Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Construction of Novel Bridged Aromatic Ring-Fused Oxazocine Frameworks via N-Heterocyclic Carbene-Catalyzed Azabenzoin Reaction and Radical-Initiated Cascade Cyclization

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Table of Contents

1. General Information

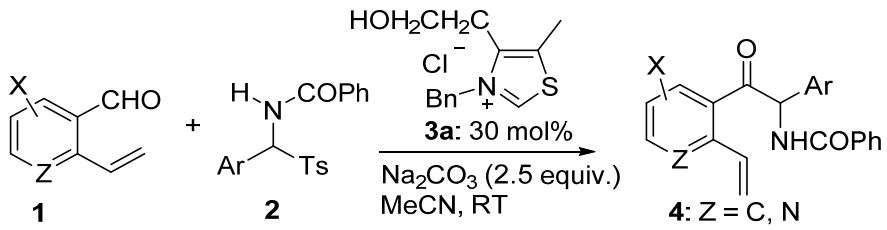
Commercially available chemical reagents were used without further purification. Anhydrous solvents were prepared by solvent purification system. Melting points were uncorrected. ^{1}H NMR (400 and 600 MHz) and ^{13}C NMR (100 and 150 MHz) were recorded in the indicated solvents using JEOL instrument. J values are reported in Hz. IR spectra were recorded using an AVATAR 360 FT-IR spectrometer. High resolution mass spectral analysis (HRMS) was performed on a LCT Premier XE (ESI) or a micrOTOF-Q II (ESI). Column chromatography was performed using 200-300 mesh silica gel eluted with the solvents as indicated.

The *o*-vinyl aromatic aldehydes **1**[1] and *N*-(aryl(tosyl)methyl)benzamides **2**[2] were prepared based on the literature methods.

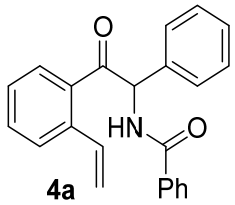
1. (a) L. Jarrige, A. Carboni, G. Dagousset, G. Levitre, E. Magnier, G. Masson, Photoredox-Catalyzed Three-Component Tandem Process: An Assembly of Complex Trifluoromethylated Phthalans and Isoindolines, *Org. Lett.* 2016, **18**, 2906−2909. (b) J. Lee, H. Y. Kim, K. Oh, Tandem Reaction Approaches to Isoquinolones from 2□Vinylbenzaldehydes and Anilines via Imine Formation−6π−Electrocyclization−Aerobic Oxidation Sequence, *Org. Lett.* 2020, **22**, 474−478.

2. (a) C. B. Schwamb, K. P. Fitzpatrick, A. C. Brueckner, H. C. Richardson, P. H.-Y. Cheong, K. A. Scheidt, Enantioselective Synthesis of α□Amidoboronates Catalyzed by Planar-Chiral NHC-Cu(I) Complexes, *J. Am. Chem. Soc*. 2018, **140**, 10644−10648. (b) B. J. Cowen, L. B. Saunders, S. J. Miller, Pyridylalanine (Pal)-Peptide Catalyzed Enantioselective Allenoate Additions to *N*-Acyl Imines, *J. Am. Chem. Soc.* 2009, **131**, 6105–6107. (c) M. S. Al Mehedi, J. J. Tepe, Diastereoselective One-Pot Synthesis of Oxazolines Using Sulfur Ylides and Acyl Imines, *J. Org. Chem*. 2019, **84**, 7219−7226.

2. Synthesis of 2-aryl-2-benzamido-1-(2-vinylaryl)-1-ethanones 4 (also namely *N*-(1-aryl-1-(2-vinylaroyl)methyl)benzamides) from NHC-catalyzed reaction of *o*-vinyl aromatic aldehydes 1 with *N*-(aryl(tosyl)methyl)benzamides 2 and characterization of 4

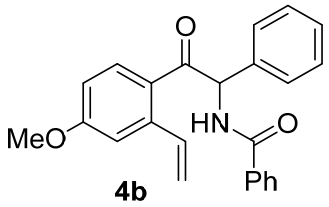


Under nitrogen atmosphere and at room temperature, *N*-(aryl(tosyl)methyl)benzamides **2** (0.5 mmol), thiazolium salt **3a** (40.5 mg, 0.15 mmol, 30 mol%), Na_2CO_3 (132.5 mg, 1.25 mmol, 2.5 equiv.) and the solution of *o*-vinyl aromatic aldehydes **1** (0.5 mmol) in dry acetonitrile (5 mL) were added successively to a dry Schlenk tube. In the sealed tube, the reaction mixture was stirred for 12 h (24 h for the reactions of 4-methoxy-2-vinylbenzaldehyde **1b** and 4-methyl-2-vinylbenzaldehyde **1c** with *N*-(phenyl(tosyl)methyl)benzamide **2a**) at room temperature. The solids in the reaction mixture were filtrated and washed with dichloromethane (10 mL×3). The combined filtrate was concentrated under reduced pressure. The residue was chromatographed on a silica gel column eluting with a mixture of petroleum ether and ethyl acetate (PE:EA from 20:1 to 3:1) to give 2-aryl-2-benzamido-1-(2-vinylaryl)-1-ethanones **4a-4o** in 31-82% yields. The 2-phenyl-2-benzamido-1-(2-vinyl-3-pyridinyl)-1-ethanone **4p** was obtained in 69% yield by chromatography eluting with a mixture of solvents from PE : EA = 20 : 1 to PE : EA : Et_3N = 30 : 10 : 0.1.



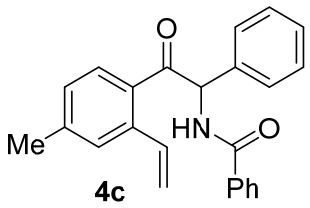
4a

2-Benzamido-2-phenyl-1-(2-vinylphenyl)-1-ethanone also (namely *N*-(1-phenyl-1-(2-vinylbenzoyl)methyl)benzamide) 4a: white solid, 136.8 mg, 80 %, mp 98-99 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 3352, 1697, 1645, 1626; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.87 (d, *J* = 7.2 Hz, 2H), 7.71 (d, *J* = 6 Hz, 1H), 7.68 (d, *J* = 7.8 Hz, 1H), 7.49-7.53 (m, 2H), 7.41-7.46 (m, 3H), 7.33 (d, *J* = 7.2 Hz, 2H), 7.25-7.31 (m, 3H), 7.22 (t, *J* = 7.8 Hz, 1H), 6.92 (dd, *J* = 17.4, 10.2 Hz, 1H), 6.56 (d, *J* = 7.2 Hz, 1H), 5.57 (dd, *J* = 17.4 Hz, 1H), 5.31 (d, *J* = 11.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.5, 166.5, 138.6, 136.2, 135.1, 134.9, 134.0, 132.2, 131.9, 129.2, 128.7, 128.6, 128.5, 128.2, 127.6, 127.5, 127.3, 117.3, 61.5; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{20}NO_2$: 342.1488, found: 342.1495.



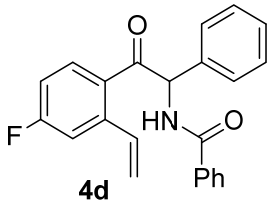
4b

2-Benzamido-2-phenyl-1-(4-methoxy-2-vinylphenyl)-1-ethanone 4b: white solid, 56.7 mg, 31 %, mp 74-75 ^{o}C (without recrystallization); IR ν (cm^{-1}) 3402, 3325, 1682, 1651; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.85 (d, J = 7.8 Hz, 2H), 7.82 (d, J = 7.8 Hz, 1H), 7.78 (d, J = 7.2 Hz, 1H), 7.50 (t, J = 7.2 Hz, 1H), 7.43 (t, J = 7.2 Hz, 2H), 7.38 (d, J = 7.8 Hz, 2H), 7.27 (t, J = 7.8 Hz, 2H), 7.23 (t, J = 8.4 Hz, 1H), 7.15 (dd, J = 17.4, 11.4 Hz, 1H), 6.97 (d, J = 3.6 Hz, 1H), 6.80 (dd, J = 7.8, 1.8 Hz, 1H), 6.62 (d, J = 6.6 Hz, 1H), 5.57 (d, J = 17.4 Hz, 1H), 5.34 (d, J = 12 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 197.1, 166.2, 162.8, 142.4, 137.3, 136.2, 134.0, 131.9, 130.8, 129.2, 128.6, 128.3, 128.1, 127.3, 126.8, 117.0, 113.6, 112.6, 60.3, 55.5; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{22}NO_3$: 372.1594, found: 372.1600.



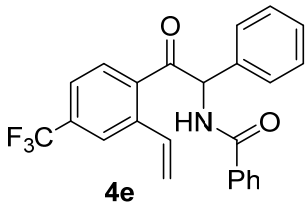
4c

2-Benzamido-2-phenyl-1-(4-methyl-2-vinylphenyl)-1-ethanone 4c: white solid, 94.5 mg, 53 %, mp 84-85 ^{o}C (without recrystallization); IR ν (cm^{-1}) 3356, 1699, 1682, 1633; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.65 (d, J = 7.8 Hz, 1H), 7.50 (t, J = 6.6 Hz, 1H), 7.43 (t, J = 7.8 Hz, 2H), 7.34 (d, J = 7.8 Hz, 2H), 7.30 (s, 1H), 7.26 (t, J = 8.4 Hz, 2H), 7.21 (t, J = 8.4 Hz, 1H), 7.10 (d, J = 8.4 Hz, 1H), 7.0 (dd, J = 17.4, 10.2 Hz, 1H), 6.69 (d, J = 7.2 Hz, 1H), 5.57 (d, J = 16.8 Hz, 1H), 5.30 (d, J = 11.4 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.7, 166.5, 143.1, 139.1, 136.7, 135.6, 134.0, 131.9, 131.8, 129.23, 129.16, 128.7, 128.5, 128.4, 128.3, 128.2, 127.3, 116.9, 61.0, 21.7; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{22}NO_2$: 356.1645, found: 356.1648.



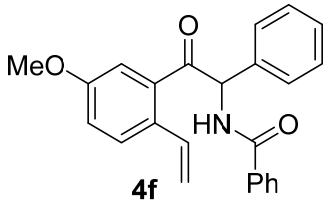
4d

2-Benzamido-2-phenyl-1-(4-fluoro-2-vinylphenyl)-1-ethanone 4d: white solid, 138.6 mg, 77 %, mp 109-110 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 3410, 3318, 1694, 1651; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.85 (d, *J* = 7.8 Hz, 2H), 7.75 (dd, *J* = 8.4, 6 Hz, 1H), 7.63 (d, *J* = 6.6 Hz, 1H), 7.51 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 2H), 7.29 (t, *J* = 8.4 Hz, 2H), 7.24 (t, *J* = 7.8 Hz, 1H), 7.18 (dd, *J* = 10.2, 2.4 Hz, 1H), 6.94-6.99 (m, 2H), 6.53 (d, *J* = 6.6 Hz, 1H), 5.60 (d, *J* = 17.4 Hz, 1H), 5.37 (d, *J* = 11.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.1, 166.6, 164.7 (d, *J* = 253 Hz), 142.1 (d, *J* = 8.7 Hz), 136.1, 134.4, 133.8, 131.9, 131.5 (d, *J* = 9.6 Hz), 131.1, 129.3, 128.7, 128.6, 128.2, 127.3, 118.3, 124.6 (d, *J* = 22 Hz), 114.5 (d, *J* = 22.1 Hz), 61.4; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{19}FNO_2$: 360.1394, found: 360.1392.



4e

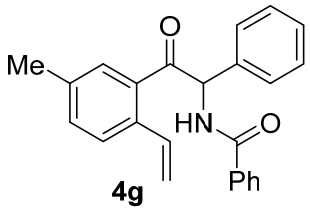
2-Benzamido-2-phenyl-1-(4-trifluoromethyl-2-vinylphenyl)-1-ethanone 4e: white solid, 135.8 mg, 66 %, 124-125 mp ^{o}C (recrystallization from acetone/*n*-hexane); IR *v* (cm^{-1}) 3366, 3267, 1709, 1645; ^{1}H NMR (600 MHz, CD_3COCD_3) δ (ppm) 8.40 (d, *J* = 6 Hz, 1H), 8.08 (d, *J* = 7.8 Hz, 1H), 7.96 (d, *J* = 7.2, 2.0 Hz, 2H), 7.89 (s, 1H), 7.70 (d, *J* = 6 Hz, 1H), 7.53 (t, *J* = 6.6 Hz, 1H), 7.44-7.46 (m, 4H), 7.32 (t, *J* = 7.8 Hz, 2H), 7.28 (t, *J* = 7.2 Hz, 1H), 6.85 (dd, *J* = 18, 11.4 Hz, 1H), 6.47 (d, *J* = 6 Hz, 1H), 5.80 (d, *J* = 16.8 Hz, 1H), 5.32 (d, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 199.2, 166.7, 140.3, 138.0, 134.7, 134.1, 133.4, 132.2 (q, *J* = 32.6 Hz), 131.6, 129.13, 129.07, 129.0, 128.6, 128.4, 127.6, 123.9 (q, *J* = 271.2 Hz), 124.0 (d, *J* = 2.9 Hz), 123.1, 118.0, 63.1; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{19}F_3NO_2$: 410.1362, found: 410.1366.



4f

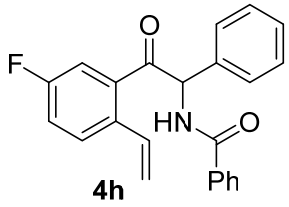
2-Benzamido-2-phenyl-1-(5-methoxy-2-vinylphenyl)-1-ethanone 4f: white solid, 121.4 mg, 65 %, mp 124-125 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 3364, 1701, 1649, 1634; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.87 (d, *J* = 8.4 Hz, 2H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.51 (t, *J* = 7.2 Hz,

1H), 7.42-7.46 (m, 3H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.27 (t, *J* = 7.8 Hz, 2H), 7.23 (t, *J* = 7.2 Hz, 1H), 7.10 (d, *J* = 2.4 Hz, 1H), 6.95 (dd, *J* = 9, 3.6 Hz, 1H), 6.82 (dd, *J* = 17.4, 12 Hz, 1H), 6.50 (d, *J* = 7.2 Hz, 1H), 5.47 (d, *J* = 17.4 Hz, 1H), 5.20 (dd, *J* = 11.4 Hz, 1H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.5, 166.5, 158.8, 136.1, 136.0, 134.3, 133.9, 131.9, 130.8, 129.2, 128.71, 128.68, 128.6, 128.2, 127.3, 118.1, 115.6, 113.4, 61.8, 55.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{22}NO_3$: 372.1594, found: 372.1588.



4g

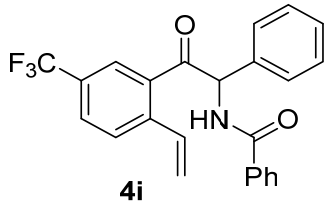
2-Benzamido-2-phenyl-1-(5-methyl-2-vinylphenyl)-1-ethanone 4g: white solid, 119.4 mg, 62 %, mp 136-137 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 3385, 1689, 1641; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.87 (d, *J* = 7.2 Hz, 2H), 7.71 (d, *J* = 6.6 Hz, 1H), 7.51 (t, *J* = 6.6 Hz, 1H), 7.49 (s, 1H), 7.45 (t, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 7.2 Hz, 1H), 7.32 (d, *J* = 7.8 Hz, 2H), 7.20-7.27 (m, 4H), 6.85 (dd, *J* = 16.8, 10.2 Hz, 1H), 6.57 (d, *J* = 7.2 Hz, 1H), 5.53 (d, *J* = 18.6 Hz, 1H), 5.24 (d, *J* = 10.2 Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.6, 166.5, 137.5, 136.2, 135.7, 135.0, 134.8, 134.0, 133.0, 131.9, 129.14, 129.06, 128.7, 128.5, 128.1, 127.4, 127.3, 116.4, 61.4, 21.2; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{22}NO_2$: 356.1645, found: 356.1641.



4h

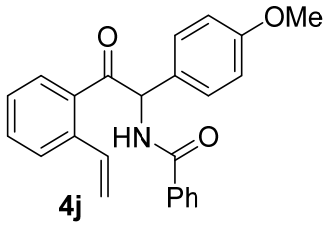
2-Benzamido-2-phenyl-1-(5-fluoro-2-vinylphenyl)-1-ethanone 4h: white solid, 127.7 mg, 71 %, mp 129-130 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 3340, 1696, 1636; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.86 (d, *J* = 7.8 Hz, 2H), 7.57 (d, *J* = 7.2 Hz, 1H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.47 (dd, *J* = 7.8, 4.8 Hz, 1H), 7.45 (t, *J* = 7.2 Hz, 2H), 7.24-7.33 (m, 6H), 7.12 (td, *J* = 8.4, 2.4 Hz, 1H), 6.84 (dd, *J* = 16.2, 11.4 Hz, 1H), 6.46 (d, *J* = 7.2 Hz, 1H), 5.53 (d, *J* = 17.4 Hz, 1H), 5.29 (d, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.6, 166.6, 161.5 (d, *J* = 248.2 Hz), 136.6 (d, *J* = 5.9 Hz), 135.5, 134.4 (d, *J* = 3.9 Hz), 133.9, 133.8, 132.0, 129.4, 129.3, 128.8, 128.7, 128.2, 127.3, 119.2 (d, *J* = 21.1 Hz), 117.4, 115.3 (d, *J* = 23 Hz), 61.9; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{19}FNO_2$: 360.1394, found:

360.1392.



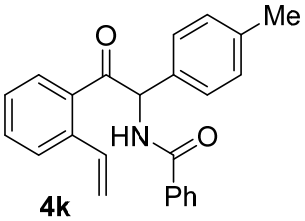
4i

2-Benzamido-2-phenyl-1-(5-trifluoromethyl-2-vinylphenyl)-1-ethanone 4e: white solid, 131.0 mg, 66 %, mp 150-151 ^{o}C (recrystallization from acetone/*n*-hexane); IR *v* (cm^{-1}) 3322, 1705, 1647; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) ^{1}H NMR (600 MHz, CD_3COCD_3) δ (ppm) 8.42 (d, *J* = 4.8 Hz, 1H), 8.21 (s, 3H), 7.95 (d, *J* = 8.4 Hz, 2H), 782 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.52 (t, *J* = 8.4 Hz, 1H), 7.43-7.48 (m, 4H), 7.33 (t, *J* = 7.8 Hz, 2H), 7.28 (t, *J* = 7.8 Hz, 1H), 6.87 (dd, *J* = 17.4, 12 Hz, 1H), 6.50 (d, *J* = 7.2 Hz, 1H), 5.78 (d, *J* = 16.8 Hz, 1H), 5.34 (d, *J* = 12 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.6, 166.7, 141.5, 135.7, 135.2, 133.7, 132.0, 129.5 (q, *J* = 32.6 Hz), 129.4, 128.9, 128.7, 128.4, 128.3, 128.2, 127.9, 127.3, 125.3 (d, *J* = 2.9 Hz), 123.6 (q, *J* = 271.2 Hz), 119.6, 62.2; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{19}F_3NO_2$: 410.1362, found: 410.1357.



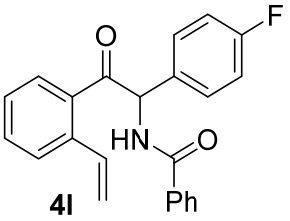
4j

2-Benzamido-2-(*p*-methoxyphenyl)-1-(2-vinylphenyl)-1-ethanone 4j: white solid, 124.4 mg, 67 %, mp 121-122 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 3406, 3333, 1697, 1647; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.86 (d, *J* = 7.8 Hz, 2H), 7.65-7.68 (m, 2H), 7.50-7.52 (m, 2H), 7.41-7.45 (m, 3H), 7.29 (t, *J* = 8.4 Hz, 1H), 7.24-7.24 (m, 2H), 6.95 (dd, *J* = 17.4, 11.4 Hz, 1H), 6.79 (d, *J* = 9.6 Hz, 2H), 6.50 (d, *J* = 7.2 Hz, 1H), 5.59 (d, *J* = 17.4 Hz, 1H), 5.31 (d, *J* = 12 Hz, 1H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 199.6, 166.3, 159.8, 137.5, 136.7, 135.1, 134.4, 131.5, 130.2, 128.5, 128.4, 127.6, 127.5, 126.6, 115.8, 114.3, 61.7, 54.7; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{22}NO_3$: 372.1594, found: 372.1598.



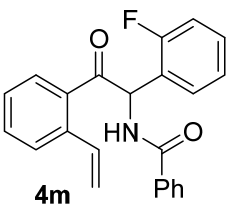
4k

2-Benzamido-2-(*p*-methylphenyl)-1-(2-vinylphenyl)-1-ethanone 4k: white solid, 144.9 mg, 82 %, mp 75-76 ^{o}C (without recrystallization); IR ν (cm^{-1}) 3349, 1686, 1640, 1622; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.86 (d, J = 6.6 Hz, 2H), 7.69 (d, J = 8.4 Hz, 1H), 7.66 (d, J = 6 Hz, 1H), 7.50-7.52 (m, 2H), 7.41-7.45 (m, 3H), 7.29 (t, J = 8.4 Hz, 1H), 7.22 (d, J = 8.4 Hz, 2H), 7.07 (d, J = 7.8 Hz, 2H), 6.95 (dd, J = 17.4, 11.4 Hz, 1H), 6.53 (d, J = 5.4 Hz, 1H), 5.59 (d, J = 16.8 Hz, 1H), 5.31 (d, J = 12 Hz, 1H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.5, 166.5, 138.5, 138.3, 138.3, 135.3, 135.1, 134.0, 33.2, 132.1, 131.8, 129.9, 128.7, 128.6, 128.2, 127.55, 127.47, 127.4, 117.1, 61.3, 21.2; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{22}NO_2$: 356.1645, found: 356.1648.



4l

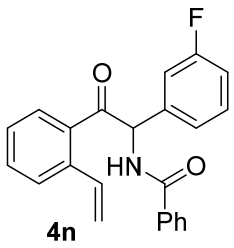
2-Benzamido-2-(*p*-fluorophenyl)-1-(2-vinylphenyl)-1-ethanone 4l: white solid, 126.7 mg, 71 %, mp 129-130 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR ν (cm^{-1}) 3325, 1688, 1636, 1630; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.86 (d, J = 8.4 Hz, 2H), 7.75 (d, J = 6 Hz, 1H), 7.64 (d, J = 8.4 Hz, 1H), 7.51-7.54 (m, 2H), 7.43-7.47 (m, 3H), 7.29-7.32 (m, 3H), 6.89-6.96 (m, 3H), 6.53 (d, J = 5.4 Hz, 1H), 5.58 (d, J = 17.4 Hz, 1H), 5.32 (d, J = 11.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.3, 166.5, 162.4 (d, J = 246.3 Hz), 138.5, 134.9, 134.7, 133.8, 132.3, 132.2 (d, J = 2.9 Hz), 132.0, 129.9 (d, J = 8.7 Hz), 128.7, 128.5, 127.6 (d, J = 3.8 Hz), 127.3, 117.6, 116.1 (d, J = 22 Hz), 60.7; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{19}FNO_2$: 360.1394, found: 360.1398.



4m

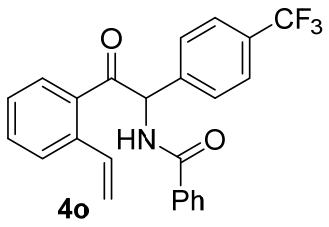
2-Benzamido-2-(*o*-fluorophenyl)-1-(2-vinylphenyl)-1-ethanone 4m: white solid, 140.5 mg, 78 %, mp

98-99 °C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 3406, 3322, 1701, 1647; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.87 (d, *J* = 7.2 Hz, 2H), 7.78 (d, *J* = 6 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.50-7.53 (m, 2H), 7.37-7.46 (m, 4H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.17-7.21 (m, 1H), 7.05 (t, *J* = 7.8 Hz, 1H), 7.0 (dd, *J* = 17.4, 10.2 Hz, 1H), 6.95 (t, *J* = 9.6 Hz, 1H), 6.75 (d, *J* = 7.2 Hz, 1H), 5.60 (d, *J* = 18.6 Hz, 1H), 5.35 (d, *J* = 12 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.2, 166.6, 160.6 (d, *J* = 247.3 Hz), 138.6, 135.0, 134.3, 133.8, 132.3, 131.9, 130.4 (d, *J* = 7.7 Hz), 130.2, 128.7, 128.4, 127.52, 127.47, 127.4, 124.8, 123.9 (d, *J* = 14.4 Hz), 117.3, 116.1 (d, *J* = 21.1 Hz), 56.2; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{19}FNO_2$: 360.1394, found: 360.1400.



4n

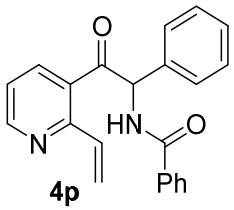
2-Benzamido-2-(*m*-fluorophenyl)-1-(2-vinylphenyl)-1-ethanone 4n: white solid, 144.3 mg, 80 %, mp 74-75 °C (without recrystallization); IR *v* (cm^{-1}) 3406, 3325, 1697, 1651; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.87 (d, *J* = 7.8 Hz, 2H), 7.77 (d, *J* = 7.2 Hz, 1H), 7.66 (d, *J* = 6.6 Hz, 1H), 7.51-7.52 (m, 2H), 7.44-7.46 (m, 3H), 7.31 (t, *J* = 8.4 Hz, 1H), 7.22 (dd, *J* = 13.8, 7.8 Hz, 1H), 7.10 (d, *J* = 8.4 Hz, 1H), 7.04 (d, *J* = 9.6 Hz, 1H), 6.89-6.94 (m, 2H), 6.55 (d, *J* = 5.4 Hz, 1H), 5.58 (d, *J* = 16.8 Hz, 1H), 5.33 (d, *J* = 11.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.0, 166.6, 163.0 (d, *J* = 246.2 Hz), 138.7 (d, *J* = 6.7 Hz), 138.6, 134.9, 134.6, 133.7, 132.4, 132.0, 130.7 (d, *J* = 7.7 Hz), 128.7, 128.6, 127.52, 127.65, 127.62, 127.3, 117.6, 115.5 (d, *J* = 20.1 Hz), 115.1 (d, *J* = 22 Hz), 61.0; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{19}FNO_2$: 360.1394, found: 360.1397.



4o

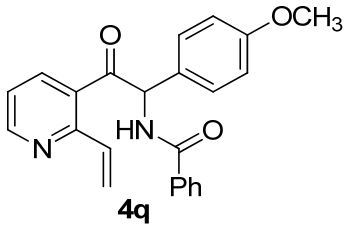
2-Benzamido-2-(*p*-trifluoromethylphenyl)-1-(2-vinylphenyl)-1-ethanone 4o: white solid, 166.3 mg, 81 %, mp 135-136 °C (recrystallization from chloroform/*n*-hexane); IR *v* (cm^{-1}) 3356, 1701, 1641; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.87 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 6 Hz, 1H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.50-7.54 (m, 4H), 7.43-7.47 (m, 5H), 7.32 (t, *J* = 6.6 Hz, 1H), 6.92 (dd, *J* = 16.8, 10.2 Hz, 1H), 6.61 (d, *J*

= 6 Hz, 1H), 5.58 (d, *J* = 16.8 Hz, 1H), 5.33 (d, *J* = 11.4 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 198.8, 166.6, 140.4, 138.7, 134.8, 133.6, 132.6, 132.1, 130.5 (q, *J* = 31.7 Hz), 128.7, 128.6, 128.5, 127.8, 127.7, 127.3, 126.0 (d, *J* = 3.8 Hz), 123.9 (q, *J* = 271 Hz), 117.8, 61.1; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{19}F_3NO_2$: 410.1362, found: 410.1366.



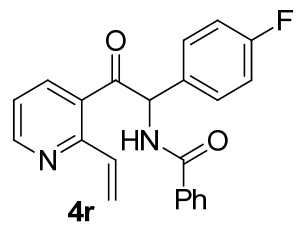
4p

2-Benzamido-2-phenyl-1-(2-vinyl-3-pyridinyl)-1-ethanone 4p: white solid, 117.6 mg, 69 %, mp 52-53 ^{o}C (without recrystallization); IR *v* (cm^{-1}) 3310, 1705, 1643; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.62 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.93 (dd, *J* = 8.4 Hz, 1H), 7.85 (dd, *J* = 6.8, 2 Hz, 2H), 7.56 (d, *J* = 6.4 Hz, 1H), 7.52 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.45 (td, *J* = 7.2, 1.6 Hz, 2H), 7.26-7.33 (m, 5H), 7.19 (dd, *J* = 7.6, 4.4 Hz, 1H), 6.99 (dd, *J* = 17.2, 10.8 Hz, 1H), 6.47 (d, *J* = 6.4 Hz, 1H), 6.38 (dd, *J* = 16.8, 1.6 Hz, 1H), 5.52 (dd, *J* = 10.8, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.1, 166.9, 153.8, 151.7, 136.3, 135.1, 133.6, 133.1, 131.9, 130.8, 129.3, 128.8, 128.6, 128.4, 127.4, 122.1, 121.9, 62.1; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{22}H_{19}N_2O_2$: 343.1441, found: 343.1443.



4q

2-Benzamido-2-(*p*-methoxyphenyl)-1-(2-vinyl-3-pyridinyl)-1-ethanone 4q: white solid, 113.5 mg, 56 %, mp 57-58^{o}C (without recrystallization); IR *v* (cm^{-1}) 3323, 1703, 1651; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.54 (d, *J* = 2.8 Hz, 1H), 7.92 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 2H), 7.70-7.78 (m, 1H), 7.32-7.42 (m, 3H), 7.16 (d, *J* = 8.8 Hz, 2H), 7.08-7.12 (m, 1H), 6.99 (dd, *J* = 16.4, 10.8 Hz, 1H), 6.72 (dd, *J* = 8.4, 2.4 Hz, 2H), 6.39 (d, *J* = 6.4 Hz, 1H), 6.35 (d, *J* = 16.8 Hz, 1H), 5.46 (d, *J* = 10.4 Hz, 1H), 3.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.1, 166.8, 159.9, 153.8, 151.7, 136.3, 133.6, 133.2, 131.9, 130.9, 129.6, 128.6, 127.3, 126.8, 122.1, 121.9, 114.8, 61.5, 55.3; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{21}N_2O_3$: 373.1546, found: 373.1543.

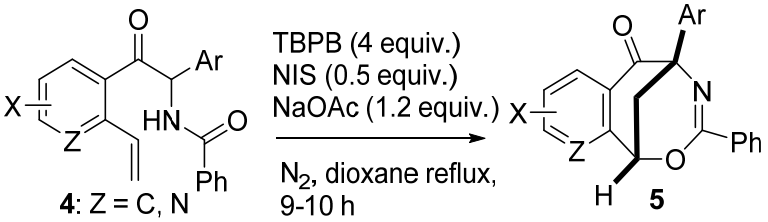


4r

2-Benzamido-2-(*p*-fluorophenyl)-1-(2-vinyl-3-pyridinyl)-1-ethanone 4r: white solid, 100.9 mg, 61 %, mp 61-62 ^{o}C (without recrystallization); IR *v* (cm^{-1}) 3315, 1705, 1651; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.58 (d, *J* = 4.4 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.79-7.83 (m, 3H), 7.46 (t, *J* = 6.8 Hz, 1H), 7.38 (t, *J* = 7.2 Hz, 2H), 7.27 (dd, *J* = 8.4, 5.6 Hz, 2H), 7.14 (dd, *J* = 7.6, 4.8 Hz, 1H), 6.88-7.00 (m, 3H), 6.46 (d, *J* = 6.8 Hz, 1H), 6.37 (dd, *J* = 16.8, 1.6 Hz, 1H), 5.49 (dd, *J* = 10.8, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.9, 166.8, 162.8 (d, *J* = 247.3 Hz), 153.9, 151.9, 136.2, 133.5, 133.0, 132.1, 131.1 (d, *J* = 2.9 Hz), 130.5, 130.1 (d, *J* = 8.6 Hz), 128.7, 127.3, 122.5, 121.9, 116.4 (d, *J* = 22.1 Hz), 61.2; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{22}H_{18}FN_2O_2$: 361.1346, found: 361.1349.

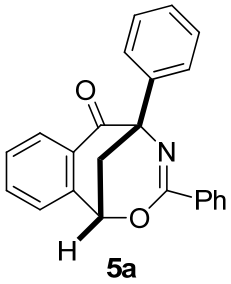
3. Radical-mediated cyclization reaction of 2-aryl-2-benzamido-1-(*o*-vinylaryl)-1-ethanones 4 and characterization of products

(1) TBPB/NIS-mediated cyclization reaction of 2-aryl-2-benzamido-1-(*o*-vinylaryl)-1-ethanones 4



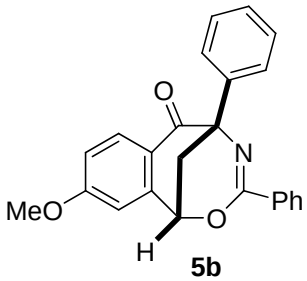
Under nitrogen atmosphere and at room temperature, 2-aryl-2-benzamido-1-(*o*-vinylaryl)-1-ethanones **4** (0.5 mmol), NaOAc (49.2 mg, 0.6 mmol, 1.2 equiv.), NIS (56.2 mg, 0.25 mmol, 50 mol%), TBPB (388.5 mg, 2 mmol, 4 equiv.) and dry 1,4-dioxane (5 mL) were added successively to a dry Schlenk tube. The reaction mixture was stirred in refluxing 1,4-dioxane for 9-10 h under the protection of nitrogen. The reaction was quenched by cooling the test tube to ambient temperature. The solids in the reaction mixture were filtrated and washed with dichloromethane (10 mL×3). The combined filtrate was concentrated under reduced pressure. The residue was chromatographed on a silica gel column eluting with a mixture of petroleum ether and ethyl acetate (PE : EA from 50 : 1 to 20 : 1) to give 3,5-diaryl-1,5-methanobenzo[f][1,3]oxazocin-6-ones **5a-5o** in 51%-92% yields. The

6,8-diphenyl-6,10-methanopyrido[3,2-f][1,3]oxazocin-5-one **5p** was obtained in 49% yield by chromatography eluting with a mixture of solvents from PE : EA = 50 : 1 to PE : EA : Et_3N = 30 : 3 : 0.1.



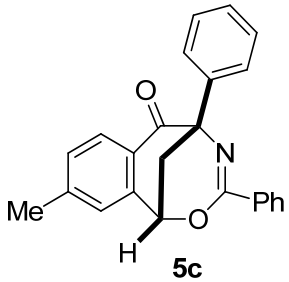
5a

3,5-Diphenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5a: white solid, 156.6 mg, 92 %, mp 193-194 ^oC (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 1697, 1626; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.15 (d, *J* = 7.6 Hz, 1H), 8.04 (dd, *J* = 6.8, 2 Hz, 2H), 7.69 (dd, *J* = 7.2, 1.6 Hz, 2H), 7.65 (td, *J* = 7.2, 1.6 Hz, 1H), 7.59 (d, *J* = 6.4 Hz, 1H), 7.51 (td, *J* = 7.2, 1.6 Hz, 1H), 7.40-7.47 (m, 3H), 7.33-7.36 (m, 3H), 5.63 (dd, *J* = 4.0, 2.0 Hz, 1H), 3.05 (dd, *J* = 13.6, 1.6 Hz, 1H), 2.45 (dd, *J* = 13.6, 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 192.7, 155.2, 142.2, 139.9, 134.5, 133.6, 131.1, 130.4, 130.3, 129.3, 129.1, 128.2, 128.1, 127.6, 127.5, 127.3, 71.7, 63.0, 34.8; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{18}NO_2$: 340.1332, found: 340.1334.



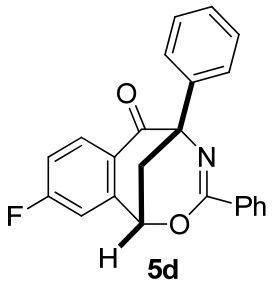
5b

9-Methoxy-3,5-diphenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5b: white solid, 94.1 mg, 51 %, mp 203-204 ^oC (recrystallization from chloroform/*n*-hexane); IR *v* (cm^{-1}) 1686, 1630; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.10 (d, *J* = 9 Hz, 1H), 8.05 (d, *J* = 7.8 Hz, 2H), 7.68 (d, *J* = 7.2 Hz, 2H), 7.40-7.45 (m, 3H), 7.32-7.36 (m, 3H), 7.04 (d, *J* = 2.4 Hz, 1H), 6.99 (dd, *J* = 8.4, 2.4 Hz, 1H), 5.55 (dd, *J* = 3.6, 2.4 Hz, 1H), 3.92 (s, 3H), 3.03 (d, *J* = 13.8 Hz, 1H), 2.41 (dd, *J* = 13.8, 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 191.9, 164.4, 154.9, 142.4, 142.2, 133.6, 131.6, 131.0, 128.2, 128.1, 127.5, 127.35, 127.28, 123.5, 115.9, 113.9, 71.9, 62.7, 55.8, 35.0; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{20}NO_3$: 370.1437, found: 370.1436.



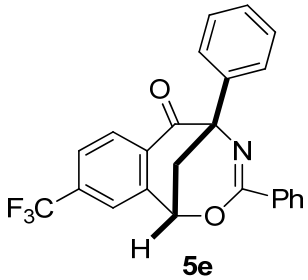
5c

9-Methyl-3,5-diphenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5c: white solid, 125.3 mg, 71 %, mp 212-213 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR ν (cm^{-1}) 1686, 1626; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.05 (d, J = 9 Hz, 2H), 8.04 (d, J = 9 Hz, 1H), 7.69 (d, J = 8.4 Hz, 2H), 7.40-7.45 (m, 3H), 7.38 (s, 1H), 7.32-7.36 (m, 3H), 7.31 (d, J = 8.4 Hz, 1H), 5.58 (s, 1H), 3.03 (d, J = 13.8 Hz, 1H), 2.46 (s, 3H), 2.43 (dd, J = 12.6, 4.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 192.6, 155.1, 145.5, 142.3, 140.0, 133.6, 131.2, 131.1, 129.8, 129.2, 128.2, 128.1, 127.9, 127.6, 127.4, 127.3, 71.8, 63.0, 35.0, 21.9; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{20}NO_2$: 354.1488, found: 354.1484.



5d

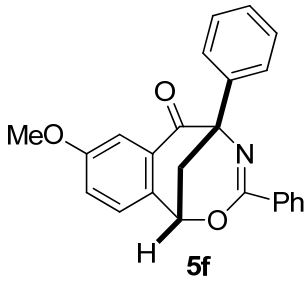
9-Fluoro-3,5-diphenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5d: white solid, 147.1 mg, 82 %, mp 217-218 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR ν (cm^{-1}) 1690, 1632; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.19 (s, 1H), 8.08 (d, J = 6.6 Hz, 2H), 7.72 (d, J = 6.6 Hz, 2H), 7.38-7.48 (m, 6H), 7.29 (d, J = 6.6 Hz, 1H), 7.19 (t, J = 7.2 Hz, 1H), 5.58 (s, 1H), 3.04 (d, J = 13.8 Hz, 1H), 2.44 (d, J = 12.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 191.4, 166.2 (d, J = 255.6 Hz), 155.0, 142.6 (d, J = 8.7 Hz), 141.8, 133.3, 132.2 (d, J = 8.7 Hz), 131.3, 128.3, 128.2, 127.3, 126.9, 117.7 (d, J = 21.5 Hz), 116.0 (d, J = 23.0 Hz), 71.2, 62.8, 34.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{17}FNO_2$: 358.1237, found: 358.1239.



5e

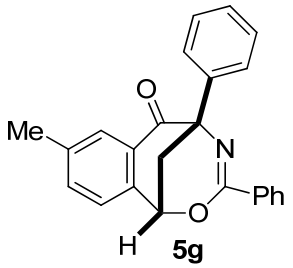
3,5-Diphenyl-9-trifluoromethyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5e: white solid, 186.1 mg,

91 %, mp 179-180 °C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 1694, 1628; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.27 (d, *J* = 8.4 Hz, 1H), 8.05 (dd, *J* = 6.8, 1.6 Hz, 2H), 7.88 (s, 1H), 7.76 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.05 (dd, *J* = 7.6, 1.2 Hz, 2H), 7.41-7.47 (m, 3H), 7.34-7.39 (m, 3H), 5.55 (dd, *J* = 3.6, 2.0 Hz, 1H), 3.06 (dd, *J* = 14.0, 2.0 Hz, 1H), 2.50 (dd, *J* = 14.4, 3.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 191.4, 155.3, 141.4, 140.4, 135.7 (q, *J* = 33 Hz), 133.1 (d, *J* = 4.4 Hz), 131.4, 129.9, 128.3, 128.2, 127.7 127.6, 127.2, 127.0 (d, *J* = 4.4 Hz), 126.4 (d, *J* = 3.0 Hz), 123.4 (q, *J* = 271.4 Hz), 71.0, 62.9, 34.3; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{17}F_3NO_2$: 408.1205, found: 408.1201.



5f

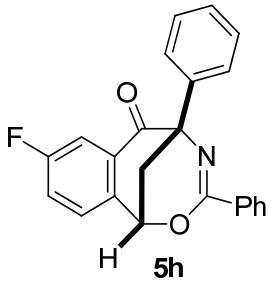
8-Methoxy-3,5-diphenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5f: white solid, 107.7 mg, 58 %, mp 165-166 °C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 1660, 1630; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.05 (d, *J* = 8.4 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 1.9 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 6.6 Hz, 1H), 7.3-7.36 (m, 3H), 7.18 (dd, *J* = 7.8, 3.0 Hz, 1H), 5.59 (s, 1H), 3.83 (s, 3H), 3.02 (dd, *J* = 13.8, 2.4 Hz, 1H), 2.42 (dd, *J* = 13.8, 4.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 192.8, 161.0, 155.4, 142.4, 133.7, 132.7, 131.8, 131.2, 130.8, 128.25, 128.17, 127.6, 127.5, 127.4, 121.9, 111.5, 71.3, 62.9, 55.7, 35.2; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{20}NO_3$: 370.1437, found: 370.1433.



5g

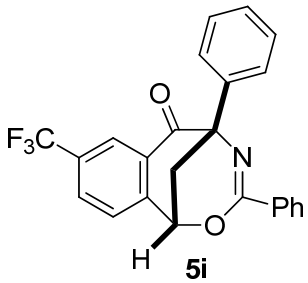
8-Methyl-3,5-diphenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5g: white solid, 141.3 mg, 80 %, mp 164-165 °C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 1697, 1630; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.04 (dd, *J* = 8.8, 2.0 Hz, 2H), 7.94 (s, 1H), 7.68 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.39-7.49 (m, 5H), 7.32-7.36 (m, 3H), 5.60 (dd, *J* = 3.2, 1.6 Hz, 1H), 3.02 (dd, *J* = 13.6, 1.6 Hz, 1H), 2.42 (dd, *J* = 13.6, 3.6 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 193.0, 155.2, 142.4, 140.5, 137.4,

135.3, 133.7, 131.1, 130.2, 129.3, 129.2, 128.3, 128.2, 127.6, 127.5, 127.4, 71.6, 63.1, 35.0, 21.4; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{20}NO_2$: 354.1488, found: 354.1487.



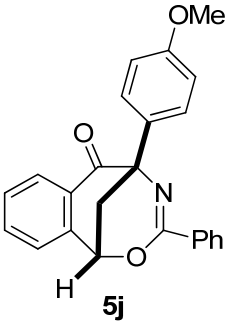
5h

8-Fluoro-3,5-diphenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5h: white solid, 163.6 mg, 92 %, mp 176-177 ^oC (recrystallization from dichloromethane/*n*-hexane); IR ν (cm^{-1}) 1699, 1628; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.09 (d, J = 6.6 Hz, 2H), 7.83 (dd, J = 7.8, 1.8 Hz, 1H), 7.73 (d, J = 8.4 Hz, 2H), 7.61 (dd, J = 9.0, 6.0 Hz, 1H), 7.49 (t, J = 7.8 Hz, 2H), 7.45 (t, J = 7.2 Hz, 1H), 7.37-7.41 (m, 3H), 7.34 (td, J = 8.4, 3.6 Hz, 1H), 5.63 (dd, J = 3.6, 2.4 Hz, 1H), 3.03 (d, J = 14.4 Hz, 1H), 2.45 (dd, J = 13.8, 3.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 191.7, 163.6 (d, J = 249.9 Hz), 155.4, 141.8, 135.9, 133.4, 132.7 (d, J = 7.2 Hz), 131.5 (d, J = 7.2 Hz), 131.3, 128.3, 128.2, 127.7, 127.6, 127.3, 121.6 (d, J = 21.6 Hz), 115.3 (d, J = 21.6 Hz), 70.9, 62.7, 34.7; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{17}FNO_2$: 358.1237, found: 358.1240.



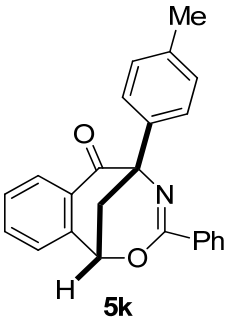
5i

3,5-Diphenyl-8-trifluoromethyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5i: white solid, 112.1 mg yielded from 0.3 mmol reactant **4i**, 92 %, mp 189-190 ^oC (recrystallization from chloroform/*n*-hexane); IR ν (cm^{-1}) 1697, 1628; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.41 (s, 1H), 8.03 (d, J = 6.6 Hz, 2H), 7.90 (d, J = 7.8 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.67 (d, J = 7.8 Hz, 2H), 7.46 (t, J = 7.8 Hz, 2H), 7.43 (t, J = 7.2 Hz, 1H), 7.34-7.38 (m, 3H), 5.69 (s, 1H), 3.05 (d, J = 13.8 Hz, 1H), 2.49 (dd, J = 13.8, 3.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 191.3, 155.3, 142.8, 141.5, 133.1, 132.7 (q, J = 33.0 Hz), 131.4, 131.1, 130.8 (d, J = 2.9 Hz), 130.1, 128.3, 128.2, 127.7, 127.6, 127.3, 126.2 (d, J = 2.9 Hz), 123.4 (q, J = 270.0 Hz), 70.9, 62.8, 34.3; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{17}F_3NO_2$: 408.1205, found: 408.1200.



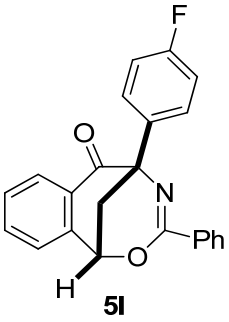
5j

5-(4-Methoxyphenyl)-3-phenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5j: white solid, 126.0 mg, 68 %, mp 180-181 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 1688, 1620; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.14 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.03 (dd, *J* = 7.2, 1.6 Hz, 2H), 7.57-7.66 (m, 4H), 7.50 (td, *J* = 7.6, 1.2 Hz, 1H), 7.41 (tt, *J* = 7.2, 1.6 Hz, 1H), 7.34 (td, *J* = 7.2, 1.2 Hz, 2H), 6.99 (dd, *J* = 9.2, 2.4 Hz, 2H), 5.63 (dd, *J* = 3.6, 2.4 Hz, 1H), 3.84 (s, 3H), 3.03 (dd, *J* = 14.0, 2.0 Hz, 1H), 2.44 (dd, *J* = 13.6, 4.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 193.0, 159.0, 155.0, 139.9, 134.44, 134.35, 133.6, 131.1, 130.4, 130.3, 129.3, 129.1, 128.4, 128.1, 127.6, 113.7, 71.7, 62.5, 55.4, 34.7; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{20}NO_3$: 370.1437, found: 370.1436.



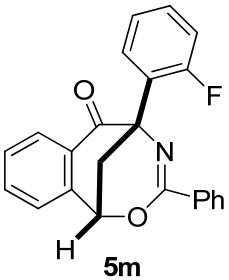
5k

5-(4-Methylphenyl)-3-phenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5k: white solid, 140.8 mg, 80 %, mp 176-177 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 1703, 1632; ^{1}H NMR (400 MHz, $CDCl_3$) 8.14 (dd, *J* = 7.6, 1.2 Hz, 1H), 8.03 (dd, *J* = 7.2, 1.6 Hz, 2H), 7.64 (td, *J* = 7.2, 1.6 Hz, 1H), 7.56-7.59 (m, 3H), 7.50 (td, *J* = 7.2, 1.6 Hz, 1H), 7.41 (tt, *J* = 7.2, 1.6 Hz, 1H), 7.34 (td, *J* = 7.6, 1.6 Hz, 2H), 7.26 (d, *J* = 7.2 Hz, 2H), 5.62 (dd, *J* = 3.6, 1.6 Hz, 1H), 3.04 (dd, *J* = 14.0, 2.0 Hz, 1H), 2.43 (dd, *J* = 13.2, 3.6 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 192.9, 155.1, 140.0, 139.3, 137.1, 134.4, 133.6, 131.1, 130.4, 130.3, 129.3, 129.1, 129.0, 128.2, 127.6, 127.2, 71.7, 62.8, 34.8, 21.4; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{20}NO_2$: 354.1488, found: 354.1492.



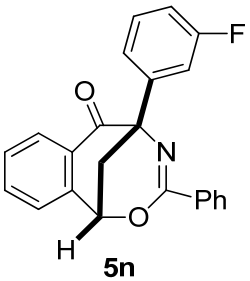
5l

5-(4-Fluorophenyl)-3-phenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5l: white solid, 153.5 mg, 86 %, mp 182-183 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 1692, 1628; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.14 (d, *J* = 7.2 Hz, 1H), 8.03 (d, *J* = 7.2 Hz, 2H), 7.64-7.67 (m, 3H), 7.59 (d, *J* = 7.2 Hz, 1H), 7.52 (t, *J* = 9 Hz, 1H), 7.42 (t, *J* = 7.2 Hz, 1H), 7.35 (t, *J* = 7.8 Hz, 2H), 7.13 (t, *J* = 9 Hz, 2H), 5.64 (s, 1H), 3.03 (dd, *J* = 13.8, 1.8 Hz, 1H), 2.43 (dd, *J* = 13.8, 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 192.6, 162.3 (d, *J* = 243.4 Hz), 155.3, 139.8, 137.9 (d, *J* = 2.9 Hz), 134.6, 133.4, 131.2, 130.3, 130.2, 129.3, 129.1, 129.0, 128.2, 127.5, 115.0 (d, *J* = 21.1 Hz), 71.6, 62.6, 34.7; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{17}FNO_2$: 358.1237, found: 358.1242.



