

Electronic Supplementary Information (ESI)

KHMDS Mediated Ring-Opening/Reconstruction of Anthranils with Arylacetonitriles: Synthesis of Multisubstituted 2-Aminoquinoline *N*-Oxides

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1. General Information

^1H , ^{13}C , and ^{19}F NMR spectra were recorded at 25 °C on a Bruker Avance III 500 MHz spectrometer operating at 500 MHz for ^1H , 125 MHz for ^{13}C , and 471 MHz for ^{19}F NMR experiments. Chemical shifts were calibrated to the residual proton and carbon resonance of the solvent, CDCl_3 (^1H δ 7.26; ^{13}C δ 77.0)/ DMSO-d_6 (^1H δ 2.50; ^{13}C δ 39.52). ^{19}F NMR chemical shifts are relative to trifluoro-toluene in CDCl_3 at $\delta = -63.72$ ppm (external reference). The following abbreviations were used to illuminate the diversities: δ = chemical shifts, J = coupling constant, s = singlet, d = doublet, t = triplet, q = quartet, sep = septet, m = multiplet, bs = broad singlet. Chemical shifts are given in ppm relative to the internal standard of tetramethylsilane (TMS). High-resolution mass spectra (HRMS) were obtained by using a TOF analyzer in ESI mode. X-ray data were taken at 273K with a Bruker APEX-II CCD single crystal diffractometer by using graphite monochromated Mo-K α radiation (0.71073 Å). Data integration was done using SAINT.^{1a} Intensities for absorption were corrected using SADABS.^{1b} Structure solution and refinement were carried out using Bruker SHELX-TL.^{1c-d} TLC analysis was performed with pre-coated TLC plates (0.2 mm, Silica gel 60 F-254, Merck). Column chromatography was done using silica gel (100-200 mesh) as an adsorbent. Unless otherwise stated, all reagents and starting materials obtained from commercial suppliers were used without further purification. Anthranils, Arylacetonitriles, KHMDS (0.5 M in toluene), LiHMDS (1.0 M in toluene) were purchased from Sigma-Aldrich, Alfa Aesar, TCI and CDH India. Toluene was distilled over sodium metal and benzophenone and stored under nitrogen. All the reactions were performed in an oven-dried glass pressure tube (capacity 15 mL) procured from the Sigma-Aldrich India (catalogue No. Z181099) under an atmosphere of N_2 . Reactions were monitored by thin-layer chromatography (TLC). The products were purified by column chromatography on silica gel using methanol and ethyl acetate as the eluent.

Preparation of Starting Materials

The C3-substituted anthranil derivatives were prepared by the reported procedure Pd-catalyzed reactions of anthranil and aryl halides.² and arylacetonitrile derivatives 2-(4-((tert-butyl)dimethylsilyloxy)phenyl)acetonitrile (**2d**),^{3a} 2-(4-(methoxymethoxy)phenyl)acetonitrile (**2e**),^{3b} 2-(4-(benzyloxy)phenyl)acetonitrile (**2f**),^{3b} 2-(4-(1H-pyrazol-1-yl)phenyl)acetonitrile (**2n**)^{3b} were prepared according to the literature procedure. Anthranil and remaining arylacetonitrile derivatives were purchased from standard commercial sources (Sigma Aldrich, and Alfa Aesar).

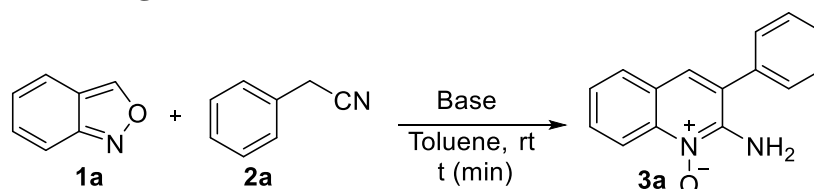
2. Experimental Section

2.1 Optimization of the reaction conditions

To the stirred solution of benzo[*c*]isoxazole (**1a**, 60 mg, 0.5 mmol) in toluene (1 mL), 2-phenylacetonitrile (**2a**, 88 mg, 0.75 mmol) and KHMDS (0.5 M in toluene) (1 mL, 0.5 mmol) were added under nitrogen atmosphere. The resulting reaction mixture was stirred at room temperature for 1 h. After 1h, the reaction mixture was quenched with saturated NH₄Cl solution, extracted with ethyl acetate (20 mL×3) and was dried over Na₂SO₄. Purification using column chromatography on silica gel gave the corresponding product 2-amino-3-phenylquinoline-1-oxide (**3a**) (ethyl acetate /methanol = 95/5) in the reported yield.

Entry	Parameter
Table S1	Base screening
Table S2	Solvent screening
Table S3	Base loading screening
Table S4	Substrate 1a and 2a ratio screening
Table S5	Reaction time screening

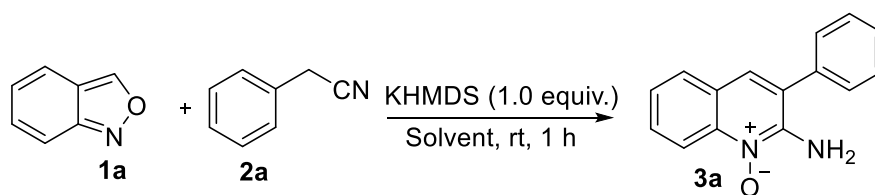
Table S1. Base screening^a



Entry	1a/2a (equiv.)	Base (equiv.)	Solvent	Temp.	Time (min)	Yield ^b (%)
1	1.0/1.5	Na ₂ CO ₃ (1.0)	Toluene	rt	180	NR ^c
2	1.0/1.5	CS ₂ CO ₃ (1.0)	Toluene	rt	180	13
3	1.0/1.5	NEt ₃ (1.0)	Toluene	rt	180	NR ^c
4	1.0/1.5	NaOH (1.0)	Toluene	rt	180	39
5	1.0/1.5	<i>t</i> -BuONa (1.0)	Toluene	rt	60	65
6	1.0/1.5	KHMDS (1.0)	-	rt	60	66

^a Reactions were carried out with **1a** (0.5 mmol, 1.0 equiv.), **2a** (0.75 mmol, 1.5 equiv.), base (0.5 mmol, 1.0 equiv.), toluene (1.0 mL) at rt for 60-180 minutes. ^b Isolated yield. ^c NR: No Reaction.

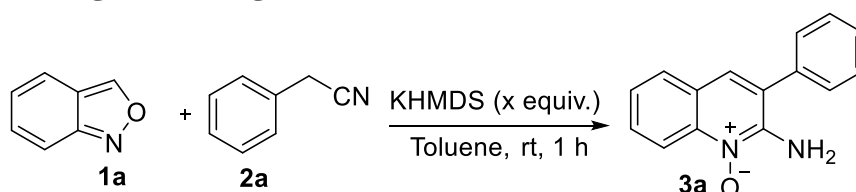
Table S2. Solvent screening^a



Entry	Solvent	3a ^b (%)
1	DCM	75
2	Xylene	72
3	CHCl ₃	55
4	DMF	66

^a Reactions were carried out with **1a** (0.5 mmol, 1.0 equiv.), **2a** (0.75 mmol, 1.5 equiv.), KHMDS (0.5 mmol, 1.0 equiv.). ^b Isolated yield.

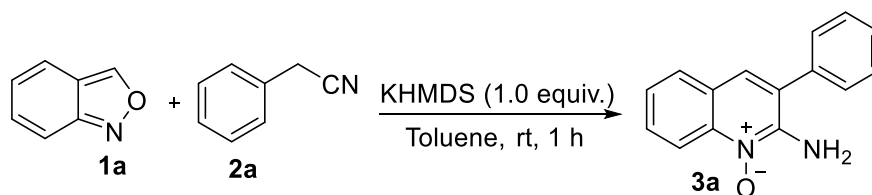
Table S3. Screening the loading of base ^a



Entry	KHMDS (equiv.)	3a ^b (%)
1	KHMDS (0.2)	51
2	KHMDS (0.5)	70
3	KHMDS (1.0)	97

^a Reactions were carried out with **1a** (0.5 mmol, 1.0 equiv.), **2a** (0.75 mmol, 1.5 equiv.), KHMDS (x equiv.). ^b Isolated yield.

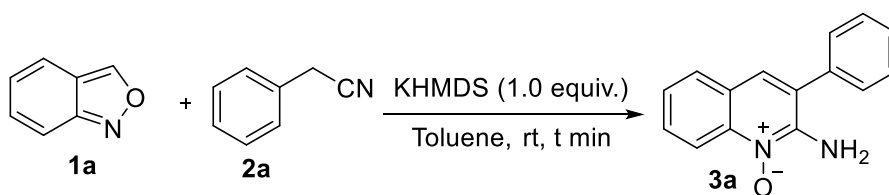
Table S4. Screening the substrate 1a and 2a ratio ^a



Entry	1a (mmol)	2a (mmol)	3a ^b (%)
1	1.0	1.0	46
2	1.0	1.5	97

^a Reactions were carried out with **1a** (x mmol), **2a** (x mmol), KHMDS (1.0 equiv.). ^b Isolated yield.

Table S5. Screening the reaction time ^a



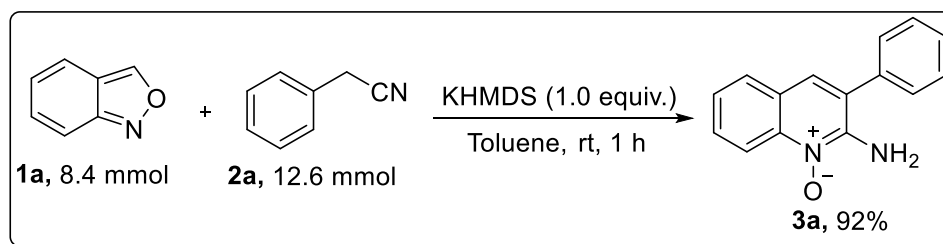
Entry	Time (min)	3a ^b (%)
1	5	55
2	10	68
3	30	82
4	60	97
5	180	96

^a Reactions were carried out with **1a** (0.5 mmol, 1.0 equiv.), **2a** (0.75 mmol, 1.5 equiv.), KHMDS (0.5 mmol, 1.0 equiv.). ^b Isolated yield.

2.2 General procedure for the synthesis of quinoline *N*-oxides (**3a** as representative example)

To the stirred solution of benzo[*c*]isoxazole (**1a**, 60 mg, 0.5 mmol) in toluene (1 mL), 2-phenylacetonitrile (**2a**, 88 mg, 0.75 mmol) and KHMDS (0.5 M in toluene) (1 mL, 0.5 mmol) were added under nitrogen atmosphere. The resulting reaction mixture was stirred at room temperature for 1 h. After design time reaction mixture was quenched with saturated NH₄Cl solution, extracted with ethyl acetate (20 mL×3) and was dried over Na₂SO₄. Purification using column chromatography on silica gel gave the corresponding product 2-amino-3-phenylquinoline-1-oxide (**3a**) (ethyl acetate /methanol = 95/5) in the reported yield.

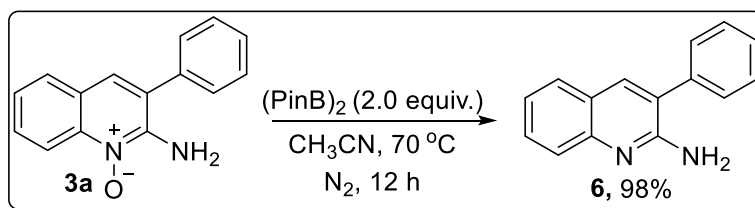
2.3 Large-scale reaction of **3a**



To the stirred solution of benzo[*c*]isoxazole (**1a**, 1 g, 8.4 mmol) in toluene (5 mL), 2-phenylacetonitrile (**2a**, 1.47 g, 12.6 mmol) and KHMDS (0.5 M in toluene) (16.8 mL, 8.4 mmol) were added under nitrogen atmosphere. The resulting reaction mixture was stirred at room temperature for 1 h. After design time reaction mixture was quenched with saturated NH₄Cl solution, extracted in ethyl acetate (20 mL×3) and was dried over Na₂SO₄. Purification using column chromatography (ethyl acetate /methanol = 95/5) on silica gel gave 2-amino-3-phenylquinoline-1-oxide **3a** as yellow solid (1.82 g, 7.7 mmol, 92%).

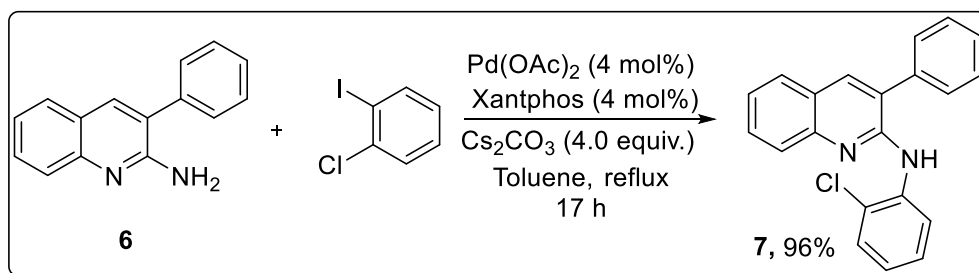
2.4 Post-functionalization of Quinoline *N*-Oxide (**3a**)

2.4.1 Reduction of 2-amino-3-phenylquinoline 1-oxide (**3a**) to 3-phenylquinolin-2-amine (**6**):⁴



To the stirred solution of 2-amino-3-phenylquinoline 1-oxide (**3a**, 118 mg, 0.5 mmol) in acetonitrile (2 mL) was added Bis(pinacolato)diboron (PinB)₂ (254 mg, 1.0 mmol) under nitrogen atmosphere. The resulting reaction mixture was stirred at 70 °C for 12 h. After design time reaction mixture was quenched with saturated NH₄Cl solution, extracted in ethyl acetate (20 mL×3) and was dried over Na₂SO₄. Purification using column chromatography (ethyl acetate /*n*-hexane = 1/1) on silica gel gave 3-phenylquinolin-2-amine (**6**) as white solid. Yield: 98% (108 mg); ¹H NMR (500 MHz, CDCl₃) δ 7.79 (s, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.57 (t, *J* = 7.7 Hz, 1H), 7.51 (dt, *J* = 15.4, 7.7 Hz, 4H), 7.44 (t, *J* = 7.0 Hz, 1H), 7.27 (dd, *J* = 8.8, 5.8 Hz, 1H), 5.05 (s, 2H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 155.2, 147.2, 137.6, 137.2, 129.6, 129.1, 128.9, 128.2, 127.5, 125.6, 125.0, 124.2, 122.8 ppm.

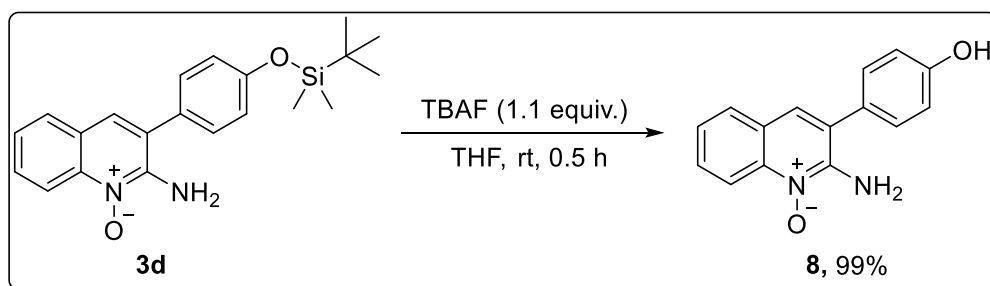
2.4.2 Synthesis of *N*-(2-chlorophenyl)-3-phenylquinolin-2-amine (**7**) from 3-phenylquinolin-2-amine (**6**):⁵



To the stirred solution of 3-phenylquinolin-2-amine (**6**, 132 mg, 0.6 mmol) and 1-chloro-2-iodobenzene (119 mg, 0.5 mmol) in toluene (2 mL) was added Pd(OAc)₂ (4.49 mg, 4 mol%), xantphos (11.6 mg, 4 mol%), Cs₂CO₃ (652 mg, 2.0 mmol) under nitrogen atmosphere. The resulting reaction mixture was reflux for 17 h. After design time reaction mixture was quenched with saturated NH₄Cl solution, extracted in ethyl acetate (20 mL×3) and was dried over Na₂SO₄. Purification using column chromatography (ethyl acetate /*n*-hexane = 98/2) on silica gel gave *N*-(2-chlorophenyl)-3-phenylquinolin-2-amine (**7**) as yellow gel. Yield: 96% (191 mg); ¹H NMR (500 MHz, DMSO-*d*₆) δ 9.03 (dd, *J* = 8.3, 1.3 Hz, 1H), 8.10 (s, 1H), 7.86 (d, *J*

= 7.2 Hz, 1H), 7.80 (d, $J = 8.3$ Hz, 1H), 7.64 (ddd, $J = 11.4, 7.0, 4.4$ Hz, 5H), 7.58 – 7.52 (m, 1H), 7.44 (dd, $J = 8.0, 1.3$ Hz, 1H), 7.40 (dd, $J = 11.3, 4.2$ Hz, 2H), 7.02 (td, $J = 7.7, 1.4$ Hz, 1H) ppm; ^{13}C { ^1H } NMR (125 MHz, DMSO- d_6) δ 150.7, 145.9, 137.2, 136.7, 136.1, 129.9, 129.5, 129.3, 129.0, 128.9, 127.9, 127.8, 126.5, 126.4, 124.2, 123.9, 122.8, 122.0, 120.4 ppm; HRMS (ESI-TOF): m/z [M+H] $^+$ calcd for $\text{C}_{21}\text{H}_{16}\text{ClN}_2^+$: 331.0997; found: 331.1004.

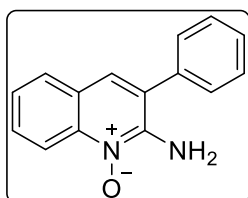
2.4.3 Procedure for the preparation of compound **8**:⁶



To the stirred solution of TBMS protected *N*-oxide (**3d**, 50 mg, 0.136 mmol, 1.0 equiv.) in THF (5 mL THF per mmol) was added tetrabutylammonium fluoride (TBAF, 1.0 M in THF, 1.1 equiv.) and the resulting solution was stirred at room temperature for 0.5 h. Upon completion the reaction (monitored by TLC) mixture the reaction mixture was quenched with water and extracted with ethyl acetate. The combined organic layers were washed with brine, dried over Na_2SO_4 , and concentrated under reduced pressure. The crude material was purified by column chromatography on silica gel (MeOH/ethyl acetate, 15:85) to give the product **8** as yellow gel. Yield: 99% (34 mg); ^1H NMR (500 MHz, DMSO- d_6) δ 8.29 (d, $J = 8.6$ Hz, 1H), 7.88 (d, $J = 7.8$ Hz, 1H), 7.68 (dd, $J = 14.3, 5.8$ Hz, 2H), 7.41 (t, $J = 9.5$ Hz, 3H), 6.98 (s, 2H), 6.93 (d, $J = 8.2$ Hz, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, DMSO- d_6) δ 157.9, 146.9, 138.0, 129.9 (2C), 128.3, 126.4, 126.2, 124.4, 124.1, 122.4, 116.8, 115.9 ppm; HRMS (ESI-TOF): m/z [M+H] $^+$ calcd for $\text{C}_{15}\text{H}_{13}\text{N}_2\text{O}_2^+$: 253.0972; found: 253.0972.

3. Characterization data for products

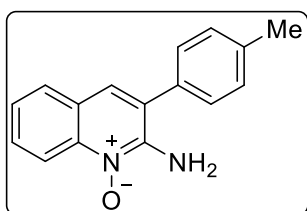
2-Amino-3-phenylquinoline 1-oxide (**3a**):



Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 95:5); Yield: 97% (96 mg), Yellow solid; mp 175-176 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.56 (d, $J = 8.8$ Hz, 1H), 7.77 – 7.69 (m, 2H), 7.57 (s, 1H), 7.53 (d, $J = 4.2$ Hz, 4H), 7.49 (dd, $J = 9.1, 4.5$ Hz, 1H), 7.43 (t, $J = 7.5$ Hz, 1H), 6.23 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 146.8, 138.9, 135.5, 130.7, 129.5, 129.1, 128.6, 128.3,

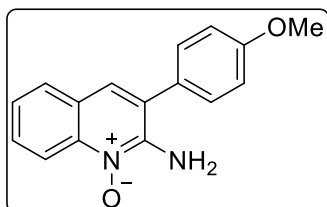
128.0, 124.9, 124.4, 122.8, 117.5, 77.2, 77.0, 76.7 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{15}H_{13}N_2O^+$: 237.1022; found: 237.1015.

2-Amino-3-(*p*-tolyl)quinoline 1-oxide (3b):



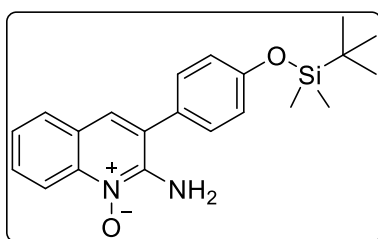
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 96:4); Yield: 62% (65 mg), Yellow solid; mp 188-189 °C; 1H NMR (500 MHz, $CDCl_3$) δ 8.53 (d, J = 8.7 Hz, 1H), 7.70 (d, J = 7.5 Hz, 2H), 7.52 (s, 1H), 7.40 (d, J = 7.6 Hz, 3H), 7.31 (d, J = 7.5 Hz, 2H), 6.27 (s, 2H), 2.41 (s, 3H) ppm; ^{13}C $\{^1H\}$ NMR (125 MHz, $CDCl_3$) δ 146.7, 139.0, 138.8, 132.6, 130.4, 130.0, 128.4, 127.9, 127.7, 124.7, 124.4, 122.8, 117.5, 21.2 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{16}H_{15}N_2O^+$: 251.1179; found: 251.1176.

2-Amino-3-(4-methoxyphenyl)quinoline 1-oxide (3c):



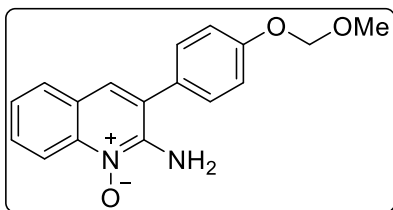
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 93:7); Yield: 58% (65 mg), Yellow solid; mp 182-183 °C; 1H NMR (500 MHz, $CDCl_3$) δ 8.51 (d, J = 8.9 Hz, 1H), 7.68 (t, J = 7.3 Hz, 2H), 7.51 (s, 1H), 7.43 (d, J = 8.6 Hz, 2H), 7.39 (t, J = 7.5 Hz, 1H), 7.02 (d, J = 8.6 Hz, 2H), 6.28 (s, 2H), 3.85 (s, 3H) ppm; ^{13}C $\{^1H\}$ NMR (125 MHz, $CDCl_3$) δ 160.1, 146.9, 138.7, 130.4, 129.8, 127.8, 127.7, 127.7, 124.7, 124.2, 122.8, 117.5, 114.8, 55.4 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{16}H_{15}N_2O_2^+$: 267.1128; found: 267.1135.

2-Amino-3-(4-((*tert*-butyldimethylsilyl)oxy)phenyl)quinoline 1-oxide (3d):



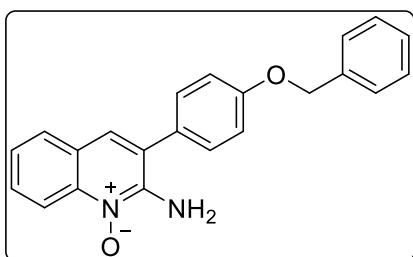
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 95:5); Yield: 80% (123 mg), Yellow solid; mp 135-136 °C; 1H NMR (500 MHz, $CDCl_3$) δ 8.52 (d, J = 8.8 Hz, 1H), 7.68 (t, J = 6.9 Hz, 2H), 7.51 (s, 1H), 7.38 (t, J = 7.7 Hz, 3H), 6.96 (d, J = 8.4 Hz, 2H), 6.26 (s, 2H), 1.01 (s, 9H), 0.25 (s, 6H) ppm; ^{13}C $\{^1H\}$ NMR (125 MHz, $CDCl_3$) δ 156.5, 146.8, 138.7, 130.4, 129.8, 128.3, 127.8, 124.7, 124.2, 122.9, 120.9, 117.5, 116.7, 25.6, 18.2, -4.4 ppm; HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{27}N_2O_2Si^+$: 367.1836; found: 367.1850.

2-Amino-3-(4-(methoxymethoxy)phenyl)quinoline 1-oxide (3e):



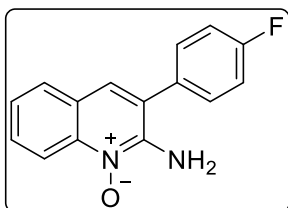
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 94:6); Yield: 95% (118 mg), Yellow solid; mp 190-191 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.53 (d, J = 8.9 Hz, 1H), 7.69 (dd, J = 7.6, 5.5 Hz, 2H), 7.51 (s, 1H), 7.44 (d, J = 8.6 Hz, 2H), 7.39 (t, J = 7.5 Hz, 1H), 7.17 (d, J = 8.7 Hz, 2H), 6.23 (s, 2H), 5.23 (s, 2H), 3.51 (s, 3H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 157.7, 146.8, 138.8, 130.4, 129.8, 128.9, 127.8, 127.6, 124.7, 124.1, 122.9, 117.6, 117.1, 94.3, 56.1 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_3^+$: 297.1234; found: 297.1237.

2-Amino-3-(4-(benzyloxy)phenyl)quinoline 1-oxide (3f):



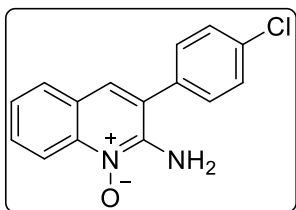
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 91:9); Yield: 68% (98 mg), Yellow gel; ^1H NMR (500 MHz, CDCl_3) δ 8.54 (d, J = 8.6 Hz, 1H), 7.70 (d, J = 7.1 Hz, 2H), 7.53 (s, 1H), 7.50 – 7.39 (m, 7H), 7.38 – 7.33 (m, 1H), 7.11 (d, J = 8.4 Hz, 2H), 6.26 (s, 2H), 5.14 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 159.3, 147.0, 138.8, 136.5, 130.5, 129.9, 128.7, 128.2, 128.0, 127.9, 127.8, 127.4, 124.8, 124.1, 122.9, 117.6, 115.8, 70.2 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{19}\text{N}_2\text{O}_2^+$: 343.1441; found: 343.1442.

2-Amino-3-(4-fluorophenyl)quinoline 1-oxide (3g):



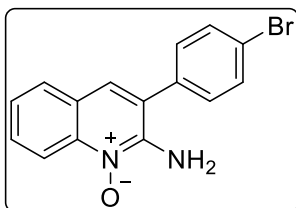
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 95:5); Yield: 80% (85 mg), Yellow solid; mp 190-191 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.44 (d, J = 8.3 Hz, 1H), 7.66 (d, J = 7.6 Hz, 2H), 7.45 (d, J = 10.2 Hz, 3H), 7.36 (t, J = 7.1 Hz, 1H), 7.10 (t, J = 8.0 Hz, 2H), 6.41 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 163.0 (d, $J_{\text{C-F}}$ = 247.5 Hz), 146.6, 138.9, 131.5 (d, $J_{\text{C-F}}$ = 3.8 Hz), 130.8, 130.5 (d, $J_{\text{C-F}}$ = 8.8 Hz), 128.1, 127.9, 124.9, 123.3, 122.7, 117.6, 116.5 (d, $J_{\text{C-F}}$ = 21.3 Hz) ppm; ^{19}F NMR (471 MHz, CDCl_3) δ -211.6 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{12}\text{FN}_2\text{O}^+$: 255.0928; found: 255.0933.

2-Amino-3-(4-chlorophenyl)quinoline 1-oxide (3h):



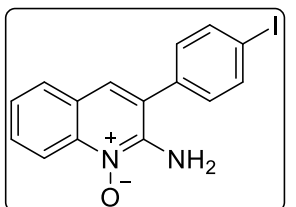
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 95:5); Yield: 76% (86 mg), Yellow solid; mp 195-196 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.46 (d, J = 8.4 Hz, 1H), 7.68 (d, J = 7.0 Hz, 2H), 7.50 (s, 1H), 7.47 – 7.30 (m, 5H), 6.42 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 146.6, 138.8, 135.0, 133.9, 130.9, 129.9, 129.5, 128.4, 127.9, 124.8, 123.1, 122.6, 117.4 ppm; HRMS (ESI-TOF): m/z [$\text{M}+\text{H}$] $^+$ calcd for $\text{C}_{15}\text{H}_{12}\text{ClN}_2\text{O}^+$: 271.0633; found: 271.0631.

2-Amino-3-(4-bromophenyl)quinoline 1-oxide (3i):



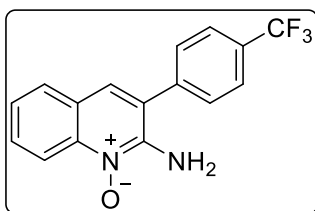
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 95:5); Yield: 64% (84 mg), Yellow solid; mp 213-214 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.54 (d, J = 8.7 Hz, 1H), 7.73 (t, J = 7.6 Hz, 2H), 7.65 (d, J = 8.2 Hz, 2H), 7.53 (s, 1H), 7.42 (dd, J = 11.8, 8.1 Hz, 3H), 6.24 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 146.4, 139.0, 134.5, 132.7, 130.9, 130.3, 128.0, 127.9, 125.0, 123.4, 123.2, 122.8, 117.7 ppm; HRMS (ESI-TOF): m/z [$\text{M}+\text{H}$] $^+$ calcd for $\text{C}_{15}\text{H}_{12}\text{BrN}_2\text{O}^+$: 315.0128; found: 315.0129.

2-Amino-3-(4-iodophenyl)quinoline 1-oxide (3j):



Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 95:5); Yield: 57% (87 mg), Yellow solid; mp 224-225 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.51 (d, J = 8.8 Hz, 1H), 7.83 (d, J = 8.1 Hz, 2H), 7.71 (t, J = 7.0 Hz, 2H), 7.51 (s, 1H), 7.41 (t, J = 7.5 Hz, 1H), 7.27 (d, J = 8.0 Hz, 2H), 6.27 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 146.2, 139.0, 138.5, 135.1, 130.8, 130.4, 128.0, 127.6, 124.9, 123.1, 122.7, 117.6, 94.9 ppm; HRMS (ESI-TOF): m/z [$\text{M}+\text{H}$] $^+$ calcd for $\text{C}_{15}\text{H}_{12}\text{IN}_2\text{O}^+$: 362.9989; found: 362.9988.

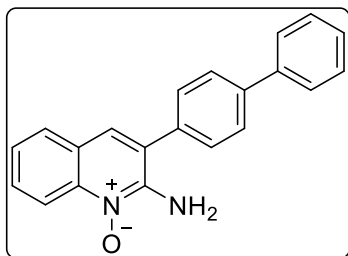
2-Amino-3-(4-(trifluoromethyl)phenyl)quinoline 1-oxide (3k):



Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 95:5); Yield: 57% (73 mg), Yellow solid; mp 192-193 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.53 (d, J = 8.7 Hz, 1H), 7.79 (d, J = 7.8 Hz, 2H), 7.74 (d, J = 7.2 Hz, 2H), 7.68 (d, J = 7.8 Hz, 2H), 7.57 (s, 1H), 7.44 (t, J = 7.4 Hz, 1H), 6.28 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 146.2, 139.2, 139.1, 131.2 (q, $J_{\text{C-F}}$ =

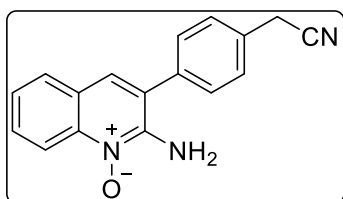
32.5 Hz), 129.2, 128.2, 128.1, 127.1, 126.4 (q, $J_{C-F} = 3.7$ Hz), 125.1, 123.8 (q, $J_{C-F} = 270$ Hz), 122.9, 122.7, 117.6 ppm; ^{19}F NMR (471 MHz, CDCl_3) δ -62.8 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{12}\text{F}_3\text{N}_2\text{O}^+$: 305.0896; found: 305.0895.

