

Supporting Information

Fe-Catalyzed Synthesis of Substituted N-Aryl Oxazolidines

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General information:

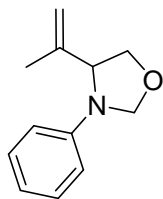
All the reagents were commercial grade and purified according to the established procedures. Organic extracts were dried over anhydrous magnesium sulphate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F₂₅₄ (0.25mm). NMR spectra were recorded in CDCl₃ with tetramethylsilane (TMS) as the internal standard for ¹H NMR (400 MHz) and for ¹³C NMR (100 MHz). The

NMR data was collected on Varian 400 MHz and Bruker 400 MHz AVIII HD spectrometers. IR spectra were recorded on NICOLET IS-10 FT-IR spectrometer. GC-MS analysis carried out on an Agilent GC-MS (7890A – 5975C VL MSD) system.

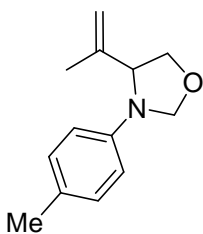
General Procedure for the Preparation of 4-Propenyl-3-Aryl Oxazolidines: To the solution of anh. FeCl₂ (0.05 mmol), allyl alcohol (1.5 mmol) and para-formaldehyde (0.6 mmol) in anh. THF (5 mL), the aryl hydroxylamine (0.5 mmol) solution was added slowly in THF (5 mL) using a syringe pump over 4 hours at 60 °C while keeping the flask under inert atmosphere using nitrogen balloon. Reactions were allowed to continue for two more hours for the complete consumption of aryl hydroxylamine. Then the mixture was filtered through celite and the filtrate was concentrated to dryness. The crude product was purified over a short column of silica gel (hexane/ethyl acetate eluents) to obtain the pure oxazolidine which was then directly analyzed by GC-MS, ESI-MS, NMR and FT-IR.

General Procedure for the Synthesis of Allyl Amino Alcohols: To the propenyl oxazolidine (obtained from the previous step) in a RB flask, 2 mL of conc. HCl was added and stirred for 2 hours. Once the reaction is completed (monitored by TLC and GC-MS), the mixture was filtered through celite and the filtrate was concentrated to dryness. The crude product was purified over a short column of silica gel (hexane/ethyl acetate eluents) and the isolated pure N-aryl amino alcohol which was then directly analyzed by GC-MS, ESI-MS, NMR and FT-IR.

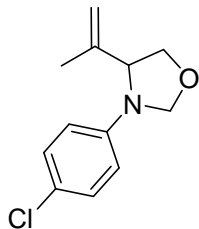
Spectral data



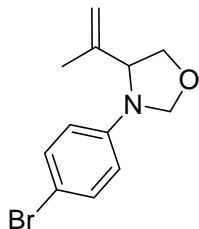
3-phenyl-4-(prop-1-en-2-yl)oxazolidine (1a): ^1H NMR (400 MHz, CDCl_3): δ 1.72 (s, 3H), 3.91 (dd, 1H, $J^1 = 8.0\text{Hz}$, $J^2 = 3.6\text{Hz}$), 4.07-4.10 (m, 1H), 4.16 (t, 1H, $J = 7.6\text{ Hz}$), 4.86 (d, 1H, $J = 2.4\text{ Hz}$), 4.92 (s, 1H), 5.03 (s, 1H), 5.09 (d, 1H, $J = 2.0\text{ Hz}$), 6.51 (d, 2H, $J = 8.0\text{ Hz}$), 6.74 (t, 1H, $J = 7.6\text{ Hz}$), 7.20 (t, 2H, $J = 7.6\text{ Hz}$); ^{13}C NMR (100 MHz, CDCl_3): δ 18.4, 63.3, 72.8, 82.4, 112.5, 112.6, 117.6, 125.7, 129.4, 144.5; GC-MS : 189.0 (M^+); IR (KBr): 2918, 2847, 1621, 1542, 1162, 1092, 811 cm^{-1} .



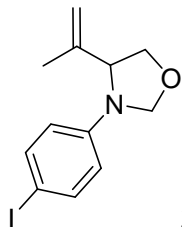
4-(prop-1-en-2-yl)-3-p-tolyloxazolidine (1b): ^1H NMR (400 MHz, CDCl_3): δ 1.73 (s, 3H), 2.43 (s, 3H), 3.90 (dd, 1H, $J^1 = 8.4\text{Hz}$, $J^2 = 4.0\text{ Hz}$), 4.04-4.07 (m, 1H), 4.17 (t, 1H, $J = 8.0\text{ Hz}$), 4.84 (d, 1H, $J = 2.0\text{ Hz}$), 4.93 (s, 1H), 5.04 (s, 1H), 5.09 (d, 1H, $J = 2.4\text{ Hz}$), 6.46 (d, 2H, $J = 8.4\text{ Hz}$), 7.02 (d, 2H, $J = 8.4\text{ Hz}$); ^{13}C NMR (100 MHz, CDCl_3): δ 18.4, 20.5, 63.5, 72.7, 82.7, 112.4, 112.6, 122.3, 125.9, 129.9, 144.6; GC-MS : 203.0 (M^+); IR (KBr): 2920, 2855, 1620, 1521, 1499, 1164, 1095, 947, 899, 801 cm^{-1} .



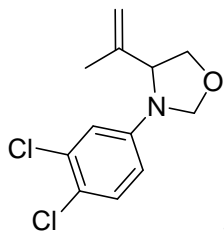
3-(4-chlorophenyl)-4-(prop-1-en-2-yl)oxazolidine (1c): ^1H NMR (400 MHz, CDCl_3): δ 1.72 (s, 3H), 3.94 (dd, 1H, $J^1 = 8.4$ Hz, $J^2 = 4.4$ Hz), 4.06-4.09 (m, 1H), 4.21 (t, 1H, $J = 7.2$ Hz), 4.85 (d, 1H, $J = 2.0$ Hz), 4.95 (brs, 1H), 5.03 (brs, 1H), 5.08 (brs, 1H), 6.44 (d, 2H, $J = 6.8$ Hz), 7.15 (d, 2H, $J = 6.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 18.3, 63.3, 72.8, 82.4, 112.9, 113.5, 122.5, 129.2, 143.8, 144.0; HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{15}\text{ClNO}$ ($\text{M} + \text{H}^+$) 224.0837, found 224.0844; IR (KBr): 2881, 2826, 1599, 1498, 1488, 1389, 1368, 1174, 1090, 942, 900, 809 cm^{-1} .



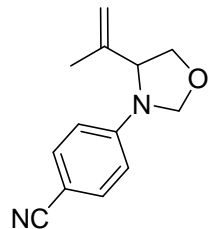
3-(4-bromophenyl)-4-(prop-1-en-2-yl)oxazolidine (1d): ^1H NMR (400 MHz, CDCl_3): δ 1.69 (s, 3H), 3.90 (dd, 1H, $J^1 = 8.4$ Hz, $J^2 = 4.0$ Hz), 4.03-4.06 (m, 1H), 4.82 (d, 1H, $J = 2.0$ Hz), 4.93 (s, 1H), 5.00 (s, 1H), 5.03 (d, 1H, $J = 2.0$ Hz), 6.37 (d, 2H, $J = 9.2$ Hz), 7.26 (d, 2H, $J = 8.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 18.3, 63.2, 72.8, 82.2, 109.6, 112.9, 114.0, 132.1, 143.9, 144.2; HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{15}\text{BrNO}$ ($\text{M} + \text{H}^+$) 268.0332; found, 268.0331; IR (KBr): 2972, 2914, 2859, 1593, 1490, 1358, 1146, 1094, 899, 807 cm^{-1} .



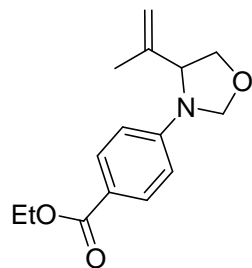
3-(4-iodophenyl)-4-(prop-1-en-2-yl)oxazolidine (1e): ^1H NMR (400 MHz, CDCl_3): δ 1.69 (s, 3H), 3.91 (dd, 1H, $J^1 = 8.4$ Hz, $J^2 = 4.0$ Hz), 4.03-4.06 (m, 1H), 4.17 (t, 1H, $J = 7.6$ Hz), 4.81 (s, 1H), 4.93 (s, 1H), 4.99 (s, 1H), 5.03 (s, 1H), 6.27 (d, 2H, $J = 8.4$ Hz), 7.44 (d, 2H, $J = 7.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 18.3, 29.9, 63.1, 72.8, 82.1, 112.9, 114.7, 124.2, 137.9, 143.8; GC-MS : 314.9 (M^+); IR (KBr): 2989, 2889, 1595, 1488, 1352, 1134, 1096, 1004, 949, 893, 805 cm^{-1} .



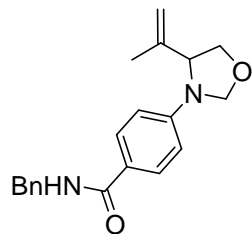
3-(3,4-dichlorophenyl)-4-(prop-1-en-2-yl)oxazolidine (1f): ^1H NMR (400 MHz, CDCl_3): δ 1.70 (s, 3H), 3.94 (dd, 1H, $J^1 = 8.4$ Hz, $J^2 = 4.0$ Hz), 4.05-4.08 (m, 1H), 4.20 (t, 1H, $J = 8.0$ Hz), 4.83 (d, 1H, $J = 2.4$ Hz), 4.97 (s, 1H), 5.02 (s, 1H), 5.04 (d, 1H, $J = 2.4$ Hz), 6.33 (dd, 1H, $J^1 = 8.8$ Hz, $J^2 = 2.8$ Hz), 6.57 (d, 1H, $J = 2.8$ Hz), 7.22 (d, 1H, $J = 8.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 18.3, 63.2, 72.8, 82.1, 112.0, 113.3, 113.8, 120.4, 130.8, 133.1, 143.4, 144.5; HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{14}\text{Cl}_2\text{NO}$ ($\text{M} + \text{H}^+$) 258.0447; found, 258.0445; IR (KBr): 2970, 2917, 2853, 1597, 1483, 1360, 1019, 795 cm^{-1} .



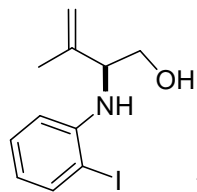
4-(4-(prop-1-en-2-yl)oxazolidin-3-yl)benzonitrile (1g): ^1H NMR (400 MHz, CDCl_3): δ 1.72 (s, 3H), 3.98 (dd, 1H, $J^1 = 8.0\text{Hz}$, $J^2 = 3.2\text{Hz}$), 4.18-4.23 (m, 2H), 4.92 (d, 1H, $J = 2.0$ Hz), 4.99 (s, 2H), 5.09 (d, 1H, $J = 2.0$ Hz), 6.48 (d, 2H, $J = 8.4$ Hz), 7.46 (d, 2H, $J = 8.4$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 18.3, 62.8, 72.8, 81.5, 105.2, 112.3, 113.6, 120.4, 133.8, 142.9, 147.5; HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{15}\text{N}_2\text{O}$ ($\text{M} + \text{H}^+$) 215.1179; found, 215.1178; IR (KBr): 2915, 2881, 2848, 2213, 1651, 1521, 1497, 1389, 1371, 1174, 1092, 1062, 942, 900, 810 cm^{-1} .



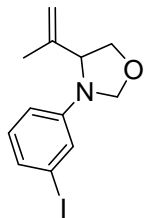
Ethyl 4-(4-(prop-1-en-2-yl)oxazolidin-3-yl)benzoate (1h): ^1H NMR (400 MHz, CDCl_3): δ 1.33 (t, 3H, $J = 7.2$ Hz), 1.70 (s, 3H), 4.18 (brs, 2H), 4.30 (q, 2H, $J = 7.2$ Hz), 4.93 (d, 2H, $J = 8.4$ Hz), 4.98 (s, 1H), 5.09 (s, 1H), 6.45 (d, 2H, $J = 8.0$ Hz), 7.88 (d, 2H, $J = 8.0$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 14.6, 18.4, 60.5, 62.8, 72.8, 81.7, 111.5, 113.2, 131.4, 131.5, 143.4, 148.1, 167.0; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{20}\text{N}_2\text{O}_3$ ($\text{M} + \text{H}^+$) 262.1438; found, 262.1440; IR (KBr): 2978, 2927, 2871, 1699, 1604, 1522, 1364, 1270, 1178, 1101, 767 cm^{-1} .



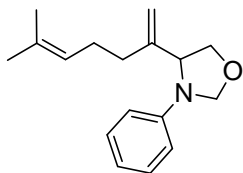
N-benzyl-4-(4-(prop-1-en-2-yl)oxazolidin-3-yl)benzamide (1i): ^1H NMR (400 MHz, CDCl_3): δ 1.23 (t, 1H, $J = 6.8$ Hz), 1.70 (s, 3H), 3.95 (d, 1H, $J = 8.0$ Hz), 4.14-4.20 (m, 2H), 4.60 (d, 2H, $J = 5.6$ Hz), 4.90 (s, 1H), 4.95 (s, 1H), 4.99 (s, 1H), 5.08 (s, 1H), 6.42 (brs, 1H), 6.47 (d, 2H, $J = 8.8$ Hz), 7.26 (d, 1H, $J = 5.2$ Hz), 7.31 (d, 3H, $J = 4.0$ Hz), 7.68 (d, 2H, $J = 8.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 18.3, 44.1, 62.8, 72.7, 81.8, 111.6, 113.1, 122.7, 127.6, 128.0, 128.7, 128.8, 138.9, 143.5, 147.3, 167.3; HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{23}\text{N}_2\text{O}_2$ ($\text{M} + \text{H}^+$) 323.1754; found, 323.1763; IR (KBr): 3317, 2912, 2868, 1612, 1518, 1359, 1303, 1201, 1169, 945, 828, 764, 729 cm^{-1} .



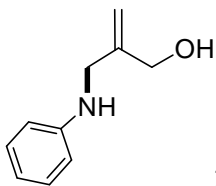
2-(2-iodophenylamino)-3-methylbut-3-en-1-ol (1k): ^1H NMR (400 MHz, CDCl_3): δ 1.77 (s, 3H), 1.94 (brs, 1H), 3.72-3.76 (m, 1H), 3.81 (brs, 1H), 3.91-3.94 (m, 1H), 4.69 (brs, 1H), 5.01 (s, 2H), 6.42-6.49 (m, 2H), 7.15 (t, 1H, $J = 7.6$ Hz), 7.65 (d, 1H, $J = 7.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 19.6, 61.3, 63.9, 86.1, 112.1, 113.9, 119.3, 129.4, 139.2, 142.2, 146.5; HRMS (ESI) calcd for $\text{C}_{11}\text{H}_{15}\text{I}\text{N}\text{O}$ ($\text{M} + \text{H}^+$) 304.0193; found, 304.0201; IR (KBr): 3376, 2923, 2856, 1587, 1501, 1451, 1313, 1008, 899, 748 cm^{-1} .



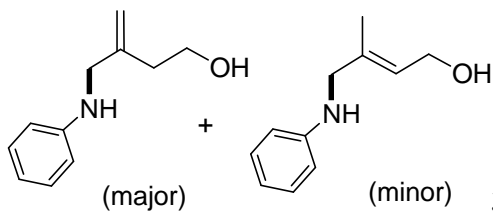
3-(3-iodophenyl)-4-(prop-1-en-2-yl)oxazolidine (11): ^1H NMR (400 MHz, CDCl_3): δ 1.71 (s, 3H), 3.91-3.94 (m, 1H), 4.05-4.08 (m, 1H), 4.17 (t, 1H, $J = 7.6$ Hz), 4.84 (s, 1H), 4.95 (s, 1H), 5.03 (d, 2H, $J = 8.0$ Hz), 6.47 (d, 1H, $J = 8.8$ Hz), 6.82 (s, 1H), 6.90 (t, 1H, $J = 8.0$ Hz), 7.06 (d, 1H, $J = 7.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 18.3, 63.0, 72.7, 82.0, 95.5, 111.7, 113.0, 121.1, 126.5, 130.8, 139.2, 143.7, 146.3; HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{15}\text{I}\text{N}\text{O}$ ($\text{M} + \text{H}^+$) 316.0193; found, 316.0190; IR (KBr): 3071, 2922, 2865, 1591, 1551, 1479, 1388, 1353, 1170, 1093, 980, 947, 758 cm^{-1} .



4-(6-methylhepta-1,5-dien-2-yl)-3-phenyloxazolidine (2a): ^1H NMR (400 MHz, CDCl_3): δ 1.60 (s, 3H), 1.68 (s, 3H), 2.07 (t, 2H, $J = 7.6$ Hz), 2.18 (t, 2H, $J = 7.6$ Hz), 3.90-3.93 (m, 1H), 4.09-4.11 (m, 1H), 4.17 (t, 1H, $J = 7.2$ Hz), 4.87 (s, 1H), 4.94 (s, 1H), 5.10 (d, 2H, $J = 8.0$ Hz), 6.50 (d, 2H, $J = 8.0$ Hz), 6.74 (t, 1H, $J = 7.6$ Hz), 7.22 (t, 2H, $J = 7.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 17.9, 25.9, 26.4, 32.0, 63.1, 73.1, 82.4, 111.0, 112.6, 117.5, 124.1, 129.3, 132.2, 145.4, 147.9; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{24}\text{N}\text{O}$ ($\text{M} + \text{H}^+$) 258.1852; found, 258.1859; IR (KBr): 2966, 2912, 2857, 1604, 1510, 1391, 1345, 1170, 1095, 949, 752 cm^{-1} .

