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Supporting Information

Iron-Catalyzed Decarbonylation Initiated [2+2+m] Annulation of Benzene-Linked 1,*n*-Enynes with Aliphatic Aldehydes

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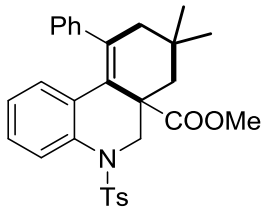
Contents

1. General information

^{1}H NMR spectra were recorded on Bruker 400 or 600 MHz spectrometer and the chemical shifts were reported in parts per million (δ) relative to internal standard TMS (0 ppm) for $CDCl_3$. The peak patterns are indicated as follows: s, singlet; d, doublet; dd, doublet of doublet; t, triplet; q, quartet; m, multiplet. The coupling constants, *J*, are reported in Hertz (Hz). ^{13}C NMR spectra were obtained at Bruker 100 MHz and referenced to the internal solvent signals (central peak is 77.0 ppm in $CDCl_3$). $CDCl_3$ was used as the NMR solvent. APEX II (Bruker Inc.) was used for HR-MS and ESI-MS. IR spectra were recorded by a Nicolet 5MX-S infrared spectrometer. Flash column chromatography was performed over silica gel 200-300. All reagents were weighed and handled in air at room temperature. All reagents were purchased from Alfa, Acros, Aldrich, and TCI and used without further purification.

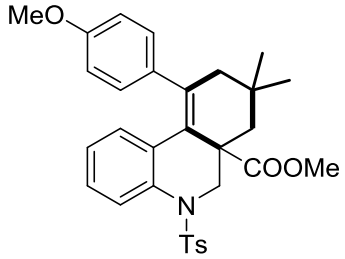
2. General procedure and characterization data for product 3 and 5

To a mixture of aliphatic aldehyde **2** or **4** (1.5 mmol), enyne **1** (0.3 mmol) and $FeCl_2$ (1.0 mg, 2.5 mol %), chlorobenzene (1.0 mL) was added under nitrogen at room temperature. Then pure *di-tert*-butyl peroxide (137 μL, 0.75 mmol) was dropped into the mixture. The resulting mixture was stirred at 120 ℃ for 2 hours. After the mixture was cooled to room temperature, the resulting solution was directly filtered through a pad of silica by EtOAc. The solvent was evaporated in vacuo to give the crude products. NMR yields were determined by ^{1}H NMR using dibromomethane as an internal standard. The residue was purified by flash column chromatography on silica gel (ethyl acetate/petroleum ether) to give the pure product **3** or **5**.

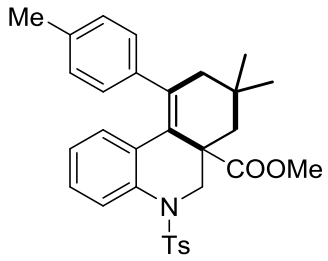


Methyl-8,8-dimethyl-10-phenyl-5-tosyl-5,7,8,9-tetrahydrophenanthridine-6a(6H)-carboxylate (3a). (93 mg, 62%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.5); IR (neat): ν_{max} 2951, 2870, 1736, 1597, 1479, 1458, 1356, 1242, 1169, 1072, 1047, 1036, 951, 920, 760, 720, 675 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.59 (d, *J* = 8.2 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 7.15-7.06 (m, 3H), 7.02-6.98 (m, 1H), 6.63 (td, *J* = 7.6, 1.1 Hz, 1H), 6.56-6.54 (m, 2H), 6.49 (dd, *J* = 7.8, 1.5 Hz, 1H), 4.56 (d, *J* = 11.6 Hz, 1H), 3.66 (d, *J* = 11.6 Hz, 1H), 3.40 (s, 3H), 2.48 (d, *J* = 17.2 Hz, 1H), 2.39 (s, 3H), 2.10 (dd, *J* = 14.0, 0.7 Hz, 1H), 2.00 (d, *J* = 17.2 Hz, 1H), 1.55 (d, *J* = 14.0 Hz, 1H), 1.04 (s, 3H), 0.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.6, 143.8, 142.4, 135.6, 135.1, 135.0, 130.9, 130.3, 129.5, 128.6, 127.9, 127.5, 127.1, 126.8, 126.7,

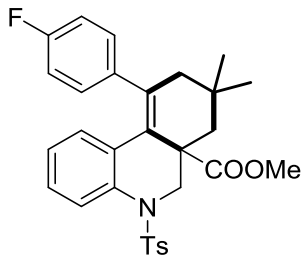
123.5, 122.7, 55.7, 52.2, 49.5, 46.3, 44.0, 29.8, 29.7, 28.2, 21.5; HRMS (ESI) calcd for $C_{30}H_{31}NNaO_4S$ [M + Na^+], 524.1866; found: 524.1873.



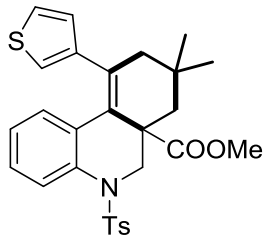
Methyl 10-(4-methoxyphenyl)-8,8-dimethyl-5-tosyl-5,6,6a,7,8,9-hexahydrophenanthridine-6a-carboxylate (3b). (83 mg, 52%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.5); IR (neat): ν_{max} 2951, 2924, 1732, 1607, 1508, 1479, 1458, 1354, 1290, 1244, 1169, 1090, 1032 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.59 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.00 (td, *J* = 7.8, 1.6 Hz, 1H), 6.66 (d, *J* = 7.6, 0.8 Hz, 1H), 6.61 (d, *J* = 8.6 Hz, 2H), 6.54 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.42 (d, *J* = 8.6 Hz, 2H), 4.55 (d, *J* = 11.8 Hz, 1H), 3.76 (s, 3H), 3.65 (d, *J* = 11.8 Hz, 1H), 3.39 (s, 3H), 2.46 (d, *J* = 17.2 Hz, 1H), 2.39 (s, 3H), 2.09 (d, *J* = 14.0 Hz, 1H), 1.97 (d, *J* = 17.2 Hz, 1H), 1.53 (d, *J* = 14.0 Hz, 1H), 1.03 (s, 3H), 0.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 158.4, 143.8, 135.7, 135.3, 134.7, 134.5, 131.0, 130.8, 129.8, 129.5, 127.6, 127.0, 126.3, 123.7, 122.8, 113.4, 55.9, 55.2, 52.2, 49.7, 46.4, 44.2, 29.9, 29.8, 28.3, 21.6; HRMS (ESI) calcd for $C_{31}H_{33}NNaO_5S$ [M + Na^+], 554.1972; found: 554.1959.



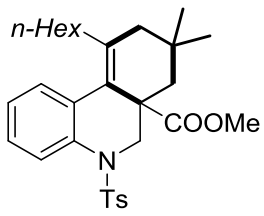
Methyl 8,8-dimethyl-10-(p-tolyl)-5-tosyl-5,6,6a,7,8,9-hexahydrophenanthridine-6a-carboxylate. (3c). (77 mg, 50%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.6); IR (neat): ν_{max} 2951, 2922, 2868, 1734, 1479, 1458, 1356, 1244, 1069, 1090, 1034 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.00 (td, *J* = 7.8, 1.4 Hz, 1H), 6.88 (d, *J* = 8.0 Hz, 2H), 6.64 (td, *J* = 7.6, 1.0 Hz, 1H), 6.52 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.45 (d, *J* = 8.0 Hz, 2H), 4.56 (d, *J* = 11.8 Hz, 1H), 3.64 (d, *J* = 11.8 Hz, 1H), 3.39 (s, 3H), 2.46 (d, *J* = 17.2 Hz, 1H), 2.39 (s, 3H), 2.28 (s, 3H), 2.09 (d, *J* = 14.0 Hz, 1H), 1.97 (d, *J* = 17.2 Hz, 1H), 1.54 (d, *J* = 14.0 Hz, 1H), 1.03 (s, 3H), 0.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.6, 143.8, 139.4, 136.3, 135.6, 135.2, 134.9, 130.9, 130.5, 129.5, 128.6, 128.5, 127.5, 127.0, 126.5, 123.5, 122.7, 55.7, 52.2, 49.5, 46.4, 44.1, 29.8, 29.6, 28.2, 21.5, 21.1; HRMS (ESI) calcd for $C_{31}H_{33}NNaO_4S$ [M + Na^+], 538.2023; found: 538.2014.



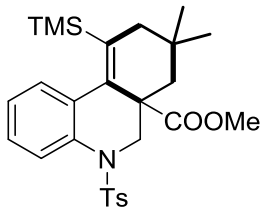
Methyl 10-(4-fluorophenyl)-8,8-dimethyl-5-tosyl-5,6,6a,7,8,9-hexahydrophenanthridine-6a-carboxylate. (3d). (98 mg, 63%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.6); IR (neat): ν_{max} 2951, 2924, 2870, 1732, 1599, 1506, 1479, 1354, 1242, 1221, 1169, 1092, 1034 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, J = 8.4, 0.7 Hz, 1H), 7.60 (d, J = 8.2 Hz, 2H), 7.25 (d, J = 8.0 Hz, 2H), 7.01 (td, J = 7.8, 1.6 Hz, 1H), 6.79-6.74 (m, 2H), 6.66 (td, J = 7.6, 1.0 Hz, 1H), 6.53-6.47 (m, 3H), 4.55 (d, J = 11.8 Hz, 1H), 3.67 (d, J = 11.8 Hz, 1H), 3.40 (s, 3H), 2.45 (d, J = 17.2 Hz, 1H), 2.39 (s, 3H), 2.11 (d, J = 14.0 Hz, 1H), 1.98 (d, J = 17.2 Hz, 1H), 1.56 (d, J = 14.0 Hz, 1H), 1.04 (s, 3H), 0.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.4, 161.1 (d, J_{C-F} = 144.8 Hz), 143.8, 138.2, 135.5 (d, J_{C-F} = 48.9 Hz), 133.9, 130.8, 130.2, 130.1, 129.5, 127.5, 127.3, 127.2, 123.6, 122.7, 114.8 (d, J_{C-F} = 21.1 Hz), 55.7, 52.2, 49.6, 46.3, 44.0, 29.8, 29.7, 28.1, 21.5; HRMS (ESI) calcd for $C_{30}H_{30}FNNaO_4S$ [M + Na^+], 542.1772; found: 542.1754.



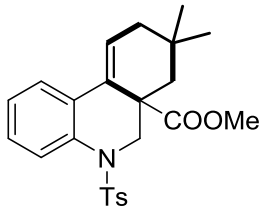
Methyl-8,8-dimethyl-10-(thiophen-3-yl)-5-tosyl-5,7,8,9-tetrahydrophenanthridine-6a(6H)-carboxylate (**3e**). (94 mg, 62%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:8, R_f = 0.5); IR (neat): ν_{max} 2949, 2868, 1738, 1732, 1352, 1242, 1169, 1092, 1033 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.77 (dd, J = 8.4, 0.6 Hz, 1H), 7.61 (d, J = 8.2 Hz, 2H), 7.23 (d, J = 8.2 Hz, 2H), 7.10-7.05 (m, 1H), 7.05 (q, J = 3.0 Hz, 1H), 6.75 (td, J = 7.8, 1.0 Hz, 1H), 6.70 (dd, J = 7.8, 1.6 Hz, 1H), 6.56 (q, J = 1.2 Hz, 1H), 6.29 (q, J = 1.2 Hz, 1H), 4.55 (d, J = 11.8 Hz, 1H), 3.67 (d, J = 11.8 Hz, 1H), 3.42 (s, 3H), 2.47 (d, J = 17.2 Hz, 1H), 2.38 (s, 3H), 2.13 (d, J = 14.0 Hz, 1H), 2.04 (d, J = 17.2 Hz, 1H), 1.55 (d, J = 14.0 Hz, 1H), 1.05 (s, 3H), 0.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.6, 143.9, 142.5, 135.7, 135.4, 130.6, 130.5, 129.6, 129.4, 128.3, 127.4, 127.1, 124.4, 123.7, 122.7, 55.9, 52.2, 49.8, 46.0, 44.1, 29.9, 29.8, 28.1, 21.5; HRMS (ESI) calcd for $C_{28}H_{29}NNaO_4S_2$ [M + Na^+], 530.1430; found: 530.1417.



Methyl-10-hexyl-8,8-dimethyl-5-tosyl-5,7,8,9-tetrahydrophenanthridine-6a(6H)-carboxylate (**3f**). (92 mg, 60%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.6); IR (neat): ν_{max} 2951, 2926, 2858, 1732, 1599, 1479, 1454, 1433, 1354, 1242, 1167, 1090, 1034, 982, 949, 814, 762, 674, 575 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.66 (dd, J = 8.2, 0.8 Hz, 1H), 7.44 (d, J = 8.2 Hz, 2H), 7.20-7.16 (m, 1H), 7.15-7.10 (m, 4H), 4.21 (d, J = 12.4 Hz, 1H), 3.72 (d, J = 12.4 Hz, 1H), 3.37 (s, 3H), 2.34 (s, 3H), 2.12-2.05 (m, 1H), 2.00 (d, J = 14.0 Hz, 1H), 1.94 (d, J = 17.2 Hz, 1H), 1.61-1.54 (m, 1H), 1.51 (d, J = 17.2 Hz, 1H), 1.40 (d, J = 14.0 Hz, 1H), 1.32-1.24 (m, 8H), 0.90 (t, J = 6.8 Hz, 3H), 0.86 (s, 3H), 0.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.4, 143.2, 136.1, 135.8, 132.6, 129.2, 129.0, 127.2, 124.6, 124.4, 124.1, 56.1, 52.0, 50.8, 44.7, 43.2, 34.3, 31.5, 30.1, 29.5, 29.3, 28.3, 27.6, 22.5, 21.3, 14.0; HRMS (ESI) calcd for $C_{30}H_{39}NNaO_4S$ [M + Na^+], 532.2492; found: 532.2494.

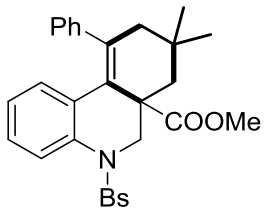


Methyl-8,8-dimethyl-5-tosyl-10-(trimethylsilyl)-5,7,8,9-tetrahydrophenanthridine-6a(6H)-carboxylate (**3g**). (52 mg, 35 %). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.5); IR (neat): ν_{max} 2951, 1738, 1732, 1358, 1248, 1169, 1072, 1034, 839, 758, 552 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.77 (dd, J = 8.2, 0.8 Hz, 1H), 7.54 (d, J = 8.2 Hz, 2H), 7.20 (td, J = 7.8, 1.8 Hz, 1H), 7.15 (d, J = 8.2 Hz, 2H), 7.05 (dd, J = 7.8, 1.8 Hz, 1H), 6.99 (td, J = 7.4, 1.0 Hz, 1H), 4.41 (d, J = 11.6 Hz, 1H), 3.47 (d, J = 11.6 Hz, 1H), 3.35 (s, 3H), 2.33 (s, 3H), 1.99 (dd, J = 14.0, 1.0 Hz, 1H), 1.95 (d, J = 17.0 Hz, 1H), 1.89 (d, J = 17.0 Hz, 1H), 1.42 (d, J = 14.0 Hz, 1H), 0.91 (s, 3H), 0.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.7, 143.6, 139.5, 135.8, 135.4, 134.6, 132.7, 130.3, 129.5, 128.4, 127.3, 123.5, 122.8, 55.9, 52.0, 50.8, 44.2, 43.1, 29.9, 29.0, 27.8, 21.4, -0.04; HRMS (ESI) calcd for $C_{27}H_{35}NNaO_4SSi$ [M + Na^+], 520.1948; found: 520.1952.

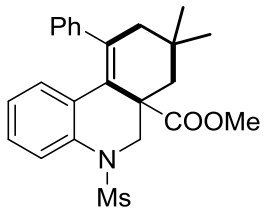


Methyl-8,8-dimethyl-5-tosyl-5,7,8,9-tetrahydrophenanthridine-6a(6H)-carboxylate (**3h**). (41 mg, 32%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:10, R_f = 0.5); IR (neat): ν_{max} 2949, 2902, 2866, 2828, 1732, 1597, 1485, 1460, 1352, 1238, 1167, 1092, 1047, 1037, 889, 814, 752, 729 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.2 Hz, 2H), 7.55 (d, J = 7.8, 1.4 Hz, 1H), 7.49 (dd, J = 8.4, 0.8 Hz, 1H), 7.26 (d, J = 8.2 Hz, 2H), 7.05 (td, J = 7.8, 1.6 Hz, 1H), 6.99 (td, J = 7.4, 1.0 Hz, 1H), 6.20 (t, J = 4.0 Hz, 1H), 4.82 (d, J = 12.0 Hz, 1H), 3.56 (s, 3H), 3.22 (d, J = 12.0 Hz, 1H), 2.38 (s, 3H), 2.29 (d, J = 13.4 Hz, 1H), 2.07 (d, J = 4.0 Hz, 2H), 1.30 (d, J = 13.4 Hz, 1H), 1.01 (s, 3H), 0.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.2, 143.7, 137.4,

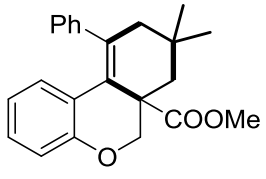
134.9, 130.4, 129.7, 127.3, 127.0, 126.3, 124.6, 123.2, 118.6, 55.7, 52.3, 45.6, 43.3, 40.2, 31.8, 28.9, 25.8, 21.5; HRMS (ESI) calcd for $C_{24}H_{27}NNaO_4S$ [M + Na^+], 448.1553; found: 448.1539.



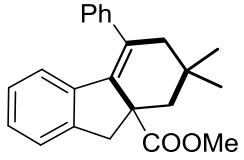
Methyl 5-((4-bromophenyl)sulfonyl)-8,8-dimethyl-10-phenyl-5,6,6a,7,8,9-hexahydrophenanthridine-6a-carboxylate. (3i). (102 mg, 60%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.4); IR (neat): ν_{max} 2951, 2868, 1732, 1574, 1447, 1389, 1360, 1242, 1172, 1088, 1068, 1034, 1012, 918 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.73 (dd, J = 8.4, 0.8 Hz, 1H), 7.60 (d, J = 8.8 Hz, 2H), 7.55 (d, J = 8.8 Hz, 2H), 7.16-7.13 (m, 3H), 7.01 (td, J = 7.8, 1.6 Hz, 1H), 6.66 (td, J = 7.6, 1.0 Hz, 1H), 6.55-6.51 (m, 3H), 4.57 (d, J = 11.8 Hz, 1H), 3.64 (d, J = 11.8 Hz, 1H), 3.39 (s, 3H), 2.48 (d, J = 17.2 Hz, 1H), 2.11 (d, J = 14.0 Hz, 1H), 2.02 (d, J = 17.2 Hz, 1H), 1.55 (d, J = 14.0 Hz, 1H), 1.05 (s, 3H), 0.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 142.2, 137.0, 135.5, 135.2, 132.2, 131.0, 130.6, 128.9, 128.4, 128.2, 127.2, 126.8, 126.6, 123.9, 122.7, 55.9, 52.3, 49.5, 46.4, 44.0, 29.8, 29.7, 28.2; HRMS (ESI) calcd for $C_{29}H_{28}BrNNaO_4S$ [M + Na^+], 588.0815; found: 588.0803.



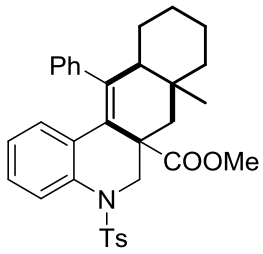
Methyl-8,8-dimethyl-5-(methylsulfonyl)-10-phenyl-5,7,8,9-tetrahydrophenanthridine-6a(6H)-carboxylate (3j). (71 mg, 56%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:5, R_f = 0.5); IR (neat): ν_{max} 2951, 2903, 2868, 1732, 1599, 1483, 1447, 1350, 1244, 1159, 962, 912, 856, 769, 758, 733, 702, 528, 513 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.62 (dd, J = 8.4, 0.8 Hz, 1H), 7.27-7.18 (m, 3H), 7.13-7.11 (m, 2H), 7.03-6.99 (m, 1H), 6.72 (dd, J = 7.9, 1.6 Hz, 1H), 6.60 (td, J = 7.6, 1.0 Hz, 1H), 4.61 (d, J = 12.3 Hz, 1H), 3.62 (d, J = 12.3 Hz, 1H), 3.47 (s, 3H), 3.00 (s, 3H), 2.53 (dd, J = 17.8, 1.0 Hz, 1H), 2.20 (dd, J = 13.8, 1.6 Hz, 1H), 2.17 (d, J = 17.8 Hz, 1H), 1.53 (d, J = 13.8 Hz, 1H), 1.10 (s, 3H), 1.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 142.7, 135.8, 135.5, 131.6, 128.8, 128.4, 127.5, 127.1, 126.9, 122.4, 118.7, 55.6, 52.2, 47.5, 47.4, 43.9, 37.5, 30.6, 29.6, 27.2; HRMS (ESI) calcd for $C_{24}H_{27}NNaO_4S$ [M + Na^+], 448.1553; found: 448.1556.



Methyl-8,8-dimethyl-10-phenyl-8,9-dihydro-6H-benzo[c]chromene-6a(7H)-carboxylate (**3k**). (47 mg, 45%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6); IR (neat): ν_{max} 2949, 2901, 2680, 1728, 1481, 1443, 1238, 1220, 1188, 754, 700 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.31-7.23 (m, 3H), 7.21-7.18 (m, 2H), 6.91 (td, *J* = 7.6, 1.6 Hz, 1H), 6.68 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.56 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.41 (td, *J* = 7.6, 1.2 Hz, 1H), 4.62 (d, *J* = 10.4 Hz, 1H), 3.98 (d, *J* = 10.4 Hz, 1H), 3.55 (s, 3H), 2.42 (dd, *J* = 18.6, 2.0 Hz, 1H), 2.19 (dd, *J* = 13.6, 2.0 Hz, 1H), 2.16 (d, *J* = 18.6 Hz, 1H), 1.28 (d, *J* = 13.6 Hz, 1H), 1.07 (s, 3H), 1.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 153.6, 143.4, 134.1, 130.3, 128.9, 128.6, 127.5, 126.8, 124.9, 121.6, 119.5, 116.0, 74.9, 52.2, 48.9, 46.1, 41.9, 31.7, 29.2, 25.6; HRMS (ESI) calcd for $C_{23}H_{24}NaO_3$ [M + Na^+], 371.1618; found: 371.1618.

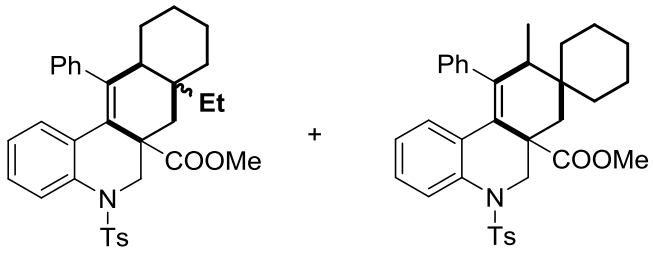


Methyl-7,7-dimethyl-5-phenyl-6,7,8,9-tetrahydro-8aH-fluorene-8a-carboxylate (**3l**). (78 mg, 83%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.7); IR (neat): ν_{max} 2951, 1728, 1254, 1202, 1169, 1026, 970, 700 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.39-7.34 (m, 2H), 7.32-7.30 (m, 1H), 7.25-7.22 (m, 2H), 7.12 (d, *J* = 7.4 Hz, 1H), 7.02 (dd, *J* = 7.4, 1.0 Hz, 1H), 6.84 (t, *J* = 7.6 Hz, 1H), 6.54 (d, *J* = 7.6 Hz, 1H), 3.58 (s, 3H), 3.31 (d, *J* = 15.8 Hz, 1H), 3.00 (d, *J* = 15.8 Hz, 1H), 2.56 (d, *J* = 13.4 Hz, 1H), 2.33 (d, *J* = 17.6 Hz, 1H), 2.15 (d, *J* = 17.6 Hz, 1H), 1.66 (d, *J* = 13.4 Hz, 1H), 1.05 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.5, 142.7, 142.2, 140.4, 136.1, 134.3, 128.5, 128.1, 126.9, 126.1, 124.4, 123.6, 55.1, 52.1, 47.6, 45.5, 32.2, 30.9, 28.1; HRMS (ESI) calcd for $C_{23}H_{24}NaO_2$ [M + Na^+], 355.1669; found: 355.1672.

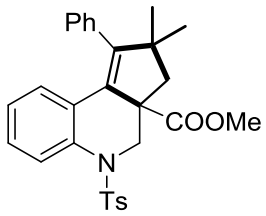


Methyl (6a,7a,11a)-7a-methyl-12-phenyl-5-tosyl-5,7,7a,8,9,10,11,11a-octahydrobenzo[j]phenanthridine-6a(6H)-carboxylate (**3m**). (84 mg, 52%, 20:20:1:1). The two major isomers were isolated and characterized. **Isomer 1:** Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:5, R_f = 0.55); IR (neat): ν_{max} 2928, 2862, 1736, 1454, 1356, 1240, 1169, 1088, 1037, 918, 762 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 8.4, 0.6 Hz, 1H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 7.15-7.05 (m, 3H), 6.98-6.94 (m, 1H), 6.63 (td, *J* = 7.6, 1.1 Hz, 1H), 6.39 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.38 (br, 2H), 4.74 (d, *J* = 11.4 Hz, 1H), 3.50 (d, *J* = 11.4 Hz, 1H), 3.38 (s, 3H), 2.40 (s, 3H), 2.11 (d, *J* = 14.6 Hz, 1H), 2.10-2.06 (m, 1H), 1.75 (dd, *J* = 14.6, 1.0 Hz, 1H), 1.65-1.50 (m, 3H), 1.44-1.27 (m, 3H), 1.12 (s, 3H), 1.07-0.97 (m, 1H), 0.88-0.75 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 143.9, 141.4, 139.9, 135.3, 134.8, 131.1, 130.5, 129.5, 129.2, 127.7, 127.5, 126.8, 126.5, 126.0, 123.3, 122.6, 58.9, 52.0,

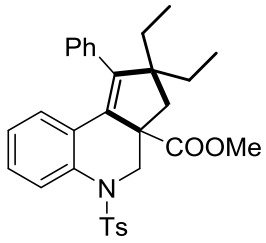
49.8, 48.2, 39.9, 37.6, 32.0, 28.7, 27.7, 26.1, 21.6, 21.5; HRMS (ESI) calcd for $C_{35}H_{35}NNaO_4S$ [M + Na^+], 564.2179; found: 564.2172. **Isomer 2:** Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:5, R_f = 0.5); IR (neat): ν_{max} 2930, 2882, 1734, 1479, 1456, 1358, 1221, 1169, 1074, 1032 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.2 Hz, 2H), 7.13-7.09 (m, 1H), 7.05-7.00 (m, 3H), 6.64 (td, *J* = 7.6, 1.1 Hz, 1H), 6.54 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.52-7.49 (m, 2H), 4.51 (d, *J* = 11.8 Hz, 1H), 3.89 (d, *J* = 11.8 Hz, 1H), 3.41 (s, 3H), 2.48 (d, *J* = 14.6 Hz, 1H), 2.40 (s, 3H), 2.21-2.17 (m, 1H), 1.83-1.79 (m, 2H), 1.73-1.66 (m, 1H), 1.62-1.48 (m, 3H), 1.26-1.22 (m, 3H), 0.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 143.8, 143.3, 140.0, 135.5, 135.0, 131.2, 130.9, 129.5, 128.3, 127.8, 127.5, 127.4, 126.6, 126.5, 123.9, 123.7, 53.1, 52.4, 50.5, 49.7, 39.9, 35.1, 32.6, 30.1, 29.8, 26.9, 26.2, 21.6, 21.3; HRMS (ESI) calcd for $C_{35}H_{35}NNaO_4S$ [M + Na^+], 564.2179; found: 564.2172.



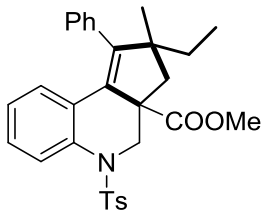
Methyl-7a-ethyl-12-phenyl-5-tosyl-5,7,7a,8,9,10,11,11a-octahydrobenzo[j]phenanthridine-6a(6H)-carboxylate(3n, 10:10:1:1**). Methyl-9'-methyl-10'-phenyl-5'-tosyl-5',9'-dihydro-6'H-spiro[cyclohexane-1,8'-phenanthridine] -6a'(7'H)-carboxylate (3o**, 1:1**).** The two major isomers were isolated and characterized**. Isomer 1.** Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.55); IR (neat): ν_{max} 2930, 2855, 1738, 1730, 1360, 1242, 1207, 1669, 1090, 1032 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.76-7.74 (m, 1H), 7.58-7.55 (m, 2H), 7.26-7.24 (m, 2H), 7.15-7.05 (m, 3H), 6.98-6.95 (m, 1H), 6.61-6.57 (m, 1H), 6.50-6.28 (m, 3H), 4.78-4.71 (m, 1H), 3.50-3.40 (m, 1H), 3.88 (s, 3H), 2.40 (s, 3H), 2.46-2.19 (m, 1H), 2.10-1.64 (m, 4H), 1.56-0.80 (m, 8H), 0.71 (t, *J* = 7.4 Hz, 1.5H), 0.64 (d, *J* = 7.0 Hz, 1.5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.4, 174.2, 143.9, 141.8, 141.5, 140.6, 139.9, 135.3, 135.2, 134.8, 131.1, 131.0, 130.5, 129.5, 127.8, 127.7, 127.6, 126.8, 126.6, 126.1, 126.0, 123.4, 122.7, 59.1, 59.0, 52.1, 50.0, 48.0, 47.9, 36.4, 35.3, 34.7, 34.5, 34.4, 33.2, 32.3, 27.7, 26.2, 26.1, 21.8, 21.7, 21.6, 12.8, 7.1; HRMS (ESI) calcd for $C_{34}H_{37}NNaO_4S$ [M + Na^+], 578.2336; found:578.2319. **Isomer 2.** Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.50); IR (neat): ν_{max} 2926, 2852, 1734, 1479, 1449, 1356, 1229, 1169, 1032 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.86-7.83 (m, 1H), 7.52-7.50 (m, 2H), 7.26-7.22 (m, 2H), 7.13-7.09 (m, 1H), 7.06-7.00 (m, 3H), 6.68-6.62 (m, 1H), 6.59-6.47 (m, 3H), 4.52 (d, *J* = 11.8 Hz, 1H), 3.75-3.71 (m, 1H), 3.41 (s, 3H), 2.41 (s, 3H), 2.33-2.16 (m, 2H), 1.92-1.65 (m, 3H), 1.50-0.84 (m, 11H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 174.6, 143.8, 143.3, 140.9, 139.9, 135.5, 134.8, 131.2, 131.1, 130.9, 129.4, 128.2, 127.8, 127.5, 127.4, 127.3, 126.5, 123.9, 123.8, 53.0, 52.4, 50.3, 49.5, 36.5, 35.9, 35.5, 35.3, 35.0, 32.6, 30.8, 29.9, 26.1, 21.6, 21.2, 21.1, 15.3, 7.2; HRMS (ESI) calcd for $C_{34}H_{37}NNaO_4S$ [M + Na^+], 578.2336; found: 578.2319.



Methyl-2,2-dimethyl-1-phenyl-5-tosyl-2,3,4,5-tetrahydro-3aH-cyclopenta[c]quinoline-3a-carboxylate (**5a**). (88 mg, 60%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.5); IR (neat): ν_{max} 2955, 2926, 1728, 1599, 1480, 1458, 1355, 1250, 1140, 1120, 1070 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.2 Hz, 2H), 7.49 (d, J = 8.4 Hz, 1H), 7.35-7.30 (m, 3H), 7.27 (d, J = 8.2 Hz, 2H), 7.00-6.95 (m, 3H), 6.71 (dd, J = 7.8, 1.4 Hz, 1H), 6.62 (t, J = 7.6 Hz, 1H), 5.03 (d, J = 12.0 Hz, 1H), 3.64 (s, 3H), 3.45 (d, J = 12.0 Hz, 1H), 2.49 (d, J = 13.4 Hz, 1H), 2.40 (s, 3H), 1.88 (d, J = 13.4 Hz, 1H), 1.26 (s, 3H), 0.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 147.6, 143.7, 137.2, 136.7, 135.9, 129.7, 129.3, 128.7, 128.4, 127.7, 127.4, 127.2, 127.0, 124.0, 122.9, 120.2, 55.7, 55.4, 52.4, 49.0, 48.1, 28.6, 27.5, 21.5; HRMS (ESI) calcd for $C_{29}H_{29}NNaO_4S$ [M + Na^+], 510.1710; found: 510.1716.



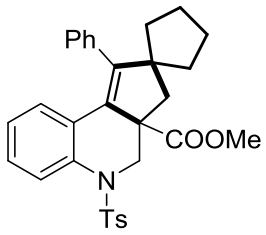
Methyl-2,2-diethyl-1-phenyl-5-tosyl-2,3,4,5-tetrahydro-3aH-cyclopenta[c]quinoline-3a-carboxylate (**5b**). (108 mg, 70%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.6); IR (neat): ν_{max} 2965, 2878, 1732, 1462, 1456, 1356, 1238, 1213, 1169, 1090, 918, 814, 752 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, J = 8.2 Hz, 2H), 7.60 (d, J = 8.4 Hz, 1H), 7.27-7.25 (m, 5H), 6.98 (td, J = 8.6, 1.0 Hz, 1H), 6.90-6.87 (m, 2H), 6.65-6.57 (m, 2H), 5.00 (d, J = 11.6 Hz, 1H), 3.56 (s, 3H), 3.44 (d, J = 11.6 Hz, 1H), 2.40 (s, 3H), 2.33 (d, J = 14.4 Hz, 1H), 1.91 (d, J = 14.4 Hz, 1H), 1.61 (q, J = 7.4 Hz, 2H), 1.28-1.21 (m, 1H), 1.15-0.92 (m, 1H), 0.96 (t, J = 7.4 Hz, 3H), 0.66 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 144.6, 143.7, 136.4, 136.3, 135.7, 132.2, 129.6, 128.8, 128.3, 128.1, 127.3, 127.2, 124.4, 122.9, 120.6, 56.6, 56.4, 55.3, 52.2, 39.9, 31.0, 30.9, 21.5, 9.44, 8.95; HRMS (ESI) calcd for $C_{31}H_{33}NNaO_4S$ [M + Na^+], 538.2023; found: 538.2027.



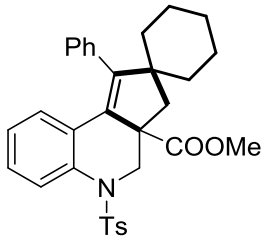
Methyl

(3a)-2-ethyl-2-methyl-1-phenyl-5-tosyl-2,3,4,5-tetrahydro-3aH-cyclopenta[c]quinoline-3a-carboxylate (**5c**, dr = 1:1). (101 mg, 67%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.5); IR

(neat): ν_{max} 2963, 2928, 2876, 1734, 1458, 1354, 1221, 1165, 1089, 914, 814, 752 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.2 Hz, 2H), 7.67 (d, J = 8.2 Hz, 2H), 7.53 (d, J = 8.40 Hz, 1H), 7.52 (d, J = 8.40 Hz, 1H), 7.33-7.25 (m, 10H), 6.99-6.90 (m, 6H), 6.69-6.60 (m, 4H), 5.03 (d, J = 11.8 Hz, 1H), 5.02 (d, J = 11.8 Hz, 1H), 3.62 (s, 3H), 3.60 (s, 3H), 3.46 (d, J = 7.6 Hz, 1H), 3.43 (d, J = 7.6 Hz, 1H), 2.63 (d, J = 13.6 Hz, 1H), 2.40 (s, 3H), 2.39 (s, 3H), 2.30 (d, J = 13.6 Hz, 1H), 1.95 (d, J = 13.6 Hz, 1H), 1.70 (d, J = 13.6 Hz, 1H), 1.61-1.47 (m, 2H), 1.30 (s, 3H), 1.20-1.13 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H), 0.85 (s, 3H), 0.71 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.7, 174.6, 147.1, 143.7, 136.9, 136.8, 136.7, 136.5, 135.8, 135.7, 130.2, 130.0, 129.6, 128.9, 128.6, 128.4, 128.3, 127.9, 127.7, 127.4, 127.3, 127.2, 127.1, 127.0, 126.9, 124.2, 124.0, 123.0, 122.9, 120.5, 120.3, 56.1, 56.0, 55.4, 55.1, 52.4, 52.3, 52.0, 51.9, 45.3, 43.9, 32.6, 31.4, 26.4, 25.5, 21.5, 9.37, 8.66; HRMS (ESI) calcd for $C_{30}H_{31}NNaO_4S$ [M + Na^+], 524.1866; found: 524.1874.

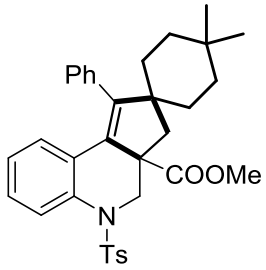


Methyl-1'-phenyl-5'-tosyl-4',5'-dihydrospiro[cyclopentane-1,2'-cyclopenta[c]quinoline]-3a'(3'H)-carboxy late (**5d**). (88 mg, 57%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.5); IR (neat): ν_{max} 2953, 2868, 1730, 1352, 1228, 1161, 1138, 1121, 1072, 989, 951, 864, 814, 754, 662, 575 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 8.4 Hz, 2H), 7.48 (dd, J = 8.4, 0.8 Hz, 1H), 7.35-7.30 (m, 3H), 7.27 (d, J = 8.2 Hz, 2H), 7.00-6.93 (m, 3H), 6.71 (dd, J = 8.0, 1.6 Hz, 1H), 6.62 (td, J = 7.6, 1.0 Hz, 1H), 5.03 (d, J = 12.0 Hz, 1H), 3.64 (s, 3H), 3.46 (d, J = 12.0 Hz, 1H), 2.54 (d, J = 13.2 Hz, 1H), 2.40 (s, 3H), 1.80 (d, J = 13.2 Hz, 1H), 1.70-1.40 (m, 7H), 1.26-1.19 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 146.0, 143.6, 137.3, 136.8, 135.7, 130.1, 129.6, 129.0, 128.4, 127.6, 127.3, 127.2, 127.0, 124.0, 123.0, 120.2, 59.1, 55.7, 55.3, 52.4, 48.2, 38.2, 36.4, 30.0, 25.8, 24.0, 23.9, 21.5; HRMS (ESI) calcd for $C_{31}H_{31}NNaO_4S$ [M + Na^+], 536.1866; found: 536.1875.

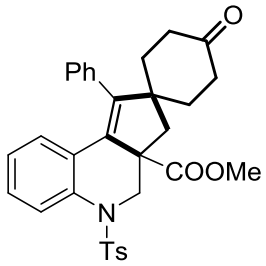


Methyl-1'-phenyl-5'-tosyl-4',5'-dihydrospiro[cyclohexane-1,2'-cyclopenta[c]quinoline]-3a'(3'H)-carboxyl ate (**5e**). (90 mg, 57%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.5); IR (neat): ν_{max} 2928, 2857, 1734, 1599, 1481, 1449, 1354, 1225, 1167, 1090, 1047, 916, 870, 814, 752, 704, 662, 575, 542 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.4 Hz, 2H), 7.48 (dd, J = 8.4, 0.6 Hz, 1H), 7.35-7.31 (m, 3H), 7.27 (d, J = 8.4 Hz, 2H), 6.97-6.93 (m, 3H), 6.65 (dd, J = 8.0, 1.6 Hz, 1H), 6.59 (td, J = 7.6, 1.0 Hz, 1H), 5.05 (d, J = 12.0 Hz, 1H), 3.62 (s, 3H), 3.44 (d, J = 12.0 Hz, 1H), 2.72 (d, J = 13.6 Hz, 1H), 2.40 (s, 3H), 1.75 (d, J = 13.6 Hz, 1H), 1.68-1.59 (m, 3H), 1.58-1.51 (m, 2H), 1.33-1.24 (m, 2H), 1.19-1.18 (m, 2H), 0.97-0.92 (m, 1H); ^{13}C

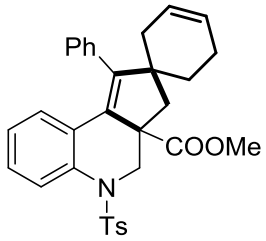
NMR (100 MHz, $CDCl_3$) δ 174.9, 146.0, 143.6, 137.3, 136.8, 135.7, 130.1, 129.6, 129.0, 128.4, 127.6, 127.3, 127.2, 127.0, 124.0, 123.0, 120.2, 59.1, 55.7, 55.3, 52.4, 48.2, 38.2, 36.4, 30.0, 25.8, 24.0, 23.9, 21.5; HRMS (ESI) calcd for $C_{32}H_{33}NNaO_4S$ [M + Na^+], 550.2023; found: 550.2032.



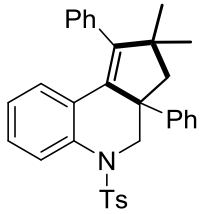
Methyl-4,4-dimethyl-1'-phenyl-5'-tosyl-4',5'-dihydrospiro[cyclohexane-1,2'-cyclopenta[c]quinoline]-3a'(3'H)-carboxylate (**5f**). (100 mg, 60%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.5); IR (neat): ν_{max} 2947, 2926, 2907, 2863, 1732, 1599, 1479, 1456, 1352, 1229, 1169, 1090, 917, 887, 864, 812, 754, 704, 662, 575 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.4 Hz, 2H), 7.48 (dd, J = 8.4, 0.6 Hz, 1H), 7.35-7.30 (m, 3H), 7.26 (d, J = 8.4 Hz, 2H), 6.97-6.93 (m, 3H), 6.71 (dd, J = 8.0, 1.6 Hz, 1H), 6.62 (td, J = 7.6, 1.0 Hz, 1H), 5.03 (d, J = 12.0 Hz, 1H), 3.62 (s, 3H), 3.43 (d, J = 12.0 Hz, 1H), 2.72 (d, J = 13.6 Hz, 1H), 2.40 (s, 3H), 1.80-1.72 (m, 1H), 1.70 (d, J = 13.6 Hz, 1H), 1.48-1.44 (m, 1H), 1.38-1.20 (m, 5H), 0.98-0.96 (m, 1H), 0.88 (s, 3H), 0.65 (s, 3H);^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 148.0, 143.6, 137.2, 136.8, 135.8, 129.8, 129.7, 128.9, 128.4, 127.9, 127.3, 127.2, 127.0, 124.0, 122.9, 120.2, 55.9, 55.3, 52.4, 52.2, 43.2, 36.1, 35.2, 33.0, 32.9, 29.8, 29.1, 23.6, 21.5; HRMS (ESI) calcd for $C_{34}H_{37}NNaO_4S$ [M + Na^+], 578.2336; found: 578.2342.



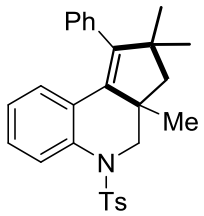
Methyl-4-oxo-1'-phenyl-5'-tosyl-4',5'-dihydrospiro[cyclohexane-1,2'-cyclopenta[c]quinoline]-3a'(3'H)-carboxylate (**5g**). (93 mg, 57%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:5, R_f = 0.4); IR (neat): ν_{max} 2951, 2932, 2864, 1730, 1718, 1458, 1352, 1227, 1161, 1090, 1074, 1051, 914, 870, 812, 663, 570, 540 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.4 Hz, 2H), 7.46 (dd, J = 8.4, 0.6 Hz, 1H), 7.37-7.34 (m, 3H), 7.30 (d, J = 8.4 Hz, 2H), 7.02-6.97 (m, 3H), 6.70 (dd, J = 8.0, 1.6 Hz, 1H), 6.63 (td, J = 7.6, 1.0 Hz, 1H), 5.09 (d, J = 12.2 Hz, 1H), 3.67 (s, 3H), 3.52 (d, J = 12.2 Hz, 1H), 3.03 (d, J = 13.4 Hz, 1H), 2.59-2.50 (m, 1H), 2.42 (s, 3H), 2.42-2.36 (m, 2H), 2.27-2.24 (m, 1H), 2.05-2.01 (m, 2H), 1.97 (d, J = 13.4 Hz, 1H), 1.64-1.52 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.2, 174.4, 145.5, 143.8, 137.4, 136.0, 135.8, 130.9, 129.8, 128.8, 128.7, 127.9, 127.8, 127.7, 126.9, 123.4, 123.1, 120.2, 55.5, 52.7, 51.0, 42.6, 38.6, 37.9, 37.0, 33.6, 21.5; HRMS (ESI) calcd for $C_{32}H_{31}NNaO_5S$ [M + Na^+], 564.1815; found: 564.1800.



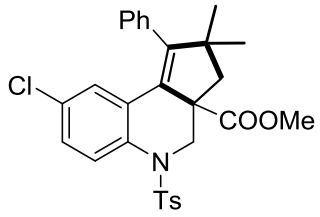
Methyl (3a')-1'-phenyl-5'-tosyl-4',5'-dihydrospiro[cyclohexane-1,2'-cyclopenta[c]quinolin]-3-ene-3a'(3'H)-carboxylate (**5h**, dr = 1:1). (66 mg, 42%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:5, R_f = 0.6); IR (neat): ν_{max} 3024, 2949, 2922, 2839, 1734, 1597, 1479, 1458, 1352, 1163, 1089, 1047, 918, 812, 748, 704, 662, 569 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.4 Hz, 2H), 7.67 (d, J = 8.4 Hz, 2H), 7.53 (d, J = 8.4 Hz, 1H), 7.46 (dd, J = 8.4, 0.6 Hz, 1H), 7.37-7.27 (m, 10H), 7.05-7.02 (m, 2H), 7.01-6.94 (m, 2H), 6.92-6.89 (m, 2H), 6.76 (dd, J = 8.0, 1.6 Hz, 1H), 6.66-6.59 (m, 3H), 5.66-5.54 (m, 4H), 5.09 (d, J = 12.0 Hz, 1H), 5.00 (d, J = 12.0 Hz, 1H), 3.66 (s, 3H), 3.62 (s, 3H), 3.49 (d, J = 12.0 Hz, 1H), 3.42 (d, J = 12.0 Hz, 1H), 2.67 (d, J = 13.8 Hz, 1H), 2.59 (d, J = 13.4 Hz, 1H), 2.42 (s, 3H), 2.41 (s, 3H), 2.38-2.34 (m, 1H), 2.14-1.94 (m, 6H), 1.79-1.72 (m, 4H), 1.53-1.47 (m, 1H), 1.33-1.23 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 174.8, 147.1, 143.7, 137.4, 136.9, 136.6, 136.4, 135.9, 130.5, 130.2, 129.7, 129.6, 128.9, 128.5, 128.4, 127.8, 127.7, 127.4, 127.3, 127.0, 126.9, 126.4, 126.3, 125.4, 124.8, 124.2, 123.5, 123.0, 122.8, 120.6, 119.8, 55.8, 55.7, 55.5, 55.1, 52.4, 50.5, 50.0, 43.9, 43.7, 36.4, 33.7, 32.5, 30.1, 23.2, 22.2, 21.5; HRMS (ESI) calcd for $C_{32}H_{31}NNaO_4S$ [M + Na^+], 548.1866; found: 548.1873.



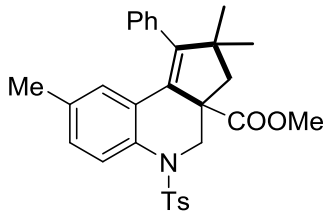
2,2-Dimethyl-1,3a-diphenyl-5-tosyl-3,3a,4,5-tetrahydro-2H-cyclopenta[c]quinoline (**5i**). (62 mg, 41%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:5, R_f = 0.3); IR (neat): ν_{max} 2955, 2926, 2866, 1728, 1599, 1481, 1458, 1354, 1254, 1140, 1120, 1072, 949, 862, 814, 754, 662 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.41-7.34 (m, 5H), 7.30-7.27 (m, 4H), 7.16-7.13 (m, 2H), 6.95 (d, J = 8.4 Hz, 2H), 6.89 (d, J = 8.4 Hz, 2H), 6.86-6.81 (m, 2H), 6.55 (td, J = 7.6, 1.0 Hz, 1H), 5.26 (d, J = 12.2 Hz, 1H), 3.64 (d, J = 12.2 Hz, 1H), 2.37 (d, J = 12.6 Hz, 1H), 2.28 (s, 3H), 2.17 (d, J = 12.6 Hz, 1H), 1.01 (s, 3H), 0.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 145.6, 143.3, 137.7, 136.3, 135.9, 132.0, 129.4, 128.7, 128.6, 128.5, 127.9, 127.8, 127.6, 127.3, 127.1, 126.4, 122.8, 122.0, 118.5, 57.5, 54.0, 51.4, 47.8, 28.9, 27.5, 21.4; HRMS (ESI) calcd for $C_{33}H_{31}NNaO_2S$ [M + Na^+], 528.1968; found: 528.1961.



