Supporting Information

Construction of Enantiopure Imine Bridged Benzo[*c*]azepinones by a Silver (I) and Chiral N-Heterocyclic Carbene Multicatalytic Reaction Sequence of *N*'-(2-Alkynylbenzylidene)hydrazides and Cyclopropanecarbaldehydes

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1. General Information

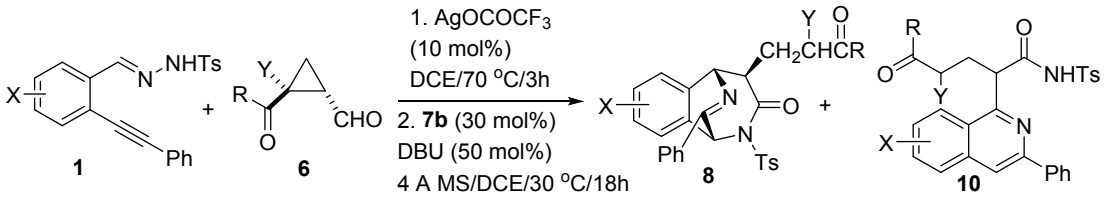
Commercially available chemical reagents were used without further purification. Anhydrous solvents were prepared by solvent purification system. Melting points were uncorrected. ^{1}H NMR (400 and 600 MHz) and ^{13}C NMR (100 and 150 MHz) were recorded in the indicated solvents using JEOL and Bruker 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 *N*'-(2-alkynylbenzylidene)hydrazides **1**[1] and cyclopropanecarbaldehydes **6** [2] were prepared based on the literature methods.

([1]. X. Cheng, X. Cao, J. Xuan, W.-J. Xiao, Silver (I)- and Base-Mediated [3 + 3]-Cycloaddition of C, N-Cyclic Azomethine Imines with Aza-oxyallyl Cations, *Org. Lett*. **2018**, *20*, 52−55. [2]. A. Hartikka, P. I. Arvidsson, Tetrazolic Acid Functionalized Dihydroindol: Rational Design of a Highly Selective Cyclopropanation Organocatalyst, *J. Org. Chem.* **2007**, *72*, 5874-5877.)

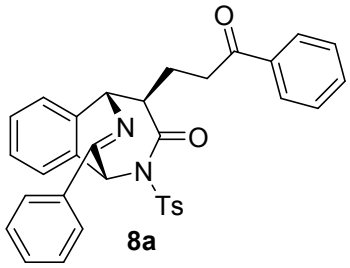
2. Experimental procedure for the reaction of *N*'-(2-alkynylbenzylidene)hydrazides with cyclopropanecarbaldehydes and characterization of products

General procedure for the enantioselective synthesis of 1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one derivatives 8 from Ag (I)/NHC catalyzed reaction of *N*'-(2-alkynylbenzylidene)hydrazides 1 and cyclopropanecarbaldehydes 6.



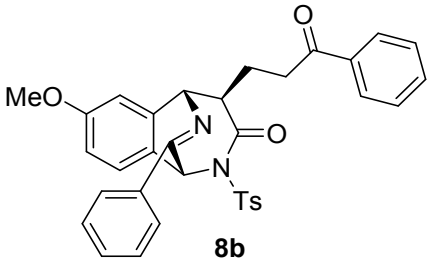
Under nitrogen atmosphere and at room temperature, $AgOCOCF_3$ (11 mg, 0.05 mmol, 0.1 equiv.), *N*'-(2-alkynylbenzylidene)hydrazides **1** (0.5 mmol), cyclopropanecarbaldehydes **6** (0.75 mmol, 1.5 equiv.) and dry dichloroethane (4 mL) were added successively to a dry Schlenk tube. The reaction mixture was stirred for 3 h at 70 °C. Then, under the protecting of nitrogen, chiral *N*-mesityl triazolium salt **7b** (73 mg, 0.15 mmol, 0.3 equiv.), activated 4A molecular sieve (300 mg), DBU (38 mg, 0.25 mmol, 0.5 equiv.) and dry dichloroethane (1 mL) were added to the test tube. In the sealed Schlenk tube, the reaction mixture was stirred

for another 18 h (30 h for the reaction of **1a** with 2-formylcyclopropane-1,1-dicarboxylate **6i**) at 30 °C. 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 acetone (petroleum ether : acetone from 5 : 1 to 4 : 1) to give the major 5,1-(azenometheno)benzo[*c*]azepin-3-one products **8** in 32-82% yields with ≥ 99% ee and minor isoquinoline products **10** in 6-24% yields. In some cases, a trace amount of pyrazolo[5,1-a]isoquinoline derivatives **11** was observed, but without isolation.



8a

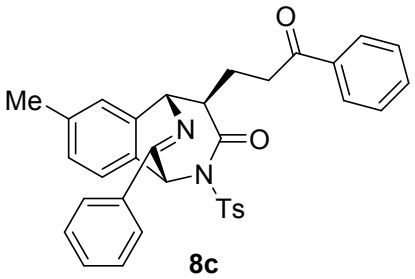
(*1R, 4R, 5S*)-4-(3-Oxo-3-phenylpropyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 8a: white solid, 74 % (202.7 mg); ee 99.8%; $[\alpha]^{20}_{D}$ = + 25.4 ° (*c* 0.5, CH_2Cl_2); mp 192-193 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.22 (d, *J* = 7.2 Hz, 2H), 7.86 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.52-7.60 (m, 5H), 7.39-7.43 (m, 3H), 7.33-7.36 (m, 2H), 7.13 (d, *J* = 8.4 Hz, 2H), 7.00 (s, 1H), 5.50 (d, *J* = 3.6 Hz, 1H), 3.13 (t, *J* = 7.8 Hz, 2H), 3.03 (td, *J* = 7.2, 3.6 Hz, 1H), 2.30-2.36 (m, 1H), 2.28 (s, 3H), 2.08-2.14 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.1, 171.8, 170.6, 144.7, 141.9, 136.8, 136.4, 135.1, 134.5, 132.9, 131.5, 129.1, 129.0, 128.9, 128.50, 128.47, 128.02, 127.97, 127.3, 126.6, 125.6, 63.1, 54.0, 50.4, 36.1, 26.8, 21.5; IR *v* (cm^{-1}) 1699, 1674; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{29}N_2O_4S$: 549.1842, found: 549.1840.



8b

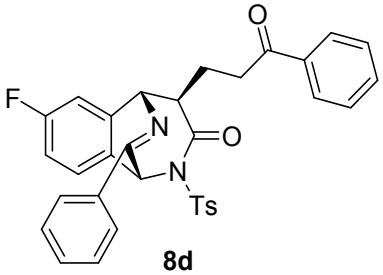
(*1R, 4R, 5S*)-7-Methoxy-4-(3-oxo-3-phenylpropyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-3H-5,1-(azenometheno)benzo[*c*]azepin-3-one 8b: white solid, 79% (228 mg); ee 99.9%; $[\alpha]^{20}_{D}$ = +30 ° (*c* 0.5, CH_2Cl_2); mp 138-139 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.21 (d, *J* = 7.2 Hz, 2H), 7.85 (d, *J* = 7.8 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.51-7.57 (m, 4H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.13 (d,

J = 8.4 Hz, 2H), 6.96 (d, *J* =1.8 Hz, 1H), 6.94 (s, 1H), 6.84 (dd, *J* = 8.4, 3.0 Hz, 1H), 5.42 (d, *J* = 3.0 Hz, 1H), 3.82 (s, 3H), 3.10-3.13 (m, 2H), 3.01 (td, *J* = 6.6, 3.0 Hz, 1H), 2.23-2.36 (m, 1H), 2.28 (s, 3H), 2.06-2.12 (m, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 199.3, 172.2, 171.1, 160.2, 144.8, 143.6, 136.8, 136.4, 135.1, 133.1, 131.6, 129.3, 129.1, 128.6, 128.1, 128.0, 127.4, 126.5, 113.5, 111.4, 63.4, 55.6, 54.0, 50.3, 36.2, 26.9, 21.6; IR *v* (cm^{-1}) 1688; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_5S$: 579.1948, found: 579.1946.



8c

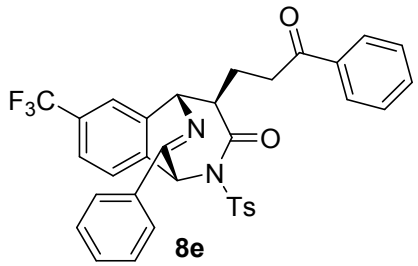
(*1R, 4R, 5S*)-7-Methyl-4-(3-oxo-3-phenylpropyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-3H-5,1-(azenometheno)benzo[*c*]azepin-3-one 8c: white solid, 82% (229.6 mg); ee 99.9%, $[\alpha]^{20}_D$ = +30.8 ^{o} (*c* 0.5, CH_2Cl_2); mp 126-127 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.21 (d, *J* = 7.6 Hz, 2H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 8.4 Hz, 2H), 7.51-7.57 (m, 4H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.40 (t, *J* = 8.0 Hz, 2H), 7.24 (s, 1H), 7.13 (d, *J* = 7.6 Hz, 3H), 6.95 (s, 1H), 5.43 (d, *J* = 2.8 Hz, 1H), 3.12 (t, *J* = 7.6 Hz, 2H), 3.01 (td, *J* = 6.4, 3.2 Hz, 1H), 2.36 (s, 3H), 2.29-2.35 (m, 1H), 2.29 (s, 3H), 2.04-2.14 (m, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 198.5, 172.1, 170.6, 145.0, 142.3, 139.0, 137.0, 136.8, 135.3, 133.0, 131.9, 131.5, 129.2, 128.9, 128.70, 128.65, 128.4, 127.9, 127.4, 126.9, 126.3, 62.0 , 54.5, 50.5, 35.9, 26.7, 20.6, 20.5; IR *v* (cm^{-1}) 1684; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_4S$: 563.1999, found: 563.2001.



8d

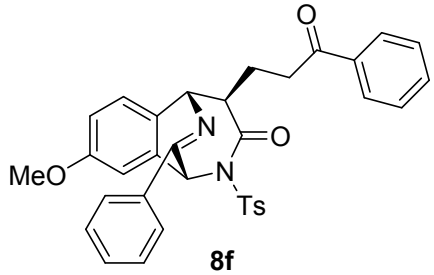
(1R, 4R, 5S)-7-Fluoro-4-(3-oxo-3-phenylpropyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-3H-5,1-(azenometheno)benzo[*c*]azepin-3-one 8d: white solid, 70% (197 mg); ee 99.7%, $[\alpha]^{20}_D$ = + 23.27 ^{o} (*c* 0.5, CH_2Cl_2); mp 165-166 ^{o}C; ^{1}H NMR (600 MHz,$CDCl_3$) δ (ppm) 8.22 (d, *J* = 7.8 Hz, 2H), 7.86 (d, *J* = 7.2 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.53-7.59 (m, 5H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.16 (dd, *J* = 8.4, 3.0 Hz, 1H), 7.14 (d, *J* = 7.8 Hz, 2H), 7.04 (td, *J* = 7.8, 1.8 Hz, 1H), 7.00 (s, 1H), 5.47 (d, *J* = 3.0 Hz, 1H), 3.11-3.13 (m,

2H), 3.03 (td, *J* = 7.2, 3.6 Hz, 1H), 2.30-2.35 (m, 1H), 2.30 (s, 3H), 2.07-2.13 (m, 1H); ^{13}C NMR (150 MHz, CD_3COCD_3) δ (ppm) 198.4, 171.7, 170.7, 162.6 (d, *J* = 246.9 Hz), 145.1, 145.0 (d, *J* = 8.6 Hz), 137.0, 136.7, 135.0, 133.0, 131.7, 131.0 (d, *J* = 1.9 Hz), 129.3, 129.2, 129.0, 128.7, 128.6, 127.9, 127.5, 114.6 (d, *J* = 21.5 Hz), 113.1 (d, *J* = 23.0 Hz), 61.8, 54.1, 49.9, 35.8, 26.5, 20.6; IR *v* (cm^{-1}) 1697, 1676; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{28}FN_2O_4S$: 567.1748, found: 567.1745.



8e

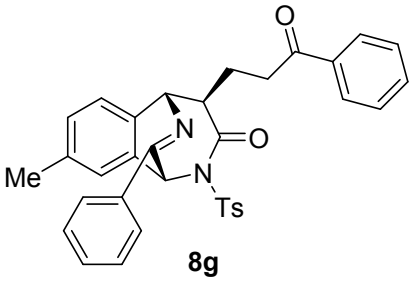
(*1R, 4R, 5S*)-4-(3-Oxo-3-phenylpropyl)-11-phenyl-2-tosyl-7-(trifluoromethyl)-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 8e: white solid, 32% (99 mg); ee 99.3%; $[\alpha]^{20}_D$ = +20.47 ^{o} (*c* 0.5, CH_2Cl_2); mp 92-93 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.21 (d, *J* = 6.6 Hz, 2H), 7.86 (d, *J* = 7.2, Hz, 2H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.71 (s, 1H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.54 (t, *J* = 7.2 Hz, 3H), 7.41 (t, *J* = 7.8 Hz, 2H), 714 (d, *J* = 9.0 Hz, 2H), 7.07 (s, 1H), 5.58 (d, *J* = 3.0 Hz, 1H), 3.08-3.18 (m, 2H), 3.05 (td, *J* =6.0, 2.4 Hz, 1H), 2.27-2.37 (m, 1H), 2.30 (s, 3H), 2.08-2.14 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.1, 171.3, 170.3, 145.2, 142.8, 138.4, 136.7, 136.0, 134.7, 133.2, 132.0, 131.3 (q, *J* = 32.6 Hz), 129.4, 129.2, 128.7, 128.6, 128.1, 127.4, 127.2, 125.2 (d, *J* = 3.8 Hz), 123.7 (q, *J* = 271.2 Hz), 122.8 (d, *J* = 3.8 Hz), 62.8, 53.8, 49.8, 36.1, 26.7, 21.6; IR *v* (cm^{-1}) 1686; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{28}F_3N_2O_4S$: 617.1716, found: 617.1718.



8f

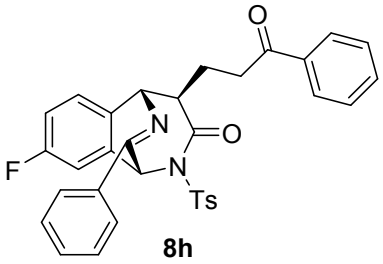
(*1R, 4R, 5S*)-8-Methoxy-4-(3-oxo-3-phenylpropyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-3H-5,1-(azenometheno)benzo[*c*]azepin-3-one 8f: white solid, 35% (101.2 mg); ee 99.9 %; $[\alpha]^{20}_D$ = +50.8 ^{o} (*c* 0.5, CH_2Cl_2); mp 202-203 ^{o}C; ^{1}H NMR (600 MHz,$CDCl_3$) δ (ppm) 8.21 (d, *J* = 6.6 Hz, 2H), 7.85 (d, *J* = 7.8 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.52-7.57 (m, 4H), 7.40 (t, *J* = 8.4 Hz 2H), 7.32 (d, *J* = 7.8 Hz 1H), 7.13 (d, *J* = 9.6 Hz, 2H) , 7.12 (d, *J* = 2.4 Hz, 1H), 6.93 (s, 1H), 6.86 (dd, *J* = 8.4, 2.4 Hz, 1H), 5.43 (d, *J* = 2.4Hz,

1H), 3.84 (s, 3H), 3.10 (t, *J* = 7.2 Hz, 2H), 3.01 (td, *J* = 6.0, 2.4 Hz 1H), 2.27-2.32 (m, 1H), 2.29 (s, 3H), 2.04-2.10 (m, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 198.5, 172.2, 170.2, 159.5, 145.1, 137.0, 136.8, 136.1, 135.3, 134.1, 133.0, 131.5, 129.2, 128.9, 128.8, 128.6, 127.9, 127.4, 126.8, 114.7, 112.3, 61.3, 55.2, 54.8, 50.9, 35.9, 26.2, 20.6; IR *v* (cm^{-1}) 1686; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{30}N_2O_5S$: 579.1948, found: 579.1950.



8g

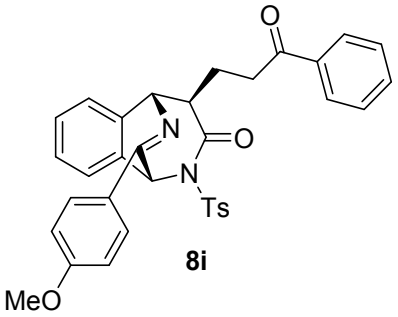
(*1R, 4R, 5S*)-8-Methyl-4-(3-oxo-3-phenylpropyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-3H-5,1-(azenometheno)benzo[*c*]azepin-3-one 8g: white solid, 65% (182.6 mg); ee 99.9%; $[\alpha]^{20}_D$ = +48 ^{o} (*c* 0.5, CH_2Cl_2); mp 222-223 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.22 (d, *J* = 7.2 Hz, 2H), 7.85 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 7.8 Hz, 2H), 7.52-7.57 (m, 4H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.40 (s, 1H), 7.30 (d, *J* = 7.8 Hz, 1H), 7.14 (d, *J* = 7.2 Hz, 1H), 7.12 (d, *J* = 8.4 Hz, 2H), 6.94 (s, 1H), 5.45 (d, *J* = 3.0 Hz, 1H), 3.10 (t, *J* = 7.2 Hz, 2H), 3.01 (td, *J* = 6.6, 3.0 Hz 1H), 2.38 (s, 3H), 2.28-2.33 (m, 1H), 2.28 (s, 3H), 2.05-2.17 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 199.2, 172.1, 170.6, 144.8, 138.9, 138.0, 136.8, 136.3, 135.2, 134.5, 133.1, 131.6, 129.5, 129.2, 129.1, 128.61, 128.58, 128.1, 127.4, 125.5, 62.8, 54.3, 50.6, 36.2, 26.8, 21.6, 21.3; IR *v* (cm^{-1}) 1699, 1670; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{30}N_2O_4S$: 563.1999, found: 563.2001.



8h

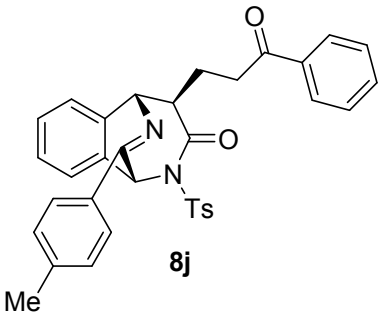
(*1R, 4R, 5S*)-8-Fluoro-4-(3-oxo-3-phenylpropyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-3H-5,1-(azenometheno)benzo[*c*]azepin-3-one 8h: white solid, 61% (173.5 mg); ee 99.8%; $[\alpha]^{20}_D$ = +19.2 ^{o} (*c* 0.5, CH_2Cl_2); mp 155-156 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.20 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.86 (dd, *J* = 8.4, 0.8 Hz, 2H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.52-7.58 (m, 4H), 7.38-7.43 (m, 3H), 7.31 (dd, *J* = 8.0, 2.4 Hz ,1H), 7.15 (d, *J* = 7.6Hz, 2H), 7.04 (td, *J* = 8.8, 2.8 Hz 1H) , 6.96 (s, 1H), 5.50 (d, *J* = 3.2 Hz, 1H), 3.12

(td, *J* = 7.2, 2.8 Hz, 2H), 3.02 (td, *J* = 6.8, 3.2 Hz, 1H), 2.27-2.36 (m, 1H), 2.29 (s, 1H), 2.05-2.14 (m, 1H); $^{13}C\{^{1}H\}$ NMR (150 MHz, CD_3COCD_3) δ (ppm) 198.5, 171.8, 170.2, 162.0 (d, *J* = 224.2 Hz), 145.2, 138.4, 137.0, 136.9, 136.6, 135.0, 133.0, 131.6, 129.3, 129.0, 128.7, 128.6, 127.9, 127.8 (d, *J* = 8.6 Hz), 127.5, 115.5 (d, *J* = 21.6 Hz), 114.2 (d, *J* = 23.0 Hz), 61.3, 54.5, 50.2, 35.8, 26.6, 20.6; IR *v* (cm^{-1}) 1701, 1670; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{27}FN_2O_4S$: 567.1748, found: 567.1738.



8i

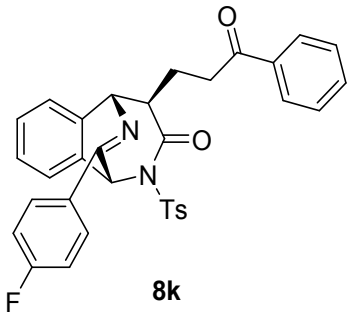
(*1R, 4R, 5S*)-11-(4-Methoxyphenyl)-4-(3-oxo-3-phenylpropyl)-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 8i: white solid, 76% (219.6 mg); ee 99.8%; $[\alpha]^{20}_D$ = +11.53 ^{o} (*c* 0.5, CH_2Cl_2); mp169-170 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.21 (d, *J* = 5.6 Hz, 2H), 7.86 (d, *J* =7.6 Hz, 2H), 7.68 (d, *J* = 8.4 Hz, 2H), 7.58-7.60 (m, 1H), 7.53(t, *J* = 7.2 Hz ,1H), 7.39-7.43 (m, 3H), 7.33-7.35 (m, 2H) , 7.13 (d, *J* = 8.8 Hz, 2H), 7.04 (d, *J* = 8.8 Hz, 2H), 6.98 (s, 1H) , 5.44 (d, *J* = 2.4 Hz, 1H), 3.91 (s, 3H), 3.10-3.14 (m, 2H), 3.00-3.04 (m, 1H), 2.30-2.37 (m, 1H), 2.28 (s, 3H), 2.06-2.15 (m, 1H); ^{13}C NMR (150 MHz, CD_3COCD_3) δ (ppm) 198.6, 172.0, 170.0, 162.7, 145.0, 142.6, 137.0, 136.8, 134.9, 133.0, 129.19, 129.17, 128.9, 128.7, 128.6, 127.93, 127.86, 127.7, 127.0, 125.7, 114.3, 61.8, 55.1, 54.4, 50.4, 35.9, 26.7, 20.6; IR *v* (cm^{-1}) 1686, 1672; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_5S$: 579.1948, found: 579.1945.



8j

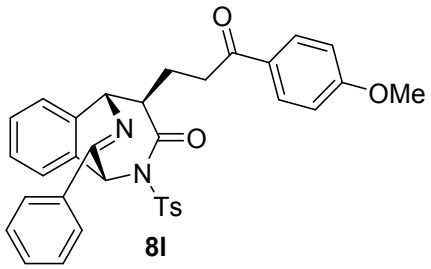
(*1S, 4R, 5S*)-4-(3-Oxo-3-phenylpropyl)-11-(*p*-tolyl)-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 8j: white solid, 71% (199.7 mg); ee 99.6%; $[\alpha]^{20}_D$ = +15.13 ^{o} (*c* 0.5, CH_2Cl_2); mp 203-204 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.11 (d, *J* = 8.4 Hz, 2H), 7.85 (d, *J* = 7.6 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.57-7.60 (m, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.36-7.42 (m, 3H), 7.33-7.35

(m, 4H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.98 (s, 1H) , 5.46 (d, *J* = 3.2 Hz, 1H), 3.11 (t, *J* = 6.8 Hz, 2H), 3.01 (td, *J* = 6.8, 3.2 Hz, 1H), 2.45 (s, 3H) , 2.30-2.36 (m, 1H), 2.28 (s, 3H), 2.05-2.14 (m, 1H); ^{13}C NMR (150 MHz, CD_3COCD_3) δ (ppm) 198.5, 171.9, 170.2, 145.0, 142.4, 142.0, 137.0, 136.8, 134.9, 133.0, 132.6, 129.6, 129.2, 128.9, 128.7, 128.6, 127.9, 127.4, 127.0, 125.7, 61.9, 54.4, 50.5, 35.9, 26.7, 20.6, 20.5; IR *v* (cm^{-1}) 1692,1674; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_4S$: 563.1999, found: 563.2001.



8k

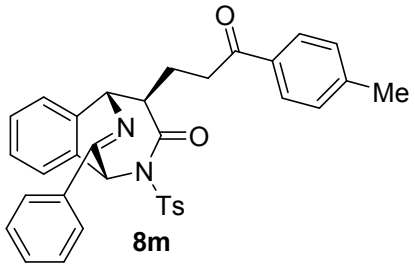
(*1S, 4R, 5S*)-11-(4-Fluorophenyl)-4-(3-oxo-3-phenylpropyl)-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 8k: white solid, 75% (212.2 mg); ee 99%; $[\alpha]^{20}_D$ = +37.13 ^{o} (*c* 0.5, CH_2Cl_2); mp197-198 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$,) δ (ppm) 8.23-8.27 (m, 2H), 7.87 (d, *J* = 8.0 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.57-7.59 (m, 1H), 7.54 (t, *J* = 7.2 Hz , 1H), 7.39-7.43 (m, 3H), 7.33-7.36 (m, 2H), 7.21 (t, *J* = 8.8 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H) , 6.95 (s, 1H), 5.48 (d, *J* = 2.4 Hz, 1H), 3.07-3.21 (m, 2H), 3.02 (td, *J* = 6.4, 2.8 Hz, 1H), 2.28-2.37 (m, 1H), 2.30 (s, 3H), 2.06-2.15 (m, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 198.5, 171.9, 169.5, 165.0 (d, *J* = 249.2 Hz), 145.1, 142.2, 137.0, 136.7, 134.6, 133.0, 131.6 (d, *J* = 2.8 Hz), 129.9 (d, *J* = 8.6 Hz), 129.2, 129.0, 128.7, 128.65, 128.0, 127.9, 127.1, 125.7, 115.8 (d, *J* = 22 Hz), 61.9, 54.5, 50.6, 35.8, 26.6, 20.6; IR *v* (cm^{-1}) 1713, 1674; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{28}FN_2O_4S$: 567.1748, found: 567.1745.



8l

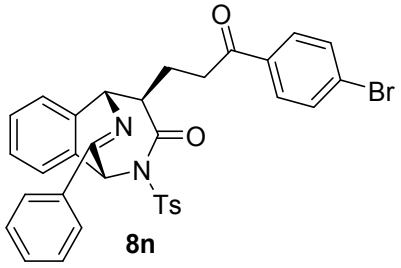
(*1R, 4R, 5S*)-4-(3-Oxo-3-(*p*-methoxyphenyl)propyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 8l: white solid, 67 % (193.6 mg); ee 99.7%; $[\alpha]^{20}_D$ = +8.27 ^{o} (*c* 0.5, CH_2Cl_2); mp 94-95 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.22 (dd, *J* = 8.4, 2.0 Hz, 2H), 7.85 (d, *J* = 8.8 Hz, 2H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.51-7.60 (m, 4H), 7.41-7.44 (m,1H), 7.33-7.35 (m, 2H), 7.13 (d, *J* = 8.4 Hz, 2H), 7.00 (s, 1H), 6.87 (d, *J* = 9.2 Hz, 2H), 5.50 (d, *J* = 3.2 Hz, 1H), 3.86 (s, 3H), 3.06-3.16 (m,

2H), 3.02 (td, *J* = 6.4, 3.2 Hz, 1H), 2.26-2.35 (m, 1H), 2.30 (s, 3H), 2.05-2.14 (m, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 197.0, 171.9, 170.5, 163.6, 145.0, 142.3, 136.8, 135.3, 134.8, 131.5, 130.2, 130.0, 129.2, 129.0, 128.9, 128.7, 127.9, 127.4, 127.1, 125.7, 113.8, 61.9, 55.1, 54.5, 50.6, 35.5, 27.0, 20.6; IR *v* (cm^{-1}) 1686, 1678; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_5S$: 579.1948, found: 579.1951.



8m

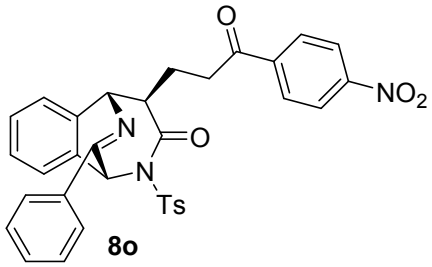
(*1R, 4R, 5S*)-4-(3-Oxo-3-(*p*-methylphenyl)propyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 8m: white solid, 75 % (211.4 mg); ee 99.7%; $[\alpha]^{20}_D$ = +12.6 ^{o} (*c* 0.5, CH_2Cl_2); mp 124-125 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.22 (d, *J* = 7.2 Hz, 2H), 7.76 (d, *J* = 7.8 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.52- 7.60 (m, 4H), 7.42-7.43 (m,1H), 7.32-7.37 (m, 2H), 7.20 (d, *J* = 7.8 Hz, 2H), 7.13 (d, *J* = 7.8 Hz, 2H), 7.00 (s, 1H), 5.49 (d, *J* =1.8 Hz ,1H), 3.09-3.12 (m, 2H), 3.02 (td, *J* = 6.6, 2.4 Hz, 1H), 2.40 (s, 3H), 2.28-2.34 (m, 1H), 2.26 (s, 3H), 2.07-2.12 (m, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 198.1, 171.9, 170.5, 145.0, 143.7, 142.3, 136.8, 135.2, 134.8, 134.6, 131.5, 129.24, 129.18, 128.96, 128.93, 128.7, 128.1, 128.0, 127.4, 127.1, 125.7, 62.0, 54.5, 50.6, 35.8, 26.8, 20.7, 20.6; IR *v* (cm^{-1}) 1686; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_4S$: 563.1999, found: 563.1993.



8n

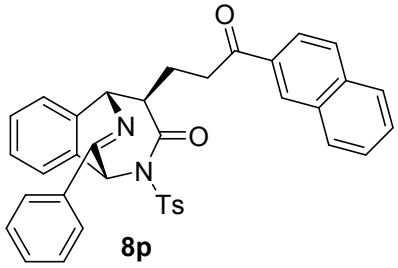
(*1R, 4R, 5S*)-4-(3-Oxo-3-(*p*-bromophenyl)propyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 8n: white solid, 80% (250 mg); ee 99.7%; $[\alpha]^{20}_D$ = +4.13 ^{o} (*c* 0.5, CH_2Cl_2); mp 172-173 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.22 (d, *J* = 7.2 Hz, 2H), 7.69 (t, *J* = 8.8 Hz, 4H), 7.52-7.61 (m, 6H), 7.42-7.34 (m ,1H), 7.34-7.36 (m, 2H), 7.14 (d, *J* = 8.2 Hz, 2H), 7.01 (s, 1H), 5.48 (d, *J* = 3.1 Hz, 1H), 3.08 (t, *J* = 7.2 Hz, 2H), 3.02 (td, *J* = 6.6, 3.2 Hz, 1H), 2.32-2.39 (m, 1H), 2.30 (s, 3H), 2.07-2.16 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 198.2, 171.9, 170.8, 144.9, 141.9, 136.3, 135.5, 135.1, 134.5, 131.9, 131.7, 129.7, 129.3, 129.14, 129.05, 128.6, 128.2, 128.1, 127.4, 126.8, 125.7,

63.2, 53.9, 50.6, 36.2, 26.8, 21.6; IR *v* (cm^{-1}) 1686; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{28}BrN_2O_4S$: 627.0947, found: 627.0951.



8o

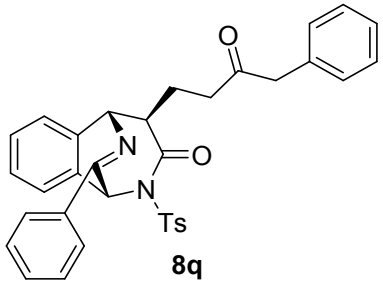
(*1R, 4R, 5S*)-4-(3-Oxo-3-(*p*-nitrophenyl)propyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 8o: white solid, 76% (225.4 mg); ee 99.6%; $[\alpha]^{20}_D$ = +7.73° (*c* 0.5, CH_2Cl_2); mp 177-178 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.22 (d, *J* = 9.6 Hz, 2H), 8.19 (d, *J* = 8.4 Hz, 2H), 7.97 (d, *J* = 9 Hz, 2H), 7.70 (d, *J* = 9 Hz, 2H), 7.59-7.60 (m, 1H), 7.56 (d, *J* = 7.2 Hz, 1H), 7.52 (t, *J* = 7.2 Hz, 2H), 7.42-7.43 (m, 1H), 7.32-7.37 (m, 2H), 7.15 (d, *J* = 7.8 Hz, 2H), 6.99 (s, 1H), 5.47 (d, *J* = 3.0 Hz, 1H), 3.14-3.17 (m, 2H), 3.03 (td, *J* = 6.6, 2.4 Hz, 1H), 2.37-2.43 (m, 1H), 2.31(s, 3H), 2.14-2.19 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 197.7, 171.8, 170.9, 150.3, 145.0, 141.7, 141.2, 136.3, 135.1, 134.5, 131.8, 129.3, 129.15, 129.1, 128.6, 128.2, 127.4, 126.8, 125.7, 123.8, 63.4, 53.8, 50.7, 36.8, 26.7, 21.7; IR *v* (cm^{-1}) 1701, 1680; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{28}N_3O_6S$: 594.1693, found: 594.1691.



8p

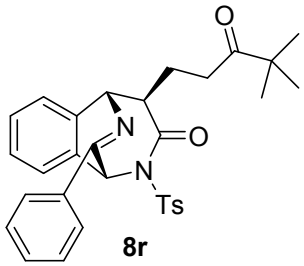
(*1R, 4R, 5S*)-4-(3-(Naphthalen-2-yl)-3-oxopropyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 8p: white solid, 81 % (242.8 mg); ee 99.6%; $[\alpha]^{20}_D$ = -12.6 ° (*c* 0.5, CH_2Cl_2); mp 107-108 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.34 (s, 1H), 8.23 (d, *J* = 7.2 Hz, 2H), 7.95 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.83-7.89 (m, 3H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.50-7.62 (m, 6H), 7.44-7.46 (m, 1H), 7.34-7.38 (m, 2H), 7.10 (d, *J* = 8.4 Hz, 2H), 7.02 (s, 1H), 5.53 (d, *J* =3.2 Hz, 1H), 3.18-3.32 (m, 2H), 3.08 (td, *J* = 6.8, 3.2 Hz, 1H), 2.37-2.46 (m, 1H), 2.22 (s, 3H), 2.14-2.19 (m, 1H); ^{13}C NMR (150 MHz, CD_3COCD_3) δ (ppm) 198.5, 171.9, 170.5, 145.0, 142.3, 136.8, 135.6, 135.3, 134.8, 134.3, 132.7, 131.6, 129.7, 129.7, 129.2, 129.0, 128.9, 128.7, 128.5, 128.4, 128.0, 127.8, 127.4, 127.1, 126.9, 125.7, 123.7, 62.0,

54.5, 50.6, 35.9, 26.9, 20.5; IR *v* (cm^{-1}) 1684; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{37}H_{31}N_2O_4S$: 599.1999, found: 599.2002.



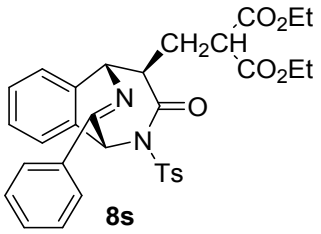
8q

(*1R, 4R, 5S*)-4-(3-Oxo-4-phenylbutyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 8q: white solid, 61 % (171.5 mg); ee 99.3 %; $[\alpha]^{20}_D$ = +37.93° (*c* 0.5, CH_2Cl_2); mp 144-145 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 8.13 (d, *J* = 8.4 Hz, 2H), 7.75-7.77 (m, 1H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.54-7.59 (m, 3H), 7.43 (d, *J* = 8.4 Hz, 1H), 7.23-7.35 (m, 6H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 7.6 Hz, 2H), 6.96 (s, 1H), 5.38 (d, *J* = 3.2 Hz, 1H), 2.83-2.88 (m, 1H), 2.69-2.74 (m, 2H), 2.29 (s, 3H), 1.70-1.76 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 207.4, 171.9, 170.7, 144.8, 141.8, 136.4 , 135.2, 134.5, 134.2, 131.6, 129.5, 129.3, 129.1, 129.0, 128.8, 128.6, 128.1, 127.4, 127.1, 126.7, 125.7, 62.8, 53.8, 50.6, 50.1, 39.4, 26.1, 21.7; IR *v* (cm^{-1}) 1715, 1688; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_4S$: 563.1999, found: 563.1996.



8r

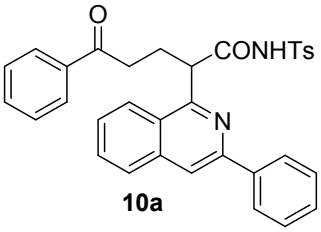
(*1R, 4R, 5S*)-4-(4,4-Dimethyl-3-oxopentyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 8r: white solid, 36% (94.3 mg); ee 99.9%; $[\alpha]^{20}_D$ = +47° (*c* 0.5, CH_2Cl_2); mp 76-77 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.19-8.22 (m, 2H), 7.68 (d, *J* = 6.4 Hz, 2H), 7.51-7.59 (m, 4H), 7.38-7.41 (m, 1H), 7.31-7.35 (m, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.98 (s, 1H), 5.40 (d, *J* = 3.2Hz, 1H), 2.93 (td, *J* = 6.8, 3.2 Hz, 1H), 2.62 (t, *J* = 7.2 Hz, 2H), 2.34 (s, 3H), 2.09-2.18 (m, 1H), 1.83-1.92 (m, 1H), 1.05 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 215.2, 171.9, 170.6, 144.8, 141.9, 136.4, 135.1, 134.6, 131.7, 129.2, 129.1, 129.0, 128.6, 128.1, 127.4, 126.7, 125.7, 63.2, 53.9, 50.5, 44.1, 34.1, 26.7, 26.5, 21.7; IR *v* (cm^{-1}) 1699; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{31}H_{33}N_2O_4S$: 529.2155, found: 529.2159.



8s

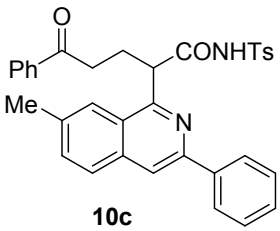
diethyl (*1R, 4R, 5S*)-2-((3-Oxo-11-phenyl-2-tosyl-2,3,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-4-yl)methyl)malonate 8s: white solid, 42% (124.1 mg); ee 99 %, $[\alpha]^{20}_{D}$ = +33.2° (c = 0.5, CH_2Cl_2); mp 121-122°C (recrystallization from EA/*n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.18 (dd, *J* =8.4, 2.4 Hz, 2H), 7.68 (dd, *J* = 6.8, 1.6 Hz, 2H), 7. 51-7.60 (m, 4H), 7.33-7.41 (m, 3H), 7.16 (d, *J* = 7.6 Hz, 2H), 6.98 (s, 1H), 5.44 (d, *J* = 3.2 Hz, 1H), 4.09-4.24 (m, 4H), 3.82 (t, *J* = 8.0 Hz, 1H), 2.93 (td, *J* = 7.2, 3.2Hz 1H), 2.33-2.40 (m, 1H), 2.35 (s, 3H), 2.17-2.25 (m, 1H), 1.24 (t, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 171.4, 171.1, 169.0, 168.9, 144.9, 141.5, 136.2, 135.2, 134.6, 131.7, 129.3, 129.1, 129.0, 128.6, 128.2, 127.5, 126.7, 125.8, 62.3, 61.61, 61.57, 52.4, 50.7, 49.9, 30.7, 21.7, 14.14, 14.11; IR *v* (cm^{-1}) 1746, 1736, 1682; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{32}H_{33}N_2O_7S$: 589.2003, found: 589.2000.

(Note: The minor products **10b**, **10q**, **10r** and **10s** with chemical yields below 10% were not fully characterized.)



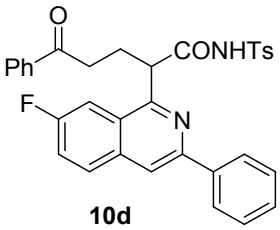
10a

***N*-Tosyl-5-oxo-5-phenyl-2-(3-phenylisoquinolin-1-yl)pentanamide 10a:** white solid, 43 mg, 16%, mp 91-92 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1703, 1684; ^{1}H NMR (600 MHz, CD_3COCD_3) δ (ppm) 11.20 (s, 1H), 8.45 (d, *J* = 8.4 Hz, 1H), 8.29 (s, 1H), 8.12 (dd, *J* = 8.4, 1.2 Hz, 2H), 8.06 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 6.6 Hz, 2H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.79 (t, *J* = 7.2 Hz, 1H), 7.68 (t, *J* = 7.8 Hz, 1H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.42-7.50 (m, 5H), 7.26 (d, *J* = 7.8 Hz, 2H), 5.00 (dd, *J* = 9.0, 5.4 Hz, 1H), 3.20-3.25 (m, 1H) , 3.12-3.17 (m, 1H), 2.44-2.55 (m, 2 H), 2.37 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 198.9, 169.9, 157.5, 149.0, 144.6, 138.3, 137.9, 136.7, 136.3, 133.3, 131.4, 129.5, 129.32, 129.29, 128.6, 128.4, 128.2, 128.1, 127.0, 125.7, 124.5, 117.3, 48.8, 35.2, 30.7, 21.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{29}N_2O_4S$: 549.1842, found: 549.1840.



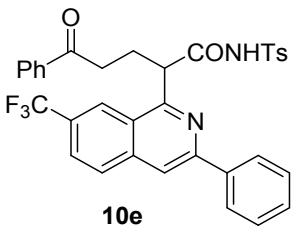
10c

***N*-Tosyl-2-(7-methyl-3-phenylisoquinolin-1-yl)-5-oxo-5-phenylpentanamide 10c:** white solid, 34.4 mg, 12%, mp 178-179 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1709, 1686; ^1H NMR (600 MHz, CD_3COCD_3) δ (ppm) 11.26 (brs, 1H), 8.24 (s, 1H), 8.20 (s, 1H), 8.10 (d, *J* = 7.2 Hz, 2H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.91 (d, *J* =6.6 Hz, 2H), 7.84 (d, *J* = 8.4, Hz, 2H), 7.60-7.64 (m, 2H), 7.42-7.50 (m, 5H), 7.26 (d, *J* = 7.8 Hz, 2H), 4.95 (dd, *J* = 9.0, 5.4 Hz, 1H), 3.17-3.23 (m, 1H), 3.08-3.13 (m, 1H), 2.54 (s, 3H), 2.50-2.56 (m, 1H), 2.42-2.48 (m, 1H), 2.37 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 198.8, 170.0, 156.6, 148.3, 144.6, 138.6, 138.4, 136.7, 136.4, 136.1, 133.6, 133.2, 129.4, 129.3, 129.1, 128.6, 128.4, 128.1, 128.0, 126.8, 125.9, 123.3, 117.1, 48.7, 35.3, 30.7, 22.3, 21.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{30}N_2O_4S$: 563.1999, found: 563.1996.



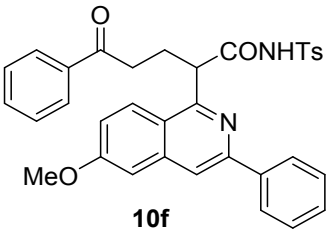
10d

***N*-Tosyl-2-(7-fluoro-3-phenylisoquinolin-1-yl)-5-oxo-5-phenylpentanamide 10d:** white solid, 45.4 mg, 16%, mp 170-171 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1715, 1688; ^1H NMR (400 MHz, CD_3COCD_3) δ (ppm) 11.04 (brs, 1H), 8.33 (s, 1H), 8.23 (dd, *J* = 10.4, 2.0 Hz, 1H), 8.16 (dd, *J* = 9.2, 6.0 Hz, 1H), 8.08-8.10 (m, 2H), 7.92-7.95 (m, 2H), 7.82 (dt, *J* = 8.4, 2.0 Hz, 2H), 7.66 (td, *J* = 8.8, 2.8 Hz, 1H), 7.61 (tt, *J* = 7.6, 2.0 Hz, 1H), 7.43-7.52 (m, 5H), 7.25 (d, *J* = 7.6 Hz, 2H), 4.95 (dd, *J* = 9.2, 4.8 Hz, 1H), 3.13-3.29 (m, 2H), 2.41-2.57 (m, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.8, 169.5, 161.6 (d, *J* = 250.1 Hz), 156.9 (d, *J* = 6.7 Hz), 148.8, 144.7, 138.0, 136.7, 136.2, 135.0, 133.3, 130.9, 130.8, 129.5, 129.4, 128.7, 128.4, 128.1, 126.9, 126.4 (d, *J* = 8.7 Hz), 122.1 (d, *J* = 25.9 Hz), 117.0, 108.5 (d, *J* = 22.0 Hz), 49.1, 35.1, 30.4, 21.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{28}FN_2O_4S$ 567.1748, found: 567.1750.



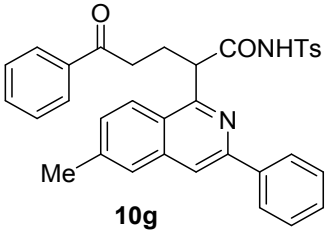
10e

***N*-Tosyl-5-oxo-5-phenyl-2-(3-phenyl-6-(trifluoromethyl)isoquinolin-1-yl)pentanamide 10e:** white solid, 53.1 mg, 17%, mp 170-171 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1701, 1674; ^1H NMR (600 MHz, CD_3COCD_3) δ (ppm) 10.94 (s, 1H), 8.96 (s, 1H), 8.42 (s, 1H), 8.28 (d, *J* =10.2 Hz, 1H), 8.12-8.13 (m, 2H), 8.00 (d, *J* = 9.0 Hz, 1H), 7.93 (d, *J* = 6.6 Hz, 2H), 7.81 (d, *J* = 7.8 Hz, 2H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.47-7.50 (m, 5H), 7.24 (d, *J* = 7.8 Hz, 2H), 5.17 (dd, *J* = 9.6, 6.0 Hz, 1H), 3.24-3.30 (m, 1H), 3.16-3.22 (m, 1H), 2.53-2.59 (m, 1H), 2.43-2.48 (m, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.5, 169.2, 158.7, 151.2, 144.8, 139.2, 137.6, 136.6, 136.0, 133.4, 130.0 (q, *J* = 32.6 Hz), 129.9, 129.5, 129.4, 128.7, 128.4, 128.1, 127.1, 127.0 (d, *J* = 2.0 Hz), 124.6, 123.7 (d, *J* = 271.2 Hz), 122.6 (d, *J* = 4.8 Hz), 116.8, 49.1, 35.2, 30.6, 21.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{28}F_3N_2O_4S$: 617.1716, found: 617.1712.



10f

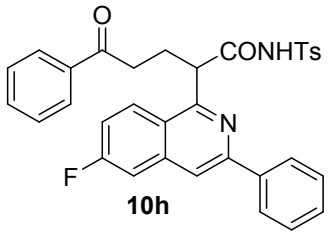
***N*-Tosyl-2-(7-methoxy-3-phenylisoquinolin-1-yl)-5-oxo-5-phenylpentanamide 10f:** white solid, 46.2 mg, 16%, mp 175-176 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1732, 1669; ^1H NMR (400 MHz, CD_3COCD_3) δ (ppm) 11.39 (brs, 1H), 8.34 (d, *J* = 9.2 Hz, 1H), 8.19 (s, 1H), 8.10 (d, *J* = 7.6 Hz, 2H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.83 (d, *J* = 8.4 Hz, 2H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.42-7.50 (m, 6H), 7.25-7.28 (m, 3H), 4.90 (dd, *J* = 8.4, 5.2 Hz, 1H), 4.00 (s, 3H), 3.06-3.22 (m, 2H), 2.39-2.54 (m, 2H), 2.36 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 198.9, 170.1, 161.7, 156.8, 149.4, 144.5, 140.2, 138.3, 136.7, 136.5, 133.3, 129.4, 129.3, 128.6, 128.4, 128.1, 127.0, 126.4, 121.3, 121.2, 116.5, 105.7, 55.7, 48.7, 35.2, 30.8, 21.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_5S$: 579.1948, found: 579.1950.



10g

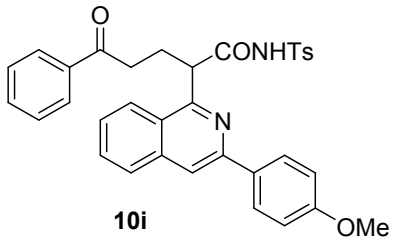
***N*-Tosyl-2-(6-Methyl-3-phenylisoquinolin-1-yl)-5-oxo-5-phenylpentanamide:** white solid, 35.7 mg, 13%,

mp 189-190 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1713, 1688; ^1H NMR (400 MHz, CD_3COCD_3) δ (ppm) 11.29 (brs, 1H), 8.32 (d, *J* = 8.8 Hz, 1H), 8.18 (s, 1H), 8.10-8.12 (m, 2H), 7.90 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.82-7.84 (m, 3H), 7.61 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.43-7.53 (m, 6H), 7.26 (d, *J* = 7.6 Hz, 2H), 4.94 (dd, *J* = 8.4, 5.6 Hz, 1H), 3.07-3.24 (m, 2H), 2.55 (s, 3H), 2.43-2.52 (m, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.9, 170.0, 157.2, 149.0, 144.6, 142.0, 138.4, 138.3, 136.7, 136.4, 133.3, 130.7, 129.4, 129.3, 129.2, 128.6, 128.4, 128.1, 127.1, 126.9, 124.3, 124.1, 116.8, 48.6, 35.2, 30.8, 22.0, 21.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_4S$: 563.1999, found: 563.2002.



10h

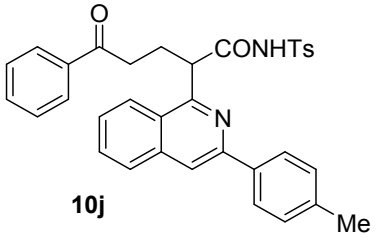
***N*-Tosyl-2-(6-fluoro-3-phenylisoquinolin-1-yl)-5-oxo-5-phenylpentanamide 10h:** white solid, 69.1 mg, 24%, mp 185-186 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1736, 1665; ^1H NMR (400 MHz, CD_3COCD_3) δ (ppm) 11.08 (brs, 1H), 8.57 (dd, *J* = 9.2, 5.6 Hz, 1H), 8.29 (s, 1H), 8.08-8.11 (m, 2H), 7.92 (d, *J* = 8.4 Hz, 2H), 7.82 (d, *J* = 8.4 Hz, 2H), 7.74 (dd, *J* = 10.0, 2.4 Hz, 1H), 7.59-7.63 (m, 1H), 7.45-7.54 (m, 6H) , 7.25 (d, *J* = 8.4 Hz, 2H), 5.00 (dd, *J* = 9.2, 5.2 Hz, 1H), 3.11-3.27 (m, 2H), 2.40-2.57 (m, 2H) , 2.37 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 199.0, 169.6, 163.8 (d, *J* = 252.8 Hz), 157.7, 150.0, 144.7, 139.7 (d, *J* =11.4 Hz), 137.9, 136.7, 136.2, 133.4, 129.6, 129.5, 129.4, 128.7, 128.4, 128.1, 128.04, 127.98, 127.0, 122.9, 118.8 (d, *J* = 24.3 Hz), 116.7 (d, *J* = 4.4 Hz), 111.4 (d, *J* = 20.1 Hz), 49.0, 35.1, 30.6, 20.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{28}FN_2O_4S$: 567.1748, found: 567.1751.



10i

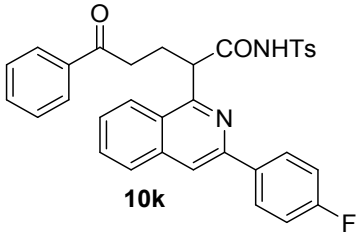
***N*-Tosyl-2-(3-(4-methoxyphenyl)isoquinolin-1-yl)-5-oxo-5-phenylpentanamide 10i:** white solid, 39 mg, 14%, mp 173-174 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1736, 1667; ^1H NMR (400 MHz, CD_3COCD_3) δ (ppm) 11.24 (brs, 1H), 8.41 (d, *J* = 8.4 Hz, 1H), 8.18 (s, 1H), 8.06 (dd, *J* = 8.8, 2.0 Hz, 2H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.91 (dd, *J* = 6.8, 1.6 Hz, 2H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.75 (t, *J* = 8.4 Hz, 1H), 7.59-7.66 (m, 2H), 7.49 (t, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 7.6 Hz, 2H), 7.01 (dd, *J* = 9.2, 2.4 Hz, 2H), 4.97 (dd, *J* = 8.4, 5.6 Hz, 1H), 3.90 (s, 3H), 3.09-3.26 (m, 2H) , 2.40-2.55 (m, 2H), 2.38 (s, 3H); ^{13}C NMR (150 MHz,

$CDCl_3$) δ (ppm) 198.9, 170.0, 160.8, 157.3, 148.7, 144.6, 138.0, 136.7, 136.3, 133.3, 131.3, 130.7, 129.5, 128.6, 128.4, 128.2, 128.11, 128.06, 128.0, 125.3, 124.5, 116.2, 114.7, 55.6, 48.6, 35.3, 30.8, 21.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_5S$: 579.1948, found: 579.1951.



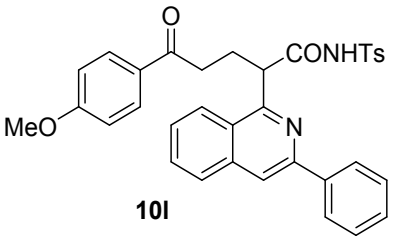
10j

***N*-Tosyl-5-oxo-5-phenyl-2-(3-(*p*-tolyl)isoquinolin-1-yl)pentanamide 10j:** white solid, 38.9 mg, 14%, mp 165-166 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1734, 1669; ^1H NMR (600 MHz, CD_3COCD_3) δ (ppm) 11.25 (s, 1H), 8.44 (d, *J* = 8.4 Hz, 1H), 8.24 (s, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 2H), 7.92 (d, *J* = 7.8 Hz, 2H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.78 (t, *J* = 7.2 Hz, 1H), 7.66 (t, *J* = 7.8 Hz,1H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 2H), 7.27 (t, *J* = 10.2 Hz, 4H), 4.99 (dd, *J* = 9.0, 5.4 Hz, 1H), 3.20-3.25 (m, 1H), 3.11-3.16 (m, 1H) , 2.43-2.54 (m, 2H), 2.42 (s, 3H) 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$,) δ (ppm) 198.9, 170.0, 157.4, 149.0, 144.6, 139.4, 138.0, 136.7, 136.3, 135.4, 133.3, 131.3, 130.1, 129.4, 128.7, 128.4, 128.2, 128.1, 126.8, 125.5, 124.5, 116.8, 48.6, 35.2, 30.8, 21.6, 21.4; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_4S$: 563.1999, found: 563.2001.



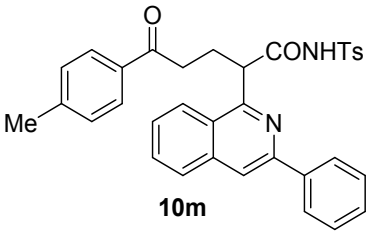
10k

***N*-Tosyl-2-(3-(4-fluorophenyl)isoquinolin-1-yl)-5-oxo-5-phenylpentanamide 10k:** white solid, 39.8 mg, 14%, mp 162-163 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1736, 1667; ^1H NMR (600 MHz, CD_3COCD_3) δ (ppm) 11.07 (s, 1H), 8.45 (d, *J* = 7.8 Hz, 1H), 8.27 (s, 1H), 8.14 (dd, *J* = 9.0, 6.0 Hz, 2H), 8.04 (d, *J* = 9.0 Hz, 1H), 7.92 (d, *J* = 7.8 Hz, 2H), 7.83 (d, *J* = 8.4 Hz, 2H), 7.79 (t, *J* = 7.8 Hz, 1H), 7.68 (t, *J* = 8.4 Hz, 1H) , 7.61 (t, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.20 (t, *J* = 9.0 Hz, 2H), 5.01(dd, *J* = 8.4, 4.8Hz, 1H), 3.20-3.26 (m, 1H), 3.13-3.18 (m, 1H), 2.49-2.55 (m, 1H), 2.41-2.47 (m, 1H), 2.83 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 198.8, 169.6, 163.6 (d, *J* = 248.4 Hz), 157.6, 148.0, 144.6, 137.8, 136.6, 136.1, 134.3, 133.3, 131.4, 129.4, 128.7 (d, *J* = 8.7 Hz), 128.6, 128.4, 128.3, 128.1, 128.0, 125.5, 124.4, 116.9, 116.2 (d, *J* = 21.6 Hz), 48.7, 35.2, 30.5, 21.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{28}FN_2O_4S$: 567.1748, found: 567.1751.



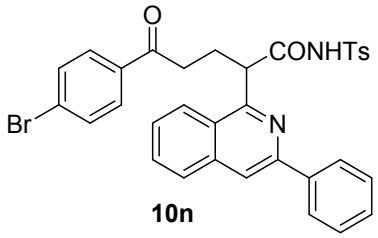
10l

***N*-Tosyl-5-(4-methoxyphenyl)-5-oxo-2-(3-phenylisoquinolin-1-yl)pentanamide 10l:** white solid, 57 mg, 20%, mp 106-107 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1724, 1655; ^1H NMR (400 MHz, CD_3COCD_3) δ (ppm) 11.20 (s, 1H), 8.46 (d, *J* = 8.0 Hz, 1H), 8.29 (s, 1H), 8.12 (dd, *J* = 8.4, 2.0 Hz, 2H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.90 (dt, *J* = 8.4, 1.6 Hz, 2H), 7.84 (d, *J* = 8.0 Hz, 2H), 7.79 (td, *J* = 8.0, 1.2Hz, 1H), 7.68 (td, *J* = 8.4, 1.6 Hz, 1H), 7.43-7.49 (m, 3H), 7.26 (d, *J* = 8.0 Hz, 2H), 6.99 (dt, *J* = 9.2, 2.4 Hz, 2H), 4.99 (dd, *J* = 8.8, 5.6 Hz, 1H), 3.88 (s, 3H), 3.03-3.19 (m, 2H), 2.41-2.55 (m, 2H), 2.38 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 197.4, 169.9, 163.7, 157.6, 149.0, 144.6, 138.3, 137.9, 136.3, 131.4, 130.4, 129.8, 129.4, 129.30, 128.26, 128.4, 128.2, 127.0, 125.7, 124.6, 117.2, 113.8, 55.6, 48.9, 34.9, 30.9, 21.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_5S$: 579.1948, found: 579.1950.



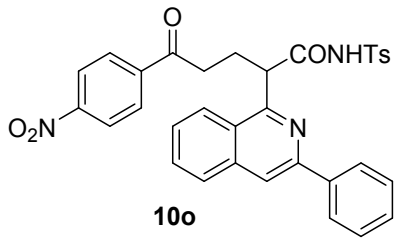
10m

***N*-Tosyl-5-oxo-2-(3-phenylisoquinolin-1-yl)-5-(*p*-tolyl)pentanamide 10m:** white solid, 49.5 mg, 18%, mp 173-174 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1728, 1657; ^1H NMR (600 MHz, CD_3COCD_3) δ (ppm) 11.20 (s, 1H), 8.45 (d, *J* = 7.8 Hz, 1H), 8.29 (s, 1H), 8.11 (d, *J* = 7.8 Hz, 2H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.79-7.84 (m, 5H), 7.68 (t, *J* = 7.8 Hz, 1H), 7.42-7.48 (m, 3H) , 7.29 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 7.8 Hz, 2H), 5.01 (dd, *J* = 9.0, 5.4 Hz, 1H), 3.16-3.21 (m, 1H), 3.08-3.13 (m, 1H), 2.42-2.54 (m, 2H), 2.39 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 198.6, 169.6, 158.2, 149.0, 144.3, 143.7, 138.8, 137.8, 137.1, 134.6, 130.7, 129.4, 129.2, 128.7, 128.6, 128.1, 128.0, 127.7, 126.8, 126.0, 125.0, 116.0, 49.8, 35.6, 27.3, 20.8, 20.7; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_4S$: 563.1999, found: 563.2001.