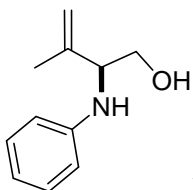


2-Phenylaminomethyl-prop-2-en-1-ol (3a): ^1H NMR (400 MHz, CDCl_3): δ 1.33-1.36 (m, 1H), 1.61 (brs, 1H), 3.88 (s, 2H), 4.23 (s, 2H), 5.20 (d, 2H, $J = 4.0$ Hz), 6.67 (d, 2H, $J = 8.0$ Hz), 6.75 (t, 1H, $J = 8.0$ Hz), 7.20 (t, 2H, $J = 8.0$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 47.0, 65.0, 112.3, 113.1, 117.8, 129.2, 145.9, 148.2; GC-MS : 163.0 (M^+); IR (KBr): 3392, 3051, 2924, 1607, 1507, 1315, 1261, 1070, 1048, 754 cm^{-1} .



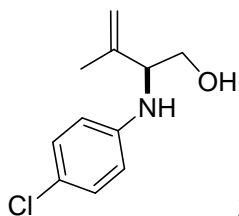
(4a+4a'):

Inseparable mixture of two isomers were obtained after column chromatography which was confirmed by NMR and GC-MS analysis as shown on pages: S49, S50 and S51. GC-MS : 177.0 (M^+).

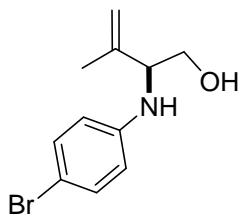


3-methyl-2-(phenylamino)but-3-en-1-ol (1a'): ^1H NMR (400 MHz, CDCl_3): δ 1.76 (s, 3H), 1.92 (brs, 1H), 3.63-3.67 (m, 1H), 3.75-3.78 (m, 1H), 3.86-3.88 (m, 1H), 4.15 (brs, 1H), 5.00 (s, 1H), 5.03 (s, 1H), 6.59 (d, 2H, $J = 7.6$ Hz), 6.70 (t, 1H, $J = 7.2$ Hz), 7.15 (t, 2H, $J = 7.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 19.7, 60.9, 64.1, 113.5, 113.8, 117.9, 129.3, 142.9, 147.5;

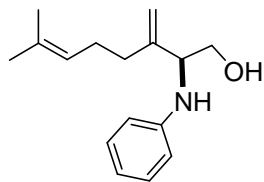
HRMS (ESI) calcd for C₁₁ H₁₆ N O (M + H⁺) 178.1226; found, 178.1229; IR (KBr): 3392, 3051, 2924, 1607, 1507, 1315, 1261, 1070, 1048, 754 cm⁻¹.



2-(4-chlorophenylamino)-3-methylbut-3-en-1-ol (1c'): ¹H NMR (400 MHz, CDCl₃): δ 1.63 (brs, 1H), 1.76 (s, 3H), 3.66-3.70 (m, 1H), 3.76-3.84 (m, 2H), 4.21 (brs, 1H), 5.02 (s, 2H), 6.51 (d, 2H, *J* = 7.6 Hz), 7.10 (d, 2H, *J* = 7.6 Hz); ¹³C NMR (100 MHz, CDCl₃): δ 19.7, 60.9, 63.9, 113.8, 114.8, 122.4, 129.2, 142.5, 146.0; GC-MS : 211.0 (M⁺); IR (KBr): 3400, 2935, 1655, 1599, 1604, 1315, 1091, 1050, 902, 816 cm⁻¹.



2-(4-bromophenylamino)-3-methylbut-3-en-1-ol (1d'): ¹H NMR (400 MHz, CDCl₃): δ 1.63 (brs, 1H), 1.77 (s, 3H), 3.69-3.70 (m, 1H), 3.78-3.83 (m, 2H), 4.24 (brs, 1H), 5.02 (s, 2H), 6.47 (d, 2H, *J* = 7.6 Hz), 7.22 (d, 2H, *J* = 7.6 Hz); ¹³C NMR (100 MHz, CDCl₃): δ 19.7, 60.9, 63.9, 113.8, 115.3, 125.2, 132.1, 142.4, 146.5; GC-MS : 256.9 (M⁺); IR (KBr): 3403, 2929, 1594, 1502, 1314, 1073, 902, 813 cm⁻¹.

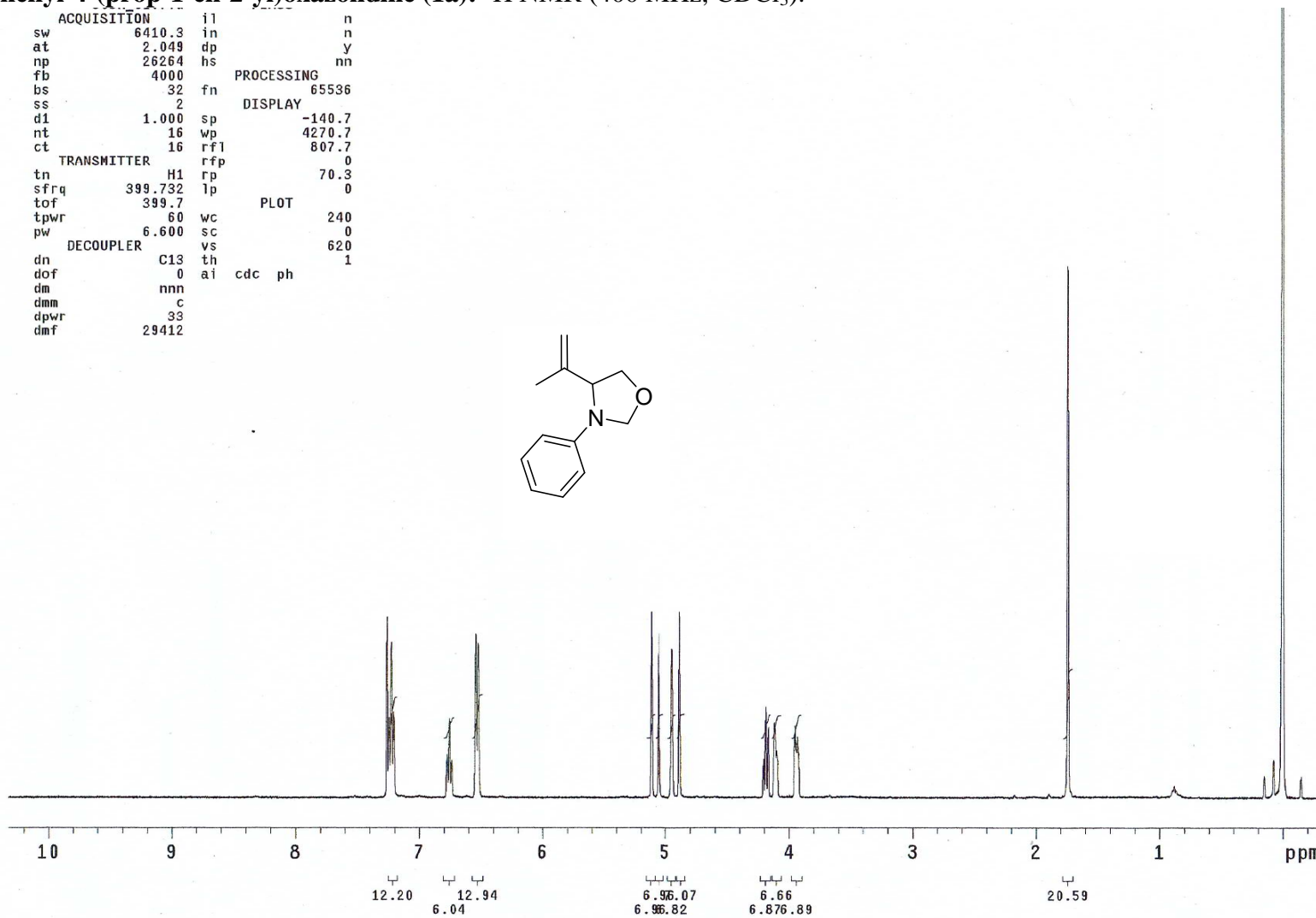
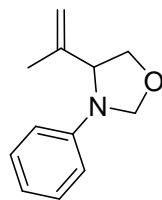


7-methyl-3-methylene-2-(phenylamino)oct-6-en-1-ol (2a'): ^1H NMR (400 MHz, CDCl_3): δ 1.61 (brs, 1H), 1.67 (s, 3H), 1.69 (s, 3H), 1.74-1.77 (m, 2H), 2.08-2.14 (m, 2H), 3.72 (t, 2H, $J = 6.4$ Hz), 4.14 (d, 2H, $J = 6.8$ Hz), 4.91 (s, 1H), 4.97 (s, 1H), 5.42 (t, 1H, $J = 6.8$ Hz), 6.56 (d, 2H, $J = 8.0$ Hz), 6.66 (t, 1H, $J = 7.2$ Hz), 7.14 (t, 2H, $J = 7.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 16.6, 18.0, 32.5, 36.3, 59.3, 59.5, 105.2, 112.5, 113.4, 117.3, 124.1, 129.3, 139.1, 145.7, 147.8; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{24}\text{NO}$ ($\text{M} + \text{H}^+$) 246.1852; found, 246.1855; IR (KBr): 3360, 3052, 2922, 2859, 1607, 1509, 1317, 1258, 993, 896, 748 cm^{-1} .

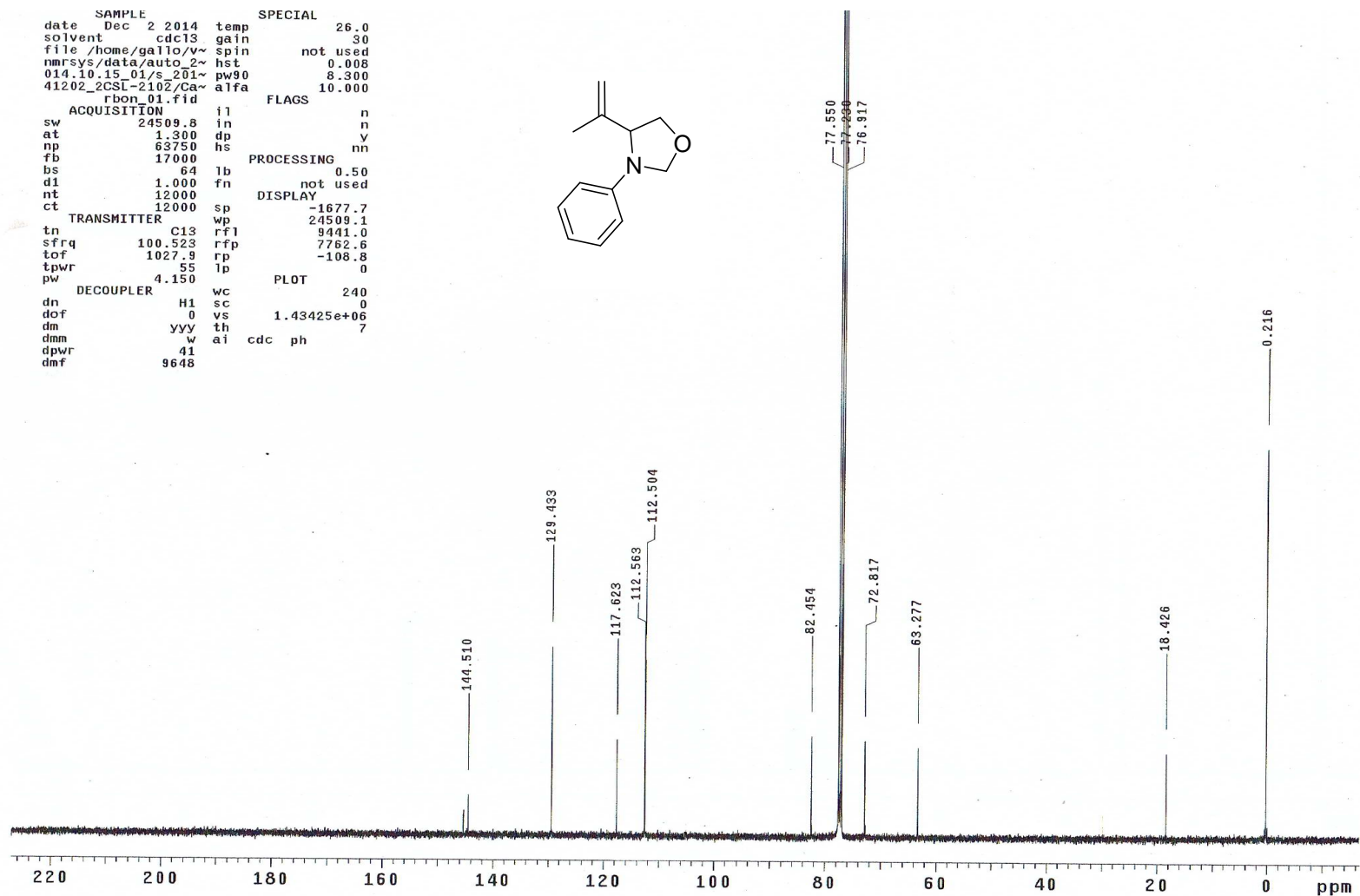
SPECTRA

3-phenyl-4-(prop-1-en-2-yl)oxazolidine (1a): ¹H NMR (400 MHz, CDCl₃):

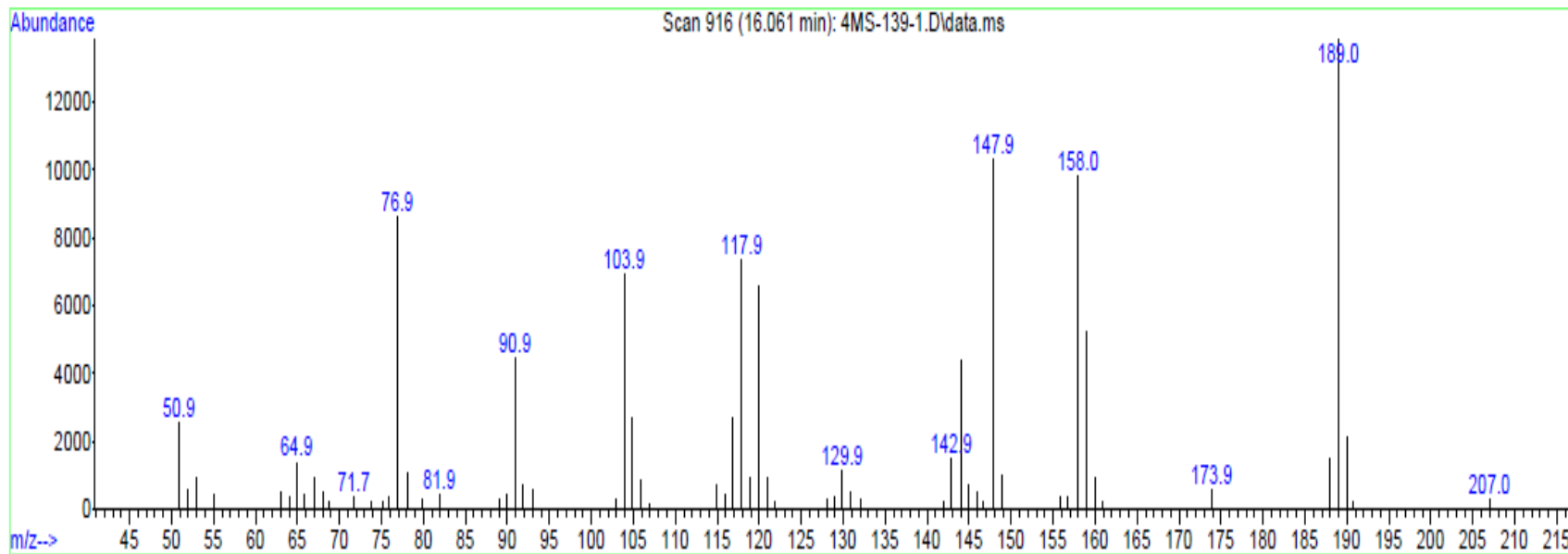
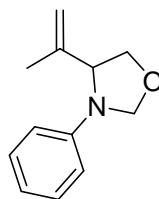
```
ACQUISITION      il      n
sw      6410.3    in      n
at      2.049    dp      y
np      26264    hs      nn
fb      4000
bs      32      fn      PROCESSING 65536
ss      2      DISPLAY
d1      1.000    sp      -140.7
nt      16      wp      4270.7
ct      16      rfl     807.7
TRANSMITTER      rfp     0
tn      H1      rp      70.3
sfrq    399.732 lp      0
tof     399.7    PLOT
tpwr    60      wc      240
pw      6.600    sc      0
DECOUPLER C13      th     620
dn      0      ai cdc ph 1
dof     0
dm      nnn
dmm     c
dpwr    33
dmf     29412
```