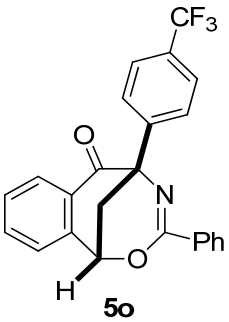
5m

5-(2-Fluorophenyl)-3-phenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5m: white solid, 128.6 mg, 72 %, mp 184-185 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 1697, 1626; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.20 (d, *J* = 7.4 Hz, 1H), 8.07 (d, *J* = 7.2 Hz, 2H), 8.05 (d, *J* = 6 Hz, 1H), 7.66 (t, *J* = 6.6 Hz, 1H), 7.59 (d, *J* = 6.6 Hz, 1H), 7.52 (t, *J* = 6.6 Hz, 1H), 7.43 (t, *J* = 7.2 Hz, 1H), 7.33-7.37 (m, 3H), 7.27 (t, *J* = 7.2 Hz, 1H), 7.08 (dd, *J* = 11.4, 9 Hz, 1H), 5.61 (s, 1H), 3.25 (d, *J* = 13.8 Hz, 1H), 2.29 (dd, *J* = 13.8, 3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.7, 160.4 (d, *J* = 244.3 Hz), 155.7, 140.0, 134.5, 133.5, 131.3, 130.3, 130.1, 129.9, 129.8, 129.4, 129.3, 129.2, 128.2, 127.6, 124.4 (d, *J* = 2.9 Hz), 115.5 (d, *J* = 21.1 Hz), 71.8, 61.5, 33.4 (d, *J* = 3.9 Hz); HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{17}FNO_2$: 358.1237, found: 358.1240.



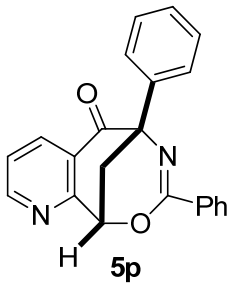
5n

5-(3-Fluorophenyl)-3-phenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5n: white solid, 144.6 mg, 81 %, mp 177-178 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR ν (cm^{-1}) 1697, 1620; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.14 (dd, J = 7.6, 1.2 Hz, 1H), 8.03 (dt, J = 6.8, 1.2 Hz, 2H), 7.66 (td, J = 7.6, 1.6 Hz, 1H), 7.59 (dd, J = 7.6, 1.2 Hz, 1H), 7.49-7.53 (m, 2H), 7.33-7.44 (m, 5H), 7.01-7.07 (m, 1H), 5.64 (dd, J = 3.6, 1.6 Hz, 1H), 3.03 (dd, J = 13.6, 2.0 Hz, 1H), 2.43 (dd, J = 13.6, 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 192.3, 163.0 (d, J = 243.4 Hz), 155.4, 145.0 (d, J = 6.7 Hz), 139.8, 136.7, 133.3, 131.3, 130.4, 130.1, 129.7 (d, J = 8.6 Hz), 129.4, 129.1, 128.2, 127.6, 122.8 (d, J = 2.0 Hz), 114.9 (d, J = 23.0 Hz), 114.4 (d, J = 21.1 Hz), 71.6, 62.8, 34.5; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{17}FNO_2$: 358.1237, found: 358.139.



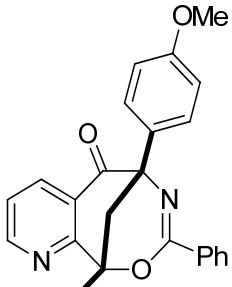
5o

3-Phenyl-5-(4-trifluoromethylphenyl)-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5o: white solid, 183.2 mg, 90 %, mp 172-173 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR ν (cm^{-1}) 1696, 1626; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.15 (d, J = 7.8 Hz, 1H), 8.04 (d, J = 7.8 Hz, 2H), 7.81 (d, J = 7.8 Hz, 2H), 7.70 (d, J = 7.8 Hz, 2H), 7.67 (t, J = 7.2 Hz, 1H), 7.61 (d, J = 6.6 Hz, 1H), 7.53 (t, J = 7.8 Hz, 1H), 7.43 (t, J = 7.2 Hz, 1H), 7.36 (t, J = 7.8 Hz, 2H), 5.66 (dd, J = 3, 2.4 Hz, 1H), 3.06 (dd, J = 13.8, 2.4 Hz, 1H), 2.43 (dd, J = 13.8, 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 192.2, 155.5, 146.1, 139.7, 134.7, 131.3, 130.4, 130.0, 129.6 (q, J = 32.5 Hz), 129.3, 129.1, 128.2, 127.8, 127.5, 125.1 (d, J = 3.3 Hz), 124.4 (q, J = 270.3 Hz), 71.5, 63.0, 34.5; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{17}F_3NO_2$: 408.1205, found: 408.1207.



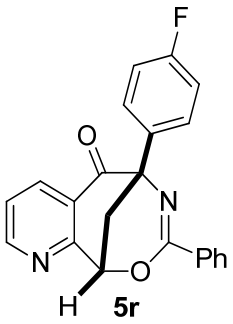
5p

6,8-Diphenyl-6,10-dihydro-6,10-methanopyrido[3,2-*f*][1,3]oxazocin-5-one 5p: white solid, 83.2 mg, 49 %, mp 178-179 ^{o}C (recrystallization from chloroform/*n*-hexane); IR *v* (cm^{-1}) 1697, 1626; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.84 (dd, *J* = 5.2, 2.0 Hz, 1H), 8.42 (dd, *J* = 7.6, 1.2 Hz, 1H), 8.08 (dd, *J* = 7.6, 1.2 Hz, 2H), 7.69 (dd, *J* = 6.8, 1.6 Hz, 2H), 7.33-7.50 (m, 7H), 5.80 (dd, *J* = 4.0, 2.0 Hz, 1H), 3.08 (dd, *J* = 13.6, 1.6 Hz, 1H), 2.51 (dd, *J* = 14.4, 3.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 192.1, 158.2, 155.6, 154.4, 141.4, 137.1, 133.1, 131.4, 128.3, 128.2, 127.73, 127.67, 127.3, 126.2, 125.4, 73.2, 62.7, 33.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{22}H_{17}N_2O_2$: 341.1284, found: 341.1287.



5q

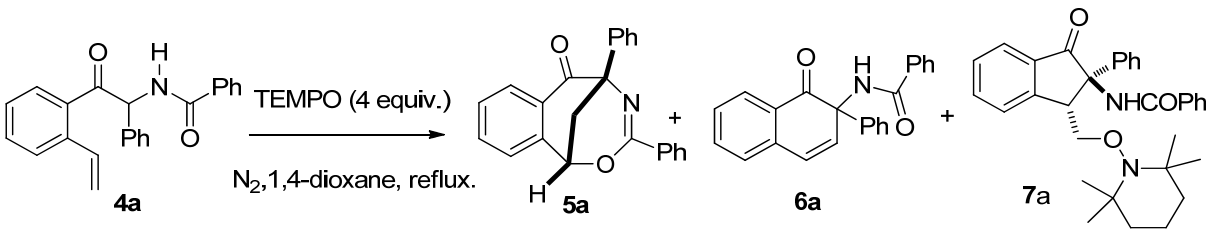
6-(4-Methoxyphenyl)-8-phenyl-6,10-dihydro-6,10-methanopyrido[3,2-*f*][1,3]oxazocin-5-one 5q: white solid, 79.6 mg, 43 %, mp 170-171 ^{o}C (recrystallization from dichloromethane /*n*-hexane); IR *v* (cm^{-1}) 1703, 1632; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.82 (dd, *J* = 5.2, 2.0 Hz, 1H), 8.39 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.07 (d, *J* = 7.2 Hz, 2H), 7.62 (d, *J* = 8.8 Hz, 2H), 7.45 (dd, *J* = 8.0, 5.2 Hz, 1H), 7.41 (d, *J* = 7.2 Hz 1H), 7.34 (t, *J* = 7.6 Hz 2H), 7.00 (d, *J* = 8.8, 2H), 5.79 (dd *J* = 4.0, 2.0 Hz, 1H), 3.83 (s, 3H), 3.05 (dd, *J* = 14.0, 2.0 Hz, 1H), 2.48 (dd, *J* = 14.0, 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 192.3, 159.1, 158.1, 155.4, 154.3, 137.2, 133.5, 133.1, 131.3, 128.4, 128.2, 127.6, 126.3, 125.4, 113.7, 73.2, 62.2, 55.4, 33.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{19}N_2O_3$: 371.1390, found: 371.1386.



5r

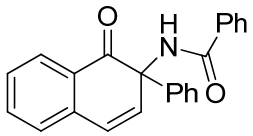
6-(4-Fluorophenyl)-8-phenyl-6,10-dihydro-6,10-methanopyrido[3,2-*f*][1,3]oxazocin-5-one 5r: white solid, 82.4 mg, 46 %, mp 165-166 ^{o}C (recrystallization from dichloromethane/*n*-hexane); IR *v* (cm^{-1}) 1703, 1632; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.84 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.39 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.06 (dd, *J* = 6.8, 1.2 Hz, 2H), 7.66 (dd, *J* = 8.8, 5.2 Hz, 2H), 7.46 (dd, *J* = 7.6, 4.8 Hz, 1H), 7.41 (d, *J* = 7.2 Hz 1H), 7.35 (t, *J* = 7.6 Hz 2H), 7.14 (t, *J* = 8.8 Hz 2H), 5.80 (dd *J* = 3.6, 2.4 Hz, 1H), 3.04 (dd, *J* = 14.0, 2.0 Hz, 1H), 2.48 (dd, *J* = 14.0, 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 192.0, 162.4 (d, *J* = 244.4 Hz), 158.1, 155.7, 154.5, 137.14, 137.09 (d, *J* = 3.8 Hz), 132.9, 131.5, 129.0 (d, *J* = 7.6 Hz), 128.2, 127.6, 126.1, 125.4, 115.1 (d, *J* = 21.1 Hz), 73.1, 62.3, 33.5; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{22}H_{16}FN_2O_2$: 359.1190, found: 359.1194.

(2) TEMPO-mediated cyclization reaction of 2-aryl-2-benzamido-1-(*o*-vinylaryl)-1-ethanones 4



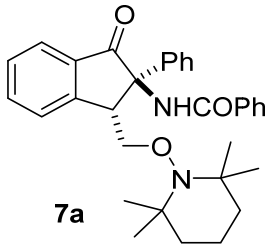
4a **5a** **6a** **7a**

Under nitrogen atmosphere and at room temperature, 2-benzamido-2-phenyl-1-(*o*-vinylphenyl)-1-ethanone **4a** (170.5 mg, 0.5 mmol) and TEMPO (312.5 mg, 2 mmol, 4 equiv.**)** were dissolved in dry 1,4-dioxane (5 mL). The reaction mixture was stirred in refluxing 1,4-dioxane for 10 h under the protection of nitrogen. The reaction was then quenched by removal of the solvents. The residue was chromatographed on a silica gel column eluting with a mixture of petroleum ether and ethyl acetate (PE : EA from 50 : 1 to 20 : 1) to give 3,5-diphenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one **5a** (60%), 2-benzamido-2-phenylnaphthalen-1-one **6a** (12%) and inden-1-one derivative **7a** (19%).



6a

2-Benzamido-2-phenylnaphthalen-1-one 6a: white solid, 20.5 mg, 12 %, mp 149-150 ^{o}C (recrystallization from chloroform/*n*-hexane); IR *v* (cm^{-1}) 3354, 1684, 1645; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.91 (d, *J* = 7.2 Hz, 1H), 7.85 (d, *J* = 6.6 Hz, 2H), 7.61 (d, *J* = 7.2 Hz, 2H), 7.56 (t, *J* = 6.0 Hz, 1H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.38 (s, 1H), 7.27-7.33 (m, 5H), 6.92 (d, *J* = 9 Hz, 1H), 6.77 (d, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 196.5, 166.6, 137.3, 136.5, 134.9, 134.2, 133.8, 132.0, 129.3, 129.1, 128.9, 128.7, 128.5, 128.1, 127.7, 127.3, 126.9, 126.4, 66.0; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{18}NO_2$: 340.1332, found: 340.1337.

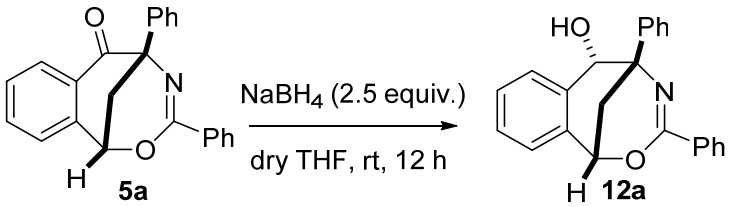


7a

(*2R*, *3R*)- and (*2S*, *3S*)-2-Benzamido-2-phenyl-3-(((2,2,6,6-tetramethyl-1-piperidinyl)oxy)methyl)-2,3-dihydroinden-1-one 7a: white solid, 47.2 mg, 19 %, mp 167-168 ^{o}C (recrystallization from chloroform/*n*-hexane); IR *v* (cm^{-1}) 3453, 1724, 1655; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.93 (d, *J* = 7.2 Hz, 1H), 7.88 (d, *J* = 6.6 Hz, 2H), 7.66-7.70 (m, 2H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.44-7.49 (m, 3H), 7.26-7.30 (m, 3H), 7.18 (d, *J* = 7.2 Hz, 1H), 7.08 (s, 1H), 5.55 (t, *J* = 7.8 Hz, 1H), 1.25-1.54 (m, 6H), 1.09 (s, 3H), 1.03 (s, 3H), 1.01 (s, 3H), 0.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 201.7, 167.2, 152.4, 137.1, 135.9, 135.7, 133.9, 132.0, 128.9, 128.8, 128.2, 127.2, 126.0, 125.7, 124.8, 76.4, 70.9, 59.8, 59.7, 49.0, 39.8, 39.7, 33.1, 32.6, 20.23, 20.22, 17.1; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{32}H_{37}N_2O_3$: 497.2798, found: 397.2802.

4. Reduction of 3,5-diphenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one 5a

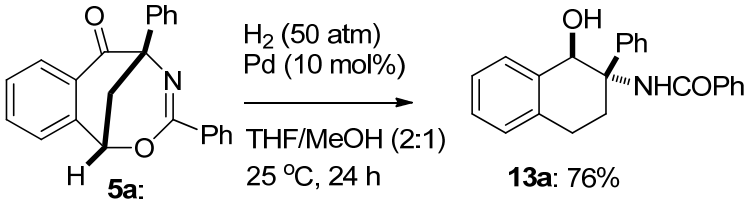
(1) Reduction of 5a by $NaBH_4$



In a flask, the 3,5-diphenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one **5a** (169.5 mg, 0.5 mmol) and $NaBH_4$ (47.3 mg, 1.25 mmol) were dissolved in dry THF (5 mL). The reaction mixture was stirred for 12 h at room temperature. The reaction was then quenched by adding water (10 mL). The resulting mixture was extracted with ethyl acetate (10×3 mL). The combined organic layer was washed by a saturated aqueous solution of NaCl (10 mL) and dried with anhydrous $MgSO_4$. After removal of $MgSO_4$ and organic solvents, the residue was chromatographed on a silica gel column eluting with a mixture of petroleum ether and ethyl acetate (petroleum ether : ethyl acetate = 20 : 1) to give 3,5-diphenyl-5,6-dihydro-1,5-methanobenzo[*f*][1,3]oxazocin-6-ol **12a** in 82% yield.

(*1S, 5S, 6S*)- and (*1R, 5R, 6R*)-3,5-Diphenyl-5,6-dihydro-1,5-methanobenzo[*f*][1,3]oxazocin-6-ol 12a: white solid, 139.9 mg, 82 %, mp 117-118 ^{o}C (without recrystallization); IR *v* (cm^{-1}) 3526, 1640; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.01 (d, *J* = 6.6 Hz, 2H), 7.79 (d, *J* = 7.8 Hz, 2H), 7.68 (d, *J* = 6.6 Hz, 1H), 7.30-7.45 (m, 9H), 5.46 (s, 1H), 5.17 (d, *J* = 11.4 Hz, 1H), 2.81 (d, *J* = 9.0 Hz, 1H), 2.69 (d, *J* = 12.6 Hz, 1H), 2.37 (d, *J* = 12.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 155.0, 145.1, 139.8, 133.7, 133.6, 131.1, 129.9, 129.1, 128.7, 128.5, 128.2, 127.7, 127.1, 126.5, 78.9, 72.6, 58.0, 34.9; HRMS (TOF-ESI): $[M + H]^{+}$ calcd for $C_{23}H_{20}NO_2$: 342.1488, found: 342.1484.

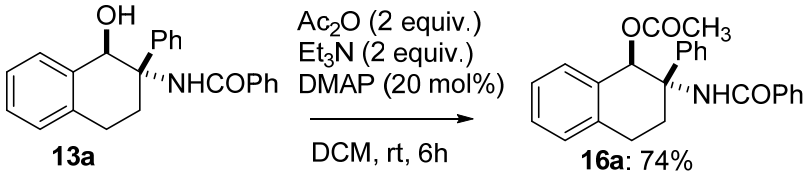
(2) Pd-C catalyzed hydrogenation reaction of compound 5a



In a glass vessel, the 3,5-diphenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one **5a** (67.8 mg, 0.2 mmol) was dissolved in THF (2 mL), followed by the addition of Pd-C (10 mol%, 32.8 mg Pd-C containing 10% w/w of Pd and 35% H_2O) and methanol (1 mL). This vessel was subsequently transferred into a steel autoclave reactor. The autoclave was purged with H_2 gas without stirring, and then was pressurized under 50 atm pressure of H_2 gas. The reaction mixture was stirred under H_2 gas (50 atm) for 24 h at 25 ^{o}C. The autoclave

was then slowly depressurized by releasing the hydrogen gas carefully. The Pd-C was filtrated and washed with dichloromethane (5 mL×3). The combined filtrate was concentrated under reduced pressure. The residue was chromatographed on a silica gel column eluting with a mixture of petroleum ether and ethyl acetate (PE : EA = 5 : 1) to give *N*-(1-hydroxy-2-phenyl-2-tetrahydronaphthalenyl)benzamide **13a** in 76% yield.

(*1R, 2S*)-and (*1S, 2R*)-*N*-(1-Hydroxy-2-phenyl-2-tetrahydronaphthalenyl)benzamide 13a: white solid, 50.9 mg, 76%, mp 217-218 ^{o}C (recrystallization from chloroform/*n*-hexane); IR *v* (cm^{-1}) 3580, 3279, 1645; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.65 (d, *J* = 6.6 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 8.4 Hz, 2H), 7.33 (t, *J* = 7.8 Hz, 2H),7.26-7.30 (m, 3H), 7.14 (d, *J* = 7.8 Hz, 1H), 5.46 (s, 1H), 6.41 (s, 1H), 4.91 (s, 1H), 2.76-2.85 (m, 3H), 2.50-2.53 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 167.7, 141.2, 136.1, 136.0, 134.5, 131.9, 129.5, 128.8, 128.7, 128.6, 128.1, 127.5, 127.1, 126.8, 126.7, 75.9, 62.0, 29.0, 26.1; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{23}H_{22}NO_2$: 344.1645, found: 344.1647.

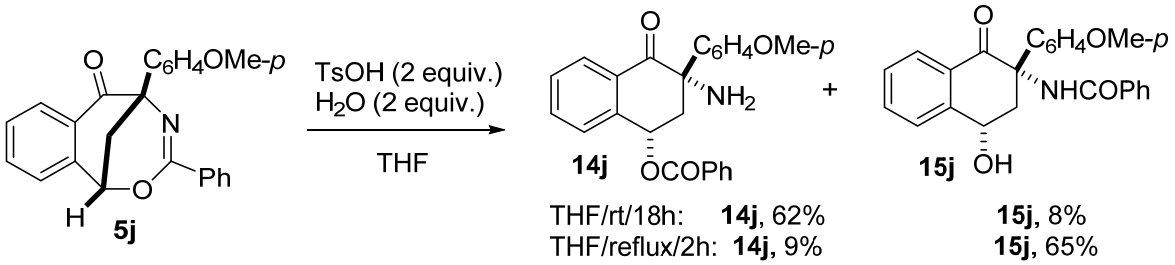


The *N*-(1-hydroxy-2-phenyl-2-tetrahydronaphthalenyl)benzamide **13a** (67.8 mg, 0.2 mmol), dichloromethane (2 mL), DMAP (4.9 mg, 0.04 mmol), Ac_2O (40.8 mg, 0.4 mmol) and Et_3N (60.7 mg, 0.6 mmol) were added successively to a flask. The reaction mixture was stirred for 6 h at room temperature. The reaction was then quenched by adding water (5 mL). The resulting mixture was extracted with DCM (10×3 mL). The combined organic layer was dried with anhydrous $MgSO_4$. After removal of $MgSO_4$ and organic solvents, the residue was chromatographed on a silica gel column eluting with a mixture of petroleum ether and ethyl acetate (petroleum ether : ethyl acetate from 5 : 1 to 3 : 1) to give 2-benzamido-2-phenyl-1-tetrahydronaphthalenyl acetate **16a** in 74% yield.

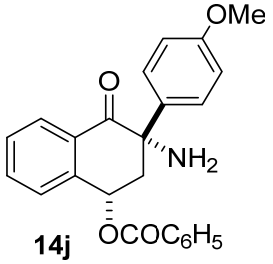
2-benzamido-2-phenyl-1-tetrahydronaphthalenyl acetate **16a:** white solid, 56.9 mg, 74%, mp 188-189 ^{o}C (recrystallization from ethyl acetate/*n*-hexane); IR *v* (cm^{-1}) 3289, 1740, 1645; ^{1}H NM-R (600 MHz, $CDCl_3$) δ (ppm) 7.55 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 7.2 Hz, 2H), 7.41 (t, *J* = 8.4 Hz, 2H), 7.22-7.36 (m, 8H), 6.38 (d, *J* = 11.4 Hz, 1H), 6.18 (s, 1H), 3.29 (d, *J* = 12.6 Hz, 1H), 3.05 (dd, *J* = 17.4, 4.8 Hz, 1H),

2.94-2.99 (m, 1H), 2.74-2.79 (m, 1H), 1.65 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 169.7, 166.7, 142.3, 137.7, 134.7, 132.1, 131.6, 129.3, 129.2, 128.6, 128.2, 127.4, 127.0, 126.7, 126.2, 73.7, 59.9, 25.9, 23.9, 20.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{25}H_{24}NO_3$: 386.1750, found: 386.1747.

5. Acidic hydrolysis of compound 5j

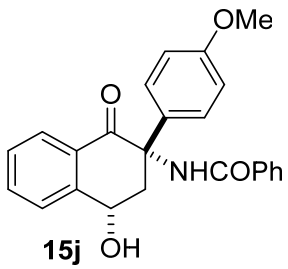


In a test flask, the 5-(4-methoxyphenyl)-3-phenyl-1,5-methanobenzo[*f*][1,3]oxazocin-6-one **5j** (73.8 mg, 0.2 mmol), TsOH (68.8 mg, 0.4 mmol) and H_2O (7.2 mg, 0.4 mmol) were dissolved in THF (2 mL). The reaction mixture was stirred for 18 h at room temperature or was stirred for 2h in refluxing THF. The reaction was then quenched by the addition of saturated aqueous solution of $NaHCO_3$ (2 mL). The resulting mixture was extracted with ethyl acetate (10×3 mL). The combined organic layer was dried with anhydrous $MgSO_4$. After removal of $MgSO_4$ and organic solvents, the residue was chromatographed on a silica gel column eluting with a mixture of petroleum ether and ethyl acetate (petroleum ether : ethyl acetate from 5 : 1 to 2 : 1) to give 3-amino-3-(*p*-methoxyphenyl)-4-oxo-1-tetrahydronaphthalenyl benzoate **14j** and *N*-(4-hydroxy-2-(*p*-methoxyphenyl)-1-oxo-2-tetrahydronaphthalenyl)benzamide **15j**. Products **14j** and **15j** were isolated in 62% and 8% yields from the reaction at room temperature, while as **14j** and **15j** were obtained in 9% and 65% yields from the reaction in refluxing THF.



(*1S, 3S*)- and (*1R, 3R*)-3-Amino-3-(*p*-methoxyphenyl)-4-oxo-1-tetrahydronaphthalenyl benzoate 14j: white solid, 47.8 mg, 62%, mp 77-78 °C (without recrystallization); IR *v* (cm^{-1}) 3370, 1721, 1692; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.22 (d, *J* = 7.8 Hz, 1H), 8.10 (d, *J* = 7.8 Hz, 2H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.56

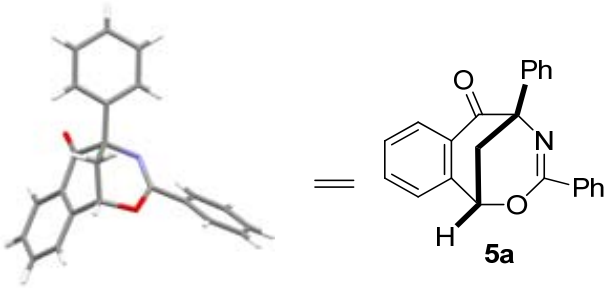
(t, *J* = 7.8 Hz, 1H), 7.46-7.48 (m, 3H), 7.35-7.37 (m, 3H), 6.86 (d, *J* = 9.6 Hz, 2H), 6.15 (dd, *J* = 10.2, 4.2 Hz, 1H), 3.75 (s, 3 H), 3.30 (dd, *J* = 12.6, 4.2 Hz, 1H), 2.46 (t, *J* = 12 Hz, 1H), 2.21 (brs, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 200.2, 166.2, 159.5, 141.6, 134.1, 133.6, 132.2, 131.5, 129.9, 129.8, 128.7, 128.0, 127.5, 126.5, 114.6, 69.0, 63.0, 55.3, 42.5; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{22}NO_4$: 388.1543, found: 388.1547.



15j

(*2S*, *4S*)- and (*2R*, *4R*)-*N*-(4-Hydroxy-2-(*p*-methoxyphenyl)-1-oxo-2-tetrahydronaphthalenyl)benzamide 15j: white solid, 50.2 mg, 65 %, mp 154-155 ^{o}C (recrystallization from chloroform/*n*-hexane); IR *v* (cm^{-1}) 3381, 1694, 1647; ^{1}H NM-R (600 MHz, $CDCl_3$) δ (ppm) 8.15 (d, *J* = 7.8 Hz, 1H), 7.74 (d, *J* = 6.6 Hz, 2H), 7.67 (s, 1H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.45-7.48 (m, 3H), 7.37-7.40 (m, 3H), 6.78 (d, *J* = 9 Hz, 2H), 4.89 (d, *J* = 7.8 Hz, 1H), 4.06 (dd, *J* = 13.2, 4.2 Hz, 1H), 3.70 (s, 3 H), 2.82 (t, *J* = 12.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 195.5, 166.7, 159.7, 146.0, 134.63, 134.60, 131.7, 130.0, 129.0, 128.6, 128.12, 128.06, 127.9, 127.1, 126.8, 114.2, 65.6, 65.0, 55.3, 41.8; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{24}H_{22}NO_4$: 388.1543, found: 388.1549.

4. X-Ray crystallography of 5a, 7a, 12a, 15j and 16a



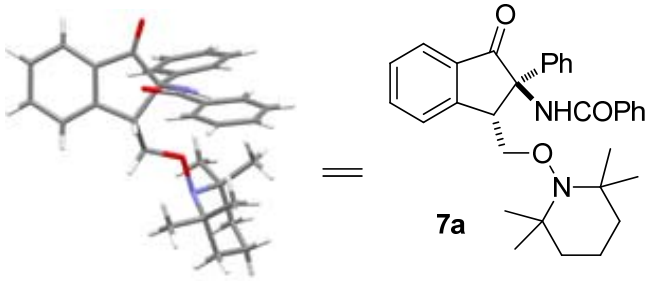
5a

Crystals of compound **5a** (CCDC 2072676) were obtained via slow evaporation of a solution containing **5a** in dichloromethane and *n*-hexane. Single-crystal diffraction intensity data of the compound **5a** was collected on a XtaLAB Synergy R (DW system, HyPix) four-circle diffractometer equipped with graphite monochromatized CuKα (λ = 1.54184) at 100.00K. Empirical absorption corrections was applied to the intensities using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The structure was solved by the program ShelXT (Sheldrick, 2015) and refined with the program ShelXL (Sheldrick, 2015). The crystal data and structure refinement results for compound **5a** are listed in the Table S1.

Table S1. Crystal data and structure refinement for 5a.

Identification code	20190725a
Empirical formula	$C_{23}H_{17}NO_2$
Formula weight	339.38
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	P 2_1 2_1 2_1
a/Å	6.0655(3)
b/Å	16.0001(7)
c/Å	17.3309(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1681.94(13)
Z	4
ρ_{calc} (g/cm^3)	1.340
μ/mm^{-1}	0.680
F(000)	712.0
Crystal size/mm^3	0.25 × 0.15 × 0.1
Radiation	CuKα (λ = 1.54184)
2 θ range for data collection/°	7.52 to 149.624
Index ranges	-6 ≤ h ≤ 7, -19 ≤ k ≤ 20, -21 ≤ l ≤ 13

Reflections collected	5875
Independent reflections	3079 [R_{int} = 0.0329, R_{sigma} = 0.0430]
Data/restraints/parameters	3079/0/235
Goodness-of-fit on F^2	1.099
Final R indexes [I≥2σ (I)]	R_1 = 0.0394, wR_2 = 0.0965
Final R indexes [all data]	R_1 = 0.0457, wR_2 = 0.1073
Largest diff. peak/hole / e $Å^{-3}$	0.19/-0.25

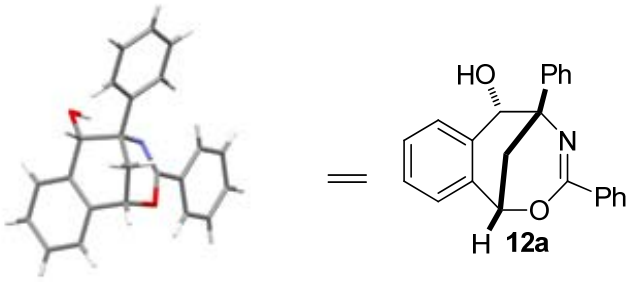


Crystals of compound **7a** (CCDC 2072678) were obtained via slow evaporation of a solution containing **7a** in dichloromethane, ethyl acetate and *n*-hexane. Single-crystal diffraction intensity data of the compound **7a** was collected on a XtaLAB Synergy R (DW system, HyPix) four-circle diffractometer equipped with graphite monochromatized CuKα (λ = 1.54184) at 100.00K. Empirical absorption corrections was applied to the intensities using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The structure was solved by the program ShelXT (Sheldrick, 2015) and refined with the program ShelXL (Sheldrick, 2015). The crystal data and structure refinement results for compound **7a** are listed in the Table S2.

Table S2. Crystal data and structure refinement for 7a.

Identification code	20190725b
Empirical formula	$C_{32}H_{36}N_2O_3$
Formula weight	496.63
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.8614(2)
b/Å	11.4704(2)
c/Å	12.8238(2)
α/°	79.9360(10)
β/°	82.2430(10)
γ/°	71.336(2)
Volume/$Å^3$	1348.26(4)

Z	2
ρ_{calc} (g/cm^3)	1.223
μ/mm^{-1}	0.617
F(000)	532.0
Crystal size/mm^3	0.25 × 0.15 × 0.15
Radiation	CuKα (λ = 1.54184)
2 θ range for data collection/°	7.026 to 151.638
Index ranges	-9 ≤ h ≤ 12, -14 ≤ k ≤ 14, -15 ≤ l ≤ 15
Reflections collected	16392
Independent reflections	5371 [R_{int} = 16392, R_{sigma} = 0.0278]
Data/restraints/parameters	5371/0/342
Goodness-of-fit on F^2	1.083
Final R indexes [I>=2σ (I)]	R_1 =0.0385, wR_2 =0.0961
Final R indexes [all data]	R_1 = 0.0458 wR_2 = 0.1048
Largest diff. peak/hole / e Å^{-3}	0.25/-0.24

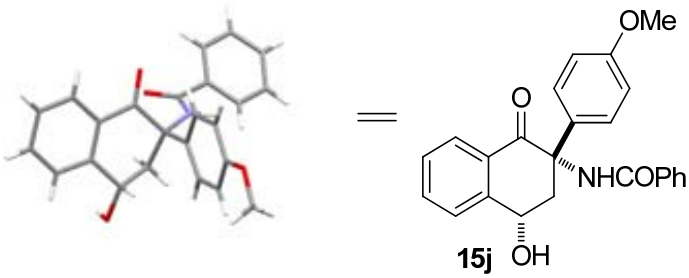


Crystals of compound **12a** (CCDC 2072679) were obtained via slow evaporation of a solution containing **12a** in acetone, dichloromethane and *n*-hexane. Single-crystal diffraction intensity data of the compound **12a** was collected on a 'XtaLAB Synergy R, DW system, HyPix' four-circle diffractometer equipped with graphite monochromatized CuKα (λ = 1.54184) at 99.99 K. Empirical absorption corrections was applied to the intensities using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The structure was solved by the program ShelXT (Sheldrick, 2015) and refined with the program ShelXL (Sheldrick, 2015). The crystal data and structure refinement results for compound **12a** are listed in the Table S3.

Table S3. Crystal data and structure refinement for 12a.

Identification code	exp_4015
Empirical formula	$C_{23}H_{19}NO_2$
Formula weight	341.39
Temperature/K	99.99(10)

Crystal system	monoclinic
Space group	Pc
a/Å	9.3804(3)
b/Å	6.3889(2)
c/Å	29.2078(9)
α/°	90
β/°	92.434(3)
γ/°	90
Volume/Å^3	1748.86(10)
Z	4
ρ_{calc} (g/cm^3)	1.297
μ/mm^{-1}	0.654
F(000)	720.0
Crystal size/mm^3	0.25 × 0.1 × 0.05
Radiation	CuKα (λ = 1.54184)
2 θ range for data collection/°	9.436 to 160.232
Index ranges	-7 ≤ h ≤ 11, -7 ≤ k ≤ 7, -36 ≤ l ≤ 36
Reflections collected	18385
Independent reflections	4745 [R_{int} = 0.0785, R_{sigma} = 0.0528]
Data/restraints/parameters	4745/4/477
Goodness-of-fit on F^2	1.068
Final R indexes [I>=2σ (I)]	R_1 = 0.0933, wR_2 = 0.2653
Final R indexes [all data]	R_1 = 0.0970, wR_2 = 0.2696
Largest diff. peak/hole / e Å^{-3}	0.58/-0.54



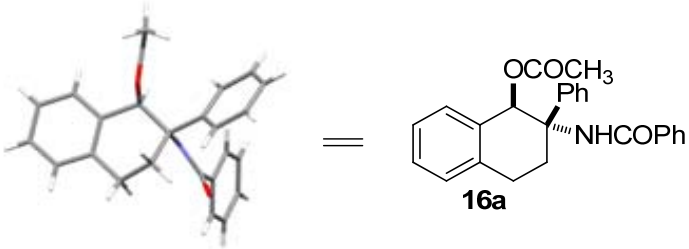
15j

Crystals of compound **15j** (CCDC 2072680) were obtained via slow evaporation of a solution containing **15j** in acetone, dichloromethane and *n*-hexane. Single-crystal diffraction intensity data of the compound **15j** was collected on a 'XtaLAB Synergy R, DW system, HyPix' four-circle diffractometer equipped with graphite monochromatized CuKα (λ = 1.54184) at 100.00 K. Empirical absorption corrections was applied to the intensities using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The structure was solved by the program ShelXT (Sheldrick, 2015) and refined with the program ShelXL (Sheldrick, 2015). The crystal data and structure refinement results for compound **15j** are listed in the Table

S4.

Table S4. Crystal data and structure refinement for 15j.

Identification code	20210317a
Empirical formula	$C_{24}H_{21}NO_4$
Formula weight	387.42
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	11.7696(5)
b/Å	12.8699(5)
c/Å	13.1051(3)
α/°	81.729(3)
β/°	79.931(3)
γ/°	89.240(3)
Volume/Å^3	1934.03(13)
Z	4
ρ_{calc} (g/cm^3)	1.331
μ/mm^{-1}	0.736
F(000)	816.0
Crystal size/mm^3	0.2 × 0.15 × 0.03
Radiation	CuKα (λ = 1.54184)
2 θ range for data collection/°	6.922 to 153.378
Index ranges	-14 ≤ h ≤ 14, -16 ≤ k ≤ 16, -13 ≤ l ≤ 16
Reflections collected	23184
Independent reflections	7740 [R_{int} = 0.0515, R_{sigma} = 0.0453]
Data/restraints/parameters	7740/0/541
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0616, wR_2 = 0.1891
Final R indexes [all data]	R_1 = 0.0730, wR_2 = 0.2003
Largest diff. peak/hole / e Å^{-3}	0.64/-0.40



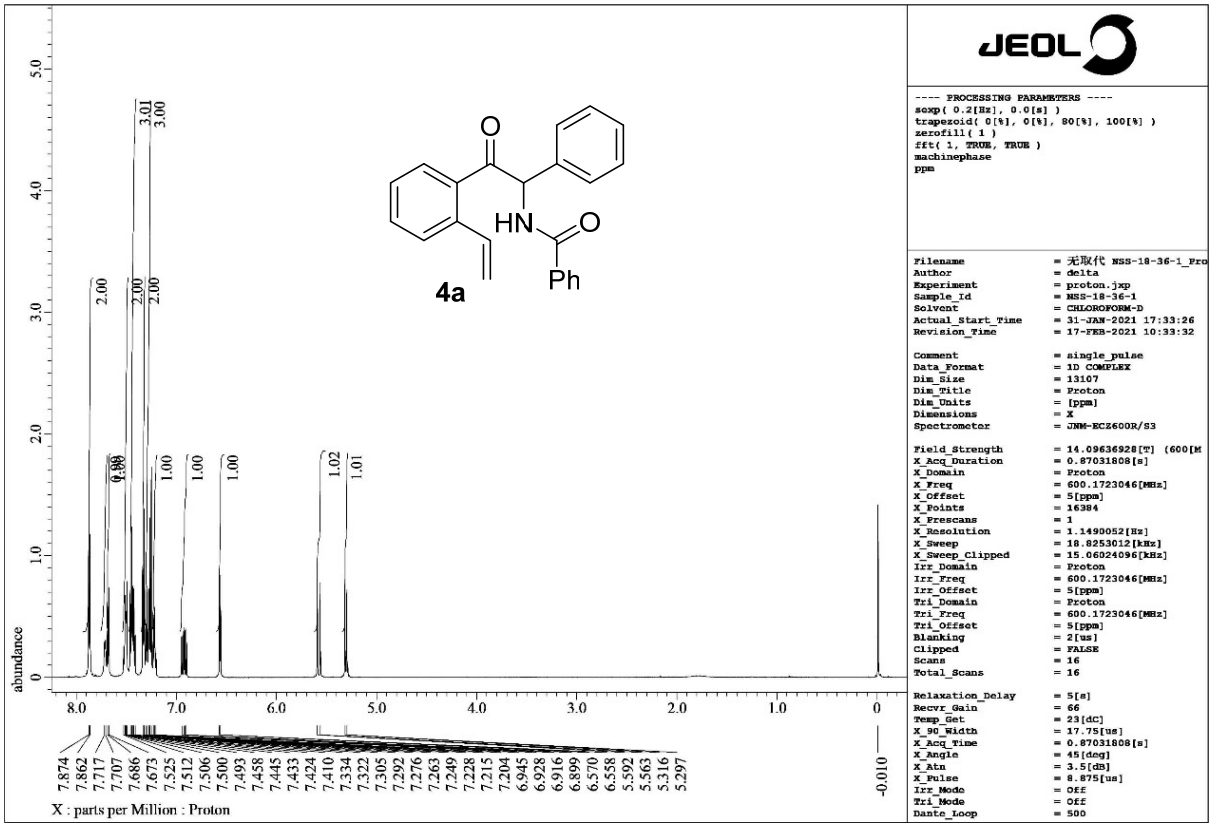
Crystals of compound **16a** (CCDC 2072681) were obtained via slow evaporation of a solution containing

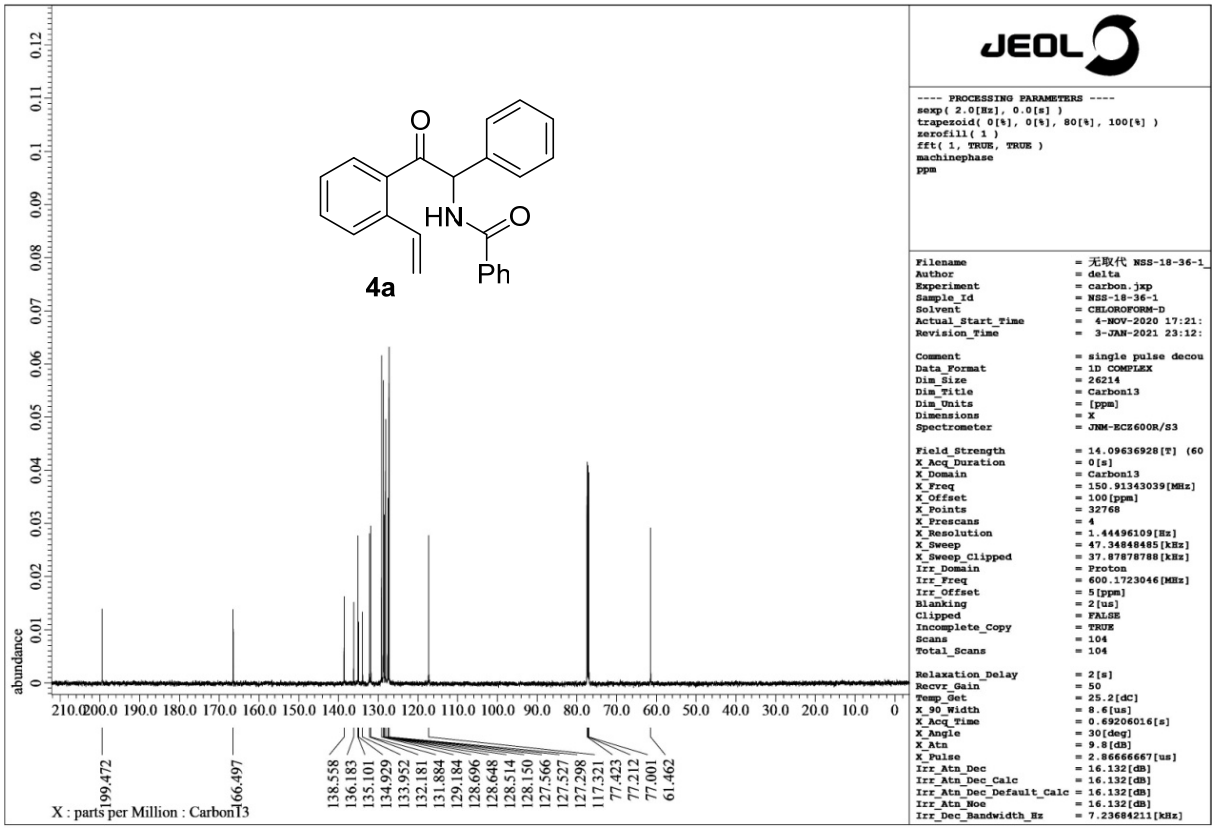
16a in chloroform-d, dichloromethane and *n*-hexane. Single-crystal diffraction intensity data of the compound **16a** was collected on a 'XtaLAB Synergy R, DW system, HyPix' four-circle diffractometer equipped with graphite monochromatized CuKα (λ = 1.54184) at 100.00 K. Empirical absorption corrections was applied to the intensities using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The structure was solved by the program ShelXT (Sheldrick, 2015) and refined with the program ShelXL (Sheldrick, 2015). The crystal data and structure refinement results for compound **16a** are listed in the Table S5.

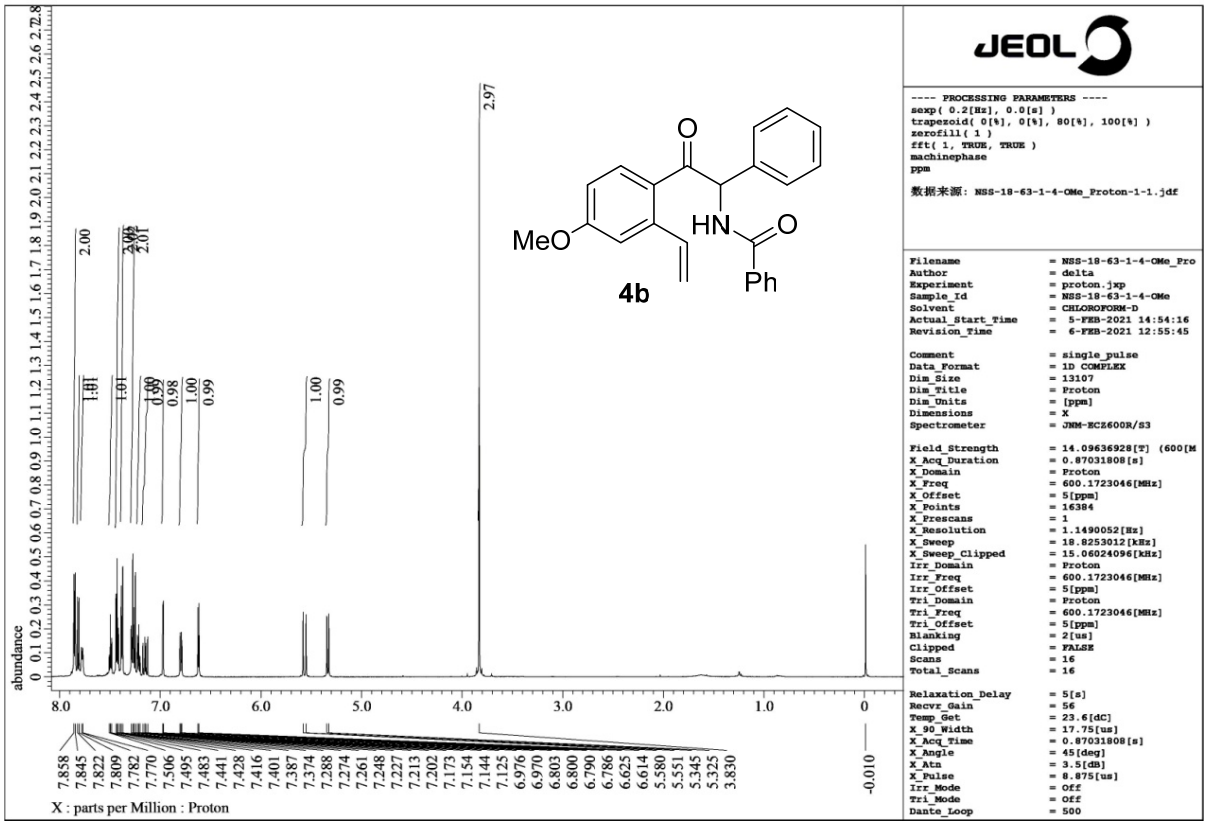
Table S5. Crystal data and structure refinement for 16a.