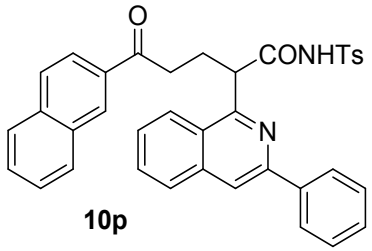
10n

***N*-Tosyl-5-oxo-5-(4-bromophenyl)-2-(3-phenylisoquinolin-1-yl)pentanamide 10n:** white solid, 45.8 mg, 15%, mp 183-184°C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1711, 1690; ^1H NMR (400 MHz, CD_3COCD_3) δ (ppm) 11.17 (s, 1H), 8.43 (d, *J* = 8.4Hz, 1H), 8.29 (s, 1H), 8.09-8.11 (m, 2H), 8.06 (d, *J* = 8.0 Hz, 1H), 7.78 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.81-7.85 (m, 4H), 7.66-7.70 (m, 3H), 7.43-7.49 (m, 3H), 7.26 (d, *J* = 8.0 Hz, 2H), 5.00 (dd, *J* = 8.8, 5.6Hz, 1H), 3.11-3.26 (m, 2H), 2.41-2.57 (m, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 197.9, 169.9, 157.4, 149.0, 144.7, 138.2, 137.9, 136.3, 135.4, 132.0, 131.4, 129.6, 129.5, 129.3, 128.5, 128.43, 128.38, 128.3, 126.9, 125.6, 124.4, 117.3, 48.6, 35.2, 30.6, 21.7; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{28}BrN_2O_4S$: 627.0947, found: 627.0944.



10o

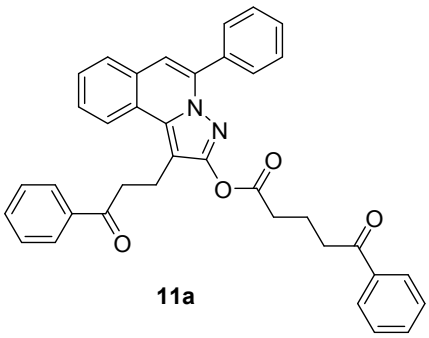
***N*-Tosyl-5-(4-nitrophenyl)-5-oxo-2-(3-phenylisoquinolin-1-yl)pentanamide 10o:** white solid, 35.4 mg, 12%, mp 188-189 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1734, 1665; ^1H NMR (600 MHz, CD_3COCD_3) δ (ppm) 11.14 (s, 1H), 8.42 (d, *J* = 9.6 Hz, 1H), 8.28-8.30 (m, 3H), 8.05-8.12 (m, 5H), 7.83 (d, *J* = 9.0 Hz, 2H), 7.79 (t, *J* = 7.2 Hz, 1H), 7.68 (t, *J* = 7.2 Hz, 1H), 7.42-7.46 (m, 3H) , 7.26 (d, *J* = 7.8 Hz, 2H), 5.02 (dd, *J* = 9.0, 6.0 Hz, 1H), 3.29-3.31 (m, 2H), 2.60-2.48 (m, 2H), 2.38 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 197.5, 169.8, 157.2, 150.5, 148.9, 144.7, 141.1, 138.0, 136.3, 131.5, 129.5, 129.42, 129.36, 129.2, 128.5, 128.4, 128.3, 126.9, 125.6, 124.3, 123.9, 117.4, 48.3, 35.8, 30.3, 21.7; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{28}N_3O_6S$: 594.1693, found: 594.1698.



10p

***N*-Tosyl-5-(2-naphthalenyl)-5-oxo-2-(3-phenylisoquinolin-1-yl)pentanamide 10p:** white solid, 47 mg,

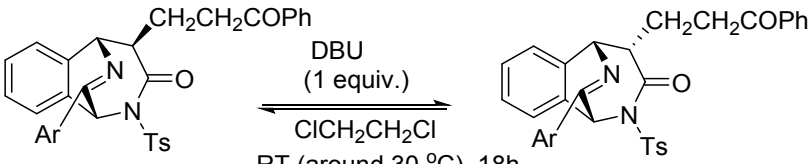
16%, mp 135-136 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1726, 1665; ^1H NMR (400 MHz, CD_3COCD_3) δ (ppm) 11.20 (s, 1H), 8.55 (s, 1H), 8.49 (d, *J* = 8.4 Hz, 1H), 8.29 (s, 1H), 8.11-8.13 (m, 2H), 8.06 (d, *J* = 8.0 Hz, 2H), 7.97-7.99 (m, 3H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.79 (td, *J* = 7.2, 1.2 Hz, 1H), 7.61-7.70 (m, 3H), 7.43-7.46 (m, 3H), 7.24 (d, *J* = 8.0 Hz, 2H), 5.06 (dd, *J* = 8.8, 5.6 Hz, 1H), 3.26-3.43 (m, 2H), 2.48-2.63 (m, 2H), 2.32 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 198.9, 170.0, 157.5, 149.0, 144.6, 138.3, 137.9, 136.3, 135.7, 134.0, 132.6, 131.4, 129.9, 129.8, 129.4, 129.3, 128.6, 128.5, 128.42, 128.37, 128.2, 127.8, 127.0, 126.9, 125.7, 124.5, 123.8, 117.3, 48.9, 35.4, 30.9, 21.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{37}H_{31}N_2O_4S$: 599.1999, found: 599.1996.



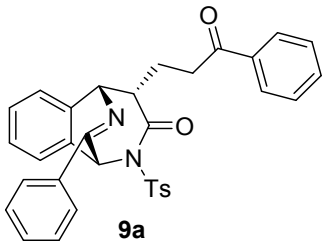
11a

1-(3-Oxo-3-phenylpropyl)-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl 5-oxo-5-phenylpentanoate 11a (This by-product was isolated from the reaction of **1a** with **6a** catalyzed by AgOTf (10 mol %), *N*-mesityl triazolium salt **7b** (30 mol%) and DBU (100 mol%), see Table 1 and entry 1)**:** white solid, 6 %, mp 106-107 °C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 1765, 1680; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.18-8.20 (m, 1H), 7.93-7.97 (m, 4H), 7.85 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.74-7.76 (m, 1H), 7.46-7.57 (m, 7H), 7.44 (d, *J* = 6.8 Hz, 2H), 7.40 (d, *J* = 7.6 Hz, 2H), 7.03 (s,1H), 3.42-3.46 (m, 2H), 3.33-3.37 (m, 2H), 3.12 (t, *J* = 6.8 Hz, 2H), 2.80 (t, *J* = 6.8 Hz, 2H), 2.19 (quint., *J* = 6.8 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 199.4, 199.2, 171.7, 155.1, 138.4, 136.8, 136.7, 136.6, 133.5, 133.3, 133.1, 129.8, 129.52, 129.48, 128.72, 128.67, 128.4, 128.2, 128.1, 127.9, 127.75, 127.70, 124.6, 122.8, 112.7, 103.6, 37.7, 37.3, 33.1, 19.2, 18.2; HRMS (TOF-ESI): $[M + Na]^+$ calcd for $C_{37}H_{30}N_2O_4Na$: 589.2097, found: 589.2099.

3. Isomerization between (*1R, 4R, 5S*)-5,1-(azenometheno)benzo[*c*]azepin-3-ones 8 and (*1R, 4S, 5S*)-5,1-(azenometheno)benzo[*c*]azepin-3-ones 9

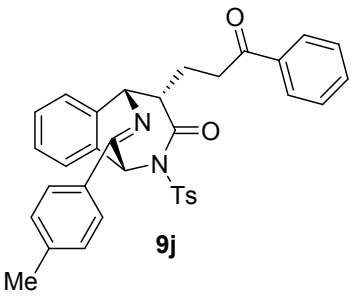


In a test tube, a mixture of (*1R, 4R, 5S*)-4-(3-oxo-3-phenylpropyl)-11-aryl-2-tosyl-5,1-(azenometheno)benzo[*c*]azepin-3-one **8a** or **8j** (0.2 mmol) and DBU (0.4 mmol, 60.8 mg) in dichloroethane (2 mL) was stirred for 18 h at room temperature (~30 °C). After removal of the solvent, the residue was chromatographed on a silica gel column eluting with a mixture of petroleum ether, dichloromethane and ethyl acetate (petroleum ether : DCM : EA = 6 : 2 : 1) to give the (*1R, 4S, 5S*)-5,1-(azenometheno)benzo[*c*]azepin-3-ones **9a** and **9j** in 49 % and 47 % yield, respectively. Meanwhile, 41% of **8a** and 42 % of **8j** were recovered.



9a

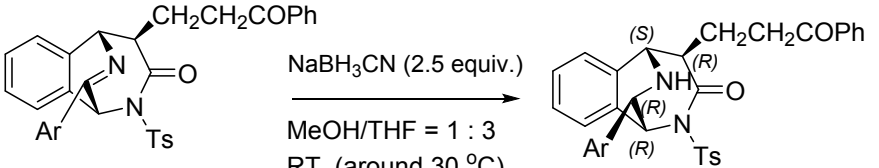
(*1R, 4S, 5S*)-4-(3-Oxo-3-phenylpropyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 9a: white solid, 54 mg, 49 %, ee 99.2%, $[\alpha]^{20}_{D}$ +49.7 ° (*c* 0.5, CH_2Cl_2), mp 90-91 °C (without recrystallization); IR *v* (cm^{-1}) 1686; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.12 (d, *J* = 7.8 Hz, 2H), 7.85 (dd, *J* = 8.4, 1.8 Hz, 2H), 7.68 (d, *J* = 7.2 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.51-7.55 (m, 4H), 7.47 (d, *J* = 6.6 Hz, 1H), 7.43 (t, *J* = 7.2 Hz, 1H), 7.40 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.37 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.10 (d, *J* = 7.8 Hz, 2H), 6.99 (s, 1H), 5.36 (d, *J* = 3.6 Hz, 1H), 3.06-3.12 (m, 2H), 2.96-3.01 (m, 1H), 2.27 (s, 3H), 1.94-2.00 (m, 1H), 1.73-1.79 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 199.1, 171.8, 170.6, 144.8, 139.8, 136.7, 136.2, 135.2, 134.8, 133.2, 131.7, 129.3, 129.1, 128.8, 128.63, 128.57, 128.3, 128.1, 127.3, 127.2, 127.0, 63.9, 50.54, 50.50, 36.8, 26.4, 21.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{28}N_2O_4S$: 549.1842, found: 549.1845.



9j

(*1R, 4S, 5S*)-4-(3-Oxo-3-phenylpropyl)-11-(p-tolyl)-2-tosyl-1,2,4,5-tetrahydro-5,1-(azenometheno)benzo[*c*]azepin-3-one 9j: white solid, 48.8 mg, 43 %, ee 99.7%, $[\alpha]^{20}_{D}$ +44.6 ^{o} (*c* 0.5, CH_2Cl_2), mp 202-203 ^{o}C (recrystallization from dichloromethane and *n*-hexane); IR *v* (cm^{-1}) 1705, 1674; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.01 (d, *J* = 7.8 Hz, 2H), 7.84 (d, *J* = 7.8 Hz, 2H), 7.67 (d, *J* = 7.2 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 2H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.36-7.46 (m, 5H), 7.32 (d, *J* = 7.8 Hz, 2H), 7.10 (d, *J* = 7.8 Hz, 2H), 6.96 (s, 1H), 5.32 (d, *J* = 3.6 Hz, 1H), 3.05-3.11 (m, 2H), 2.95-3.00 (m, 1H), 2.44 (s, 3H), 2.27 (s, 3H), 1.93-1.99 (m, 1H), 1.73-1.78 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 199.1, 171.8, 170.3, 144.7, 142.2, 139.8, 136.7, 136.2, 134.9, 133.1, 132.3, 129.8, 129.2, 128.7, 128.6, 128.5, 128.2, 128.0, 127.2, 127.1, 1269, 63.7, 50.5, 50.4, 36.8, 26.3, 21.5; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{31}N_2O_4S$: 563.1999, found: 563.2002.

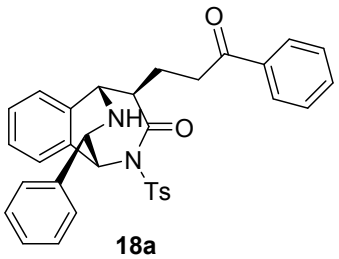
4. Reduction of (*1R, 4R, 5S*)-5,1-(azenometheno)benzo[*c*]azepin-3-ones 8



8a: Ar = Ph
8j: Ar = *p*-MeC_6H_4-

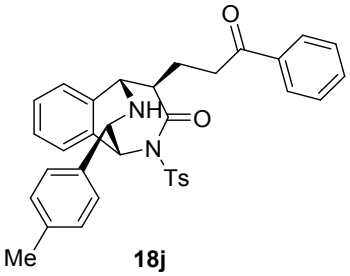
18a: 62%, ee: 99.4 %, dr: 20 :1
18j: 58%, ee: 99.6%, dr: 31 : 1

In a test tube, a mixture of 4-(3-oxo-3-phenylpropyl)-11-aryl-2-tosyl-5,1-(azenometheno)benzo[*c*]azepin-3-ones **8** (0.2 mmol) and $NaBH_3CN$ (0.5 mmol, 31 mg) in methanol (1 mL) and THF (3 mL) was stirred for 18 h at room temperature (around 30 ^{o}C). After removal of the solvents, the residue was chromatographed on a silica gel column eluting with a mixture of petroleum ether and acetone (petroleum ether : acetone = 4 : 1) to give the 4-(3-oxo-3-phenylpropyl)-11-aryl-2-tosyl-5,1-(epiminomethano)benzo[*c*]azepin-3-ones **18** in 58%-62 % yield with > 99% ee and 22 : 1 -31 : 1 dr.



18a

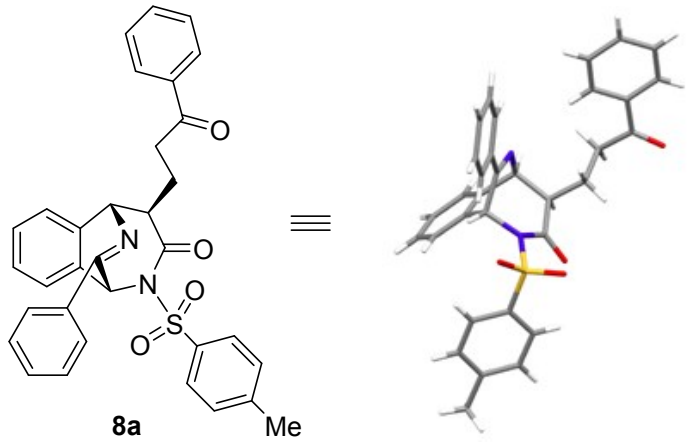
(*1R, 4R, 5S, 11R*)-4-(3-Oxo-3-phenylpropyl)-11-phenyl-2-tosyl-1,2,4,5-tetrahydro-5,1-(epiminomethano)benzo[*c*]azepin-3-one 18a: white solid, 67.7 mg, 62%, ee 99.4%, $[\alpha]^{20}_{D}$ = -63.87 ^{o} (c = 0.5, CH_2Cl_2), mp 169-170 ^{o}C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 3364, 1682; ^{1}H NMR (400 MHz, CD_2Cl_2) δ (ppm) 7.96 (dd, *J* = 7.2, 1.6 Hz, 2H), 7.55-7.61 (m, 4H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.40-7.43 (m, 2H), 7.36-7.39 (m, 4H), 7.28 (dd, *J* = 6.4, 2.0 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.8 Hz, 2H), 6.00 (d, *J* = 3.2 Hz, 1H), 4.55 (d, *J* = 2.8 Hz, 1H), 4.26 (s, 1H), 3.28 (t, *J* = 6.8 Hz, 2H), 2.47-2.54 (m, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 200.2, 174.3, 143.7, 140.9, 140.2, 137.1, 136.9, 136.8, 133.2, 129.8, 129.0, 128.8, 128.7, 128.5, 128.2, 128.1, 128.0, 127.8, 126.0, 124.9, 61.4, 59.7, 56.4, 55.7, 37.8, 27.2, 21.6; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{33}H_{31}N_2O_4S$: 551.1999, found: 551.1997.



18j

(*1R, 4R, 5S, 11R*)-4-(3-Oxo-3-phenylpropyl)-11-(*p*-tolyl)-2-tosyl-1,2,4,5-tetrahydro-5,1-(epiminomethano)benzo[*c*]azepin-3-one 18j: white solid, 65.6 mg, 58%, ee 99.6 %, $[\alpha]^{20}_{D}$ = -60.4^{o} (c = 0.5, CH_2Cl_2), mp 200-201 ^{o}C (recrystallization from EA/*n*-hexane); IR *v* (cm^{-1}) 3383, 1682; ^{1}H NMR (400 MHz, CD_2Cl_2) δ (ppm) 7.89 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.47-7.53 (m, 2H), 7.40 (t, *J* = 8.0 Hz, 2H), 7.32-7.36 (m, 4H), 7.20 (dd, *J* = 5.6, 2.4 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 8.4 Hz, 2H), 5.88 (d, *J* = 3.2 Hz, 1H), 4.45 (d, *J* = 2.4 Hz, 1H), 4.19 (s, 1H), 3.20 (t, *J* = 6.8 Hz, 2H), 2.37-2.48 (m, 3H), 2.32 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 200.2, 174.4, 143.6, 140.2, 137.9, 137.4, 137.2, 136.9, 136.8, 133.2, 129.7, 129.4, 128.8, 128.7, 128.6, 128.2, 128.1, 127.9, 126.0, 124.8, 61.2, 59.8, 56.4, 55.7, 37.8, 27.2, 21.7, 21.3; HRMS (TOF-ESI): $[M + H]^+$ calcd for $C_{34}H_{33}N_2O_4S$: 565.2155, found: 565.2154.

4. X-Ray crystallography of 8a, 9j, 10a, 11a and 18j

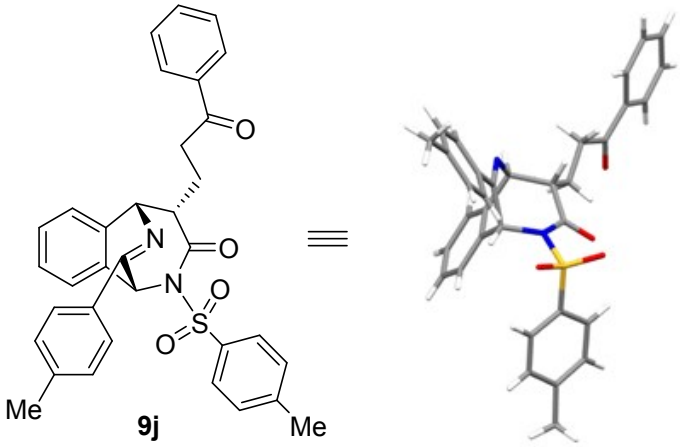


Crystals of compound **8a** (CCDC 1991926) were obtained by slow evaporation of a solution of **8a** in dichloromethane and *n*-hexane. Single-crystal diffraction intensity data of the compound **8a** was collected on a SuperNova (Dual, Cu at home/near, AtlasS2) diffractometer with CuKα radiation (λ = 1.54184 Å) at 100.01 K. The structure was solved by the program ShelXS (Sheldrick, 2008) and refined with the program ShelXL (Sheldrick, 2015). The crystal data and structure refinement results for compound **8a** are listed in the Table S1.

Table S1. Crystal data and structure refinement for 8a.

Identification code	20181204e
Empirical formula	$C_{33}H_{28}N_2O_4S$
Formula weight	548.63
Temperature/K	100.01(10)
Crystal system	triclinic
Space group	P1
a/Å	8.0643(3)
b/Å	9.5772(5)
c/Å	9.7272(5)
α/°	71.192(4)
β/°	74.716(4)
γ/°	76.923(4)
Volume/Å^3	677.74(6)
Z	1
ρ_{calc} (g/cm^3)	1.344
μ/mm^{-1}	1.404
F(000)	288.0
Crystal size/mm^3	0.4 × 0.2 × 0.1
Radiation	CuKα (λ = 1.54184)
2 θ range for data collection/°	9.818 to 143.582

Index ranges	$-9 \le h \le 6$, $-11 \le k \le 10$, $-11 \le l \le 10$
Reflections collected	4408
Independent reflections	3099 [R_{int} = 0.0308, R_{sigma} = 0.0362]
Data/restraints/parameters	3099/3/362
Goodness-of-fit on F^2	1.032
Final R indexes [I≥2σ (I)]	R_1 = 0.0318, wR_2 = 0.0851
Final R indexes [all data]	R_1 = 0.0323, wR_2 = 0.0857
Largest diff. peak/hole / e $Å^{-3}$	0.20/-0.38
Flack parameter	0.013(15)



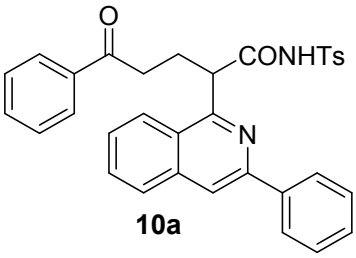
9j

Crystals of compound **9j** (CCDC 1991927) were obtained by slow evaporation of a solution of **9j** in dichloromethane and *n*-hexane. Single-crystal diffraction intensity data of the compound **9j** was collected on a 'XtaLAB Synergy R, DW system, HyPix' diffractometer with CuKα radiation (λ = 1.54184 Å) at 100 K. 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 **9j** are listed in the Table S2.

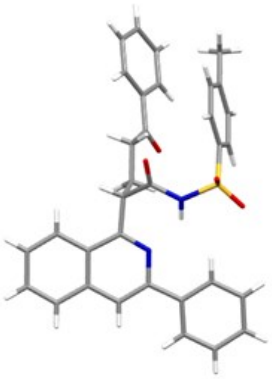
Table S2. Crystal data and structure refinement for 9j.

Identification code	20190612a
Empirical formula	$C_{34}H_{30}N_2O_4S$
Formula weight	562.66
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	10.52860(10)
b/Å	10.84520(10)
c/Å	23.4899(2)
α/°	90

β/°	90
γ/°	90
Volume/Å^3	2682.19(4)
Z	4
ρ_{calc} (g/cm^3)	1.393
μ/mm^{-1}	1.433
F(000)	1184.0
Crystal size/mm^3	0.3 × 0.25 × 0.2
Radiation	CuKα (λ = 1.54184)
2 θ range for data collection/°	7.528 to 151.576
Index ranges	-5 ≤ h ≤ 13, -12 ≤ k ≤ 13, -29 ≤ l ≤ 28
Reflections collected	14855
Independent reflections	5354 [R_{int} = 0.0317, R_{sigma} = 0.0317]
Data/restraints/parameters	5354/0/372
Goodness-of-fit on F^2	1.071
Final R indexes [I≥2σ (I)]	R_1 = 0.0330, wR_2 = 0.0850
Final R indexes [all data]	R_1 = 0.0370, wR_2 = 0.0906
Largest diff. peak/hole / e Å^{-3}	0.28/-0.39
Flack parameter	-0.005(7)



10a

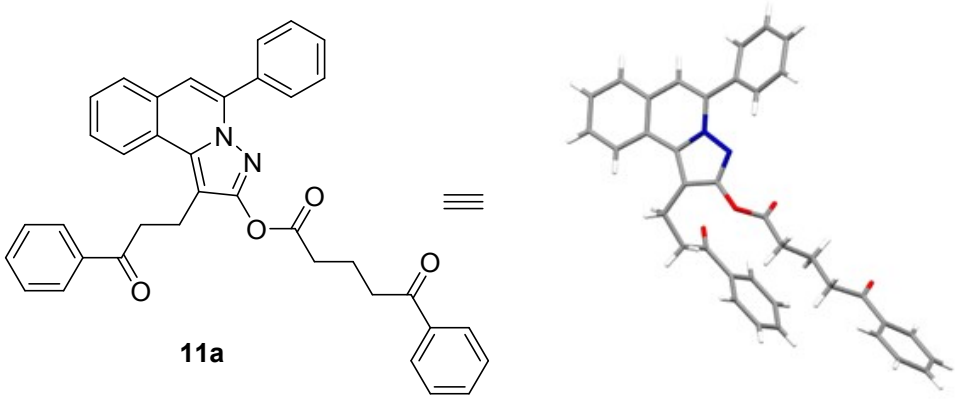


Crystals of compound **10a** (CCDC 2019566) were obtained by slow evaporation of a solution of **10a** in ethyl acetate, *n*-hexane and dichloromethane. Single-crystal diffraction intensity data of the compound **10a** was collected on a 'XtaLAB Synergy R, DW system, HyPix' diffractometer with CuKα radiation (λ = 1.54184 Å) at 100.01 K. 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 **10a** are listed in the Table S3.

Table S3. Crystal data and structure refinement for 10a.

Identification code	20200727i
Empirical formula	$C_{33}H_{28}N_2O_4S$

Formula weight	548.63
Temperature/K	100.01(10)
Crystal system	triclinic
Space group	P-1
a/Å	8.47632(19)
b/Å	11.6836(2)
c/Å	15.0430(2)
α/°	68.2289(16)
β/°	85.3090(17)
γ/°	72.4618(19)
Volume/Å^3	1318.44(5)
Z	2
ρ_{calc} (g/cm^3)	1.382
μ/mm^{-1}	1.444
F(000)	576.0
Crystal size/mm^3	0.2 × 0.2 × 0.2
Radiation	CuKα (λ = 1.54184)
2 θ range for data collection/°	8.522 to 151.49
Index ranges	-10 ≤ h ≤ 10, -14 ≤ k ≤ 14, -18 ≤ l ≤ 18
Reflections collected	15701
Independent reflections	5265 [Rint = 0.0381, Rsigma = 0.0372]
Data/restraints/parameters	5265/0/367
Goodness-of-fit on F^2	1.072
Final R indexes [I>=2σ (I)]	R_1 = 0.0361, wR_2 = 0.0947
Final R indexes [all data]	R_1 = 0.0397, wR_2 = 0.0980
Largest diff. peak/hole / e Å^{-3}	0.40/-0.45



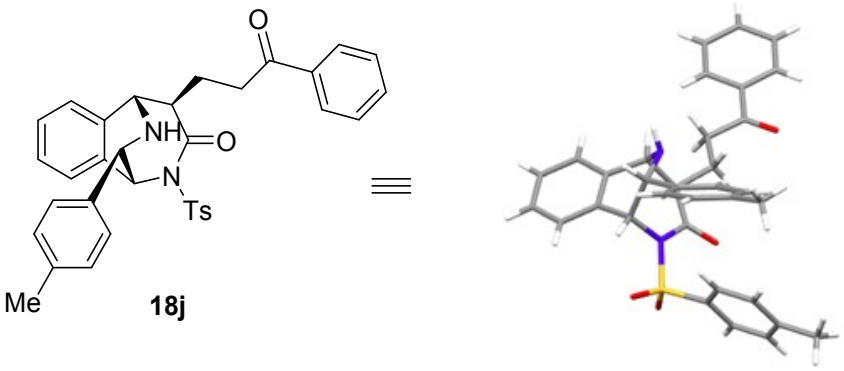
11a

Crystals of compound **11a** (CCDC 1991928) were obtained by slow evaporation of a solution of **11a** in ethyl acetate and *n*-hexane. Single-crystal diffraction intensity data of the compound **11a** was collected on a SuperNova (Dual, Cu at home/near, AtlasS2) diffractometer with CuKα radiation (λ = 1.54184 Å) at 100.01

K. 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 **11a** are listed in the Table S4.

Table S4. Crystal data and structure refinement for 11a.

Identification code	20181225c
Empirical formula	$C_{37}H_{30}N_2O_4$
Formula weight	566.63
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	Pn
a/Å	5.30440(10)
b/Å	18.4193(3)
c/Å	14.2352(2)
α/°	90
β/°	97.8080(10)
γ/°	90
Volume/Å^3	1377.93(4)
Z	2
ρ_{calc} (g/cm^3)	1.366
μ/mm^{-1}	0.712
F(000)	596.0
Crystal size/mm^3	0.3 × 0.2 × 0.03
Radiation	CuKα (λ = 1.54184)
2 θ range for data collection/°	7.896 to 144.092
Index ranges	$-6 \le h \le 6$, $-20 \le k \le 22$, $-17 \le l \le 15$
Reflections collected	9415
Independent reflections	4206 [R_{int} = 0.0343, R_{sigma} = 0.0363]
Data/restraints/parameters	4206/2/388
Goodness-of-fit on F^2	1.035
Final R indexes [I≥2σ (I)]	R_1 = 0.0297, wR_2 = 0.0743
Final R indexes [all data]	R_1 = 0.0311, wR_2 = 0.0756
Largest diff. peak/hole / e Å^{-3}	0.15/-0.18
Flack parameter	0.00(13)



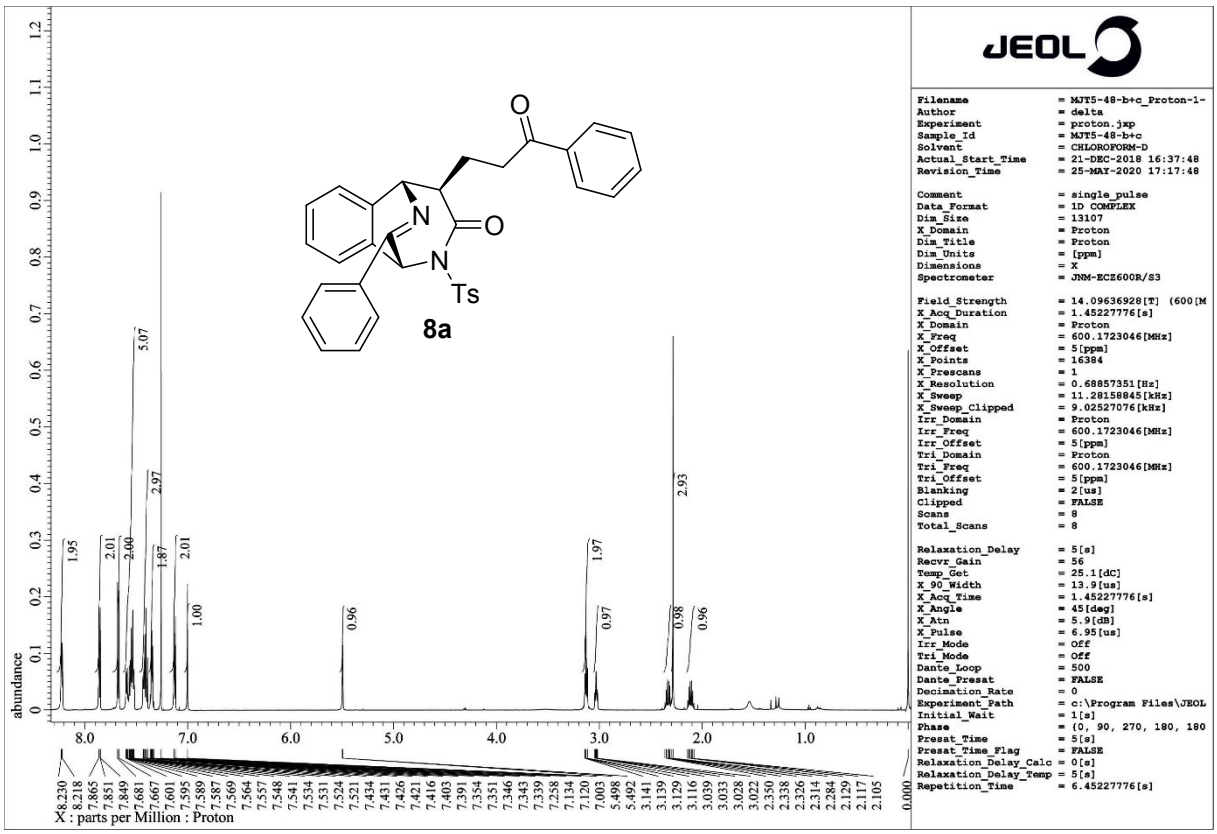
Crystals of compound **18j** (CCDC 2024858) were obtained by slow evaporation of a solution of **18j** in ethyl acetate and *n*-hexane. Single-crystal diffraction intensity data of the compound **18j** was collected on a 'XtaLAB Synergy R, DW system, HyPix' diffractometer with CuKα radiation (λ = 1.54184) at 277 K. The structure was solved by the program 'ShelXT (Sheldrick, 2015)' and refined with the program 'ShelXT (Sheldrick, 2015)'. The crystal data and structure refinement results for compound **18j** are listed in the Table S5.

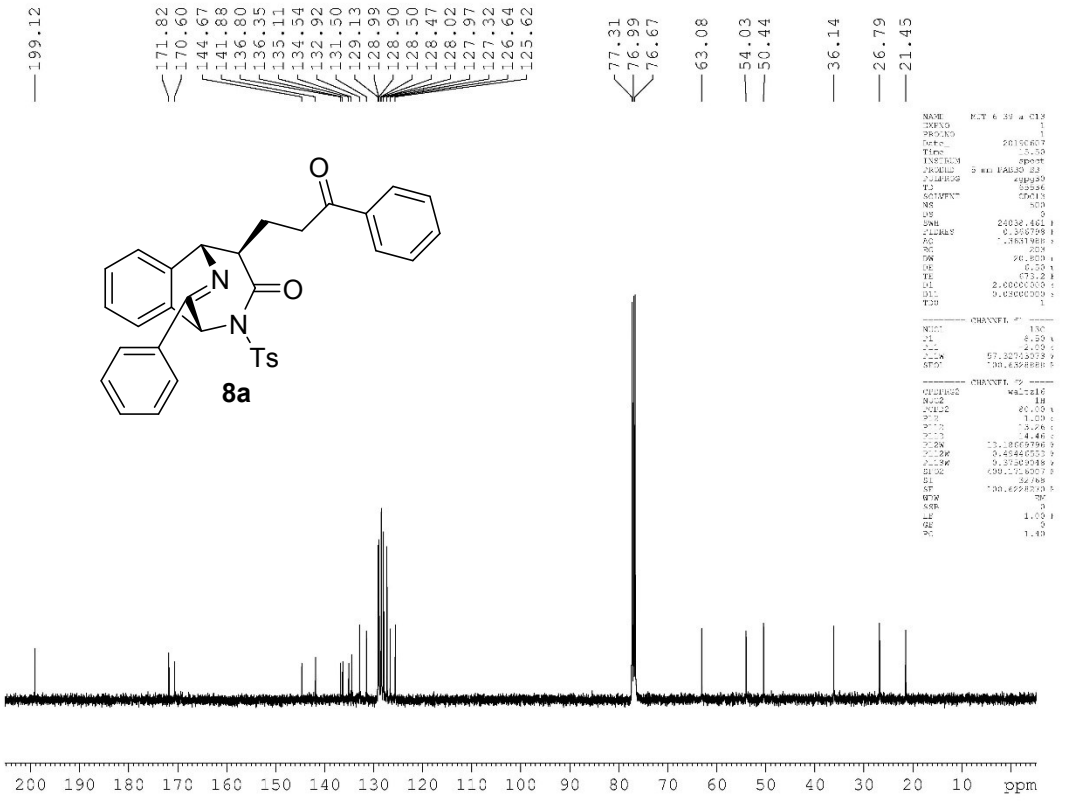
Table S5. Crystal data and structure refinement for 18j.

Identification code	20200816a
Empirical formula	$C_{34}H_{32}N_2O_4S$
Formula weight	564.67
Temperature/K	277(8)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.98984(6)
b/Å	13.05864(11)
c/Å	32.2030(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2939.42(4)
Z	4
ρ_{calc} (g/cm^3)	1.276
μ/mm^{-1}	1.308
F(000)	1192.0
Crystal size/mm^3	0.5 × 0.03 × 0.02
Radiation	CuKα (λ = 1.54184)
2 θ range for data collection/°	7.304 to 151.99
Index ranges	$-8 \le h \le 8$, $-16 \le k \le 16$, $-39 \le l \le 40$
Reflections collected	56786

Independent reflections	6060 [R_{int} = 0.0771, R_{sigma} = 0.0292]
Data/restraints/parameters	6060/48/364
Goodness-of-fit on F^2	1.068
Final R indexes [I≥2σ (I)]	R_1 = 0.0451, wR_2 = 0.1280
Final R indexes [all data]	R_1 = 0.0471, wR_2 = 0.1303
Largest diff. peak/hole / e Å^{-3}	0.30/-0.34
Flack parameter	0.004(8)

5. ^{1}H and ^{13}C NMR spectra of products

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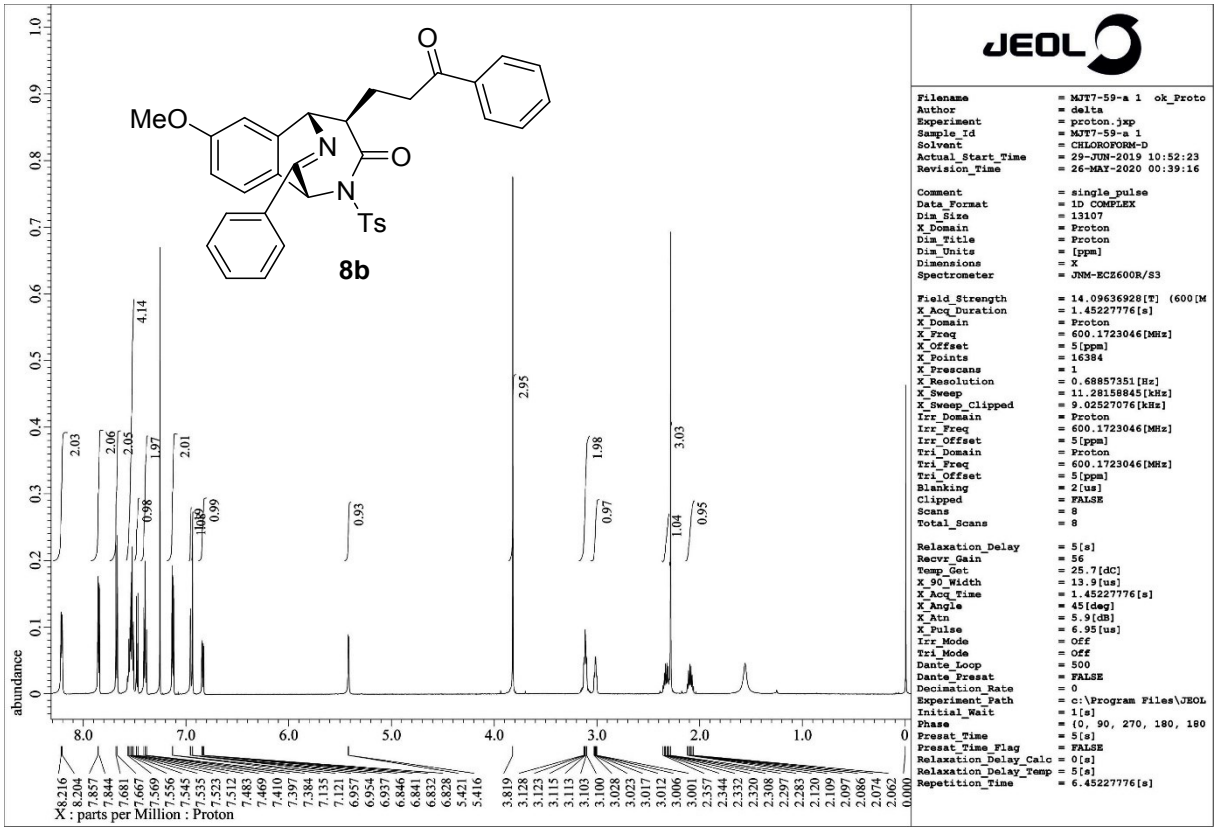
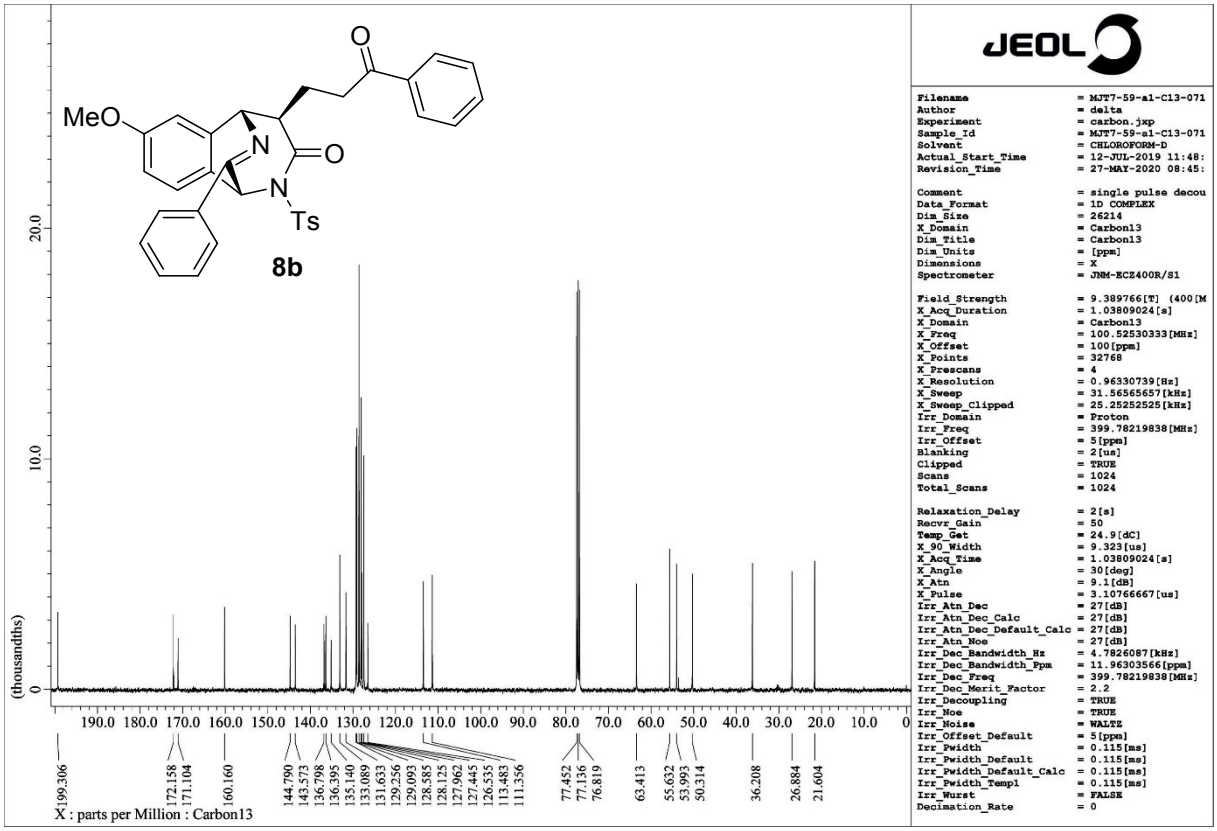
171.82
170.60
144.67
141.88
136.80
136.35
135.11
134.54
132.92
131.50
129.13
128.99
128.90
128.50
128.47
128.02
127.97
127.32
126.64
125.62
77.31
76.99
76.67
63.08
54.03
50.44
36.14
26.79
21.45
O
N
O
N
Ts
8a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


MeO
O
N
O
N
Ts
8b
abundance
4.14
2.03
2.06
2.05
1.97
2.01
0.98
1.02
0.99
0.93
2.95
1.98
0.97
3.03
1.04
0.95
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : Proton
JEOL
Filename = MJT7-59-a 1 ok_Proto
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-59-a 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-JUN-2019 10:52:23
Revision_Time = 26-MAY-2020 00:39:16
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 1.45227776[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.68857351[Hz]
X_Sweep = 11.28158845[kHz]
X_Sweep_Clipped = 9.02527076[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 = 25.7[dC]
X_90_Width = 13.9[us]
X_Acq_Time = 1.45227776[s]
X_Angle = 45[deg]
X_Atn = 5.9[dB]
X_Pulse = 6.95[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.45227776[s]


MeO
N
O
O
N
Ts
8b
(thousandths)
X : parts per Million : Carbon13
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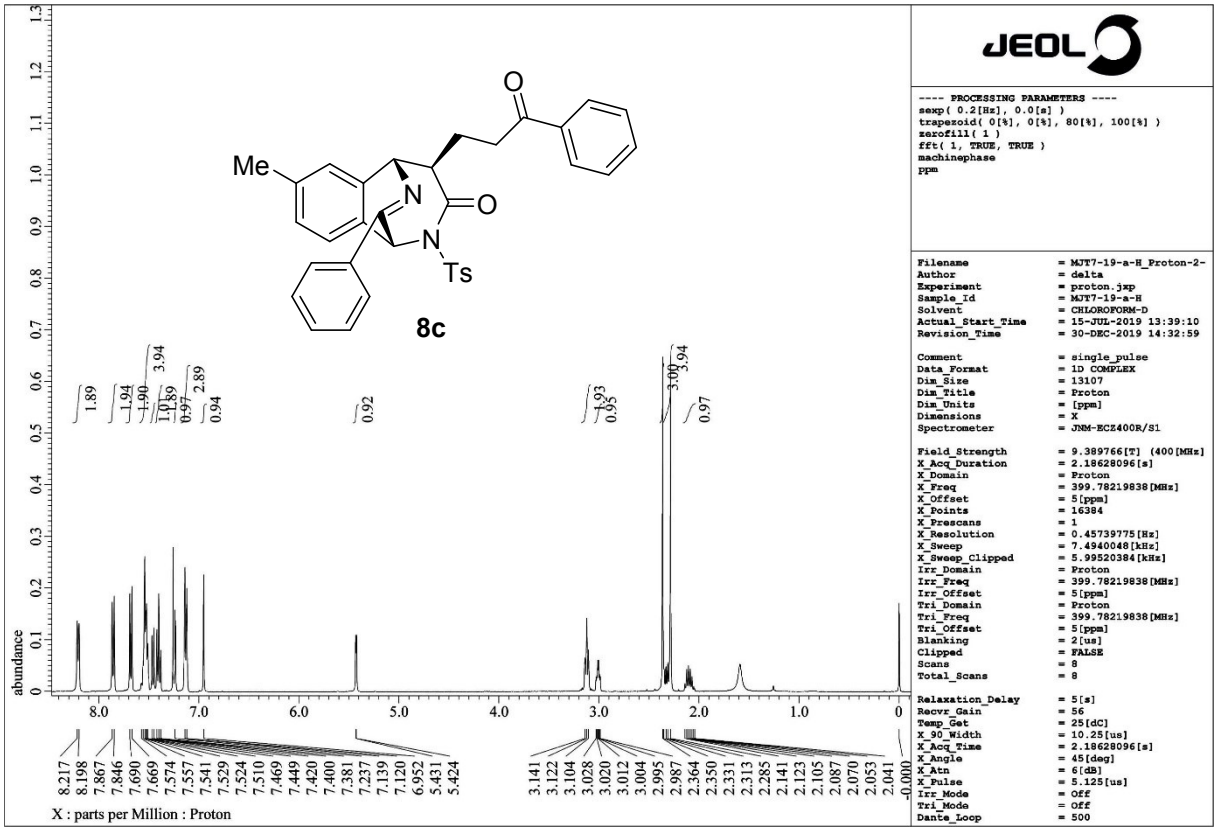
Filename = MJT7-59-a1-C13-071
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-59-a1-C13-071
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-JUL-2019 11:48:
Revision_Time = 27-MAY-2020 08:45:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
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 = 24.9[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]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Templ = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


Me
N
O
O
N
Ts
8c
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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Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-19-a-H
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-JUL-2019 13:39:10
Revision_Time = 30-DEC-2019 14:32:59
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Data_Format = 1D COMPLEX
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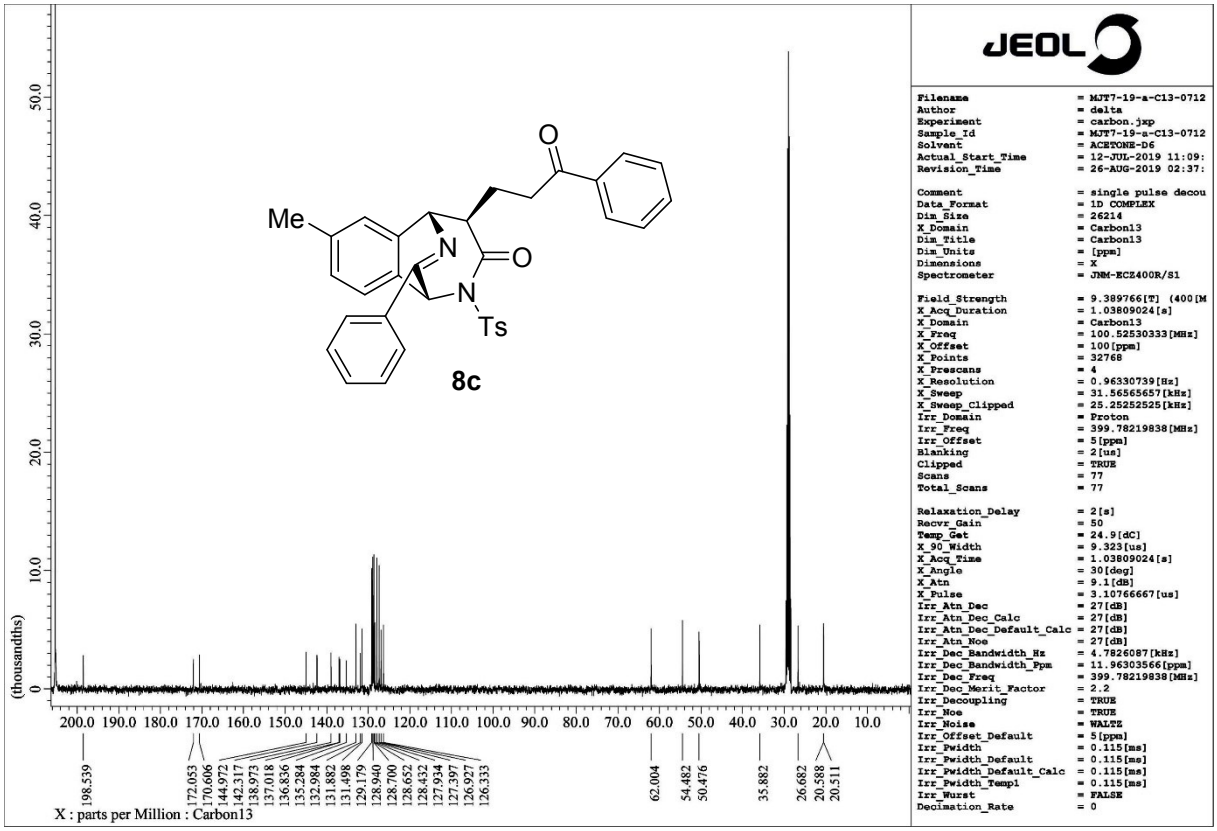
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 2.18628096[s]
X_Domain = Proton
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.9952038[kHz]
Irr_Domain = 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 = 25[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
N
O
N
Ts
O
8c
(thousandths)
X : parts per Million : Carbon13
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172.053
170.606
144.972
142.317
138.973
137.018
136.836
135.284
132.984
131.882
131.498
129.179
128.940
128.700
128.652
128.432
127.934
127.397
126.927
126.333
62.004
54.482
50.476
35.882
26.682
20.588
20.511
Filename = MJT7-19-a-C13-0712
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-19-a-C13-0712
Solvent = ACETONE-D6
Actual_Start_Time = 12-JUL-2019 11:09:
Revision_Time = 26-AUG-2019 02:37:
Comment = single pulse decou
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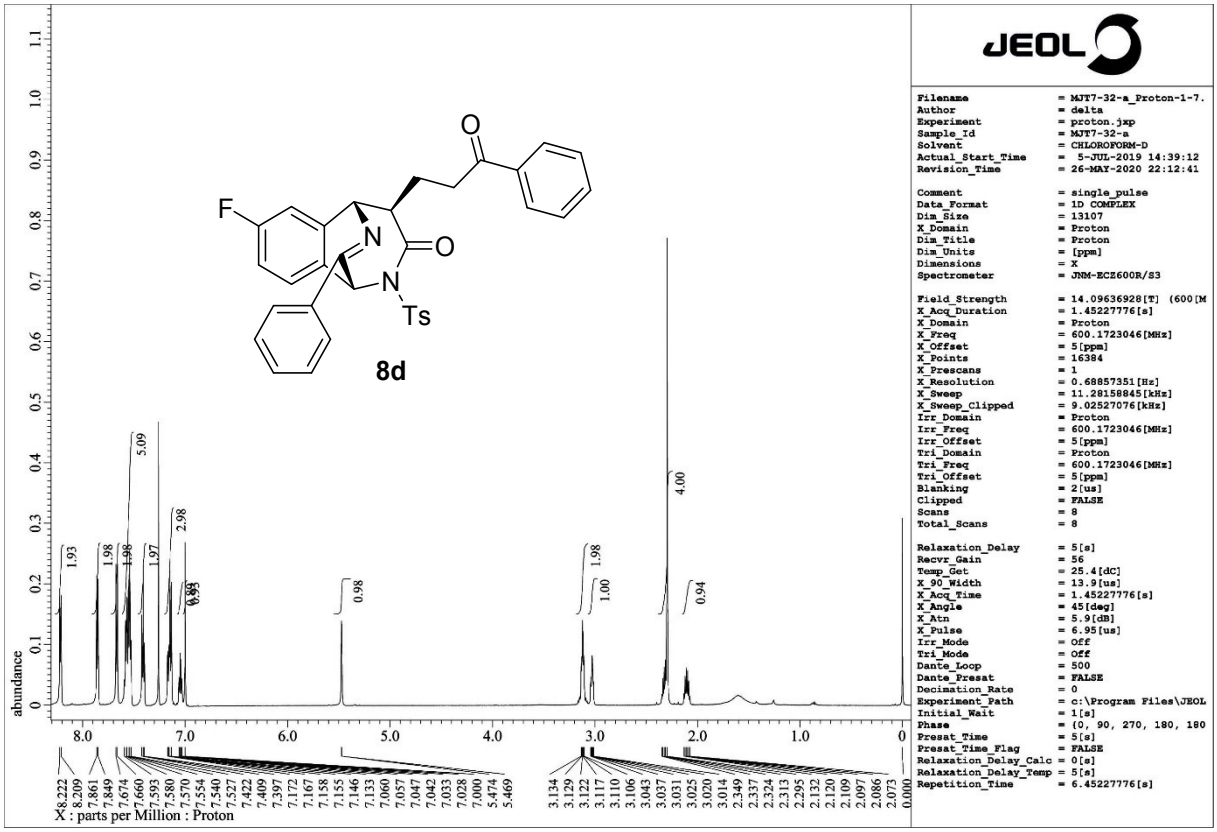
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[M
X_Acq_Duration = 1.03809024[s]
X_Domain = Carbon13
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = TRUE
Scans = 77
Total_Scans = 77
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.9[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]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Templ = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


F
N
O
N
Ts
O
8d
abundance
X : parts per Million : Proton
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1.98
1.98
1.98
1.97
5.09
2.98
0.98
1.98
1.00
4.00
0.94
8.222
8.209
7.861
7.849
7.674
7.660
7.593
7.580
7.570
7.554
7.540
7.527
7.422
7.409
7.397
7.172
7.167
7.158
7.155
7.146
7.133
7.060
7.057
7.047
7.042
7.033
7.028
7.000
5.474
5.469
3.134
3.129
3.122
3.117
3.110
3.106
3.043
3.037
3.031
3.025
3.020
3.014
2.349
2.337
2.324
2.313
2.295
2.132
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2.097
2.086
2.073
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Author = delta
Experiment = proton.jxp
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Revision_Time = 26-MAY-2020 22:12:41
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X_Acq_Duration = 1.45227776[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.68857351[Hz]
X_Sweep = 11.28158845[kHz]
X_Sweep_Clipped = 9.02527076[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 = 25.4[dC]
X_90_Width = 13.9[us]
X_Acq_Time = 1.45227776[s]
X_Angle = 45[deg]
X_Atn = 5.9[dB]
X_Pulse = 6.95[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
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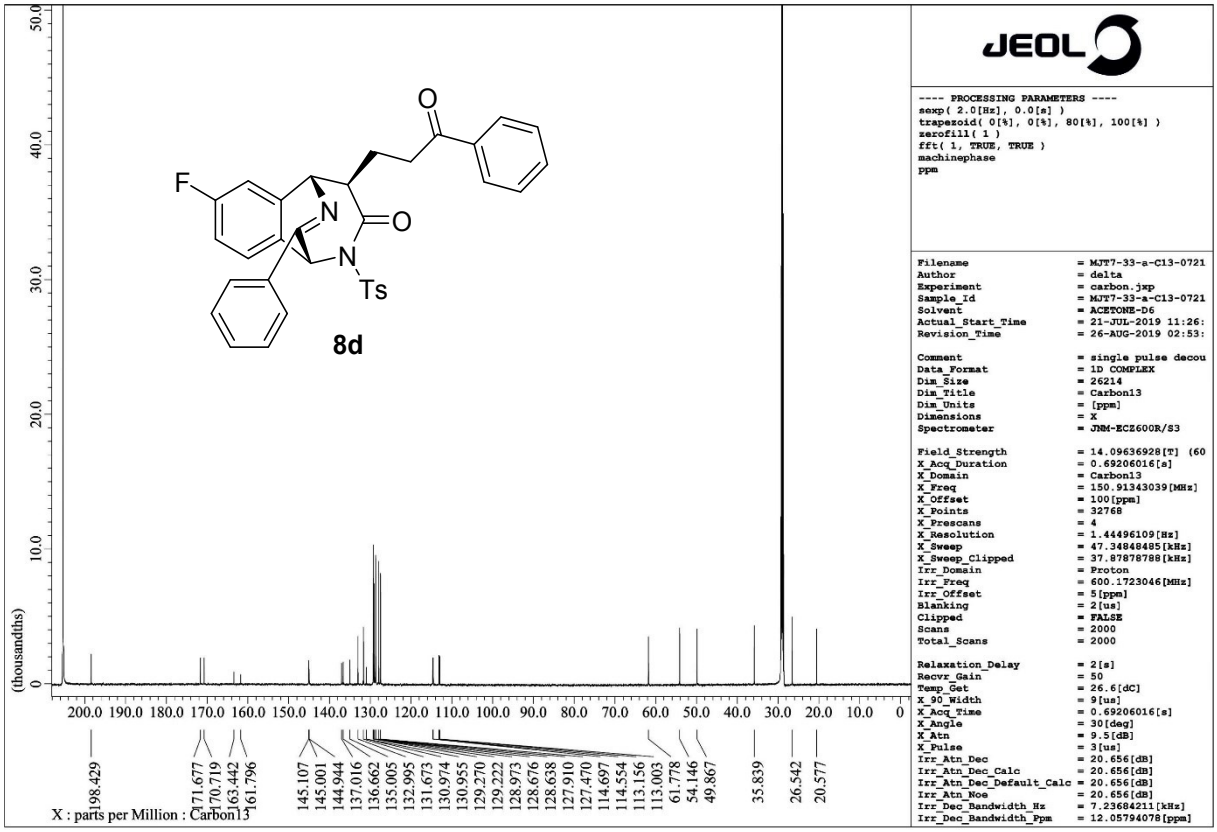
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.45227776[s]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O
N
O
N
Ts
8d
(thousandths)
X : parts per Million : Carbon13
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170.719
163.442
161.796
145.107
145.001
144.944
137.016
136.662
135.005
132.995
131.673
130.974
130.955
129.270
129.222
128.973
128.676
128.638
127.910
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113.003
61.778
54.146
49.867
35.839
26.542
20.577
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Author = delta
Experiment = carbon.jxp
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Actual_Start_Time = 21-JUL-2019 11:26:
Revision_Time = 26-AUG-2019 02:53:
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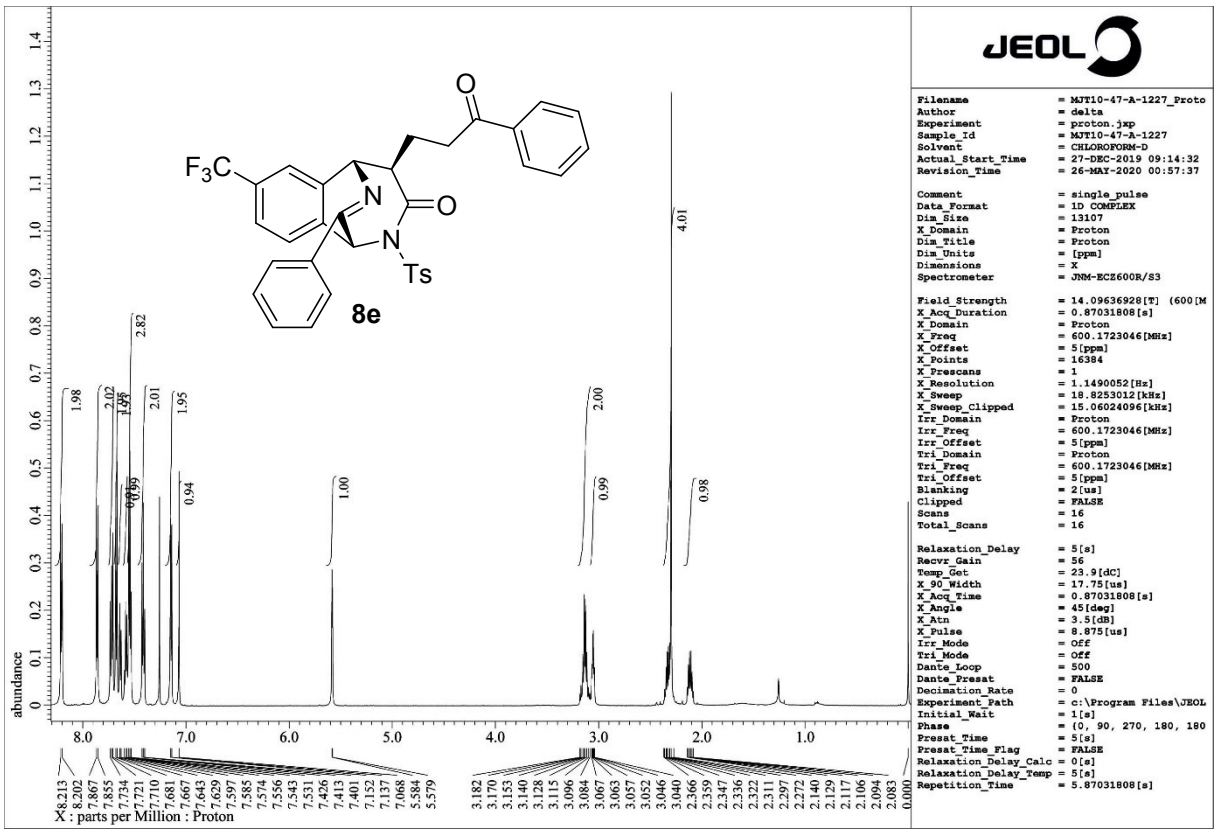
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (60
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 2000
Total_Scans = 2000
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 26.6[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.5[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 20.656[dB]
Irr_Atn_Dec_Calc = 20.656[dB]
Irr_Atn_Dec_Default_Calc = 20.656[dB]
Irr_Atn_Noe = 20.656[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]


