Regioselective Synthesis of Tetrahydroquinolines *via Syn*- and *Anti*-Nucleopalladation-Initiated Cascade Processes

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Supporting Information

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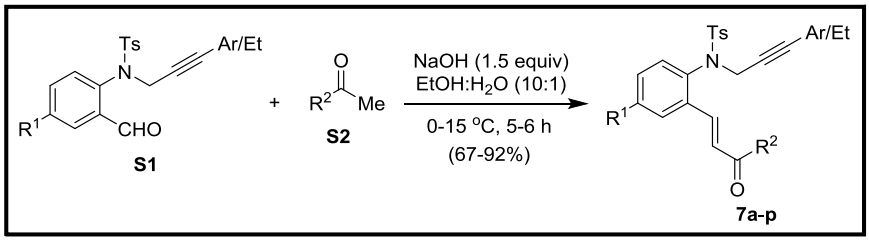
1. General Information

All reagents and solvents were purchased from commercial suppliers (Avra, Alfa Aesar, Sigma-Aldrich, CDH, Merck) and used without further purification. All reactions were carried out in oven-dried glassware under a nitrogen atmosphere. The reactions were monitored by thin layer chromatography using Merck silica gel 60 F_{254} and visualized by UV detection or using *p*-anisaldehyde stain or molecular iodine. Silica gel (230-400 mesh) was used for flash column chromatography. Melting points were recorded on a melting point apparatus in capillaries and are uncorrected. ^{1}H and ^{13}C-NMR spectra were recorded in $CDCl_3$ at room temperature on a Brucker Avance 300 spectrometer operating at 300 MHz for ^{1}H and 75 MHz for ^{13}C. In some cases Brucker 400 MHz NMR instruments was used. Chemical shifts (δ) are expressed in ppm using TMS as an internal standard and coupling constants (*J*) are given in Hz. Infrared (IR) spectra were obtained using an Agilent Cary 630 FTIR Spectrometer with a diamond ATR accessory for solid and liquid samples, requiring no sample preparation and the major frequencies were reported in cm^{-1}. Elemental analyses were determined at the CAI de Microanálisis Elemental, Universidad Complutense, by using a Leco 932 CHNS combustion microanalyzer. ESI-MS spectra were obtained with a JMS-T100LC (JEOL) instrument.

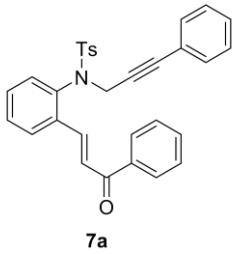
2. General Procedure for the Synthesis of Compounds 7a-p[1]



To a solution of methyl ketone **S2** (2.75 mmol, 1.1 equiv) in 10:1 EtOH/H_2O (15 mL) mixture was stirred with NaOH (3.75 mmol, 1.5 equiv) at 0 ^{o}C. After 10 minutes, aldehyde **S1** (2.5 mmol, 1.0 equiv) was added and stirring was continued at 10-15 ^{o}C for 5-6 h. After completion of the reaction, the reaction mixture was poured into ice water and acidified with 1.5 N HCl. The aqueous suspension was extracted with DCM (2 x 60 mL), washed with water and brine. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by flash column chromatography using petroleum ether and ethyl acetate mixture as eluent (90:10, v/v) to obtain the desired products **7a**-**p**.

[1] P. Vinoth, M. Karuppasamy, B. S. Vachan, I. Muthukrishnan, C. U. Maheswari, S. Nagarajan, V. Pace, A. Roller, N. Bhuvanesh and V. Sridharan, *Org. Lett.*, 2019, **21**, 3465–3469.

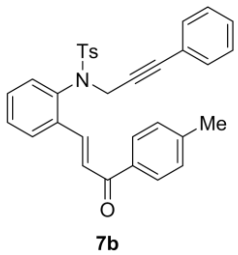
(*E*)-4-Methyl-*N*-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenyl)-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (7a):[1]



7a

Yellow solid; mp: 114-115 ^{o}C; yield: 1.104 g, 90%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.33 (s, 3H), 4.45 (brs, 1H), 4.88 (brs, 1H), 7.13-7.17 (m, 3H), 7.18-7.27 (m, 4H), 7.33-7.53 (m, 6H), 7.58 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.82 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.98-8.04 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ* 21.5, 42.6, 82.9, 86.1, 122.2, 125.0, 127.6, 128.2, 128.5, 128.6, 128.8, 129.4, 129.6, 130.2, 130.6, 131.5, 132.8, 135.9, 136.2, 137.9, 138.8, 140.5, 144.0, 191.2. *One aromatic carbon is merged with others.

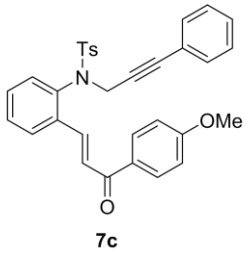
(*E*)-4-Methyl-*N*-(2-(3-oxo-3-(*p*-tolyl)prop-1-en-1-yl)phenyl)-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (7b):[1]



7b

Off-white solid; mp: 101-102 ^{o}C; yield: 1.072 g, 85%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.26 (s, 3H), 2.37 (s, 3H), 4.42 (brs, 1H), 4.71 (brs, 1H), 7.07-7.38 (m, 13H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.74 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.92 (d, *J* = 15.9 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ* 21.5, 21.7, 42.6, 82.9, 86.0, 122.2, 125.1, 127.6, 128.2, 128.3, 128.5, 129.0, 129.3, 129.6, 130.3, 130.5, 131.5, 135.4, 135.9, 136.3, 138.7, 140.0, 143.6, 144.0, 190.7. *One aromatic carbon is merged with others.

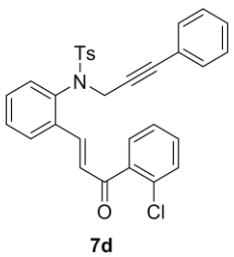
(*E*)-*N*-(2-(3-(4-Methoxyphenyl)-3-oxoprop-1-en-1-yl)phenyl)-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (7c):[1]



7c

Yellow viscous liquid; yield: 1.198 g, 92%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.33 (s, 3H), 3.90 (s, 3H), 4.50 (brs, 1H), 4.79 (brs, 1H), 6.98 (d, *J* = 9.0 Hz, 2H), 7.14-7.27 (m, 7H), 7.31-7.45 (m, 4H), 7.67 (d, *J* = 8.1 Hz, 2H), 7.80 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.97 (d, *J* = 15.9 Hz, 1H), 8.02 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.5, 42.6, 55.5, 82.9, 86.0, 113.9, 122.2, 125.0, 127.7, 128.2, 128.3, 128.5, 129.3, 129.6, 130.2, 130.4, 130.8, 131.2, 131.5, 136.0, 136.4, 138.6, 139.5, 144.0, 163.4, 189.4.

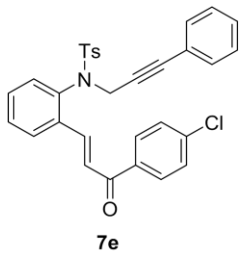
(*E*)-*N*-(2-(3-(2-Chlorophenyl)-3-oxoprop-1-en-1-yl)phenyl)-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (7d):[1]



7d

Yellow solid; mp: 124-125 ^{o}C; yield: 1.010 g, 77%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.32 (s, 3H), 4.36 (brs, 1H), 4.59 (brs, 1H), 6.98 (d, *J* = 16.2 Hz, 1H), 7.03-7.08 (m, 2H), 7.14-7.25 (m, 6H), 7.22-7.44 (m, 6H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 16.2 Hz, 1H), 7.75 (dd, *J* = 8.1, 1.5 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ* 21.6, 42.6, 82.7, 86.0, 122.1, 126.8, 127.5, 128.1, 128.3, 128.6, 129.4, 129.6, 129.7, 129.8, 130.3, 131.0, 131.3, 131.5, 135.7, 135.8, 138.5, 138.9, 142.5, 144.0, 194.0. *Two aromatic carbons are merged with others.

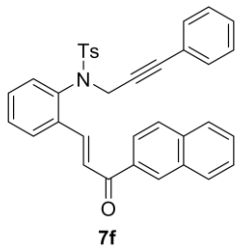
(*E*)-*N*-(2-(3-(4-Chlorophenyl)-3-oxoprop-1-en-1-yl)phenyl)-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (7e):[1]



7e

Yellow solid; mp: 122-123 °C; yield: 1.039 g, 79%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.29 (s, 3H), 4.46 (brs, 1H), 4.64 (brs, 1H), 7.03-7.08 (m, 3H), 7.12-7.23 (m, 4H), 7.24-7.41 (m, 6H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.75 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.98 (d, *J* = 15.9 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ* 21.6, 42.7, 82.8, 86.1, 122.1, 124.7, 127.7, 128.2, 128.6, 128.9, 129.4, 129.6, 129.9, 130.3, 130.8, 131.5, 135.8, 136.1, 136.2, 138.9, 139.1, 141.1, 144.1, 190.2. *One aromatic carbon is merged with others.

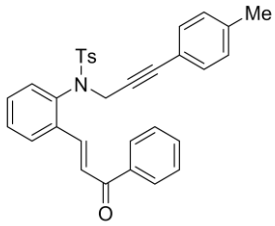
(*E*)-4-Methyl-*N*-(2-(3-(naphthalen-1-yl)-3-oxoprop-1-en-1-yl)phenyl)-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (7f):[1]



7f

Yellow solid; mp: 109-110 °C; yield: 1.204 g, 89%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.24 (s, 3H), 4.45 (brs, 1H), 4.65 (brs, 1H), 7.04-7.20 (m, 9H), 7.29 (td, *J* = 7.5, 1.5 Hz, 1H), 7.37 (td, *J* = 7.5, 1.5 Hz, 1H), 7.43 (d, *J* = 16.2 Hz, 1H), 7.47-7.55 (m, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.79-7.88 (m, 3H), 7.96-8.01 (m, 2H), 8.01 (d, *J* = 16.2 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.5, 42.7, 82.9, 86.1, 122.2, 124.8, 125.3, 126.8, 127.7, 127.8, 128.2, 128.3, 128.4, 128.5, 128.6, 129.4, 129.6, 129.8, 130.2, 130.6, 130.7, 131.5, 132.6, 135.1, 135.5, 135.9, 136.4, 138.8, 140.5, 144.0, 191.4.

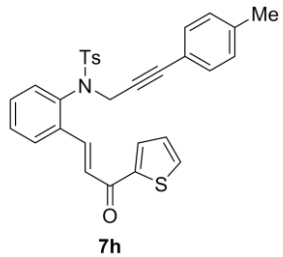
(*E*)-4-Methyl-*N*-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenyl)-*N*-(3-(*p*-tolyl)prop-2-yn-1-yl)benzenesulfonamide (7g):[1]



7g

Off-white solid; mp: 99-100 °C; yield: 1.060 g, 84%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.30 (s, 3H), 2.34 (s, 3H), 4.50 (brs, 1H), 4.74 (brs, 1H), 7.00-7.06 (m, 4H), 7.15 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.22 (d, *J* = 8.1 Hz, 2H), 7.32-7.52 (m, 5H), 7.58 (tt, *J* = 8.1, 1.5 Hz, 1H), 7.66 (d, *J* = 8.1 Hz, 2H), 7.81 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.98-8.04 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.4, 21.5, 42.7, 82.2, 86.2, 119.1, 125.0, 127.6, 128.2, 128.6, 128.9, 129.0, 129.3, 129.6, 130.3, 130.6, 131.4, 132.7, 135.9, 136.3, 137.9, 138.7, 138.8, 140.6, 144.0, 191.3.

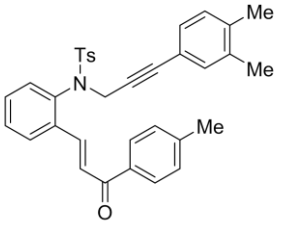
(*E*)-4-Methyl-*N*-(2-(3-oxo-3-(thiophen-2-yl)prop-1-en-1-yl)phenyl)-*N*-(3-(*p*-tolyl)prop-2-yn-1-yl)benzenesulfonamide (7h):[1]



7h

Colourless solid; mp: 204-205 °C; yield: 1.136 g, 89%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.30 (s, 3H), 2.34 (s, 3H), 4.50 (brs, 1H), 4.78 (brs, 1H), 7.02 (d, *J* = 8.4 Hz, 2H), 7.06 (d, *J* = 8.4 Hz, 2H), 7.16-7.29 (m, 4H), 7.30-7.45 (m, 3H), 7.67-7.69 (m, 3H), 7.78 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.88 (dd, *J* = 3.9, 1.2 Hz, 1H), 8.04 (d, *J* = 15.9 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.4, 21.5, 42.7, 82.2, 86.2, 119.1, 124.5, 127.9, 128.2, 128.3, 129.0, 129.3, 129.6, 130.4, 130.6, 131.4, 132.4, 133.9, 135.9, 136.0, 138.7, 138.8, 139.5, 144.0, 145.2, 182.4.

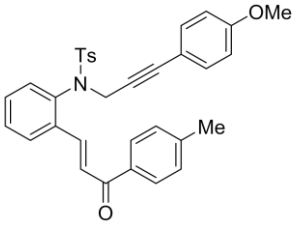
(*E*)-*N*-(3-(3,4-Dimethylphenyl)prop-2-yn-1-yl)-4-methyl-*N*-(2-(3-oxo-3-(*p*-tolyl)prop-1-en-1-yl)phenyl)benzenesulfonamide (7i):



7i

Pale brown viscous liquid; yield: 1.041 g, 78%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.16 (s, 3H), 2.20 (s, 3H), 2.35 (s, 3H), 2.44 (s, 3H), 4.47 (brs, 1H), 4.79 (brs, 1H), 6.88-6.99 (m, 3H), 7.16 (d, *J* = 7.8 Hz, 1H), 7.22-7.44 (m, 7H), 7.67 (d, *J* = 8.1 Hz, 2H), 7.81 (d, *J* = 6.6 Hz, 1H), 7.92 (d, *J* = 7.8 Hz, 2H), 7.99 (d, *J* = 15.9 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ* 19.5, 19.7, 21.5, 21.7, 42.7, 81.9, 86.3, 119.4, 125.0, 127.6, 128.3, 128.9, 129.0, 129.3, 129.5, 129.6, 130.3, 130.5, 132.6, 135.4, 136.0, 136.3, 136.5, 137.5, 138.7, 140.0, 143.5, 143.9, 190.7; Anal Calcd for $C_{34}H_{31}NO_3S$: C, 76.52; H, 5.86; N, 2.62. Found: C, 76.41; H, 5.74; N, 2.68. *One aromatic carbon is merged with others.

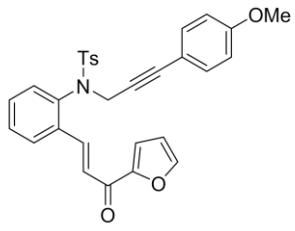
(*E*)-*N*-(3-(4-Methoxyphenyl)prop-2-yn-1-yl)-4-methyl-*N*-(2-(3-oxo-3-(*p*-tolyl)prop-1-en-1-yl)phenyl)benzenesulfonamide (7j):[1]



7j

Off-white solid; mp: 116-117 ^{o}C; yield: 0.895 g, 67%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.33 (s, 3H), 2.43 (s, 3H), 3.76 (s, 3H), 4.49 (brs, 1H), 4.75 (brs, 1H), 6.73 (d, *J* = 8.8 Hz, 2H), 7.09 (d, *J* = 8.8 Hz, 2H), 7.15 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.30 (td, *J* = 8.4, 1.6 Hz, 1H), 7.36 (d, *J* = 16.0 Hz, 1H), 7.41 (td, *J* = 8.4, 1.6 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.80 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.91 (d, *J* = 8.4 Hz, 2H), 8.00 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.7, 20.9, 41.9, 54.4, 80.6, 85.1, 113.0, 113.5, 124.2, 126.7, 127.4, 128.2, 128.4, 128.5, 128.7, 129.5, 129.6, 132.1, 134.5, 135.1, 135.5, 137.9, 139.2, 142.7, 143.1, 158.9, 189.8.

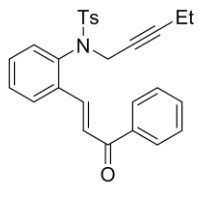
(*E*)-*N*-(2-(3-(Furan-2-yl)-3-oxoprop-1-en-1-yl)phenyl)-*N*-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (7k):



7k

Grey solid; mp: 116-117 ^{o}C; yield: 1.049 g, 82%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.35 (s, 3H), 3.77 (s, 3H), 4.52 (brs, 1H), 4.75 (brs, 1H), 6.58-6.60 (m, 1H), 6.75 (d, *J* = 9.0 Hz, 2H), 7.13 (d, *J* = 9.0 Hz, 2H), 7.19 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.23-7.28 (m, 3H), 7.34-7.42 (m, 3H), 7.65-7.70 (m, 3H), 7.79 (dd, *J* = 7.5, 1.5 Hz, 1H), 8.09 (d, *J* = 15.9 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): 21.5, 42.7, 55.3, 81.5, 86.0, 112.5, 113.8, 114.3, 118.0, 124.0, 127.7, 128.2, 129.3, 129.6, 130.5, 130.6, 133.0, 136.0, 136.1, 138.8, 139.4, 144.0, 146.6, 153.4, 159.7, 178.1; Anal Calcd for $C_{30}H_{25}NO_5S$: C, 70.43; H, 4.93; N, 2.74. Found: C, 70.18; H, 4.71; N, 2.72.

(*E*)-4-Methyl-*N*-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenyl)-*N*-(pent-2-yn-1-yl)benzenesulfonamide (7l):

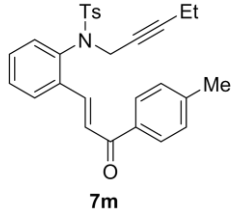


7l

Yellow viscous liquid; yield: 0.920 g, 83%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 0.92 (t, *J* = 7.5 Hz, 3H), 1.95-2.02 (m, 2H), 2.34 (s, 3H), 4.31 (brs, 1H), 4.43 (brs, 1H), 7.09 (d, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.30-7.45 (m, 3H), 7.50-7.65 (m, 5H), 7.80 (d, *J* = 6.6 Hz, 1H), 7.94-8.03 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): 12.2, 13.4, 21.5, 42.3, 73.0, 88.1, 124.8, 127.5,

128.2, 128.5, 128.9, 129.2, 129.5, 130.3, 130.5, 132.8, 135.9, 136.2, 137.9, 138.8, 140.8, 143.8, 191.4; Anal Calcd for $C_{27}H_{25}NO_3S$: C, 73.11; H, 5.68; N, 3.16. Found: C, 72.83; H, 5.55; N, 3.08.

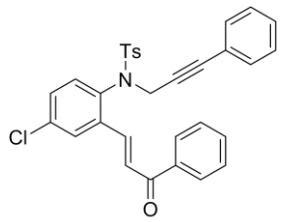
(*E*)-4-Methyl-*N*-(2-(3-oxo-3-(*p*-tolyl)prop-1-en-1-yl)phenyl)-*N*-(pent-2-yn-1-yl)benzenesulfonamide (7m):



7m

Pale yellow viscous liquid; yield: 1.030 g, 90%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 0.92 (t, *J* = 7.5 Hz, 3H), 1.95-2.03 (m, 2H), 2.34 (s, 3H), 2.45 (s, 3H), 4.31 (brs, 1H), 4.46 (brs, 1H), 7.10 (d, *J* = 7.5, 1H), 7.22 (d, *J* = 8.1 Hz, 2H), 7.30-7.44 (m, 5H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.91-7.96 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): 12.2, 13.4, 21.5, 21.7, 42.3, 73.0, 88.1, 124.8, 127.5, 128.2, 129.0, 129.2, 129.3, 129.4, 130.3, 130.4, 135.4, 136.0, 136.3, 138.8, 140.2, 143.6, 143.8, 190.7; Anal Calcd for $C_{28}H_{27}NO_3S$: C, 73.50; H, 5.95; N, 3.06. Found: C, 73.23; H, 5.96; N, 2.99.

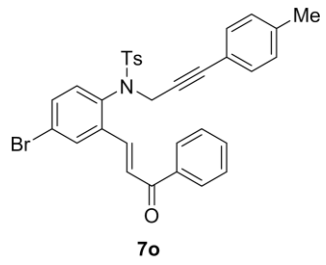
(*E*)-*N*-(4-Chloro-2-(3-oxo-3-phenylprop-1-en-1-yl)phenyl)-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (7n):[1]



7n

Yellow viscous liquid; yield: 0.971 g, 74%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.25 (s, 3H), 4.42 (brs, 1H), 4.68 (brs, 1H), 7.03-7.26 (m, 9H), 7.29 (d, *J* = 15.9 Hz, 1H), 7.41-7.46 (t, *J* = 6.9 Hz, 2H), 7.52 (d, *J* = 7.5 Hz, 1H), 7.58 (d, *J* = 8.1 Hz, 2H), 7.70 (d, *J* = 2.4 Hz, 1H), 7.85 (d, *J* = 15.9 Hz, 1H), 7.92 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): 21.5, 42.6, 82.5, 86.3, 122.0, 125.7, 127.4, 128.2, 128.3, 128.6, 128.7, 128.8, 129.7, 130.4, 131.5, 131.6, 133.0, 135.3, 135.6, 137.1, 137.6, 138.0, 138.9, 144.2, 190.5.

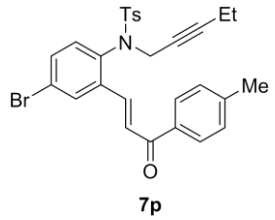
(*E*)-*N*-(4-Bromo-2-(3-oxo-3-phenylprop-1-en-1-yl)phenyl)-4-methyl-*N*-(3-(*p*-tolyl)prop-2-yn-1-yl)benzenesulfonamide (7o):[1]



7o

Colourless solid; mp: 97-98 ^{o}C; yield: 1.066 g, 73%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.30 (s, 3H), 2.32 (s, 3H), 4.46 (brs, 1H), 4.73 (brs, 1H), 7.02-7.07 (m, 5H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 16.0 Hz, 1H), 7.46 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.48-7.53 (m, 2H), 7.60 (tt, *J* = 7.2, 1.6 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.89-7.93 (m, 2H), 7.98-8.00 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ* 21.4, 21.5, 42.6, 81.8, 86.5, 118.9, 123.4, 125.7, 128.2, 128.6, 128.8, 129.0, 129.7, 130.4, 131.4, 131.8, 133.0, 133.4, 135.6, 137.6, 138.3, 138.8, 144.1, 190.5. *Two aromatic carbons are merged with others.

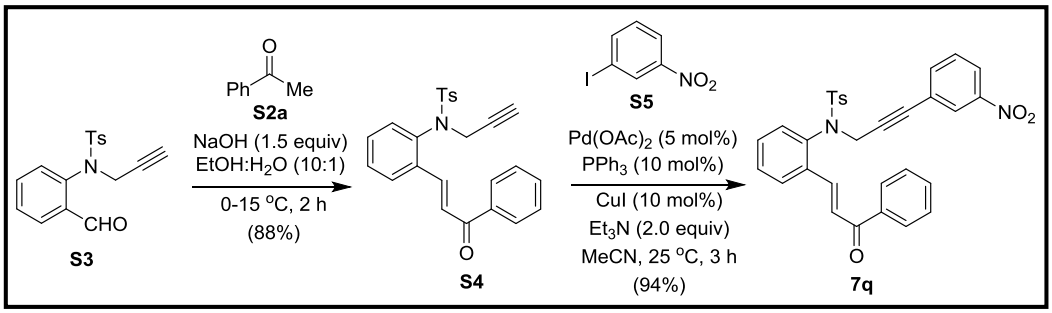
(*E*)-*N*-(4-Bromo-2-(3-oxo-3-(*p*-tolyl)prop-1-en-1-yl)phenyl)-4-methyl-*N*-(pent-2-yn-1-yl)benzenesulfonamide (7p):



7p

Pale brown viscous liquid; yield: 1.046 g, 78%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 0.94 (s, 3H), 1.97-2.04 (m, 2H), 2.33 (s, 3H), 2.45 (s, 3H), 4.30 (brs, 1H), 4.41 (brs, 1H), 6.98 (d, *J* = 8.4, 1H), 7.23 (d, *J* = 8.4 Hz, 2H), 7.31-7.36 (m, 3H), 7.45 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.83 (d, *J* = 15.9 Hz, 1H), 7.90-7.94 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): 12.2, 13.4, 21.5, 21.7, 42.2, 72.8, 88.4, 123.3, 125.6, 128.2, 129.0, 129.4, 129.6, 130.3, 132.0, 133.2, 135.1, 135.7, 137.6, 138.4, 138.5, 143.9, 144.1, 189.9; Anal Calcd for $C_{28}H_{26}BrNO_3S$: C, 62.69; H, 4.89; N, 2.61. Found: C, 62.53; H, 4.82; N, 2.49.

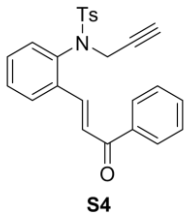
3. Synthesis of (*E*)-4-Methyl-*N*-(3-(3-nitrophenyl)prop-2-yn-1-yl)-*N*-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenyl)benzenesulfonamide 7q[1]



To a solution of acetophenone **S2a** (2.75 mmol, 1.1 equiv) in 10:1 EtOH/H_2O mixture (15 mL) was added NaOH (3.75 mmol, 1.5 equiv) at 0 ^{o}C. After 10 minutes of stirring, aldehyde **S3** (2.5 mmol, 1.0 equiv) was added and stirring was continued at 10-15 ^{o}C for 2 h. After completion of the reaction, the reaction mixture was poured into ice water and acidified with 1.5 N HCl. The aqueous suspension was extracted with DCM (2 x 60 mL), washed with water and brine. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by flash column chromatography using petroleum ether and ethyl acetate mixture as eluent (90:10, v/v) to deliver compound **S4**.