Identification code	20210310c
Empirical formula	$C_{25}H_{23}NO_3$
Formula weight	385.44
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.0089(3)
b/Å	12.1614(4)
c/Å	17.3949(2)
α/°	90.1962(19)
β/°	100.0512(19)
γ/°	107.208(3)
Volume/Å^3	1988.11(10)
Z	4
ρ_{calc} (g/cm^3)	1.288
μ/mm^{-1}	0.674
F(000)	816.0
Crystal size/mm^3	0.25 × 0.25 × 0.15
Radiation	CuKα (λ = 1.54184)
2 θ range for data collection/°	7.624 to 152.898
Index ranges	-12 ≤ h ≤ 12, -15 ≤ k ≤ 14, -19 ≤ l ≤ 21
Reflections collected	24382
Independent reflections	8030 [R_{int} = 0.0451, R_{sigma} = 0.0409]
Data/restraints/parameters	8030/1/557
Goodness-of-fit on F^2	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0575, wR_2 = 0.1520
Final R indexes [all data]	R_1 = 0.0641, wR_2 = 0.1577
Largest diff. peak/hole / e Å^{-3}	0.48/-0.38

7. ^{1}H and ^{13}C NMR spectra of products





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trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-18-63-1-4-OMe_Proton-1-1.jdf
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Filename	= NSS-18-63-1-4-OMe_Pro
Author	= delta
Experiment	= proton.jxp
Sample_Id	= NSS-18-63-1-4-OMe
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-FEB-2021 14:54:16
Revision_Time	= 6-FEB-2021 12:55:45
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Dimensions	= X
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Field_Strength	= 14.09636928[T] (600[M
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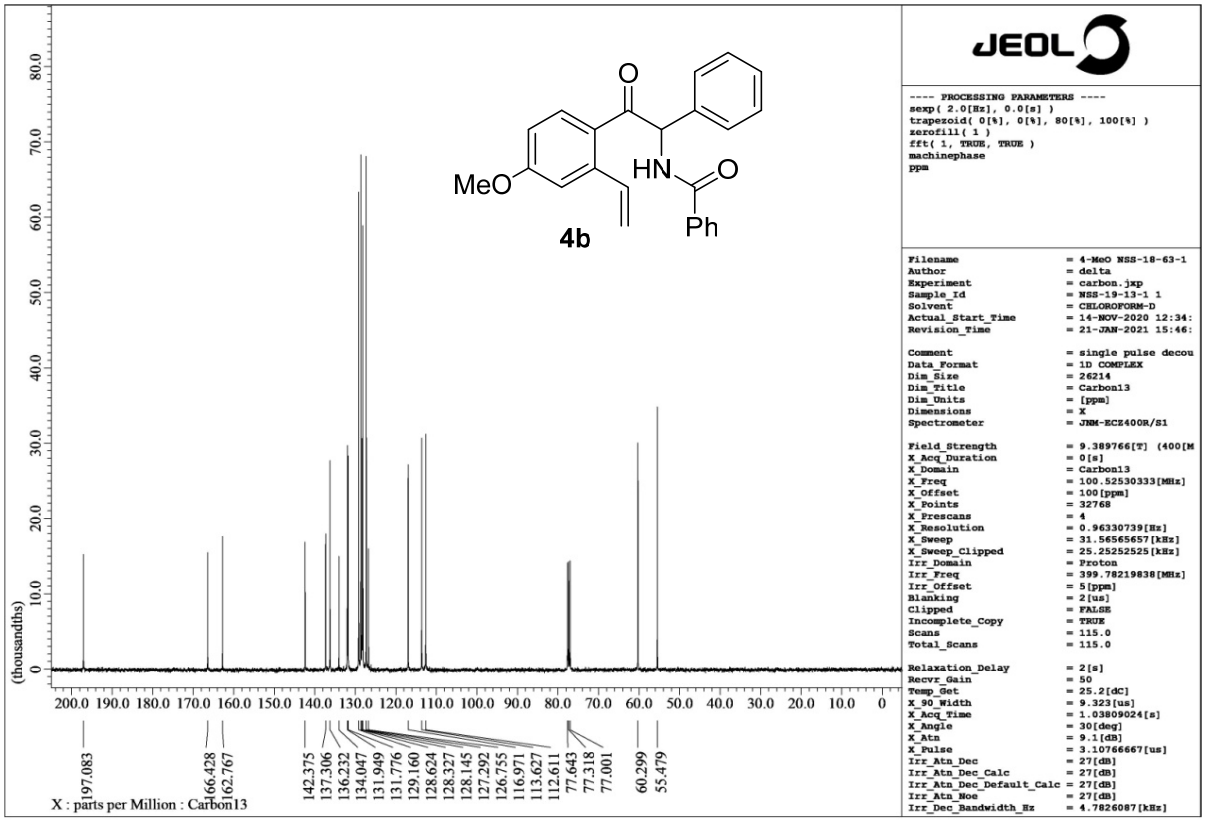
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 1.1490052[Hz]
X_Sweep	= 18.8253012[kHz]
X_Sweep_Clipped	= 15.06024096[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 23.6[dC]
X_90_Width	= 17.75[us]
X_Acq_Time	= 0.87031808[s]
X_Angle	= 45[deg]
X_Atn	= 3.5[dB]
X_Pulse	= 8.875[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500

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zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
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Author	= delta
Experiment	= carbon.jxp
Sample_Id	= NSS-19-13-1 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-NOV-2020 12:34:
Revision_Time	= 21-JAN-2021 15:46:
Comment	= single pulse decou
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Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400R/S1
Field_Strength	= 9.389766[T] (400[M
X_Acq_Duration	= 0[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Incomplete_Copy	= TRUE
Scans	= 115.0
Total_Scans	= 115.0
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 25.2[dC]
X_90_Width	= 9.323[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 9.1[dB]
X_Pulse	= 3.10766667[us]
Irr_Atn_Dec	= 27[dB]
Irr_Atn_Dec_Calc	= 27[dB]
Irr_Atn_Dec_Default_Calc	= 27[dB]
Irr_Atn_Noe	= 27[dB]
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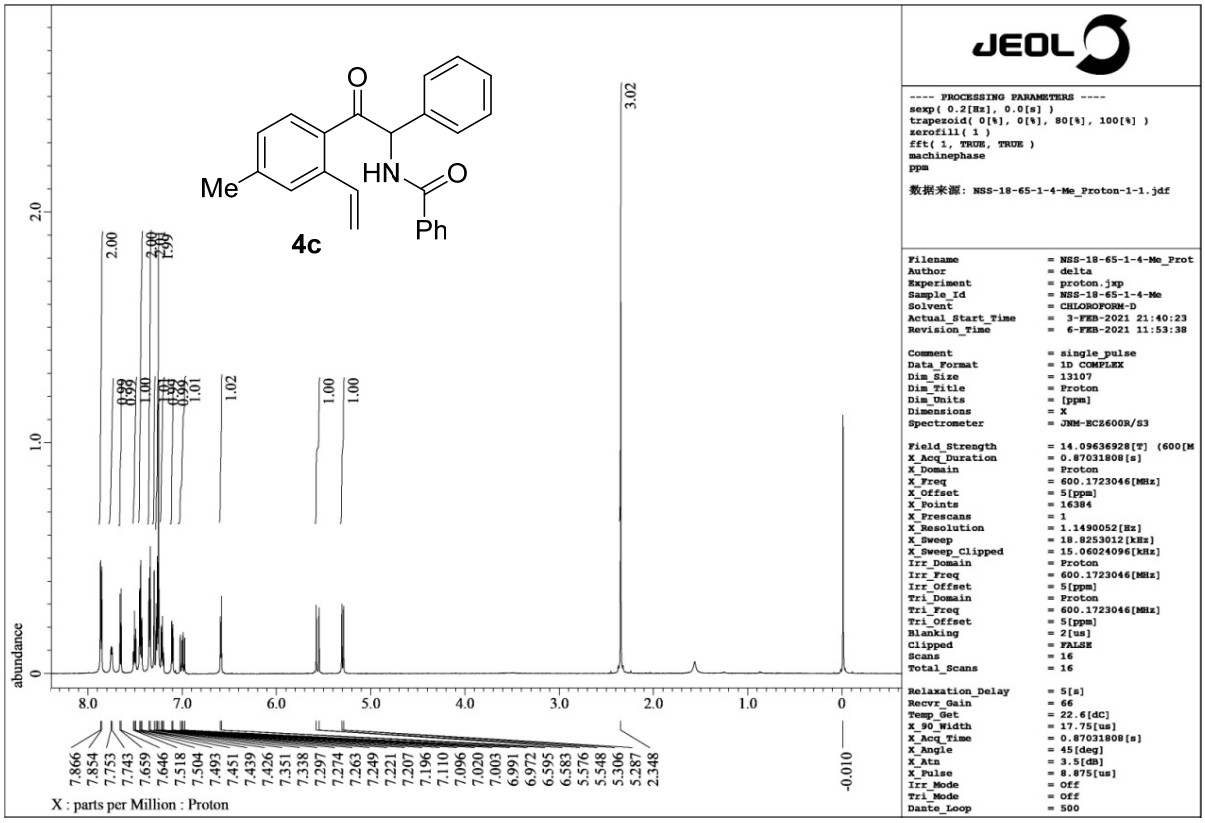
4c
Me
HN
O
Ph
abundance
X : parts per Million : Proton
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trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
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Filename = NSS-18-65-1-4-Me_Prot
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-18-65-1-4-Me
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-FEB-2021 21:40:23
Revision_Time = 6-FEB-2021 11:53:38
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Dim_Units = [ppm]
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Spectrometer = JNM-ECZ600R/S3
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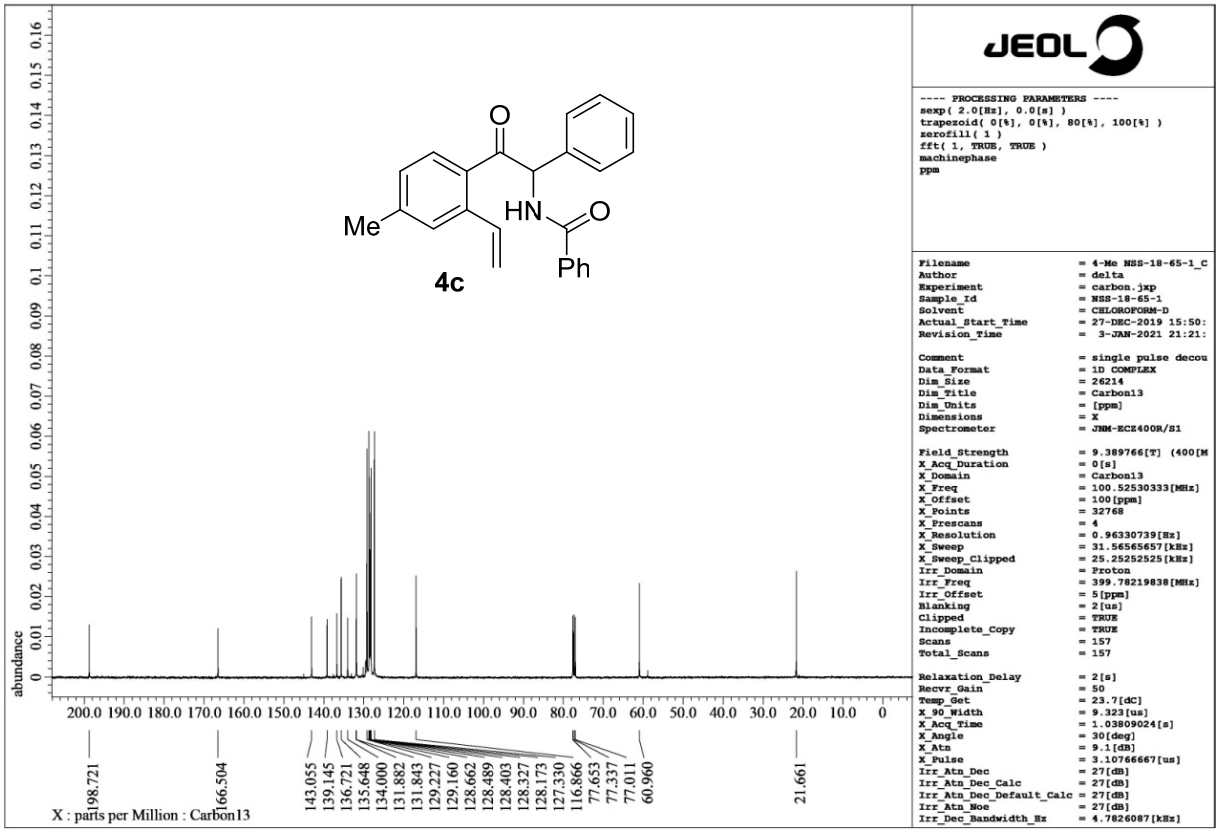
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 22.6[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500


4c
Me
HN
O
Ph
abundance
X : parts per Million : Carbon13
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zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
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Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-18-65-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-DEC-2019 15:50:
Revision_Time = 3-JAN-2021 21:21:
Comment = single pulse decou
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Dim_Title = Carbon13
Dim_Units = [ppm]
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Spectrometer = JNM-ECZ400R/S1
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X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
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X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
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Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
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Incomplete_Copy = TRUE
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Total_Scans = 157
Relaxation_Delay = 2[s]
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X_Acq_Time = 1.03809024[s]
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X_Pulse = 3.10766667[us]
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Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
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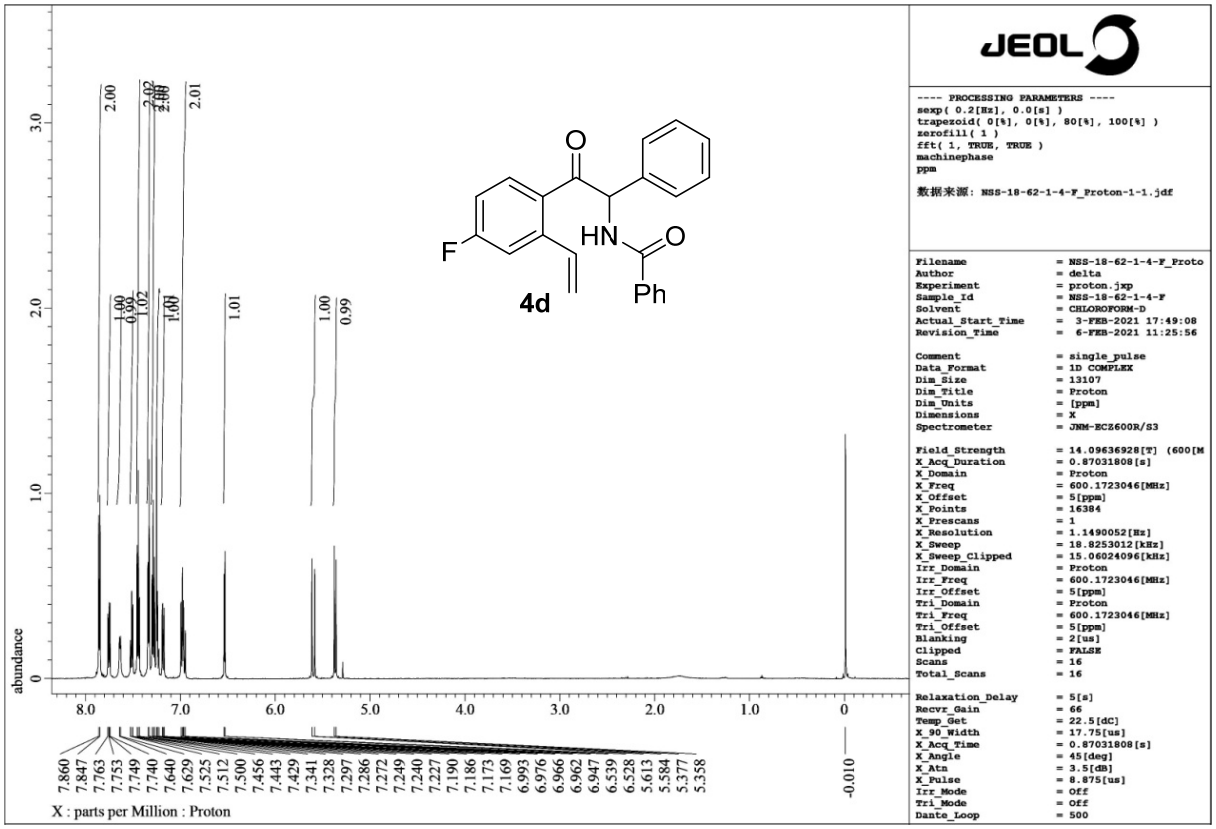


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---- PROCESSING PARAMETERS ----
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fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-18-62-1-4-F_Proton-1-1.jdf

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Author                  = delta
Experiment              = proton.jxp
Sample_Id               = NSS-18-62-1-4-F
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  3-FEB-2021 17:49:08
Revision_Time           =  6-FEB-2021 11:25:56

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Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 0.87031808[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 1.1490052[Hz]
X_Sweep                 = 18.8253012[kHz]
X_Sweep_Clipped         = 15.06024096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 5[s]
Recvr_Gain              = 66
Temp_Get                = 22.5[dC]
X_90_Width              = 17.75[us]
X_Acq_Time              = 0.87031808[s]
X_Angle                 = 45[deg]
X_Atn                   = 3.5[dB]
X_Pulse                 = 8.875[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
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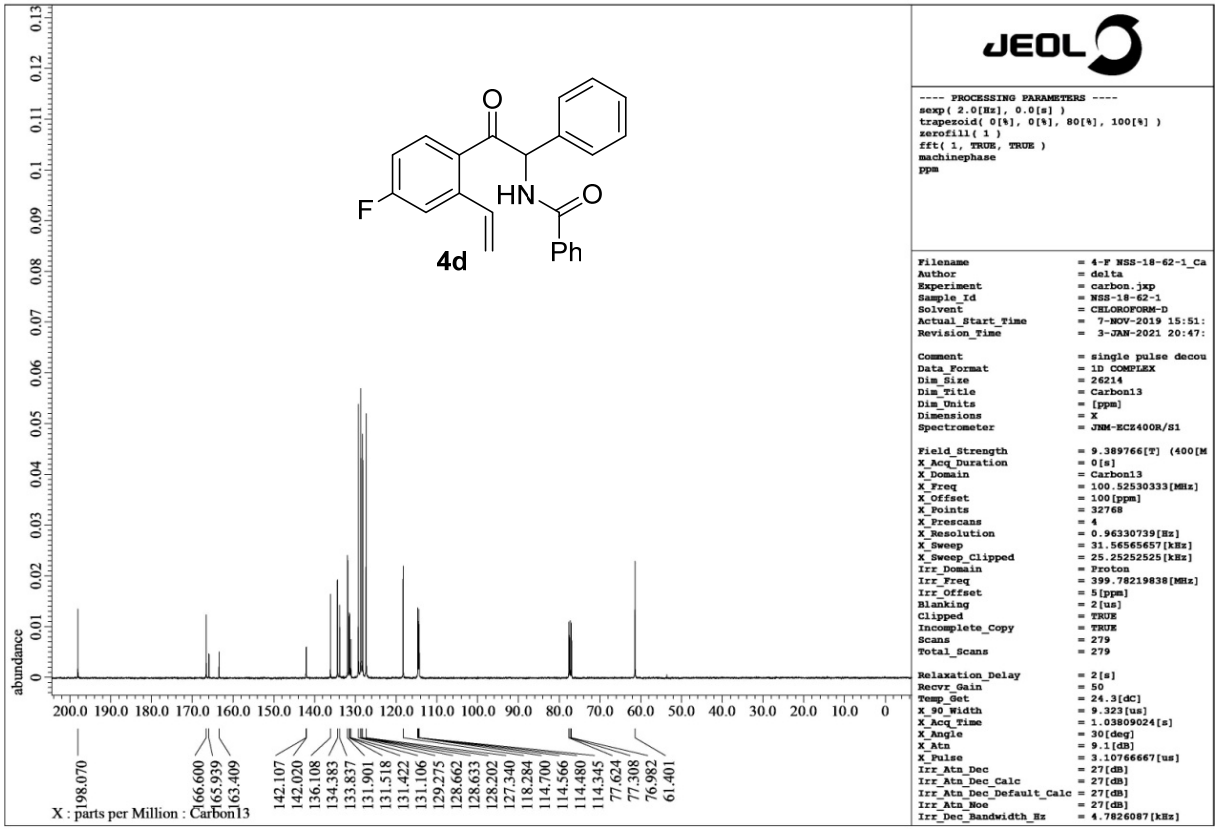


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fft( 1, TRUE, TRUE )
machinephase
ppm

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Author                  = delta
Experiment              = carbon.jxp
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Actual_Start_Time       =  7-NOV-2019 15:51:
Revision_Time           =  3-JAN-2021 20:47:

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X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
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Total_Scans             = 279

Relaxation_Delay        = 2[s]
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Temp_Get                = 24.3[dC]
X_90_Width              = 9.323[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 9.1[dB]
X_Pulse                 = 3.10766667[us]
Irr_Atn_Dec             = 27[dB]
Irr_Atn_Dec_Calc        = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe             = 27[dB]
Irr_Dec_Bandwidth_Hz    = 4.7826087[kHz]
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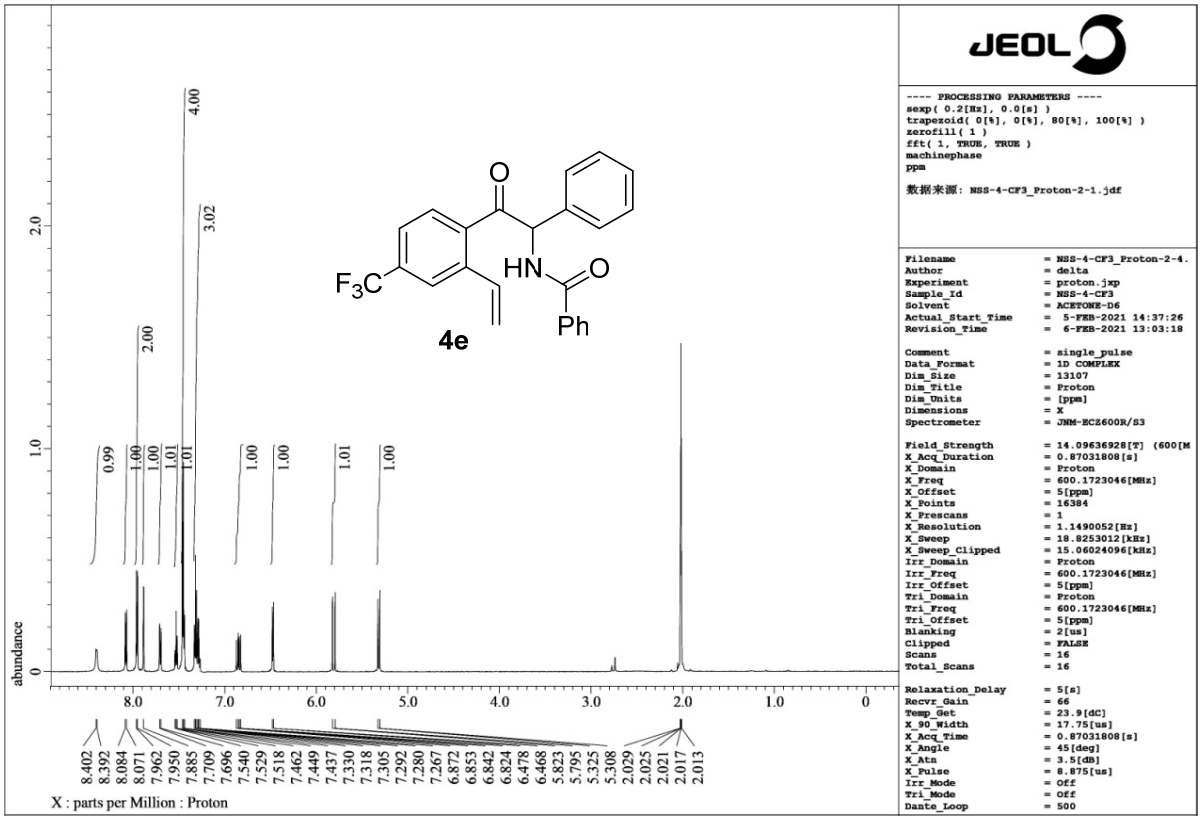
4e
abundance
X : parts per Million : Proton
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fft(1, TRUE, TRUE)
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Author = delta
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Revision_Time = 6-FEB-2021 13:03:18
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Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
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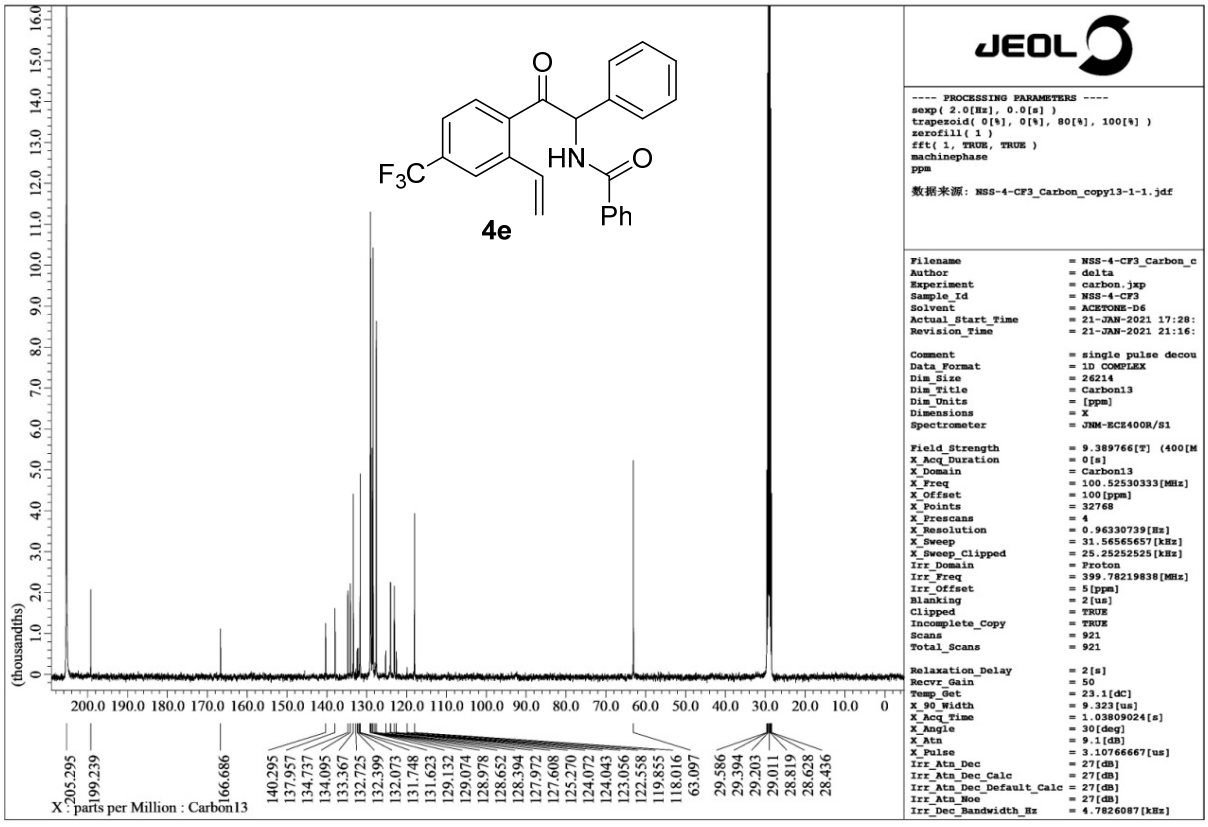
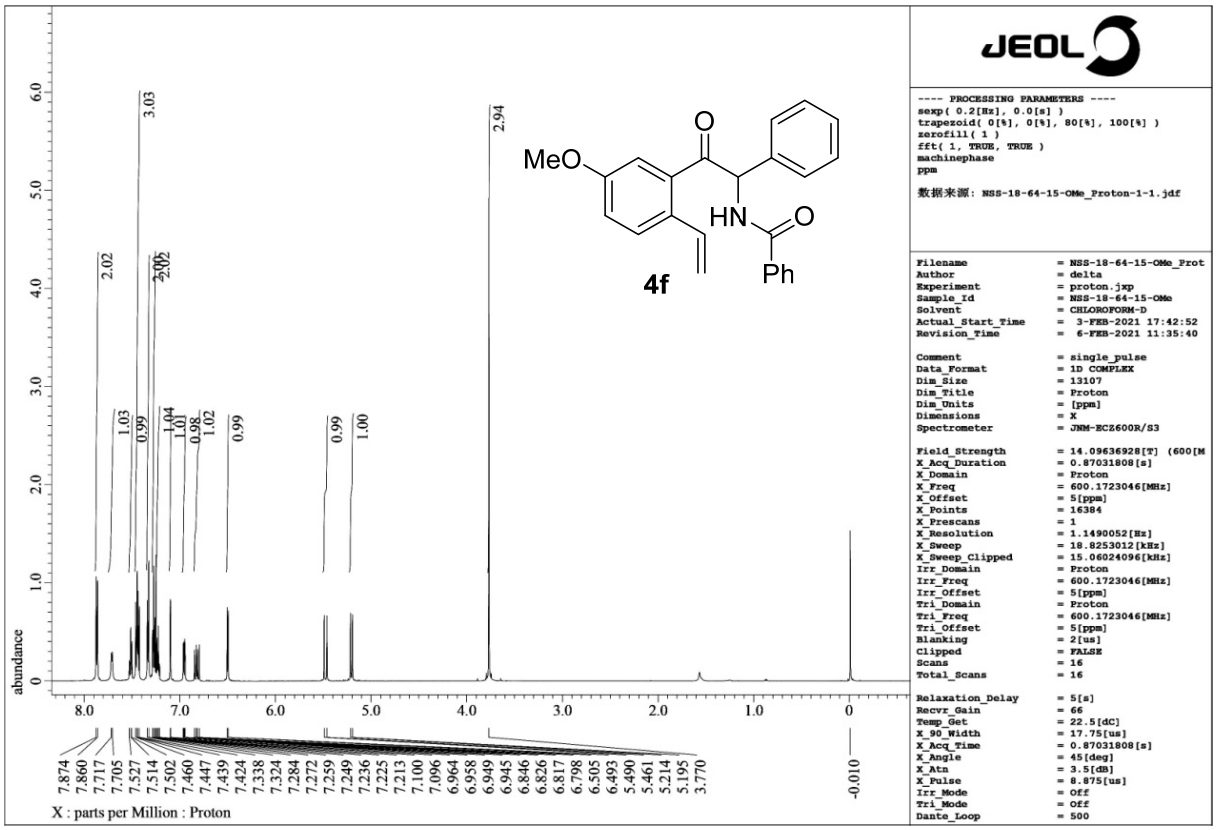
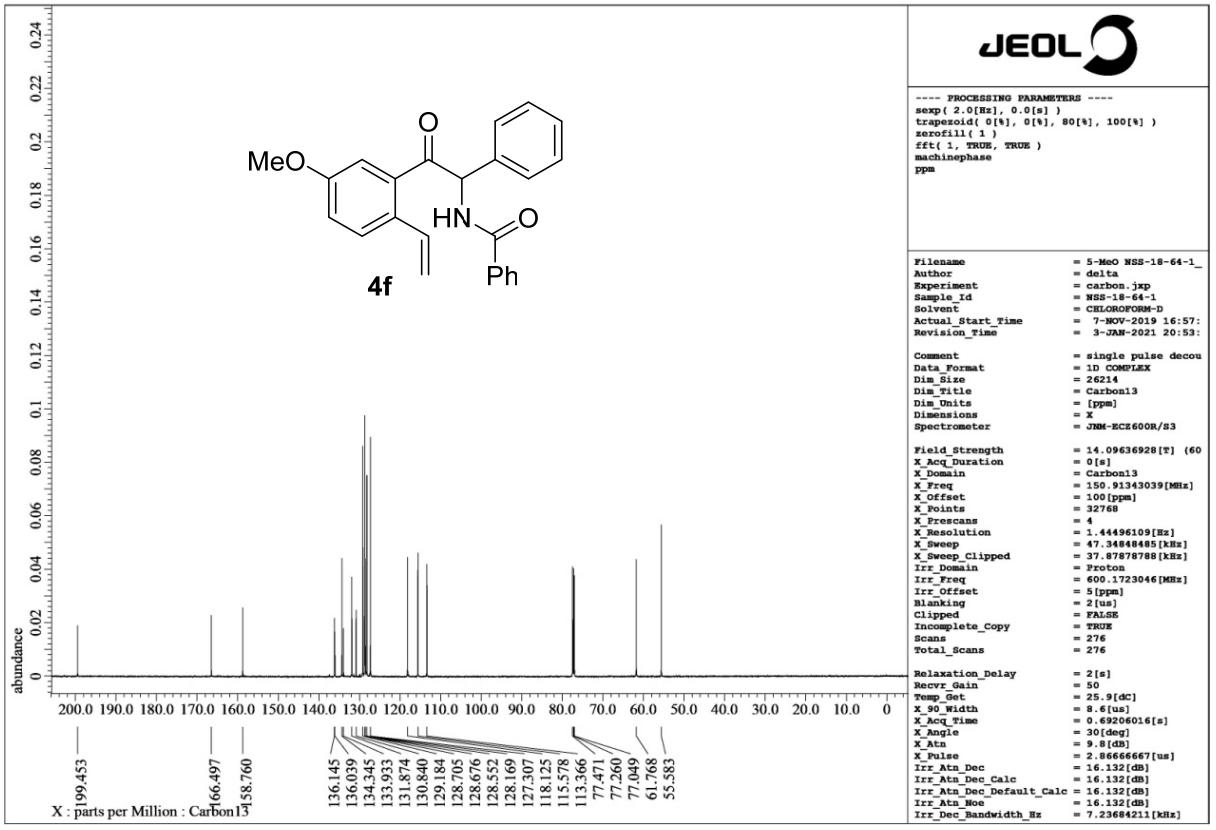
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 23.9[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

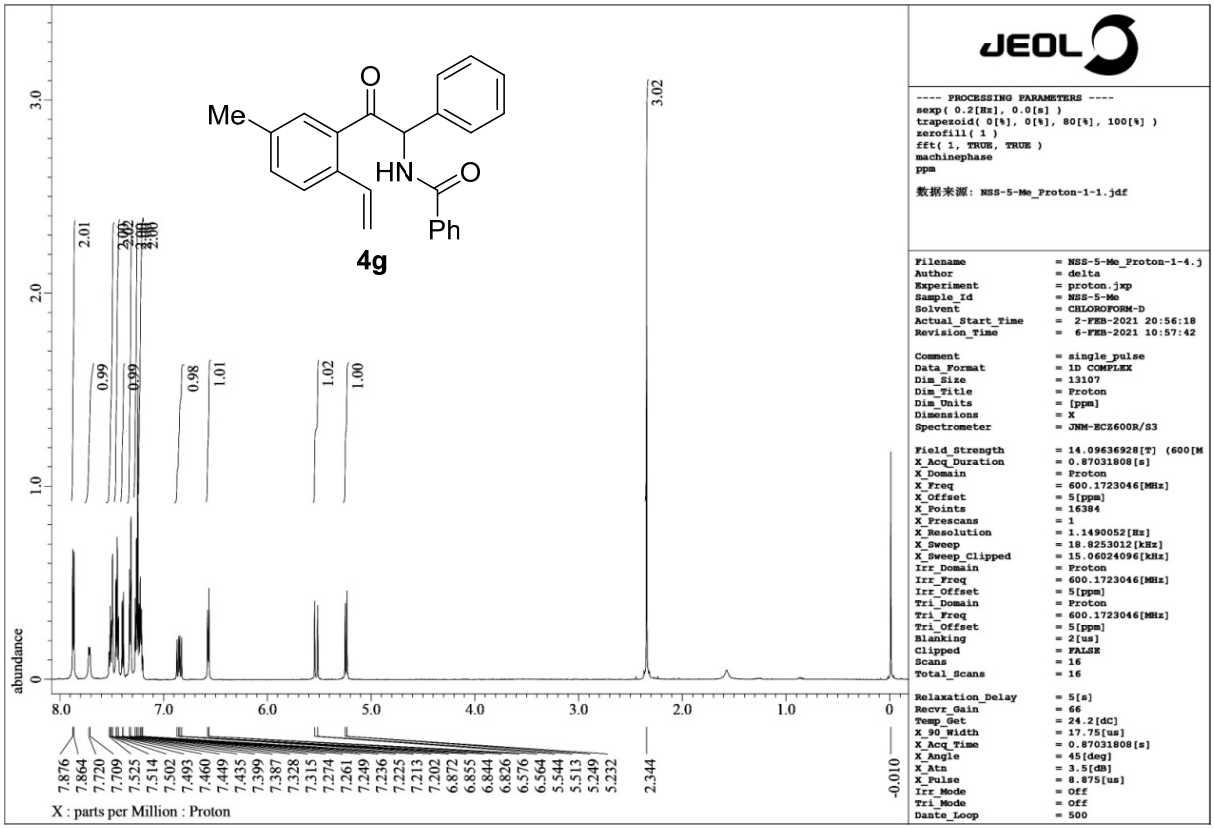

4e
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-4-CF3_Carbon_copy13-1-1.jdf
Filename = NSS-4-CF3_Carbon_c
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-4-CF3
Solvent = ACETONE-D6
Actual_Start_Time = 21-JAN-2021 17:28:
Revision_Time = 21-JAN-2021 21:16:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Incomplete_Copy = TRUE
Scans = 921
Total_Scans = 921
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 23.1[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]

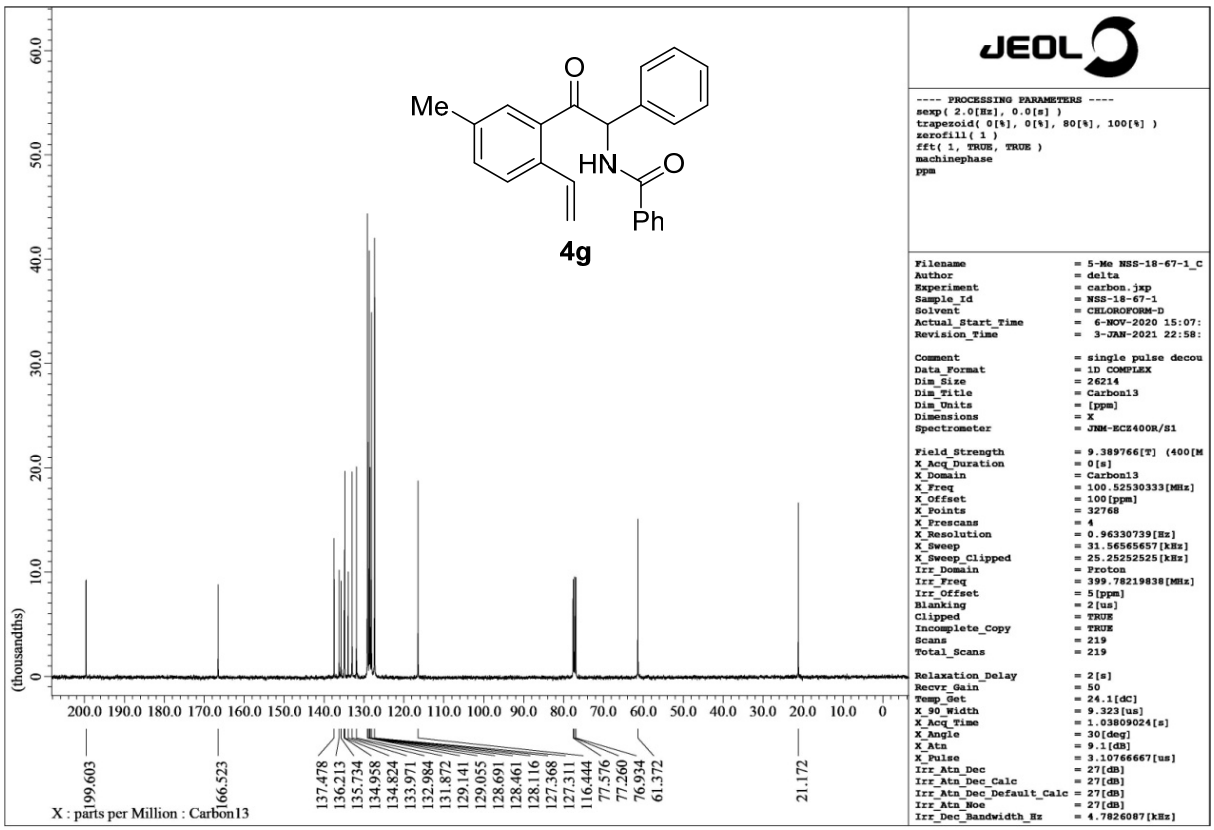


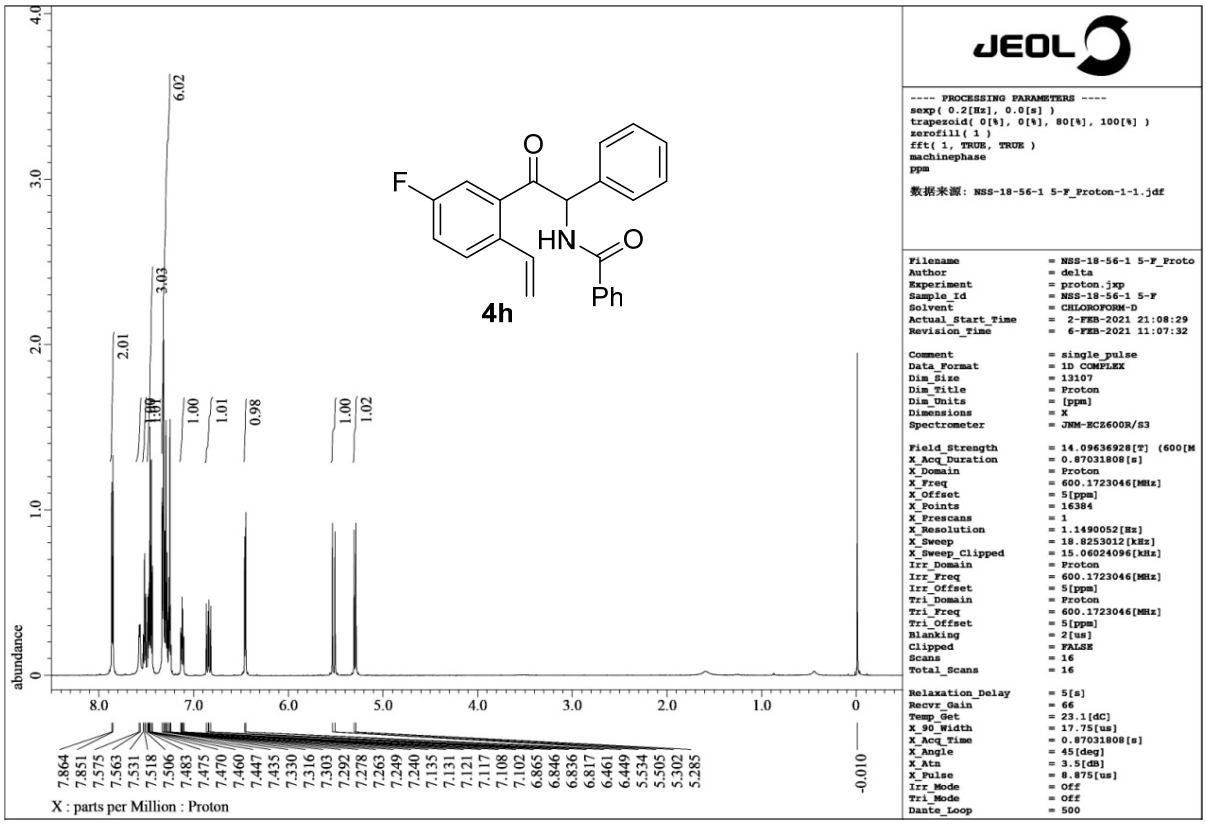

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-18-64-15-OMe_Proton-1-1.jdf

Filename                = NSS-18-64-15-OMe_Prot
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = NSS-18-64-15-OMe
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  3-FEB-2021 17:42:52
Revision_Time           =  6-FEB-2021 11:35:40

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 0.87031808[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 1.1490052[Hz]
X_Sweep                 = 18.8253012[kHz]
X_Sweep_Clipped         = 15.06024096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 5[s]
Recvr_Gain              = 66
Temp_Get                = 22.5[dC]
X_90_Width              = 17.75[us]
X_Acq_Time              = 0.87031808[s]
X_Angle                 = 45[deg]
X_Atn                   = 3.5[dB]
X_Pulse                 = 8.875[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
```

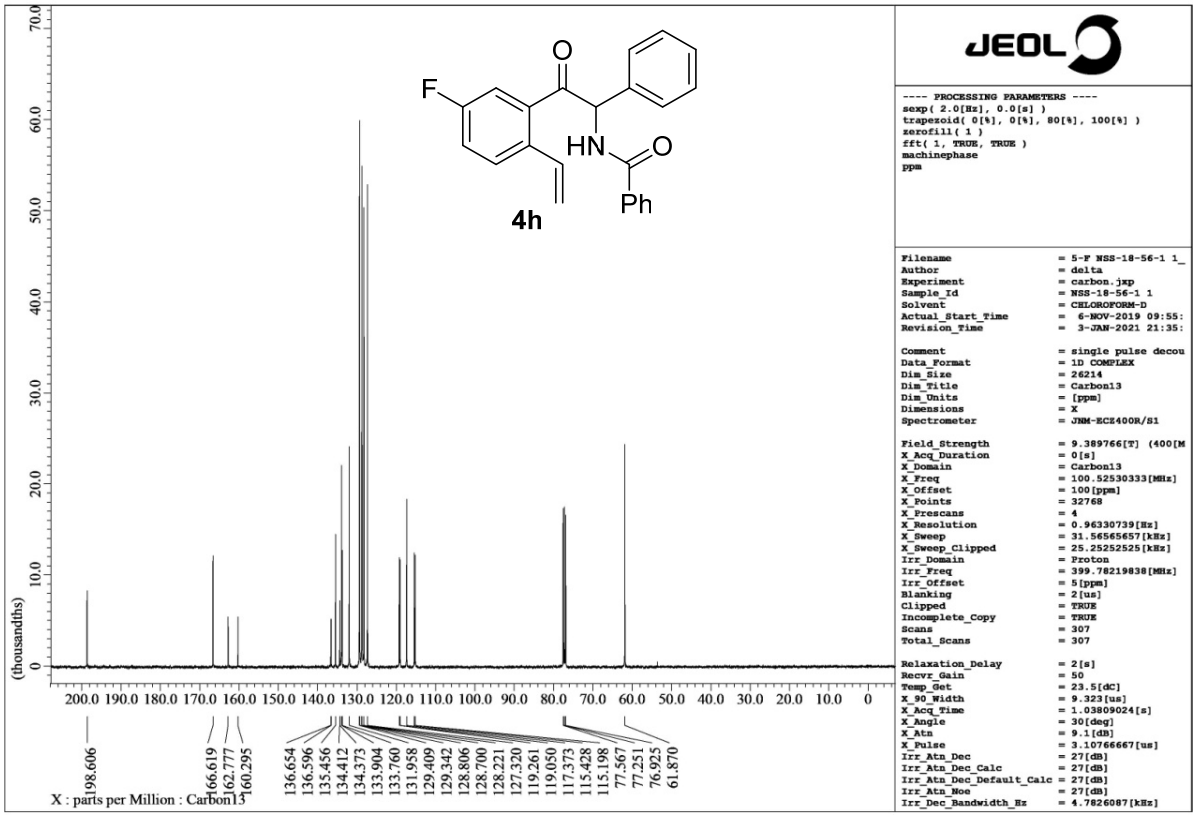


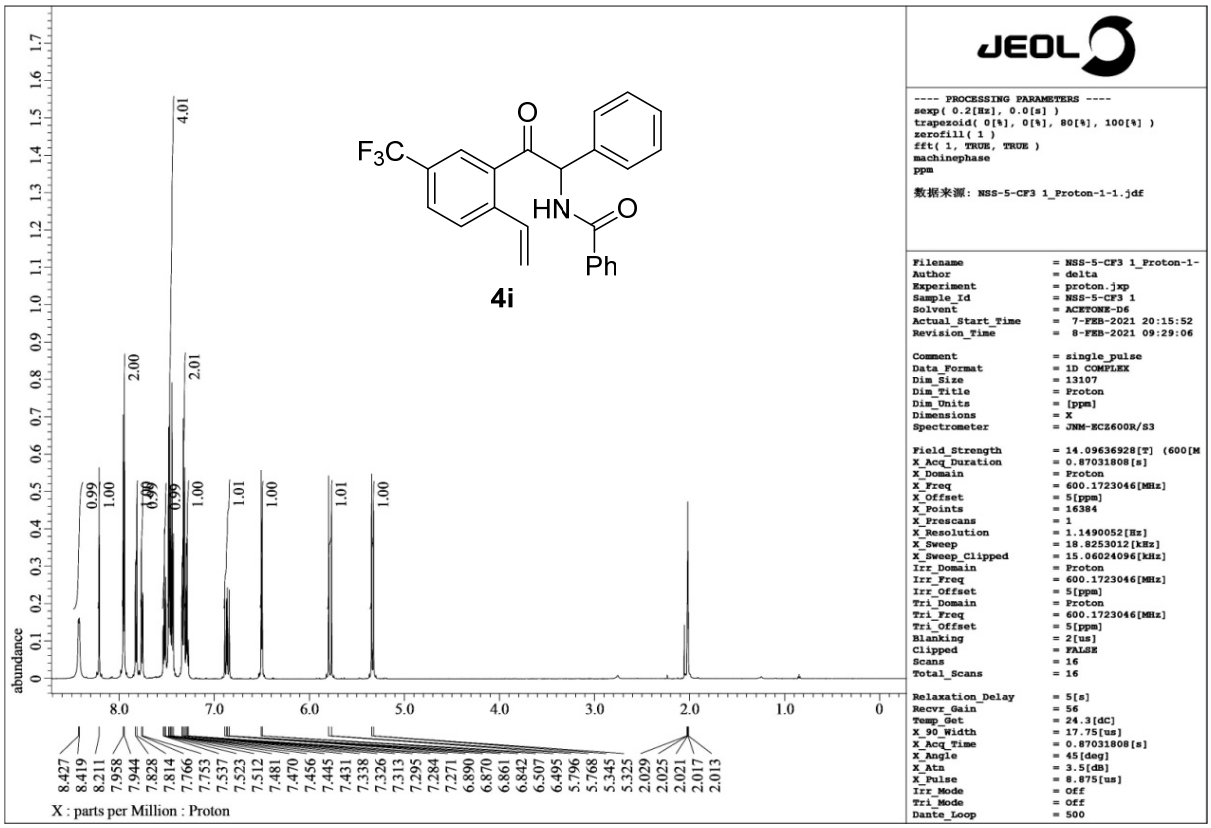

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename                = 5-MeO NSS-18-64-1_
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = NSS-18-64-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  7-NOV-2019 16:57:
Revision_Time           =  3-JAN-2021 20:53:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (60
X_Acq_Duration          = 0[s]
X_Domain                = Carbon13
X_Freq                  = 150.91343039[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 1.44496109[Hz]
X_Sweep                 = 47.34848485[kHz]
X_Sweep_Clipped         = 37.87878788[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Incomplete_Copy         = TRUE
Scans                   = 276
Total_Scans             = 276

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 25.9[dC]
X_90_Width              = 8.6[us]
X_Acq_Time              = 0.69206016[s]
X_Angle                 = 30[deg]
X_Atn                   = 9.8[dB]
X_Pulse                 = 2.86666667[us]
Irr_Atn_Dec             = 16.132[dB]
Irr_Atn_Dec_Calc        = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe             = 16.132[dB]
Irr_Dec_Bandwidth_Hz    = 7.23684211[kHz]
```


Me
O
HN
O
Ph
4g
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-5-Me_Proton-1-1.jdf
Filename = NSS-5-Me_Proton-1-4.j
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-5-Me
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-FEB-2021 20:56:18
Revision_Time = 6-FEB-2021 10:57:42
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.0602496[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 24.2[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