3-phenyl-4-(prop-1-en-2-yl)oxazolidine (1a): ^{13}C NMR (100 MHz, CDCl_3):

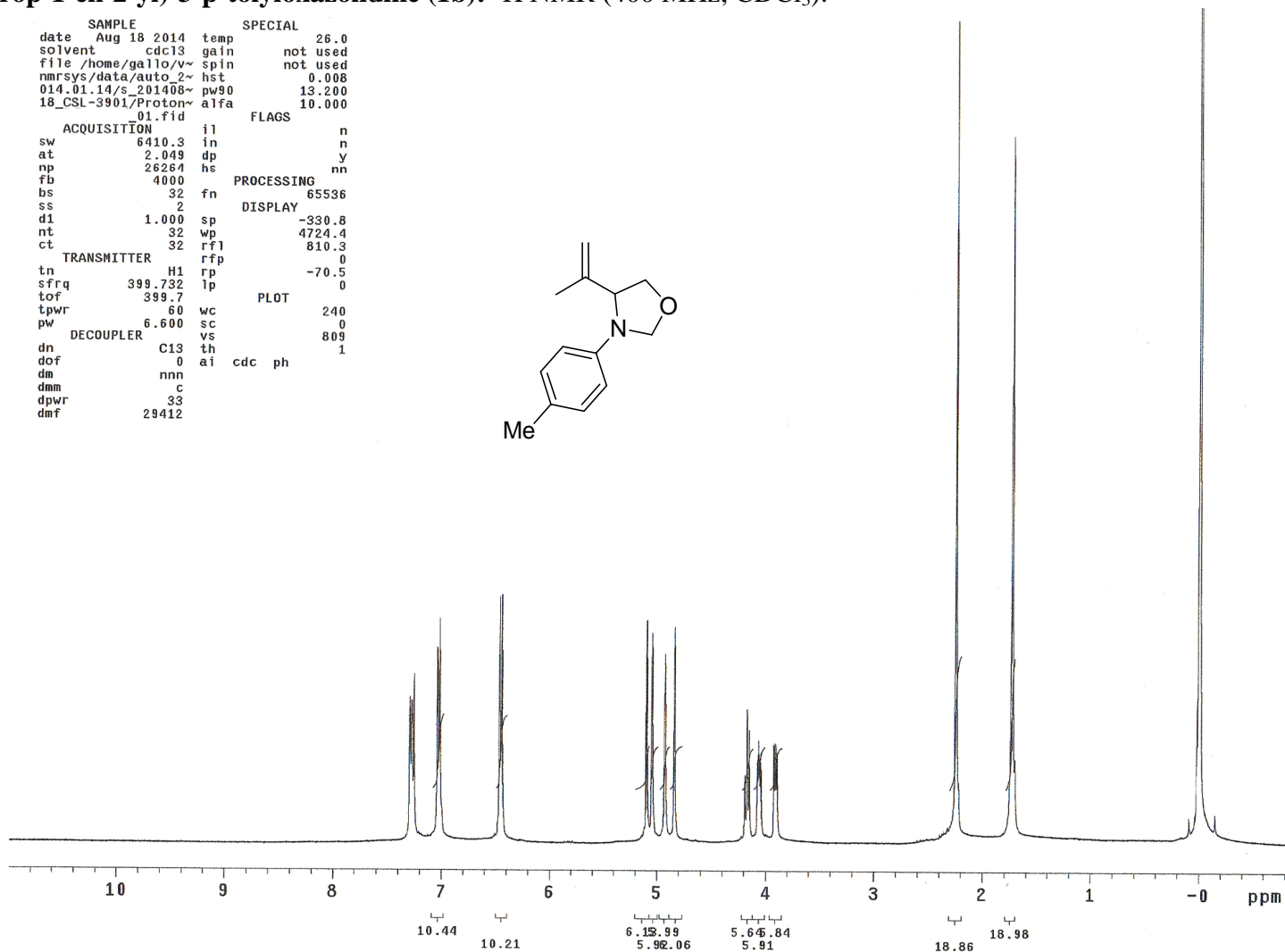
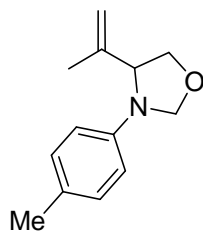


3-phenyl-4-(prop-1-en-2-yl)oxazolidine (1a): GC-MS analysis

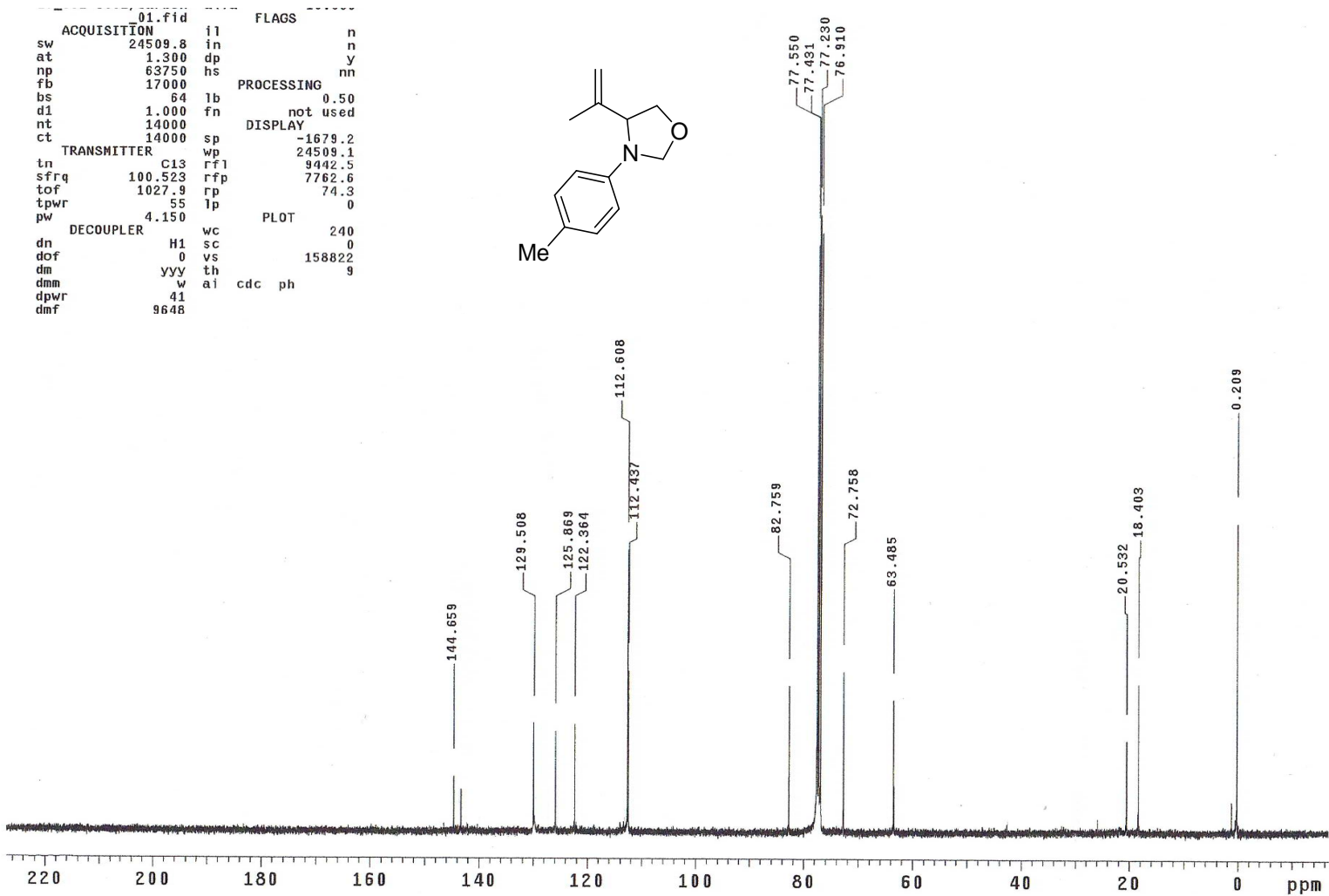


4-(prop-1-en-2-yl)-3-p-tolyloxazolidine (1b): ^1H NMR (400 MHz, CDCl_3):

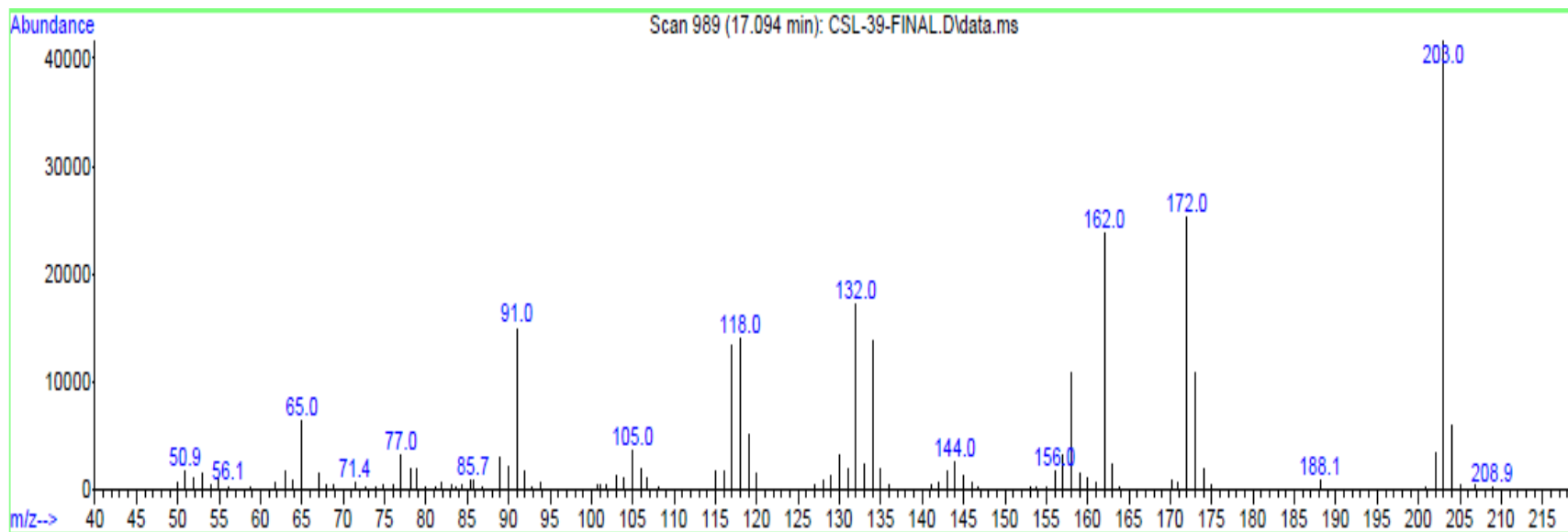
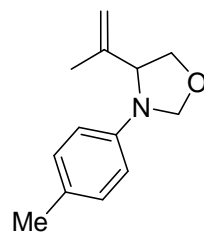
SAMPLE		SPECIAL	
date	Aug 18 2014	temp	26.0
solvent	cdcl3	gain	not used
file	/home/gallo/v~	spin	not used
nmr sys	/data/auto 2~	hst	0.008
014_01_14/s_201408~		pw90	13.200
18_CSL-3901/Proton~		alfa	10.000
01.fid		FLAGS	
ACQUISITION		PROCESSING	
sw	6410.3	il	n
at	2.049	in	n
np	26264	dp	y
fb	4000	hs	nn
bs	32	fn	65536
ss	2	DISPLAY	
d1	1.000	sp	-330.8
nt	32	wp	4724.4
ct	32	rfl	810.3
TRANSMITTER		rfp	0
tn	H1	rp	-70.5
sfrq	399.732	lp	0
tof	399.7	PLOT	
tpwr	60	wc	240
pw	6.600	sc	0
DECOUPLER		vs	809
dn	C13	th	1
dof	0	ai	cdc ph
dm	nnn		
dmm	c		
dpwr	33		
dmf	29412		



4-(prop-1-en-2-yl)-3-p-tolyloxazolidine (1b): ^{13}C NMR (100 MHz, CDCl_3):

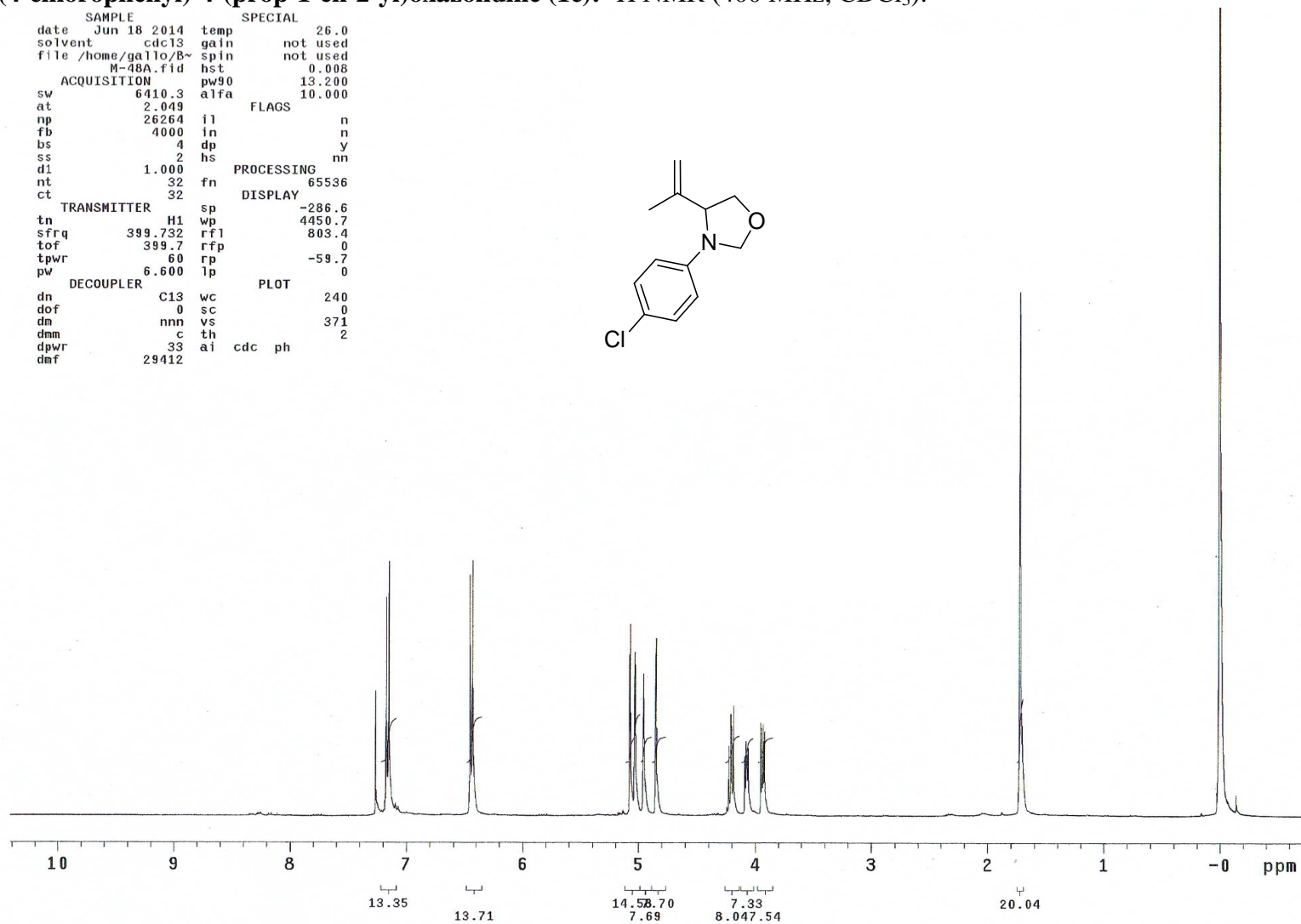
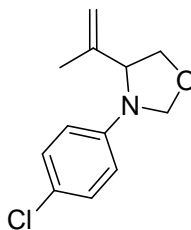


