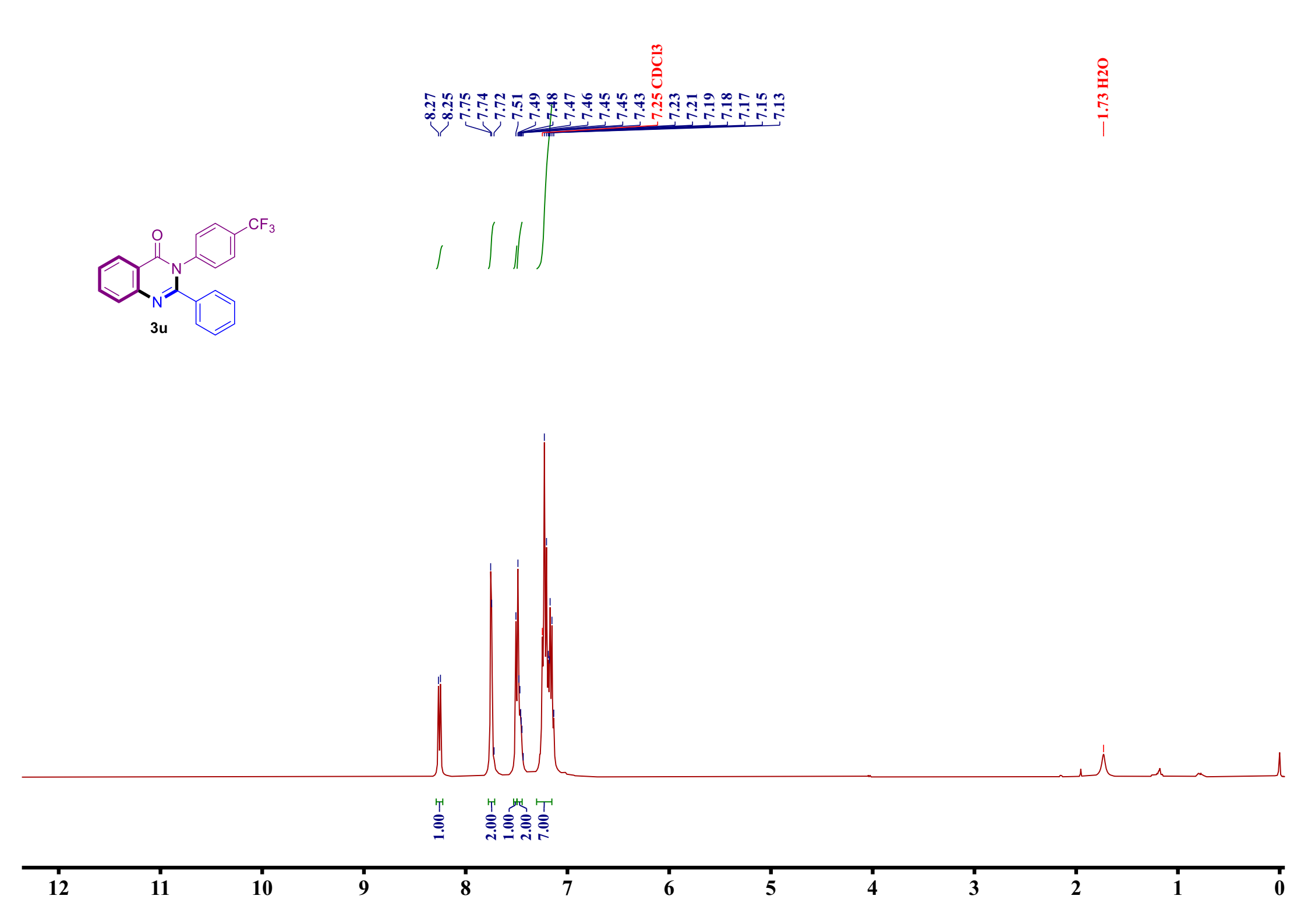
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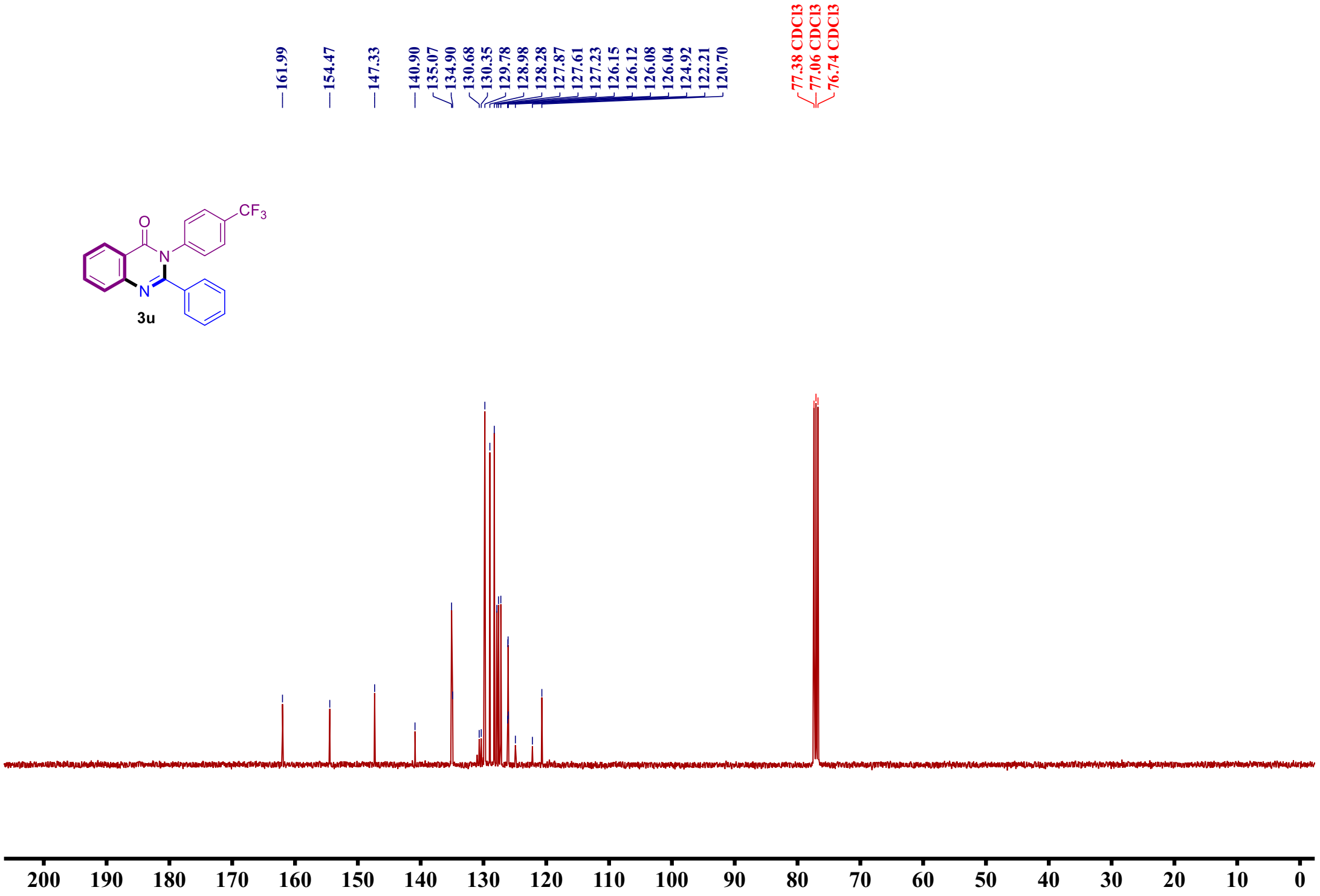
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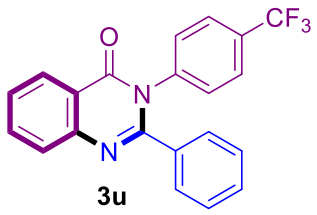

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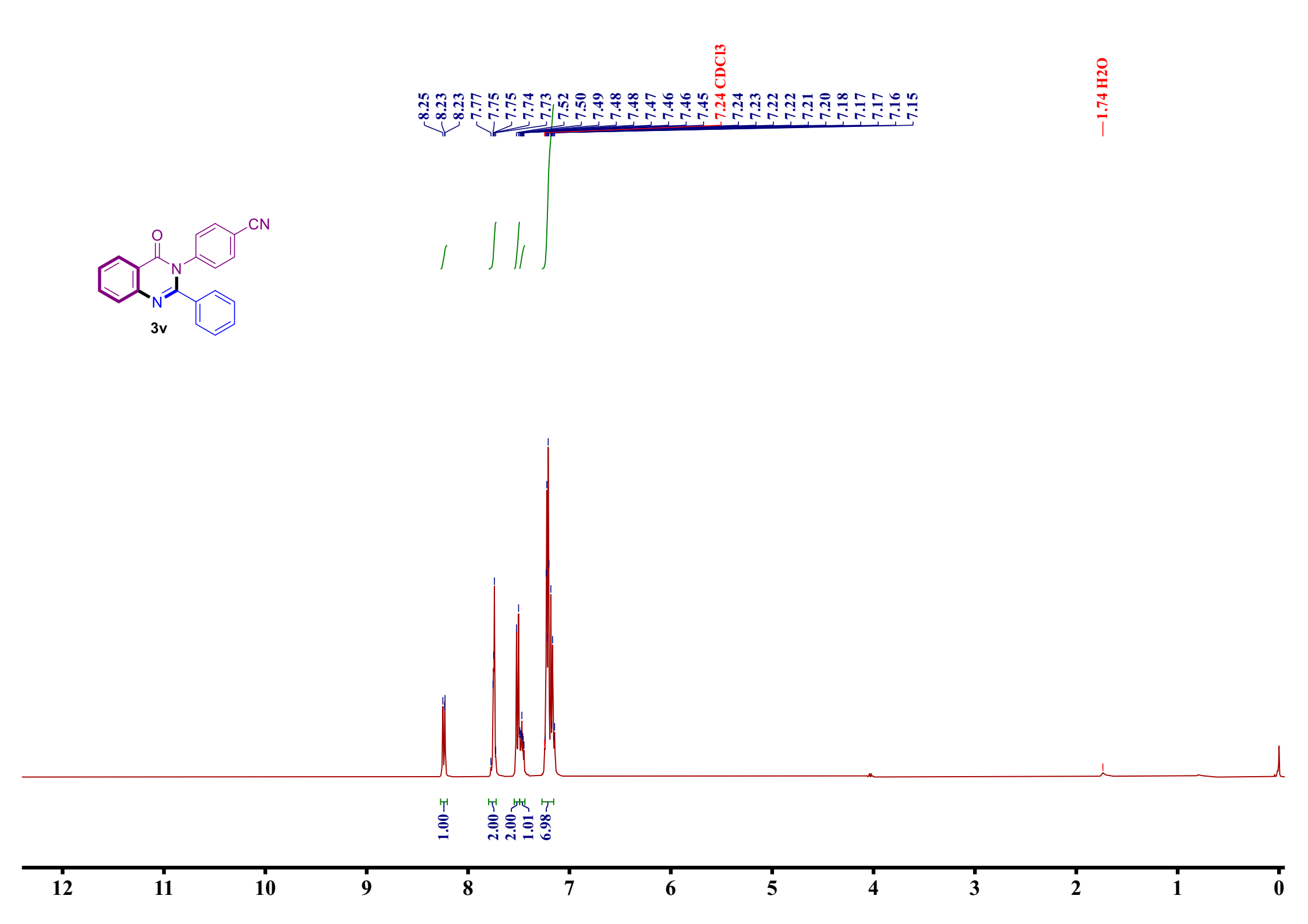
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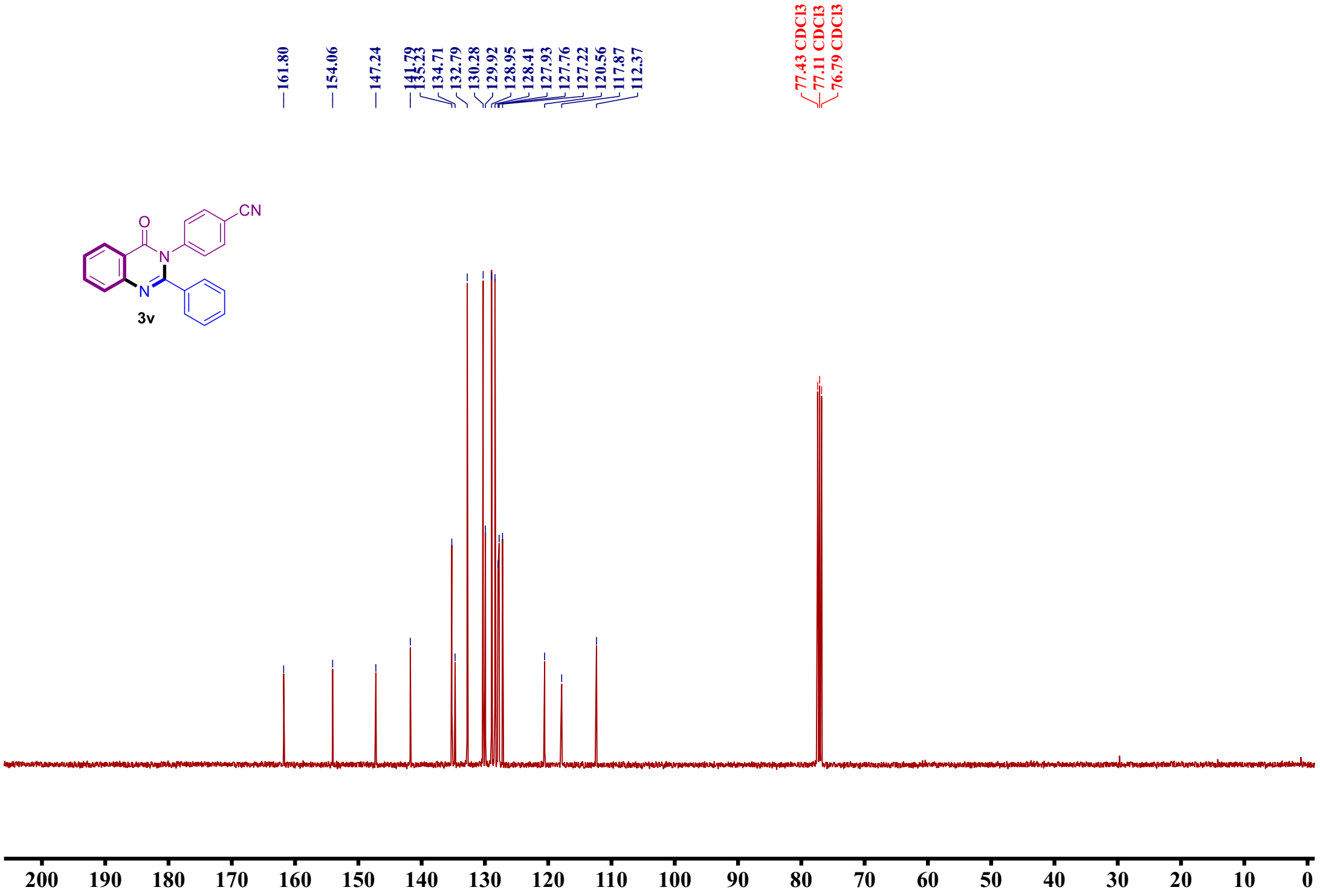
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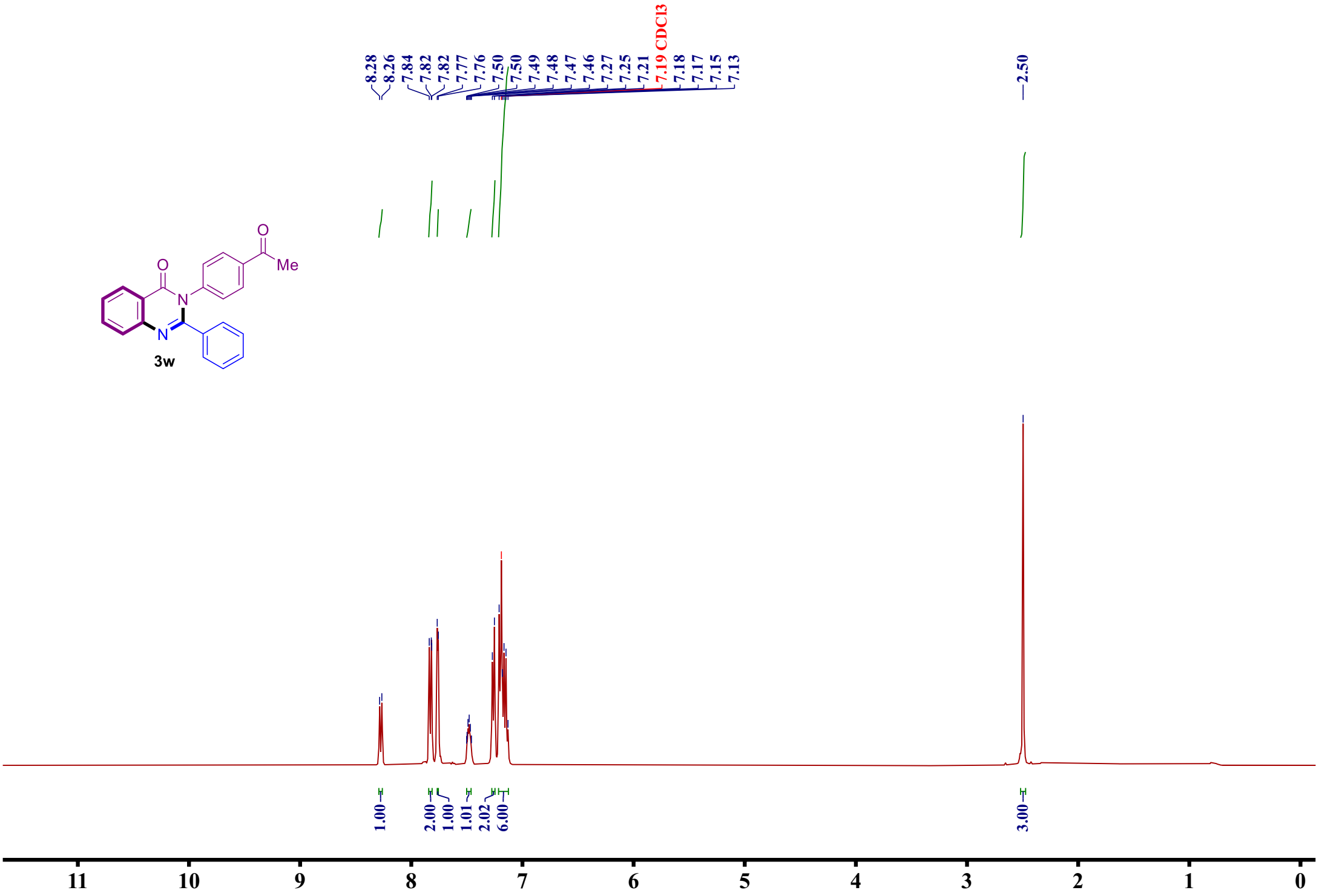