3-([1,1'-Biphenyl]-4-yl)-2-aminoquinoline 1-oxide (3l):



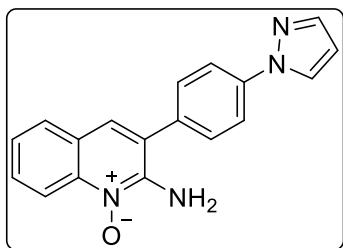
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 95:5); Yield: 61% (80 mg), Yellow solid; mp 223-224 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.55 (d, $J = 8.5$ Hz, 1H), 7.71 (d, $J = 5.8$ Hz, 4H), 7.62 (d, $J = 7.4$ Hz, 2H), 7.57 (d, $J = 5.3$ Hz, 3H), 7.48 (t, $J = 7.4$ Hz, 2H), 7.40 (d, $J = 3.1$ Hz, 2H), 6.38 (s, 2H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 146.7, 141.8, 140.0, 138.9, 134.4, 130.6, 129.0, 129.0, 128.9, 128.0, 127.9, 127.8, 127.0, 124.7, 124.0, 122.8, 117.5 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{21}\text{H}_{17}\text{N}_2\text{O}^+$: 313.1335; found: 313.1331.

2-Amino-3-(4-(cyanomethyl)phenyl)quinoline 1-oxide (3m):



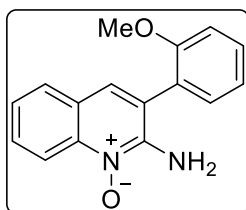
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 90:10); Yield: 39% (45 mg), Yellow solid; mp 140-141 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.56 (d, $J = 8.6$ Hz, 1H), 7.74 (d, $J = 7.7$ Hz, 2H), 7.58 (d, $J = 6.5$ Hz, 3H), 7.52 (d, $J = 8.0$ Hz, 2H), 7.44 (t, $J = 7.5$ Hz, 1H), 6.23 (s, 2H), 3.85 (s, 2H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 146.6, 138.9, 135.3, 131.0, 129.4, 129.1, 129.0, 128.6, 128.0, 125.0, 123.4, 122.6, 117.4, 117.3, 23.4 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{14}\text{N}_3\text{O}^+$: 276.1131; found: 276.1132.

3-(4-(1H-pyrazol-1-yl)phenyl)-2-aminoquinoline 1-oxide (3n):



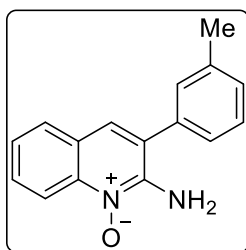
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 88:12); Yield: 46% (58 mg), Yellow gel; ^1H NMR (500 MHz, CDCl_3) δ 8.50 (d, $J = 8.7$ Hz, 1H), 7.97 (s, 1H), 7.82 (d, $J = 8.1$ Hz, 2H), 7.75 (s, 1H), 7.70 (d, $J = 6.8$ Hz, 2H), 7.58 (d, $J = 6.2$ Hz, 3H), 7.41 (t, $J = 7.3$ Hz, 1H), 6.50 (bs, 3H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 147.1, 141.6, 140.5, 138.8, 133.1, 131.0, 129.8, 129.2, 127.9, 126.7, 124.9, 123.6, 122.6, 119.7, 117.4, 108.2 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{15}\text{N}_4\text{O}^+$: 303.1240; found: 303.1241.

2-Amino-3-(2-methoxyphenyl)quinoline 1-oxide (3o):



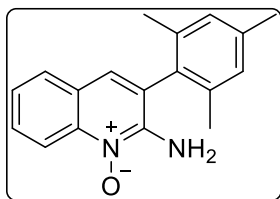
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 92:8); Yield: 47% (53 mg), Yellow solid; mp 197-198 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.56 (d, *J* = 8.6 Hz, 1H), 7.69 (d, *J* = 7.1 Hz, 2H), 7.54 (s, 1H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 7.2 Hz, 1H), 7.31 (d, *J* = 7.1 Hz, 1H), 7.10 (t, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 8.3 Hz, 1H), 6.14 (s, 2H), 3.80 (s, 3H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.8, 147.3, 138.9, 131.4, 130.8, 130.5, 129.2, 127.9, 124.5, 124.1, 122.7, 122.0, 121.4, 117.5, 111.5, 55.6 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₁₆H₁₅N₂O₂⁺: 267.1128; found: 267.1135.

2-Amino-3-(*m*-tolyl)quinoline 1-oxide (3p):



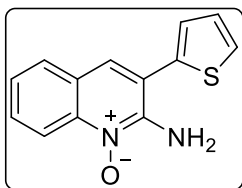
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 93:7); Yield: 58% (61 mg), Yellow oil; ¹H NMR (500 MHz, CDCl₃) δ 8.51 (d, *J* = 8.7 Hz, 1H), 7.75 – 7.66 (m, 2H), 7.55 (s, 1H), 7.39 (dd, *J* = 9.6, 7.5 Hz, 2H), 7.34 – 7.21 (m, 3H), 6.40 (s, 2H), 2.41 (s, 3H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 156.8, 147.4, 138.9, 131.4, 130.8, 130.5, 129.5, 127.8, 124.5, 124.0, 122.7, 122.0, 121.4, 117.5, 111.5, 55.6 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₁₆H₁₅N₂O⁺: 251.1179; found: 251.1178.

2-Amino-3-mesitylquinoline 1-oxide (3q):



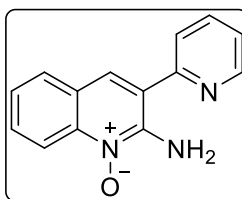
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 95:5); Yield: 36% (42 mg), Yellow oil; ¹H NMR (500 MHz, DMSO-d₆) δ 8.34 (d, *J* = 8.5 Hz, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.72 (t, *J* = 7.8 Hz, 1H), 7.54 (s, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.04 (s, 2H), 6.69 (s, 2H), 2.32 (s, 3H), 1.98 (s, 6H) ppm; ¹³C {¹H} NMR (125 MHz, DMSO-d₆) δ 146.5, 138.4, 137.5, 136.2, 131.3, 129.9, 128.5, 128.2, 126.8, 123.9, 122.7, 122.3, 116.7, 20.7, 19.7 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₁₈H₁₉N₂O⁺: 279.1492; found: 279.1485.

2-Amino-3-(thiophen-2-yl)quinoline 1-oxide (3r):



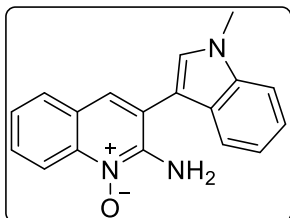
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 93:7); Yield: 96% (98 mg), Yellow oil; ^1H NMR (500 MHz, CDCl_3) δ 8.44 (d, $J = 8.7$ Hz, 1H), 7.62 (dd, $J = 16.8, 9.1$ Hz, 3H), 7.41 – 7.28 (m, 3H), 7.12 – 7.02 (m, 1H), 6.63 (s, 2H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 146.5, 138.7, 136.4, 130.8, 128.4, 127.9, 127.8, 127.0, 126.9, 124.7, 122.2, 117.3, 117.2 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{11}\text{N}_2\text{OS}^+$: 243.0587; found: 243.0588.

2-Amino-3-(pyridin-2-yl)quinoline 1-oxide (3s):



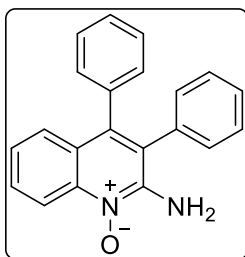
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 93:7); Yield: 78% (78 mg), Yellow solid; mp 158-159 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.67 (d, $J = 4.7$ Hz, 1H), 8.53 (d, $J = 8.6$ Hz, 1H), 8.48 (s, 2H), 8.04 (s, 1H), 7.90 (d, $J = 8.1$ Hz, 1H), 7.86 (td, $J = 7.8, 1.8$ Hz, 1H), 7.77 – 7.68 (m, 2H), 7.38 (dd, $J = 11.1, 3.9$ Hz, 1H), 7.33 (ddd, $J = 7.2, 4.9, 1.0$ Hz, 1H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 155.2, 148.2, 147.8, 139.4, 137.4, 131.4, 128.4, 126.9, 124.3, 122.8, 122.1, 121.6, 119.3, 117.4 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{14}\text{H}_{12}\text{N}_3\text{O}^+$: 238.0975; found: 238.0978.

2-Amino-3-(1-methyl-1H-indol-3-yl)quinoline 1-oxide (3t):



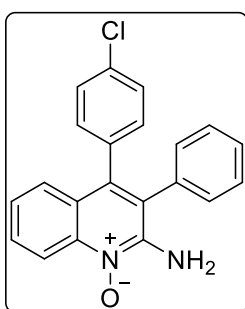
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 87:13); Yield: 54% (66 mg), Yellow solid; mp 149-150 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.49 (d, $J = 8.0$ Hz, 1H), 7.77 – 7.64 (m, 3H), 7.59 (d, $J = 7.3$ Hz, 1H), 7.46 – 7.37 (m, 2H), 7.33 (s, 2H), 7.20 (t, $J = 6.8$ Hz, 1H), 6.65 (s, 2H), 3.87 (s, 3H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 148.1, 138.2, 137.1, 130.4, 129.9, 128.2, 127.6, 126.0, 124.7, 122.8, 122.6, 120.6, 119.6, 118.3, 117.0, 109.9, 109.0, 33.0 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{16}\text{N}_3\text{O}^+$: 290.1288; found: 290.1289.

2-Amino-3,4-diphenylquinoline 1-oxide (3ba):



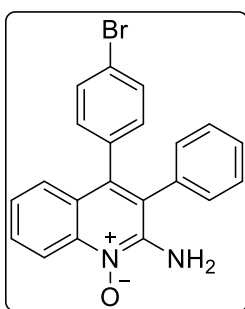
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 93:7); Yield: 66% (86 mg), Yellow solid; mp 233-234 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.75 (d, *J* = 8.3 Hz, 1H), 7.57 (t, *J* = 7.1 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.29 – 7.19 (m, 6H), 7.16 (dd, *J* = 9.8, 8.6 Hz, 3H), 7.12 – 7.07 (m, 2H), 4.94 (s, 2H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 155.6, 148.7, 145.1, 136.4, 135.3, 130.3, 130.0, 129.8, 129.6, 128.8, 127.8, 127.4, 126.9, 124.1, 123.7, 123.4, 122.9 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₆N₂NaO⁺: 335.1155; found: 335.1154.

2-Amino-4-(4-chlorophenyl)-3-phenylquinoline 1-oxide (3ca):



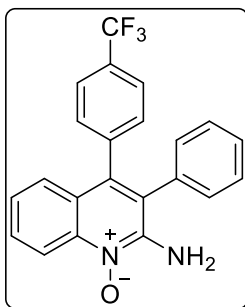
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 94:6); Yield: 73% (106 mg), Yellow gel; ¹H NMR (500 MHz, CDCl₃) δ 7.75 (d, *J* = 8.4 Hz, 1H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.29 (t, *J* = 7.1 Hz, 3H), 7.27 – 7.22 (m, 3H), 7.17 (t, *J* = 7.4 Hz, 1H), 7.13 (d, *J* = 7.0 Hz, 2H), 7.05 (d, *J* = 8.3 Hz, 2H), 5.00 (s, 2H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 155.5, 146.8, 146.6, 135.6, 135.2, 133.4, 131.3, 130.2, 129.7, 128.9, 128.1, 127.8, 126.4, 125.6, 123.5, 123.4, 122.8 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₆ClN₂O⁺: 347.0946; found: 347.0947.

2-Amino-4-(4-bromophenyl)-3-phenylquinoline 1-oxide (3da):



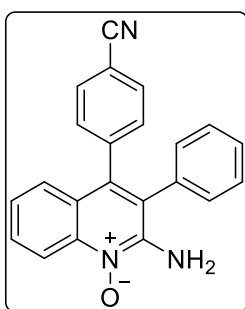
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 94:6); Yield: 76% (125 mg), Yellow solid; mp 191-192 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.74 (d, *J* = 8.2 Hz, 1H), 7.60 – 7.54 (m, 1H), 7.39 (d, *J* = 8.3 Hz, 2H), 7.32 – 7.27 (m, 3H), 7.24 (d, *J* = 6.0 Hz, 1H), 7.19 – 7.15 (m, 1H), 7.15 – 7.11 (m, 2H), 6.99 (d, *J* = 8.3 Hz, 2H), 4.88 (s, 2H) ppm; ¹³C {¹H} NMR (125 MHz, CDCl₃) δ 155.5, 147.1, 146.5, 135.7, 135.7, 131.7, 131.0, 130.2, 129.7, 129.2, 128.9, 127.8, 126.4, 125.8, 123.4, 122.7, 121.6 ppm; HRMS (ESI-TOF): *m/z* [M+H]⁺ calcd for C₂₁H₁₅BrN₂NaO⁺: 413.0260; found: 413.0261.

2-Amino-3-phenyl-4-(4-(trifluoromethyl)phenyl)quinoline 1-oxide (3ea):



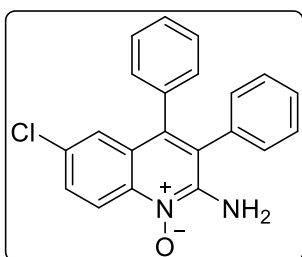
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 94:6); Yield: 75% (120 mg), White solid; mp 242-243 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.75 (d, $J = 8.3$ Hz, 1H), 7.58 (t, $J = 7.4$ Hz, 1H), 7.52 (d, $J = 7.8$ Hz, 2H), 7.32 – 7.21 (m, 6H), 7.18 (d, $J = 7.3$ Hz, 1H), 7.14 (d, $J = 7.2$ Hz, 2H), 4.92 (s, 2H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 155.4, 147.3, 146.2, 140.7, 135.5, 130.4, 130.2, 129.7, 128.9, 127.9, 127.3, 126.2, 126.2 (q, $J_{\text{C-F}} = 270$ Hz), 126.1, 124.8 (q, $J_{\text{C-F}} = 3.7$ Hz), 123.4, 123.2, 122.8 ppm; ^{19}F NMR (471 MHz, CDCl_3) δ -162.5 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{16}\text{F}_3\text{N}_2\text{O}^+$: 381.1209; found: 381.1208.

2-Amino-4-(4-cyanophenyl)-3-phenylquinoline 1-oxide (3fa):



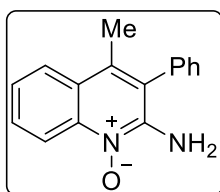
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 92:8); Yield: 67% (95 mg), Yellow oil; ^1H NMR (500 MHz, CDCl_3) δ 7.78 (d, $J = 8.4$ Hz, 1H), 7.63 – 7.58 (m, 1H), 7.56 (d, $J = 8.1$ Hz, 2H), 7.29 – 7.23 (m, 5H), 7.19 (d, $J = 3.1$ Hz, 2H), 7.11 (d, $J = 6.6$ Hz, 2H), 5.24 (s, 2H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 155.3, 146.2, 146.2, 141.8, 134.8, 131.7, 130.8, 130.2, 130.2, 129.1, 128.3, 126.0, 125.3, 123.5, 123.2, 122.6, 118.5, 111.6 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{16}\text{N}_3\text{O}^+$: 338.1288; found: 338.1287.

2-Amino-6-chloro-3,4-diphenylquinoline 1-oxide (3ga):



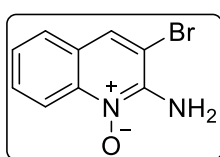
Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 94:6); Yield: 61% (89 mg), Yellow solid; mp 240-241 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.61 (d, $J = 8.9$ Hz, 1H), 7.65 (d, $J = 8.6$ Hz, 1H), 7.41 (s, 1H), 7.27 (dd, $J = 9.0, 3.2$ Hz, 6H), 7.13 (d, $J = 6.8$ Hz, 2H), 7.08 (d, $J = 3.5$ Hz, 2H), 6.04 (s, 2H) ppm; ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 138.4, 137.5, 135.0, 133.8, 131.0, 130.5, 130.3, 130.0, 129.1, 129.0, 128.5, 128.1, 128.0, 126.1, 124.1, 123.9, 119.4 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{21}\text{H}_{16}\text{ClN}_2\text{O}^+$: 347.0946; found: 347.0951.

2-Amino-4-methyl-3-phenylquinoline 1-oxide (3ha):



Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 95:5); Yield: 62% (65 mg), Yellow gel; ^1H NMR (500 MHz, CDCl_3) δ 8.55 (d, J = 8.6 Hz, 1H), 7.91 (d, J = 8.2 Hz, 1H), 7.74 (t, J = 7.7 Hz, 1H), 7.55 (t, J = 7.2 Hz, 2H), 7.52 – 7.43 (m, 2H), 7.30 (d, J = 7.2 Hz, 2H), 6.23 (s, 2H), 2.36 (s, 3H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 147.7, 138.3, 137.0, 134.0, 130.9, 129.7 (2C), 129.1, 124.7, 124.6, 123.6, 122.8, 117.4, 16.0 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{15}\text{N}_2\text{O}^+$: 251.1179; found: 251.1178.

2-Amino-3-bromoquinoline 1-oxide (5):



Following the general synthetic procedure. The reaction mixture was purified by silica gel column chromatography (EtOAc: MeOH, 94:6); Yield: 47% (47 mg), Yellow oil; ^1H NMR (500 MHz, CDCl_3) δ 8.51 (d, J = 8.7 Hz, 1H), 7.94 (s, 1H), 7.74 (t, J = 7.9 Hz, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.44 (t, J = 7.5 Hz, 1H), 6.42 (s, 2H) ppm; ^{13}C { ^1H } NMR (125 MHz, CDCl_3) δ 146.3, 139.0, 131.2, 130.6, 127.2, 125.5, 122.7, 117.8, 104.2 ppm; HRMS (ESI-TOF): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_9\text{H}_8\text{BrN}_2\text{O}^+$: 238.9815; found: 238.9816.

4. Single Crystal X-ray Structure of 3a

Crystallization: Crystal of compound **3a** (15 mg) was grown in a 2 mL mixture of solvents EtOH:*n*-hexane (1:3) by slow evaporation method for 7 days.

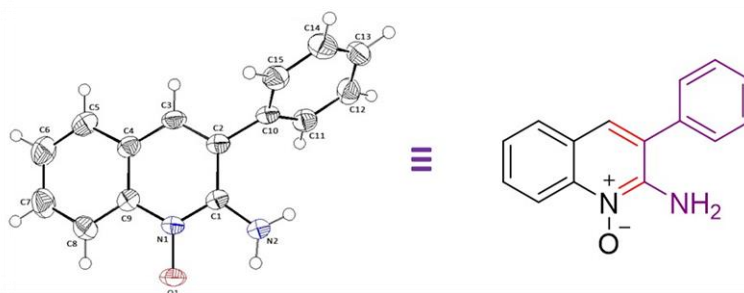


Figure S1: X-ray crystallography of **3a** (the ellipsoid contour probability level is 50%).

Table S6: Crystal data and structure refinement for **3a**.

CCDC Number	2308996
Empirical formula	$\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}$
Formula weight	236.27

Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 10.8378(11) Å	$\alpha = 90^\circ$
	b = 7.4709(7) Å	$\beta = 103.094(3)^\circ$
	c = 15.5056(15) Å	$\gamma = 90^\circ$
Volume / Z	1222.8(2) Å ³ / 4	
Calculated density	1.283 Mg/m ³	
Absorption coefficient	0.082 mm ⁻¹	
F(000)	496	
Crystal size	0.586 x 0.230 x 0.013 mm	
Theta range for data collection	3.042 to 25.699 deg.	
Limiting indices	-13<=h<=13, -9<=k<=9, -18<=l<=18	
Reflections collected / unique	36266 / 2315 [R(int) = 0.0836]	
Completeness to theta	= 25.242 99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.745 and 0.669	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2315 / 0 / 163	
Goodness-of-fit on F ²	1.175	
Final R indices [I>2sigma(I)]	R ₁ = 0.0708, wR ₂ = 0.1826	
R indices (all data)	R ₁ = 0.0894, wR ₂ = 0.1948	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.212 and -0.339 e.Å ⁻³	

Single Crystal X-ray Structure of **3ga**

Crystallization: Crystal of compound **3ga** (15 mg) was grown in a 2 mL mixture of solvents CHCl₃:*n*-hexane (1:4) by slow evaporation method for 5 days.

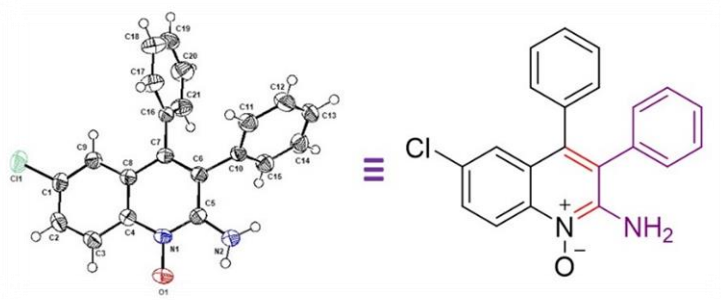


Figure S2: X-ray crystallography of **3ga** (the ellipsoid contour probability level is 50%).

Table S7: Crystal data and structure refinement for **3ga**.

CCDC Number	2308997	
Empirical formula	C ₂₁ H ₁₅ ClN ₂ O	
Formula weight	346.80	
Temperature	299(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Orthorhombic, P 21 21 21	
Unit cell dimensions	a = 7.2658(2) Å	alpha = 90°
	b = 7.9217(2) Å	beta = 90°
	c = 29.7691(10) Å	gamma = 90°
Volume	1713.43(9) Å ³	
Z, Calculated density	4, 1.344 Mg/m ³	
Absorption coefficient	0.234 mm ⁻¹	
F(000)	720	
Crystal size	0.309 x 0.196 x 0.053 mm	
Theta range for data collection	2.661 to 27.112 deg.	
Limiting indices	-9<=h<=9, -10<=k<=10, -38<=l<=38	
Reflections collected / unique	52147 / 3787 [R(int) = 0.0308]	
Completeness to theta	= 25.242 99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.7113	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3787 / 2 / 232	
Goodness-of-fit on F ²	1.154	
Final R indices [I>2sigma(I)]	R ₁ = 0.0373, wR ₂ = 0.0894	
R indices (all data)	R ₁ = 0.0383, wR ₂ = 0.0900	

Absolute structure parameter	0.024(12)
Extinction coefficient	n/a
Largest diff. peak and hole	0.211 and -0.224 e.A ⁻³

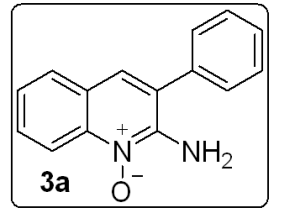
5. References

1. (a) *SAINT-Plus, version 6.45*, Bruker AXS Inc., Madison, WI, 2003; (b) G. M. Sheldrick, *SADABS, Program for Empirical Absorption Correction of Area Detector Data*, University of Gottingen, Germany, 1997; (c) *SMART (version 5.625), SHELX-TL (version 6.12)*, Bruker AXS Inc., Madison, WI, 2000; (d) G. M. Sheldrick, *SHELXS-97*, University of Gottingen, Germany, 1997.
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6. NMR Spectra

8.568
8.550
7.737
7.729
7.722
7.714
7.565
7.538
7.530
7.508
7.500
7.491
7.482
7.473
7.440
7.426
7.411
7.260
6.234

¹H NMR (500 MHz, CDCl₃)

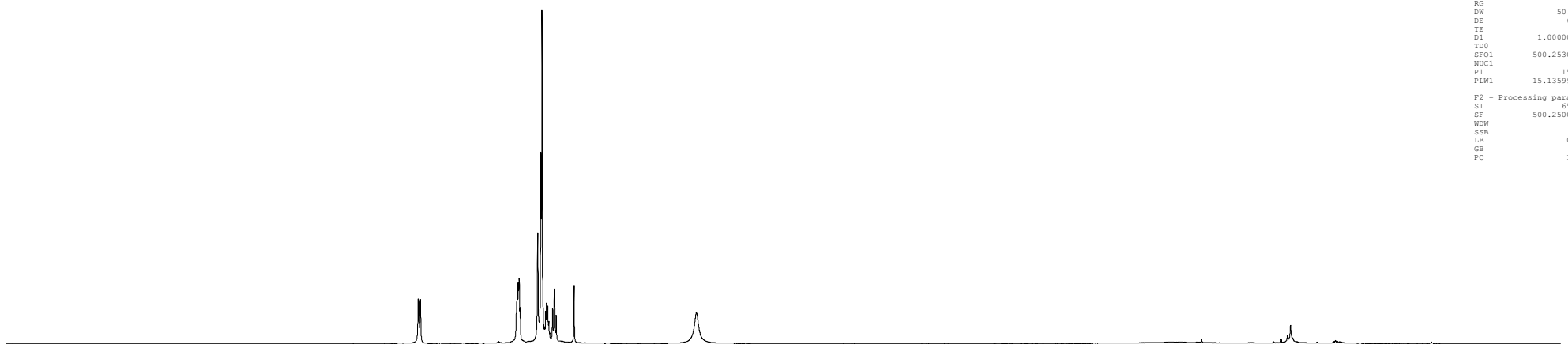


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PROCNO       1

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SOLVENT      CDCl3
NS           16
DS           0
SWH          10000.000 Hz
FIDRES       0.305176 Hz
AQ           3.2767959 sec
RG           287
DW           50.000 usec
DE           6.50 usec
TE           0 K
D1           1.00000000 sec
TDO         1
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P1           15.10 usec
PL1         15.1359968 W

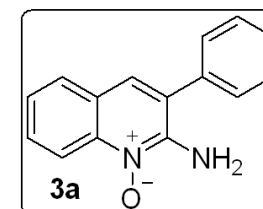
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1.03
2.13
1.05
4.07
1.11
1.05
2.00

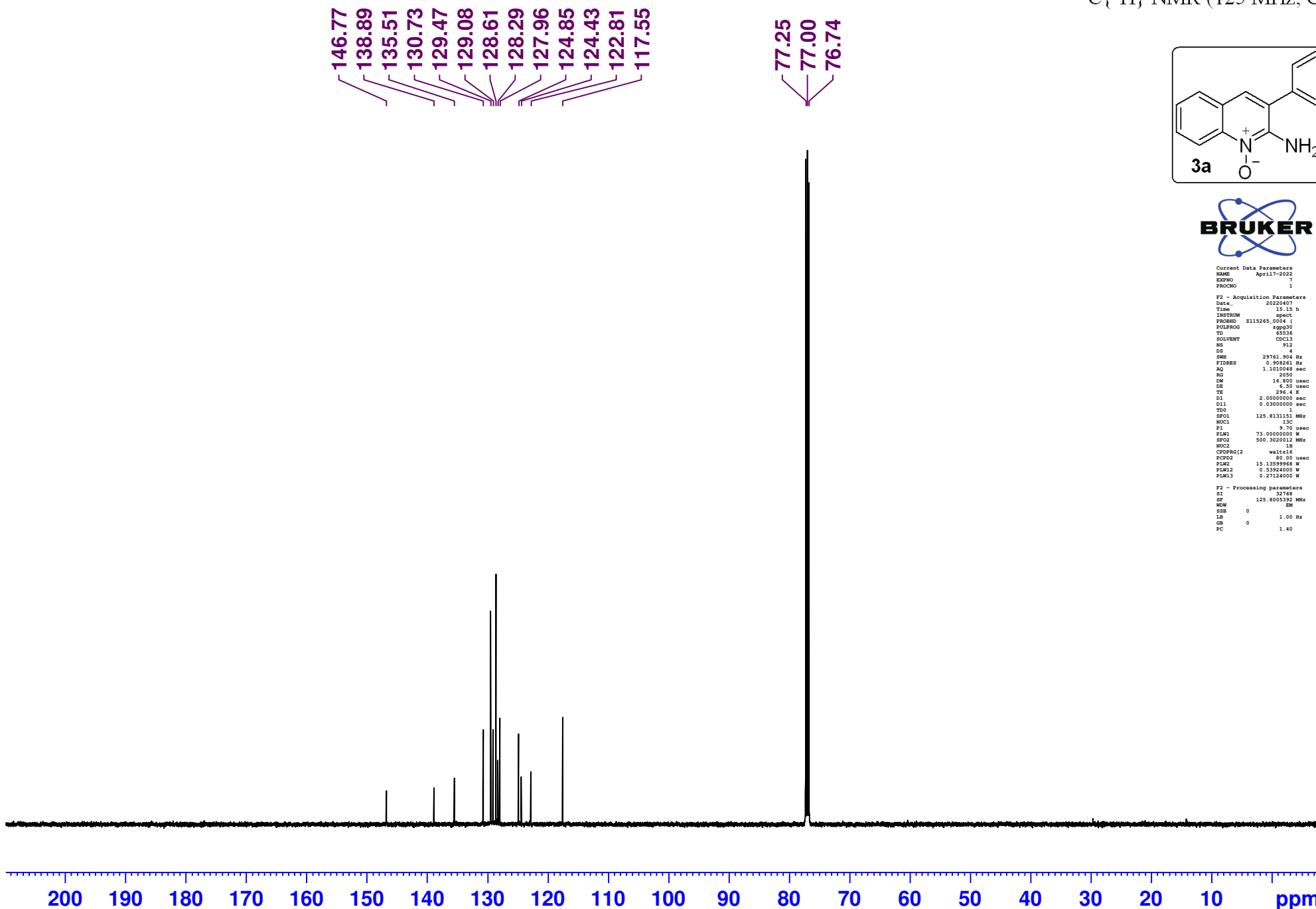
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



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EXPNO    7
PROCNO   1

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Time     15:15 h
INSTRUM  spect
PROBHD   5115265.004 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        912
DS        4
SWH       29761.904 Hz
FIDRES    0.998261 Hz
AQ        1.1010048 sec
RG         2000
DW        16.800 usec
DE        6.50 usec
TE        296.4 K
D1        2.00000000 sec
d11       0.03000000 sec
TDO       1
SFO1      125.811111 MHz
NUC1      13C
P1        73.00000000 sec
PLA1      0.00000000 W
SFO2      500.3020012 MHz
NUC2      1H
CPDPRG2   waltz16
PCPD2     80.00 usec
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PLM12     0.53924000 W
PLM13     0.27154000 W

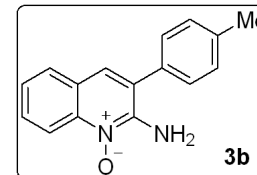
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SSB       0
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PC        1.40
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8.535
8.518
7.704
7.689
7.519
7.406
7.391
7.315
7.300
7.260
6.268

2.414

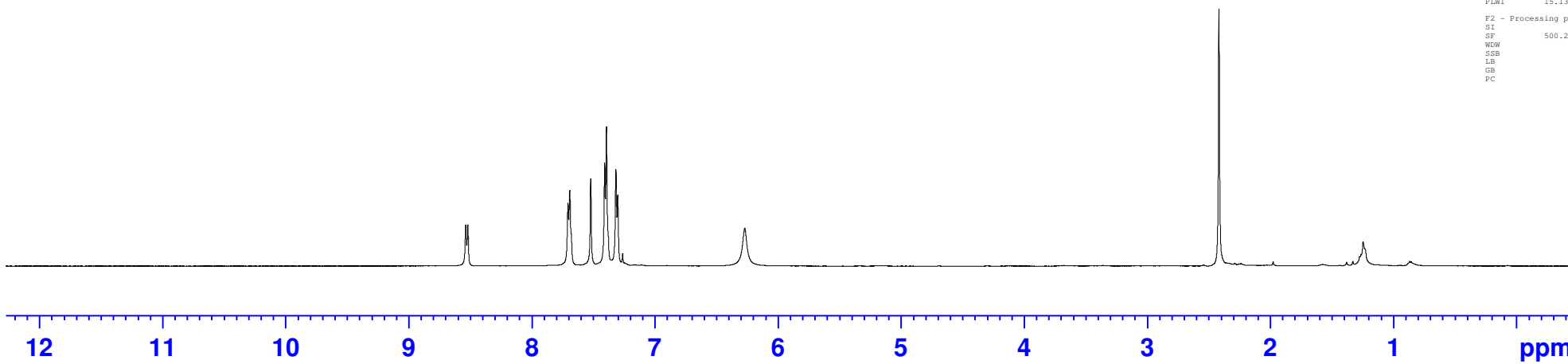
¹H NMR (500 MHz, CDCl₃)



