**Supporting Information**

# Ni-Catalzyed Alkene Carboacylation via Amide C-N Bond Activation

James A. Walker Jr.,[†] Kevin L. Vickerman,[†] Jenna N. Humke and Levi M. Stanley*

Department of Chemistry, Iowa State University, Ames, IA 50011, United States

Email: lstanley@iastate.edu

## Table of Contents



## General Experimental Details

All air-sensitive procedures were conducted under inert atmosphere in a nitrogen-filled dry box or by standard Schlenk techniques. All reactions were performed under an atmosphere of nitrogen unless otherwise stated. All glassware for moisture sensitive reactions were dried at 140 °C in an oven. Tetrahydrofuran, methylene chloride and *N,N*-dimethylformamide were degassed by purging with argon for 45 minutes and dried with a solvent purification system by passing through a one-meter column of activated alumina. Anhydrous 1,4-dioxane was purchased from

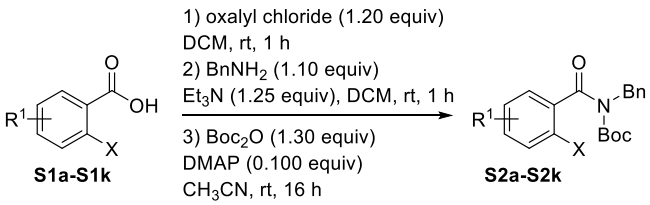
Sigma Aldrich. Flash column chromatography was performed on SiliFlash® P60 silica gel (40-63 μm, 60Å) or using a Teledyne Isco Combiflash® R*f* system with Redi*Sep* GoldTM columns using hexanes/ethyl acetate, dichloromethane/methanol, or pentane/ether mixtures as eluents. Reactions products were visualized on TLC by UV light or by staining with $KMnO_4$.

HRMS (ESI) analysis was performed at the Iowa State University Chemical Instrumentation Facility on an Agilent 6540 QTOF spectrometer. NMR spectra were acquired on Varian MR-400 and Bruker Avance III 600 spectrometers at the Iowa State University Chemical Instrumentation Facility. Chemical shifts are reported in ppm relative to a residual solvent peak ($CDCl_3$ = 7.26 ppm for $^1H$ and 77.16 ppm for $^{13}C$). $^{19}F$ NMR shifts are reported based on indirect reference to $CDCl_3$.[1]

**Materials**

2-iodobenzoic acid (**S1a**) was purchased from Sigma Aldrich. 2-Iodo-5-methylbenzoic acid (**S1b**), 2-bromo-4-methylbenzoic acid (**S1c**), 2-iodo-5-methoxybenzoic acid (**S1d**), 2-bromo-4-methoxybenzoic acid (**S1e**), 2-bromo-6-fluorobenzoic acid (**S1f**), 2-bromo-4-fluorobenzoic acid (**S1g**), 2-bromo-3-fluorobenzoic acid (**S1h**), 2-bromo-5-(trifluoromethyl)benzoic acid (**S1i**), 2-iodo-4-(trifluoromethyl)benzoic acid (**S1j**), and 2-bromo-4,5-difluorobenzoic acid (**S1k**) were purchased from Combi-Blocks. Arylboronic acid pinacol esters were synthesized according to known a literature procedure.[2] Tetrakis(triphenylphosphine), cesium fluoride, and di-*tert*-butyl dicarbonate were purchased from Ak Scientific. Tribasic potassium phosphate was purchased from Sigma Aldrich. Bis(1,5-cyclooctadiene)nickel(0), and 1,3-bis(2,6-di-i-propylphenyl)-4,5-dihydroimidazol-2-ylidine were purchased from Strem Chemicals.

**General Procedure A: Synthesis of *o*-Halobenzamides S2a-S2k:**

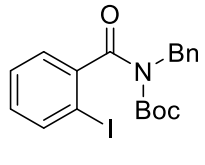



**S1a**; $R^1$ = H, X = I
**S1b**; $R^1$ = 5-Me, X = I
**S1c**; $R^1$ = 4-Me, X= Br
**S1d**; $R^1$ = 5-MeO, X= I
**S1e**; $R^1$ = 4-MeO, X = Br
**S1f**; $R^1$ = 6-F, X = Br
**S1g**; $R^1$ = 4-F, X= Br
**S1h**; $R^1$ = 3-F, X= Br
**S1i**; $R^1$ = 5-$CF_3$, X= Br
**S1j**; $R^1$ = 4-$CF_3$, X = I
**S1k**; $R^1$ = 4,5-F, X = Br

**S2a**; $R^1$ = H, X= I
**S2b**; $R^1$ = 5-Me, X = I
**S2c**; $R^1$ = 4-Me, X = Br
**S2d**; $R^1$ = 5-MeO, X = I
**S2e**; $R^1$ = 4-MeO, X = Br
**S2f**; $R^1$ = 6-F, X = Br
**S2g**; $R^1$ = 4-F, X = Br
**S2h**; $R^1$ = 3-F, X = Br
**S2i**; $R^1$ = 5-$CF_3$, X = Br
**S2j**; $R^1$ = 4-$CF_3$, X = I
**S2k**; $R^1$ = 4,5-F, X = Br

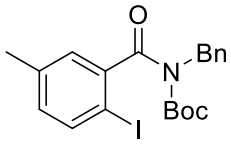
*o*-Halobenzamides (**S2a-S2k**) were prepared from the appropriate *o*-halobenzoic acid (**S1a-S1k**). To the appropriate *o*-halobenzoic acid (**S1a-S1k**) in anhydrous DCM (0.3 M) at 0 °C under $N_2$ was added 2 M oxalyl chloride (1.20 equiv) dropwise and a catalytic amount of DMF (1-2 drops). The reaction was allowed to warm to room temperature and stirred for 1 h. The solvent was removed under reduced pressure to afford the corresponding crude acid chloride. To the crude acid chloride was added DCM (0.9 M) and triethylamine (1.25 equiv). Next, a solution of benzylamine (1.10 equiv) in DCM (0.5 M) was added dropwise. The reaction mixture was stirred at room temperature for 1 h, then diluted with ethyl acetate, and washed successively with 1M HCl and brine. The organic layer was dried over anhydrous sodium sulfate, and concentrated under reduced pressure. The resulting crude material was used directly in the next step. To the round-bottom flask containing the crude benzamide was added DMAP (0.10 equiv), acetonitrile (0.2 M) and $Boc_2O$ (1.30 equiv). The reaction flask was then flushed with $N_2$ and allowed to stir at room temperature for 16 h. The reaction was quenched by addition of water, and extracted with ethyl acetate (3x). The organic layers were combined, dried over $Na_2SO_4$, filtered, and evaporated under reduced

pressure. The resulting crude *o*-halobenzamides (**S2a-S2k**) were used directly in the next step without further purification.



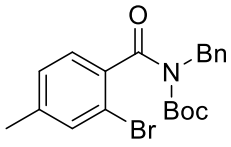
**S2a**

***tert*-butyl benzyl(2-iodobenzoyl)carbamate (S2a):** Prepared according to general procedure A from *o*-iodobenzoic acid **S1a** (7.61 g, 30.7 mmol). The reactions afforded crude product **S2a** as white solid in 80% yield (10.7 g, 24.7 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.14 (s, 9H), 5.05 (s, 2H), 7.07 (td, *J* = 7.1, 1.5 Hz, 1H), 7.17 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.29 (d, *J* = 7.2 Hz, 1H), 7.31-7.38 (m, 3H), 7.47 (d, *J* = 8.0 Hz, 2H), 7.80 (d, *J* = 8.0 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.5, 47.6, 83.9, 91.7, 127.0, 127.6, 127.9, 128.5, 128.6, 130.3, 137.5, 139.2, 144.6, 15.1, 171.6. **HRMS** (ESI): Calcd. for $C_{19}H_{21}INO_3^+$ ([M+H]$^+$): 438.0561, Found: 438.0556.



**S2b**

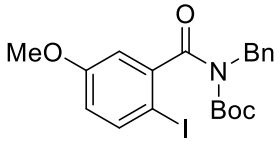
***tert*-butyl benzyl(2-iodo-5-methylbenzoyl)carbamate (S2b):** Prepared according to general procedure A from 2-iodo-5-methylbenzoic acid **S1b** (2.62 g, 10.0 mmol). The reactions afforded crude product **S2b** as a colorless oil in 91% yield (4.01 g, 9.10 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.16 (s, 9H), 2.30 (s, 3H), 5.05 (s, 2H), 6.90 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.01 (d, *J* = 1.5 Hz, 1H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.32-7.38 (m, 2H), 7.48 (d, *J* = 7.2 Hz, 2H), 7.66 (d, *J* = 8.1 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 21.0, 27.5, 48.0, 83.7, 87.5, 127.5, 127.9, 128.5, 128.6, 131.3, 137.5, 138.1, 138.9, 144.3, 152.1, 171.8. **HRMS** (ESI): Calcd. for $C_{20}H_{23}INO_3^+$ ([M+H]$^+$): 452.0717, Found: 452.0720.



**S2c**

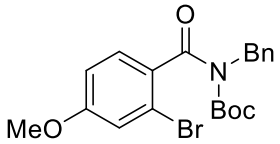
***tert*-butyl benzyl(2-bromo-4-methylbenzoyl)carbamate (S2c):** Prepared according to general procedure A from 2-bromo-4-methylbenzoic acid **S1c** (2.15 g, 10.0 mmol). The reactions afforded crude product **S2c** as a colorless oil in 83% yield (3.36 g, 8.32 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.17 (s, 9H), 2.35 (s, 3H), 5.05 (s, 2H), 7.12-7.18 (m, 2H), 7.26-7.30 (m, 1H), 7.32-7.37 (m, 3H), 7.45-7.47 (m, 2H). **$^{13}$C**

**NMR** (101 MHz, $CDCl_3$) δ 27.5, 48.0, 83.6, 118.5, 127.4, 127.7, 128.0, 128.4, 128.5, 133.0, 133.1, 137.5, 137.6, 140.9, 152.3, 170.5. **HRMS** (ESI): Calcd. for $C_{20}H_{23}BrNO_3^+$ ($[M+H]^+$): 404.0856, Found: 404.0828.



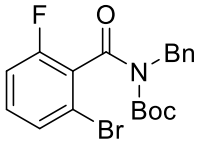
**S2d**

***tert*-butyl benzyl(2-iodo-5-methoxybenzoyl)carbamate (S2d):** Prepared according to general procedure A from 2-iodo-5-methoxybenzoic acid **S1d** (2.78 g, 10.0 mmol). The reactions afforded crude product **S2d** as a colorless oil in 81% yield (3.79 g, 8.10 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.17 (s, 9H), 3.75 (s, 3H), 5.04 (s, 2H), 6.67 (dd, *J* = 8.7, 3.0 Hz, 1H) 6.74 (d, *J* = 3.0 Hz, 1H), 7.28 (d, *J* = 7.3 Hz, 1H), 7.31-7.37 (m, 2H), 7.47 (d, *J* = 7.3 Hz, 2H), 7.63 (d, *J* = 8.7 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.5, 48.0, 55.6, 80.1, 83.8, 112.9, 116.9, 127.5, 128.5, 128.6, 137.4, 139.8, 145.2, 152.0, 159.7, 171.3. **HRMS** (ESI): Calcd. for $C_{20}H_{23}INO_4^+$ ($[M+H]^+$): 468.0666, Found: 468.0665.



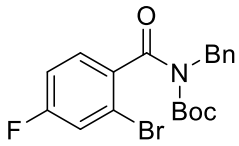
**S2e**

***tert*-butyl benzyl(2-bromo-4-methoxybenzoyl)carbamate (S2e):** Prepared according to general procedure A from 2-bromo-4-methoxybenzoic acid **S1e** (2.31 g, 10.0 mmol). The reactions afforded crude product **S2e** as a yellow oil in 90% yield (3.80 g, 9.00 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.19 (s, 9H), 3.81 (s, 3H), 5.03 (s, 2H), 6.86 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.07 (d, *J* = 2.4 Hz, 1H), 7.21 (d, *J* = 8.6 Hz, 1H), 7.26-7.29 (m, 1H), 7.31-7.35 (m, 2H), 7.42-7.46 (m, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.6, 48.2, 53.6, 55.8, 83.5, 113.2, 118.1, 119.7, 127.5, 128.5, 129.2, 132.6, 137.7, 152.4, 160.7, 170.5. **HRMS** (ESI): Calcd. for $C_{20}H_{22}BrNO_4^+Na$ ($[M+Na]^+$): 442.0624, Found: 442.0587.



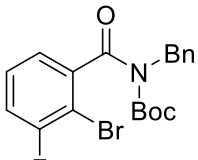
**S2f**

***tert*-butyl benzyl(2-bromo-6-fluorobenzoyl)carbamate (S2f):** Prepared according to general procedure A from 2-bromo-6-fluorobenzoic acid **S1f** (2.19 g, 10.0 mmol). The reactions afforded crude product **S2f** as a white solid in 75% yield (3.05 g, 7.50 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.18 (s, 9H), 5.10 (s, 2H), 7.04-7.08 (m, 1H), 7.21 (m, 1H), 7.24-7.30 (m, 1H), 7.31-7.37 (m, 3H), 7.41-7.45 (m, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.5, 47.6, 84.2, 114.6 (d, $J$ = 21.2 Hz, 1C), 119.2 (d, $J$ = 5.05 Hz, 1C), 127.5, 128.1, 128.3 (d, $J$ = 4.04 Hz, 1C), 128.5, 129.7, (d, $J$ = 21.2 Hz, 1C), 130.6 (d, $J$ = 8.08 Hz, 1C), 137.2, 151.6, 158.4 (d $J$ = 252.5 Hz, 1C), 165.4. **$^{19}$F NMR** ($CDCl_3$, 376 MHz): δ -114.1 (m, 1F). **HRMS** (ESI): Calcd. for $C_{19}H_{19}BrFNO_3^+Na$ ($[M+Na]^+$): 430.0425, Found: 430.0387.



**S2g**

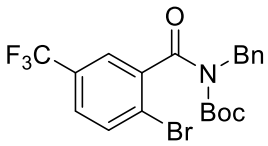
**tert-butyl benzyl(2-bromo-4-fluorobenzoyl)carbamate (S2g):** Prepared according to general procedure A from 2-bromo-4-fluorobenzoic acid **S1g** (2.19 g, 10.0 mmol). The reactions afforded crude product **S2g** as a white solid in 85% yield (3.47 g, 8.50 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.20 (s, 9H), 5.04 (s, 2H), 7.06 (td, $J$ = 8.0, 2.5 Hz, 1H), 7.24-7.36 (m, 5H), 7.43-7.45 (m, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.6, 48.1, 84.0. 114.7 (d, $J$ = 21.2, 1C), 119.3 (d, $J$ = 9.09 Hz, 1C), 120.0 (d, $J$ = 13.1 Hz, 1C), 120.2 (d, $J$ = 14.1 Hz, 1C), 127.6, 128.5, 129.2, 136.7 (d, $J$ = 4.04 Hz, 1C), 137.4, 152.1, 162.5 (d, $J$ = 254.5 Hz, 1C), 169.6. **$^{19}$F NMR** ($CDCl_3$, 376 MHz): δ -109.4 (m, 1F). **HRMS** (ESI): Calcd. for $C_{19}H_{19}BrFNO_3^+Na$ ($[M+Na]^+$): 430.0425, Found: 430.0384.



**S2h**

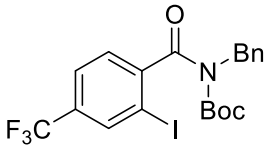
***tert*-butyl benzyl(2-bromo-3-fluorobenzoyl)carbamate (S2h):** Prepared according to general procedure A from 2-bromo-3-fluorobenzoic acid **S1h** (2.19 g, 10.0 mmol). The reactions afforded crude product **S2h** as a white solid in 84% yield (3.43 g, 8.40 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.17 (s, 9H), 5.06 (s, 2H), 7.04 (dt, $J$ =

7.6, 1.0 Hz, 1H), 7.14 (td, *J* = 8.4, 1.4 Hz, 1H), 7.27-7.37 (m, 4H), 7.42-7.47 (m, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.5, 47.9, 84.1, 106.4 (d, *J* = 23.2 Hz, 1C), 116.7 (d, *J* = 22.2 Hz, 1C), 122.8 (d, *J* = 3.0 Hz, 1C), 127.7, 128.5, 128.6, 128.9 (d, *J* = 8.1 Hz, 1C), 137.3, 142.6, 151.9, 159.0 (d, *J* = 248.5 Hz, 1C), 169.1. **$^{19}$F NMR** ($CDCl_3$, 376 MHz): δ -106.1 (m, 1F). **HRMS** (ESI): Calcd. for $C_{19}H_{19}BrFNO_3^+Na$ ($[M+Na]^+$): 430.0425, Found: 430.0393.



**S2i**

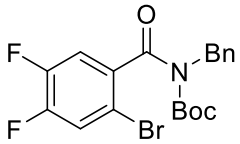
***tert*-butyl benzyl(2-bromo-5-(trifluoromethyl)benzoyl)carbamate (S2i):** Prepared according to general procedure A from 2-bromo-5-(trifluoromethyl)benzoic acid **S1i** (2.69 g, 10.0 mmol). The reactions afforded crude product **S2i** as a white solid in 88% yield (4.03 g, 8.80 mmol). **$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 1.16 (s, 9H), 5.07 (s, 2H), 7.28-7.38 (m, 3H), 7.45-7.51 (m, 4H), 7.67 (d, *J* = 8.2 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.5, 48.0, 84.4, 122.5, 124.7 (q, *J* = 3.8 Hz, 1C), 126.1 (q, *J* = 274.0 Hz, 1C), 126.8 (q, *J* = 3.7 Hz, 1C), 127.7, 128.6, 128.6, 130.3, 133.3, 137.1, 141.4, 151.7, 168.9. **$^{19}$F NMR** ($CDCl_3$, 376 MHz): δ -62.9 (s, 3F). **HRMS** (ESI): Calcd. for $C_{20}H_{19}BrF_3NO_3^+Na$ ($[M+Na]^+$): 480.0393, Found: 480.0344.



**S2j**

***tert*-butyl benzyl(2-iodo-4-(trifluoromethyl)benzoyl)carbamate (S2j):** Prepared according to general procedure A from 2-iodo-4-(trifluoromethyl)benzoic acid **S1j** (3.16 g, 10.0 mmol). The reactions afforded crude product **S2j** as a colorless oil in 91% yield (4.60 g, 9.10 mmol). **$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 1.19 (s, 9H), 5.08 (s, 2H), 7.27-7.38 (m, 4H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.64 (dd, *J* = 8.0, 0.9 Hz, 1H), 8.06 (s, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.6, 47.8, 84.5, 91.1, 122.7 (q, *J* = 274.7, 1C), 124.5 (d, *J* = 22.2 Hz, 1C), 126.9 (d, *J* = 11.1 Hz, 1C), 127.7 (q, *J* = 6.1 Hz, 1C), 128.6 (m, 1C), 128.7 (d, *J* = 9.1 Hz, 1C), 132.0 (q, *J* = 33.3 Hz, 1C), 135.9 (dd, *J* = 15.2, 4.0 Hz,

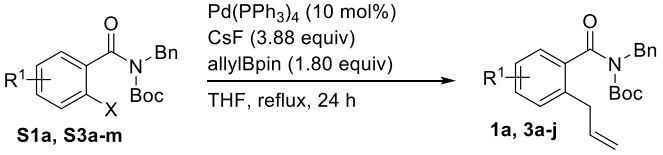
1C), 137.1, 148.1, 151.6, 170.5. **$^{19}$F NMR** ($CDCl_3$, 376 MHz): δ -62.8 (s, 3F). **HRMS** (ESI): Calcd. for $C_{20}H_{20}F_3INO_3^+$ ([M+H]$^+$): 506.0434, Found: 506.0450.



**S2k**

***tert*-butyl benzyl(2-bromo-4,5-difluorobenzoyl)carbamate (S2k):** Prepared according to general procedure A from 2-bromo-4,5-difluorobenzoic acid **S1k** (2.37 g, 10.0 mmol). The reactions afforded crude product **S2k** as a white solid in 74% yield (3.16 g, 7.40 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.24 (s, 9H), 5.03 (s, 2H), 7.14 (dd, *J* = 9.8, 7.9 Hz, 1H), 7.27-7.43 (m, 6H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.6, 48.1, 84.4, 112.6 (dd, *J* = 7.4, 4.1 Hz, 1C), 116.9, 117.1 (d, *J* = 2.0 Hz, 1C), 127.7, 128.5, 128.6 (d, *J* = 2.0 Hz, 1C), 137.0 (dd, *J* = 6.1, 5.1 Hz, 1C), 137.1, 149.7 (dd, *J* = 252.5, 13.1 Hz, 1C), 150.4 (dd, *J* = 257.6, 14.1 Hz, 1C), 151.9, 168.4. **$^{19}$F NMR** ($CDCl_3$, 376 MHz): δ -137.8 (m, 1F), -133.4 (m, 1F). **HRMS** (ESI): Calcd. for $C_{19}H_{19}BrF_2NO_3^+$ ([M+H]$^+$): 426.0511, Found: 426.0502.

**General Procedure B: Synthesis of *o*-Allylbenzamides 1a, 3a-j**

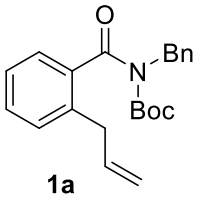



**S2a**; $R^1$ = H, X = I
**S2b**; $R^1$ = 5-Me, X = I
**S2c**; $R^1$ = 4-Me, X = Br
**S2d**; $R^1$ = 5-MeO, X = I
**S2e**; $R^1$ = 4-MeO, X = Br
**S2f**; $R^1$ = 6-F, X = Br
**S2g**; $R^1$ = 4-F, X= Br
**S2h**; $R^1$ = 3-F, X = Br
**S2i**; $R^1$ = 5-$CF_3$, X = Br
**S2j**; $R^1$ = 4-$CF_3$, X = I
**S2k**; $R^1$ = 4,5-F, X = Br

**1a**; $R^1$ = H
**3a**; $R^1$ = 5-Me
**3b**; $R^1$ = 5-MeO
**3c**; $R^1$ = 5-$CF_3$
**3d**; $R^1$ = 4-MeO
**3e**; $R^1$ = 4-Me
**3f**; $R^1$ = 4-F
**3g**; $R^1$ = 4-$CF_3$
**3h**; $R^1$ = 3-F
**3i**; $R^1$ = 6-F
**3j**; $R^1$ = 4,5-F

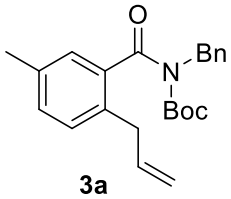
*o*-Allylbenzamides (**1a, 3a-j**) were prepared according to the following procedure. A round-bottom flask was charged with 3.00 mmol of *o*-iodobenzamide (**S2a-S2k**), CsF (1.77 g, 11.6

mmol), $Pd(PPh_3)_4$ (0.347 g, 0.300 mmol), and THF (37.5 mL). The resulting solution was stirred at room temperature for 30 minutes. Then 2-allyl-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (allylBpin) (0.907 g, 5.40 mmol) in THF (37.5 mL) was added. The resulting solution was stirred at reflux for 24 hours. The reaction mixture was diluted with hexanes (100 mL) followed by water (100 mL). The layers were separated, and the organic layer extracted with hexanes (2 x 100 mL). The combined organic layers were washed with water (200 mL) and brine (200 mL), dried over $Na_2SO_4$, filtered, and concentrated under reduced pressure. Purifications of the crude products were carried out by flash column chromatography to give *o*-allylbenzamides **1a, 3a-j**.



**1a**

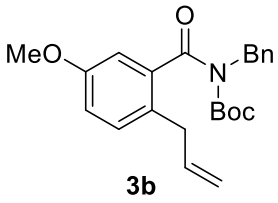
***tert*-butyl (2-allylbenzoyl)(benzyl)carbamate (1a):** Prepared according to general procedure B from *tert*-butyl benzyl(2-iodobenzoyl)carbamate **S2a** (1.31 g, 3.00 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes EtOAc) to give **1a** as a colorless oil in 79% yield (0.830 g, 2.37 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.08 (s, 9H), 3.45 (d, $J$ = 6.8 Hz, 1H), 5.03 (s, 2H), 5.03-5.10 (m, 2H), 5.92 (ddt, $J$ = 17.0, 10.0, 6.8 Hz, 1H), 7.12 (d, $J$ = 7.6 Hz, 1H), 7.19 (t, $J$ = 7.6 Hz, 1H), 7.22-7.37 (m, 5H), 7.45 (d, $J$ = 7.4 Hz, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.5, 37.6, 48.1, 83.4, 116.6, 125.9, 126.1, 127.5, 128.4, 128.6, 129.6, 129.8, 136.6, 137.3, 137.9, 138.2, 153.0, 172.4. **HRMS** (ESI): Calcd. for $C_{22}H_{26}NO_3^+$ ($[M+H]^+$): 352.1907, Found: 352.1883.



**3a**

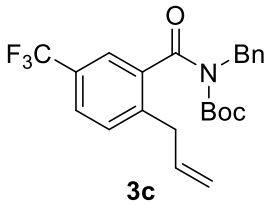
***tert*-butyl (2-allyl-5-methylbenzoyl)(benzyl)carbamate (3a):** Prepared according to general procedure B from *tert*-butyl (2-iodo-5-methylbenzoyl)(benzyl)carbamate **S2b** (1.35 g, 3.00 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10

Hexanes:EtOAc) to give **3a** as a colorless oil in 78% yield (0.856 g, 2.34 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.09 (s, 9H), 2.30 (s, 3H), 3.41 (d, *J* = 8.0 Hz, 2H), 5.03 (s, 2H), 5.01-5.08 (m, 2H), 5.91 (ddt, *J* = 17.0, 10.0, 8.0 Hz, 1H), 6.96 (s, 1H), 7.11-7.16 (m, 2H), 7.26-7.30 (m, 1H), 7.33-7.37 (m, 2H), 7.45-7.47 (m, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 20.9, 27.4, 37.2, 48.1, 83.3, 116.2, 126.7, 127.5, 128.4, 128.5, 129.8, 130.3, 134.3, 135.4, 136.81, 137.9, 137.9, 153.1, 172.5. **HRMS** (ESI): Calcd. for $C_{23}H_{28}NO_3^+$ ($[M+H]^+$): 366.2064, Found: 366.2024.



**3b**

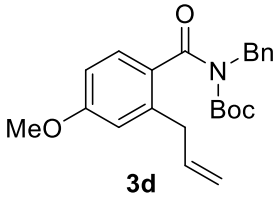
***tert*-butyl (2-allyl-5methoxybenzoyl)(benzyl)carbamate (3b):** Prepared according to general procedure B from *tert*-butyl benzyl(2-iodo-5-methoxybenzoyl)carbamate **S2d** (1.40 g, 3.00 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **3b** as a dark-green oil in 61% yield (0.698 g, 1.83 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.14 (s, 9H), 3.38 (d, *J* = 6.8 Hz, 2H), 3.76 (s, 3H), 5.02-5.08 (m, 2H), 5.04 (s, 2H), 5.91 (ddt, *J* = 17.0, 10.1, 6.8 Hz, 1H), 6.69 (d, *J* = 2.8 Hz, 1H), 6.89 (dd, *J* = 8.5, 2.8 Hz, 1H), 7.16 (d, *J* = 8.5 Hz, 1H), 7.28-7.31 (m, 1H), 7.34-7.38 (m, 2H), 7.46-7.48 (m, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.5, 36.7, 48.1, 55.5, 83.4, 111.5, 115.4, 116.1, 127.5, 128.4, 128.5, 129.2, 130.9, 136.9, 137.8, 138.9, 152.9, 157.6, 172.1. **HRMS** (ESI): Calcd. for $C_{23}H_{27}NO_4^+Na$ ($[M+Na]^+$): 404.1832, Found: 404.1786.



**3c**

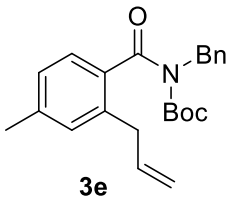
***tert*-butyl (2-allyl-5-(trifluoromethyl)benzoyl)(benzyl)carbamate (3c):** Prepared according to general procedure B from *tert*-butyl benzyl(2-bromo-5-(trifluoromethyl)benzoyl)carbamate **S2i** (1.37 g, 3.00 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 95:5 hexanes:EtOAc) to give **3c** as a colorless oil as an 84:16 mixture of **3c** and the olefin

isomerization product in 70% yield (0.879 g, 2.10 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.10 (s, 9H), 3.46 (d, *J* = 6.8 Hz, 2H), 5.05 (s, 2H), 5.06-5.11 (m, 2H), 5.81-5.93 (m, 1H), 7.27-7.40 (m, 5H), 7.45 (d, *J* = 7.2 Hz, 2H) 7.58 (dd, *J* = 7.9, 3.1 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.3, 37.3, 48.0, 83.9, 117.4, 122.9 (q, *J* = 3.7 Hz, 1C), 125.9 (q, *J* = 3.8 Hz, 1C), 127.0 (q, *J* = 273.4 Hz, 1C), 127.6, 128.3, 128.5, 128.7, 130.2, 131.5, 135.2, 137.3, 138.7, 141.0, 152.3, 170.8,. **$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -62.6 (m, 1F). **HRMS** (ESI): Calcd. for $C_{23}H_{25}F_3NO_3^+$ ($[M+H]^+$): 420.1781, Found: 420.1720.



**3d**

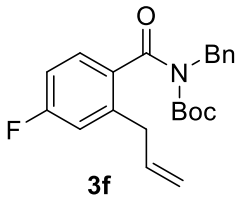
***tert*-butyl benzyl(2-allyl-4-methoxybenzoyl)carbamate (3d):** Prepared according to general procedure B from *tert*-butyl benzyl(2-bromo-4-methoxybenzoyl)carbamate **S2e** (1.26 g, 3.00 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **3d** as a colorless oil in 34% yield (0.386 g, 1.01 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.13 (s, 9H), 3.48 (d, *J* = 6.8 Hz, 2H), 3.80 (s, 3H), 4.99 (s, 2H), 5.04-5.12 (m, 2H), 5.92 (ddt, *J* = 17.2, 10.0, 6.8 Hz, 1H), 6.70 (dd, *J* = 8.5, 2.4 Hz, 1H), 6.78 (d, *J* = 2.4 Hz, 1H), 7.12 (d, *J* = 8.5 Hz, 1H), 7.24-7.29 (m, 1H), 7.31-7.35 (m, 2H), 7.42-7.44 (m, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.6, 37.7, 48.4, 55.4, 83.1, 110.9, 115.5, 116.6, 127.5, 128.3, 128.4, 128.5, 130.5, 136.5, 138.0, 140.2, 153.3, 160.8, 172.4. **HRMS** (ESI): Calcd. for $C_{23}H_{27}NO_4^+Na$ ($[M+Na]^+$): 404.1832, Found: 404.1782.



**3e**

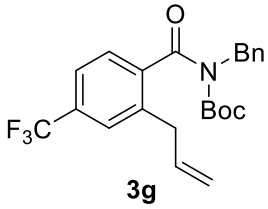
***tert*-butyl (2-allyl-4-methylbenzoyl)(benzyl)carbamate (3e):** Prepared according to general procedure B from *tert*-butyl benzyl(2-bromo-4-methylbenzoyl)carbamate **S2c** (1.21 g, 3.00 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10

hexanes:EtOAc) to give **3e** as a colorless oil in 28% yield (0.310 g, 0.848 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.11 (s, 9H), 2.34 (s, 3H), 3.44 (d, *J* = 8.0 Hz, 2H), 5.01 (s, 2H), 5.05-5.10 (m, 2H), 5.93 (ddt, *J* = 17.0, 10.0, 6.9 Hz, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 7.05-7.07 (m, 1H), 7.24-7.30 (m, 1H), 7.30-7.37 (m, 2H), 7.44 (d, *J* = 8.0 Hz, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 21.5, 27.5, 37.6, 48.2, 83.2, 116.3, 126.4, 126.5, 127.5, 128.3, 128.5, 130.6, 135.3, 136.8 137.5, 138.0, 139.8, 153.1, 172.6. **HRMS** (ESI): Calcd. for $C_{23}H_{28}NO_3^+$ ($[M+H]^+$): 366.2064, Found: 366.2027.



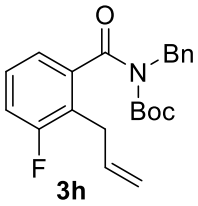
**3f**

**tert-butyl (2-allyl-4-fluorobenzoyl)(benzyl)carbamate (3f):** Prepared according to general procedure B from *tert*-butyl benzyl(2-bromo-4-fluorobenzoyl)carbamate **S2g** (1.22 g, 3.00 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **3f** as a colorless oil in 51% yield (0.568 g, 1.54 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.14 (s, 9H), 3.44 (d, *J* = 6.9 Hz, 2H), 5.01 (s, 2H), 5.06-5.12 (m, 2H), 5.89 (ddt, *J* = 17.4, 9.6, 6.9 Hz, 1H), 6.89 (td, *J* = 8.5, 2.4 Hz, 1H), 6.97 (dd, *J* = 9.8, 2.4 Hz, 1H), 7.12 (dd, *J* = 8.5, 5.7 Hz, 1H), 7.26-7.30 (m, 1H), 7.32-7.36 (m, 2H), 7.42-7.44 (m, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.6, 37.4, 48.2, 83.6, 112.8 (d, *J* = 21.2 Hz, 1C), 116.7 (d, *J* = 22.2 Hz, 1C), 117.4, 127.61, 128.1 (d, *J* = 9.1 Hz, 1C), 128.4, 128.6, 134.3 (d, *J* = 3.0 Hz, 1C), 135.6, 137.7 140.6 (d, *J* = 7.1 Hz, 1C), 152.9, 163.3 (d, *J* = 250.5 Hz, 1C), 171.6. **$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -110.9 (m, 1F). **HRMS** (ESI): Calcd. for $C_{22}H_{24}FNO_3^+Na$ ($[M+Na]^+$): 392.1632, Found: 392.1596.



**3g**

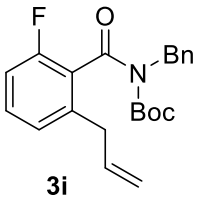
***tert*-butyl (2-allyl-4-(trifluoromethyl)benzoyl)(benzyl)carbamate (3g):** Prepared according to general procedure B from *tert*-butyl benzyl(2-iodo-4-(trifluoromethyl)benzoyl)carbamate **S2j** (1.52 g, 3.00 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexnaes:EtOAc to 90:10 hexanes:EtOAc) to give **3g** as a colorless oil in 81% yield (1.02 g, 2.43 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.12 (s, 9H), 3.45 (d, *J* = 6.8 Hz, 2H), 5.05 (s, 2H), 5.06-5.12 (m, 2H), 5.89 (ddt, *J* = 16.8, 10.3, 6.8 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.27-7.32 (m, 1H), 7.34-7.38 (m, 2H), 7.43-7.51 (m, 4H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 22.5, 37.4, 47.9, 84.1, 117.7, 122.9 (q, *J* = 3.75 Hz, 1C), 126.1, 126.5 (q, *J* = 4.0 Hz, 1C), 127.0 (q, *J* = 274.1 Hz, 1C), 127.7, 128.5, 128.6, 131.2, 135.2, 137.5, 137.9, 141.8, 152.4, 171.1. **$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -62.6 (s, 3F). **HRMS** (ESI): Calcd. for $C_{23}H_{24}F_3NO_3^+Na$ ($[M+Na]^+$): 442.1600, Found: 442.1550.



**3h**

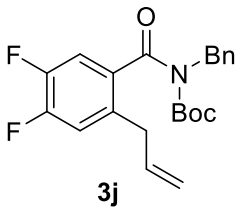
***tert*-butyl (2-allyl-3-fluorobenzoyl)(benzyl)carbamate (3h):** Prepared according to general procedure B from *tert*-butyl benzyl(3-fluoro-2-bromobenzoyl)carbamate **S2h** (1.22 g, 3.00 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **3h** as a colorless oil in 71% yield (0.787 g, 2.13 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.12, (s, 9H), 3.43 (d, *J* = 6.0 Hz, 2H), 4.97-5.05 (m, 2H), 5.03 (s, 2H), 5.89 (ddt, *J* = 17.1, 10.0, 6.6 Hz, 1H), 6.93 (dd, *J* = 7.6, 0.6 Hz, 1H), 7.05-7.09 (m, 1H), 7.18 (m, 1H), 7.27-7.30 (m, 1H), 7.33-7.37 (m, 2H), 7.43-7.45 (m, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.5, 30.7, 48.0, 83.8, 116.27, 116.3, 116.5, 121.7 (d, *J* = 3.0 Hz, 1C), 124.6 (d, *J* = 17.2 Hz, 1C), 127.4 (d, *J* = 9.1 Hz, 1C), 127.6, 128.5 (d, *J* = 15.2 Hz, 1C), 135.2, 137.7, 140.4 (d, *J* = 5.1 Hz, 1C), 152.7, 161.4 (d, *J* = 248.5 Hz, 1C),

170.9 (d, $J$ = 3.0 Hz, 1C). **$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -116.6 (m, 1F). **HRMS** (ESI): Calcd. for $C_{22}H_{24}FNO_3^+Na$ ($[M+Na]^+$): 392.1632, Found: 392.1587.



**3i**

***tert*-butyl (2-allyl-6-fluorobenzoyl)(benzyl)carbamate (3i):** Prepared according to general procedure B from *tert*-butyl benzyl(2-bromo-6-fluorobenzoyl)carbamate **S2f** (1.22 g, 3.00 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **3i** as a colorless oil in 89% yield (0.984 g, 2.66 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.16 (s, 9H), 3.37 (dd, $J$ = 22.6, 7.2 Hz, 2H), 4.99-5.05 (m, 2H), 5.09 (d, $J$ = 4.6 Hz, 2H), 5.86 (ddt, $J$ = 17.6, 9.6, 6.8 Hz, 1H), 6.91 (t, $J$ = 9.6 Hz, 1H), 7.03 (d, $J$ = 7.6 Hz, 1H), 7.24-7.30 (m, 2H), 7.32-7.36 (m, 2H), 7.42-7.44 (m, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.4 (d, $J$ = 4.0 Hz, 1C), 37.4, 47.6, 83.7, 112.9, 113.1, 116.9, 125.3 (d, $J$ = 2.0 Hz, 1C), 126.9 (d, $J$ = 17.2 Hz, 1C), 127.8 (d, $J$ = 74.7 Hz, 1C), 128.5, 130.1 (d, $J$ = 8.1 Hz, 1C), 135.8 (d, $J$ = 6.1 Hz, 1C), 137.6, 139.1 (d, $J$ = 3.0 Hz, 1C), 152.1, 158.3 (d, $J$ = 247.5 Hz, 1C), 167.25. **$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -117.7 (m, 1F). **HRMS** (ESI): Calcd. for $C_{22}H_{24}FNO_3^+Na$ ($[M+Na]^+$): 392.1632, Found: 392.1598.

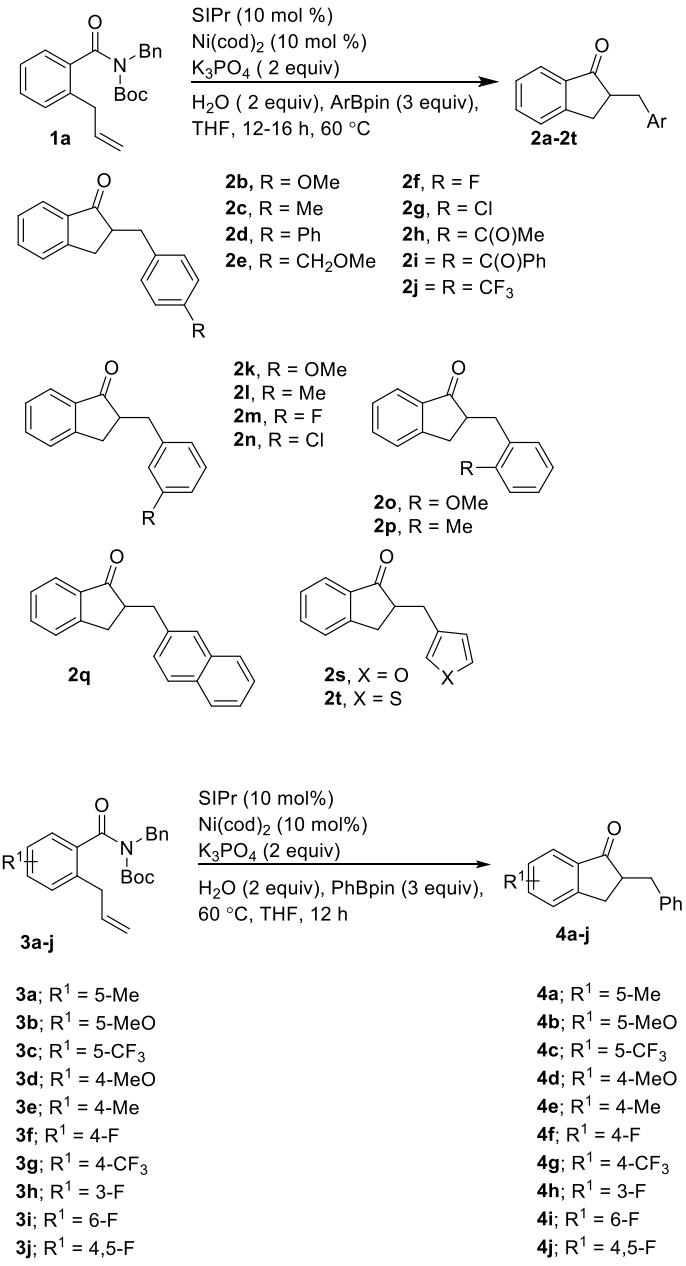


**3j**

***tert*-butyl (2-allyl-4,5-difluorobenzoyl)(benzyl)carbamate (3j):** Prepared according to general procedure B from *tert*-butyl benzyl(4,5-difluoro-2-bromobenzoyl)carbamate **S2k** (1.28 g, 3.00 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 DCM:EtOAc to 90:10 DCM:EtOAc) to give **3j** as a colorless oil in 61% yield (0.709 g, 1.83 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 1.19 (s, 9H), 3.36 (d, $J$ = 6.8 Hz, 2H), 5.00 (s, 2H), 5.03-5.10 (m, 2H), 5.84 (ddt, $J$ = 16.9, 10.2, 6.8 Hz, 1H), 6.97 (dd, $J$ = 10.2, 7.8 Hz, 1H), 7.06 (dd, $J$ = 11.2, 7.6 Hz, 1H), 7.27-7.31 (m, 1H), 7.33-7.38 (m, 2H), 7.39-7.43 (m, 2H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 27.5, 36.6, 48.1,

83.9, 115.3 (d, $J$ = 19.2 Hz, 1C), 117.4, 118.5 (d, $J$ = 18.2 Hz, 1C), 127.6, 128.36 (d, $J$ = 29.3 Hz, 1C), 128.37 (d, $J$ = 10.1 Hz, 1C), 134.2 (dd, $J$ = 5.1 Hz, 1C), 134.5 (dd, $J$ = 5.1 Hz, 1C), 135.3, 137.3, 148.2 (dd, $J$ = 249.6, 13.2 Hz, 1C), 150.5 (dd, $J$ = 248.2, 12.6 Hz, 1C), 152.4, 170.1. **$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -141.3 (m, 1F) -135.8 (m, 1F). **HRMS** (ESI): Calcd. for $C_{22}H_{23}F_2NO_3{}^+Na$ ($[M+Na]^+$): 410.1538, Found: 410.1492.

**General Procedure C: Synthesis of 2-Benzyl-2,3-dihydro-1*H*-inden-1-ones 2a-2t, 4a-4j**

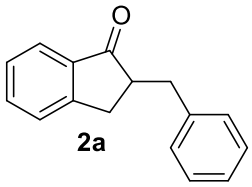



**3a**; $R^1$ = 5-Me
**3b**; $R^1$ = 5-MeO
**3c**; $R^1$ = 5-$CF_3$
**3d**; $R^1$ = 4-MeO
**3e**; $R^1$ = 4-Me
**3f**; $R^1$ = 4-F
**3g**; $R^1$ = 4-$CF_3$
**3h**; $R^1$ = 3-F
**3i**; $R^1$ = 6-F
**3j**; $R^1$ = 4,5-F

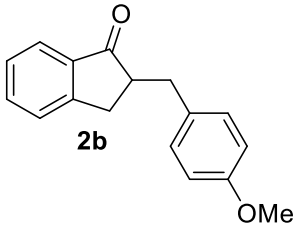
**4a**; $R^1$ = 5-Me
**4b**; $R^1$ = 5-MeO
**4c**; $R^1$ = 5-$CF_3$
**4d**; $R^1$ = 4-MeO
**4e**; $R^1$ = 4-Me
**4f**; $R^1$ = 4-F
**4g**; $R^1$ = 4-$CF_3$
**4h**; $R^1$ = 3-F
**4i**; $R^1$ = 6-F
**4j**; $R^1$ = 4,5-F

2-benzyl-2,3-dihydro-1*H*-inden-1-ones **2a-2t, 4a-4j** were prepared by the following procedure. A 1-dram vial was charged with 0.100 mmol of the appropriate *o*-allylbenzamide **1a, 3a-3j**, $Ni(cod)_2$ (2.8 mg, 0.010 mmol ), SIPr (3.9 mg, 0.010 mmol), $K_3PO_4$ (42.5 mg, 0.200 mmol), $H_2O$ (3.6 µL, 0.20 mmol), the appropriate ArBpin (0.300 mmol), and THF (0.10-0.20 mL, 0.50-1.0 M). The

resulting solution stirred at 60 °C for 12-16 hours. Upon completion of the reaction, the reaction mixture was filtered through a short plug of silica gel eluting with 70:30 hexanes:EtOAc and concentrated under reduced pressure. The crude product was purified by column chromatography with a gradient of 100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc over a 25 minute period on a Combiflash system.

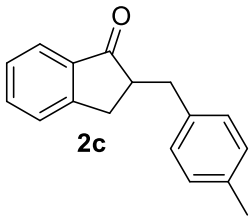



**2-benzyl-2,3-dihydro-1*H*-inden-1-one (2a):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and phenylboronic acid pinacol ester (61.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2a** as a colorless oil in 97% yield (21.6 mg, 0.097 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.68 (dd, *J* = 14.0, 10.4 Hz, 1H), 2.88 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.97-3.06 (m, 1H), 3.18 (dd, *J* = 17.2, 7.8 Hz, 1H), 3.42 (dd, *J* = 14.0, 4.2 Hz, 1H), 7.20-7.34 (m, 5H), 7.35-7.43 (m, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.80 (d, *J* = 7.6 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.3, 37.1, 49.1, 124.1, 126.5, 126.7, 127.5, 128.6, 129.0, 134.9, 136.7, 139.8, 153.7, 207.9. **HRMS** (ESI): Calcd. for $C_{16}H_{14}O^+Na$ ($[M+Na]^+$): 245.0937, Found: 245.0902.

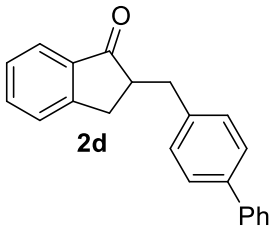



**2-(4-methoxybenzyl)-2,3-dihydro-1*H*-inden-1-one (2b):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 4-methoxyphenylboronic acid pinacol ester (70.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAC to 90:10 hexanes:EtOAc) to give **2b** as a colorless oil in 98% yield (24.8 mg, 0.098 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.65 (dd, *J* = 14.0, 10.1 Hz, 1H), 2.86 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.93-3.00

(m, 1H), 3.17 (dd, *J* = 17.2, 7.7 Hz, 1H), 3.31 (dd, *J* = 14.0, 4.3 Hz, 1H), 3.79 (s, 3H), 6.84 (ddd, *J* = 8.7, 3.0, 2.1 Hz, 2H), 7.16 (ddd, *J* = 8.7, 3.0, 2.0 Hz, 2H), 7.35-7.41 (m, 2H), 7.57 (ddd, *J* = 7.6, 7.6, 1.2 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.2, 36.2, 49.3, 55.4, 114.0, 124.1, 126.7, 127.5, 130.0, 131.7, 134.9, 136.7, 153.8, 158.3, 208.1. **HRMS** (ESI): Calcd. for $C_{17}H_{17}O_2^+$ ($[M+H]^+$): 253.1223, Found: 253.1225.

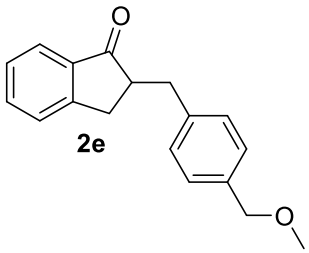



**2-(4-methylbenzyl)-2,3-dihydro-1*H*-inden-1-one (2c):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 4-tolylboronic acid pinacol ester (65.4 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2c** as a colorless oil in 99% yield (23.4 mg, 0.099 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.33 (s, 3H), 2.64 (dd, *J* = 14.0, 10.4 Hz, 1H), 2.86 (dd, *J* = 17.2, 3.9 Hz, 1H), 2.95-3.02 (m, 1H), 3.17 (dd, *J* = 17.2, 7.8 Hz, 1H), 3.36 (dd, *J* = 14.0, 4.2 Hz, 1H), 7.10-7.15 (m, 4H), 7.35-7.41 (m, 2H), 7.57 (ddd, *J* = 7.6, 7.6, 1.1 Hz, 1H), 7.78 (d, *J* = 7.7 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 21.3, 32.3, 36.7, 49.2, 124.1, 126.6, 127.5, 128.9, 129.3, 134.8, 136.0, 136.66, 136.73, 153.8, 208.1. **HRMS** (ESI): Calcd. for $C_{17}H_{17}O^+$ ($[M+H]^+$): 237.1274, Found: 237.1272.

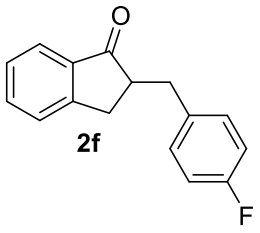



**2-([1,1'-biphenyl]-4-ylmethyl)-2,3-dihydro-1*H*-inden-1-one (2d):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 4-biphenylboronic acid pinacol ester (84.1 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2d** as a colorless oil in 94% yield (27.9 mg, 0.094 mmol). **$^1$H NMR** (400

MHz, $CDCl_3$) δ 2.73 (dd, *J* = 14.0, 10.4 Hz, 1H), 2.91 (dd, *J* = 17.2, 4.0 Hz, 1H), 3.02-3.08 (m, 1H), 3.23 (dd, *J* = 17.2, 7.8 Hz, 1H), 3.44 (dd, *J* = 14.0, 4.3 Hz, 1H), 7.32-7.46 (m, 7H), 7.53-7.60 (m, 5H), 7.81 (d, *J* = 7.5 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.4, 36.8, 49.0, 124.2, 126.7, 127.1, 127.3, 127.4, 127.6, 128.9, 129.5, 135.0, 136.7, 138.9, 139.4, 141.0, 153.8, 207.9. **HRMS** (ESI): Calcd. for $C_{22}H_{19}O^+$ ($[M+H]^+$): 299.1430, Found: 299.1433.

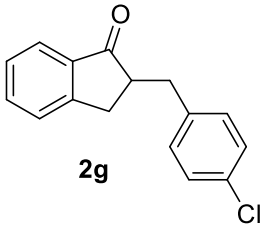



**2-(4-(methoxymethyl)benzyl)-2,3-dihydro-1*H*-inden-1-one (2e):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 4-(methoxymethyl)phenylboronic acid pinacol ester (74.4 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2e** as a colorless oil in 78% yield (20.7 mg, 0.078 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.68 (dd, *J* = 13.8, 11.0 Hz, 1H), 2.84 (dd, *J* = 17.2, 3.8 Hz, 1H), 2.96-3.03 (m, 1H), 3.16 (dd, *J* = 17.1, 7.8 Hz, 1H), 3.36-3.40 (m, 4H), 4.42 (s, 2H), 7.22-7.28 (m, 4H), 7.34-7.40 (m, 2H), 7.56 (dd, *J* = 7.5, 7.5 Hz, 1H), 7.78 (d, *J* = 7.7 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.3, 36.8, 49.0, 58.3, 74.6, 124.2, 126.7, 127.6, 128.2, 129.1, 134.9, 136.4, 136.8, 138.2, 153.8, 207.91. **HRMS** (ESI): Calcd. for $C_{18}H_{19}O_2^+$ ($[M+H]^+$): 267.1380, Found: 267.1383.

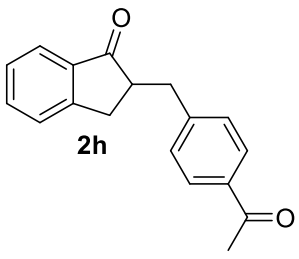



**2-(4-fluorobenzyl)-2,3-dihydro-1*H*-inden-1-one (2f):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 4-fluorophenylboronic acid pinacol ester (66.7 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2f** as a colorless

oil in 98% yield (23.6 mg, 0.098 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.70 (dd, *J* = 14.0, 10.0 Hz, 1H), 2.83 (dd, *J* = 17.1, 4.0 Hz, 1H), 2.93-3.00 (m, 1H), 3.18 (dd, *J* = 17.1, 7.8 Hz, 1H), 3.33 (dd, *J* = 14.0, 4.3 Hz, 1H), 6.95-7.00 (m, 2H), 7.18-7.21 (m, 2H), 7.35-7.41 (m, 2H), 7.57 (ddd, *J* = 7.7, 7.7, 1.0 Hz, 1H), 7.77 (d, *J* = 7.6 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.2, 36.2, 49.0, 115.4 (d, *J* = 21.0 Hz), 124.2, 126.7, 127.6, 130.5 (d, *J* = 7.8 Hz), 135.0, 135.3 (d, *J* = 3.2 Hz), 136.6, 153.6, 161.6 (d, *J* = 243 Hz), 207.7. **$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -116.9 (m, 1F). **HRMS** (ESI): Calcd. for $C_{16}H_{14}FO^+$ ($[M+H]^+$): 241.1023, Found: 241.1023.

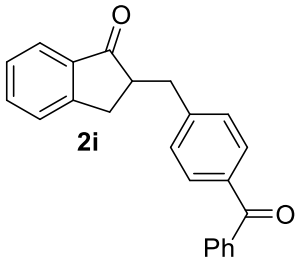



**2-(4-chlorobenzyl)-2,3-dihydro-1*H*-inden-1-one (2g):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 4-chlorophenylboronic acid pinacol ester (71.5 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2g** as a colorless oil in 85% yield (21.8 mg, 0.085 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.70 (dd, *J* = 14.0, 10.0 Hz, 1H), 2.83 (dd, *J* = 17.2, 4.2 Hz, 1H), 2.94-3.00 (m, 1H), 3.18 (dd, *J* = 17.1, 7.8 Hz, 1H), 3.34 (dd, *J* = 14.0, 4.4 Hz, 1H), 7.18 (d, *J* = 8.5, 2H), 7.26 (d, *J* = 8.5 Hz, 2H), 7.36-7.42 (m, 2H), 7.58 (td, *J* = 7.6, 1.2 Hz, 1H), 7.78 (d, *J* = 7.7 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.2, 36.4, 48.8, 124.3, 126.7, 127.7, 128.8, 130.4, 132.3, 135.1, 136.6, 138.1, 153.6, 207.6. **HRMS** (ESI): Calcd. for $C_{16}H_{14}ClO^+$ ($[M+H]^+$): 257.0728, Found: 257.0726.

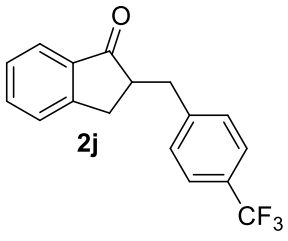



**2-(4-acetylbenzyl)-2,3-dihydro-1*H*-inden-1-one (2h):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 4-acetylboronic acid pinacol ester (73.8 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10

hexanes:EtOAc) to give **2h** as a white solid in 76 % yield (20.1 mg, 0.076 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.58 (s, 3H), 2.75-2.85 (m, 2H), 2.98-3.05 (m, 1H), 3.18 (dd, *J* = 17.1, 7.9 Hz, 1H), 3.42 (dd, *J* = 14.0, 4.4 Hz, 1H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.39 (dd, *J* = 7.5., 7.5 Hz, 2H), 7.58 (dd, *J* = 7.5, 7.5 Hz, 1H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.90 (d, *J* = 7.7 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 23.7, 32.2, 37.0, 48.6, 124.2, 126.7, 127.7, 128.8, 129.3, 135.1, 135.7, 136.5, 145.5, 153.5, 197.9, 207.4. **HRMS** (ESI): Calcd. for $C_{18}H_{17}O_2^+$ ([M+H]$^+$): 265.1223, Found: 265.1226.

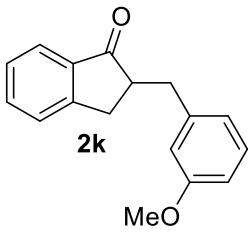



**2-(4-benzoylbenzyl)-2,3-dihydro-1*H*-inden-1-one (2i):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 4-benzoylphenylboronic acid pinacol ester (92.5 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 80:20 hexanes:EtOAc) to give **2i** as a white solid in 54% yield (17.5 mg, 0.054 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.80 (dd, *J* = 14.0, 10.2 Hz, 1H), 2.87 (dd, *J* = 17.1, 3.9 Hz, 1H), 3.02-3.08 (m, 1H), 3.22 (dd, *J* = 17.0, 7.8 Hz, 1H), 3.47 (dd, *J* = 17.0, 4.3 Hz, 1H), 7.36-7.43 (m, 4H), 7.47-7.50 (m, 2H), 7.57-7.61 (m, 2H), 7.75-7.80 (m, 5H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.3, 37.1, 48.7, 124.2, 126.7, 127.7, 128.4, 129.0, 130.1, 130.6, 132.4, 135.1, 135.9, 136.5, 137.8, 144.9, 153.5, 196.5, 207.4. **HRMS** (ESI): Calcd. for $C_{23}H_{19}O_2^+$ ([M+H]$^+$): 327.1380, Found: 327.1382.

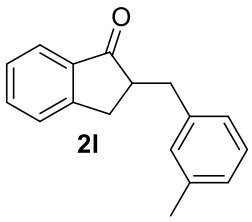



**2-(4-(trifluoromethyl)benzyl)-2,3-dihydro-1*H*-inden-1-one (2j):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 4-(trifluoromethyl)phenylboronic acid pinacol ester (81.6 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2j** as colorless oil in 69% yield (19.9 mg, 0.069 mmol). **$^1$H NMR**

(400 MHz, $CDCl_3$) δ 2.74-2.85 (m, 2H), 2.93-3.00 (m, 1H), 3.20 (dd, *J* = 17.0, 7.8 Hz, 1H), 3.43 (dd, *J* = 14.0, 4.3 Hz, 1H), 7.35-7.42 (m, 4H), 7.55-7.61 (m, 3H), 7.79 (d, *J* = 7.7 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.3, 36.9, 48.7, 110.2, 124.3, 125.6 (q, *J* = 3.8 Hz), 126.7, 127.8, 129.1 (q, *J* = 235 Hz), 129.4, 132.6, 135.2, 136.5, 143.9, 207.31. **$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -62.4 (s, 1F). **HRMS** (ESI): Calcd. for $C_{17}H_{14}F_3O^+$ ($[M+H]^+$): 291.0991, Found: 291.0992.

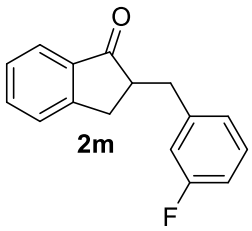



**2-(3-methoxybenzyl)-2,3-dihydro-1*H*-inden-1-one (2k):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 3-methoxyphenylboronic acid pinacol ester (70.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2k** as a colorless oil in 96% yield (24.3 mg, 0.096 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.64 (dd, *J* = 13.9, 10.5 Hz, 1H), 2.87 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.96-3.03 (m, 1H), 3.18 (dd, *J* = 17.2, 7.8 Hz, 1H), 3.38 (dd, *J* = 14.0, 4.2 Hz, 1H), 3.79 (s, 3H), 6.75-6.85 (m, 3H), 7.22 (dd, *J* = 7.9, 7.9 Hz, 1H), 7.35-7.42 (m, 2H), 7.57 (ddd, *J* = 7.6, 7.6, 1.2 Hz, 1H), 7.78 (d, *J* = 7.7 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.4, 37.2, 49.0, 55.3, 111.8, 114.7, 121.4, 124.2, 126.7, 127.6, 129.6, 135.0, 136.7, 141.4, 153.8, 160.0, 207.9. **HRMS** (ESI): Calcd. for $C_{17}H_{17}O_2^+$ ($[M+H]^+$): 253.1223, Found: 253.1227.

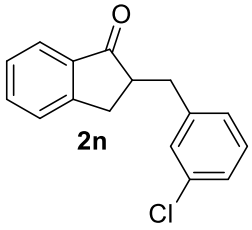



**2-(3-methylbenzyl)-2,3-dihydro-1*H*-inden-1-one (2l):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 3-tolylboronic acid pinacol ester (65.4 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2l** as a white solid in

85% yield (20.0 mg, 0.085 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.34 (s, 3), 2.61 (dd, *J* = 13.9, 10.6 Hz, 1H), 2.86 (dd, *J* = 17.2, 3.9 Hz, 1H), 2.96-3.03 (m, 1H), 3.17 (dd, *J* = 17.2, 7.7 Hz, 1H), 3.38 (dd, *J* = 13.9, 4.1 Hz, 1H), 7.03-7.07 (m, 3H), 7.19 (dd, *J* = 7.5 Hz, 1H), 7.36-7.42 (m, 2H), 7.58 (d, *J* = 7.7 Hz, 1H) 7.79 (d, *J* = 7.6 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 21.5, 32.4, 37.1, 49.1, 124.1, 126.0, 126.8, 127.2, 127.6, 128.6, 129.8, 134.8, 136.7, 138.3, 139.8, 153.8, 208.0. **HRMS** (ESI): Calcd. for $C_{17}H_{17}O^+$ ($[M+H]^+$): 237.1274, Found: 237.1276.

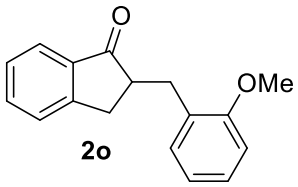



**2-(3-fluorobenzyl)-2,3-dihydro-1*H*-inden-1-one (2m):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 3-fluorophenylboronic acid pinacol ester (66.7 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2m** as a colorless oil in 67% yield (16.1 mg, 0.067 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.68 (dd, *J* = 14.0, 10.3 Hz, 1H), 2.84 (dd, *J* = 17.1, 4.1 Hz, 1H), 2.95-3.02 (m, 1H), 3.20 (dd, *J* = 17.2, 7.8 Hz, 1H), 3.38 (dd, *J* = 14.0, 4.3 Hz, 1H), 6.89-6.97 (m, 2H), 7.02 (d, *J* = 7.6 Hz, 1H), 7.23-7.28 (m, 1H), 7.36-7.42 (m, 2H), 7.58 (ddd, *J* = 7.7, 7.7, 1.1 Hz, 1H), 7.78 (d, *J* = 7.7 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.3, 36.8, 48.8, 113.4 (d, *J* = 21.0 Hz), 115.9 (d, *J* = 21.0 Hz), 124.2, 124.7 (d, *J* = 2.8 Hz), 126.7, 127.7, 130.1 (d, *J* = 8.3 Hz), 135.6, 136.6, 142.3 (d, *J* = 7.2 Hz), 153.6, 163.0 (d, *J* = 245 Hz), 207.5. **$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -113.3 (m, 1F). **HRMS** (ESI): Calcd. for $C_{16}H_{14}FO^+$ ($[M+H]^+$): 241.1023, Found: 241.1023.



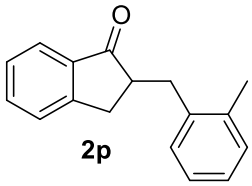

**2-(3-chlorobenzyl)-2,3-dihydro-1*H*-inden-1-one (2n):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 3-chlorophenylboronic acid pinacol ester (71.6

mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2n** as a colorless oil in 54% yield (13.9 mg, 0.054 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.65 (dd, *J* = 14.0, 10.4 Hz, 1H), 2.84 (dd, *J* = 17.0, 4.1 Hz, 1H), 2.95-3.01 (m, 1H), 3.20 (dd, *J* = 17.2, 7.7 Hz, 1H), 3.37 (dd, *J* = 14.1, 4.2 Hz, 1H), 7.13 (ddd, *J* = 7.0, 1.7, 1.7 Hz, 1H), 7.18-7.25 (m, 3H), 7.36-7.43 (m, 2H), 7.58 (ddd, *J* = 7.6, 7.6, 1.2 Hz, 1H), 7.78 (d, *J* = 7.7 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.3, 36.8, 48.8, 124.2, 126.74, 126.75, 127.2, 127.7, 129.1, 130.0, 134.4, 135.1, 136.6, 141.9, 153.5, 207.4. **HRMS** (ESI): Calcd. for $C_{16}H_{14}ClO^+$ ($[M+H]^+$): 257.0728, Found: 257.0725.



**2o**

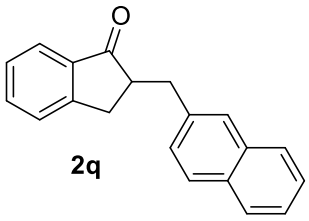
**2-(2-methoxybenzyl)-2,3-dihydro-1*H*-inden-1-one (2o):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 2-methoxyphenylboronic acid pinacol ester (70.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2o** as a colorless oil in 50% yield (12.6 mg, 0.050 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.63 (dd, *J* = 13.6, 9.9 Hz, 1H), 2.86 (dd, *J* = 20.5, 7.2 Hz, 1H), 3.07-3.16 (m, 2H), 3.42 (dd, *J* = 13.6, 4.2 Hz, 1H), 3.82 (s, 3H), 6.86-6.92 (m, 2H), 7.17-7.24 (m, 2H), 7.34-7.40 (m, 2H), 7.56 (ddd, *J* = 7.6, 7.6, 1.2 Hz, 1H) 7.78 (d, *J* = 7.9 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 31.9, 32.5, 47.7, 55.3, 110.4, 120.6, 124.1, 126.7, 127.4, 127.8, 128.3, 130.6, 134.7, 136.9, 154.0, 157.9, 208.5. **HRMS** (ESI): Calcd. for $C_{17}H_{17}O_2^+$ ($[M+H]^+$): 253.1223, Found: 253.1221.