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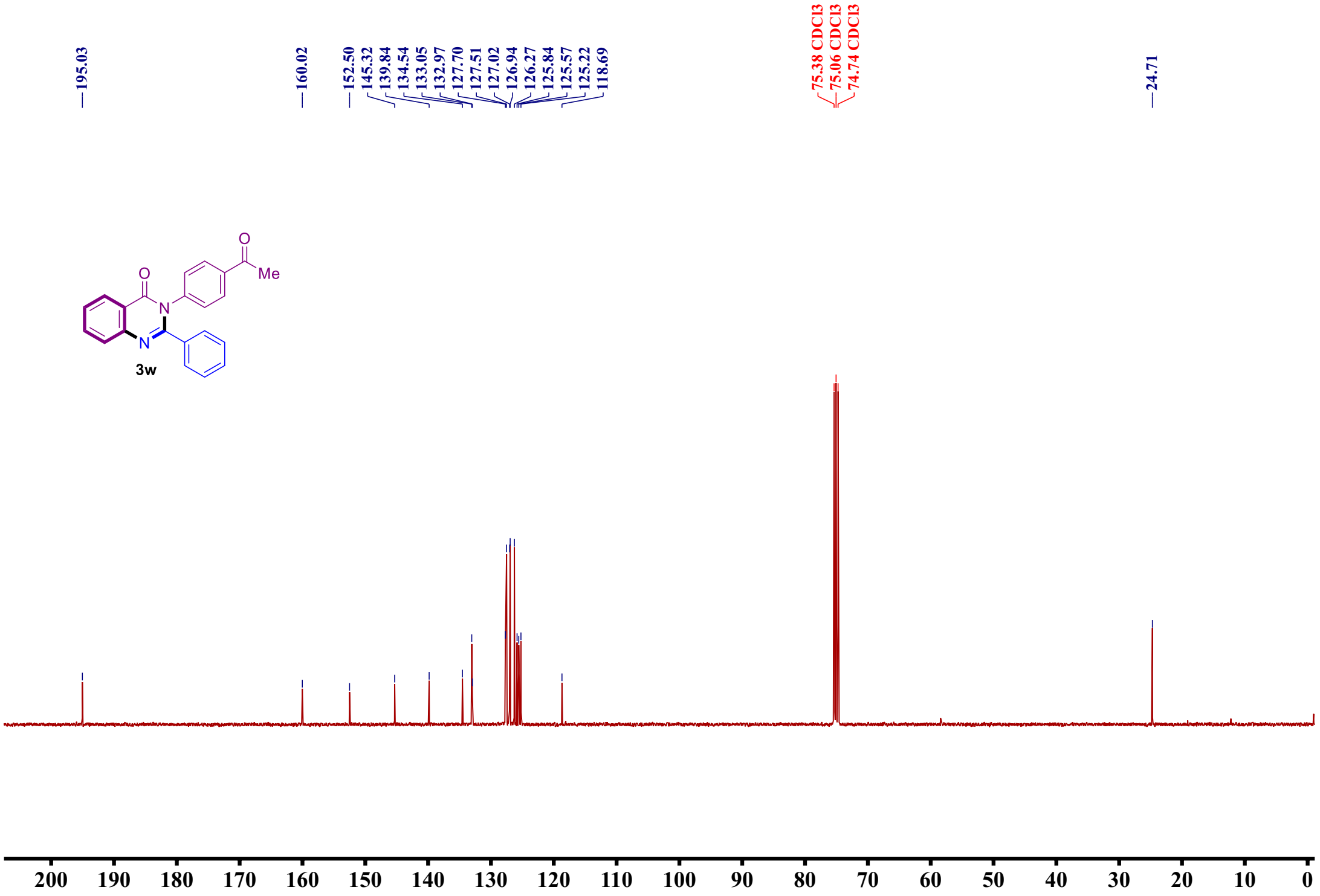
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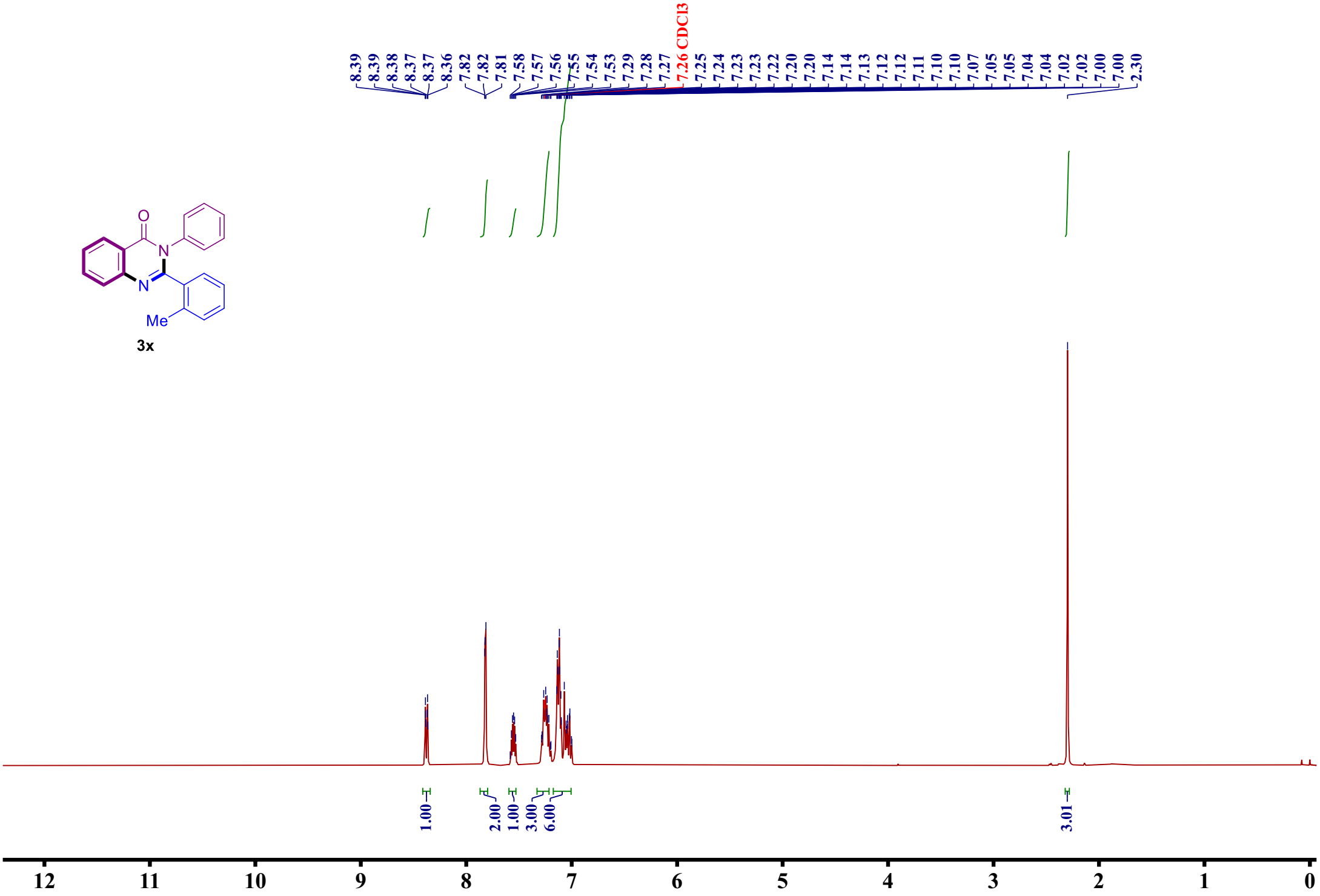
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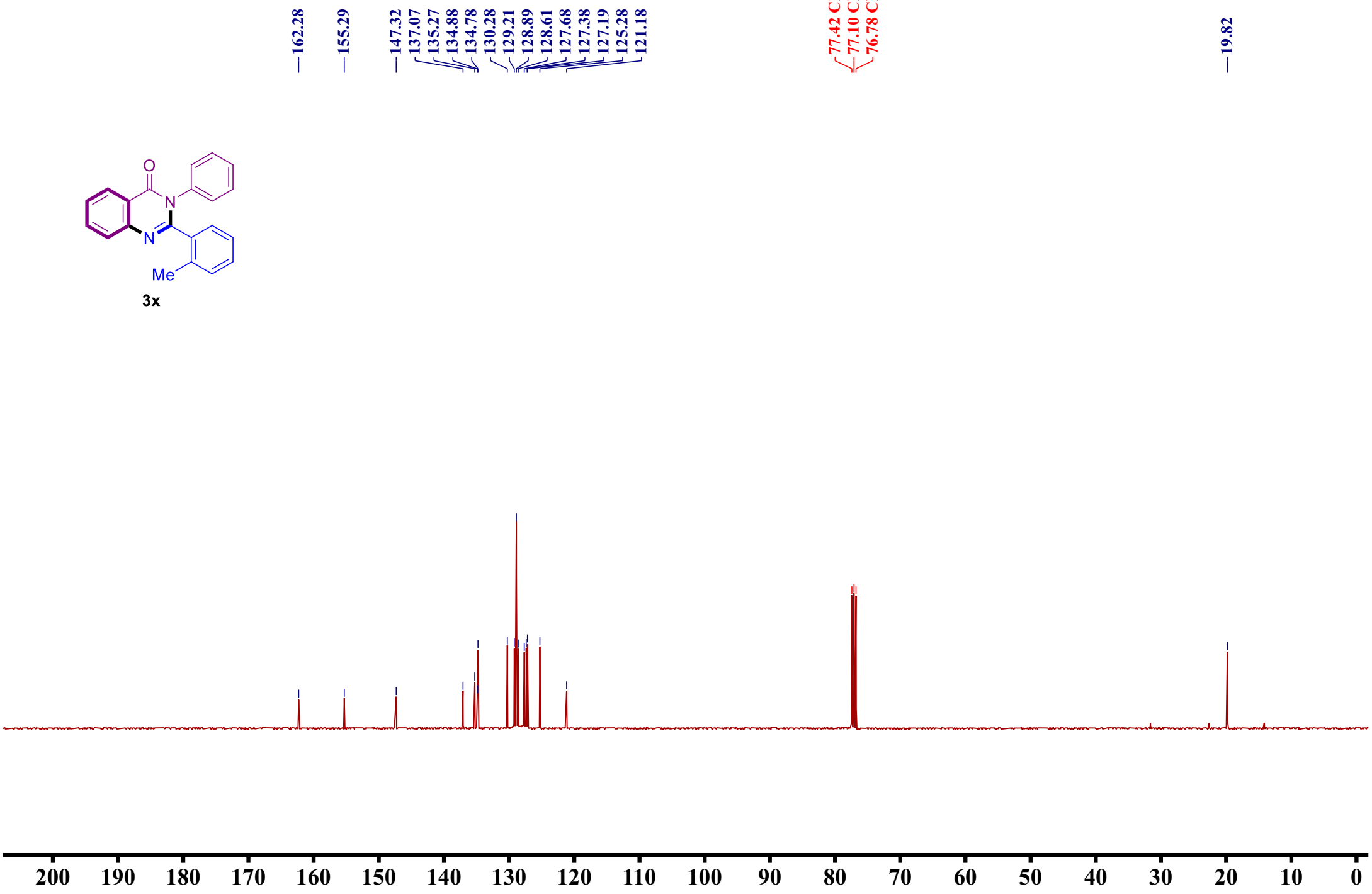
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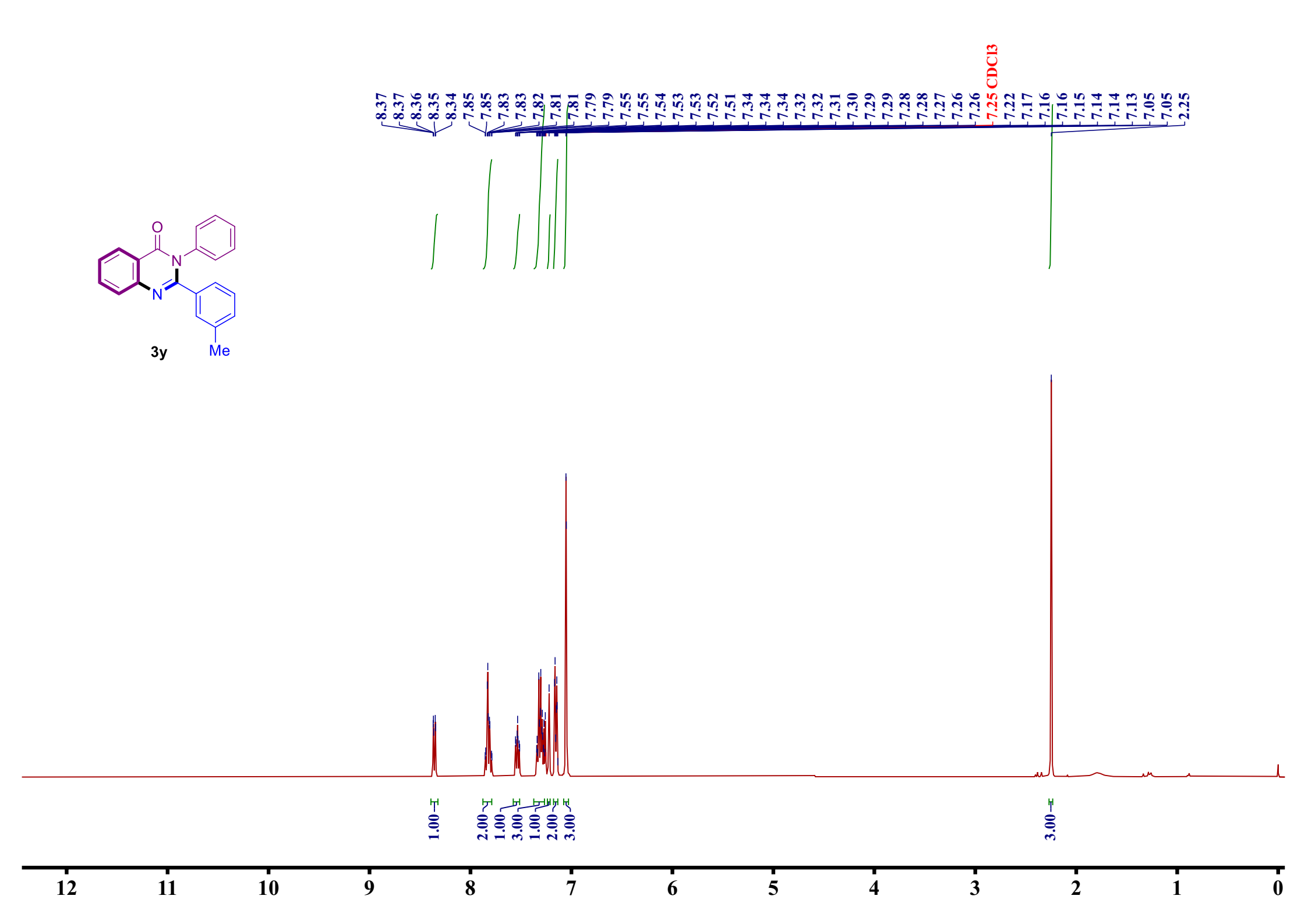
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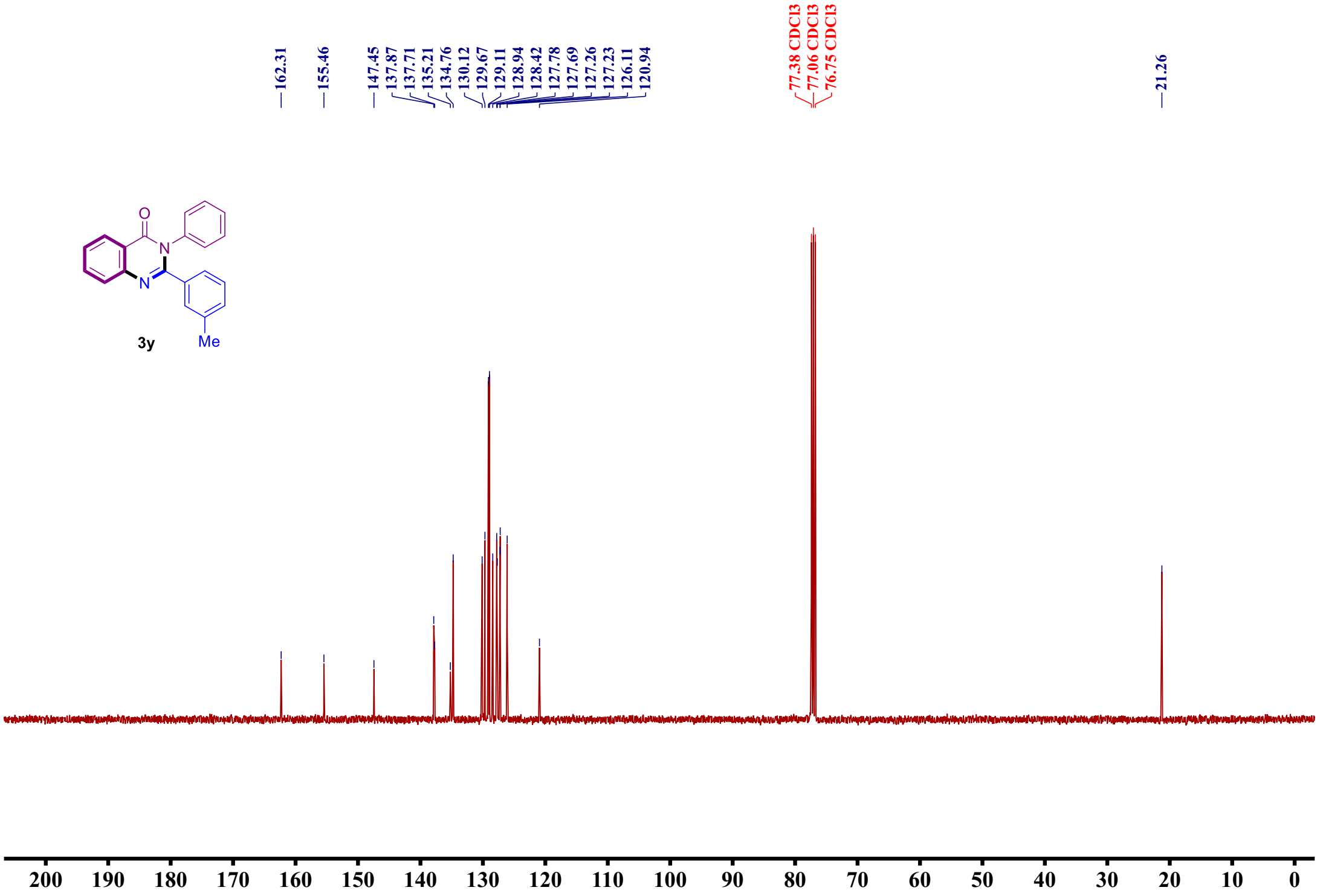
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Me
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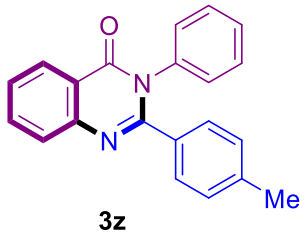
