

Supporting Information

Synthesis of a Versatile 1*H*-indene-3-carboxylate Scaffold Enabled by Visible-Light Promoted Wolff Rearrangement of 1-Diazonaphthalen-2(1*H*)-ones

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I. General Information

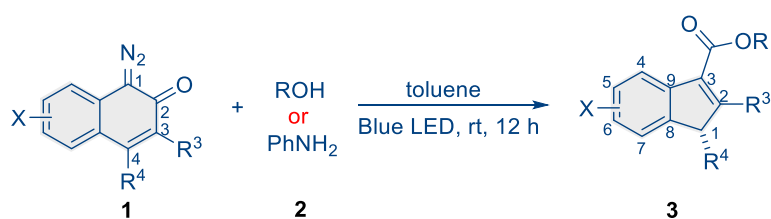
Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co., China. All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. Anhydrous acetonitrile was purified by the Innovative® solvent purification system or purchased from Energy Chemical. Analytical grade dichloromethane (DCM), 1,2-dichloroethane (DCE), tetrahydrofuran (THF), toluene, ethyl acetate, and cyclohexane were purchased from Energy Chemical. These solvents were directly used as received. β -naphthols, and 15-crown-5 were purchased from Energy Chemical and Leyan. Blue LED reactor was purchased from Shenzhen synled Tech. Co. Ltd. ^1H , and ^{13}C spectra were collected on a Bruker AV 300 and 400 MHz NMR spectrometer using residue solvent peaks as an internal standard (^1H NMR: CDCl_3 at 7.26 ppm; ^{13}C NMR: CDCl_3 at 77.0 ppm). Mass spectra were collected on an Agilent GC/MS 5975C system, a MALDI Micro MX mass spectrometer, or an API QSTAR XL System.

II. Synthesis of 1-Diazonaphthalen-2(1*H*)-ones

All the phthalazine 1-Diazonaphthalen-2(1*H*)-ones used this work are known compounds and were synthesized according to the literature procedure.¹

III. Visible-Light-Promoted Sequential Reaction of 1-Diazonaphthalen-2(1*H*)-ones

General Procedure A.

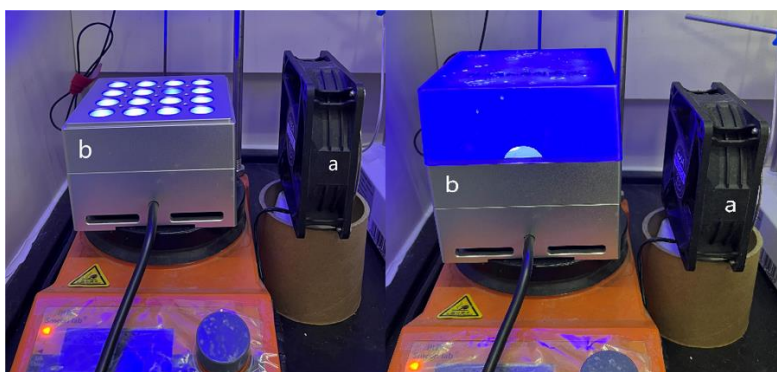


An oven-dried 4-mL vial equipped with a magnetic stirring bar was charged with the 1-diazonaphthalen-2(1*H*)-one **1** (0.1 mmol, 1.0 equiv), the alcohol **2** or aniline, and toluene (1.0 mL). The mixture was stirred at RT under the irradiation of 24 W blue LED for 12 h, and the reaction progress was monitored by TLC. Upon completion (12 h), the mixture was directly subjected to flash column chromatography on silica gel (eluent: hexanes/EtOAc = 10:1) to give the desired product **3**.

Note: For **3a–3e**, 20 equiv of alcohol was used; For **3f–3h** and **3j–3k**, 5 equiv of alcohol was used; For **3i**, 10 equiv of alcohol was used; For **3y**, 3.0 equiv of aniline was used; For **3z**, 3.0 equiv of phenol was used in anhydrous toluene.

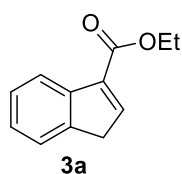
¹ A. Biswas, S. Pan and R. Samanta, *Org. Lett.*, 2022, **24**, 1631–1636.

The images of the photo-reactor in current study:



a: An additional fan was adopted to help cool the reaction mixture.

b: The photo reactor with a built-in fan (24 W output power with a peak power at 467.5 nm; beam angle: 45°; lumen: 130–140).



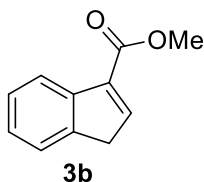
Ethyl 1H-indene-3-carboxylate (3a) was prepared as a light-yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 15.2 mg, 81% yield).

¹H NMR (300 MHz, CDCl₃) δ 7.97 (d, *J* = 7.6 Hz, 1H), 7.42 – 7.40 (m, 2H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.22 – 7.17 (m, 1H), 4.31 (q, *J* = 7.1 Hz, 2H), 3.45 (d, *J* = 1.7 Hz, 2H), 1.34 (t, *J* = 7.1 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 164.2, 144.4, 143.4, 140.8, 136.5, 126.7, 125.5, 123.8, 122.5, 60.5, 38.4, 14.4 ppm.

It's a known compound.²

² V. V. Kozhukhova, S. A. Kalyuzhnaya, Y. G. Yatluk and A. L. Suvorov, *Russ. J. Org. Chem.*, 2004, **40**, 773–774.

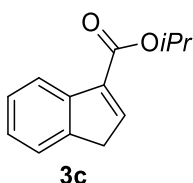


Methyl 1*H*-indene-3-carboxylate (3b) was prepared as a light-yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 12.2 mg, 70% yield).

¹H NMR (300 MHz, CDCl₃) δ 7.97 (d, *J* = 7.6 Hz, 1H), 7.42 – 7.39 (m, 2H), 7.31 – 7.17 (m, 2H), 3.84 (s, 3H), 3.46 (d, *J* = 1.9 Hz, 2H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 164.6, 144.6, 143.4, 140.7, 136.1, 126.7, 125.6, 123.8, 122.4, 51.6, 38.5 ppm.

It's a known compound.³



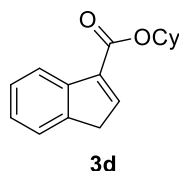
Isopropyl 1*H*-indene-3-carboxylate (3c) was prepared as a light-yellow oil according to the General Procedure 1 (eluent: hexanes/EtOAc = 10:1, 12.7 mg, 63% yield).

¹H NMR (300 MHz, CDCl₃) δ 7.97 (d, *J* = 7.6 Hz, 1H), 7.42 – 7.37 (m, 2H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.21 – 7.16 (m, 1H), 5.23 – 5.15 (m, 1H), 3.443 – 3.437 (m, 2H), 1.32 (d, *J* = 6.2 Hz, 6H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 163.8, 144.2, 143.5, 140.9, 136.9, 126.6, 125.5, 123.8, 122.5, 67.9, 38.3, 22.0 ppm.

HRMS (ESI+) Calcd for C₁₃H₁₅O₂ [M+H]⁺: 203.1072, found: 203.1076.

³ I. Honzíčková, J. Vinklárek, C. C. Romão, Z. Růžicková and Jan Honzíček, *New J. Chem.*, 2016, **40**, 245–256.

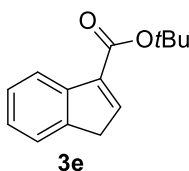


Cyclohexyl 1*H*-indene-3-carboxylate (3d) was prepared as a red oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 17.4 mg, 72% yield).

¹H NMR (300 MHz, CDCl₃) δ 7.97 (d, *J* = 7.6 Hz, 1H), 7.40 – 7.18 (m, 4H), 4.98 – 4.95 (m, 1H), 3.443 – 3.438 (m, 2H), 1.92 – 1.35 (m, 10H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 163.7, 144.2, 143.5, 140.9, 137.0, 126.6, 125.5, 123.8, 122.5, 72.8, 38.3, 31.7, 25.5, 23.8 ppm.

HRMS (ESI+) Calcd for C₁₆H₁₉O₂ [M+H]⁺: 243.1385, found: 243.1393.

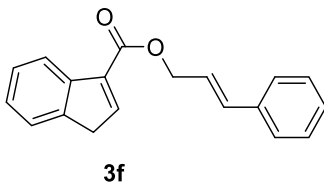


Tert-butyl 1*H*-indene-3-carboxylate (3e) was prepared as a light-yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 9.5 mg, 44% yield).

¹H NMR (300 MHz, CDCl₃) δ 7.94 (d, *J* = 7.6 Hz, 1H), 7.39 (d, *J* = 7.4 Hz, 1H), 7.33 – 7.25 (m, 2H), 7.20 – 7.15 (m, 1H), 3.42 (d, *J* = 1.8 Hz, 2H), 1.55 (s, 9H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 163.6, 143.8, 143.6, 141.0, 137.9, 126.6, 125.4, 123.8, 122.5, 81.0, 38.1, 28.3 ppm.

HRMS (ESI+) Calcd for C₁₄H₁₇O₂ [M+H]⁺: 217.1229, found: 217.1230.



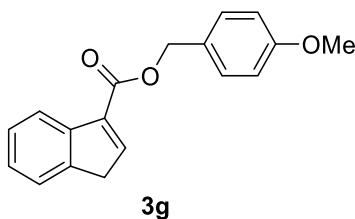
Cinnamyl 1*H*-indene-3-carboxylate (3f) was prepared as a light-yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 17.8 mg, 65% yield).

¹H NMR (300 MHz, CDCl₃) δ 8.08 (d, *J* = 7.6 Hz, 1H), 7.51 – 7.46 (m, 2H), 7.43 – 7.38

(m, 2H), 7.36 – 7.22 (m, 5H), 6.74 (d, J = 16 Hz, 1H), 6.46 – 6.36 (m, 1H), 4.98 – 4.96 (m, 2H), 3.52 (s, 2H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 163.9, 144.9, 143.4, 140.7, 136.3, 136.2, 134.3, 128.7, 128.2, 126.74, 126.72, 125.7, 123.9, 123.3, 122.5, 65.2, 38.5 ppm.

HRMS (ESI+) Calcd for $\text{C}_{19}\text{H}_{17}\text{O}_2$ $[\text{M}+\text{H}]^+$: 277.1229, found: 277.1226.

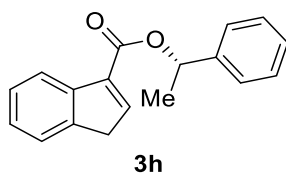


4-Methoxybenzyl 1H-indene-3-carboxylate (3g) was prepared as a pink solid according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 17.3 mg, 62% yield).

^1H NMR (300 MHz, CDCl_3) δ 7.96 (d, J = 7.6 Hz, 1H), 7.42 – 7.18 (m, 6H), 6.86 – 6.83 (m, 2H), 5.22 (s, 2H), 3.74 (s, 3H), 3.43 (d, J = 1.7 Hz, 2H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 164.0, 159.6, 144.8, 143.4, 140.7, 136.2, 130.1, 128.2, 126.7, 125.6, 123.8, 122.5, 114.0, 66.0, 55.3, 38.4 ppm.

HRMS (ESI+) Calcd for $\text{C}_{18}\text{H}_{17}\text{O}_3$ $[\text{M}+\text{H}]^+$: 281.1178, found: 281.1183.

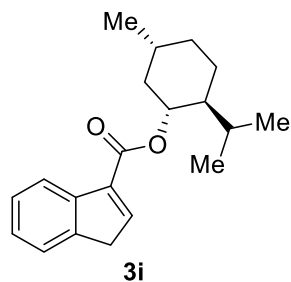


(S)-1-Phenylethyl 1H-indene-3-carboxylate (3h) was prepared as a light-yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 14.6 mg, 55% yield).

^1H NMR (300 MHz, CDCl_3) δ 8.06 (d, J = 7.6 Hz, 1H), 7.51 – 7.44 (m, 4H), 7.39 – 7.23 (m, 5H), 6.14 (q, J = 6.5 Hz, 1H), 3.51 (s, 2H), 1.69 (d, J = 6.6 Hz, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 163.4, 144.8, 143.5, 141.8, 140.8, 136.5, 128.6, 127.9, 126.7, 126.1, 125.6, 123.8, 122.5, 72.5, 38.4, 22.5 ppm.

HRMS (ESI+) Calcd for $\text{C}_{18}\text{H}_{17}\text{O}_2$ $[\text{M}+\text{H}]^+$: 265.1229, found: 265.1223.

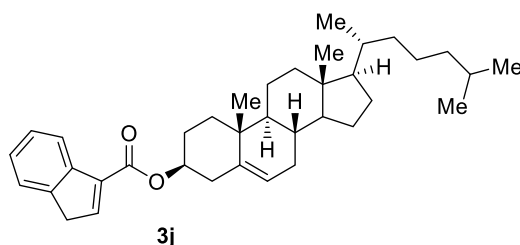


(1*R*,2*S*,5*R*)-2-iso-propyl-5-methylcyclohexyl 1*H*-indene-3-carboxylate (3i) was prepared as a light-yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 18.1 mg, 62% yield).

¹H NMR (300 MHz, CDCl₃) δ 7.97 (d, *J* = 7.3 Hz, 1H), 7.39 (s, 2H), 7.28 – 7.26 (m, 1H), 7.20 – 7.16 (m, 1H), 4.91 – 4.84 (m, 1H), 3.44 (s, 2H), 2.07 (d, *J* = 9.9 Hz, 1H), 1.93 – 1.92 (m, 1H), 1.68 – 1.64 (m, 2H), 1.52 – 1.49 (m, 3H), 1.11 – 1.04 (m, 2H), 0.87 – 0.85 (m, 6H), 0.75 – 0.71 (m, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 158.6, 139.0, 138.3, 135.8, 131.6, 121.4, 120.3, 118.6, 117.3, 69.1, 42.1, 35.9, 33.2, 29.1, 26.3, 21.3, 18.4, 16.9, 15.6, 11.3 ppm.

HRMS (ESI⁺) Calcd for C₂₀H₂₇O₂ [M+H]⁺: 299.2011, found: 299.2016.



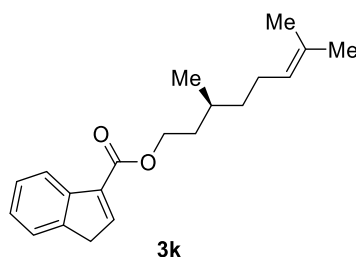
(3*S*,8*S*,9*S*,10*R*,13*R*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 1*H*-indene-3-carboxylate (3j) was prepared as a white solid according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 30.6 mg, 58% yield).

¹H NMR (300 MHz, CDCl₃) δ 7.97 (d, *J* = 7.5 Hz, 1H), 7.41 – 7.39 (m, 2H), 7.31 – 7.26 (t, *J* = 7.17 Hz, 1H), 7.21 – 7.16 (m, 1H), 5.36 (d, *J* = 4.3 Hz, 1H), 4.85 – 4.74 (m, 1H), 3.44 (d, *J* = 1.4 Hz, 2H), 2.42 (d, *J* = 7.8 Hz, 2H), 1.97 – 1.93 (m, 2H), 1.90 – 1.86 (m, 1H), 1.80 – 1.73 (m, 1H), 1.71 – 1.66 (m, 1H), 1.52 – 1.43 (m, 7H), 1.29 – 1.26 (m, 3H), 1.21 – 1.18 (m, 3H), 1.16 – 1.05 (m, 5H), 1.01 (s, 4H), 0.85 (d, *J* = 6.5 Hz, 3H), 0.81 – 0.76 (m, 8H), 0.62

(s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 158.5, 139.1, 138.3, 135.7, 134.5, 131.6, 121.4, 120.3, 118.6, 117.6, 117.3, 69.0, 51.5, 50.9, 44.9, 37.1, 34.6, 34.3, 33.2, 33.1, 31.9, 31.5, 31.0, 30.6, 26.8, 26.7, 23.1, 22.8, 22.78, 19.1, 18.7, 17.7, 17.4, 15.9, 14.2, 13.5, 6.7 ppm.

HRMS (ESI+) Calcd for $\text{C}_{37}\text{H}_{56}\text{NO}_2$ $[\text{M}+\text{NH}_4]^+$: 546.4311, found: 546.4304.

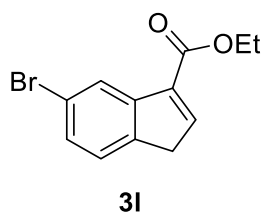


(S)-3,7-dimethyloct-6-en-1-yl 1H-indene-3-carboxylate (3k) was prepared as a light-yellow solid according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 21.2 mg, 71% yield).

^1H NMR (300 MHz, CDCl_3) δ 7.97 (d, J = 7.6 Hz, 1H), 7.42 – 7.38 (m, 2H), 7.28 (t, J = 7.6 Hz, 1H), 7.21 – 7.16 (m, 1H), 5.05 – 5.01 (m, 1H), 4.35 – 4.22 (m, 2H), 3.45 – 3.44 (m, 2H), 1.99 – 1.89 (m, 2H), 1.80 – 1.71 (m, 1H), 1.62 – 1.53 (m, 8H), 0.90 (d, J = 6.4 Hz, 3H), 0.80 – 0.76 (m, 2H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 159.1, 139.2, 138.2, 135.6, 131.3, 126.2, 121.5, 120.3, 119.4, 118.6, 117.3, 57.9, 33.2, 31.8, 30.4, 24.4, 20.5, 20.2, 14.3, 12.5 ppm.

HRMS (ESI+) Calcd for $\text{C}_{20}\text{H}_{27}\text{O}_2$ $[\text{M}+\text{H}]^+$: 299.2011, found: 299.2006.



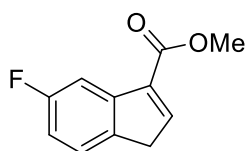
Ethyl 5-bromo-1H-indene-3-carboxylate (3l) was prepared as a light-yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 16.6 mg, 62% yield).

^1H NMR (400 MHz, CDCl_3) δ 8.19 (d, J = 1.8 Hz, 1H), 7.47 (t, J = 1.8 Hz, 1H), 7.38 – 7.36 (m, 1H), 7.32 – 7.30 (m, 1H), 4.37 (q, J = 7.1 Hz, 2H), 3.47 (d, J = 1.4 Hz, 2H), 1.42 (t, J =

7.1 Hz, 3H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 163.7, 145.6, 142.8, 142.1, 135.7, 128.4, 125.7, 125.1, 120.6, 60.7, 38.2, 14.4 ppm.

HRMS (ESI+) Calcd for $\text{C}_{12}\text{H}_{12}\text{BrO}_2$ $[\text{M}+\text{H}]^+$: 267.0021, found: 267.0026.



3m

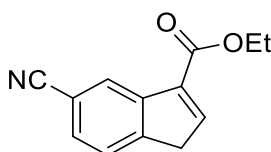
Methyl 5-fluoro-1H-indene-3-carboxylate (3m) was prepared as a yellow solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 12.5 mg, 65% yield).

^1H NMR (300 MHz, CDCl_3) δ 7.68 – 7.64 (m, 1H), 7.45 (s, 1H), 7.32 – 7.28 (m, 1H), 6.91 – 6.85 (m, 1H), 3.83 (s, 3H), 3.42 (s, 2H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 163.1, 161.3 (d, $^1J_{\text{C-F}} = 240$ Hz), 145.5, 141.4 (d, $^3J_{\text{C-F}} = 10$ Hz), 137.5 (d, $^4J_{\text{C-F}} = 3$ Hz), 134.6 (d, $^4J_{\text{C-F}} = 3$ Hz), 123.4 (d, $^3J_{\text{C-F}} = 9$ Hz), 111.5 (d, $^2J_{\text{C-F}} = 23$ Hz), 108.7 (d, $^2J_{\text{C-F}} = 25$ Hz), 50.7, 36.9 ppm.

^{19}F NMR (375 MHz, CDCl_3) δ -116.4 ppm.

HRMS (ESI+) Calcd for $\text{C}_{11}\text{H}_{10}\text{FO}_2$ $[\text{M}+\text{H}]^+$: 193.0665, found: 193.0659.



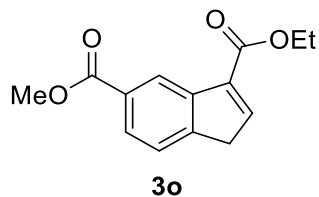
3n

Ethyl 5-cyano-1H-indene-3-carboxylate (3n) was prepared as a yellow solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 11 mg, 49% yield).

^1H NMR (400 MHz, CDCl_3) δ 8.33 (s, 1H), 7.58 – 7.56 (m, 3H), 4.40 (q, $J = 7.2$ Hz, 2H), 3.62 (d, $J = 1.4$ Hz, 2H), 1.43 (t, $J = 7.2$ Hz, 3H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 163.3, 148.2, 146.0, 141.6, 135.5, 129.5, 126.2, 124.5, 119.5, 110.7, 60.9, 38.9, 14.3 ppm.

HRMS (ESI+) Calcd for C₁₃H₁₂NO₂ [M+H]⁺: 214.0868, found: 214.0859.

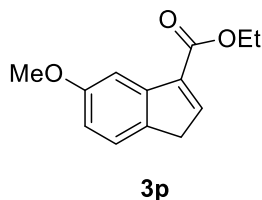


3-Ethyl 5-methyl 1H-indene-3,5-dicarboxylate (3o) was prepared as a white solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 13 mg, 53% yield).

¹H NMR (300 MHz, CDCl₃) δ 8.68 (s, 1H), 7.98 (d, *J* = 7.8 Hz, 1H), 7.53 – 7.50 (m, 2H), 4.40 (q, *J* = 7.1 Hz, 2H), 3.94 (s, 3H), 3.57 (s, 2H), 1.43 (t, *J* = 7.1 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 167.5, 163.8, 148.4, 145.0, 141.1, 136.1, 128.9, 127.2, 123.7, 123.6, 60.7, 52.1, 38.5, 14.3 ppm.

HRMS (ESI+) Calcd for C₁₄H₁₅O₄ [M+H]⁺: 247.0970, found: 247.0963.

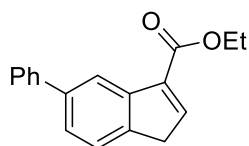


Ethyl 5-methoxy-1H-indene-3-carboxylate (3p) was prepared as a light-yellow solid according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 18.2 mg, 83% yield).

¹H NMR (300 MHz, CDCl₃) δ 7.65 – 7.64 (m, 1H), 7.48 (s, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 6.84 – 6.81 (m, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 3.86 (s, 3H), 3.45 (s, 2H), 1.41 (t, *J* = 7.1 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 164.2, 159.0, 145.8, 142.2, 136.1, 135.5, 124.2, 112.4, 107.4, 60.5, 55.5, 37.8, 14.4 ppm.

HRMS (ESI+) Calcd for C₁₃H₁₅O₃ [M+H]⁺: 219.1021, found: 219.1012.



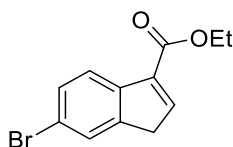
3q

Ethyl 5-phenyl-1H-indene-3-carboxylate (3q) was prepared as a colorless oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 23.5 mg, 87% yield).

¹H NMR (300 MHz, CDCl₃) δ 8.31 (s, 1H), 7.68 – 7.65 (m, 2H), 7.55 – 7.50 (m, 3H), 7.49 – 7.42 (m, 2H), 7.37 – 7.32 (m, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.56 (d, *J* = 1.8 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 164.2, 144.9, 142.5, 141.7, 141.5, 140.0, 136.4, 128.7, 127.4, 127.1, 124.8, 124.0, 121.3, 60.6, 38.2, 14.4 ppm.

HRMS (ESI+) Calcd for C₁₈H₁₇O₂ [M+H]⁺: 265.1229, found: 265.1221.



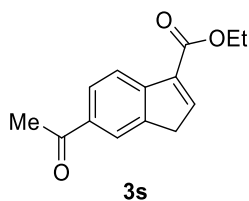
3r

Ethyl 6-bromo-1H-indene-3-carboxylate (3r) was prepared as a light-yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 21 mg, 79% yield).

¹H NMR (300 MHz, CDCl₃) δ 7.90 (d, *J* = 8.2 Hz, 1H), 7.60 (s, 1H), 7.49 – 7.43 (m, 2H), 4.37 (q, *J* = 7.1 Hz, 2H), 3.50 (s, 2H), 1.40 (t, *J* = 7.1 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 163.8, 145.4, 144.4, 139.8, 135.9, 129.8, 127.1, 123.8, 119.9, 60.7, 38.2, 14.4 ppm.

HRMS (ESI+) Calcd for C₁₂H₁₂BrO₂ [M+H]⁺: 267.0021, found: 269.0007.

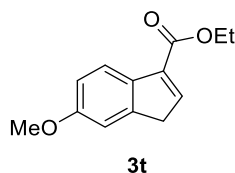


Ethyl 6-acetyl-1H-indene-3-carboxylate (3s) was prepared as a white solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 21 mg, 69% yield).

¹H NMR (300 MHz, CDCl₃) δ 8.12 – 8.07 (m, 2H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.63 (s, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.59 (s, 2H), 2.64 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 198.2, 163.7, 147.8, 145.5, 143.5, 136.2, 134.6, 127.7, 123.4, 122.3, 60.7, 38.6, 26.8, 14.3 ppm.

HRMS (ESI+) Calcd for C₁₄H₁₅O₃ [M+H]⁺: 231.1021, found: 231.1014.

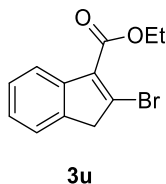


Ethyl 6-methoxy-1H-indene-3-carboxylate (3t) was prepared as a white solid according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 16.5 mg, 75% yield).

¹H NMR (300 MHz, CDCl₃) δ 7.92 (d, *J* = 8.5 Hz, 1H), 7.32 (t, *J* = 2.0 Hz, 1H), 7.05 (s, 1H), 6.93 – 6.89 (m, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 3.84 (s, 3H), 3.48 (d, *J* = 1.3 Hz, 2H), 1.40 (t, *J* = 7.1 Hz, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 164.3, 158.4, 145.3, 142.1, 136.1, 133.9, 122.9, 112.3, 110.1, 60.4, 55.5, 38.3, 14.4 ppm.

HRMS (ESI+) Calcd for C₁₃H₁₅O₃ [M+H]⁺: 219.1021, found: 219.1014.



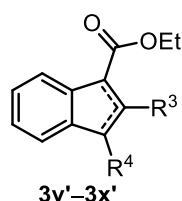
Ethyl 2-bromo-1H-indene-3-carboxylate (3u) was prepared as a white solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 15 mg, 56% yield).

¹H NMR (300 MHz, CD₂Cl₂) δ 7.77 (d, *J* = 7.4 Hz, 1H), 7.31 (d, *J* = 7.3 Hz, 1H), 7.25 – 7.13 (m, 2H), 4.32 (q, *J* = 7.1 Hz, 2H), 3.70 (s, 2H), 1.35 (t, *J* = 7.1 Hz, 3H) ppm.

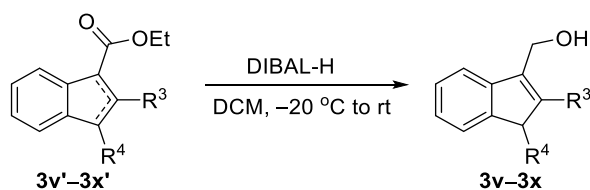
¹³C NMR (75 MHz, CD₂Cl₂) δ 163.0, 141.5, 140.9, 133.8, 133.5, 126.9, 125.6, 123.2, 121.8, 60.9, 47.3, 14.1 ppm.

It's a known compound and not very stable.⁴

General Procedure B.

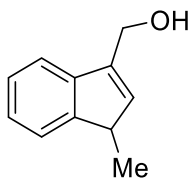


Note: In initial synthesis, 3v'-3x' were obtained as a mixture of isomers, thus the ester groups in the corresponding products was reduced by DIBAL-H to get cleaner NMR spectra.



To a solution of 3v'-3x' (0.2 mmol) in anhydrous DCM (2.0 mL), DIBAL-H (for 3v'-3x': 2.0 equiv, for 3x': 4.0 equiv, 1.0 M in *n*-hexane) was added dropwise under a nitrogen atmosphere at -20 °C and then the resulting reaction mixture was slowly warmed to room temperature and stirred for additional 2 h at the same temperature. After completion, the reaction was quenched with HCl (1M) solution at 0 °C and the mixture was extracted with DCM (3 × 30 mL). The combined organic phases were washed with brine, dried over Na₂SO₄, and concentrated in vacuo, the mixture was directly subjected to flash column chromatography on silica gel (eluent: hexanes/ethyl acetate = 5:1) to give the desired product 3v-3x.

⁴ C. Yu, X. Ma, B. Chen, B. Tang, R. S. Paton and G. Zhang, *Eur. J. Org. Chem.*, 2017, **11**, 1561–1565.



3v

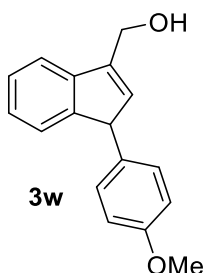
(1-Methyl-1H-inden-3-yl) methanol (3v) was prepared as a light-yellow oil according to the General Procedure B (eluent: hexanes/EtOAc = 5:1, 17.6 mg, 46% yield).

For the major isomer:

¹H NMR (400 MHz, CDCl₃) δ 7.39 (d, *J* = 7.3 Hz, 1H), 7.24 – 7.21 (m, 2H), 7.15 – 7.12 (m, 1H), 6.11 (s, 1H), 3.81 – 3.77 (m, 1H), 3.72 – 3.68 (m, 1H), 3.53 – 3.50 (m, 1H), 2.08 – 2.07 (s, 3H), 1.71 (s, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 146.2, 145.0, 141.1, 130.7, 127.0, 125.0, 123.2, 119.2, 63.9, 51.9, 13.1, ppm.

HRMS (ESI+) Calcd for C₁₁H₁₃O [M+H]⁺: 161.0966, found: 161.0965.



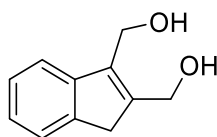
3w

(1-(4-Methoxyphenyl)-1H-inden-3-yl) methanol (3w) was prepared as a yellow solid according to the General Procedure B (eluent: hexanes/EtOAc = 5:1, 45 mg, 89% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.57 – 7.53 (m, 4H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.25 (t, *J* = 7.4 Hz, 1H), 6.98 (d, *J* = 8.7 Hz, 2H), 6.51 (d, *J* = 1.96 Hz, 1H), 3.98 – 3.97 (m, 1H), 3.89 – 3.86 (m, 1H), 3.84 (s, 3H), 3.77 – 3.74 (m, 1H), 1.75 (s, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 159.4, 145.5, 145.3, 144.2, 131.6, 128.9, 128.2, 127.1, 125.3, 123.7, 120.7, 114.1, 64.1, 55.4, 52.2 ppm.

HRMS (ESI+) Calcd for C₁₇H₁₇O₂ [M+H]⁺: 253.1229, found: 253.1227.



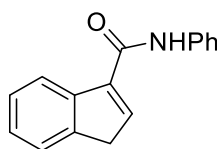
3x

(1*H*-Indene-2,3-diyl) dimethanol (3x) was prepared as a yellow solid according to the General Procedure B (eluent: hexanes/EtOAc = 5:1, 11.1 mg, 32% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.23 – 7.13 (m, 4H), 7.08 – 7.04 (m, 1H), 6.58 (s, 1H), 4.43 – 4.33 (m, 3H), 4.05 – 4.01 (m, 1H), 3.50 – 3.46 (m, 1H), 3.39 – 3.34 (m, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 150.0, 143.9, 143.7, 130.2, 127.3, 125.2, 123.2, 121.3, 63.7, 60.7, 53.9 ppm.

HRMS (ESI+) Calcd for C₁₁H₁₂NaO₂ [M+Na]⁺: 199.0735, found: 199.0732.



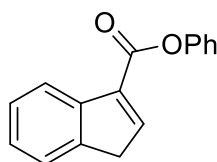
3y

N-phenyl-1*H*-indene-3-carboxamide (3y) was prepared as a white solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 39 mg, 83% yield).

¹H NMR (400 MHz, DMSO) δ 10.21 (s, 1H), 7.95 (d, *J* = 8.72 Hz, 1H), 7.79 (d, *J* = 7.64 Hz, 2H), 7.54 (d, *J* = 7.32 Hz, 1H), 7.42 – 7.41 (m, 1H), 7.38 – 7.32 (m, 3H), 7.28 – 7.24 (m, 1H), 7.10 (t, *J* = 7.36 Hz, 1H), 3.63 (d, *J* = 1.16 Hz, 2H) ppm.

¹³C NMR (100 MHz, DMSO) δ 163.4, 143.9, 142.1, 139.5, 139.4, 139.0, 129.1, 126.7, 125.7, 124.4, 124.0, 122.4, 120.6, 38.6 ppm.

It's a known compound.³



3z

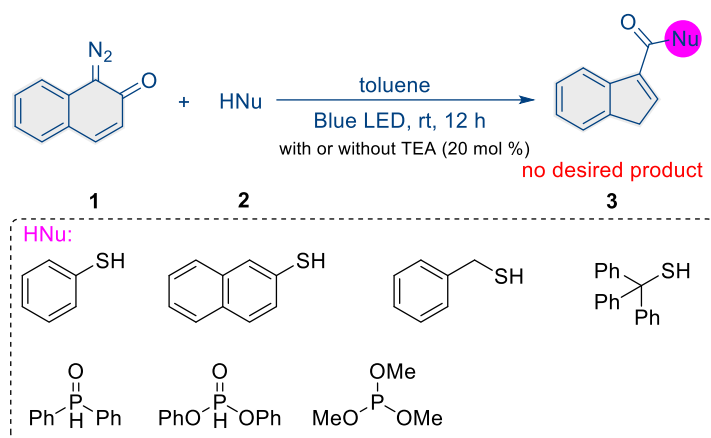
Phenyl 1*H*-indene-3-carboxylate (3z) was prepared as a white solid according to the General Procedure A (eluent: hexanes/EtOAc = 10:1, 13 mg, 55% yield).

^1H NMR (300 MHz, CDCl_3) δ 8.11 (d, $J = 7.6$ Hz 1H), 7.69 (s, 1H), 7.51 (d, $J = 7.6$ Hz, 1H), 7.46 – 7.35 (m, 3H), 7.32 – 7.21 (m, 4H), 3.61 (s, 2H) ppm.

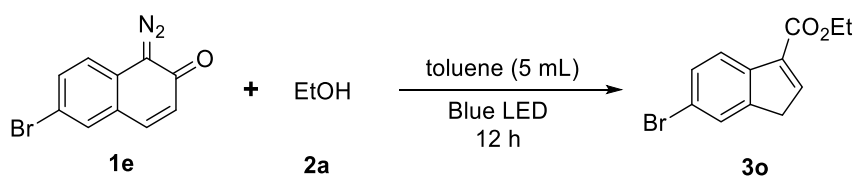
^{13}C NMR (75 MHz, CDCl_3) δ 162.3, 150.6, 146.3, 143.3, 140.5, 135.7, 129.6, 126.9, 126.0, 125.9, 123.9, 122.5, 121.8, 38.8 ppm.

HRMS (ESI+) Calcd for $\text{C}_{16}\text{H}_{13}\text{O}_2$ $[\text{M}+\text{H}]^+$: 237.0916, found: 237.0907.

IV. Unsuccessful Nucleophiles

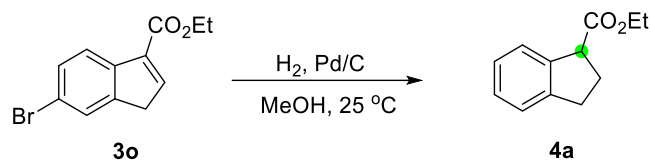


V. The Procedure for Synthetic Transformation

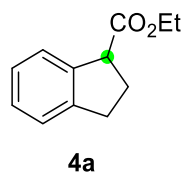


An oven-dried test tube equipped with a magnetic stirring bar was charged with the **1e** (4.42 mmol, 1.1 g), **2a** (20 equiv, 5.2 mL), and toluene (5 mL). The mixture was stirred at 25 °C under the irradiation of Blue LED for 12 h, and the reaction progress was monitored by TLC. Upon completion (12 h), the mixture was directly subjected to flash column chromatography on silica gel (eluent: hexanes/ethyl acetate = 10:1) to give the desired product **3o**.

General Procedure C.



In a nitrogen atmosphere of glovebox, an oven-dried test tube equipped with a magnetic stirring bar was charged with **3o** (0.2 mmol, 54 mg), Pd/C (5%, 10 mg, 10 % on carbon), and anhydrous MeOH (2.0 mL). Then, the reaction mixture was removed from glovebox and then attached with a H₂ balloon. The resulting suspension was stirred at room temperature for 4 h. Upon completion (monitored by TLC), the reaction mixture was filtered through a short plug of celite, and the filter cake was washed with DMC (10 mL). The combined filtrates were concentrated under reduced pressure to get the crude product. The desired product **4a** was obtained after purification on silica gel flash column chromatography (eluent: hexanes/ethyl acetate = 10:1).



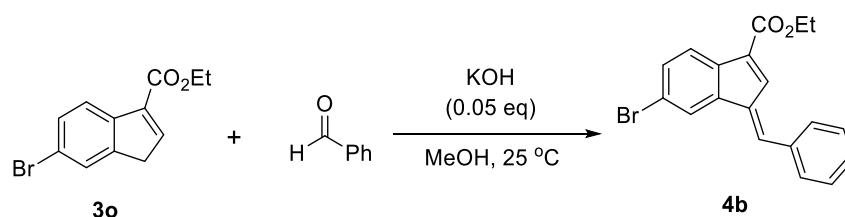
Ethyl 2,3-dihydro-1*H*-indene-1-carboxylate (**4a**, **racemic**) was prepared as a colorless oil according to the General Procedure C (eluent: hexanes/EtOAc = 10:1, 34 mg, 89% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.39 – 7.37 (m, 1H), 7.25 – 7.15 (m, 3H), 4.22 – 4.16 (m, 2H), 4.04 (t, *J* = 7.2 Hz, 1H), 3.14 – 3.06 (m, 1H), 2.95 – 2.87 (m, 1H), 2.49 – 2.28 (m, 2H), 1.28 (t, *J* = 7.1 Hz, 3H) ppm.