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EXPNO    10
PROCNO    1

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Time      20.31 h
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PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         4
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         80.6
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1      500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.1359968 W

F2 - Processing parameters
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SF         500.2500149 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



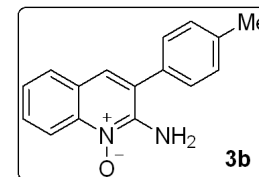
1.06
2.19
1.13
3.19
2.13
2.00
3.28

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

146.73
138.99
138.78
132.59
130.42
130.04
128.39
127.85
127.74
124.68
124.37
122.82
117.51

77.25
76.99
76.74

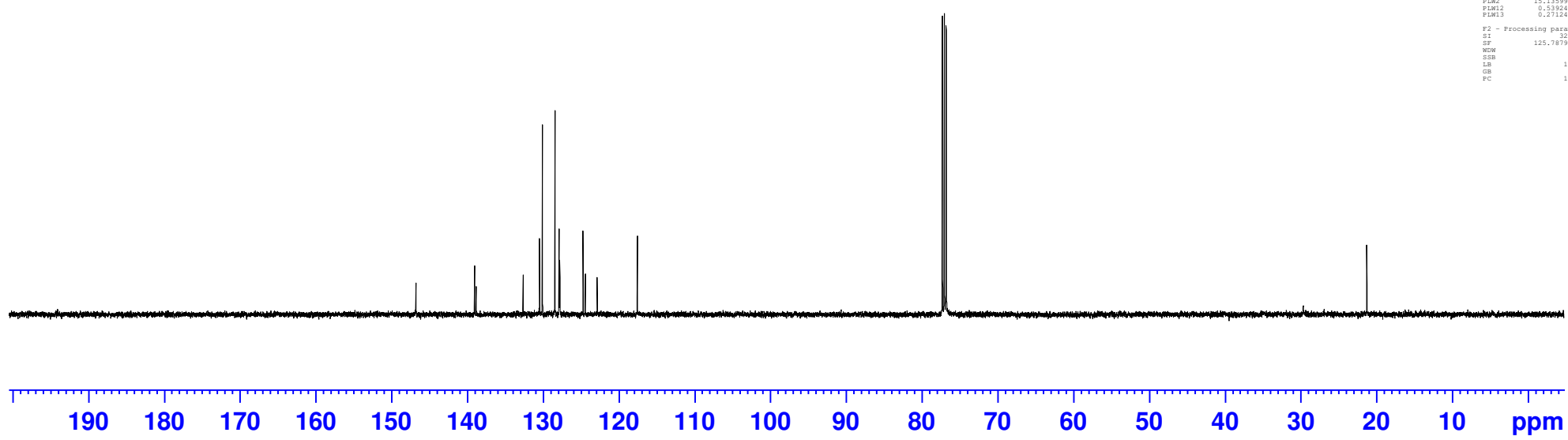
21.21



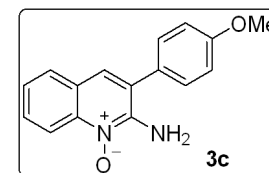
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PROCNO        1

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PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
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DS            4
SWE           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG            1030
DM            16.800 usec
DE            6.50 usec
TE            0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1
SF01          125.8005413 MHz
NUC1          13C
P1            9.70 usec
PLM1          73.0000000 W
SFO2          500.2550010 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         80.00 usec
PLM2          15.13599968 W
PLM12         0.53924000 W
PLM13         0.27124000 W

F2 - Processing parameters
SI            32768
SF            125.7879719 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
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¹H NMR (500 MHz, CDCl₃)



Current Data Parameters
NAME Jun6-2022
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220606
Time 12.07 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 114
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TDO 1
SFO1 500.3030894 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.524
8.506
7.697
7.681
7.668
7.505
7.442
7.425
7.402
7.387
7.372
7.260
7.025
7.007
6.282

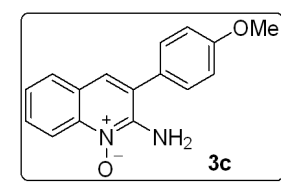
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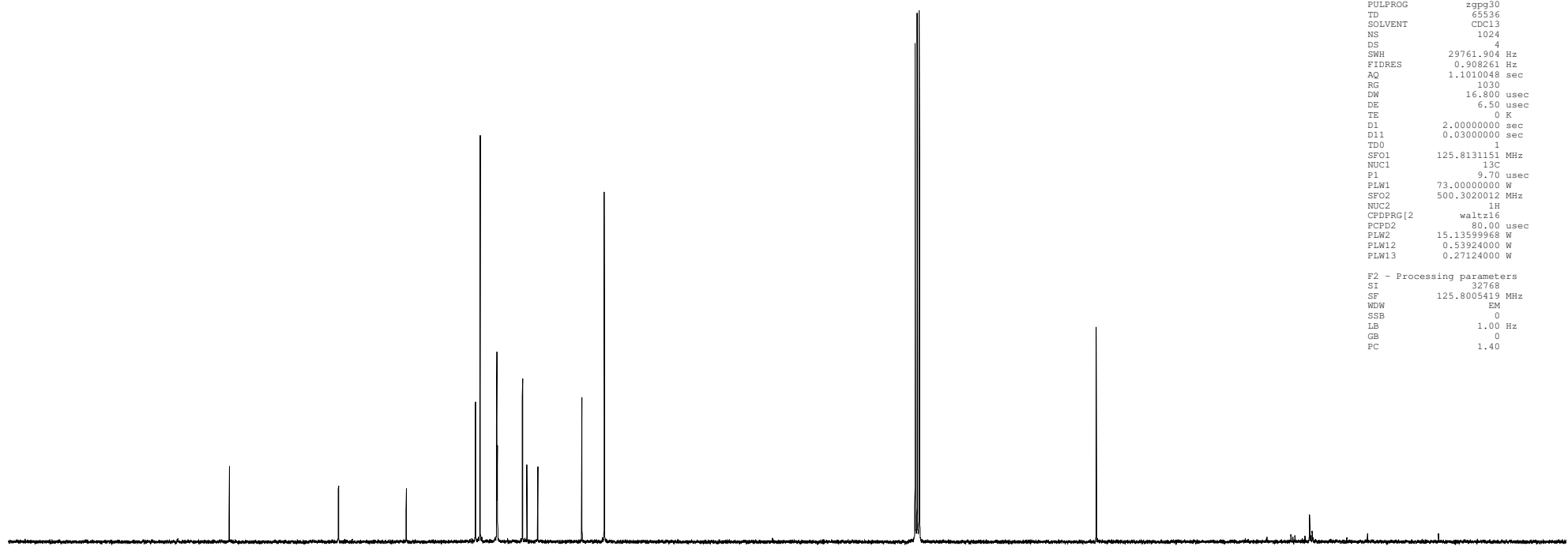
1.00
2.06
1.03
1.99
1.02
2.02
1.96

3.20

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



160.11
146.92
138.74
130.37
129.81
127.80
127.75
127.71
124.69
124.16
122.85
117.52
114.81
77.25
77.00
76.74
55.37



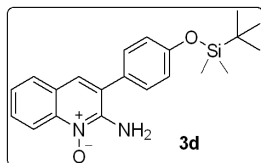
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PROCNO 1

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TD 65536
SOLVENT cdcl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 1030
DW 16.800 usec
DE 6.50 usec
TE 0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
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NUC1 13C
P1 9.70 usec
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SF02 500.3020012 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
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PLW12 0.53924000 W
PLW13 0.27124000 W

F2 - Processing parameters
SI 32768
SF 125.8005419 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

^1H NMR (500 MHz, CDCl_3)



8.530
8.512
7.696
7.680
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7.400
7.386
7.369
7.260
6.968
6.951
6.255

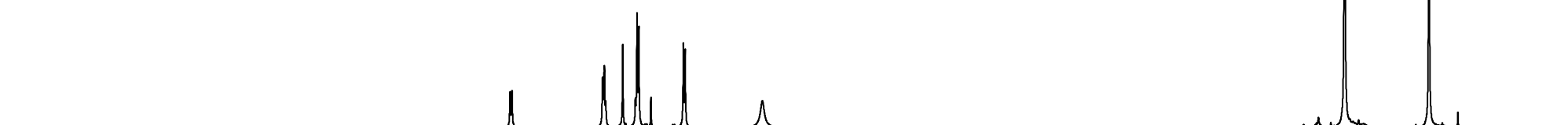
1.006
0.246



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EXPNO 2
PROCNO 1

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PULPROG zg30
TE 65536
SOLVENT CDCl_3
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DS 2
SWH 10000.000 Hz
FREQES 0.305176 Hz
AQ 3.276799 sec
RG 80.6
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TPO 1
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NUC1 1H
F1 15.10 usec
PWL 15.13599968 W

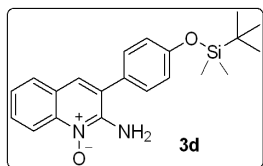
F2 - Processing parameters
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WVW EM
SFB 0
LF 0.30 Hz
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PC 1.00



12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

1.00
2.06
1.04
3.03
2.01
2.02
9.10
5.90

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

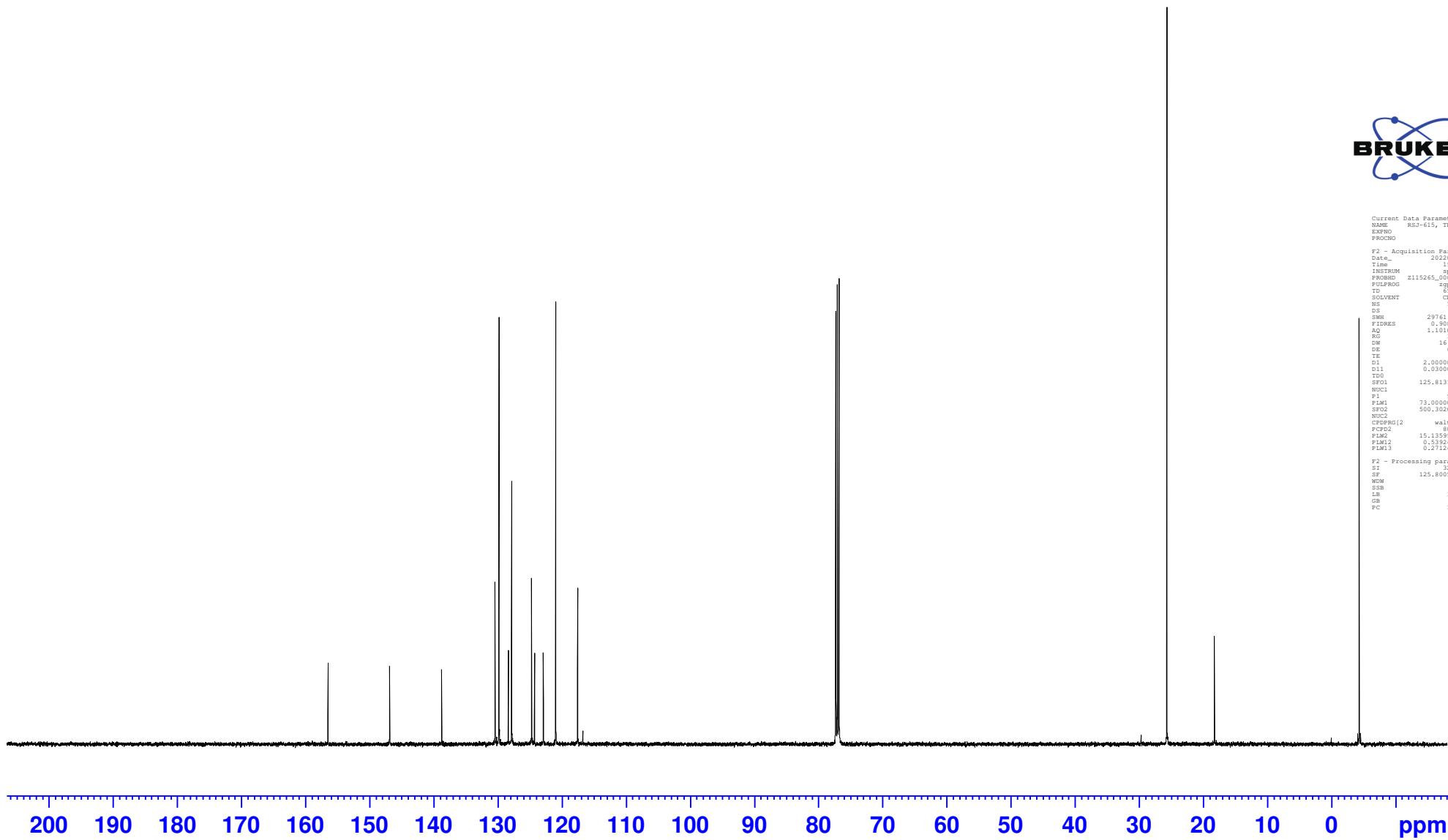


156.45
146.85
138.72
130.39
129.78
128.30
127.81
124.70
124.23
122.86
120.92
117.51
116.68

77.25
77.00
76.74

25.60
18.18

-4.39



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Current Data Parameters
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EXPNO 3
PROCNO 1

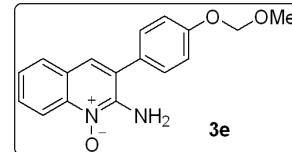
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FIDRES 0.998261 Hz
AQ 1.1010048 sec
RG 1030
DM 16.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SF01 125.8131151 MHz
NUC1 13C
P1 9.70 usec
PLM1 73.00000000 W
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
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PLM12 0.53924000 W
PLM13 0.27124000 W

F2 - Processing parameters
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SF 125.8005420 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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8.539
8.521
7.704
7.692
7.688
7.678
7.507
7.450
7.433
7.410
7.394
7.380
7.260
7.179
7.162
6.235
5.227

3.505

¹H NMR (500 MHz, CDCl₃)

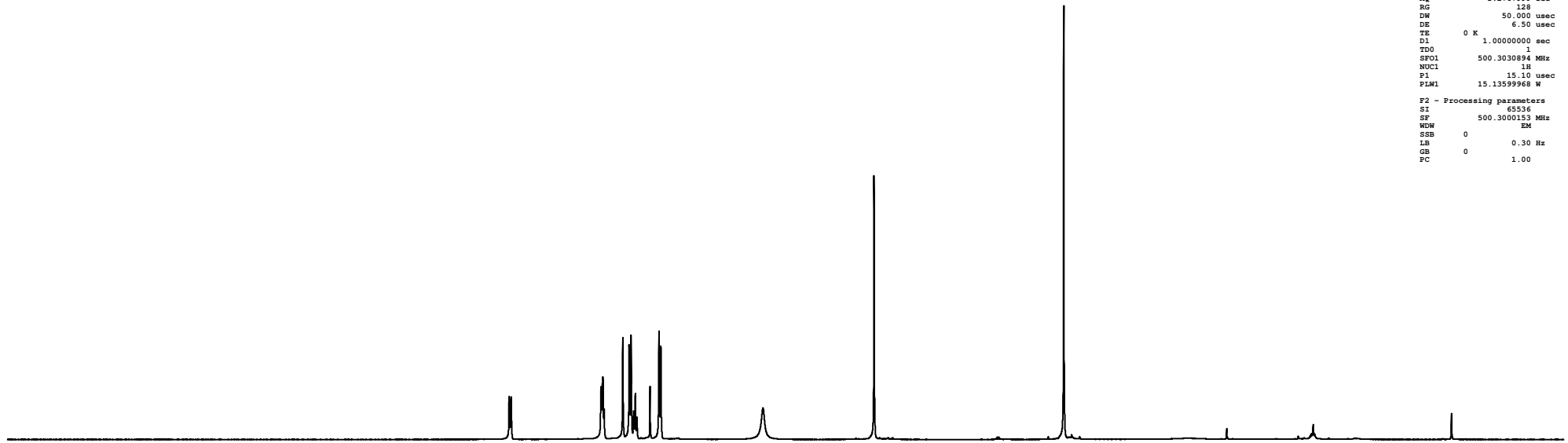


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Current Data Parameters
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PROCNO       1

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PULPROG      zg30
TD           65536
SOLVENT      CDCl3
NS           4
DS           2
SWH          10000.000 Hz
FIDRES       0.305176 Hz
AQ           3.2167999 sec
RG           128
DW           50.000 usec
DE           6.50 usec
TE           0 K
D1           1.00000000 sec
TDO          1
SFO1         500.3030894 MHz
NUC1         1H
F1           15.10 usec
PLM1         15.13599968 W

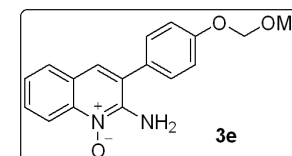
F2 - Processing parameters
SI           65536
SF           500.3000153 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```



12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

1.00
2.04
1.07
2.03
0.98
2.01
1.95
2.02
3.00

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

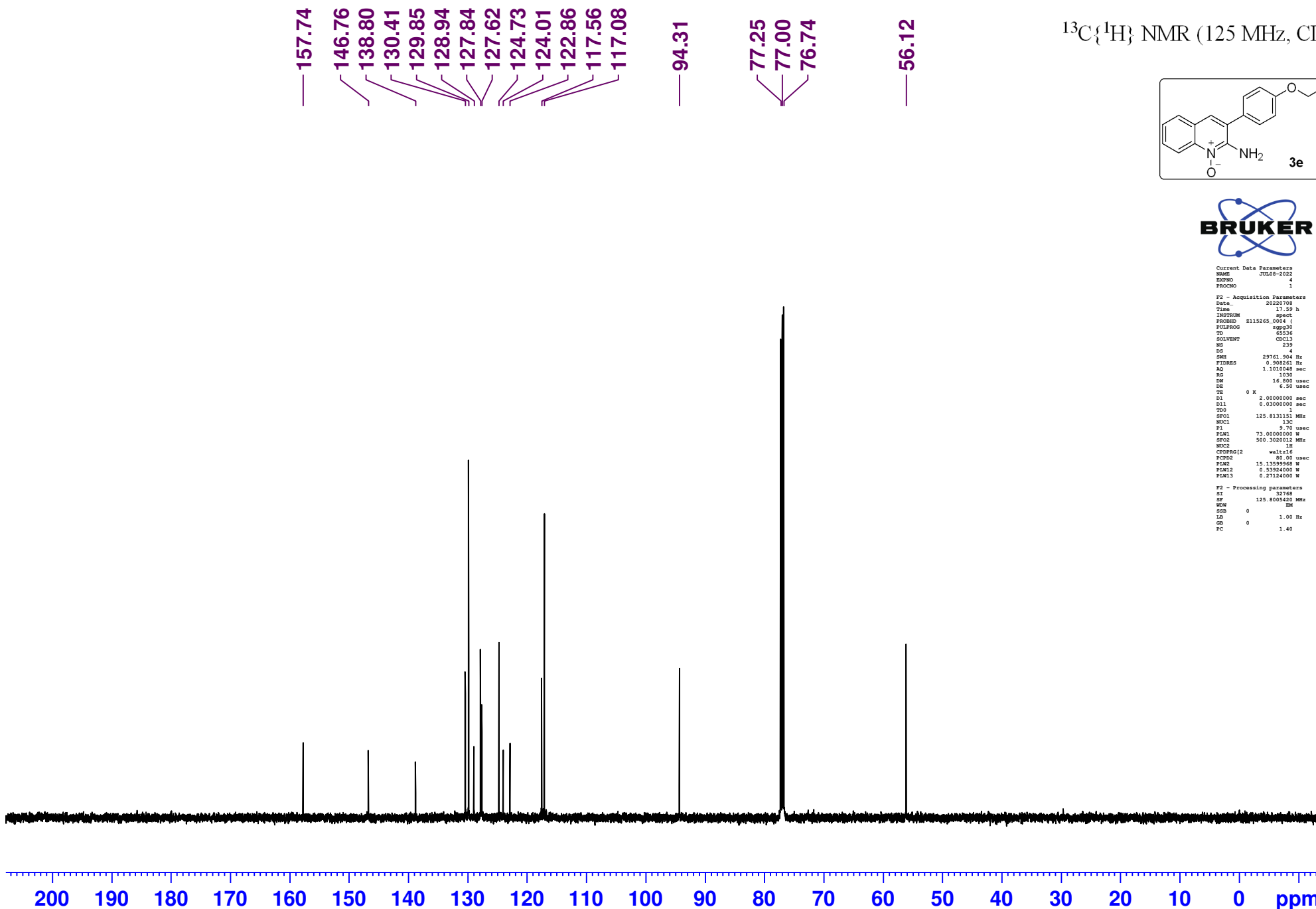


```
Current Data Parameters
NAME          JUL08-2022
EXPNO         4
PROCNO        1

F2 - Acquisition Parameters
Date_         20220708
Time          17:59 h
INSTRUM       spect
PROBHD        mmh5mm
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            239
DS            4
SWH           29761.904 Hz
FIDRES        0.998261 Hz
AQ            1.1010048 sec
RG            1030
DSW           16.800 usec
DE            6.50 usec
TE            0 K

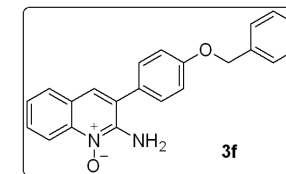
D1            2.0000000 sec
D11           0.0300000 sec
TDO           1
SFO1          125.811111 MHz
NUC1          13C
P1            9.70 usec
PL1           73.0000000 W
SFO2          500.3020012 MHz
NUC2          1H
PCPDPRG2     waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27184000 W

F2 - Processing parameters
SI            32768
SF            125.800420 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```



8.551
8.534
7.710
7.696
7.529
7.472
7.457
7.435
7.418
7.404
7.372
7.358
7.344
7.260
7.122
7.106
6.261
— 5.139

¹H NMR (500 MHz, CDCl₃)

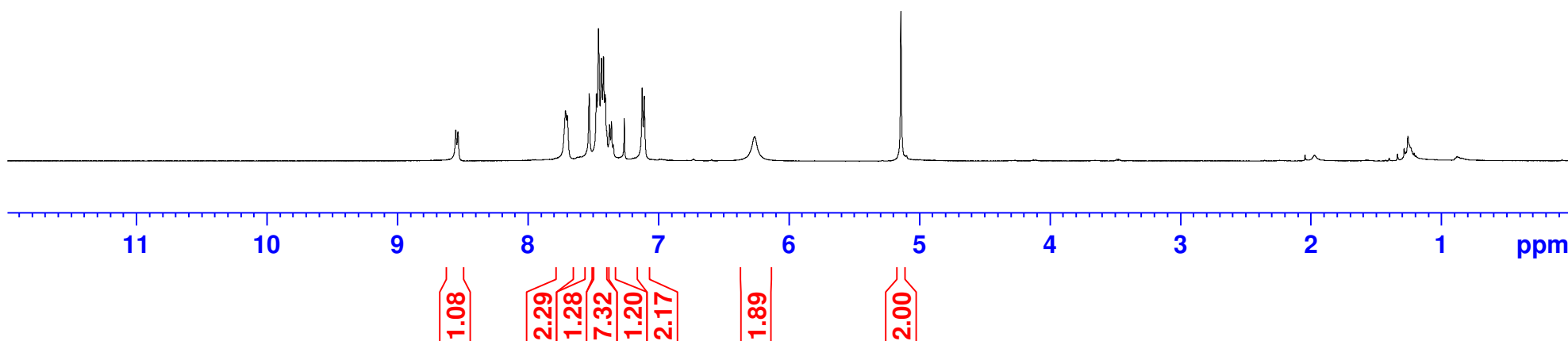


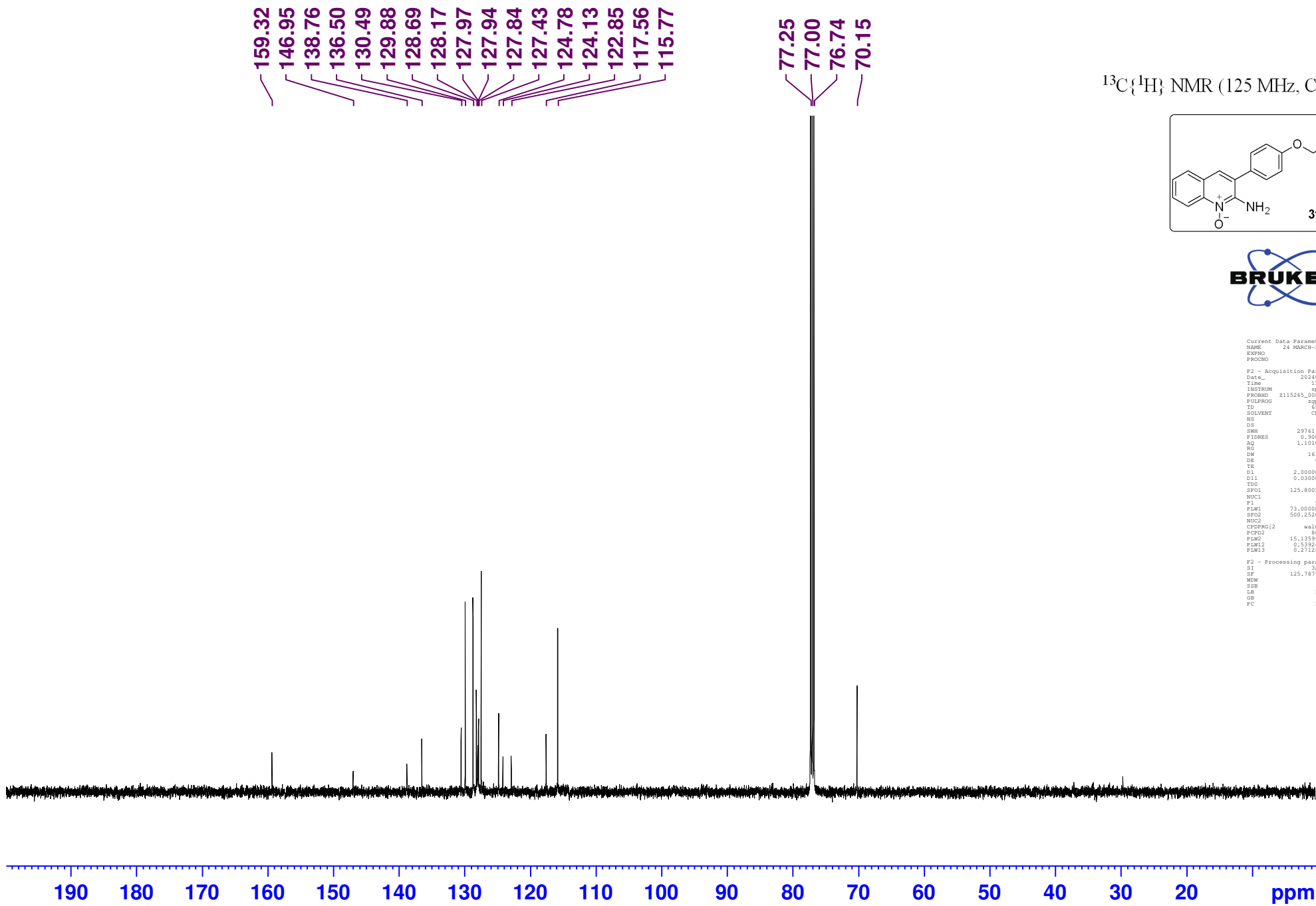
```

Current Data Parameters
NAME      24 MARCH-2024
EXPNO    3
PROCNO   1

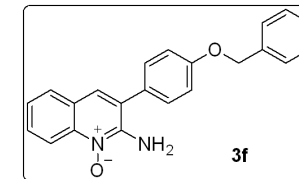
F2 - Acquisition Parameters
Date_    20240324
Time     15.08 h
INSTRUM  spect
PROBHD   Z115265_0004 (
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        0
SWH       10000.000 Hz
FIDRES    0.305176 Hz
AQ        3.2767999 sec
RG        144
DW        50.000 usec
DE        6.50 usec
TE        0 K
D1        1.00000000 sec
TDO       1
SF01      500.2530890 MHz
NUC1      1H
P1        15.10 usec
PL1       15.1359968 W

F2 - Processing parameters
SI        65536
SF        500.2500146 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```





$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```

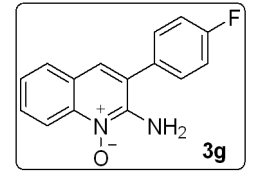
Current Data Parameters
NAME      24 MARCH-2024
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20240324
Time      15.31 h
INSTRUM    spect
PROBHD     Z115265_0004 (
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         392
DS         4
SWE        29761.904 Hz
FIDRES     0.908261 Hz
AQ         1.1010048 sec
RG         1030
DM         16.800 usec
DE         6.50 usec
TE         0 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1
SF01       125.8005413 MHz
NUC1       13C
P1         9.70 usec
PL1        73.0000000 W
SFO2       500.2550010 MHz
NUC2       1H
CPCPRG2    waltz16
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27124000 W

F2 - Processing parameters
SI         32768
SF         125.7879674 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

8.452
8.435
7.668
7.652
7.637
7.464
7.444
7.374
7.360
7.345
7.260
7.118
7.102
7.086
6.407

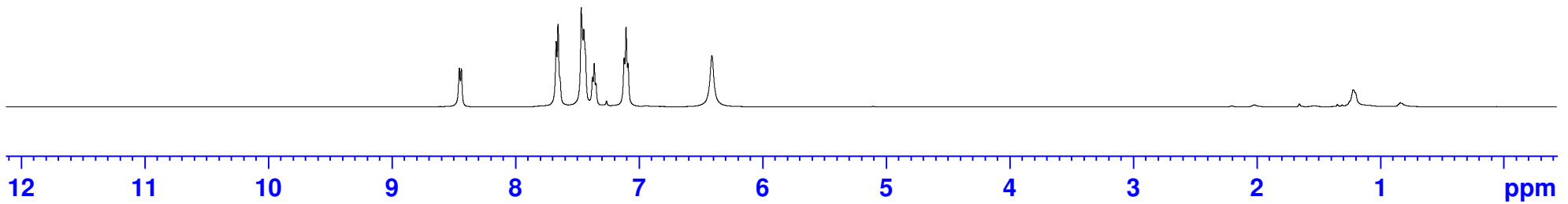
^1H NMR (500 MHz, CDCl_3)



```
Current Data Parameters
NAME          3g
EXPNO         17
PROCNO        1

F2 - Acquisition Parameters
Date_         20240117
Time          23.07 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            4
DS            0
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG            71.8
DW            50.000 usec
DE            6.50 usec
TE            0 K
D1            1.00000000 sec
TDO           1
SFO1          500.2530890 MHz
NUC1           1H
P1            15.10 usec
PL1           15.1359968 W

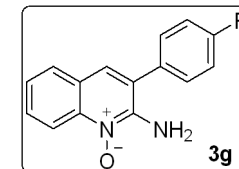
F2 - Processing parameters
SI            65536
SF            500.2500183 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```



1.00
2.09
3.01
1.03
2.02
2.01

163.98
 162.00
 146.59
 138.91
 131.53
 131.50
 130.77
 130.55
 130.48
 128.08
 127.93
 124.91
 123.32
 122.73
 117.55
 116.57
 116.40
 77.25
 77.00
 76.74

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

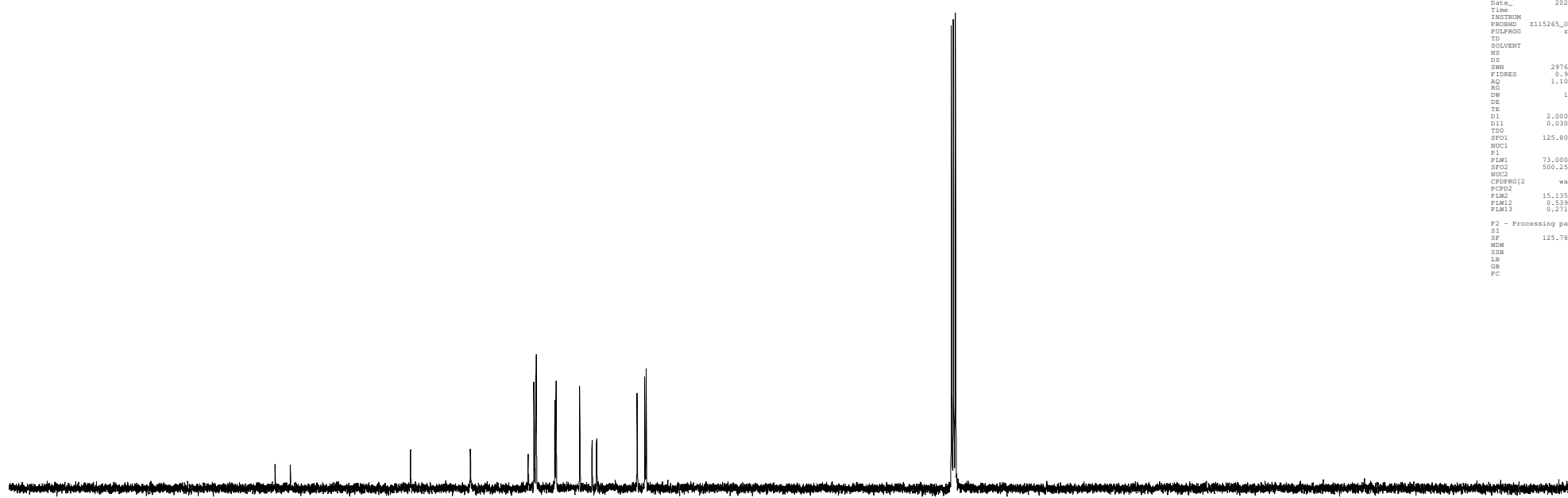