To a stirred solution of compound **S4** (2.5 mmol, 1.0 equiv) in MeCN (50 mL) were added 3-nitroiodobenzene **S5** (3 mmol, 1.2 equiv), $Pd(OAc)_2$ (0.125 mmol, 5 mol%), PPh_3 (0.25 mmol, 10 mol%), CuI (0.25 mmol, 10 mol%), and Et_3N (5.0 mmol, 2.0 equiv) successively. The resulting mixture was degassed with nitrogen and stirred at room temperature for 3 h. After completion of the reaction, as indicated by TLC, the reaction mixture was filtered through a pad of celite and the celite bed was washed well with ethyl acetate (100 mL). The filtrate was washed with water, brine and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness under reduced pressure and the crude mixture was chromatographed over silica using petroleum ether and ethyl acetate mixture (93:7, v/v) as eluent to obtain the desired product **7q**.

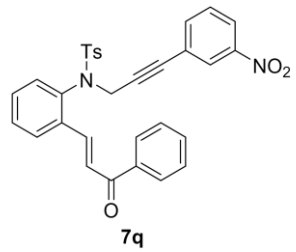
(*E*)-4-methyl-*N*-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenyl)-*N*-(prop-2-yn-1-yl)benzenesulfonamide (S4):[1]



S4

Off-white solid; mp: 137-138 °C; yield: 1.006 g, 88%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.17 (t, *J* = 2.4 Hz, 1H), 2.33 (s, 3H), 4.35 (brs, 1H), 4.44 (brs, 1H), 7.14 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.23 (d, *J* = 6.9 Hz, 2H), 7.33-7.46 (m, 3H), 7.50-7.54 (m, 2H), 7.58-7.62 (m, 3H), 7.80 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.90 (d, *J* = 15.9 Hz, 1H), 8.00 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ* 21.5, 41.7, 74.3, 124.9, 127.6, 128.2, 128.6, 128.8, 129.4, 129.6, 130.4, 130.7, 132.8, 135.6, 136.0, 137.9, 138.5, 140.3,144.1, 191.0. *One aromatic carbon is merged with others.

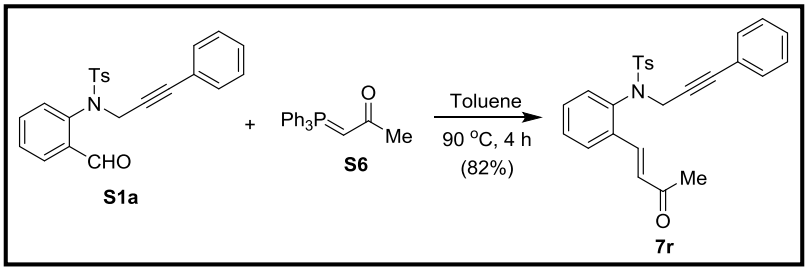
(*E*)-4-Methyl-*N*-(3-(3-nitrophenyl)prop-2-yn-1-yl)-*N*-(2-(3-oxo-3-phenylprop-1-en-1-yl)phenyl)benzenesulfonamide (7q):



7q

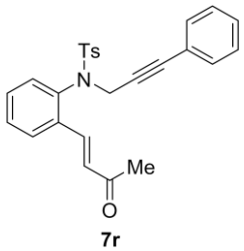
Pale brown solid; mp: 82-83 °C; yield: 1.261 g, 94%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.34 (s, 3H), 4.62 (brs, 1H), 4.71 (brs, 1H), 7.17 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.25-7.28 (m, 2H), 7.37-7.44 (m, 3H), 7.46-7.53 (m, 5H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.84 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.98-8.01 (m, 4H), 8.09-8.12 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.5, 42.5, 83.6, 85.8, 123.3, 123.9, 124.7, 126.3, 127.6, 128.2, 128.6, 128.7, 129.3, 129.6, 129.7, 130.2, 130.8, 132.9, 135.8, 136.2, 137.3, 137.8, 138.7, 140.2, 144.3, 147.9, 190.6; Anal Calcd for $C_{31}H_{24}N_2O_5S$: C, 69.39; H, 4.51; N, 5.22. Found: C, 69.02; H, 4.62; N, 5.14.

4. Synthesis of (*E*)-4-Methyl-*N*-(2-(3-oxobut-1-en-1-yl)phenyl)-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide 7r[1]



A mixture of aldehyde **S1a** (2 mmol, 1.0 equiv) and Wittig ylide **S6** (3 mmol, 1.5 equiv) in toluene (10 mL) was heated at 90 °C for 5 h. After cooling, the solvent was evaporated to dryness and the residue was treated with ether. The solidified $OPPh_3$ was removed by filtration and the filtrate was concentrated to afford the crude product, which was purified by flash column chromatography eluting with petroleum ether-ethyl acetate mixture (85:15, v/v) to obtain the pure compound **7r**.

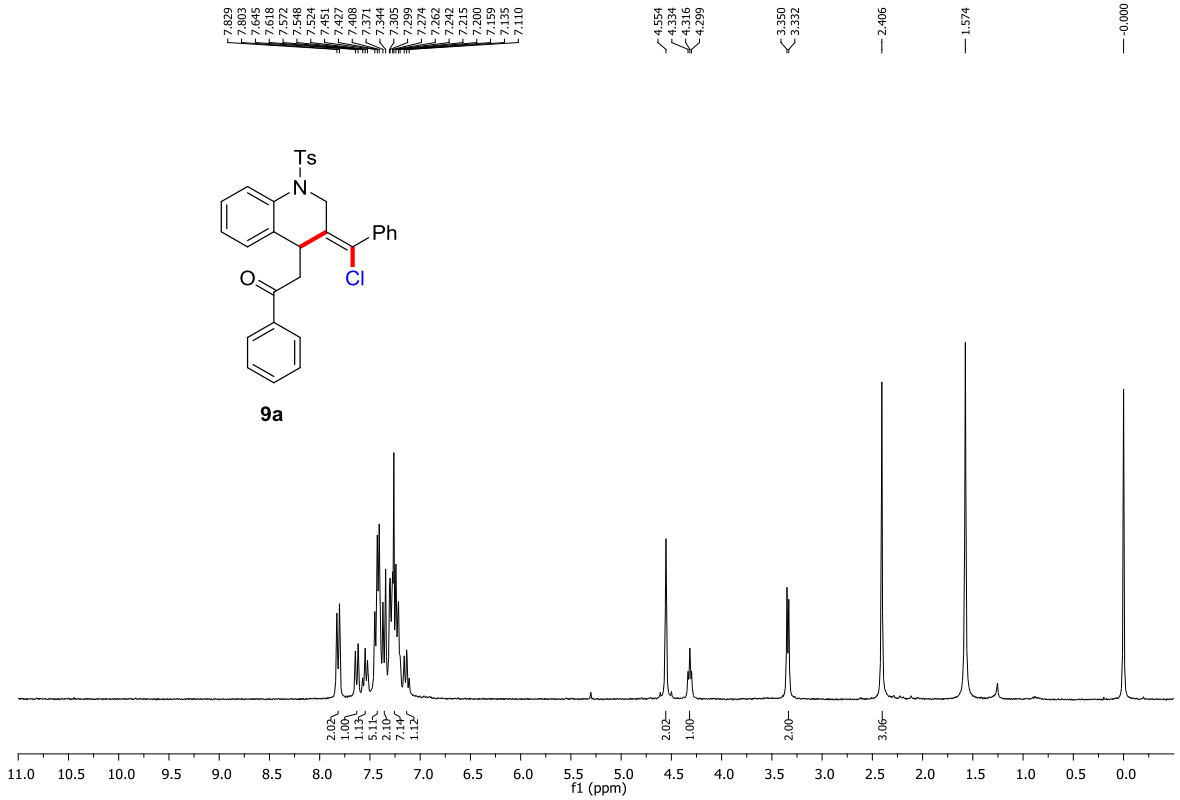
(*E*)-4-Methyl-*N*-(2-(3-oxobut-1-en-1-yl)phenyl)-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (7r):[1]

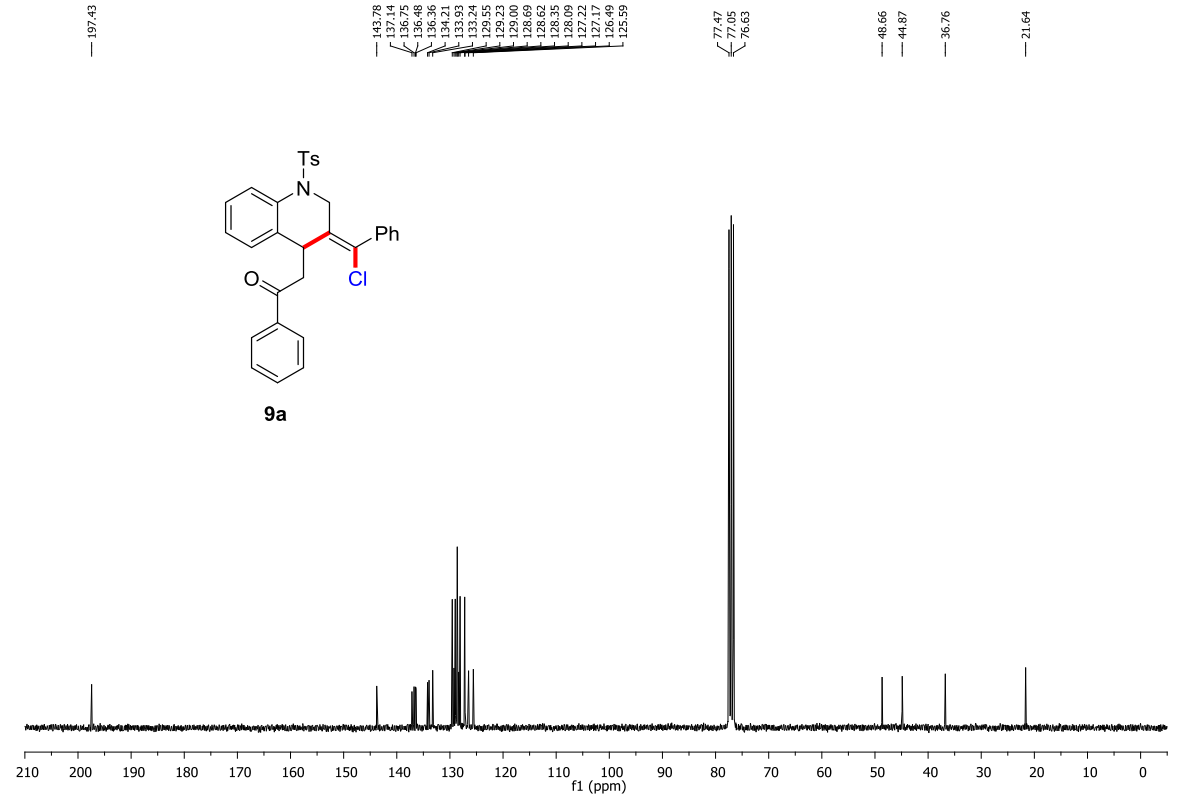


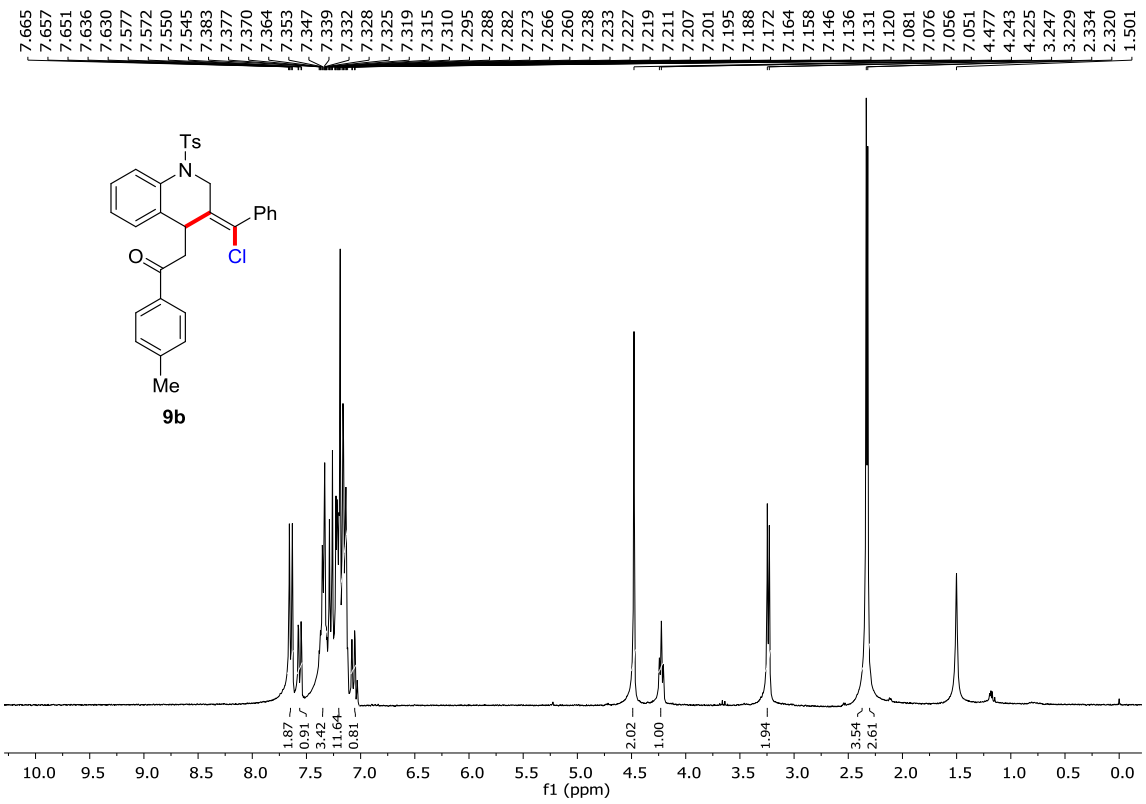
7r

Pale yellow solid; mp 139-140 ^{o}C; yield: 0.704 g, 82%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.24 (s, 3H), 2.35 (s, 3H), 4.57 (s, 2H), 6.54 (d, *J* = 16.5 Hz, 1H), 6.98 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.09 (dd, *J* = 8.1, 1.5 Hz, 2H), 7.15-7.29 (m, 6H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.68 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.87 (d, *J* = 16.5 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.6, 26.5, 42.8, 82.8, 86.0, 122.1, 127.2, 128.2, 128.3, 128.7, 129.4, 129.5, 129.6, 129.8, 130.8, 131.4, 135.9, 136.0, 138.7, 139.5, 144.2, 199.0.

5. Copies of ^{1}H and ^{13}C NMR Spectra



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7.572
7.550
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7.377
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7.353
7.347
7.339
7.332
7.328
7.325
7.319
7.315
7.310
7.295
7.288
7.282
7.273
7.266
7.260
7.238
7.233
7.227
7.219
7.211
7.207
7.201
7.195
7.188
7.172
7.164
7.158
7.146
7.136
7.131
7.120
7.081
7.076
7.056
7.051
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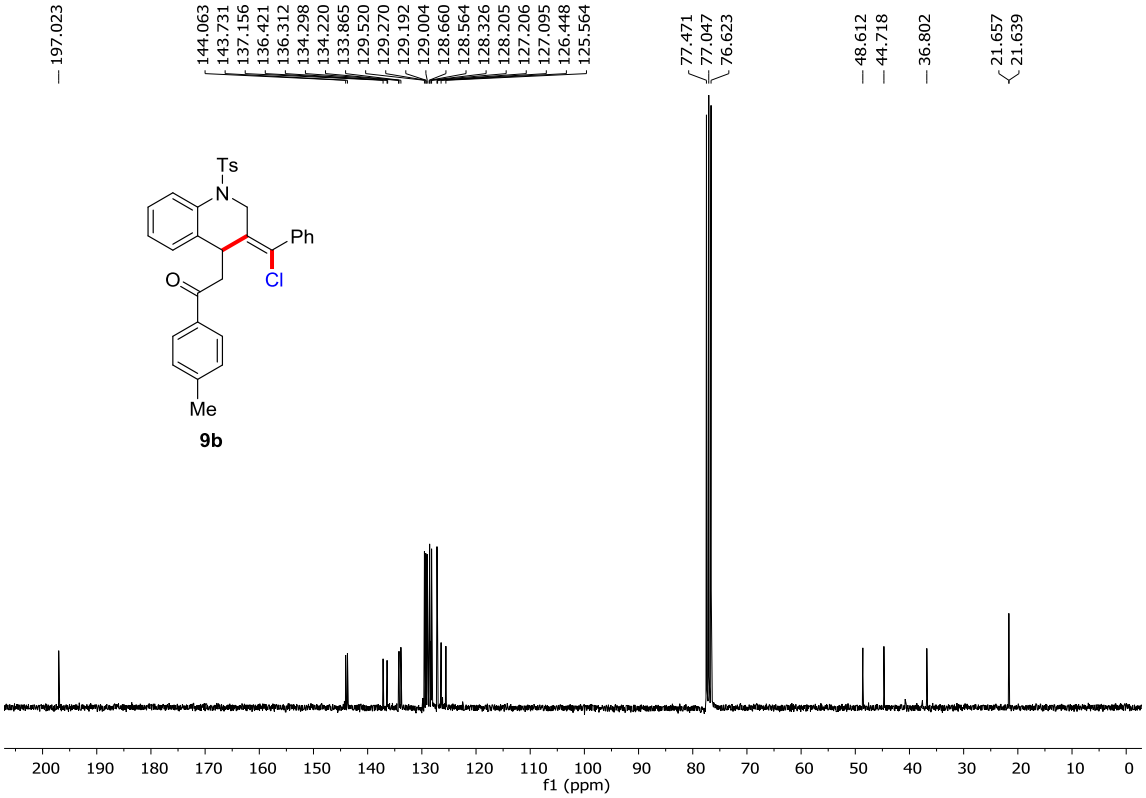
4.243
4.225
3.247
3.229
2.334
2.320
1.501
Ts
N
Ph
Cl
O
Me
9b
1.87
0.91
3.42
11.64
0.81
2.02
1.00
1.94
3.54
2.61
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.660
128.564
128.326
128.205
127.206
127.095
126.448
125.564
77.471
77.047
76.623
48.612
44.718
36.802
21.657
21.639
Ts
N
Ph
Cl
O
Me
9b
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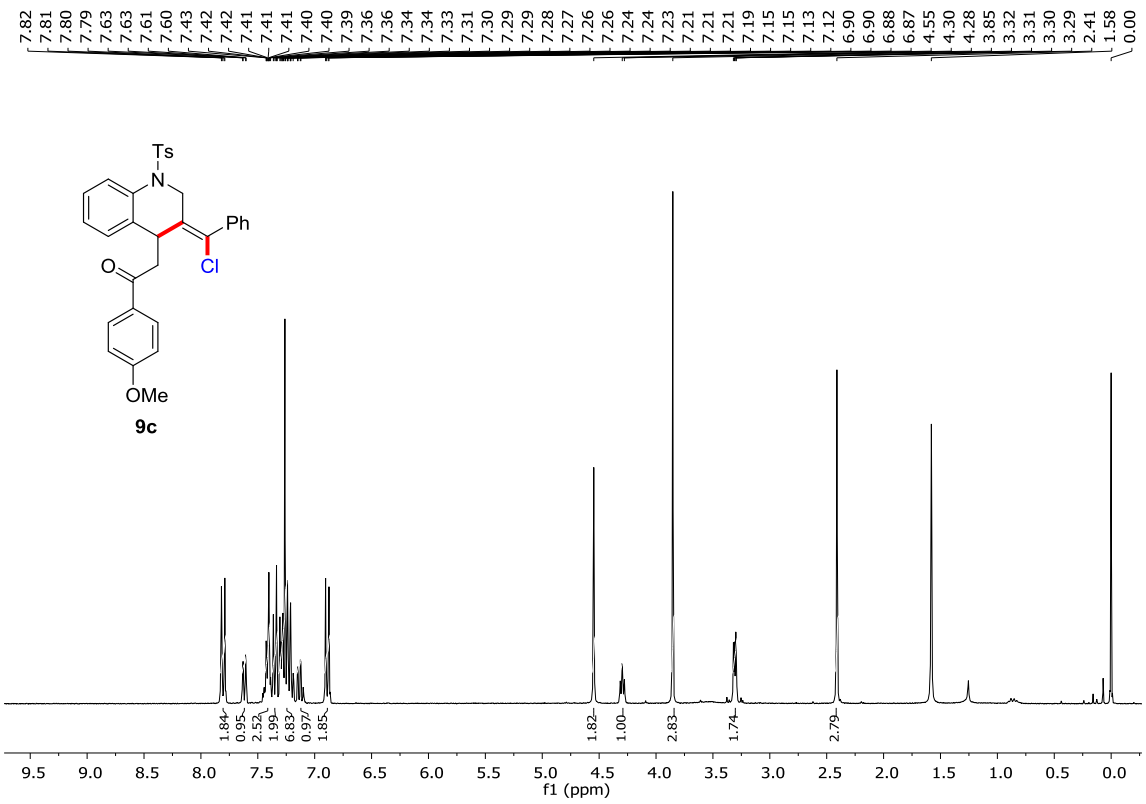
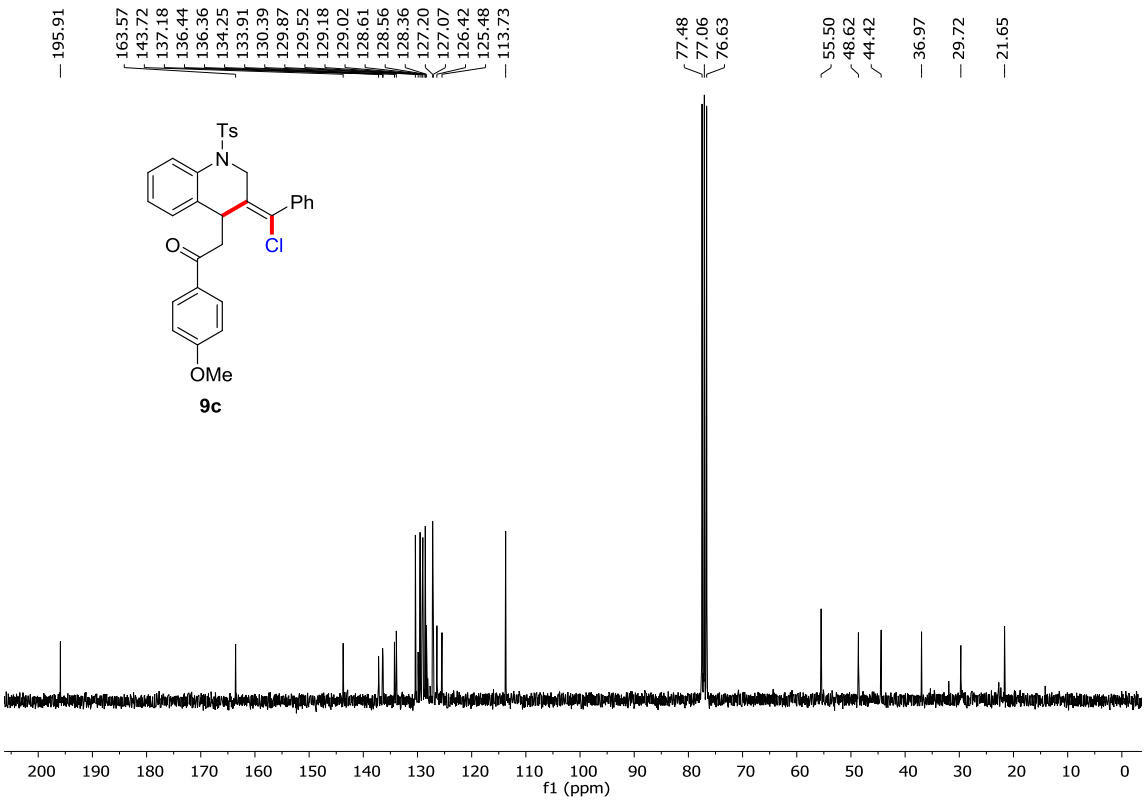
f1 (ppm)


7.82 7.81 7.80 7.79 7.63 7.63 7.61 7.60 7.43 7.42 7.42 7.41 7.41 7.41 7.40 7.40 7.39 7.36 7.36 7.34 7.34 7.33 7.31 7.30 7.29 7.29 7.28 7.27 7.26 7.26 7.24 7.24 7.23 7.21 7.21 7.21 7.19 7.15 7.15 7.13 7.12 6.90 6.90 6.88 6.87 4.55 4.30 4.28 3.85 3.32 3.31 3.30 3.29 2.41 1.58 0.00
Ts
N
Ph
Cl
O
OMe
9c
1.84 0.95 2.52 1.90 6.83 0.97 1.85 1.82 1.00 2.83 1.74 2.79
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