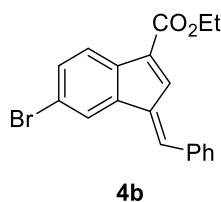
¹³C NMR (100 MHz, CDCl₃) δ 173.9, 144.1, 140.9, 127.5, 126.4, 124.7, 124.69, 60.8, 50.2, 31.8, 28.7, 14.3 ppm.

HRMS (ESI+) Calcd for C₁₂H₁₅O₂ [M+H]⁺: 191.1072, found: 191.1068.

General Procedure D



The aldehyde (1.1 equiv) was added to a solution of **3o** (0.2 mmol, 54 mg, 1.0 equiv) in MeOH (2.0 mL). Under vigorously stirring, KOH (0.01 mmol, 0.6 mg, 5 mol %) was added to the resulted solution. The reaction was smoothly proceeded, and the yellow product **4b** was precipitated immediately under the bottom of the vial. Upon completion (10 min, monitored by TLC), the mixture was directly subjected to flash column chromatography on silica gel (eluent: hexanes/ethyl acetate = 10:1) to give the desired product **4b**.

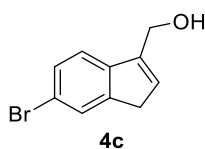


Ethyl (E)-1-benzylidene-6-bromo-1H-indene-3-carboxylate (4b) was prepared as a yellow solid according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 47.6 mg, 65% yield, *E/Z* >100:1 by crude ^1H NMR).

^1H NMR (300 MHz, CDCl_3) δ 7.84 – 7.89 (m, 2H), 7.73 (s, 1H), 7.67 (s, 1H), 7.62 (d, *J* = 7.2 Hz, 2H), 7.49 – 7.42 (m, 4H), 4.38 (q, *J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ 164.5, 139.3, 137.2, 136.9, 135.9, 135.8, 135.6, 133.6, 130.7, 130.6, 129.9, 129.1, 123.7, 122.5, 120.1, 60.8, 14.4 ppm.

HRMS (ESI+) Calcd for $\text{C}_{11}\text{H}_{13}\text{O}_2$ [$\text{M}+\text{H}$] $^+$: 355.0334, found: 355.0325.

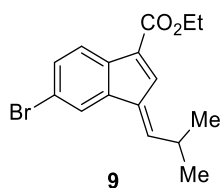


(6-Bromo-1H-inden-3-yl) methanol (4c) was prepared as a yellow solid according to the General Procedure B (eluent: hexanes/EtOAc = 5:1, 55 mg, 49% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.57 (s, 1H), 7.42 – 7.39 (m, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 6.42 (s, 1H), 4.65 (d, *J* = 1.4 Hz, 2H), 3.33 (d, *J* = 1.3 Hz, 2H), 1.93 (s, 1H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 146.6, 143.5, 142.3, 129.9, 129.3, 127.2, 120.7, 119.2, 59.6, 37.7 ppm.

HRMS (ESI+) Calcd for C₁₀H₁₀BrO [M+H]⁺: 224.9915, found: 226.9897.

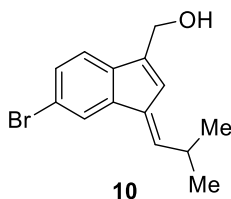


Ethyl (E)-6-bromo-1-(2-methylpropylidene)-1H-indene-3-carboxylate (9) was prepared as a yellow oil according to the General Procedure D (eluent: hexanes/EtOAc = 10:1, 45 mg, 70% yield, *E/Z* = 5:1 based on the crude ¹H NMR).

¹H NMR (400 MHz, CDCl₃) δ 7.82 (d, *J* = 8.2 Hz, 1H), 7.71 (d, *J* = 1.7 Hz, 1H), 7.58 (s, 1H), 7.43 – 7.41 (m, 1H), 6.73 (d, *J* = 10.2 Hz, 1H), 4.40 – 4.35 (m, 2H), 3.16 – 3.11 (m, 1H), 1.41 (t, *J* = 7.12 Hz, 3H), 1.19 (d, *J* = 6.64 Hz, 6H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 164.5, 147.5, 138.5, 137.7, 135.8, 133.5, 132.8, 130.2, 123.5, 122.4, 119.9, 60.7, 30.3, 23.0, 14.4 ppm.

HRMS (ESI+) Calcd for C₁₆H₁₈BrO₂ [M+H]⁺: 321.0490, found: 321.0485.



(E)-6-bromo-1-(2-methylpropylidene)-1H-inden-3-ylmethanol (10) was prepared as a yellow oil according to the General Procedure B (eluent: hexanes/EtOAc = 10:1, 130 mg, 81% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.68 (d, *J* = 1.7 Hz, 1H), 7.36 – 7.33 (m, 1H), 7.16 (d, *J* = 8.0 Hz, 1H), 6.73 (s, 1H), 6.41 (d, *J* = 10.0 Hz, 1H), 4.72 (s, 2H), 3.06 – 2.97 (m, 1H), 1.91 (s, 1H), 1.15 (d, *J* = 6.6 Hz, 6H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 146.7, 143.7, 140.6, 139.6, 136.2, 129.5, 122.5, 121.5, 120.3, 119.4, 59.7, 29.8, 23.2 ppm.

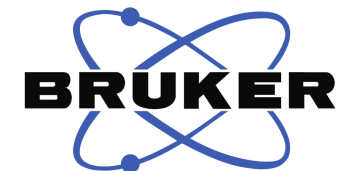
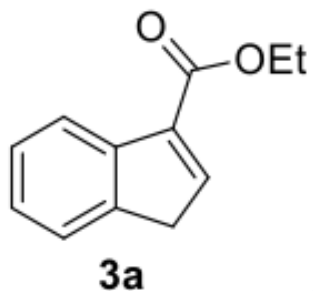
It's a known compound.⁵

⁵ J. Jo, M. Jeong, J.-S. Ahn, J. Akter, H.-S. Kim, Y.-G. Suh and H. Yun, *J. Org. Chem.*, 2019, **84**, 10953–10961.

7.987
7.962
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7.403
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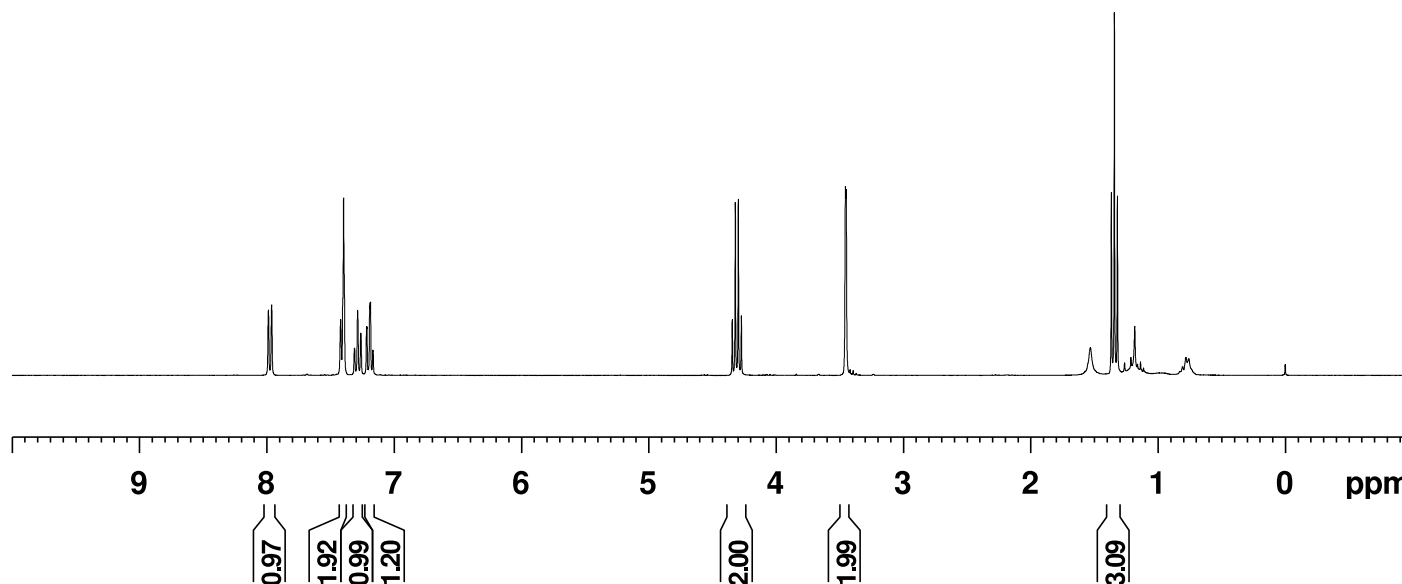


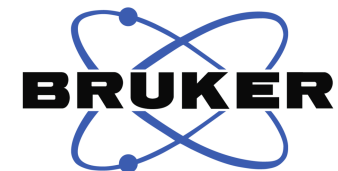
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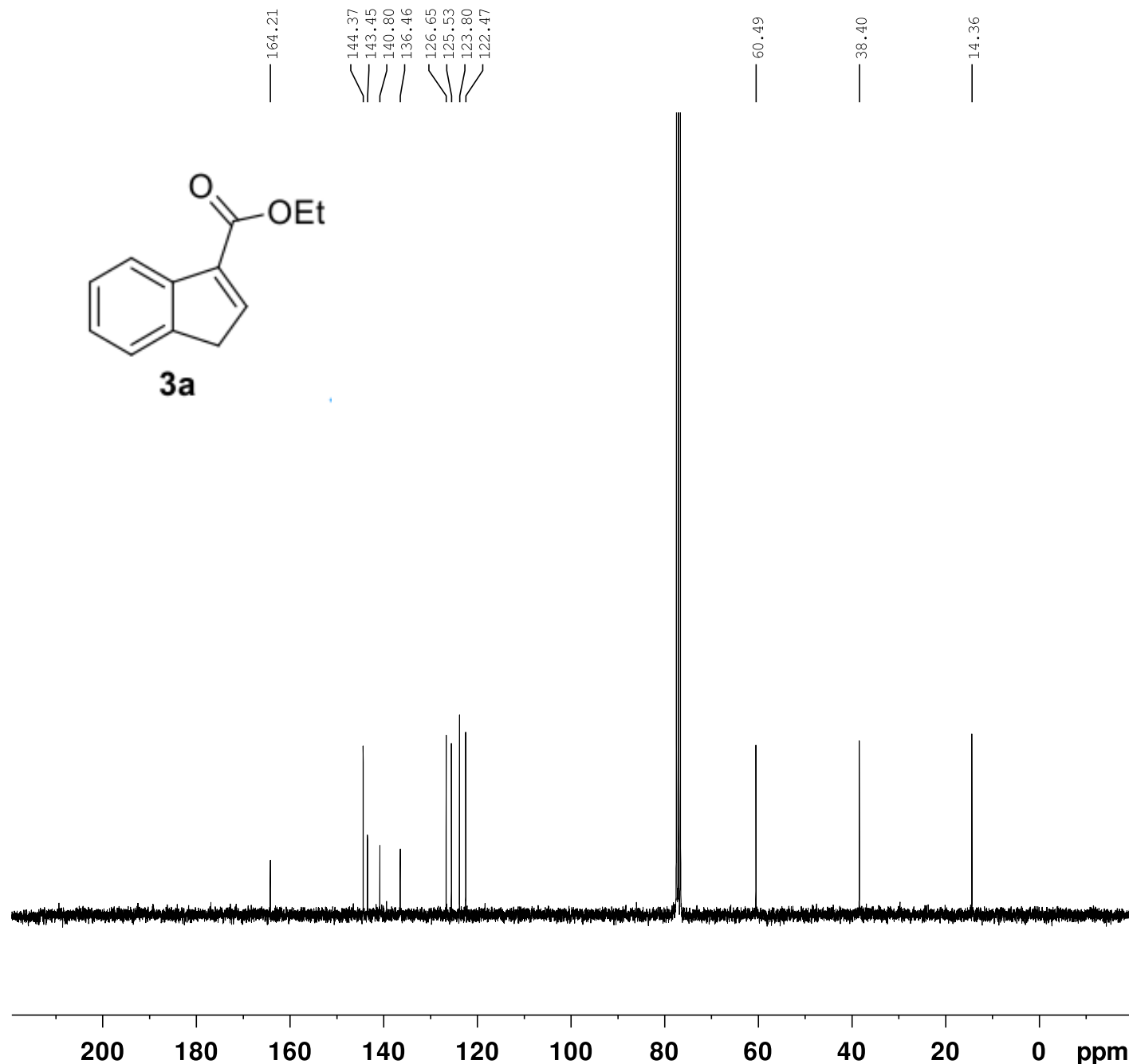
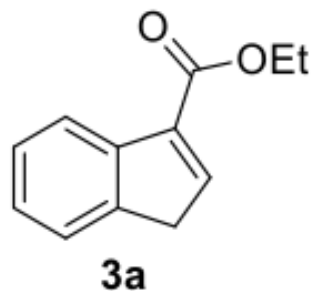
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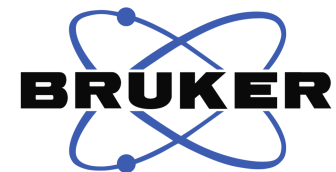
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GB 0
PC 1.40



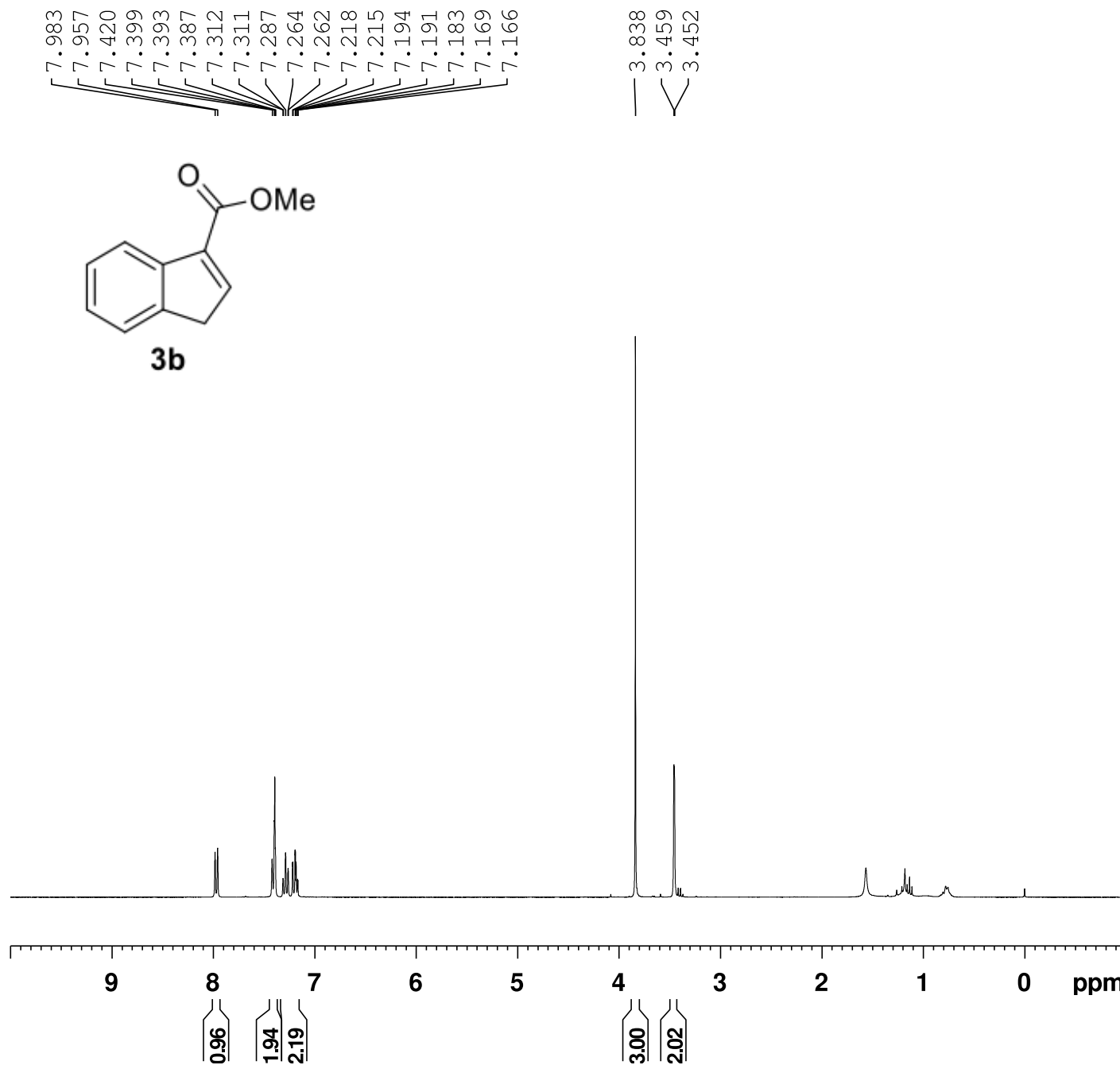


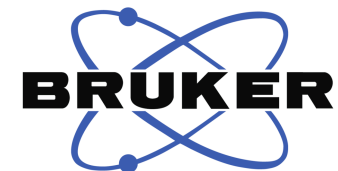
Current Data Parameters
 NAME HNMR-YX-1-p40 (B1)
 EXPNO 368
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220707
 Time 16.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.091699 Hz
 AQ 5.4525952 sec
 RG 181
 DW 83.200 usec
 DE 6.50 usec
 TE -59.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1318534 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 14.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1300302 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





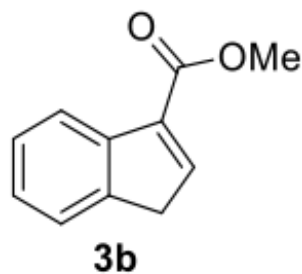
Current Data Parameters
NAME CNMR-YX-1-p40 (B1)
EXPNO 384
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220708
Time 21.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

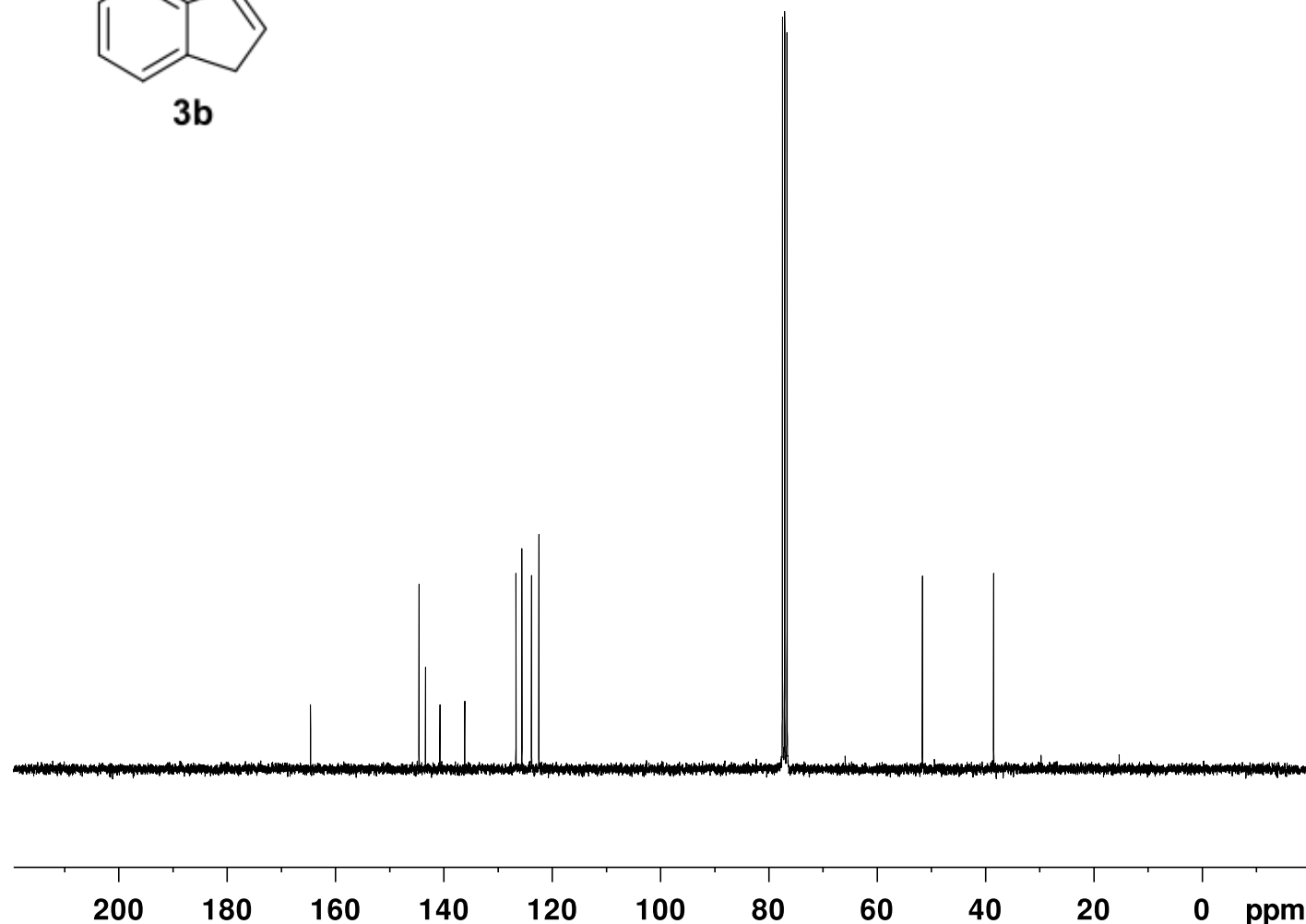
===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

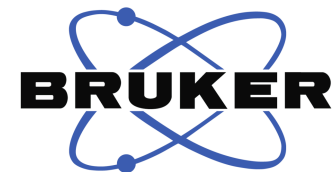
F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



164.60
144.57
143.37
140.71
136.14
126.68
125.59
123.81
122.44

51.62
38.47





Current Data Parameters
 NAME HNMR-YX-1-p40 (B3)
 EXPNO 367
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220707
 Time 16.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.091699 Hz
 AQ 5.4525952 sec
 RG 203
 DW 83.200 usec
 DE 6.50 usec
 TE -59.1 K
 D1 1.00000000 sec
 TD0 1

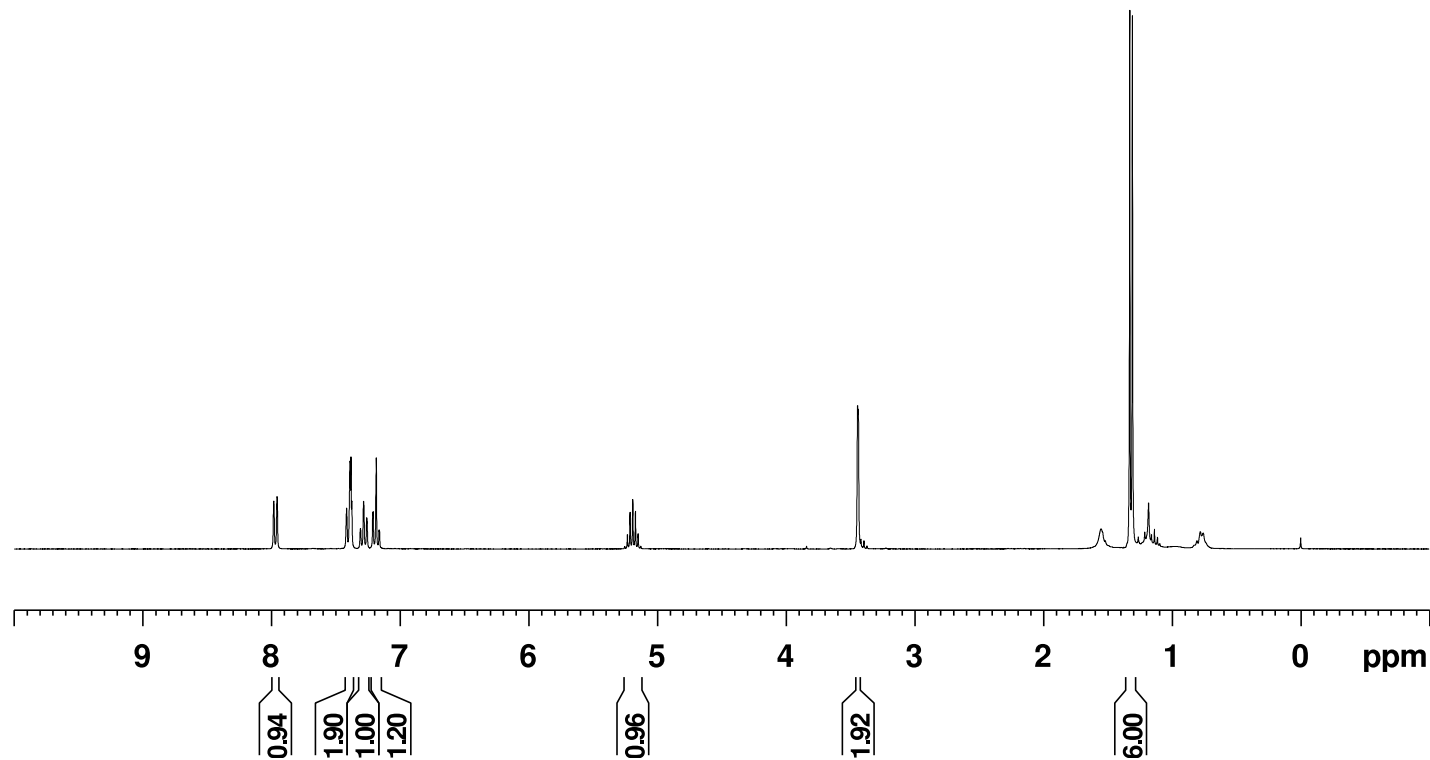
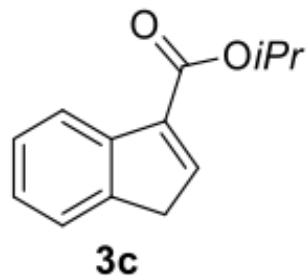
===== CHANNEL f1 =====
 SFO1 300.1318534 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 14.00000000 W

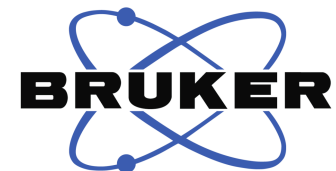
F2 - Processing parameters
 SI 65536
 SF 300.1300296 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7.981
7.956
7.415
7.388
7.381
7.375
7.307
7.284
7.259
7.212
7.209
7.184
7.163
7.159
5.233
5.212
5.191
5.170
5.149

3.444
3.438

1.329
1.308





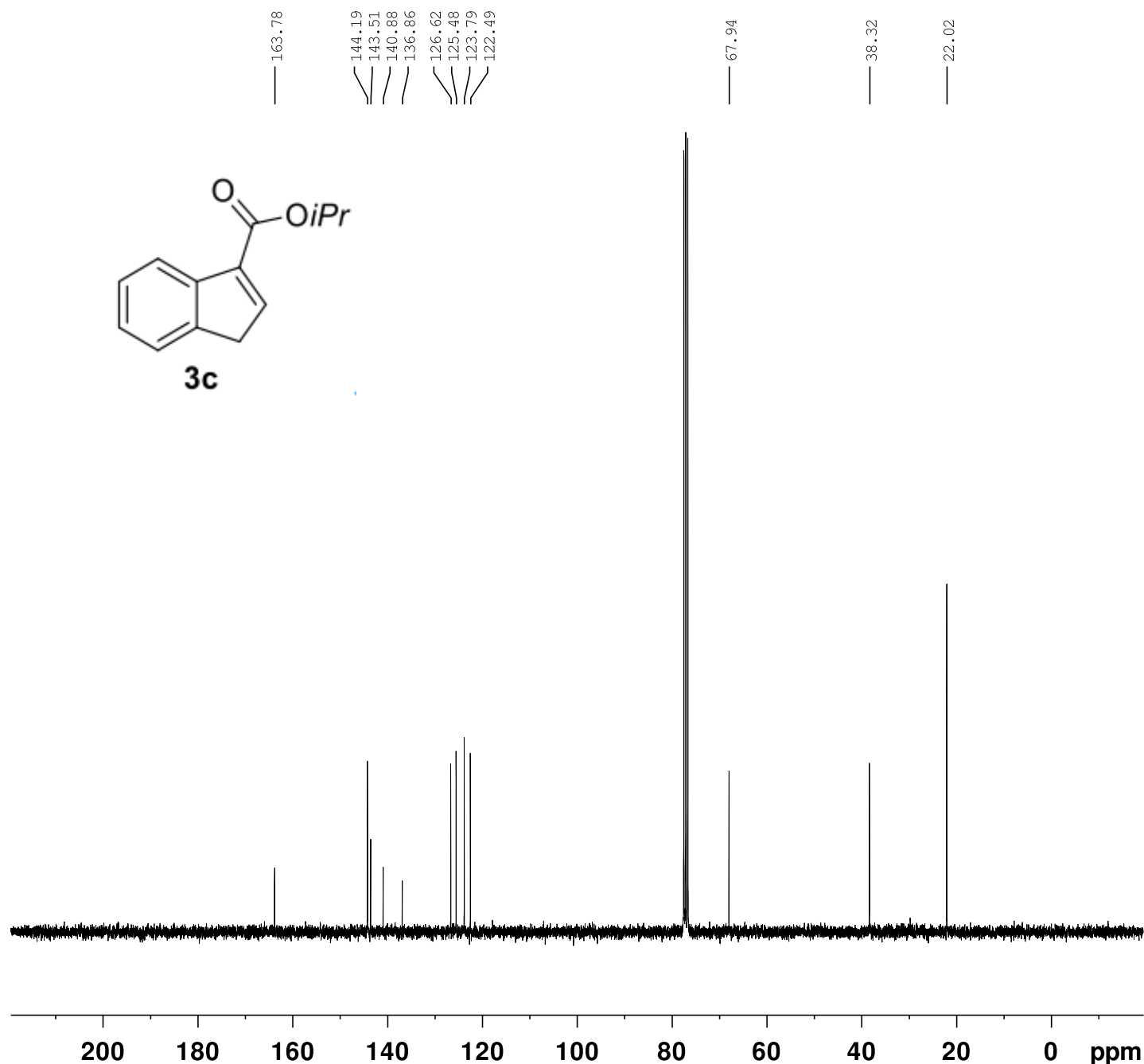
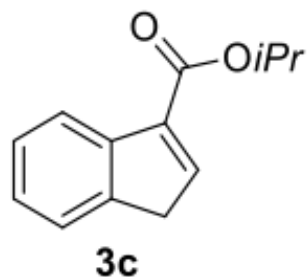
Current Data Parameters
NAME CNMR-YX-1-p40 (B3)
EXPNO 383
PROCNO 1

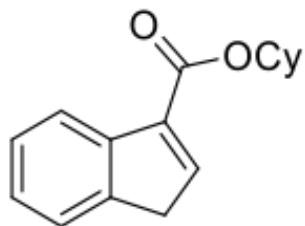
F2 - Acquisition Parameters
Date_ 20220708
Time 21.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

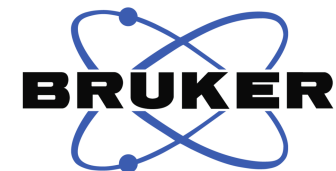




3d

7.986
7.960
7.398
7.392
7.283
7.181

4.977
4.964
4.950
3.443
3.438
1.916
1.908
1.889
1.879
1.752
1.742
1.720
1.710
1.593
1.582
1.551
1.519
1.507
1.488
1.479
1.447
1.437
1.415
1.404
1.394

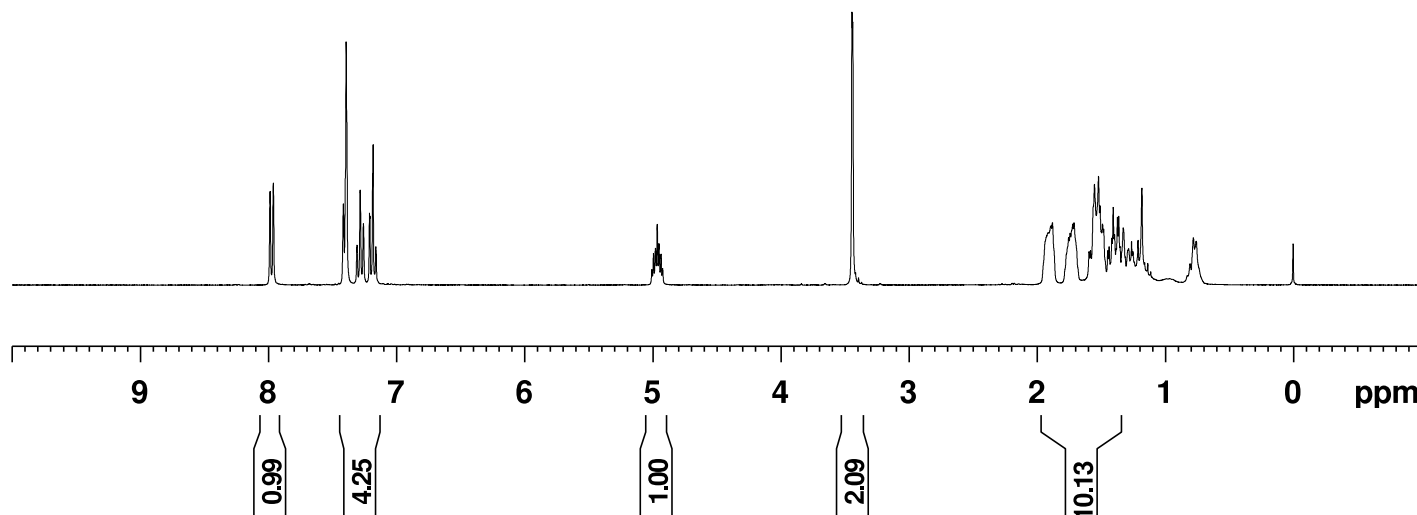


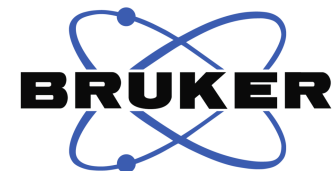
Current Data Parameters
NAME HNMR-YX-1-p40 (B6)
EXPNO 200
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220629
Time 10.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300309 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





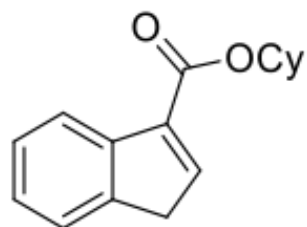
Current Data Parameters
 NAME CNMR-YX-1-p40 (B6)
 EXPNO 201
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220629
 Time 10.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 300
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175317 sec
 RG 203
 DW 27.733 usec
 DE 6.50 usec
 TE -59.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

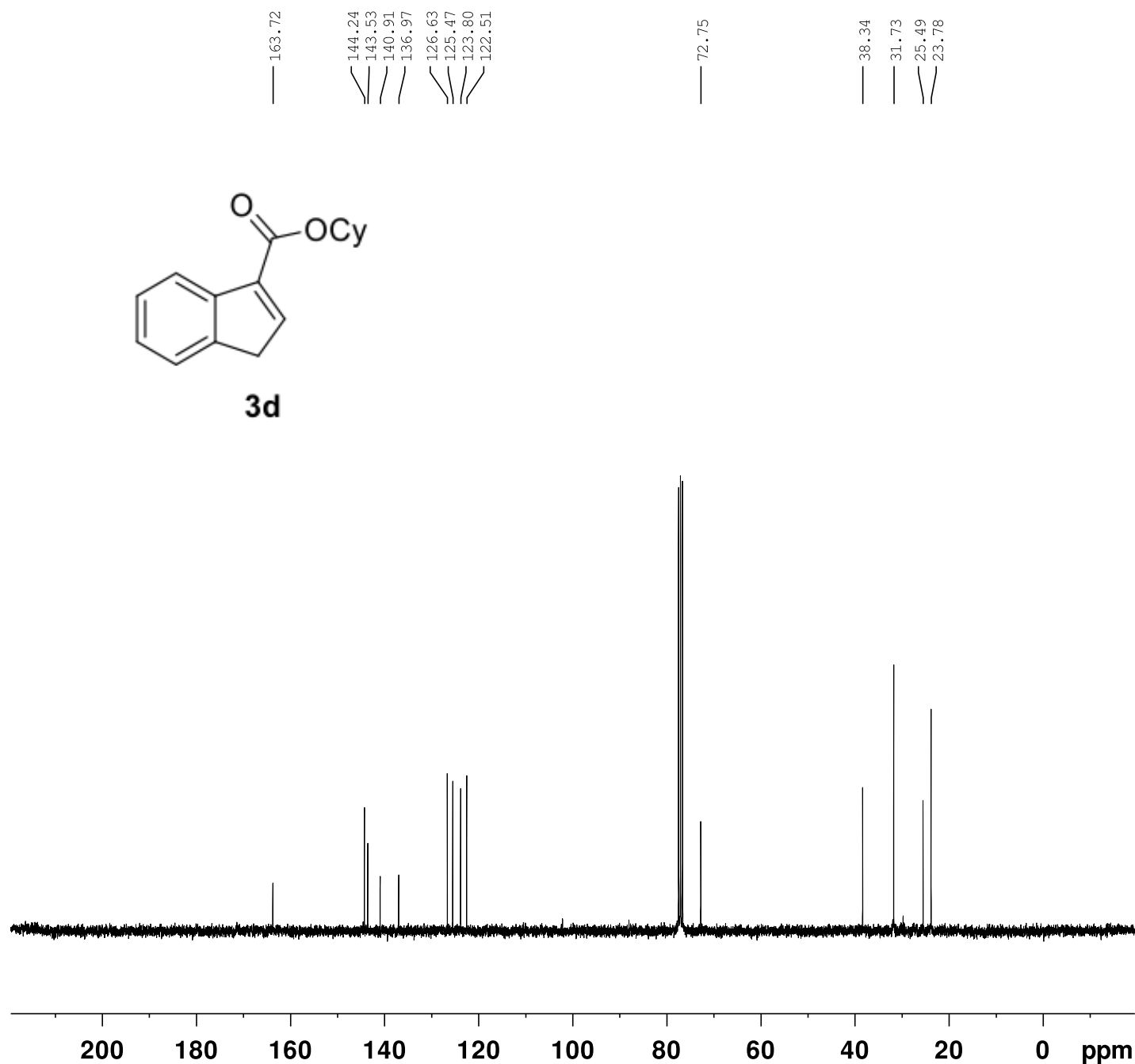
===== CHANNEL f1 =====
 SFO1 75.4752949 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 34.20000076 W