**2p**

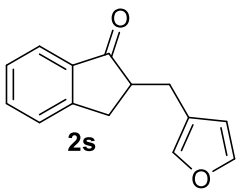
**2-(2-methylbenzyl)-2,3-dihydro-1*H*-inden-1-one (2p):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 2-

tolylboronic acid pinacol ester (65.4 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2p** as a colorless oil in 90% yield (21.3 mg, 0.090 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.38 (s, 3H), 2.59 (dd, *J* = 14.5, 11.1 Hz, 1H), 2.87 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.99-3.06 (m, 1H), 3.21 (dd, *J* = 17.2, 7.8 Hz, 1H), 3.49 (dd, *J* = 14.5, 4.1 Hz, 1H), 7.14-7.21 (m, 4H), 7.37-7.44 (m, 2 H), 7.59 (ddd, *J* = 7.6, 7.6, 1.1 Hz, 1H) 7.81 (d, *J* = 7.6 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 19.6, 32.8, 34.6, 47.7, 124.1, 124.3, 126.1, 126.6, 126.8, 127.5, 129.1, 130.6, 135.0, 136.6, 138.1, 153.7, 208.1. **HRMS** (ESI): Calcd. for $C_{17}H_{17}O^+$ ($[M+H]^+$): 237.1274, Found: 237.1273.



**2q**

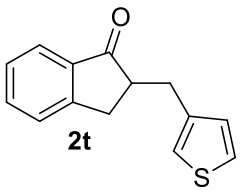
**2-(naphthalen-2-ylmethyl)-2,3-dihydro-1*H*-inden-1-one (2q):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 2-naphthylboronic acid pinacol ester (76.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 DCM:EtOAc to 90:10 DCM:EtOAc) to give **2q** as a white solid in 99% (27.0 mg, 0.099 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.84 (dd, *J* = 14.1, 10.0 Hz, 1H), 2.92 (dd, *J* = 16.5, 3.2 Hz, 1H), 3.06-3.23 (m, 2H), 3.57 (dd, *J* = 14.1, 4.1 Hz, 1H), 7.34-7.50 (m, 5H), 7.57 (dt, *J* = 7.7, 1.2 Hz, 1H), 7.68 (broad s, 1H), 7.76-7.84 (m, 4H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.3, 37.3, 49.0, 124.2, 125.6, 126.2, 126.7, 127.4, 127.5, 127.6, 127.61, 127.8, 128.4, 132.3, 133.7, 135.0, 136.7, 137.3, 153.8, 208.0. **HRMS** (ESI): Calcd. for $C_{20}H_{16}O^+Na$ ($[M+Na]^+$): 295.1093, Found: 295.1057.



**2s**

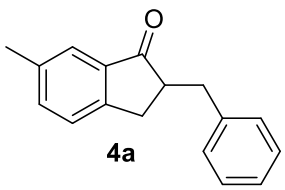
**2-(furan-3-ylmethyl)-2,3-dihydro-1*H*-inden-1-one (2s):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 3-furanylboronic acid pinacol ester (58.2 mg, 0.300 mmol). The crude reaction mixture was purified

by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2s** as a colorless oil in 63% yield (13.4 mg, 0.063 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.67 (dd, *J* = 14.2, 8.8 Hz, 1H), 2.89 (dd, *J* = 16.6, 4.2 Hz, 1H), 2.87-2.95 (m, 2H), 3.08 (dd, *J* = 14.2, 3.7 Hz, 1H), 3.26 (dd, *J* = 16.6, 7.2 Hz, 1H), 6.27 (s, 1H), 7.32 (t, *J* = 1.6 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.42 (d, *J* = 7.7 Hz, 1H), 7.57 (td, *J* = 7.6, 1.2 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 26.2, 32.4, 47.8, 111.3, 122.3, 124.1, 126.7, 127.6, 135.0, 136.8, 139.8, 143.1, 153.8, 208.0. **HRMS** (ESI): Calcd. for $C_{14}H_{13}O_2^+$ ($[M+H]^+$): 213.0910, Found: 213.0916.



**2t**

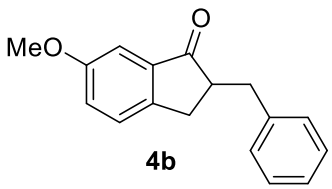
**2-(thiophen-3-ylmethyl)-2,3-dihydro-1*H*-inden-1-one (2t):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **1a** (35.1 mg, 0.100 mmol) and 3-thienylboronic acid pinacol ester (63.0 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **2t** as a white solid in 88% yield (20.1 g, 0.088 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.82 (dd, *J* = 14.4, 9.8 Hz, 1H), 2.88 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.96-3.02 (m, 1H), 3.25 (dd, *J* = 17.2, 7.7 Hz, 1H), 3.33 (dd, *J* = 14.4, 4.1 Hz, 1H), 6.98 (dd, *J* = 4.9, 1.2 Hz, 1H), 7.00-7.02 (m, 1H), 7.25 (dd, *J* = 4.9, 3.0 Hz, 1H), 7.37 (t, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 7.7 Hz, 1H), 7.57 (td, *J* = 7.6, 1.2 Hz, 1H), 7.77 (d, *J* = 7.7 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 31.5, 32.5, 48.3, 121.5, 124.1, 125.8, 126.7, 127.5, 128.4, 134.9, 136.7, 139.8, 153.8, 207.9. **HRMS** (ESI): Calcd. for $C_{14}H_{13}OS^+$ ($[M+H]^+$): 229.0682, Found: 222.0684.



**4a**

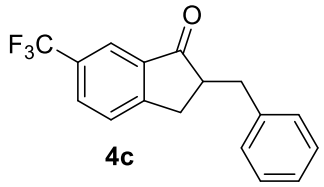
**2-benzyl-6-methyl-2,3-dihydro-1*H*-inden-1-one (4a):** Prepared according to general procedure C from *tert*-butyl (2-allyl-5-methyl)(benzyl)carbamate **3a** (36.5 mg, 0.100 mmol) and phenylboronic acid pinacol ester (61.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash

column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **4a** as a colorless oil in 92% yield (21.7 mg, 0.092 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 2.66 (dd, *J* = 14.0, 10.4 Hz, 1H), 2.81 (dd, *J* = 17.0, 3.8 Hz, 1H), 2.97-3.04 (m, 1H), 3.13 (dd, *J* = 17.0, 7.8 Hz, 1H), 3.40 (dd, *J* = 14.0, 4.2 Hz, 1H), 7.21-7.36 (m, 6H), 7.40 (dd, *J* = 7.8. 1.1 Hz, 1H), 7.59 (s, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 21.2, 32.0, 37.2, 49.4, 124.1, 126.4, 126.4, 128.6, 129.0, 136.2, 136.8, 137.5, 139.9, 151.1, 208.1. **HRMS** (ESI): Calcd. for $C_{17}H_{17}O^+$ ($[M+H]^+$): 237.1274, Found: 237.1270.



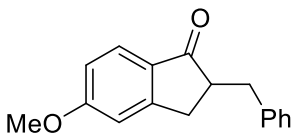
**4b**

**2-benzyl-6-methoxy-2,3-dihydro-1*H*-inden-1-one (4b):** Prepared according to a modified version of general procedure C from *tert*-butyl (2-allyl-5-methoxy)(benzyl)carbamate **3b** (38.1 mg, 0.100 mmol) and phenylboronic acid pinacol ester (61.2 mg, 0.300 mmol). Upon completion of the reaction, the reaction mixture was filtered through a short plug of silica gel. The filtrate was concentrated under reduced pressure. To the crude product was dissolved in DCM (2.0 mL). The resulting solution was cooled to 0 °C, and TFA (0.400 mL) was added slowly. The mixture was allowed to warm to room temperature and stirred for 1 h. The reaction was concentrated under reduced pressure. The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **4b** as a white solid in 96% yield (24.0 mg, 0.096 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.66 (dd, *J* = 14.0, 10.2 Hz, 1H), 2.78 (dd, *J* = 16.4, 3.2 Hz, 1H), 2.97-3.07 (m, 1H), 3.09 (dd, *J* = 16.4, 7.6 Hz, 1H), 3.39 (dd, *J* = 14.0, 4.2 Hz, 1H), 3.84 (s, 3H), 7.17 (dd, *J* = 8.3, 2.5 Hz, 1H), 7.19-7.33 (m, 6H) **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 31.6, 37.2, 49.8, 55.7, 105.2, 124.4, 126.5, 127.4, 128.6, 129.0, 137.8, 139.8, 146.6, 159.5, 208.0 **HRMS** (ESI): Calcd. for $C_{17}H_{17}O_2^+$ ($[M+H]^+$): 253.1223, Found: 253.1226.



**4c**

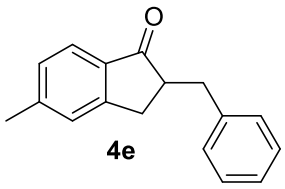
**2-benzyl-6-(trifuoromethyl)-2,3-dihydro-1*H*-inden-1-one (4c):** Prepared according to general procedure C from *tert*-butyl (2-allyl-5-(trifluoromethyl)benzoyl)(benzyl)carbamate **3c** (41.9 mg, 0.100 mmol) and phenylboronic acid pinacol ester (61.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **4c** as a white solid in 51% yield (14.8 mg, 0.051 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.73 (dd, *J* = 14.0, 10.1 Hz, 1H), 2.93 (dd, *J* = 17.6, 4.0 Hz, 1H), 3.05-3.12 (m, 1H), 3.24 (dd, *J* = 17.6, 7.9 Hz, 1H), 3.40 (dd, *J* = 14.0, 4.4 Hz, 1H), 7.21-7.25(m, 3H), 7.28-7.34 (m, 2H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.81 (dd, *J* = 8.0, 1.3 Hz, 1H), 8.04 (s, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.3, 36.9, 49.4, 121.4 (q, *J* = 4.0 Hz, 1H), 126.6 (q, *J* = 274 Hz, 1C), 126.7, 127.5, 128.8, 129.0. 130.5 (q, *J* = 33.3 Hz, 1C), 131.4 (q, *J* = 3.0 Hz, 1C), 137.1, 139.2, 156.9, 206.6. **$^{19}$F NMR** ($CDCl_3$, 376 MHz): δ -62.5 (s, 1F). **HRMS** (ESI): Calcd. for $C_{17}H_{14}F_3O^+$ ($[M+H]^+$): 291.0991, Found: 291.0995.



**4d**

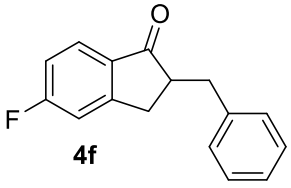
**2-benzyl-5-methoxy-2,3-dihydro-1*H*-inden-1-one (4d):** Prepared according to general procedure C from *tert*-butyl (2-allylbenzoyl)(benzyl)carbamate **3d** (38.1 mg, 0.100 mmol) and phenylboronic acid pinacol ester (61.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **4d** as a white solid in 88% yield (22.2 mg, 0.088 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.65 (dd, *J* = 14.0, 10.4 Hz, 1H), 2.80 (dd, *J* = 17.2, 3.8 Hz, 1H), 2.96-3.02 (m, 1H), 3.11 (dd, *J* = 17.2, 7.8 Hz, 1H), 3.39 (dd, *J* = 14.0, 4.2 Hz, 1H), 3.86 (s, 3H), 6.82 (s, 1H), 6.90 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.19-7.32 (m, 5H), 7.72 (d, *J* = 8.5 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.3, 37.3, 49.2, 55.7, 109.8,

115.5, 125.8, 126.4, 128.6, 129.0, 129.9, 139.9, 156.7, 165.5, 206.1. **HRMS** (ESI): Calcd. for $C_{17}H_{17}O_2^+$ ($[M+H]^+$): 253.1223, Found: 253.1226.



**4e**

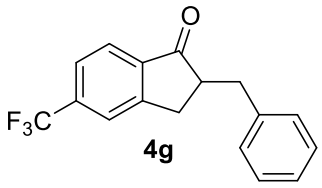
**2-benzyl-5-methyl-2,3-dihydro-1*H*-inden-1-one (4e):** Prepared according to general procedure C from *tert*-butyl (2-allyl-4-methylbenzoyl)(benzyl)carbamate **3e** (36.5 mg, 0.100 mmol) and phenylboronic acid pinacol ester (61.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **4e** as a colorless oil in 97% yield (22.9 mg, 0.097 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.42 (s, 3H), 2.65 (dd, *J* = 14.0, 10.5 Hz, 1H), 2.81 (dd, *J* = 17.1, 3.7 Hz, 1H), 2.95-3.02 (m, 1H), 3.11 (dd, *J* = 17.1, 7.7 Hz, 1H), 3.39 (dd, *J* = 13.9, 4.1 Hz, 1H), 7.17-7.32 (m, 7H), 7.68 (d, *J* = 7.8 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 22.2, 32.1, 37.3, 49.2, 123.9, 126.4, 127.0, 128.6, 128.8, 129.1, 134.4, 139.9, 146.1, 154.3, 207.4. **HRMS** (ESI): Calcd. for $C_{17}H_{17}O^+$ ($[M+H]^+$): 237.1274, Found: 237.1276.



**4f**

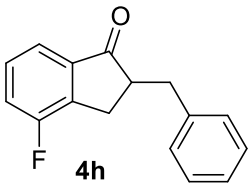
**2-benzyl-5-fluoro-2,3-dihydro-1*H*-inden-1-one (4f):** Prepared according to general procedure C from *tert*-butyl (2-allyl-4-fluorobenzoyl)(benzyl)carbamate **3f** (36.9 mg, 0.100 mmol) and phenylboronic acid pinacol ester (61.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **4f** as a yellow oil in 99% yield (23.8 mg, 0.099 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.69 (dd, *J* = 14.0, 10.2 Hz, 1H), 2.85 (dd, *J* = 17.3, 3.8 Hz, 1H), 2.98-3.07 (m, 1H), 3.15 (dd, *J* = 17.3, 7.8 Hz, 1H), 3.38 (dd, *J* = 14.0, 4.3 Hz, 1H), 7.02-7.95 (m, 2H), 7.19-7.25 (m, 3H), 7.27-7.33 (m, 2H), 7.78 (dd, *J* = 8.2, 5.3 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.2 (d, *J* = 2.0 Hz, 1C), 37.1, 49.3,

113.3 (d, $J$ = 22.2 Hz, 1C), 115.9 (d, $J$ = 24.2 Hz, 1C), 126.4 (d, $J$ = 11.1 Hz, 1C), 126.6, 128.7, 129.0, 133.1 (d, $J$ = 2.0 Hz, 1C), 139.4, 156.6 (d, $J$ = 10.1 Hz, 1C), 167.3 (d, $J$ = 257.6 Hz, 1C), 206.0. **$^{19}$F NMR** ($CDCl_3$, 376 MHz): δ -102.7 (m, 1F). **HRMS** (ESI): Calcd. for $C_{16}H_{14}FO^+$ ($[M+H]^+$): 241.1023, Found: 241.1027.



**4g**

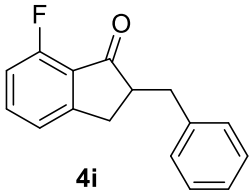
**2-benzyl-5-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4g):** Prepared according to general procedure C from *tert*-butyl(2-allyl-4-(trifluoromethyl)(benzyl)carbamate **3g** (41.9 mg, 0.100 mmol) and phenylboronic acid pinacol ester (61.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **4g** as a white solid in 85% yield (24.7 mg, 0.085 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.73 (dd, $J$ = 14.0, 10.1 Hz, 1H), 2.93 (dd, $J$ = 17.4, 4.0 Hz, 1H), 3.03-3.11 (m, 1H), 3.24 (dd, $J$ = 17.4, 7.8 Hz, 1H), 3.39 (dd, $J$ = 14.0, 4.4 Hz, 1H), 7.20-7.25 (m, 3H), 7.28-7.34 (m, 2H), 7.63 (d, $J$ = 8.0 Hz, 1H), 7.67 (s, 1H), 7.88 (d, $J$ = 8.0 Hz, 1H) **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.2, 36.9, 49.4, 123.9 (q, $J$ = 4.0 Hz, 1C), 124.7, 125.2 (q, $J$ = 4.0 Hz, 1C), 126.5 (q, $J$ = 274.7 Hz, 1C), 126.7, 128.8, 129.0, 136.2 (q, $J$ = 31.3 Hz, 1C), 139.2, 139.31-139.35 (m, 1C), 153.8, 206.9. **$^{19}$F NMR** ($CDCl_3$, 376 MHz): δ -62.9 (s, 3F). **HRMS** (ESI): Calcd. for $C_{17}H_{14}F_3O^+$ ($[M+H]^+$): 291.0991, Found: 291.0978.



**4h**

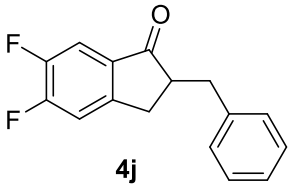
**2-benzyl-4-fluoro-2,3-dihydro-1*H*-inden-1-one (4h):** Prepared according to general procedure C from *tert*-butyl(2-allyl-3-fluorobenzoyl)(benzyl)carbamate **3h** (36.9 mg, 0.100 mmol) and phenylboronic acid pinacol ester (61.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **4h** as a

yellow oil in 95% yield (22.8 mg, 0.095 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.71 (dd, *J* = 14.0, 10.2 Hz, 1H), 2.85 (dd, *J* = 17.5, 4.0 Hz, 1H), 3.00-3.06 (m, 1H), 3.20 (dd, *J* = 17.5, 7.8 Hz, 1H), 3.39 (dd, *J* = 14.0, 4.3 Hz, 1H), 7.21-7.27 (m, 4H), 7.29-7.33 (m, 2H), 7.34-7.39 (m, 1H), 7.58 (d, *J* = 7.5 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 28.0, 37.0, 49.0, 119.9, 121.0 (d, *J* = 20.2 Hz, 1C), 126.6, 128.7, 129.0, 129.5 (d, *J* = 6.1 Hz, 1C), 139.3, 139.5 (d, *J* = 8.1 Hz, 1C), 139.6 (d, *J* = 8.1 Hz, 1C), 160.2 (d, *J* = 251.5 Hz, 1C), 206.6. **$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -118.9 (m, 1F). **HRMS** (ESI): Calcd. for $C_{16}H_{14}FO^+$ ($[M+H]^+$): 241.1023, Found: 241.1019.



**4i**

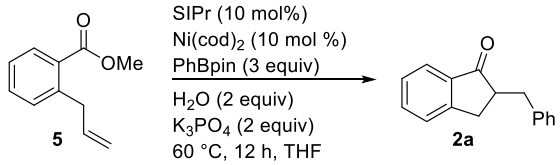
**2-benzyl-4-fluoro-2,3-dihydro-1*H*-inden-1-one (4i):** Prepared according to general procedure C from *tert*-butyl(2-allyl-6-fluorobenzoyl)(benyl)carbamate **3i** (36.9 mg, 0.100 mmol) and phenylboronic acid pinacol ester (61.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **4i** as a yellow oil in 84% yield (20.2 mg, 0.084 mmol). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 2.70 (dd, *J* = 14.0, 10.2 Hz, 1H), 2.87 (dd, *J* = 17.3, 4.2 Hz, 1H), 3.00-3.06 (m, 1H), 3.17 (dd, *J* = 17.3, 7.9 Hz, 1H), 3.39 (dd, *J* = 14.0, 4.3 Hz, 1H), 6.97 (t, *J* = 9.0 Hz, 1H), 7.16 (d, *J* = 7.3 Hz, 1H), 7.19-7.33 (m, 5H), 7.54 (m, 1H) **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 32.2, 37.0, 49.6, 114.4 (d, *J* = 19.2 Hz, 1C), 122.5 (d, *J* = 5.1 Hz, 1C), 124.5 (d, *J* = 13.1 Hz, 1C), 126.6, 128.7, 129.1, 136.7-136.9 (m, 1C), 139.4, 155.8 (d, *J* = 2.0 Hz, 1C), 159.2 (d, *J* = 265.6 Hz, 1C), 204.1 (d, *J* = 1.0 Hz, 1C). **$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -114.4 (m, 1F). **HRMS** (ESI): Calcd. for $C_{16}H_{14}FO^+$ ($[M+H]^+$): 241.1023, Found: 241.1018.



**4j**

**2-benzyl-5,6-difluoro-2,3-dihydro-1*H*-inden-1-one (4j):** Prepared according to general procedure C from *tert*-butyl(2-allyl-4,5-difluorobenzoyl)(benyl)carbamate **3j** (38.7 mg, 0.100 mmol) and phenylboronic acid pinacol ester (61.2 mg, 0.300 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **4j** as a off-white solid in 46% yield (11.9 mg, 0.046 mmol). **$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 2.70 (dd, *J* = 14.0, 10.0 Hz, 1H), 2.82 (dd, *J* = 17.0, 1.2 Hz, 1H), 2.99-3.08 (m, 1H), 3.13 (ddd, *J* = 17.0, 7.7, 0.6 Hz, 1H), 3.36 (dd, *J* = 14.0, 4.3 Hz, 1H), 7.17 (dd, *J* = 9.4, 6.7 Hz, 1H), 7.20-7.24 (m, 3H), 7.27-7.33 (m, 2H), 7.54 (dd, *J* = 8.2, 0.4 Hz, 1H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 31.8 (d, *J* = 1.0 Hz, 1C), 40.0, 49.4 (d, *J* = 1.0 Hz, 1C), 112.2 (dd, *J* = 17.2, 2.0 Hz, 1C), 114.9 (d, *J* = 18.2 Hz, 1C), 126.7, 128.7, 129.0, 133.0 (dd, *J* = 6.1, 3.0 Hz, 1C), 139.1, 150.3 (dd, *J* = 8.1, 3.0 Hz, 1C), 150.8 (dd, *J* = 252.5, 14.1 Hz, 1C), 155.4 (dd, *J* = 260.6, 14.1 Hz, 1C), 205.7 (d, *J* = 2.0 Hz, 1C). **$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -136.8 (m, 1F), -125.2 (m, 1F). **HRMS** (ESI): Calcd. for $C_{16}H_{13}F_2O^+$ ($[M+H]^+$): 259.0929, Found: 259.0918.

**Nickel-Catalyzed Carboacylation of Methyl-2-Allylbenzoate 5**

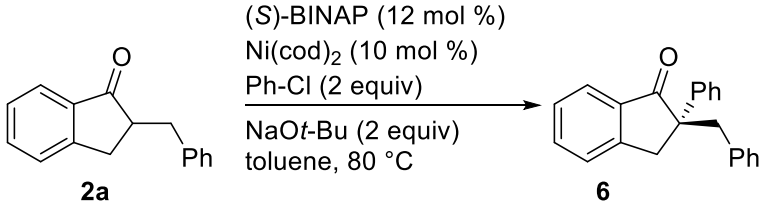


**5** **2a**

A 1-dram vial was charged with 0.100 mmol of methyl 2-allylbenzoate **5** (17.6 mg, 0.100 mmol), $Ni(cod)_2$ (2.8 mg, 0.010 mmol), SIPr (3.9 mg, 0.010 mmol), $K_3PO_4$ (42.5 mg, 0.200 mmol), $H_2O$ (3.6 μL, 0.20 mmol), phenylboronic acid pinacol ester (61.2 mg, 0.300 mmol), and THF (0.100 mL). The resulting solution stirred at 60 °C for 12 hours. Upon completion of the reaction, the

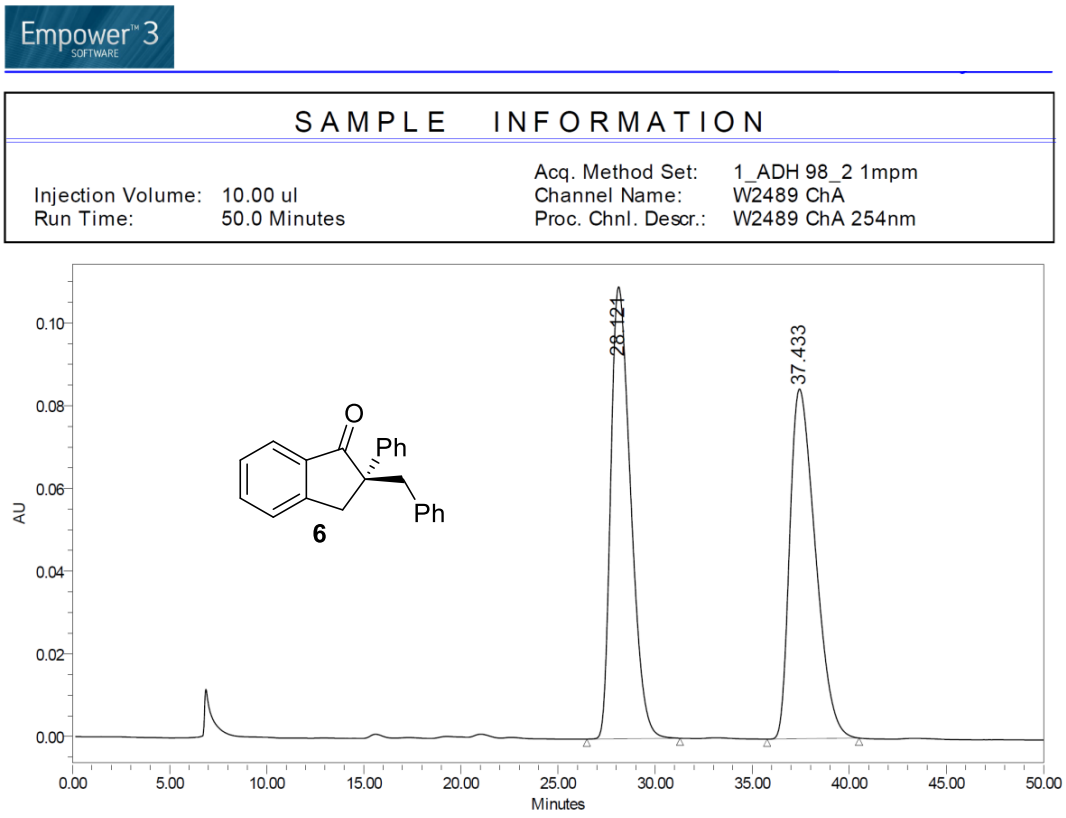
reaction mixture was filtered through a plug of silica with 70:30 hexanes:EtOAc. The crude product was purified by column chromatography with a gradient of 100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc over a 25 minute period on a Combiflash system to **2a** as colorless oil in 50% yield (11.0 mg, 0.049 mmol). NMR data match those reported for synthesis of **2a** from benzamide **1a**.

**Enantioselective α-Arylation of 2a to Form (*S*)-2-Benzyl-2-phenyl-2,3-dihydro-1*H*-inden-1-one 6**




2-Benzyl-2-phenyl-2,3-dihydro-1*H*-inden-1-one **6** was prepared according to a known literature procedure.[3] Inside of a glovebox, to a 1-dram vial containing a magnetic stir bar was added $Ni(cod)_2$ (5.5 mg, 0.020 mmol), (*S*)-BINAP (14.9 mg, 0.024 mmol), NaO*t*Bu (38.4 mg, 0.400 mmol), chlorobenzene (40.5 μL, 0.400 mmol), **2a** (44.5 mg, 0.200 mmol), and toluene (1.00 mL). The vial was sealed with a cap containing a PTFE septum and removed from the glovebox. The reaction was stirred at 80 °C for 36 h. Upon completion, the reaction was cooled to room temperature. The reaction was quenched with a saturated aqueous $NH_4Cl$ solution and extracted with $Et_2O$ (2 x 10 mL). The combined organic layers were dried over $Na_2SO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by flash column chromatography (98:2, hexanes:EtOAc) to give **6** as a white solid in 65% yield (39.0 mg, 0.130 mmol). The enantiomeric excess was determined by HPLC analysis (254 nm, 25 °C) $t_R$ 27.2 min (minor); $t_R$ 36.0 min (major) [Chiracel AD-H (0.46 cm x 25 cm)(from Daicel Chemical Ind., Ltd.)

hexane/*i*-PrOH, 98:2, 1.0 mL/min] to be 98% ee. NMR data are consistent with known literature values.[3]

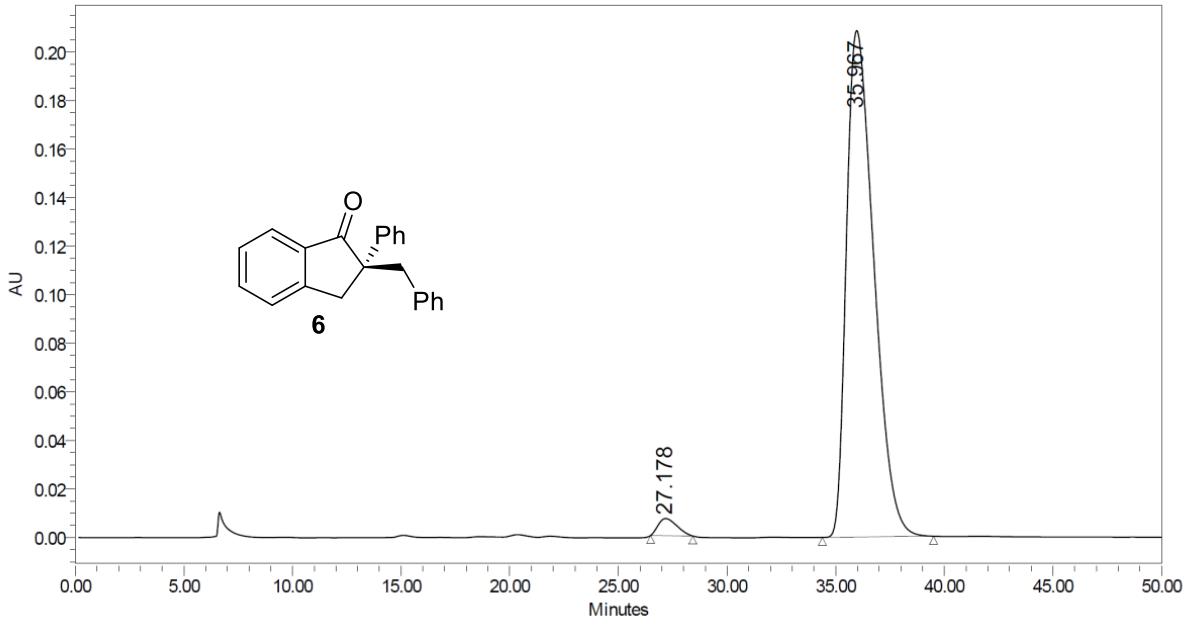



| | RT | Area | % Area | Height | Int Type |
|---|---|---|---|---|---|
| 1 | 28.121 | 7785708 | 50.28 | 109316 | bb |
| 2 | 37.433 | 7700176 | 49.72 | 84584 | bb |

Empower™ 3 SOFTWARE

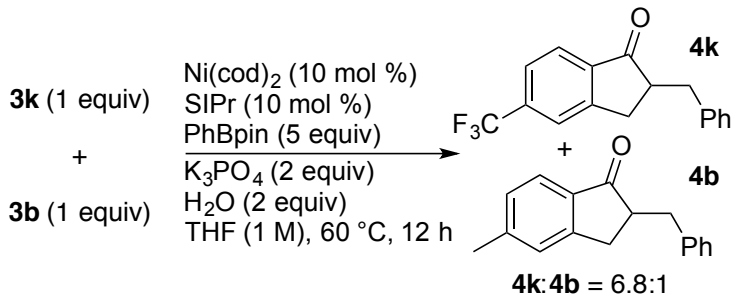
## SAMPLE INFORMATION

| | | | |
|---|---|---|---|
| Injection Volume: | 10.00 ul | Acq. Method Set: | 1_ADH 98_2 1mpm |
| Run Time: | 50.0 Minutes | Channel Name: | W2489 ChA |
| | | Proc. Chnl. Descr.: | W2489 ChA 254nm |

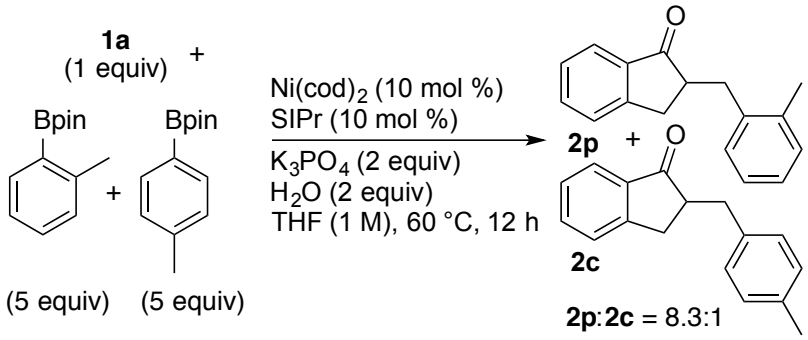



| | RT | Area | % Area | Height | Int Type |
|---|---|---|---|---|---|
| 1 | 27.178 | 420907 | 2.25 | 7035 | bb |
| 2 | 35.967 | 18255606 | 97.75 | 208617 | bb |

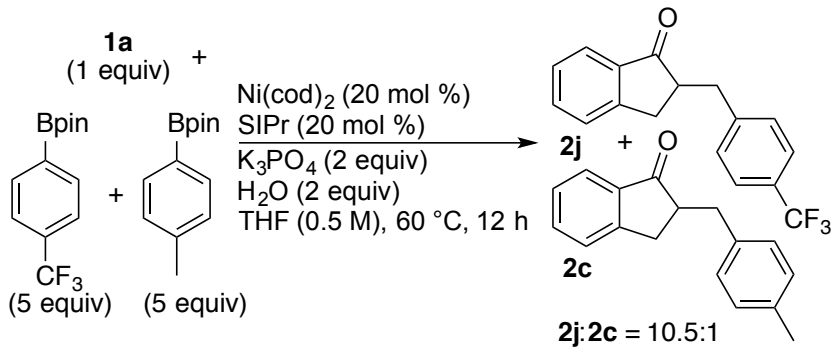
**Experimental Procedures for Competition Experiments:**



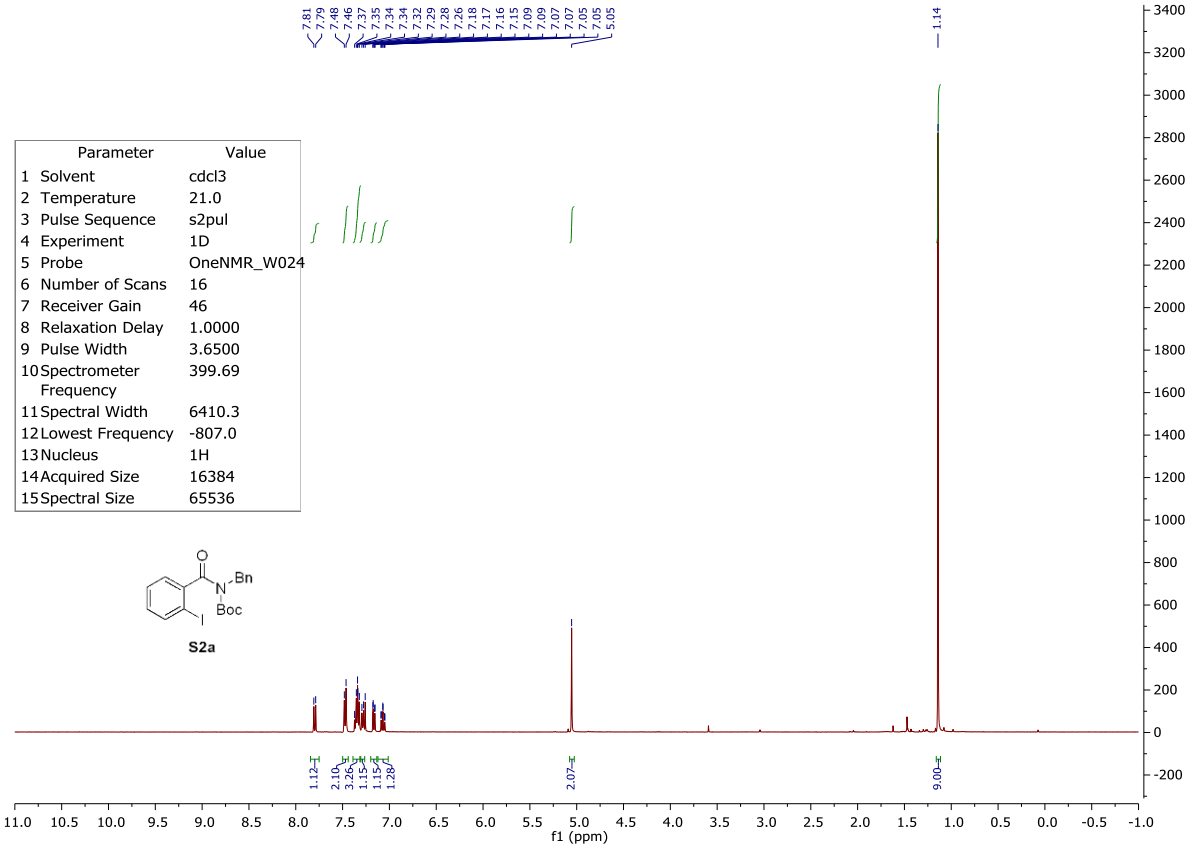

A competition experiment generating 2-benzyl-2,3-dihydro-1*H*-inden-1-ones **4b** and **4k** was carried out by the following procedure. A 1-dram vial was charged with *o*-allylbenzamides **3b** (36.5 mg, 0.100 mmol) and **3k** (41.9 mg, 0.100 mmol), $Ni(cod)_2$ (2.8 mg, 0.010 mmol), SIPr (3.9 mg, 0.010 mmol), $K_3PO_4$ (42.4 mg, 0.200 mmol), $H_2O$ (3.6 μL, 0.20 mmol), phenylboronic acid pinacol ester (102 mg, 0.500 mmol), and THF (0.10 mL). The resulting solution was stirred at 60 °C for 12 hours. Upon completion of the reaction, the reaction mixture was filtered through a plug of silica with hexanes:EtOAc (70:30), and concentrated under reduced pressure. The crude mixture was dissolved in $CDCl_3$ with $CH_2Br_2$ as internal standard. The ratio of products **4k:4b** was determined to be 6.8:1 by $^1H$ NMR spectroscopy. The NMR yields of **4k** and **4b** were determined to be 75% and 11%, respectively.

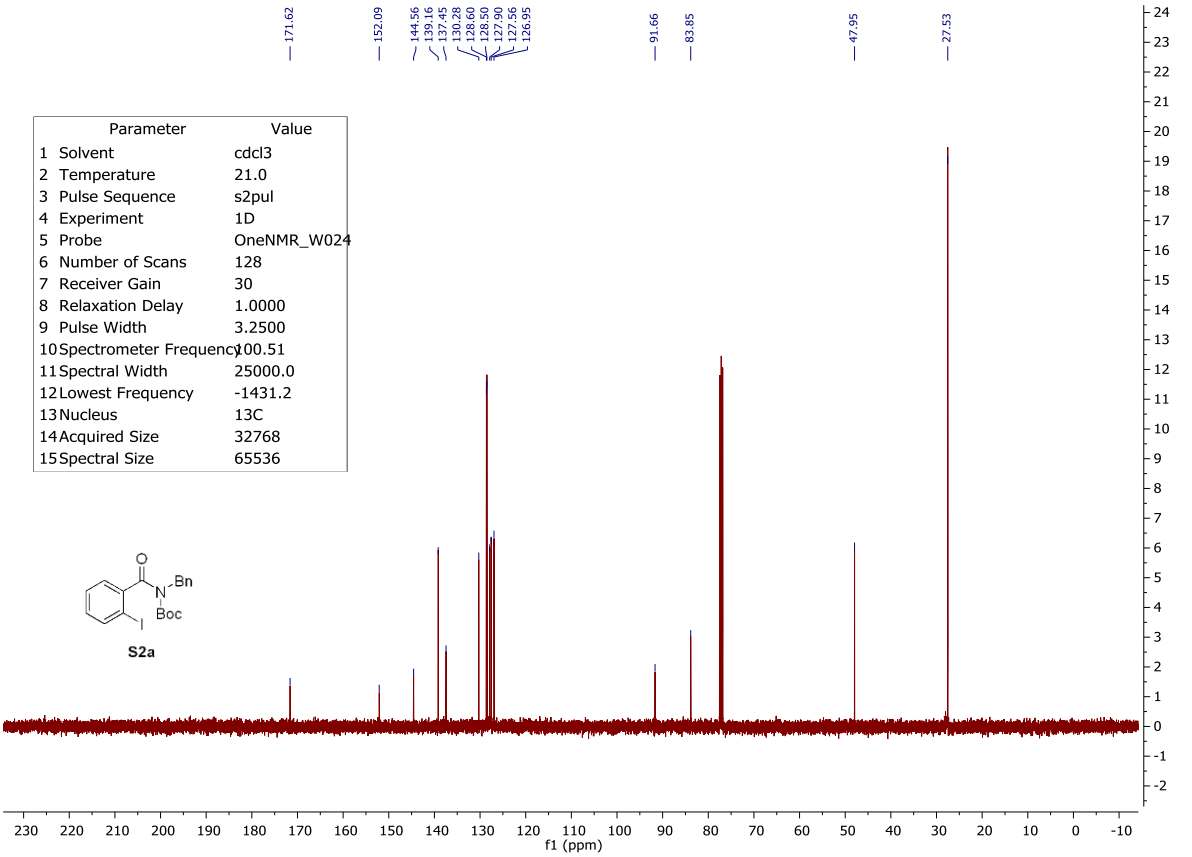


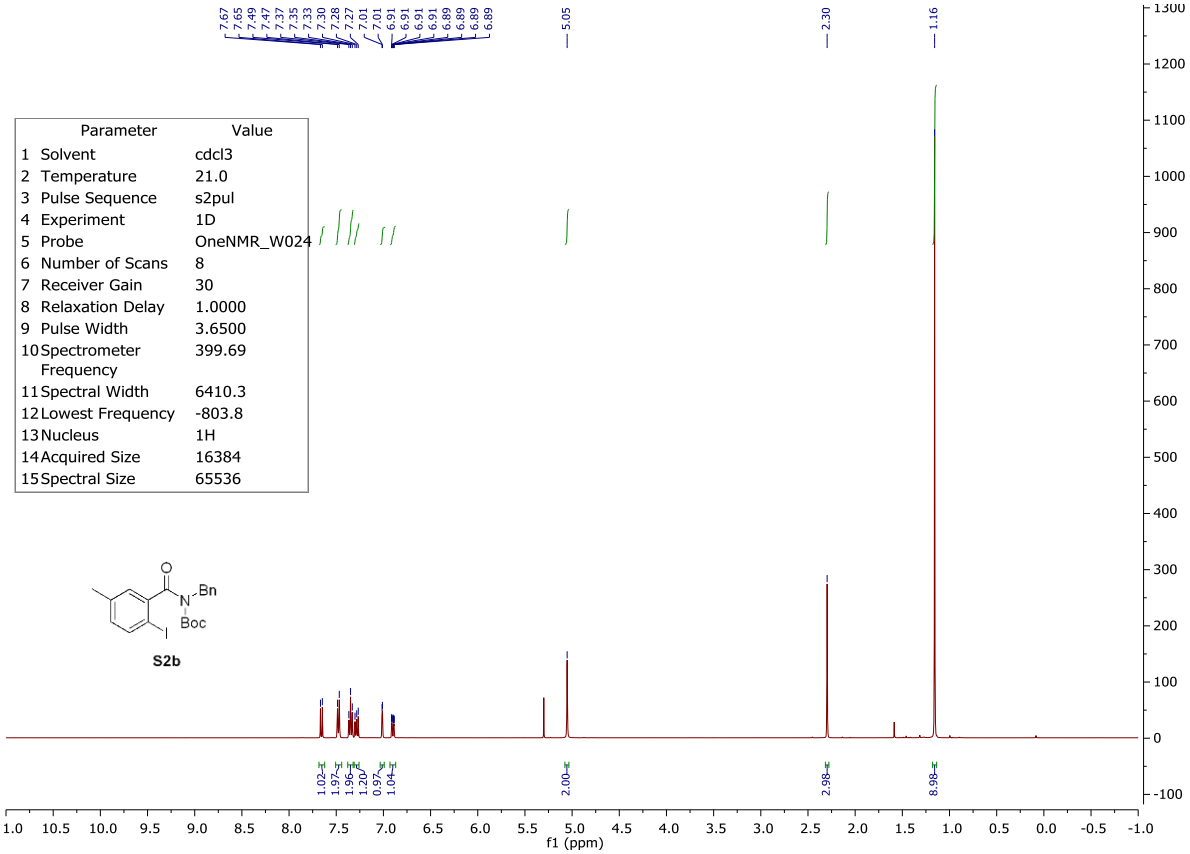

A competition experiment generating 2-benzyl-2,3-dihydro-1*H*-inden-1-ones **2p** and **2c** was carried out by the following procedure. A 1-dram vial was charged with *o*-allylbenzamide **1a** (35.1 mg, 0.100 mmol), $Ni(cod)_2$ (2.8 mg, 0.010 mmol), SIPr (3.9 mg, 0.010 mmol), $K_3PO_4$ (42.5 mg, 0.200 mmol), $H_2O$ (3.6 μL, 0.20 mmol), 4-tolylboronic acid pinacol ester (109 mg, 0.500 mmol), 2-tolylboronic acid pinacol ester (109 mg, 0.500 mmol), and THF (0.10 mL). The resulting solution was stirred at 60 °C for 12 hours. Upon completion of the reaction, the reaction mixture was filtered through a plug of silica with hexanes:EtOAc (70:30), and concentrated under reduced pressure. The crude mixture was dissolved in $CDCl_3$ with $CH_2Br_2$ as internal standard. The ratio of products **2p:2c** was determined to be 8.3:1 by $^1H$ NMR spectroscopy. The NMR yields of **2p** and **2c** were determined to be 58% and 7%, respectively.




A competition experiment generating 2-benzyl-2,3-dihydro-1*H*-inden-1-ones **2j** and **2c** was carried out by the following procedure. A 1-dram vial was charged with *o*-allylbenzamide **1a** (35.1 mg, 0.100 mmol), $Ni(cod)_2$ (2.8 mg, 0.010 mmol), SIPr (3.9 mg, 0.010 mmol), $K_3PO_4$ (42.5 mg, 0.200 mmol), $H_2O$ (3.6 μL, 0.20 mmol), 4-tolylboronic acid pinacol ester (109 mg, 0.500 mmol), 4-(trifluoromethyl)phenylboronic acid pinacol ester (136 mg, 0.500 mmol), and THF (0.10 mL). The resulting solution was stirred at 60 °C for 12 hours. Upon completion of the reaction, the reaction mixture was filtered through a plug of silica with hexanes:EtOAc (70:30), and concentrated under reduced pressure. The crude mixture was dissolved in $CDCl_3$ with $CH_2Br_2$ as internal standard. The ratio of products **2j:2c** was determined to be 10.5:1 by $^1H$ NMR spectroscopy. The NMR yields of **2j** and **2c** were determined to be 84% and 8%, respectively.


7.81
7.79
7.48
7.46
7.37
7.35
7.34
7.34
7.32
7.29
7.28
7.26
7.18
7.17
7.16
7.15
7.09
7.09
7.07
7.07
7.05
7.05
5.05
1.14
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 46
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -807.0
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
N
Bn
Boc
I
S2a
1.12
2.10
3.26
1.15
1.15
1.28
2.07
9.00
f1 (ppm)

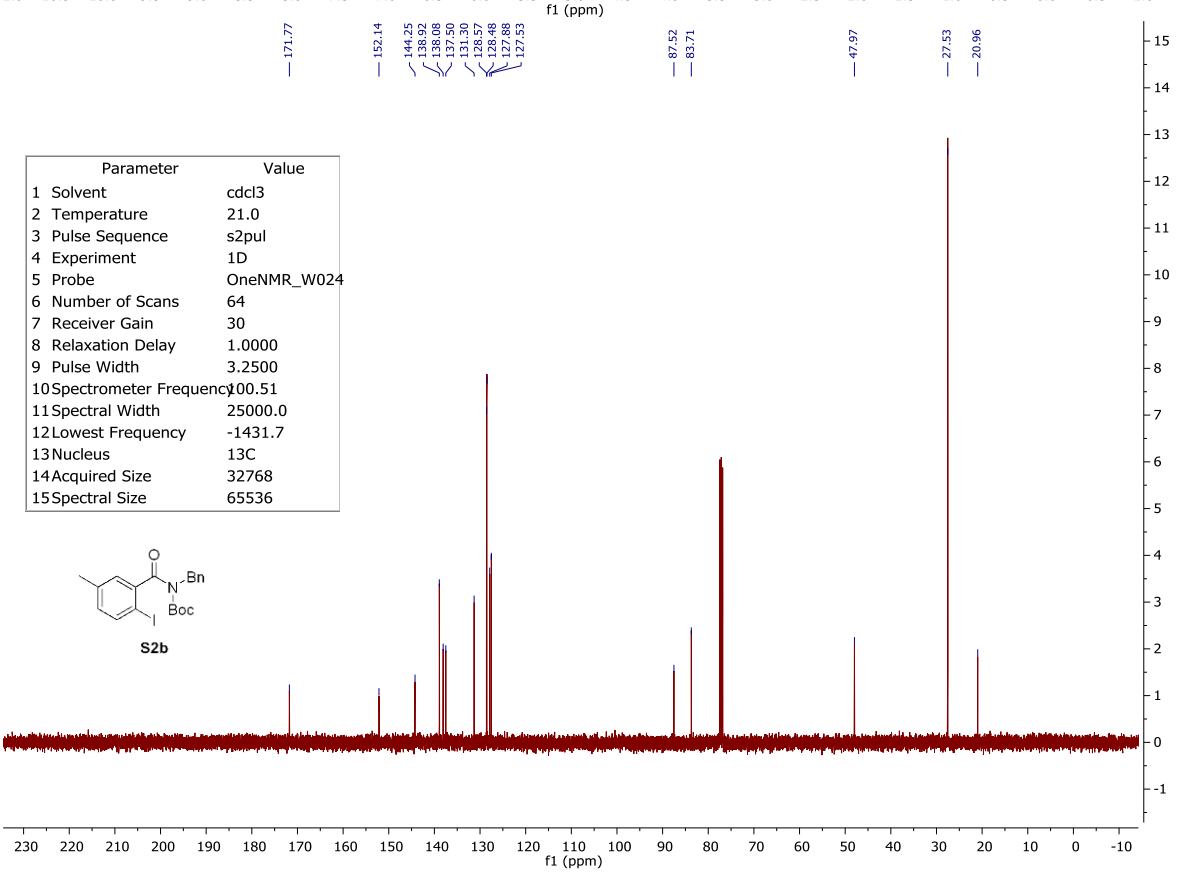

171.62
152.09
144.56
139.16
137.45
130.28
128.60
128.50
127.90
127.56
126.95
91.66
83.85
47.95
27.53
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 128
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1431.2
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
N
Bn
Boc
I
S2a
f1 (ppm)




| Parameter | Value |
|---|---|
| 1 Solvent | cdcl3 |
| 2 Temperature | 21.0 |
| 3 Pulse Sequence | s2pul |
| 4 Experiment | 1D |
| 5 Probe | OneNMR_W024 |
| 6 Number of Scans | 8 |
| 7 Receiver Gain | 30 |
| 8 Relaxation Delay | 1.0000 |
| 9 Pulse Width | 3.6500 |
| 10 Spectrometer Frequency | 399.69 |
| 11 Spectral Width | 6410.3 |
| 12 Lowest Frequency | -803.8 |
| 13 Nucleus | 1H |
| 14 Acquired Size | 16384 |
| 15 Spectral Size | 65536 |



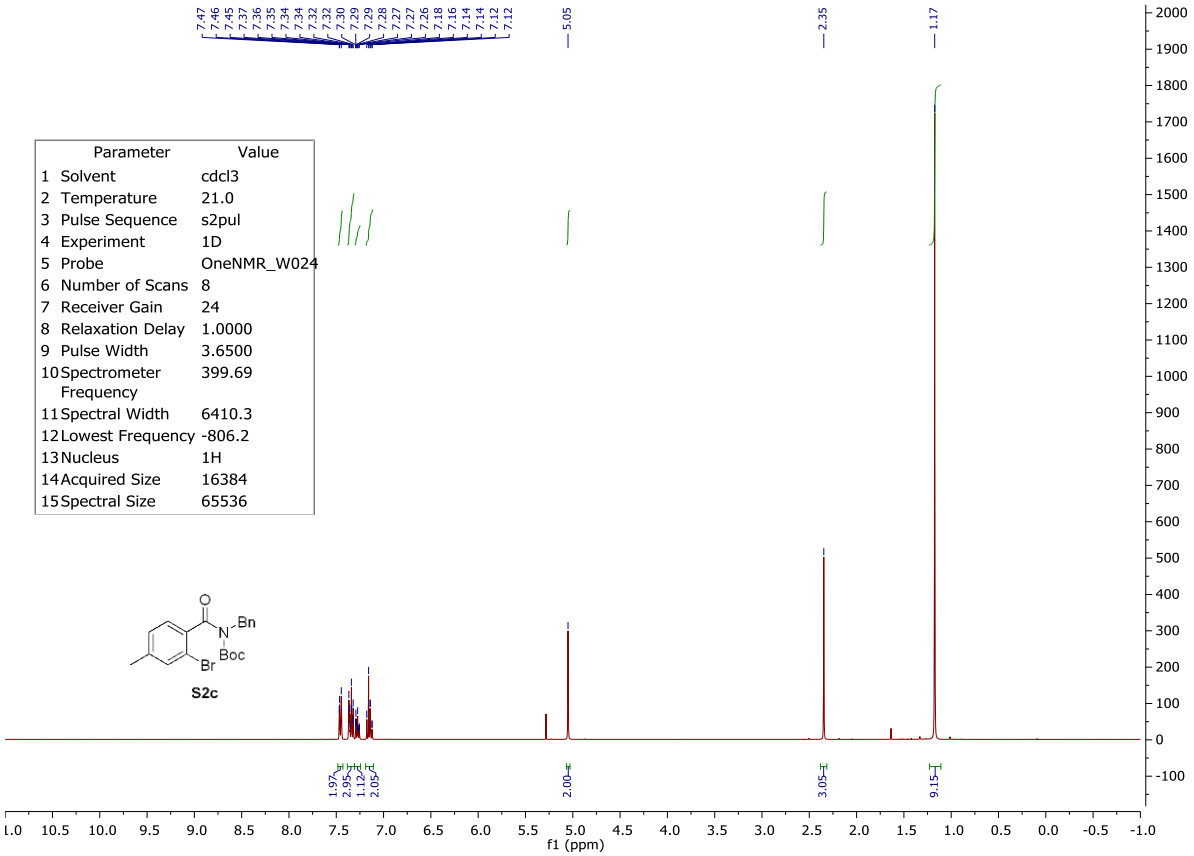

**S2b**

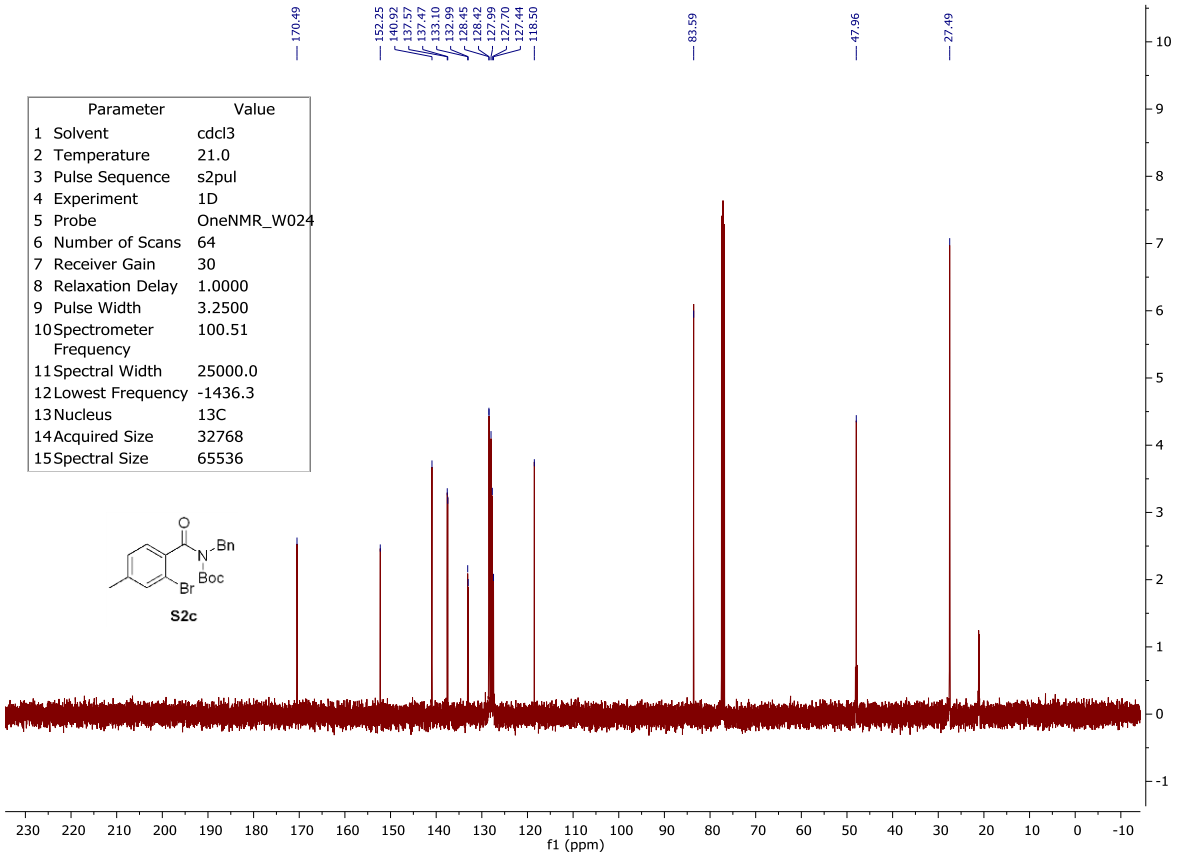


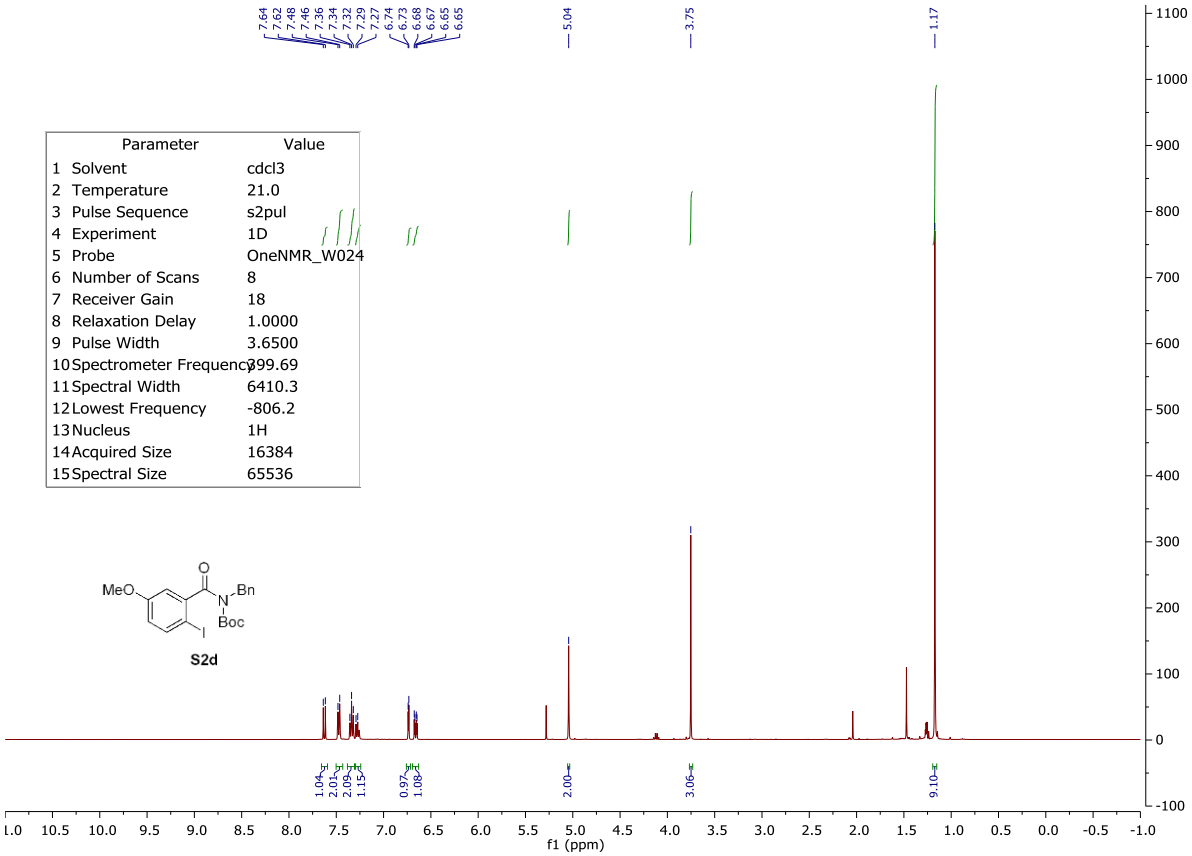

| Parameter | Value |
|---|---|
| 1 Solvent | cdcl3 |
| 2 Temperature | 21.0 |
| 3 Pulse Sequence | s2pul |
| 4 Experiment | 1D |
| 5 Probe | OneNMR_W024 |
| 6 Number of Scans | 64 |
| 7 Receiver Gain | 30 |
| 8 Relaxation Delay | 1.0000 |
| 9 Pulse Width | 3.2500 |
| 10 Spectrometer Frequency | 100.51 |
| 11 Spectral Width | 25000.0 |
| 12 Lowest Frequency | -1431.7 |
| 13 Nucleus | 13C |
| 14 Acquired Size | 32768 |
| 15 Spectral Size | 65536 |




**S2b**


7.47 7.46 7.45 7.37 7.36 7.35 7.34 7.34 7.32 7.32 7.30 7.29 7.29 7.28 7.27 7.27 7.26 7.18 7.16 7.14 7.14 7.12 7.12
5.05
2.35
1.17
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 24
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
N
Bn
Boc
Br
S2c
1.97
2.95
1.12
2.05
2.00
3.05
9.15
f1 (ppm)

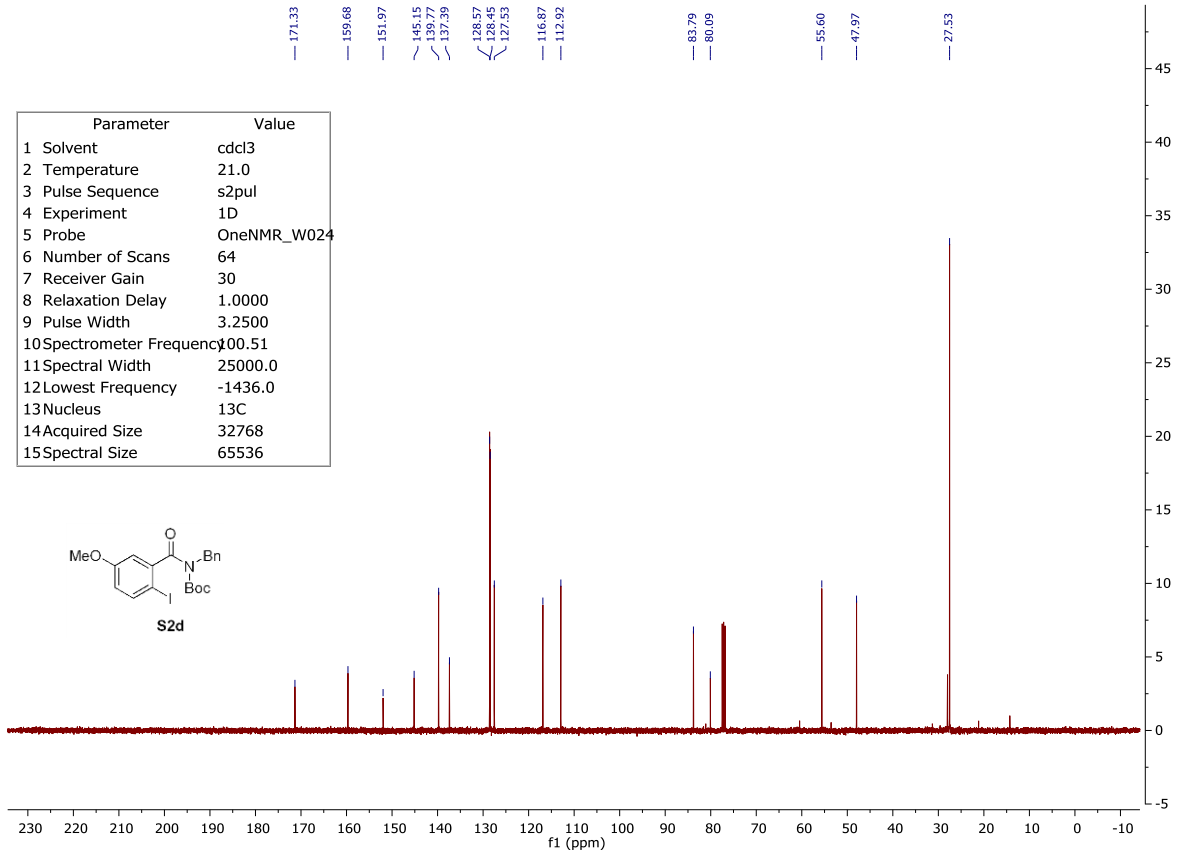

170.49
152.25
140.92
137.57
137.47
133.10
132.99
128.45
128.42
127.99
127.70
127.44
118.50
83.59
47.96
27.49
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 64
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1436.3
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
N
Bn
Boc
Br
S2c
f1 (ppm)




| | Parameter | Value |
|---|---|---|
| 1 | Solvent | cdcl3 |
| 2 | Temperature | 21.0 |
| 3 | Pulse Sequence | s2pul |
| 4 | Experiment | 1D |
| 5 | Probe | OneNMR_W024 |
| 6 | Number of Scans | 8 |
| 7 | Receiver Gain | 18 |
| 8 | Relaxation Delay | 1.0000 |
| 9 | Pulse Width | 3.6500 |
| 10 | Spectrometer Frequency | 399.69 |
| 11 | Spectral Width | 6410.3 |
| 12 | Lowest Frequency | -806.2 |
| 13 | Nucleus | 1H |
| 14 | Acquired Size | 16384 |
| 15 | Spectral Size | 65536 |