195.91 163.57 143.72 137.18 136.44 136.36 134.25 133.91 130.39 129.87 129.52 129.18 129.02 128.61 128.56 128.36 127.20 127.07 126.42 125.48 113.73 77.48 77.06 76.63 55.50 48.62 44.42 36.97 29.72 21.65
Ts
N
Ph
Cl
O
OMe
9c
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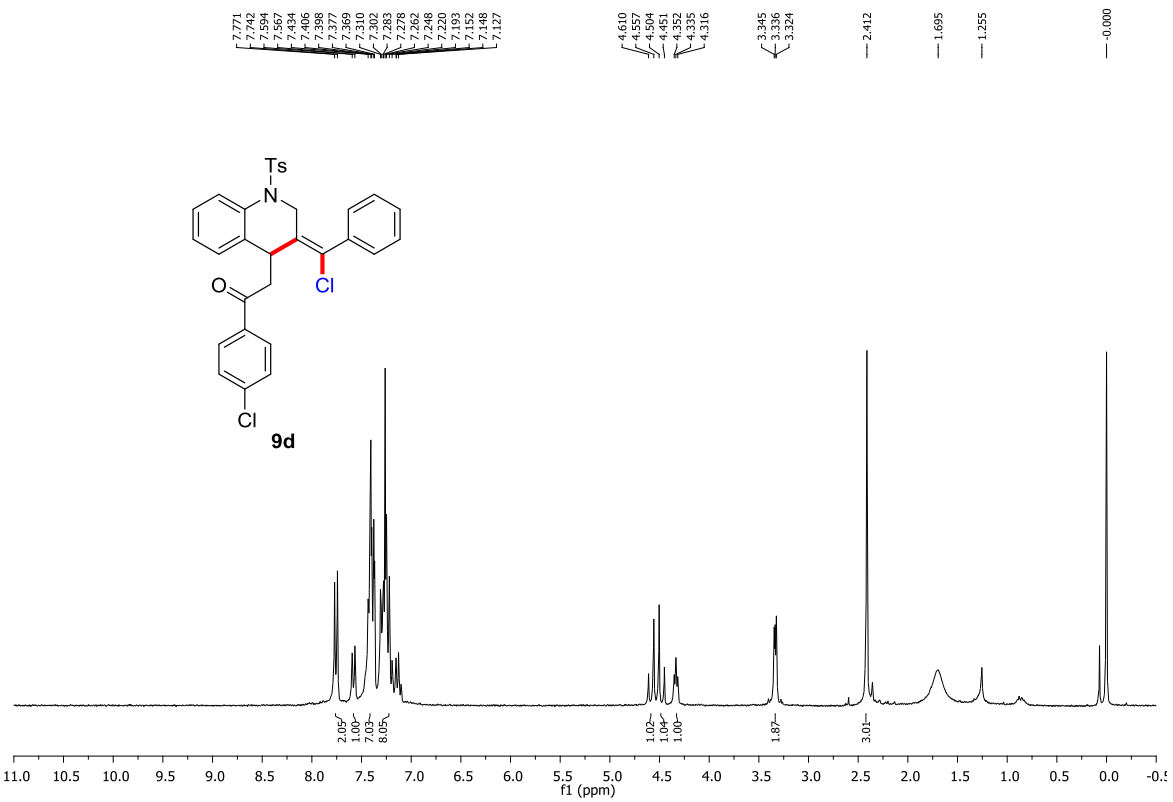
f1 (ppm)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7.220
7.193
7.152
7.148
7.127
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4.557
4.504
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4.352
4.335
4.316
3.345
3.336
3.324
2.412
1.695
1.255
0.000
Ts
N
O
Cl
Cl
9d
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1.00
7.03
8.05
1.02
1.04
1.00
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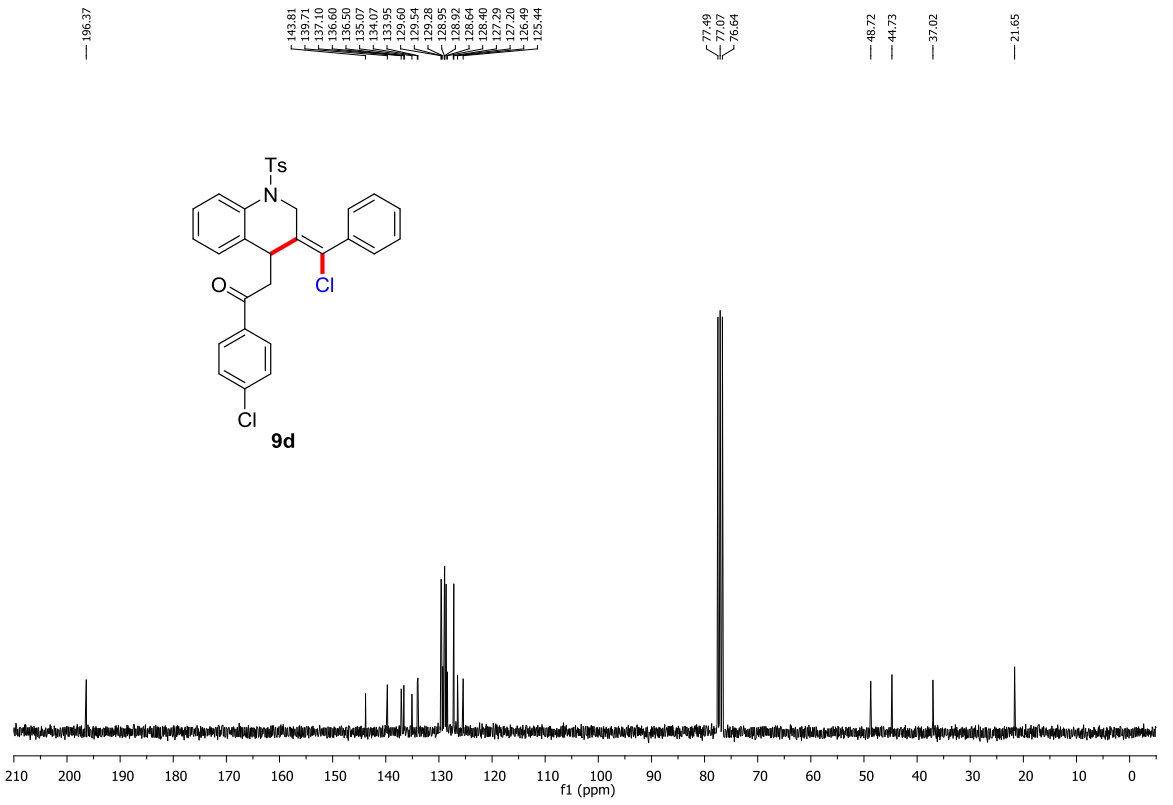
3.01
f1 (ppm)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136.50
135.07
134.07
133.95
129.60
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129.28
128.95
128.92
128.64
128.40
127.29
127.20
126.49
125.44
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77.07
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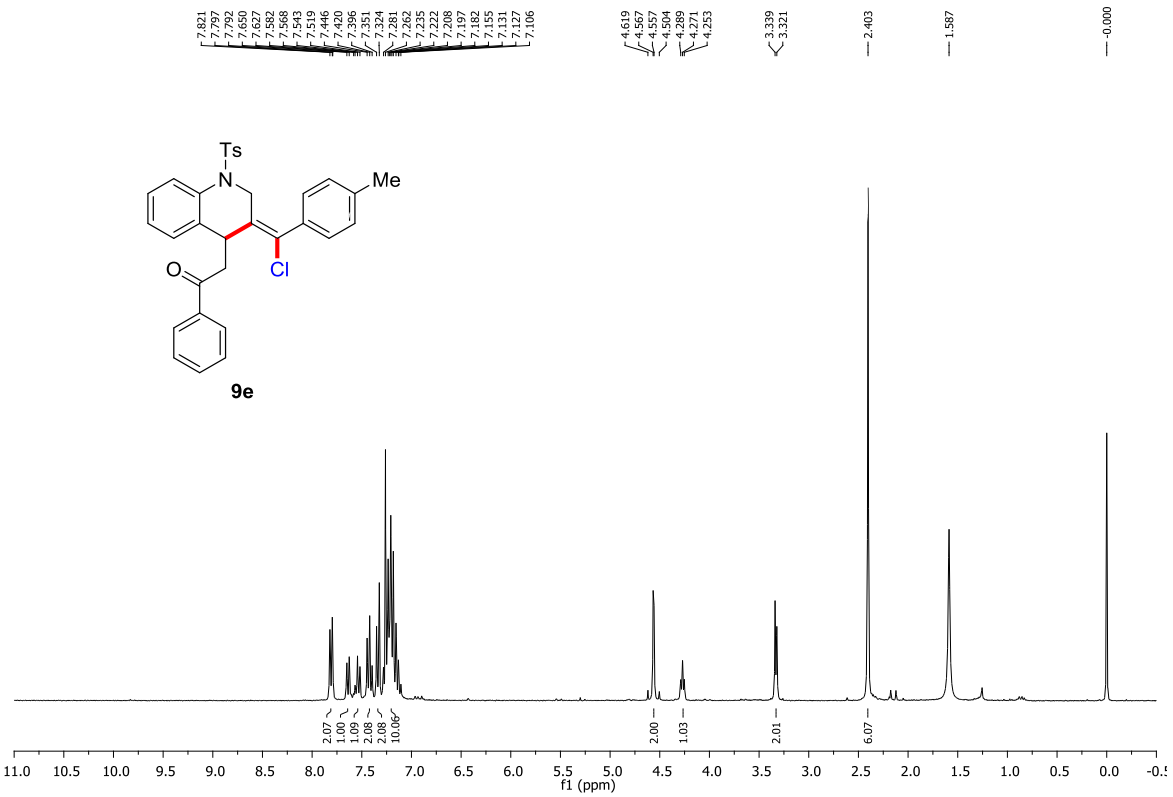
48.72
44.73
37.02
21.65
Ts
N
O
Cl
Cl
9d
f1 (ppm)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7.106
4.619
4.567
4.557
4.504
4.289
4.271
4.253
3.339
3.321
2.403
1.587
0.000
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Me
Cl
O
9e
2.07
1.00
1.09
2.08
2.08
10.06
2.00
1.03
2.01
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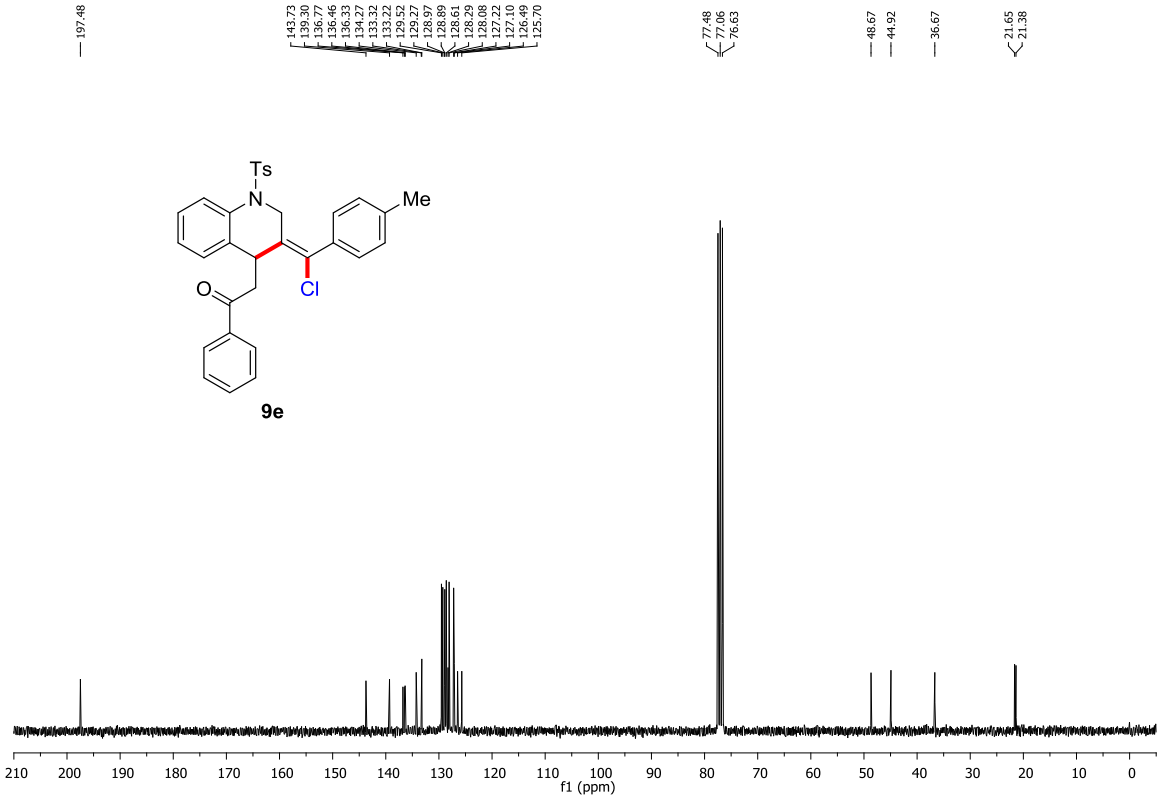
f1 (ppm)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129.27
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126.49
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77.06
76.63
48.67
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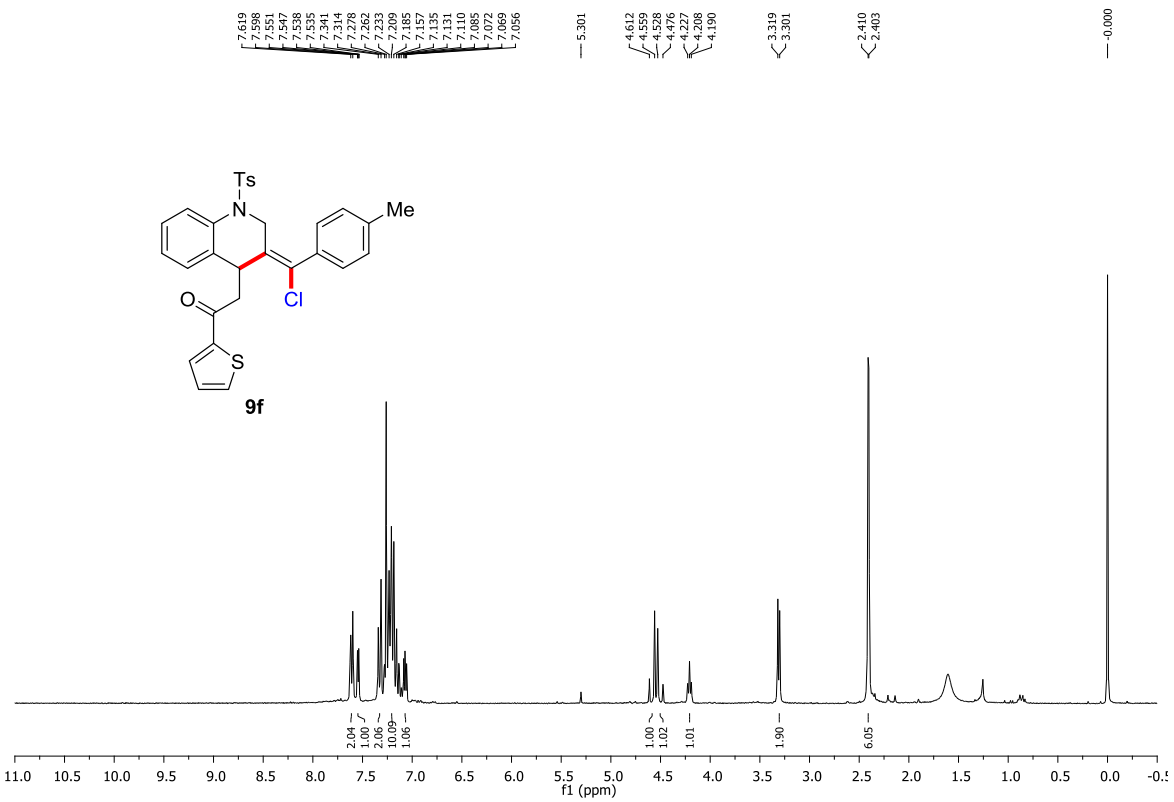
O
9e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.157
7.135
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7.085
7.072
7.069
7.056
5.301
4.612
4.559
4.528
4.476
4.227
4.208
4.190
3.319
3.301
2.410
2.403
0.000
Ts
N
Me
Cl
O
S
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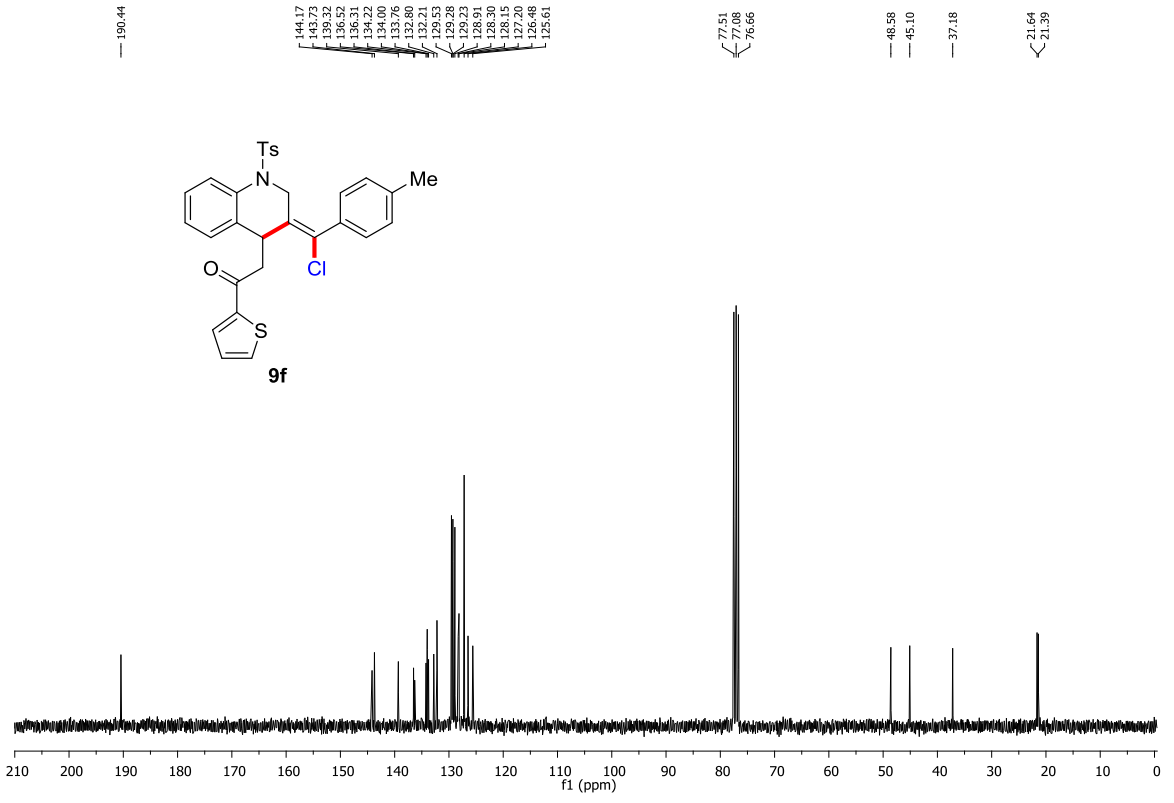
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127.20
126.48
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77.08
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21.39
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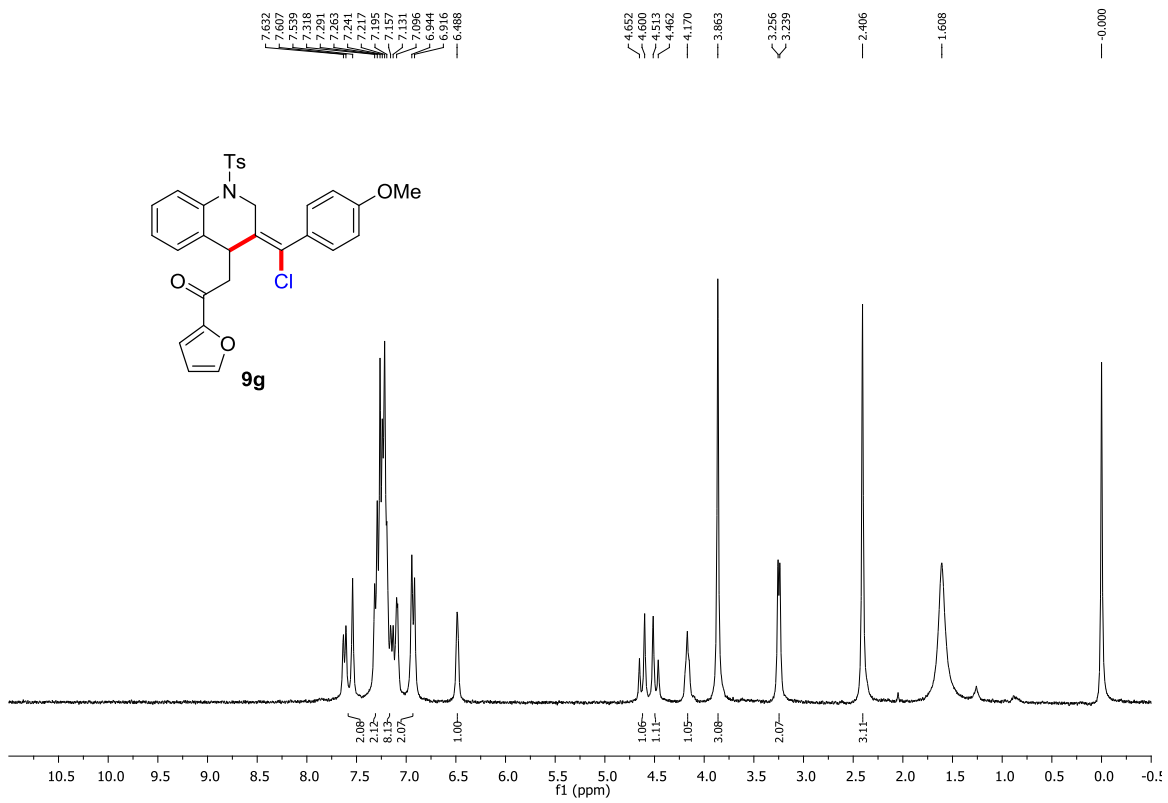
Me
Cl
O
S
9f
f1 (ppm)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7.157
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7.096
6.944
6.916
6.488
4.652
4.600
4.513
4.462
4.170
3.863
3.256
3.239
2.406
1.608
0.000
Ts
N
OMe
Cl
O
O
9g
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1.06
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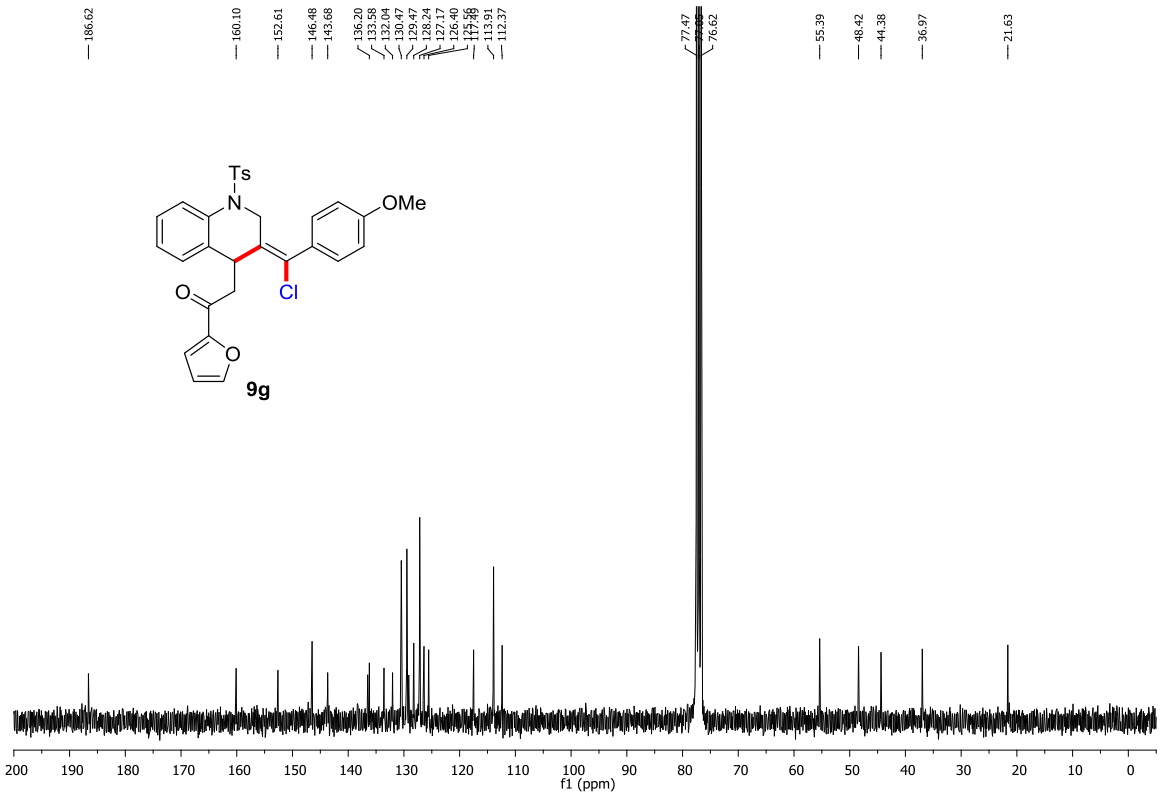
f1 (ppm)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117.48
113.91
112.37
77.47
77.05
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44.38
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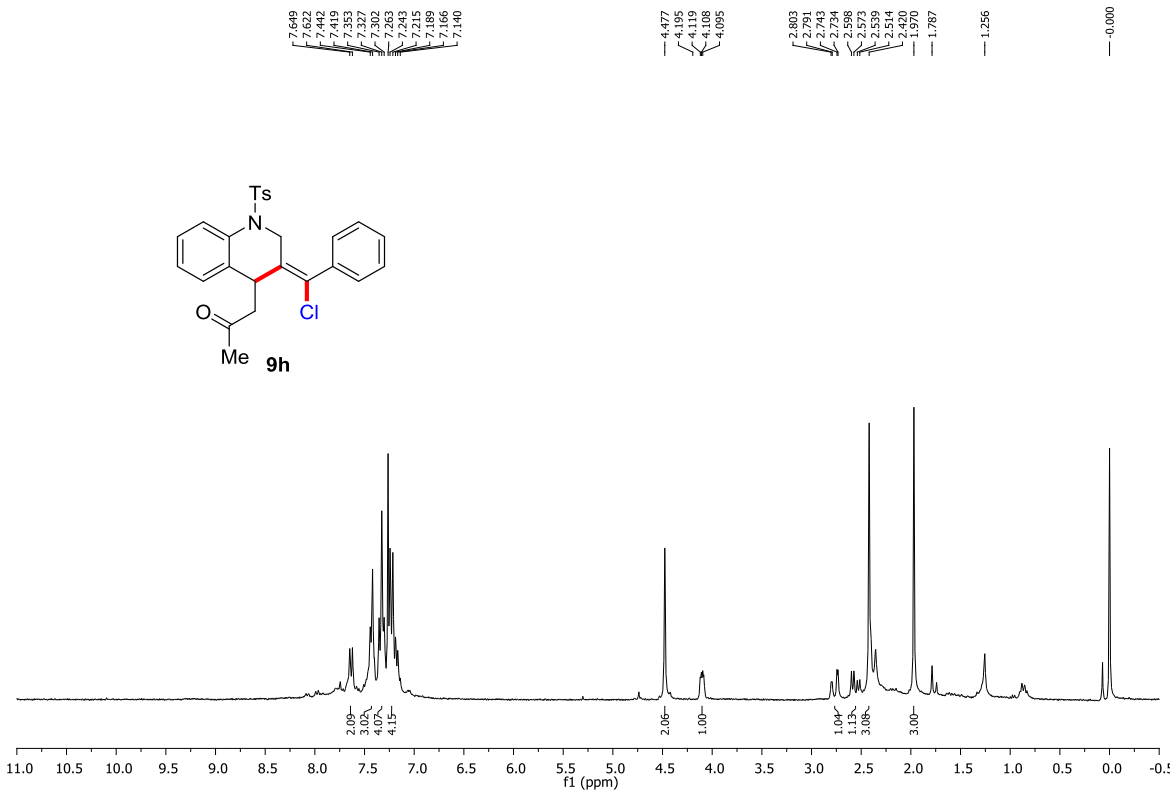
Ts
N
OMe
Cl
O
O
9g
f1 (ppm)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4.477
4.195
4.119
4.108
4.095
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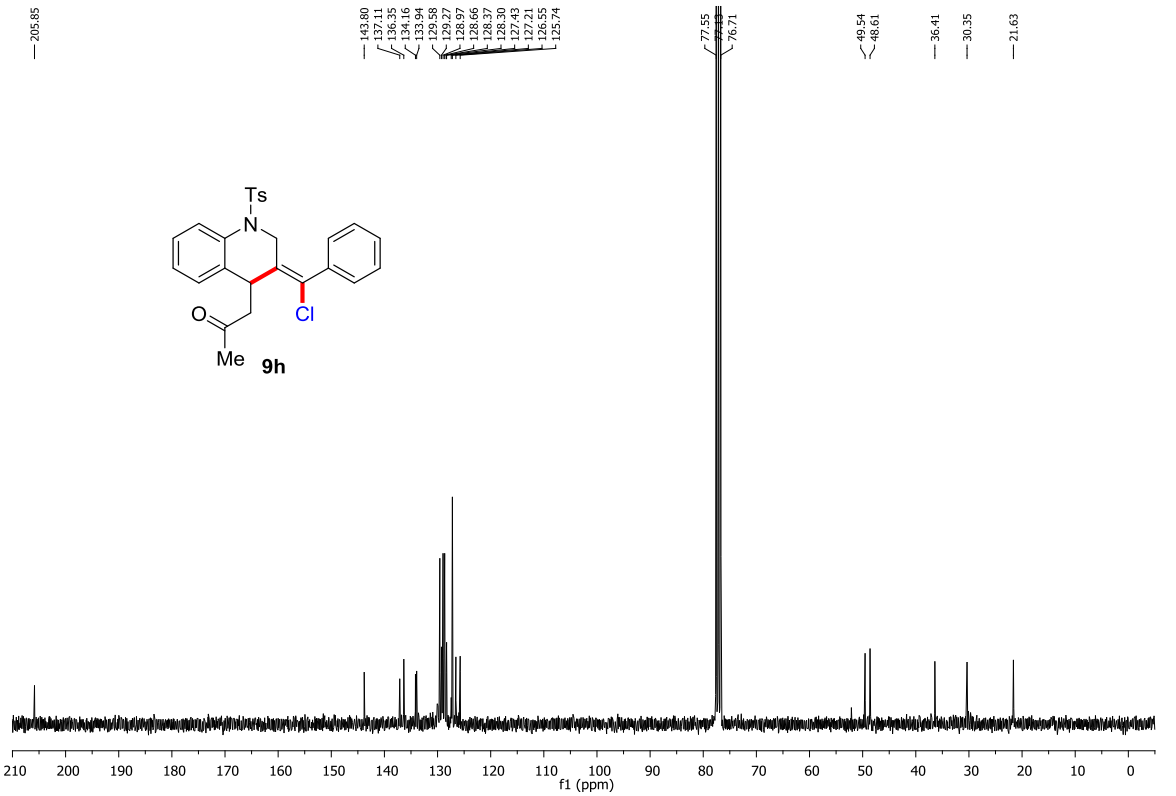