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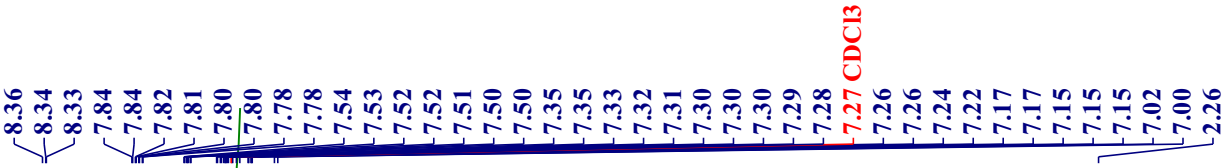
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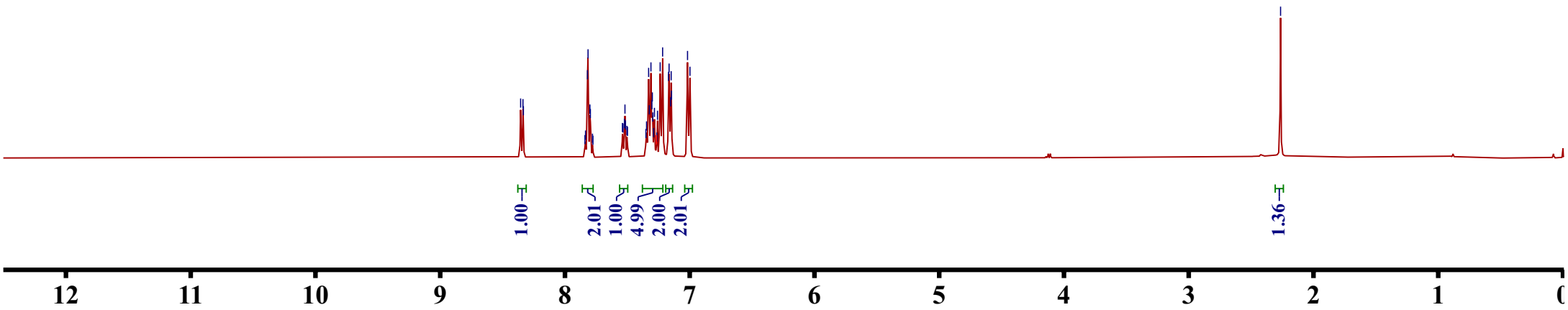
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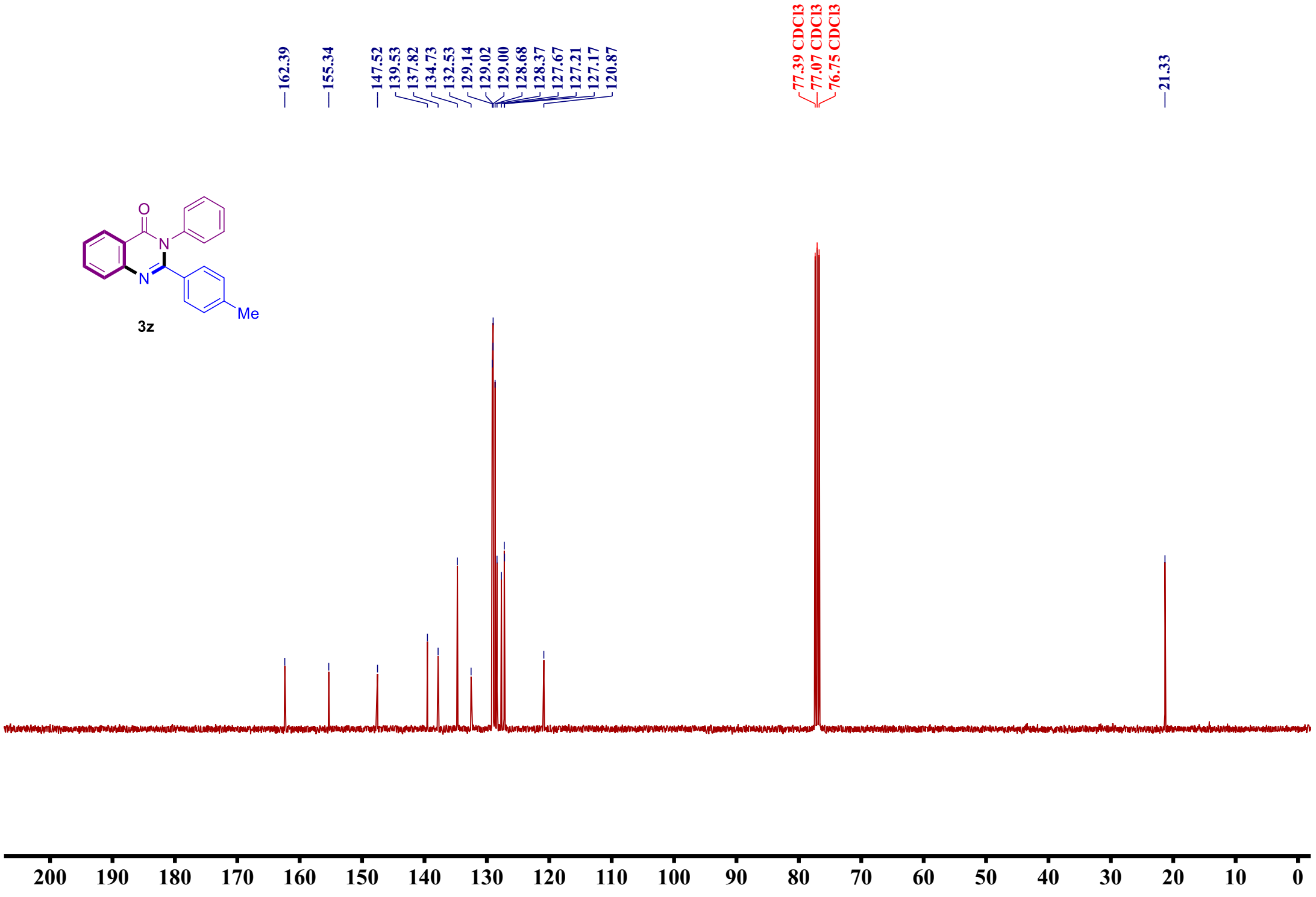
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77.07 CDCl3
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Me
3z
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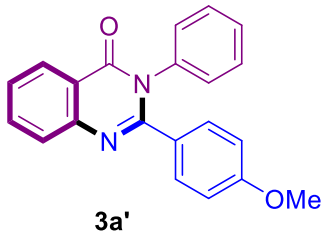