F3C
O
N
O
N
Ts
8e
abundance
X : parts per Million : Proton
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8.202
7.867
7.855
7.734
7.721
7.710
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7.629
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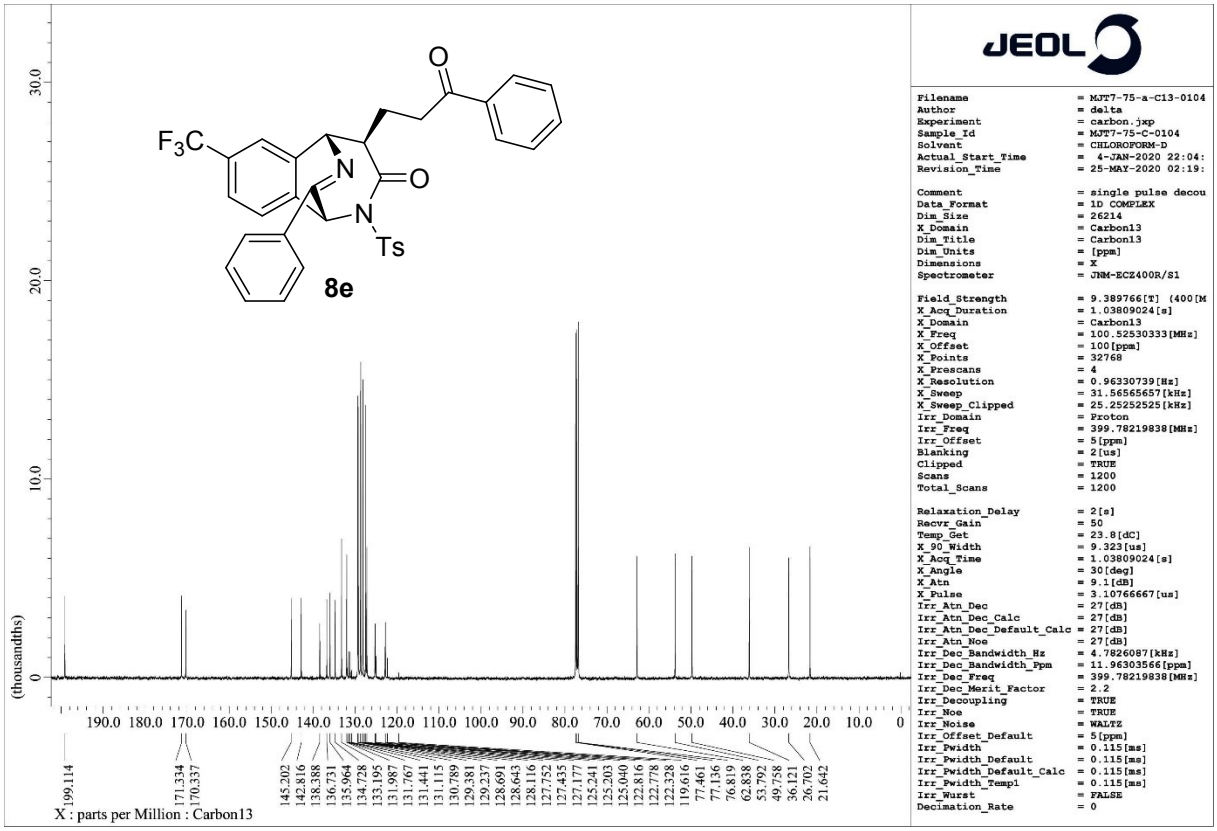
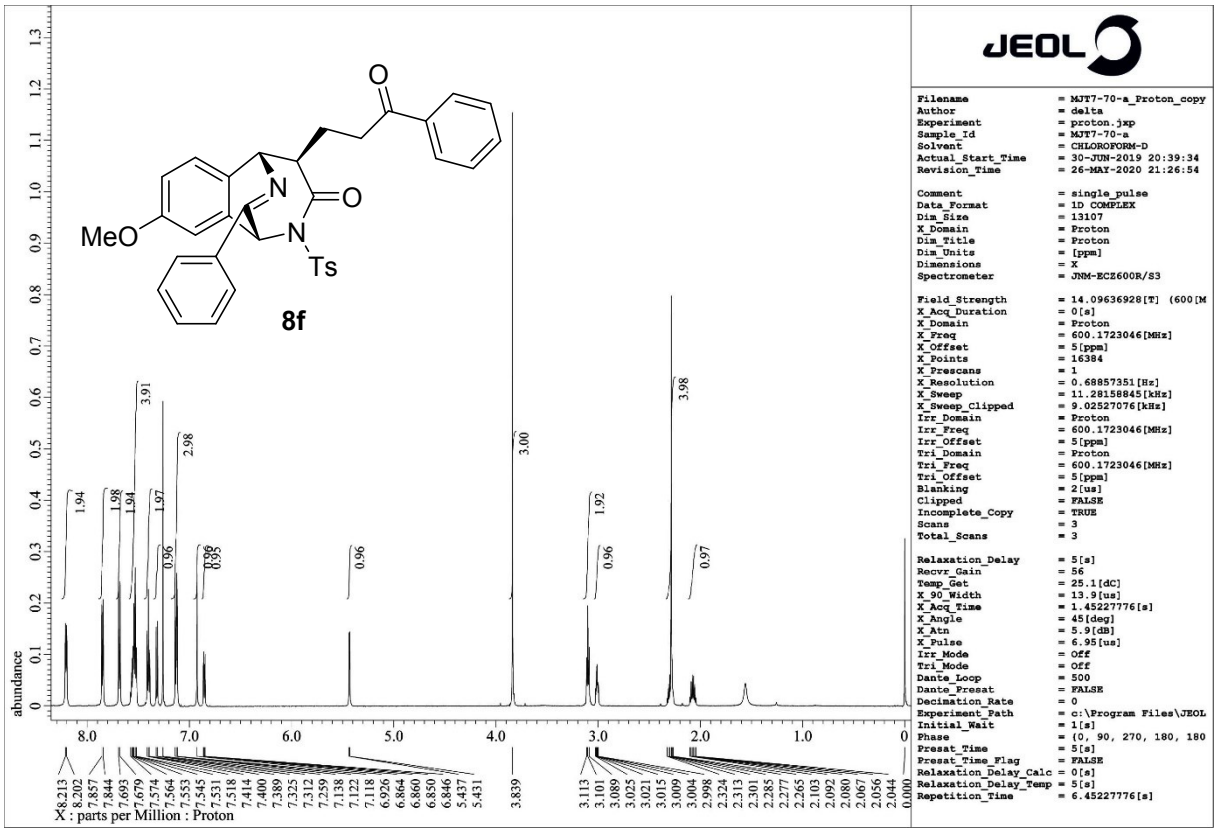
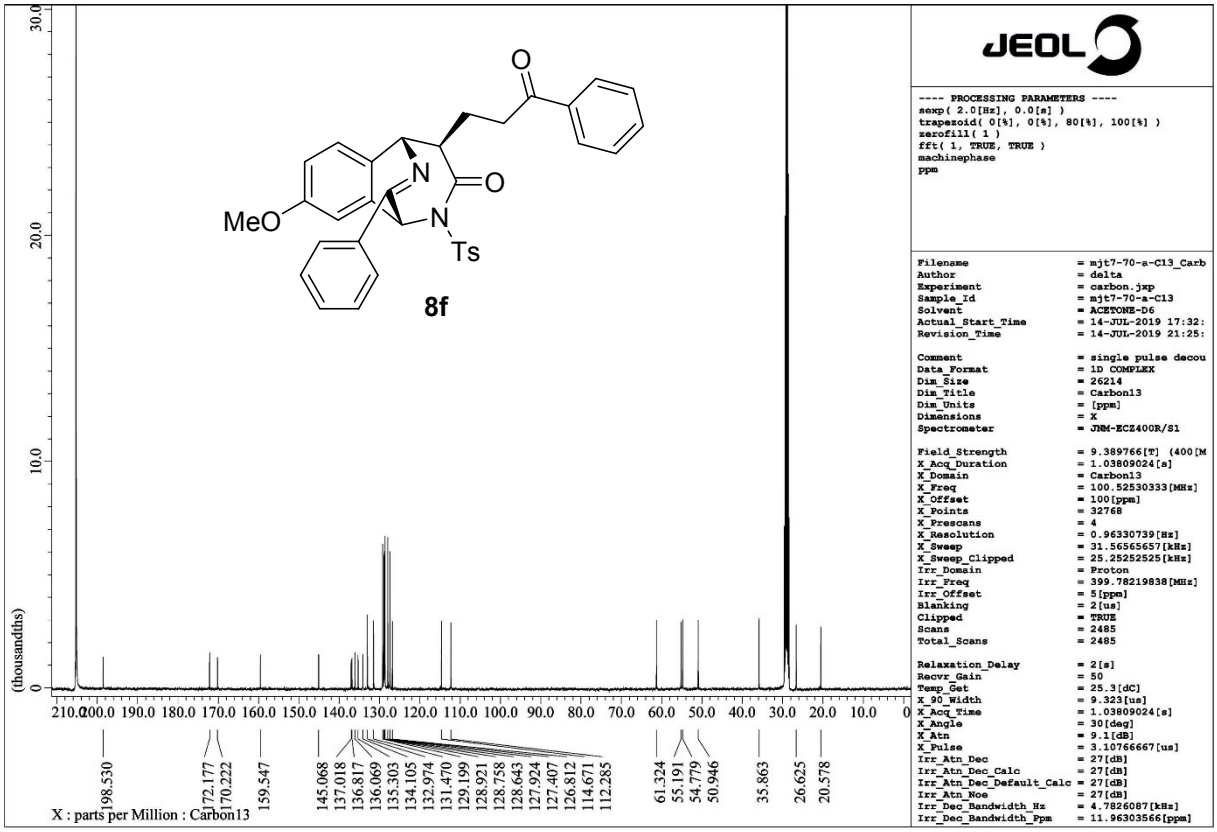
7.574
7.556
7.543
7.531
7.426
7.413
7.401
7.152
7.137
7.068
5.584
5.579
3.182
3.170
3.153
3.140
3.128
3.115
3.096
3.084
3.067
3.063
3.057
3.052
3.046
3.040
2.366
2.359
2.347
2.336
2.322
2.311
2.297
2.272
2.140
2.129
2.117
2.106
2.094
2.083
0.000
1.98
2.02
1.98
2.82
0.95
2.01
1.95
0.94
1.00
2.00
0.99
4.01
0.98
Filename = MJT10-47-A-1227_Proto
Author = delta
Experiment = proton.jxp
Sample_Id = MJT10-47-A-1227
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-DEC-2019 09:14:32
Revision_Time = 26-MAY-2020 00:57:37
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 5.87031808[s]

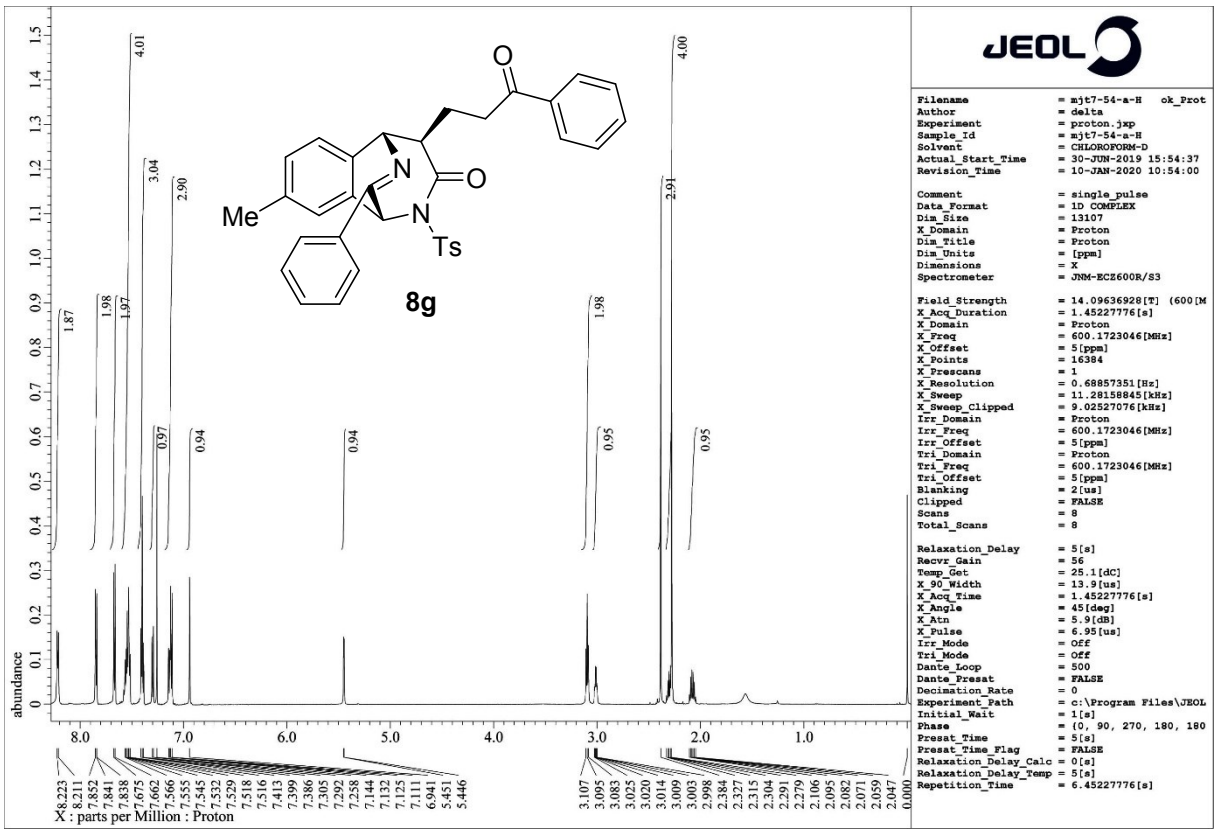

F3C
O
N
O
N
Ts
8e
(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = MJT7-75-a-C13-0104
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-75-C-0104
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-JAN-2020 22:04:
Revision_Time = 25-MAY-2020 02:19:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
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 = 1200
Total_Scans = 1200
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]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


MeO
O
N
O
N
Ts
8f
abundance
X : parts per Million : Proton
JEOL
Filename = MJT7-70-a_Proton_copy
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-70-a
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-JUN-2019 20:39:34
Revision_Time = 26-MAY-2020 21:26:54
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 0.68857351[Hz]
X_Sweep = 11.28158845[kHz]
X_Sweep_Clipped = 9.02527076[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 = 3
Total_Scans = 3
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 25.1[dC]
X_90_Width = 13.9[us]
X_Acq_Time = 1.45227776[s]
X_Angle = 45[deg]
X_Atn = 5.9[dB]
X_Pulse = 6.95[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.45227776[s]

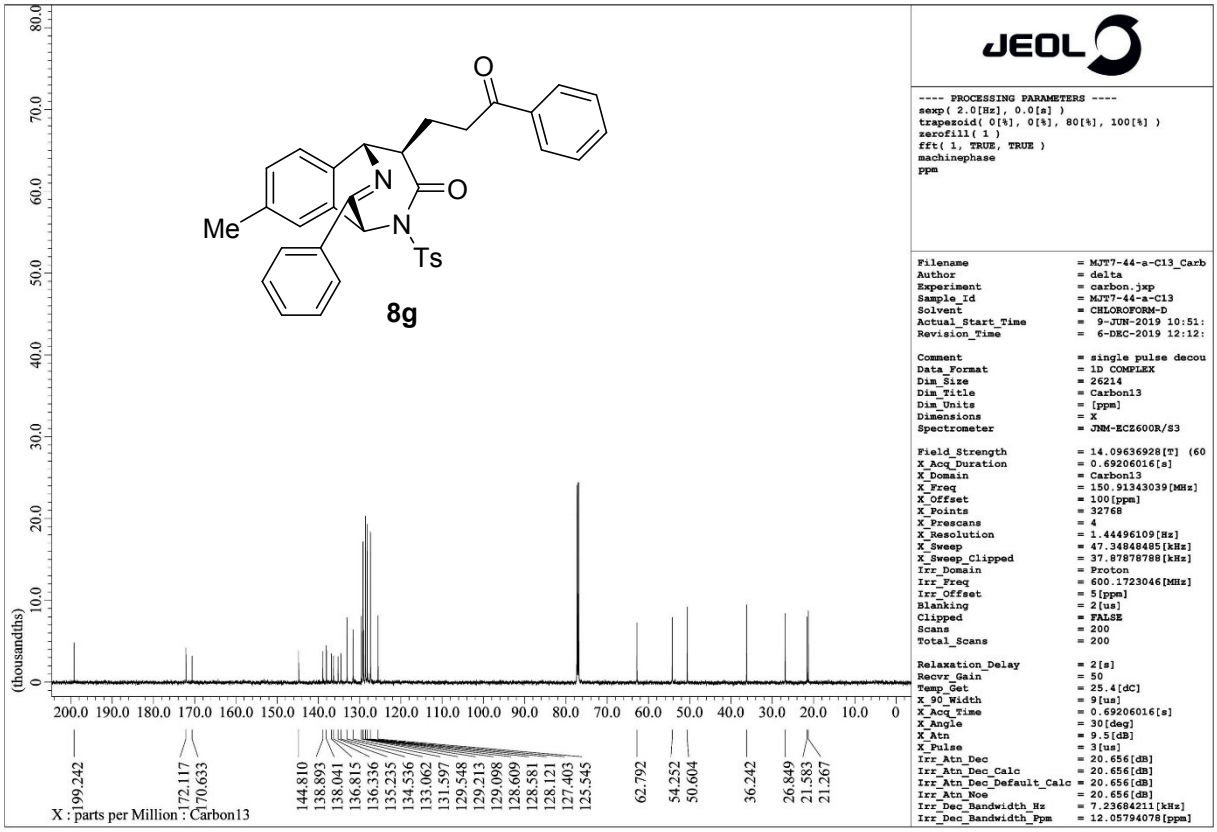


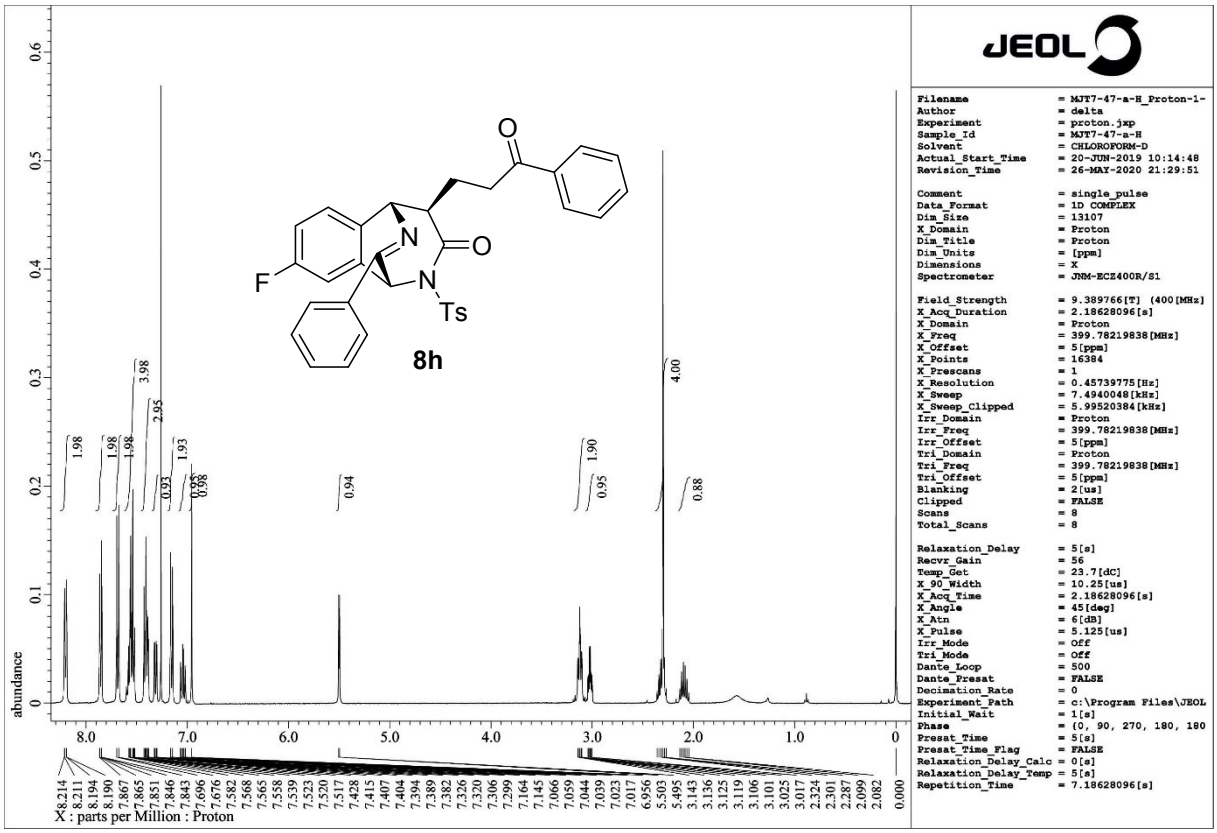

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

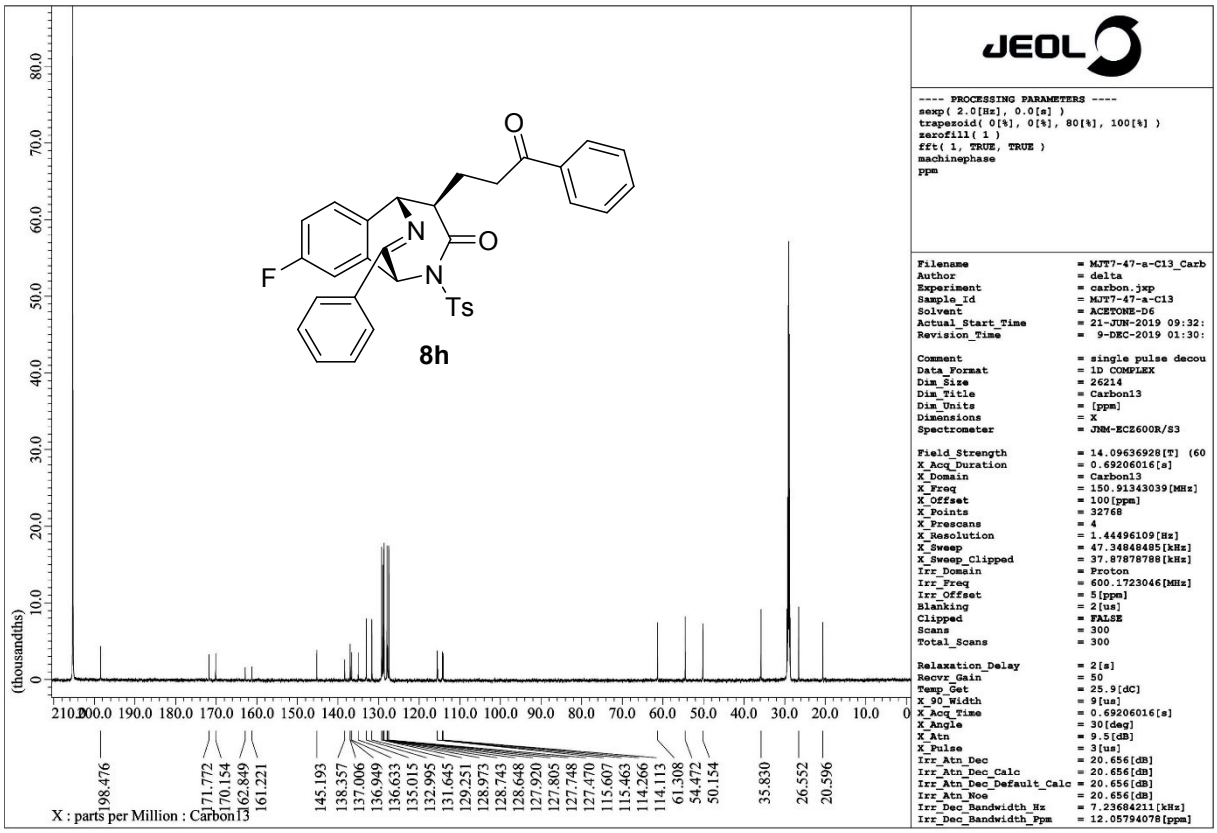
Filename	= mjt7-70-a-C13_Carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= mjt7-70-a-C13
Solvent	= ACETONE-D6
Actual_Start_Time	= 14-JUL-2019 17:32:
Revision_Time	= 14-JUL-2019 21:25:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= 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	= 2485
Total_Scans	= 2485
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 25.3[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]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]

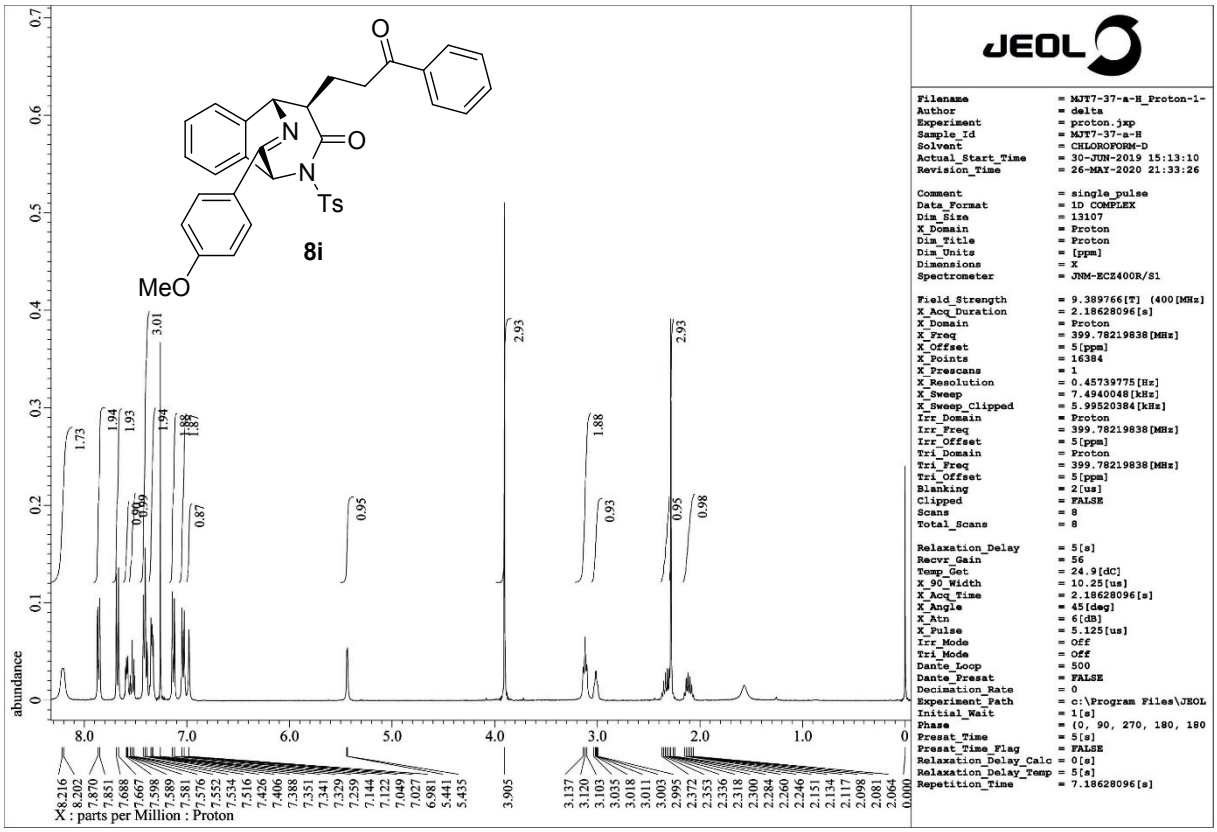


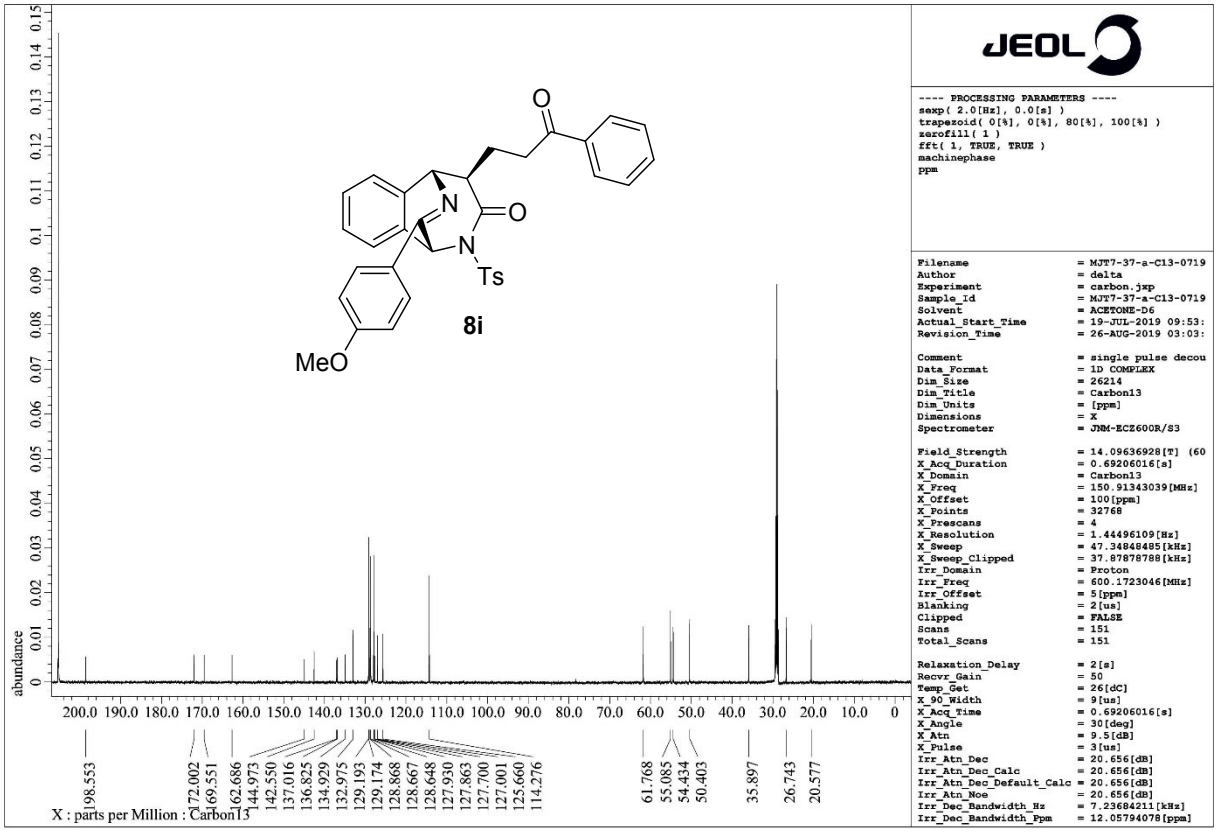
Filename	= mjt7-54-a-H ok_Prot
Author	= delta
Experiment	= proton.jxp
Sample_Id	= mjt7-54-a-H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-JUN-2019 15:54:37
Revision_Time	= 10-JAN-2020 10:54:00
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 1.45227776[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68857351[Hz]
X_Sweep	= 11.28158845[kHz]
X_Sweep_Clipped	= 9.02527076[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	= 25.1[dC]
X_90_Width	= 13.9[us]
X_Acq_Time	= 1.45227776[s]
X_Angle	= 45[deg]
X_Atn	= 5.9[dB]
X_Pulse	= 6.95[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 6.45227776[s]

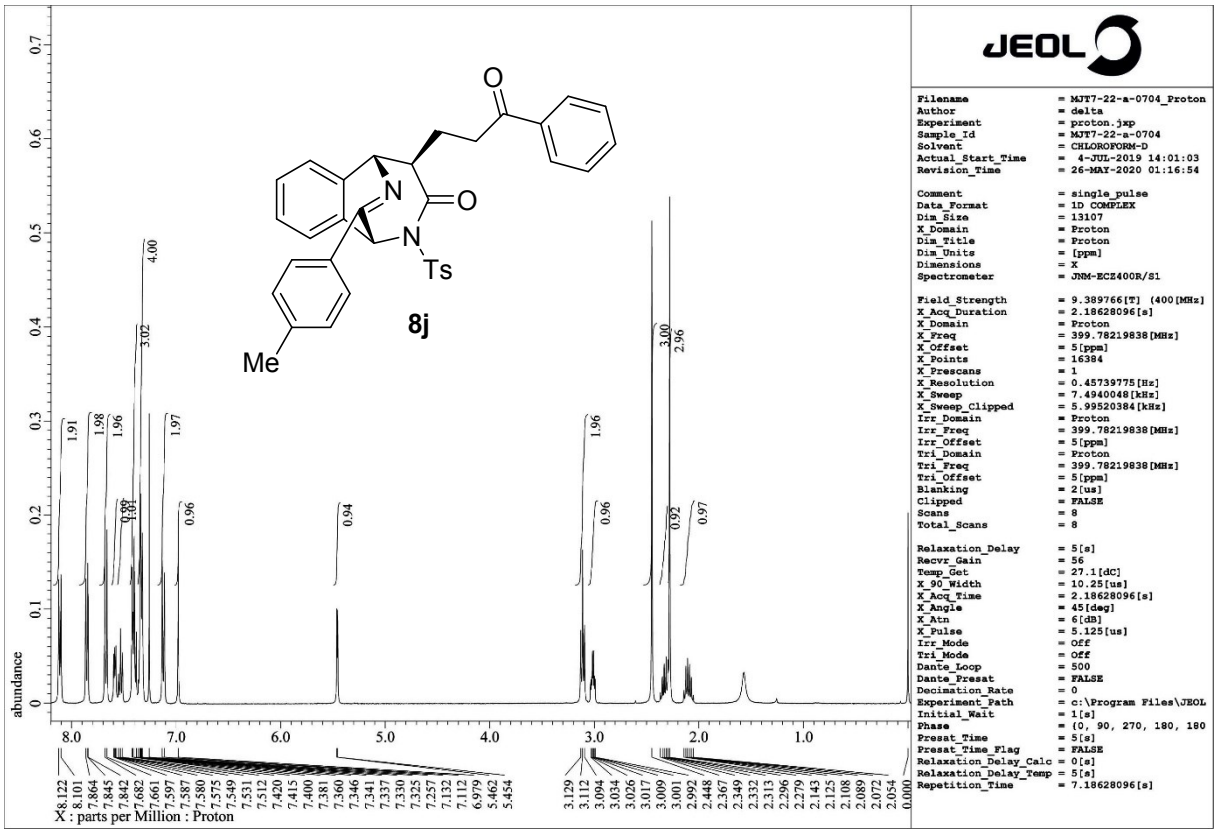

Me
N
O
N
Ts
O
8g
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = MJT7-44-a-C13_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-44-a-C13
Solvent = CHLOROFORM-D
Actual_Start_Time = 9-JUN-2019 10:51:
Revision_Time = 6-DEC-2019 12:12:
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 = 0.69206016[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 = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.4[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.5[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 20.656[dB]
Irr_Atn_Dec_Calc = 20.656[dB]
Irr_Atn_Dec_Default_Calc = 20.656[dB]
Irr_Atn_Noe = 20.656[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]

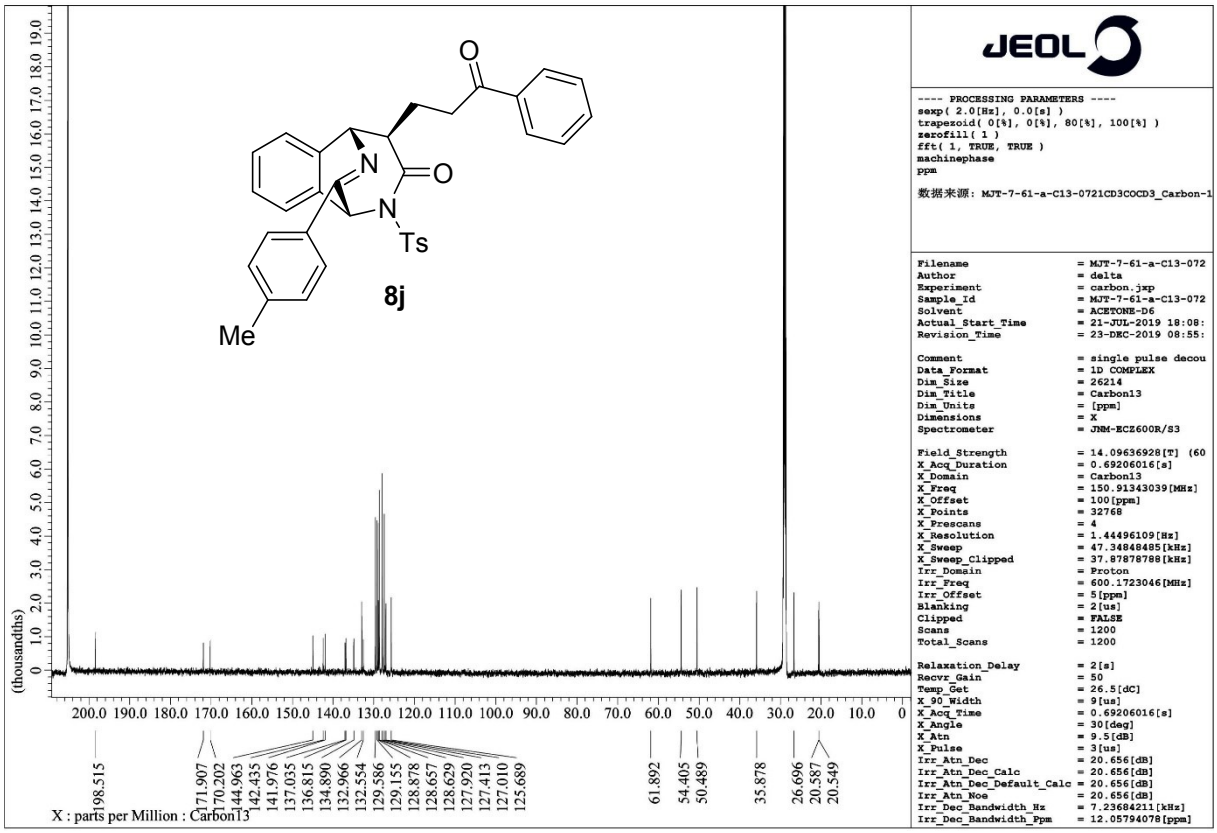

F
N
O
N
Ts
O
8h
abundance
X : parts per Million : Proton
Filename = MJT7-47-a-H_Proton-1-
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-47-a-H
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-JUN-2019 10:14:48
Revision_Time = 26-MAY-2020 21:29:51
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 23.7[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

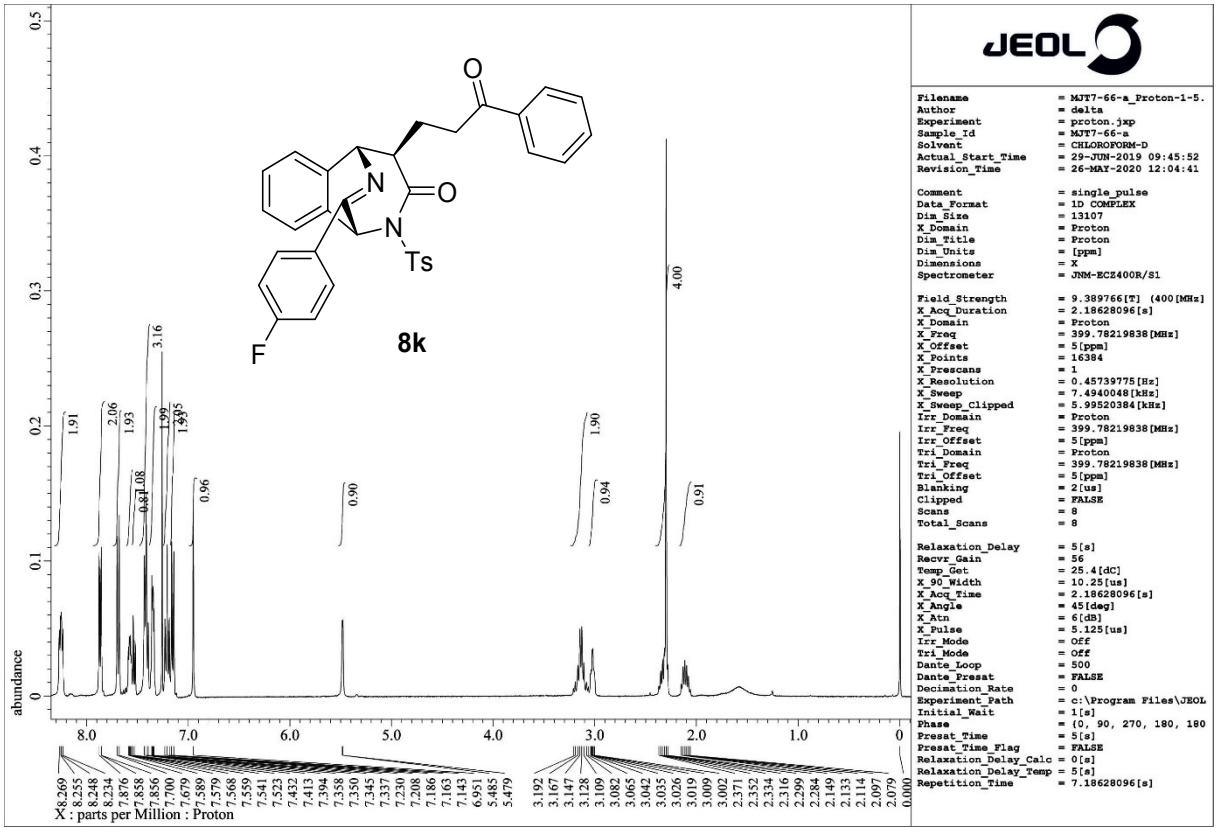

8h
F
Ts
(thousandths)
X : parts per Million : Carbon13
198.476
171.772
170.154
162.849
161.221
145.193
138.357
137.006
136.949
136.633
135.015
132.995
131.645
129.251
128.973
128.743
128.648
127.920
127.805
127.748
127.470
115.607
115.463
114.266
114.113
61.308
54.472
50.154
35.830
26.552
20.596
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = MJT7-47-a-C13_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-47-a-C13
Solvent = ACETONE-D6
Actual_Start_Time = 21-JUN-2019 09:32:
Revision_Time = 9-DEC-2019 01:30:
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 = 0.69206016[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 = 300
Total_Scans = 300
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.9[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.5[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 20.656[dB]
Irr_Atn_Dec_Calc = 20.656[dB]
Irr_Atn_Dec_Default_Calc = 20.656[dB]
Irr_Atn_Noe = 20.656[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]

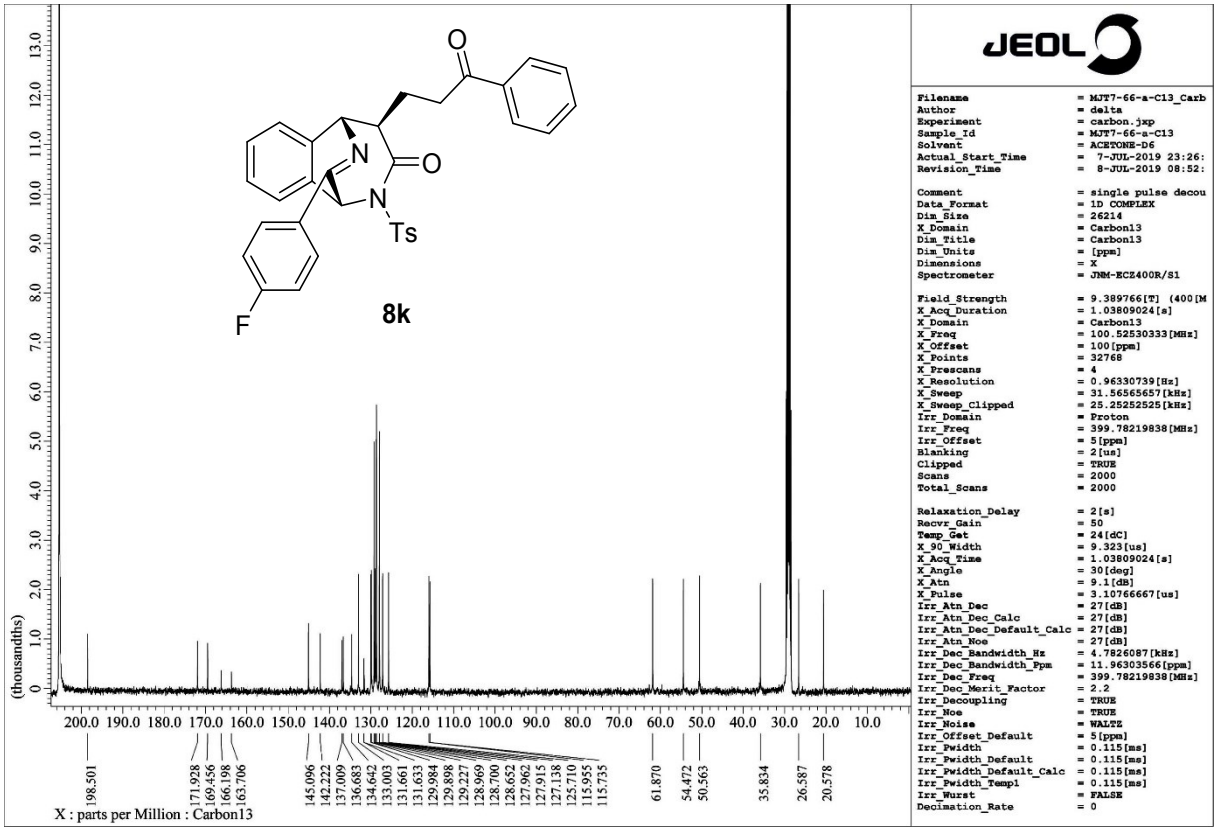

8i
MeO
Ts
abundance
X : parts per Million : Proton
8.216
8.202
7.870
7.851
7.688
7.667
7.598
7.589
7.581
7.576
7.552
7.534
7.516
7.426
7.406
7.388
7.351
7.341
7.329
7.259
7.144
7.122
7.049
7.027
6.981
5.441
5.435
3.905
3.137
3.120
3.103
3.035
3.018
3.011
3.003
2.995
2.372
2.353
2.336
2.318
2.300
2.284
2.260
2.246
2.151
2.134
2.117
2.098
2.081
2.064
2.000
Filename = MJT7-37-a-H_Proton-1-
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-37-a-H
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-JUN-2019 15:13:10
Revision_Time = 26-MAY-2020 21:33:26
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 24.9[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]


8i
MeO
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
Filename = MJT7-37-a-C13-0719
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-37-a-C13-0719
Solvent = ACETONE-D6
Actual_Start_Time = 19-JUL-2019 09:53:
Revision_Time = 26-AUG-2019 03:03:
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 = 151
Total_Scans = 151
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 26[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.5[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 20.656[dB]
Irr_Atn_Dec_Calc = 20.656[dB]
Irr_Atn_Dec_Default_Calc = 20.656[dB]
Irr_Atn_Noe = 20.656[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]


8j
Me
abundance
X : parts per Million : Proton
Filename = MJT7-22-a-0704_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-22-a-0704
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-JUL-2019 14:01:03
Revision_Time = 26-MAY-2020 01:16:54
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 27.1[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

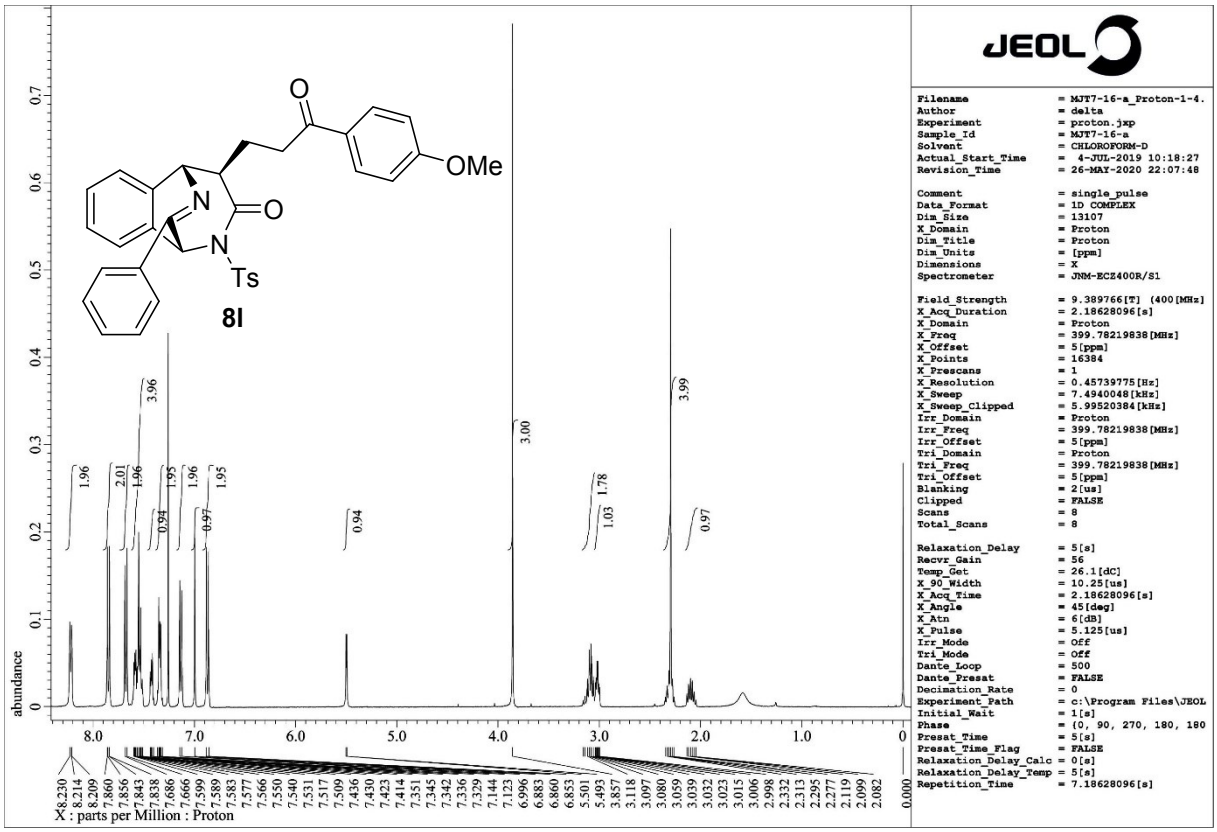

O
N
O
N
Ts
Me
8j
(thousandths)
X : parts per Million : Carbon13
198.515
171.907
170.202
144.963
142.435
141.976
137.035
136.815
134.890
132.966
132.554
129.586
129.155
128.878
128.657
128.629
127.920
127.413
127.010
125.689
61.892
54.405
50.489
35.878
26.696
20.587
20.549
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: MJT-7-61-a-C13-0721CD3COCD3_Carbon-1
Filename = MJT-7-61-a-C13-072
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT-7-61-a-C13-072
Solvent = ACETONE-D6
Actual_Start_Time = 21-JUL-2019 18:08:
Revision_Time = 23-DEC-2019 08:55:
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 = 1200
Total_Scans = 1200
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 26.5[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.5[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 20.656[dB]
Irr_Atn_Dec_Calc = 20.656[dB]
Irr_Atn_Dec_Default_Calc = 20.656[dB]
Irr_Atn_Noe = 20.656[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]


O
N
O
N
Ts
F
8k
abundance
X : parts per Million : Proton
8.269
8.255
8.248
8.234
7.876
7.858
7.856
7.700
7.679
7.589
7.579
7.568
7.559
7.541
7.523
7.432
7.413
7.394
7.358
7.350
7.345
7.337
7.230
7.208
7.186
7.163
7.143
6.951
5.485
5.479
3.192
3.167
3.147
3.128
3.109
3.082
3.065
3.042
3.035
3.026
3.019
3.009
3.002
2.371
2.352
2.334
2.316
2.299
2.284
2.149
2.133
2.114
2.097
2.079
2.000
1.91
2.06
1.93
1.96
1.95
3.16
1.08
0.81
0.96
0.90
1.90
0.94
4.00
0.91
JEOL
Filename = MJT7-66-a_Proton-1-5.
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-66-a
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-JUN-2019 09:45:52
Revision_Time = 26-MAY-2020 12:04:41
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 25.4[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]



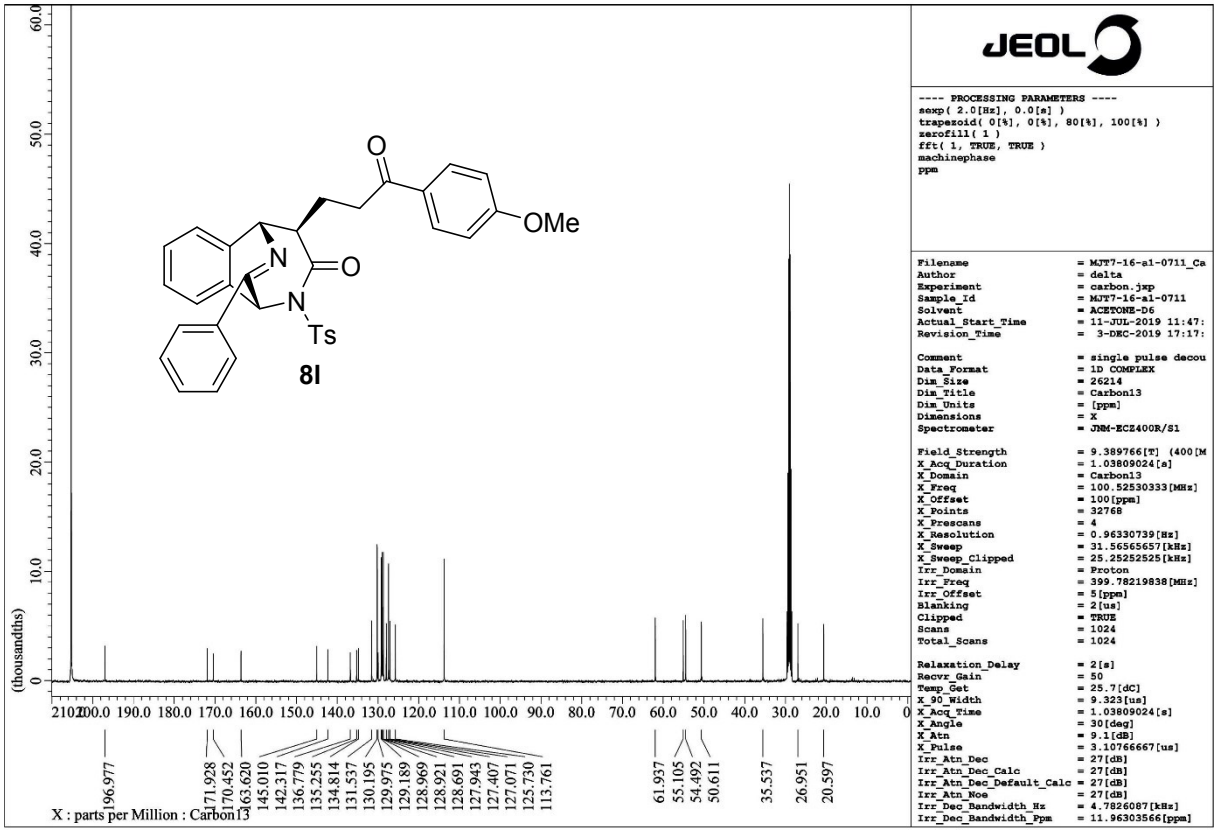
JEOL

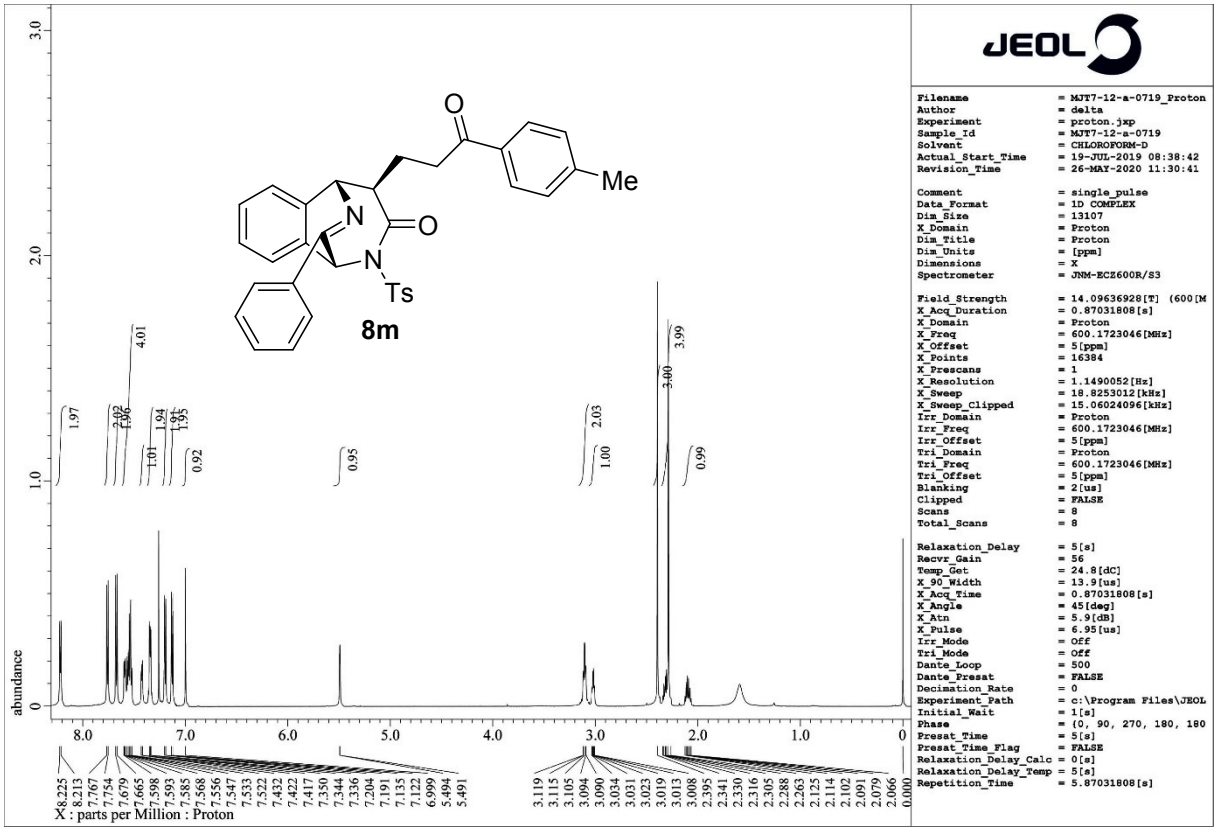
Filename	= MJT7-66-a-C13_Carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= MJT7-66-a-C13
Solvent	= ACETONE-D6
Actual_Start_Time	= 7-JUL-2019 23:26:
Revision_Time	= 8-JUL-2019 08:52:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [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	= 2000
Total_Scans	= 2000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 24[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]
Irr_Dec_Freq	= 399.78219838[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 0.115[ms]
Irr_Pwidth_Default	= 0.115[ms]
Irr_Pwidth_Default_Calc	= 0.115[ms]
Irr_Pwidth_Temp1	= 0.115[ms]
Irr_Wurst	= FALSE
Decimation_Rate	= 0