2.791
2.743
2.734
2.598
2.573
2.539
2.514
2.420
1.970
1.787
1.256
0.000
Ts
N
O
Me
Cl
9h
2.09
3.02
4.07
4.15
2.06
1.00
1.04
1.13
3.08
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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127.21
126.55
125.74
77.55
77.13
76.71
49.54
48.61
36.41
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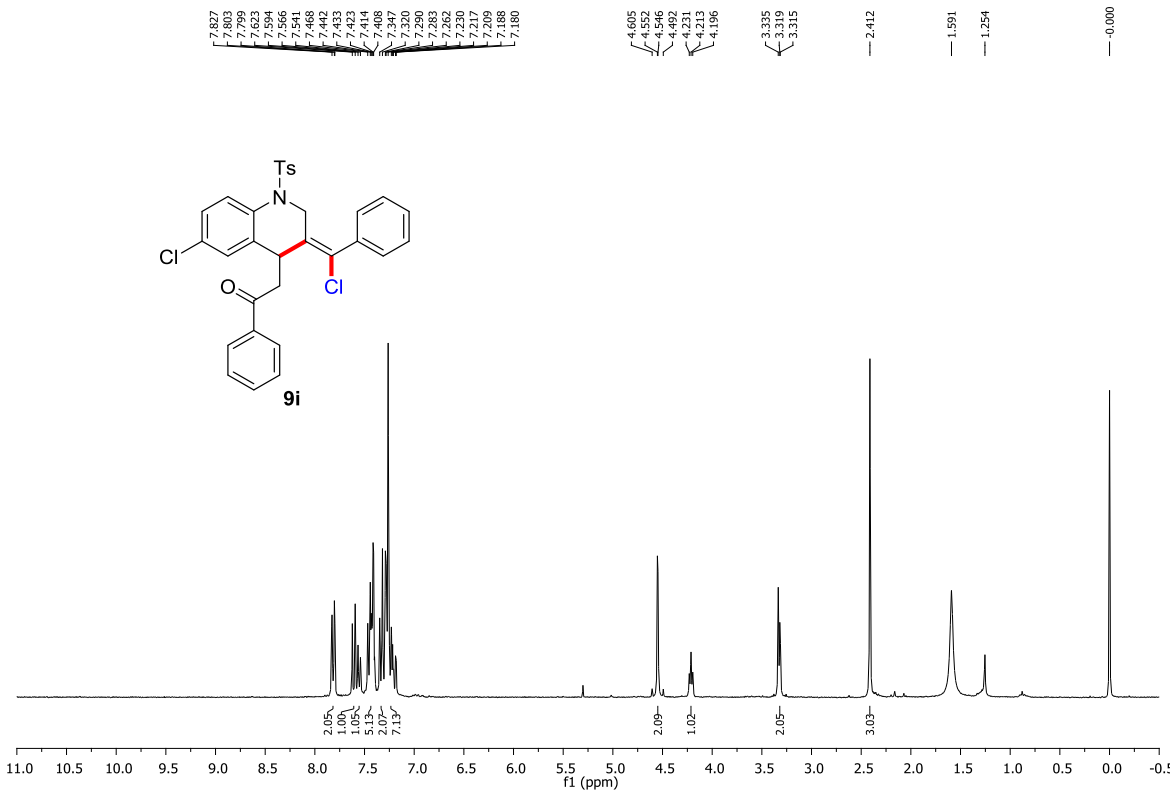
N
O
Me
Cl
9h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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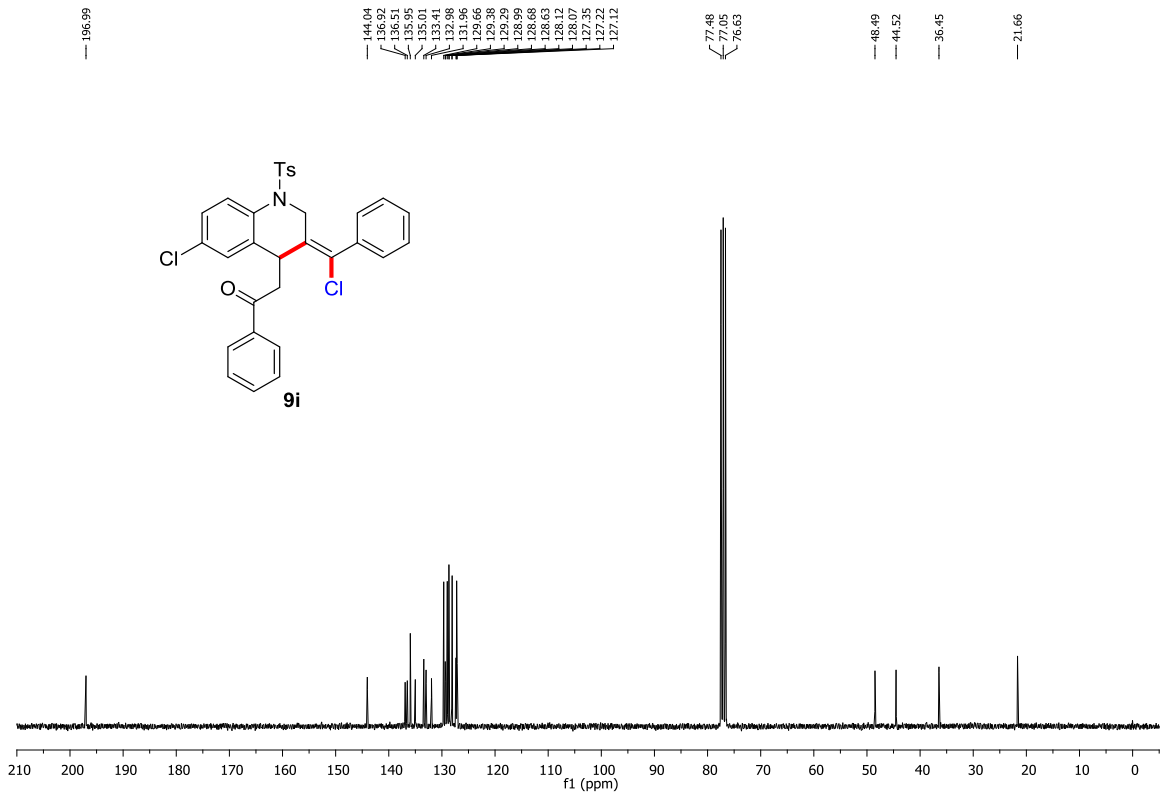
7.414
7.408
7.347
7.320
7.290
7.283
7.262
7.230
7.217
7.209
7.188
7.180
4.605
4.552
4.546
4.492
4.231
4.213
4.196
3.335
3.319
3.315
2.412
1.591
1.254
0.000
Ts
N
Cl
O
Cl
9i
2.05
1.00
1.05
5.13
2.07
7.13
2.09
1.02
2.05
3.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.68
128.63
128.12
128.07
127.35
127.22
127.12
77.48
77.05
76.63
48.49
44.52
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Ts
N
Cl
O
Cl
9i
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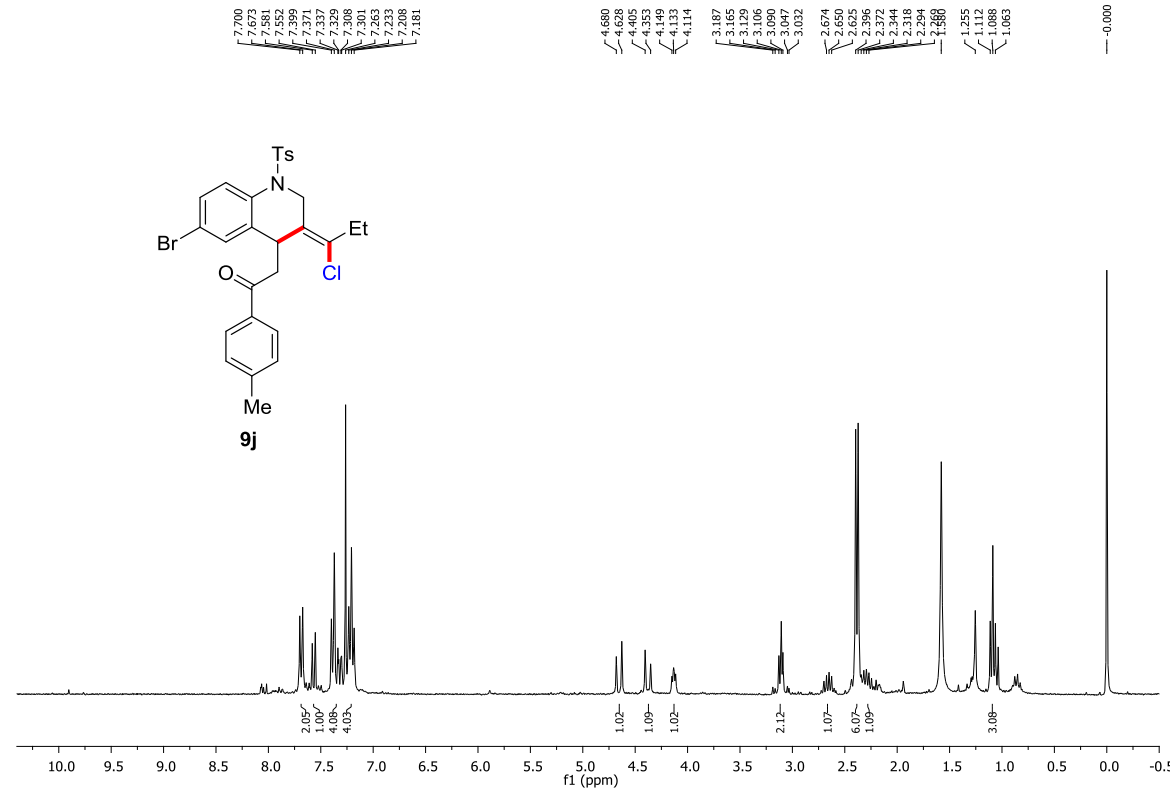
f1 (ppm)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7.181
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4.628
4.405
4.353
4.149
4.133
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3.187
3.165
3.129
3.106
3.090
3.047
3.032
2.674
2.650
2.625
2.396
2.372
2.344
2.318
2.294
1.255
1.112
1.088
1.063
-0.000
Ts
N
Br
Et
Cl
O
Me
9j
2.05
1.00
4.08
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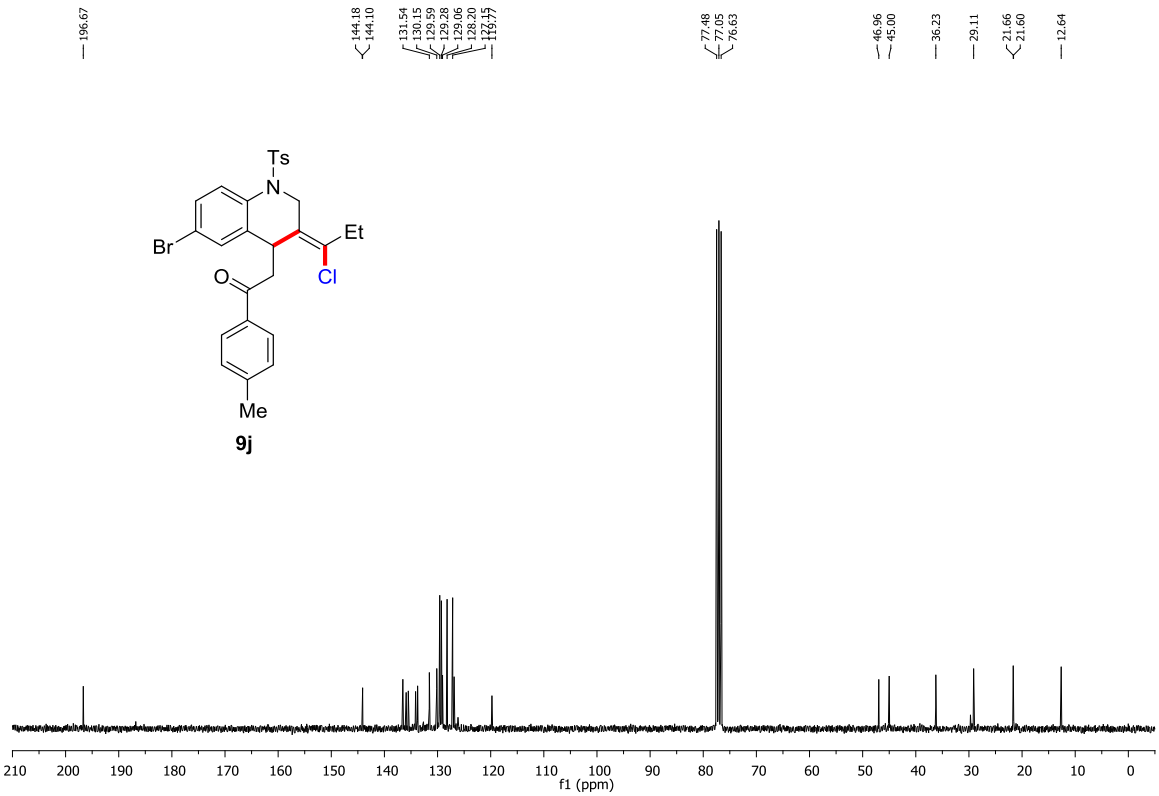
1.02
1.09
1.02
2.12
1.07
6.07
1.09
3.08
f1 (ppm)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77.05
76.63
46.96
45.00
36.23
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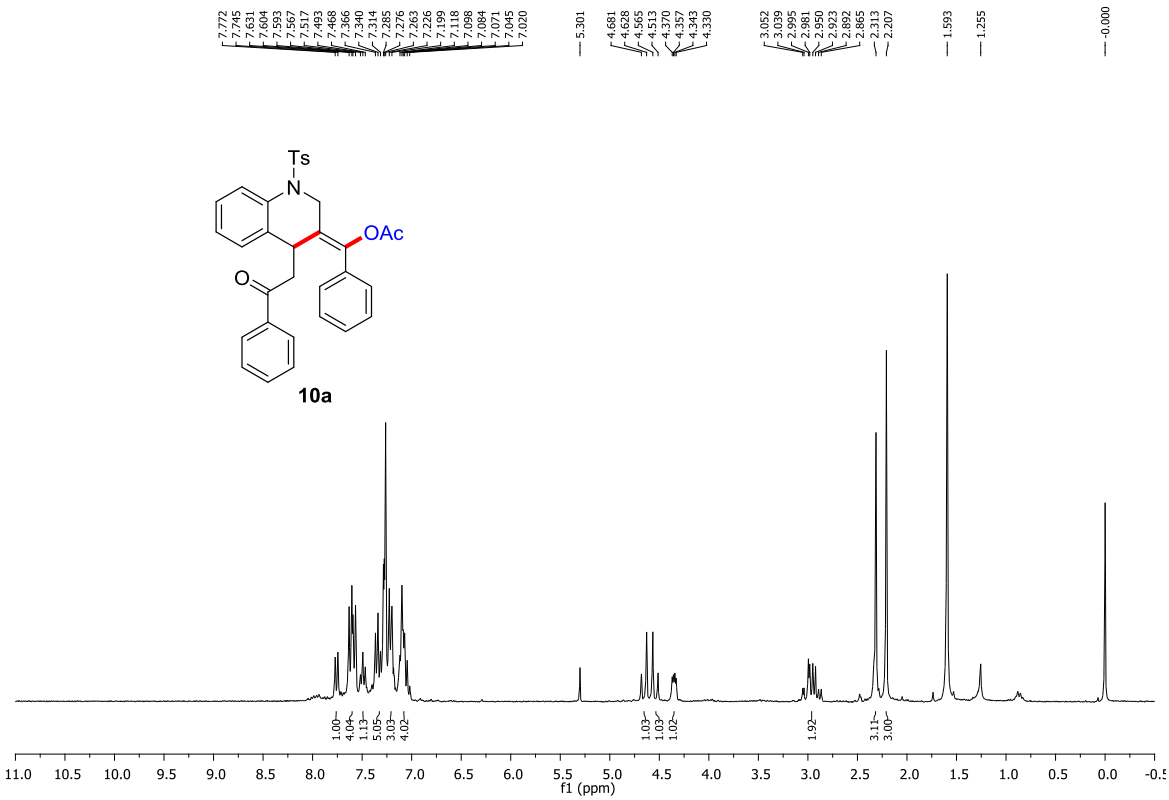
21.66
21.60
12.64
Ts
N
Br
Et
Cl
O
Me
9j
f1 (ppm)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7.071
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4.370
4.357
4.343
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3.039
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2.865
2.313
2.207
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0.000
Ts
N
OAc
O
10a
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3.03
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1.03
1.03
1.02
1.92
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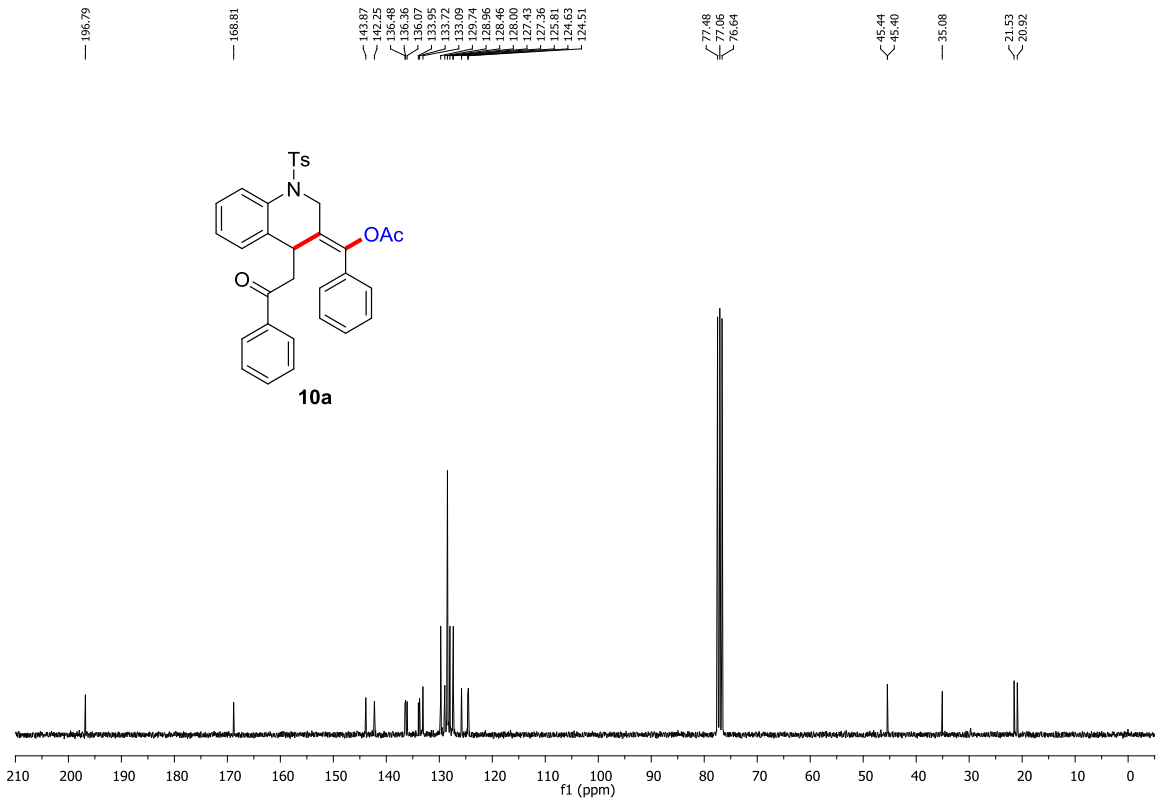
f1 (ppm)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128.00
127.43
127.36
125.81
124.63
124.51
77.48
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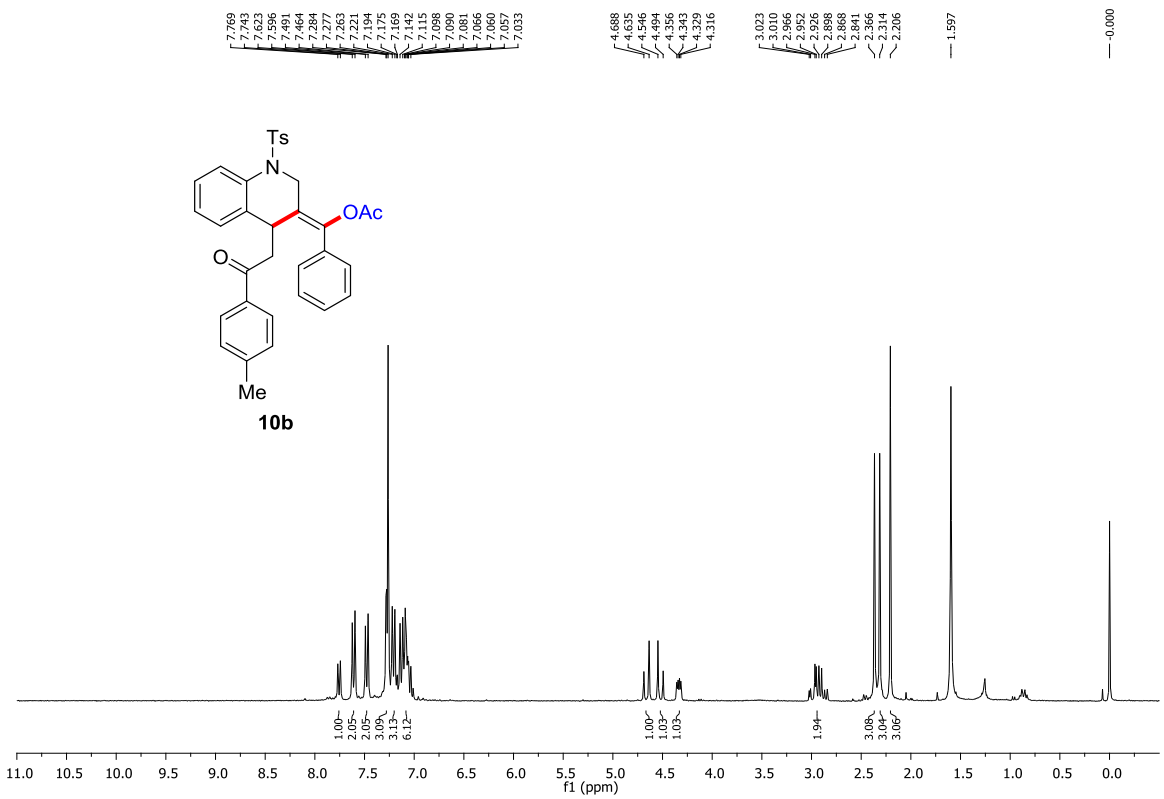
45.40
35.08
21.53
20.92
Ts
N
OAc
O
10a
f1 (ppm)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7.081
7.066
7.060
7.057
7.033
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0.000
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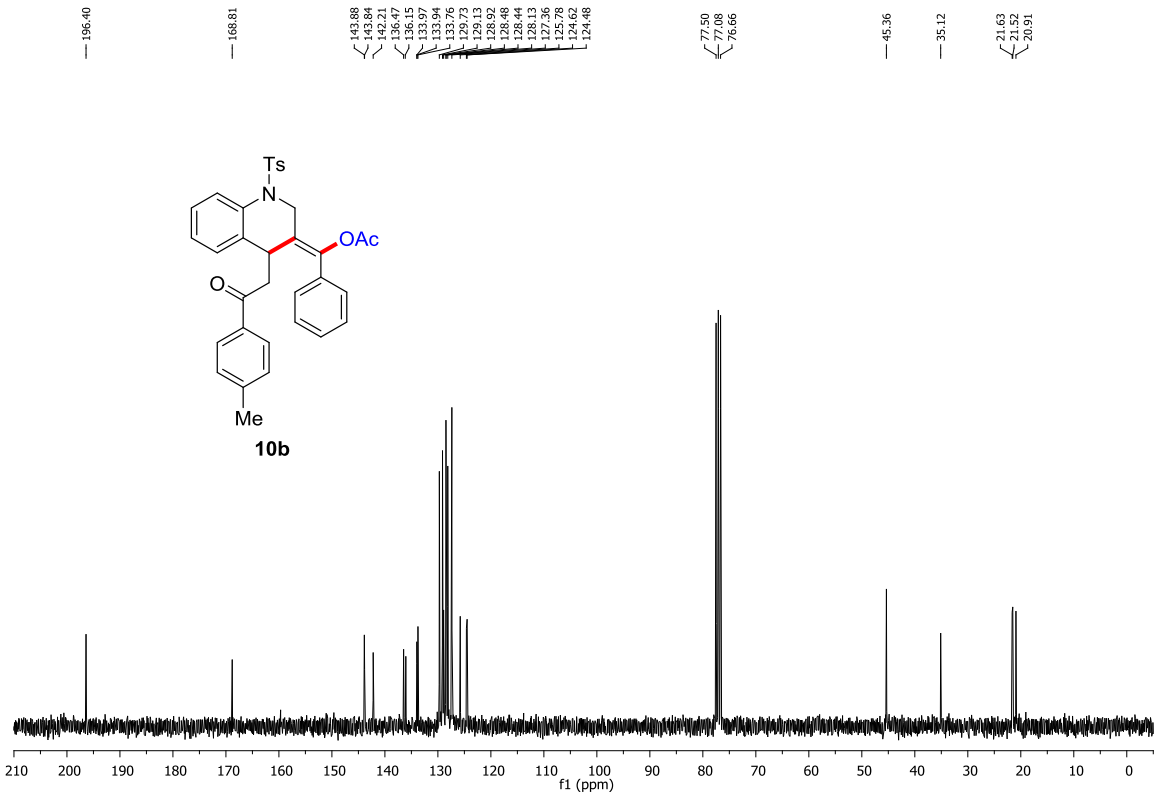
OAc
O
Me
10b
1.00
2.05
2.05
3.09
3.13
6.12
1.00
1.03
1.03
1.94
3.08
3.04
3.06
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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124.62
124.48
77.50
77.08
76.66
45.36
35.12
21.63
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OAc
O
Me
10b
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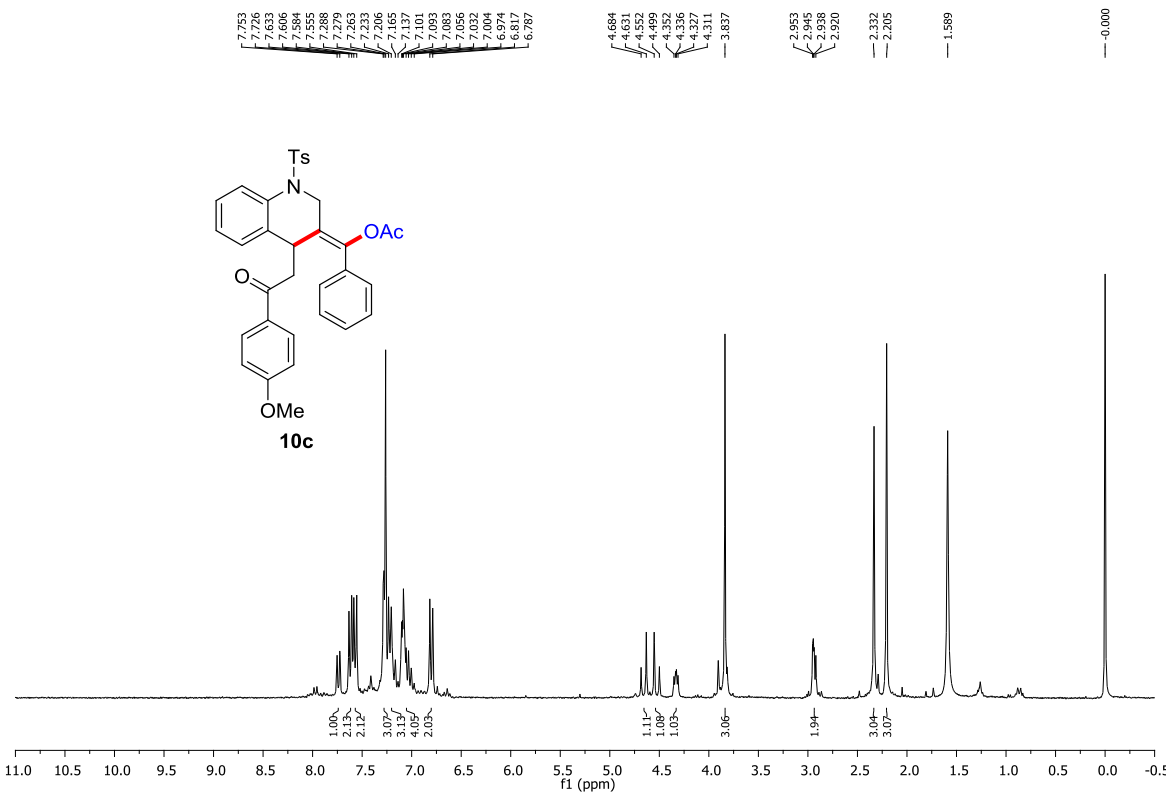
f1 (ppm)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2.332