2,2,3a-Trimethyl-1-phenyl-5-tosyl-3,3a,4,5-tetrahydro-2H-cyclopenta[c]quinoline (**5j**). (52 mg, 39%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:10, R_f = 0.6); IR (neat): ν_{max} 2957, 2924, 2866, 1350, 1161, 1136, 1121, 1069, 991, 953, 864, 814 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.4 Hz, 2H), 7.47 (dd, J = 8.6, 0.6 Hz, 1H), 7.31-7.26 (m, 5H), 6.99-6.95 (m, 3H), 6.65 (dd, J = 8.0, 1.6 Hz, 1H), 6.58 (td, J = 7.6, 1.0 Hz, 1H), 4.47 (d, J = 11.6 Hz, 1H), 3.33 (d, J = 11.6 Hz, 1H), 2.40 (s, 3H), 1.99 (d, J = 13.2 Hz, 1H), 1.77 (d, J = 13.2 Hz, 1H), 1.35 (s, 3H), 1.28 (s, 3H), 0.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 143.6, 137.5, 137.4, 135.8, 134.9, 129.7, 128.9, 128.4, 128.3, 127.2, 126.9, 123.1, 122.5, 119.8, 59.3, 51.4, 47.7, 43.1, 29.5, 24.4, 21.5; HRMS (ESI) calcd for $C_{28}H_{29}NNaO_2S$ [M + Na^+], 466.1811; found: 466.1800.

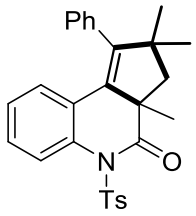


Methyl-8-chloro-2,2-dimethyl-1-phenyl-5-tosyl-2,3,4,5-tetrahydro-3aH-cyclopenta[c]quinoline-3a-carboxylate. (**5k**). (84 mg, 54%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.5); IR (neat): ν_{max} 2951, 2920, 1734, 1560, 1356, 1254, 1223, 1161, 1123, 1069, 991, 951, 864, 820 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.4 Hz, 2H), 7.47 (d, J = 9.0 Hz, 1H), 7.40-7.38 (m, 3H), 7.32 (d, J = 8.4 Hz, 2H), 7.01-6.98 (m, 2H), 6.95 (dd, J = 9.0, 2.6 Hz, 1H), 6.64 (d, J = 2.6 Hz, 1H), 5.05 (d, J = 12.0 Hz, 1H), 3.68 (s, 3H), 3.42 (d, J = 12.0 Hz, 1H), 2.52 (d, J = 13.4 Hz, 1H), 2.44 (s, 3H), 1.90 (d, J = 13.4 Hz, 1H), 1.28 (s, 3H), 0.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 149.2, 144.0, 136.8, 135.9, 134.4, 129.8, 128.6, 128.4, 127.6, 127.4, 127.2, 127.0, 125.3, 121.3, 55.5, 55.1, 52.5, 48.9, 48.1, 28.4, 27.3, 21.5; HRMS (ESI) calcd for $C_{29}H_{28}ClNNaO_4S$ [M + Na^+], 544.1320; found: 544.1314.

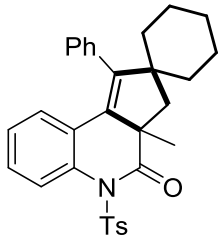


Methyl-2,2,8-trimethyl-1-phenyl-5-tosyl-2,3,4,5-tetrahydro-3aH-cyclopenta[c]quinoline-3a-carboxylate (**5l**). (69 mg, 46%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.5); IR (neat): ν_{max} 2957, 2924, 2864, 1734, 1597, 1483, 1458, 1350, 1234, 1220, 1163, 1090, 1040, 866, 812 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.4 Hz, 2H), 7.37 (d, J = 8.6 Hz, 1H), 7.35-7.31 (m, 3H), 7.27 (d, J = 8.4

Hz, 2H), 7.00-6.97 (m, 2H), 6.78 (dd, *J* = 8.6, 1.6 Hz, 1H), 6.46 (d, *J* = 8.6 Hz, 1H), 5.00 (d, *J* = 12.0 Hz, 1H), 3.65 (s, 3H), 3.41 (d, *J* = 12.0 Hz, 1H), 2.48 (d, *J* = 13.4 Hz, 1H), 2.40 (s, 3H), 1.87 (d, *J* = 13.4 Hz, 1H), 1.86 (s, 3H), 1.26 (s, 3H), 0.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 147.5, 143.6, 137.3, 136.8, 133.4, 132.2, 129.6, 129.4, 128.7, 128.4, 128.3, 128.2, 127.2, 127.0, 123.7, 120.0, 55.6, 55.5, 52.4, 49.1, 48.0, 28.6, 27.4, 21.5, 20.5; HRMS (ESI) calcd for $C_{30}H_{31}NNaO_4S$ [M + Na^+], 524.1866; found: 524.1852.



2,2,3a-Trimethyl-1-phenyl-5-tosyl-2,3,3a,5-tetrahydro-4H-cyclopenta[c]quinolin-4-one (**5m**). (74 mg, 54%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.6); IR (neat): ν_{max} 2961, 2930, 2868, 1718, 1597, 1364, 1175, 1086, 746, 704, 654, 559 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.4 Hz, 2H), 7.47 (dd, *J* = 8.2, 0.6 Hz, 1H), 7.38-7.30 (m, 5H), 7.24 (td, *J* = 7.4, 1.4 Hz, 1H), 7.10-7.08 (m, 2H), 6.97 (td, *J* = 7.6, 1.0 Hz, 1H), 6.75 (dd, *J* = 7.6, 1.4 Hz, 1H), 2.41 (s, 3H), 2.25 (d, *J* = 13.8 Hz, 1H), 1.84 (d, *J* = 13.8 Hz, 1H), 1.27 (s, 3H), 1.16 (s, 3H), 0.64 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.0, 149.2, 144.7, 136.7, 135.3, 134.8, 131.6, 129.1, 128.9, 128.4, 128.2, 127.4, 127.2, 127.1, 126.0, 125.8, 124.0, 54.7, 49.2, 48.3, 29.1, 28.4, 24.5, 21.5; HRMS (ESI) calcd for $C_{28}H_{27}NNaO_3S$ [M + Na^+], 480.1604; found: 480.1610.

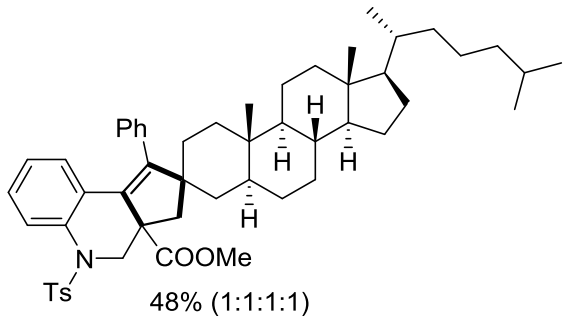


3a'-Methyl-1'-phenyl-5'-tosyl-3',3a'-dihydrospiro[cyclohexane-1,2'-cyclopenta[c]quinolin]-4'(5'H)-one (5n). (106 mg, 71%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:7, R_f = 0.5); IR (neat): ν_{max} 2924, 2849, 1718, 1647, 1597, 1454, 1366, 1175, 1084, 790, 702, 654, 570 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.4 Hz, 2H), 7.68 (dd, *J* = 8.2, 0.6 Hz, 1H), 7.39-7.33 (m, 3H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.23 (td, *J* = 7.8, 1.6 Hz, 1H), 7.05-7.02 (m, 2H), 6.95 (td, *J* = 7.6, 1.0 Hz, 1H), 6.70 (dd, *J* = 7.6, 1.4 Hz, 1H), 2.41 (s, 3H), 2.29 (d, *J* = 14.0 Hz, 1H), 1.88 (d, *J* = 14.0 Hz, 1H), 1.64-1.60 (m, 1H), 1.57-1.51 (m, 3H), 1.38-1.19 (m, 3H), 1.14 (s, 3H), 0.98-0.83 (m, 2H), 0.53-0.50 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.1, 149.9, 144.7, 136.6, 135.5, 134.6, 132.0, 129.3, 129.1, 128.6, 128.1, 127.4, 127.2, 127.1, 126.1, 125.9, 124.0, 54.9, 52.8, 43.6, 36.1, 36.0, 25.3, 25.1, 23.1, 22.3, 21.6; HRMS (ESI) calcd for $C_{31}H_{31}NNaO_3S$ [M + Na^+], 520.1917; found: 520.1923.

3. Synthesis of product 7

To a mixture of alkyl aldehyde **6** (0.9 mmol), enyne **1a** (0.3 mmol) and $FeCl_2$ (1.0 mg, 2.5 mol %), chlorobenzene (1.0 mL) was added under nitrogen at room temperature. Then pure *di-tert*-butyl peroxide (137 μL,

0.75 mmol) was dropped into the mixture. The resulting mixture was stirred at 120 ℃ for 2 hours. After the mixture was cooled to room temperature, the resulting solution was directly filtered through a pad of silica by EtOAc. The solvent was evaporated in vacuo to give the crude products. The residue was purified by flash column chromatography on silica gel (ethyl acetate/petroleum ether) to give the product **7**.



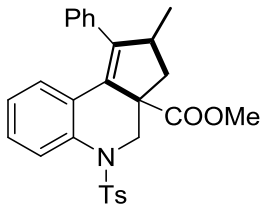
48% (1:1:1:1)

Methyl (5S,8R,9S,10S,13R,14S,17R)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-1'-phenyl-5'-tosyl-1,2,4,4',5,5',6,7,8,9,10,11,12,13,14,15,16,17-octadecahydrospiro[cyclopenta[a]phenanthrene-3,2'-cyclopenta[c]quinoline]-3a'(3'H)-carboxylate (**7**, dr = 1:1:1:1). (117 mg, 48%). **Isomer 1 (1:1)**: Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:5, R_f = 0.55); IR (neat): ν_{max} 2932, 2886, 2855, 1734, 1599, 1477, 1458, 1356, 1228, 1167, 1090, 1072, 952, 870, 814, 756, 662, 573 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.4 Hz, 1H), 7.66 (d, J = 8.4 Hz, 1H), 7.51 (d, J = 8.4 Hz, 0.5H), 7.48 (d, J = 8.4 Hz, 0.5H), 7.33-7.29 (m, 3H), 7.26 (d, J = 8.4 Hz, 2H), 6.97-6.91 (m, 3H), 6.63 (td, J = 7.6, 1.6 Hz, 1H), 6.59 (td, J = 7.6, 1.6 Hz, 1H), 5.03 (d, J = 12.0 Hz, 0.5H), 5.01 (d, J = 12.0 Hz, 0.5H), 3.61 (s, 1.5H), 3.59 (s, 1.5H), 3.43 (d, J = 12.0 Hz, 1H), 2.75 (d, J = 13.6 Hz, 0.5H), 2.69 (d, J = 13.6 Hz, 0.5H), 2.40 (s, 3H), 1.97-1.93 (m, 1H), 1.81-1.74 (m, 2H), 1.63-1.45 (m, 6H), 1.34-0.98 (m, 20H), 0.91-0.86 (m, 4H), 0.87 (s, 3H), 0.85 (s, 3H), 0.74-0.64 (m, 2H), 0.62 (s, 3H), 0.51 (s, 1.5H), 0.49 (s, 1.5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 147.8, 147.7, 143.6, 137.2, 137.0, 136.8, 136.6, 135.8, 129.9, 129.8, 129.7, 129.6, 129.0, 128.9, 128.4, 128.3, 127.9, 127.3, 127.2, 127.1, 127.0, 124.2, 124.0, 122.9, 122.8, 120.3, 120.1, 56.5, 56.2, 56.0, 55.9, 55.4, 55.3, 54.5, 54.4, 53.1, 53.0, 52.4, 44.8, 44.6, 43.2, 42.5, 42.2, 39.9, 39.5, 36.7, 36.1, 35.7, 35.6, 35.4, 35.3, 34.7, 32.5, 32.0, 29.6, 28.9, 28.7, 28.2, 27.9, 26.8, 24.1, 23.8, 22.8, 22.5, 21.5, 20.9, 18.6, 12.0, 11.4; HRMS (ESI) calcd for $C_{53}H_{69}NNaO_4S$ [M + Na^+], 838.4840; found: 838.4828. **Isomer 2 (1:1)**. Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:5, R_f = 0.5); IR (neat): ν_{max} 2930, 2866, 1734, 1597, 1448, 1356, 1240, 1161, 1121, 1092, 1070, 949, 864, 814, 750, 662, 571 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.4 Hz, 1H), 7.66 (d, J = 8.4 Hz, 1H), 7.45 (d, J = 8.4 Hz, 0.5H), 7.42 (d, J = 8.4 Hz, 0.5H), 7.32-7.26 (m, 5H), 7.05-6.91 (m, 3H), 6.72 (td, J = 7.6, 1.6 Hz, 0.5H), 6.70 (td, J = 7.6, 1.6 Hz, 0.5H), 6.63-6.57 (m, 1H), 4.89 (d, J = 12.0 Hz, 0.5H), 4.87 (d, J = 12.0 Hz, 0.5H), 3.66 (s, 1.5H), 3.65 (s, 1.5H), 3.42 (d, J = 12.2 Hz, 0.5H), 3.40 (d, J = 12.2 Hz, 0.5H), 2.42 (d, J = 12.2 Hz, 1H), 2.40 (s, 3H), 2.39 (d, J = 14.2 Hz, 0.5H), 2.08 (d, J = 14.2 Hz, 0.5H), 1.89-1.71 (m, 4H), 1.59-1.48 (m, 4H), 1.33-0.94 (m, 18H), 0.88-0.84 (m, 12H), 0.68 (s, 1.5H), 0.67 (s, 1.5H), 0.58 (s, 1.5H), 0.57 (s, 1.5H), 0.34-0.30 (m, 1H), 0.20-0.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ

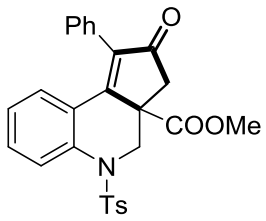
175.0, 149.6, 149.5, 143.6, 139.5, 139.4, 137.7, 137.6, 136.1, 130.1, 129.9, 129.8, 128.9, 128.3, 127.8, 127.4, 127.3, 127.2, 127.0, 125.0, 124.7, 123.2, 123.1, 120.7, 120.4, 56.4, 56.3, 56.2, 55.4, 55.1, 55.0, 54.4, 54.3, 53.3, 52.5, 50.5, 50.4, 42.5, 41.5, 41.4, 41.1, 40.8, 40.0, 39.6, 36.2, 35.7, 35.6, 35.4, 35.1, 34.8, 34.7, 34.4, 33.7, 32.1, 31.8, 29.1, 28.6, 28.2, 28.0, 24.1, 23.8, 22.9, 22.6, 21.6, 20.8, 20.7, 18.7, 12.1, 11.5, 11.4; HRMS (ESI) calcd for $C_{53}H_{69}NNaO_4S$ [M + Na^+], 838.4840; found: 838.4828.

4. Synthesis of products 10, 11, 13 and 14

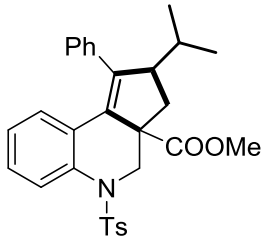
To a mixture of alkyl aldehyde **8** or **12** (1.5 mmol), enyne **1a** (0.3 mmol) and $FeCl_2$ (1.0 mg, 2.5 mol %), chlorobenzene (1.0 mL) was added under nitrogen at room temperature. Then pure *di-tert*-butyl peroxide (137 μL, 0.75 mmol) was dropped into the mixture. The resulting mixture was stirred at 120 ℃ for 2 hours. After the mixture was cooled to room temperature, the resulting solution was directly filtered through a pad of silica by EtOAc. The solvent was evaporated in vacuo to give the crude products. NMR yields were determined by ^{1}H NMR using dibromomethane as an internal standard. The residue was purified by flash column chromatography on silica gel (ethyl acetate/petroleum ether) to give the pure product **10, 11** and **13**. The product **14** was detected by crude ^{1}H NMR, GC-MS and HRMS (ESI).



Methyl (3a)-2-methyl-1-phenyl-5-tosyl-2,3,4,5-tetrahydro-3aH-cyclopenta[c]quinoline-3a-carboxylate (**10**, 1:1). (47 mg, 33%). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:5, R_f = 0.6); IR (neat): ν_{max} 2955, 2924, 2868, 1732, 1599, 1479, 1456, 1352, 1246, 1167, 1090, 1074, 1047 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 8.4 Hz, 2H), 7.60 (dd, J = 8.4, 0.6 Hz, 1H), 7.50 (dd, J = 8.6, 1.0 Hz, 1H), 7.33-7.22 (m, 10H), 7.11-7.07 (m, 3H), 6.98 (d, J = 8.4 Hz, 2H), 6.93-6.90 (m, 2H), 6.82 (dd, J = 7.6, 1.0 Hz, 1H), 6.75 (td, J = 7.6, 1.0 Hz, 1H), 6.68 (td, J = 7.6, 1.0 Hz, 1H), 5.02 (d, J = 12.0 Hz, 1H), 4.81 (d, J = 12.0 Hz, 1H), 3.74 (d, J = 12.6 Hz, 1H), 3.65 (s, 3H), 3.56 (s, 3H), 3.43 (d, J = 12.0 Hz, 1H), 3.46-3.40 (m, 1H), 2.91-2.87 (m, 1H), 2.77 (q, J = 7.4 Hz, 1H), 2.39 (s, 3H), 2.34 (s, 3H), 2.30-2.23 (m, 2H), 1.54-1.49 (m, 1H), 1.20 (d, J = 7.0 Hz, 3H), 0.84 (d, J = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 174.2, 144.7, 144.2, 143.7, 143.6, 137.7, 137.2, 136.8, 135.9, 129.8, 129.7, 129.6, 128.5, 128.3, 128.2, 128.0, 127.9, 127.6, 127.5, 127.4, 127.3, 127.2, 127.0, 125.9, 124.0, 123.9, 123.0, 122.7, 120.3, 58.4, 57.2, 55.8, 55.1, 52.5, 52.4, 45.3, 43.6, 42.4, 41.0, 21.5, 19.8, 19.4; HRMS (ESI) calcd for $C_{28}H_{27}NNaO_4S$ [M + Na^+], 496.1553; found: 496.1555.

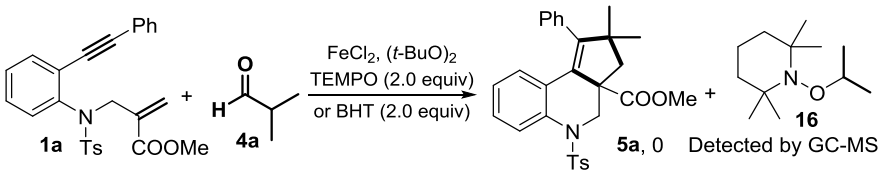


Methyl (3a)-2-methyl-1-phenyl-5-tosyl-2,3,4,5-tetrahydro-3aH-cyclopenta[c]quinoline-3a-carboxylate (11). (48 mg). Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:2, R_f = 0.3); IR (neat): ν_{max} 2953, 2926, 2870, 1730, 1709, 1599, 1477, 1460, 1352, 1238, 1167, 1070, 758, 735, 700, 658 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.77 (dd, J = 8.6, 0.6 Hz, 1H), 7.68 (d, J = 8.4 Hz, 2H), 7.35-7.33 (m, 3H), 7.29-7.27 (m, 2H), 7.26-7.23 (m, 1H), 7.13-7.11 (m, 2H), 7.08 (dd, J = 7.8, 1.5 Hz, 1H), 6.83 (td, J = 7.6, 1.0 Hz, 1H), 5.17 (d, J = 12.2 Hz, 1H), 3.58 (s, 3H), 3.55 (d, J = 12.2 Hz, 1H), 3.00 (d, J = 18.6 Hz, 1H), 2.53 (d, J = 18.6 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.3, 171.5, 159.2, 144.5, 137.1, 136.4, 135.5, 131.5, 130.2, 129.9, 128.8, 128.6, 128.5, 128.4, 127.2, 123.4, 121.8, 121.4, 53.1, 53.0, 49.8, 44.3, 21.5; HRMS (ESI) calcd for $C_{27}H_{23}NNaO_5S$ [M + Na^+], 496.1189; found: 496.1195.



Methyl 2-isopropyl-1-phenyl-5-tosyl-3,3a,4,5-tetrahydro-2H-cyclopenta[c]quinoline-3a-carboxylate (13). (48 mg, 32%). **Isomer 1:** Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:5, R_f = 0.6); IR (neat): ν_{max} 2953, 2930, 2870, 1734, 1458, 1352, 1242, 1204, 1167, 1092, 1070, 1045 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 8.4 Hz, 2H), 7.53 (dd, J = 8.2, 1.0 Hz, 1H), 7.35-7.29 (m, 3H), 7.24 (d, J = 8.4 Hz, 2H), 7.03-6.96 (m, 4H), 6.67 (td, J = 7.6, 1.0 Hz, 1H), 5.03 (d, J = 11.8 Hz, 1H), 3.59 (s, 3H), 3.43 (d, J = 11.8 Hz, 1H), 2.91-2.87 (m, 1H), 2.40 (s, 3H), 2.33 (dd, J = 14.2, 4.2 Hz, 1H), 2.02 (dd, J = 14.2, 10.0 Hz, 1H), 1.91-1.84 (m, 1H), 0.87 (d, J = 6.8 Hz, 3H), 0.83 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 143.6, 143.0, 137.7, 137.0, 135.7, 131.7, 129.7, 128.4, 127.5, 127.4, 127.3, 127.0, 124.1, 122.9, 120.2, 57.3, 56.9, 55.7, 52.2, 31.8, 28.1, 21.6, 21.5, 16.1; HRMS (ESI) calcd for $C_{30}H_{31}NNaO_4S$ [M + Na^+], 524.1866; found: 524.1850; **Isomer 2:** Isolated by flash column chromatography (ethyl acetate/petroleum ether = 1:5, R_f = 0.55); IR (neat): ν_{max} 2945, 2924, 2868, 1732, 1590, 1460, 1385, 1354, 1229, 1169, 1090, 1028 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 8.2 Hz, 1H), 7.58 (d, J = 8.2 Hz, 2H), 7.29-7.22 (m, 6H), 7.08 (t, J = 7.4 Hz, 1H), 6.97-6.93 (br, 1H), 6.76-6.70 (m, 2H), 4.85 (d, J = 11.8 Hz, 1H), 3.55-3.52 (m, 5H), 2.43-2.37 (m, 1H), 2.36 (s, 3H), 1.84-1.59 (m, 2H), 0.83 (d, J = 6.8 Hz, 3H), 0.39 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.4, 143.7, 142.3, 136.2, 135.8, 130.9,129.5, 128.3, 127.9, 127.5, 127.4, 127.3, 125.6, 123.7, 123.0, 57.5, 56.0, 53.8, 52.4, 33.4, 27.1, 21.5, 20.9, 15.4; HRMS (ESI) calcd for $C_{30}H_{31}NNaO_4S$ [M + Na^+], 524.1866; found: 524.1850.

5. The radical trapping experiment



To a mixture of isobutyraldehyde **4a** (1.5 mmol), enyne **1a** (0.3 mmol), $FeCl_2$ (1.0 mg, 2.5 mol %) and **TEMPO** or **BHT** (0.6 mmol), chlorobenzene (1.0 mL) was added under nitrogen at room temperature. Then pure di-*tert*-butyl peroxide (137 μL, 0.75 mmol) was dropped into the mixture. The resulting mixture was stirred at 120 ℃ for 2 hours. After the mixture was cooled to room temperature, the resulting solution was directly filtered through a pad of silica by EtOAc. The solvent was evaporated in vacuo to give the crude products. NMR yields were determined by ^{1}H NMR using dibromomethane as an internal standard. **4a** was almost recovered, and **5a** was not detected by ^{1}H NMR. Moreover, the TEMPO-*iso*propyl adduct **16** was detected by GC-MS when TEMPO was added.

6. X-ray crystallography data for 3m.

Figure S1: ORTER drawing of 3m

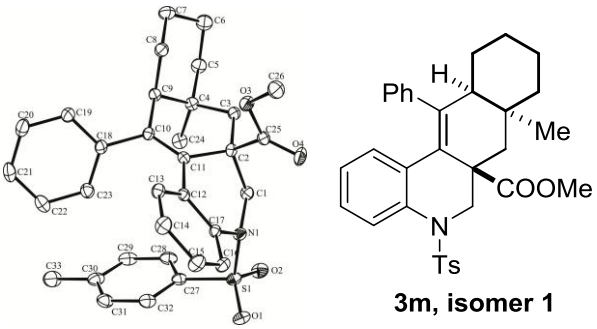


Table S1 Crystal data and structure refinement for 3m-isomer 1

Identification code	**3m-isomer 1**
Empirical formula	$C_{33}H_{35}NO_4S$
Formula weight	541.68
Temperature/K	180.01(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.4186(13)
b/Å	11.3388(8)
c/Å	16.9081(14)

α/°	90
β/°	107.550(9)
γ/°	90
Volume/Å^3	2818.4(4)
Z	4
ρ_{calc}g/cm^3	1.277
μ/mm^{-1}	0.154
F(000)	1152.0
Crystal size/mm^3	0.15 × 0.1 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/ °	6.14 to 52.042
Index ranges	-18 ≤ h ≤ 19, -13 ≤ k ≤ 13, -20 ≤ l ≤ 13
Reflections collected	14537
Independent reflections	5526 [R_{int} = 0.0586, R_{sigma} = 0.0800]
Data/restraints/parameters	5526/0/355
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0534, wR_2 = 0.1076
Final R indexes [all data]	R_1 = 0.1051, wR_2 = 0.1358
Largest diff. peak/hole / e Å^{-3}	0.29/-0.40

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3m-isomer 1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ}tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	7206.5(17)	6640(2)	7519.7(16)	27.4(6)
C2	7915.3(17)	7111(2)	8298.3(15)	22.9(6)
C3	7638.7(18)	8382(2)	8469.8(16)	26.7(6)
C4	7130.0(17)	8480(2)	9122.7(16)	28.0(6)
C5	7016.5(19)	9787(2)	9310.5(19)	35.7(7)
C6	7896(2)	10423(2)	9770.8(19)	42.6(8)
C7	8400(2)	9750(2)	10552.0(19)	41.5(8)
C8	8574.8(18)	8479(2)	10352.7(17)	29.8(6)
C9	7676.7(17)	7833(2)	9916.3(16)	24.8(6)
C10	7842.9(16)	6548(2)	9723.9(15)	22.9(6)

C11	7988.5(16)	6247(2)			9007.2(15)	21.4(6)
C12	8286.6(16)	5080(2)			8793.8(16)	21.4(6)
C13	8964.4(17)	4431(2)			9362.6(17)	26.1(6)
C14	9326.3(19)	3429(2)			9121.1(17)	34.0(7)
C15	9044.0(19)	3074(2)			8300.8(18)	34.6(7)
C16	8392.1(18)	3717(2)			7720.7(17)	28.8(6)
C17	8002.1(16)	4708(2)			7966.7(15)	21.5(6)
C18	7769.6(17)	5642(2)			10342.9(16)	25.2(6)
C19	8209(2)	5780(2)			11188.9(17)	33.9(7)
C20	8097(2)	4958(2)			11755.7(18)	39.6(8)
C21	7537(2)	4000(3)			11497.6(19)	38.3(7)
C22	7102(2)	3843(2)			10663(2)	38.0(7)
C23	7215.5(18)	4667(2)			10094.3(18)	31.6(7)
C24	6170.0(18)	7939(2)			8801.6(19)	34.9(7)
C25	8837.1(18)	7160(2)			8126.8(17)	25.7(6)
C26	10420.6(19)	7337(3)			8719.6(19)	40.7(8)
C27	5830.6(17)	4288(2)			7589.3(17)	28.6(6)
C28	5219.8(18)	5062(2)			7776.5(19)	35.5(7)
C29	4802.2(19)	4746(3)			8362(2)	40.4(8)
C30	4981.2(19)	3675(3)			8769.9(19)	39.0(8)
C31	5594.2(19)	2909(3)			8574.4(19)	38.0(7)
C32	6017.1(18)	3213(2)			7986.9(18)	34.4(7)
C33	4534(2)	3341(3)			9413(2)	55.1(9)
N1	7317.3(14)	5366.7(17)			7363.1(13)	25.2(5)
O1	6601.5(12)	3624.2(16)			6507.9(11)	35.9(5)
O2	5826.5(13)	5560.2(16)			6307.8(12)	39.3(5)
O3	9520.1(12)	7343.0(16)			8820.2(11)	31.7(5)
O4	8946.8(13)	7049.3(17)			7458.2(12)	38.4(5)
S1	6367.0(5)	4686.9(6)			6844.2(4)	29.7(2)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3m-isomer 1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}

C1	25.8(14)	28.3(15)	25.8(15)	3.4(12)	4.3(12)	1.9(12)
C2	22.7(13)	25.3(14)	20.9(14)	2.3(11)	6.8(11)	1.6(11)
C3	30.6(15)	23.5(14)	25.7(15)	2.4(11)	8.0(12)	0.6(12)
C4	27.4(14)	26.6(14)	30.2(16)	-0.2(12)	8.9(12)	3.4(12)
C5	40.2(17)	28.5(15)	39.7(18)	-1.4(13)	14.0(14)	7.2(13)
C6	56(2)	26.9(15)	48(2)	-3.5(14)	19.6(16)	5.4(15)
C7	52(2)	30.5(16)	39.7(18)	-8.9(14)	11.3(15)	-4.8(14)
C8	32.5(15)	28.9(15)	27.4(15)	-0.3(12)	7.9(12)	0.6(12)
C9	27.9(14)	22.0(13)	27.4(15)	0.0(11)	12.7(12)	2.1(11)
C10	22.6(13)	24.7(13)	20.9(14)	1.2(11)	6.0(11)	0.9(11)
C11	17.8(12)	21.7(13)	23.5(14)	2.4(11)	4.2(11)	0.1(10)
C12	18.6(12)	23.9(14)	23.2(14)	0.5(11)	8.3(11)	-1.9(11)
C13	24.1(14)	29.9(15)	24.8(15)	1.1(12)	8.3(12)	1.4(12)
C14	33.0(16)	36.2(16)	29.8(17)	4.8(13)	4.8(13)	10.1(13)
C15	36.6(16)	35.0(16)	33.3(17)	-3.5(13)	12.3(14)	10.7(13)
C16	29.7(15)	34.1(16)	23.7(15)	-4.4(12)	9.6(12)	0.0(12)
C17	19.1(12)	24.9(13)	21.6(14)	0.4(11)	7.8(11)	-1.1(11)
C18	27.8(14)	25.5(14)	26.4(15)	0.1(11)	14.3(12)	4.0(12)
C19	47.4(18)	29.3(15)	27.8(16)	-1.7(12)	15.8(14)	-1.7(13)
C20	59(2)	35.7(17)	27.2(17)	4.0(13)	18.5(15)	11.8(16)
C21	48.8(19)	35.6(17)	40.6(19)	12.9(14)	28.5(16)	10.1(15)
C22	37.7(17)	31.8(16)	49(2)	7.4(14)	20.5(15)	-0.8(13)
C23	30.4(15)	33.8(16)	31.5(16)	2.2(13)	10.9(13)	-2.0(13)
C24	26.5(15)	37.1(16)	40.4(18)	2.5(13)	9.0(13)	7.8(13)
C25	31.2(15)	20.1(14)	25.1(16)	4.9(11)	7.2(13)	1.4(11)
C26	28.5(16)	55(2)	42.1(19)	-4.2(15)	16.1(14)	-9.7(14)
C27	23.1(14)	29.5(15)	31.9(16)	-7.4(12)	6.3(12)	-2.5(12)
C28	26.4(15)	31.1(16)	46.1(19)	-8.3(13)	6.6(14)	-0.3(12)
C29	24.3(15)	41.5(18)	57(2)	-18.7(16)	14.2(15)	-3.2(13)
C30	30.6(16)	45.7(19)	44.3(19)	-16.5(15)	16.6(14)	-12.4(14)
C31	34.0(17)	35.3(16)	46.9(19)	-6.8(14)	15.4(15)	-9.3(13)
C32	26.5(15)	34.6(17)	43.6(18)	-9.1(14)	12.8(14)	-3.0(12)
C33	53(2)	60(2)	65(2)	-18.6(18)	36.9(19)	-18.2(17)

N1	26.9(12)	25.1(12)	21.3(12)	-0.8(9)	3.9(10)	0.8(9)
O1	34.5(11)	38.3(11)	32.9(11)	-13.5(9)	7.0(9)	-0.9(9)
O2	34.5(11)	42.5(12)	30.4(11)	-0.1(9)	-6.0(9)	3.9(9)
O3	22.4(10)	46.4(12)	26.3(11)	-4.0(9)	7.3(8)	-5.8(8)
O4	41.5(12)	53.9(13)	24.1(11)	1.8(9)	16.2(10)	-1.2(10)
S1	26.2(4)	33.3(4)	26.0(4)	-5.1(3)	2.4(3)	0.1(3)

Table 4 Bond Lengths for 3m-isomer 1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.531(3)	C16	C17	1.396(4)
C1	N1	1.487(3)	C17	N1	1.437(3)
C2	C3	1.555(3)	C18	C19	1.395(4)
C2	C11	1.526(3)	C18	C23	1.383(4)
C2	C25	1.535(4)	C19	C20	1.385(4)
C3	C4	1.539(4)	C20	C21	1.374(4)
C4	C5	1.537(4)	C21	C22	1.380(4)
C4	C9	1.539(4)	C22	C23	1.389(4)
C4	C24	1.542(4)	C25	O3	1.335(3)
C5	C6	1.525(4)	C25	O4	1.199(3)
C6	C7	1.520(4)	C26	O3	1.449(3)
C7	C8	1.523(4)	C27	C28	1.392(4)
C8	C9	1.543(3)	C27	C32	1.380(4)
C9	C10	1.531(3)	C27	S1	1.762(3)
C10	C11	1.341(3)	C28	C29	1.381(4)
C10	C18	1.495(3)	C29	C30	1.382(4)
C11	C12	1.481(3)	C30	C31	1.394(4)
C12	C13	1.398(3)	C30	C33	1.502(4)
C12	C17	1.398(3)	C31	C32	1.386(4)
C13	C14	1.380(4)	N1	S1	1.654(2)
C14	C15	1.383(4)	O1	S1	1.4247(19)
C15	C16	1.382(4)	O2	S1	1.4289(19)

Table 5 Bond Angles for 3m-isomer 1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	C1	C2	113.66(19)	C12	C17	N1	119.7(2)
C1	C2	C3	108.6(2)	C16	C17	C12	120.5(2)
C1	C2	C25	108.2(2)	C16	C17	N1	119.8(2)
C11	C2	C1	108.4(2)	C19	C18	C10	121.7(2)
C11	C2	C3	114.1(2)	C23	C18	C10	120.4(2)
C11	C2	C25	108.6(2)	C23	C18	C19	117.8(2)
C25	C2	C3	108.9(2)	C20	C19	C18	120.7(3)
C4	C3	C2	115.4(2)	C21	C20	C19	120.7(3)
C3	C4	C24	111.2(2)	C20	C21	C22	119.5(3)
C5	C4	C3	109.4(2)	C21	C22	C23	119.8(3)
C5	C4	C9	110.3(2)	C18	C23	C22	121.5(3)
C5	C4	C24	107.4(2)	O3	C25	C2	111.7(2)
C9	C4	C3	109.1(2)	O4	C25	C2	125.2(2)
C9	C4	C24	109.4(2)	O4	C25	O3	123.1(3)
C6	C5	C4	115.0(2)	C28	C27	S1	119.7(2)
C7	C6	C5	110.4(2)	C32	C27	C28	120.2(3)
C6	C7	C8	111.2(2)	C32	C27	S1	120.1(2)
C7	C8	C9	111.2(2)	C29	C28	C27	119.5(3)
C4	C9	C8	111.5(2)	C28	C29	C30	121.3(3)
C10	C9	C4	110.6(2)	C29	C30	C31	118.4(3)
C10	C9	C8	111.7(2)	C29	C30	C33	121.1(3)
C11	C10	C9	121.2(2)	C31	C30	C33	120.4(3)
C11	C10	C18	121.8(2)	C32	C31	C30	120.9(3)
C18	C10	C9	116.9(2)	C27	C32	C31	119.6(3)
C10	C11	C2	123.6(2)	C1	N1	S1	114.58(16)
C10	C11	C12	126.6(2)	C17	N1	C1	118.51(19)
C12	C11	C2	109.7(2)	C17	N1	S1	118.58(16)
C13	C12	C11	121.7(2)	C25	O3	C26	115.2(2)
C13	C12	C17	118.2(2)	N1	S1	C27	105.79(12)
C17	C12	C11	119.1(2)	O1	S1	C27	107.36(12)
C14	C13	C12	121.0(2)	O1	S1	N1	108.36(11)
C13	C14	C15	120.2(2)	O1	S1	O2	120.17(12)

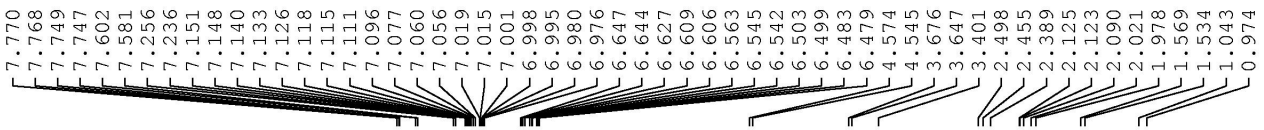
C16	C15	C14	120.0(2)	O2	S1	C27	108.79(13)
C15	C16	C17	120.0(2)	O2	S1	N1	105.52(11)

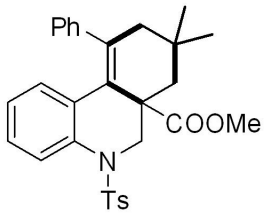
Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3m-isomer 1.

Atom	*x*	*y*	*z*	U(eq)
H1A	6592	6767	7575	33
H1B	7247	7099	7034	33
H3A	8196	8871	8654	32
H3B	7249	8720	7942	32
H5A	6734	10202	8780	43
H5B	6591	9844	9645	43
H6A	8288	10493	9405	51
H6B	7753	11228	9921	51
H7A	8035	9759	10944	50
H7B	8987	10145	10823	50
H8A	8895	8060	10872	36
H8B	8972	8469	9989	36
H9	7301	7828	10306	30
H13	9179	4682	9924	31
H14	9771	2982	9520	41
H15	9298	2388	8136	41
H16	8209	3484	7155	35
H19	8589	6446	11378	41
H20	8409	5057	12329	48
H21	7451	3449	11891	46
H22	6725	3174	10477	46
H23	6906	4558	9521	38
H24A	6218	7079	8780	52
H24B	5863	8242	8245	52
H24C	5819	8153	9176	52
H26A	10536	6568	8507	61
H26B	10875	7485	9257	61

H26C	10460	7955	8327	61
H28	5091	5803	7504	43
H29	4383	5274	8487	48
H31	5724	2169	8848	46
H32	6433	2684	7859	41
H33A	4932	3554	9965	83
H33B	4423	2488	9390	83
H33C	3954	3761	9304	83

7. Copies of ^{1}H NMR and ^{13}C NMR spectra for new compounds





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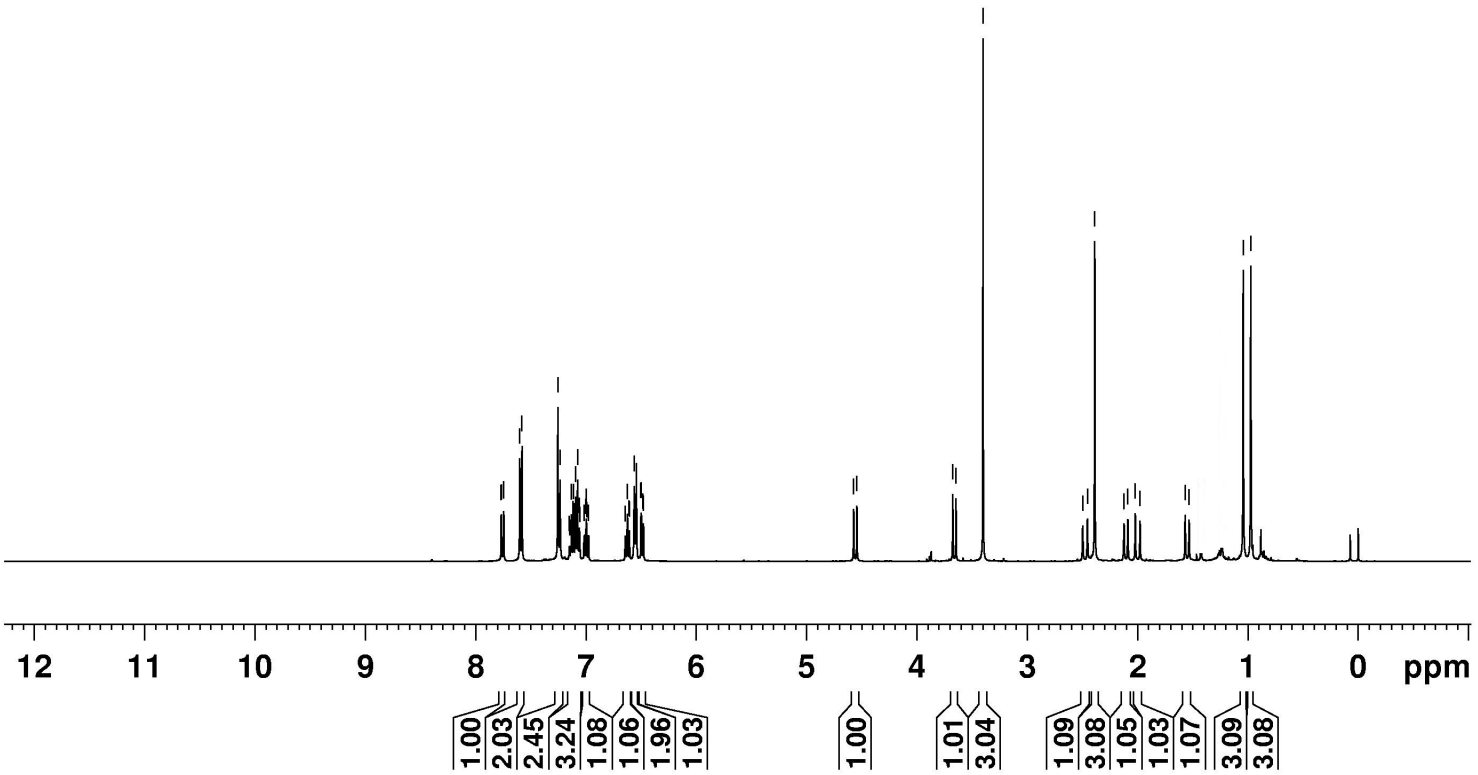

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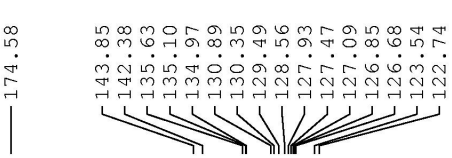
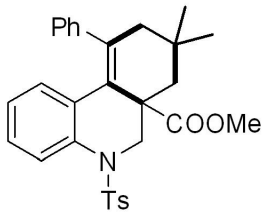
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	18
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	25.48
DW	62.400 usec
DE	6.50 usec
TE	555.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.2324716 MHz
NUC1	1H
P1	9.60 usec
SI	65536
SF	400.2300110 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





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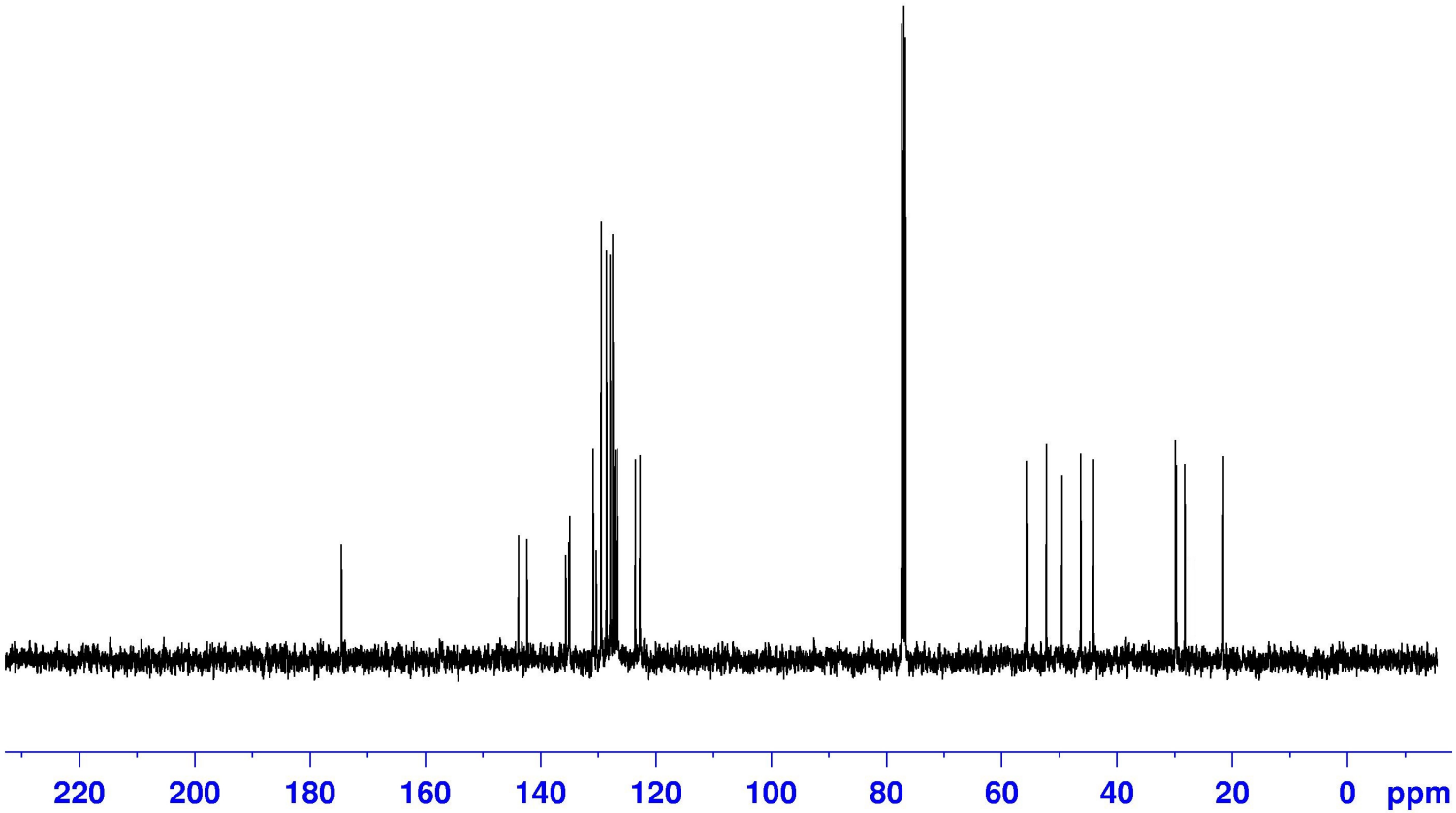

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EXPNO	2
PROCNO	1
Date_	20160816
Time	10.28
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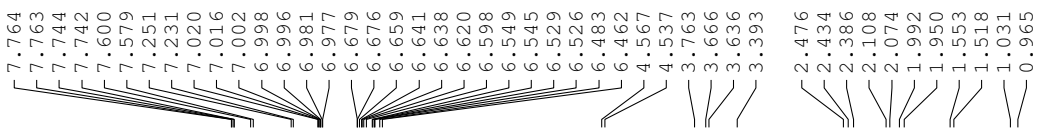
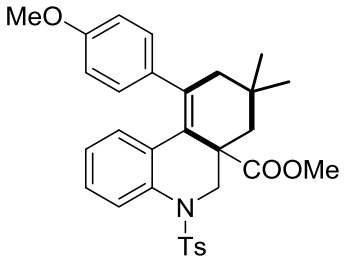
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	24
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	294.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127787 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40





3b

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EXPNO                       1
PROCNO                      1
Date_                20160623
Time                    17.08
INSTRUM                 spect
PROBHD    5 mm PADUL 13C
PULPROG                  zg30
TD                      32768
SOLVENT                 CDCl3
NS                          8
DS                          0
SWH                  6393.862 Hz
FIDRES               0.195125 Hz
AQ                   2.5625076 sec
RG                       90.5
DW                     78.200 usec
DE                      6.50 usec
TE                     296.9 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      13.10 usec
PL1                      1.80 dB
PL1W              8.92857742 W
SFO1             400.1326008 MHz
SI                      32768
SF               400.1300100 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
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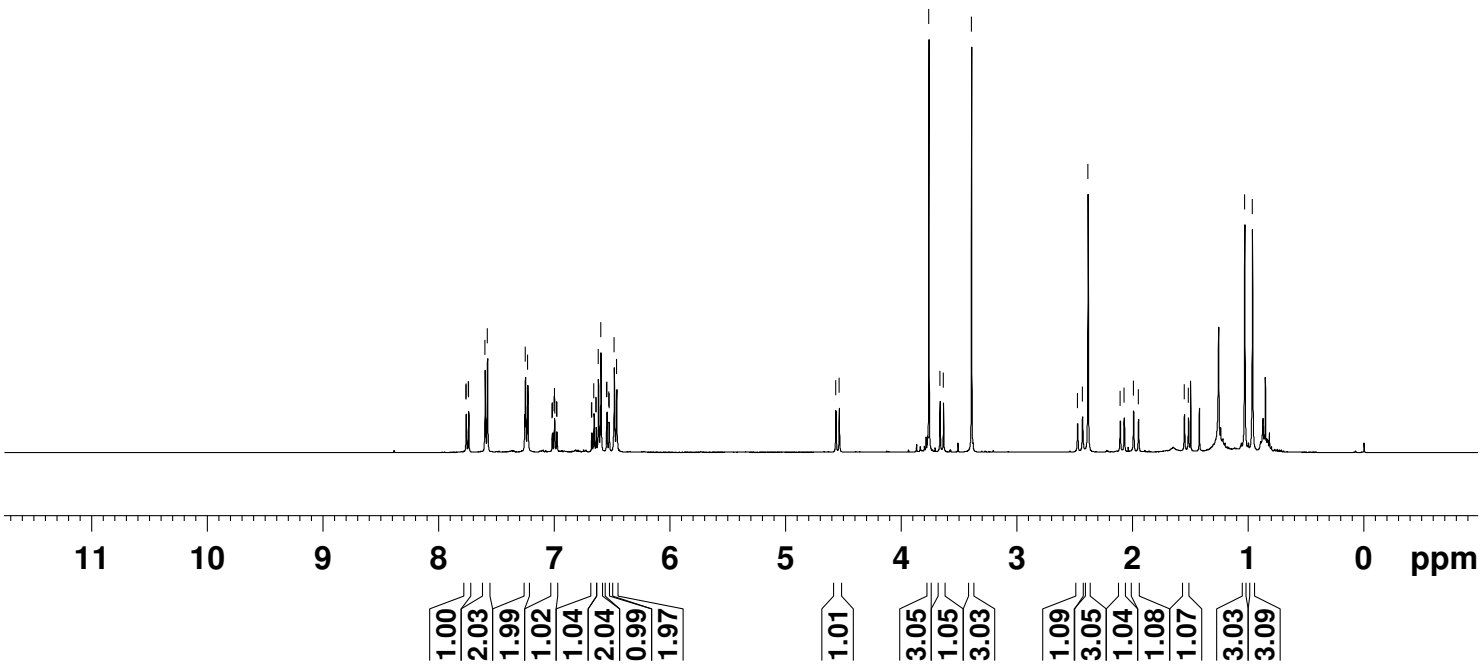