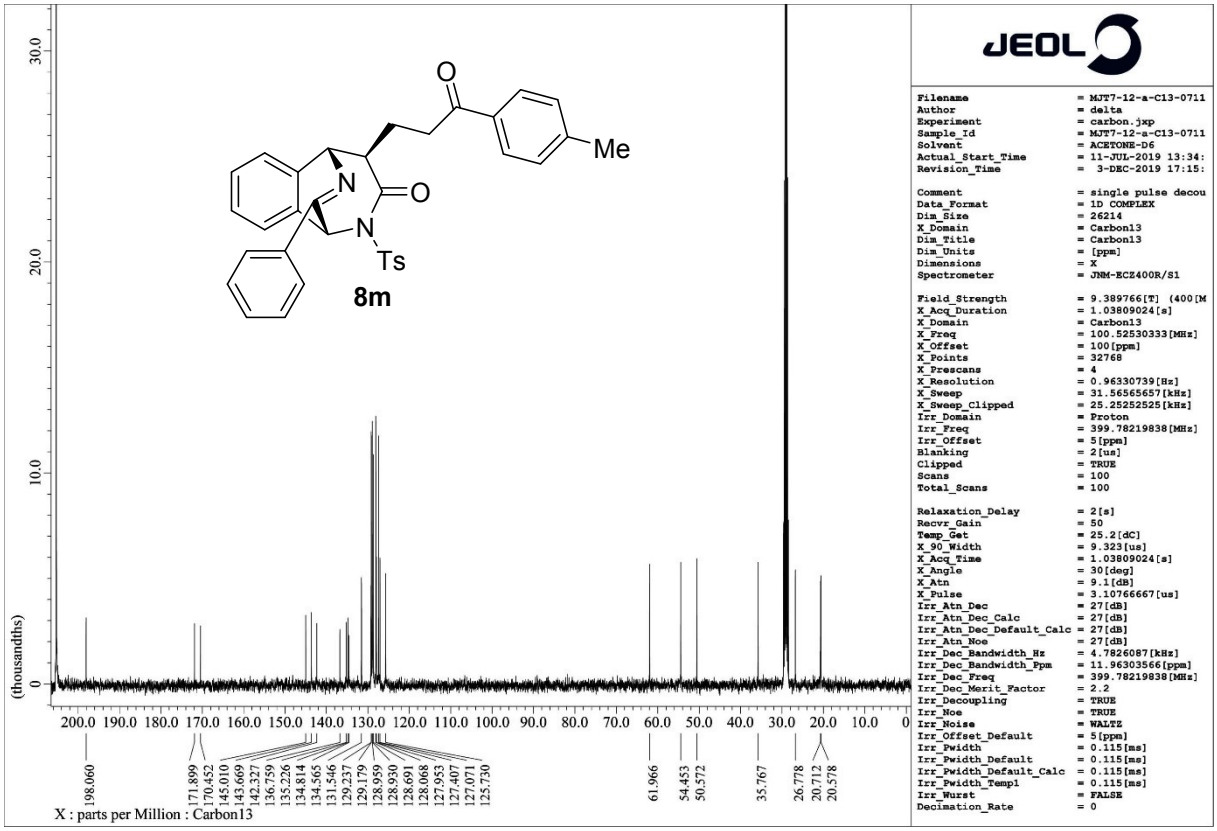


JEOL

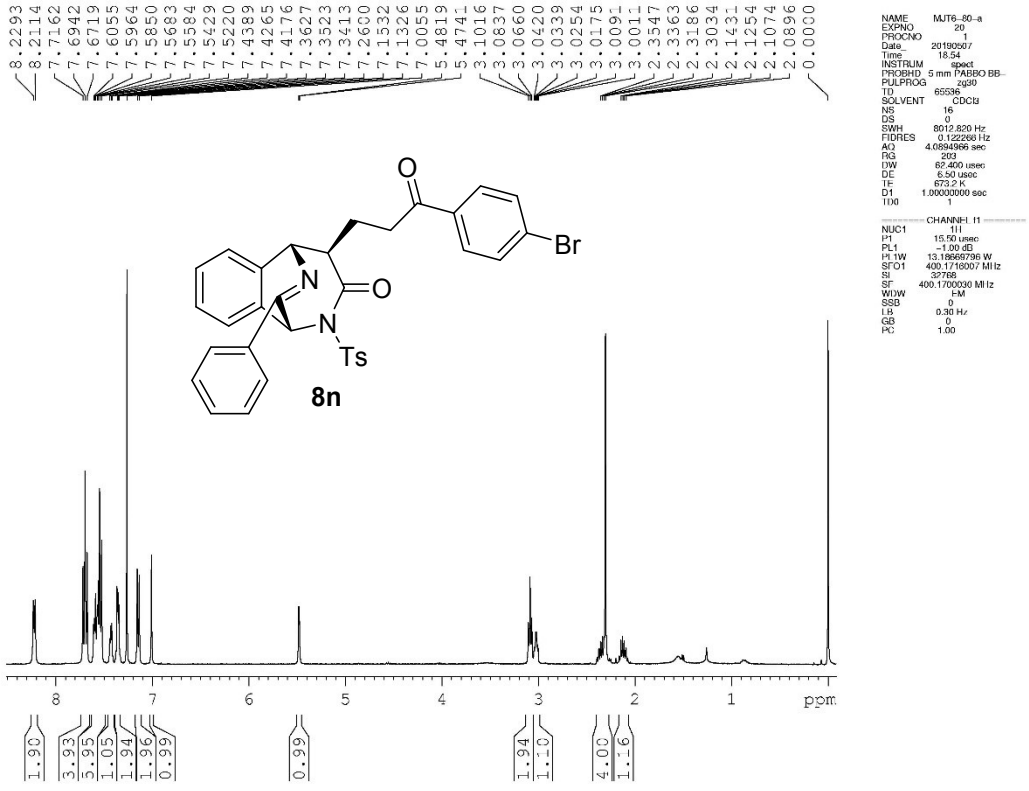
Filename	= MJT7-16-a_Proton-1-4.
Author	= delta
Experiment	= proton.jxp
Sample_Id	= MJT7-16-a
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 4-JUL-2019 10:18:27
Revision_Time	= 26-MAY-2020 22:07:48
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [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	= 26.1[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
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 7.18628096[s]


OMe
N
O
N
Ts
8l
(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 = MJT7-16-a1-0711_Ca
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-16-a1-0711
Solvent = ACETONE-D6
Actual_Start_Time = 11-JUL-2019 11:47:
Revision_Time = 3-DEC-2019 17:17:
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 = 25.7[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]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]

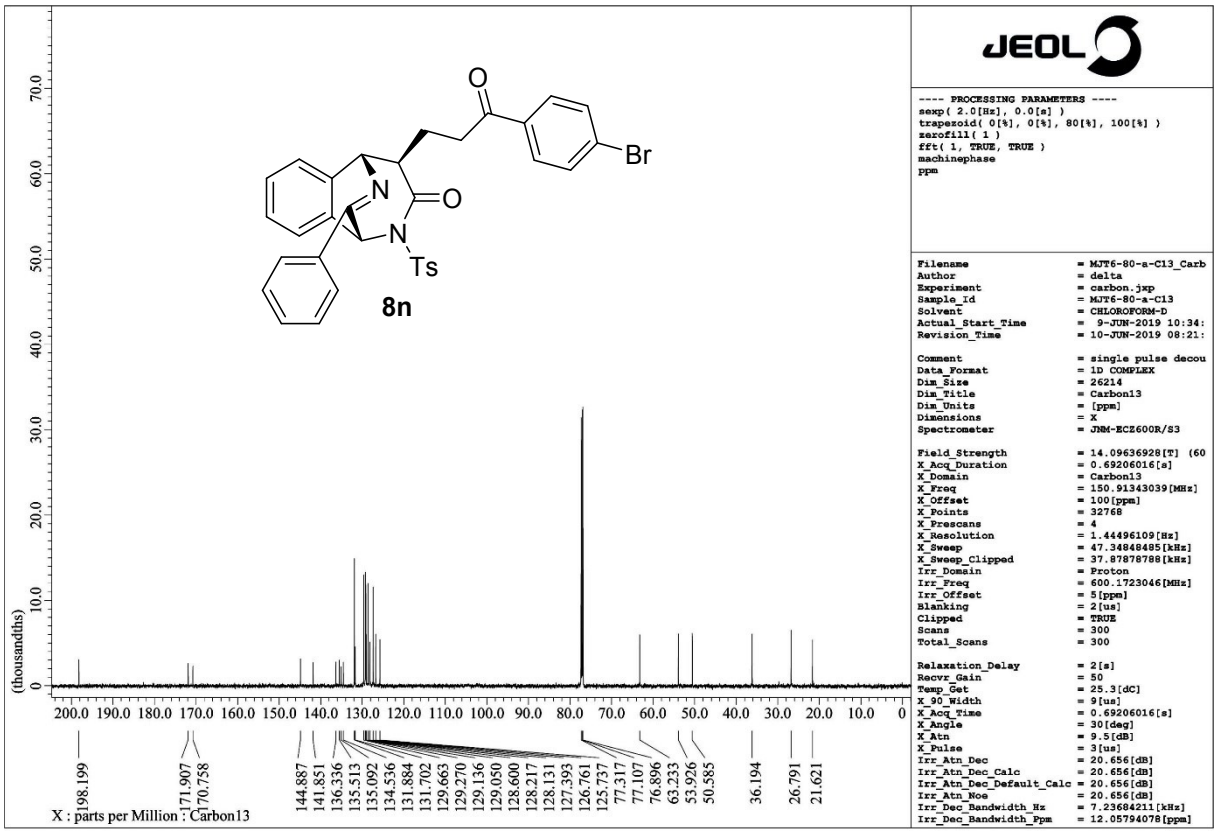

Me
N
O
N
Ts
8m
abundance
X : parts per Million : Proton
Filename = MJT7-12-a-0719_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-12-a-0719
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUL-2019 08:38:42
Revision_Time = 26-MAY-2020 11:30:41
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 24.8[dC]
X_90_Width = 13.9[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 5.9[dB]
X_Pulse = 6.95[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 5.87031808[s]

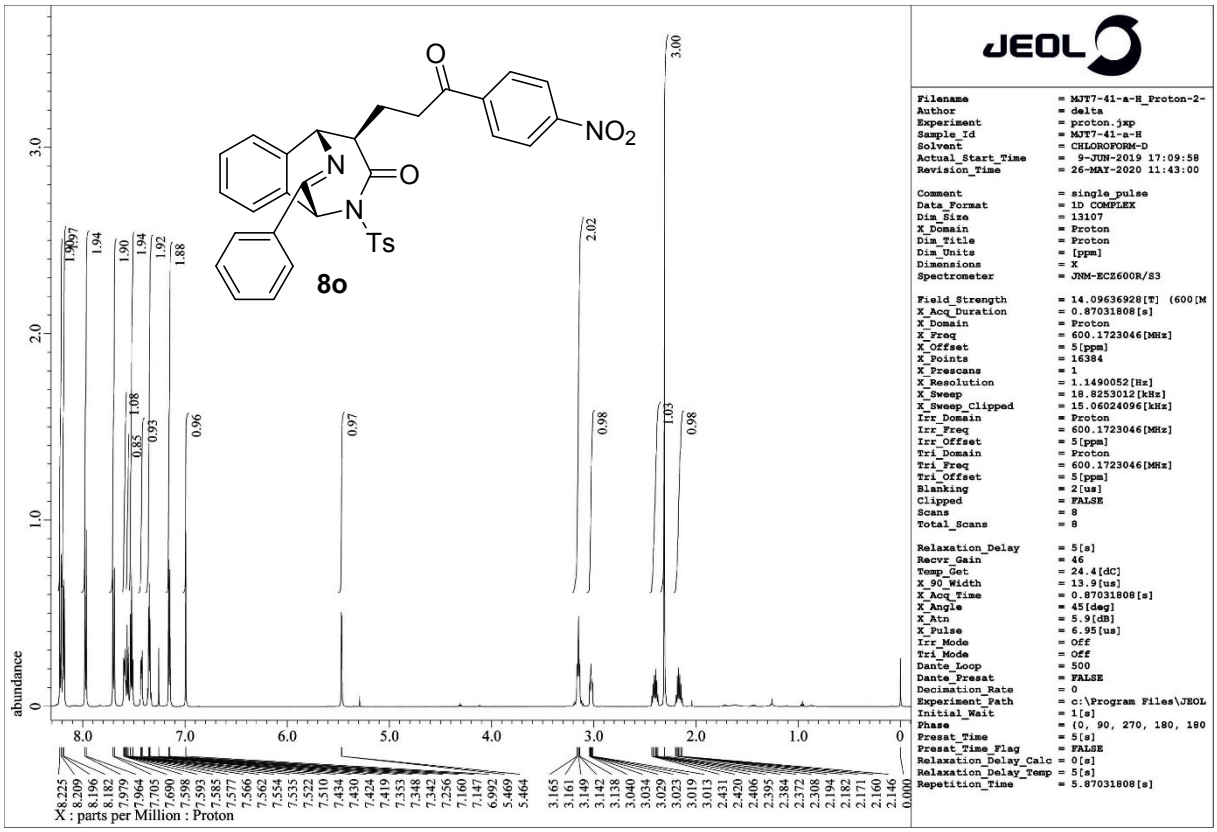


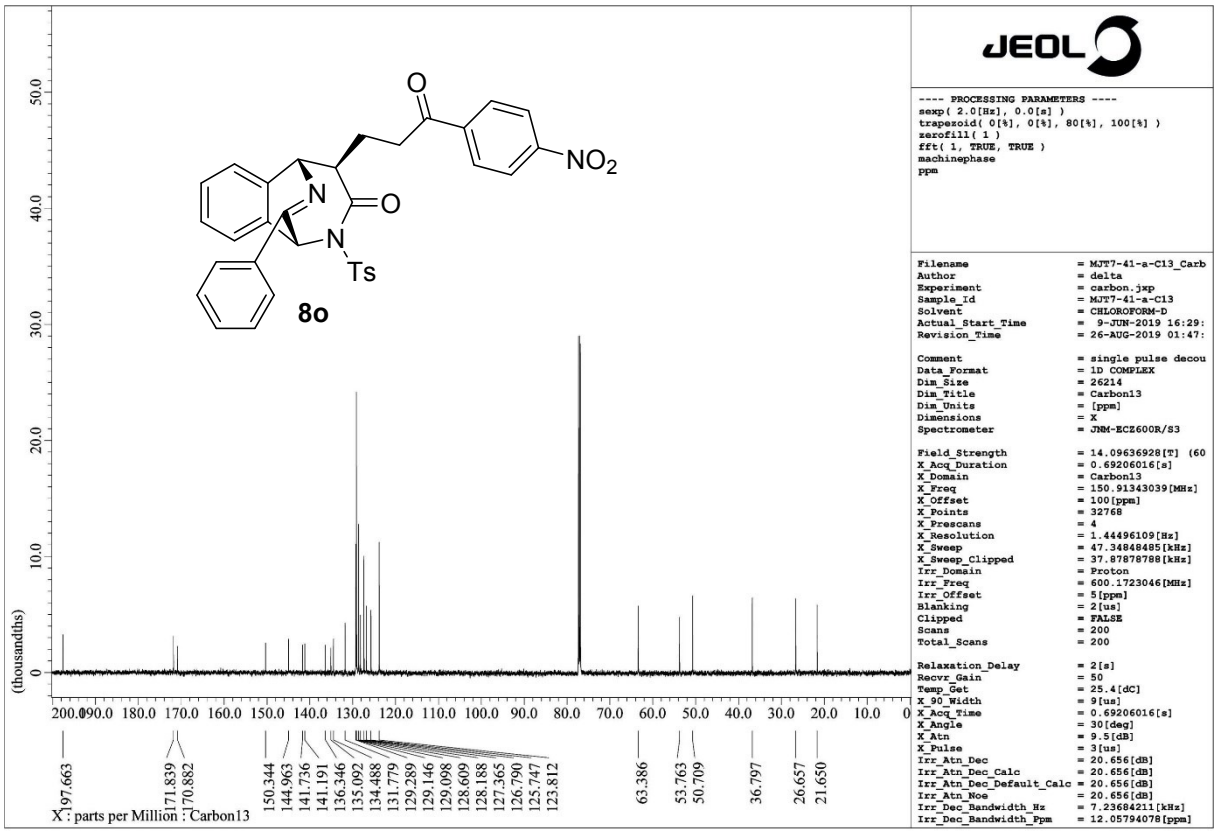

```
Filename                = MJT7-12-a-C13-0711
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = MJT7-12-a-C13-0711
Solvent                 = ACETONE-D6
Actual_Start_Time       = 11-JUL-2019 13:34:
Revision_Time           =  3-DEC-2019 17:15:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Carbon13
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                   = 100
Total_Scans             = 100

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]
Irr_Dec_Bandwidth_Hz    = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm   = 11.96303566[ppm]
Irr_Dec_Freq            = 399.78219838[MHz]
Irr_Dec_Merit_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = TRUE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 0.115[ms]
Irr_Pwidth_Default      = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1        = 0.115[ms]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
```

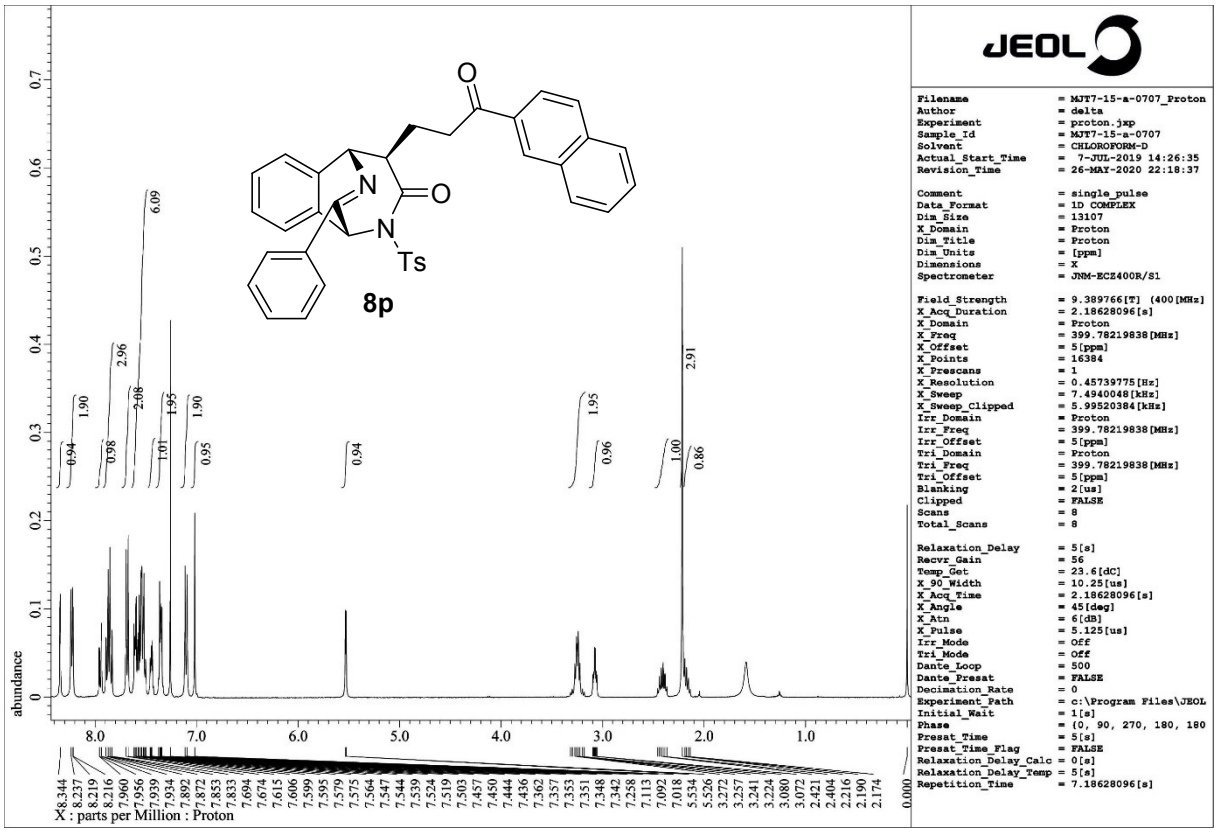


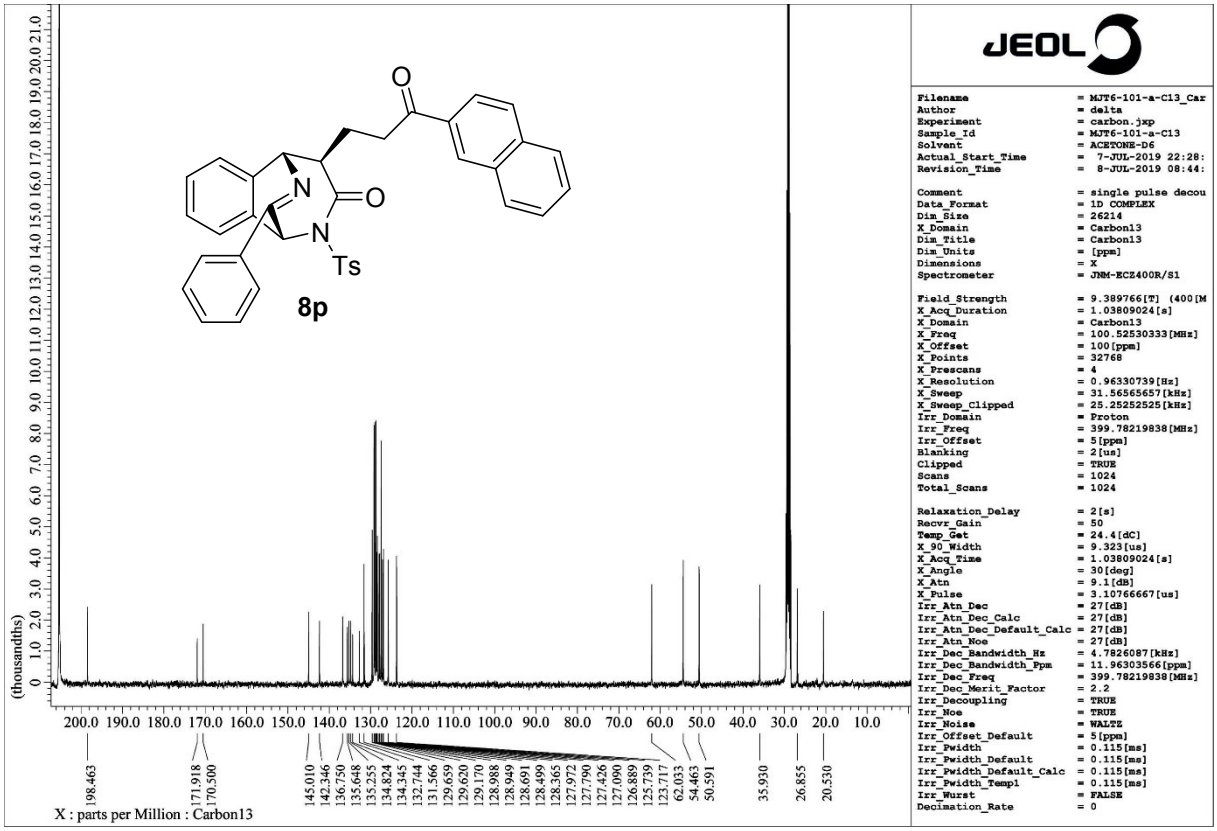

```
NAME            MJT6-80-a
EXPNO                  20
PROCNO                  1
Date_            20190507
Time                18.54
INSTRUM              spect
PROBHD  5 mm PABBO BB-
PULPROG             zgpg
TD                  65536
SOLVENT            CDCl3
NS                     16
DS                      0
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                    203
DW                82.400 usec
DE                 6.50 usec
TE                 673.2 K
D1               1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                15.50 usec
PL1               -1.00 dB
PL1W        13.18666796 W
SFO1        400.1716007 MHz
SI                  32768
SF          400.1700030 MHz
WDW                 EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                  1.00
```

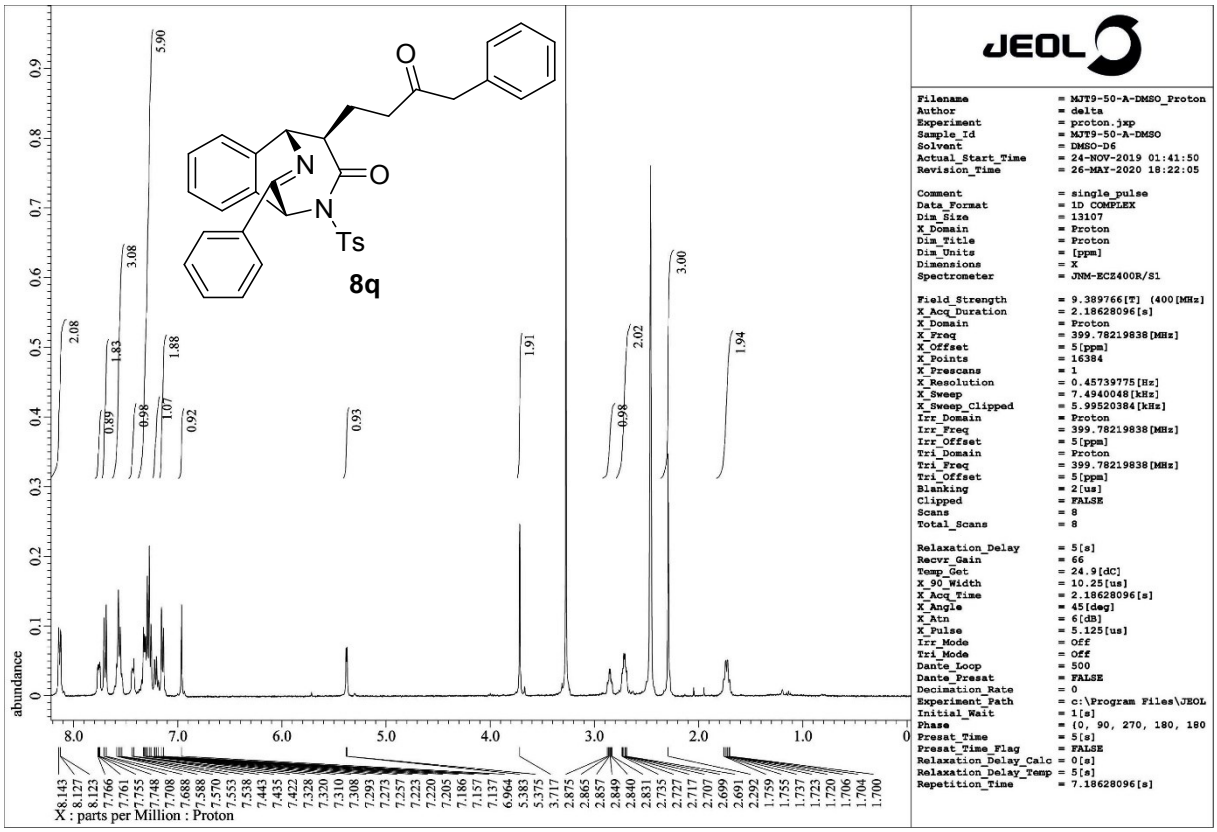

8n
(thousandths)
X : parts per Million : Carbon13
198.199
171.907
170.758
144.887
141.851
136.336
135.513
135.092
134.536
131.884
131.702
129.663
129.270
129.136
129.050
128.600
128.217
128.131
127.393
126.761
125.737
77.317
77.107
76.896
63.233
53.926
50.585
36.194
26.791
21.621
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = MJT6-80-a-C13_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT6-80-a-C13
Solvent = CHLOROFORM-D
Actual_Start_Time = 9-JUN-2019 10:34:
Revision_Time = 10-JUN-2019 08:21:
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 = TRUE
Scans = 300
Total_Scans = 300
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.3[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.5[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 20.656[dB]
Irr_Atn_Dec_Calc = 20.656[dB]
Irr_Atn_Dec_Default_Calc = 20.656[dB]
Irr_Atn_Noe = 20.656[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]

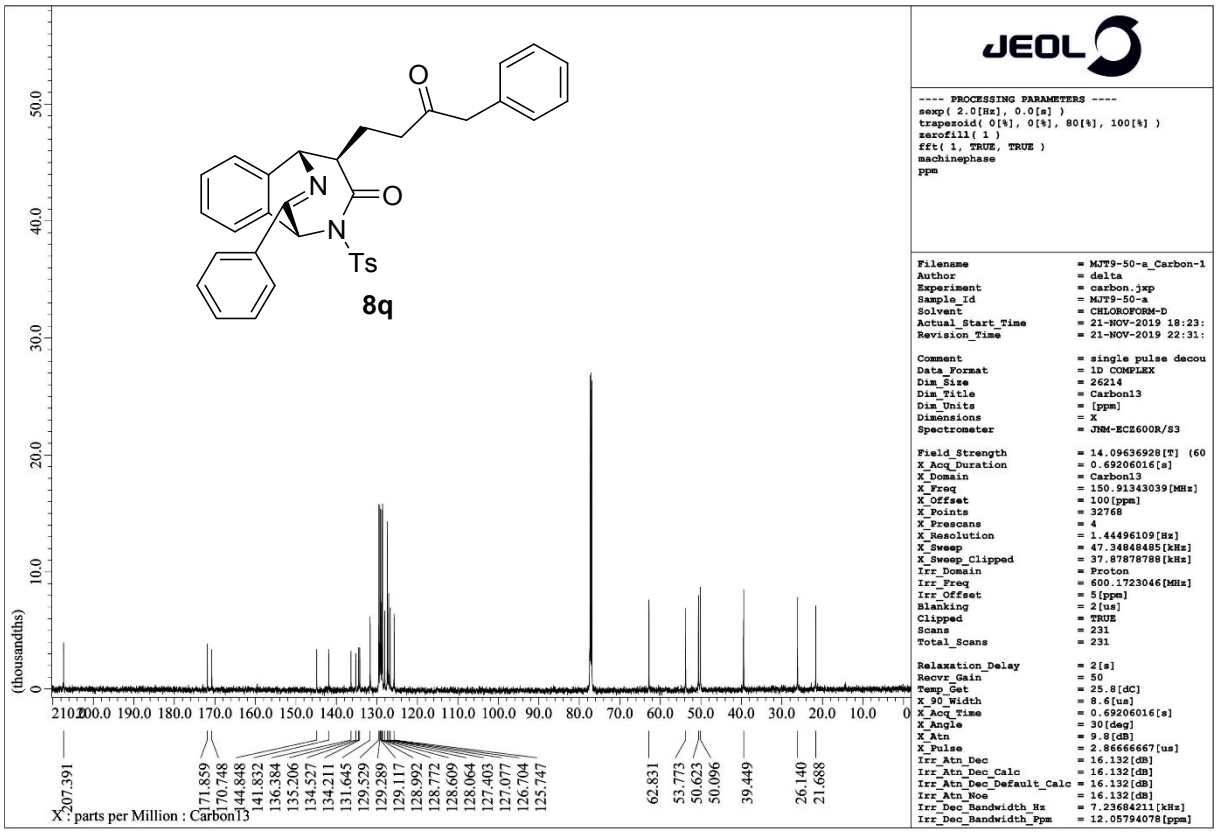

8o
abundance
X : parts per Million : Proton
8.225
8.209
8.196
8.182
7.979
7.964
7.705
7.690
7.598
7.593
7.585
7.577
7.566
7.562
7.554
7.535
7.522
7.510
7.434
7.430
7.424
7.419
7.353
7.348
7.342
7.256
7.160
7.147
6.992
5.469
5.464
3.165
3.161
3.149
3.142
3.138
3.040
3.034
3.029
3.023
3.019
3.013
2.431
2.420
2.406
2.395
2.384
2.372
2.308
2.194
2.182
2.171
2.160
2.146
0.000
1.97
1.97
1.94
1.90
1.94
1.92
1.88
1.08
0.85
0.93
0.96
0.97
2.02
0.98
3.00
1.03
0.98
Filename = MJT7-41-a-H_Proton-2-
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-41-a-H
Solvent = CHLOROFORM-D
Actual_Start_Time = 9-JUN-2019 17:09:58
Revision_Time = 26-MAY-2020 11:43:00
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 24.4[dC]
X_90_Width = 13.9[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 5.9[dB]
X_Pulse = 6.95[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 5.87031808[s]

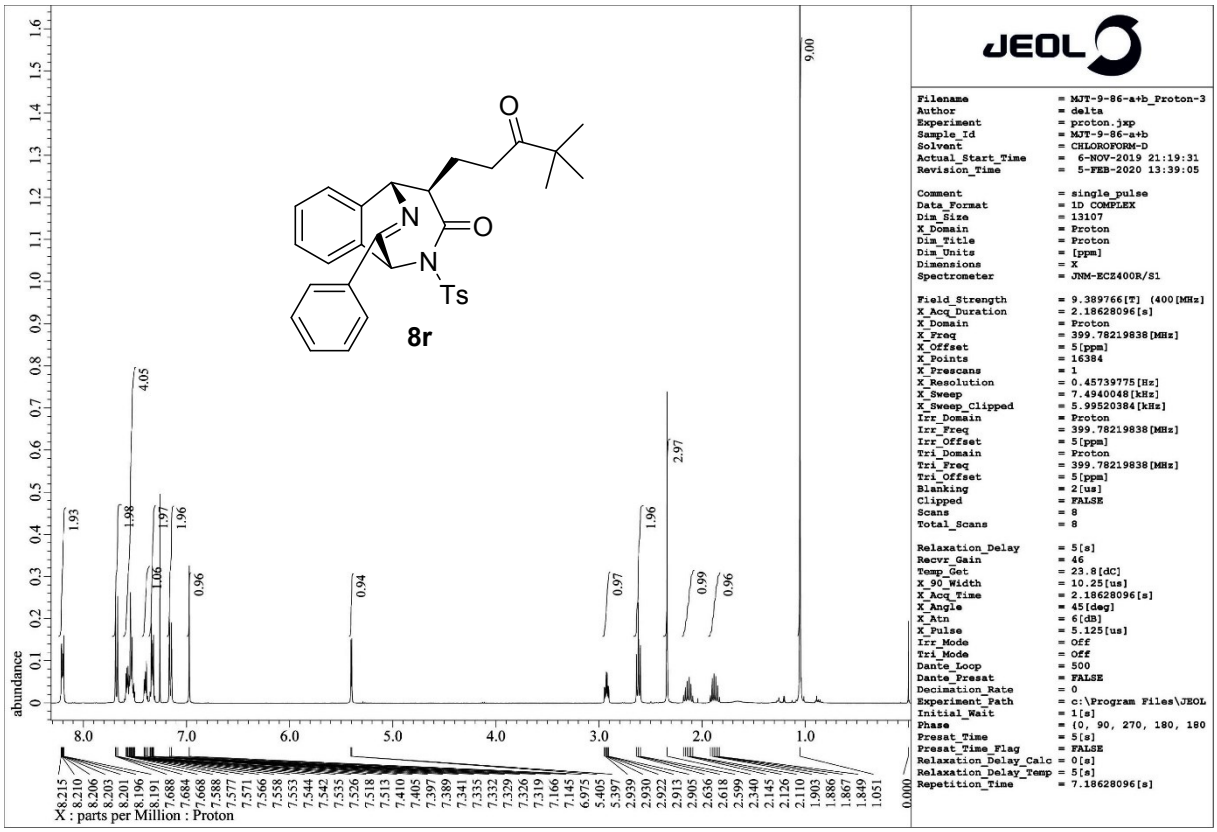

8o
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = MJT7-41-a-C13_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-41-a-C13
Solvent = CHLOROFORM-D
Actual_Start_Time = 9-JUN-2019 16:29:
Revision_Time = 26-AUG-2019 01:47:
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 = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.4[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.5[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 20.656[dB]
Irr_Atn_Dec_Calc = 20.656[dB]
Irr_Atn_Dec_Default_Calc = 20.656[dB]
Irr_Atn_Noe = 20.656[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]

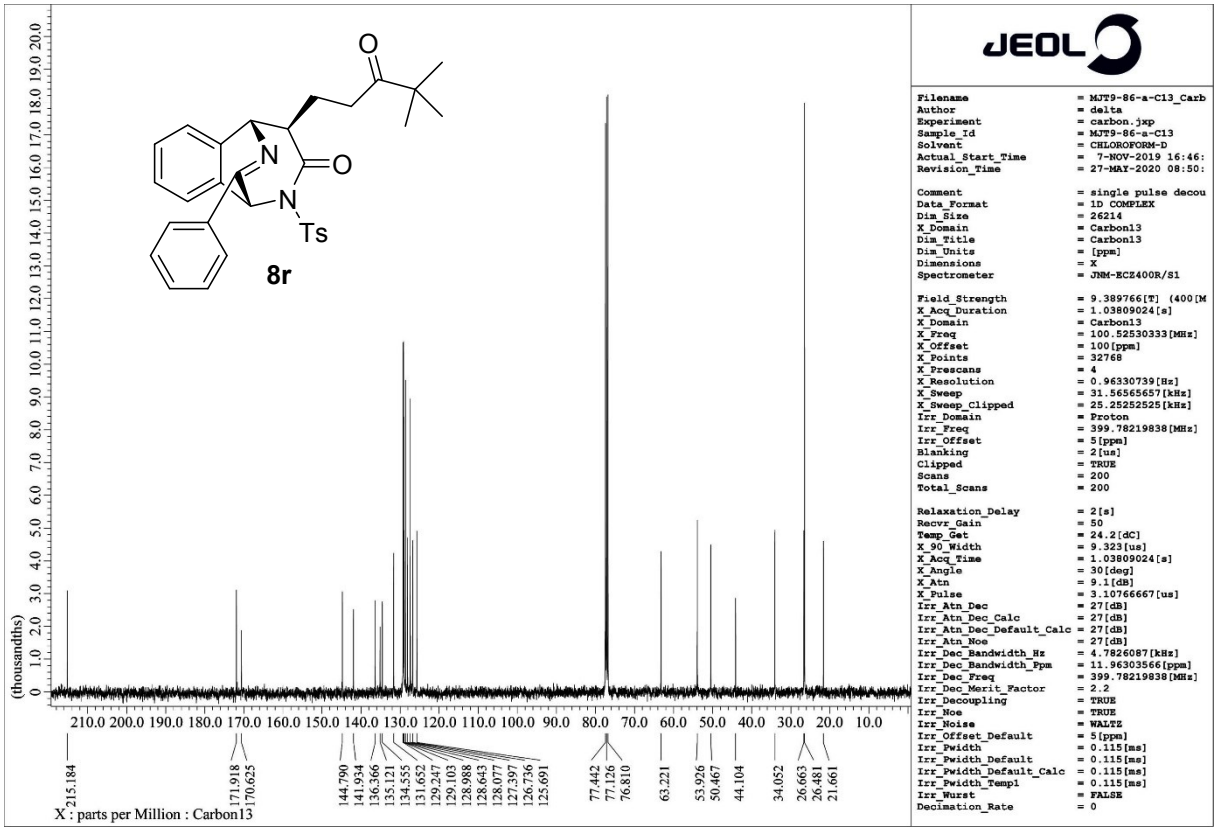

8p
abundance
X : parts per Million : Proton
Filename = MJT7-15-a-0707_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-15-a-0707
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-JUL-2019 14:26:35
Revision_Time = 26-MAY-2020 22:18:37
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 23.6[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

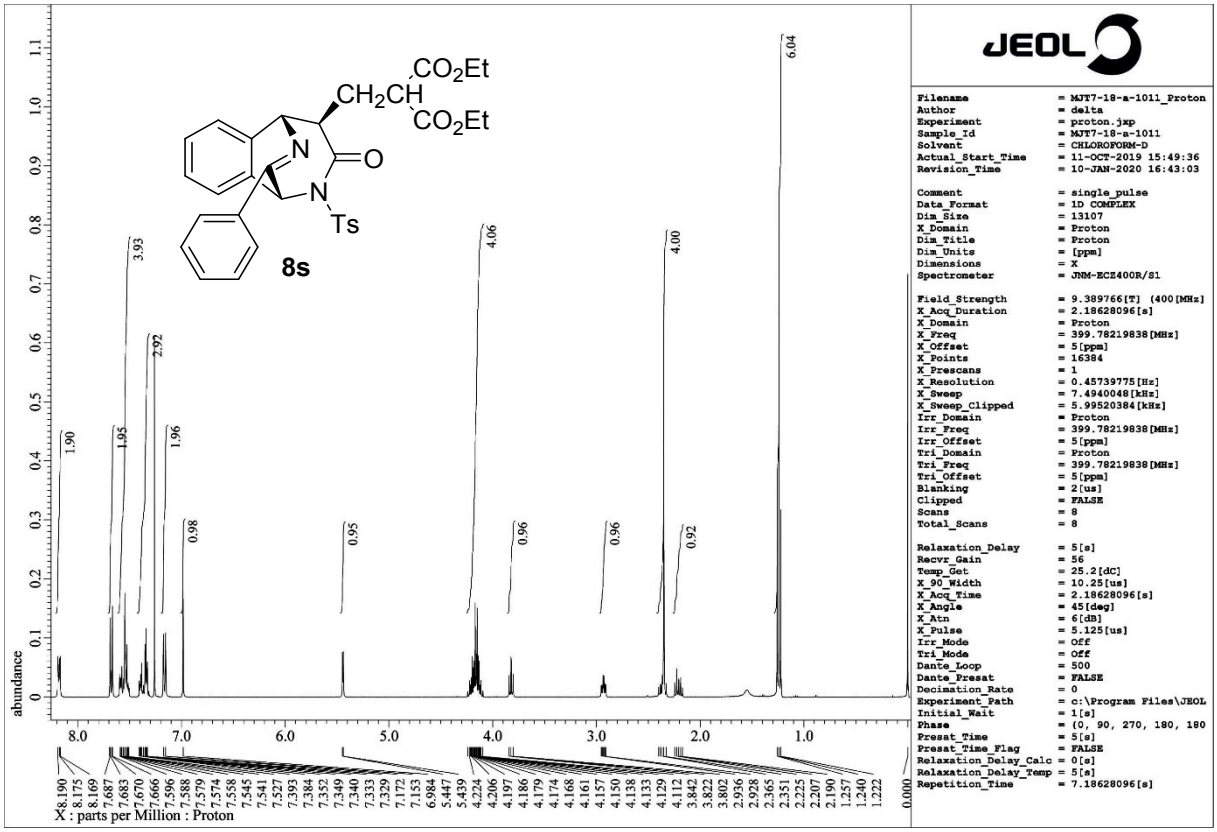

8p
(thousandths)
X : parts per Million : Carbon13
Filename = MJT6-101-a-C13_Car
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT6-101-a-C13
Solvent = ACETONE-D6
Actual_Start_Time = 7-JUL-2019 22:28:
Revision_Time = 8-JUL-2019 08:44:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
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 = 24.4[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]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

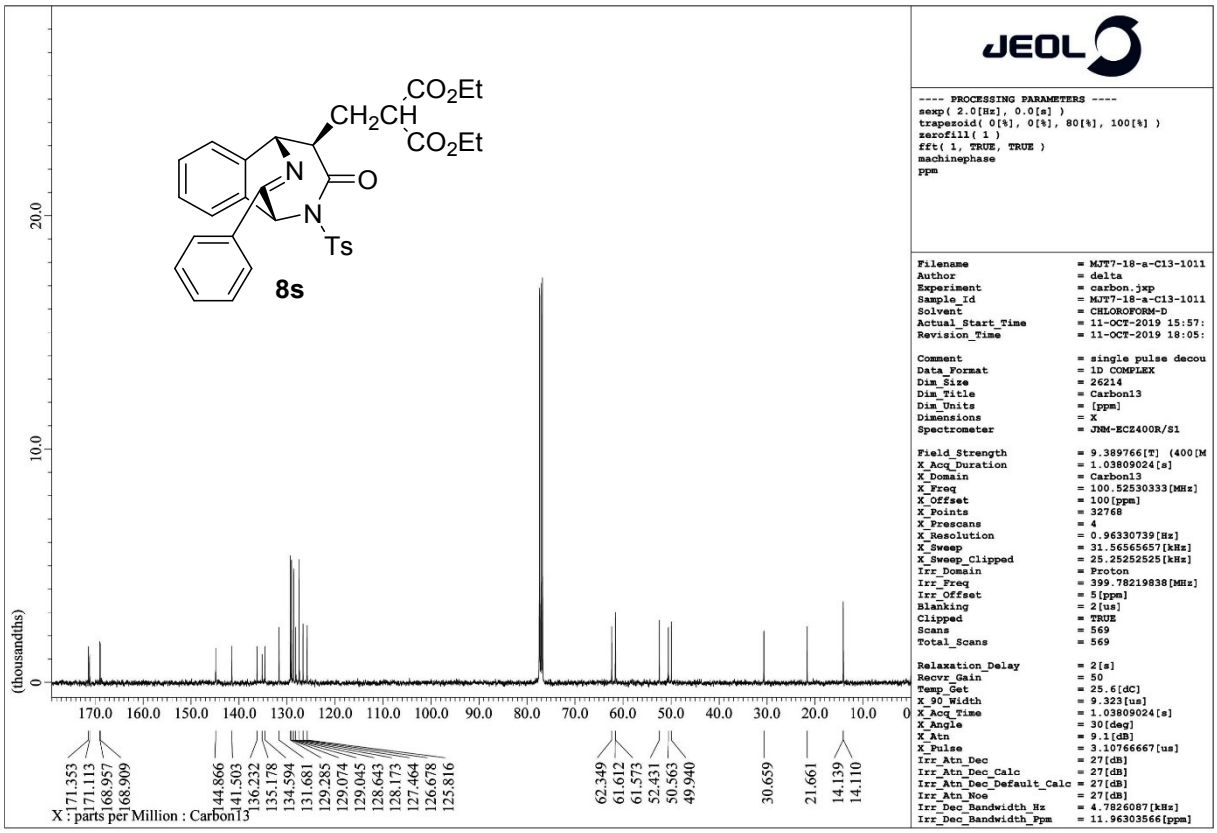

8q
abundance
X : parts per Million : Proton
Filename = MJT9-50-A-DMSO_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = MJT9-50-A-DMSO
Solvent = DMSO-D6
Actual_Start_Time = 24-NOV-2019 01:41:50
Revision_Time = 26-MAY-2020 18:22:05
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 24.9[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

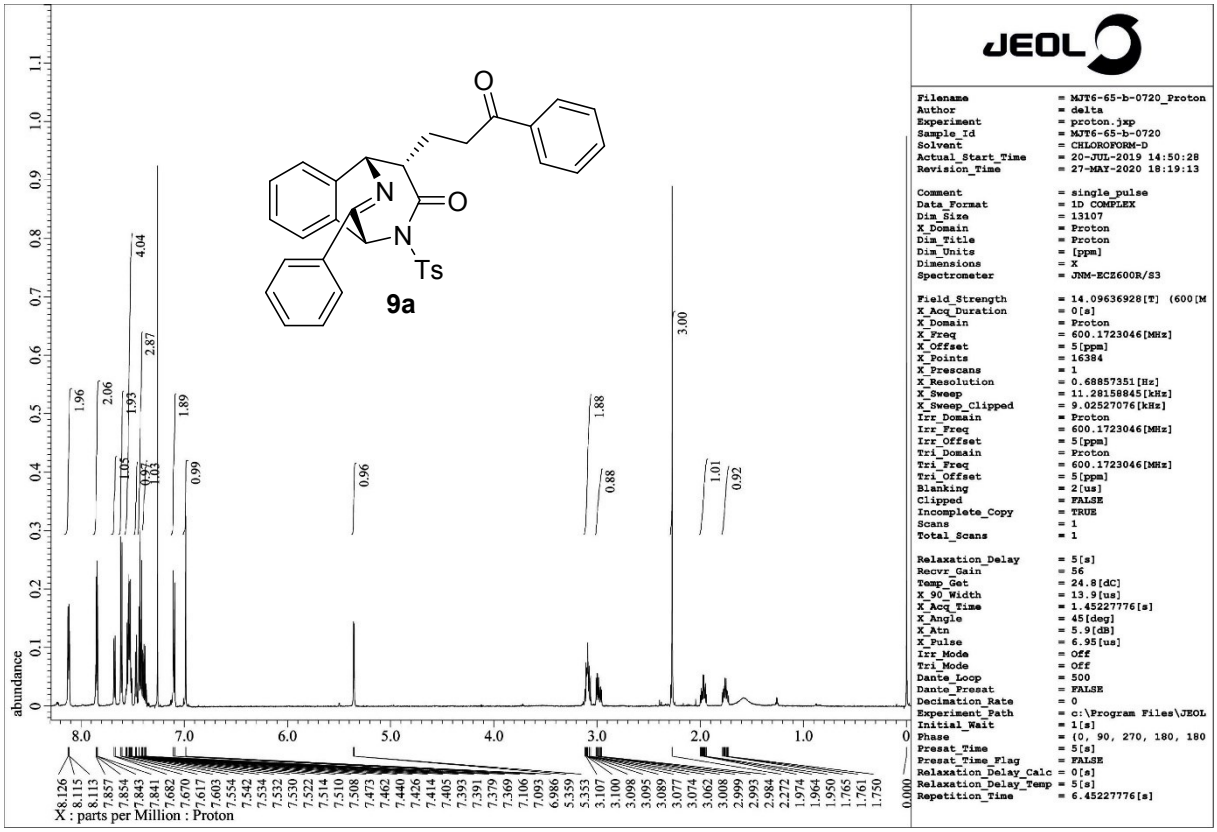

O
N
O
N
Ts
8q
(thousandths)
X : parts per Million : Carbon13
207.391
171.859
170.748
144.848
141.832
136.384
135.206
134.527
134.211
131.645
129.529
129.289
129.117
128.992
128.772
128.609
128.064
127.403
127.077
126.704
125.747
62.831
53.773
50.623
50.096
39.449
26.140
21.688
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = MJT9-50-a_Carbon-1
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT9-50-a
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-NOV-2019 18:23:
Revision_Time = 21-NOV-2019 22:31:
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 = TRUE
Scans = 231
Total_Scans = 231
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]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]

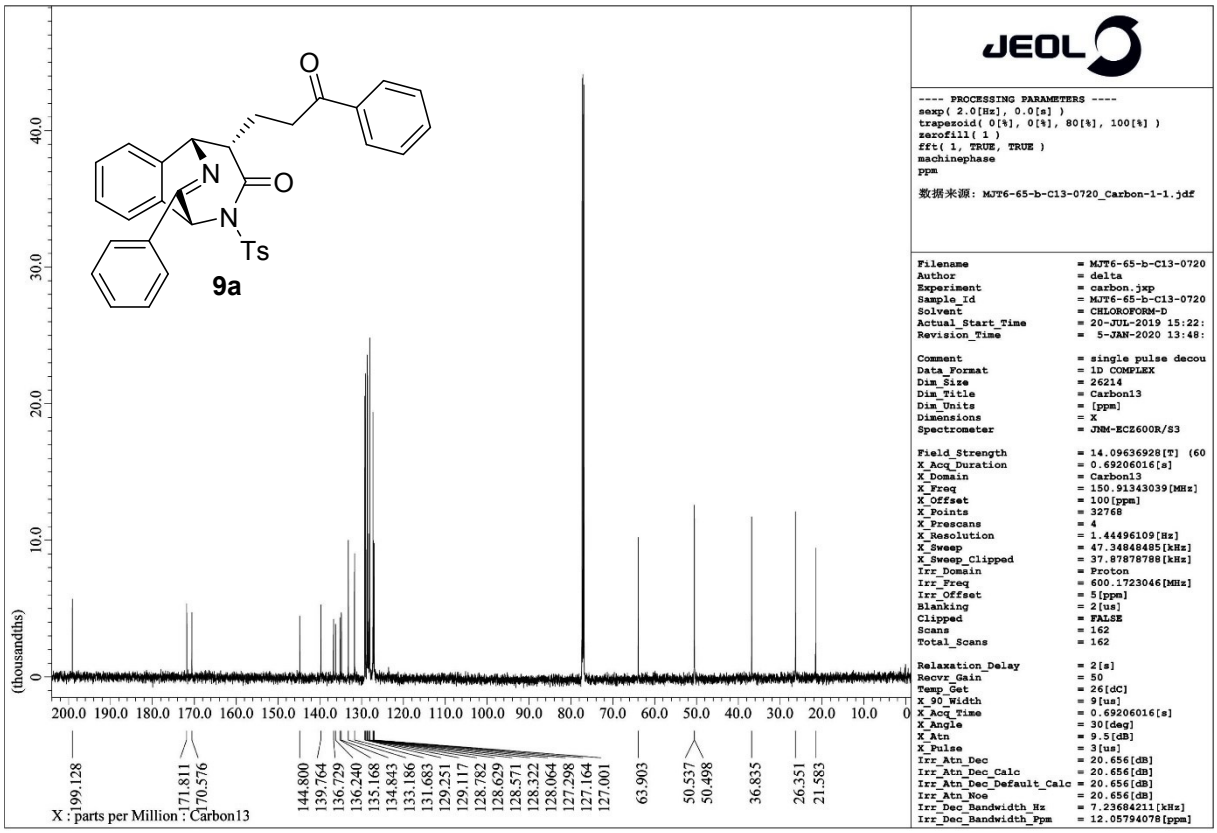

O
N
O
N
Ts
8r
abundance
X : parts per Million : Proton
9.00
4.05
2.97
1.93
1.98
1.97
1.96
1.06
0.96
0.94
0.97
1.96
0.99
0.96
8.215
8.210
8.206
8.203
8.201
8.196
8.191
7.688
7.684
7.668
7.588
7.577
7.571
7.566
7.558
7.553
7.544
7.542
7.535
7.526
7.518
7.513
7.410
7.405
7.397
7.389
7.341
7.335
7.332
7.329
7.326
7.319
7.166
7.145
6.975
5.405
5.397
2.939
2.930
2.922
2.913
2.905
2.636
2.618
2.599
2.340
2.145
2.126
2.110
1.903
1.886
1.867
1.849
1.051
0.000
Filename = MJT-9-86-a+b_Proton-3
Author = delta
Experiment = proton.jxp
Sample_Id = MJT-9-86-a+b
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-NOV-2019 21:19:31
Revision_Time = 5-FEB-2020 13:39:05
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 23.8[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

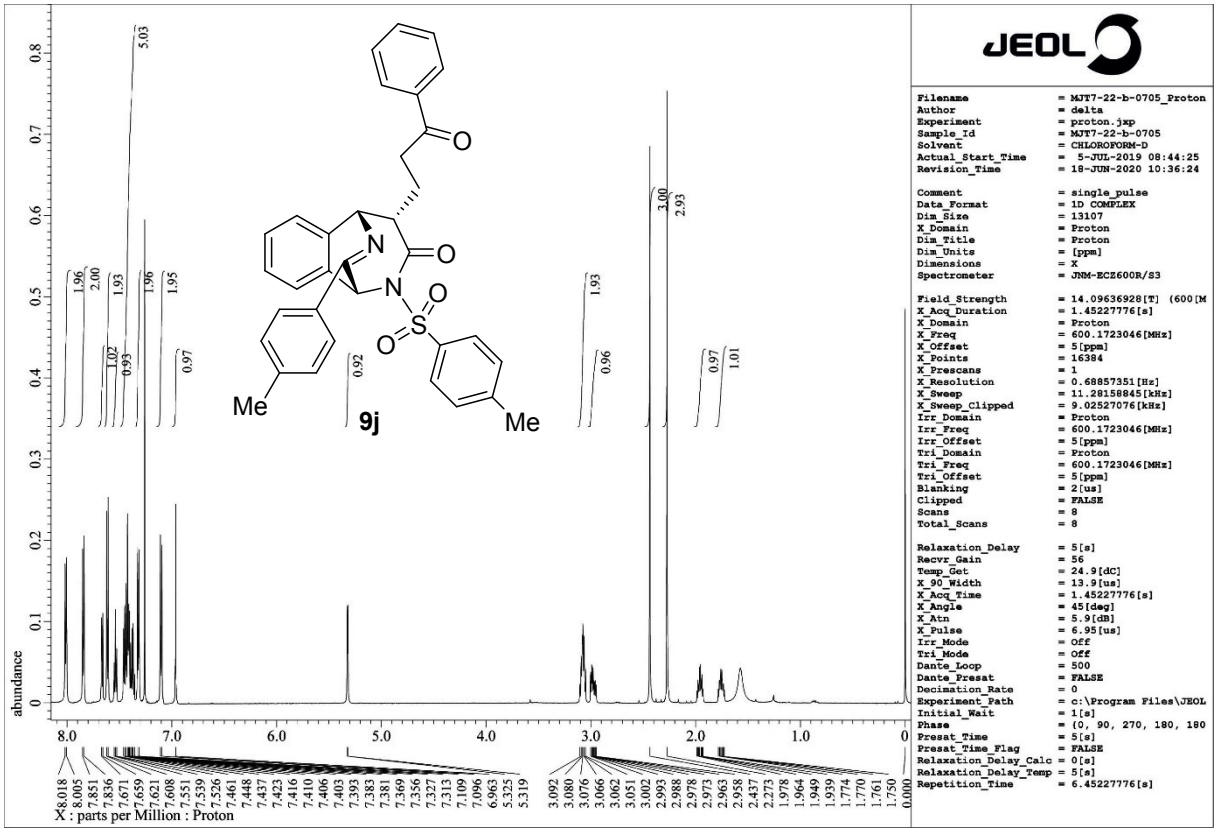

8r
(thousandths)
X : parts per Million : Carbon13
Filename = MJT9-86-a-C13_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT9-86-a-C13
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-NOV-2019 16:46:
Revision_Time = 27-MAY-2020 08:50:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
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 = 200
Total_Scans = 200
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]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

