Supporting Information

Testing the Limits of Radical-Anionic CH-Amination: a 10-Million-Fold Decrease in Basicity Opens a New Path to Hydroxyisoindolines via a Mixed C-N/C-O-Forming Cascade

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1) General information

Unless otherwise noted, all ^{1}H NMRs were run on BRUKER AV 400 MHz, BRUKER AV 500 MHz, or BRUKER AV 600 MHz spectrometer at 298 K. Proton chemical shifts are given relative to the residual proton signal of $CDCl_3$ (7.26 ppm), DMSO (2.50 ppm), CD_3CN (1.94 ppm), CD_3OD (4.78, 3.31 ppm), $(CD_3)_2CO$ (2.05 ppm). Carbon chemical shifts were internally referenced to $CDCl_3$ (77.23 ppm), DMSO (39.51 ppm), CD_3CN (118.69, 1.39 ppm), CD_3OD (49.15 ppm), $(CD_3)_2CO$ (206.26, 29.84 ppm) signal. Data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, and m = multiplet), coupling constant (Hz), and integration. High resolution mass spectra (HRMS) were obtained on an Agilent 6200 Series TOF.

Materials: Acetonitrile, benzene, diethyl-ether, dichloromethane, DMF, toluene and tetrahydrofuran (THF) were obtained from a SPS-4 Solvent Purification System. Hexanes for column chromatography and preparatory thin layer chromatography were distilled prior to use. All other solvents were used as purchased. Unless otherwise specified, all reagents were used as is from suppliers without further purification. Column chromatography was performed using silica gel (60 Å) and preparatory thin layer chromatography was performed using a 1000 μm glass backed plate containing UV dye. All TLC analysis was visualized by UV light (254 nm). $AlCl_3$ was purchased from AlfaAesar and freshly sublimed before use. $Pd(PPh_3)_4$ was purchased from SigmaAldrich and stored under Ar at -25°C.

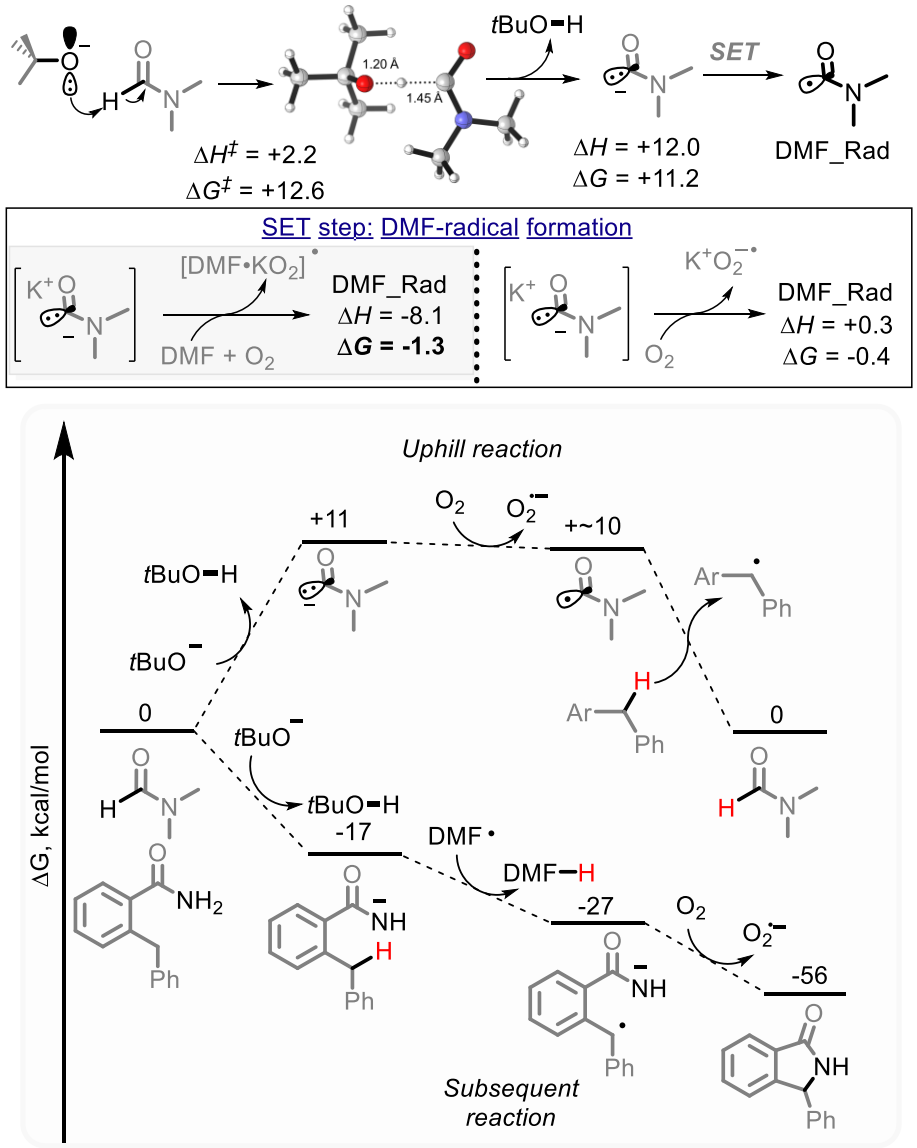
2) Thermodynamic Data

2a) Generation of DMF radical

We suggest that the chemical species responsible for the formation of the bis-benzylic C-centered radical to be $C(O)N(CH_3)_2$ radical, which is generated from DMF. While we were unable to find the p*K*a of *t*-BuOH in DMF, literature reports[1] the p*K*a 1-butanol in DMF to be 33.3. It is reasonable to estimate the p*K*a of *t*-BuOH in DMF to be ca. 34-35. The p*K*a of DMF in DMF was found to be 38[1], making DMF approximately 3-4 pKa units less acid than *t*-BuOH. Although this makes the initial deprotonation of H-C(O)NMe_2 uphill, a small amount of DMF anion can be formed at the equilibrium. Calculations show that, although the deprotonation is endergonic by 11.2 kcal/mol, the activation barrier for deprotonation of DMF is relatively low (12.6 kcal/mol, Scheme 9).

Drapeau and co-workers noted the formamide proton shift, via ^1H and ^{13}C NMR when *t*-BuOK was added to wet DMF-d_7.[2] Their computational work additionally highlighted two interesting points regarding the impact of counter ions. First, the cation stabilizes the DMF anion, assisting in deprotonation. Second, a cation of a certain size (i.e., Li) can stabilize the DMF anion and increase the barrier for its oxidation to the DMF radical.[2] Our experimental results also suggest that reaction is slow in the presence of Na and, to a greater extent, Li counterions (Table 1, Entry 1, 7-10).

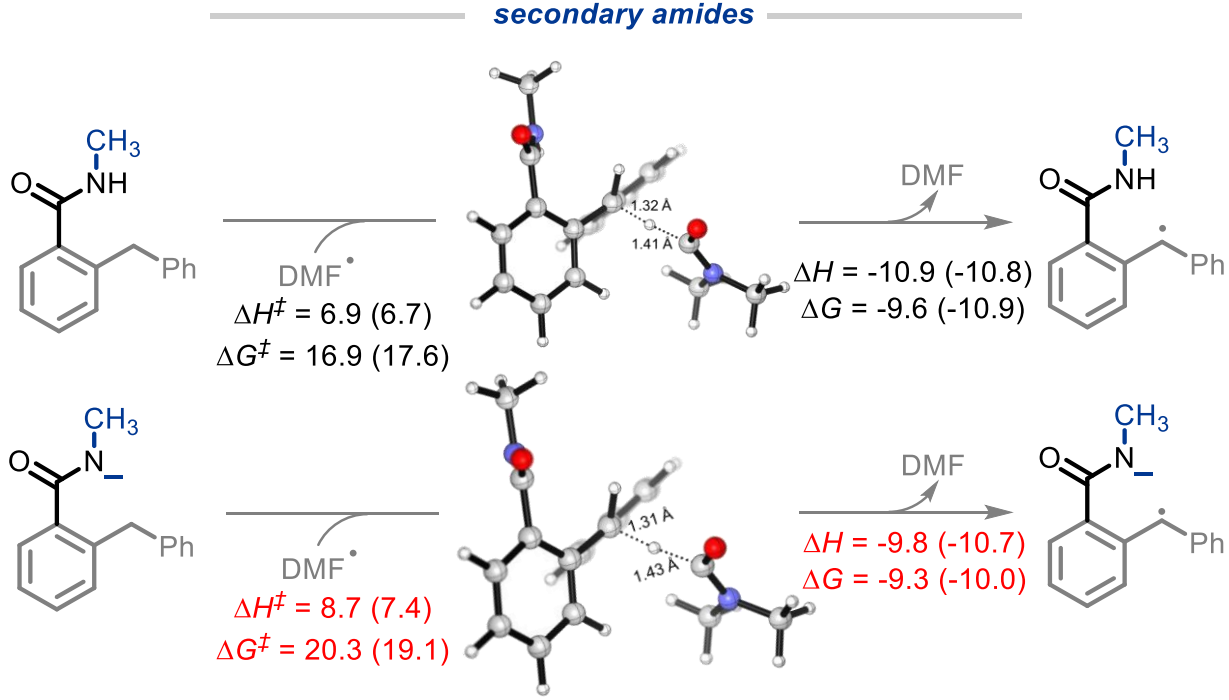
Our calculations show that the oxidation of DMF anion by oxygen is slightly exergonic (with the inclusion of K^+). This makes the combined deprotonation and oxidation of DMF endergonic by ~10 kcal/mol, which would allow only small quantities of DMF radical to be present at a given time. If the propagation step of the cascade is fast, then the initial penalty of forming the DMF radical is a small price to pay when all sequential steps in the cascade reactions are favorable and efficient. Overall, the generation of DMF radical imposes a ~10kcal/mol penalty needed to initiate an otherwise exergonic sequence. Interestingly, calculations suggest that the activation barrier for proton abstraction from DMF is almost entirely entropic (enthalpy of activation is only 2.2 kcal/mol). The TS Gibbs energy (12.6 kcal/mol) is only 1.4 kcal/mol higher than the Gibbs energy of the product, suggesting that the deprotonation should be rapidly reversible.



Scheme S1. Gibbs energy changes associated with the DMF and amide deprotonation, radical formation from DMF and with the C-N bond forming process; all energies in kcal/mol.

2b) Secondary amide HAT

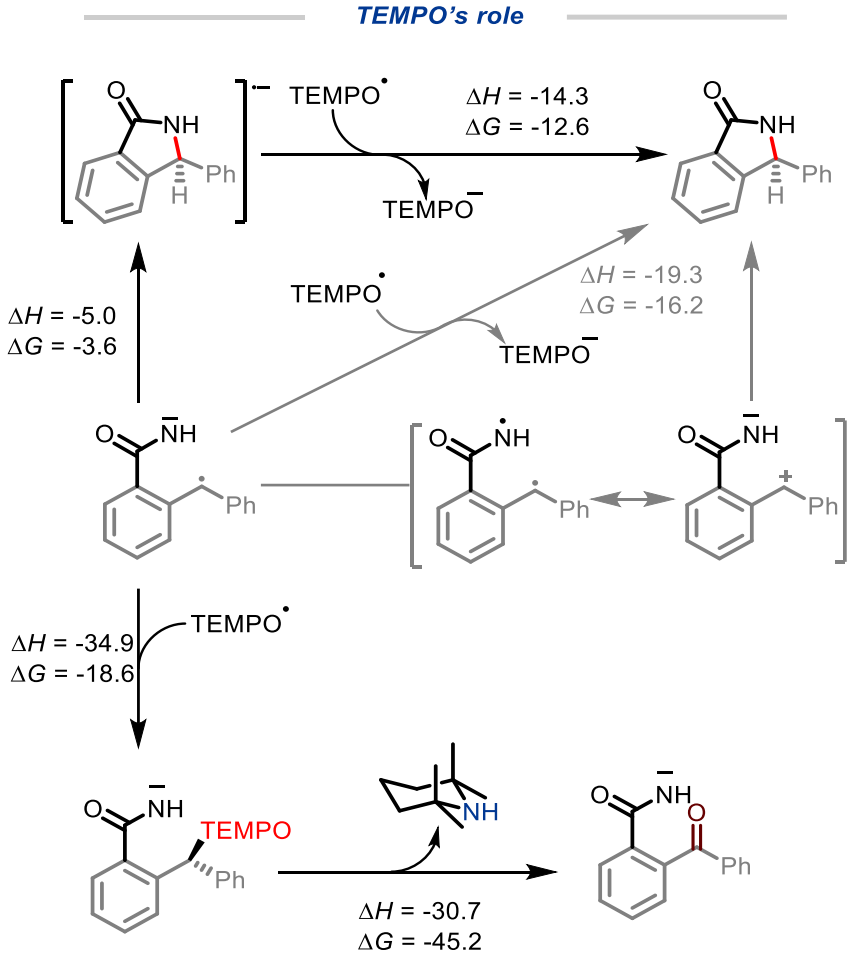
Since we get back the unreacted starting material, the reaction is stalling out in the initial stages of the cascade. Yet our calculations find that each of the three initiation steps, i.e., the deprotonation (ΔG = -16.0), HAT (ΔG = -9.3), and the radical-anion cyclization (ΔG = -5.9), for **1r** are thermodynamically favorable. Our analysis suggests that the barrier for the H-abstraction is about 1.2 kcal/mol higher for the secondary amides than it is for the primary amides. Such difference in the barrier should correspond to a ca. 10-fold rate decrease for this step, providing a possible explanation for the low reactivity of the secondary amide substrates under the reaction conditions.



Scheme S2. Thermodynamics for HAT of amide **1r**. Numbers in parenthesis are for primary amide **1a**. All energies reported in kcal/mol.

2c) Oxidation via TEMPO

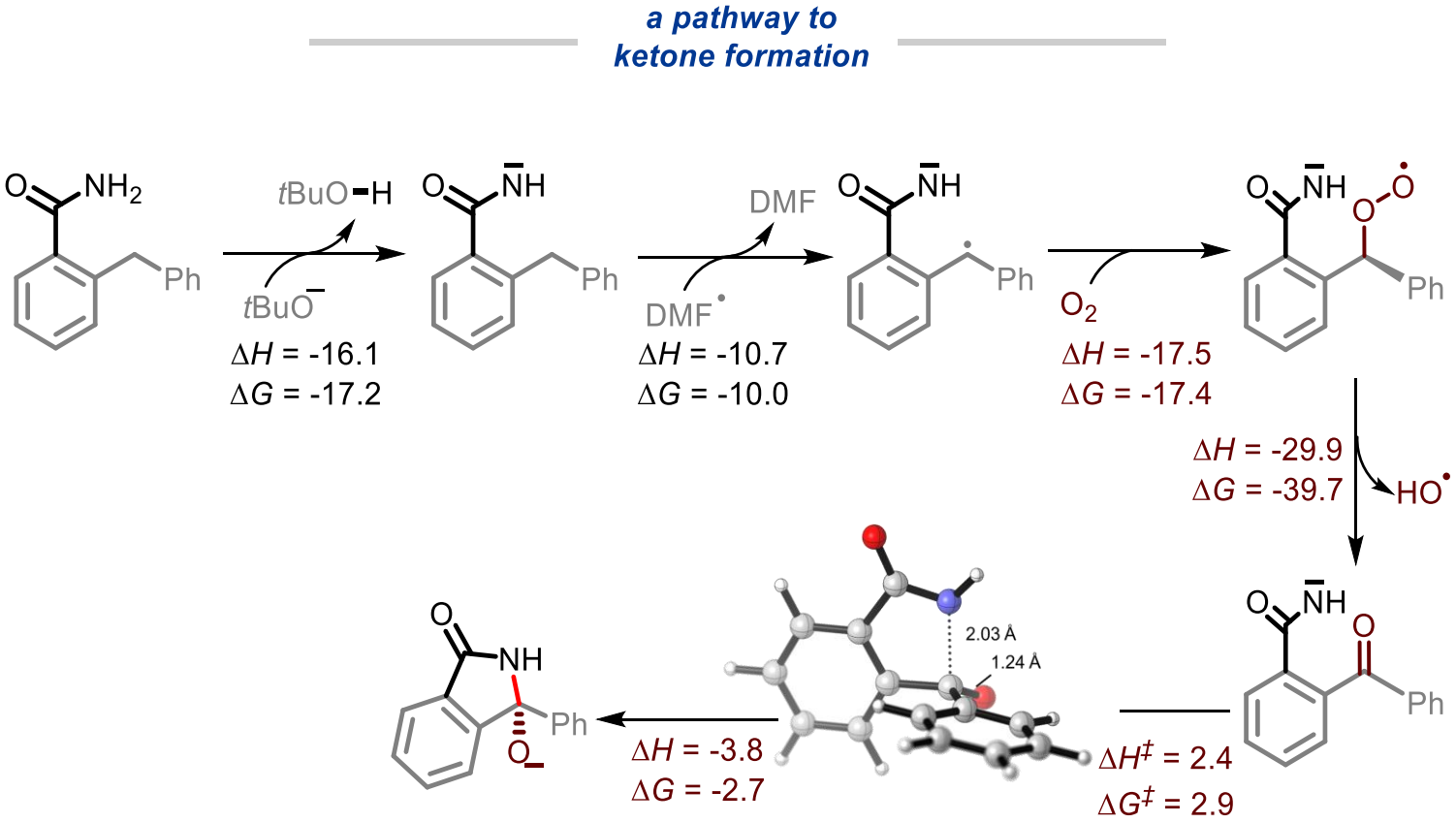
While exploring the potential roles of TEMPO, we considered that it may be used as an oxidant. If the radical anion intermediate were to form *in situ*, oxidation via TEMPO is possible (ΔG = -16.2 kcal/mol) according to the calculations



Scheme S3. Thermodynamics for the oxidation of **1a** via TEMPO into the initial cyclic intermediate. All energies reported in kcal/mol.

2d) Formation of a ketone intermediate

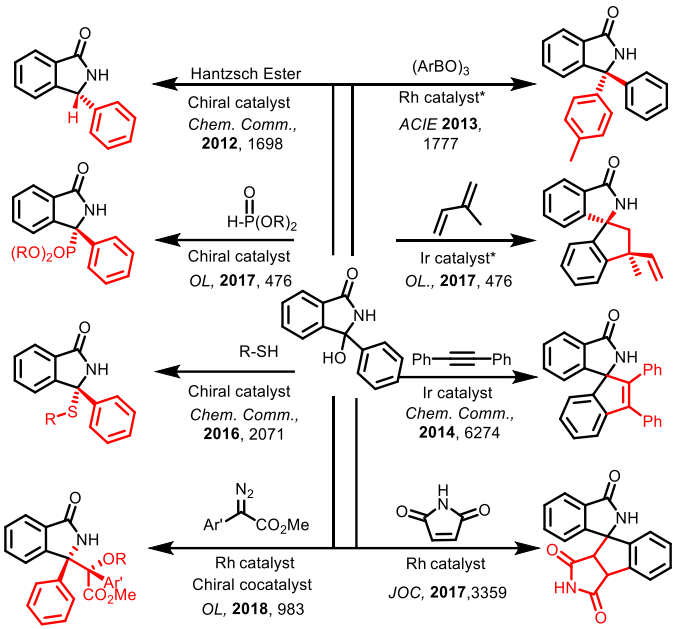
While exploring possible pathways for the formation of our cyclic product, we considered the formation of a ketone intermediate. Our calculations show that formation and cyclization of a ketone intermediate is favorable. However, an intramolecular cyclization followed by oxidation with O_2 will likely occure before an intermolecular addition of O_2.



Scheme S4. Thermodynamics of **1a** for the formation of a ketone intermediate. All energies reported in kcal/mol.

2e) Post Synthetic Modifications

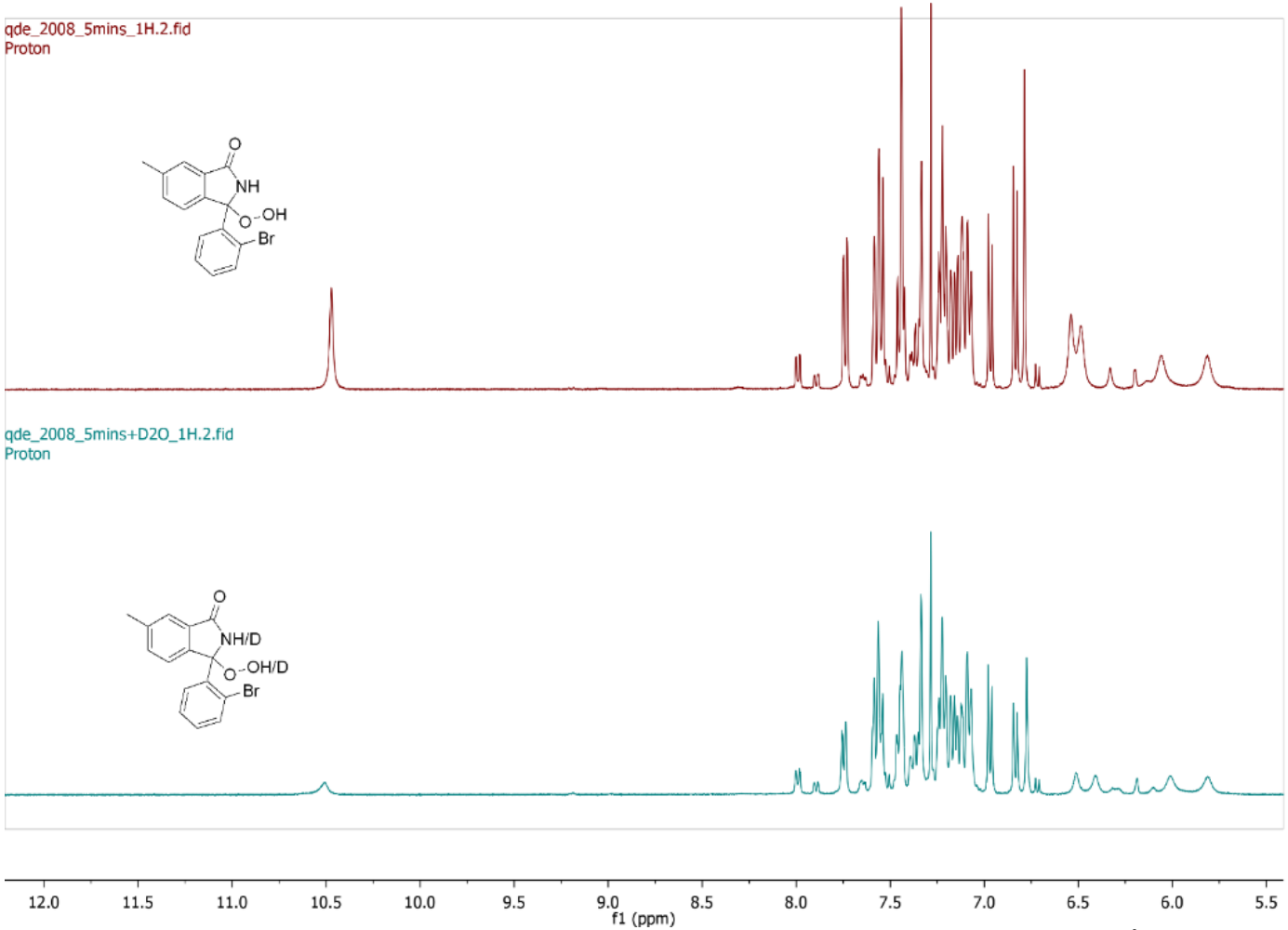
A variety of post-synthetic modifications of the core hydroxyisoindoline structure are possible including enantioselective transformations mediated by chiral phosphoric acids.[3-4] Transition metal catalysis was also utilized for making chiral isoindolinones and spiroisoindolinones.[5]



Scheme S5. Post-synthetic modifications for 3-hydroxyisoindolinone.

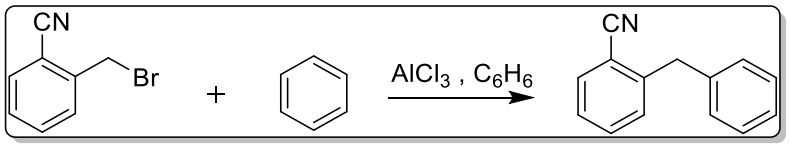
3) Experimental Details

3a) Hydroperoxide crude reaction mixture

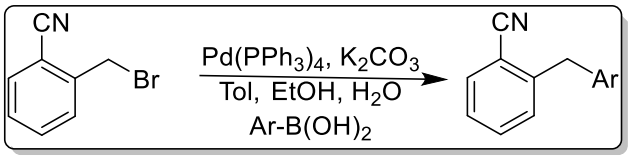


Scheme S6. To a 10 mL round bottom flask charged was a stir bar was added **1p** (20 mg, 0.0657 mmol), 4Å MS, DMF (2.6 mL), and *t*BuOK (3 eq). After 10 mins the reaction was quenched with NH_4Cl and worked up with EtOAc, the organic layers were collected and dried over Na_2SO_4. Top: Crude spectra with hydroperoxide signal at ~10.5ppm. Bottom: after addition of D_2O to the crude sample.

3b) Procedures, spectral data and copies of NMR's for amide precursors



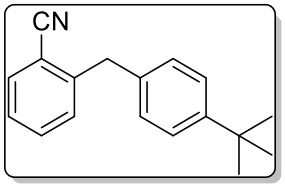
2-benzylbenzonitrile: To a flask charged with a stir bar and $AlCl_3$ (1.364 g, 10.2 mmol) in 12 mL of dry benzene was added 2-(bromomethyl)-1-benzonitrile (1 g, 5.1 mmol) in an ice bath. The reaction mixture was warmed to room temp and then heated to reflux for 45 mins. When all the starting material were consumed as monitored by TLC, the rxn mixture was cooled to room temp and poured into ice and then acidified with 1 N HCl. The organic materials were extracted with CH_2Cl_2. The combined organic extracts were washed with H_2O then brine and dried over $MgSO_4$. The solvents were removed under reduced pressure and purified by column chromatography (10% EtOAc/90% Hex) to afford the desired product (553 mg, 2.86 mmol) in 71% yield.[1] ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 (d, *J* = 7.7 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.24 – 7.19 (m, 2H), 7.18 (d, *J* = 3.0 Hz, 1H), 7.15 (d, *J* = 7.0 Hz, 4H), 4.09 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.93, 138.83, 132.95, 132.89, 130.07, 128.99, 128.75, 128.36, 126.84, 126.74, 118.25, 112.51, 40.18. Spectra data matched those previously reported.[6]



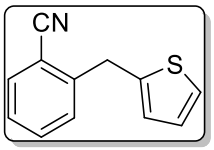
General Procedure 1:

To a two-neck round bottom flask equipped with a magnetic stirring bar and reflux condenser was charged with 2-(bromomethyl)benzonitrile (150 mg, 765 mmol), aryl boronic acid (1.5 eq), K_2CO_3 (4 eq), toluene (5 mL), EtOH (2 mL), H_2O (1 mL). The solution was allowed to stir during outgassing with argon for 30 mins. The outlet needle was removed and the solution was kept under inert atmosphere for the remainder of the reaction. $Pd(PPh_3)_4$ (4 mol %) was then added to the solution and the reaction was allowed to stir at reflux for 8 hours. Upon completion, the mixture was diluted with ethyl acetate (10 mL) and H_2O (5 mL) and added to a separatory funnel. The aqueous solution was extracted with EtOAc (1 x 15 mL). The organic layer was collected and washed with

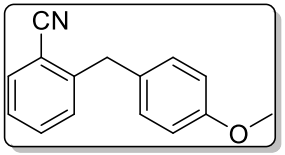
H_2O (2 x 10 mL) and brine (1 x 20 mL). The organic layer was collected and dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was then subjected to column chromatography, with hexanes as the eluent, to afford the desired product.



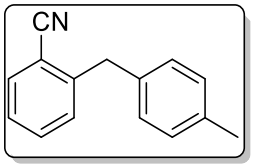
2-(4-(tert-butyl)Benzyl)benzonitrile: Following **general procedure 1** with 2-(Bromomethyl)benzonitrile and (4-(tertbutyl)phenyl)boronic acid provided the desired compound in 190 mg (yield 99%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.64 (d, *J* = 7.7 Hz, 1H), 7.52 (t, *J* = 8.3 Hz, 1H), 7.40 (d, *J* = 8.3 Hz, 2H), 7.32 (dd, *J* = 17.5, 7.7 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 4.23 (s, 2H), 1.37 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 149.50, 145.19, 135.80, 132.93, 132.85, 130.10, 128.64, 126.76, 125.65, 118.30, 112.51, 39.72, 34.43, 31.40. Spectra matches those previously reported. [7]



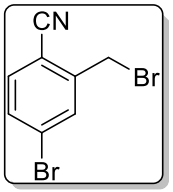
2-(thiophene-2-ylmethyl)benzonitrile: Following **general procedure 1** with 2-(Bromomethyl)benzonitrile and 2-thienylboronic acid provided the desired compound in 145 mg (yield 95%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.63 (d, *J* = 8.9 Hz, 1H), 7.53 (t, *J* = 7.7 Hz, 1H), 7.37 (d, *J* = 7.4 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 6.4 Hz, 1H), 6.95 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.92 (d, *J* = 3.4 Hz, 1H), 4.39 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.12, 141.07, 133.12, 132.93, 129.80, 127.23, 127.10, 126.16, 124.69, 117.88, 112.26, 34.40. [M+H] 200.0456, found 200.0528.



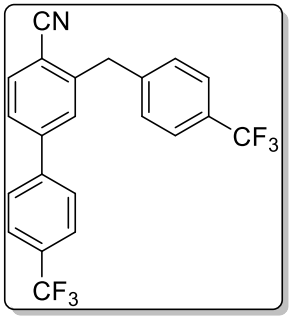
2-(4-methoxybenzyl)benzonitrile: Following **general procedure 1** with 2-(Bromomethyl)benzonitrile and (4-methoxyphenol)boronic acid provided the desired compound in 182 mg (yield 99%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 (d, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 8.3 Hz, 1H), 7.30 – 7.24 (m, 1H), 7.18 (d, *J* = 8.7 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 4.14 (s, 2H), 3.77 (s,2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.41, 145.47, 132.97, 132.90 , 130.93, 130.01, 129.97, 126.76, 118.31, 114.14, 112.38, 55.24, 39.37. Spectra matched those previously reported.[6]



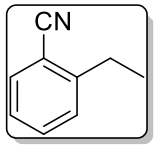
2-(4-methylbenzyl)benzonitrile: Following **general procedure 1** with 2-(Bromomethyl)benzonitrile and (4-methylphenol)boronic acid provided the desired compound in 279 mg (yield 98%). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.63 (d, *J* = 7.0 Hz, 1H), 7.48 (s, 1H), 7.32 – 7.24 (m, 2H), 7.12 (s, 4H), 4.17 (s, 2H), 2.32 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 145.32, 136.31, 135.78, 132.90, 132.87, 130.00, 129.42, 128.88, 126.71, 118.23, 112.53, 39.81, 21.04. Spectra matched those previously reported.[6]



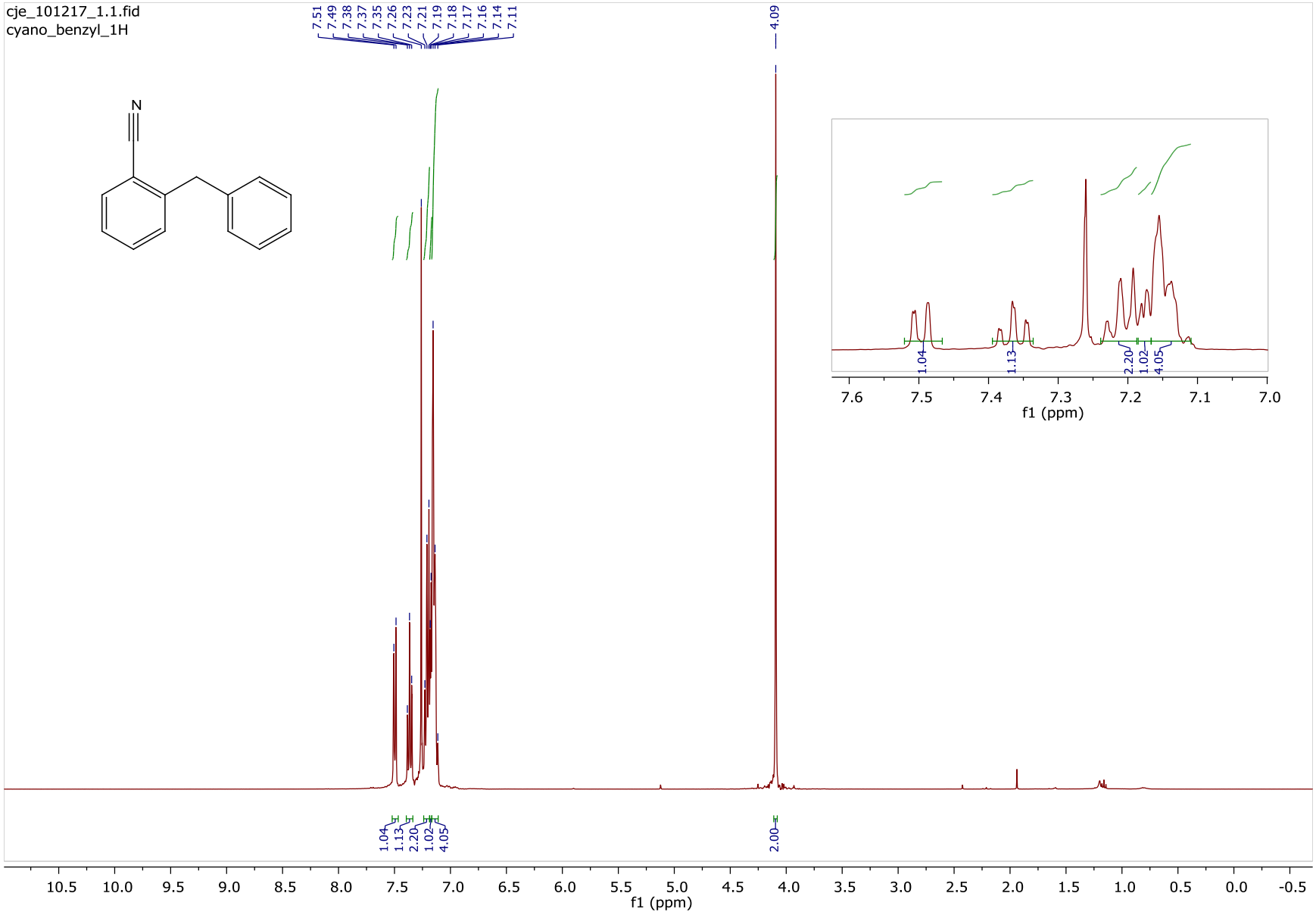
4-bromo-2-(bromomethyl)benzonitrile: To a dry solution of 4-bromo-2-methylbenzonitrile (2g, 10.2 mmol) in $CHCl_3$ (11 mL) under argon NBS (2.180 g, 12.24 mmol) and benzoyl peroxide (100mg, 1 mmol) were added. The reaction mixture was stirred at 85˚C for 24 hours. After that, the reaction mixture was cooled to room temp and the precipitate was filtered off and washed with EtOAc. The solvent was evaporated and the residue purified by column chromatography and recrystallized from cyclohexane. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 1.8 Hz, 1H), 7.57 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.52 (d, *J* = 8.3 Hz, 1H), 4.57 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.01, 134.41, 133.89, 132.53, 128.34, 116.33, 111.42, 28.41.7. Spectra matched those previously reported.[2]



4'-(trifluoromethyl)-3-(4-trifluoromethyl)benzyl-[1,1'-biphenyl]-4-carbonitrile: Following **general procedure 1**. 4-bromo-2-(bromomethyl)benzonitrile and 4-(trifluoromethyl)-phenyl boronic acid were coupled together to give the desired product in 175 mg(yield 79%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 8.3 Hz, 2H), 7.62 – 7.57 (m, 3H), 7.56 (d, *J* = 1.5 Hz, 1H), 7.43 (d, *J* = 8.1 Hz, 2H), 4.36 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.71, 144.65, 142.74 (d, *J* = 2.5 Hz), 133.86, 130.99, 130.67, 129.53, 129.40, 129.21, 129.06, 127.82, 126.33, 126.18 (q, *J* = 3.7 Hz), 125.92 (q, *J* = 3.8 Hz), 125.65, 125.53, 122.95, 122.83, 120.24, 120.13, 117.99, 112.44, 40.21. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.45, -62.60. [M+H] 406.0952, found 406.1673.



2-ethylbenzonitrile: 1-bromo-2-ethylbenzene (555 mg, 3 mmol) and CuCN (672 mg, 7.5 mmol) were added to a two-neck round bottom flask equipped with a stir bar and a water condenser. NMP (4 mL) was added and the solution was left to mix at 195^{o}C for 20 mins. Upon consumption of starting material the reaction vessel was brought to room temp and worked up with NH_4OH 10% and $CHCl_3$. The organic layers were collected and condensed under reduced pressure and after purifying via column chromatography on silica gel with EtOAc: Hex (5:95) as an eluent yielded the desired product in 64% yield (253.4 mg).[6] ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.62 (d, *J* = 7.8 Hz, 1H), 7.55 (td, *J* = 7.6, 1.4 Hz, 1H), 7.37 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.31 (td, *J* = 7.6, 1.2 Hz, 1H), 2.90 (q, *J* = 7.6 Hz, 2H), 1.33 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 148.01, 132.93, 132.73, 128.84, 126.38, 118.08, 111.99, 27.74, 15.06. Spectra matches those previously reported.[8]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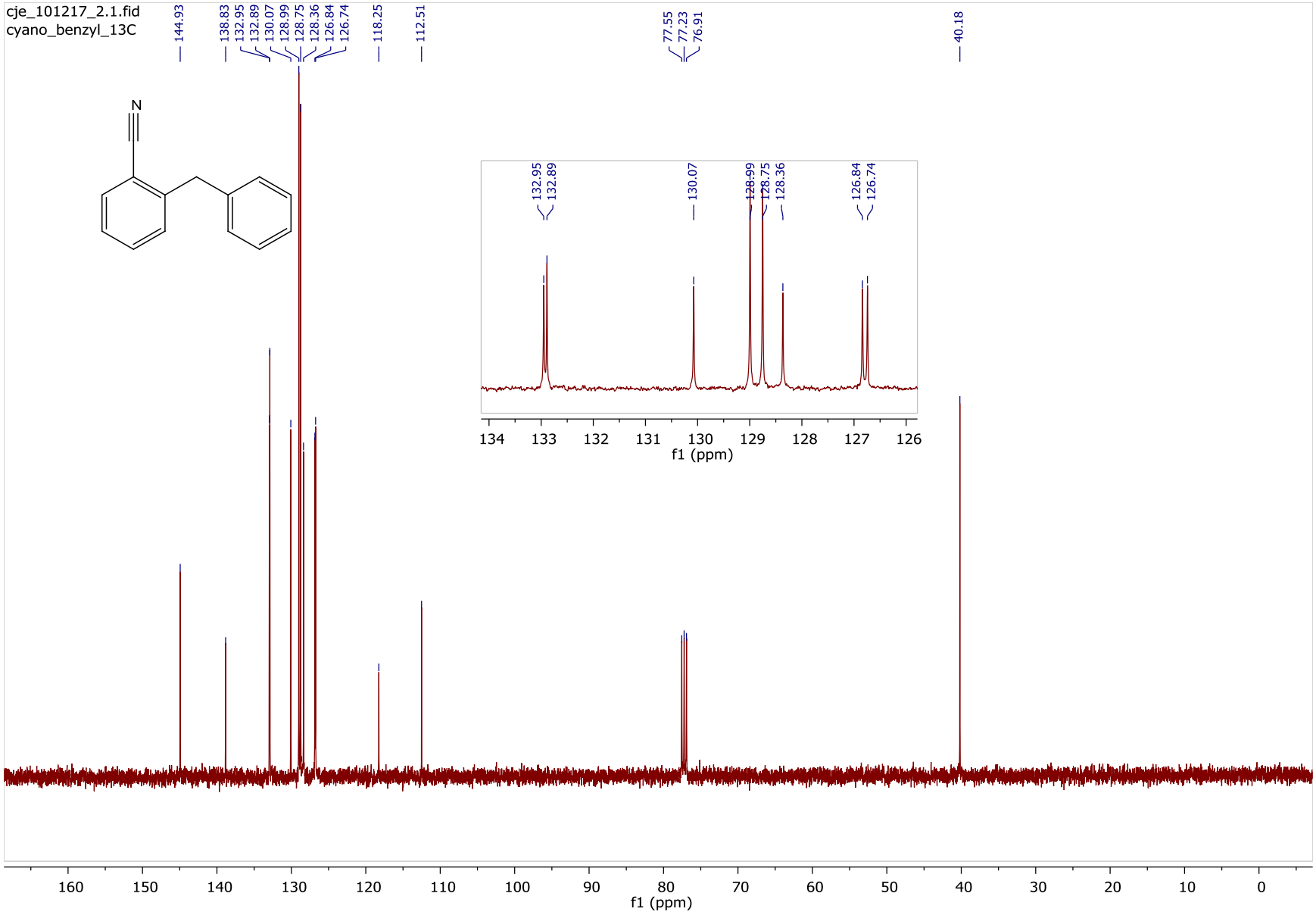
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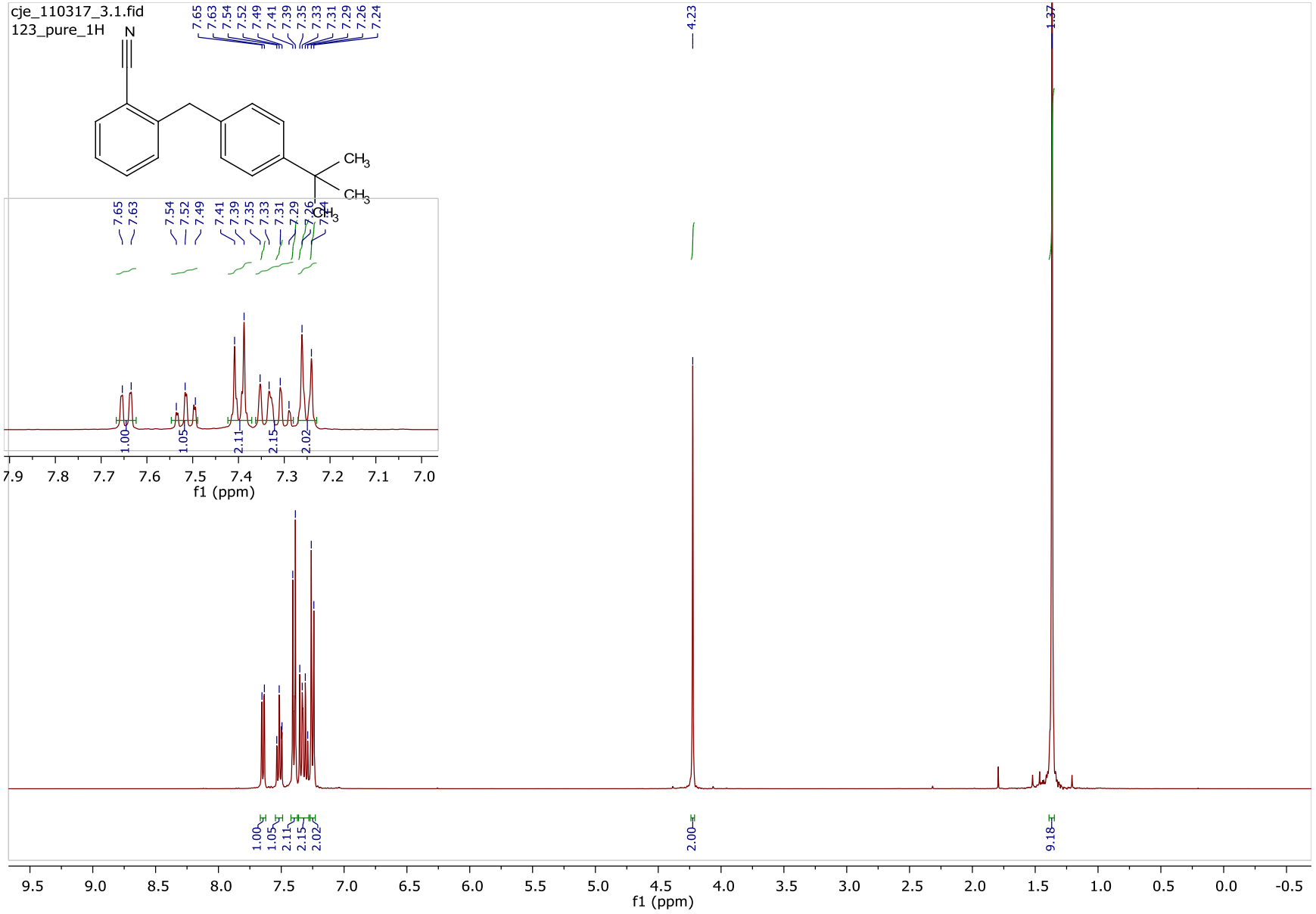
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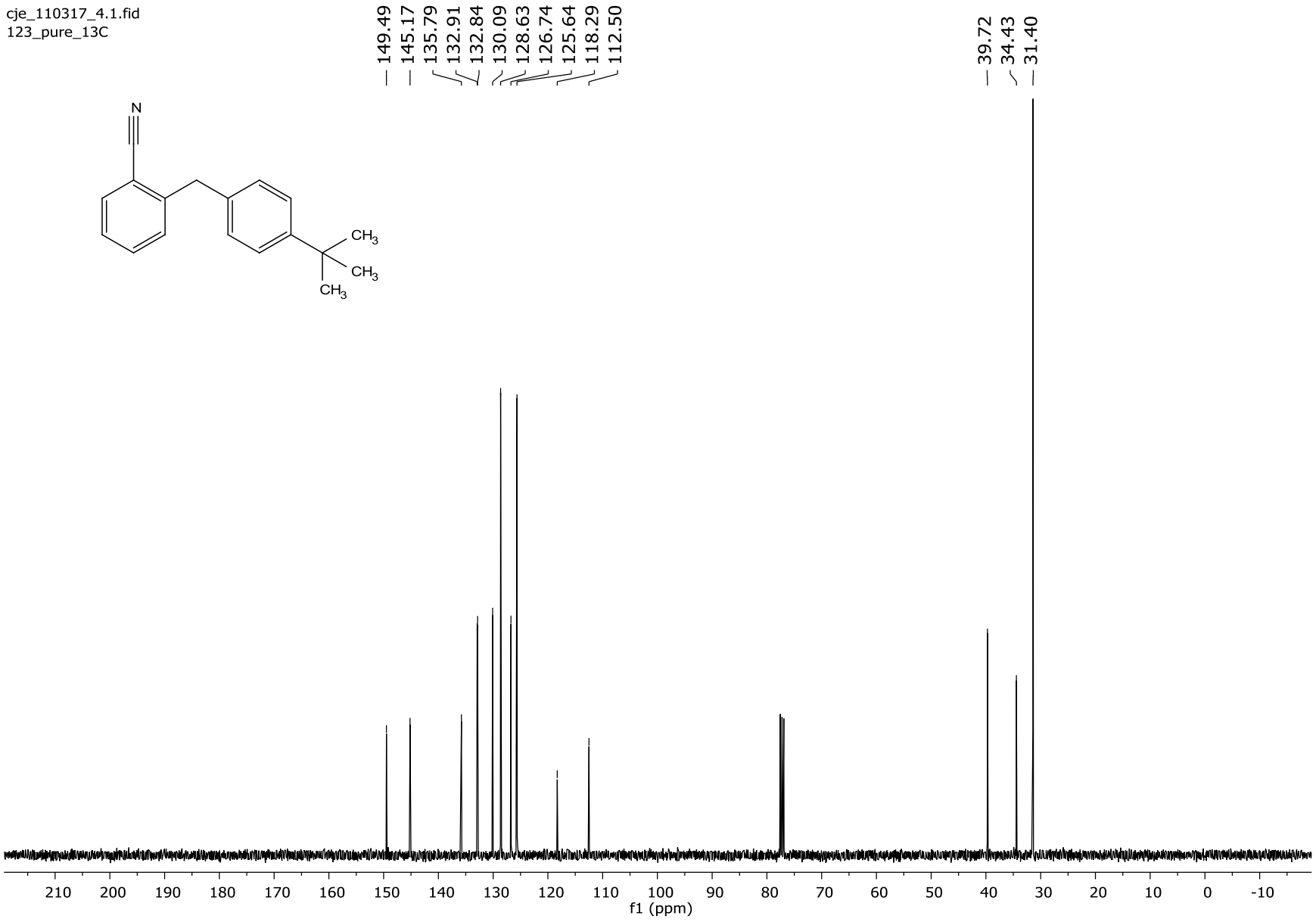
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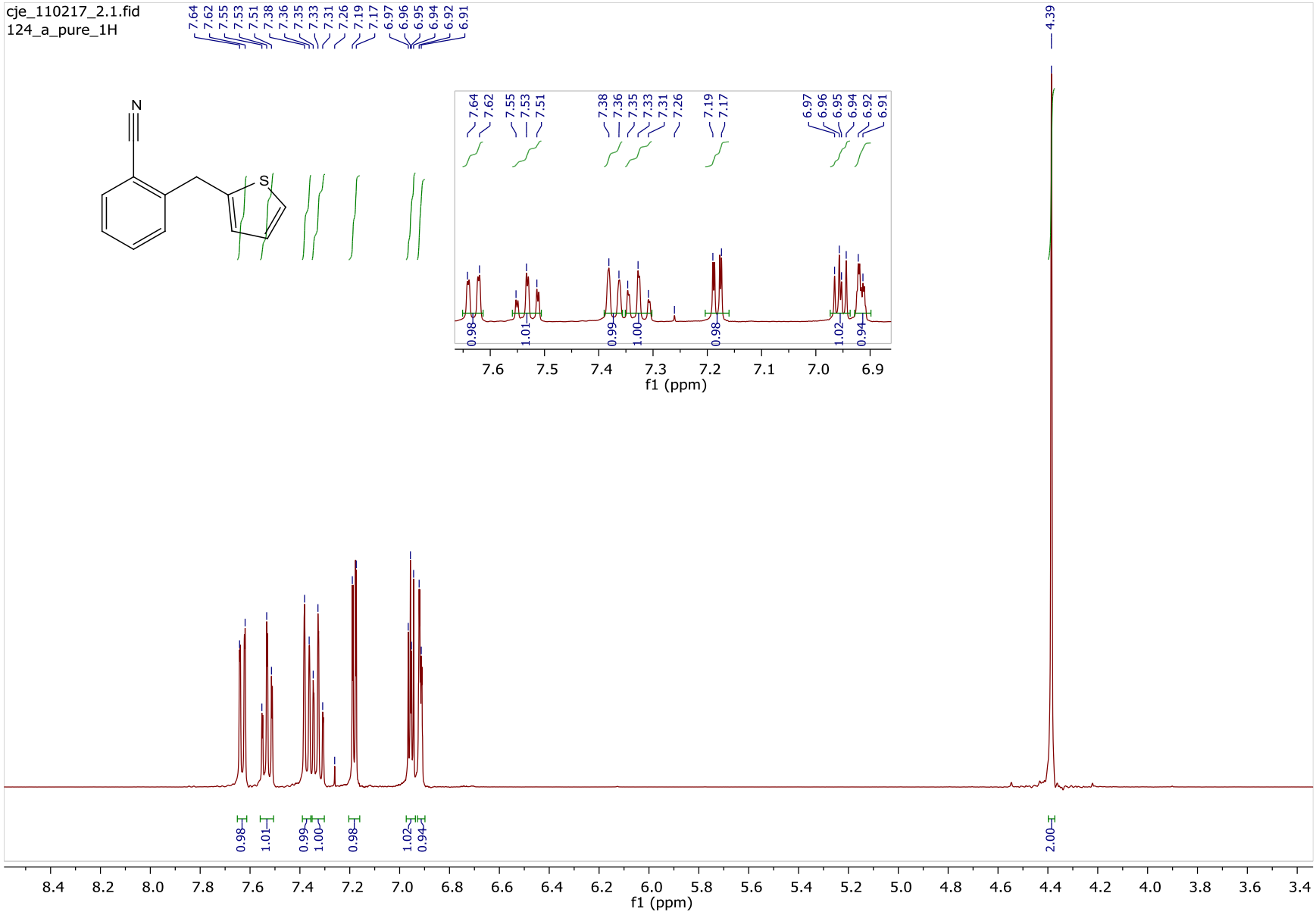
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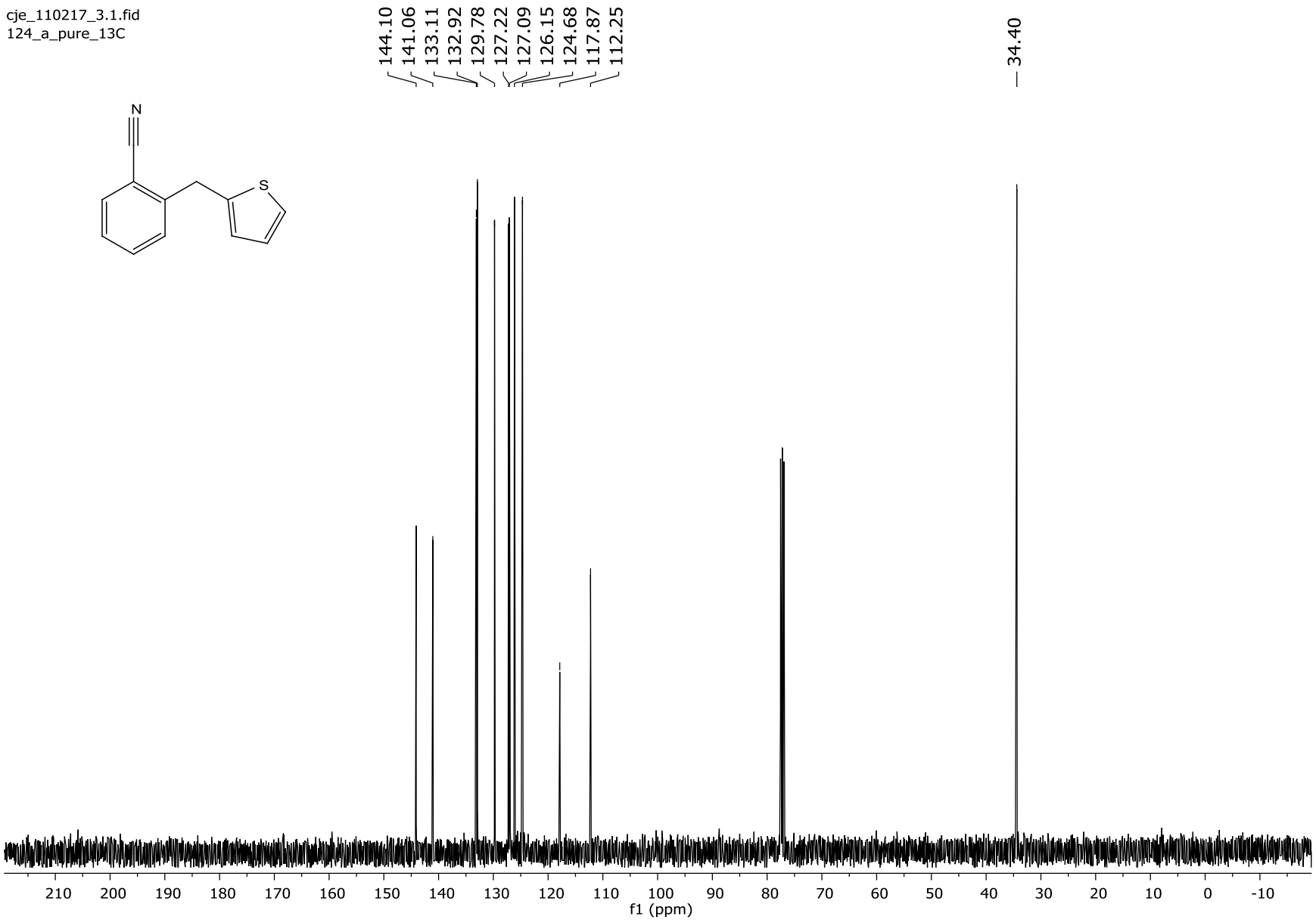
f1 (ppm)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126.15
124.68
117.87
112.25
34.40
N
S
210
200
190
180
170
160
150
140
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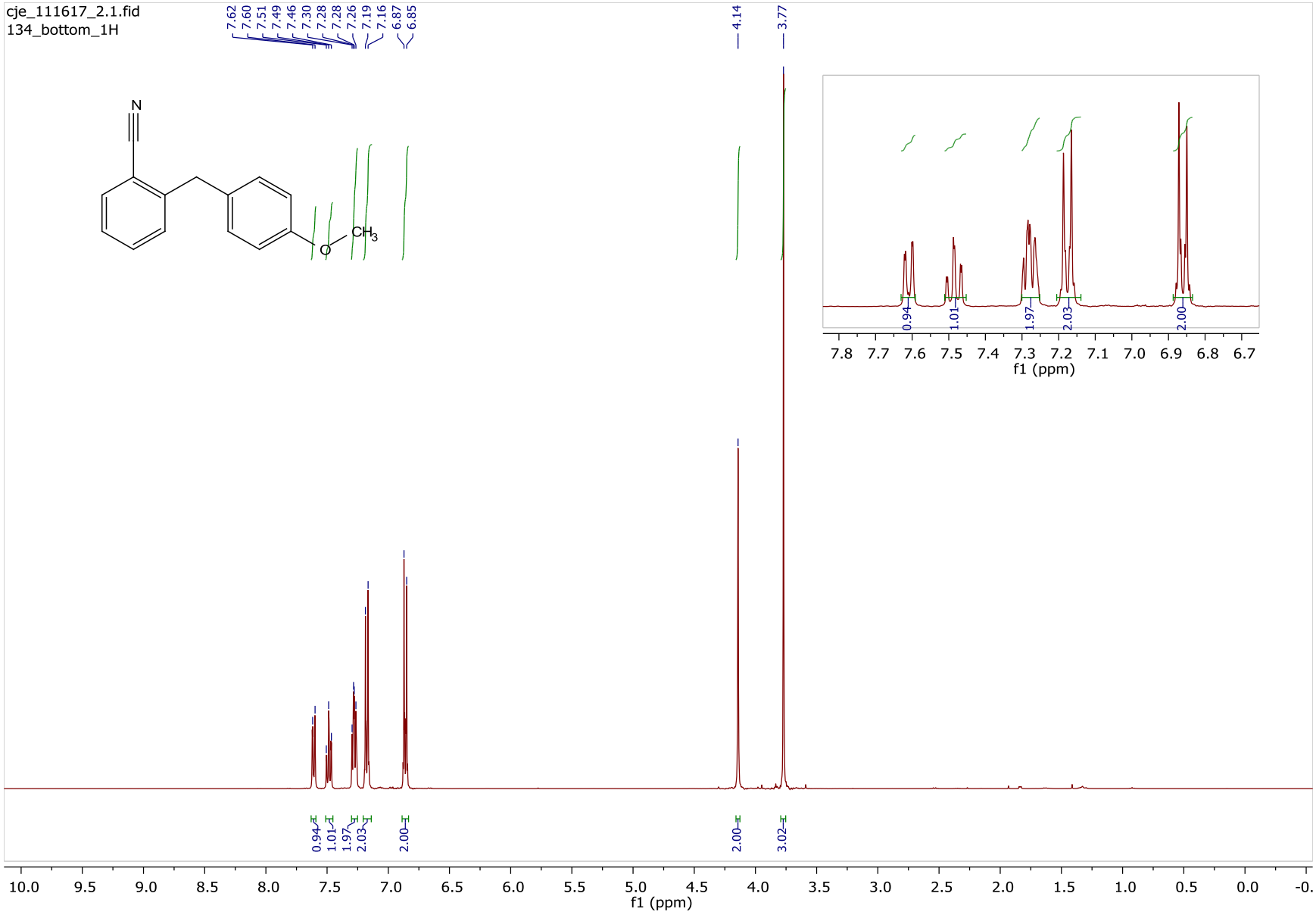
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.49
7.46
7.30
7.28
7.28
7.26
7.19
7.16
6.87
6.85
4.14
3.77
N
CH3
O
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1.01
1.97
2.03
2.00
3.02
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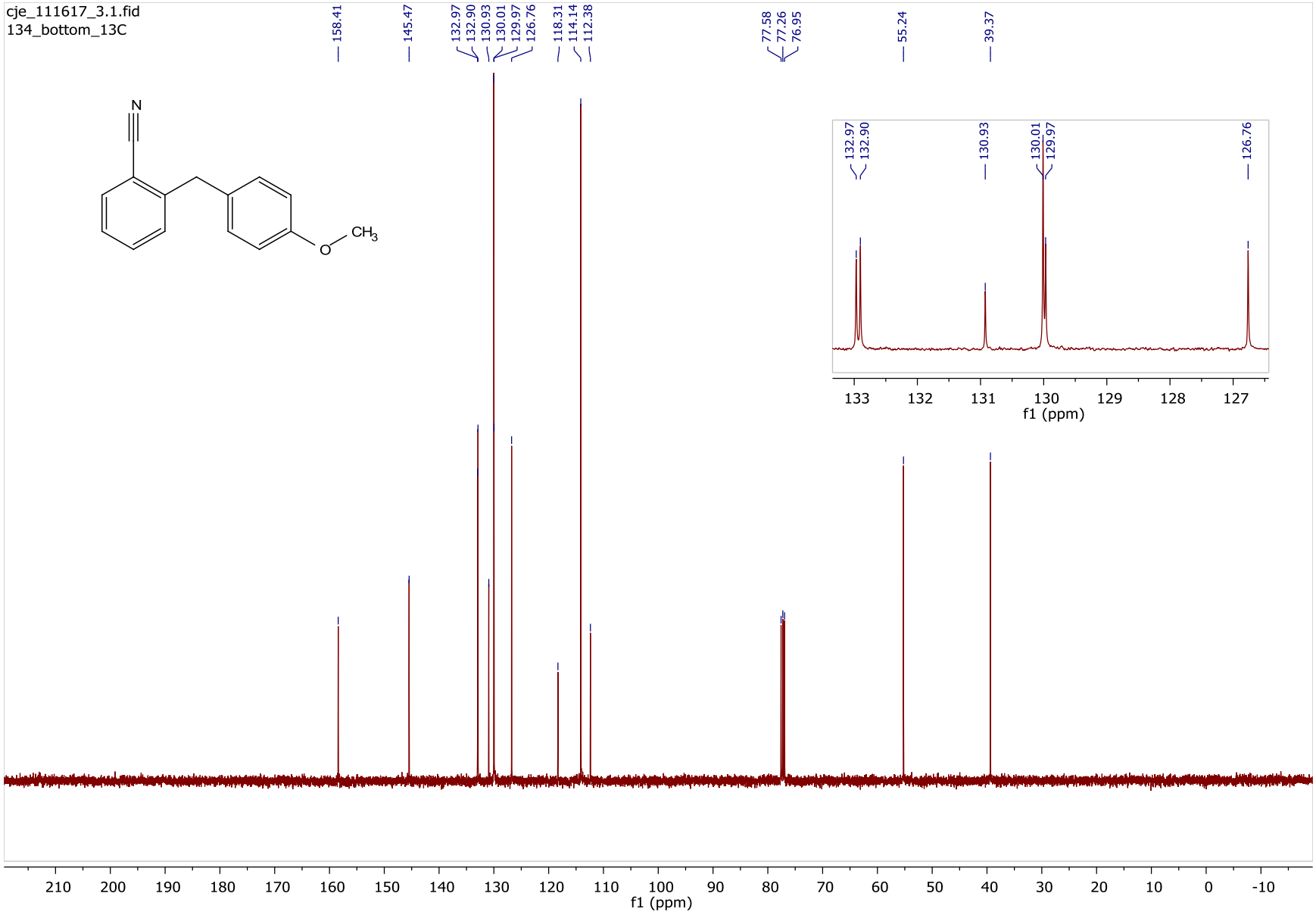
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O
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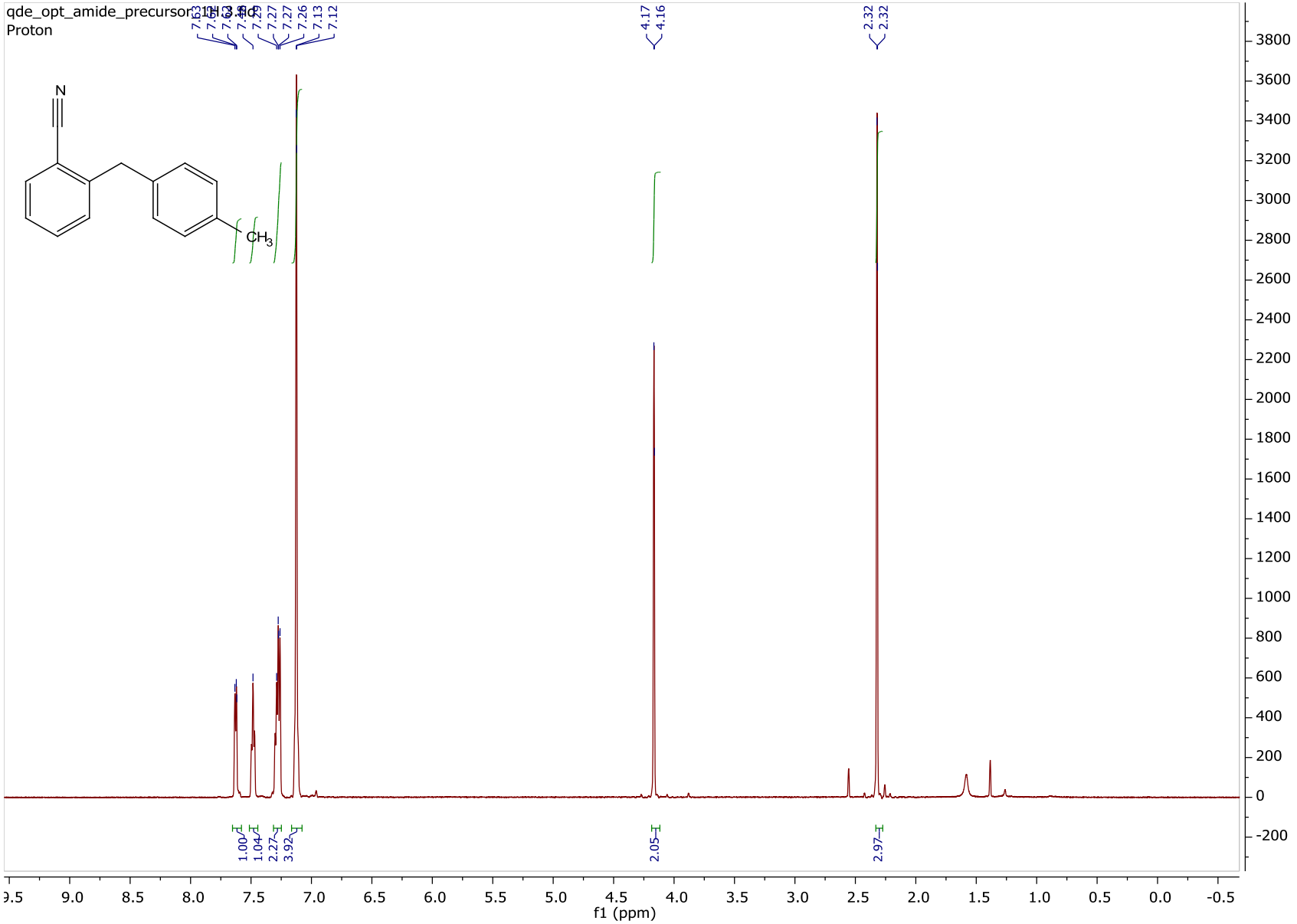
f1 (ppm)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7.27
7.27
7.26
7.13
7.12
4.17
4.16
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2.32
N
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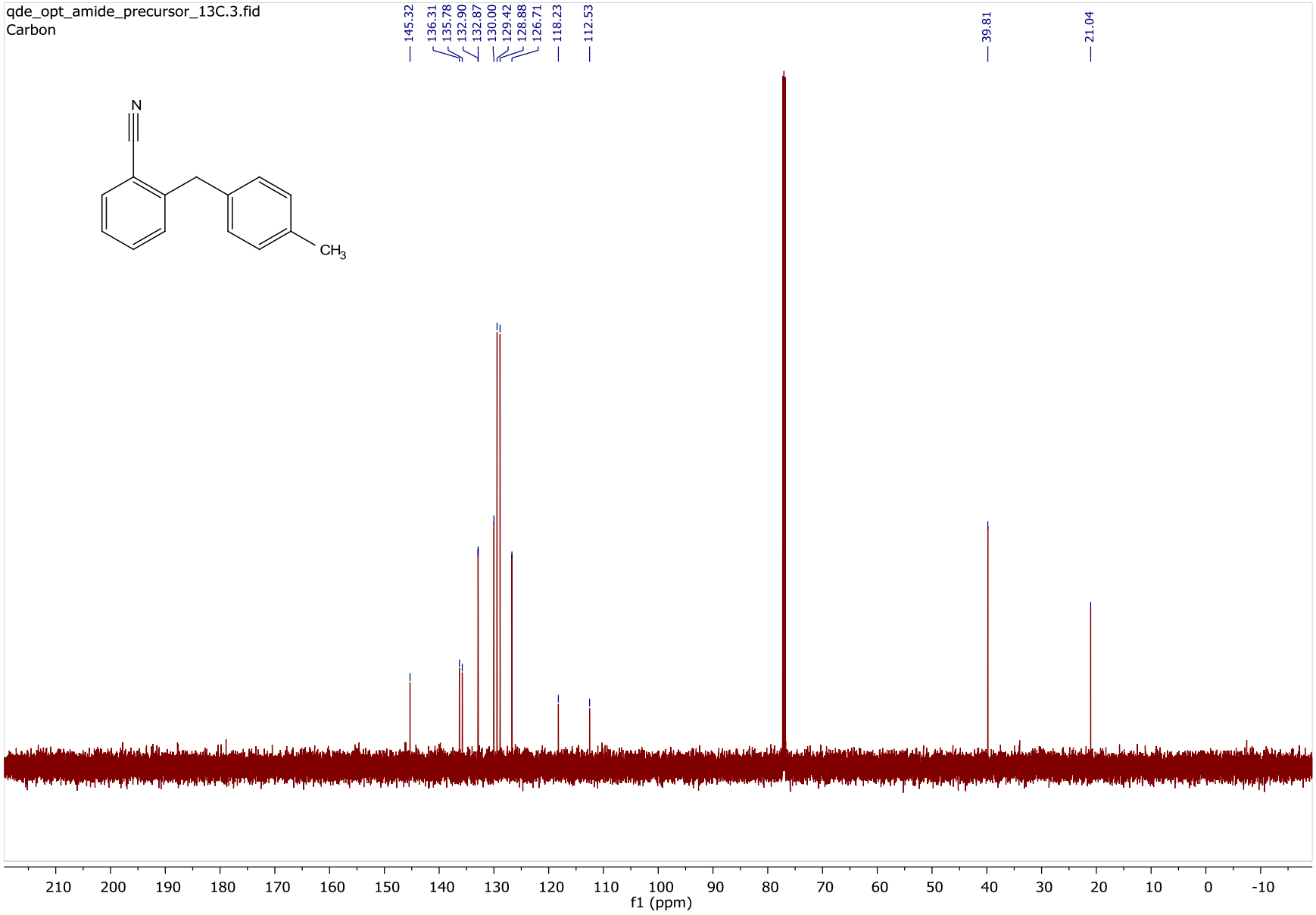
1.04
2.27
3.92
2.05
2.97
f1 (ppm)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126.71
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39.81
21.04
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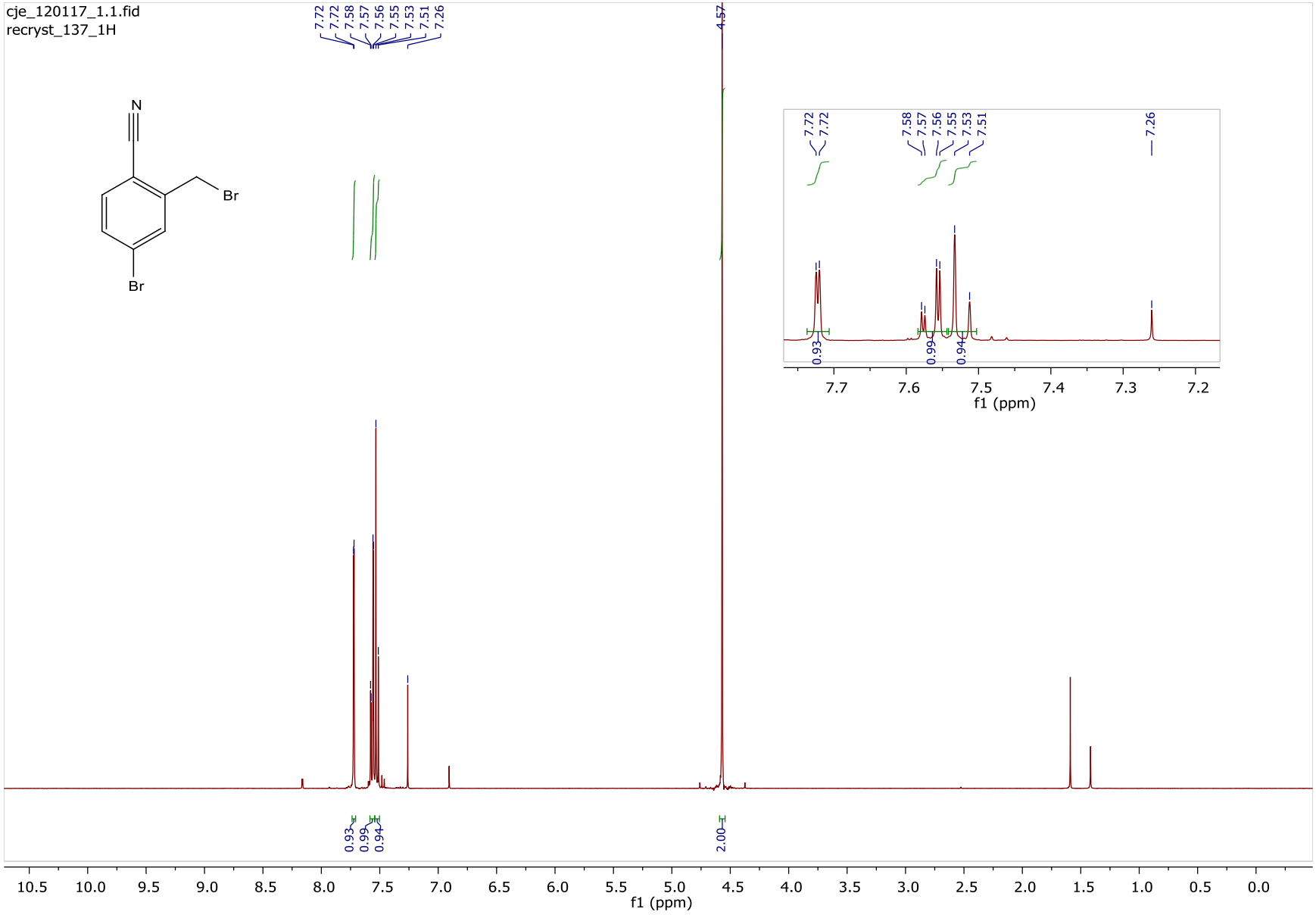
f1 (ppm)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7.56
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7.53
7.51
7.26
4.57
N
Br
Br
0.93
0.99
0.94
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
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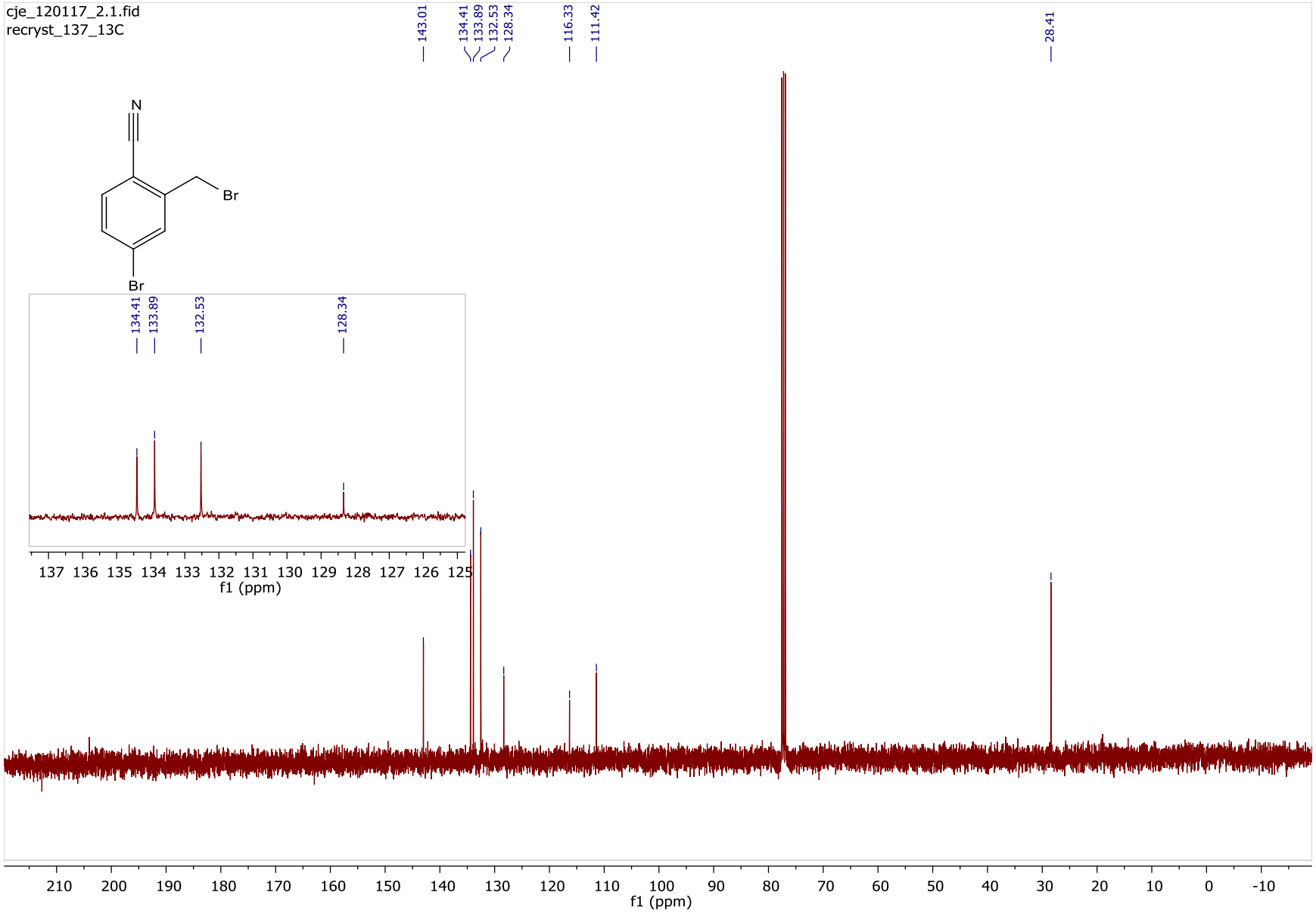
f1 (ppm)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28.41
N
Br
Br
134.41
133.89
132.53
128.34
137 136 135 134 133 132 131 130 129 128 127 126 125
f1 (ppm)
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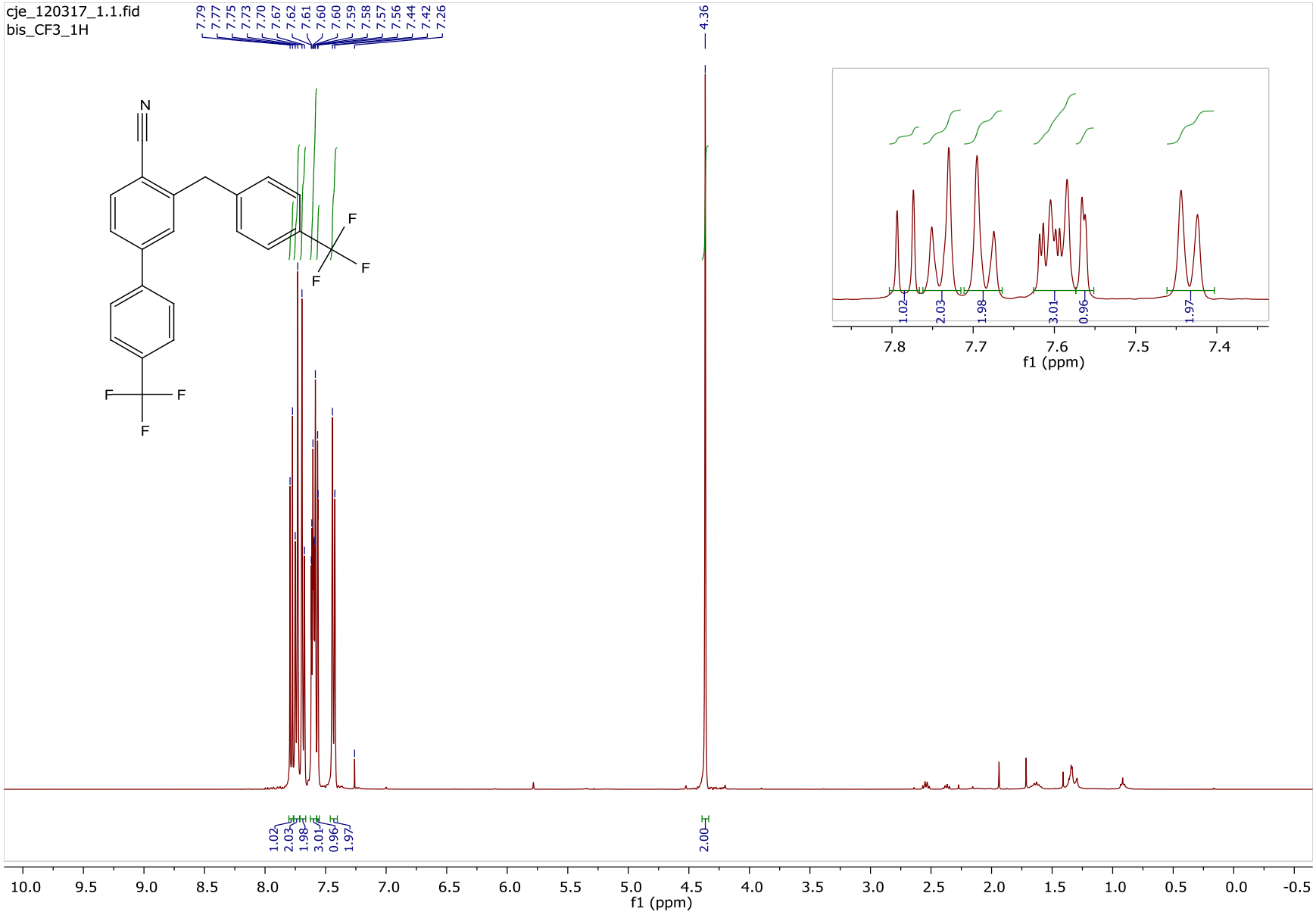
f1 (ppm)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7.77
7.75
7.73
7.70
7.67
7.62
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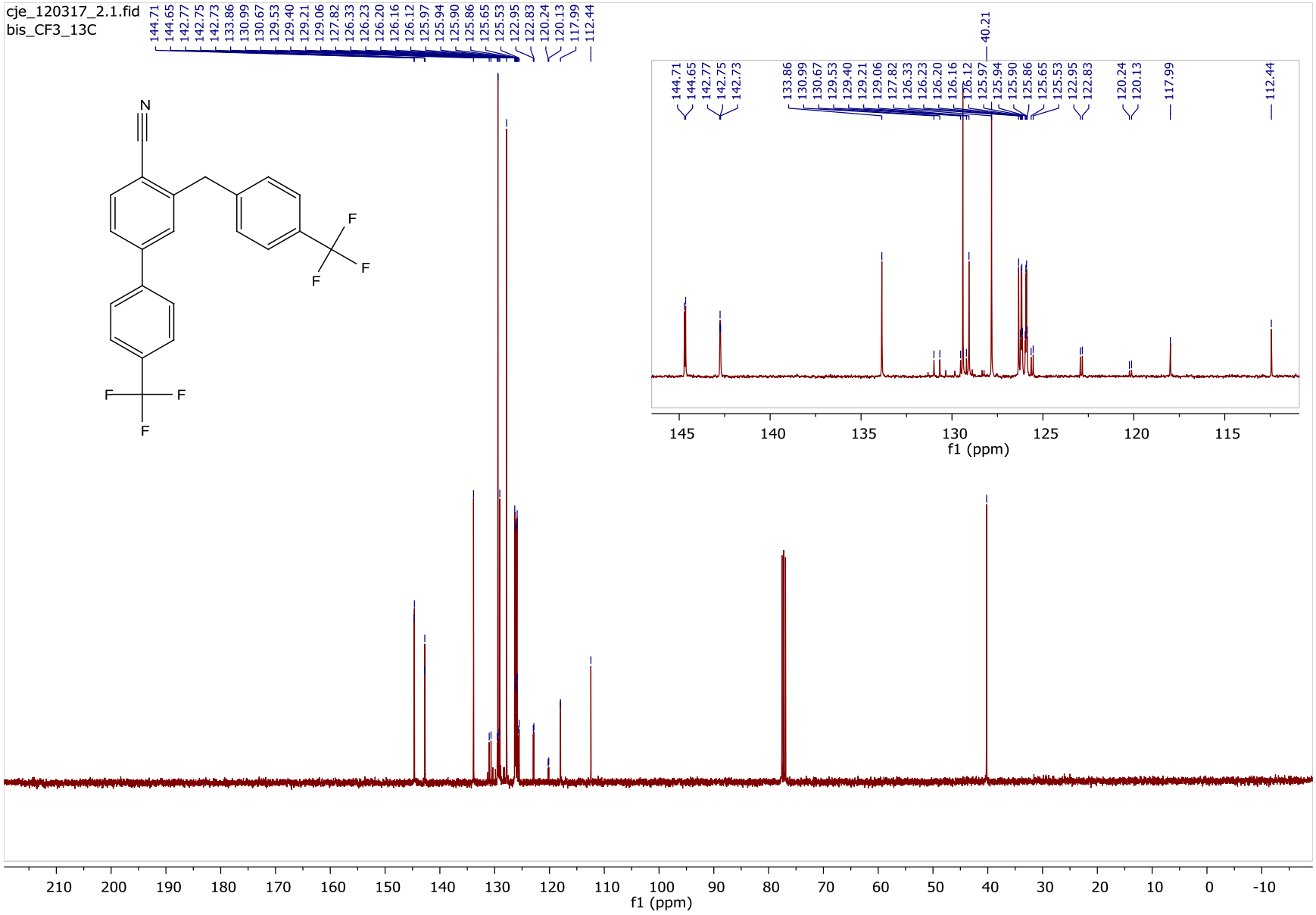
7.58
7.57
7.56
7.44
7.42
7.26
4.36
N
F
F
F
F
F
F
1.02
2.03
1.98
3.01
0.96
1.97
2.00
f1 (ppm)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142.73
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130.99
130.67
129.53
129.40
129.21
129.06
127.82
126.33
126.23
126.20
126.16
126.12
125.97
125.94
125.90
125.86
125.65
125.53
122.95
122.83
120.24
120.13
117.99
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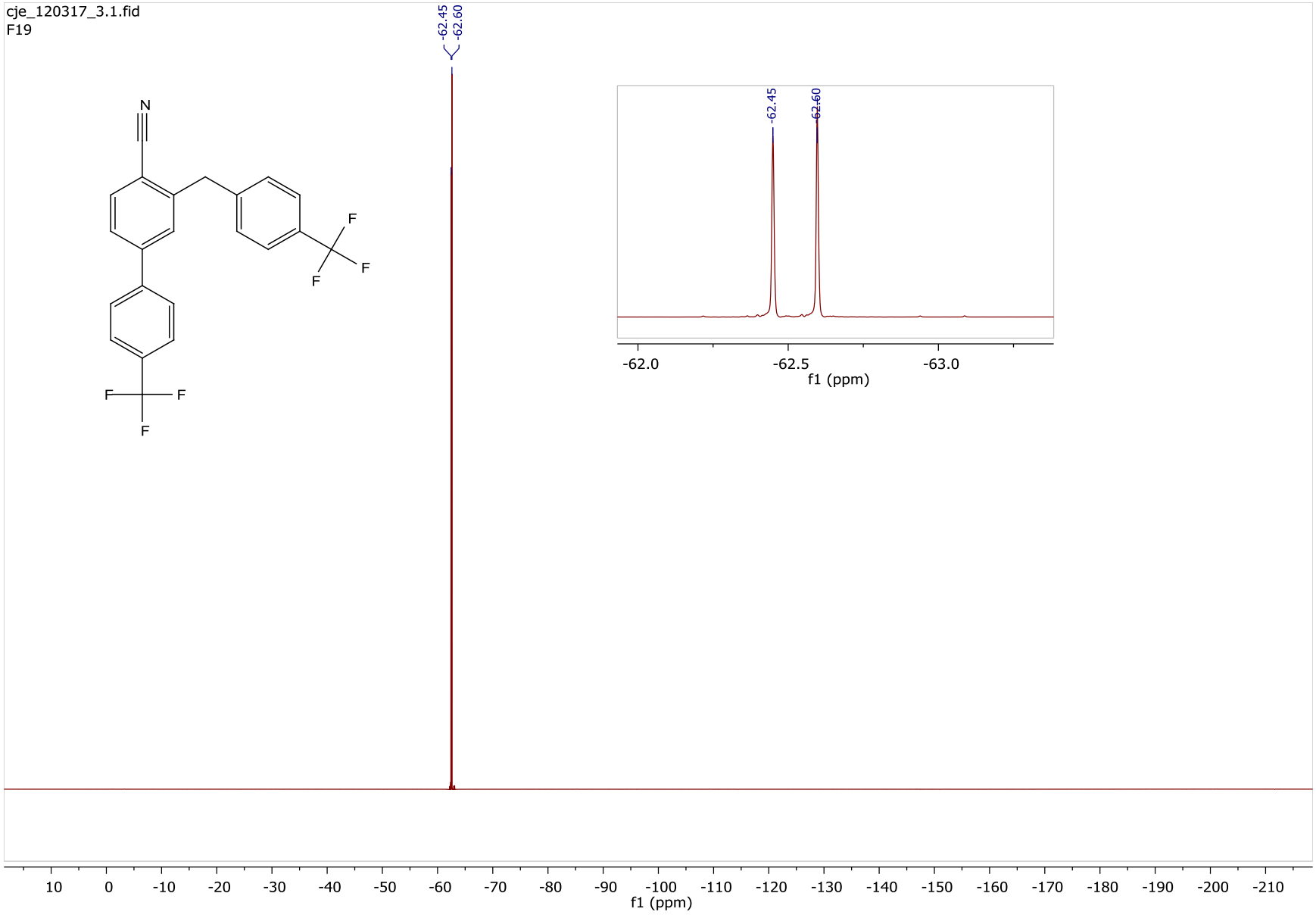
N
F
F
F
F
F
F
f1 (ppm)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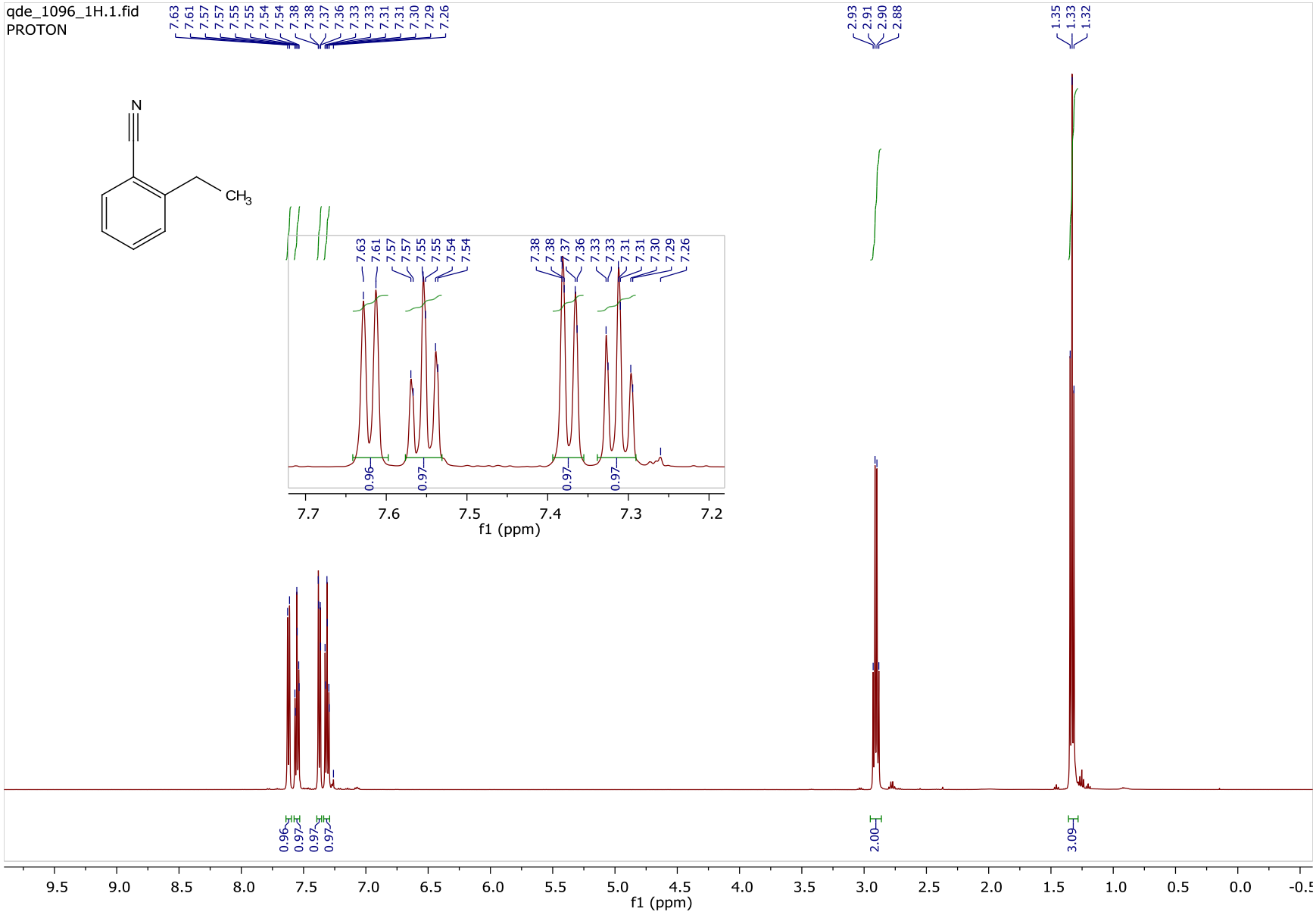
-62.60
N
F
F
F
F
F
F
-62.45
-62.60
-62.0
-62.5
-63.0
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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PROTON
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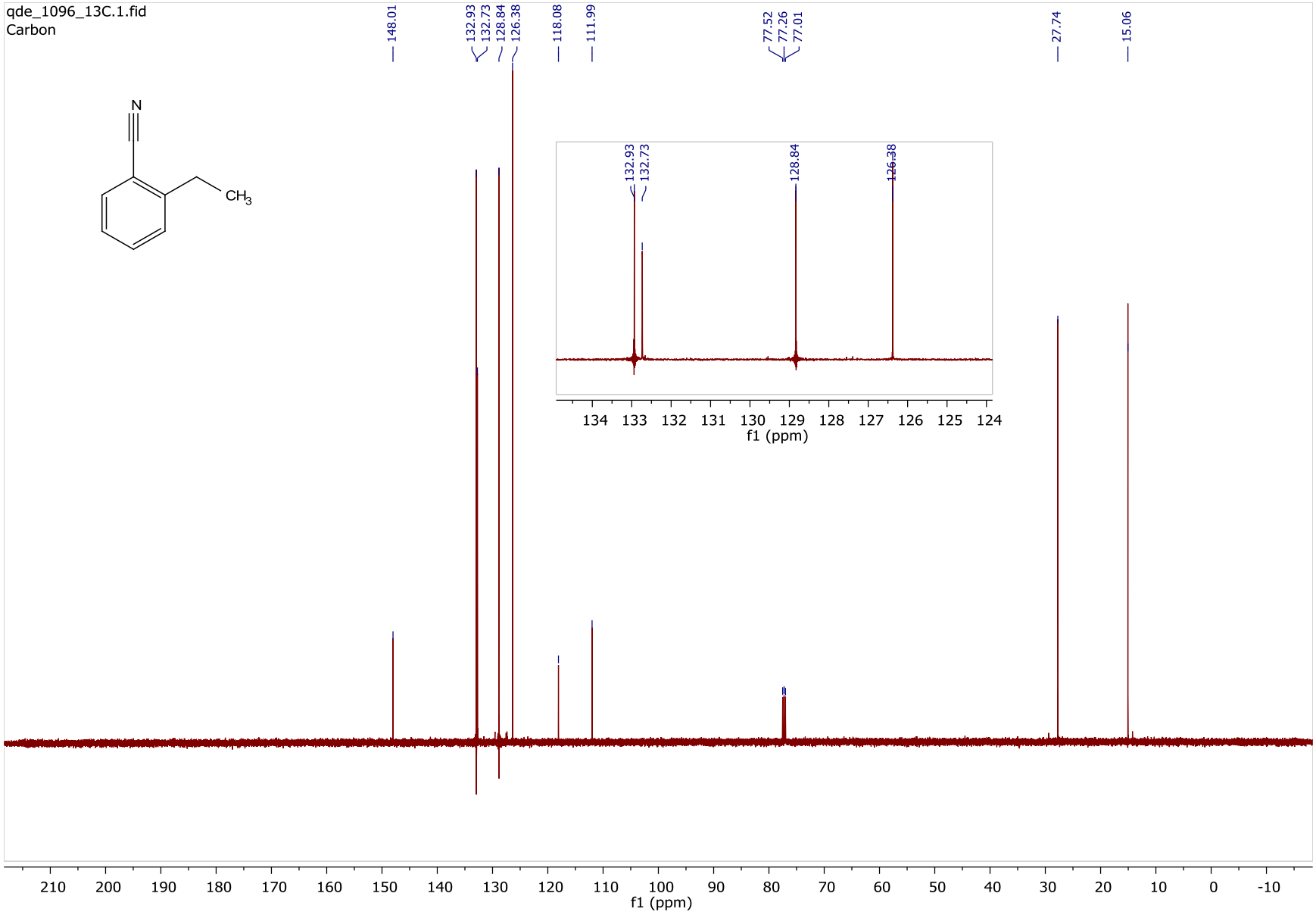
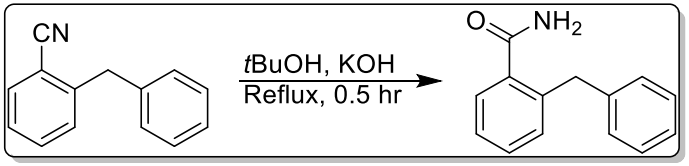
2.93 2.91 2.90 2.88
1.35 1.33 1.32
N
CH3
0.96 0.97 0.97 0.97
2.00
3.09
f1 (ppm)