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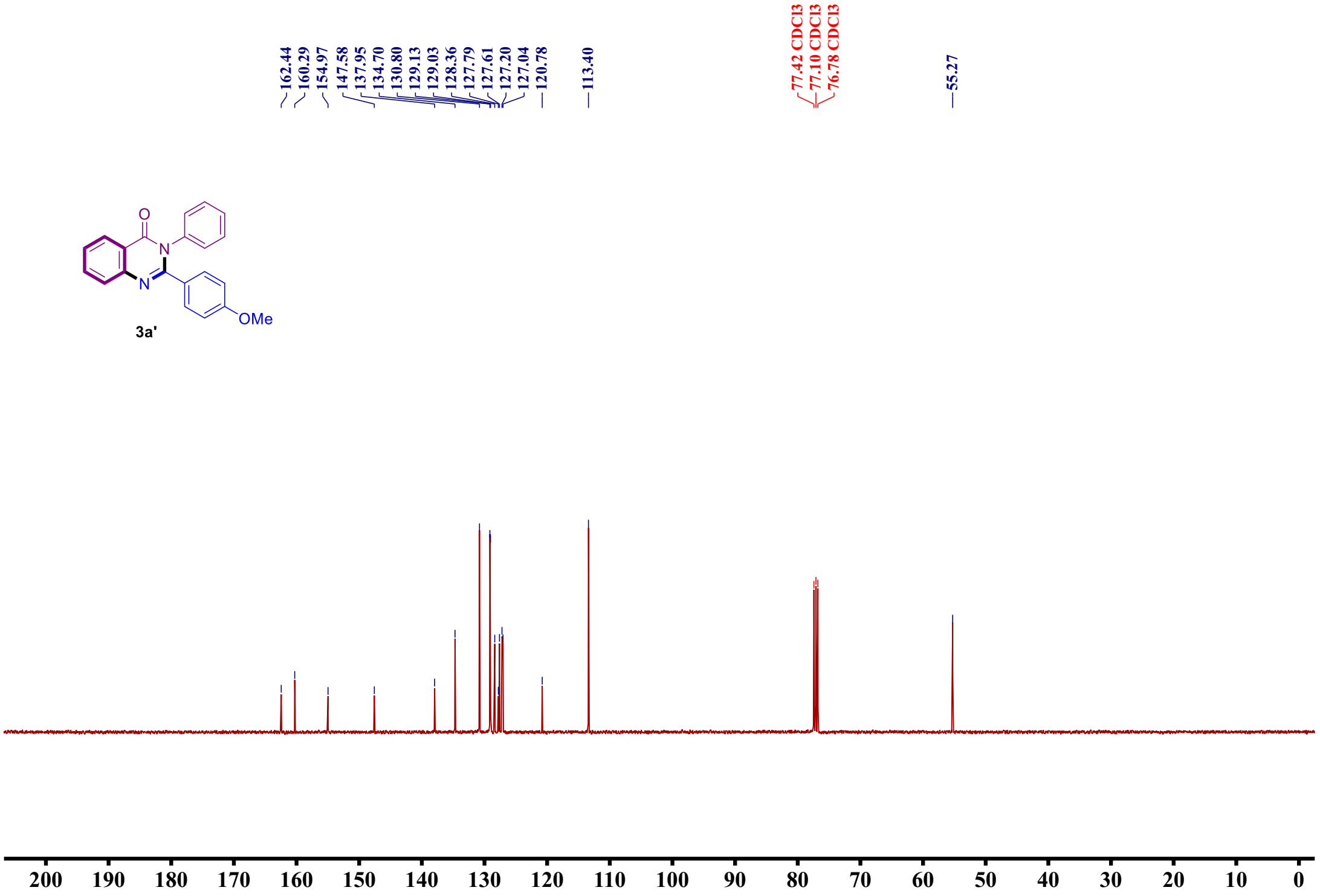
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120.78
113.40
77.42 CDCl3
77.10 CDCl3
76.78 CDCl3
55.27
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3a'
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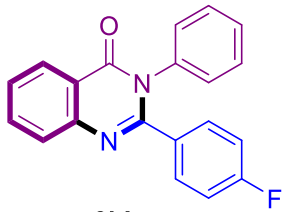
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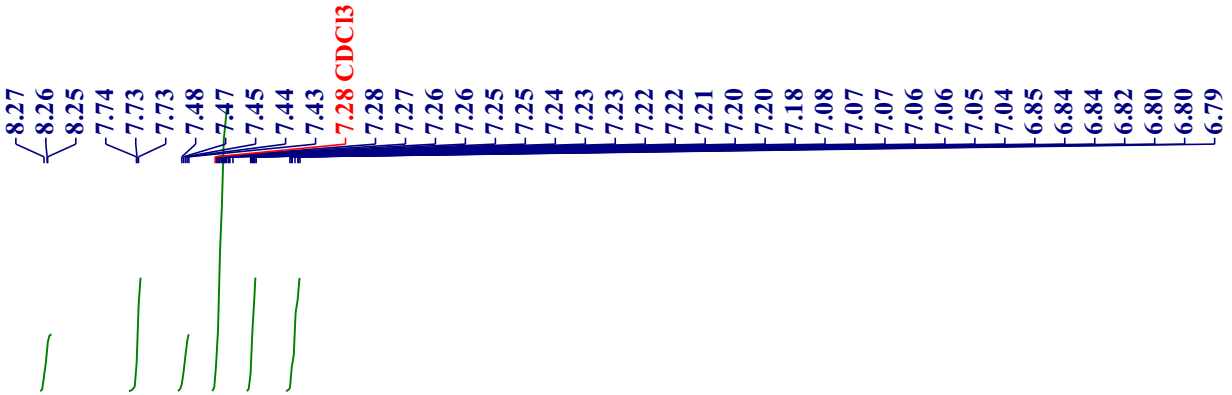
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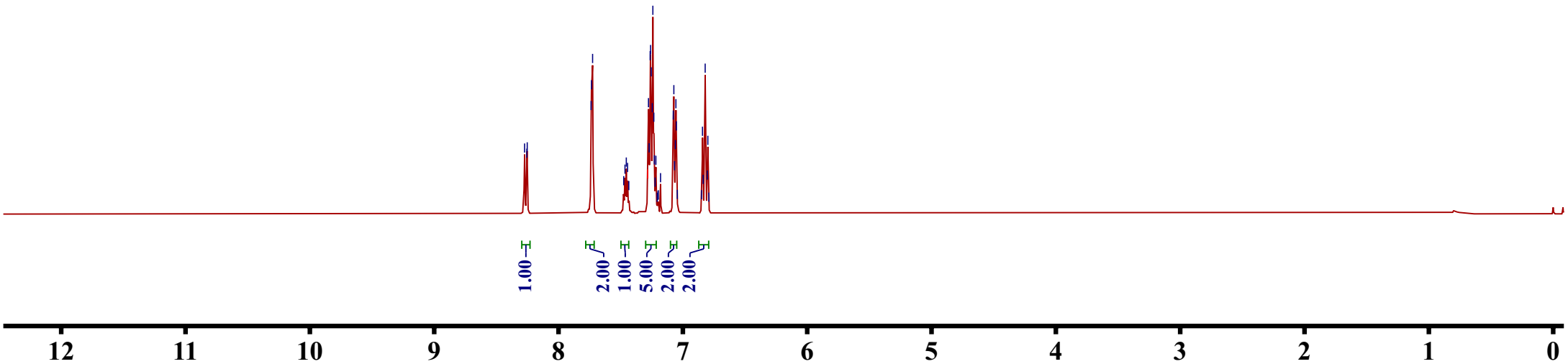