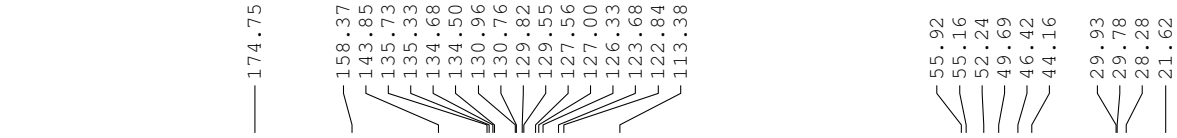

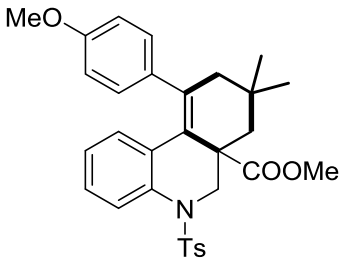

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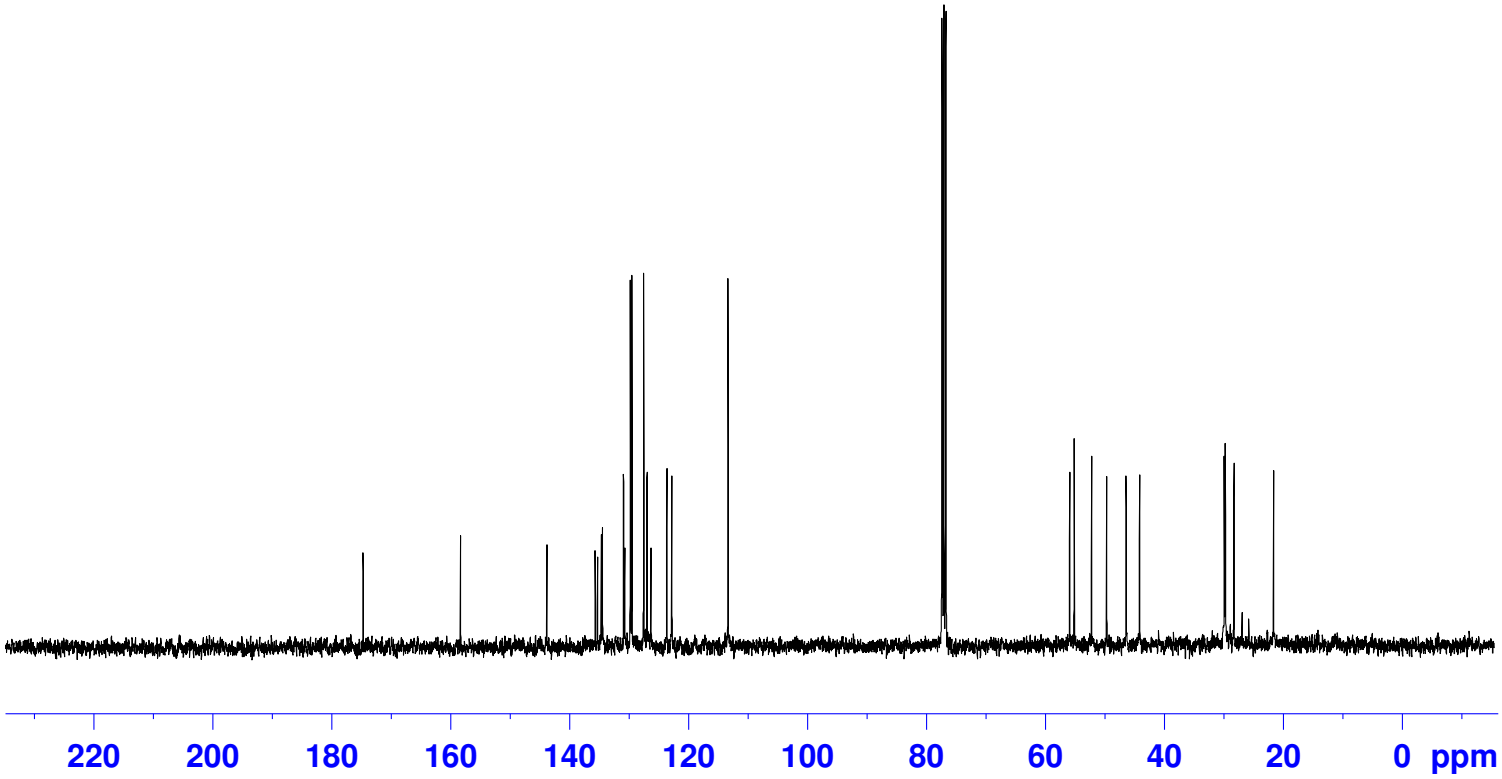


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EXPNO                           2
PROCNO                          1
Date_                    20160623
Time                        17.11
INSTRUM                     spect
PROBHD          5 mm PADUL 13C
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                            96
DS                             4
SWH                    25252.525 Hz
FIDRES                 0.385323 Hz
AQ                     1.2976629 sec
RG                          2050
DW                        19.800 usec
DE                         8.00 usec
TE                        297.7 K
D1                     2.00000000 sec
D11                    0.03000000 sec
TD0                            10

======== CHANNEL f1 ========
NUC1                          13C
P1                         13.50 usec
PL1                         3.00 dB
PL1W                43.93649673 W
SFO1                100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                          1H
PCPD2                      80.00 usec
PL2                         1.80 dB
PL12                       17.19 dB
PL13                       18.46 dB
PL2W                 8.92857742 W
PL12W                0.25809658 W
PL13W                0.19265592 W
SFO2                400.1316005 MHz
SI                         32768
SF                  100.6127690 MHz
WDW                           EM
SSB                            0
LB                          3.00 Hz
GB                             0
PC                          1.40
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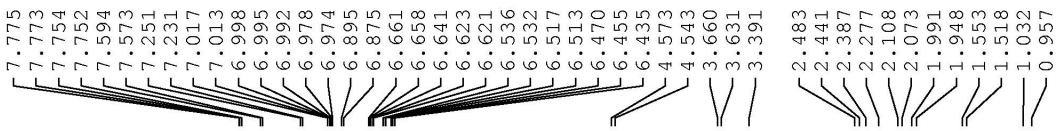

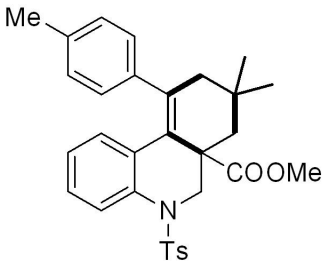

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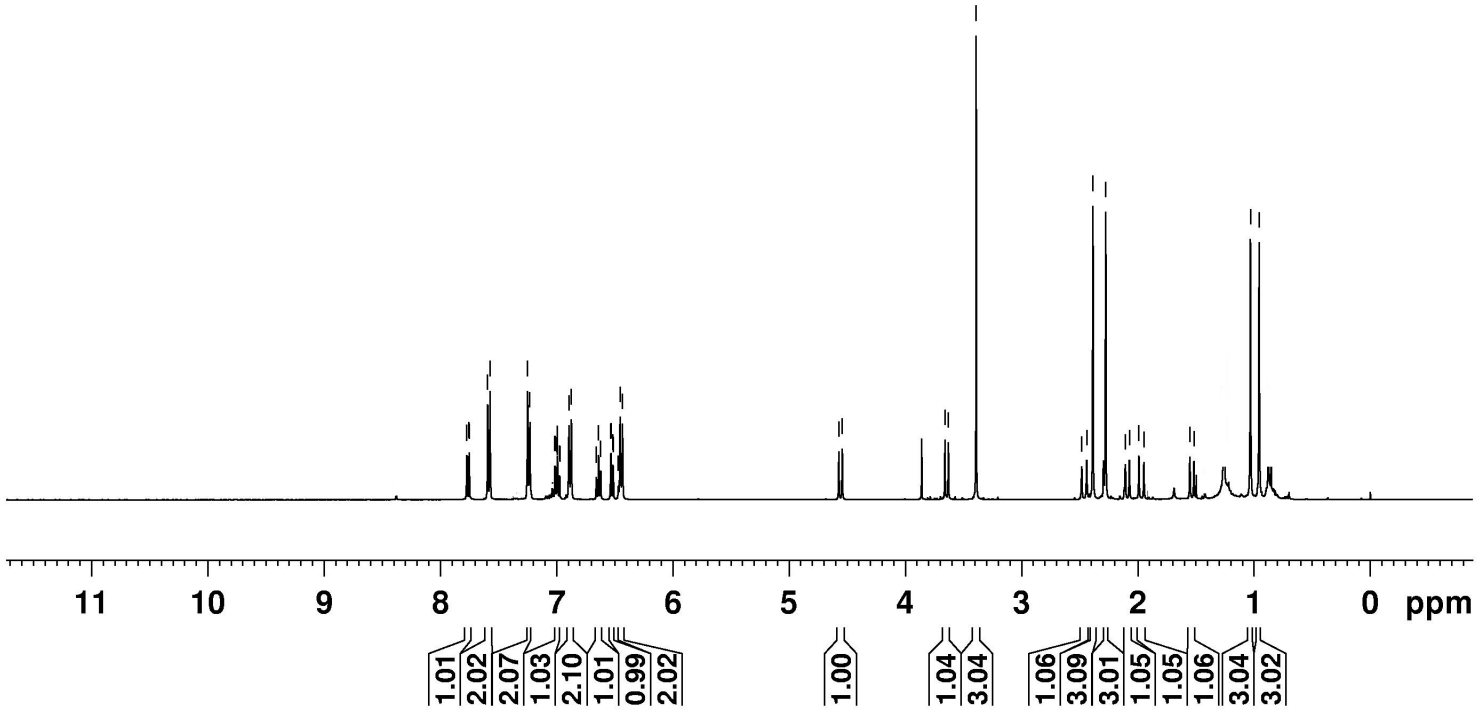

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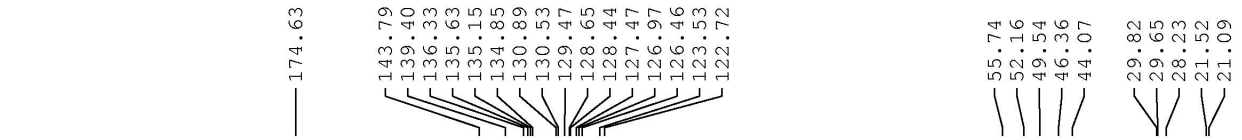
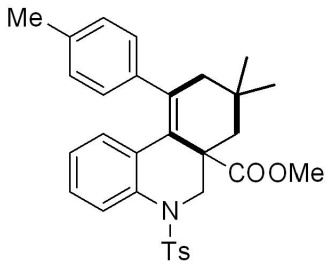
EXPNO	1
PROCNO	1
Date_	20160816
Time	15.34
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDC13
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	64
DW	78.200 usec
DE	6.50 usec
TE	296.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300132 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





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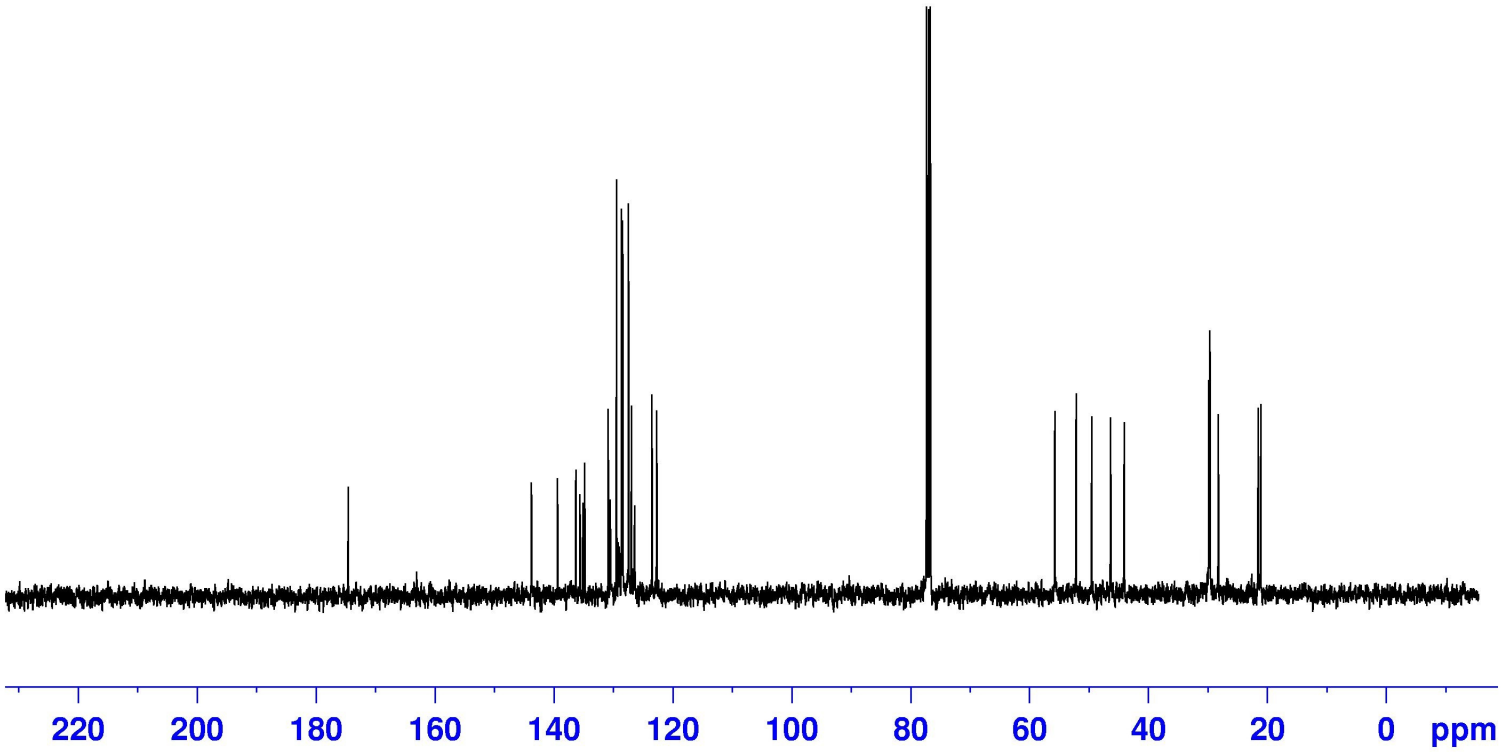

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EXPNO	2
PROCNO	1
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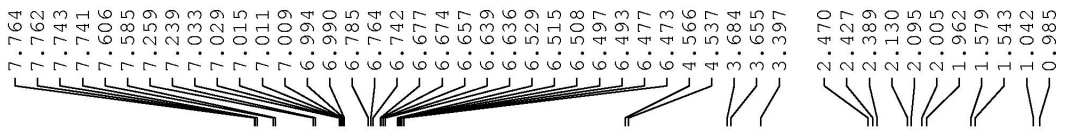
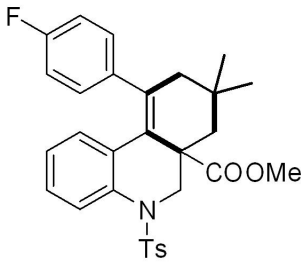
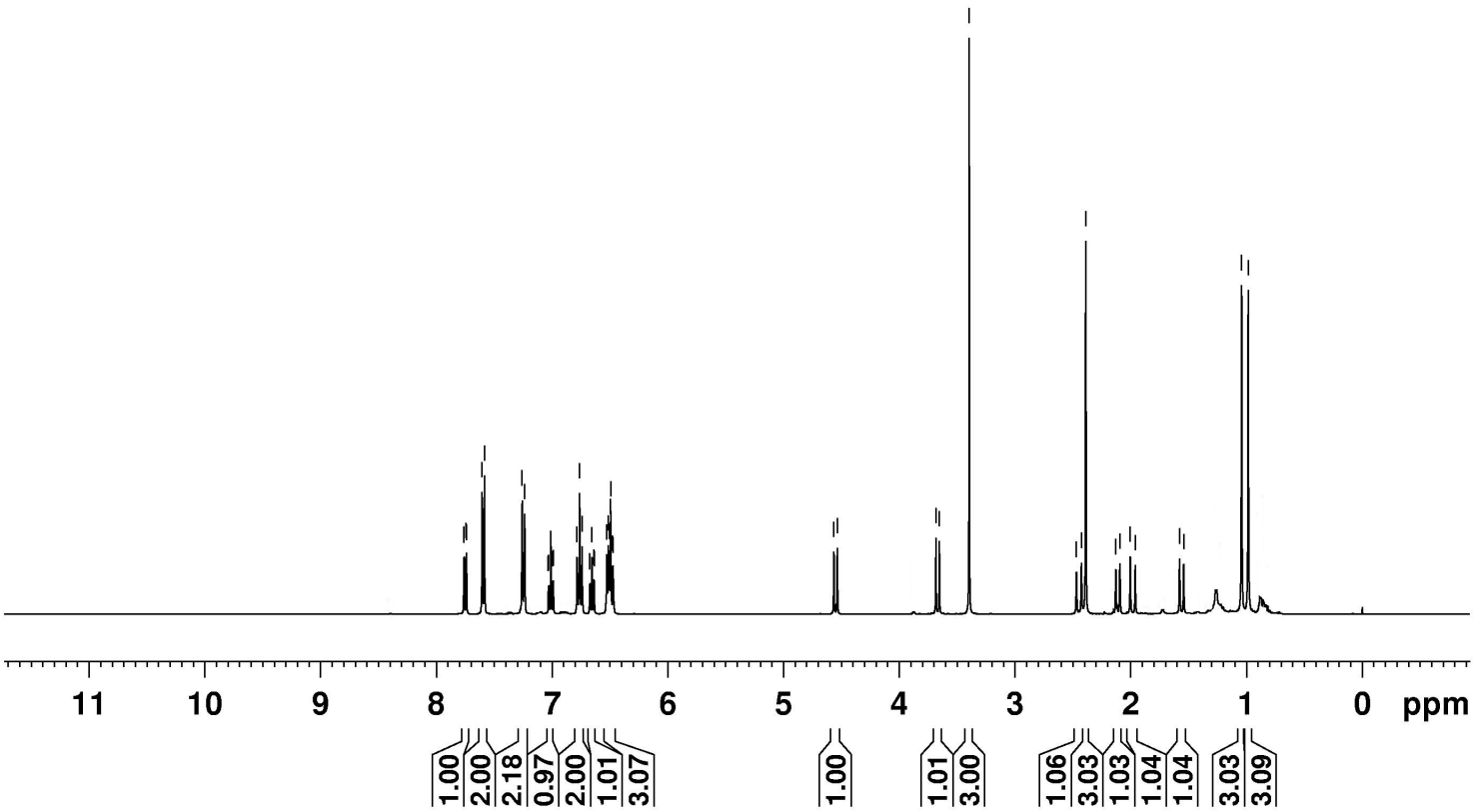
Time	15.41
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	48
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	297.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127784 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

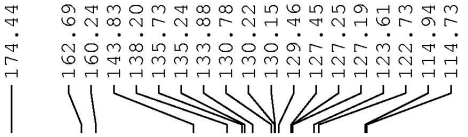


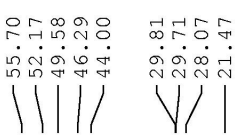


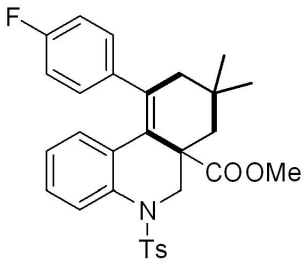
3d



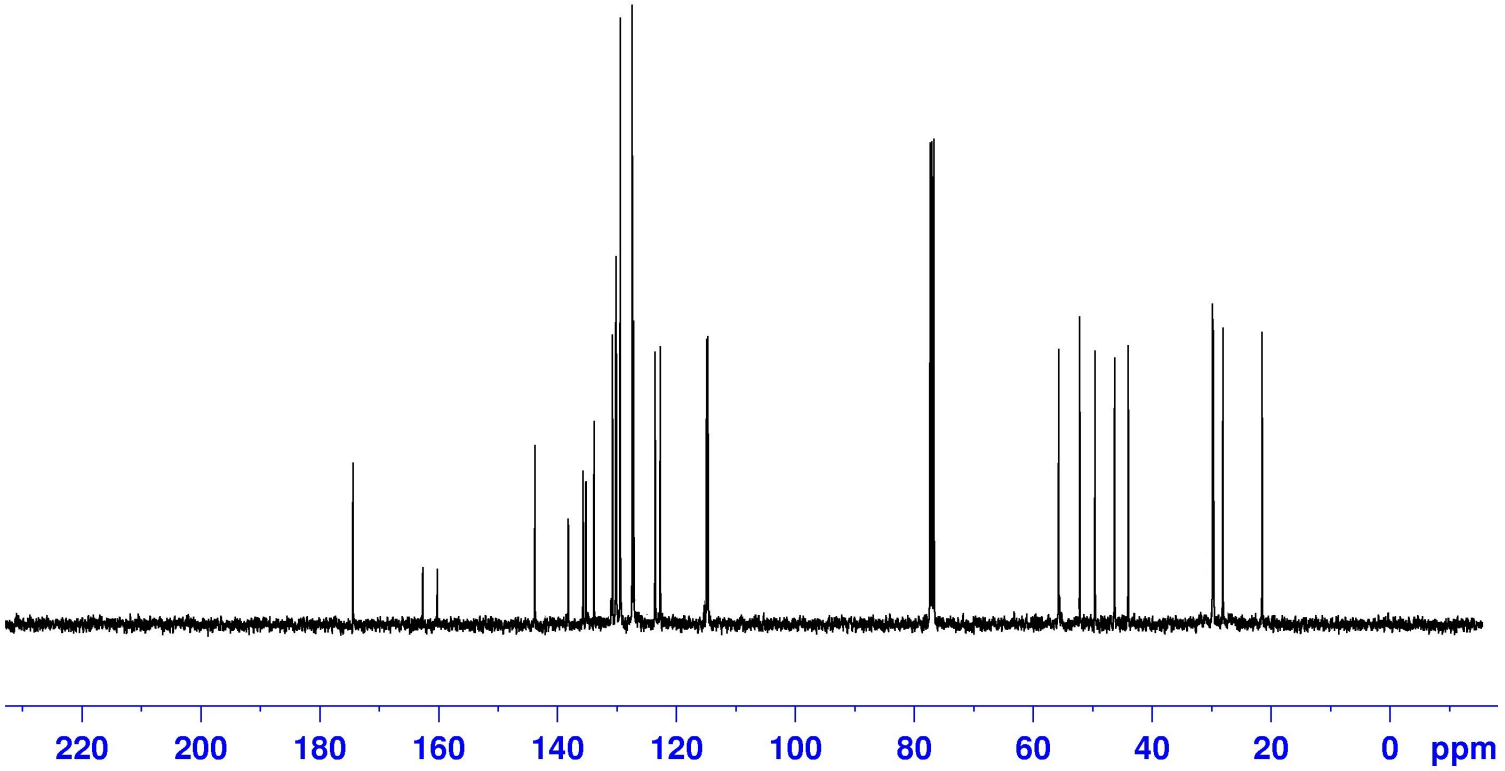
NAME	lly-798-3p-20160817	
EXPNO	1	
PROCNO	1	
Date_	20160817	
Time	13.11	
INSTRUM	spect	
PROBHD	5 mm PADUL 13C	
PULPROG	zg30	
TD	32768	
SOLVENT	CDCl3	
NS	8	
DS	0	
SWH	6393.862	Hz
FIDRES	0.195125	Hz
AQ	2.5625076	sec
RG	57	
DW	78.200	usec
DE	6.50	usec
TE	296.9	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	13.10	usec
PL1	1.80	dB
PL1W	8.92857742	W
SFO1	400.1326008	MHz
SI	32768	
SF	400.1300078	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



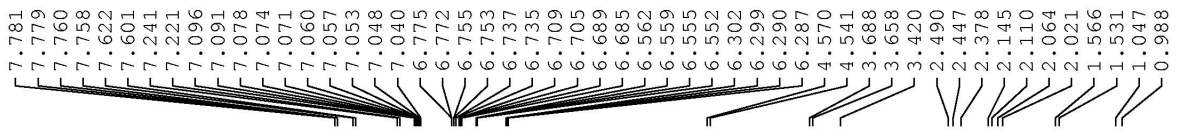


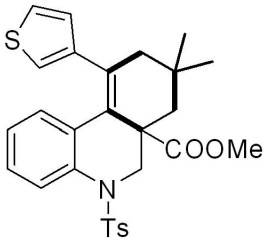


3d



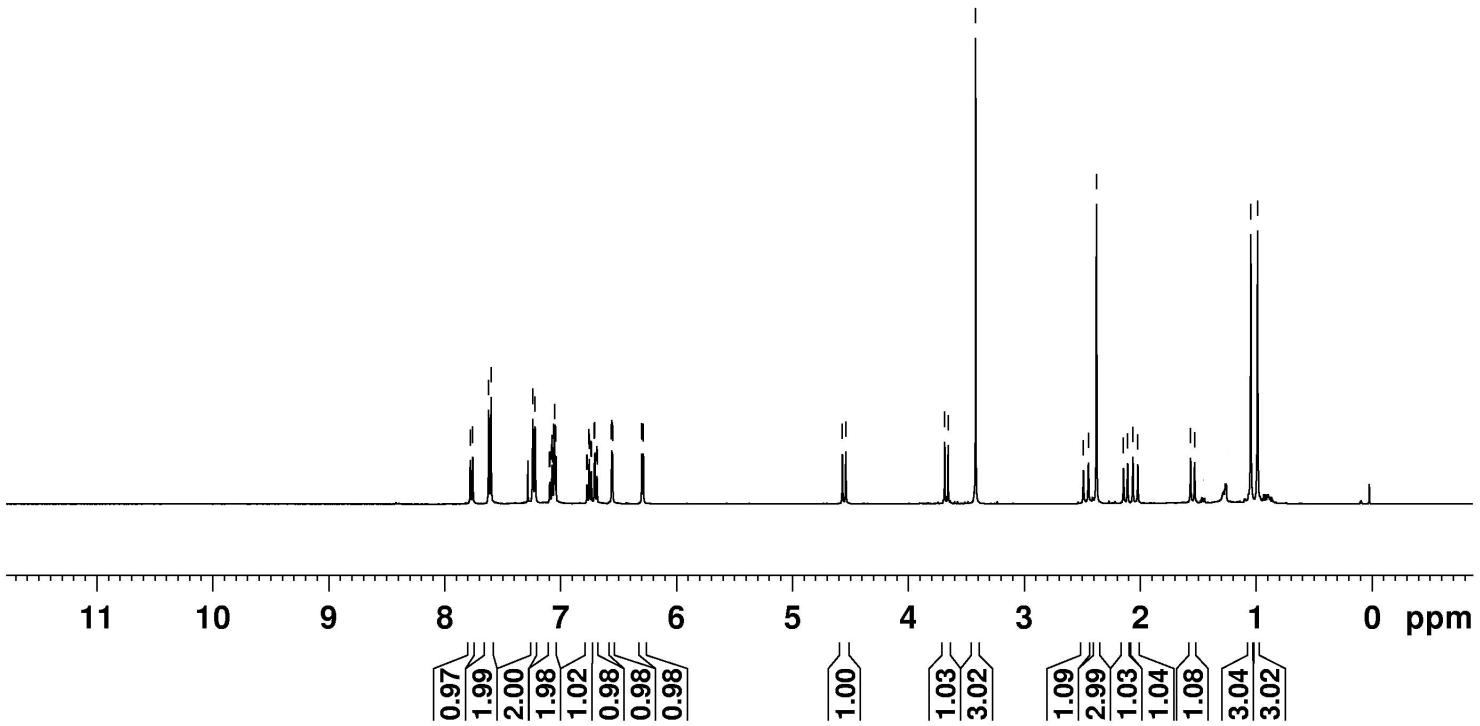
NAME	lly-798-3p-20160817
EXPNO	2
PROCNO	1
Date_	20160817
Time	13.18
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	80
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	296.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127806 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

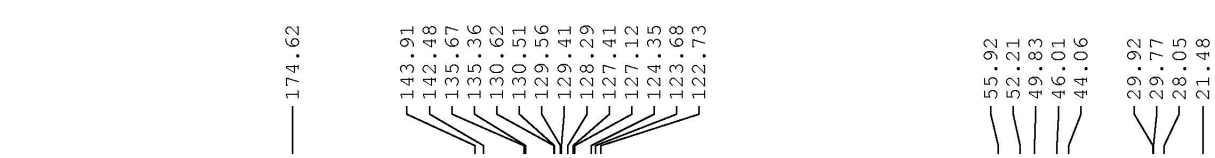


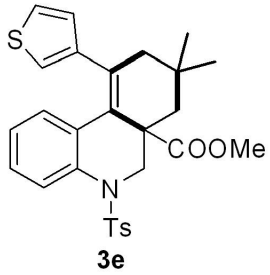


3e

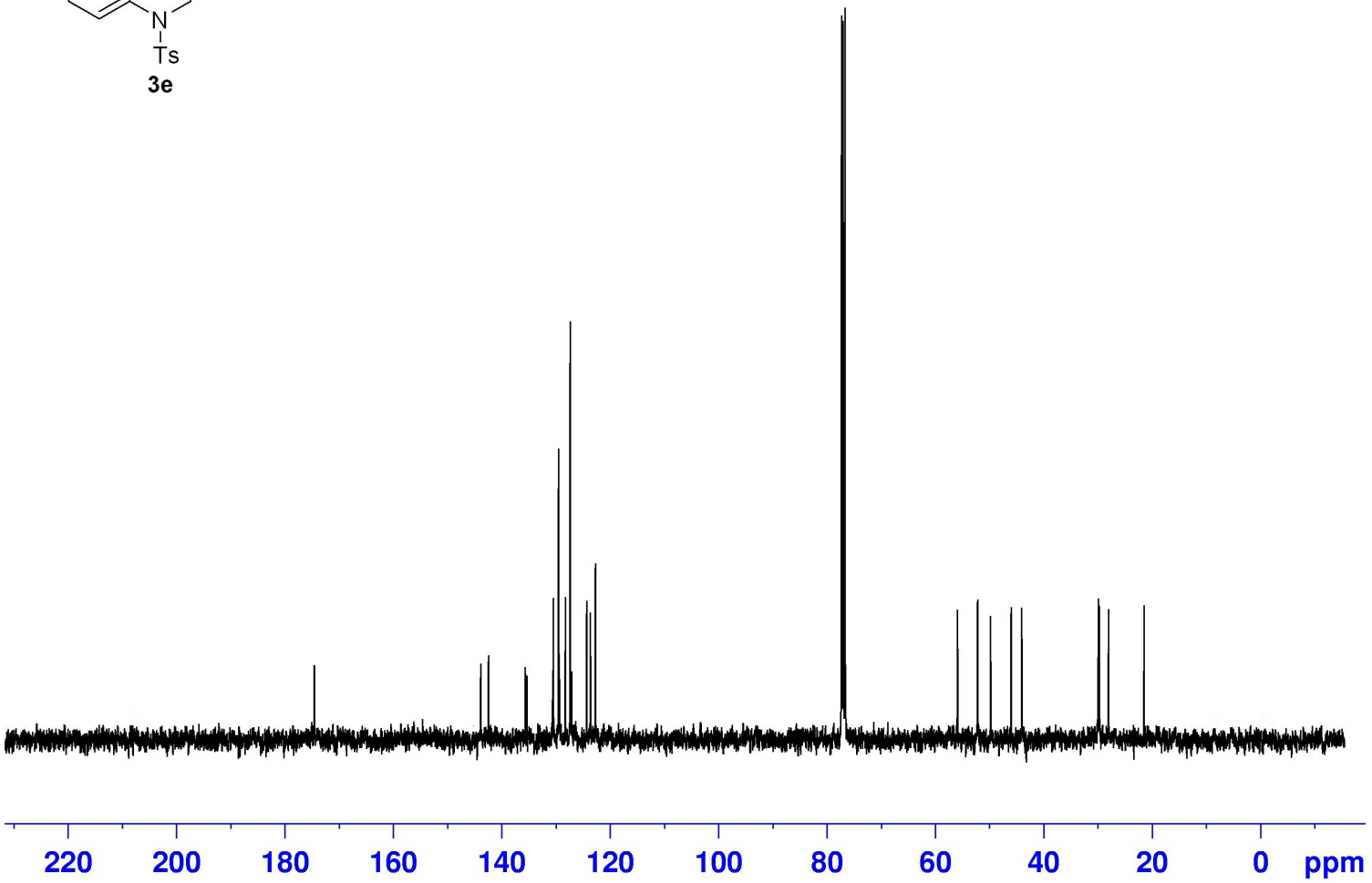
NAME	lly-781-2p-20160816
EXPNO	1
PROCNO	1
Date_	20160816
Time	22.05
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	128
DW	78.200 usec
DE	6.50 usec
TE	297.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



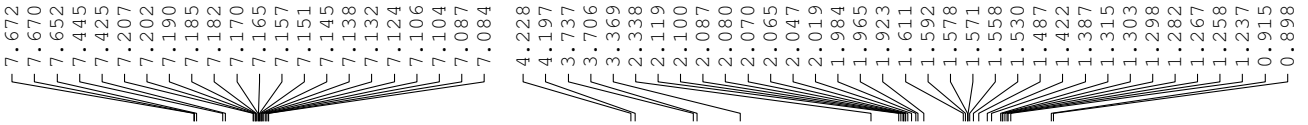


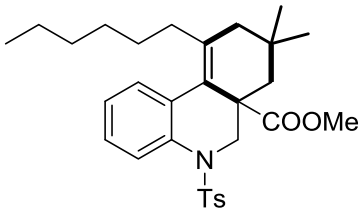


3e

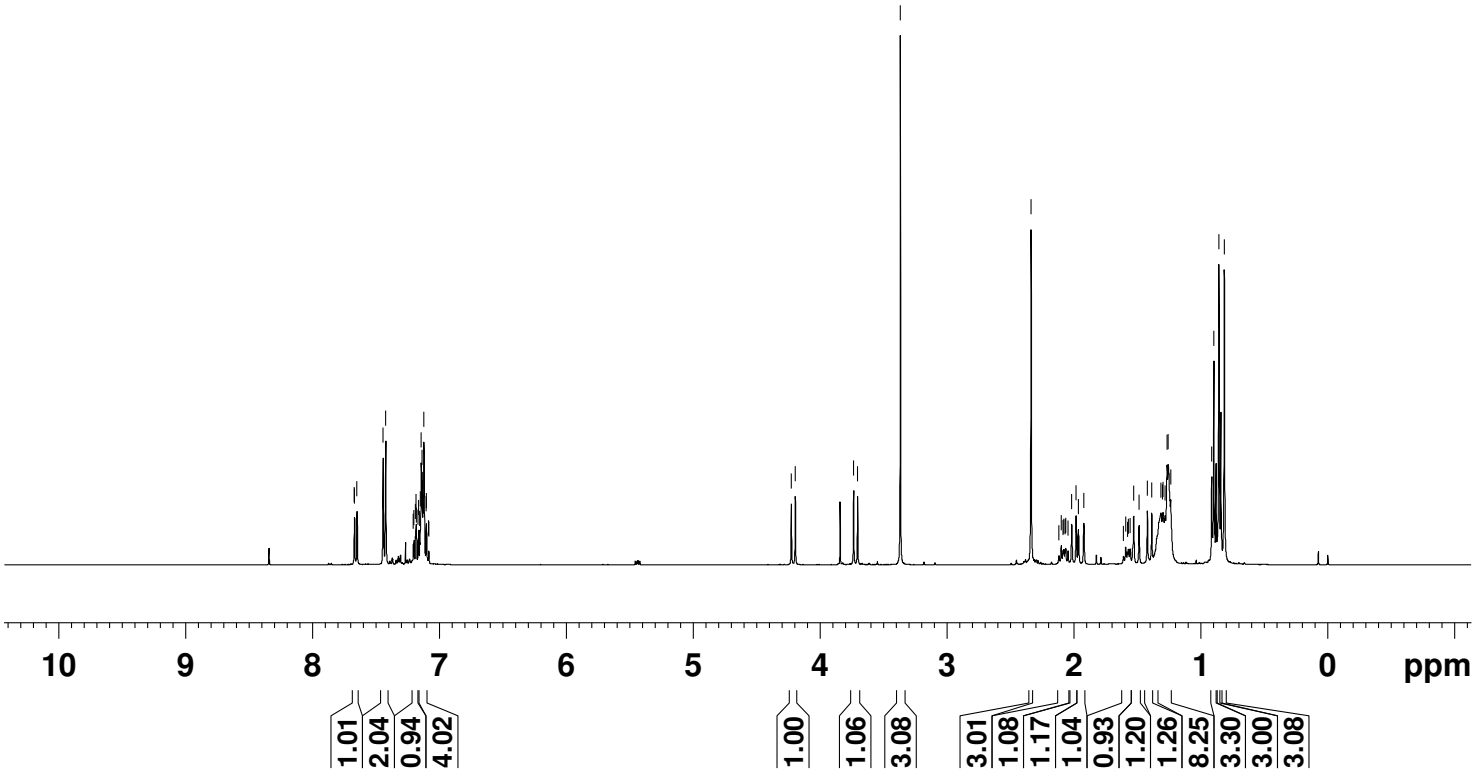


NAME	lly-781-2p-20160816
EXPNO	2
PROCNO	1
Date_	20160816
Time	22.12
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	56
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127737 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

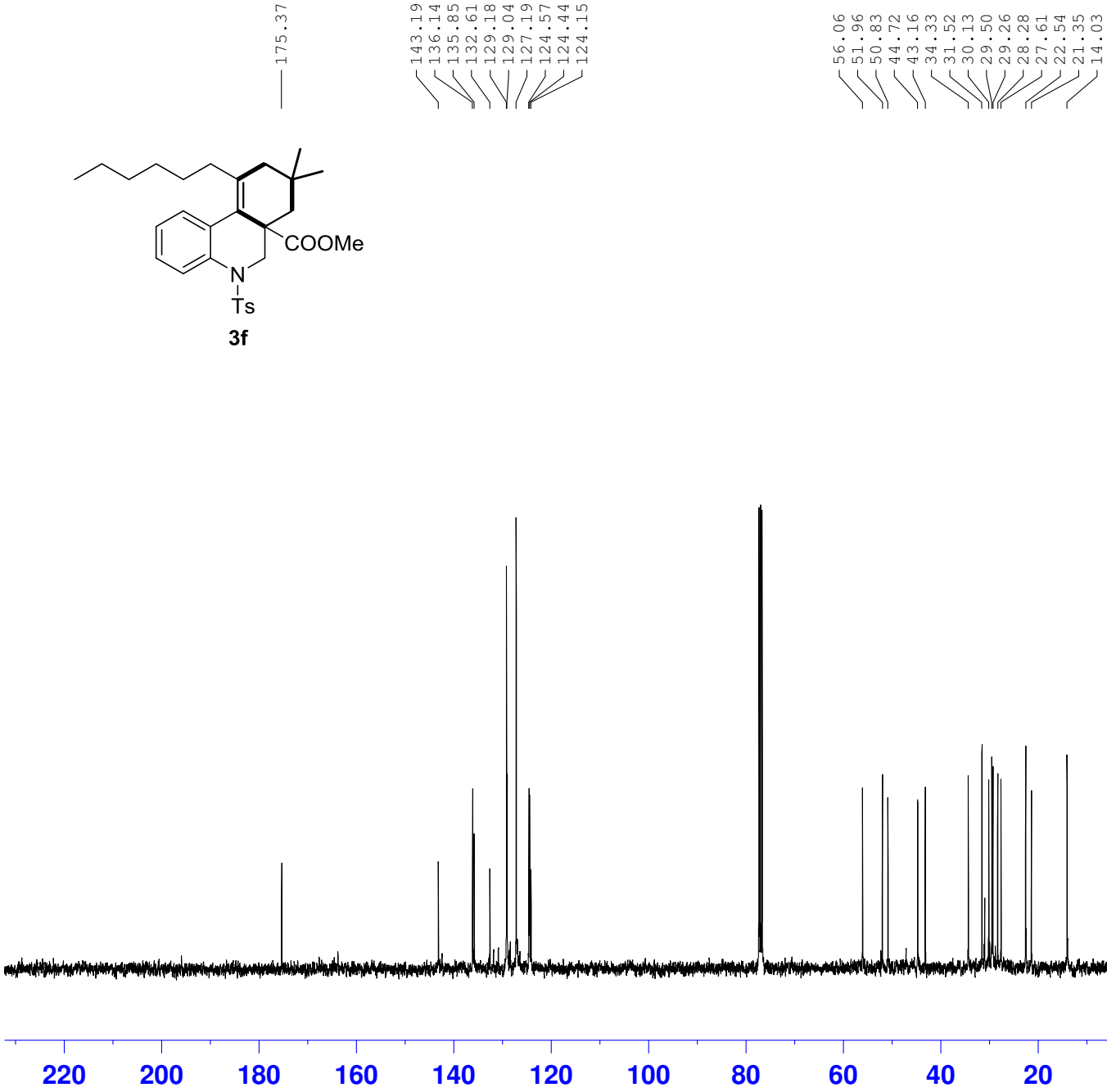




3f

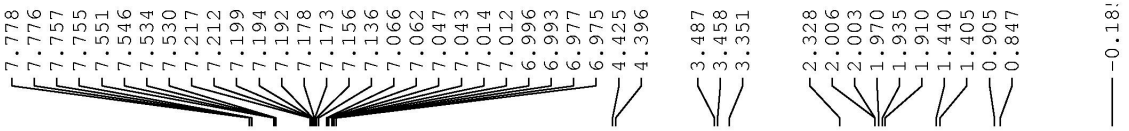


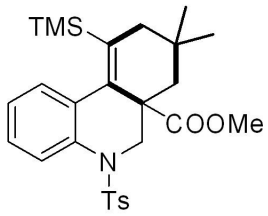
NAME	lly-770-2p-20160426
EXPNO	1
PROCNO	1
Date_	20160426
Time	16.53
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	50.8
DW	78.200 usec
DE	6.50 usec
TE	296.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300061 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

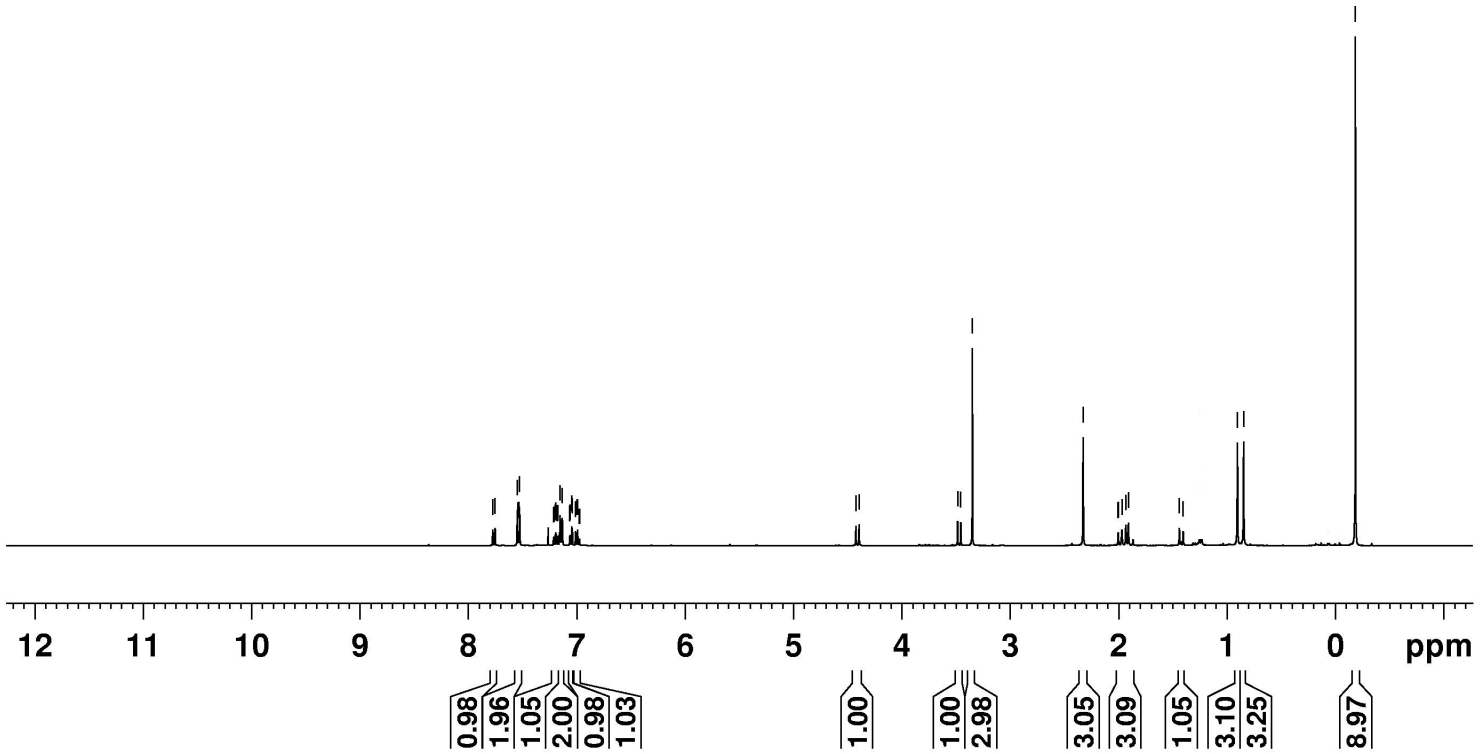
NAME	lly-770-2p-20160426
EXPNO	2
PROCNO	1
Date_	20160426
Time	16.56
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	48
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	297.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127778 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