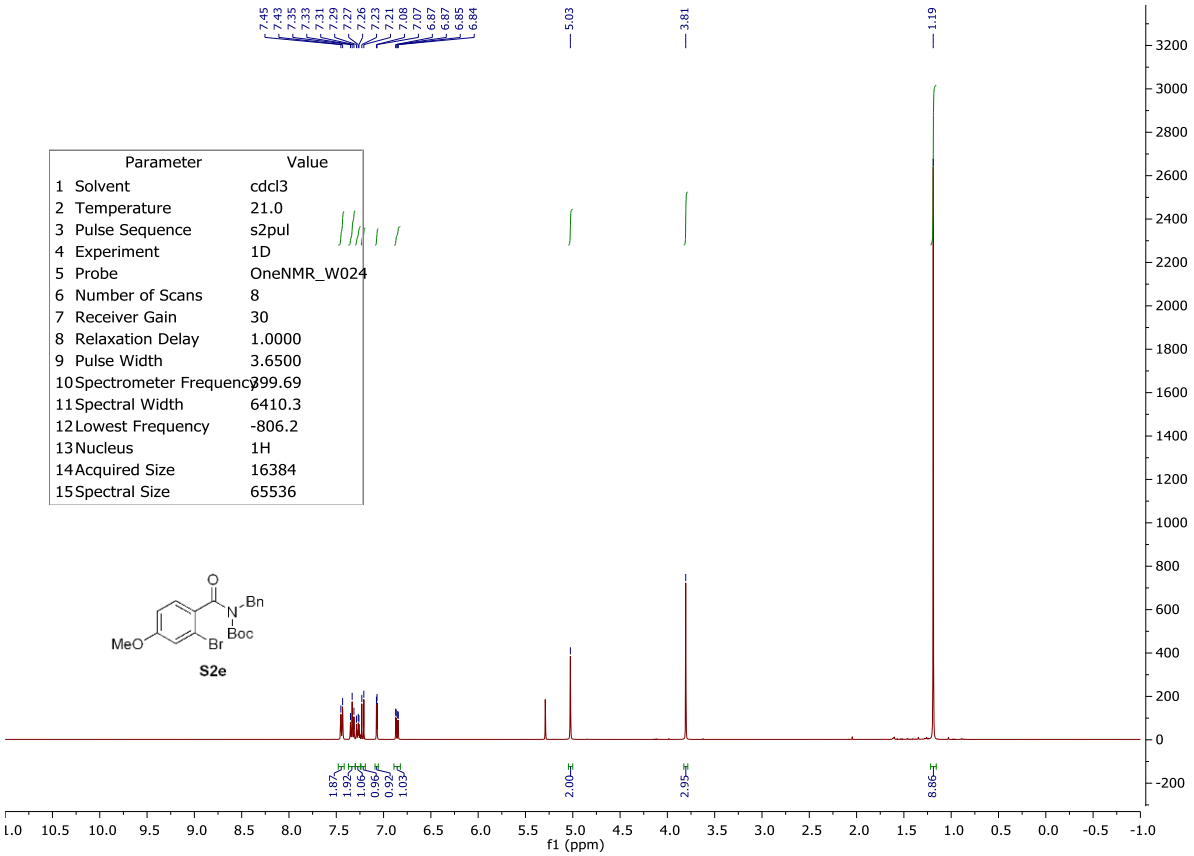

**S2d**

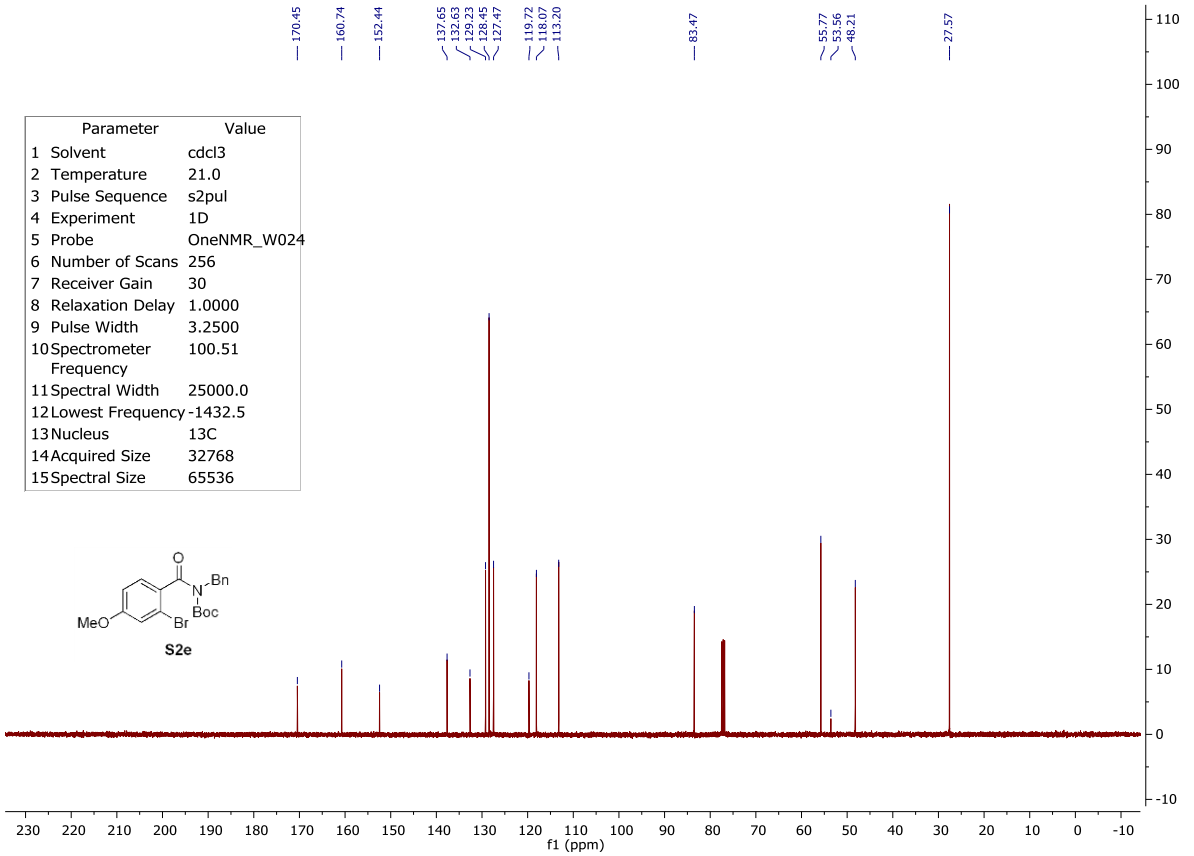


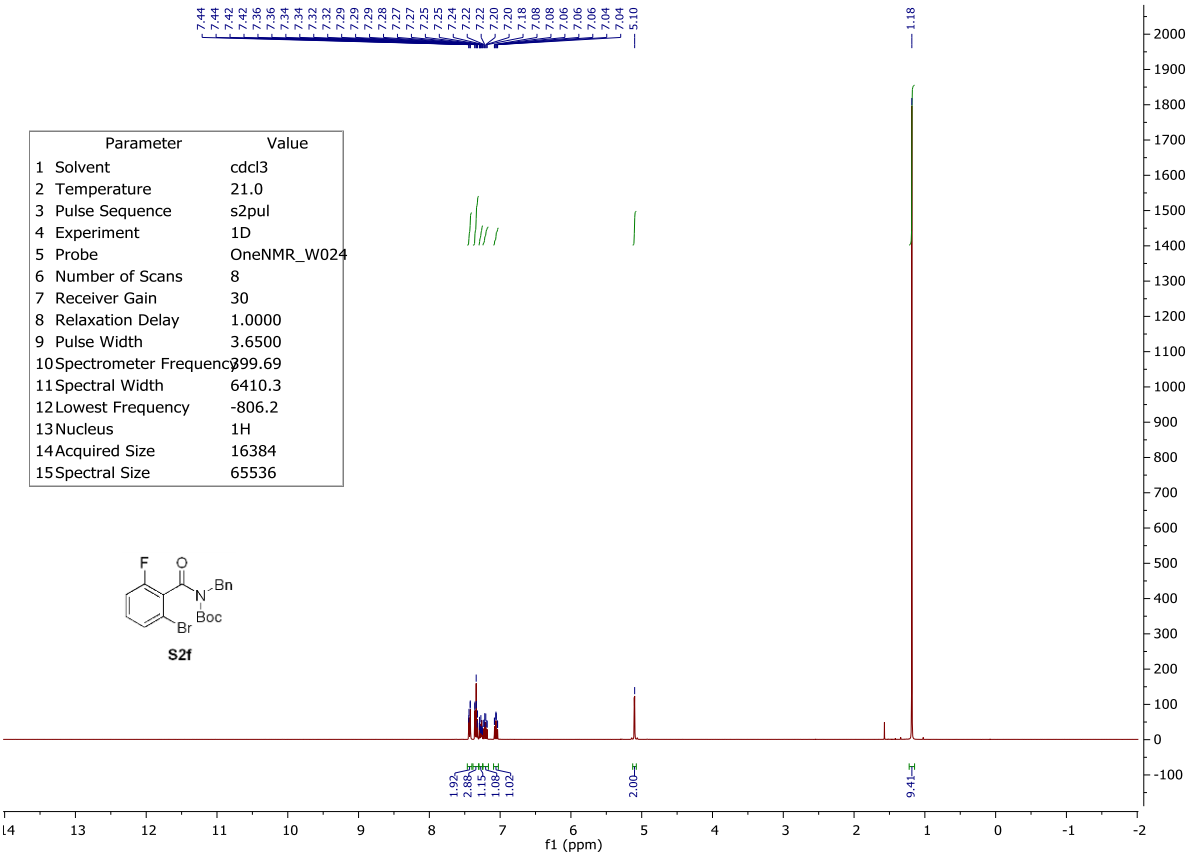

| | Parameter | Value |
|---|---|---|
| 1 | Solvent | cdcl3 |
| 2 | Temperature | 21.0 |
| 3 | Pulse Sequence | s2pul |
| 4 | Experiment | 1D |
| 5 | Probe | OneNMR_W024 |
| 6 | Number of Scans | 64 |
| 7 | Receiver Gain | 30 |
| 8 | Relaxation Delay | 1.0000 |
| 9 | Pulse Width | 3.2500 |
| 10 | Spectrometer Frequency | 100.51 |
| 11 | Spectral Width | 25000.0 |
| 12 | Lowest Frequency | -1436.0 |
| 13 | Nucleus | 13C |
| 14 | Acquired Size | 32768 |
| 15 | Spectral Size | 65536 |




**S2d**


7.45
7.43
7.35
7.33
7.31
7.29
7.27
7.26
7.23
7.21
7.08
7.07
6.87
6.87
6.85
6.84
5.03
3.81
1.19
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
N
Bn
Boc
MeO
Br
S2e
1.87
1.92
1.06
0.98
0.92
1.03
2.00
2.95
8.86
f1 (ppm)

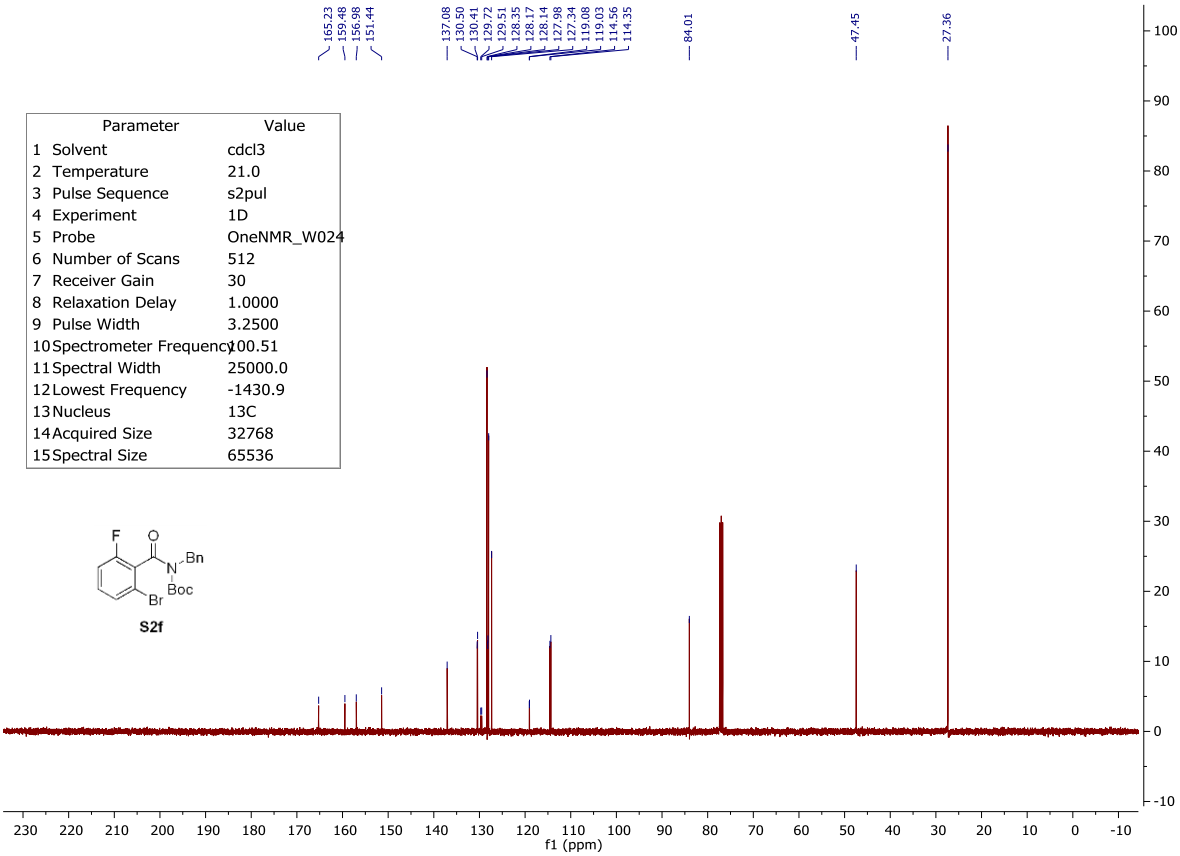

170.45
160.74
152.44
137.65
132.63
129.23
128.45
127.47
119.72
118.07
113.20
83.47
55.77
53.56
48.21
27.57
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1432.5
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
N
Bn
Boc
MeO
Br
S2e
f1 (ppm)




| Parameter | Value |
|---|---|
| 1 Solvent | cdcl3 |
| 2 Temperature | 21.0 |
| 3 Pulse Sequence | s2pul |
| 4 Experiment | 1D |
| 5 Probe | OneNMR_W024 |
| 6 Number of Scans | 8 |
| 7 Receiver Gain | 30 |
| 8 Relaxation Delay | 1.0000 |
| 9 Pulse Width | 3.6500 |
| 10 Spectrometer Frequency | 399.69 |
| 11 Spectral Width | 6410.3 |
| 12 Lowest Frequency | -806.2 |
| 13 Nucleus | 1H |
| 14 Acquired Size | 16384 |
| 15 Spectral Size | 65536 |



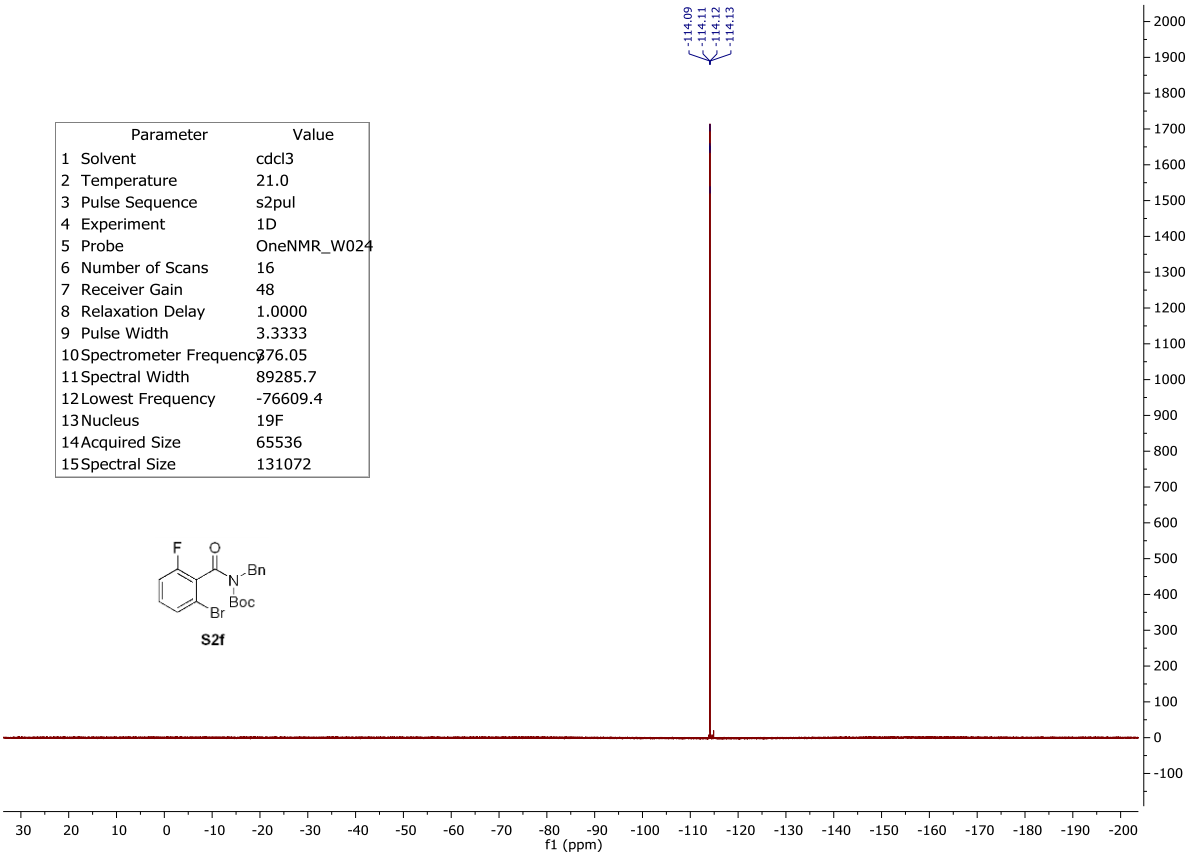

**S2f**

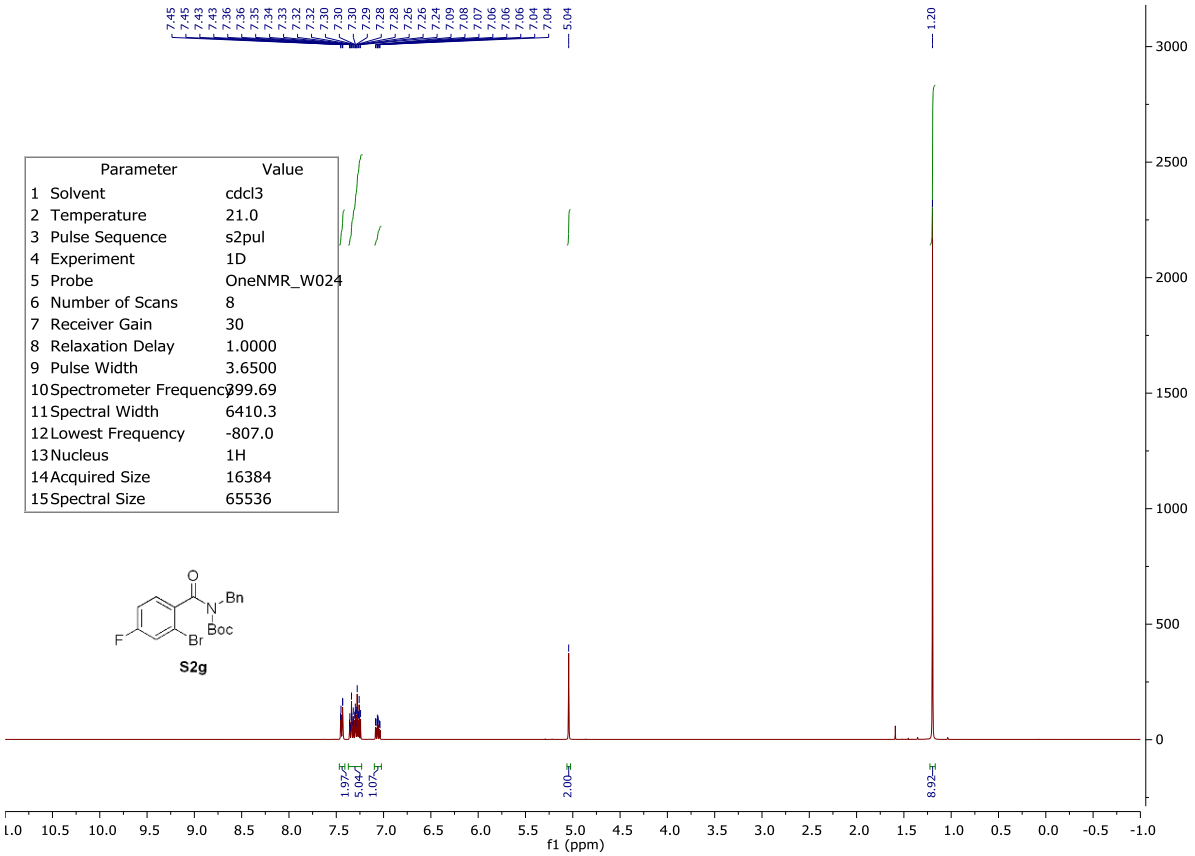


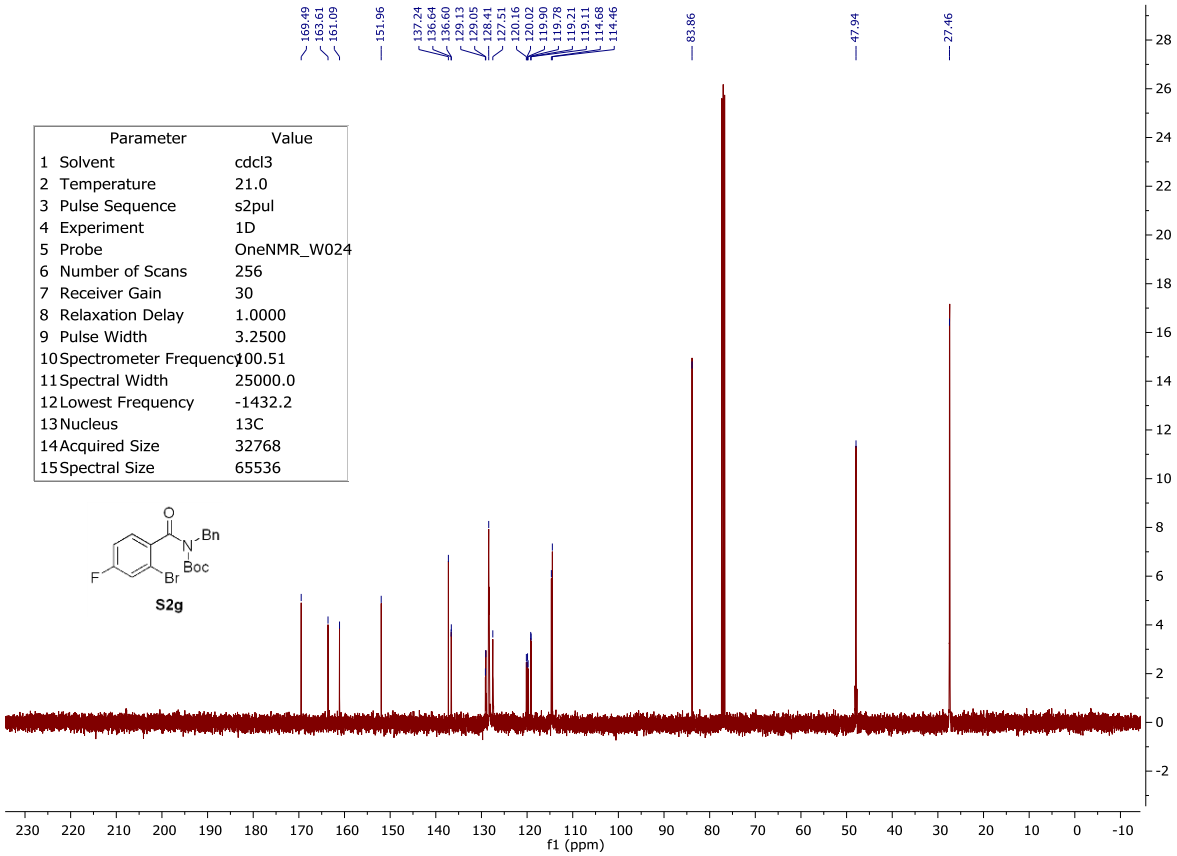

| Parameter | Value |
|---|---|
| 1 Solvent | cdcl3 |
| 2 Temperature | 21.0 |
| 3 Pulse Sequence | s2pul |
| 4 Experiment | 1D |
| 5 Probe | OneNMR_W024 |
| 6 Number of Scans | 512 |
| 7 Receiver Gain | 30 |
| 8 Relaxation Delay | 1.0000 |
| 9 Pulse Width | 3.2500 |
| 10 Spectrometer Frequency | 100.51 |
| 11 Spectral Width | 25000.0 |
| 12 Lowest Frequency | -1430.9 |
| 13 Nucleus | 13C |
| 14 Acquired Size | 32768 |
| 15 Spectral Size | 65536 |

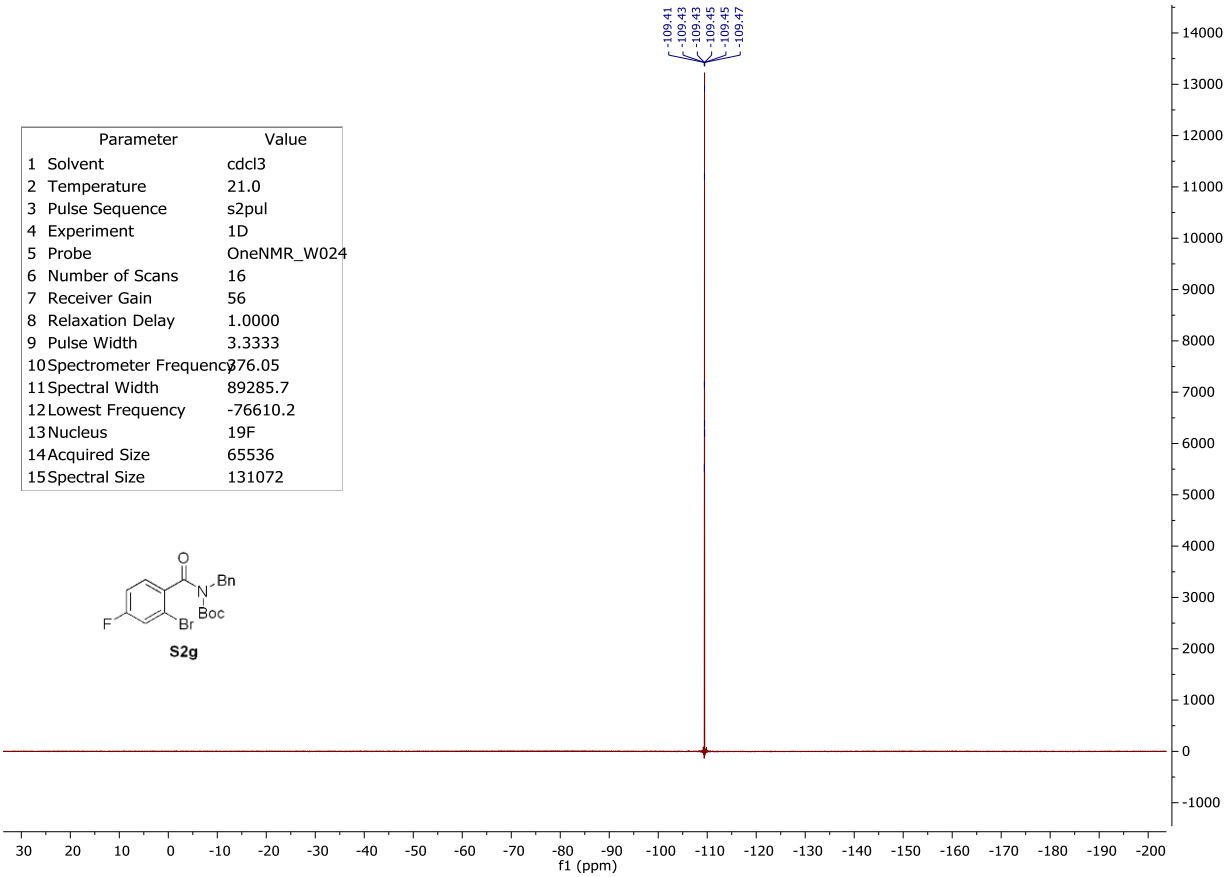



**S2f**


-114.09
-114.11
-114.12
-114.13
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 48
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76609.4
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
F
O
N
Bn
Boc
Br
S2f
f1 (ppm)


7.45 7.45 7.43 7.43 7.36 7.36 7.35 7.34 7.33 7.32 7.32 7.30 7.30 7.30 7.29 7.28 7.28 7.26 7.26 7.24 7.09 7.08 7.07 7.06 7.06 7.06 7.04 7.04
5.04
1.20
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -807.0
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
N
Bn
Boc
F
Br
S2g
1.97
5.04
1.07
2.00
8.92
f1 (ppm)

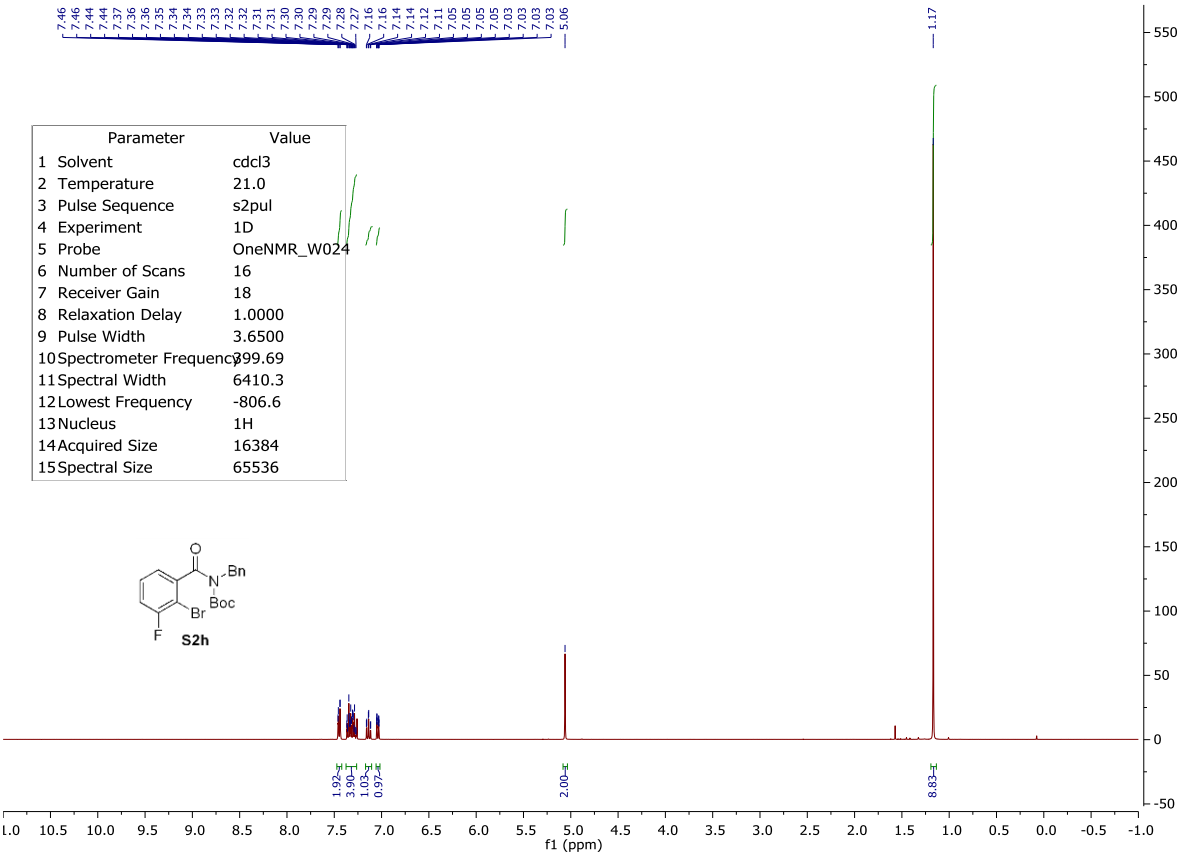

169.49 163.61 161.09 151.96 137.24 136.64 136.60 129.13 129.05 128.41 127.51 120.16 120.02 119.90 119.78 119.21 119.11 114.68 114.46
83.86
47.94
27.46
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1432.2
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
N
Bn
Boc
F
Br
S2g
f1 (ppm)

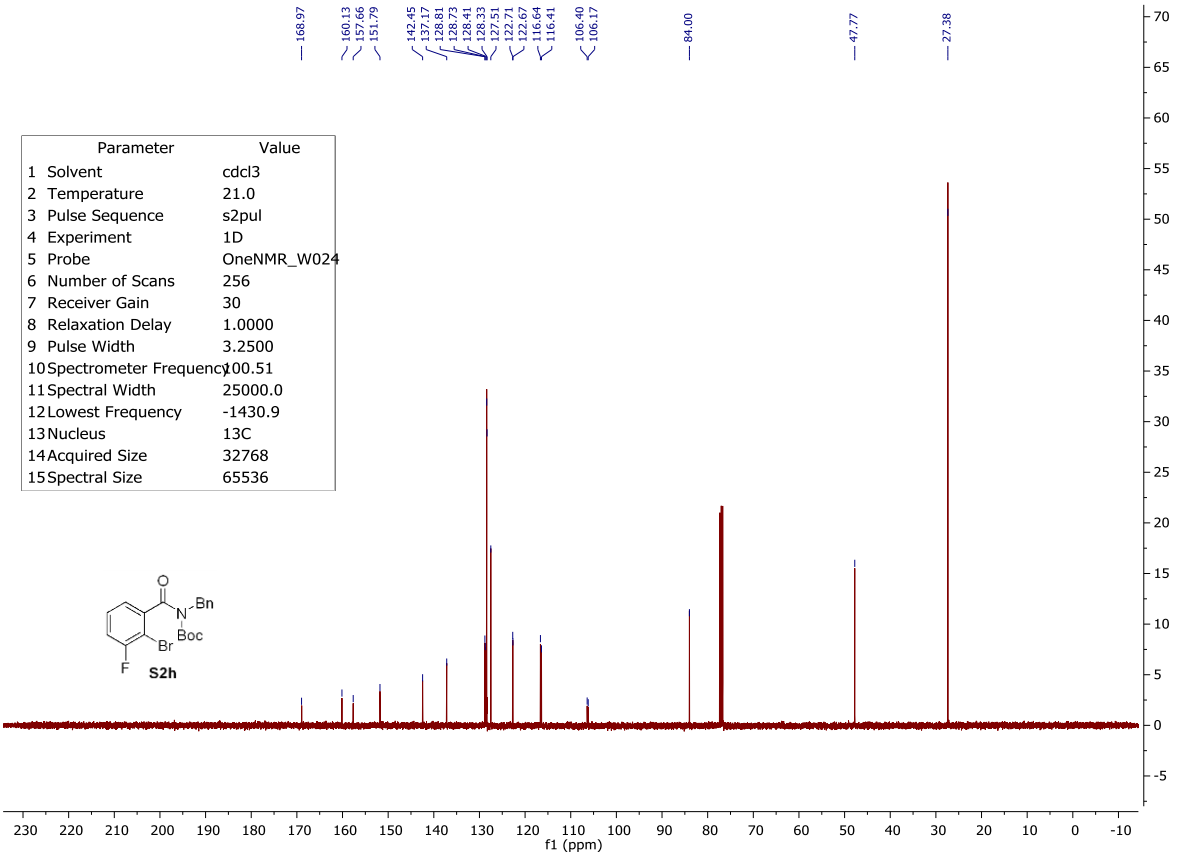


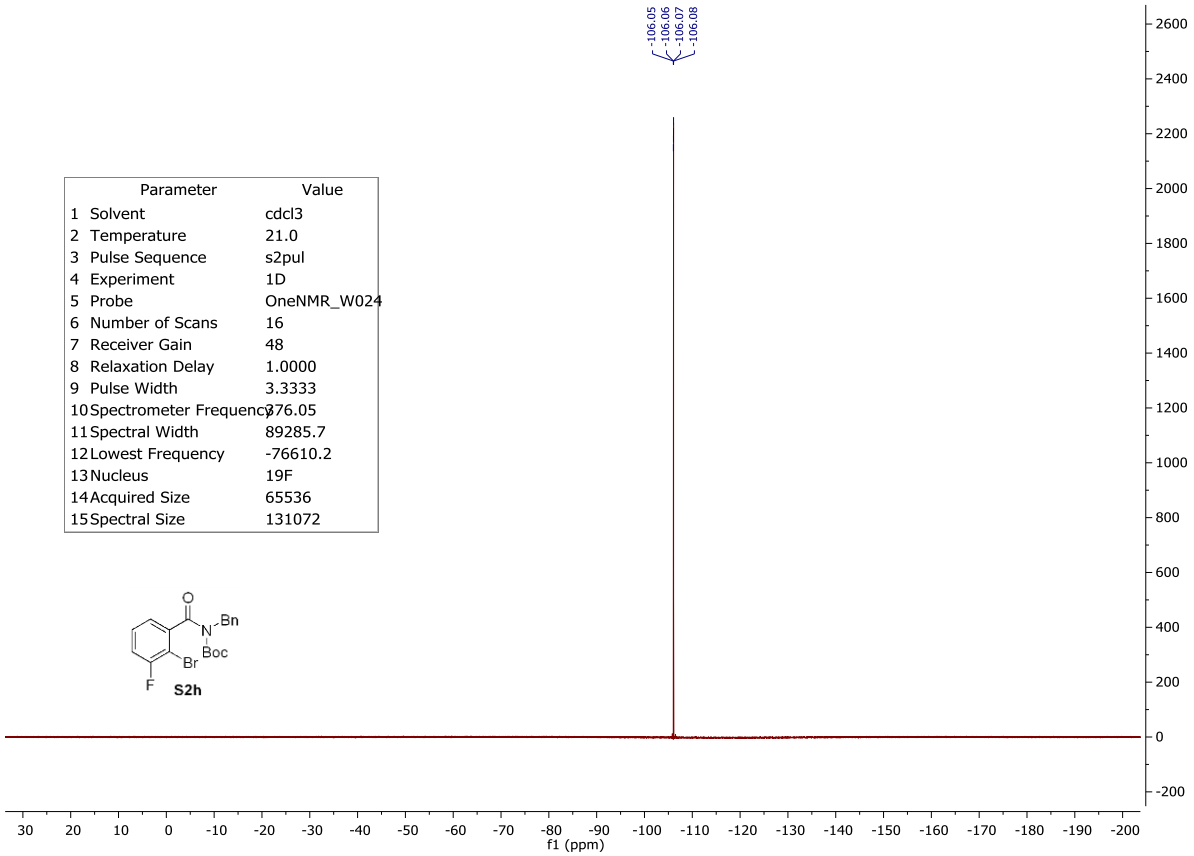

| Parameter | Value |
|---|---|
| 1 Solvent | cdcl3 |
| 2 Temperature | 21.0 |
| 3 Pulse Sequence | s2pul |
| 4 Experiment | 1D |
| 5 Probe | OneNMR_W024 |
| 6 Number of Scans | 16 |
| 7 Receiver Gain | 56 |
| 8 Relaxation Delay | 1.0000 |
| 9 Pulse Width | 3.3333 |
| 10 Spectrometer Frequency | 376.05 |
| 11 Spectral Width | 89285.7 |
| 12 Lowest Frequency | -76610.2 |
| 13 Nucleus | 19F |
| 14 Acquired Size | 65536 |
| 15 Spectral Size | 131072 |

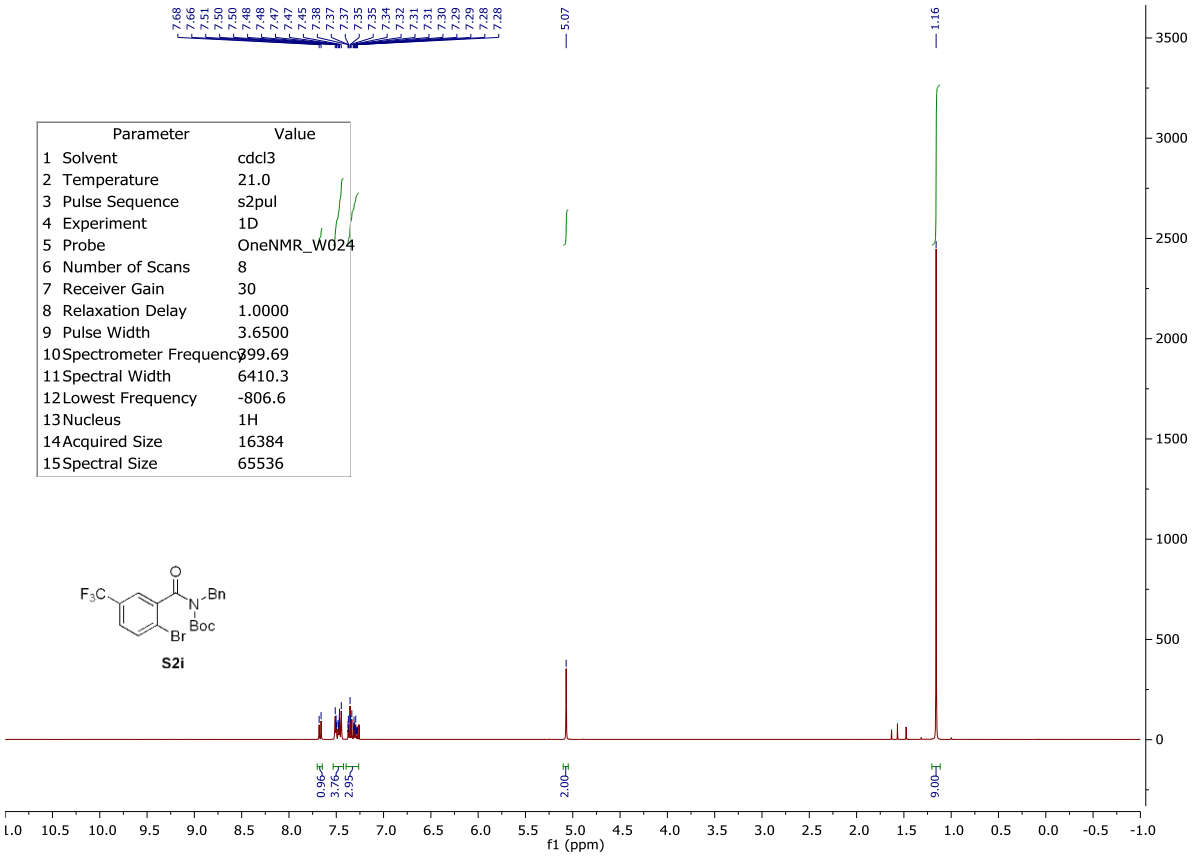


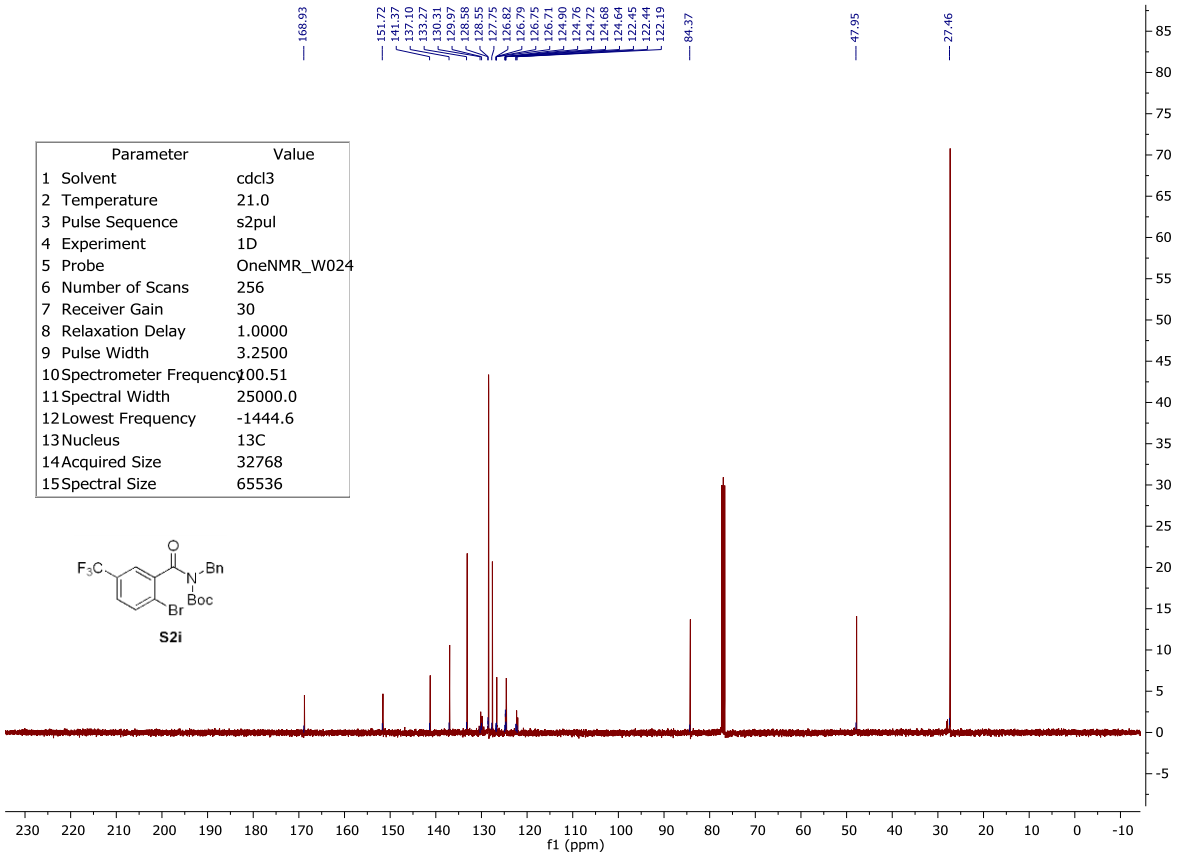

**S2g**

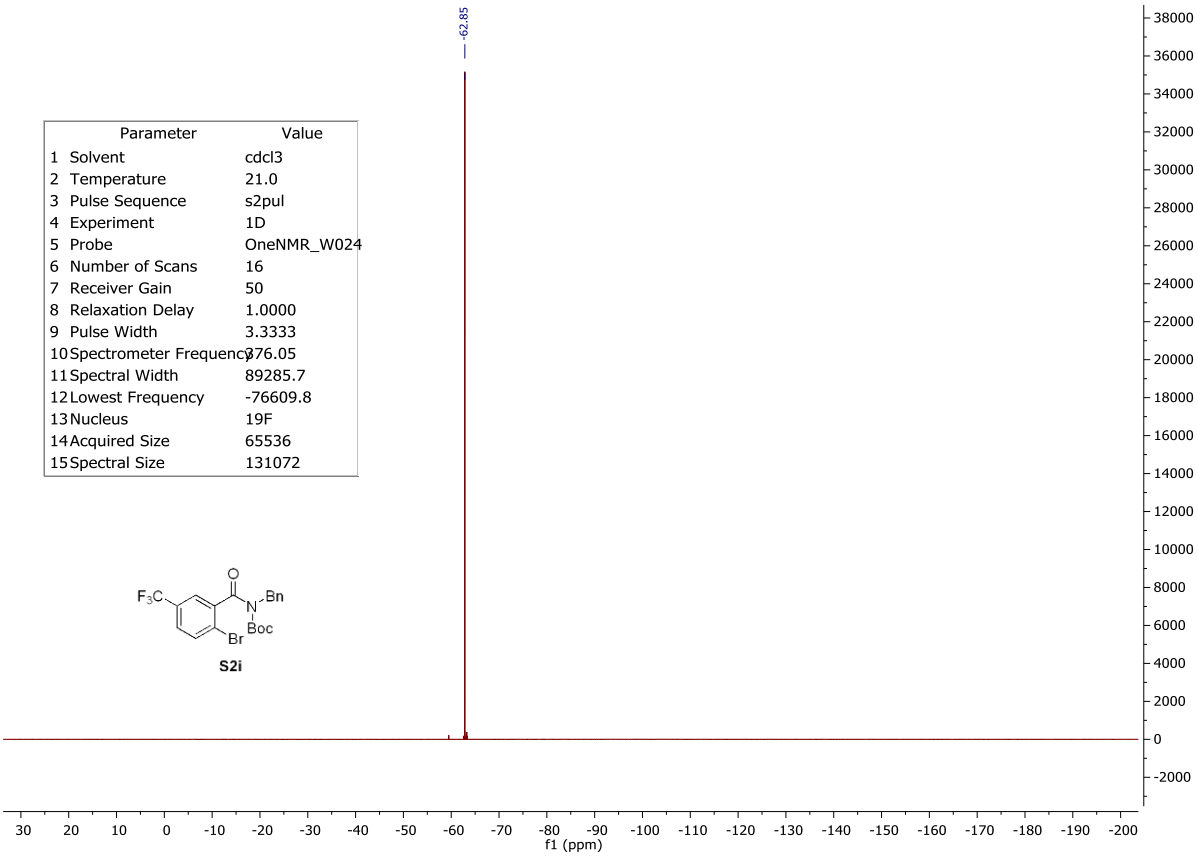

7.46 7.46 7.44 7.44 7.37 7.36 7.36 7.35 7.34 7.34 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.30 7.29 7.29 7.28 7.27 7.16 7.16 7.14 7.14 7.12 7.11 7.05 7.05 7.05 7.03 7.03 7.03 7.03 5.06
1.17
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 18
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.6
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
N
Bn
Boc
Br
F
S2h
1.92
3.90
1.03
0.97
2.00
8.83
f1 (ppm)


168.97
160.13
157.66
151.79
142.45
137.17
128.81
128.73
128.41
128.33
127.51
122.71
122.67
116.64
116.41
106.40
106.17
84.00
47.77
27.38
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1430.9
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
N
Bn
Boc
Br
F
S2h
f1 (ppm)


-106.05
-106.06
-106.07
-106.08
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 48
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76610.2
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
O
N
Bn
Boc
Br
F
S2h
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


7.68 7.66 7.51 7.50 7.50 7.48 7.48 7.47 7.47 7.45 7.38 7.37 7.37 7.35 7.35 7.34 7.32 7.31 7.31 7.30 7.29 7.29 7.28 7.28
5.07
1.16
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.6
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
F3C
Bn
N
Boc
Br
S2i
0.96
3.76
2.95
2.00
9.00
f1 (ppm)

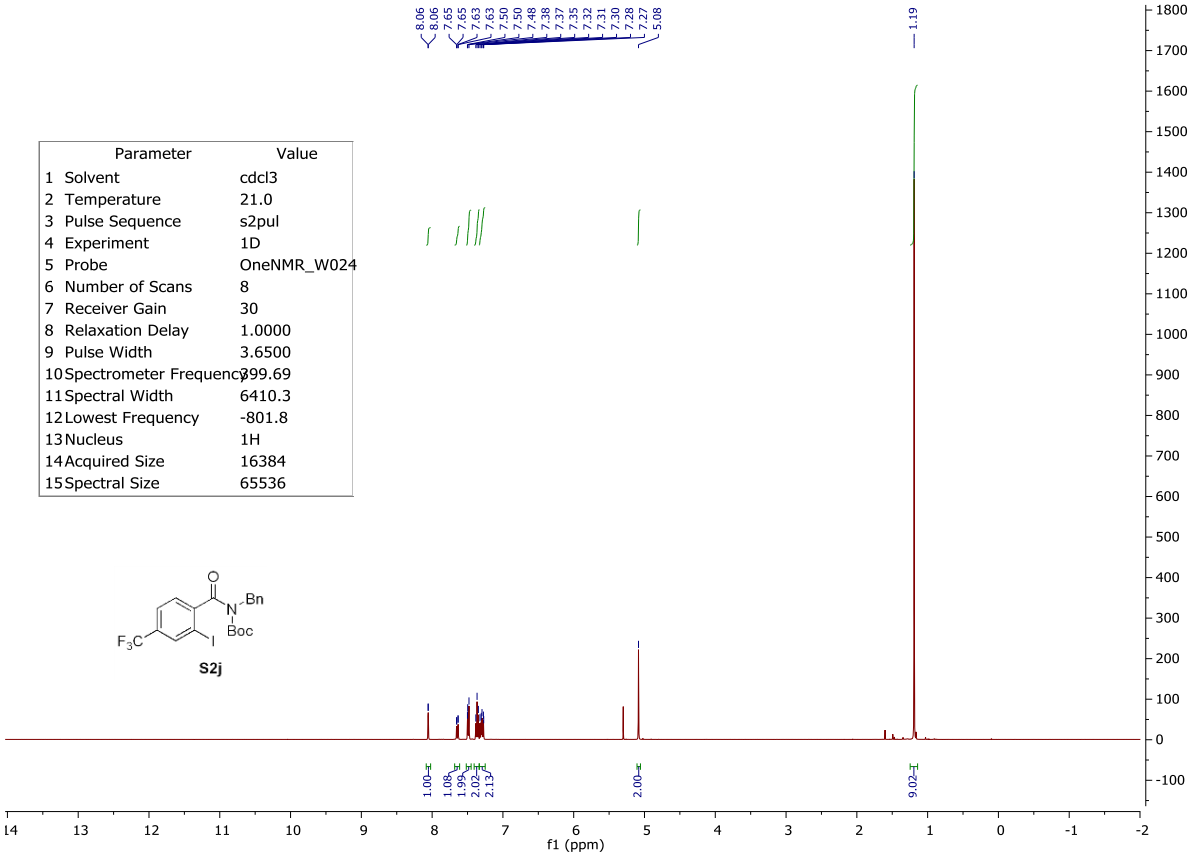

168.93
151.72 141.37 137.10 133.27 130.31 129.97 128.58 128.55 127.75 126.82 126.79 126.75 126.71 124.90 124.76 124.72 124.68 124.64 122.45 122.44 122.19
84.37
47.95
27.46
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1444.6
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
F3C
Bn
N
Boc
Br
S2i
f1 (ppm)

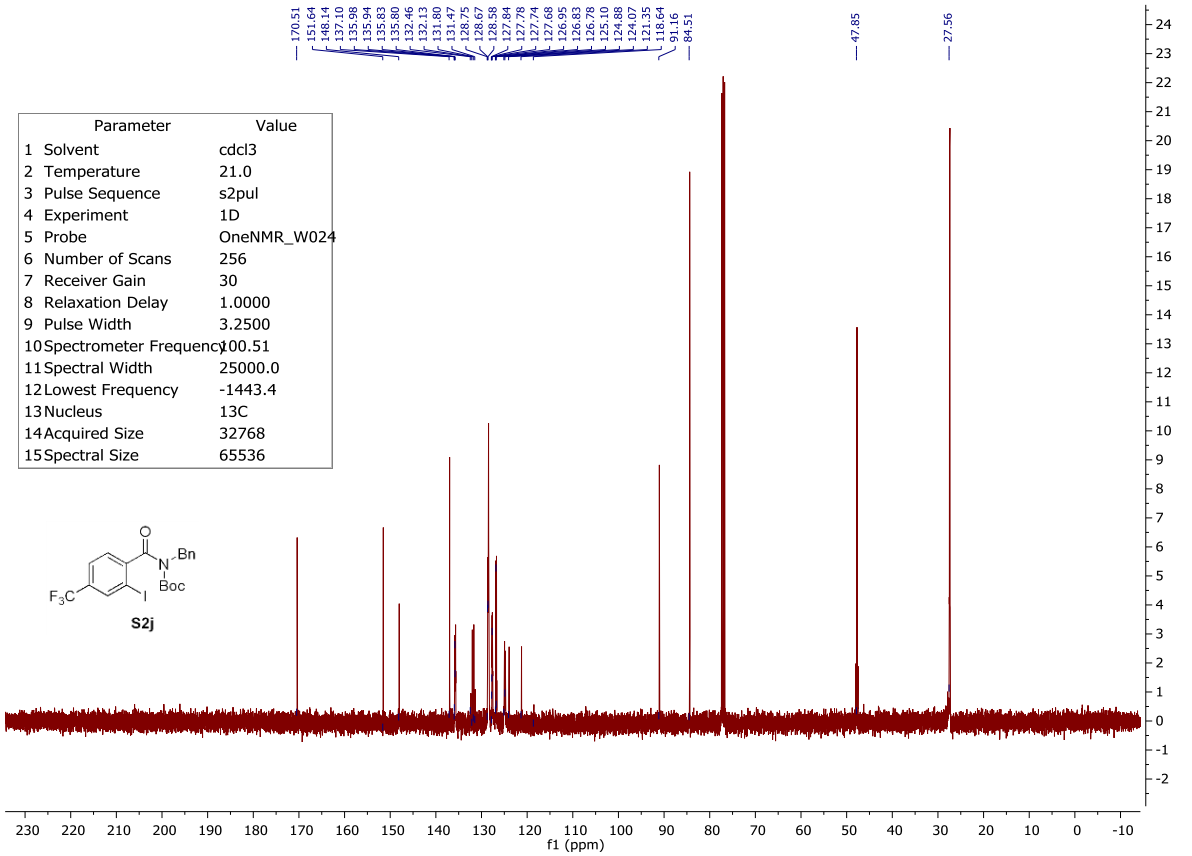



| | Parameter | Value |
|---|---|---|
| 1 | Solvent | cdcl3 |
| 2 | Temperature | 21.0 |
| 3 | Pulse Sequence | s2pul |
| 4 | Experiment | 1D |
| 5 | Probe | OneNMR_W024 |
| 6 | Number of Scans | 16 |
| 7 | Receiver Gain | 50 |
| 8 | Relaxation Delay | 1.0000 |
| 9 | Pulse Width | 3.3333 |
| 10 | Spectrometer Frequency | 376.05 |
| 11 | Spectral Width | 89285.7 |
| 12 | Lowest Frequency | -76609.8 |
| 13 | Nucleus | 19F |
| 14 | Acquired Size | 65536 |
| 15 | Spectral Size | 131072 |

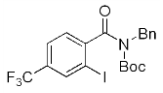



**S2i**

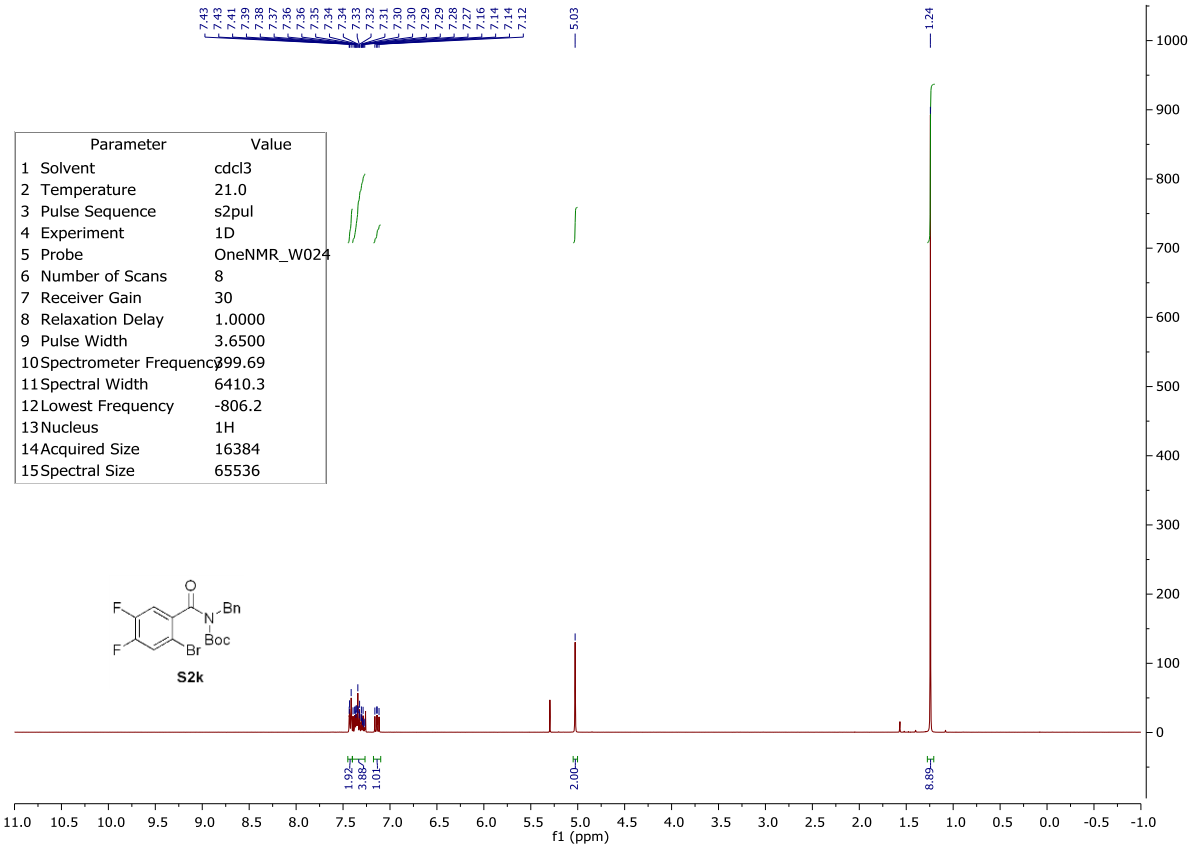

8.06
8.06
7.65
7.65
7.63
7.63
7.50
7.50
7.48
7.38
7.37
7.35
7.32
7.31
7.30
7.28
7.27
5.08
1.19
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -801.8
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
Bn
N
Boc
F3C
I
S2j
1.00
1.08
1.99
2.02
2.13
2.00
9.02
f1 (ppm)


170.51
151.64
148.14
137.10
135.98
135.94
135.83
135.80
132.46
132.13
131.80
131.47
128.75
128.67
128.58
127.84
127.78
127.74
127.68
126.95
126.83
126.78
125.10
124.88
124.07
121.35
118.64
91.16
84.51
47.85
27.56
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1443.4
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
Bn
N
Boc
F3C
I
S2j
f1 (ppm)

| | Parameter | Value |
|---|---|---|
| 1 | Solvent | cdcl3 |
| 2 | Temperature | 21.0 |
| 3 | Pulse Sequence | s2pul |
| 4 | Experiment | 1D |
| 5 | Probe | OneNMR_W024 |
| 6 | Number of Scans | 16 |
| 7 | Receiver Gain | 44 |
| 8 | Relaxation Delay | 1.0000 |
| 9 | Pulse Width | 3.3333 |
| 10 | Spectrometer Frequency | 376.05 |
| 11 | Spectral Width | 89285.7 |
| 12 | Lowest Frequency | -76605.3 |
| 13 | Nucleus | 19F |
| 14 | Acquired Size | 65536 |
| 15 | Spectral Size | 131072 |



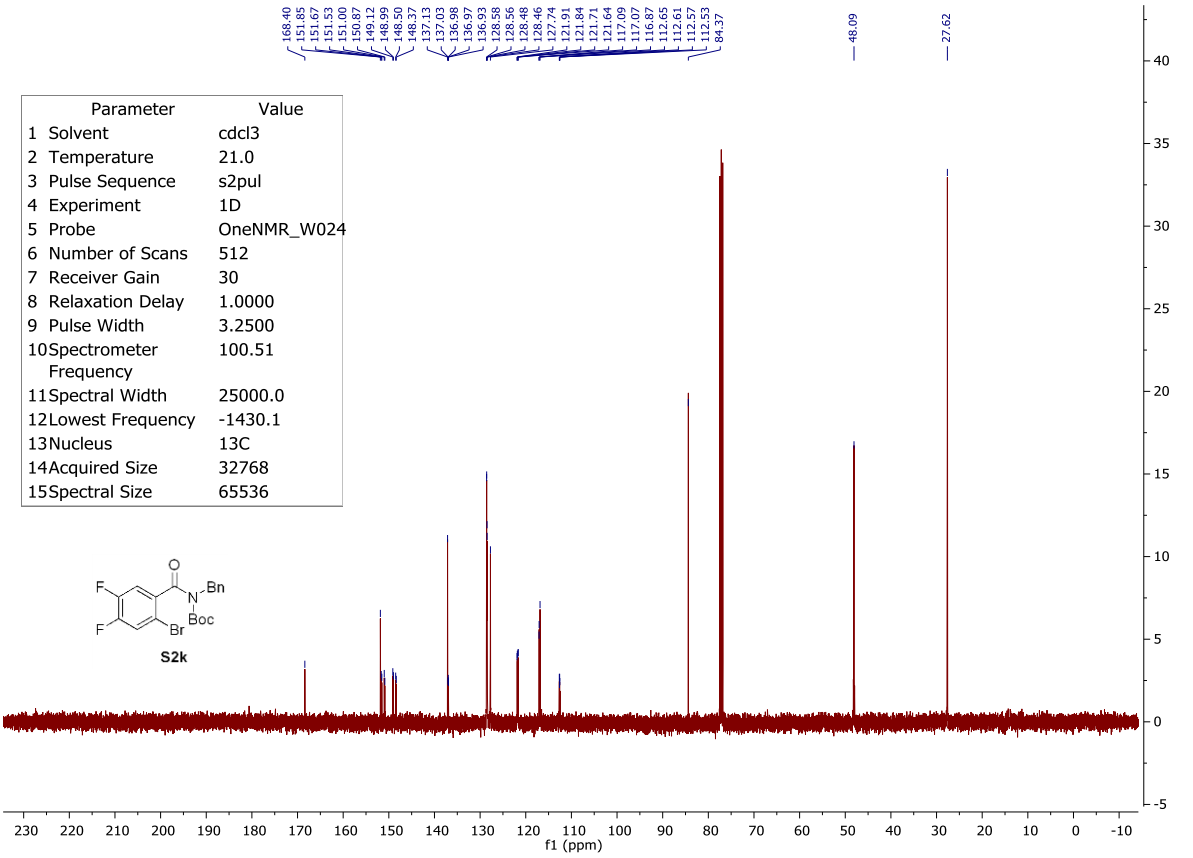

**S2j**




| Parameter | Value |
|---|---|
| 1 Solvent | cdcl3 |
| 2 Temperature | 21.0 |
| 3 Pulse Sequence | s2pul |
| 4 Experiment | 1D |
| 5 Probe | OneNMR_W024 |
| 6 Number of Scans | 8 |
| 7 Receiver Gain | 30 |
| 8 Relaxation Delay | 1.0000 |
| 9 Pulse Width | 3.6500 |
| 10 Spectrometer Frequency | 399.69 |
| 11 Spectral Width | 6410.3 |
| 12 Lowest Frequency | -806.2 |
| 13 Nucleus | 1H |
| 14 Acquired Size | 16384 |
| 15 Spectral Size | 65536 |