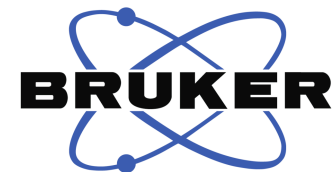
===== CHANNEL f2 =====
 SFO2 300.1312005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 14.00000000 W
 PLW12 0.17284000 W
 PLW13 0.14000000 W

F2 - Processing parameters
 SI 32768
 SF 75.4677485 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



3d





Current Data Parameters
NAME HNMR-YX-1-p40 (B4)
EXPNO 370
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220707
Time 16.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

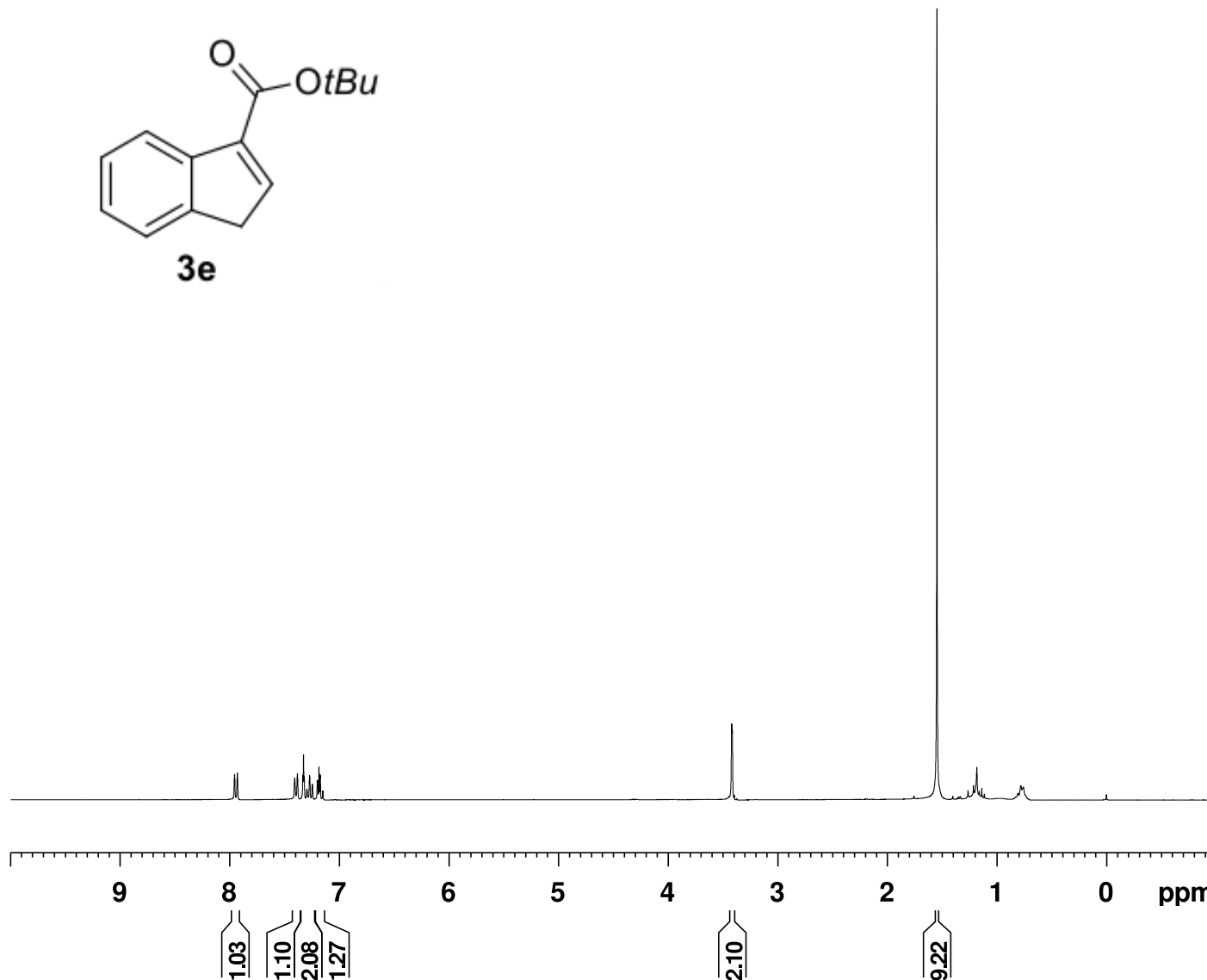
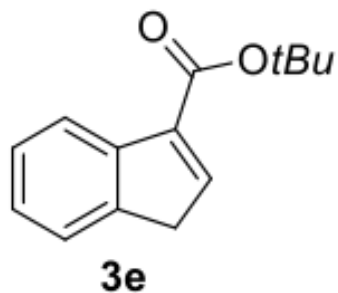
===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

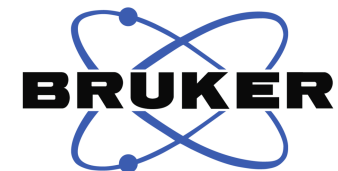
F2 - Processing parameters
SI 65536
SF 300.1300292 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.956
7.930
7.407
7.382
7.333
7.326
7.320
7.295
7.270
7.247
7.201
7.197
7.176
7.173
7.152
7.148

3.420
3.414

1.546





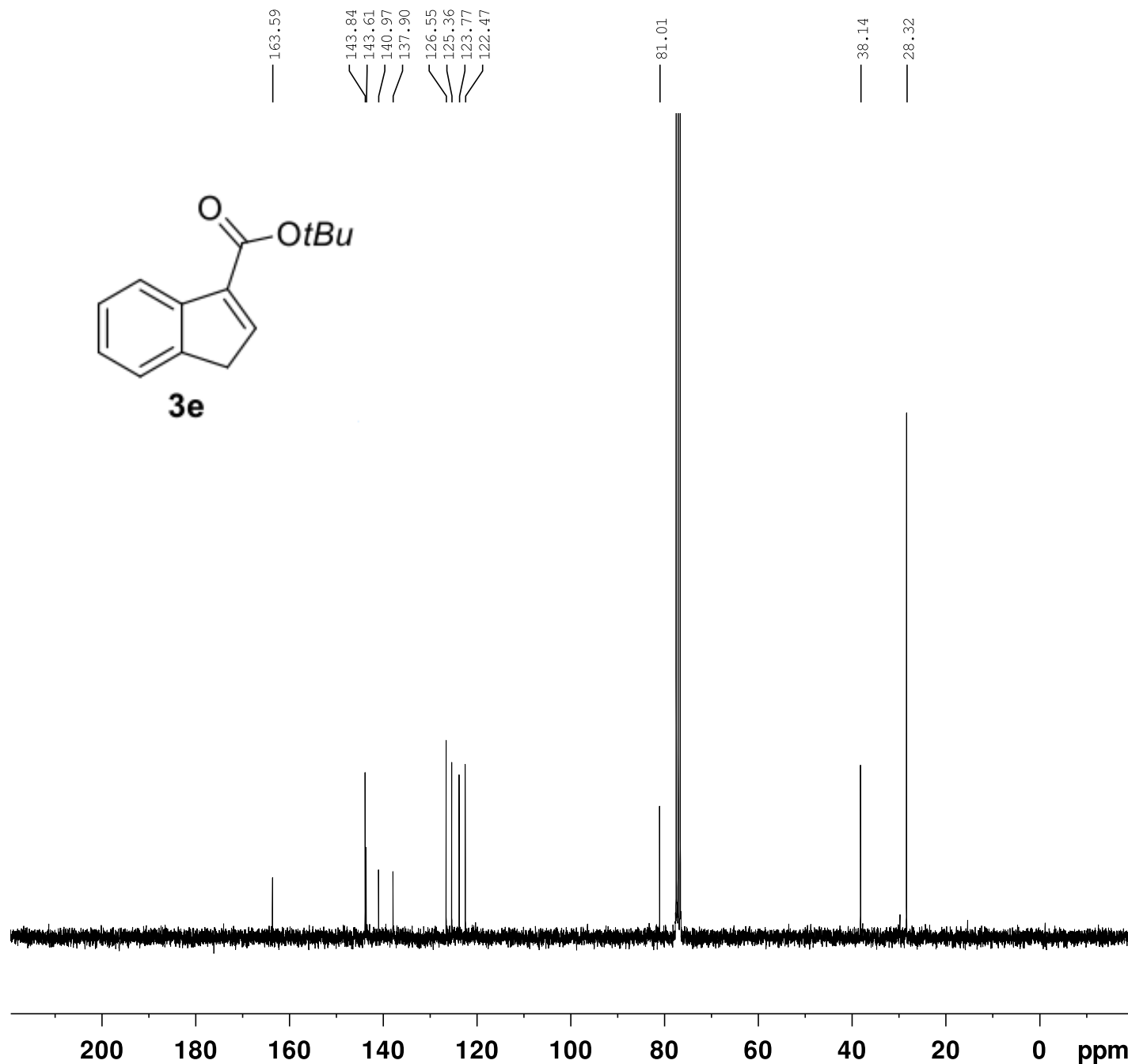
Current Data Parameters
NAME CNMR-YX-1-p40 (B4)
EXPNO 382
PROCNO 1

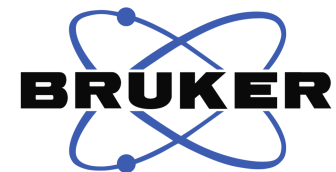
F2 - Acquisition Parameters
Date_ 20220708
Time 20.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



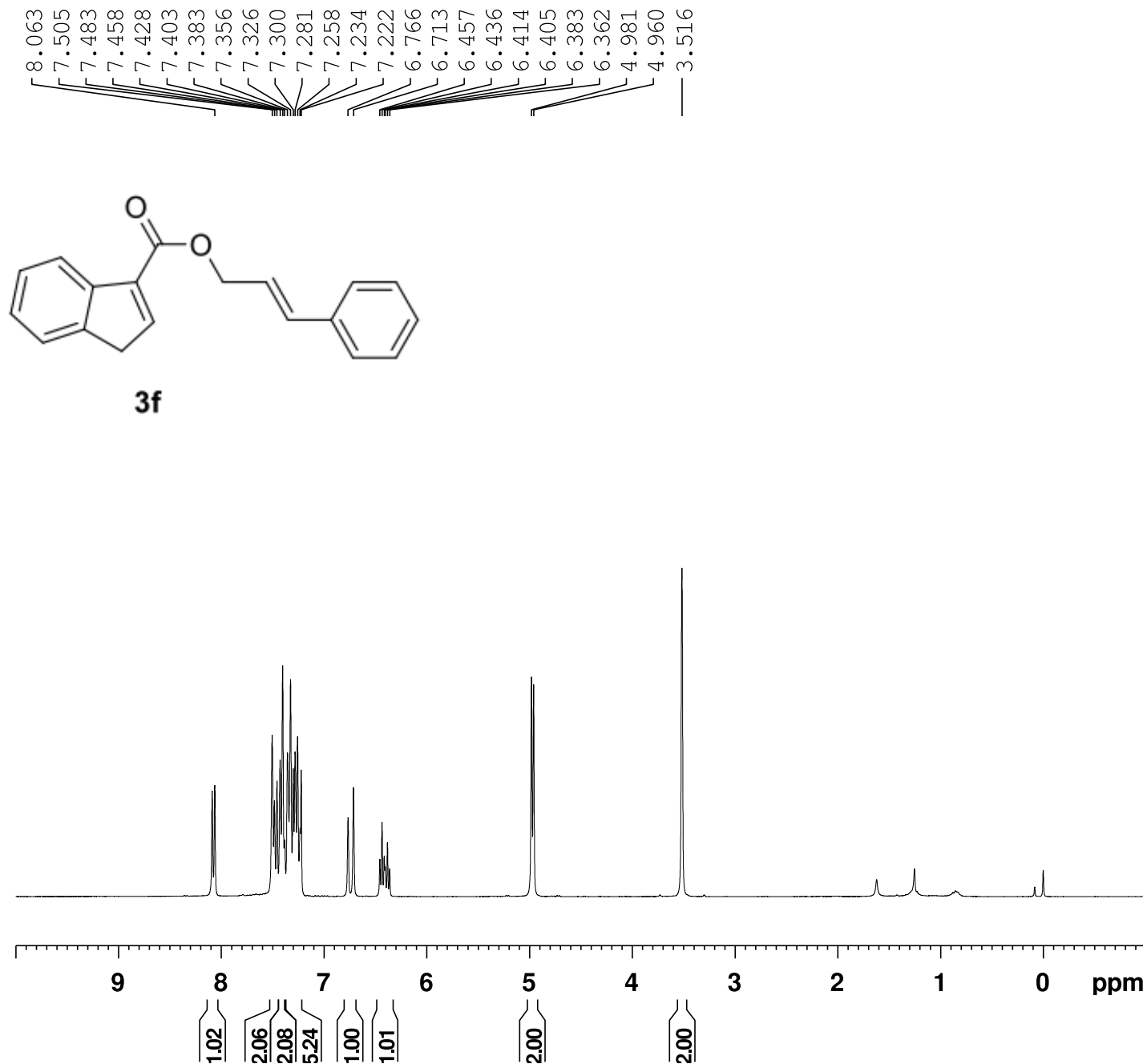


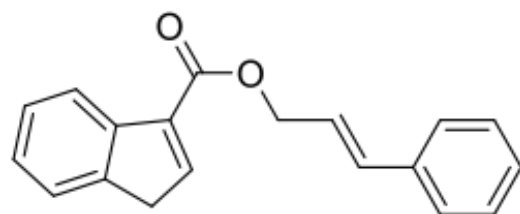
Current Data Parameters
 NAME HNMR-YX-3-p91
 EXPNO 103
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230406
 Time 16.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.091699 Hz
 AQ 5.4525952 sec
 RG 128
 DW 83.200 usec
 DE 6.50 usec
 TE 289.6 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1318534 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 14.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1300180 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





3f

163.91
144.92
143.42
140.74
136.26
136.16
134.36
128.69
128.16
126.75
126.72
125.66
123.87
123.29
122.52

65.15

38.53



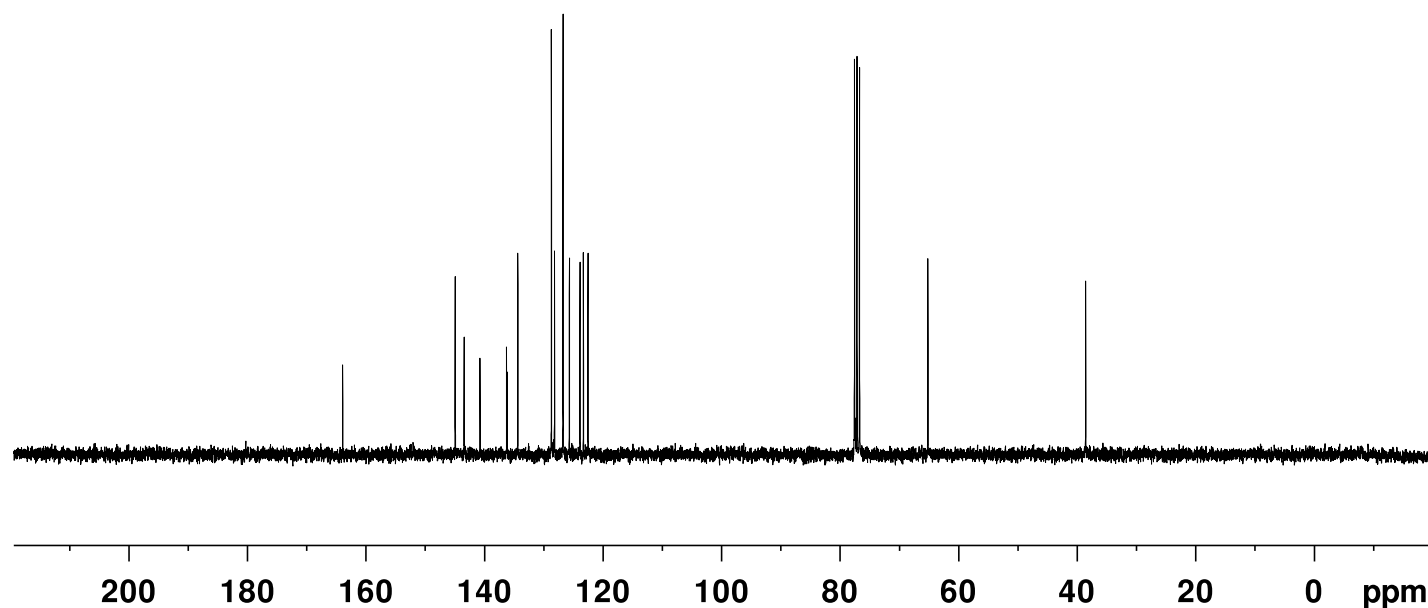
Current Data Parameters
NAME CNMR-YX-3-p91
EXPNO 104
PROCNO 1

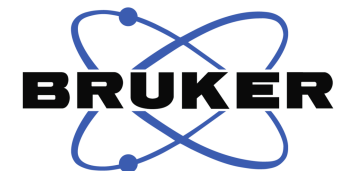
F2 - Acquisition Parameters
Date_ 20230406
Time 21.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 290.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



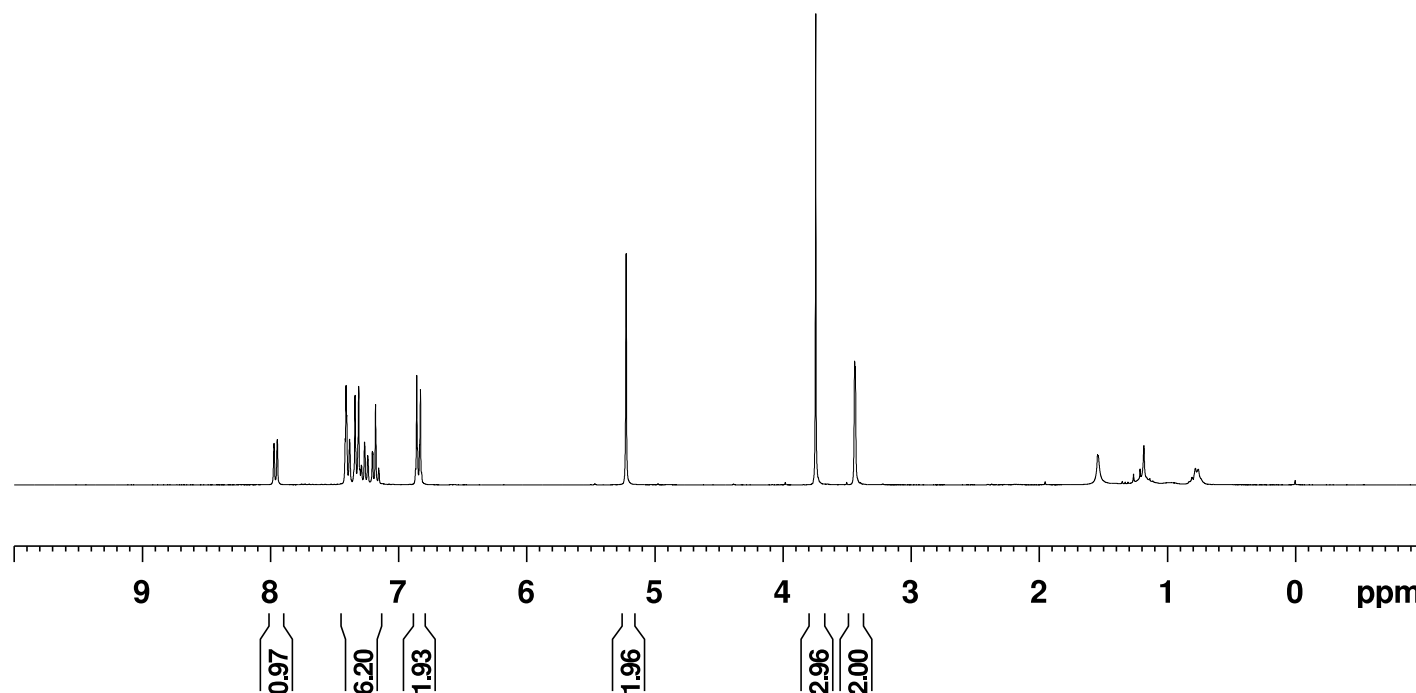
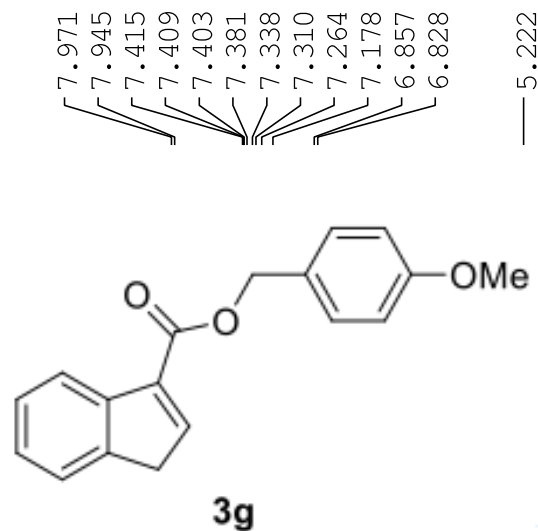


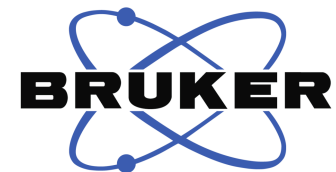
Current Data Parameters
 NAME HNMR-YX-1-p40 (B5)
 EXPNO 202
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220630
 Time 9.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.091699 Hz
 AQ 5.4525952 sec
 RG 181
 DW 83.200 usec
 DE 6.50 usec
 TE -59.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1318534 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 14.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1300316 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





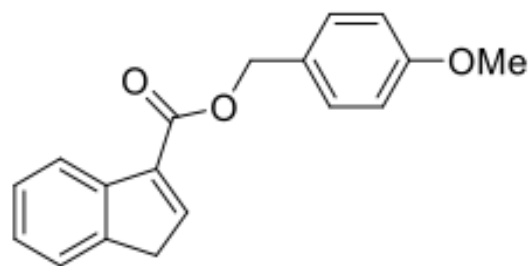
Current Data Parameters
 NAME CNMR-YX-1-p40 (B5)
 EXPNO 203
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220630
 Time 9.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 300
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175317 sec
 RG 203
 DW 27.733 usec
 DE 6.50 usec
 TE -59.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

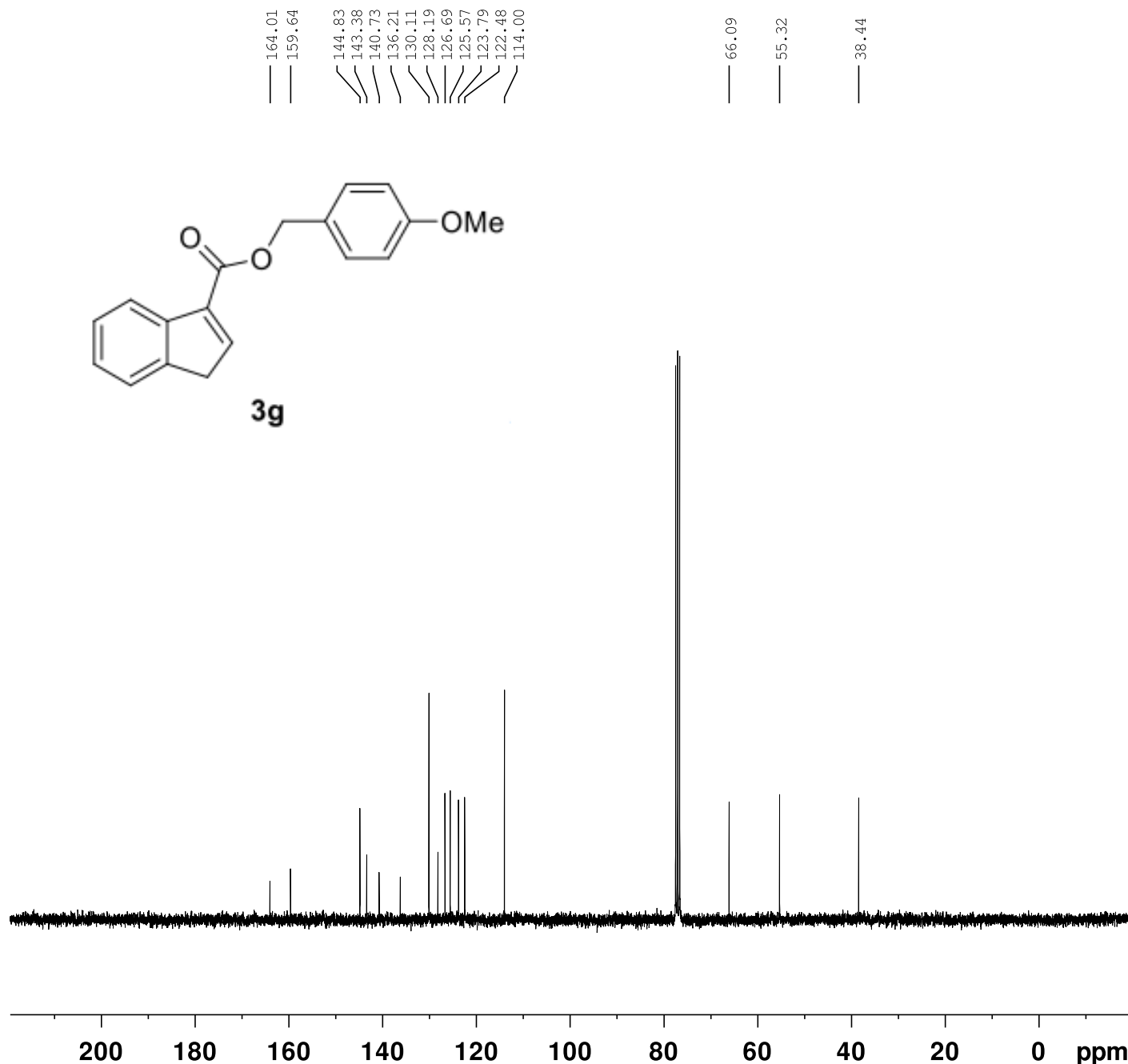
===== CHANNEL f1 =====
 SFO1 75.4752949 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 34.20000076 W

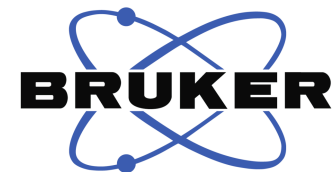
===== CHANNEL f2 =====
 SFO2 300.1312005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 14.00000000 W
 PLW12 0.17284000 W
 PLW13 0.14000000 W

F2 - Processing parameters
 SI 32768
 SF 75.4677485 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



3g





Current Data Parameters
 NAME HNMR-YX-3-p92
 EXPNO 58
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230331
 Time 23.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.091699 Hz
 AQ 5.4525952 sec
 RG 144
 DW 83.200 usec
 DE 6.50 usec
 TE 291.1 K
 D1 1.00000000 sec
 TD0 1

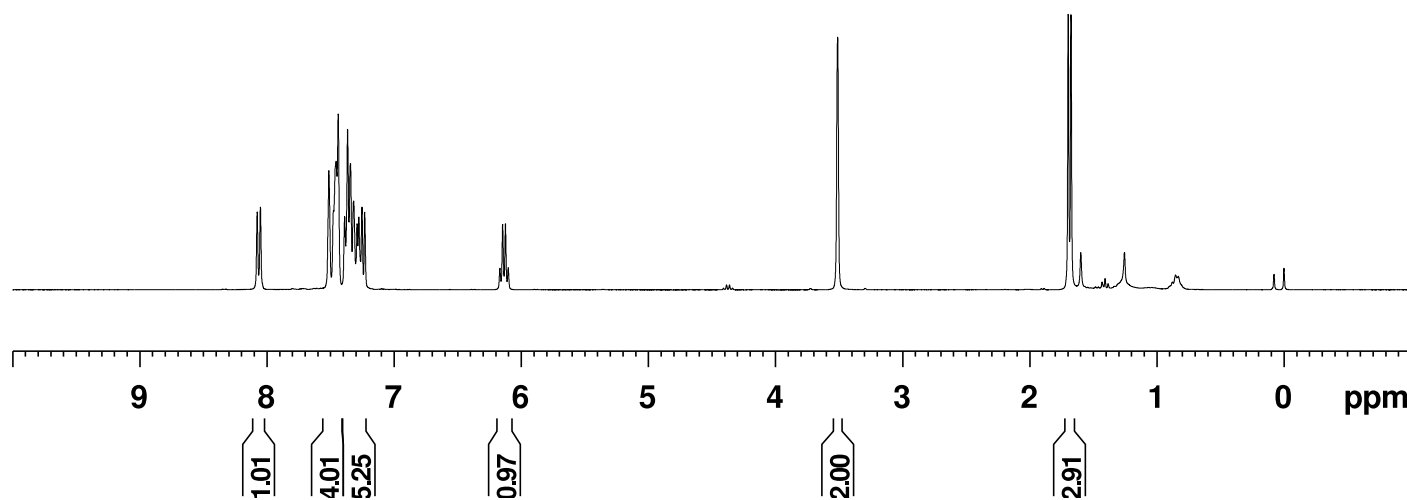
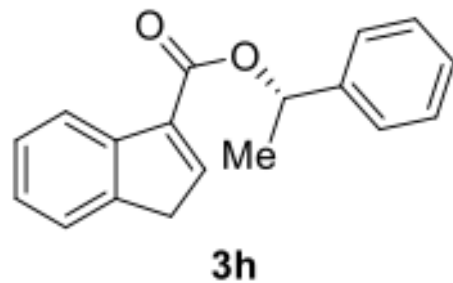
===== CHANNEL f1 =====
 SFO1 300.1318534 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 14.00000000 W

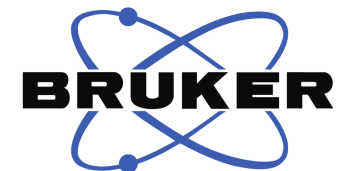
F2 - Processing parameters
 SI 65536
 SF 300.1300151 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.077
8.052
7.513
7.477
7.457
7.440
7.389
7.366
7.344
7.318
7.291
7.277
7.253
7.232
6.168
6.146
6.124
6.102

— 3.511

1.697
1.675





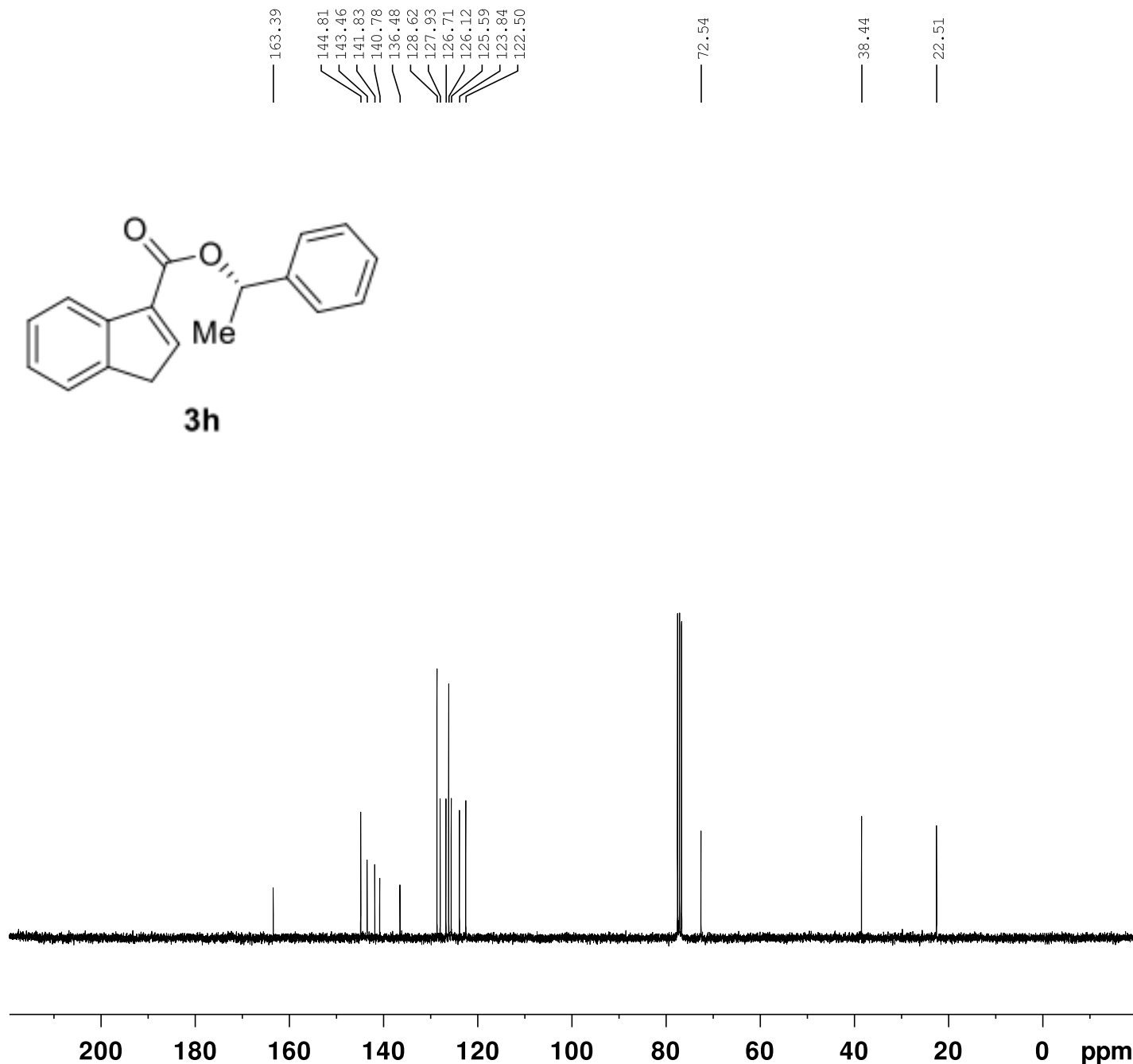
Current Data Parameters
 NAME CNMR-YX-3-p92
 EXPNO 59
 PROCNO 1

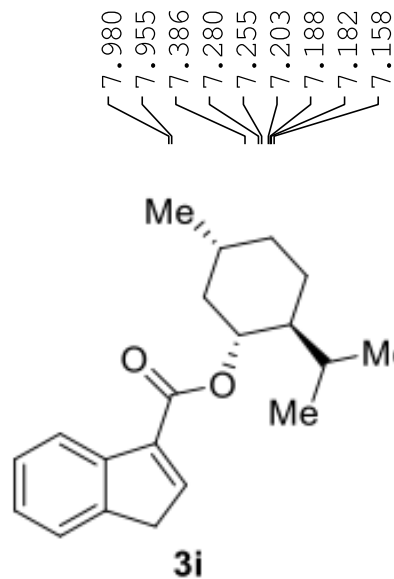
F2 - Acquisition Parameters
 Date_ 20230331
 Time 23.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 250
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175317 sec
 RG 203
 DW 27.733 usec
 DE 6.50 usec
 TE 291.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 75.4752949 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 34.20000076 W

===== CHANNEL f2 =====
 SFO2 300.1312005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 14.00000000 W
 PLW12 0.17284000 W
 PLW13 0.14000000 W

F2 - Processing parameters
 SI 32768
 SF 75.4677485 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

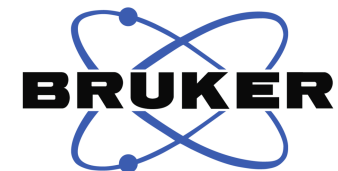




7.980
7.955
7.386
7.280
7.255
7.203
7.188
7.182
7.158

4.912
4.877
4.863
4.841

3.443
2.092
2.059
1.929
1.915
1.683
1.644
1.523
1.492
1.107
1.080
1.044
0.868
0.860
0.854
0.750
0.738
0.720