4-(prop-1-en-2-yl)-3-p-tolyloxazolidine (1b): GC-MS analysis



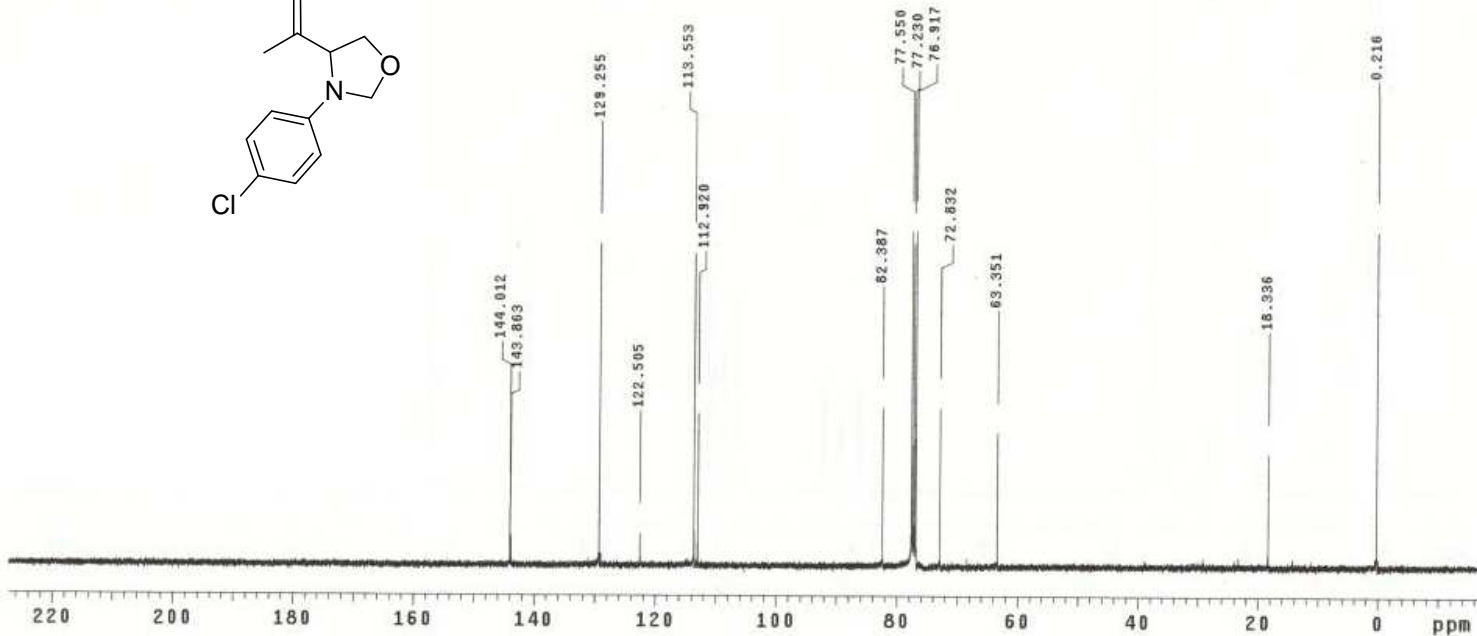
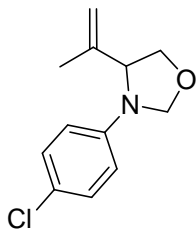
3-(4-chlorophenyl)-4-(prop-1-en-2-yl)oxazolidine (1c): ¹H NMR (400 MHz, CDCl₃):

SAMPLE		SPECIAL	
date	Jun 18 2014	temp	26.0
solvent	cdc13	gain	not used
file	/home/gallo/B~	spin	not used
	M-48A.fid	hst	0.008
ACQUISITION		pw90	13.200
sw	6410.3	alfa	10.000
at	2.049	FLAGS	
np	26264	il	n
fb	4000	in	n
bs	4	dp	y
ss	2	hs	nn
d1	1.000	PROCESSING	
nt	32	fn	65536
ct	32	DISPLAY	
TRANSMITTER		sp	-286.6
tn	H1	wp	4450.7
sfrq	399.732	rfl	803.4
tof	399.7	rfp	0
tpwr	60	rp	-59.7
pw	6.600	lp	0
DECOUPLER		PLOT	
dn	C13	wc	240
dof	0	sc	0
dm	nnn	vs	371
dmm	c	th	2
dpwr	33	ai	cdc ph
dmr	29412		

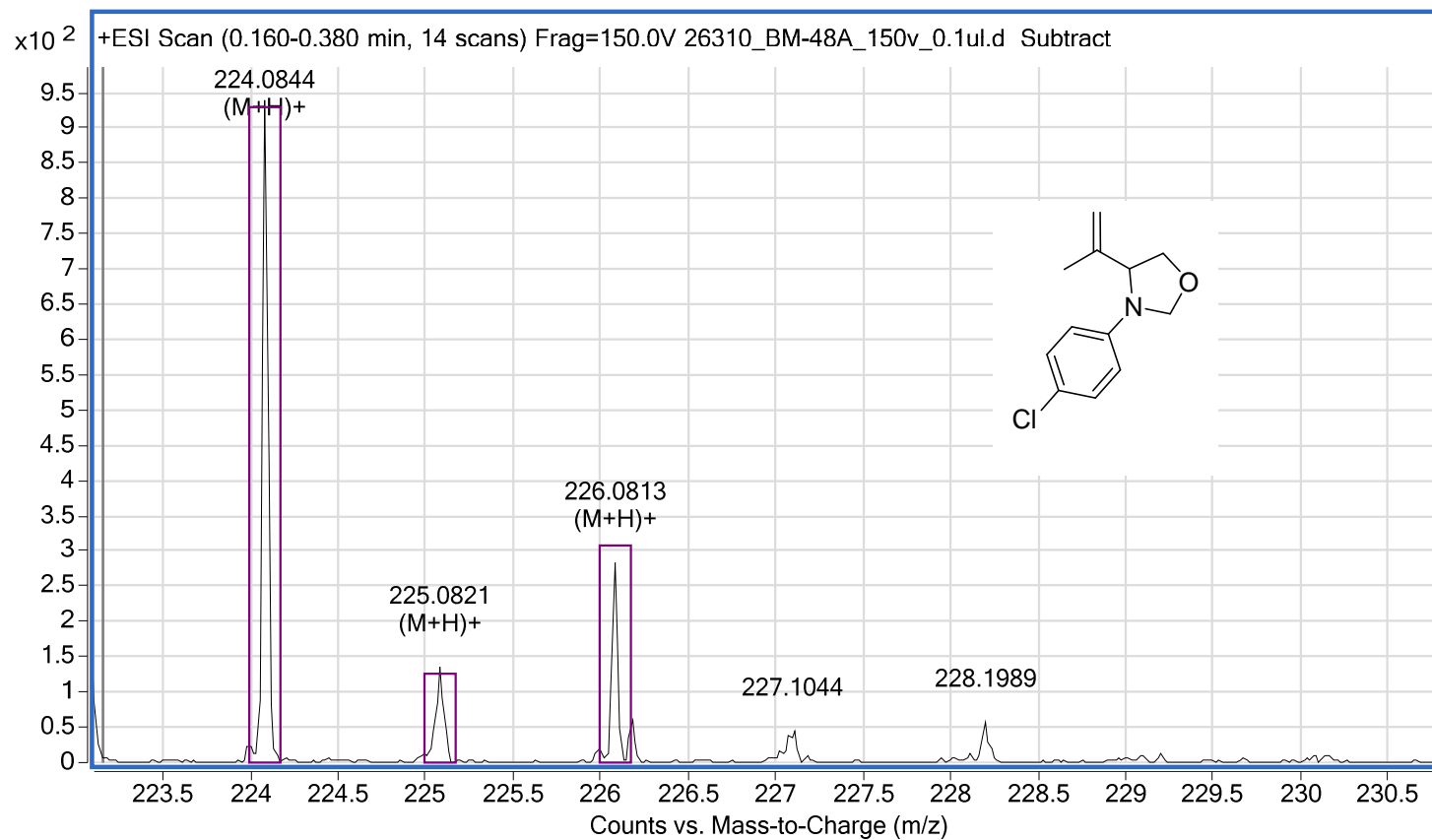


3-(4-chlorophenyl)-4-(prop-1-en-2-yl)oxazolidine (1c): ¹³C NMR (100 MHz, CDCl₃):

```
SAMPLE SPECIAL
data Jun 18 2014 temp 26.0
solvent cdc13 gain 30
file exp spln not used
ACQUISITION hst 0.008
sw 24509.6 pw90 8.300
at 1.300 alfa 10.000
np 63750
fb 17000 il l
bs 32 in n
d1 1.000 dp y
nt 8000 hs nn
ct 3072
TRANSMITTER lb 0.50
tn C13 fn not used
sfrq 100.523 DISPLAY
tof 1027.9 sp -1677.7
tpwr 55 wp 24509.1
pw 4.150 rfl 9441.0
DECOUPLER H1 rfp 7762.6
dn 0 rp 95.0
dof 0 lp 0
dm yyy PLOT
dmm w wc 240
dpwr 41 sc 0
dmf 9648 vs 58669
al cdc ph th 4
```



3-(4-chlorophenyl)-4-(prop-1-en-2-yl)oxazolidine (1c): HR-MS analysis

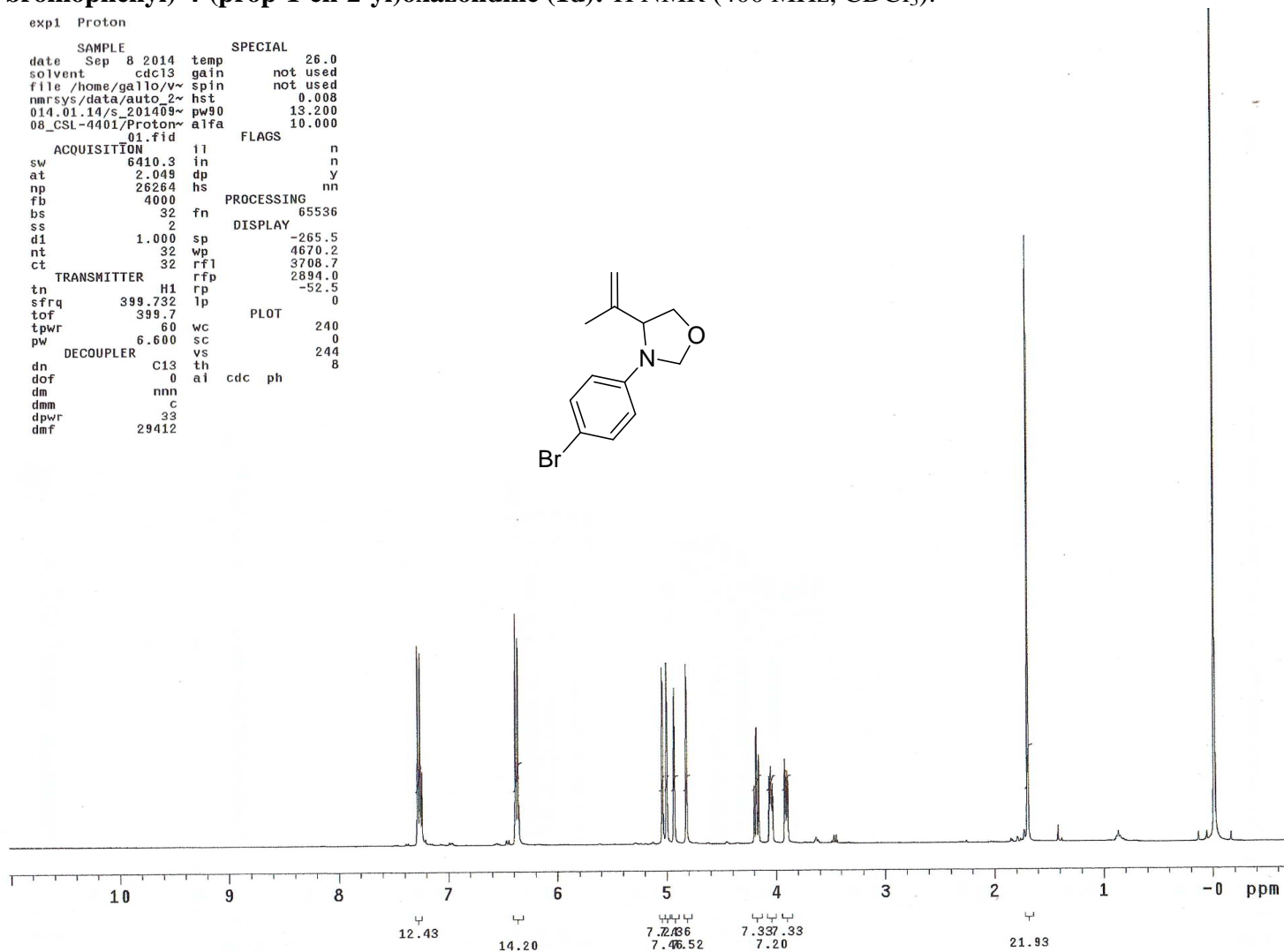
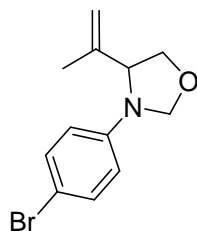


3-(4-bromophenyl)-4-(prop-1-en-2-yl)oxazolidine (1d): ^1H NMR (400 MHz, CDCl_3):

```

exp1 Proton
SAMPLE
date Sep 8 2014 temp 26.0
solvent cdc13 gain not used
file /home/gallo/v spin not used
nmrSYS/data/auto_2 hst 0.008
014.01.14/s_201409 pw90 13.200
08_CSL-4401/Proton alfa 10.000
01.fid
SPECIAL
ACQUISITION
sw 6410.3 in n
at 2.049 dp y
np 26264 hs nn
fb 4000
bs 32 fn PROCESSING 65536
ss 2 DISPLAY
d1 1.000 sp -265.5
nt 32 wp 4670.2
ct 32 rfl 3708.7
TRANSMITTER
tn H1 rfp 2894.0
sfrq 399.732 lp -52.5
tof 399.7 PLOT
tpwr 60 wc 240
pw 6.600 sc 0
DECOUPLER C13 th 244
dn 0 ai cdc ph 8
dof nnn
dm c
dmm 33
dpwr 29412
dmf

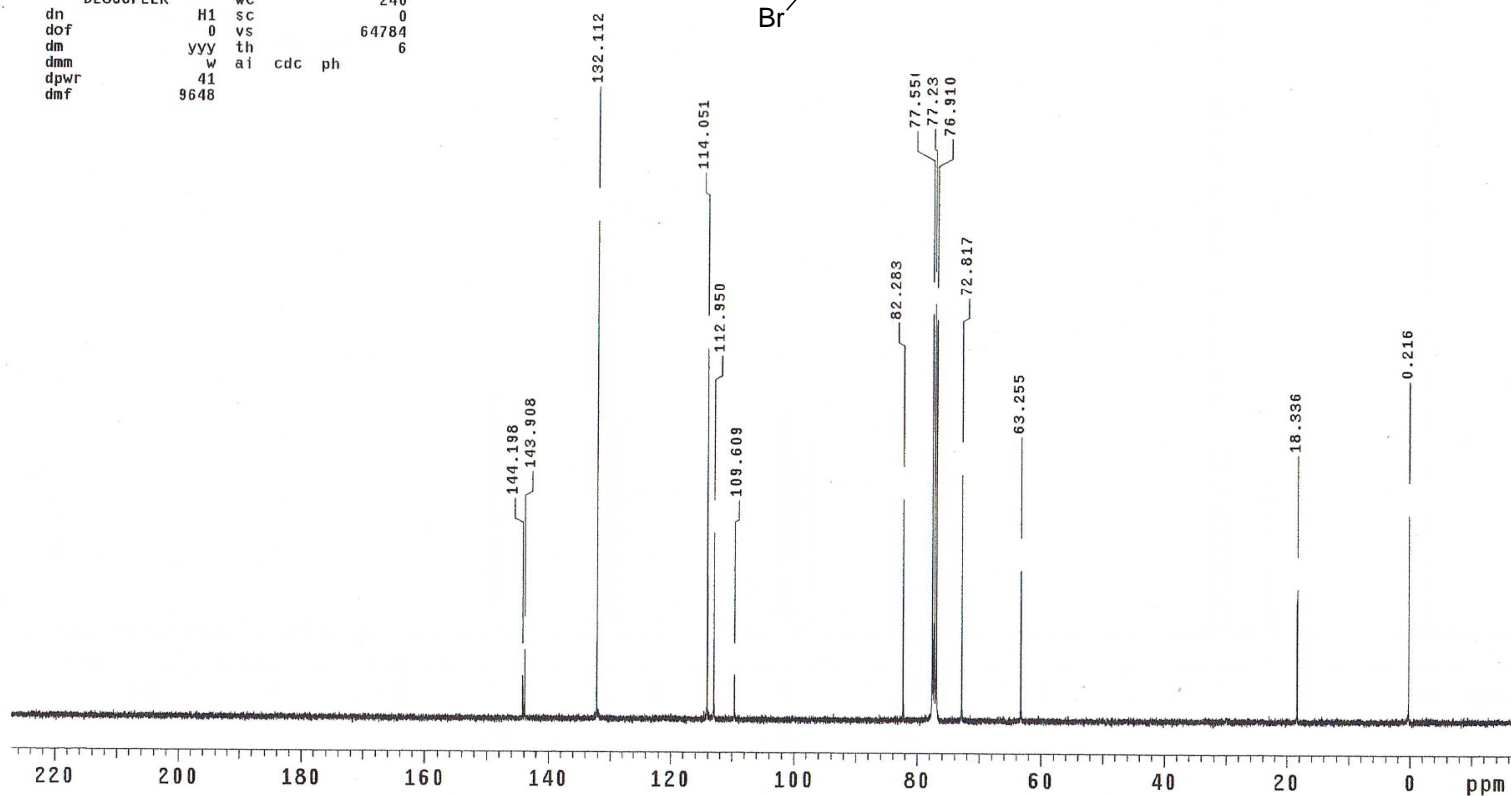
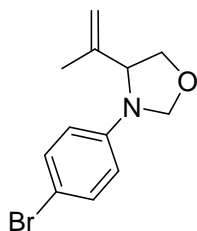
```