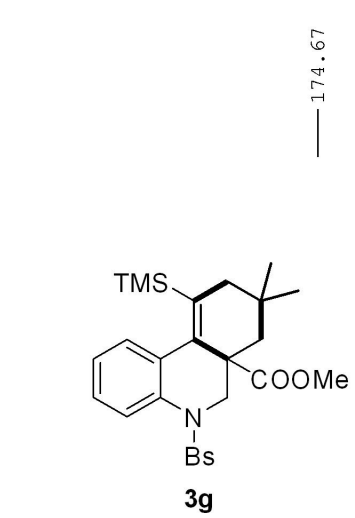




3g

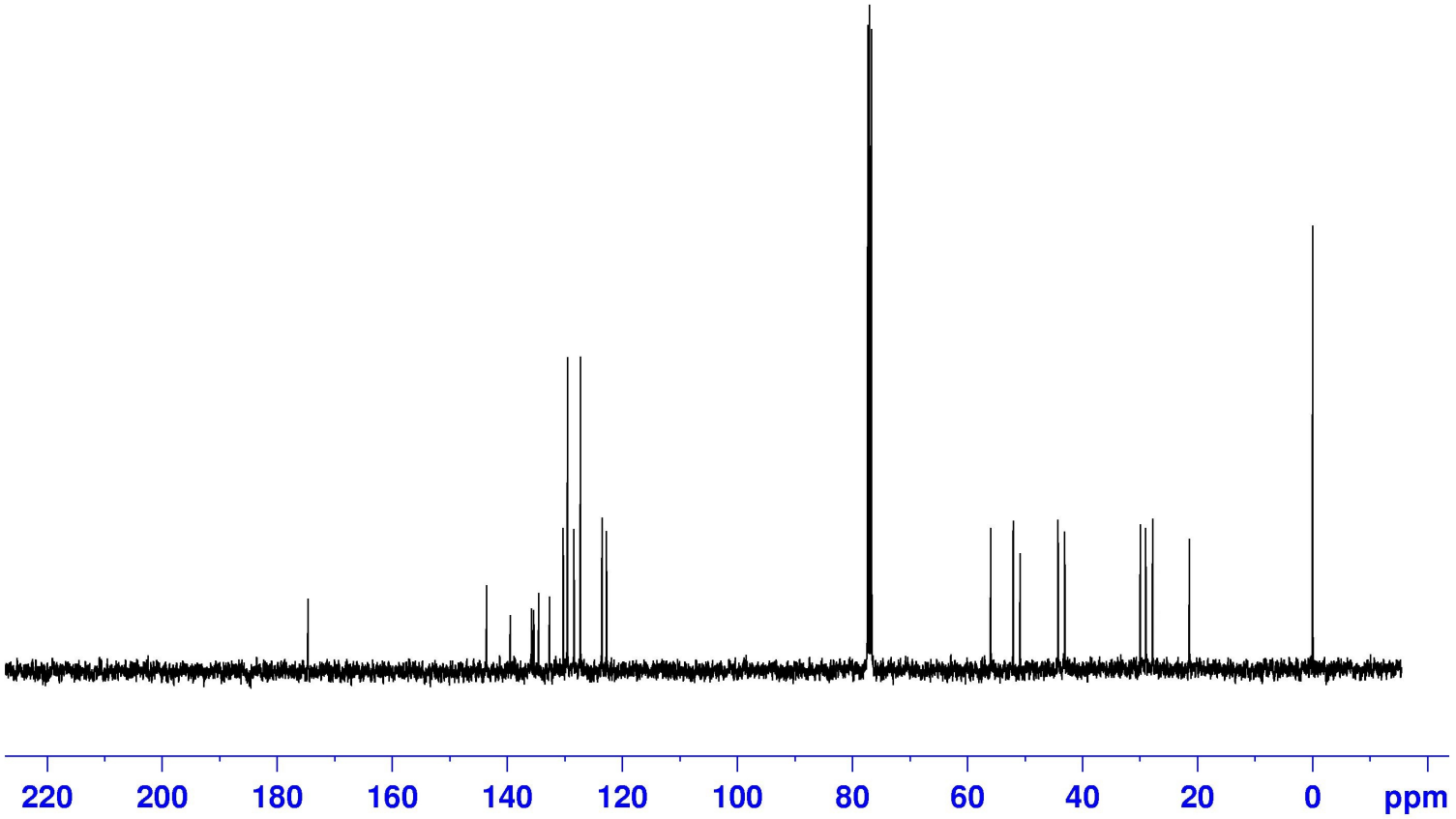
```
NAME      lly-773-5ap-20160819
EXPNO                    1
PROCNO                   1
Date_             20160819
Time                 9.36
INSTRUM             spect
PROBHD    5 mm PADUL 13C
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ                2.5625076 sec
RG                     114
DW                  78.200 usec
DE                   6.50 usec
TE                  296.0 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  13.10 usec
PL1                  1.80 dB
PL1W           8.92857742 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300073 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



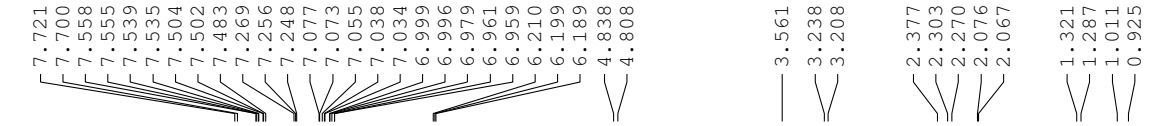


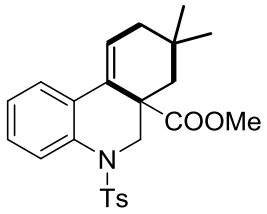
3g

174.67
143.61
139.51
135.80
135.42
134.57
132.69
130.30
129.55
128.44
127.29
123.55
122.77
55.94
52.03
50.84
44.23
43.08
29.93
28.99
27.78
21.39
-0.04



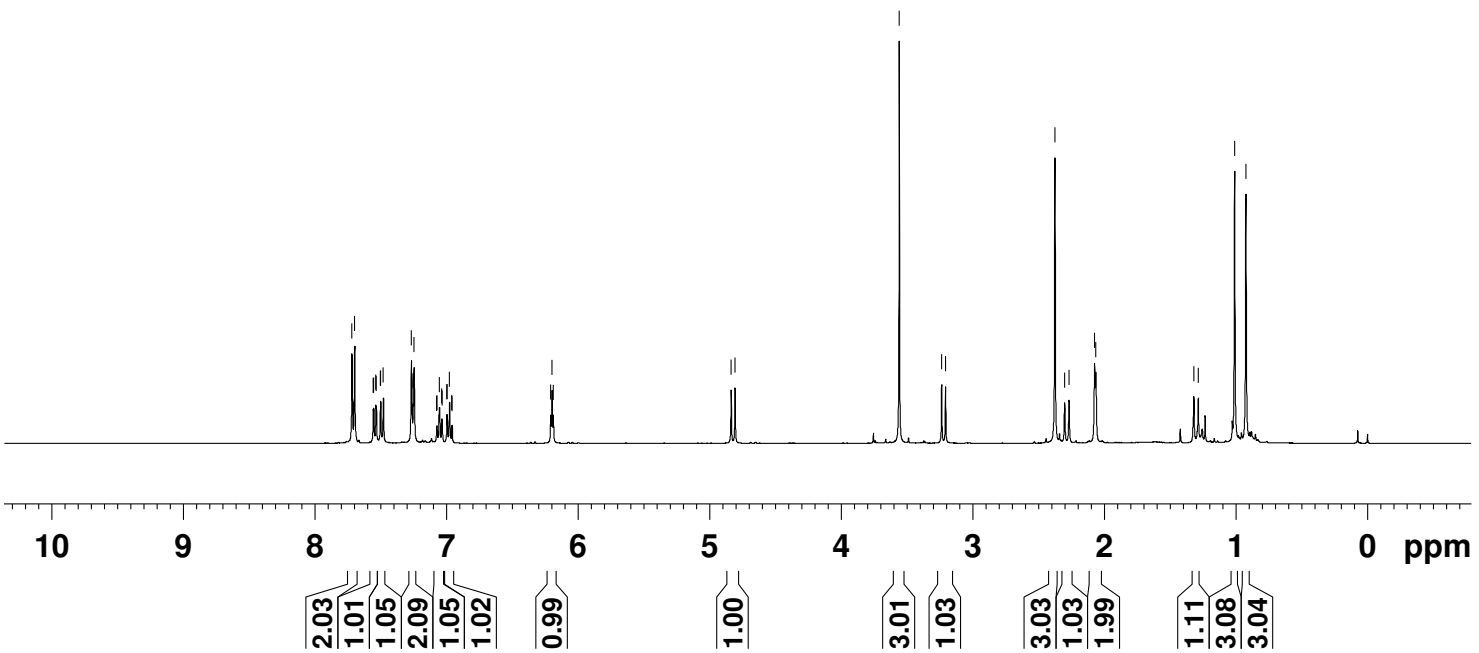
NAME	lly-773-5ap-20160819
EXPNO	2
PROCNO	1
Date_	20160819
Time	17.24
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	48
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	297.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127734 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

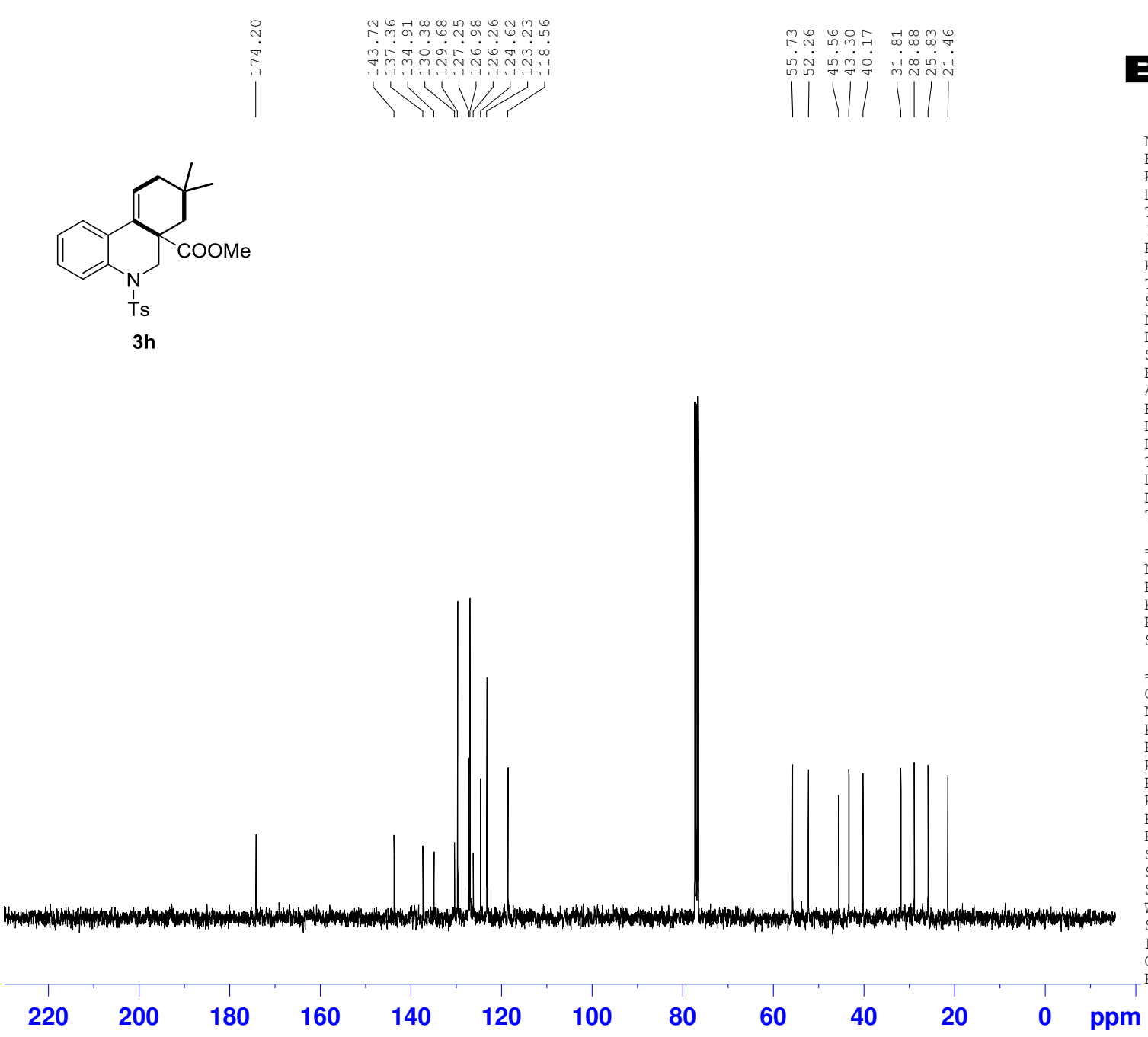




3h

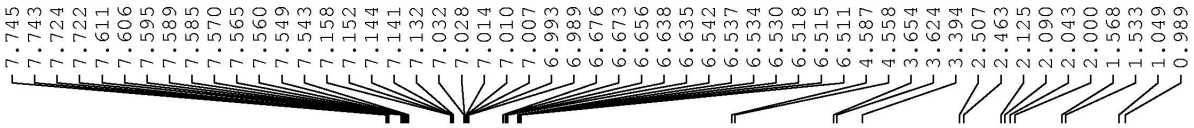
```
NAME      lly-781-1p-20160519
EXPNO                       1
PROCNO                      1
Date_                20160519
Time                    16.48
INSTRUM                 spect
PROBHD    5 mm PADUL 13C
PULPROG                  zg30
TD                      32768
SOLVENT                 CDCl3
NS                          8
DS                          0
SWH                  6393.862 Hz
FIDRES               0.195125 Hz
AQ                   2.5625076 sec
RG                        114
DW                     78.200 usec
DE                      6.50 usec
TE                     297.6 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     13.10 usec
PL1                     1.80 dB
PL1W             8.92857742 W
SFO1           400.1326008 MHz
SI                      32768
SF             400.1300112 MHz
WDW                        EM
SSB                         0
LB                      0.30 Hz
GB                          0
PC                      1.00
```

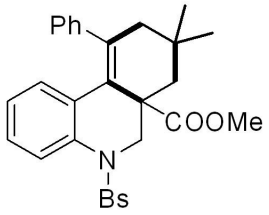




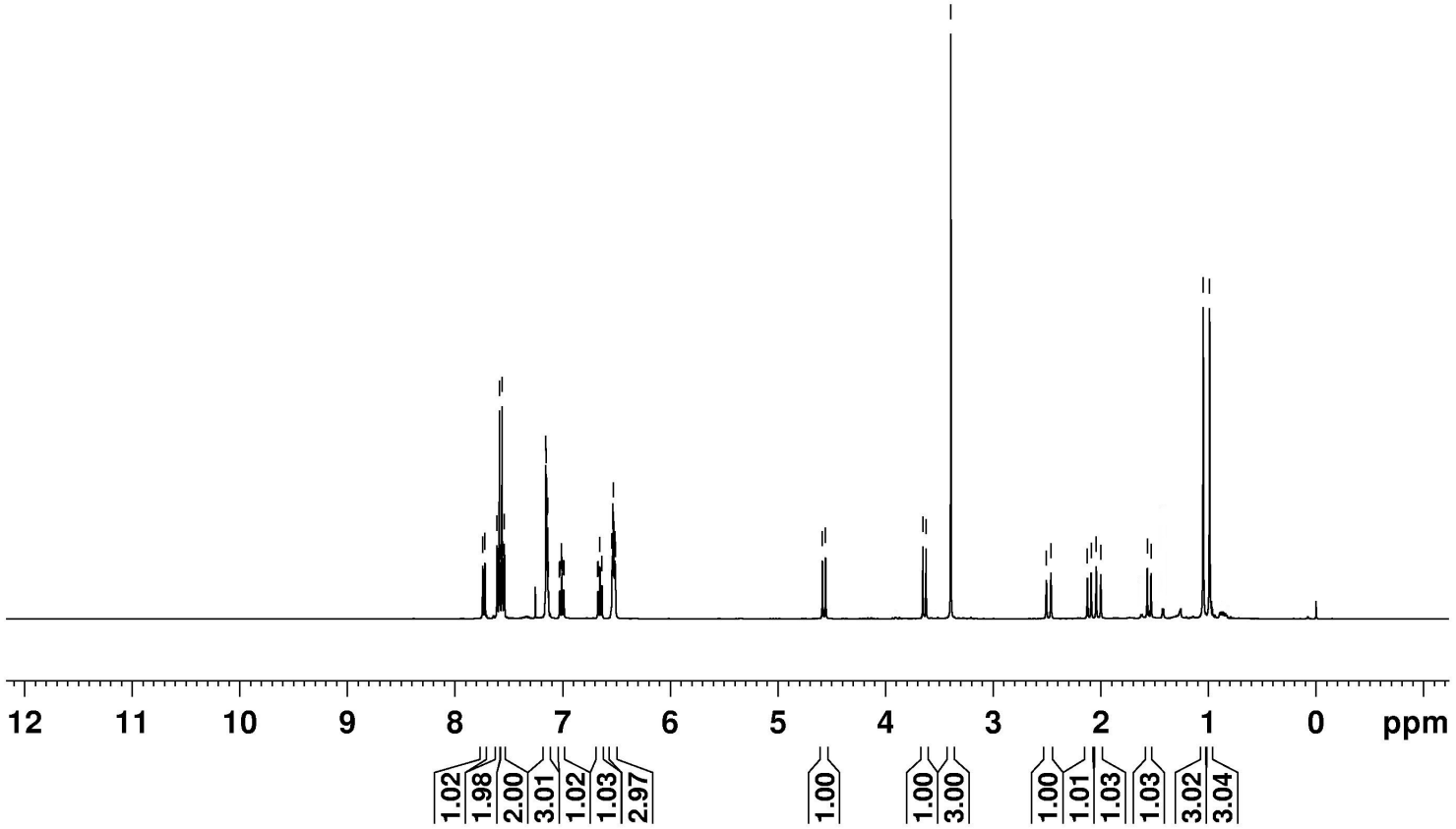
BRUKER

NAME	lly-781-1p-20160519
EXPNO	2
PROCNO	1
Date_	20160519
Time	16.51
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	40
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	298.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127761 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

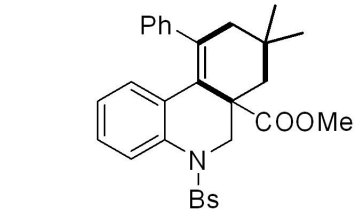




3i

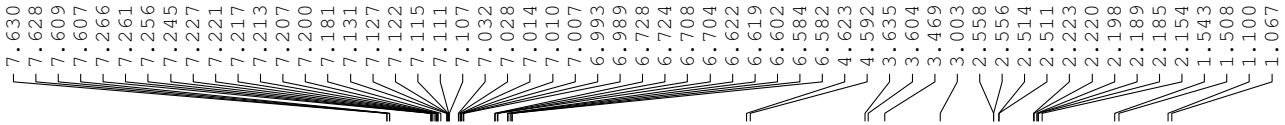


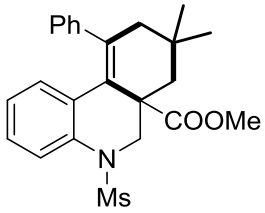
NAME	lly-801-1p-20160817
EXPNO	1
PROCNO	1
Date_	20160817
Time	14.21
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	90.5
DW	78.200 usec
DE	6.50 usec
TE	295.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300113 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



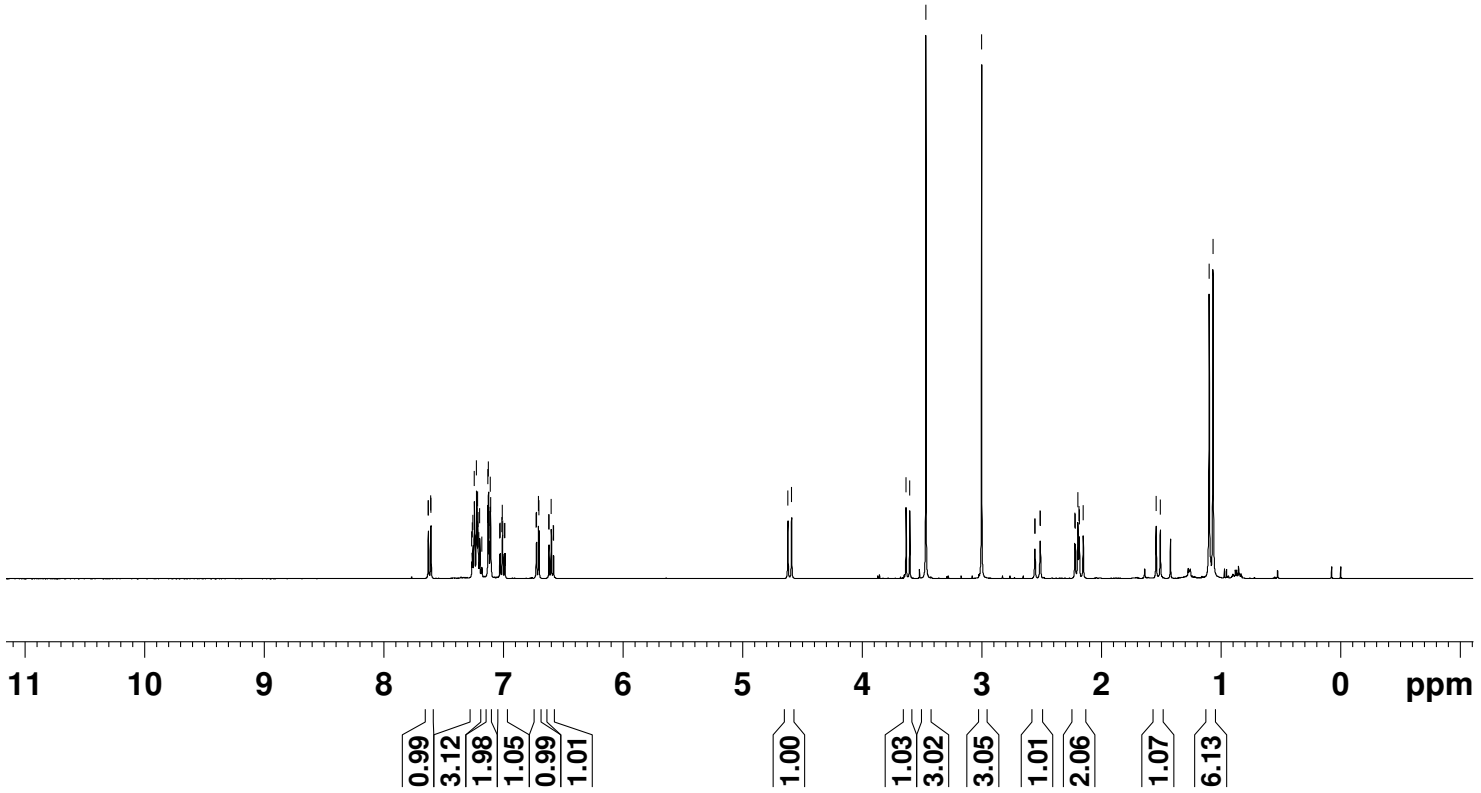
3i

NAME	lly-801-1p-20160817
EXPNO	2
PROCNO	1
Date_	20160817
Time	14.35
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	72
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	296.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127774 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

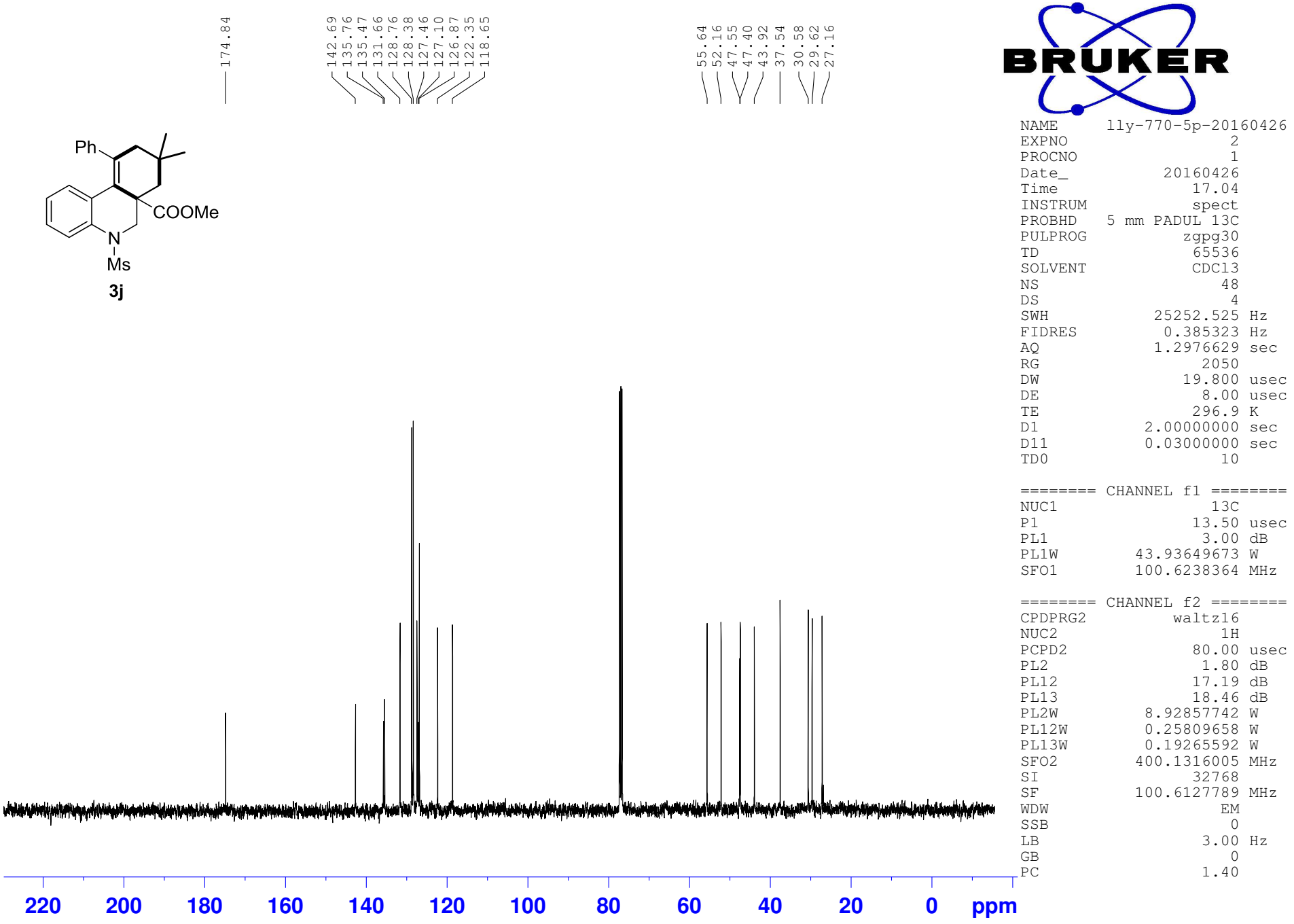




3j

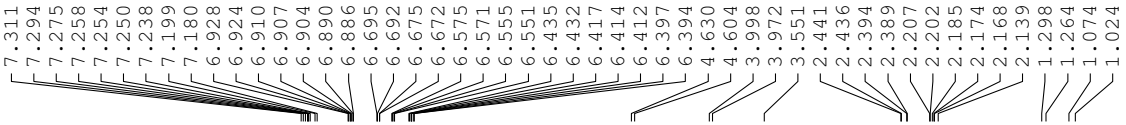


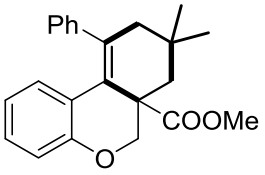
NAME	lly-770-5p-20160426
EXPNO	1
PROCNO	1
Date_	20160426
Time	17.02
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	80.6
DW	78.200 usec
DE	6.50 usec
TE	296.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300110 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



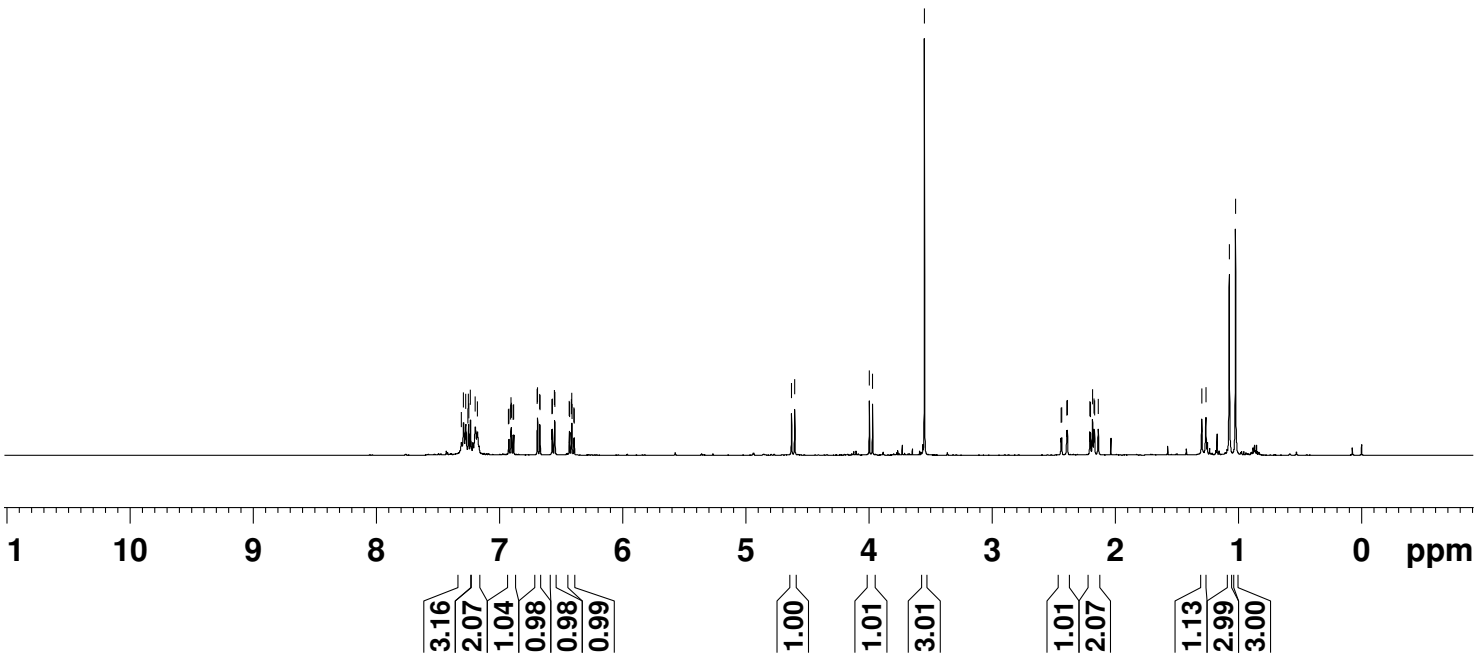
BRUKER

NAME	lly-770-5p-20160426
EXPNO	2
PROCNO	1
Date_	20160426
Time	17.04
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	48
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	296.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127789 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

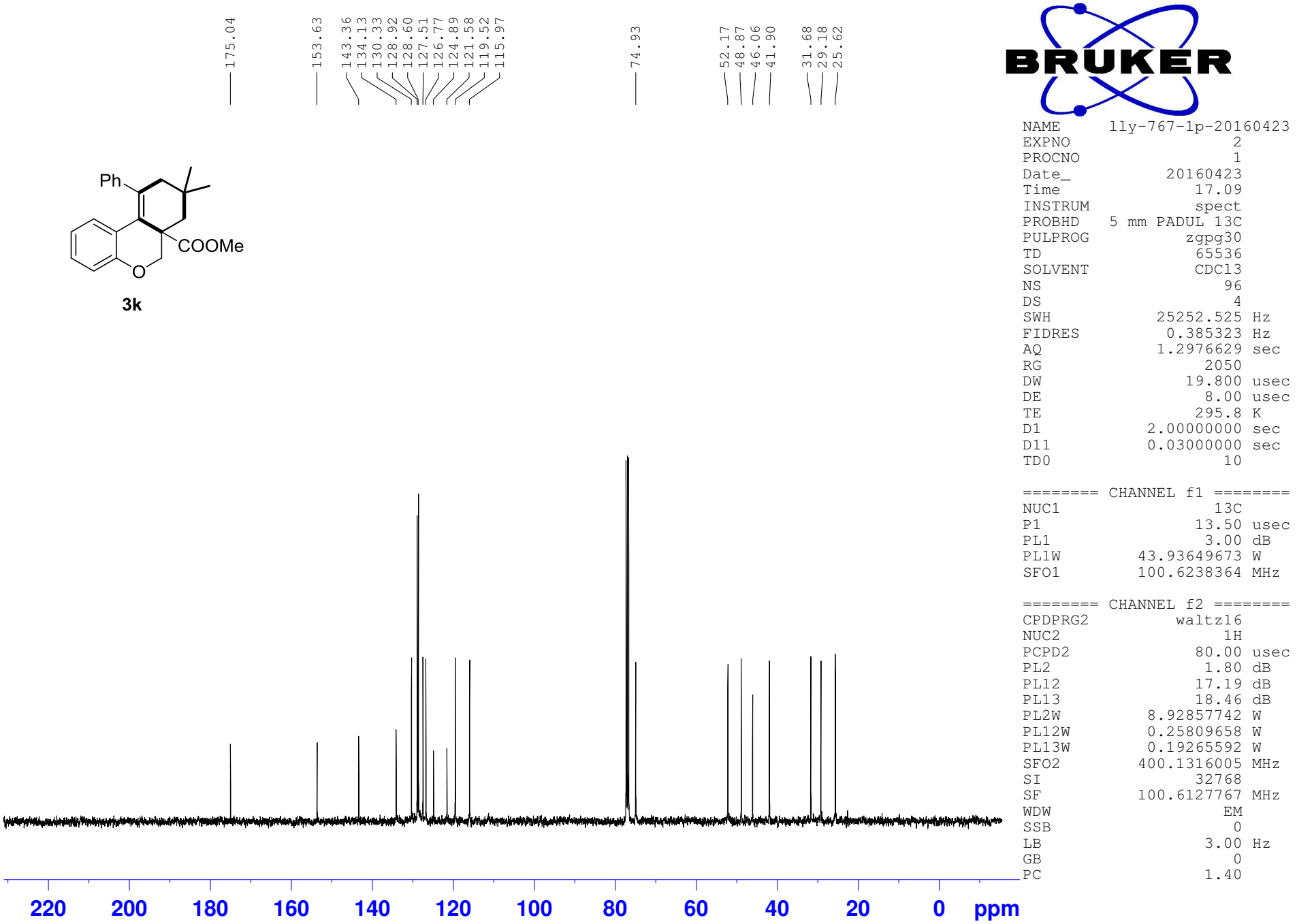




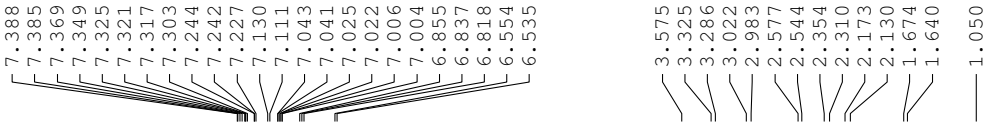
3k

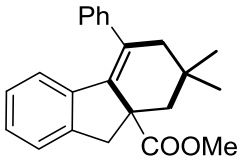


NAME	lly-767-1p-20160423
EXPNO	1
PROCNO	1
Date_	20160423
Time	17.07
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	90.5
DW	78.200 usec
DE	6.50 usec
TE	295.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300184 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

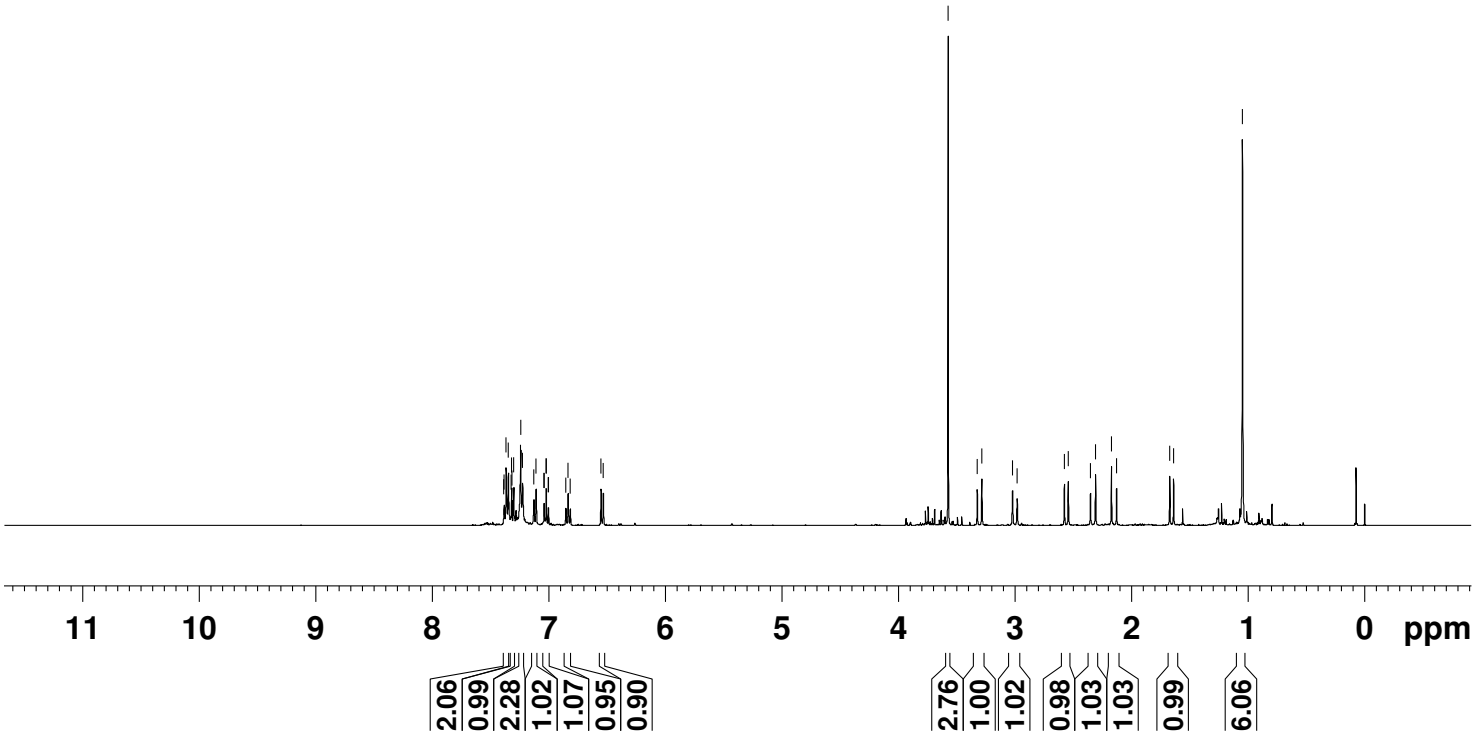



```
NAME        lly-767-1p-20160423
EXPNO                         2
PROCNO                        1
Date_                  20160423
Time                      17.09
INSTRUM                   spect
PROBHD    5 mm PADUL 13C
PULPROG                 zgpg30
TD                         65536
SOLVENT                   CDCl3
NS                           96
DS                            4
SWH                   25252.525 Hz
FIDRES                 0.385323 Hz
AQ                    1.2976629 sec
RG                         2050
DW                       19.800 usec
DE                        8.00 usec
TE                       295.8 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                          10

======== CHANNEL f1 ========
NUC1                        13C
P1                        13.50 usec
PL1                        3.00 dB
PL1W                43.93649673 W
SFO1                100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                     80.00 usec
PL2                        1.80 dB
PL12                      17.19 dB
PL13                      18.46 dB
PL2W                 8.92857742 W
PL12W                0.25809658 W
PL13W                0.19265592 W
SFO2                400.1316005 MHz
SI                         32768
SF                  100.6127767 MHz
WDW                          EM
SSB                           0
LB                         3.00 Hz
GB                            0
PC                         1.40
```

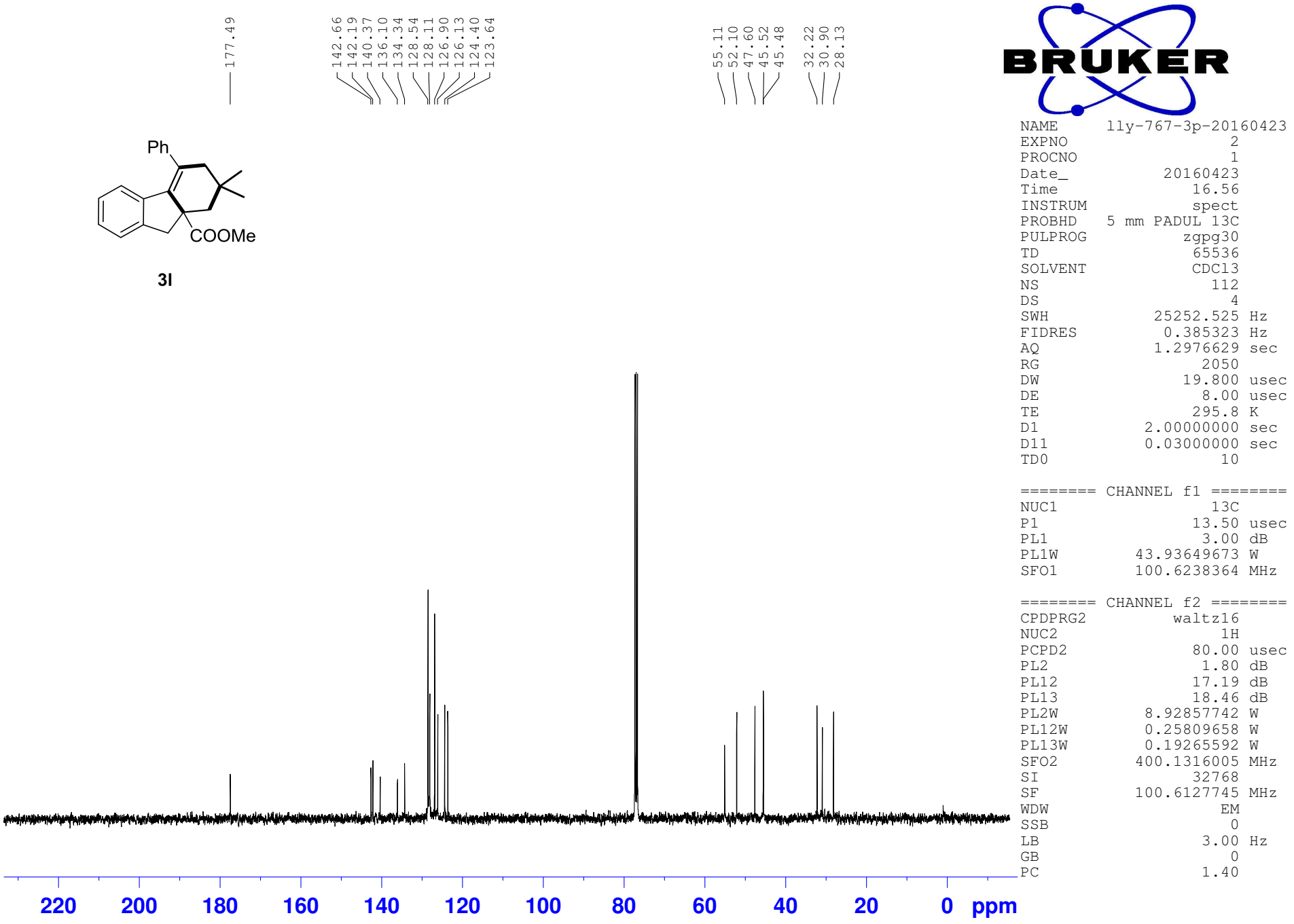




3l



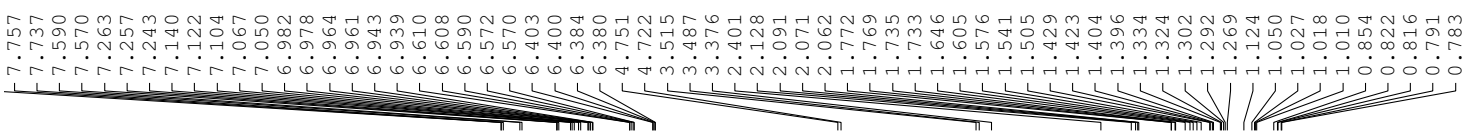