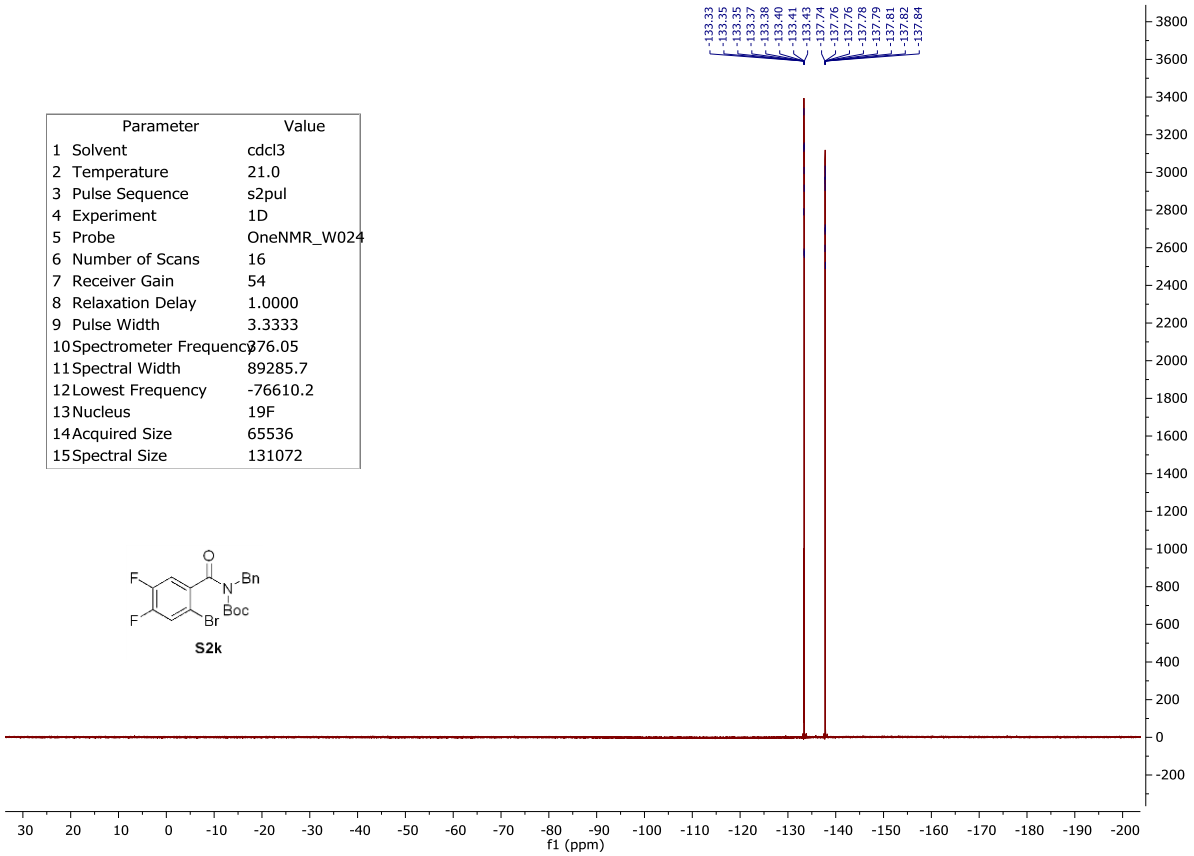

**S2k**

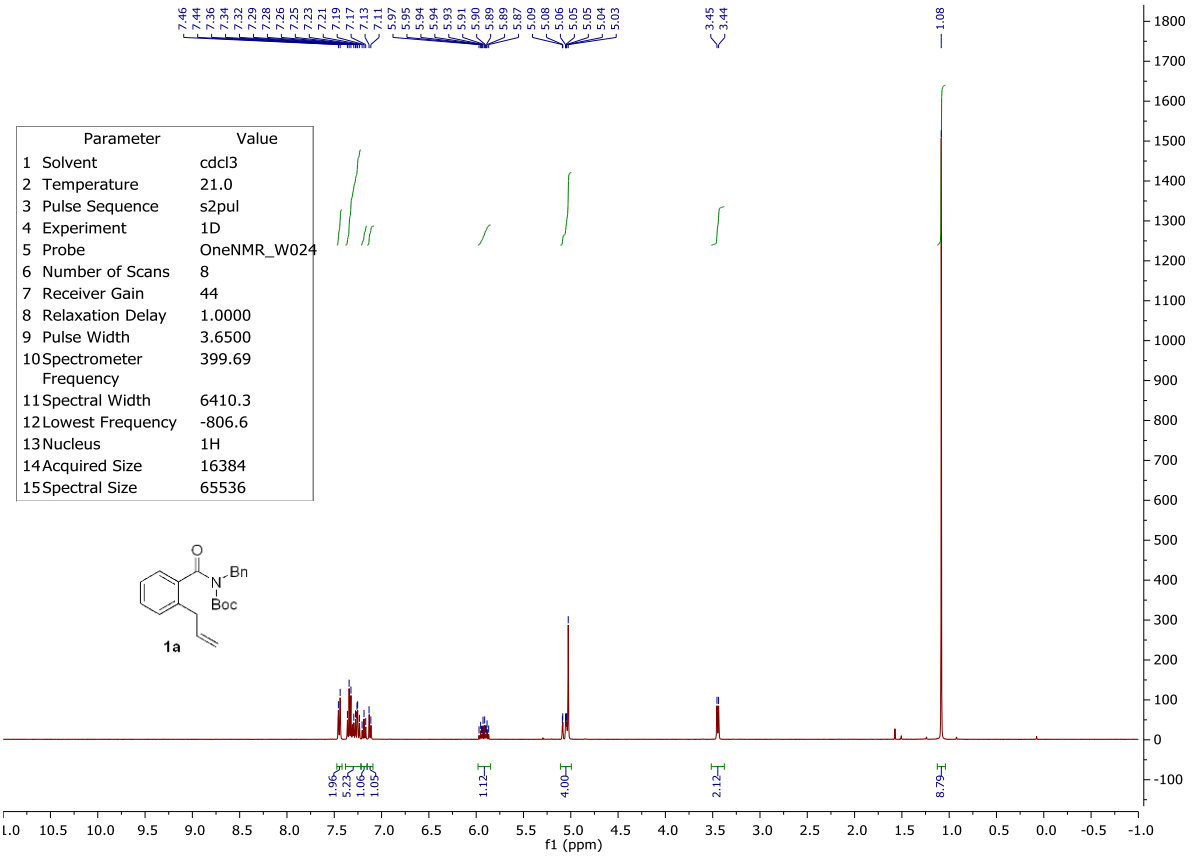


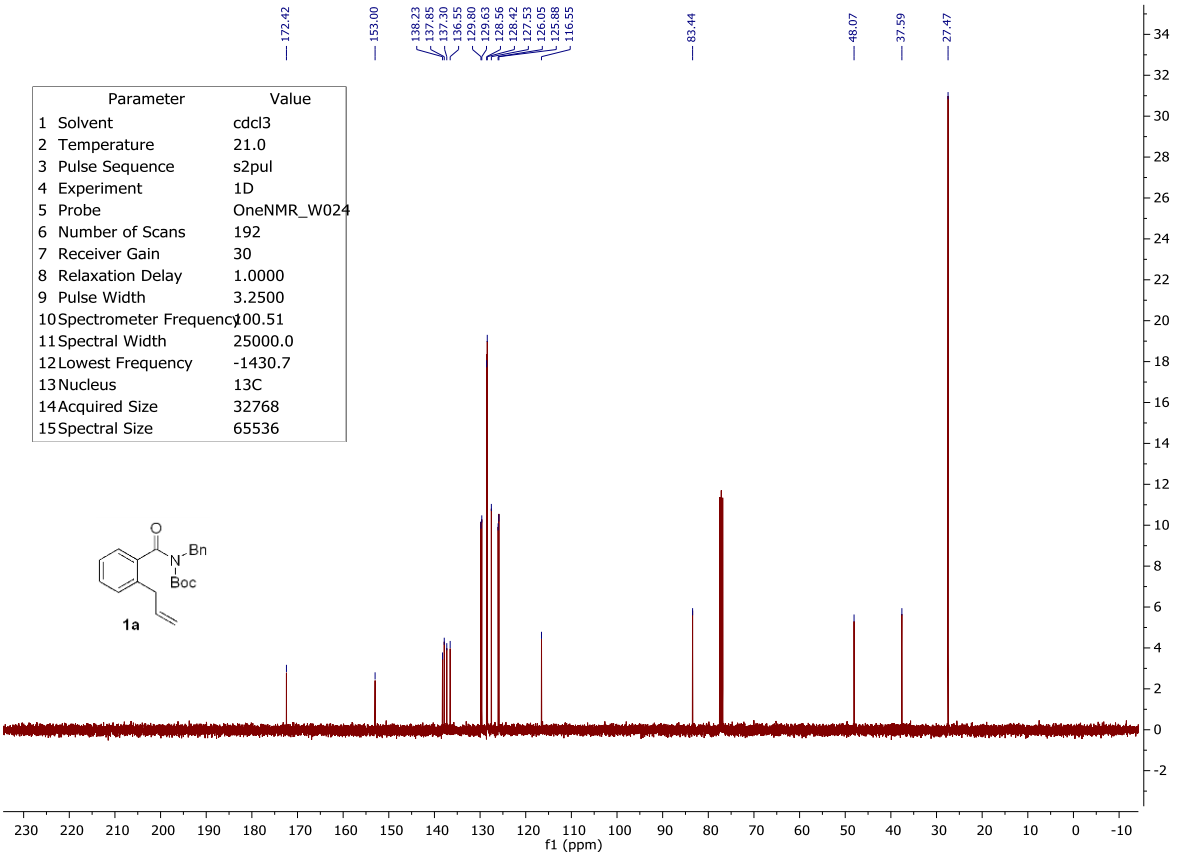

| Parameter | Value |
|---|---|
| 1 Solvent | cdcl3 |
| 2 Temperature | 21.0 |
| 3 Pulse Sequence | s2pul |
| 4 Experiment | 1D |
| 5 Probe | OneNMR_W024 |
| 6 Number of Scans | 512 |
| 7 Receiver Gain | 30 |
| 8 Relaxation Delay | 1.0000 |
| 9 Pulse Width | 3.2500 |
| 10 Spectrometer Frequency | 100.51 |
| 11 Spectral Width | 25000.0 |
| 12 Lowest Frequency | -1430.1 |
| 13 Nucleus | 13C |
| 14 Acquired Size | 32768 |
| 15 Spectral Size | 65536 |

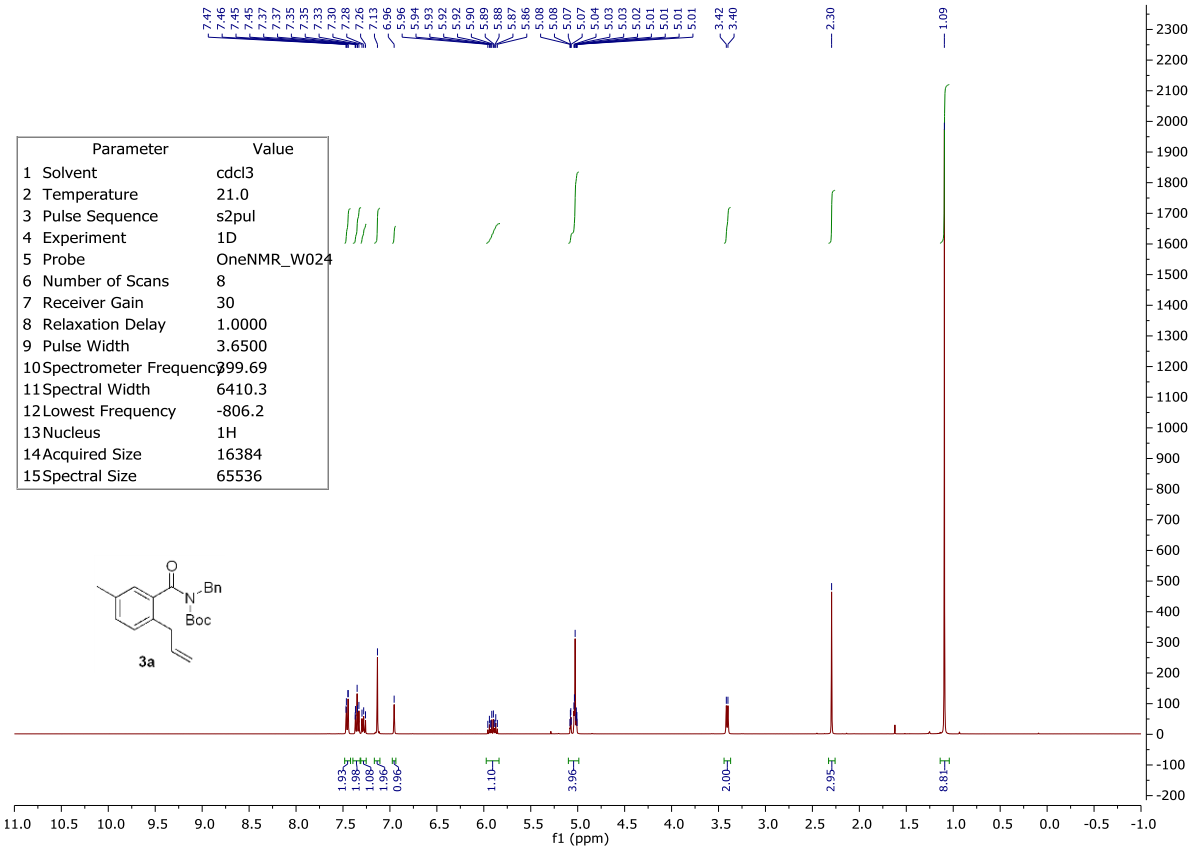


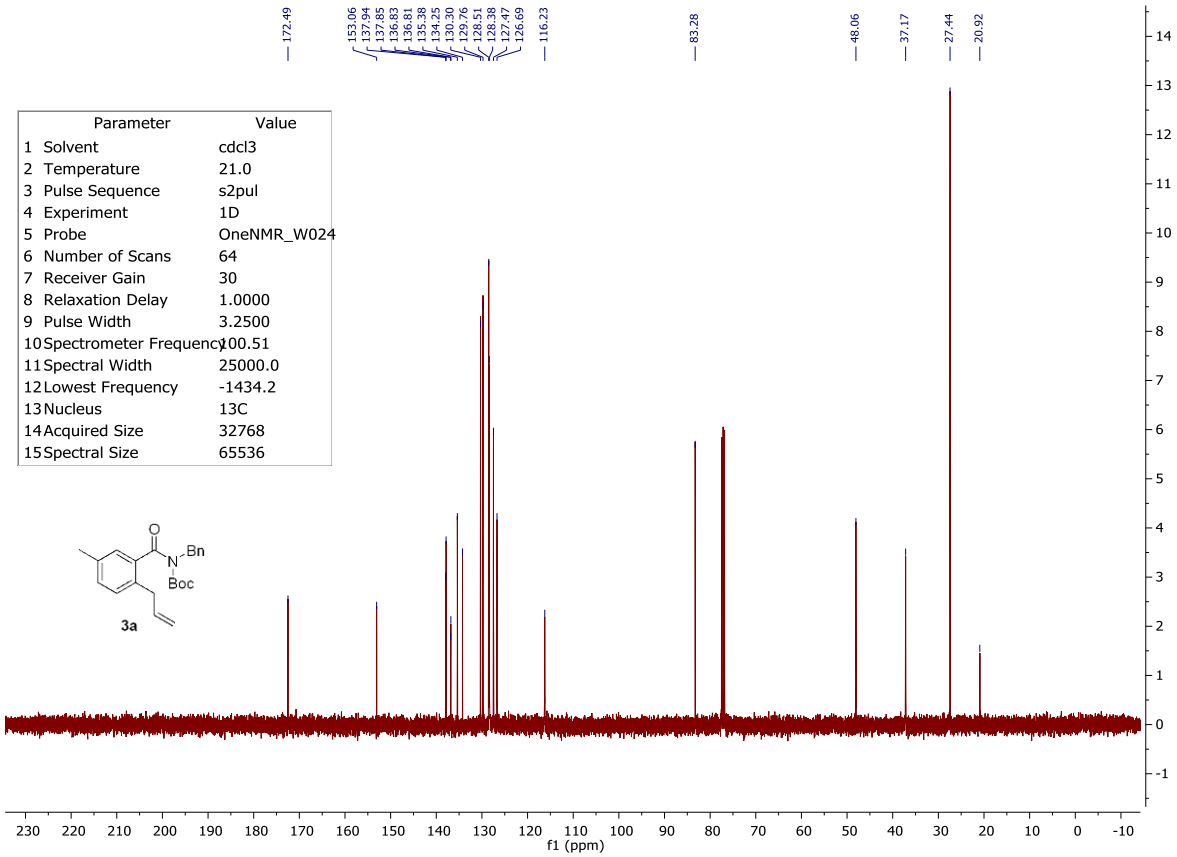

**S2k**

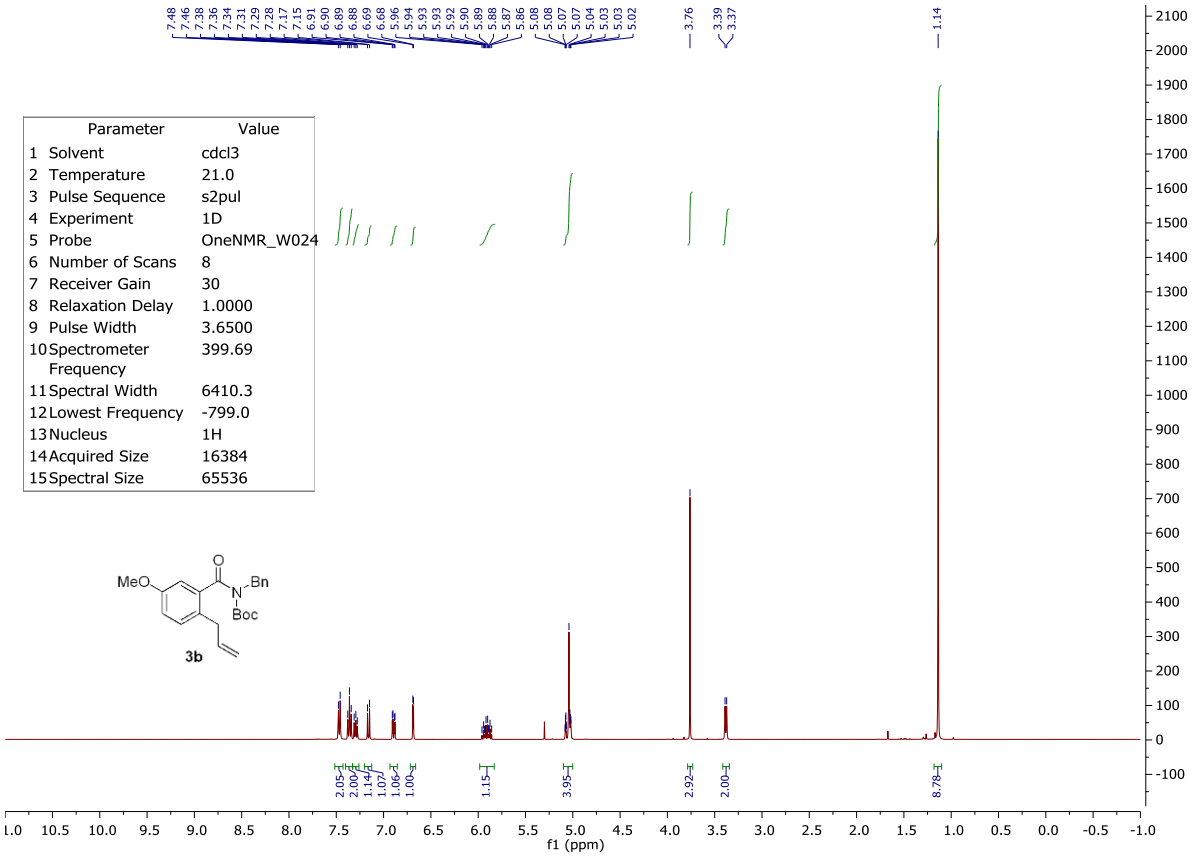

-133.33
-133.35
-133.35
-133.37
-133.38
-133.40
-133.41
-133.43
-137.74
-137.76
-137.76
-137.78
-137.79
-137.81
-137.82
-137.84
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 54
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76610.2
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
O
N
Bn
Boc
F
F
Br
S2k
f1 (ppm)

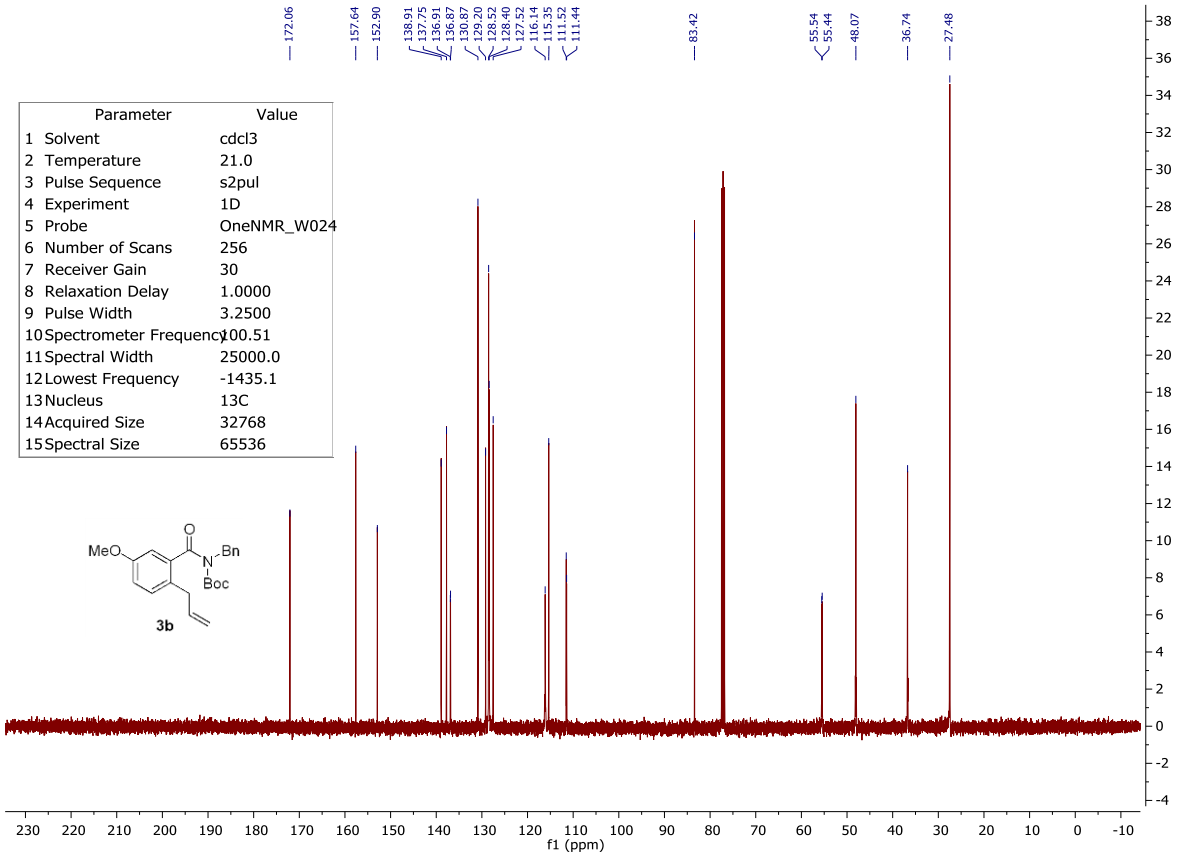

7.46 7.44 7.36 7.34 7.32 7.29 7.28 7.26 7.25 7.23 7.21 7.19 7.17 7.13 7.11 5.97 5.95 5.94 5.94 5.93 5.91 5.90 5.89 5.89 5.87 5.09 5.08 5.06 5.05 5.05 5.04 5.03 3.45 3.44 1.08
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 44
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.6
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
N
Bn
Boc
1a
1.96 5.23 1.06 1.05 1.12 4.00 2.12 8.79
f1 (ppm)

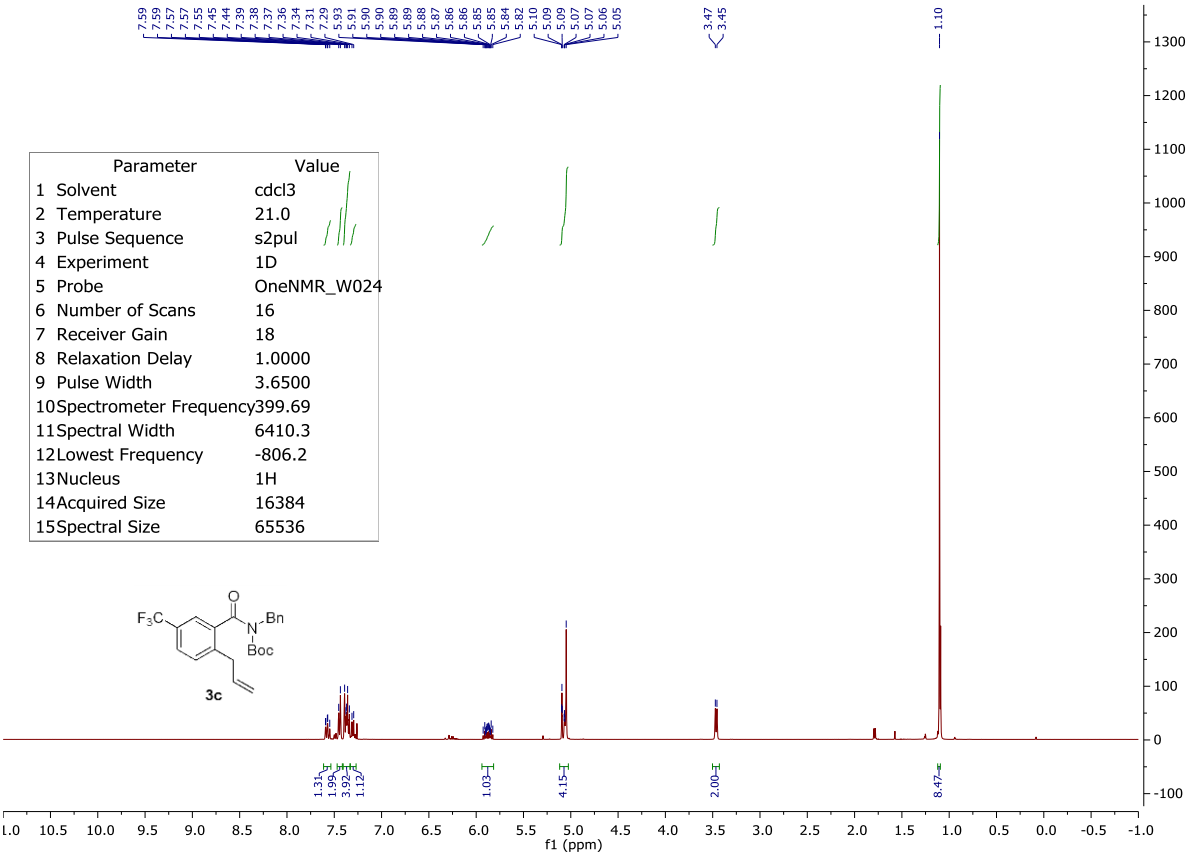

172.42 153.00 138.23 137.85 137.30 136.55 129.80 129.63 128.56 128.42 127.53 126.05 125.88 116.55 83.44 48.07 37.59 27.47
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 192
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1430.7
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
N
Bn
Boc
1a
f1 (ppm)

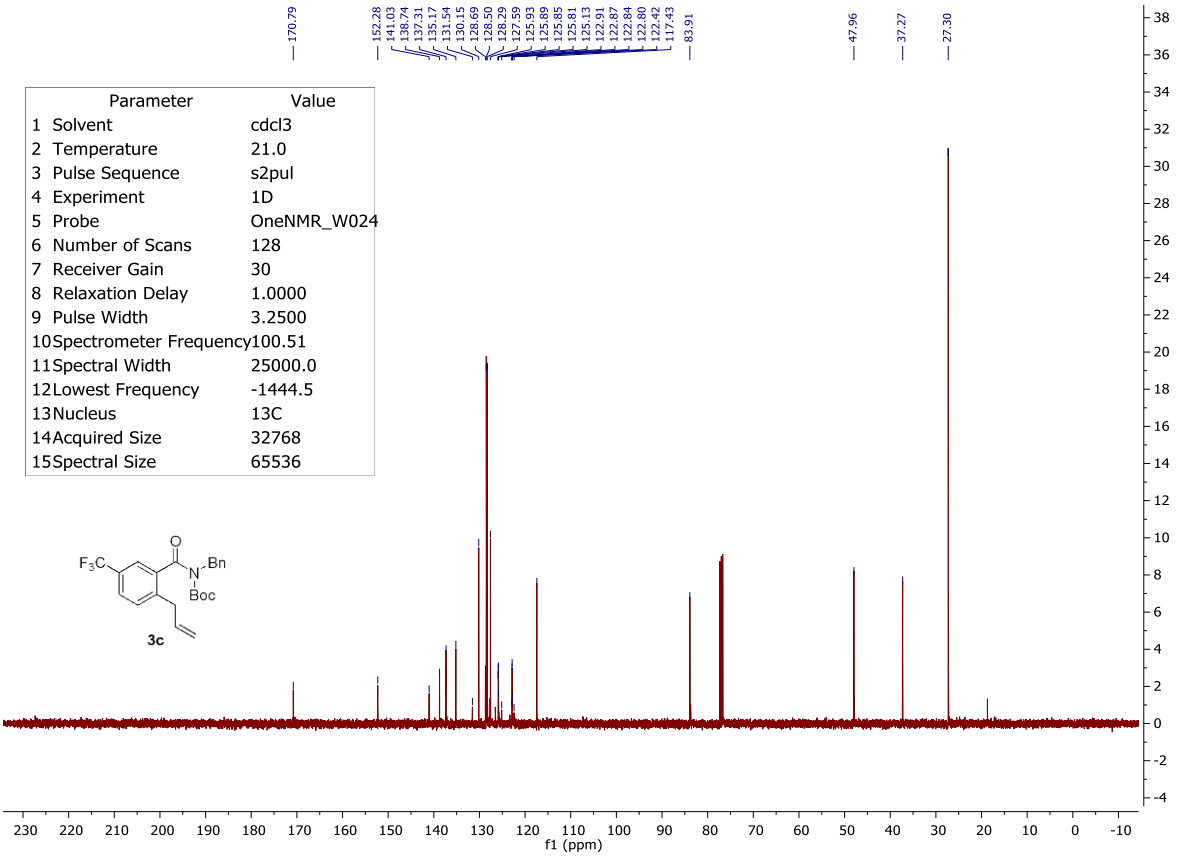

7.47 7.46 7.45 7.45 7.37 7.37 7.35 7.35 7.33 7.30 7.28 7.26 7.13 6.96 5.96 5.94 5.93 5.92 5.90 5.89 5.88 5.87 5.86 5.08 5.07 5.07 5.04 5.03 5.03 5.02 5.01 5.01 5.01 5.01 3.42 3.40 2.30 1.09
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
N
Bn
Boc
3a
1.93 1.98 1.08 1.96 0.96 1.10 3.96 2.00 2.95 8.81
f1 (ppm)

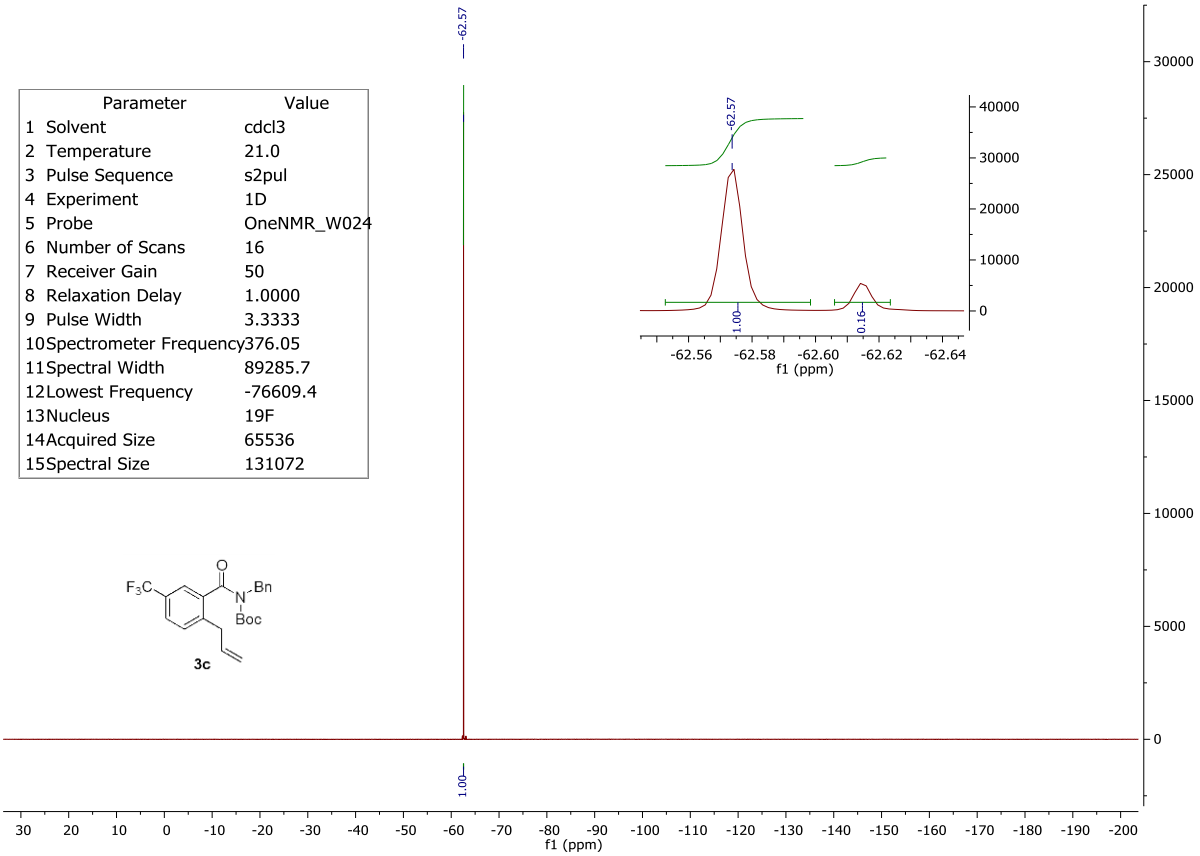

172.49 153.06 137.94 137.85 136.83 136.81 135.38 134.25 130.30 129.76 128.51 128.38 127.47 126.69 116.23 83.28 48.06 37.17 27.44 20.92
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 64
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1434.2
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
N
Bn
Boc
3a
f1 (ppm)

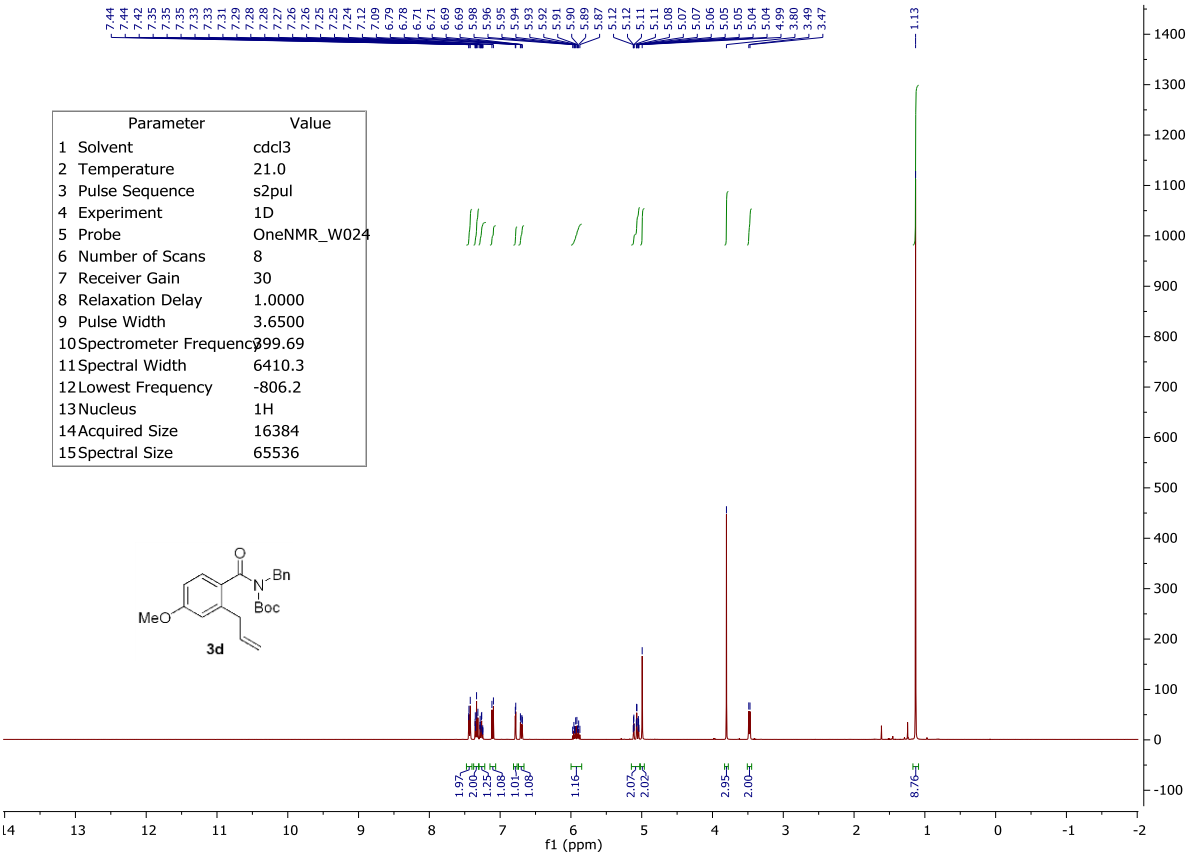

7.48 7.46 7.38 7.36 7.34 7.31 7.29 7.28 7.17 7.15 6.91 6.90 6.89 6.88 6.69 6.68 5.96 5.94 5.93 5.93 5.92 5.90 5.89 5.88 5.87 5.86 5.08 5.08 5.07 5.07 5.04 5.03 5.03 5.02
3.76 3.39 3.37
1.14
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -799.0
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
MeO
N
Bn
Boc
O
3b
2.05 2.00 1.14 1.07 1.06 1.00 1.15 3.95 2.92 2.00 8.78
f1 (ppm)

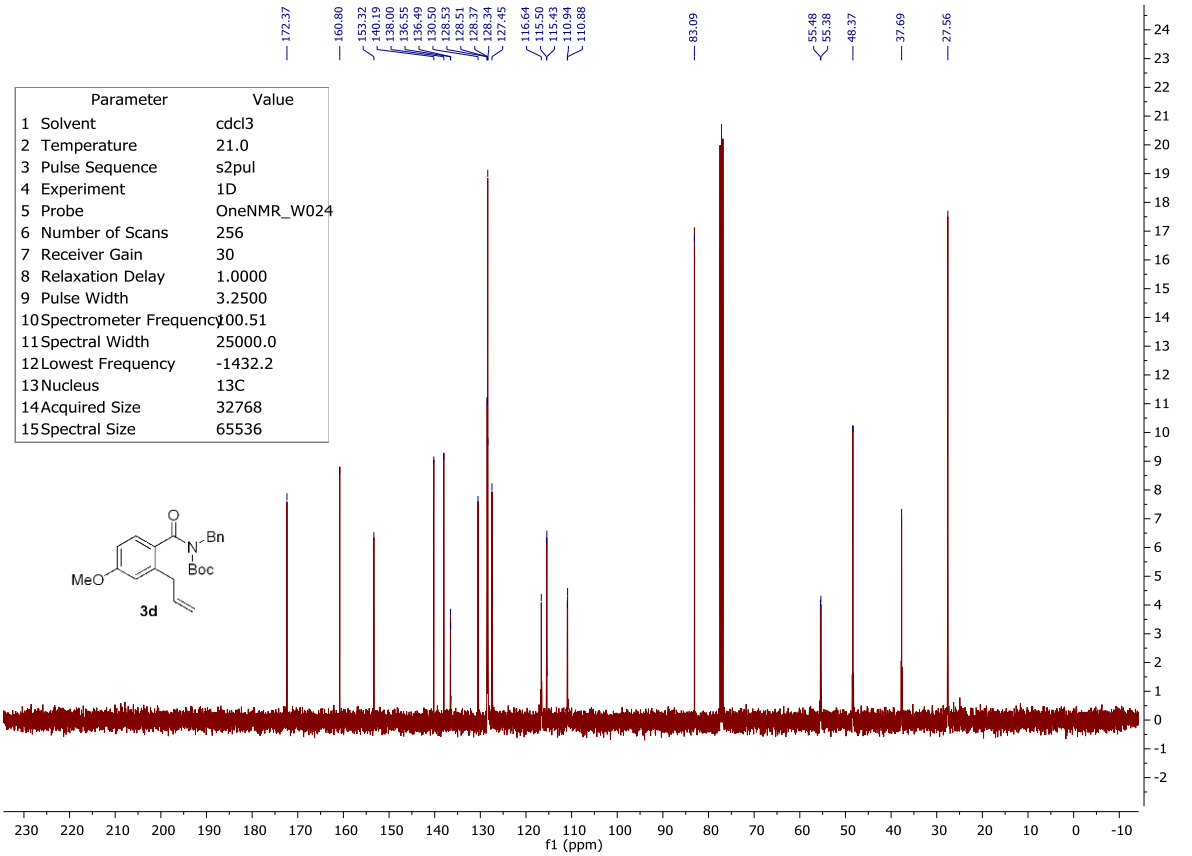

172.06
157.64
152.90
138.91 137.75 136.91 136.87 130.87 129.20 128.52 128.40 127.52 116.14 115.35 111.52 111.44
83.42
55.54 55.44
48.07
36.74
27.48
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1435.1
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
MeO
N
Bn
Boc
O
3b
f1 (ppm)

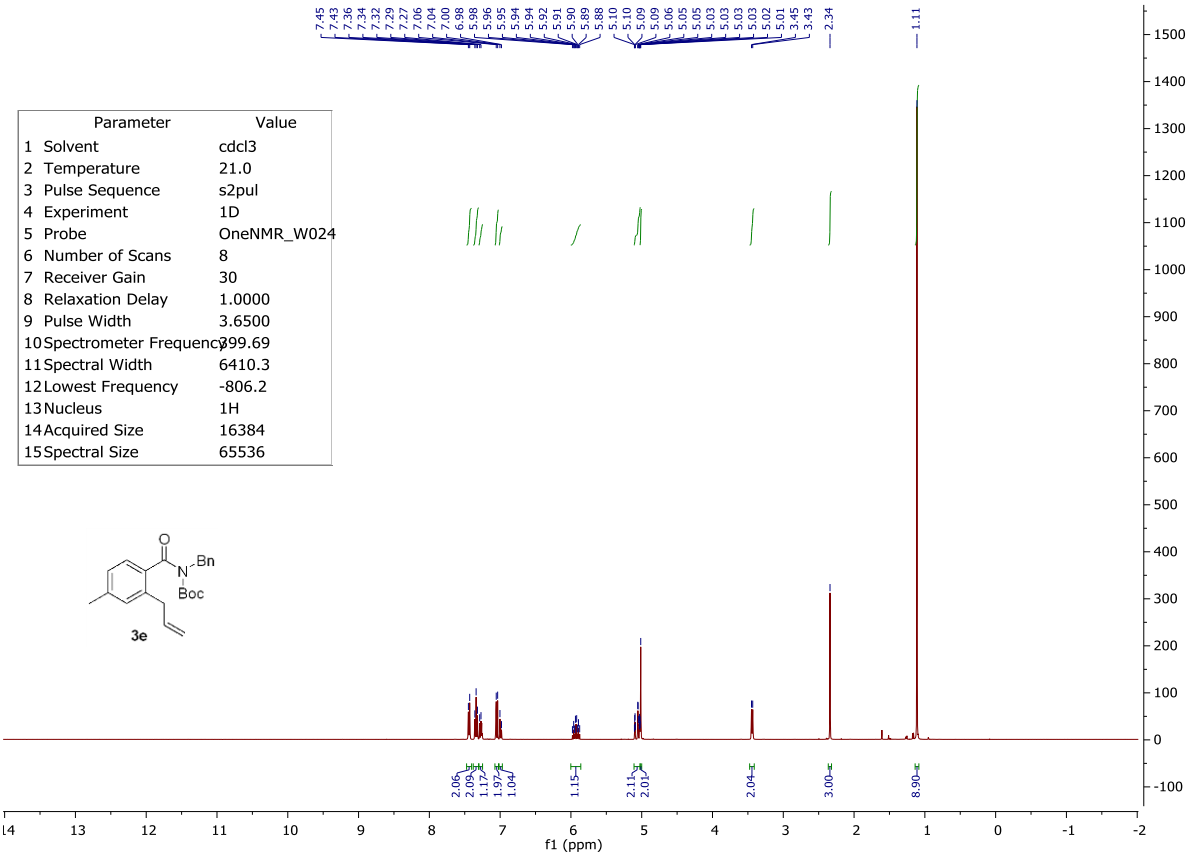

7.59 7.59 7.57 7.57 7.55 7.45 7.44 7.39 7.38 7.37 7.36 7.34 7.31 7.29 5.93 5.91 5.90 5.90 5.89 5.89 5.88 5.87 5.86 5.86 5.85 5.85 5.84 5.82 5.10 5.09 5.09 5.07 5.07 5.06 5.05
3.47 3.45
1.10
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 18
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
F3C
O
N
Bn
Boc
3c
1.31 1.95 3.92 1.12 1.03 4.15 2.00 8.47
f1 (ppm)

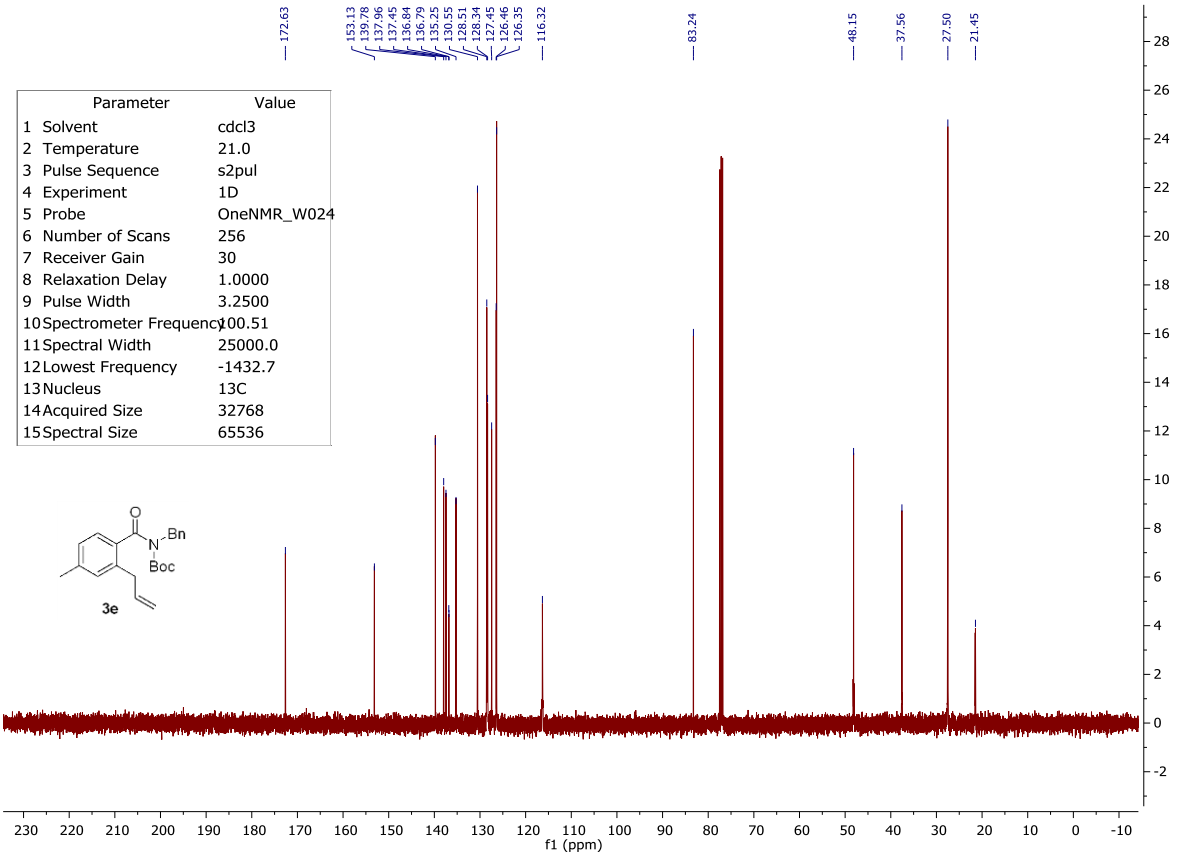

170.79
152.28 141.03 138.74 137.31 135.17 131.54 130.15 128.69 128.50 128.29 127.59 125.93 125.89 125.85 125.81 125.13 122.91 122.87 122.84 122.80 122.42 117.43
83.91
47.96
37.27
27.30
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 128
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1444.5
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
F3C
O
N
Bn
Boc
3c
f1 (ppm)

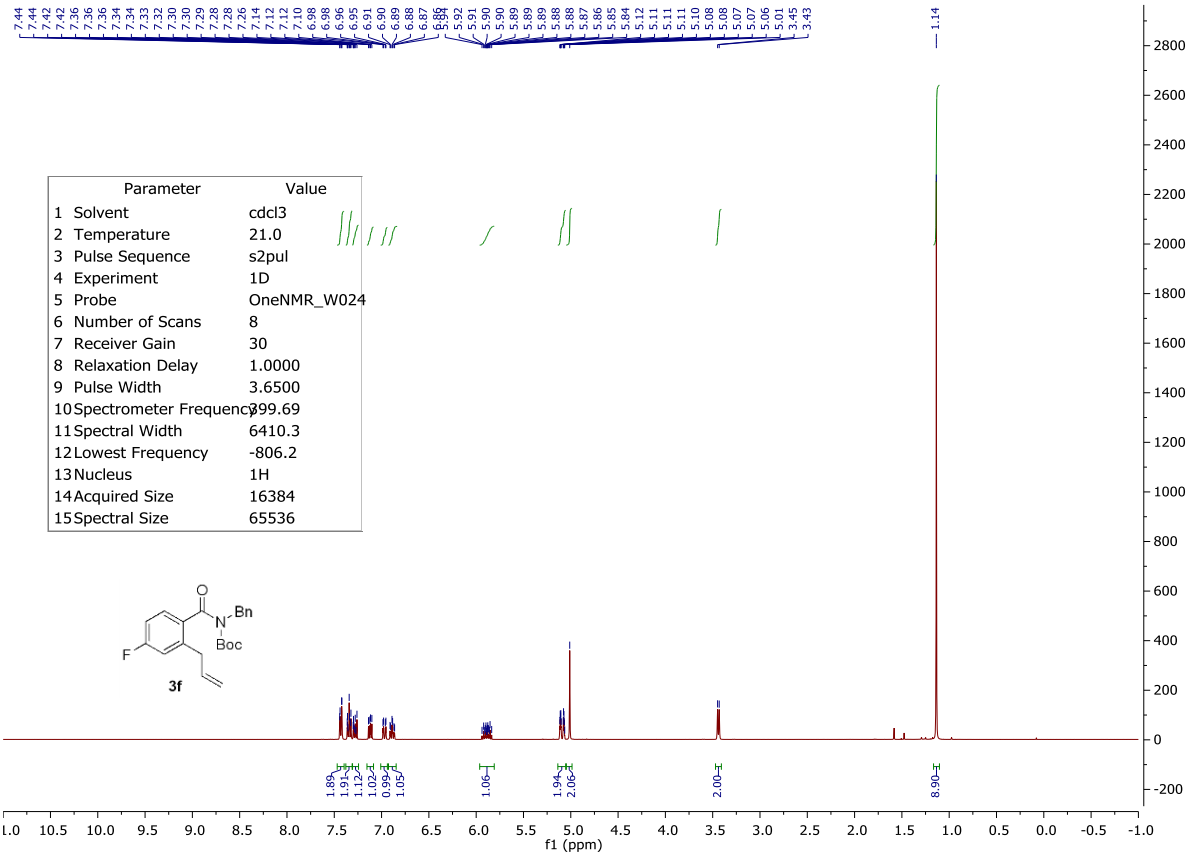

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 50
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76609.4
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
-62.57
1.00
0.16
f1 (ppm)
F3C
O
N
Bn
Boc
3c

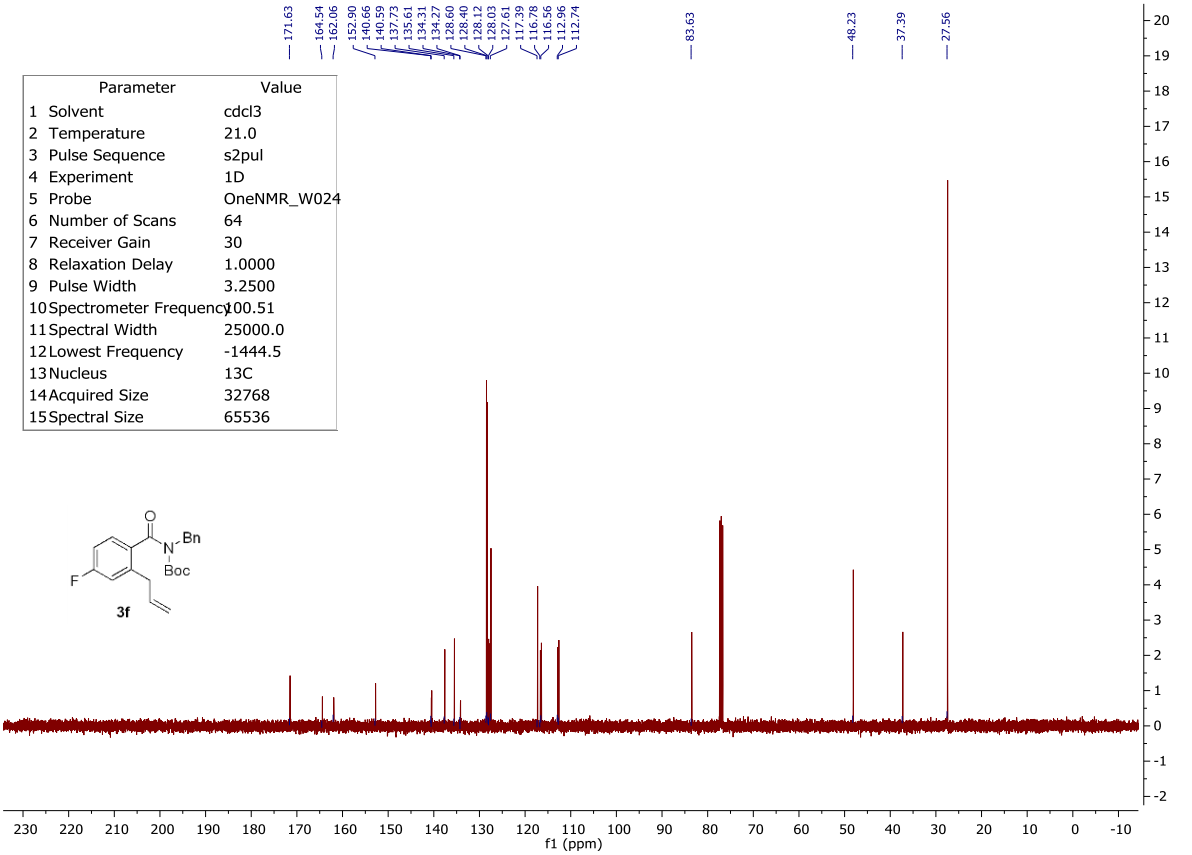

7.44 7.44 7.42 7.35 7.35 7.35 7.33 7.33 7.31 7.29 7.28 7.28 7.27 7.26 7.26 7.25 7.25 7.24 7.12 7.09 6.79 6.78 6.71 6.71 6.69 6.69 5.98 5.96 5.95 5.94 5.93 5.92 5.91 5.90 5.89 5.87 5.12 5.12 5.11 5.11 5.08 5.07 5.07 5.06 5.05 5.05 5.04 5.04 4.99 3.80 3.49 3.47
1.13
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
MeO
N
Bn
Boc
O
3d
1.97 2.00 1.25 1.08 1.01 1.08 1.16 2.07 2.02 2.95 2.00 8.76
f1 (ppm)

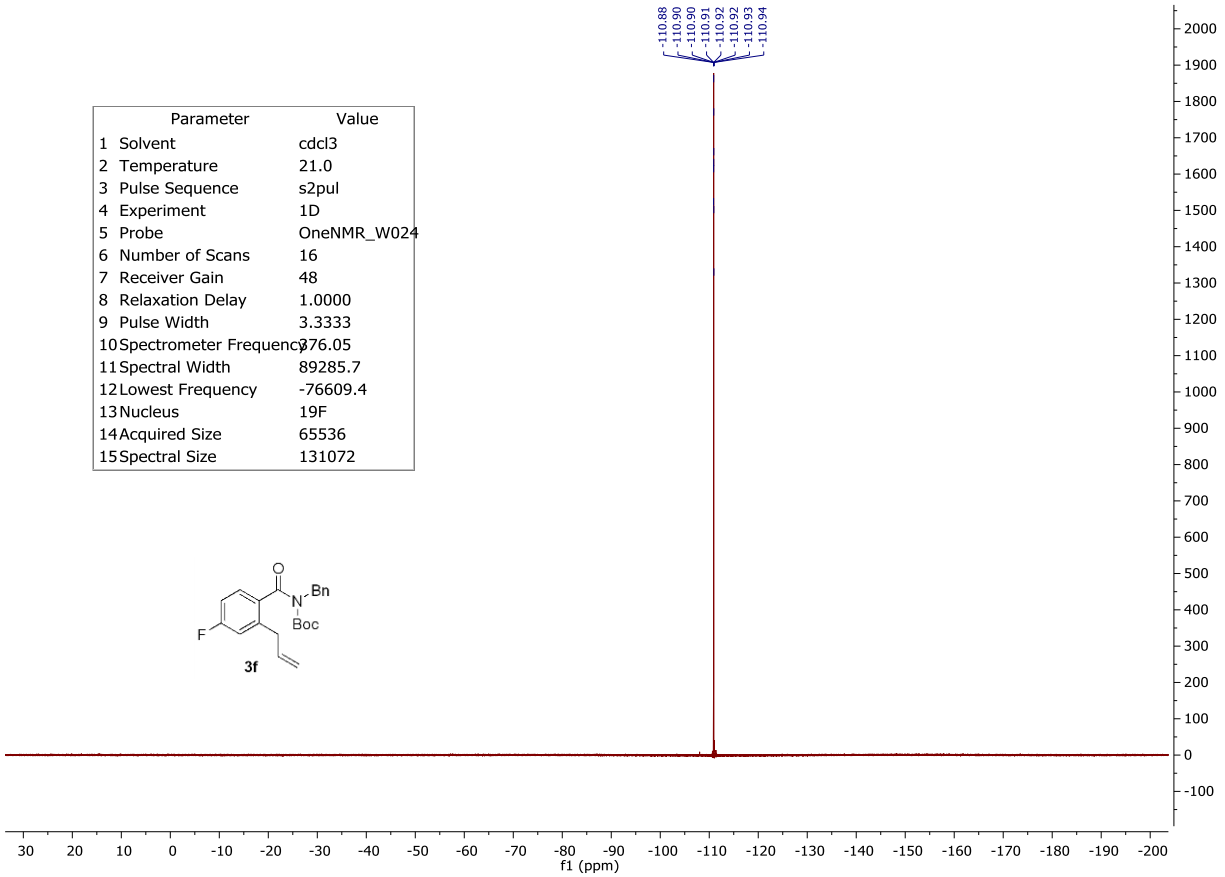

172.37 160.80 153.32 140.19 138.00 136.55 136.49 130.50 128.53 128.51 128.37 128.34 127.45 116.64 115.50 115.43 110.94 110.88 83.09 55.48 55.38 48.37 37.69 27.56
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1432.2
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
MeO
N
Bn
Boc
O
3d
f1 (ppm)

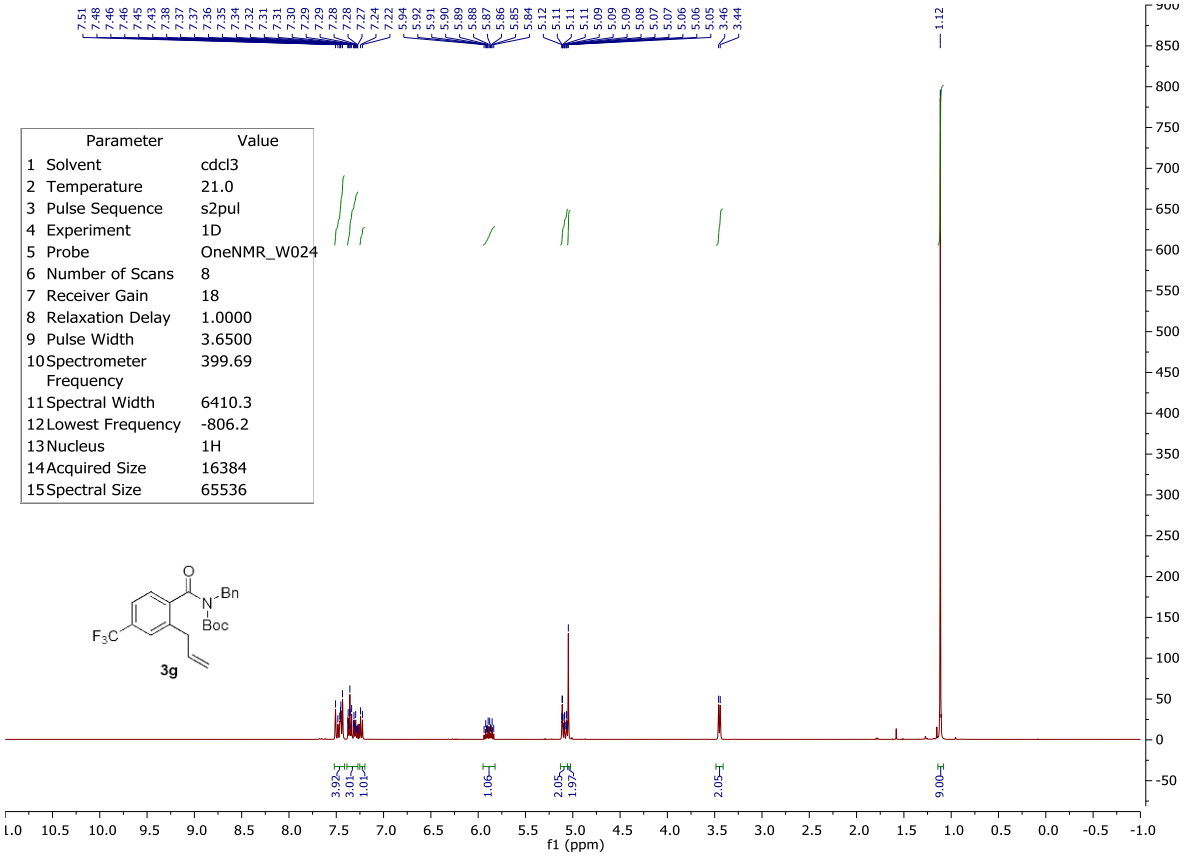

7.45 7.43 7.36 7.34 7.32 7.29 7.27 7.06 7.04 7.00 6.98 5.98 5.96 5.95 5.94 5.94 5.92 5.91 5.90 5.89 5.88 5.10 5.10 5.09 5.09 5.06 5.05 5.05 5.03 5.03 5.03 5.03 5.02 5.01 3.45 3.43 2.34 1.11
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
N
Bn
Boc
3e
2.06 2.05 1.17 1.97 1.04 1.15 2.11 2.01 2.04 3.00 8.90
f1 (ppm)

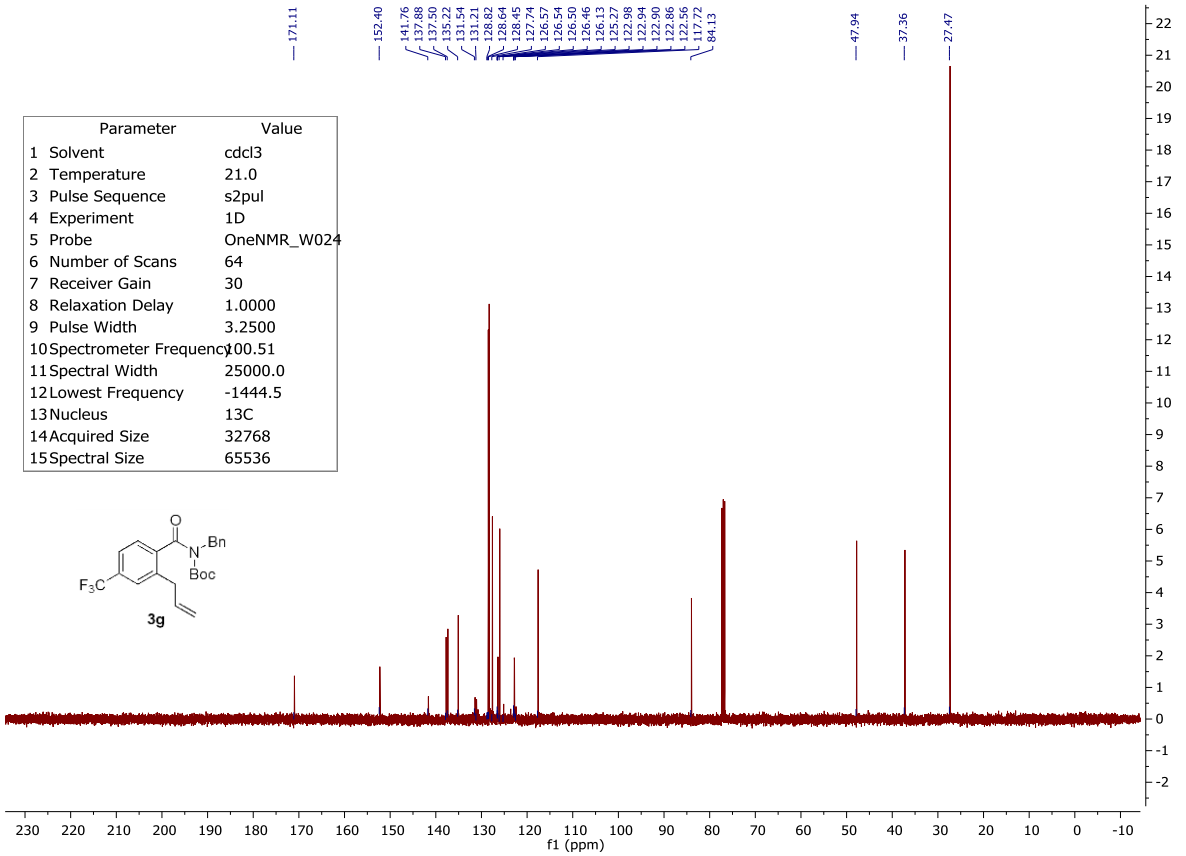

172.63 153.13 139.78 137.96 137.45 136.84 136.79 135.25 130.55 128.51 128.34 127.45 126.46 126.35 116.32 83.24 48.15 37.56 27.50 21.45
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1432.7
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
N
Bn
Boc
3e
f1 (ppm)


Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
3f
f1 (ppm)

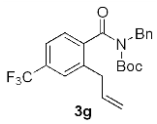

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 64
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1444.5
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
3f
f1 (ppm)


-110.88
-110.90
-110.90
-110.91
-110.92
-110.92
-110.93
-110.94
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 48
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76609.4
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
O
N
Bn
Boc
F
3f
f1 (ppm)

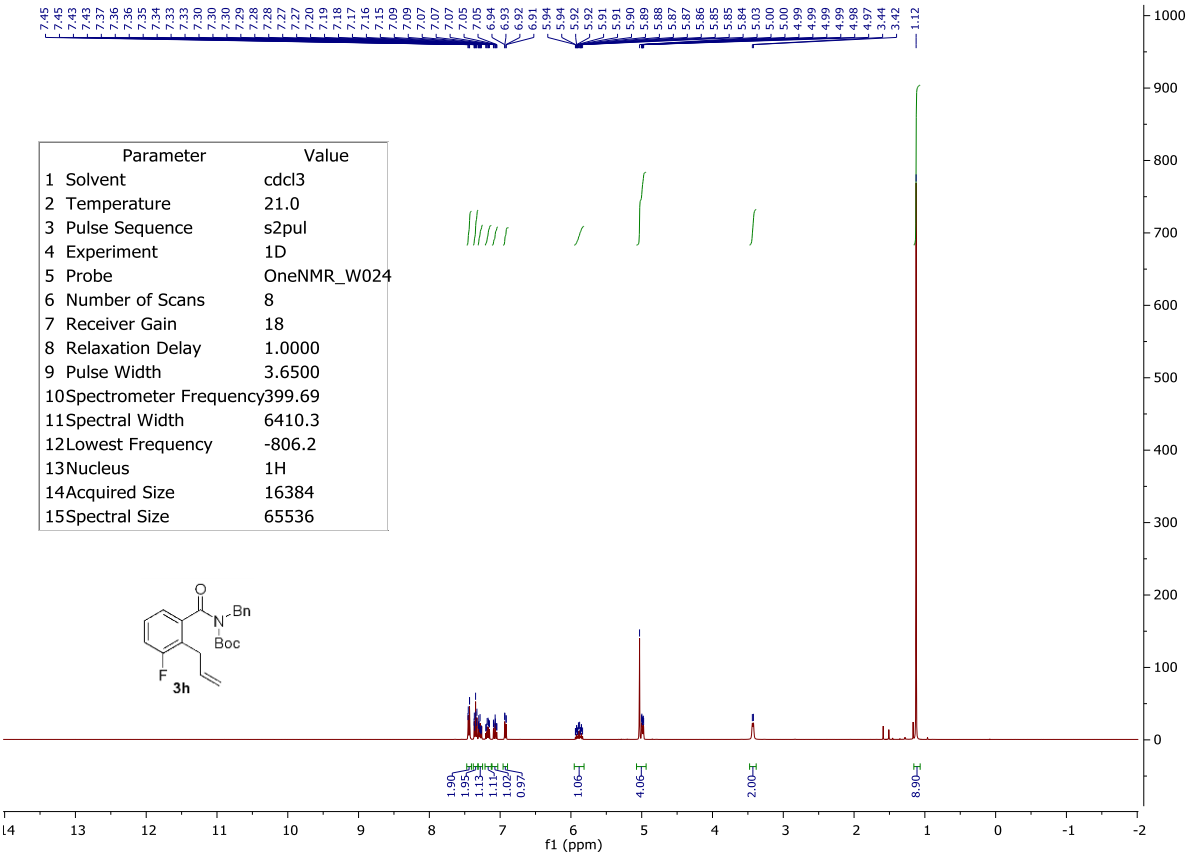

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 18
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
Bn
N
Boc
O
F3C
3g
f1 (ppm)

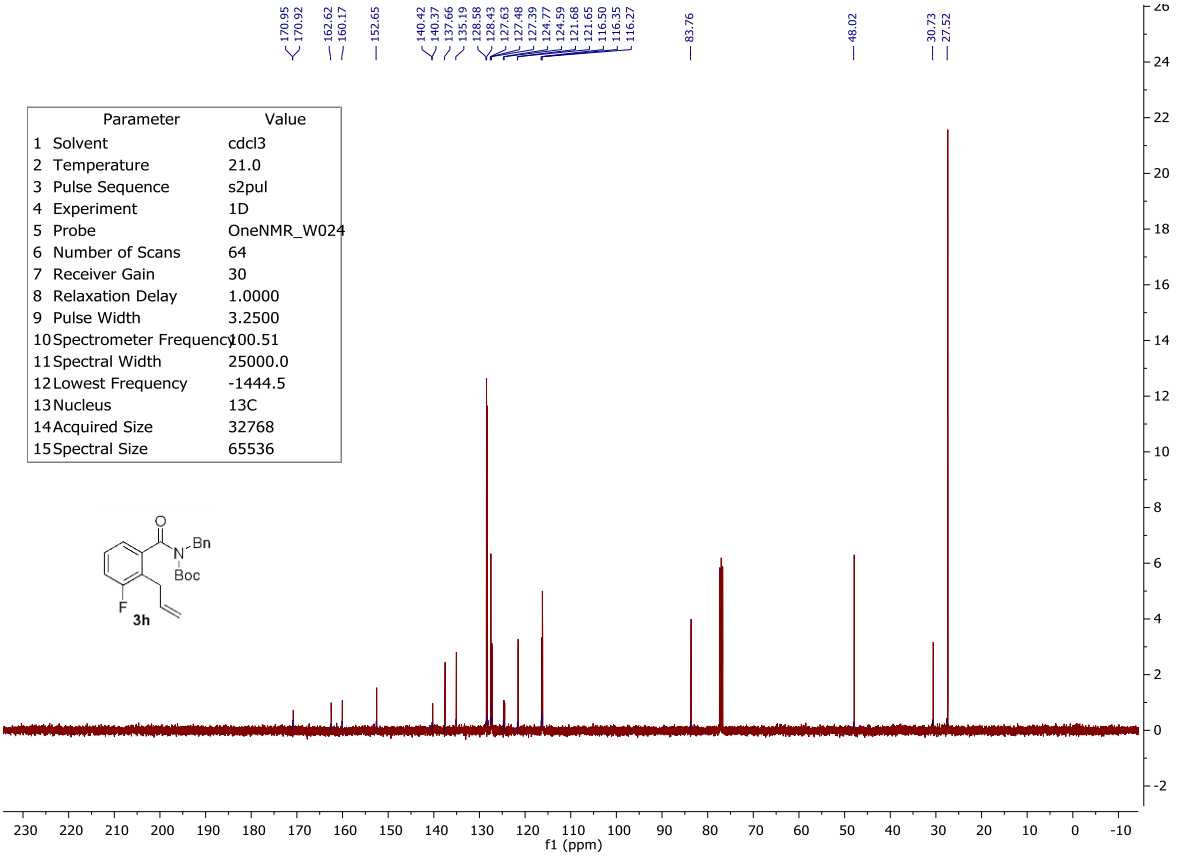

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 64
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1444.5
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
Bn
N
Boc
O
F3C
3g
f1 (ppm)

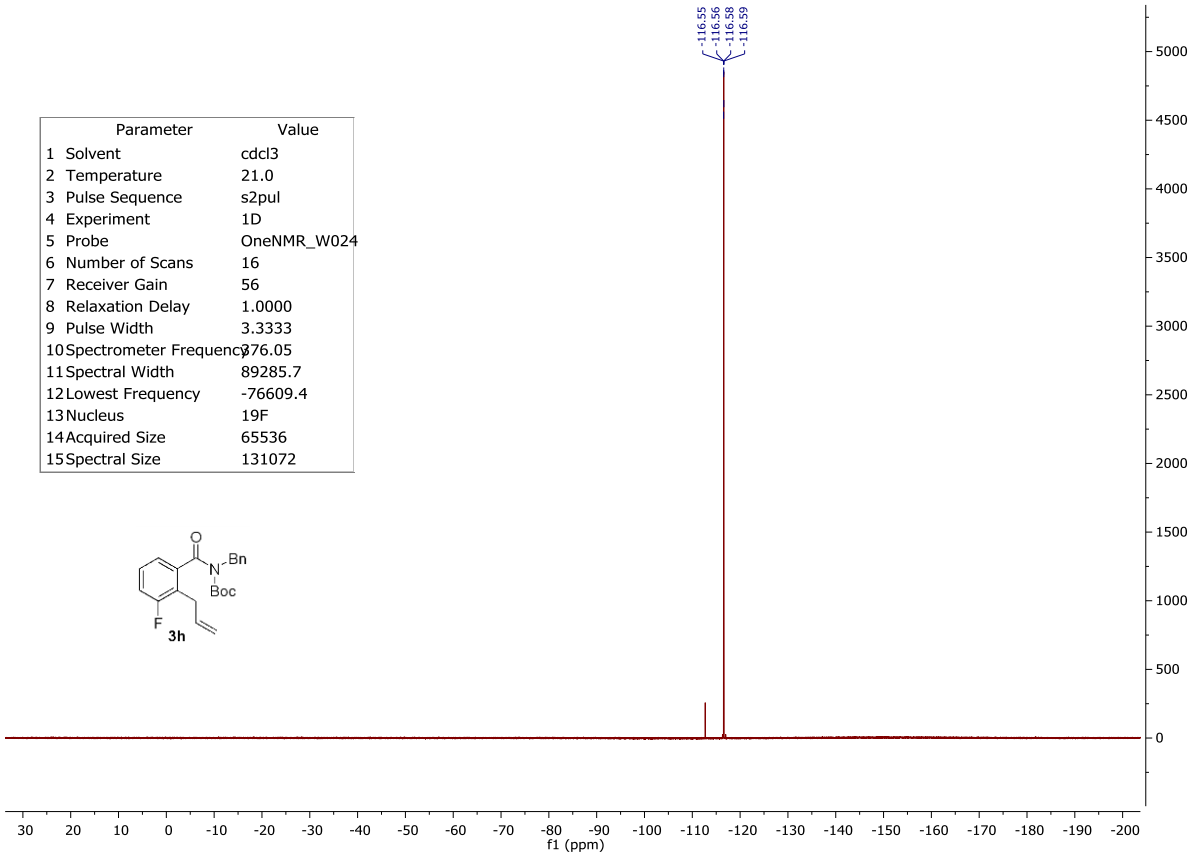
| | Parameter | Value |
|---|---|---|
| 1 | Solvent | cdcl3 |
| 2 | Temperature | 21.0 |
| 3 | Pulse Sequence | s2pul |
| 4 | Experiment | 1D |
| 5 | Probe | OneNMR_W024 |
| 6 | Number of Scans | 16 |
| 7 | Receiver Gain | 48 |
| 8 | Relaxation Delay | 1.0000 |
| 9 | Pulse Width | 3.3333 |
| 10 | Spectrometer Frequency | 376.05 |
| 11 | Spectral Width | 89285.7 |
| 12 | Lowest Frequency | -76609.4 |
| 13 | Nucleus | 19F |
| 14 | Acquired Size | 65536 |
| 15 | Spectral Size | 131072 |

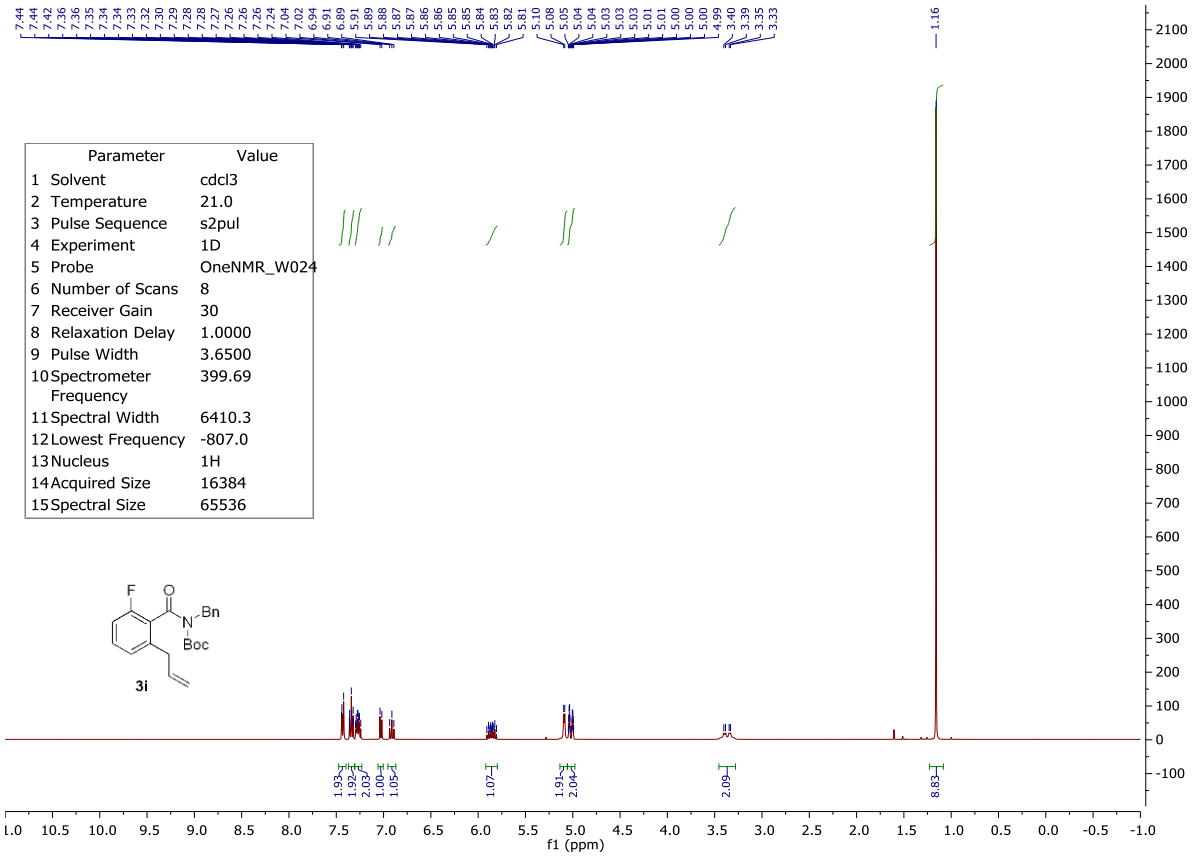


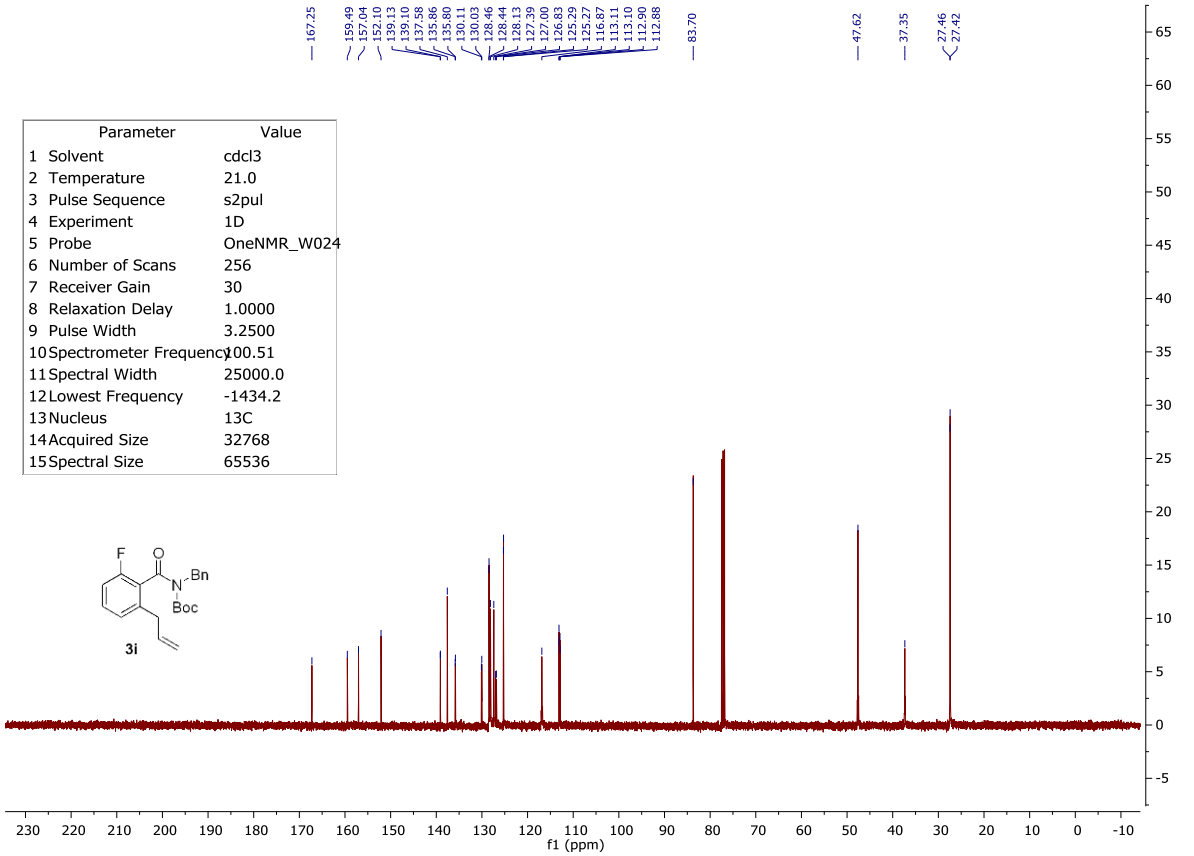

**3g**

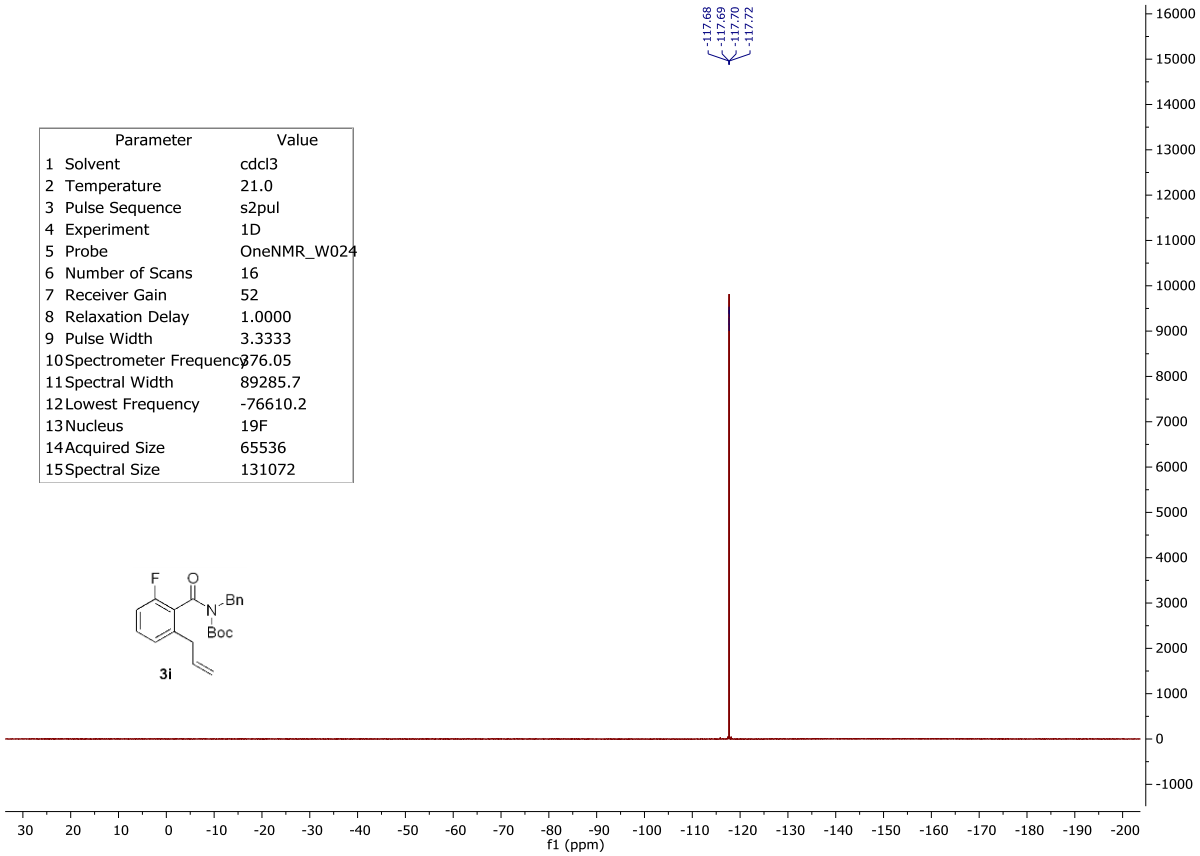

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 18
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
Bn
Boc
F
3h
f1 (ppm)

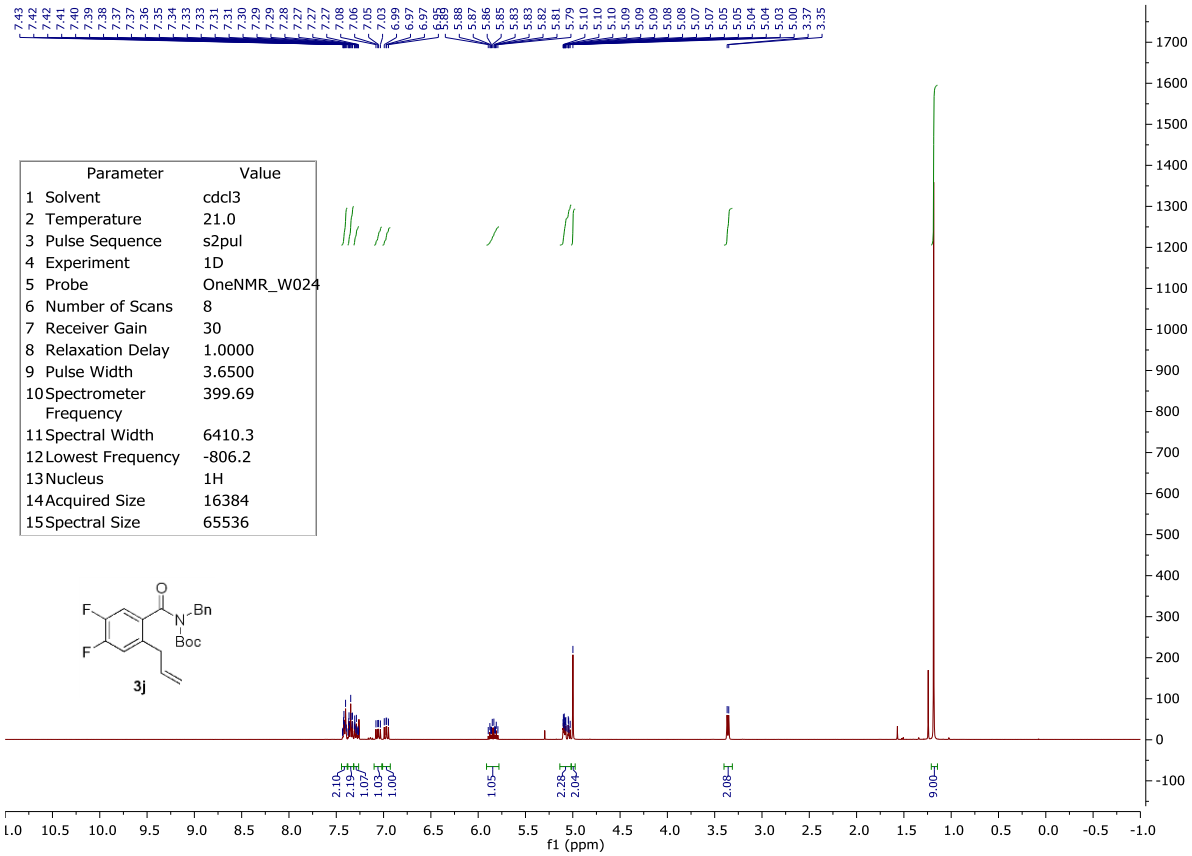

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 64
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1444.5
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
Bn
Boc
F
3h
f1 (ppm)

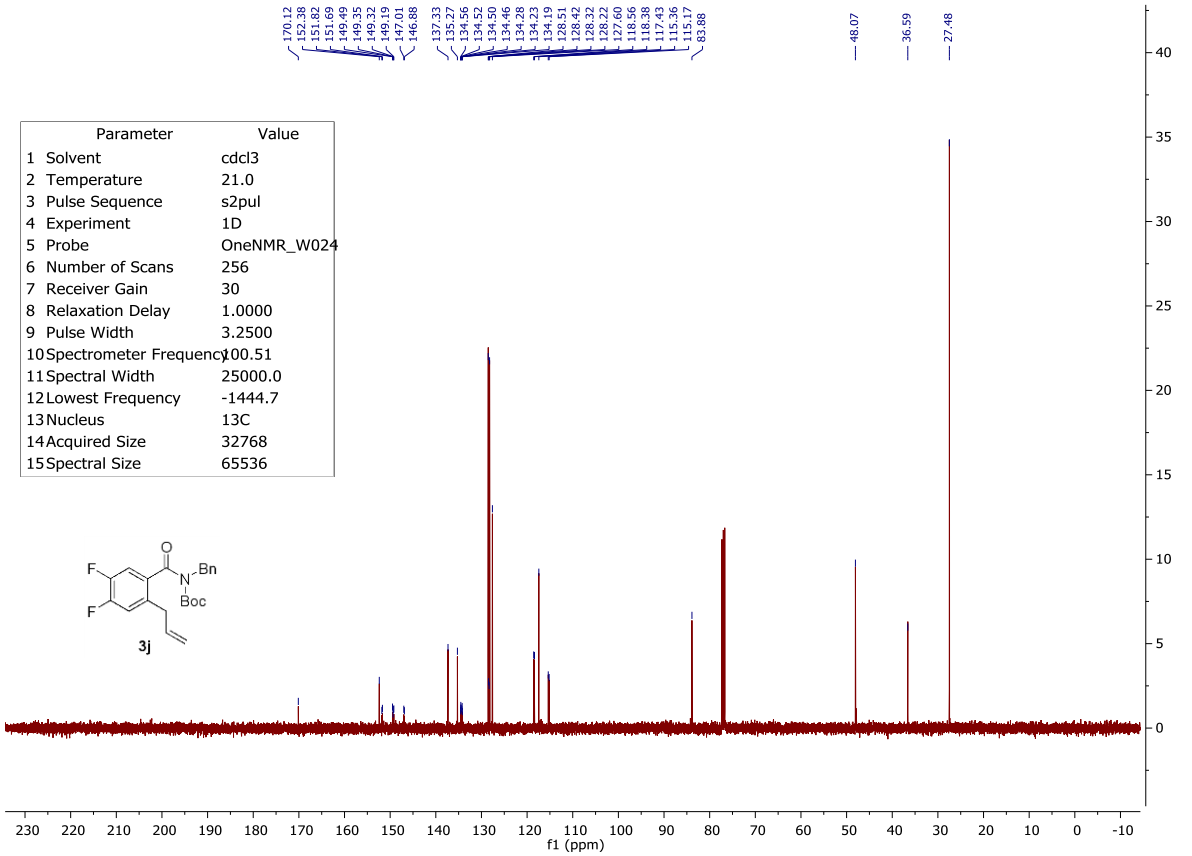

-116.55
-116.56
-116.58
-116.59
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 56
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76609.4
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
O
N
Bn
Boc
F
3h
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

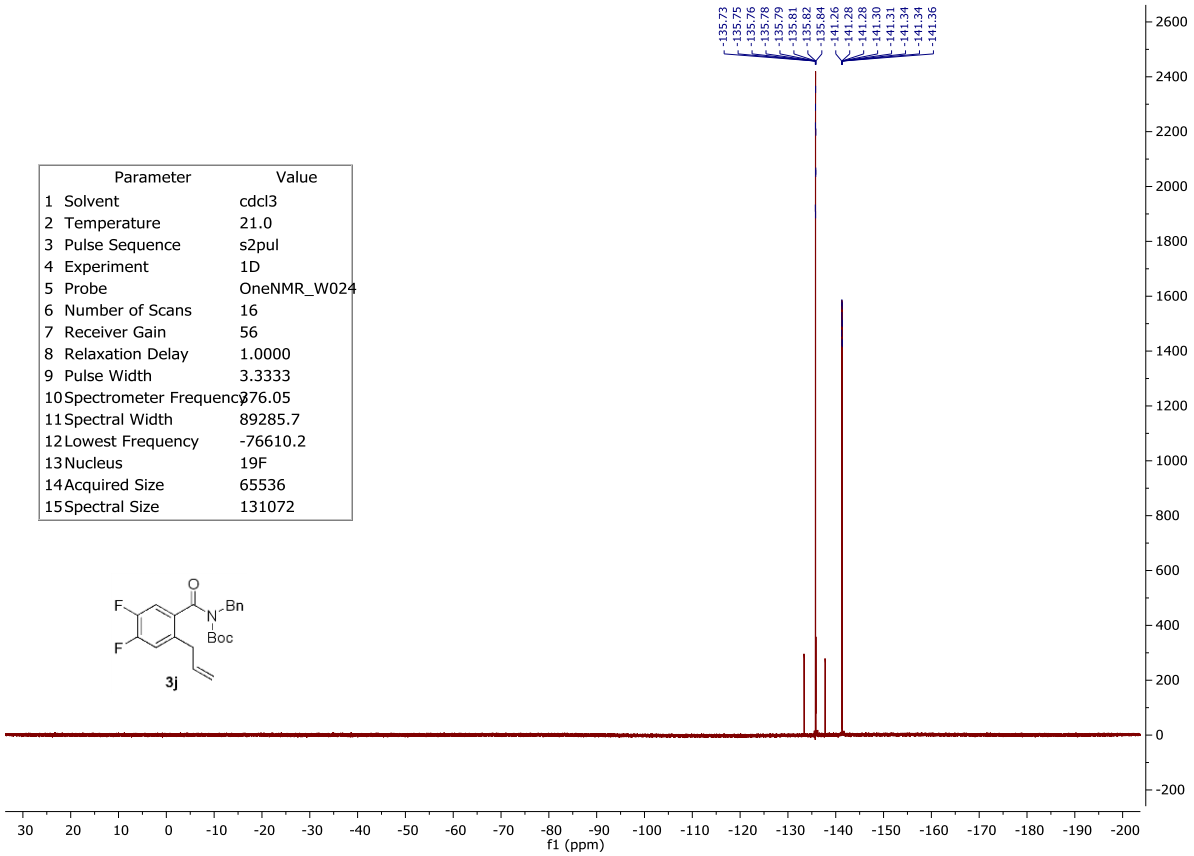

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -807.0
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
F
O
N
Bn
Boc
3i
f1 (ppm)

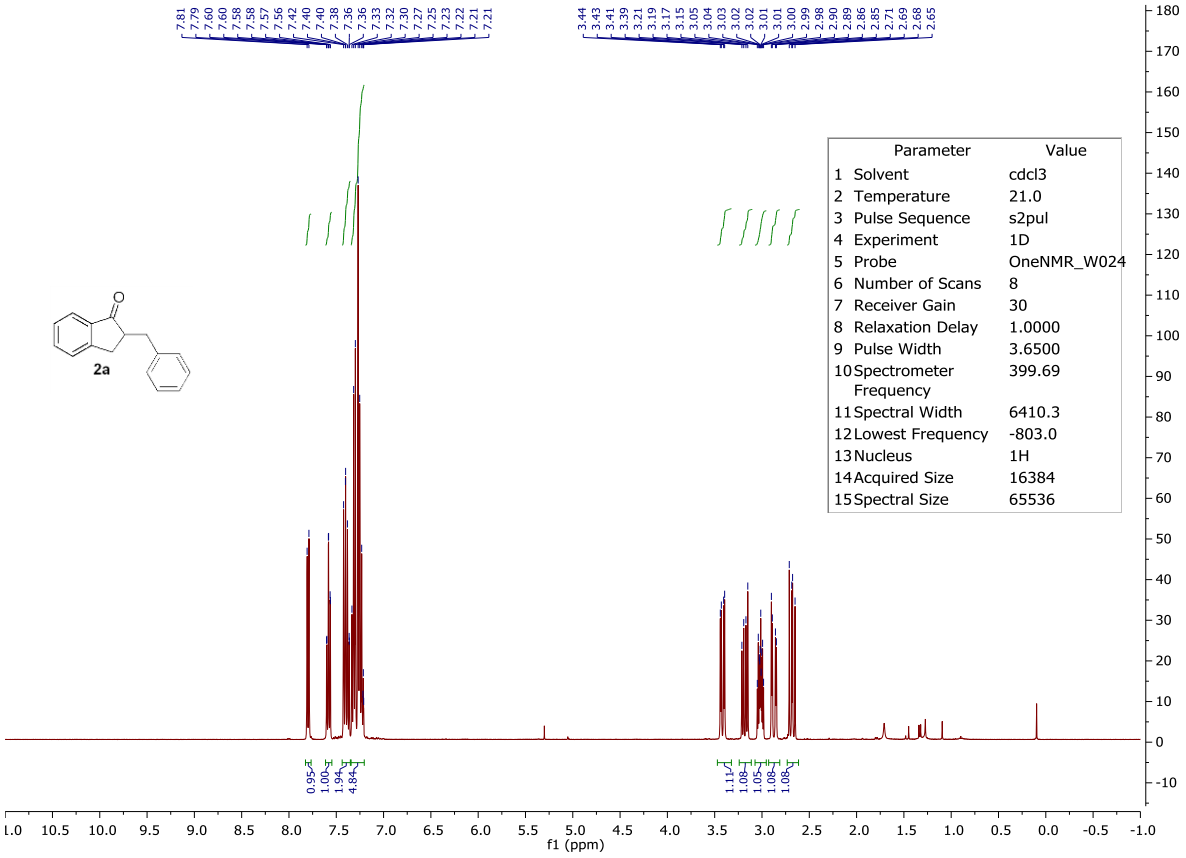

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1434.2
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
F
O
N
Bn
Boc
3i
f1 (ppm)

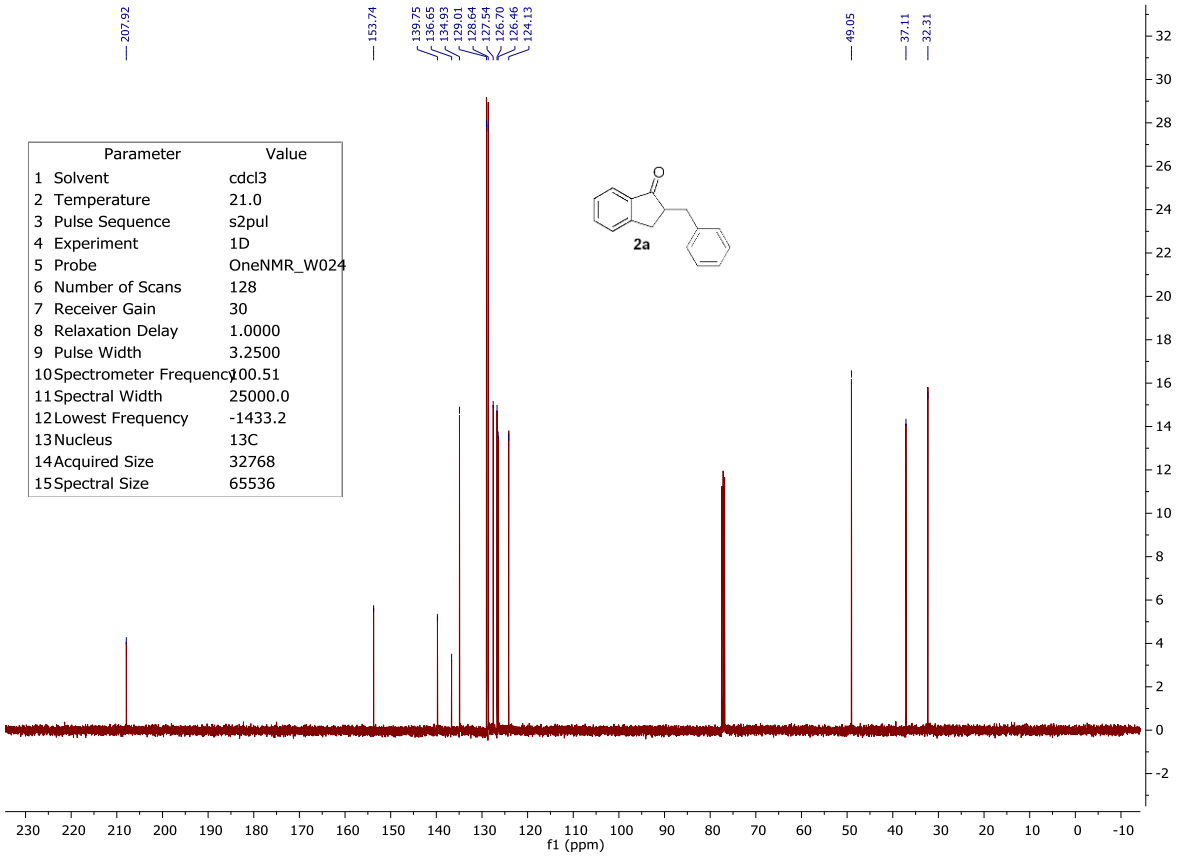

-117.68
-117.69
-117.70
-117.72
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 52
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76610.2
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
F
O
N
Bn
Boc
3i
f1 (ppm)

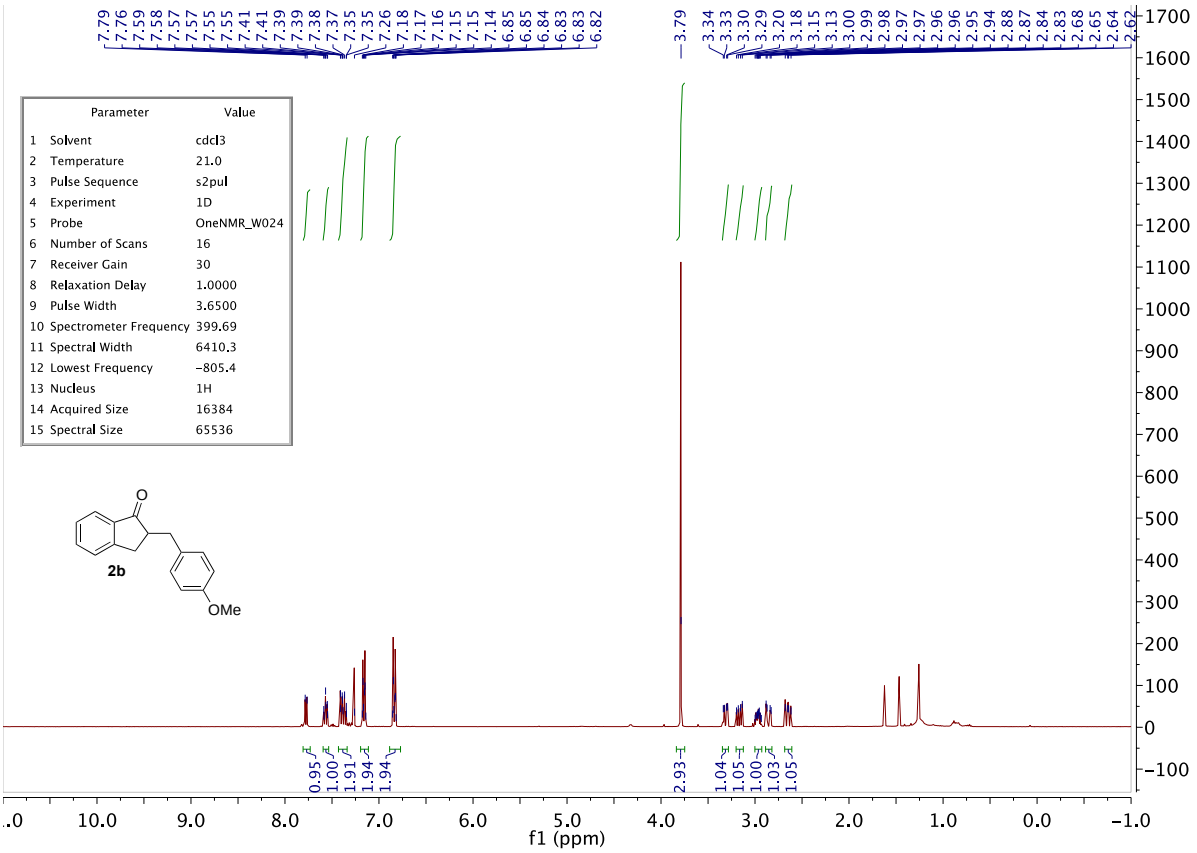

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
F
F
O
N
Bn
Boc
3j
f1 (ppm)

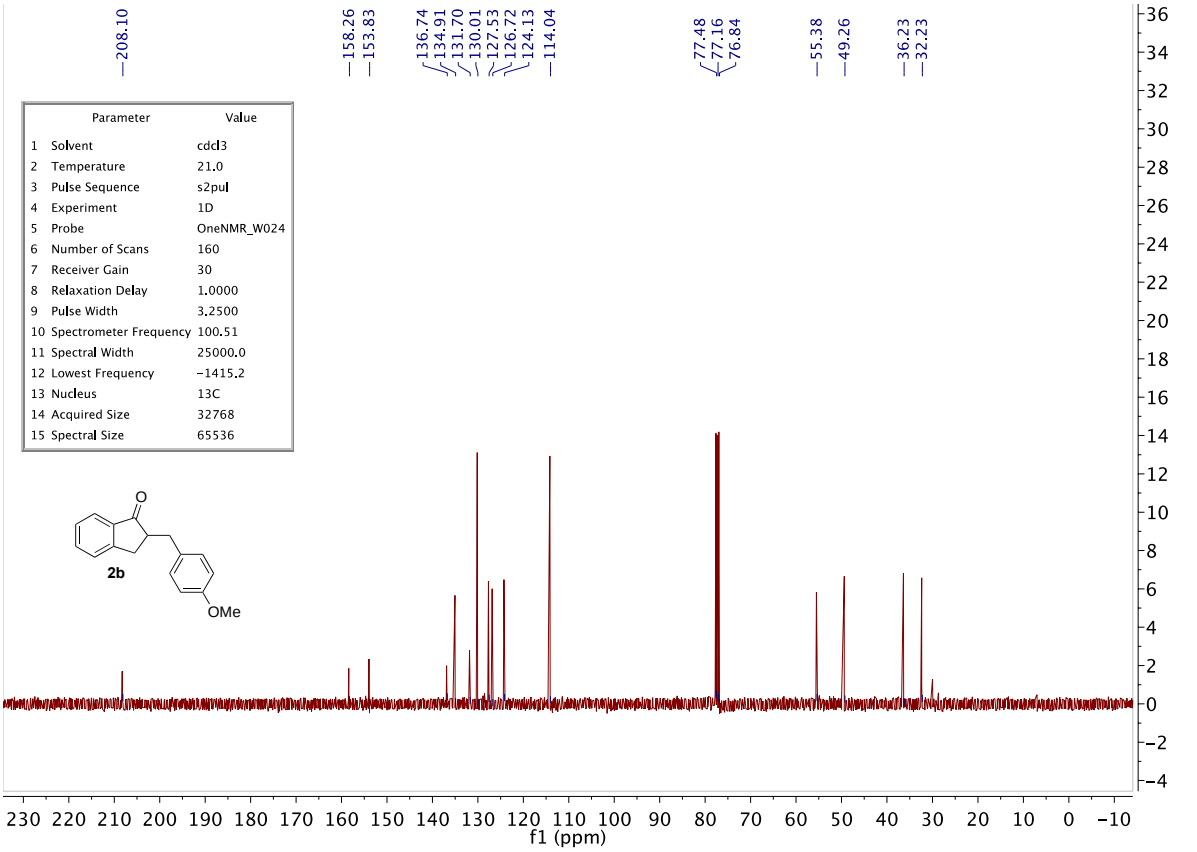

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1444.7
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
F
F
O
N
Bn
Boc
3j
f1 (ppm)

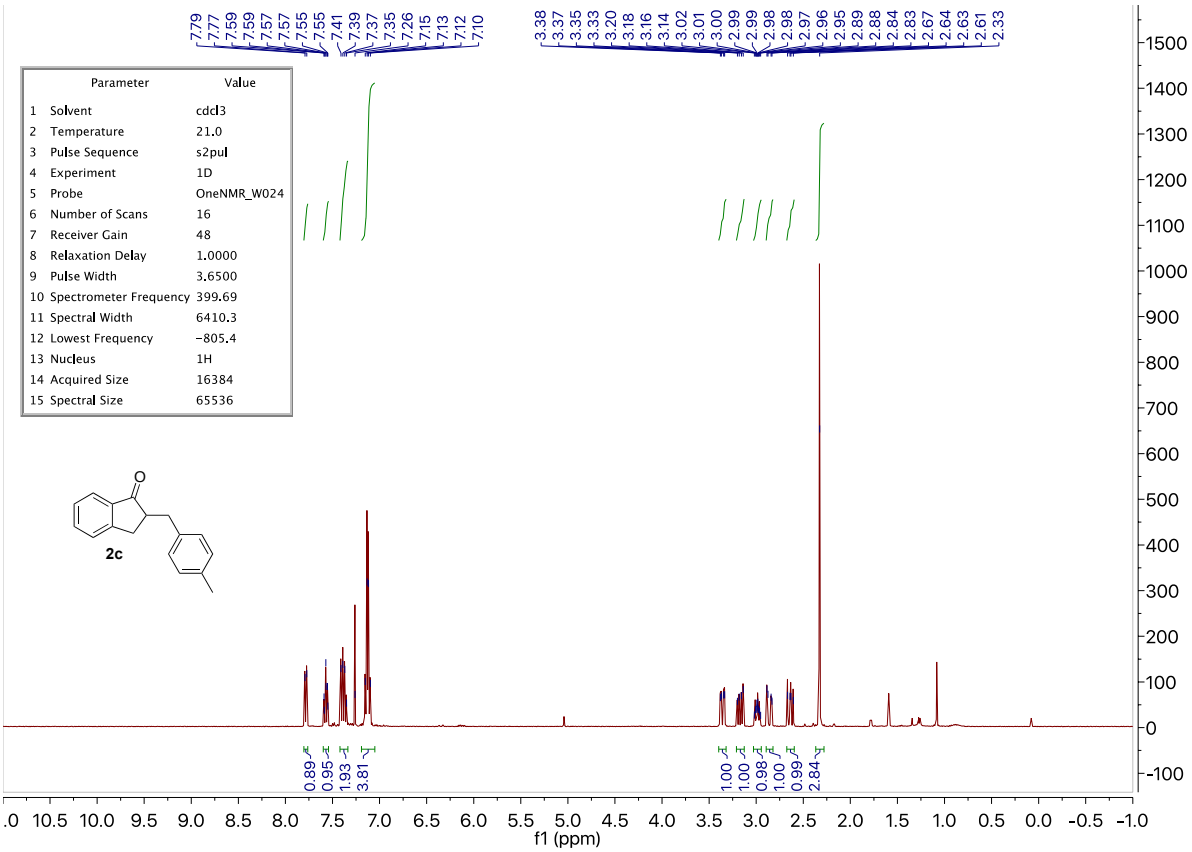

-135.73
-135.75
-135.76
-135.78
-135.79
-135.81
-135.82
-135.84
-141.26
-141.28
-141.30
-141.31
-141.34
-141.34
-141.36
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 56
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76610.2
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
F
F
O
N
Bn
Boc
3j
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

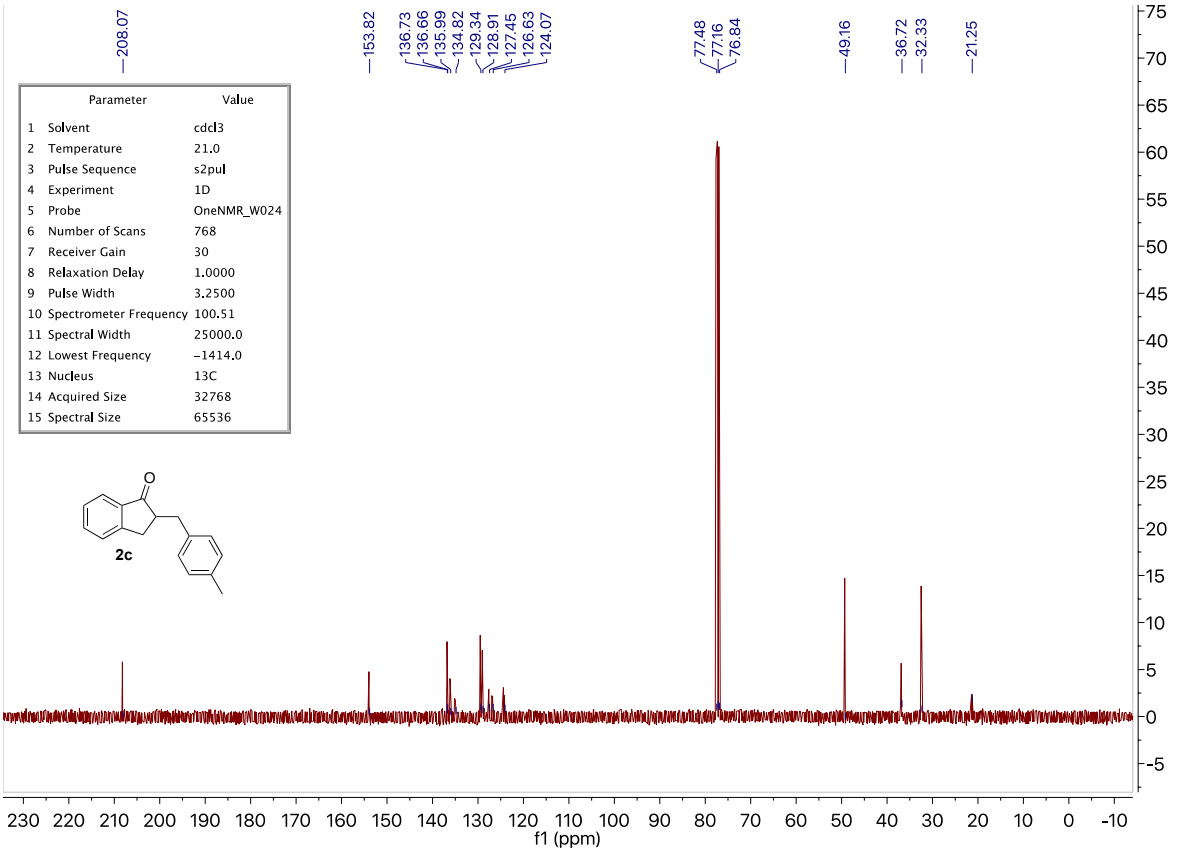

7.81 7.79 7.60 7.60 7.60 7.58 7.58 7.58 7.57 7.56 7.42 7.40 7.40 7.38 7.36 7.36 7.33 7.32 7.30 7.27 7.25 7.23 7.22 7.21 7.21
3.44 3.43 3.41 3.39 3.21 3.19 3.17 3.15 3.05 3.04 3.03 3.02 3.02 3.01 3.01 3.00 2.99 2.98 2.90 2.89 2.86 2.85 2.71 2.69 2.68 2.65
2a
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -803.0
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
0.95 1.00 1.94 4.84 1.11 1.08 1.05 1.08 1.08
f1 (ppm)

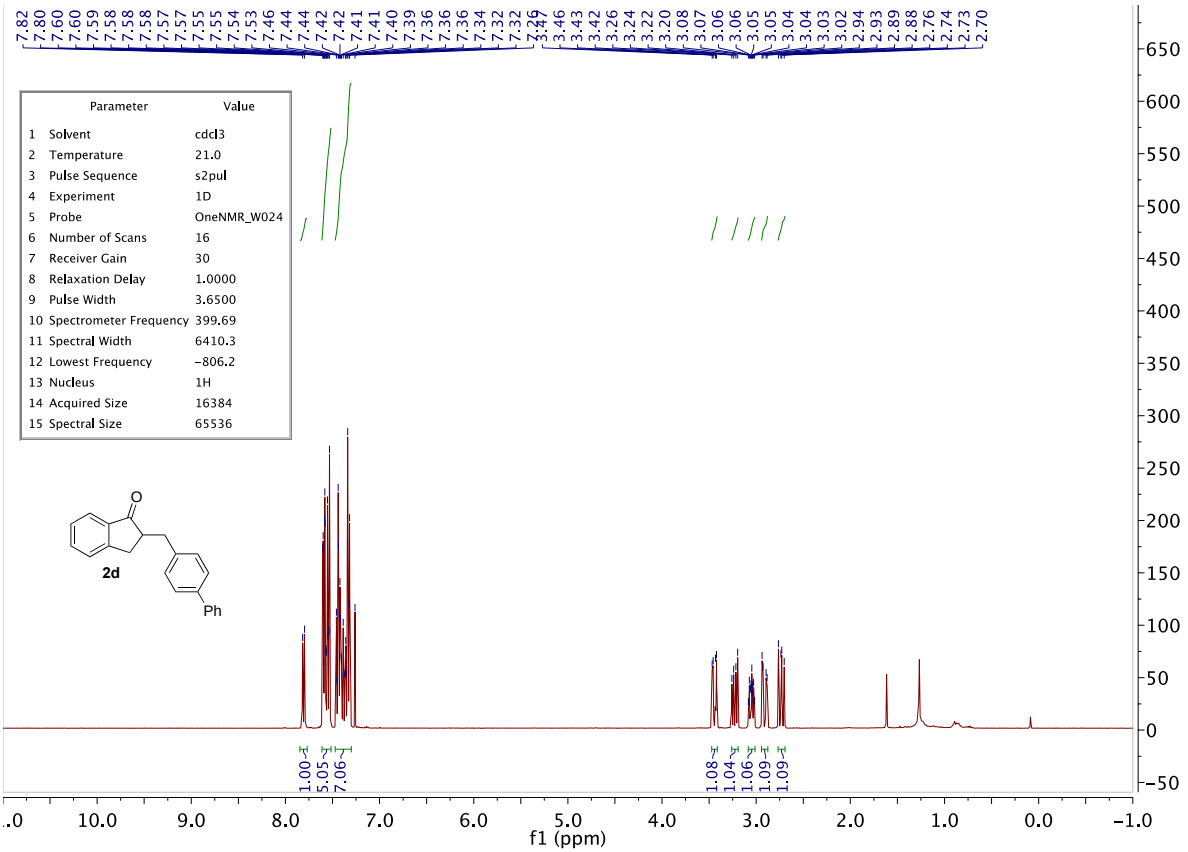

207.92 153.74 139.75 136.65 134.93 129.01 128.64 127.54 126.70 126.46 124.13 49.05 37.11 32.31
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 128
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1433.2
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
2a
f1 (ppm)

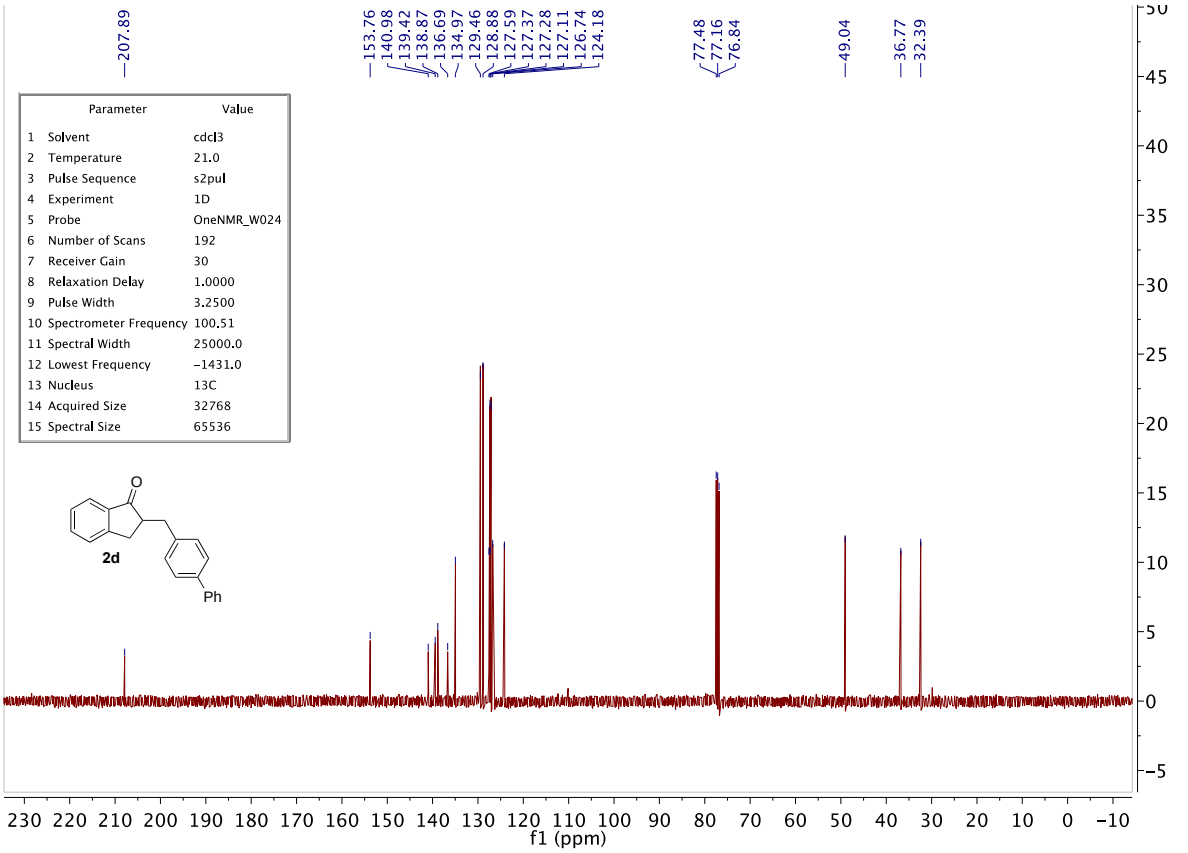

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -805.4
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
2b
OMe
f1 (ppm)

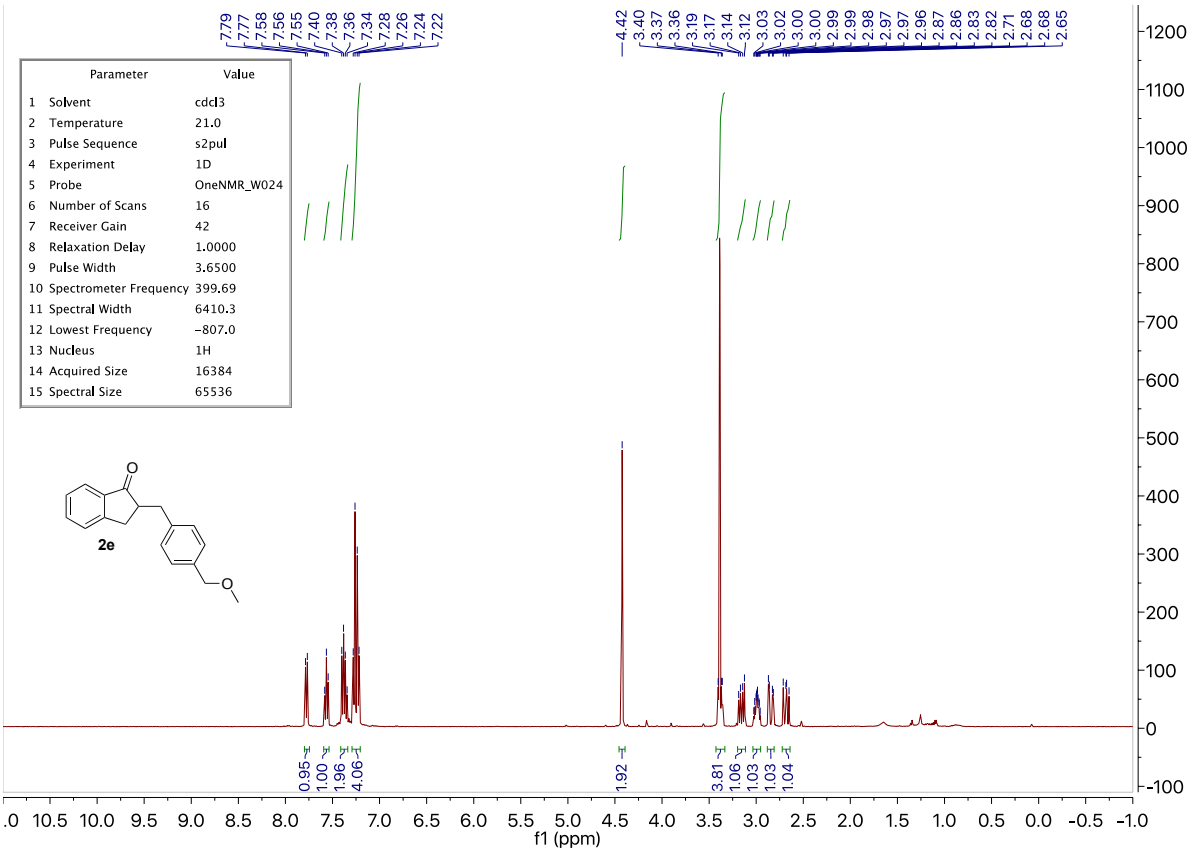

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 160
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1415.2
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
2b
OMe
f1 (ppm)

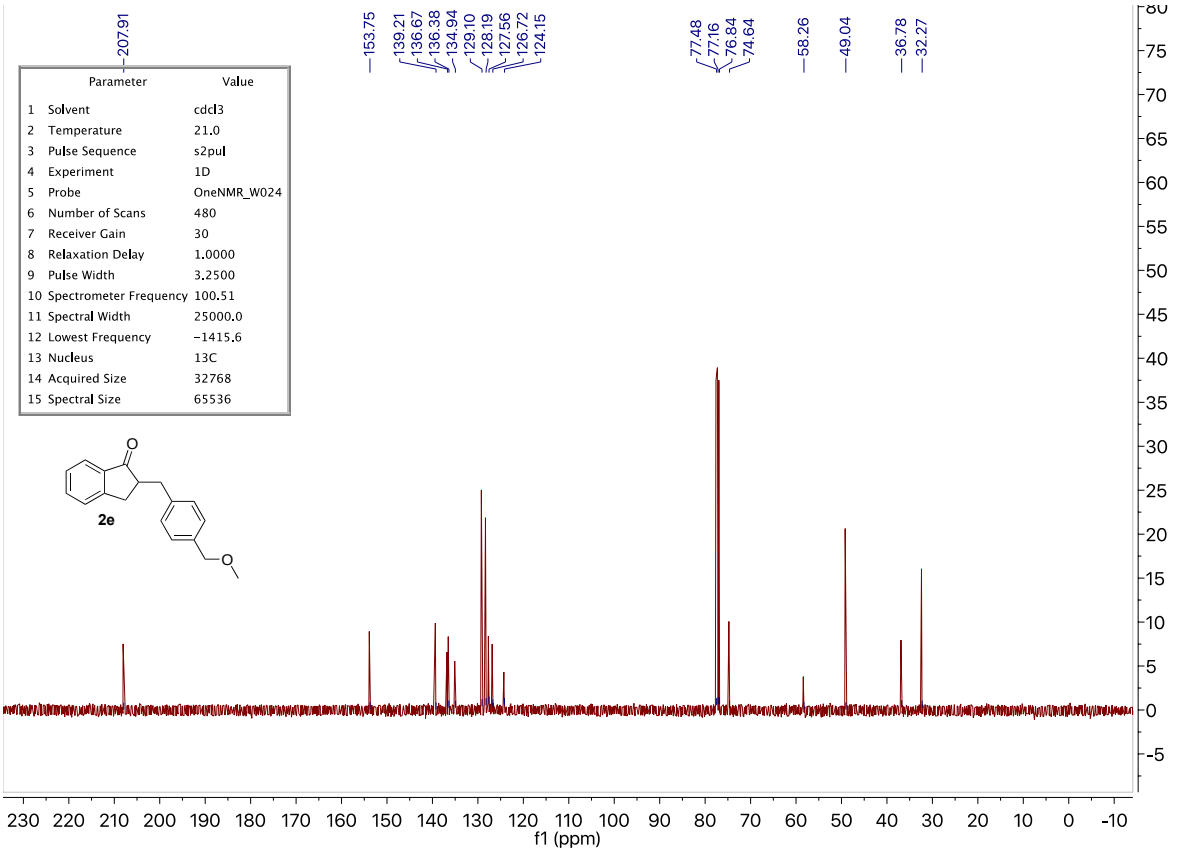

7.79 7.77 7.59 7.59 7.57 7.57 7.55 7.55 7.41 7.39 7.37 7.35 7.26 7.15 7.13 7.12 7.10
3.38 3.37 3.35 3.33 3.20 3.18 3.16 3.14 3.02 3.01 3.00 2.99 2.99 2.98 2.98 2.97 2.96 2.95 2.89 2.88 2.84 2.83 2.67 2.64 2.63 2.61 2.33
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 48
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -805.4
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
2c
0.89 0.95 1.93 3.81 1.00 1.00 0.98 1.00 0.99 2.84
f1 (ppm)