qde_1096_13C.1.fid
Carbon
148.01
132.93
132.73
128.84
126.38
118.08
111.99
77.52
77.26
77.01
27.74
15.06
N
CH3
f1 (ppm)

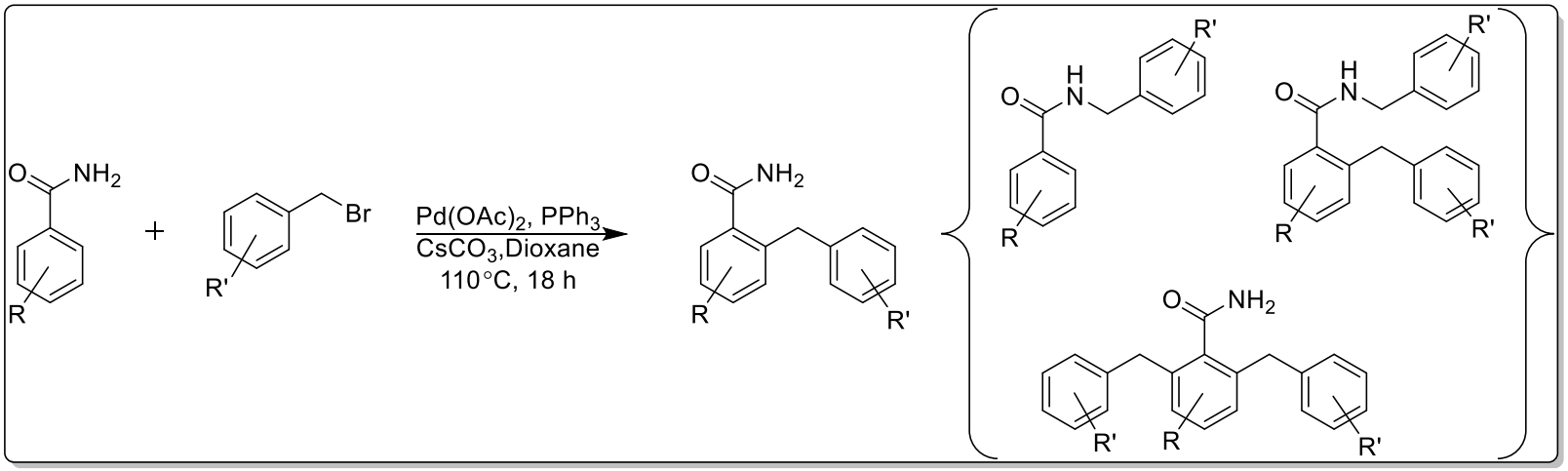
3b Procedures, spectral data and copies of NMR's for amides

General Procedure 2



In a round bottom flask equipped with a stir bar and a condenser was added benzonitrile and enough *t*BuOH to make a 1mM solution. To this stirred solution was added finely ground KOH (3.7 eq). The reaction was left to reflux for 30 minutes, cooled to room temp, and poured into a brine solution and extracted with $CHCl_3$. The collected organic layers were dried, concentrated under reduced pressure, and purified via column chromatography on silica gel.[9]

General Procedure 3

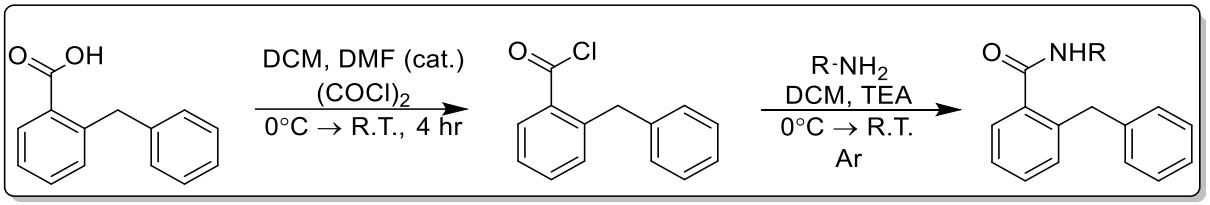


In an oven dried screw-cap vial equipped with a magnetic stir bar, benzamide (1 eq) was dissolved in dioxane (2 mM) under argon. Followed by the addition of $CsCO_3$ (1.2 eq), benzyl bromide (1 eq), $Pd(OAc)_2$ (5 mol %), and PPh_3 (10 mol %). The resulting reaction mixture was heated at 110^{o}C for 18 hours. The reaction mixture was cooled to room temp and extracted with ethyl acetate. The organic

layers were combined, dried with $MgSO_4$, concentrated under reduced pressure, and purified by column chromatography on silica gel (1.5 EA : 3.5 Hex) to give the desired product.[10]

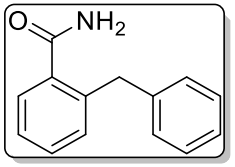
See reference 7 for a more detailed descriptions of side product yields and isolation

General Procedure 4

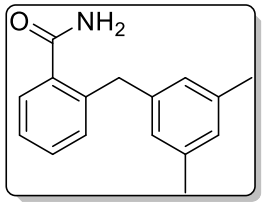


General Proceudre 4 A: In a round bottom flask equipped with a stir bar was added 2-benzylbenzoic acid (500 mg, 2.3) dissolved in dry DCM (8 mL) under Ar. 1 drop of DMF (cat.) was added at 0°C, followed by the dropwise addition of Oxalyl chloride (404 µL, 4.71 mmol). Upon complete addition of oxalyl chloride, the reaction was brought to room temperature and allowed to stir for 4 hours. Upon completion the reaction was concentrated under reduced pressure and the crude acyl chloride was dissolved in the minimal amount of dry inert DCM needed. The solution was cooled to 0°C and the corresponding amine (2.6 mmol), TEA (5.2 mmol), and 1 mL of dry inert DCM were added to an addition funnel and added dropwise to the stirred chilled solution. Upon complete addition the reaction was allowed to stir at room temperature overnight and then washed with 1M NaOH and extracted with DCM, concentrated under reduced pressure, and purified by column chromatography on silica gel to give the desired secondary benzamide.[11]

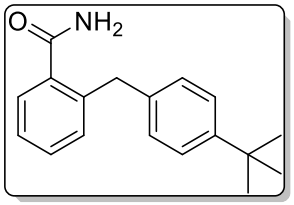
General Procedure 4 B: To a solution of 2-benzylbenzoic acid (43 mg, 0.203 mmol) in dry DCM at 0°C under Ar was added dropwise oxalyl chloride followed by a catalytic amount of dry DMF (1 drop). The reaction was allowed to mix for 4 hr and the solvent then removed to afford crude acyl chloride. The crude solvent was then dissolved in the minimal amount of EtoAc which was then added dropwise into a solution of methoxyaminde hydrochloride (20 mg, 243 mmol) and K_2CO_3 (56 mg, 0.405 mmol) dissolved in EtOAc (1 mL) and water (0.5 mL) at 0°C . The reaction was allowed to mix overnight and then the phases separated and the aqueous layer extracted with EtOAc. The collected organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure. Purified on silica gel with by eluting with a 25:75:1 mixture of EtOAc:Hex:TEA.[12]



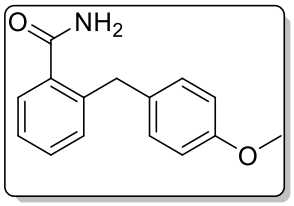
2-benzylbenzamide: following **general procedure 2** with 2-benzylbenzonitrile (92 mg, 0.5 mmol) and after purification via column chromatography yielded the desired product in 71% yield (75 mg, 0.355 mmol) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.37 (td, *J* = 7.5, 1.5 Hz, 1H), 7.30 – 7.27 (m, 2H), 7.26 – 7.22 (m, 2H), 7.21 – 7.15 (m, 3H), 5.58 (s, 2H), 4.25 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.96, 140.76, 139.01, 135.41, 131.18, 130.46, 128.98, 128.52, 127.39, 126.38, 126.17, 38.79. Spectra matched those previously reported.[6]



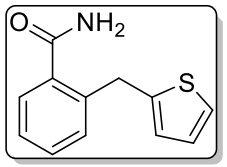
2-(3,5-dimethylbenzyl)benzamide: following **general procedure 3** with benzamide (199mg, 1 mmol) and 3,5-dimethylbenzyl bromide (121 mg, 1 mmol) and after purification via column chromatography yielded the desired product in 31% yield (73 mg, 0.301 mmol) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.37 (td, *J* = 7.5, 1.5 Hz, 1H), 7.29 – 7.25 (m, 1H), 7.25 – 7.20 (m, 1H), 6.86 – 6.73 (m, 3H), 5.79 (d, *J* = 76.3 Hz, 2H), 4.17 (s, 2H), 2.26 (d, *J* = 0.7 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.92, 140.58, 138.95, 138.05, 135.38, 131.20, 130.44, 127.88, 127.48, 126.72, 126.29, 38.62, 21.31. [M+H] 240.1310, found 240.1410



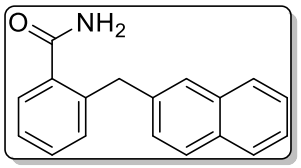
2-(4-(tert-butyl)benzyl)benzamide: following **general procedure 2** with 2-(4-(tert-butyl)benzyl)benzonitrile (51 mg, 0.2 mmol) and after purification via column chromatography yielded the desired product in 73% yield (39 mg, 0.146 mmol). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.47 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.36 (td, *J* = 7.4, 1.5 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.24 (dd, *J* = 7.9, 6.3 Hz, 2H), 7.14 – 7.09 (m, 2H), 6.15 (d, *J* = 259.5 Hz, 2H), 4.21 (s, 2H), 1.30 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 172.57, 149.10, 139.12, 137.79, 135.68, 131.27, 130.51, 128.68, 127.60, 126.43, 125.59, 38.38, 34.51, 31.53. [M+H] 268.1628, found 268.1183.



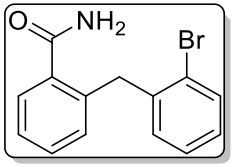
2-(4-(methoxyl)benzyl)benzamide: following **general procedure 2** with 2-(4-methoxy)benzylbenzonitrile (103mg, 0.461 mmol) and after purification via column chromatography yielded the desired product in 50% yield (56 mg, 0.232 mmol). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 7.6 Hz, 1H), 7.36 (td, *J* = 7.5, 1.2 Hz, 1H), 7.25 (d, *J* = 8.6 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 1H), 7.10 (d, *J* = 8.6 Hz, 2H), 6.81 (d, *J* = 8.6 Hz, 2H), 5.90 (d, *J* = 139.6 Hz, 2H), 4.17 (s, 2H), 3.76 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.31, 158.17, 139.59, 135.56, 133.01, 131.19, 130.58, 130.11, 127.57, 126.46, 114.11, 55.41, 38.11. [M+H] 242.1103, found 242.1232.



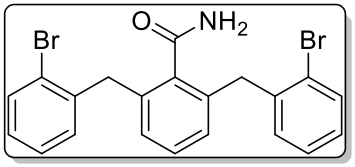
2-(thiophen-2-ylmethyl)benzamide: following **General Procedure 2** with 2-(thiophen-2-ylmethyl)benzonitrile (60 mg, 0.301 mmol) and after purification via column chromatography yielded the desired product in 32% yield (21 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 (d, *J* = 7.5 Hz, 1H), 7.44 – 7.36 (m, 1H), 7.35 – 7.28 (m, 2H), 7.17 – 7.12 (m, 1H), 6.90 (dd, *J* = 5.0, 3.4 Hz, 1H), 6.81 – 6.77 (m, 2H), 5.83 (d, *J* = 54.1 Hz, 2H), 4.42 (s, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 171.68, 143.78, 138.62, 130.86, 130.75, 127.57, 126.88, 126.84, 125.52, 124.22, 33.29. [M+H] 218.0561, found 218.0654.



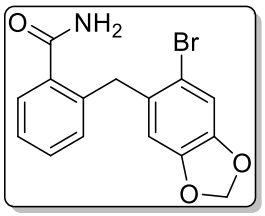
2-(napthalen-2-ylmethyl)benzamide): following **general procedure 3** with benzamide (221 mg, 1 mmol) and 2 bromomethylnapthelene (121mg, 1 mmol) and after purification via column chromatography yielded the desired product in 15 % yield (39 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.77 (dd, *J* = 16.5, 8.8 Hz, 3H), 7.59 (s, 1H), 7.50 – 7.40 (m, 3H), 7.36 (q, *J* = 7.9 Hz, 2H), 7.28 – 7.23 (m, 2H), 5.95 (d, *J* = 160.9 Hz, 2H), 4.40 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 172.36, 139.08, 138.50, 135.67, 133.73, 132.24, 131.39, 130.63, 128.30, 127.82, 127.77, 127.58, 127.36, 126.60, 126.19, 125.62, 39.10. [M+H] 262.1154, found 262.1248.



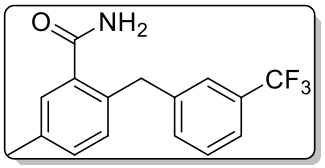
2-(2-bromobenzyl)benzamide): following **general procedure 3** with benzamide (400 mg, 3.3 mmol) and 2 bromobenzylbromide (825 mg, 3.3 mmol) after purification via column chromatography yielded the desired product in 19 % yield (181 mg) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (dd, *J* = 8.4, 1.4 Hz, 1H), 7.50 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.34 (td, *J* = 7.5, 1.6 Hz, 1H), 7.30 – 7.25 (m, 1H), 7.25 – 7.18 (m, 1H), 7.11 – 7.03 (m, 3H), 6.04 (d, *J* = 155.1 Hz, 2H), 4.35 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 172.16, 140.20, 137.89, 135.71, 133.04, 131.37, 130.76, 130.68, 128.19, 127.74, 127.44, 126.67, 125.21, 39.15. [M+H] 290.0102, found 290.0186.



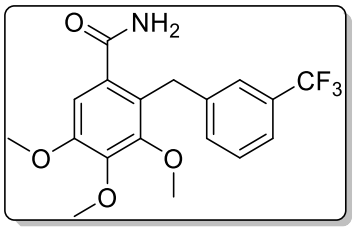
2,6-bis(2-bromobenzyl)benzamide: following **general procedure 3** with benzamide (400 mg, 3.3 mmol) and 2 bromobenzylbromide (825 mg, 3.3 mmol) after purification via column chromatography yielded the desired product in 6 % yield (29 mg). See reference 3 for additional detail on product isolation. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.23 (td, *J* = 7.5, 1.3 Hz, 2H), 7.18 (t, *J* = 7.7 Hz, 1H), 7.13 – 7.06 (m, 4H), 6.87 (d, *J* = 7.7 Hz, 2H), 6.01 (d, *J* = 231.7 Hz, 2H), 4.22 (s, 4H). [M+H] 457.9677, found 457.9707



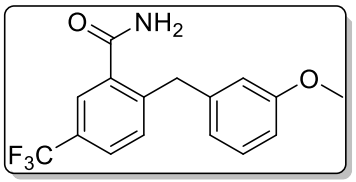
2-((6-bromobenzo[d][1,3]dioxol-5-yl)methyl)benzamide: following **general procedure 3** with benzamide (400 mg, 3.3 mmol) and 5-bromo-6-(bromomethyl)benzo[d][1,3]dioxole (971 mg, 3.3 mmol) after purification by column chromatography yielded the product in 9 % yield (101 mg) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.38 – 7.33 (m, 1H), 7.28 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.12 – 7.08 (m, 1H), 7.02 (s, 1H), 5.93 (s, 2H), 4.25 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.88, 147.68, 147.12, 138.28, 135.48, 133.29, 130.80, 130.73, 127.42, 126.71, 115.20, 112.92, 111.00, 101.85, 38.84. Spectra matched previously reported data. [10]



5-methyl-2-(3-trifluoromethyl)benzyl)benzamide: following **general procedure 3** with 3-methylbenzamide (400 mg, 2.96 mmol) and 1-(bromomethyl)-3-(trifluoromethyl)benzene (707 mg, 2.96 mmol). After purification the desired product ed product was obtained in 24 % yield (204 mg). After purification the desired product was yielded in 23% yield (204 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 – 7.41 (m, 2H), 7.39 – 7.32 (m, 2H), 7.29 (d, *J* = 1.9 Hz, 1H), 7.19 (dd, *J* = 8.0, 1.9 Hz, 1H), 7.10 (d, *J* = 7.8 Hz, 1H), 5.78 (s, 2H), 4.25 (s, 2H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 172.04, 142.25, 136.68, 135.67, 135.15, 132.67, 131.64, 131.32, 129.00, 128.14, 125.79, 125.76, 123.14, 123.10, 38.34, 21.09. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.49. .Spectra matched previously reported data. [10]

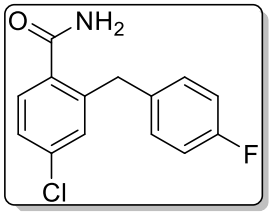


3,4,5-trimethoxy-2(3-trifluoromethyl)benzyl)benzamide: following **general procedure 3** with 3,4,5-trimethoxybenzamide (500 mg, 2.36 mmol) and 1-(bromomethyl)-3-(trifluoromethyl)benzene (564 mg, 2.36 mmol) after purification via column chromatography (60 EtOAc : 40 Hex) yielded the product in 12% yield (104 mg) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.47 (d, *J* = 1.8 Hz, 1H), 7.42 – 7.38 (m, 2H), 7.36 – 7.31 (m, 1H), 6.82 (s, 1H), 5.82 (d, *J* = 145.6 Hz, 2H), 4.21 (s, 2H), 3.87 (s, 3H), 3.68 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 171.90, 152.94, 152.58, 144.36, 142.80, 132.30, 131.52, 130.61, 128.93, 125.64, 125.62, 125.01, 122.95, 122.93, 106.84, 61.02, 56.40, 32.50. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.45. Spectra matched previously reported data. [10]

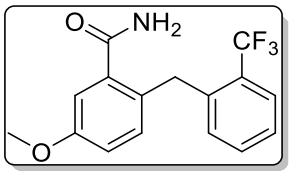


2-(3-methoxybenzyl)-5-(trifluoromethyl)benzamide: following **general procedure 3** with 3-(trifluoromethoxy)benzamide (400 mg, 2.12 mmol) and 1-(bromomethyl)-3-methoxybenzene (425 mg, 2.12 mmol) after purification via column chromatography yielded the desired product in 21 % yield (136 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (d, *J* = 2.0 Hz, 1H), 7.63 – 7.58 (m, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.20 (t, *J* = 7.9 Hz, 1H), 6.78 – 6.69 (m, 3H), 6.03 (d, *J* = 175.1 Hz, 2H), 4.24 (s, 2H), 3.76 (s,

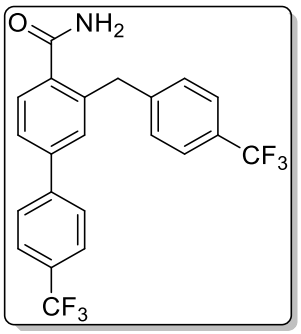
3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.76, 160.05, 143.19, 141.37, 136.18, 131.83, 129.91, 121.52, 115.17, 111.85, 55.36, 38.85. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.57. Spectra matched previously reported data [10]



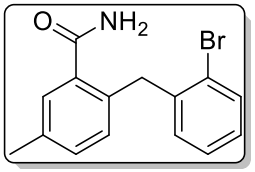
4-chloro-2-(4-fluorobenzyl)benzamide: Following **general procedure 3** with 4-chlorobenzamide (450 mg, 2.892 mmol) and 1-(bromomethyl)-4-fluorobenzene (545 mg, 2.892 mmol). After purification via column chromatography yielded the desired product in 0.5% yield (37 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 8.1 Hz, 1H), 7.22 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.17 (d, *J* = 2.1 Hz, 1H), 7.16 – 7.11 (m, 2H), 6.99 – 6.93 (m, 2H), 5.93 (d, *J* = 154.2 Hz, 3H), 4.16 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.17, 162.94, 160.51, 141.66, 136.66, 135.70, 135.67, 133.71, 131.17, 130.72, 130.64, 128.87, 126.83, 115.71, 115.50, 37.93. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -116.57 (ddd, *J* = 14.1, 8.9, 5.4 Hz). [M+H] 264.0513, found 264.0598.



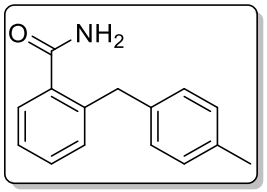
5-methoxy-2-(2-(trifluoromethyl)benzyl)benzamide: following **general procedure 3** with 3-methoxybenzamide (632 mg, 2.646 mmol) and 1-methyl-2-(trifluoromethyl)benzene (400 mg, 2.646 mmol) and after purification via column chromatography yielded the desired product in 13% yield (107 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 27.1 Hz, 4H), 7.17 – 6.86 (m, 3H), 5.90 (d, *J* = 141.4 Hz, 2H), 4.21 (s, 2H), 3.80 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 171.61, 158.07, 142.24, 136.16, 132.41 (d, *J* = 1.2 Hz), 132.34, 130.76, 130.51, 130.26, 128.85, 125.53 (d, *J* = 3.9 Hz), 122.95 (d, *J* = 3.7 Hz), 116.02, 113.05, 55.48, 37.77. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.48. [M+H] 310.0977, found 210.1079.



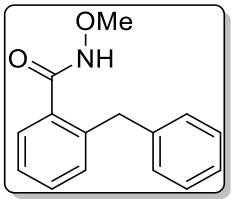
4'-(trifluoromethyl)-3-(4-trifluooromethyl)benzyl)-[1, 1'-biphenyl]-4-carboxamide: following **general procedure 2** with 4'-(trifluoromethyl)-3-(4-trifluoromethyl)benzyl-[1,1'-biphenyl]-4-carbonitrile (104 mg, 0.260 mmol after purification in DCM:MeOH (97:3)) yielded the desired product in 88% yield (97 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.67 – 7.58 (m, 3H), 7.56 – 7.49 (m, 3H), 7.45 (d, *J* = 1.8 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 5.72 (s, 2H), 4.39 (s, 2H). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.37, -62.53. ^{13}C NMR (151 MHz, Acetone-d_6) δ 171.68, 146.02, 143.77, 140.82, 139.56, 136.00, 129.73, 129.62, 129.20, 128.99, 128.59, 127.65, 125.78 (q, *J* = 3.8 Hz), 125.51, 125.39, 125.16, 125.07 (q, *J* = 3.9 Hz), 38.02. [M+H] 424.1058, found 424.0944.



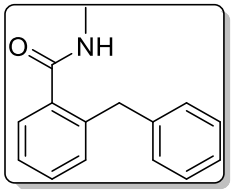
2-(2-bromobenzyl)-5-methylbenzamide: following **general procedure 3** with 3-methylbenzamide (5.00 g, 37 mmol) and 2 bromobenzylbromide (9.25 g, 37 mmol) after purification via column chromatography yielded the desired product in 23.3 % yield (2.62 g) ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.57 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.34 (d, *J* = 1.9 Hz, 1H), 7.21 (td, *J* = 7.5, 1.3 Hz, 1H), 7.18 – 7.14 (m, 1H), 7.11 – 7.04 (m, 2H), 6.97 (d, *J* = 7.9 Hz, 1H), 5.66 (d, *J* = 44.6 Hz, 2H), 4.30 (s, 2H), 2.35 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 171.88, 140.28, 136.25, 135.36, 134.53, 132.86, 131.27, 131.06, 130.63, 127.97, 127.93, 127.54, 125.01, 38.65, 20.90. Spectra matched those previously reported. [10]



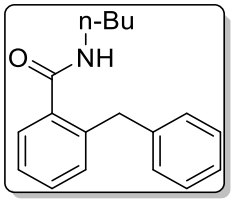
2-(4-methylbenzyl)benzamide: following **general procedure 2.** with 2-(4-methylbenzyl)benzonitrile (201 mg, 0.97 mmol) and after purification via column chromatography yielded the desired product in 96% yield (209 mg, 0.93 mmol). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.47 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.38 – 7.33 (m, 1H), 7.22 (t, *J* = 8.0 Hz, 2H), 7.07 (s, 4H), 5.87 (d, *J* = 115.4 Hz, 2H), 4.19 (s, 2H), 2.30 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 172.39, 139.19, 137.72, 135.70, 135.52, 131.10, 130.44, 129.28, 128.87, 127.46, 126.33, 38.39, 21.06. [M+H] 226.1154, found 226.1154.



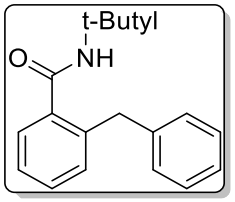
2-benzyl-N-methoxybenzamide following **general procedure 4 B** 2-benzylbenzoicacid and methoxyaminde hydrochloride**.** Yielded the desired product was yielded in 56% yield (26 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.62 (s, 1H), 7.38 – 7.30 (m, 2H), 7.27 – 7.17 (m, 5H), 7.17 – 7.10 (m, 3H), 4.16 (s, 2H), 3.65 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.70, 140.64, 140.03, 132.87, 131.22, 130.86, 129.21, 128.59, 127.83, 126.42, 126.31, 64.42, 38.83. Spectra matched those previously reported.[13]



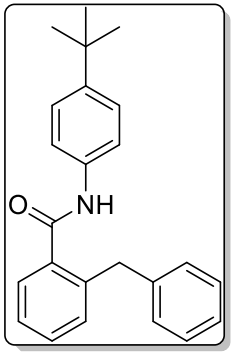
2-benzyl-N-methylbenzamide following **general procedure 4 B** with 2-benzylbenzoicacid (28 mg, 0.132 mmol) and methyl amine (4.9 mg, 0.158 mmol). Yielded the desired product in 84% yield (25 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 (ddt, *J* = 7.2, 5.9, 1.4 Hz, 2H), 7.28 – 7.24 (m, 1H), 7.24 – 7.18 (m, 3H), 7.18 – 7.14 (m, 3H), 5.75 (s, 1H), 4.15 (s, 2H), 2.82 (dd, *J* = 4.9, 1.6 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 170.78, 140.90, 138.87, 136.82, 130.96, 129.98, 128.97, 128.45, 127.12, 126.40, 126.14, 38.98, 26.58. [M+H] 226.1154, found 226.1243.



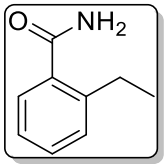
2-benzyl-N-butylbenzamide: following **general procedure 4 A** with 2-benzylbenzoicacid (250 mg, 1.18 mmol) and n-butylamine (95 mg, 1.3 mmol) after purfication (20: 80:1 EtOAc:Hex:TEA) yielded the desired product in 96% yield (304 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.29 (m, 2H), 7.26 (dd, *J* = 8.2, 6.4 Hz, 2H), 7.23 – 7.19 (m, 2H), 7.19 – 7.14 (m, 3H), 6.03 (s, 1H), 4.17 (s, 2H), 3.27 (td, *J* = 7.1, 5.7 Hz, 2H), 1.46 – 1.37 (m, 2H), 1.36 – 1.15 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.01, 140.94, 138.72, 137.07, 130.90, 129.80, 128.97, 128.42, 127.22, 126.29, 126.07, 39.54, 38.84, 31.47, 20.10, 13.80. [M+H] 268.1058, found 268.1716.



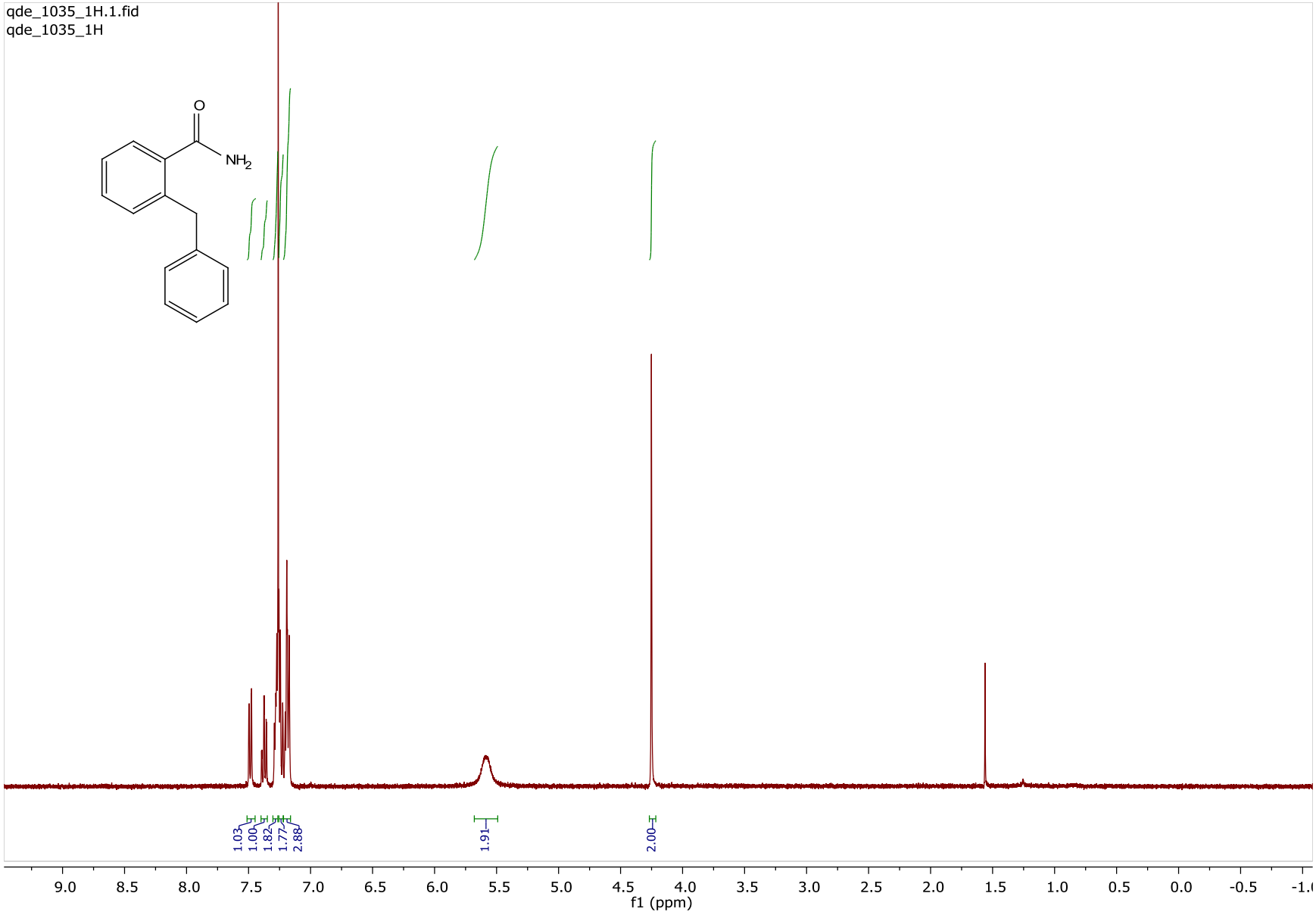
2-benzyl-N-(tert-butyl)benzamide: following **general procedure 4 A** with 2-benzylbenzoicacid (250 mg, 1.18 mmol) and tert-butylamine (95 mg, 1.3 mmol) after purfication (20: 80:1 EtOAc:Hex:TEA) yielded the desired product in 85% yield (278 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.31 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.27 – 7.22 (m, 2H), 7.22 – 7.18 (m, 1H), 7.18 – 7.15 (m, 2H), 7.15 – 7.13 (m, 1H), 5.43 (s, 1H), 4.19 (s, 2H), 1.29 (s, 8H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.48, 141.08, 138.14, 138.00, 131.00, 129.58, 128.90, 128.52, 127.33, 126.37, 126.11, 51.58, 38.79, 28.65. Spectra matched those previously reported. [14]



2-benzyl-N-(4-(tert-butyl)phenyl)benzamide: following **general procedure 4 A** with with 2-benzylbenzoicacid (250 mg, 1.18 mmol) and 4-tert-butylaniline (194 mg, 1.3 mmol) after purfication (20: 80:1 EtOAc:Hex:TEA) yielded the desired product in 68% yield (276 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 – 7.44 (m, 1H), 7.38 – 7.31 (m, 2H), 7.29 (s, 4H), 7.25 – 7.19 (m, 4H), 7.18 – 7.11 (m, 3H), 4.18 (s, 2H), 1.28 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.88, 147.53, 140.66, 138.60, 136.94, 135.14, 131.22, 130.37, 128.92, 128.67, 127.49, 126.62, 126.31, 125.83, 119.78, 38.95, 34.43, 31.40. [M+H] 344.1936, found 344.2034



2-ethylbenzamide: following **general procedure 2** with 2-ethylbenzonitrile (107 mg, 0.82 mmol) yielded the desired product in >99% yield (122 mg) after purification via column chromatography DMC:MeOH (97:3). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.43 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.38 (td, *J* = 7.5, 1.4 Hz, 1H), 7.30 (ddd, *J* = 8.9, 1.6, 0.9 Hz, 1H), 7.23 (td, *J* = 7.5, 1.3 Hz, 1H), 6.08 (d, *J* = 198.6 Hz, 2H), 2.87 (q, *J* = 7.5 Hz, 2H), 1.27 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 172.59, 142.50, 135.11, 130.36, 129.62, 126.92, 26.37, 15.95. [M+H] 150.0841, found 150.0926.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5.0
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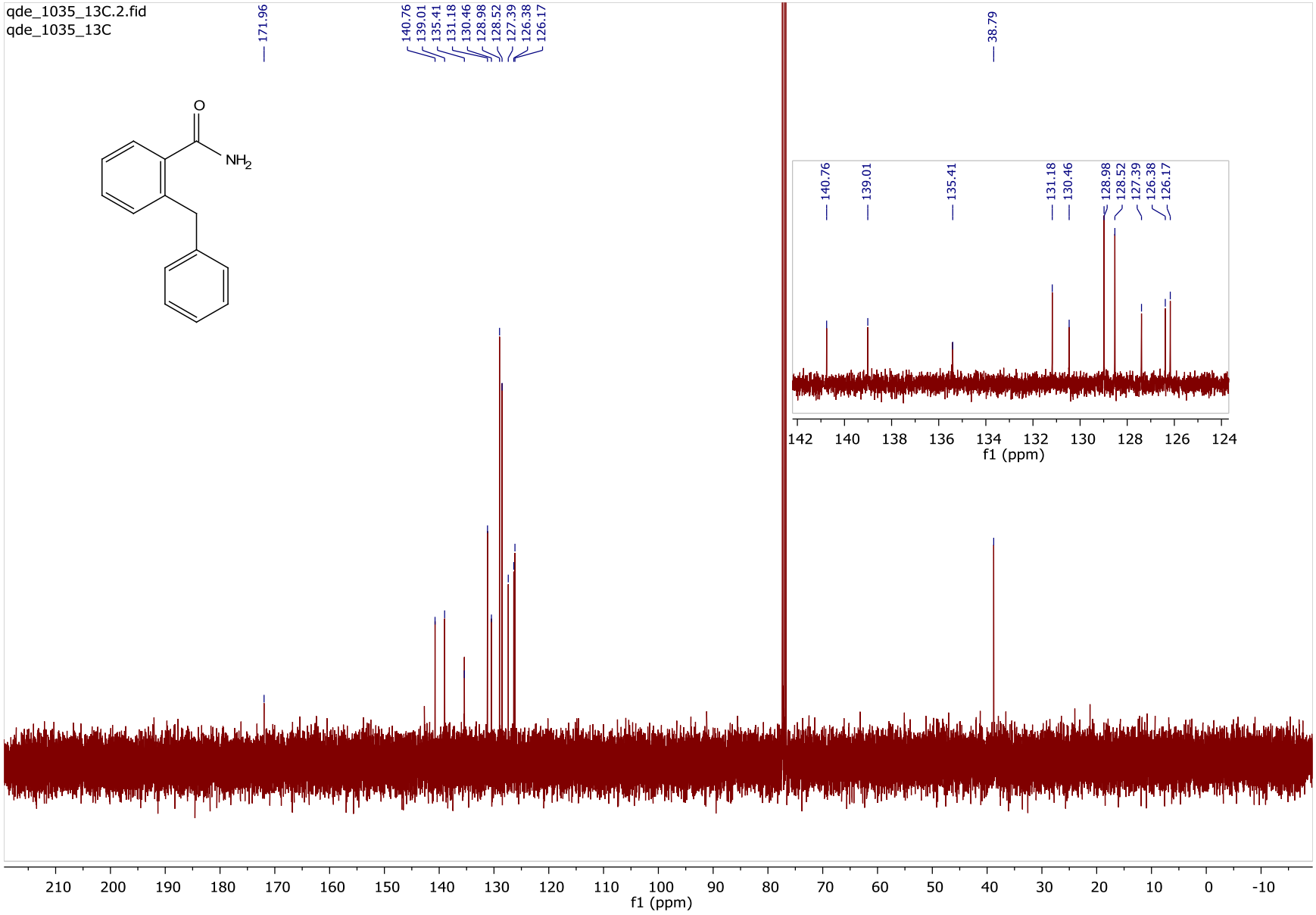
f1 (ppm)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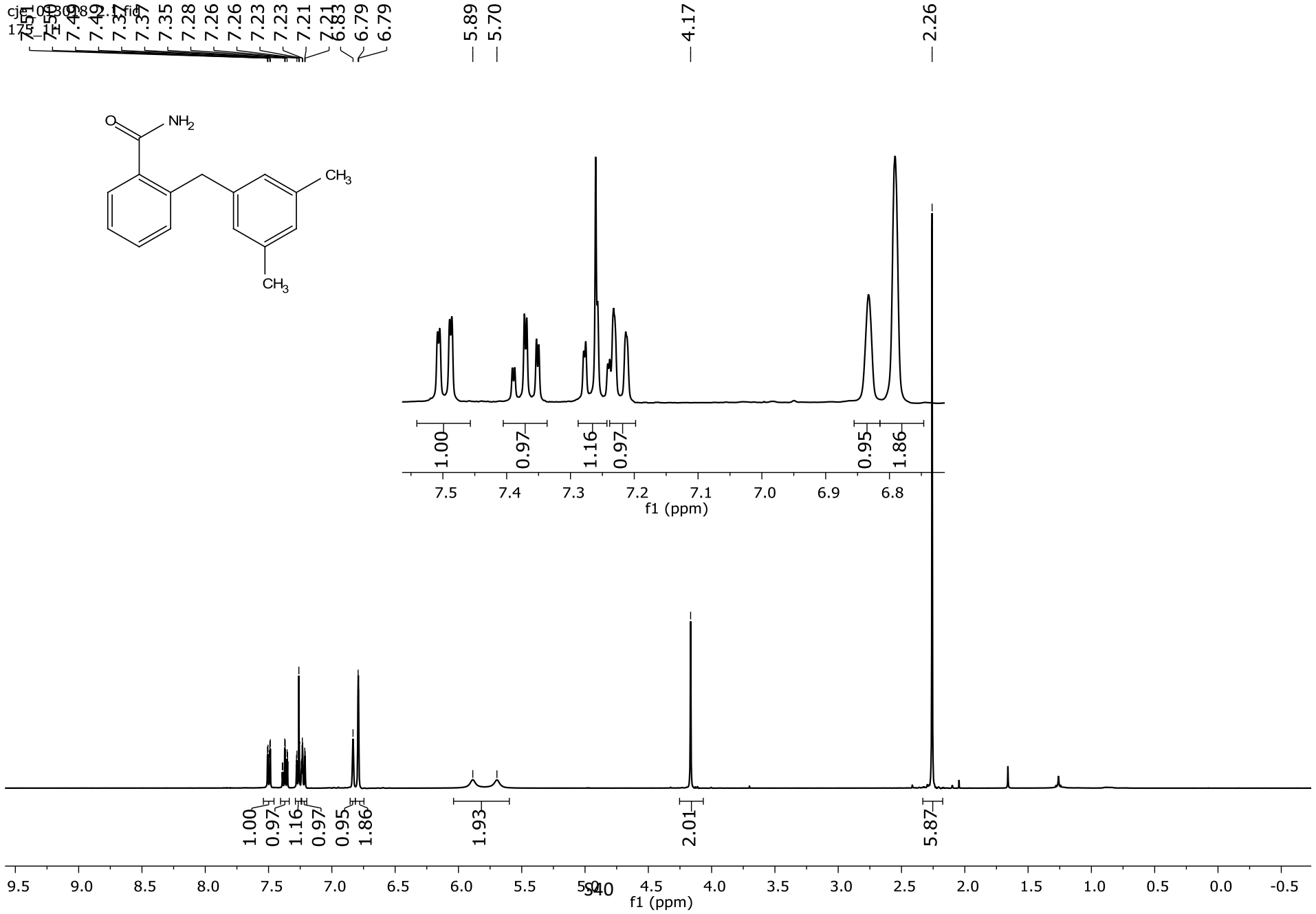
O
NH2
f1 (ppm)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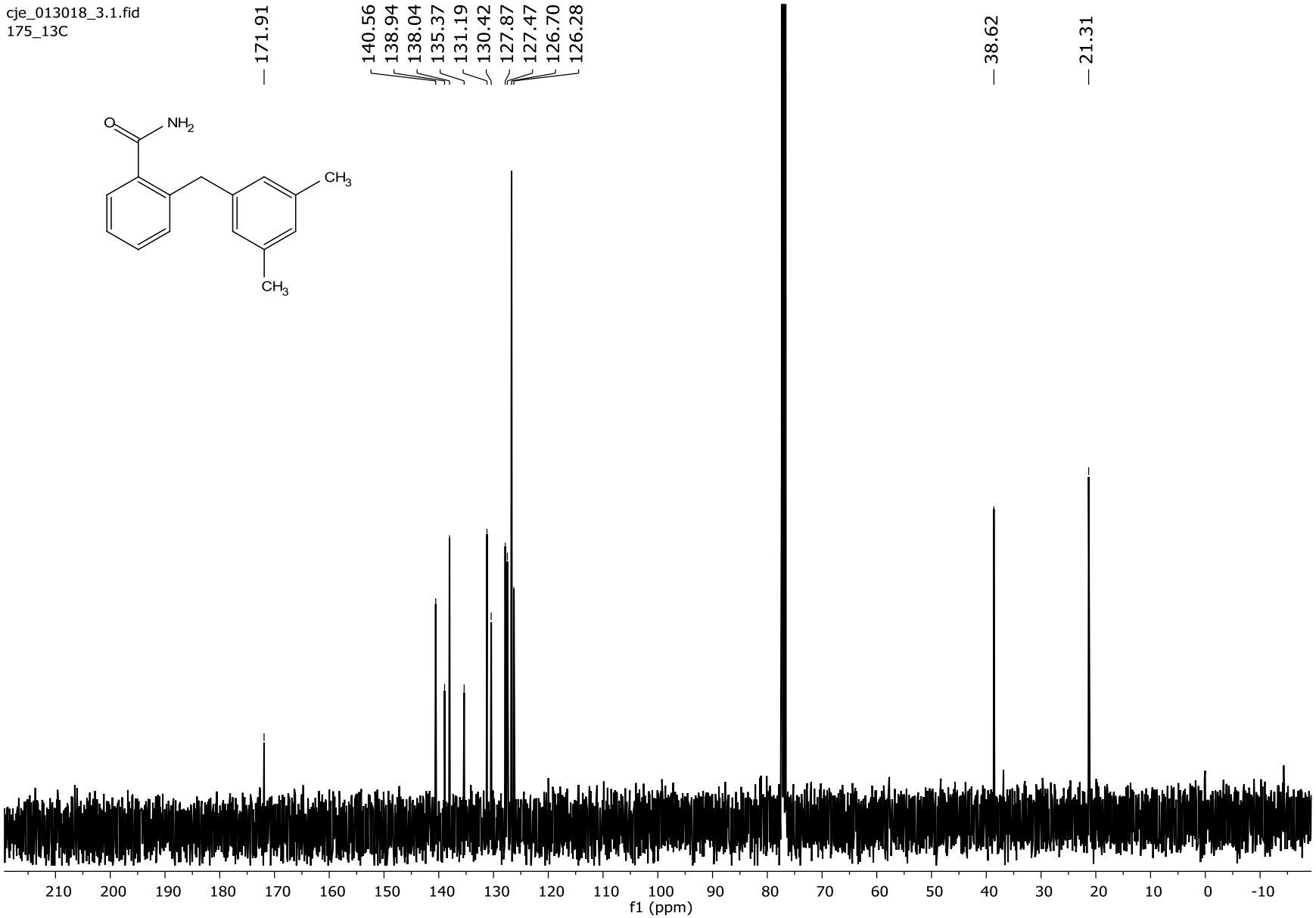
f1 (ppm)
f1 (ppm)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200
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180
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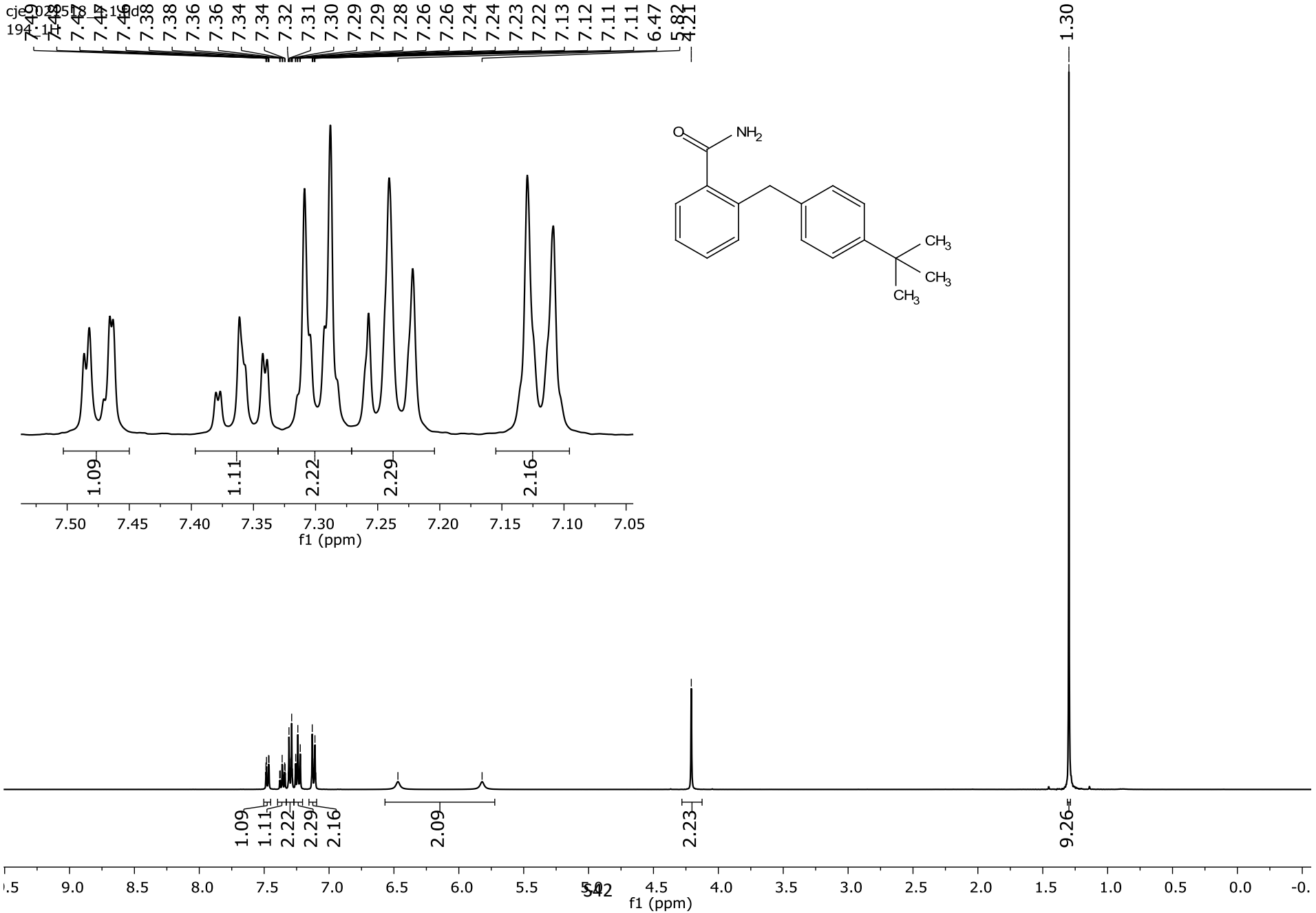
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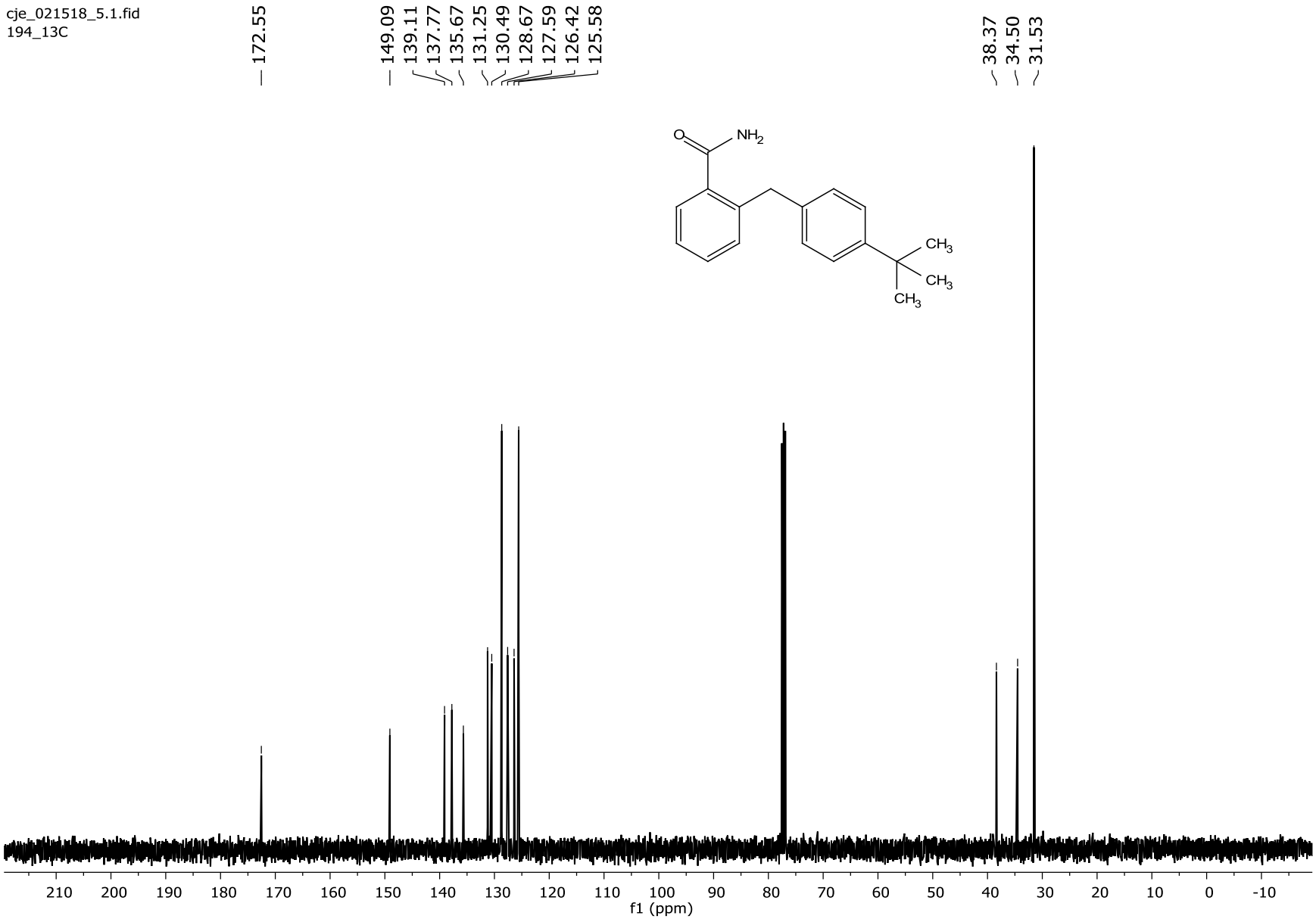
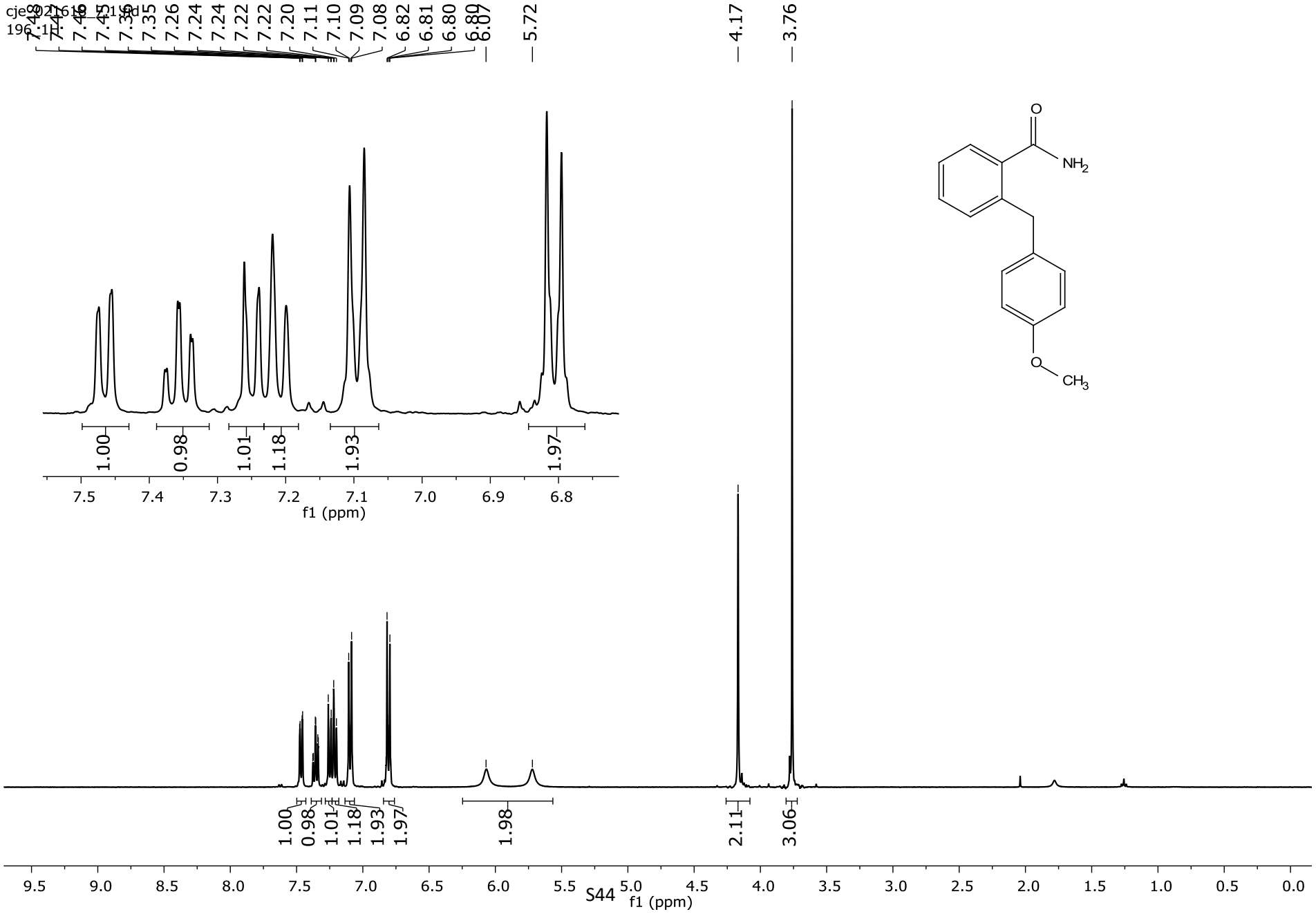
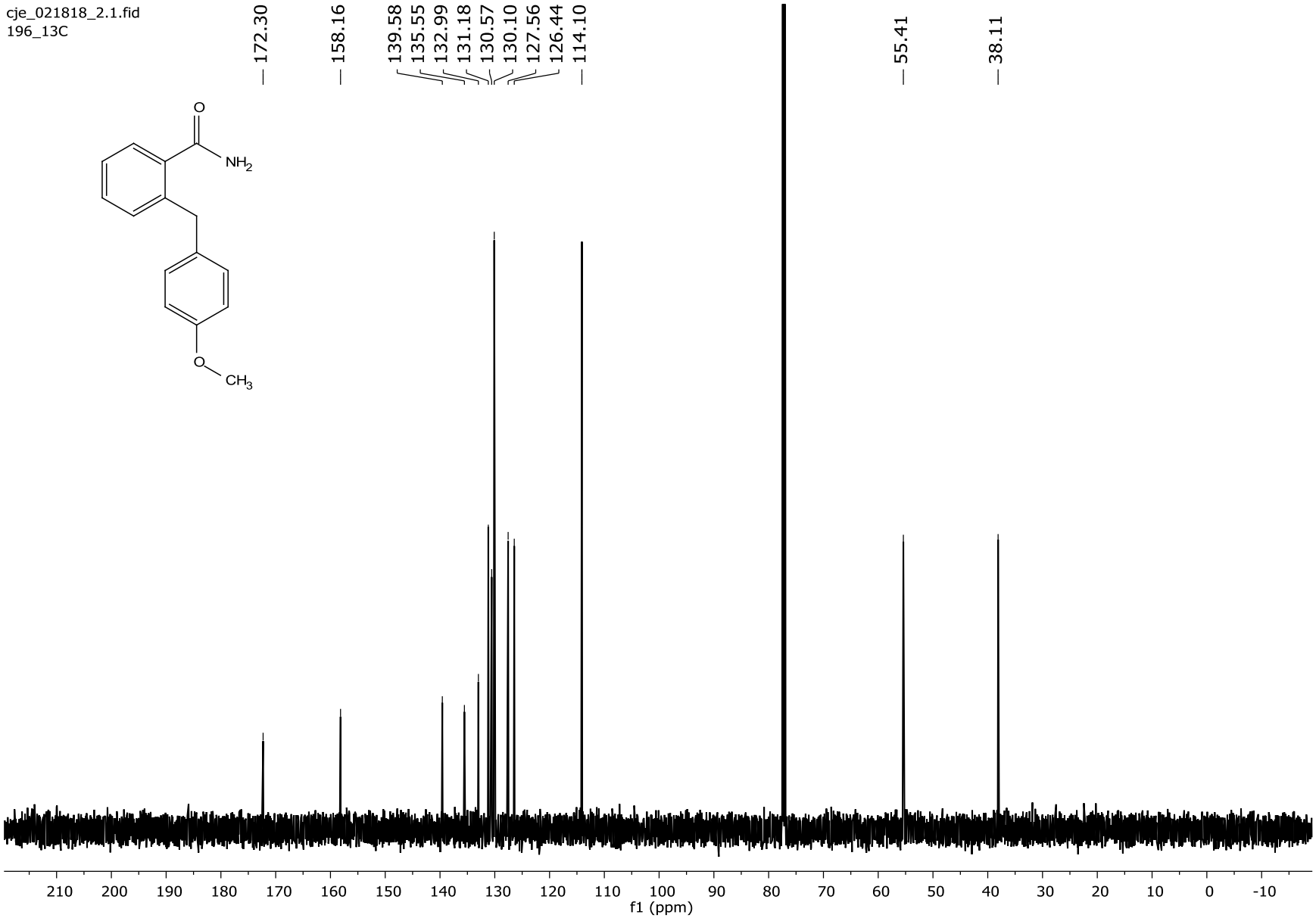
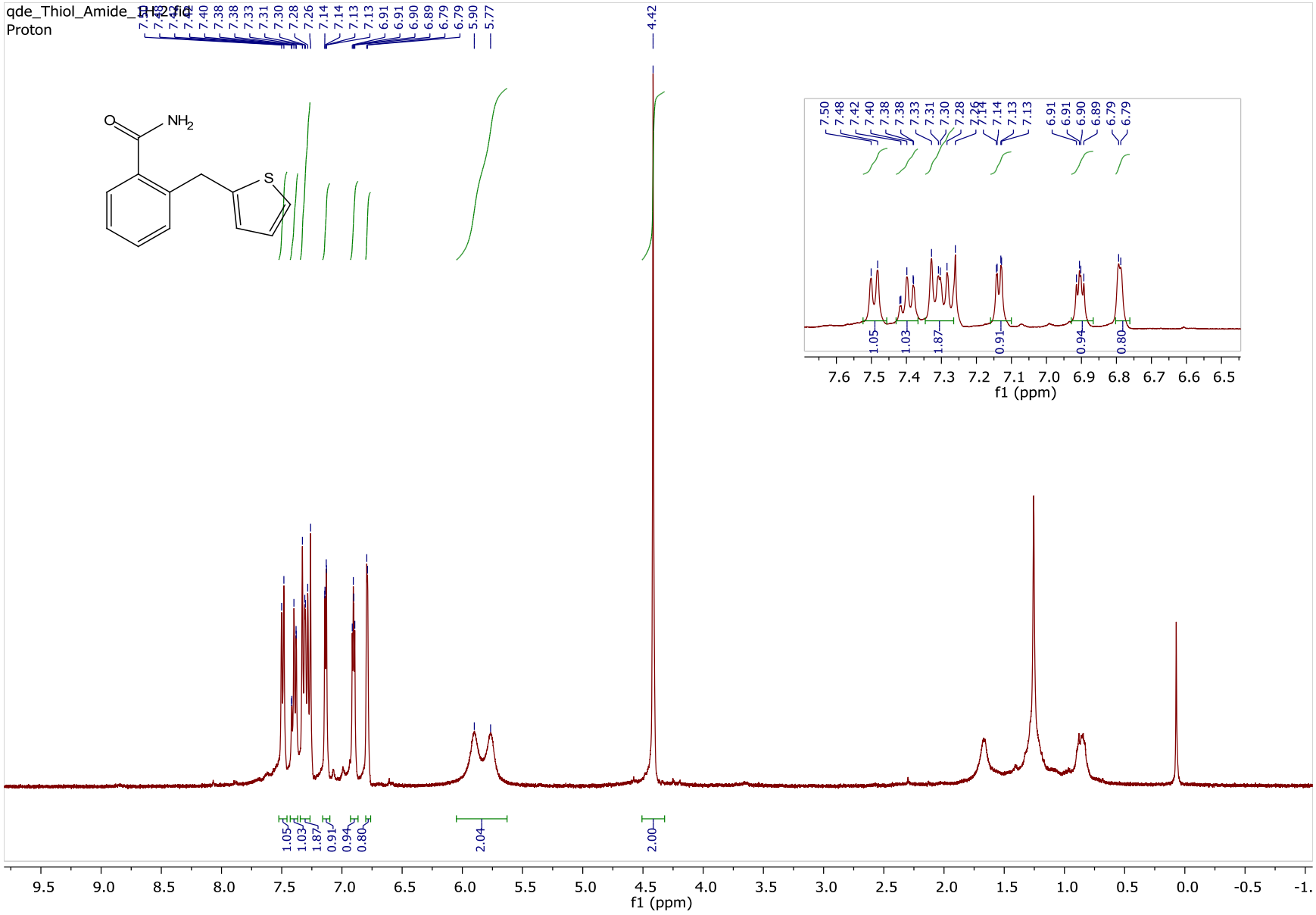
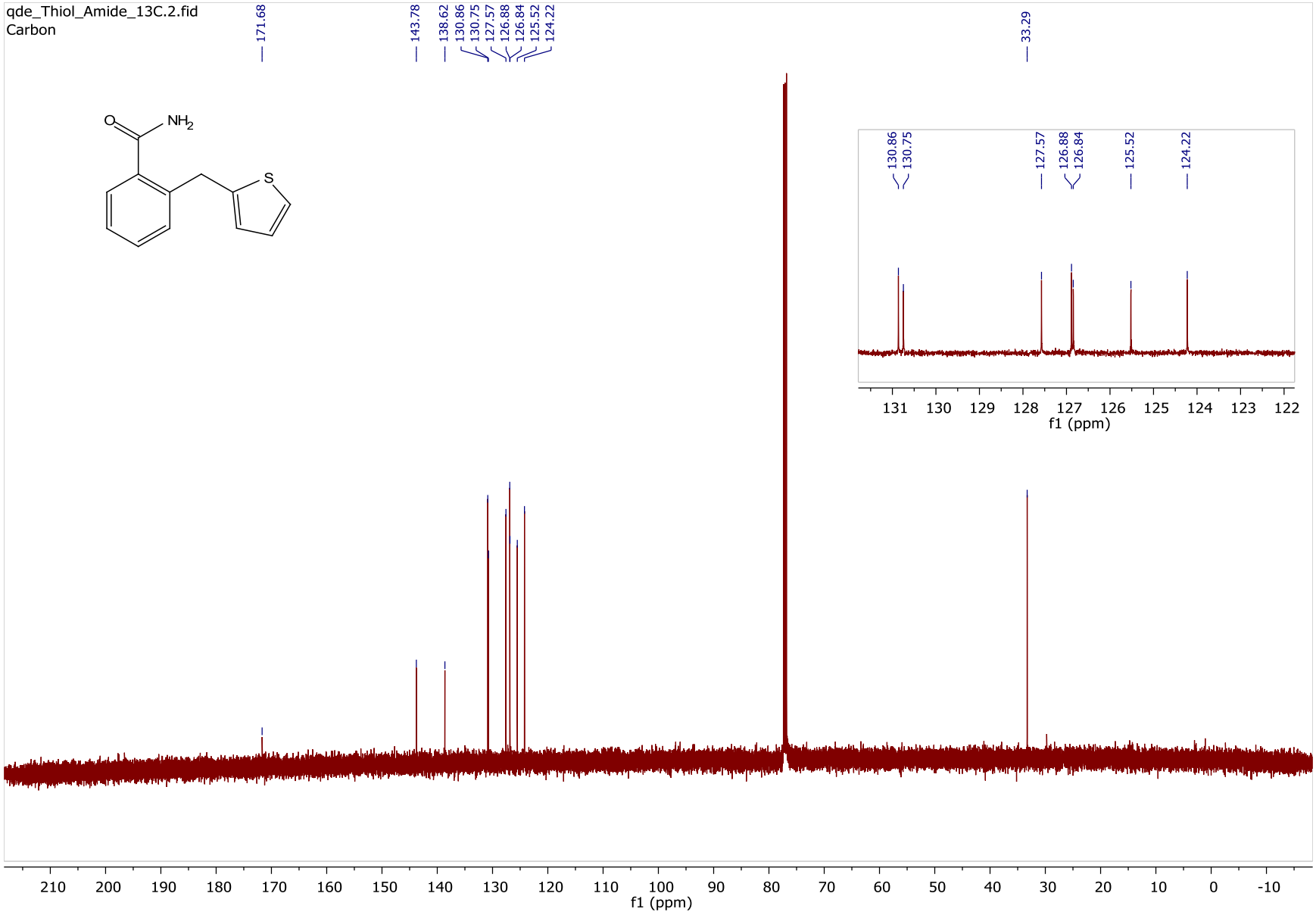
7.26
7.26
7.24
7.24
7.23
7.22
7.13
7.12
7.11
7.11
6.47
5.82
4.21
1.30
O
NH2
CH3
CH3
CH3
1.09
1.11
2.22
2.29
2.16
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
f1 (ppm)
1.09
1.11
2.22
2.29
2.16
2.09
2.23
9.26
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

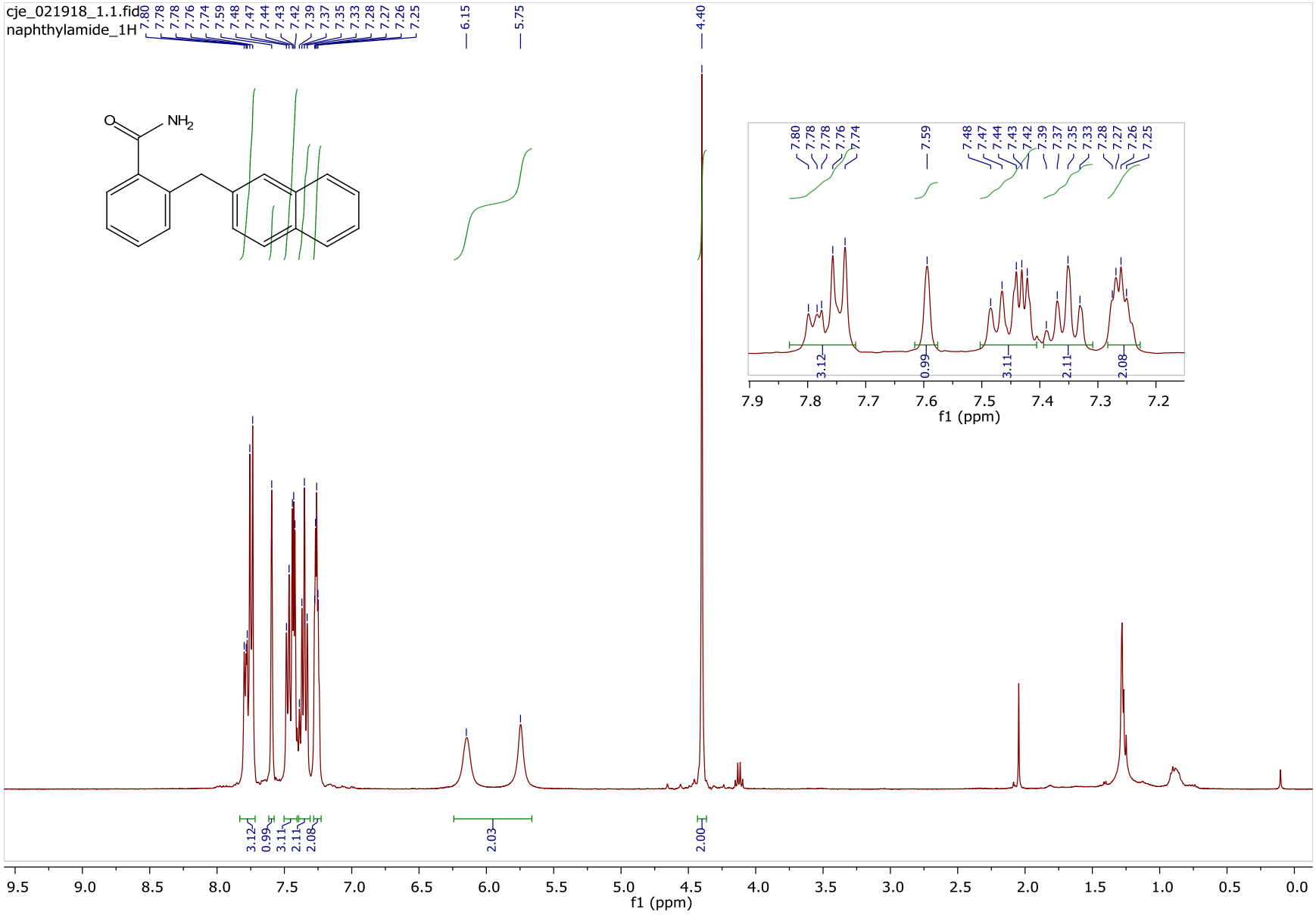

cje_021518_5.1.fid
194_13C
172.55
149.09
139.11
137.77
135.67
131.25
130.49
128.67
127.59
126.42
125.58
38.37
34.50
31.53
O
NH2
CH3
CH3
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