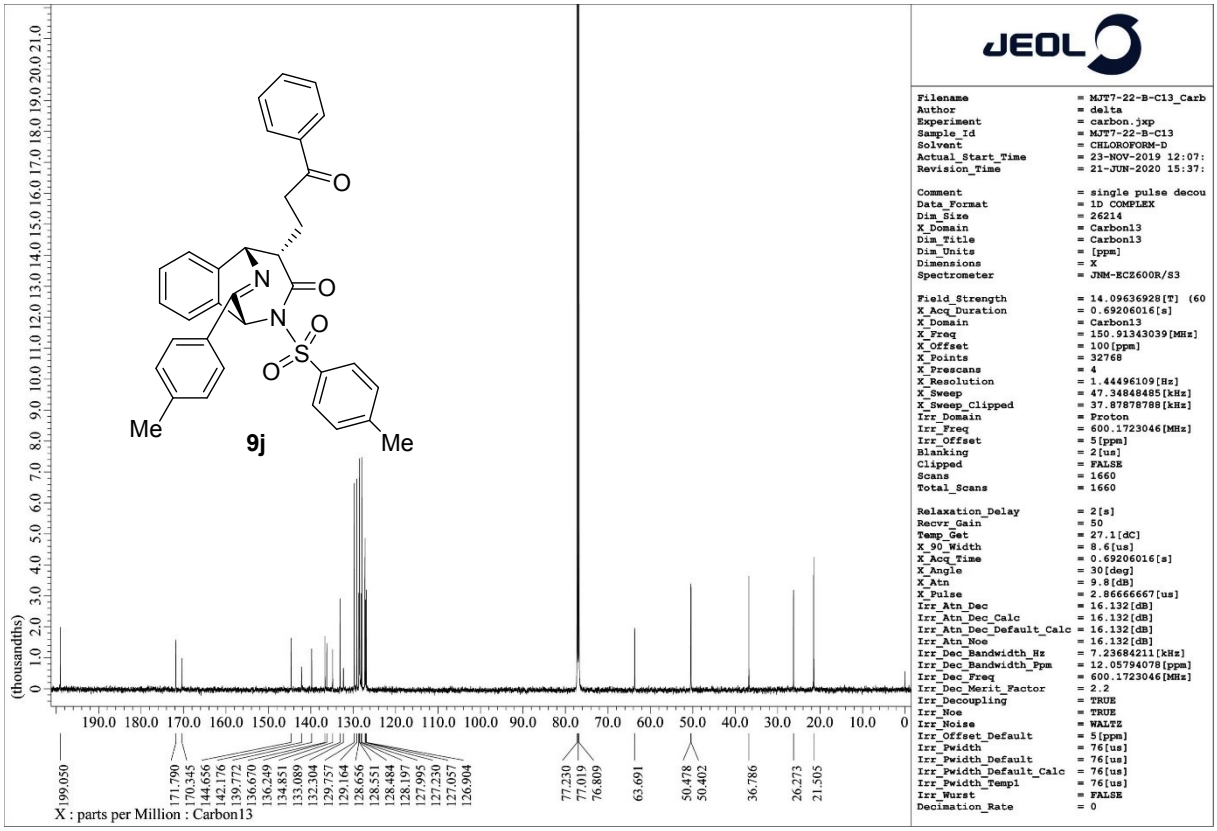

8s
abundance
X : parts per Million : Proton
Filename = MJT7-18-a-1011_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-18-a-1011
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-OCT-2019 15:49:36
Revision_Time = 10-JAN-2020 16:43:03
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 25.2[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]


8s
(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 = MJT7-18-a-C13-1011
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-18-a-C13-1011
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-OCT-2019 15:57:
Revision_Time = 11-OCT-2019 18:05:
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 = 569
Total_Scans = 569
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.6[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]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]


9a
abundance
X : parts per Million : Proton
Filename = MJT6-65-b-0720_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = MJT6-65-b-0720
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-JUL-2019 14:50:28
Revision_Time = 27-MAY-2020 18:19:13
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 0.68857351[Hz]
X_Sweep = 11.28158845[kHz]
X_Sweep_Clipped = 9.02527076[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 = 1
Total_Scans = 1
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 24.8[dC]
X_90_Width = 13.9[us]
X_Acq_Time = 1.45227776[s]
X_Angle = 45[deg]
X_Atn = 5.9[dB]
X_Pulse = 6.95[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.45227776[s]

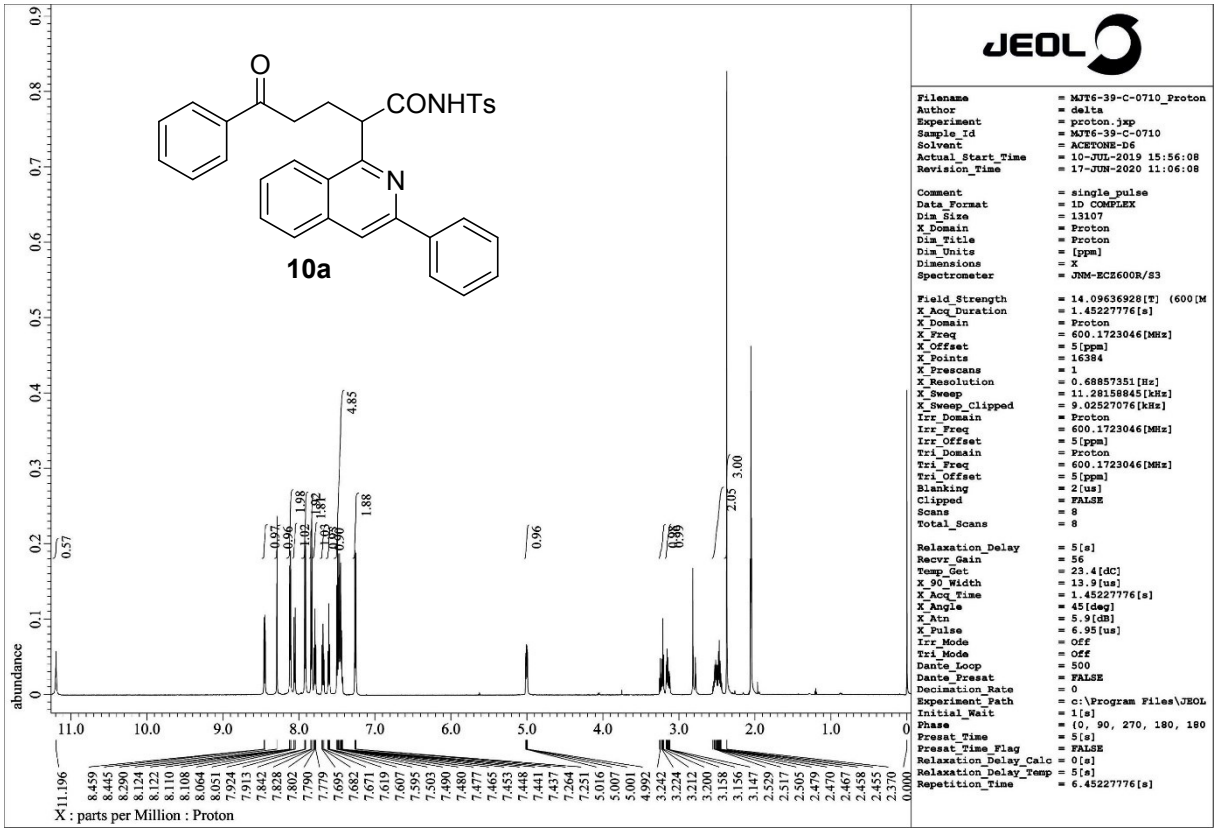

9a
(thousandths)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
数据来源: MJT6-65-b-C13-0720_Carbon-1-1.jdf
Filename = MJT6-65-b-C13-0720
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT6-65-b-C13-0720
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-JUL-2019 15:22:
Revision_Time = 5-JAN-2020 13:48:
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 = 0.69206016[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 = 162
Total_Scans = 162
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 26[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.5[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 20.656[dB]
Irr_Atn_Dec_Calc = 20.656[dB]
Irr_Atn_Dec_Default_Calc = 20.656[dB]
Irr_Atn_Noe = 20.656[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]


9j
Me
Me
abundance
X : parts per Million : Proton
Filename = MJT7-22-b-0705_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-22-b-0705
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-JUL-2019 08:44:25
Revision_Time = 18-JUN-2020 10:36:24
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S3
Field_Strength = 14.09636928[T] (600[M
X_Acq_Duration = 1.45227776[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.68857351[Hz]
X_Sweep = 11.28158845[kHz]
X_Sweep_Clipped = 9.02527076[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 = 24.9[dC]
X_90_Width = 13.9[us]
X_Acq_Time = 1.45227776[s]
X_Angle = 45[deg]
X_Atn = 5.9[dB]
X_Pulse = 6.95[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.45227776[s]



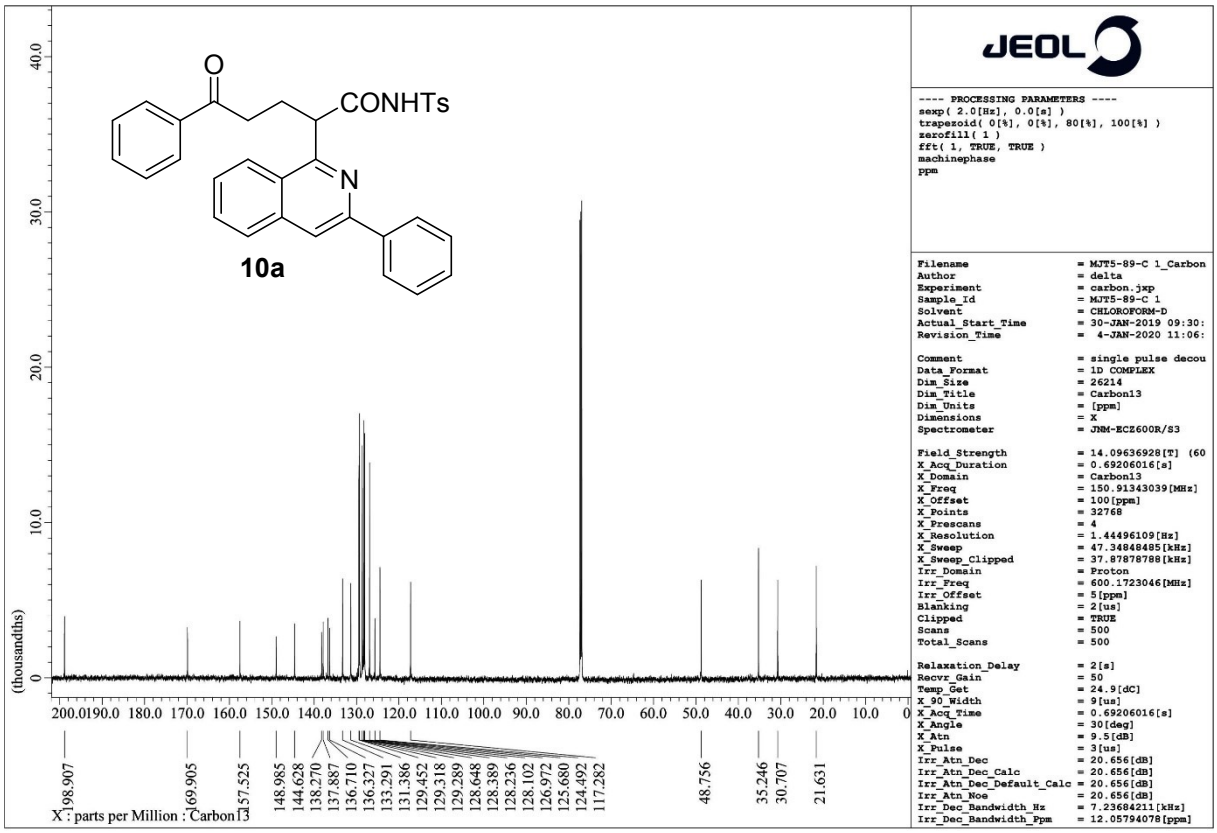
JEOL

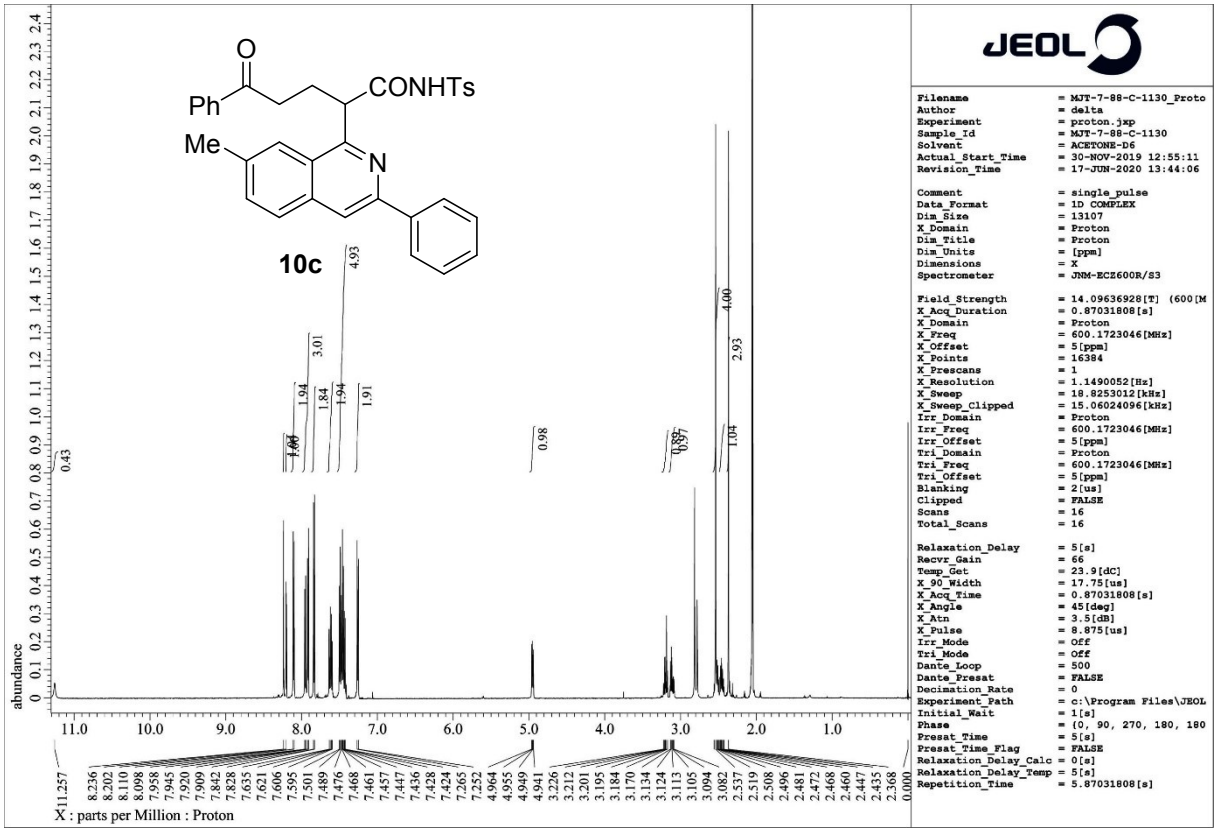
Filename	= MJT7-22-B-C13_Carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= MJT7-22-B-C13
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-NOV-2019 12:07:
Revision_Time	= 21-JUN-2020 15:37:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
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	= 1660
Total_Scans	= 1660
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 27.1[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]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0

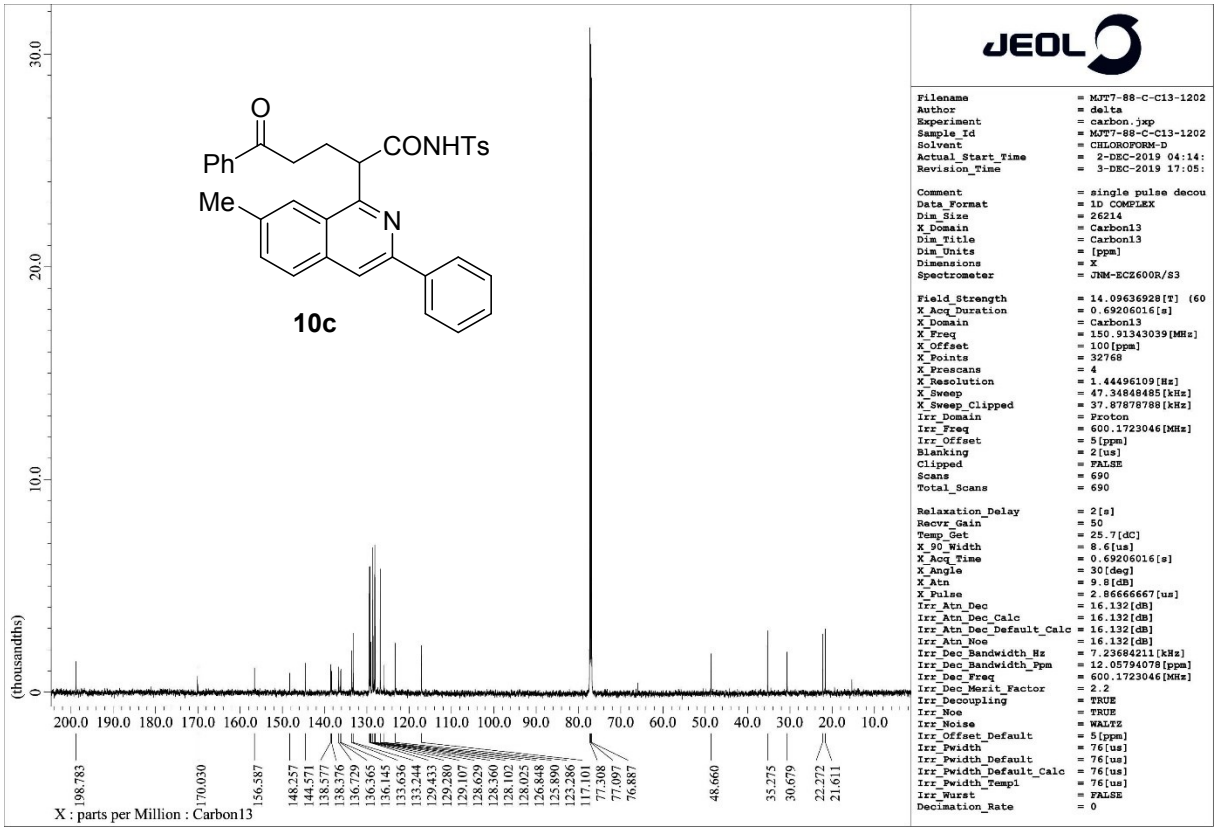


JEOL

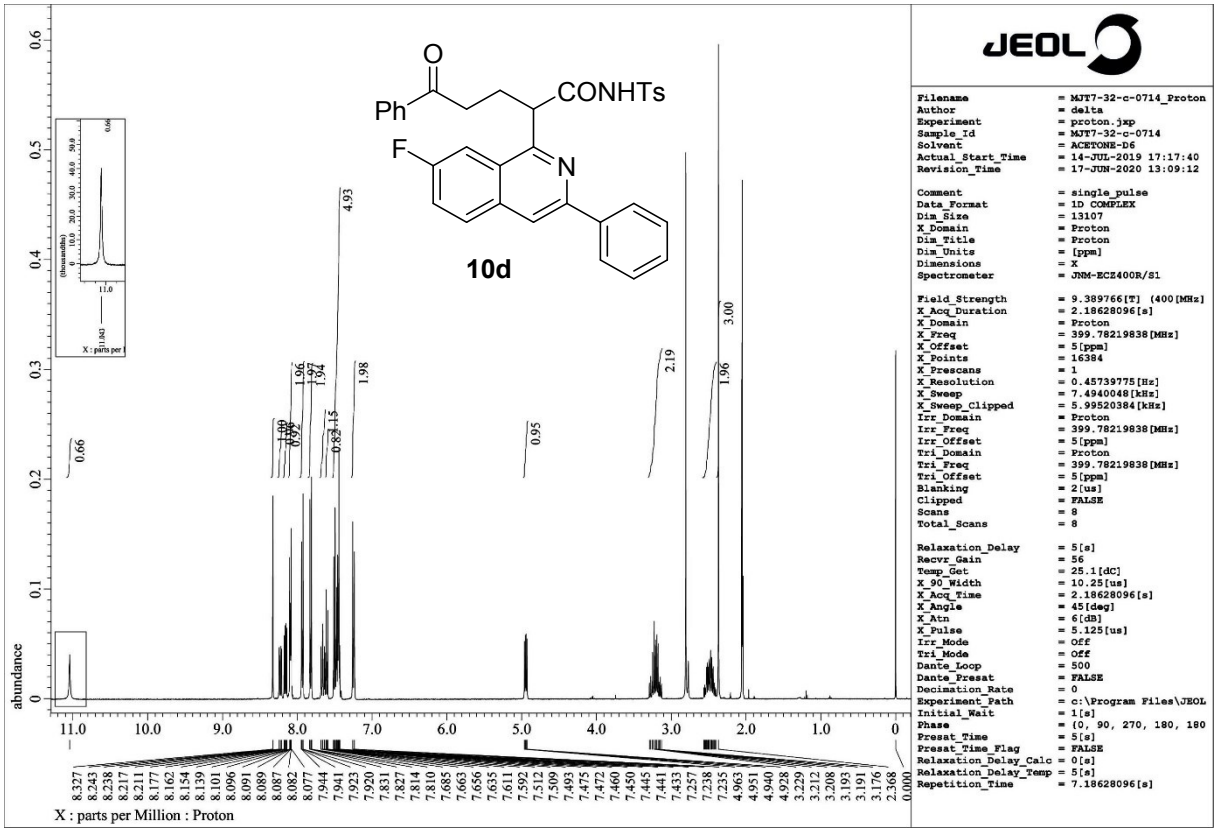
Filename	= MJT6-39-C-0710_Proton
Author	= delta
Experiment	= proton.jxp
Sample_Id	= MJT6-39-C-0710
Solvent	= ACETONE-D6
Actual_Start_Time	= 10-JUL-2019 15:56:08
Revision_Time	= 17-JUN-2020 11:06:08
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 1.45227776[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68857351[Hz]
X_Sweep	= 11.28158845[kHz]
X_Sweep_Clipped	= 9.02527076[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	= 13.9[us]
X_Acq_Time	= 1.45227776[s]
X_Angle	= 45[deg]
X_Atn	= 5.9[dB]
X_Pulse	= 6.95[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 9[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 6.45227776[s]


O
CONHTs
N
10a
(thousandths)
X : parts per Million : Carbon13
198.907
169.905
157.525
148.985
144.628
138.270
137.887
136.710
136.327
133.291
131.386
129.452
129.318
129.289
128.648
128.389
128.236
128.102
126.972
125.680
124.492
117.282
48.756
35.246
30.707
21.631
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = MJT5-89-C 1_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT5-89-C 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-JAN-2019 09:30:
Revision_Time = 4-JAN-2020 11:06:
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 = TRUE
Scans = 500
Total_Scans = 500
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.9[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.5[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 20.656[dB]
Irr_Atn_Dec_Calc = 20.656[dB]
Irr_Atn_Dec_Default_Calc = 20.656[dB]
Irr_Atn_Noe = 20.656[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]

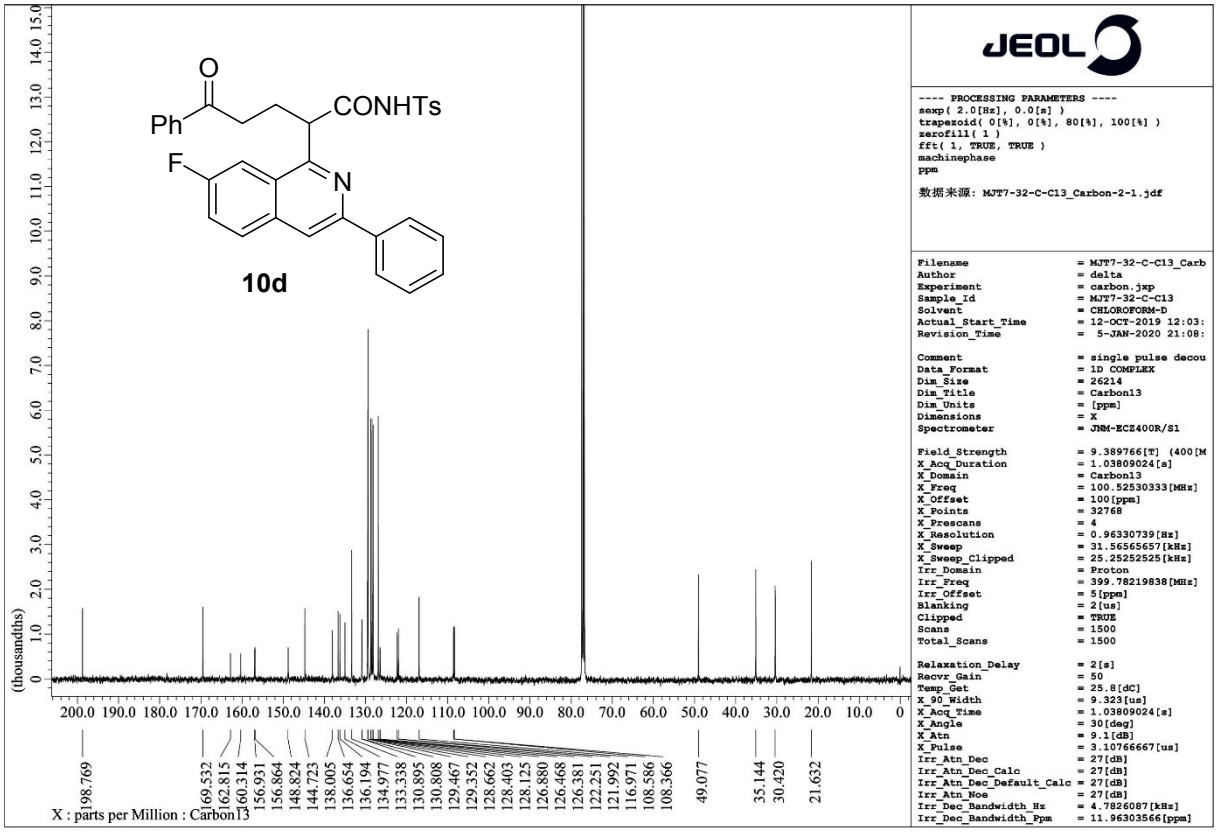

O
Ph
CONHTs
Me
N
10c
abundance
X : parts per Million : Proton
0.43
1.94
1.84
1.94
1.91
3.01
4.93
0.98
0.97
1.04
2.93
4.00
Filename = MJT-7-88-C-1130_Proto
Author = delta
Experiment = proton.jxp
Sample_Id = MJT-7-88-C-1130
Solvent = ACETONE-D6
Actual_Start_Time = 30-NOV-2019 12:55:11
Revision_Time = 17-JUN-2020 13:44:06
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 23.9[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 5.87031808[s]

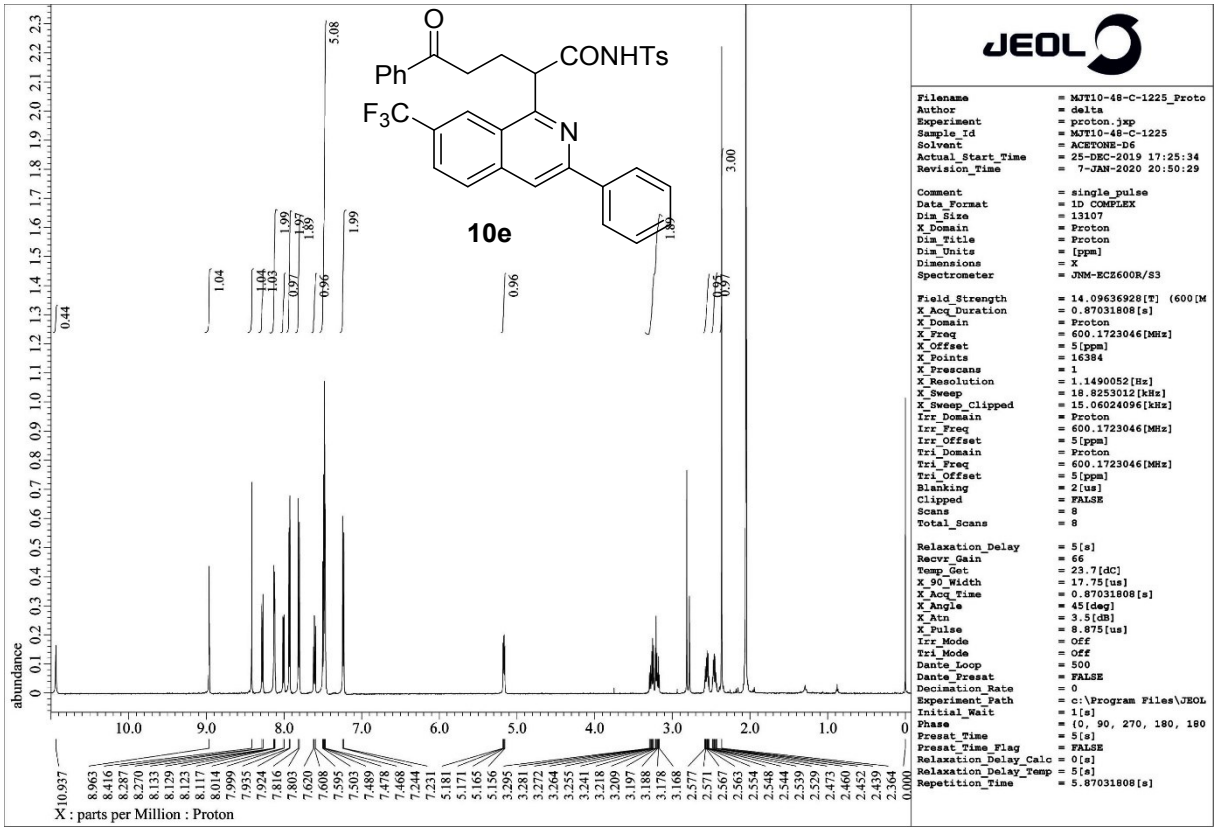


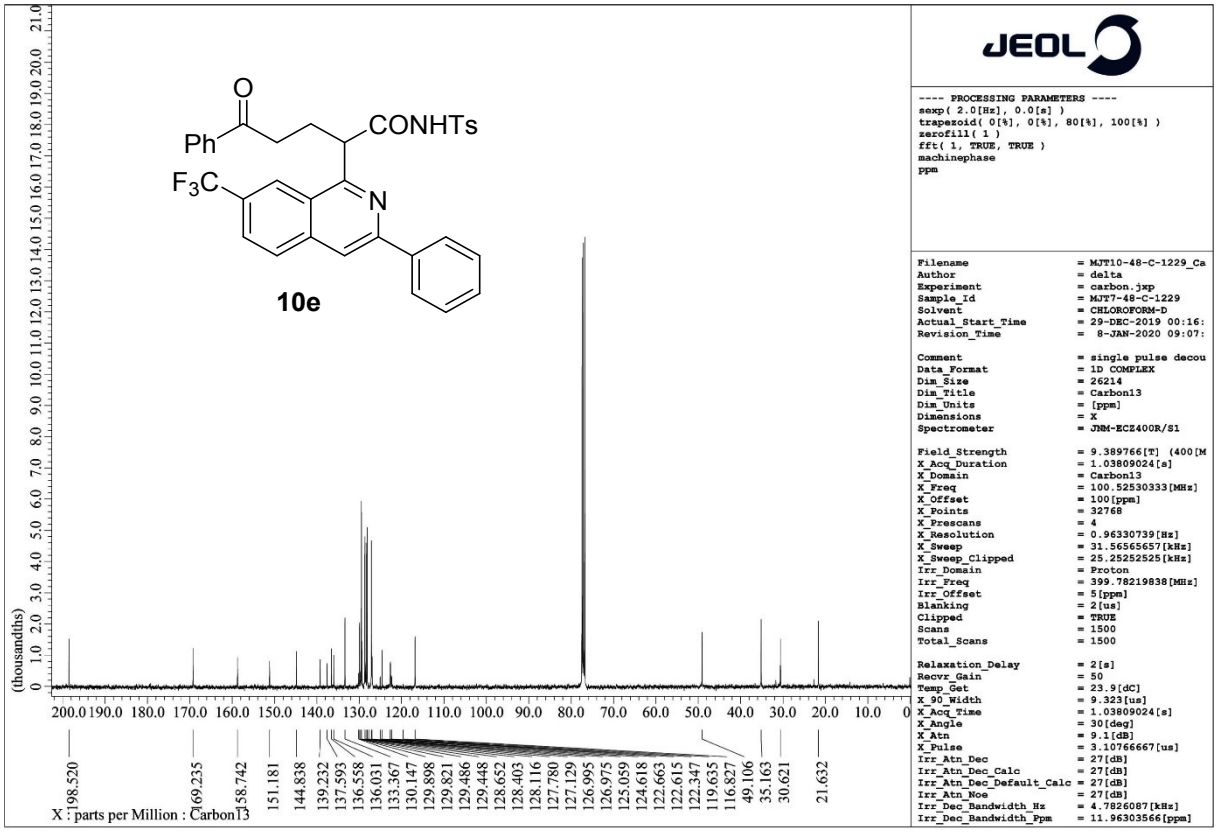

```
Filename                = MJT7-88-C-C13-1202
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = MJT7-88-C-C13-1202
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  2-DEC-2019 04:14:
Revision_Time           =  3-DEC-2019 17:05:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Carbon13
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                   = 690
Total_Scans             = 690

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 25.7[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]
Irr_Dec_Bandwidth_Ppm   = 12.05794078[ppm]
Irr_Dec_Freq            = 600.1723046[MHz]
Irr_Dec_Merit_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = TRUE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 76[us]
Irr_Pwidth_Default      = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1        = 76[us]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
```

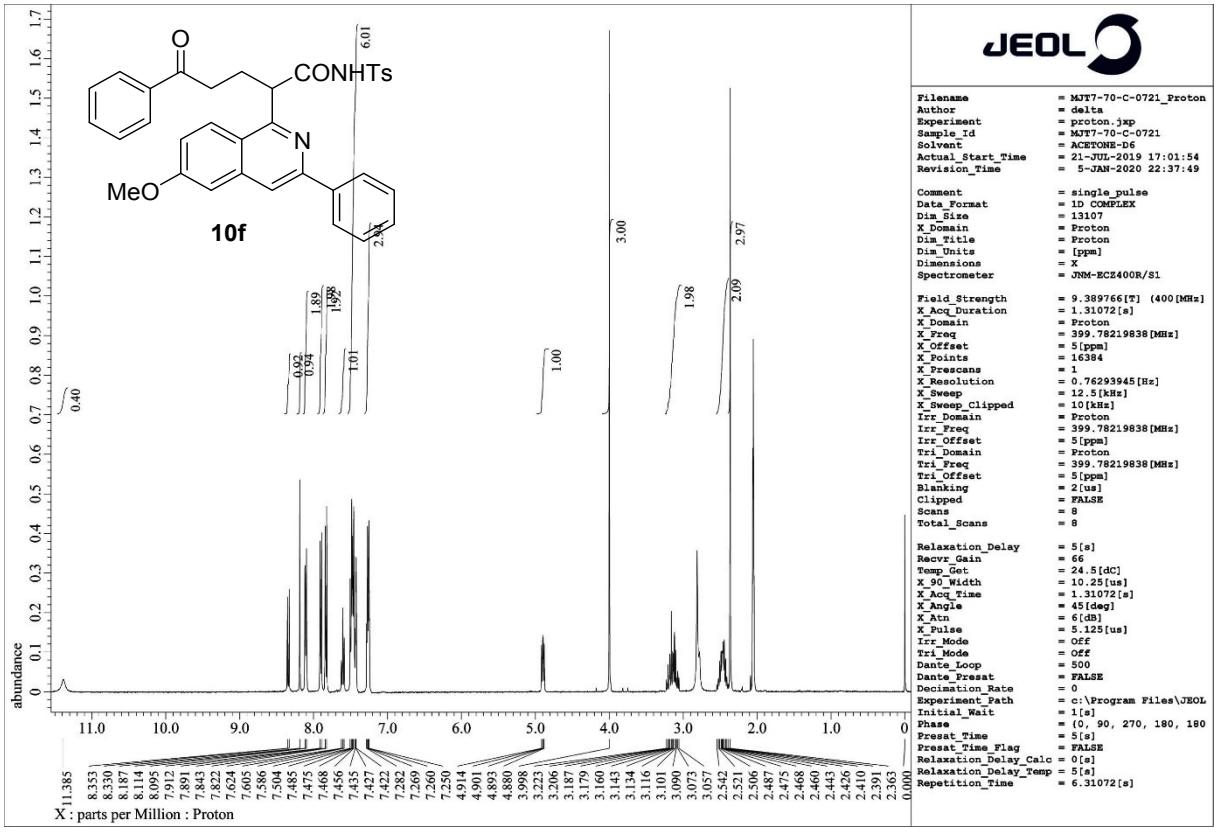


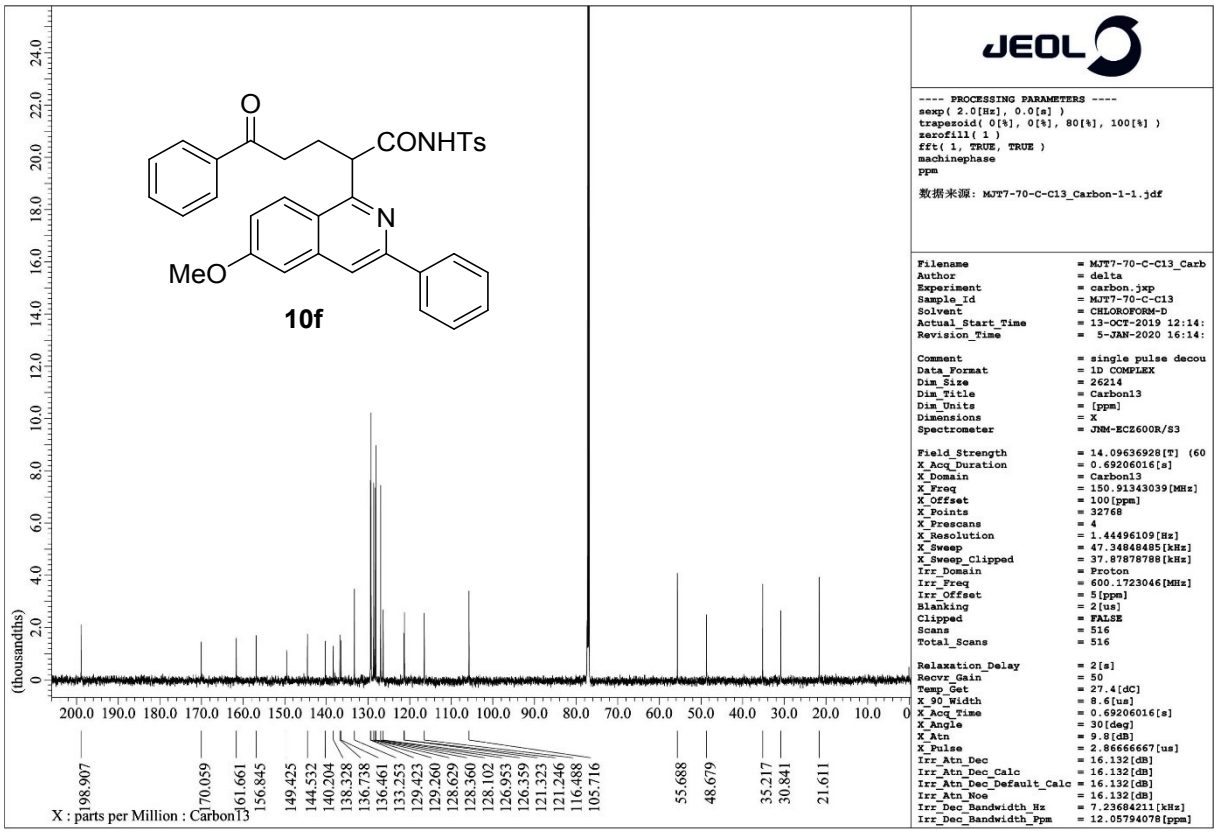

```
Filename                = MJT7-32-c-0714_Proton
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = MJT7-32-c-0714
Solvent                 = ACETONE-D6
Actual_Start_Time       = 14-JUL-2019 17:17:40
Revision_Time           = 17-JUN-2020 13:09:12

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
X_Domain                = Proton
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                = 25.1[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
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = c:\Program Files\JEOL
Initial_Wait            = 1[s]
Phase                   = (0, 90, 270, 180, 180
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 9[s]
Relaxation_Delay_Temp   = 5[s]
Repetition_Time         = 7.18628096[s]
```


O
Ph
CONHTs
F
N
10d
(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: MJT7-32-C-C13_Carbon-2-1.jdf
Filename = MJT7-32-C-C13_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-32-C-C13
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-OCT-2019 12:03:
Revision_Time = 5-JAN-2020 21:08:
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 = 1500
Total_Scans = 1500
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.8[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]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]


O
Ph
CONHTs
F3C
N
10e
abundance
X : parts per Million : Proton
Filename = MJT10-48-C-1225_Proto
Author = delta
Experiment = proton.jxp
Sample_Id = MJT10-48-C-1225
Solvent = ACETONE-D6
Actual_Start_Time = 25-DEC-2019 17:25:34
Revision_Time = 7-JAN-2020 20:50:29
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 5.87031808[s]


O
Ph
CONHTs
F3C
N
10e
(thousandths)
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
Filename = MJT10-48-C-1229_Ca
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-48-C-1229
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-DEC-2019 00:16:
Revision_Time = 8-JAN-2020 09:07:
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 = 1500
Total_Scans = 1500
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]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]

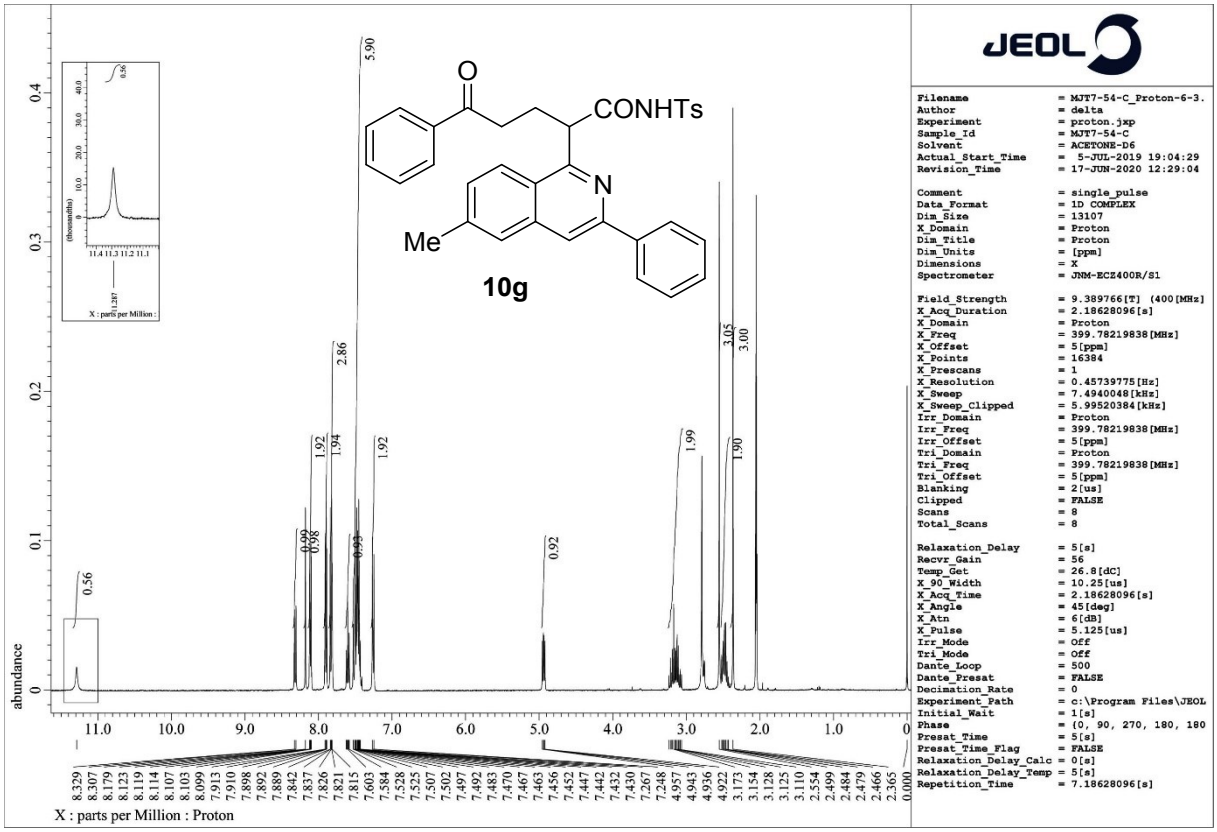

O
CONHTs
N
MeO
10f
abundance
X : parts per Million : Proton
JEOL
Filename = MJT7-70-C-0721_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-70-C-0721
Solvent = ACETONE-D6
Actual_Start_Time = 21-JUL-2019 17:01:54
Revision_Time = 5-JAN-2020 22:37:49
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 1.31072[s]
X_Domain = Proton
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.76293945[Hz]
X_Sweep = 12.5[kHz]
X_Sweep_Clipped = 10[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 = 24.5[dC]
X_90_Width = 10.25[us]
X_Acq_Time = 1.31072[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 5.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.31072[s]



JEOL

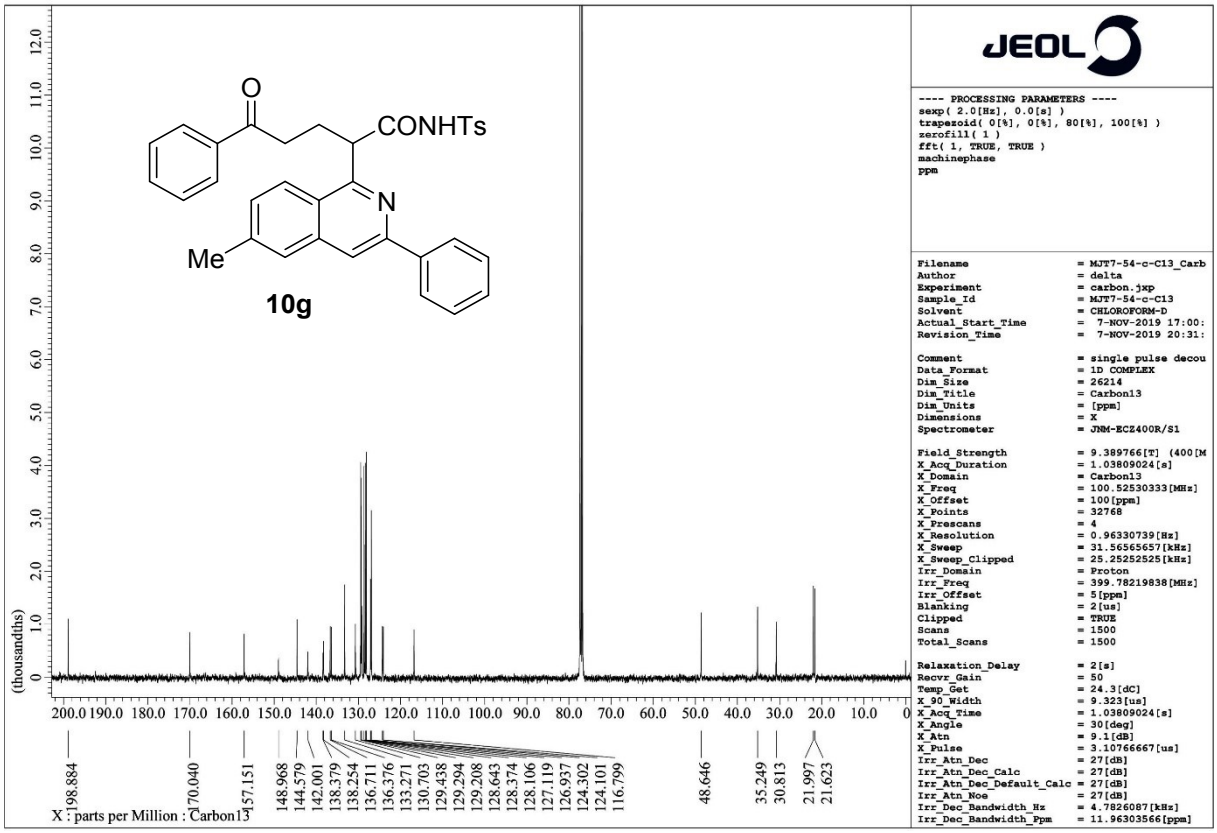
```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

数据来源: MJT7-70-C-C13_Carbon-1-1.jdf
```

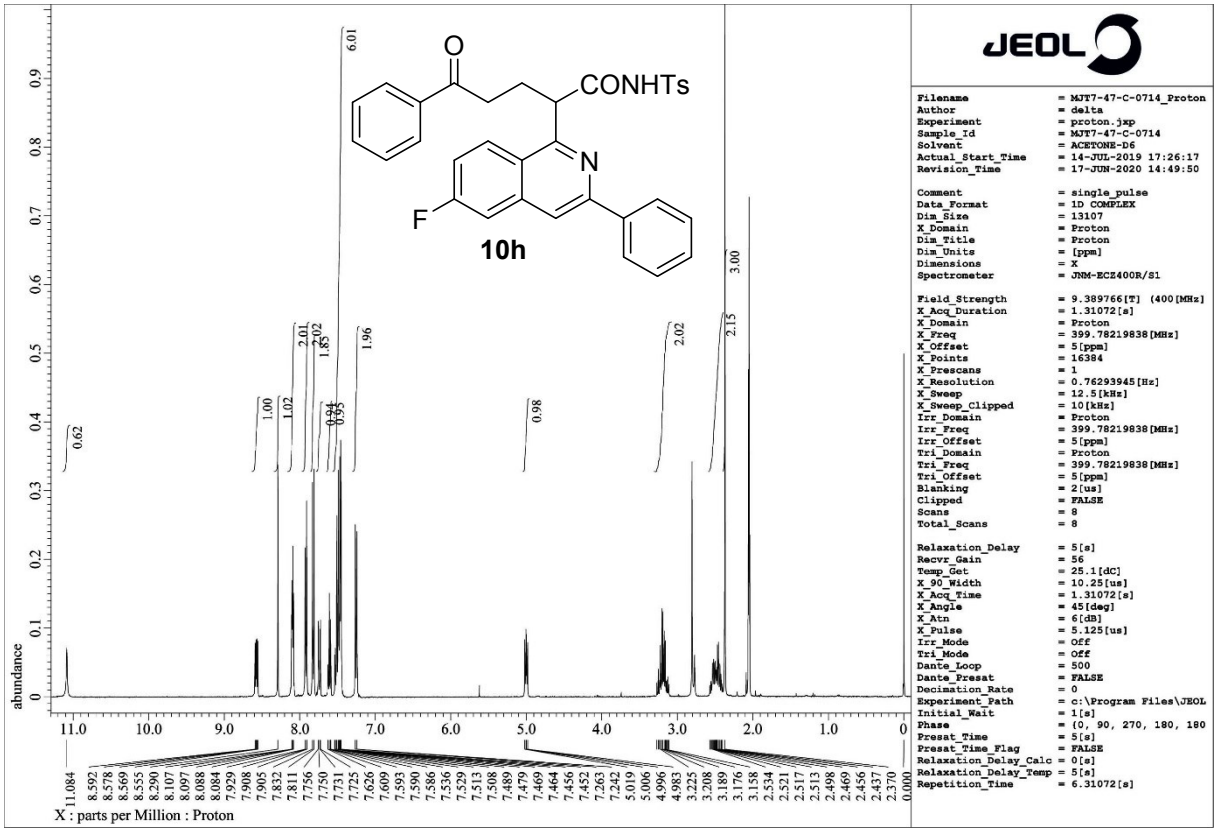
Filename	= MJT7-70-C-C13_Carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= MJT7-70-C-C13
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-OCT-2019 12:14:
Revision_Time	= 5-JAN-2020 16:14:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 262214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 516
Total_Scans	= 516
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 27.4[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]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]

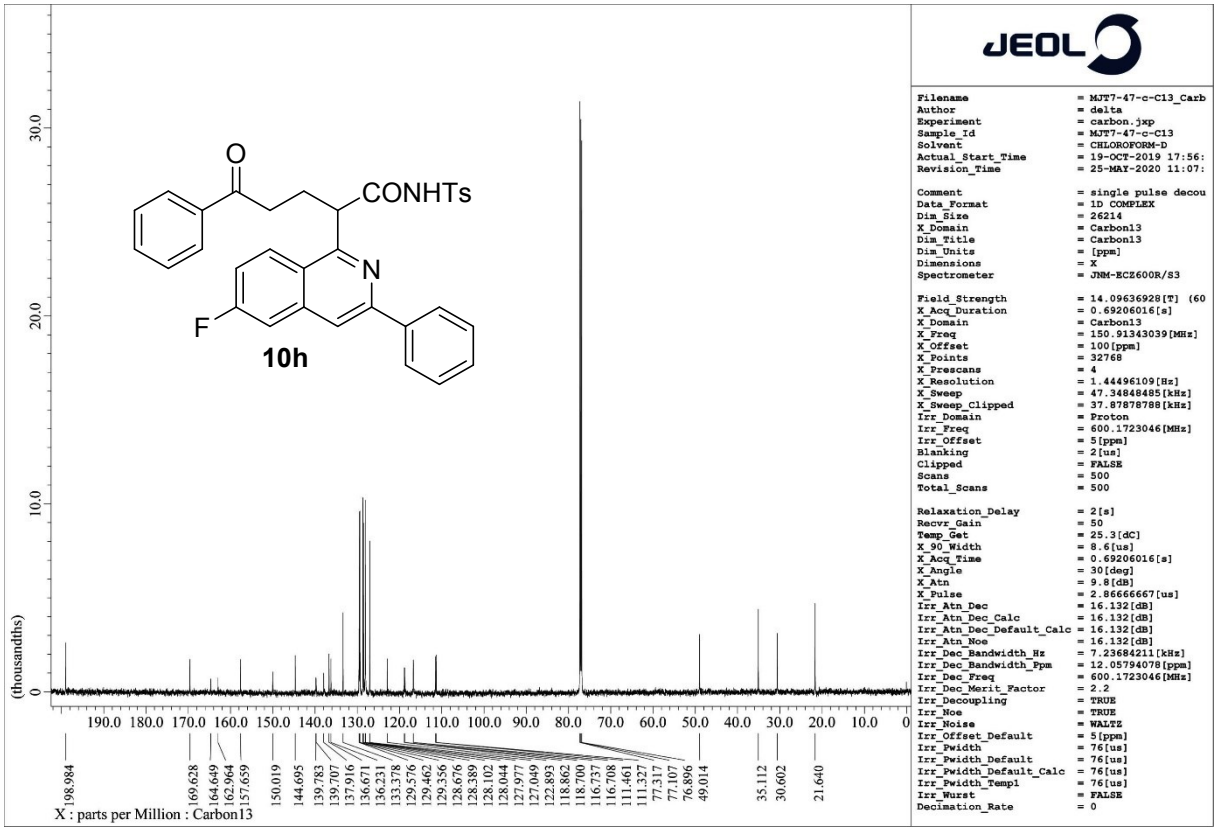


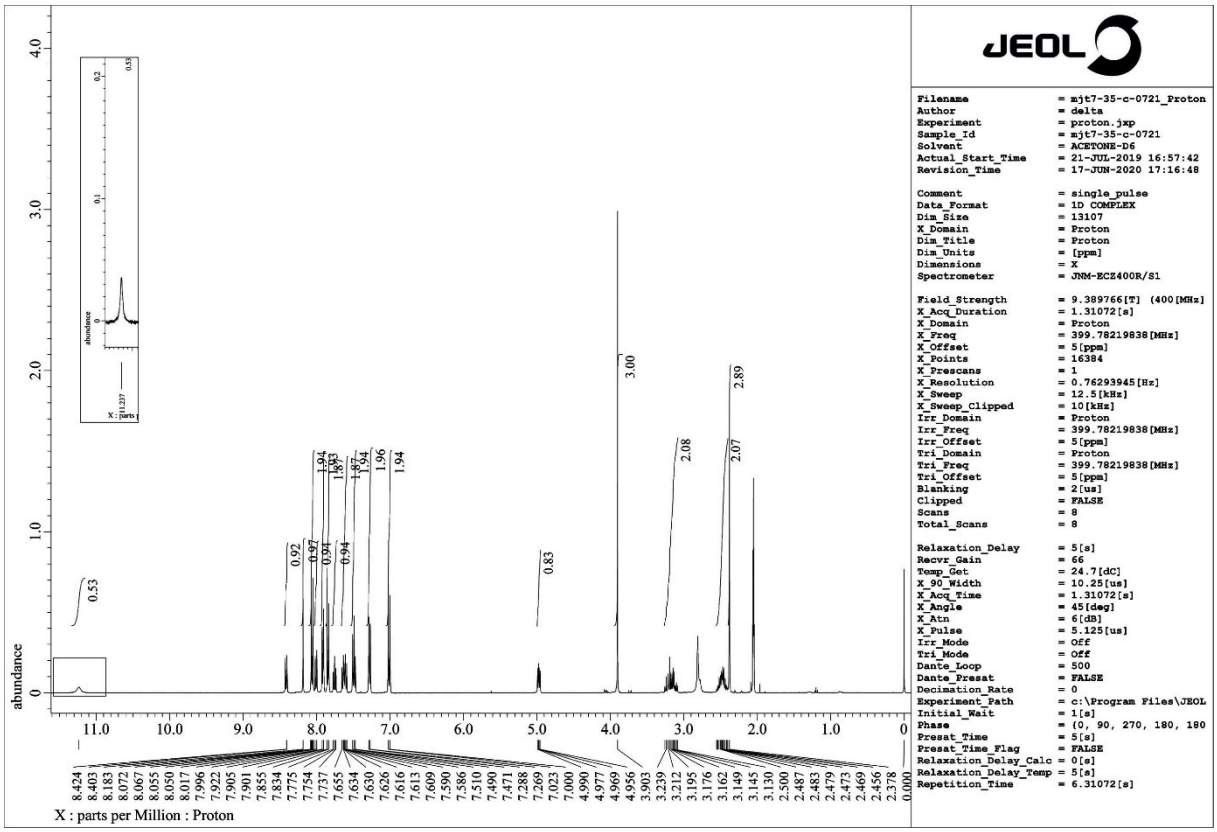
JEOL

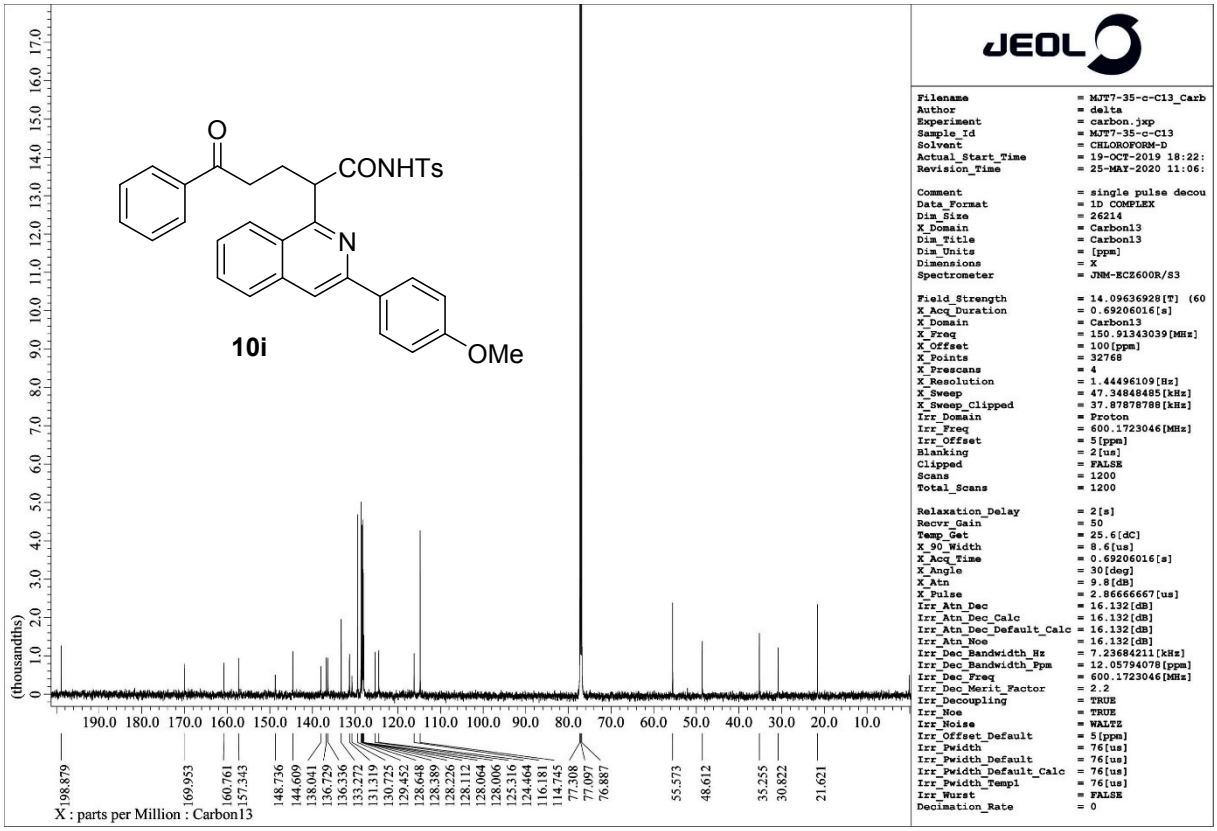
Filename	= MJT7-54-C_Proton-6-3.
Author	= delta
Experiment	= proton.jxp
Sample_Id	= MJT7-54-C
Solvent	= ACETONE-D6
Actual_Start_Time	= 5-JUL-2019 19:04:29
Revision_Time	= 17-JUN-2020 12:29:04
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [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	= 26.8[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
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 7.18628096[s]