```

Current Data Parameters
NAME          3g
EXPNO        3
PROCNO       1

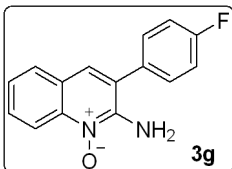
F2 - Acquisition Parameters
Date_        20240228
Time        22.22 h
INSTRUM     spect
PROBHD      Z115265_0004 (
PULPROG     zgpg30
TD          65536
SOLVENT     CDCl3
NS          328
DS          4
SWE         29761.904 Hz
FIDRES     0.908261 Hz
AQ         1.1010048 sec
RG          1030
DM         16.800 usec
DE         6.50 usec
TE         0 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1
SFO1       125.8005413 MHz
NUC1        13C
P1         9.70 usec
PLM1       73.0000000 W
SFO2       500.2550010 MHz
NUC2        1H
CPDPRG2     waltz16
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27124000 W

F2 - Processing parameters
SI          32768
SF          125.7879711 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
  
```



190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

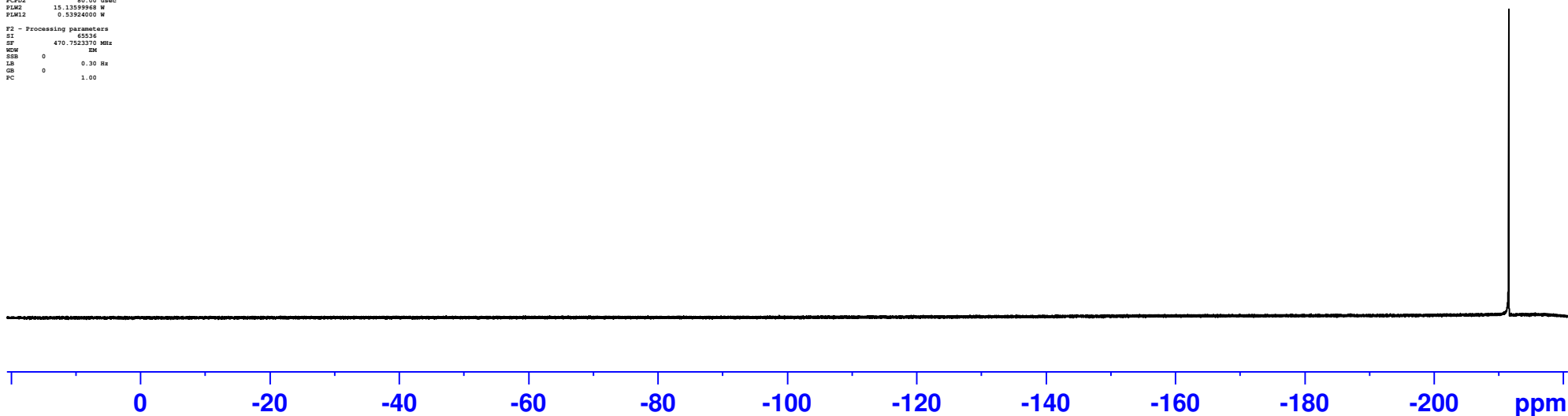
^{19}F NMR (471 MHz, CDCl_3)



```
Current Data Parameters
NAME          19F NMR
EXPNO        1
PROCNO       1

F2 - Acquisition Parameters
Date_         20230623
Time          11:59 h
INSTRUM      spect
PROBHD       zhl1269_0004 (
PULPROG      zgpg30g_2
TD           131072
SOLVENT      CDCl3
NS           78
DS           4
SWH          112636.367 Hz
FIDRES       1.723953 Hz
AQ           0.576718 sec
RG           362
RW           4.400 usec
DE           6.50 usec
TE           0 K
D1           1.0000000 sec
D11          0.0300000 sec
D12          0.0000200 sec
TDO          1
SFO1         470.7052618 MHz
NUC1         19F
P1           15.00 usec
PL1          27.0000000 dB
SFO2         500.3050012 MHz
NUC2         1H
CPCPG2       waltz16
PL2          15.13599968 dB
PL12         0.13954000 dB

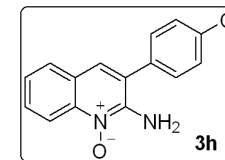
F2 - Processing parameters
SI           65536
SF           470.7523370 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
```



— -211.61

8.469
8.452
7.690
7.676
7.503
7.422
7.383
7.369
7.260
6.423

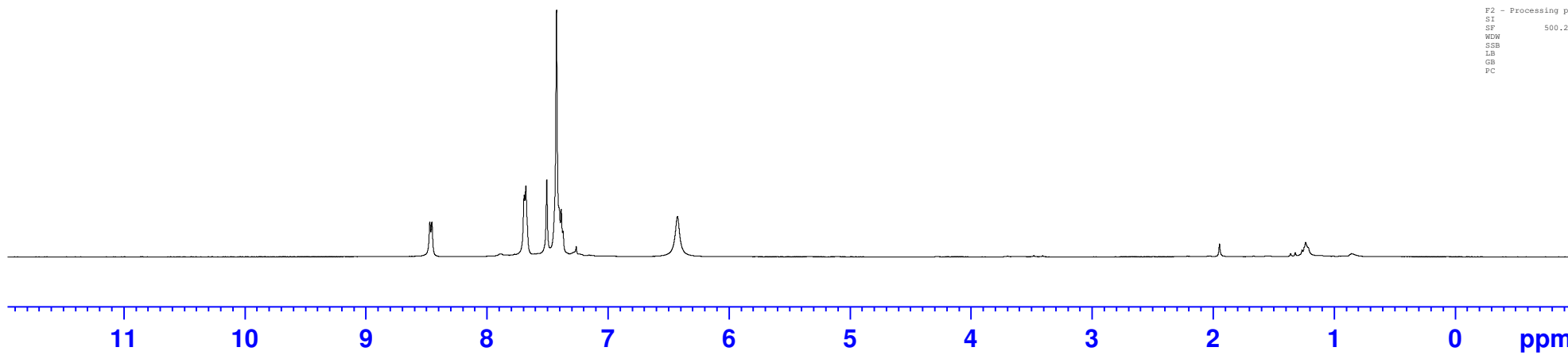
^1H NMR (500 MHz, CDCl_3)



```
Current Data Parameters
NAME          3h
EXPNO         8
PROCNO        1

F2 - Acquisition Parameters
Date_         20240117
Time          16.43 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            4
DS            0
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG            80.6
DW            50.000 usec
DE            6.50 usec
TE            0 K
D1            1.00000000 sec
TD0           1
SF01          500.2530890 MHz
NUC1          1H
P1            15.10 usec
PLM1          15.1359968 W

F2 - Processing parameters
SI            65536
SF            500.2500148 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```

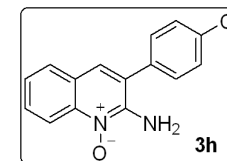


1.04
2.18
1.18
5.18
2.00

146.58
138.84
135.04
133.86
130.85
129.92
129.51
128.36
127.91
124.83
123.13
122.56
117.43

77.25
76.99
76.74

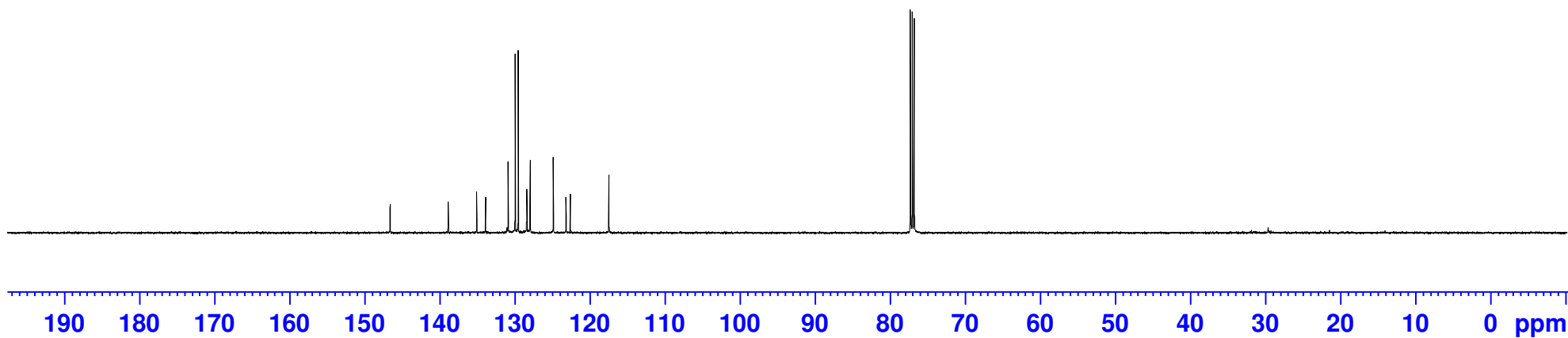
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME          3h
EXPNO         9
PROCNO        1

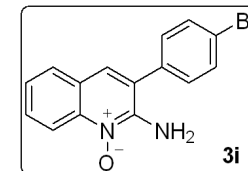
F2 - Acquisition Parameters
Date_         20240117
Time_        17.18 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            616
DS            4
SWE           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG            1030
DM            16.800 usec
DE            6.50 usec
TE            0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
SF01          125.8005413 MHz
NUC1          13C
P1            9.70 usec
PL1          73.00000000 W
SFO2          500.2520010 MHz
NUC2          1H
CPCPRG2       waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27124000 W

F2 - Processing parameters
SI            32768
SF            125.7879755 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```



8.546
8.529
7.743
7.729
7.713
7.662
7.645
7.534
7.441
7.425
7.417
7.401
7.260
6.237

¹H NMR (500 MHz, CDCl₃)

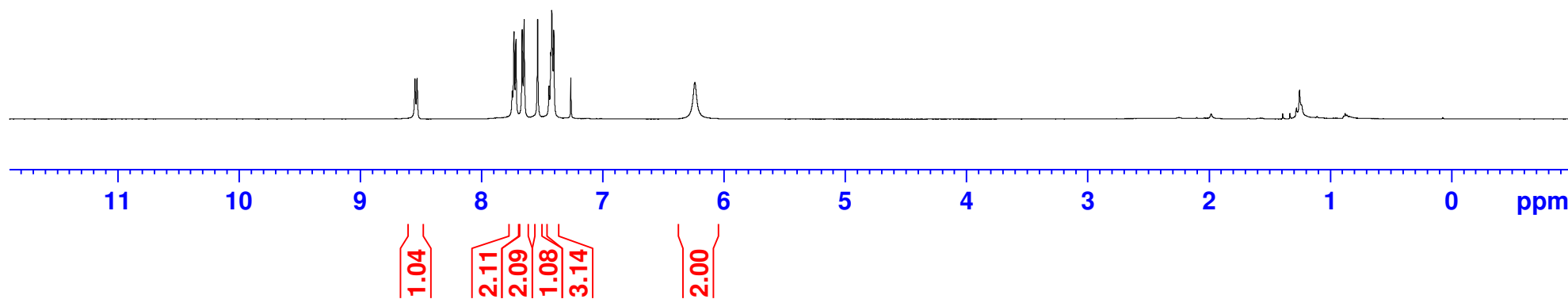


```

Current Data Parameters
NAME          3i
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20240117
Time          13.37 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767959 sec
RG            228
DW            50.000 usec
DE            6.50 usec
TE            0 K
D1            1.00000000 sec
TDO           1
SF01          500.2530890 MHz
NUC1          1H
P1            15.10 usec
PL1           15.1359968 W

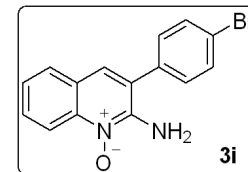
F2 - Processing parameters
SI            65536
SF            500.2500144 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



146.34
139.03
134.46
132.67
130.91
130.27
127.99
127.91
125.01
123.38
123.15
122.77
117.66

77.25
77.00
76.74

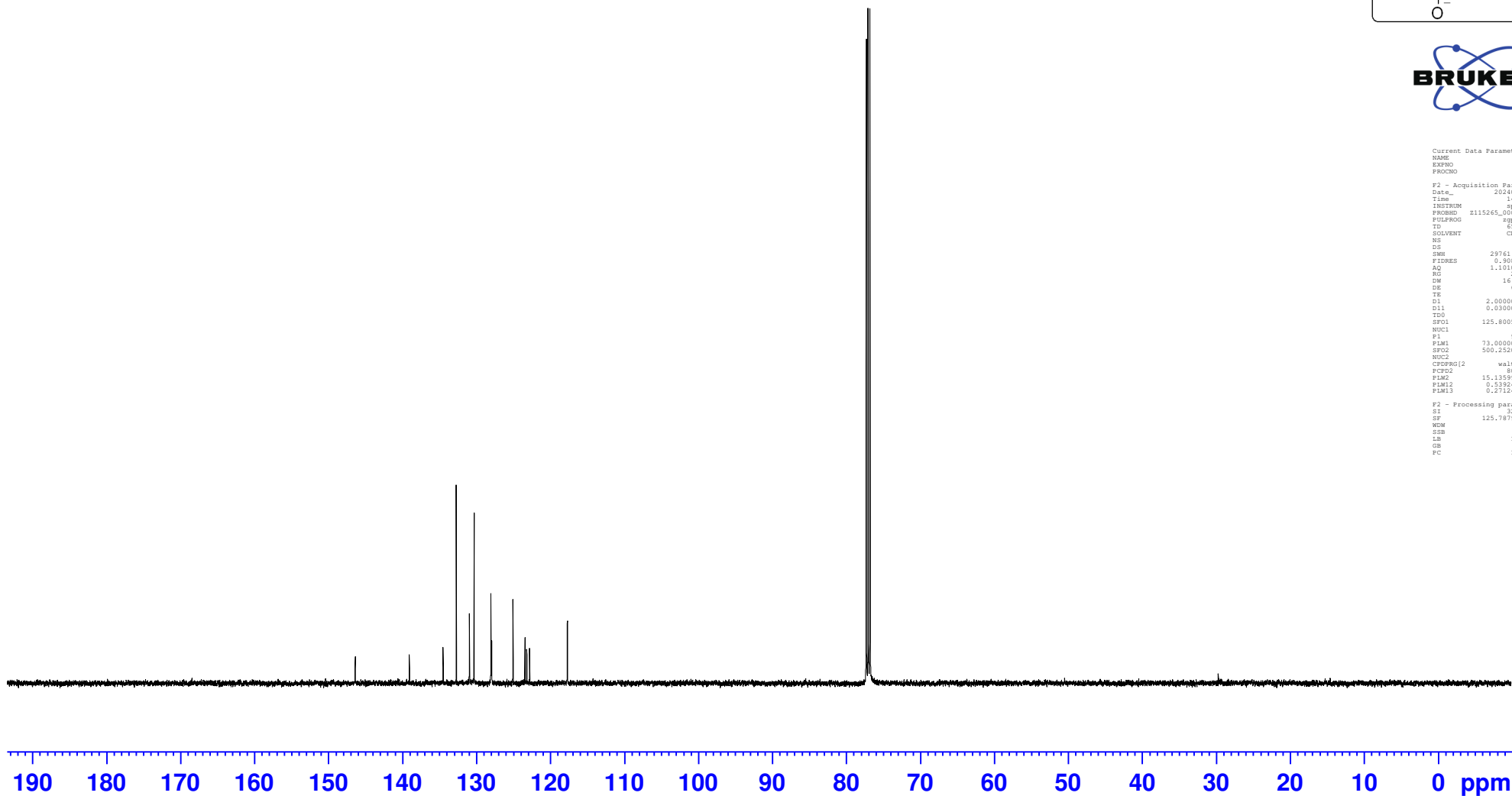
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME          3i
EXPNO         3
PROCNO        1

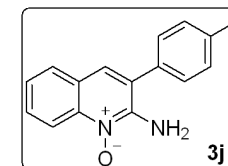
F2 - Acquisition Parameters
Date_         20240117
Time          14.10 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            577
DS            4
SWE           29761.904 Hz
FIDRES        0.998261 Hz
AQ            1.1010048 sec
RG            2050
DM            16.800 usec
DE            6.50 usec
TE            0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1
SF01          125.8005413 MHz
NUC1          13C
P1            9.70 usec
PLM1          73.0000000 W
SFO2          500.2550010 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         80.00 usec
PLM2          15.13599968 W
PLM12         0.53924000 W
PLM13         0.27124000 W

F2 - Processing parameters
SI            32768
SF            125.7879665 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```



8.520
8.503
7.836
7.820
7.726
7.713
7.698
7.509
7.423
7.407
7.393
7.274
7.258
6.266

¹H NMR (500 MHz, CDCl₃)

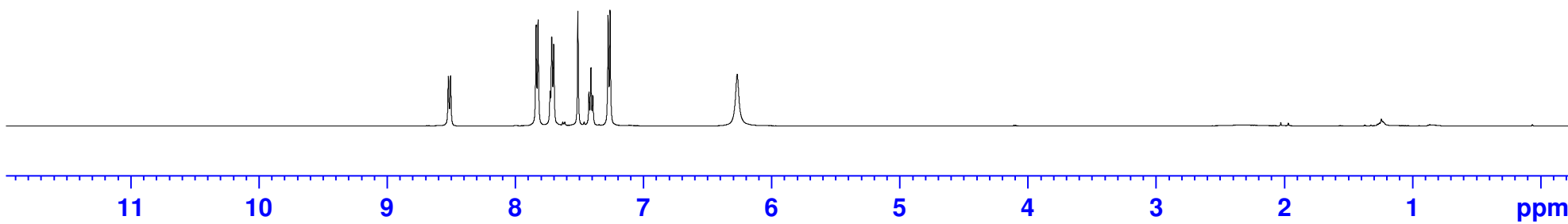


```

Current Data Parameters
NAME          3j
EXPNO        14
PROCNO       1

F2 - Acquisition Parameters
Date_        20240117
Time         22.14 h
INSTRUM      spect
PROBHD       Z115265_0004 (
PULPROG      zg30
TD           65536
SOLVENT      CDCl3
NS           4
DS           0
SWH          10000.000 Hz
FIDRES       0.305176 Hz
AQ           3.2767999 sec
RG           161
DW           50.000 usec
DE           6.50 usec
TE           0 K
D1           1.00000000 sec
TDO         1
SF01         500.2530890 MHz
NUC1         1H
P1           15.10 usec
PL1         15.13559968 W

F2 - Processing parameters
SI           65536
SF           500.2500138 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```



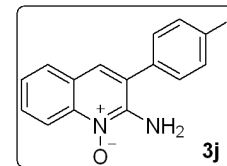
1.01
2.00
2.07
1.02
1.10
2.10
2.00

146.17
138.95
138.52
135.06
130.80
130.34
127.97
127.64
124.91
123.14
122.72
117.60

94.92

77.25
77.00
76.74

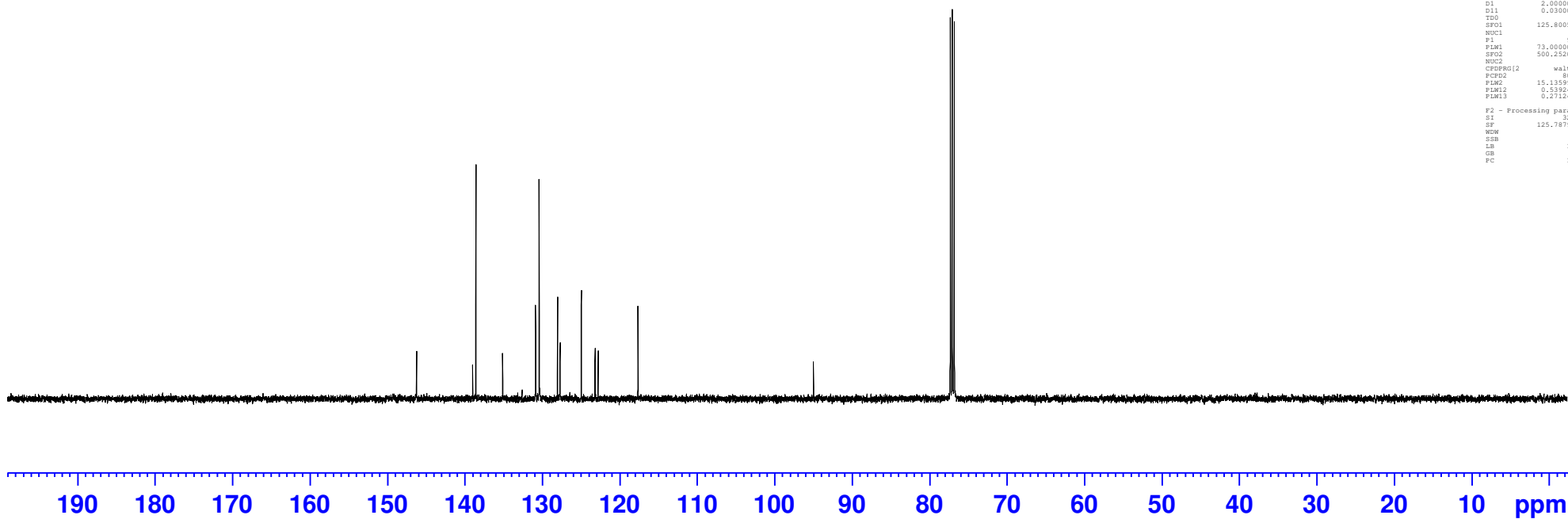
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME          3j
EXPNO         15
PROCNO        1

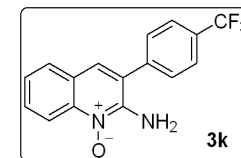
F2 - Acquisition Parameters
Date_         20240117
Time          22.22 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            112
DS            4
SWE           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG            2050
DM            16.800 usec
DE            6.50 usec
TE            0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
SF01          125.8005413 MHz
NUC1          13C
P1            9.70 usec
PLM1          73.00000000 W
SFO2          500.2550010 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         80.00 usec
PLM2          15.13599968 W
PLM12         0.53924000 W
PLM13         0.27124000 W

F2 - Processing parameters
SI            32768
SF            125.7879719 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```



8.534
8.517
7.796
7.781
7.748
7.733
7.685
7.669
7.572
7.455
7.440
7.426
7.260
6.280

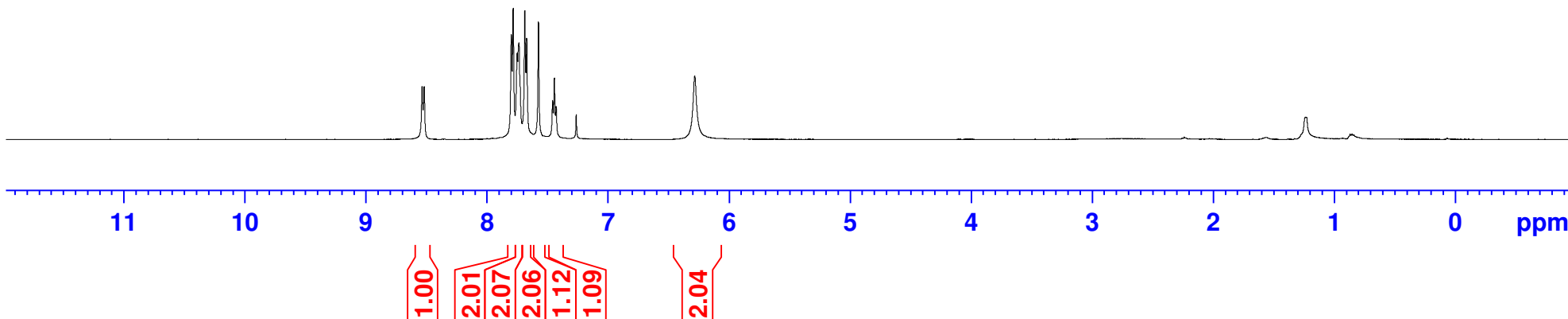
^1H NMR (500 MHz, CDCl_3)



```
Current Data Parameters
NAME          3k
EXPNO         4
PROCNO        1

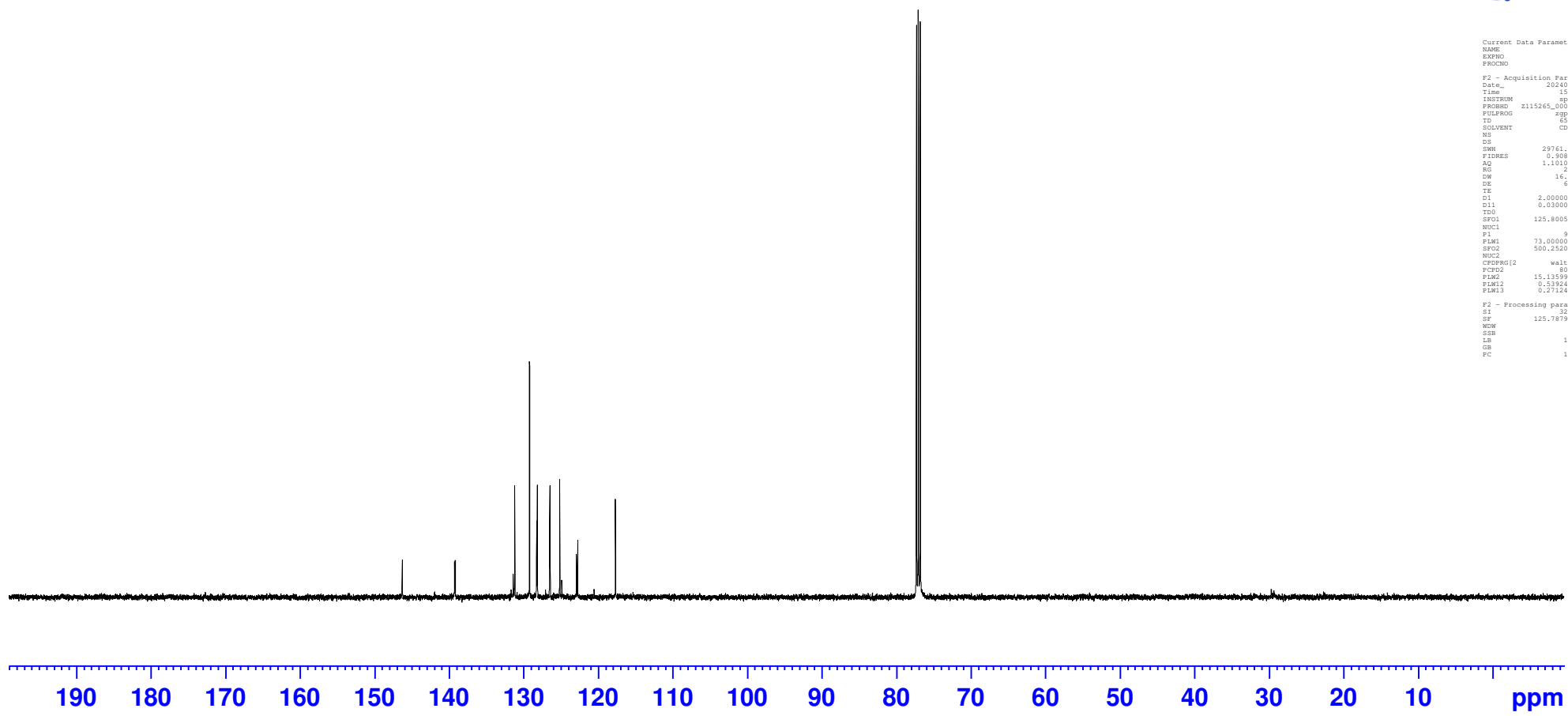
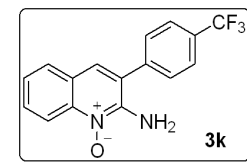
F2 - Acquisition Parameters
Date_         20240117
Time          15.05 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            4
DS            0
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767959 sec
RG            228
DW            50.000 usec
DE            6.50 usec
TE            0 K
D1            1.00000000 sec
TDO           1
SF01          500.2530890 MHz
NUC1          1H
P1            15.10 usec
PL1           15.1359968 W

F2 - Processing parameters
SI            65536
SF            500.2500149 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```



146.24
 139.23
 139.14
 131.63
 131.37
 131.15
 131.11
 130.85
 129.16
 128.20
 128.11
 127.01
 126.48
 126.45
 126.42
 126.39
 125.12
 124.84
 122.87
 122.71
 122.68
 120.51
 117.64
 77.25
 77.00
 76.74

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



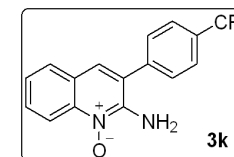
```

Current Data Parameters
NAME          3k
EXPNO        5
PROCNO       1

F2 - Acquisition Parameters
Date_        20240117
Time        15.41 h
INSTRUM     spect
PROBHD      Z115265_0004 (
PULPROG     zgpg30
TD          65536
SOLVENT     CDCl3
NS          646
DS          4
SWE         29761.904 Hz
FIDRES     0.998261 Hz
AQ         1.1010048 sec
RG          2030
DM         16.800 usec
DE         6.50 usec
TE          0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SF01       125.8005413 MHz
NUC1        13C
P1         9.70 usec
PLM1       73.00000000 W
SFO2       500.2550010 MHz
NUC2        1H
CPCPRG2     waltz16
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27124000 W

F2 - Processing parameters
SI          32768
SF         125.7879674 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

^{19}F NMR (471 MHz, CDCl_3)