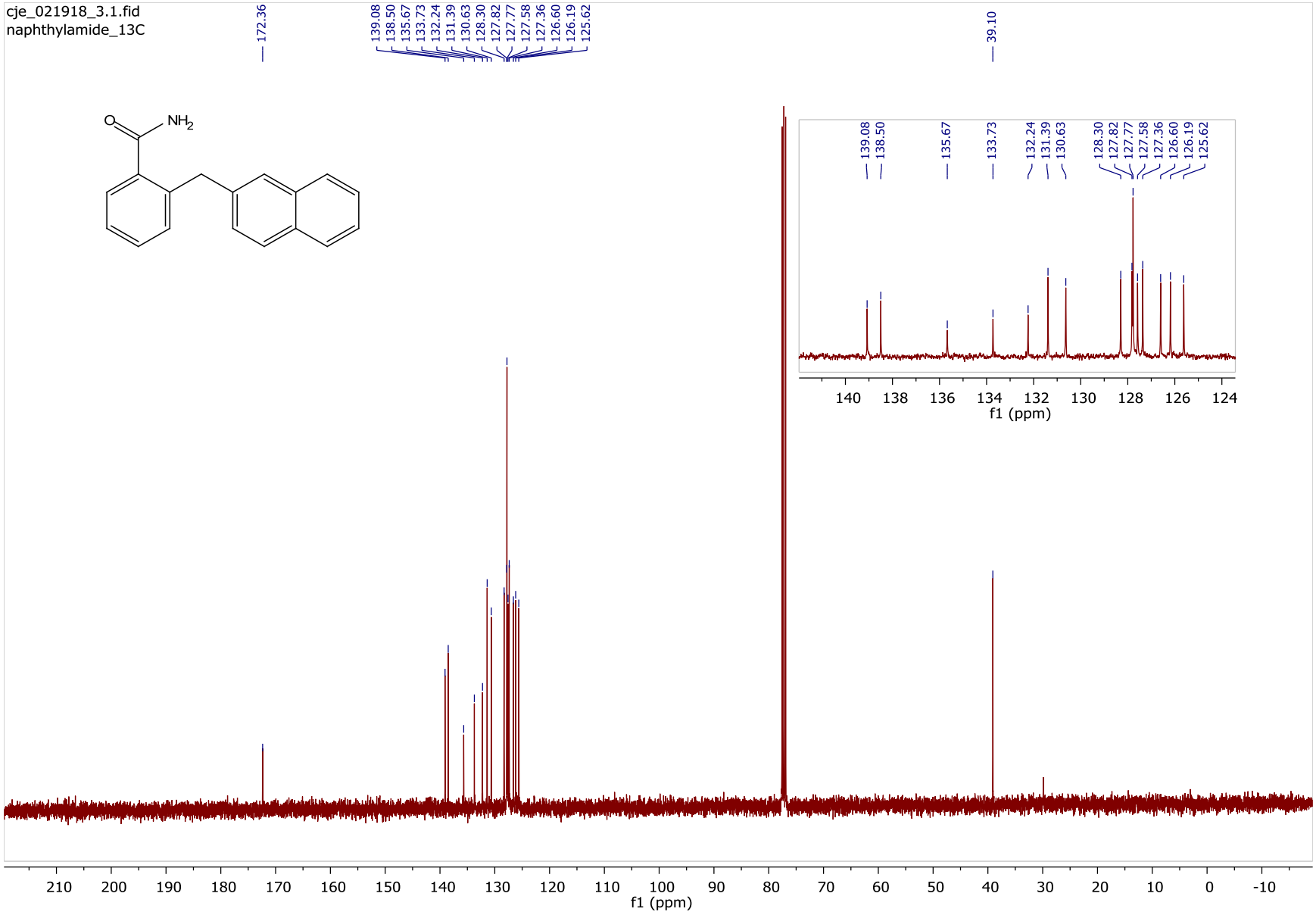

7.48
7.47
7.46
7.45
7.36
7.35
7.26
7.24
7.24
7.22
7.22
7.20
7.11
7.10
7.09
7.08
6.82
6.81
6.80
6.80
6.07
5.72
4.17
3.76
NH2
O
O
CH3
1.00
0.98
1.01
1.18
1.93
1.97
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
f1 (ppm)
1.00
0.98
1.01
1.18
1.93
1.97
1.98
2.11
3.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

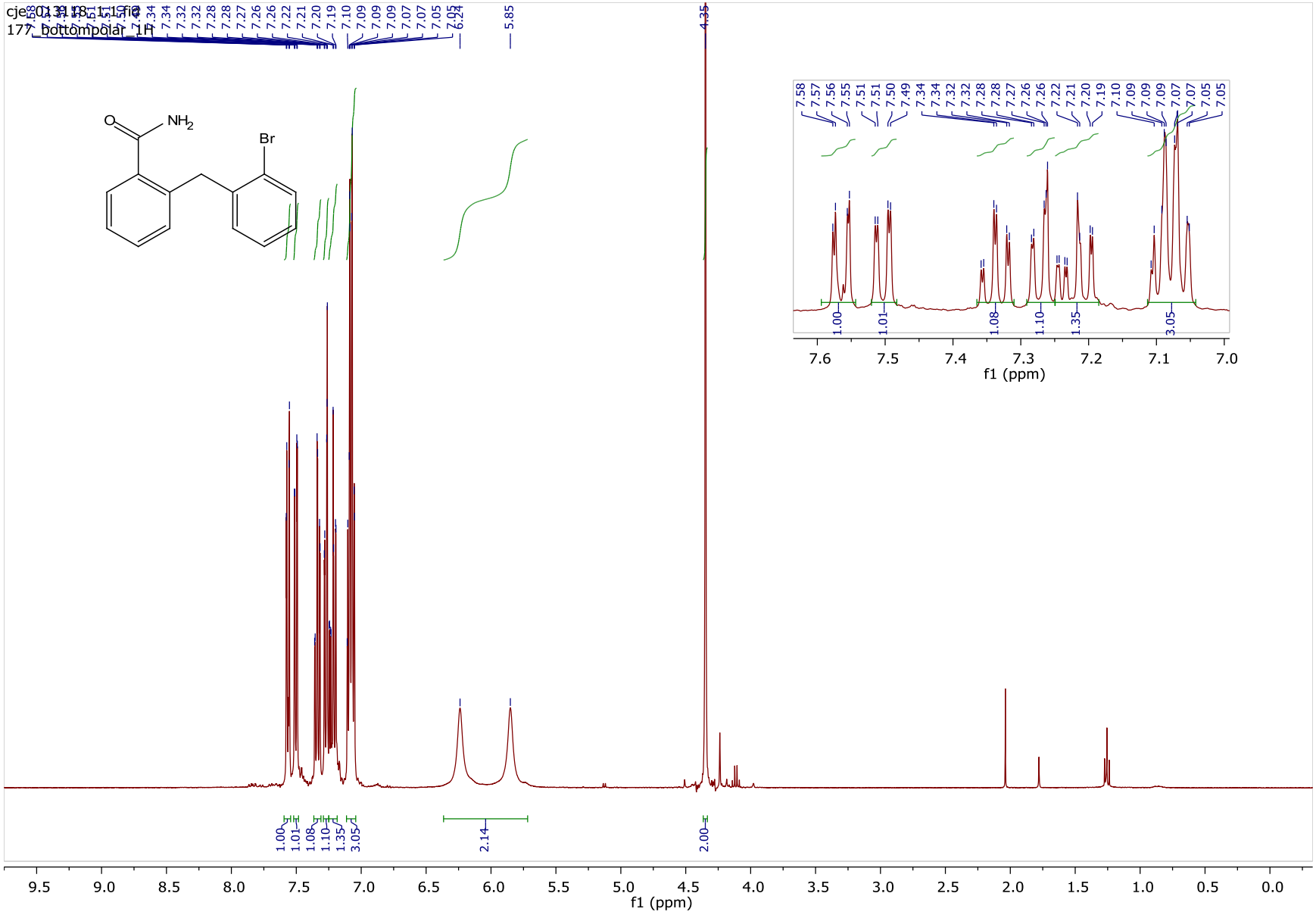

cje_021818_2.1.fid
196_13C
172.30
158.16
139.58
135.55
132.99
131.18
130.57
130.10
127.56
126.44
114.10
55.41
38.11
O
NH2
O
CH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

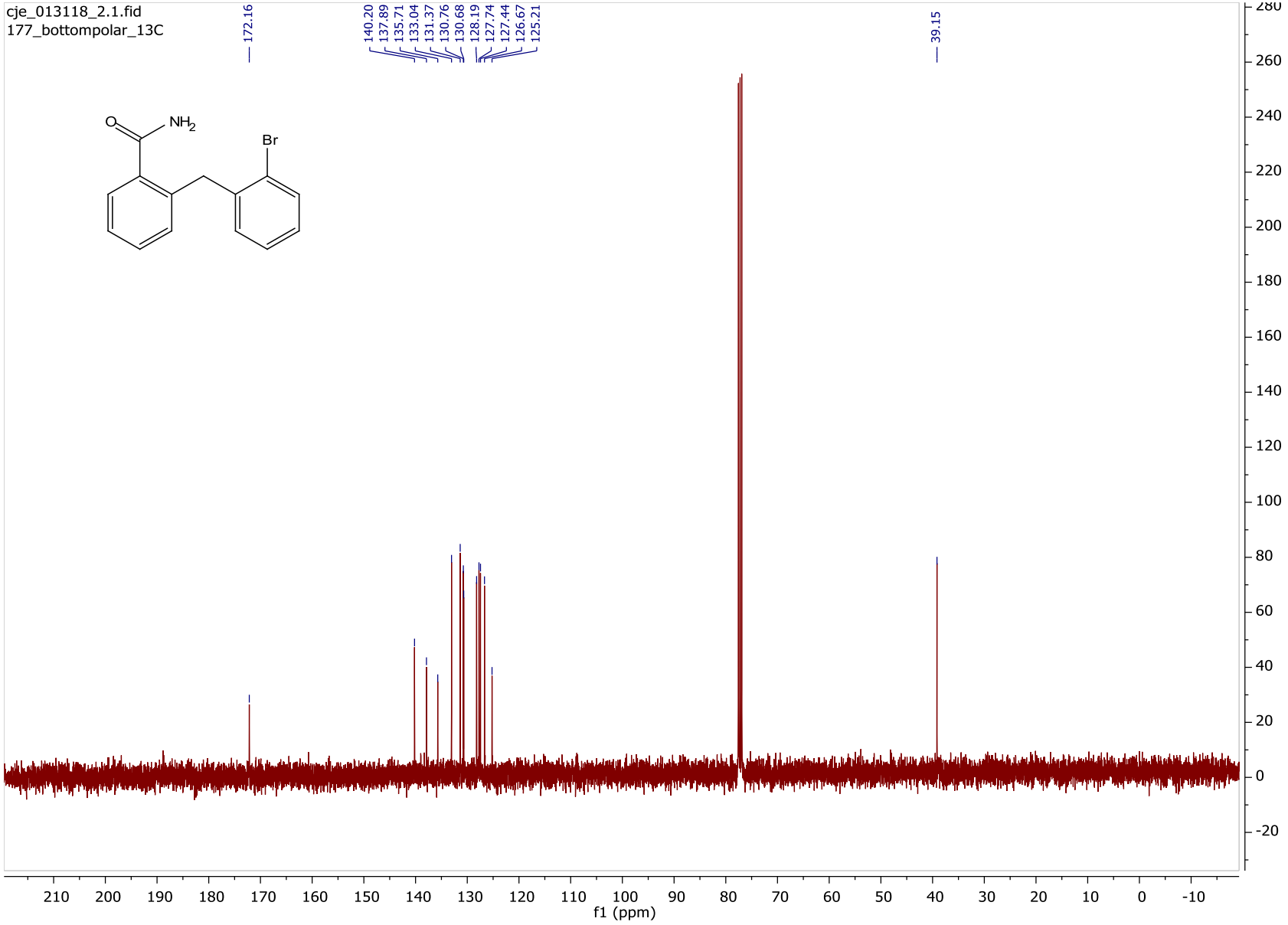

qde_Thiol_Amide_1H.2.fid
Proton
O
NH2
S
7.50
7.48
7.42
7.40
7.38
7.38
7.33
7.31
7.30
7.28
7.26
7.14
7.14
7.13
7.13
6.91
6.91
6.90
6.89
6.79
6.79
5.90
5.77
4.42
1.05
1.03
1.87
0.91
0.94
0.80
2.04
2.00
f1 (ppm)

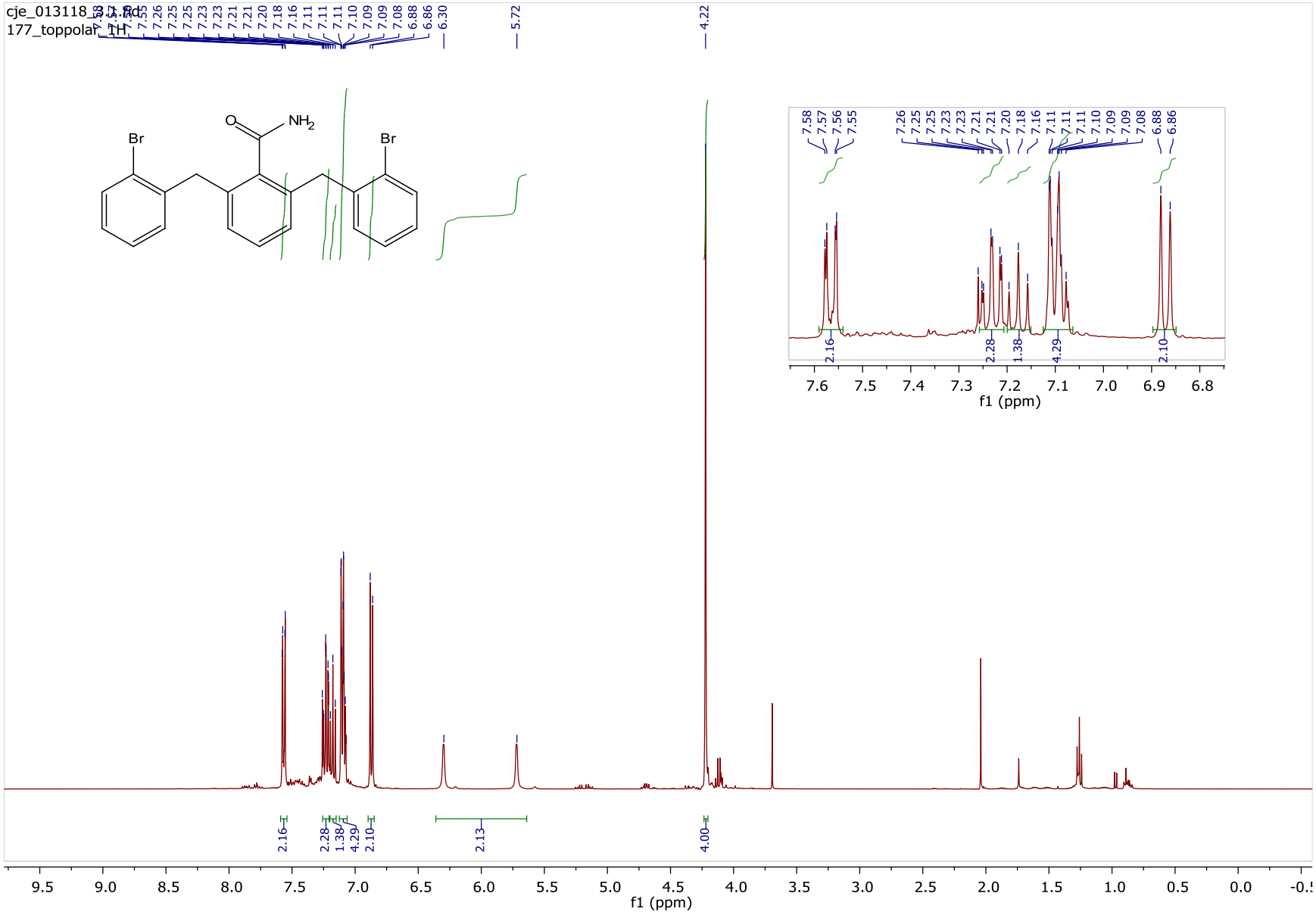

qde_Thiol_Amide_13C.2.fid
Carbon
171.68
143.78
138.62
130.86
130.75
127.57
126.88
126.84
125.52
124.22
33.29
O
NH2
S
f1 (ppm)

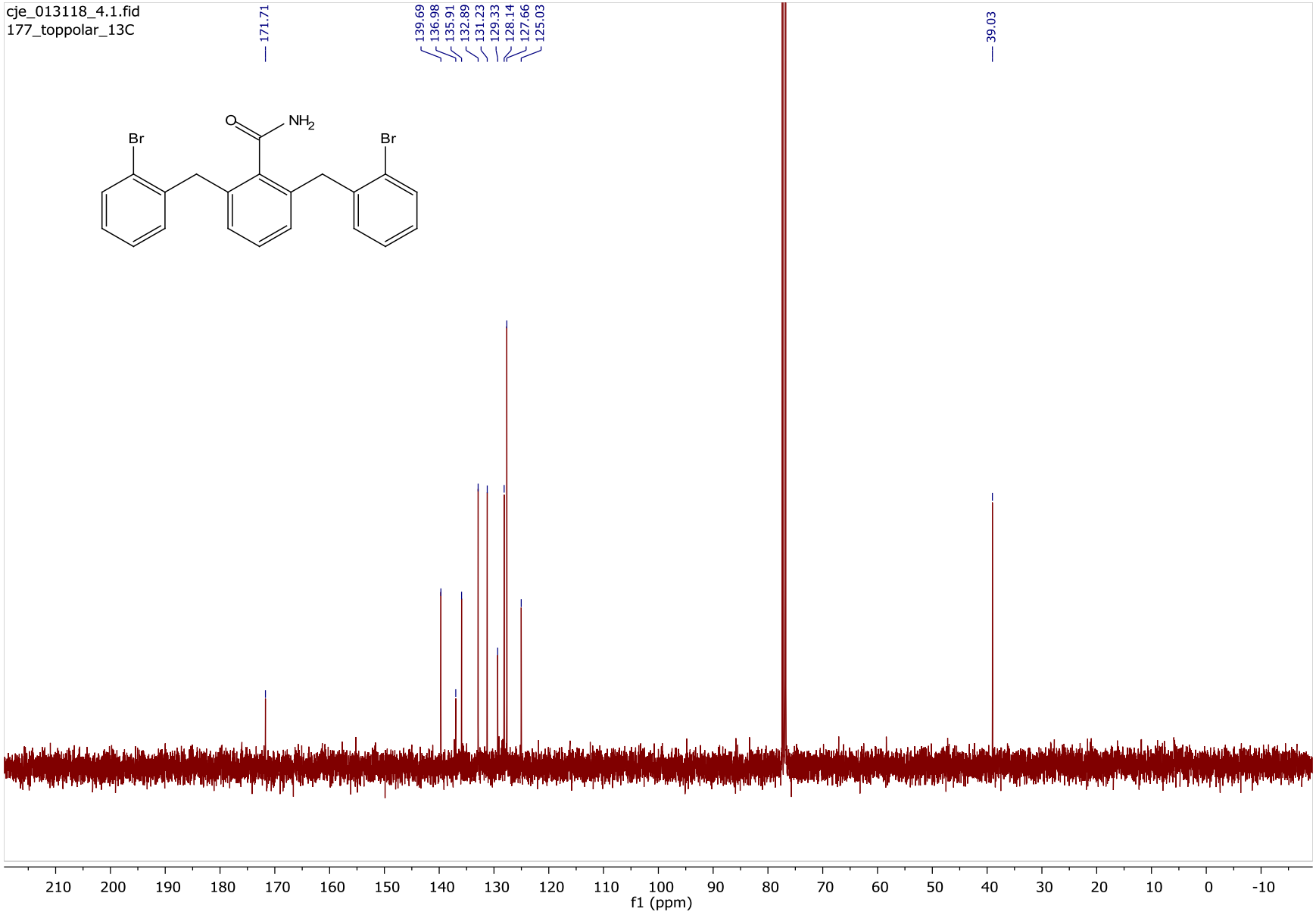

cje_021918_1.1.fid
naphthylamide_1H
7.80
7.78
7.78
7.76
7.74
7.59
7.48
7.47
7.44
7.43
7.42
7.39
7.37
7.35
7.33
7.28
7.27
7.26
7.25
6.15
5.75
4.40
O
NH2
3.12
0.99
3.11
2.11
2.08
2.03
2.00
f1 (ppm)

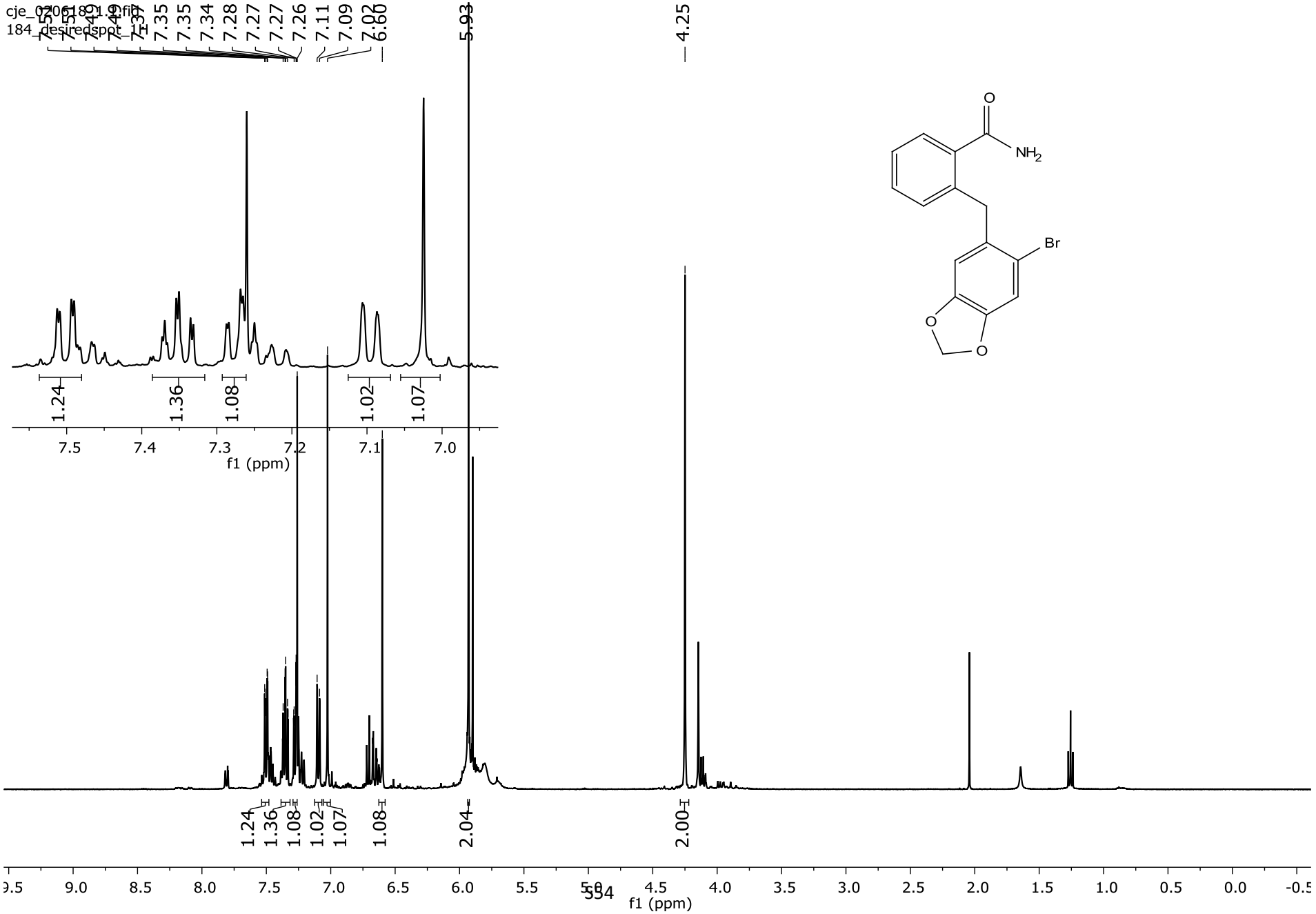

cje_021918_3.1.fid
naphthylamide_13C
172.36
139.08
138.50
135.67
133.73
132.24
131.39
130.63
128.30
127.82
127.77
127.58
127.36
126.60
126.19
125.62
39.10
O
NH2
f1 (ppm)
f1 (ppm)

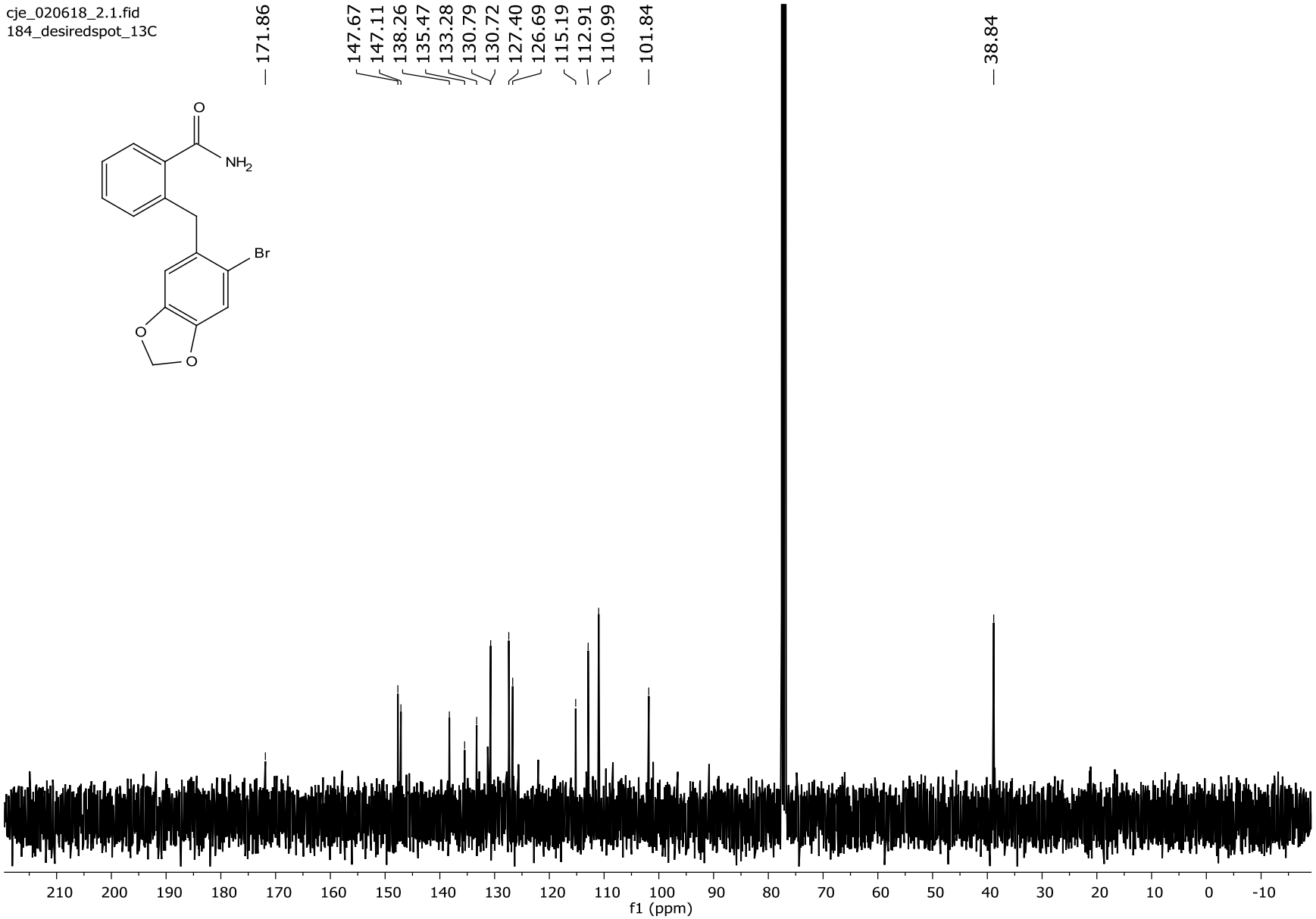

O
NH2
Br
f1 (ppm)

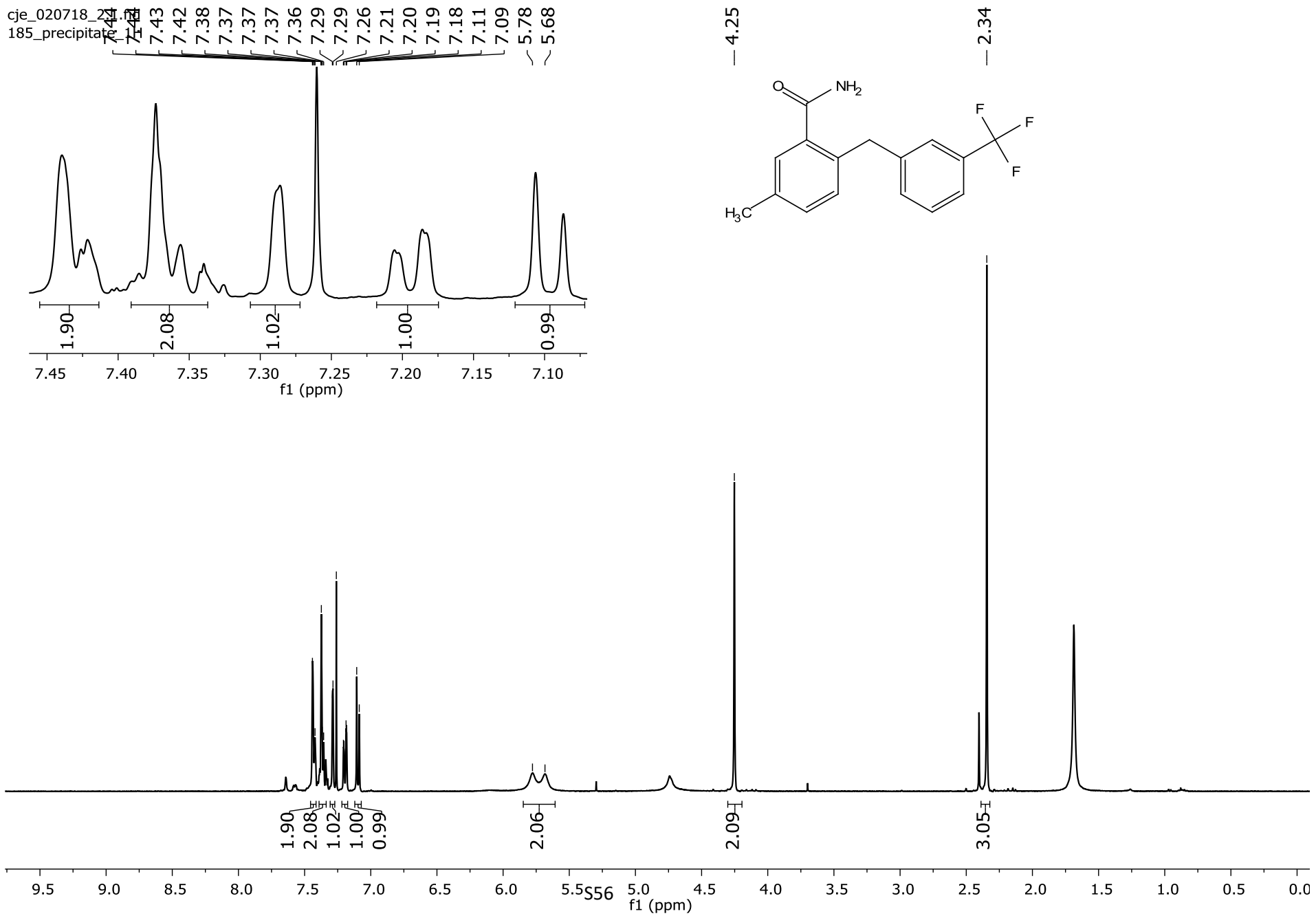

cje_013118_2.1.fid
177_bottompolar_13C
172.16
140.20
137.89
135.71
133.04
131.37
130.76
130.68
128.19
127.74
127.44
126.67
125.21
39.15
O
NH2
Br
f1 (ppm)

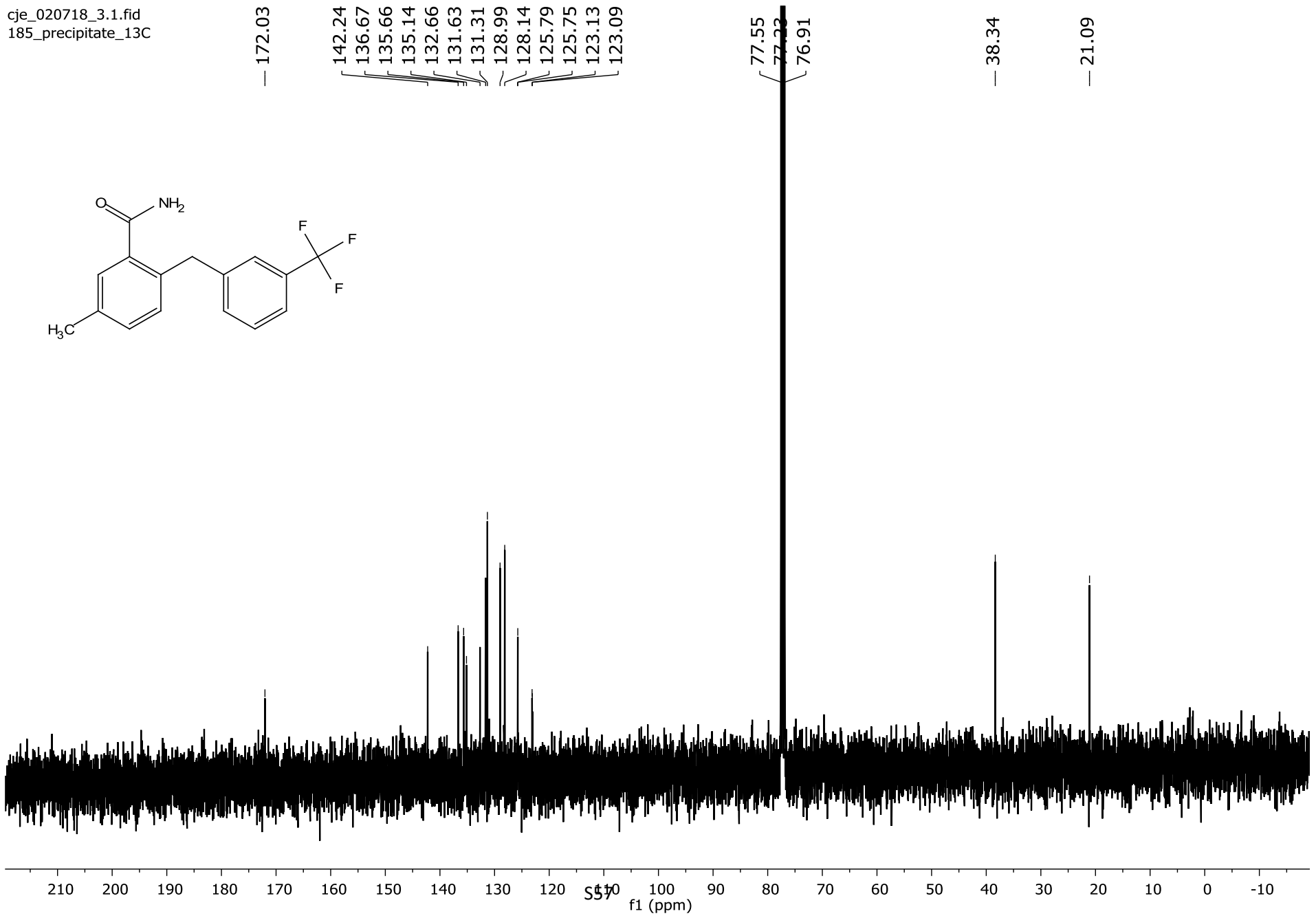

cje_013118_1H.fid
177_toppolar_1H
7.58
7.57
7.56
7.55
7.26
7.25
7.25
7.23
7.23
7.21
7.21
7.20
7.18
7.16
7.11
7.11
7.11
7.10
7.09
7.09
7.08
6.88
6.86
6.30
5.72
4.22
O
NH2
Br
Br
2.16
2.28
1.38
4.29
2.10
2.13
4.00
f1 (ppm)

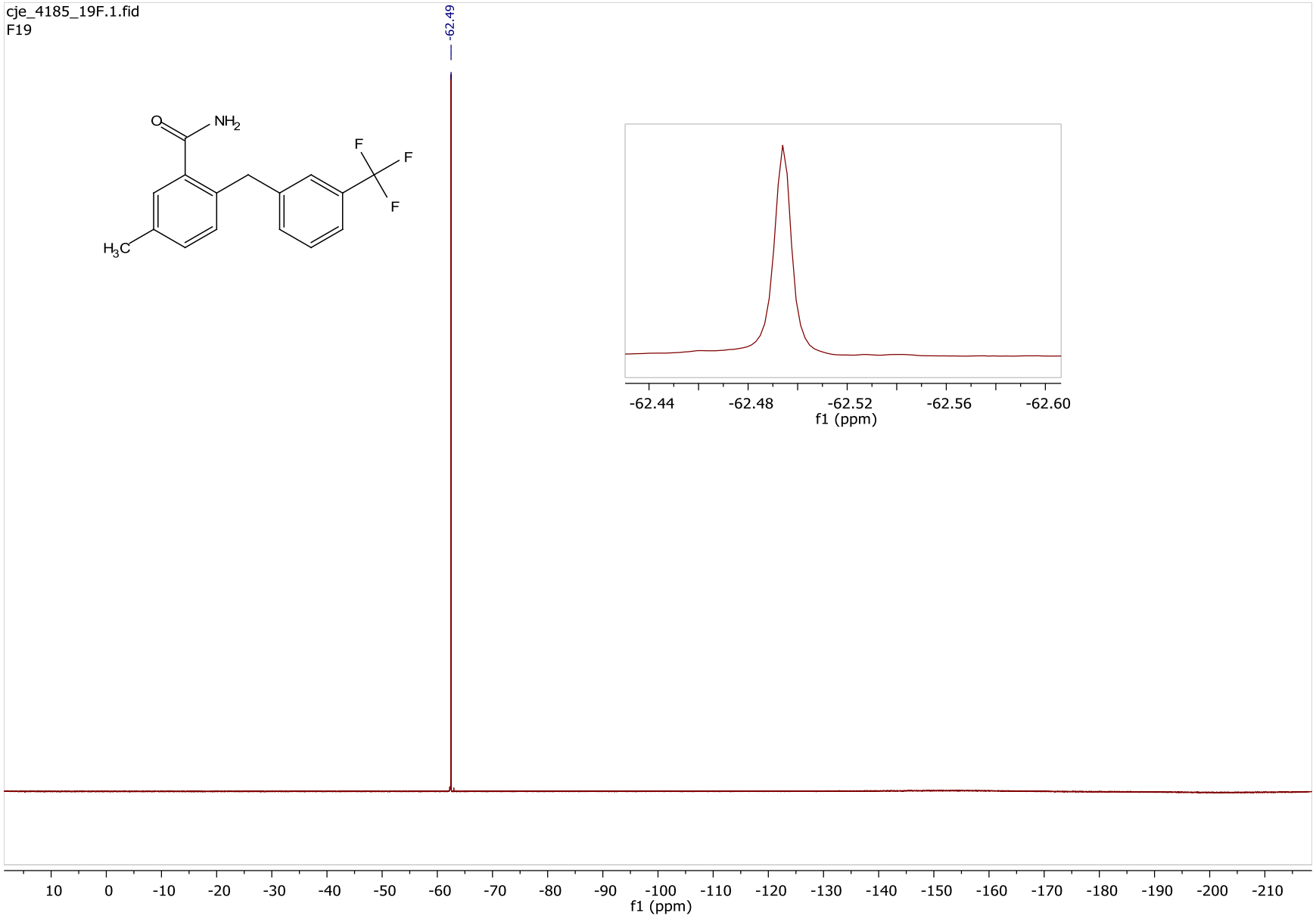

cje_013118_4.1.fid
177_toppolar_13C
171.71
139.69
136.98
135.91
132.89
131.23
129.33
128.14
127.66
125.03
39.03
O
NH2
Br
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

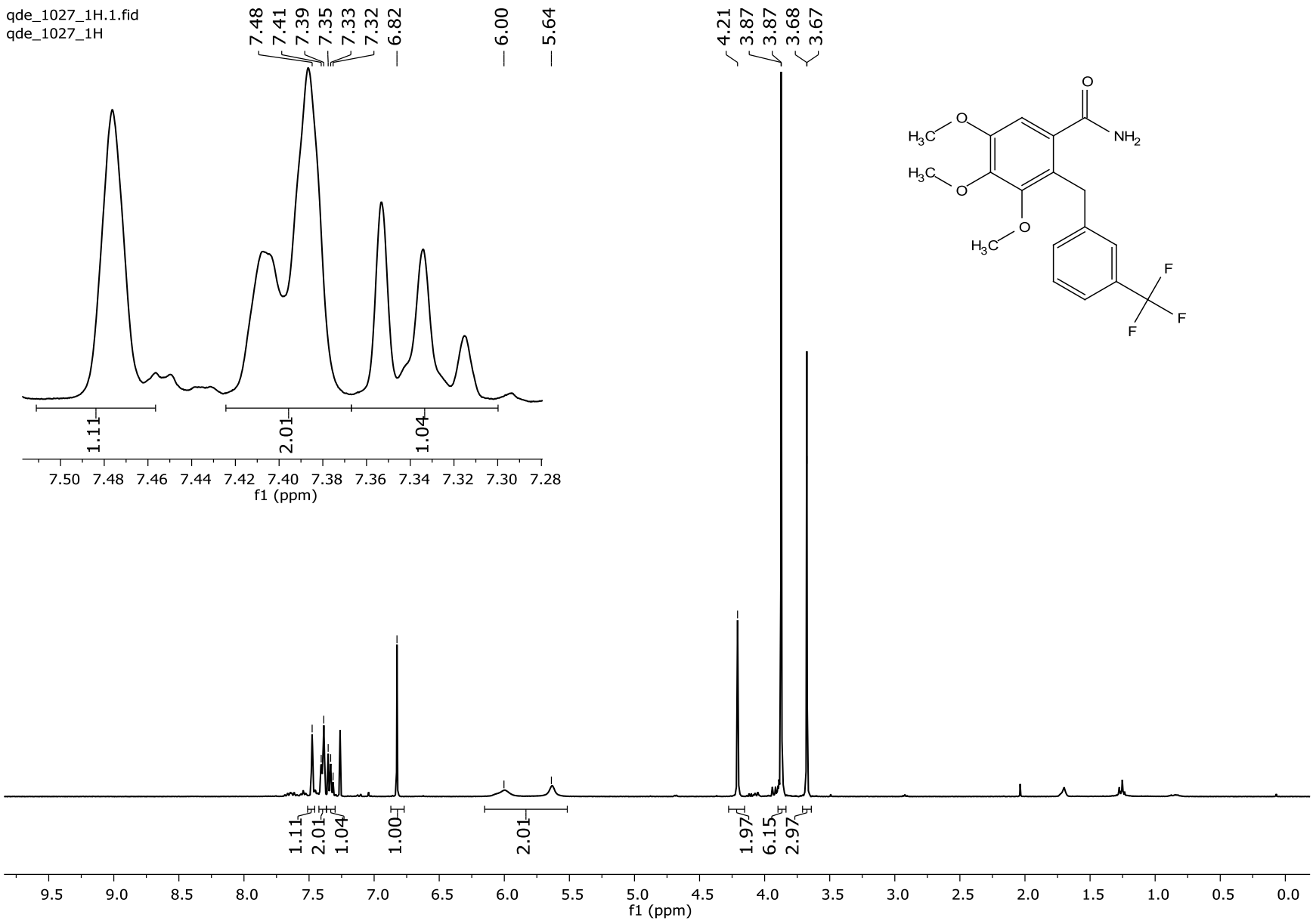

cje_020518_1.10.fid
184_desiredspot_1.3.7
7.55
7.55
7.49
7.49
7.37
7.35
7.35
7.34
7.28
7.27
7.27
7.26
7.11
7.09
7.02
6.80
5.93
4.25
1.24
1.36
1.08
1.02
1.07
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)
1.24
1.36
1.08
1.02
1.07
1.08
2.04
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
O
NH2
Br
O
O
O


cje_020618_2.1.fid
184_desiredspot_13C
171.86
147.67
147.11
138.26
135.47
133.28
130.79
130.72
127.40
126.69
115.19
112.91
110.99
101.84
38.84
O
NH2
Br
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

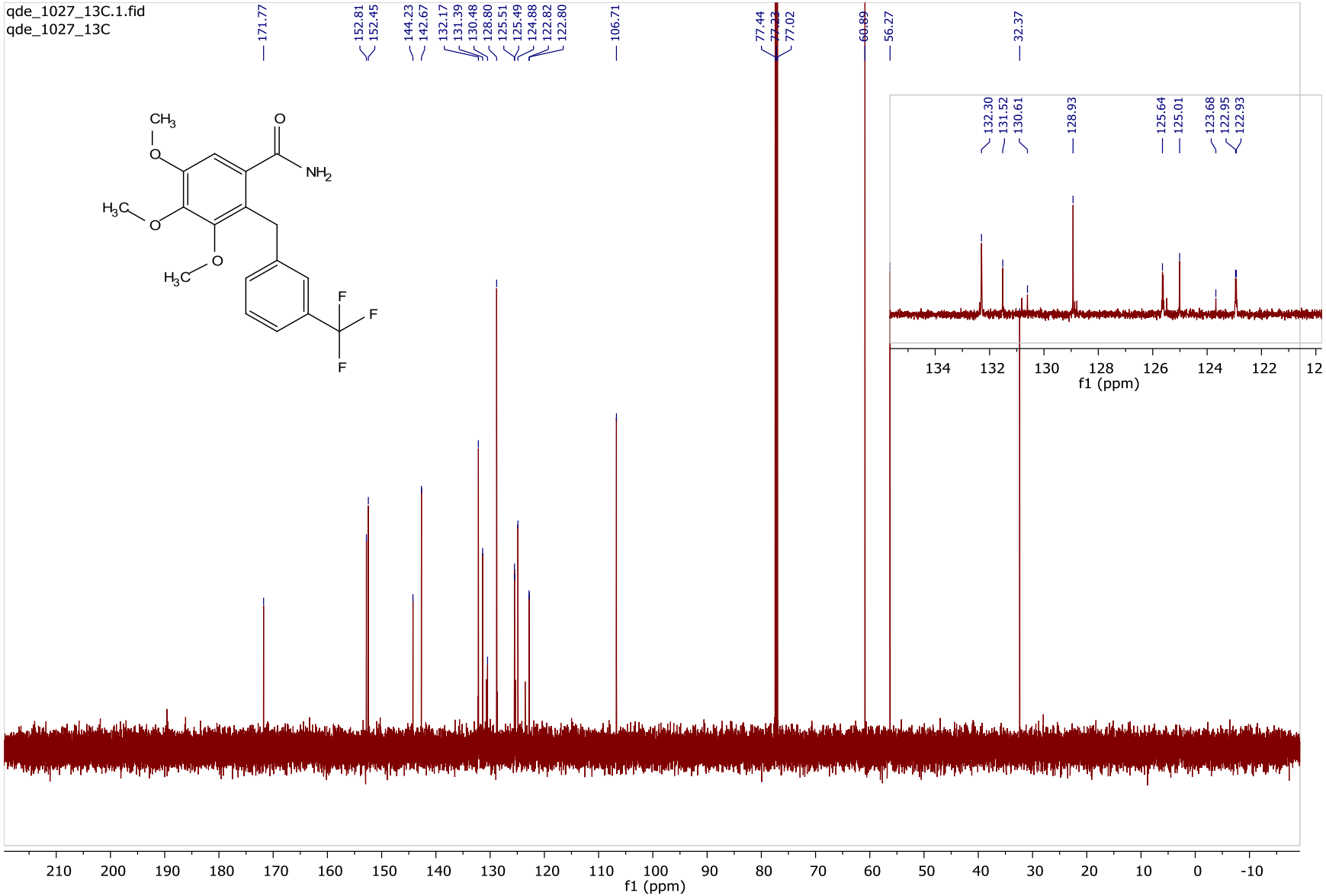

cje_020718_2-1-13
185_precipitate_1-1
7.44
7.43
7.43
7.42
7.38
7.37
7.37
7.37
7.36
7.29
7.29
7.26
7.21
7.20
7.19
7.18
7.11
7.09
5.78
5.68
4.25
2.34
O
NH2
F
F
F
H3C
1.90
2.08
1.02
1.00
0.99
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
f1 (ppm)
1.90
2.08
1.02
1.00
0.99
2.06
2.09
3.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

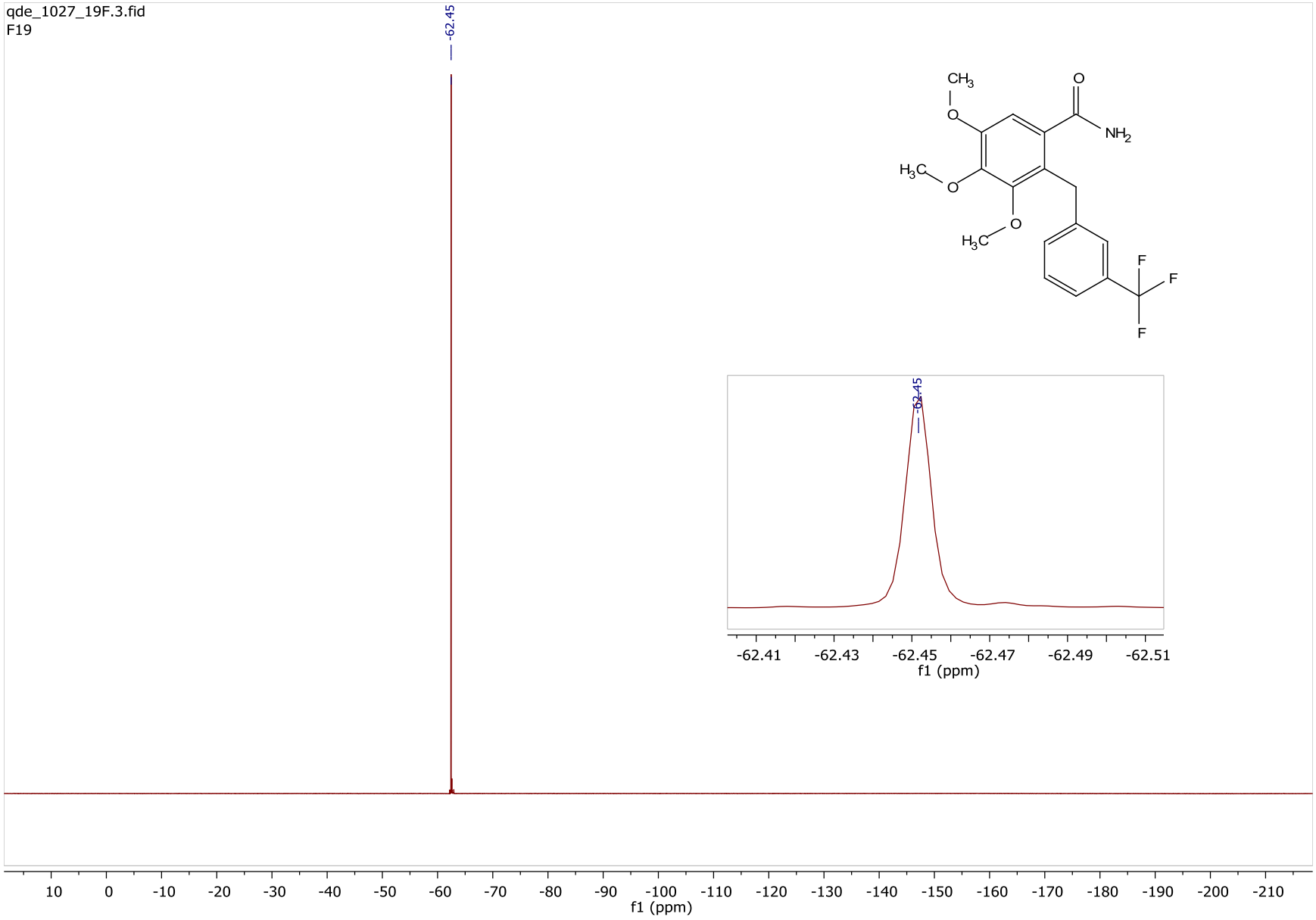

cje_020718_3.1.fid
185_precipitate_13C
172.03
142.24
136.67
135.66
135.14
132.66
131.63
131.31
128.99
128.14
125.79
125.75
123.13
123.09
77.55
77.23
76.91
38.34
21.09
O
NH2
F
F
F
H3C
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

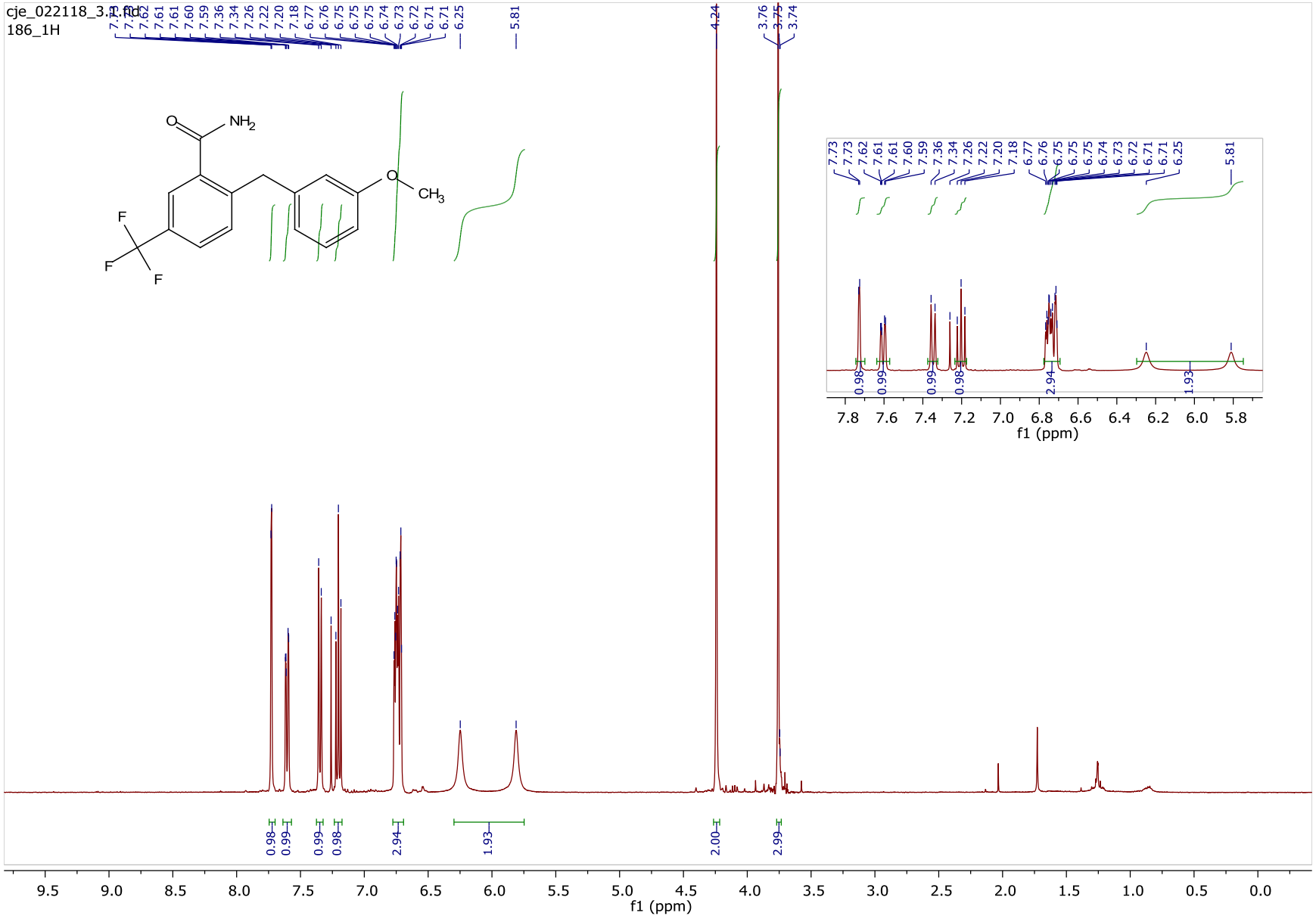

cje_4185_19F.1.fid
F19
-62.49
O
NH2
F
F
F
H3C
-62.44
-62.48
-62.52
-62.56
-62.60
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

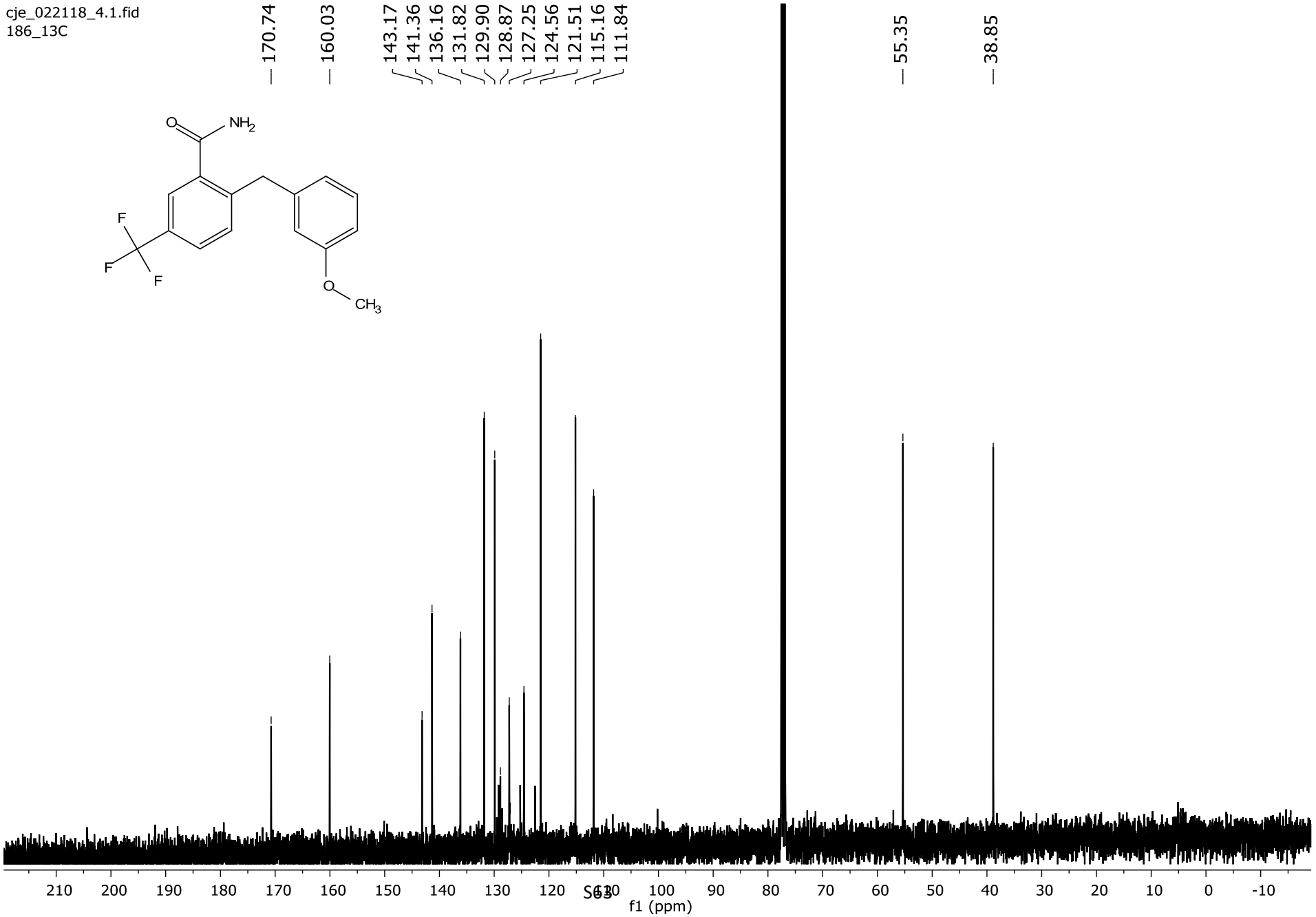

qde_1027_1H.1.fid
qde_1027_1H
7.48
7.41
7.39
7.35
7.33
7.32
6.82
6.00
5.64
4.21
3.87
3.87
3.68
3.67
1.11
2.01
1.04
7.50 7.48 7.46 7.44 7.42 7.40 7.38 7.36 7.34 7.32 7.30 7.28
f1 (ppm)
O
NH2
H3C
O
H3C
O
O
H3C
F
F
F
1.11
2.01
1.04
1.00
2.01
1.97
6.15
2.97
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

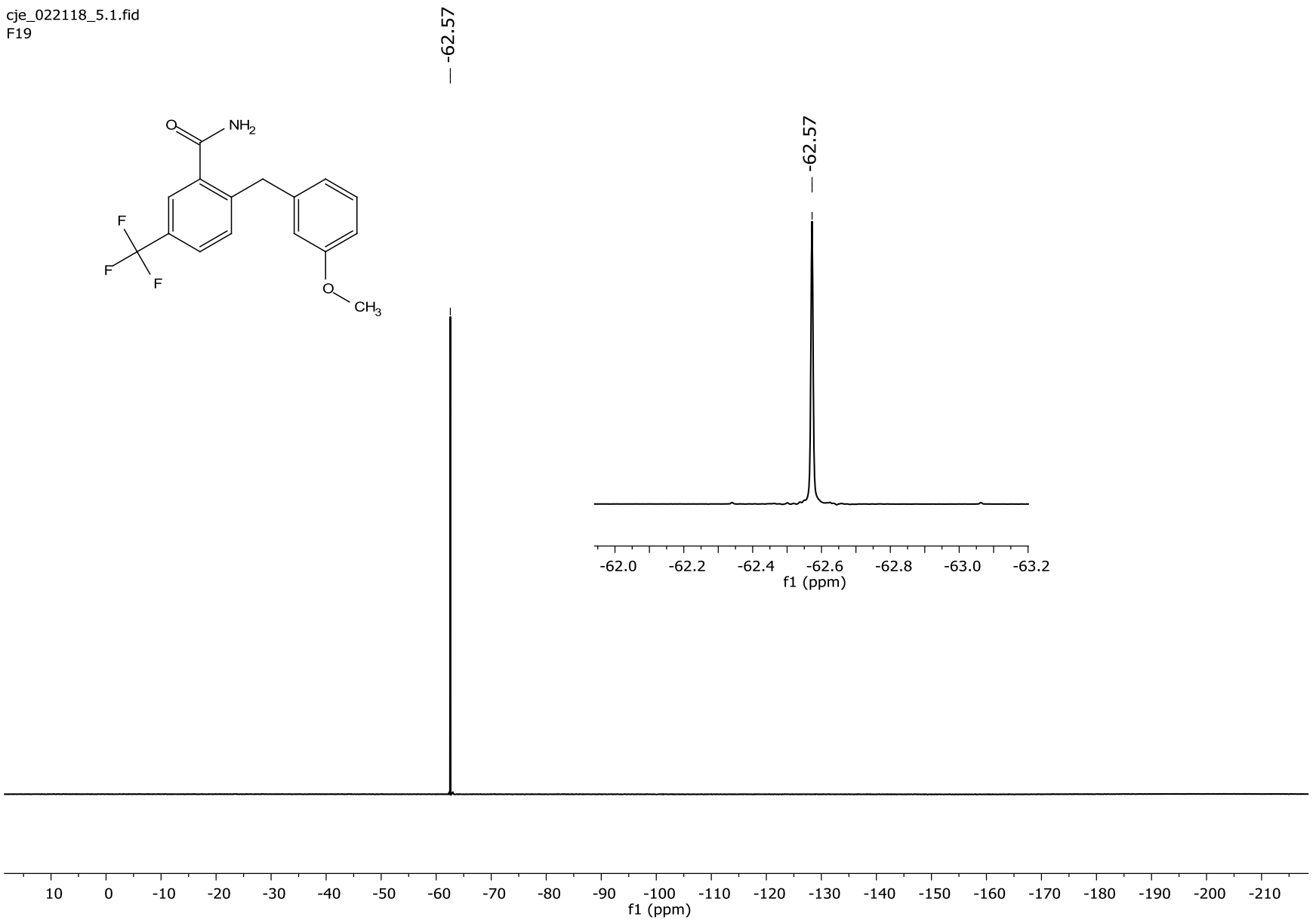
Z

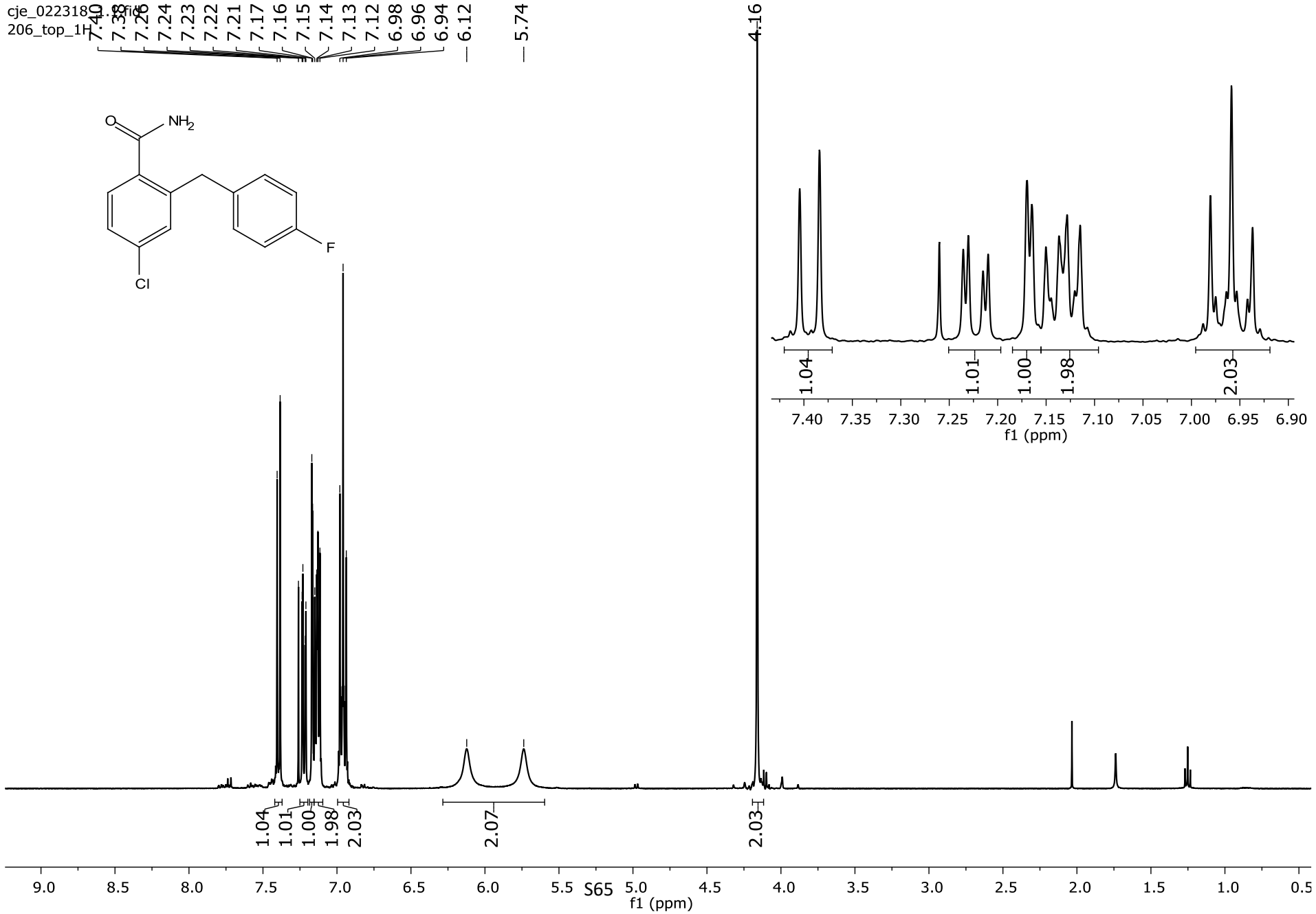

qde_1027_13C.1.fid
qde_1027_13C
171.77
152.81
152.45
144.23
142.67
132.17
131.39
130.48
128.80
125.51
125.49
124.88
122.82
122.80
106.71
77.44
77.23
77.02
60.89
56.27
32.37
132.30
131.52
130.61
128.93
125.64
125.01
123.68
122.95
122.93
f1 (ppm)
f1 (ppm)

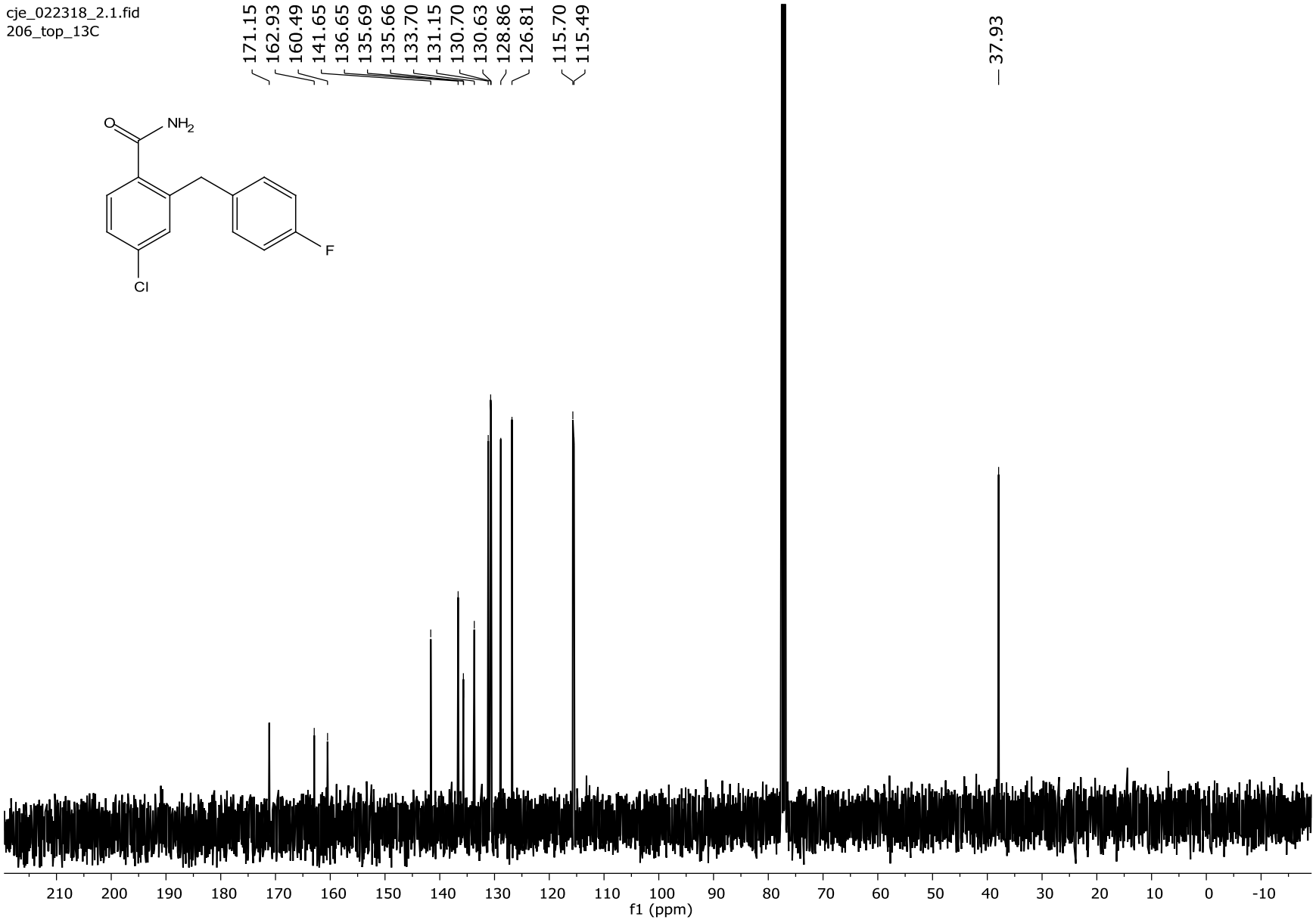

qde_1027_19F.3.fid
F19
-62.45
CH3
O
O
NH2
H3C
O
O
H3C
F
F
F
-62.45
-62.41
-62.43
-62.45
-62.47
-62.49
-62.51
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

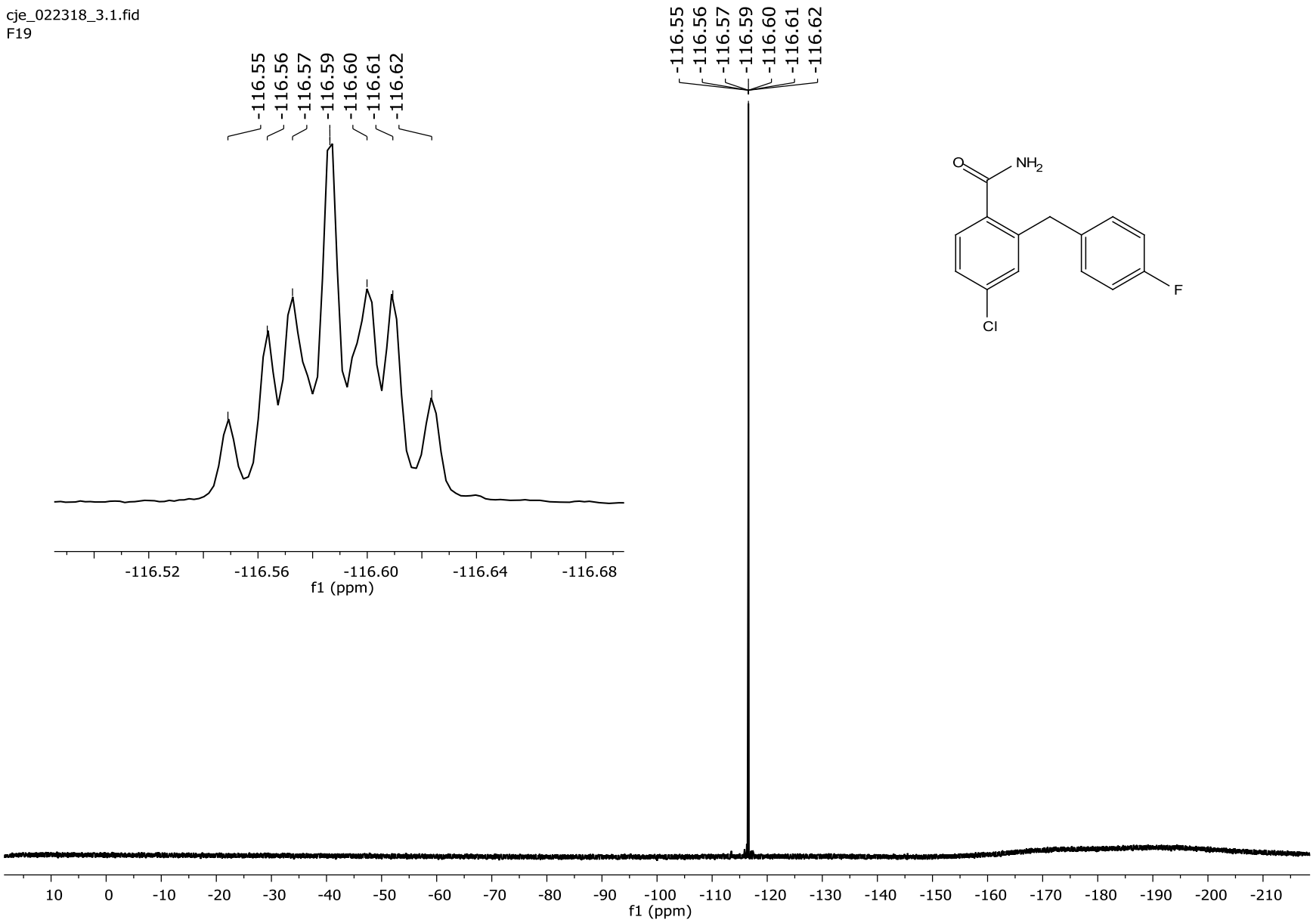

cje_022118_3_1.fid
186_1H
7.73 7.73 7.62 7.61 7.61 7.60 7.59 7.36 7.34 7.26 7.22 7.20 7.18 6.77 6.76 6.75 6.75 6.75 6.74 6.73 6.72 6.71 6.71 6.25
5.81
4.24
3.76 3.75 3.74
O
NH2
O
CH3
F
F
F
0.98 0.99 0.99 0.98 2.94 1.93 2.00 2.99
f1 (ppm)
0.98 0.99 0.99 0.98 2.94 1.93
f1 (ppm)

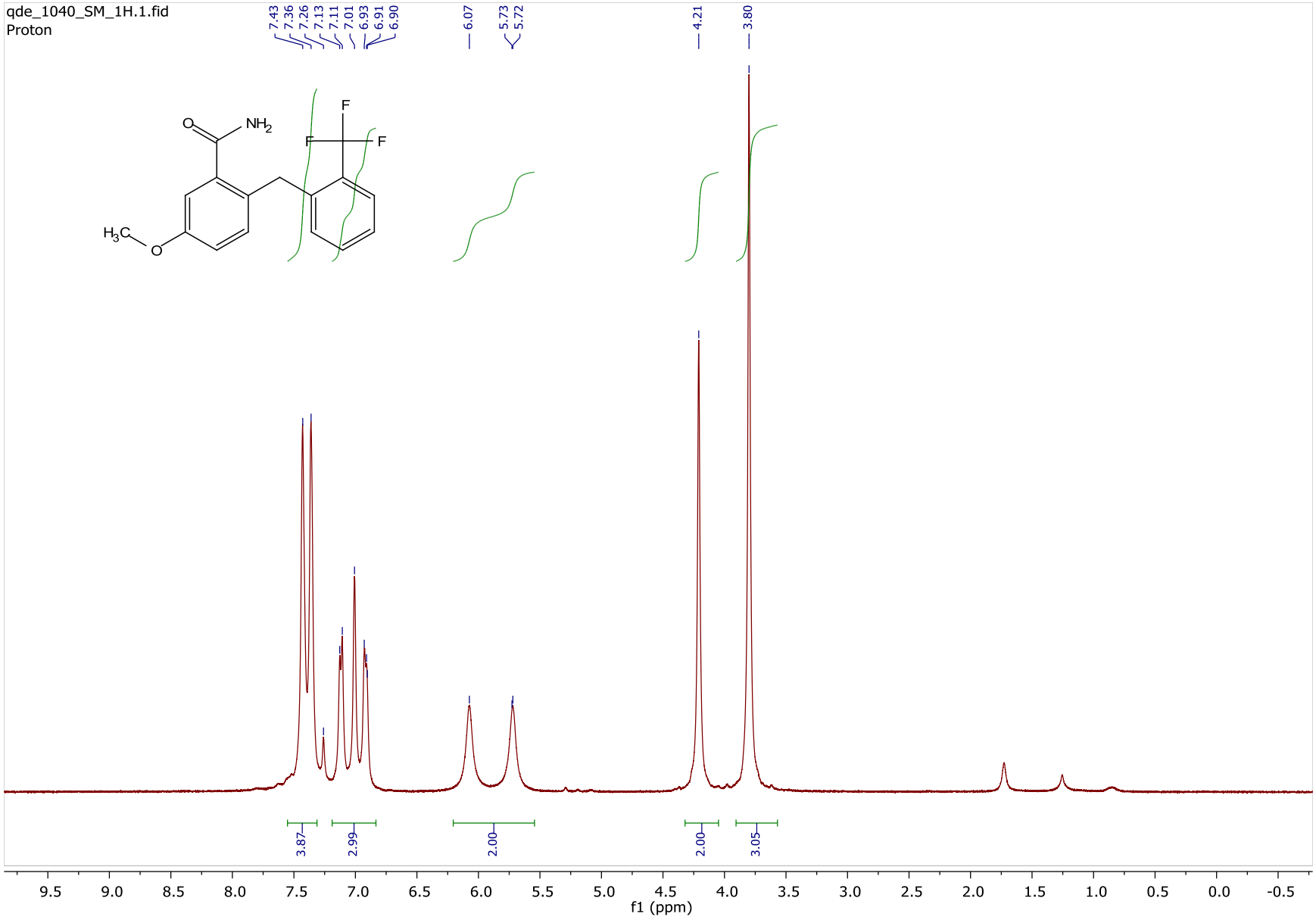

cje_022118_4.1.fid
186_13C
170.74
160.03
143.17
141.36
136.16
131.82
129.90
128.87
127.25
124.56
121.51
115.16
111.84
55.35
38.85
O
NH2
F
F
F
O
CH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

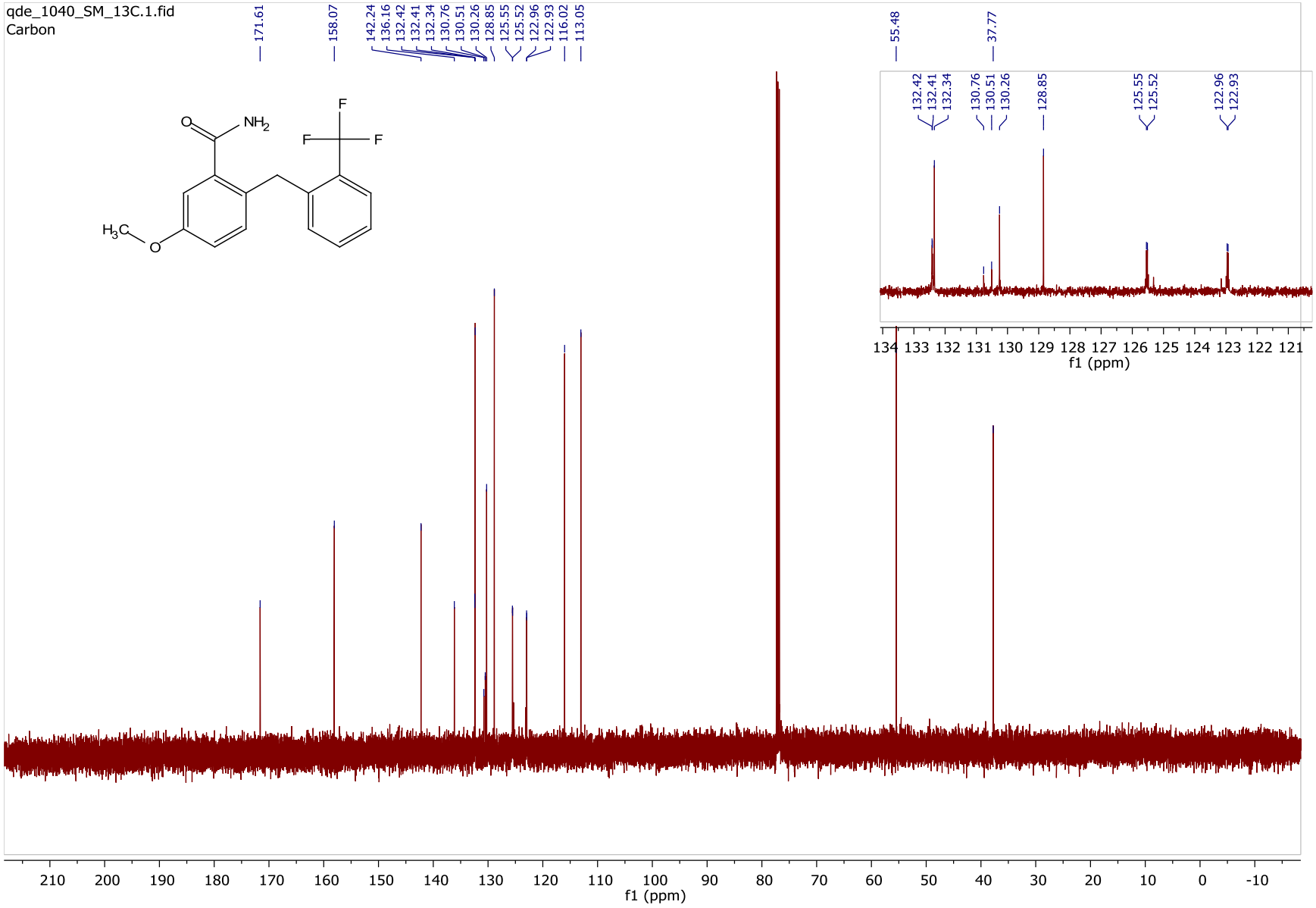

cje_022118_5.1.fid
F19
-62.57
O
NH2
F
F
F
O
CH3
-62.57
-62.0
-62.2
-62.4
-62.6
-62.8
-63.0
-63.2
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