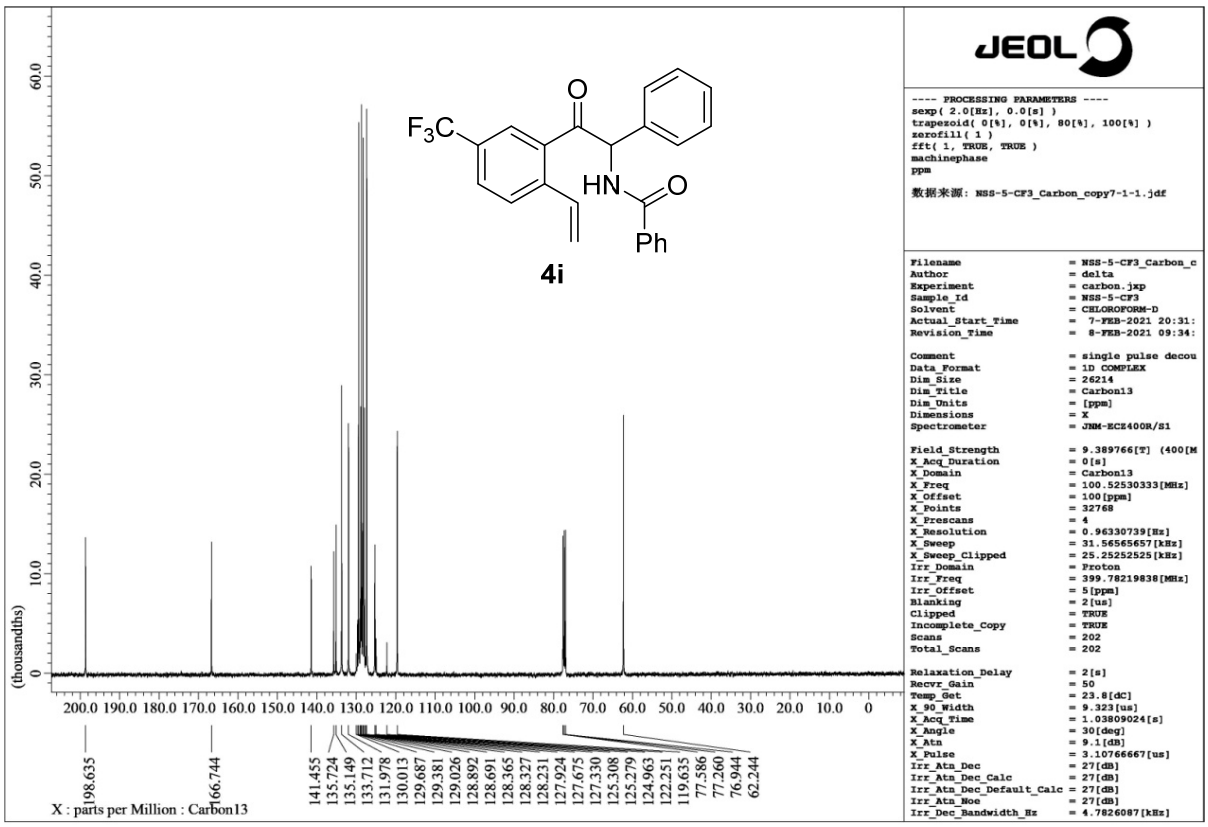

Me
O
HN
O
Ph
4g
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 5-Me NSS-18-67-1_C
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-18-67-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-NOV-2020 15:07:
Revision_Time = 3-JAN-2021 22:58:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Incomplete_Copy = TRUE
Scans = 219
Total_Scans = 219
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.1[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]


4h
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-56-1 5-F_Proton-1-1.jdf
Filename = NSS-18-56-1 5-F_Proto
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-18-56-1 5-F
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-FEB-2021 21:08:29
Revision_Time = 6-FEB-2021 11:07:32
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 23.1[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

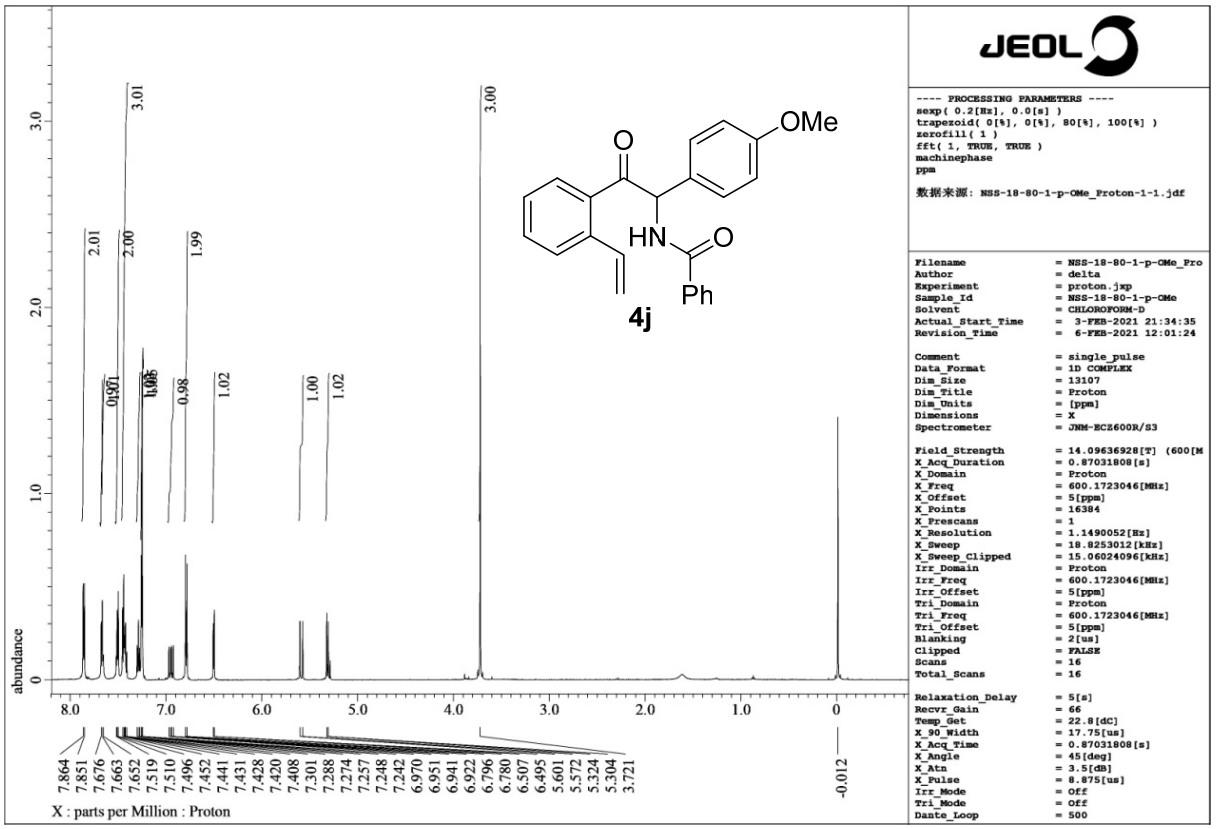

4h
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 5-F NSS-18-56-1 1_
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-18-56-1 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-NOV-2019 09:55:
Revision_Time = 3-JAN-2021 21:35:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Incomplete_Copy = TRUE
Scans = 307
Total_Scans = 307
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 23.5[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]

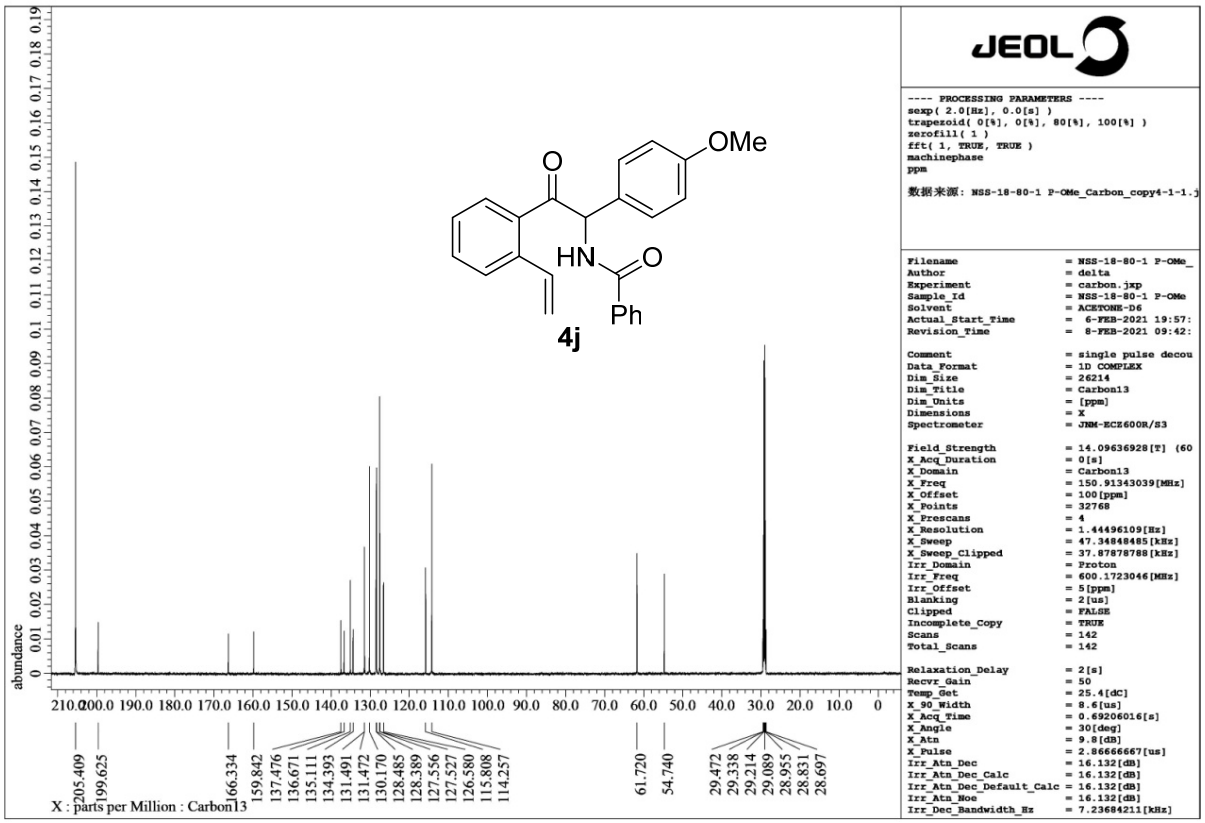


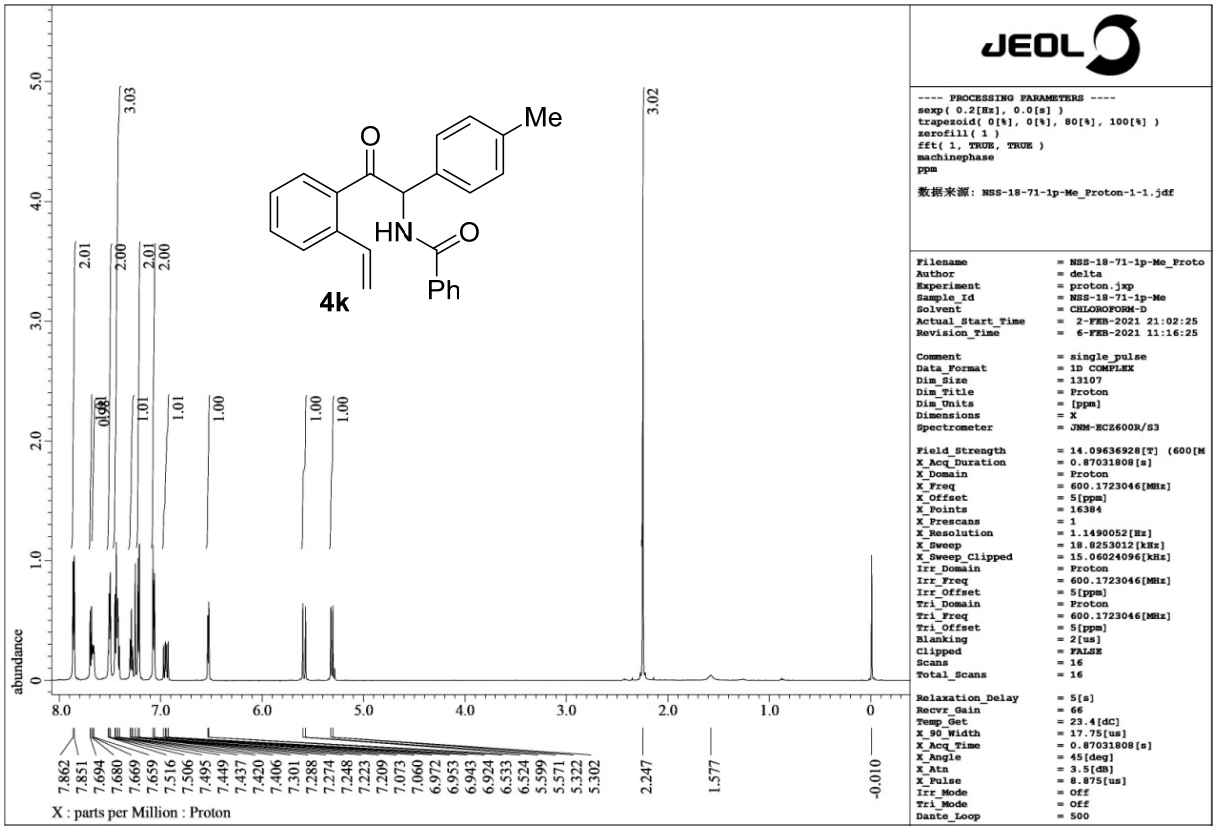

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-5-CF3 1_Proton-1-1.jdf

Filename                = NSS-5-CF3 1_Proton-1-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = NSS-5-CF3 1
Solvent                 = ACETONE-D6
Actual_Start_Time       =  7-FEB-2021 20:15:52
Revision_Time           =  8-FEB-2021 09:29:06

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 0.87031808[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 1.1490052[Hz]
X_Sweep                 = 18.8253012[kHz]
X_Sweep_Clipped         = 15.06024096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 24.3[dC]
X_90_Width              = 17.75[us]
X_Acq_Time              = 0.87031808[s]
X_Angle                 = 45[deg]
X_Atn                   = 3.5[dB]
X_Pulse                 = 8.875[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
```



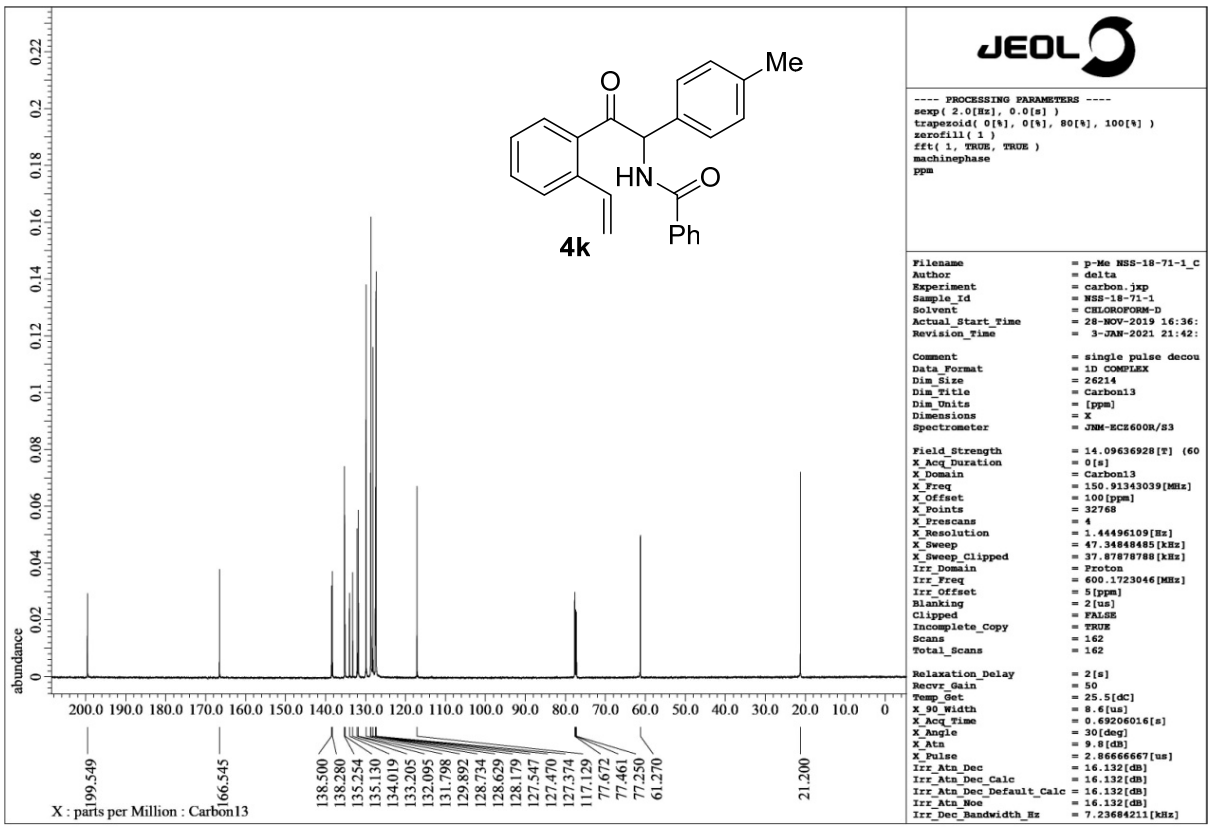

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-5-CF3_Carbon_copy7-1-1.jdf

Filename                = NSS-5-CF3_Carbon_c
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = NSS-5-CF3
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  7-FEB-2021 20:31:
Revision_Time           =  8-FEB-2021 09:34:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400R/S1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 0[s]
X_Domain                = Carbon13
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = TRUE
Incomplete_Copy         = TRUE
Scans                   = 202
Total_Scans             = 202

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 23.8[dC]
X_90_Width              = 9.323[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 9.1[dB]
X_Pulse                 = 3.10766667[us]
Irr_Atn_Dec             = 27[dB]
Irr_Atn_Dec_Calc        = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe             = 27[dB]
Irr_Dec_Bandwidth_Hz    = 4.7826087[kHz]
```


4j
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-80-1-p-OMe_Proton-1-1.jdf
Filename = NSS-18-80-1-p-OMe_Pro
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-18-80-1-p-OMe
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-FEB-2021 21:34:35
Revision_Time = 6-FEB-2021 12:01:24
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 22.8[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

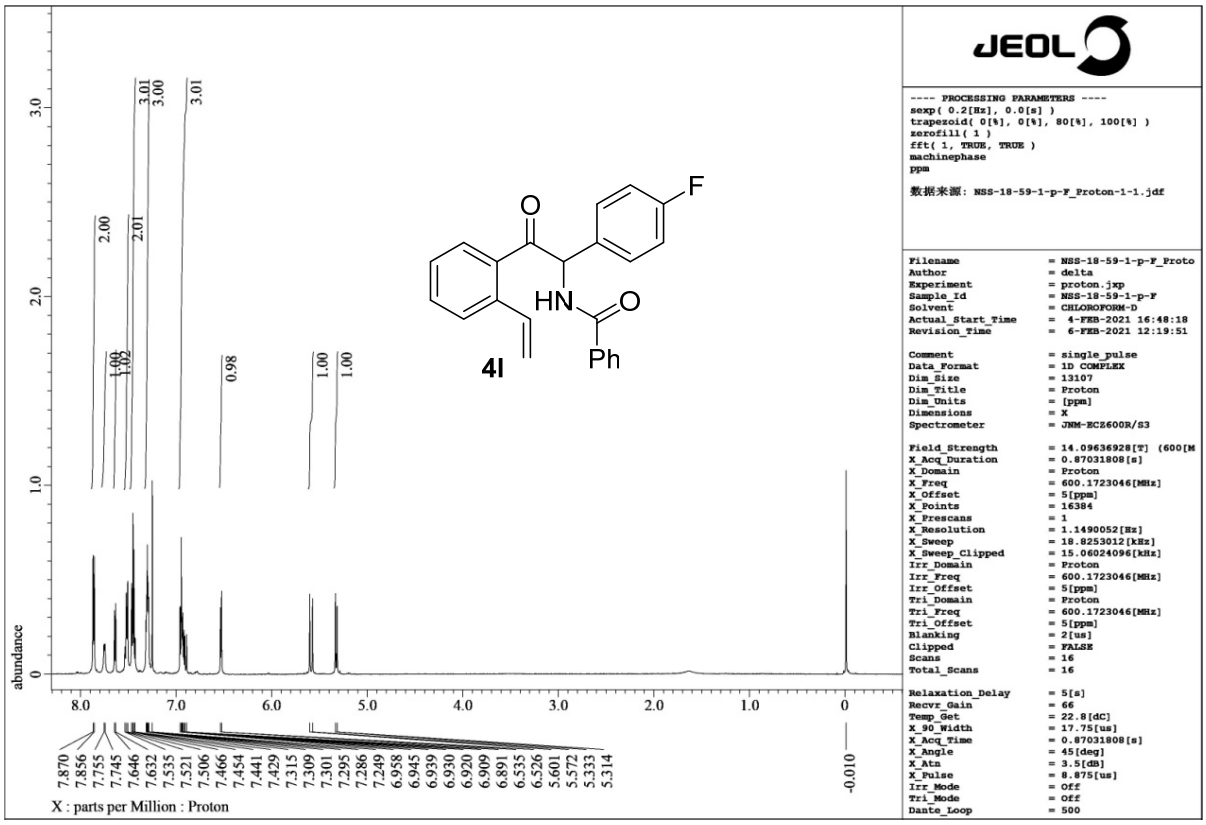

4j
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-80-1 P-OMe_Carbon_copy4-1-1.j
Filename = NSS-18-80-1 P-OMe_
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-18-80-1 P-OMe
Solvent = ACETONE-D6
Actual_Start_Time = 6-FEB-2021 19:57:
Revision_Time = 8-FEB-2021 09:42:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 142
Total_Scans = 142
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.4[dC]
X_90_Width = 8.6[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.8[dB]
X_Pulse = 2.86666667[us]
Irr_Atn_Dec = 16.132[dB]
Irr_Atn_Dec_Calc = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe = 16.132[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]

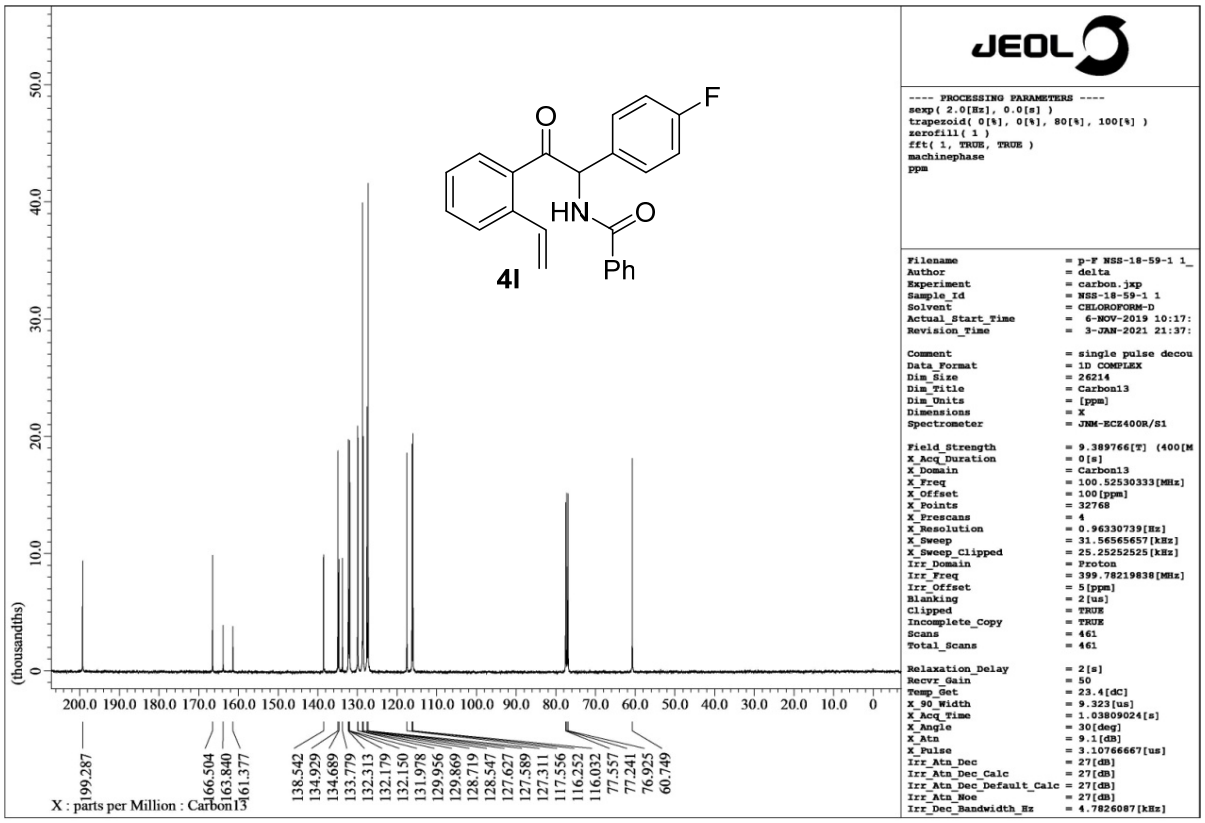


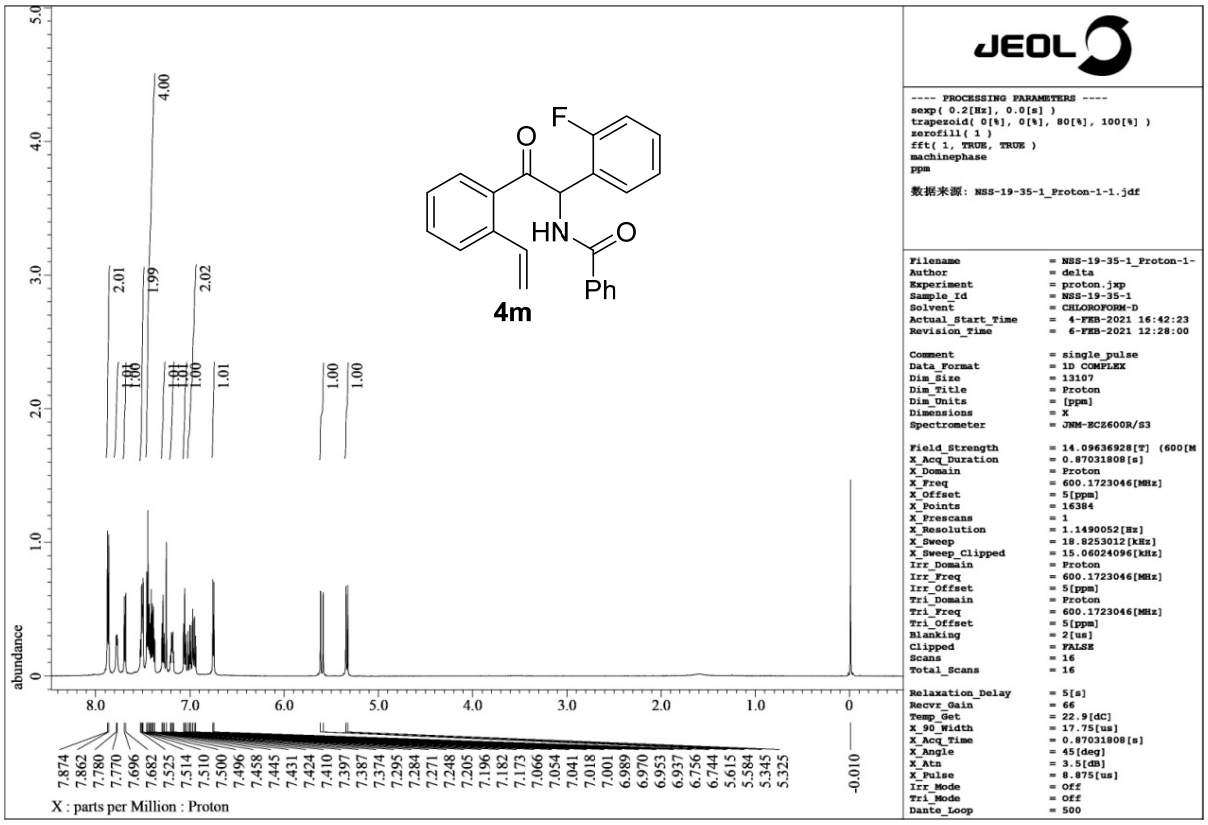

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-18-71-1p-Me_Proton-1-1.jdf

Filename              = NSS-18-71-1p-Me_Proto
Author                = delta
Experiment            = proton.jxp
Sample_Id             = NSS-18-71-1p-Me
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  2-FEB-2021 21:02:25
Revision_Time         =  6-FEB-2021 11:16:25

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 0.87031808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 1.1490052[Hz]
X_Sweep               = 18.8253012[kHz]
X_Sweep_Clipped       = 15.06024096[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 23.4[dC]
X_90_Width            = 17.75[us]
X_Acq_Time            = 0.87031808[s]
X_Angle               = 45[deg]
X_Atn                 = 3.5[dB]
X_Pulse               = 8.875[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
```



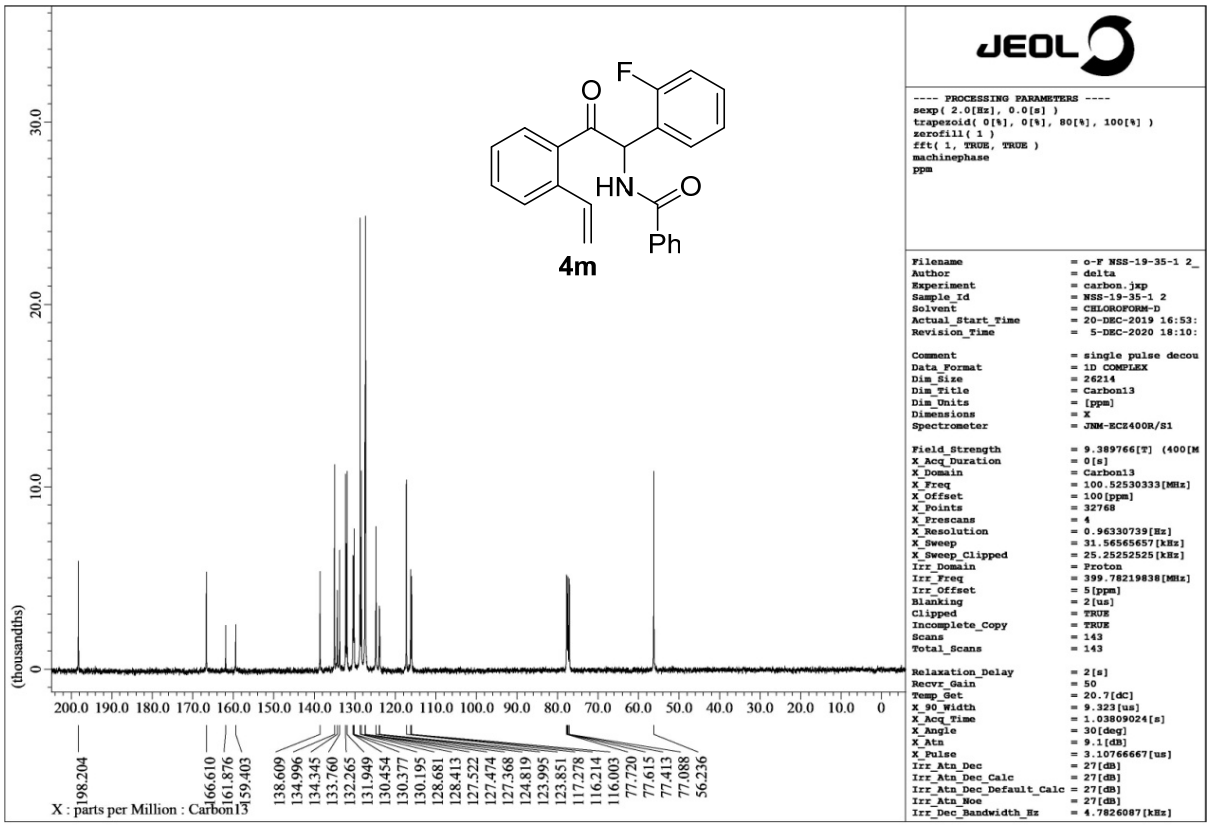

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename              = p-Me NSS-18-71-1_C
Author                = delta
Experiment            = carbon.jxp
Sample_Id             = NSS-18-71-1
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 28-NOV-2019 16:36:
Revision_Time         =  3-JAN-2021 21:42:

Comment               = single pulse decou
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
Dim_Title             = Carbon13
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (60
X_Acq_Duration        = 0[s]
X_Domain              = Carbon13
X_Freq                = 150.91343039[MHz]
X_Offset              = 100[ppm]
X_Points              = 32768
X_Prescans            = 4
X_Resolution          = 1.44496109[Hz]
X_Sweep               = 47.34848485[kHz]
X_Sweep_Clipped       = 37.87878788[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Incomplete_Copy       = TRUE
Scans                 = 162
Total_Scans           = 162

Relaxation_Delay      = 2[s]
Recvr_Gain            = 50
Temp_Get              = 25.5[dC]
X_90_Width            = 8.6[us]
X_Acq_Time            = 0.69206016[s]
X_Angle               = 30[deg]
X_Atn                 = 9.8[dB]
X_Pulse               = 2.86666667[us]
Irr_Atn_Dec           = 16.132[dB]
Irr_Atn_Dec_Calc      = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe           = 16.132[dB]
Irr_Dec_Bandwidth_Hz  = 7.23684211[kHz]
```


4l
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-59-1-p-F_Proton-1-1.jdf
Filename = NSS-18-59-1-p-F_Proto
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-18-59-1-p-F
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-FEB-2021 16:48:18
Revision_Time = 6-FEB-2021 12:19:51
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 22.8[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

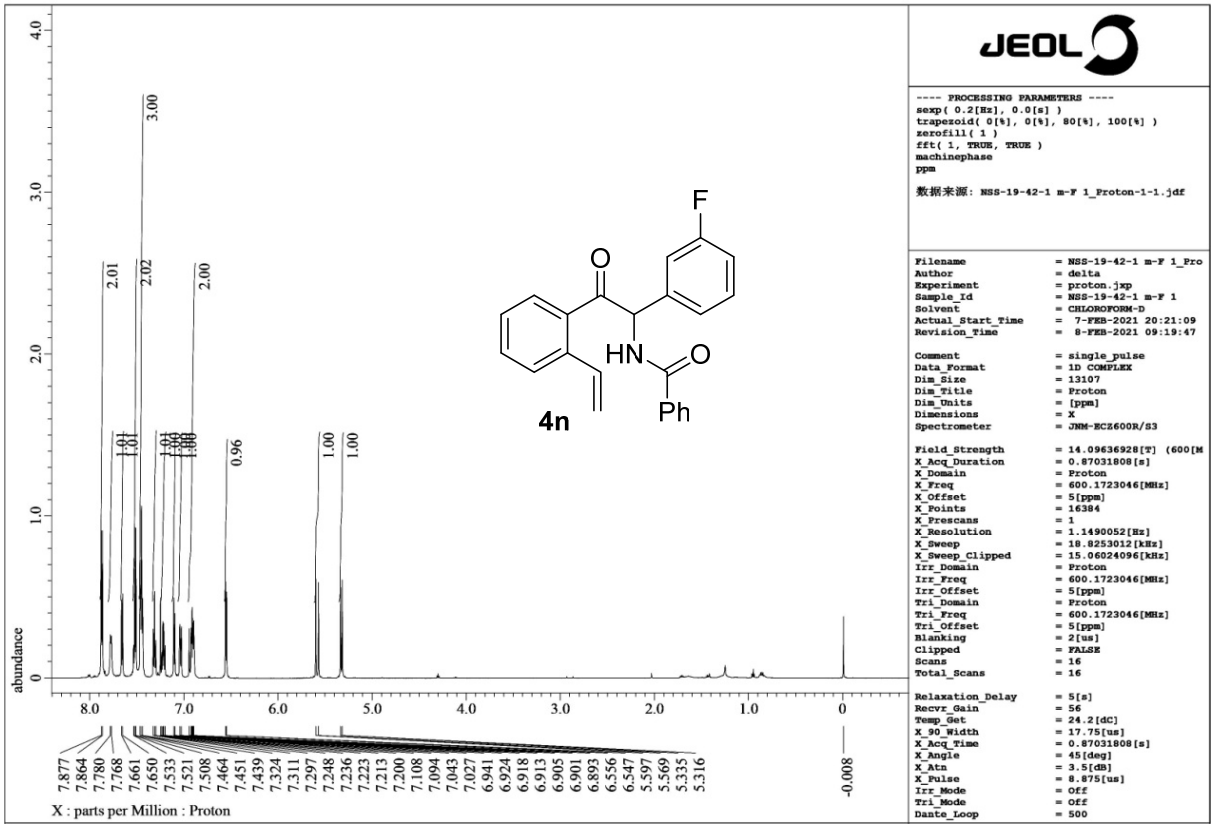

4l
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = p-F NSS-18-59-1 1_
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-18-59-1 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-NOV-2019 10:17:
Revision_Time = 3-JAN-2021 21:37:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Incomplete_Copy = TRUE
Scans = 461
Total_Scans = 461
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 23.4[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]



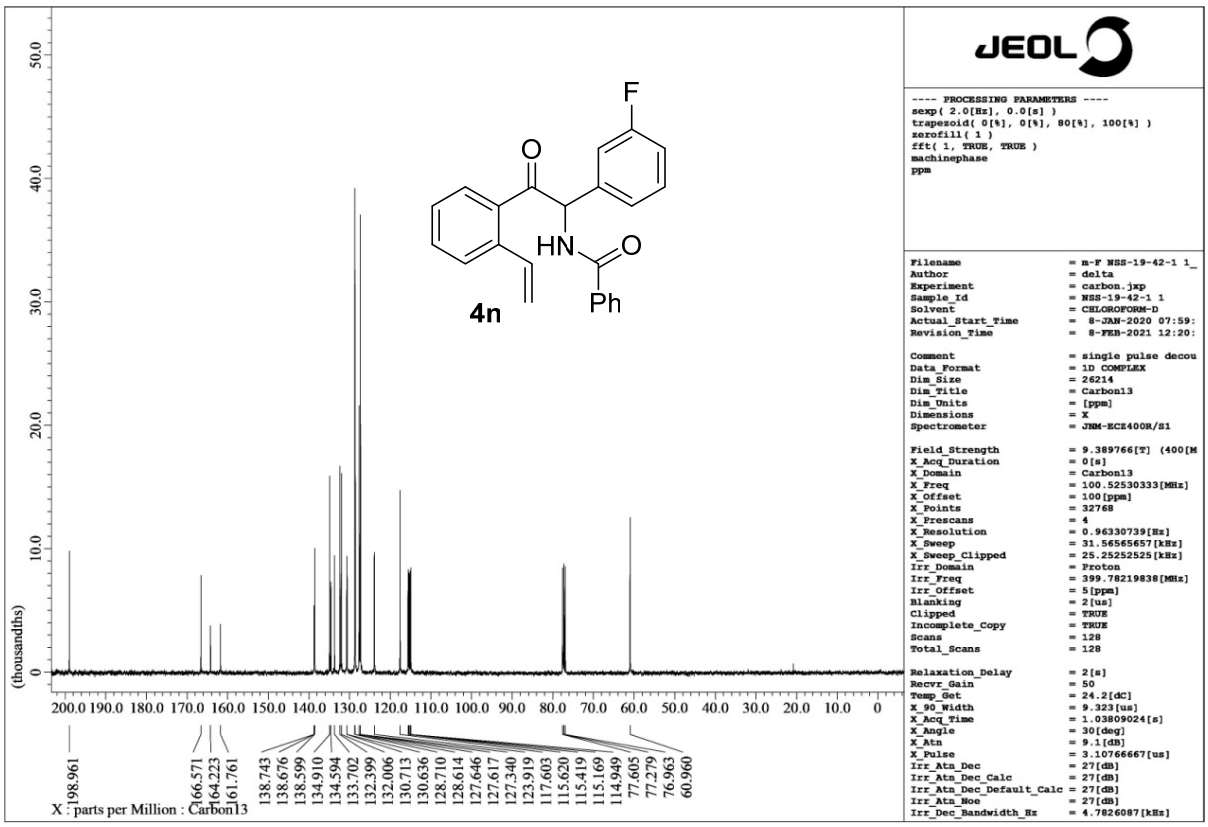

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-19-35-1_Proton-1-1.jdf

Filename              = NSS-19-35-1_Proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = NSS-19-35-1
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  4-FEB-2021 16:42:23
Revision_Time         =  6-FEB-2021 12:28:00

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S3

Field_Strength        = 14.09636928[T] (600[M
X_Acq_Duration        = 0.87031808[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 1.1490052[Hz]
X_Sweep               = 18.8253012[kHz]
X_Sweep_Clipped       = 15.06024096[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 22.9[dC]
X_90_Width            = 17.75[us]
X_Acq_Time            = 0.87031808[s]
X_Angle               = 45[deg]
X_Atn                 = 3.5[dB]
X_Pulse               = 8.875[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
```



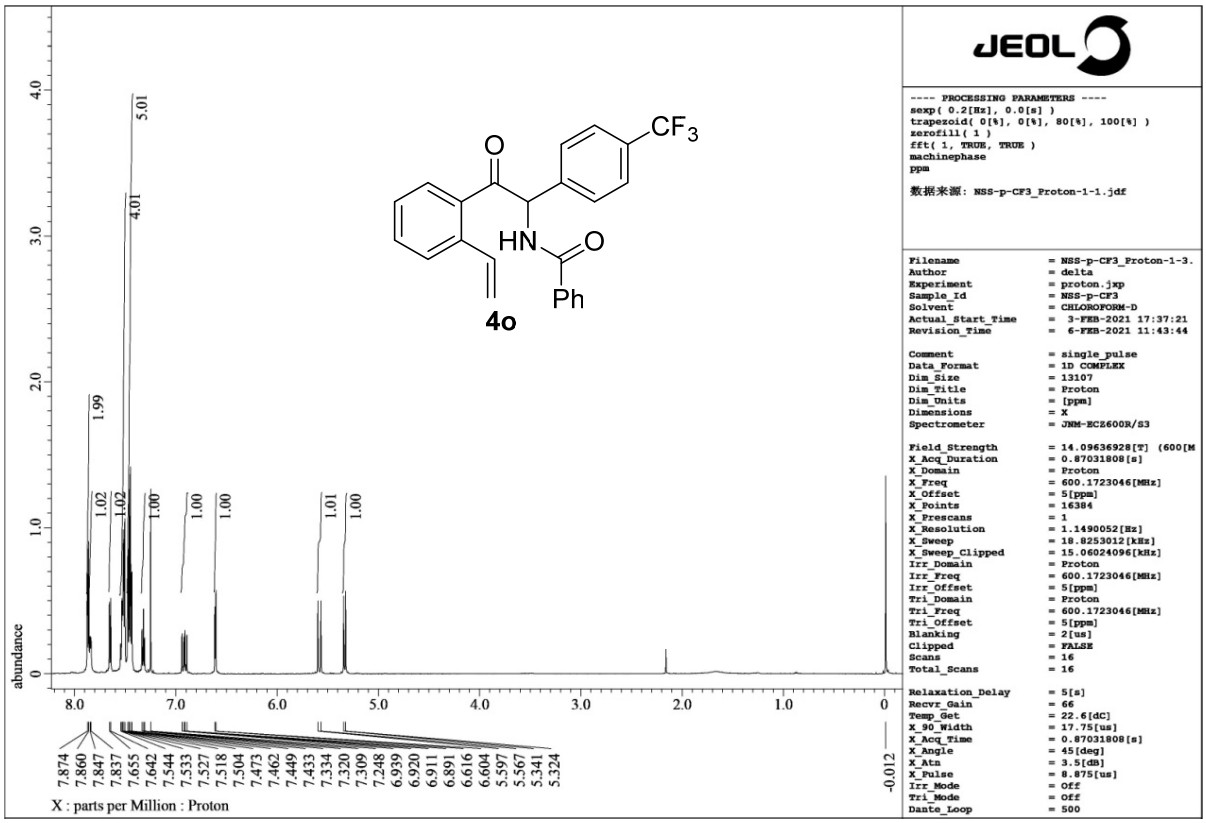

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename              = o-F NSS-19-35-1 2_
Author                = delta
Experiment            = carbon.jxp
Sample_Id             = NSS-19-35-1 2
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 20-DEC-2019 16:53:
Revision_Time         =  5-DEC-2020 18:10:

Comment               = single pulse decou
Data_Format           = 1D COMPLEX
Dim_Size              = 26214
Dim_Title             = Carbon13
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400R/S1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 0[s]
X_Domain              = Carbon13
X_Freq                = 100.52530333[MHz]
X_Offset              = 100[ppm]
X_Points              = 32768
X_Prescans            = 4
X_Resolution          = 0.96330739[Hz]
X_Sweep               = 31.56565657[kHz]
X_Sweep_Clipped       = 25.25252525[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Blanking              = 2[us]
Clipped               = TRUE
Incomplete_Copy       = TRUE
Scans                 = 143
Total_Scans           = 143

Relaxation_Delay      = 2[s]
Recvr_Gain            = 50
Temp_Get              = 20.7[dC]
X_90_Width            = 9.323[us]
X_Acq_Time            = 1.03809024[s]
X_Angle               = 30[deg]
X_Atn                 = 9.1[dB]
X_Pulse               = 3.10766667[us]
Irr_Atn_Dec           = 27[dB]
Irr_Atn_Dec_Calc      = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe           = 27[dB]
Irr_Dec_Bandwidth_Hz  = 4.7826087[kHz]
```

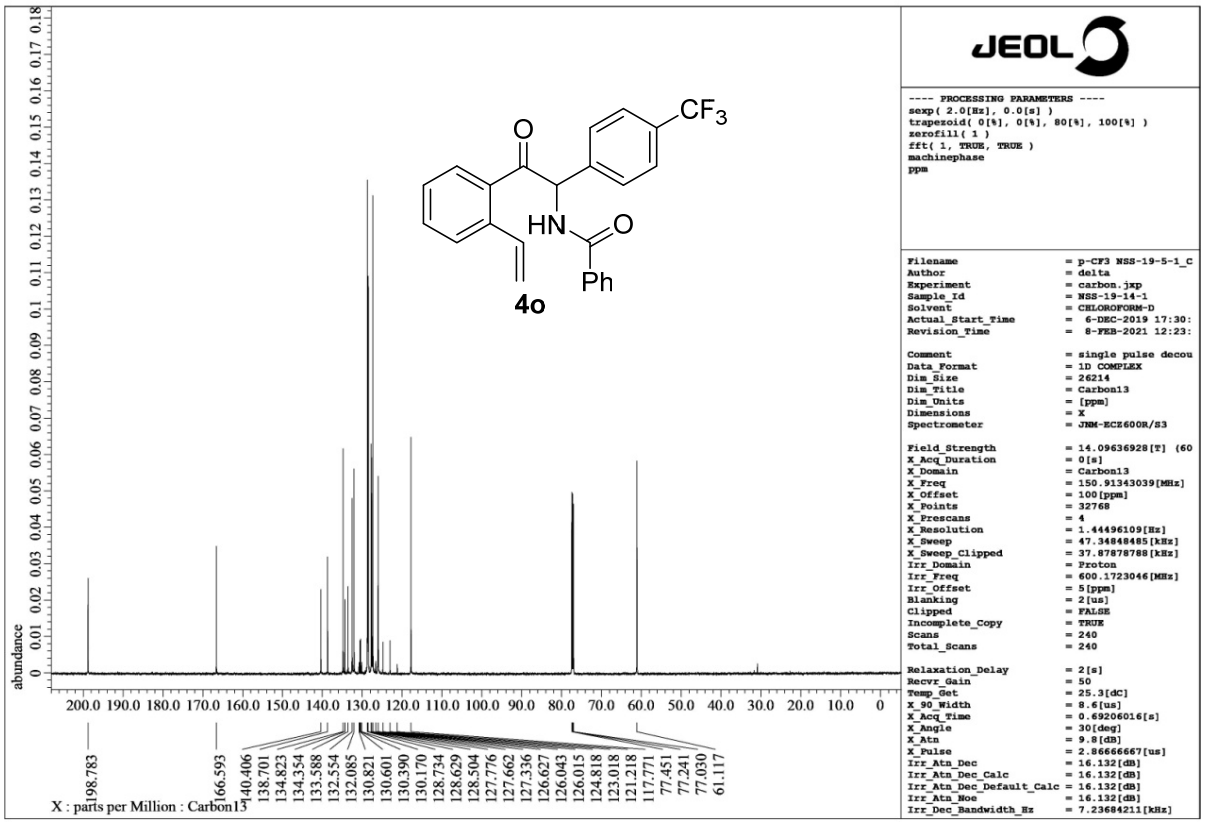


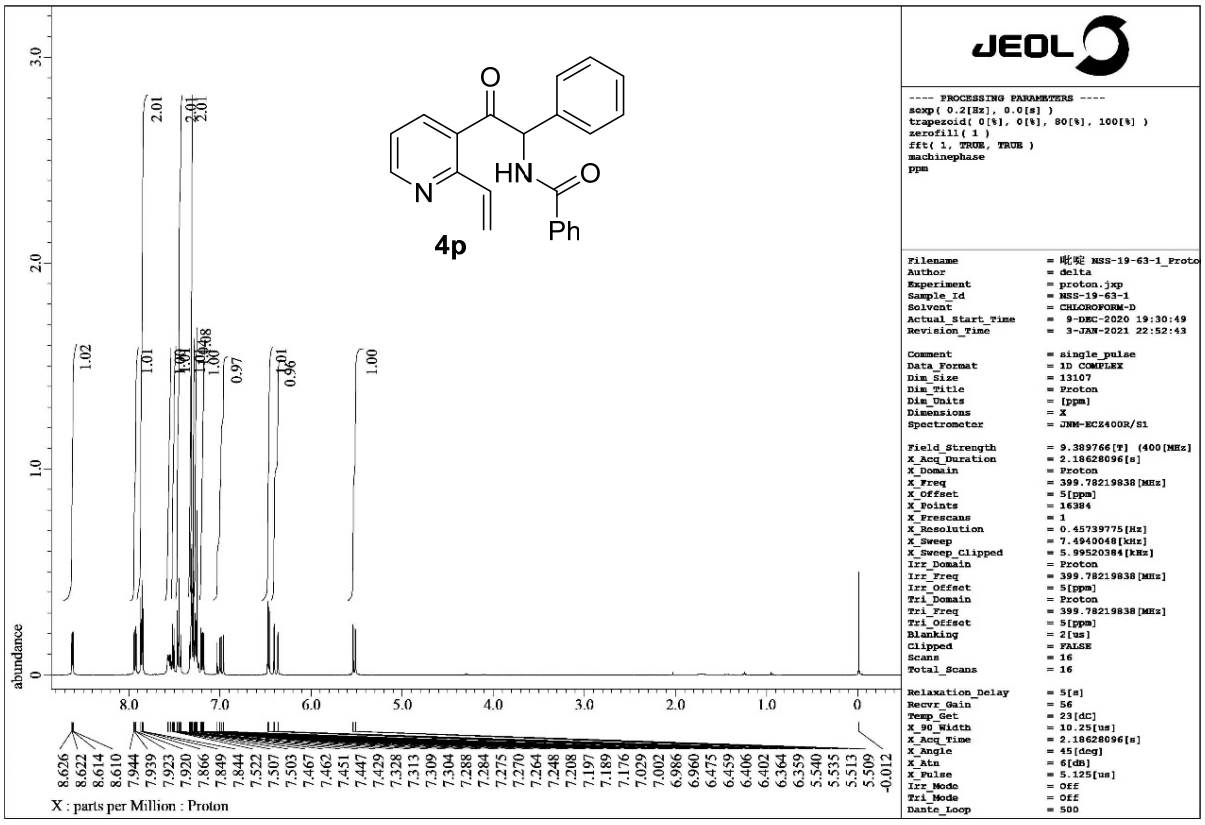

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-19-42-1 m-F 1_Proton-1-1.jdf