O
CONHTs
N
Me
10g
(thousandths)
X : parts per Million : Carbon13
198.884
170.040
157.151
148.968
144.579
142.001
138.379
138.254
136.711
136.376
133.271
130.703
129.438
129.294
129.208
128.643
128.374
128.106
127.119
126.937
124.302
124.101
116.799
48.646
35.249
30.813
21.997
21.623
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = MJT7-54-c-C13_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-54-c-C13
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-NOV-2019 17:00:
Revision_Time = 7-NOV-2019 20:31:
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 = 1500
Total_Scans = 1500
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]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]


O
CONHTs
N
F
10h
abundance
X : parts per Million : Proton
6.01
3.00
2.15
2.02
2.01
2.02
1.85
1.96
1.00
1.02
0.94
0.95
0.98
0.62
11.084
8.592
8.578
8.569
8.555
8.290
8.107
8.097
8.088
8.084
7.929
7.908
7.905
7.832
7.811
7.756
7.750
7.731
7.725
7.626
7.609
7.593
7.590
7.586
7.536
7.529
7.513
7.508
7.489
7.479
7.469
7.464
7.456
7.452
7.263
7.242
5.019
5.006
4.996
4.983
3.225
3.208
3.189
3.176
3.158
2.534
2.521
2.517
2.513
2.498
2.469
2.456
2.437
2.370
0.000
Filename = MJT7-47-C-0714_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-47-C-0714
Solvent = ACETONE-D6
Actual_Start_Time = 14-JUL-2019 17:26:17
Revision_Time = 17-JUN-2020 14:49:50
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 1.31072[s]
X_Domain = Proton
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.76293945[Hz]
X_Sweep = 12.5[kHz]
X_Sweep_Clipped = 10[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 = 25.1[dC]
X_90_Width = 10.25[us]
X_Acq_Time = 1.31072[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 5.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.31072[s]

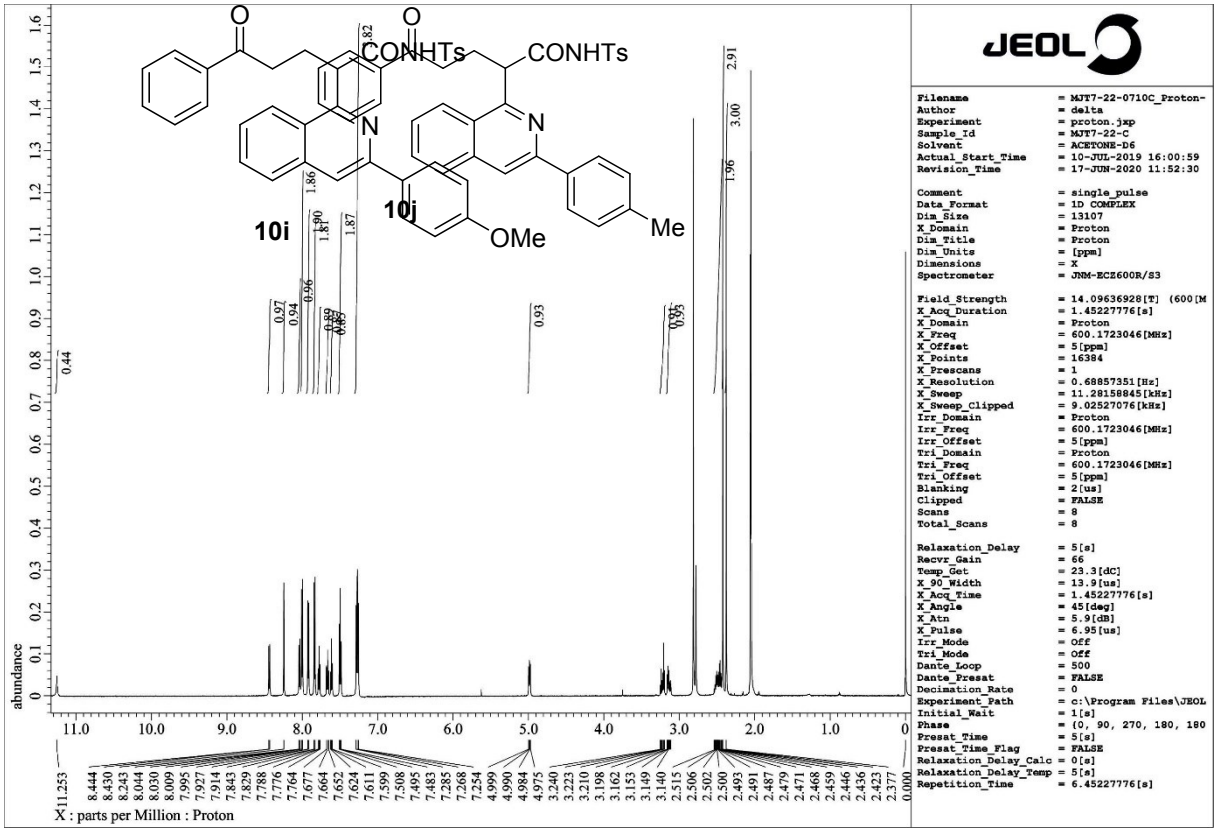

O
CONHTs
N
F
10h
(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = MJT7-47-c-C13_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-47-c-C13
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-OCT-2019 17:56:
Revision_Time = 25-MAY-2020 11:07:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
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 = 500
Total_Scans = 500
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]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0


abundance
X : parts per Million : Proton
JEOL
Filename = mjt7-35-c-0721_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = mjt7-35-c-0721
Solvent = ACETONE-D6
Actual_Start_Time = 21-JUL-2019 16:57:42
Revision_Time = 17-JUN-2020 17:16:48
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400R/S1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 1.31072[s]
X_Domain = Proton
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.76293945[Hz]
X_Sweep = 12.5[kHz]
X_Sweep_Clipped = 10[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 = 24.7[dC]
X_90_Width = 10.25[us]
X_Acq_Time = 1.31072[s]
X_Angle = 45[deg]
X_Atn = 6[dB]
X_Pulse = 5.125[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.31072[s]



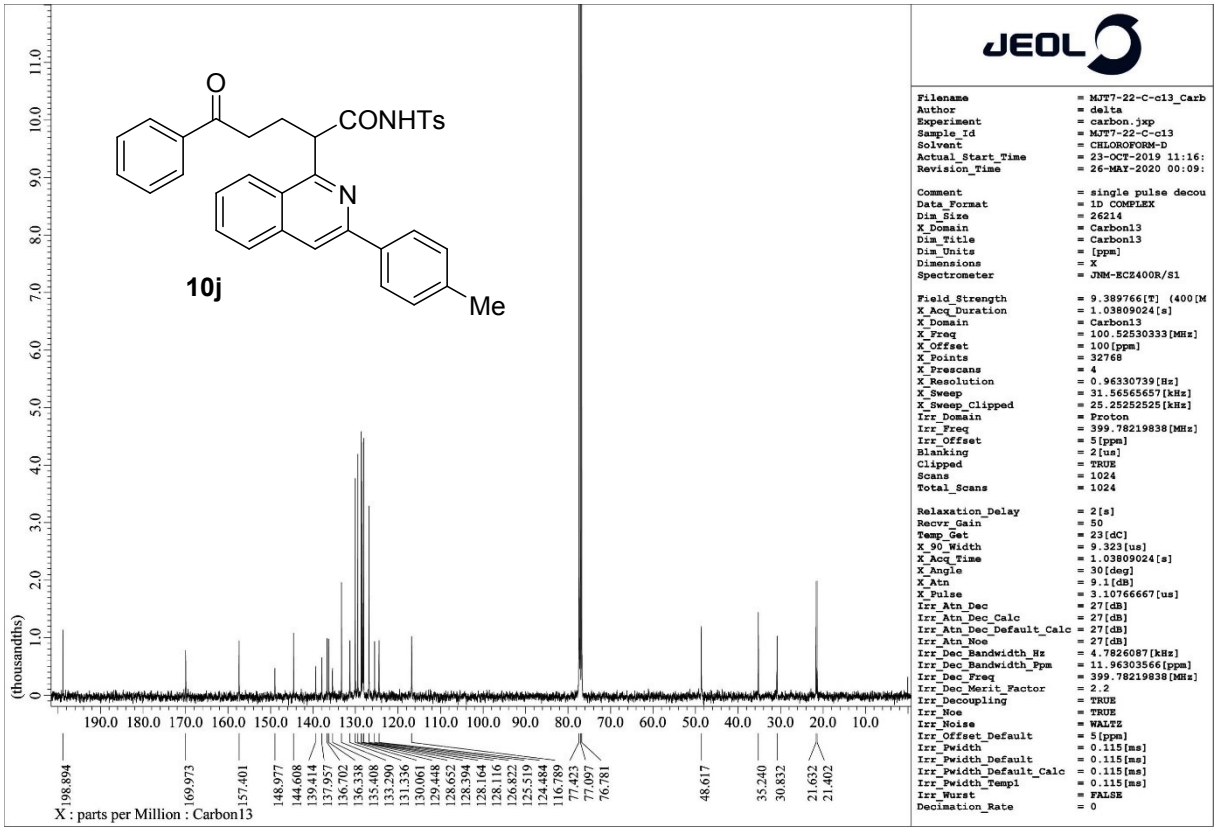
JEOL

Filename	= MJT7-35-c-C13_Carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= MJT7-35-c-C13
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 19-OCT-2019 18:22:
Revision_Time	= 25-MAY-2020 11:06:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
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	= 1200
Total_Scans	= 1200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 25.6[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]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Templ	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0



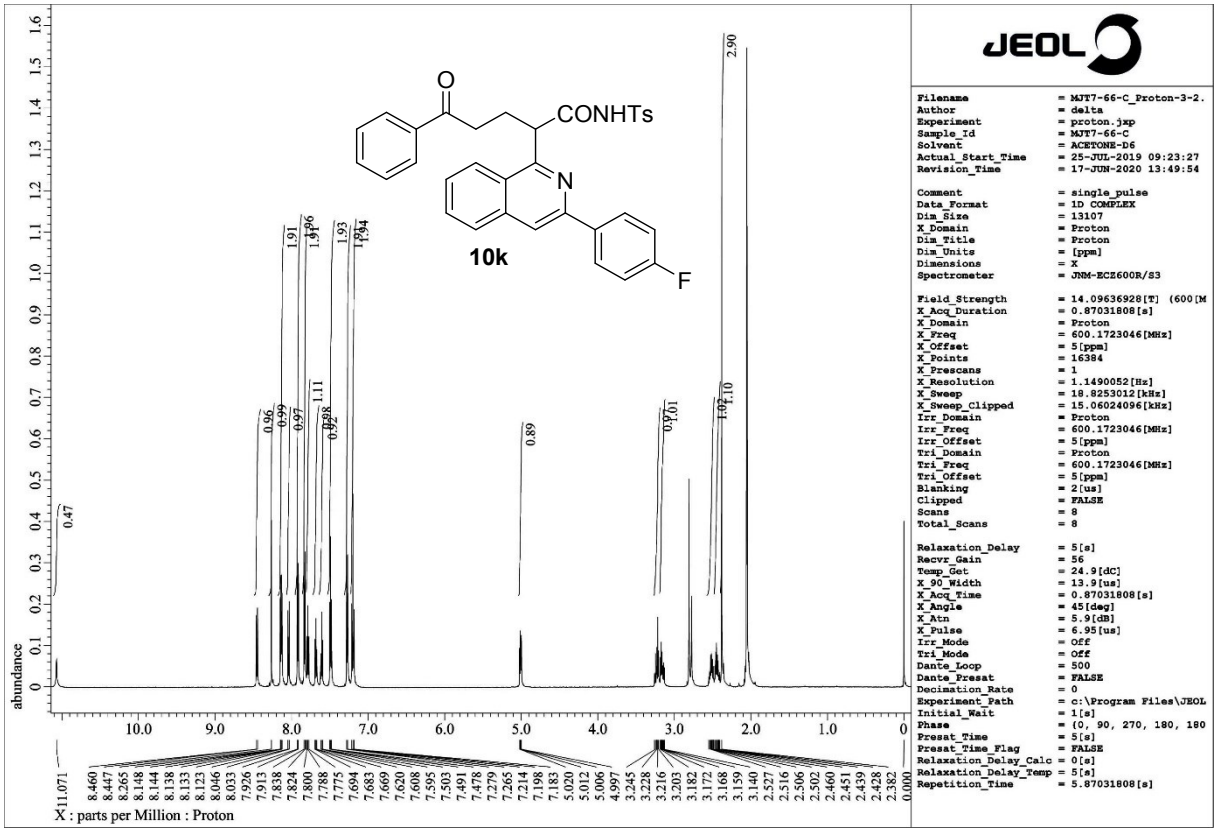
JEOL

Filename	= MJT7-22-0710C_Proton-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= MJT7-22-C
Solvent	= ACETONE-D6
Actual_Start_Time	= 10-JUL-2019 16:00:59
Revision_Time	= 17-JUN-2020 11:52:30
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (600[M
X_Acq_Duration	= 1.45227776[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68857351[Hz]
X_Sweep	= 11.28158845[kHz]
X_Sweep_Clipped	= 9.02527076[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	= 23.3[dC]
X_90_Width	= 13.9[us]
X_Acq_Time	= 1.45227776[s]
X_Angle	= 45[deg]
X_Atn	= 5.9[dB]
X_Pulse	= 6.95[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 9[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 6.45227776[s]



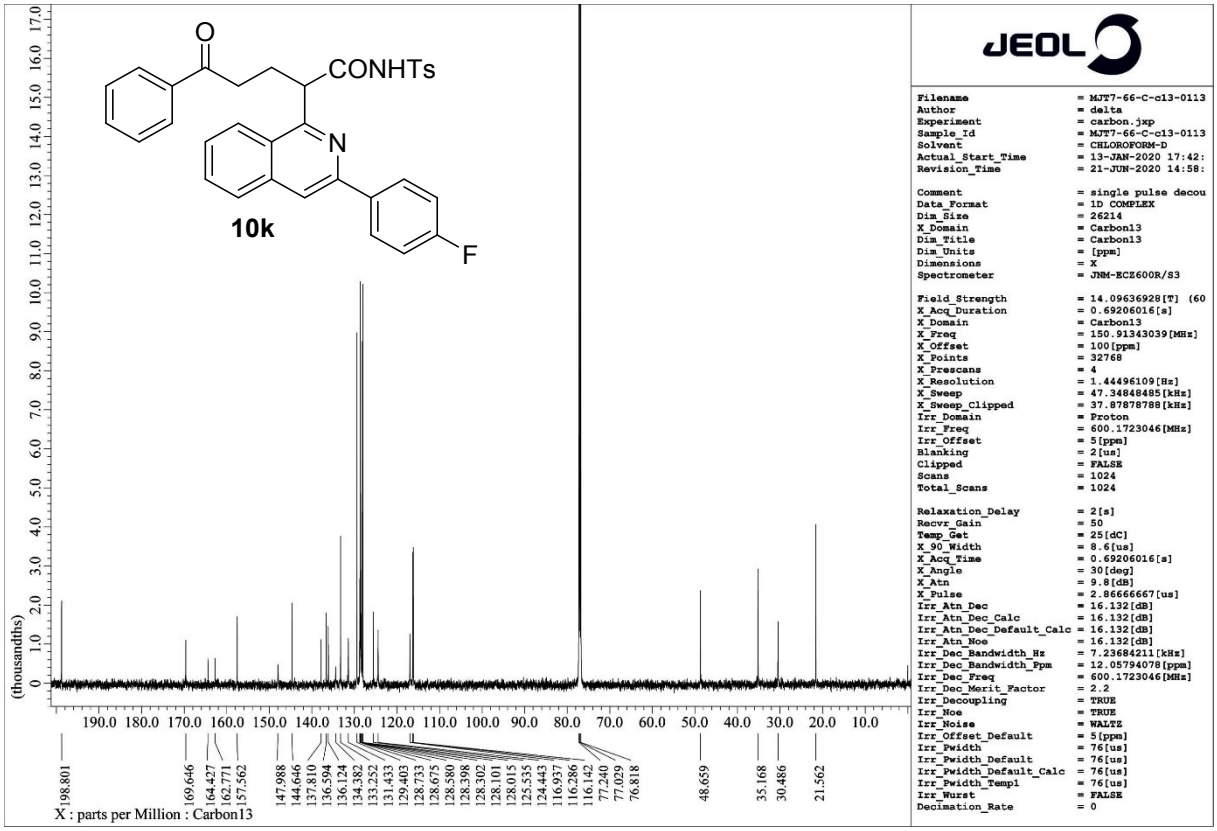
JEOL

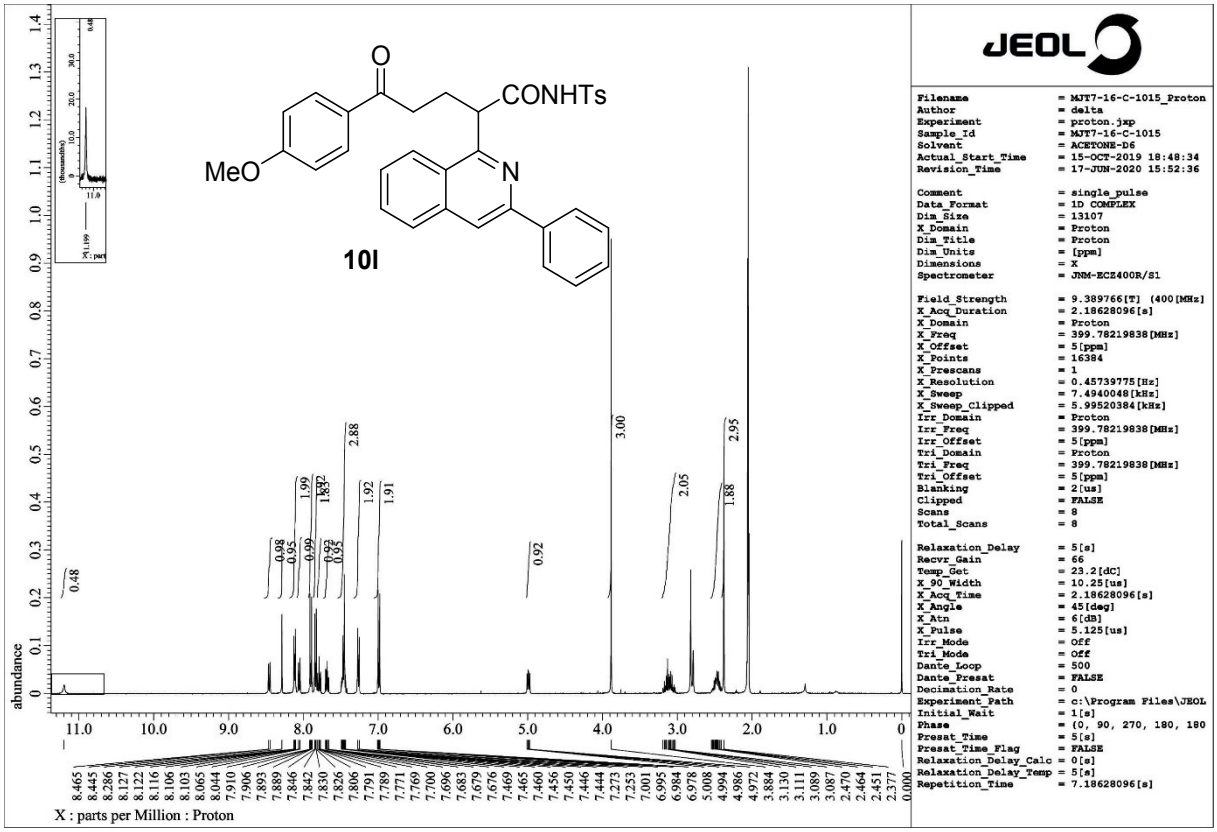
Filename	= MJT7-22-C-c13_Carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= MJT7-22-C-c13
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-OCT-2019 11:16:
Revision_Time	= 26-MAY-2020 00:09:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
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	= 23[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]
Irr_Dec_Freq	= 399.78219838[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 0.115[ms]
Irr_Pwidth_Default	= 0.115[ms]
Irr_Pwidth_Default_Calc	= 0.115[ms]
Irr_Pwidth_Temp1	= 0.115[ms]
Irr_Wurst	= FALSE
Decimation_Rate	= 0

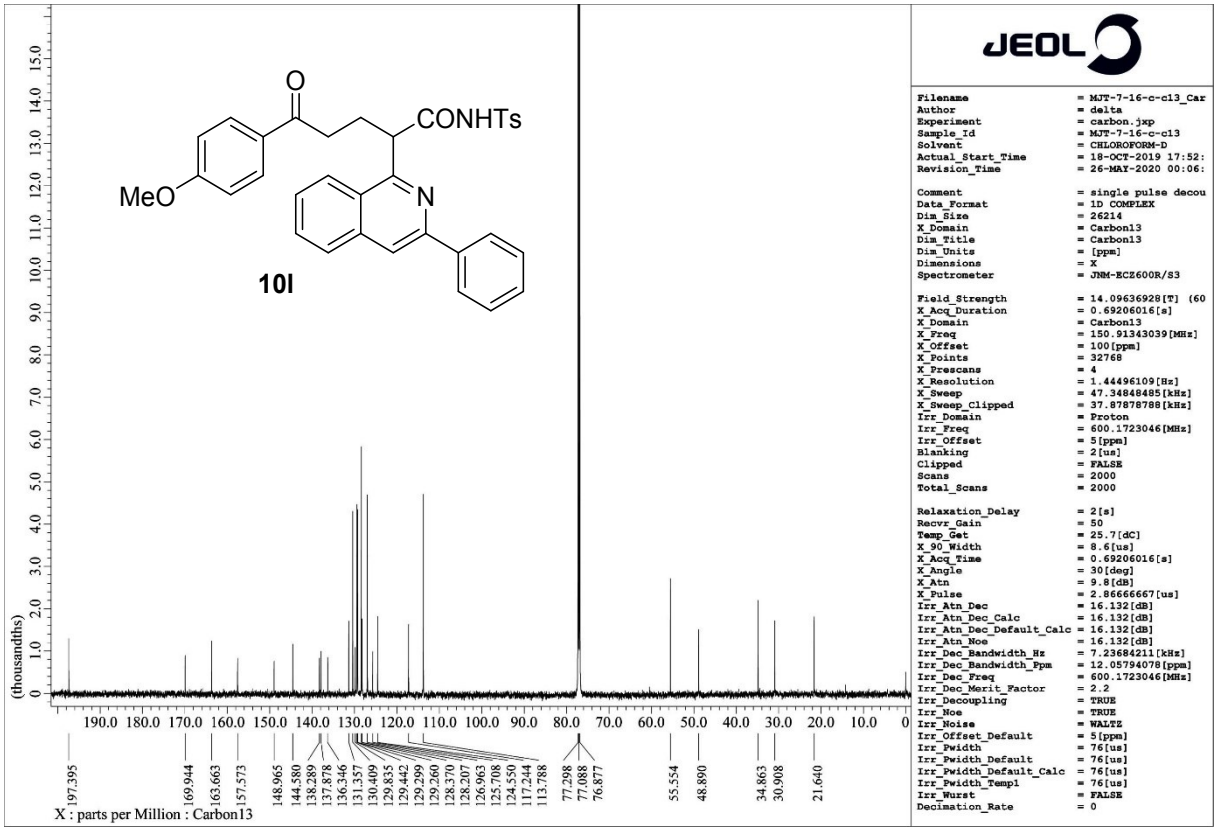


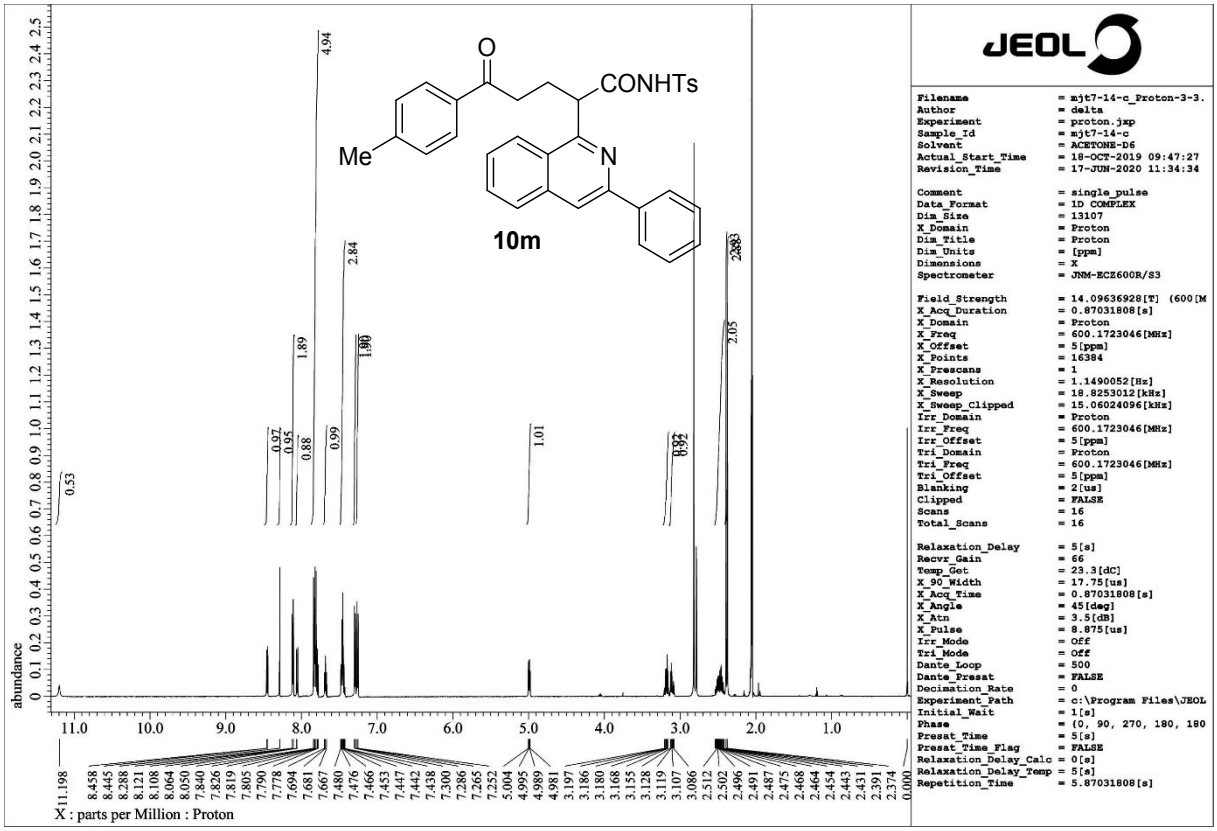
JEOL

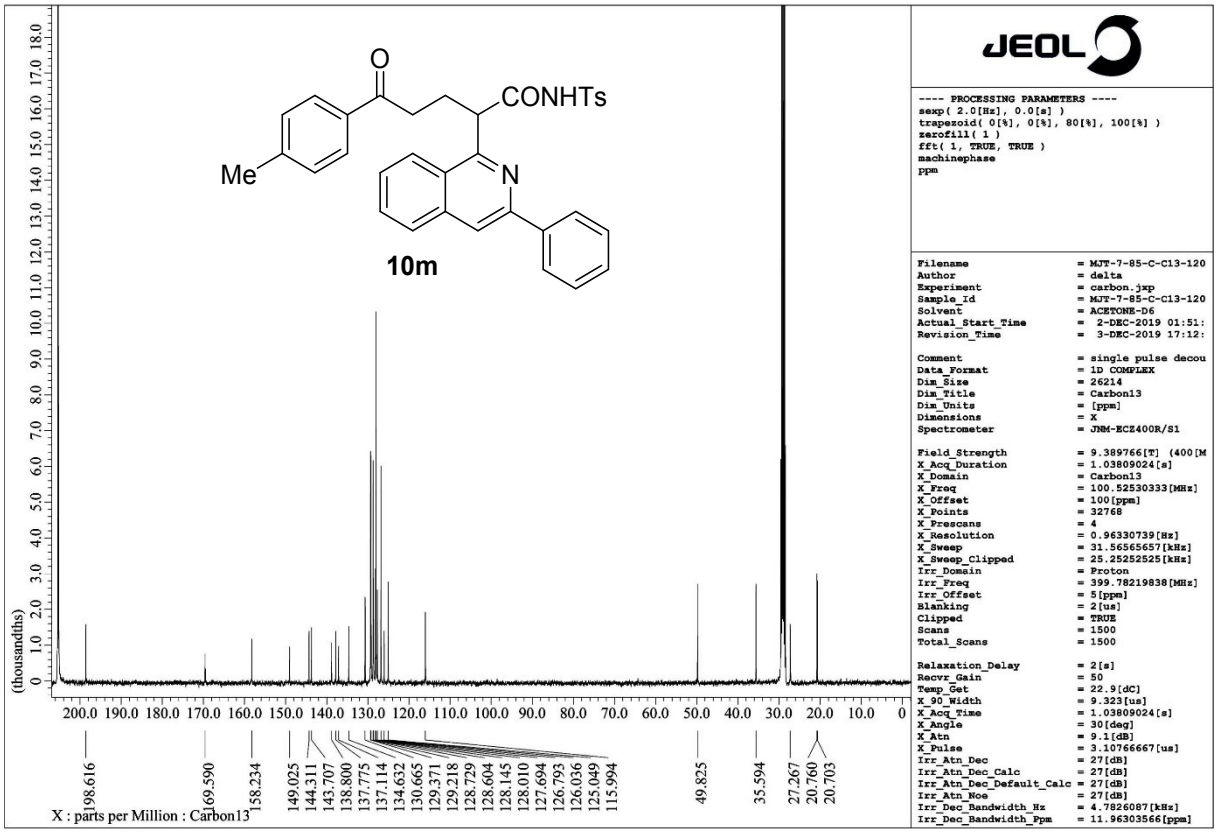
Filename	= MJT7-66-C_Proton-3-2.
Author	= delta
Experiment	= proton.jxp
Sample_Id	= MJT7-66-C
Solvent	= ACETONE-D6
Actual_Start_Time	= 25-JUL-2019 09:23:27
Revision_Time	= 17-JUN-2020 13:49:54
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [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	= 24.9[dC]
X_90_Width	= 13.9[us]
X_Acq_Time	= 0.87031808[s]
X_Angle	= 45[deg]
X_Atn	= 5.9[dB]
X_Pulse	= 6.95[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 5.87031808[s]


O
CONHTs
N
F
10k
(thousandths)
X : parts per Million : Carbon13
198.801
169.646
164.427
162.771
157.562
147.988
144.646
137.810
136.594
136.124
134.382
133.252
131.433
129.403
128.733
128.675
128.580
128.398
128.302
128.101
128.015
125.535
124.443
116.937
116.286
116.142
77.240
77.029
76.818
48.659
35.168
30.486
21.562
JEOL
Filename = MJT7-66-C-c13-0113
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-66-C-c13-0113
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-JAN-2020 17:42:
Revision_Time = 21-JUN-2020 14:58:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
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 = 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]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0


O
CONHTs
MeO
N
10l
abundance
X : parts per Million : Proton
0.48
0.98
0.95
0.99
0.99
0.93
0.92
1.99
1.93
2.88
1.92
1.91
0.92
3.00
2.05
2.95
1.88
JEOL
Filename = MJT7-16-C-1015_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-16-C-1015
Solvent = ACETONE-D6
Actual_Start_Time = 15-OCT-2019 18:48:34
Revision_Time = 17-JUN-2020 15:52:36
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 23.2[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

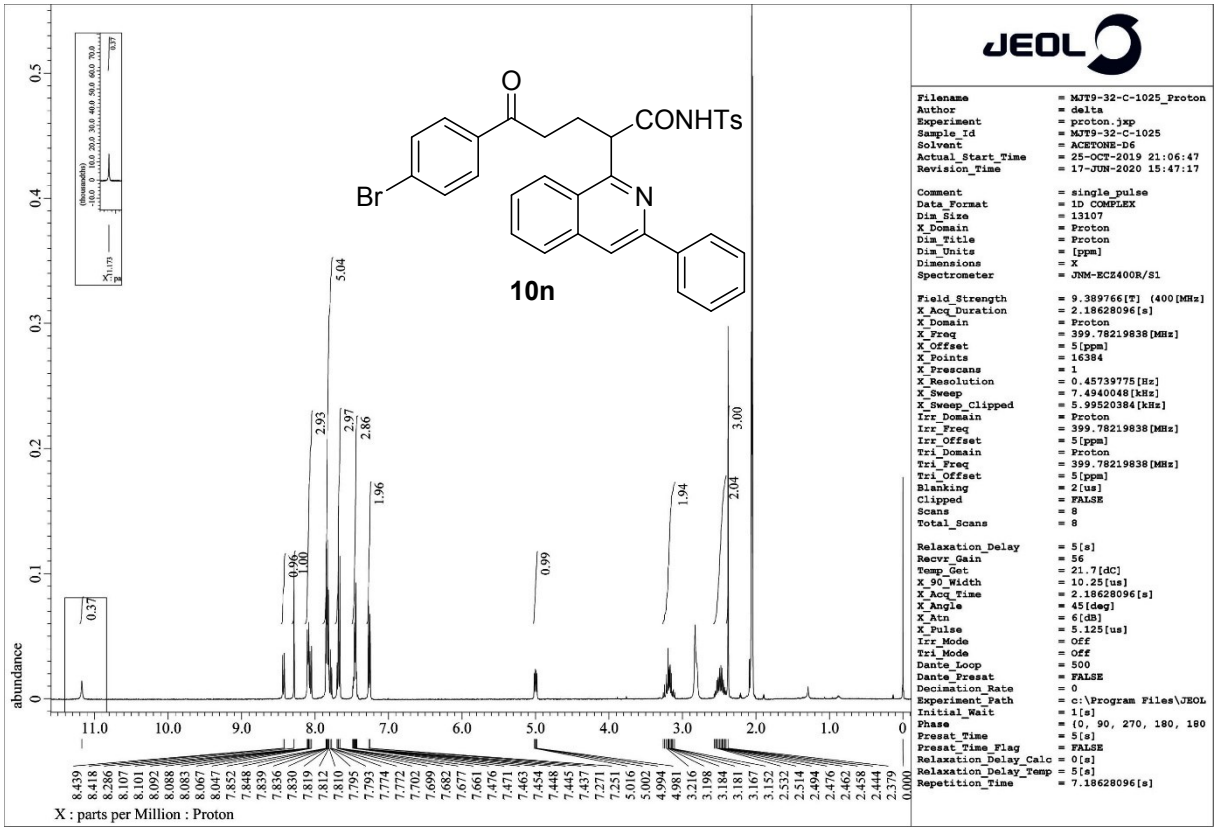

O
CONHTs
MeO
N
10l
(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = MJT-7-16-c-c13_Car
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT-7-16-c-c13
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-OCT-2019 17:52:
Revision_Time = 26-MAY-2020 00:06:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
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 = 2000
Total_Scans = 2000
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.7[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]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0


O
CONHTs
Me
N
10m
abundance
X : parts per Million : Proton
JEOL
Filename = mjt7-14-c_Proton-3-3.
Author = delta
Experiment = proton.jxp
Sample_Id = mjt7-14-c
Solvent = ACETONE-D6
Actual_Start_Time = 18-OCT-2019 09:47:27
Revision_Time = 17-JUN-2020 11:34:34
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 23.3[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 5.87031808[s]

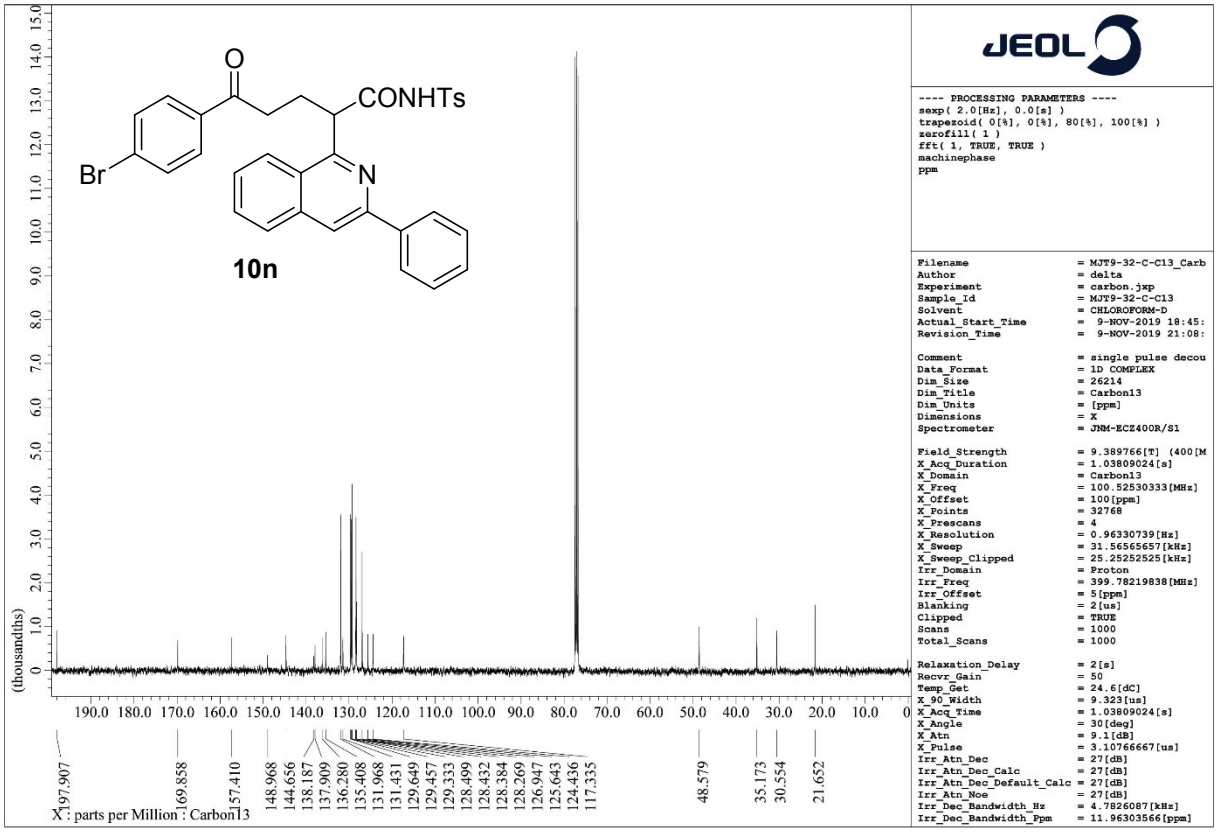


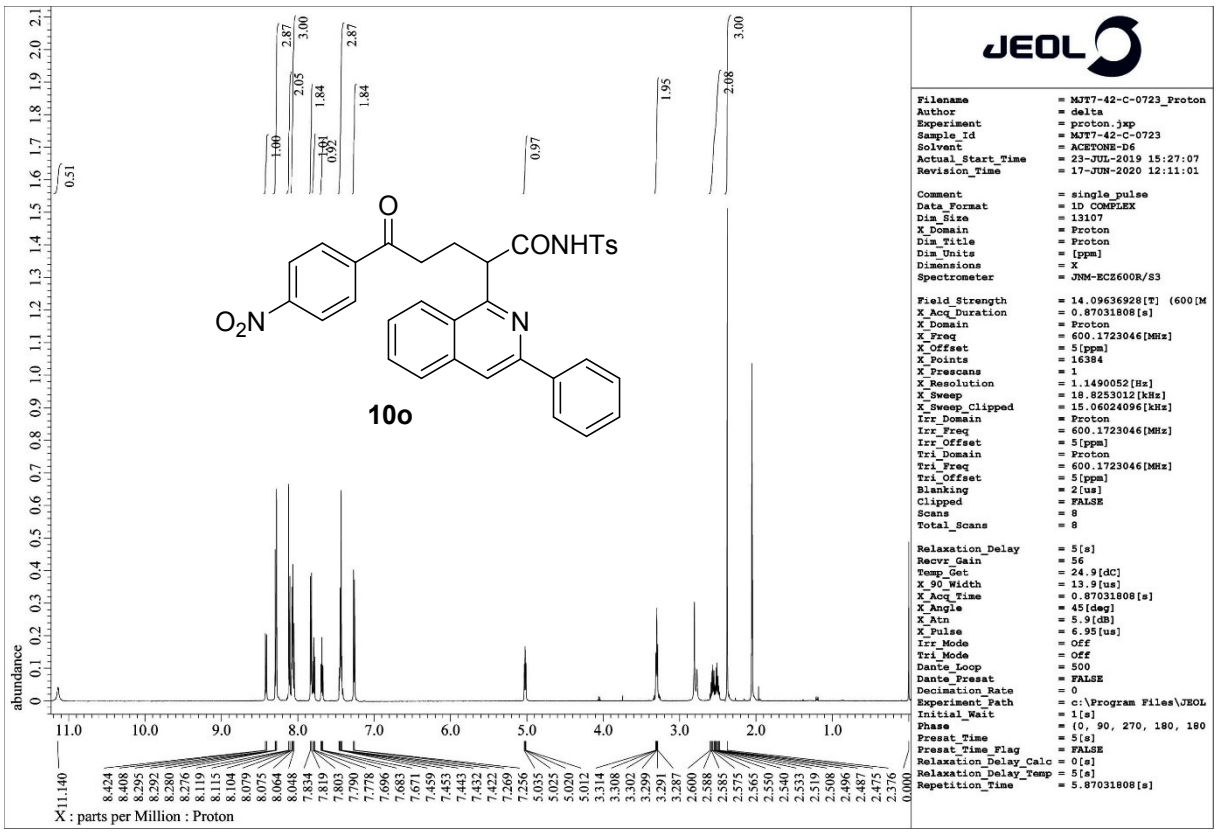

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

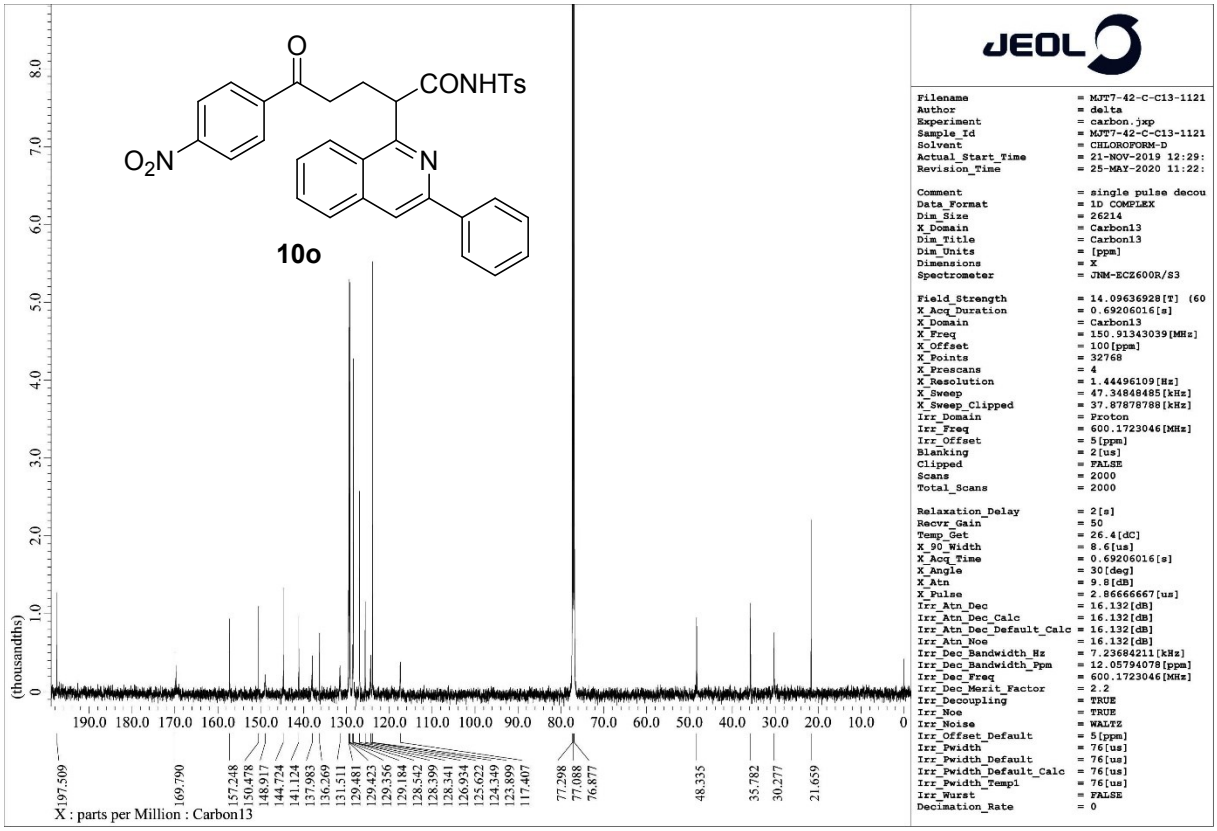
Filename	= MJT-7-85-C-C13-120
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= MJT-7-85-C-C13-120
Solvent	= ACETONE-D6
Actual_Start_Time	= 2-DEC-2019 01:51:
Revision_Time	= 3-DEC-2019 17:12:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
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	= 1500
Total_Scans	= 1500
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.9[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]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]

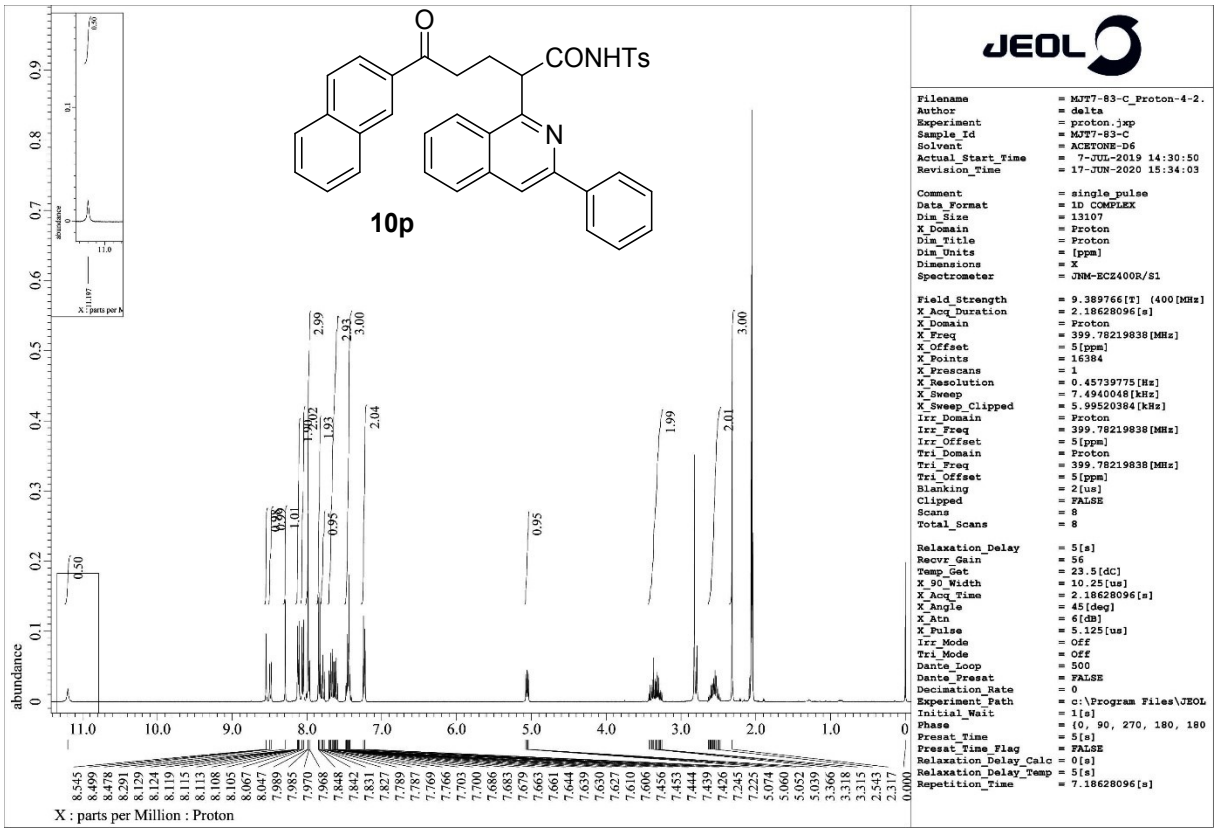


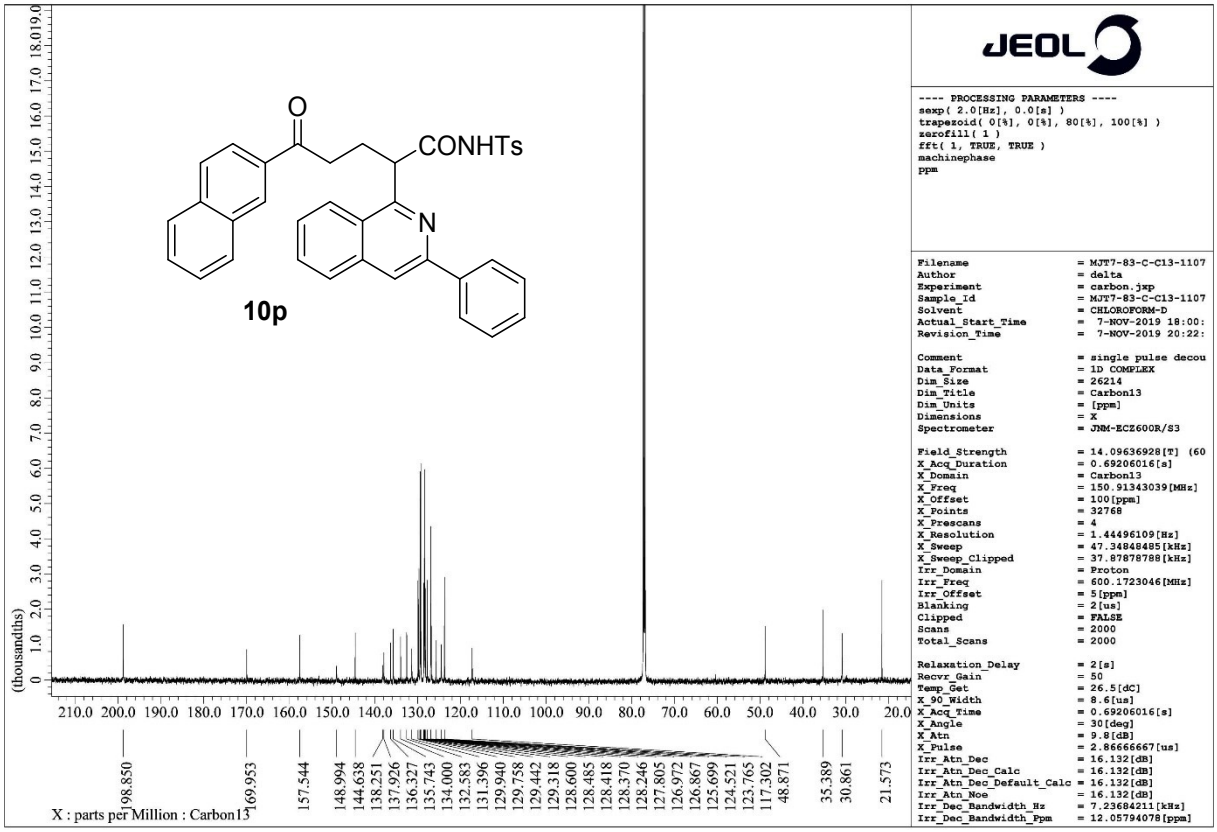
Filename	= MJT9-32-C-1025_Proton
Author	= delta
Experiment	= proton.jxp
Sample_Id	= MJT9-32-C-1025
Solvent	= ACETONE-D6
Actual_Start_Time	= 25-OCT-2019 21:06:47
Revision_Time	= 17-JUN-2020 15:47:17
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [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	= 21.7[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
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 7.18628096[s]


O
CONHTs
Br
N
10n
(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 = MJT9-32-C-C13_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT9-32-C-C13
Solvent = CHLOROFORM-D
Actual_Start_Time = 9-NOV-2019 18:45:
Revision_Time = 9-NOV-2019 21:08:
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 = 1000
Total_Scans = 1000
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]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]


O
CONHTs
O2N
N
10o
abundance
X : parts per Million : Proton
Filename = MJT7-42-C-0723_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-42-C-0723
Solvent = ACETONE-D6
Actual_Start_Time = 23-JUL-2019 15:27:07
Revision_Time = 17-JUN-2020 12:11:01
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 24.9[dC]
X_90_Width = 13.9[us]
X_Acq_Time = 0.87031808[s]
X_Angle = 45[deg]
X_Atn = 5.9[dB]
X_Pulse = 6.95[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 5.87031808[s]

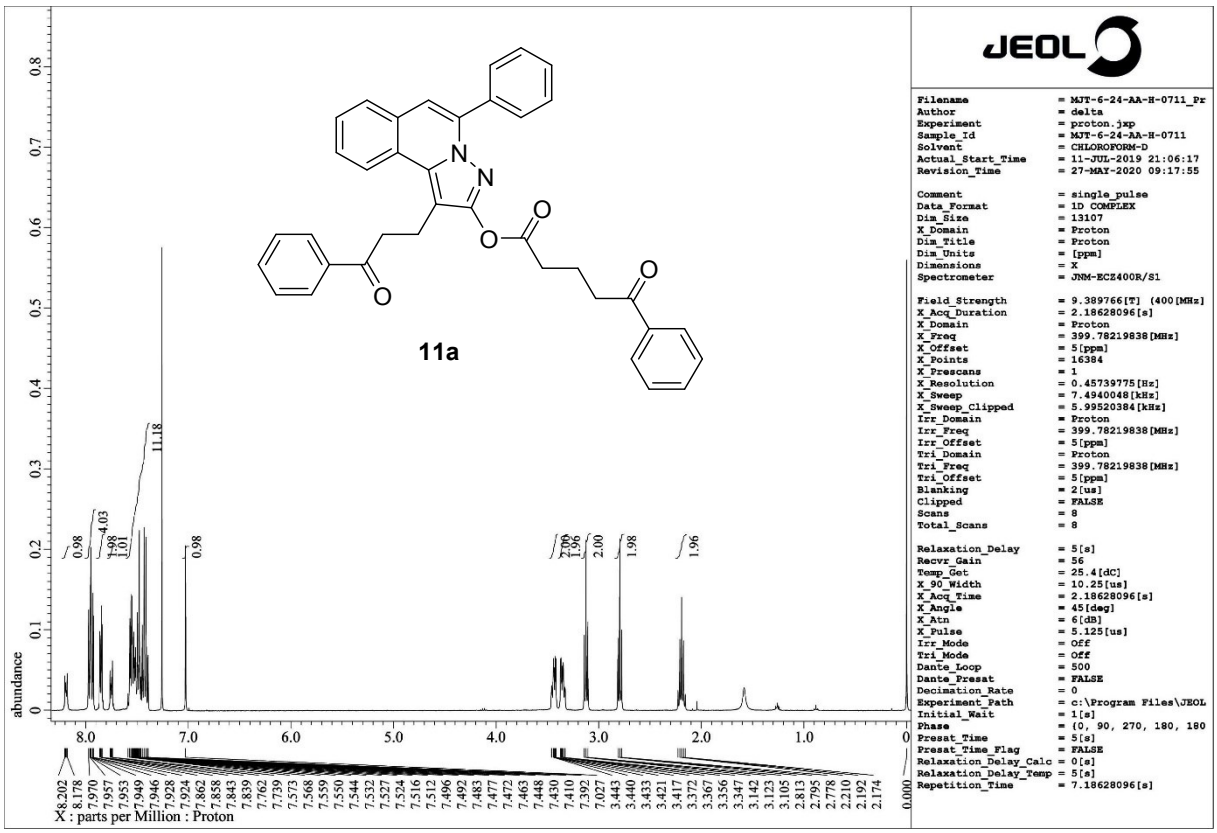

O
CONHTs
O_2N
N
10o
(thousandths)
X : parts per Million : Carbon13
Filename = MJT7-42-C-C13-1121
Author = delta
Experiment = carbon.jxp
Sample_Id = MJT7-42-C-C13-1121
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-NOV-2019 12:29:
Revision_Time = 25-MAY-2020 11:22:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
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 = 2000
Total_Scans = 2000
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 26.4[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]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0