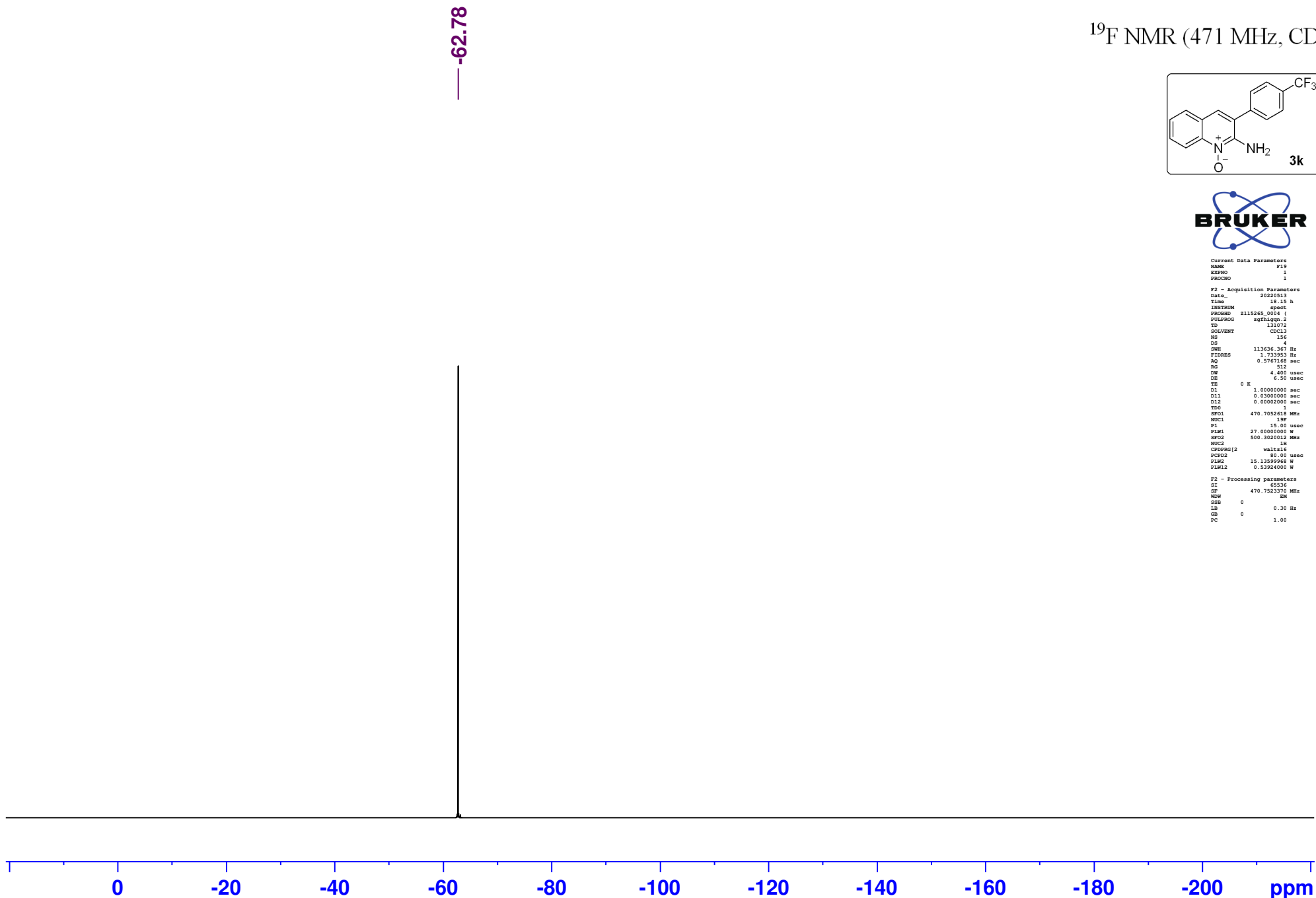


```
Current Data Parameters
NAME          F19
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20220513
Time          18:15 h
INSTRUM       spect
PROBHD        115265_004 (
PULPROG       sgfbhiqu_2
TD            131072
SOLVENT       CDCl3
NS            156
DS            4
SWH           113634.367 Hz
FIDRES        1.723993 Hz
AQ            0.5767168 sec
RG            512
DE            4.400 usec
TE            0 K

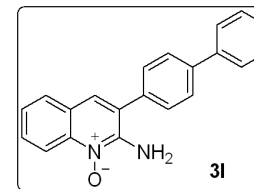
D1            1.0000000 sec
D11           0.0300000 sec
D12           0.0000200 sec
TD0           1
SF01          470.7052618 MHz
NUC1           19F
P1            15.00 usec
PIW1          27.0000000 W
SFO2          500.3020102 MHz
NUC2           1H
CFOPRG12      waltz16
PCPD2         80.00 usec
PLW2          13.13599668 W
PLW12         0.13364000 W

F2 - Processing parameters
SI            65536
SF            470.7523770 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```



8.555
8.538
7.717
7.705
7.630
7.616
7.578
7.567
7.491
7.477
7.462
7.401
7.395
7.260
6.384

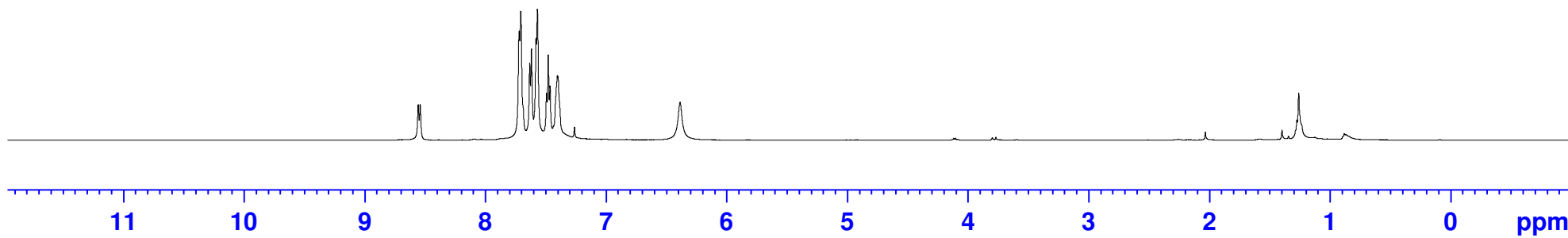
^1H NMR (500 MHz, CDCl_3)



```
Current Data Parameters
NAME          3I
EXPNO         6
PROCNO        1

F2 - Acquisition Parameters
Date_         20240117
Time          15.45 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            4
DS            0
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG            80.6
DW            50.000 usec
DE            6.50 usec
TE            0 K
D1            1.00000000 sec
TDO           1
SF01          500.2530890 MHz
NUC1           1H
P1            15.10 usec
PLM1          15.13599968 W

F2 - Processing parameters
SI            65536
SF            500.2500148 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```

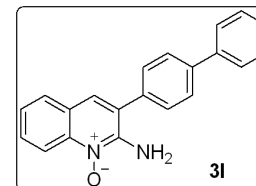


1.01
4.18
2.22
3.41
2.29
2.29
2.00

146.66
141.81
139.95
138.84
134.36
130.60
128.94
128.90
127.96
127.91
127.80
127.00
124.74
123.97
122.77
117.51

77.25
77.00
76.74

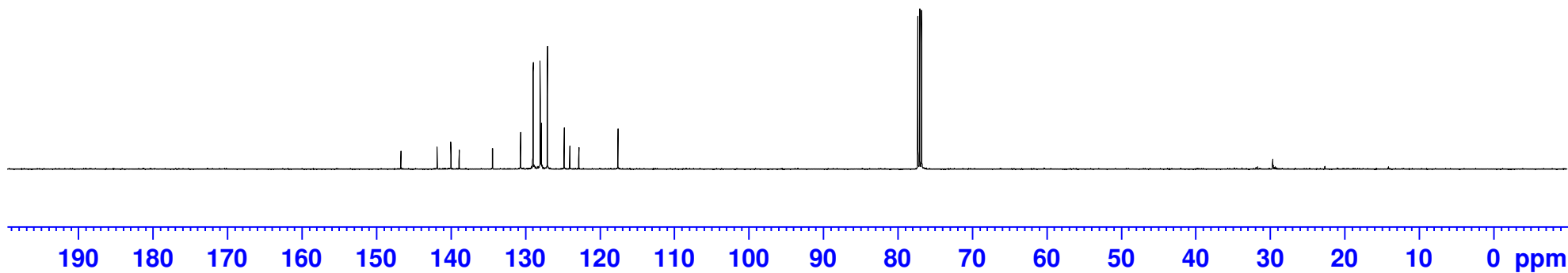
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME          31
EXPNO         7
PROCNO        1

F2 - Acquisition Parameters
Date_         20240117
Time          16.39 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            973
DS            4
SWE           29761.904 Hz
FIDRES        0.998261 Hz
AQ            1.1010048 sec
RG            1030
DM            16.800 usec
DE            6.50 usec
TE            0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1
SFO1          125.8055413 MHz
NUC1          13C
P1            9.70 usec
PLM1          73.0000000 W
SFO2          500.2520010 MHz
NUC2          1H
CPCPRG1[2]   waltz16
PCPD2         80.00 usec
PLM2         15.13599968 W
PLM12         0.53924000 W
PLM13         0.27124000 W

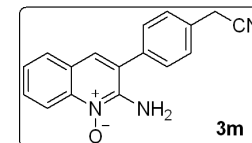
F2 - Processing parameters
SI            32768
SF            125.7879756 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```



8.567
8.550
7.762
7.747
7.732
7.582
7.569
7.532
7.516
7.459
7.444
7.429
7.260
6.228

3.854

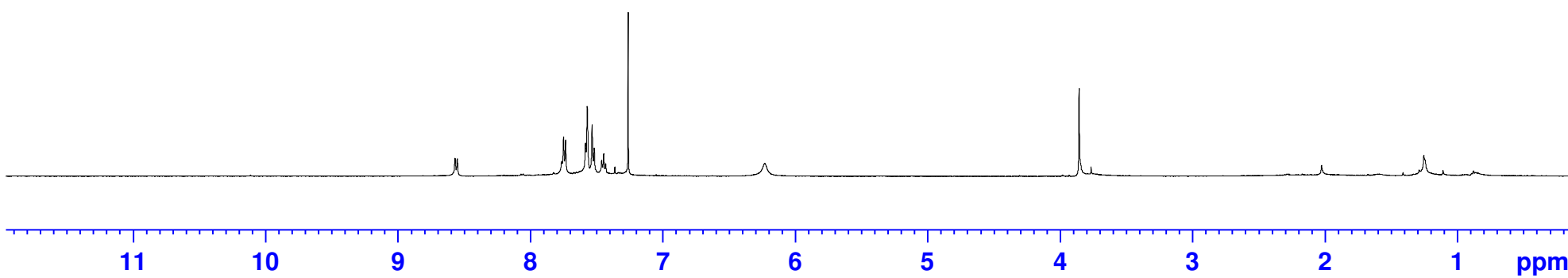
¹H NMR (500 MHz, CDCl₃)



```
Current Data Parameters
NAME          3m
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20240228
Time          12.04 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            9
DS            0
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767959 sec
RG            322
DW            50.000 usec
DE            6.50 usec
TE            0 K
D1            1.00000000 sec
TDO           1
SFO1          500.2530890 MHz
NUC1          1H
P1            15.10 usec
PL1           15.1359968 W

F2 - Processing parameters
SI            65536
SF            500.2500169 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```



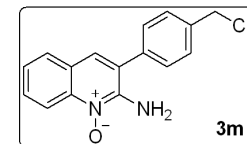
1.14
2.12
2.95
2.09
1.37
2.00
2.09

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

146.62
138.86
135.34
130.97
129.39
129.14
129.02
128.55
127.99
124.96
123.43
122.63
117.43
117.31

77.25
76.99
76.74

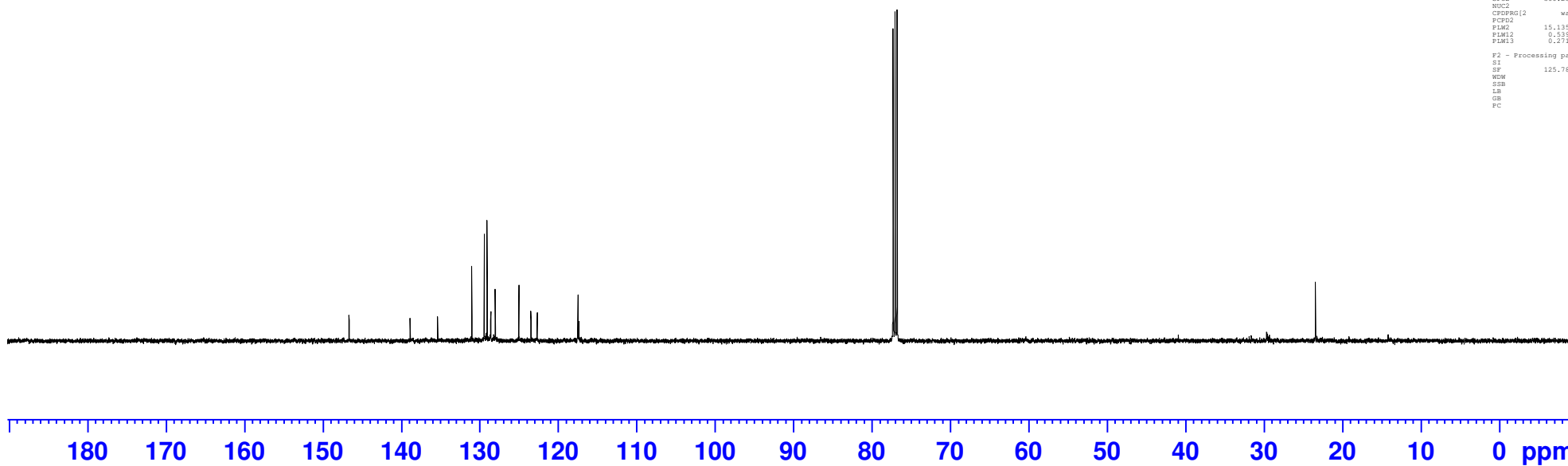
23.38



```
Current Data Parameters
NAME          3m
EXPNO         5
PROCNO        1

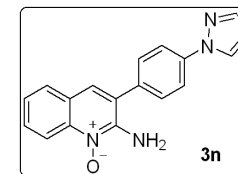
F2 - Acquisition Parameters
Date_         20230314
Time          16.00 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            215
DS            4
SWE           29761.904 Hz
FIDRES       0.908261 Hz
AQ           1.1010048 sec
RG            1030
DM           16.800 usec
DE           6.50 usec
TE           295.1 K
D1           2.0000000 sec
D11          0.0300000 sec
TD0           1
SFO1         125.8005413 MHz
NUC1          13C
P1            9.70 usec
PLM1         73.0000000 W
SFO2         500.2520010 MHz
NUC2           1H
CPDPRG2       waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27124000 W

F2 - Processing parameters
SI            32768
SF           125.7879728 MHz
WDW          EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```



8.508
8.491
7.970
7.830
7.813
7.749
7.709
7.695
7.588
7.576
7.420
7.406
7.391
7.260
6.502

^1H NMR (500 MHz, CDCl_3)

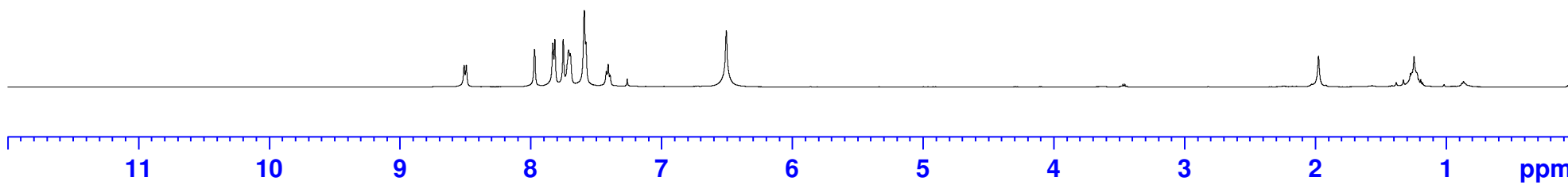


```

Current Data Parameters
NAME      24 MARCH-2024
EXPNO     5
PROCNO    1

F2 - Acquisition Parameters
Date_     20240324
Time      15.36 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         4
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         114
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SF01       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PLM1       15.1359968 W

F2 - Processing parameters
SI         65536
SF         500.2500146 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

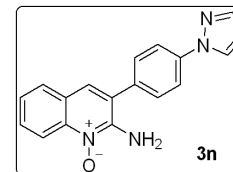


1.02
1.08
2.13
1.04
2.05
3.11
1.09
3.00

147.09
141.58
140.48
138.80
133.13
131.02
129.78
129.15
127.93
126.67
124.93
123.55
122.56
119.70
117.39
108.17

77.25
77.00
76.74

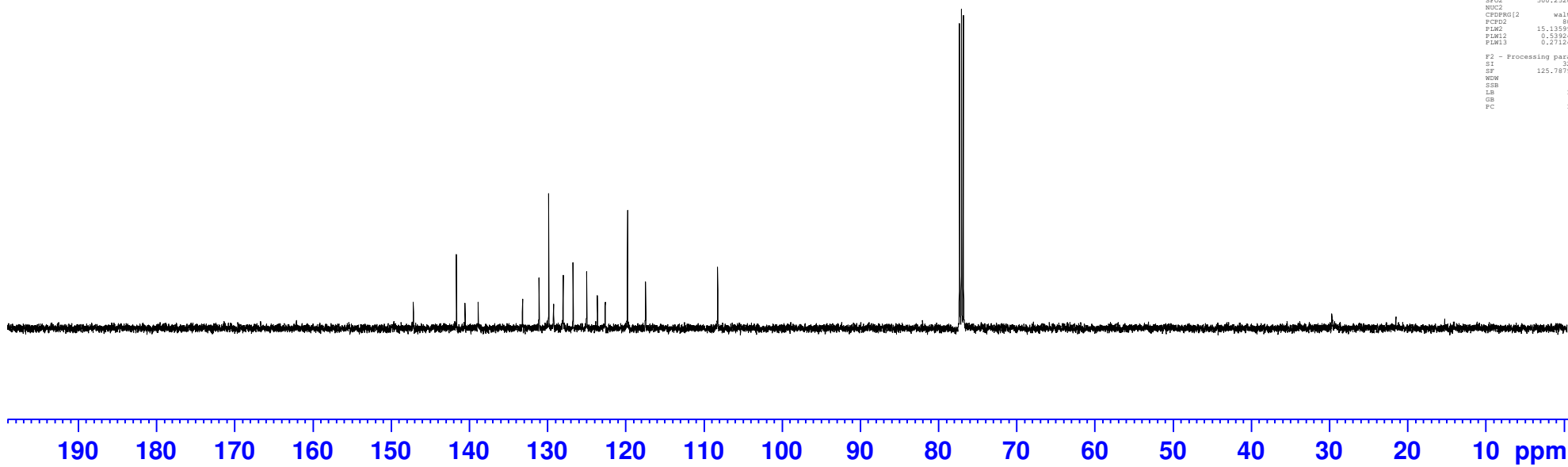
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME      24 MAR08-2024
EXPNO     6
PROCNO    1

F2 - Acquisition Parameters
Date_     20240324
Time      15:41 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         59
DS         4
SWE        29761.904 Hz
FIDRES    0.998261 Hz
AQ         1.1010048 sec
RG         1030
DM         16.800 usec
DE         6.50 usec
TE         0 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1
SF01       125.8005413 MHz
NUC1       13C
P1         9.70 usec
PL1        73.0000000 W
SFO2       500.2550010 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27124000 W

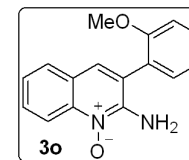
F2 - Processing parameters
SI         32768
SF         125.7879729 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
```



8.568
8.551
7.701
7.687
7.545
7.479
7.464
7.448
7.406
7.392
7.377
7.314
7.300
7.260
7.110
7.096
7.081
7.055
7.038
6.138

3.796

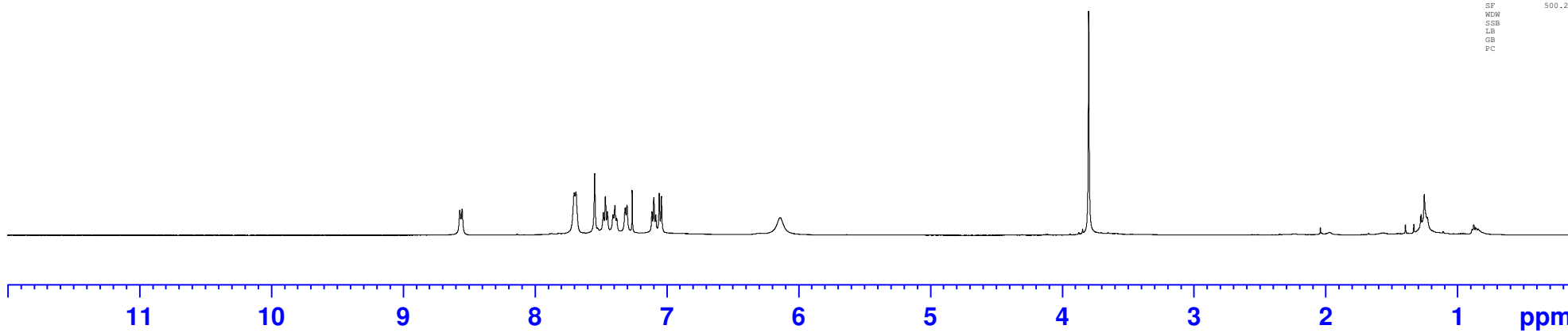
¹H NMR (500 MHz, CDCl₃)



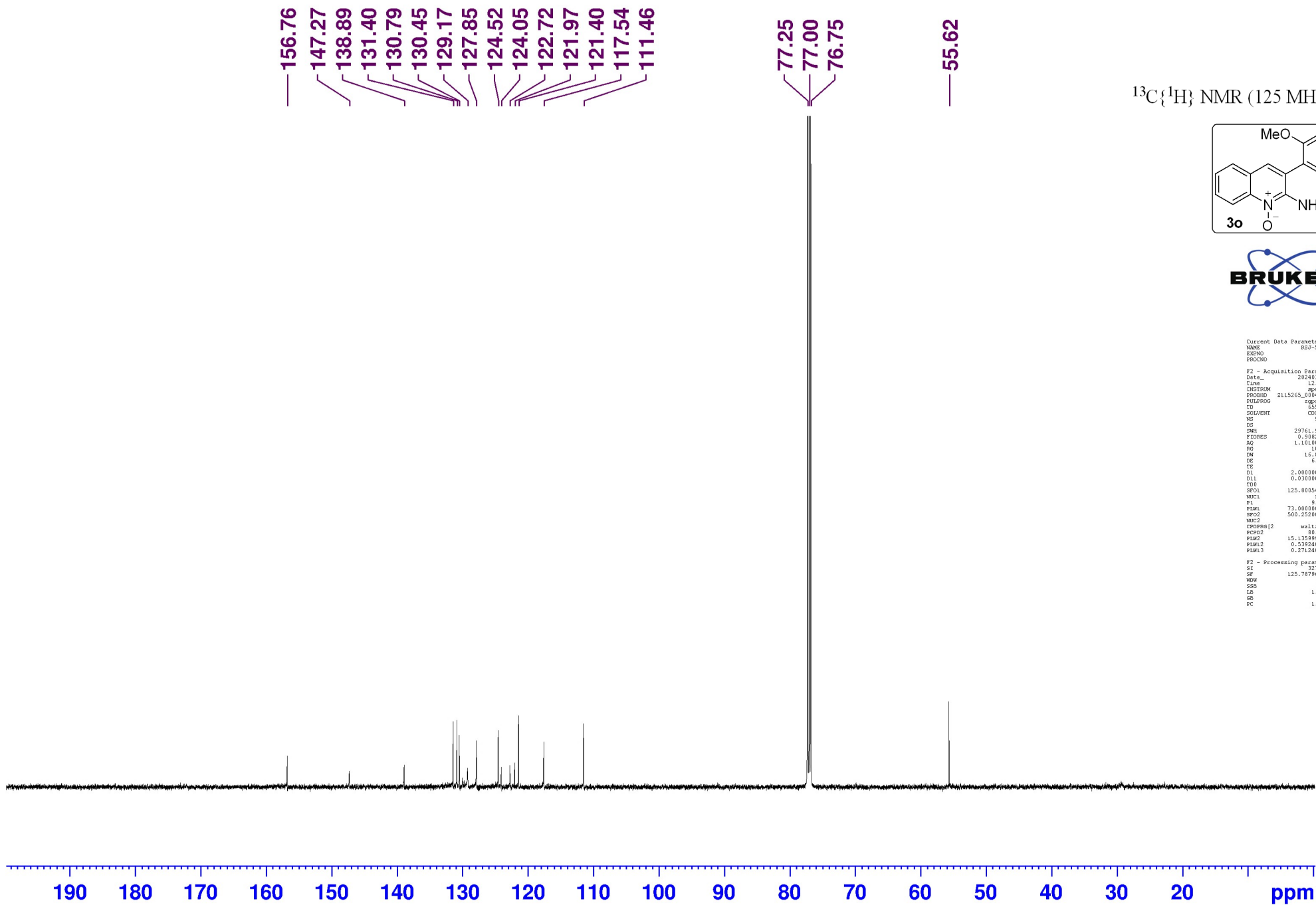
```
Current Data Parameters
NAME      RSJ-576
EXPNO     8
PROCNO    1

F2 - Acquisition Parameters
Date_     20240322
Time      12.06 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767959 sec
RG         181
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1      500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.1359968 W

F2 - Processing parameters
SI         65536
SF         500.2500145 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



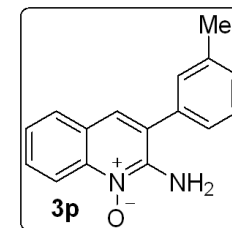
1.03
2.11
1.05
1.37
1.22
1.15
1.10
1.09
1.93
3.00



8.514
8.497
7.699
7.692
7.685
7.553
7.405
7.390
7.385
7.371
7.300
7.285
7.269
7.259
7.255
6.396

2.414

^1H NMR (500 MHz, CDCl_3)

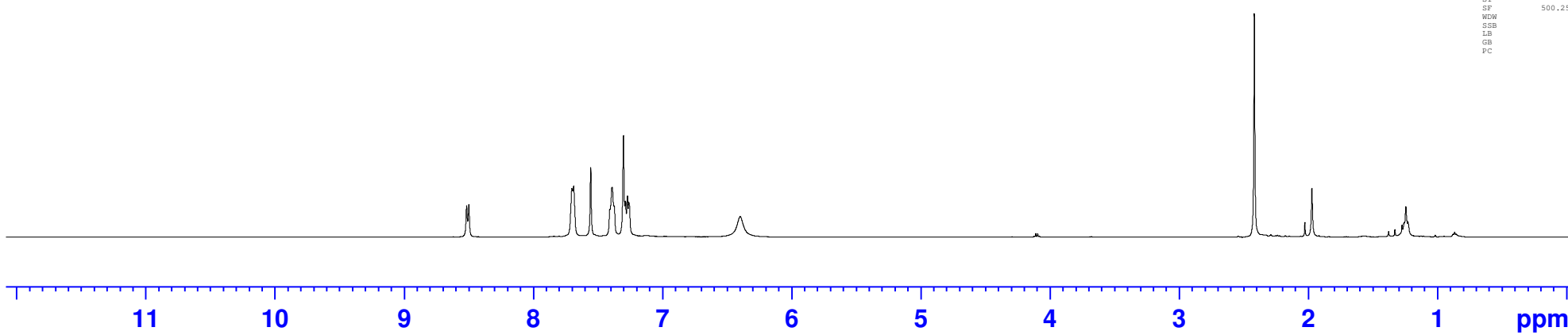


```

Current Data Parameters
NAME          3p
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20240118
Time          9.45 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            4
DS            0
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG            71.8
DW            50.000 usec
DE            6.50 usec
TE            0 K
D1            1.00000000 sec
TDO          1
SFO1          500.2530890 MHz
NUC1          1H
P1            15.10 usec
PL1           15.1359968 W

F2 - Processing parameters
SI            65536
SF            500.2500138 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



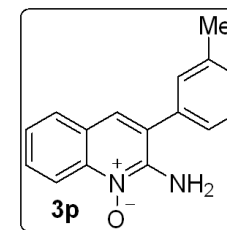
1.04
2.19
1.12
2.18
3.39
2.00
3.14

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

147.03
139.29
138.72
135.27
130.67
129.76
129.25
129.17
128.64
127.85
125.50
124.72
124.62
122.65
117.36

77.25
76.99
76.74

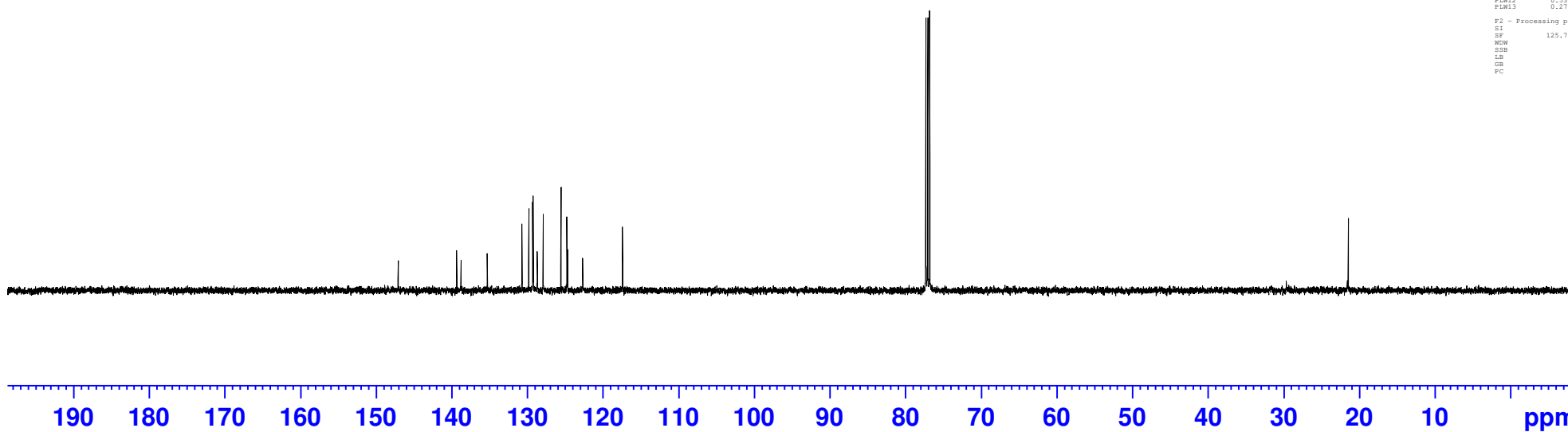
21.38



```
Current Data Parameters
NAME          3p
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20240118
Time_         9:50 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            50
DS            4
SWE           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG            1030
DM            16.800 usec
DE            6.50 usec
TE            0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1
SF01          125.8005413 MHz
NUC1          13C
P1            9.70 usec
PLM1          73.0000000 W
SFO2          500.2550010 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         80.00 usec
PLM2          15.13599968 W
PLM12         0.53924000 W
PLM13         0.27124000 W

F2 - Processing parameters
SI            32768
SF            125.7879747 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

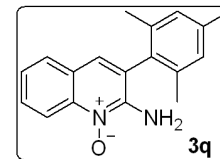


8.345
8.328
7.872
7.856
7.731
7.716
7.700
7.538
7.440
7.425
7.410
7.037
6.693

3.342

2.503
2.500
2.497
2.316
1.985

¹H NMR (500 MHz, DMSO-d₆)



```
Current Data Parameters
NAME      RSJ-1022
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20240322
Time      13.04 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         181
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1      500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13599968 W

F2 - Processing parameters
SI         65536
SF         500.2500061 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

0.99
1.18
1.36
1.14
1.31
2.26
2.11

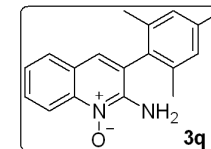
3.43
6.38



$^{13}\text{C} \{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6)

146.53
138.40
137.46
136.23
131.26
129.90
128.49
128.22
126.83
123.88
122.67
122.32
116.73

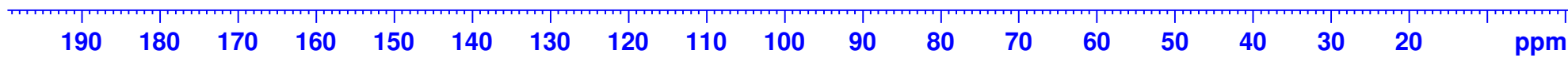
40.02
39.85
39.68
39.52
39.35
39.18
39.01
20.73
19.65



```
Current Data Parameters
NAME      RUP-1022
EXPNO    15
PROCNO    1

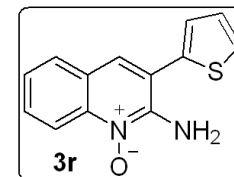
F2 - Acquisition Parameters
Date_     20240313
Time      8.37 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         10000
DS         4
SWE        29761.904 Hz
FIDRES    0.908261 Hz
AQ         1.1010048 sec
RG         1030
DM         16.800 usec
DE         6.50 usec
TE         0 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1
SFO1       125.8005413 MHz
NUC1       13C
P1         9.70 usec
PL1        73.0000000 W
SFO2       500.2550010 MHz
NUC2       1H
PCPDPRG2   waltz16
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27124000 W

F2 - Processing parameters
SI         32768
SF         125.7980262 MHz
RG         64
SBB        0
LB         1.00 Hz
GB         0
PC         1.40
```



8.451
8.433
7.647
7.634
7.619
7.595
7.366
7.356
7.345
7.330
7.315
7.295
7.290
7.260
7.076
7.069
7.061
6.635

¹H NMR (500 MHz, CDCl₃)