Filename                = NSS-19-42-1 m-F 1_Pro
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = NSS-19-42-1 m-F 1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  7-FEB-2021 20:21:09
Revision_Time           =  8-FEB-2021 09:19:47

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 0.87031808[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 1.1490052[Hz]
X_Sweep                 = 18.8253012[kHz]
X_Sweep_Clipped         = 15.06024096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Set                = 24.2[dC]
X_90_Width              = 17.75[us]
X_Acq_Time              = 0.87031808[s]
X_Angle                 = 45[deg]
X_Atn                   = 3.5[dB]
X_Pulse                 = 8.875[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
```



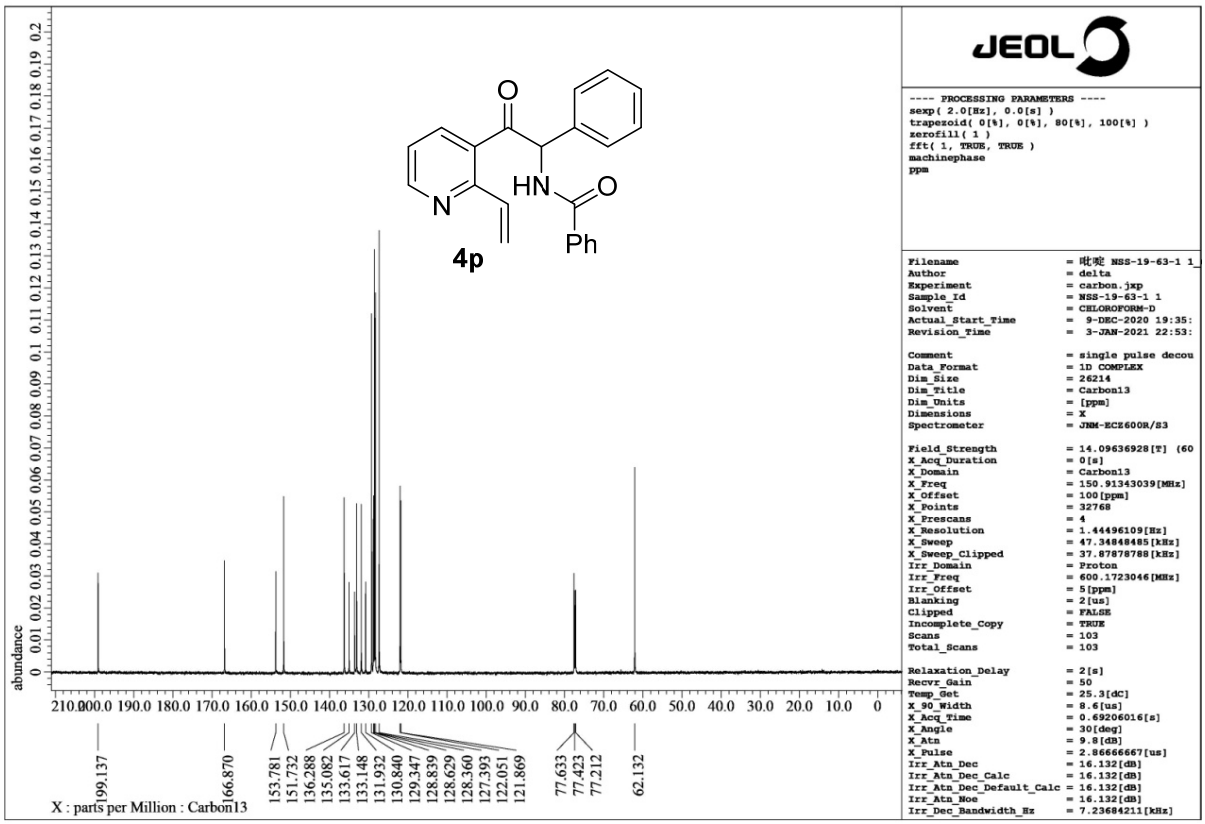

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename                = m-F NSS-19-42-1 1_
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = NSS-19-42-1 1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  8-JAN-2020 07:59:
Revision_Time           =  8-FEB-2021 12:20:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400R/S1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 0[s]
X_Domain                = Carbon13
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = TRUE
Incomplete_Copy         = TRUE
Scans                   = 128
Total_Scans             = 128

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Set                = 24.2[dC]
X_90_Width              = 9.323[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 9.1[dB]
X_Pulse                 = 3.10766667[us]
Irr_Atn_Dec             = 27[dB]
Irr_Atn_Dec_Calc        = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe             = 27[dB]
Irr_Dec_Bandwidth_Hz    = 4.7826087[kHz]
```


JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-p-CF3_Proton-1-1.jdf
Filename = NSS-p-CF3_Proton-1-3.
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-p-CF3
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-FEB-2021 17:37:21
Revision_Time = 6-FEB-2021 11:43:44
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 22.6[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
4o
abundance
X : parts per Million : Proton

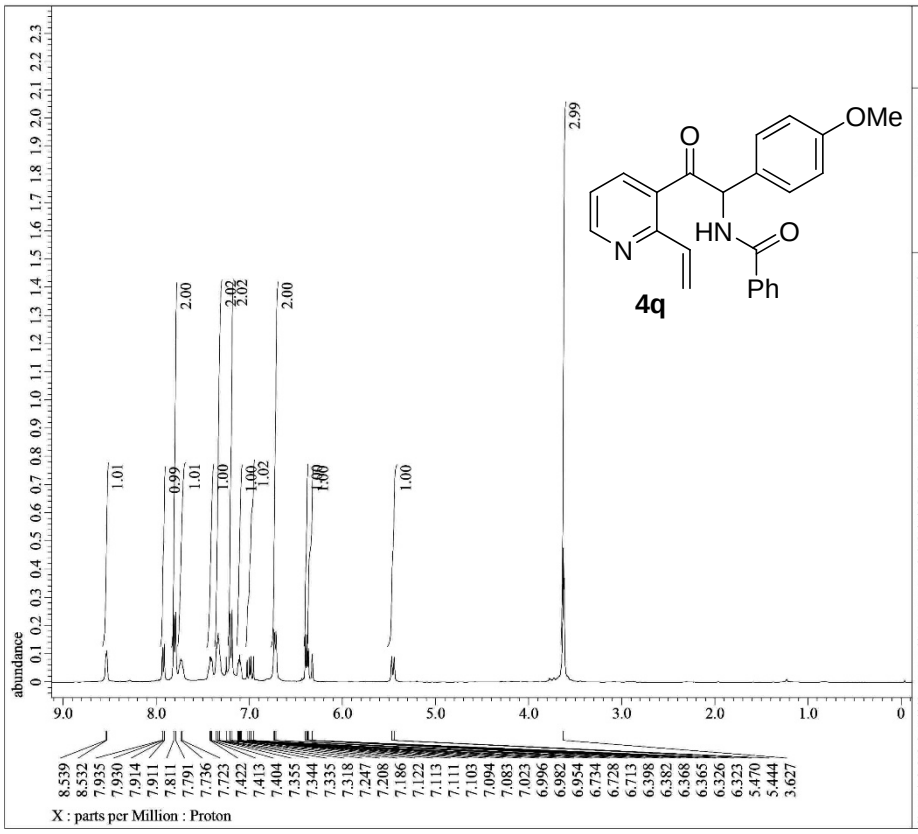

JEOL
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = p-CF3 NSS-19-5-1_C
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-19-14-i
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-DEC-2019 17:30:
Revision_Time = 8-FEB-2021 12:23:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 240
Total_Scans = 240
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.3[dC]
X_90_Width = 8.6[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.8[dB]
X_Pulse = 2.86666667[us]
Irr_Atn_Dec = 16.132[dB]
Irr_Atn_Dec_Calc = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe = 16.132[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
4o
abundance
X : parts per Million : Carbon13




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename                = 吡啶 NSS-19-63-1_Proto
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = NSS-19-63-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  9-DEC-2020 19:30:49
Revision_Time           =  3-JAN-2021 22:52:43

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400R/S1

Field_Strength          = 9.389766[T] (400[MHz]
X_Acq_Duration          = 2.18628096[s]
X_Domain                = Proton
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45739775[Hz]
X_Sweep                 = 7.4940048[kHz]
X_Sweep_Clipped         = 5.99520384[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 23[dC]
X_90_Width              = 10.25[us]
X_Acq_Time              = 2.18628096[s]
X_Angle                 = 45[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 5.125[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
```

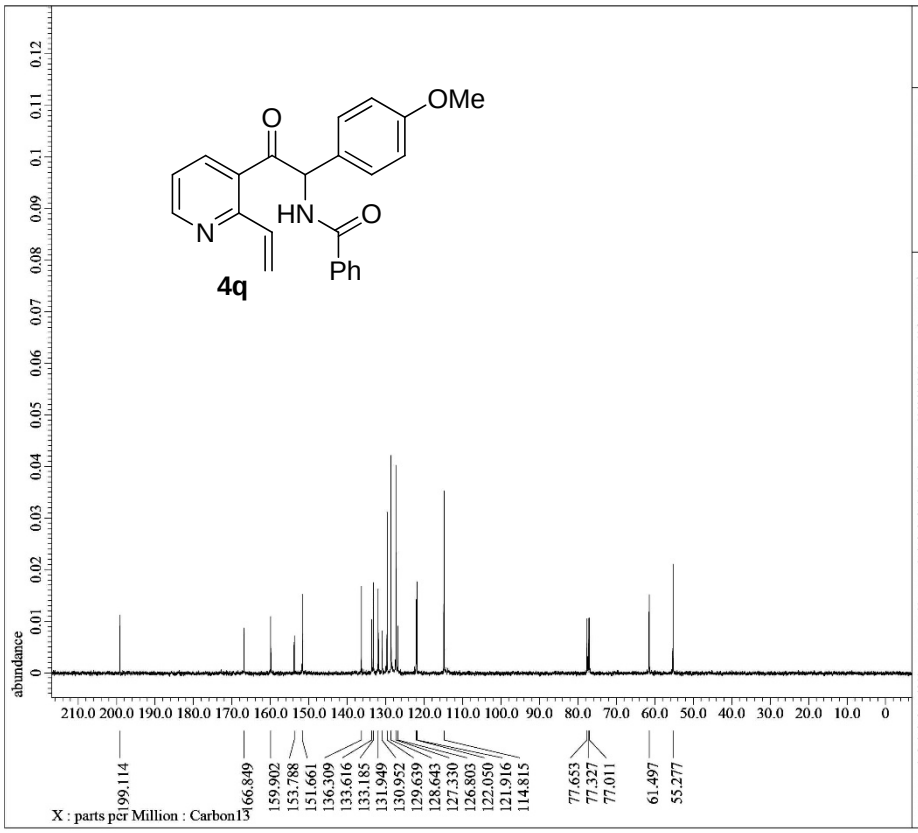



```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename                = 吡啶 NSS-19-63-1 1_
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = NSS-19-63-1 1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  9-DEC-2020 19:35:
Revision_Time           =  3-JAN-2021 22:53:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (60
X_Acq_Duration          = 0[s]
X_Domain                = Carbon13
X_Freq                  = 150.91343039[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 1.44496109[Hz]
X_Sweep                 = 47.34848485[kHz]
X_Sweep_Clipped         = 37.87878788[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Incomplete_Copy         = TRUE
Scans                   = 103
Total_Scans             = 103

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 25.3[dC]
X_90_Width              = 8.6[us]
X_Acq_Time              = 0.69206016[s]
X_Angle                 = 30[deg]
X_Atn                   = 9.8[dB]
X_Pulse                 = 2.86666667[us]
Irr_Atn_Dec             = 16.132[dB]
Irr_Atn_Dec_Calc        = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe             = 16.132[dB]
Irr_Dec_Bandwidth_Hz    = 7.23684211[kHz]
```



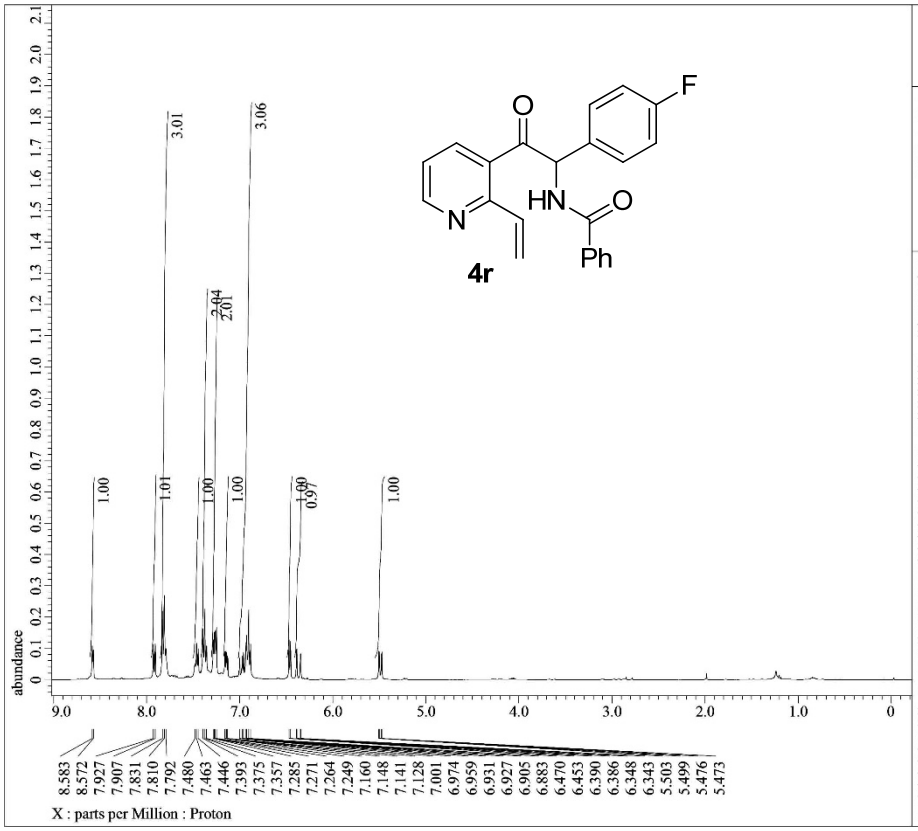

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= NSS-21-p-OMe yi_Proto
Author	= delta
Experiment	= proton.jxp
Sample_Id	= NSS-21-p-OMe yi
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-APR-2021 16:39:59
Revision_Time	= 5-MAY-2021 23:33:06
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400R/S1
Field_Strength	= 9.389766[T] (400[MHz]
X_Acq_Duration	= 2.18628096[s]
X_Domain	= Proton
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45739775[Hz]
X_Sweep	= 7.4940048[kHz]
X_Sweep_Clipped	= 5.99520384[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 23[dC]
X_90_Width	= 10.25[us]
X_Acq_Time	= 2.18628096[s]
X_Angle	= 45[deg]
X_Atn	= 6[dB]
X_Pulse	= 5.125[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500

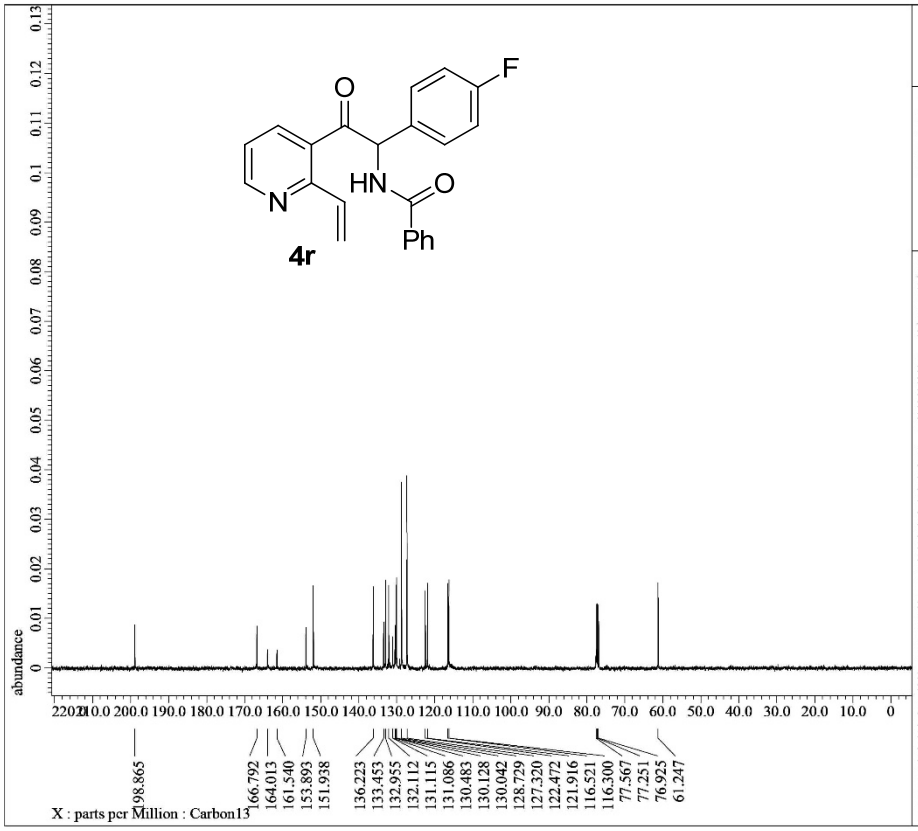



```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

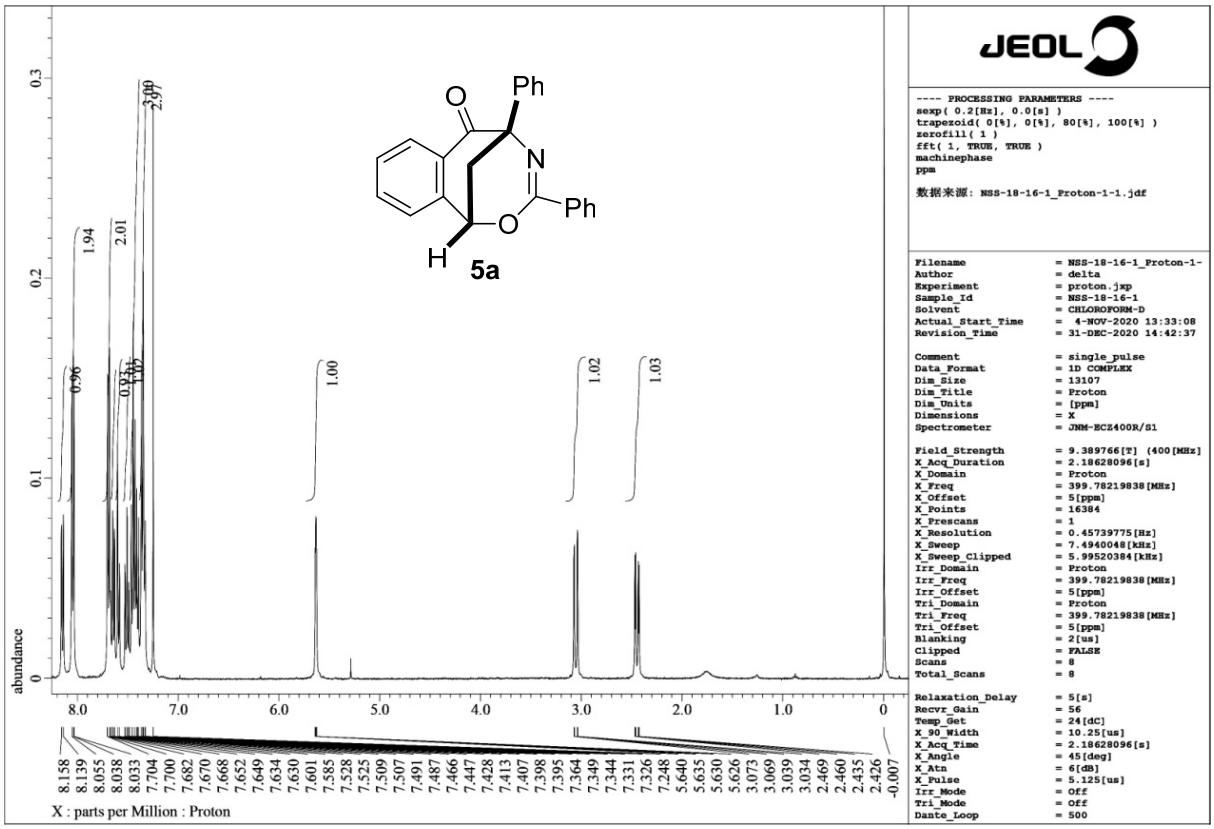
Filename	= NSS-21-p-OMe yi_Ca
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= NSS-21-p-OMe yi
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-APR-2021 16:41:
Revision_Time	= 5-MAY-2021 23:37:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400R/S1
Field_Strength	= 9.389766[T] (400[M
X_Acq_Duration	= 0[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Incomplete_Copy	= TRUE
Scans	= 50
Total_Scans	= 50
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 23.3[dC]
X_90_Width	= 9.323[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 9.1[dB]
X_Pulse	= 3.10766667[us]
Irr_Atn_Dec	= 27[dB]
Irr_Atn_Dec_Calc	= 27[dB]
Irr_Atn_Dec_Default_Calc	= 27[dB]
Irr_Atn_Noe	= 27[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]

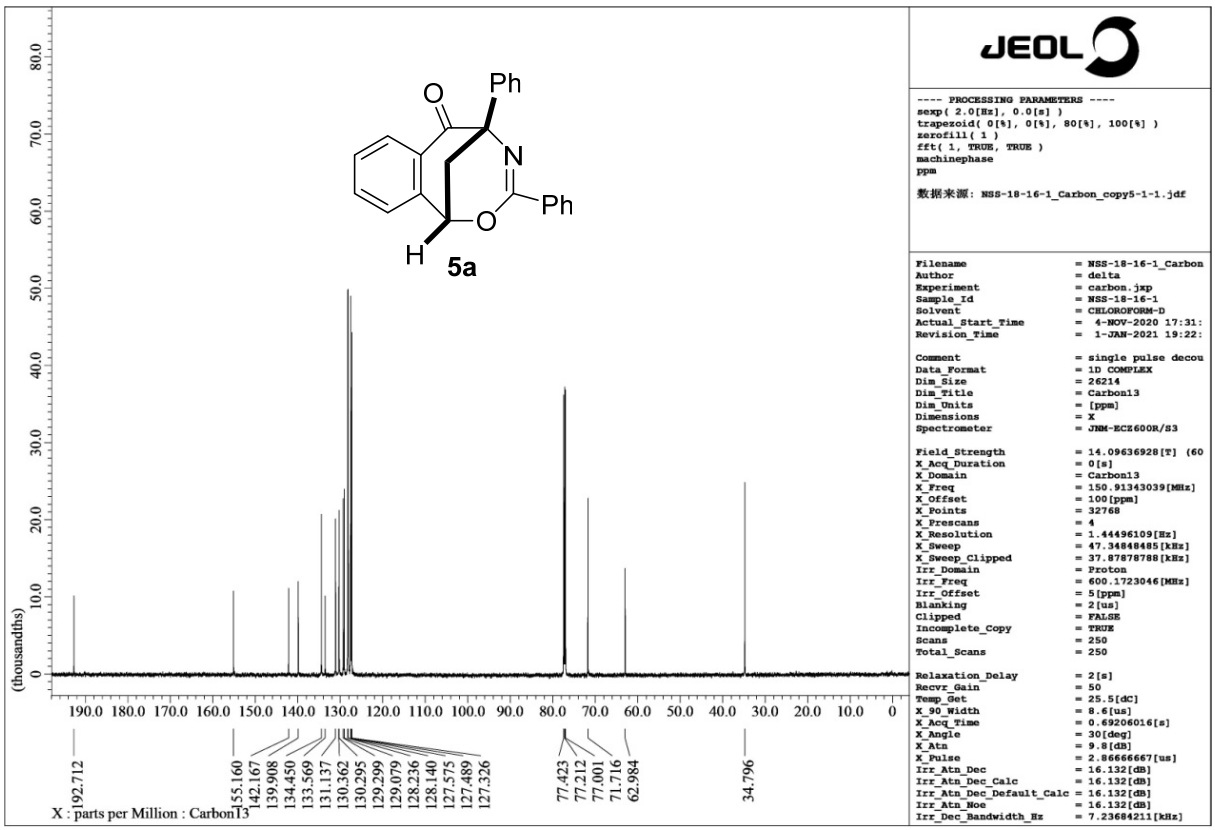


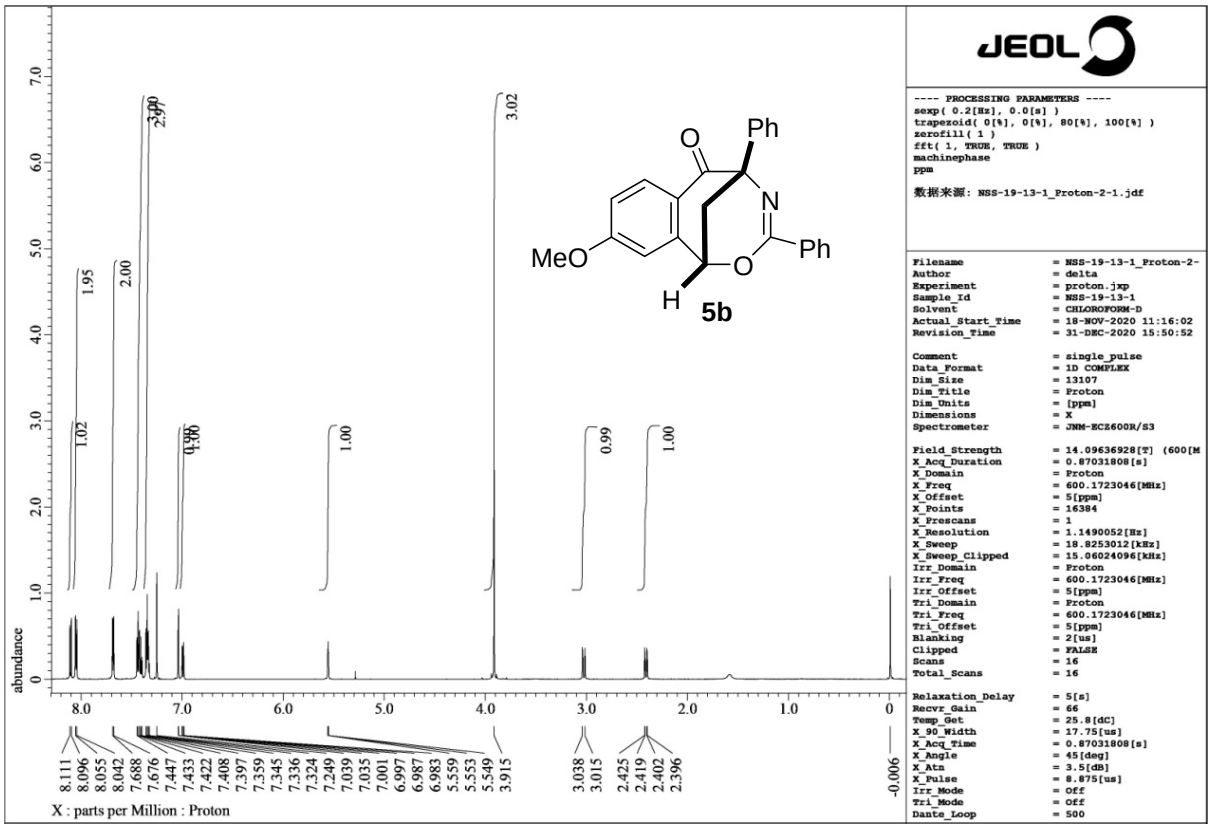

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename                = NSS-21-BD-F-yI_Proton
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = NSS-21-BD-F-yI
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 29-APR-2021 10:57:37
Revision_Time           =  5-MAY-2021 23:08:42

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400R/S1

Field_Strength          = 9.389766[T] (400[MHz]
X_Acq_Duration          = 0[s]
X_Domain                = Proton
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45739775[Hz]
X_Sweep                 = 7.4940048[kHz]
X_Sweep_Clipped         = 5.99520384[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Incomplete_Copy         = TRUE
Scans                   = 6
Total_Scans             = 6

Relaxation_Delay        = 5[s]
Recvr_Gain              = 36
Temp_Get                = 23.3[dC]
X_90_Width              = 10.25[us]
X_Acq_Time              = 2.18628096[s]
X_Angle                 = 45[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 5.125[us]
Irr_Mode                = Off
Tri_Mode                = Off
```

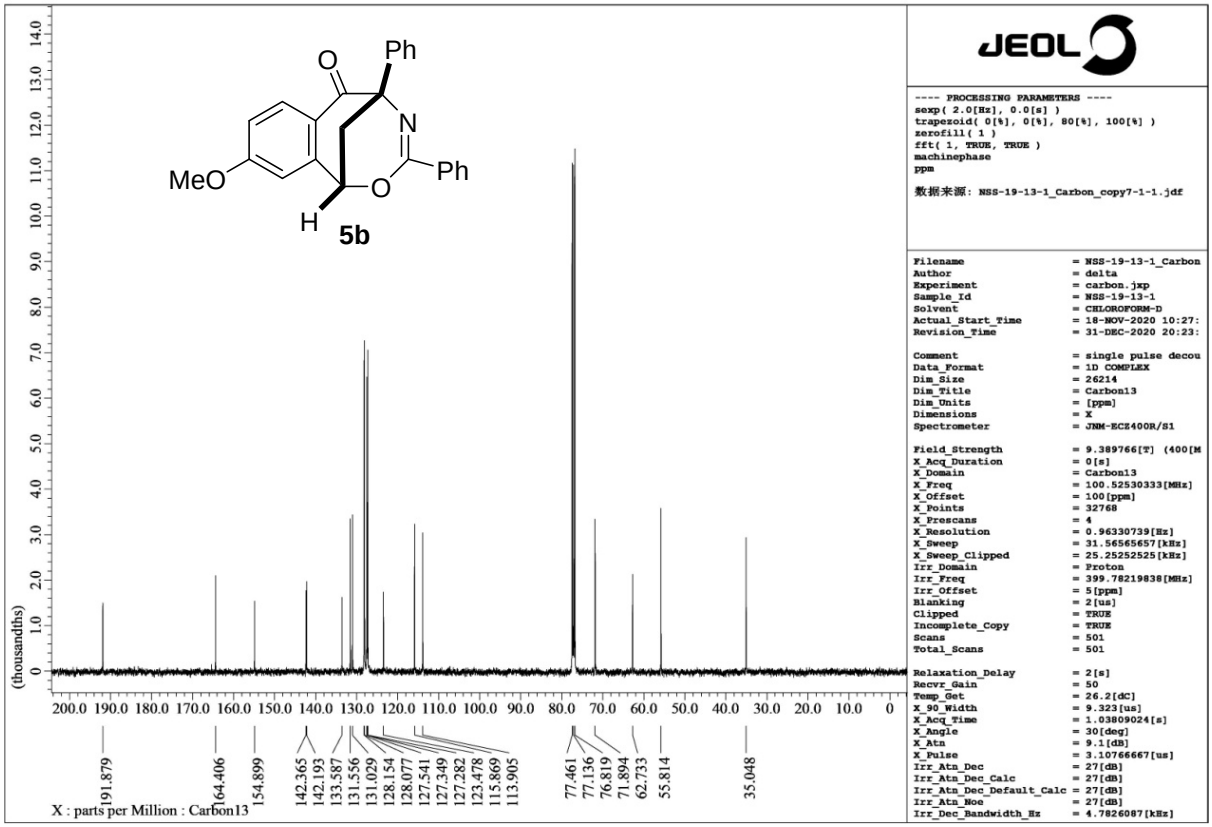


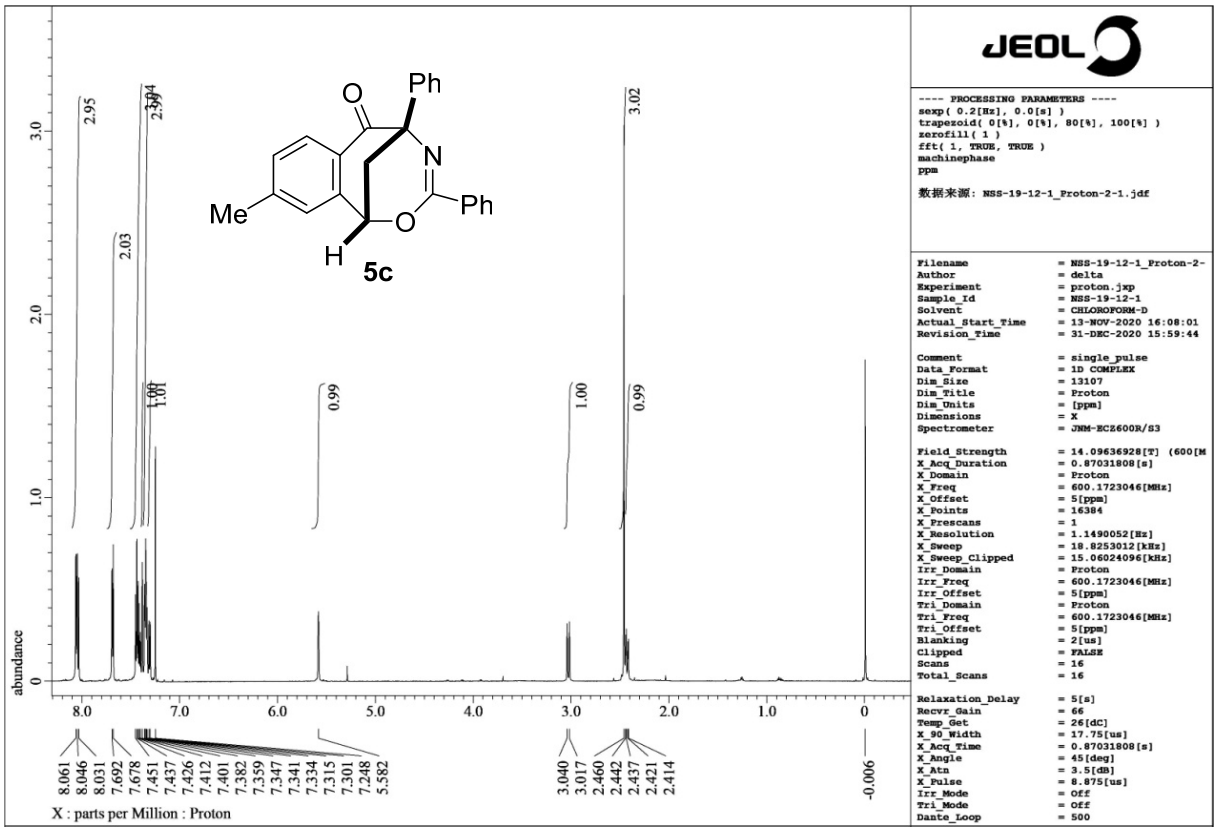

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename                = NSS-21-BD-F-yI_Car
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = NSS-21-BD-F-yI
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 29-APR-2021 10:58:
Revision_Time           =  5-MAY-2021 23:43:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400R/S1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 0[s]
X_Domain                = Carbon13
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = TRUE
Incomplete_Copy         = TRUE
Scans                   = 52
Total_Scans             = 52

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 23.6[dC]
X_90_Width              = 9.323[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 9.1[dB]
X_Pulse                 = 3.10766667[us]
Irr_Atn_Dec             = 27[dB]
Irr_Atn_Dec_Calc        = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe             = 27[dB]
Irr_Dec_Bandwidth_Hz    = 4.7826087[kHz]
```

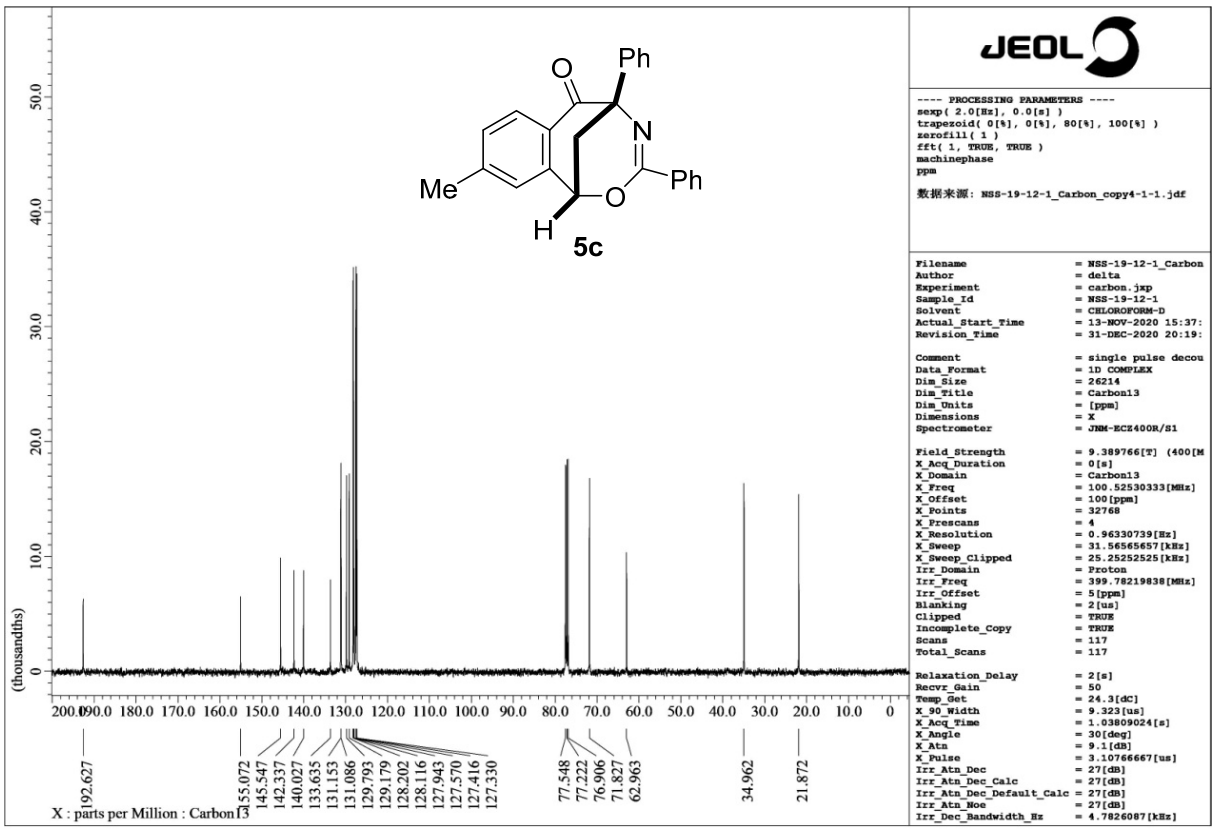

O
Ph
N
Ph
O
H
5a
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-16-1_Proton-1-1.jdf
Filename = NSS-18-16-1_Proton-1-
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-18-16-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-NOV-2020 13:33:08
Revision_Time = 31-DEC-2020 14:42:37
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 2.18628096[s]
X_Domain = Proton
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 24[dC]
X_90_Width = 10.25[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 5.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

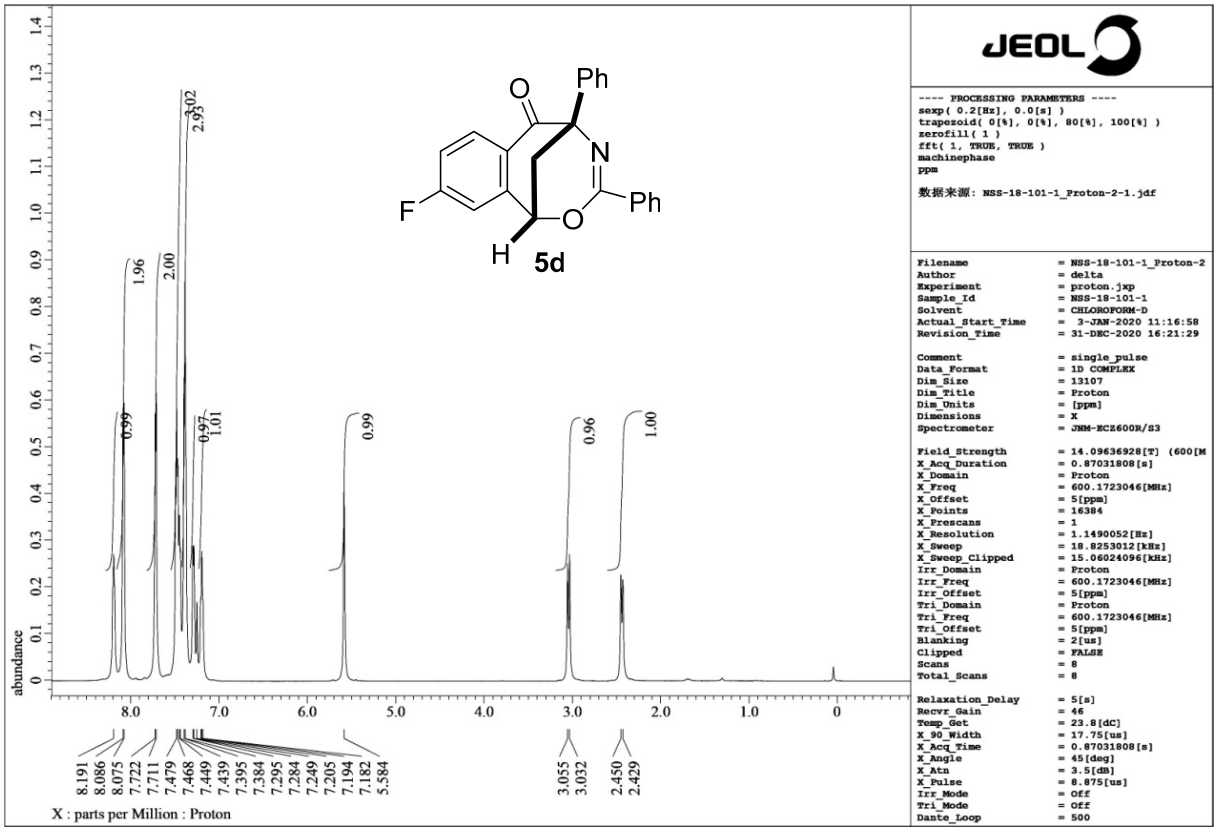

O
Ph
N
Ph
O
H
5a
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-16-1_Carbon_copy5-1-1.jdf
Filename = NSS-18-16-1_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-18-16-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-NOV-2020 17:31:
Revision_Time = 1-JAN-2021 19:22:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 250
Total_Scans = 250
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.5[dC]
X_90_Width = 8.6[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.8[dB]
X_Pulse = 2.86666667[us]
Irr_Atn_Dec = 16.132[dB]
Irr_Atn_Dec_Calc = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe = 16.132[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]

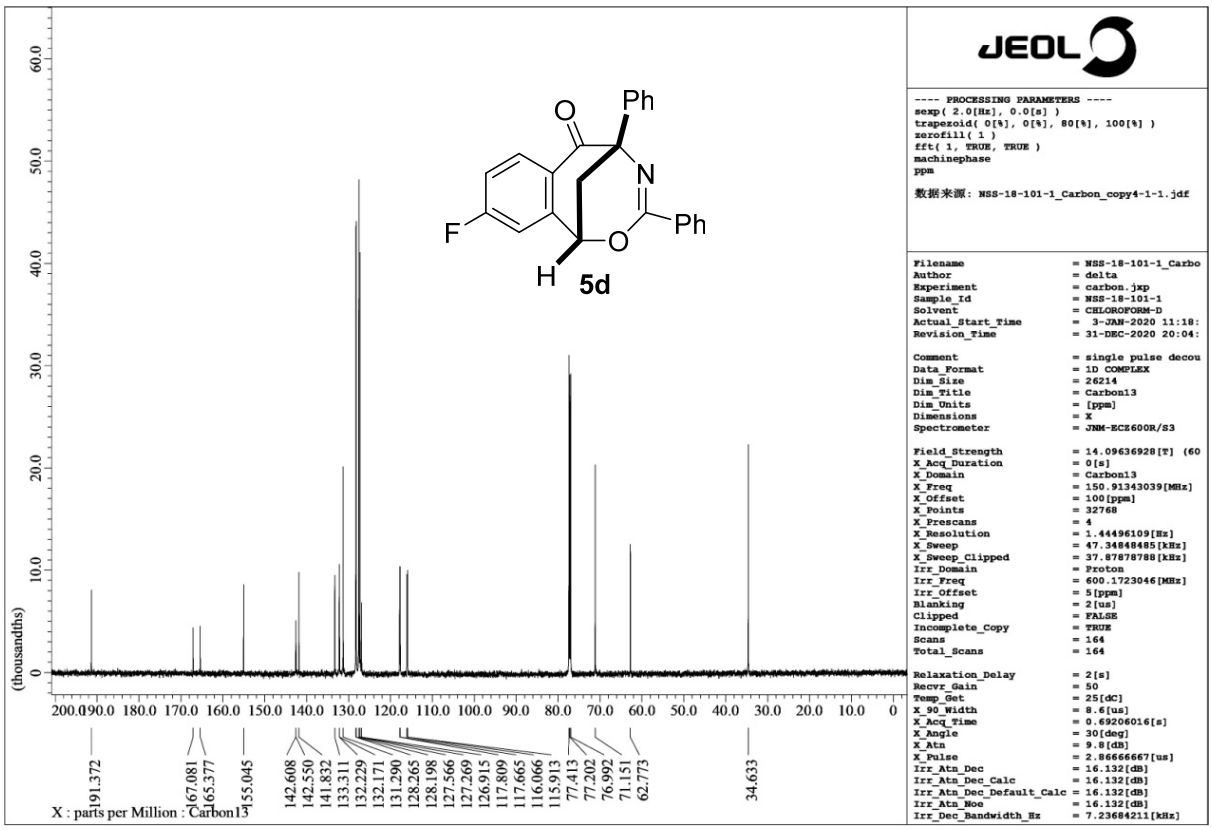

JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-13-1_Proton-2-1.jdf
Filename = NSS-19-13-1_Proton-2-
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-19-13-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-NOV-2020 11:16:02
Revision_Time = 31-DEC-2020 15:50:52
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 25.8[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
MeO
Ph
N
O
Ph
H
5b
abundance
X : parts per Million : Proton

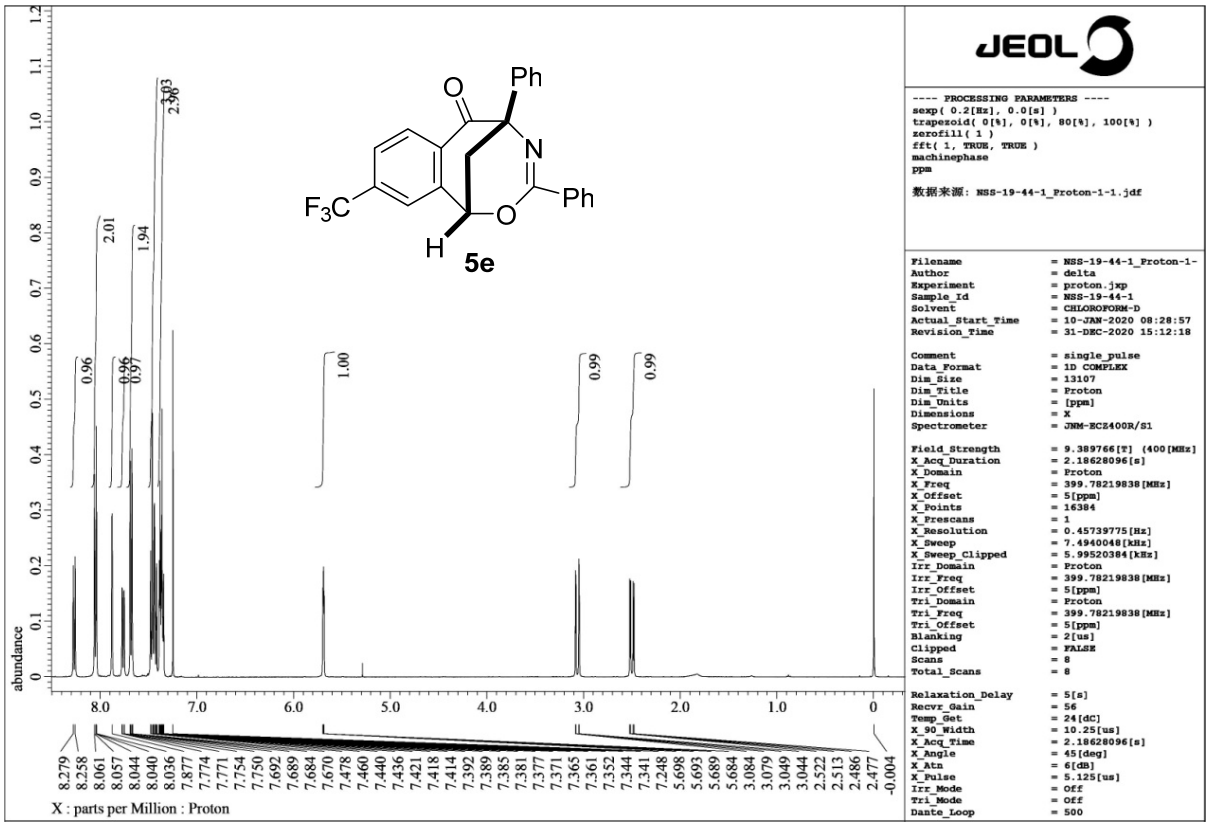

JEOL
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-13-1_Carbon_copy7-1-1.jdf
Filename = NSS-19-13-1_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-19-13-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-NOV-2020 10:27:
Revision_Time = 31-DEC-2020 20:23:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Incomplete_Copy = TRUE
Scans = 501
Total_Scans = 501
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 26.2[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
MeO
Ph
N
O
Ph
H
5b
(thousandths)
X : parts per Million : Carbon13