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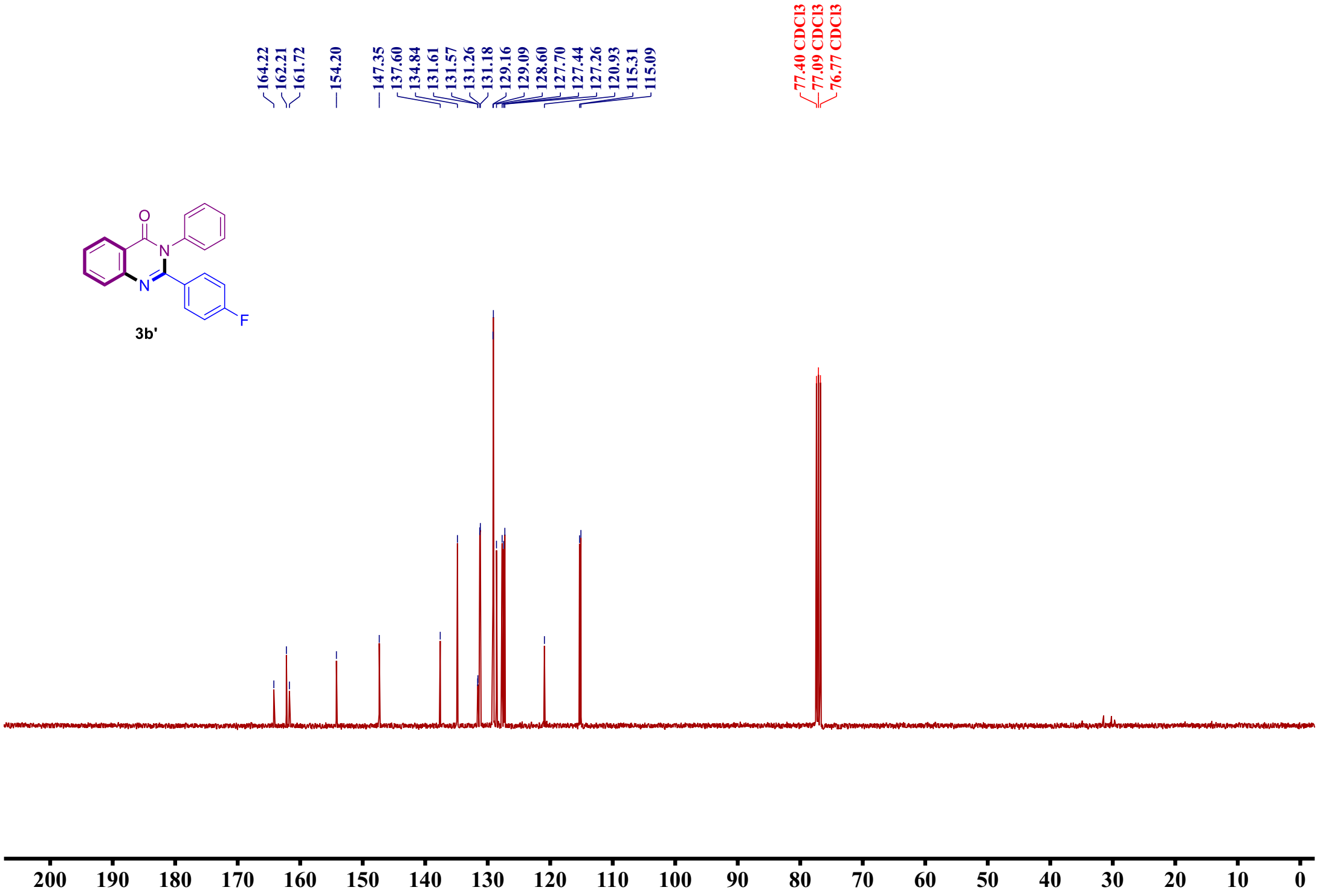
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77.09 CDCl3
76.77 CDCl3
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N
F
3b'
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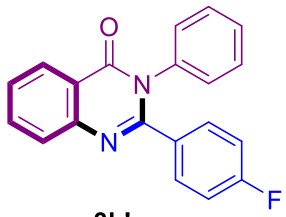

3b'

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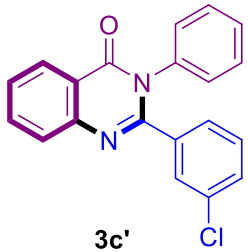

3c'

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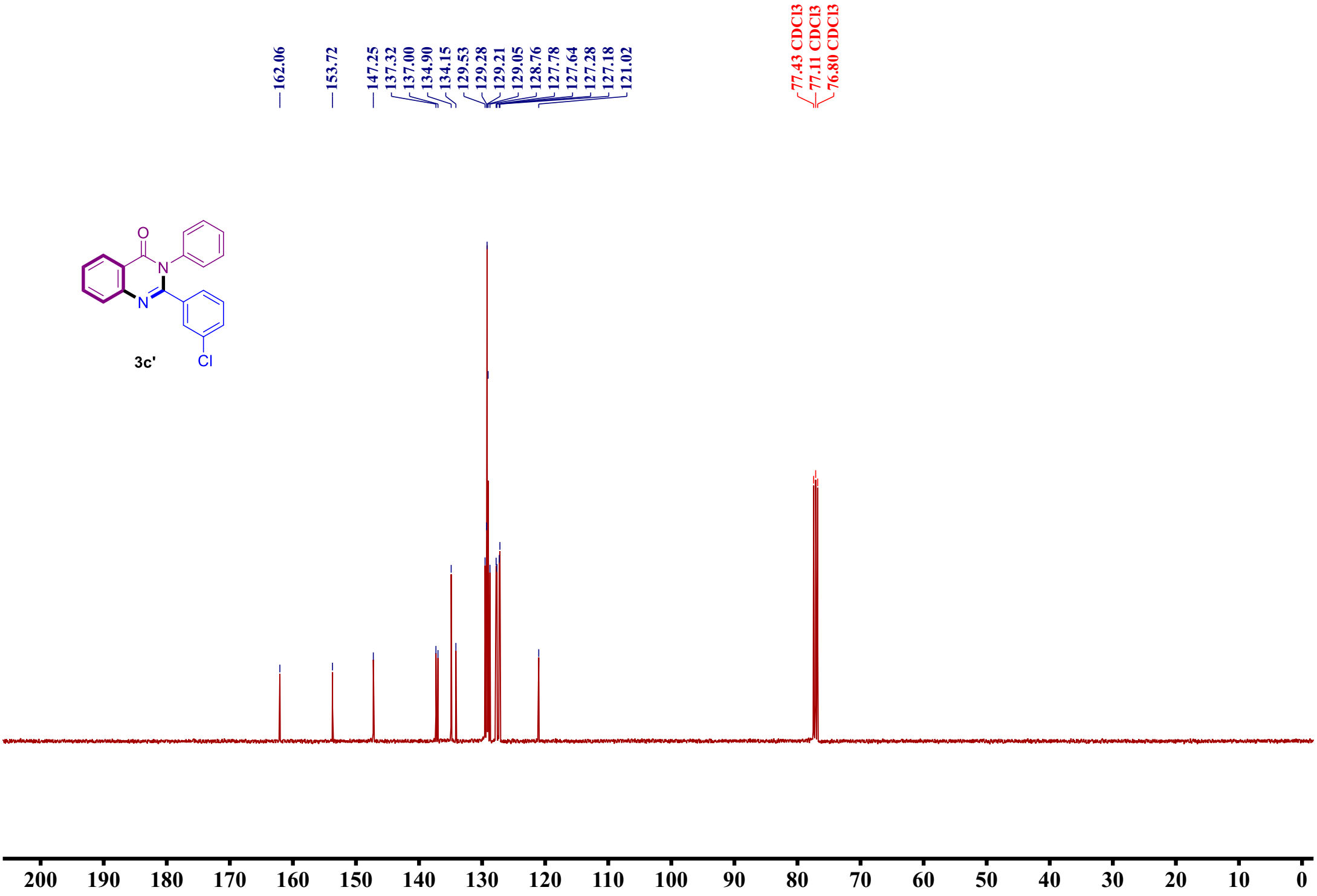
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Cl