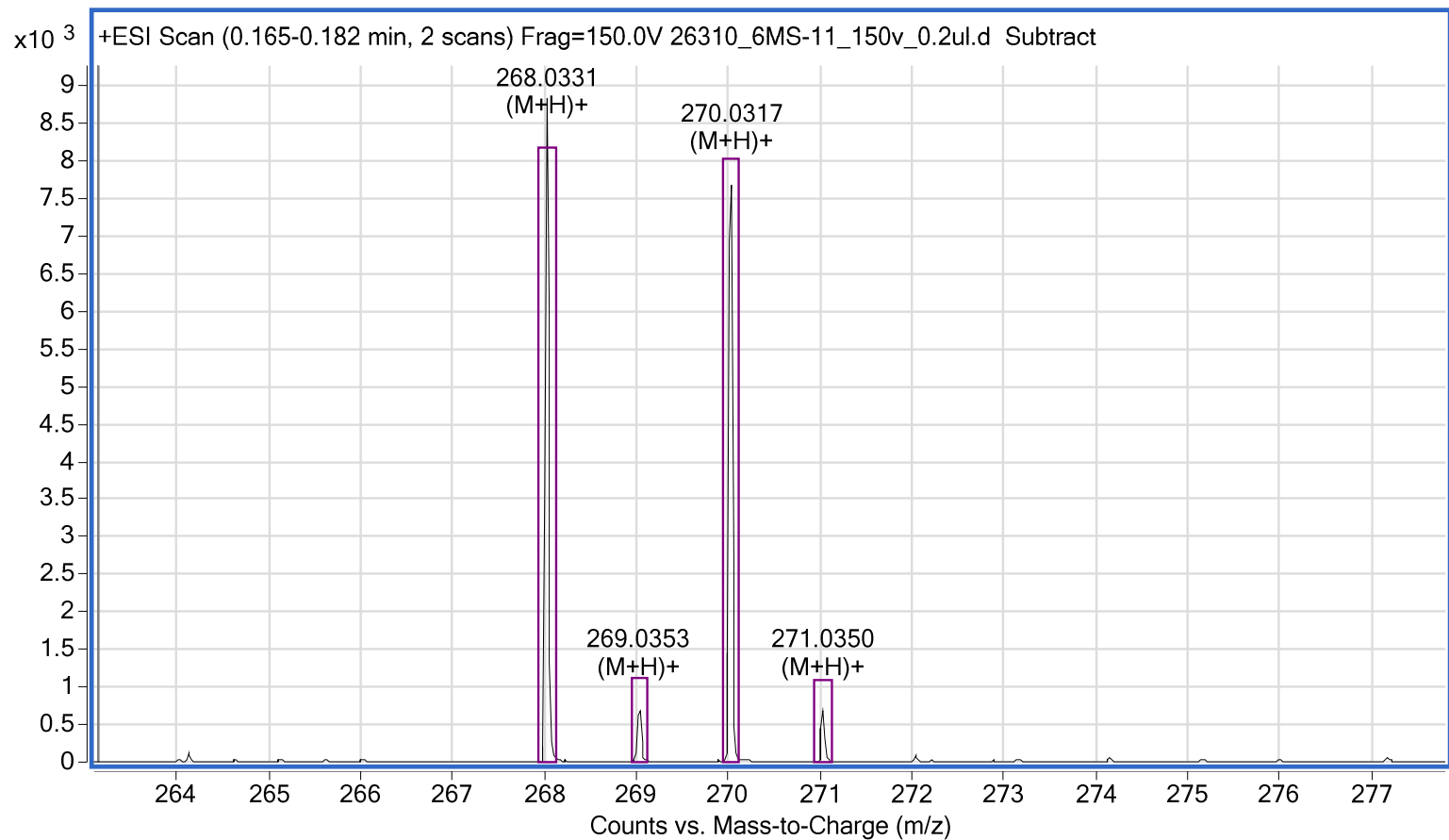
3-(4-bromophenyl)-4-(prop-1-en-2-yl)oxazolidine (1d): ^{13}C NMR (100 MHz, CDCl_3):

```

ACQUISITION  f1      n
sw          24509.8 in      n
at          1.300  in      n
np          63750  dp      y
fb          17000  hs      nn
bs          64    lb      0.50
di          1.000  fn      not used
nt          5000  DISPLAY
ct          5000  sp      -1679.2
                wp      24509.1
                rfl      9442.5
TRANSMITTER  C13    rfp      7762.6
                rp      72.7
                lp      0
                PLOT
pw          4.150  wc      240
                dn      H1    sc      0
                dof     0    vs      64784
                dm      yy   th      6
                dmm     w    ai      cdc ph
                dpwr    41
                dmf     9648
    
```

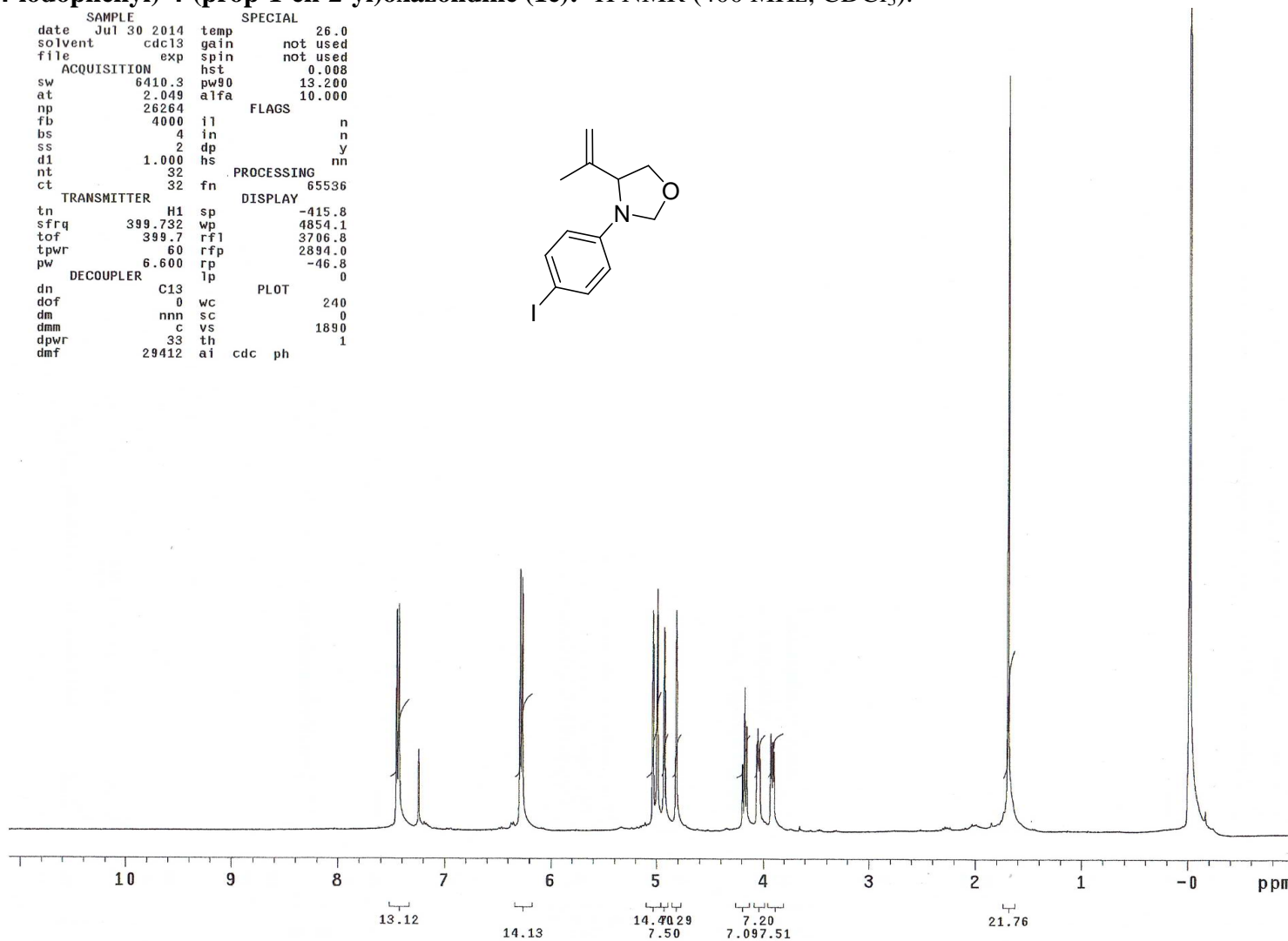
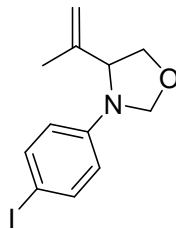


3-(4-bromophenyl)-4-(prop-1-en-2-yl)oxazolidine (1d): HR-MS analysis

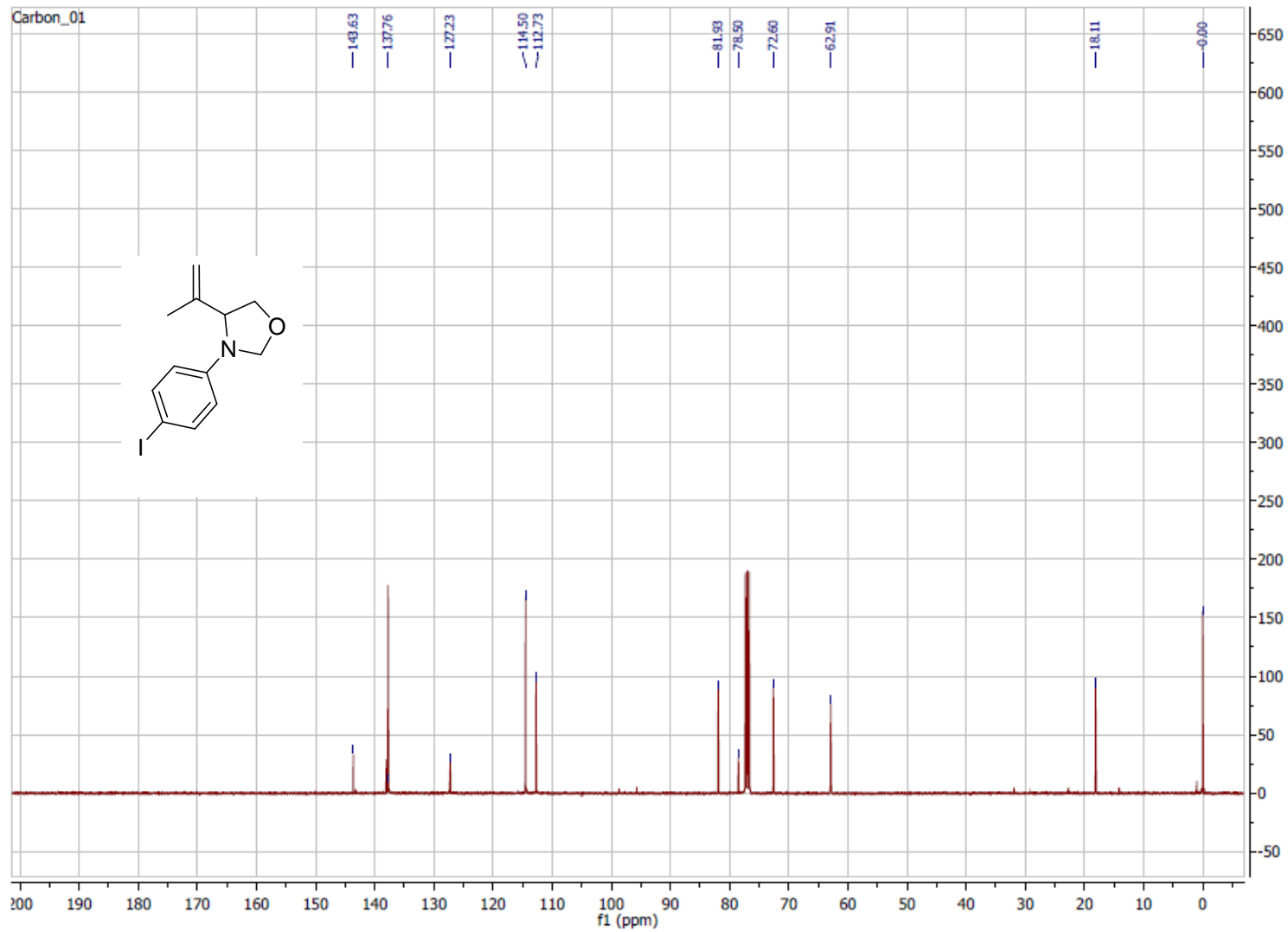


3-(4-iodophenyl)-4-(prop-1-en-2-yl)oxazolidine (1e): ¹H NMR (400 MHz, CDCl₃):

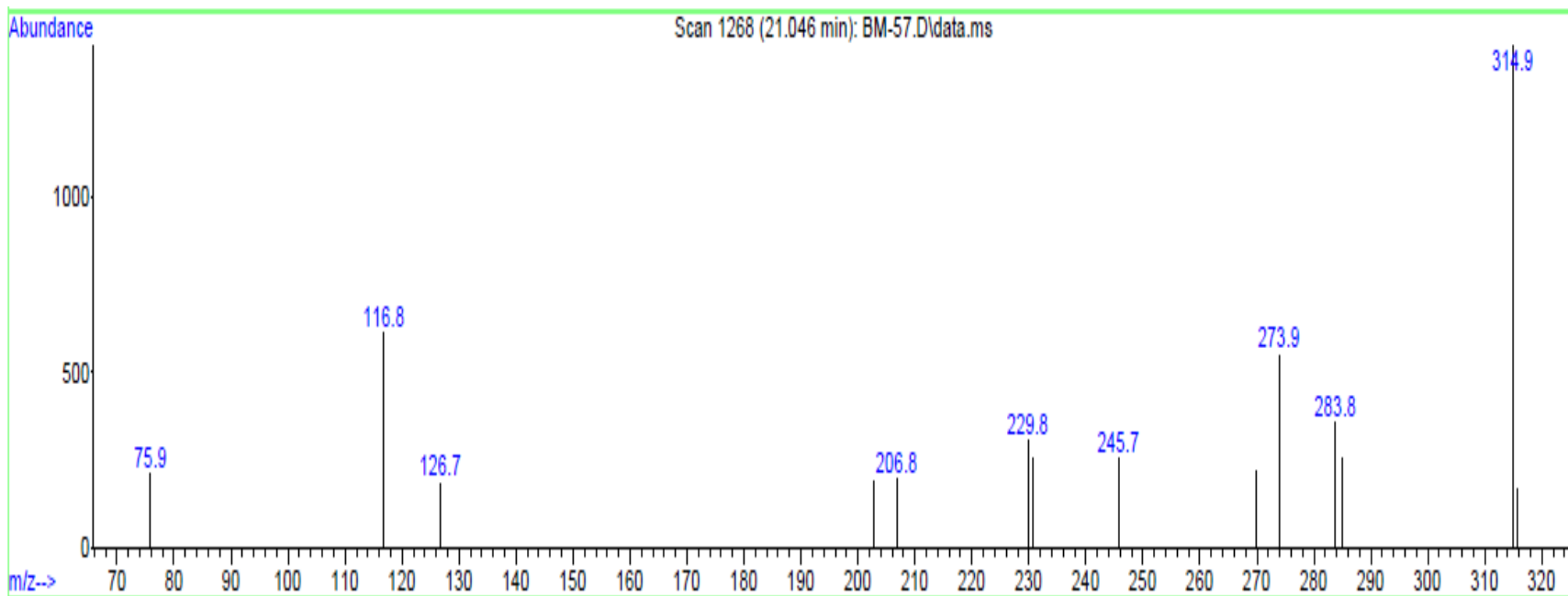
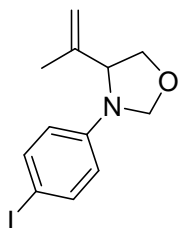
SAMPLE		SPECIAL	
date	Jul 30 2014	temp	26.0
solvent	cdcl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	6410.3	pw90	13.200
at	2.049	alfa	10.000
np	26264	FLAGS	
fb	4000	il	n
bs	4	in	n
ss	2	dp	y
d1	1.000	hs	nn
nt	32	PROCESSING	
ct	32	fn	65536
TRANSMITTER		DISPLAY	
tn	H1	sp	-415.8
sfrq	399.732	wp	4854.1
tof	399.7	rfl	3706.8
tpwr	60	rfp	2894.0
pw	6.600	rp	-46.8
DECOUPLER		lp	0
dn	C13	PLOT	
dof	0	wc	240
dm	nnn	sc	0
dmm	c	vs	1890
dpwr	33	th	1
dmf	29412	ai	cdc ph



3-(4-iodophenyl)-4-(prop-1-en-2-yl)oxazolidine (1e): ^{13}C NMR (100 MHz, CDCl_3):