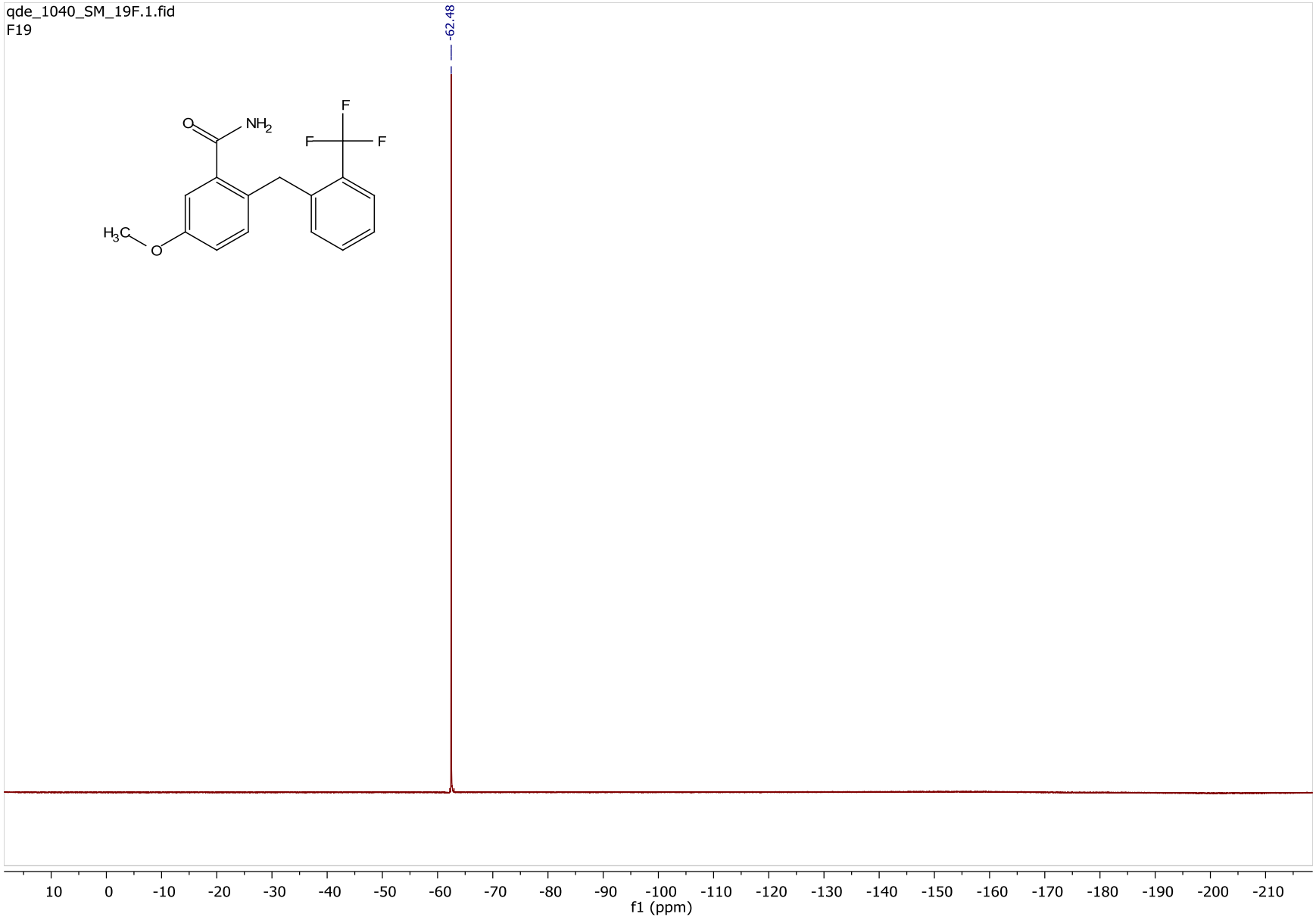

cje_022318_1.10.fid
206_top_1H
7.40
7.38
7.26
7.24
7.23
7.22
7.21
7.17
7.16
7.15
7.14
7.13
7.12
6.98
6.96
6.94
6.12
5.74
4.16
O
NH2
F
Cl
1.04
1.01
1.00
1.98
2.03
2.07
2.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
f1 (ppm)

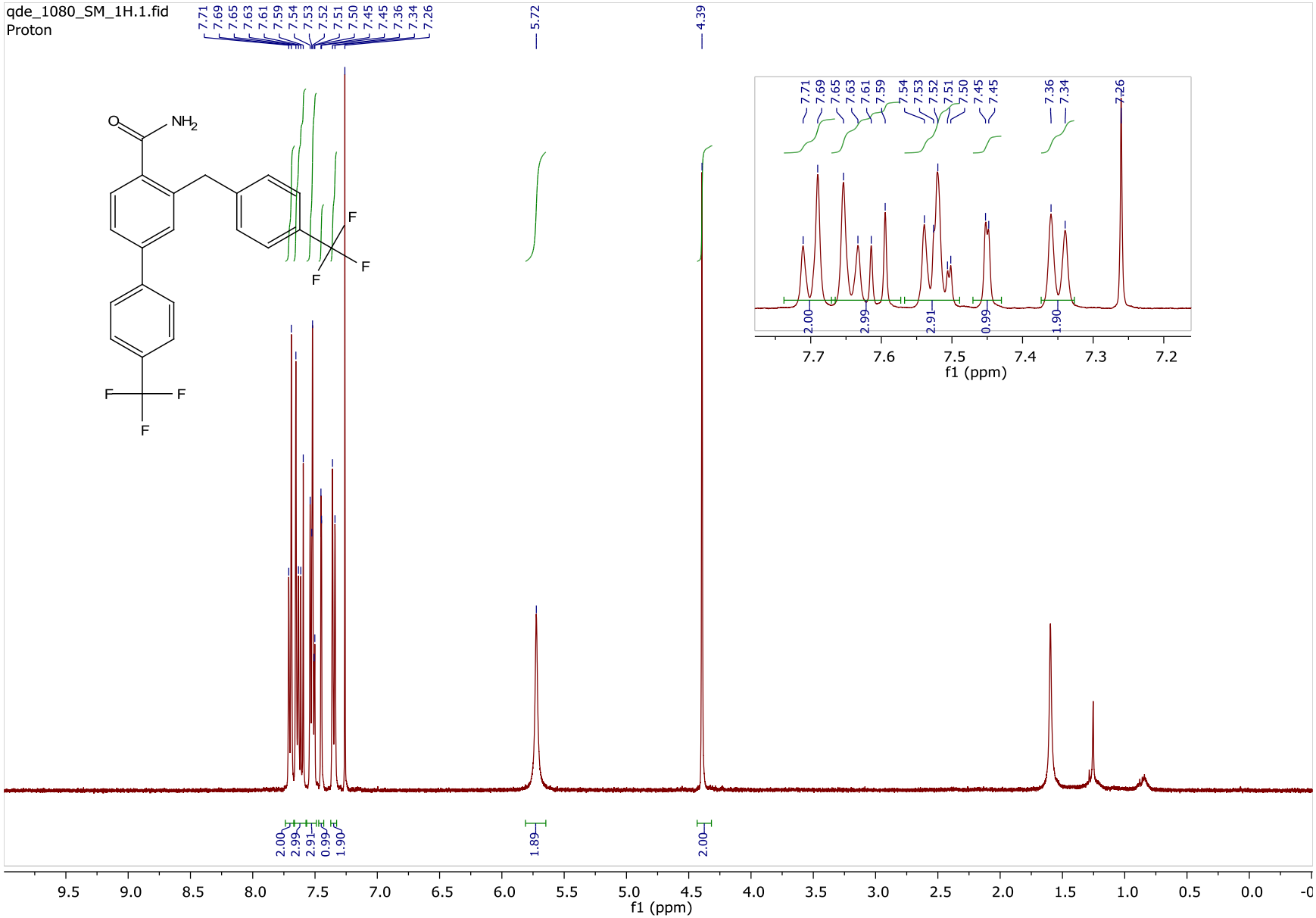

cje_022318_2.1.fid
206_top_13C
171.15
162.93
160.49
141.65
136.65
135.69
135.66
133.70
131.15
130.70
130.63
128.86
126.81
115.70
115.49
37.93
O
NH2
F
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

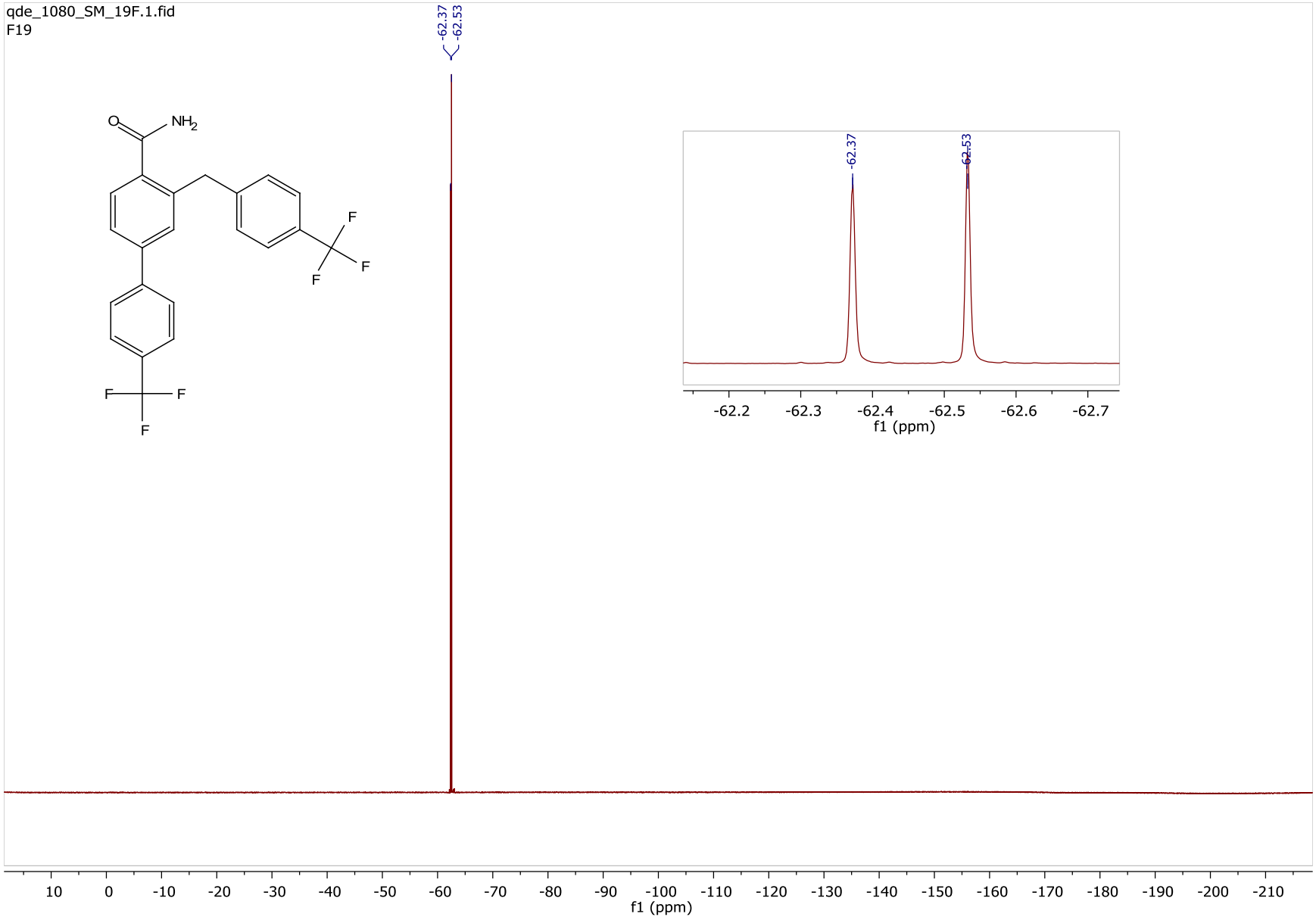

cje_022318_3.1.fid
F19
-116.55
-116.56
-116.57
-116.59
-116.60
-116.61
-116.62
-116.52
-116.56
-116.60
-116.64
-116.68
f1 (ppm)
O
NH2
F
Cl
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

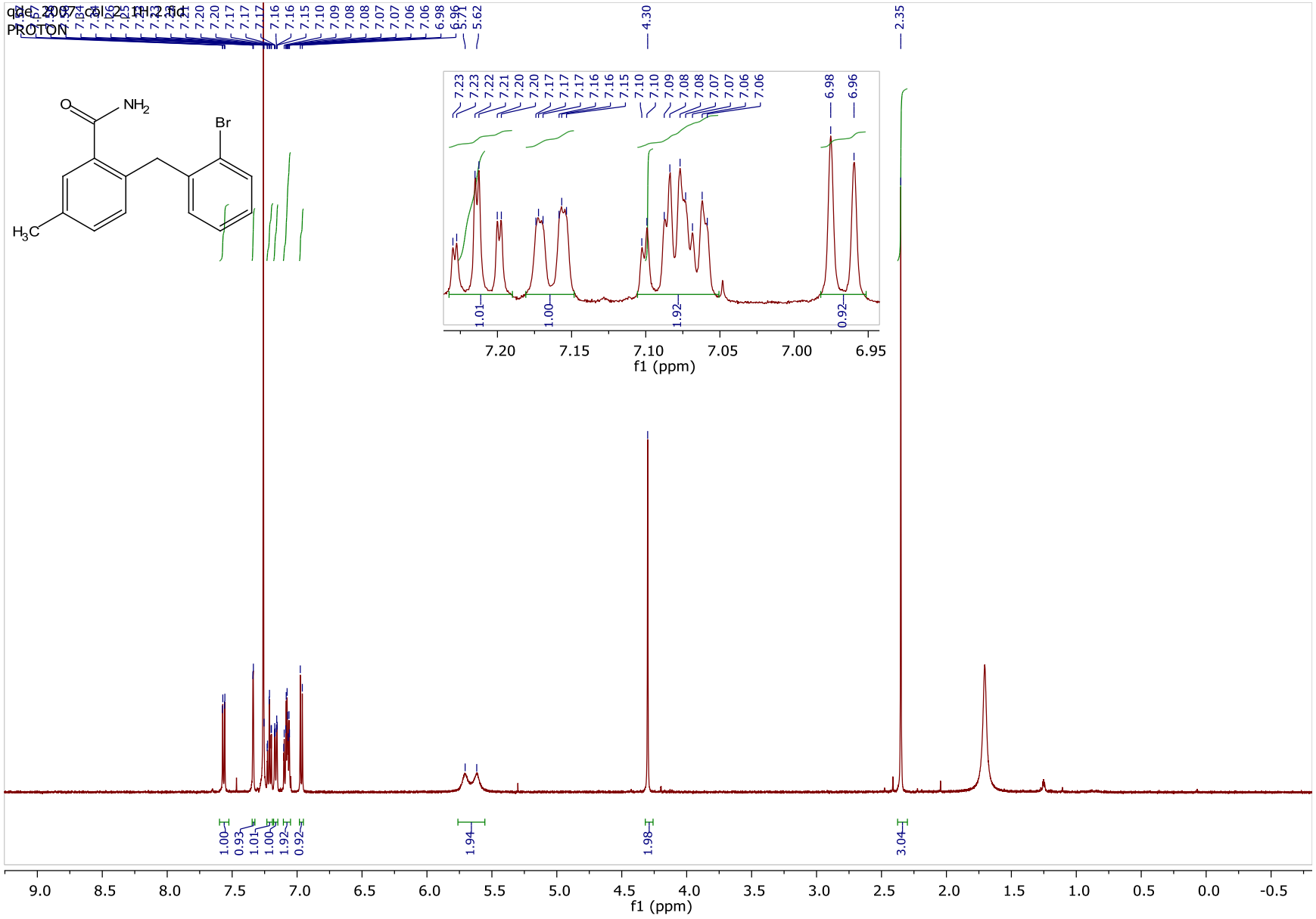

qde_1040_SM_1H.1.fid
Proton
7.43
7.36
7.26
7.13
7.11
7.01
6.93
6.91
6.90
6.07
5.73
5.72
4.21
3.80
O
NH2
F
F
F
H3C
O
3.87
2.99
2.00
2.00
3.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

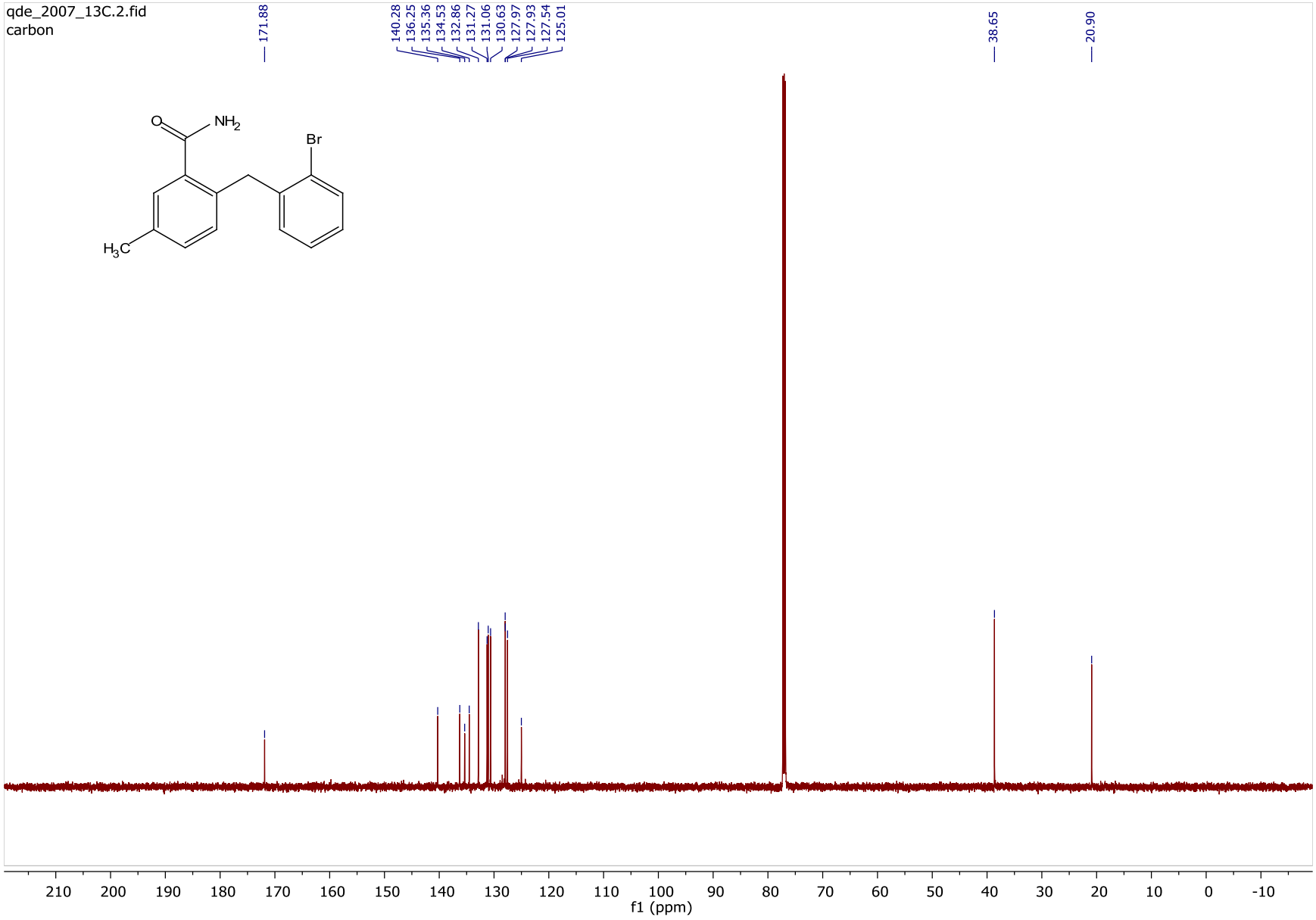

qde_1040_SM_13C.1.fid
Carbon
171.61
158.07
142.24
136.16
132.42
132.41
132.34
130.76
130.51
130.26
128.85
125.55
125.52
122.96
122.93
116.02
113.05
55.48
37.77
O
NH2
F
F
F
H3C
O
f1 (ppm)

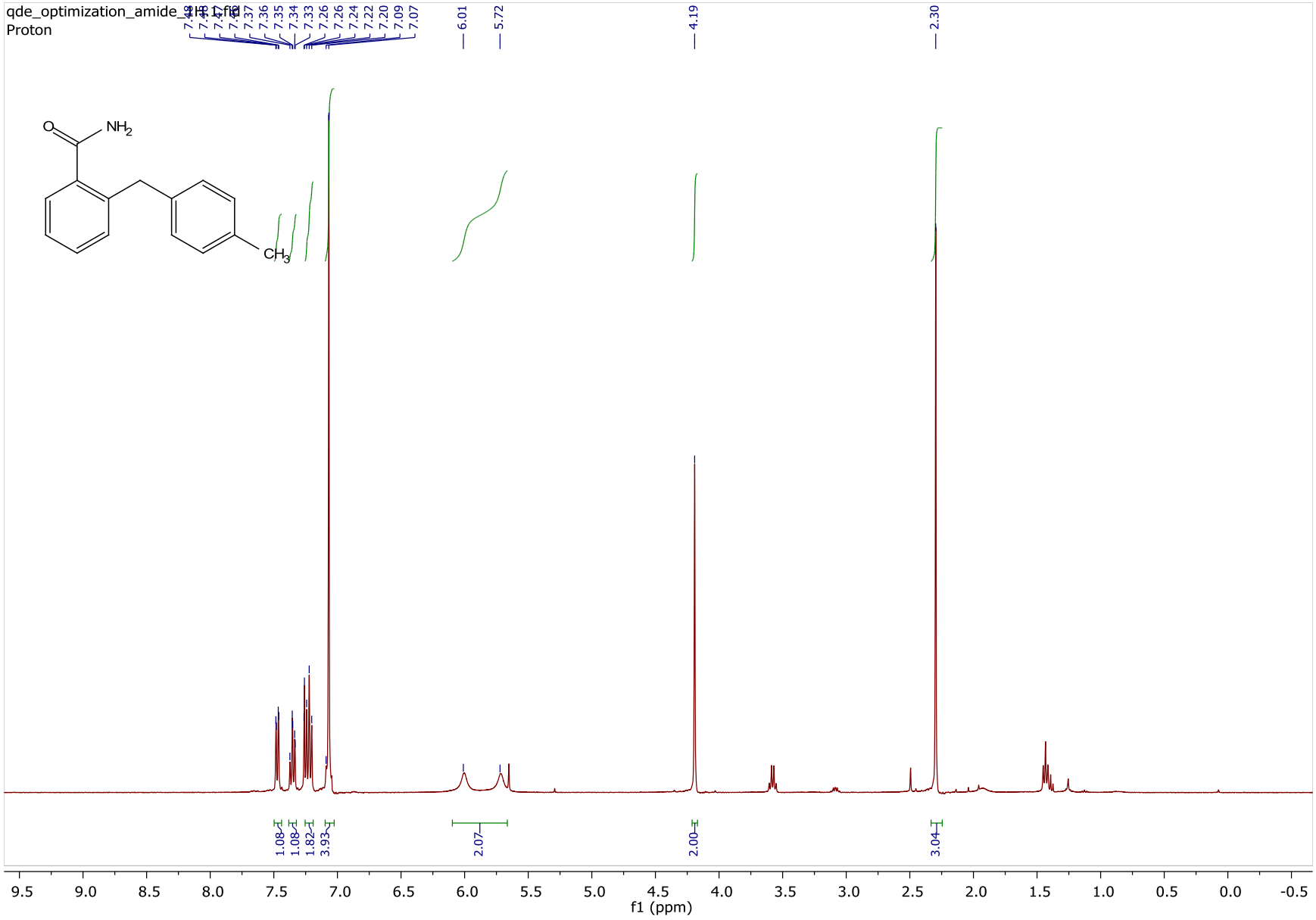

qde_1040_SM_19F.1.fid
F19
-62.48
O
NH2
F
F
F
H3C
O
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

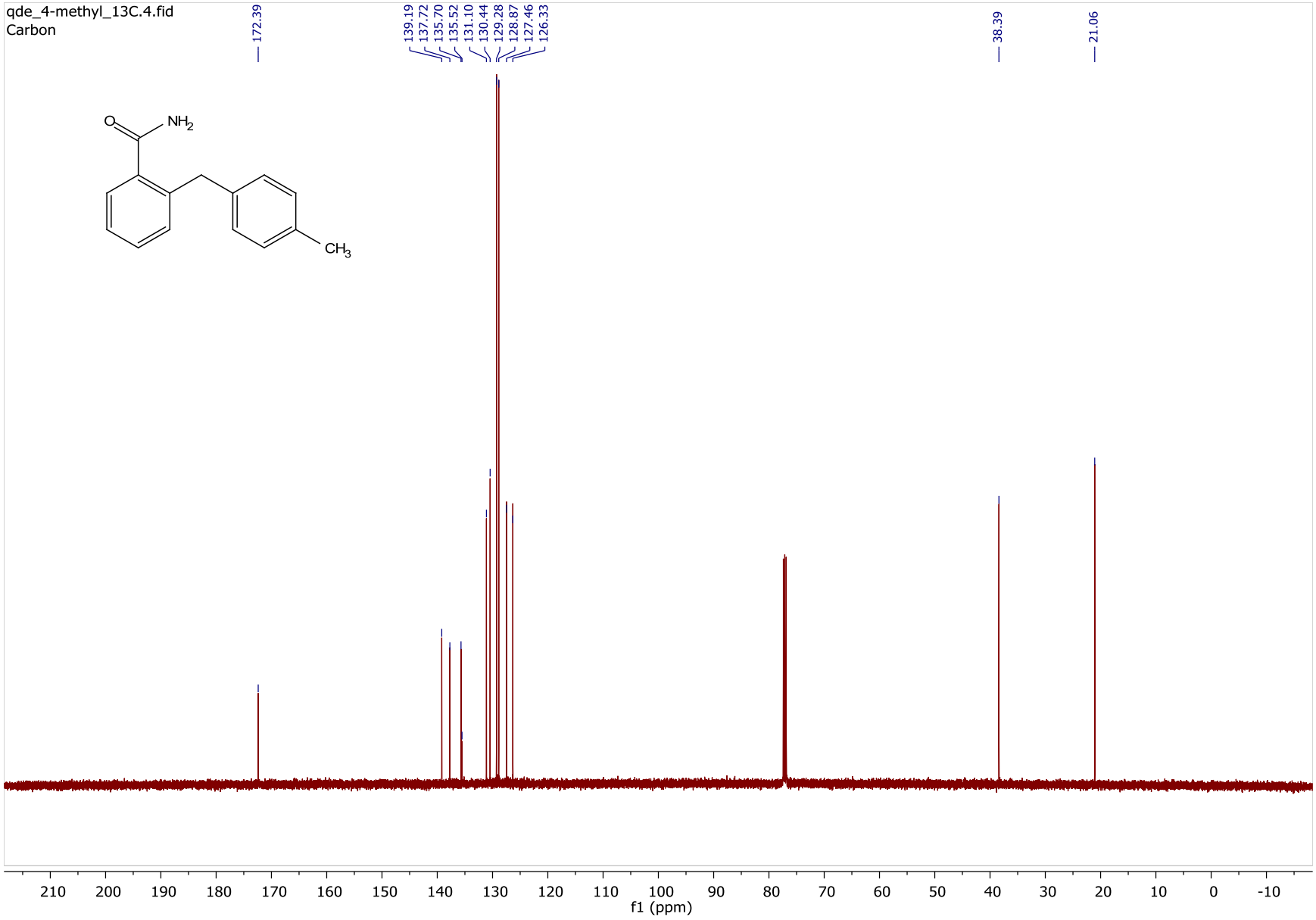

qde_1080_SM_1H.1.fid
Proton
7.71
7.69
7.65
7.63
7.61
7.59
7.54
7.53
7.52
7.51
7.50
7.45
7.45
7.36
7.34
7.26
5.72
4.39
O
NH2
F
F
F
F
F
F
2.00
2.99
2.91
0.99
1.90
1.89
2.00
f1 (ppm)

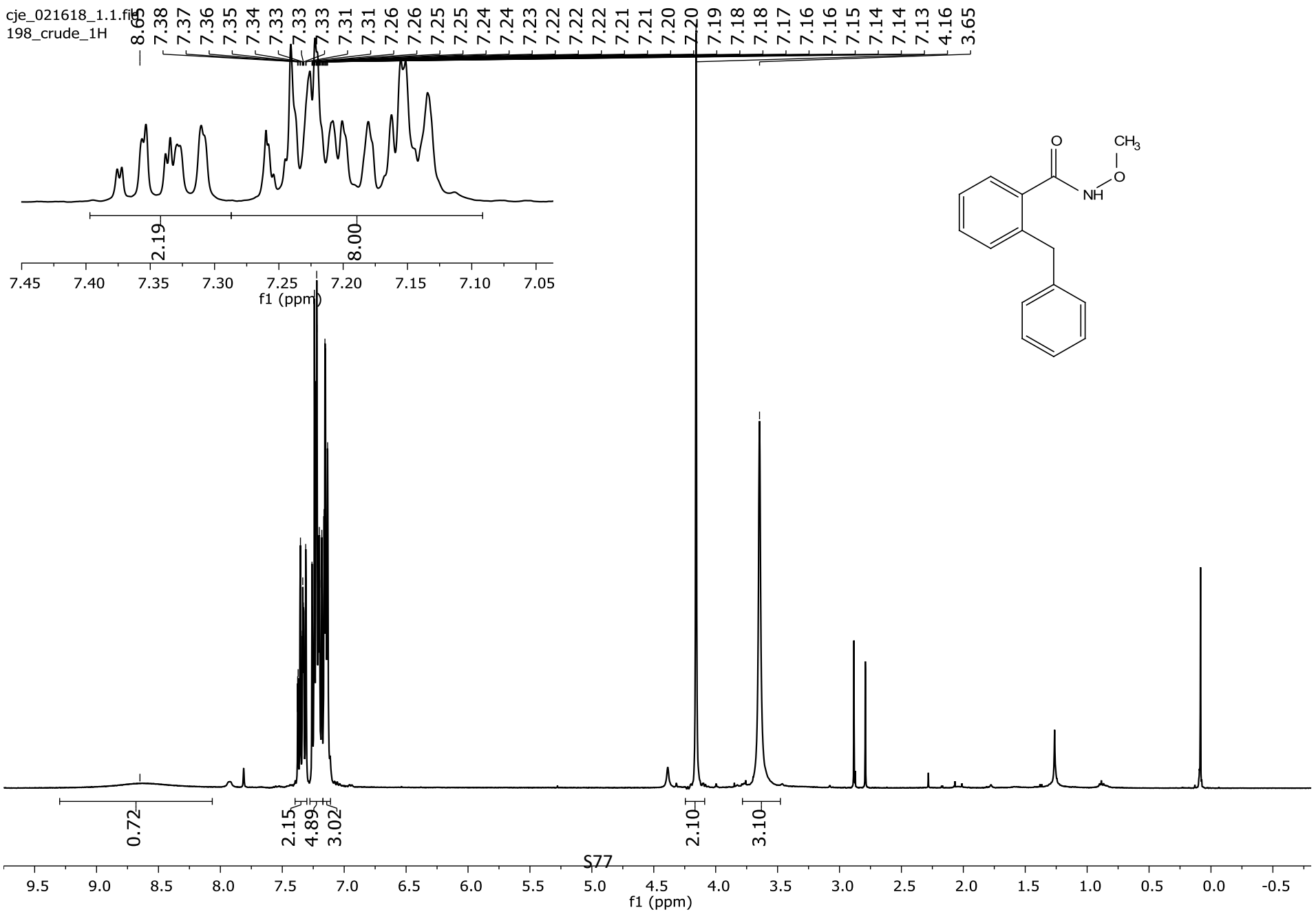

qde_1080_SM_19F.1.fid
F19
-62.37
-62.53
O
NH2
F
F
F
F
F
F
-62.37
-62.53
-62.2
-62.3
-62.4
-62.5
-62.6
-62.7
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

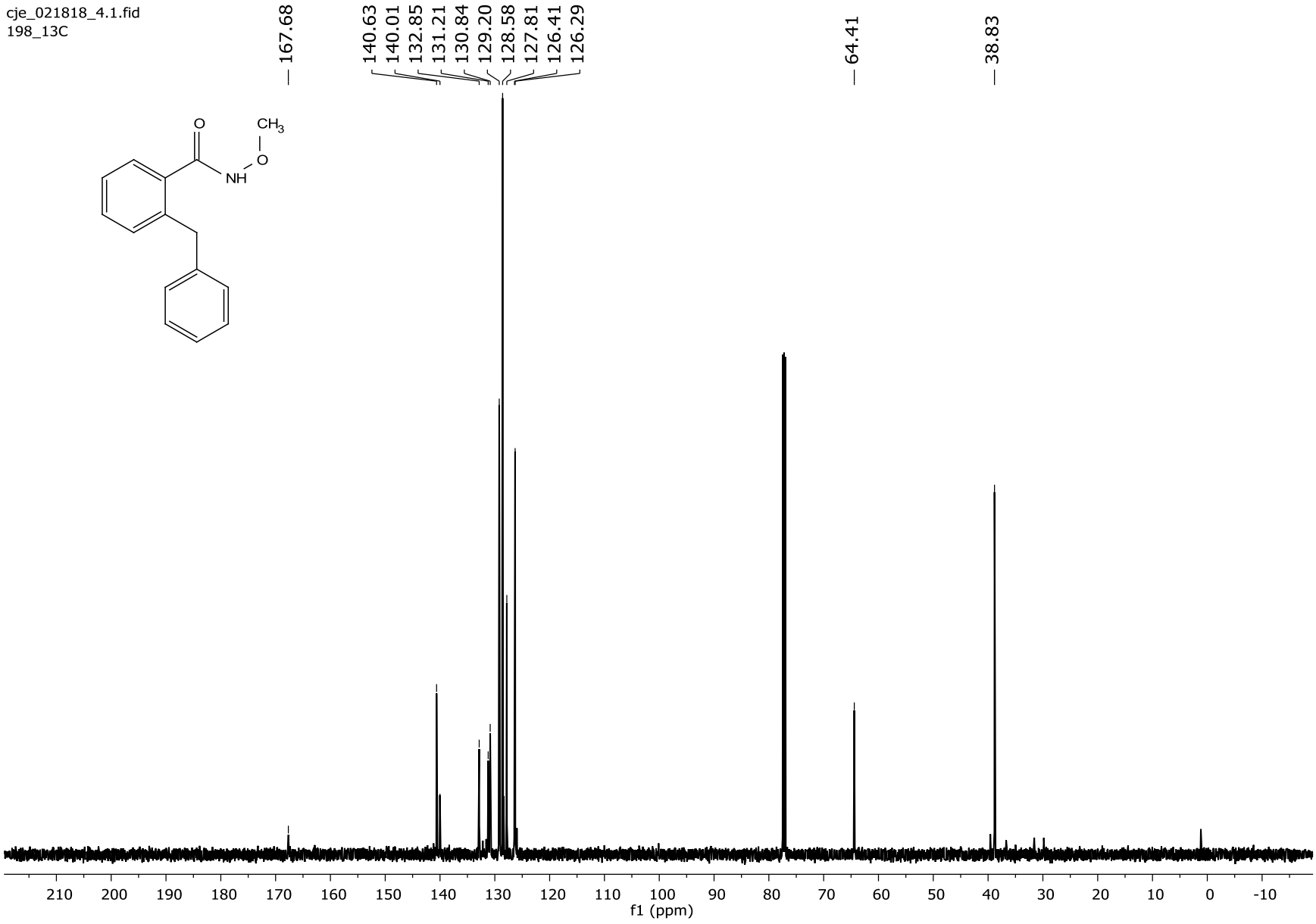

PROTON
O
NH2
Br
H3C
7.23
7.23
7.22
7.21
7.20
7.20
7.17
7.17
7.17
7.16
7.16
7.15
7.10
7.10
7.09
7.08
7.08
7.07
7.07
7.06
7.06
6.98
6.96
1.01
1.00
1.92
0.92
7.20
7.15
7.10
7.05
7.00
6.95
f1 (ppm)
4.30
2.35
5.62
6.96
1.00
0.93
1.01
1.00
1.92
0.92
1.94
1.98
3.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

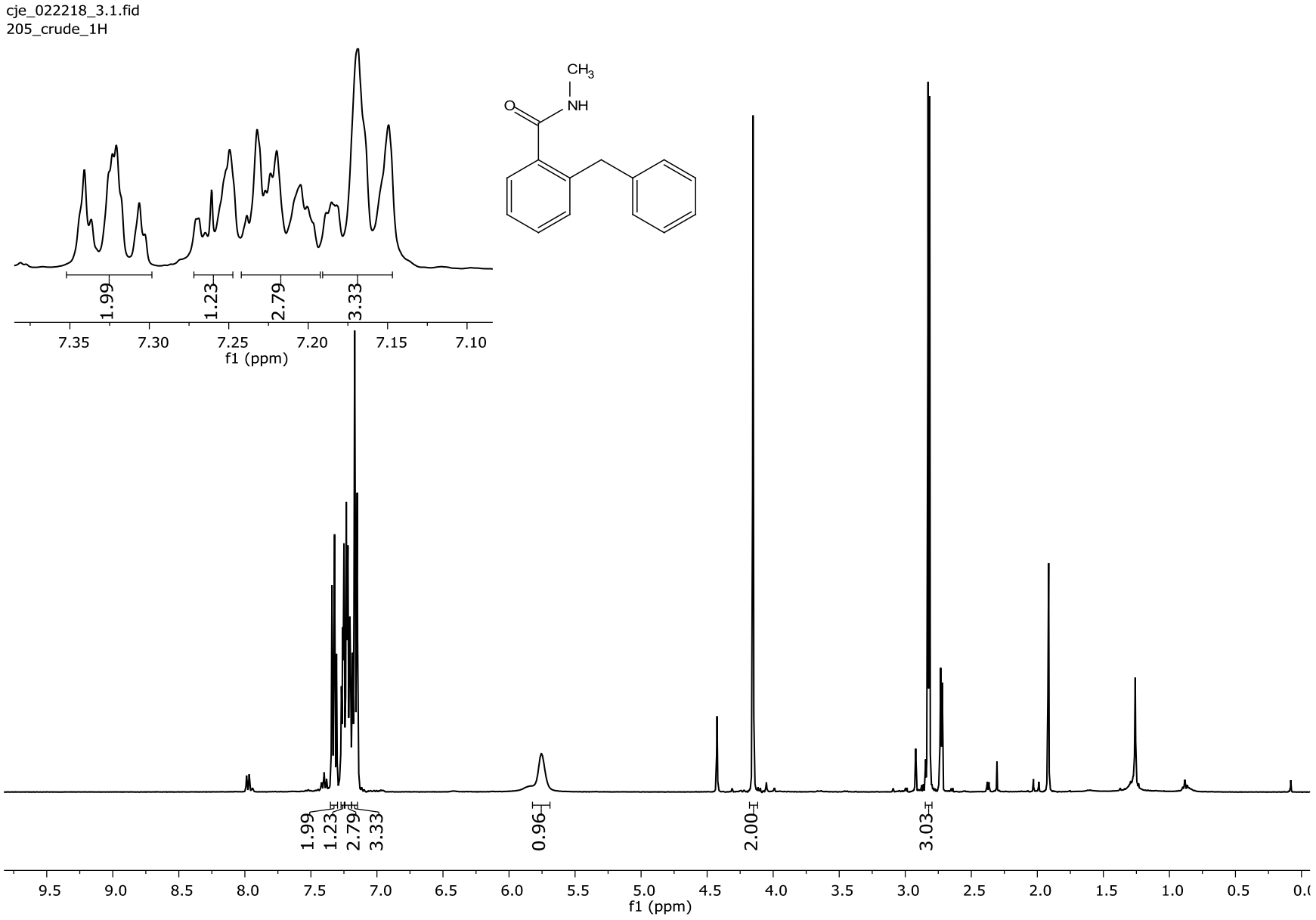

qde_2007_13C.2.fid
carbon
171.88
140.28
136.25
135.36
134.53
132.86
131.27
131.06
130.63
127.97
127.93
127.54
125.01
38.65
20.90
O
NH2
Br
H3C
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

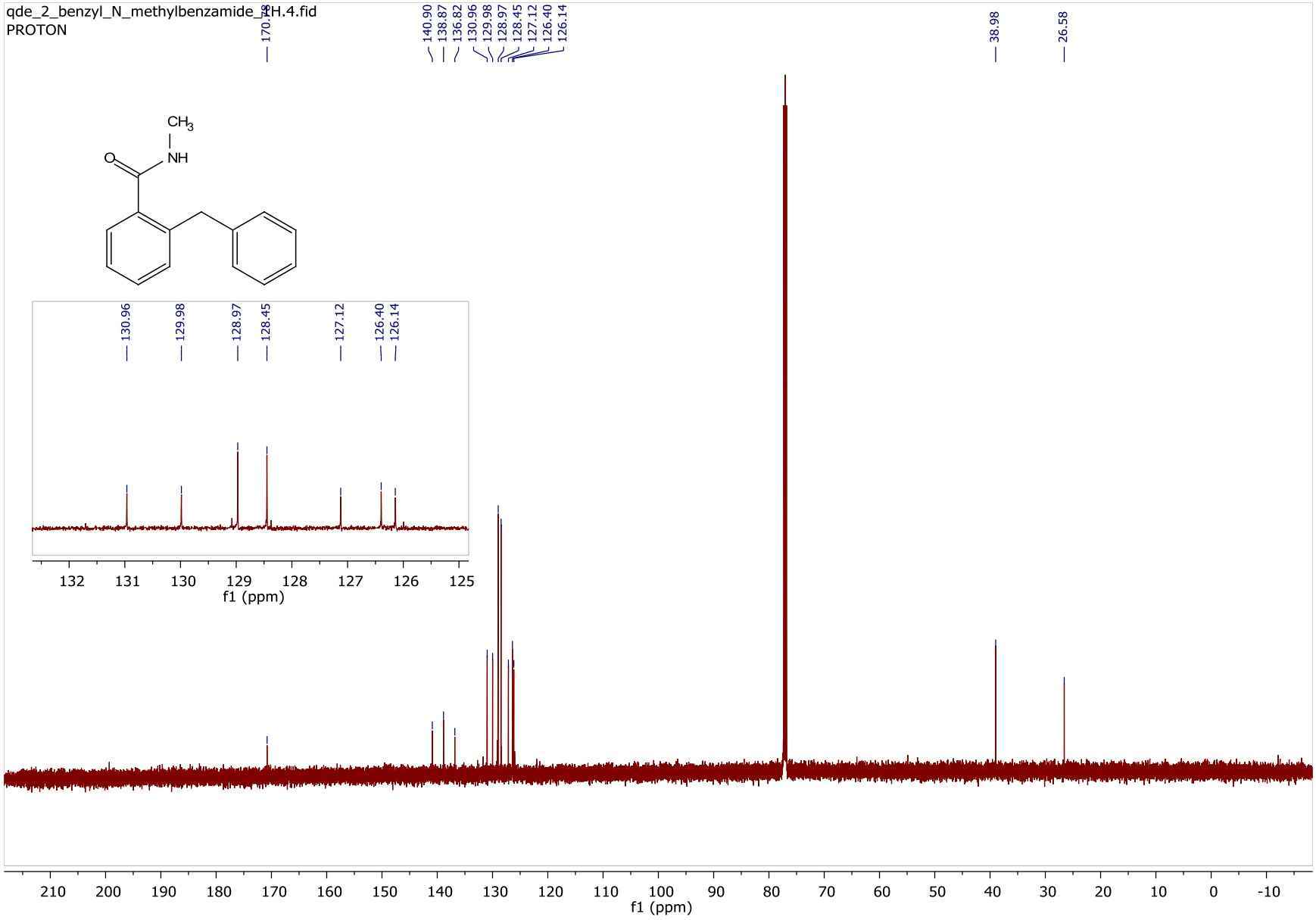

qde_optimization_amide_1_fid
Proton
7.48
7.41
7.40
7.37
7.36
7.35
7.34
7.33
7.26
7.26
7.24
7.22
7.20
7.09
7.07
6.01
5.72
4.19
2.30
O
NH2
CH3
1.08
1.08
1.82
3.93
2.07
2.00
3.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

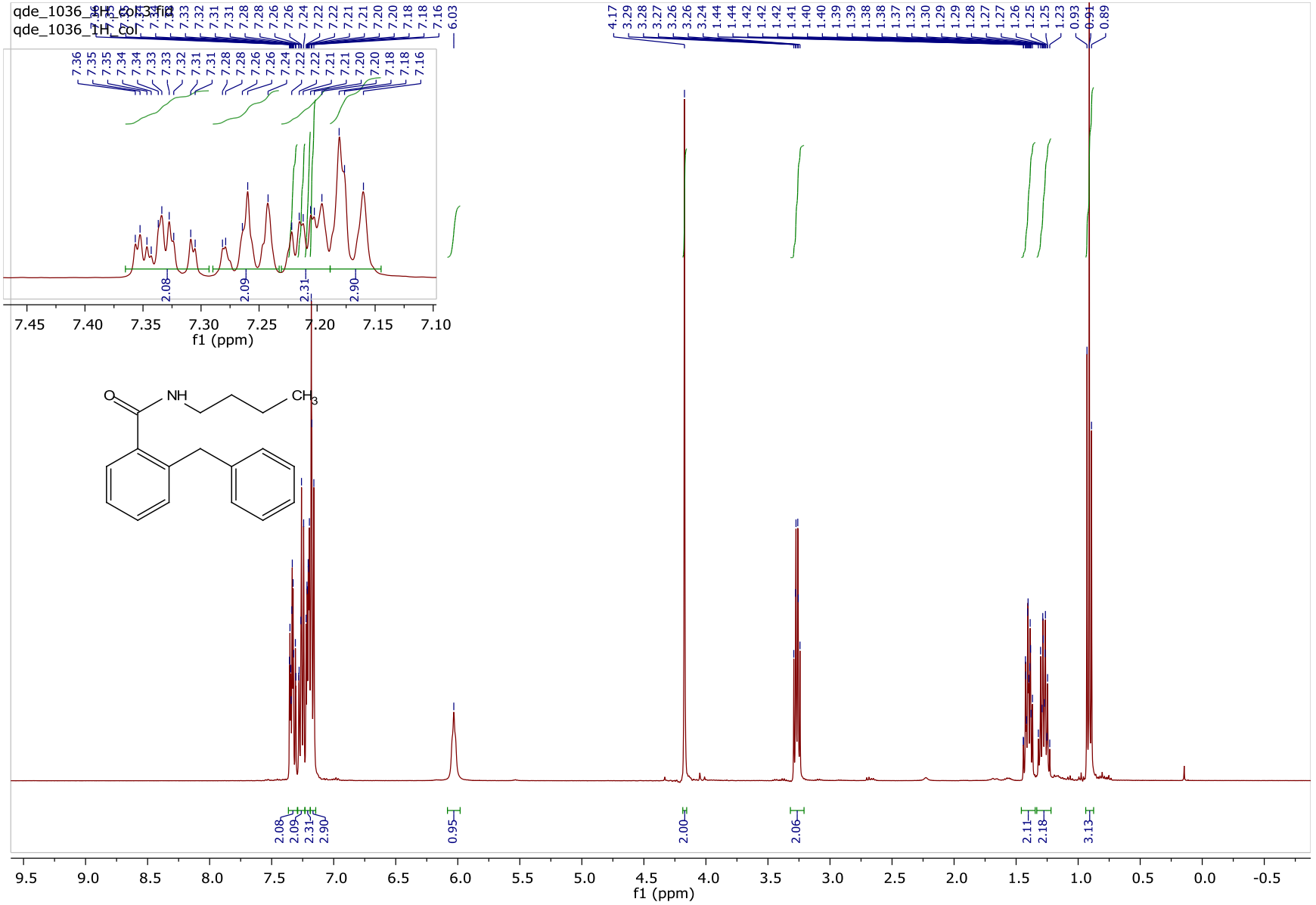

qde_4-methyl_13C.4.fid
Carbon
172.39
139.19
137.72
135.70
135.52
131.10
130.44
129.28
128.87
127.46
126.33
38.39
21.06
O
NH2
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

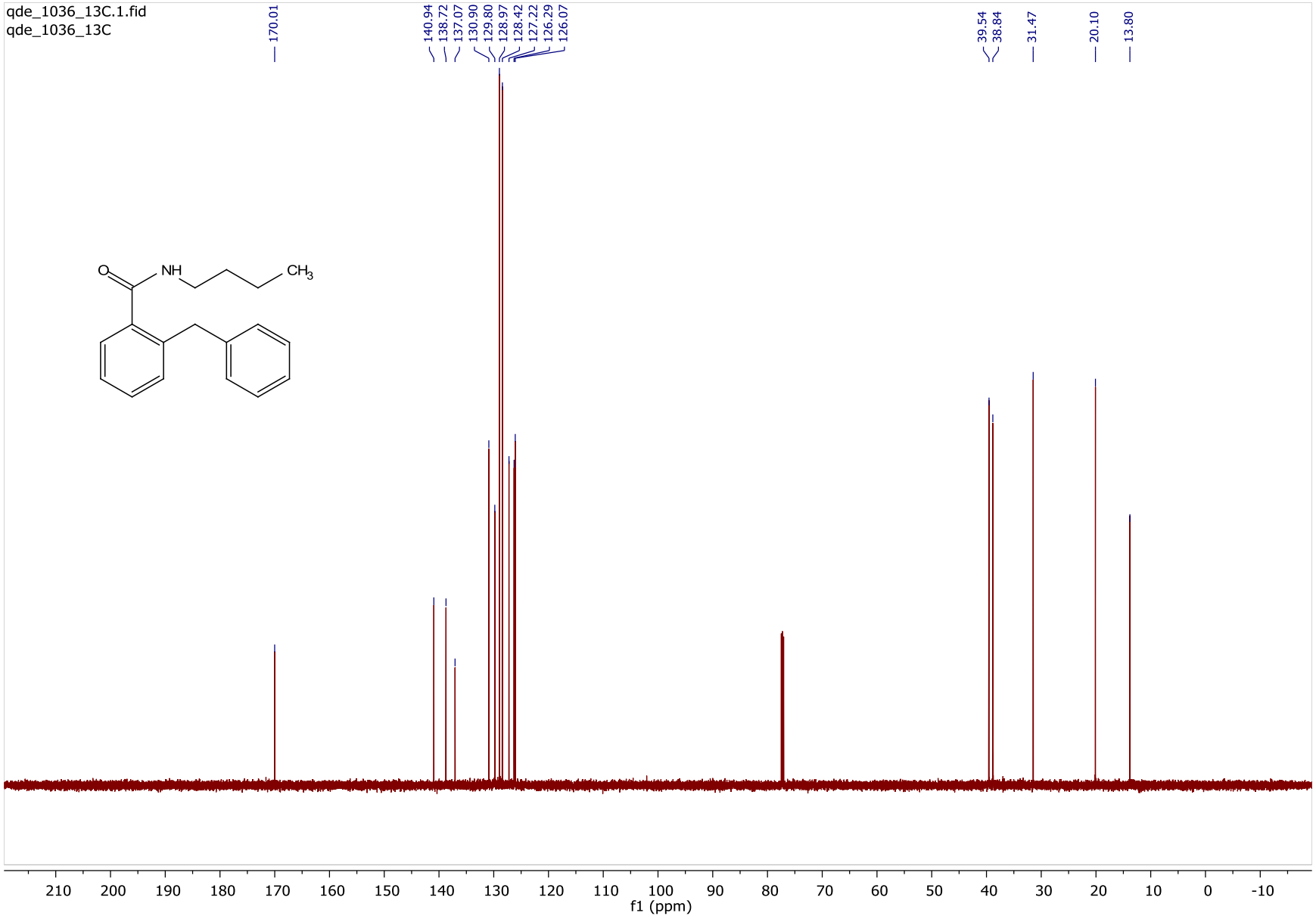

cje_021618_1.1.fid
198_crude_1H
8.65
7.38
7.37
7.36
7.35
7.34
7.33
7.33
7.33
7.31
7.31
7.26
7.26
7.25
7.25
7.24
7.24
7.23
7.22
7.22
7.22
7.21
7.21
7.20
7.20
7.19
7.18
7.18
7.17
7.16
7.16
7.15
7.14
7.14
7.13
4.16
3.65
2.19
8.00
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
f1 (ppm)
O
CH3
O
NH
0.72
2.15
4.89
3.02
2.10
3.10
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

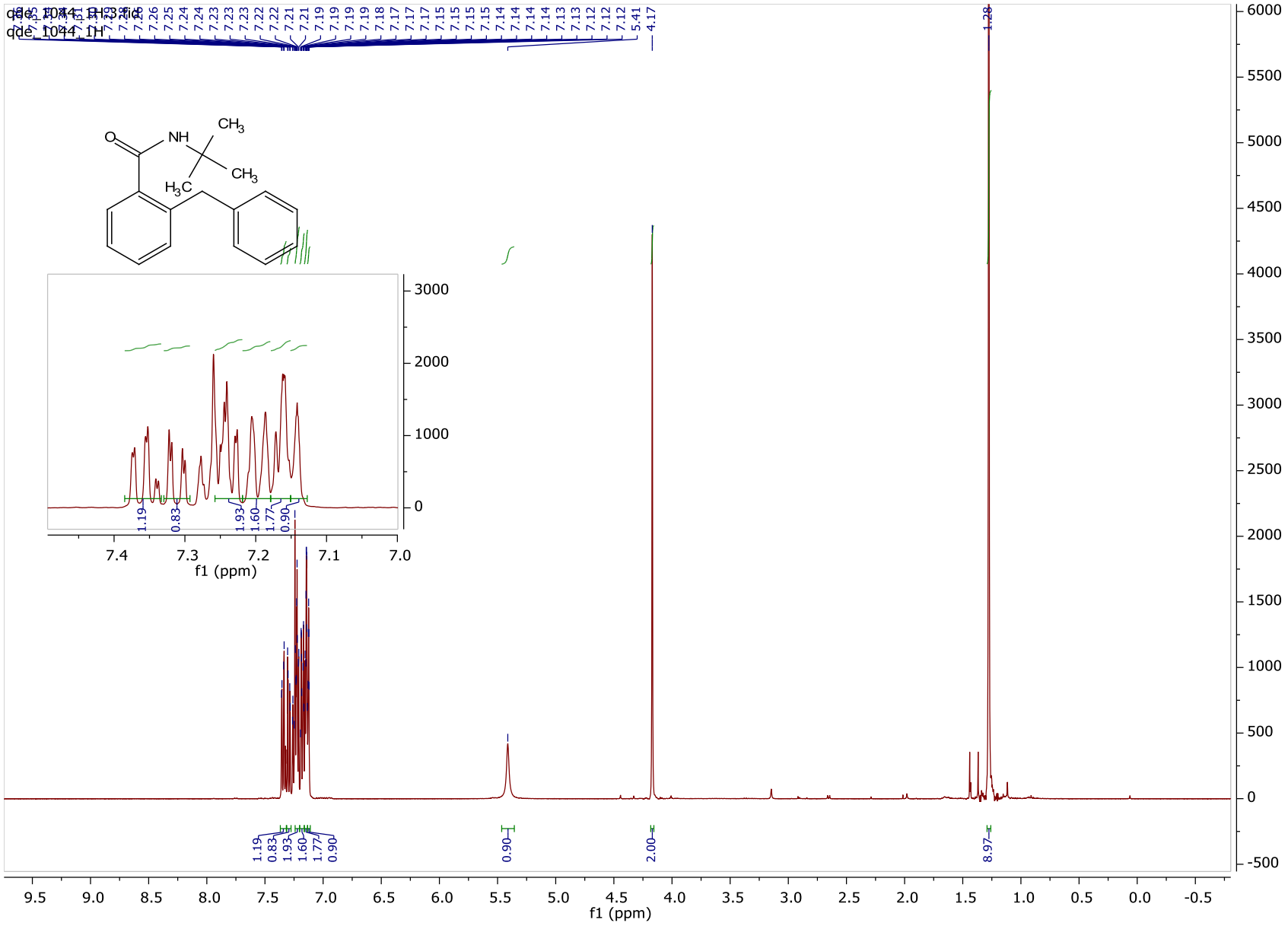

cje_021818_4.1.fid
198_13C
167.68
140.63
140.01
132.85
131.21
130.84
129.20
128.58
127.81
126.41
126.29
64.41
38.83
O
CH3
O
NH
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

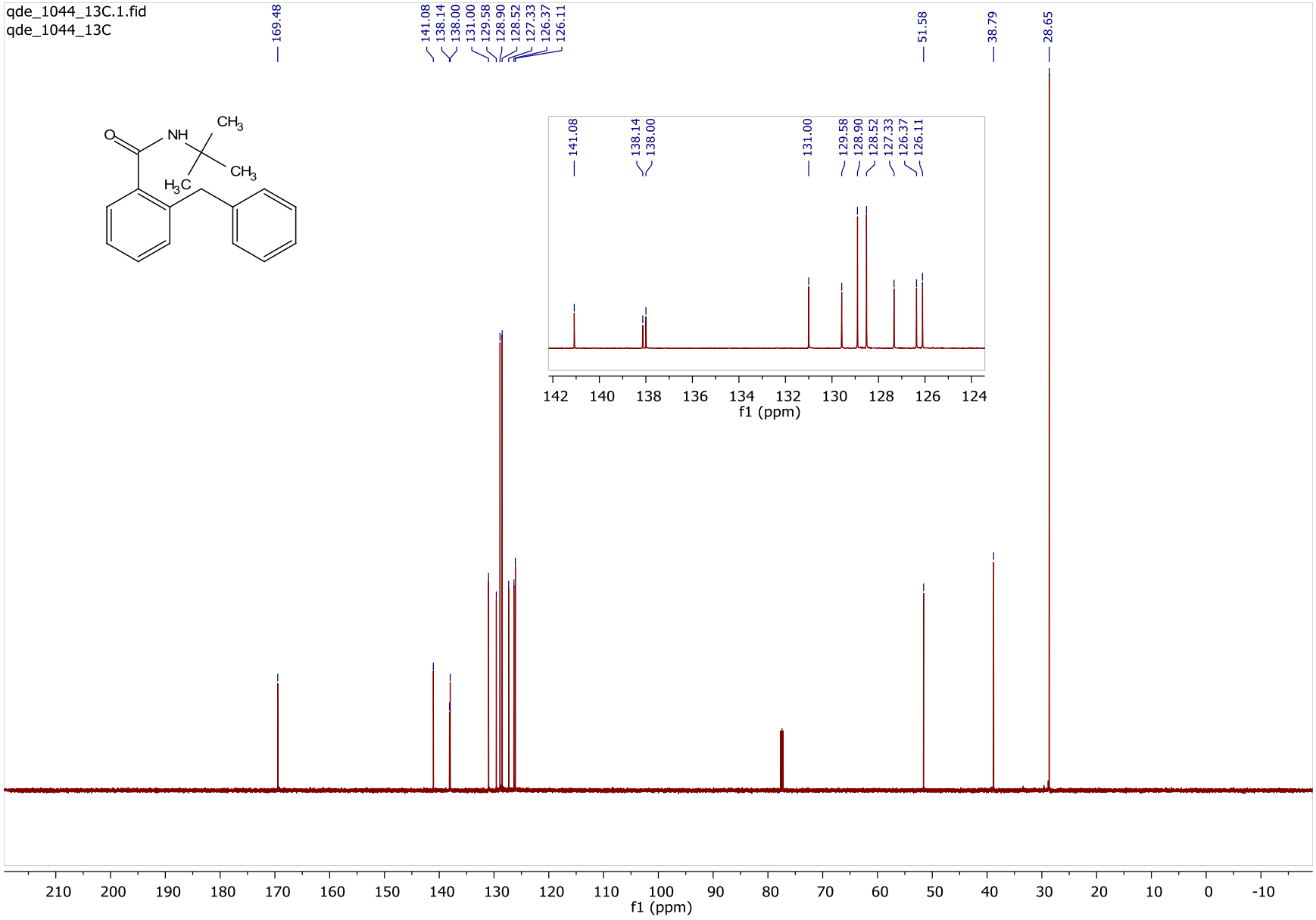

cje_022218_3.1.fid
205_crude_1H
CH3
NH
O
1.99
1.23
2.79
3.33
7.35
7.30
7.25
7.20
7.15
7.10
f1 (ppm)
0.96
2.00
3.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

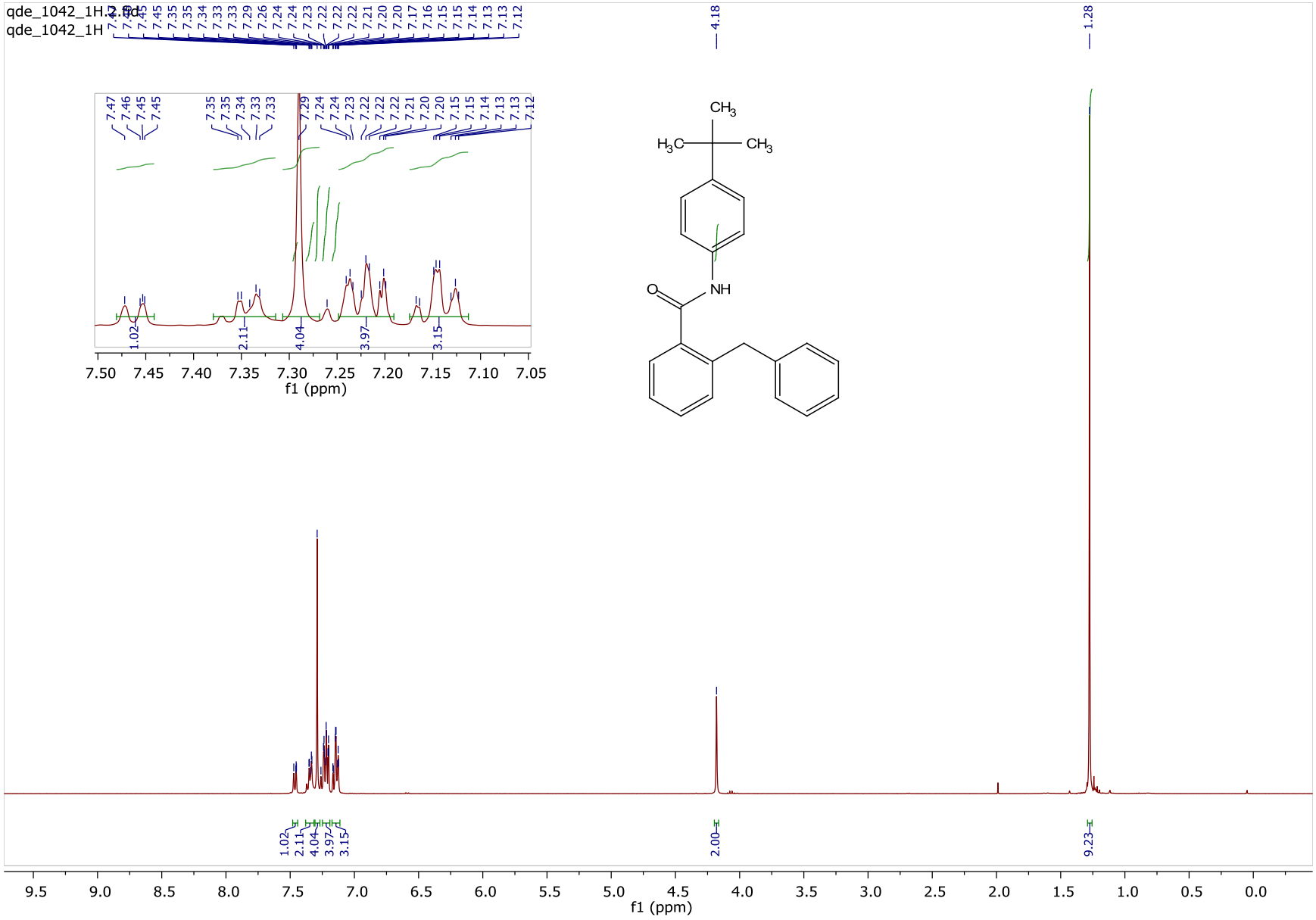

qde_2_benzyl_N_methylbenzamide_2H.4.fid
PROTON
170.78
140.90
138.87
136.82
130.96
129.98
128.97
128.45
127.12
126.40
126.14
38.98
26.58
CH3
NH
O
f1 (ppm)

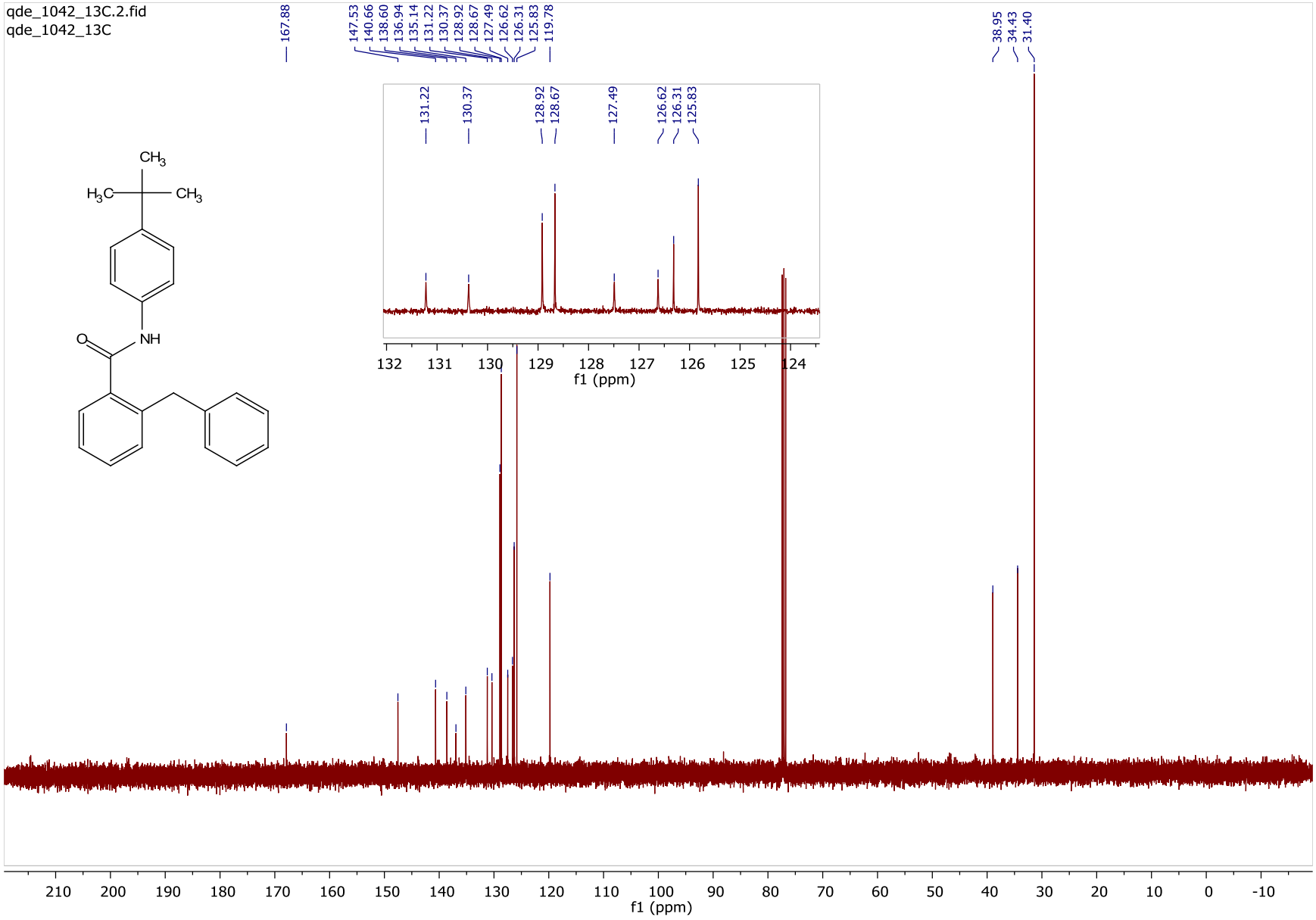

qde_1036_1H_col_13.fid
qde_1036_1H_col
f1 (ppm)
O
NH
CH3

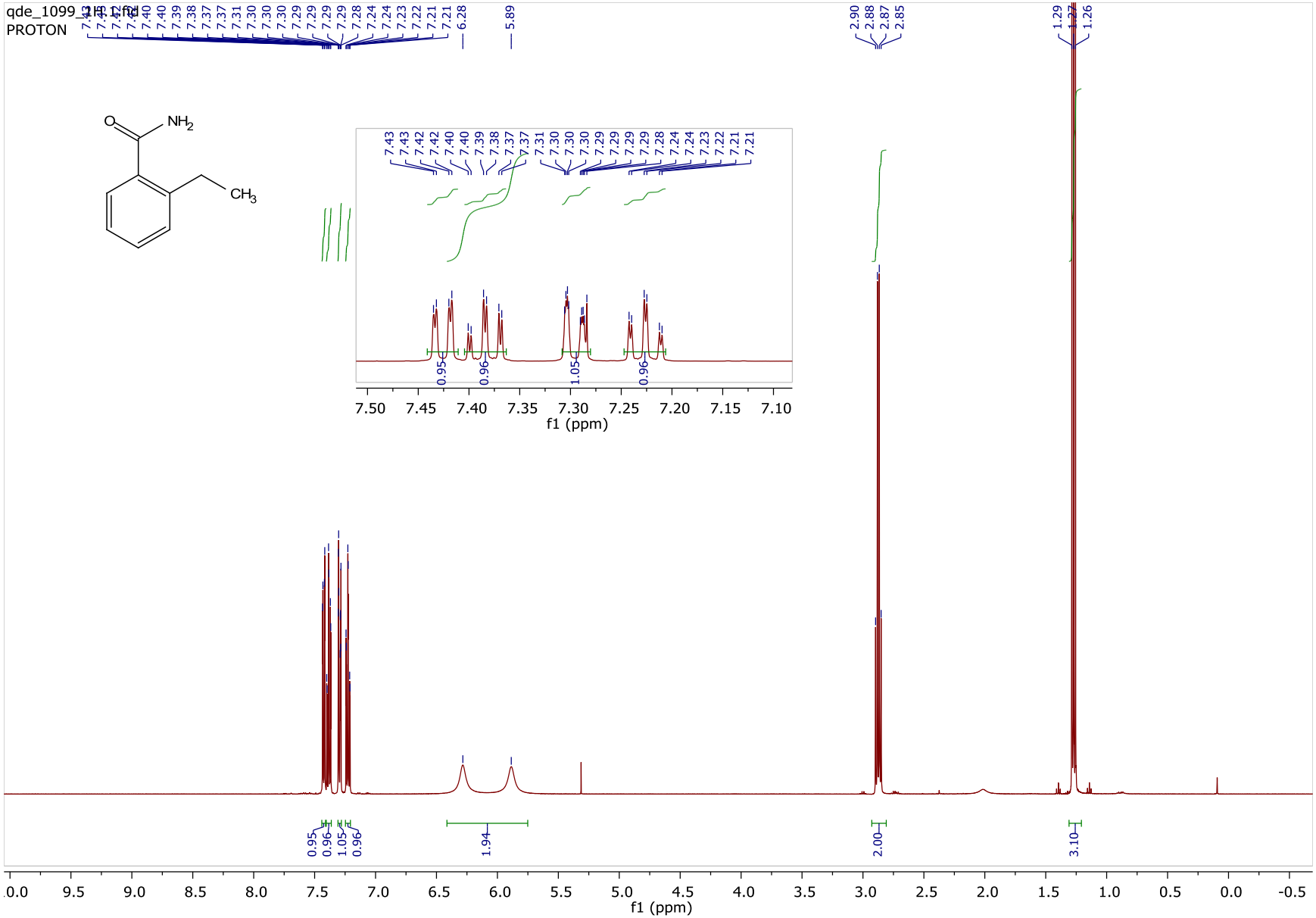

qde_1036_13C.1.fid
qde_1036_13C
170.01
140.94
138.72
137.07
130.90
129.80
128.97
128.42
127.22
126.29
126.07
39.54
38.84
31.47
20.10
13.80
O
NH
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

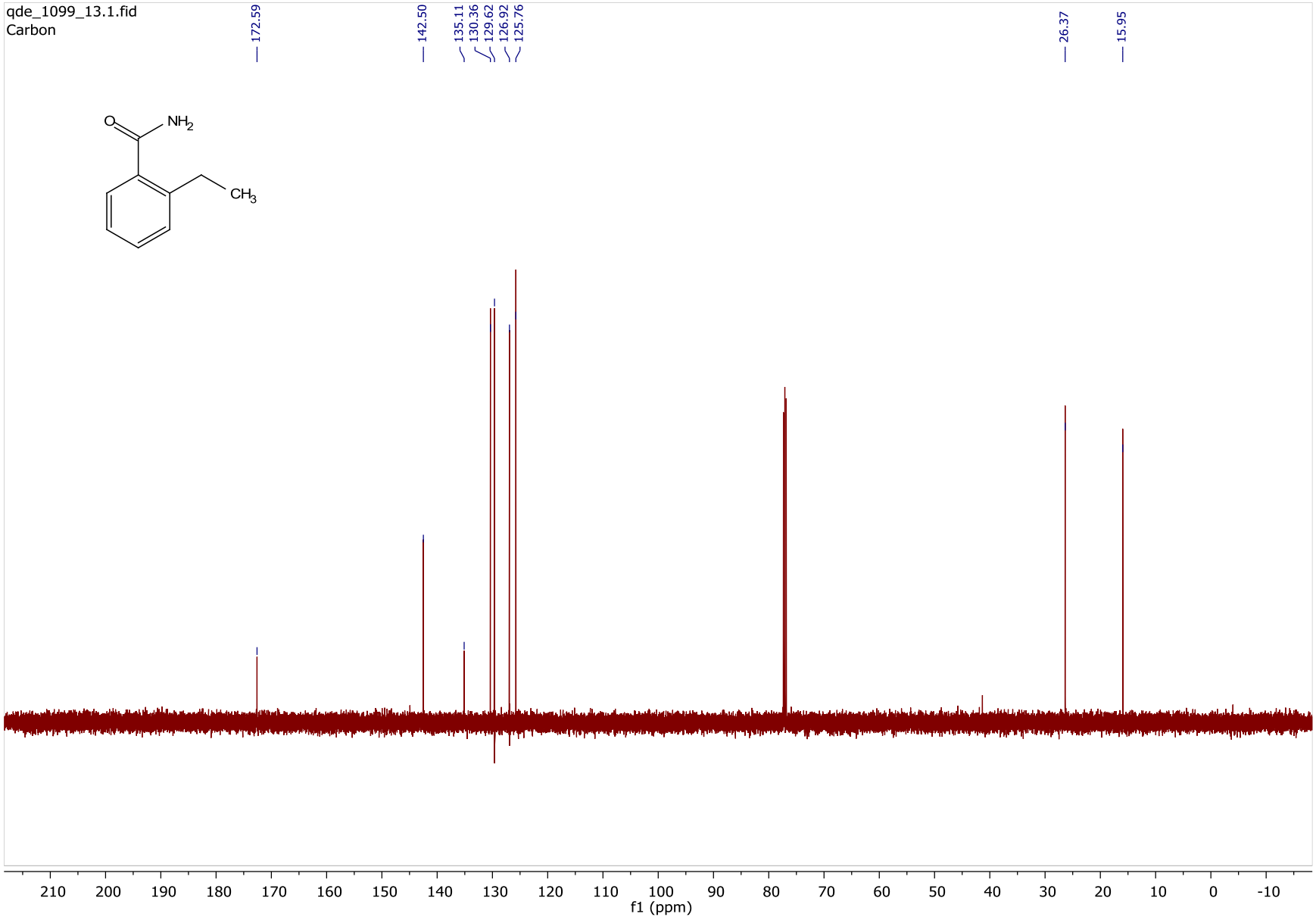

qde_1044_1H
qde_1044_1H
O
NH
CH3
CH3
H3C
1.19
0.83
1.93
1.60
1.77
0.90
0.90
2.00
8.97
f1 (ppm)


qde_1044_13C.1.fid
qde_1044_13C
169.48
141.08
138.14
138.00
131.00
129.58
128.90
128.52
127.33
126.37
126.11
51.58
38.79
28.65
O
NH
CH3
CH3
H3C
f1 (ppm)
f1 (ppm)


qde_1042_1H
qde_1042_1H
4.18
1.28
CH3
H3C
CH3
O
NH
1.02
2.11
4.04
3.97
3.15
2.00
9.23
f1 (ppm)
f1 (ppm)

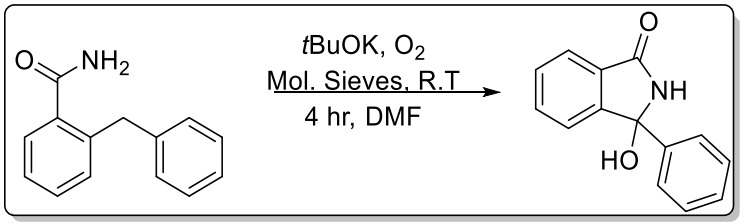

qde_1042_13C.2.fid
qde_1042_13C
167.88
147.53
140.66
138.60
136.94
135.14
131.22
130.37
128.92
128.67
127.49
126.62
126.31
125.83
119.78
38.95
34.43
31.40
CH3
H3C
CH3
NH
O
f1 (ppm)
f1 (ppm)


qde_1099_1H_1.fid
PROTON
O
NH2
CH3
f1 (ppm)


qde_1099_13.1.fid
Carbon
172.59
142.50
135.11
130.36
129.62
126.92
125.76
26.37
15.95
O
NH2
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

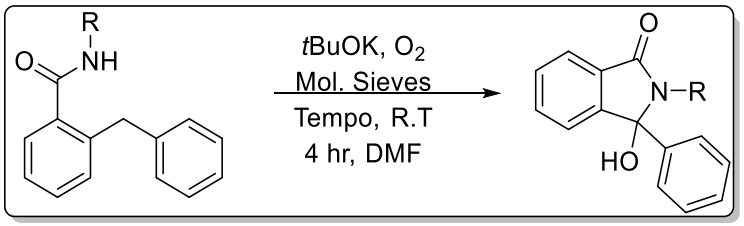
2d) Procedures, spectral data and copies of NMR's for C(sp^3)-H amination products

General procedure 5

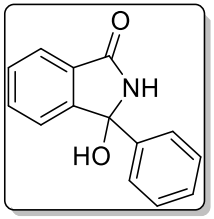


To a 20 mL scintillation vial equipped with a magnetic stir bar was added 4Å-molecular sieves (3x mass of starting amide), primary amide (1.0 eq) and DMF (concentration from 0.025M). The flask was then purged with O_2 and fitted with a balloon of O_2 for the duration of the reaction. To this mixture was then added *t*-BuOK (3.0 equivalents) at room temperature and the mixture was allowed to stir vigorously. Upon completion of the reaction (monitored by TLC), the mixture was transferred to a separatory funnel and diluted with EtOAc. The resulting mixture was washed with ammonium chloride (6 x 15 mL) to remove DMF. The solvent was removed under reduced pressure and purified by silica gel chromatography (DCM: MeOH 98:2) to afford the desired product.

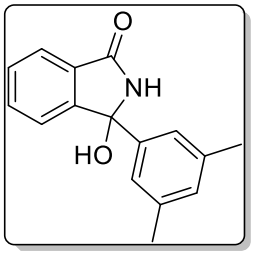
General procedure 6



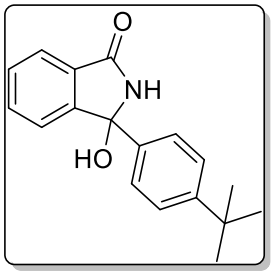
To a 20 mL scintillation vial equipped with a magnetic stir bar was added 4Å-molecular sieves (3x mass of starting amide), primary amide (1.0 eq), Tempo (1.0 eq) and DMF (concentration from 0.025M). The flask was then purged with O_2 and fitted with a balloon of O_2 for the duration of the reaction. To this mixture was then added *t*-BuOK (3.0 equivalents) at room temperature and the mixture was allowed to stir vigorously. Upon completion of the reaction (monitored by TLC), the mixture was transferred to a separatory funnel and diluted with EtOAc. The resulting mixture was washed with ammonium chloride (6 x 15 mL) to remove DMF. The solvent was removed under reduced pressure and purified by silica gel chromatography (DCM: MeOH 98:2) to afford the desired product.



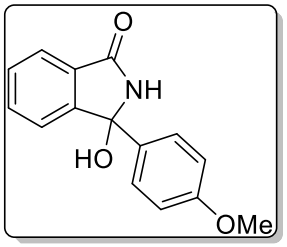
3-hydroxy-3-phenylisoindolin-1-one: following **general procedure 5** with 2-benzylbenzamide (37 mg, 0.175 mmol) yielded the desired product in 87% yield (34 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 (dt, *J* = 7.5, 1.0 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.48 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.40 (dt, *J* = 7.5, 0.9 Hz, 1H), 7.37 – 7.30 (m, 4H), 7.26 (s, 1H), 7.01 (s, 1H), 4.44 (s, 1H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.97, 150.15, 140.00, 133.46, 129.77, 129.62, 128.86, 128.84, 125.72, 123.89, 123.12, 88.39. Matched previously reported spectra.[15]



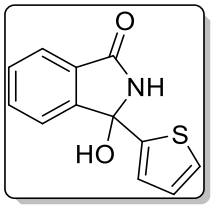
3-(3,5-dimethylphenyl)-3-hydroxyisoindolin-1-one: following **general procedure 5** with 2-(3,5 – dimethylbenzyl)benzamide (35 mg, 0.146 mmol) yielded the desired product in 64% yield (24 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 (dd, *J* = 7.4, 1.1 Hz, 1H), 7.51 (td, *J* = 7.5, 1.2 Hz, 1H), 7.42 (td, *J* = 7.5, 1.1 Hz, 1H), 7.37 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.16 (d, *J* = 1.6 Hz, 2H), 6.94 (s, 1H), 6.71 (s, 1H), 3.99 (s, 1H), 2.28 (s, 6H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.80, 150.22, 139.83, 138.59, 133.44, 130.53, 129.73, 129.63, 123.89, 123.37, 123.10, 88.32, 21.58. Spectra matched those previously reported.[16]



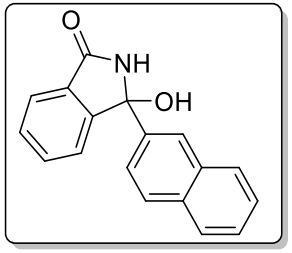
3-(4-(*tert*-butyl)phenyl)-3-hydroxyisoindolin-1-one: following **general procedure 5** with 3-(4-(*tert*-butyl)benzyl)benzamide (35 mg, 0.131 mmol) yielded the diesred product in 84% yield (31 mg) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 – 7.52 (m, 1H), 7.52 – 7.45 (m, 3H), 7.39 – 7.33 (m, 4H), 7.17 (s,1H), 4.78 (d, *J* = 41.1 Hz, 1H), 1.30 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.16, 151.77, 150.26, 137.11, 133.27, 129.63, 129.51, 125.74, 125.43, 123.76, 123.13, 88.43, 34.74, 31.46. Spectra matched those previously reported.[16]



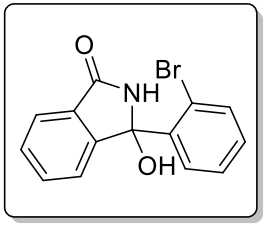
3-hydroxy-3-(4-methoxyphenyl)isoindolin-1-one: following **general procedure 5** with 2-(4-methoxybenzyl)benzamide (30 mg, 0.124 mmol) yielded the desired product in 39% yield (14 mg). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.62 (d, *J* = 7.5 Hz, 1H), 7.50 (td, *J* = 7.5, 1.2 Hz, 1Hz), 7.45 (d, *J* = 8.9 Hz, 2H), 7.39 (td, *J* = 7.5, 1.1 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 6.92 (s, 1H), 6.85 (d, *J* = 8.8 Hz, 2H), 4.15 (s, 1H), 3.78 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.66, 159.77, 150.08, 133.20, 129.44, 129.31, 126.80, 123.61, 122.76, 113.92, 88.06, 55.27. Matched previously reported spectra.[17]



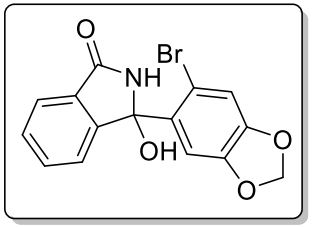
3-hydroxy-3-(thiophen-2-yl)isoindolin-1-one: following **general procedure 5** with 2-(thiophen-2-ylmethyl)benzamide (25 mg, 0.115 mmol) yielded the desired product in 85 % yield (23mg). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.61 – 7.53 (m, 3H), 7.51 (s, 1H), 7.45 – 7.40 (m, 1H), 7.33 – 7.28 (m, 1H), 7.08 (d, *J* = 3.5 Hz, 1H), 6.98 – 6.93 (m, 1H), 5.15 (s, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.60, 149.05, 144.11, 133.20, 129.67, 128.90, 127.05, 126.12, 124.79, 123.66, 122.80, 86.87. Matched previously reported spectra.[15]



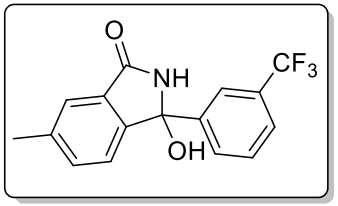
3-hydroxy-3-(naphthalen -2-yl)isoindolin-1-one: Following **general procedure** 5 with 2-(napthalen-2-ylmethyl)benzamide) (18 mg, 0.069 mmol) yielded the desired product in 70% yield (12.6 mg). ^{1}H NMR (400 MHz, Acetone-d_6) δ 8.29 (s, 1H), 8.27 (d, *J* = 1.8 Hz, 1H), 8.00 – 7.95 (m, 1H), 7.89 (t, *J* = 8.6 Hz, 2H), 7.77 – 7.69 (m, 1H), 7.61 – 7.46 (m, 5H), 7.42 (d, *J* = 7.4 Hz, 1H), 6.03 (s, 1H). ^{13}C NMR (151 MHz, Acetone-d_6) δ 168.35, 150.84, 139.40, 133.23, 133.14, 132.46, 130.94, 129.10, 128.26, 128.01, 127.49, 126.23, 124.44, 123.97, 122.97, 122.81, 87.66. Spectra matched those previously reported.[18]



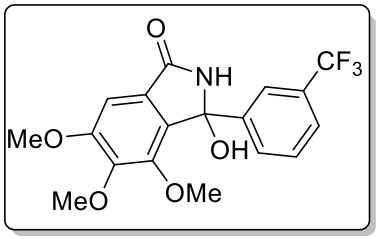
3-(2-bromophenyl)-3-hydroxyisoindolin-1-one: Following **general procedure** 5 with 2-(2-bromobenzyl)benzamide (33mg, 0.114 mmol) yielded the desired product in 81% yield (27 mg). ^{1}H NMR (400 MHz, Acetonitrile-d_3) δ 8.25 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.73 – 7.62 (m, 1H), 7.57 – 7.51 (m, 3H), 7.50 – 7.45 (m, 1H), 7.28 (s, 1H), 7.25 (td, *J* = 7.6, 1.8 Hz, 1H), 7.18 – 7.13 (m, 1H), 4.84 (s, 1H). ^{13}C NMR (151 MHz, Acetonitrile-d_3) δ 169.58, 148.88, 137.95, 134.89, 132.71, 132.62, 130.32, 129.72, 129.54, 127.58, 122.71, 122.44, 120.58, 86.72. [M+H$^+$] 303.9895, found 303.9968.