```
NAME      lly-767-3p-20160423
EXPNO                       1
PROCNO                      1
Date_              20160423
Time                   16.52
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 6393.862 Hz
FIDRES              0.195125 Hz
AQ                2.5625076 sec
RG                       128
DW                    78.200 usec
DE                     6.50 usec
TE                    295.3 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.10 usec
PL1                     1.80 dB
PL1W             8.92857742 W
SFO1           400.1326008 MHz
SI                     32768
SF             400.1300170 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
```

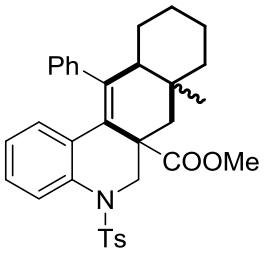


3l

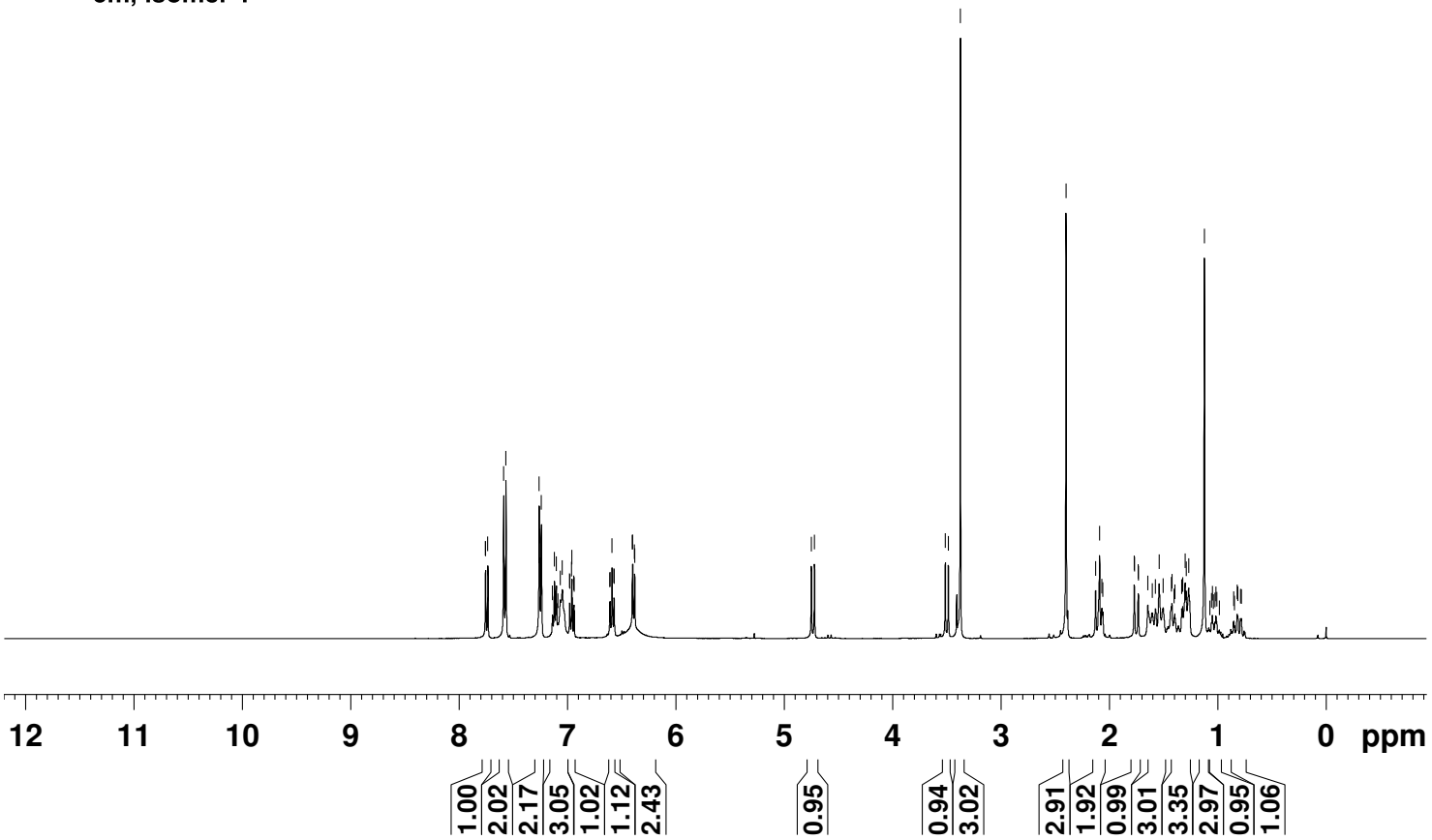
BRUKER

NAME	lly-767-3p-20160423
EXPNO	2
PROCNO	1
Date_	20160423
Time	16.56
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	112
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	295.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127745 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40



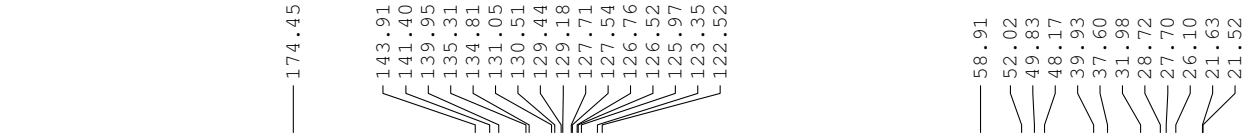


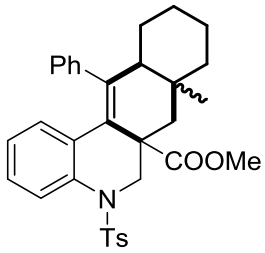
3m, isomer 1



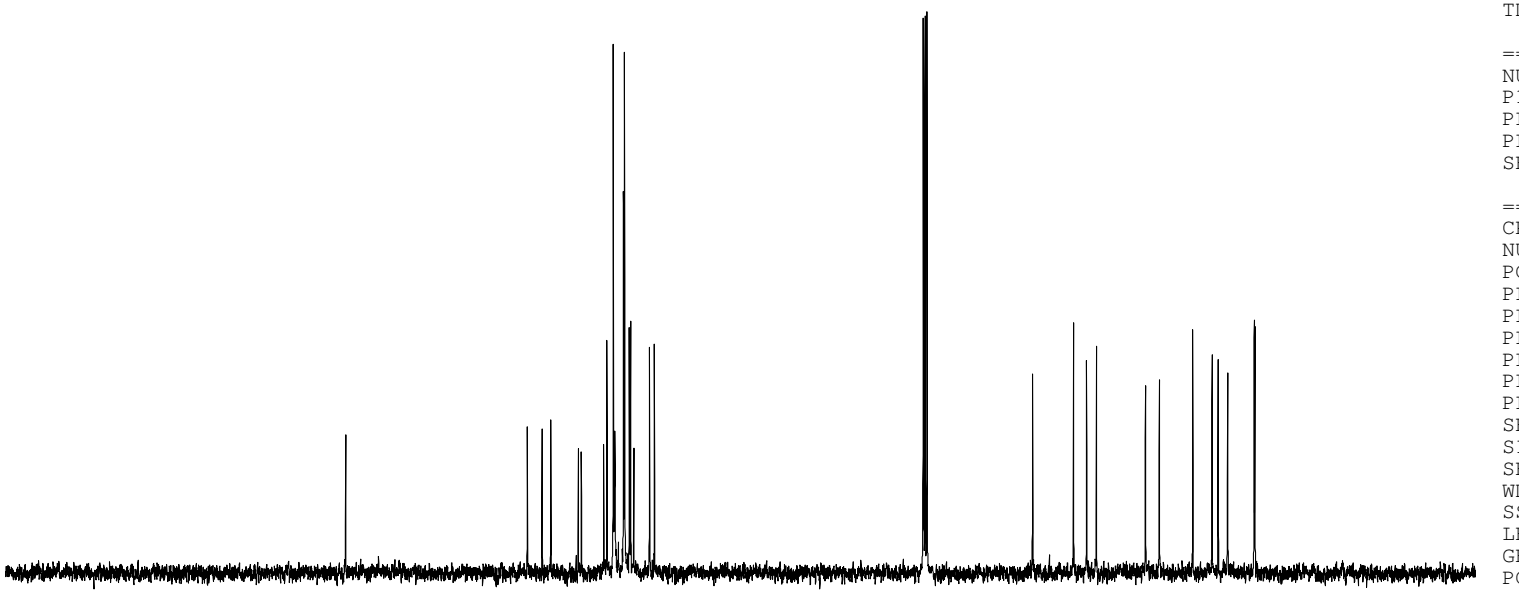
BRUKER

NAME	lly-789-3aap-20160530
EXPNO	1
PROCNO	1
Date_	20160530
Time	16.47
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	64
DW	78.200 usec
DE	6.50 usec
TE	297.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300108 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

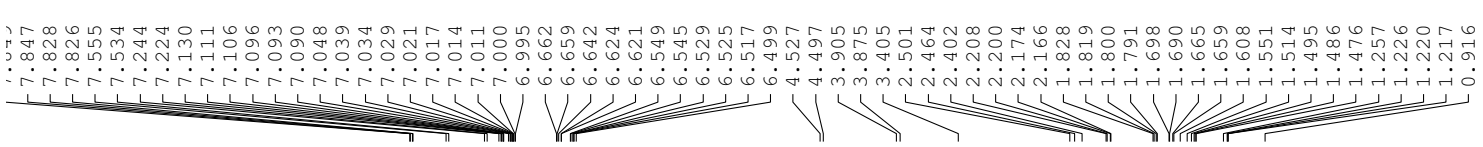


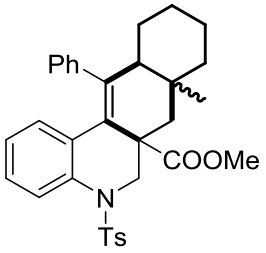


3m, isomer 1

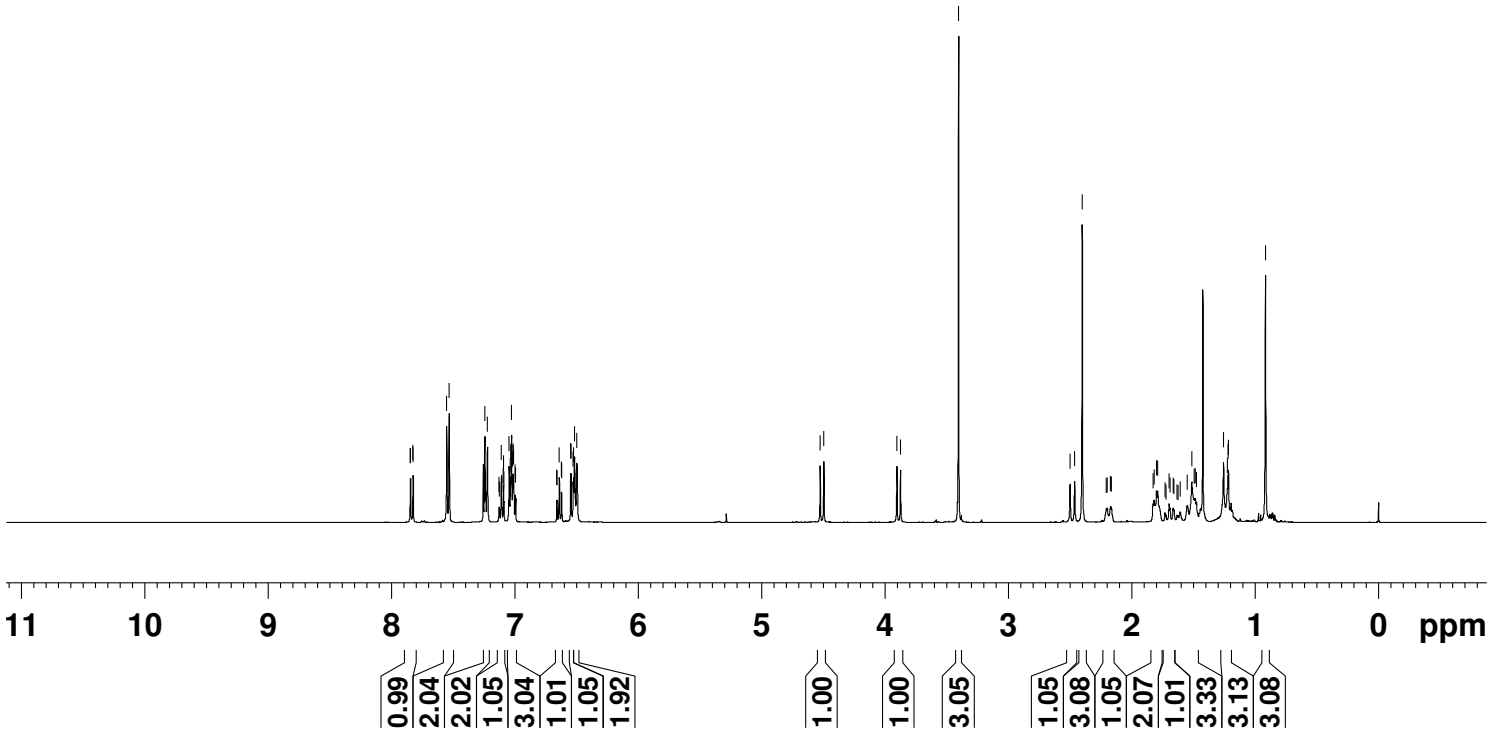


NAME	lly-789-3aap-20160530
EXPNO	2
PROCNO	1
Date_	20160530
Time	16.49
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	297.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127795 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

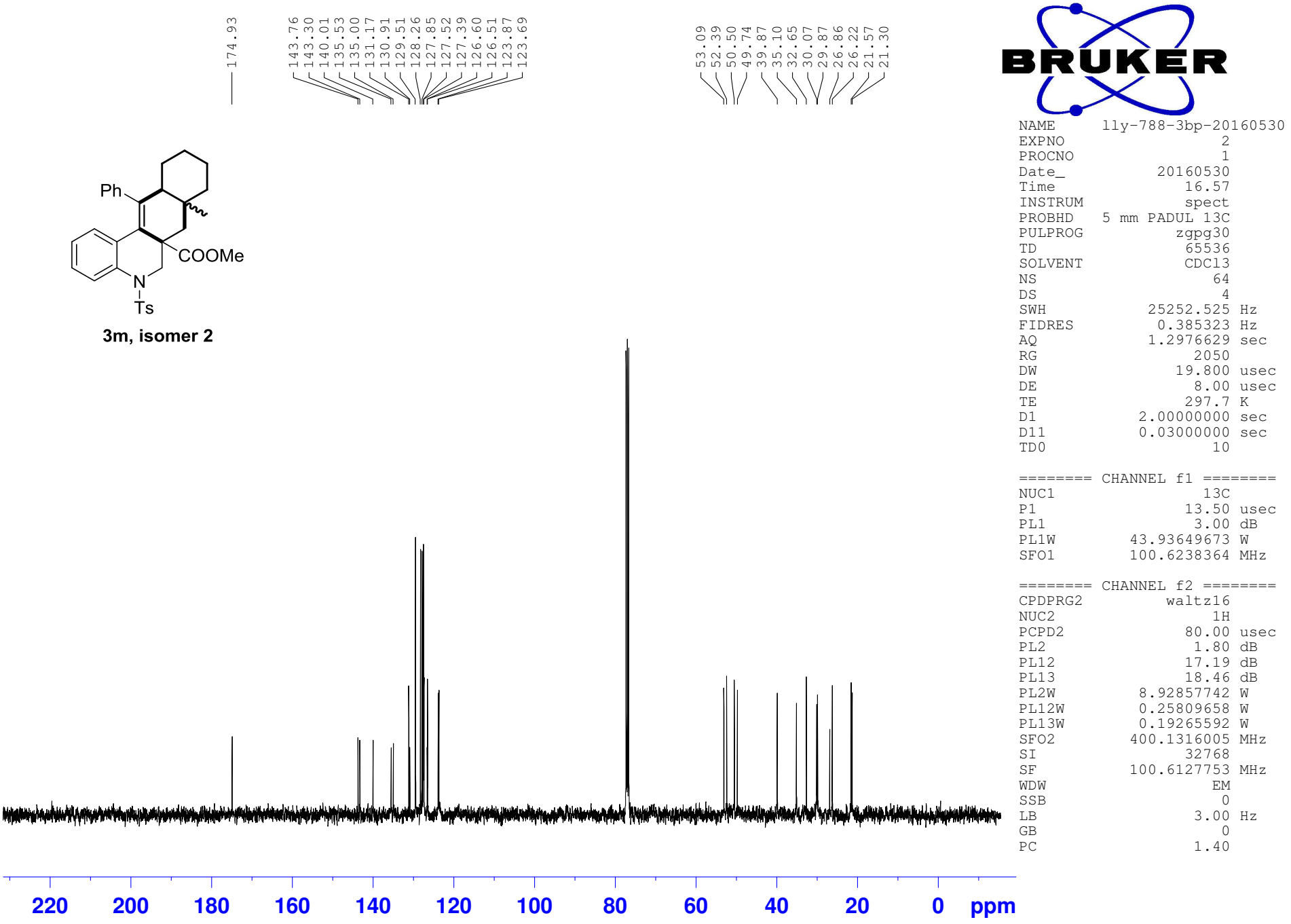




3m, isomer 2

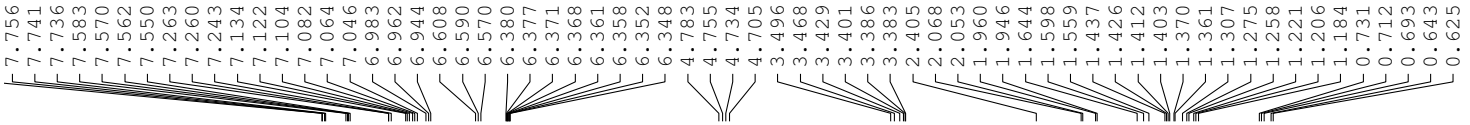


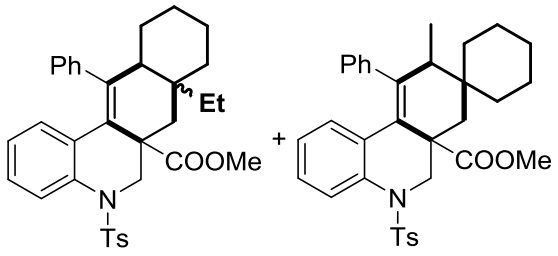

```
NAME      lly-788-3bp20160530
EXPNO                       1
PROCNO                      1
Date_              20160530
Time                    9.59
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 6393.862 Hz
FIDRES              0.195125 Hz
AQ                2.5625076 sec
RG                       101
DW                    78.200 usec
DE                     6.50 usec
TE                    296.8 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.10 usec
PL1                     1.80 dB
PL1W           8.92857742 W
SFO1          400.1326008 MHz
SI                     32768
SF            400.1300107 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
```



BRUKER

NAME	lly-788-3bp-20160530
EXPNO	2
PROCNO	1
Date_	20160530
Time	16.57
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	297.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127753 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40





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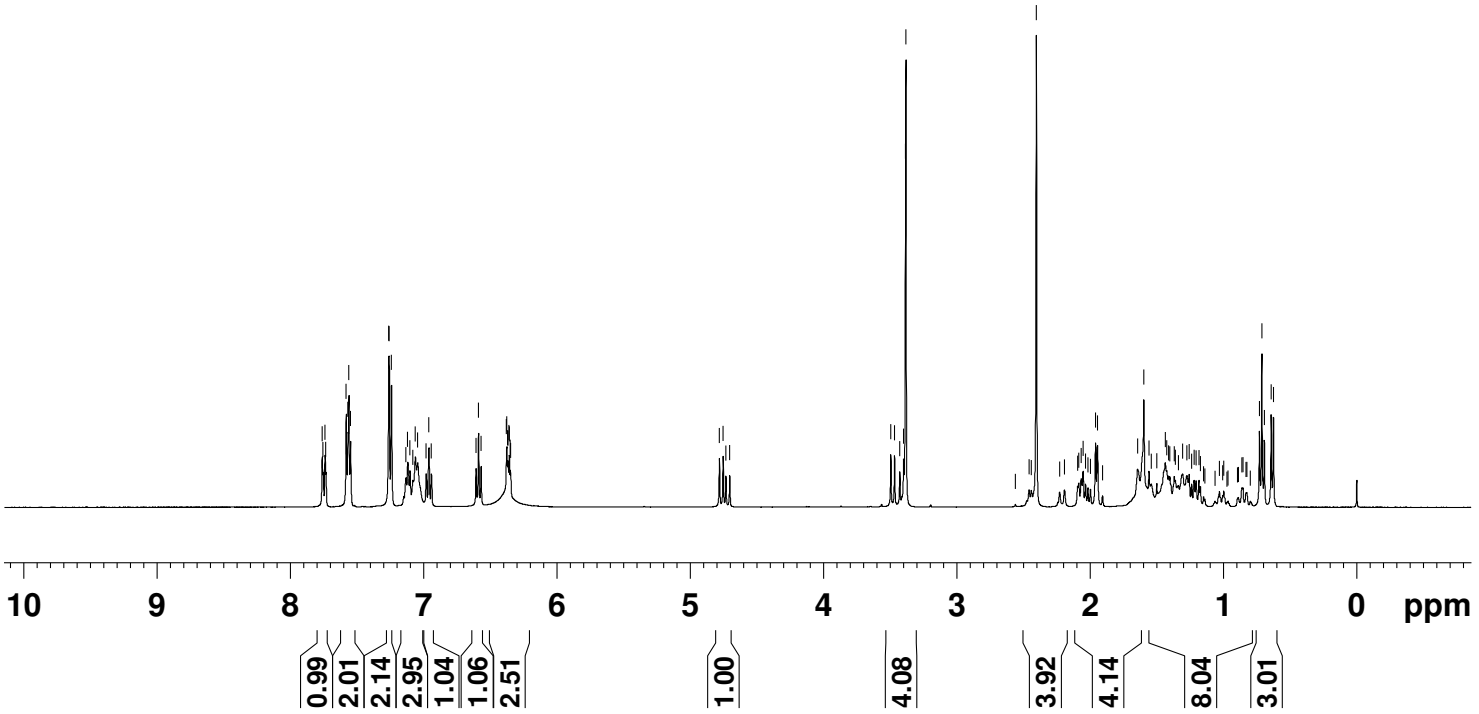
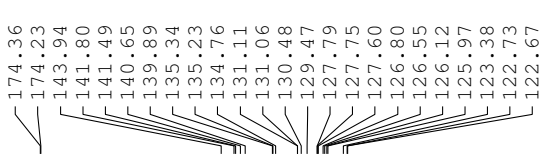
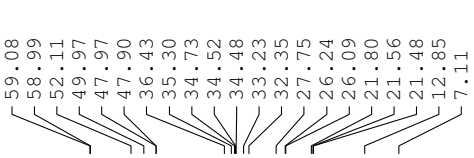
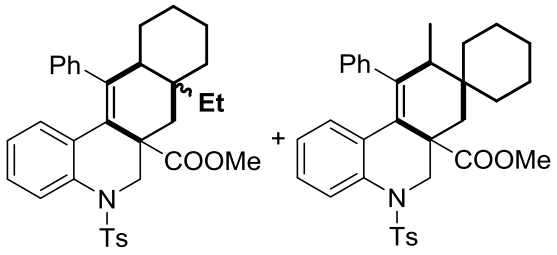
isomer 1




```
NAME        lly-795-1amp-20160617
EXPNO                           1
PROCNO                          1
Date_                    20160617
Time                         9.22
INSTRUM                     spect
PROBHD    5 mm PADUL 13C
PULPROG                      zg30
TD                          32768
SOLVENT                     CDCl3
NS                              8
DS                              0
SWH                      6393.862 Hz
FIDRES                   0.195125 Hz
AQ                       2.5625076 sec
RG                            128
DW                          78.200 usec
DE                           6.50 usec
TE                          297.1 K
D1                     1.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                           1H
P1                          13.10 usec
PL1                          1.80 dB
PL1W                 8.92857742 W
SFO1                400.1326008 MHz
SI                          32768
SF                  400.1300100 MHz
WDW                            EM
SSB                             0
LB                           0.30 Hz
GB                              0
PC                           1.00
```

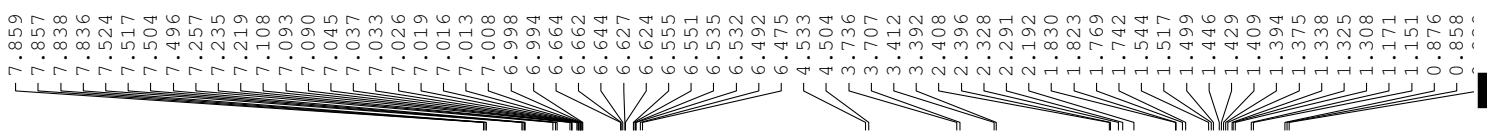


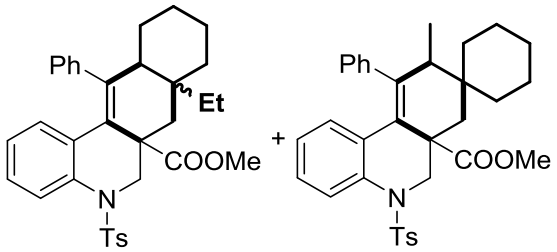




isomer 1

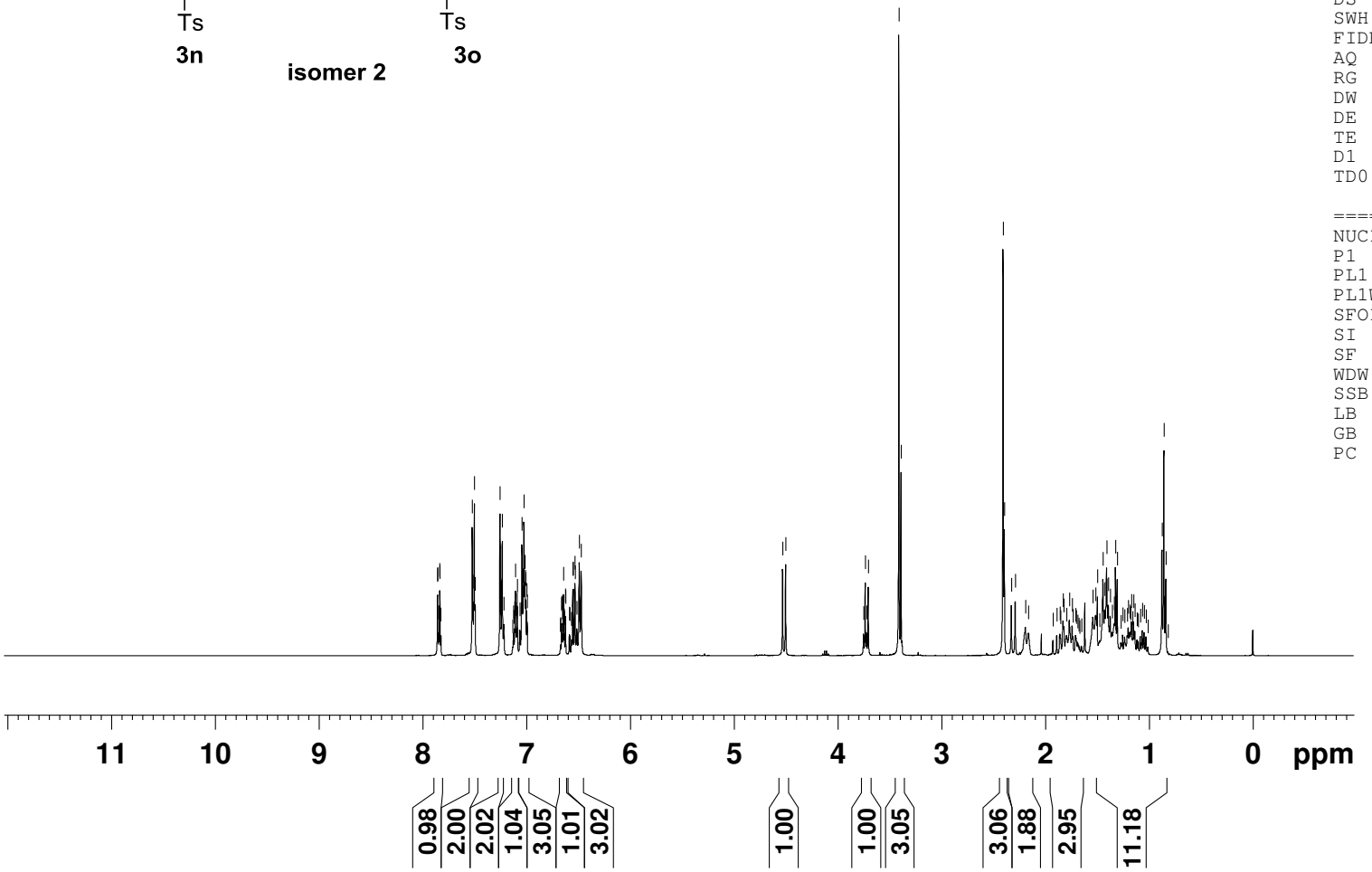

```
NAME        lly-795-1amp-20160617
EXPNO                           2
PROCNO                          1
Date_                    20160617
Time                         9.26
INSTRUM                     spect
PROBHD    5 mm PADUL 13C
PULPROG                    zgpg30
TD                          65536
SOLVENT                     CDCl3
NS                            432
DS                              4
SWH                     25252.525 Hz
FIDRES                   0.385323 Hz
AQ                       1.2976629 sec
RG                           2050
DW                         19.800 usec
DE                          8.00 usec
TE                         297.7 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                             10

======== CHANNEL f1 ========
NUC1                          13C
P1                         13.50 usec
PL1                         3.00 dB
PL1W                43.93649673 W
SFO1               100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                          1H
PCPD2                      80.00 usec
PL2                         1.80 dB
PL12                       17.19 dB
PL13                       18.46 dB
PL2W                8.92857742 W
PL12W               0.25809658 W
PL13W               0.19265592 W
SFO2               400.1316005 MHz
SI                          32768
SF                 100.6127742 MHz
WDW                            EM
SSB                             0
LB                         3.00 Hz
GB                              0
PC                         1.40
```

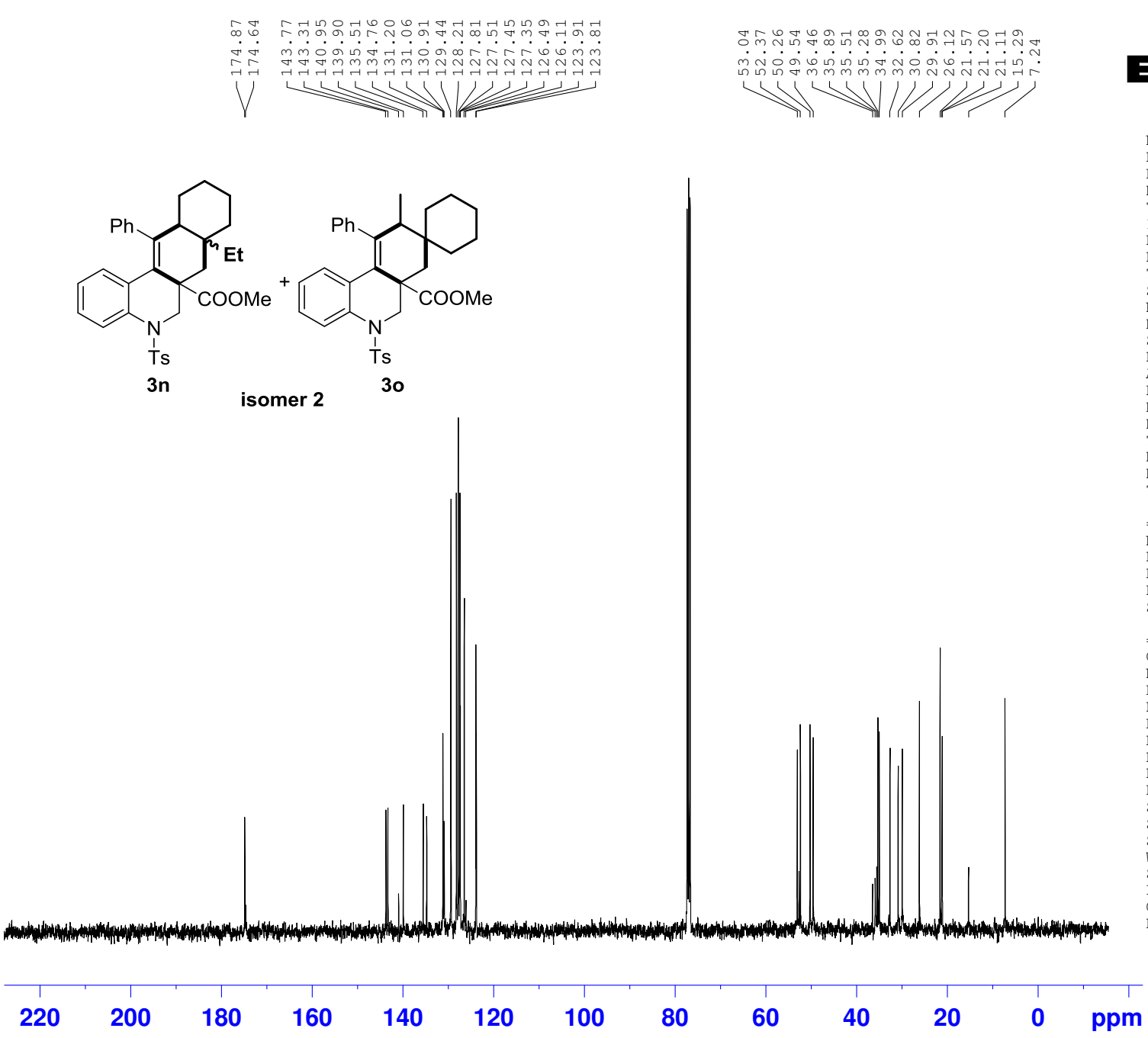




3n **isomer 2** **3o**

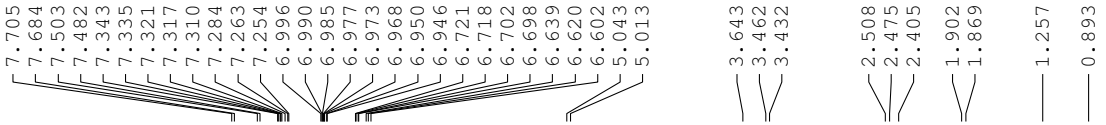
NAME	lly-795-1bmp-20160617
EXPNO	1
PROCNO	1
Date_	20160617
Time	16.42
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	64
DW	78.200 usec
DE	6.50 usec
TE	297.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300106 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

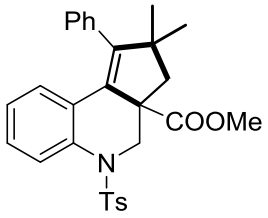




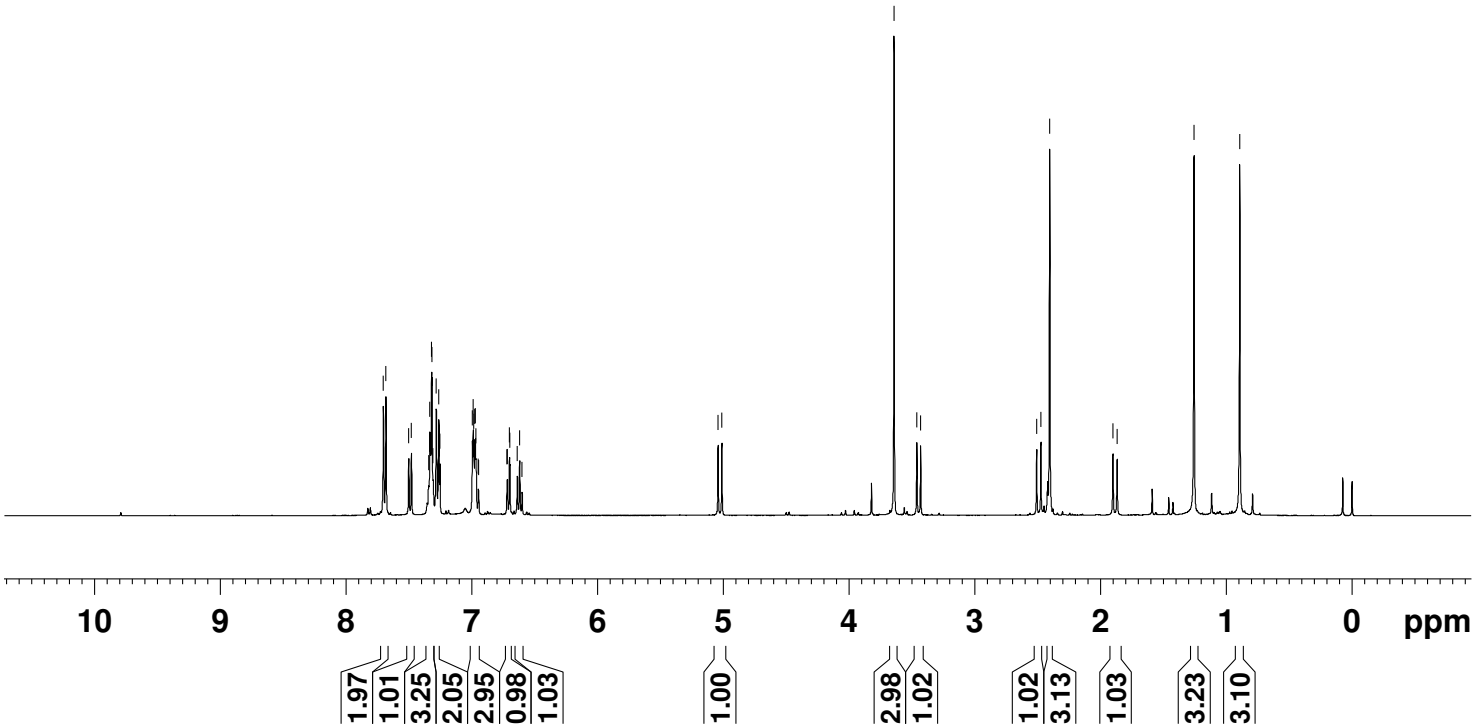
BRUKER

NAME	lly-795-1bmp-20160617
EXPNO	2
PROCNO	1
Date_	20160617
Time	16.45
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	176
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127758 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

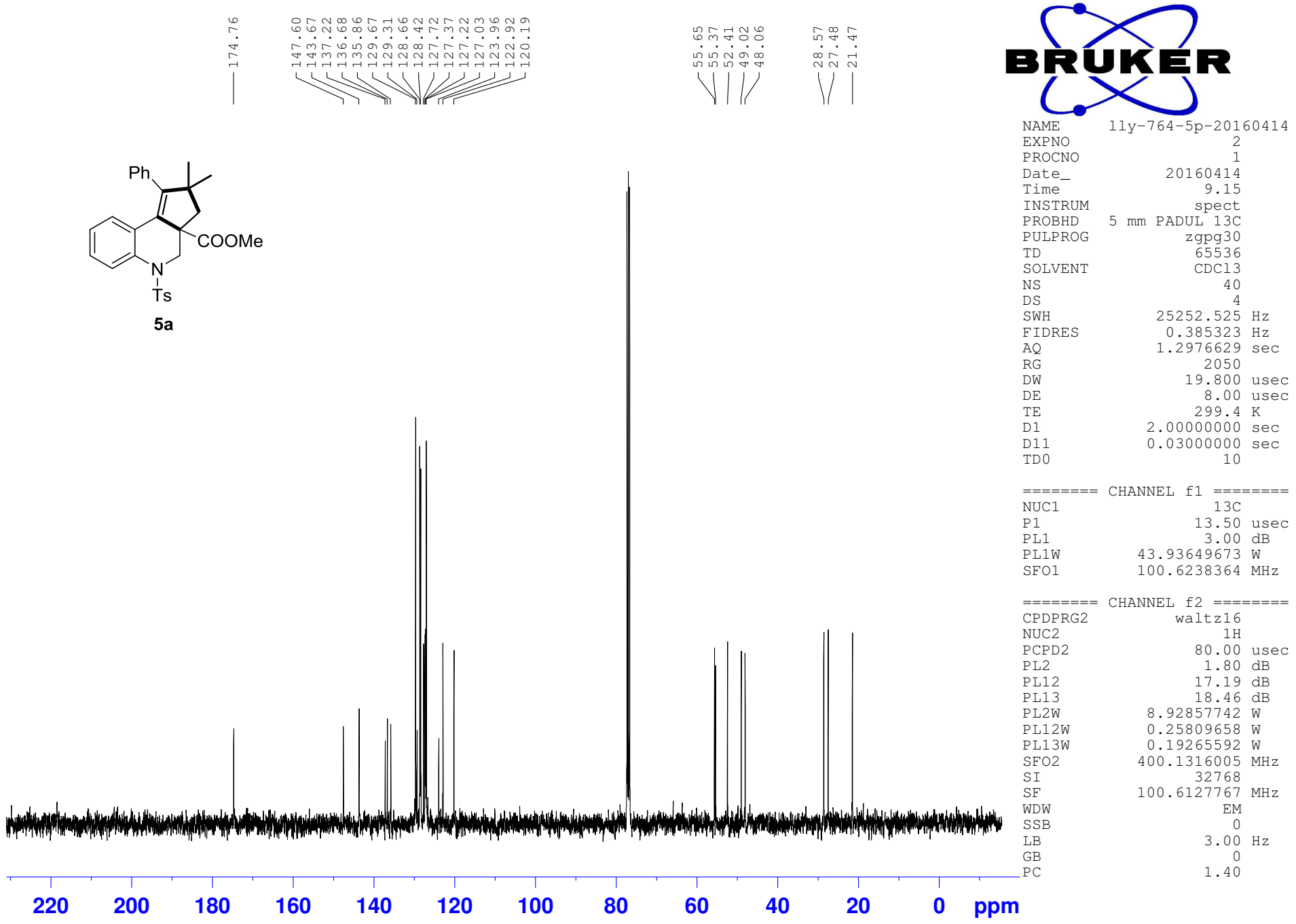




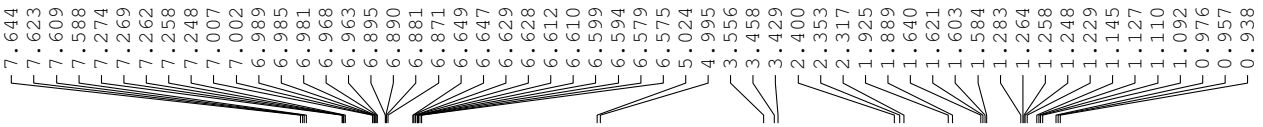
5a

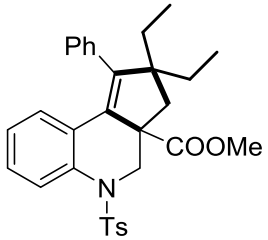



```
NAME      lly-764-5p-20160413
EXPNO                       1
PROCNO                      1
Date_                20160413
Time                    16.34
INSTRUM                 spect
PROBHD    5 mm PADUL 13C
PULPROG                  zg30
TD                      32768
SOLVENT                 CDCl3
NS                          8
DS                          0
SWH                  6393.862 Hz
FIDRES               0.195125 Hz
AQ                   2.5625076 sec
RG                        144
DW                     78.200 usec
DE                      6.50 usec
TE                     298.2 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      13.10 usec
PL1                      1.80 dB
PL1W               8.92857742 W
SFO1             400.1326008 MHz
SI                      32768
SF               400.1300119 MHz
WDW                        EM
SSB                         0
LB                      0.30 Hz
GB                          0
PC                      1.00
```

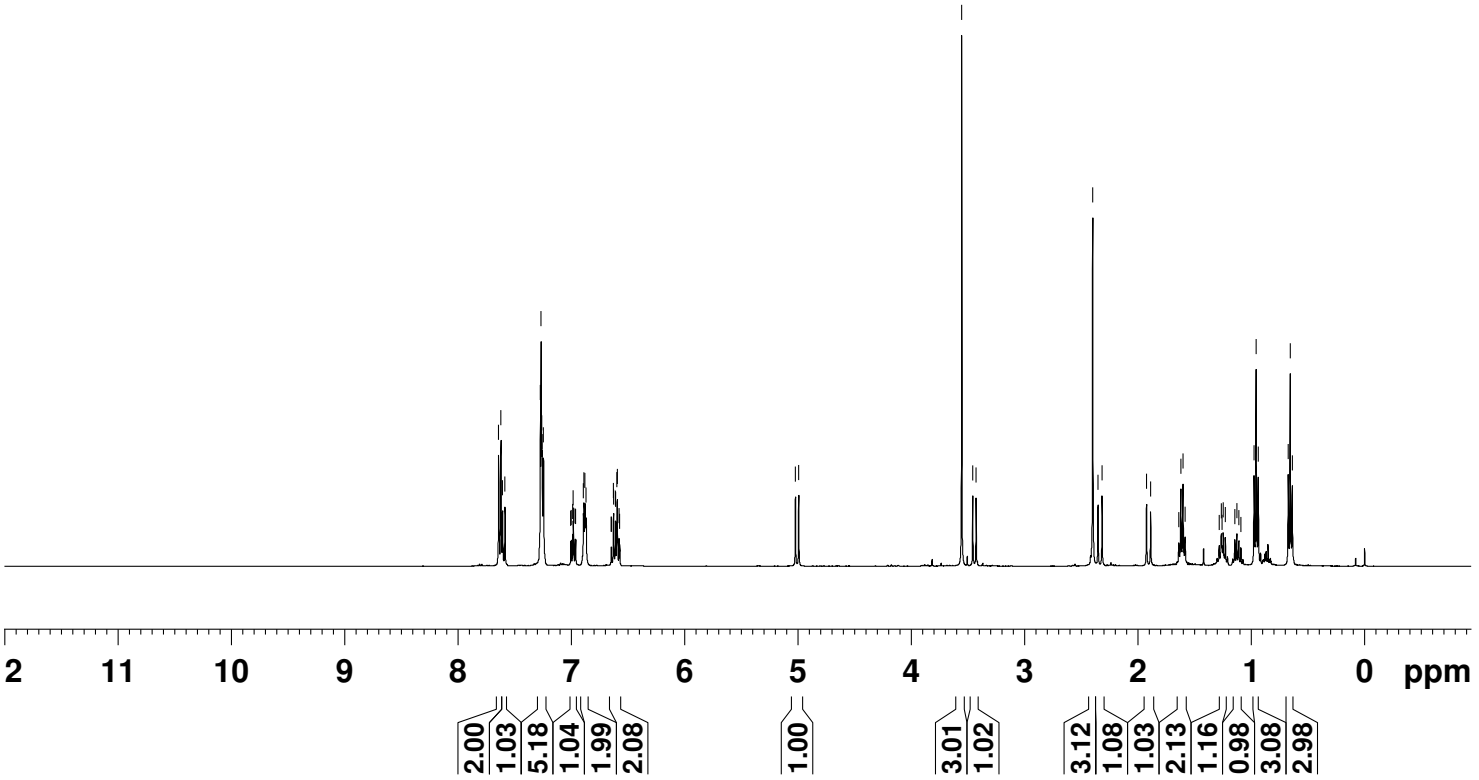



```
NAME      lly-764-5p-20160414
EXPNO                       2
PROCNO                      1
Date_              20160414
Time                    9.15
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      40
DS                       4
SWH              25252.525 Hz
FIDRES            0.385323 Hz
AQ               1.2976629 sec
RG                    2050
DW                  19.800 usec
DE                   8.00 usec
TE                  299.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     10

======== CHANNEL f1 ========
NUC1                   13C
P1                   13.50 usec
PL1                   3.00 dB
PL1W         43.93649673 W
SFO1         100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   1.80 dB
PL12                 17.19 dB
PL13                 18.46 dB
PL2W          8.92857742 W
PL12W         0.25809658 W
PL13W         0.19265592 W
SFO2         400.1316005 MHz
SI                   32768
SF           100.6127767 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```

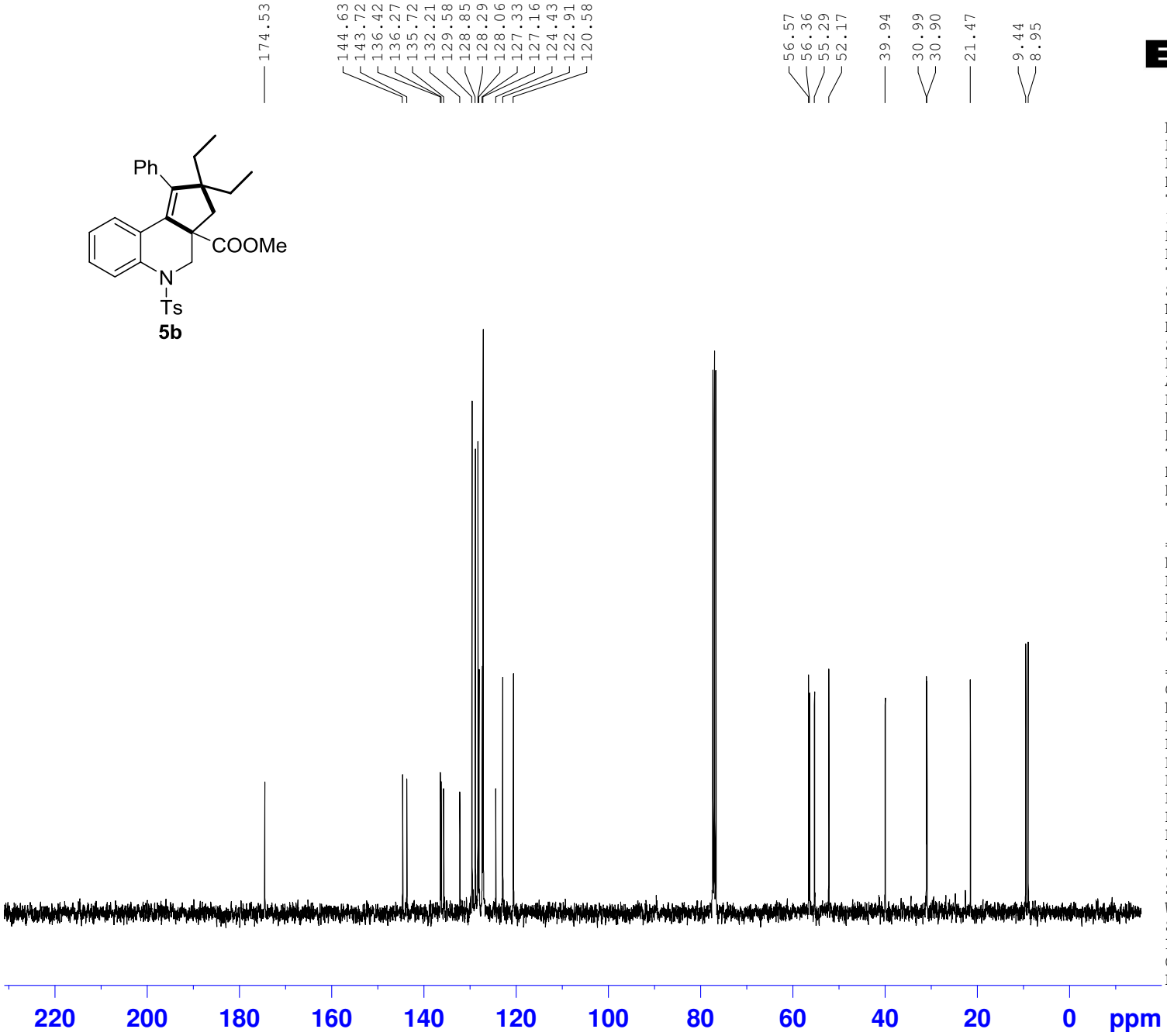




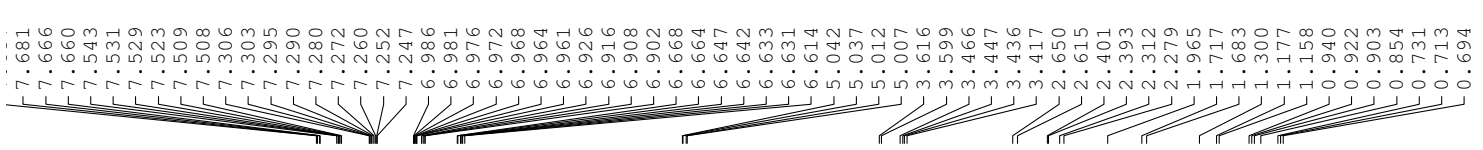
5b

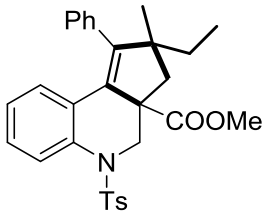



```
NAME      lly-768-3p-20160424
EXPNO                       1
PROCNO                      1
Date_              20160424
Time                   16.47
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                6393.862 Hz
FIDRES            0.195125 Hz
AQ                2.5625076 sec
RG                     71.8
DW                   78.200 usec
DE                    6.50 usec
TE                   295.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.10 usec
PL1                     1.80 dB
PL1W           8.92857742 W
SFO1          400.1326008 MHz
SI                    32768
SF            400.1300131 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



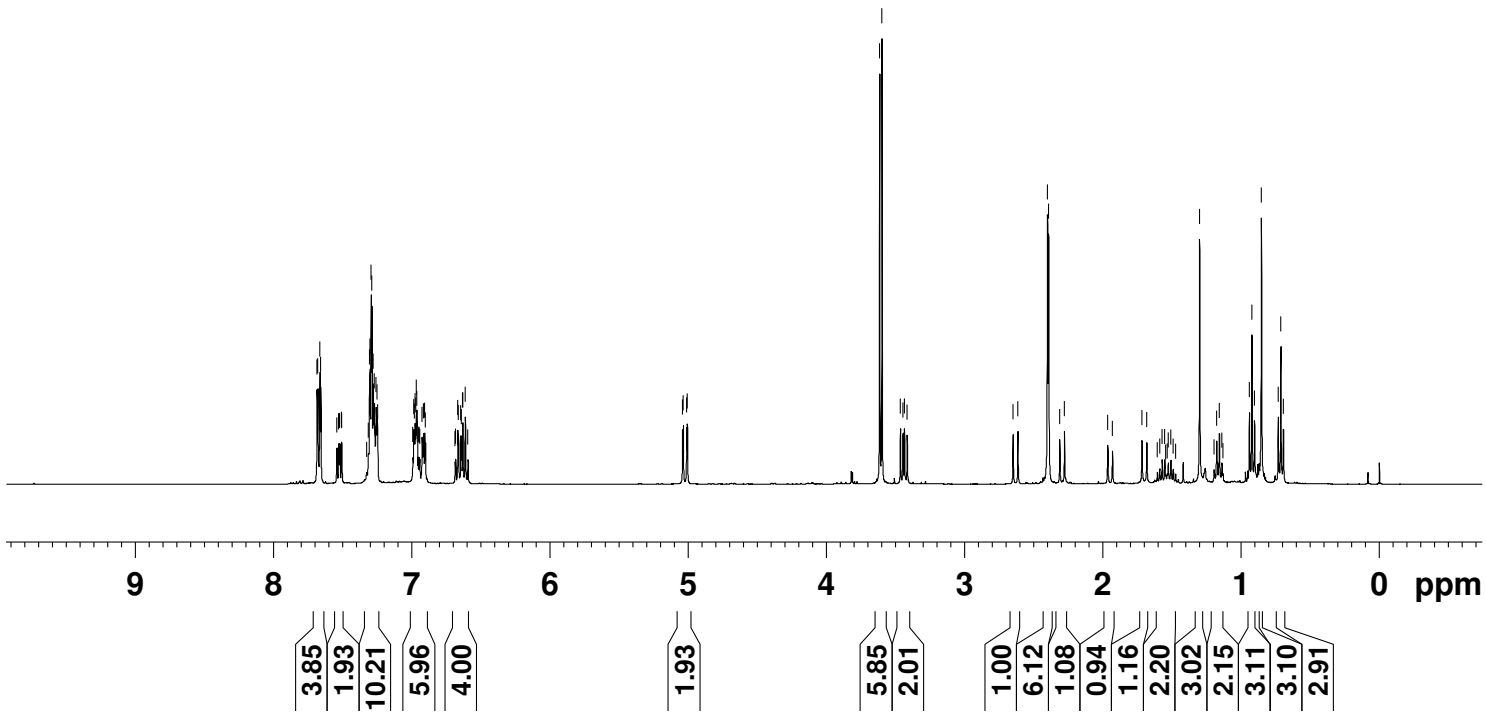

```
NAME        lly-768-3p-20160424
EXPNO                         2
PROCNO                        1
Date_                  20160424
Time                      16.49
INSTRUM                   spect
PROBHD    5 mm PADUL 13C
PULPROG                 zgpg30
TD                         65536
SOLVENT                   CDCl3
NS                           48
DS                            4
SWH                   25252.525 Hz
FIDRES                0.385323 Hz
AQ                    1.2976629 sec
RG                         2050
DW                       19.800 usec
DE                        8.00 usec
TE                       295.8 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           10