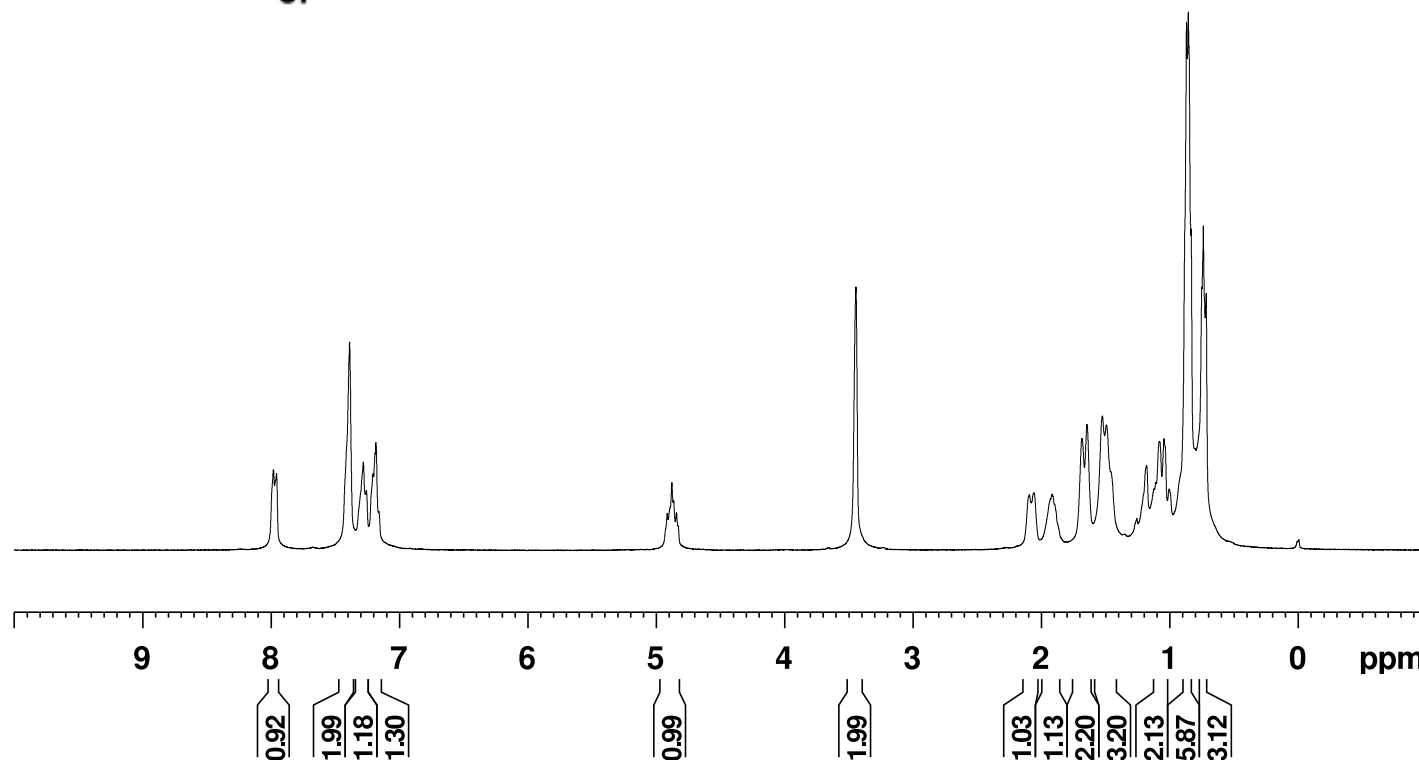


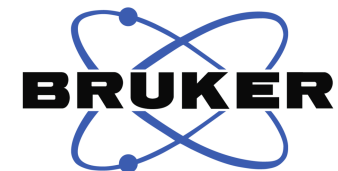
Current Data Parameters
NAME HNMR-YX-1-p50
EXPNO 374
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220708
Time 14.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.452592 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300311 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





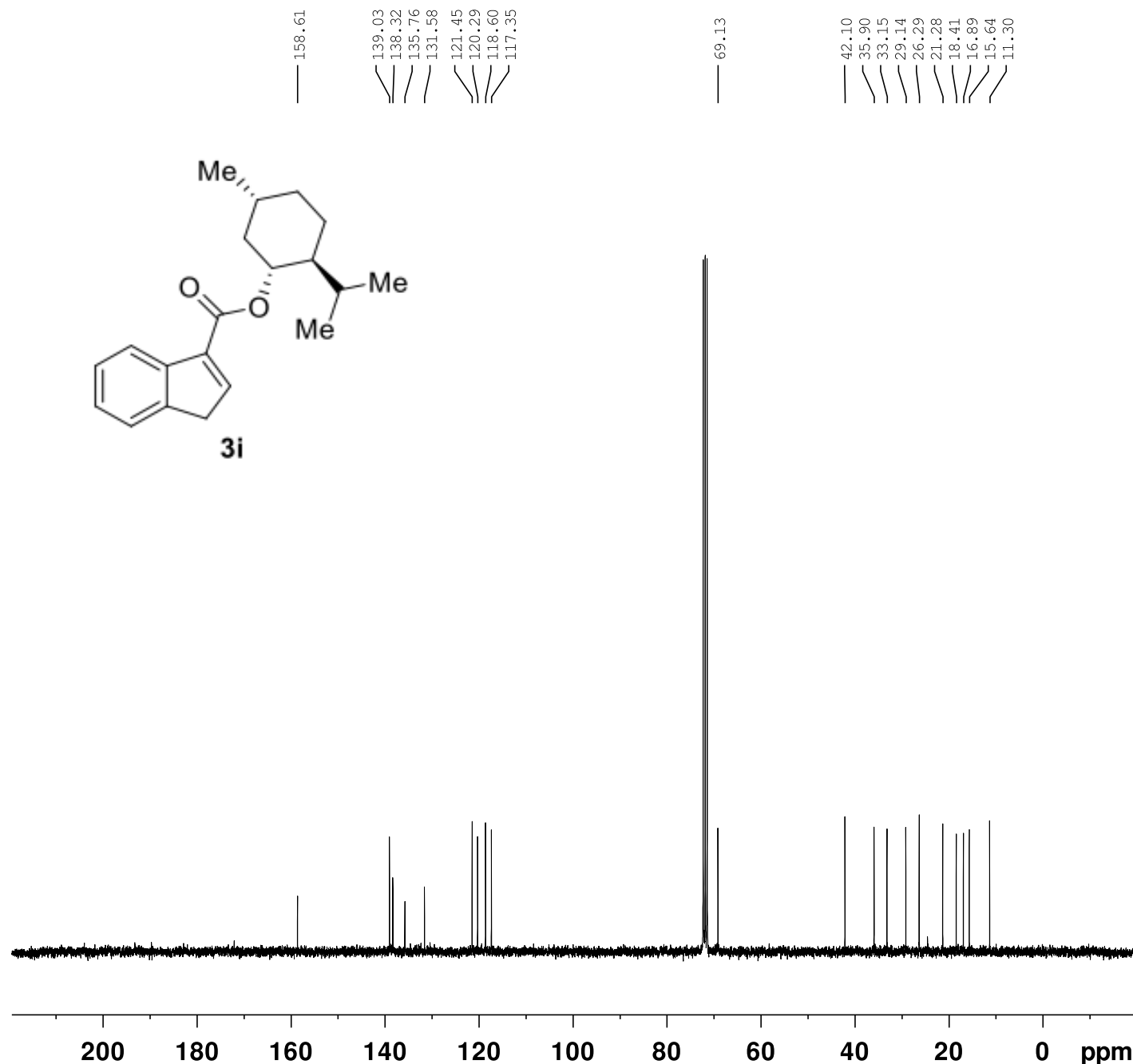
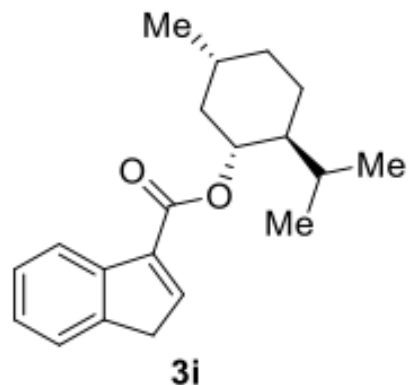
Current Data Parameters
NAME CNMR-YX-1-p50
EXPNO 389
PROCNO 1

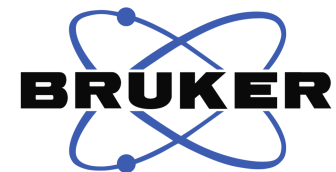
F2 - Acquisition Parameters
Date_ 20220709
Time 3.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 600
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



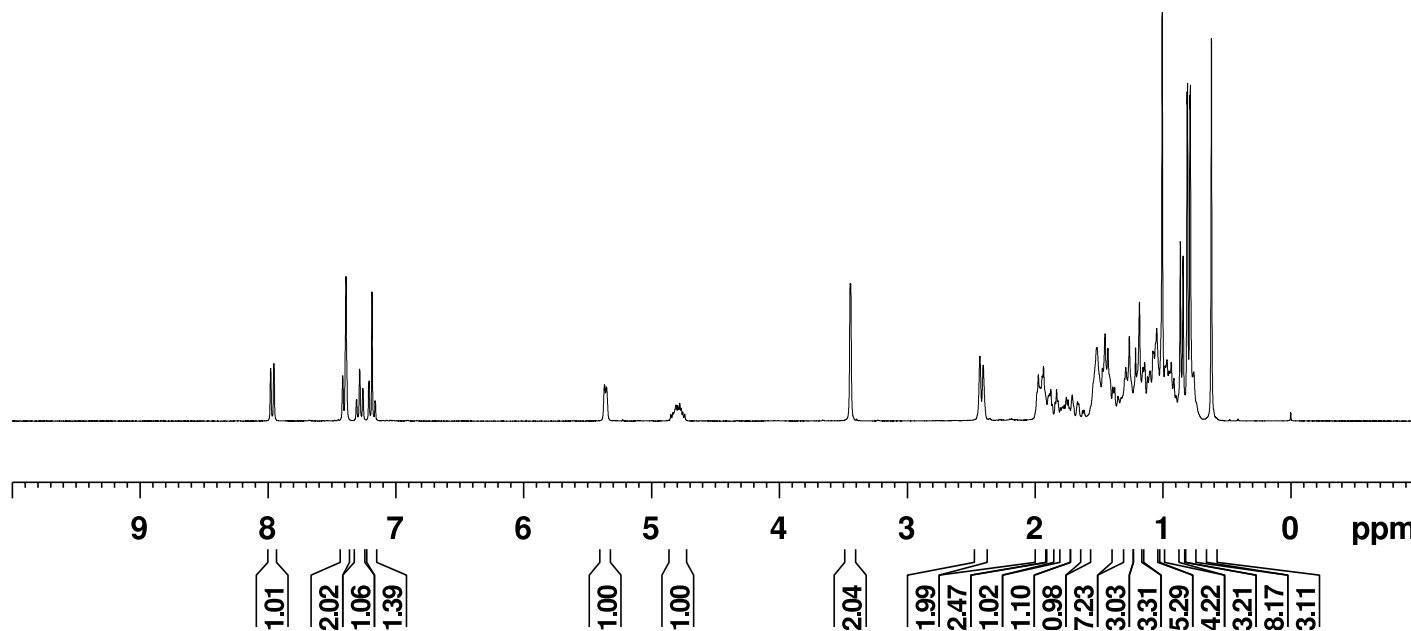
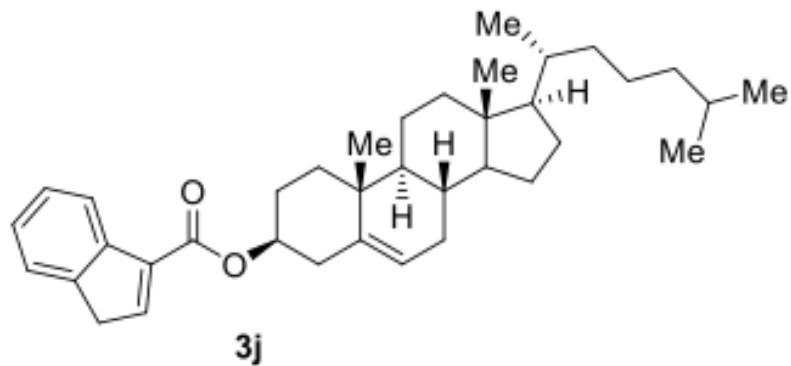
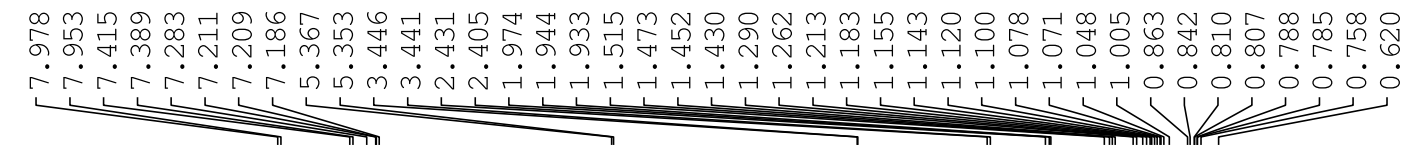


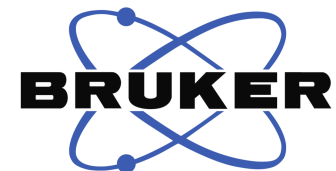
Current Data Parameters
 NAME HNMR-YX-1-p42
 EXPNO 375
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220708
 Time 14.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.091699 Hz
 AQ 5.4525952 sec
 RG 128
 DW 83.200 usec
 DE 6.50 usec
 TE -59.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1318534 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 14.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1300296 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





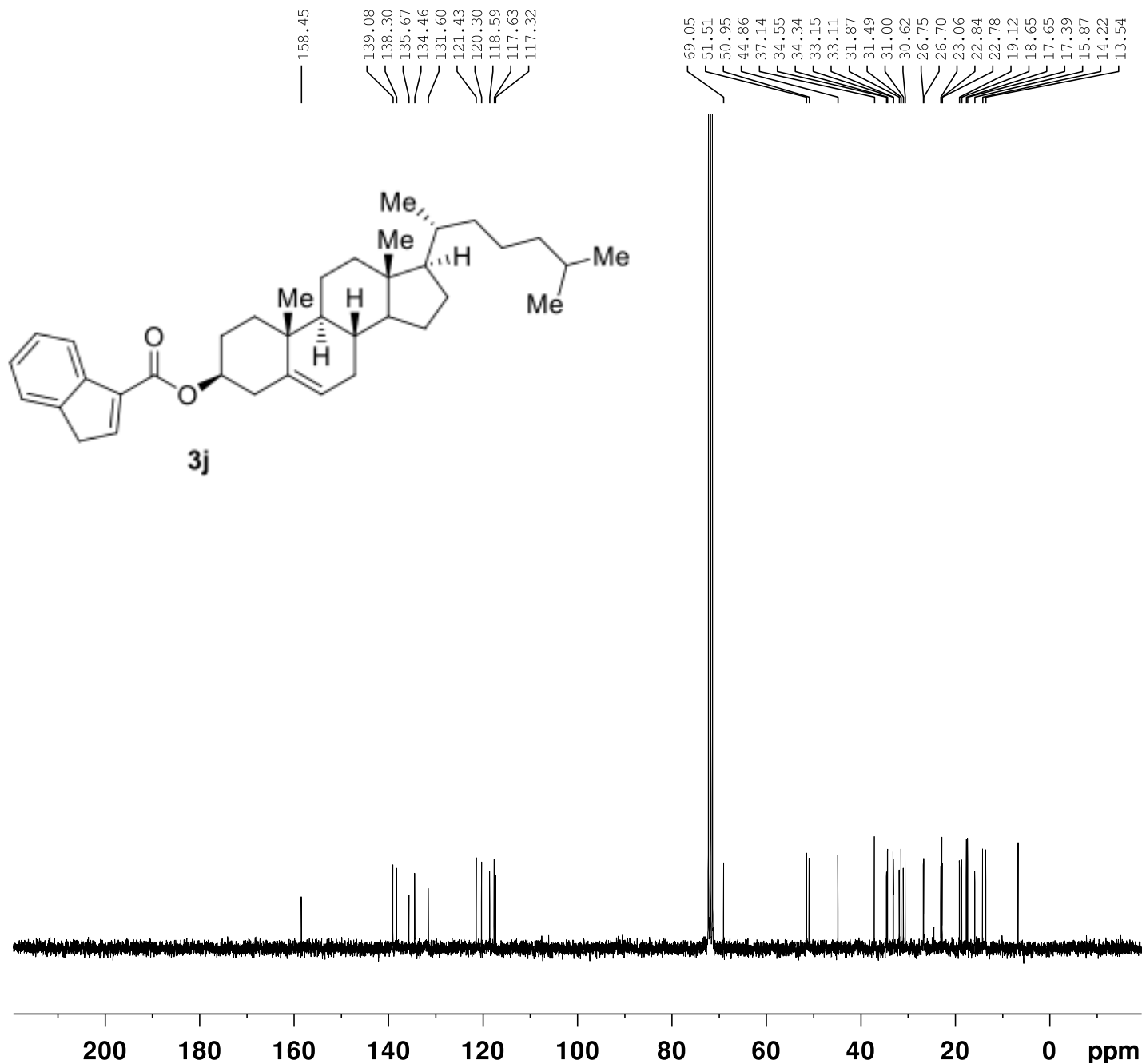
Current Data Parameters
NAME CNMR-YX-1-p42
EXPNO 390
PROCNO 1

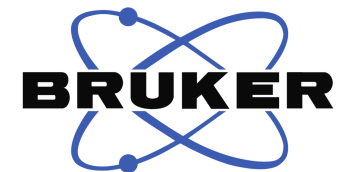
F2 - Acquisition Parameters
Date_ 20220709
Time 4.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 600
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



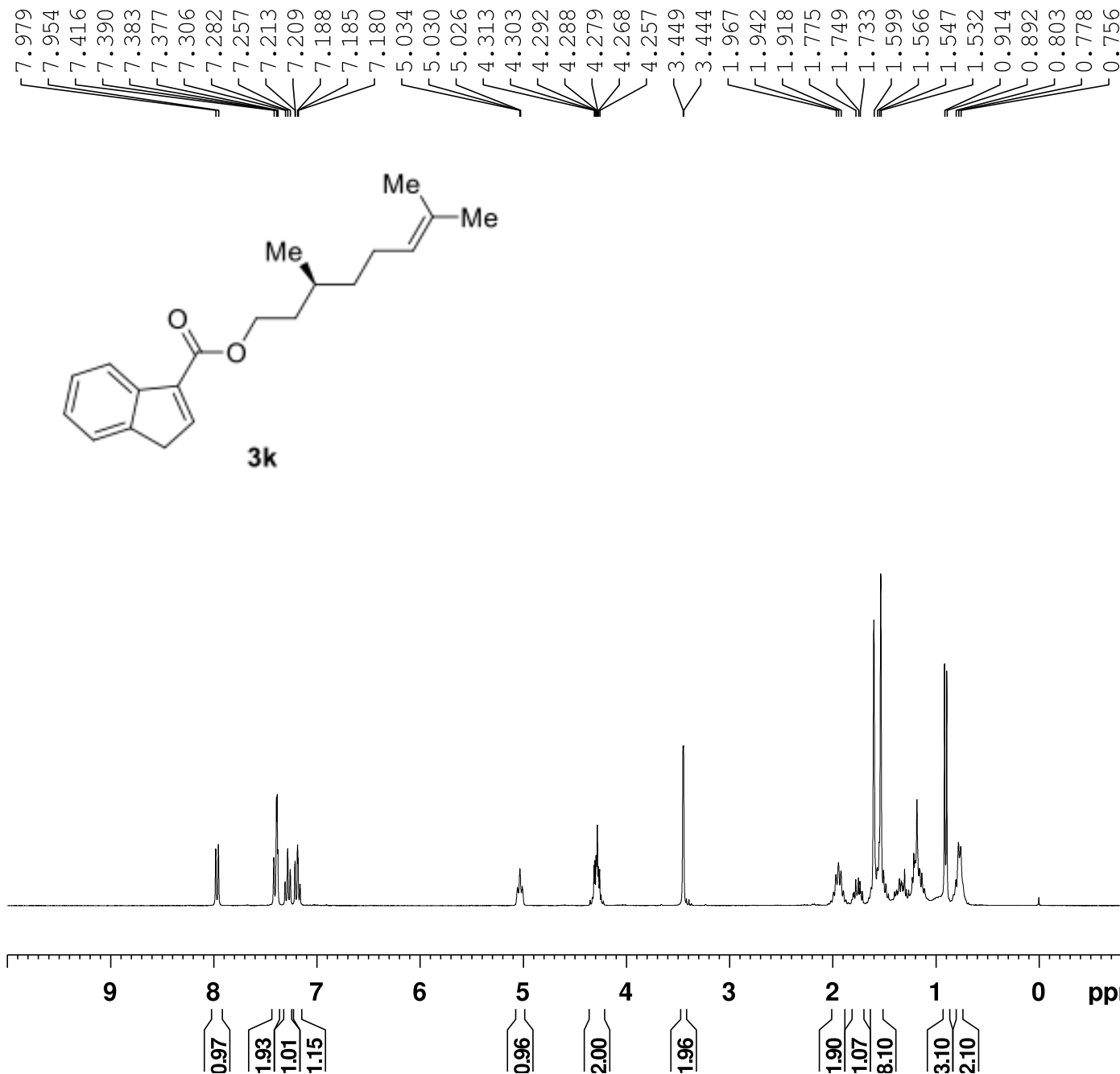


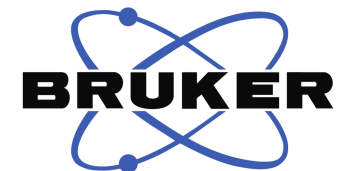
Current Data Parameters
 NAME HNMR-YX-1-p46
 EXPNO 373
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220708
 Time 14.11
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.091699 Hz
 AQ 5.4525952 sec
 RG 114
 DW 83.200 usec
 DE 6.50 usec
 TE -59.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1318534 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 14.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1300315 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





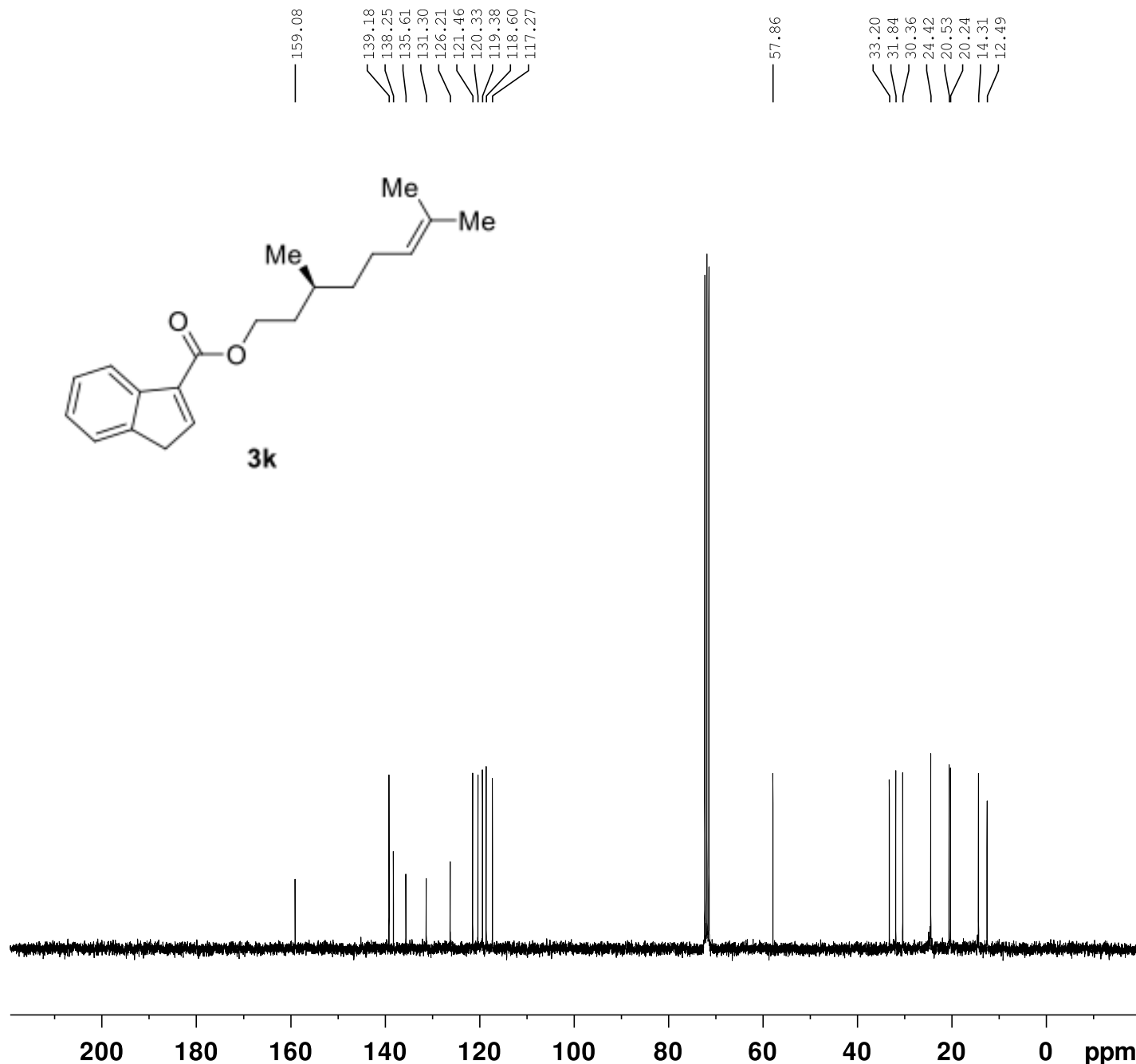
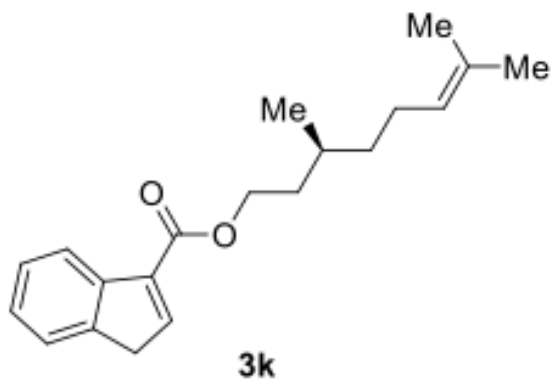
Current Data Parameters
 NAME CNMR-YX-1-p46
 EXPNO 388
 PROCNO 1

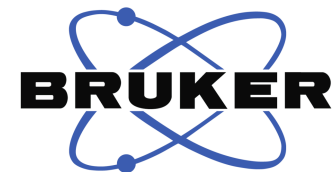
F2 - Acquisition Parameters
 Date_ 20220709
 Time 2.50
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 600
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175317 sec
 RG 203
 DW 27.733 usec
 DE 6.50 usec
 TE -59.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 75.4752949 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 34.20000076 W

===== CHANNEL f2 =====
 SFO2 300.1312005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 14.00000000 W
 PLW12 0.17284000 W
 PLW13 0.14000000 W

F2 - Processing parameters
 SI 32768
 SF 75.4677485 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

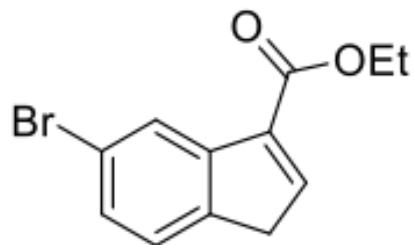




Current Data Parameters
NAME HNMR-YX-3-p84
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230329
Time 3.04 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 81.1688
DW 61.000 usec
DE 13.54 usec
TE 293.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

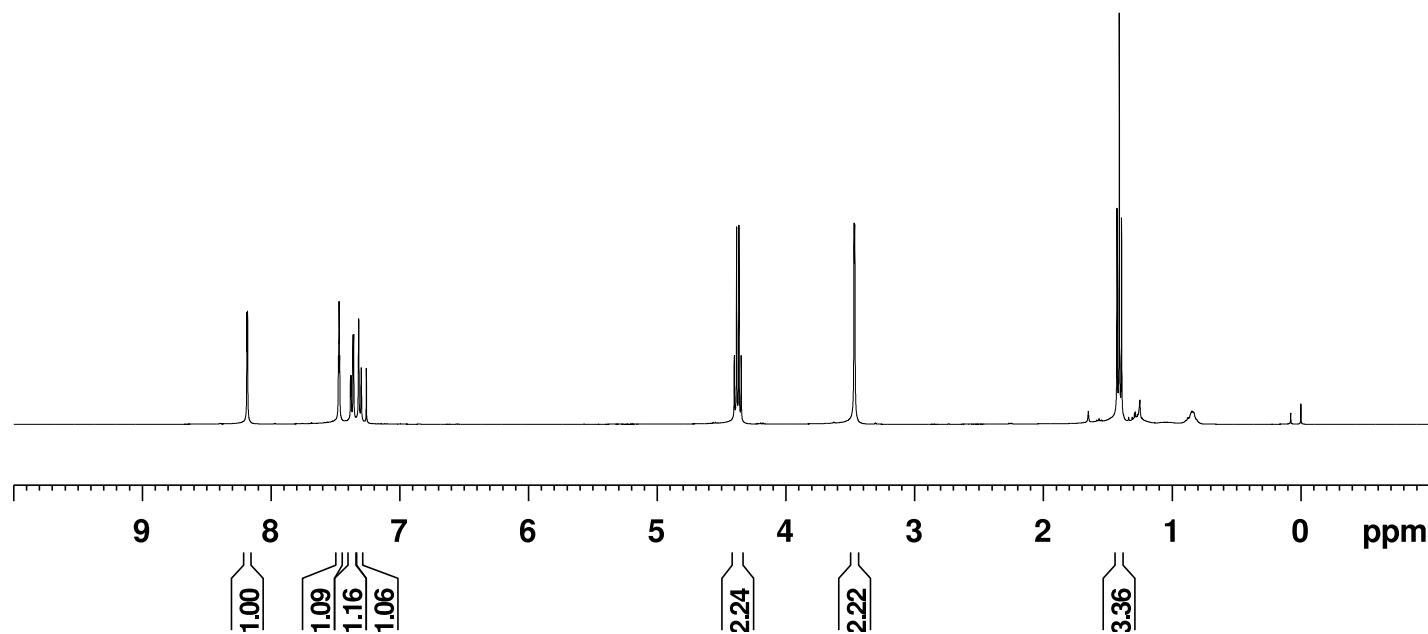


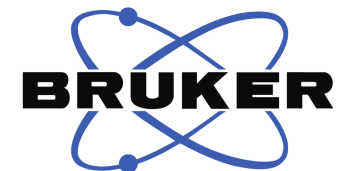
31

8.187
8.183
7.477
7.472
7.467
7.383
7.378
7.363
7.358
7.320
7.300
7.260

4.401
4.383
4.366
4.348
3.470
3.466

1.428
1.410
1.393

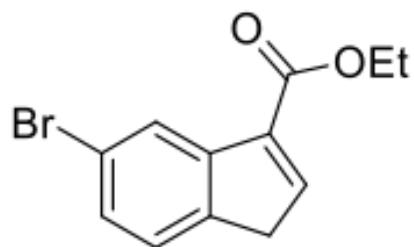




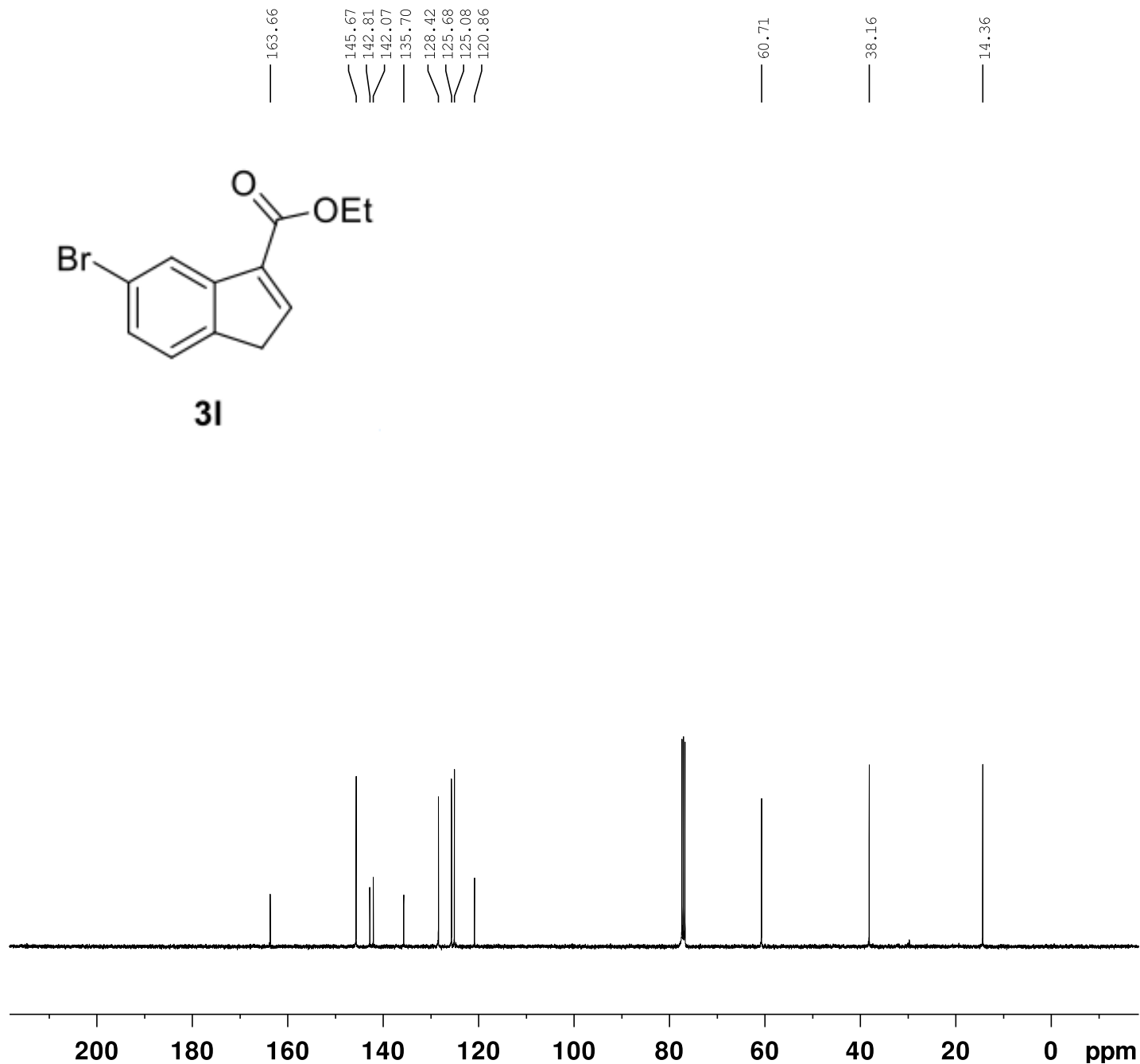
Current Data Parameters
NAME CNMR-YX-3-p84
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230329
Time 3.28 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 50.1934
DW 21.000 usec
DE 6.50 usec
TE 293.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

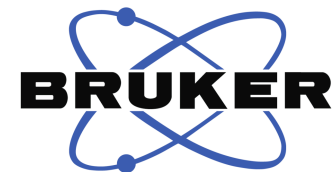
F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



3l



S45



Current Data Parameters
 NAME HNMR-YX-3-p79
 EXPNO 25
 PROCNO 1

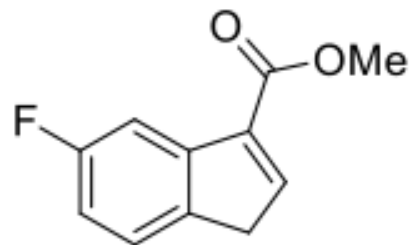
F2 - Acquisition Parameters
 Date_ 20230327
 Time 14.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.091699 Hz
 AQ 5.4525952 sec
 RG 144
 DW 83.200 usec
 DE 6.50 usec
 TE 290.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1318534 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 14.00000000 W

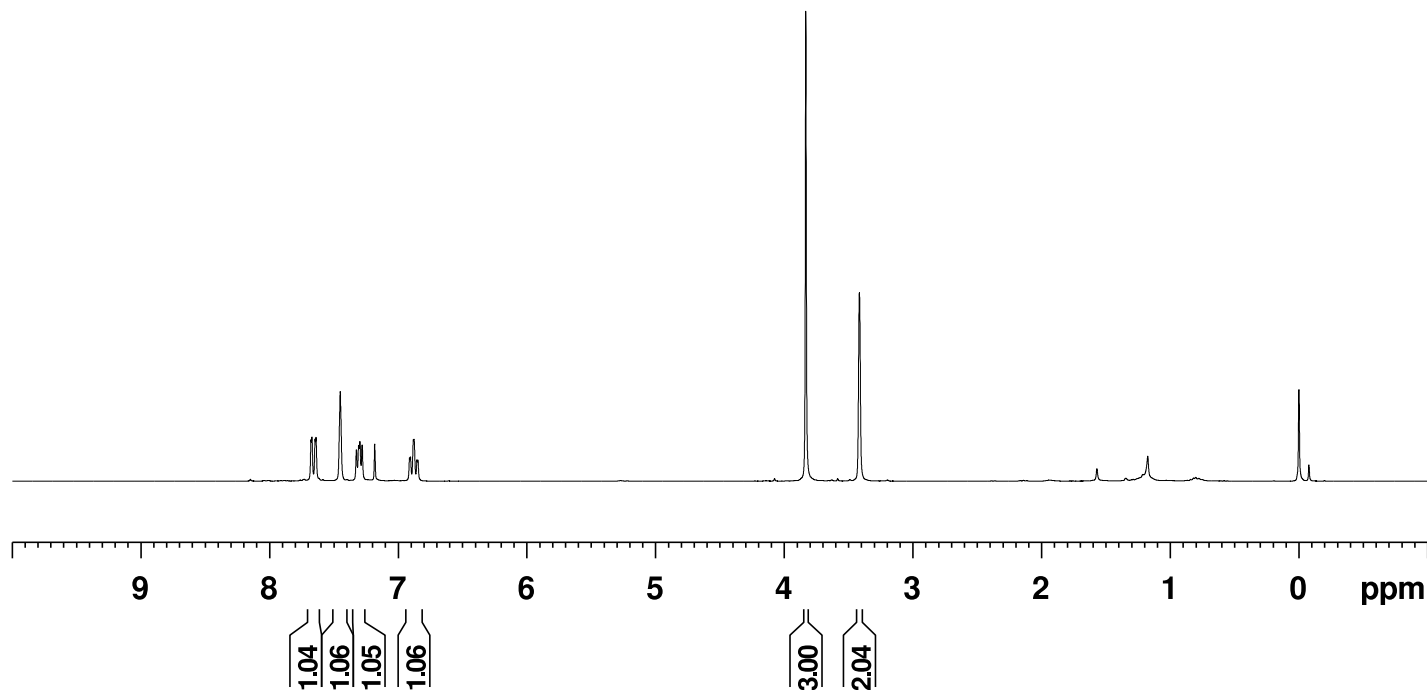
F2 - Processing parameters
 SI 65536
 SF 300.1300301 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