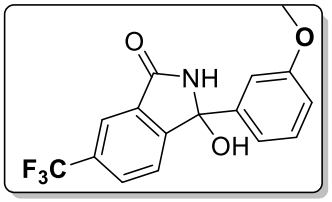
3-(6-bromobenzo[*d*][1,3] dioxol-5-yl)-3-hydroxyisoindolin-1-one: Following **general procedure 5** with 2-((6-bromobenzo[*d*][1,3]dioxol-5-yl)methyl)benzamide (32 mg, 0.096 mmol) yielded the desired product in 75% yield (24 mg). ^{1}H NMR (600 MHz, Acetone-d_6) δ 7.96 (s, 1H), 7.86 (s, 1H), 7.70 – 7.65 (m, 1H), 7.54 (dtd, *J* = 28.2, 7.4, 1.2 Hz, 2H), 7.24 (dt, *J* = 7.5, 0.9 Hz, 1H), 7.02 (s, 1H), 6.13 (q, *J* = 1.0 Hz, 2H), 5.97 (s, 1H). ^{13}C NMR (151 MHz, Acetone-d_6) δ 169.07, 149.36, 148.39, 147.43, 133.11, 132.32, 132.20, 129.06, 122.49, 122.31, 114.14, 111.48, 109.62, 102.37, 86.50. [M+H$^+$] 347.9793, found 347.9878



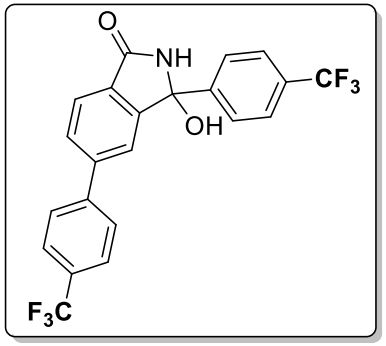
3-hydroxy-6-methyl-3-(3-trifluoromethyl)phenyl)isoindolin-1-one: Following **general procedure** 5 with 5-methyl-2-(3-(trifluoromethyl)benzyl)benzamide (25 mg, 0.085 mmol) yielded the desired product in 79% yield (21 mg).^{1}H NMR (400 MHz, Acetonitrile-d_3) δ 7.88 (tt, J = 1.8, 0.8 Hz, 1H), 7.73 (dt, J = 7.8, 1.7 Hz, 1H), 7.65 (ddt, J = 7.8, 1.8, 1.0 Hz, 1H), 7.59 – 7.51 (m, 2H), 7.43 (s, 2H), 7.38 (ddd, J = 7.8, 1.6, 0.8 Hz, 2H), 7.20 (d, J = 7.8 Hz, 1H), 4.90 (s, 1H), 2.42 (d, J = 0.9 Hz, 3H). ^{13}C NMR (151 MHz, Acetonitrile-d_3) δ 168.74, 147.05, 143.01, 140.15, 133.78, 130.42, 130.14, 129.58, 129.44, 125.00, 124.97, 123.41, 123.22, 122.51, 122.22, 122.19, 87.00, 20.33. ^{19}F NMR (376 MHz, Acetone-d_6) δ -63.03. [M+H$^+$] 308.0820, found 308.0916.



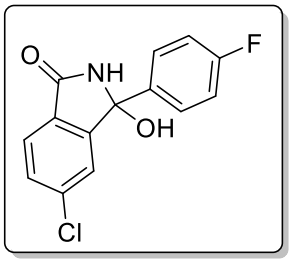
3-hydroxy-4,5,6-trimethoxy-3-(3-(trifluoromethyl)phenyl)isoindolin-1-one: Following **general procedure 5** with 3,4,5-trimethoxy-2-(3-(trifluoromethyl)benzyl)benzamide (31.2 mg, 0.084 mmol) yielded the desired product in 90% yield (28 mg).^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, J = 1.9 Hz, 1H), 7.61 (d, J = 7.9 Hz, 1H), 7.53 (dd, J = 14.5, 3.9 Hz, 2H), 7.40 (t, J = 7.8 Hz, 1H), 6.88 (d, J = 2.7 Hz, 1H), 5.13 (s, 1H), 3.83 – 3.81 (m, 3H), 3.81 (d, J = 0.9 Hz, 3H), 3.44 (d, J = 0.8 Hz, 3H). ^{13}C NMR (151 MHz, Acetonitrile-*d3*) δ 173.57, 161.60, 153.92, 151.65, 147.95, 139.47, 135.16, 134.88, 134.31, 131.39, 130.65, 130.02, 128.85, 128.25, 107.03, 91.65, 65.66, 65.51, 61.41. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -57.69. [M+H] 384.0981, found 384.1048.



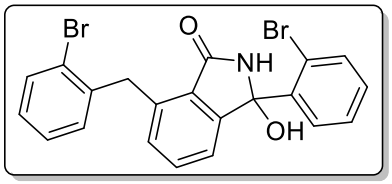
3-hydroxy-3-(3-methoxyphenyl)-6-(trifluoromethyl)isoindolin-1-one: Following **general procedure** 5 with 2-(3-methoxybenzyl)-5-trifluoromethyl)benzamide (50 mg, 0.162 mmol)yielded the desired product in 90% yield (47 mg) . ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 (s, 1H), 7.71 (d, J = 8.0 Hz, 2H), 7.45 (d, J = 7.9 Hz, 1H), 7.23 (t, J = 8.0 Hz, 1H), 7.12 (t, J = 2.1 Hz, 1H), 7.03 (d, J = 7.7 Hz, 1H), 6.83 (dd, J = 8.3, 2.5 Hz, 1H), 5.09 (s, 1H), 3.76 (s, 3H). ^{13}C NMR (101 MHz, Acetone-*d6*) δ 167.74, 160.87, 155.13, 143.36, 132.54, 132.04, 131.72, 130.46, 126.29, 124.93, 123.59, 120.74, 118.67, 114.41, 112.48, 88.42, 55.56. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.54. [M+H] 324.0769, found 324.0548.



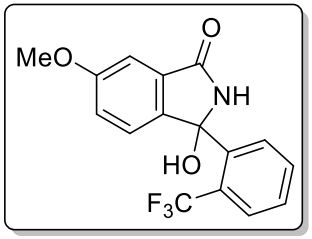
3-hydroxy-3,5-bis(4-(trifluoromethyl)phenyl)isoindolin-1-one: Following **general procedure 5** with 4'-(trifluoromethyl)-3-(4-(trifluoromethyl)benzyl)-[1,1'-biphenyl]-4-carboxamide (50 mg, 0.118 mmol) yielded the desired product in 60% yield (31 mg).^{1}H NMR (400 MHz, Acetone-d_6) δ 8.53 (s, 1H), 7.90 (d, J = 1.6 Hz, 1H), 7.88 (d, J = 1.4 Hz, 2H), 7.85 (d, J = 5.1 Hz, 2H), 7.81 (d, J = 8.8 Hz, 2H), 7.78 (s, 1H), 7.75 – 7.72 (m, 3H), 6.37 (s, 1H). ^{13}C NMR (101 MHz, Acetone-d_6) δ 169.28, 152.55, 147.74, 145.34, 145.09, 132.01, 130.11, 129.39, 128.07, 127.19, 126.71, 125.15, 123.04, 88.67. ^{19}F NMR (376 MHz, Chloroform-d) δ -62.63, -62.72. [M+H] 438.0850, found 438.0895.



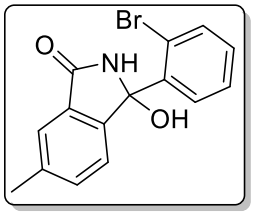
5-chloro-3-(4-fluorophenyl)-3-hydroxyisoindolin-1-one: Following **general procedure 5** with 4-chloro-2-(fluorobenzyl)benzamide (25 mg, 0.095 mmol) yielded the desired product in 68% yield (18 mg)^{1}H NMR (400 MHz, Acetone-d_6) δ 8.40 (s, 1H), 7.70 (d, J = 8.1 Hz, 1H), 7.68 – 7.63 (m, 2H), 7.55 (dd, J = 8.0, 1.8 Hz, 1H), 7.39 (d, J = 1.8 Hz, 1H), 7.19 – 7.11 (m, 2H), 6.14 (s, 1H). ^{13}C NMR (101 MHz, Acetone-d_6) δ 167.15, 163.86, 161.43, 152.54, 138.02, 129.58, 129.37, 127.94, 127.85, 124.63, 123.06, 115.14, 114.93, 86.89. ^{19}F NMR (376 MHz, Chloroform-d) δ -112.69 (tt, J = 8.7, 5.2 Hz). [M+H] 278.0306, found 278.0814.



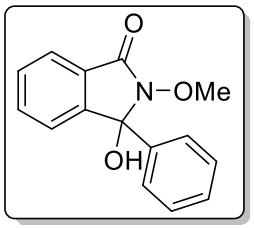
7-(2-bromobenzyl)-3-(2-bromophenyl)-3-hydroxyisoindolin-1-one:Following **general procedure 5** with 2,6-bis (2-bromobenzyl)benzamide (20 mg, 0.0436 mmol) yielded the desired product in 78% yield (16.3 mg) ^{1}H NMR (500 MHz, Chloroform-d) δ 8.00 (dd, J = 8.0, 1.7 Hz, 1H), 7.56 (ddd, J = 7.8, 6.2, 1.3 Hz, 2H), 7.43 (t, J = 7.6 Hz, 1H), 7.36 (td, J = 7.6, 1.3 Hz, 1H), 7.23 – 7.19 (m, 2H), 7.19 – 7.14 (m, 2H), 7.12 – 7.10 (m, 1H), 7.08 (ddd, J = 8.0, 6.9, 2.1 Hz, 1H), 6.75 (s, 1H), 4.57 (dd, J = 133.0, 16.1 Hz, 2H), 3.99 (s, 1H). ^{13}C NMR (126 MHz, Chloroform-d) δ 170.54, 148.85, 139.71, 139.69, 137.32, 135.15, 133.07, 132.93, 131.51, 130.85, 130.38, 129.40, 128.16, 128.06, 127.55, 127.51, 125.04, 121.38, 121.01, 86.67, 35.83. [M+H] 471.9470, found 471.9265.



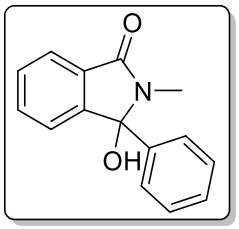
3-hydroxy-6-methoxy-3-2(-(trilfluoromethyl)phenyl)isoindolin-1-one: Following **general procedure 5** with 5-methoxy-2-(2-trifluoromethyl)benzyl)benzamide (25 mg, 0.081 mmol) yielded the ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (s, 1H), 7.63 (dd, *J* = 25.8, 7.8 Hz, 2H), 7.47 (t, *J* = 7.8 Hz, 1H), 7.25 – 7.20 (m, 2H), 7.08 (dd, *J* = 8.4, 2.5 Hz, 1H), 6.59 (s, 1H), 3.86 (s, 3H), 3.30 (s, 1H). ^{13}C NMR (151 MHz, Acetone-d_6) δ 168.08, 161.14, 143.95, 142.29, 132.46, 130.09, 129.88, 129.74, 129.33, 125.32, 124.84 – 124.49 (m), 123.88, 123.52, 122.26 (q, *J* = 3.9 Hz), 119.64, 106.48, 86.91, 55.23. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.57. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.57. [M+H] 324.0769, found 324.0545.



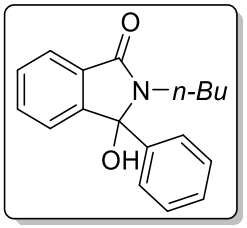
3-(2-bromophenyl)-3-hydroxy-6-methylisoindolin-1-one: Following **general procedure 5** with 2-(2-bromobenzyl)-5-methylbenzamide (20 mg, 0.066 mmol) yielded the desired product in 86% yield (18 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.57 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.48 (dd, *J* = 1.8, 0.9 Hz, 1H), 7.37 (ddd, *J* = 9.4, 7.1, 1.3 Hz, 2H), 7.26 – 7.18 (m, 2H), 6.88 (s, 1H), 4.35 (s, 1H), 2.42 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.17, 145.50, 140.10, 137.35, 135.10, 133.86, 131.61, 130.26, 129.31, 127.41, 123.99, 122.88, 121.01, 87.57, 21.43. [M+H] 318.0051, found 318.0143.



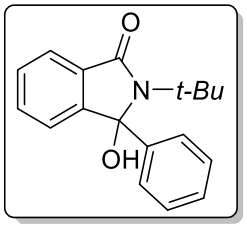
3-hydroxy-2-methoxy-3-phenylisoindolin-1-one: Following **general procedure 6** with 2-benzyl-*N*-methoxybenzamide (22.8 mg, 0.0945 mmol) yielded the desired product in 31% yield (7.48 mg) ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.83 – 7.77 (m, 1H), 7.54 (td, *J* = 7.5, 1.2 Hz, 1H), 7.51 – 7.46 (m, 3H), 7.39 – 7.34 (m, 3H), 7.29 (d, *J* = 7.5 Hz, 1H), 3.90 (s, 3H), 3.69 (s, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.93, 145.93, 137.69, 133.49, 129.97, 128.91, 128.65, 127.96, 126.27, 123.79, 122.79, 90.90, 65.61. Spectra Matched those previously published.[19]



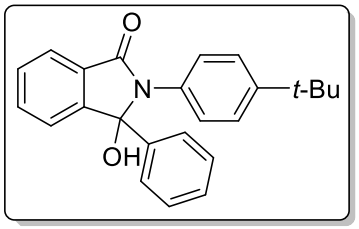
3-hydroxy-2-methyl-3-phenylisoindolin-1-one: Following **general procedure 6** with 2-benzyl-N-methylbenzamide (30 mg, 0.013 mmol) yielded the desired product in (74% 22 mg) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.34 (tdd, *J* = 11.4, 5.3, 2.8 Hz, 7H), 3.62 (s, 1H), 2.62 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.12, 149.17, 138.20, 132.72, 130.24, 129.48, 128.80, 128.59, 126.13, 123.27, 122.94, 91.23, 24.08.Spectra Matched those previously published.[19]



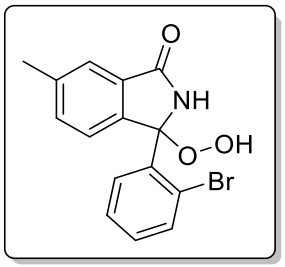
2-butyl-3-hydroxy-3-phenylisoindolin-1-one: Following **general procedure 6** with 2-benzyl-N-butylbenzamide (50 mg, 0.187 mmol) yielded the desired product in 87% yield (46 mg).[1]H NMR (500 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 7.5 Hz, 1H), 7.43 (td, *J* = 7.5, 1.2 Hz, 1H), 7.39 – 7.34 (m, 3H), 7.33 – 7.28 (m, 3H), 7.27 – 7.22 (m, 1H), 4.53 (s, 1H), 3.35 – 3.23 (m, 1H), 2.87 (ddd, *J* = 14.0, 9.7, 5.9 Hz, 1H), 1.45 – 1.30 (m, 1H), 1.22 – 1.07 (m, 3H), 0.75 (t, *J* = 7.1 Hz, 3H). [13]C NMR (126 MHz, Chloroform-*d*) δ 168.00, 149.20, 138.89, 132.48, 130.56, 129.29, 128.41, 126.26, 123.12, 122.73, 91.37, 39.35, 30.64, 20.44, 13.65. Spectra Matched those previously reported.[19]



2-(*tert*-butyl)-3-hydroxy-3-phenylisoindolin-1-one: Following **general procedure 6** with 2-benzyl-*N*-(*tert*-butyl)benzamide (50 mg, 0.187 mmol) yielded the desired product in 54% yield (28.4 mg) [1]H NMR (500 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 7.5 Hz, 2H), 7.67 – 7.61 (m, 1H), 7.58 – 7.49 (m, 3H), 7.45 – 7.40 (m, 3H), 5.73 (s, 1H), 1.16 (s, 9H). [13]C NMR (126 MHz, Chloroform-*d*) δ 197.92, 167.06, 138.79, 137.15 (d, *J* = 14.0 Hz), 133.39, 130.24, 130.21, 129.89, 128.55, 128.46, 127.48, 51.91, 28.23. [M+H] 282.1416, found 282.1371.

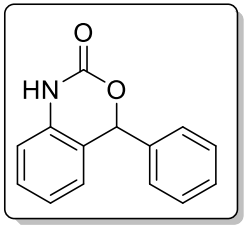


2-(4-(*tert*-butyl)phenyl)-3-hydroxy-3-phenylisoindolin-1-one: Following **general procedure 6** 2-benzyl-*N*-(4-(*tert*-butyl)phenyl)benzamide (50 mg, 0.146 mmol) yielded the desired product in 55% yield (29 mg). [1]H NMR (400 MHz, Chloroform-*d*) δ 7.63 (d, *J* = 7.7 Hz, 1H), 7.50 – 7.41 (m, 3H), 7.36 (d, *J* = 8.7 Hz, 2H), 7.32 – 7.26 (m, 5H), 7.22 (d, *J* = 8.8 Hz, 2H), 4.61 (s, 1H), 1.30 (s, 9H). [13]C NMR (101 MHz, Chloroform-*d*) δ 167.63, 148.70 (d, *J* = 6.5 Hz), 139.08, 133.08, 133.00, 129.70, 129.46, 128.44, 128.19, 126.12, 125.41, 124.69, 123.78, 122.59, 93.05, 34.39, 31.31. [M+H] 358.1279, found 358.1560.

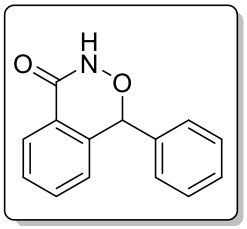


3-(2-bromophenyl)-3-hydroperoxy-6-methylisoindolin-1-one: Following an adapted procedure[20] in which a round bottom flask charged with a stir bar was added 3-(2-bromophenyl)-3-hydrxy-6-methylisoindolin-1-one (106 mg, 0.3 mmol) and 2 mL of diethyl ether. Then in succession 10M H_2SO_4 (0.123 mL) and 30% H_2O_2 (0.093 mL, 3 mmol) was added and the reaction was allowed to mix for 4 hours at room temperature. The reaction was then diluted with ethyl acetate, washed with saturated K_2CO_3, and concentrated down. The crude mixture was purified by silica gel chromatography (DCM:MeOH, 97:3). Desired product obtained in 68% (68.5 mg) yield. [1]H NMR (400 MHz, Chloroform-*d*) δ 9.82 (s, 1H), 7.89 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.63 – 7.58 (m, 2H), 7.42 – 7.29 (m, 4H), 7.24 (td, *J* = 7.6, 1.7 Hz, 1H), 2.46 (s, 3H). [13]C NMR (151 MHz, Chloroform-*d*) δ

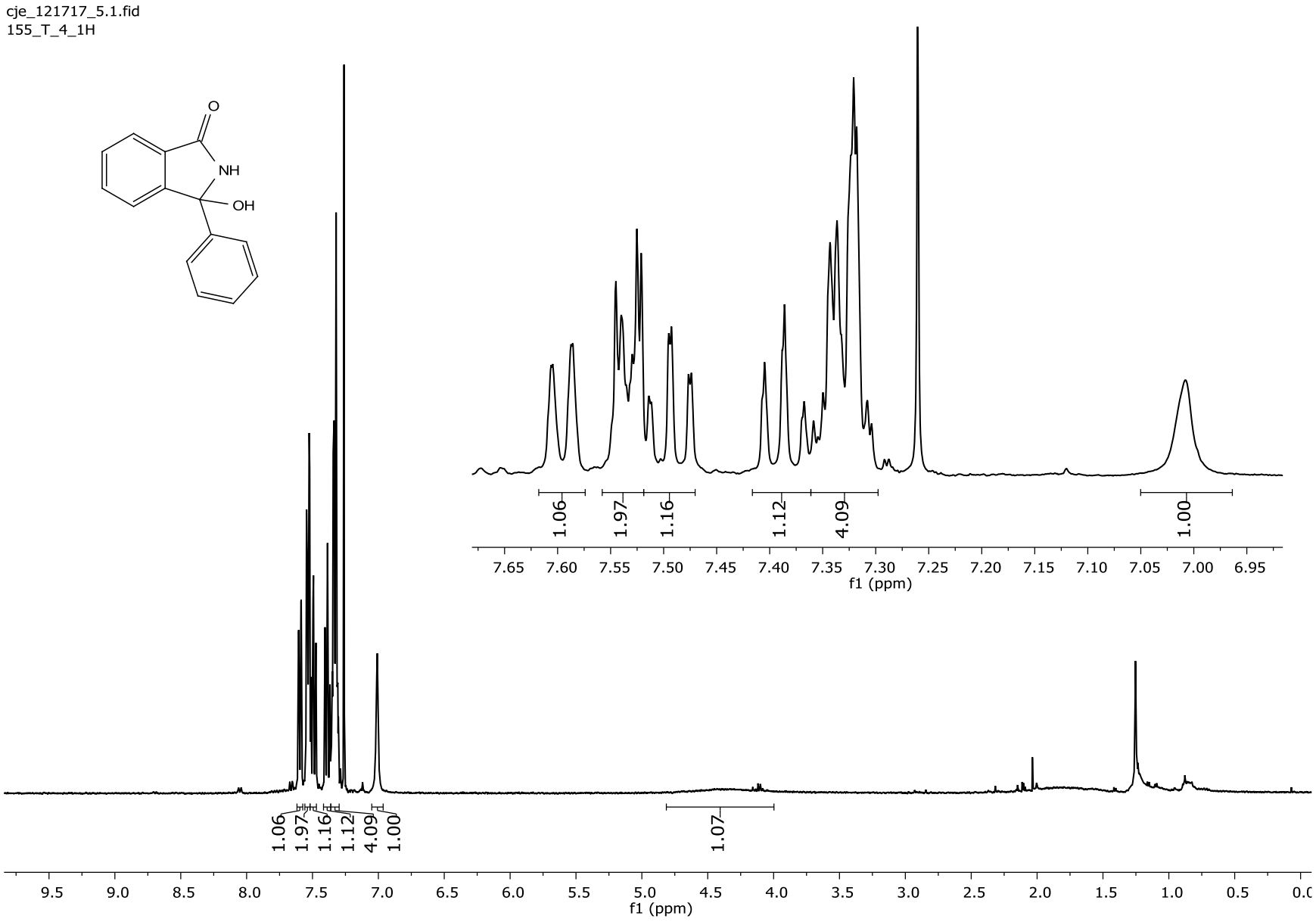
171.73, 140.95, 140.71, 135.35, 134.63, 133.74, 132.32, 130.54, 130.03, 127.48, 124.27, 123.35, 121.29, 96.53, 21.46. [M+H] 334.0001, found 334.0075.



4-phenyl-1,4-dihydro-2*H*-benzo[d][1,3]oxazin-2-one: Following **general procedure 5** with 2-benzylbenzonitrile (20mg, 0.103 mmol) yielded the desired product in 12% yield (2.5 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (s, 1H), 7.43 – 7.38 (m, 3H), 7.38 – 7.33 (m, 2H), 7.32 – 7.27 (m, 1H), 7.03 (td, *J* = 7.6, 1.1 Hz, 1H), 6.87 (dd, *J* = 7.9, 1.1 Hz, 2H), 6.38 (s, 1H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 137.56, 135.46, 129.68, 129.42, 129.02, 127.95, 126.22, 123.64, 121.35, 114.33, 81.44. Spectra Matched those previously reported.[21]



1-phenyl-1*H*-benzo[d][1,2]oxazin-4(3*H*)-one: Following **general procedure 5** with 2-benzylbenzonitrile (20mg, 0.103 mmol) yielded the desired product in 11% yield (2.4 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.68 (s, 1H), 8.22 – 8.13 (m, 1H), 7.58 – 7.48 (m, 2H), 7.43 (dd, *J* = 5.0, 1.8 Hz, 3H), 7.39 – 7.33 (m, 2H), 6.93 – 6.85 (m, 1H), 6.16 (d, *J* = 0.0 Hz, 1H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 166.62, 140.20, 136.48, 133.35, 129.63, 129.18, 128.94, 128.66, 127.66, 126.30, 125.52, 83.15. [M+H] = 226.0863, found 226.0864.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OH
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1.16
1.12
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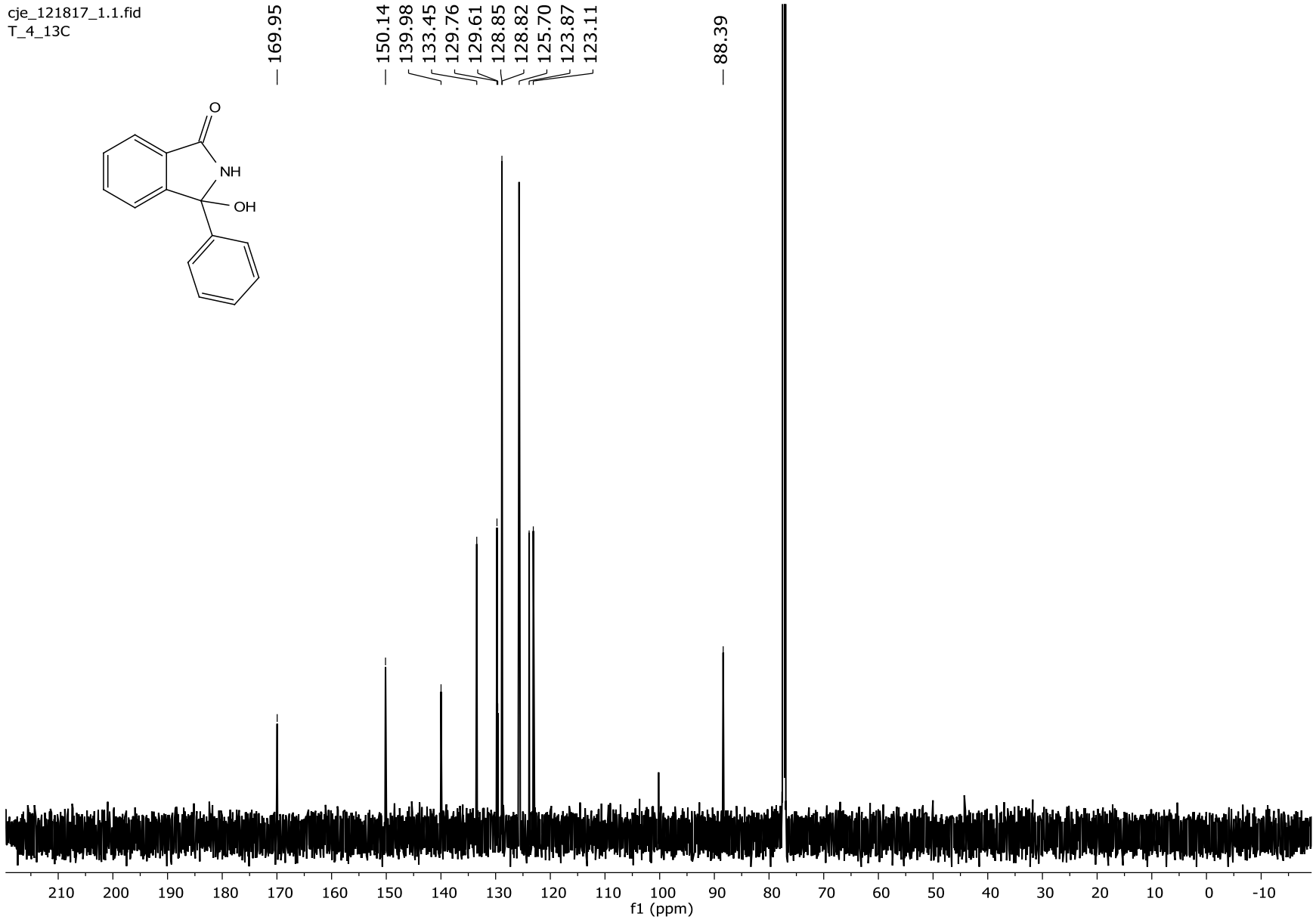
1.00
1.07
f1 (ppm)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88.39
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OH
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190
180
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160
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100
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f1 (ppm)

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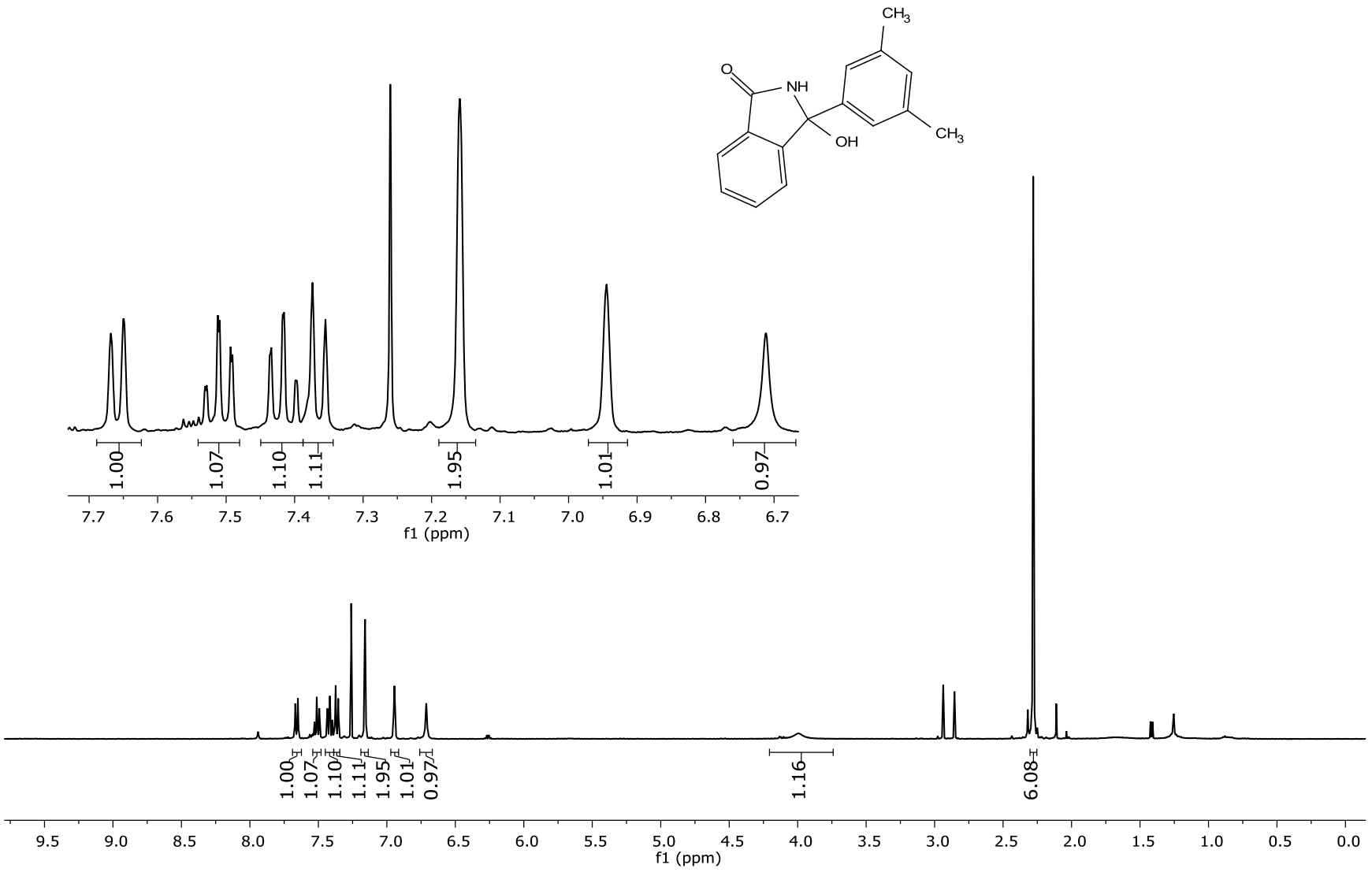
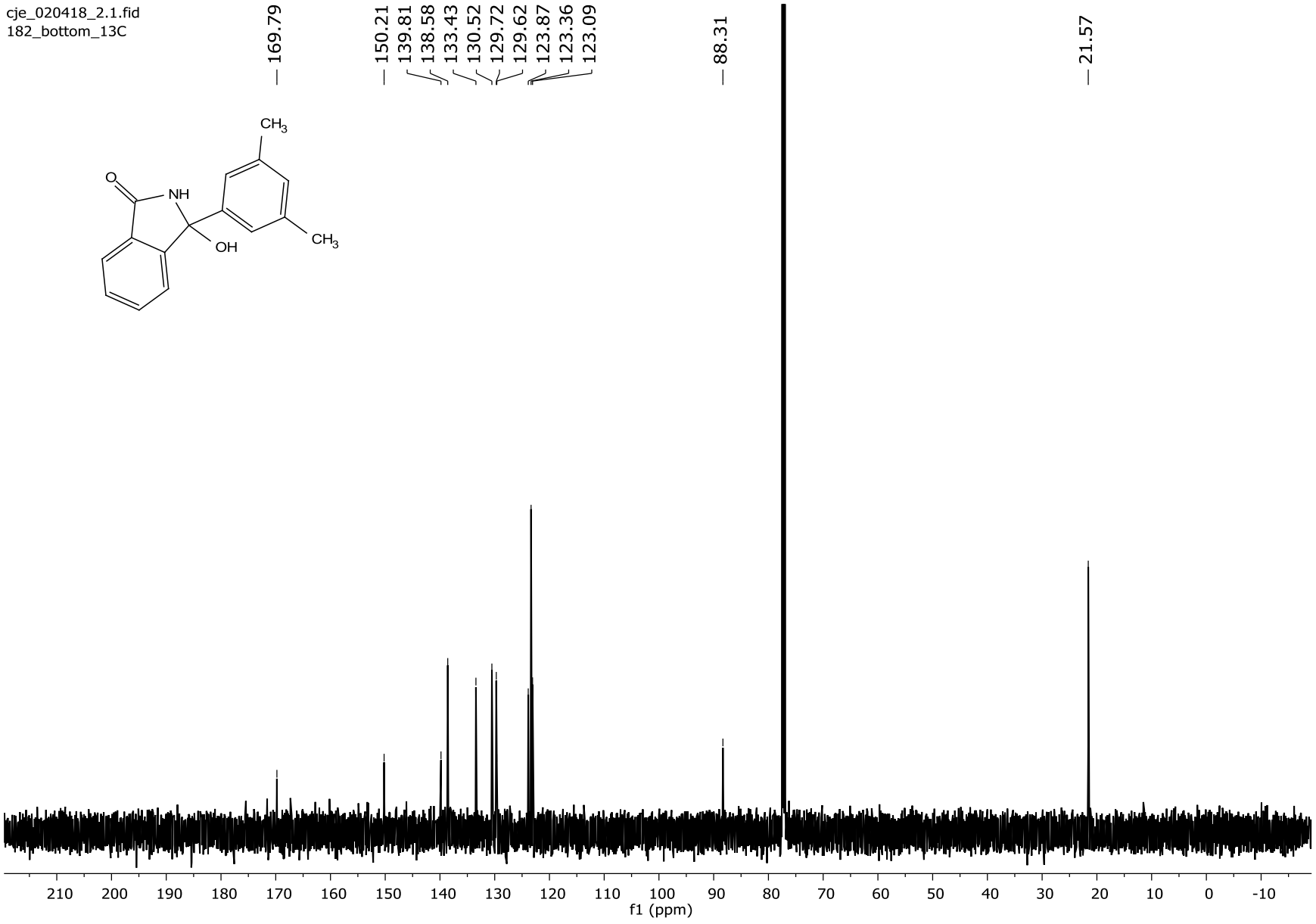
182_bottom_1H

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129.72
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123.36
123.09
88.31
21.57
CH3
O
NH
OH
CH3
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200
190
180
170
160
150
140
130
120
110
100
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30
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10
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f1 (ppm)

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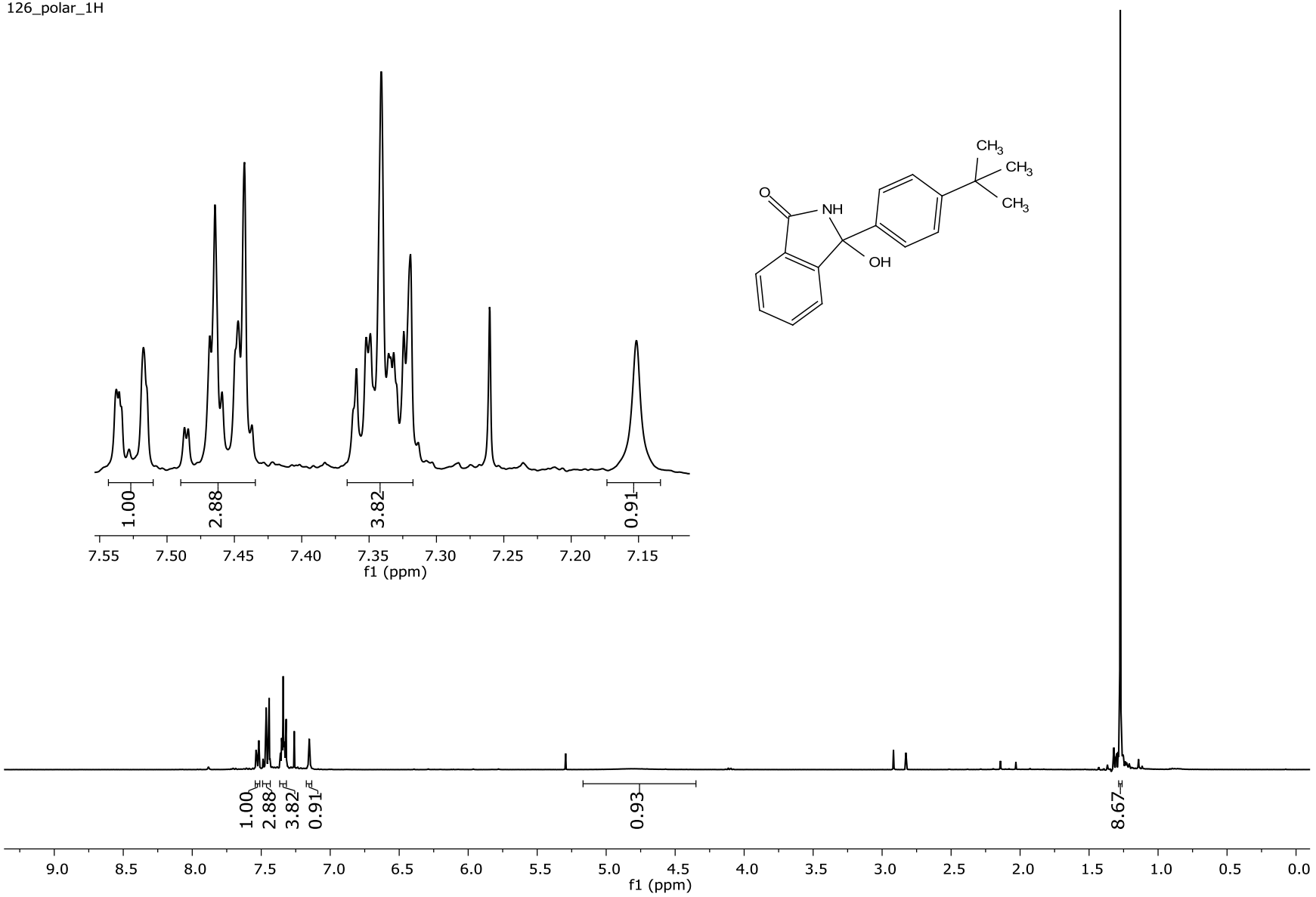

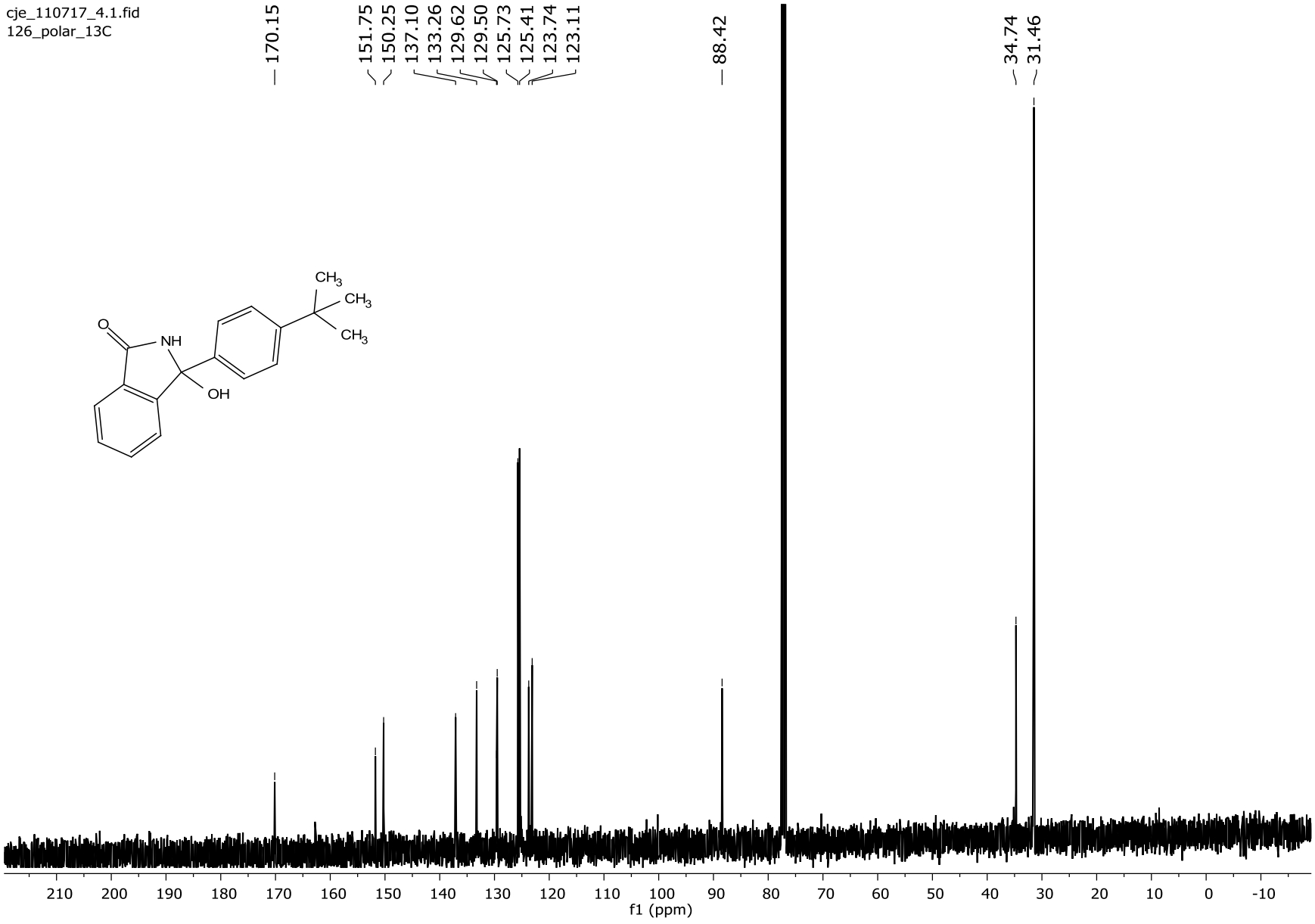
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137.10
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123.74
123.11
88.42
34.74
31.46
CH3
CH3
CH3
O
NH
OH
210
200
190
180
170
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140
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100
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80
70
60
50
40
30
20
10
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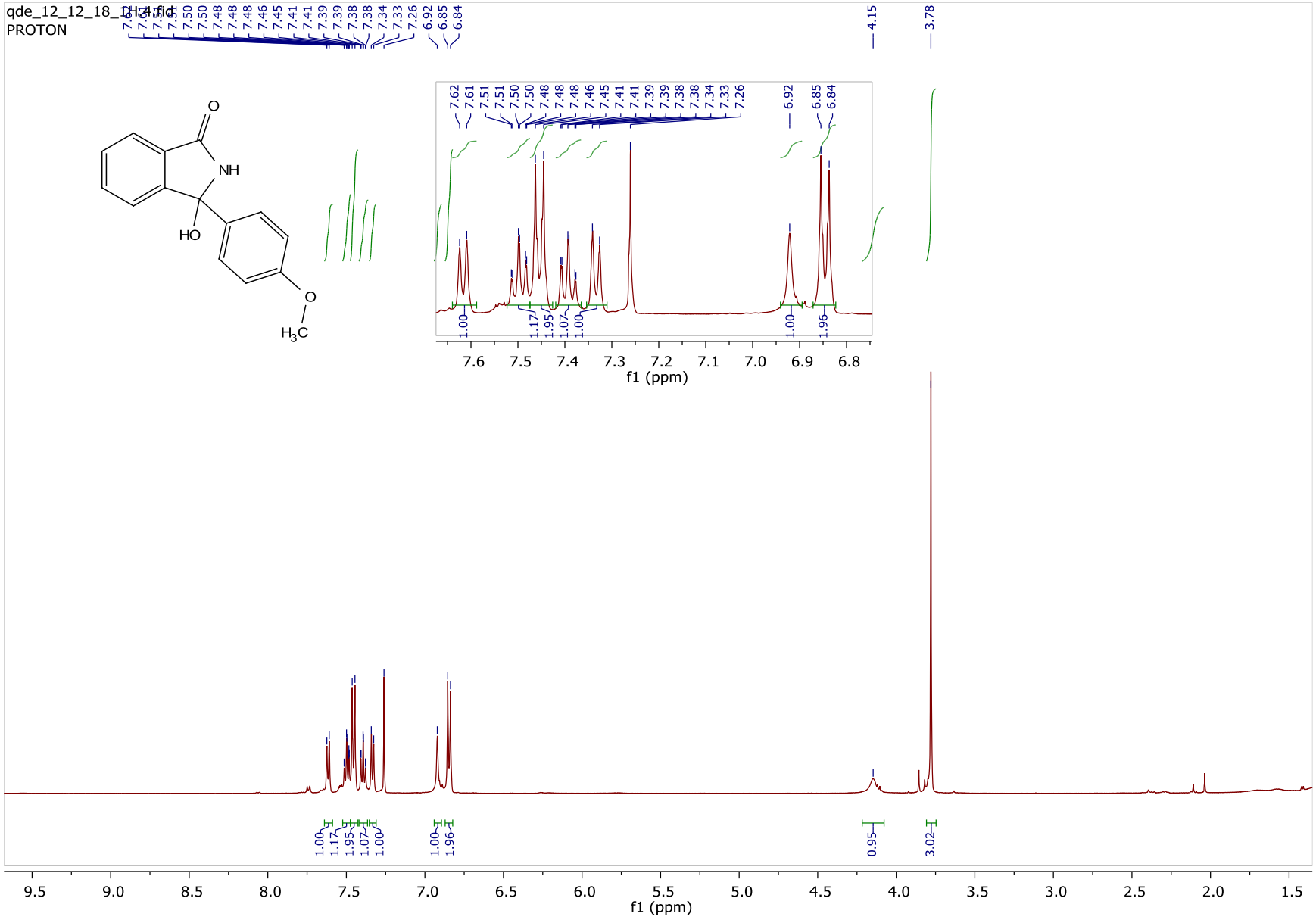
-10
f1 (ppm)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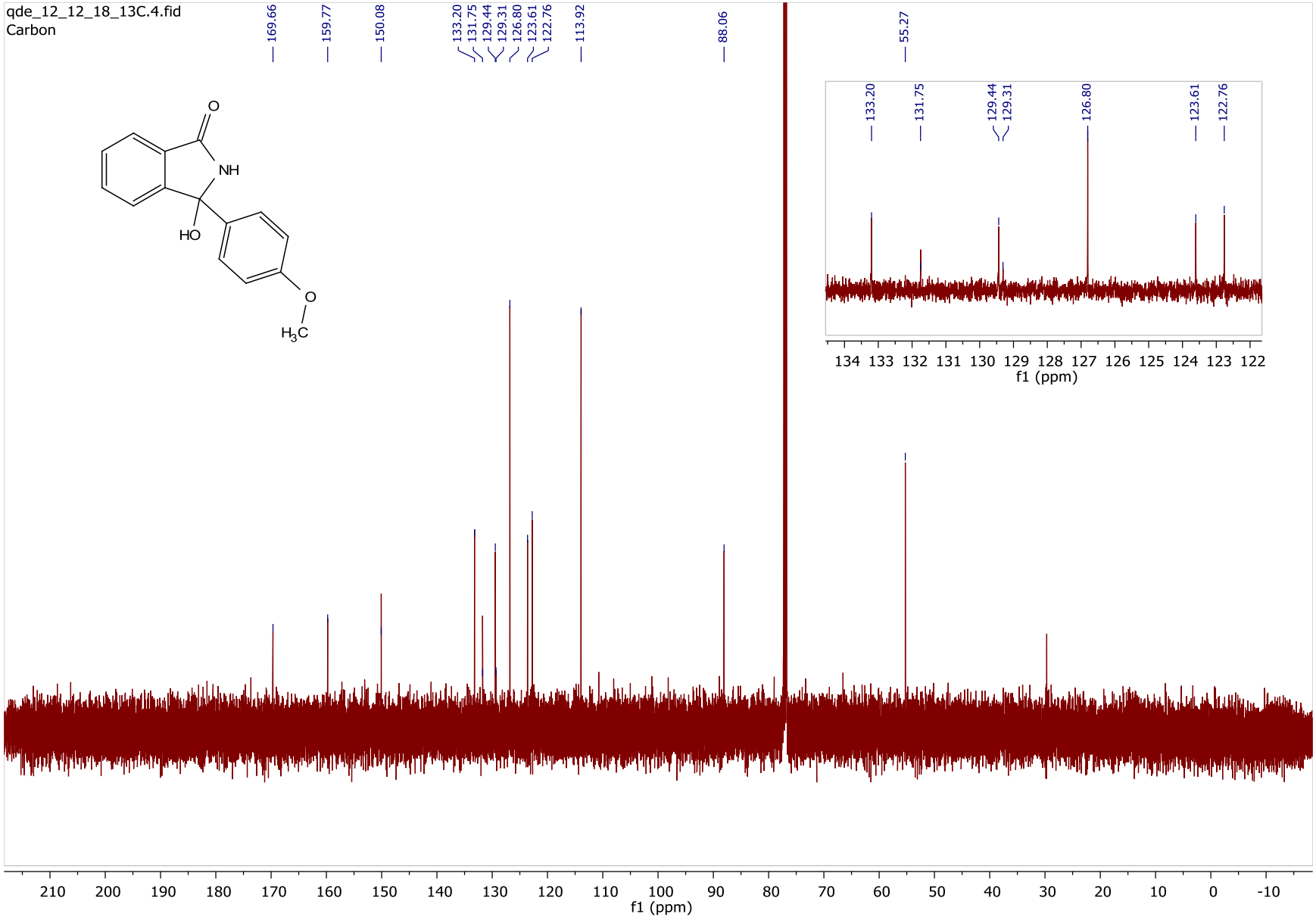
4.15
3.78
O
NH
HO
O
H3C
1.00 1.17 1.95 1.07 1.00 1.00 1.96
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)
1.00 1.17 1.95 1.07 1.00 1.00 1.96 0.95 3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)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133.20
131.75
129.44
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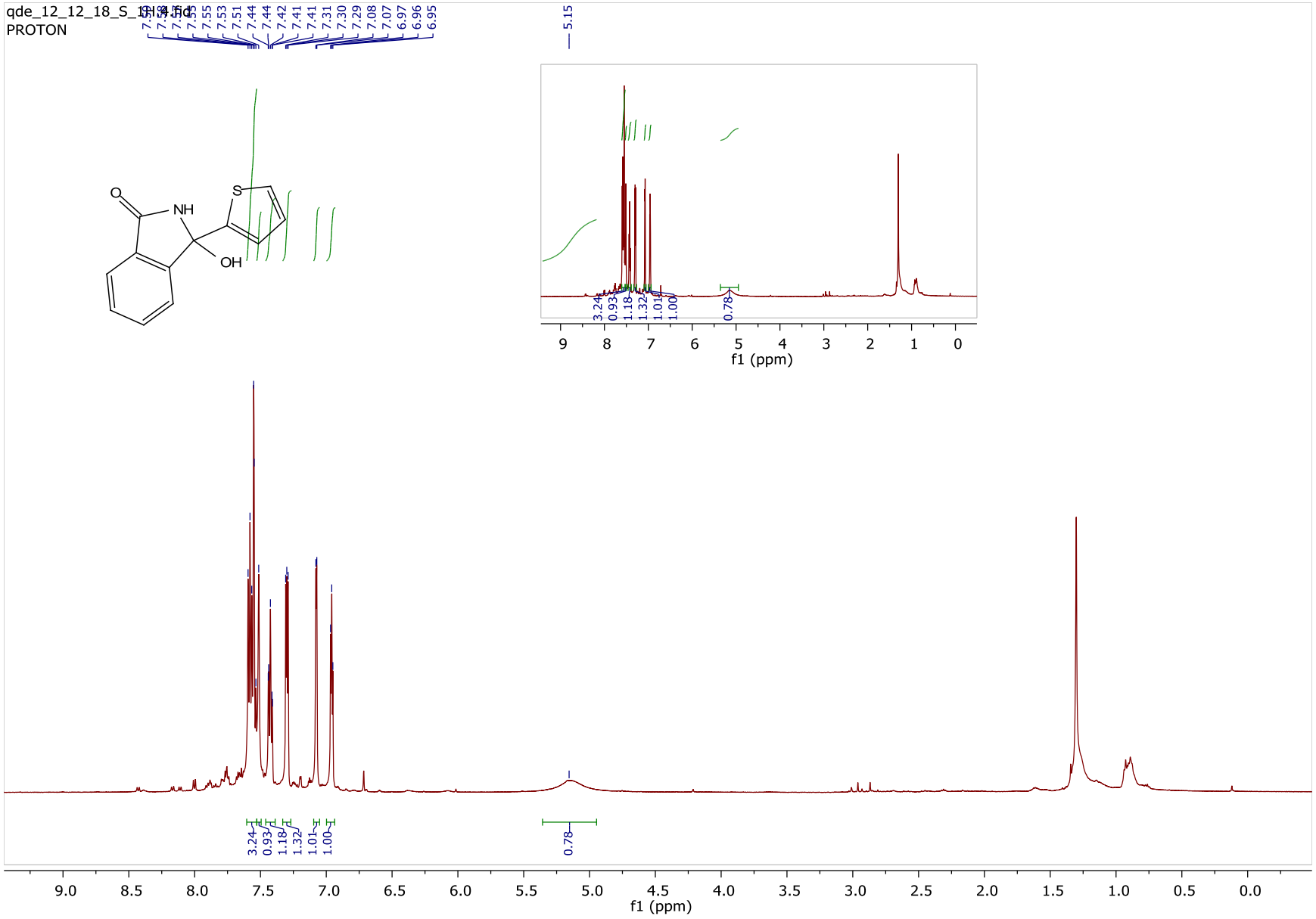
55.27
O
NH
HO
O
H3C
f1 (ppm)


qde_12_12_18_S_1H_3.fid
PROTON
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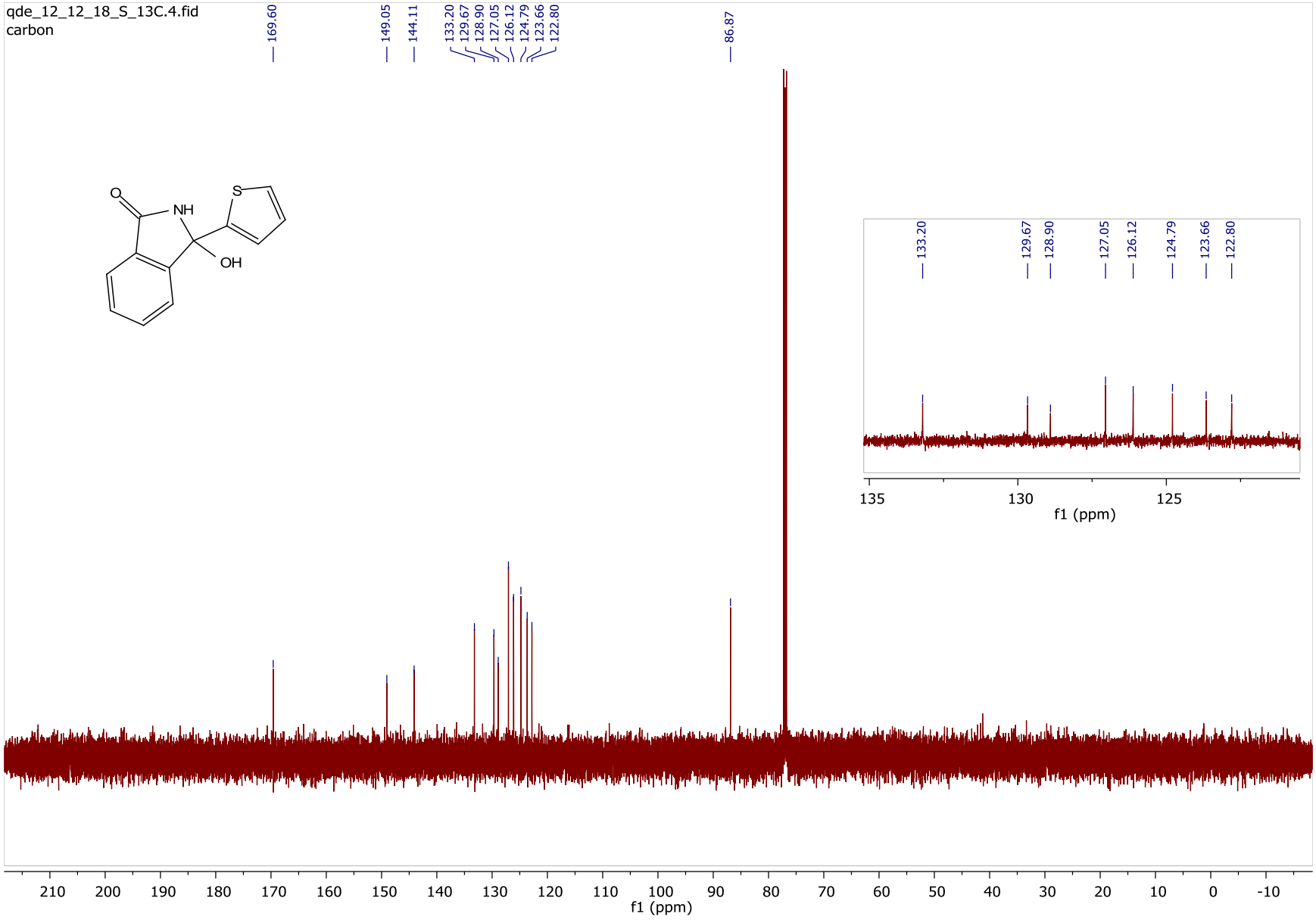
5.15
O
NH
S
OH
3.24
0.93
1.18
1.32
1.01
1.00
0.78
f1 (ppm)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144.11
133.20
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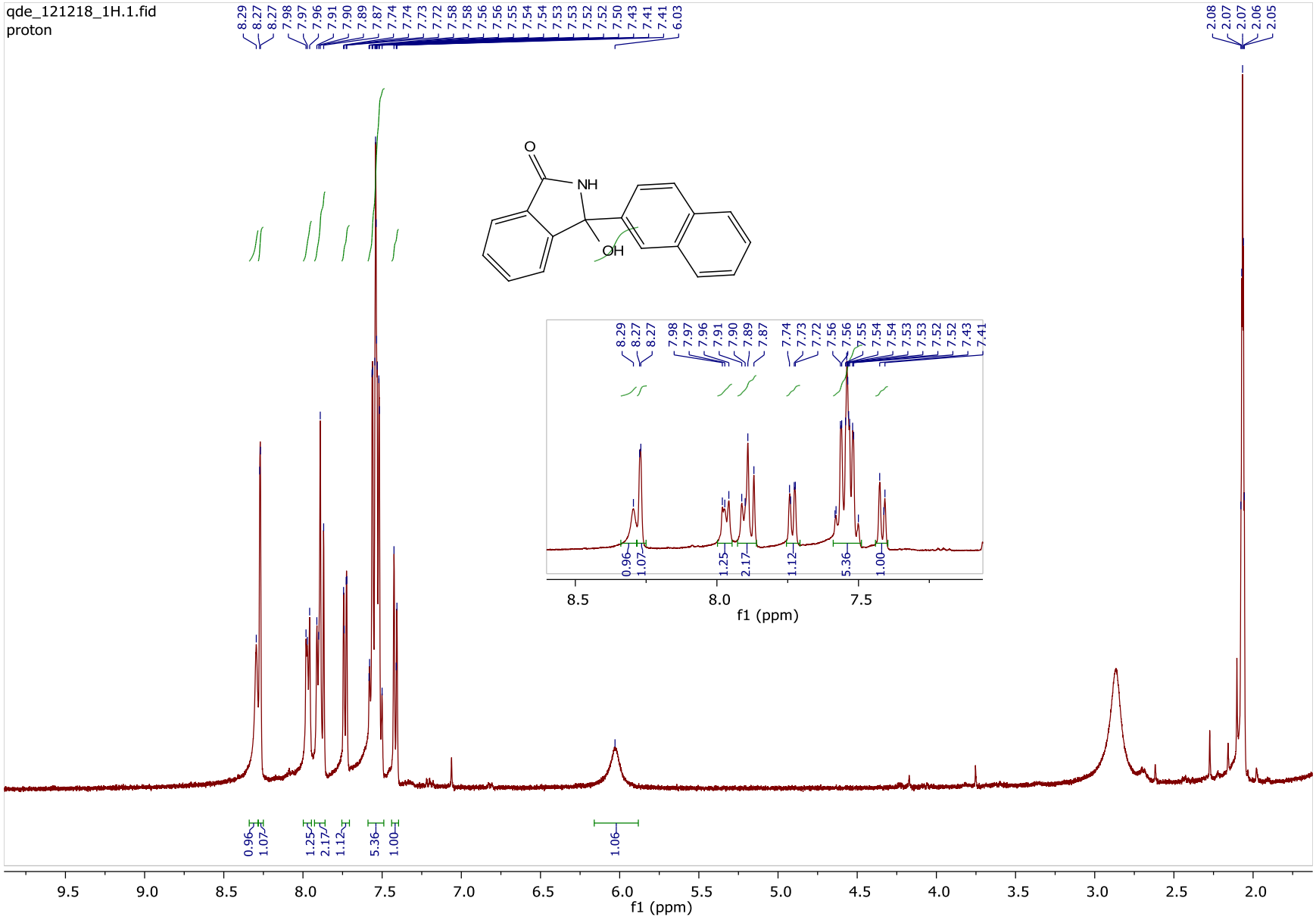
124.79
123.66
122.80
86.87
O
NH
OH
S
f1 (ppm)
f1 (ppm)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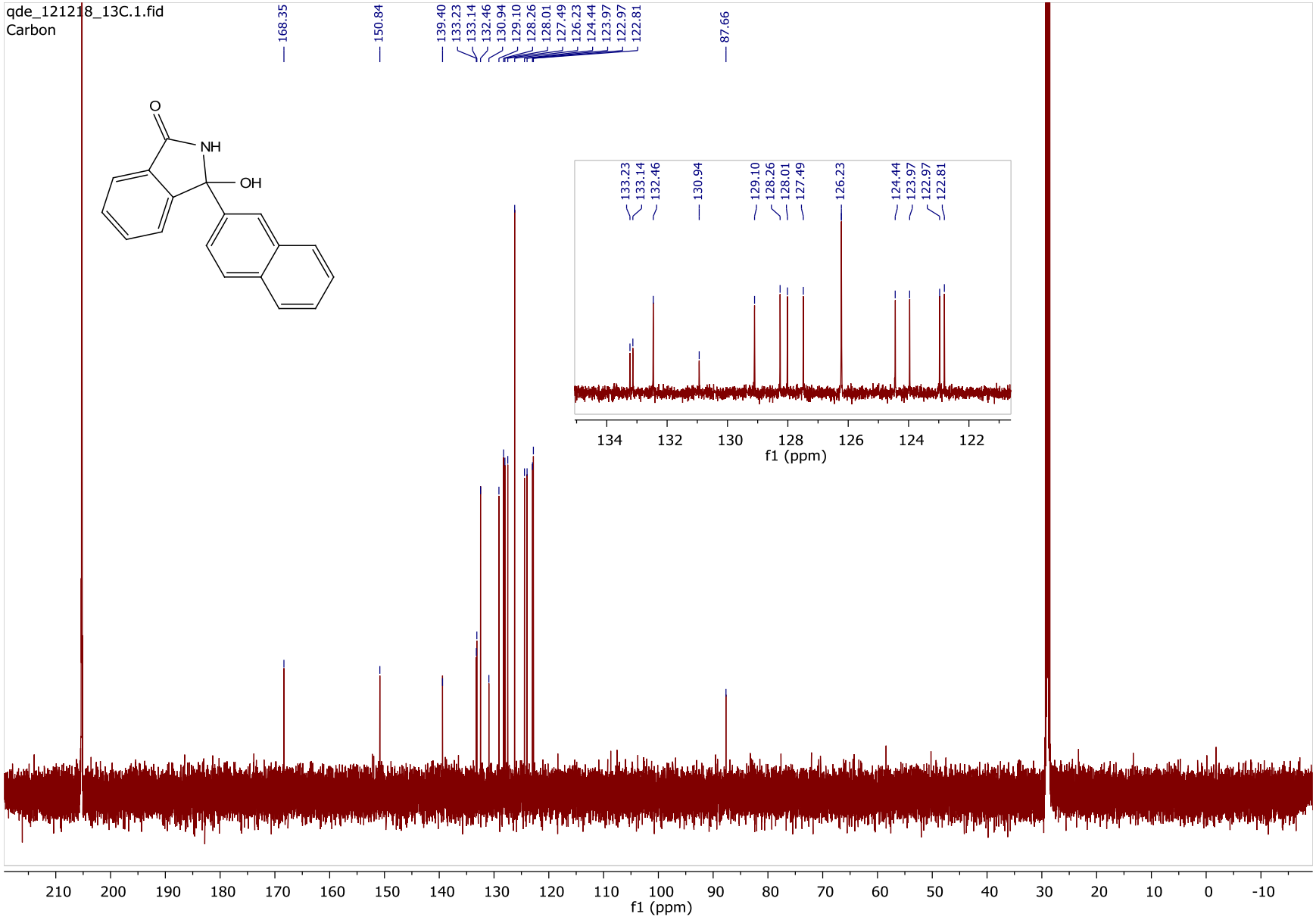
proton
O
NH
OH
f1 (ppm)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Carbon
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128.01
127.49
126.23
124.44
123.97
122.97
122.81
87.66
O
NH
OH
133.23
133.14
132.46
130.94
129.10
128.26
128.01
127.49
126.23
124.44
123.97
122.97
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200
190
180
170
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40
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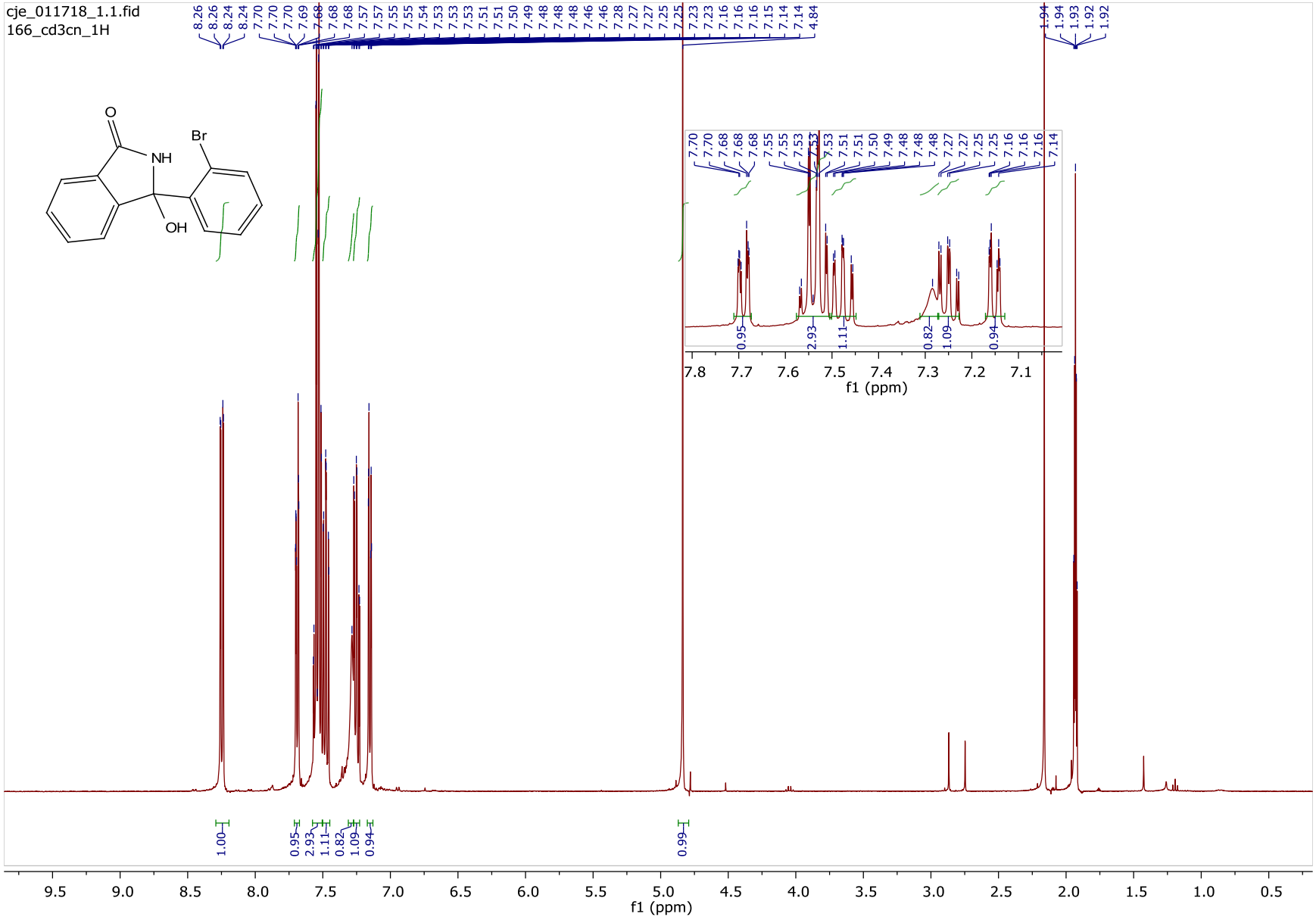
f1 (ppm)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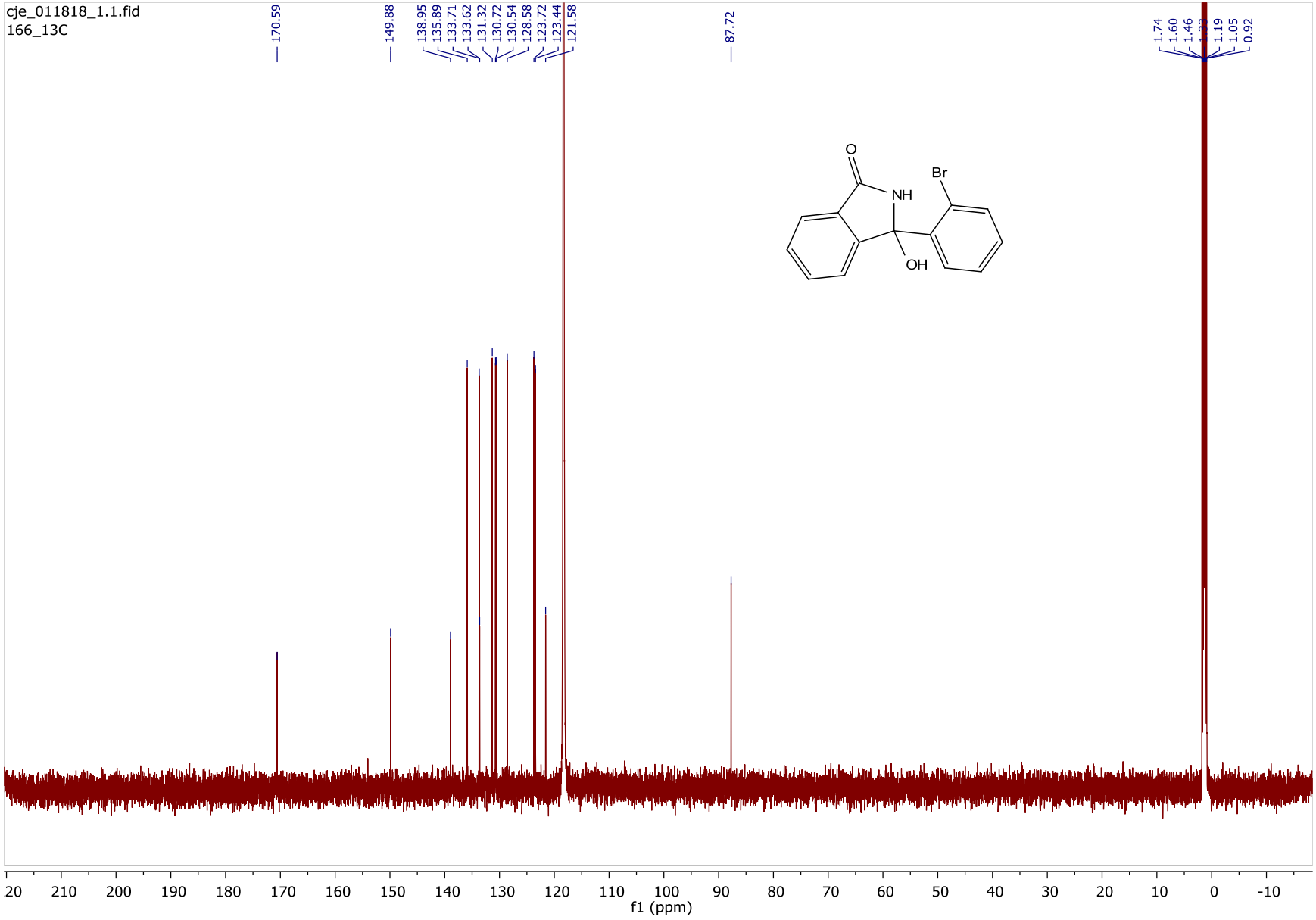
O
NH
Br
OH
f1 (ppm)
f1 (ppm)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133.62
131.32
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130.54
128.58
123.72
123.44
121.58
87.72
1.74
1.60
1.46
1.33
1.19
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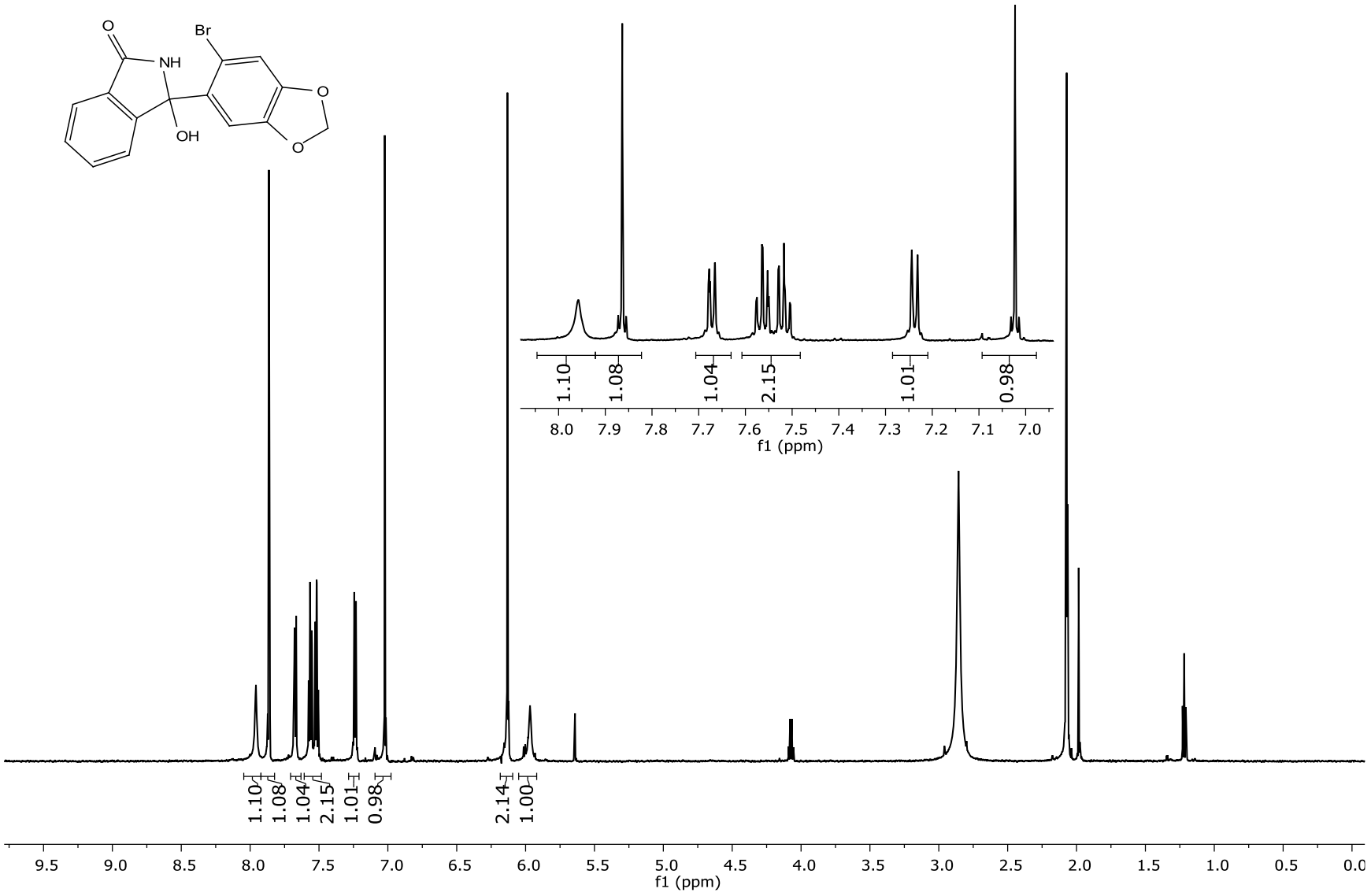
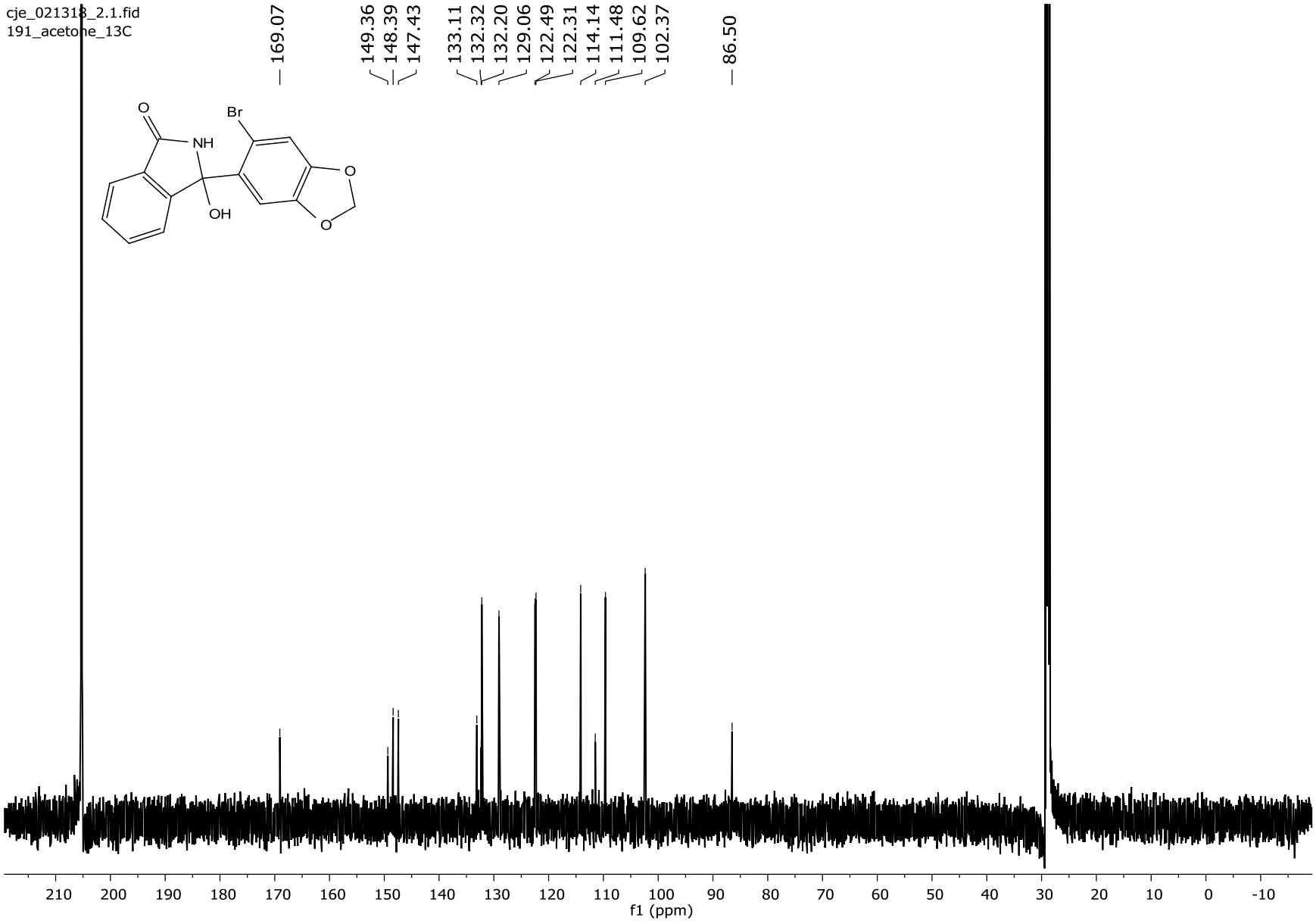
0.92
O
NH
Br
OH
f1 (ppm)