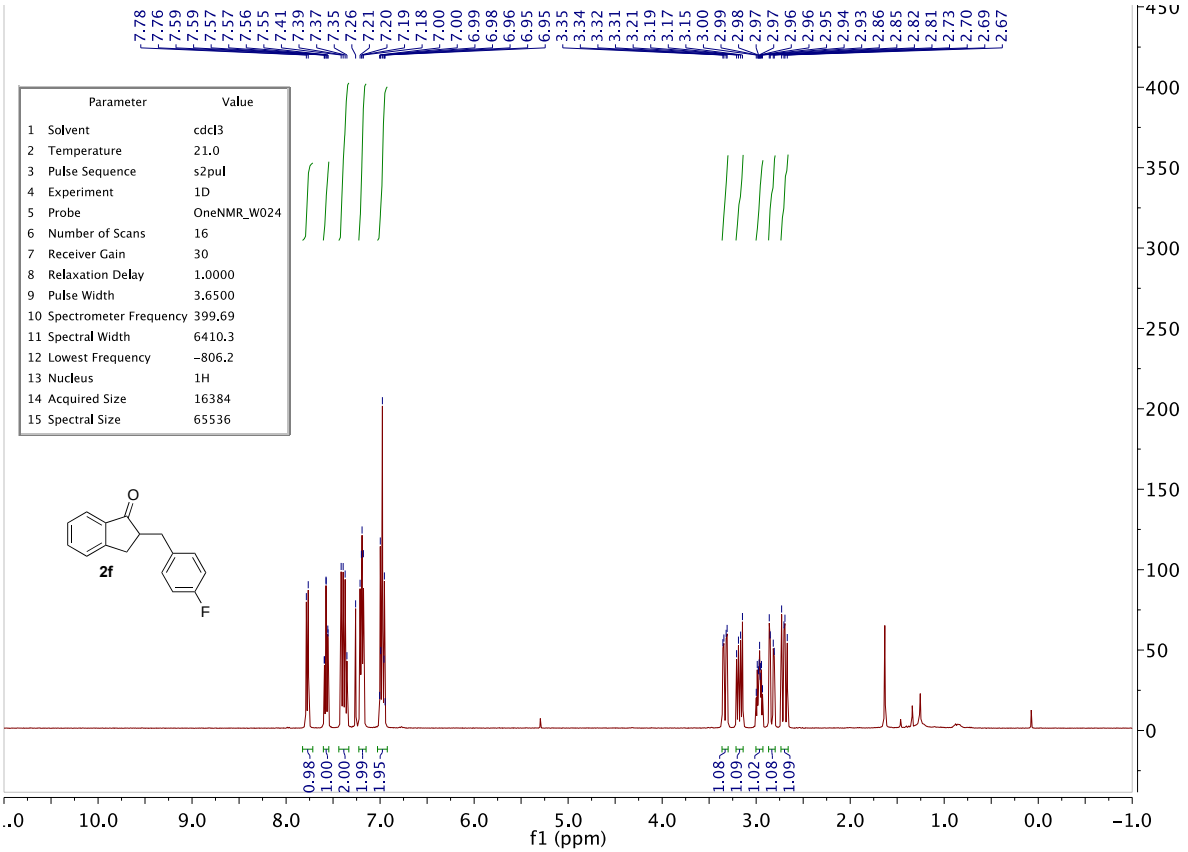

208.07
153.82
136.73 136.66 135.99 134.82 129.34 128.91 127.45 126.63 124.07
77.48 77.16 76.84
49.16
36.72 32.33
21.25
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 768
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1414.0
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
2c
f1 (ppm)

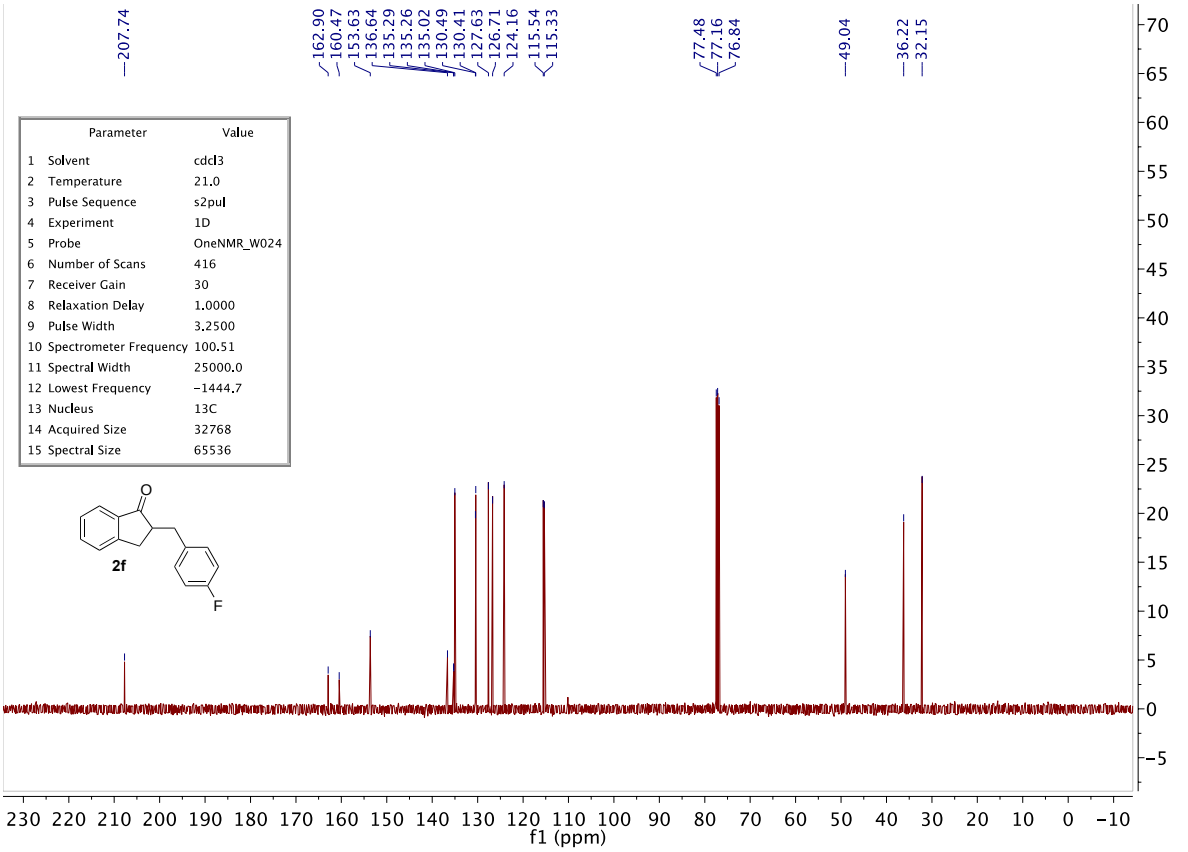

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
2d
Ph
f1 (ppm)

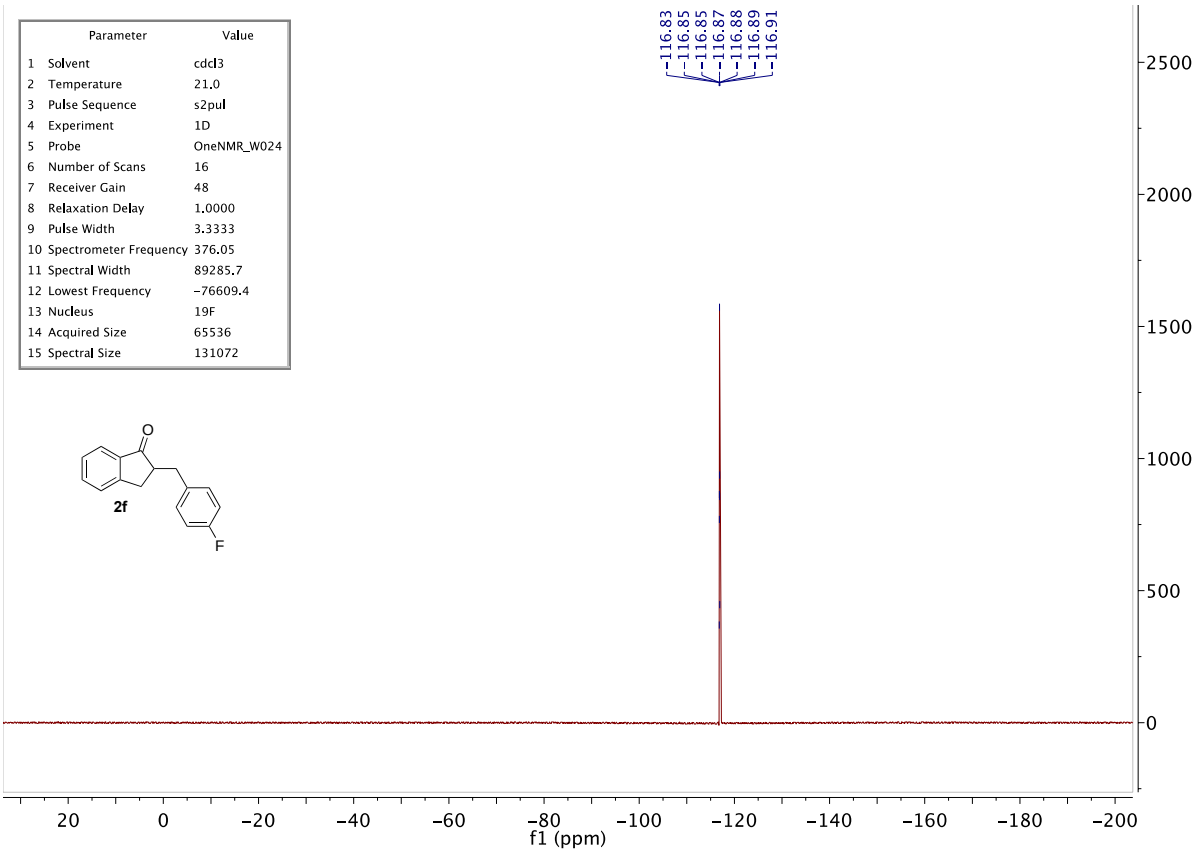

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 192
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1431.0
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
2d
Ph
f1 (ppm)

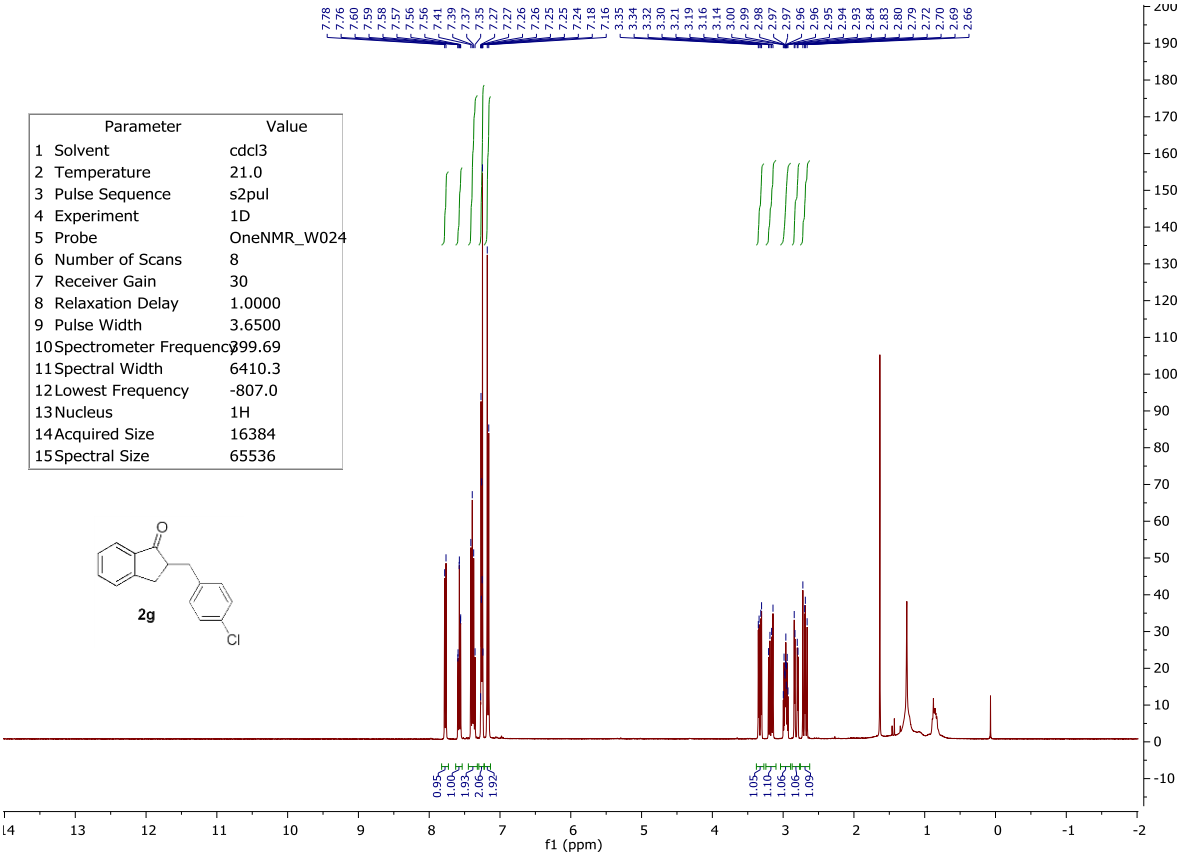

7.79
7.77
7.58
7.56
7.55
7.40
7.38
7.36
7.34
7.28
7.26
7.24
7.22
4.42
3.40
3.37
3.36
3.19
3.17
3.14
3.12
3.03
3.02
3.00
3.00
2.99
2.99
2.98
2.97
2.97
2.96
2.87
2.86
2.83
2.82
2.71
2.68
2.68
2.65
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 42
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -807.0
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
2e
O
0.95
1.00
1.96
4.06
1.92
3.81
1.06
1.03
1.03
1.04
f1 (ppm)

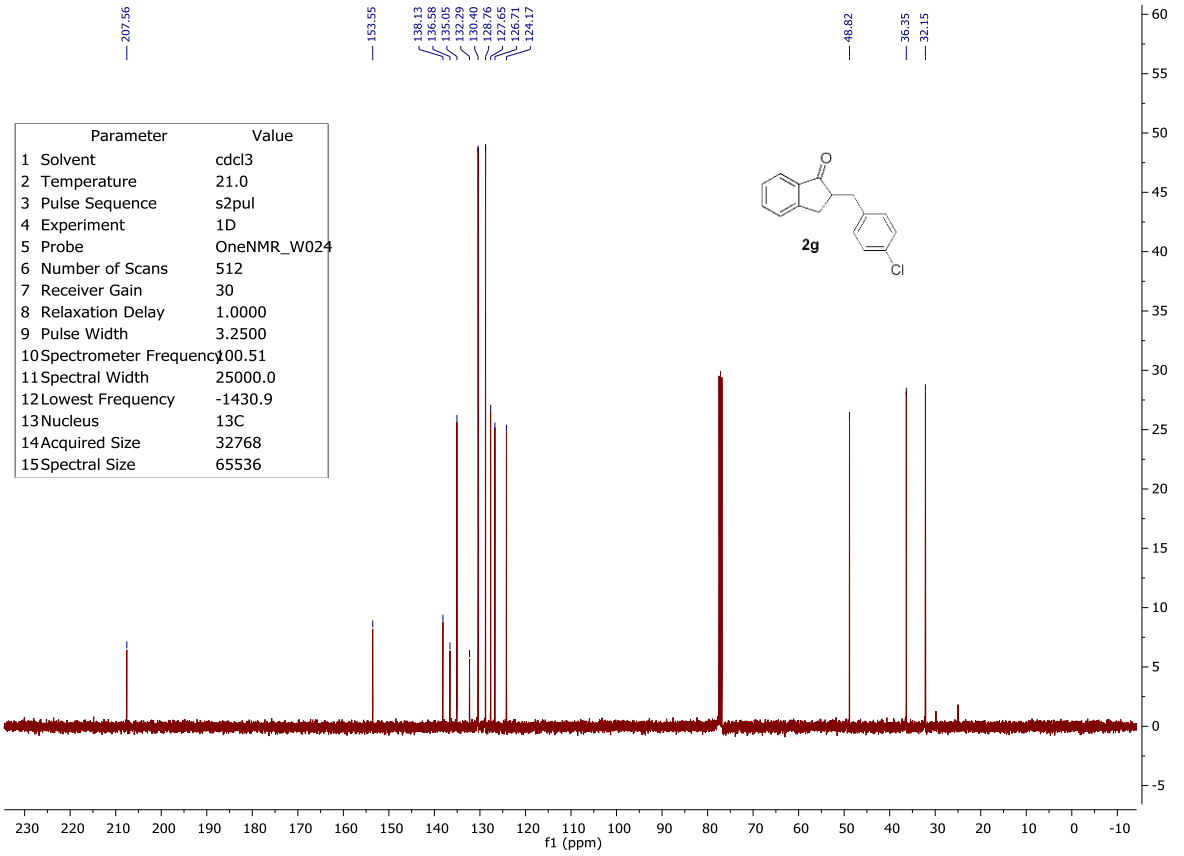

207.91
153.75
139.21
136.67
136.38
134.94
129.10
128.19
127.56
126.72
124.15
77.48
77.16
76.84
74.64
58.26
49.04
36.78
32.27
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 480
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1415.6
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
2e
O
f1 (ppm)

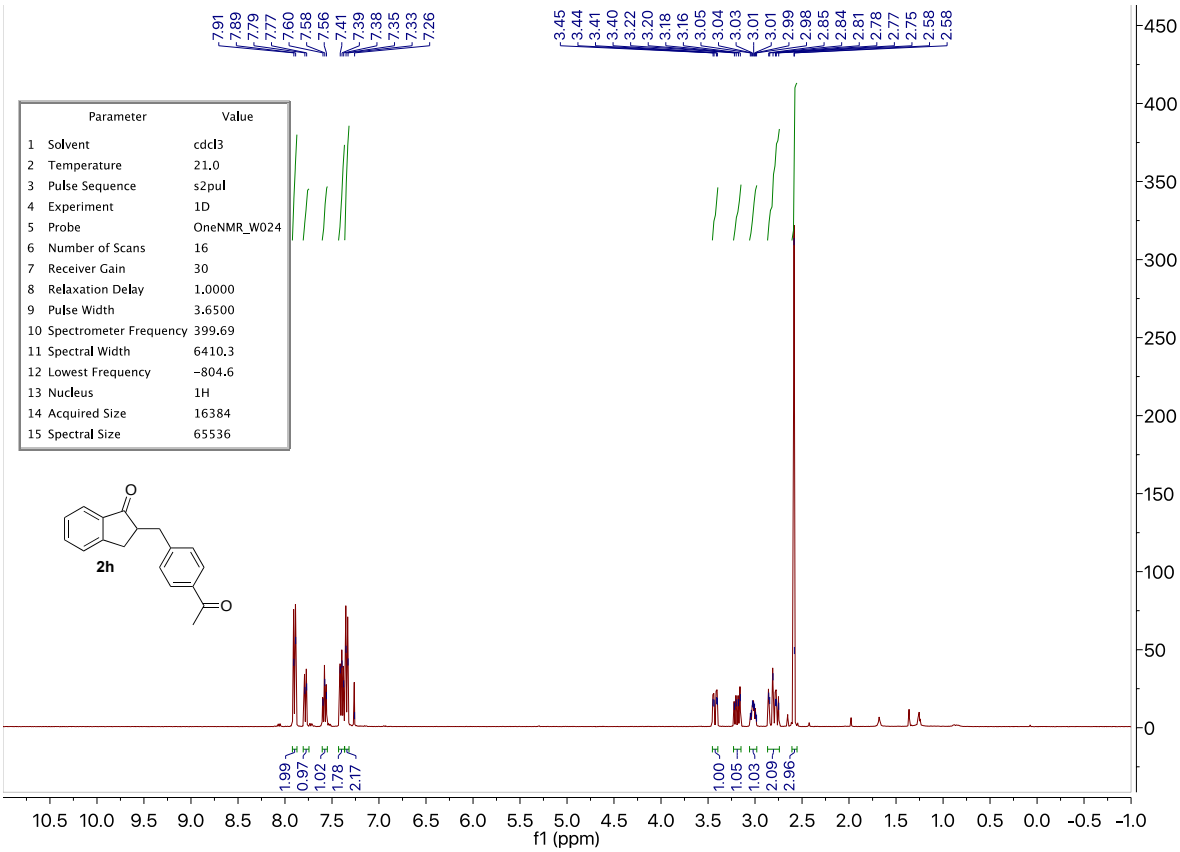

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
2f
f1 (ppm)

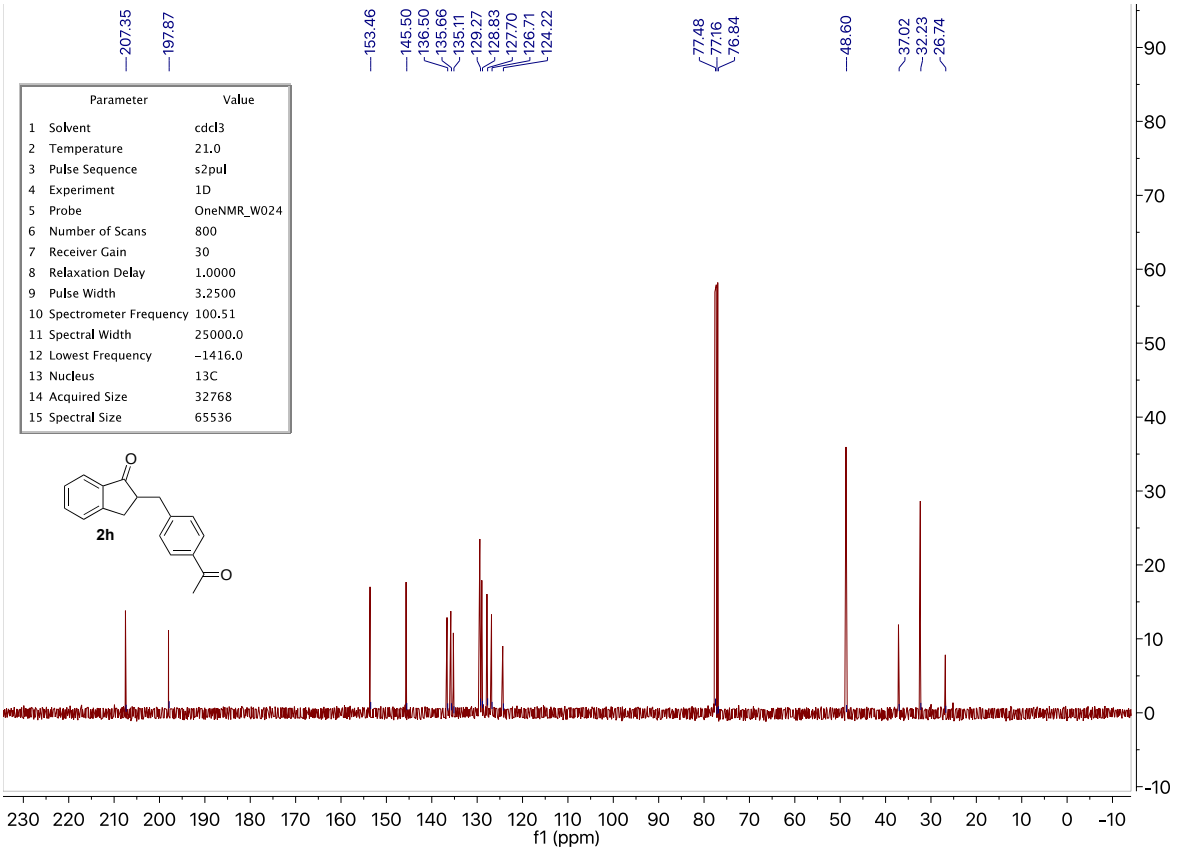

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 416
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1444.7
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
2f
f1 (ppm)

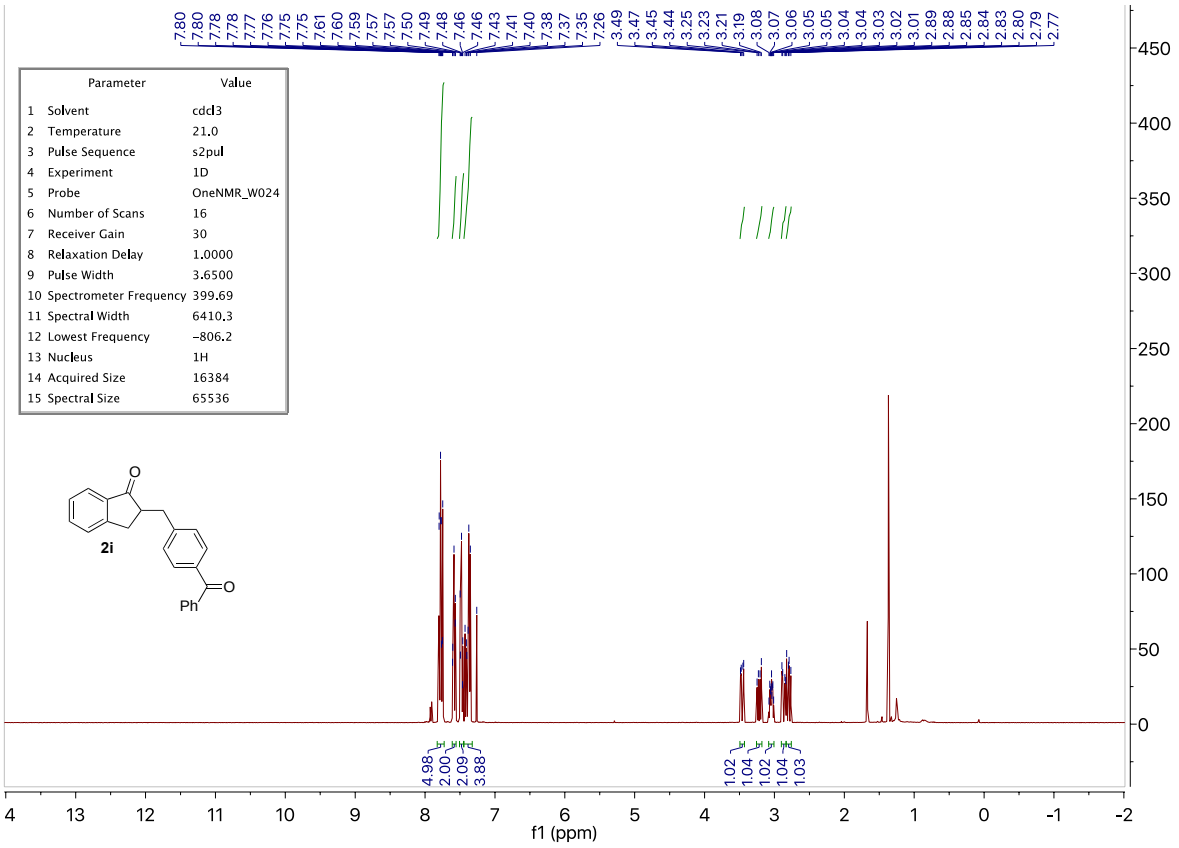

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 48
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76609.4
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
-116.83
-116.85
-116.85
-116.87
-116.88
-116.89
-116.91
2f
O
F
2500
2000
1500
1000
500
0
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

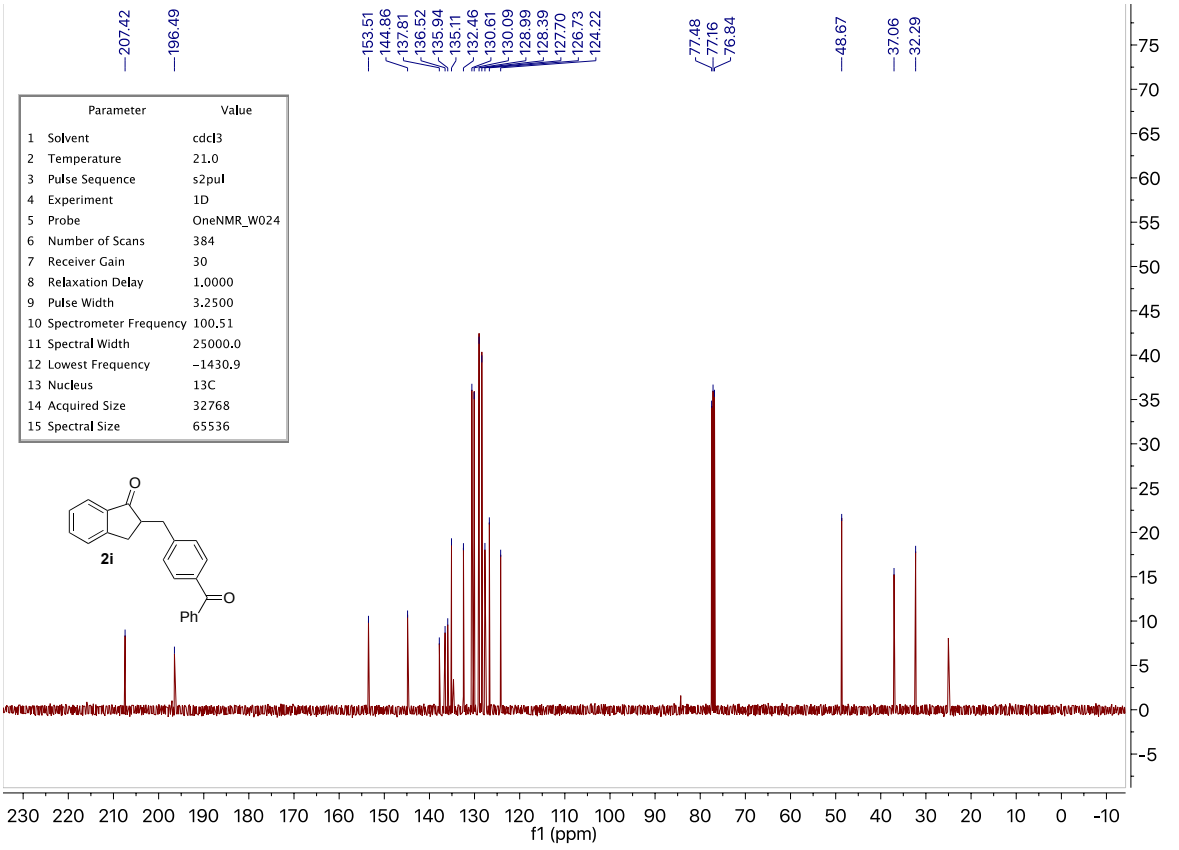

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -807.0
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
2g
Cl
f1 (ppm)

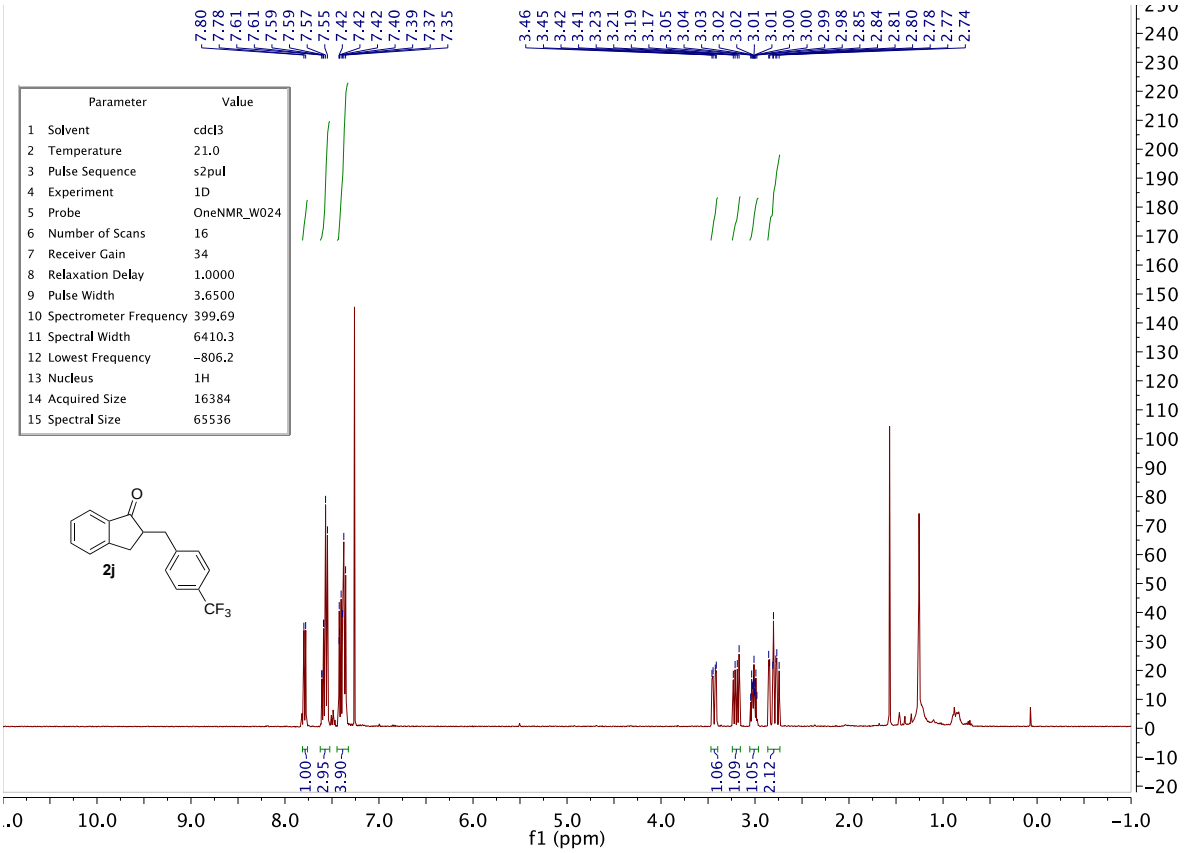

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 512
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1430.9
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
2g
Cl
f1 (ppm)

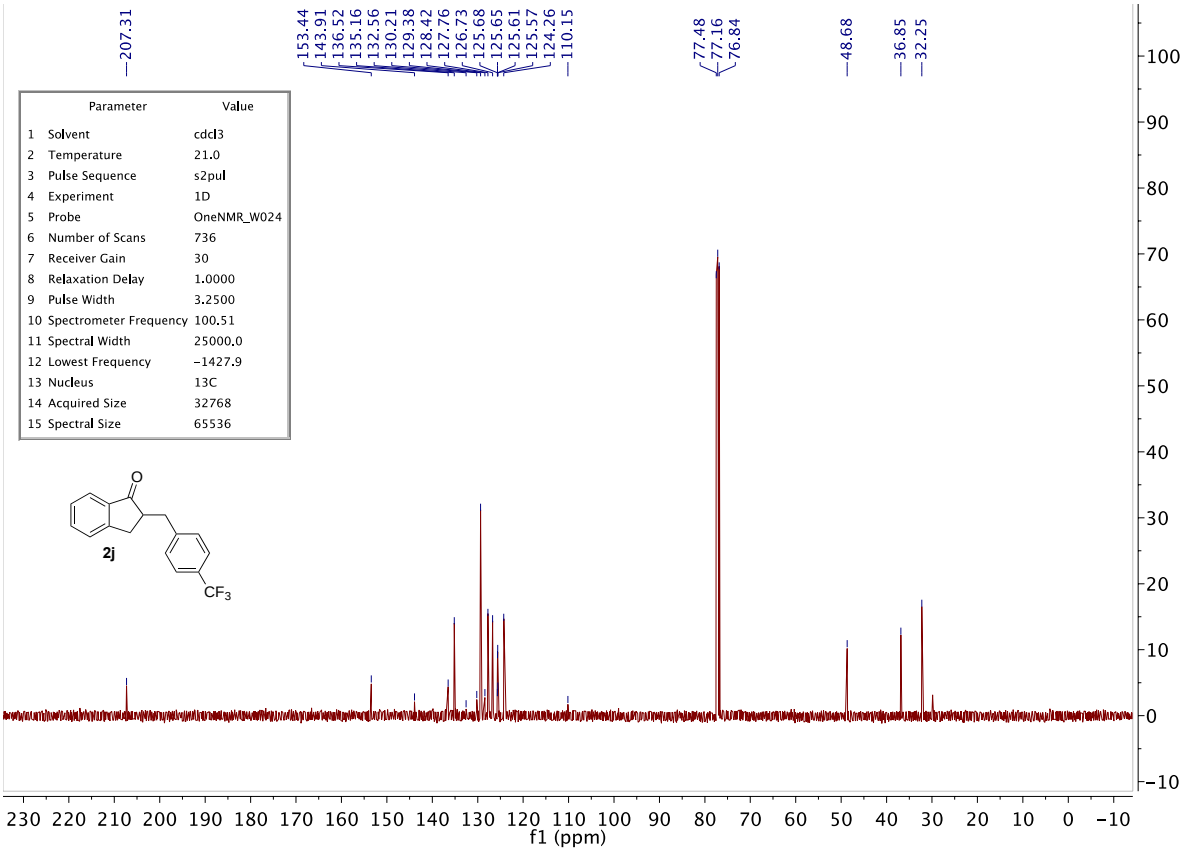

7.91
7.89
7.79
7.77
7.60
7.58
7.56
7.41
7.39
7.38
7.35
7.33
7.26
3.45
3.44
3.41
3.40
3.22
3.20
3.18
3.16
3.05
3.04
3.03
3.01
3.01
2.99
2.98
2.85
2.84
2.81
2.78
2.77
2.75
2.58
2.58
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -804.6
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
2h
O
1.99
0.97
1.02
1.78
2.17
1.00
1.05
1.03
2.09
2.96
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 -1.0
f1 (ppm)
450
400
350
300
250
200
150
100
50
0

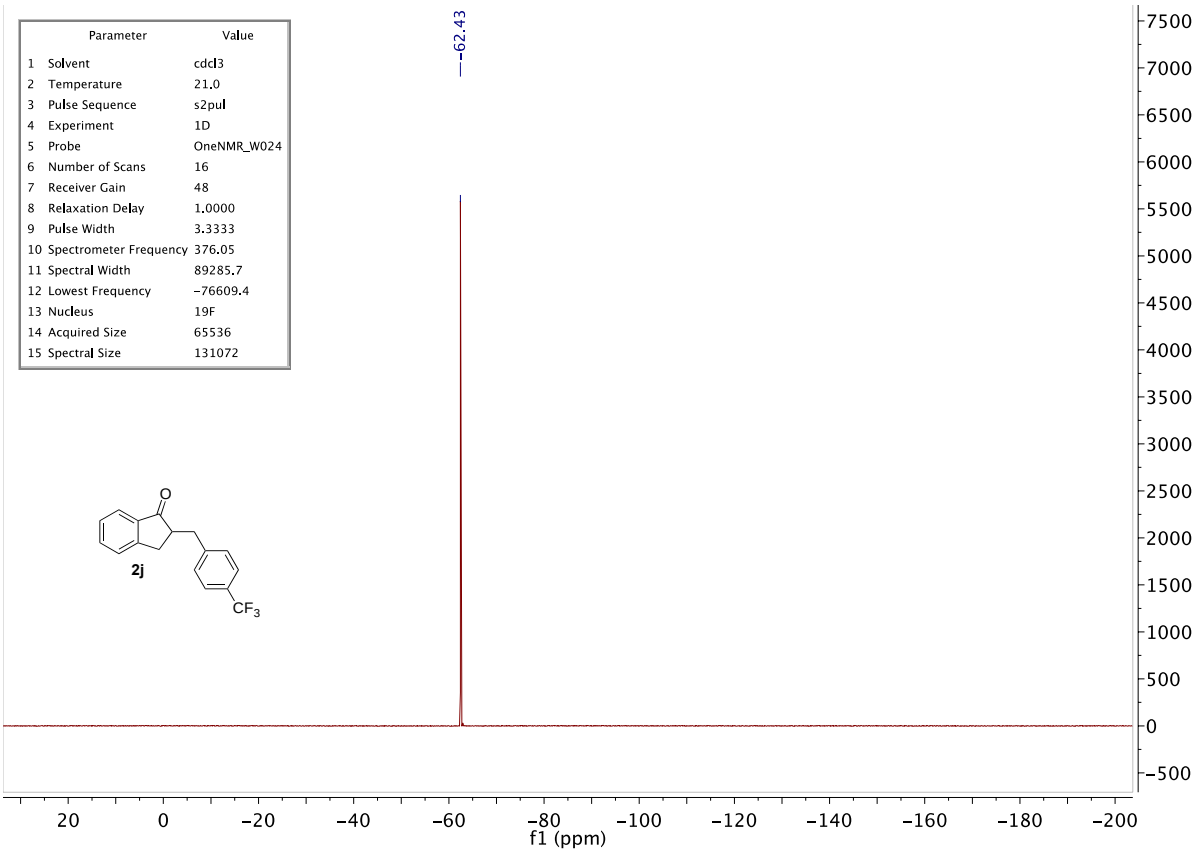

207.35
197.87
153.46
145.50
136.50
135.66
135.11
129.27
128.83
127.70
126.71
124.22
77.48
77.16
76.84
48.60
37.02
32.23
26.74
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 800
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1416.0
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
2h
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
90
80
70
60
50
40
30
20
10
0
-10

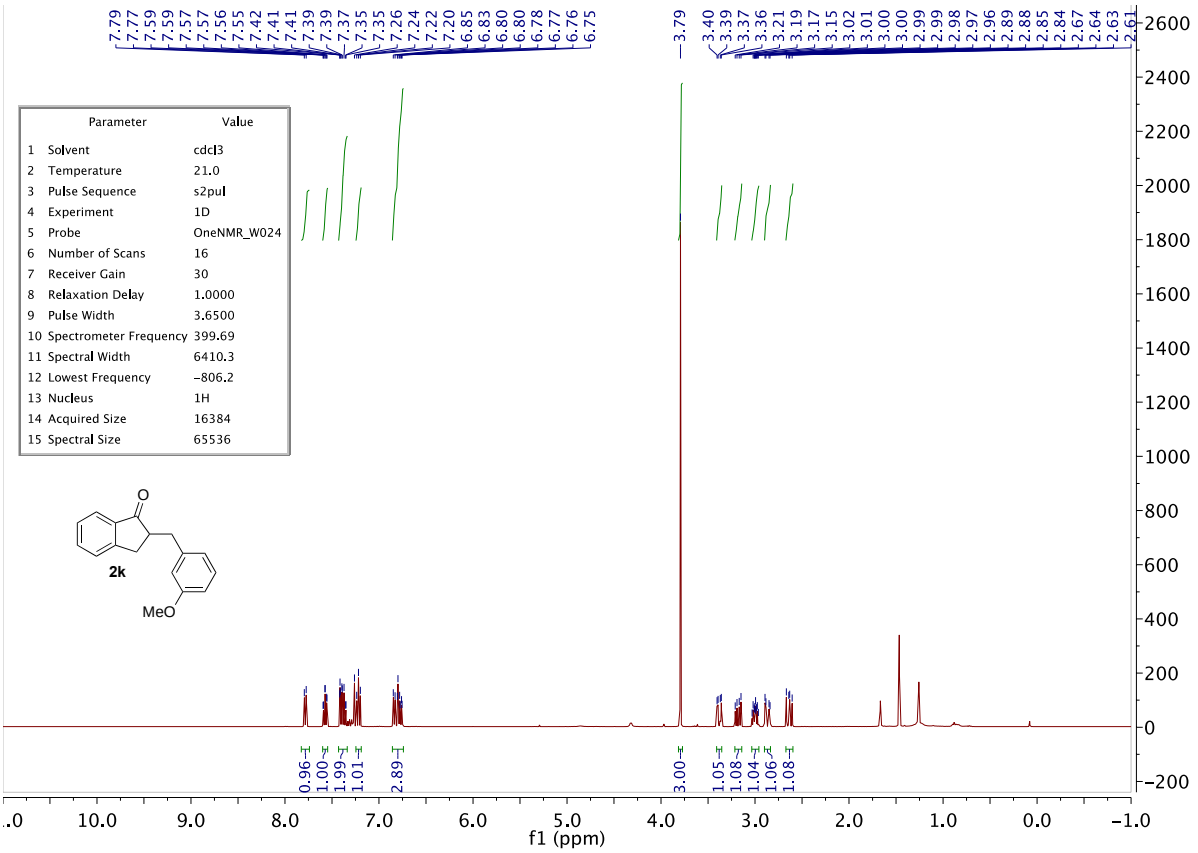

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
2i
Ph
f1 (ppm)

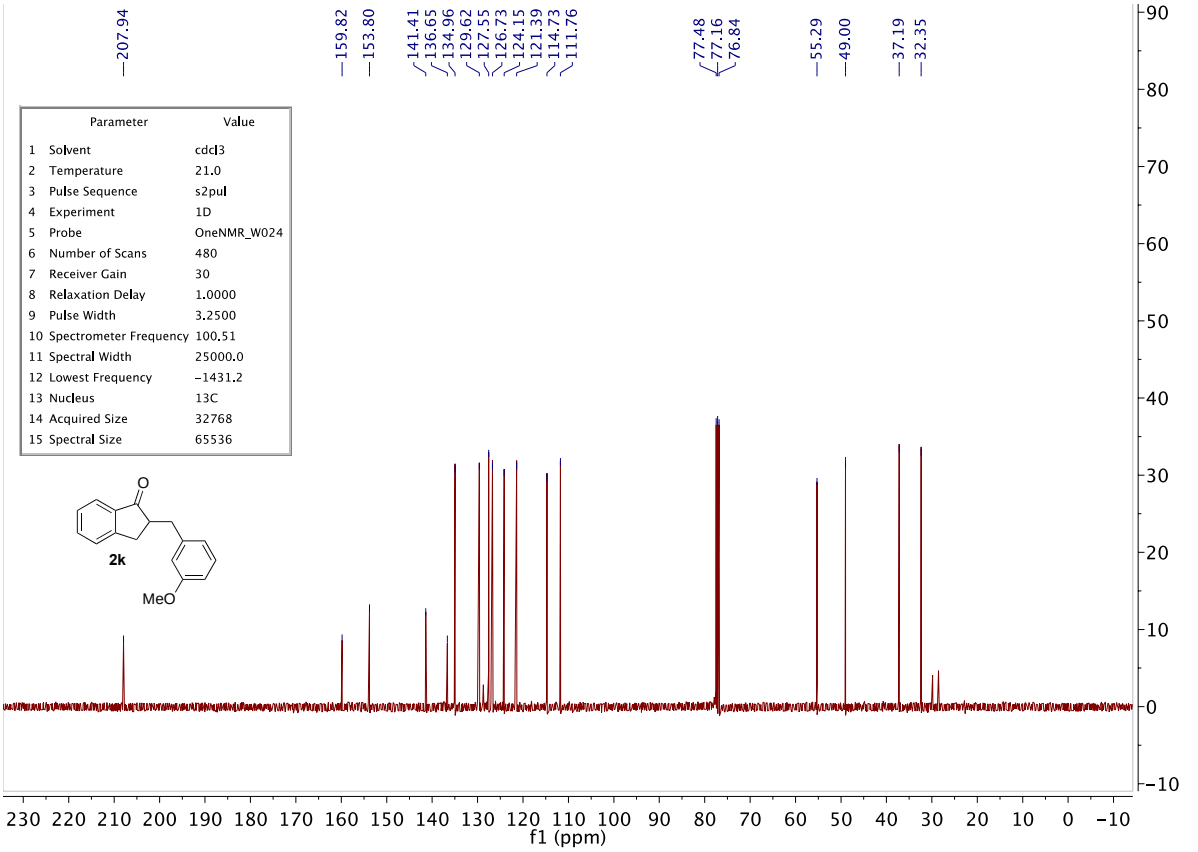

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 384
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1430.9
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
2i
Ph
f1 (ppm)

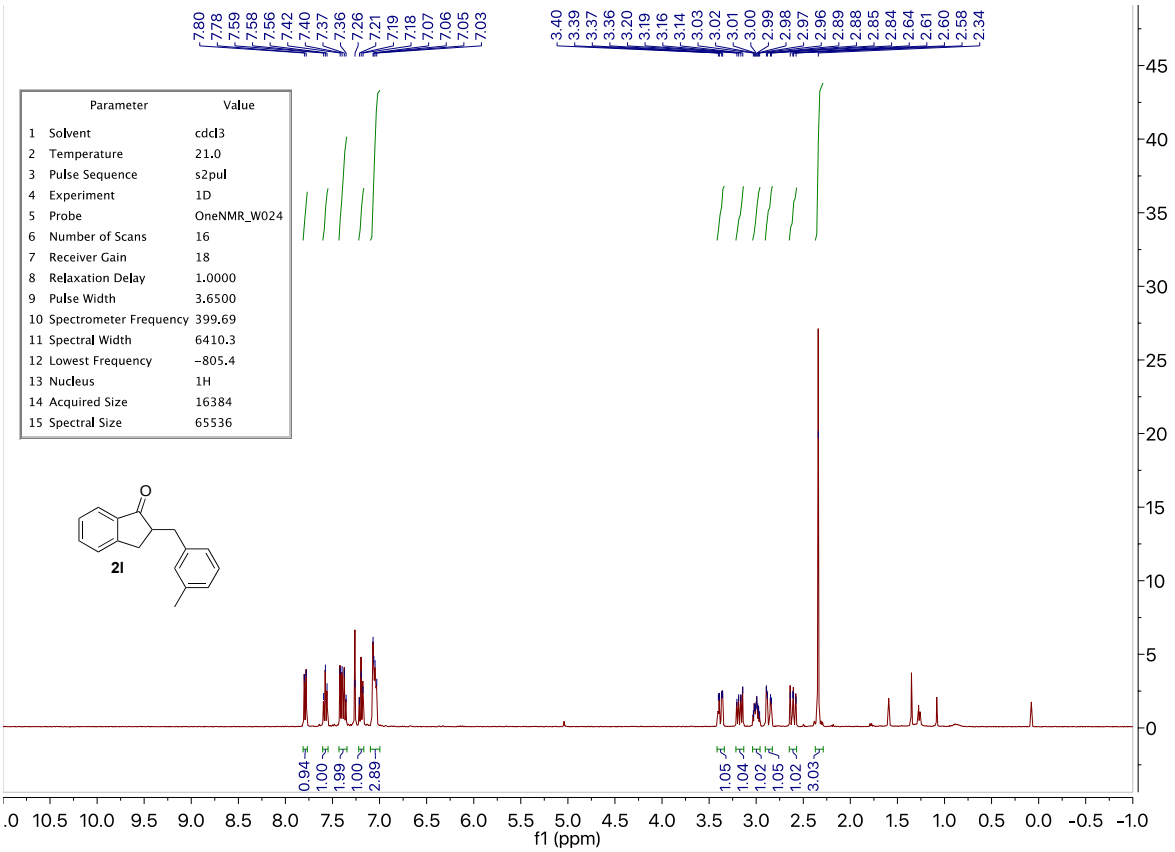

7.80 7.78 7.61 7.61 7.59 7.59 7.57 7.55 7.42 7.42 7.40 7.39 7.37 7.35
3.46 3.45 3.42 3.41 3.23 3.21 3.19 3.17 3.05 3.04 3.03 3.02 3.02 3.01 3.01 3.00 3.00 2.99 2.98 2.85 2.84 2.81 2.80 2.78 2.77 2.74
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 34
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
2j
CF3
1.00 2.95 3.90 1.06 1.09 1.05 2.12
f1 (ppm)

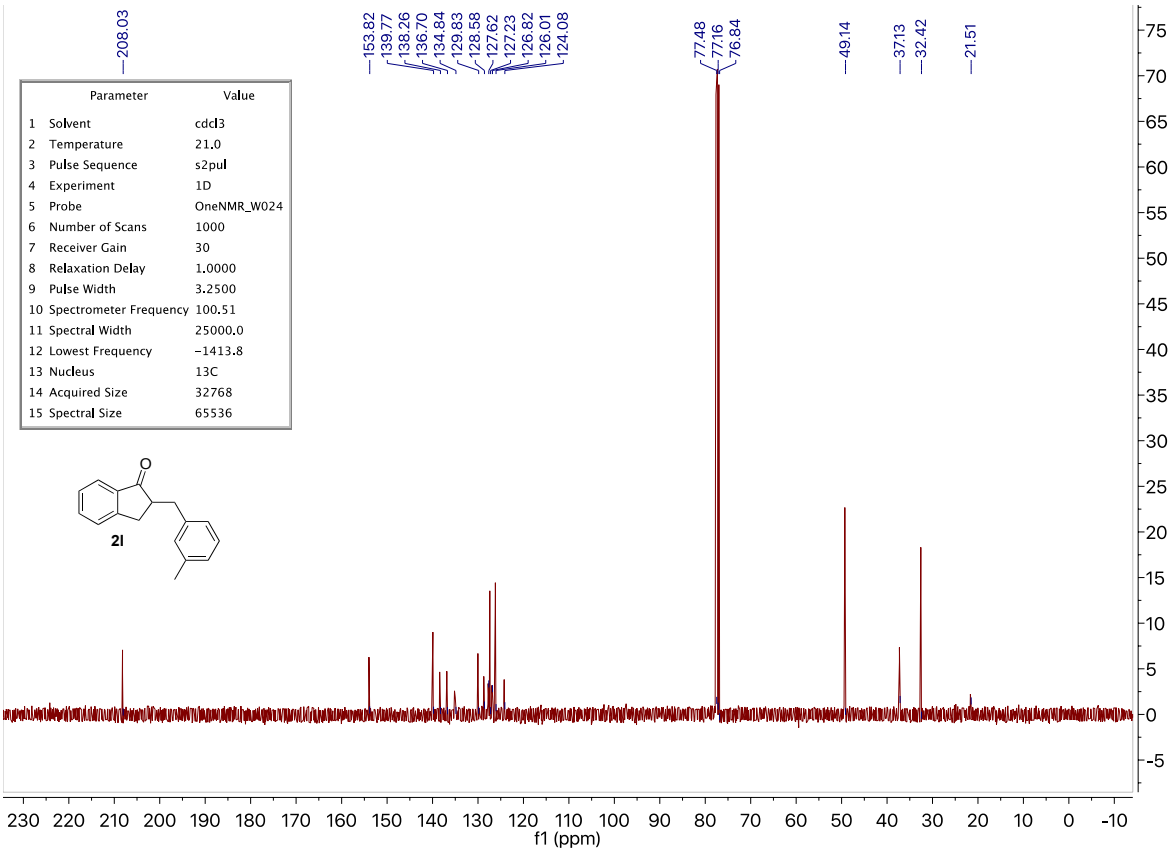

207.31
153.44 143.91 136.52 135.16 132.56 130.21 129.38 128.42 127.76 126.73 125.68 125.65 125.61 125.57 124.26 110.15
77.48 77.16 76.84
48.68
36.85 32.25
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 736
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1427.9
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
2j
CF3
f1 (ppm)

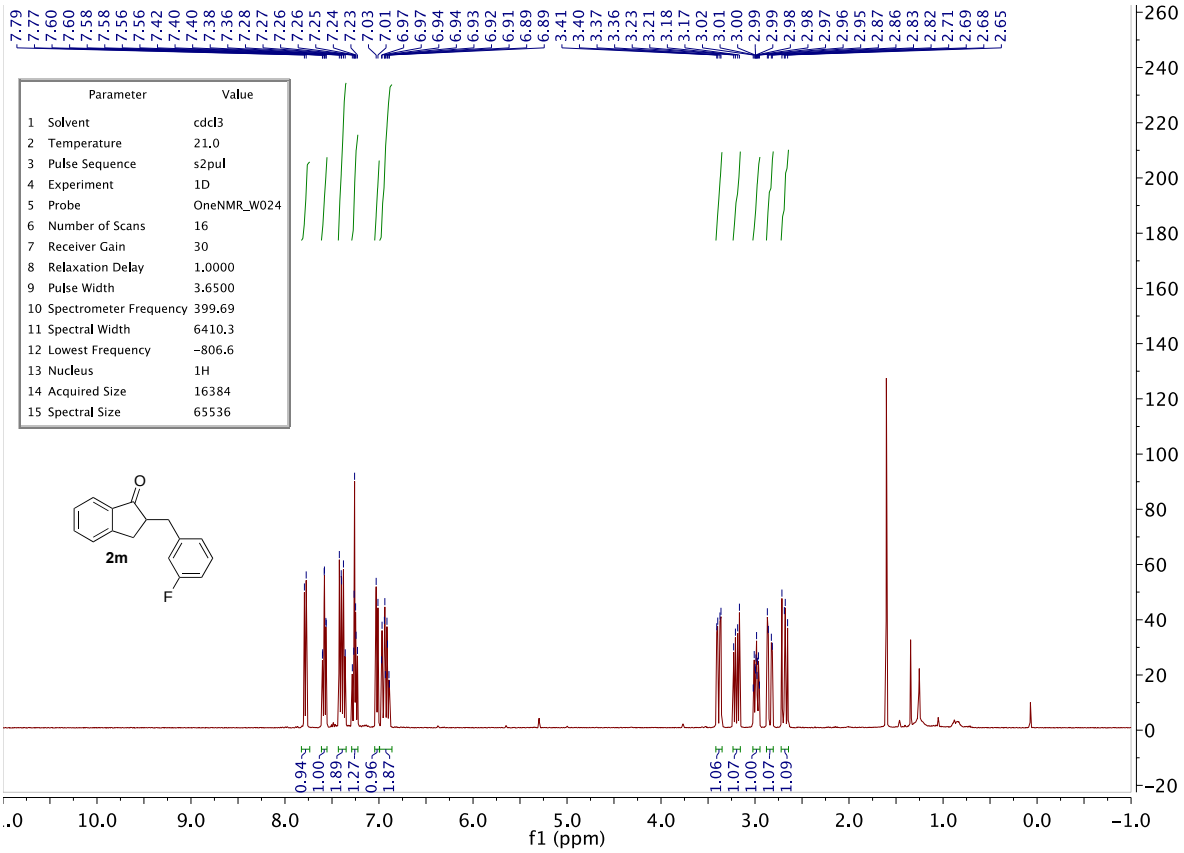

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 48
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76609.4
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
-62.43
O
2j
CF3
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

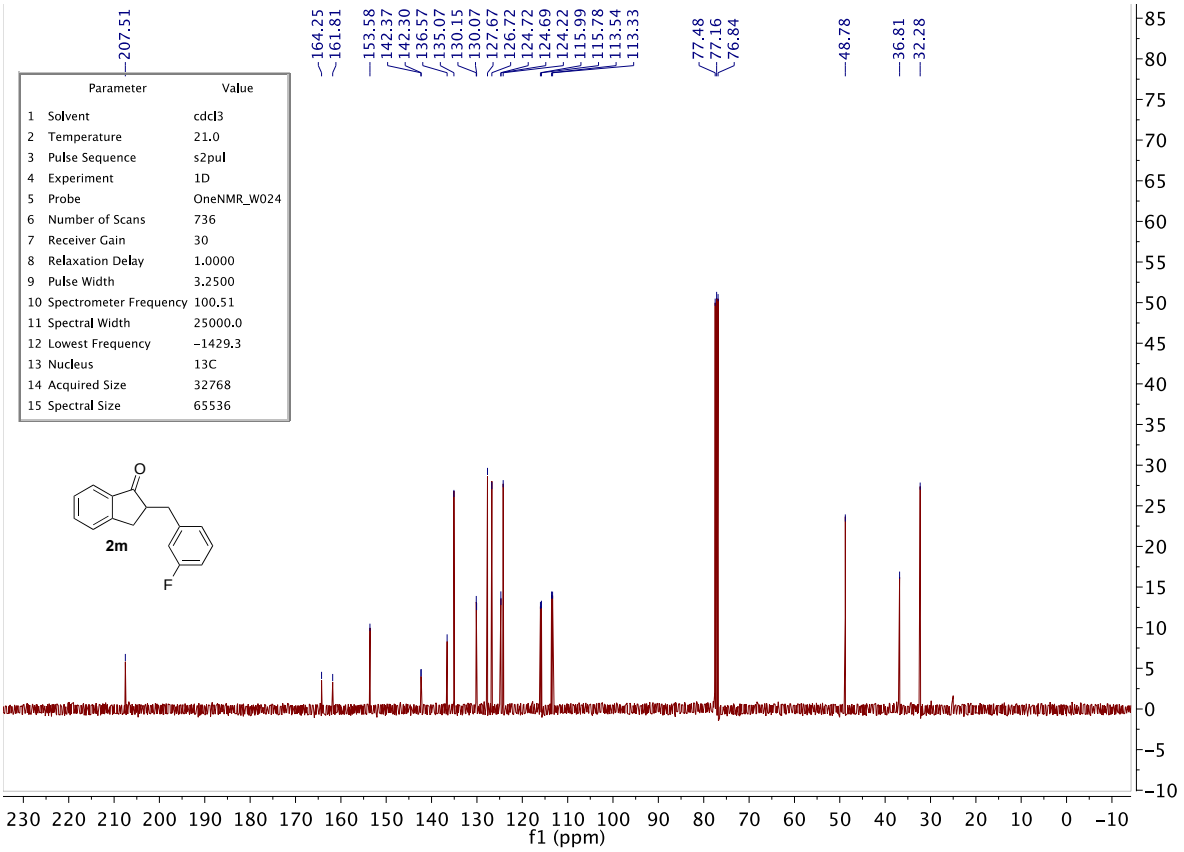

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
2k
MeO
f1 (ppm)

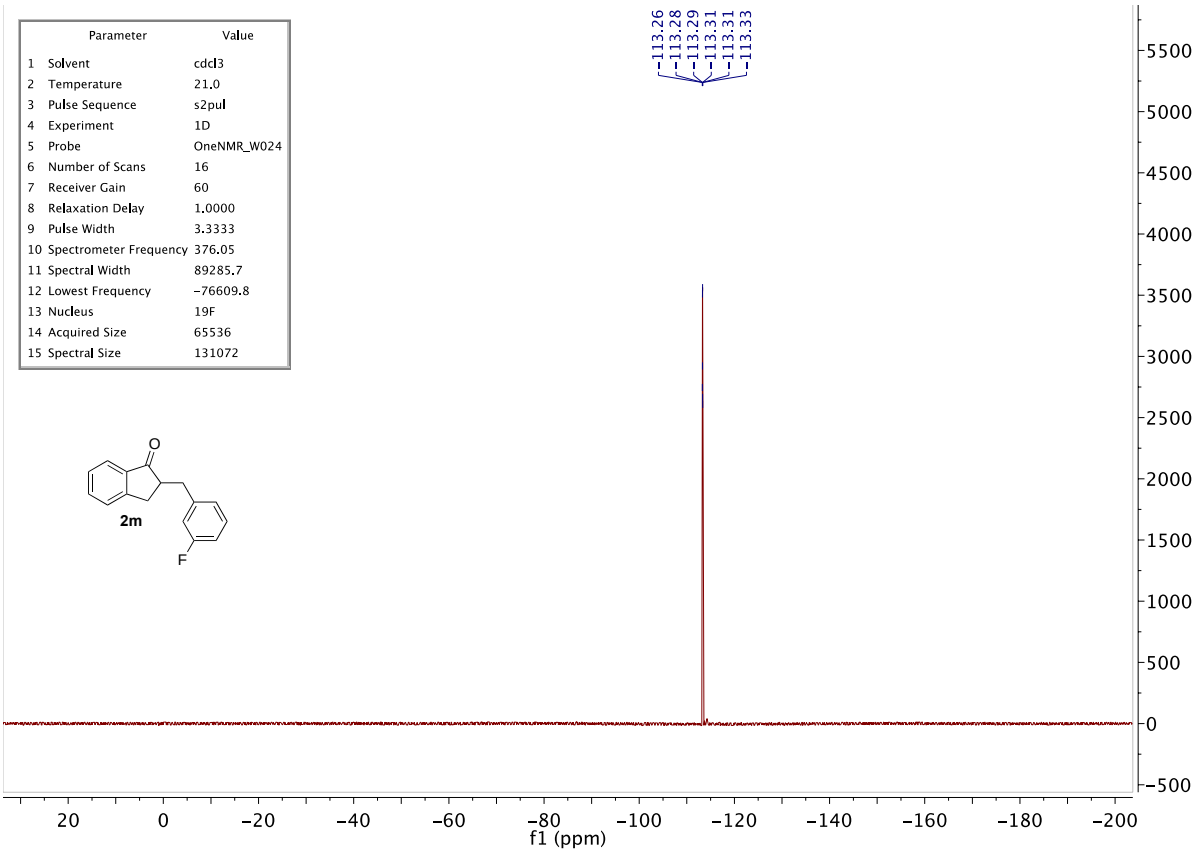

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 480
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1431.2
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
2k
MeO
f1 (ppm)

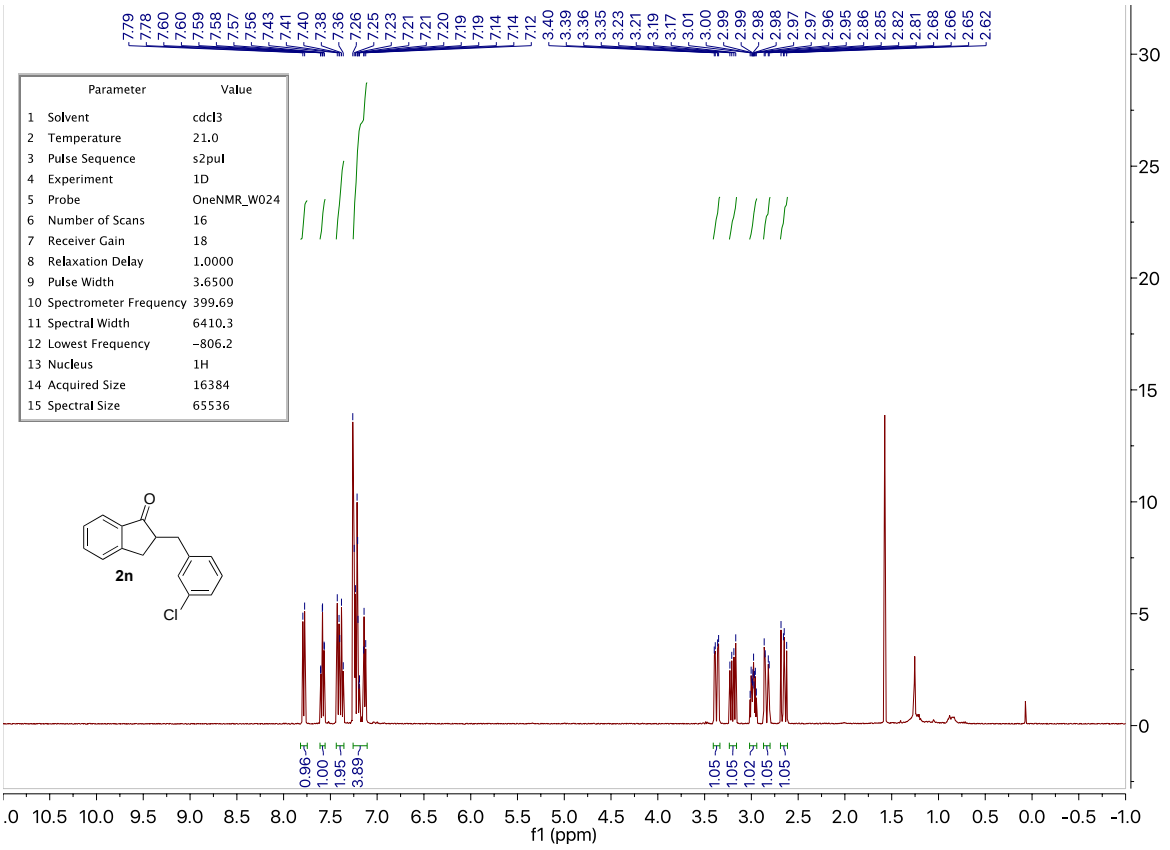

7.80 7.78 7.59 7.58 7.56 7.42 7.40 7.37 7.36 7.26 7.21 7.19 7.18 7.07 7.06 7.05 7.03
3.40 3.39 3.37 3.36 3.20 3.19 3.16 3.14 3.03 3.02 3.01 3.00 2.99 2.98 2.97 2.96 2.89 2.88 2.85 2.84 2.64 2.61 2.60 2.58 2.34
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 18
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -805.4
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
2l
0.94 1.00 1.99 1.00 2.89
1.05 1.04 1.02 1.05 1.02 3.03
f1 (ppm)