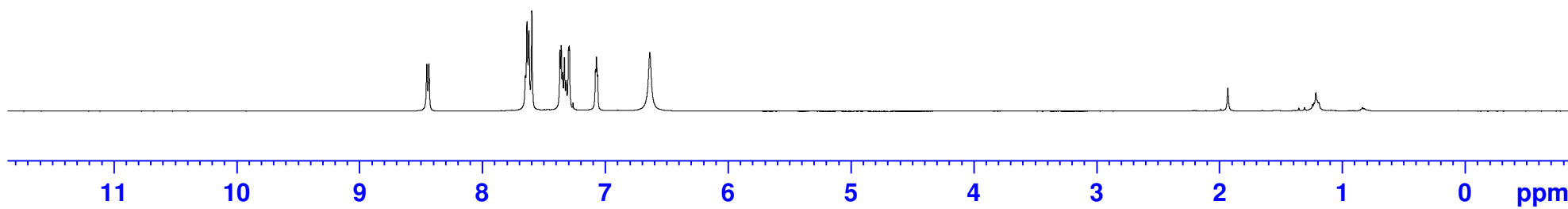


```

Current Data Parameters
NAME          3r
EXPNO        12
PROCNO       1

F2 - Acquisition Parameters
Date_        20240117
Time         21.55 h
INSTRUM      spect
PROBHD       Z115265_0004 (
PULPROG      zg30
TD           65536
SOLVENT      CDCl3
NS           4
DS           0
SWH          10000.000 Hz
FIDRES       0.305176 Hz
AQ           3.2767999 sec
RG           64
DW           50.000 usec
DE           6.50 usec
TE           0 K
D1           1.00000000 sec
TDO         1
SF01         500.2530890 MHz
NUC1         1H
P1           15.10 usec
PLM1         15.1359968 W

F2 - Processing parameters
SI           65536
SF           500.2500157 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```

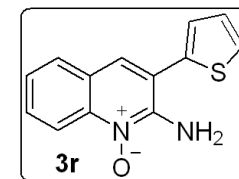


1.05
2.09
1.00
3.14
1.06
2.07

146.54
138.71
136.40
130.78
128.42
127.94
127.82
127.01
126.88
124.72
122.21
117.32
117.23

77.25
77.00
76.74

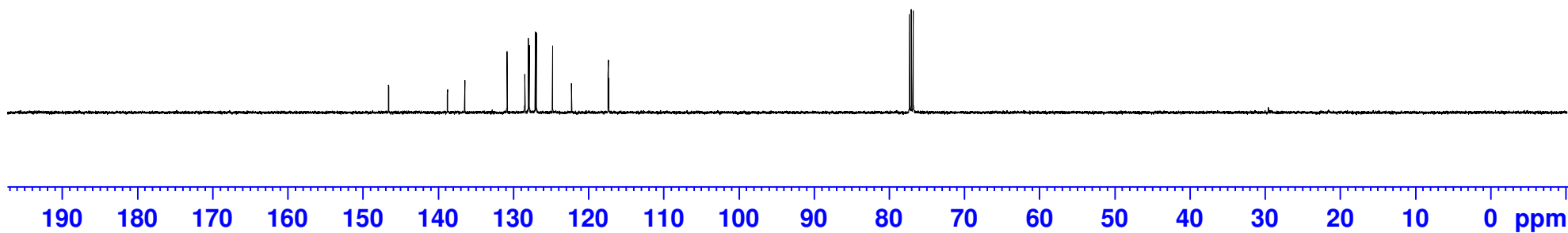
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



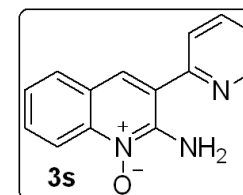
```
Current Data Parameters
NAME          3r
EXPNO         13
PROCNO        1

F2 - Acquisition Parameters
Date_         20240117
Time_        21.59 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            38
DS            4
SWE           29761.904 Hz
FIDRES        0.998261 Hz
AQ            1.1010048 sec
RG            1030
DM            16.800 usec
DE            6.50 usec
TE            0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
SFO1          125.8005413 MHz
NUC1          13C
P1            9.70 usec
PLM1          73.00000000 W
SFO2          500.2550010 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         80.00 usec
PLM2          15.13599969 W
PLM12         0.53924000 W
PLM13         0.27124000 W

F2 - Processing parameters
SI            32768
SF            125.7879865 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```



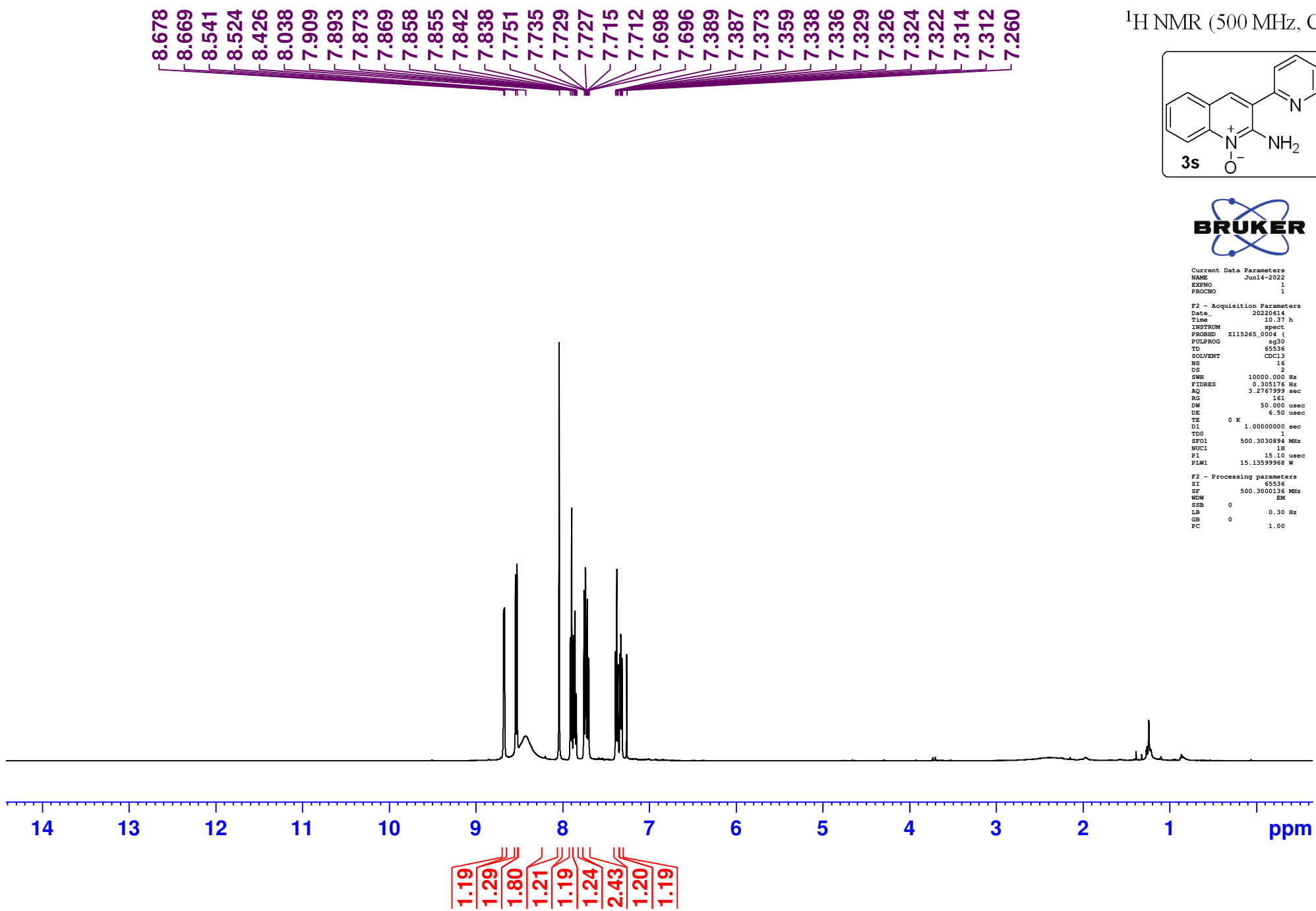
¹H NMR (500 MHz, CDCl₃)



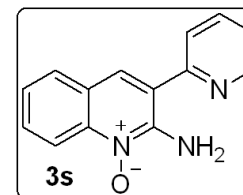
Current Data Parameters
NAME Jun14-2022
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220614
Time 10:37 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.216799 sec
RG 161
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TDO 1
SFO1 500.3030894 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000136 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

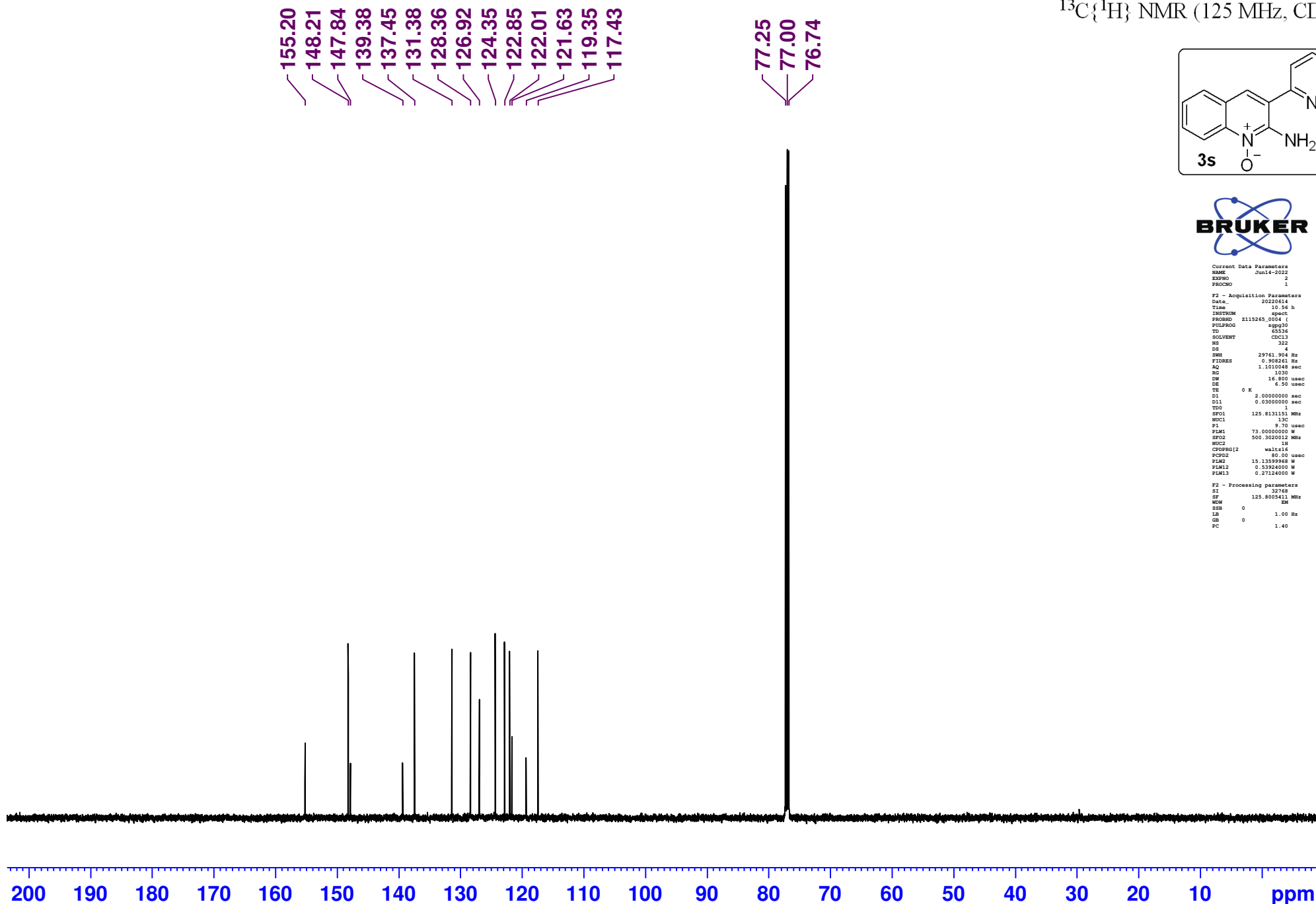


```
Current Data Parameters
NAME      Jun14-2022
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20220614
Time     10:56 h
INSTRUM  spect
PROBHD   zgpg30
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        322
DS        4
SWH       29761.904 Hz
FIDRES    0.998261 Hz
AQ         1.1010048 sec
RG         1030
RW         16.800 usec
DE         6.50 usec
TE         0 K

D1         2.0000000 sec
D11        0.0300000 sec
TDO        1
SFO1       125.8131151 MHz
NUC1       13C
P1         9.70 usec
PLA1       73.0000000 W
SFO2       500.3020012 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2      80.00 usec
PLM2       15.13599968 W
PLM12      0.53924000 W
PLM13      0.27154000 W

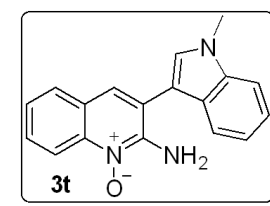
F2 - Processing parameters
SI         32768
SF         125.8003411 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```



8.496
8.480
7.735
7.683
7.670
7.594
7.579
7.423
7.407
7.394
7.326
7.260
7.209
7.196
6.650

3.866

¹H NMR (500 MHz, CDCl₃)

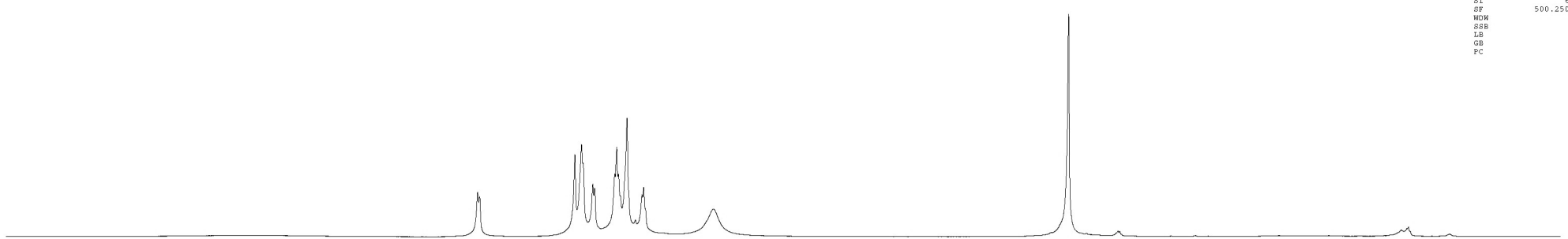


```

Current Data Parameters
NAME      24 MARCH-2024
EXPNO     13
PROCNO    1

F2 - Acquisition Parameters
Date_     20240325
Time      7.42 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         64
DN         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TD0        1
SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13599966 W

F2 - Processing parameters
SI         65536
SF         500.2500151 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



12 11 10 9 8 7 6 5 4 3 2 1 ppm

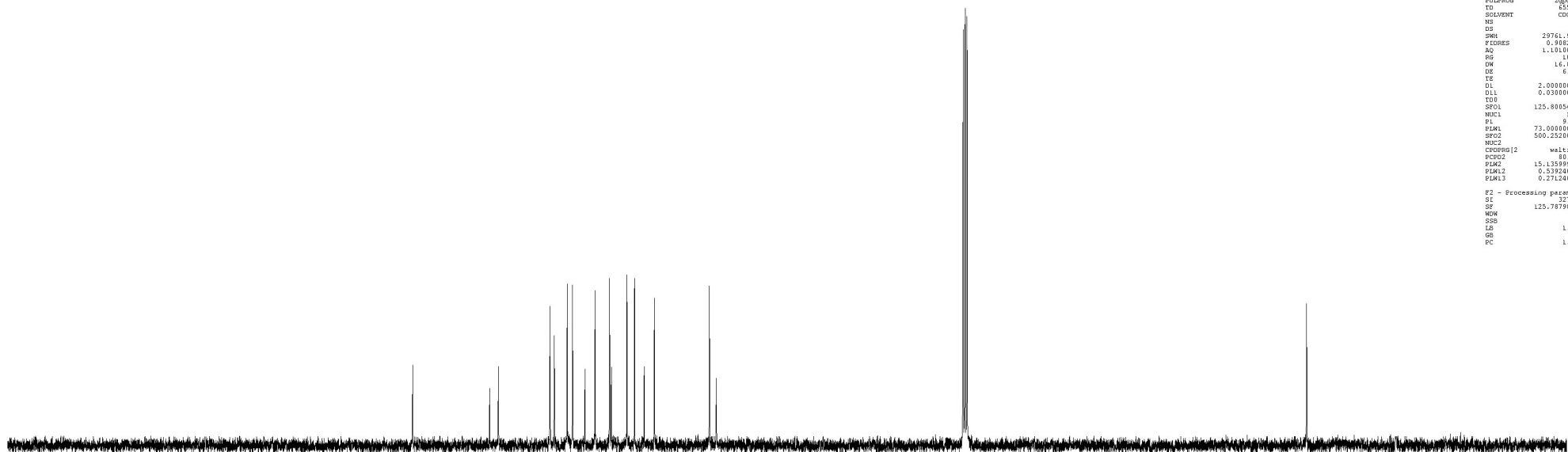
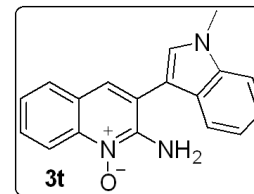
1.00 3.08 1.15 2.37 2.01 1.04 2.13 3.15

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

148.14
138.22
137.10
130.44
129.90
128.24
127.56
125.95
124.65
122.78
122.56
120.55
119.57
118.33
117.01
109.92
109.03

77.25
77.00
76.74

33.01



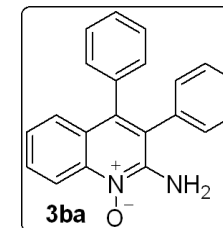
```
Current Data Parameters
NAME      24 MARCH 2024
EXPNO    11
PROCNO   1

F2 - Acquisition Parameters
Date_    20240323
Time     7.47 h
PROBHD   spect
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        63
DS        4
SFORES   29761.904 Hz
AQ        0.908261 Hz
RG        1.101040 sec
DM        16.800 usec
DE        6.50 usec
TE        0 K
DIL       2.00000000 sec
D1L       0.03000000 sec
TD0       1
SFO1     125.805413 MHz
NUC1      13C
PL        9.70 usec
P1M1     73.00000000 M
SFO2     500.132013 MHz
NUC2      1H
CROSSP2  waltz16
PCPD2    80.00 usec
P1M2     15.1359965 M
P1M3     0.53924000 M
P1M4     0.27124000 M

F2 - Processing parameters
SI        32768
SF        125.7878810 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

¹H NMR (500 MHz, CDCl₃)

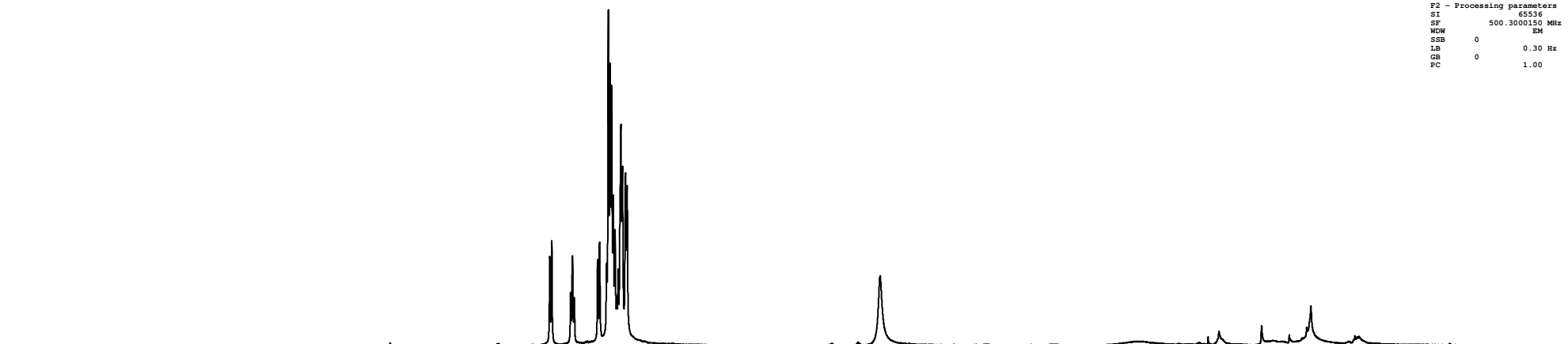


Current Data Parameters
NAME Jan03-2023
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230105
Time 11.23 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.216799 sec
RG 256
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TDO 1
SFO1 500.3030894 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000150 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.760
7.743
7.580
7.566
7.552
7.350
7.335
7.274
7.260
7.246
7.233
7.217
7.202
7.188
7.176
7.155
7.153
7.139
7.115
7.112
7.100
4.939

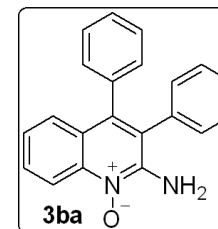


12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

1.00
1.06
1.10
6.39
3.17
2.14

2.07

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

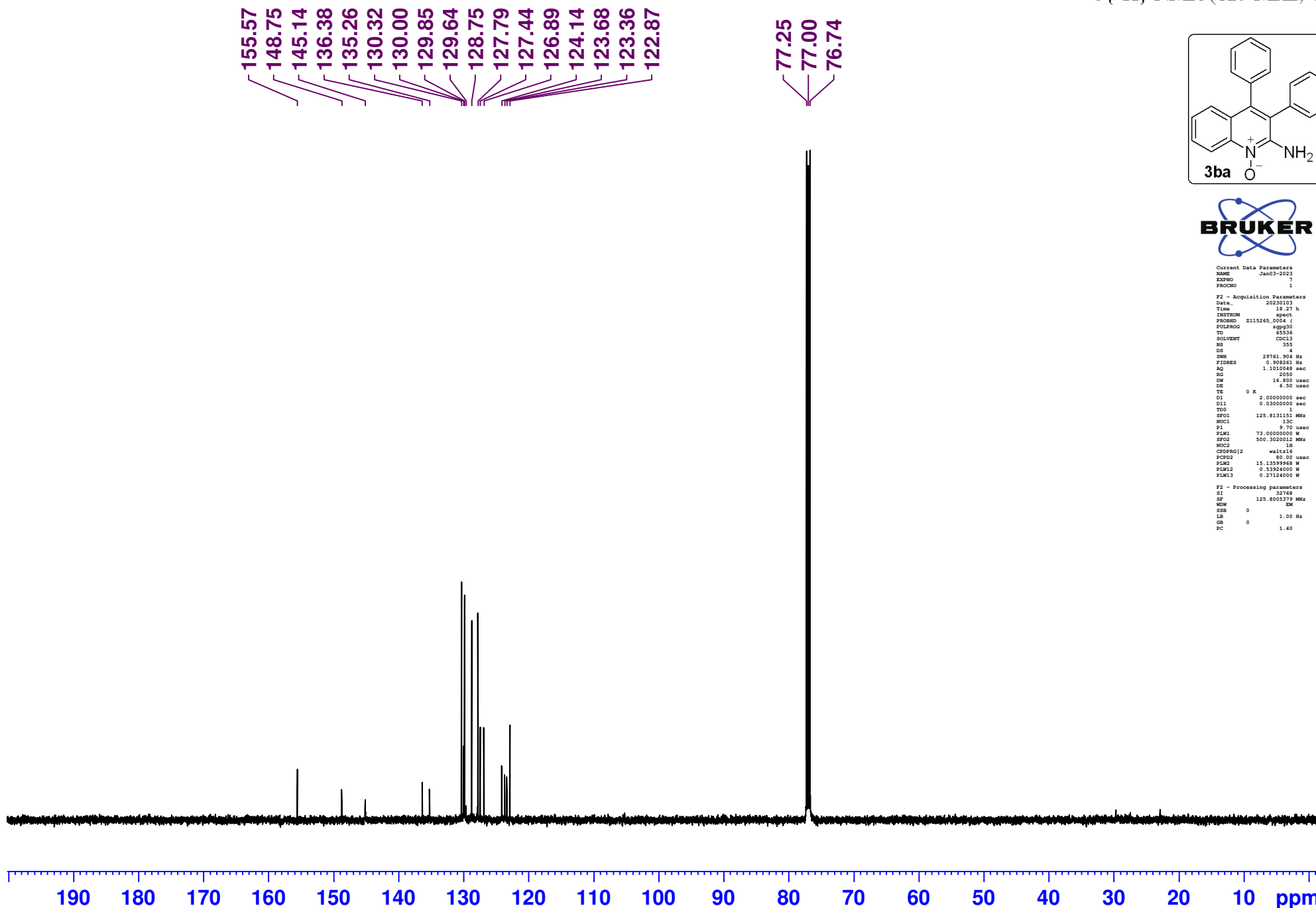


```
Current Data Parameters
NAME          Jan03-2023
EXPNO        7
PROCNO       1

F2 - Acquisition Parameters
Date_        20230103
Time         18:27 h
INSTRUM      spect
PROBHD       5mmQNP1H1
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           355
DS           4
SWH          29761.904 Hz
FIDRES       0.998261 Hz
AQ           1.1010048 sec
RG           2000
DW           16.800 usec
DE           6.50 usec
TE           0 K

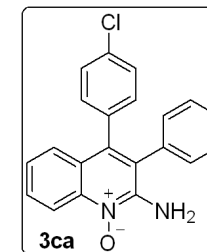
D1           2.0000000 sec
D11          0.0300000 sec
TDO          1
SFO1         125.811111 MHz
NUC1         13C
P1           73.0000000 usec
PL1          0.27154000 W
SFO2         500.3020012 MHz
NUC2         1H
PCPDPRG2     waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27154000 W

F2 - Processing parameters
SI           32768
SF           125.800379 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
```



7.755
7.738
7.590
7.576
7.561
7.304
7.289
7.276
7.260
7.241
7.224
7.188
7.173
7.158
7.134
7.120
7.055
7.039
5.000

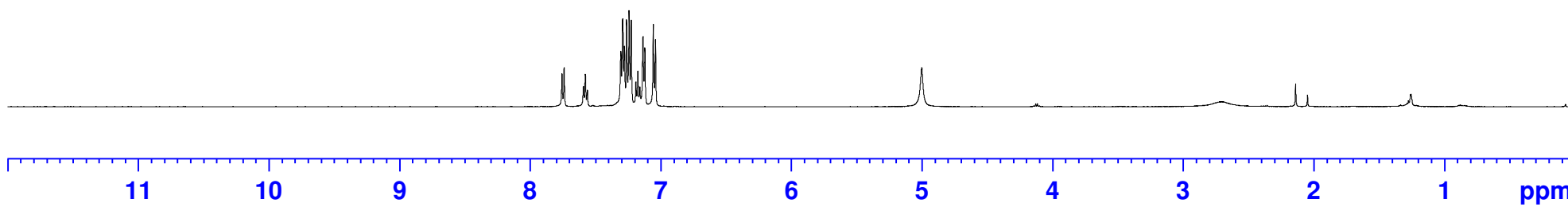
¹H NMR (500 MHz, CDCl₃)



Current Data Parameters
NAME 24 MARCH-2024
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240324
Time 23.32 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767959 sec
RG 287
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TDO 1
SFO1 500.2530890 MHz
NUC1 1H
P1 15.10 usec
PL1 15.13559968 W

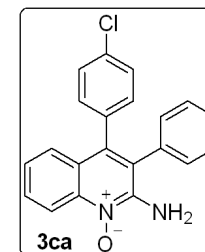
F2 - Processing parameters
SI 65536
SF 500.2500132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.02
1.05
3.27
3.45
1.18
2.00
1.98

2.07

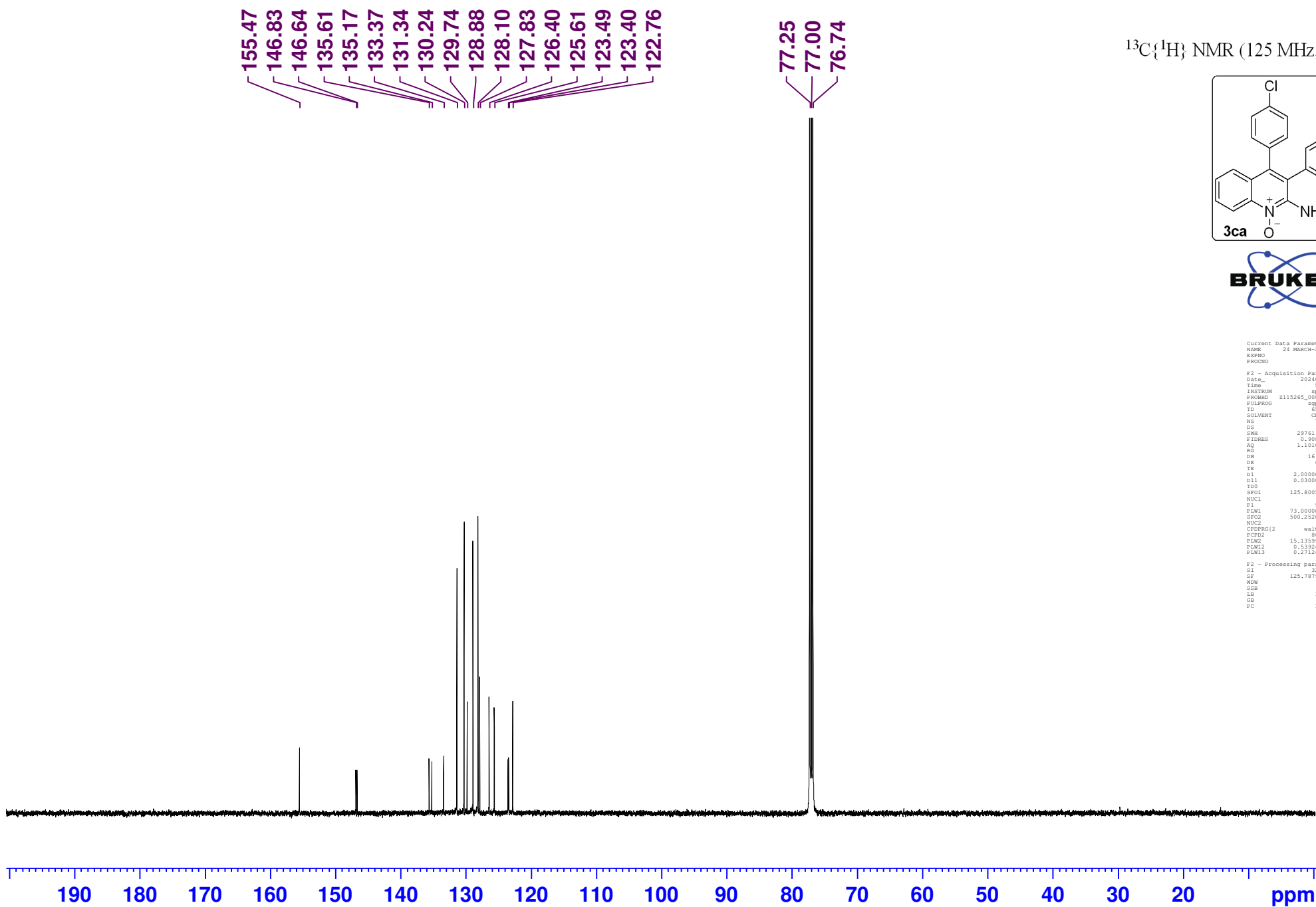
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME      24 MARCH-2024
EXPNO     10
PROCNO    1

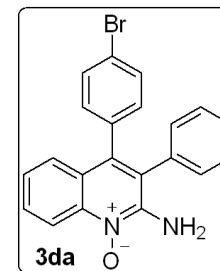
F2 - Acquisition Parameters
Date_     20240325
Time      5:51 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         7000
DS         4
SWE        29761.904 Hz
FIDRES    0.998261 Hz
AQ         1.1010048 sec
RG         1030
DM         16.800 usec
DE         6.50 usec
TE         0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SFO1      125.8005413 MHz
NUC1       13C
P1         9.70 usec
PL1        73.00000000 W
SFO2      500.2550010 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     80.00 usec
PLM2      15.13599968 W
PLM12     0.53924000 W
PLM13     0.27124000 W

F2 - Processing parameters
SI         32768
SF         125.7879650 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```



7.752
7.736
7.589
7.587
7.573
7.559
7.556
7.395
7.378
7.306
7.299
7.292
7.285
7.282
7.277
7.260
7.244
7.186
7.184
7.170
7.154
7.139
7.136
7.122
6.998
6.981
4.882

¹H NMR (500 MHz, CDCl₃)

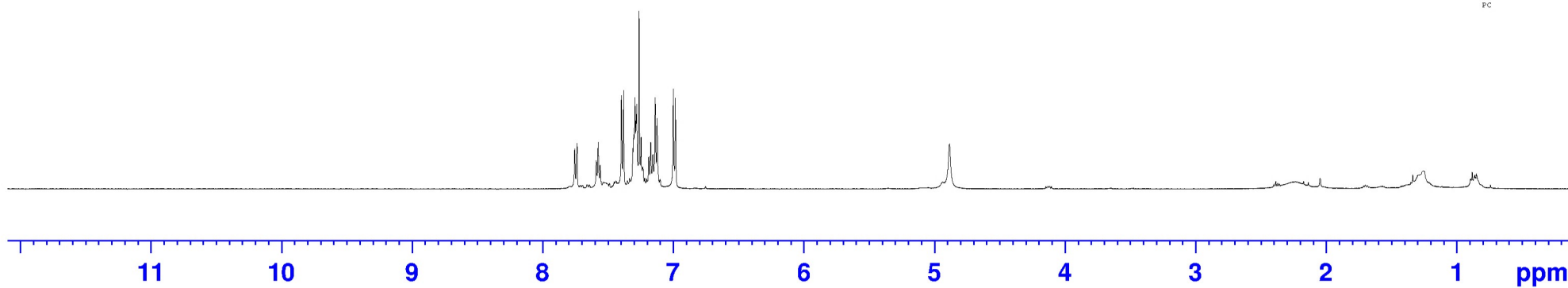