Ph
O
N
Me
O
Ph
H
5c
2.95
2.03
2.94
2.94
1.00
1.01
0.99
1.00
0.99
3.02
abundance
8.061
8.046
8.031
7.692
7.678
7.451
7.437
7.426
7.412
7.401
7.382
7.359
7.347
7.341
7.334
7.315
7.301
7.248
5.582
3.040
3.017
2.460
2.442
2.437
2.421
2.414
-0.006
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-12-1_Proton-2-1.jdf
Filename = NSS-19-12-1_Proton-2-
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-19-12-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-NOV-2020 16:08:01
Revision_Time = 31-DEC-2020 15:59:44
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 26[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

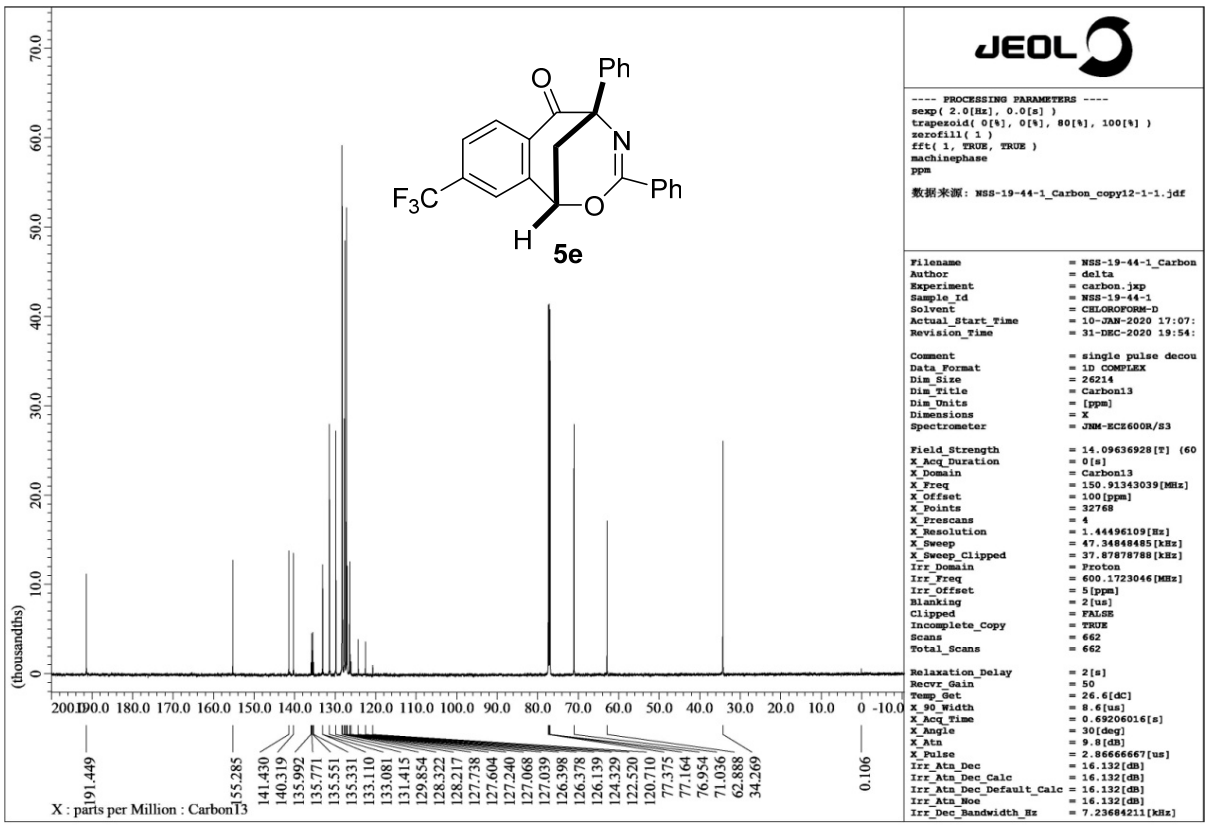

Ph
O
N
Me
O
Ph
H
5c
(thousandths)
192.627
155.072
145.547
142.337
140.027
133.635
131.153
131.086
129.793
129.179
128.202
128.116
127.943
127.570
127.416
127.330
77.548
77.222
76.906
71.827
62.963
34.962
21.872
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-12-1_Carbon_copy4-1-1.jdf
Filename = NSS-19-12-1_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-19-12-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-NOV-2020 15:37:
Revision_Time = 31-DEC-2020 20:19:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Incomplete_Copy = TRUE
Scans = 117
Total_Scans = 117
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.3[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]


O
Ph
N
F
O
Ph
H
5d
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-101-1_Proton-2-1.jdf
Filename = NSS-18-101-1_Proton-2
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-18-101-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-JAN-2020 11:16:58
Revision_Time = 31-DEC-2020 16:21:29
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 23.8[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

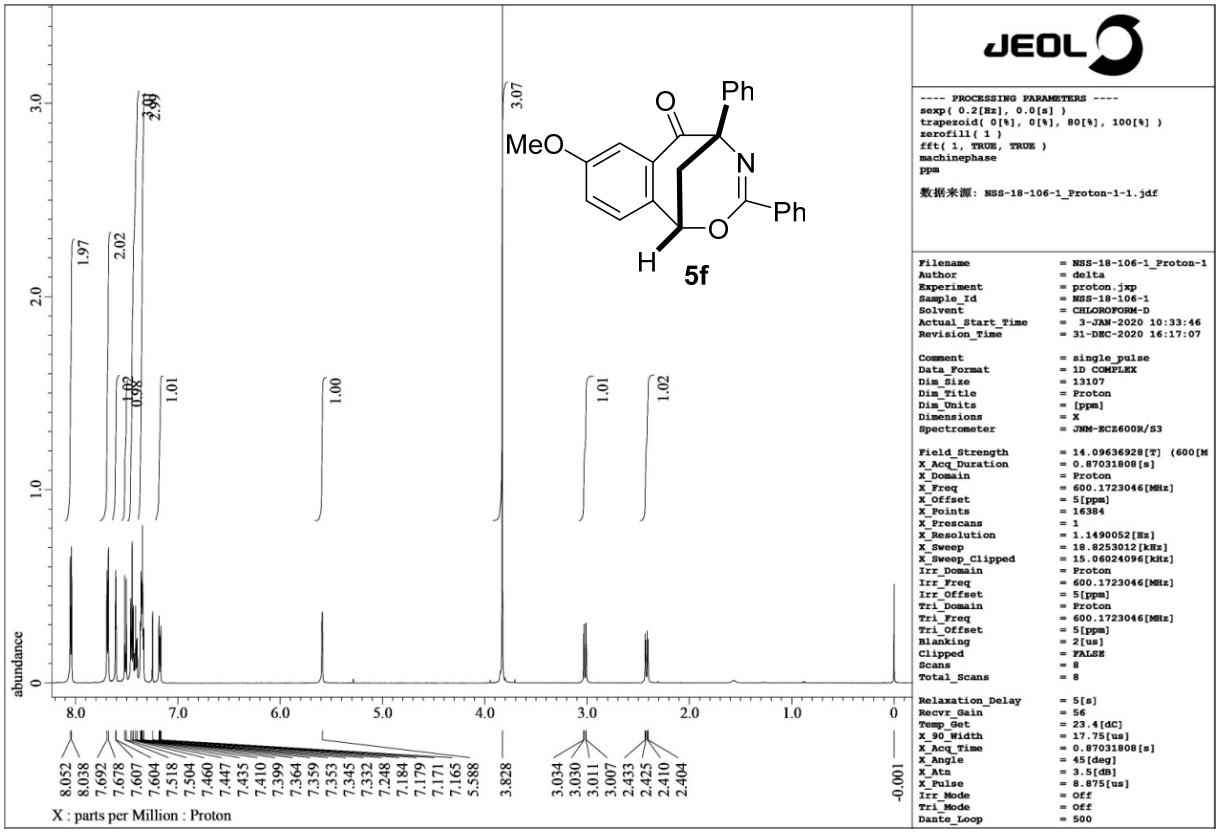

O
Ph
N
F
O
Ph
H
5d
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-101-1_Carbon_copy4-1-1.jdf
Filename = NSS-18-101-1_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-18-101-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-JAN-2020 11:18:
Revision_Time = 31-DEC-2020 20:04:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 164
Total_Scans = 164
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25[dC]
X_90_Width = 8.6[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.8[dB]
X_Pulse = 2.86666667[us]
Irr_Atn_Dec = 16.132[dB]
Irr_Atn_Dec_Calc = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe = 16.132[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]

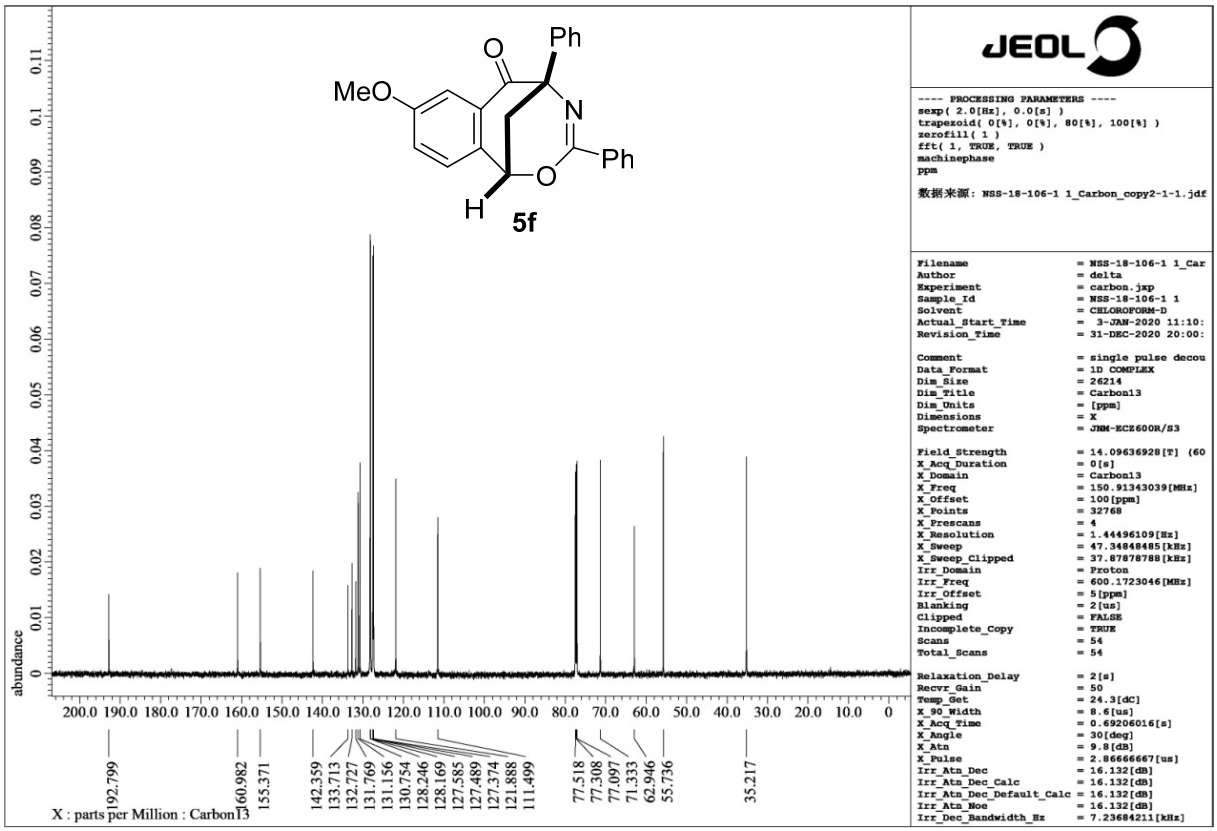


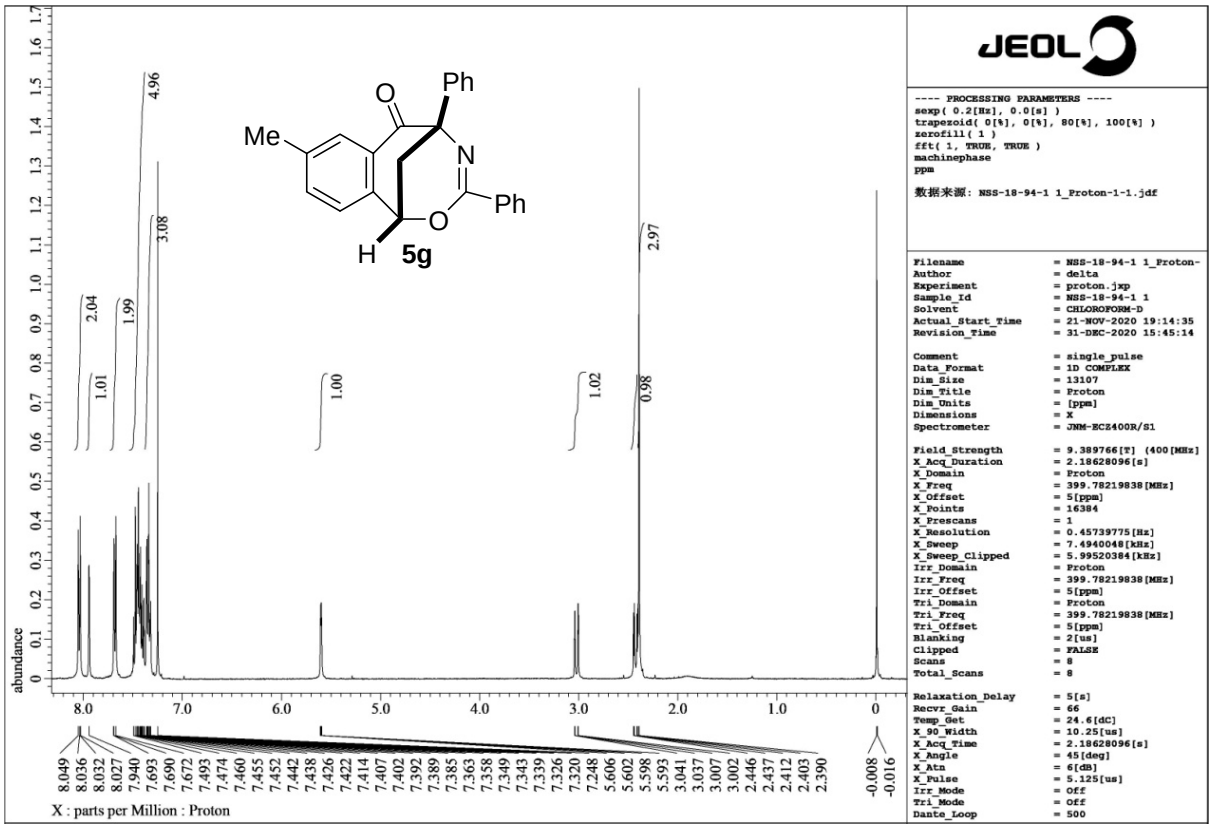

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-19-44-1_Proton-1-1.jdf

Filename                = NSS-19-44-1_Proton-1-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = NSS-19-44-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 10-JAN-2020 08:28:57
Revision_Time           = 31-DEC-2020 15:12:18

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400R/S1

Field_Strength          = 9.389766[T] (400[MHz]
X_Acq_Duration          = 2.18628096[s]
X_Domain                = Proton
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45739775[Hz]
X_Sweep                 = 7.4940048[kHz]
X_Sweep_Clipped         = 5.99520384[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 24[dC]
X_90_Width              = 10.25[us]
X_Acq_Time              = 2.18628096[s]
X_Angle                 = 45[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 5.125[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
```

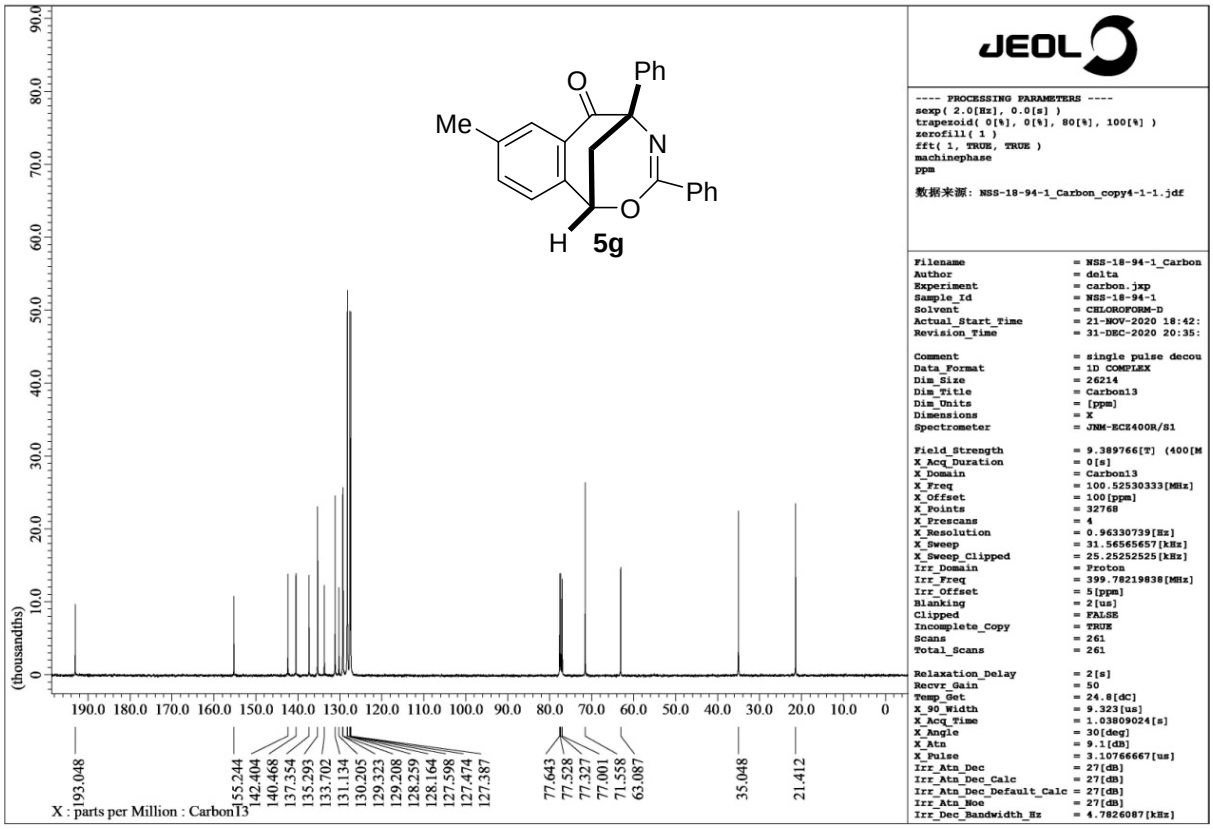


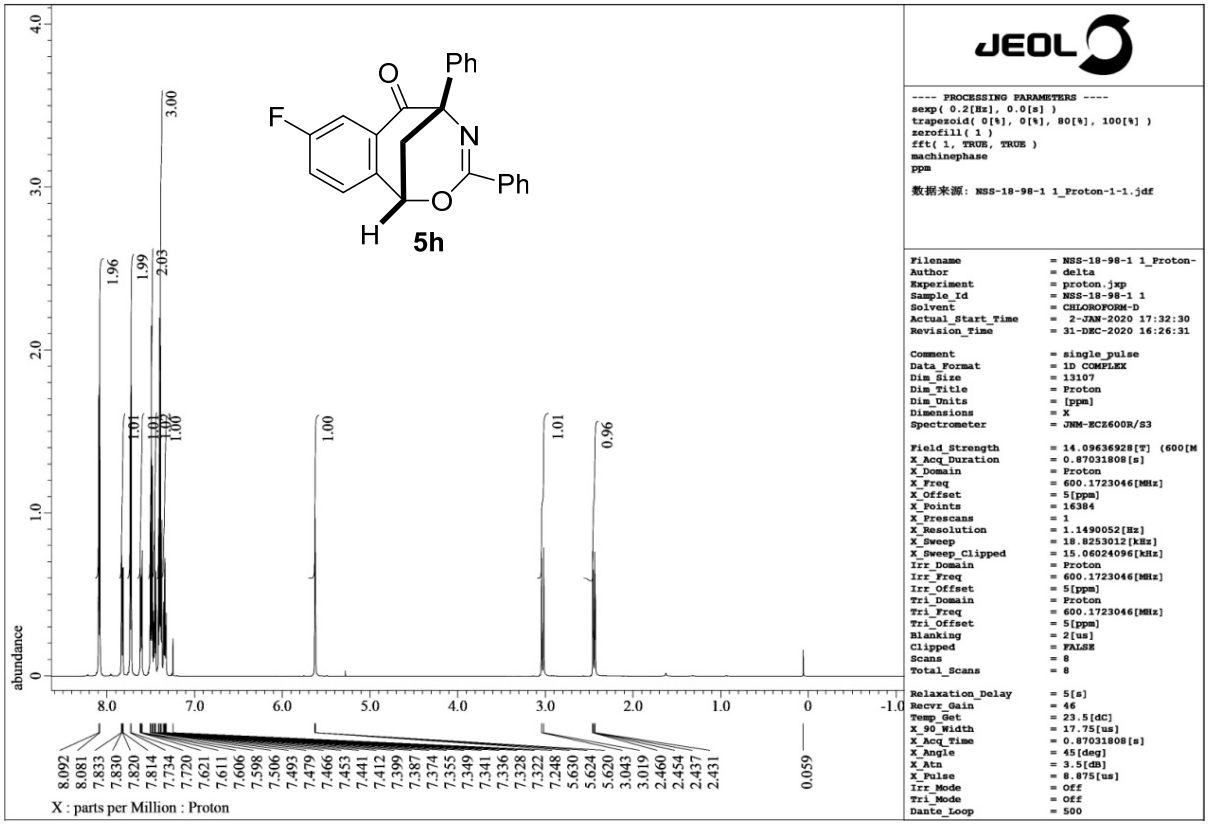

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-19-44-1_Carbon_copy12-1-1.jdf

Filename                = NSS-19-44-1_Carbon
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = NSS-19-44-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 10-JAN-2020 17:07:
Revision_Time           = 31-DEC-2020 19:54:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (60
X_Acq_Duration          = 0[s]
X_Domain                = Carbon13
X_Freq                  = 150.91343039[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 1.44496109[Hz]
X_Sweep                 = 47.34848485[kHz]
X_Sweep_Clipped         = 37.87878788[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Incomplete_Copy         = TRUE
Scans                   = 662
Total_Scans             = 662

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 26.6[dC]
X_90_Width              = 8.6[us]
X_Acq_Time              = 0.69206016[s]
X_Angle                 = 30[deg]
X_Atn                   = 9.8[dB]
X_Pulse                 = 2.86666667[us]
Irr_Atn_Dec             = 16.132[dB]
Irr_Atn_Dec_Calc        = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe             = 16.132[dB]
Irr_Dec_Bandwidth_Hz    = 7.23684211[kHz]
```

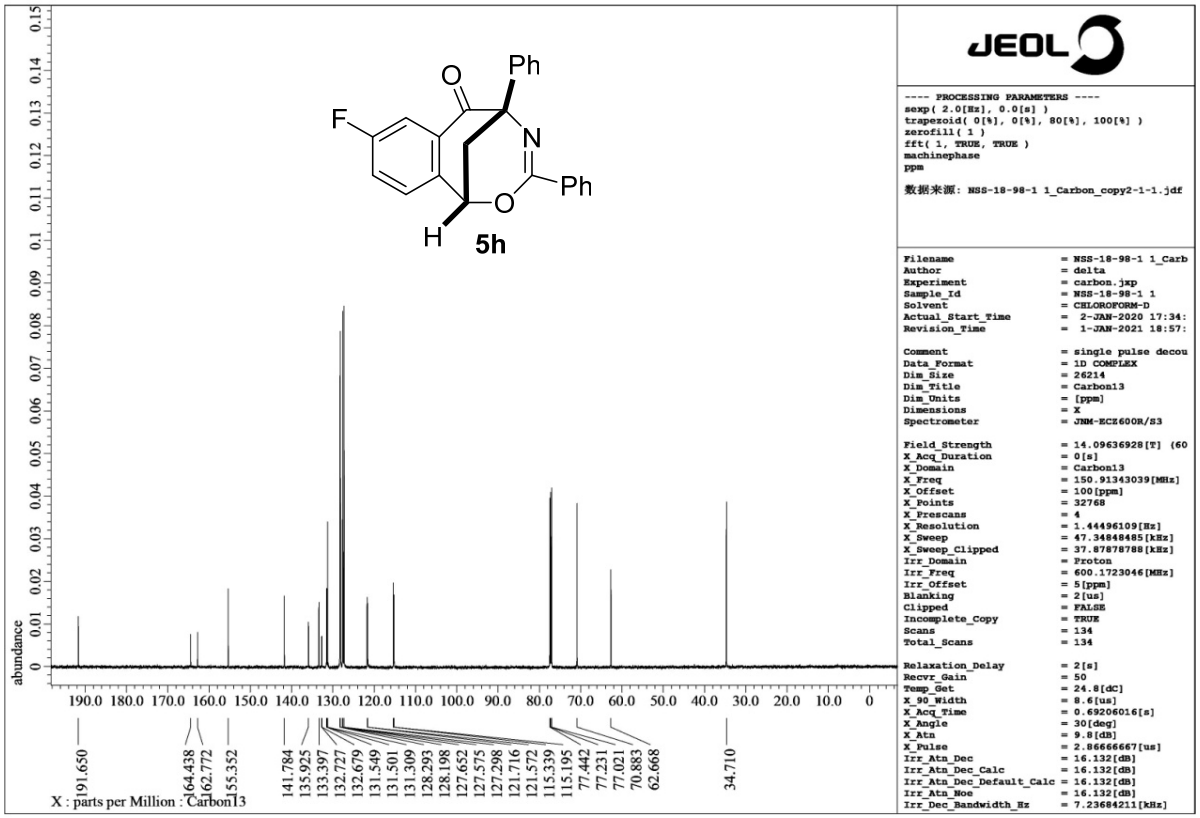

MeO
O
Ph
N
Ph
O
H
5f
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-106-1_Proton-1-1.jdf
Filename = NSS-18-106-1_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-18-106-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-JAN-2020 10:33:46
Revision_Time = 31-DEC-2020 16:17:07
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 23.4[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

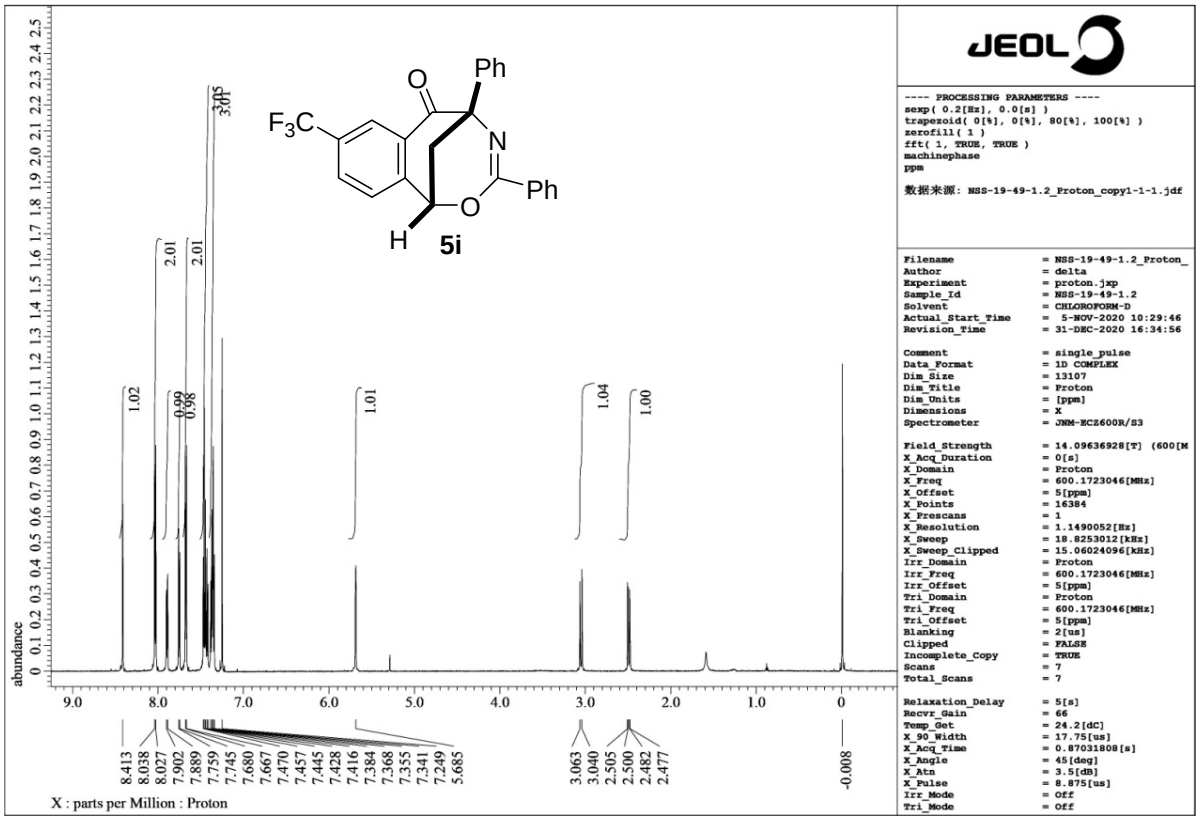

MeO
O
Ph
N
Ph
O
H
5f
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-106-1 1_Carbon_copy2-1-1.jdf
Filename = NSS-18-106-1 1_Car
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-18-106-1 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-JAN-2020 11:10:
Revision_Time = 31-DEC-2020 20:00:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 56
Total_Scans = 56
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.3[dC]
X_90_Width = 8.6[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.8[dB]
X_Pulse = 2.86666667[us]
Irr_Atn_Dec = 16.132[dB]
Irr_Atn_Dec_Calc = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe = 16.132[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]

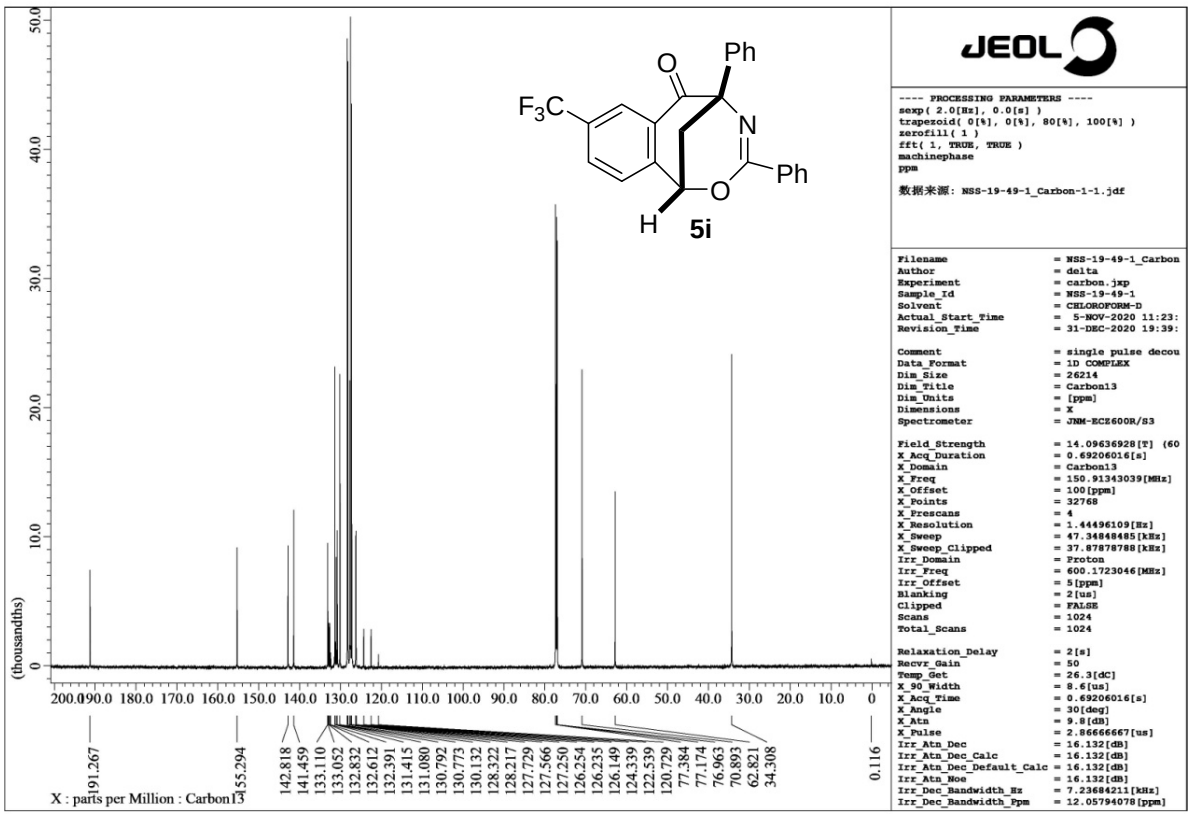

Me
O
Ph
N
Ph
O
H
5g
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-94-1 1_Proton-1-1.jdf
Filename = NSS-18-94-1 1_Proton-
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-18-94-1 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-NOV-2020 19:14:35
Revision_Time = 31-DEC-2020 15:45:14
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 2.18628096[s]
X_Domain = Proton
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 24.6[dC]
X_90_Width = 10.25[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 5.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

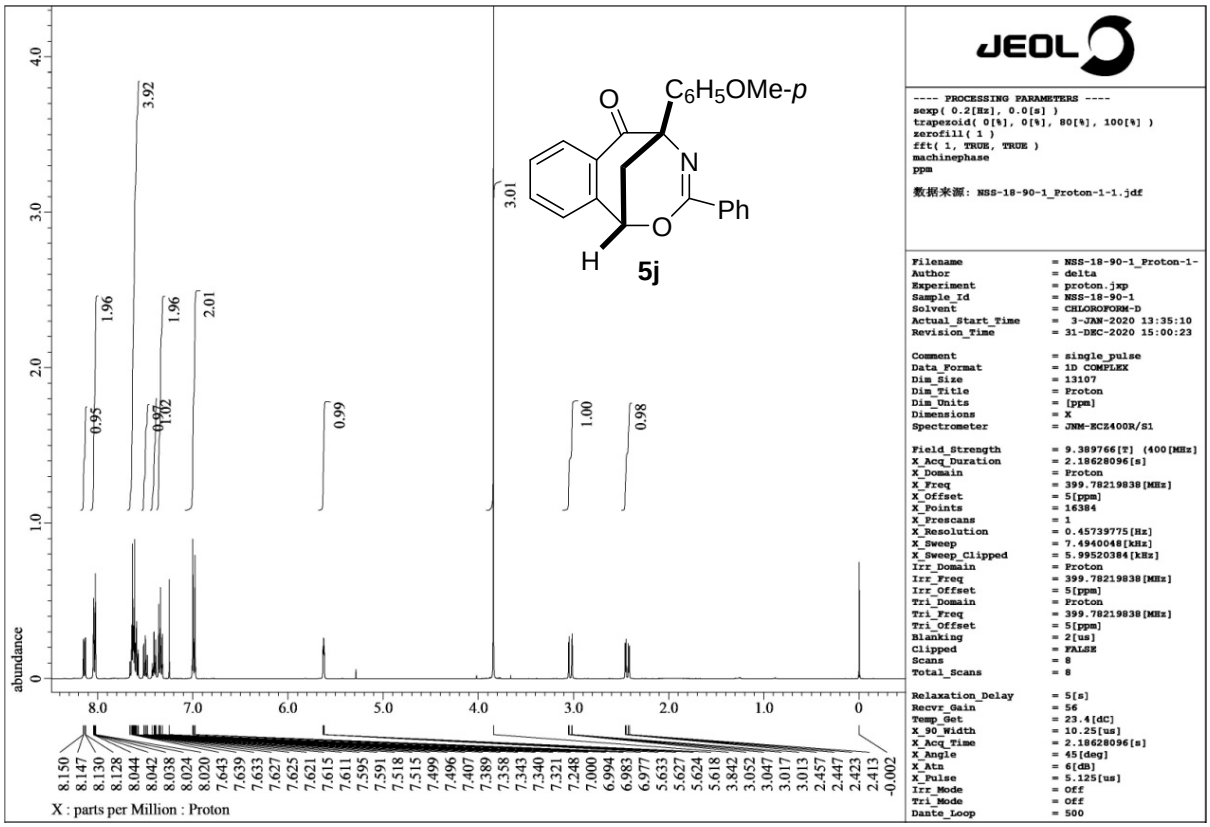

Me
O
Ph
N
Ph
O
H
5g
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-94-1_Carbon_copy4-1-1.jdf
Filename = NSS-18-94-1_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-18-94-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-NOV-2020 18:42:
Revision_Time = 31-DEC-2020 20:35:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 261
Total_Scans = 261
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.8[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]

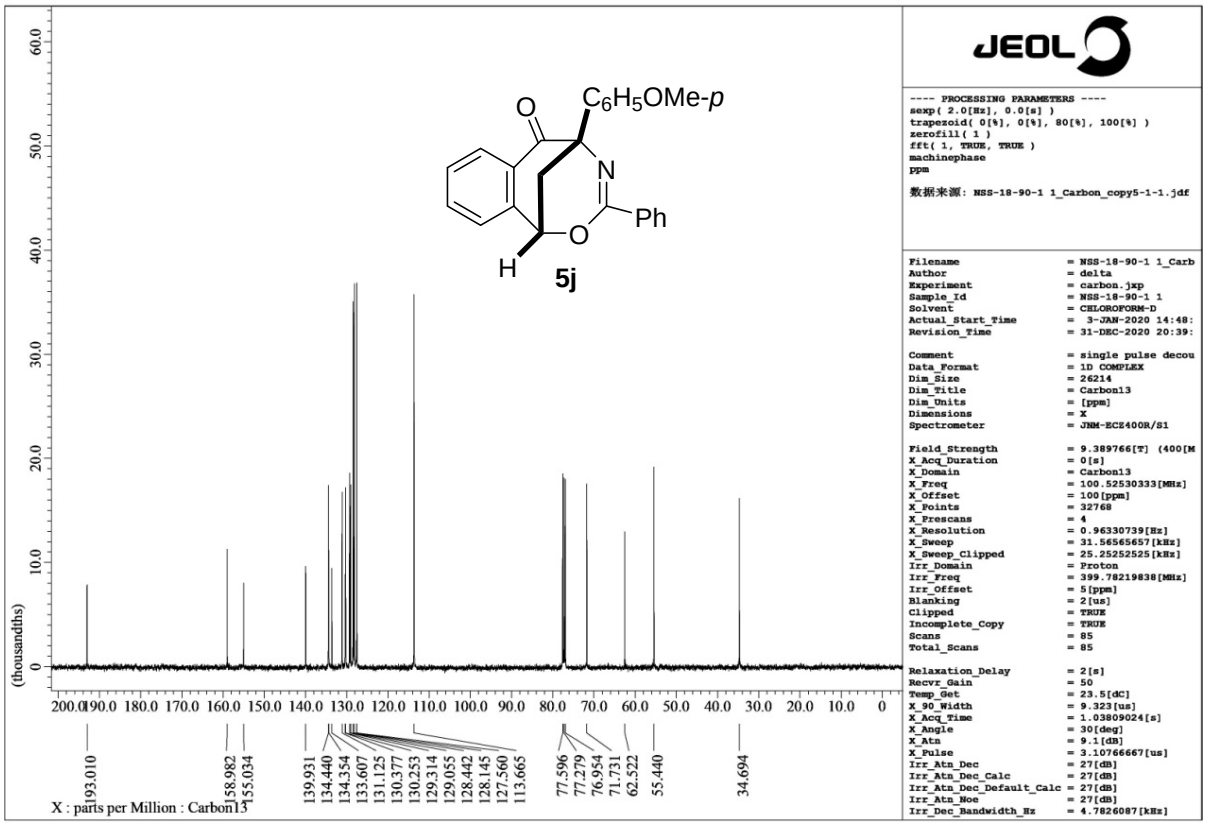

Ph
O
F
N
Ph
O
H
5h
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-98-1 1_Proton-1-1.jdf
Filename = NSS-18-98-1 1_Proton-
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-18-98-1 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-JAN-2020 17:32:30
Revision_Time = 31-DEC-2020 16:26:31
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 23.5[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

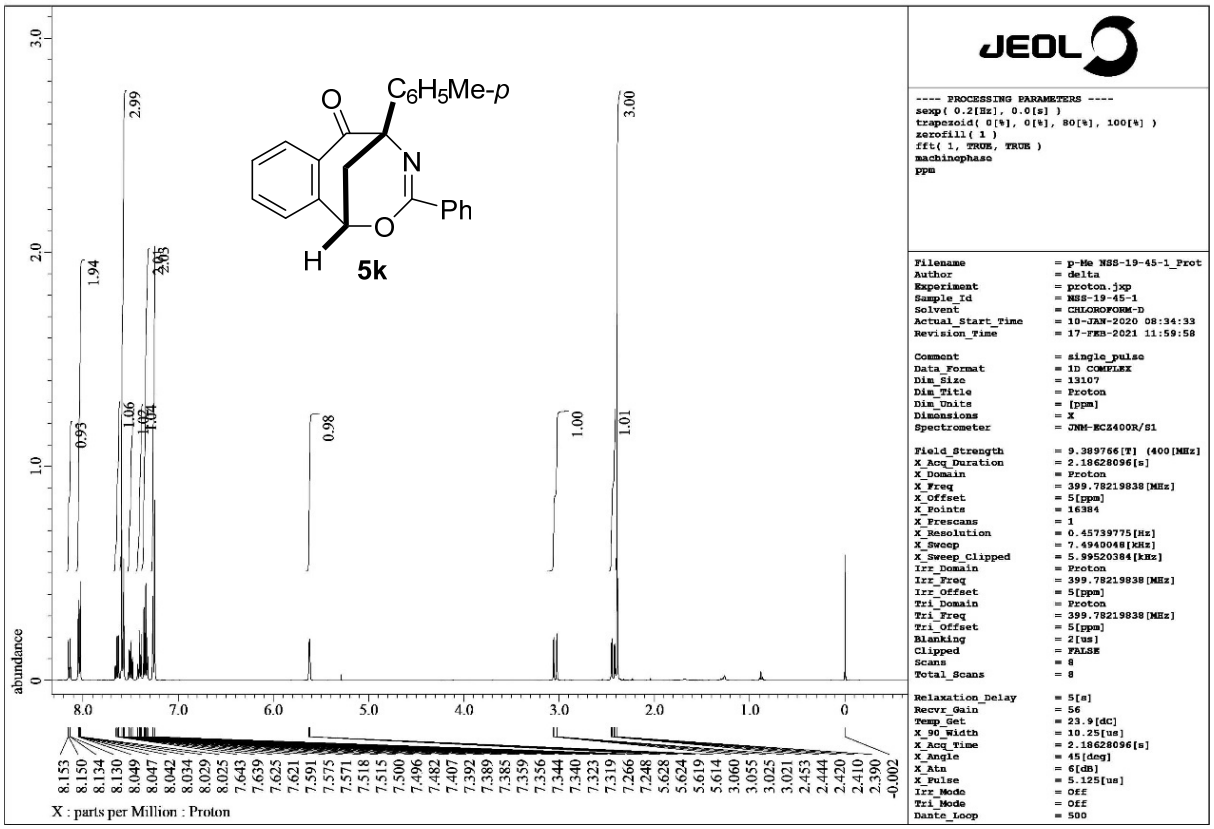

Ph
O
F
N
Ph
O
H
5h
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-98-1 1_Carbon_copy2-1-1.jdf
Filename = NSS-18-98-1 1_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-18-98-1 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-JAN-2020 17:34:
Revision_Time = 1-JAN-2021 18:57:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 134
Total_Scans = 134
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.8[dC]
X_90_Width = 8.6[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.8[dB]
X_Pulse = 2.86666667[us]
Irr_Atn_Dec = 16.132[dB]
Irr_Atn_Dec_Calc = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe = 16.132[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]

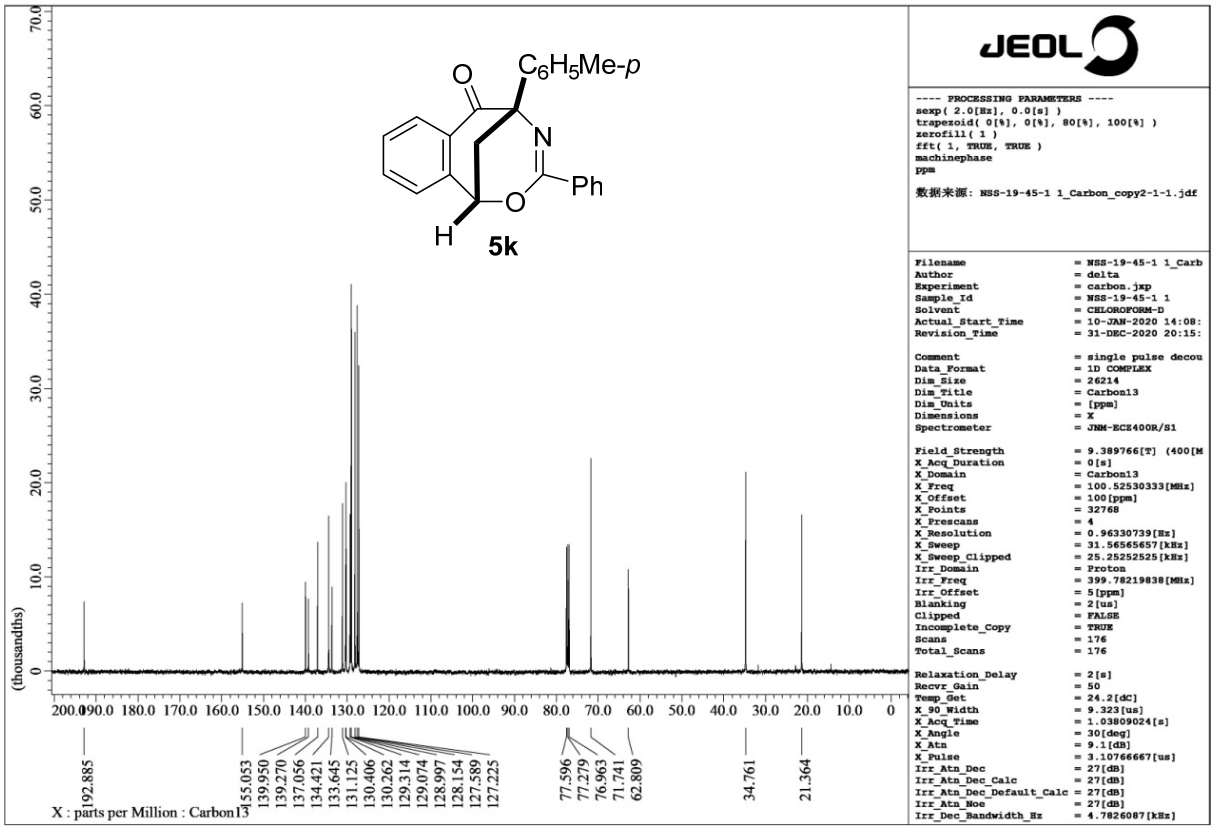

Ph
O
F3C
N
Ph
O
H
5i
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-49-1.2_Proton_copy1-1-1.jdf
Filename = NSS-19-49-1.2_Proton_
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-19-49-1.2
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-NOV-2020 10:29:46
Revision_Time = 31-DEC-2020 16:34:56
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 7
Total_Scans = 7
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 24.2[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off

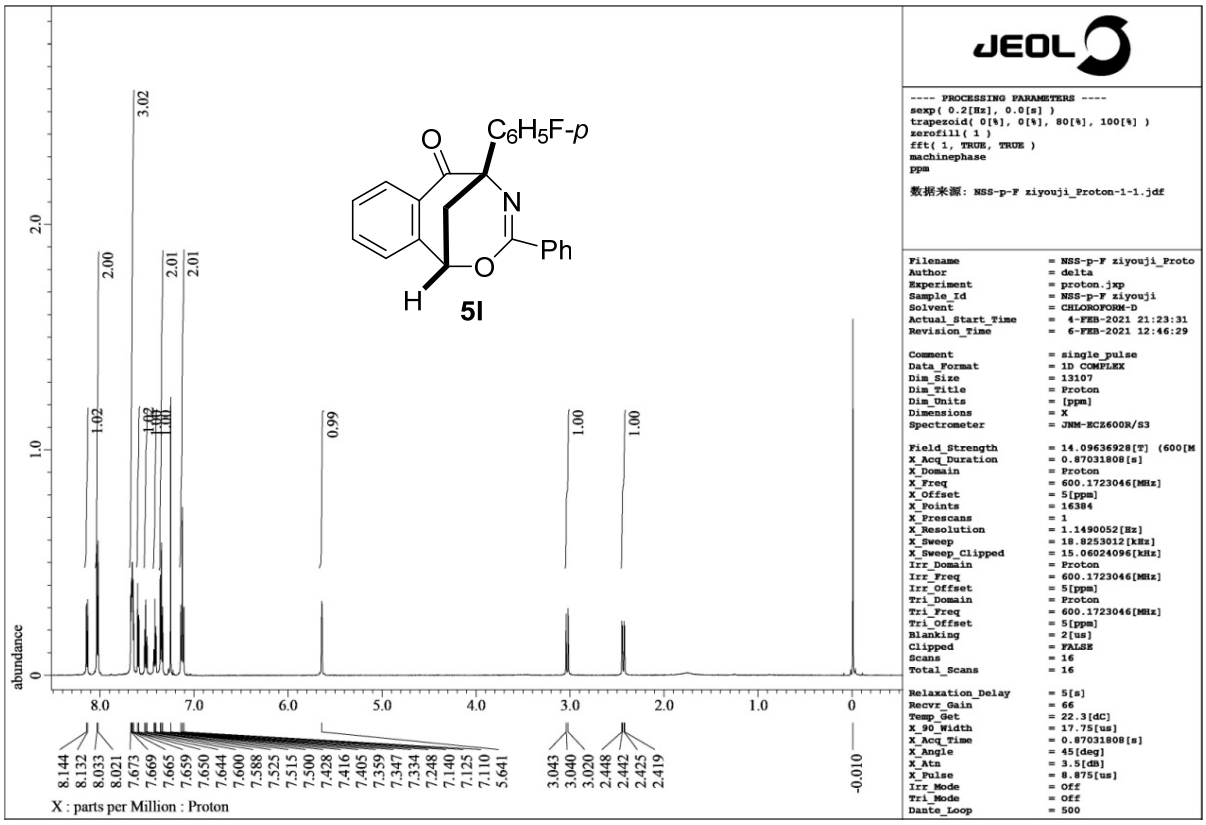

Ph
O
F3C
N
Ph
O
H
5i
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-49-1_Carbon-1-1.jdf
Filename = NSS-19-49-1_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-19-49-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-NOV-2020 11:23:
Revision_Time = 31-DEC-2020 19:39:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 26.3[dC]
X_90_Width = 8.6[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.8[dB]
X_Pulse = 2.86666667[us]
Irr_Atn_Dec = 16.132[dB]
Irr_Atn_Dec_Calc = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe = 16.132[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]