2.205
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-0.000
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O
OMe
10c
1.00
2.13
2.12
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2.03
1.11
1.08
1.03
3.06
1.94
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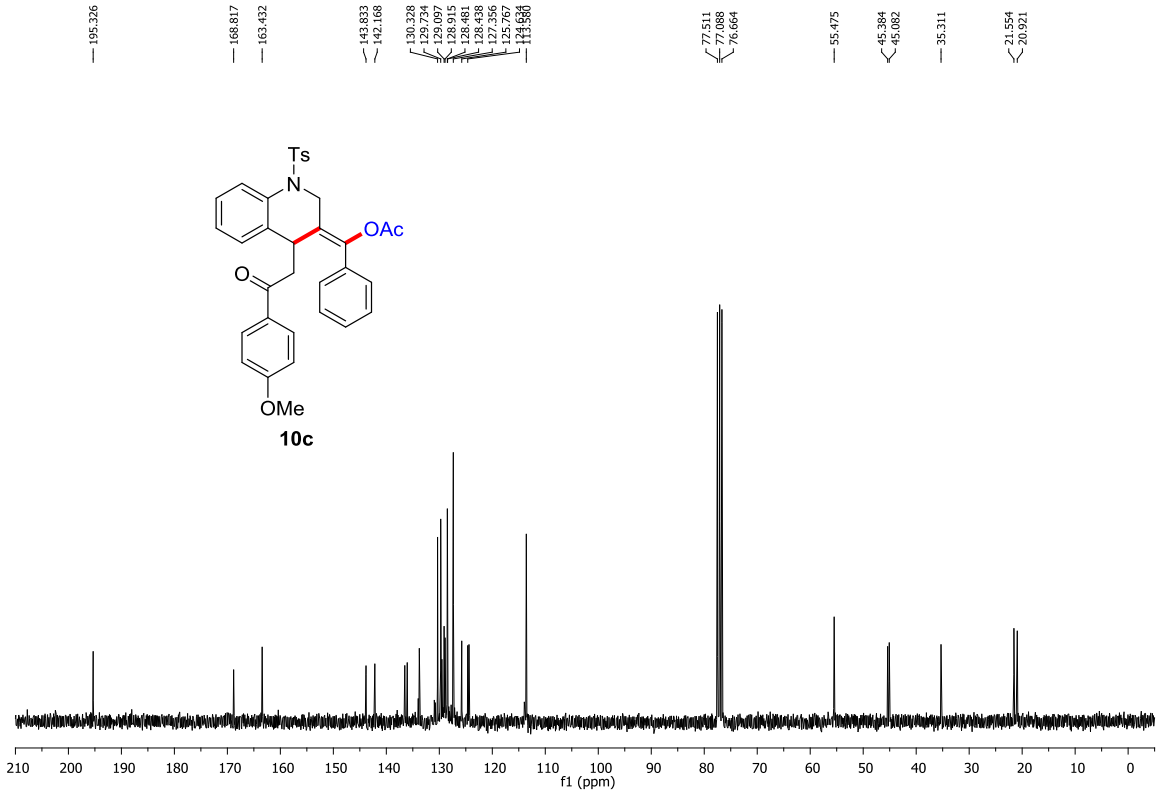
3.07
f1 (ppm)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77.088
76.664
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35.311
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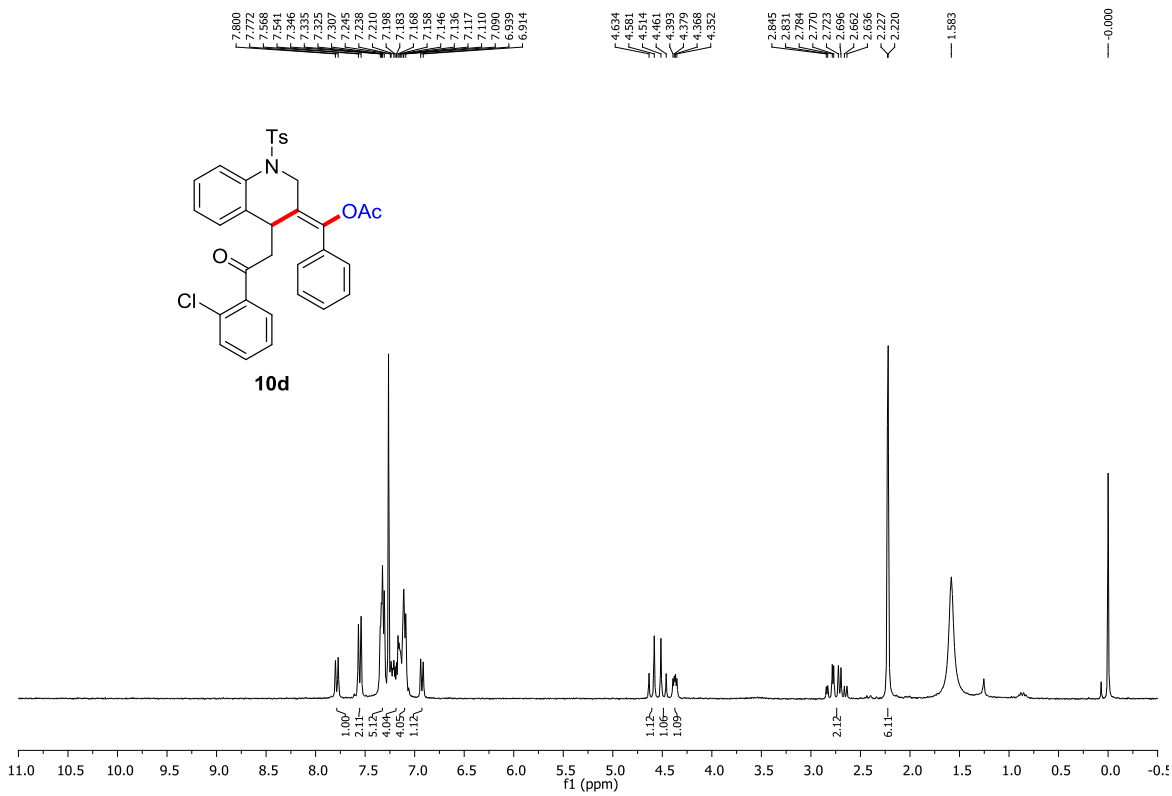
Ts
N
OAc
O
OMe
10c
f1 (ppm)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7.168
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7.110
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6.914
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2.220
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-0.000
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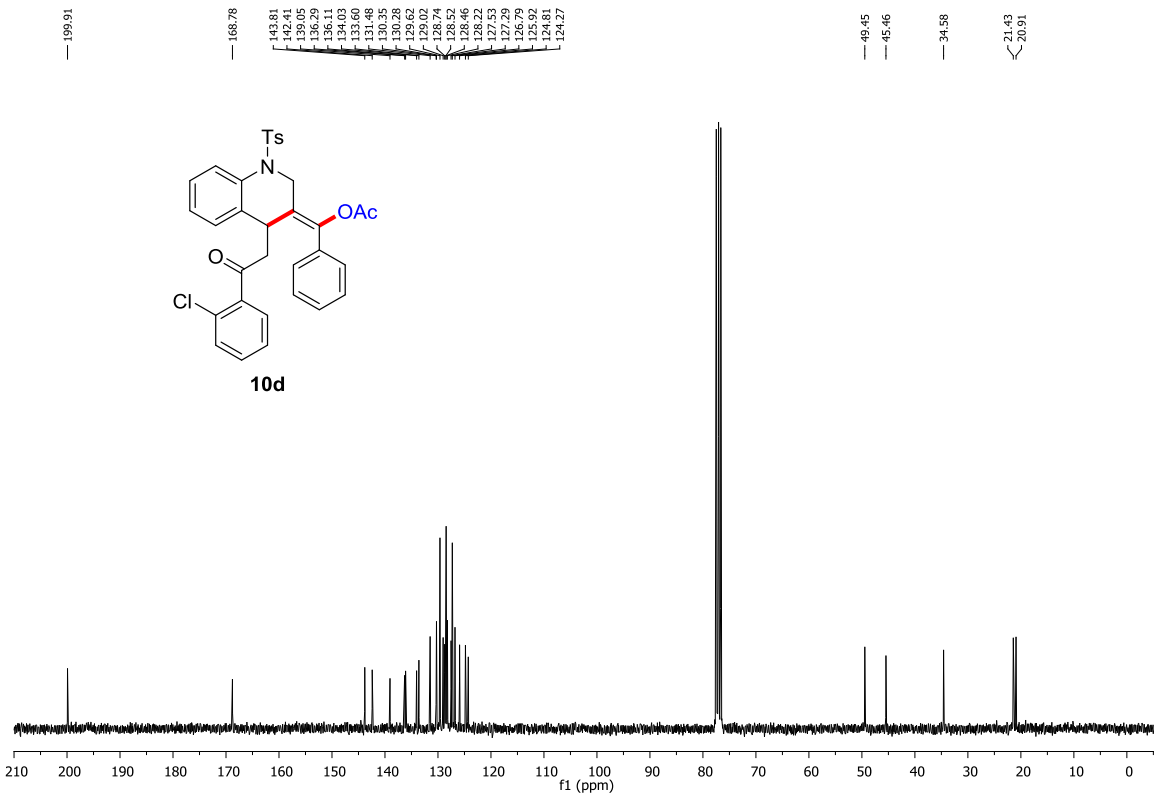
OAc
O
Cl
10d
1.00
2.11
5.13
4.04
4.05
1.12
1.12
1.06
1.09
2.12
6.11
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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124.27
49.45
45.46
34.58
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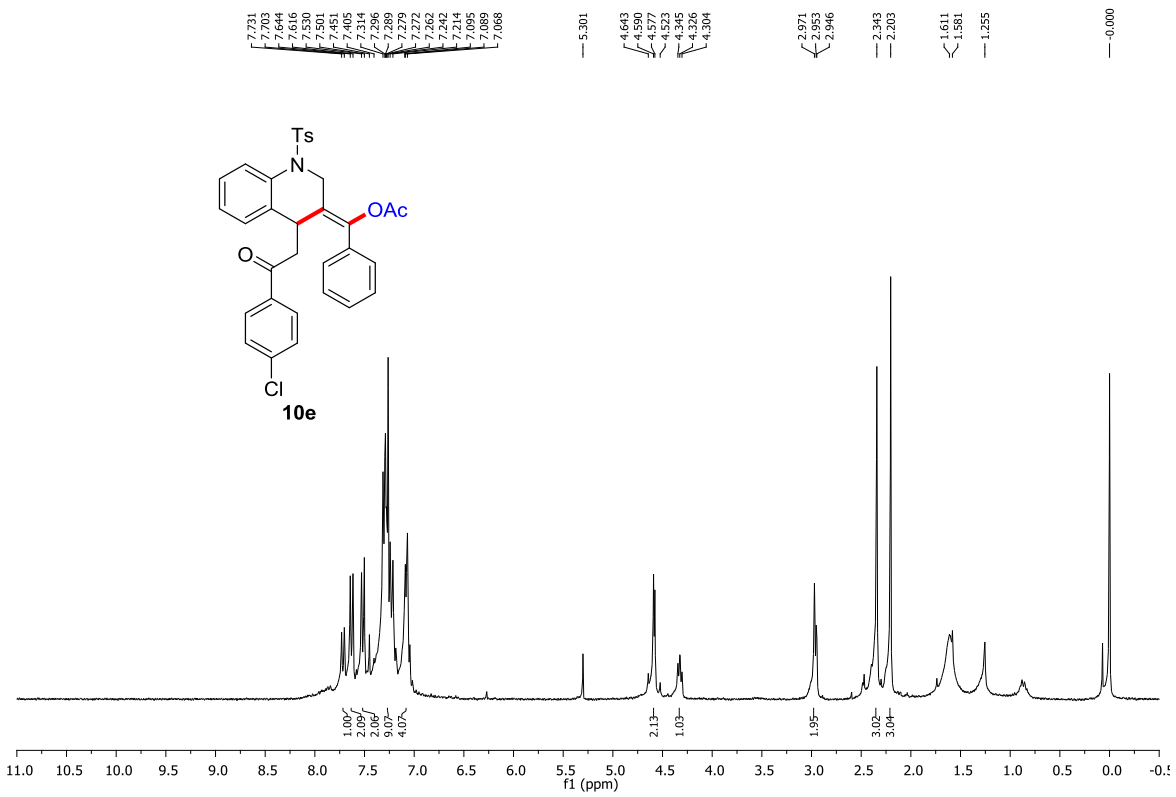
OAc
O
Cl
10d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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4.345
4.326
4.304
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2.953
2.946
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1.611
1.581
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OAc
O
Cl
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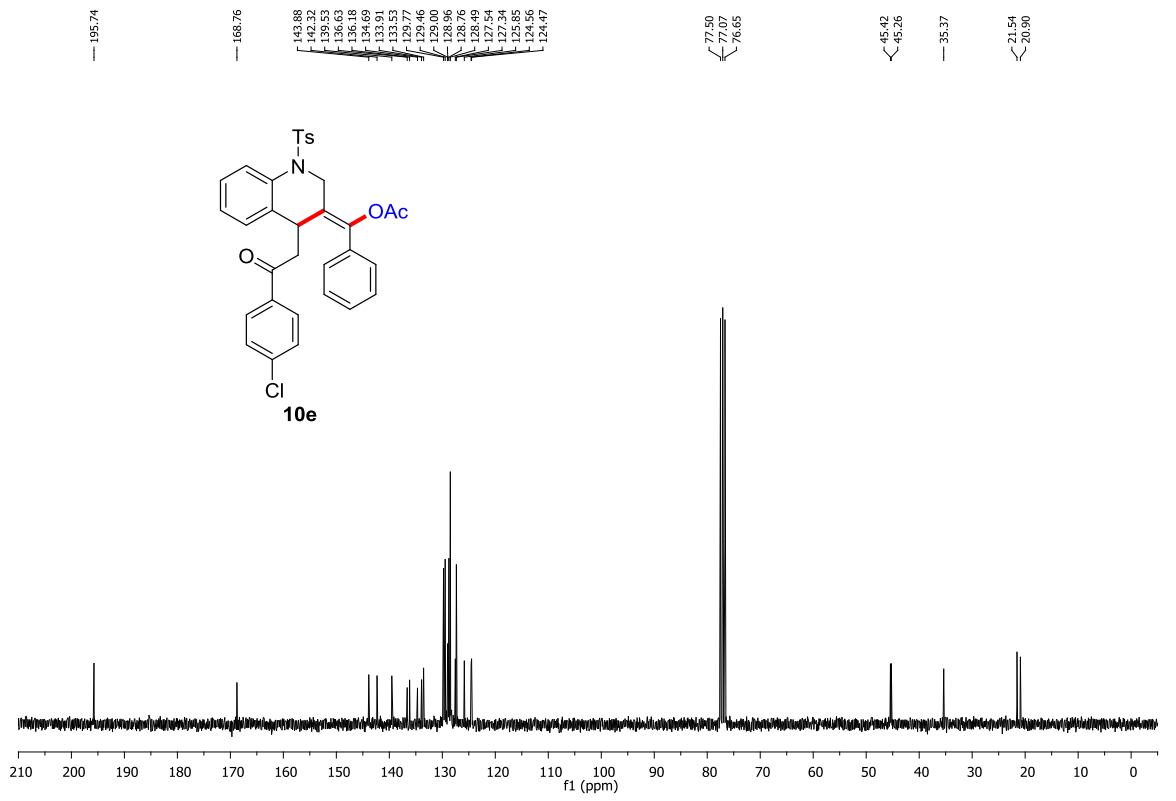
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128.49
127.54
127.34
125.85
124.56
124.47
77.50
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45.26
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21.54
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Ts
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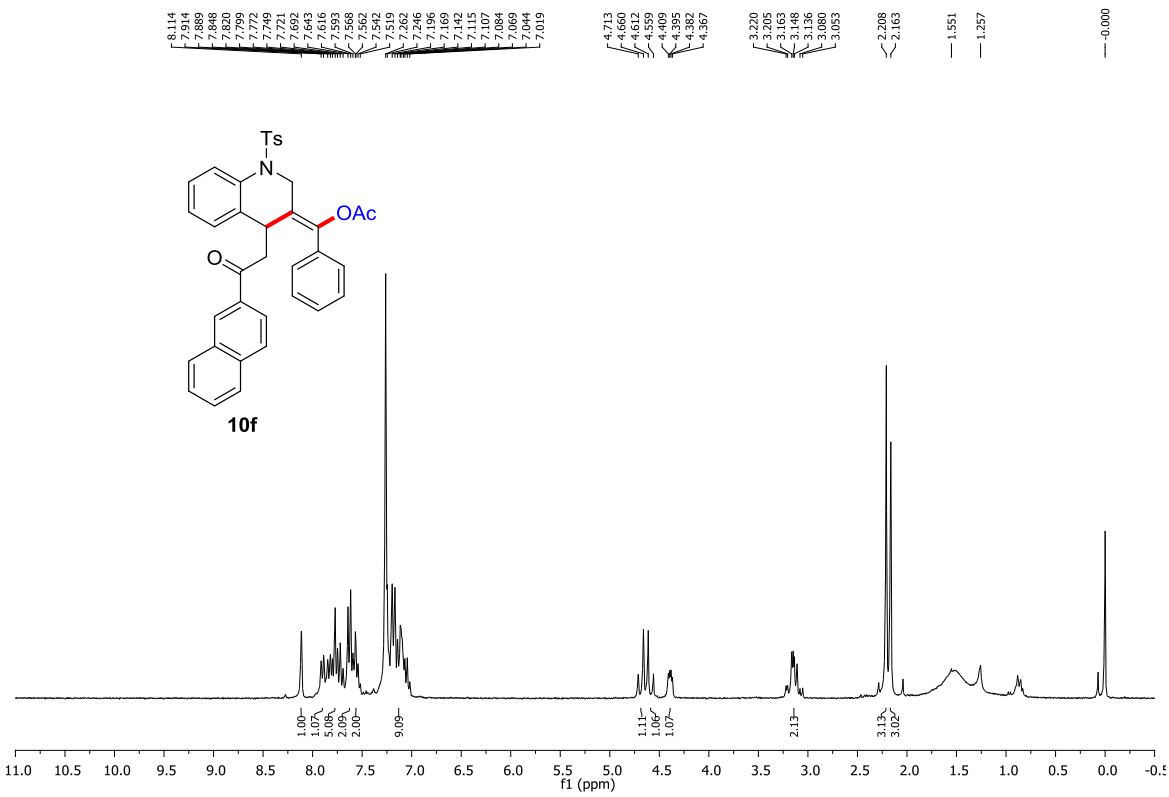
OAc
O
Cl
10e
f1 (ppm)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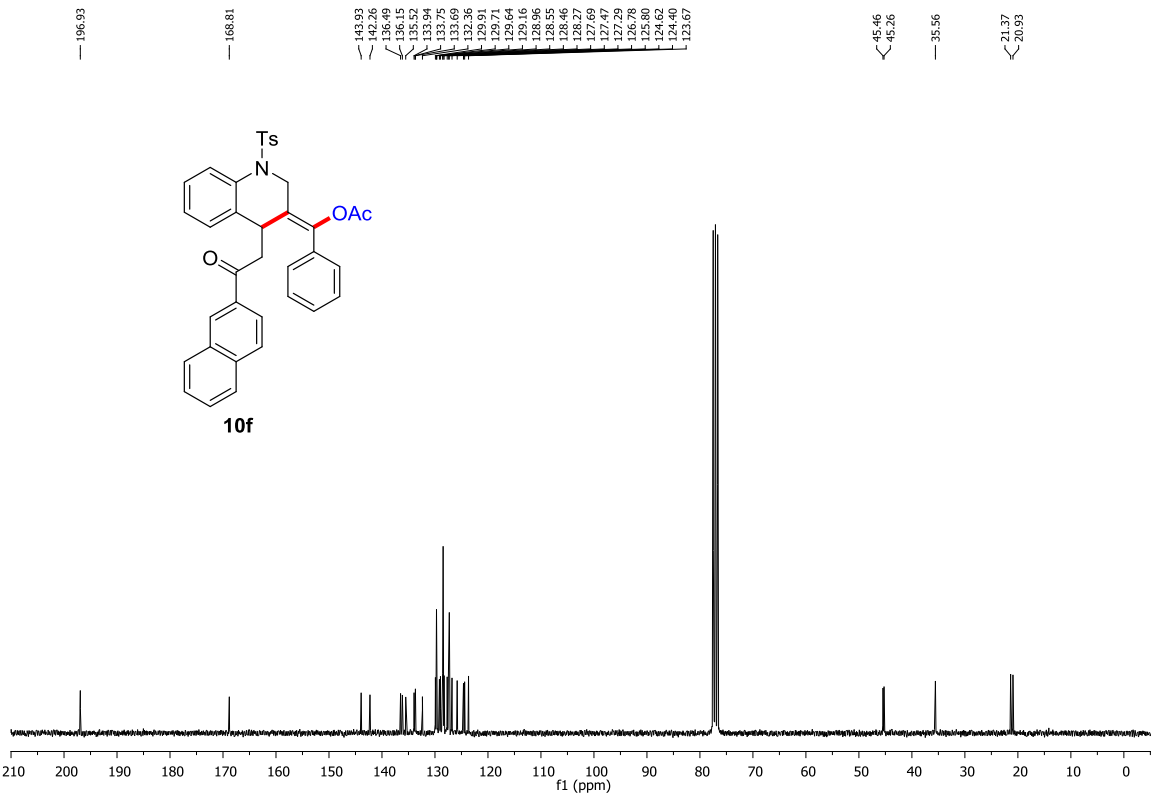
10f
f1 (ppm)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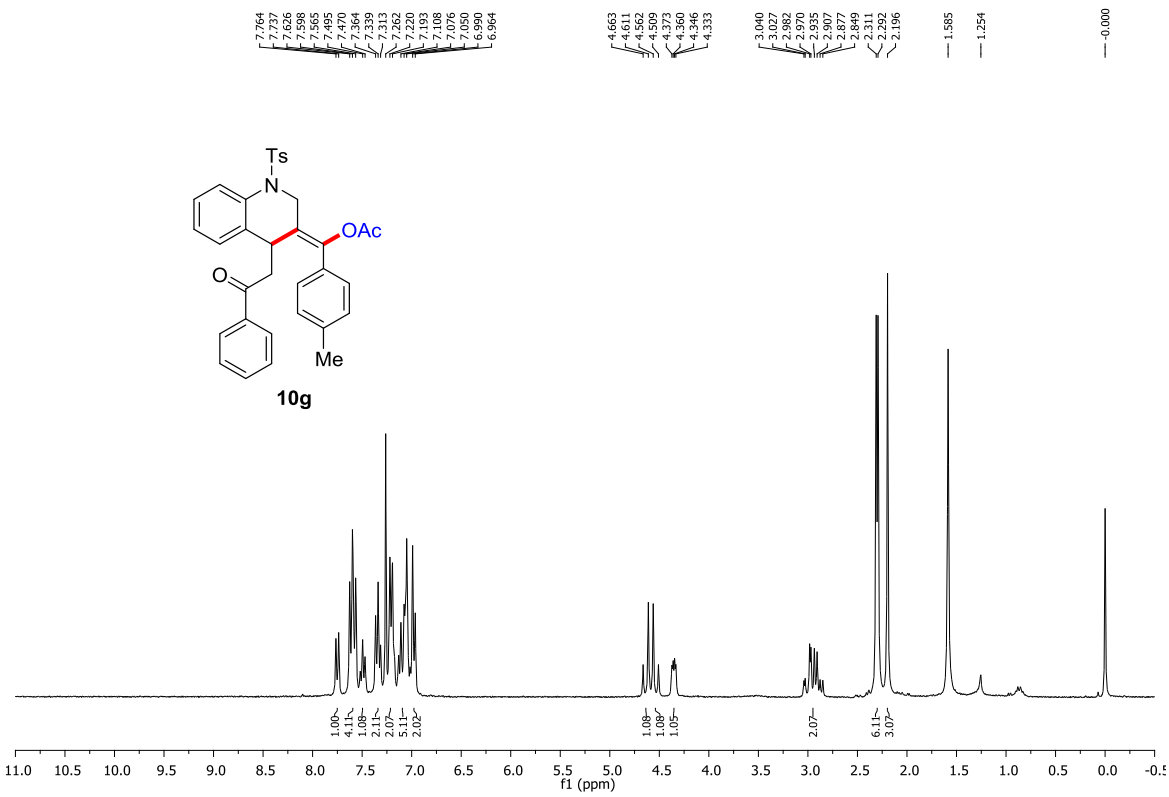
f1 (ppm)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7.050
6.990
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1.254
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N
OAc
O
Me
10g
1.00
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1.08
2.11
2.07
5.11
2.02
1.08
1.08
1.05
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6.11
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6.5
6.0
5.5
5.0
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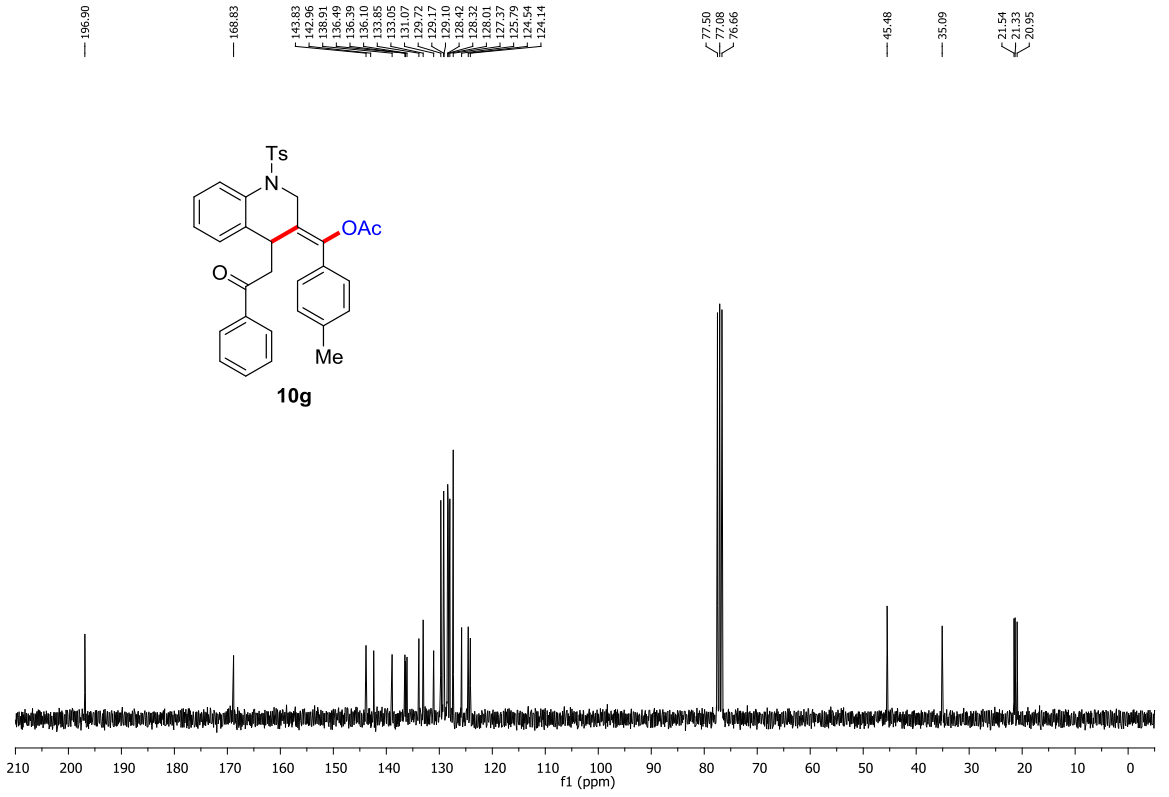
f1 (ppm)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136.39
136.10
133.85
133.05
131.07
129.72
129.17
129.10
128.42
128.32
128.01
127.37
125.79
124.54
124.14
77.50
77.08
76.66
45.48
35.09
21.54
21.33
20.95
Ts
N
OAc
O
Me
10g
210
200
190
180
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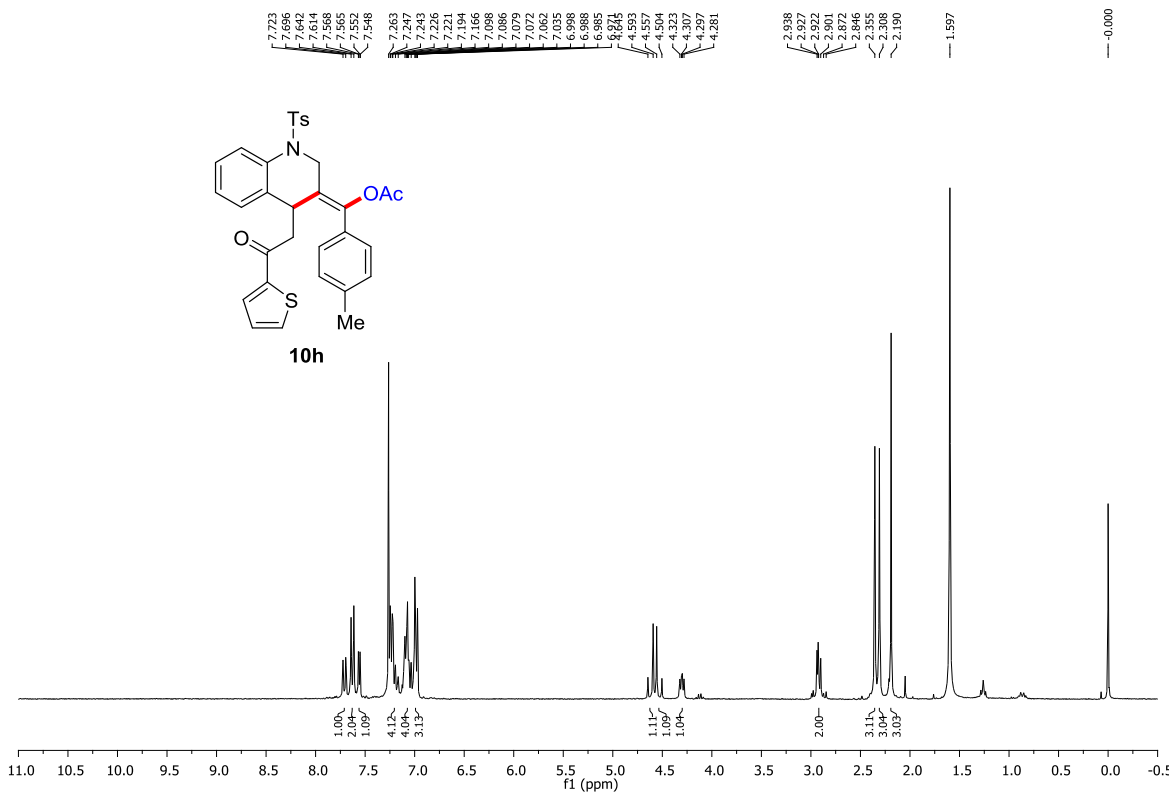
Ts
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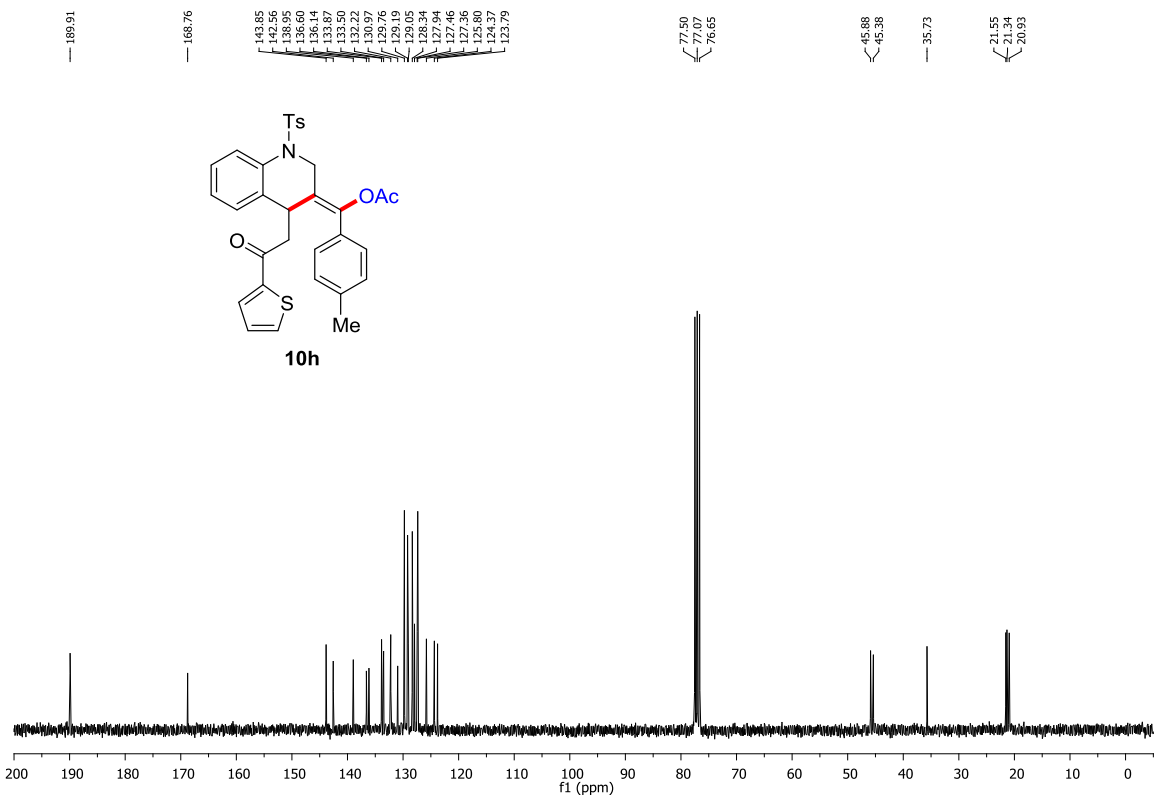
O
S
Me
10h