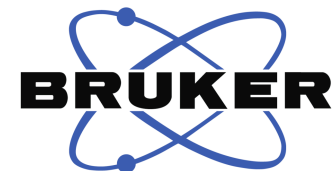
7.678
7.671
7.646
7.639
7.451
7.325
7.308
7.298
7.281
7.183
6.912
6.905
6.882
6.878
6.854
6.847

— 3.833
— 3.416



3m

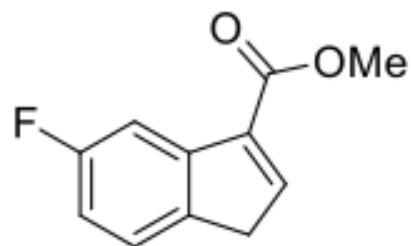




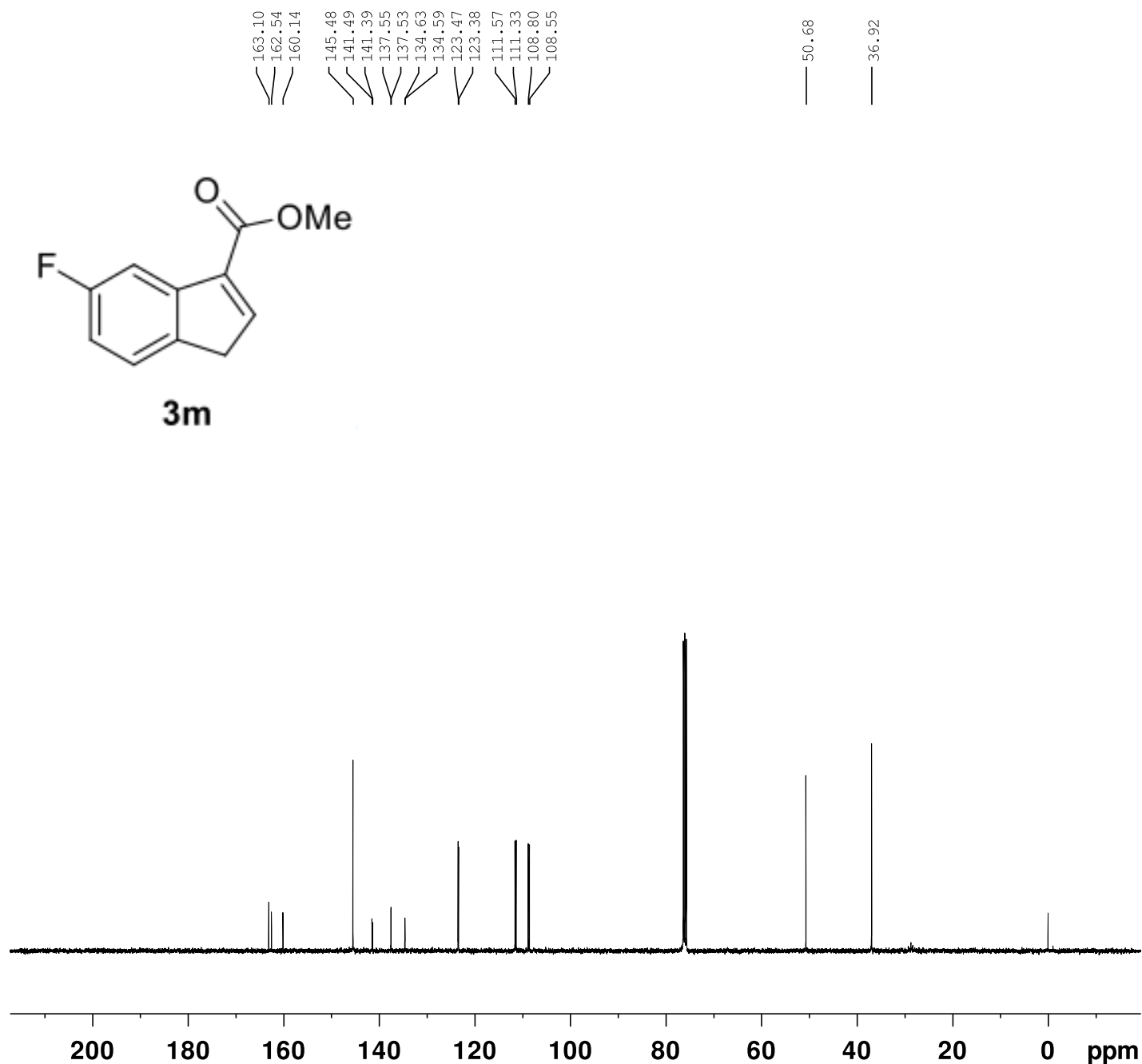
Current Data Parameters
 NAME CNMR-YX-3-p79
 EXPNO 1
 PROCNO 1

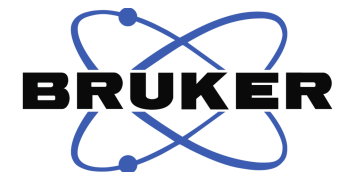
F2 - Acquisition Parameters
 Date_ 20230329
 Time 2.30 h
 INSTRUM Avance
 PROBHD Z116098_0833 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 400
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 50.1934
 DW 21.000 usec
 DE 6.50 usec
 TE 293.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6228298 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 87.89900208 W
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 20.73200035 W
 PLW12 0.25595000 W
 PLW13 0.12874000 W

F2 - Processing parameters
 SI 32768
 SF 100.6128746 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



3m

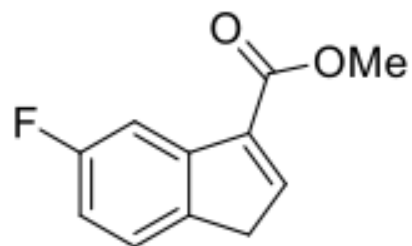




Current Data Parameters
NAME FNMN-YX-3-p79
EXPNO 2
PROCNO 1

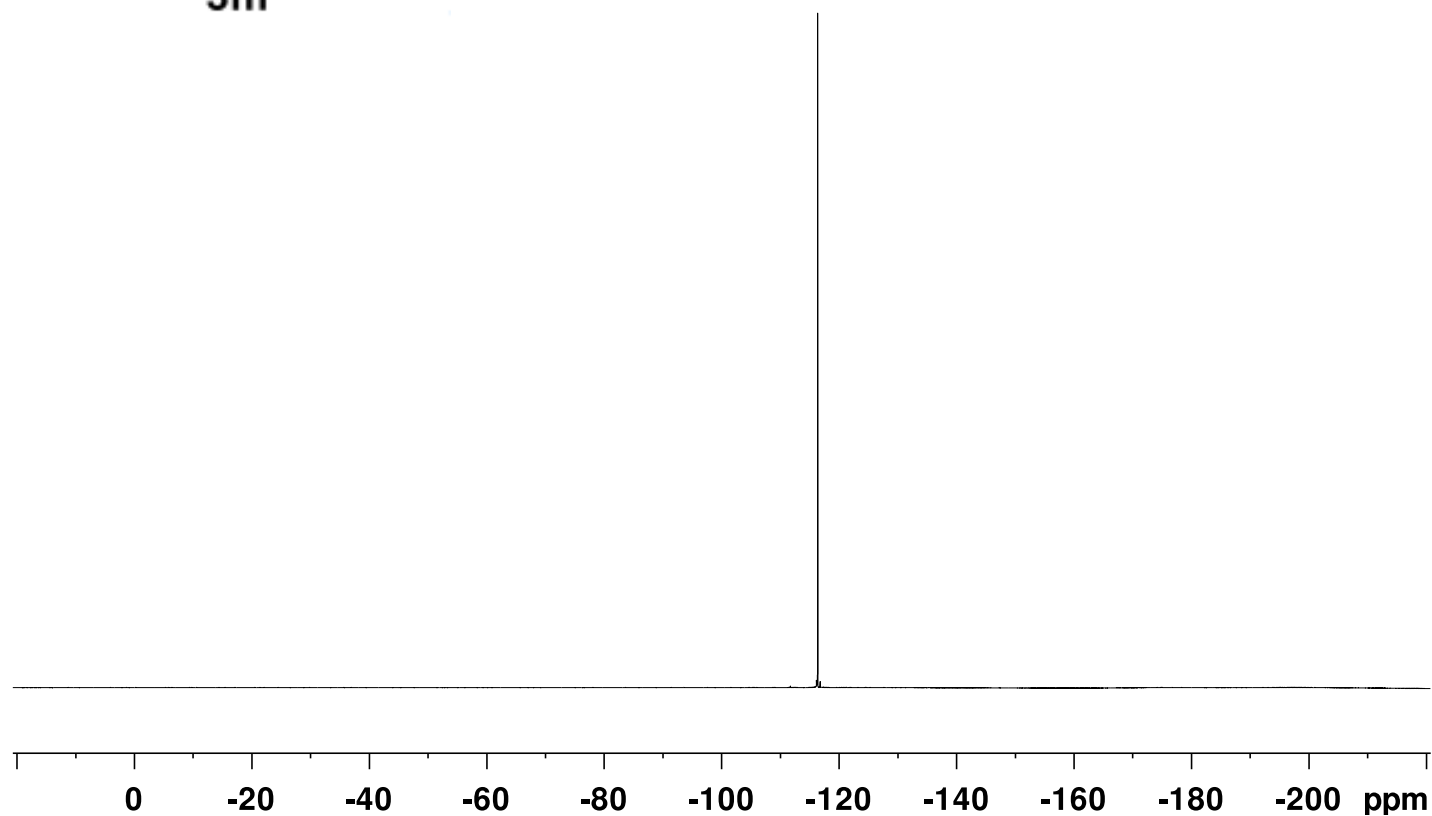
F2 - Acquisition Parameters
Date_ 20230324
Time 22.03 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 293.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 376.4607164 MHz
NUC1 19F
P1 18.00 usec
PLW1 16.73100090 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W

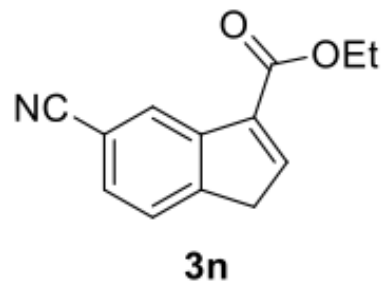
F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3m

— -116.37

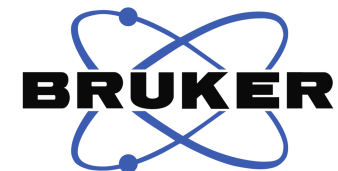




8.334
7.582
7.561
7.278

4.429
4.411
4.393
4.375
3.624
3.620

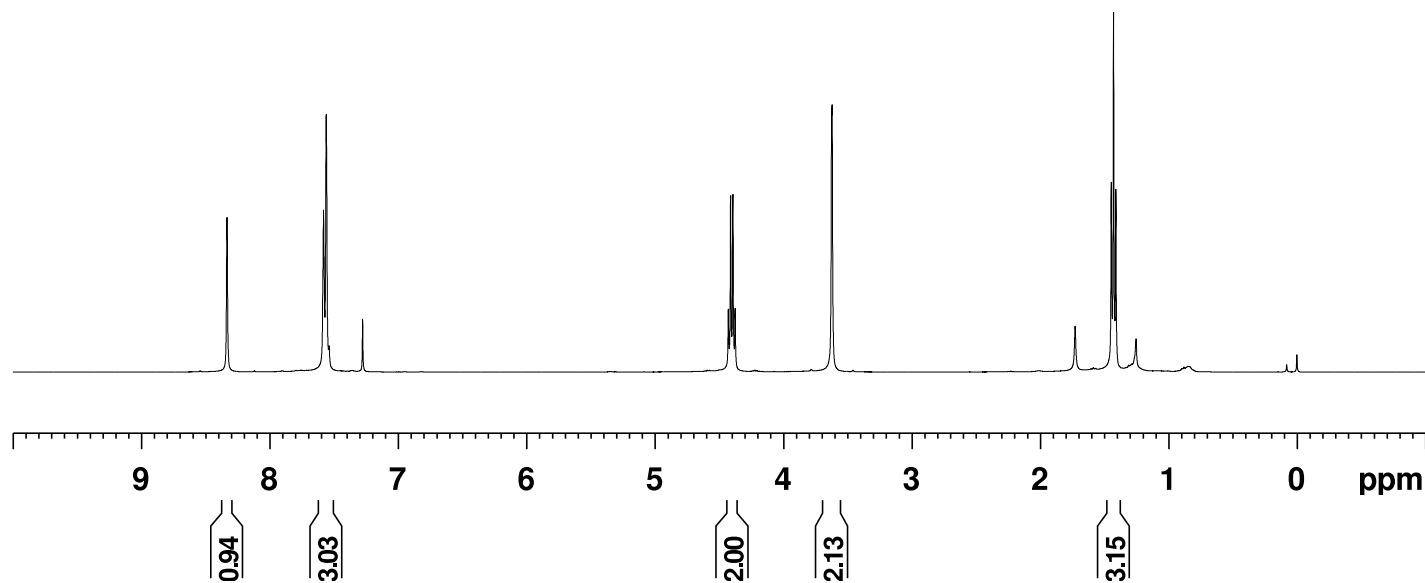
1.446
1.428
1.410

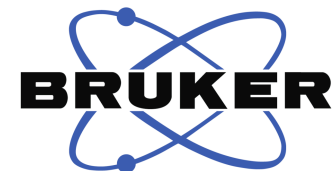


Current Data Parameters
NAME HNMR-YX-3-p95
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230331
Time 21.38 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 95.2744
DW 61.000 usec
DE 13.54 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

F2 - Processing parameters
SI 65536
SF 400.1300030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

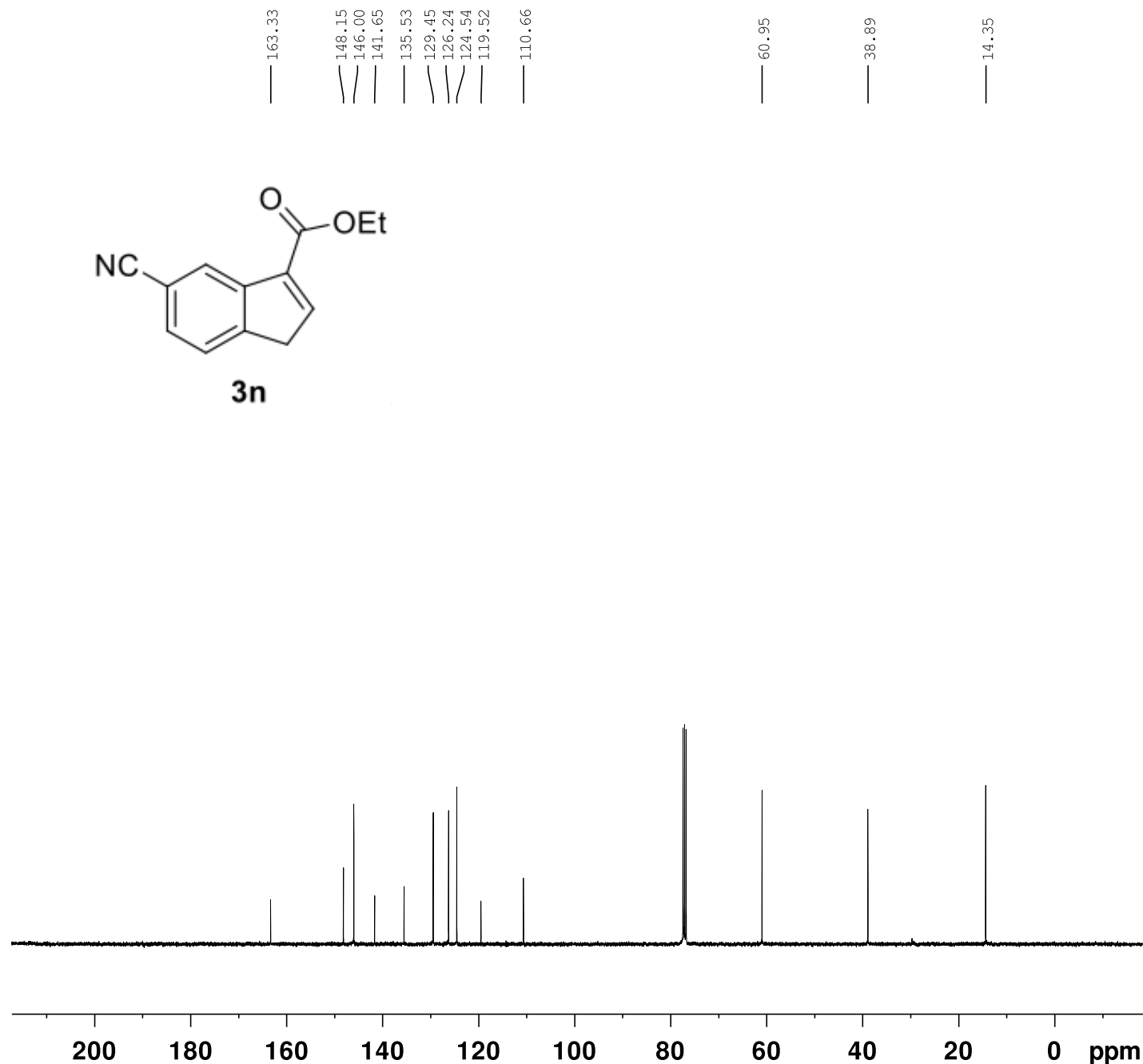
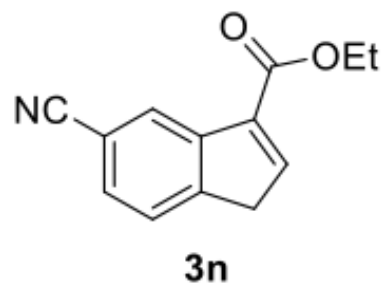


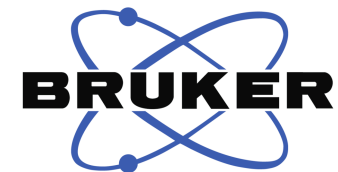


Current Data Parameters
NAME CNMR-YX-3-p95
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230401
Time 8.21 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 51.55
DW 21.000 usec
DE 6.50 usec
TE 294.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



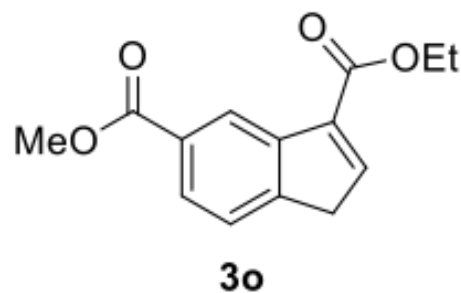


Current Data Parameters
 NAME HNMR-YX-4-p5
 EXPNO 80
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230404
 Time 13.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.091699 Hz
 AQ 5.4525952 sec
 RG 114
 DW 83.200 usec
 DE 6.50 usec
 TE 291.5 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1318534 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 14.00000000 W

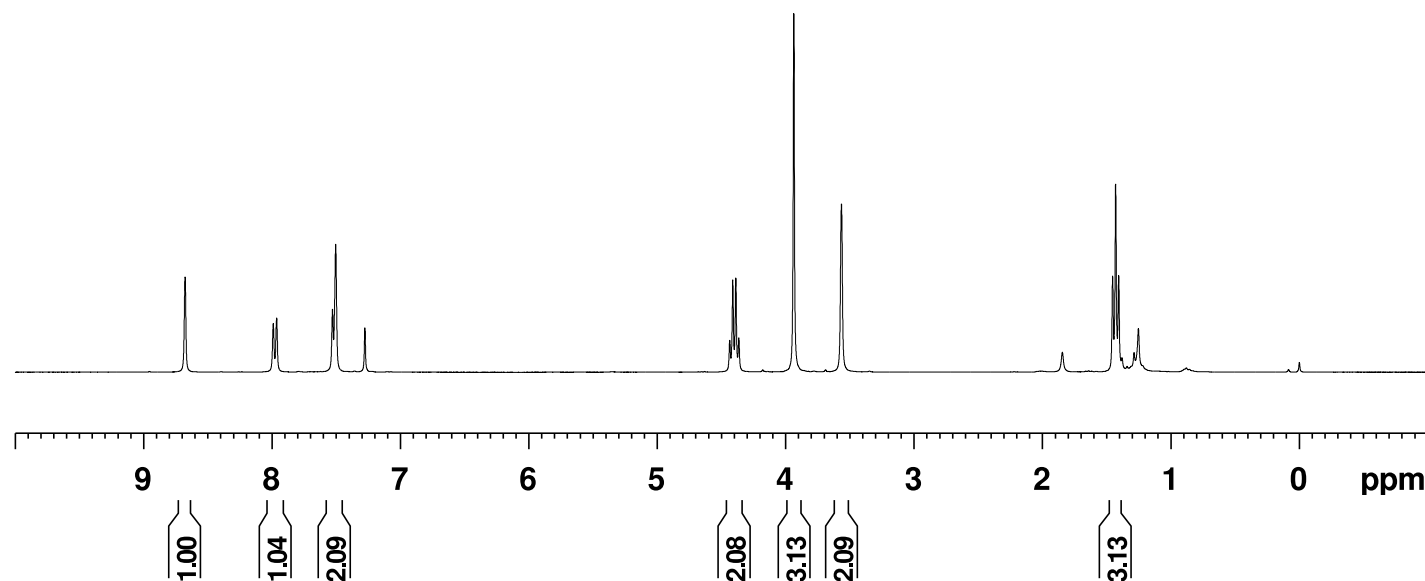
F2 - Processing parameters
 SI 65536
 SF 300.130015 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

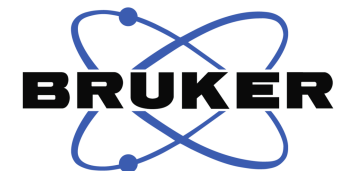


8.677
 7.990
 7.964
 7.529
 7.504
 7.277

4.436
 4.412
 4.389
 4.365
 3.937
 3.565

1.454
 1.430
 1.407





Current Data Parameters
NAME CNMR-YX-4-p5
EXPNO 81
PROCNO 1

F2 - Acquisition Parameters

Date_ 20230404
Time 13.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 292.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====

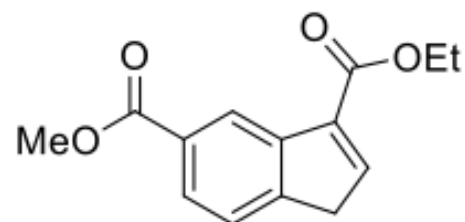
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====

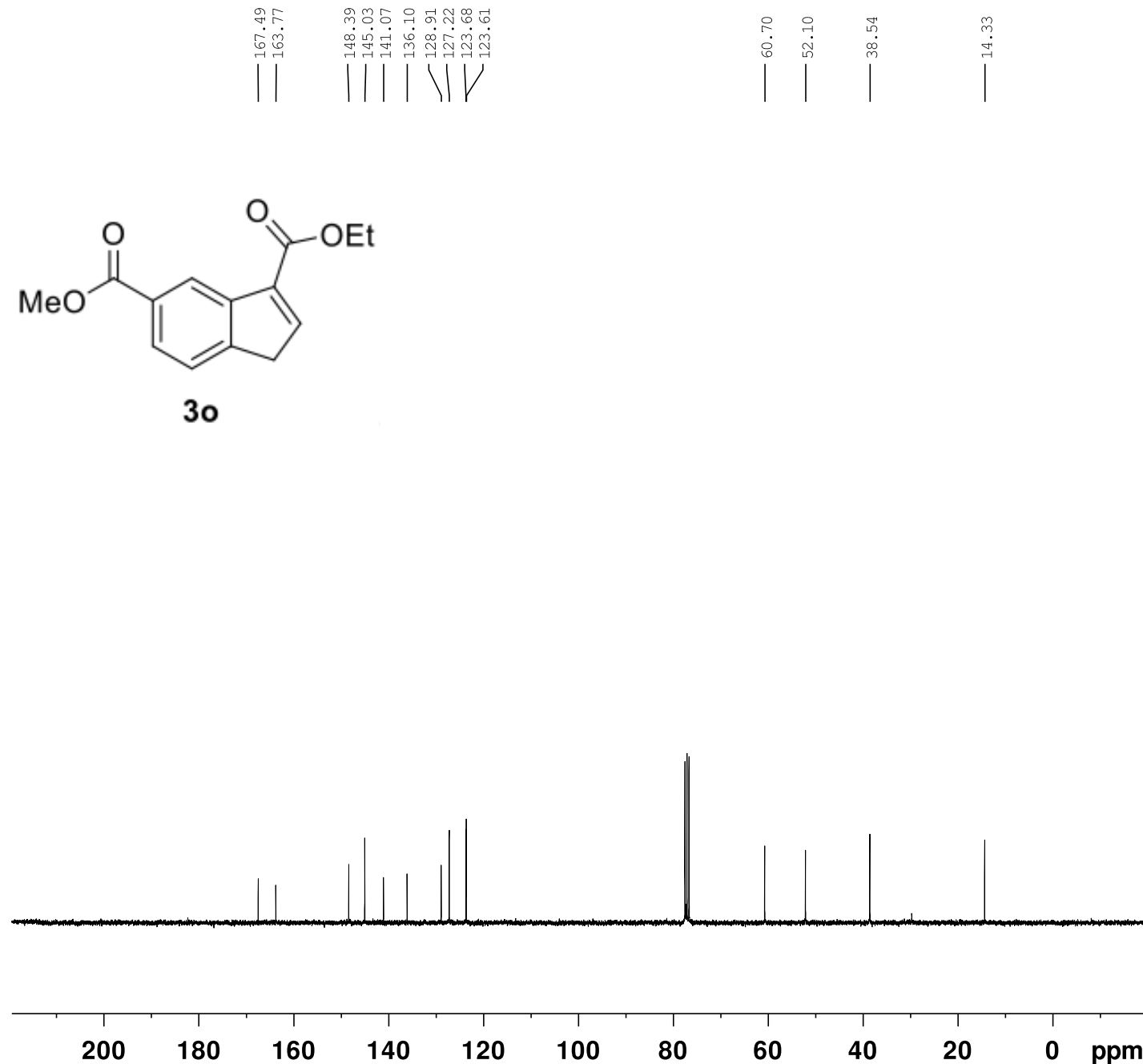
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

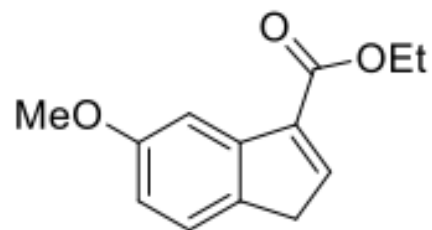
F2 - Processing parameters

SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



3o



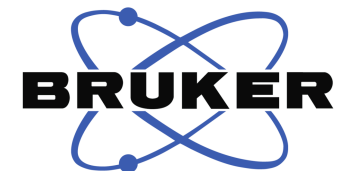


3p

7.647
7.640
7.478
7.352
7.325
6.843
6.836
6.816
6.809

4.402
4.378
4.354
4.331
3.859
3.449

1.431
1.407
1.383

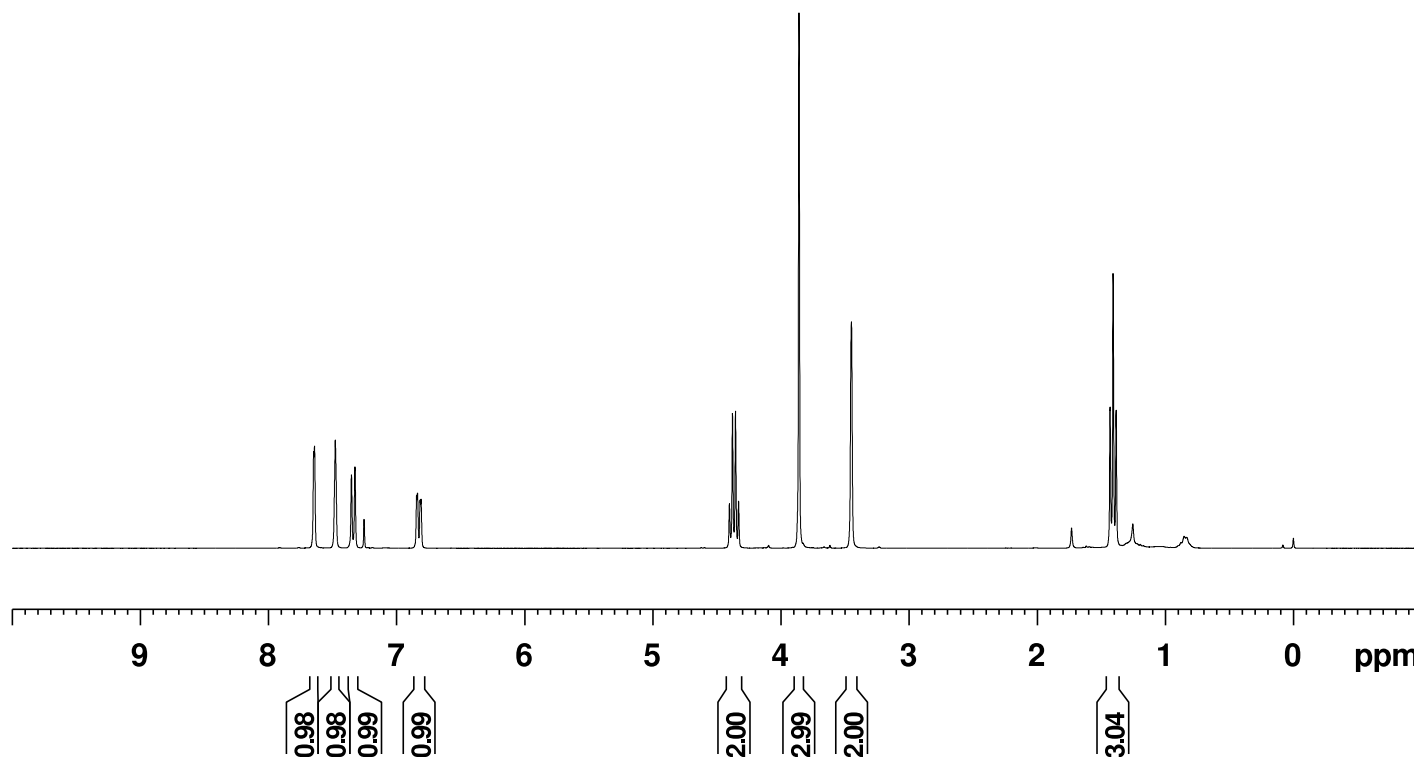


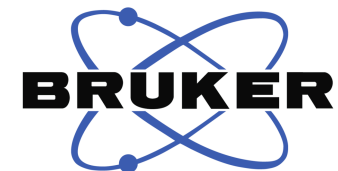
Current Data Parameters
NAME HNMR-YX-3-p85
EXPNO 54
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230331
Time 16.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 114
DW 83.200 usec
DE 6.50 usec
TE 289.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.130087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





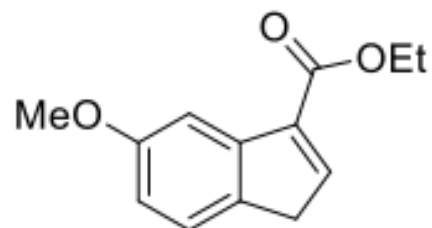
Current Data Parameters
 NAME CNMR-YX-3-p85
 EXPNO 55
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230331
 Time 17.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 250
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175317 sec
 RG 203
 DW 27.733 usec
 DE 6.50 usec
 TE 290.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

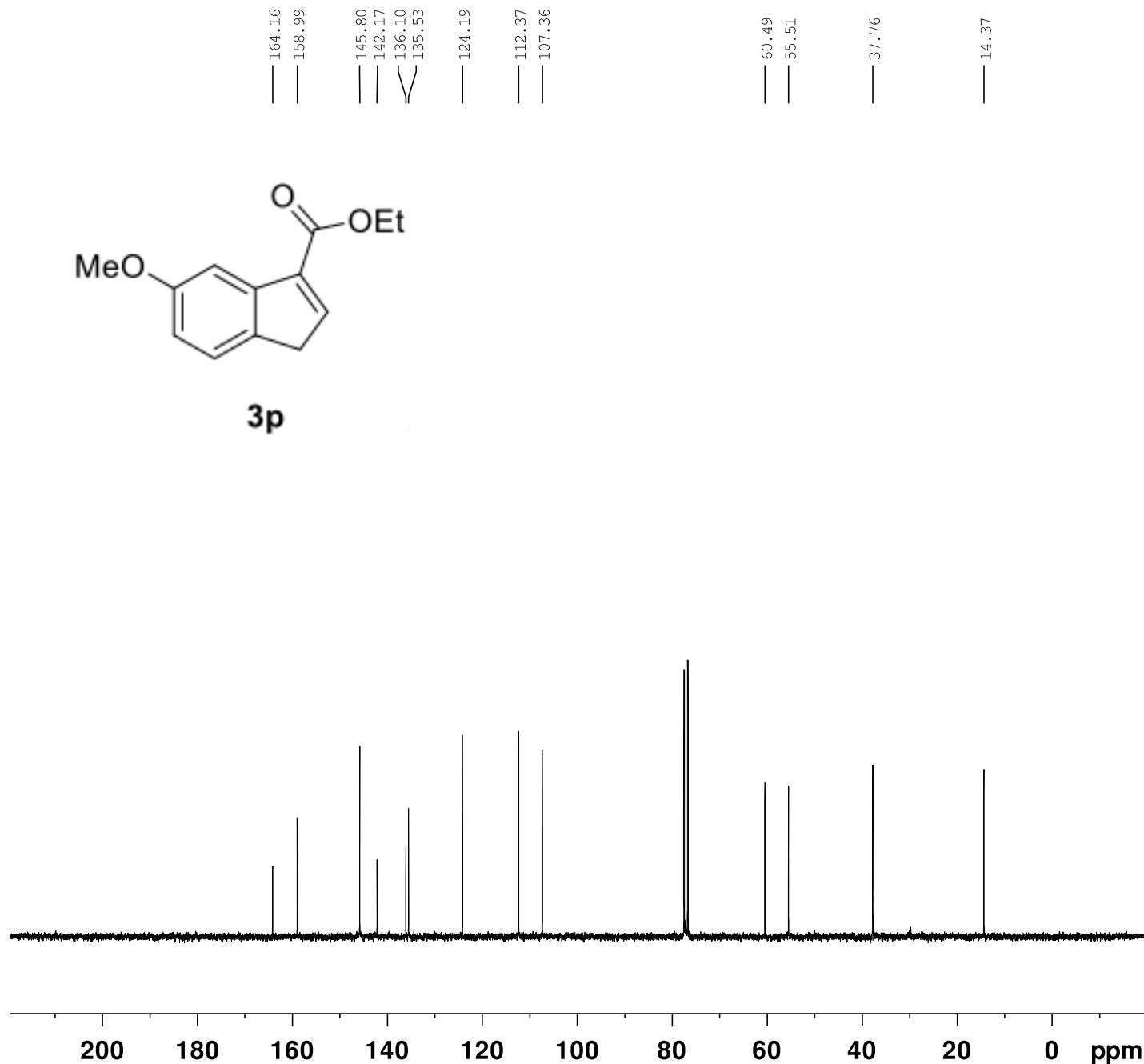
===== CHANNEL f1 =====
 SFO1 75.4752949 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 34.20000076 W

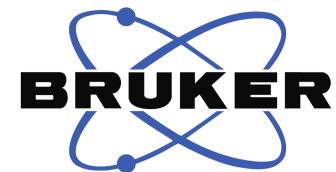
===== CHANNEL f2 =====
 SFO2 300.1312005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 14.00000000 W
 PLW12 0.17284000 W
 PLW13 0.14000000 W

F2 - Processing parameters
 SI 32768
 SF 75.4677485 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



3p





Current Data Parameters
NAME HNMR-YX-1-p75
EXPNO 460
PROCNO 1

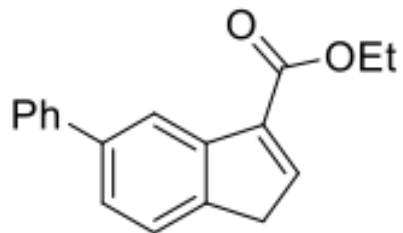
F2 - Acquisition Parameters
Date_ 20220721
Time 13.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

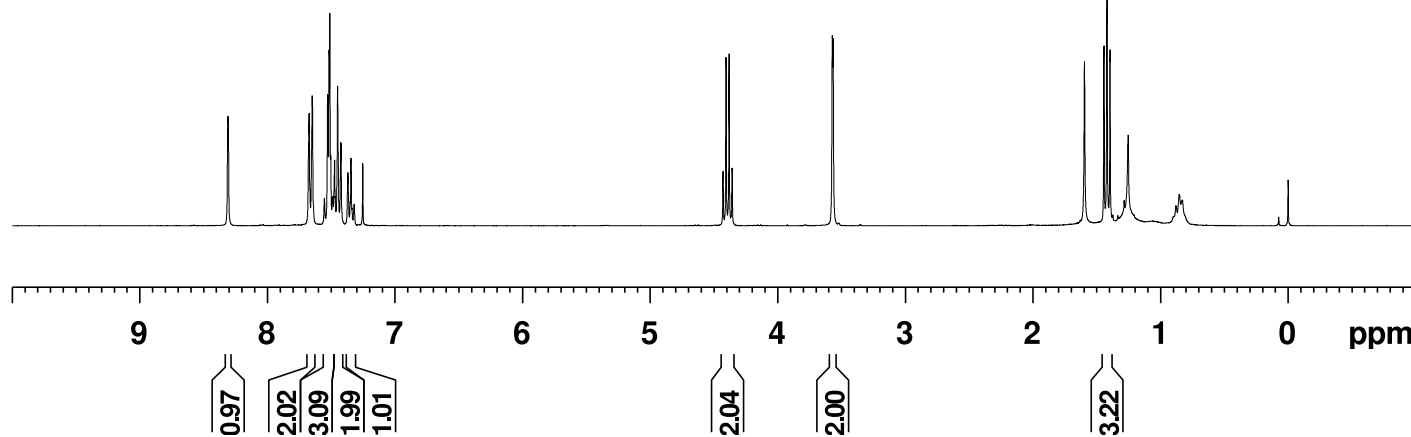
F2 - Processing parameters
SI 65536
SF 300.130094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