cje_021318_1.1.fid
191_acetone_1H

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147.43
133.11
132.32
132.20
129.06
122.49
122.31
114.14
111.48
109.62
102.37
86.50
O
NH
Br
OH
O
O
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200
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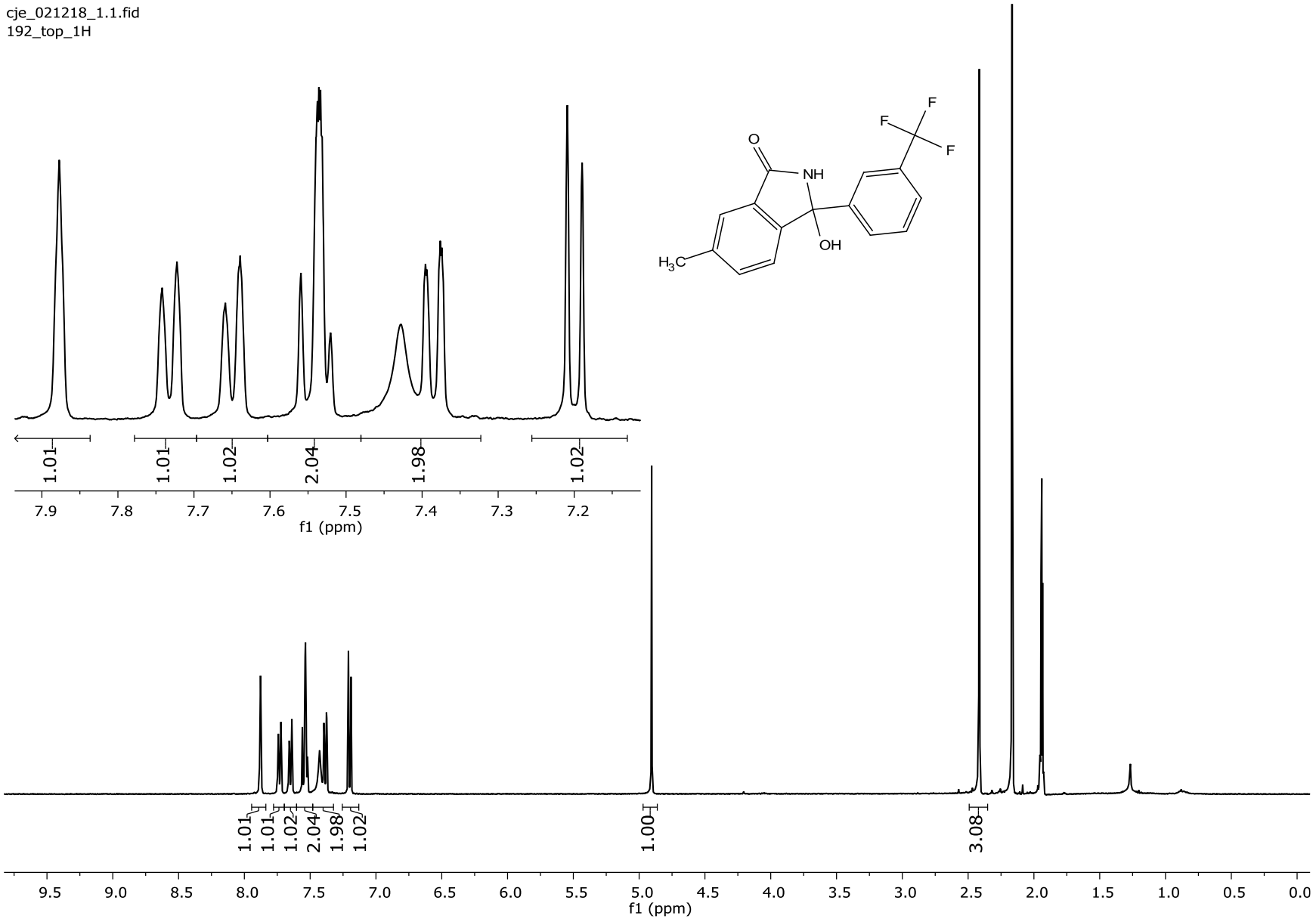
f1 (ppm)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F
F
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NH
OH
H3C
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1.02
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7.8
7.7
7.6
7.5
7.4
7.3
7.2
f1 (ppm)
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1.01
1.02
2.04
1.98
1.02
1.00
3.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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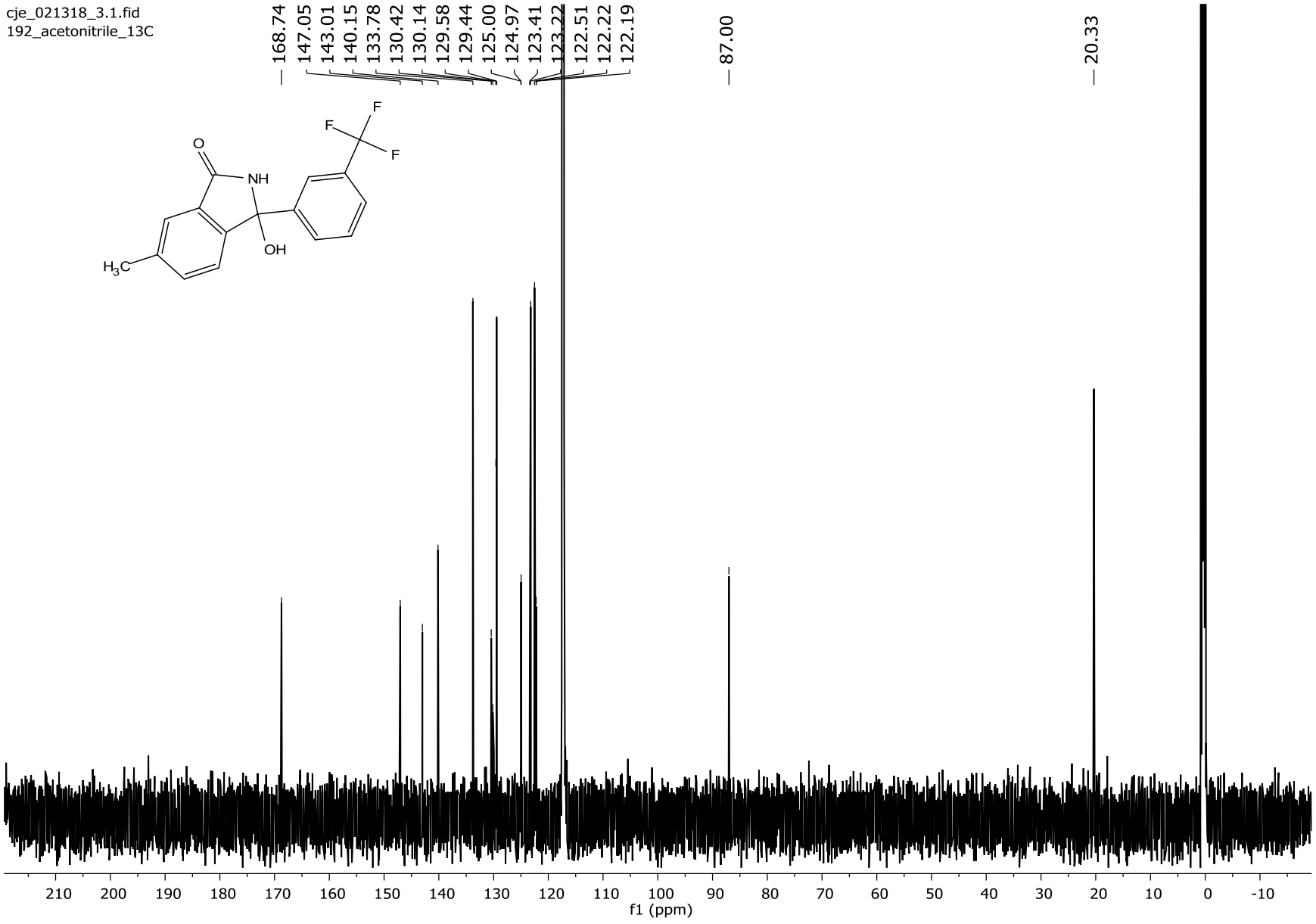
0.0
f1 (ppm)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87.00
20.33
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NH
OH
F
F
F
H3C
210
200
190
180
170
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120
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30
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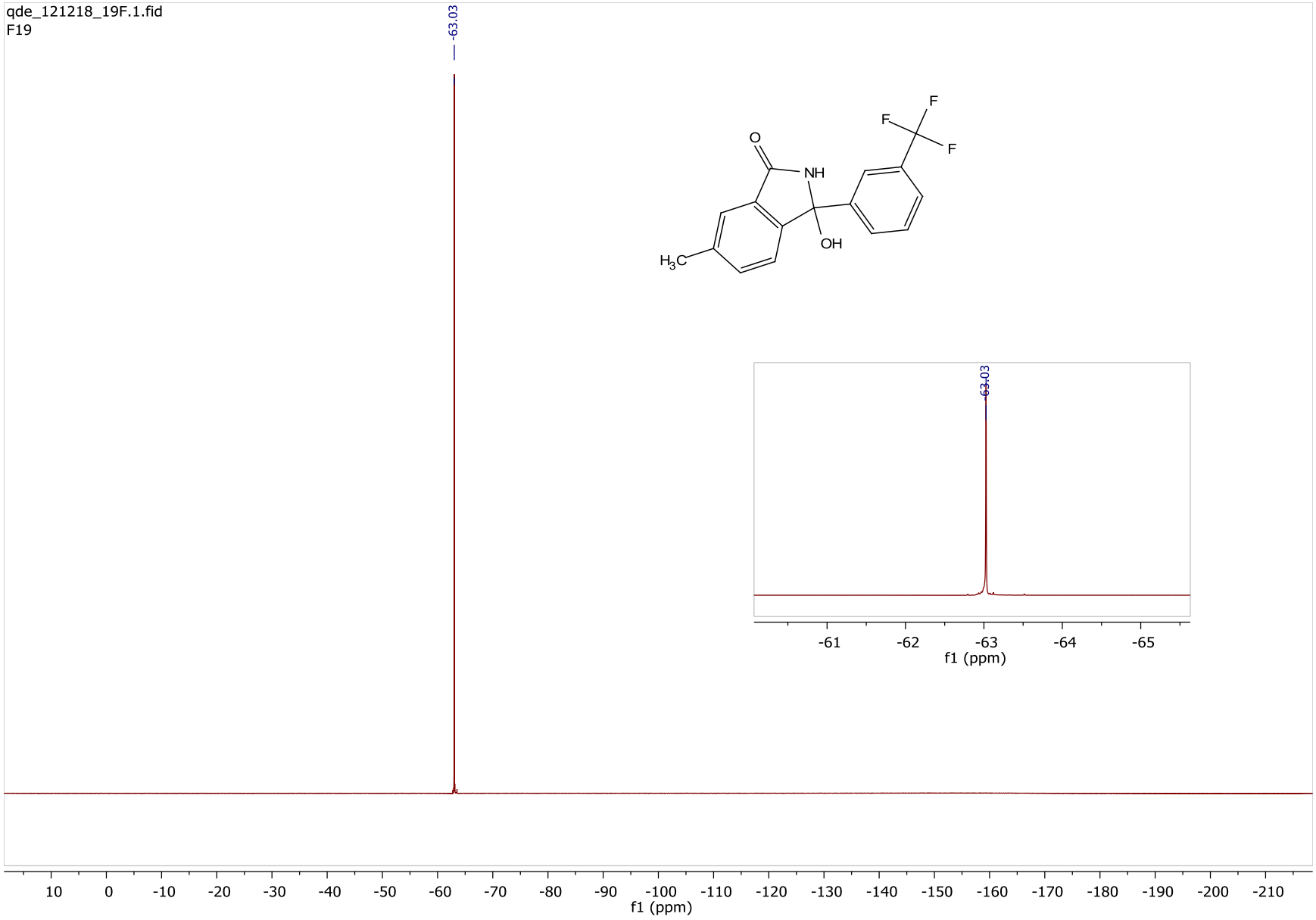
f1 (ppm)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-63.03
F
F
F
O
NH
OH
H3C
-63.03
-61
-62
-63
-64
-65
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
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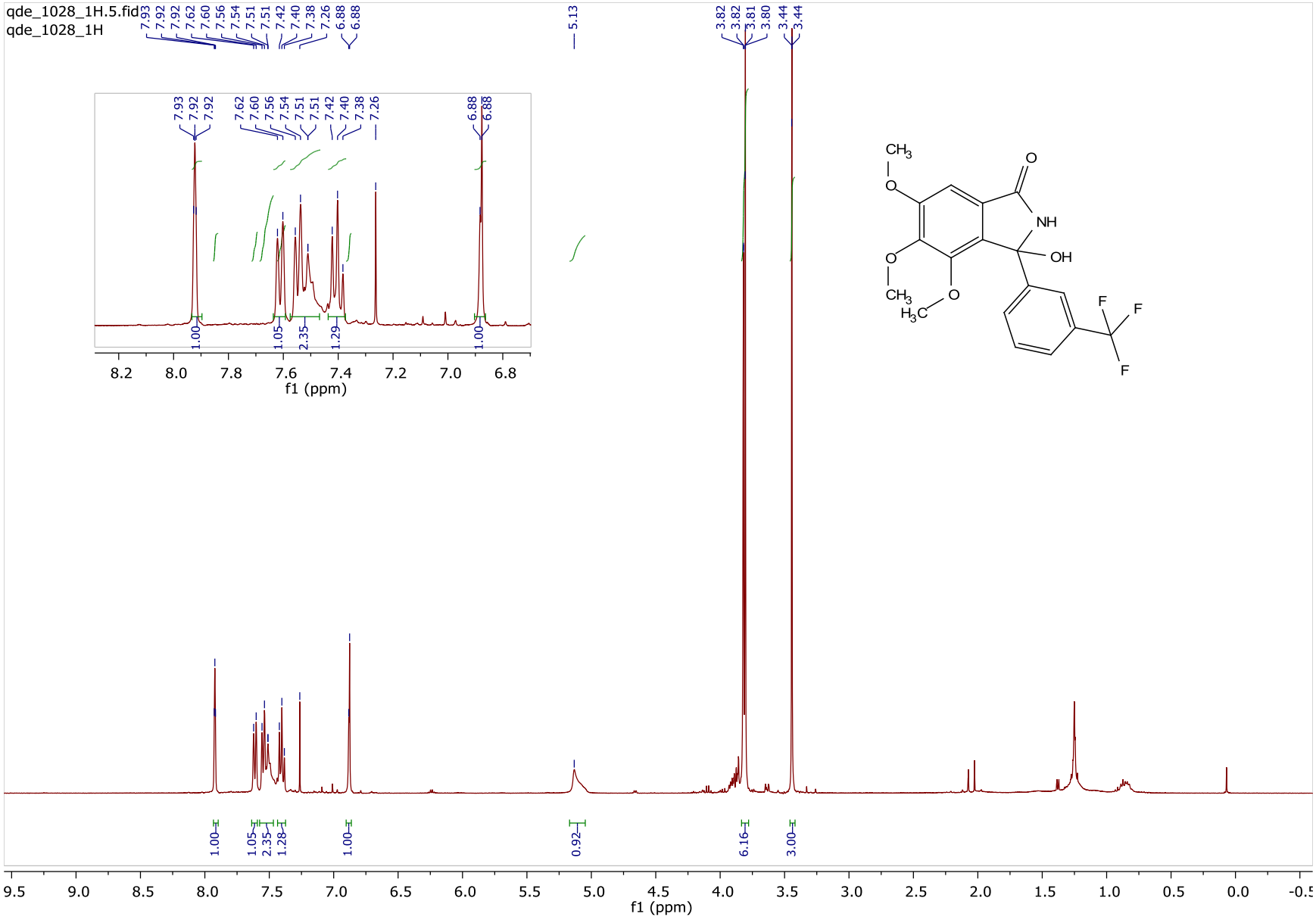
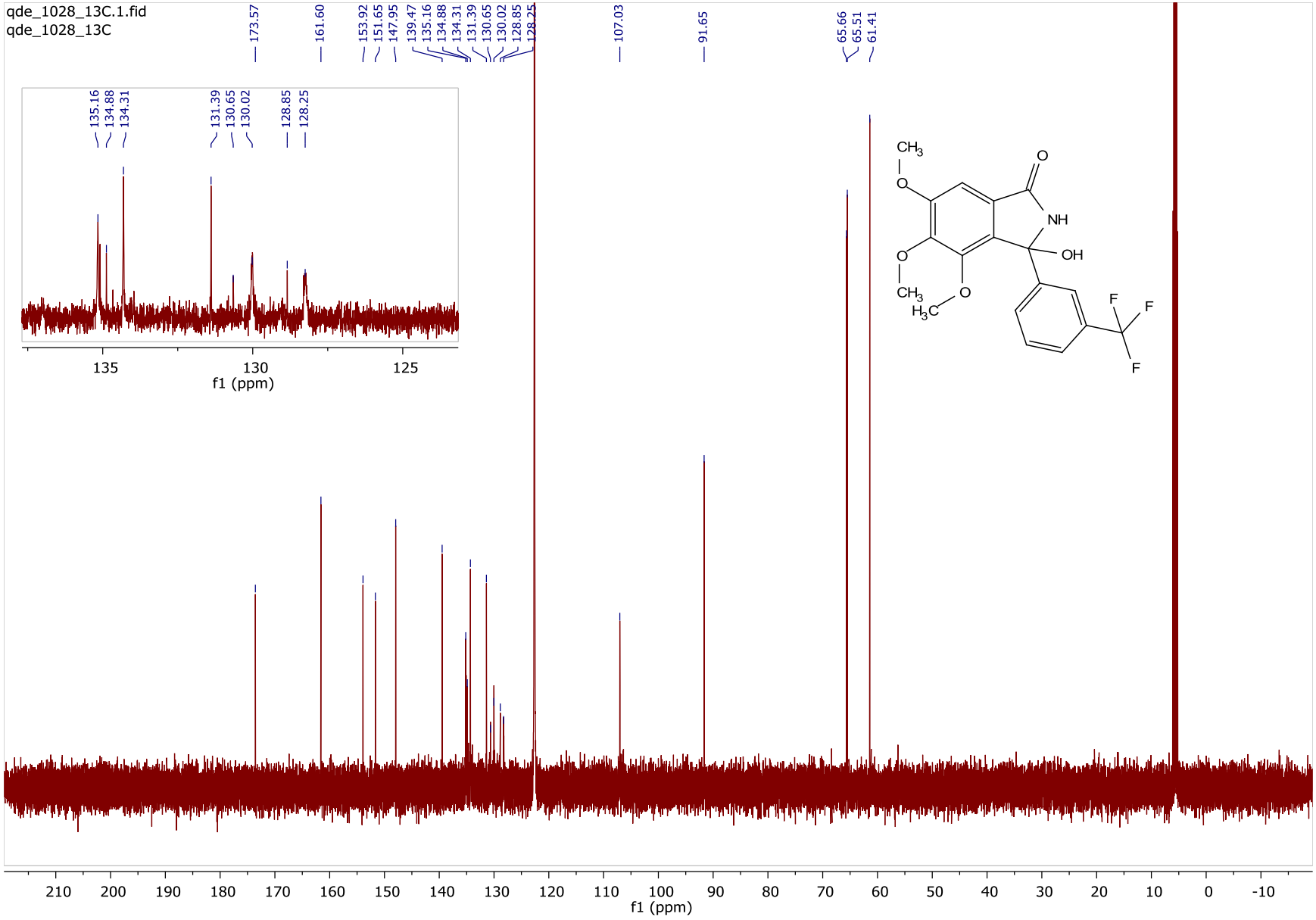
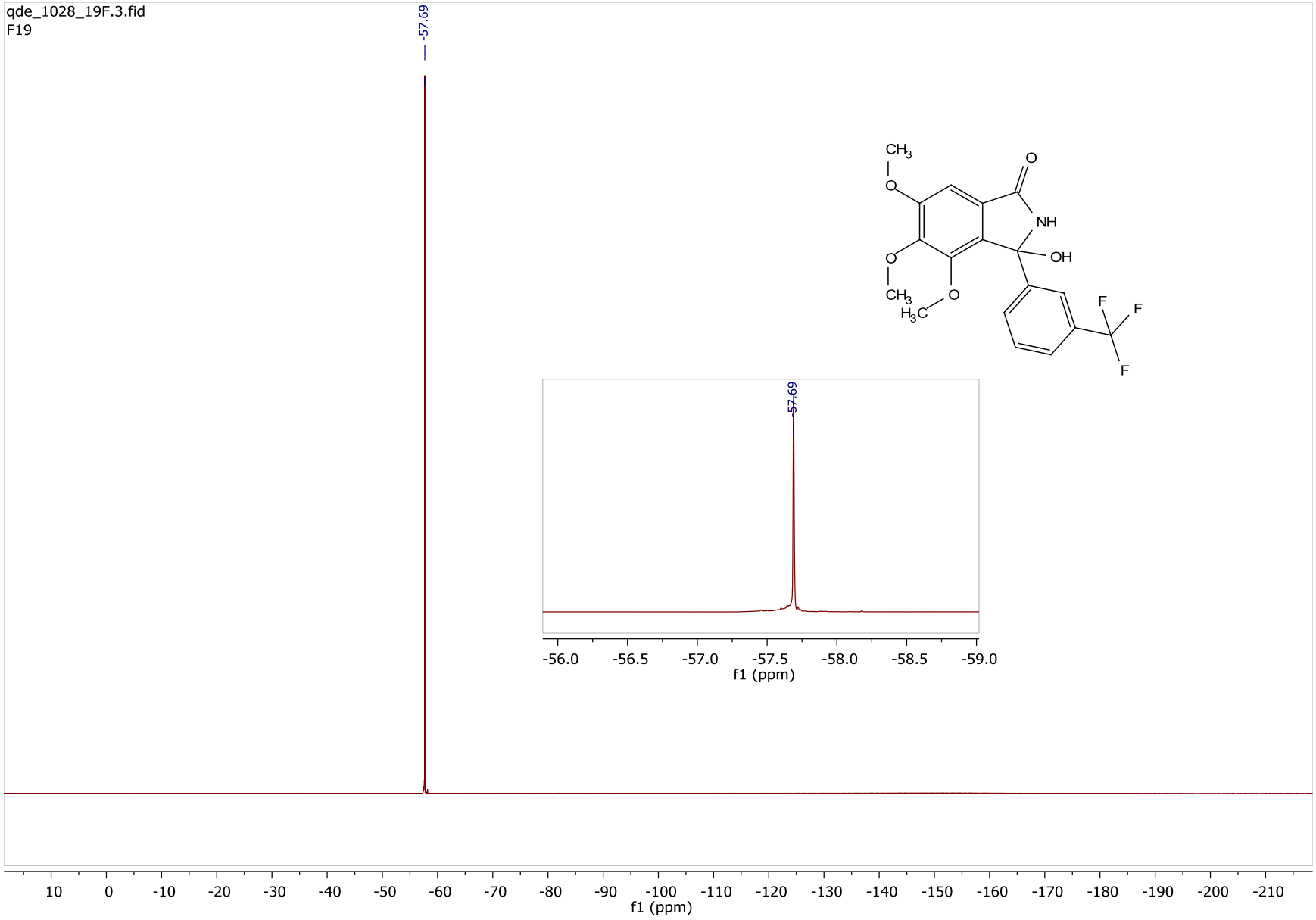
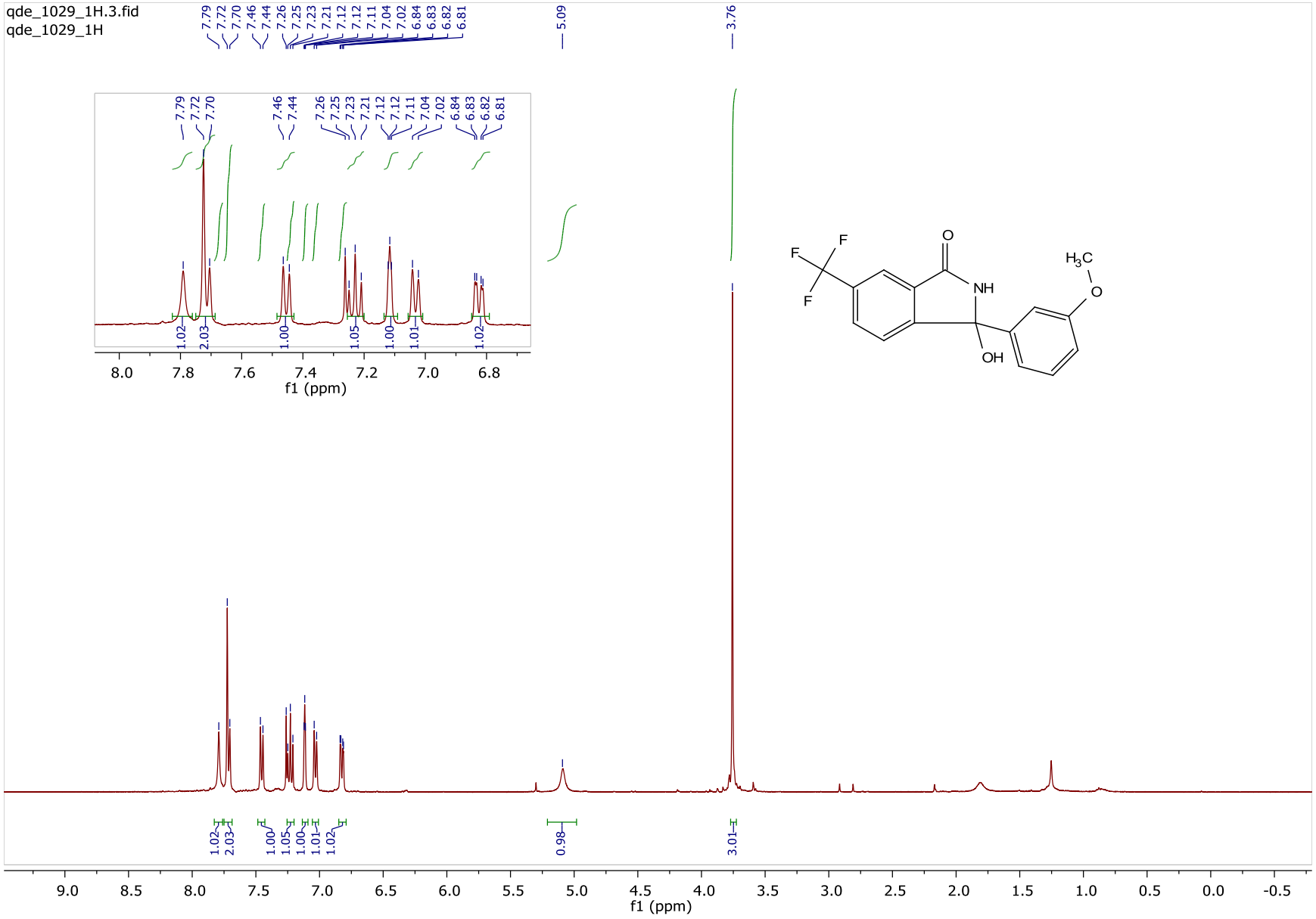
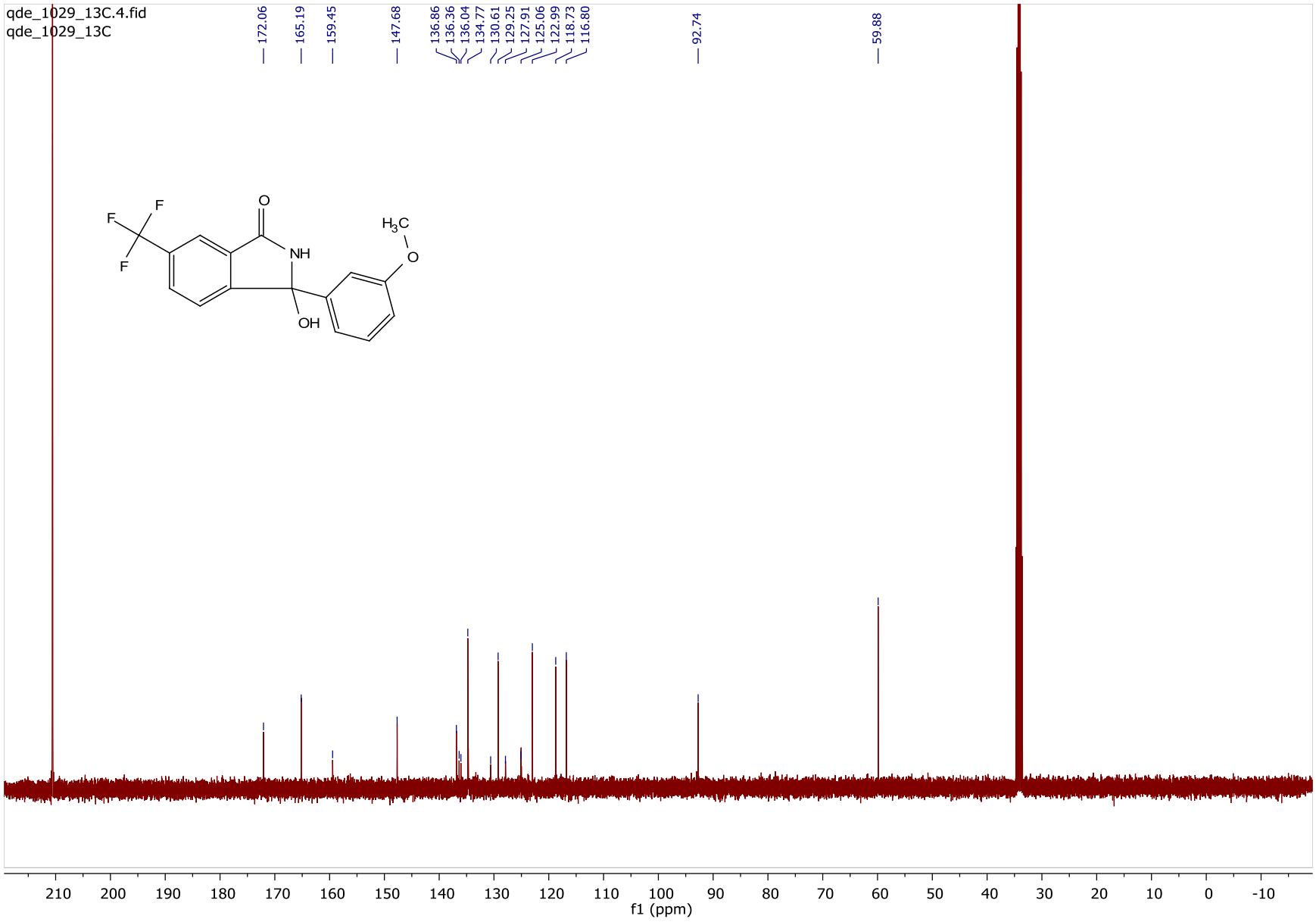
-190
-200
-210
f1 (ppm)

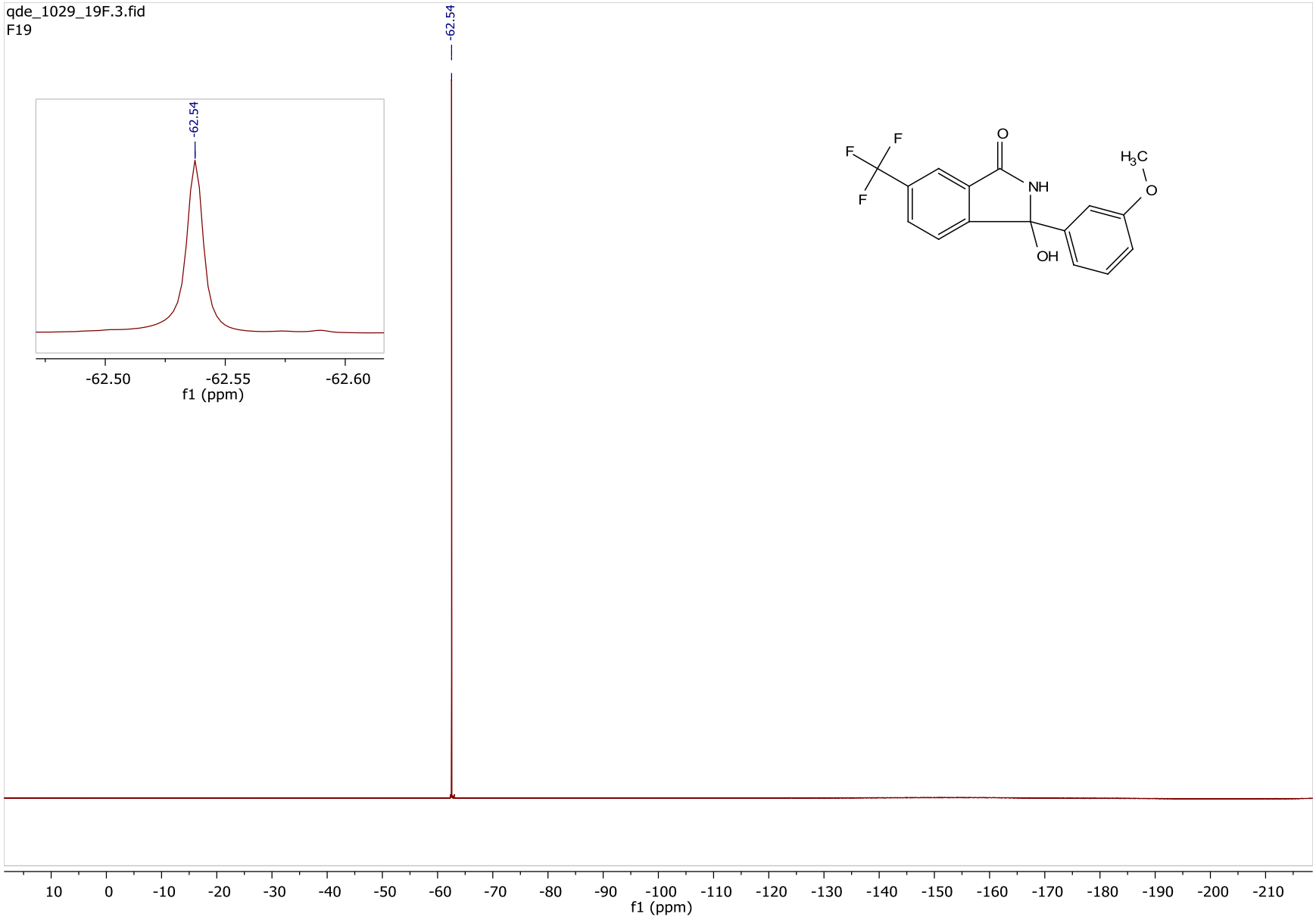

qde_1028_1H.5.fid
qde_1028_1H
7.93 7.92 7.92 7.62 7.60 7.56 7.54 7.51 7.51 7.42 7.40 7.38 7.26 6.88 6.88
5.13
3.82 3.82 3.81 3.80 3.44 3.44
1.00 1.05 2.35 1.29 1.00
8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8
f1 (ppm)
CH3
O
O
NH
OH
O
CH3
H3C
O
F
F
F
1.00 1.05 2.35 1.28 1.00 0.92 6.16 3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


qde_1028_13C.1.fid
qde_1028_13C
173.57
161.60
153.92
151.65
147.95
139.47
135.16
134.88
134.31
131.39
130.65
130.02
128.85
128.25
107.03
91.65
65.66
65.51
61.41
f1 (ppm)
CH3
O
NH
OH
F
H3C

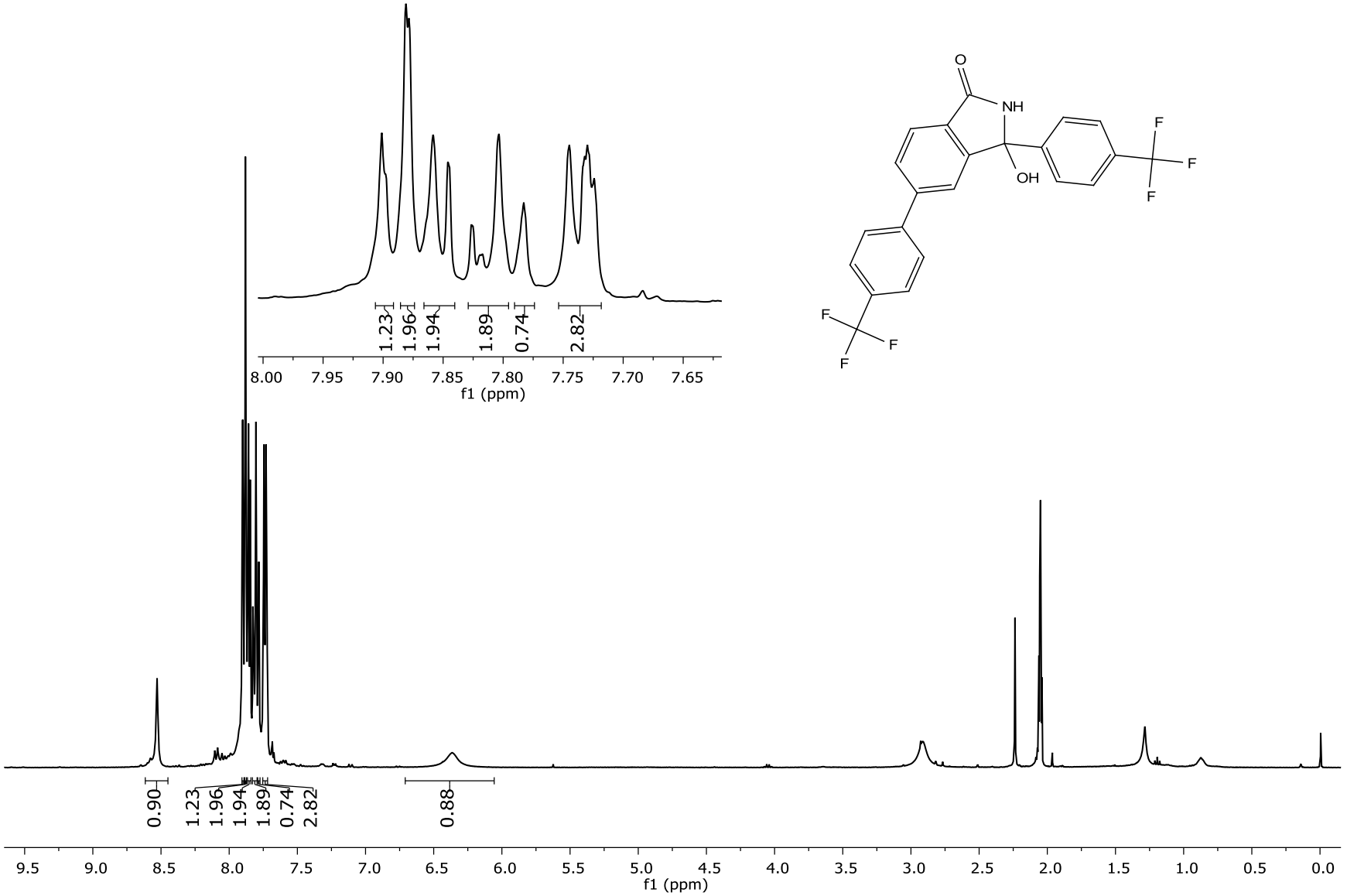

qde_1028_19F.3.fid
F19
-57.69
CH3
O
O
NH
OH
O
CH3
H3C
O
F
F
F
-57.69
-56.0
-56.5
-57.0
-57.5
-58.0
-58.5
-59.0
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

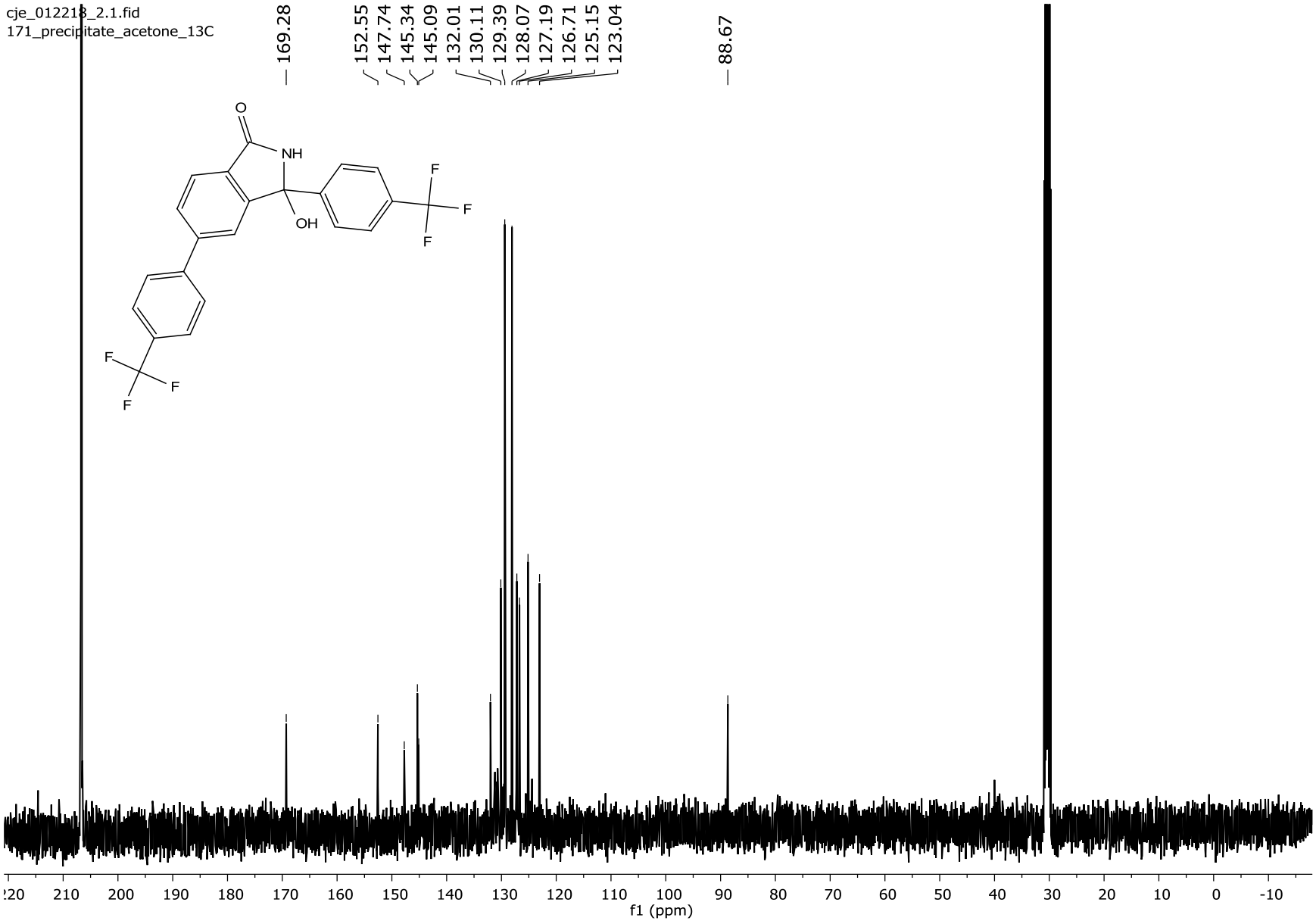

qde_1029_1H.3.fid
qde_1029_1H
7.79
7.72
7.70
7.46
7.44
7.26
7.25
7.23
7.21
7.12
7.12
7.11
7.04
7.02
6.84
6.83
6.82
6.81
5.09
3.76
1.02
2.03
1.00
1.05
1.00
1.01
1.02
0.98
3.01
f1 (ppm)
F
F
F
O
NH
OH
H3C
O

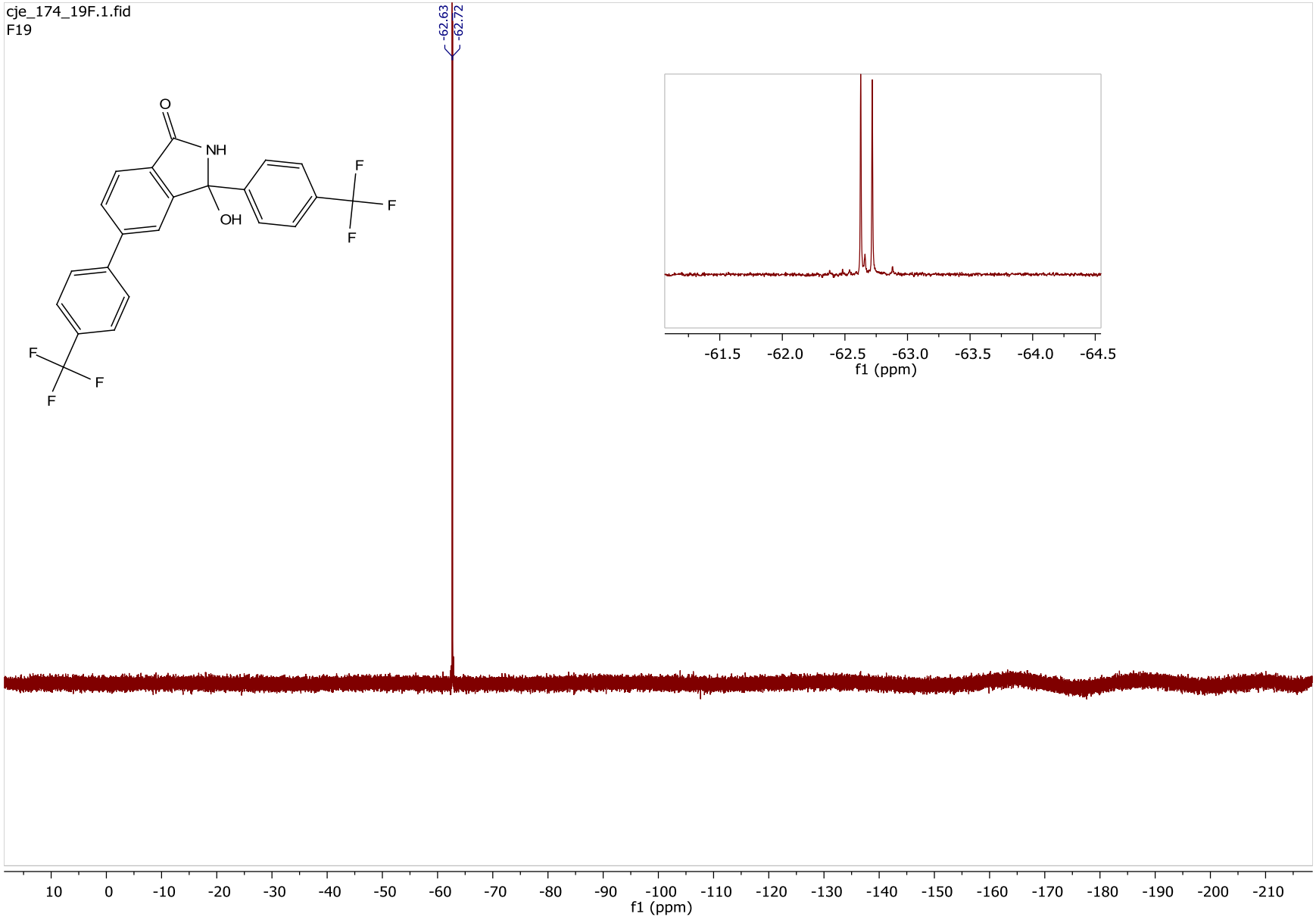

qde_1029_13C.4.fid
qde_1029_13C
172.06
165.19
159.45
147.68
136.86
136.36
136.04
134.77
130.61
129.25
127.91
125.06
122.99
118.73
116.80
92.74
59.88
F
F
F
O
NH
OH
H3C
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

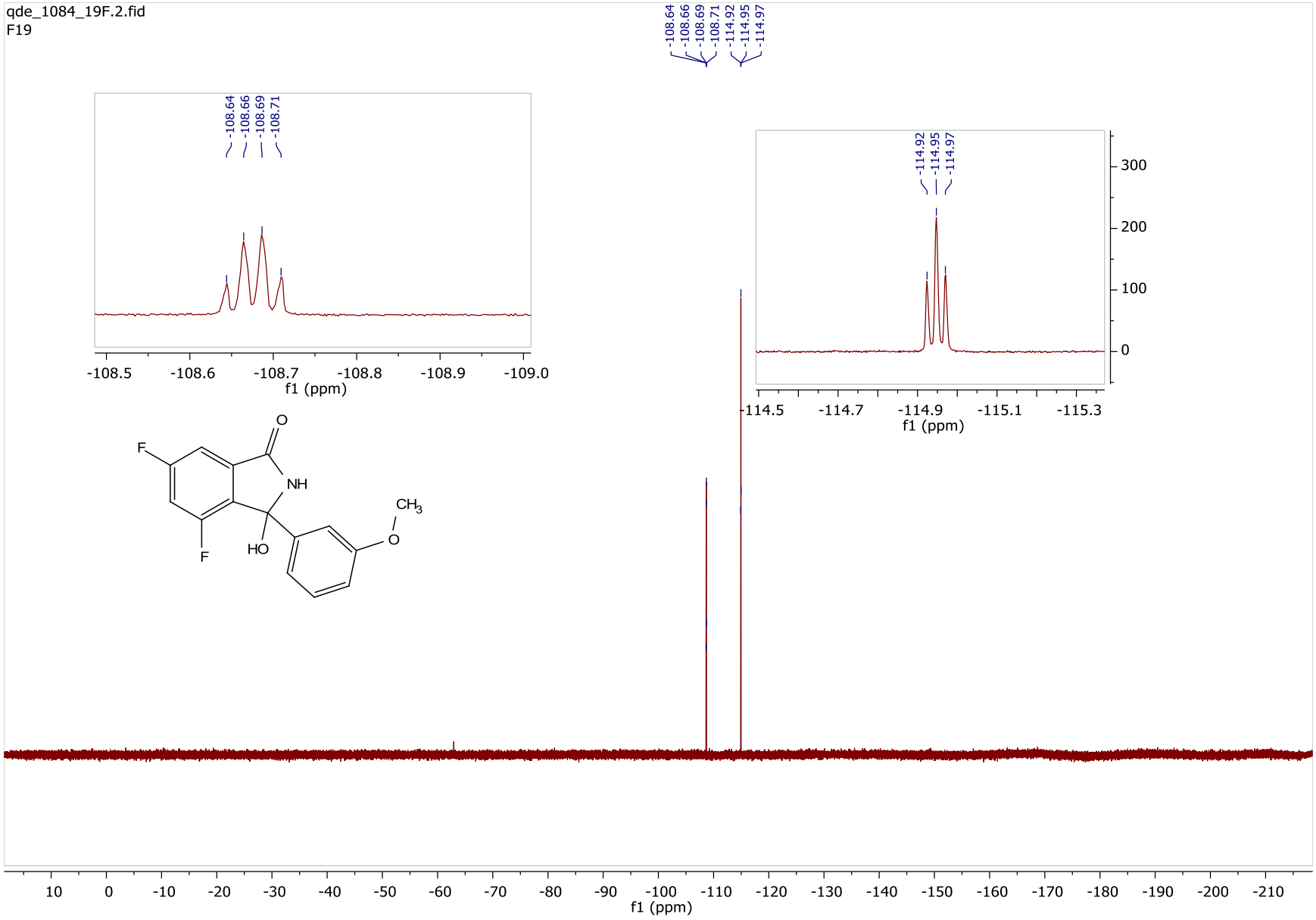

qde_1029_19F.3.fid
F19
-62.54
-62.54
-62.50
-62.55
-62.60
f1 (ppm)
F
F
F
O
NH
OH
H3C
O
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

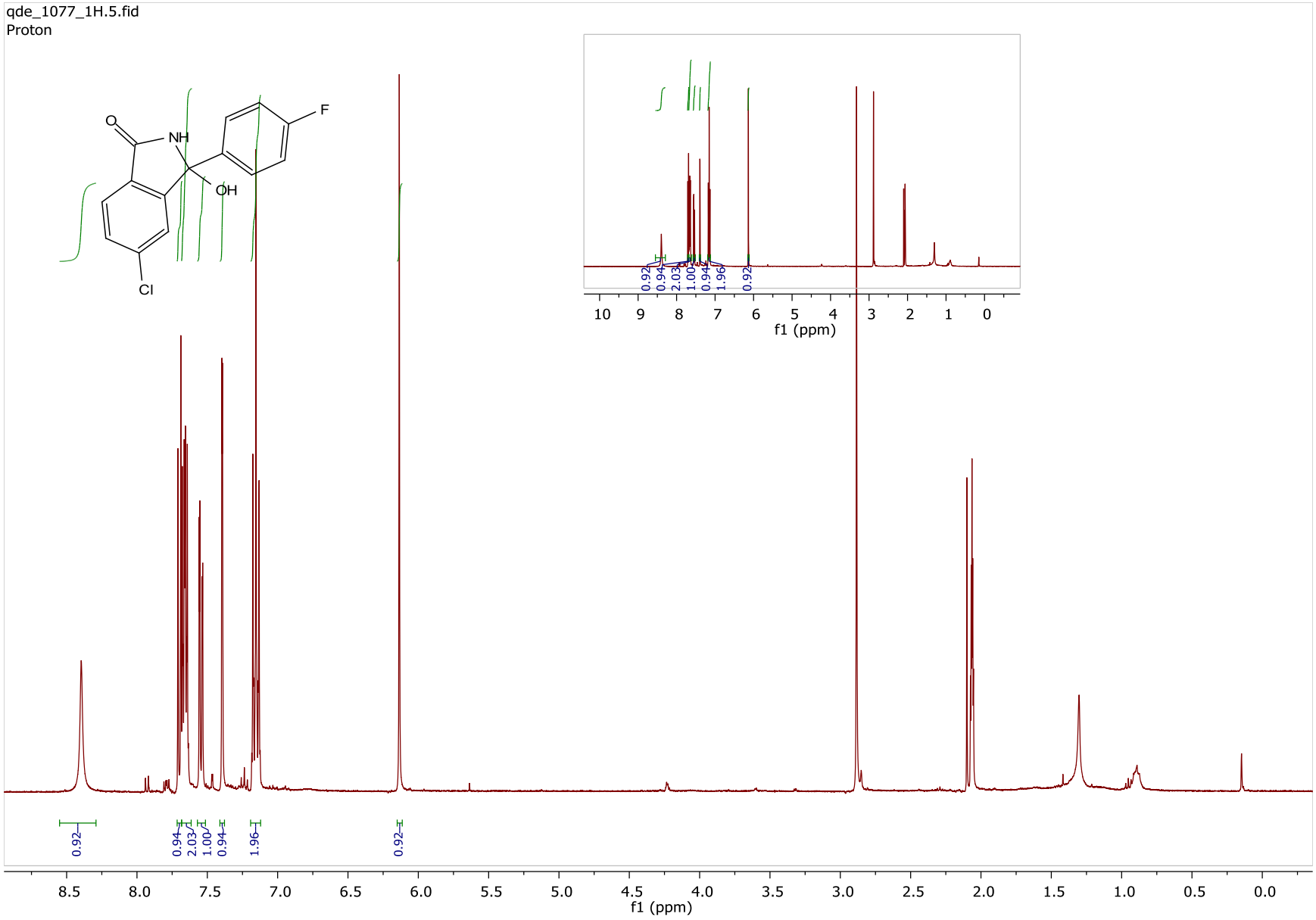
cje_012218_1.1.fid
171_precipitate_acetone_1H

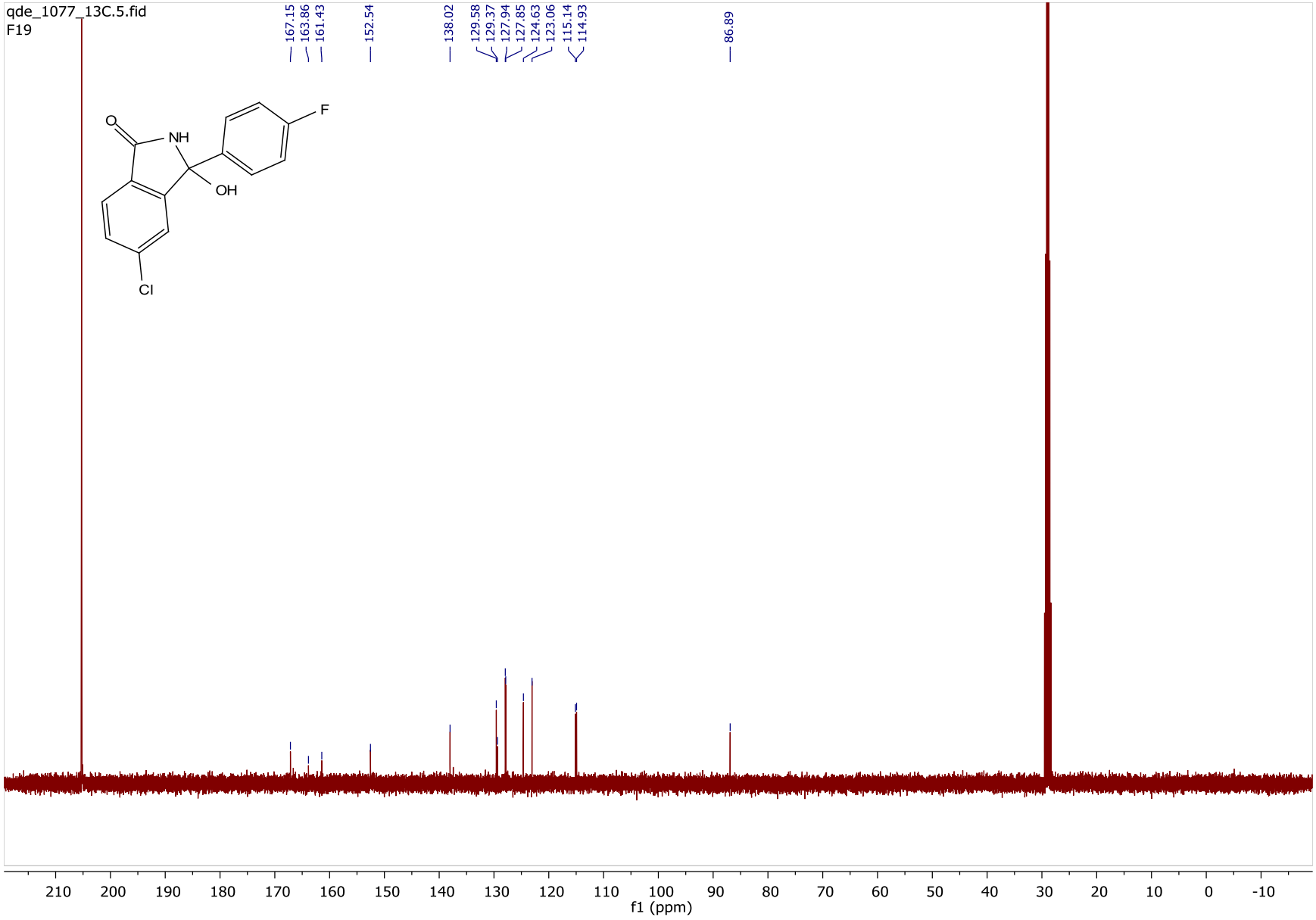


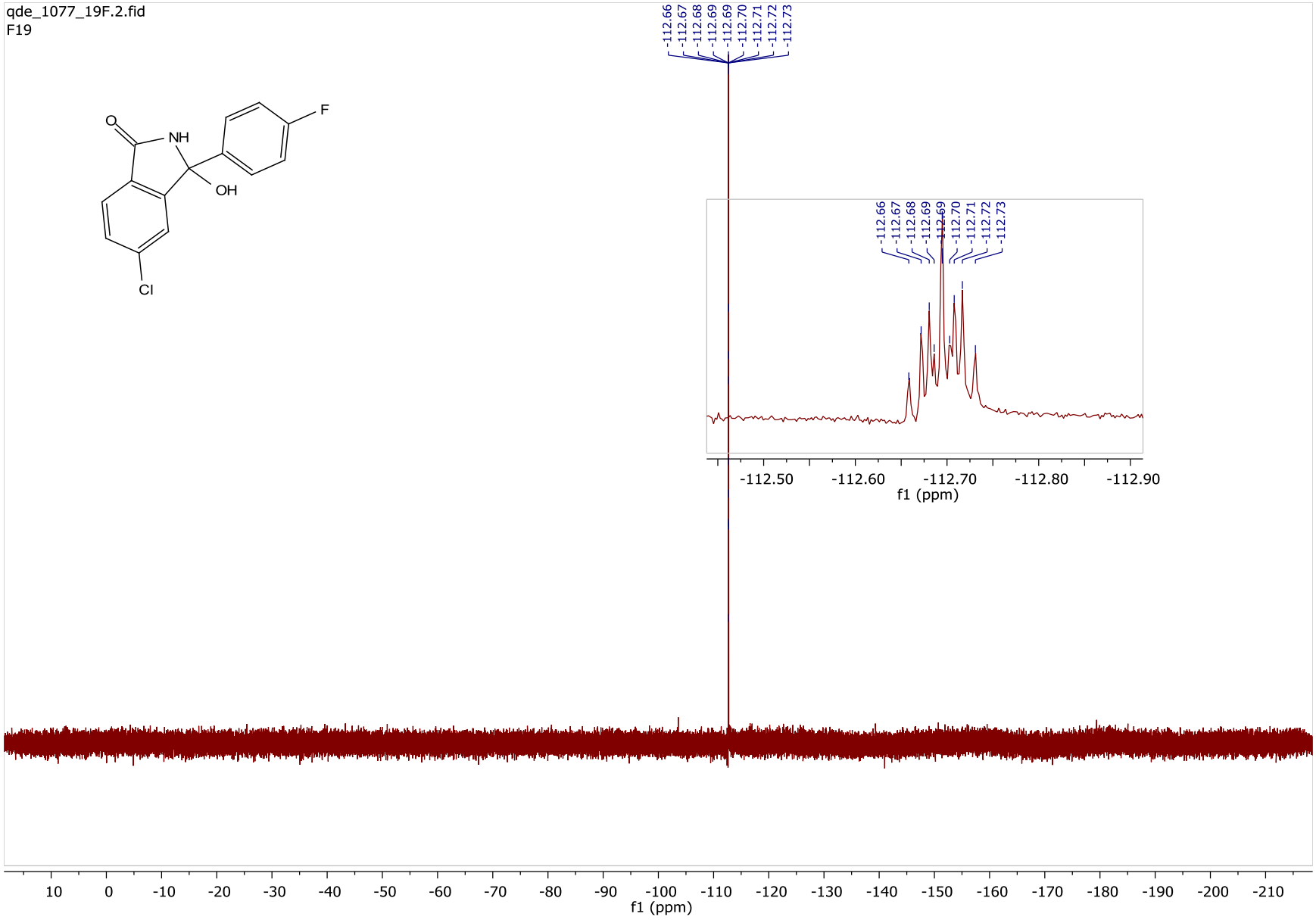

cje_012218_2.1.fid
171_precipitate_acetone_13C
169.28
152.55
147.74
145.34
145.09
132.01
130.11
129.39
128.07
127.19
126.71
125.15
123.04
88.67
O
NH
OH
F
F
F
F
F
F
f1 (ppm)

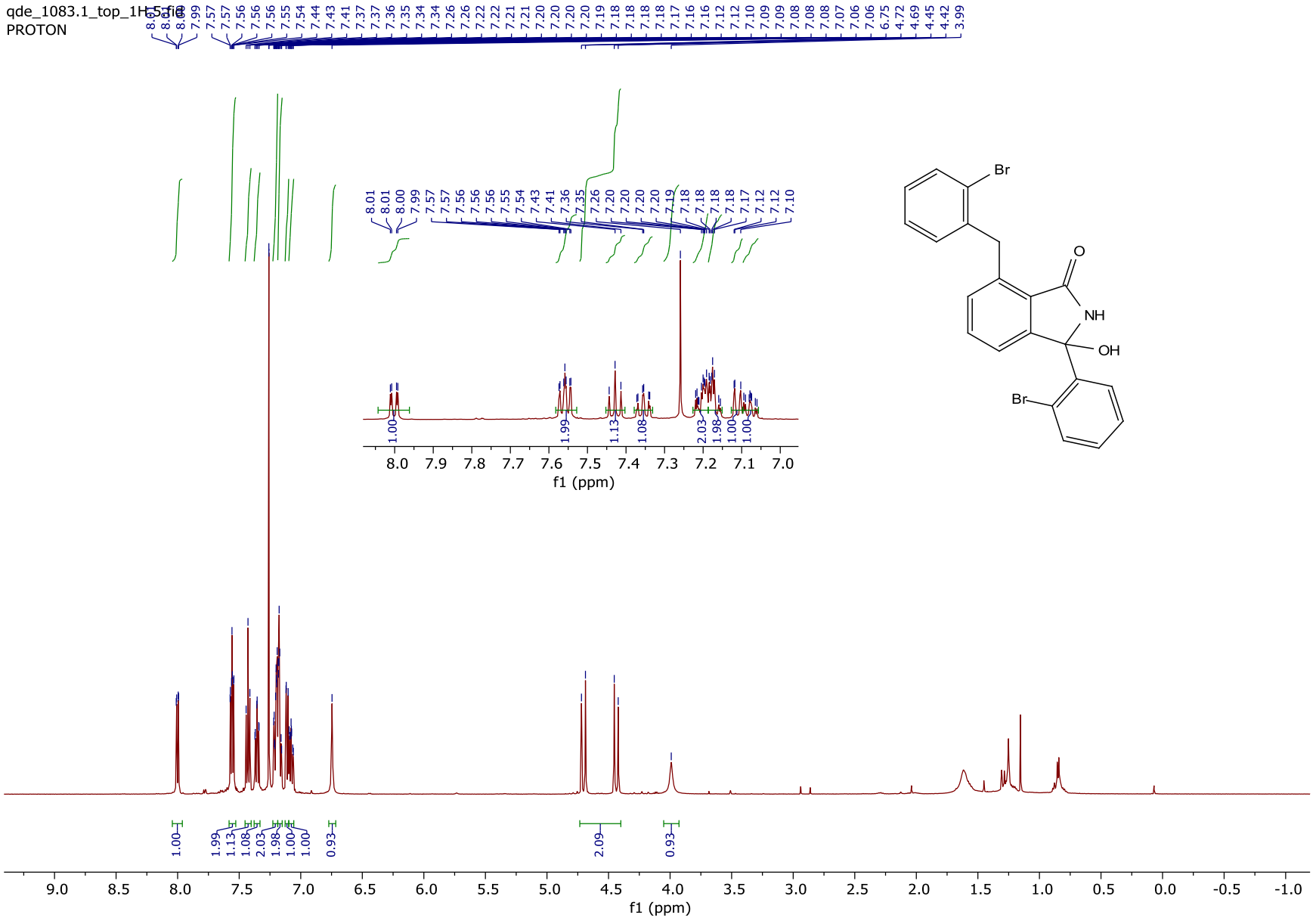

cje_174_19F.1.fid
F19
-62.63
-62.72
O
NH
OH
F
F
F
F
F
F
-61.5
-62.0
-62.5
-63.0
-63.5
-64.0
-64.5
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

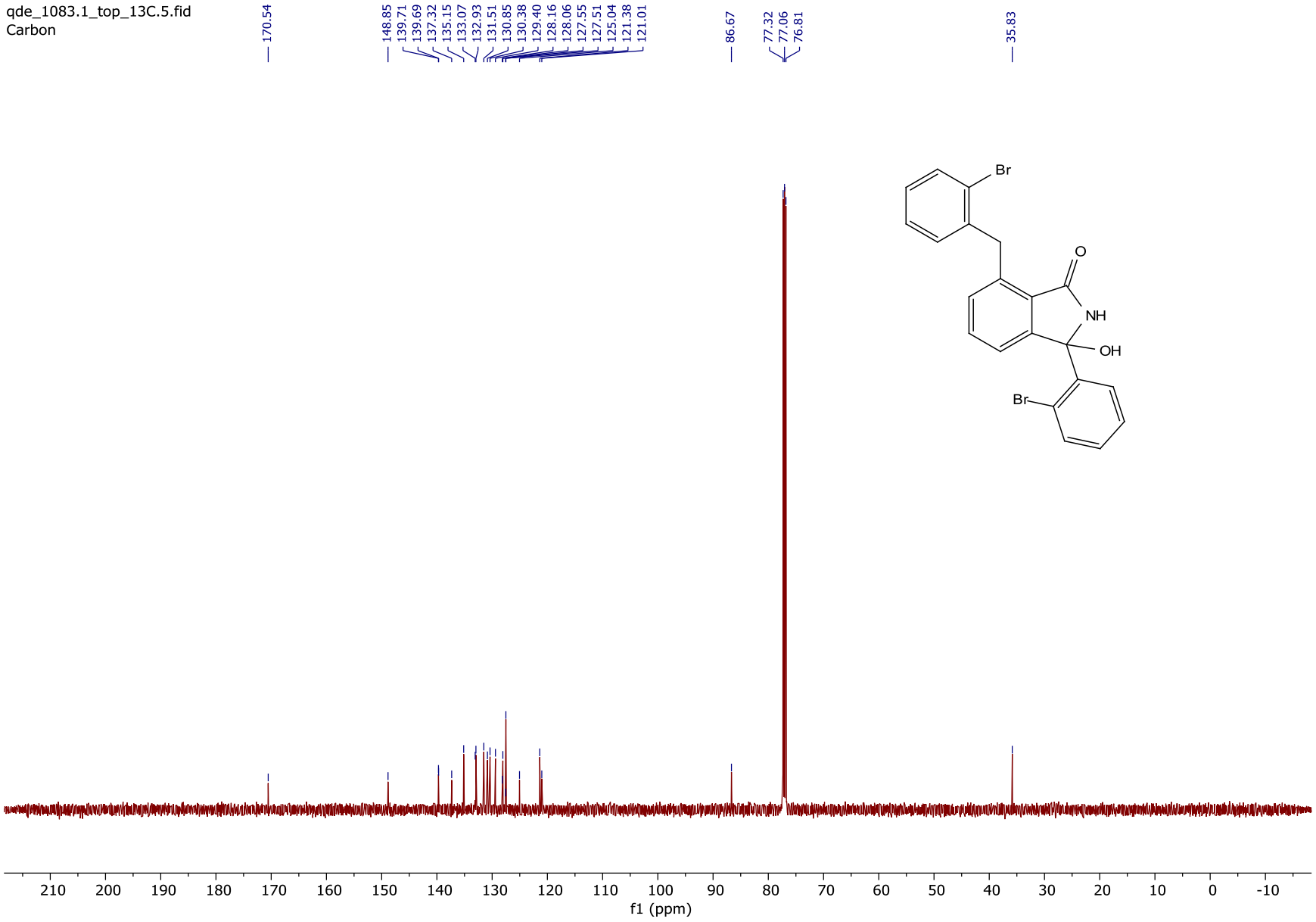

qde_1084_19F.2.fid
F19
-108.64
-108.66
-108.69
-108.71
-114.92
-114.95
-114.97
-108.5
-108.6
-108.7
-108.8
-108.9
-109.0
f1 (ppm)
-114.5
-114.7
-114.9
-115.1
-115.3
f1 (ppm)
300
200
100
0
O
NH
CH3
O
HO
F
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

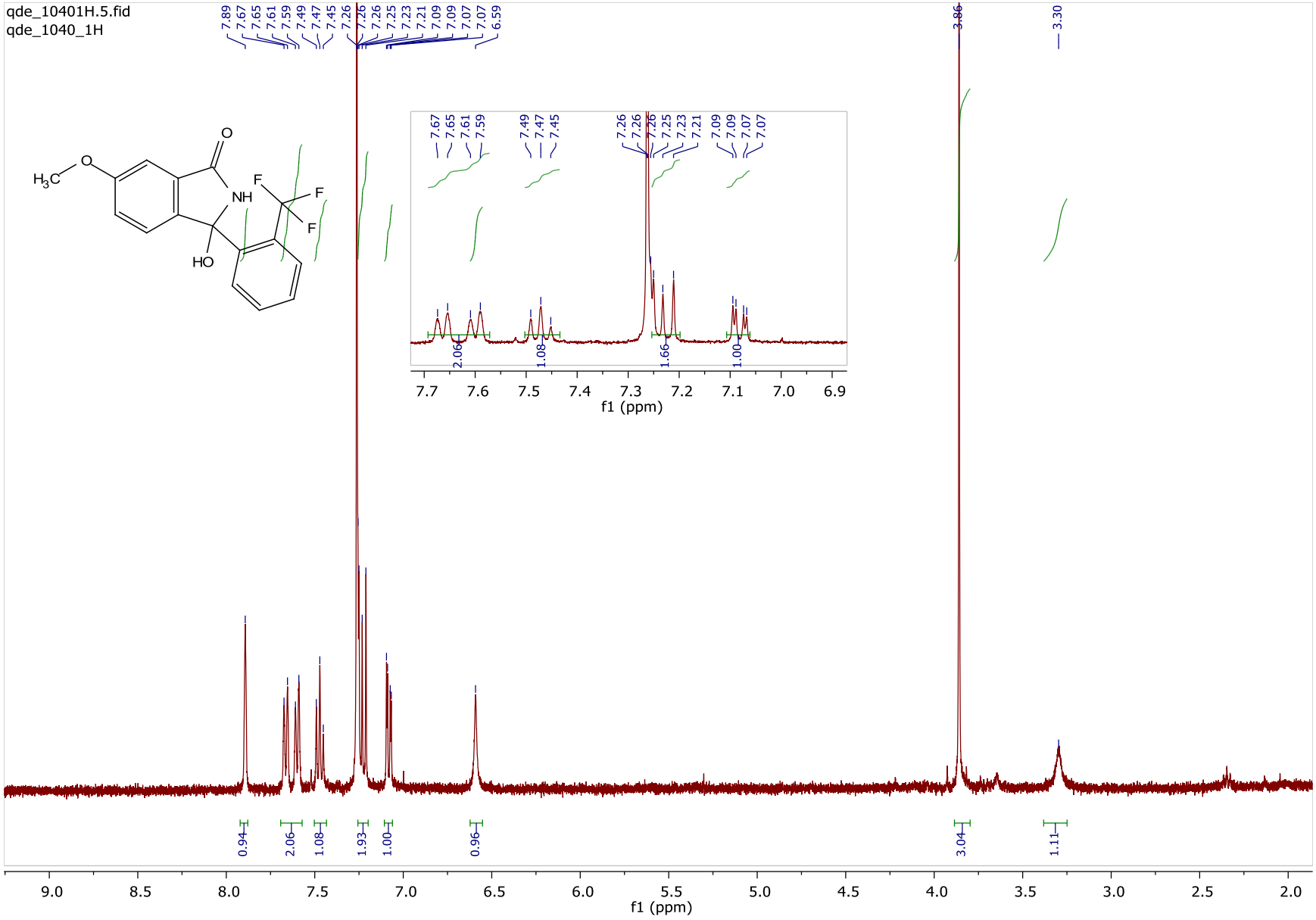

qde_1077_1H.5.fid
Proton
O
NH
OH
F
Cl
0.92
0.94
2.03
1.00
0.94
1.96
0.92
f1 (ppm)
f1 (ppm)

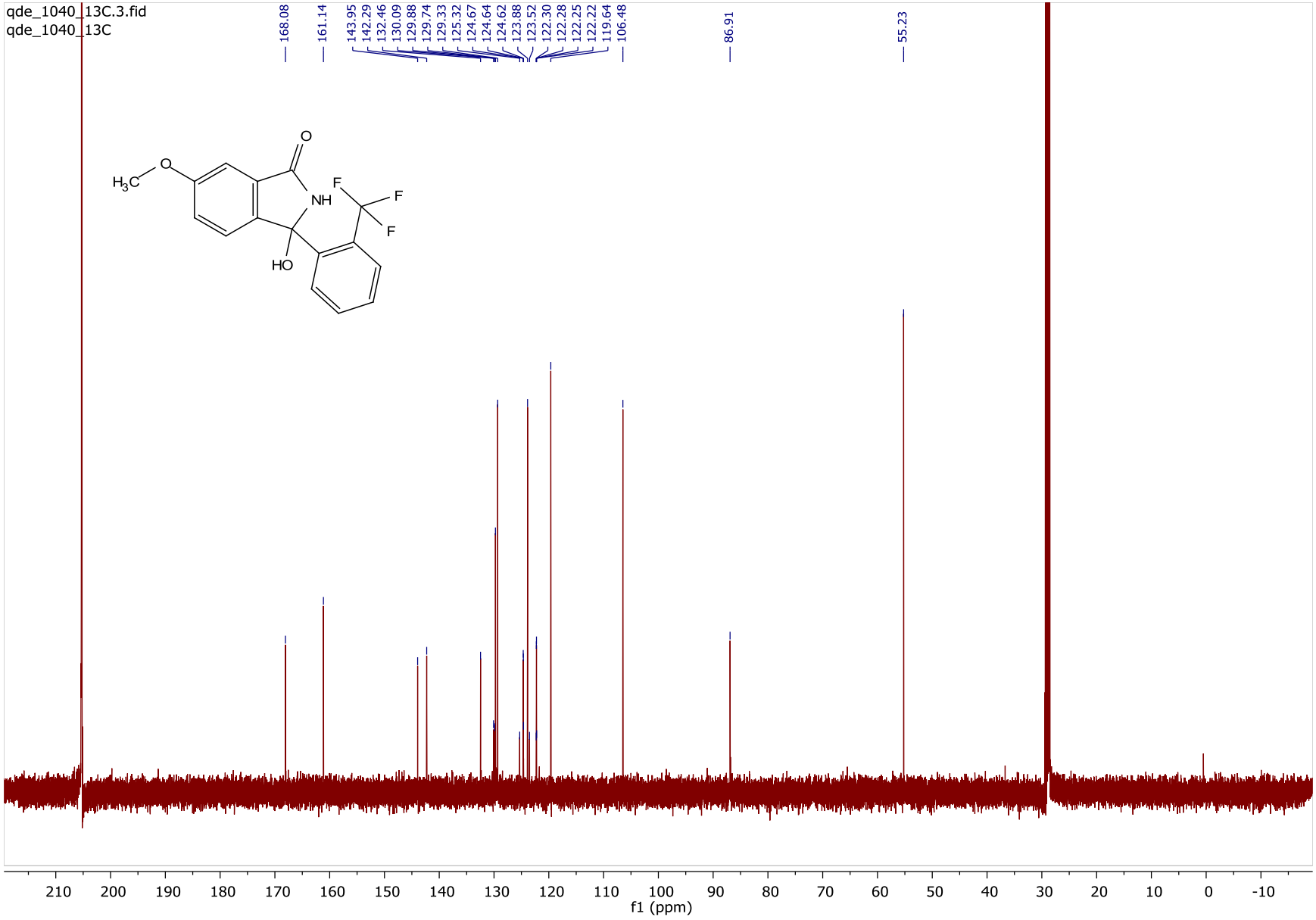

qde_1077_13C.5.fid
F19
167.15
163.86
161.43
152.54
138.02
129.58
129.37
127.94
127.85
124.63
123.06
115.14
114.93
86.89
O
NH
OH
F
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

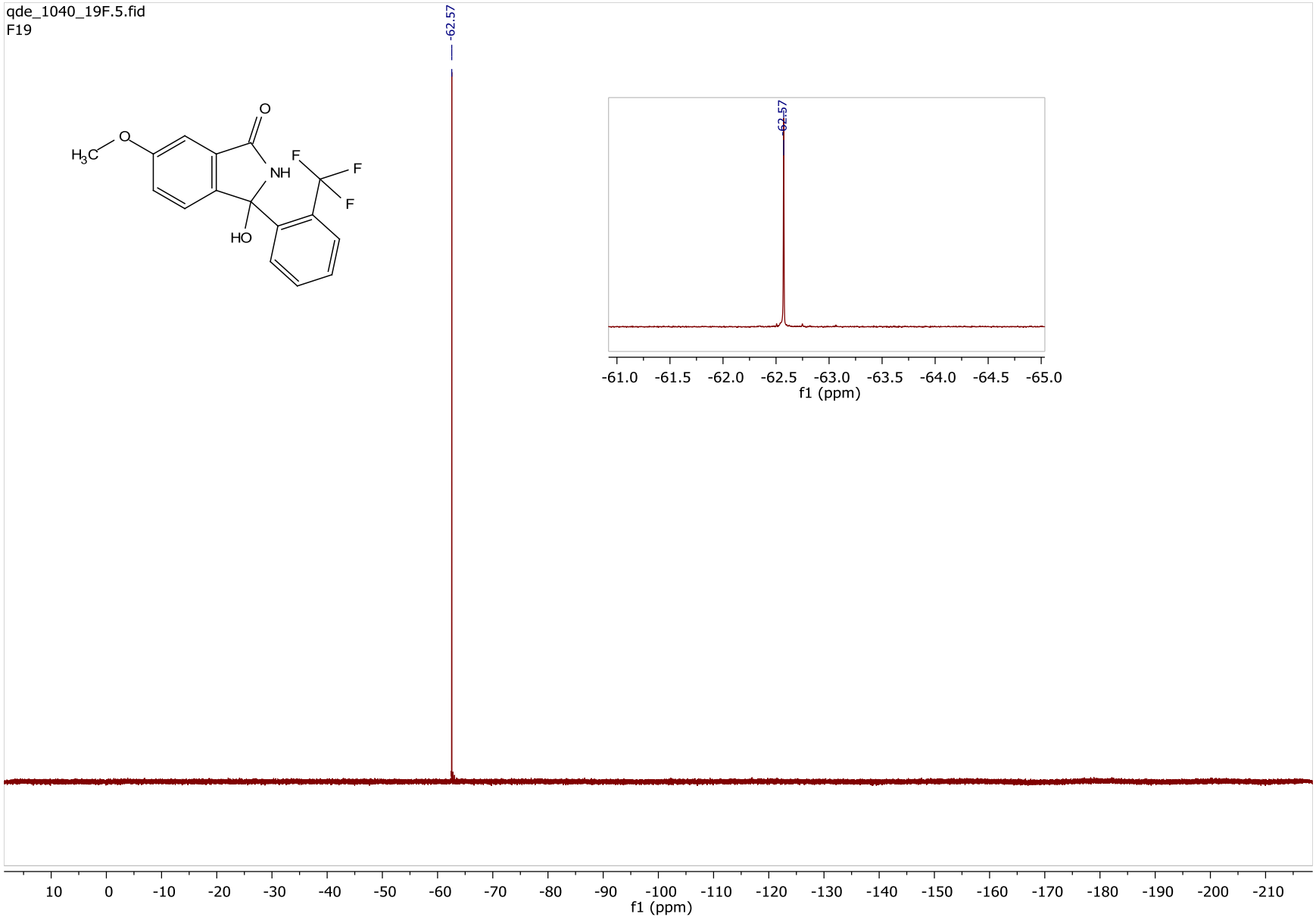

qde_1077_19F.2.fid
F19
-112.66
-112.67
-112.68
-112.69
-112.69
-112.70
-112.71
-112.72
-112.73
O
NH
OH
F
Cl
-112.50
-112.60
-112.70
-112.80
-112.90
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

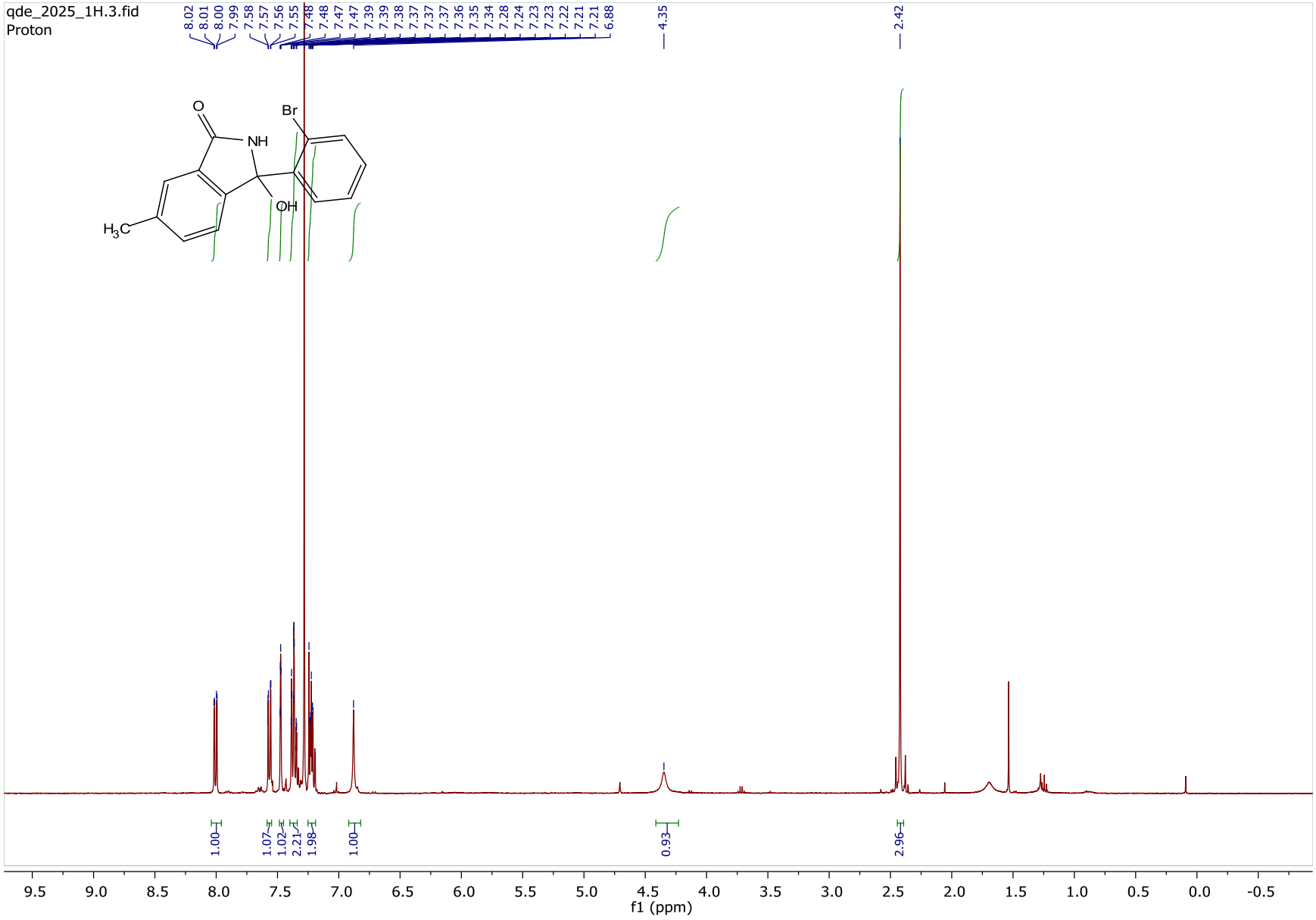

qde_1083.1_top_1H_5.fid
PROTON
Br
O
NH
OH
Br
f1 (ppm)
f1 (ppm)