f1 (ppm)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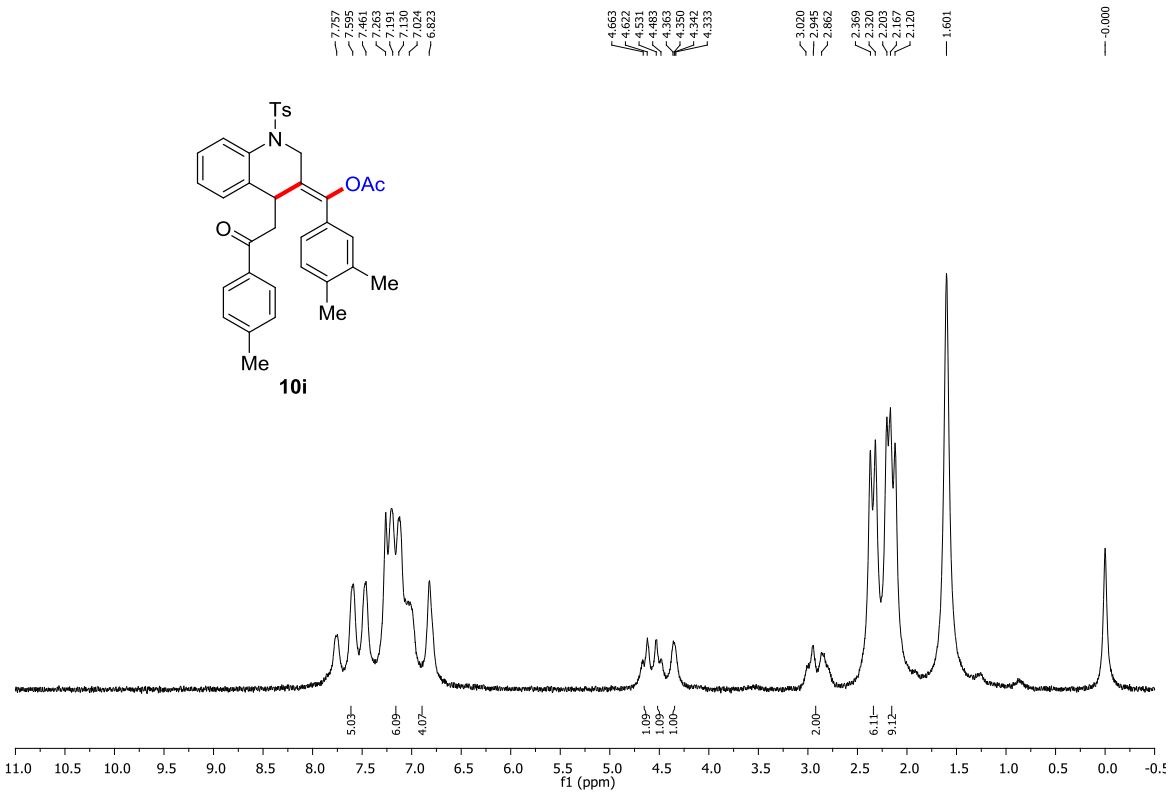
O
S
Me
10h
f1 (ppm)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4.350
4.342
4.333
3.020
2.945
2.862
2.369
2.320
2.203
2.167
2.120
1.601
-0.000
Ts
N
OAc
O
Me
Me
Me
10i
5.03
6.09
4.07
1.09
1.09
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2.00
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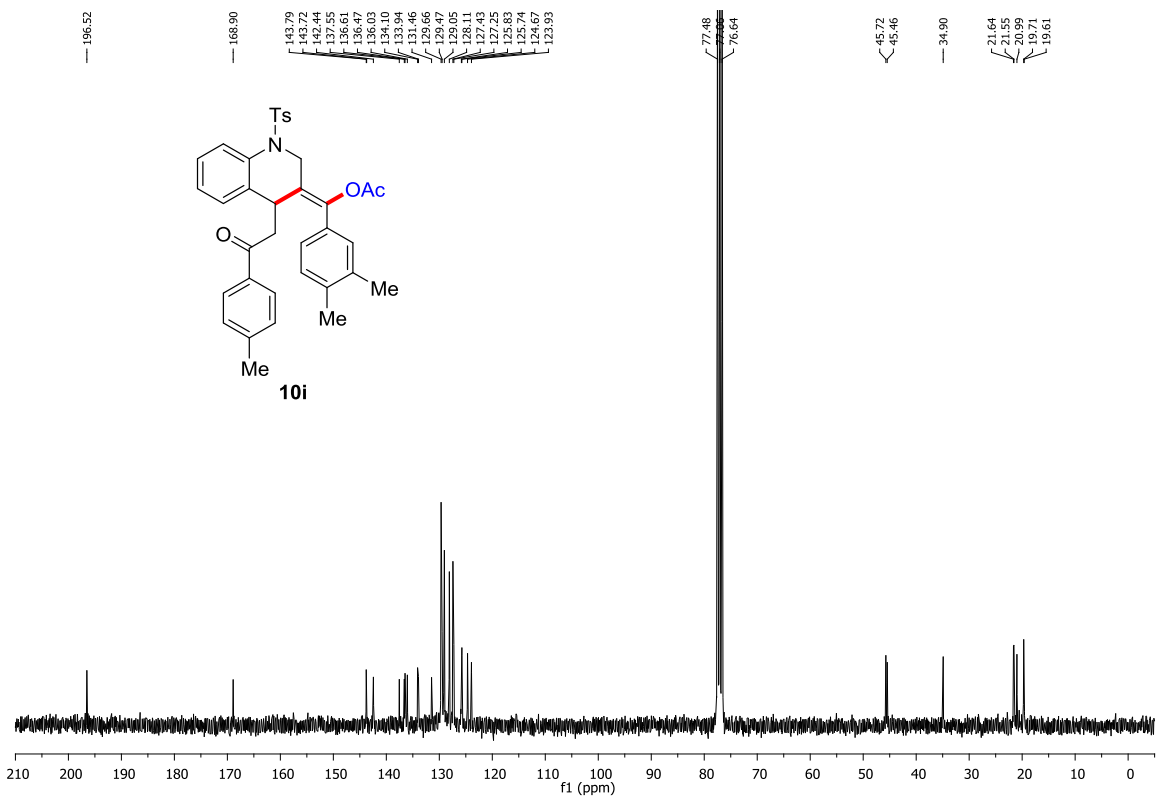
9.12
f1 (ppm)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134.10
134.04
131.46
129.66
129.47
129.05
128.11
127.43
127.25
125.83
125.74
124.67
123.93
77.48
77.16
76.84
76.64
45.72
45.46
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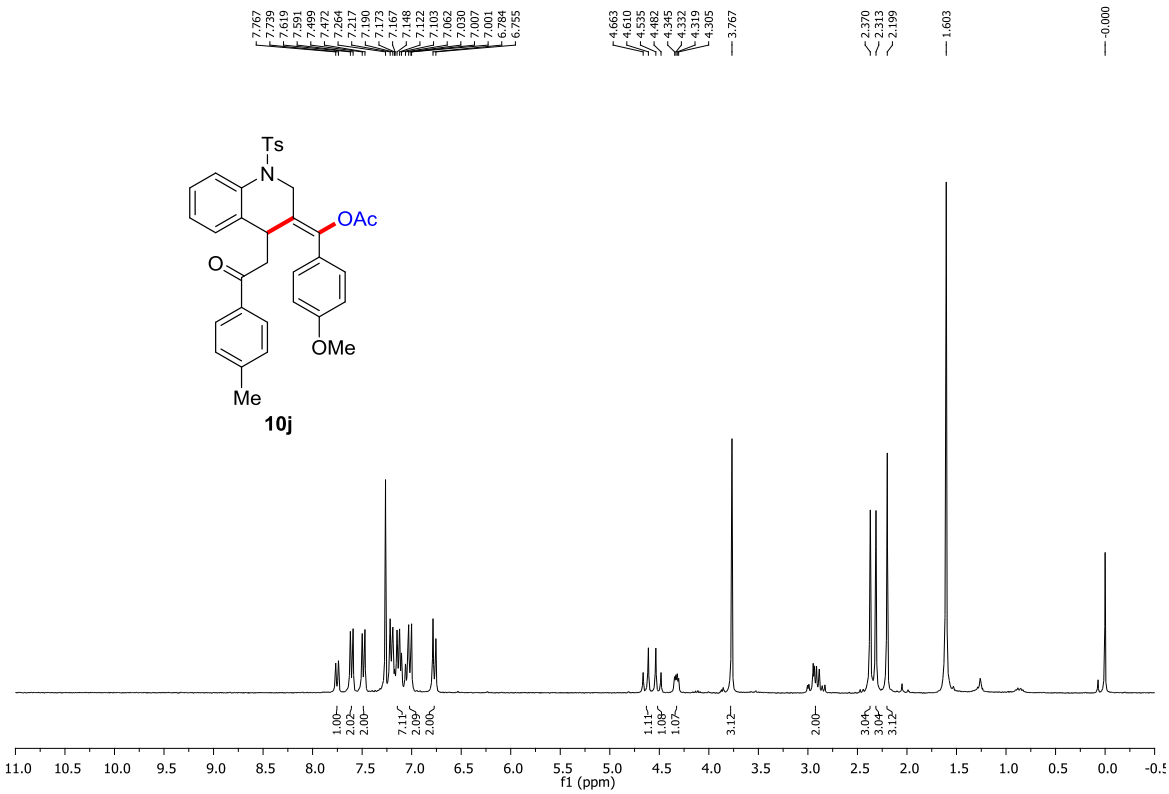
20.99
19.71
19.61
Ts
N
OAc
O
Me
Me
Me
10i
f1 (ppm)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7.217
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7.173
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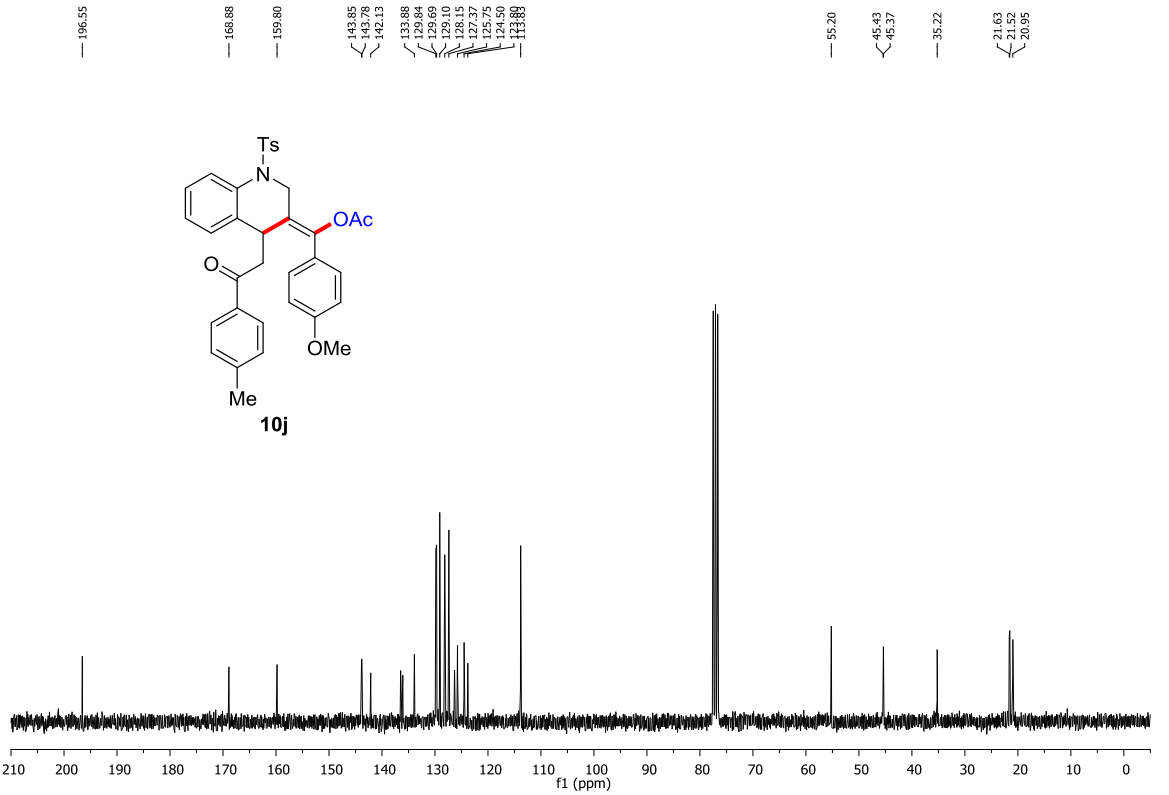
7.148
7.122
7.103
7.062
7.030
7.007
7.001
6.784
6.755
4.663
4.610
4.535
4.482
4.345
4.332
4.319
4.305
3.767
2.370
2.313
2.199
1.603
-0.000
Ts
N
OAc
O
OMe
Me
10j
1.00
2.02
2.00
7.11
2.09
2.00
1.11
1.08
1.07
3.12
2.00
3.04
3.04
3.12
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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142.13
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129.84
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128.15
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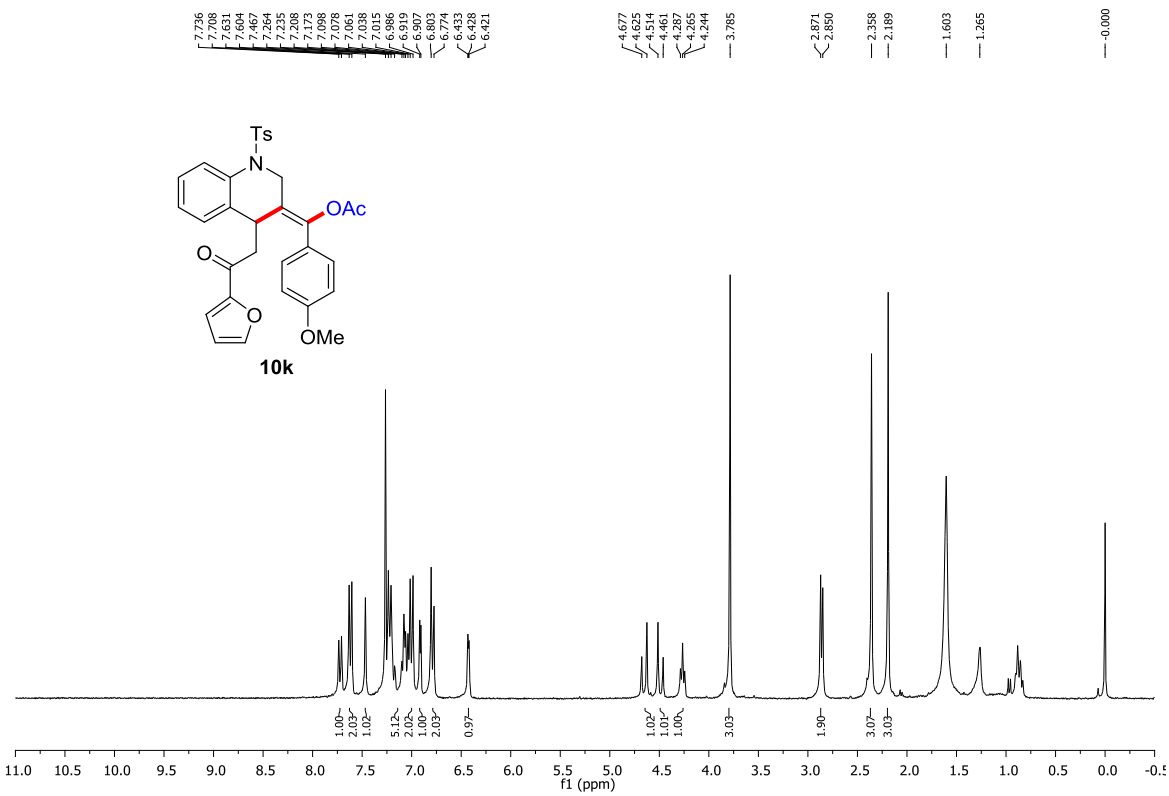
125.75
124.50
55.20
45.43
45.37
35.22
21.63
21.52
20.95
Ts
N
OAc
O
OMe
Me
10j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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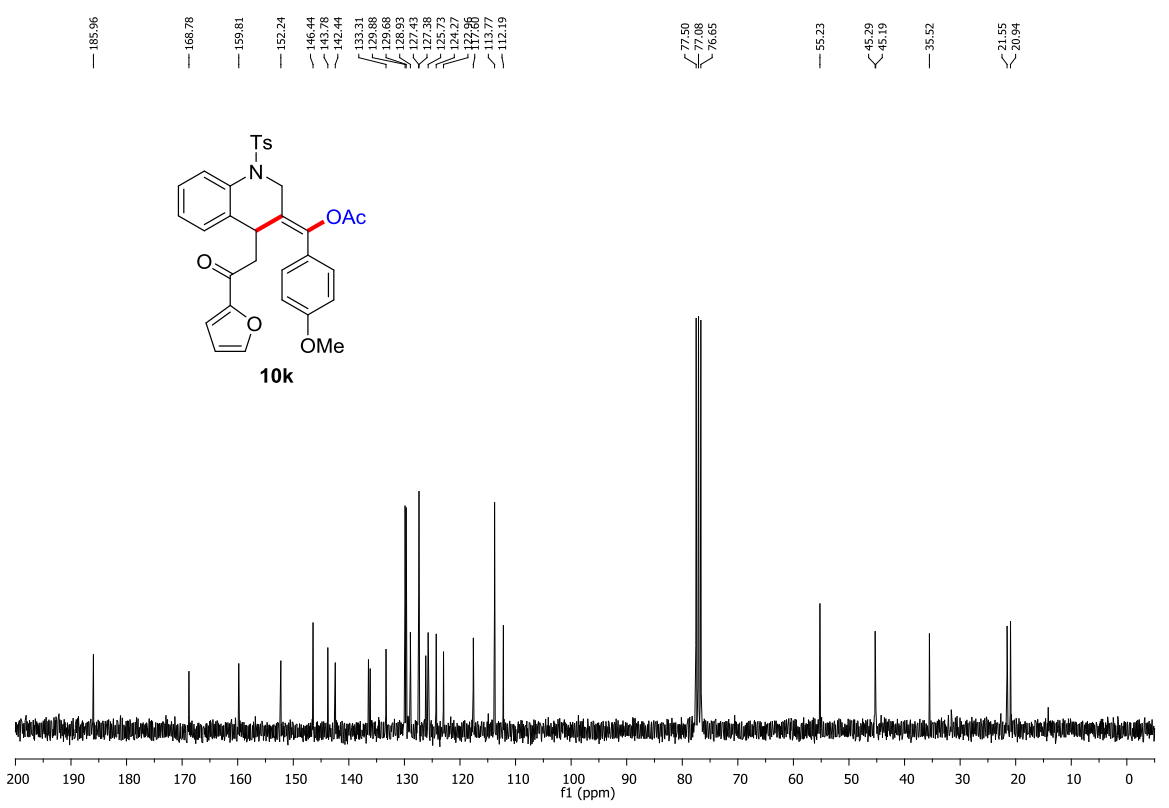
7.038
7.015
6.986
6.919
6.907
6.803
6.774
6.433
6.428
6.421
4.677
4.625
4.514
4.461
4.287
4.265
4.244
3.785
2.871
2.850
2.358
2.189
1.603
1.265
-0.000
Ts
N
OAc
O
O
OMe
10k
1.00
2.03
1.02
5.12
2.02
1.00
2.03
0.97
1.03
1.01
1.00
3.03
1.90
3.07
3.03
f1 (ppm)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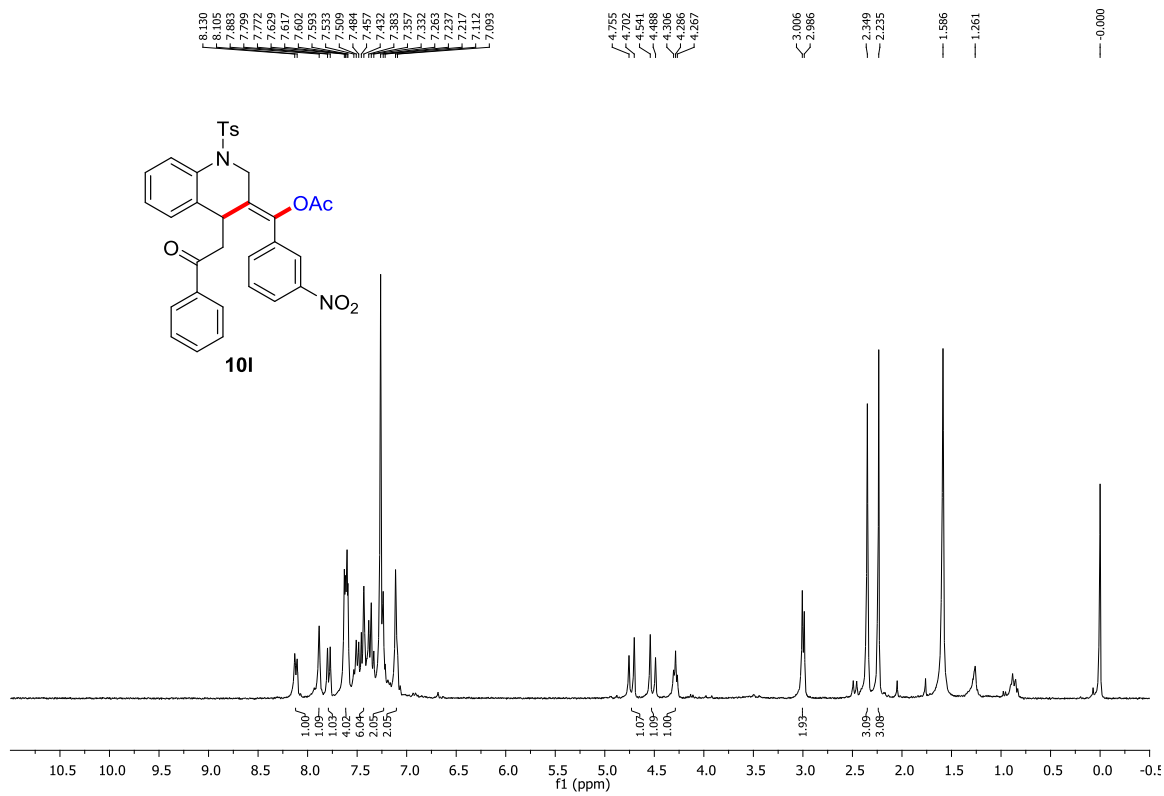
168.78
159.81
152.24
146.44
143.78
142.44
133.31
129.88
129.68
128.93
127.43
127.38
125.73
124.27
113.77
112.19
77.50
77.08
76.65
55.23
45.29
45.19
35.52
21.55
20.94
Ts
N
OAc
O
O
OMe
10k
f1 (ppm)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8.105
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7.772
7.629
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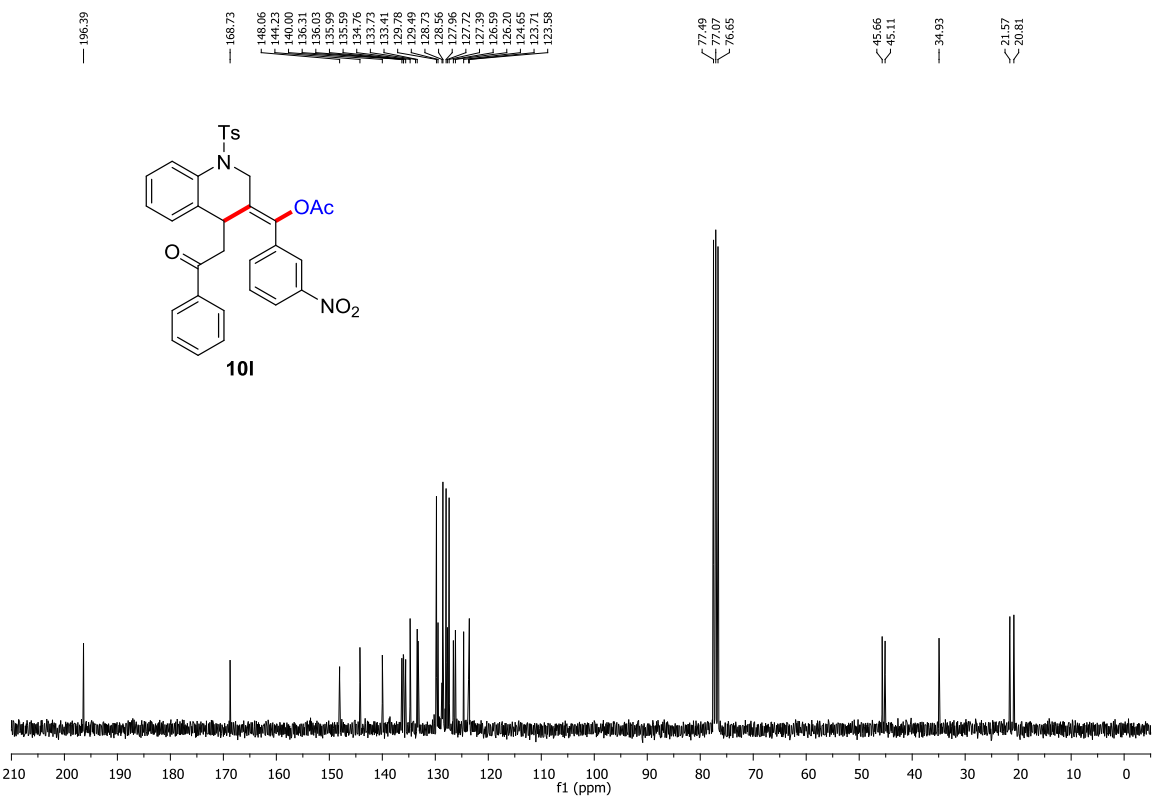
7.602
7.593
7.533
7.509
7.484
7.457
7.432
7.383
7.357
7.332
7.263
7.237
7.217
7.112
7.093
4.755
4.702
4.541
4.488
4.306
4.286
4.267
3.006
2.986
2.349
2.235
1.586
1.261
-0.000
Ts
N
OAc
O
NO2
10l
1.00
1.09
1.03
4.02
6.04
2.05
2.05
1.07
1.09
1.00
1.93
3.09
3.08
f1 (ppm)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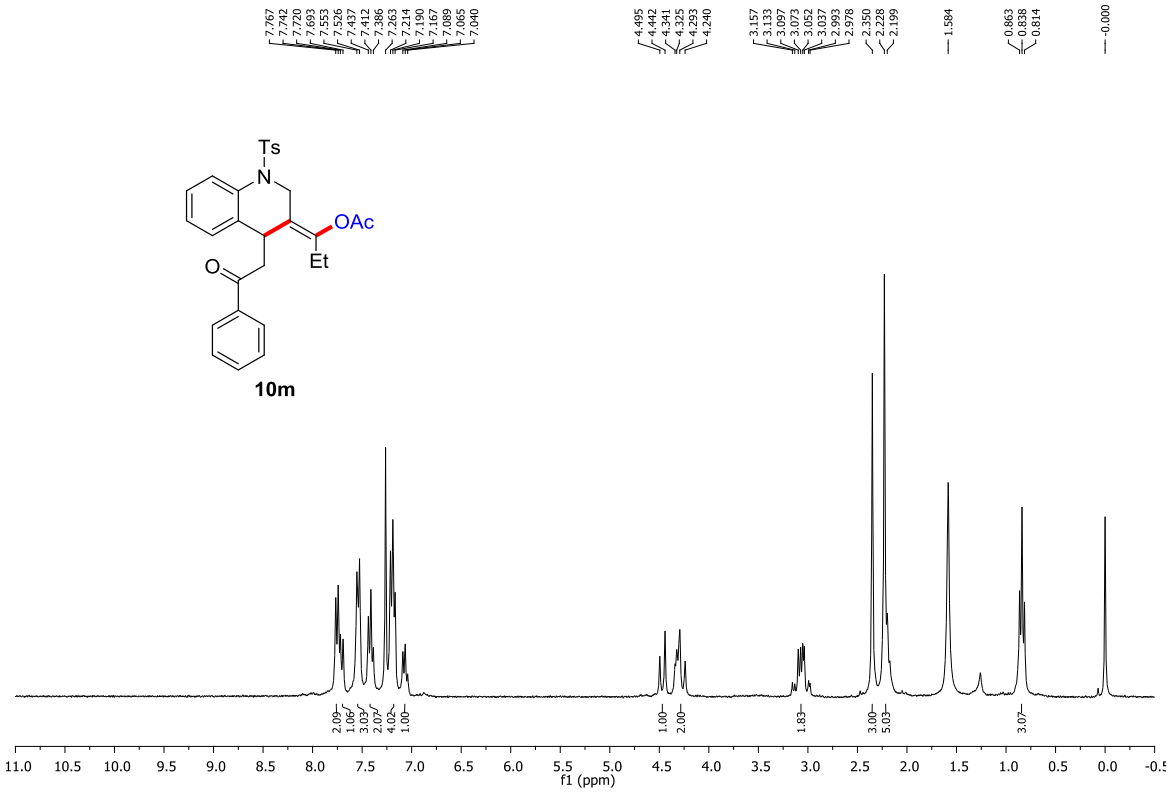
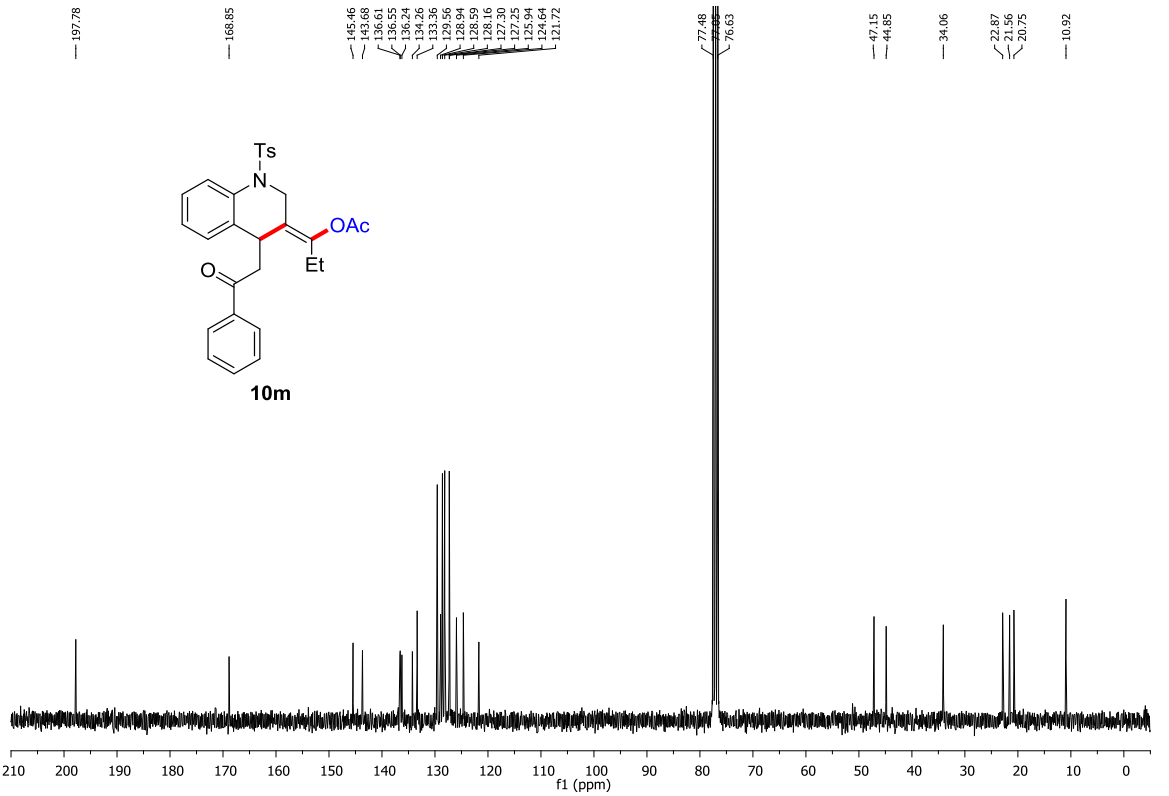
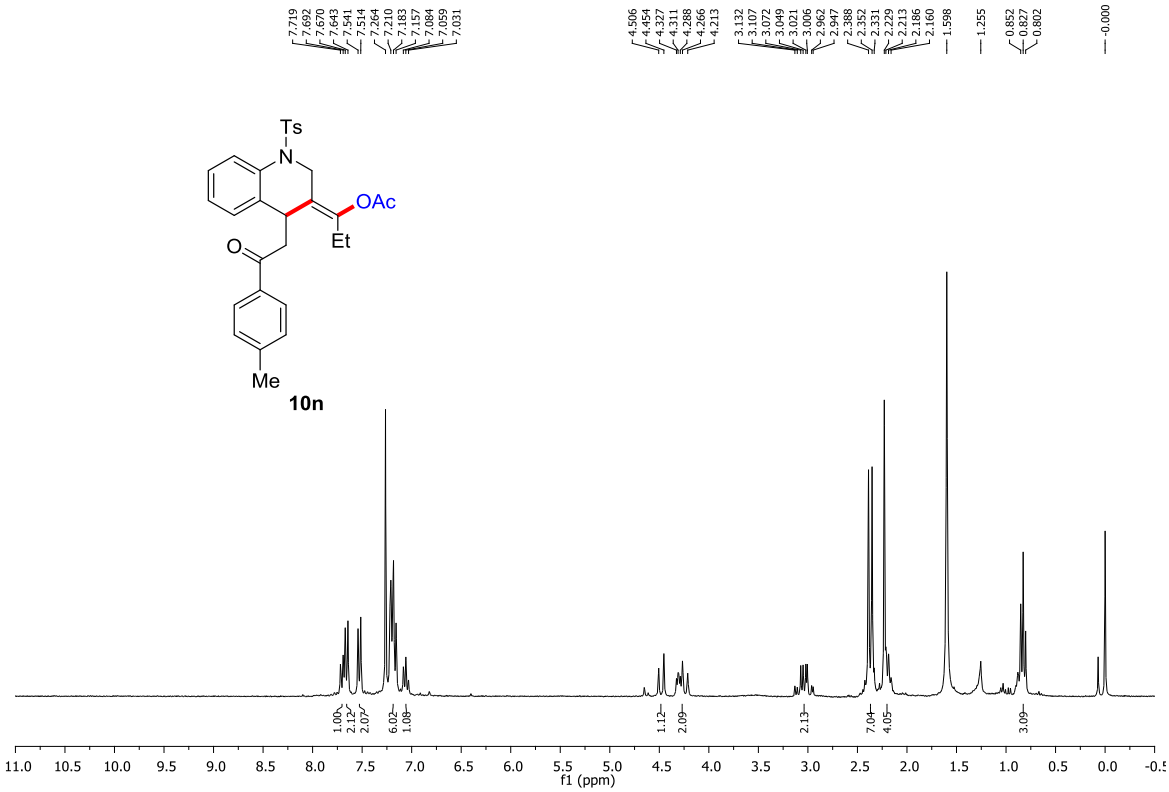
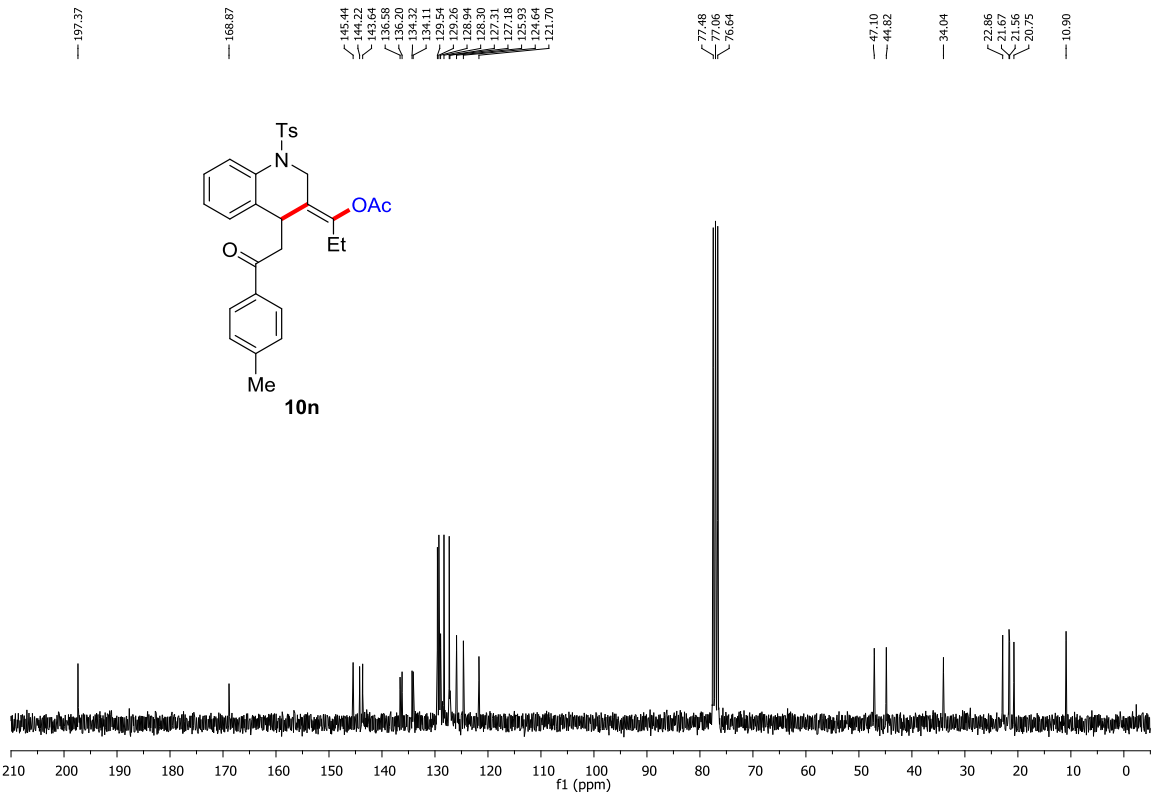
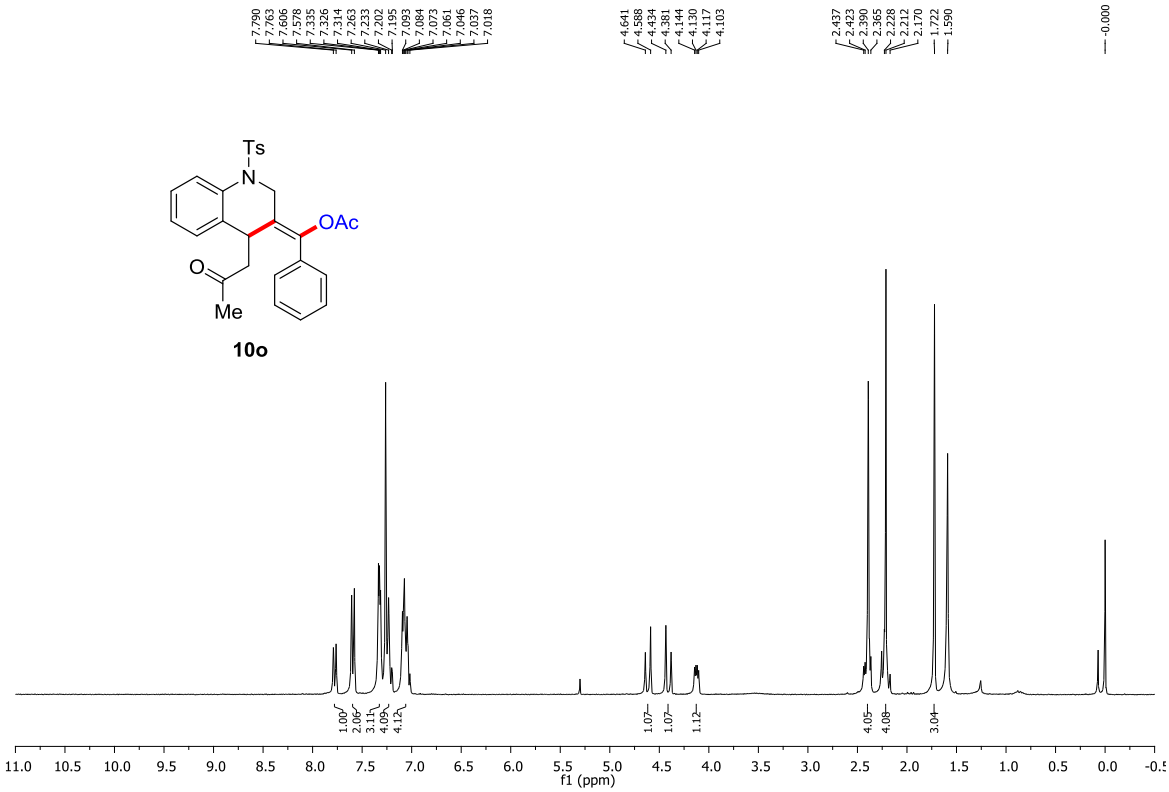
148.06
144.23
140.00
136.31
136.03
135.99
135.59
134.76
133.73
133.41
129.78
129.49
128.73
128.56
127.96
127.72
127.39
126.59
126.20
124.65
123.71
123.58
77.49
77.07
76.65
45.66
45.11
34.93
21.57
20.81
Ts
N
OAc
O
NO2
10l
f1 (ppm)