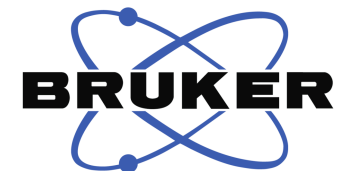
7.673
7.649
7.553
7.527
7.517
7.511
7.504
7.491
7.485
7.473
7.468
7.450
7.424
7.369
7.365
7.351
7.344
7.320
7.253
4.429
4.405
4.381
4.358
3.572
3.567

1.443
1.420
1.396



3q





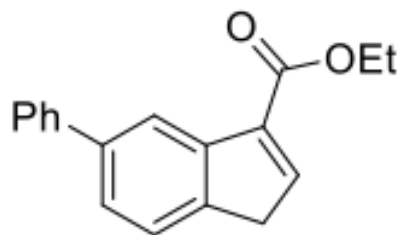
Current Data Parameters
 NAME CNMR-YX-1-p75
 EXPNO 469
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220721
 Time 23.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 200
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175317 sec
 RG 203
 DW 27.733 usec
 DE 6.50 usec
 TE -59.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

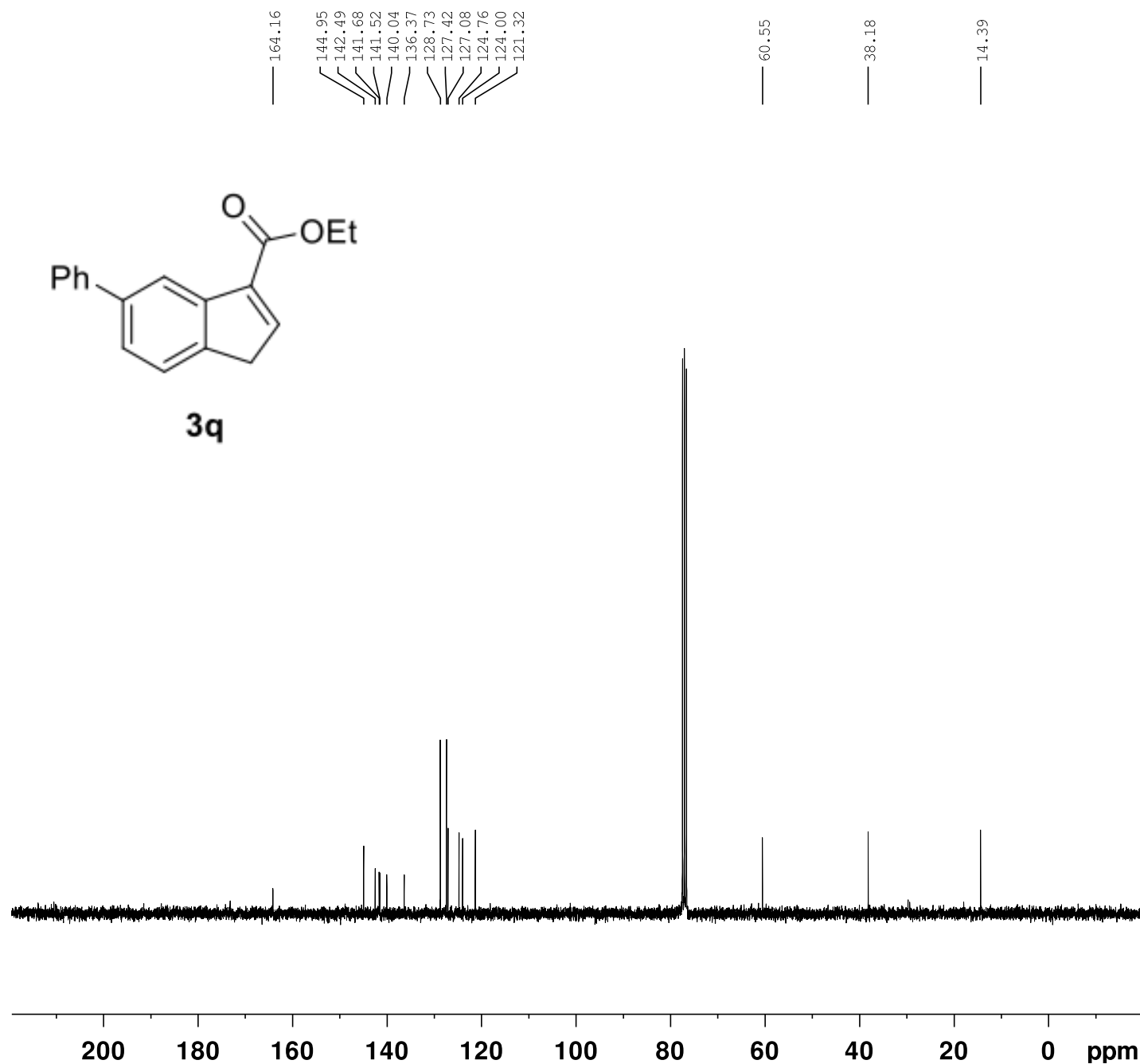
===== CHANNEL f1 =====
 SFO1 75.4752949 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 34.20000076 W

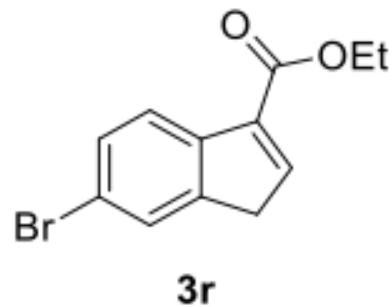
===== CHANNEL f2 =====
 SFO2 300.1312005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 14.00000000 W
 PLW12 0.17284000 W
 PLW13 0.14000000 W

F2 - Processing parameters
 SI 32768
 SF 75.4677485 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



3q

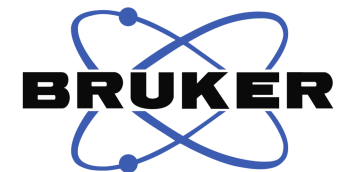




7.911
7.884
7.596
7.490
7.462
7.429
7.262

4.403
4.379
4.355
4.332
— 3.497

1.428
1.405
1.381

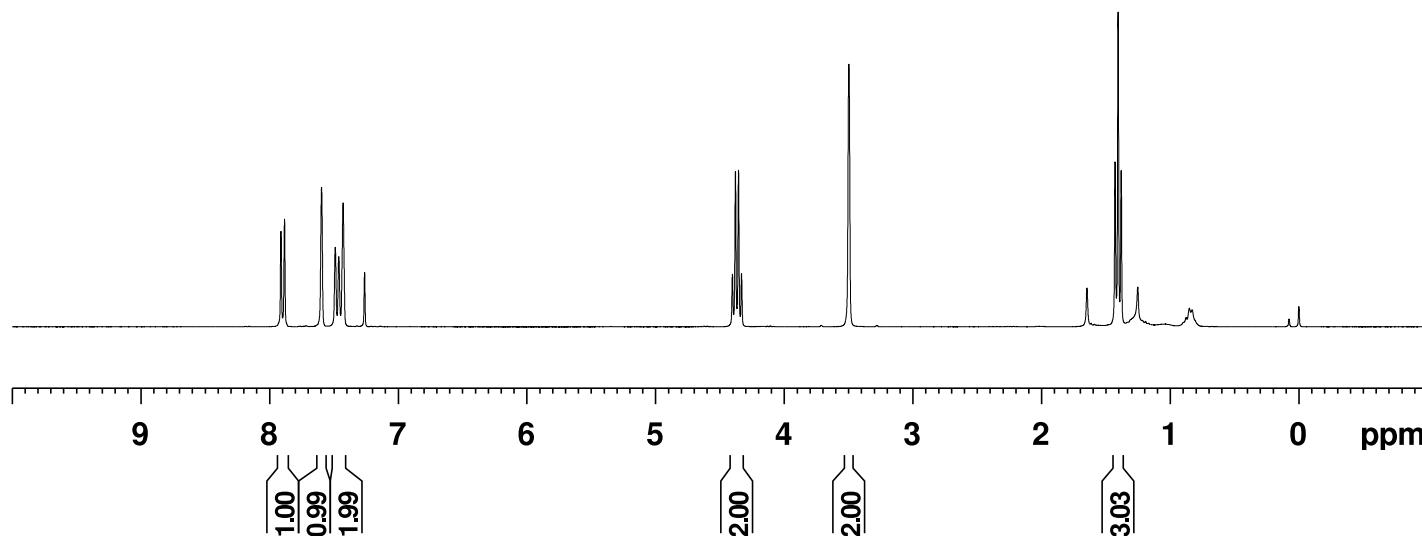


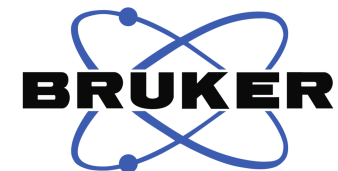
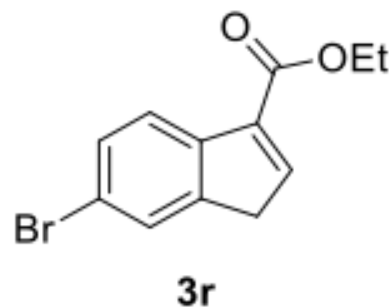
Current Data Parameters
NAME HNMR-YX-3-p89
EXPNO 56
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230331
Time 21.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE 291.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.130063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





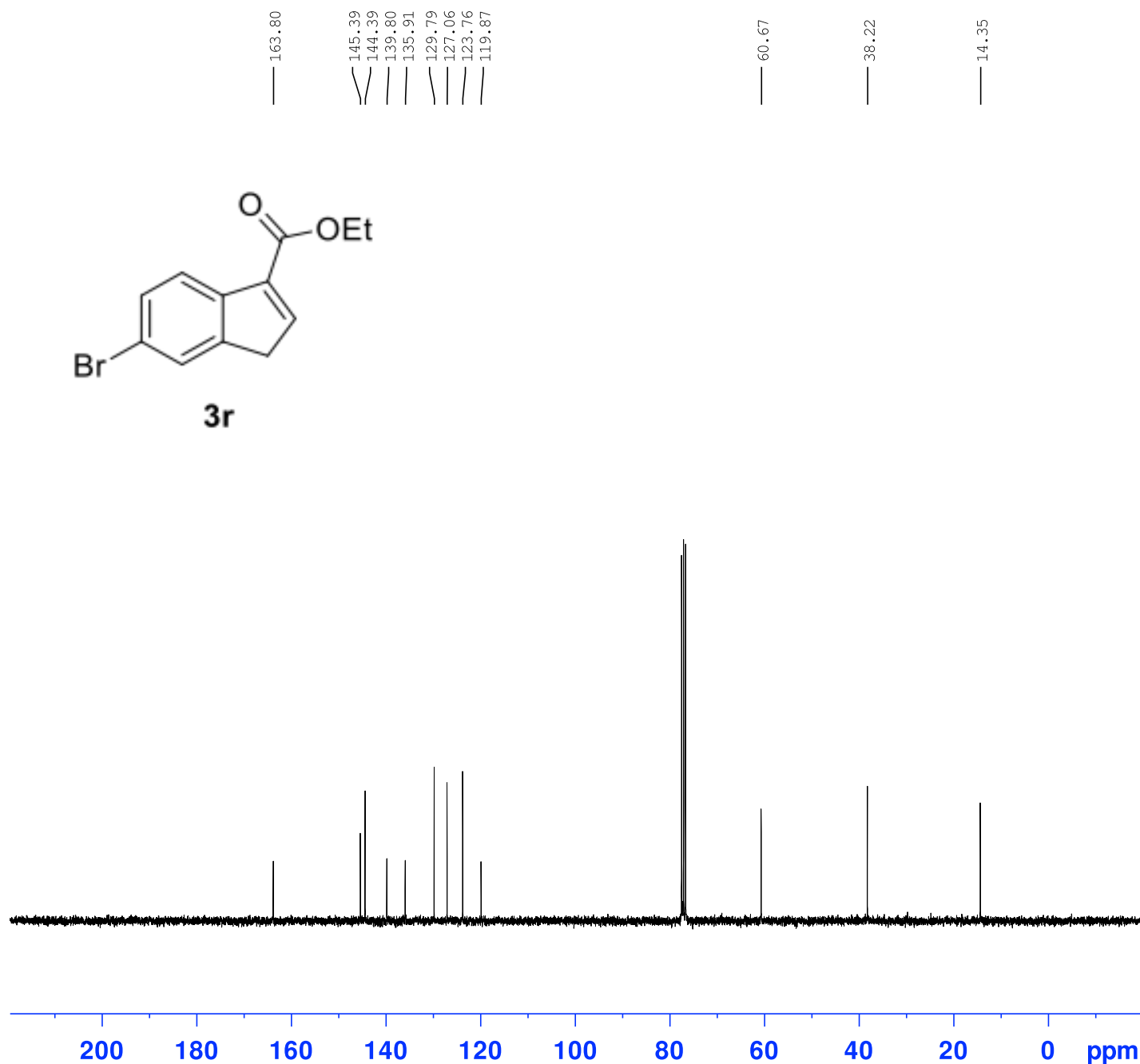
Current Data Parameters
 NAME CNMR-YX-3-p89
 EXPNO 57
 PROCNO 1

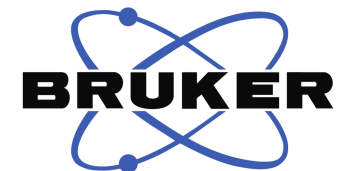
F2 - Acquisition Parameters
 Date_ 20230331
 Time 22.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 250
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175317 sec
 RG 203
 DW 27.733 usec
 DE 6.50 usec
 TE 291.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 75.4752949 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 34.20000076 W

===== CHANNEL f2 =====
 SFO2 300.1312005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 14.00000000 W
 PLW12 0.17284000 W
 PLW13 0.14000000 W

F2 - Processing parameters
 SI 32768
 SF 75.4677485 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



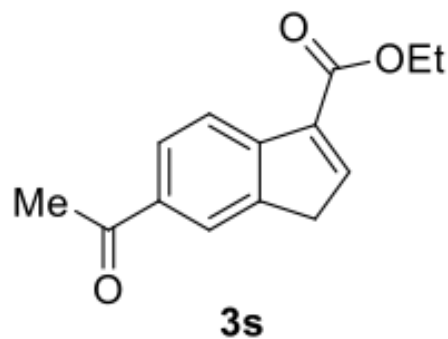


Current Data Parameters
 NAME HNMR-YX-4-pl6
 EXPNO 140
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230411
 Time 13.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.091699 Hz
 AQ 5.4525952 sec
 RG 101
 DW 83.200 usec
 DE 6.50 usec
 TE 292.6 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1318534 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 14.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1300013 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

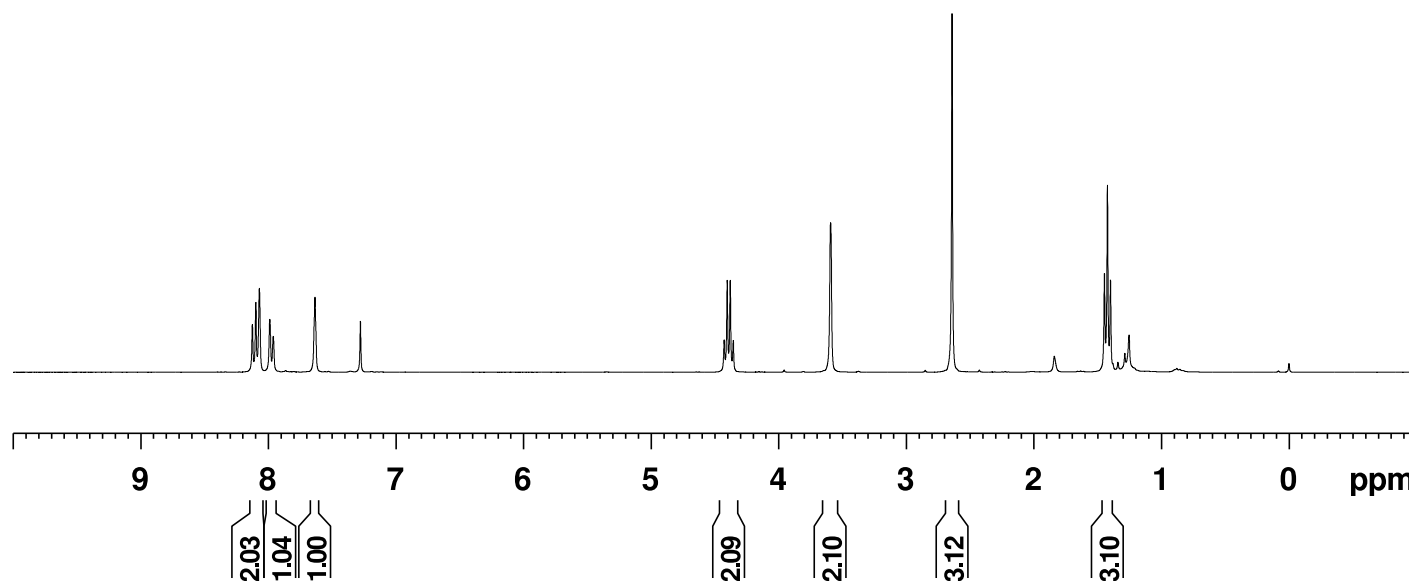


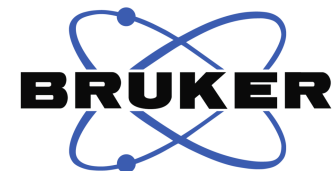
8.125
8.098
8.070
7.988
7.961
7.634
7.278

4.427
4.403
4.379
4.356
3.593

2.641

1.446
1.423
1.399





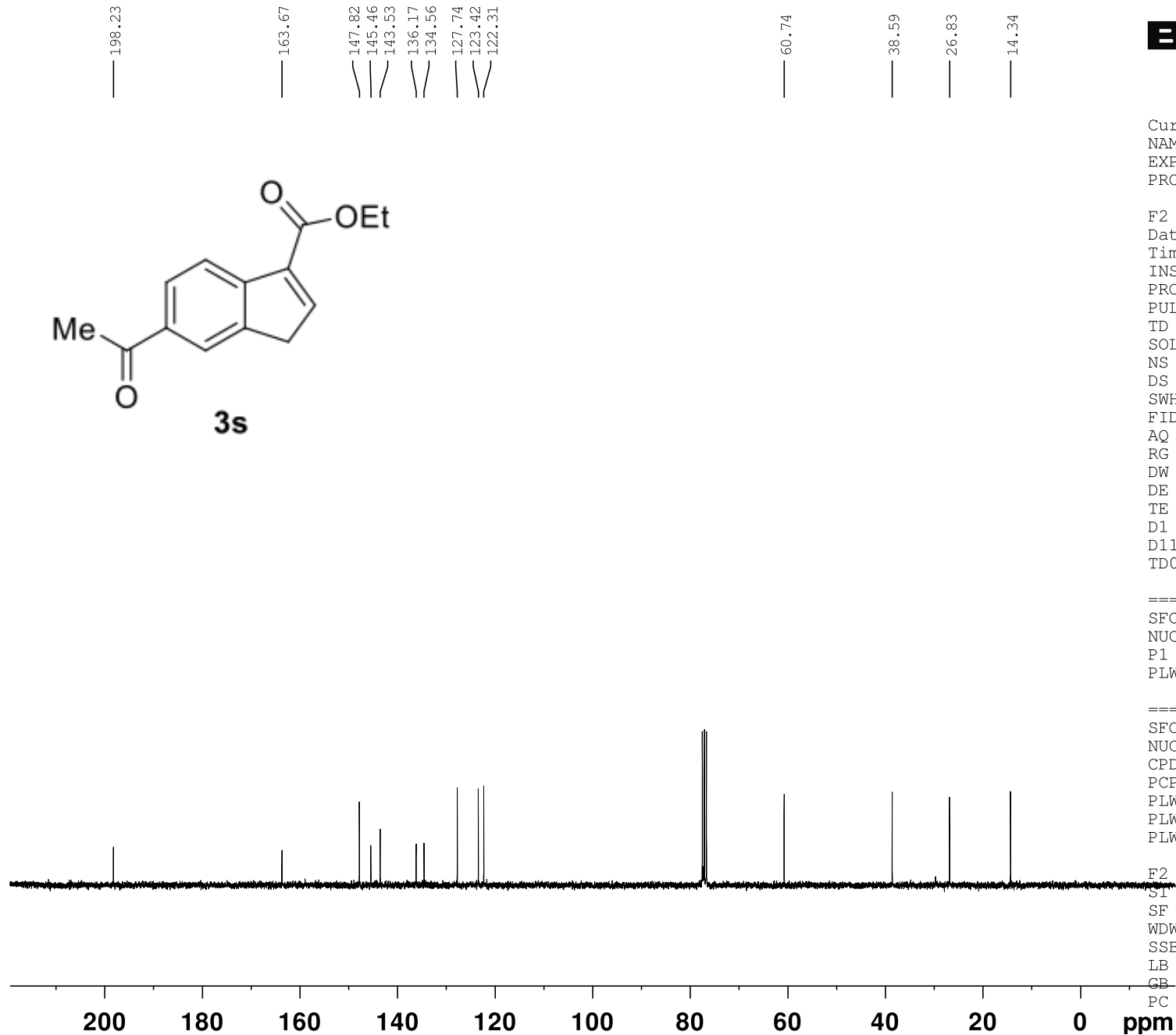
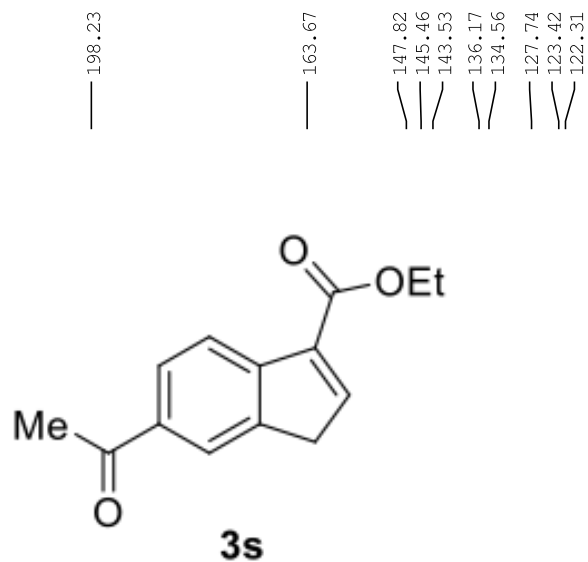
Current Data Parameters
NAME CNMR-YX-4-pl6
EXPNO 141
PROCNO 1

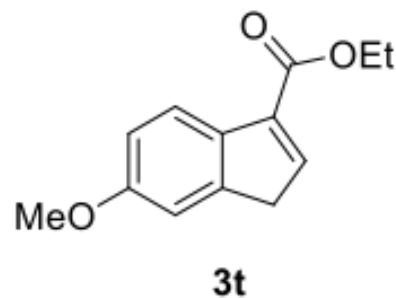
F2 - Acquisition Parameters
Date_ 20230411
Time 14.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 100
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 293.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





7.933
7.905
7.329
7.323
7.316
7.055
7.048
6.927
6.920
6.899
6.891

4.399
4.375
4.352
4.328
3.840
3.483
3.479

1.428
1.404
1.381

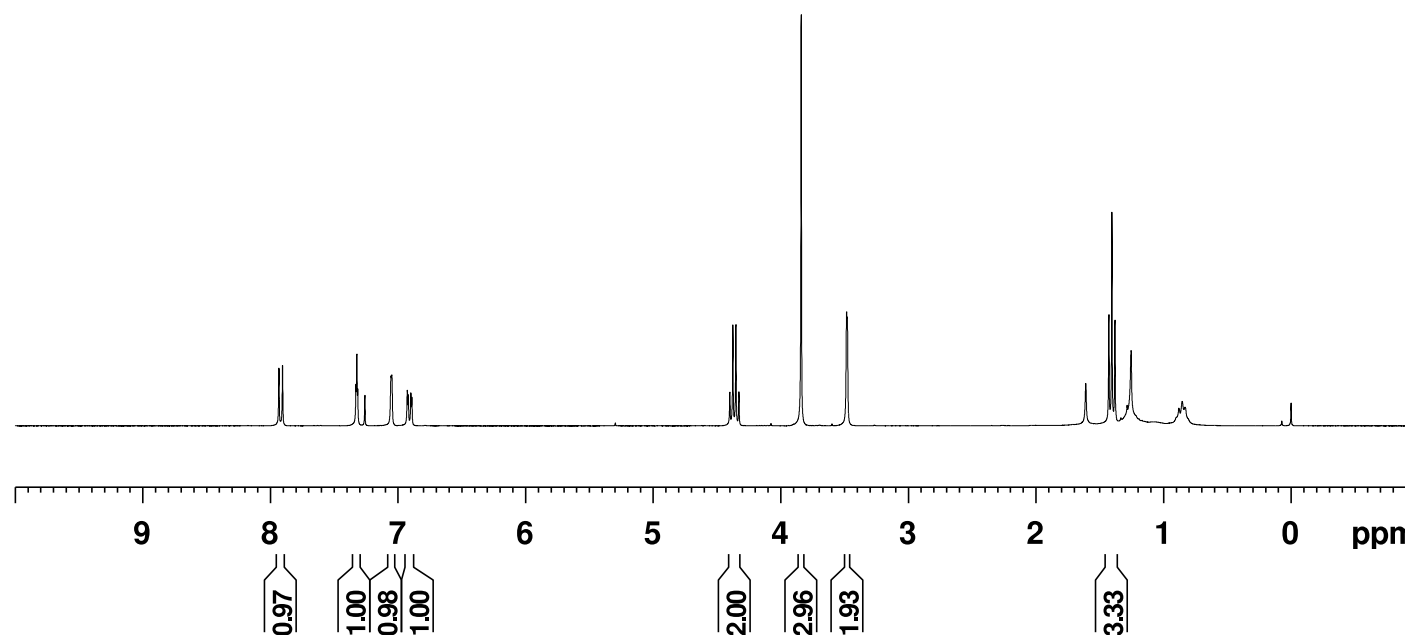


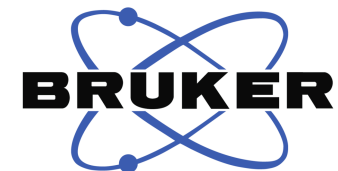
Current Data Parameters
NAME HNMR-YX-1-p68
EXPNO 499
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220725
Time 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.130072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





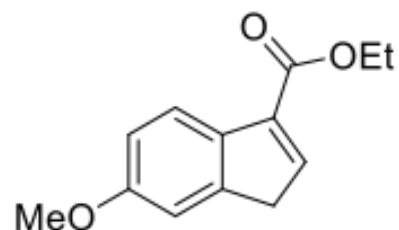
Current Data Parameters
NAME CNMR-YX-1-p68
EXPNO 69
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220725
Time 21.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

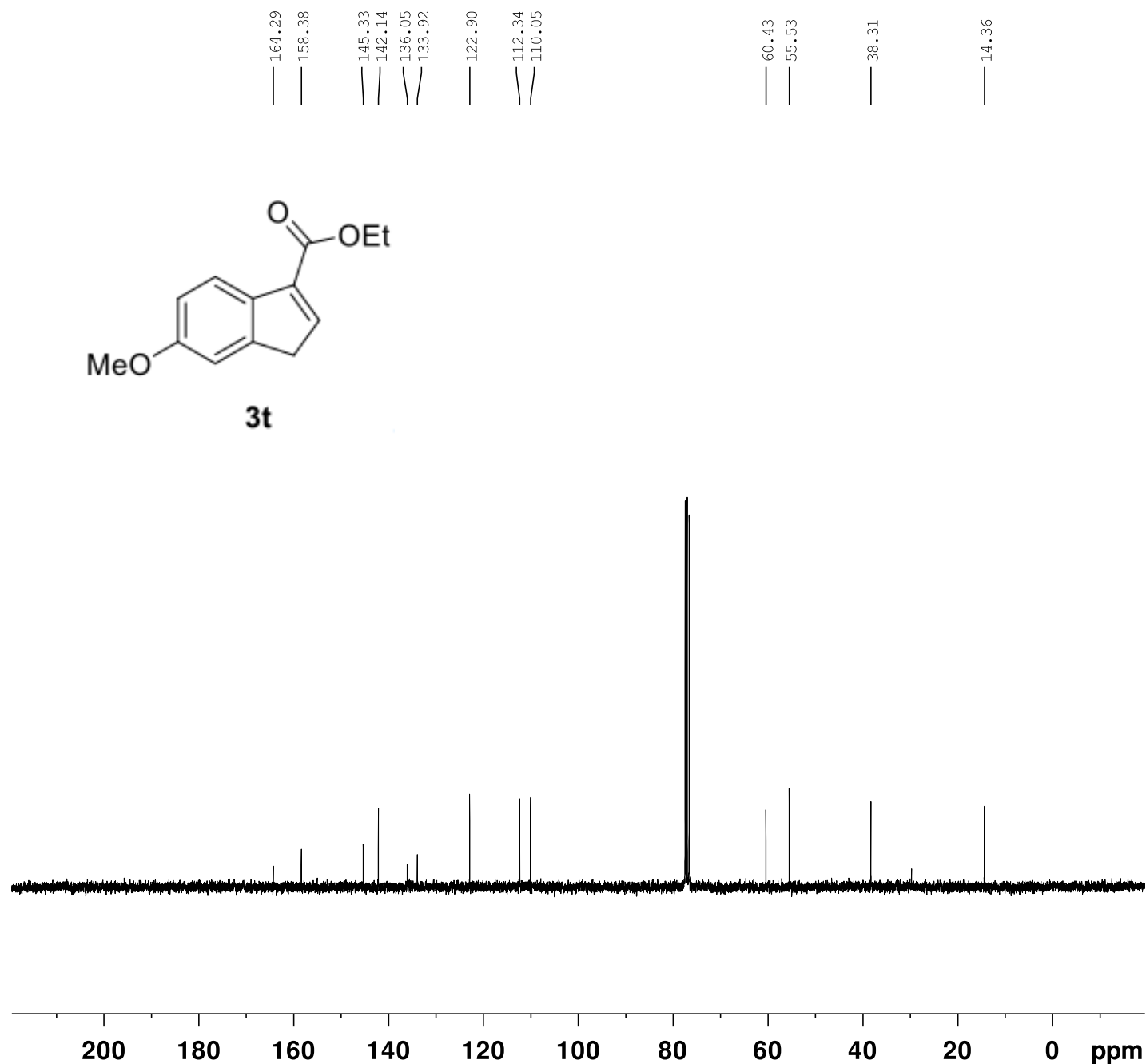
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



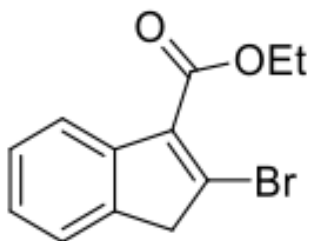
3t



7.784
7.759
7.325
7.300
7.251
7.228
7.203
7.179
7.175
7.154
7.150
7.130
7.126

4.356
4.332
4.308
4.285
3.695

1.369
1.345
1.322



3u

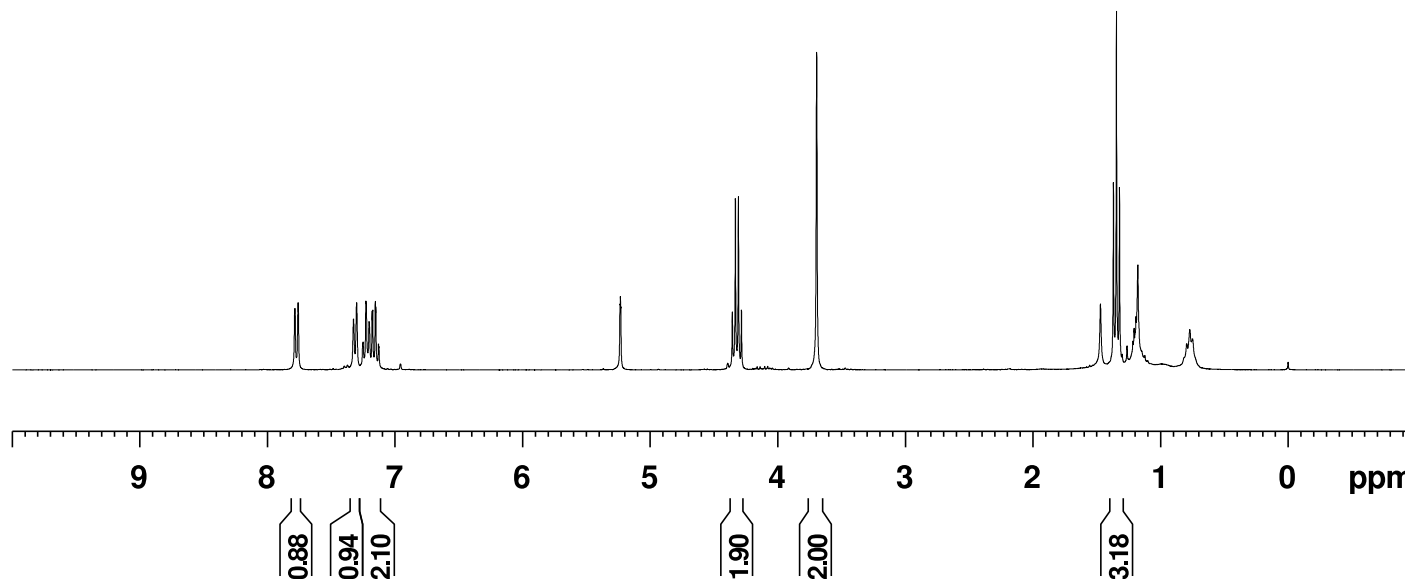


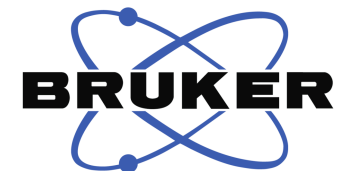
Current Data Parameters
NAME HNMR-YX-1-p70
EXPNO 446
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220719
Time 14.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300375 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME CNMR-YX-1-p70
EXPNO 450
PROCNO 1

F2 - Acquisition Parameters

Date_ 20220720
Time 15.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 200
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====

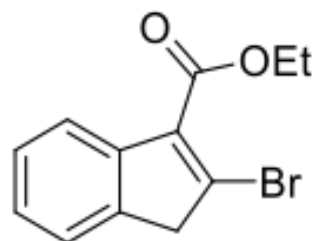
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====

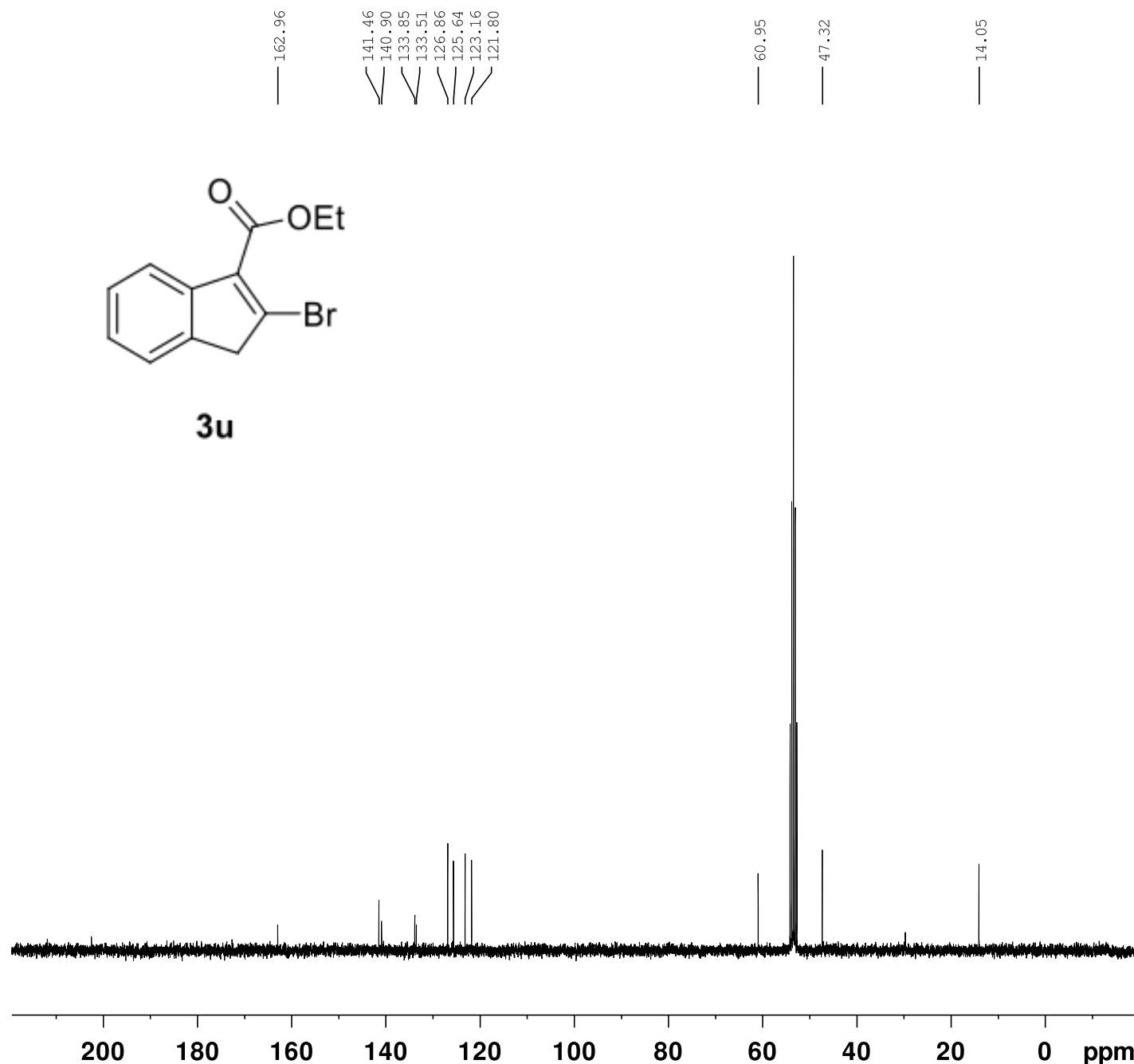
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters

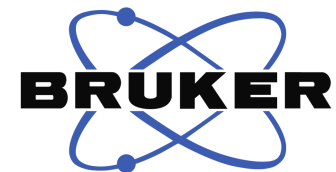
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



3u



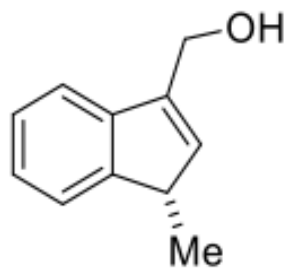
S64



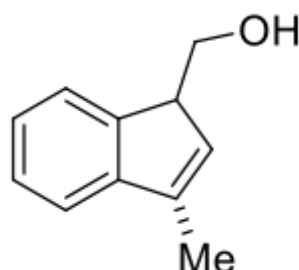
Current Data Parameters
 NAME HNMR-YX-3-p36
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230207
 Time 18.45 h
 INSTRUM Avance
 PROBHD Z116098_0833 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 65.4108
 DW 61.000 usec
 DE 13.54 usec
 TE 294.3 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1324708 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 20.73200035 W

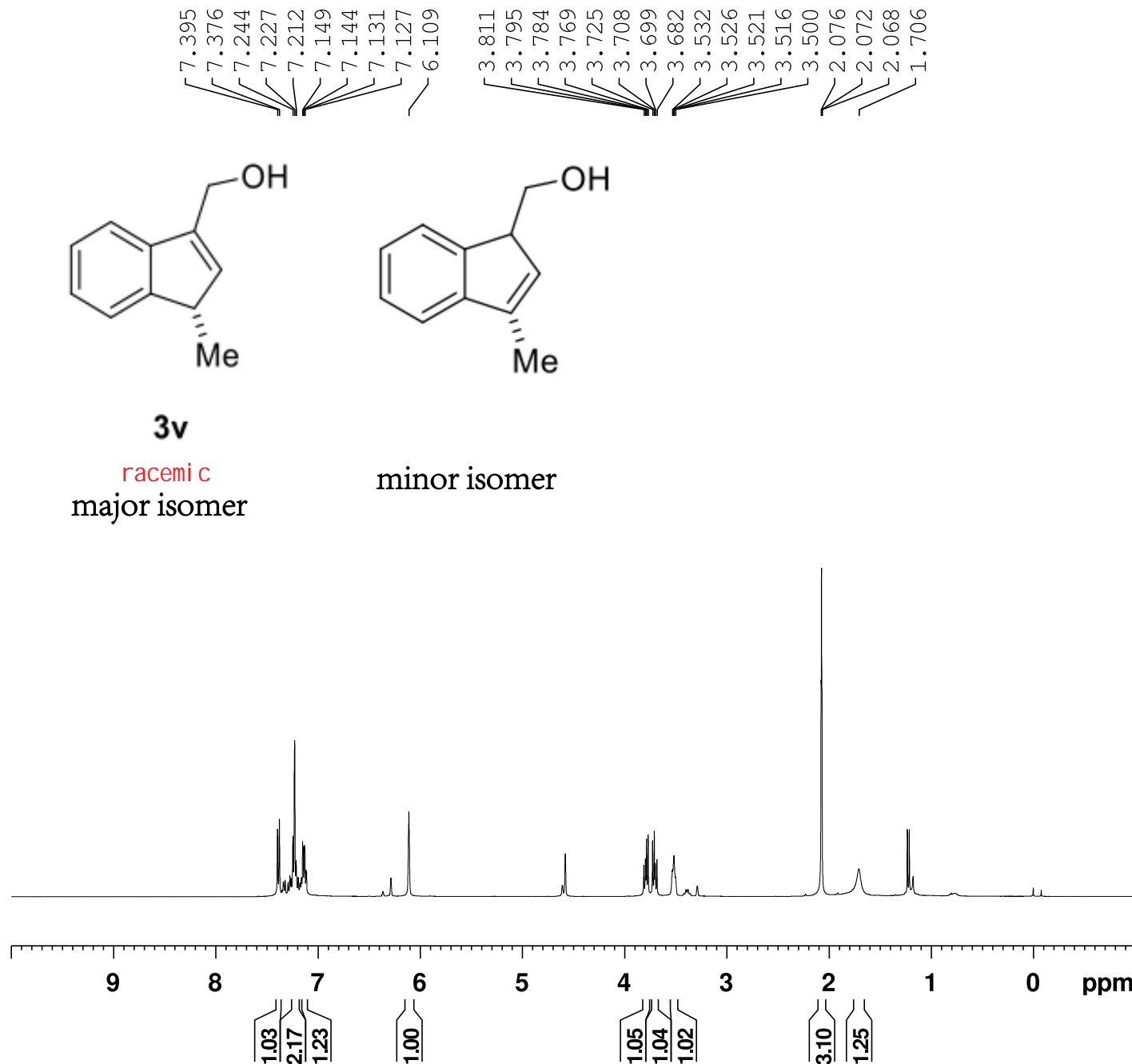
F2 - Processing parameters
 SI 65536
 SF 400.1300541 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

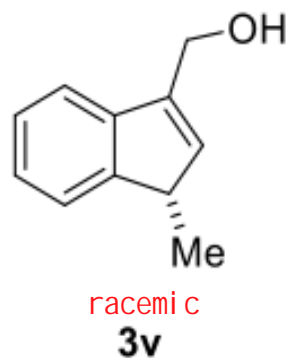


3v
 racemic
 major isomer



minor isomer



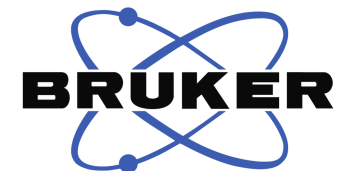


146.17
145.00
141.08
130.73
127.03
125.01
123.16
119.23

63.94

51.91

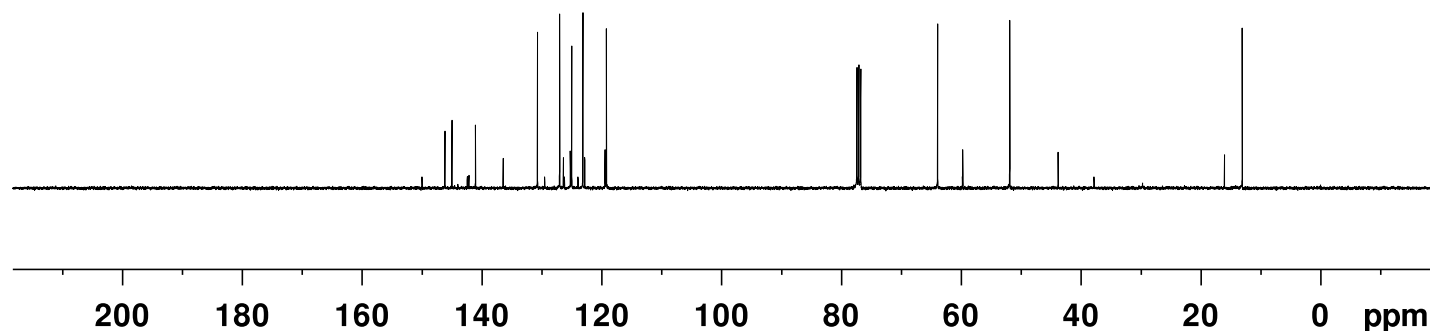
13.10

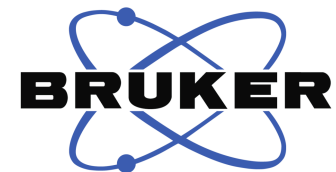


Current Data Parameters
NAME CNMR-YX-3-p36
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230208
Time 1.03 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 51.55
DW 21.000 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

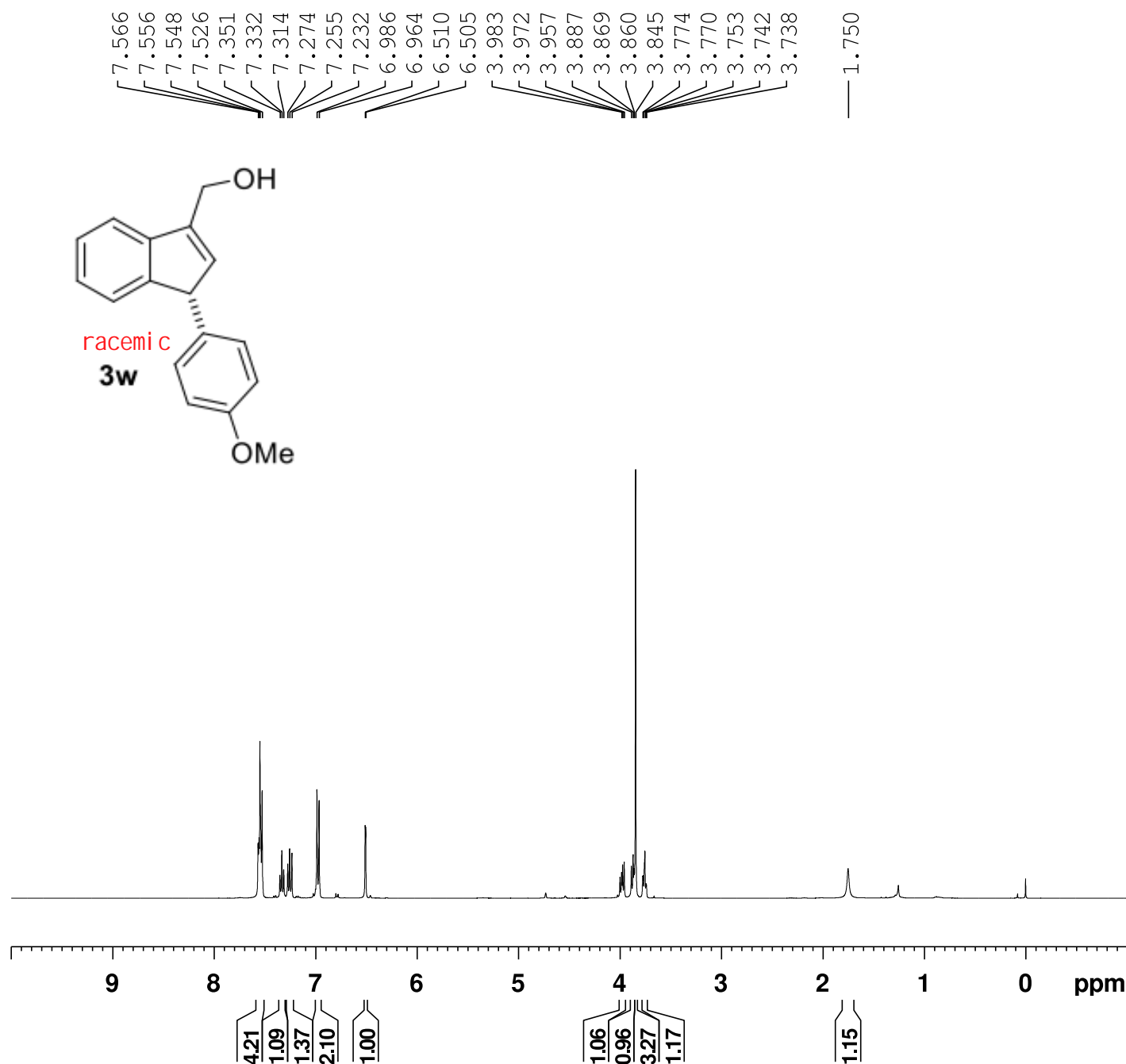
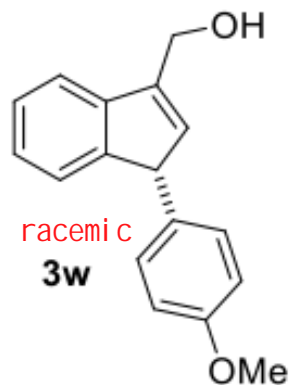


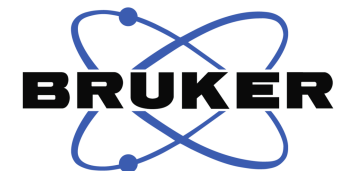


Current Data Parameters
NAME HNMR-YX-3-p44
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230214
Time 19.12 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 77.1605
DW 61.000 usec
DE 13.54 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

F2 - Processing parameters
SI 65536
SF 400.1300209 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

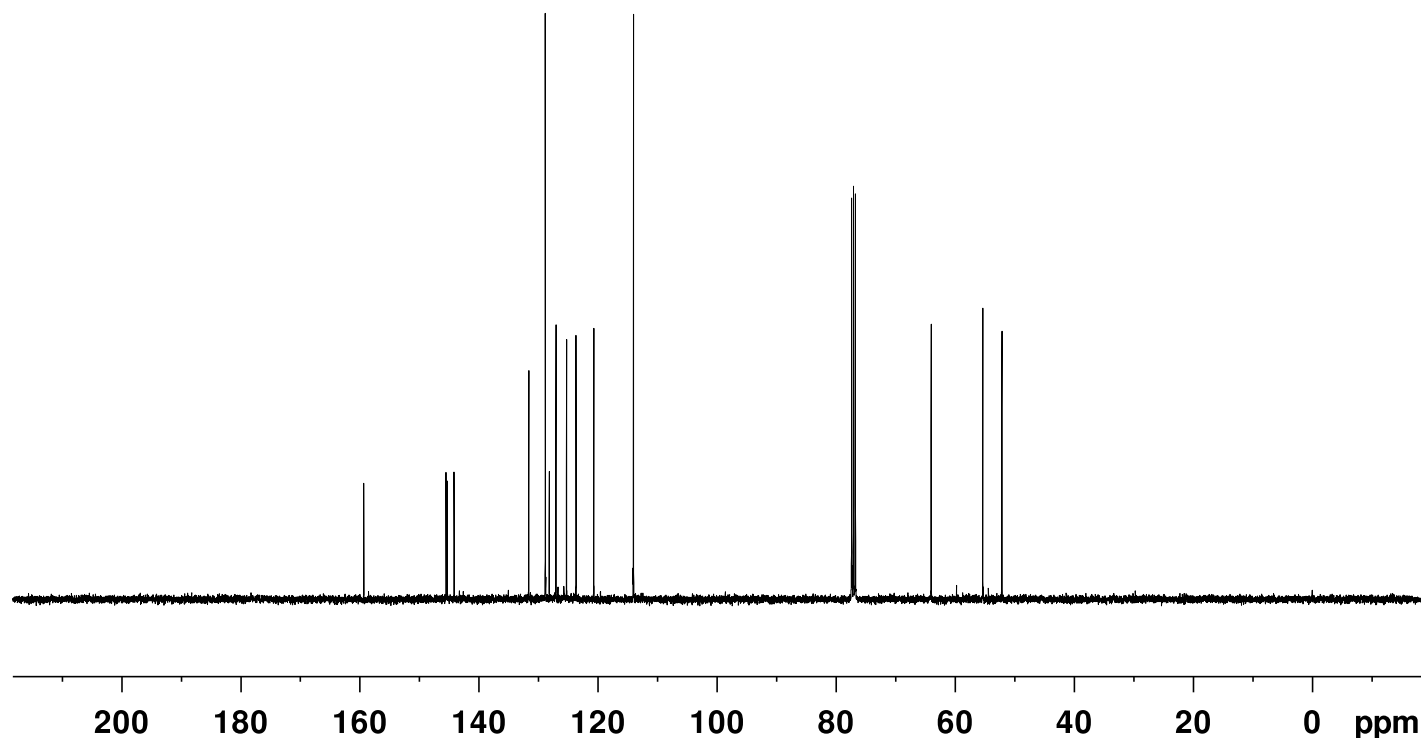
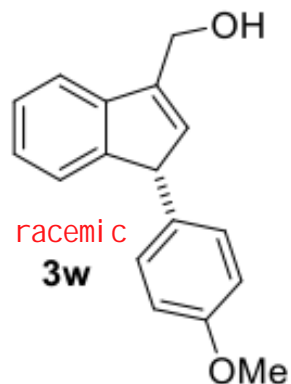


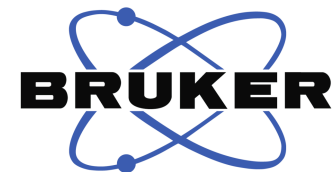


Current Data Parameters
NAME CNMR-YX-3-p44
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230215
Time 3.52 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 48.6724
DW 21.000 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

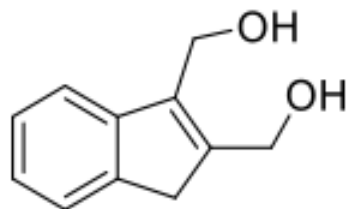




Current Data Parameters
NAME HNMR-YX-3-p35 (A)
EXPNO 1
PROCNO 1

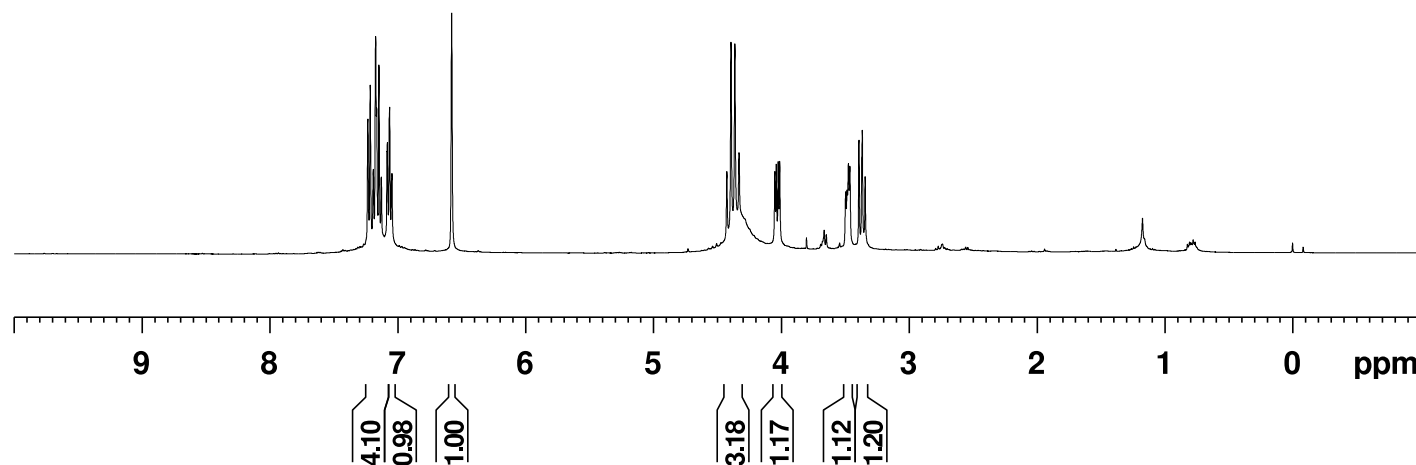
F2 - Acquisition Parameters
Date_ 20230207
Time 18.26 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 42.5532
DW 61.000 usec
DE 13.54 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

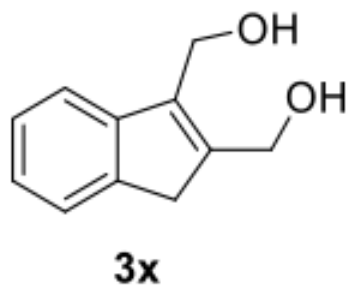
F2 - Processing parameters
SI 65536
SF 400.1300547 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3x

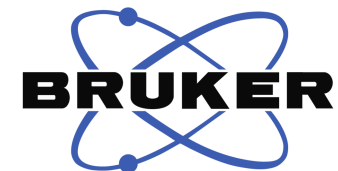
7.233
7.214
7.190
7.172
7.164
7.146
7.127
7.083
7.080
7.065
7.062
7.047
7.044
6.577
4.425
4.392
4.362
4.330
4.050
4.038
4.023
4.012
3.495
3.484
3.474
3.463
3.392
3.365
3.343





149.98
143.87
143.69
130.20
127.28
125.20
123.20
121.27

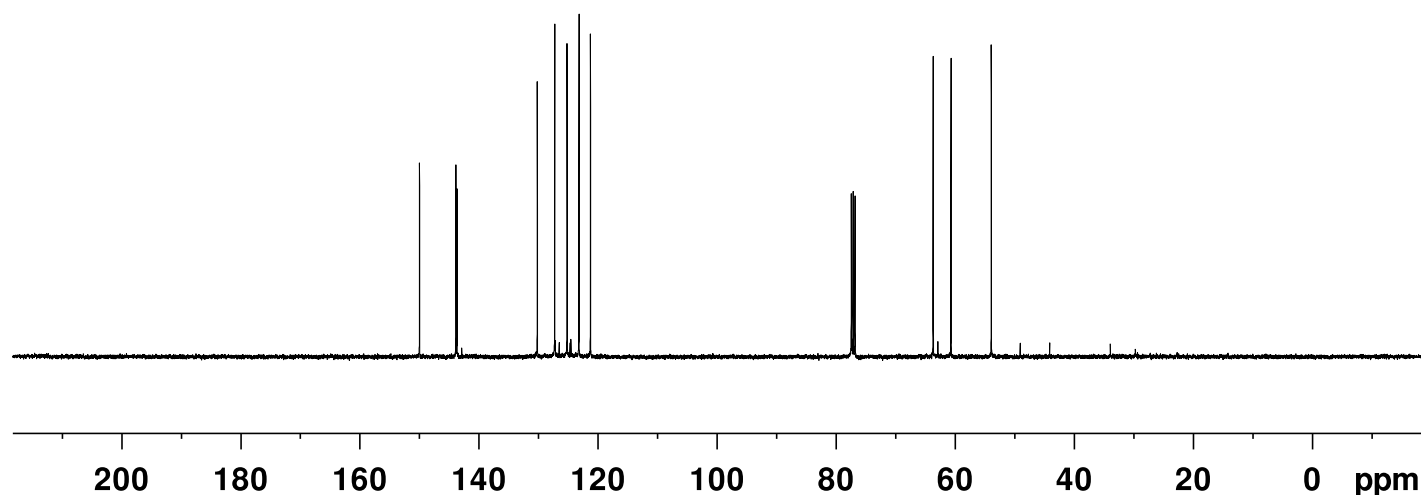
63.71
60.72
53.95



Current Data Parameters
NAME CNMR-YX-3-p35 (A)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230209
Time 0.02 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 50.1934
DW 21.000 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

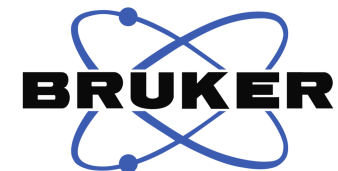
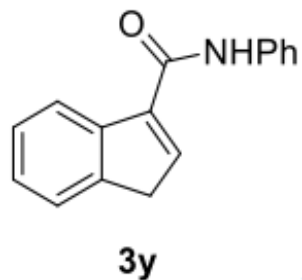
F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



S70

10.206
7.958
7.939
7.801
7.782
7.550
7.532
7.422
7.418
7.413
7.380
7.361
7.341
7.335
7.316
7.284
7.281
7.265
7.263
7.247
7.244
7.120
7.101
7.083

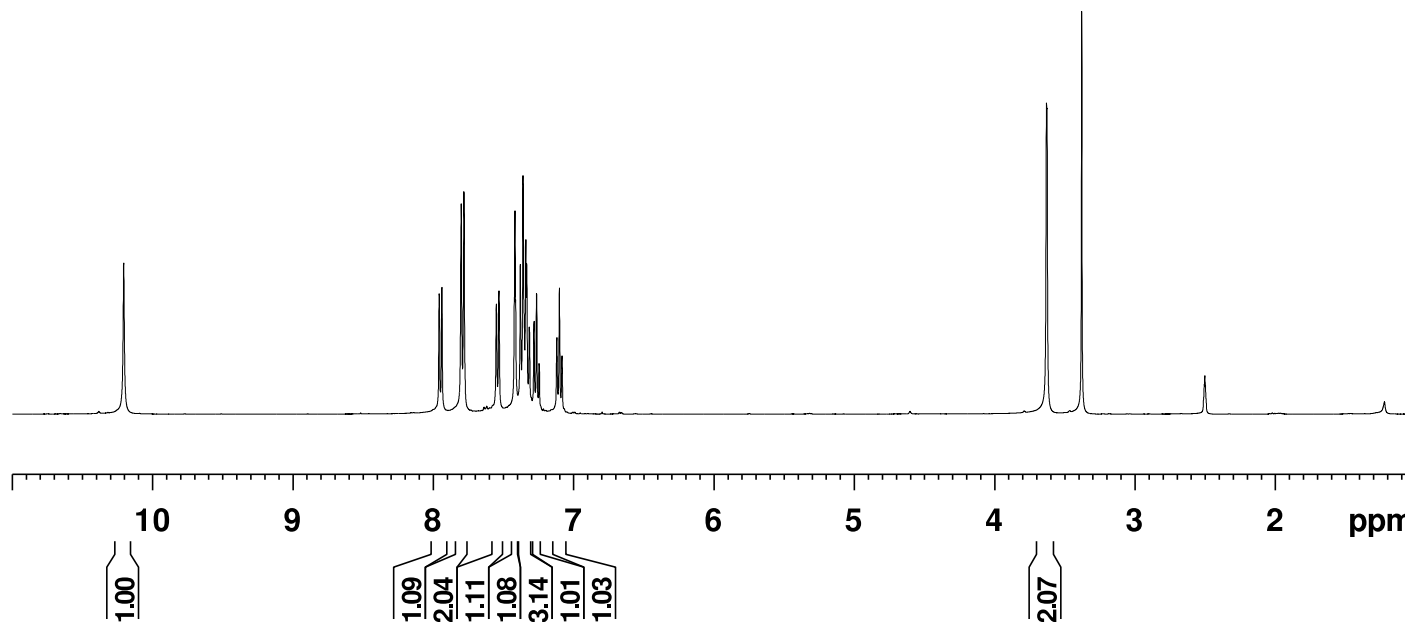
3.631
3.628

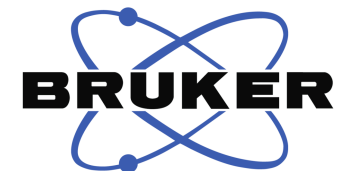


Current Data Parameters
NAME HNMR-YX-3-p55
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230228
Time 3.44 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 93.7735
DW 61.000 usec
DE 13.54 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

F2 - Processing parameters
SI 65536
SF 400.1300025 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

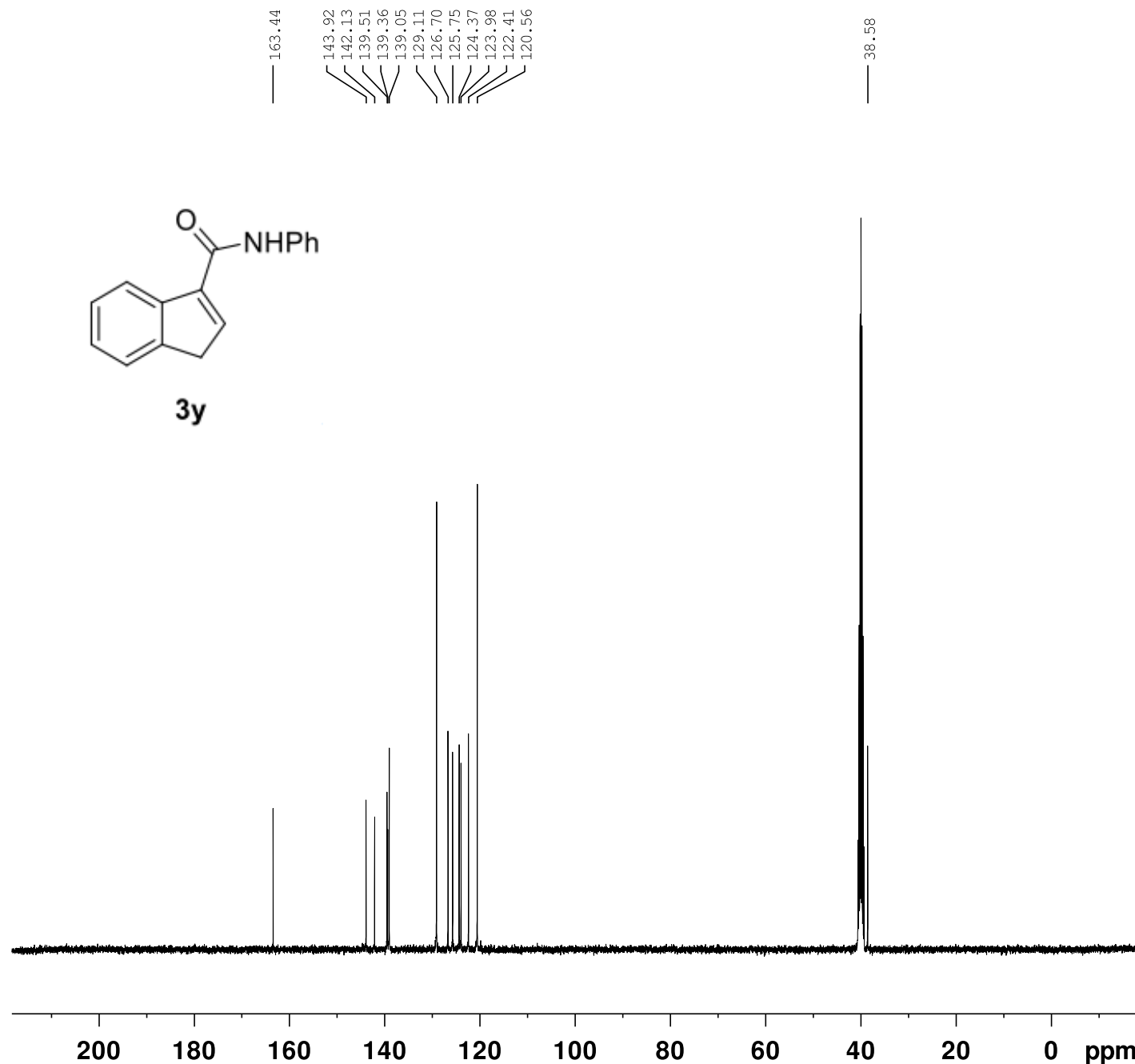
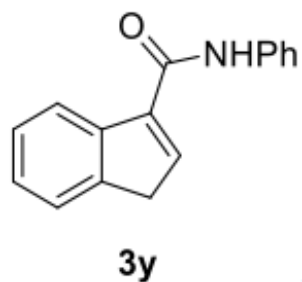




Current Data Parameters
 NAME CNMR-YX-3-p55
 EXPNO 2
 PROCNO 1

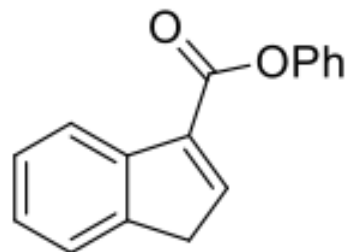
F2 - Acquisition Parameters
 Date_ 20230228
 Time 4.08 h
 INSTRUM Avance
 PROBHD Z116098_0833 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 400
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 51.55
 DW 21.000 usec
 DE 6.50 usec
 TE 295.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6228298 MHz
 NUC1 ¹³C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 87.89900208 W
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 20.73200035 W
 PLW12 0.25595000 W
 PLW13 0.12874000 W

F2 - Processing parameters
 SI 32768
 SF 100.6127685 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

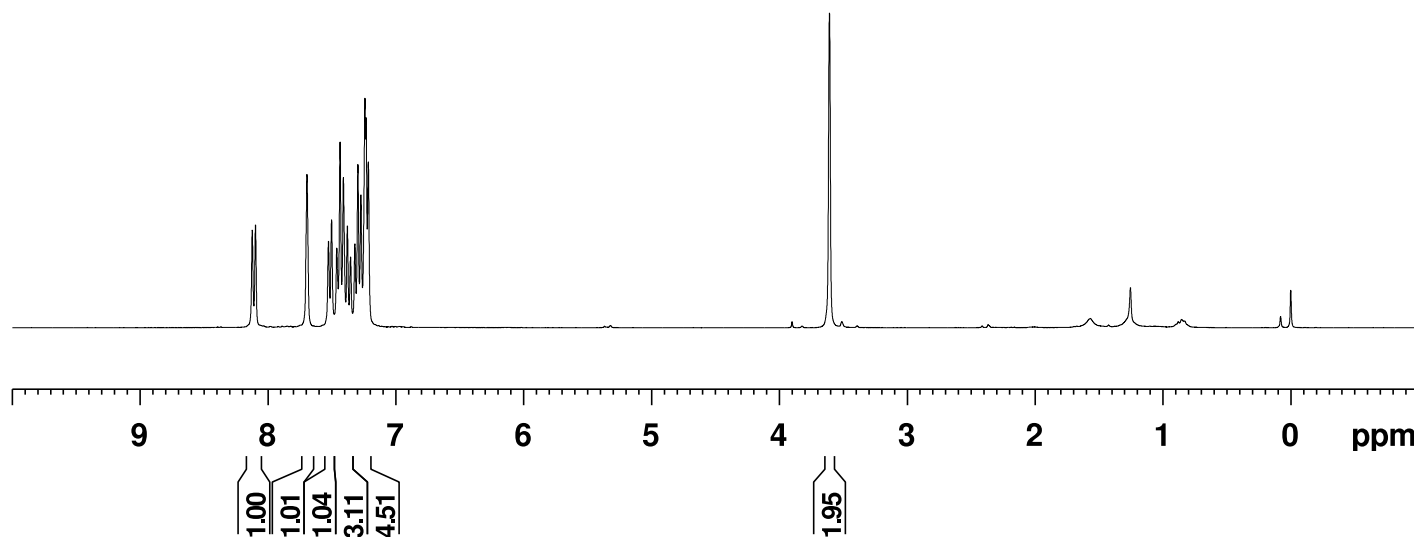


8.123
8.097
7.695
7.527
7.502
7.462
7.436
7.410
7.379
7.354
7.320
7.296
7.273
7.241
7.232
7.215

— 3.608



3z

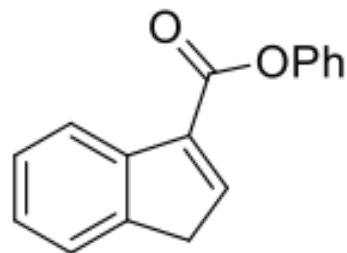


Current Data Parameters
NAME HNMR-YX-3-p83
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230403
Time 13.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

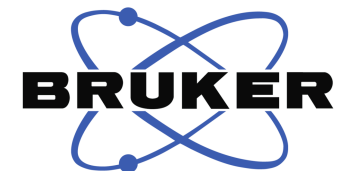
F2 - Processing parameters
SI 65536
SF 300.1300155 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3z

162.35
150.60
146.34
143.30
140.50
135.68
129.56
126.87
125.96
125.87
123.91
122.53
121.83

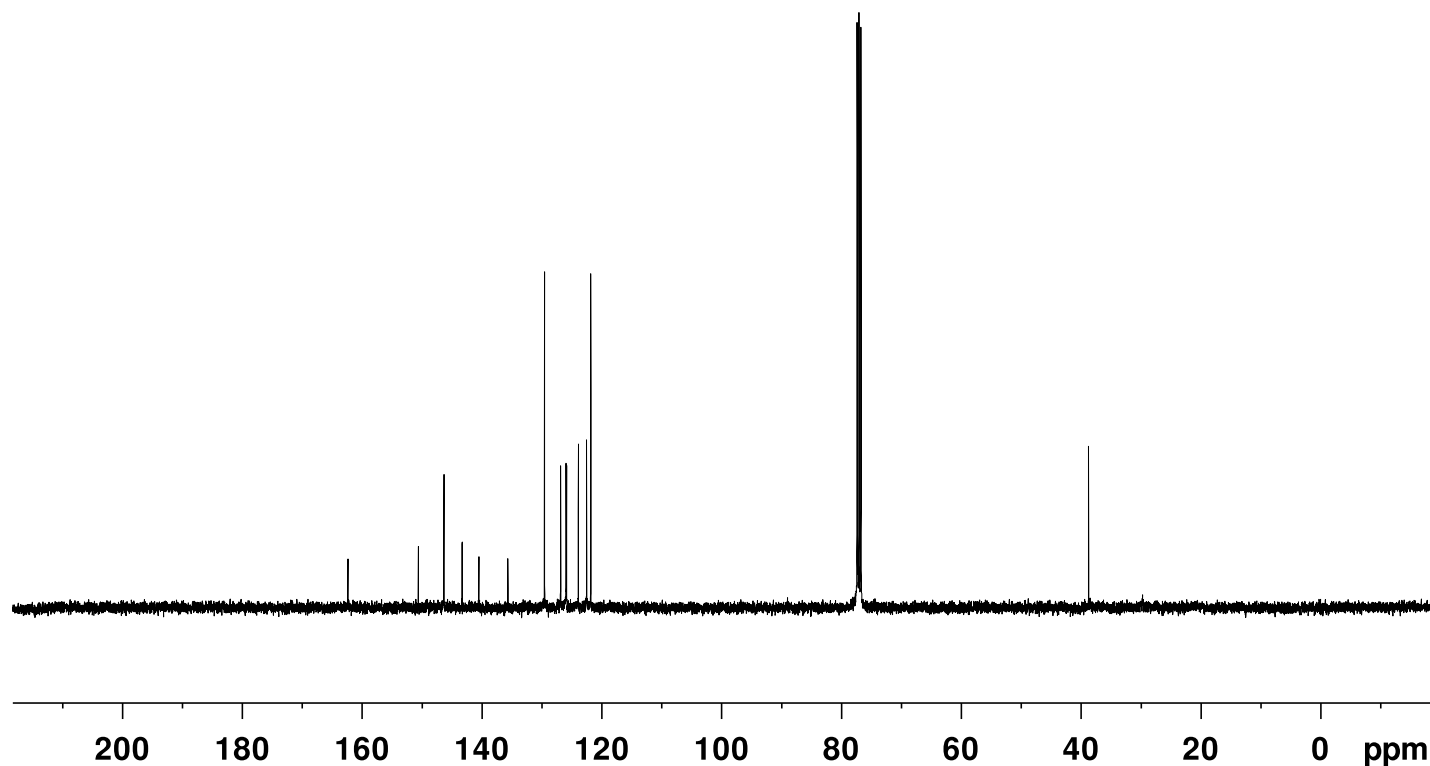
38.76

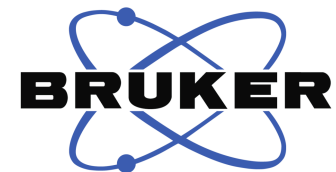


Current Data Parameters
NAME CNMR-YX-3-p83
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230329
Time 4.24 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 46.0295
DW 21.000 usec
DE 6.50 usec
TE 293.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