O
CONHTs
N
10p
abundance
X : parts per Million : Proton
Filename = MJT7-83-C_Proton-4-2.
Author = delta
Experiment = proton.jxp
Sample_Id = MJT7-83-C
Solvent = ACETONE-D6
Actual_Start_Time = 7-JUL-2019 14:30:50
Revision_Time = 17-JUN-2020 15:34:03
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 23.5[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

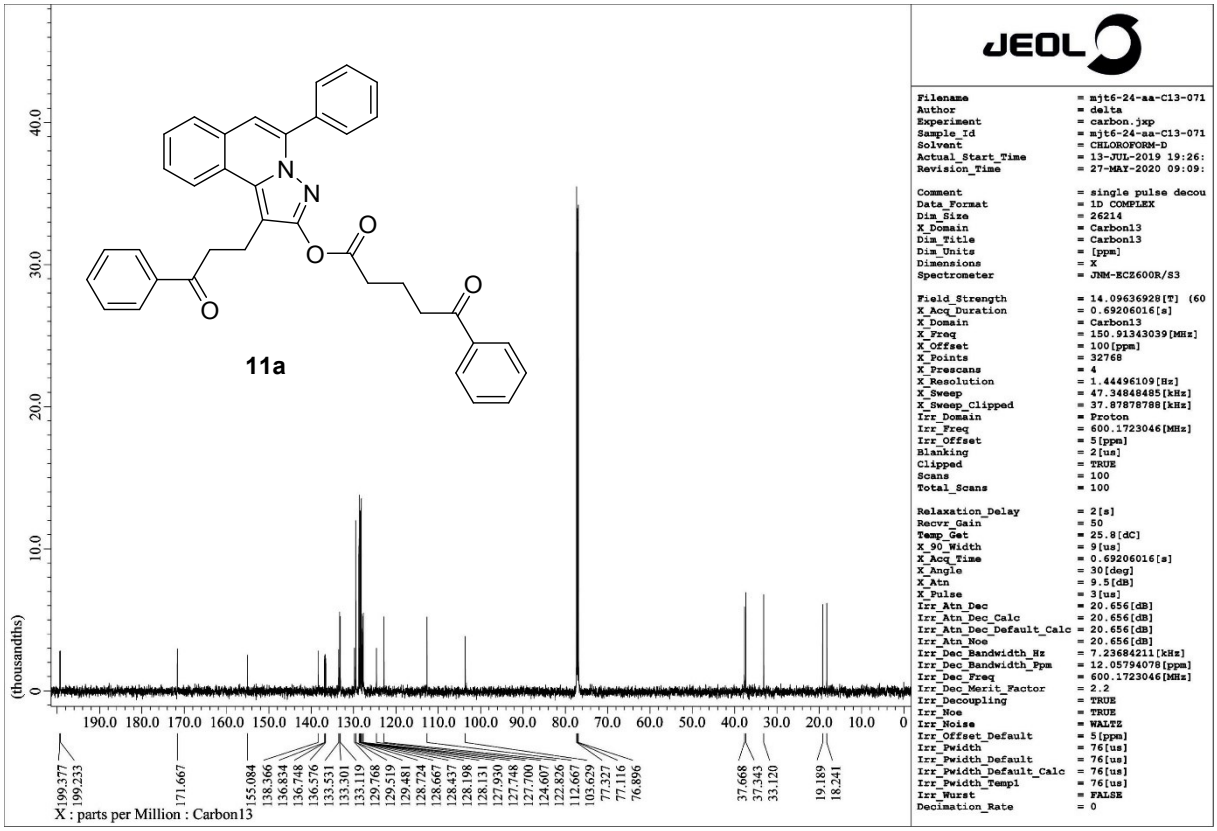


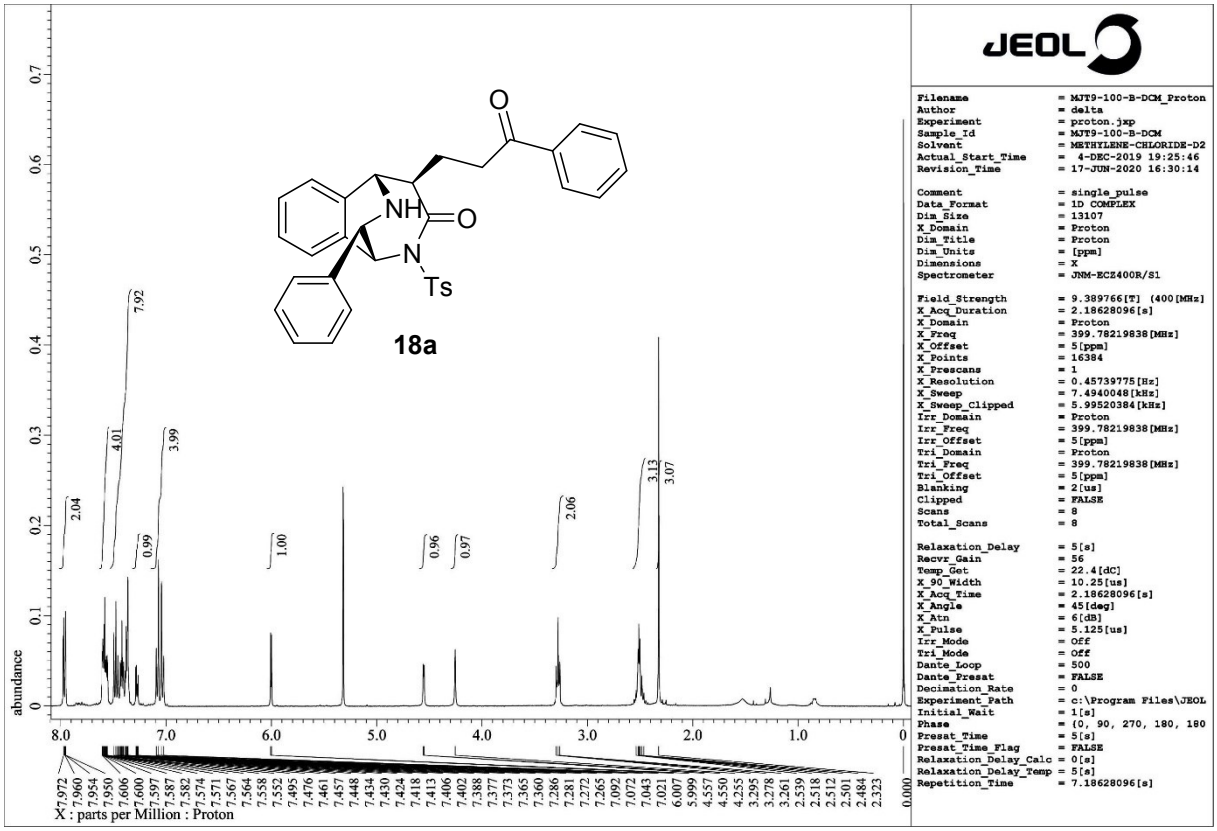

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

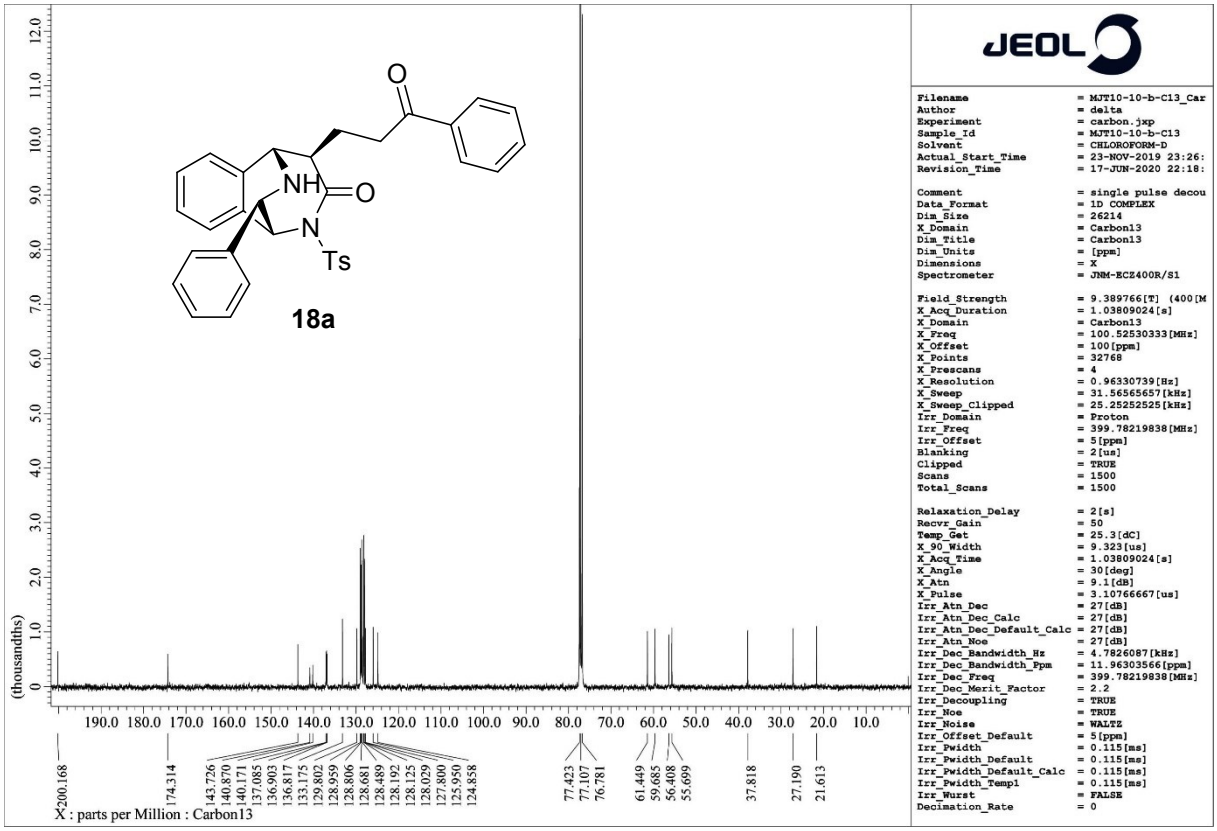
Filename	= MJT7-83-C-C13-1107
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= MJT7-83-C-C13-1107
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-NOV-2019 18:00:
Revision_Time	= 7-NOV-2019 20:22:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.69206016[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	= 2000
Total_Scans	= 2000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 26.5[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]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]



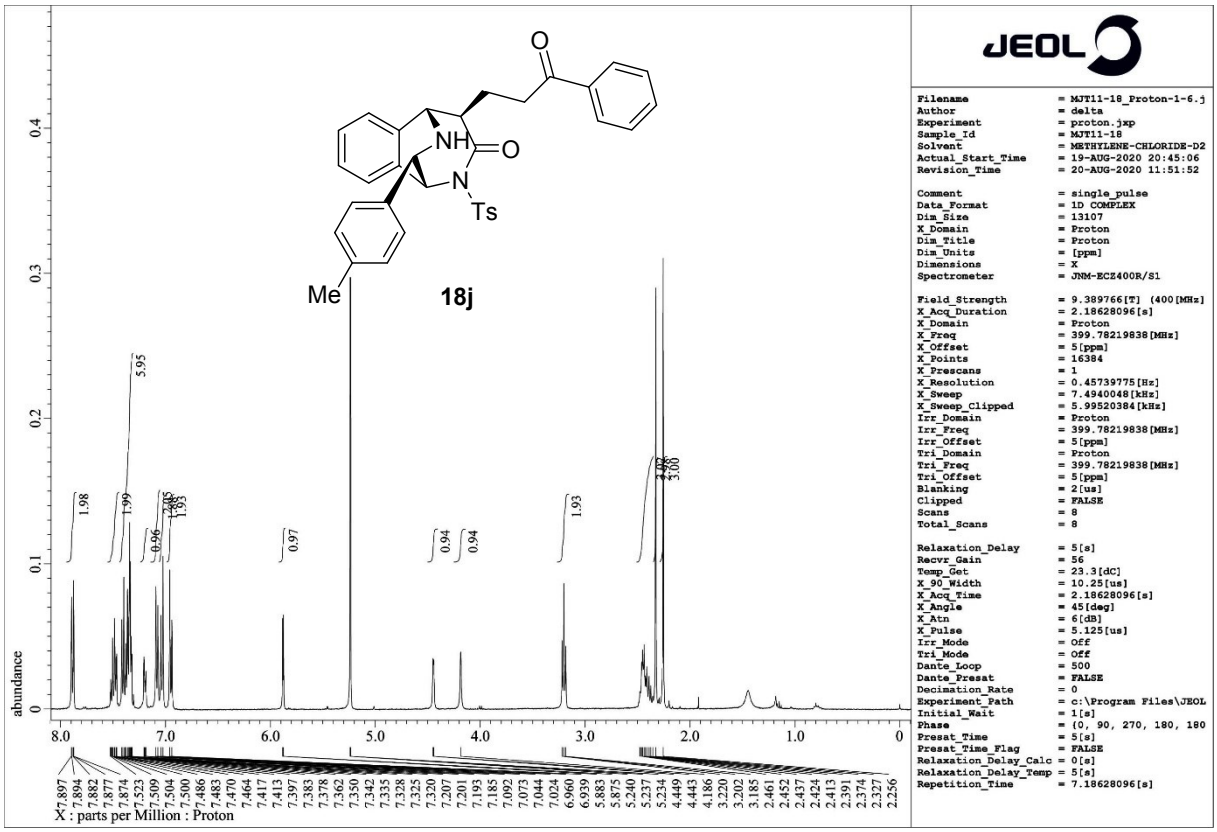
Filename	= MJT-6-24-AA-H-0711_Pr
Author	= delta
Experiment	= proton.jxp
Sample_Id	= MJT-6-24-AA-H-0711
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-JUL-2019 21:06:17
Revision_Time	= 27-MAY-2020 09:17:55
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
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	= 25.4[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
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 180
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 7.18628096[s]


11a
(thousandths)
X : parts per Million : Carbon13
199.377
199.233
171.667
155.084
138.366
136.834
136.748
136.576
133.531
133.301
133.119
129.768
129.519
129.481
128.724
128.667
128.437
128.198
128.131
127.930
127.748
127.700
124.607
122.826
112.667
103.629
77.327
77.116
76.896
37.668
37.343
33.120
19.189
18.241
Filename = mjt6-24-aa-C13-071
Author = delta
Experiment = carbon.jxp
Sample_Id = mjt6-24-aa-C13-071
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-JUL-2019 19:26:
Revision_Time = 27-MAY-2020 09:09:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
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 = TRUE
Scans = 100
Total_Scans = 100
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25.8[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 9.5[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 20.656[dB]
Irr_Atn_Dec_Calc = 20.656[dB]
Irr_Atn_Dec_Default_Calc = 20.656[dB]
Irr_Atn_Noe = 20.656[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0

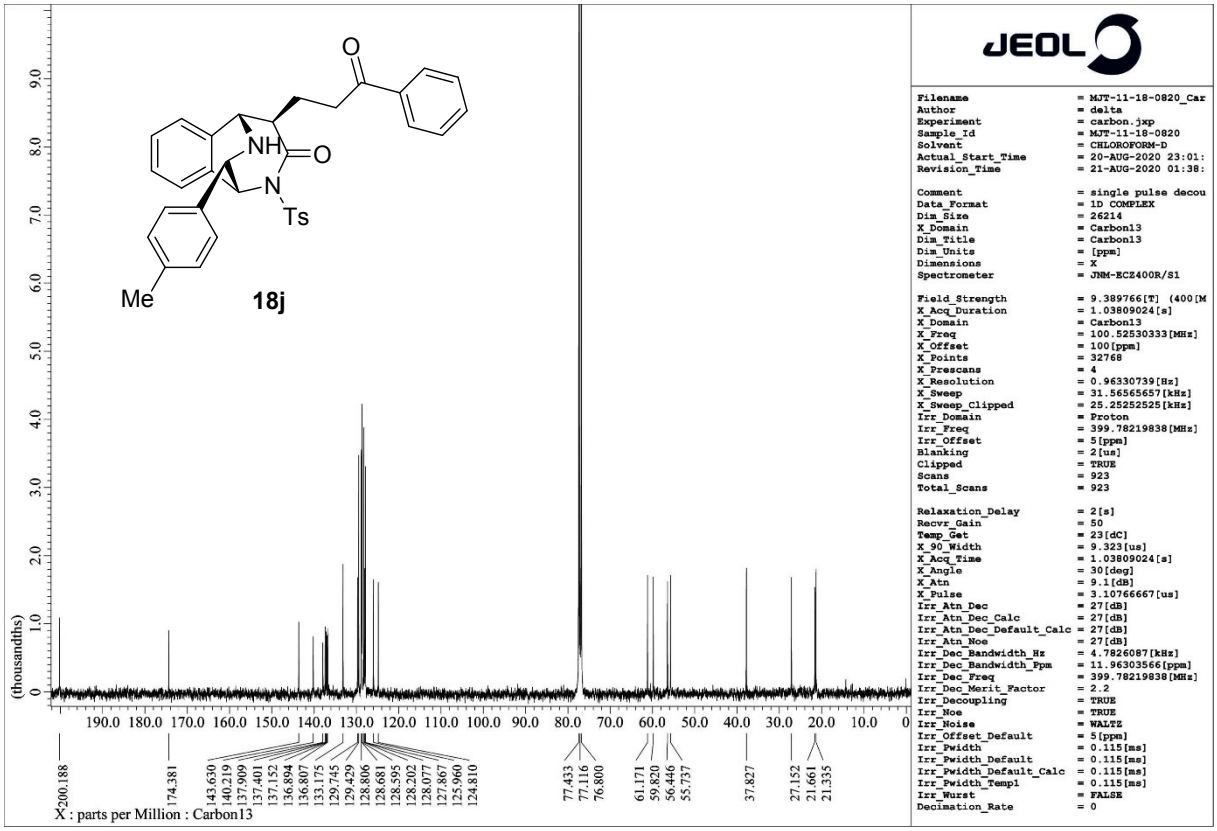

18a
abundance
X : parts per Million : Proton
7.92
4.01
3.99
2.04
0.99
1.00
0.96
0.97
2.06
3.13
3.07
7.972
7.960
7.954
7.950
7.606
7.600
7.597
7.587
7.582
7.574
7.571
7.567
7.564
7.558
7.552
7.495
7.476
7.461
7.457
7.448
7.434
7.430
7.424
7.418
7.413
7.406
7.402
7.388
7.377
7.373
7.365
7.360
7.286
7.281
7.272
7.265
7.092
7.072
7.043
7.021
6.007
5.999
4.557
4.550
4.255
3.295
3.278
3.261
2.539
2.518
2.512
2.501
2.484
2.323
0.000
Filename = MJT9-100-B-DCM_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = MJT9-100-B-DCM
Solvent = METHYLNE-CHLORIDE-D2
Actual_Start_Time = 4-DEC-2019 19:25:46
Revision_Time = 17-JUN-2020 16:30:14
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
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 = 22.4[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
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JEOL
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]



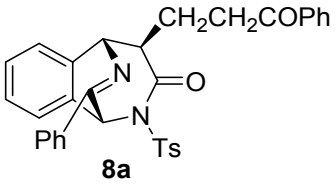

```
Filename                = MJT10-10-b-C13_Car
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = MJT10-10-b-C13
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 23-NOV-2019 23:26:
Revision_Time           = 17-JUN-2020 22:18:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Carbon13
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                   = 1500
Total_Scans             = 1500

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 25.3[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]
Irr_Dec_Bandwidth_Ppm   = 11.96303566[ppm]
Irr_Dec_Freq            = 399.78219838[MHz]
Irr_Dec_Merit_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = TRUE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 0.115[ms]
Irr_Pwidth_Default      = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Templ        = 0.115[ms]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
```



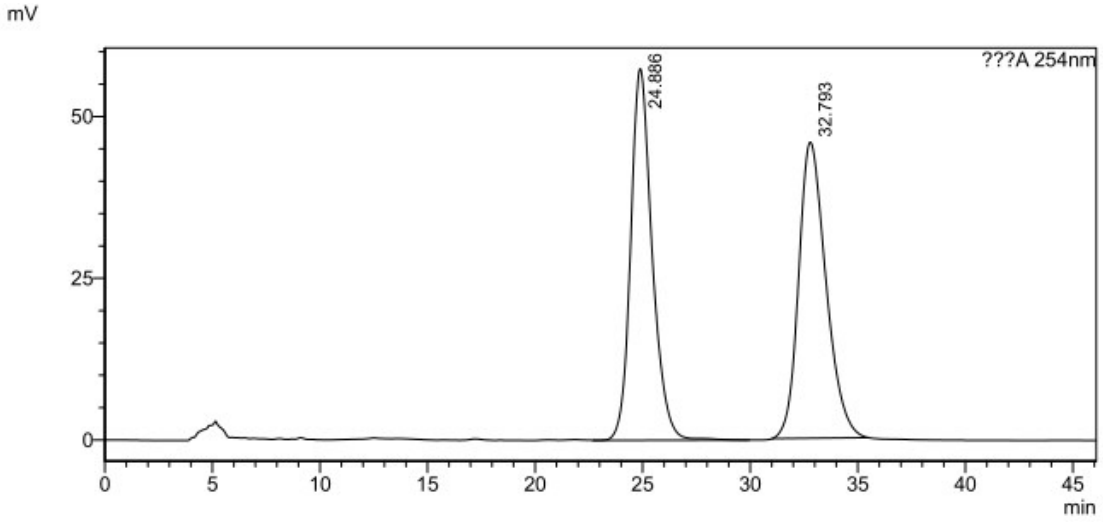

```
Filename                = MJT11-18_Proton-1-6.j
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = MJT11-18
Solvent                 = METHYLENE-CHLORIDE-D2
Actual_Start_Time       = 19-AUG-2020 20:45:06
Revision_Time           = 20-AUG-2020 11:51:52

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
X_Domain                = Proton
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                = 23.3[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
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = c:\Program Files\JEOL
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 5[s]
Repetition_Time         = 7.18628096[s]
```



6. HPLC spectra of products 8 and 9



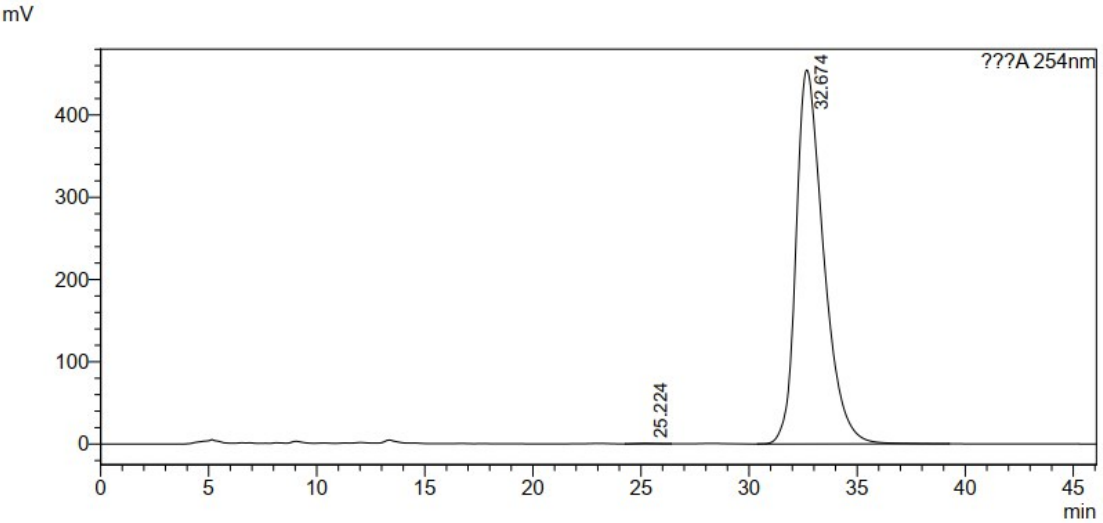
IA column, 70 : 30 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 ^{o}C, 99.8% ee.



<Peak Table>

???A 254nm

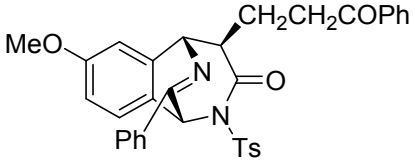
Peak#	Ret. Time	Area	Height	Conc.
1	24.886	3994994	57428	49.676
2	32.793	4047169	45758	50.324
Total		8042162	103186	



<Peak Table>

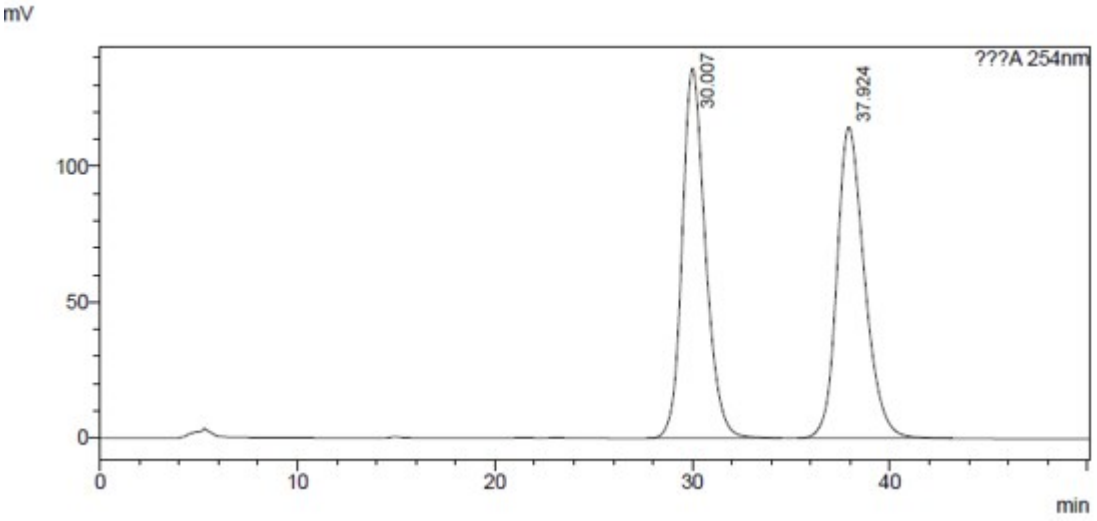
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	25.224	32822	572	0.081
2	32.674	40300694	454587	99.919
Total		40333516	455159	



8b

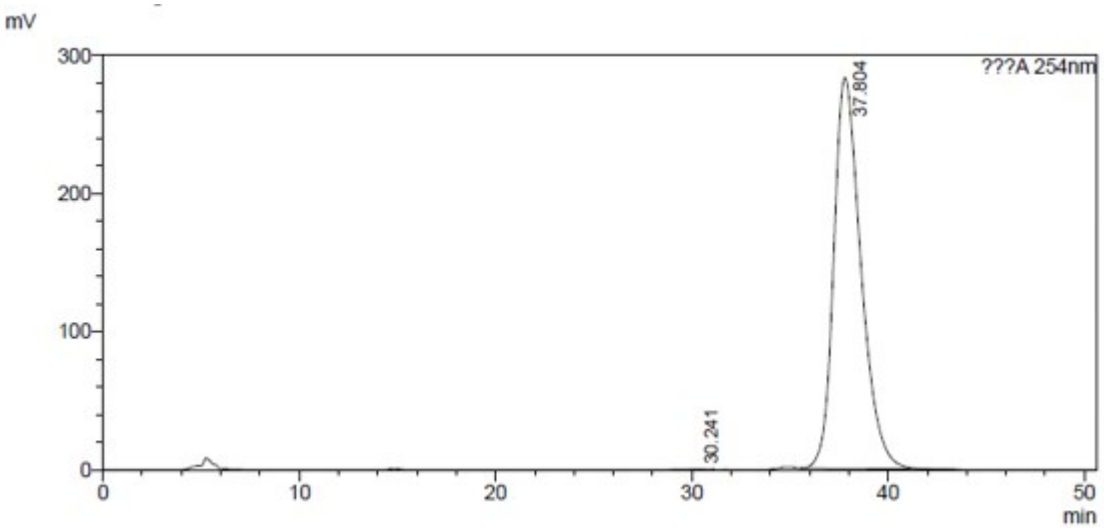
IA column, 70 : 30 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 °C, 99.9% ee.



<Peak Table>

???A 254nm

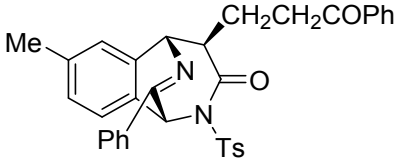
Peak#	Ret. Time	Area	Height	Conc.
1	30.007	11140710	136235	50.031
2	37.924	11127123	114603	49.969
Total		22267833	250838	



<Peak Table>

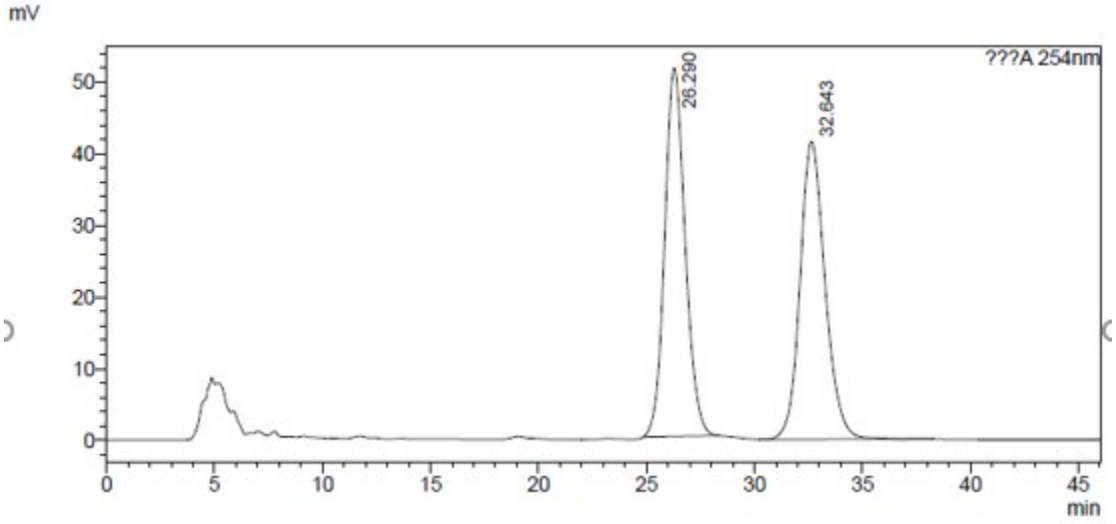
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	30.241	14612	254	0.053
2	37.804	27342326	283143	99.947
Total		27356939	283397	



8c

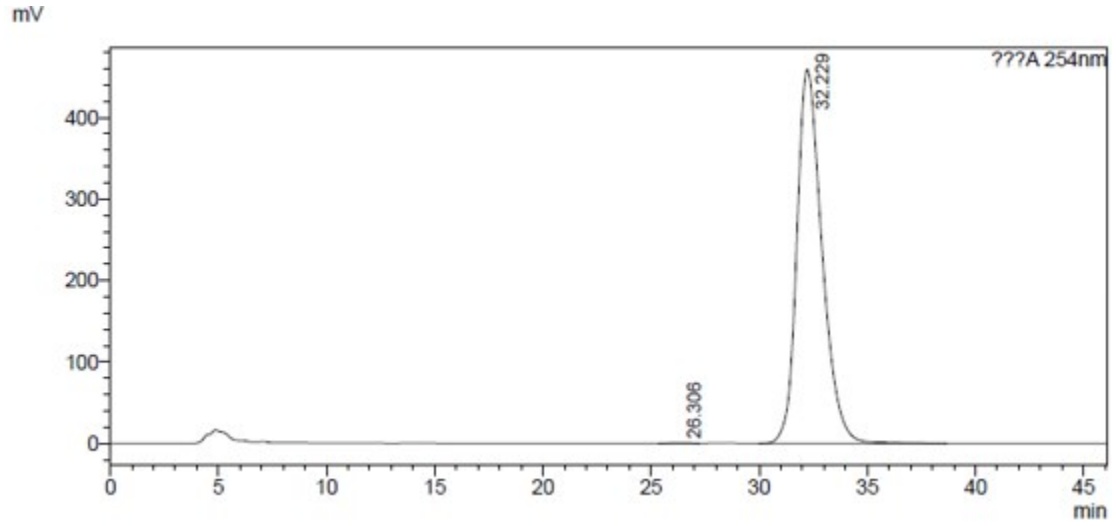
IA column, 75 : 25 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 °C, 99.9% ee.



<Peak Table>

???A 254nm

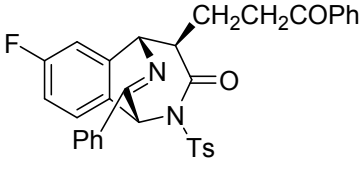
Peak#	Ret. Time	Area	Height	Conc.
1	26.290	3381867	51428	50.206
2	32.643	3354060	41563	49.794
Total		6735927	92991	



<Peak Table>

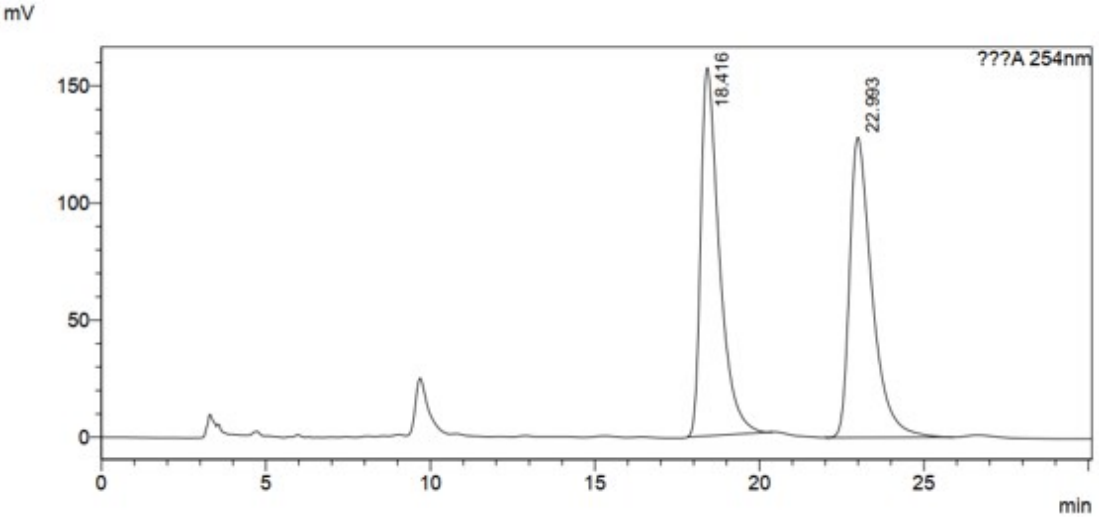
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	26.306	22071	411	0.059
2	32.229	37287344	459228	99.941
Total		37309416	459638	



8d

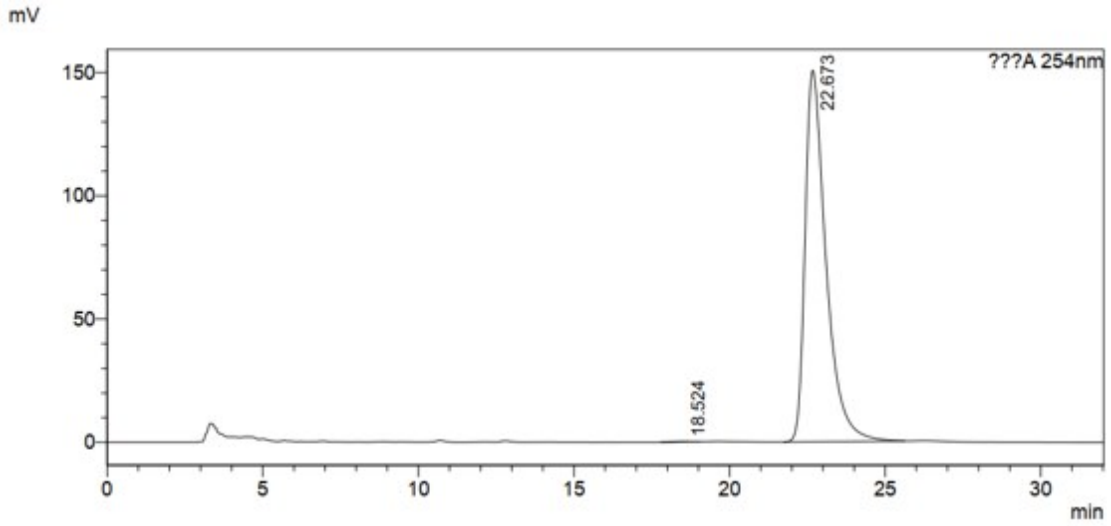
IB column, 90 : 10 hexane : IPA, flow rate: 1.0 ml/min, 254 nm, 25 °C, 99.7% ee.



<Peak Table>

???A 254nm

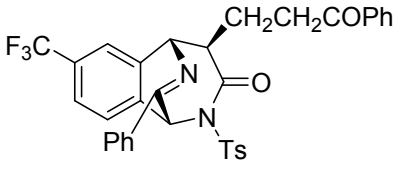
Peak#	Ret. Time	Area	Height	Conc.
1	18.416	6188499	157196	50.374
2	22.993	6096616	128155	49.626
Total		12285115	285351	



<Peak Table>

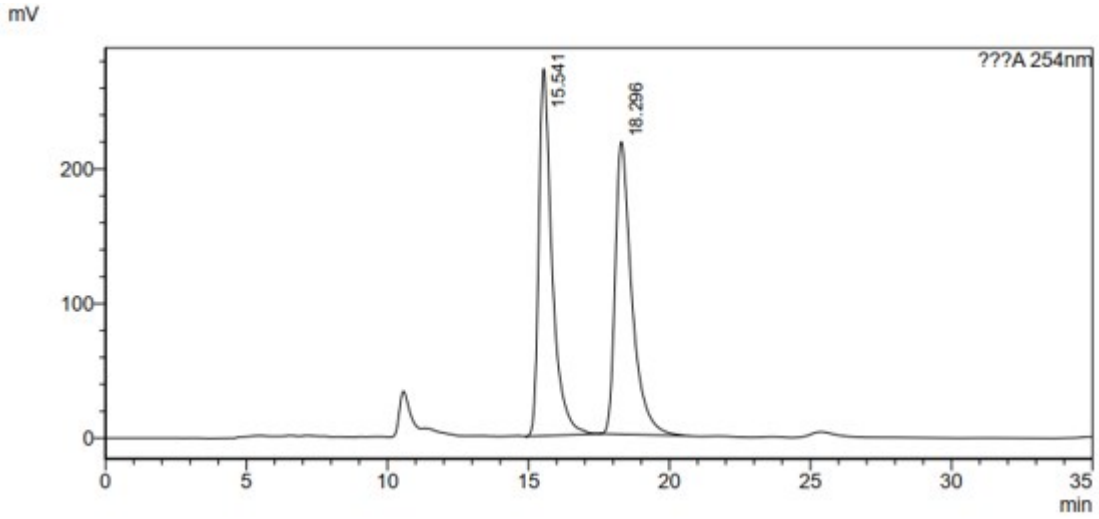
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	18.524	9396	255	0.133
2	22.673	7034017	150705	99.867
Total		7043413	150961	



8e

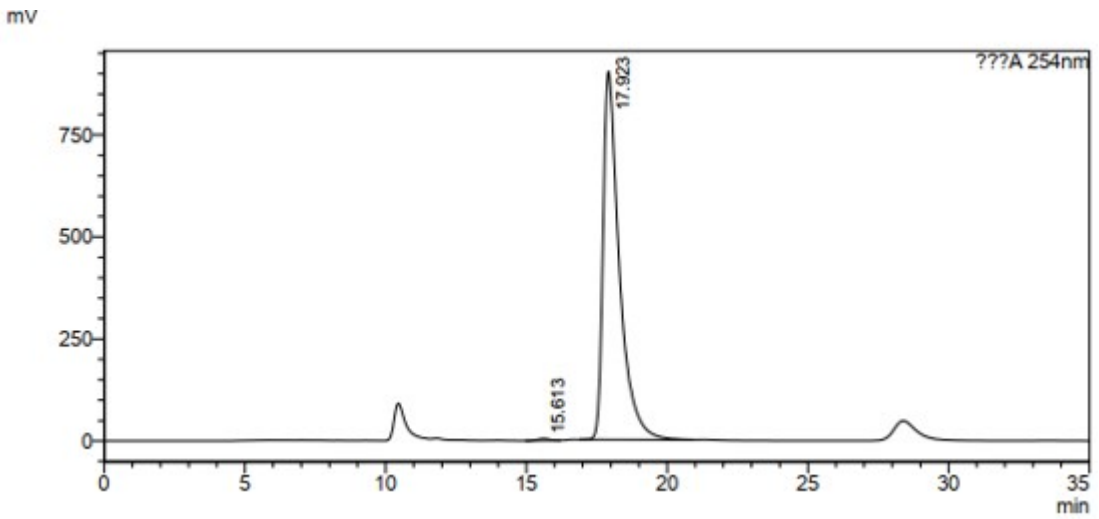
IB column, 80 : 20 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 °C, 99.3% ee.



<Peak Table>

???A 254nm

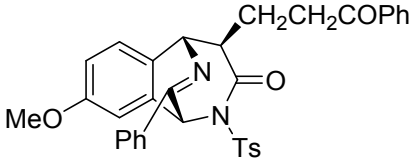
Peak#	Ret. Time	Area	Height	Conc.
1	15.541	8957801	272781	50.073
2	18.296	8931532	217174	49.927
Total		17889333	489955	



<Peak Table>

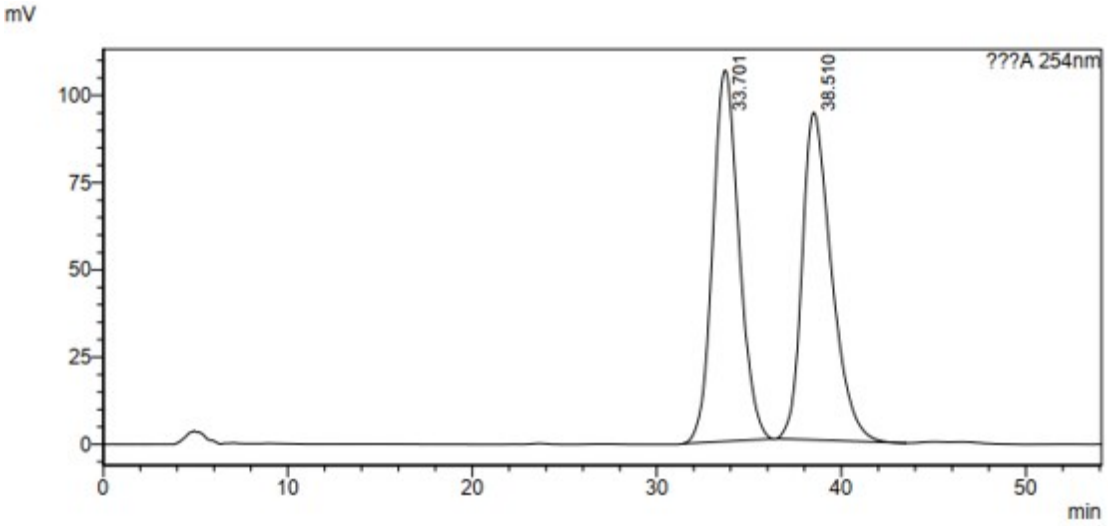
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	15.613	136294	4700	0.374
2	17.923	36278455	902146	99.626
Total		36414750	906845	



8f

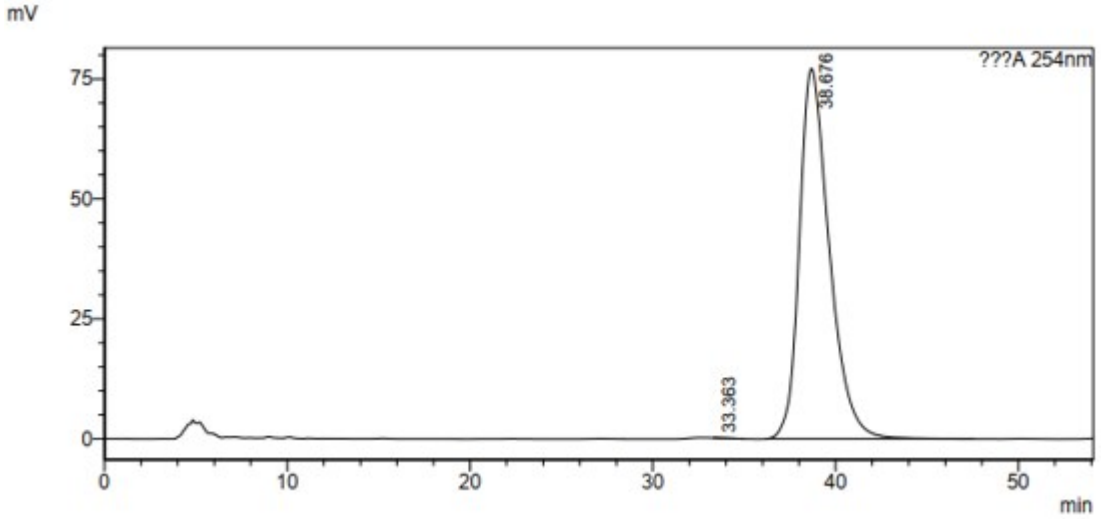
IA column, 75 : 25 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 °C, 99.9% ee.



<Peak Table>

???A 254nm

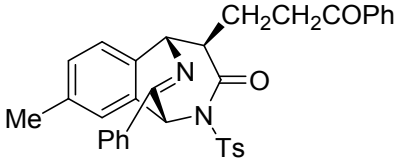
Peak#	Ret. Time	Area	Height	Conc.
1	33.701	10530053	106422	50.361
2	38.510	10379196	93848	49.639
Total		20909249	200271	



<Peak Table>

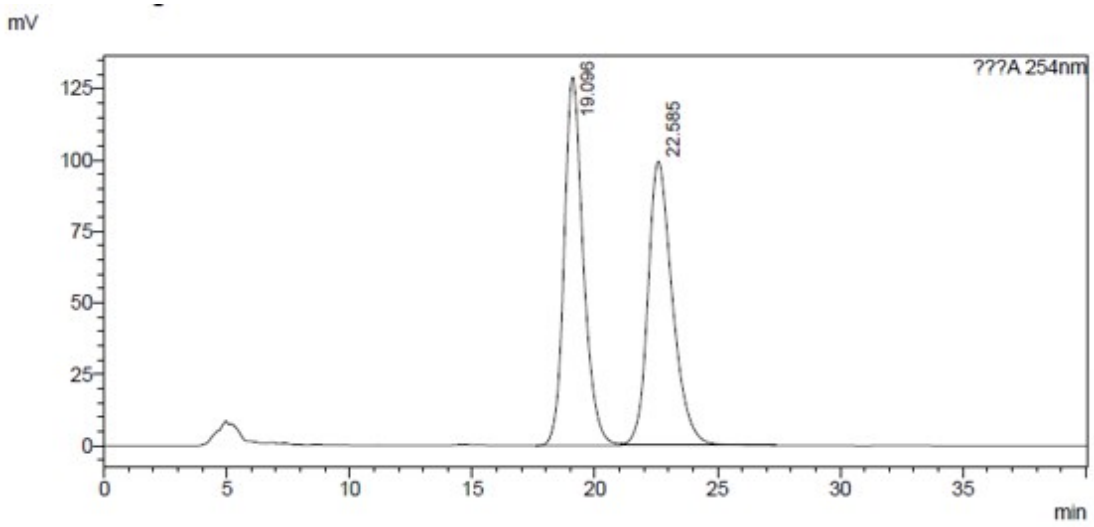
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	33.363	614	0	0.007
2	38.676	8798743	77144	99.993
Total		8799357	77144	



8g

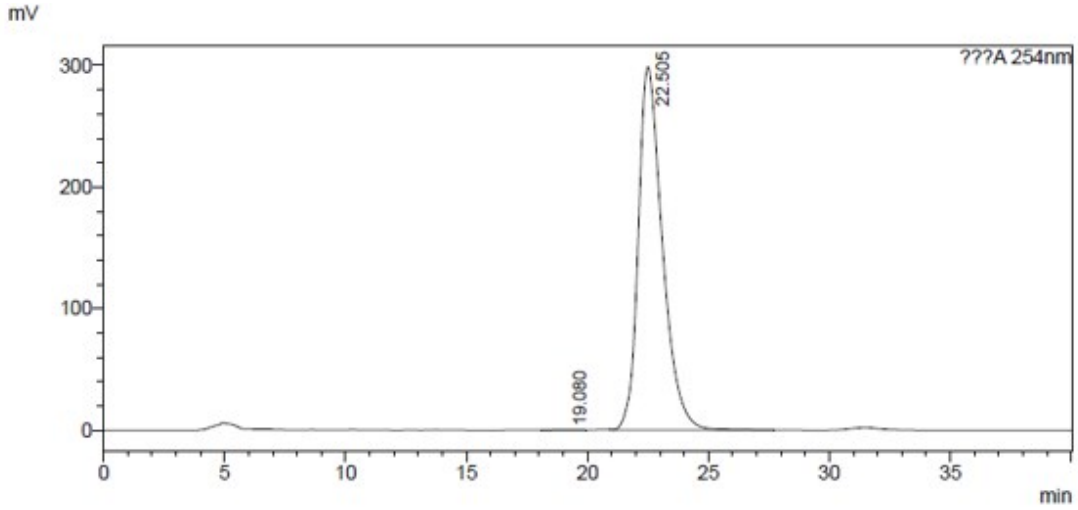
IA column, 70 : 30 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 °C, 99.9% ee.



<Peak Table>

???A 254nm

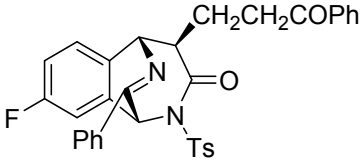
Peak#	Ret. Time	Area	Height	Conc.
1	19.096	7016413	128983	50.312
2	22.585	6929295	99413	49.688
Total		13945708	228396	



<Peak Table>

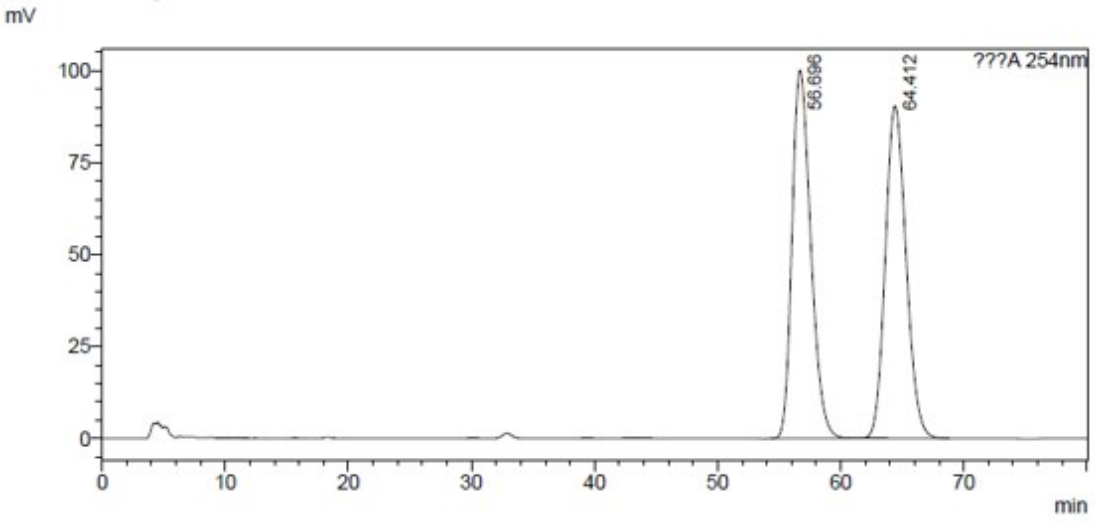
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	19.080	10803	177	0.052
2	22.505	20727371	298682	99.948
Total		20738175	298859	



8h

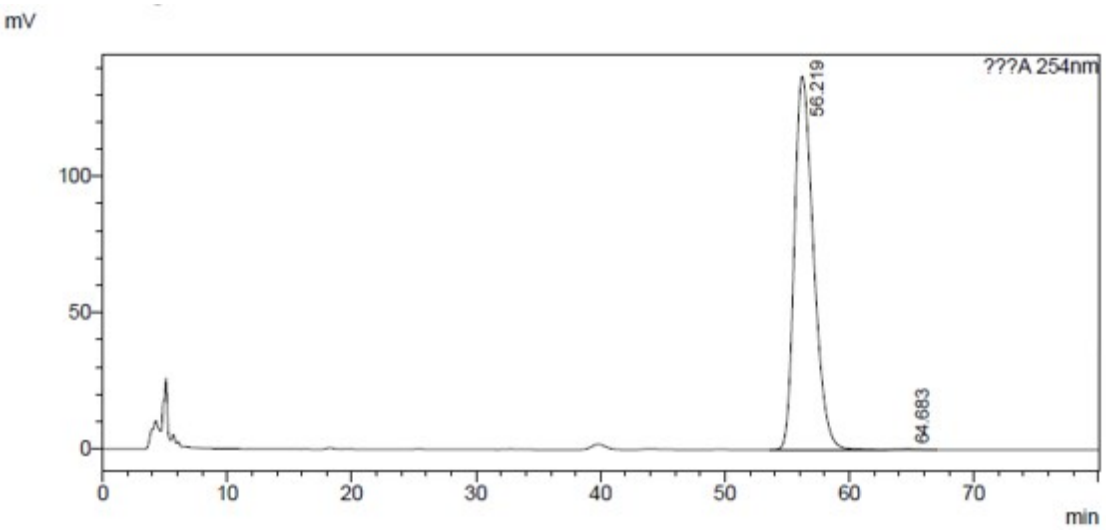
AD-H column, 80 : 20 hexane : IPA, flow rate: 0.8 ml/min, 254 nm, 25 ^{o}C, 99.8% ee.



<Peak Table>

???A 254nm

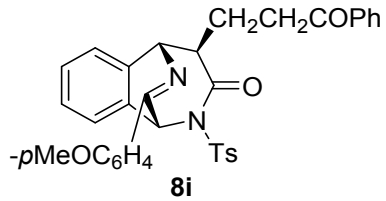
Peak#	Ret. Time	Area	Height	Conc.
1	56.696	10586686	100158	49.954
2	64.412	10606181	90348	50.046
Total		21192867	190506	



<Peak Table>

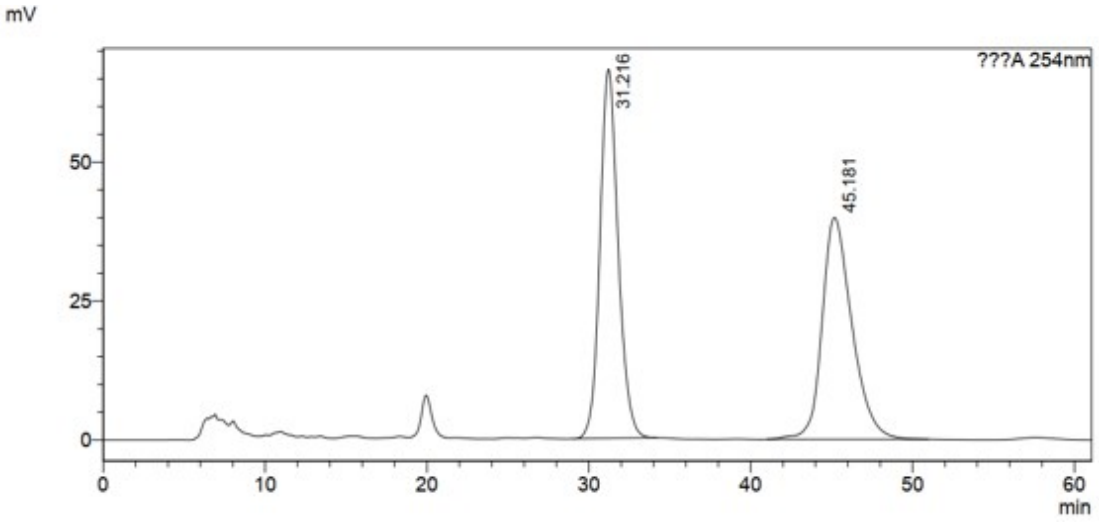
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	56.219	14653748	137066	99.888
2	64.683	16363	156	0.112
Total		14670111	137222	



8i

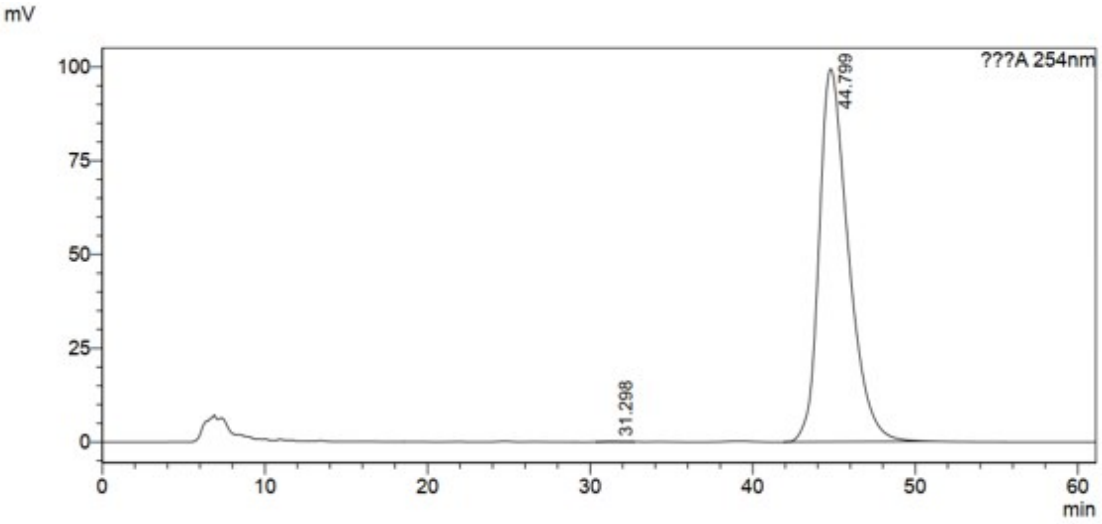
IA column, 60 : 40 hexane : IPA, flow rate: 0.5 ml/min, 254 nm, 25 °C, 99.9% ee.