Ts
N
OAc
Et
O
10m
f1 (ppm)


Ts
N
OAc
Et
O
10m
f1 (ppm)


Ts
N
OAc
Et
O
Me
10n
f1 (ppm)


Ts
N
OAc
Et
O
Me
10n
f1 (ppm)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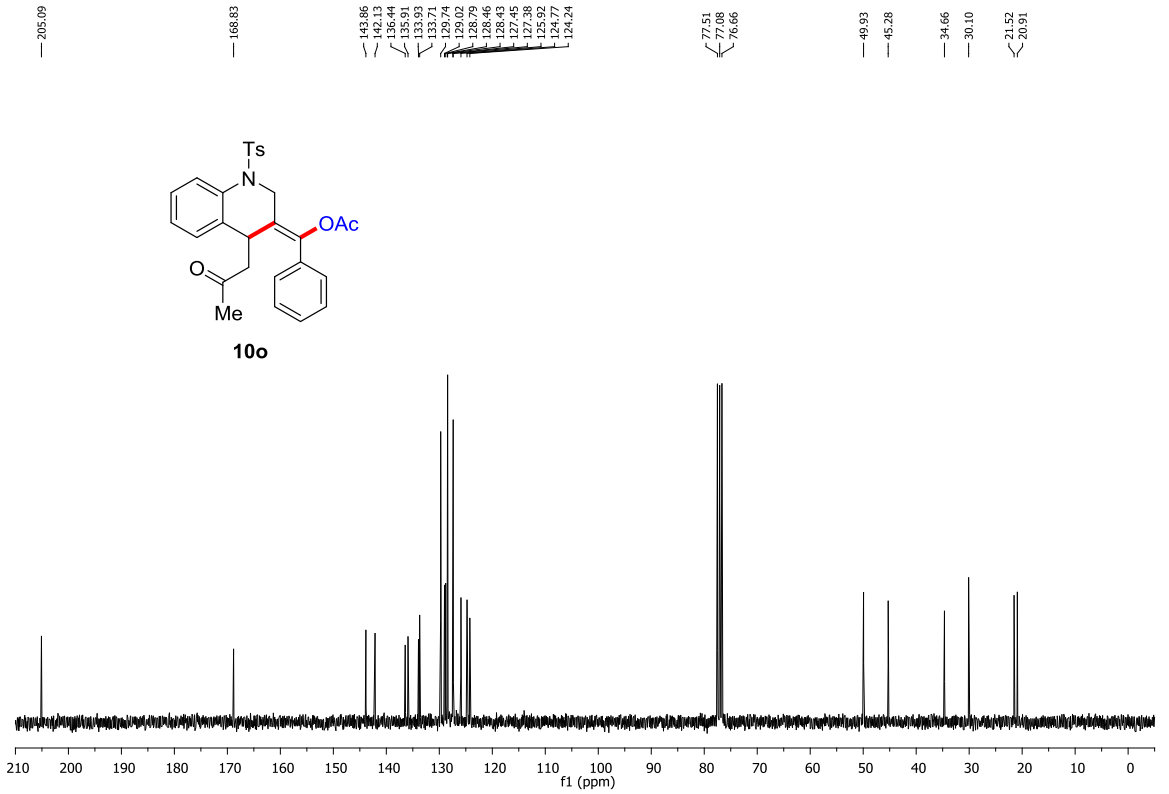
7.093
7.084
7.073
7.061
7.046
7.037
7.018
4.641
4.588
4.434
4.381
4.344
4.130
4.117
4.103
2.437
2.423
2.390
2.365
2.228
2.212
2.170
1.722
1.590
0.000
Ts
N
OAc
O
Me
10o
1.09
2.06
3.15
4.09
4.12
1.07
1.07
1.12
4.05
4.08
3.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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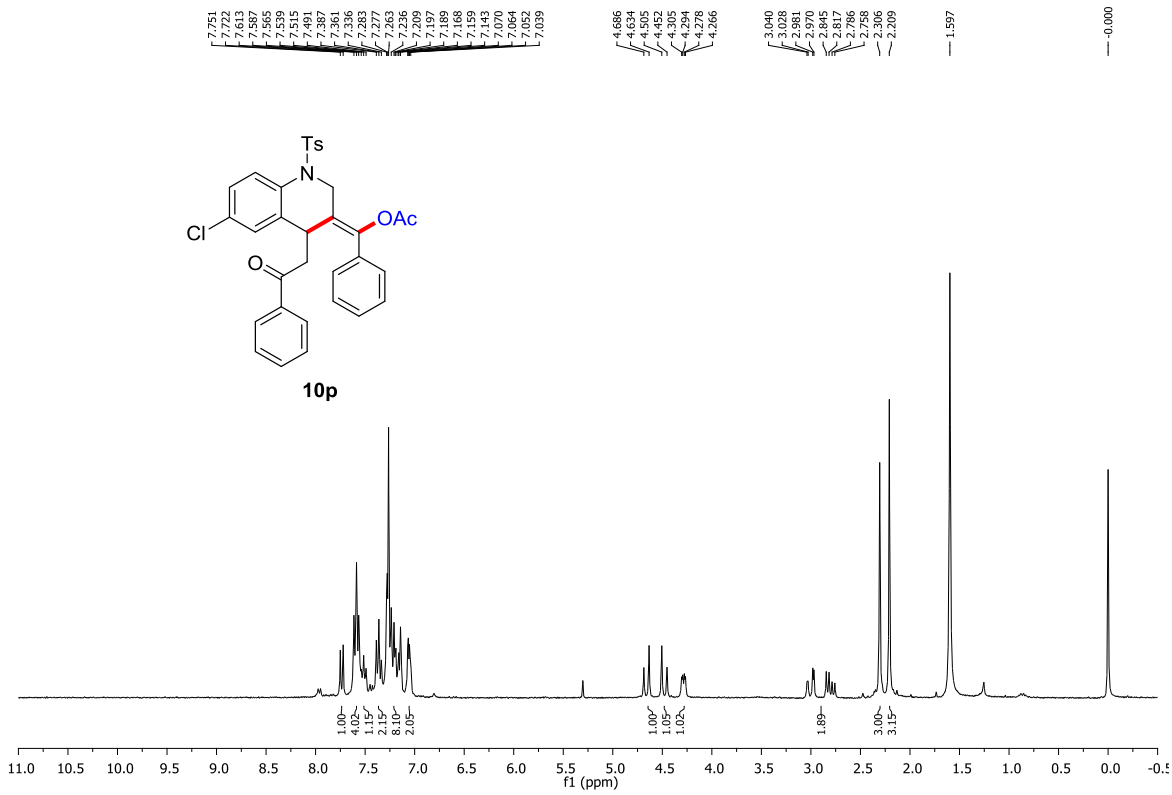
136.44
135.91
133.93
133.71
129.74
129.02
128.79
128.46
128.43
127.45
127.38
125.92
124.77
124.24
77.51
77.08
76.66
49.93
45.28
34.66
30.10
21.52
20.91
Ts
N
OAc
O
Me
10o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.277
7.263
7.236
7.209
7.197
7.188
7.168
7.159
7.143
7.070
7.064
7.052
7.039
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4.634
4.505
4.452
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4.278
4.266
3.040
3.028
2.981
2.970
2.845
2.817
2.786
2.758
2.306
2.209
1.597
-0.000
Ts
N
Cl
OAc
O
10p
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4.02
1.15
2.15
8.10
2.05
1.05
1.05
1.02
1.89
3.00
3.15
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10.5
10.0
9.5
9.0
8.5
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7.5
7.0
6.5
6.0
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5.0
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2.0
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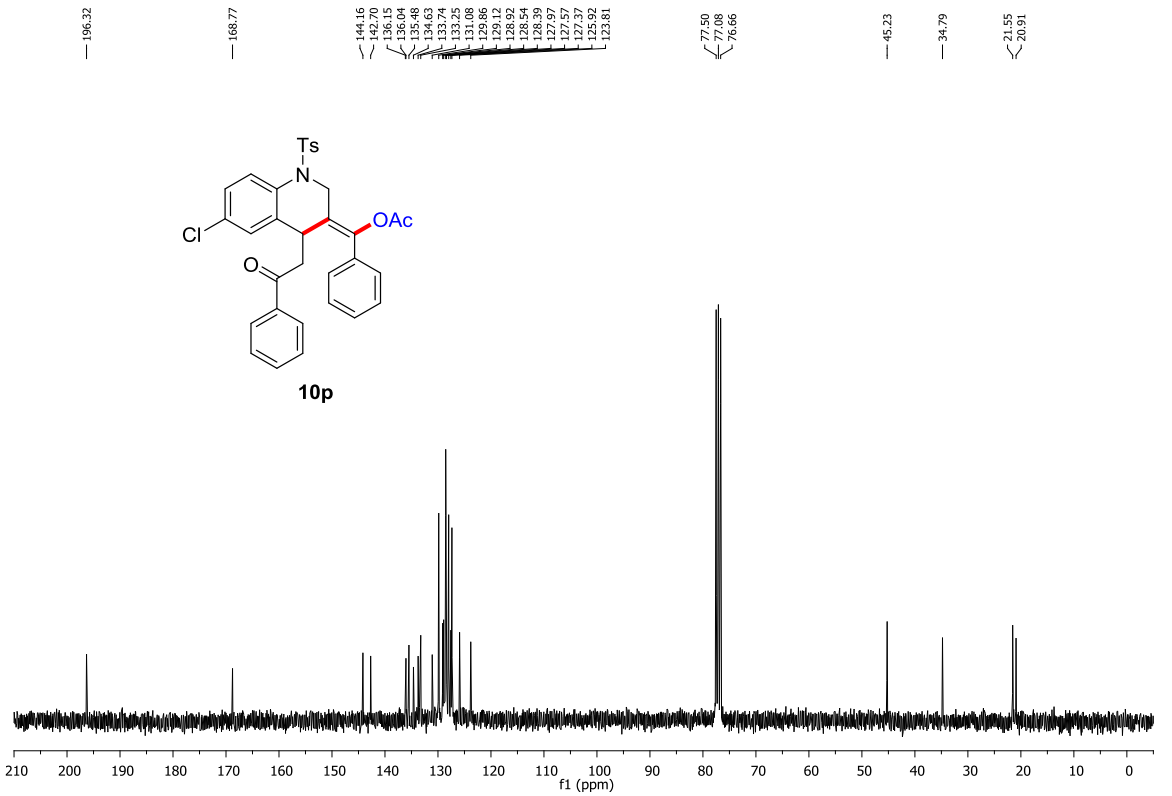
-0.5
f1 (ppm)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134.63
133.74
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131.08
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129.12
128.92
128.54
128.39
127.97
127.57
127.37
125.92
123.81
77.50
77.08
76.66
45.23
34.79
21.55
20.91
Ts
N
Cl
OAc
O
10p
210
200
190
180
170
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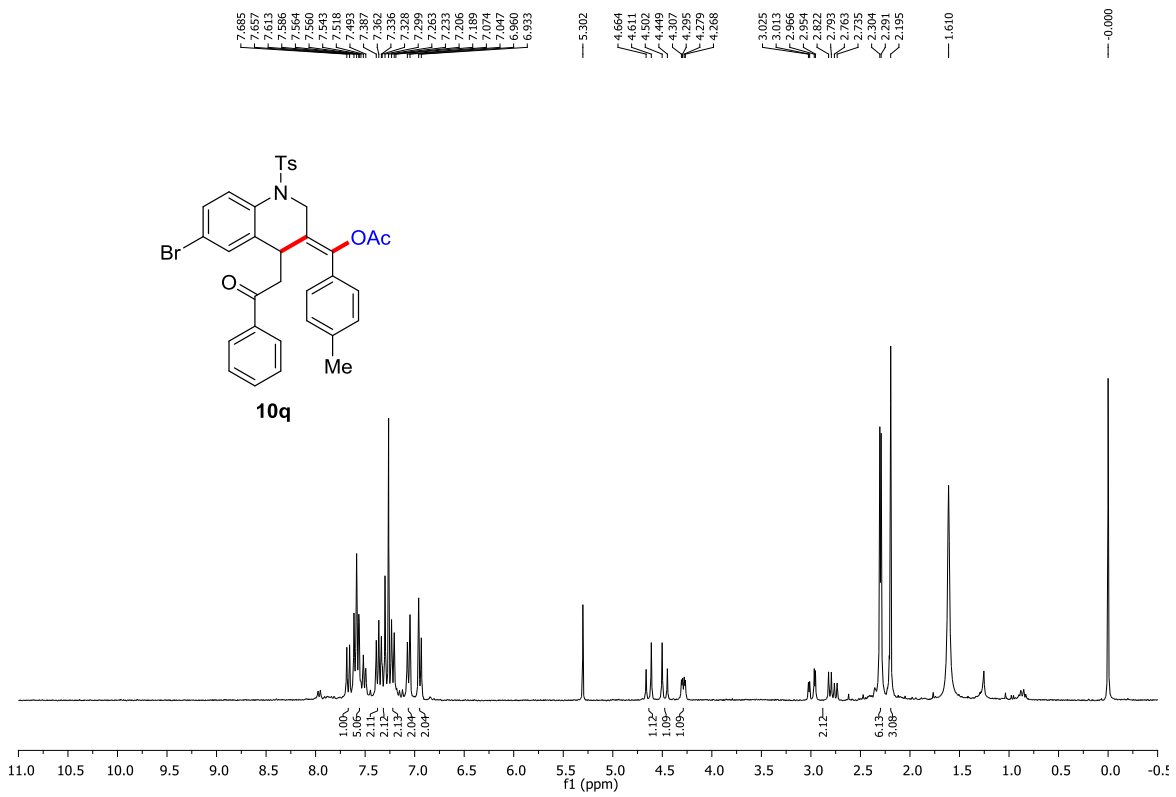
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.336
7.328
7.299
7.263
7.233
7.206
7.189
7.074
7.047
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6.933
5.302
4.664
4.611
4.502
4.449
4.307
4.295
4.279
4.268
3.025
3.013
2.966
2.954
2.822
2.793
2.763
2.735
2.304
2.291
2.195
1.610
-0.000
Ts
N
Br
OAc
O
Me
10q
1.00
5.06
2.11
2.12
2.13
2.04
2.04
1.12
1.09
1.09
2.12
6.13
3.08
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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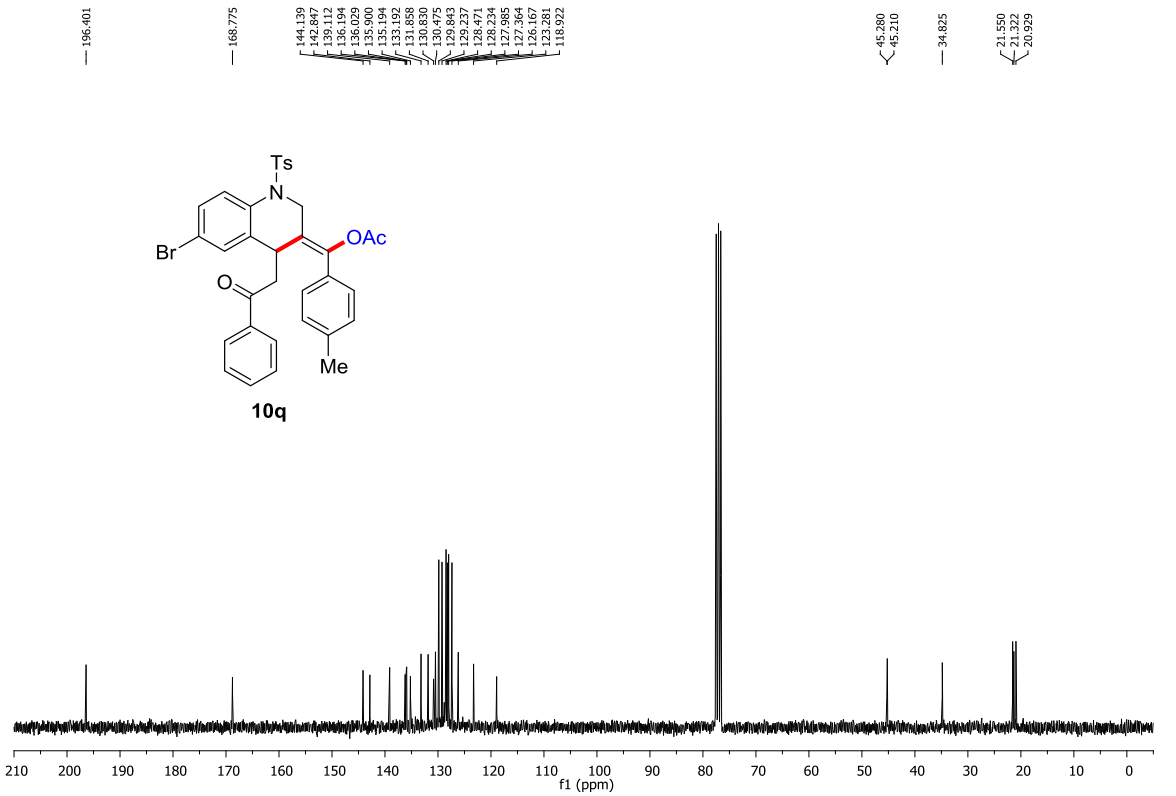
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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133.192
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130.475
129.843
129.237
128.471
128.234
127.985
127.364
126.167
123.281
118.922
45.280
45.210
34.825
21.550
21.322
20.929
Ts
N
Br
OAc
O
Me
10q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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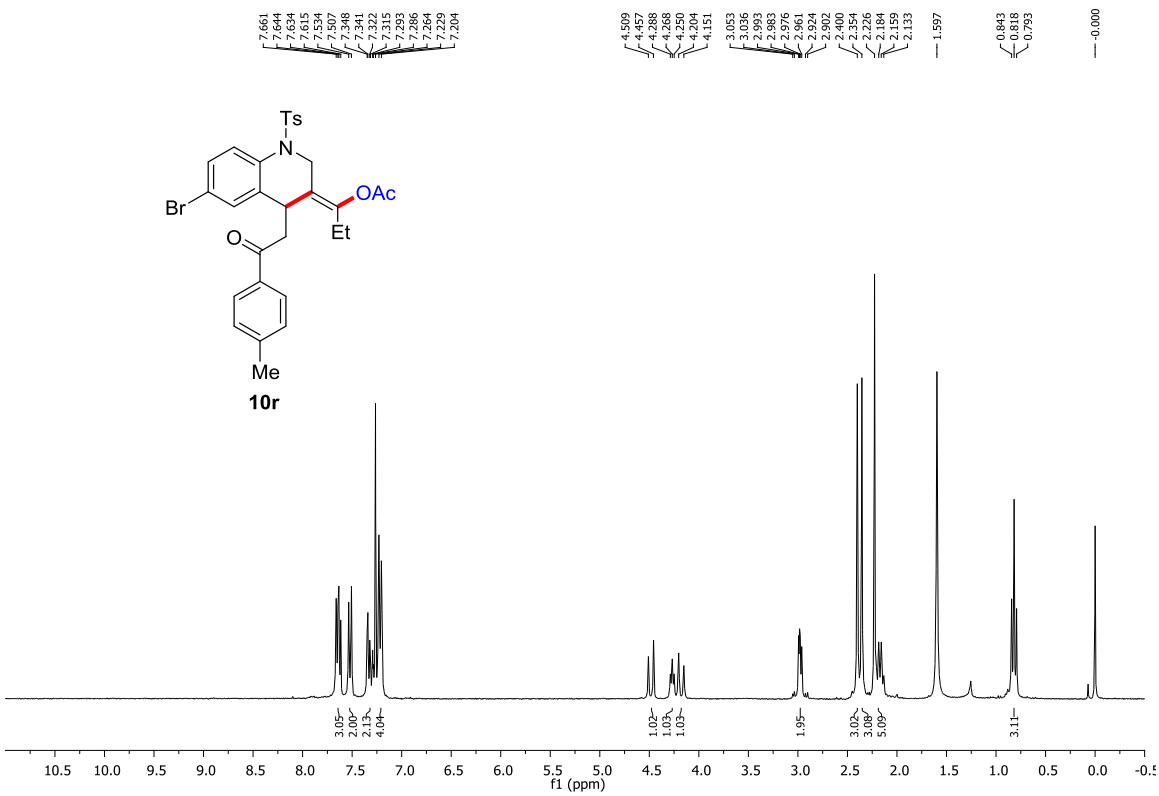
f1 (ppm)