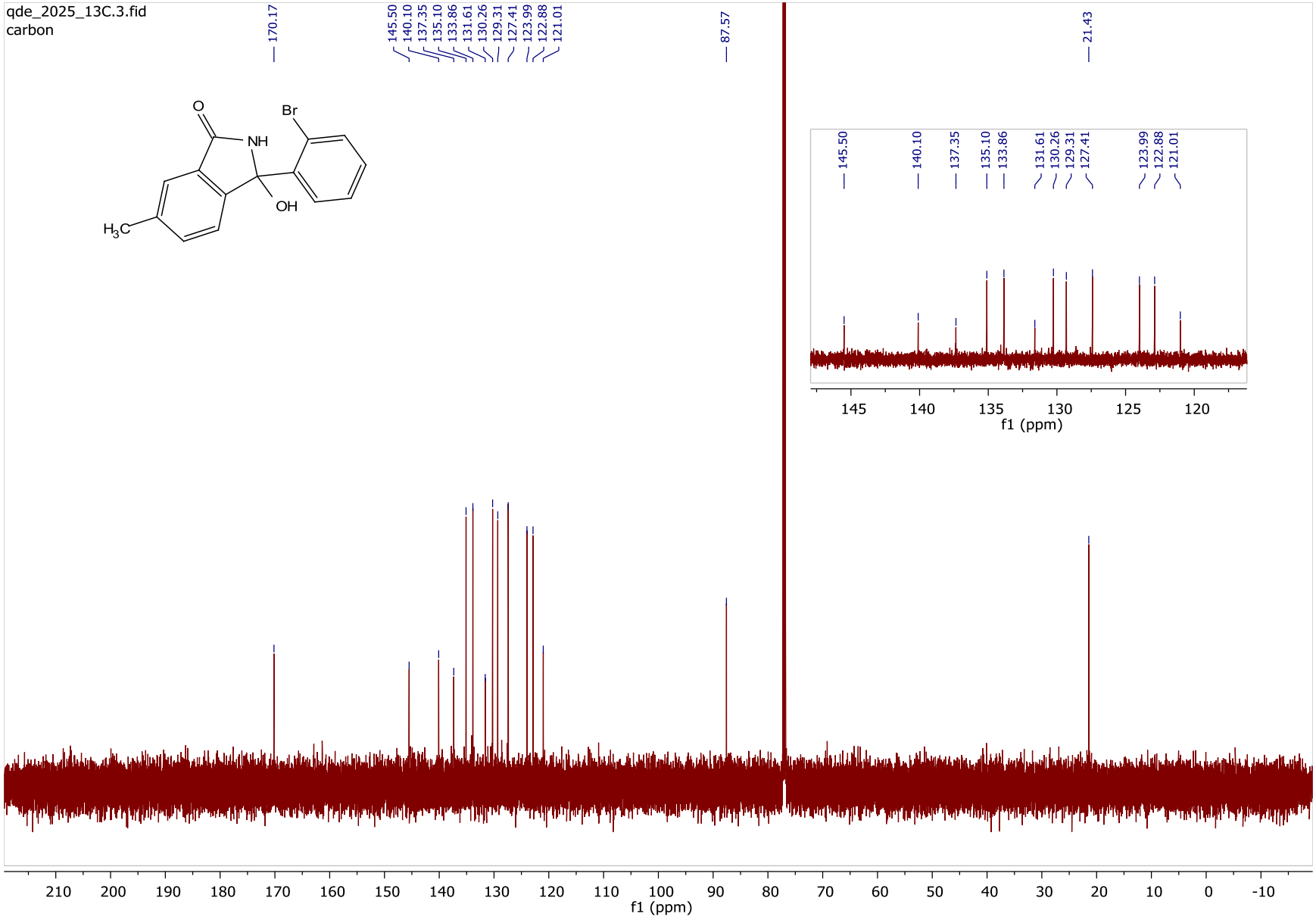

qde_1083.1_top_13C.5.fid
Carbon
170.54
148.85
139.71
139.69
137.32
135.15
133.07
132.93
131.51
130.85
130.38
129.40
128.16
128.06
127.55
127.51
125.04
121.38
121.01
86.67
77.32
77.06
76.81
35.83
Br
O
NH
OH
Br
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

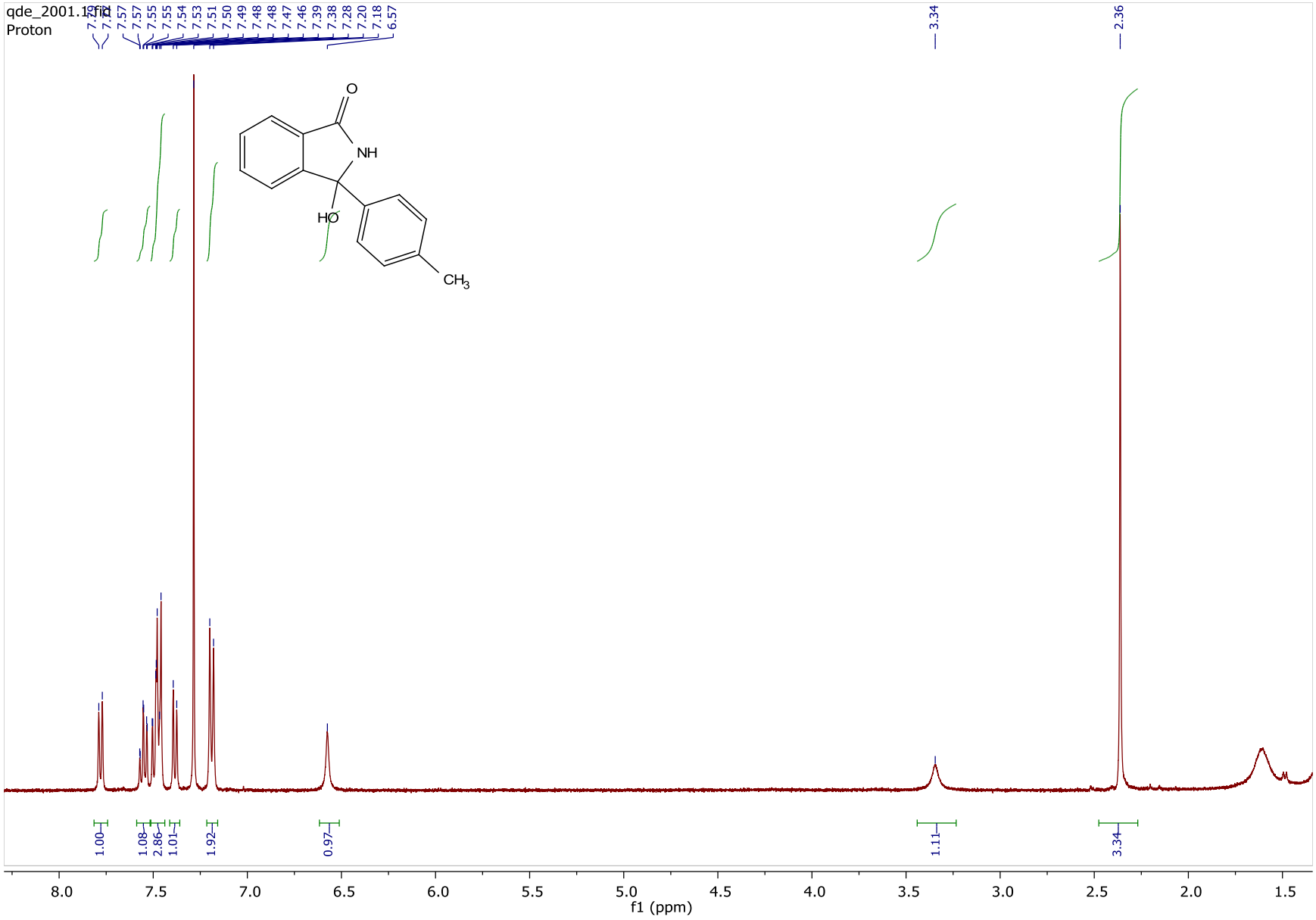

qde_10401H.5.fid
qde_1040_1H
7.89 7.67 7.65 7.61 7.59 7.49 7.47 7.45 7.26 7.26 7.26 7.25 7.23 7.21 7.09 7.09 7.07 7.07 6.59
3.86
3.30
O
H3C
O
NH
F
F
F
HO
2.06
1.08
1.66
1.00
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
0.94
2.06
1.08
1.93
1.00
0.96
3.04
1.11
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0
f1 (ppm)

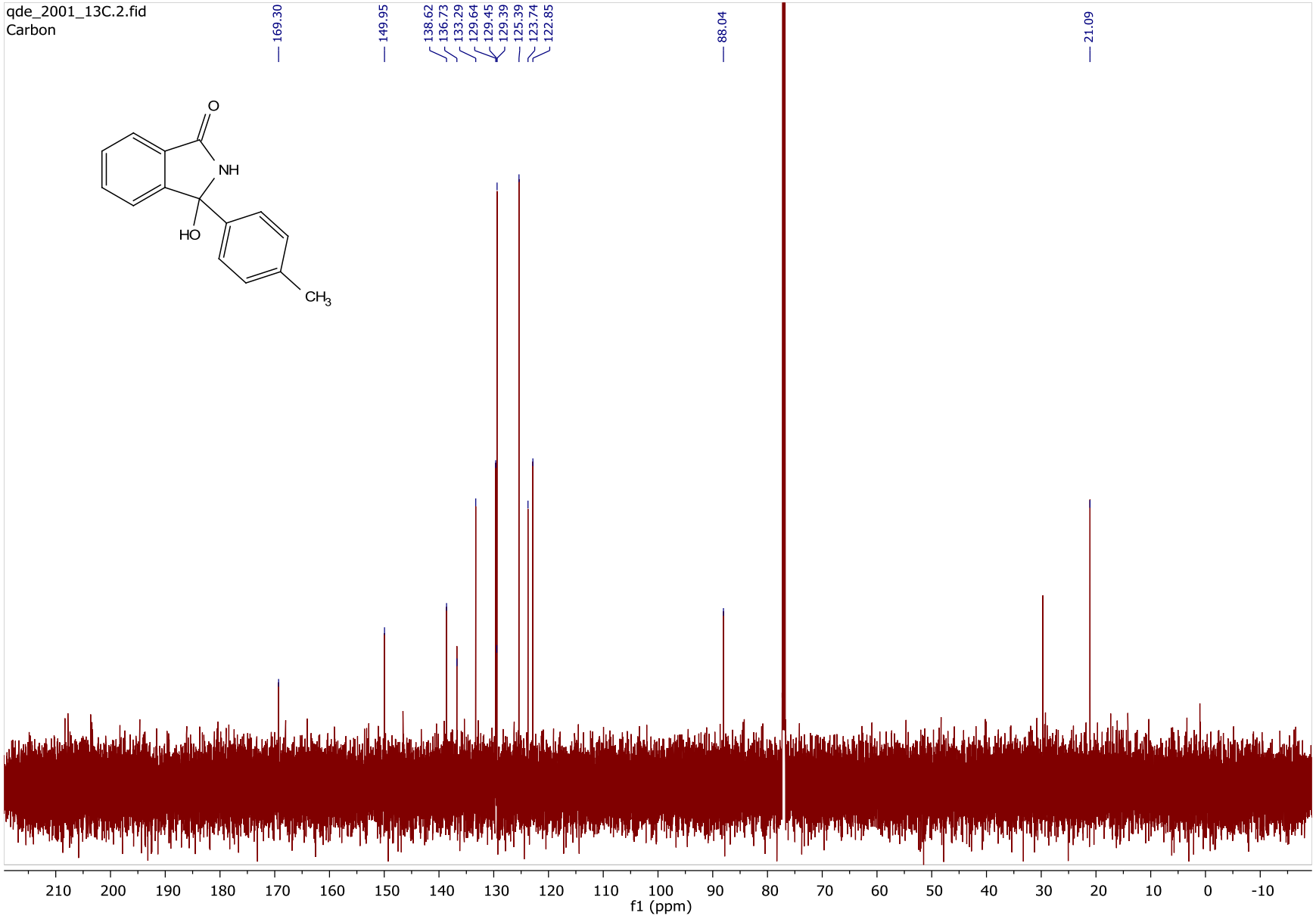

qde_1040_13C.3.fid
qde_1040_13C
168.08
161.14
143.95
142.29
132.46
130.09
129.88
129.74
129.33
125.32
124.67
124.64
124.62
123.88
123.52
122.30
122.28
122.25
122.22
119.64
106.48
86.91
55.23
O
O
H3C
NH
F
F
F
HO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

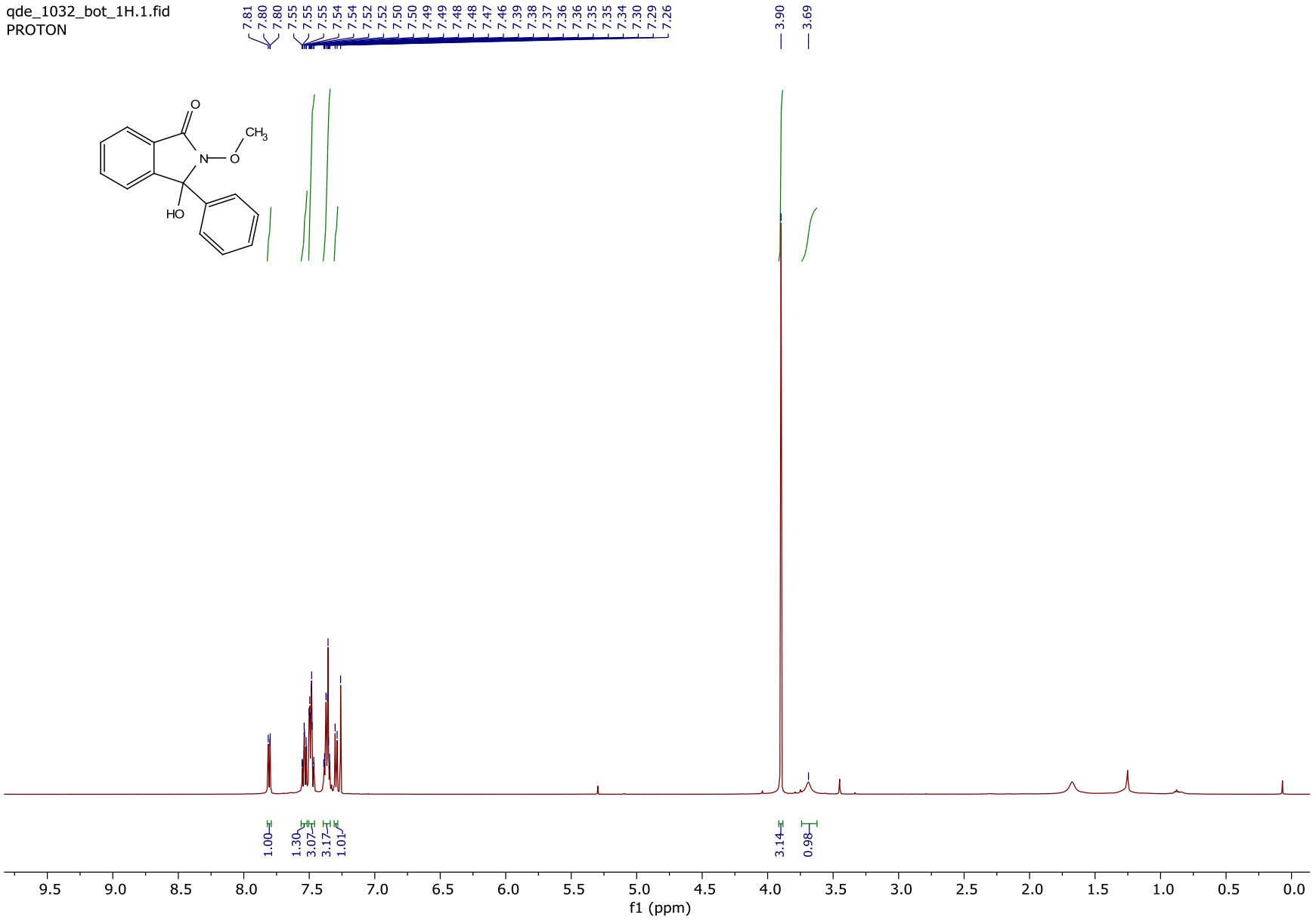

qde_1040_19F.5.fid
F19
-62.57
O
O
H3C
NH
F
F
F
HO
-62.57
-61.0 -61.5 -62.0 -62.5 -63.0 -63.5 -64.0 -64.5 -65.0
f1 (ppm)
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

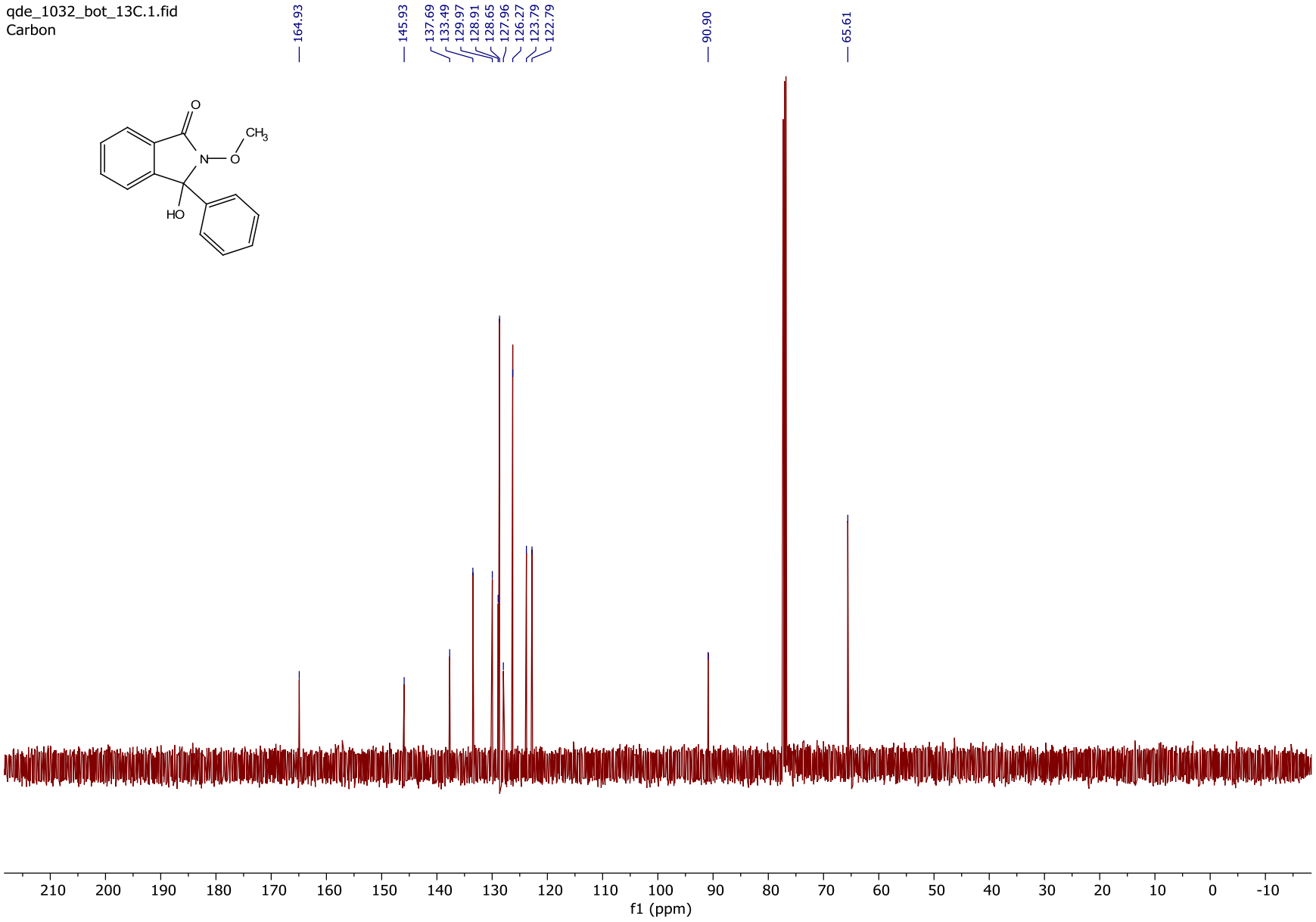

qde_2025_1H.3.fid
Proton
8.02
8.01
8.00
7.99
7.58
7.57
7.56
7.55
7.48
7.48
7.47
7.47
7.39
7.39
7.38
7.37
7.37
7.37
7.36
7.35
7.34
7.28
7.24
7.23
7.23
7.22
7.21
7.21
6.88
4.35
2.42
O
NH
Br
OH
H3C
1.00
1.07
1.02
2.21
1.98
1.00
0.93
2.96
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

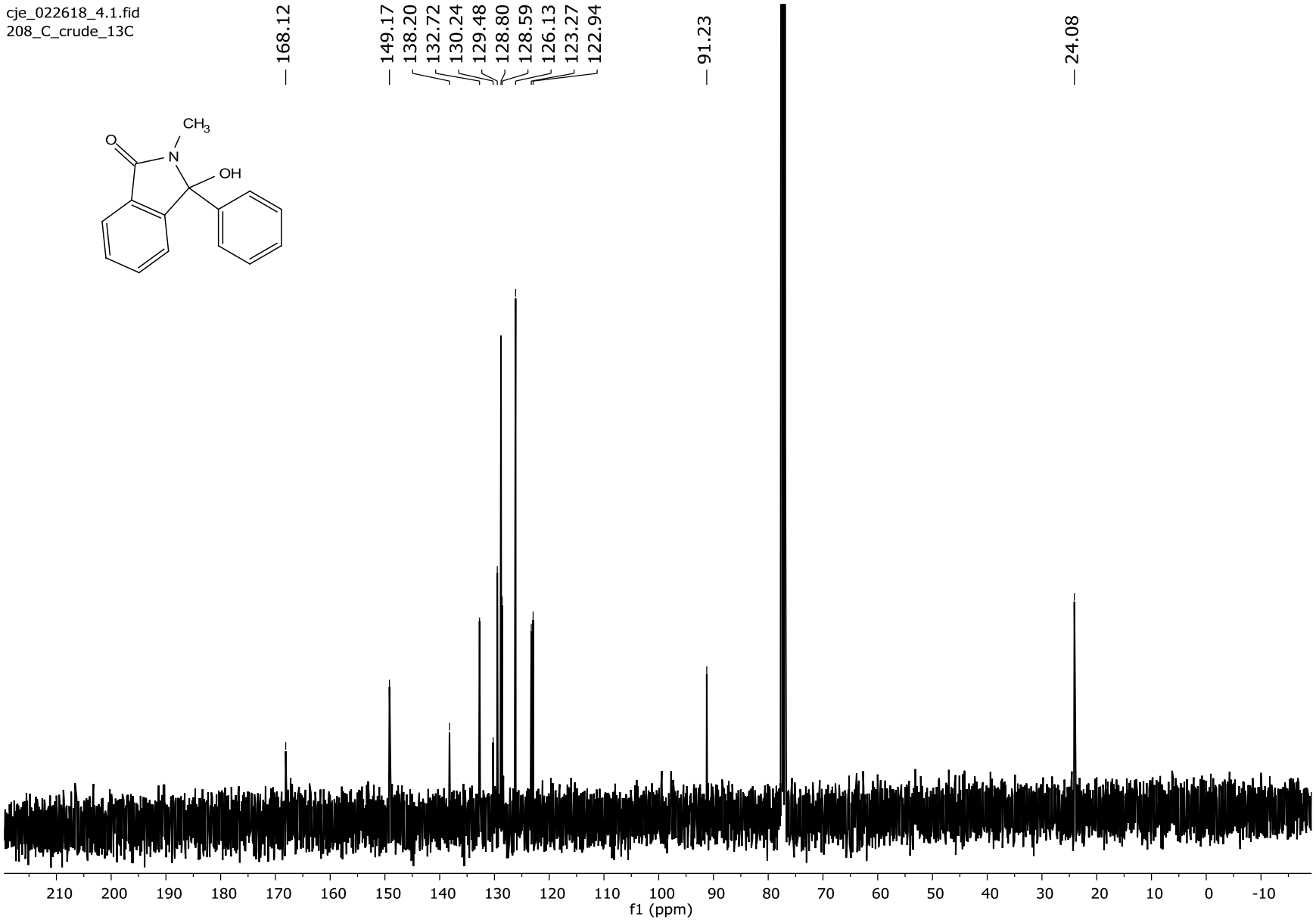

qde_2025_13C.3.fid
carbon
170.17
145.50
140.10
137.35
135.10
133.86
131.61
130.26
129.31
127.41
123.99
122.88
121.01
87.57
21.43
O
NH
Br
OH
H3C
f1 (ppm)

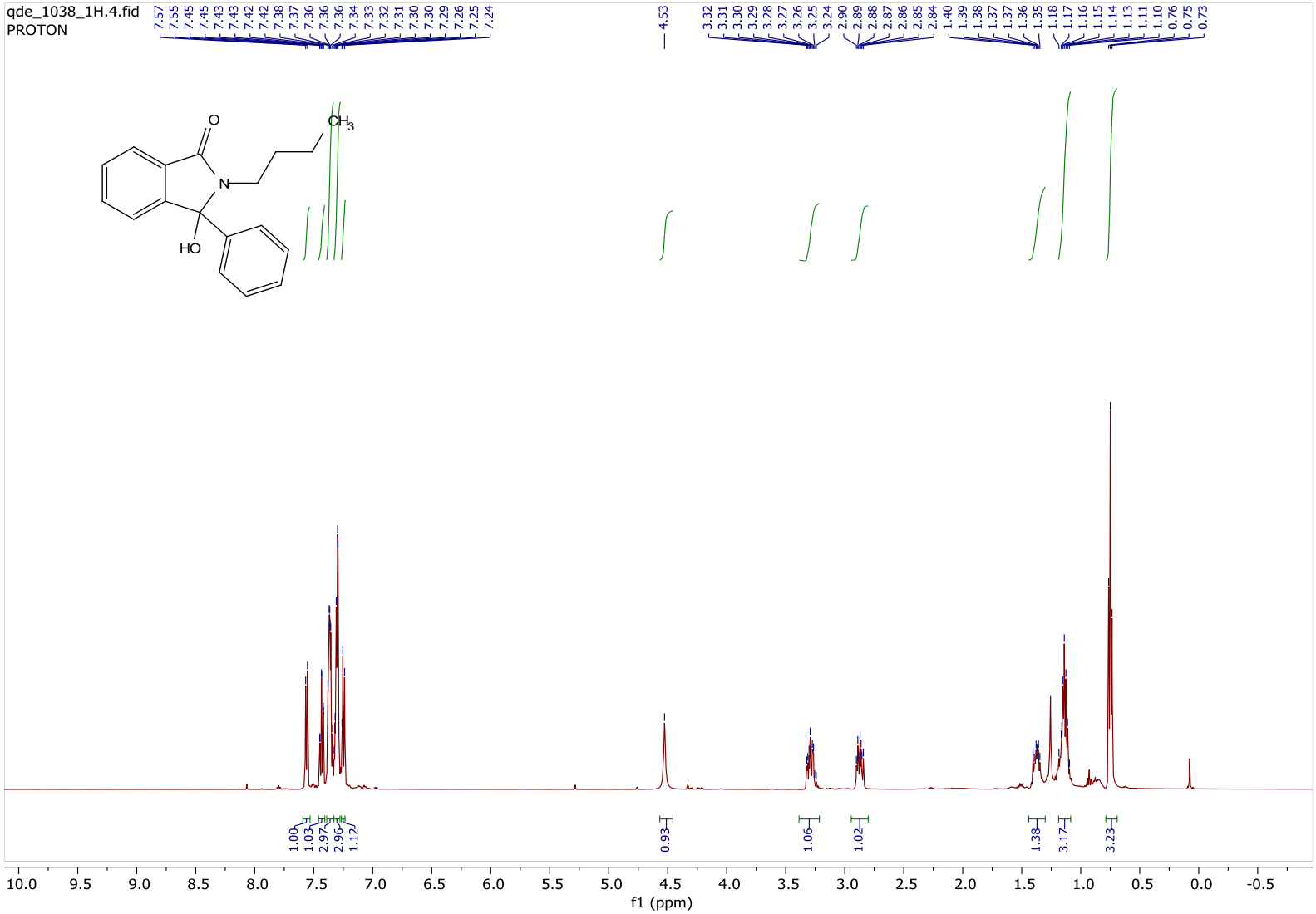

qde_2001.1.fid
Proton
7.81
7.80
7.57
7.55
7.55
7.54
7.53
7.51
7.50
7.49
7.48
7.48
7.47
7.46
7.39
7.38
7.28
7.20
7.18
6.57
3.34
2.36
O
NH
HO
CH3
1.00
1.08
2.86
1.01
1.92
0.97
1.11
3.34
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)

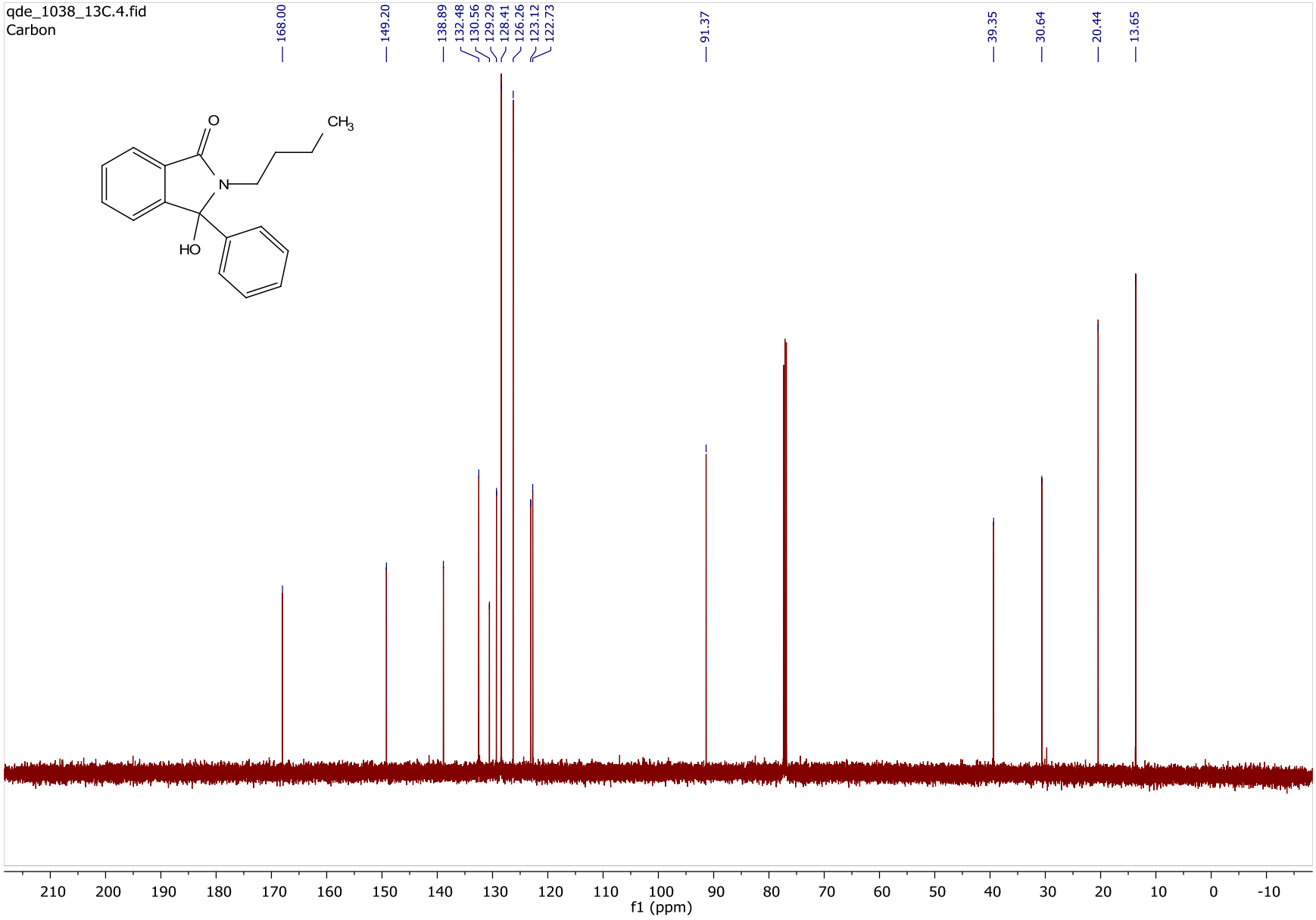

qde_2001_13C.2.fid
Carbon
169.30
149.95
138.62
136.73
133.29
129.64
129.45
129.39
125.39
123.74
122.85
88.04
21.09
O
NH
HO
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

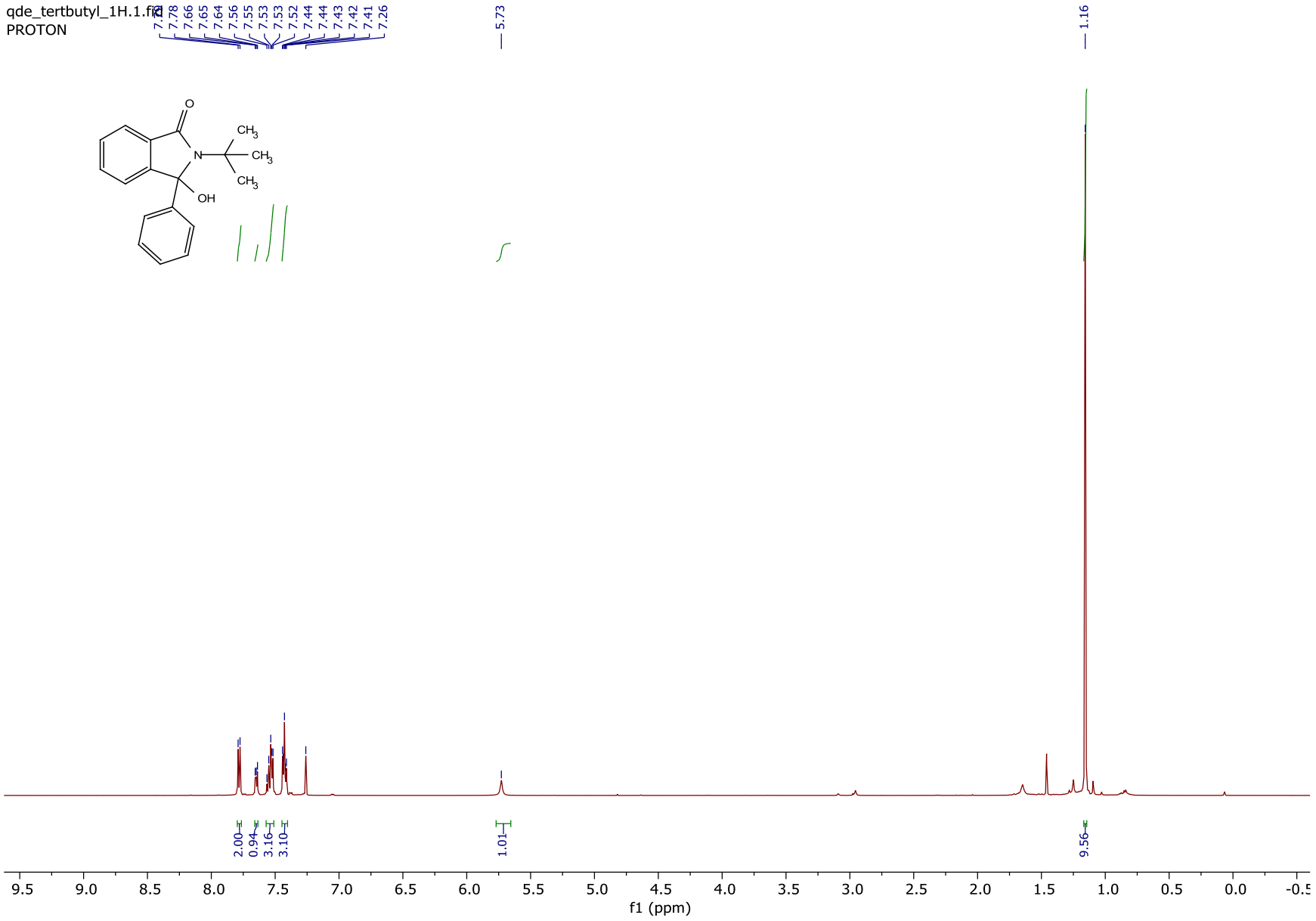

qde_1032_bot_1H.1.fid
PROTON
7.81
7.80
7.80
7.55
7.55
7.55
7.54
7.54
7.52
7.52
7.50
7.50
7.49
7.49
7.48
7.48
7.47
7.46
7.39
7.38
7.37
7.36
7.36
7.35
7.35
7.34
7.30
7.29
7.26
3.90
3.69
O
CH3
N
O
HO
1.00
1.30
3.07
3.17
1.01
3.14
0.98
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

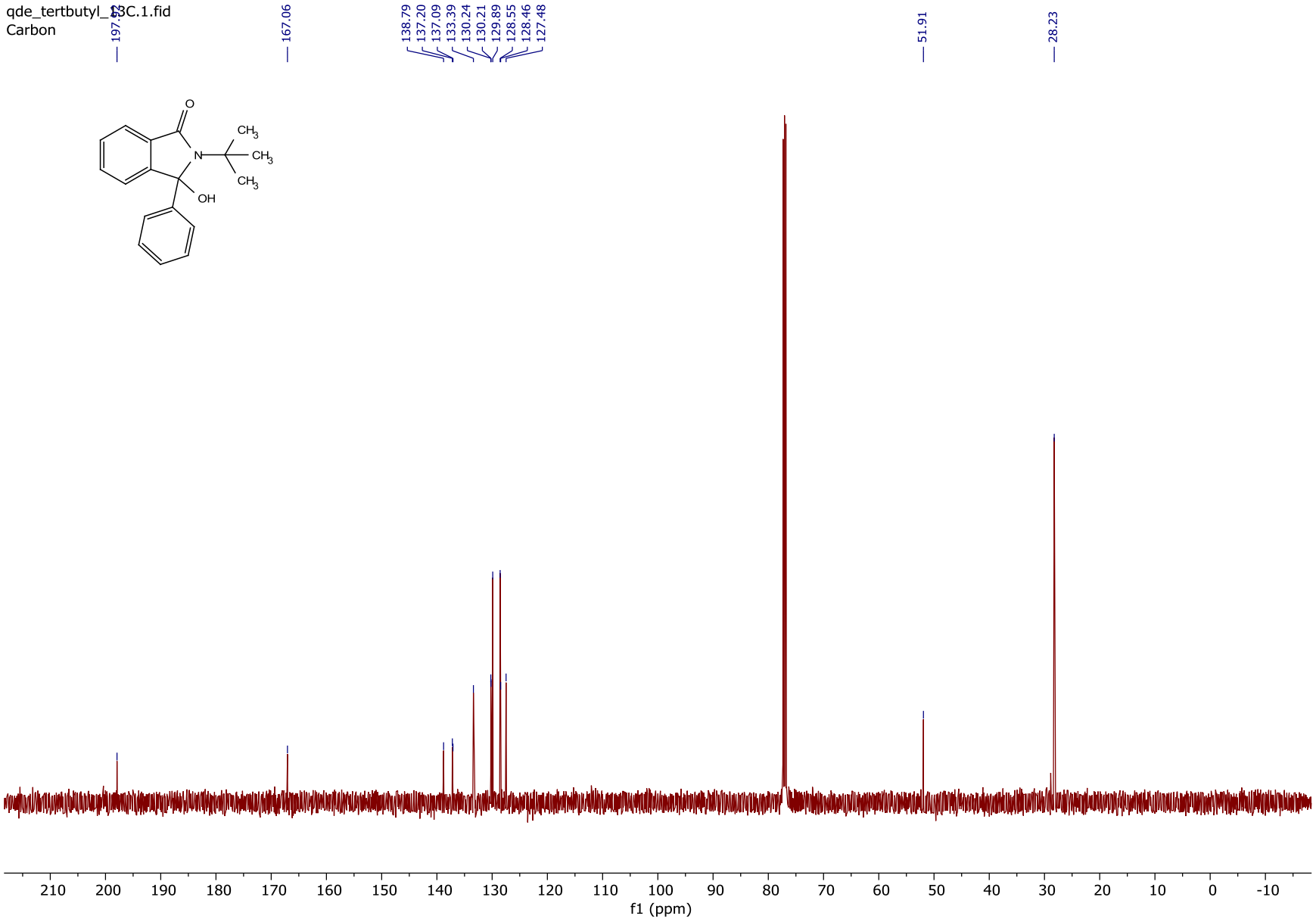

qde_1032_bot_13C.1.fid
Carbon
164.93
145.93
137.69
133.49
129.97
128.91
128.65
127.96
126.27
123.79
122.79
90.90
65.61
O
N
O
CH3
HO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

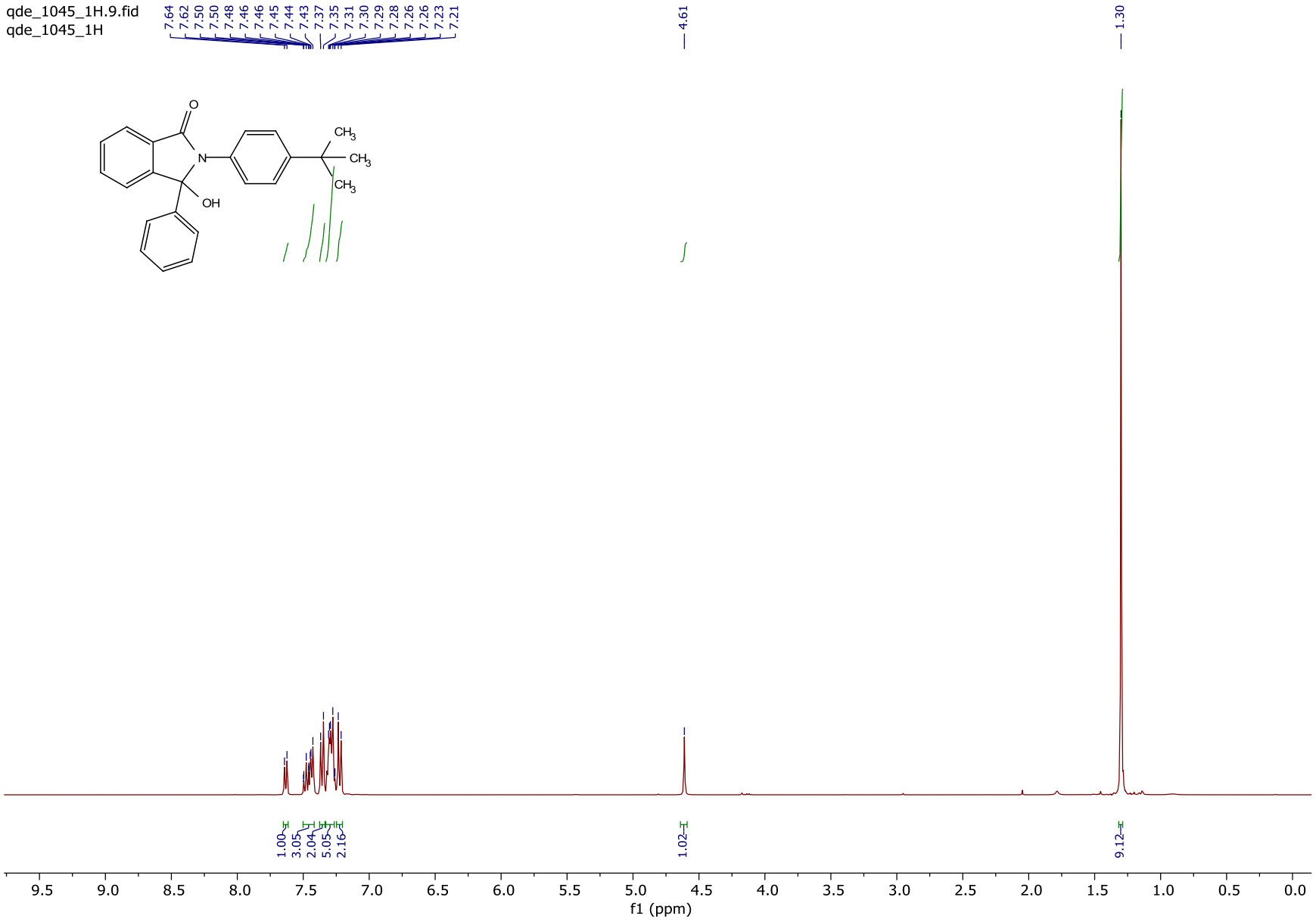

cje_022618_4.1.fid
208_C_crude_13C
168.12
149.17
138.20
132.72
130.24
129.48
128.80
128.59
126.13
123.27
122.94
91.23
24.08
CH3
O
N
OH
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

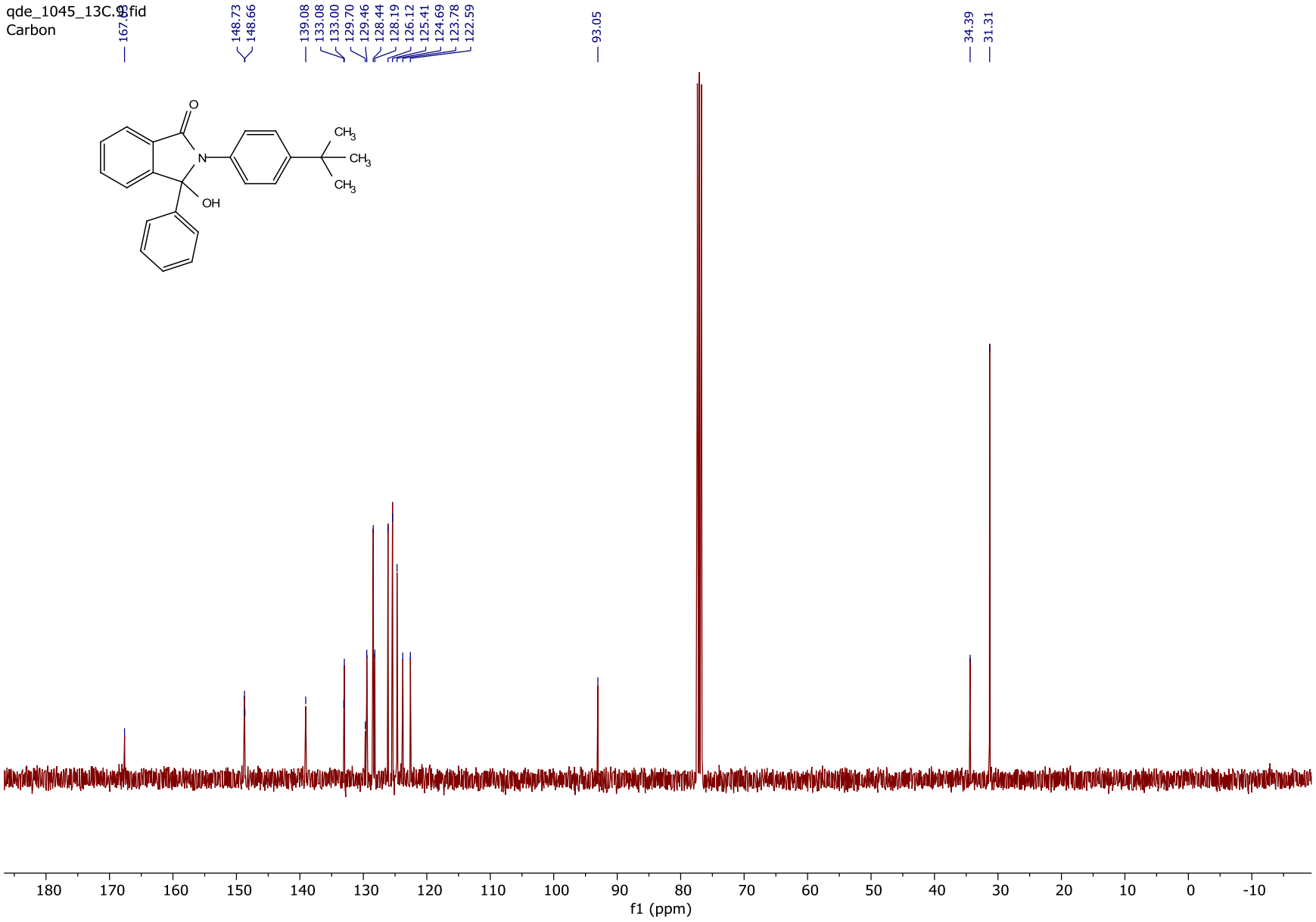

qde_1038_1H.4.fid
PROTON
7.57 7.55 7.45 7.45 7.43 7.43 7.42 7.42 7.38 7.37 7.36 7.36 7.36 7.34 7.33 7.32 7.31 7.30 7.30 7.29 7.26 7.25 7.24
4.53
3.32 3.31 3.30 3.29 3.28 3.27 3.26 3.25 3.24 2.90 2.89 2.88 2.87 2.86 2.85 2.84
1.40 1.39 1.38 1.37 1.37 1.36 1.35 1.18 1.17 1.16 1.15 1.14 1.13 1.11 1.10 0.76 0.75 0.73
O
CH3
N
HO
1.00 1.03 2.97 2.96 1.12
0.93
1.06
1.02
1.38
3.17
3.23
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

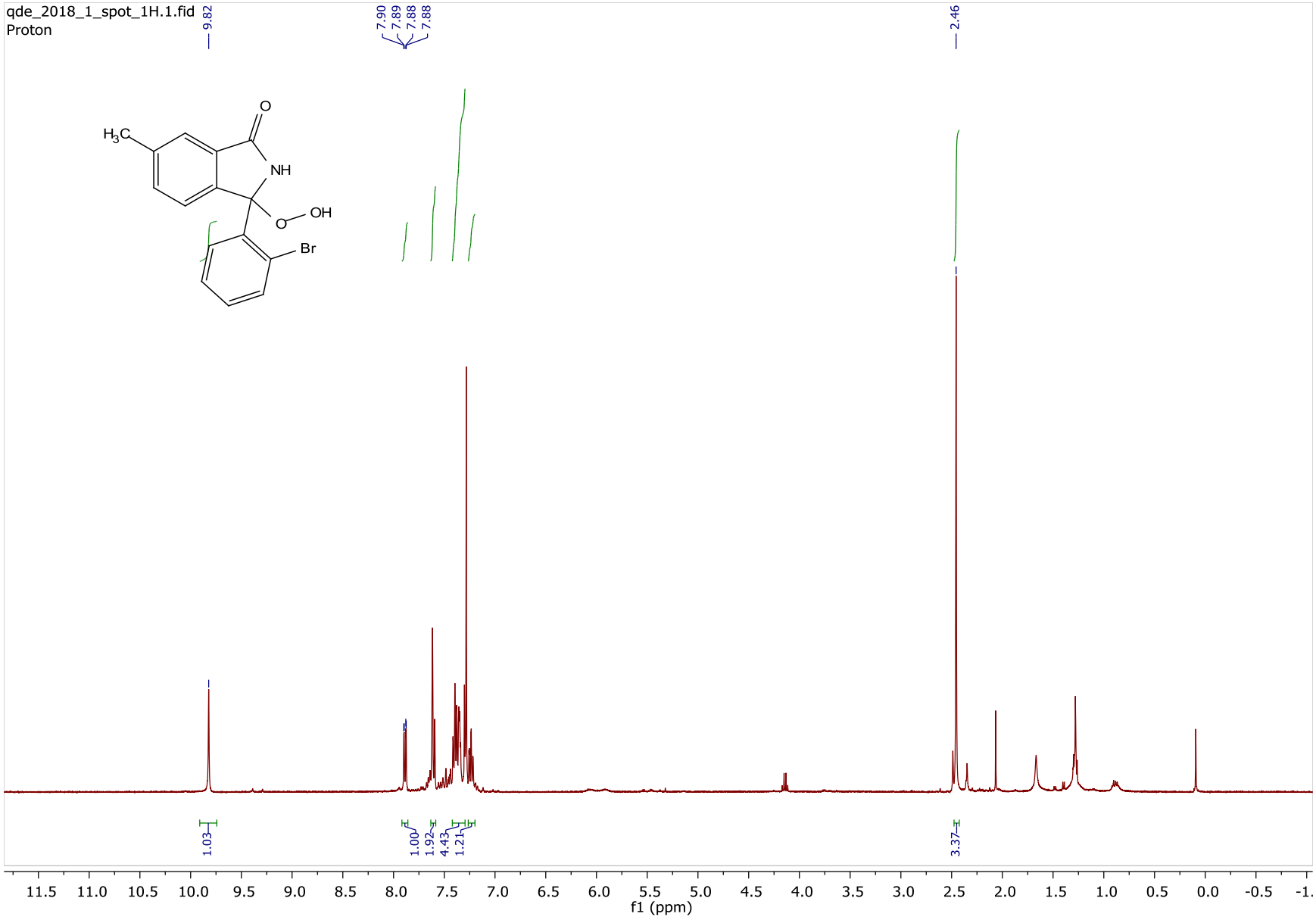

qde_1038_13C.4.fid
Carbon
168.00
149.20
138.89
132.48
130.56
129.29
128.41
126.26
123.12
122.73
91.37
39.35
30.64
20.44
13.65
O
CH3
N
HO
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

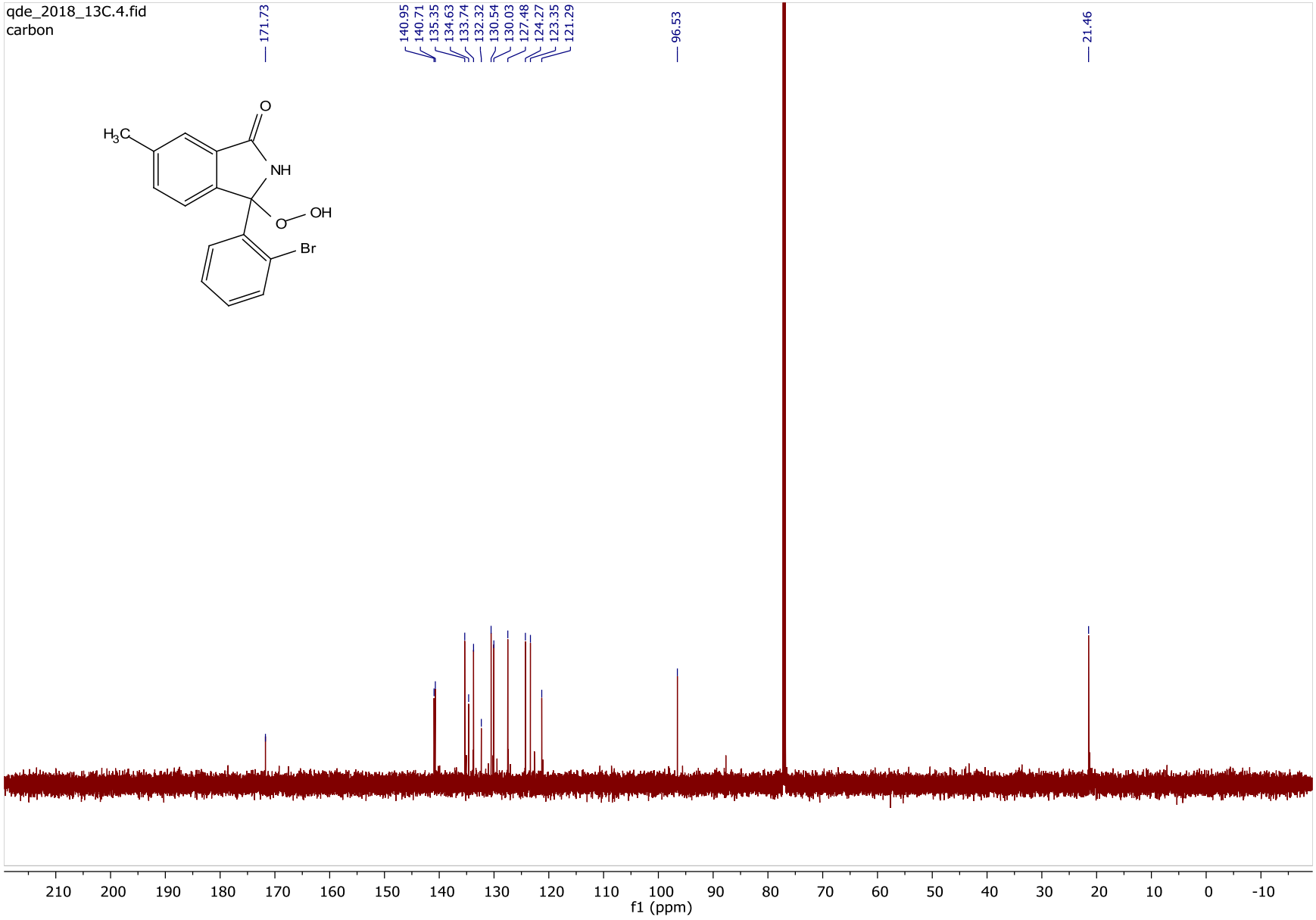

qde_tertbutyl_1H.1.fid
PROTON
7.78
7.66
7.65
7.64
7.56
7.55
7.53
7.53
7.52
7.44
7.44
7.43
7.42
7.41
7.26
5.73
1.16
O
N
CH3
CH3
CH3
OH
2.00
0.94
3.16
3.10
1.01
9.56
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


qde_tertbutyl_13C.1.fid
Carbon
197.43
167.06
138.79
137.20
137.09
133.39
130.24
130.21
129.89
128.55
128.46
127.48
51.91
28.23
O
N
CH3
CH3
CH3
OH
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

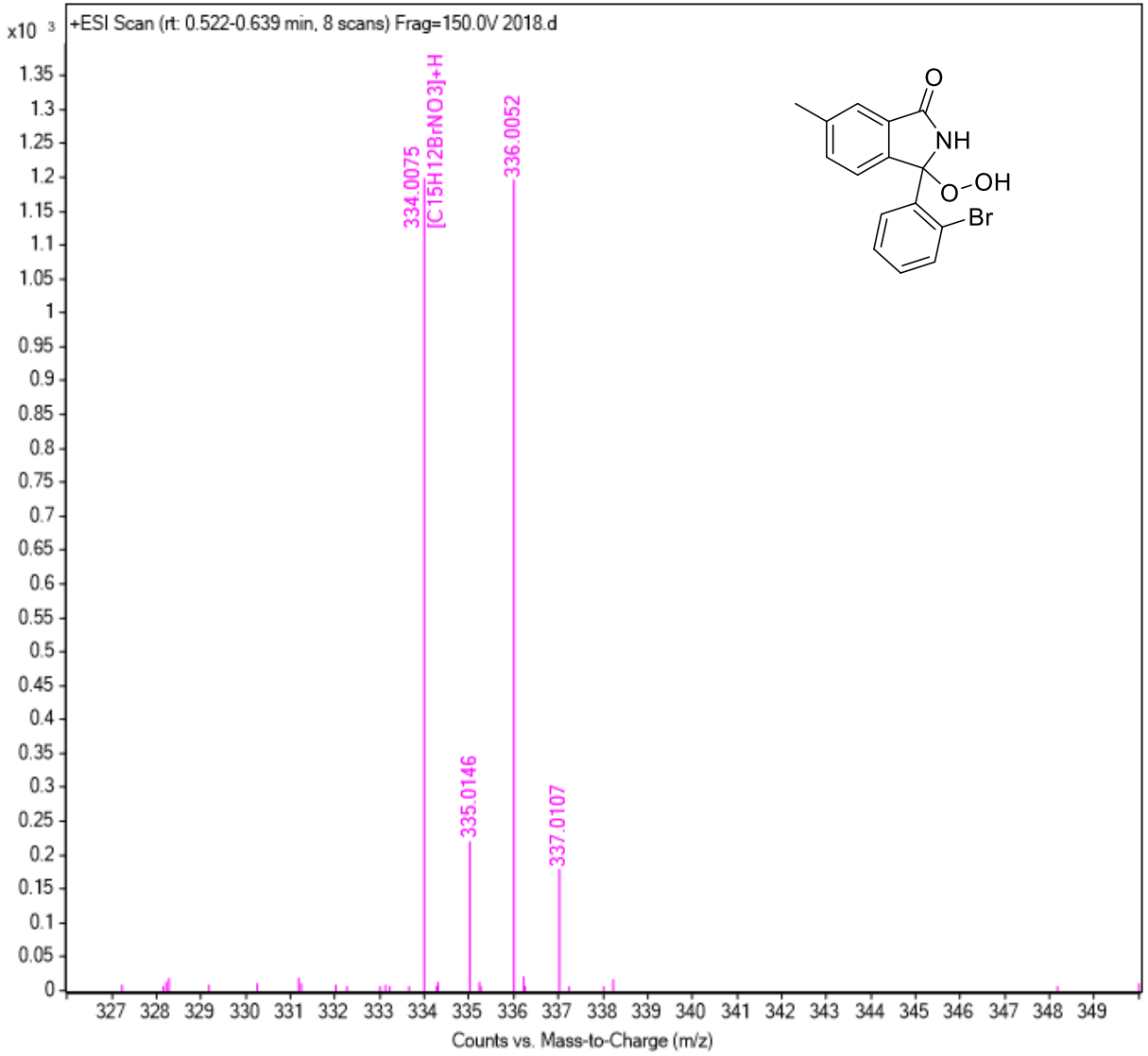

qde_1045_1H.9.fid
qde_1045_1H
7.64
7.62
7.50
7.50
7.48
7.46
7.46
7.45
7.44
7.43
7.37
7.35
7.31
7.30
7.29
7.28
7.26
7.26
7.23
7.21
4.61
1.30
O
N
OH
CH3
CH3
CH3
1.00
3.05
2.04
5.05
2.16
1.02
9.12
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

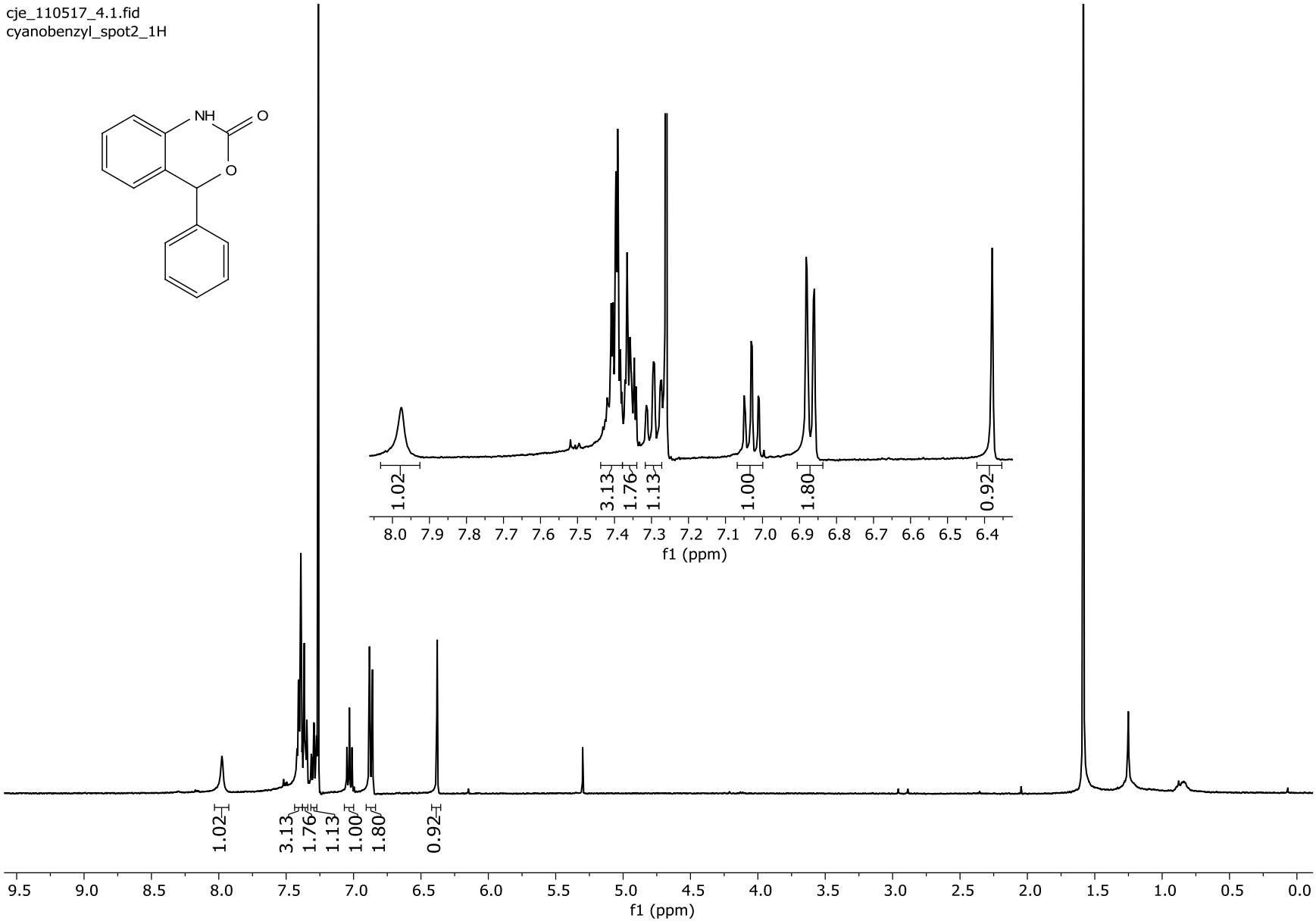

qde_1045_13C.2.fid
Carbon
167.80
148.73
148.66
139.08
133.08
133.00
129.70
129.46
128.44
128.19
126.12
125.41
124.69
123.78
122.59
93.05
34.39
31.31
O
N
OH
CH3
CH3
CH3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

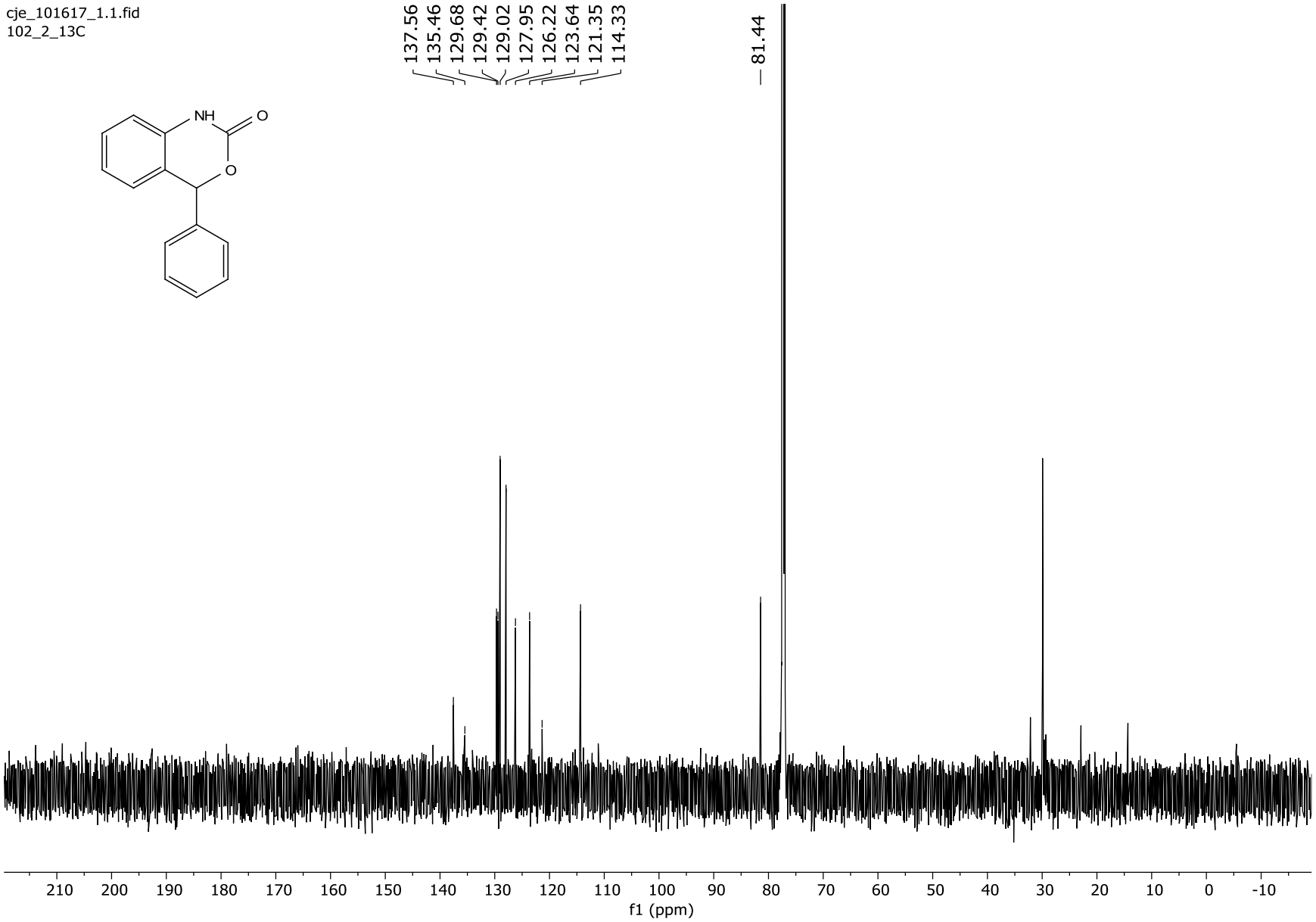

qde_2018_1_spot_1H.1.fid
Proton
9.82
7.90
7.89
7.88
7.88
2.46
O
H3C
NH
O
OH
Br
1.03
1.00
1.92
4.43
1.21
3.37
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

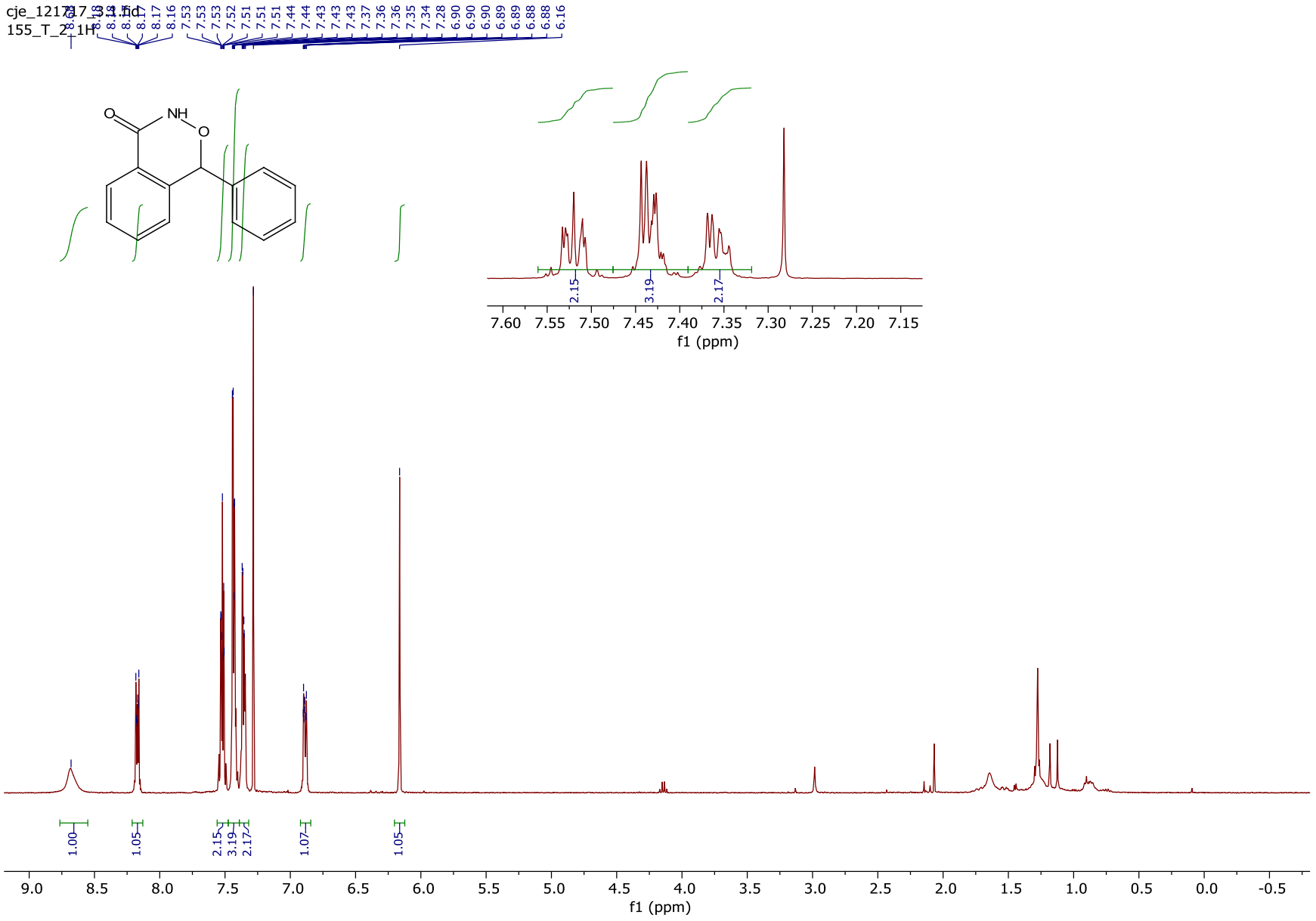

qde_2018_13C.4.fid
carbon
171.73
140.95
140.71
135.35
134.63
133.74
132.32
130.54
130.03
127.48
124.27
123.35
121.29
96.53
21.46
O
H3C
NH
O
OH
Br
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

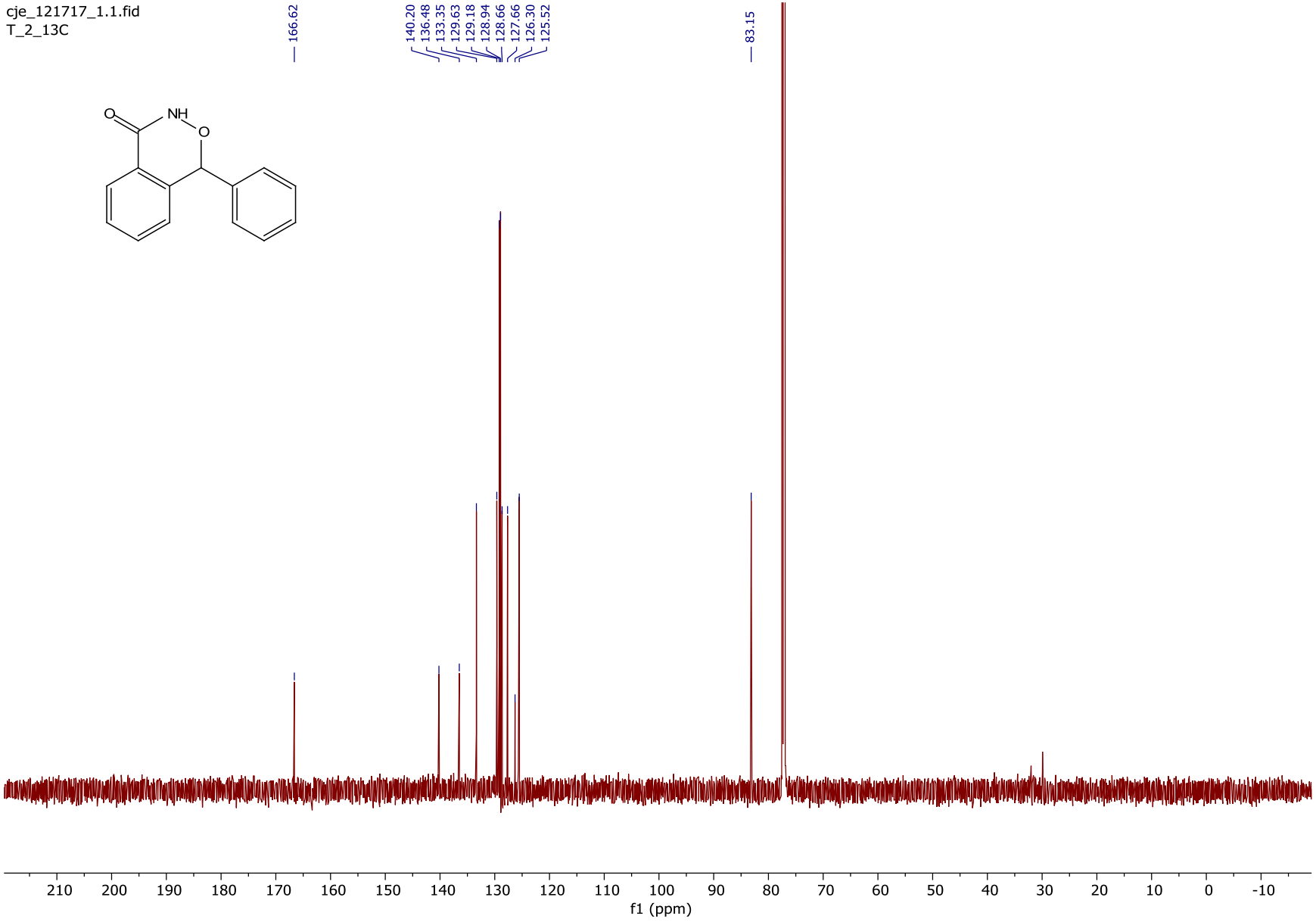
Sample Name	1/26/19	**Position**		**Instrument Name**	Instrument 1
User Name		**Inj Vol**	Unknown / Injection Program	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	2018.d
ACQ Method	DART POS.m	**Comment**		**Acquired Time**	1/26/2019 4:35:43 PM (UTC-05:00)

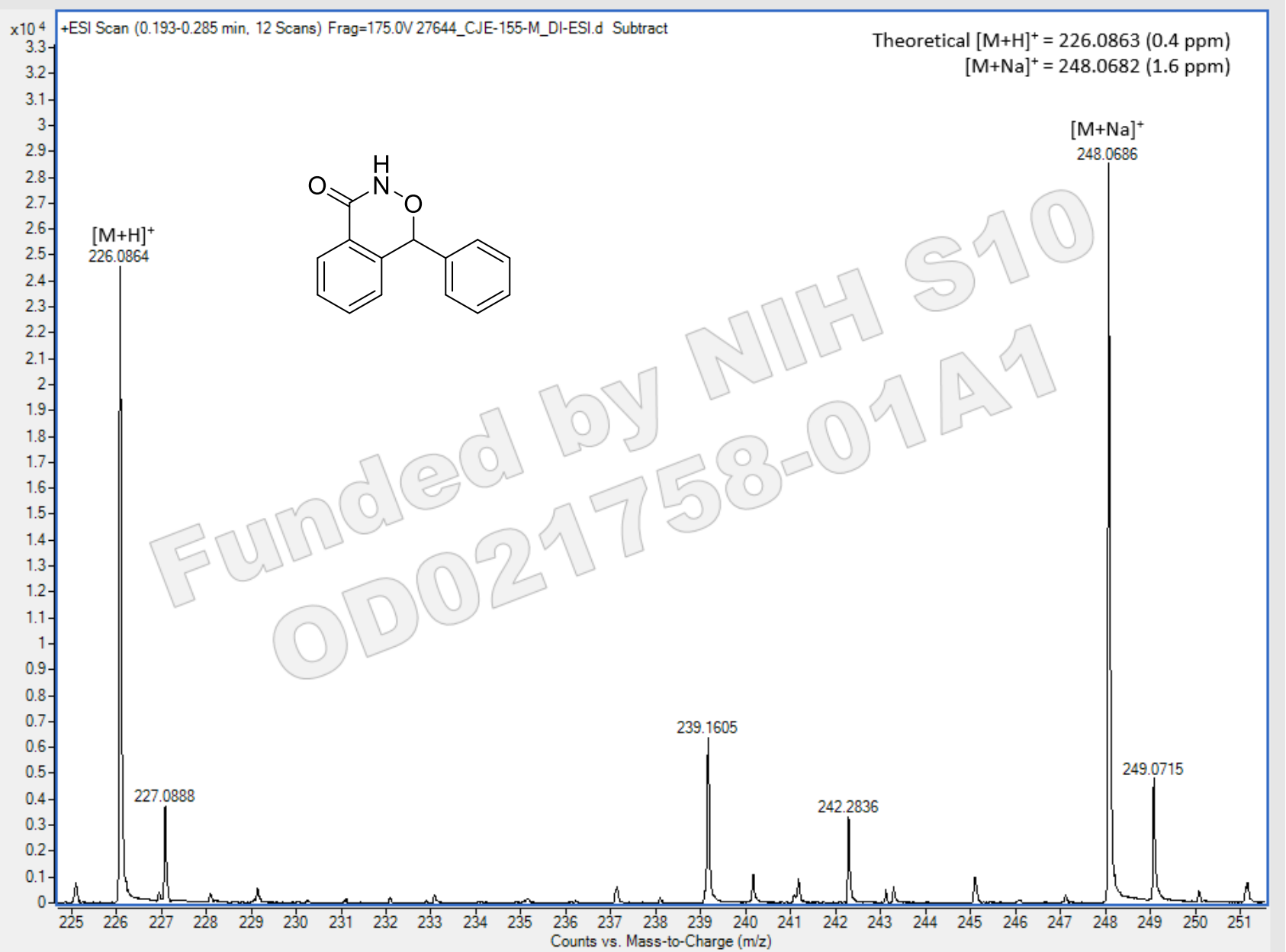


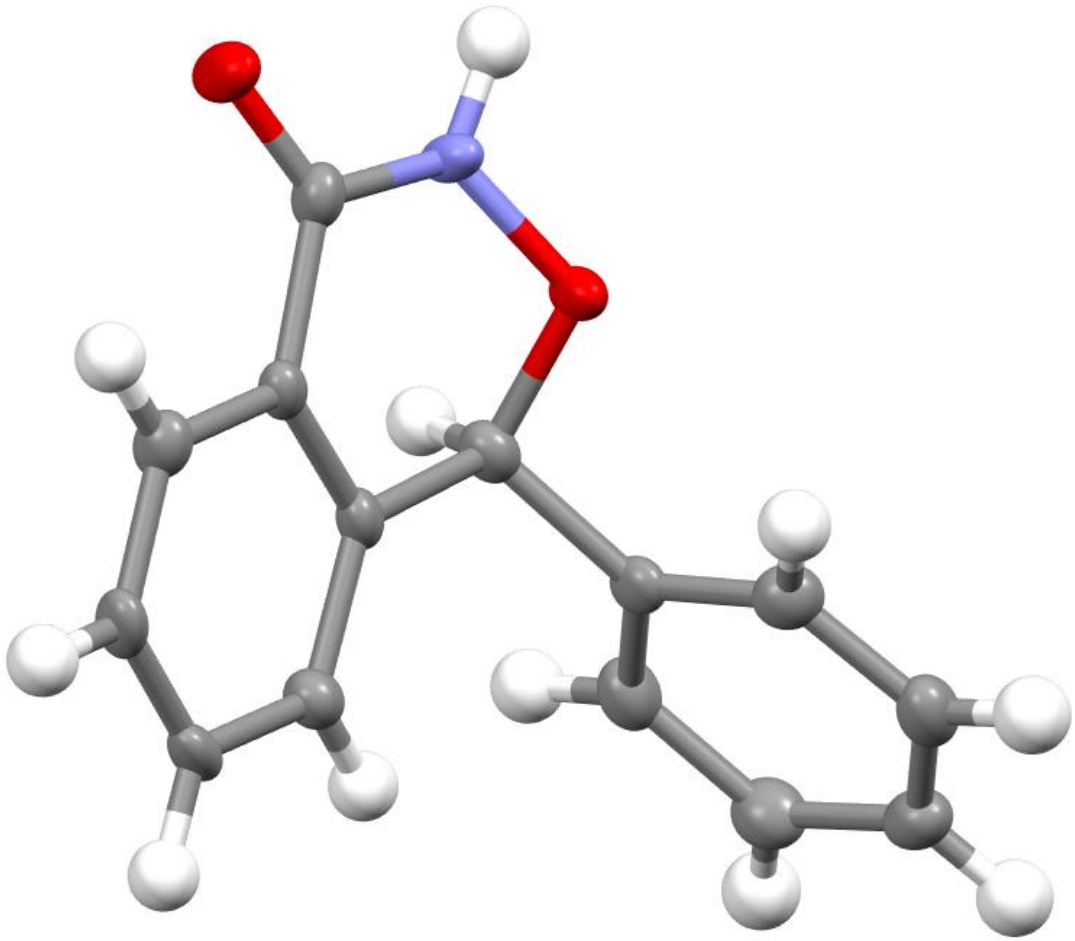

cje_110517_4.1.fid
cyanobenzyl_spot2_1H
NH
O
O
1.02
3.13
1.76
1.13
1.00
1.80
0.92
f1 (ppm)


cje_101617_1.1.fid
102_2_13C
137.56
135.46
129.68
129.42
129.02
127.95
126.22
123.64
121.35
114.33
81.44
NH
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


cje_121717_13
155_T_2_1H
8.18
8.18
8.17
8.17
8.16
7.53
7.53
7.53
7.52
7.51
7.51
7.51
7.44
7.44
7.43
7.43
7.43
7.37
7.36
7.36
7.35
7.34
7.28
6.90
6.90
6.89
6.89
6.88
6.88
6.16
O
NH
O
2.15
3.19
2.17
7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15
f1 (ppm)
1.00
1.05
2.15
3.19
2.17
1.07
1.05
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


cje_121717_1.1.fid
T_2_13C
166.62
140.20
136.48
133.35
129.63
129.18
128.94
128.66
127.66
126.30
125.52
83.15
O
NH
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


+ESI Scan (0.193-0.285 min, 12 Scans) Frag=175.0V 27644_CJE-155-M_DI-ESI.d Subtract
x10 4
Theoretical [M+H]+ = 226.0863 (0.4 ppm)
[M+Na]+ = 248.0682 (1.6 ppm)
[M+H]+
226.0864
[M+Na]+
248.0686
227.0888
239.1605
242.2836
249.0715
Counts vs. Mass-to-Charge (m/z)
Funded by NIH S10
OD021758-01A1



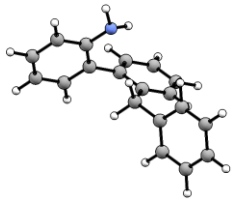
Scheme S7: Crystal Structure of 1-phenyl-1*H*-benzo[d][1,2]oxazin-4(3*H*)-one (**6a**). Carbon = grey, Oxygen = red, Nitrogen = Blue.