<Peak Table>

???A 254nm

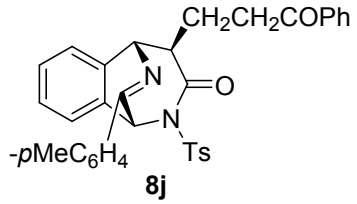
Peak#	Ret. Time	Area	Height	Conc.
1	31.216	5190634	66456	50.315
2	45.181	5125661	39917	49.685
Total		10316295	106373	



<Peak Table>

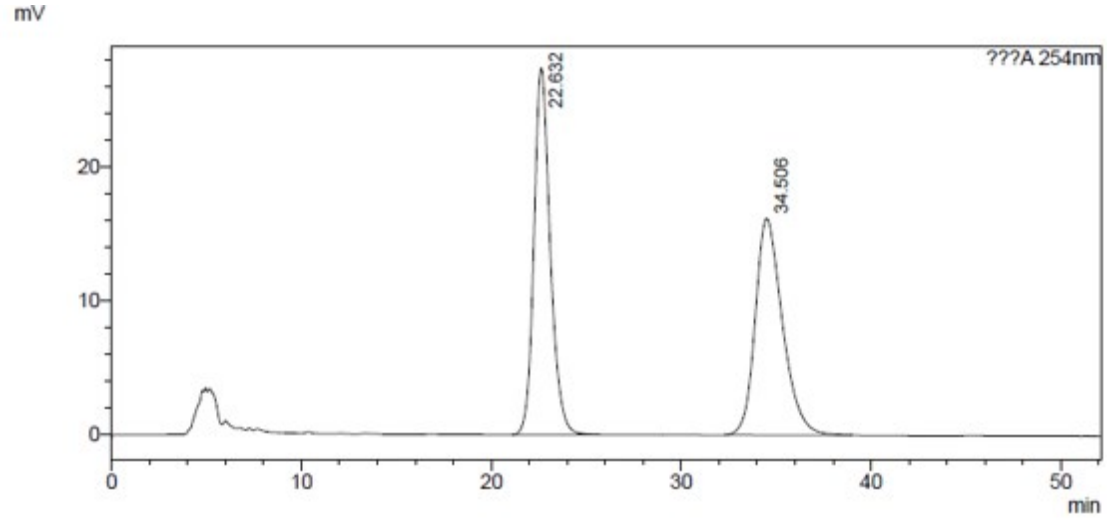
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	31.298	9397	139	0.075
2	44.799	12456086	99413	99.925
Total		12465483	99552	



8j

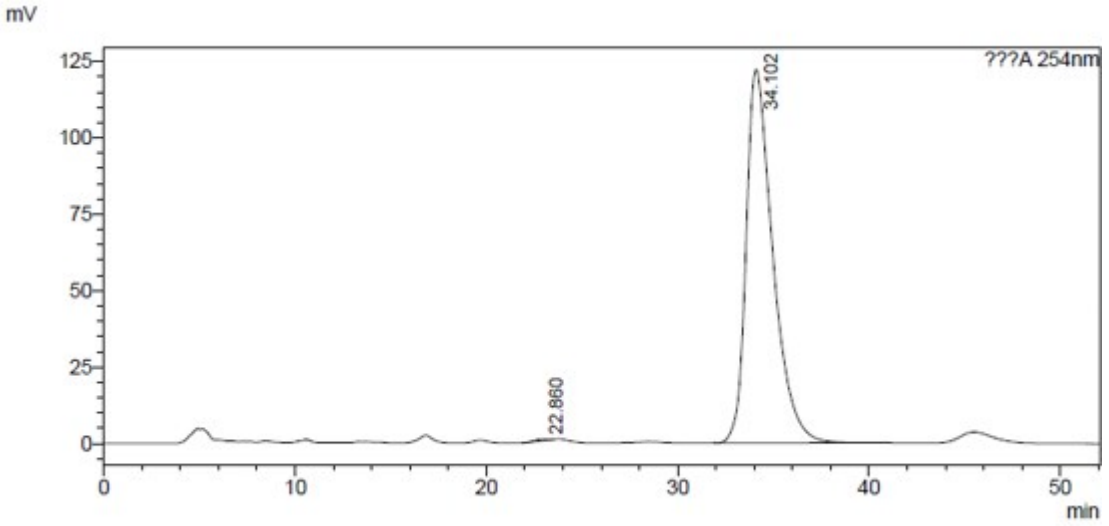
IA column, 70 : 30 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 °C, 99.6 % ee.



<Peak Table>

???A 254nm

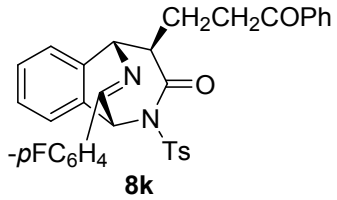
Peak#	Ret. Time	Area	Height	Conc.
1	22.632	1634451	27392	50.299
2	34.506	1614992	16167	49.701
Total		3249443	43559	



<Peak Table>

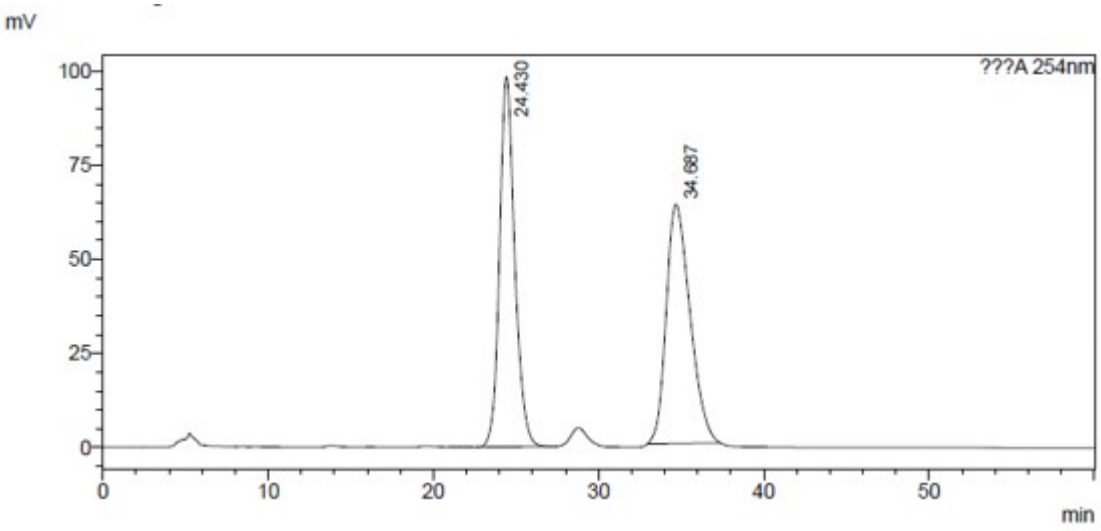
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	22.860	20942	551	0.176
2	34.102	11866905	122311	99.824
Total		11887847	122862	



8k

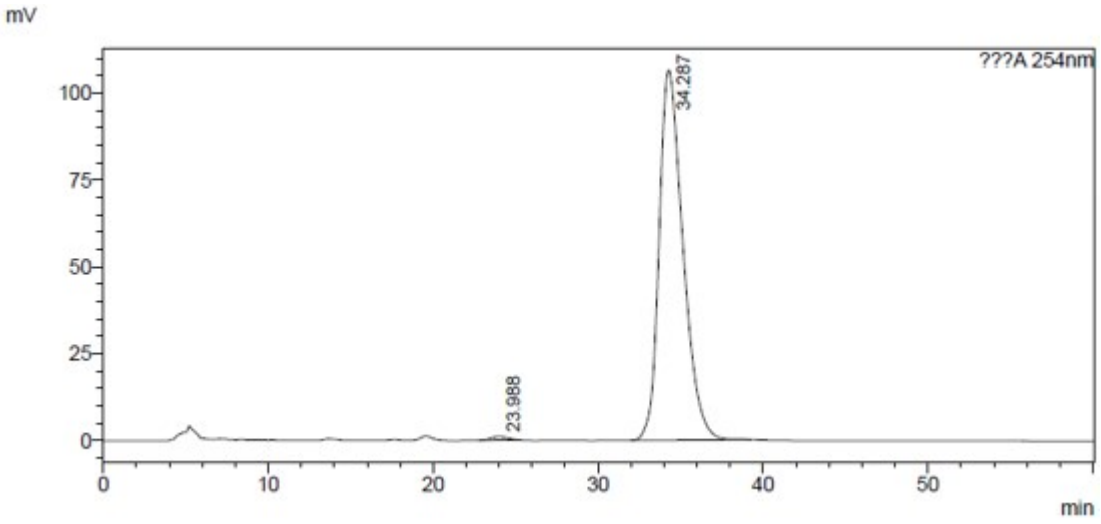
IA column, 70 : 30 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 °C, 99% ee.



<Peak Table>

???A 254nm

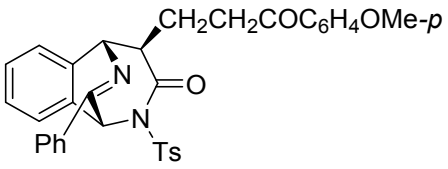
Peak#	Ret. Time	Area	Height	Conc.
1	24.430	6297130	98421	49.669
2	34.687	6380936	63587	50.331
Total		12678066	162008	



<Peak Table>

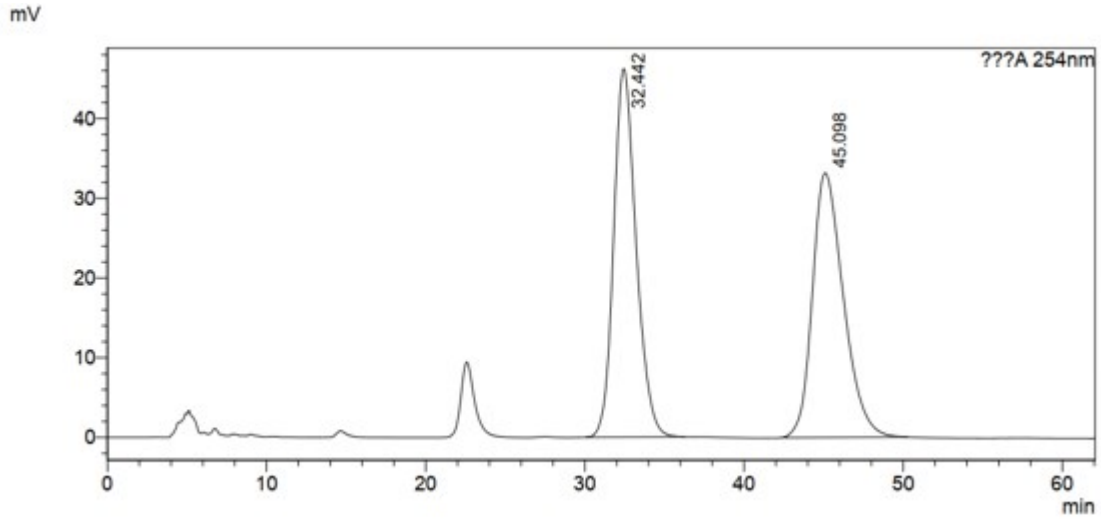
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	23.988	74327	1078	0.689
2	34.287	10707442	106538	99.311
Total		10781769	107616	



8l

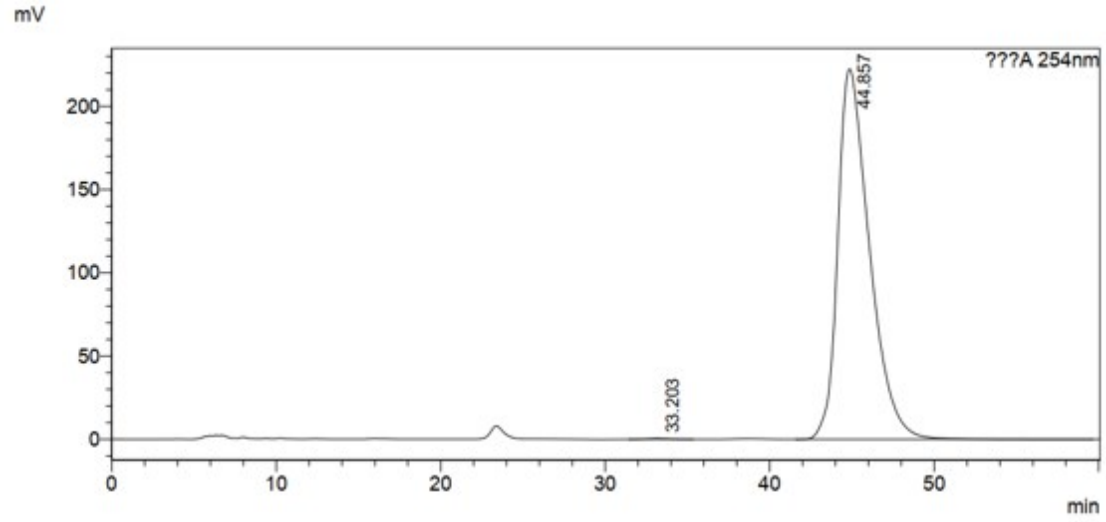
IA column, 70 : 30 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 °C, 99.7% ee.



<Peak Table>

???A 254nm

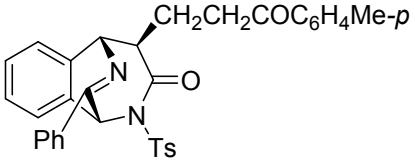
Peak#	Ret. Time	Area	Height	Conc.
1	32.442	4538054	46214	50.176
2	45.098	4506251	33206	49.824
Total		9044305	79420	



<Peak Table>

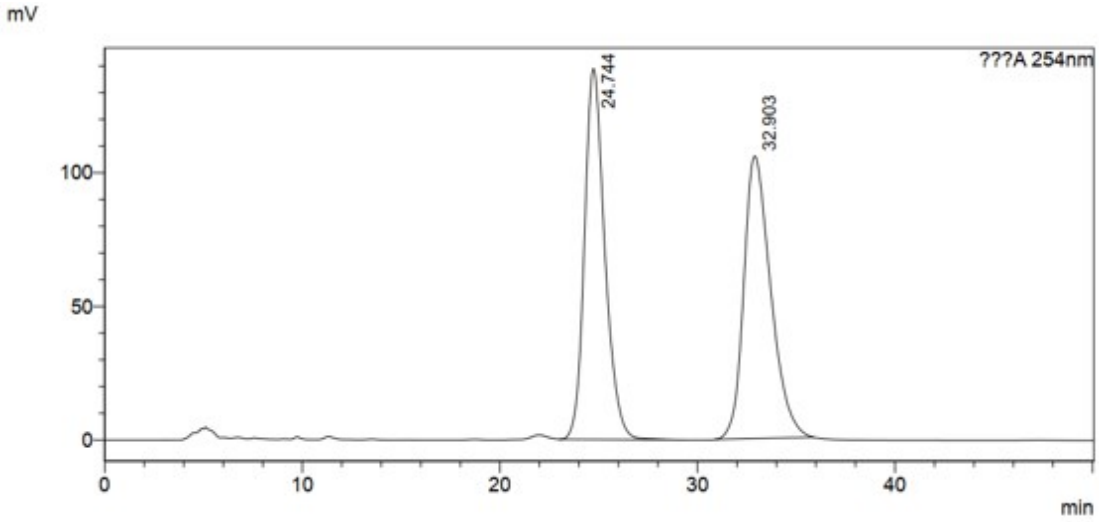
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	33.203	51092	590	0.171
2	44.857	29853100	222555	99.829
Total		29904192	223145	



8m

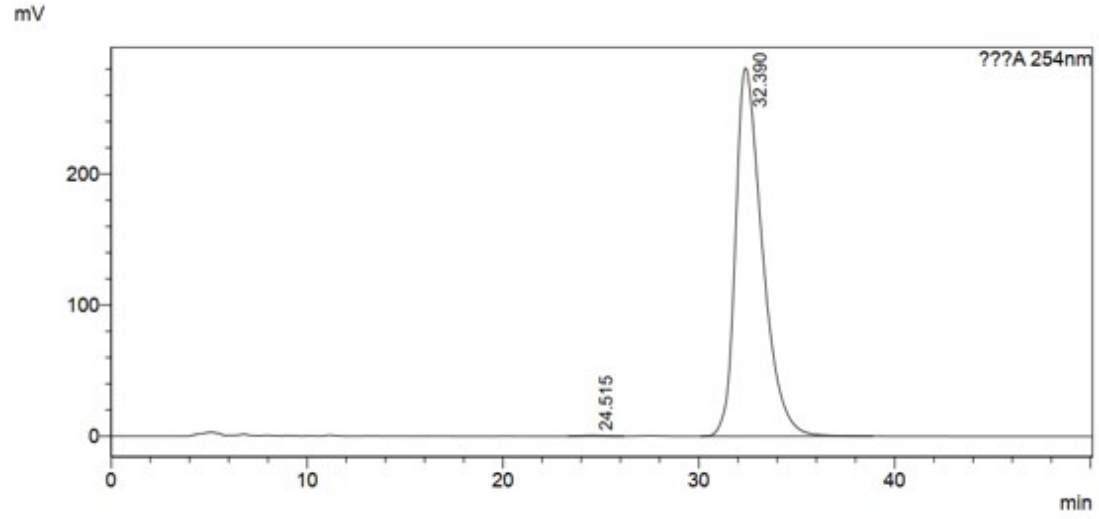
IA column, 70 : 30 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 °C, 99.7% ee.



<Peak Table>

???A 254nm

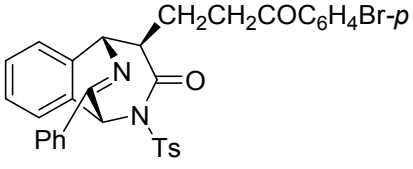
Peak#	Ret. Time	Area	Height	Conc.
1	24.744	9921881	138776	49.719
2	32.903	10033881	105756	50.281
Total		19955763	244532	



<Peak Table>

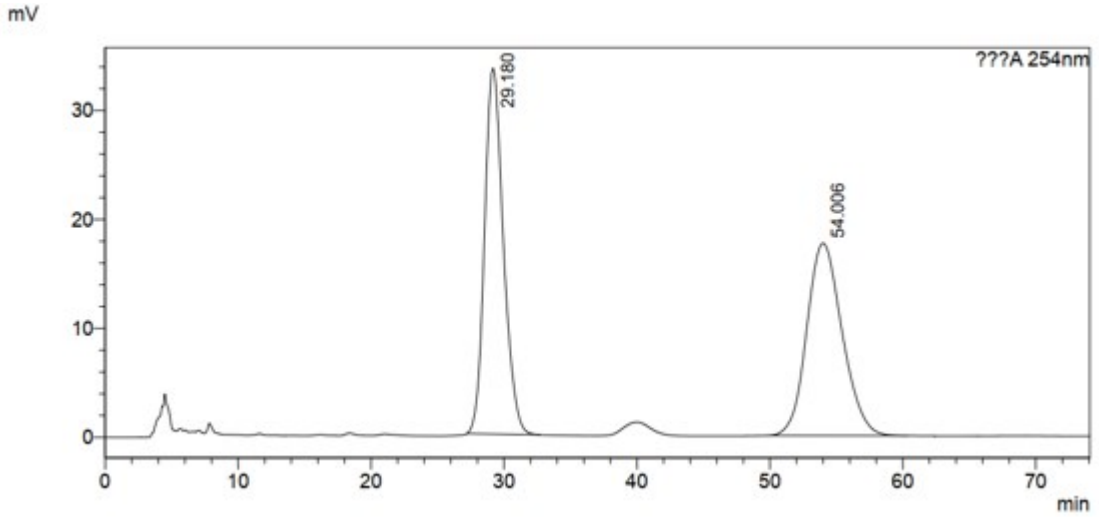
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	24.515	43438	595	0.162
2	32.390	26839660	281093	99.838
Total		26883098	281688	



8n

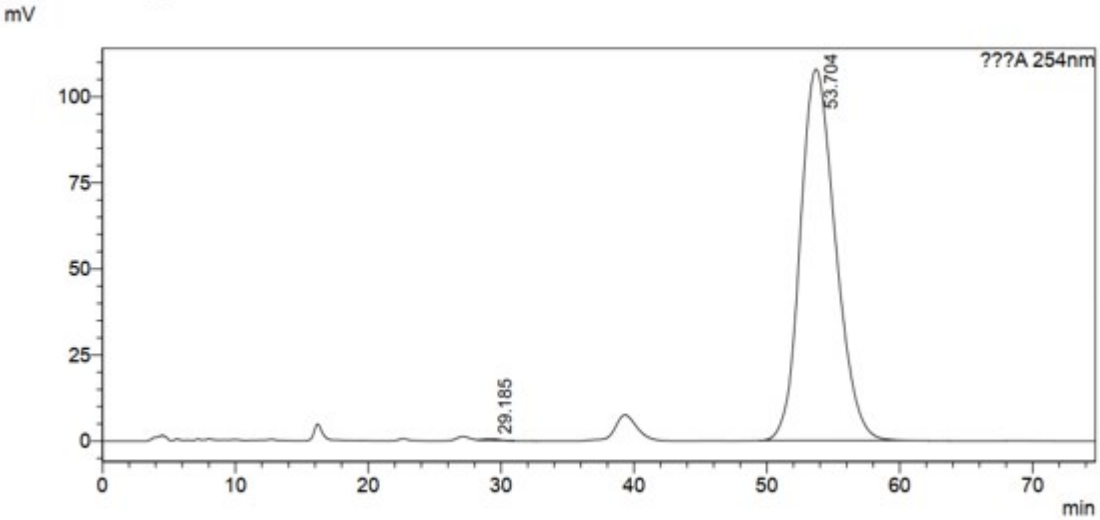
IA column, 70 : 30 hexane : IPA, flow rate: 0.8 ml/min, 254 nm, 25 °C, 99.7% ee.



<Peak Table>

???A 254nm

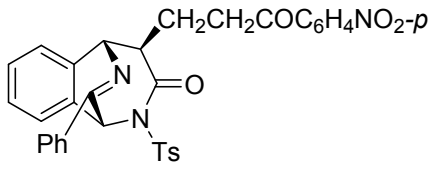
Peak#	Ret. Time	Area	Height	Conc.
1	29.180	3304216	33572	50.268
2	54.006	3268989	17659	49.732
Total		6573205	51231	



<Peak Table>

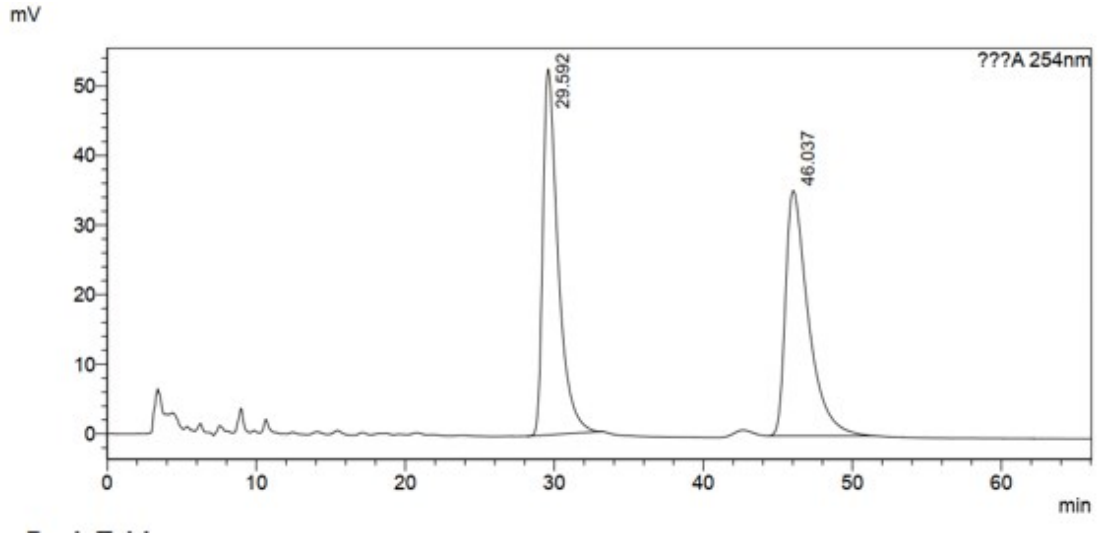
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	29.185	27894	403	0.141
2	53.704	19824844	107841	99.859
Total		19852738	108243	



8o

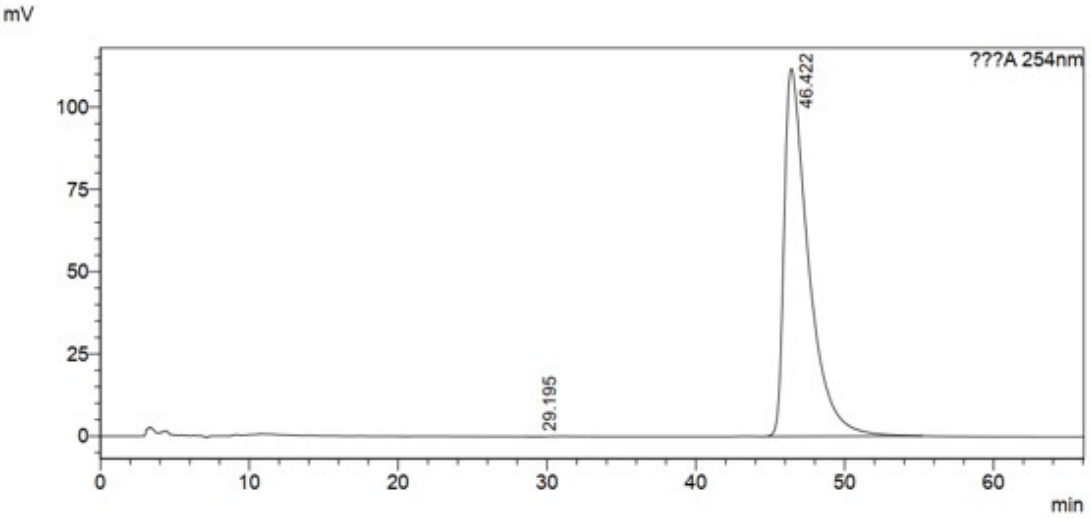
IB column, 85 : 15 hexane : IPA, flow rate: 1.0 ml/min, 254 nm, 25 °C, 99.9% ee.



<Peak Table>

???A 254nm

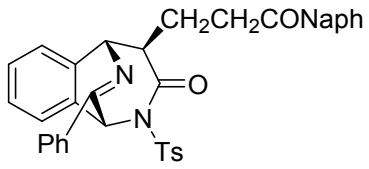
Peak#	Ret. Time	Area	Height	Conc.
1	29.592	3728545	52596	49.792
2	46.037	3759653	35242	50.208
Total		7488197	87839	



<Peak Table>

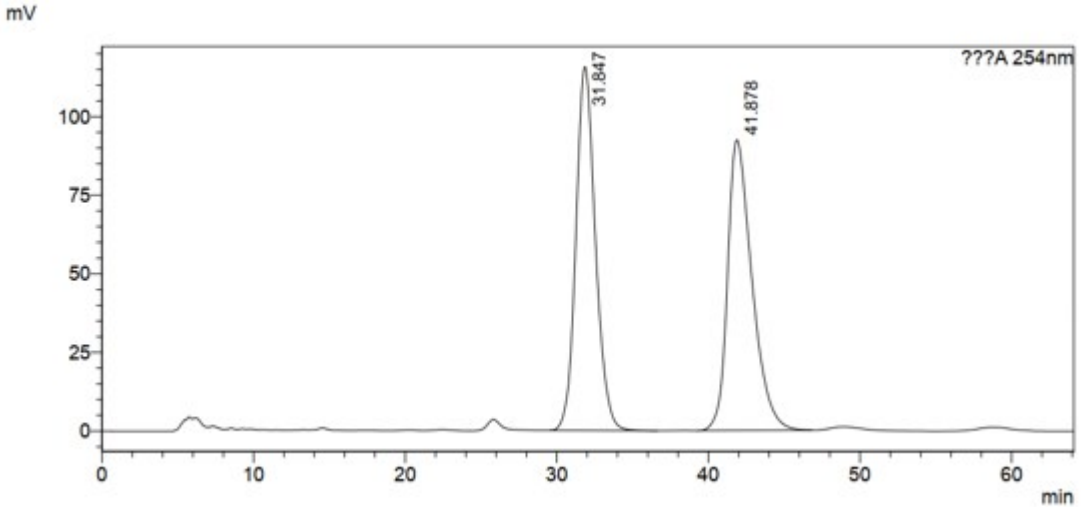
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	29.195	196	9	0.002
2	46.422	12662826	111792	99.998
Total		12663023	111801	



8p

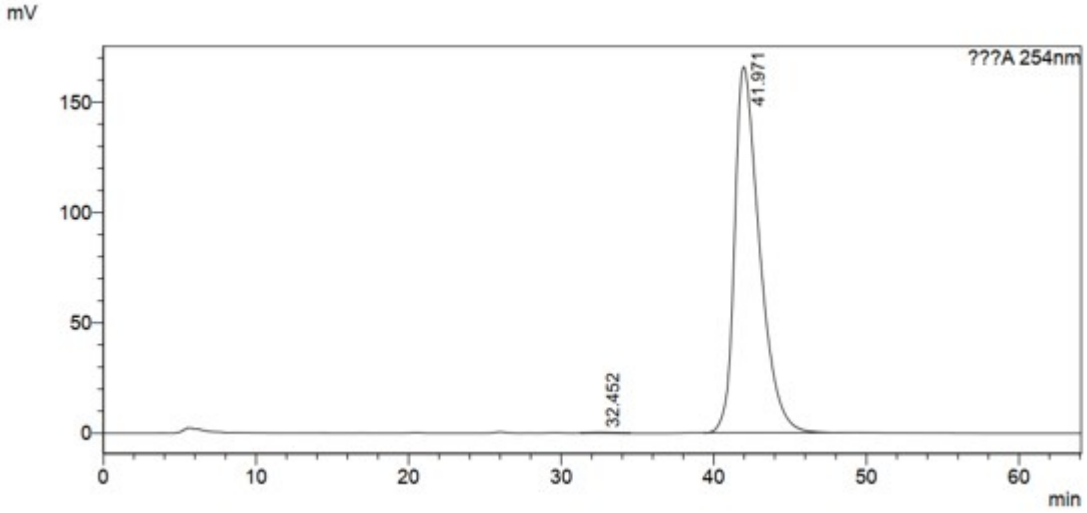
IA column, 65 : 35 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 ^{o}C, 99.6% ee.



<Peak Table>

???A 254nm

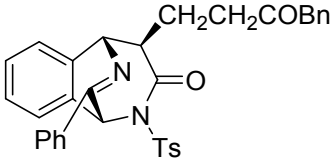
Peak#	Ret. Time	Area	Height	Conc.
1	31.847	10359140	115660	50.010
2	41.878	10354905	92432	49.990
Total		20714045	208092	



<Peak Table>

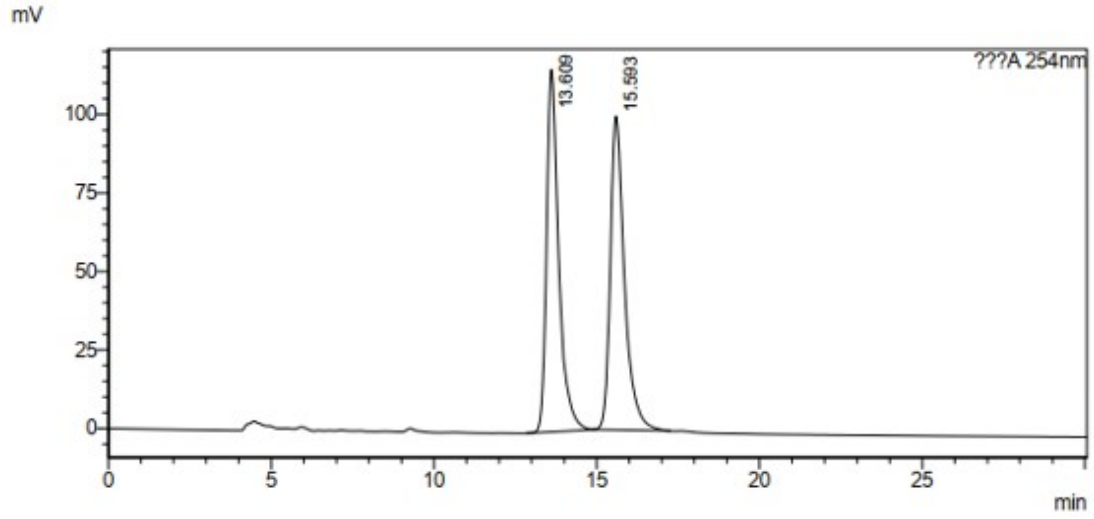
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	32.452	34790	321	0.184
2	41.971	18850250	165915	99.816
Total		18885040	166236	



8q

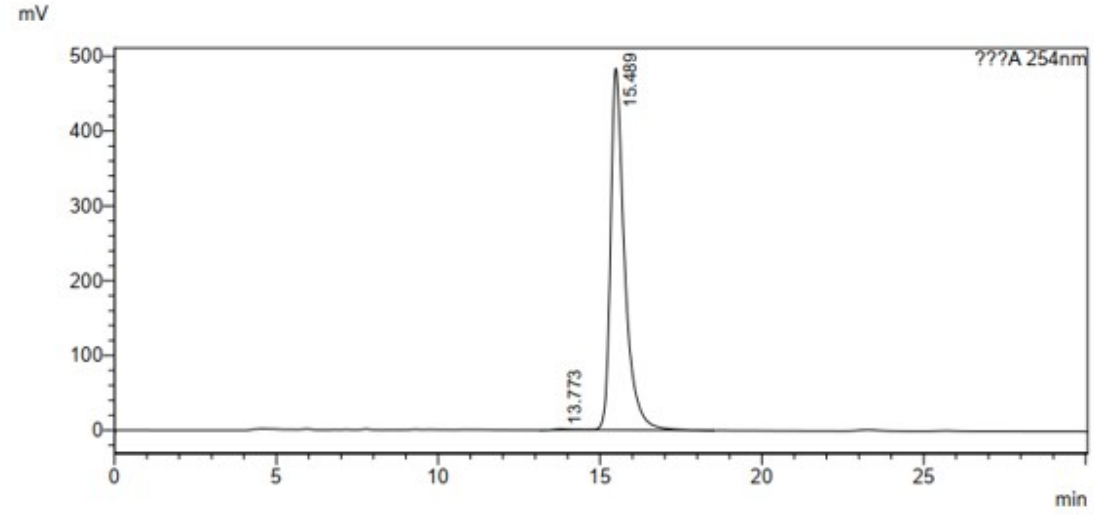
IA column, 70 : 30 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 °C, 99.3% ee.



<Peak Table>

???A 254nm

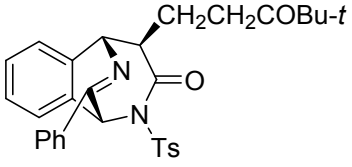
Peak#	Ret. Time	Area	Height	Conc.
1	13.609	2998334	115390	49.770
2	15.593	3026090	99872	50.230
Total		6024424	215261	



<Peak Table>

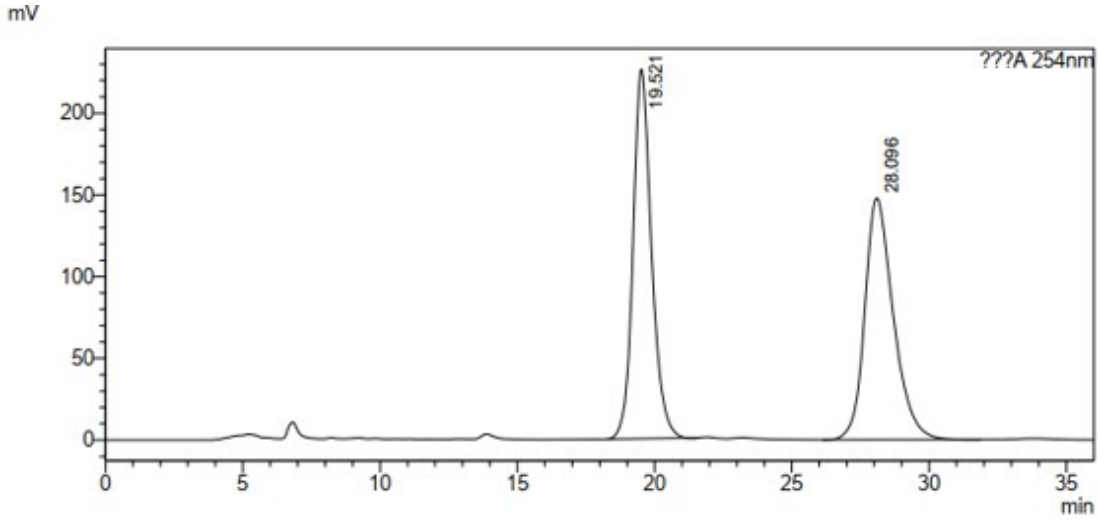
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	13.773	49282	1321	0.337
2	15.489	14559836	483588	99.663
Total		14609118	484910	



8r

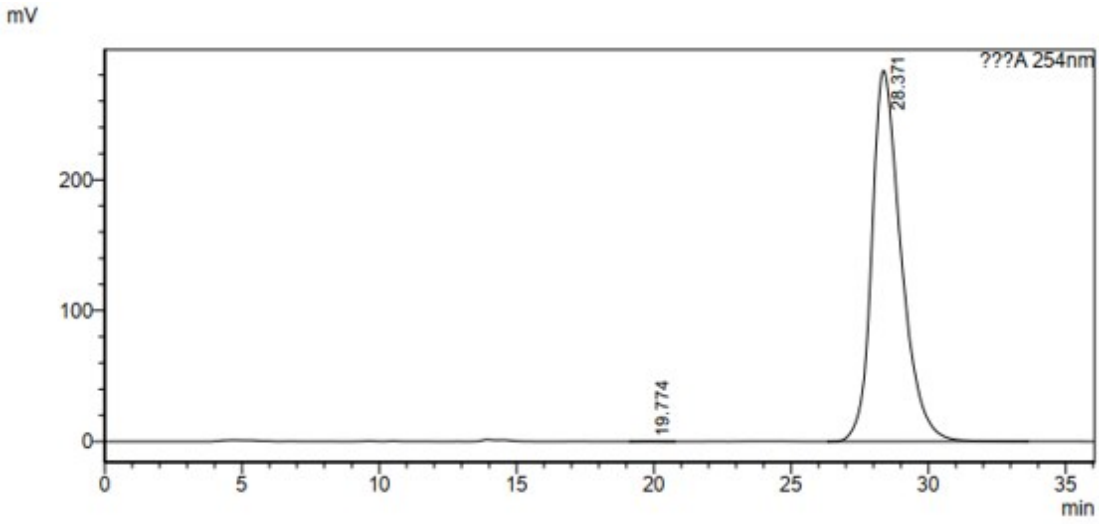
IA column, 75 : 25 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 °C, 99.9% ee.



<Peak Table>

???A 254nm

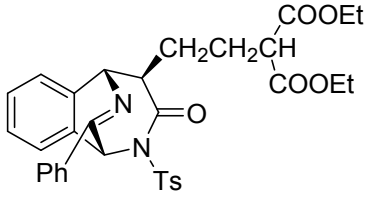
Peak#	Ret. Time	Area	Height	Conc.
1	19.521	10575857	226054	49.699
2	28.096	10703930	147797	50.301
Total		21279787	373851	



<Peak Table>

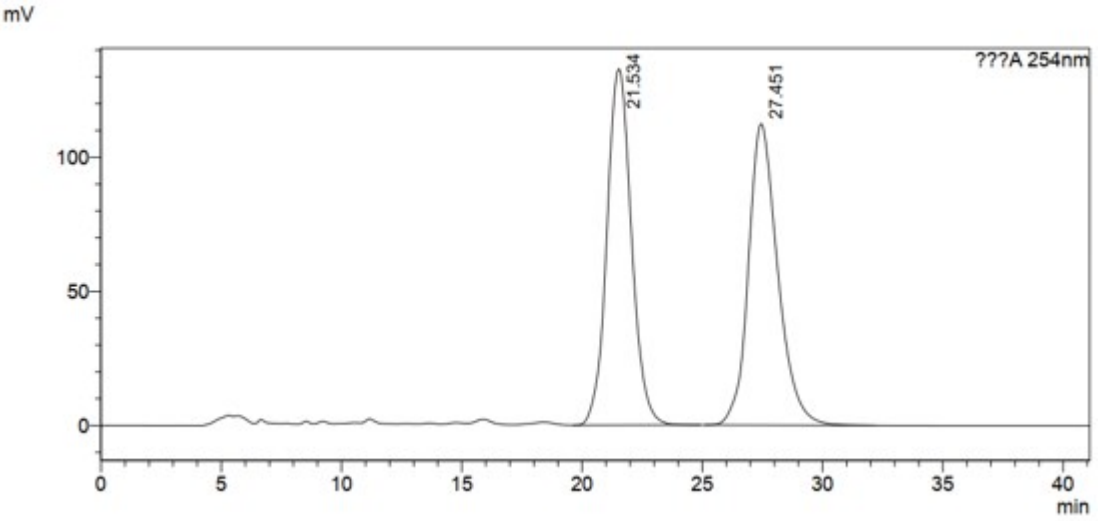
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	19.774	10569	250	0.050
2	28.371	21044259	283387	99.950
Total		21054827	283637	



8s

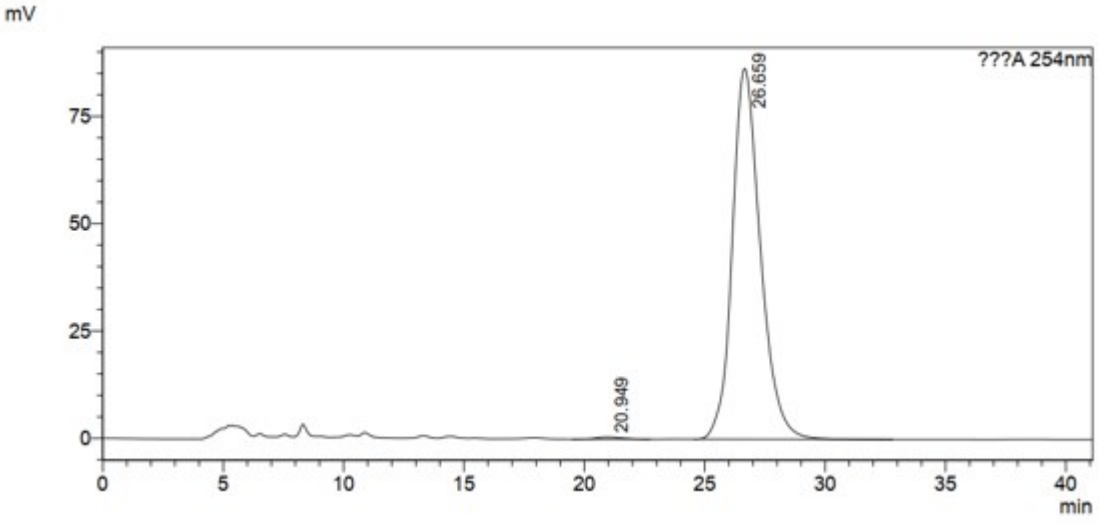
IA column, 70 : 30 hexane : IPA, flow rate: 0.8 ml/min, 254 nm, 25 °C, 99% ee.



<Peak Table>

???A 254nm

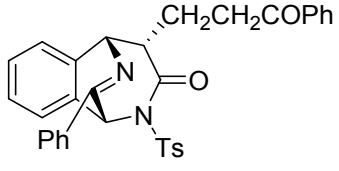
Peak#	Ret. Time	Area	Height	Conc.
1	21.534	9474410	132823	49.818
2	27.451	9543538	112354	50.182
Total		19017948	245177	



<Peak Table>

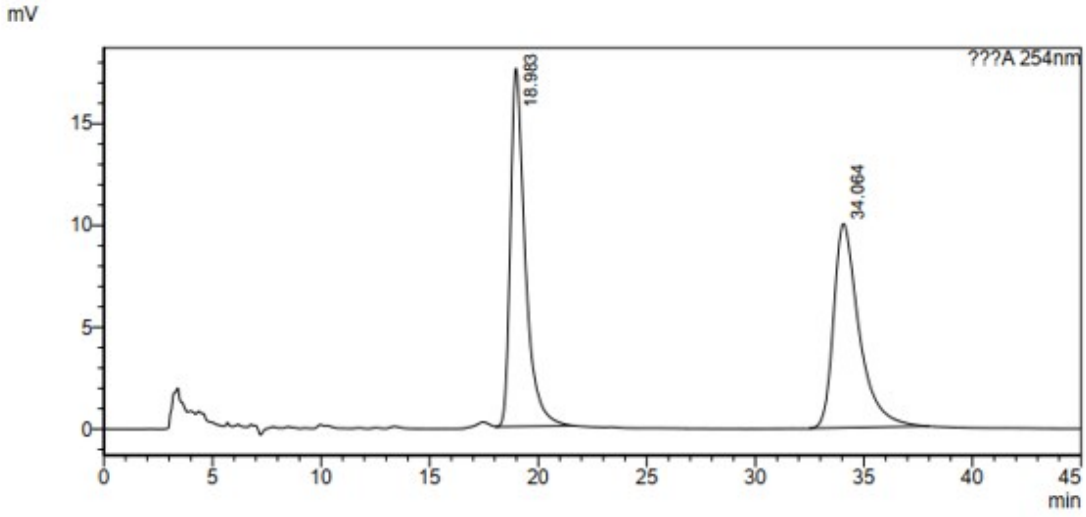
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	20.949	37931	488	0.537
2	26.659	7026737	86380	99.463
Total		7064668	86869	



9a

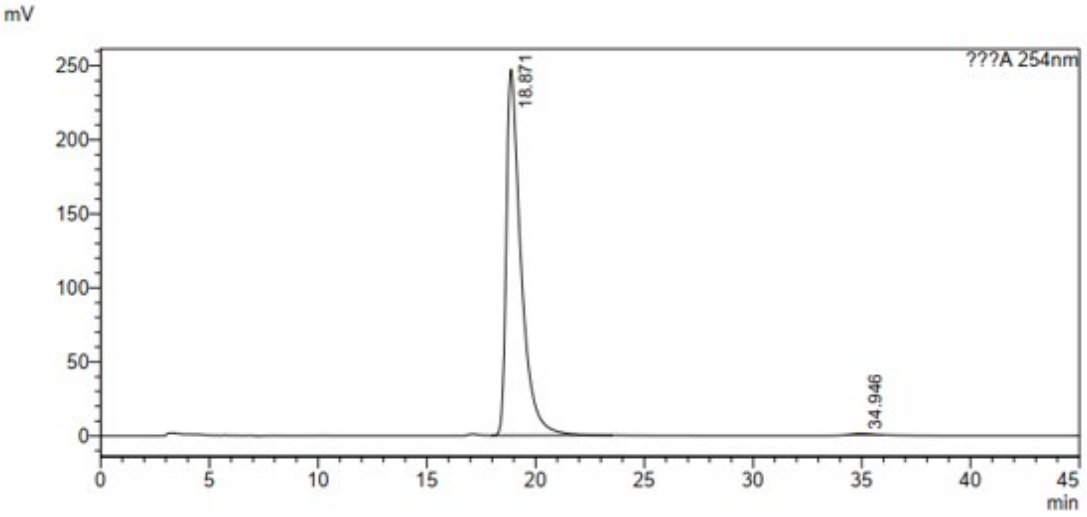
IB column, 85 : 15 hexane : IPA, flow rate: 1.0 ml/min, 254 nm, 25 °C, 99.2% ee.



<Peak Table>

???A 254nm

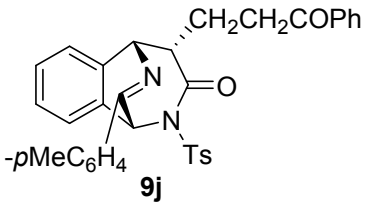
Peak#	Ret. Time	Area	Height	Conc.
1	18.983	830236	17590	50.325
2	34.064	819513	10021	49.675
Total		1649749	27611	



<Peak Table>

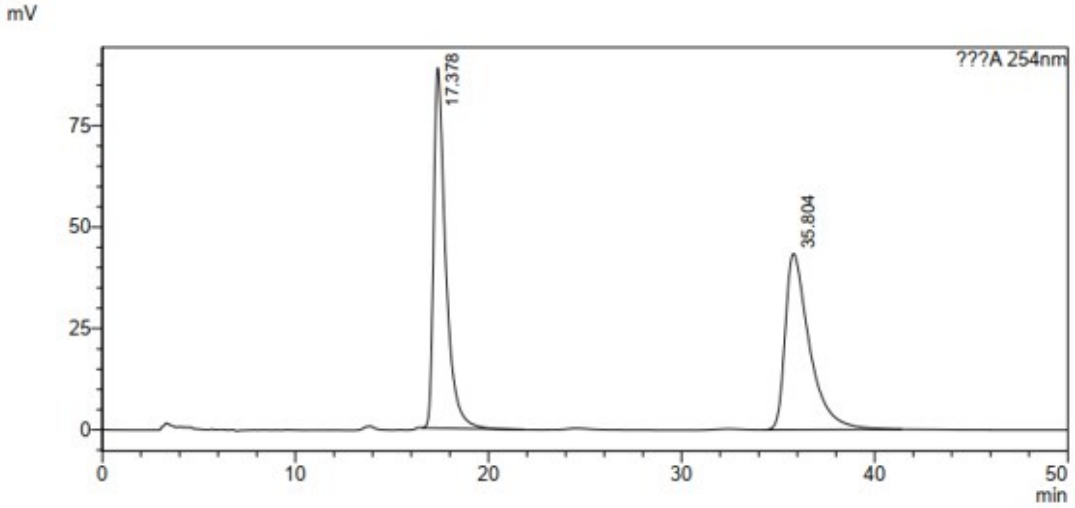
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	18.871	11616707	247464	99.589
2	34.946	47895	823	0.411
Total		11664603	248287	



9j

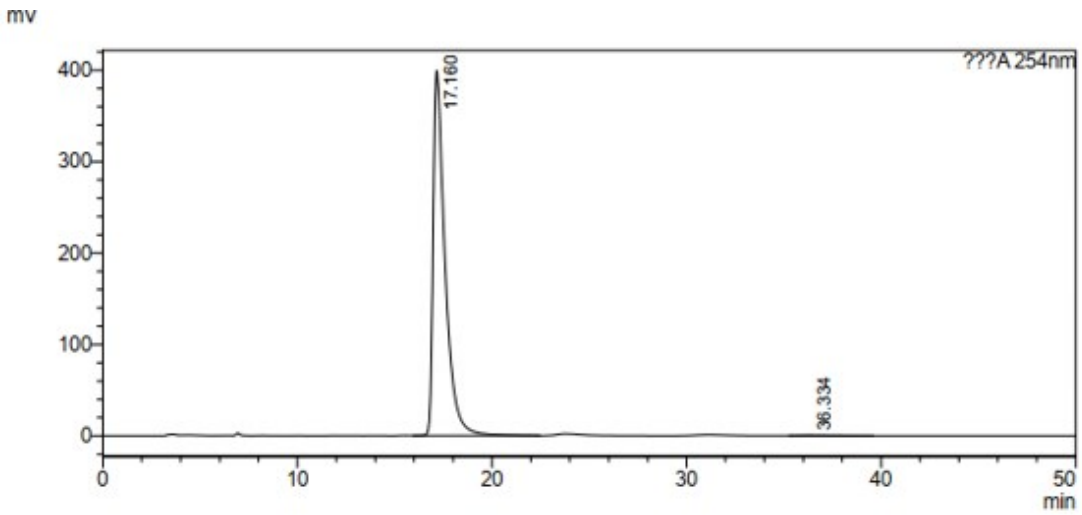
IB column, 85 : 15 hexane : IPA, flow rate: 1.0 ml/min, 254 nm, 25 °C, 99.7% ee.



<Peak Table>

???A 254nm

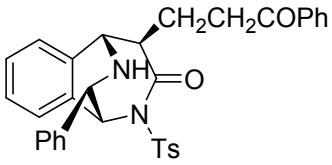
Peak#	Ret. Time	Area	Height	Conc.
1	17.378	3853424	88874	50.255
2	35.804	3814387	43456	49.745
Total		7667811	132330	



<Peak Table>

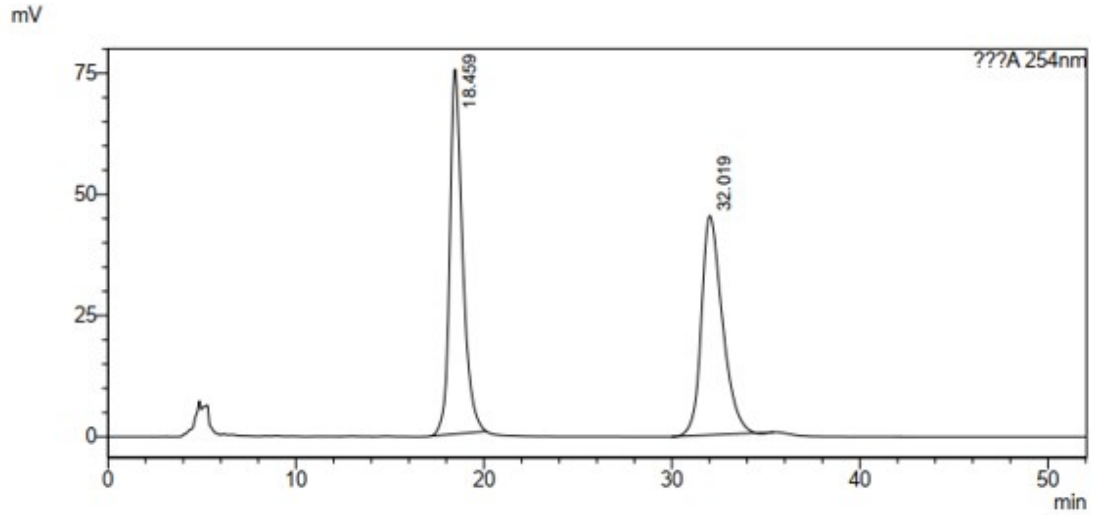
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	17.160	16962180	399163	99.835
2	36.334	28078	299	0.165
Total		16990258	399462	



18a

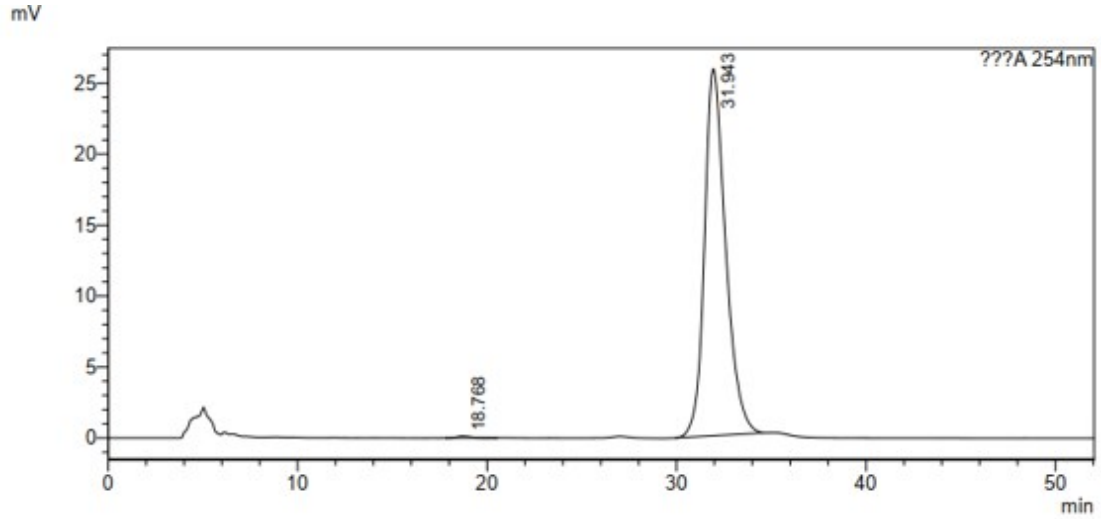
IA column, 70 : 30 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25 ºC, 99.4% ee.



<Peak Table>

???A 254nm

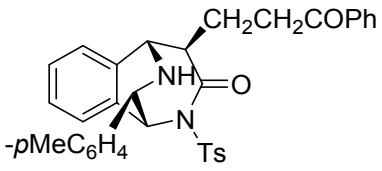
Peak#	Ret. Time	Area	Height	Conc.
1	18.459	3575638	75262	50.397
2	32.019	3519266	45236	49.603
Total		7094904	120497	



<Peak Table>

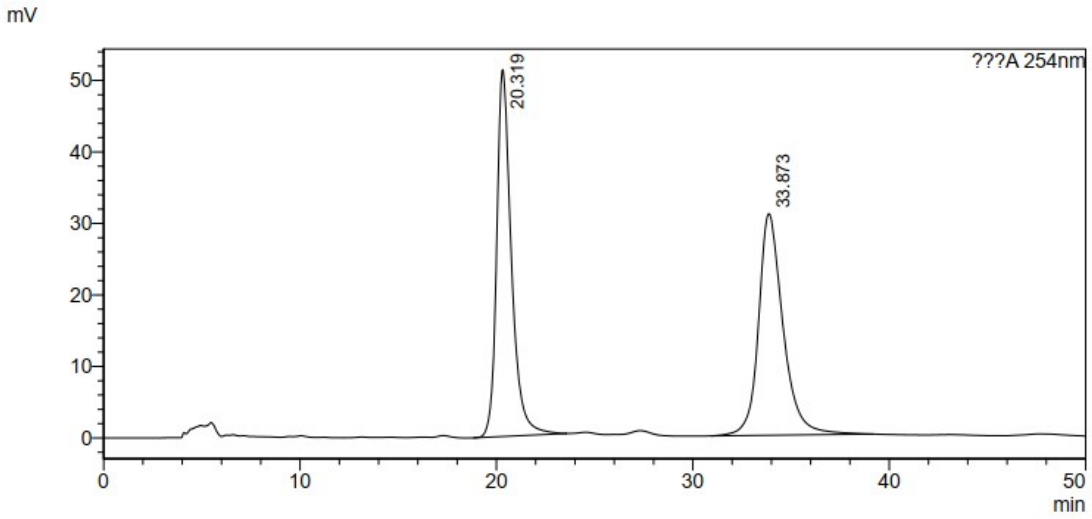
???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	18.768	6241	129	0.310
2	31.943	2008720	25857	99.690
Total		2014961	25986	



18j

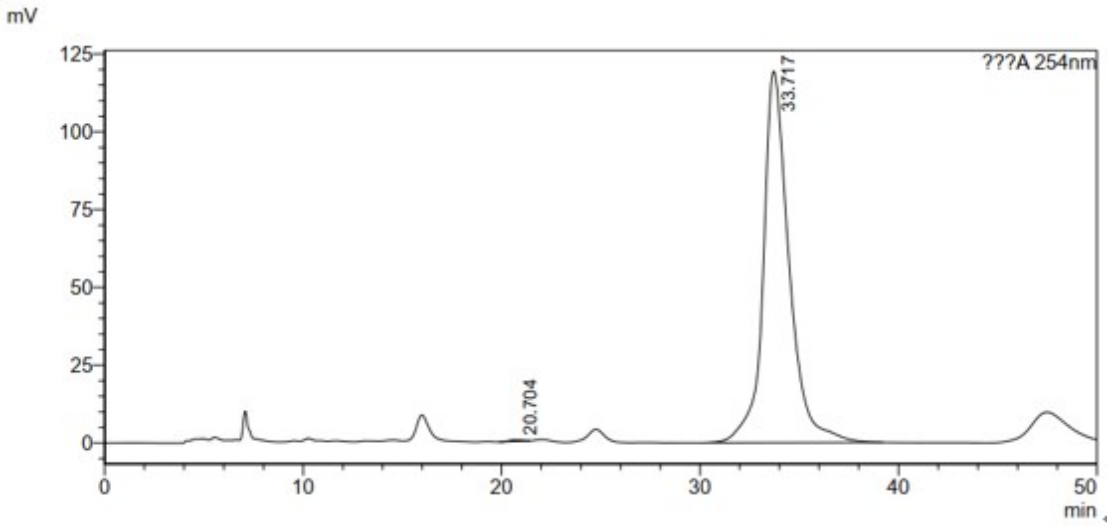
IA column, 70:30 hexane : IPA, flow rate: 0.7 ml/min, 254 nm, 25℃, 99.6 % ee.



<Peak Table>

???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	20.319	2661753	51318	49.665
2	33.873	2697656	30982	50.335
Total		5359408	82301	



<Peak Table>

???A 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	20.704	21413	481	0.197
2	33.717	10866535	119345	99.803
Total		10887948	119826	