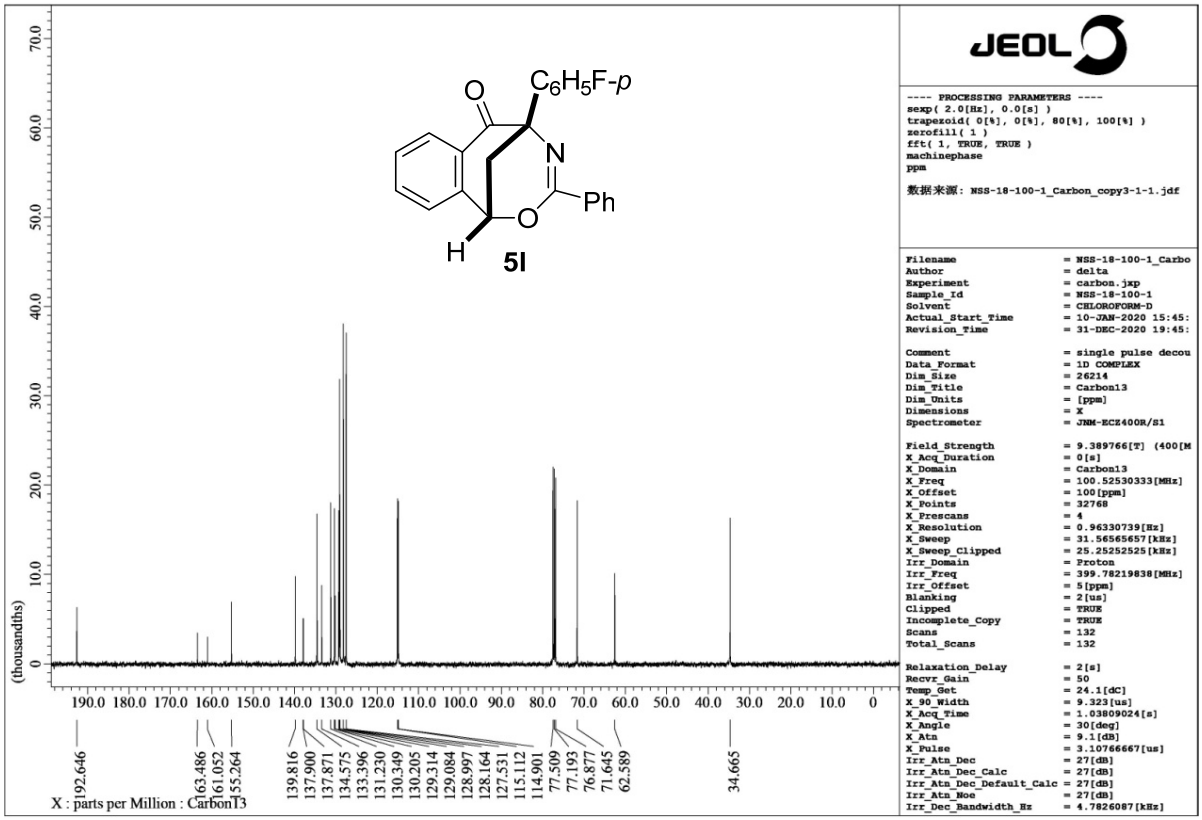

C6H5OMe-p
O
N
Ph
O
H
5j
3.01
3.92
1.96
1.96
2.01
0.95
0.97
1.02
0.99
1.00
0.98
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-90-1_Proton-1-1.jdf
Filename = NSS-18-90-1_Proton-1-
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-18-90-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-JAN-2020 13:35:10
Revision_Time = 31-DEC-2020 15:00:23
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 2.18628096[s]
X_Domain = Proton
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 23.4[dC]
X_90_Width = 10.25[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 5.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

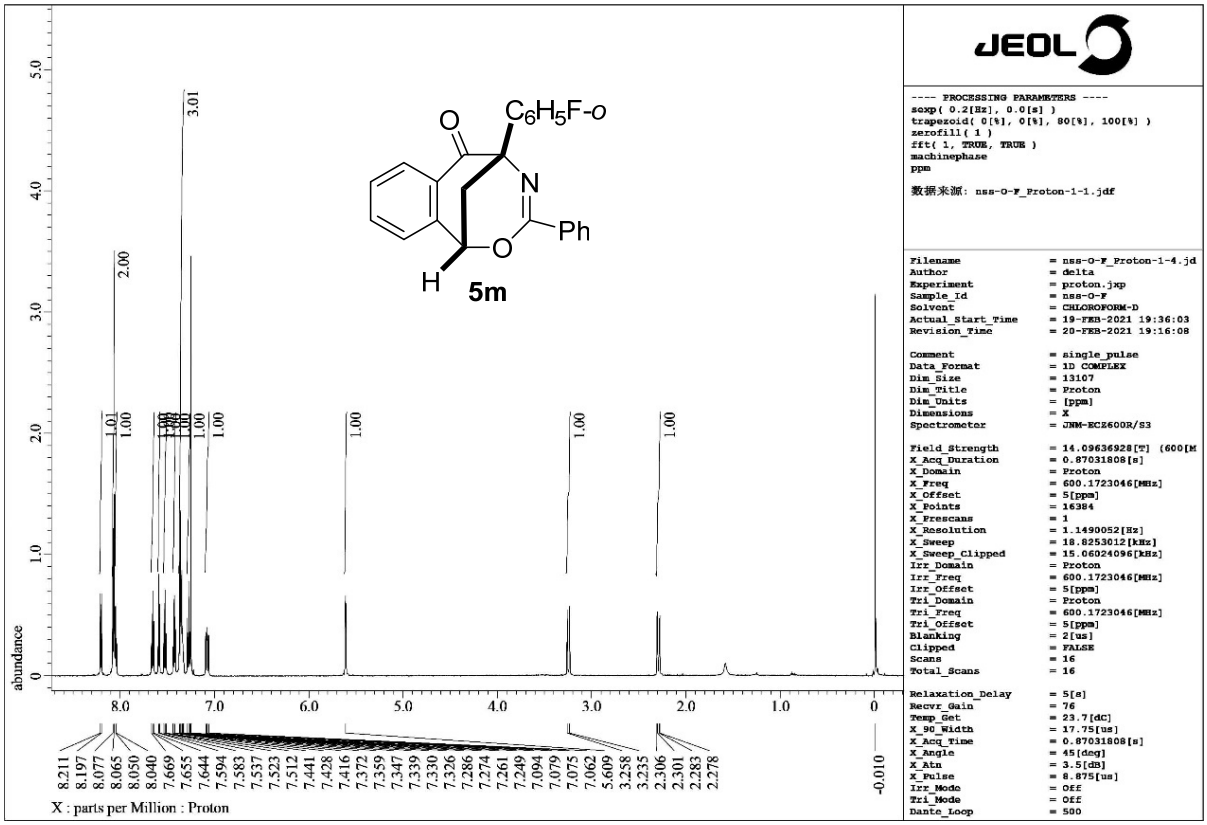

C6H5OMe-p
O
N
Ph
O
H
5j
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-90-1 1_Carbon_copy5-1-1.jdf
Filename = NSS-18-90-1 1_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-18-90-1 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-JAN-2020 14:48:
Revision_Time = 31-DEC-2020 20:39:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Incomplete_Copy = TRUE
Scans = 85
Total_Scans = 85
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 23.5[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]

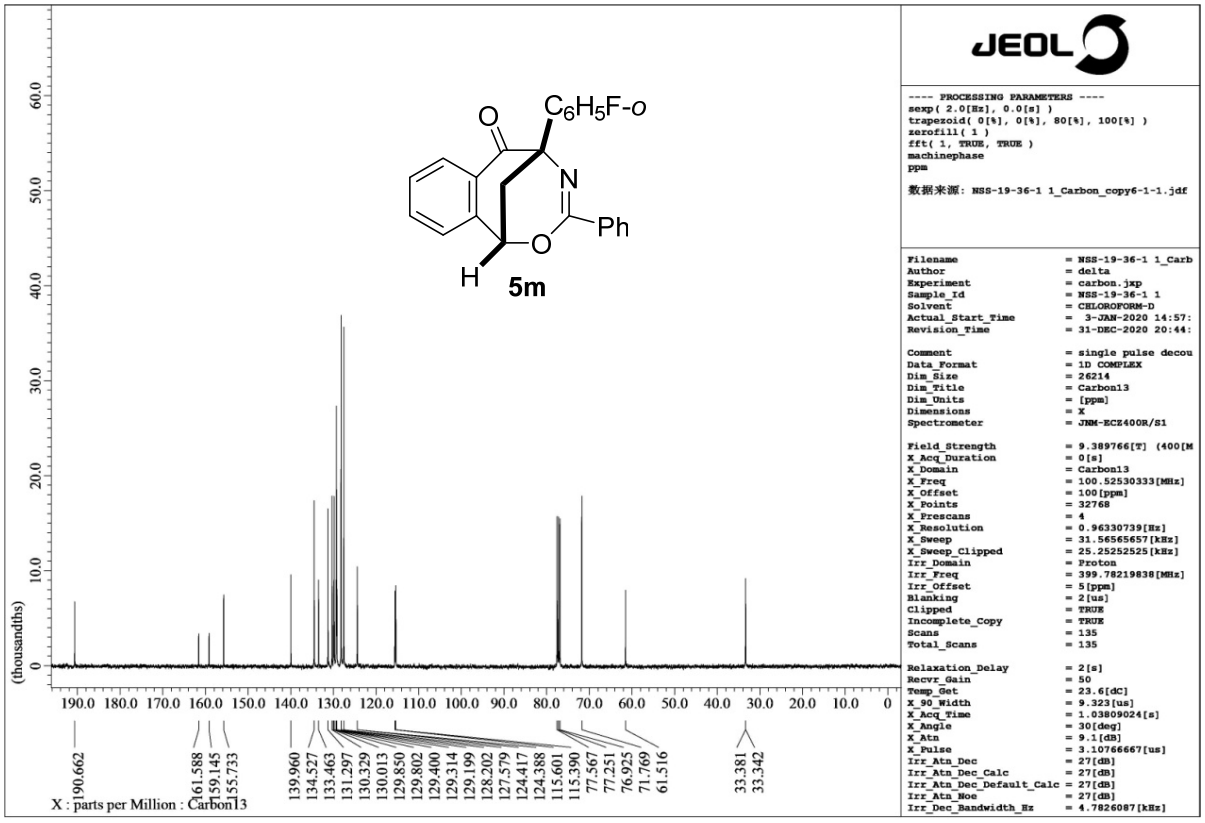

C6H5Me-p
O
N
Ph
O
H
5k
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = p-Me NSS-19-45-1_Prot
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-19-45-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-JAN-2020 08:34:33
Revision_Time = 17-FEB-2021 11:59:58
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 2.18628096[s]
X_Domain = Proton
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 23.9[dC]
X_90_Width = 10.25[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 5.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

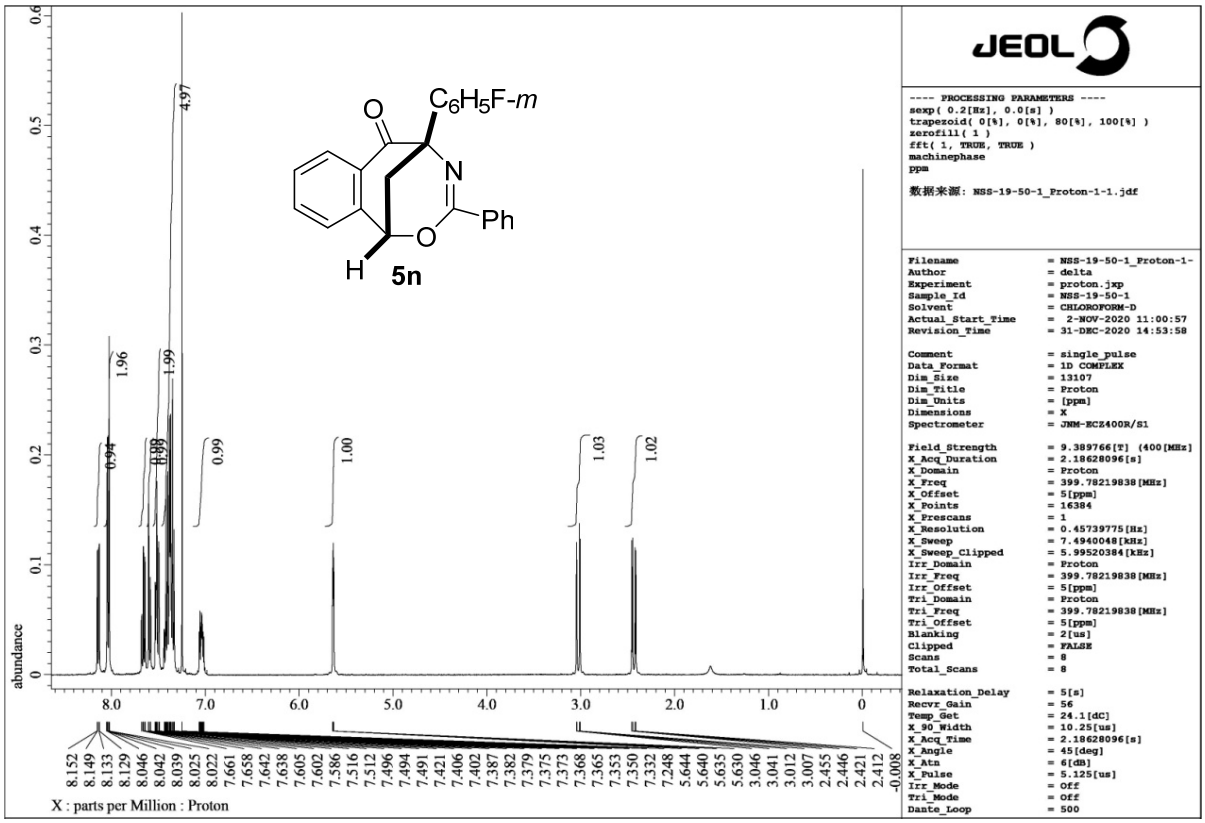

C6H5Me-p
O
N
Ph
O
H
5k
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-45-1 1_Carbon_copy2-1-1.jdf
Filename = NSS-19-45-1 1_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-19-45-1 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-JAN-2020 14:08:
Revision_Time = 31-DEC-2020 20:15:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 176
Total_Scans = 176
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.2[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]

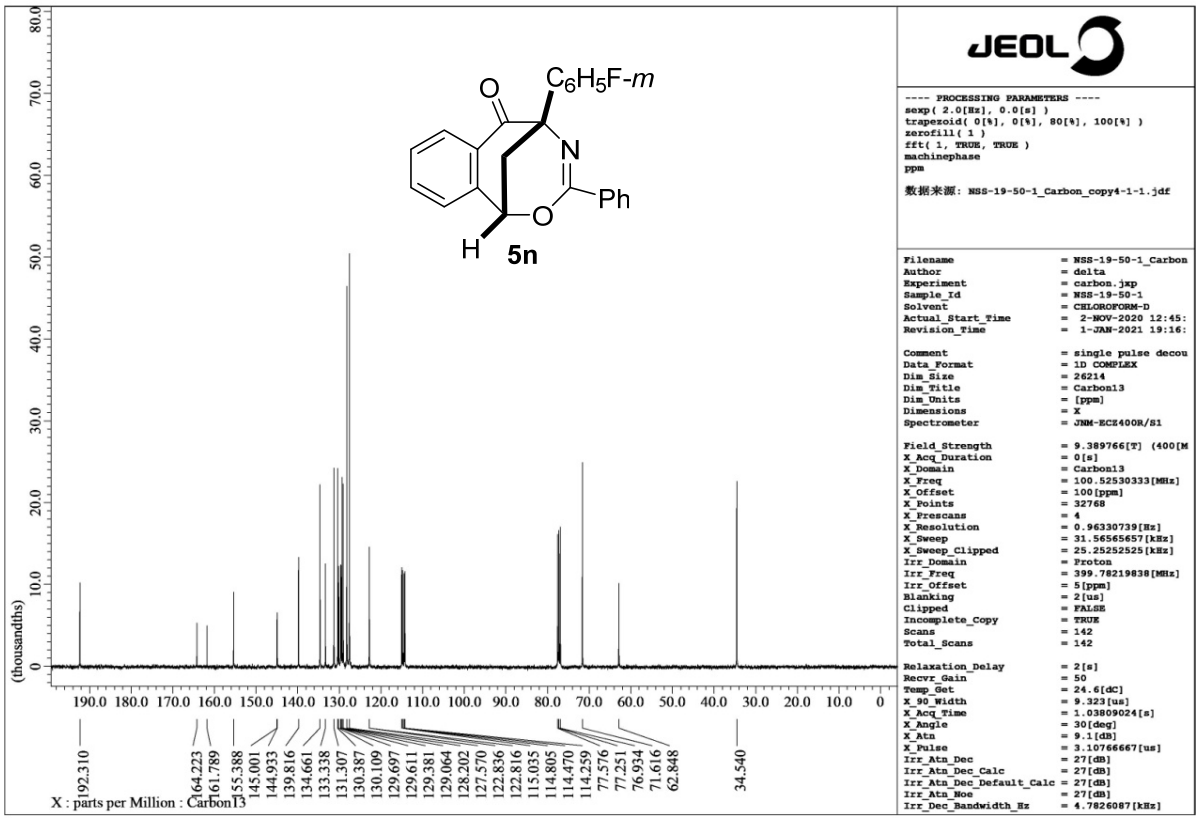

C6H5F-p
O
N
Ph
O
H
5l
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-p-F ziyouji_Proton-1-1.jdf
Filename = NSS-p-F ziyouji_Proto
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-p-F ziyouji
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-FEB-2021 21:23:31
Revision_Time = 6-FEB-2021 12:46:29
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 22.3[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

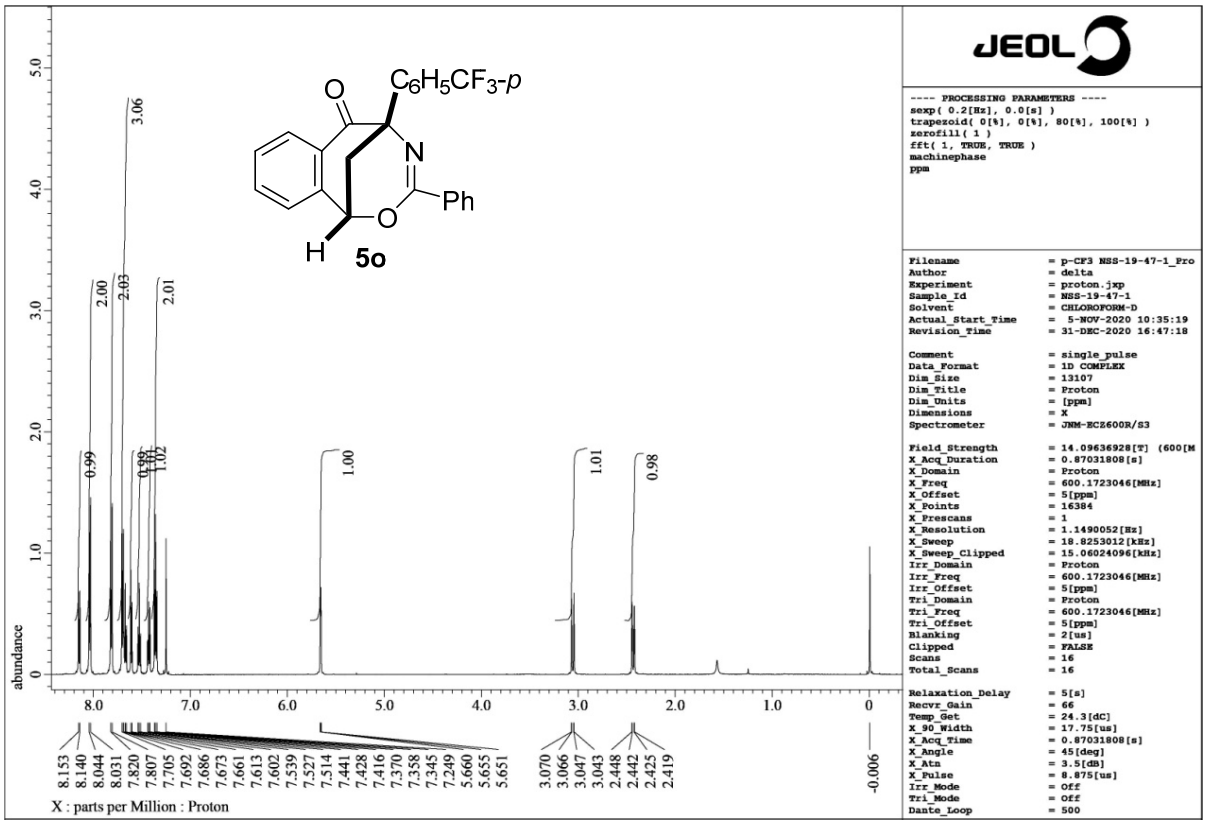

C6H5F-p
O
N
Ph
O
H
5l
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-18-100-1_Carbon_copy3-1-1.jdf
Filename = NSS-18-100-1_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-18-100-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-JAN-2020 15:45:
Revision_Time = 31-DEC-2020 19:45:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Incomplete_Copy = TRUE
Scans = 132
Total_Scans = 132
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.1[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]

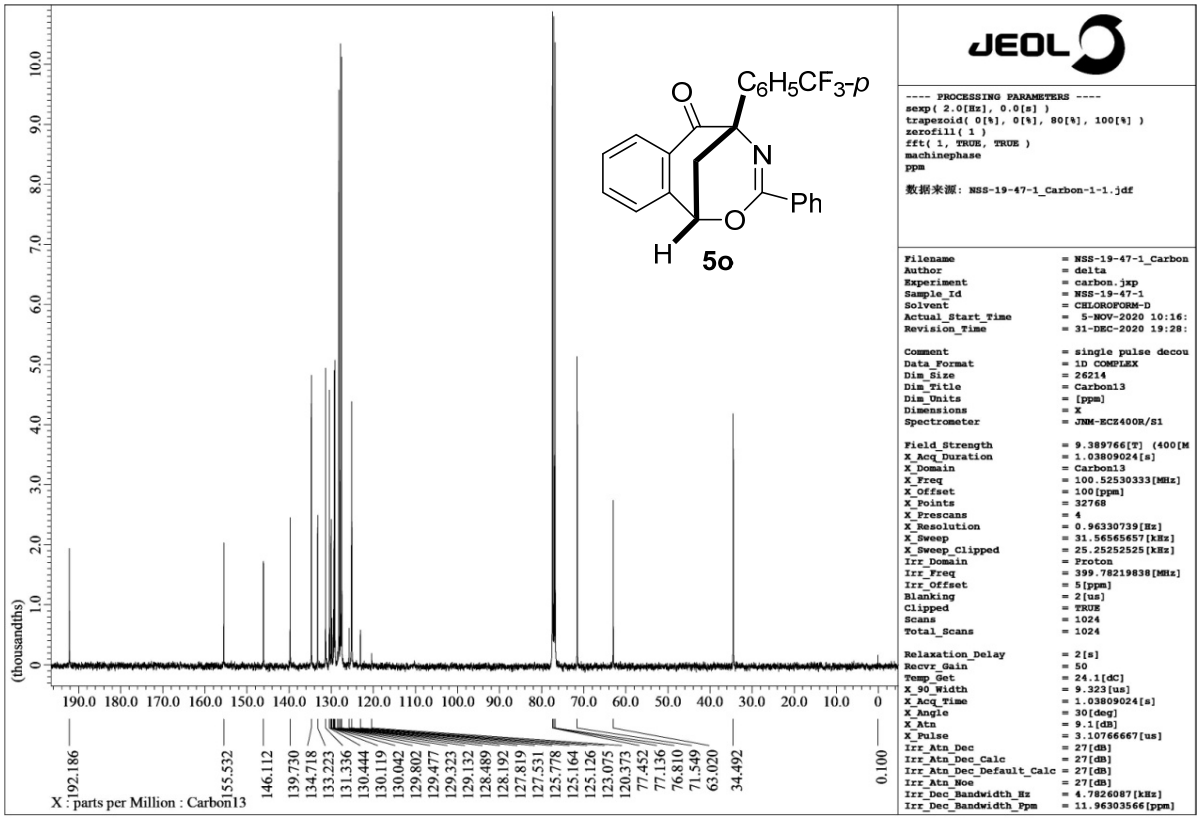

C6H5F-o
5m
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: nss-O-F_Proton-1-1.jdf
Filename = nss-O-F_Proton-1-4.jd
Author = delta
Experiment = proton.jxp
Sample_Id = nss-O-F
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-FEB-2021 19:36:03
Revision_Time = 20-FEB-2021 19:16:08
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 76
Temp_Get = 23.7[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

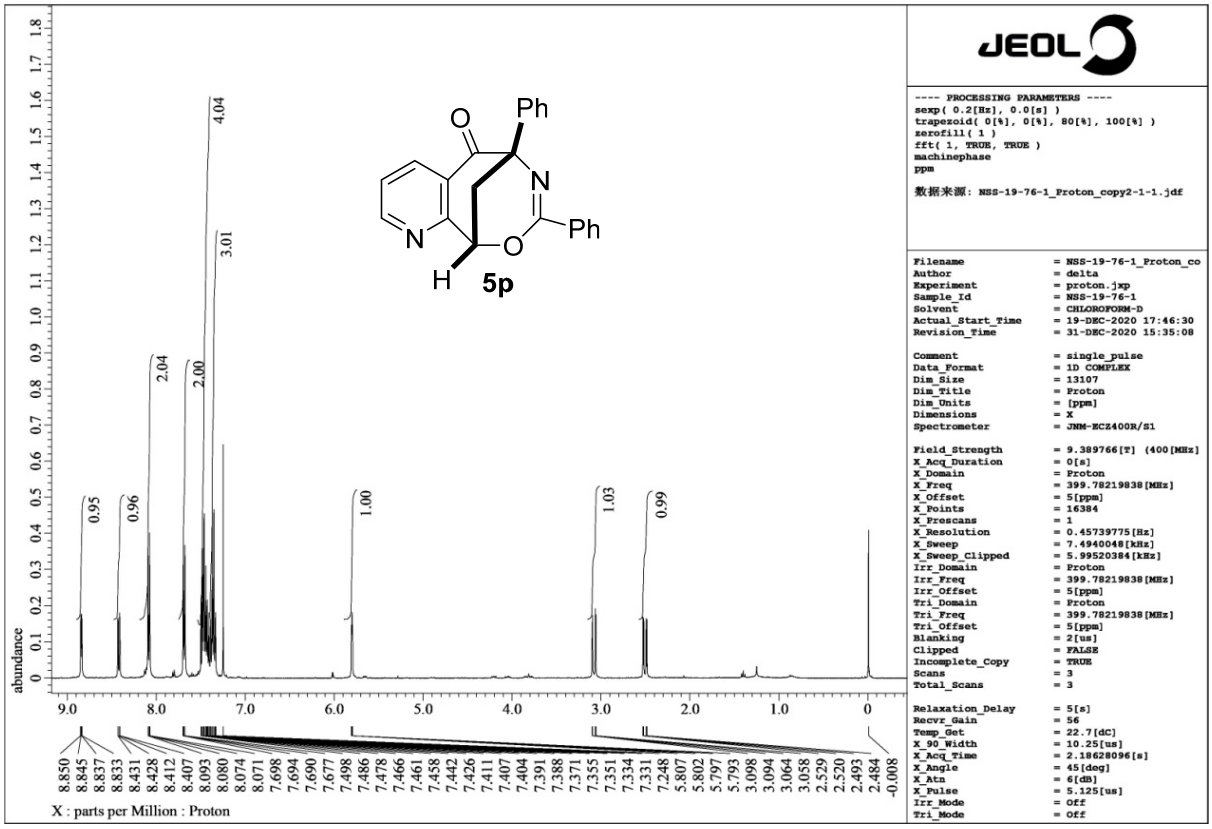

C6H5F-o
5m
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-36-1 1_Carbon_copy6-1-1.jdf
Filename = NSS-19-36-1 1_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-19-36-1 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-JAN-2020 14:57:
Revision_Time = 31-DEC-2020 20:44:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Incomplete_Copy = TRUE
Scans = 135
Total_Scans = 135
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 23.6[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]

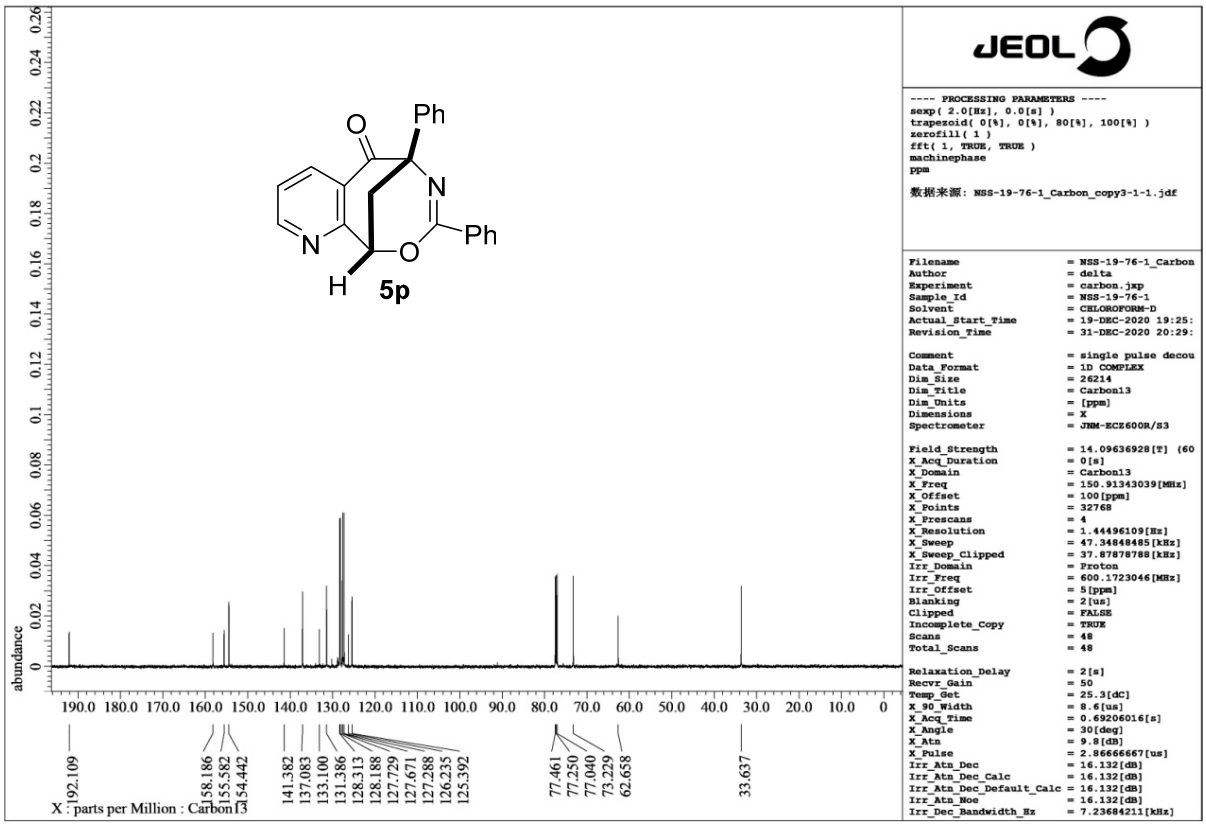

C6H5F-m
O
N
Ph
O
H
5n
4.97
1.96
1.99
0.94
0.98
0.99
1.00
1.03
1.02
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-50-1_Proton-1-1.jdf
Filename = NSS-19-50-1_Proton-1-
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-19-50-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-NOV-2020 11:00:57
Revision_Time = 31-DEC-2020 14:53:58
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 2.18628096[s]
X_Domain = Proton
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 24.1[dC]
X_90_Width = 10.25[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 5.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

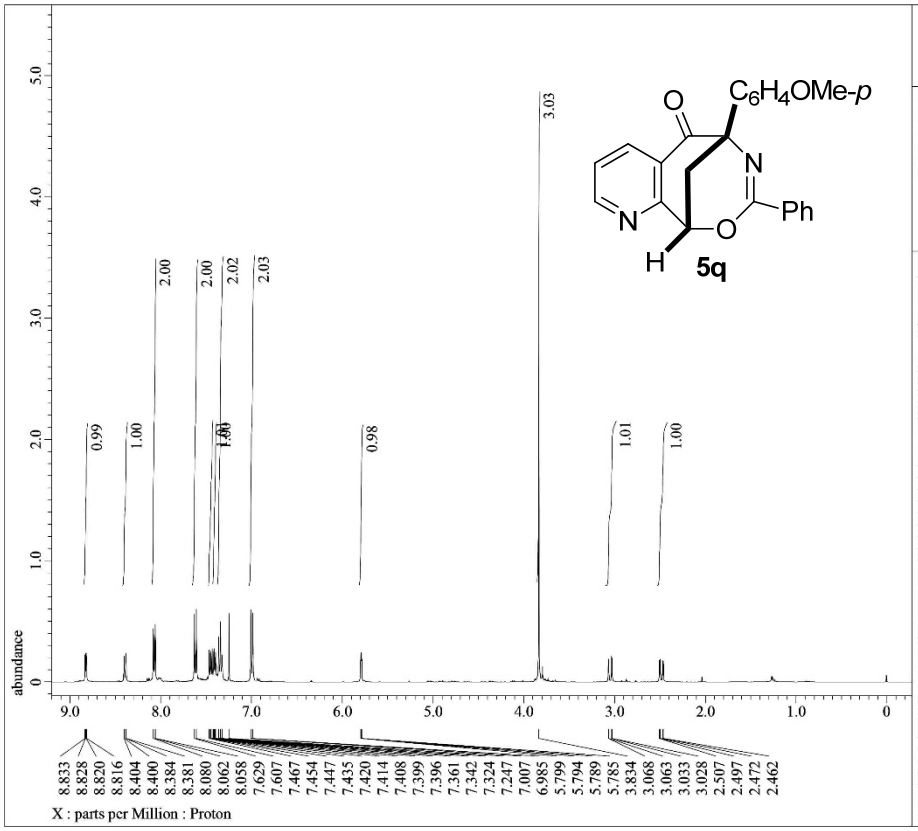

C6H5F-m
O
N
Ph
O
H
5n
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-50-1_Carbon_copy4-1-1.jdf
Filename = NSS-19-50-1_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-19-50-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-NOV-2020 12:45:
Revision_Time = 1-JAN-2021 19:16:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 142
Total_Scans = 142
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.6[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]


C6H5CF3-p
Ph
5o
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = p-CF3 NSS-19-47-1_Pro
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-19-47-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-NOV-2020 10:35:19
Revision_Time = 31-DEC-2020 16:47:18
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 24.3[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

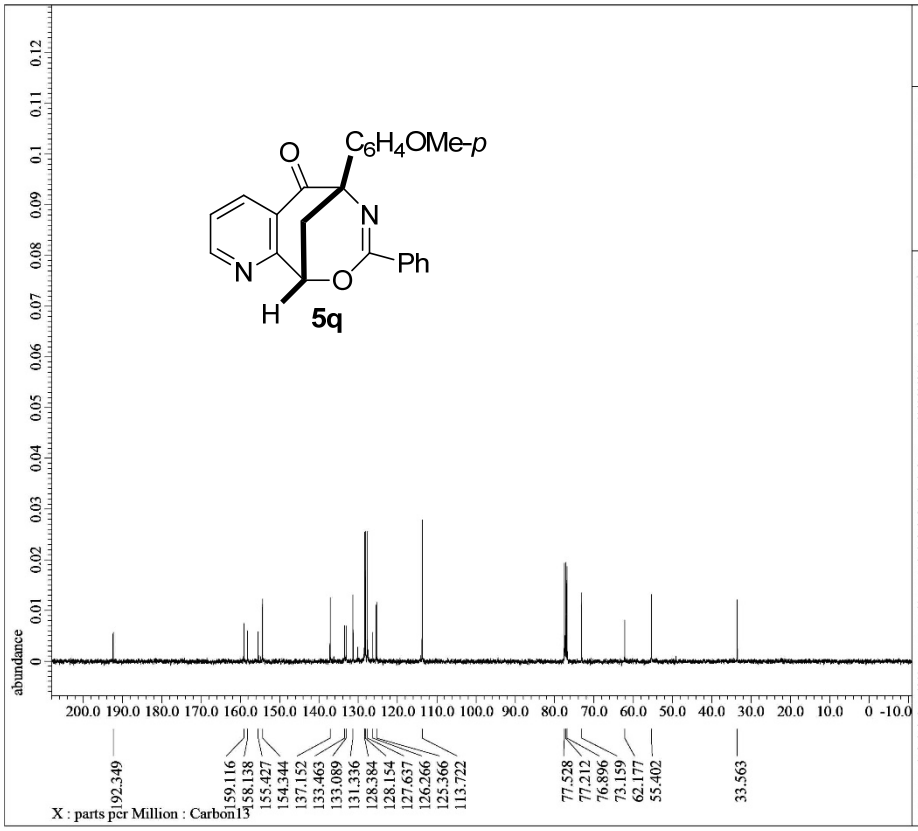

C6H5CF3-p
Ph
5o
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-47-1_Carbon-1-1.jdf
Filename = NSS-19-47-1_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-19-47-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-NOV-2020 10:16:
Revision_Time = 31-DEC-2020 19:28:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 1.03809024[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.1[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]


O
Ph
N
N
O
Ph
H
5p
4.04
3.01
2.04
2.00
0.95
0.96
1.00
1.03
0.99
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-76-1_Proton_copy2-1-1.jdf
Filename = NSS-19-76-1_Proton_co
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-19-76-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-DEC-2020 17:46:30
Revision_Time = 31-DEC-2020 15:35:08
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 0[s]
X_Domain = Proton
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 3
Total_Scans = 3
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22.7[dC]
X_90_Width = 10.25[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 5.125[us]
Irr_Mode = Off
Tri_Mode = Off

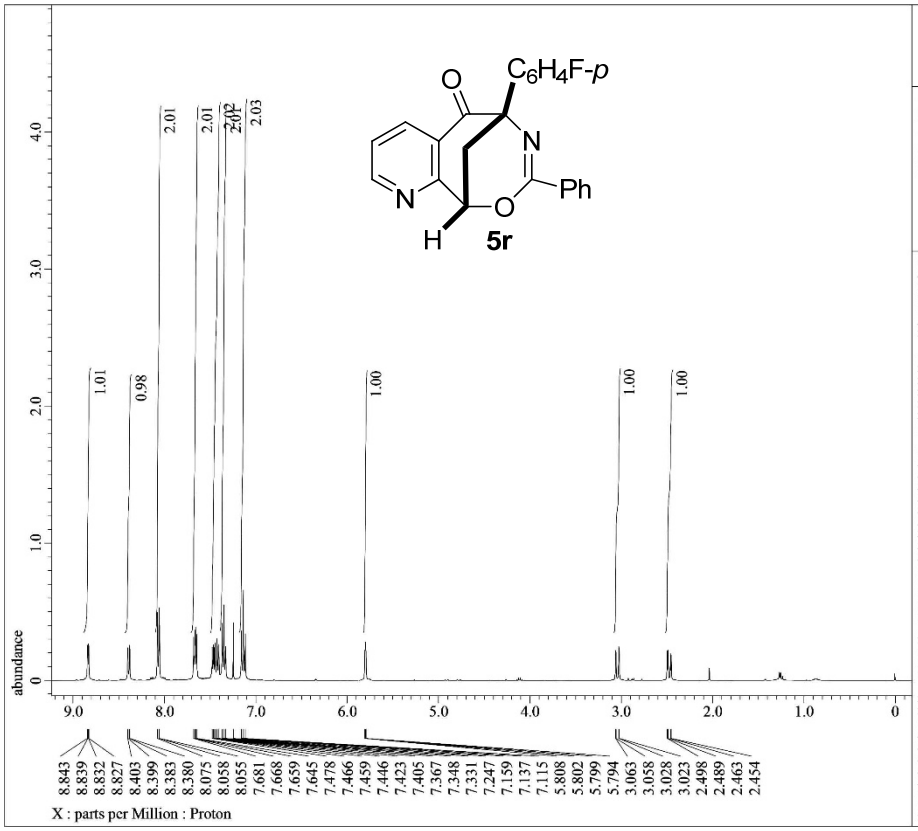

O
Ph
N
N
O
Ph
H
5p
abundance
X : parts per Million : Carbon13
192.109
158.186
155.582
154.442
141.382
137.083
133.100
131.386
128.313
128.188
127.729
127.671
127.288
126.235
125.392
77.461
77.250
77.040
73.229
62.658
33.637
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-19-76-1_Carbon_copy3-1-1.jdf
Filename = NSS-19-76-1_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-19-76-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-DEC-2020 19:25:
Revision_Time = 31-DEC-2020 20:29:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 48
Total_Scans = 48
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.3[dC]
X_90_Width = 8.6[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.8[dB]
X_Pulse = 2.86666667[us]
Irr_Atn_Dec = 16.132[dB]
Irr_Atn_Dec_Calc = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe = 16.132[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]

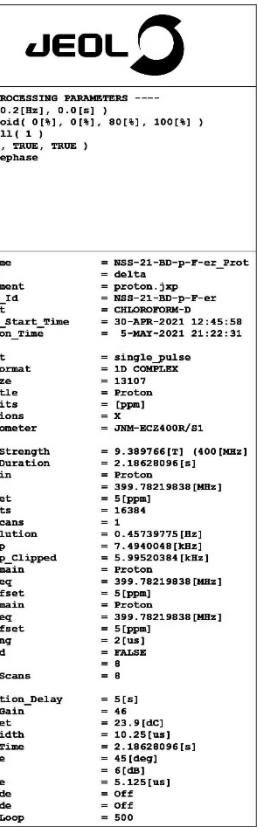



```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename                = NSS-21-BD-p-OMe-er_Pr
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = NSS-21-BD-p-OMe-er
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 30-APR-2021 12:36:27
Revision_Time           =  5-MAY-2021 21:33:29

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400R/S1

Field_Strength          = 9.389766[T] (400[MHz]
X_Acq_Duration          = 2.18628096[s]
X_Domain                = Proton
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45739775[Hz]
X_Sweep                 = 7.4940048[kHz]
X_Sweep_Clipped         = 5.99520384[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 46
Temp_Get                = 23.7[dC]
X_90_Width              = 10.25[us]
X_Acq_Time              = 2.18628096[s]
X_Angle                 = 45[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 5.125[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
```



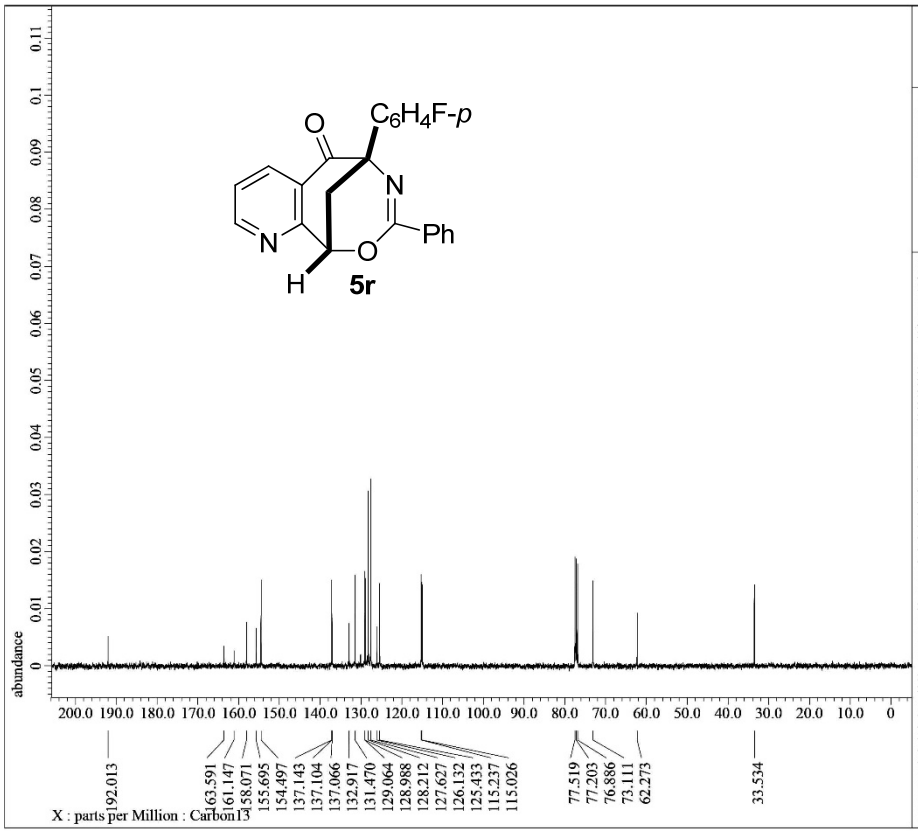

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename                = NSS-21-BD-p-OMe-er
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = NSS-21-BD-p-OMe-er
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 30-APR-2021 12:37:
Revision_Time           =  5-MAY-2021 23:56:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400R/S1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 0[s]
X_Domain                = Carbon13
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = TRUE
Incomplete_Copy         = TRUE
Scans                   = 39
Total_Scans             = 39