======== CHANNEL f1 ========
NUC1                         13C
P1                         13.50 usec
PL1                         3.00 dB
PL1W                43.93649673 W
SFO1                100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL2                        1.80 dB
PL12                      17.19 dB
PL13                      18.46 dB
PL2W                 8.92857742 W
PL12W                0.25809658 W
PL13W                0.19265592 W
SFO2                400.1316005 MHz
SI                         32768
SF                  100.6127795 MHz
WDW                          EM
SSB                           0
LB                         3.00 Hz
GB                            0
PC                         1.40
```

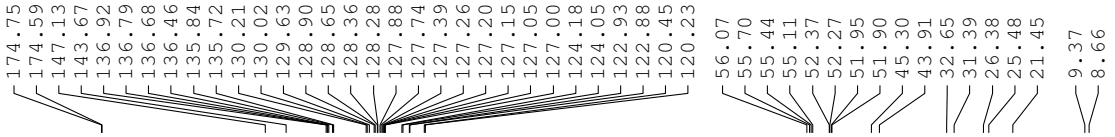


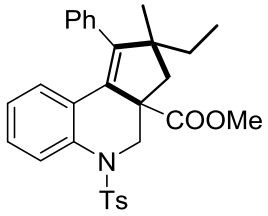


5c (1:1)

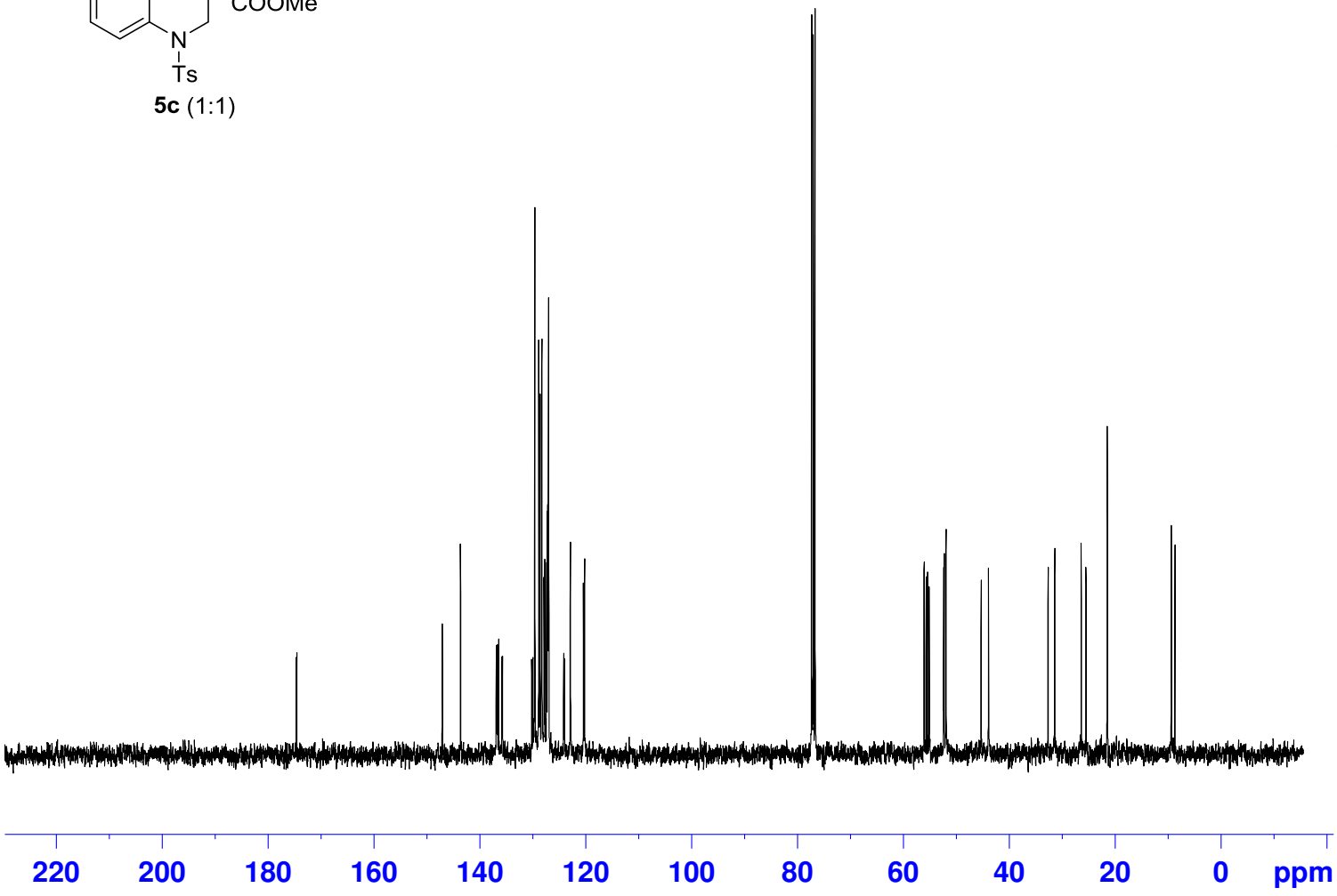
```
NAME      lly-768-2p-20160424
EXPNO                       1
PROCNO                      1
Date_              20160424
Time                   17.05
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                6393.862 Hz
FIDRES            0.195125 Hz
AQ                2.5625076 sec
RG                      71.8
DW                    78.200 usec
DE                     6.50 usec
TE                    295.3 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.10 usec
PL1                     1.80 dB
PL1W           8.92857742 W
SFO1          400.1326008 MHz
SI                     32768
SF            400.1300146 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
```



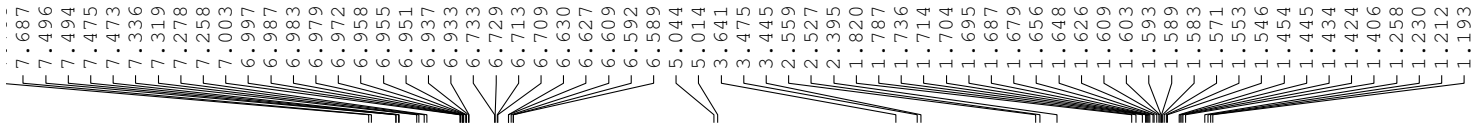


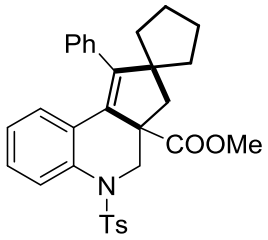


5c (1:1)




```
NAME        lly-768-2p-20160424
EXPNO                         2
PROCNO                        1
Date_                  20160424
Time                      17.07
INSTRUM                   spect
PROBHD    5 mm PADUL 13C
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                          72
DS                           4
SWH                  25252.525 Hz
FIDRES                0.385323 Hz
AQ                    1.2976629 sec
RG                        2050
DW                      19.800 usec
DE                       8.00 usec
TE                      295.9 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          10

======== CHANNEL f1 ========
NUC1                        13C
P1                        13.50 usec
PL1                        3.00 dB
PL1W               43.93649673 W
SFO1               100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                       1.80 dB
PL12                     17.19 dB
PL13                     18.46 dB
PL2W                8.92857742 W
PL12W               0.25809658 W
PL13W               0.19265592 W
SFO2               400.1316005 MHz
SI                        32768
SF                 100.6127815 MHz
WDW                          EM
SSB                           0
LB                        3.00 Hz
GB                            0
PC                        1.40
```



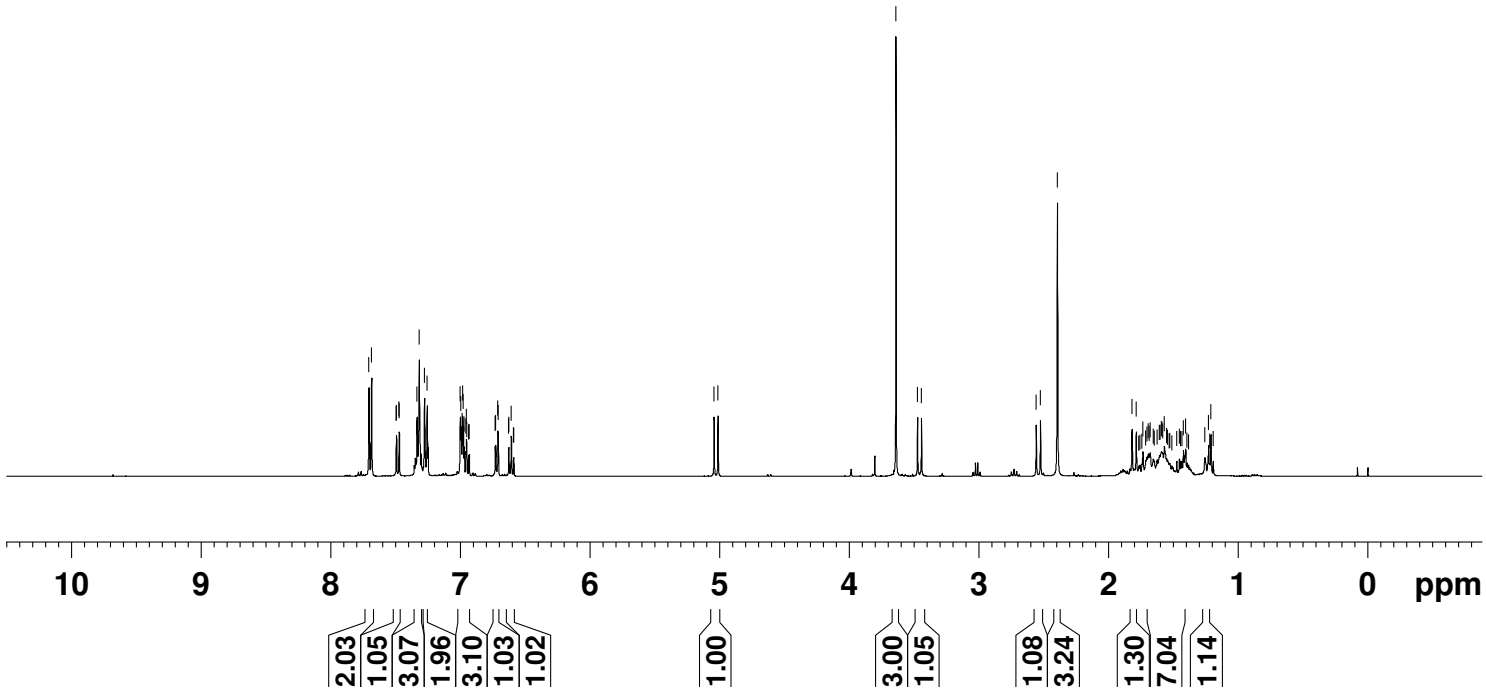


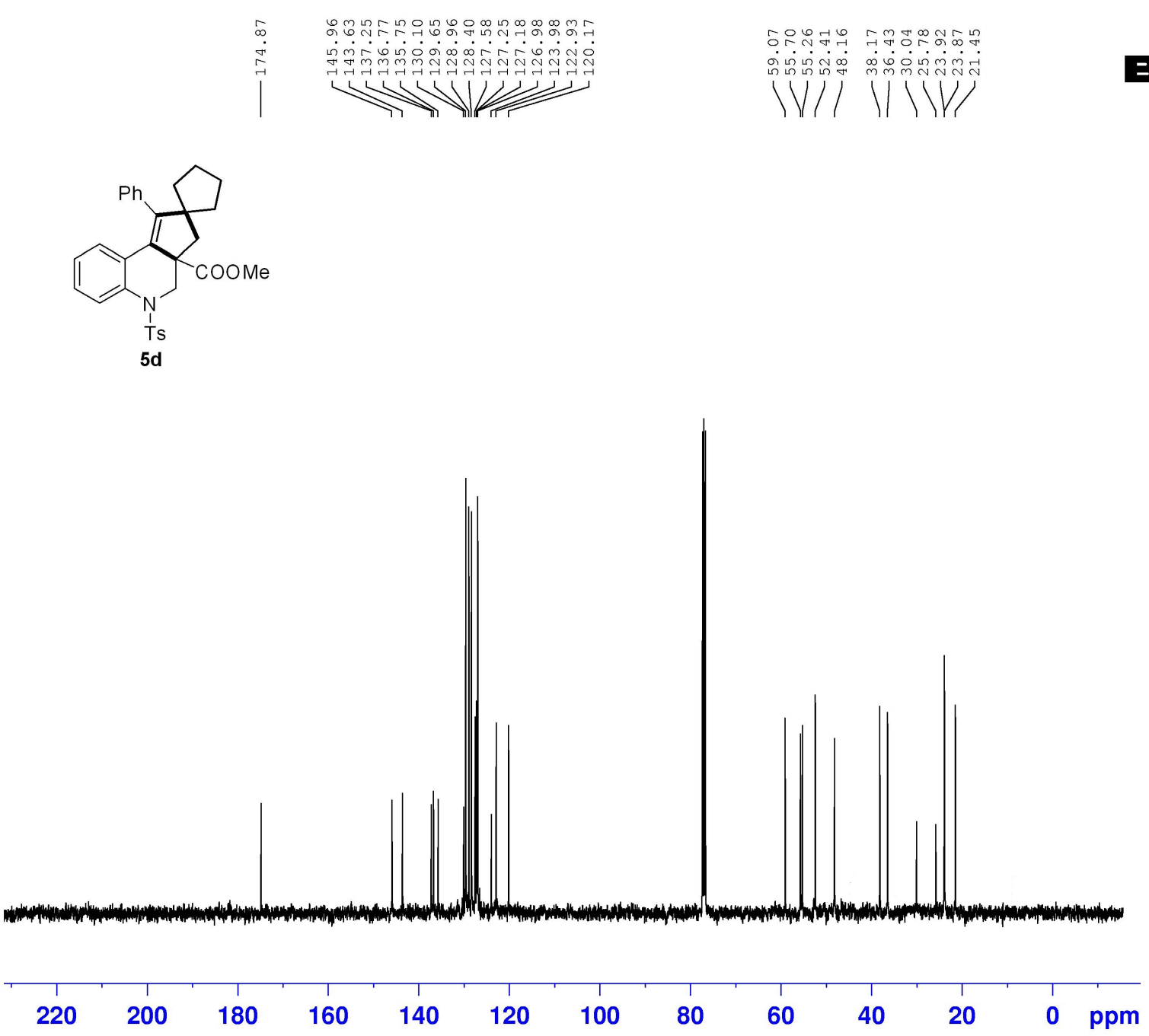
5d

NAME	lly-767-5p-20160423
EXPNO	1
PROCNO	1
Date_	20160423
Time	16.41
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	71.8
DW	78.200 usec
DE	6.50 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1

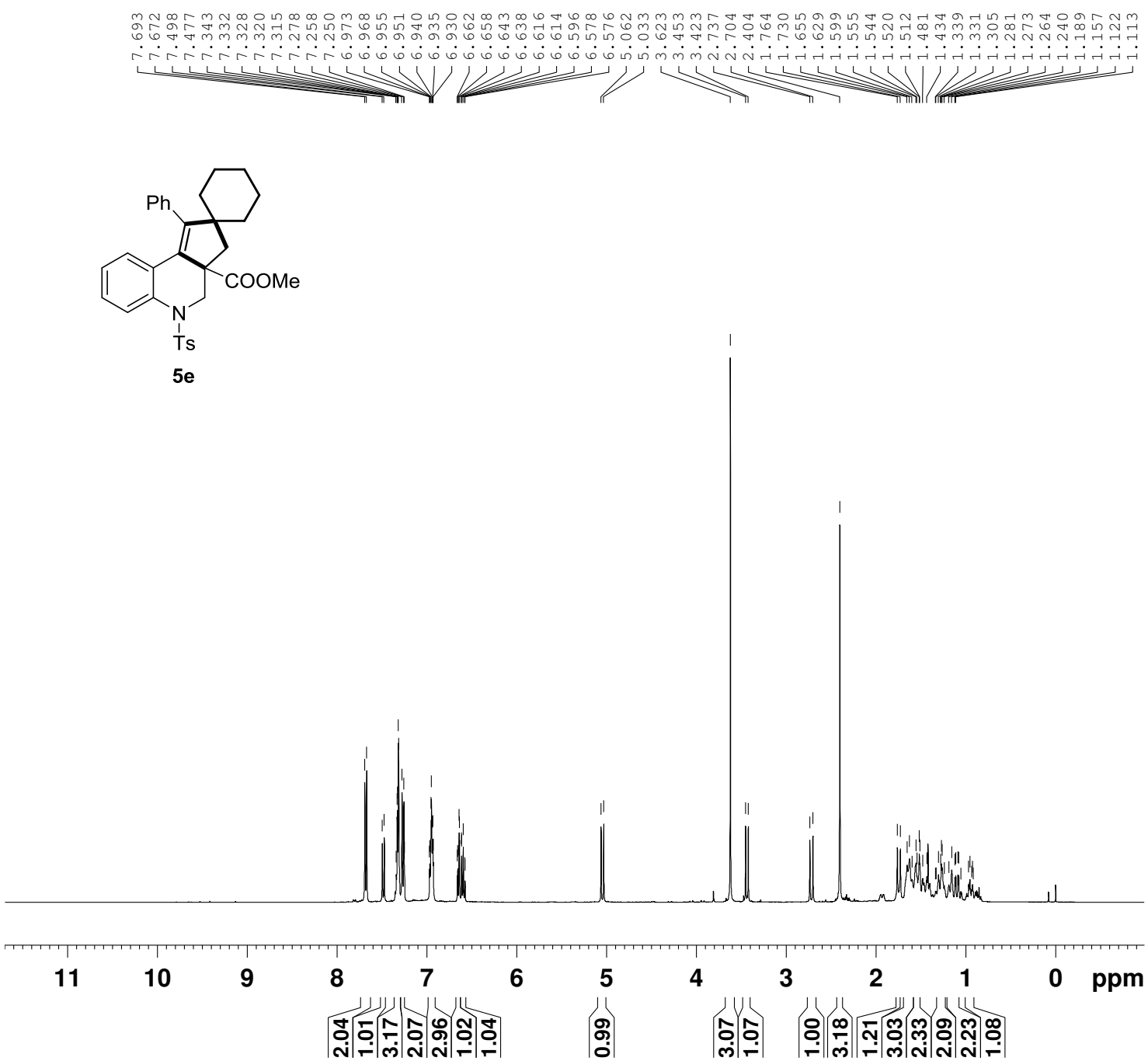
======== CHANNEL f1 ========

NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300134 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



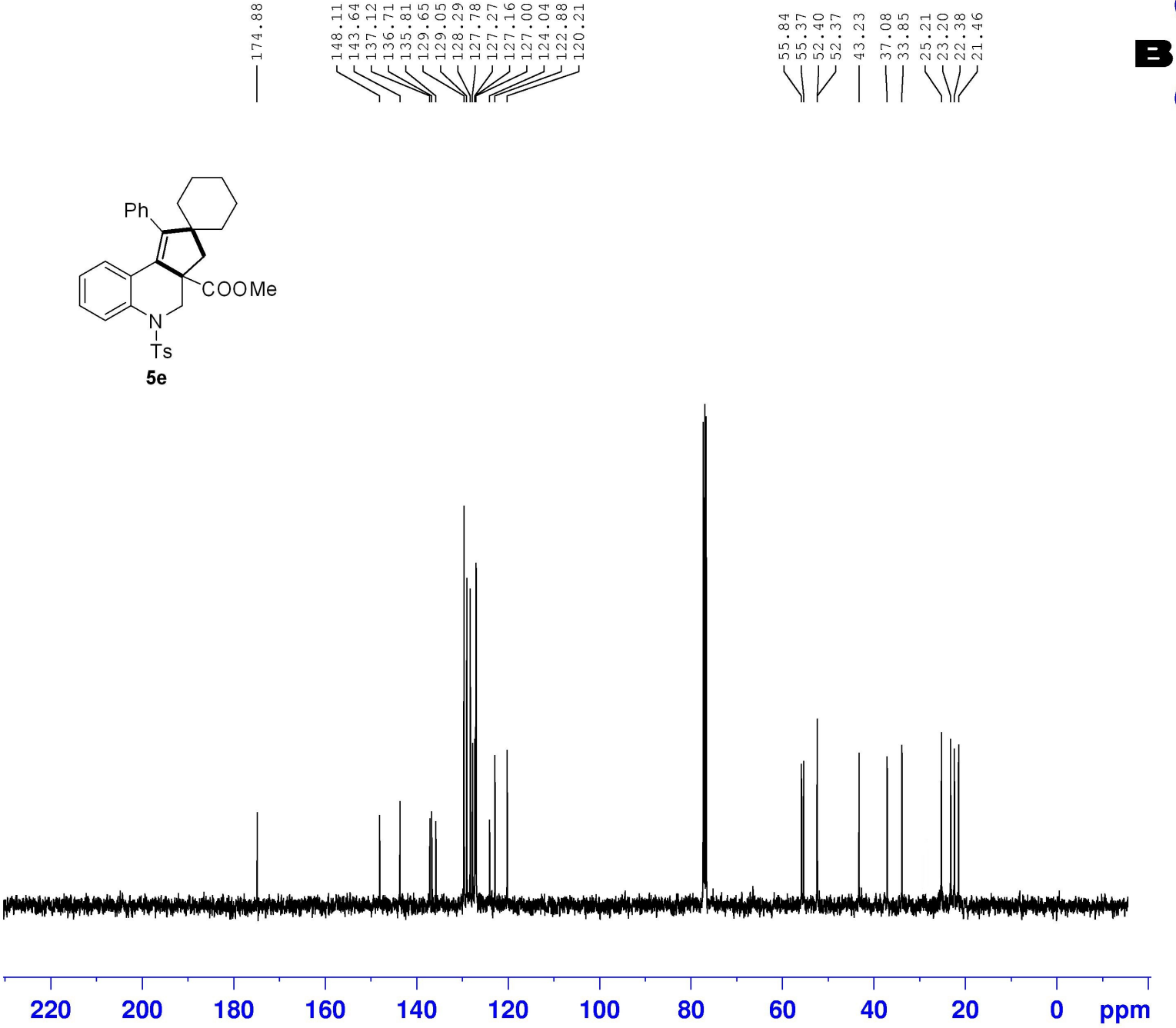


NAME	lly-767-5p-20160818
EXPNO	2
PROCNO	1
Date_	20160818
Time	14.23
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	48
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	295.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
========	CHANNEL f1 ========
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
========	CHANNEL f2 ========
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127811 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40



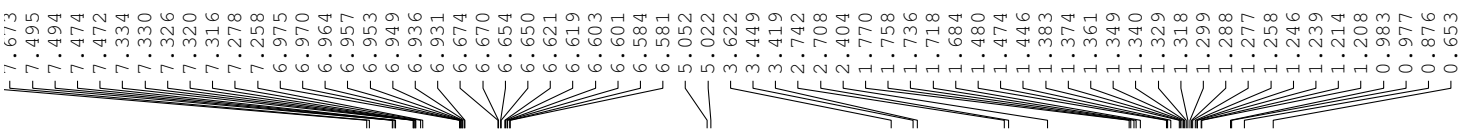
BRUKER

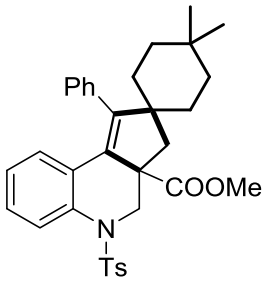
NAME	lly-764-2p-20160413
EXPNO	1
PROCNO	1
Date_	20160413
Time	9.35
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	71.8
DW	78.200 usec
DE	6.50 usec
TE	297.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300134 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



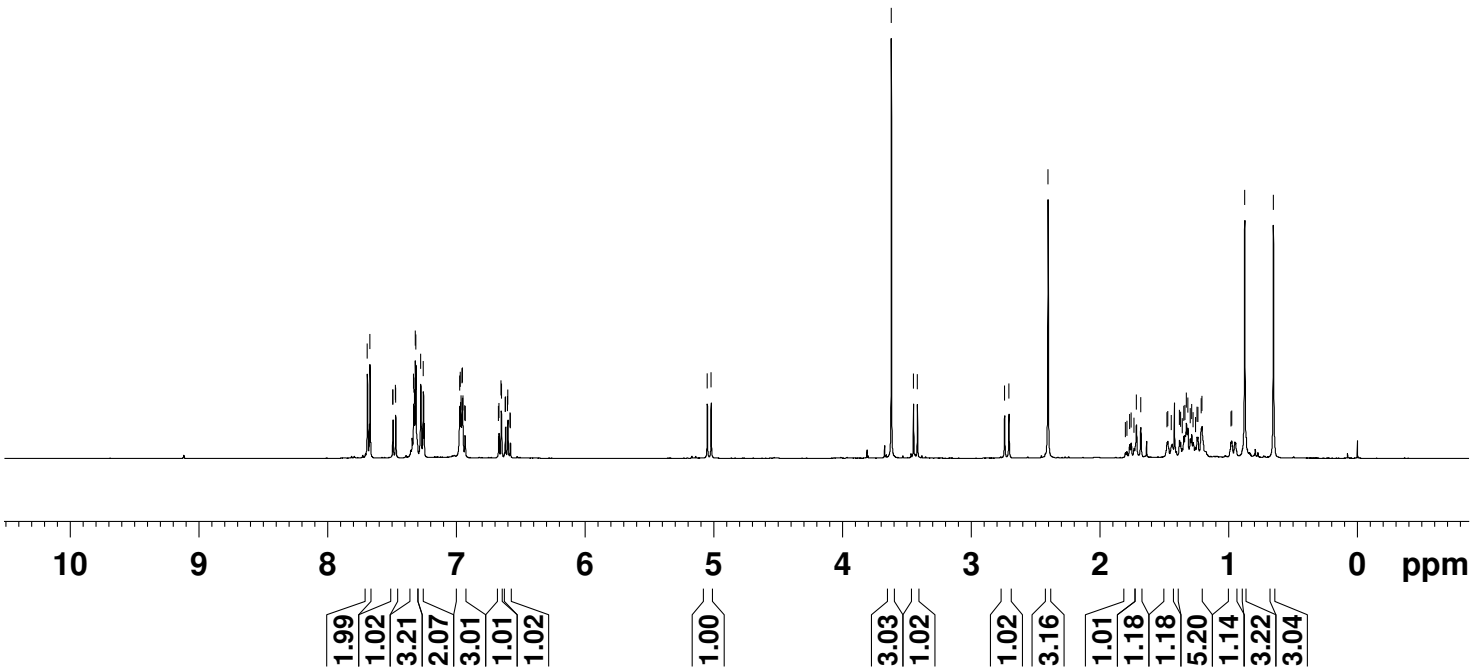
BRUKER

NAME	lly-764-2p-20160818
EXPNO	2
PROCNO	1
Date_	20160818
Time	9.54
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	40
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	297.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127789 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40



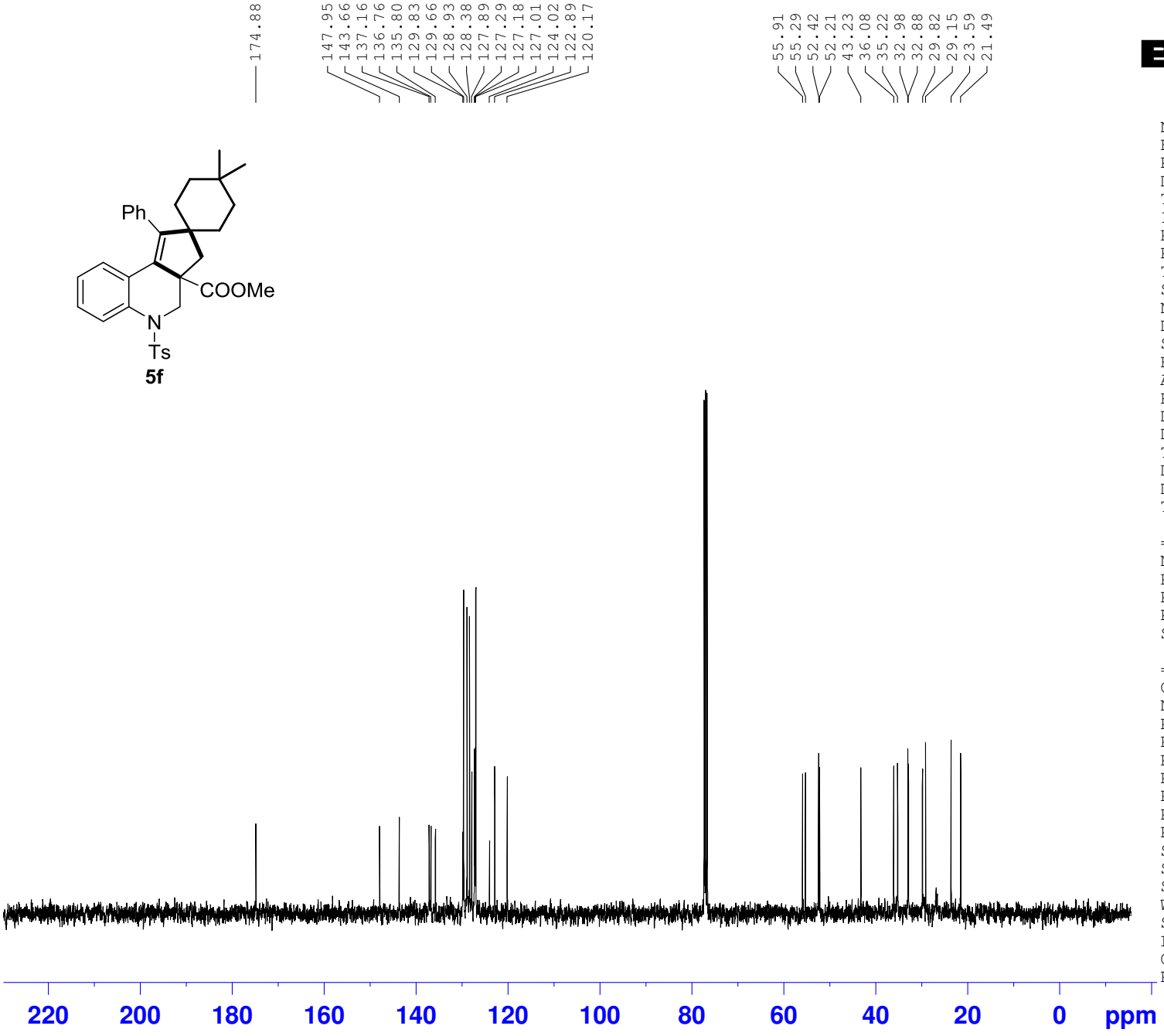


5f

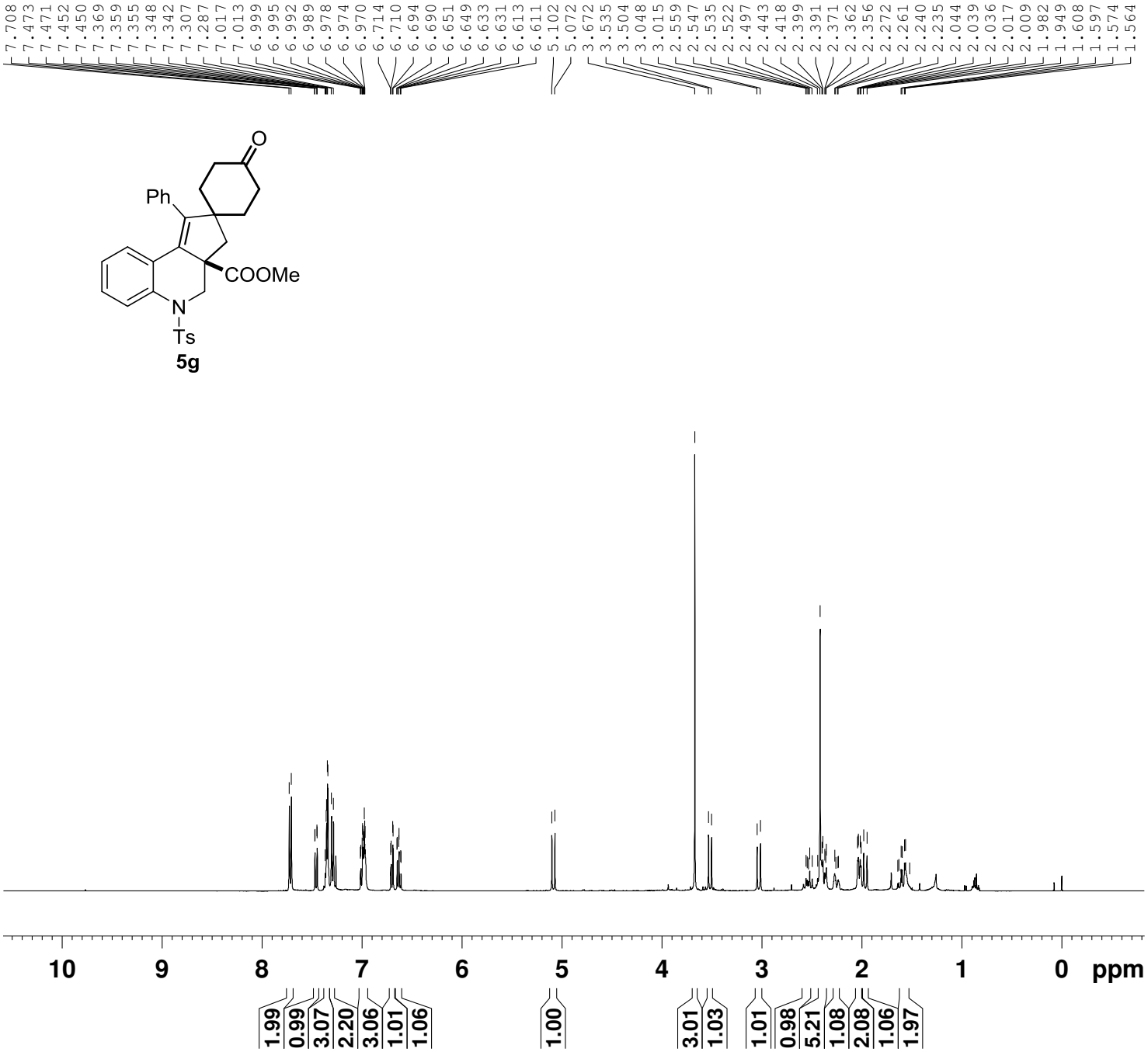


NAME	lly-773-4p-20160505
EXPNO	1
PROCNO	1
Date_	20160505
Time	9.23
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	80.6
DW	78.200 usec
DE	6.50 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1

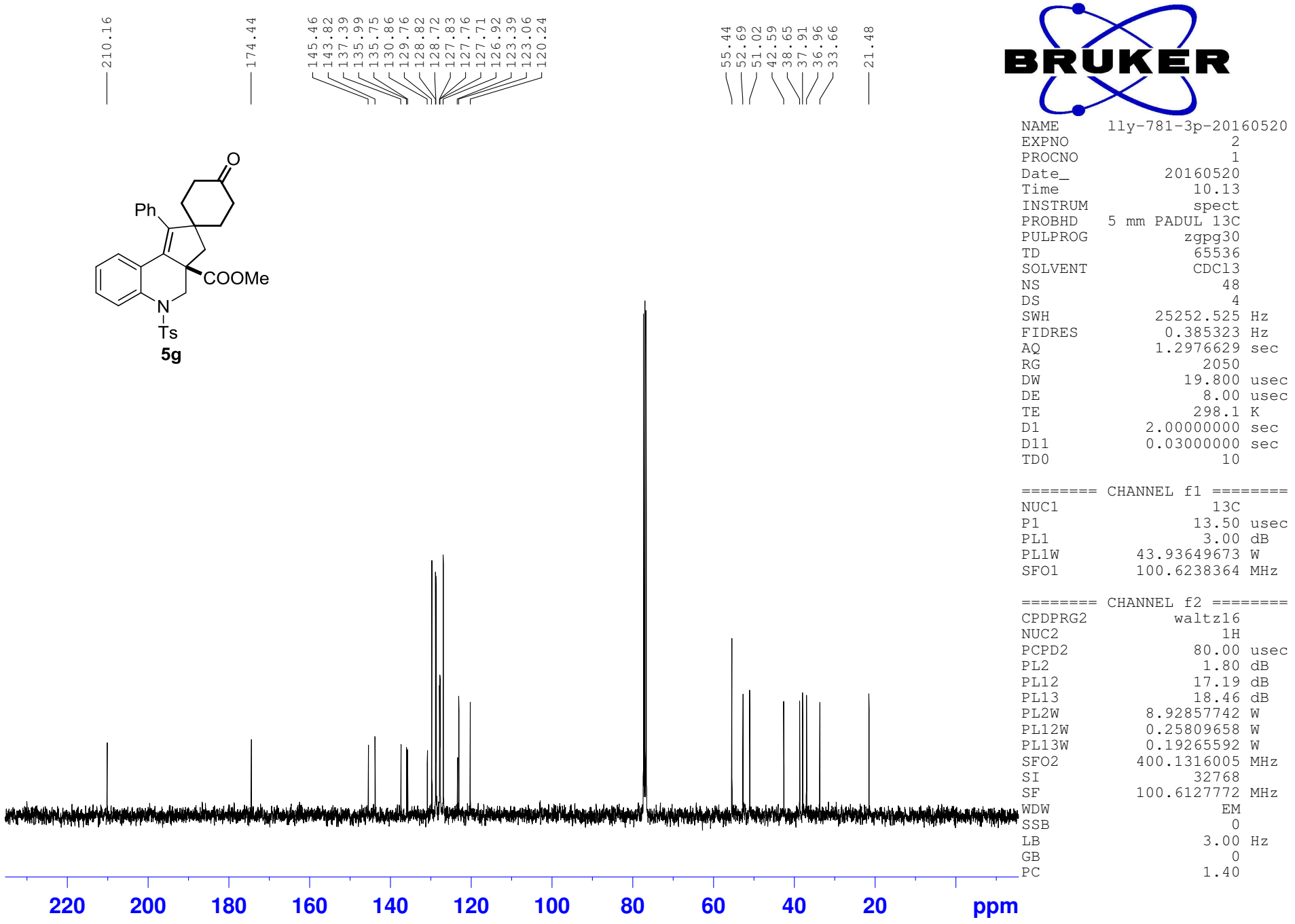
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300133 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
NAME      lly-773-4p-20160505
EXPNO                       2
PROCNO                      1
Date_              20160505
Time                    9.26
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      32
DS                       4
SWH               25252.525 Hz
FIDRES             0.385323 Hz
AQ                1.2976629 sec
RG                     2050
DW                   19.800 usec
DE                    8.00 usec
TE                   297.4 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                     10

======== CHANNEL f1 ========
NUC1                   13C
P1                   13.50 usec
PL1                   3.00 dB
PL1W           43.93649673 W
SFO1          100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   1.80 dB
PL12                 17.19 dB
PL13                 18.46 dB
PL2W           8.92857742 W
PL12W          0.25809658 W
PL13W          0.19265592 W
SFO2          400.1316005 MHz
SI                   32768
SF            100.6127775 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```

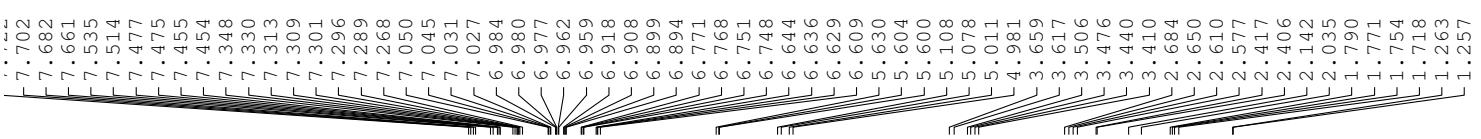


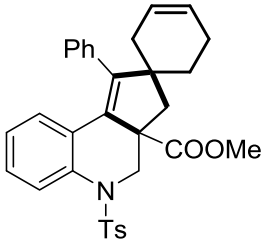