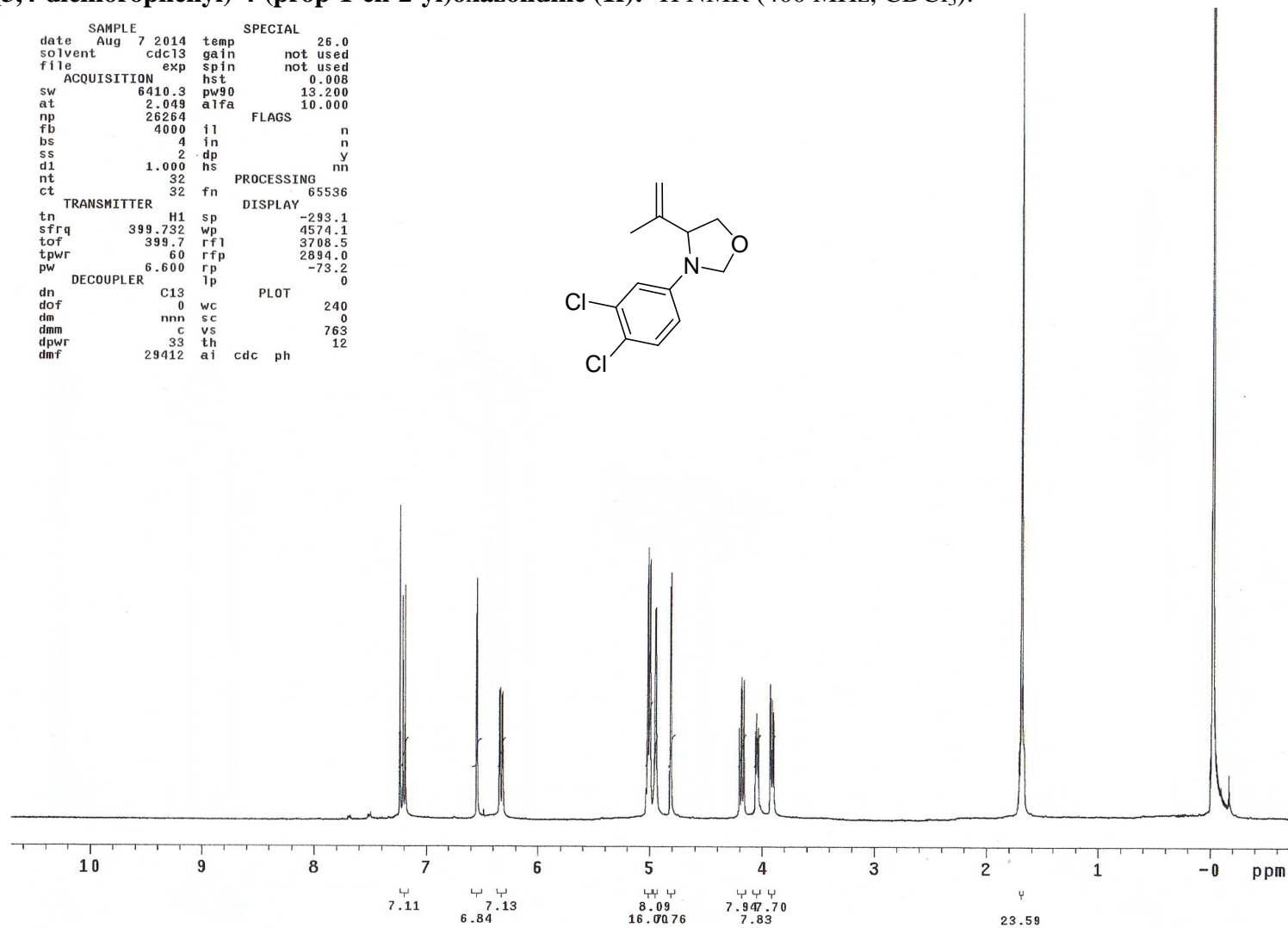
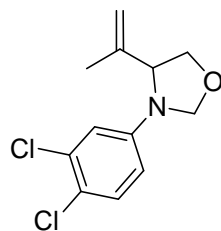


3-(4-iodophenyl)-4-(prop-1-en-2-yl)oxazolidine (1e): GC-MS analysis

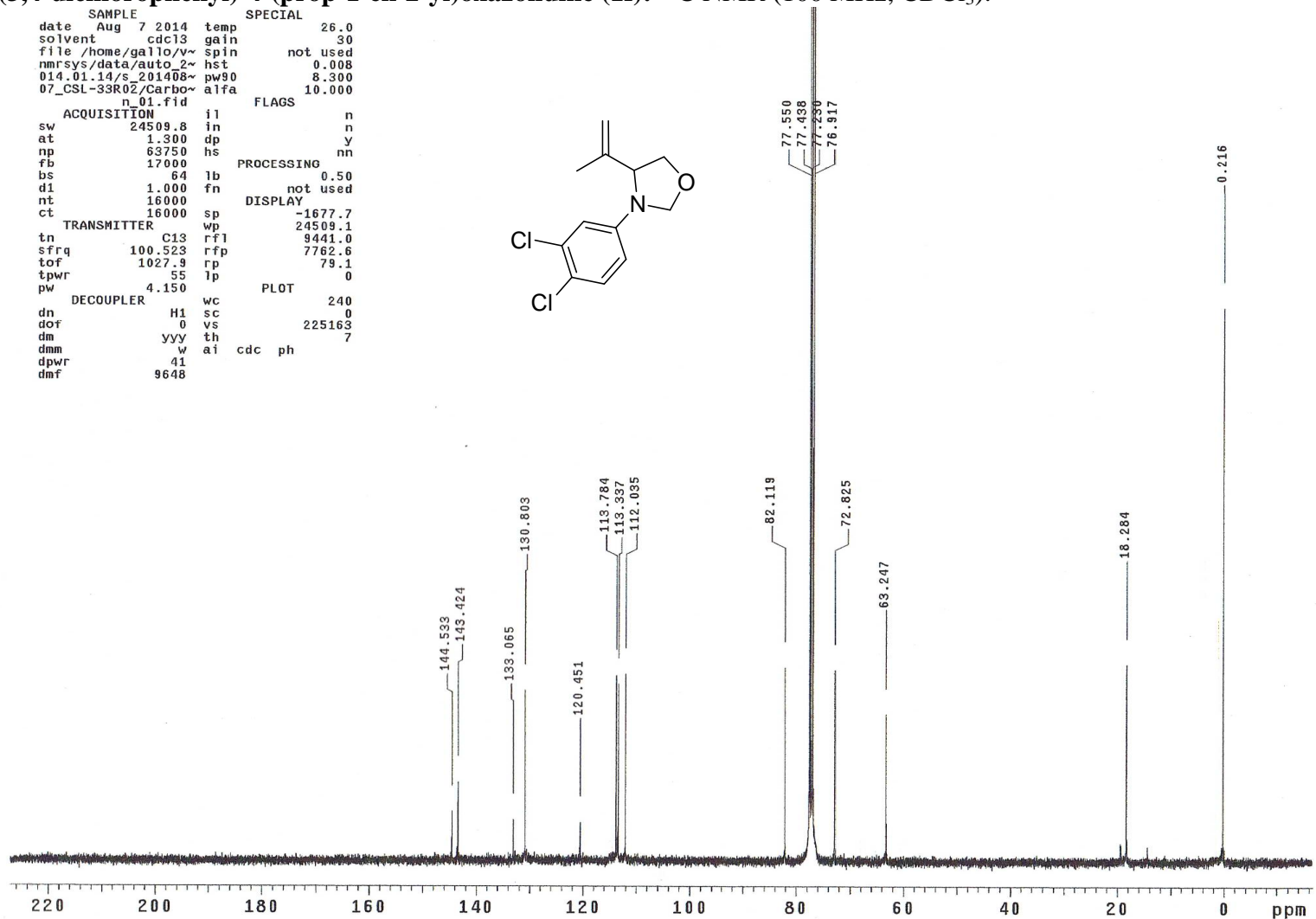


3-(3,4-dichlorophenyl)-4-(prop-1-en-2-yl)oxazolidine (1f): ¹H NMR (400 MHz, CDCl₃):

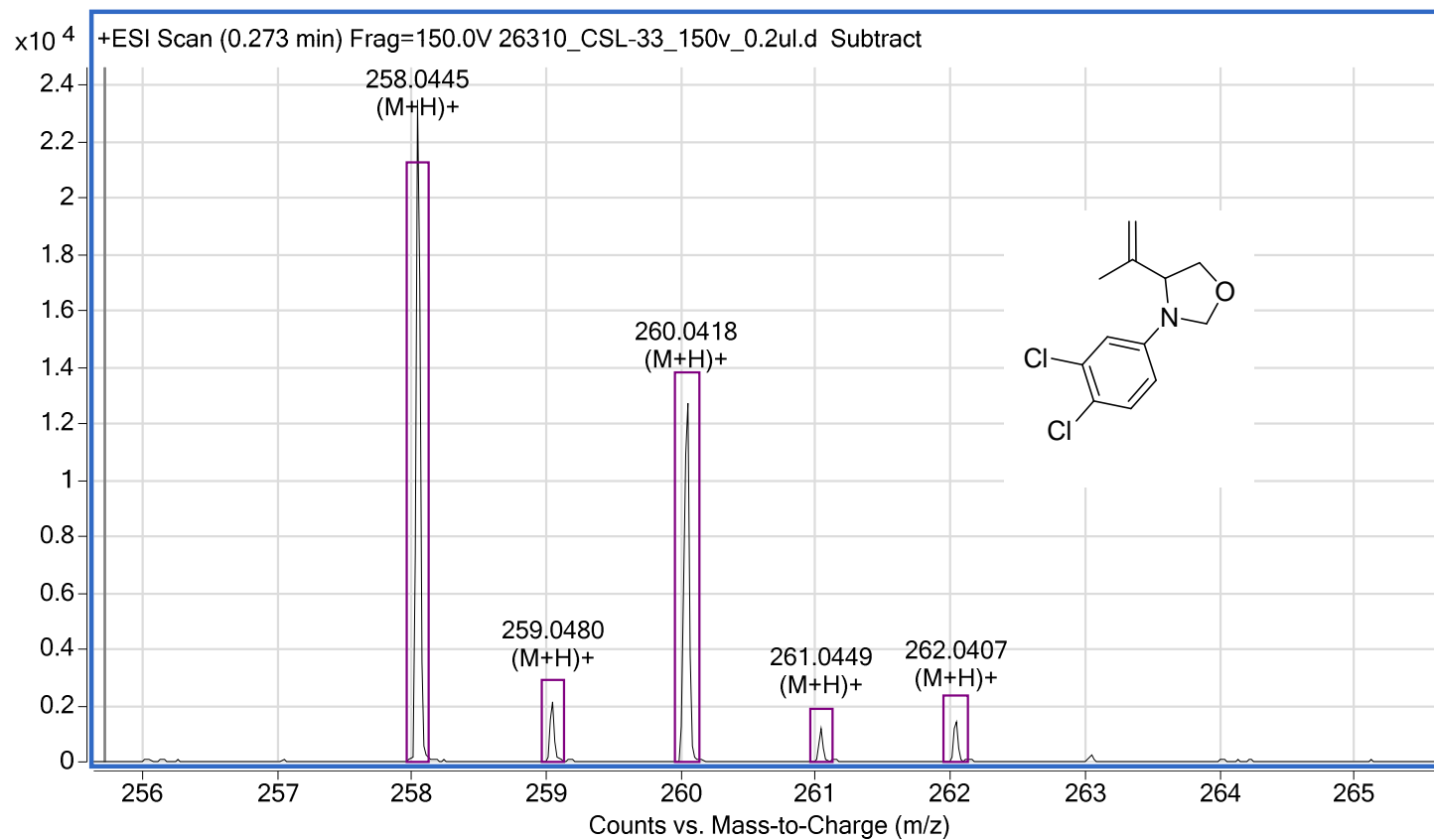
SAMPLE		SPECIAL	
date	Aug 7 2014	temp	26.0
solvent	cdc13	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	6410.3	pw90	13.200
at	2.049	alfa	10.000
np	26264	FLAGS	
fb	4000	il	n
bs	4	in	n
ss	2	dp	y
d1	1.000	hs	nn
nt	32	PROCESSING	
ct	32	fn	65536
TRANSMITTER		DISPLAY	
tn	H1	sp	-293.1
sfrq	399.732	wp	4574.1
tof	399.7	rfl	3708.5
tpwr	60	rff	2894.0
pw	6.600	rp	-73.2
DECOUPLER		tp	0
dn	C13	PLOT	
dof	0	wc	240
dm	nnn	sc	0
dmm	c	vs	763
dpwr	33	th	12
dmf	29412	ai	cdc ph



3-(3,4-dichlorophenyl)-4-(prop-1-en-2-yl)oxazolidine (1f): ¹³C NMR (100 MHz, CDCl₃):



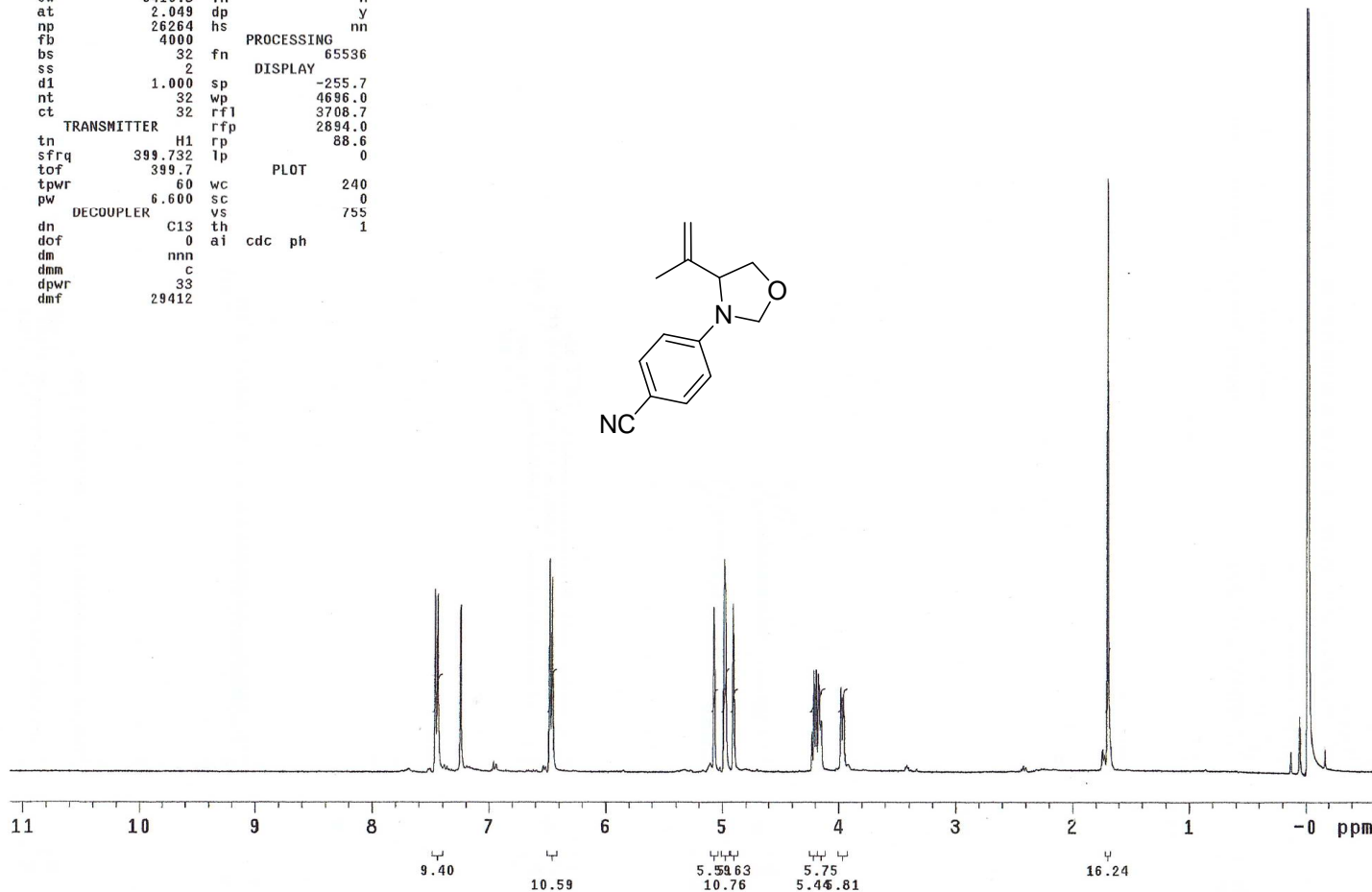
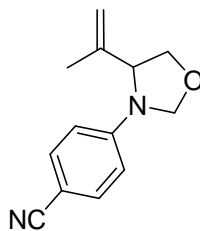
3-(3,4-dichlorophenyl)-4-(prop-1-en-2-yl)oxazolidine (1f): HR-MS analysis