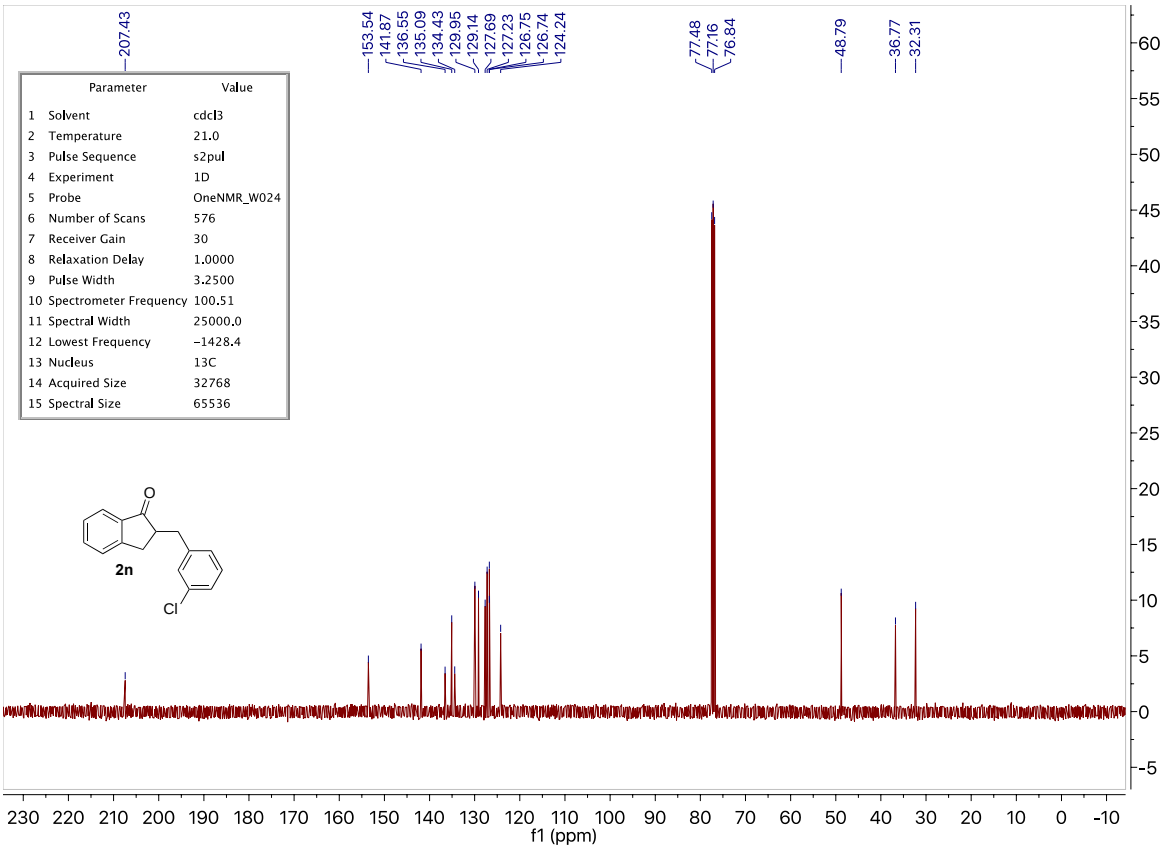

208.03
153.82 139.77 138.26 136.70 134.84 129.83 128.58 127.62 127.23 126.82 126.01 124.08
77.48 77.16 76.84
49.14
37.13
32.42
21.51
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 1000
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1413.8
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
2l
f1 (ppm)

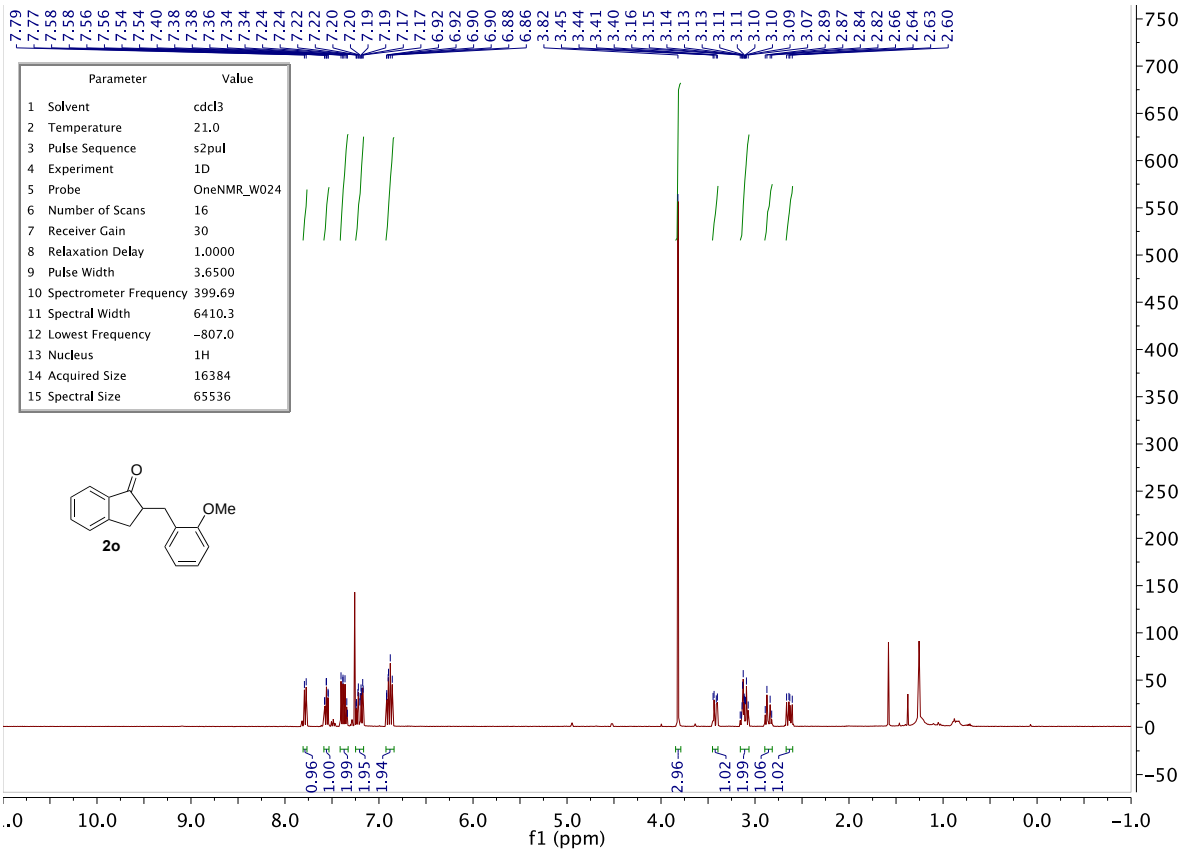

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.6
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
2m
f1 (ppm)

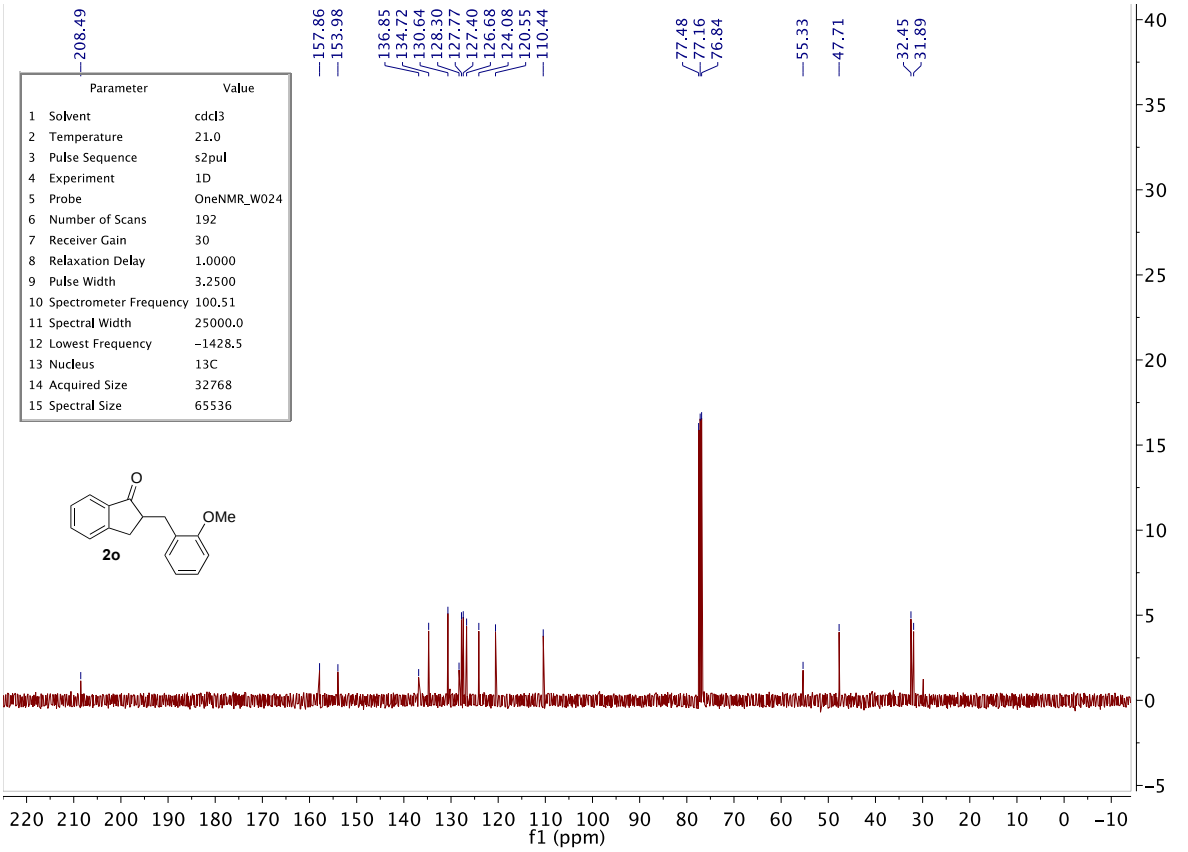

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 736
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1429.3
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
2m
f1 (ppm)

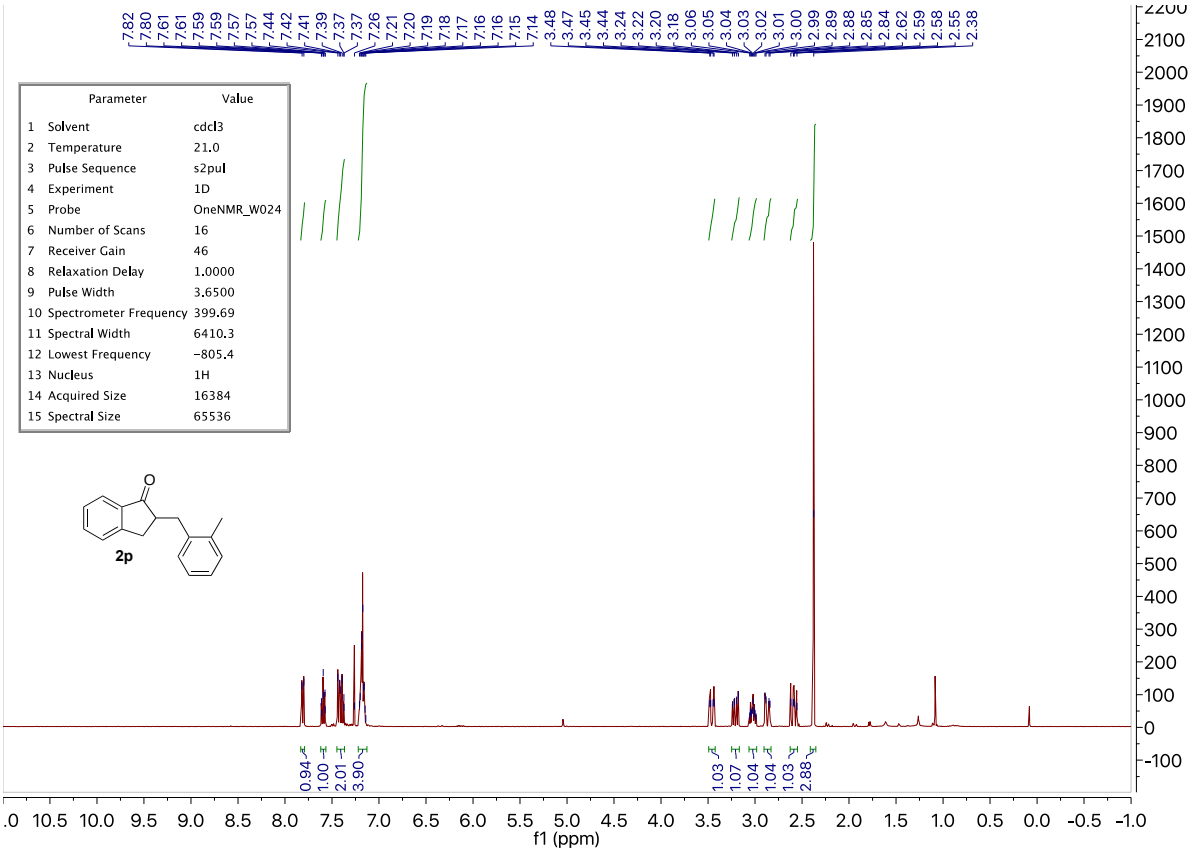

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 60
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76609.8
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
-113.26
-113.28
-113.29
-113.31
-113.31
-113.33
O
F
2m
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

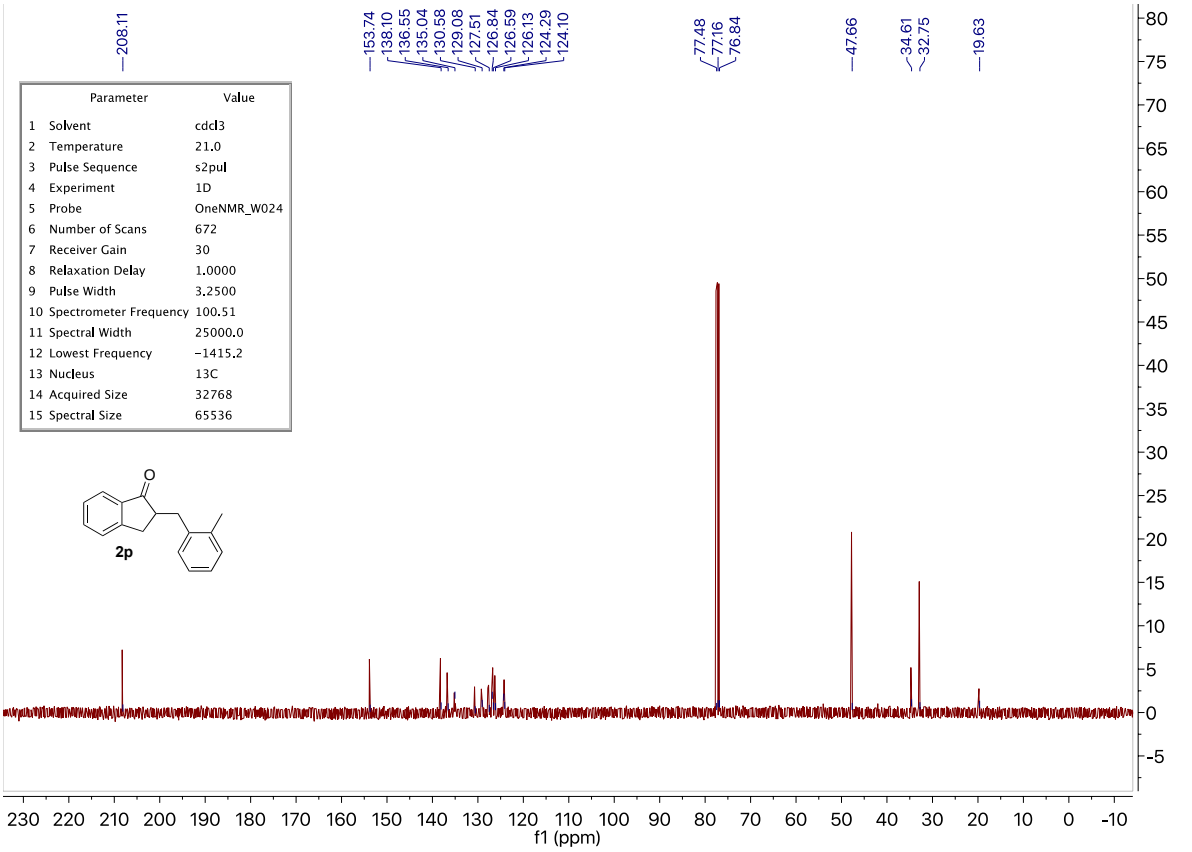

7.79 7.78 7.60 7.60 7.59 7.58 7.57 7.56 7.43 7.41 7.40 7.38 7.36 7.26 7.25 7.23 7.21 7.21 7.20 7.19 7.19 7.14 7.12 3.40 3.39 3.36 3.35 3.23 3.21 3.19 3.17 3.01 3.00 2.99 2.99 2.98 2.98 2.97 2.97 2.96 2.95 2.86 2.85 2.82 2.81 2.68 2.66 2.65 2.62
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 18
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
2n
Cl
0.96 1.00 1.95 3.89 1.05 1.05 1.02 1.05 1.05
f1 (ppm)

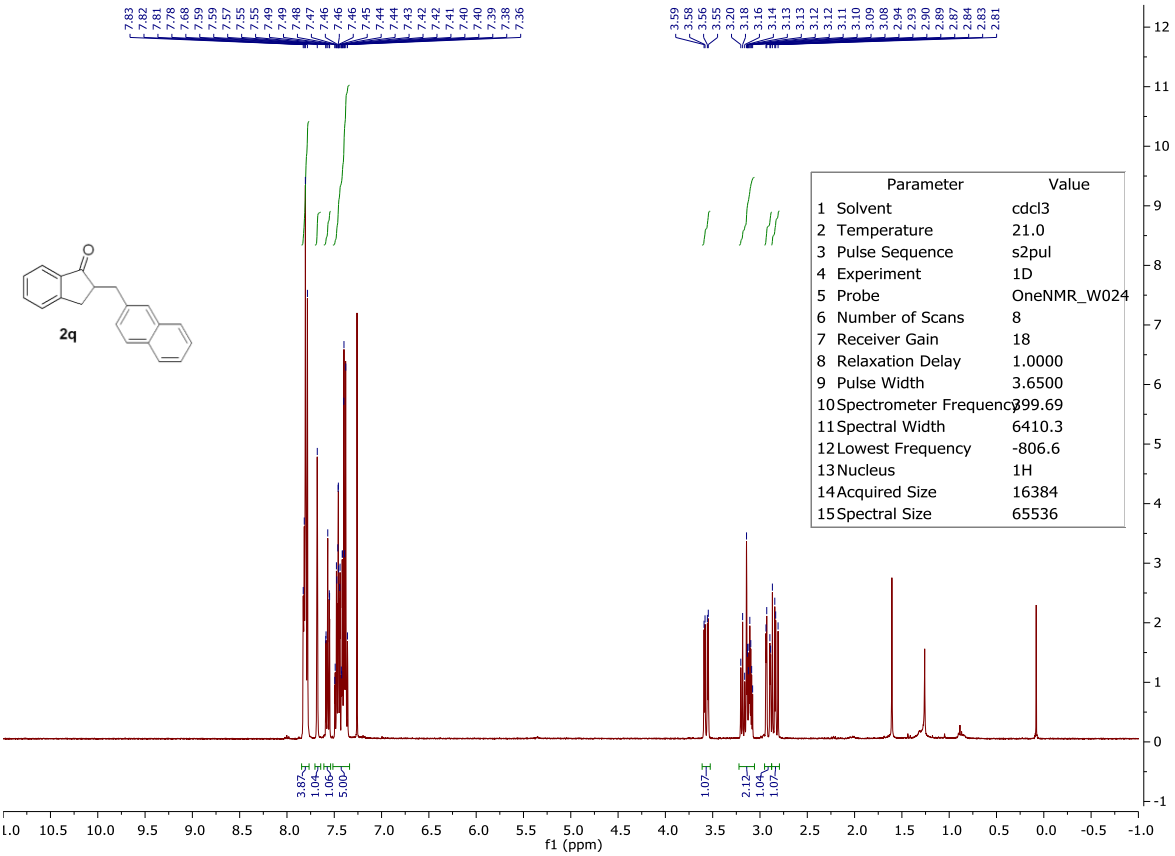

207.43
153.54 141.87 136.55 135.09 134.43 129.95 129.14 127.69 127.23 126.75 126.74 124.24
77.48 77.16 76.84
48.79
36.77
32.31
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 576
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1428.4
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
2n
Cl
f1 (ppm)

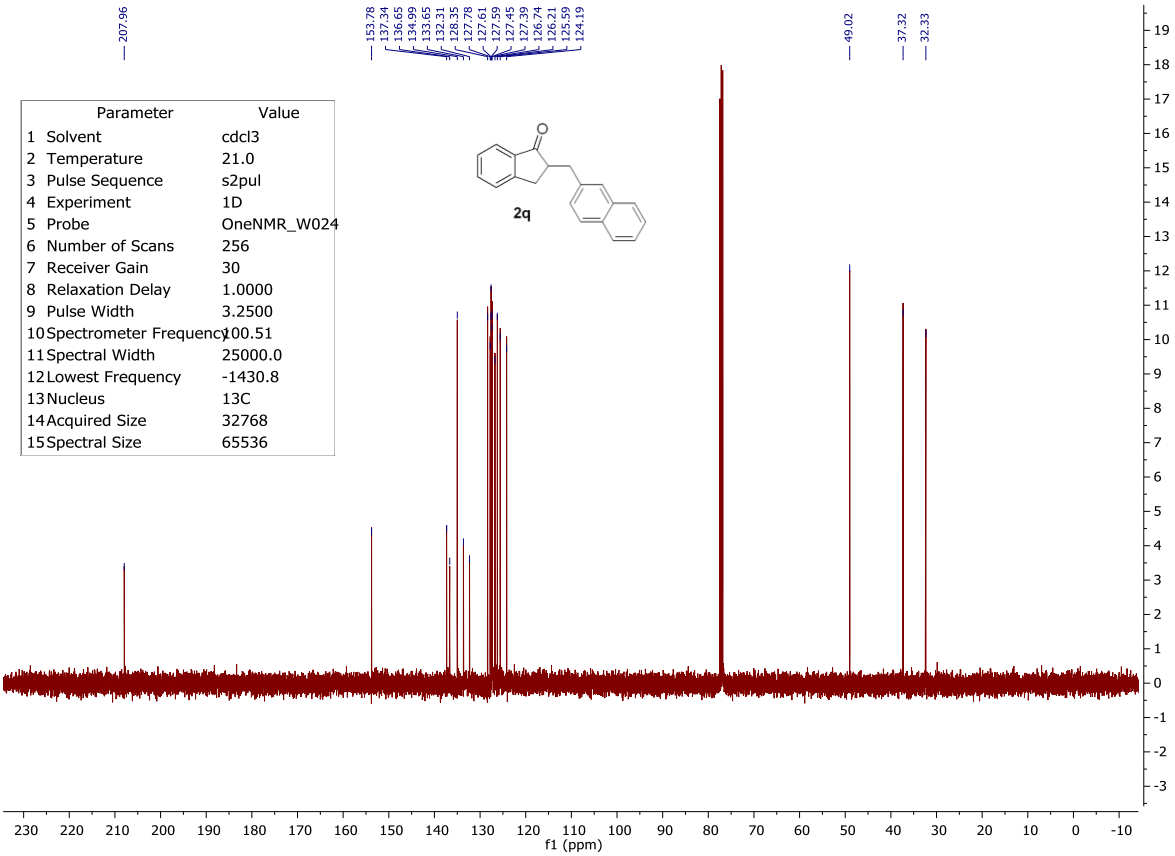

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -807.0
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
OMe
2o
f1 (ppm)

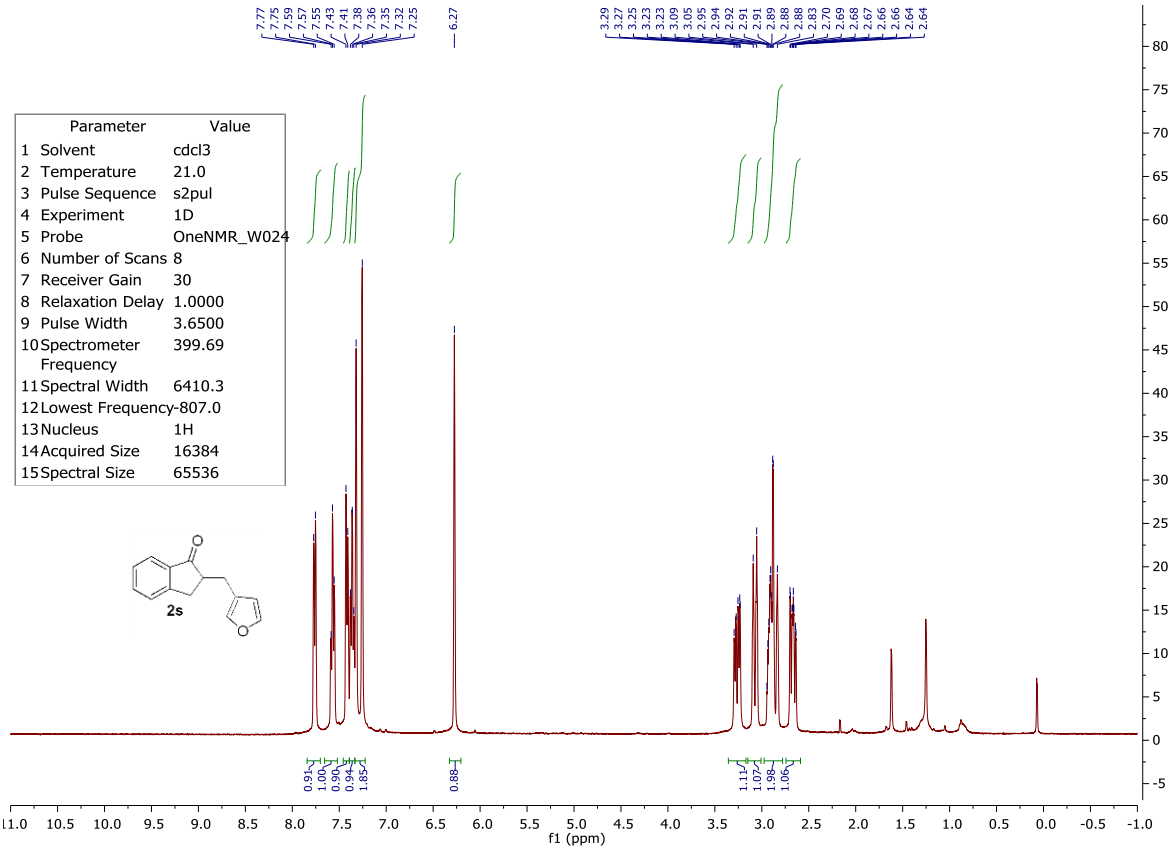

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 192
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1428.5
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
OMe
2o
f1 (ppm)

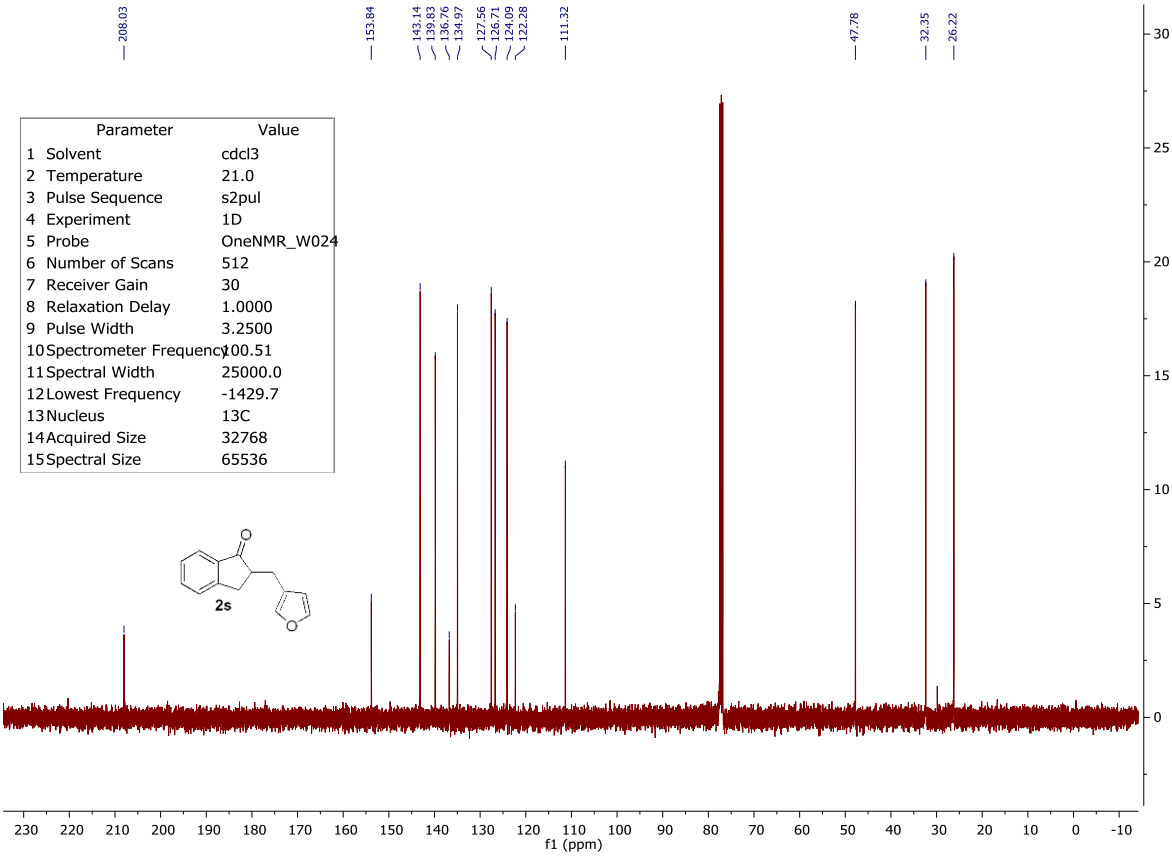

7.82 7.80 7.61 7.61 7.59 7.59 7.57 7.57 7.44 7.42 7.41 7.39 7.37 7.37 7.26 7.21 7.20 7.19 7.18 7.17 7.16 7.16 7.15 7.14 3.48 3.47 3.45 3.44 3.24 3.22 3.20 3.18 3.06 3.05 3.04 3.03 3.02 3.01 3.00 2.99 2.89 2.88 2.85 2.84 2.62 2.59 2.58 2.55 2.38
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 46
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -805.4
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
2p
0.94 1.00 2.01 3.90 1.03 1.07 1.04 1.04 1.03 2.88
f1 (ppm)

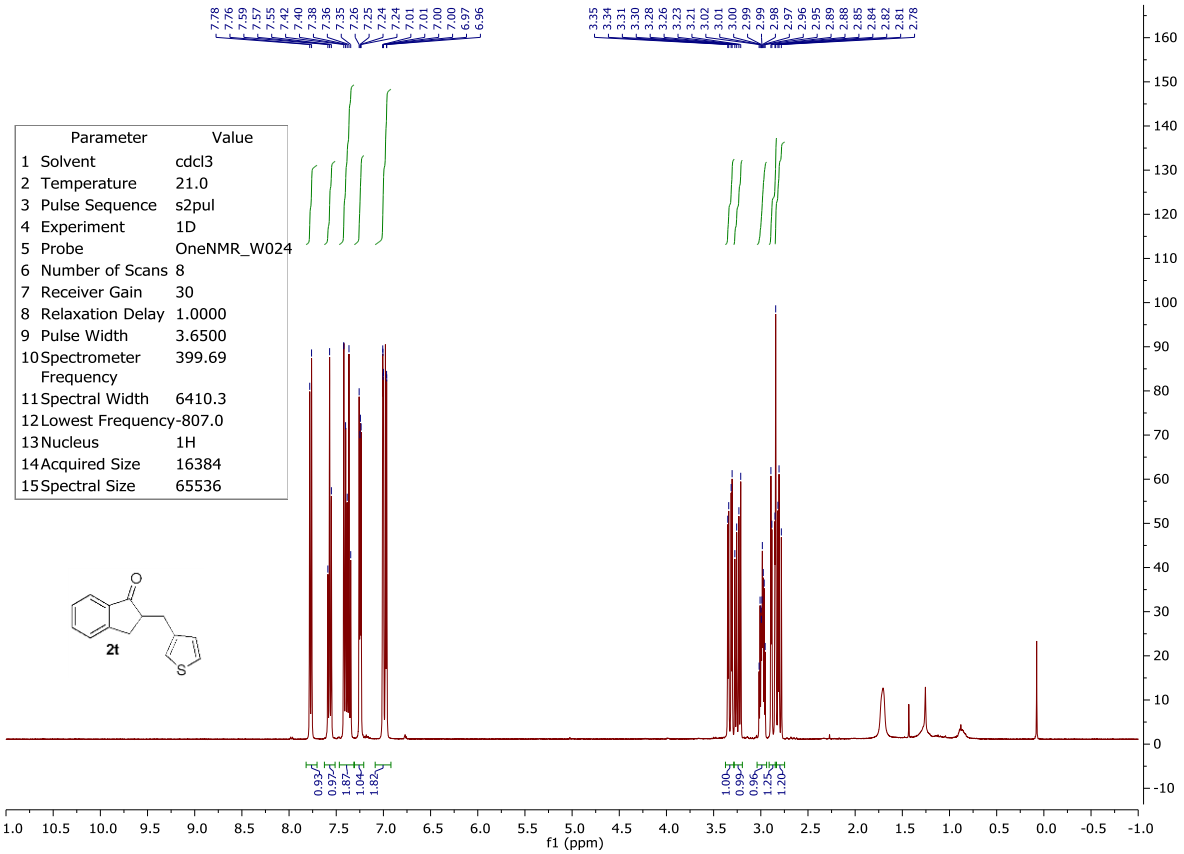

208.11
153.74 138.10 136.55 135.04 130.58 129.08 127.51 126.84 126.59 126.13 124.29 124.10
77.48 77.16 76.84
47.66
34.61 32.75
19.63
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 672
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1415.2
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
2p
f1 (ppm)

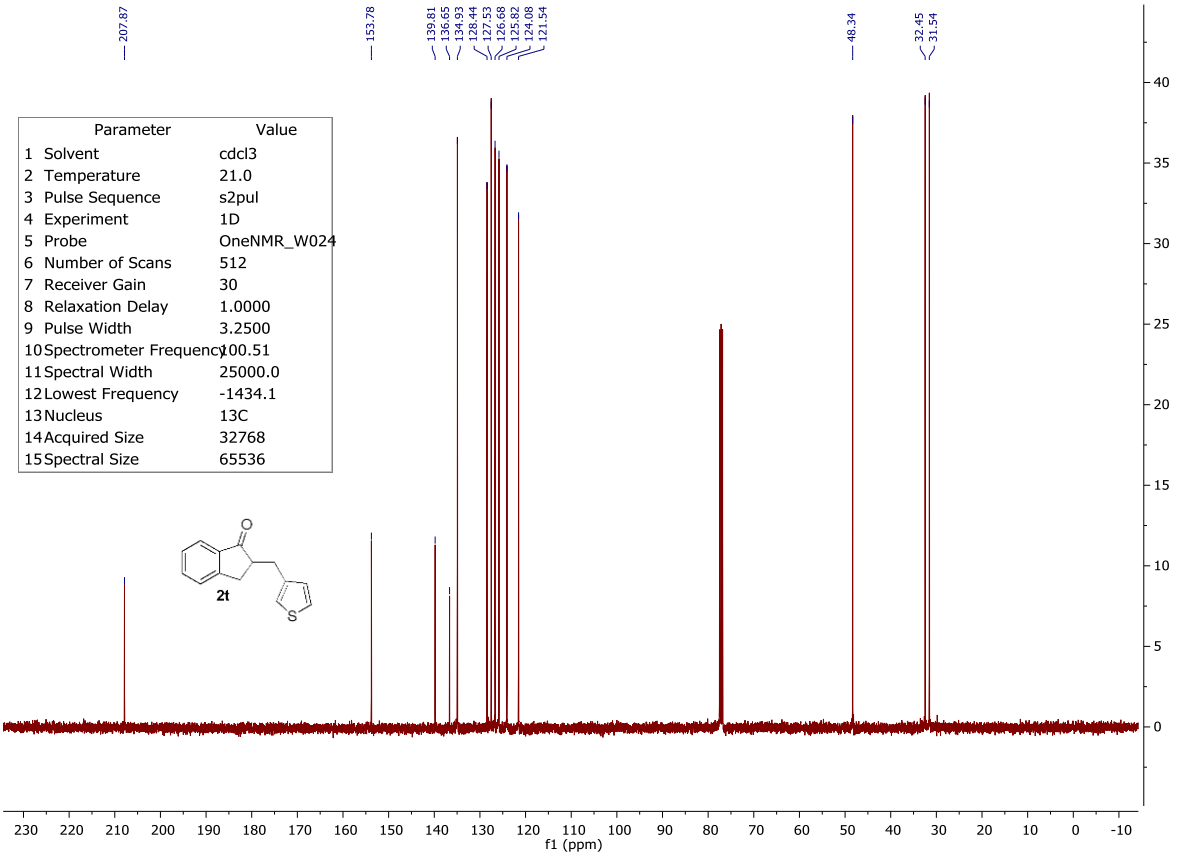

7.83 7.82 7.81 7.78 7.68 7.59 7.59 7.57 7.55 7.55 7.49 7.49 7.48 7.47 7.46 7.46 7.46 7.45 7.44 7.44 7.43 7.42 7.42 7.41 7.40 7.40 7.39 7.38 7.36
3.59 3.58 3.56 3.55 3.20 3.18 3.16 3.14 3.13 3.13 3.12 3.12 3.11 3.10 3.09 3.08 2.94 2.93 2.90 2.89 2.87 2.84 2.83 2.81
2q
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 18
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.6
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
3.87 1.04 1.06 5.00 1.07 2.12 1.04 1.07
f1 (ppm)

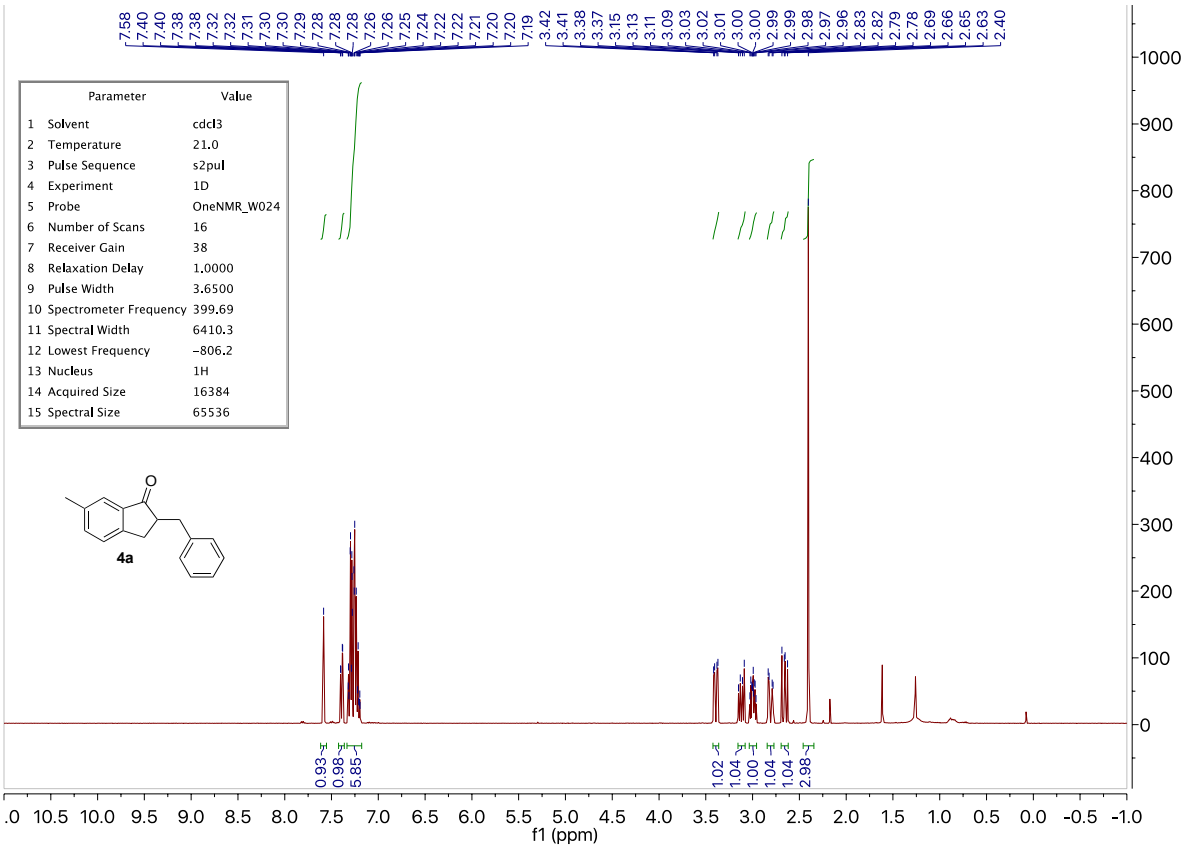

207.96
153.78 137.34 136.65 134.99 133.65 132.31 128.35 127.78 127.61 127.59 127.45 127.39 126.74 126.21 125.59 124.19
49.02 37.32 32.33
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1430.8
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
2q
f1 (ppm)

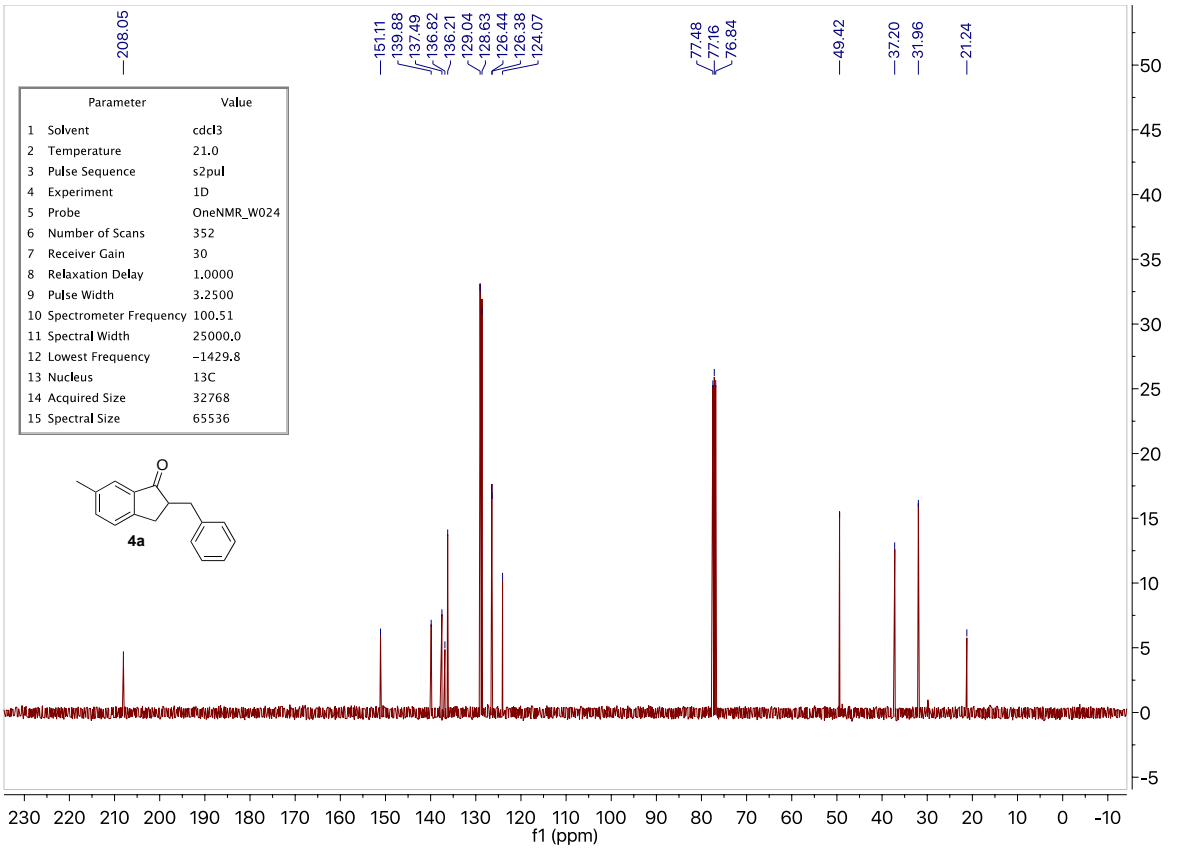

7.77
7.75
7.59
7.57
7.55
7.43
7.41
7.38
7.36
7.35
7.32
7.25
6.27
3.29
3.27
3.25
3.23
3.23
3.09
3.05
2.95
2.94
2.92
2.91
2.91
2.89
2.88
2.88
2.83
2.70
2.69
2.68
2.67
2.66
2.66
2.64
2.64
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -807.0
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
2s
0.91
1.00
0.90
0.94
1.85
0.88
1.11
1.07
1.98
1.06
f1 (ppm)

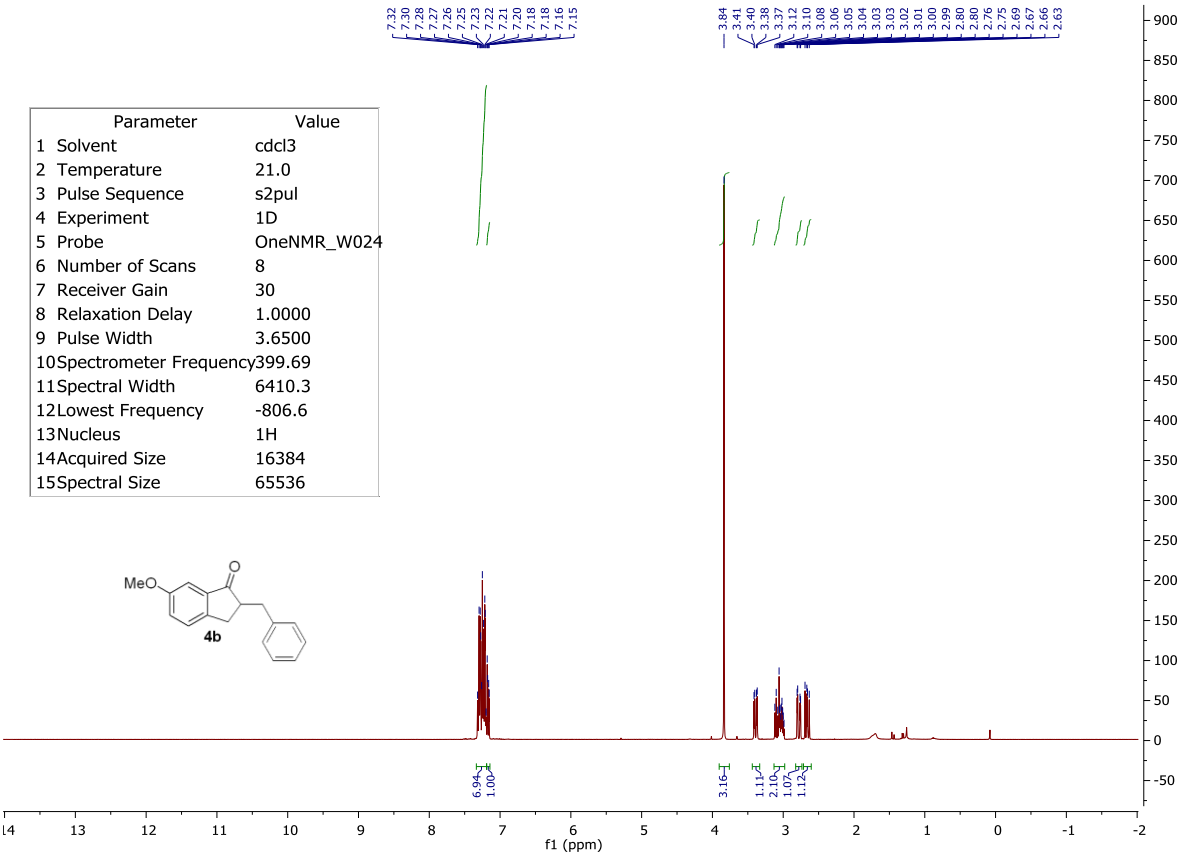

208.03
153.84
143.14
139.83
136.76
134.97
127.56
126.71
124.09
122.28
111.32
47.78
32.35
26.22
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 512
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1429.7
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
2s
f1 (ppm)

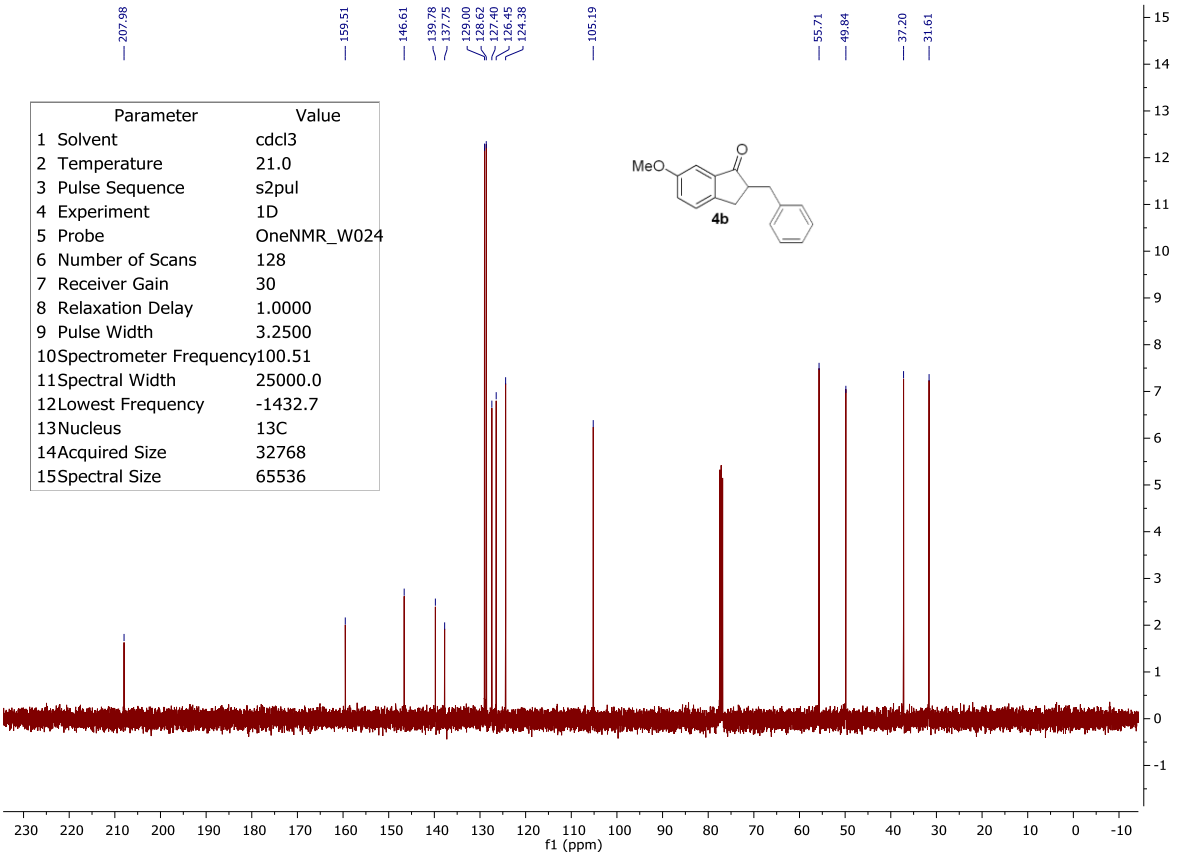

7.78 7.76 7.59 7.57 7.55 7.42 7.40 7.38 7.36 7.35 7.26 7.25 7.24 7.24 7.01 7.01 7.00 7.00 6.97 6.96
3.35 3.34 3.31 3.30 3.28 3.26 3.23 3.21 3.02 3.01 3.00 2.99 2.99 2.98 2.97 2.96 2.95 2.89 2.88 2.85 2.84 2.82 2.81 2.78
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -807.0
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
2t
0.93 0.97 1.87 1.04 1.82
1.00 0.99 0.96 1.25 1.20
f1 (ppm)

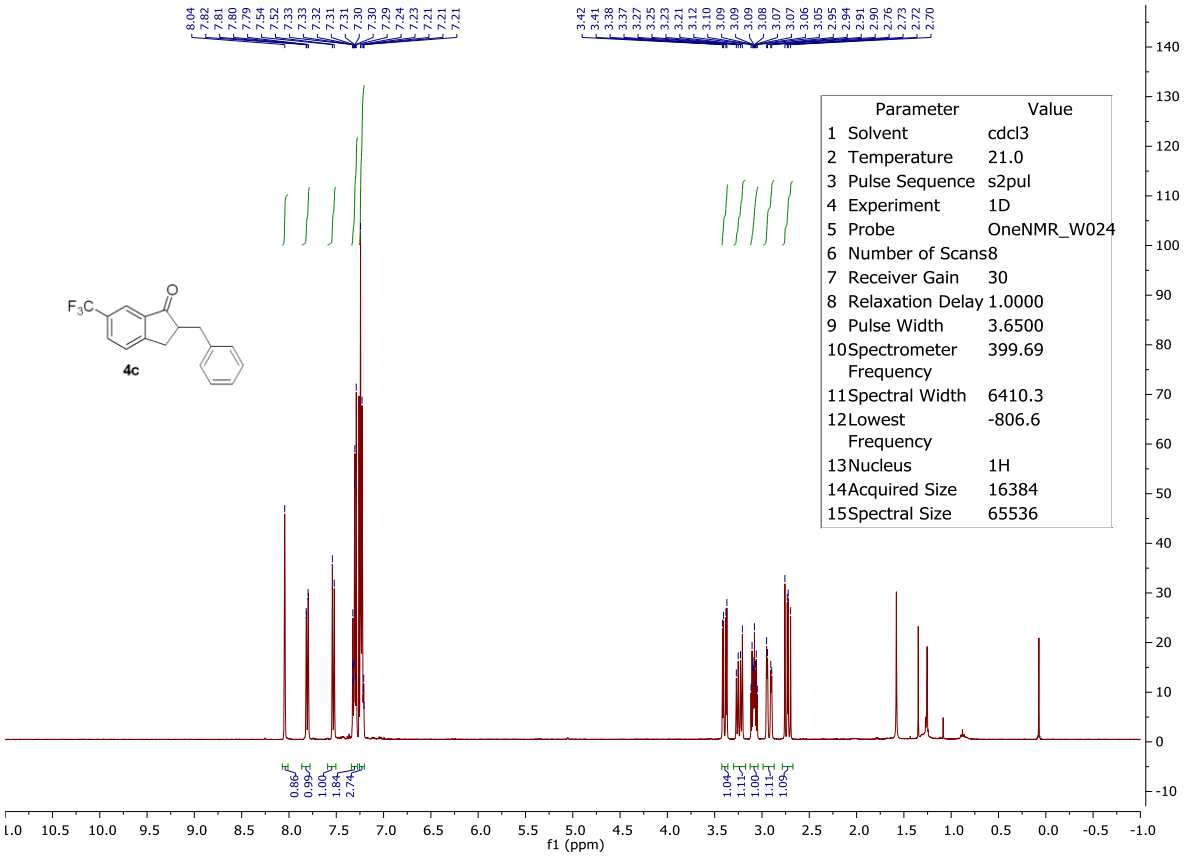

207.87
153.78
139.81 136.65 134.93 128.44 127.53 126.68 125.82 124.08 121.54
48.34
32.45 31.54
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 512
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1434.1
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
2t
f1 (ppm)

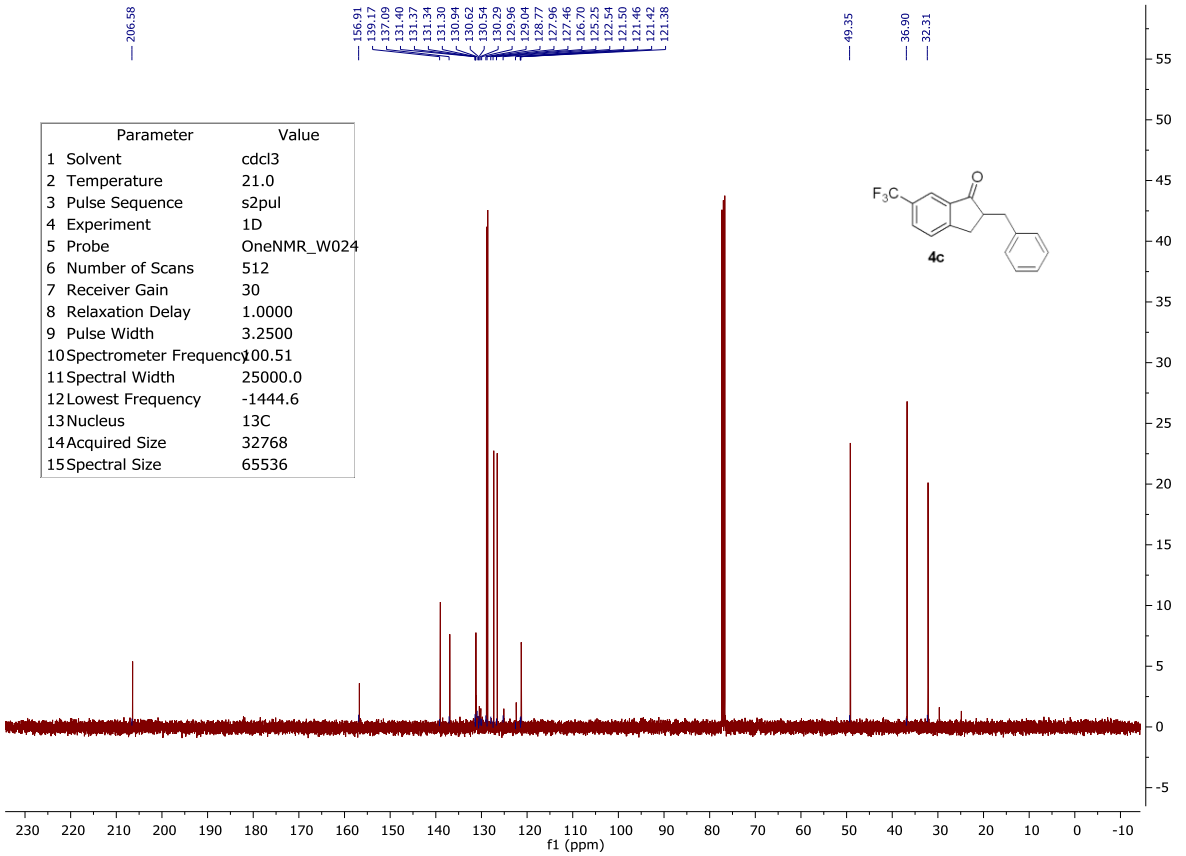

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 38
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
4a
f1 (ppm)

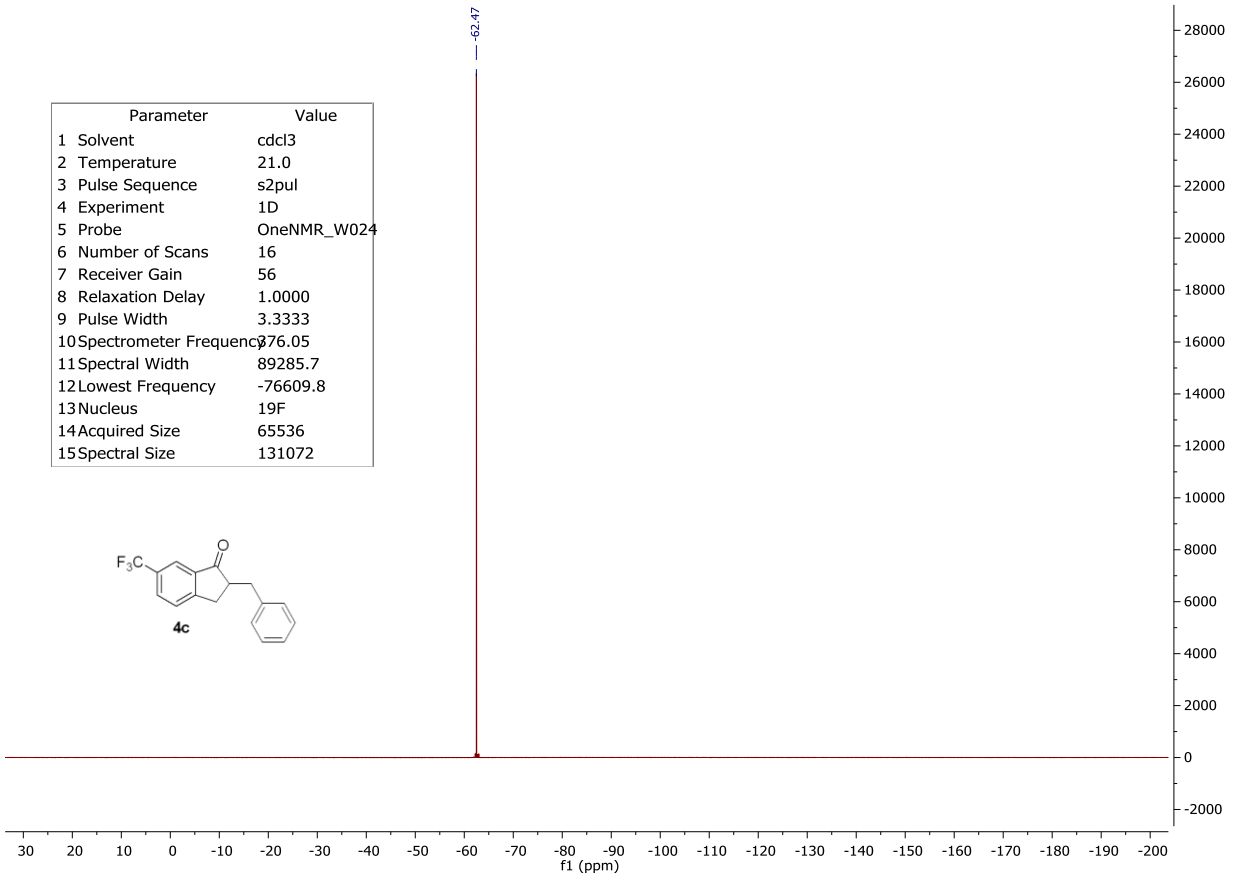

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 352
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1429.8
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
4a
f1 (ppm)


7.32 7.30 7.28 7.27 7.26 7.25 7.23 7.22 7.21 7.20 7.18 7.16 7.15
3.84 3.41 3.40 3.38 3.37 3.12 3.10 3.08 3.06 3.05 3.04 3.03 3.03 3.02 3.01 3.00 2.99 2.80 2.80 2.76 2.75 2.69 2.67 2.66 2.63
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.6
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
MeO
O
4b
6.94 1.00
3.16 1.11 2.10 1.07 1.12
f1 (ppm)


207.98 159.51 146.61 139.78 137.75 129.00 128.62 127.40 126.45 124.38 105.19 55.71 49.84 37.20 31.61
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 128
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1432.7
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
MeO
O
4b
f1 (ppm)


8.04 7.82 7.81 7.80 7.79 7.54 7.52 7.33 7.32 7.31 7.31 7.30 7.30 7.29 7.24 7.23 7.21 7.21 7.21
3.42 3.41 3.38 3.37 3.27 3.25 3.23 3.21 3.12 3.10 3.09 3.09 3.09 3.08 3.07 3.07 3.06 3.05 2.95 2.94 2.91 2.90 2.76 2.73 2.72 2.70
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.6
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
F3C
O
4c
0.86 0.99 1.00 1.84 2.74
1.04 1.11 1.00 1.11 1.09
f1 (ppm)

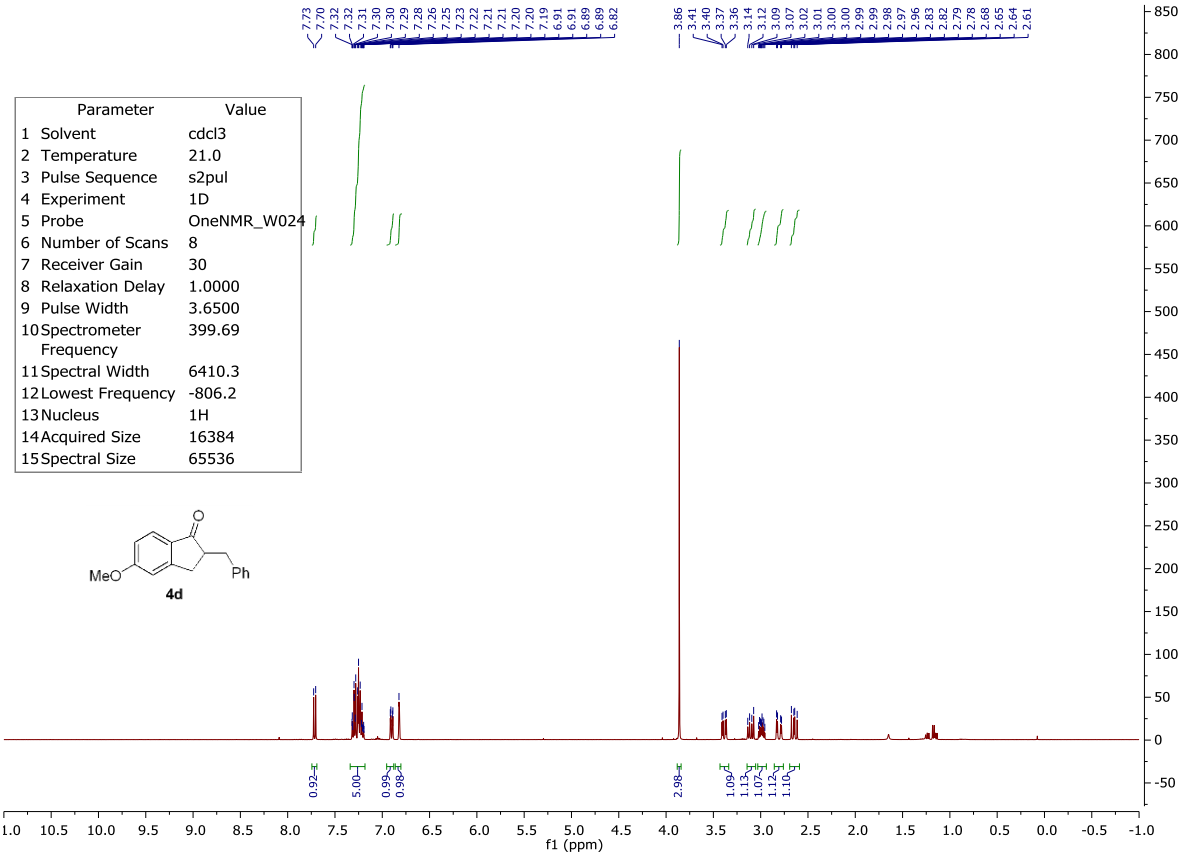

206.58
156.91 139.17 137.09 131.40 131.37 131.34 131.30 130.94 130.62 130.54 130.29 129.96 129.04 128.77 127.96 127.46 126.70 125.25 122.54 121.50 121.46 121.42 121.38
49.35
36.90
32.31
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 512
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1444.6
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
F3C
O
4c
f1 (ppm)