```

Current Data Parameters
NAME      26 MARCH-2024
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20240326
Time      21.01 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         322
DN         50.000 usec
DE         6.50 usec
TE         298.2 K
D1         1.0000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PLM1       15.13599968 W

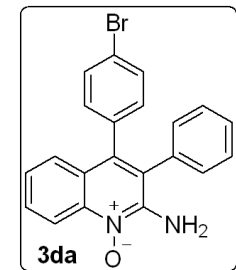
F2 - Processing parameters
SI         65536
SF         500.2500139 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



1.05
1.28
1.89
3.20
1.09
1.45
2.02
1.90

2.12

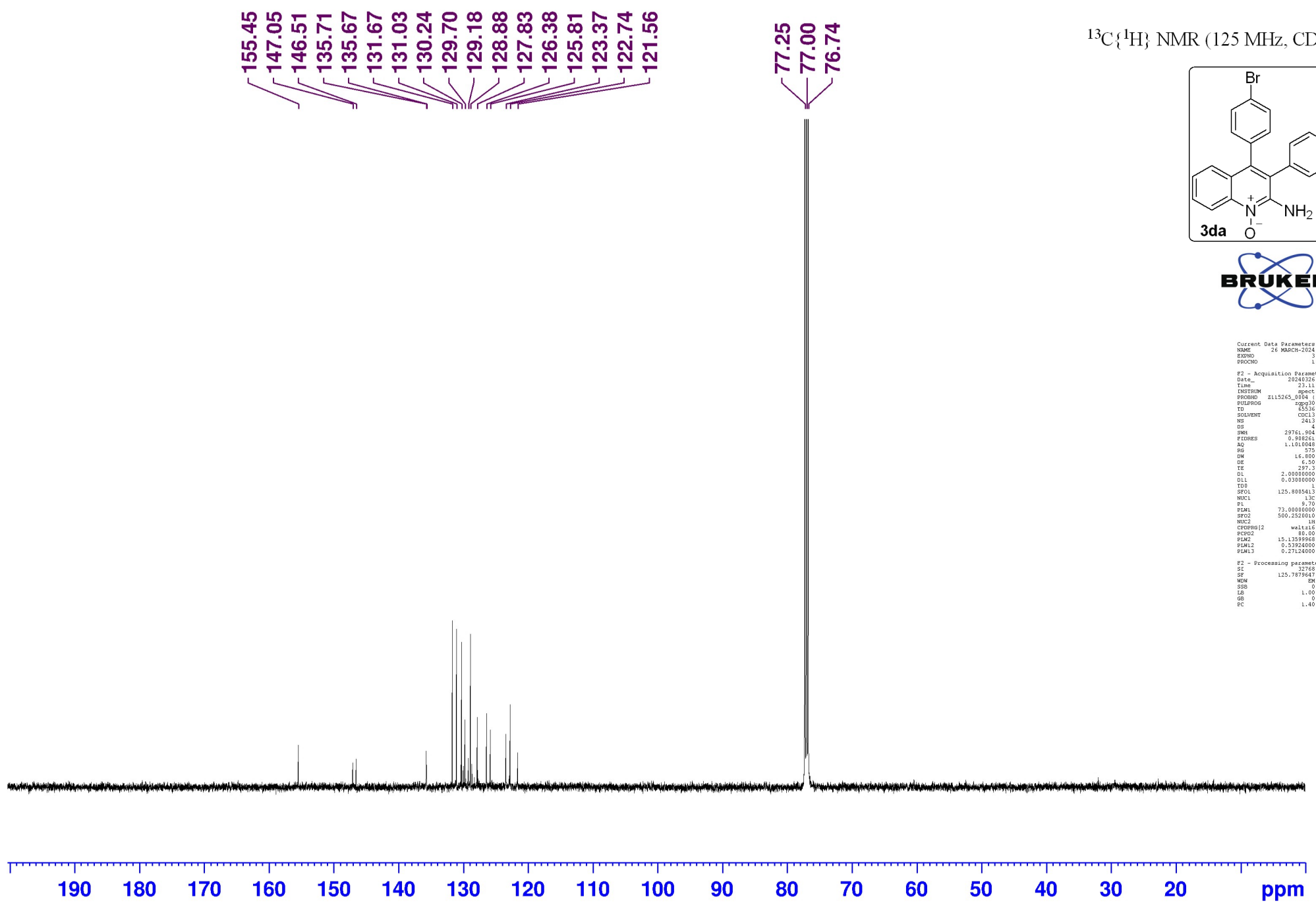
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



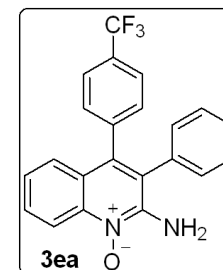
```
Current Data Parameters
NAME      26 MARCH 2024
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20240326
Time     23.11 h
PROBHD   spect
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        243
DS        4
SFO1     29761.904 Hz
FIDRES   0.908261 Hz
AQ        1.1010408 sec
RG         575
DM        16.800 usec
DE         5.50 usec
TE        297.3 K
DQ        2.00000000 sec
DIL       0.03000000 sec
TOP
SFO1     125.8005413 MHz
NUC1      13C
PL        9.70 usec
PWL1     73.00000000 M
SFO2     500.1320113 MHz
NUC2      1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PWL2     15.1359965 M
PWL3     0.53924000 M
PWL4     0.27124000 M

F2 - Processing parameters
SI        32768
SF        125.7879647 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```



^1H NMR (500 MHz, CDCl_3)

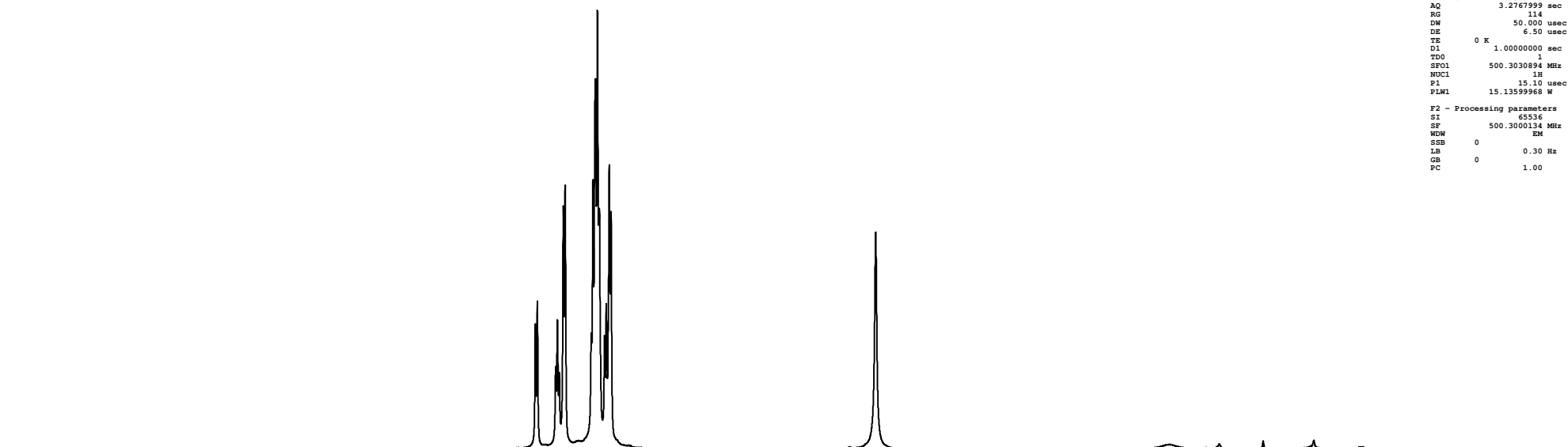


Current Data Parameters
NAME Jan11-2023
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230111
Time 16.19 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 8
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.276799 sec
RG 114
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.0000000 sec
TDO 1
SFO1 500.3030894 MHz
NUC1 ^1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

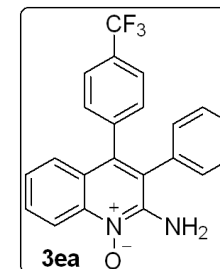
7.762
7.746
7.593
7.578
7.563
7.530
7.514
7.296
7.282
7.261
7.245
7.233
7.229
7.185
7.171
7.146
7.131
4.923



12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

1.00
1.05
1.93
6.05
1.00
2.01
1.99

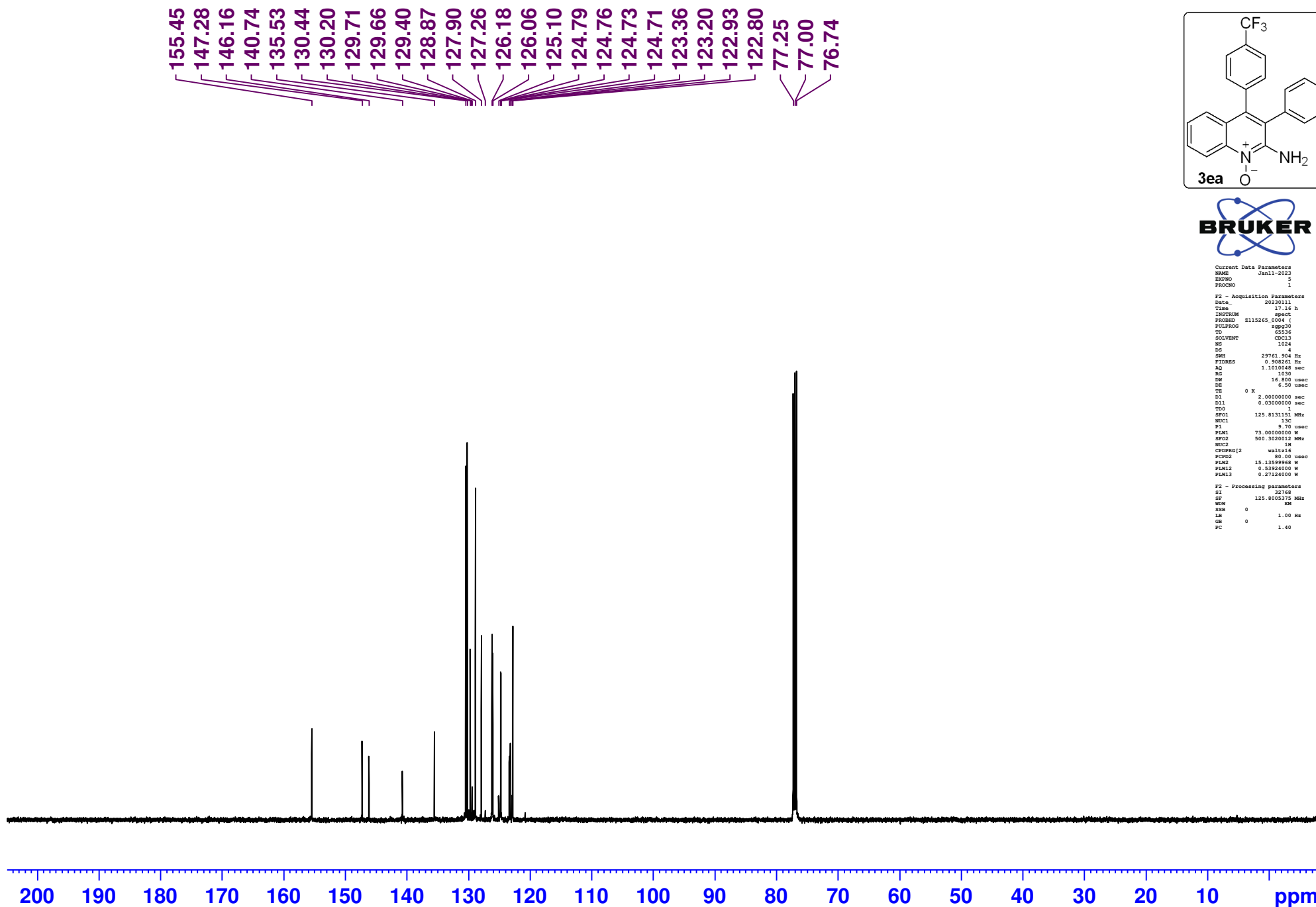
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



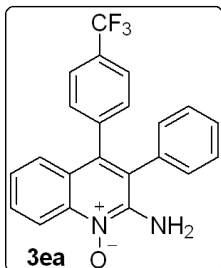
```
Current Data Parameters
NAME      Jan11-2023
EXPNO    5
PROCNO   1

F2 - Acquisition Parameters
Date_    20230111
Time     17:16 h
INSTRUM  spect
PROBHD   1H1269.004 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH       29761.904 Hz
FIDRES    0.998261 Hz
AQ         1.1010048 sec
RG         1030
DW         16.800 usec
DE         6.50 usec
TE         0 K
D1         2.0000000 sec
d11        0.0300000 sec
TDO        1
SFO1       125.811111 MHz
NUC1        13C
P1         73.0000000 usec
PLA1        0.0000000 M
SFO2       500.3020012 MHz
NUC2        1H
CPDPRG2    waltz16
PCPD2      80.00 usec
PLM2       15.1359968 M
PLM12      0.53924000 M
PLM13      0.27154000 M

F2 - Processing parameters
SI         32768
SF         125.800375 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```



^{19}F NMR (471 MHz, CDCl_3)

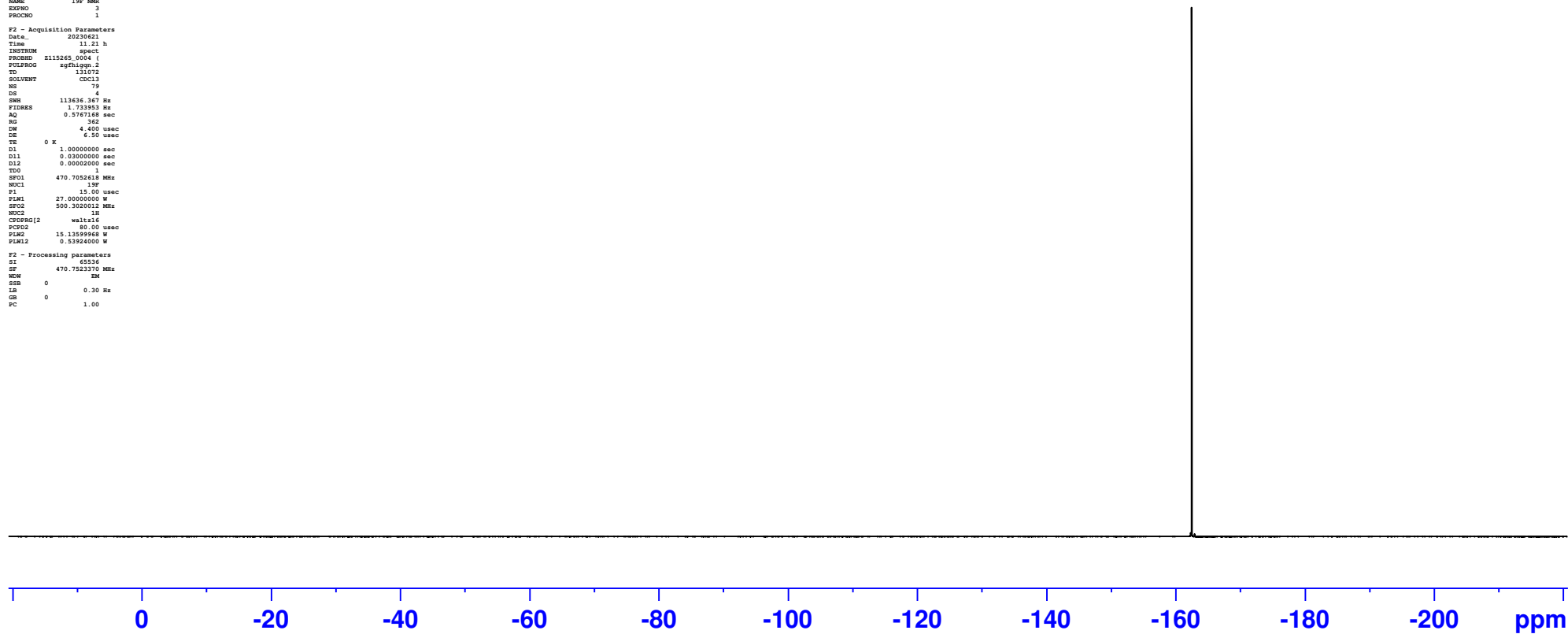


```
Current Data Parameters
NAME      19F NMR
EXPNO    3
PROCNO    1

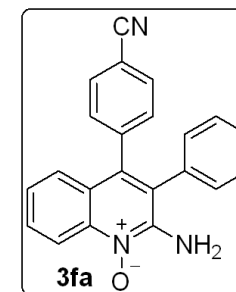
F2 - Acquisition Parameters
Date_     20230621
Time      11:21:31
INSTRUM   spect
PROBHD    E115265_0004 (
PULPROG   zgpg30
TD        131072
SOLVENT   CDCl3
NS        79
DS        4
SWH       113626.367 Hz
FIDRES    1.733953 Hz
AQ        0.5767168 sec
RG        362
DW        4.400 usec
DE        6.50 usec
TE        0 K
D1        1.0000000 sec
D11       0.0300000 sec
D12       0.0000200 sec
TD0       1
SFO1      470.7052618 MHz
NUC1      19F
P1        15.00 usec
PLM1      27.0000000 W
SFO2      500.1350012 MHz
NUC2      1H
CPCPG2    waltz16
PCPD2     80.00 usec
PLM2      15.1359988 W
PLM12     0.5392400 W

F2 - Processing parameters
SI        65536
SF        470.7583370 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```

-162.51



¹H NMR (500 MHz, CDCl₃)

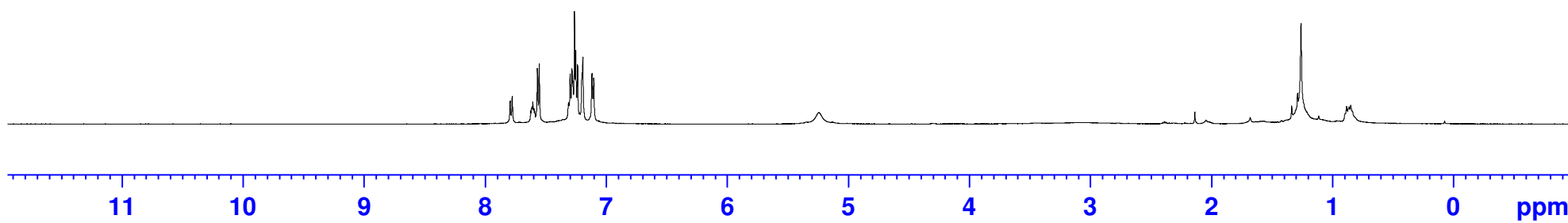


```
Current Data Parameters
NAME          3ha
EXPNO         5
PROCNO        1

F2 - Acquisition Parameters
Date_         20230114
Time          13.06 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767959 sec
RG            287
DW            50.000 usec
DE            6.50 usec
TE            0 K
D1            1.00000000 sec
TD0           1
SF01          500.3030894 MHz
NUC1          1H
P1            15.10 usec
PLM1          15.13559968 W

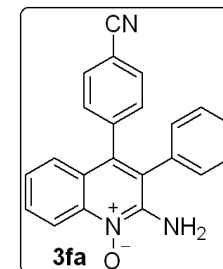
F2 - Processing parameters
SI            65536
SF            500.3000147 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```

7.791
7.774
7.621
7.615
7.611
7.605
7.598
7.595
7.588
7.567
7.550
7.309
7.295
7.281
7.273
7.260
7.250
7.234
7.197
7.190
7.115
7.101
5.241



1.00
1.08
2.04
5.42
1.99
2.04
2.00

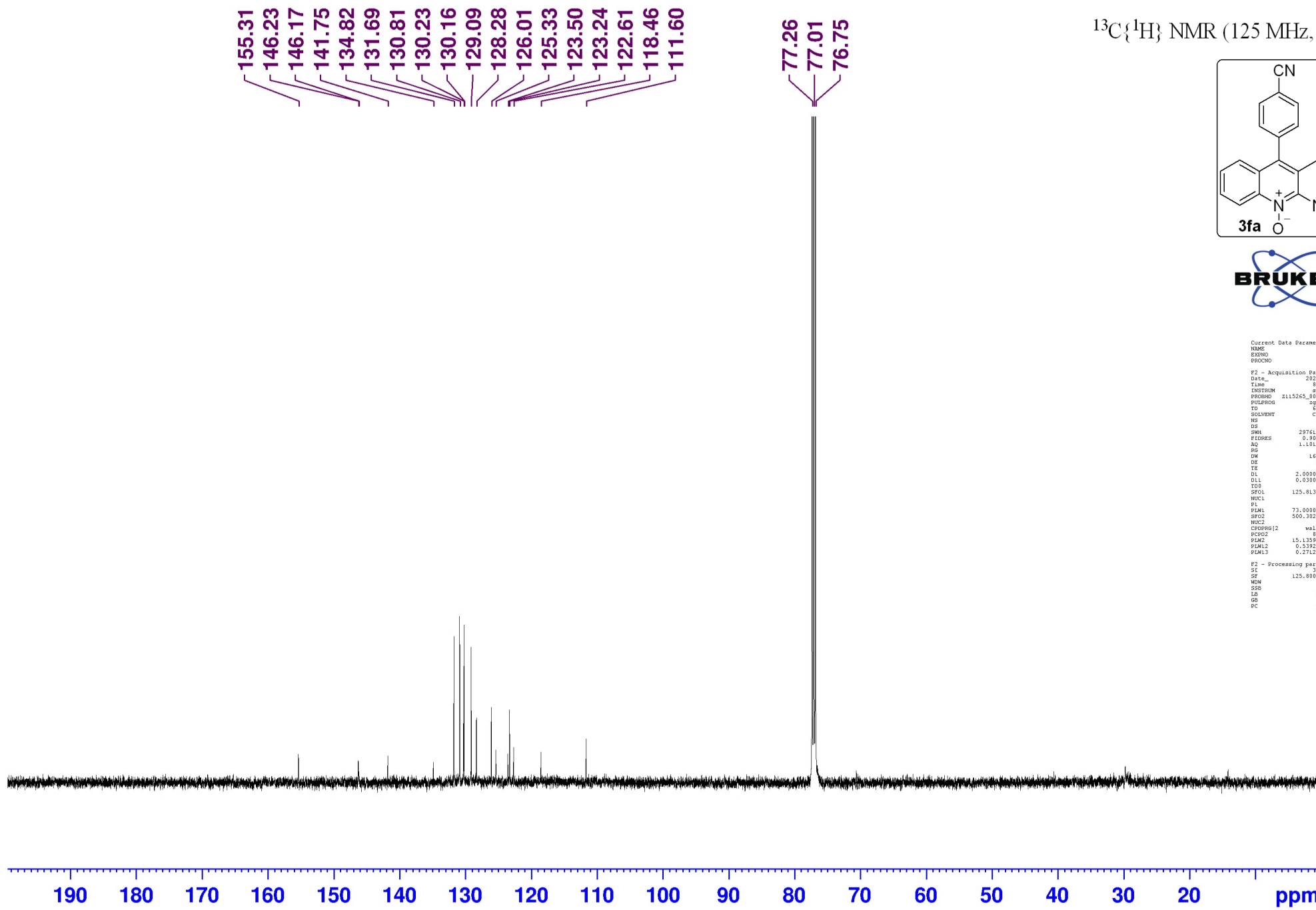
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME      3fa
EXPNO     7
PROCNO    1

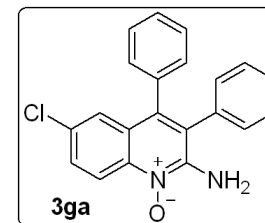
F2 - Acquisition Parameters
Date_     09240219
Time      8.21 h
PROBHD    spect
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         3000
DS         2
SFO1      29761.904 Hz
FIDRES    0.908261 Hz
AQ         1.101048 sec
RG         1030
DM         16.800 usec
DE         6.50 usec
TE         0 K
DQ         2.0000000 sec
DIL        0.03000000 sec
TOP        1
SFO1      125.8131151 MHz
NUC1       13C
PL         9.70 usec
PWL1      73.00000000 M
SFO2      500.1328011 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     80.00 usec
PWL2      15.11539965 M
PWL3      0.53924000 M
PWL4      0.27124000 M

F2 - Processing parameters
SI         32768
SF         125.805336 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```



8.621
8.603
7.659
7.642
7.409
7.298
7.283
7.275
7.267
7.263
7.259
7.141
7.127
7.081
7.075
6.041

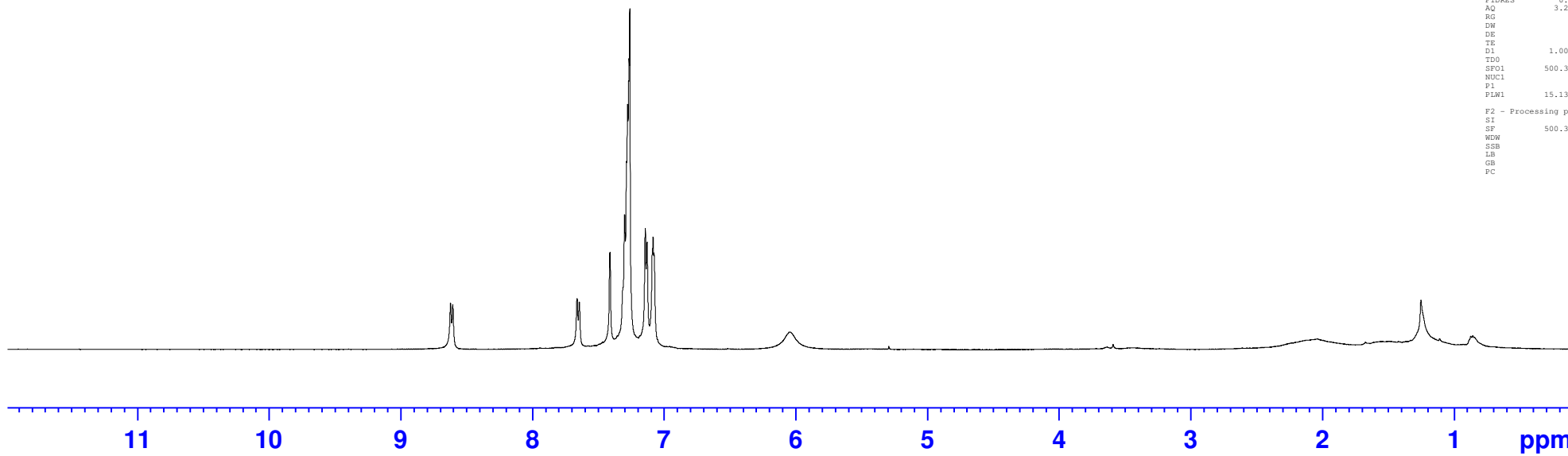
^1H NMR (500 MHz, CDCl_3)



```
Current Data Parameters
NAME      RSJ-638-FINAL
EXPNO     4
PROCNO    1

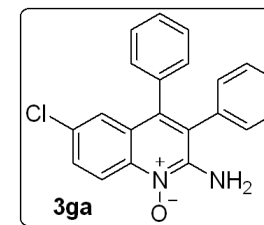
F2 - Acquisition Parameters
Date_     20220808
Time      14.58 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10000.000 Hz
FIDRES    0.305176 Hz
AQ         3.2767999 sec
RG         181
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1      500.3030894 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13599968 W

F2 - Processing parameters
SI         65536
SF         500.3000157 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



1.13
1.25
1.32
6.56
2.32
2.39
1.87

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME          Aug 25-2023
EXPNO        8
PROCNO       1

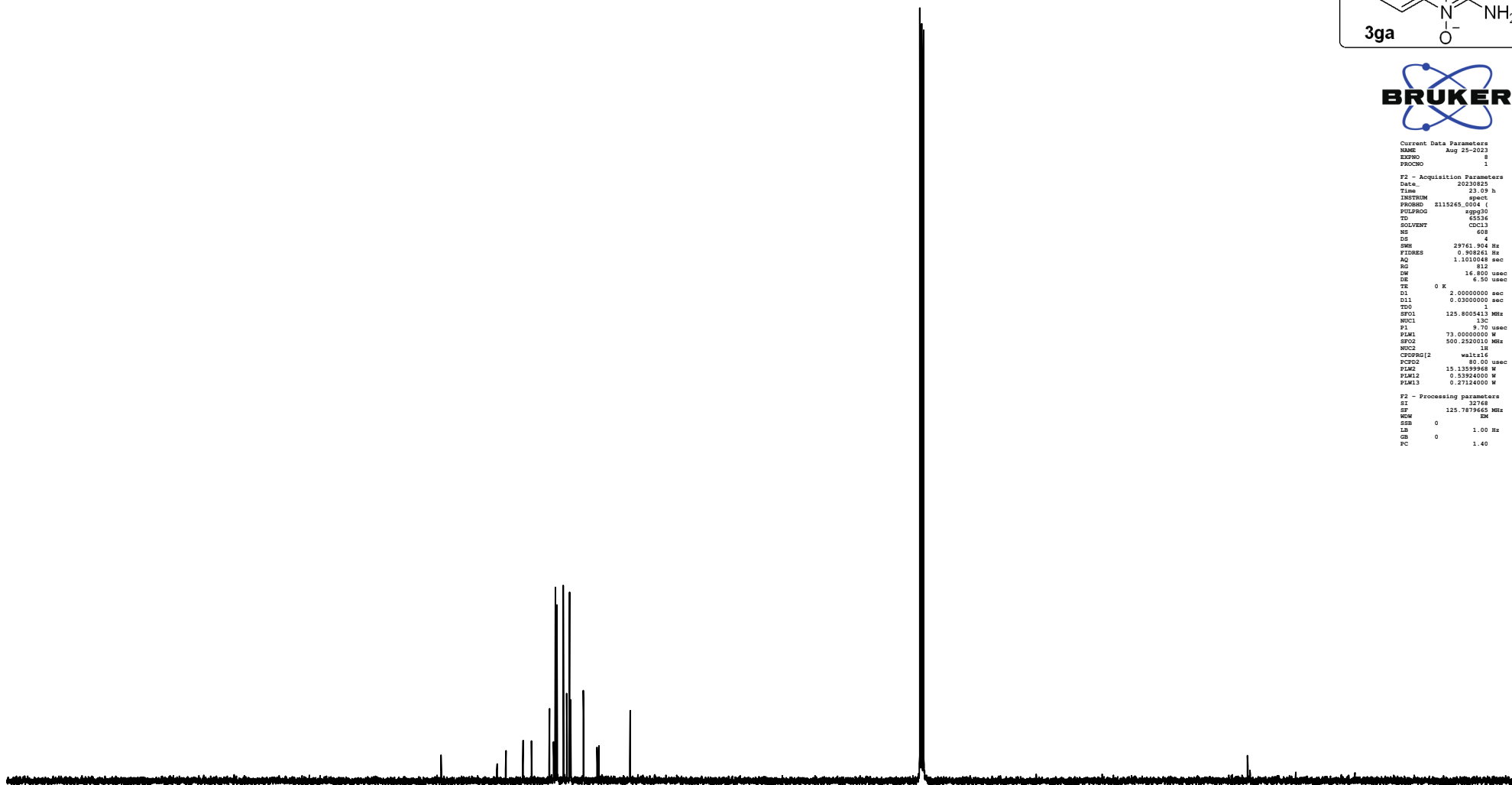
F2 - Acquisition Parameters
Date_        20230825
Time         23.09 h
INSTRUM      spect
PROBHD       5mmBBO
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           608
DS           4
SWH          29761.904 Hz
FIDRES       0.998261 Hz
AQ           1.1010048 sec
RG           812
DSW          16.800 usec
DE           6.50 usec
TE           0 K

D1           2.0000000 sec
D11          0.0300000 sec
TDO          1
SFO1         125.8005413 MHz
NUC1         13C
P1           73.0000000 usec
PLA1         0.27154000 W
SFO2         500.2520010 MHz
NUC2         1H
CPDPRG2      waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27154000 W

F2 - Processing parameters
SI           32768
SF           125.7679665 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
```