4-(4-(prop-1-en-2-yl)oxazolidin-3-yl)benzonitrile (1g): ¹H NMR (400 MHz, CDCl₃):

```

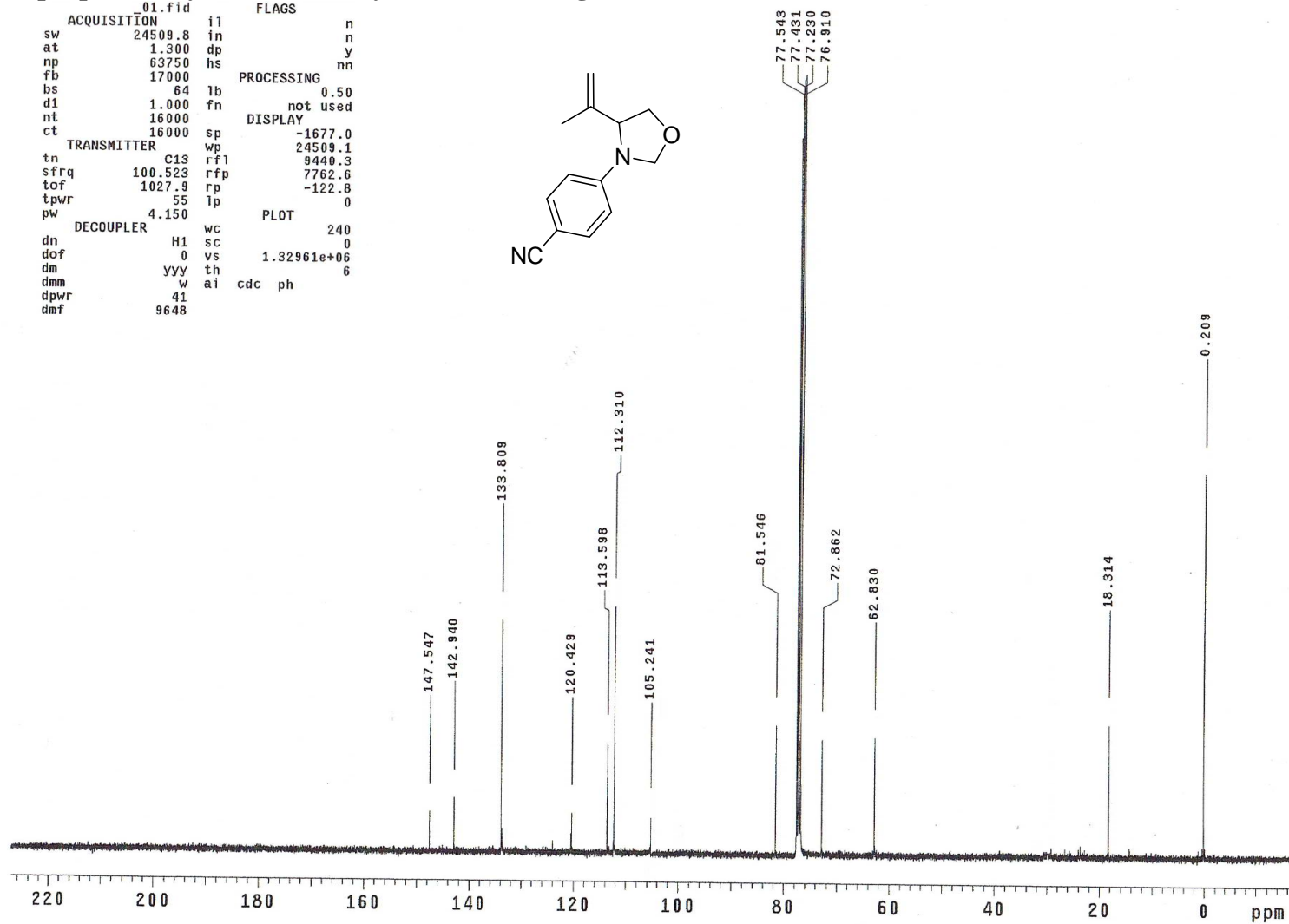
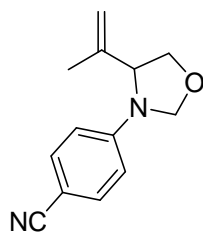
SAMPLE          SPECIAL
date Sep 19 2014 temp 26.0
solvent cdc13 gain not used
file /home/gallo/v~ spin not used
nmrSYS/data/auto_2~ hst 0.008
014_01.14/s_201409~ pw90 13.200
19_CSL-5201/Proton~ a1fa 10.000
01.fid          FLAGS
ACQUISITION    il n
sw 6410.3 in n
at 2.049 dp y
np 26264 hs nn
fb 4000          PROCESSING
bs 32 fn 65536
ss 2            DISPLAY
dl 1.000 sp -255.7
nt 32 wp 4696.0
ct 32 rf1 3708.7
TRANSMITTER    rfp 2894.0
tn H1 rp 88.6
sfrq 399.732 lp 0
tof 399.7          PLOT
tpwr 60 wc 240
pw 6.600 sc 0
DECOUPLER      vs 755
dn C13 th 1
dof 0 ai cdc ph
dm nnn
dmm c
dpwr 33
dmf 29412
    
```



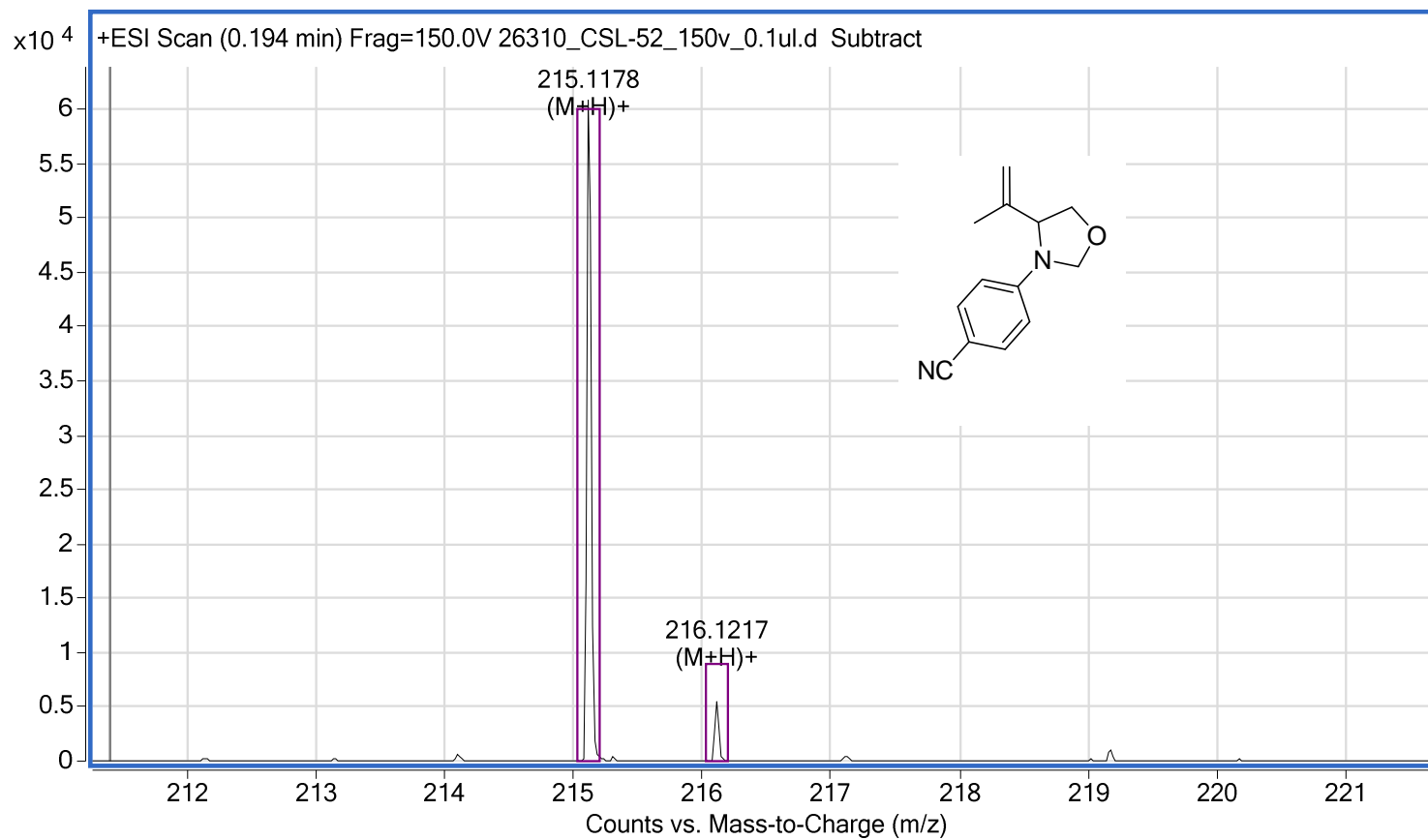
4-(4-(prop-1-en-2-yl)oxazolidin-3-yl)benzotrile (1g): ^{13}C NMR (100 MHz, CDCl_3):

```

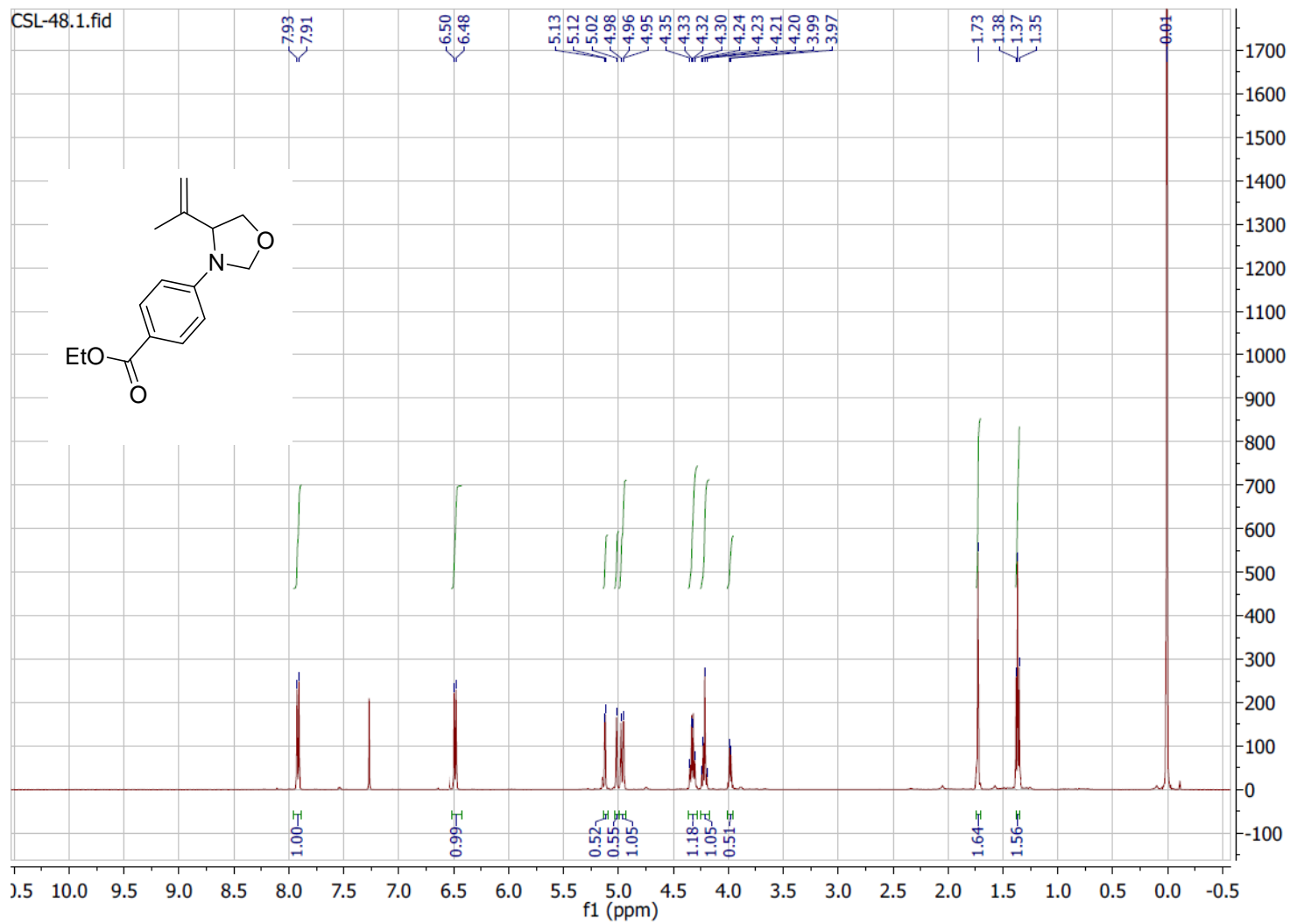
01.fid      FLAGS
ACQUISITION i1          n
sw          24509.8     in          n
at          1.300      dp          y
np          63750      hs          nn
fb          17000
bs          64         lb          0.50
d1          1.000      fn          not used
nt          16000      DISPLAY
ct          16000      sp          -1677.0
TRANSMITTER wp          24509.1
tn          C13        rf1         9440.3
sfrq       100.523     rfp         7762.6
tof        1027.9     rp          -122.8
tpwr       55         lp          0
pw         4.150      PLOT
DECOUPLER  wc          240
dn          H1        sc          0
dof         0         vs          1.32961e+06
dm          yyy       th          6
dmm         w         ai          cdc ph
dpwr       41
dmf        9648
    
```



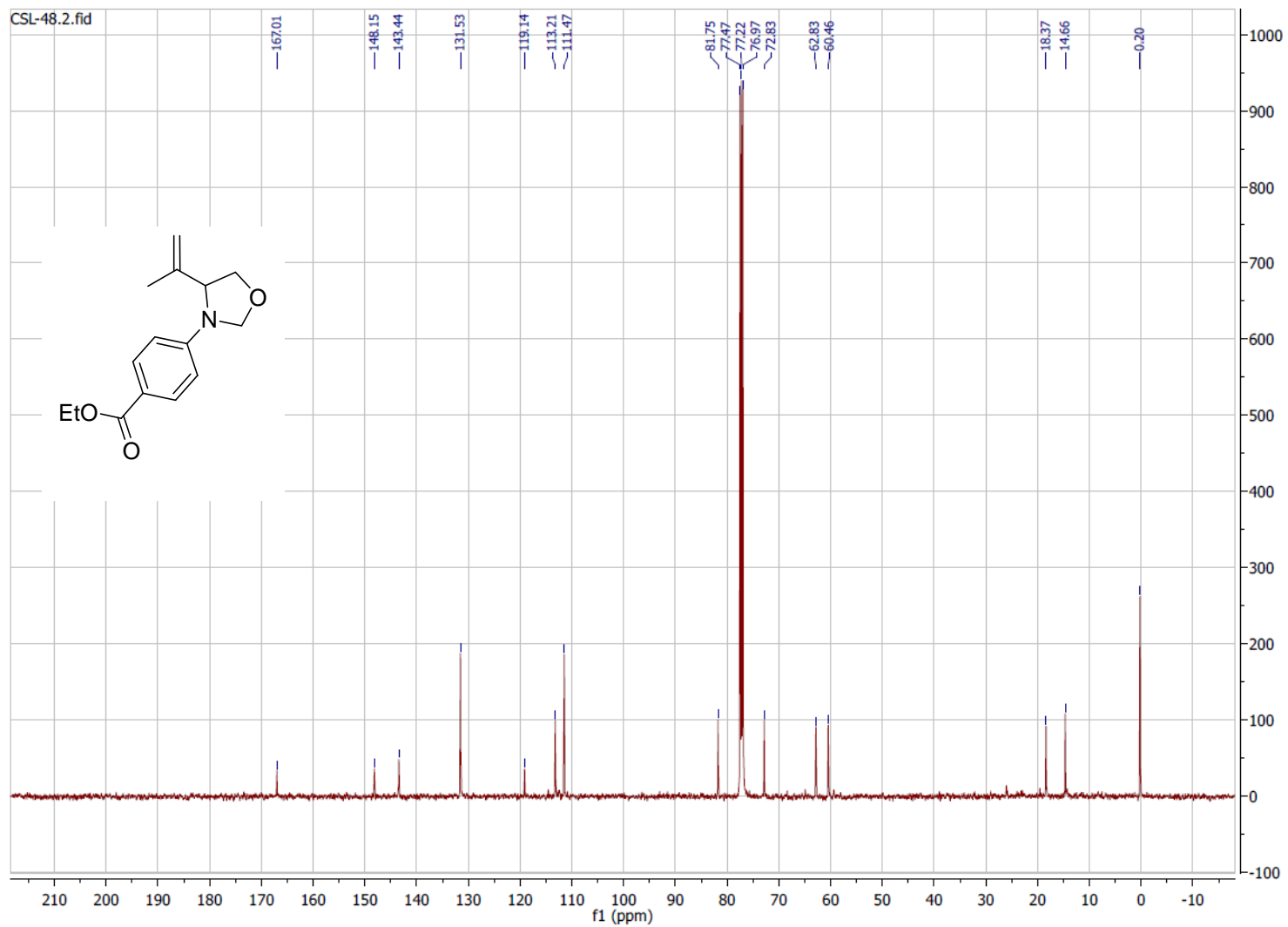
4-(4-(prop-1-en-2-yl)oxazolidin-3-yl)benzonitrile (1g): HR-MS analysis