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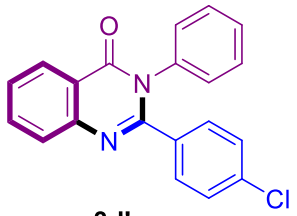

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7.08
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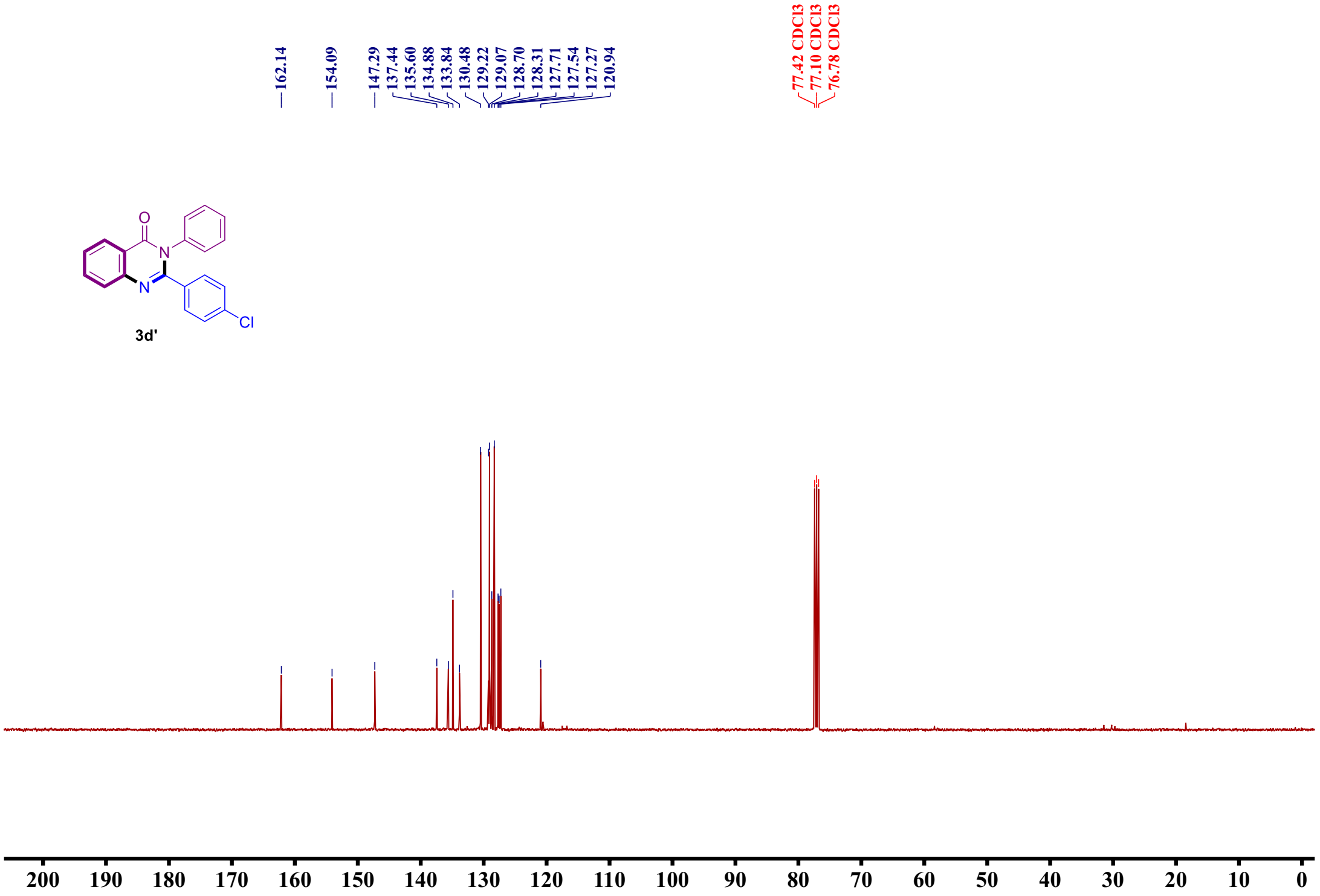
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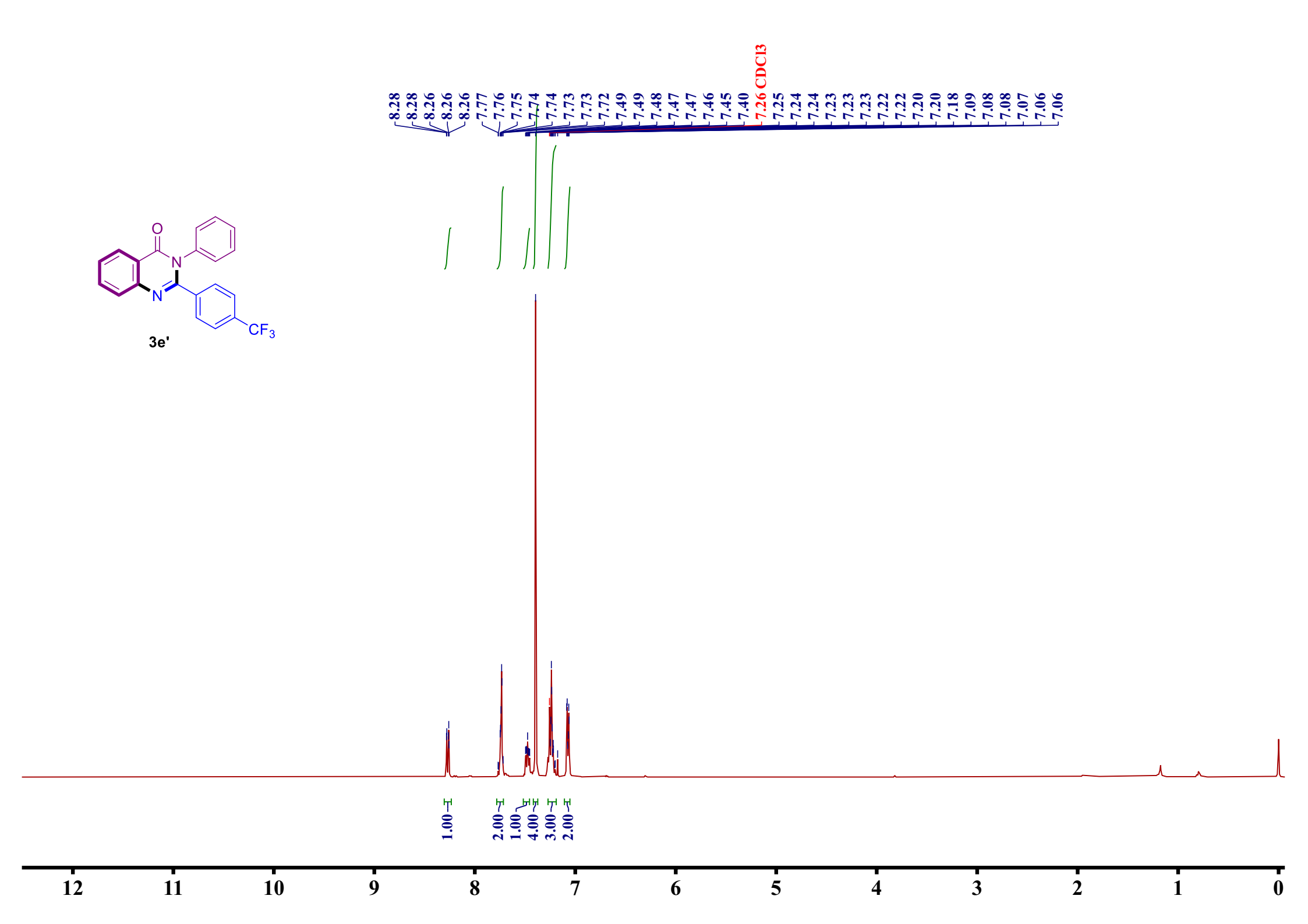
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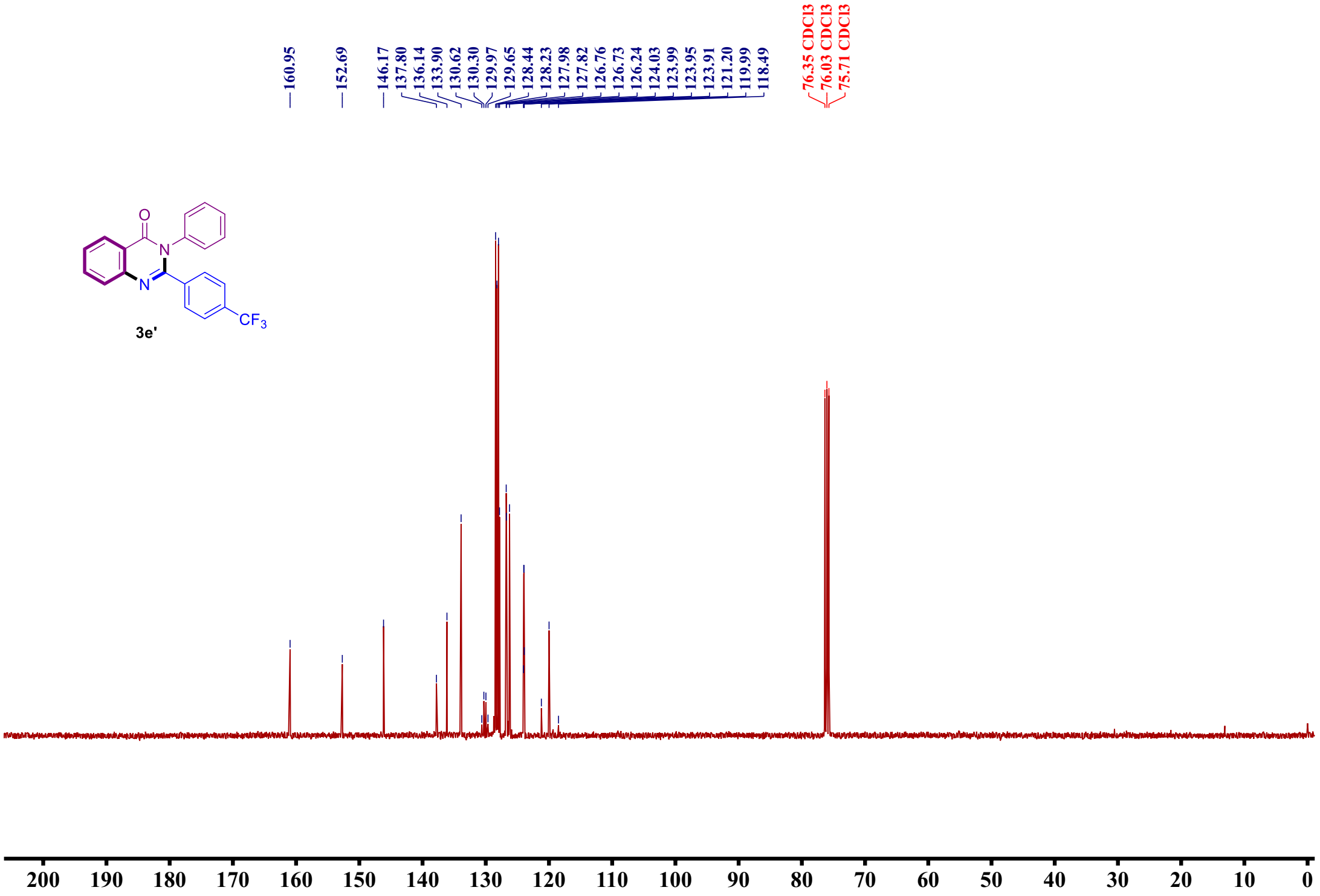
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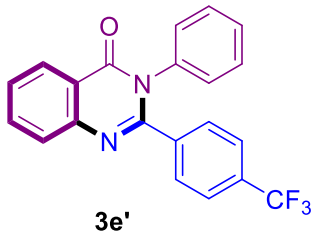