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 23.9[dC]
X_90_Width              = 9.323[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 9.1[dB]
X_Pulse                 = 3.10766667[us]
Irr_Atn_Dec             = 27[dB]
Irr_Atn_Dec_Calc        = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe             = 27[dB]
Irr_Dec_Bandwidth_Hz    = 4.7826087[kHz]
```

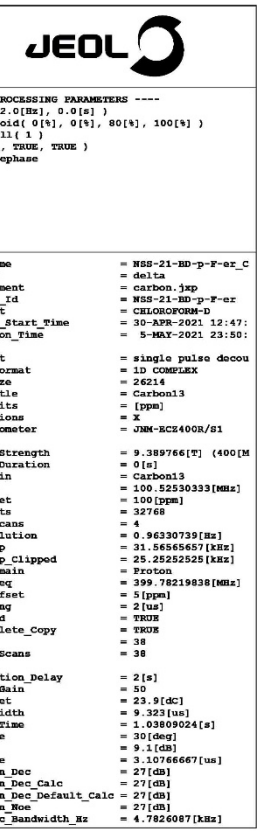




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

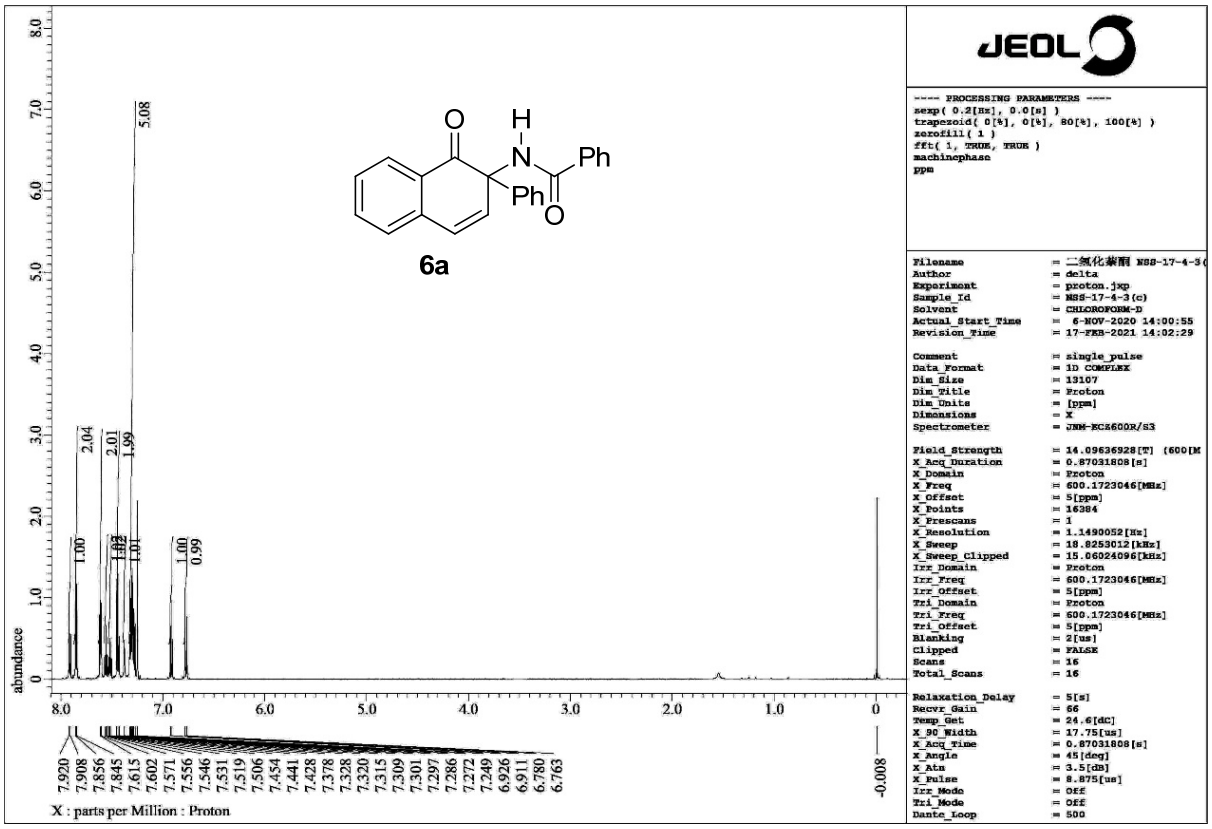
Filename	= NSS-21-BD-p-F-er_Prot
Author	= delta
Experiment	= proton.jxp
Sample_Id	= NSS-21-BD-p-F-er
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-APR-2021 12:45:58
Revision_Time	= 5-MAY-2021 21:22:31
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400R/S1
Field_Strength	= 9.389766[T] (400[MHz]
X_Acq_Duration	= 2.18628096[s]
X_Domain	= Proton
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45739775[Hz]
X_Sweep	= 7.4940048[kHz]
X_Sweep_Clipped	= 5.99520384[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 23.9[dC]
X_90_Width	= 10.25[us]
X_Acq_Time	= 2.18628096[s]
X_Angle	= 45[deg]
X_Atn	= 6[dB]
X_Pulse	= 5.125[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500

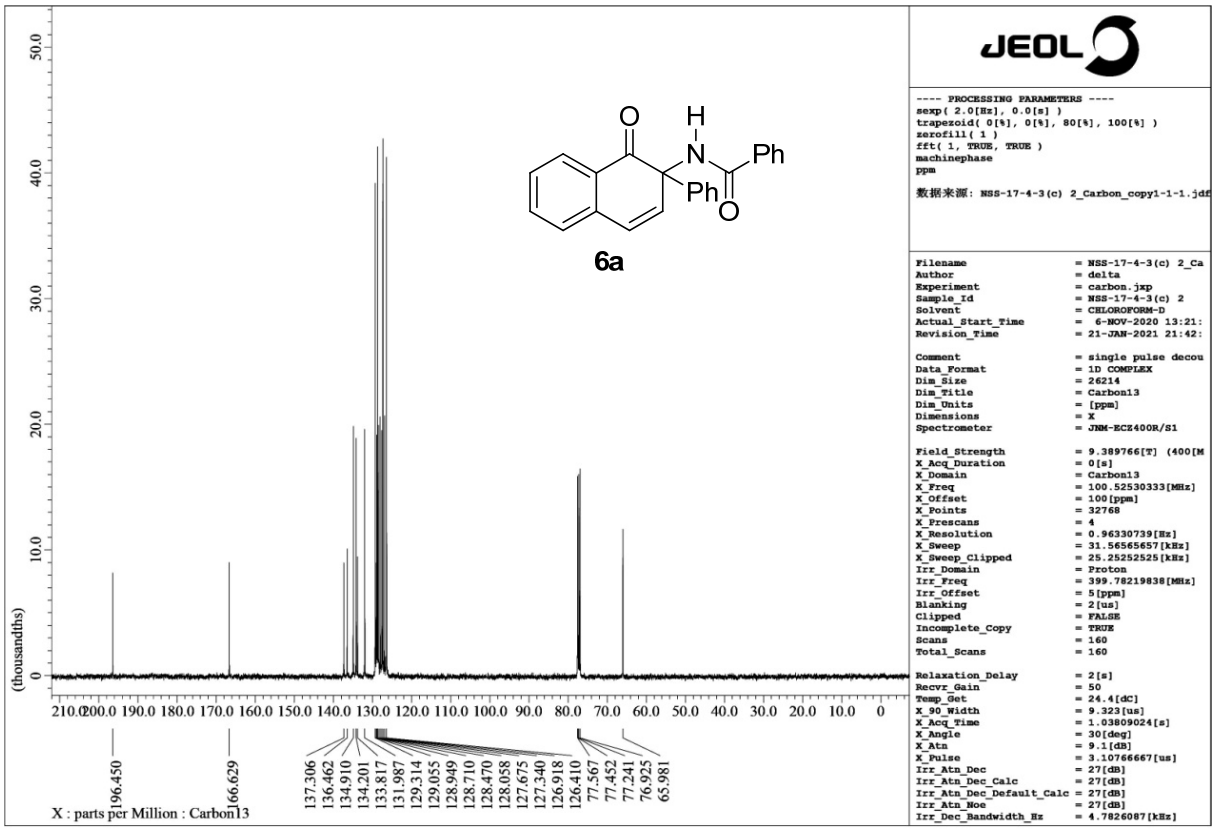


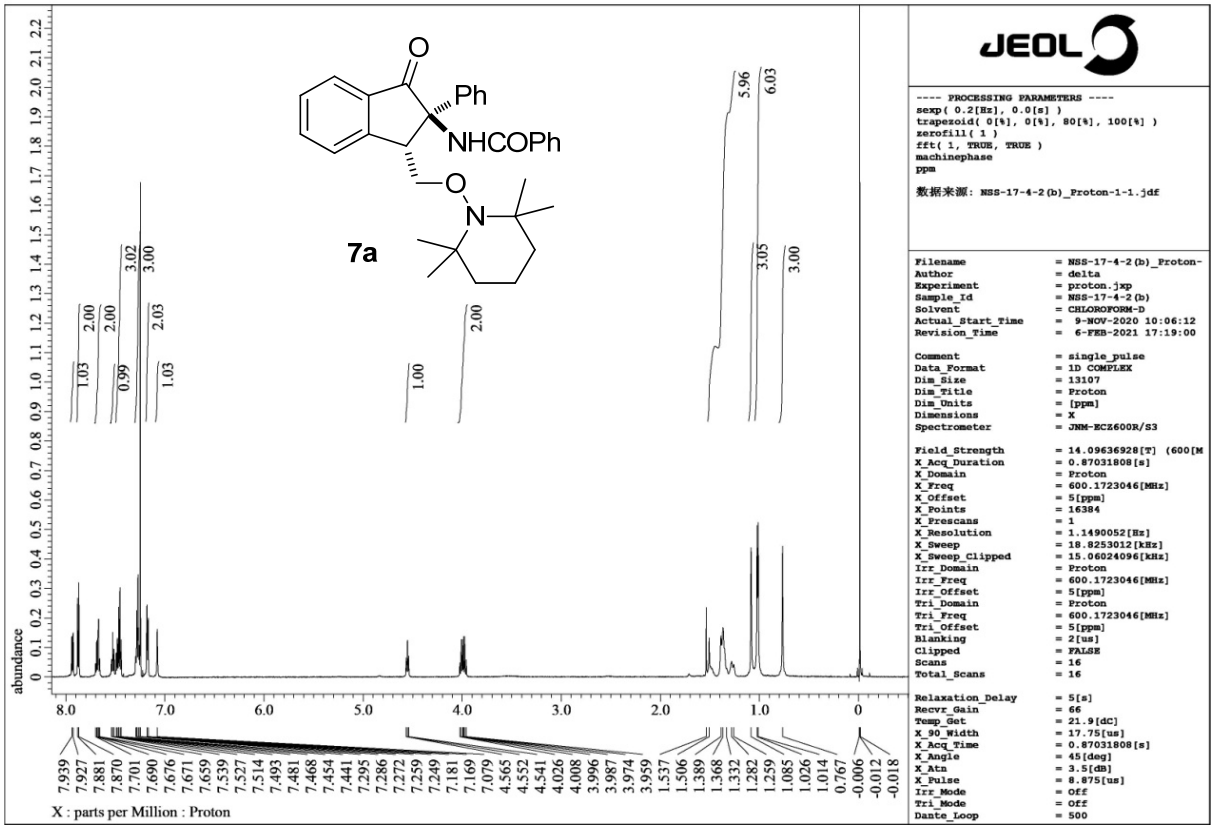


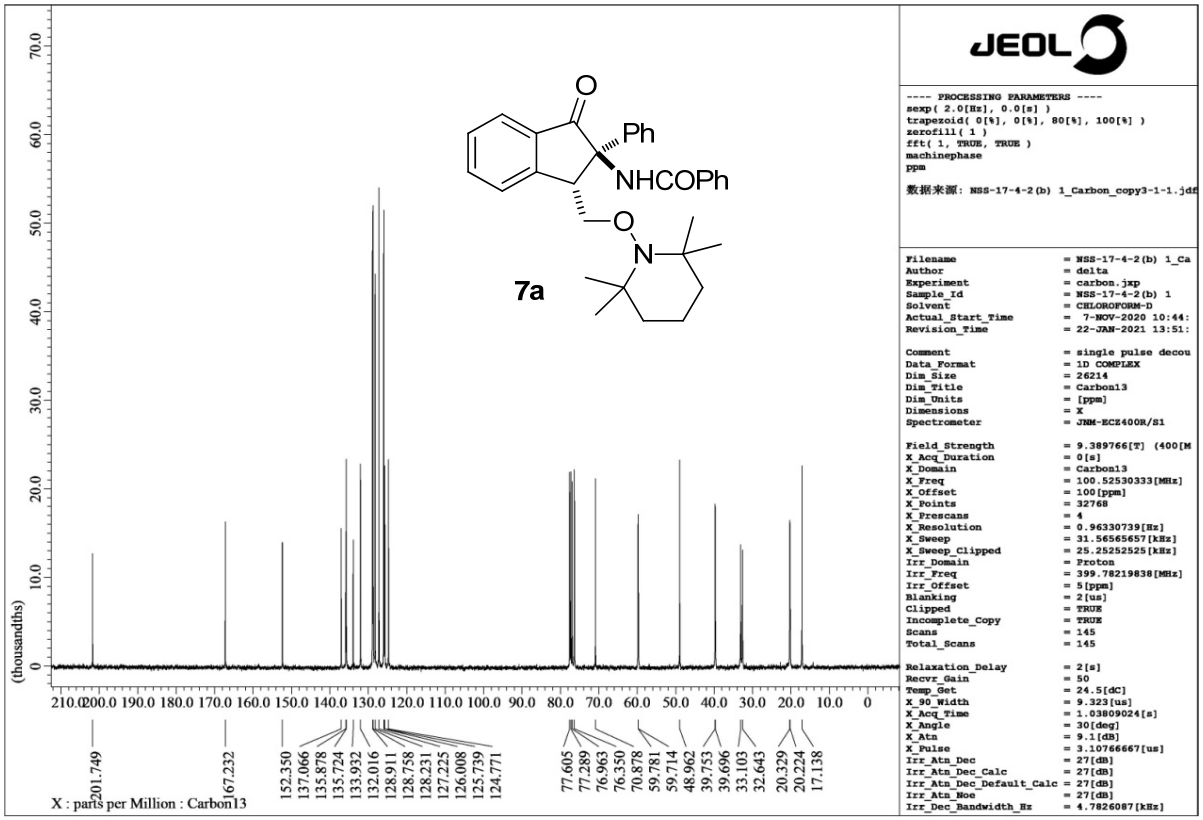
```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

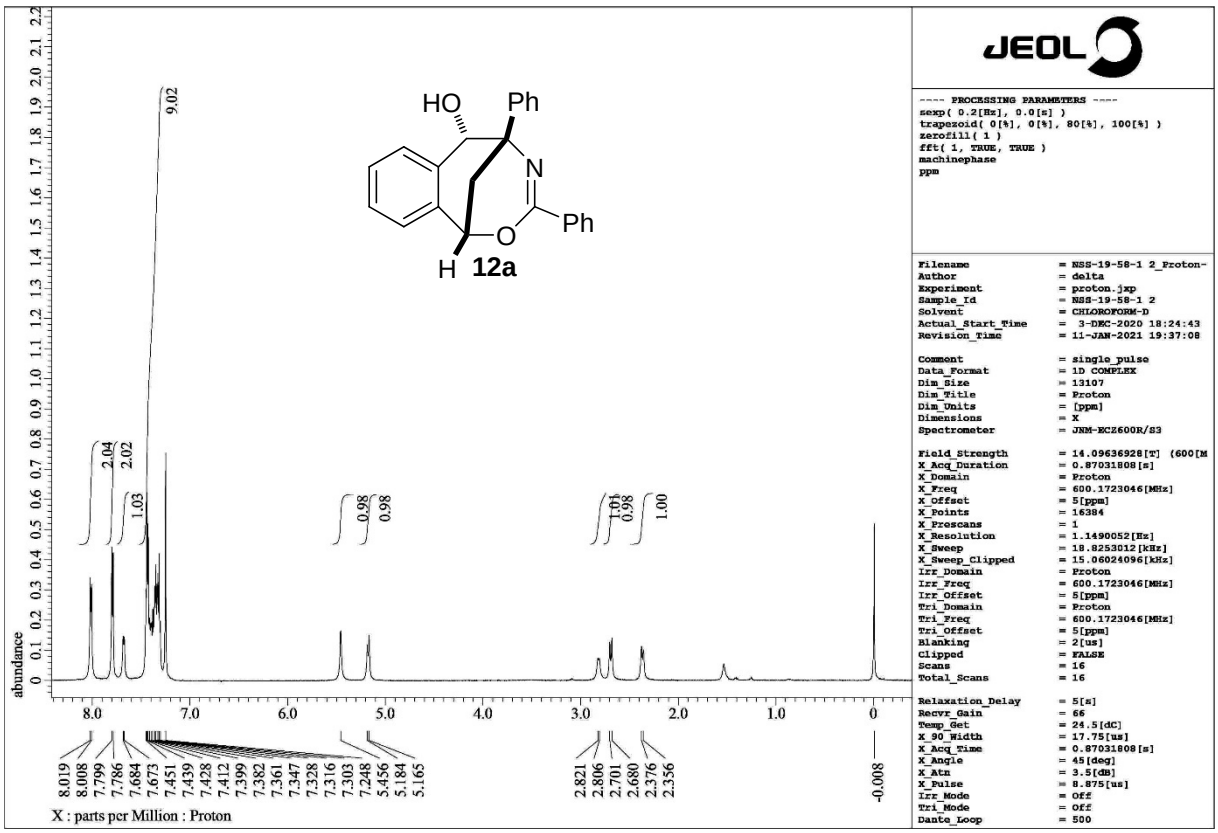
Filename	= NSS-21-BD-p-F-er_C
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= NSS-21-BD-p-F-er
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-APR-2021 12:47:
Revision_Time	= 5-MAY-2021 23:50:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400R/S1
Field_Strength	= 9.389766[T] (400[M
X_Acq_Duration	= 0[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Incomplete_Copy	= TRUE
Scans	= 38
Total_Scans	= 38
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 23.9[dC]
X_90_Width	= 9.323[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 9.1[dB]
X_Pulse	= 3.10766667[us]
Irr_Atn_Dec	= 27[dB]
Irr_Atn_Dec_Calc	= 27[dB]
Irr_Atn_Dec_Default_Calc	= 27[dB]
Irr_Atn_Noe	= 27[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]


6a
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 二氢化萘酮 NSS-17-4-3(
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-17-4-3(c)
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-NOV-2020 14:00:55
Revision_Time = 17-FEB-2021 14:02:29
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 19107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECS600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 24.6[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

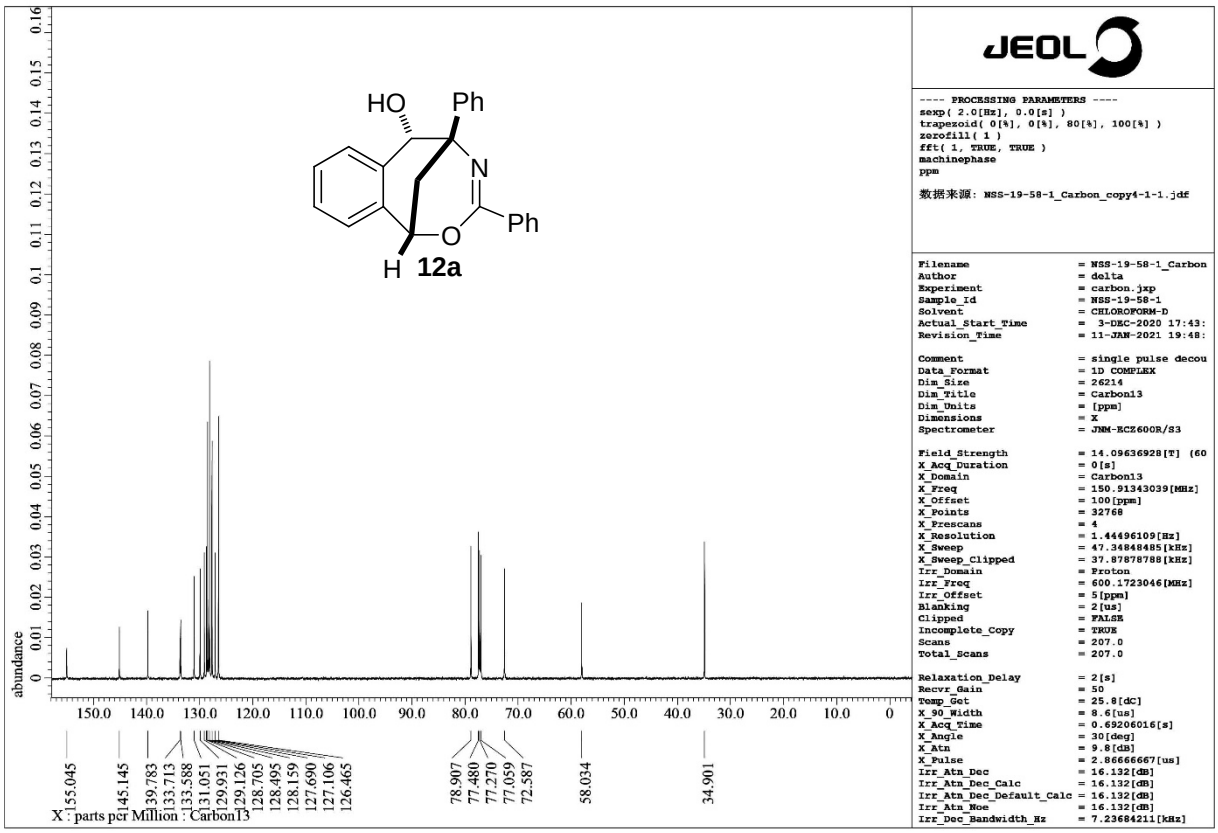

6a
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-17-4-3(c) 2_Carbon_copy1-1-1.jdf
Filename = NSS-17-4-3(c) 2_Ca
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-17-4-3(c) 2
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-NOV-2020 13:21:
Revision_Time = 21-JAN-2021 21:42:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 160
Total_Scans = 160
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.4[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]


O
Ph
NHCOPh
O
N
7a
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-17-4-2(b)_Proton-1-1.jdf
Filename = NSS-17-4-2(b)_Proton-
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-17-4-2(b)
Solvent = CHLOROFORM-D
Actual_Start_Time = 9-NOV-2020 10:06:12
Revision_Time = 6-FEB-2021 17:19:00
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 21.9[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

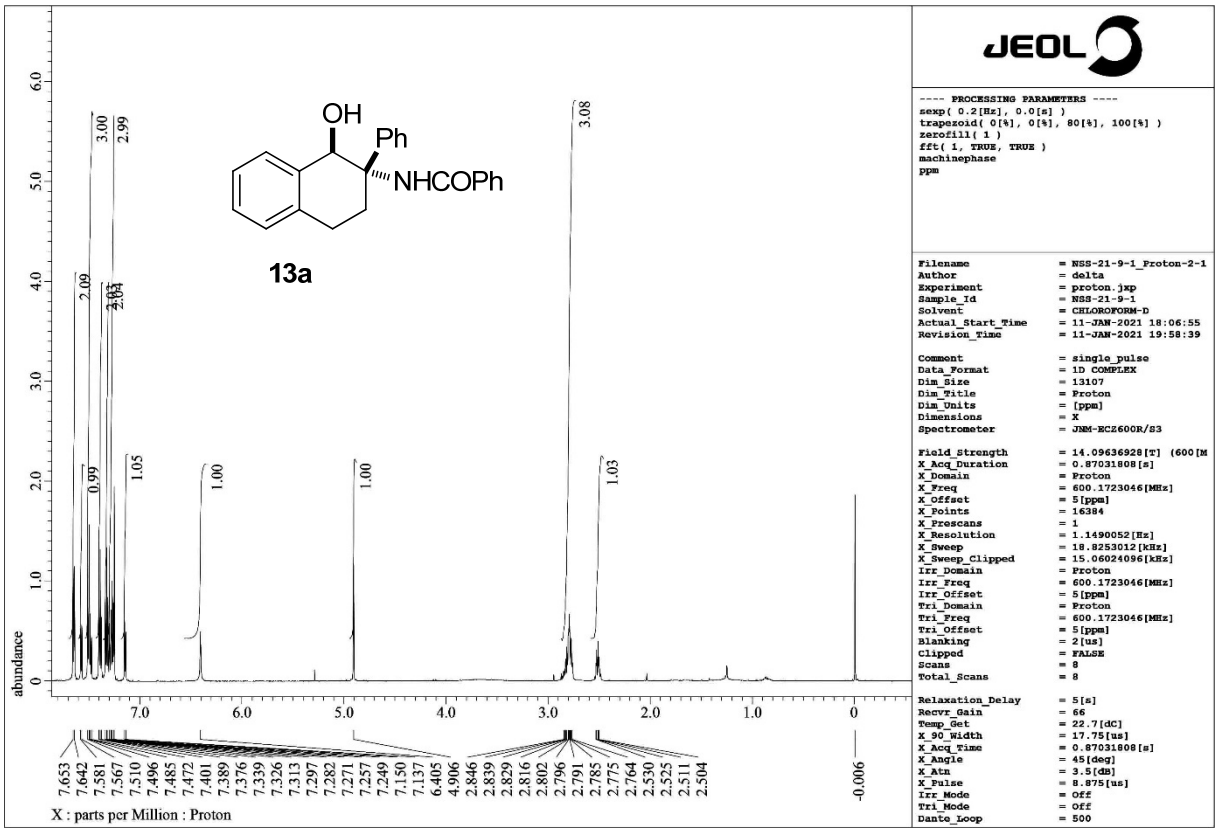

O
Ph
NHCOPh
O
N
7a
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-17-4-2(b) 1_Carbon_copy3-1-1.jdf
Filename = NSS-17-4-2(b) 1_Ca
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-17-4-2(b) 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-NOV-2020 10:44:
Revision_Time = 22-JAN-2021 13:51:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.7821938[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Incomplete_Copy = TRUE
Scans = 145
Total_Scans = 145
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.5[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]

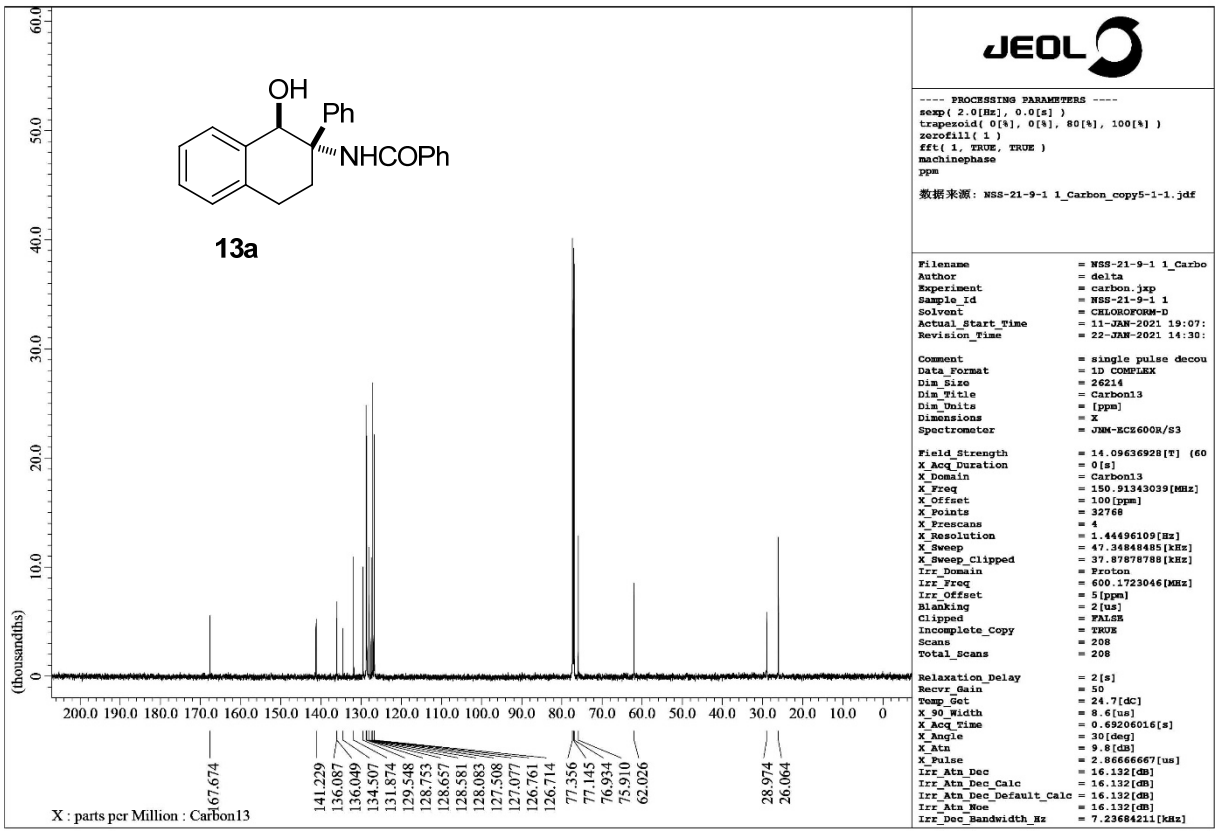


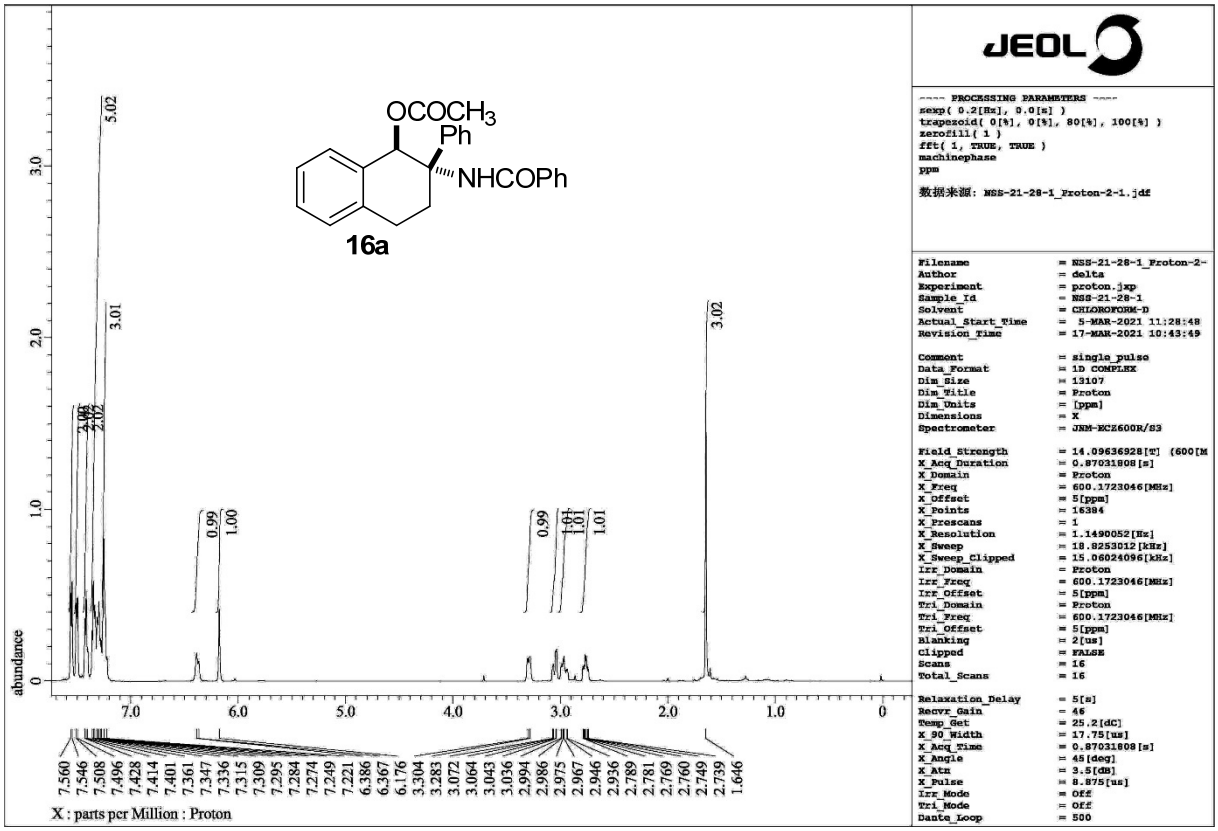

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename                = NSS-19-58-1 2_Proton-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = NSS-19-58-1 2
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  3-DEC-2020 18:24:43
Revision_Time           = 11-JAN-2021 19:37:08

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 0.87031808[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 1.1490052[Hz]
X_Sweep                 = 18.8253012[kHz]
X_Sweep_Clipped         = 15.06024096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 5[s]
Recvr_Gain              = 66
Temp_Get                = 24.5[dC]
X_90_Width              = 17.75[us]
X_Acq_Time              = 0.87031808[s]
X_Angle                 = 45[deg]
X_Atn                   = 3.5[dB]
X_Pulse                 = 8.875[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
```

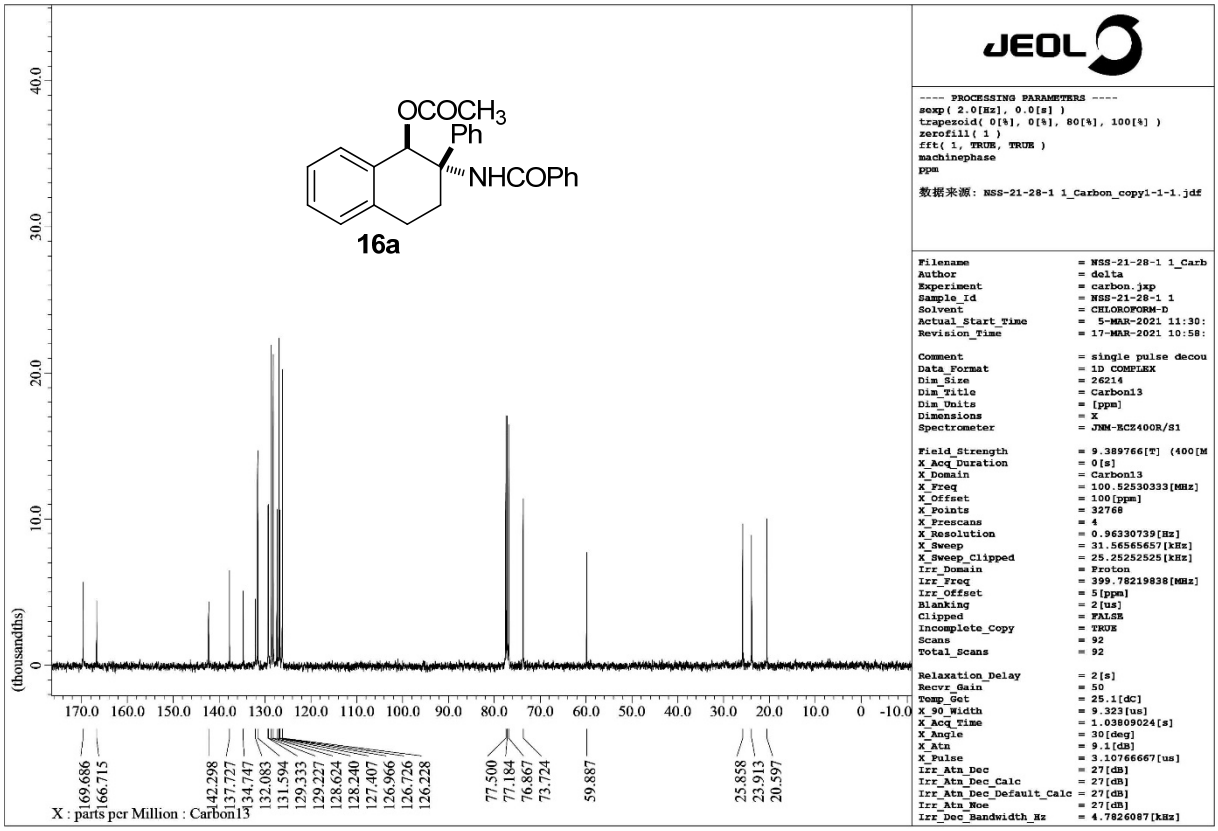


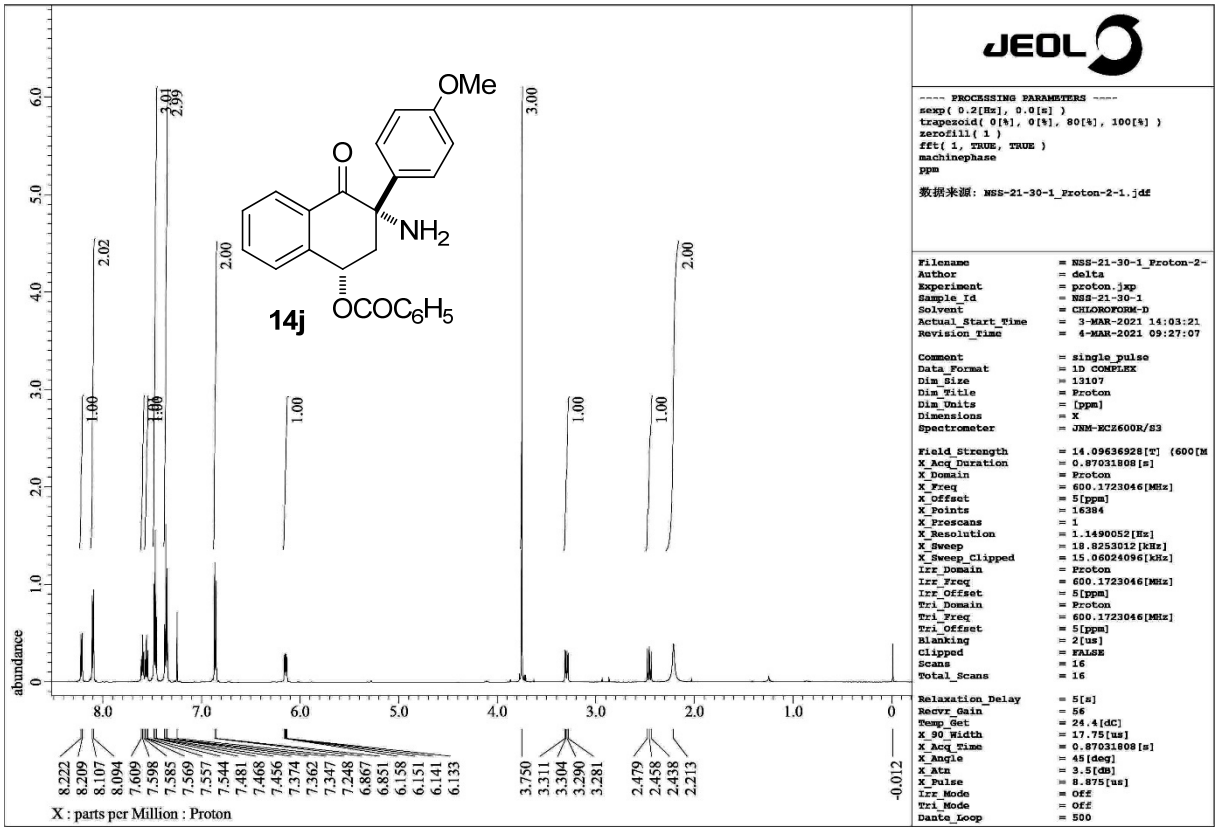

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-19-58-1_Carbon_copy4-1-1.jdf

Filename                = NSS-19-58-1_Carbon
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = NSS-19-58-1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  3-DEC-2020 17:43:
Revision_Time           = 11-JAN-2021 19:48:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ600R/S3

Field_Strength          = 14.09636928[T] (60
X_Acq_Duration          = 0[s]
X_Domain                = Carbon13
X_Freq                  = 150.91343039[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 1.44496109[Hz]
X_Sweep                 = 47.34848485[kHz]
X_Sweep_Clipped         = 37.87878788[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Incomplete_Copy         = TRUE
Scans                   = 207.0
Total_Scans             = 207.0

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 25.8[dC]
X_90_Width              = 8.6[us]
X_Acq_Time              = 0.69206016[s]
X_Angle                 = 30[deg]
X_Atn                   = 9.8[dB]
X_Pulse                 = 2.86666667[us]
Irr_Atn_Dec             = 16.132[dB]
Irr_Atn_Dec_Calc        = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe             = 16.132[dB]
Irr_Dec_Bandwidth_Hz    = 7.23684211[kHz]
```

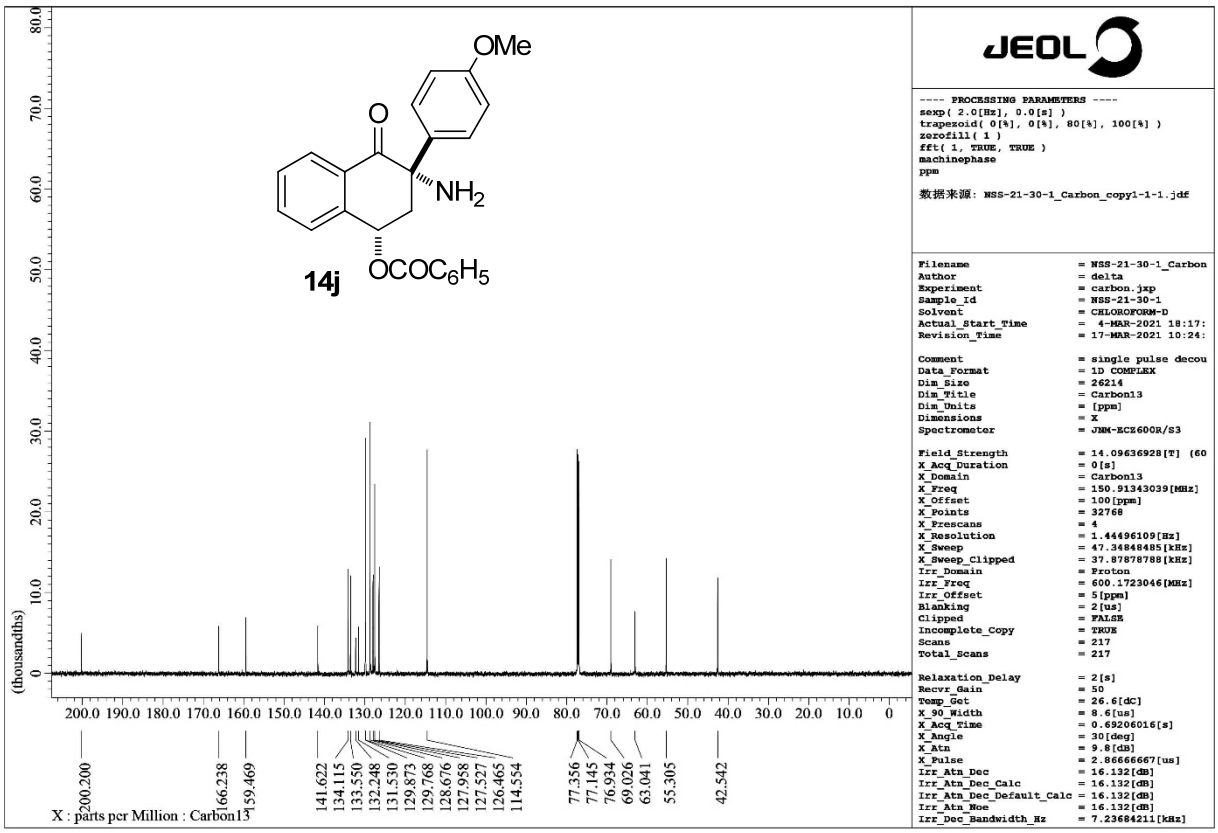

OH
Ph
NHCOPh
13a
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = NSS-21-9-1_Proton-2-1
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-21-9-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-JAN-2021 18:06:55
Revision_Time = 11-JAN-2021 19:58:39
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 66
Temp_Get = 22.7[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500

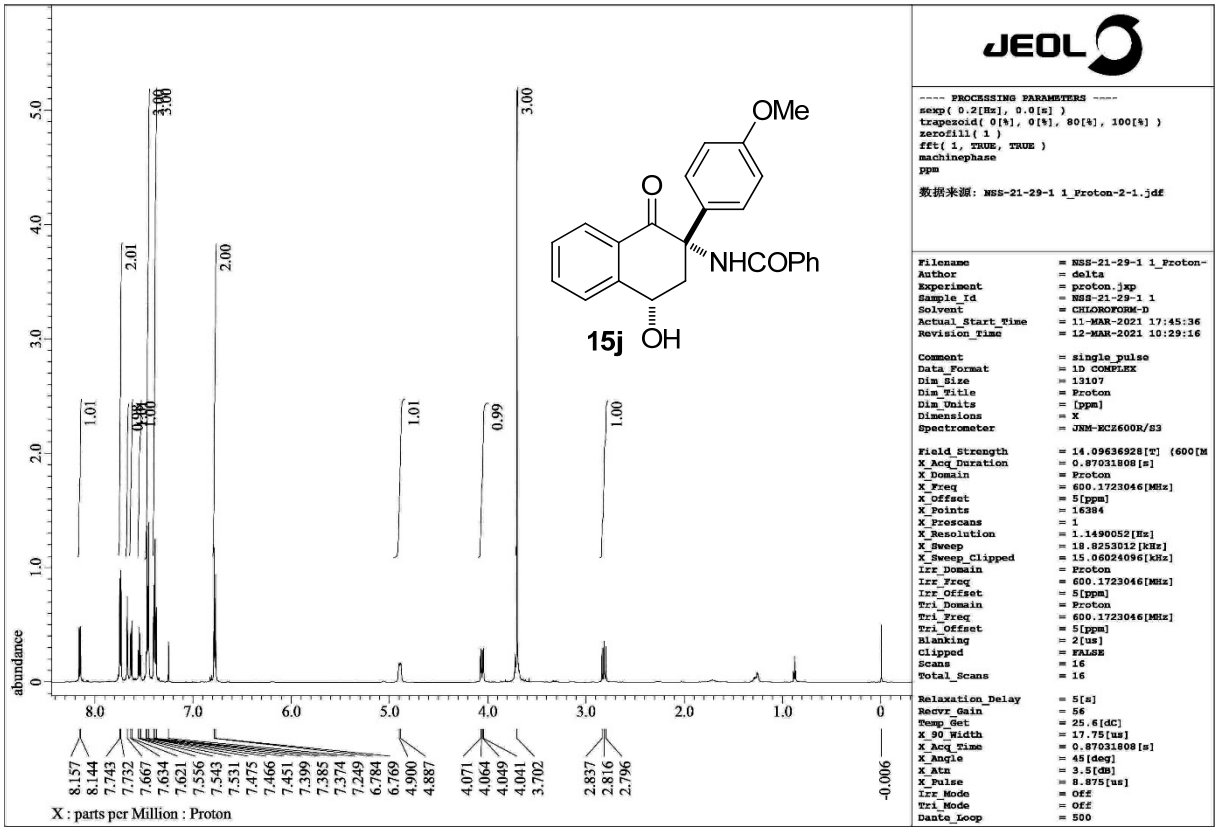

OH
Ph
NHCOPh
13a
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-21-9-1 1_Carbon_copy5-1-1.jdf
Filename = NSS-21-9-1 1_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-21-9-1 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-JAN-2021 19:07:
Revision_Time = 22-JAN-2021 14:30:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 208
Total_Scans = 208
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.7[dC]
X_90_Width = 8.6[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.8[dB]
X_Pulse = 2.86666667[us]
Irr_Atn_Dec = 16.132[dB]
Irr_Atn_Dec_Calc = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe = 16.132[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]


OCOCH3
Ph
NHCOPh
16a
5.02
3.01
3.02
0.99
1.00
0.99
1.01
1.01
1.01
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.560 7.546 7.508 7.496 7.428 7.414 7.401 7.361 7.347 7.336 7.315 7.309 7.295 7.284 7.274 7.249 7.221 6.386 6.367 6.176 3.304 3.283 3.072 3.064 3.043 3.036 2.994 2.986 2.975 2.967 2.946 2.936 2.789 2.781 2.769 2.760 2.749 2.739 1.646
X : parts per Million : Proton
JEOL
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-21-28-1_Proton-2-1.jdf
Filename = NSS-21-28-1_Proton-2-
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-21-28-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-MAR-2021 11:28:48
Revision_Time = 17-MAR-2021 10:43:49
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 25.2[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500


OCOCH3
Ph
NHCOPh
16a
(thousandths)
40.0
30.0
20.0
10.0
0
170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
169.686 166.715 142.298 137.727 134.747 132.083 131.594 129.333 129.227 128.624 128.240 127.407 126.966 126.726 126.228 77.500 77.184 76.867 73.724 59.887 25.858 23.913 20.597
X : parts per Million : Carbon13
JEOL
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-21-28-1 1_Carbon_copy1-1-1.jdf
Filename = NSS-21-28-1 1_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-21-28-1 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-MAR-2021 11:30:
Revision_Time = 17-MAR-2021 10:58:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 92
Total_Scans = 92
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.1[dC]
X_90_Width = 9.323[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 9.1[dB]
X_Pulse = 3.10766667[us]
Irr_Atn_Dec = 27[dB]
Irr_Atn_Dec_Calc = 27[dB]
Irr_Atn_Dec_Default_Calc = 27[dB]
Irr_Atn_Noe = 27[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]

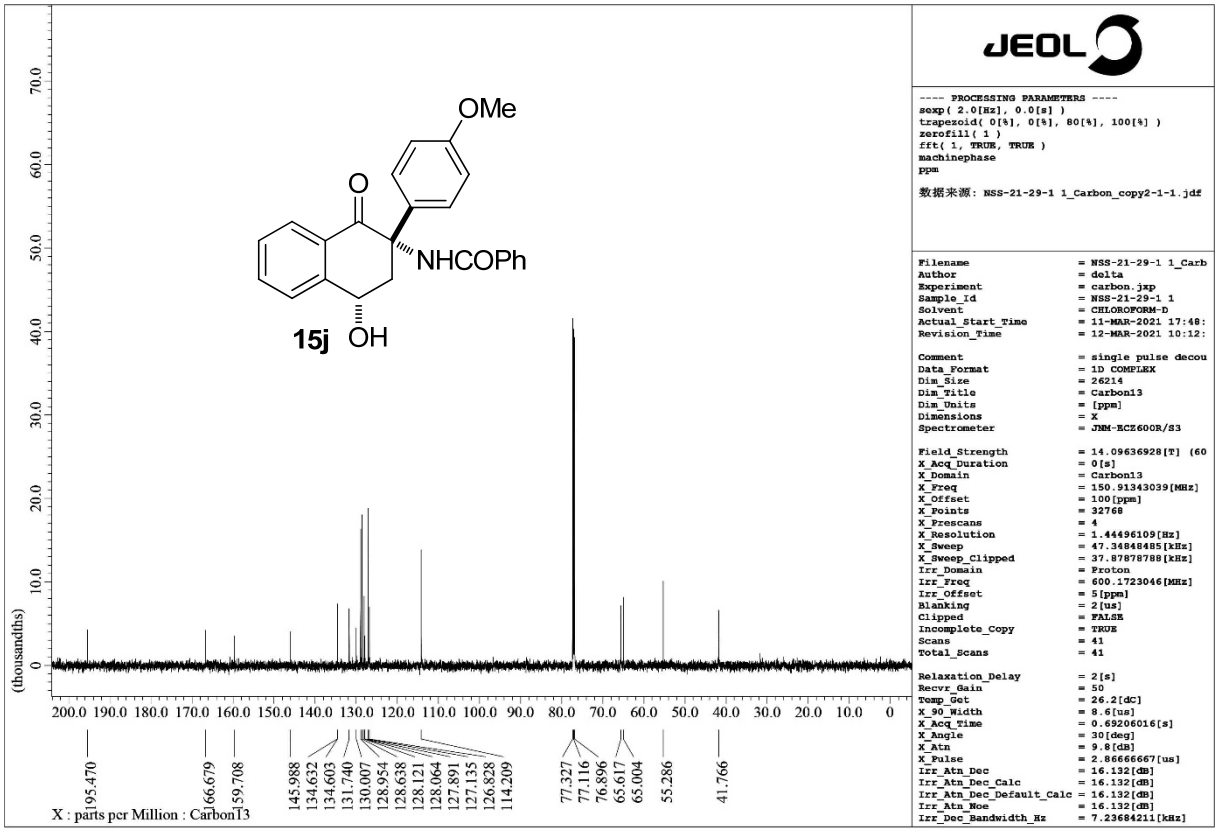

OMe
O
NH2
OCOC6H5
14j
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-21-30-1_Proton-2-1.jdf
Filename = NSS-21-30-1_Proton-2-
Author = delta
Experiment = proton.jxp
Sample_Id = NSS-21-30-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-MAR-2021 14:03:21
Revision_Time = 4-MAR-2021 09:27:07
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 0.87031808[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 1.1490052[Hz]
X_Sweep = 18.8253012[kHz]
X_Sweep_Clipped = 15.06024096[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 24.4[dC]
X_90_Width = 17.75[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 8.875[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500


OMe
O
NH2
OCOC6H5
14j
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: NSS-21-30-1_Carbon_copy1-1-1.jdf
Filename = NSS-21-30-1_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = NSS-21-30-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-MAR-2021 18:17:
Revision_Time = 17-MAR-2021 10:24:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 217
Total_Scans = 217
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 26.6[dC]
X_90_Width = 8.6[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.8[dB]
X_Pulse = 2.86666667[us]
Irr_Atn_Dec = 16.132[dB]
Irr_Atn_Dec_Calc = 16.132[dB]
Irr_Atn_Dec_Default_Calc = 16.132[dB]
Irr_Atn_Noe = 16.132[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-21-29-1 1_Proton-2-1.jdf
```

Filename	= NSS-21-29-1 1_Proton-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= NSS-21-29-1 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-MAR-2021 17:45:36
Revision_Time	= 12-MAR-2021 10:29:16
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 0.87031808[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 1.1490052[Hz]
X_Sweep	= 18.8253012[kHz]
X_Sweep_Clipped	= 15.06024096[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 25.6[dC]
X_90_Width	= 17.75[us]
X_Acq_Time	= 0.87031808[s]
X_Angle	= 45[deg]
X_Atn	= 3.5[dB]
X_Pulse	= 8.875[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: NSS-21-29-1 1_Carbon_copy2-1-1.jdf
```

Filename	= NSS-21-29-1 1_Carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= NSS-21-29-1 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-MAR-2021 17:48:
Revision_Time	= 12-MAR-2021 10:12:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Incomplete_Copy	= TRUE
Scans	= 41
Total_Scans	= 41
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 26.2[dC]
X_90_Width	= 8.6[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 9.8[dB]
X_Pulse	= 2.86666667[us]
Irr_Atn_Dec	= 16.132[dB]
Irr_Atn_Dec_Calc	= 16.132[dB]
Irr_Atn_Dec_Default_Calc	= 16.132[dB]
Irr_Atn_Noe	= 16.132[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]