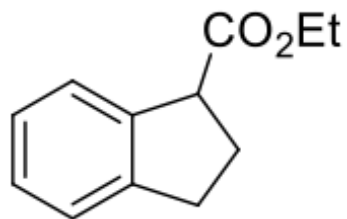


Current Data Parameters
 NAME HNMR-YX-3-p32
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230207
 Time 18.20 h
 INSTRUM Avance
 PROBHD Z116098_0833 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 86.8056
 DW 61.000 usec
 DE 13.54 usec
 TE 294.3 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1324708 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 20.73200035 W

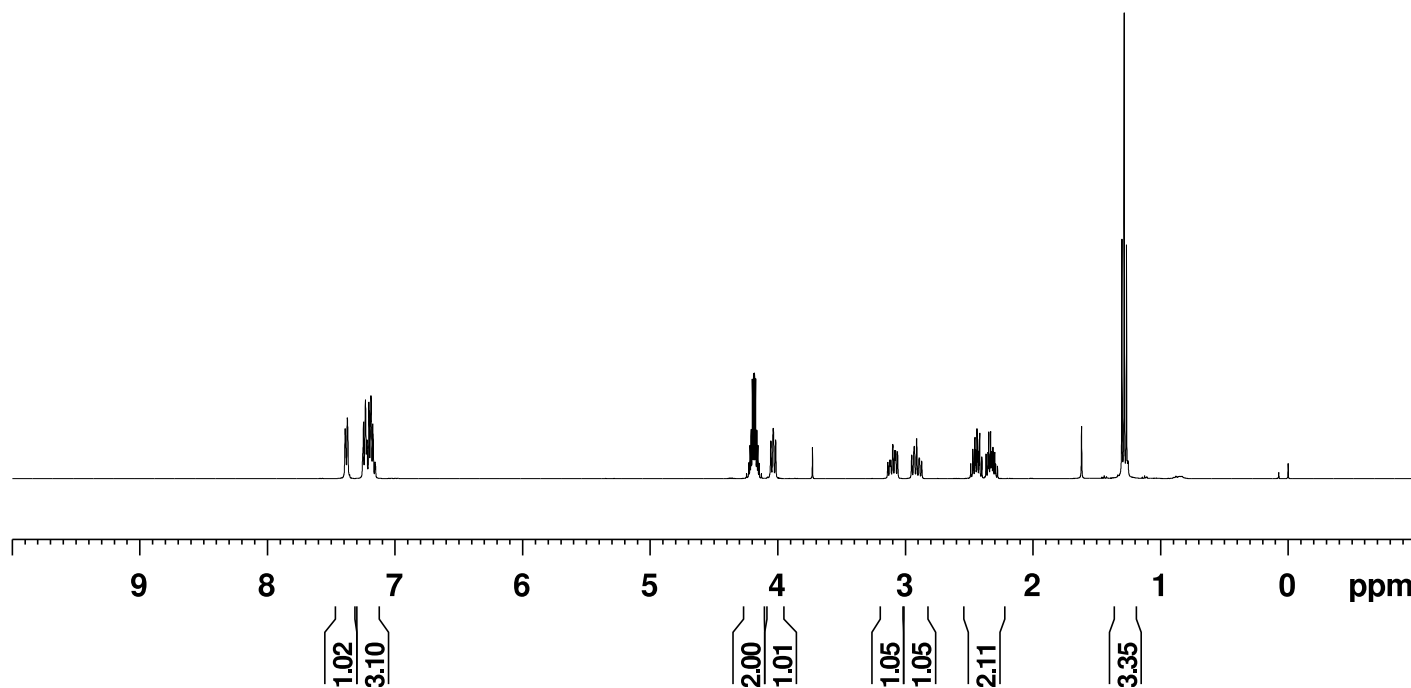
F2 - Processing parameters
 SI 65536
 SF 400.1300149 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

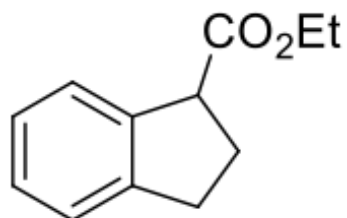
7.391
7.374
7.371
7.247
7.232
7.223
7.219
7.205
7.202
7.193
7.188
7.175
7.171
4.218
4.209
4.200
4.191
4.182
4.173
4.164
4.155
4.054
4.036
4.017
3.099
3.083
3.075
2.931
2.911
2.471
2.455
2.449
2.439
2.433
2.417
2.346
2.332
2.314
1.303
1.285
1.267



4a

racemic





4a

racemic

173.94

144.15
140.87

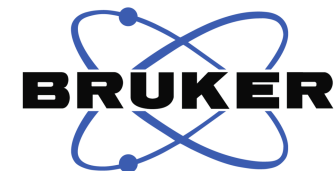
127.49
126.41
124.75
124.69

60.77

50.23

31.78
28.66

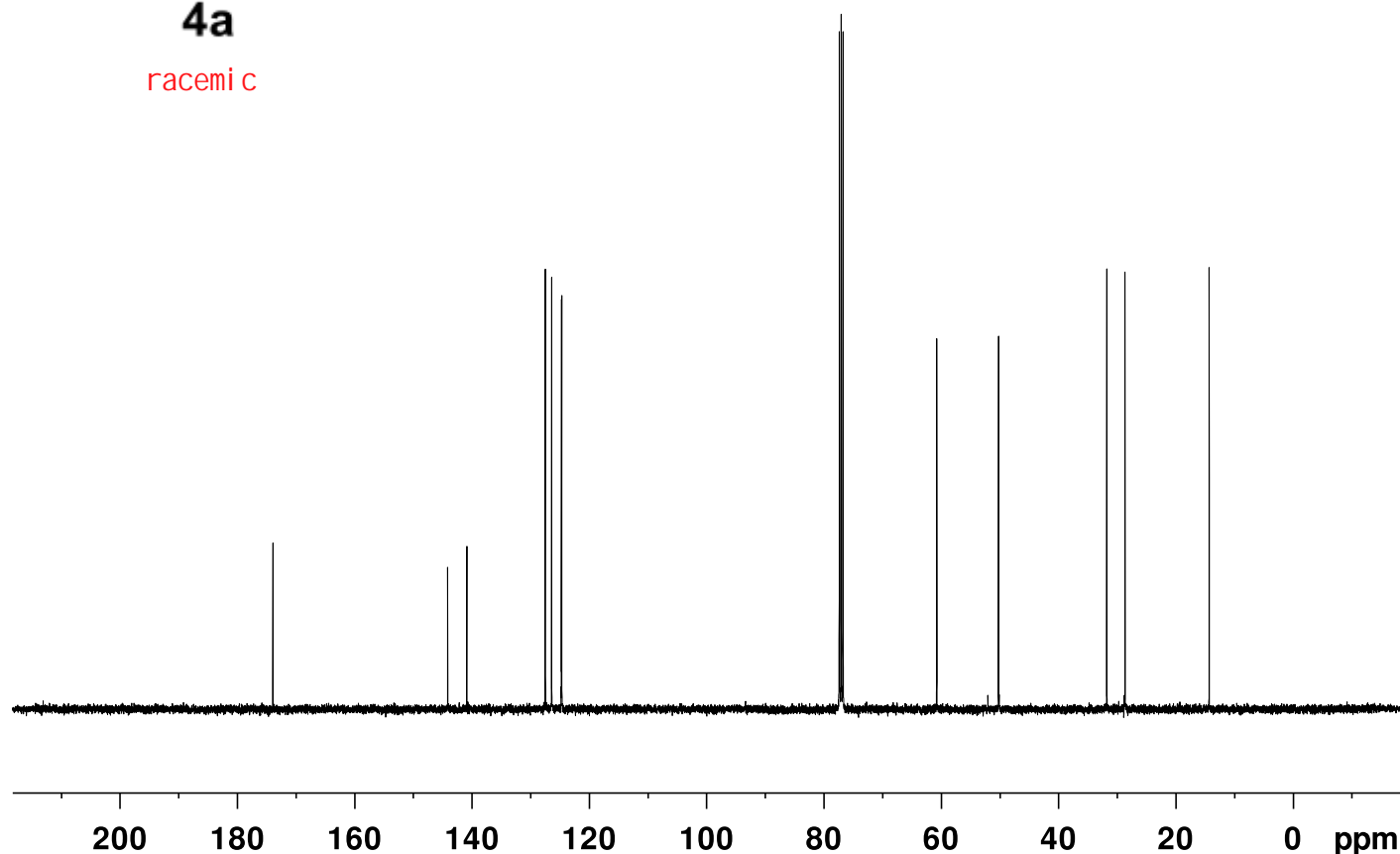
14.31

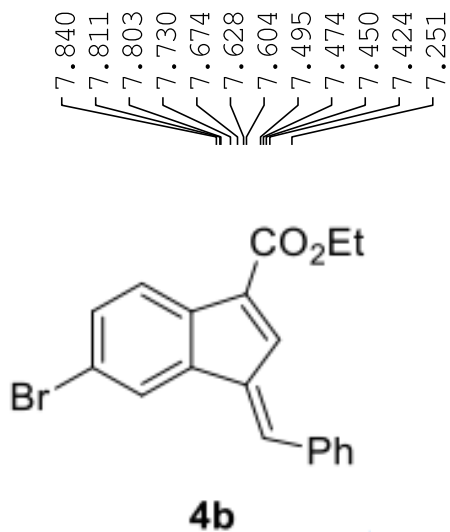


Current Data Parameters
NAME CNMR-YX-3-p32
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230208
Time 3.25 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 48.6724
DW 21.000 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



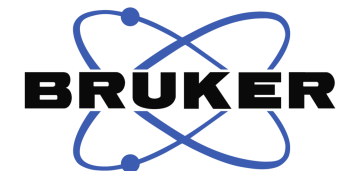


Chemical shift values (ppm) for the aliphatic region:

4.416, 4.392, 4.368, 4.344

Chemical shift values (ppm) for the aliphatic region:

1.434, 1.410, 1.387

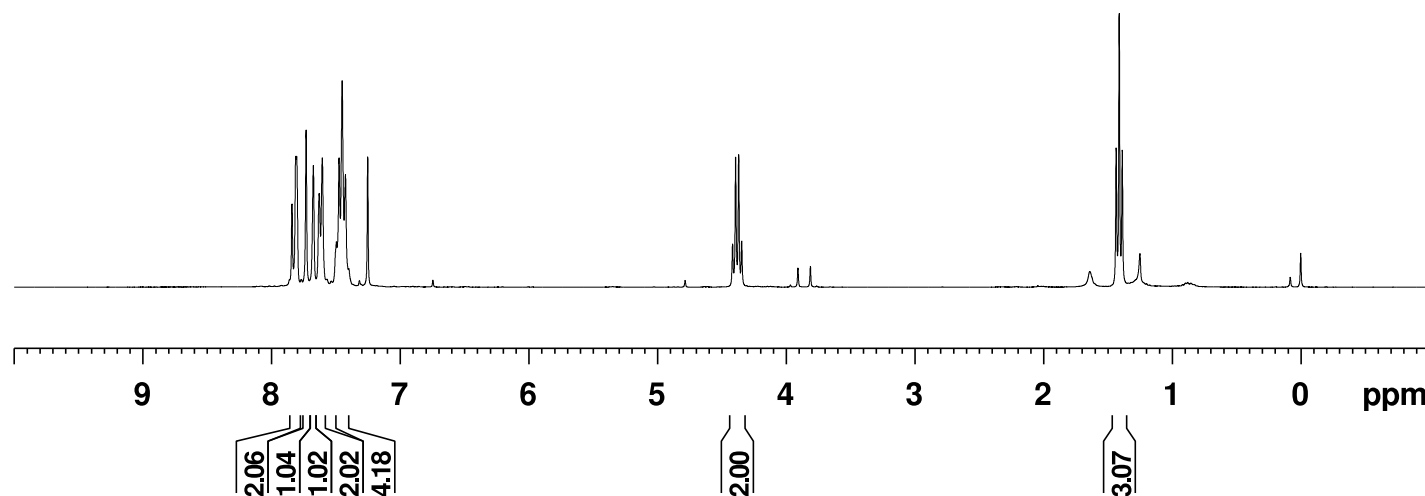


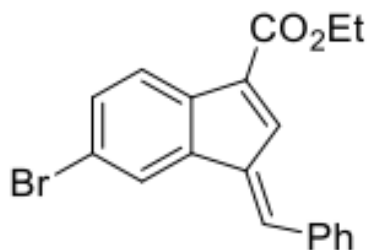
Current Data Parameters
 NAME HNMR-YX-3-p93
 EXPNO 71
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230403
 Time 13.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.091699 Hz
 AQ 5.4525952 sec
 RG 161
 DW 83.200 usec
 DE 6.50 usec
 TE 291.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1318534 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 14.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.130093 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



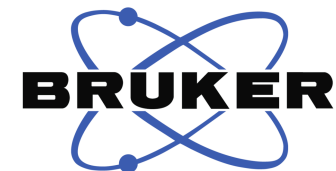


4b

164.45
139.29
137.22
136.94
135.85
135.80
135.60
133.60
130.75
130.60
129.88
129.08
123.68
122.55
120.06

60.80

14.43



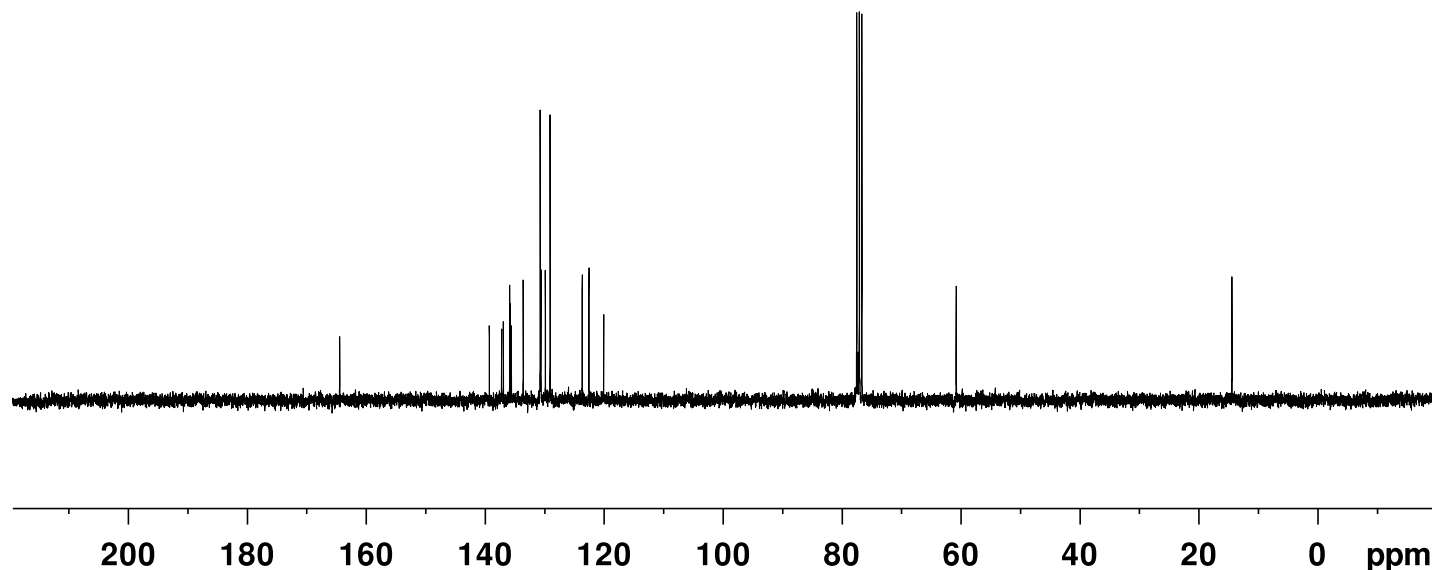
Current Data Parameters
NAME CNMR-YX-3-p93
EXPNO 72
PROCNO 1

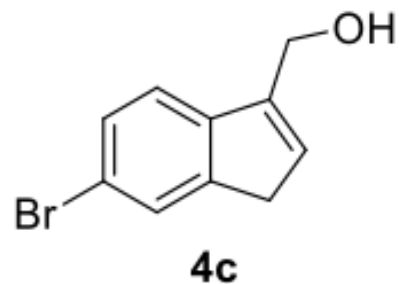
F2 - Acquisition Parameters
Date_ 20230403
Time 13.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 120
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 291.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



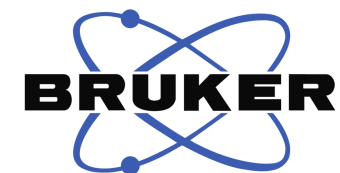
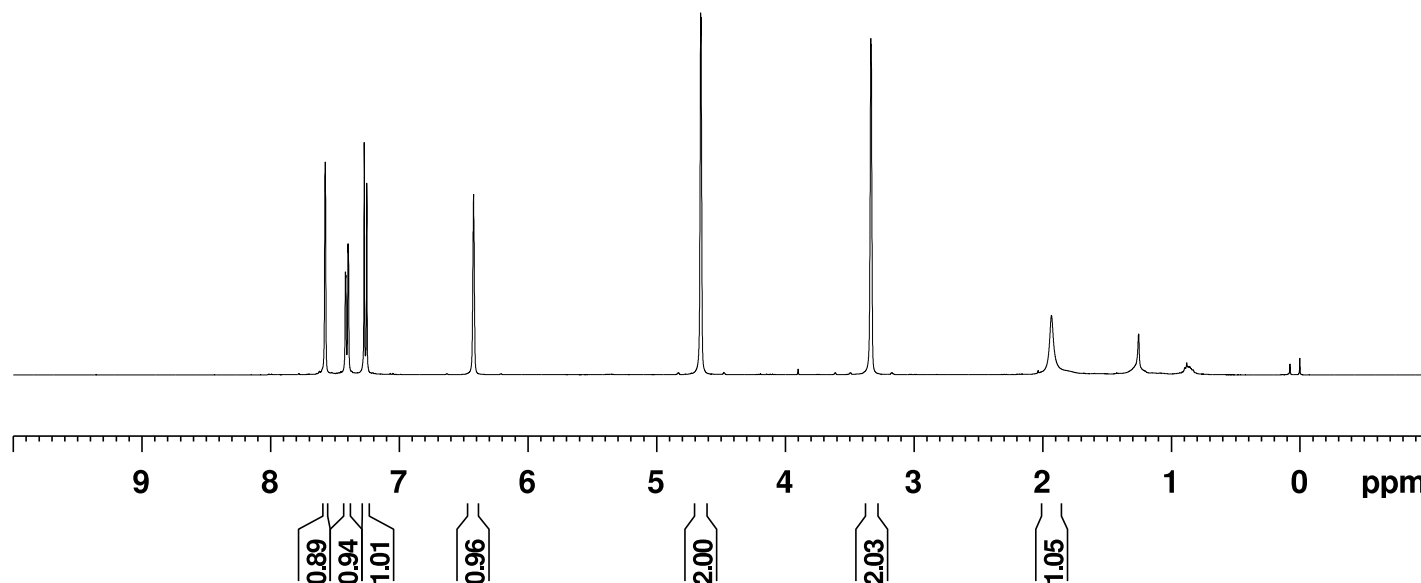


7.575
7.418
7.414
7.398
7.394
7.272
7.252
6.421

4.657
4.653

3.334
3.331

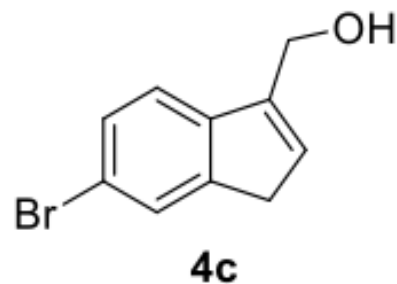
1.930



Current Data Parameters
NAME HNMR-YX-3-p34
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230207
Time 18.40 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 88.0902
DW 61.000 usec
DE 13.54 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

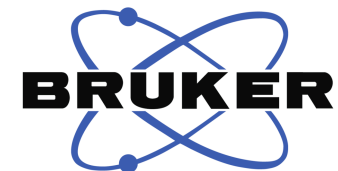
F2 - Processing parameters
SI 65536
SF 400.1300123 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



146.55
143.45
142.32
129.94
129.25
127.20
120.70
119.20

59.62

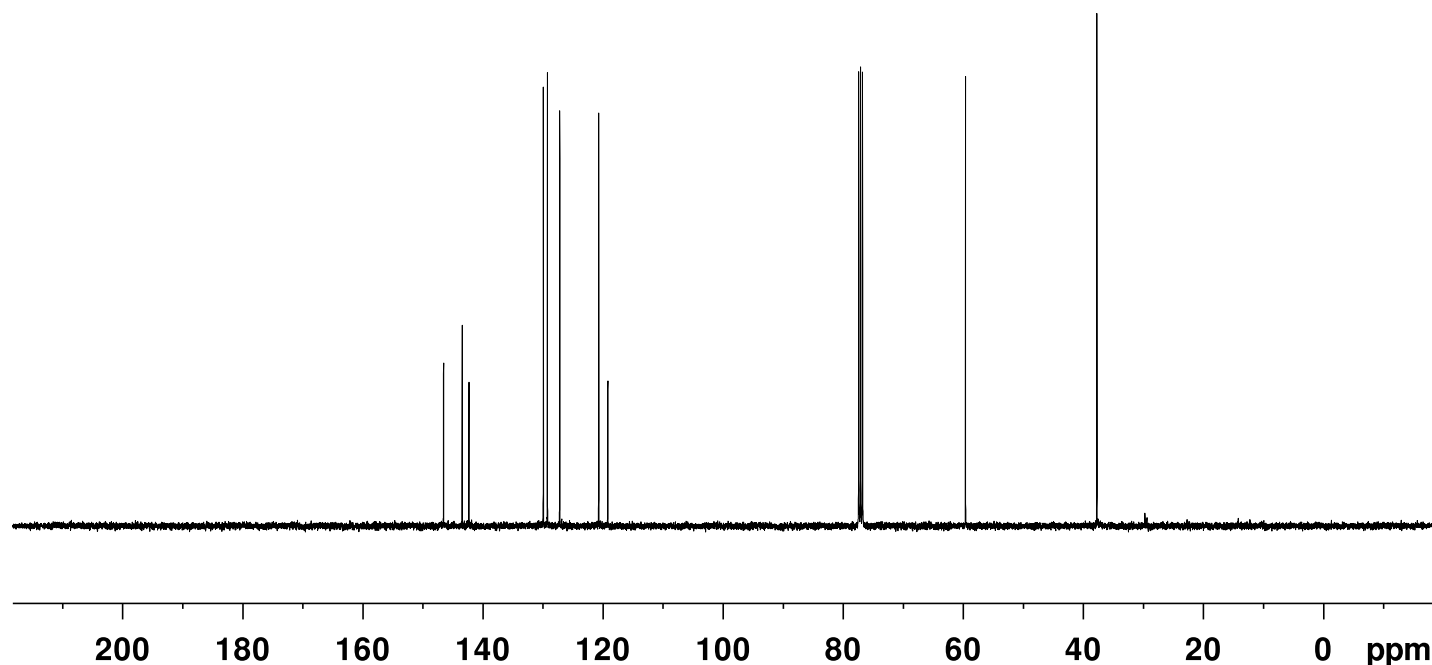
37.74



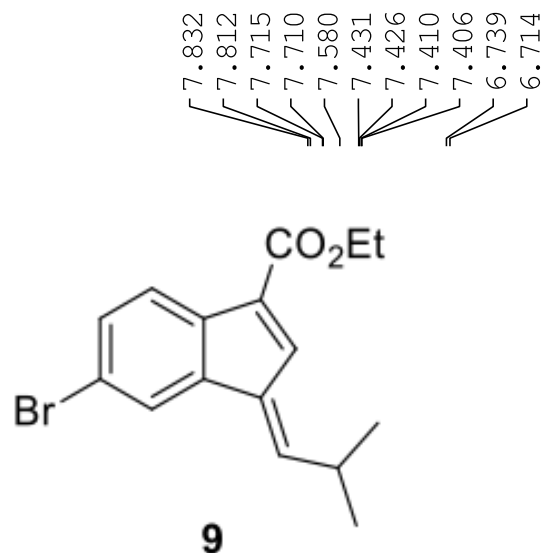
Current Data Parameters
NAME CNMR-YX-3-p34
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230208
Time 0.36 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 50.1934
DW 21.000 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



S80

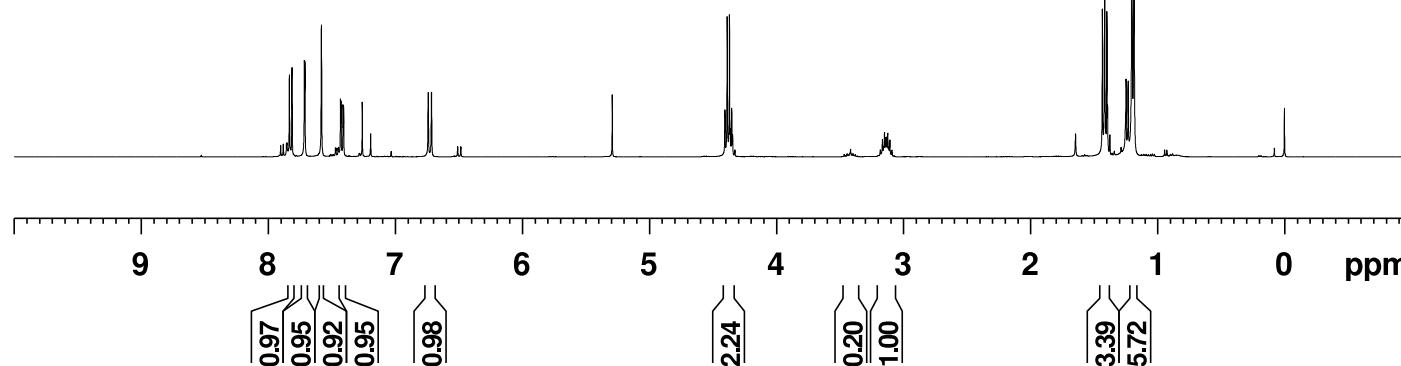
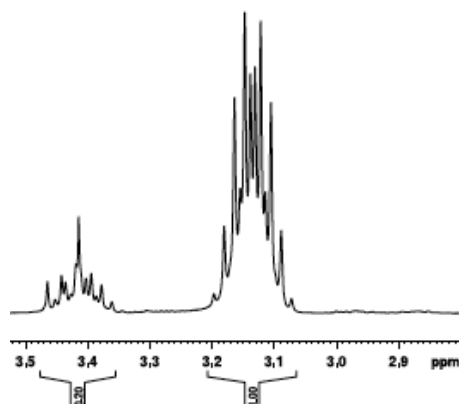


E : Z = 5 : 1

7.832
7.812
7.715
7.710
7.580
7.431
7.426
7.410
7.406
6.739
6.714

4.404
4.386
4.368
4.362
4.351
3.164
3.155
3.148
3.139
3.131
3.122
3.115
3.106
1.433
1.415
1.397
1.201
1.184

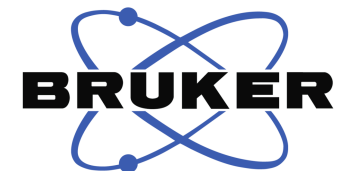
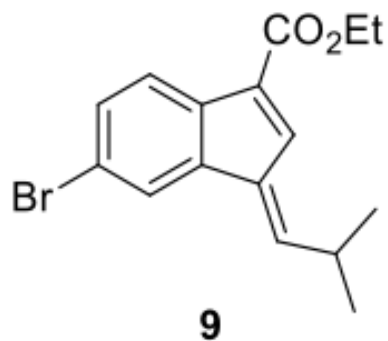
3.164
3.155
3.148
3.139
3.131
3.122
3.115
3.106



Current Data Parameters
NAME HNMR-YX-3-p43
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230213
Time 19.33 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 62.5
DW 61.000 usec
DE 13.54 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

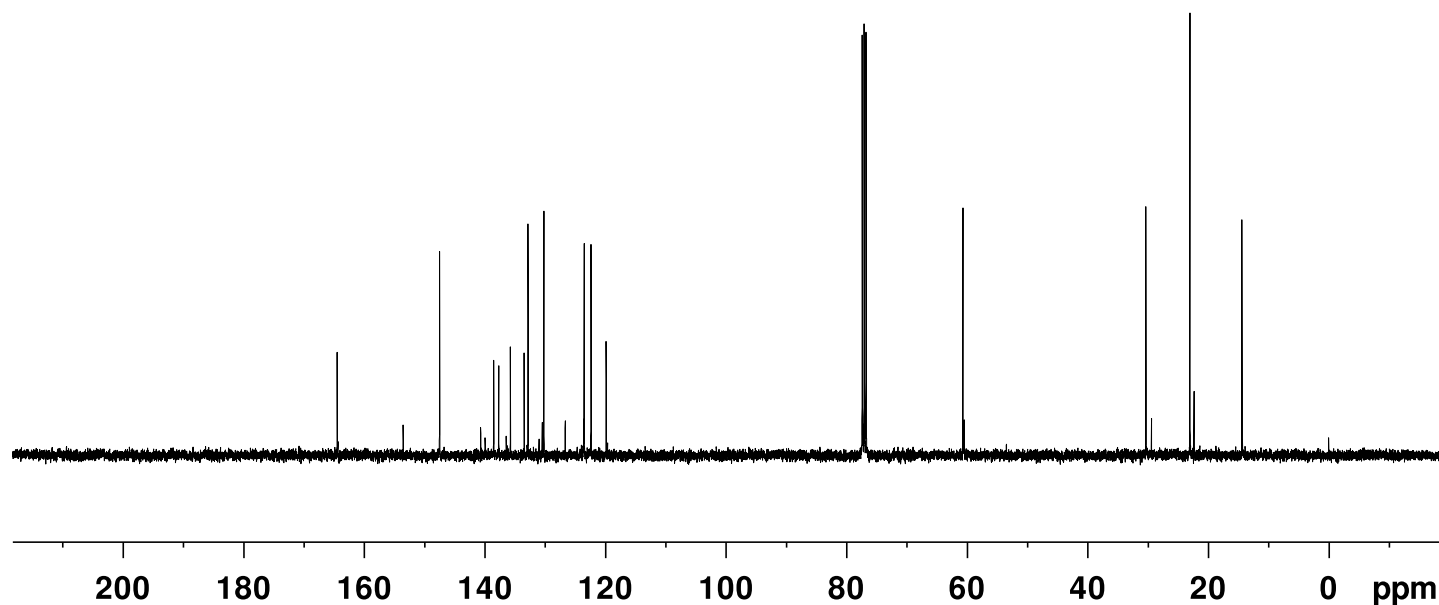
F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

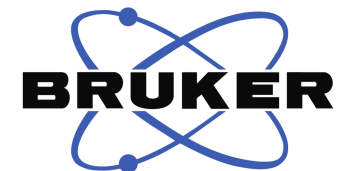


Current Data Parameters
 NAME CNMR-YX-3-p43
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230214
 Time 19.26 h
 INSTRUM Avance
 PROBHD Z116098_0833 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 100
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 53.2129
 DW 21.000 usec
 DE 6.50 usec
 TE 294.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6228298 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 87.89900208 W
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 20.73200035 W
 PLW12 0.25595000 W
 PLW13 0.12874000 W

F2 - Processing parameters
 SI 32768
 SF 100.6127685 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

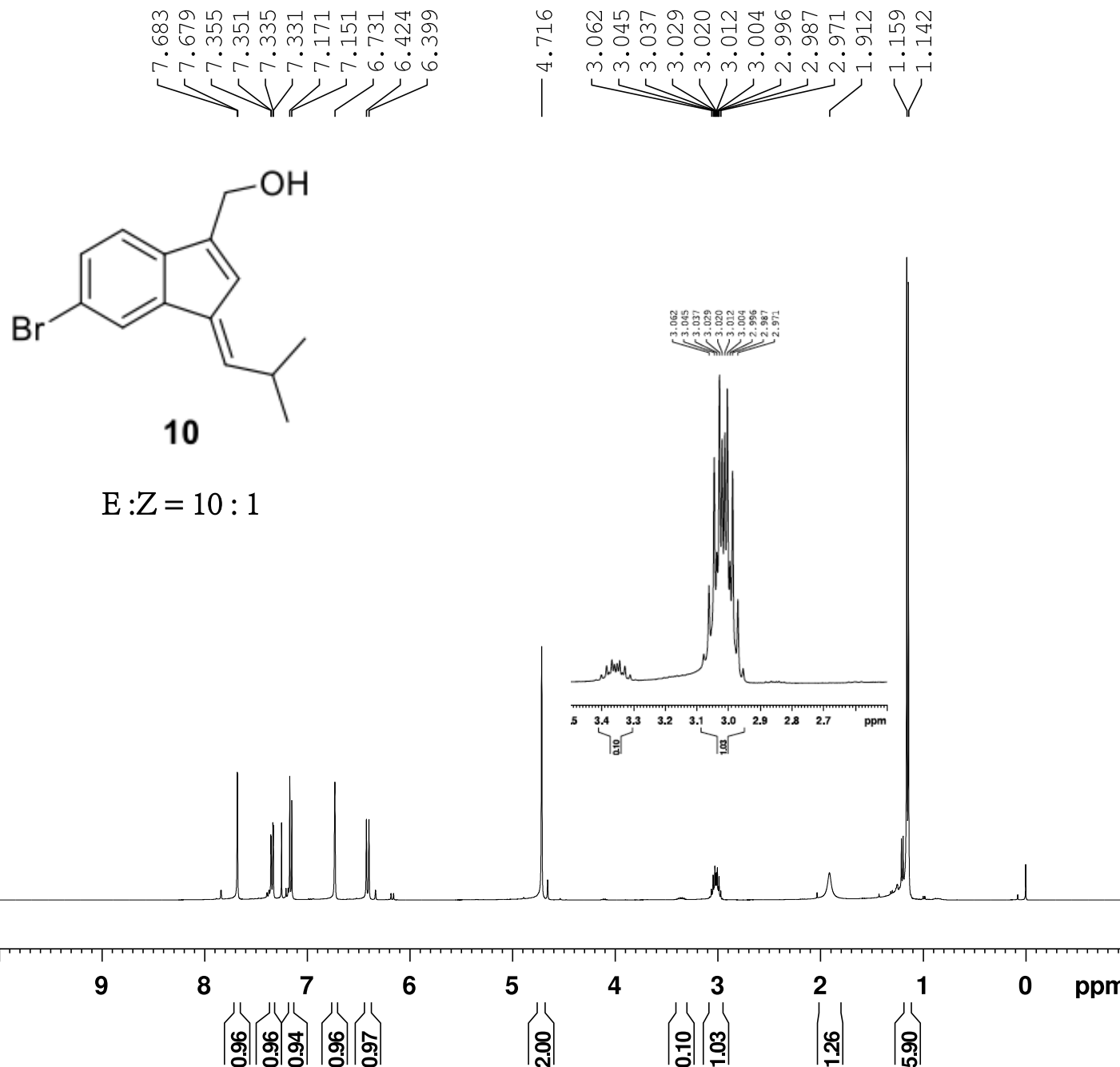


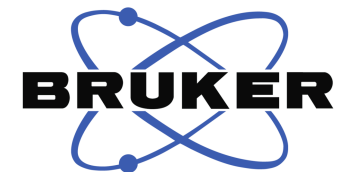


Current Data Parameters
 NAME HNMR-YX-3-p53
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230221
 Time 20.36 h
 INSTRUM Avance
 PROBHD Z116098_0833 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 70.8617
 DW 61.000 usec
 DE 13.54 usec
 TE 294.6 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1324708 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 20.73200035 W

F2 - Processing parameters
 SI 65536
 SF 400.1300136 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
 NAME CNMR-YX-3-p53
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230222
 Time 4.20 h
 INSTRUM Avance
 PROBHD Z116098_0833 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 100
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 50.1934
 DW 21.000 usec
 DE 6.50 usec
 TE 295.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6228298 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 87.89900208 W
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 20.73200035 W
 PLW12 0.25595000 W
 PLW13 0.12874000 W

F2 - Processing parameters
 SI 32768
 SF 100.6127685 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

146.71
 143.69
 140.60
 139.59
 136.17
 129.55
 122.47
 121.55
 120.35
 119.45

59.68

29.78

23.19