4) Computational Details

DFT calculations were carried with the *Gaussian 09* software package,[22] using the (U)M06-2X DFT functional[23] (with an ultrafine integration grid of 99,590 points) with the 6-311++G(d,p) basis set for all atoms. A broken-spin approach was used when necessary. Grimme's D3 version (zero damping) for empirical dispersion[24] was also included. Frequency calculations were conducted for all structures, confirming if a structure is either a minimum or a TS. The self-consistent reaction field (SCRF) correction was applied through the SMD[25] solvent model for N,N-dimethyl-formamide (DMF) to evaluate solvent effects. Natural Bond Orbital[26] (NBO) analysis was performed on key structures. Unless otherwise noted, all results presented are at the (SMD=DMF)/UM06-2X/6-31+G(d,p)/int=ultrafine level of theory. The Gibbs Free energy values are reported at 298 K, unless noted otherwise. Three-dimensional structures and orbital plots were produced with CYLView 1.0.1,[27] and Chemcraft 1.7[28]. Geometries, energies and frequencies presented in this SI were organized with ESIgen.[29]

4a) Structures and energies for all species calculated at the (SMD=DMF)/UM06-2X(D3)/6-31+G(d,p) level of theory

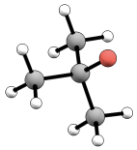
Calculated geometries (in cartesian coordinates) with their respective energies (in hartree), charge, multiplicity and stoichiometry.



# of imaginary frequencies: 0
E = -788.756905881
symmetry c1

C	-0.648983000	3.231020000	-0.119462000
C	-1.103236000	1.911436000	-0.068278000
C	-0.210716000	0.841015000	0.039596000
C	1.172257000	1.117471000	0.092190000
C	1.617612000	2.442209000	0.046804000

C	0.714894000	3.501245000	-0.057477000
H	-1.365540000	4.042964000	-0.203341000
H	-2.171425000	1.718272000	-0.107086000
H	2.685873000	2.639941000	0.089983000
H	1.077243000	4.524278000	-0.092119000
C	2.171495000	0.012667000	0.201216000
C	2.817957000	-0.236473000	1.415373000
C	2.491420000	-0.776971000	-0.924304000
C	3.756231000	-1.259624000	1.546434000
H	2.568561000	0.385280000	2.272171000
C	3.434155000	-1.808622000	-0.787207000
C	4.056647000	-2.047321000	0.433668000
H	4.243180000	-1.438182000	2.499756000
H	3.675864000	-2.416117000	-1.656005000
H	4.784626000	-2.849865000	0.512344000
C	-0.680555000	-0.604553000	0.124003000
H	-0.247647000	-1.158767000	-0.717620000
H	-0.261302000	-1.047748000	1.035406000
C	-2.177849000	-0.783024000	0.124112000
C	-2.874400000	-0.963379000	-1.075426000
C	-2.901448000	-0.737796000	1.320838000
C	-4.263823000	-1.092005000	-1.081717000
H	-2.321044000	-1.000750000	-2.011425000
C	-4.290474000	-0.866269000	1.320207000
H	-2.369533000	-0.598030000	2.259622000
C	-4.976178000	-1.042770000	0.117239000
H	-4.789271000	-1.232688000	-2.022020000
H	-4.836907000	-0.830480000	2.258356000
H	-6.057411000	-1.144686000	0.114787000
N	1.844450000	-0.577532000	-2.141432000
H	1.504417000	0.363851000	-2.303496000
H	2.339133000	-0.944095000	-2.946144000



t-BuO anion
# of imaginary frequencies: 0
E = -233.055756257
symmetry c1

C	0.000140000	0.000017000	0.136547000
C	-0.784690000	1.210640000	-0.432298000
H	-0.333223000	2.142407000	-0.068447000
H	-0.806349000	1.245168000	-1.531063000
H	-1.819874000	1.178271000	-0.069358000
C	1.441056000	0.074027000	-0.432482000
H	1.931495000	0.986202000	-0.069456000
H	2.021922000	-0.783259000	-0.068996000
H	1.481832000	0.075688000	-1.531242000
C	-0.656497000	-1.284498000	-0.432500000
H	-0.112220000	-2.165546000	-0.069212000
H	-1.689457000	-1.358293000	-0.069200000
H	-0.674979000	-1.320526000	-1.531253000
O	0.000100000	-0.000153000	1.496578000

O_2 triplet
# of imaginary frequencies: 0
E = -150.274457668
symmetry c1

O	0.000000000	0.000000000	0.598885000
O	0.000000000	0.000000000	-0.598885000

O_2 radical-anion
# of imaginary frequencies: 0
E = -150.386381107

symmetry c1

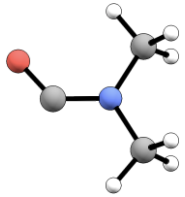
O	0.000000000	0.000000000	0.661784000
O	0.000000000	0.000000000	-0.661784000

# of imaginary frequencies: 0

E = -0.495993926274

symmetry oh

H	0.000000000	0.000000000	0.000000000



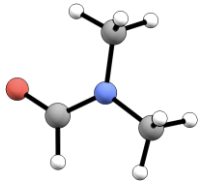
DMF-radical

# of imaginary frequencies: 0

E = -247.761752075

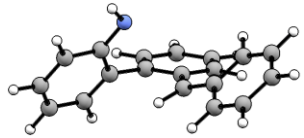
symmetry c1

C	-0.868488000	-0.646799000	0.000011000
O	-1.990011000	-0.196560000	-0.000015000
N	0.311877000	-0.049109000	0.000048000
C	0.443469000	1.408266000	-0.000007000
H	0.991623000	1.726723000	0.891691000
H	0.992133000	1.726561000	-0.891448000
H	-0.548089000	1.860223000	-0.000314000
C	1.546174000	-0.820305000	-0.000013000
H	1.304749000	-1.883716000	-0.000039000
H	2.134768000	-0.580231000	-0.890787000
H	2.134835000	-0.580288000	0.890733000



DMF
# of imaginary frequencies: 0
E = -248.421191015
symmetry c1

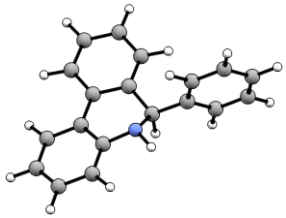
C	-0.859139000	-0.642000000	0.000046000
H	-0.768332000	-1.740442000	0.000047000
O	-1.955090000	-0.083857000	-0.000082000
N	0.335459000	-0.022644000	0.000253000
C	0.439027000	1.424287000	-0.000012000
H	0.982410000	1.761194000	0.889230000
H	0.980740000	1.761053000	-0.890343000
H	-0.562184000	1.854030000	0.000792000
C	1.579335000	-0.768929000	-0.000087000
H	1.367223000	-1.839913000	-0.000110000
H	2.168460000	-0.523299000	-0.889973000
H	2.168848000	-0.523412000	0.889564000



# of imaginary frequencies: 0
E = -787.600489204
symmetry c1

C	0.041646000	3.574976000	-0.083229000
C	0.738189000	2.386542000	-0.269356000
C	0.082429000	1.134655000	-0.254557000
C	-1.329691000	1.108431000	-0.049379000
C	-2.005973000	2.318993000	0.131350000
C	-1.339118000	3.545992000	0.118738000

H	0.573135000	4.521775000	-0.112400000
H	1.801732000	2.426889000	-0.482589000
H	-3.080223000	2.294589000	0.297951000
H	-1.893932000	4.468274000	0.264330000
C	-2.101115000	-0.163861000	-0.043576000
C	-3.107242000	-0.335690000	-0.995975000
C	-1.861896000	-1.170472000	0.970031000
C	-3.905898000	-1.482350000	-1.057811000
H	-3.258011000	0.458396000	-1.726737000
C	-2.694487000	-2.339574000	0.863855000
C	-3.672839000	-2.486088000	-0.106624000
H	-4.670301000	-1.590590000	-1.820355000
H	-2.542897000	-3.130692000	1.597394000
H	-4.267971000	-3.397476000	-0.123075000
C	0.777477000	-0.095170000	-0.536817000
H	0.173739000	-0.904372000	-0.940005000
C	2.166726000	-0.394426000	-0.331886000
C	3.012985000	0.336840000	0.537962000
C	2.719535000	-1.528541000	-0.978413000
C	4.341597000	-0.030718000	0.716875000
H	2.612483000	1.171032000	1.104605000
C	4.049015000	-1.885344000	-0.800191000
H	2.081211000	-2.119840000	-1.630462000
C	4.874116000	-1.134188000	0.043940000
H	4.965728000	0.541457000	1.397506000
H	4.446640000	-2.754570000	-1.316322000
H	5.913310000	-1.414188000	0.186729000
N	-0.944115000	-0.988874000	1.930560000
H	-0.958573000	-1.808598000	2.539900000



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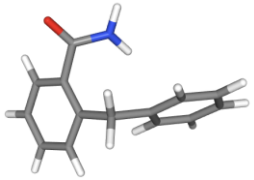
symmetry c1

C	-0.350888000	3.421088000	-0.070414000
C	-0.867595000	2.115591000	0.101823000
C	-0.039352000	1.009300000	0.146882000
C	1.387399000	1.143982000	0.006543000
C	1.894061000	2.480791000	-0.136741000
C	1.042342000	3.573616000	-0.175922000
H	-1.014520000	4.278905000	-0.104828000
H	-1.940804000	1.979921000	0.220743000
H	2.963293000	2.643489000	-0.239591000
H	1.466834000	4.568463000	-0.297722000
C	2.220858000	-0.017899000	0.036314000
C	3.650150000	0.007711000	0.126689000
C	1.616871000	-1.316209000	-0.100627000
C	4.405516000	-1.161571000	0.098027000
H	4.160856000	0.960583000	0.233707000
C	2.380784000	-2.471023000	-0.114870000
C	3.792891000	-2.414447000	-0.021941000
H	5.488749000	-1.094264000	0.174626000
H	1.875161000	-3.429831000	-0.219865000
H	4.379954000	-3.327249000	-0.041914000
C	-0.548998000	-0.382641000	0.479284000
H	-0.373663000	-0.551814000	1.558530000
C	-2.025912000	-0.576731000	0.220413000
C	-2.512481000	-0.673146000	-1.088848000

C	-2.927953000	-0.636578000	1.284364000
C	-3.877589000	-0.825115000	-1.326368000
H	-1.814377000	-0.626867000	-1.920629000
C	-4.297475000	-0.782565000	1.049966000
H	-2.555551000	-0.564804000	2.303805000
C	-4.774815000	-0.877752000	-0.256553000
H	-4.243339000	-0.899282000	-2.346549000
H	-4.987750000	-0.824799000	1.887560000
H	-5.838585000	-0.994043000	-0.442359000
N	0.224202000	-1.359539000	-0.304460000
H	-0.142551000	-2.300041000	-0.182415000

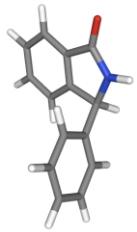


Charge 0
Multiplicity 1
Stoichiometry C14H13NO
Electronic Energy (Eh) -671.095843776
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	2.892342	-1.210623	-1.171683
C	1.689006	-1.118378	-0.468020
C	1.552618	-0.222783	0.597718
C	2.645697	0.585210	0.936816
C	3.847482	0.494721	0.237043
C	3.975544	-0.406349	-0.822064
H	2.978305	-1.912206	-1.996470
H	0.852781	-1.748910	-0.758214
H	4.682135	1.132155	0.514470

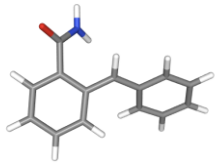
H	4.909640	-0.476193	-1.371402
C	0.270393	-0.111098	1.408807
H	0.362546	-0.766384	2.283290
H	0.190773	0.910344	1.793289
C	-0.994053	-0.497873	0.671996
C	-1.440943	-1.823361	0.752421
C	-1.767930	0.416100	-0.064782
C	-2.603905	-2.242469	0.111408
H	-0.861517	-2.534299	1.336932
C	-2.952850	0.000733	-0.683406
C	-3.366607	-1.325408	-0.612061
H	-2.919155	-3.278934	0.186579
H	-3.545454	0.731786	-1.225648
H	-4.279955	-1.638202	-1.108530
H	2.547707	1.296511	1.753999
C	-1.428404	1.878871	-0.198065
O	-2.272365	2.745218	0.025501
N	-0.172951	2.173817	-0.595389
H	0.478490	1.458500	-0.889724
H	0.082935	3.143611	-0.731628



Charge 0
Multiplicity 1
Stoichiometry C14H11NO
Electronic Energy (Eh) -669.897532149
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	3.719273	-0.742142	-0.500963
C	2.486278	-0.477352	-1.100892
C	1.492854	0.205254	-0.397389
C	1.741905	0.625915	0.912856
C	2.973160	0.366100	1.510297
C	3.964847	-0.320146	0.804650
H	4.487377	-1.271504	-1.057057
H	2.295623	-0.799554	-2.121814
H	3.160323	0.698106	2.527262
H	4.924661	-0.520468	1.271385
C	0.138058	0.439576	-1.041202
H	0.233187	0.300501	-2.125075
C	-0.940322	-0.476214	-0.491638
C	-0.987094	-1.864837	-0.453419
C	-1.976960	0.284885	0.039062
C	-2.108606	-2.464209	0.124531
H	-0.178250	-2.467957	-0.857239
C	-3.097511	-0.301219	0.618222
C	-3.153192	-1.694126	0.654483
H	-2.172465	-3.547495	0.166261
H	-3.897735	0.308893	1.027170
H	-4.010809	-2.189974	1.098457
H	0.970037	1.160227	1.462190
C	-1.644216	1.728416	-0.134451
N	-0.427407	1.749777	-0.745475
O	-2.313375	2.700949	0.194992
H	0.036060	2.613782	-0.998031

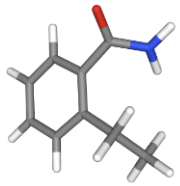


Charge 0
Multiplicity 2
Stoichiometry C14H12NO
Electronic Energy (Eh) -670.452844506
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	3.574266	-0.988448	-0.827554
C	2.211543	-0.804779	-0.627574
C	1.734987	0.240465	0.201765
C	2.695288	1.104593	0.785392
C	4.054736	0.910631	0.585402
C	4.505231	-0.142407	-0.217651
H	3.914812	-1.791958	-1.474187
H	1.508708	-1.450396	-1.143844
H	4.768741	1.582451	1.052809
H	5.568360	-0.293549	-0.377407
C	0.344899	0.513045	0.433123
H	0.122066	1.496983	0.836251
C	-0.776305	-0.374630	0.223520
C	-0.635183	-1.777664	0.342732
C	-2.087951	0.130675	0.008650
C	-1.725760	-2.630171	0.240149
H	0.340054	-2.193066	0.573341
C	-3.178062	-0.736052	-0.068528
C	-3.007277	-2.114777	0.031404
H	-1.578729	-3.700925	0.345724
H	-4.167536	-0.315788	-0.222060

H	-3.863147	-2.777891	-0.043152
H	2.348742	1.926302	1.407265
C	-2.402782	1.593371	-0.169726
O	-3.380640	2.101443	0.377053
N	-1.590975	2.291558	-0.992519
H	-1.791314	3.267535	-1.169130
H	-0.834589	1.854746	-1.501014

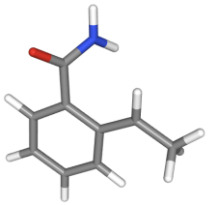


Charge 0
Multiplicity 1
Stoichiometry C9H11NO
Electronic Energy (Eh) -479.417331875
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	-0.540262	1.798947	0.688423
H	-0.121025	2.296858	1.569977
H	-1.520598	1.412825	0.979121
C	0.387680	0.665005	0.306304
C	1.766463	0.921036	0.259985
C	-0.045727	-0.640948	0.023599
C	2.684663	-0.072531	-0.063779
H	2.118732	1.922890	0.496124
C	0.880656	-1.649091	-0.274564
C	2.240964	-1.369179	-0.332461
H	3.745221	0.159722	-0.093943
H	0.519452	-2.655419	-0.467440

H	2.949317	-2.154548	-0.577371
C	-1.493263	-1.058954	0.062251
O	-1.866409	-1.996988	0.764537
N	-2.334146	-0.367740	-0.735981
H	-1.996672	0.327261	-1.386686
H	-3.310862	-0.630431	-0.771392
C	-0.698195	2.834023	-0.430904
H	-1.361921	3.644109	-0.114136
H	0.269634	3.272050	-0.694978
H	-1.118847	2.384921	-1.336825

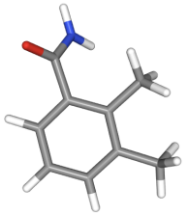


Charge 0
Multiplicity 2
Stoichiometry C9H10NO
Electronic Energy (Eh) -478.768607869
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	-0.717967	1.752113	-0.189065
H	0.213732	2.279795	-0.356549
C	-0.685546	0.339205	-0.033761
C	-1.899068	-0.399129	0.054818
C	0.530153	-0.414355	-0.021699
C	-1.907628	-1.782786	0.128036
H	-2.842592	0.137283	0.048210
C	0.500254	-1.805447	0.022140
C	-0.706828	-2.500904	0.104225

H	-2.854953	-2.310023	0.194171
H	1.441671	-2.347249	0.007200
H	-0.710122	-3.584994	0.153056
C	1.898826	0.210773	-0.053081
O	2.765865	-0.189906	-0.828535
N	2.130554	1.192289	0.845564
H	1.443178	1.456451	1.537778
H	3.050558	1.610888	0.891963
C	-1.981603	2.545022	-0.201966
H	-1.765500	3.613189	-0.263174
H	-2.616574	2.281657	-1.059718
H	-2.583745	2.369279	0.698499

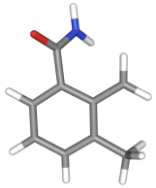


Charge 0
Multiplicity 1
Stoichiometry C9H11NO
Electronic Energy (Eh) -479.421009786
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	0.146308	-2.068247	-0.285881
H	0.865774	-2.505852	-0.983000
H	-0.854324	-2.245616	-0.682218
C	0.428593	-0.597383	-0.092085
C	1.768696	-0.161201	-0.007939
C	-0.594842	0.362748	-0.022308

C	2.045176	1.201422	0.125906
C	-0.299163	1.726574	0.083987
C	1.021786	2.148121	0.164236
H	3.081224	1.523804	0.194497
H	-1.113861	2.444178	0.114283
H	1.255746	3.204105	0.259752
C	-2.059098	0.008493	-0.057577
O	-2.834812	0.563926	-0.833972
N	-2.466776	-0.910019	0.844019
H	-1.830031	-1.321559	1.511960
H	-3.441805	-1.178807	0.874014
H	0.236759	-2.618713	0.658847
C	2.901699	-1.153819	-0.064913
H	2.771254	-1.952500	0.673011
H	2.964693	-1.631970	-1.049090
H	3.855569	-0.658587	0.131031

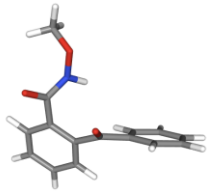


Charge 0
Multiplicity 2
Stoichiometry C9H10NO
Electronic Energy (Eh) -478.767396395
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	0.170128	-2.021323	-0.319393
H	-0.836259	-2.387538	-0.475163
C	0.435728	-0.653270	-0.100332

C	1.792151	-0.190011	-0.002417
C	-0.607821	0.324793	-0.026606
C	2.045986	1.168694	0.131339
C	-0.312272	1.679074	0.076942
C	1.011075	2.110023	0.163138
H	3.077380	1.504253	0.203882
H	-1.127680	2.395725	0.107439
H	1.236682	3.167186	0.260618
C	-2.070571	-0.028873	-0.053776
O	-2.853609	0.552439	-0.803655
N	-2.472677	-0.975021	0.822101
H	-1.836484	-1.388786	1.489507
H	-3.453498	-1.218734	0.871135
H	0.975426	-2.741912	-0.377682
C	2.935630	-1.165840	-0.063176
H	2.855057	-1.926131	0.721578
H	2.959592	-1.693361	-1.023439
H	3.887188	-0.644660	0.062351

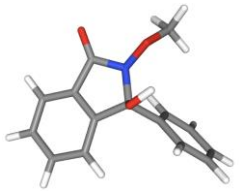


Charge 0
Multiplicity 1
Stoichiometry C15H13NO3
Electronic Energy (Eh) -859.509647817
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	3.552357	0.141129	-1.527621

C	2.294079	-0.149110	-1.002349
C	1.996860	0.185920	0.324254
C	2.966428	0.809227	1.120315
C	4.226774	1.080545	0.598716
C	4.519370	0.748410	-0.726886
H	3.776744	-0.108332	-2.559967
H	1.542296	-0.618810	-1.630080
H	4.981384	1.551442	1.221133
H	5.502256	0.964927	-1.134890
C	-0.225148	-1.134628	0.325035
C	0.313043	-2.406525	0.102425
C	-1.600005	-0.923463	0.133241
C	-0.508379	-3.460332	-0.291689
H	1.373420	-2.577048	0.266167
C	-2.416637	-1.981690	-0.266097
C	-1.873777	-3.247650	-0.477684
H	-0.082451	-4.446246	-0.448874
H	-3.477649	-1.806116	-0.417998
H	-2.516094	-4.065200	-0.789716
H	2.722411	1.069011	2.145968
C	-2.253127	0.420511	0.324581
O	-3.212314	0.589662	1.063865
N	-1.746049	1.389991	-0.478544
H	-0.896836	1.275286	-1.022845
C	-3.214507	3.042390	-1.117834
H	-2.927312	2.947813	-2.169834
H	-4.079205	2.409431	-0.900403
H	-3.444993	4.083512	-0.885948
O	-2.116300	2.695992	-0.267410
C	0.641564	-0.051591	0.904169
O	0.232988	0.608288	1.846250

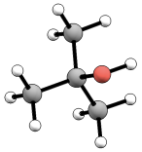


Charge 0
Multiplicity 1
Stoichiometry C15H13NO3
Electronic Energy (Eh) -859.520983928
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	2.933080	-0.646089	-1.691072
C	1.717727	-0.190662	-1.188211
C	1.429436	-0.312319	0.175697
C	2.361803	-0.906175	1.026738
C	3.582617	-1.359957	0.520924
C	3.870838	-1.230366	-0.835615
H	3.150595	-0.543192	-2.749952
H	0.989931	0.268919	-1.852461
H	4.304878	-1.815692	1.191587
H	4.820142	-1.582797	-1.227739
C	-1.073028	-0.771044	0.301866
C	-1.178236	-2.147414	0.429569
C	-2.110083	-0.015830	-0.237408
C	-2.369987	-2.746744	0.010733
H	-0.366697	-2.740512	0.842198
C	-3.296007	-0.601974	-0.662152
C	-3.414918	-1.986162	-0.528267
H	-2.487882	-3.822110	0.103212
H	-4.098193	-0.003073	-1.082701
H	-4.326132	-2.482104	-0.847629

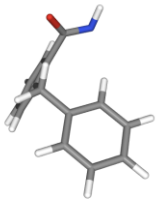
H	2.136941	-1.017855	2.082592
C	-1.706477	1.416672	-0.240303
O	-2.365517	2.406882	-0.488195
N	-0.357964	1.398359	0.082837
C	0.998082	3.218623	-0.368640
H	1.850141	2.604850	-0.672793
H	0.383602	3.476879	-1.234831
H	1.347634	4.126253	0.125789
O	0.206404	2.536481	0.614291
C	0.074708	0.138440	0.708182
O	0.060625	0.258346	2.106697
H	0.671365	0.974249	2.348289



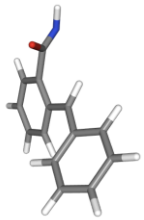
# of imaginary frequencies: 0
E = -233.583655796
symmetry c1

C	0.007620000	0.000000000	0.015772000
C	-0.665552000	1.256740000	-0.532878000
H	-0.189344000	2.153030000	-0.122641000
H	-0.594001000	1.292787000	-1.624735000
H	-1.728143000	1.273724000	-0.262904000
C	1.496263000	-0.000089000	-0.303042000
H	1.976583000	0.888745000	0.118553000
H	1.976491000	-0.888931000	0.118638000
H	1.655544000	-0.000151000	-1.385672000
C	-0.665705000	-1.256660000	-0.532880000
H	-0.189576000	-2.153011000	-0.122684000
H	-1.728285000	-1.273537000	-0.262862000
H	-0.594205000	-1.292689000	-1.624741000
O	-0.076089000	0.000005000	1.449110000

H -1.012106000 0.000049000 1.694340000



Charge -1
Multiplicity 1
Stoichiometry C14H12NO(-1)
Electronic Energy (Eh) -670.594658717
Number of Imaginary Frequencies 0

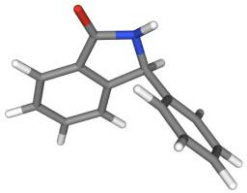


Charge -1
Multiplicity 2
Stoichiometry C14H11NO(-1)
Electronic Energy (Eh) -669.952241577
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	-4.019175	-0.975531	-0.525965
C	-2.653702	-1.178353	-0.669684
C	-1.710587	-0.255904	-0.149421
C	-2.216754	0.859066	0.563962
C	-3.585686	1.051658	0.710027
C	-4.497447	0.146499	0.159302

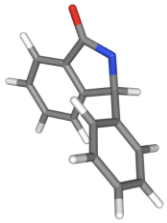
H	-4.716681	-1.694815	-0.945611
H	-2.288137	-2.054758	-1.199296
H	-3.945955	1.910408	1.269439
H	-5.565219	0.305355	0.274752
C	-0.312698	-0.539677	-0.319097
H	-0.071923	-1.567711	-0.573192
C	0.804231	0.362229	-0.186304
C	0.672385	1.760004	-0.364025
C	2.109465	-0.162805	0.030596
C	1.771101	2.607509	-0.287501
H	-0.297987	2.177602	-0.611877
C	3.200228	0.702696	0.092051
C	3.043271	2.083462	-0.048225
H	1.637028	3.675622	-0.432497
H	4.189012	0.283669	0.258103
H	3.905801	2.740422	0.013901
H	-1.531715	1.553763	1.038224
C	2.328375	-1.651715	0.255656
O	1.663453	-2.191379	1.184741
N	3.214266	-2.208516	-0.551157
H	3.280235	-3.193734	-0.280011



Charge -1
Multiplicity 2
Stoichiometry C14H11NO(-1)
Electronic Energy (Eh) -669.960117547
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	3.615721	-0.958634	-0.282323
C	2.426207	-0.735955	-0.978344
C	1.449718	0.122290	-0.465185
C	1.686708	0.765258	0.755673
C	2.873855	0.544212	1.452682
C	3.842295	-0.319574	0.936578
H	4.366889	-1.625227	-0.696480
H	2.254686	-1.230538	-1.932013
H	3.044233	1.048822	2.399558
H	4.768225	-0.487918	1.478591
C	0.135393	0.309920	-1.209164
H	0.296274	0.019872	-2.254676
C	-0.977304	-0.517249	-0.573812
C	-1.139244	-1.878339	-0.533258
C	-1.877234	0.379367	0.080943
C	-2.244624	-2.423345	0.189886
H	-0.432056	-2.537034	-1.035608
C	-2.979374	-0.168199	0.817053
C	-3.131993	-1.547458	0.851365
H	-2.397970	-3.496800	0.232084
H	-3.679440	0.483230	1.333533
H	-3.968069	-1.969937	1.406295
H	0.938026	1.440501	1.164190
C	-1.493084	1.720783	-0.191449
N	-0.405746	1.670596	-1.119049
O	-1.968532	2.810850	0.205128
H	0.275436	2.415598	-1.007014

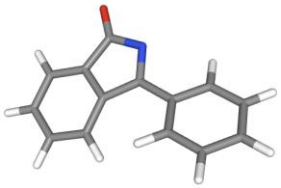


Charge -1
Multiplicity 1
Stoichiometry C14H10NO(-1)
Electronic Energy (Eh) -669.398080987
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	3.697758	-0.735764	-0.509485
C	2.463675	-0.460133	-1.104293
C	1.475847	0.241002	-0.408082
C	1.745084	0.667887	0.897574
C	2.974106	0.395369	1.494562
C	3.956239	-0.308769	0.792031
H	4.456726	-1.278239	-1.066307
H	2.266782	-0.789736	-2.122271
H	3.169315	0.733179	2.508573
H	4.915655	-0.517593	1.256258
C	0.114836	0.495014	-1.037636
H	0.224964	0.325970	-2.120256
C	-0.930662	-0.466695	-0.490998
C	-0.975219	-1.856138	-0.435246
C	-1.965258	0.304826	0.023294
C	-2.097562	-2.455140	0.147004
H	-0.164505	-2.465892	-0.828391
C	-3.085056	-0.281465	0.605410
C	-3.142840	-1.676798	0.662161

H	-2.160216	-3.538355	0.203230
H	-3.889427	0.331539	1.004345
H	-4.002793	-2.166834	1.110161
H	0.983223	1.221993	1.440950
C	-1.596272	1.755930	-0.185325
N	-0.406988	1.834094	-0.781709
O	-2.344857	2.698819	0.172480

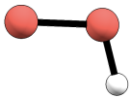


Charge -1
Multiplicity 2
Stoichiometry C14H9NO(-1)
Electronic Energy (Eh) -668.788434504
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

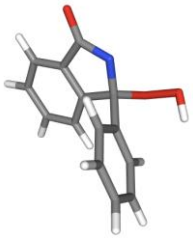
C	3.405418	-1.409047	0.405250
C	2.044309	-1.114597	0.437011
C	1.566716	0.146654	0.029587
C	2.512227	1.105047	-0.390639
C	3.870355	0.806811	-0.419895
C	4.327819	-0.454331	-0.027022
H	3.747728	-2.387138	0.731733
H	1.352634	-1.858908	0.816644
H	4.577417	1.560592	-0.755283
H	5.388264	-0.686587	-0.051346
C	0.146492	0.484443	0.056232
C	-0.986923	-0.425938	-0.009444

C	-1.153918	-1.814256	-0.170483
C	-2.131537	0.405857	0.046900
C	-2.445642	-2.328208	-0.232730
H	-0.308795	-2.488746	-0.262529
C	-3.422718	-0.114621	-0.014241
C	-3.577205	-1.492705	-0.147054
H	-2.584491	-3.398728	-0.356394
H	-4.286823	0.543798	0.032270
H	-4.570639	-1.928696	-0.197237
H	2.161357	2.083350	-0.704265
C	-1.639159	1.796706	0.135394
N	-0.261168	1.770126	0.125603
O	-2.343235	2.827413	0.209250



HO_2 radical
# of imaginary frequencies: 0
E = -150.860925779
symmetry cs

O	0.055418000	0.709676000	0.000000000
O	0.055418000	-0.600185000	0.000000000
H	-0.886686000	-0.875921000	0.000000000



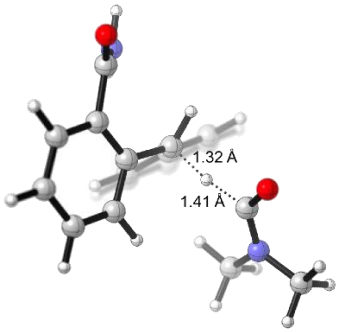
Charge -1
Multiplicity 1

Stoichiometry C14H10NO3(-1)
Electronic Energy (Eh) -819.7134128459999
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	3.372476	-1.291661	-0.077698
C	2.175281	-0.830875	-0.624577
C	1.395471	0.113540	0.056193
C	1.833624	0.580914	1.297036
C	3.027669	0.114621	1.849645
C	3.802241	-0.820714	1.163923
H	3.967980	-2.019762	-0.620971
H	1.842967	-1.211404	-1.587852
H	3.354626	0.487798	2.816062
H	4.733632	-1.179416	1.591998
C	0.060127	0.573953	-0.529002
C	-1.045496	-0.456742	-0.287133
C	-1.138824	-1.807719	-0.594010
C	-2.076215	0.213010	0.354584
C	-2.313325	-2.477781	-0.228872
H	-0.335110	-2.338711	-1.097352
C	-3.244154	-0.441988	0.722573
C	-3.352717	-1.804593	0.422935
H	-2.419105	-3.535365	-0.453028
H	-4.047119	0.089228	1.226707
H	-4.251373	-2.349595	0.697844
H	1.233333	1.315694	1.823998
C	-1.640012	1.655547	0.514441
N	-0.412678	1.815216	0.011677
O	-2.365890	2.516400	1.054952
O	0.167062	0.592356	-1.977283
O	1.161296	1.531751	-2.372954

H	1.972297	0.993899	-2.357078

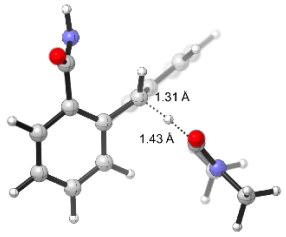


Charge 0
Multiplicity 2
Stoichiometry C17H19N2O2
Electronic Energy (Eh) -918.842500867
Number of Imaginary Frequencies 1

Molecular Geometry in Cartesian Coordinates

C	1.326162	-3.028000	1.561011
C	0.536327	-1.947088	1.167422
C	0.666458	-1.397065	-0.117378
C	1.607927	-1.965236	-0.995269
C	2.396583	-3.040730	-0.599870
C	2.261338	-3.577242	0.684040
H	1.207374	-3.442018	2.558263
H	-0.187140	-1.531853	1.863624
H	3.118526	-3.463000	-1.293052
H	2.875941	-4.417050	0.993647
C	-0.096748	-0.209436	-0.571420
H	0.791092	0.766926	-0.641013
H	-0.359670	-0.267664	-1.630211
C	-1.181340	0.354921	0.284315

C	-0.832224	1.095630	1.425211
C	-2.547344	0.245509	-0.039018
C	-1.797733	1.701439	2.223085
H	0.220993	1.206397	1.675456
C	-3.513629	0.881957	0.747753
C	-3.147411	1.599799	1.881548
H	-1.496552	2.264872	3.101204
H	-4.558704	0.796518	0.464534
H	-3.906804	2.078647	2.491827
H	1.716906	-1.547938	-1.994232
C	1.578498	1.898409	-0.944358
O	1.171876	2.612202	-1.839822
N	2.692163	2.019953	-0.221163
C	3.051412	1.082635	0.831559
H	3.994290	0.584601	0.582563
H	3.173169	1.619907	1.777462
H	2.271651	0.329834	0.947579
C	3.637752	3.104160	-0.471009
H	3.768520	3.694657	0.440960
H	4.605613	2.687426	-0.767153
H	3.254147	3.741132	-1.267091
C	-3.060061	-0.542301	-1.216399
O	-3.923037	-0.081914	-1.961790
N	-2.549365	-1.782468	-1.373599
H	-2.886133	-2.362340	-2.131392
H	-1.909327	-2.187920	-0.704085

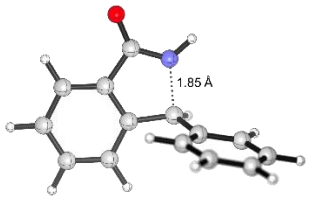


Charge -1
Multiplicity 2
Stoichiometry C17H18N2O2(-1)
Electronic Energy (Eh) -918.340155694
Number of Imaginary Frequencies 1

Molecular Geometry in Cartesian Coordinates

C	-1.767120	2.933987	1.503289
C	-0.842949	1.953068	1.141245
C	-0.835557	1.418618	-0.156637
C	-1.781556	1.903304	-1.078772
C	-2.704495	2.879412	-0.716457
C	-2.704736	3.399163	0.581302
H	-1.750781	3.337433	2.511932
H	-0.117373	1.607648	1.872049
H	-3.425008	3.237277	-1.446580
H	-3.423565	4.161280	0.866825
C	0.076244	0.329934	-0.586618
H	-0.688446	-0.727976	-0.717465
H	0.398921	0.454984	-1.621906
C	1.166053	-0.143950	0.313494
C	0.823702	-0.868003	1.469072
C	2.528054	0.033753	0.004647
C	1.796346	-1.386437	2.318403
H	-0.229489	-1.030298	1.694311
C	3.498744	-0.517875	0.850704
C	3.146366	-1.209533	2.006745
H	1.504275	-1.936355	3.208429
H	4.546198	-0.391205	0.589679
H	3.916776	-1.615227	2.656343
H	-1.785808	1.500893	-2.089772
C	-1.238735	-2.020076	-0.977772

O	-0.640273	-2.706151	-1.783403
N	-2.324336	-2.333889	-0.267592
C	-2.938611	-1.410550	0.672095
H	-3.977746	-1.222930	0.382653
H	-2.925132	-1.838634	1.679927
H	-2.395370	-0.465098	0.677911
C	-2.947588	-3.648266	-0.384895
H	-2.896092	-4.170199	0.576210
H	-3.997654	-3.533104	-0.670796
H	-2.423534	-4.228026	-1.144119
C	3.009918	0.798099	-1.220492
O	3.818196	0.191245	-1.979079
N	2.548904	2.031278	-1.330520
H	2.969998	2.429181	-2.175120

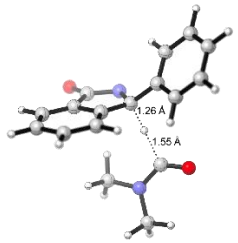


Charge -1
Multiplicity 2
Stoichiometry C14H11NO(-1)
Electronic Energy (Eh) -669.923449958
Number of Imaginary Frequencies 1

Molecular Geometry in Cartesian Coordinates

C	2.861754	-0.740288	1.499648
C	1.627274	-0.526548	0.912276
C	1.518395	-0.027101	-0.434855
C	2.754610	0.289950	-1.096949
C	3.976664	0.070332	-0.493444

C	4.063984	-0.459393	0.816985
H	2.901666	-1.132138	2.514454
H	0.721420	-0.748596	1.472965
H	4.887963	0.308023	-1.038783
H	5.026695	-0.627088	1.288782
C	0.262222	0.309478	-1.028132
H	0.310976	0.498357	-2.101038
C	-0.984459	-0.400582	-0.581051
C	-1.211231	-1.771452	-0.712527
C	-1.961296	0.402382	0.014708
C	-2.417727	-2.314279	-0.264198
H	-0.453834	-2.411215	-1.159173
C	-3.162450	-0.132706	0.472460
C	-3.392541	-1.500329	0.323347
H	-2.598526	-3.380300	-0.368892
H	-3.900209	0.515150	0.938160
H	-4.325207	-1.937158	0.668219
H	2.715675	0.698817	-2.105727
C	-1.523688	1.832535	0.149402
N	-0.393557	1.973957	-0.543387
O	-2.144435	2.673426	0.828375
H	0.154706	2.819045	-0.398270



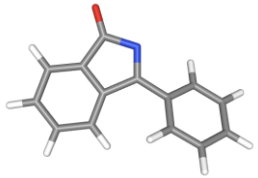
Charge -1
Multiplicity 2
Stoichiometry C17H16N2O2(-1)
Electronic Energy (Eh) -917.152966363

Number of Imaginary Frequencies 1

Molecular Geometry in Cartesian Coordinates

C	3.657153	0.628460	-1.189482
C	2.304273	0.566006	-0.861974
C	1.853157	-0.264854	0.175590
C	2.797643	-1.011474	0.891619
C	4.153389	-0.946042	0.566505
C	4.589195	-0.129635	-0.477065
H	3.985851	1.277548	-1.996357
H	1.593565	1.185345	-1.401852
H	4.870269	-1.536423	1.130646
H	5.644271	-0.078227	-0.729622
C	0.390288	-0.341086	0.508749
H	0.064859	0.876219	0.573092
C	-0.539963	-0.881989	-0.544473
C	-0.686576	-0.635921	-1.909390
C	-1.428931	-1.727805	0.120492
C	-1.737300	-1.265471	-2.584885
H	-0.013059	0.023192	-2.449850
C	-2.478403	-2.352583	-0.543931
C	-2.626912	-2.114230	-1.912813
H	-1.867664	-1.090755	-3.649295
H	-3.164222	-3.004366	-0.008437
H	-3.436249	-2.585649	-2.463002
H	2.455988	-1.646496	1.702778
C	-1.026760	-1.749653	1.570678
N	0.050882	-0.967344	1.742374
O	-1.638196	-2.409450	2.442663
C	-0.302123	2.377234	0.442276
O	0.566602	3.191446	0.193990
N	-1.625302	2.558725	0.418638

C	-2.552059	1.511949	0.819673
H	-3.280286	1.928366	1.522607
H	-3.087809	1.112087	-0.049118
H	-2.007322	0.709705	1.318949
C	-2.212358	3.833469	0.017560
H	-2.967803	3.657597	-0.754478
H	-2.688911	4.317004	0.876739
H	-1.430075	4.480969	-0.377879

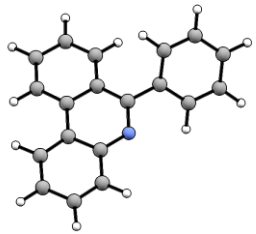


Charge 0
Multiplicity 1
Stoichiometry C14H9NO
Electronic Energy (Eh) -668.661461561
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	3.365457	-1.354999	0.567712
C	2.008947	-1.038638	0.581964
C	1.567332	0.170852	0.027825
C	2.495653	1.057297	-0.539037
C	3.846019	0.727467	-0.566815
C	4.282390	-0.478507	-0.012620
H	3.705767	-2.285160	1.011715
H	1.305146	-1.712866	1.058668
H	4.559532	1.409591	-1.018459
H	5.337964	-0.732659	-0.030766
C	0.148183	0.544663	0.062065

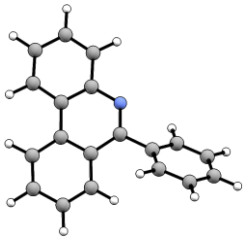
C	-1.004685	-0.411659	-0.027711
C	-1.107056	-1.779695	-0.227865
C	-2.146731	0.384307	0.060845
C	-2.398011	-2.327521	-0.297933
H	-0.237998	-2.418028	-0.344448
C	-3.422347	-0.139916	-0.011713
C	-3.534955	-1.527875	-0.185060
H	-2.511175	-3.396340	-0.450234
H	-4.302005	0.493316	0.054239
H	-4.518024	-1.984028	-0.244943
H	2.145326	1.991961	-0.966143
C	-1.658274	1.795477	0.177123
N	-0.227933	1.782716	0.160901
O	-2.317566	2.803460	0.268925



# of imaginary frequencies: 0
E = -786.446242950
symmetry c1

C	0.017613000	3.488678000	-0.322312000
C	0.671132000	2.267874000	-0.290329000
C	-0.030948000	1.043199000	-0.084443000
C	-1.461381000	1.119213000	-0.000125000
C	-2.092689000	2.369276000	-0.033050000
C	-1.373304000	3.556141000	-0.171803000
H	0.593572000	4.396989000	-0.480245000
H	1.742428000	2.249113000	-0.452074000
H	-3.174535000	2.425881000	0.036940000

H	-1.889394000	4.510950000	-0.191034000
C	-2.214266000	-0.140440000	0.078074000
C	-3.610413000	-0.203960000	0.200883000
C	-1.464974000	-1.356276000	-0.010732000
C	-4.295224000	-1.416960000	0.217052000
H	-4.185288000	0.713585000	0.286396000
C	-2.189974000	-2.584770000	-0.009821000
C	-3.567230000	-2.613436000	0.102047000
H	-5.376089000	-1.433359000	0.315684000
H	-1.618277000	-3.506270000	-0.088939000
H	-4.087339000	-3.568167000	0.106393000
C	0.603167000	-0.245038000	-0.038617000
C	2.063021000	-0.420088000	0.002967000
C	2.924680000	0.427981000	0.734671000
C	2.656494000	-1.531014000	-0.639228000
C	4.296169000	0.196414000	0.792146000
H	2.509954000	1.256878000	1.300314000
C	4.028609000	-1.756853000	-0.585524000
H	2.017959000	-2.212965000	-1.191926000
C	4.865586000	-0.892386000	0.125541000
H	4.923839000	0.863981000	1.376820000
H	4.449408000	-2.614235000	-1.104742000
H	5.935930000	-1.069666000	0.169420000
N	-0.114084000	-1.408294000	-0.069628000

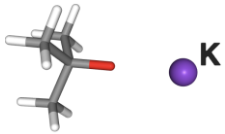


# of imaginary frequencies: 0
E = -786.3641596

symmetry c1

C	-0.118194000	3.433733000	-0.286055000
C	-0.729352000	2.201614000	-0.225860000
C	0.038223000	1.026186000	-0.071666000
C	1.448043000	1.117154000	-0.019426000
C	2.049917000	2.391718000	-0.073044000
C	1.280345000	3.527427000	-0.196411000
H	-0.714581000	4.329958000	-0.409461000
H	-1.805922000	2.134467000	-0.313397000
H	3.127064000	2.487634000	-0.030332000
H	1.759537000	4.498745000	-0.240147000
C	2.214015000	-0.113321000	0.051618000
C	3.622620000	-0.158065000	0.115231000
C	1.501126000	-1.330977000	0.037216000
C	4.289206000	-1.364041000	0.151672000
H	4.196249000	0.759848000	0.136110000
C	2.198962000	-2.556195000	0.071484000
C	3.573863000	-2.574503000	0.126178000
H	5.371890000	-1.378204000	0.200037000
H	1.620413000	-3.473133000	0.058421000
H	4.106014000	-3.518283000	0.153810000
C	-0.570168000	-0.293794000	-0.011972000
C	-2.053070000	-0.458670000	0.013344000
C	-2.661679000	-1.318751000	-0.903483000
C	-2.837021000	0.183455000	0.975468000
C	-4.037261000	-1.522559000	-0.869090000
H	-2.052074000	-1.821786000	-1.645876000
C	-4.210716000	-0.033501000	1.018079000
H	-2.370311000	0.839985000	1.701986000
C	-4.814189000	-0.881482000	0.092659000
H	-4.501673000	-2.184211000	-1.591414000
H	-4.808823000	0.459122000	1.776135000
H	-5.885483000	-1.044601000	0.123030000

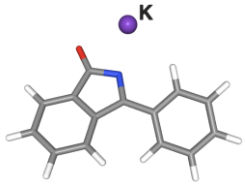
N 0.121381000 -1.391729000 0.015062000



Charge 0
Multiplicity 1
Stoichiometry C4H9KO
Electronic Energy (Eh) -832.891286275
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	-1.100135	0.000040	0.000150
C	-1.647186	-1.292465	0.643791
H	-1.281551	-1.374161	1.674812
H	-2.744637	-1.332002	0.663463
H	-1.281289	-2.164613	0.088038
C	-1.648198	1.203763	0.796617
H	-1.283670	1.159071	1.830276
H	-1.282077	2.137302	0.351859
H	-2.745671	1.240276	0.819560
C	-1.646785	0.088025	-1.441102
H	-1.281733	1.005675	-1.918594
H	-1.280116	-0.763894	-2.026896
H	-2.744239	0.089586	-1.485392
O	0.272007	0.000883	0.000680
K	2.631724	-0.000025	0.000037

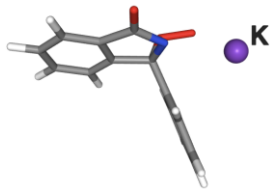


Charge 0
Multiplicity 2
Stoichiometry C14H9KNO
Electronic Energy (Eh) -1268.61654961
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	3.874735	0.503561	0.502599
C	2.493203	0.663231	0.490059
C	1.650760	-0.354716	0.000296
C	2.248978	-1.529992	-0.492988
C	3.632984	-1.685424	-0.478758
C	4.454331	-0.673970	0.022402
H	4.503509	1.298637	0.893482
H	2.046982	1.574729	0.875811
H	4.072216	-2.597778	-0.871984
H	5.532871	-0.798822	0.033735
C	0.203947	-0.164309	-0.007993
C	-0.833533	-1.182445	0.017732
C	-0.851629	-2.585376	0.116790
C	-2.059059	-0.473401	-0.000948
C	-2.082234	-3.232963	0.153726
H	0.061107	-3.168685	0.180446
C	-3.289890	-1.126987	0.035278
C	-3.295311	-2.517395	0.104635
H	-2.108645	-4.316391	0.228917
H	-4.218773	-0.562659	0.017940

H	-4.236740	-3.057825	0.133634
H	1.632981	-2.310997	-0.925980
C	-1.708688	0.953619	-0.026640
N	-0.338068	1.074930	-0.018445
O	-2.498355	1.935143	-0.055444
K	-0.608619	3.756502	-0.137393

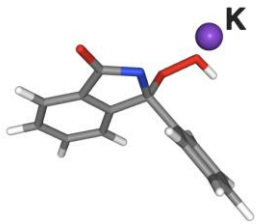


Charge 0
Multiplicity 2
Stoichiometry C14H9KNO3
Electronic Energy (Eh) -1418.9003511300002
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	-2.678618	-2.441111	0.267086
C	-1.636956	-1.653011	0.754019
C	-1.051016	-0.676576	-0.060574
C	-1.515336	-0.511453	-1.369648
C	-2.559403	-1.300922	-1.854948
C	-3.145097	-2.265688	-1.036518
H	-3.128812	-3.191121	0.910483
H	-1.288425	-1.797834	1.772041
H	-2.911422	-1.160032	-2.872487
H	-3.959422	-2.878459	-1.411253
C	0.120575	0.170133	0.416506
C	1.479522	-0.494431	0.268619

C	1.942711	-1.747428	0.642289
C	2.298956	0.430541	-0.361020
C	3.281099	-2.048554	0.360881
H	1.299290	-2.474792	1.130691
C	3.625608	0.140992	-0.646355
C	4.110530	-1.118249	-0.275137
H	3.681190	-3.019646	0.636883
H	4.264014	0.866763	-1.142495
H	5.143087	-1.381731	-0.484771
H	-1.048532	0.233342	-2.009067
C	1.463050	1.666429	-0.618303
N	0.204399	1.456331	-0.178991
O	1.904226	2.684345	-1.168542
O	-0.030764	0.324640	1.922534
O	-1.102109	0.981621	2.239076
K	-2.319282	2.304227	0.097736

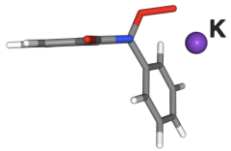


Charge 0
Multiplicity 1
Stoichiometry C14H10KNO3
Electronic Energy (Eh) -1419.54079777
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	-2.455630	-2.721594	0.178331
C	-1.471511	-1.864617	0.667657

C	-1.020029	-0.785326	-0.103472
C	-1.566080	-0.584927	-1.373508
C	-2.549412	-1.446037	-1.865986
C	-2.998664	-2.514180	-1.091335
H	-2.799129	-3.551341	0.789210
H	-1.051450	-2.035126	1.656241
H	-2.963936	-1.278515	-2.855874
H	-3.765957	-3.181527	-1.472285
C	0.077502	0.134903	0.428157
C	1.473409	-0.471526	0.307054
C	1.999557	-1.677820	0.748827
C	2.248099	0.450077	-0.382191
C	3.347118	-1.937134	0.470413
H	1.396966	-2.403115	1.289119
C	3.584243	0.201241	-0.665286
C	4.129336	-1.011189	-0.228976
H	3.792221	-2.871278	0.800307
H	4.184816	0.926009	-1.208268
H	5.170922	-1.240683	-0.434414
H	-1.210287	0.244440	-1.977885
C	1.364018	1.638734	-0.693143
N	0.127010	1.408485	-0.230475
O	1.770853	2.647554	-1.296867
O	-0.095928	0.282140	1.866352
O	-1.361968	0.896188	2.110025
H	-1.919199	0.132250	2.343479
K	-2.168391	2.648885	0.150966



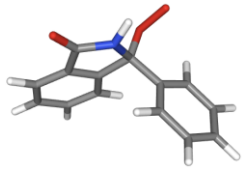
Charge -1

Multiplicity 1
Stoichiometry C14H9KNO3(-1)
Electronic Energy (Eh) -1419.0426205599997
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	-2.664571	-2.358196	0.243733
C	-1.720734	-1.480738	0.776303
C	-0.990814	-0.626797	-0.058901
C	-1.229327	-0.666588	-1.436155
C	-2.174842	-1.545450	-1.973157
C	-2.895825	-2.394167	-1.134225
H	-3.229053	-3.010388	0.904862
H	-1.551167	-1.418481	1.845873
H	-2.345767	-1.564263	-3.046031
H	-3.634049	-3.075343	-1.547814
C	0.090940	0.291530	0.536045
C	1.456832	-0.383084	0.416700
C	1.934650	-1.579829	0.934942
C	2.262019	0.439774	-0.356435
C	3.259777	-1.933293	0.651639
H	1.305172	-2.227959	1.540179
C	3.577446	0.097900	-0.647464
C	4.072329	-1.105488	-0.132817
H	3.664090	-2.862941	1.042492
H	4.201255	0.748052	-1.255721
H	5.095853	-1.404440	-0.341255
H	-0.670404	-0.003175	-2.091380
C	1.432322	1.647691	-0.739448
N	0.208730	1.536459	-0.225959
O	1.896343	2.574990	-1.445098
O	-0.123146	0.477610	1.914799

O	-1.402562	1.118678	2.149542
K	-2.406492	2.119679	0.057474

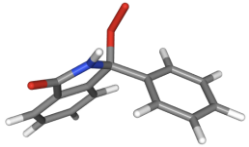


Charge -1
Multiplicity 1
Stoichiometry C14H10NO3(-1)
Electronic Energy (Eh) -819.708193378
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	3.597346	-0.883212	-0.393914
C	2.414264	-0.312062	-0.861856
C	1.430153	0.107126	0.036129
C	1.641319	-0.056403	1.406948
C	2.824816	-0.628622	1.877375
C	3.806522	-1.044145	0.977656
H	4.360730	-1.198119	-1.100041
H	2.244327	-0.159455	-1.922386
H	2.978407	-0.749059	2.946074
H	4.728814	-1.487529	1.341743
C	0.100447	0.639759	-0.501820
C	-0.993150	-0.417816	-0.409317
C	-1.035601	-1.692230	-0.958494
C	-2.053297	0.068952	0.347797
C	-2.181822	-2.461268	-0.734678
H	-0.207336	-2.083369	-1.543506
C	-3.195268	-0.687515	0.581519
C	-3.248566	-1.968074	0.027450

H	-2.246272	-3.460278	-1.155795
H	-4.015584	-0.293758	1.174879
H	-4.123207	-2.590830	0.188580
H	0.878637	0.267520	2.110957
C	-1.723905	1.462953	0.779844
N	-0.449225	1.687845	0.363931
O	-2.449988	2.242303	1.387642
H	-0.060002	2.617456	0.248107
O	0.193003	1.072744	-1.814088
O	1.045299	2.254685	-1.809049

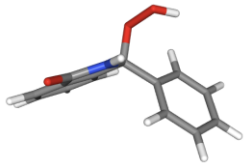


Charge 0
Multiplicity 2
Stoichiometry C14H10NO3
Electronic Energy (Eh) -819.563269559
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	3.516509	-1.144904	-0.208873
C	2.301352	-0.720847	-0.743199
C	1.453362	0.094849	0.012499
C	1.823800	0.472775	1.304914
C	3.040787	0.045805	1.835199
C	3.889648	-0.762083	1.079832
H	4.172414	-1.773473	-0.803332
H	2.022765	-1.023965	-1.747715
H	3.323588	0.347805	2.838952
H	4.838121	-1.092043	1.492605
C	0.094474	0.501540	-0.523961

C	-1.026255	-0.487715	-0.259885
C	-1.094065	-1.841300	-0.551035
C	-2.083373	0.177587	0.349711
C	-2.271924	-2.512814	-0.207331
H	-0.267656	-2.366503	-1.021397
C	-3.254237	-0.480481	0.698935
C	-3.335796	-1.844348	0.409114
H	-2.360635	-3.573901	-0.418727
H	-4.072839	0.046162	1.179901
H	-4.233947	-2.396340	0.667651
H	1.163133	1.097913	1.898532
C	-1.696799	1.607195	0.534223
N	-0.428089	1.716267	0.012620
O	-2.336338	2.505508	1.048506
H	0.119186	2.566722	0.080337
O	0.166217	0.603138	-2.004675
O	0.938571	1.581628	-2.373333

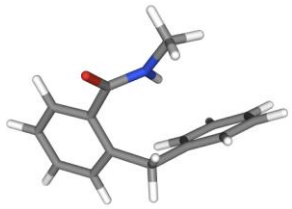


Charge 0
Multiplicity 1
Stoichiometry C14H11NO3
Electronic Energy (Eh) -820.208434809
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	3.436559	-1.257715	-0.138671
C	2.232816	-0.808326	-0.678844
C	1.419587	0.068757	0.047634

C	1.816379	0.481177	1.321046
C	3.019547	0.026041	1.860964
C	3.832793	-0.841320	1.132749
H	4.063486	-1.933643	-0.712230
H	1.926247	-1.144561	-1.666368
H	3.320667	0.353533	2.851463
H	4.770660	-1.191449	1.553097
C	0.084969	0.508269	-0.538926
C	-1.048014	-0.477198	-0.287240
C	-1.133197	-1.822689	-0.612528
C	-2.092773	0.179345	0.352403
C	-2.311571	-2.494391	-0.271449
H	-0.319565	-2.343507	-1.108821
C	-3.264558	-0.479230	0.699232
C	-3.362189	-1.834375	0.376286
H	-2.411684	-3.548683	-0.510524
H	-4.072915	0.042193	1.202976
H	-4.261828	-2.385585	0.631610
H	1.186343	1.155435	1.893453
C	-1.699030	1.604148	0.564627
N	-0.437000	1.717327	0.048559
O	-2.344709	2.492777	1.095696
H	0.090950	2.581258	0.082867
O	0.166240	0.614641	-1.964179
O	1.084989	1.655815	-2.275457
H	1.926582	1.172896	-2.369607



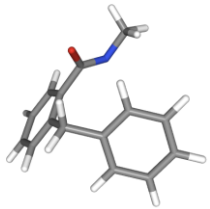
Charge 0

Multiplicity 1
Stoichiometry C15H15NO
Electronic Energy (Eh) -710.385249935
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	2.812404	-1.643430	-1.096008
C	1.611500	-1.550309	-0.389907
C	1.460339	-0.617779	0.641946
C	2.535669	0.227015	0.943686
C	3.736195	0.136857	0.240016
C	3.879100	-0.801044	-0.783948
H	2.910706	-2.374219	-1.893626
H	0.786554	-2.208894	-0.649520
H	4.557225	0.803810	0.487173
H	4.811564	-0.870852	-1.336060
C	0.173099	-0.509581	1.444095
H	0.208307	-1.248965	2.253120
H	0.144385	0.474742	1.922360
C	-1.098160	-0.745097	0.653553
C	-1.657031	-2.029162	0.624393
C	-1.770817	0.284330	-0.028212
C	-2.834987	-2.294744	-0.070303
H	-1.158140	-2.829417	1.166083
C	-2.968948	0.023833	-0.700965
C	-3.496844	-1.263546	-0.737021
H	-3.240942	-3.301936	-0.080020
H	-3.482465	0.841347	-1.199335
H	-4.420623	-1.458437	-1.273080
H	2.424175	0.969547	1.731088
C	-1.285700	1.711006	-0.021597
O	-2.006029	2.632182	0.369071

N	-0.036798	1.913612	-0.479922
H	0.490738	1.129854	-0.841866
C	0.578383	3.227018	-0.467361
H	0.032410	3.923444	-1.110528
H	0.595197	3.632790	0.548524
H	1.601514	3.132238	-0.831635

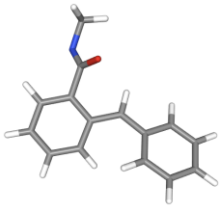


Charge -1
Multiplicity 1
Stoichiometry C15H14NO(-1)
Electronic Energy (Eh) -709.882095233
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	-3.251990	-0.398583	-0.171080
C	-2.101767	-0.321923	0.616859
C	-1.347806	0.855732	0.667025
C	-1.771064	1.956435	-0.088882
C	-2.920291	1.884291	-0.875066
C	-3.665381	0.703715	-0.919176
H	-3.823867	-1.322169	-0.200703
H	-1.764937	-1.184061	1.188398
H	-3.235915	2.749286	-1.451665
H	-4.560934	0.645554	-1.530913
C	-0.082283	0.939905	1.499612
H	-0.070490	1.894461	2.036295
H	-0.078228	0.126281	2.227935

C	1.169194	0.854752	0.644251
C	1.914965	2.014583	0.406275
C	1.567000	-0.350715	0.031220
C	3.046454	1.999502	-0.410765
H	1.601220	2.946225	0.872356
C	2.697071	-0.353144	-0.793573
C	3.440565	0.806980	-1.014003
H	3.612219	2.912643	-0.572603
H	2.995523	-1.285490	-1.265325
H	4.319700	0.777399	-1.651641
H	-1.193372	2.878353	-0.058017
C	0.815634	-1.650543	0.269789
O	0.602973	-1.993184	1.470932
N	0.465054	-2.296499	-0.824511
C	-0.259128	-3.525887	-0.553786
H	-0.552849	-3.997315	-1.497767
H	0.338693	-4.255056	0.016284
H	-1.172962	-3.355739	0.039296

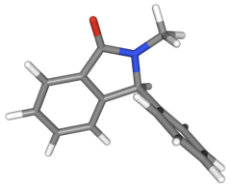


Charge -1
Multiplicity 2
Stoichiometry C15H13NO(-1)
Electronic Energy (Eh) -709.237638929
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	-4.043849	-1.477046	-0.508454

C	-2.661439	-1.435497	-0.624285
C	-1.910389	-0.339346	-0.128937
C	-2.623726	0.691898	0.531114
C	-4.007864	0.639934	0.649681
C	-4.730408	-0.434609	0.123405
H	-4.591473	-2.325829	-0.908033
H	-2.133310	-2.250919	-1.112405
H	-4.528155	1.440017	1.168616
H	-5.811507	-0.466711	0.217345
C	-0.481071	-0.374119	-0.270246
H	-0.057306	-1.351977	-0.480049
C	0.457285	0.714244	-0.164030
C	0.084212	2.062578	-0.379077
C	1.834206	0.429697	0.063175
C	1.018610	3.090151	-0.328101
H	-0.942935	2.298948	-0.636453
C	2.756160	1.474185	0.102760
C	2.361614	2.802254	-0.075966
H	0.701268	4.114330	-0.502102
H	3.802247	1.240179	0.282057
H	3.096571	3.600745	-0.032355
H	-2.085449	1.515765	0.987209
C	2.304882	-0.990995	0.322269
O	1.776018	-1.609716	1.291687
N	3.238867	-1.421572	-0.502488
C	3.682149	-2.774989	-0.212735
H	4.425105	-3.085206	-0.955213
H	4.144504	-2.865095	0.783373
H	2.857994	-3.505555	-0.231509

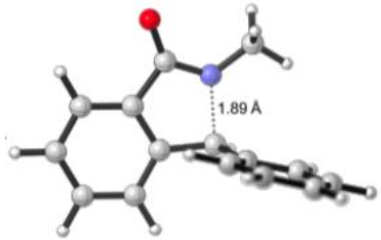


Charge -1
Multiplicity 2
Stoichiometry C15H13NO(-1)
Electronic Energy (Eh) -709.248901614
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	3.643411	-1.053241	-0.420278
C	2.465129	-0.667070	-1.065547
C	1.428261	-0.063723	-0.352112
C	1.589494	0.160822	1.021084
C	2.764825	-0.216071	1.665881
C	3.796039	-0.827881	0.946320
H	4.441018	-1.523902	-0.988063
H	2.350010	-0.837161	-2.133923
H	2.879393	-0.033466	2.730584
H	4.712178	-1.121829	1.450069
C	0.125960	0.308181	-1.050238
H	0.298810	0.240100	-2.134061
C	-1.020641	-0.585676	-0.597784
C	-1.204141	-1.931251	-0.786299
C	-1.931854	0.210381	0.166298
C	-2.346739	-2.565413	-0.206071
H	-0.486636	-2.512611	-1.364198
C	-3.077552	-0.425588	0.749817
C	-3.252012	-1.787039	0.551626
H	-2.516150	-3.628263	-0.344594

H	-3.791649	0.147600	1.335553
H	-4.119198	-2.274986	0.993902
H	0.787801	0.637211	1.582420
C	-1.507070	1.569716	0.146268
N	-0.371008	1.636392	-0.698116
O	-1.997290	2.589339	0.688494
C	0.500968	2.782424	-0.703919
H	1.019058	2.852967	-1.666668
H	-0.106173	3.678944	-0.564194
H	1.262451	2.754521	0.091749

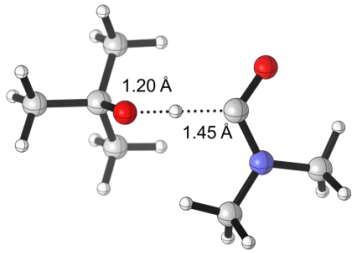


Charge -1
Multiplicity 2
Stoichiometry C15H13NO(-1)
Electronic Energy (Eh) -709.215365339
Number of Imaginary Frequencies 1

Molecular Geometry in Cartesian Coordinates

C	2.723110	-1.052997	1.547678
C	1.509111	-0.792259	0.932012
C	1.449139	-0.338046	-0.433098
C	2.709570	-0.124246	-1.087197
C	3.908598	-0.391802	-0.457573
C	3.945327	-0.869831	0.875071
H	2.726597	-1.404756	2.577743
H	0.584056	-0.940490	1.485326

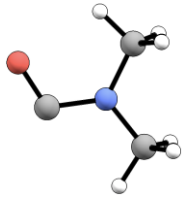
H	4.839466	-0.232440	-0.997938
H	4.890031	-1.074977	1.368035
C	0.222023	0.046108	-1.050092
H	0.293548	0.247149	-2.119507
C	-1.071517	-0.570907	-0.603875
C	-1.410591	-1.913983	-0.772465
C	-1.970132	0.288455	0.039190
C	-2.648454	-2.375926	-0.316717
H	-0.713586	-2.596629	-1.253107
C	-3.200236	-0.167722	0.505596
C	-3.542973	-1.507086	0.316627
H	-2.915029	-3.420469	-0.450800
H	-3.874926	0.519027	1.009779
H	-4.501559	-1.878759	0.667135
H	2.707448	0.245857	-2.111625
C	-1.414869	1.669406	0.223855
N	-0.326970	1.781050	-0.532366
O	-1.905073	2.509667	1.009507
C	0.606789	2.858674	-0.330439
H	0.942759	2.930894	0.714764
H	1.486181	2.685776	-0.960132
H	0.175027	3.828113	-0.610604



# of imaginary frequencies: 1
E = -481.469626540
symmetry c1

C	-1.265781000	-0.724962000	0.391509000

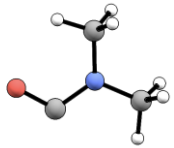
H	0.051970000	-0.294506000	0.807884000
O	-1.617867000	-1.910117000	0.189810000
N	-2.173596000	0.278982000	0.091582000
C	-3.490975000	0.031656000	-0.455702000
H	-4.275705000	0.406363000	0.215717000
H	-3.613199000	0.530992000	-1.426630000
H	-3.615042000	-1.044377000	-0.586720000
C	-1.825454000	1.664593000	0.308969000
H	-0.817264000	1.712671000	0.728275000
H	-1.847577000	2.235547000	-0.630767000
H	-2.525639000	2.144753000	1.007127000
O	1.155706000	0.078102000	1.104348000
C	1.991979000	0.044573000	-0.014065000
C	2.092711000	-1.389221000	-0.565583000
H	1.097337000	-1.756950000	-0.839794000
H	2.742259000	-1.449049000	-1.448034000
H	2.496793000	-2.055613000	0.205724000
C	3.388186000	0.522984000	0.397345000
H	4.091108000	0.513748000	-0.445494000
H	3.334107000	1.544778000	0.790766000
H	3.788036000	-0.123114000	1.187297000
C	1.454114000	0.969966000	-1.123447000
H	1.380654000	1.998302000	-0.749909000
H	2.103706000	0.971180000	-2.007876000
H	0.452226000	0.650994000	-1.436068000



DMF-anion
# of imaginary frequencies: 0
E = -247.873748625

symmetry c1

C	-0.870759000	-0.826288000	0.000031000
O	-1.935167000	-0.159377000	-0.000030000
N	0.311799000	-0.065930000	0.000056000
C	0.339626000	1.382942000	0.000000000
H	0.858977000	1.773222000	0.887076000
H	0.858847000	1.773166000	-0.887186000
H	-0.690988000	1.743566000	0.000070000
C	1.602082000	-0.706269000	-0.000025000
H	1.459441000	-1.790704000	-0.000346000
H	2.193431000	-0.432253000	-0.886648000
H	2.193338000	-0.432786000	0.886842000



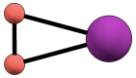
DMF-K

# of imaginary frequencies: 0

E = -847.703955297

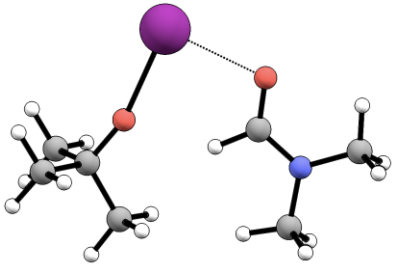
symmetry c1

C	0.118616000	-0.113606000	-0.054277000
O	-0.425173000	1.035060000	-0.050920000
N	1.497501000	-0.126002000	-0.015465000
C	2.317824000	1.070699000	0.042909000
H	2.894416000	1.106842000	0.977216000
H	3.029643000	1.096554000	-0.792353000
H	1.664860000	1.942616000	-0.009555000
C	2.225344000	-1.373325000	0.000763000
H	1.512847000	-2.200360000	-0.043913000
H	2.907849000	-1.447451000	-0.856960000
H	2.825450000	-1.473069000	0.915943000
K	-2.625626000	-0.206642000	0.020466000



KO_2 radical
# of imaginary frequencies: 0
E = -750.216537034
symmetry c2v

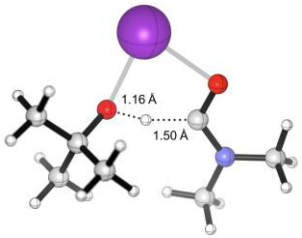
O	0.000000000	0.662500000	-1.334483000
O	0.000000000	-0.662500000	-1.334483000
K	0.000000000	0.000000000	1.123776000



# of imaginary frequencies: 0
E = -1081.32876519
symmetry c1

C	2.304643000	-0.705036000	0.011095000
C	3.242341000	-0.697398000	-1.215488000
H	3.808095000	0.242172000	-1.239827000
H	3.957777000	-1.530876000	-1.215786000
H	2.645362000	-0.754874000	-2.133997000
C	3.176704000	-0.636278000	1.283422000
H	3.740484000	0.304766000	1.292187000
H	2.532732000	-0.651674000	2.171342000
H	3.891310000	-1.466901000	1.360820000
C	1.542910000	-2.048433000	0.024080000
H	0.874460000	-2.085879000	0.893826000
H	0.926565000	-2.132098000	-0.880116000
H	2.210281000	-2.919716000	0.066125000

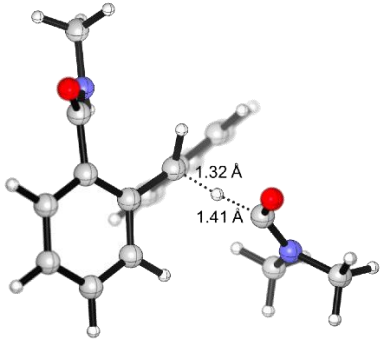
O	1.430633000	0.352447000	-0.037293000
K	0.456916000	2.550071000	-0.041280000
O	-1.913725000	1.409379000	0.060496000
C	-1.752240000	0.178857000	0.005141000
H	-0.735280000	-0.250995000	-0.037977000
N	-2.749529000	-0.714762000	-0.005540000
C	-2.485778000	-2.140362000	-0.081008000
H	-2.889638000	-2.645847000	0.802299000
H	-2.957031000	-2.562773000	-0.974494000
H	-1.409144000	-2.311363000	-0.130452000
C	-4.141893000	-0.309420000	0.050776000
H	-4.665674000	-0.646547000	-0.849923000
H	-4.624241000	-0.757818000	0.925529000
H	-4.196133000	0.776230000	0.119807000



# of imaginary frequencies: 1
E = -1081.30814840
symmetry c1

C	1.424647000	0.310829000	-0.127355000
H	-0.003134000	0.005738000	-0.454281000
O	1.720991000	1.494597000	0.212269000
N	2.410583000	-0.635269000	-0.071551000
C	3.770119000	-0.357389000	0.352426000
H	4.033619000	-0.959379000	1.231332000
H	4.480814000	-0.596234000	-0.448717000
H	3.848837000	0.700834000	0.602197000
C	2.137836000	-2.001155000	-0.461250000

H	1.100493000	-2.077209000	-0.794868000
H	2.795147000	-2.312395000	-1.283516000
H	2.294434000	-2.692190000	0.377665000
O	-1.144837000	0.093899000	-0.645253000
C	-1.938869000	-0.829203000	0.064862000
C	-1.276570000	-1.193416000	1.402410000
H	-1.089170000	-0.287882000	1.992773000
H	-1.916888000	-1.859500000	1.991955000
H	-0.316546000	-1.697832000	1.241602000
C	-2.137817000	-2.098881000	-0.771882000
H	-2.770324000	-2.830898000	-0.255982000
H	-2.609117000	-1.846315000	-1.728129000
H	-1.170671000	-2.569080000	-0.982500000
C	-3.298357000	-0.177754000	0.333753000
H	-3.763884000	0.124311000	-0.610947000
H	-3.980116000	-0.862337000	0.851641000
H	-3.175567000	0.715942000	0.958181000
K	-0.596166000	2.571850000	-0.183234000



Charge 0
Multiplicity 2
Stoichiometry C18H21N2O2
Electronic Energy (Eh) -958.131447002
Number of Imaginary Frequencies 1

Molecular Geometry in Cartesian Coordinates

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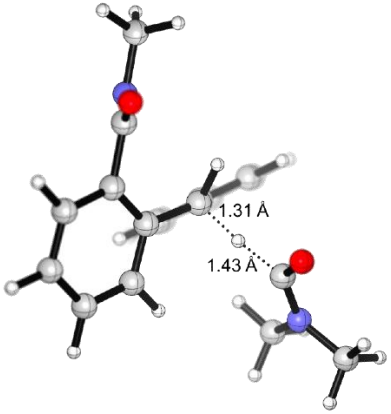
C	-0.401615	1.783655	1.457411
C	-0.520361	1.414556	0.108291
C	-1.215950	2.275342	-0.760798
C	-1.779134	3.459330	-0.296038
C	-1.658592	3.813944	1.050978
H	-0.858453	3.242890	2.967985
H	0.136146	1.141208	2.149234
H	-2.313244	4.108313	-0.984172
H	-2.097198	4.737921	1.415364
C	0.003445	0.136273	-0.430503
H	-1.061695	-0.599741	-0.692805
H	0.385722	0.242070	-1.448869
C	0.838238	-0.751512	0.430561
C	0.218310	-1.503542	1.441529
C	2.219893	-0.926315	0.227537
C	0.939986	-2.396747	2.227353
H	-0.853056	-1.389910	1.597558
C	2.936797	-1.847049	0.999180
C	2.306419	-2.575418	2.003045
H	0.434433	-2.963249	3.003738
H	3.998529	-1.976756	0.809899
H	2.874649	-3.278517	2.604115
H	-1.314128	2.000808	-1.809131
C	-2.020657	-1.512760	-1.181807
O	-1.660778	-2.235018	-2.090441
N	-3.216183	-1.442142	-0.596003
C	-3.497030	-0.539637	0.509432
H	-4.291951	0.158582	0.228027
H	-3.823382	-1.115310	1.381663
H	-2.602234	0.025340	0.771603

C	-4.318853	-2.293866	-1.031839
H	-4.614557	-2.963401	-0.217841
H	-5.174535	-1.670241	-1.308029
H	-4.001686	-2.882077	-1.892235
C	2.998210	-0.157034	-0.807040
O	3.767757	-0.723913	-1.585359
N	2.833908	1.180687	-0.802075
H	2.233866	1.605724	-0.106916
C	3.525661	2.032357	-1.751015
H	3.239453	1.782519	-2.777021
H	3.254760	3.067770	-1.545854
H	4.609545	1.919058	-1.657459



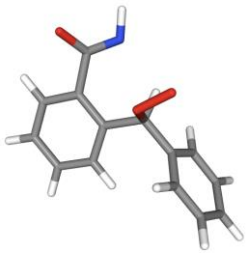
Charge -1
Multiplicity 2
Stoichiometry C18H20N2O2(-1)
Electronic Energy (Eh) -957.6256069339998
Number of Imaginary Frequencies 1

Molecular Geometry in Cartesian Coordinates

C	-1.333931	2.950890	1.853150
C	-0.621576	1.825179	1.437613

C	-0.644853	1.417141	0.095245
C	-1.403038	2.175144	-0.816078
C	-2.115495	3.295774	-0.400775
C	-2.087315	3.689155	0.940414
H	-1.296632	3.252049	2.896349
H	-0.037430	1.264605	2.161858
H	-2.694081	3.864785	-1.123137
H	-2.642202	4.563570	1.266818
C	0.033516	0.192863	-0.397816
H	-0.944398	-0.629952	-0.687386
H	0.456977	0.335993	-1.394076
C	0.914318	-0.604103	0.502502
C	0.332103	-1.335625	1.552546
C	2.301388	-0.715148	0.286252
C	1.096764	-2.148023	2.384530
H	-0.744076	-1.269220	1.706598
C	3.055780	-1.559765	1.110530
C	2.470696	-2.262944	2.160481
H	0.622586	-2.698391	3.192058
H	4.121740	-1.653597	0.919465
H	3.078829	-2.899935	2.796621
H	-1.430007	1.870562	-1.860525
C	-1.828680	-1.630072	-1.196222
O	-1.402567	-2.313491	-2.107047
N	-3.033331	-1.674443	-0.622389
C	-3.410158	-0.804372	0.479916
H	-4.268340	-0.187629	0.192666
H	-3.684887	-1.408153	1.351184
H	-2.577826	-0.153068	0.746311
C	-4.051545	-2.615746	-1.078896
H	-4.321554	-3.294048	-0.263230
H	-4.944370	-2.066633	-1.394125
H	-3.660050	-3.190321	-1.917726

C	3.028623	0.037354	-0.815446
O	3.716205	-0.652142	-1.624823
N	2.885411	1.347362	-0.784707
C	3.608237	2.031530	-1.842906
H	3.458678	3.112710	-1.751465
H	4.692295	1.836197	-1.815712
H	3.272086	1.729709	-2.848157

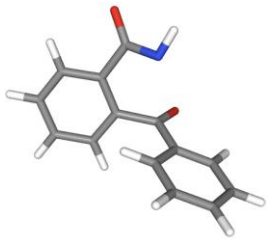


Charge -1
Multiplicity 2
Stoichiometry C14H11NO3(-1)
Electronic Energy (Eh) -820.260286021
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	-3.619034	0.249157	-1.467167
C	-2.284934	-0.144105	-1.365469
C	-1.688019	-0.300475	-0.112075
C	-2.441746	-0.069254	1.041975
C	-3.778620	0.315065	0.940418
C	-4.369275	0.478523	-0.313339
H	-4.073654	0.367397	-2.446291
H	-1.699997	-0.329551	-2.263355
H	-4.357883	0.489797	1.842264
H	-5.410063	0.778654	-0.390209
C	-0.225992	-0.668348	-0.053618

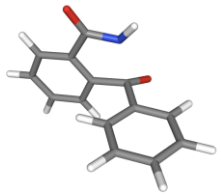
C	0.746173	0.495432	-0.003012
C	0.293115	1.794873	0.252239
C	2.126005	0.261615	-0.168794
C	1.182730	2.865098	0.329475
H	-0.768599	1.978678	0.386234
C	3.007843	1.341681	-0.059398
C	2.548319	2.636250	0.173258
H	0.808761	3.867262	0.516119
H	4.071742	1.149563	-0.163590
H	3.253248	3.460471	0.235192
H	-1.986990	-0.188636	2.021567
C	2.747987	-1.105769	-0.448526
O	3.732376	-1.422518	0.274624
N	2.212035	-1.777954	-1.450286
H	2.744926	-2.647106	-1.542663
H	0.043902	-1.326471	-0.881491
O	0.048566	-1.448266	1.164062
O	-0.478061	-2.635821	1.106618



Charge -1
Multiplicity 1
Stoichiometry C14H10NO2(-1)
Electronic Energy (Eh) -744.5946426380001
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	-4.047540	-0.172812	-0.345514
C	-2.821994	-0.325118	-0.988058
C	-1.635195	0.016749	-0.330540
C	-1.685839	0.514384	0.976043
C	-2.912706	0.663722	1.620099
C	-4.093840	0.321640	0.960083
H	-4.966309	-0.437457	-0.860272
H	-2.770950	-0.709215	-2.002266
H	-2.946738	1.044520	2.636270
H	-5.049574	0.439904	1.462340
C	-0.332832	-0.154068	-1.051921
C	0.908345	0.463672	-0.455402
C	1.048390	1.847174	-0.613578
C	1.932982	-0.287806	0.137089
C	2.209596	2.493815	-0.194297
H	0.245466	2.418058	-1.075157
C	3.098958	0.373557	0.536625
C	3.240804	1.750905	0.381254
H	2.308671	3.567649	-0.322147
H	3.894244	-0.220225	0.976893
H	4.151337	2.244275	0.709004
H	-0.767029	0.773347	1.494739
C	1.816431	-1.785299	0.390998
O	2.894099	-2.442448	0.429634
N	0.580905	-2.211755	0.570582
H	0.632150	-3.221033	0.732021
O	-0.287968	-0.650130	-2.164983

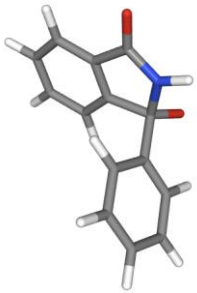


Charge -1
Multiplicity 1
Stoichiometry C14H10NO2(-1)
Electronic Energy (Eh) -744.588985631
Number of Imaginary Frequencies 1

Molecular Geometry in Cartesian Coordinates

C	-3.903949	-0.171472	0.155959
C	-2.731724	-0.136231	0.910108
C	-1.482397	-0.204335	0.287711
C	-1.423696	-0.327666	-1.104644
C	-2.595461	-0.370916	-1.860728
C	-3.839748	-0.289478	-1.233723
H	-4.868542	-0.110789	0.652347
H	-2.768101	-0.056839	1.992546
H	-2.535693	-0.469554	-2.940954
H	-4.751635	-0.321789	-1.822874
C	-0.236950	-0.173512	1.168687
C	1.076286	-0.514396	0.479706
C	1.544156	-1.826523	0.430755
C	1.817025	0.512404	-0.105878
C	2.748893	-2.102747	-0.221051
H	0.970807	-2.628144	0.890119
C	3.015857	0.241424	-0.760109
C	3.482550	-1.073088	-0.817305
H	3.116068	-3.124124	-0.265565
H	3.573618	1.057381	-1.211572
H	4.418116	-1.297483	-1.321517
H	-0.461191	-0.388110	-1.606306
C	1.205457	1.883311	0.040354
O	1.677088	2.875159	-0.560792
N	0.164489	1.795596	0.854397

H	-0.407782	2.637015	0.910810
O	-0.363948	-0.443584	2.376184



Charge -1
Multiplicity 1
Stoichiometry C14H10NO2(-1)
Electronic Energy (Eh) -744.600519096
Number of Imaginary Frequencies 0

Molecular Geometry in Cartesian Coordinates

C	-3.798651	-0.546502	0.325086
C	-2.597899	-0.240689	0.973028
C	-1.475140	0.152434	0.246489
C	-1.569017	0.229970	-1.149162
C	-2.762022	-0.075836	-1.801483
C	-3.884214	-0.465978	-1.064065
H	-4.666508	-0.847945	0.905930
H	-2.502078	-0.292869	2.053577
H	-2.819511	-0.009466	-2.884625
H	-4.814962	-0.703574	-1.571419
C	-0.155930	0.456712	1.014031
C	0.965856	-0.449004	0.453386
C	1.102617	-1.826602	0.580361
C	1.941316	0.290539	-0.207675

C	2.233838	-2.437733	0.030896
H	0.349450	-2.417580	1.096684
C	3.072523	-0.301635	-0.759717
C	3.210934	-1.685445	-0.635021
H	2.360323	-3.513301	0.119927
H	3.822393	0.296138	-1.271040
H	4.079753	-2.184248	-1.054049
H	-0.701626	0.536800	-1.731050
C	1.553795	1.736938	-0.176974
O	2.203702	2.680006	-0.639011
N	0.367253	1.783438	0.454752
H	-0.081913	2.660509	0.689195
O	-0.281717	0.441051	2.325077

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