```
NAME      lly-781-3p-20160520
EXPNO                       1
PROCNO                      1
Date_              20160520
Time                   10.09
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 6393.862 Hz
FIDRES              0.195125 Hz
AQ                2.5625076 sec
RG                       101
DW                    78.200 usec
DE                     6.50 usec
TE                    297.4 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.10 usec
PL1                     1.80 dB
PL1W           8.92857742 W
SFO1          400.1326008 MHz
SI                     32768
SF            400.1300084 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                     1.00
```



BRUKER

NAME	lly-781-3p-20160520
EXPNO	2
PROCNO	1
Date_	20160520
Time	10.13
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	48
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	298.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127772 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40





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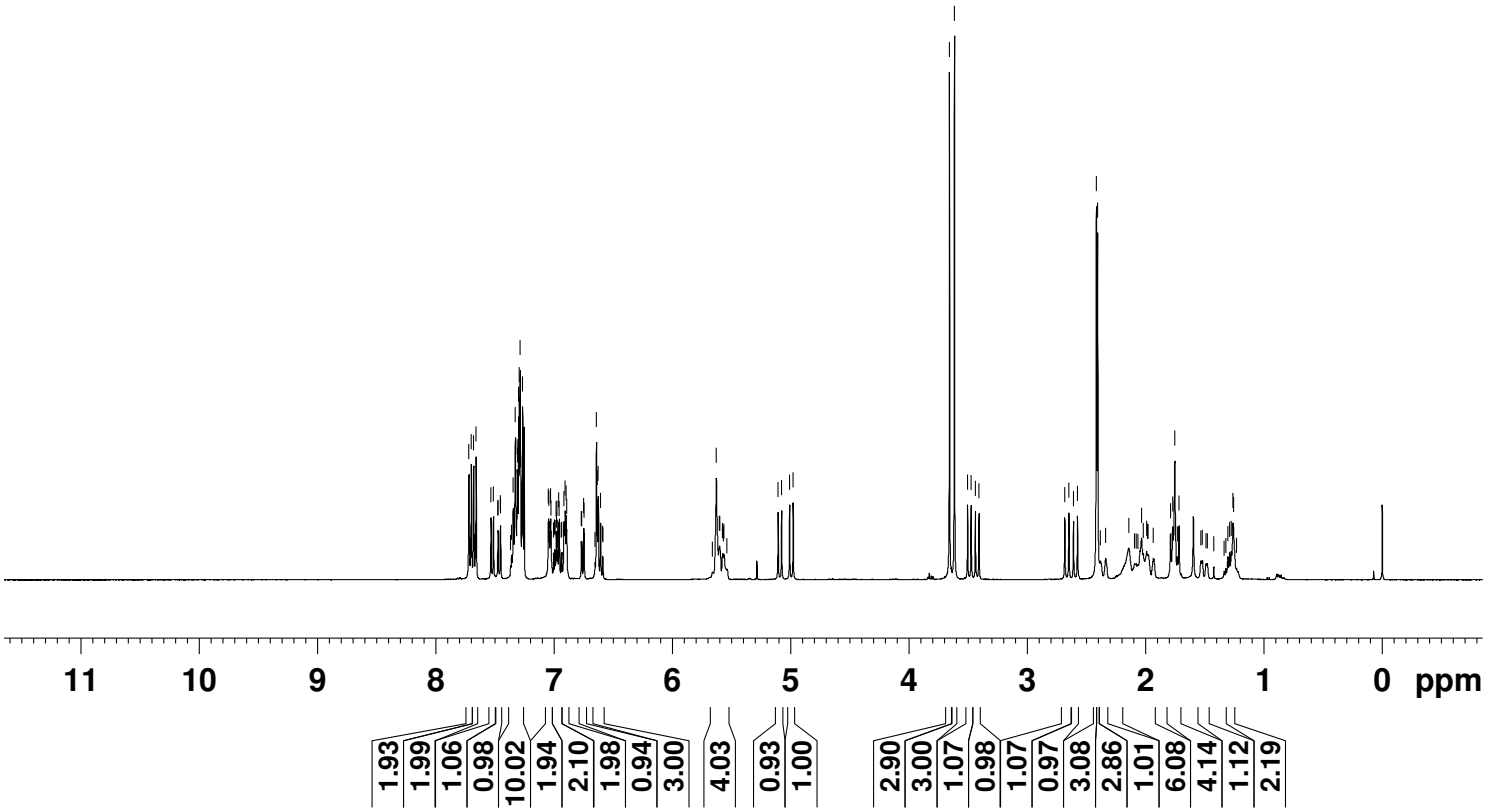
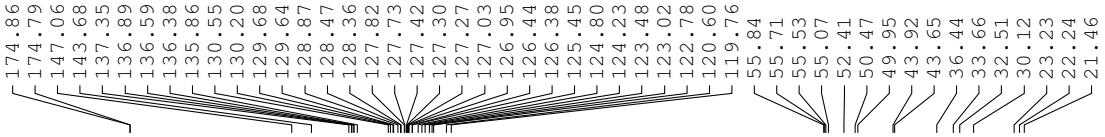
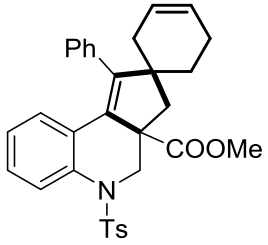
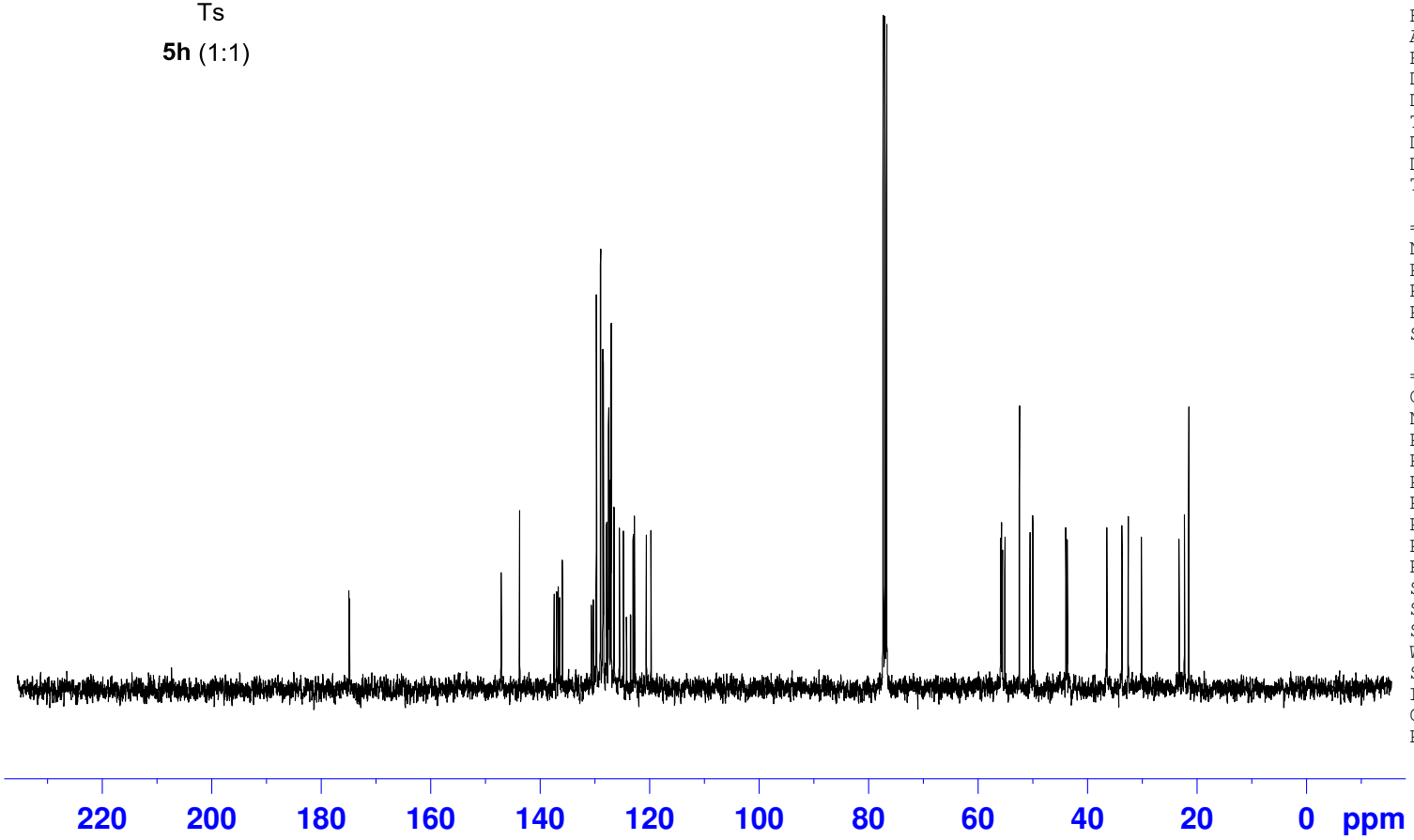


NAME	lly-769-2ap-20160531
EXPNO	1
PROCNO	1
Date_	20160531
Time	16.19
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	161
DW	78.200 usec
DE	6.50 usec
TE	297.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300117 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

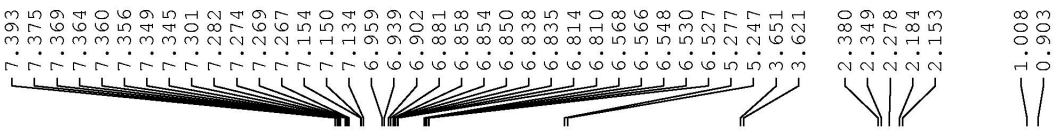


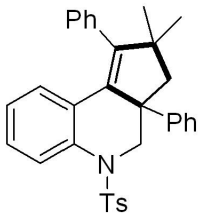


5h (1:1)



NAME	lly-769-2ap-20160602
EXPNO	2
PROCNO	1
Date_	20160602
Time	9.27
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	56
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	297.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127802 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40





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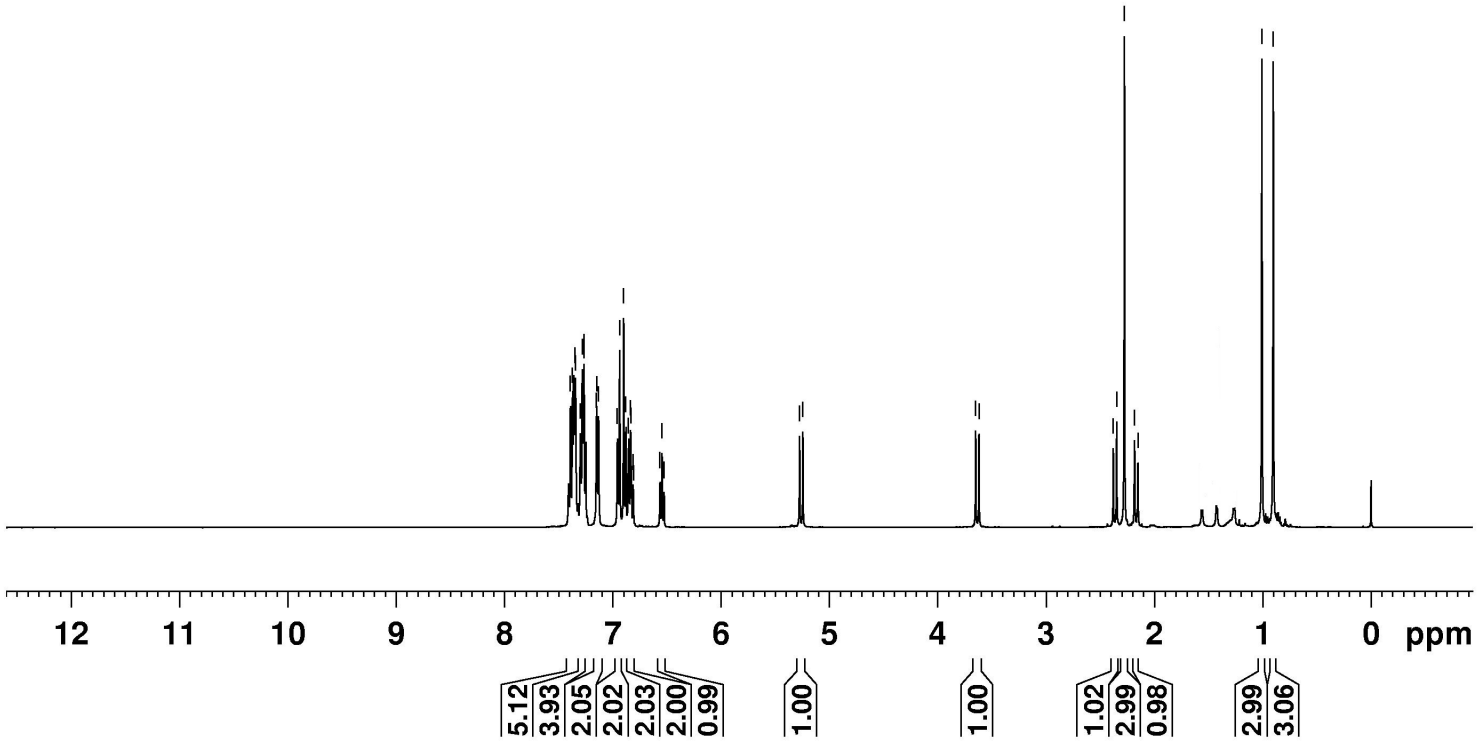
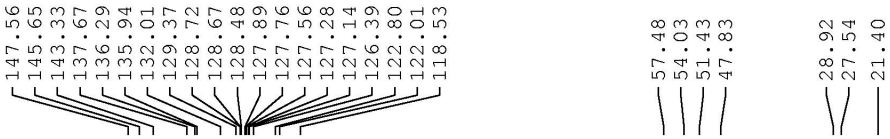
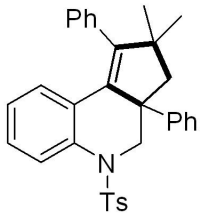


NAME	lly-771-4p-20160819
EXPNO	1
PROCNO	1
Date_	20160819
Time	10.16
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	128
DW	78.200 usec
DE	6.50 usec
TE	297.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300139 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





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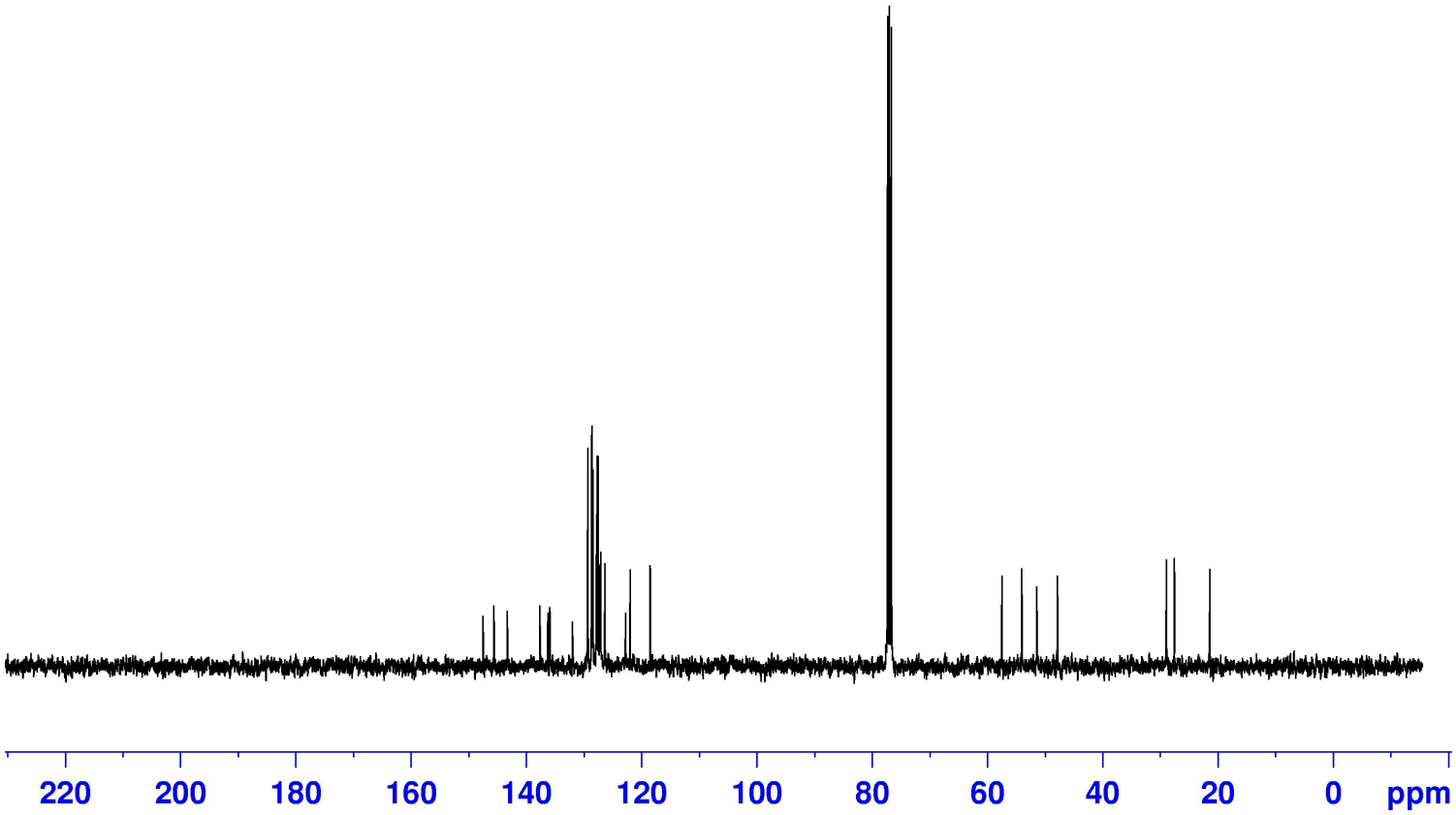
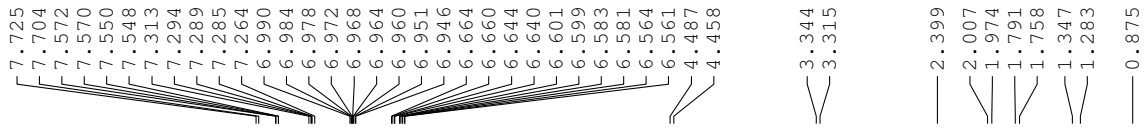
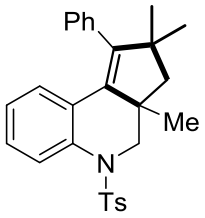


NAME	lly-771-4p-20160819
EXPNO	2
PROCNO	1
Date_	20160819
Time	10.32
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	297.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127734 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

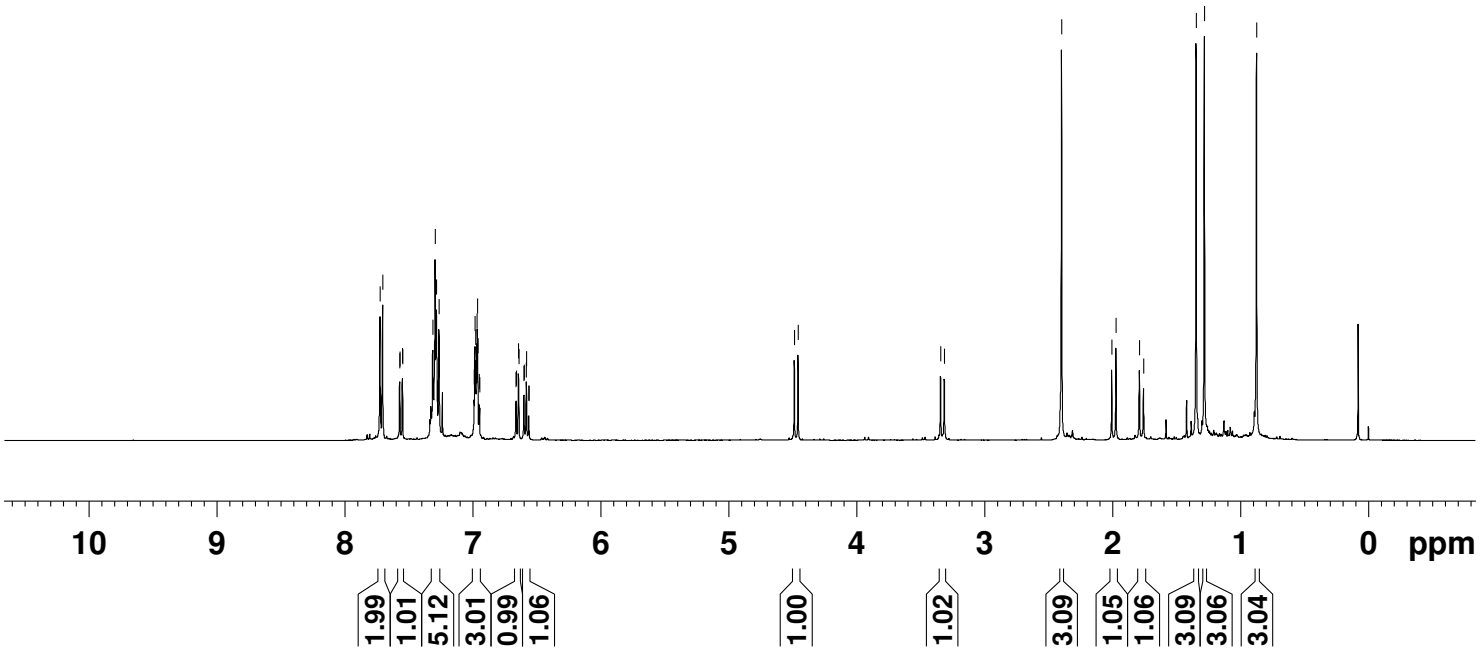


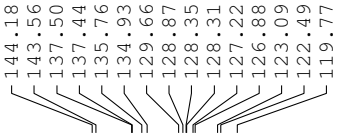


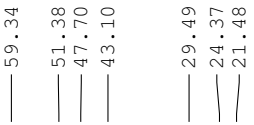
5j

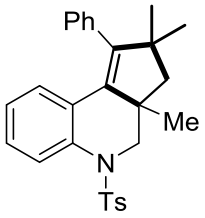
```
NAME      lly-786-1p-20160526
EXPNO                       1
PROCNO                      1
Date_              20160526
Time                   16.56
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                6393.862 Hz
FIDRES            0.195125 Hz
AQ                2.5625076 sec
RG                     80.6
DW                   78.200 usec
DE                    6.50 usec
TE                   297.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.10 usec
PL1                     1.80 dB
PL1W           8.92857742 W
SFO1          400.1326008 MHz
SI                    32768
SF            400.1300187 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```









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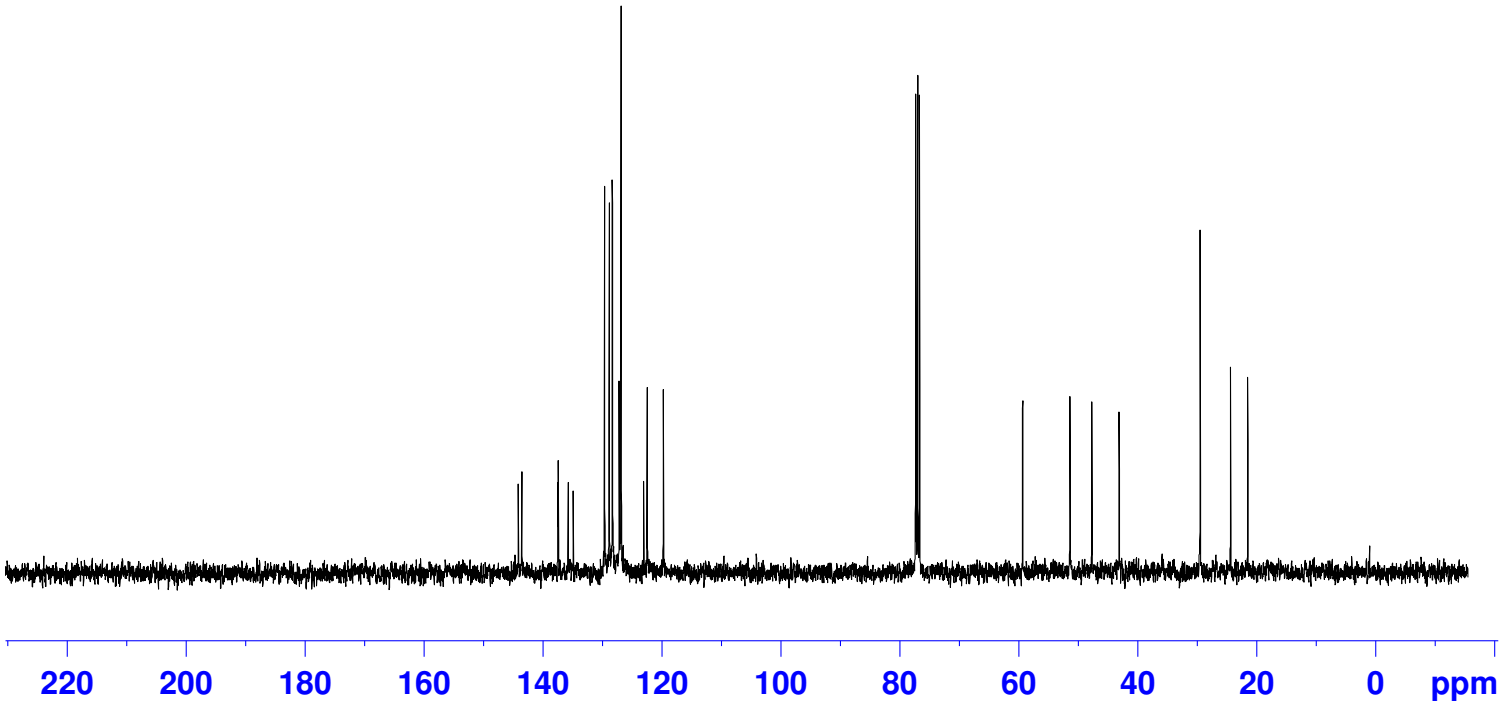
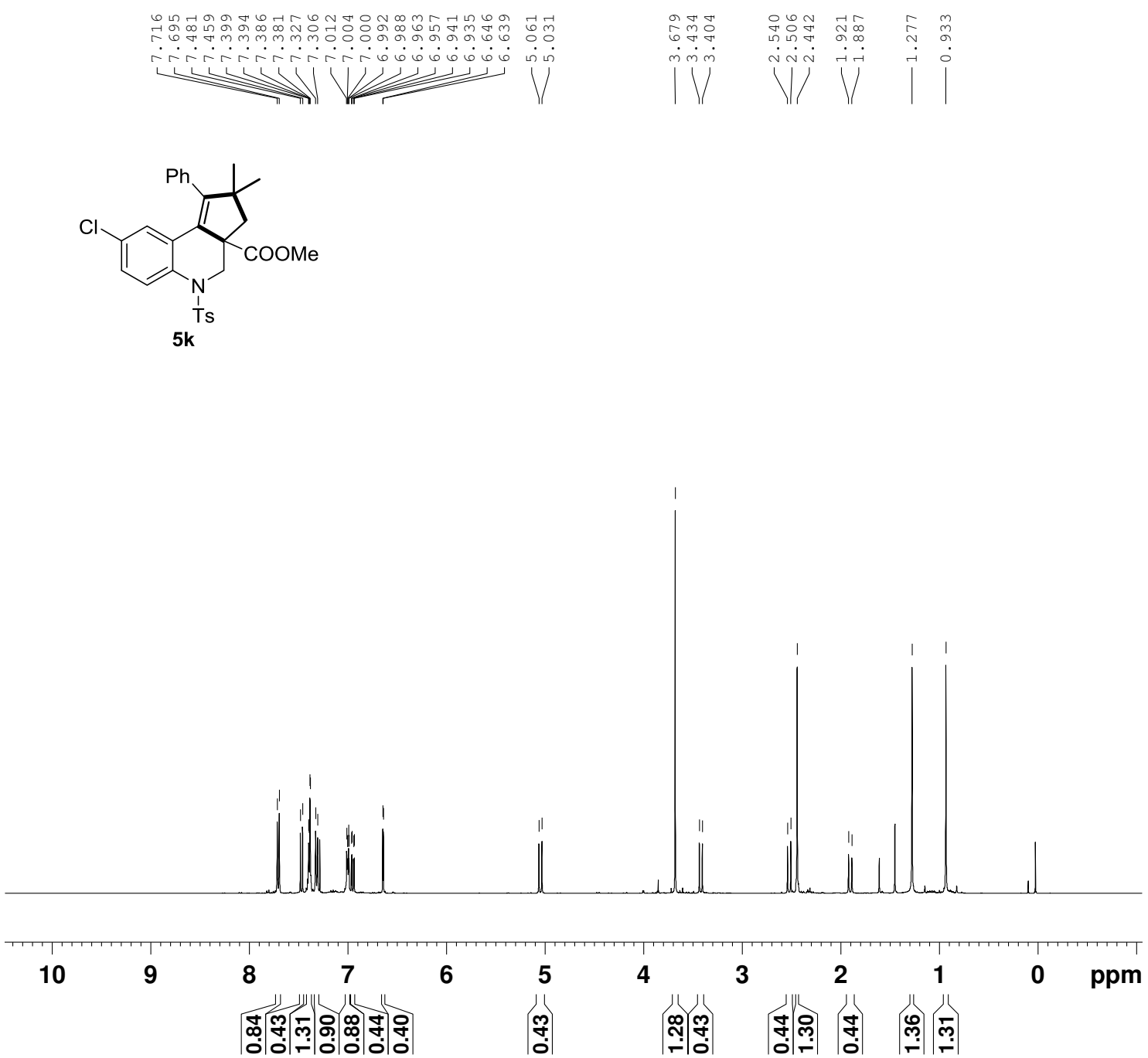
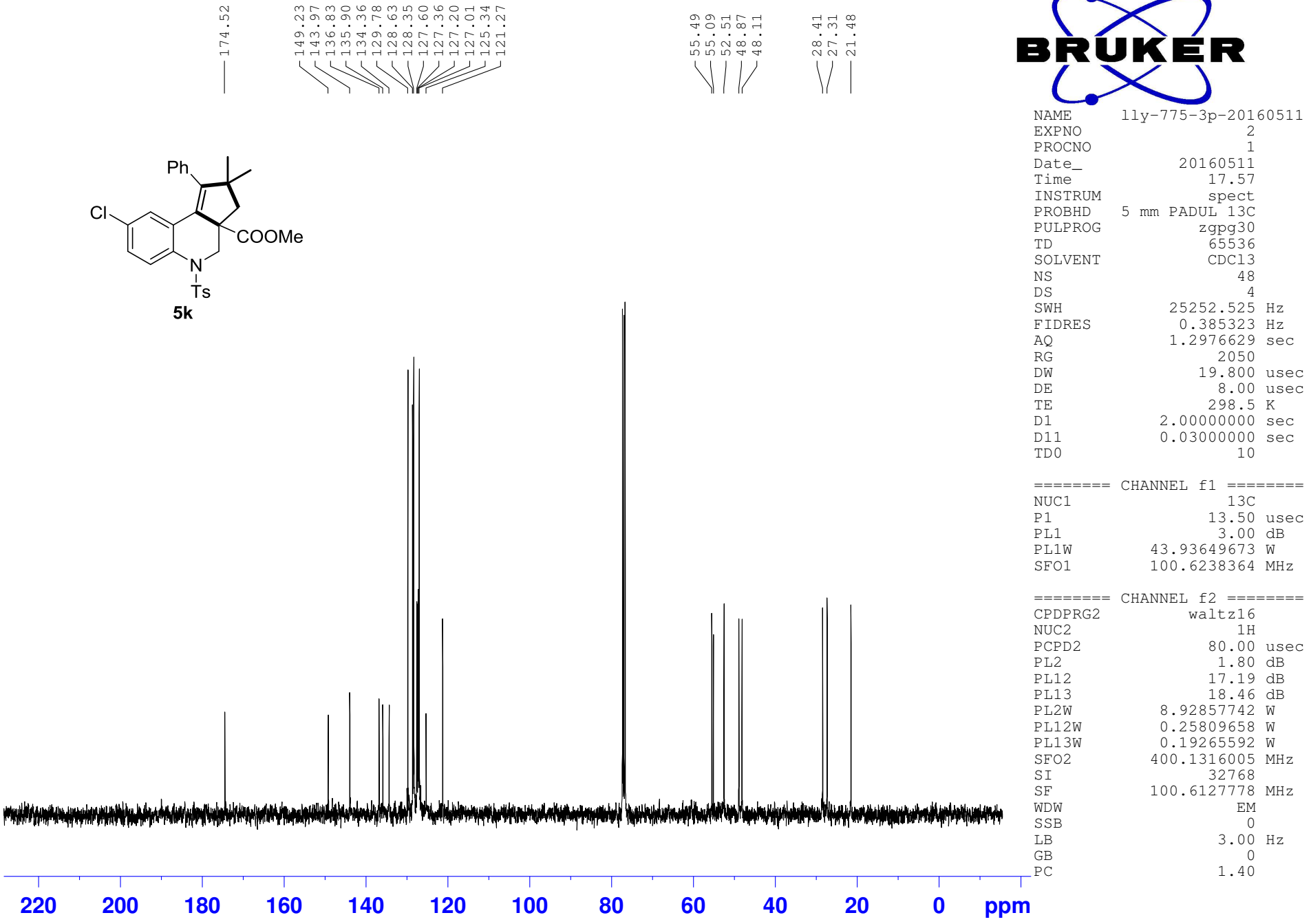



```
NAME          lly-786-1p-20160526
EXPNO                           2
PROCNO                          1
Date_                    20160526
Time                        16.59
INSTRUM                     spect
PROBHD          5 mm PADUL 13C
PULPROG                    zgpg30
TD                          65536
SOLVENT                     CDCl3
NS                             32
DS                              4
SWH                    25252.525 Hz
FIDRES                  0.385323 Hz
AQ                     1.2976629 sec
RG                          2050
DW                        19.800 usec
DE                         8.00 usec
TE                        297.8 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                            10

======== CHANNEL f1 ========
NUC1                          13C
P1                         13.50 usec
PL1                         3.00 dB
PL1W                43.93649673 W
SFO1                100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                          1H
PCPD2                      80.00 usec
PL2                         1.80 dB
PL12                       17.19 dB
PL13                       18.46 dB
PL2W                 8.92857742 W
PL12W                0.25809658 W
PL13W                0.19265592 W
SFO2                400.1316005 MHz
SI                         32768
SF                  100.6127781 MHz
WDW                           EM
SSB                            0
LB                          3.00 Hz
GB                             0
PC                          1.40
```

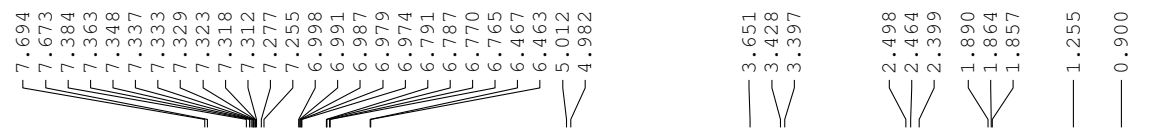


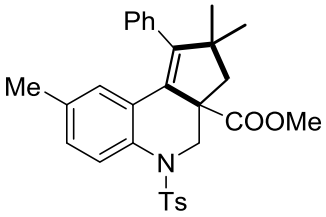

```
NAME      lly-775-3p-20160511
EXPNO                       1
PROCNO                      1
Date_              20160511
Time                    9.46
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 6393.862 Hz
FIDRES              0.195125 Hz
AQ                2.5625076 sec
RG                       203
DW                    78.200 usec
DE                     6.50 usec
TE                    297.2 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.10 usec
PL1                     1.80 dB
PL1W             8.92857742 W
SFO1           400.1326008 MHz
SI                     32768
SF             400.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



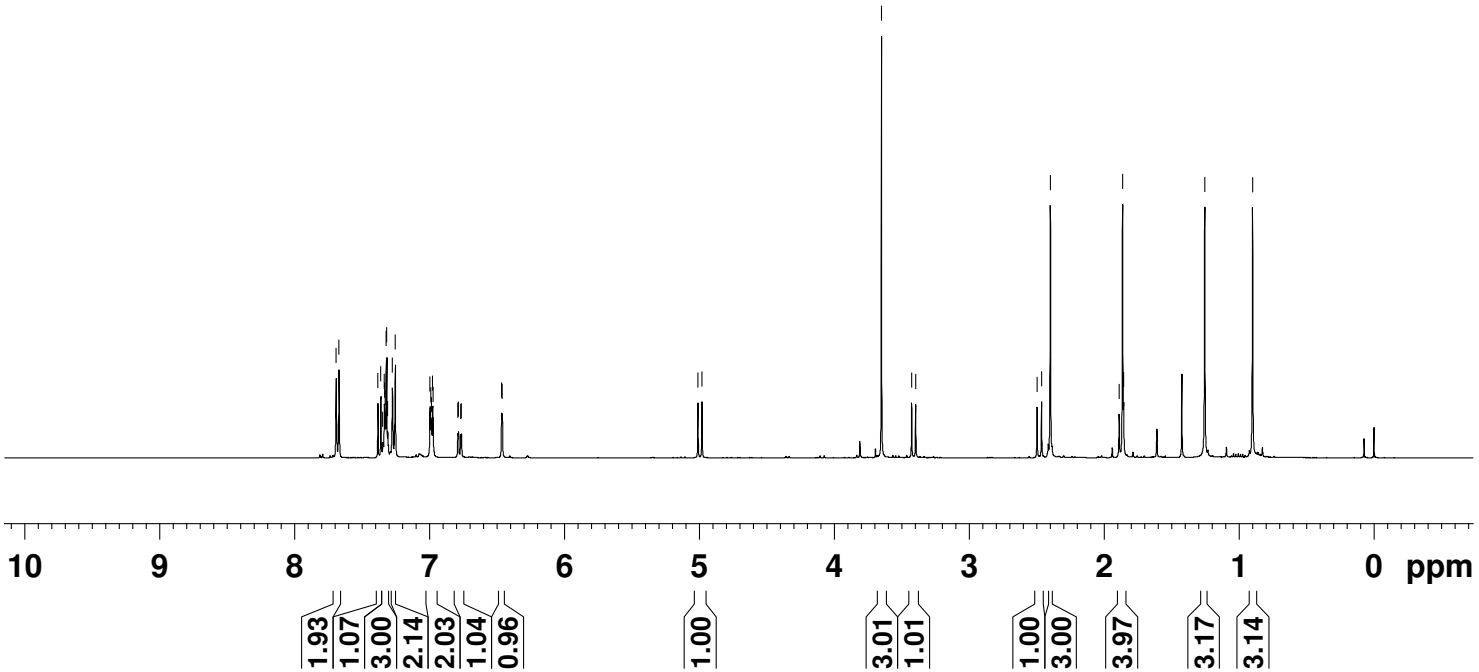
BRUKER

NAME	lly-775-3p-20160511
EXPNO	2
PROCNO	1
Date_	20160511
Time	17.57
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	48
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127778 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

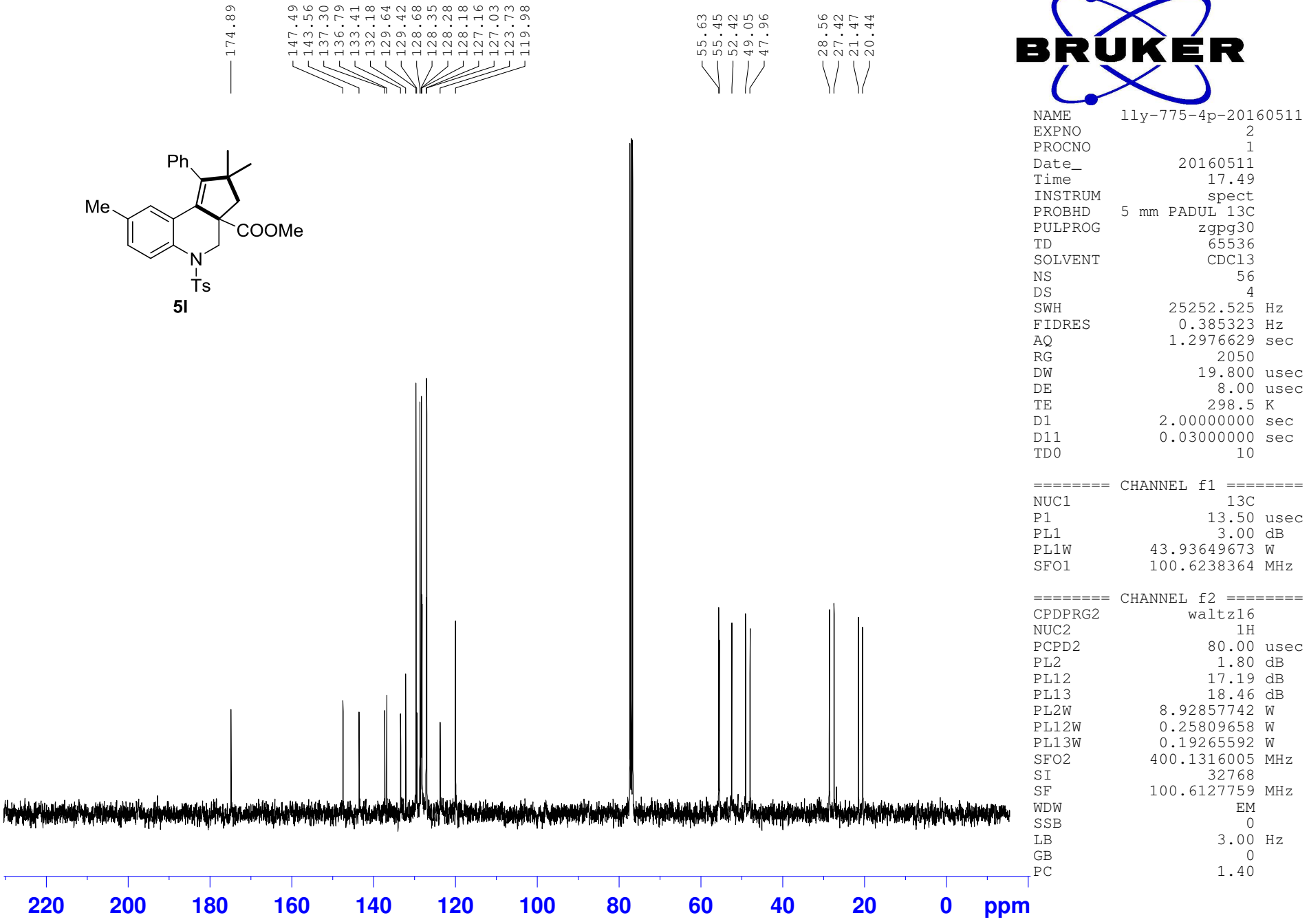




5l

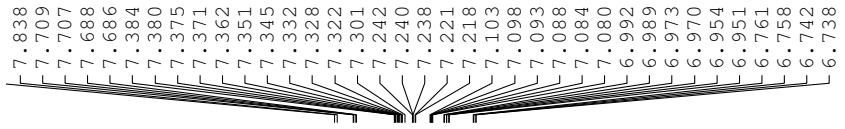


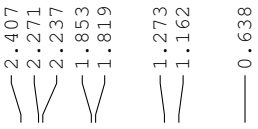

```
NAME      lly-775-4p-20160511
EXPNO                       1
PROCNO                      1
Date_              20160511
Time                    9.50
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 6393.862 Hz
FIDRES              0.195125 Hz
AQ                2.5625076 sec
RG                       128
DW                    78.200 usec
DE                     6.50 usec
TE                    297.2 K
D1               1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.10 usec
PL1                     1.80 dB
PL1W             8.92857742 W
SFO1           400.1326008 MHz
SI                     32768
SF             400.1300116 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

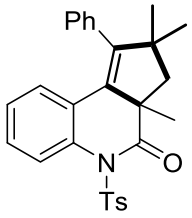


BRUKER

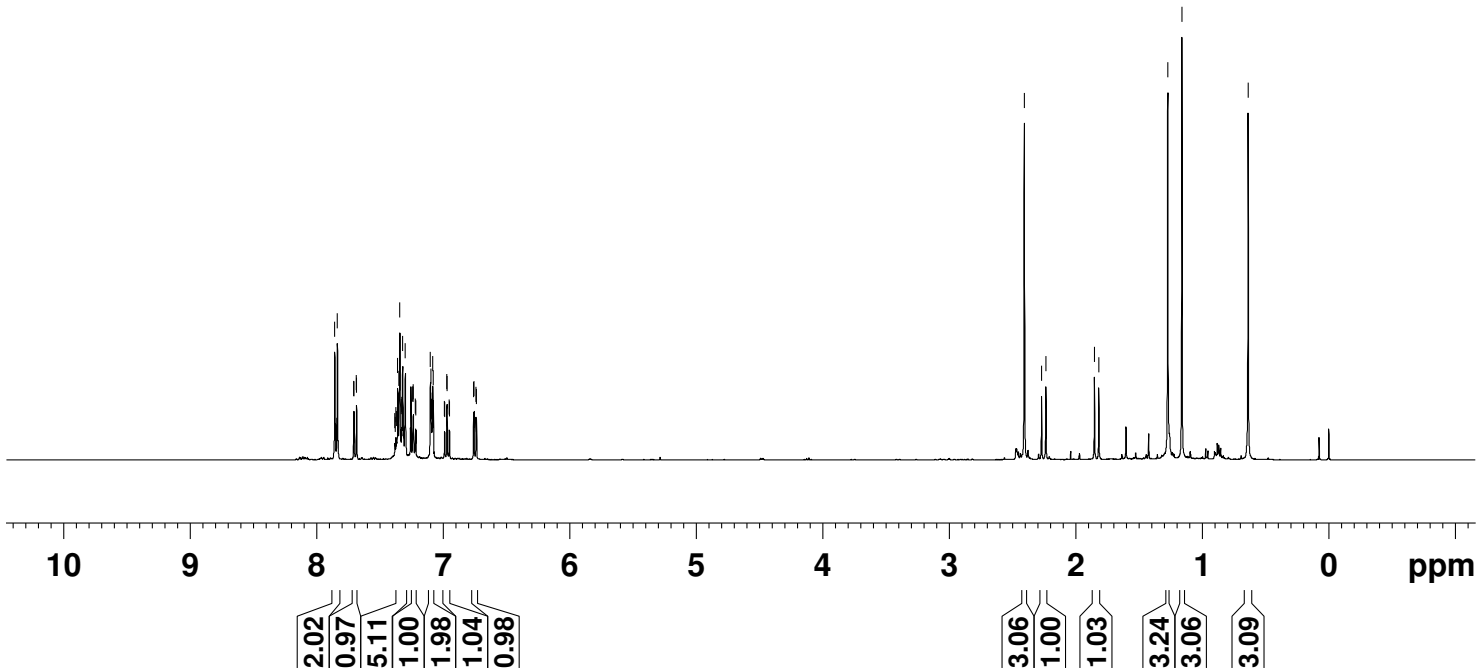
NAME	lly-775-4p-20160511
EXPNO	2
PROCNO	1
Date_	20160511
Time	17.49
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	56
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127759 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40



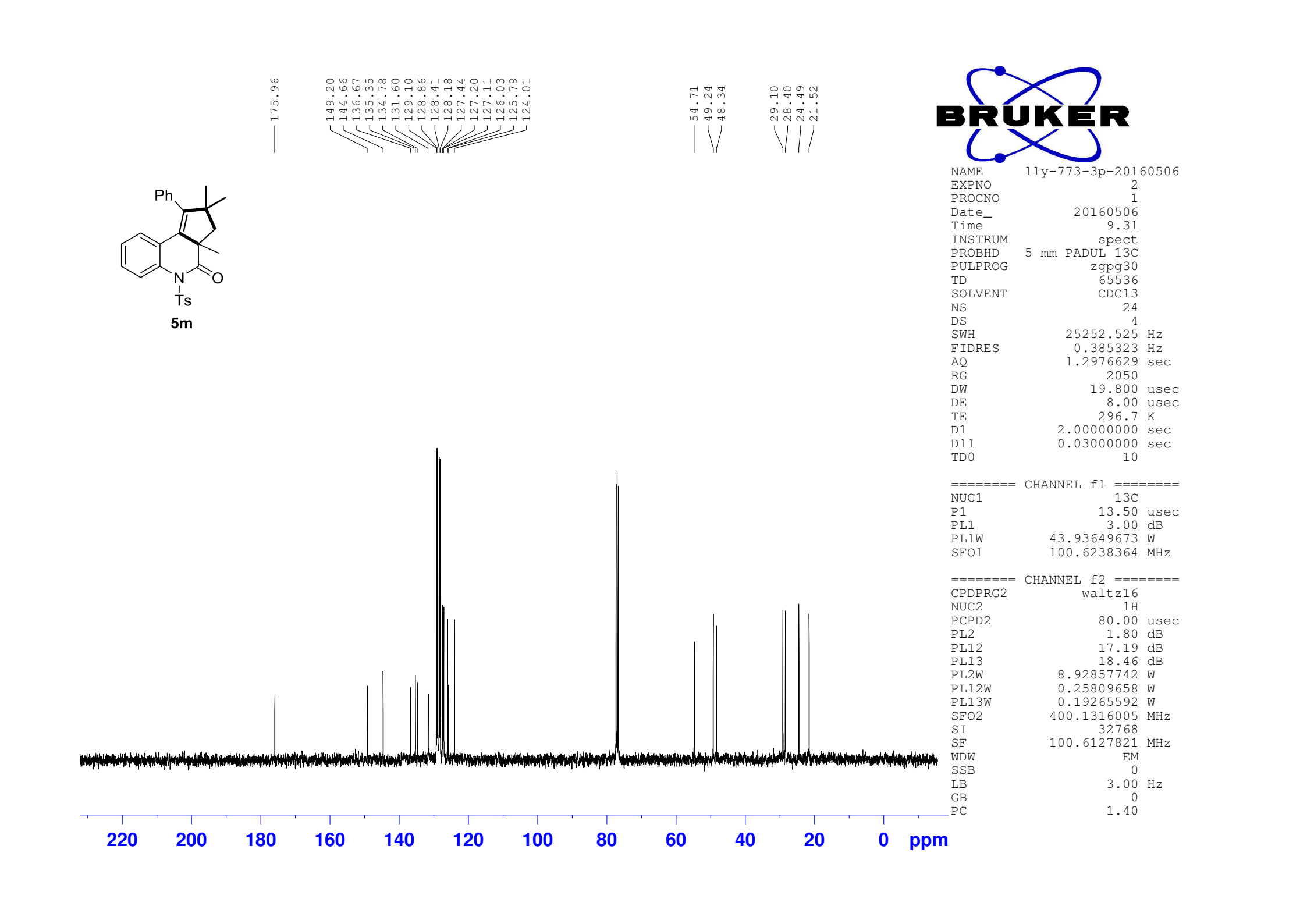




5m

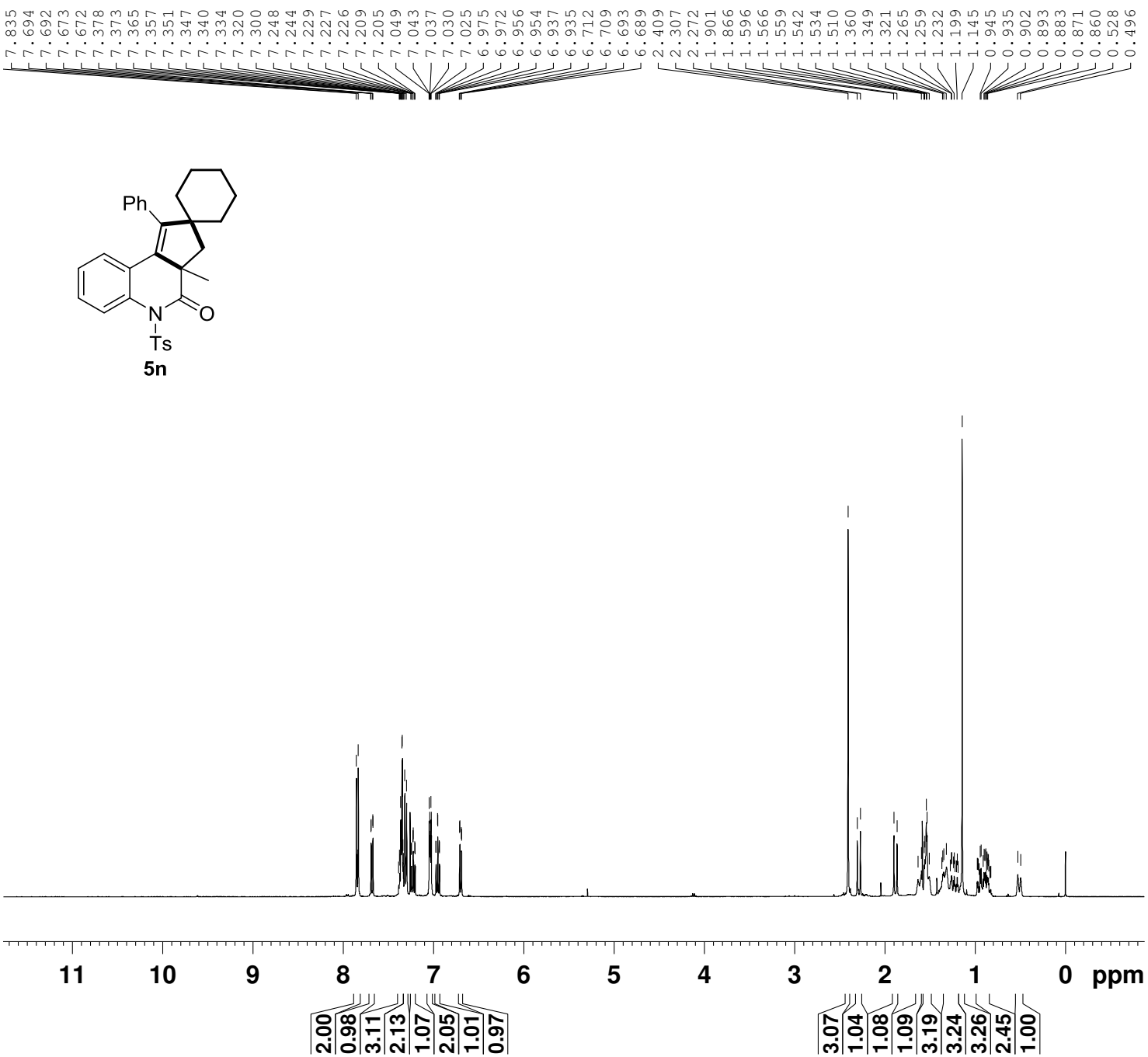


NAME	lly-773-3p-20160505
EXPNO	1
PROCNO	1
Date_	20160505
Time	16.52
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	114
DW	78.200 usec
DE	6.50 usec
TE	296.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300108 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	lly-773-3p-20160506
EXPNO	2
PROCNO	1
Date_	20160506
Time	9.31
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	24
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	296.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127821 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

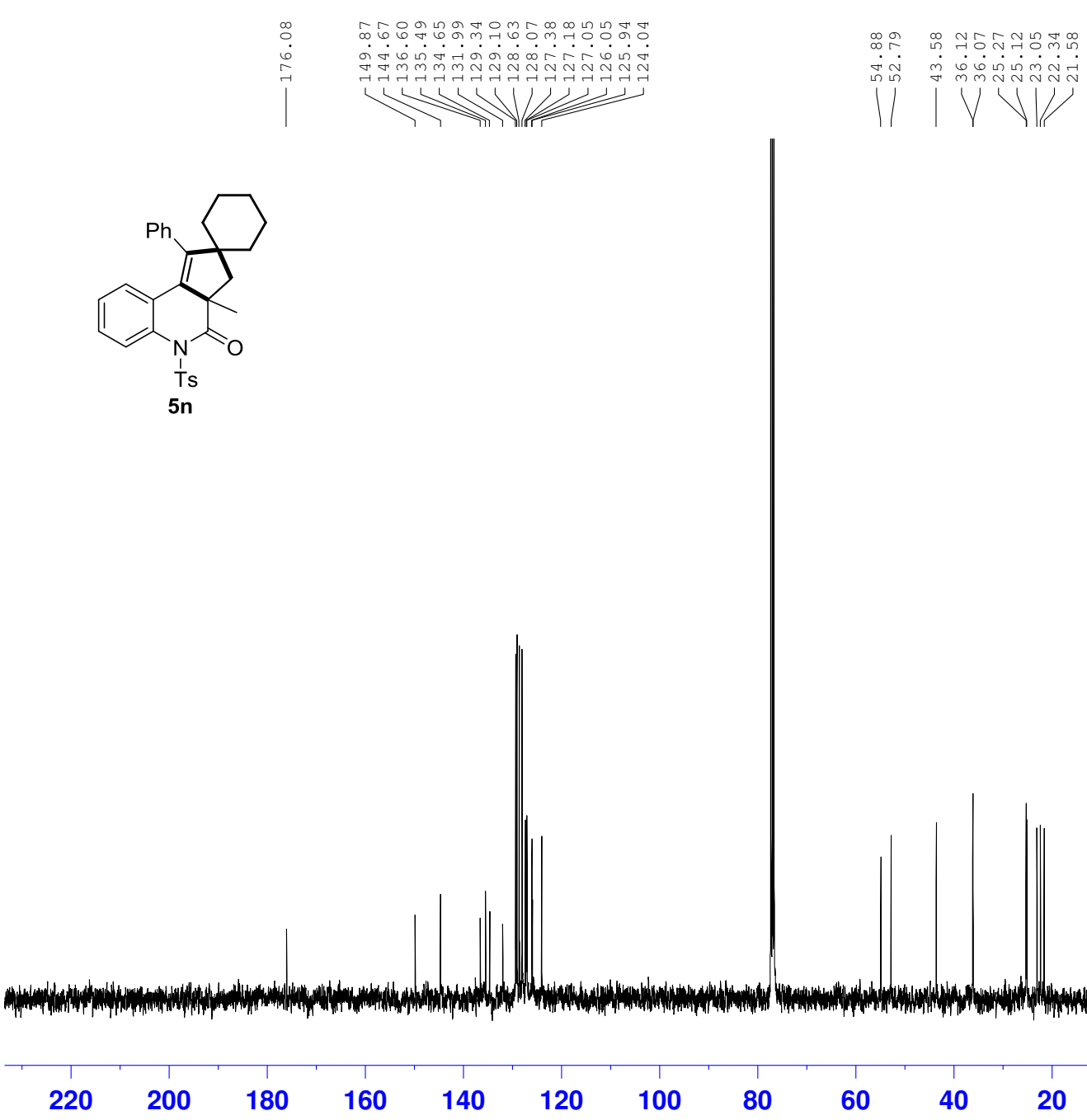


BRUKER

NAME	lly-765-3ap-20160415
EXPNO	1
PROCNO	1
Date_	20160415
Time	17.01
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	203
DW	78.200 usec
DE	6.50 usec
TE	294.7 K
D1	1.00000000 sec
TD0	1