146.79
138.66
137.39
134.91
133.67
131.07
130.44
130.20
129.95
129.03
128.53
128.14
127.99
126.11
124.13
123.90
119.35

77.25
76.99
76.74

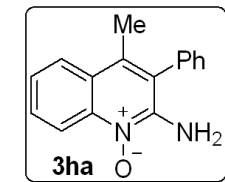


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

8.558
8.540
7.921
7.905
7.759
7.744
7.728
7.568
7.554
7.539
7.512
7.498
7.483
7.471
7.456
7.441
7.311
7.297
7.260
6.227

2.356

¹H NMR (500 MHz, CDCl₃)

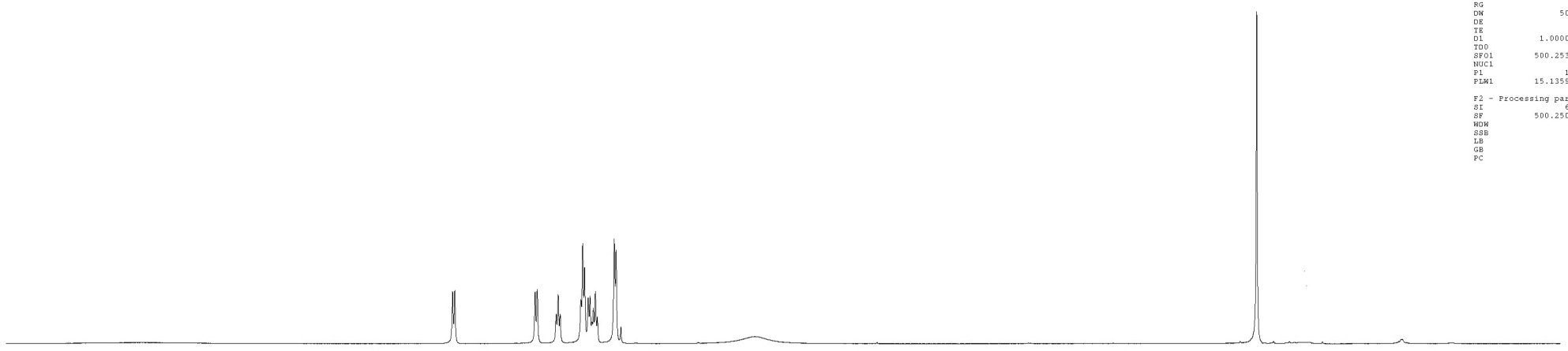


```

Current Data Parameters
NAME      24 MARCH-2024
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20240324
Time      14.54 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         4
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         144
DN         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1       500.2530890 MHz
NUC1       1H
P1         15.10 usec
PLM1       15.13599968 W

F2 - Processing parameters
SI         65536
SF         500.2500146 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



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

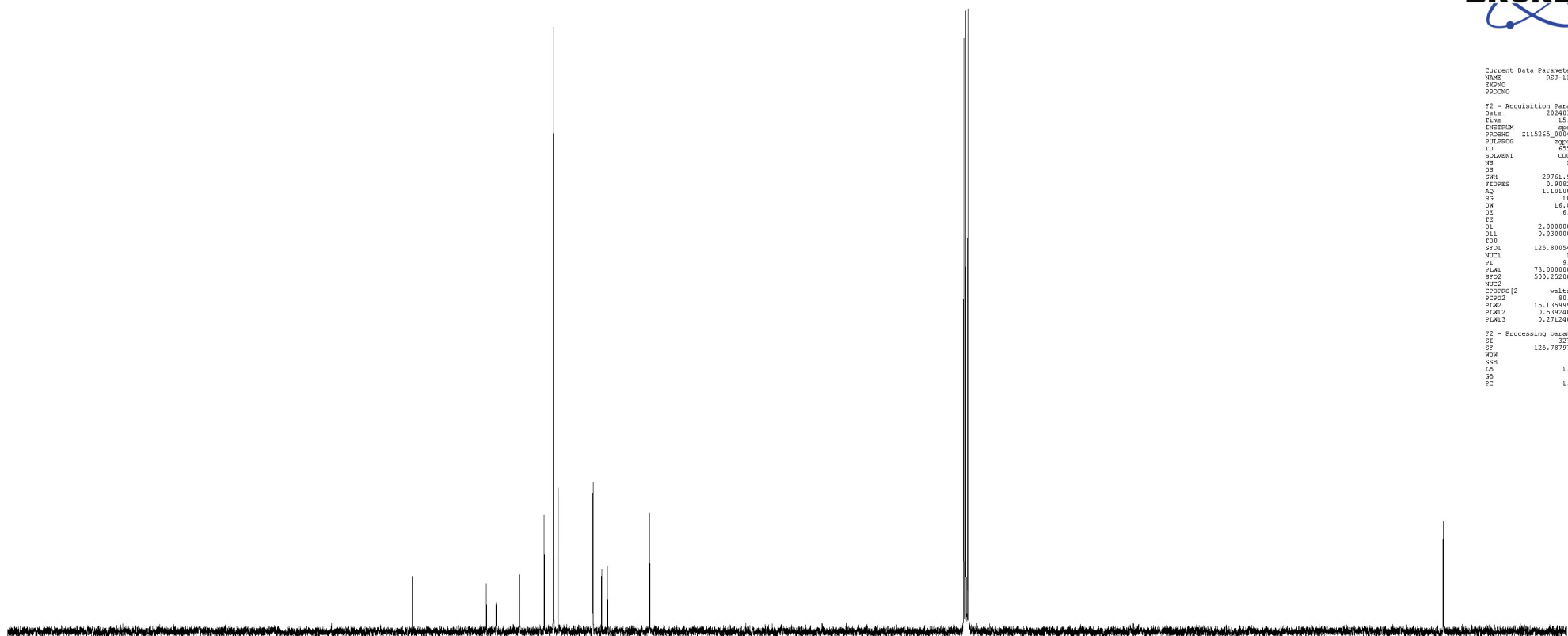
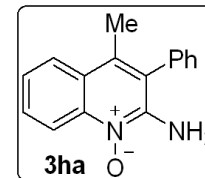
1.17 1.21 1.21 2.38 2.36 2.32 1.90 3.39

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)

147.74
138.30
137.04
134.04
130.90
129.71
129.10
124.70
124.64
123.56
122.81
117.43

77.25
77.00
76.74

15.96



```
Current Data Parameters
NAME      R02-1136
EXPNO     2
PROCNO    1

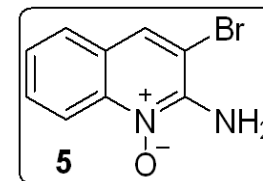
F2 - Acquisition Parameters
Date_     20240324
Time      15.04 h
PROBHD    spect
PULPROG   zgpg30
TD         65536
SOLVENT   cdcl3
NS         140
DS         4
SFO1      29761.904 Hz
FIDRES    0.908261 Hz
AQ         1.1010408 sec
RG         1030
DM         16.900 usec
DE         6.50 usec
TE         0 K
DQ         2.00000000 sec
DLL        0.03000000 sec
TOP
SFO1      125.8005413 MHz
NUC1       13C
PL         9.70 usec
P1M1      73.00000000 M
SFO2      500.1320113 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     80.00 usec
P1M2      15.1359965 M
P1M12     0.53924000 M
P1M13     0.27124000 M

F2 - Processing parameters
SI         32768
SF         125.7879701 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

8.518
8.501
7.935
7.759
7.743
7.727
7.677
7.661
7.454
7.439
7.424
7.260
6.422

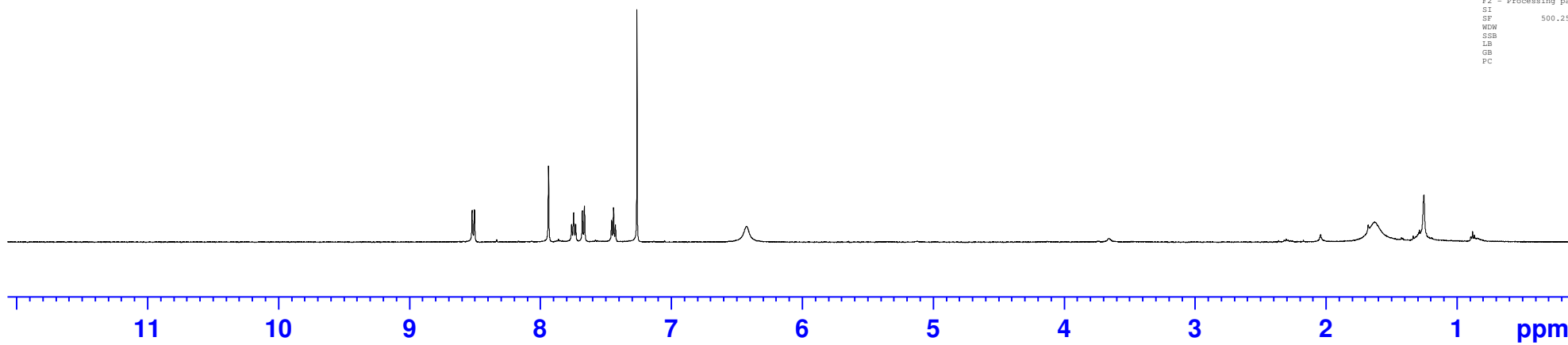
^1H NMR (500 MHz, CDCl_3)



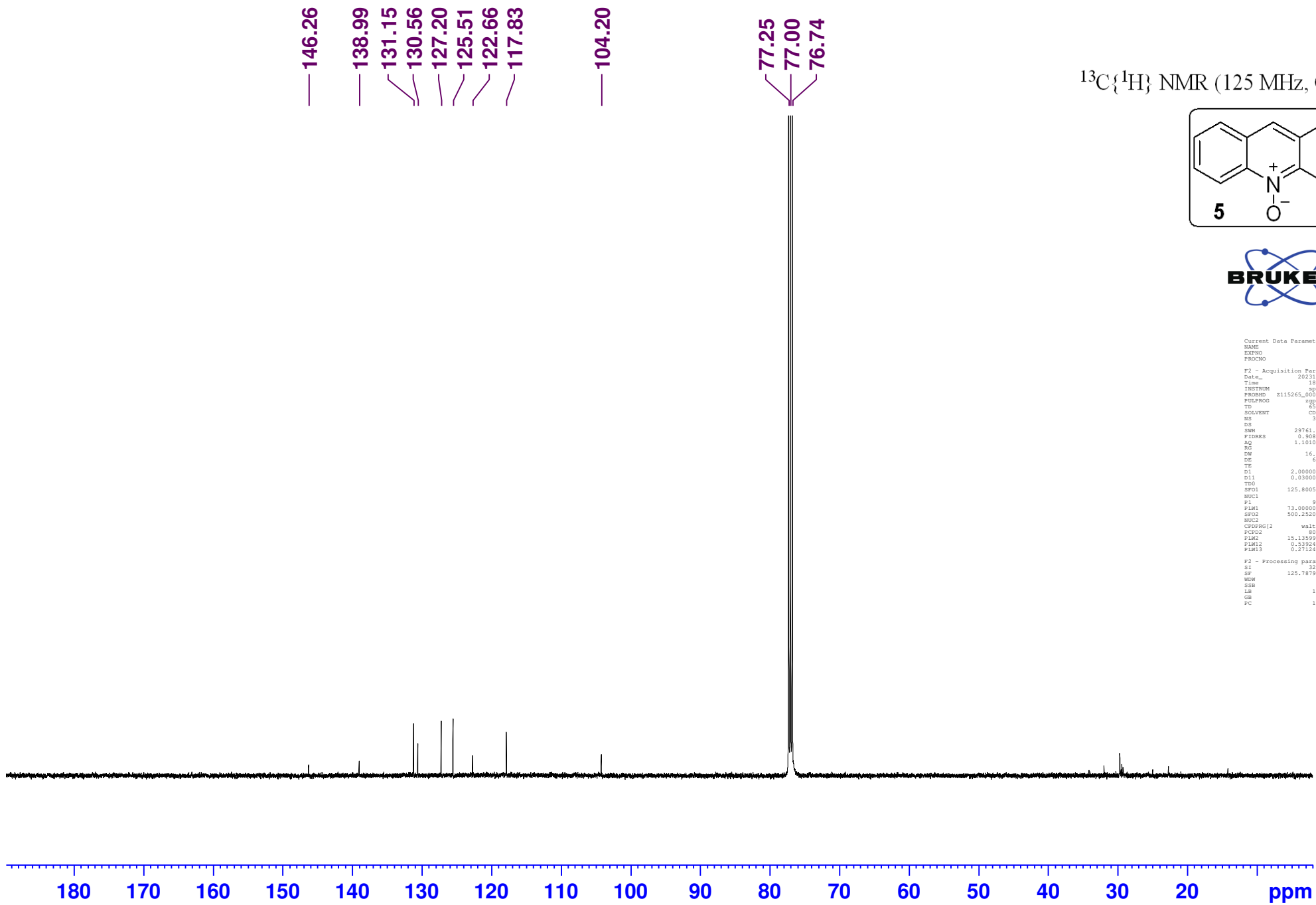
```
Current Data Parameters
NAME          5
EXPNO         3
PROCNO        1

F2 - Acquisition Parameters
Date_         20240119
Time          11.01 h
INSTRUM       spect
PROBHD        Z115265_0004 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767959 sec
RG            322
DW            50.000 usec
DE            6.50 usec
TE            0 K
D1            1.00000000 sec
TDO           1
SF01          500.2530890 MHz
NUC1           1H
P1            15.10 usec
PLM1          15.1359968 W

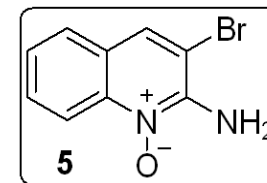
F2 - Processing parameters
SI            65536
SF            500.2500140 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```



1.05
1.05
1.11
1.08
1.11
1.96



$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```

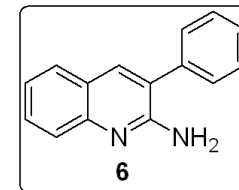
Current Data Parameters
NAME          5
EXPNO        7
PROCNO       1

F2 - Acquisition Parameters
Date_        20231126
Time         18.25 h
INSTRUM      spect
PROBHD       Z115265_0004 (
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           3500
DS           4
SWE          29761.904 Hz
FIDRES       0.908261 Hz
AQ           1.1010048 sec
RG           912
DM           16.800 usec
DE           6.50 usec
TE           0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0          1
SF01         125.8005413 MHz
NUC1         13C
P1           9.70 usec
PLM1         73.00000000 W
SFO2         500.2550010 MHz
NUC2         1H
CPDPRG2      waltz16
PCPD2        80.00 usec
PLM2         15.13599968 W
PLM12        0.53924000 W
PLM13        0.27124000 W

F2 - Processing parameters
SI           32768
SF           125.7879647 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

7.788
7.710
7.693
7.657
7.642
7.585
7.571
7.555
7.539
7.524
7.519
7.504
7.488
7.451
7.437
7.423
7.289
7.275
7.269
7.260
5.048

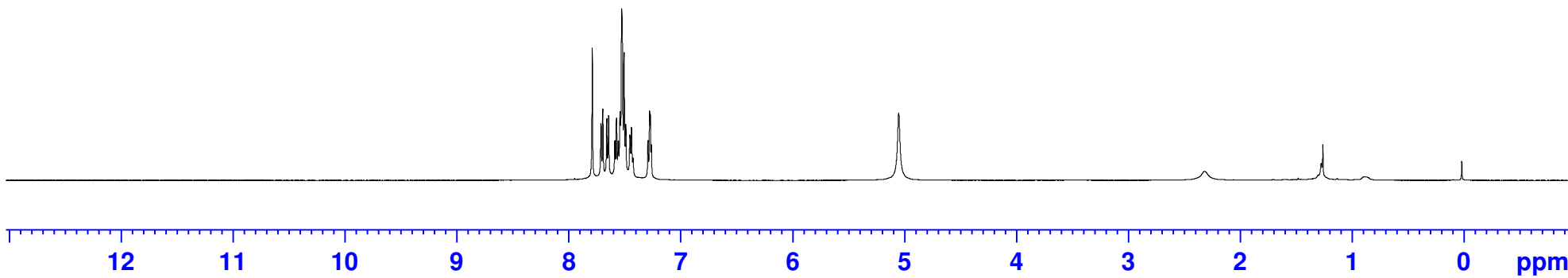
¹H NMR (500 MHz, CDCl₃)



```
Current Data Parameters
NAME      RSJ-642
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20220808
Time      14.36 h
INSTRUM   spect
PROBHD    Z115265_0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         2
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         181
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1      500.3030894 MHz
NUC1       1H
P1         15.10 usec
PL1        15.13599968 W

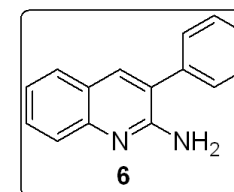
F2 - Processing parameters
SI         65536
SF         500.3000113 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



1.00
0.98
1.08
1.12
3.81
1.01
1.29

2.04

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3)



```
Current Data Parameters
NAME      Aug08-2022
EXPNO    3
PROCNO   1

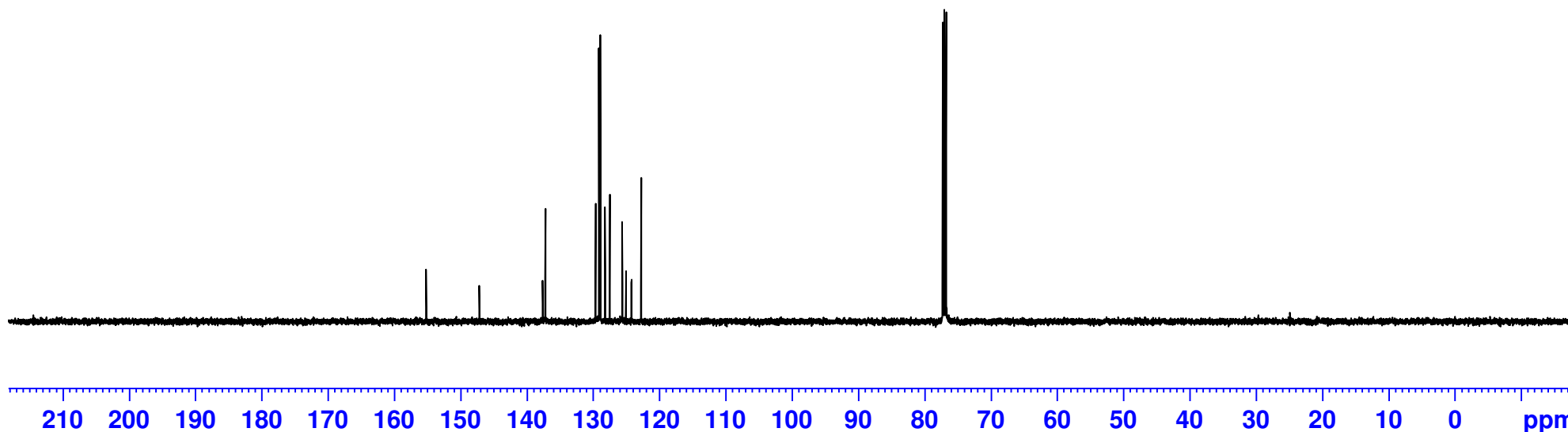
F2 - Acquisition Parameters
Date_    20220808
Time     14:52 h
INSTRUM  spect
PROBHD   5115265.004 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        249
DS        4
SWH       29761.904 Hz
FIDRES    0.998261 Hz
AQ         1.1010048 sec
RG         2050
DW         16.800 usec
DE         6.50 usec
TE        0 K

D1        2.0000000 sec
D11       0.0300000 sec
TDO       1
SFO1      125.811111 MHz
NUC1      13C
P1         9.70 usec
PLA1      73.0000000 dB
SFO2      500.3020012 MHz
NUC2      1H
CPDPRG2   waltz16
PCPD2     80.00 usec
PLM2      15.13599968 dB
PLM12     0.53924000 dB
PLM13     0.27154000 dB

F2 - Processing parameters
SI         32768
SF         125.8005411 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

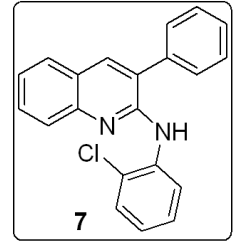
155.19
147.18
137.61
137.20
129.62
129.13
128.89
128.20
127.48
125.61
125.02
124.22
122.76

77.25
77.00
76.74



¹H NMR (500 MHz, DMSO-d₆)

9.039
9.025
9.022
8.103
7.867
7.853
7.803
7.787
7.674
7.672
7.660
7.657
7.653
7.644
7.641
7.636
7.621
7.606
7.571
7.568
7.565
7.558
7.554
7.543
7.540
7.537
7.446
7.443
7.430
7.427
7.414
7.399
7.385
7.383
7.042
7.039
7.026
7.024
7.011
7.008
3.415
2.500



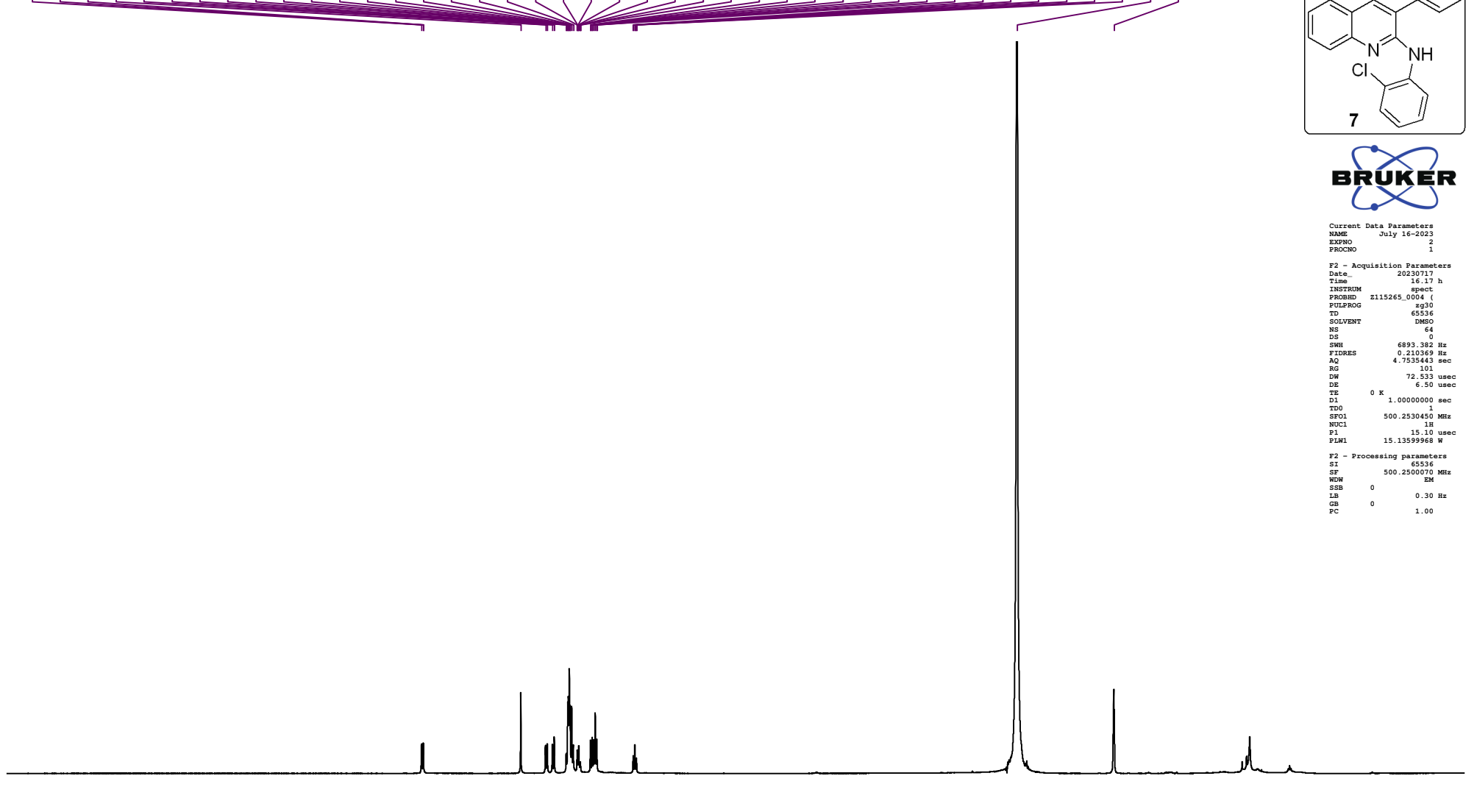
Current Data Parameters
NAME July 16-2023
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230717
Time 16:17 h
INSTRUM spect
PROBHD Z115265_0004 (1930
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 0
SWH 6893.382 Hz
FIDRES 0.210369 Hz
AQ 4.7535443 sec
RG 101
DW 72.533 usec
DE 6.50 usec
TE 0 K
DI 1.00000000 sec
TDO 1
SFO1 500.2530450 MHz
NUC1 1H
F1 15.10 usec
PLM1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.2500070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

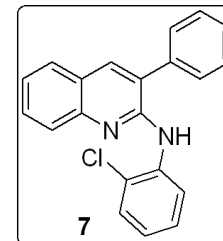
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

1.01
1.00
1.00
1.03
5.32
1.12
1.03
2.11
1.03



150.65
145.91
137.15
136.73
136.11
129.89
129.53
129.27
129.00
128.85
127.86
127.81
126.53
126.41
124.16
123.89
122.82
121.98
120.44

40.02
39.85
39.68
39.51
39.35
39.18
39.01

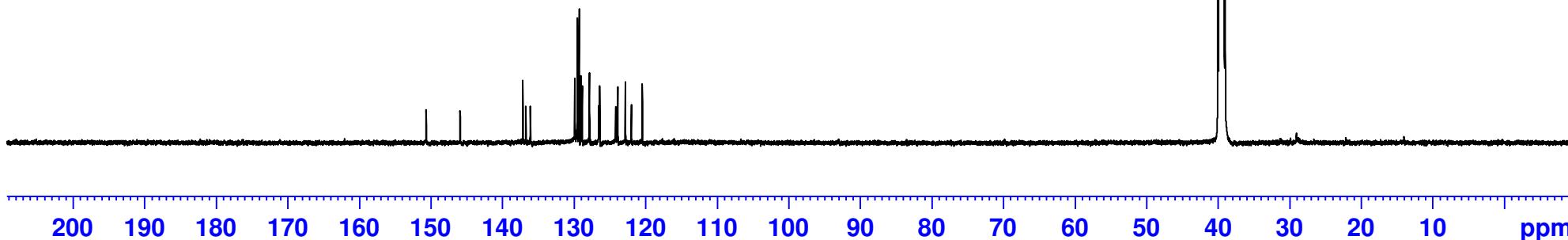


```
Current Data Parameters
NAME      July 16-2023
EXPNO    4
PROCNO   1

F2 - Acquisition Parameters
Date_    20230718
Time     7.20 h
INSTRUM  spect
PROBHD   1H125AS.004 (
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        10000
DS        4
SWH       29761.904 Hz
FIDRES    0.398261 Hz
AQ        1.1010048 sec
RG         1030
DW         16.800 usec
DE         6.50 usec
TE        0 K

D1        2.0000000 sec
D11       0.0300000 sec
TDO       1
SFO1      125.8005413 MHz
NUC1       13C
P1         73.0000000 usec
PLA1      0.0000000 M
SFO2      500.2520010 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     80.00 usec
PLM2      15.13599968 M
PLM12     0.53924000 M
PLM13     0.27124000 M

F2 - Processing parameters
SI         32768
SF         125.780199 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

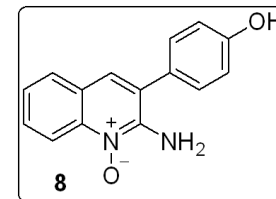


8.302
8.285
7.888
7.873
7.703
7.687
7.670
7.663
7.425
7.404
7.387
6.982
6.936
6.919

3.430

2.500

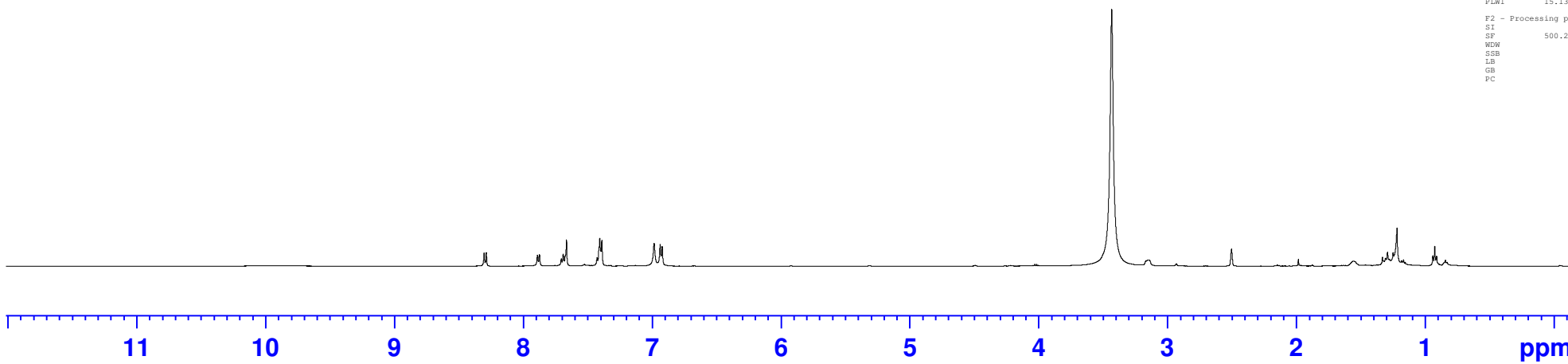
^1H NMR (500 MHz, DMSO- d_6)



Current Data Parameters
NAME 8
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230821
Time 12.42 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 80.6
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.0000000 sec
TDO 1
SFO1 500.2530890 MHz
NUC1 1H
P1 15.10 usec
PL1 15.1359968 W

F2 - Processing parameters
SI 65536
SF 500.2500068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

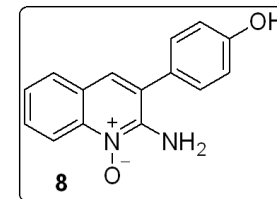


1.03
1.09
2.22
3.18
2.00
2.09

$^{13}\text{C} \{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6)

— 157.91
— 146.94
138.01
129.91
128.30
126.42
126.21
124.43
124.14
122.35
116.76
115.94

40.02
39.85
39.69
39.52
39.35
39.18
39.02



```
Current Data Parameters
NAME      8
EXPNO    4
PROCNO   1

F2 - Acquisition Parameters
Date_    2023081
Time     13.39 h
INSTRUM  spect
PROBHD   Z115265_0004 (
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       1024
DS       4
SWE      29761.904 Hz
FIDRES   0.998261 Hz
AQ       1.1010048 sec
RG       1030
DM       16.800 usec
DE       6.50 usec
TE       0 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1
SFO1     125.8005413 MHz
NUC1     13C
P1       9.70 usec
PLW1     73.0000000 W
SFO2     500.2550010 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLW2     15.13599968 W
PLW12    0.53924000 W
PLW13    0.27124000 W

F2 - Processing parameters
SI       32768
SF       125.7980162 MHz
RG       64
SBB      0
LB       1.00 Hz
GB       0
PC       1.40
```