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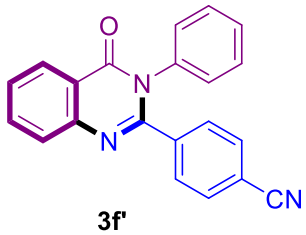
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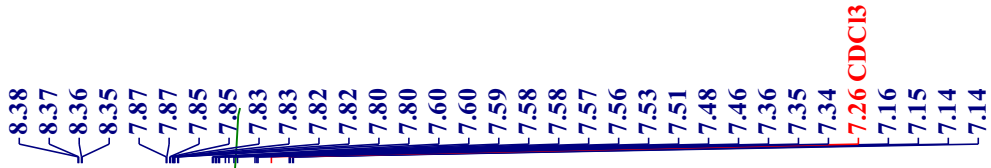
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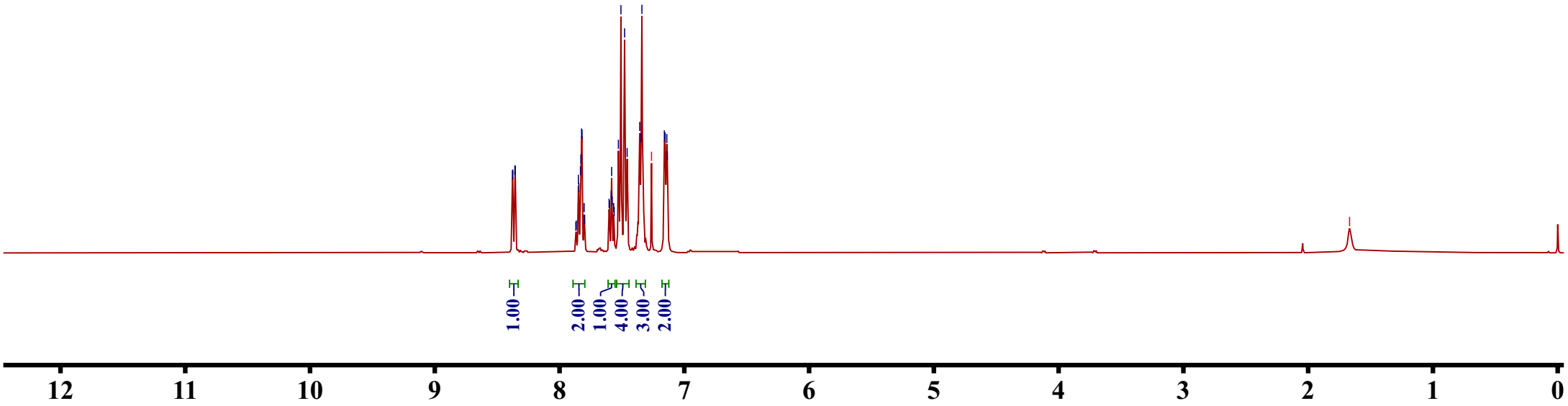
1.67 H2O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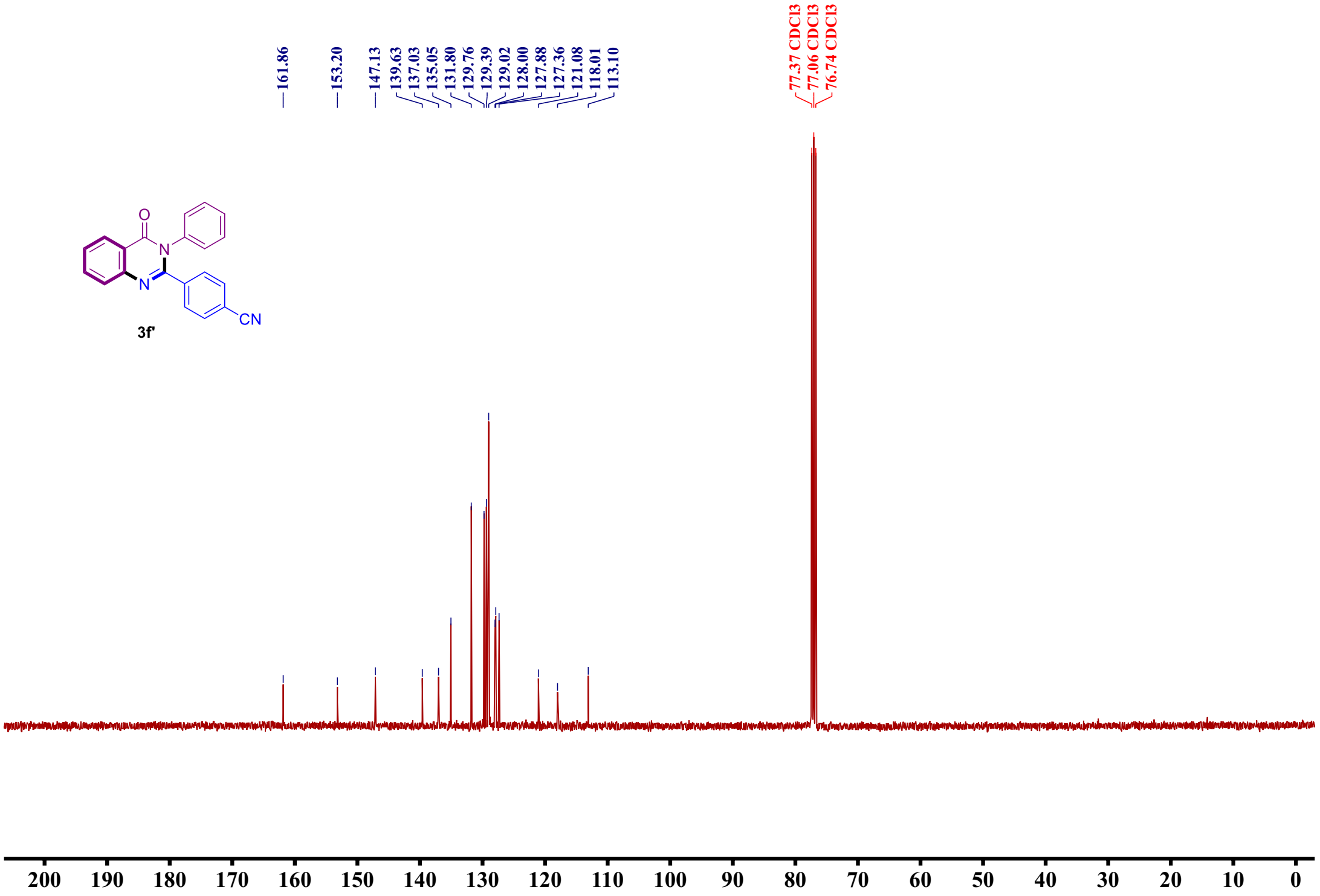
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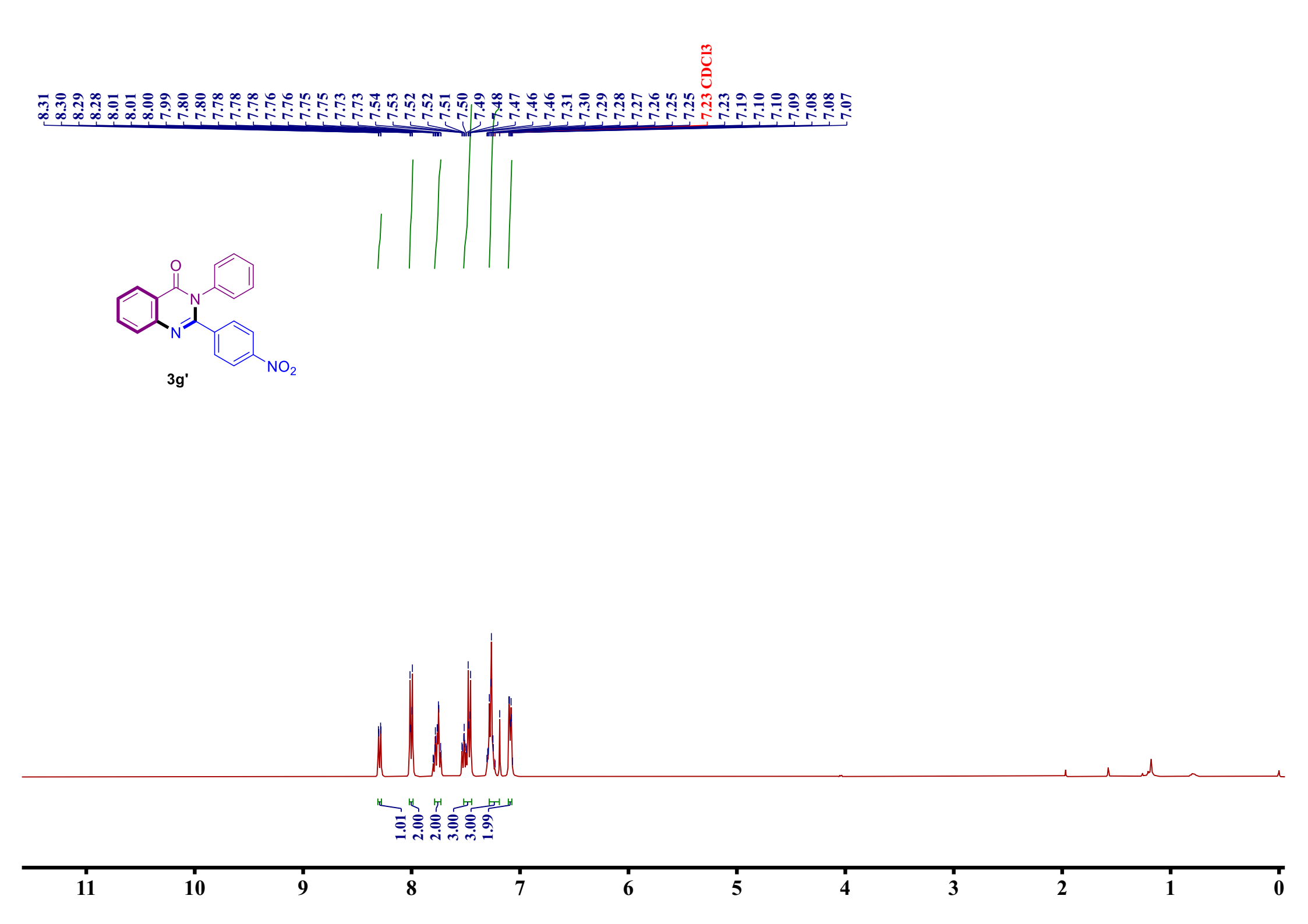
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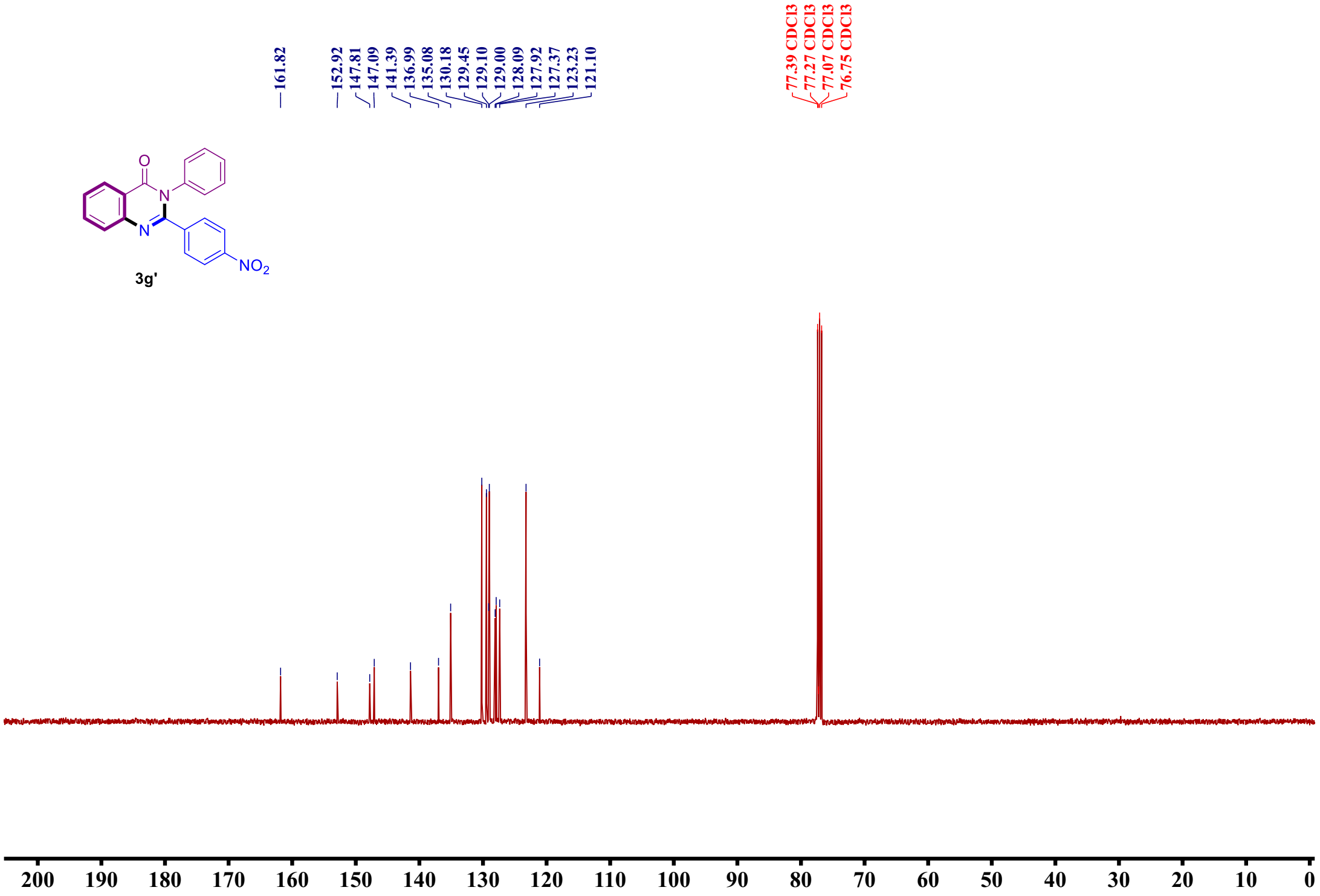