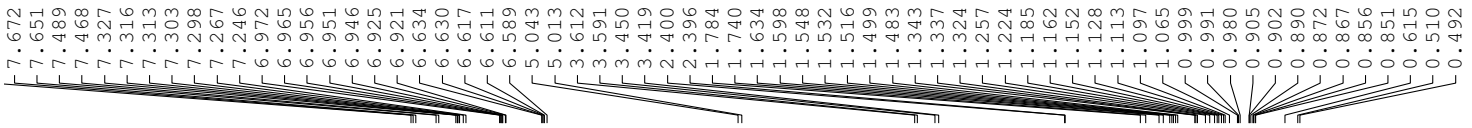
======== CHANNEL f1 ========

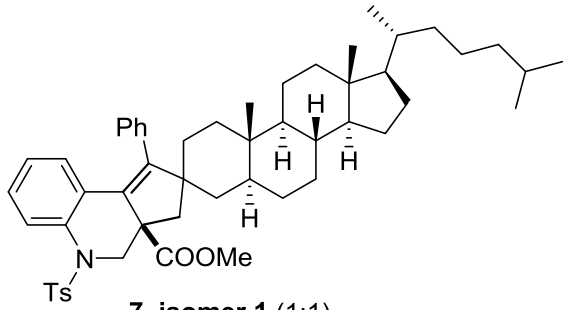
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300094 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



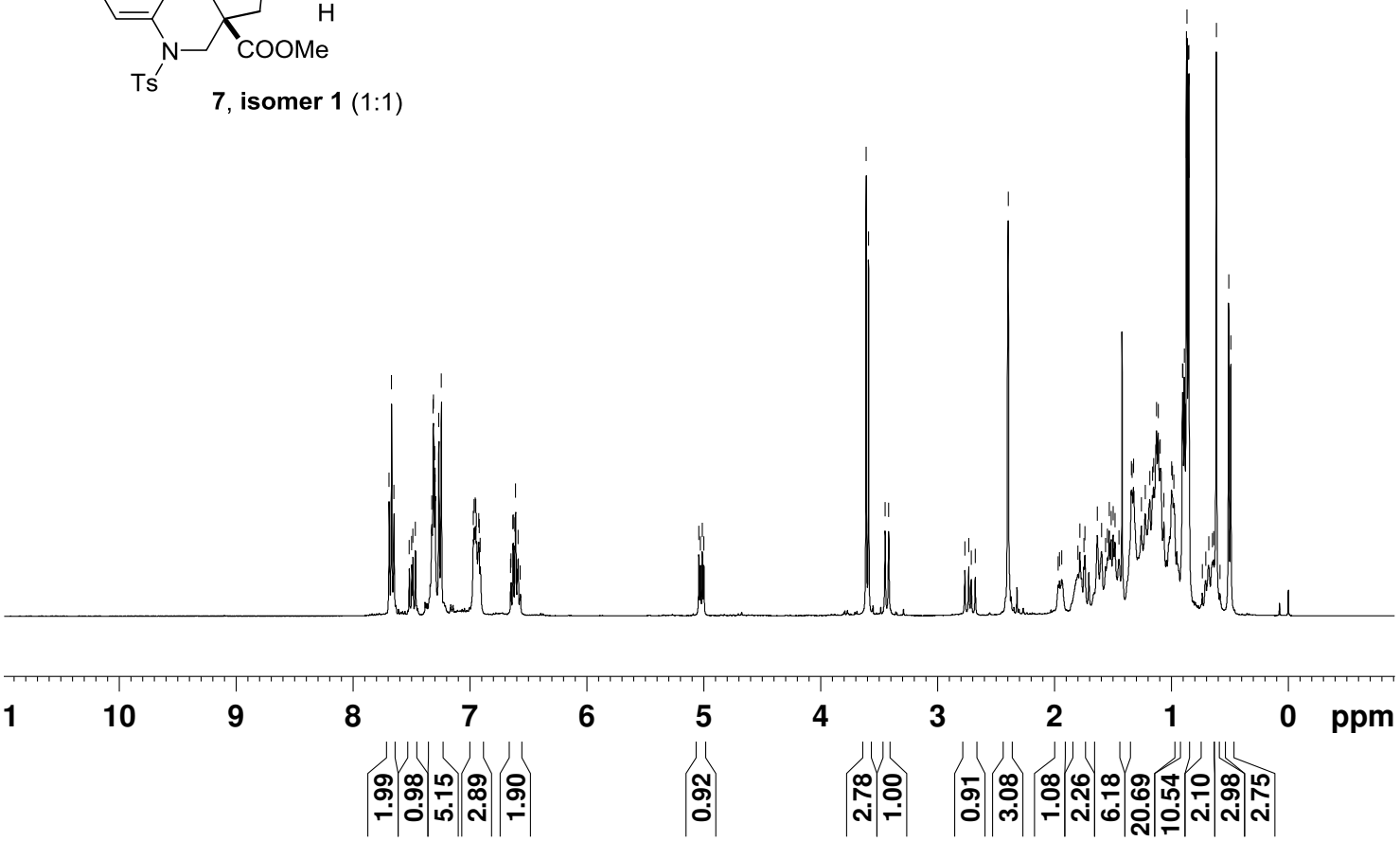
BRUKER

NAME	lly-765-3ap-20160418
EXPNO	2
PROCNO	1
Date_	20160418
Time	9.47
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	96
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	294.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127742 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

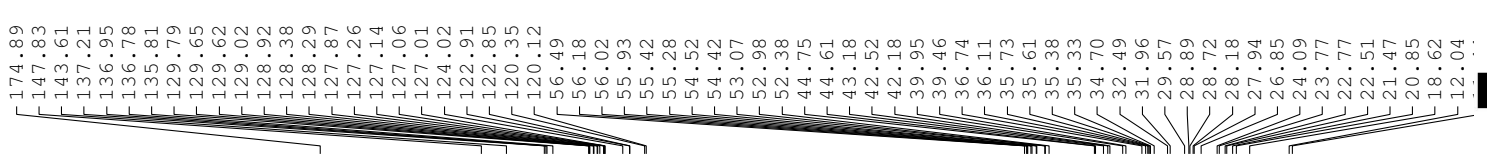


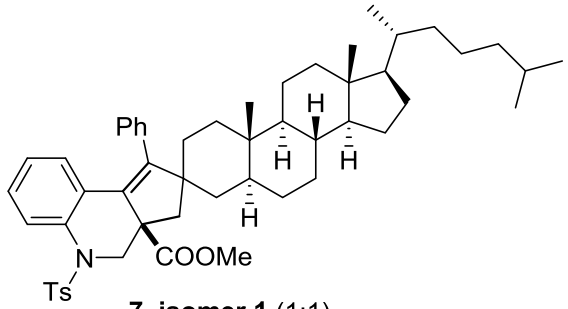


7, **isomer 1** (1:1)



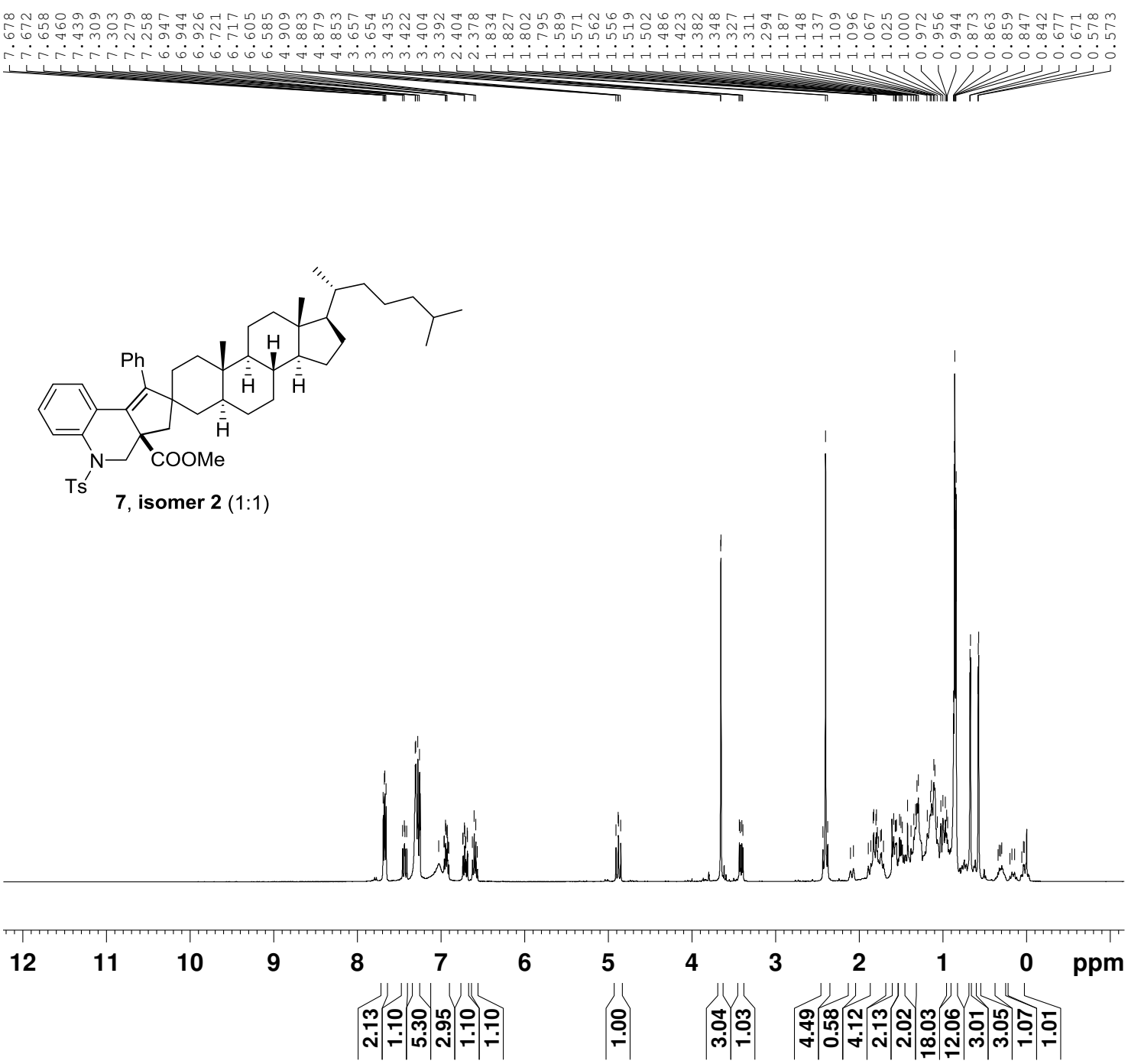
NAME	lly-793-3ap-20160606
EXPNO	1
PROCNO	1
Date_	20160606
Time	16.32
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	45.2
DW	78.200 usec
DE	6.50 usec
TE	298.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300155 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





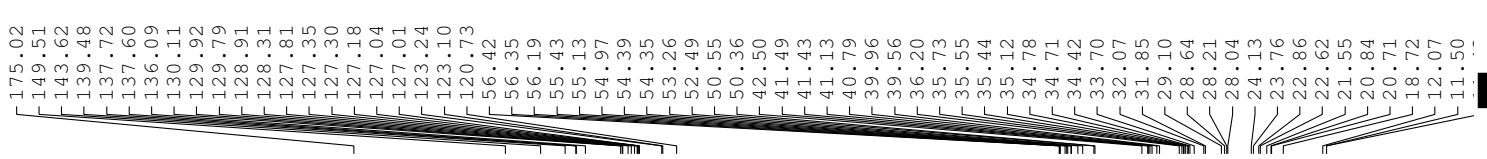
7, **isomer 1** (1:1)

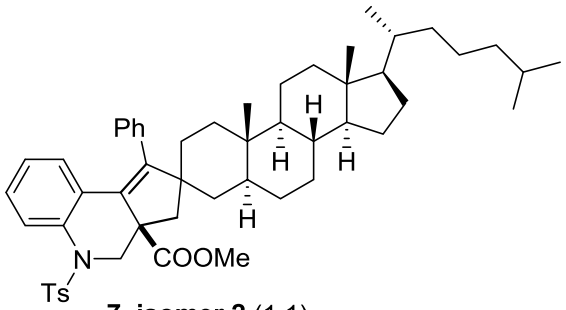

```
NAME      lly-793-3ap-20160607
EXPNO                        2
PROCNO                       1
Date_             20160607
Time                     8.52
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      200
DS                        4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                     2050
DW                   19.800 usec
DE                    8.00 usec
TE                   298.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      10

======== CHANNEL f1 ========
NUC1                    13C
P1                    13.50 usec
PL1                    3.00 dB
PL1W          43.93649673 W
SFO1         100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   1.80 dB
PL12                 17.19 dB
PL13                 18.46 dB
PL2W           8.92857742 W
PL12W          0.25809658 W
PL13W          0.19265592 W
SFO2         400.1316005 MHz
SI                   32768
SF           100.6127788 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```



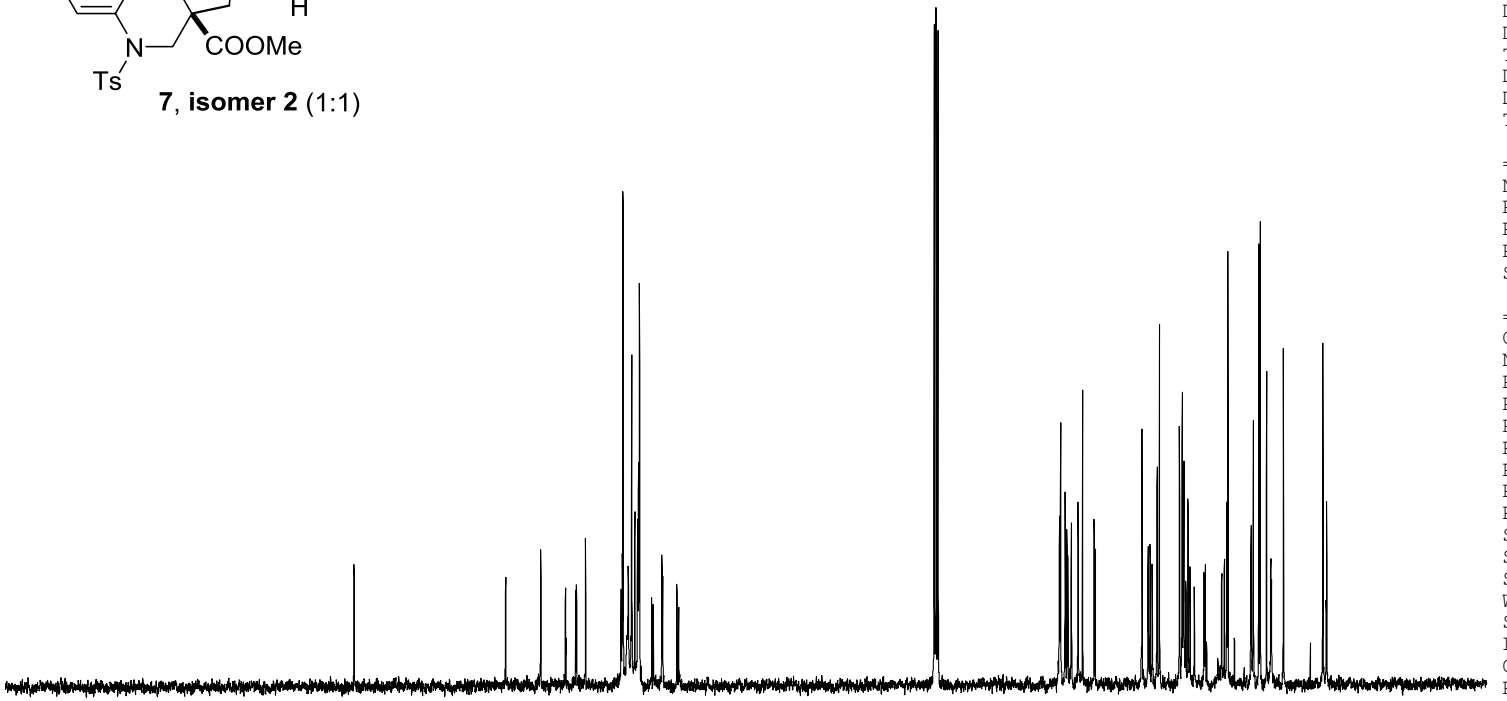
BRUKER

NAME	lly-793-3bp-20160606
EXPNO	1
PROCNO	1
Date_	20160606
Time	16.36
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	45.2
DW	78.200 usec
DE	6.50 usec
TE	298.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300133 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

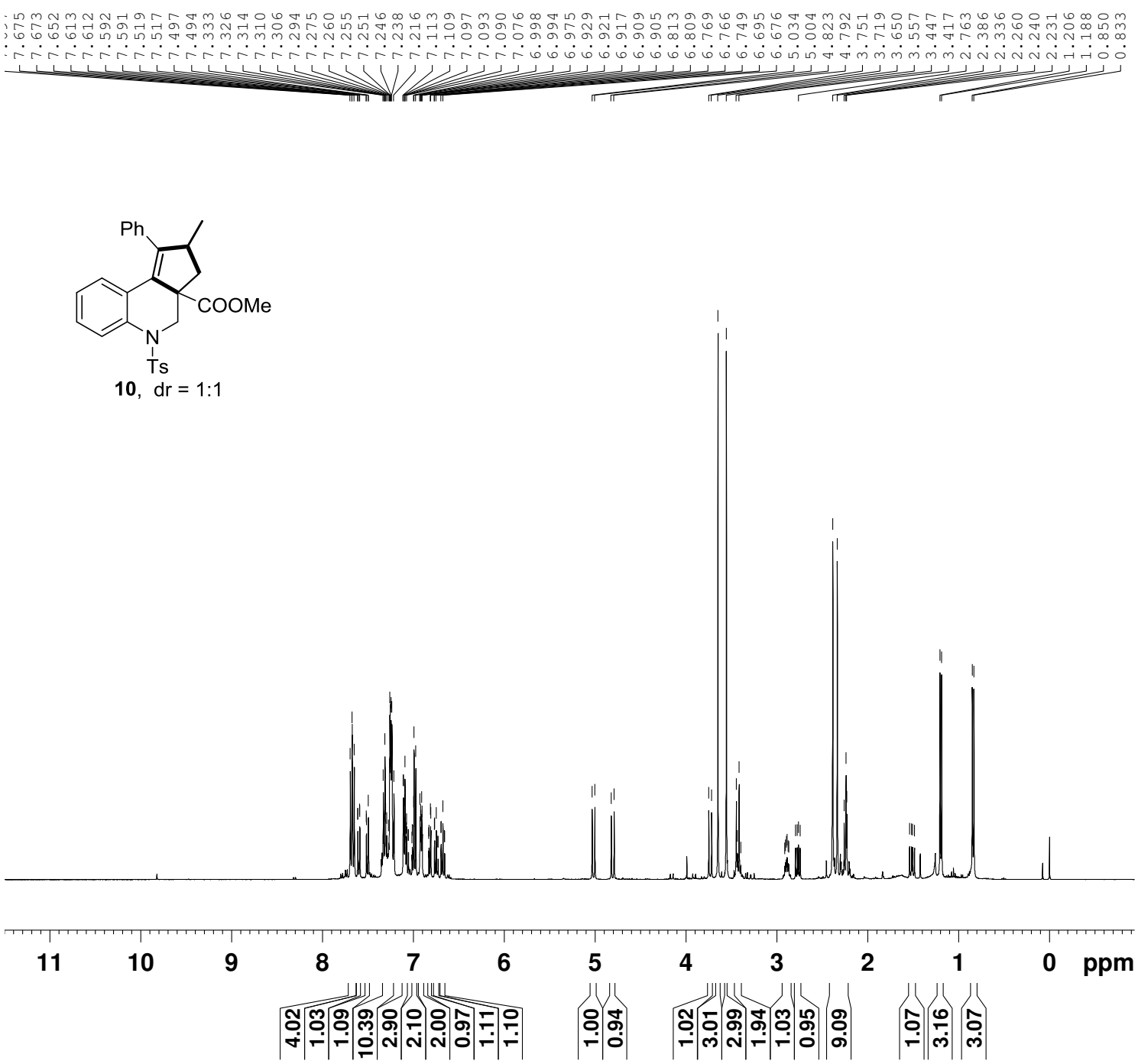




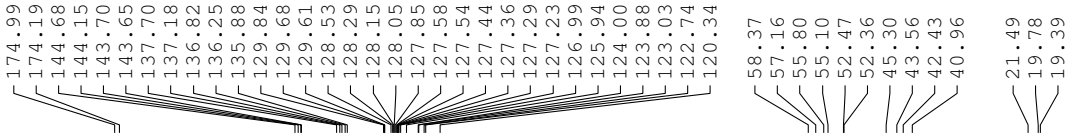
7, **isomer 2** (1:1)

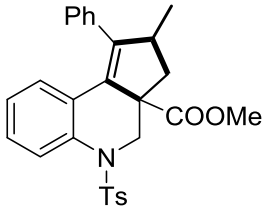



```
NAME      lly-793-3b-p-20160607
EXPNO                         2
PROCNO                        1
Date_              20160607
Time                      9.13
INSTRUM                 spect
PROBHD    5 mm PADUL 13C
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         200
DS                           4
SWH                25252.525 Hz
FIDRES              0.385323 Hz
AQ                 1.2976629 sec
RG                        2050
DW                      19.800 usec
DE                       8.00 usec
TE                      298.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          10

======== CHANNEL f1 ========
NUC1                       13C
P1                       13.50 usec
PL1                       3.00 dB
PL1W              43.93649673 W
SFO1             100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    80.00 usec
PL2                       1.80 dB
PL12                     17.19 dB
PL13                     18.46 dB
PL2W               8.92857742 W
PL12W              0.25809658 W
PL13W              0.19265592 W
SFO2             400.1316005 MHz
SI                       32768
SF               100.6127690 MHz
WDW                        EM
SSB                         0
LB                       3.00 Hz
GB                          0
PC                       1.40
```



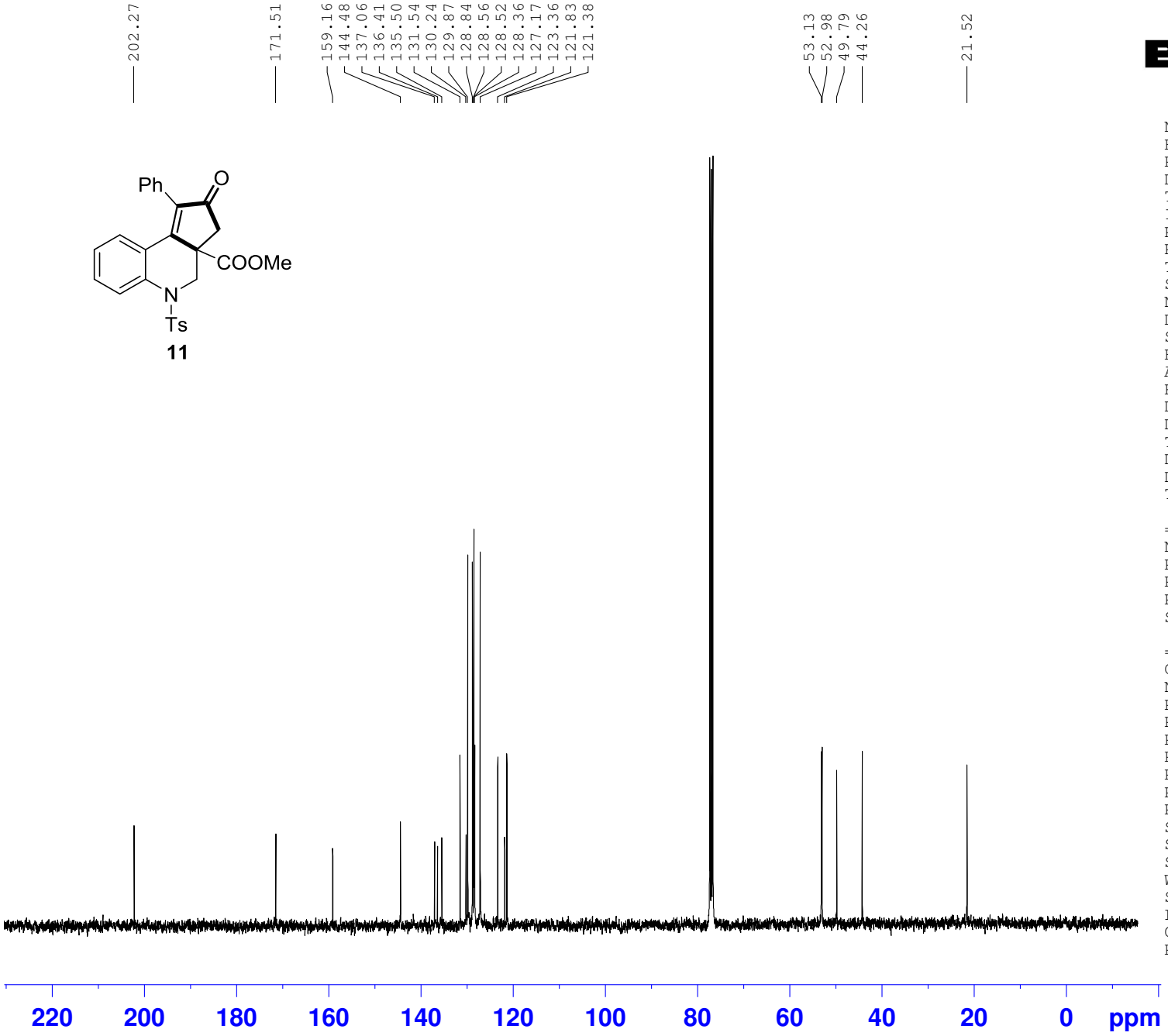

```
NAME      lly-769-1p-20160425
EXPNO                       1
PROCNO                      1
Date_              20160425
Time                   17.21
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 6393.862 Hz
FIDRES              0.195125 Hz
AQ                2.5625076 sec
RG                       128
DW                    78.200 usec
DE                     6.50 usec
TE                    296.2 K
D1               1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.10 usec
PL1                     1.80 dB
PL1W             8.92857742 W
SFO1           400.1326008 MHz
SI                     32768
SF             400.1300117 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```





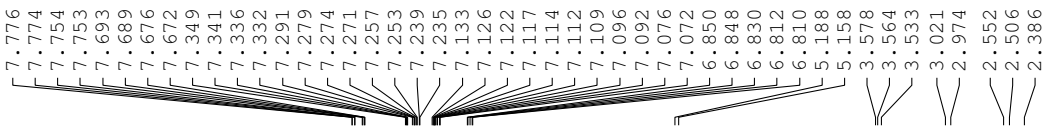
10, dr = 1:1

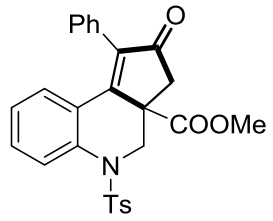

```
NAME      lly-769-1p-20160425
EXPNO                      2
PROCNO                     1
Date_               20160425
Time                   17.25
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG             zgpg30
TD                      65536
SOLVENT               CDCl3
NS                         96
DS                          4
SWH                25252.525 Hz
FIDRES             0.385323 Hz
AQ                 1.2976629 sec
RG                      2050
DW                    19.800 usec
DE                     8.00 usec
TE                    297.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        10

======== CHANNEL f1 ========
NUC1                      13C
P1                      13.50 usec
PL1                      3.00 dB
PL1W             43.93649673 W
SFO1            100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     1.80 dB
PL12                   17.19 dB
PL13                   18.46 dB
PL2W              8.92857742 W
PL12W             0.25809658 W
PL13W             0.19265592 W
SFO2            400.1316005 MHz
SI                      32768
SF              100.6127757 MHz
WDW                        EM
SSB                         0
LB                      3.00 Hz
GB                          0
PC                      1.40
```



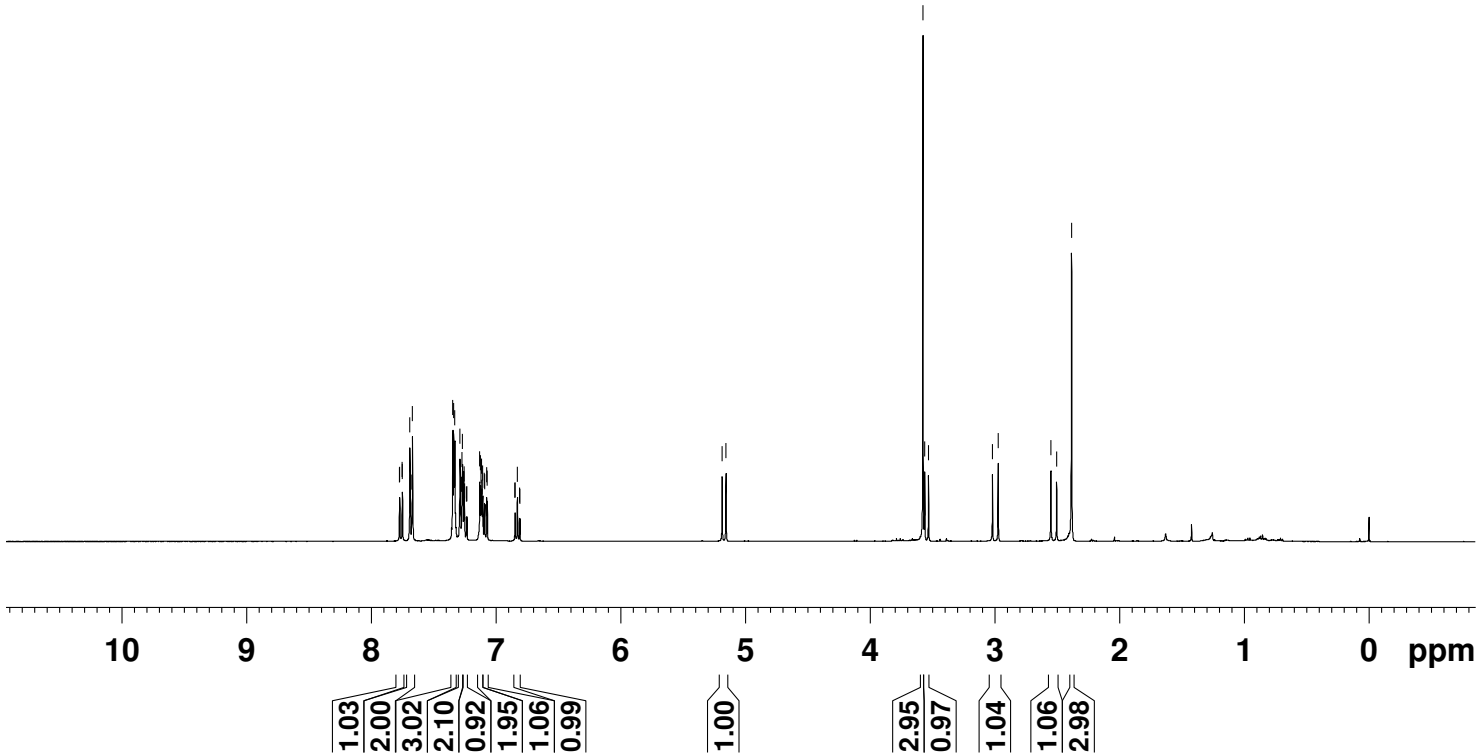
BRUKER

NAME	lly-769-7bp-20160503
EXPNO	2
PROCNO	1
Date_	20160503
Time	16.19
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	232
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	297.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127753 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

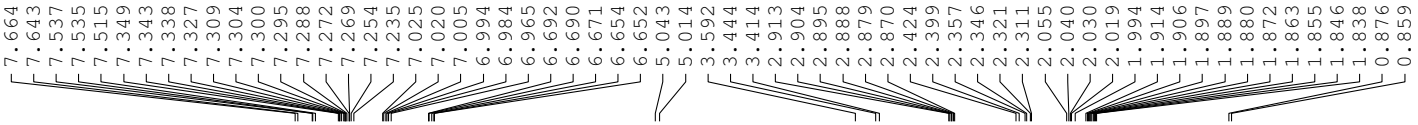


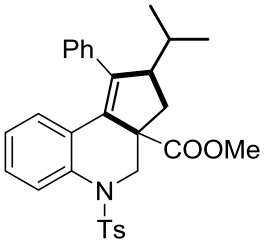


11

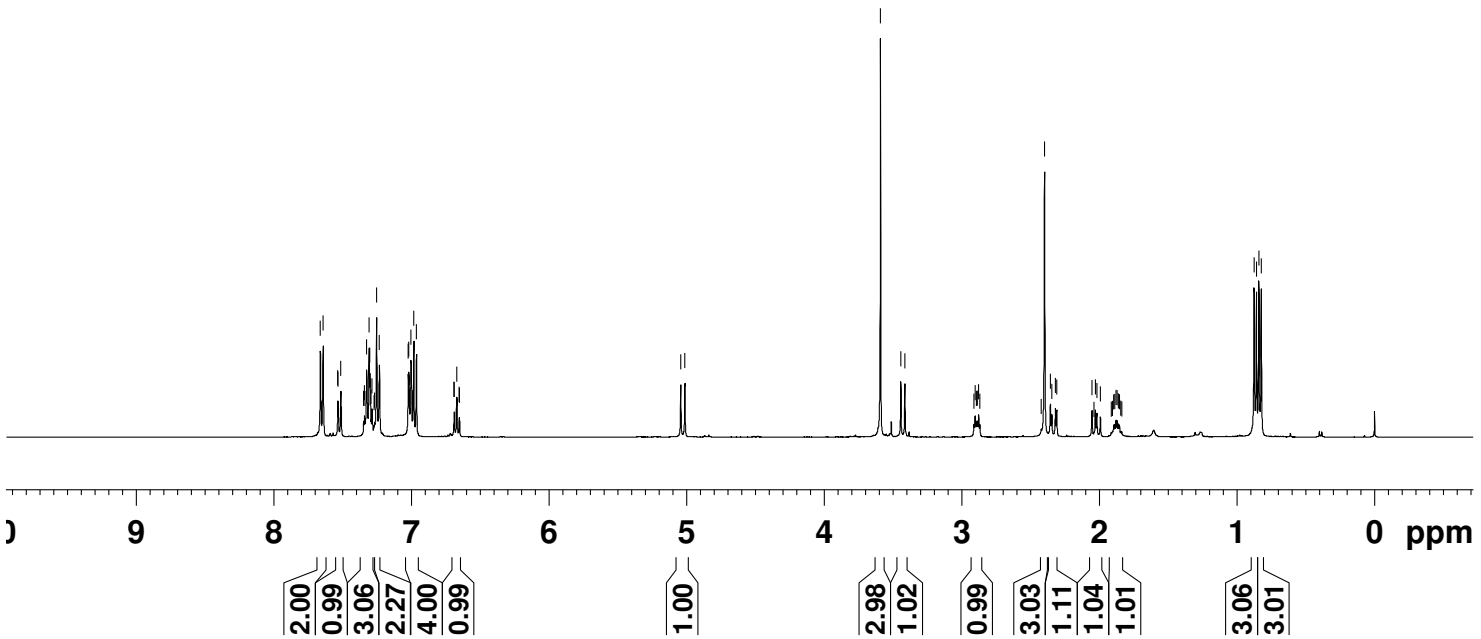


NAME	lly-769-7bp-20160503
EXPNO	1
PROCNO	1
Date_	20160503
Time	16.16
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	181
DW	78.200 usec
DE	6.50 usec
TE	296.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300092 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

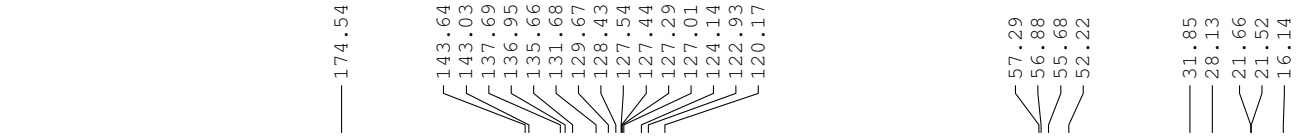


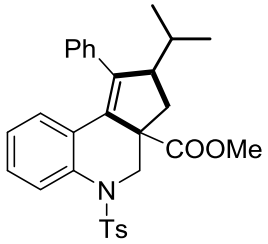


13, isomer 1

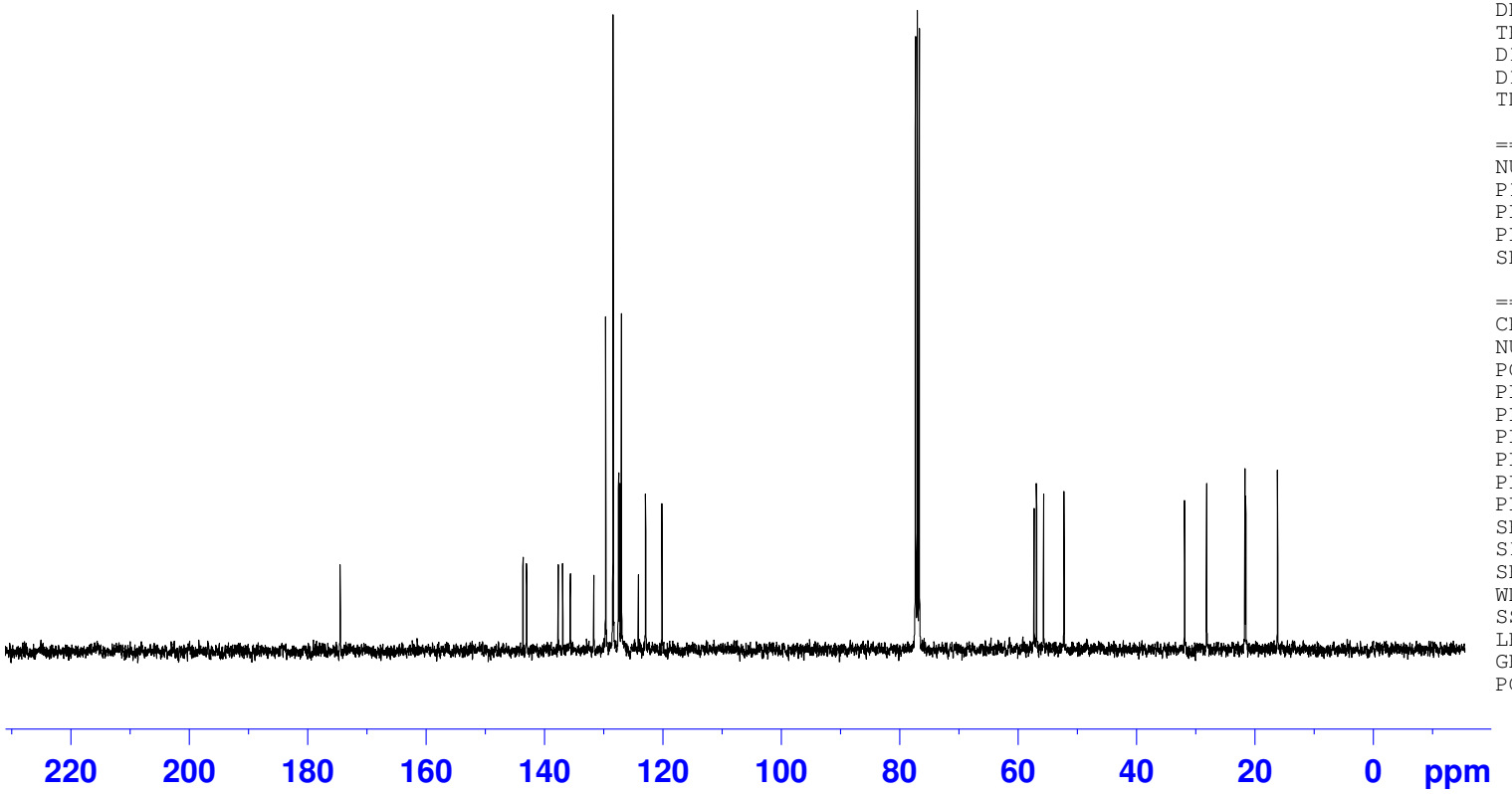


NAME	lly-769-2cp-20160601
EXPNO	1
PROCNO	1
Date_	20160601
Time	16.35
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	128
DW	78.200 usec
DE	6.50 usec
TE	297.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300121 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

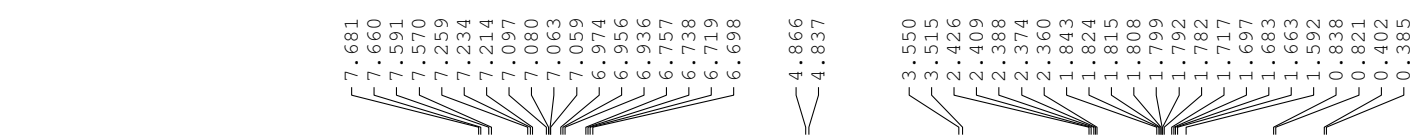


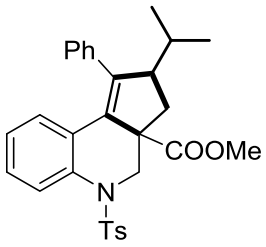


13, isomer 1

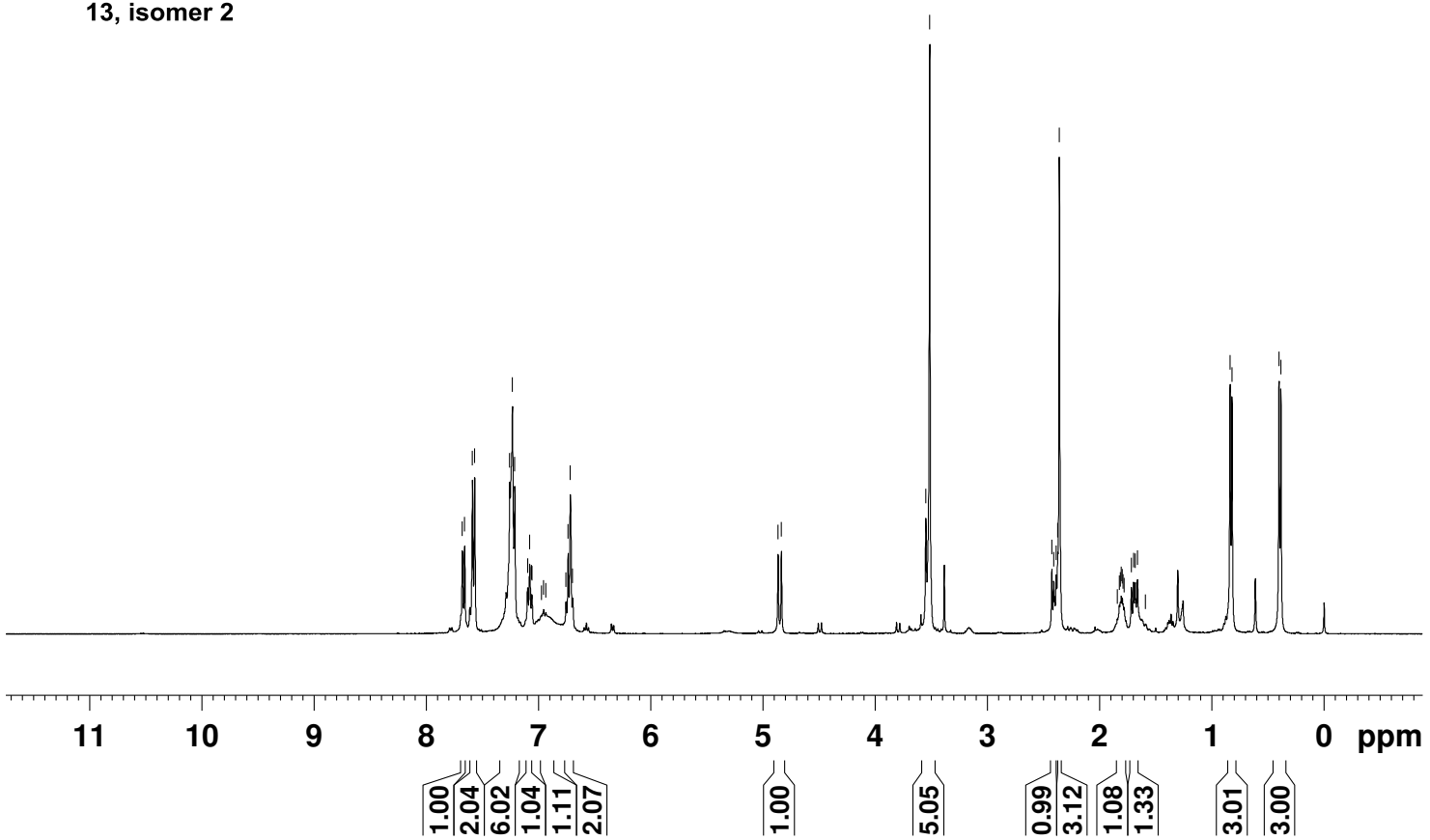



```
NAME      lly-769-2cp-20160602
EXPNO                        2
PROCNO                       1
Date_             20160602
Time                     9.36
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      176
DS                        4
SWH              25252.525 Hz
FIDRES            0.385323 Hz
AQ               1.2976629 sec
RG                     2050
DW                   19.800 usec
DE                    8.00 usec
TE                   298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      10

======== CHANNEL f1 ========
NUC1                    13C
P1                    13.50 usec
PL1                    3.00 dB
PL1W          43.93649673 W
SFO1         100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   1.80 dB
PL12                 17.19 dB
PL13                 18.46 dB
PL2W           8.92857742 W
PL12W          0.25809658 W
PL13W          0.19265592 W
SFO2         400.1316005 MHz
SI                   32768
SF           100.6127738 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```

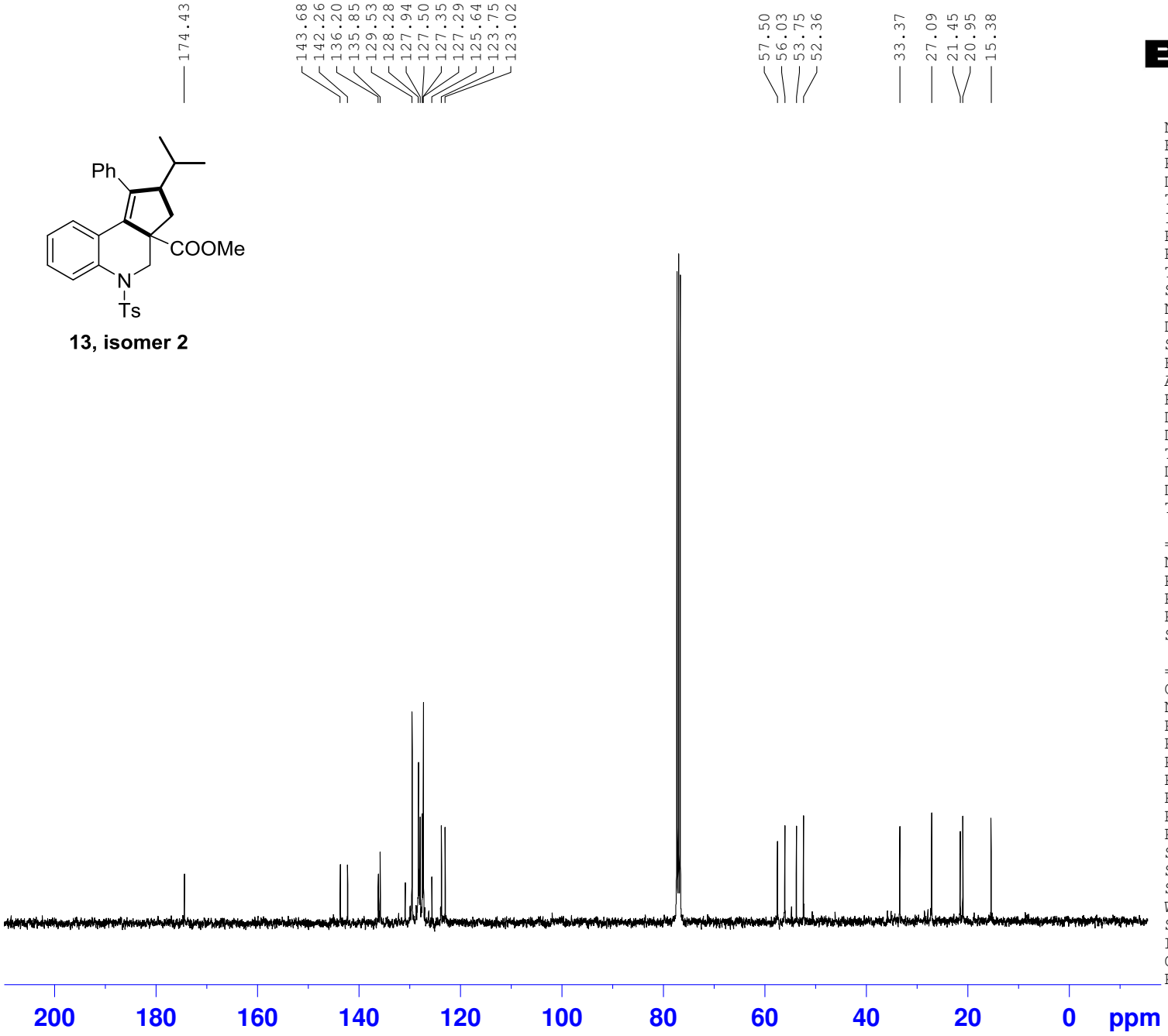




13, isomer 2



NAME	lly-797-2n-20160622
EXPNO	1
PROCNO	1
Date_	20160622
Time	16.08
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	181
DW	78.200 usec
DE	6.50 usec
TE	298.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.10 usec
PL1	1.80 dB
PL1W	8.92857742 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	lly-797-2n-20160622
EXPNO	2
PROCNO	1
Date_	20160622
Time	16.10
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	320
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	8.00 usec
TE	298.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	10
======== CHANNEL f1 ========	
NUC1	13C
P1	13.50 usec
PL1	3.00 dB
PL1W	43.93649673 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.80 dB
PL12	17.19 dB
PL13	18.46 dB
PL2W	8.92857742 W
PL12W	0.25809658 W
PL13W	0.19265592 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40