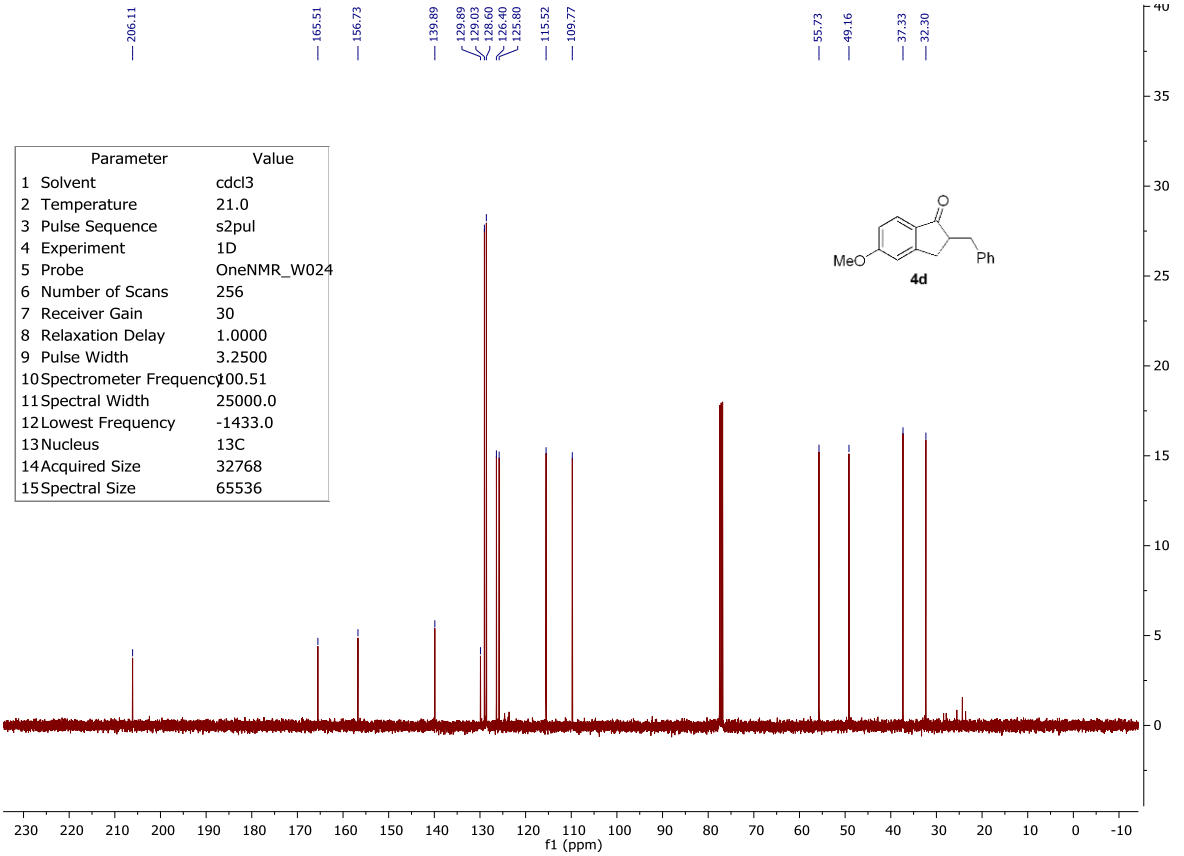


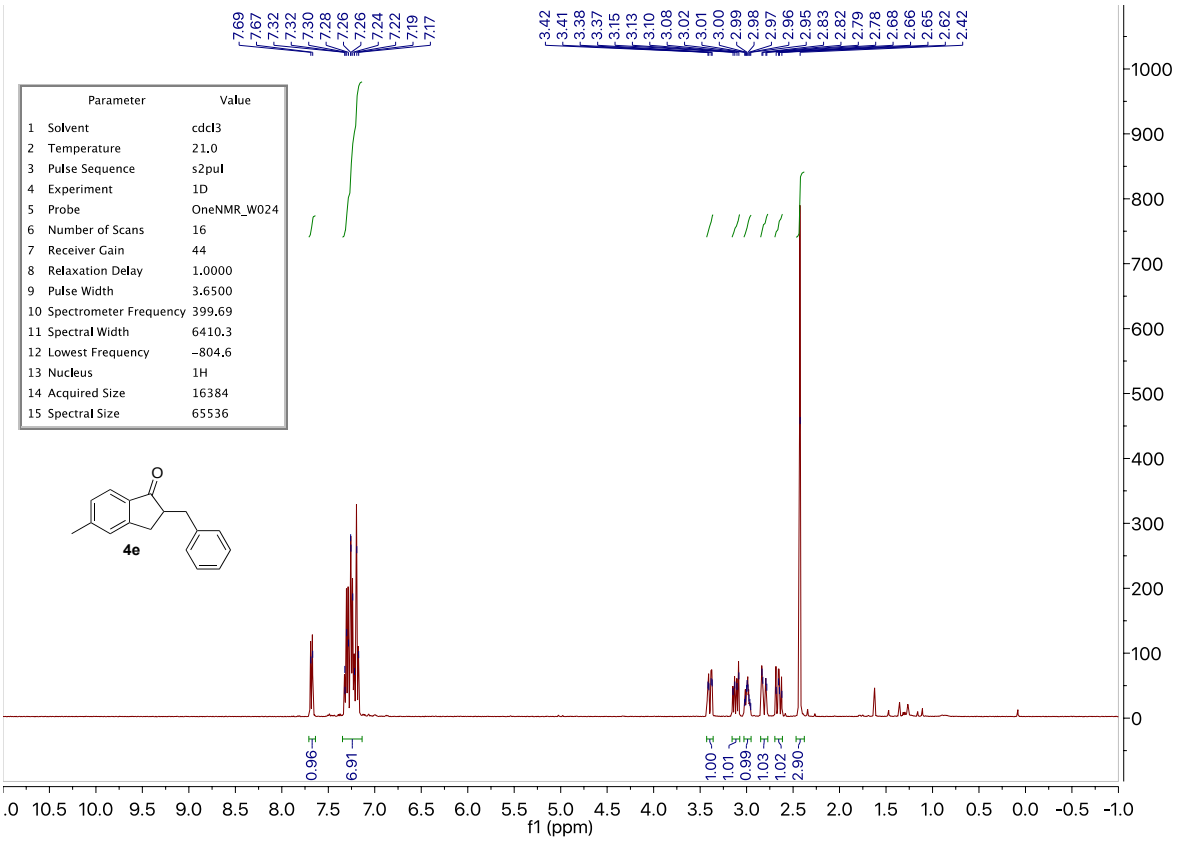

| Parameter | Value |
|---|---|
| 1 Solvent | cdcl3 |
| 2 Temperature | 21.0 |
| 3 Pulse Sequence | s2pul |
| 4 Experiment | 1D |
| 5 Probe | OneNMR_W024 |
| 6 Number of Scans | 16 |
| 7 Receiver Gain | 56 |
| 8 Relaxation Delay | 1.0000 |
| 9 Pulse Width | 3.3333 |
| 10 Spectrometer Frequency | 376.05 |
| 11 Spectral Width | 89285.7 |
| 12 Lowest Frequency | -76609.8 |
| 13 Nucleus | 19F |
| 14 Acquired Size | 65536 |
| 15 Spectral Size | 131072 |

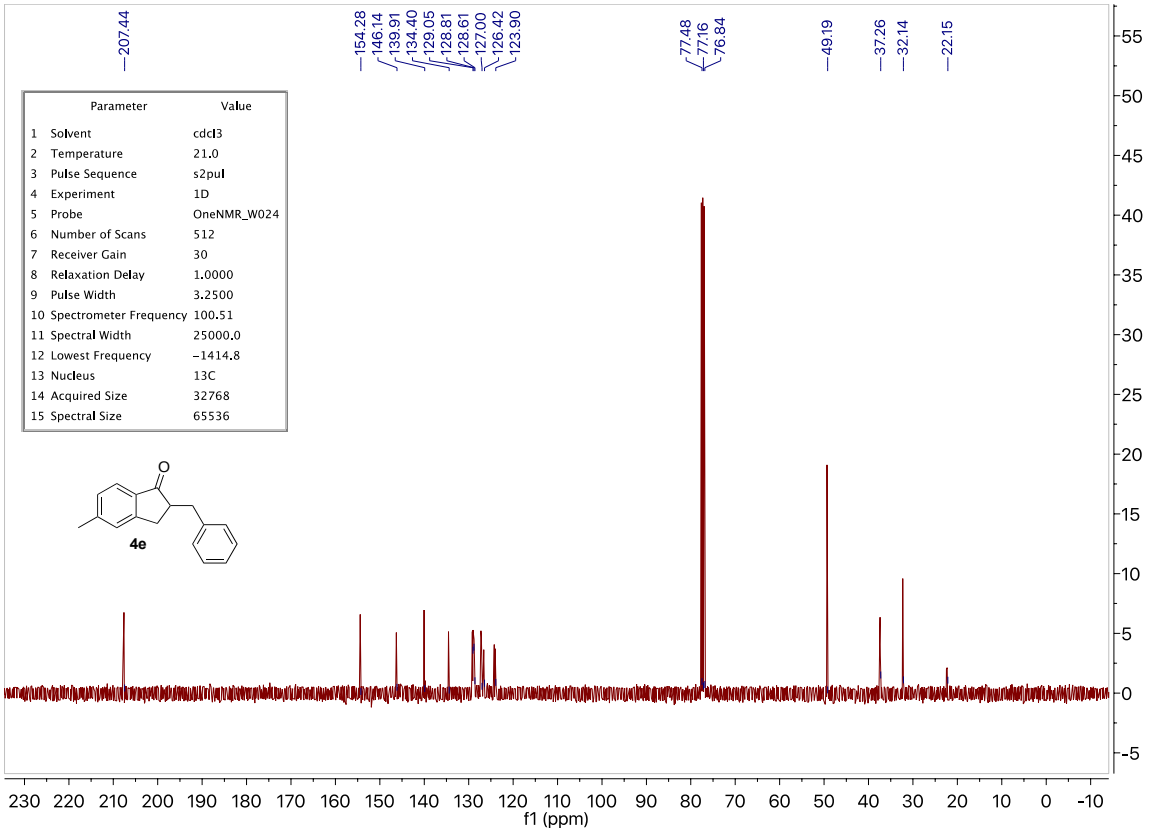


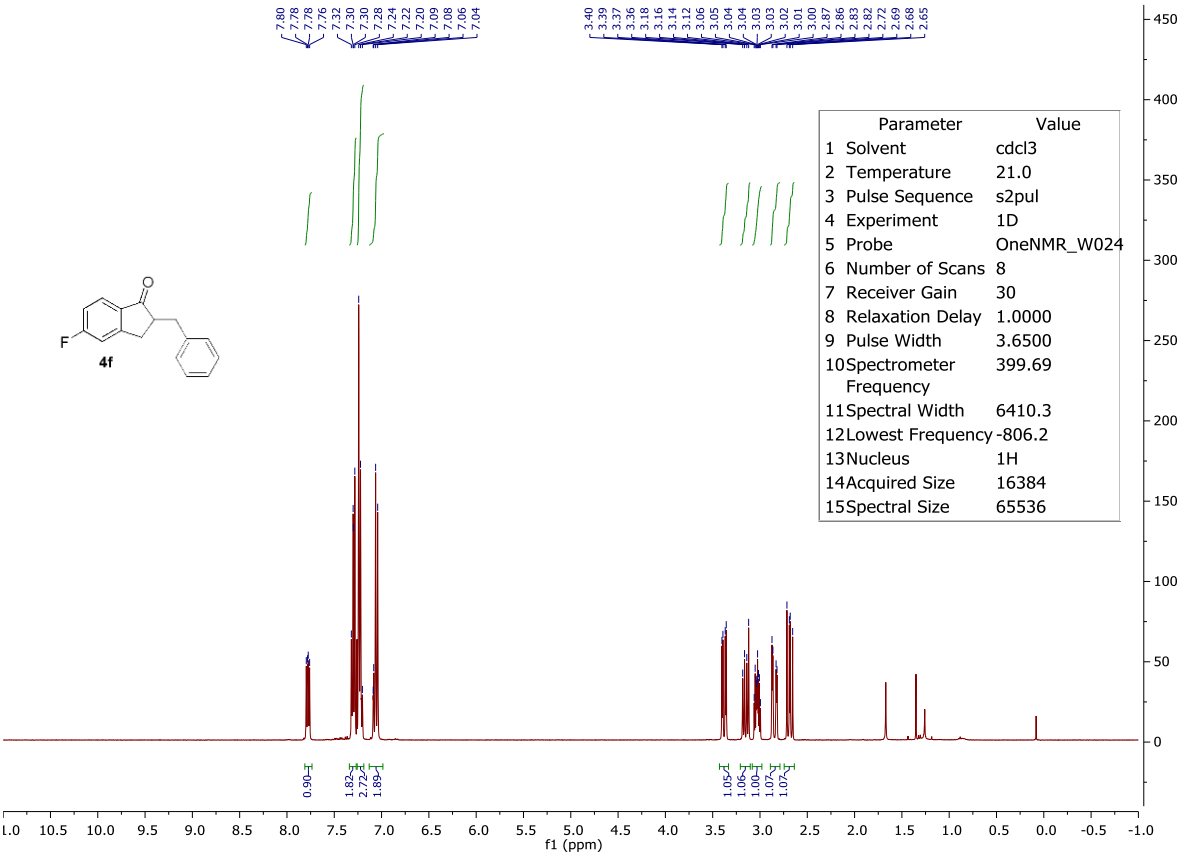

**4c**

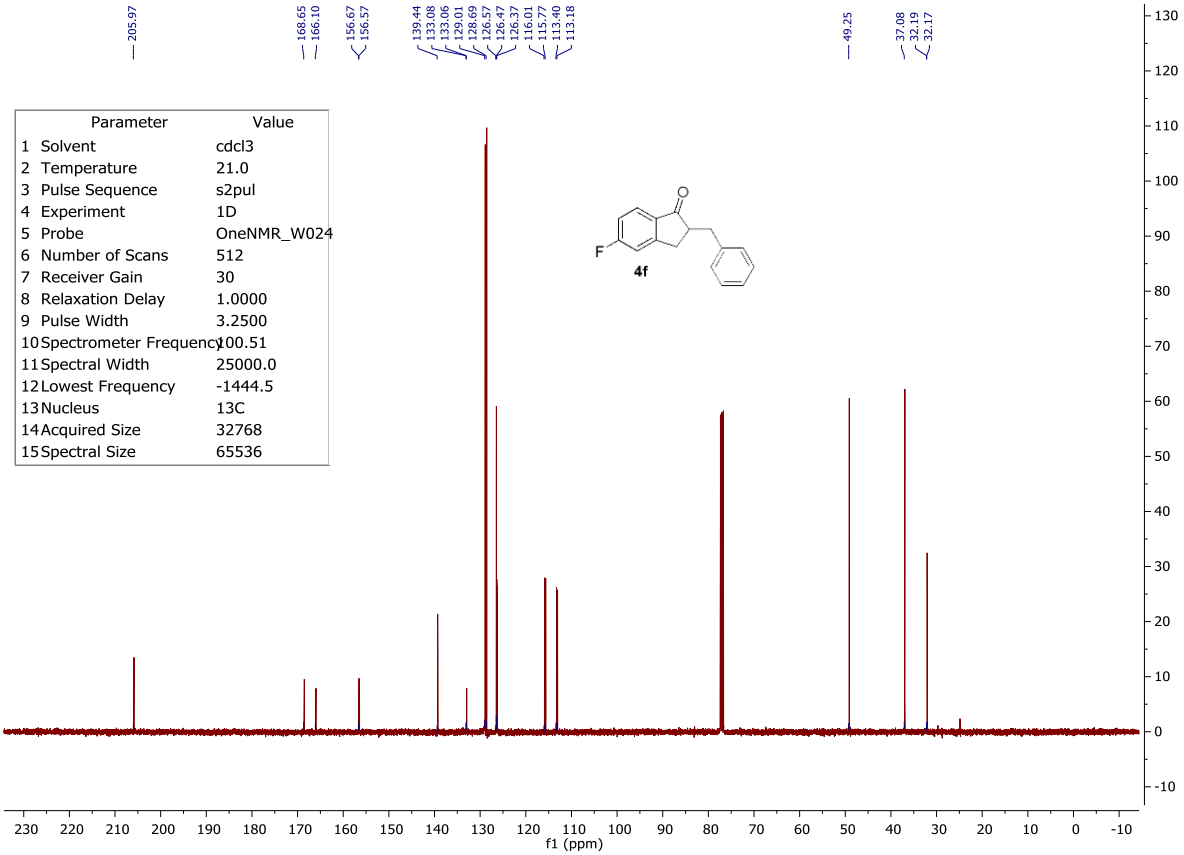

7.73 7.70 7.32 7.32 7.31 7.30 7.30 7.29 7.28 7.26 7.25 7.23 7.22 7.21 7.21 7.20 7.20 7.19 6.91 6.91 6.89 6.89 6.82
3.86 3.41 3.40 3.37 3.36 3.14 3.12 3.09 3.07 3.02 3.01 3.00 3.00 2.99 2.99 2.98 2.97 2.96 2.83 2.82 2.79 2.78 2.68 2.65 2.64 2.61
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
MeO
Ph
4d
0.92 5.00 0.99 0.98 2.98 1.09 1.13 1.07 1.12 1.10
f1 (ppm)

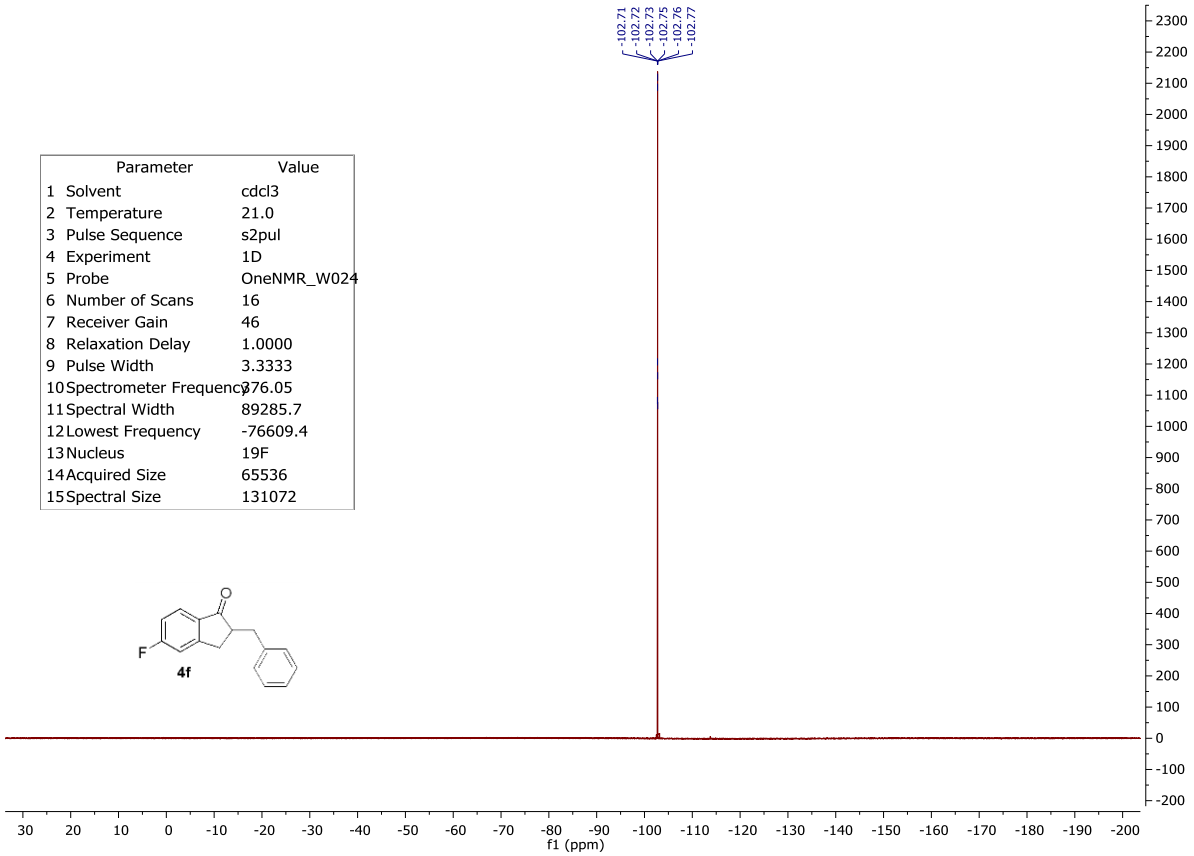

206.11 165.51 156.73 139.89 129.89 129.03 128.60 126.40 125.80 115.52 109.77 55.73 49.16 37.33 32.30
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1433.0
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
MeO
Ph
4d
f1 (ppm)

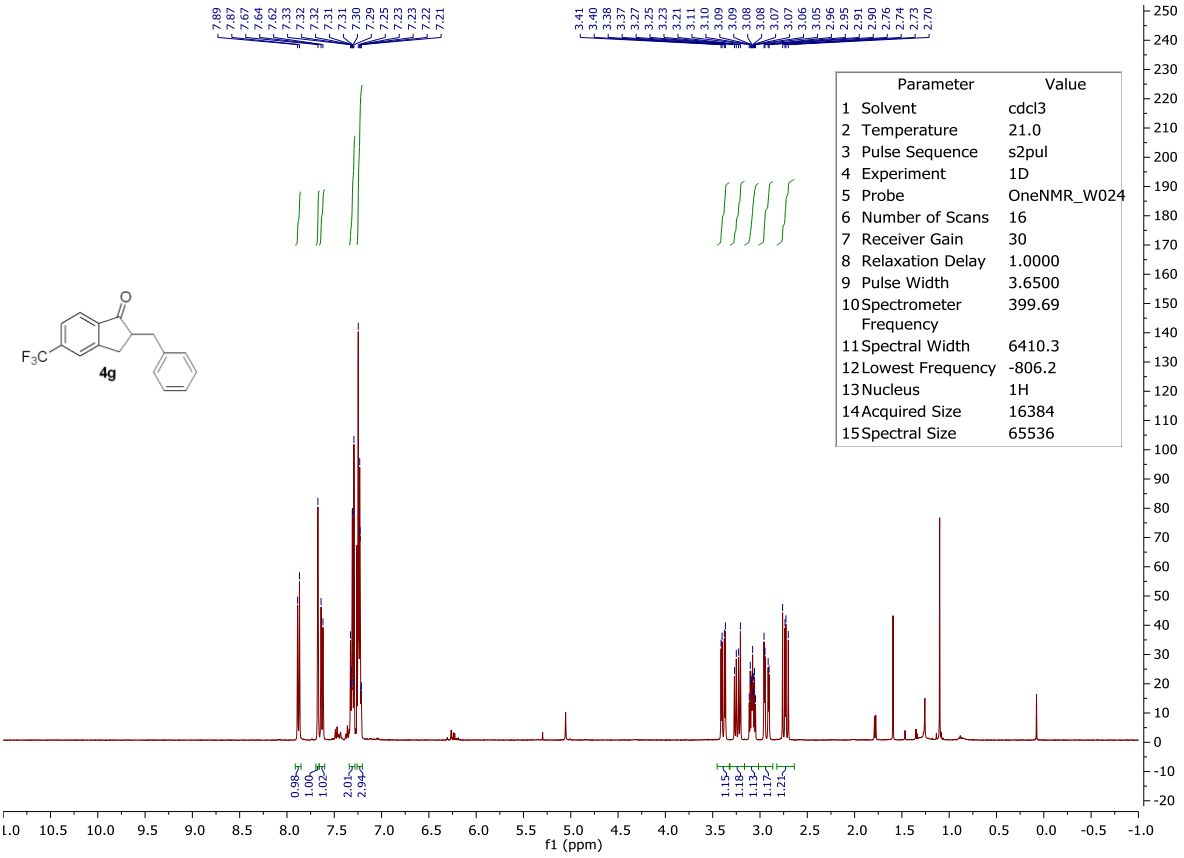

7.69
7.67
7.32
7.32
7.30
7.28
7.26
7.26
7.24
7.22
7.19
7.17
3.42
3.41
3.38
3.37
3.15
3.13
3.10
3.08
3.02
3.01
3.00
2.99
2.98
2.97
2.96
2.95
2.83
2.82
2.79
2.78
2.68
2.66
2.65
2.62
2.42
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 44
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -804.6
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
O
4e
0.96
6.91
1.00
1.01
0.99
1.03
1.02
2.90
f1 (ppm)

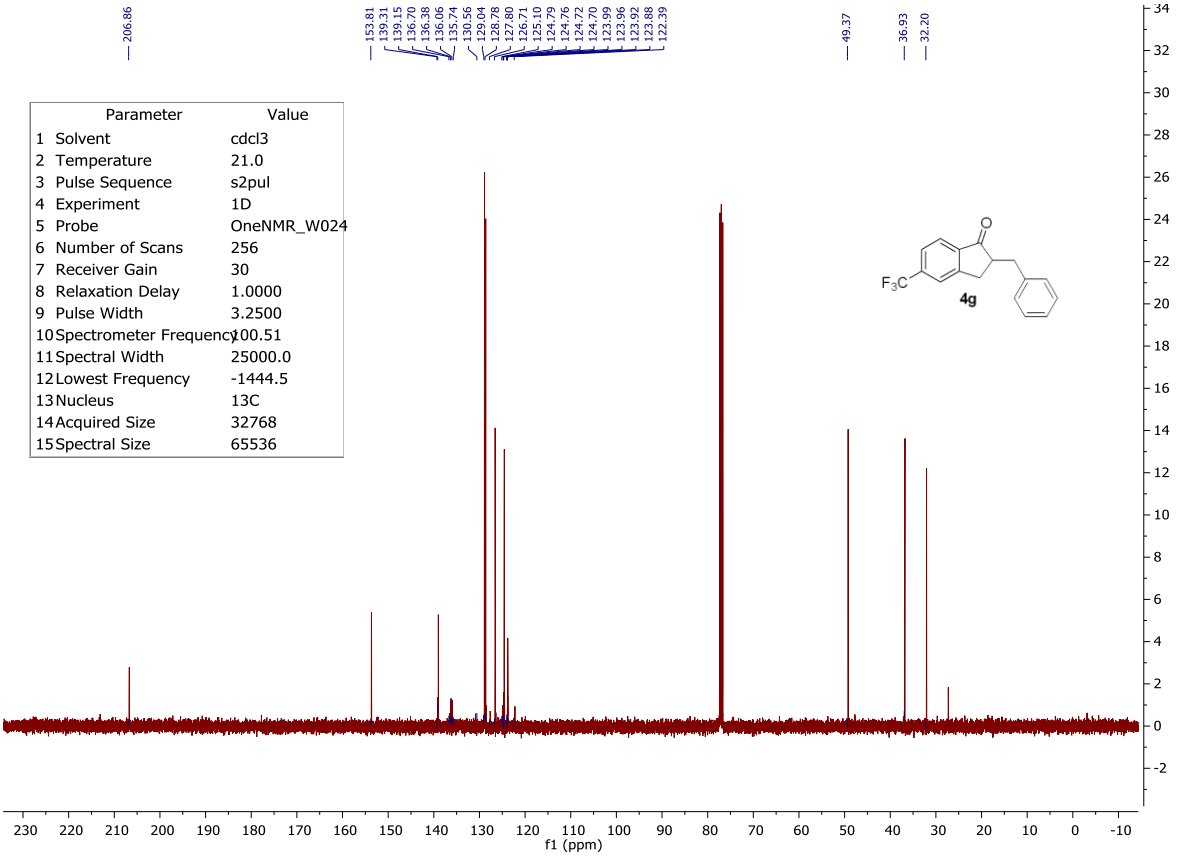

207.44
154.28
146.14
139.91
134.40
129.05
128.81
128.61
127.00
126.42
123.90
77.48
77.16
76.84
49.19
37.26
32.14
22.15
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 512
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1414.8
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
O
4e
f1 (ppm)

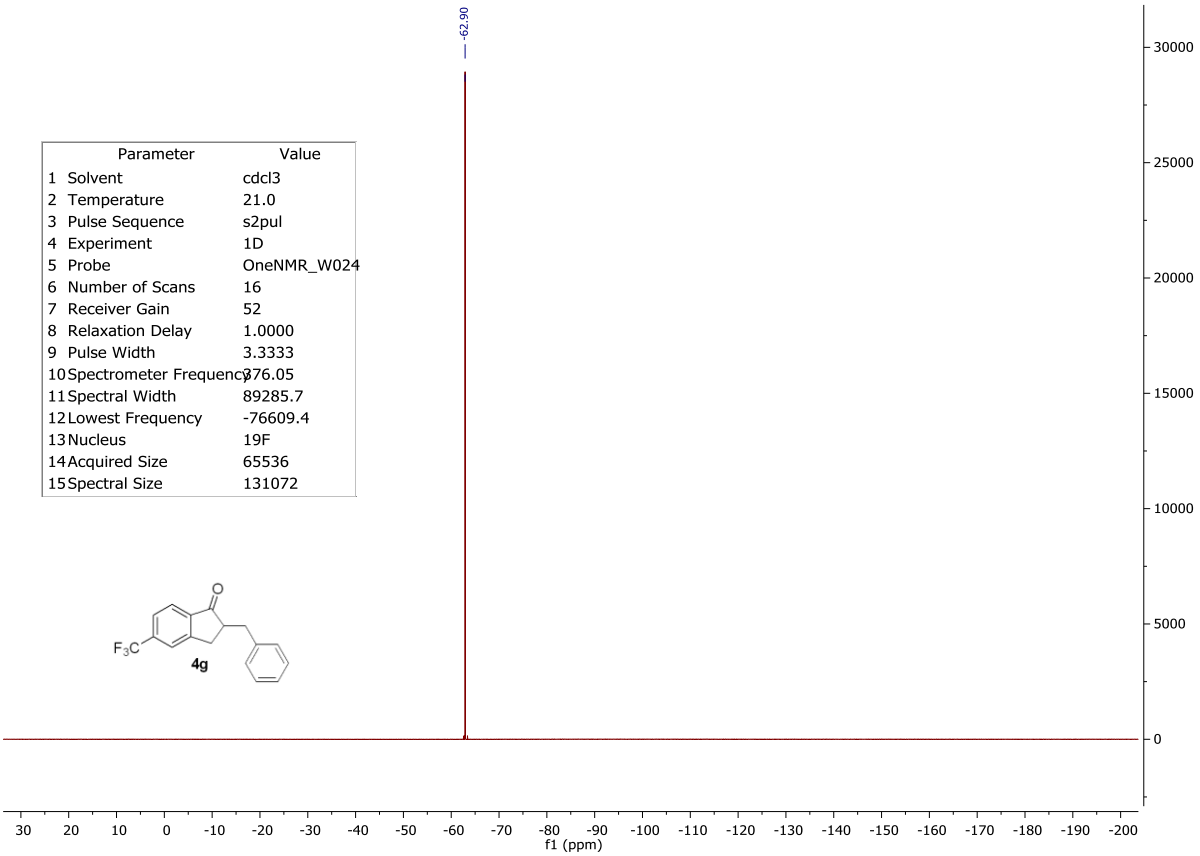

7.80 7.78 7.78 7.76 7.32 7.30 7.30 7.28 7.24 7.22 7.20 7.09 7.08 7.06 7.04
3.40 3.39 3.37 3.36 3.18 3.16 3.14 3.12 3.06 3.05 3.04 3.04 3.03 3.03 3.02 3.01 3.00 2.87 2.86 2.83 2.82 2.72 2.69 2.68 2.65
F
4f
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
0.90 1.82 2.72 1.89 1.05 1.06 1.00 1.07 1.07
f1 (ppm)


205.97
168.65 166.10 156.67 156.57 139.44 133.08 133.06 129.01 128.69 126.57 126.47 126.37 116.01 115.77 113.40 113.18
49.25
37.08 32.19 32.17
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 512
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1444.5
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
F
4f
f1 (ppm)


-102.71
-102.72
-102.73
-102.75
-102.76
-102.77
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 46
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76609.4
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
F
4f
f1 (ppm)


7.89 7.87 7.67 7.64 7.62 7.33 7.32 7.32 7.31 7.31 7.30 7.29 7.25 7.23 7.22 7.21
3.41 3.40 3.38 3.37 3.27 3.25 3.23 3.21 3.11 3.10 3.09 3.09 3.08 3.08 3.07 3.07 3.06 3.05 2.96 2.95 2.91 2.90 2.76 2.74 2.73 2.70
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
F3C
4g
0.98 1.00 1.02 2.01 2.94 1.15 1.18 1.13 1.17 1.21
f1 (ppm)

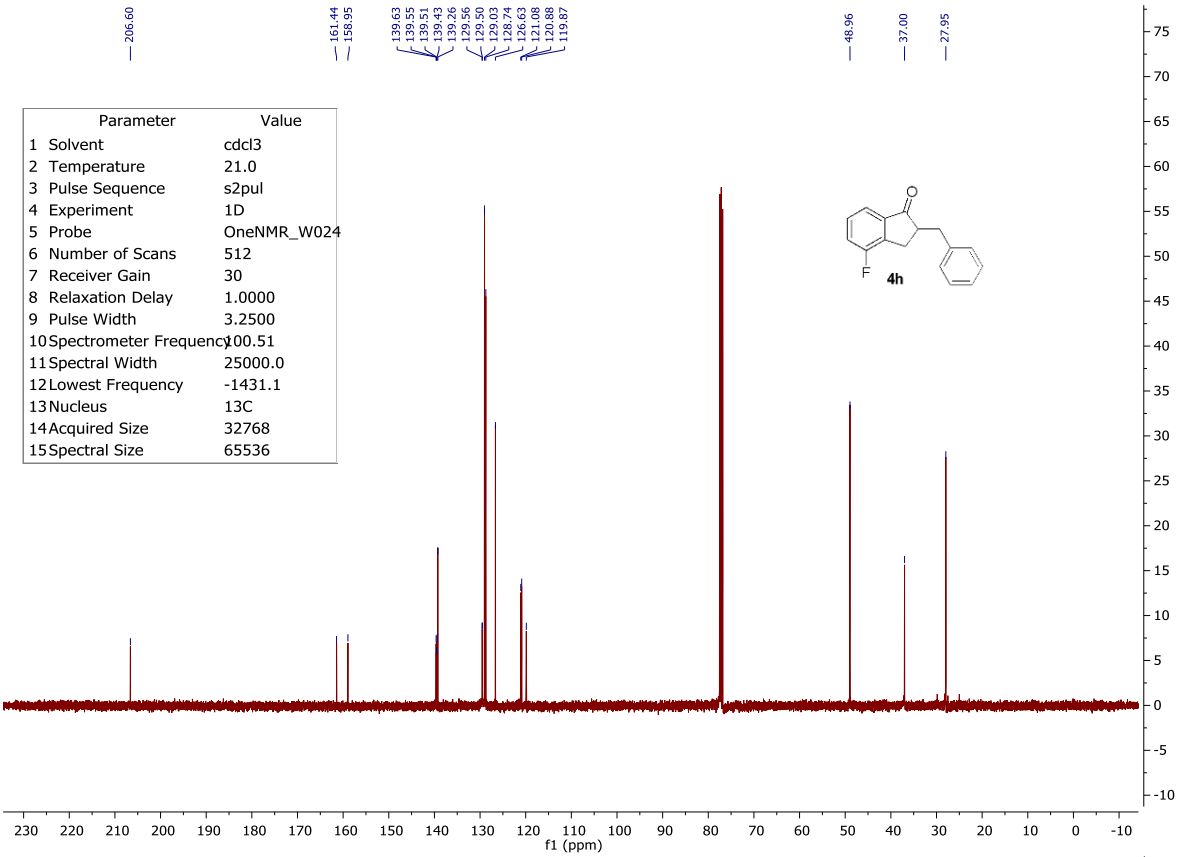

206.86
153.81 139.31 139.15 136.70 136.38 136.06 135.74 130.56 129.04 128.78 127.80 126.71 125.10 124.79 124.76 124.72 124.70 123.99 123.96 123.92 123.88 122.39
49.37
36.93
32.20
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 256
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1444.5
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
F3C
4g
f1 (ppm)

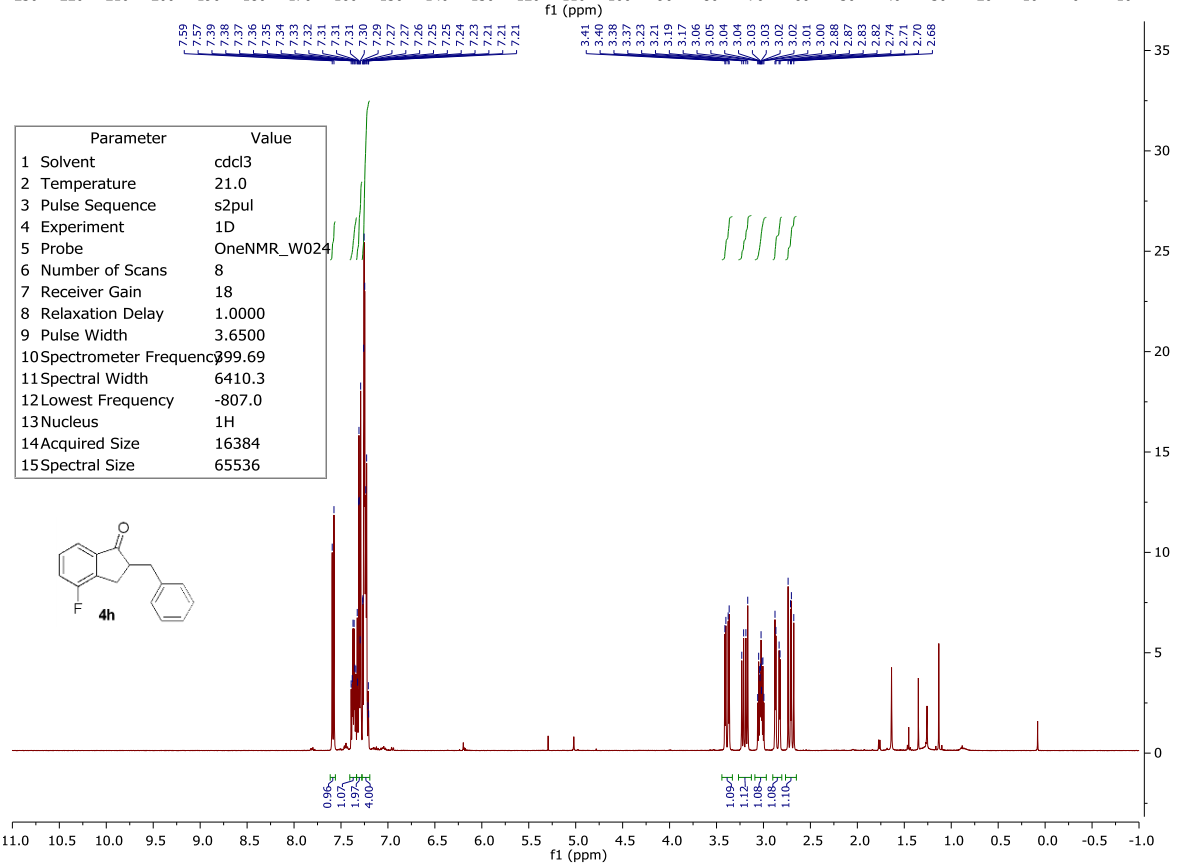


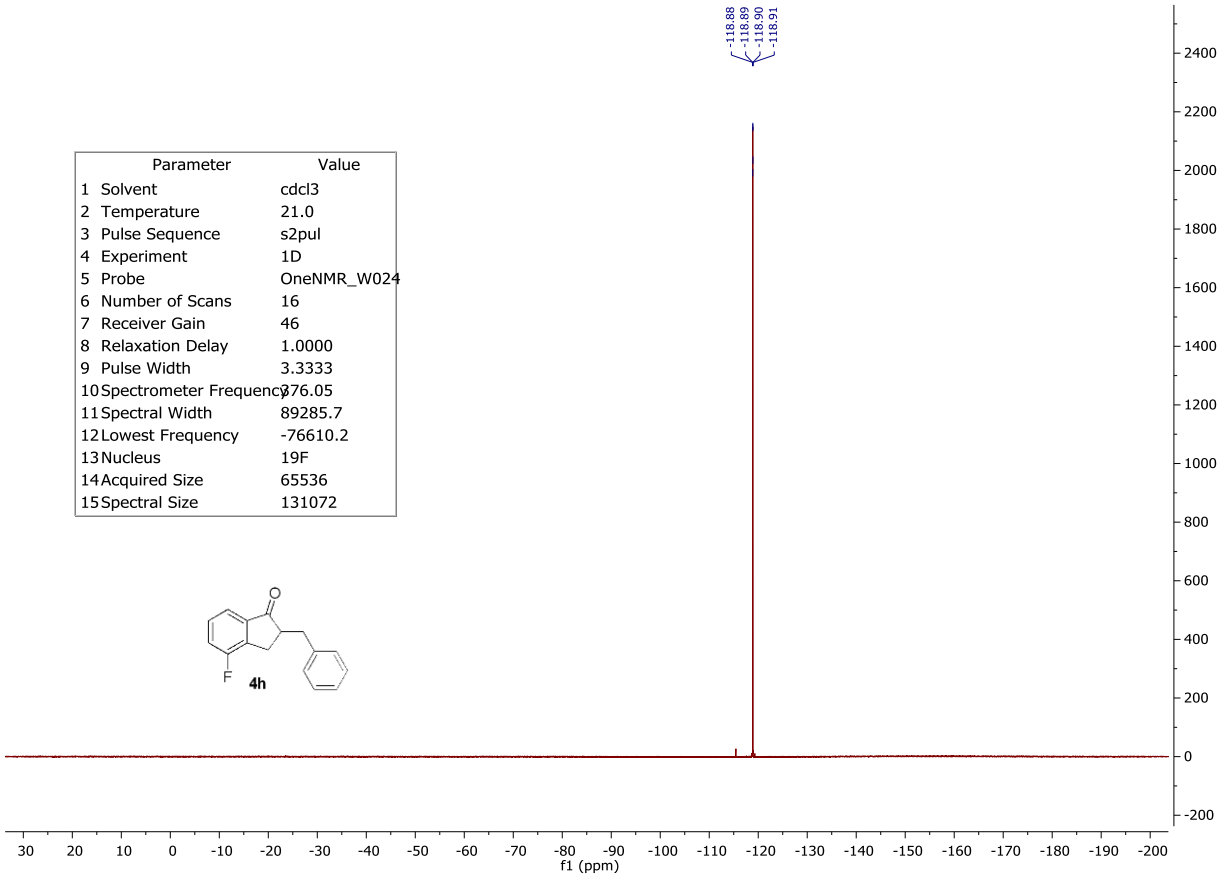

| | Parameter | Value |
|---|---|---|
| 1 | Solvent | cdcl3 |
| 2 | Temperature | 21.0 |
| 3 | Pulse Sequence | s2pul |
| 4 | Experiment | 1D |
| 5 | Probe | OneNMR_W024 |
| 6 | Number of Scans | 16 |
| 7 | Receiver Gain | 52 |
| 8 | Relaxation Delay | 1.0000 |
| 9 | Pulse Width | 3.3333 |
| 10 | Spectrometer Frequency | 376.05 |
| 11 | Spectral Width | 89285.7 |
| 12 | Lowest Frequency | -76609.4 |
| 13 | Nucleus | 19F |
| 14 | Acquired Size | 65536 |
| 15 | Spectral Size | 131072 |

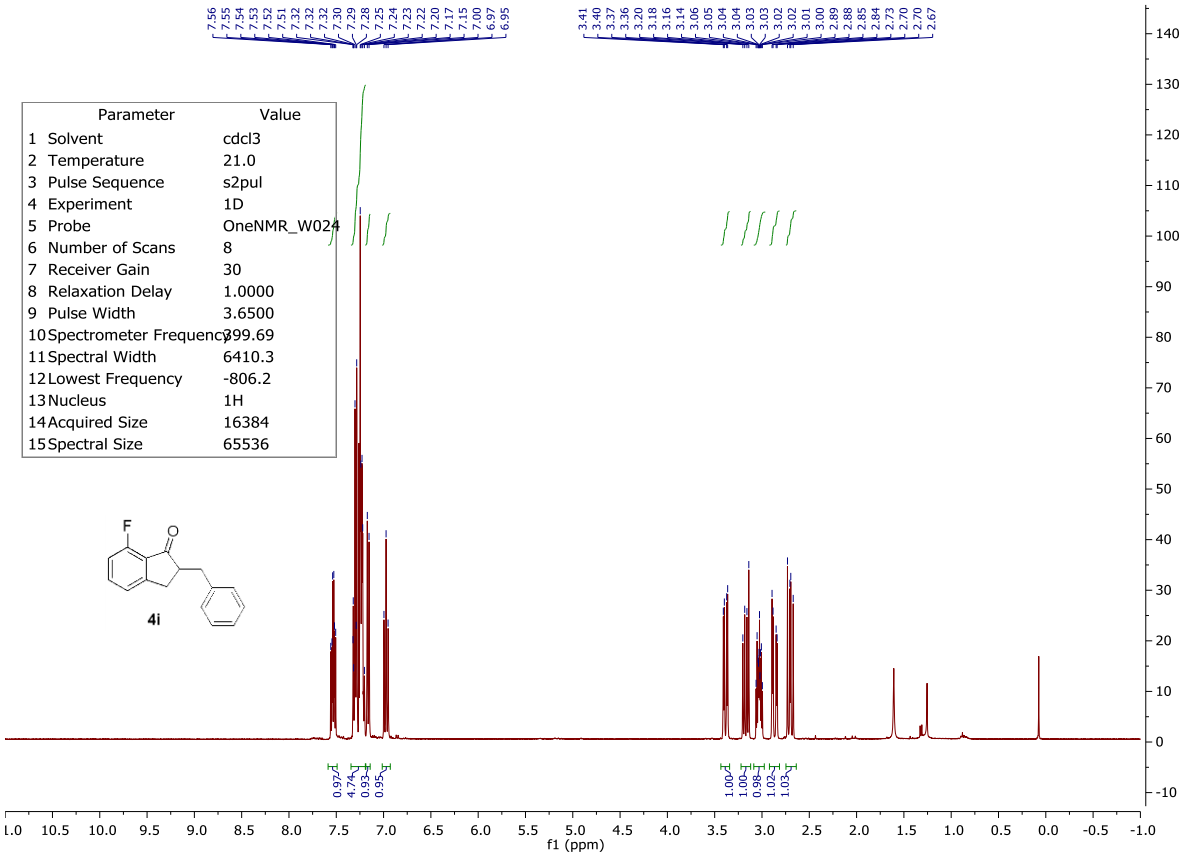


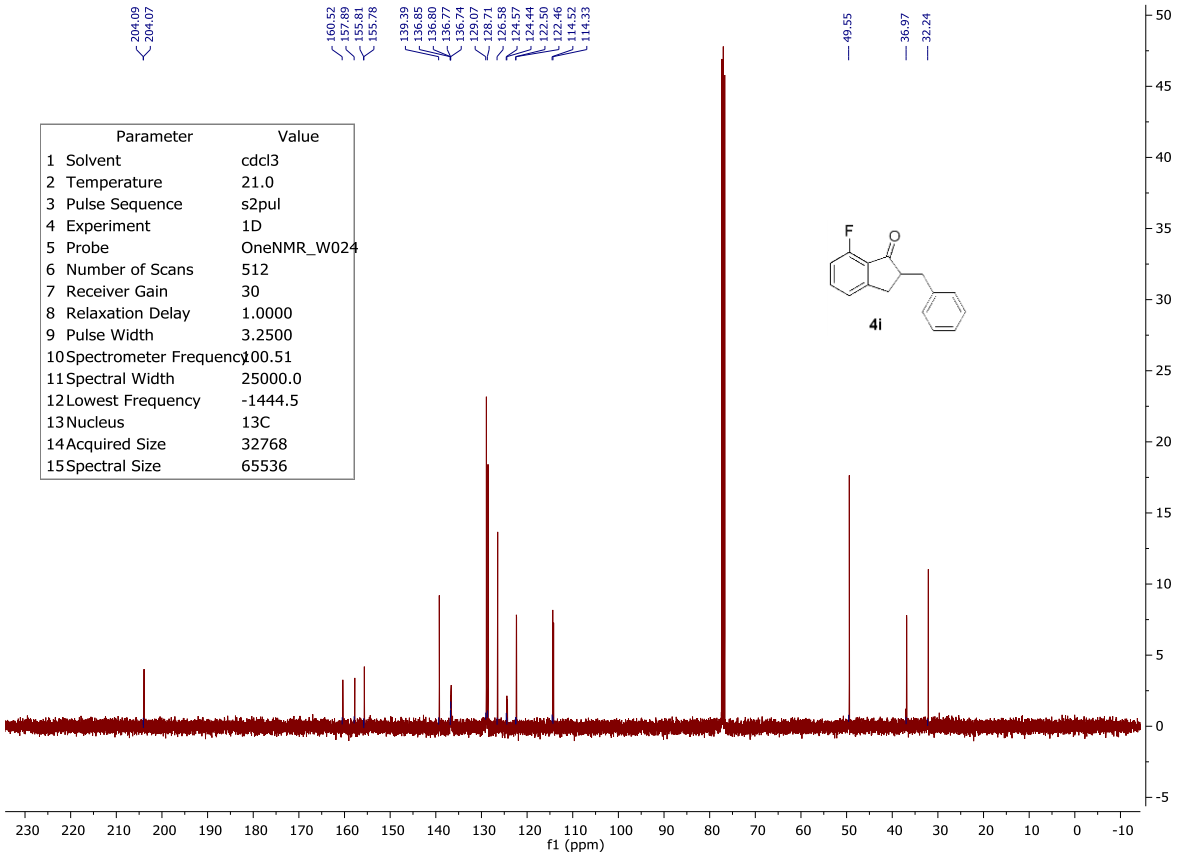

**4g**

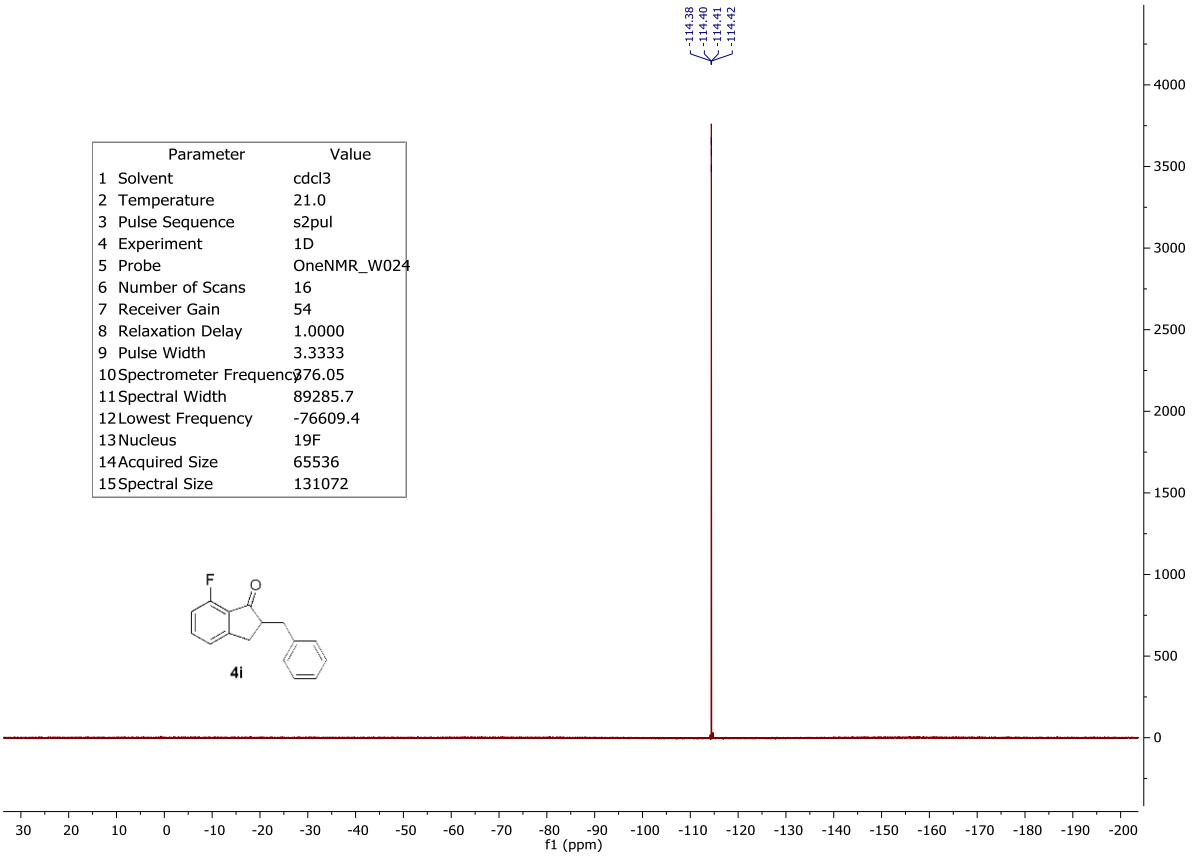

206.60
161.44
158.95
139.63
139.55
139.51
139.43
139.26
129.56
129.50
129.03
128.74
126.63
121.08
120.88
119.87
48.96
37.00
27.95
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 512
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1431.1
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
F
4h
f1 (ppm)

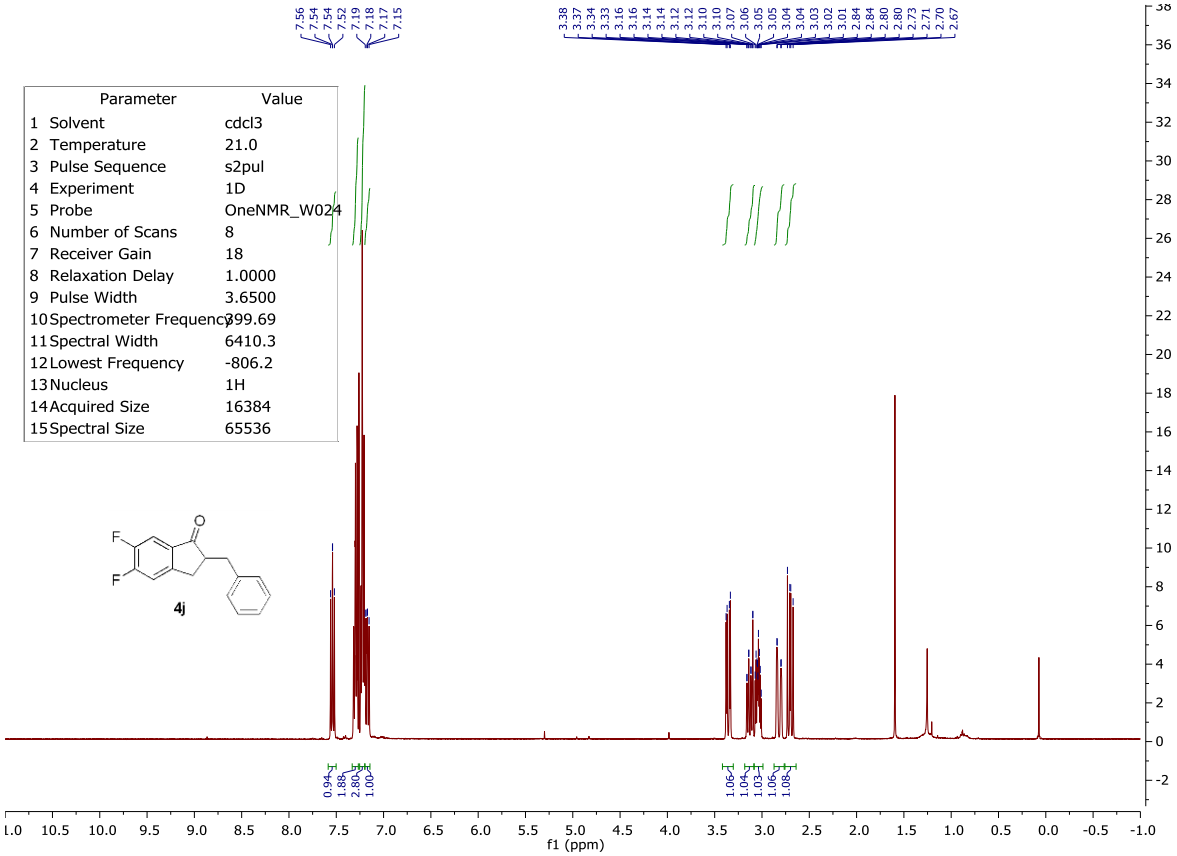

7.59
7.57
7.39
7.38
7.37
7.36
7.35
7.34
7.33
7.32
7.31
7.31
7.31
7.30
7.29
7.27
7.27
7.26
7.25
7.25
7.24
7.23
7.21
7.21
7.21
3.41
3.40
3.38
3.37
3.23
3.21
3.19
3.17
3.06
3.05
3.04
3.04
3.03
3.03
3.02
3.02
3.01
3.00
2.88
2.87
2.83
2.82
2.74
2.71
2.70
2.68
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 18
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -807.0
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
F
4h
0.96
1.07
1.97
4.00
1.09
1.12
1.08
1.08
1.10
f1 (ppm)

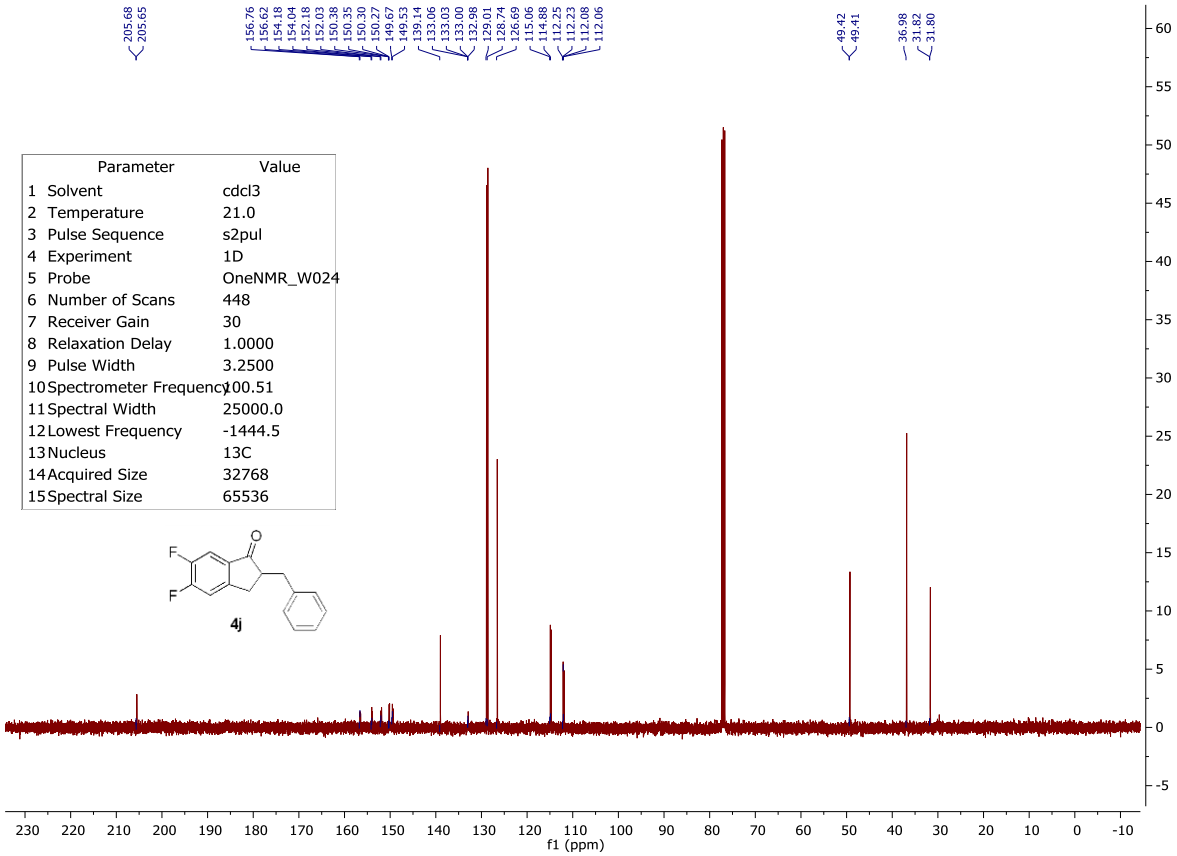

-118.88
-118.89
-118.90
-118.91
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 46
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76610.2
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
F
4h
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

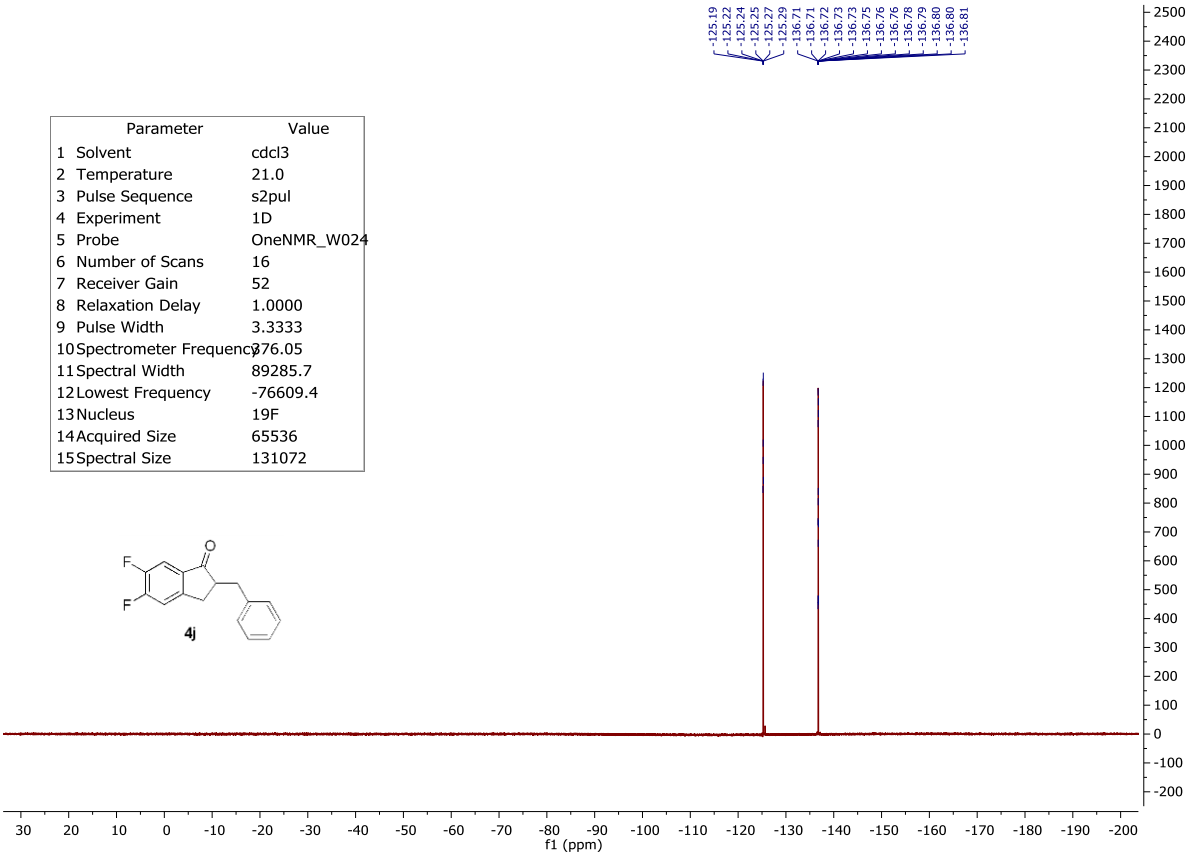

Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
4i
f1 (ppm)


Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 512
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1444.5
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
4i
f1 (ppm)


-114.38
-114.40
-114.41
-114.42
Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 16
7 Receiver Gain 54
8 Relaxation Delay 1.0000
9 Pulse Width 3.3333
10 Spectrometer Frequency 376.05
11 Spectral Width 89285.7
12 Lowest Frequency -76609.4
13 Nucleus 19F
14 Acquired Size 65536
15 Spectral Size 131072
F
O
4i
4000
3500
3000
2500
2000
1500
1000
500
0
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 8
7 Receiver Gain 18
8 Relaxation Delay 1.0000
9 Pulse Width 3.6500
10 Spectrometer Frequency 399.69
11 Spectral Width 6410.3
12 Lowest Frequency -806.2
13 Nucleus 1H
14 Acquired Size 16384
15 Spectral Size 65536
4j
f1 (ppm)


Parameter Value
1 Solvent cdcl3
2 Temperature 21.0
3 Pulse Sequence s2pul
4 Experiment 1D
5 Probe OneNMR_W024
6 Number of Scans 448
7 Receiver Gain 30
8 Relaxation Delay 1.0000
9 Pulse Width 3.2500
10 Spectrometer Frequency 100.51
11 Spectral Width 25000.0
12 Lowest Frequency -1444.5
13 Nucleus 13C
14 Acquired Size 32768
15 Spectral Size 65536
4j
f1 (ppm)




## References


1. Harris, R. K.; Becker, E. D.; De Menezes, S. M. C.; Goodfellow, R.; Granger, P. *Pure Appl. Chem.* **2001**, *73*, 1795-1818.
2. Incerti–Pradillos, C. A.; Kabeshov, M. A.; Malkov, A. V. *Angew. Chem. Int. Ed.* **2013**, *52*, 5338-5341.
3. Ge, S.; Hartwig, J. F. *J. Am. Chem. Soc.* **2011**, *133*, 16330-16333.