Ts
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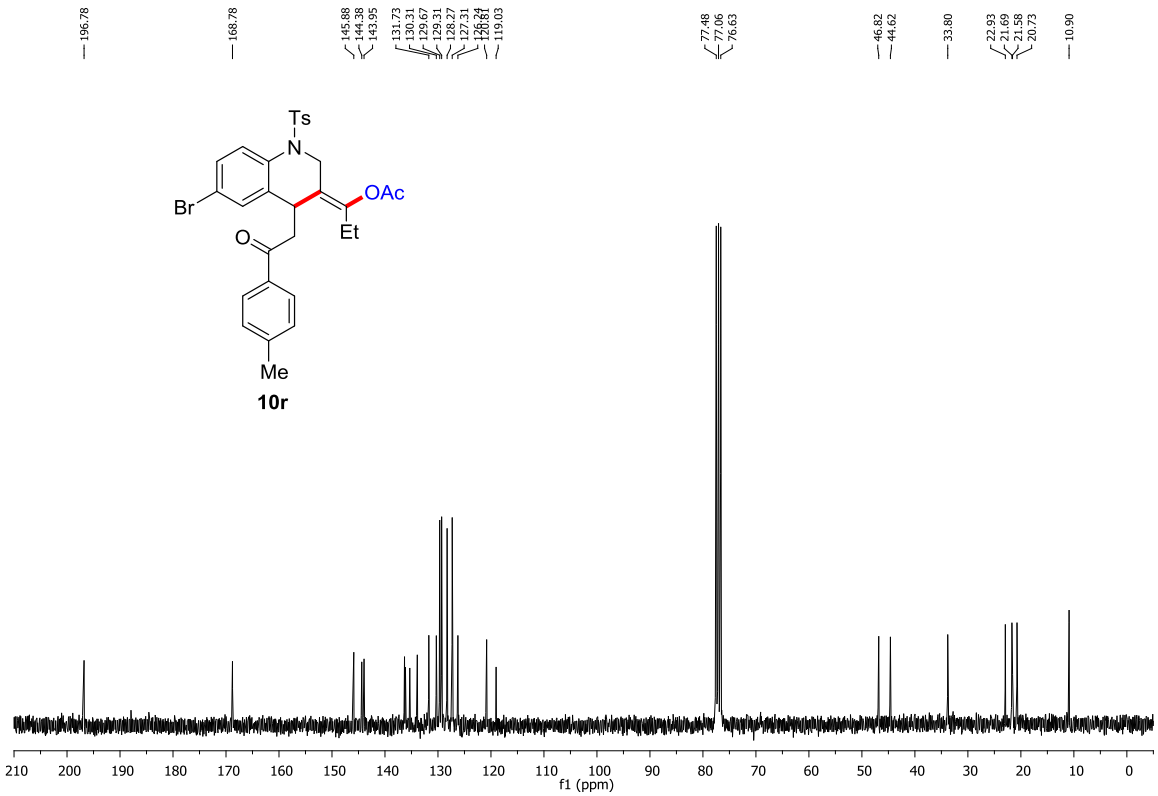
Br
OAc
Et
O
Me
10r
f1 (ppm)


Ts
N
Br
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Et
O
Me
10r
f1 (ppm)