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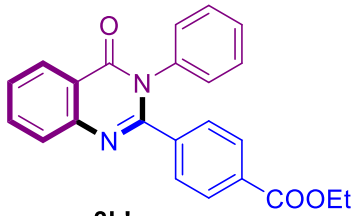

3h'

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4.25
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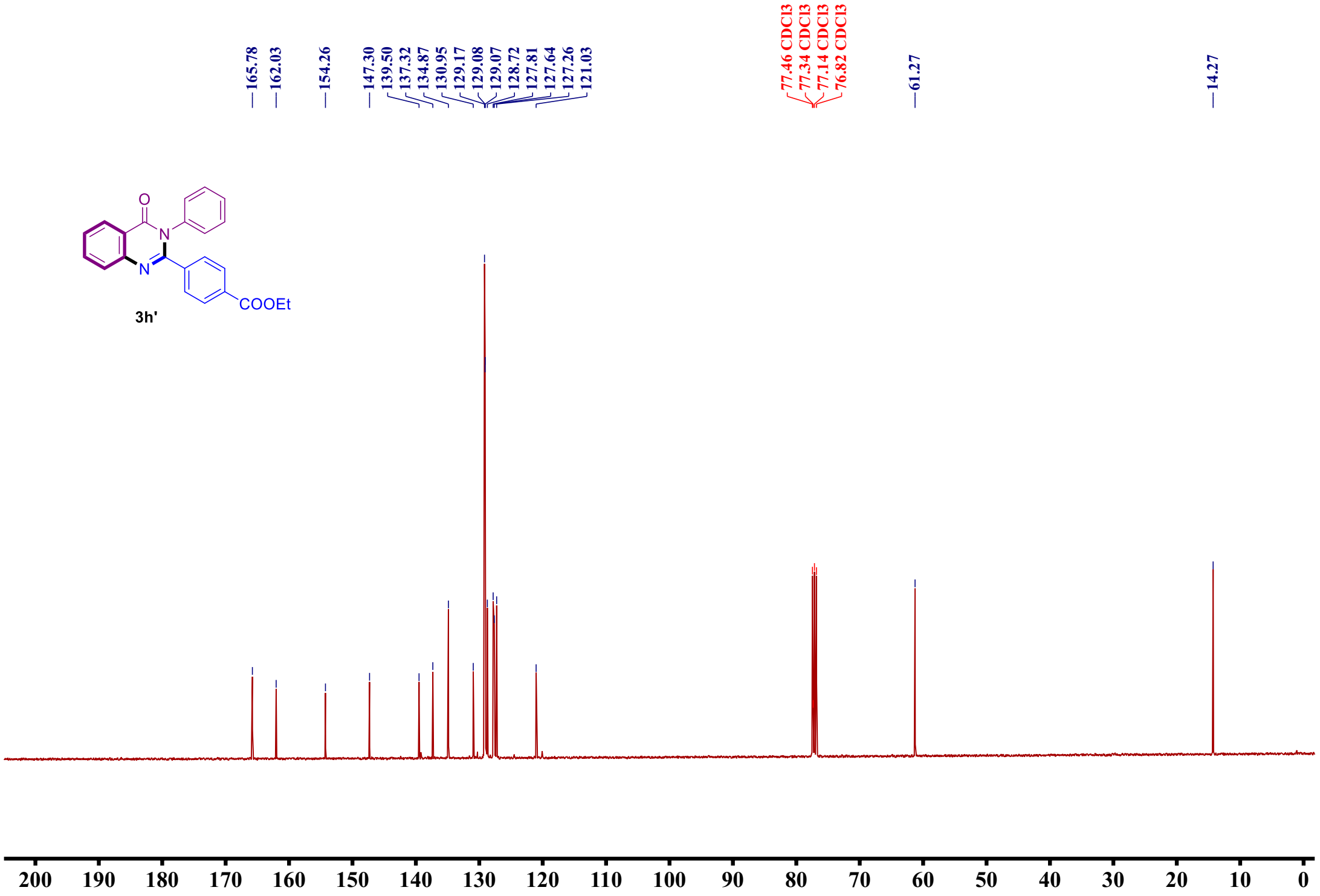
2.00
3.00

11 10 9 8 7 6 5 4 3 2 1 0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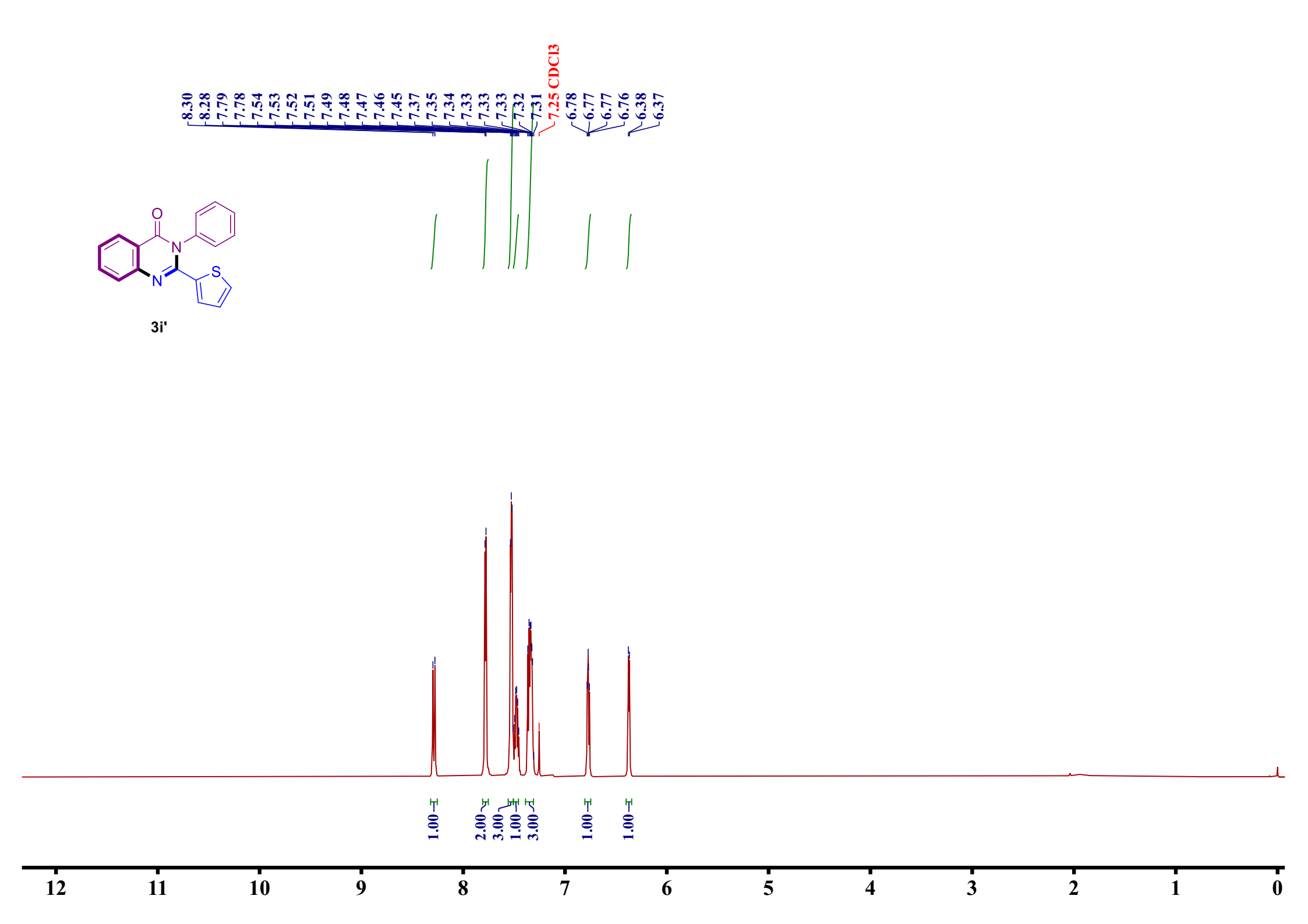
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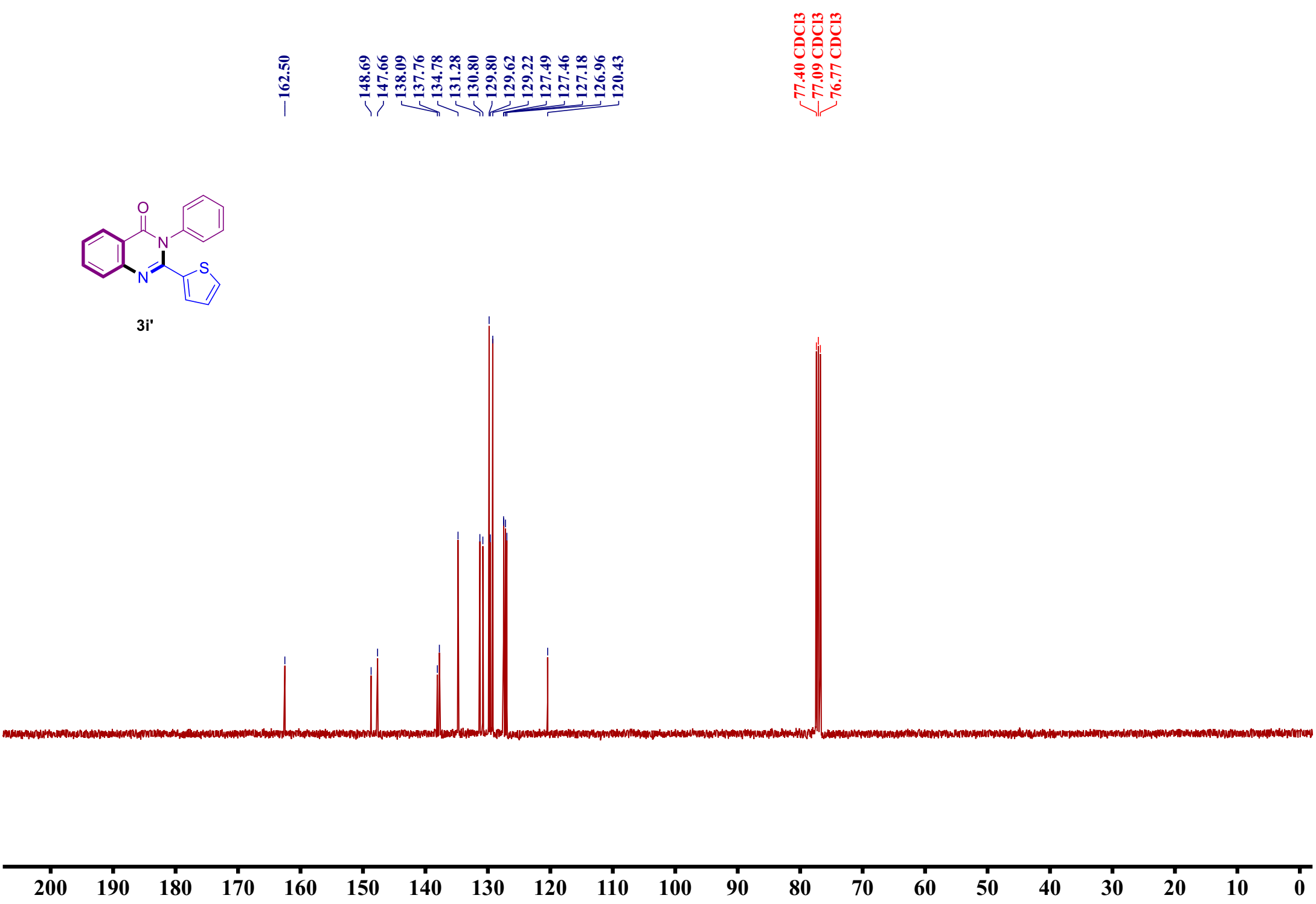
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