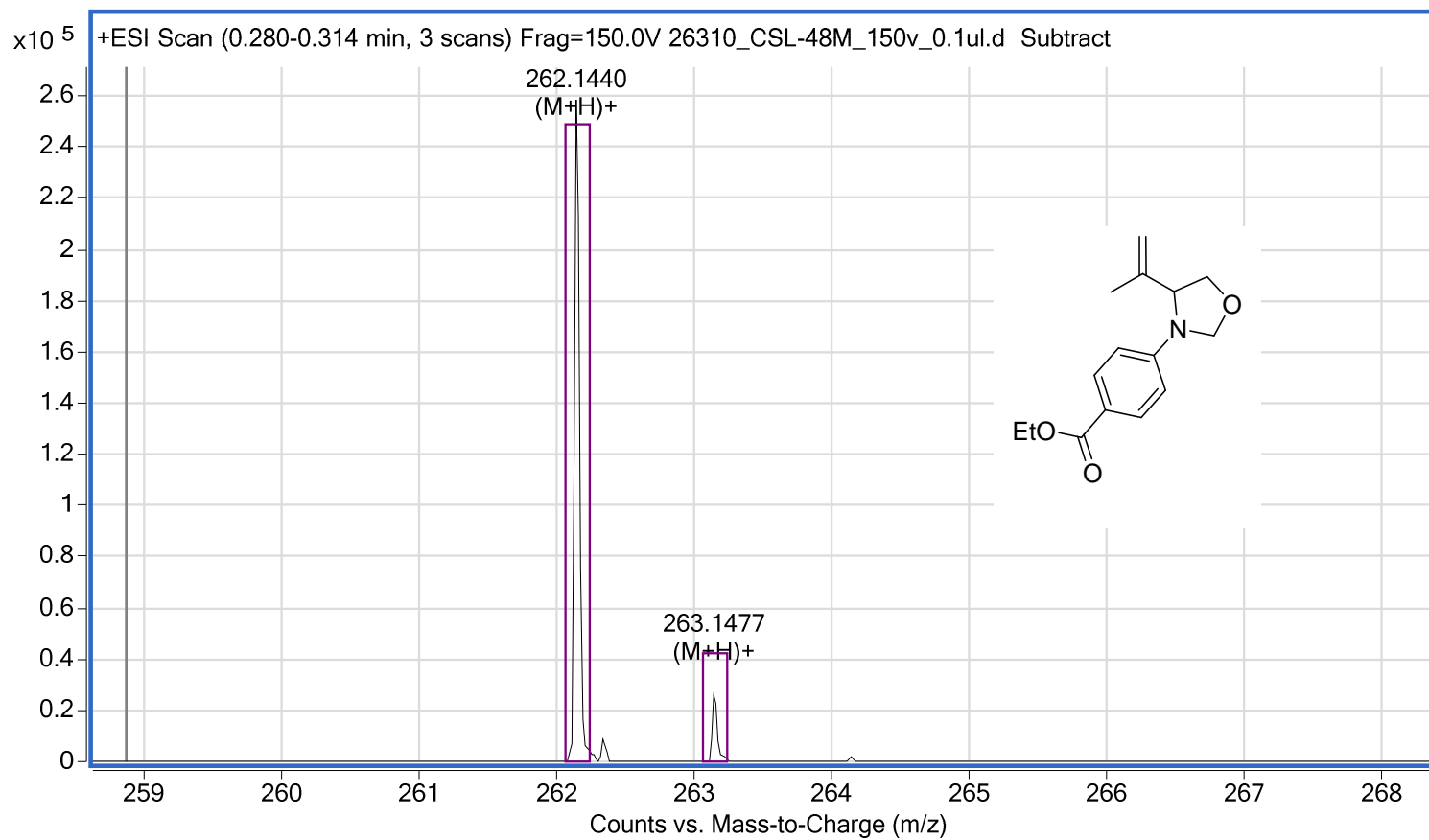
Ethyl 4-(4-(prop-1-en-2-yl)oxazolidin-3-yl)benzoate (1h): ^1H NMR (400 MHz, CDCl_3)



Ethyl 4-(4-(prop-1-en-2-yl)oxazolidin-3-yl)benzoate (1h): ^{13}C NMR (100 MHz, CDCl_3)



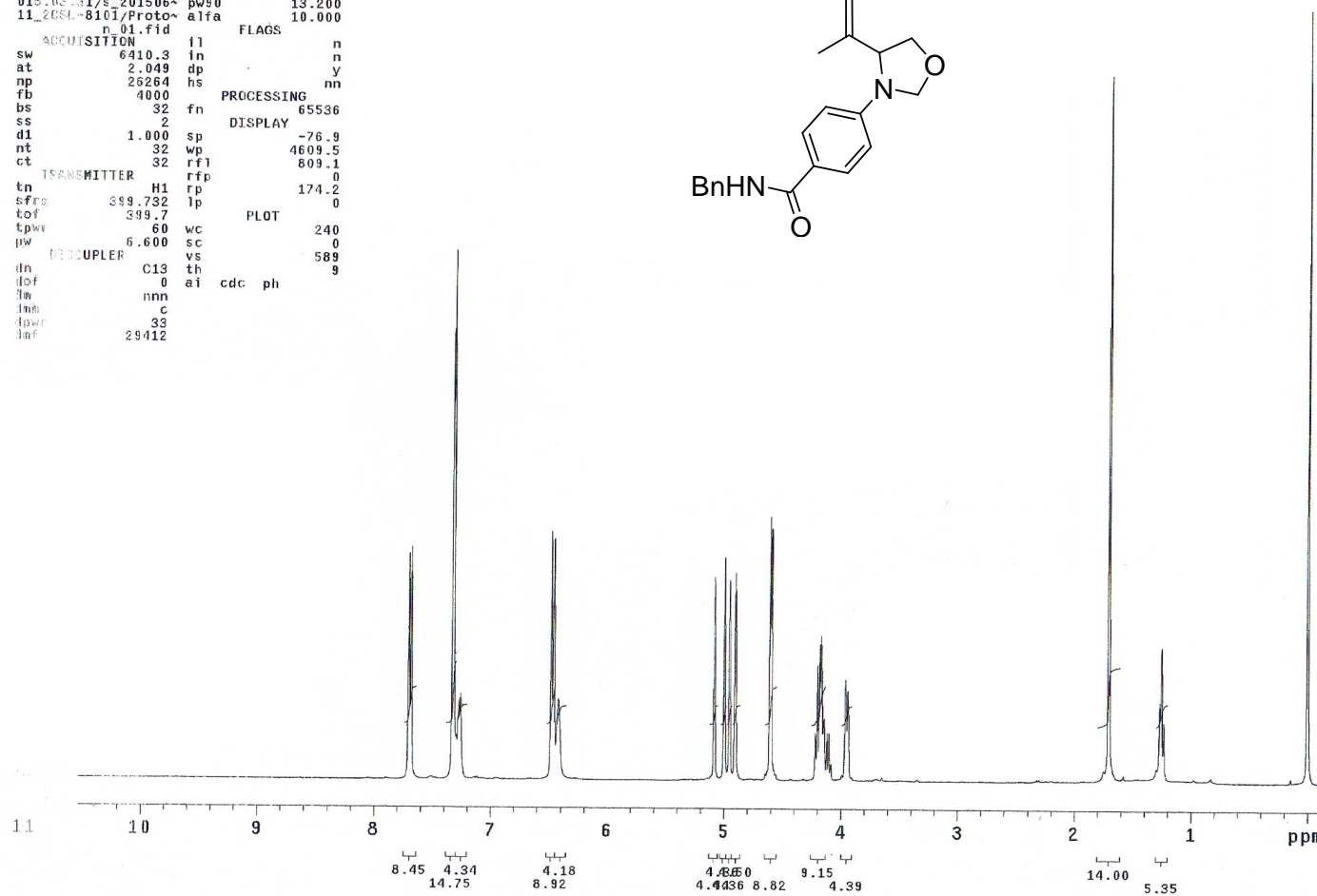
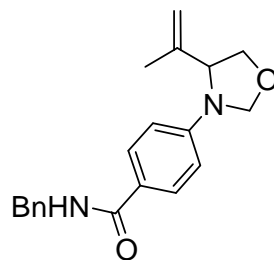
Ethyl 4-(4-(prop-1-en-2-yl)oxazolidin-3-yl)benzoate (1h): HR-MS analysis



N-benzyl-4-(4-(prop-1-en-2-yl)oxazolidin-3-yl)benzamide (1i): ¹H NMR (400 MHz, CDCl₃)

```

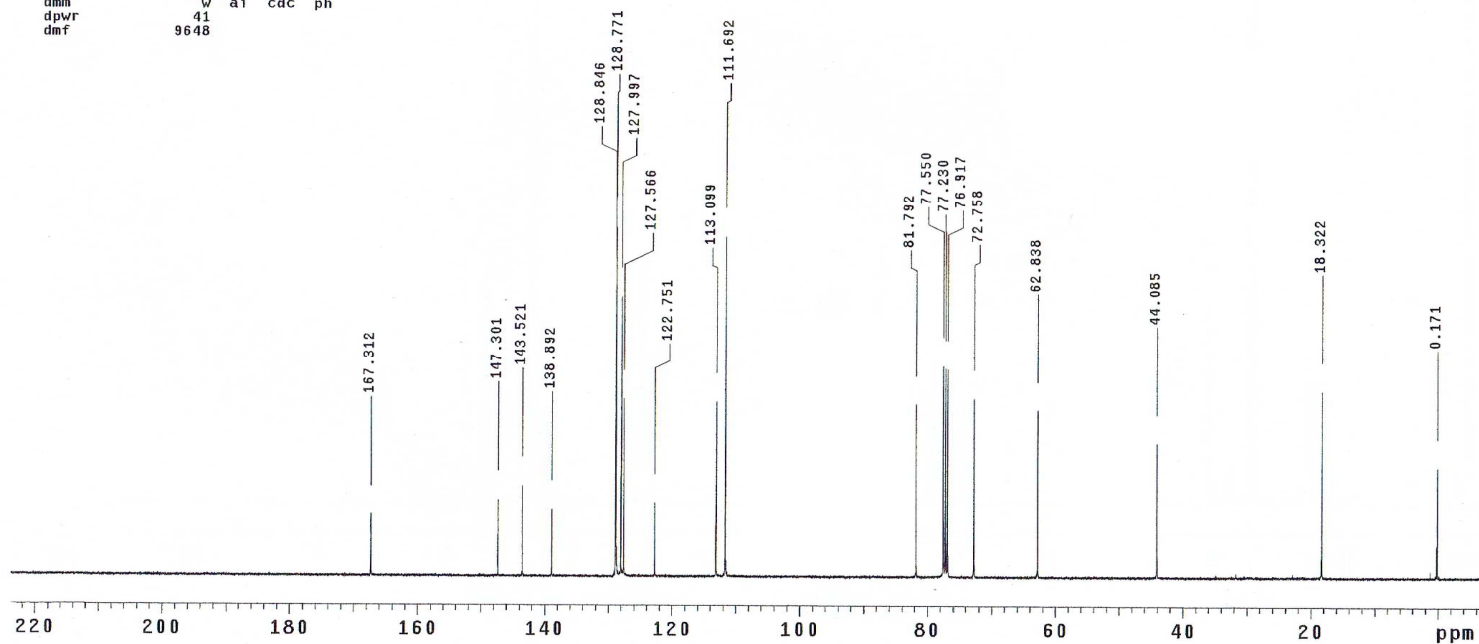
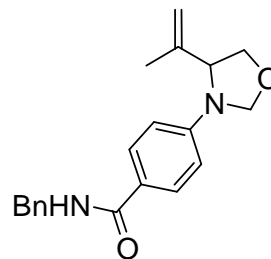
exp21 Proton
SAMPLE
date Jun 11 2015 temp 25.0
solvent cdc13 gain not used
file /home/gallo/v~ spin not used
nmrsys/data/auto_2~ hst 0.008
015_05_31/s_201506~ pw90 13.200
11_20SL-8101/Proto~ alfa 10.000
n_01.fid
ACQUISITION
sw 6410.3 in n
at 2.049 dp y
np 2624 hs nn
fb 4000
bs 32 fn PROCESSING 65536
ss 2 DISPLAY -76.9
d1 1.000 sp wp 4609.5
nt 32 rfl 809.1
ct 32 rfp 0
TRANSMITTER H1 rp 174.2
sfpc 399.732 lp 0
tof 399.7
tpwr 60 wc PLOT 240
pw 6.600 sc 0
DECOUPLER C13 th 589
dn 0 ai cdc ph 9
dof 0
fn nnn
fnh c
dprf 33
3nf 29412
    
```



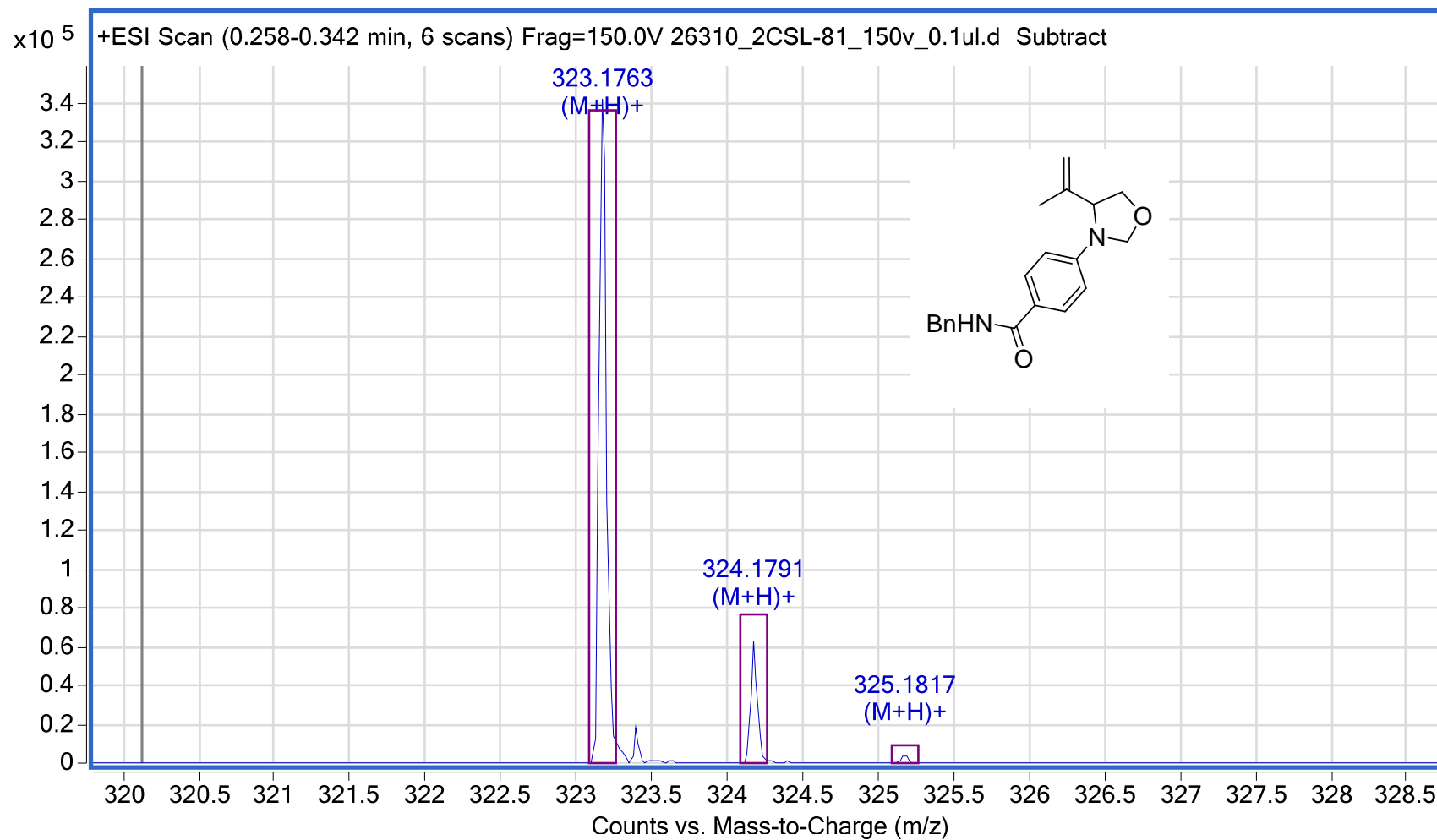
N-benzyl-4-(4-(prop-1-en-2-yl)oxazolidin-3-yl)benzamide (1i): ^{13}C NMR (100 MHz, CDCl_3)

```

exp21 Carbon
SAMPLE
date Jun 11 2015 temp SPECIAL 25.0
solvent cdc13 gain 30
file /home/gallo/v~ spin not used
nmrSYS/data/auto_2~ hst 0.008
015_03.31/s_201506~ pw90 8.300
11_2CSL-8101/Carbo~ alfa 10.000
n_01.fid
ACQUISITION i1 FLAGS n
sw 24509.8 in n
at 1.300 dp Y
np 63750 hs nn
fb 17000
bs 64 lb PROCESSING 0.50
dl 1.000 fn not used
nt 12000 DISPLAY
ct 12000 sp -684.4
TRANSMITTER wp 23166.4
tn C13 rfp 9447.0
sfrq 100.528 rfp 7762.6
tof 1027.9 rfp 63.2
tpwr 55 lp 0
pw DECOUPLER 4.150 PLOT 240
dn H1 sc 0
dof 0 vs 372415
dm YYY th 7
dmm w ai cdc ph
dpwr 41
dmf 9648
  
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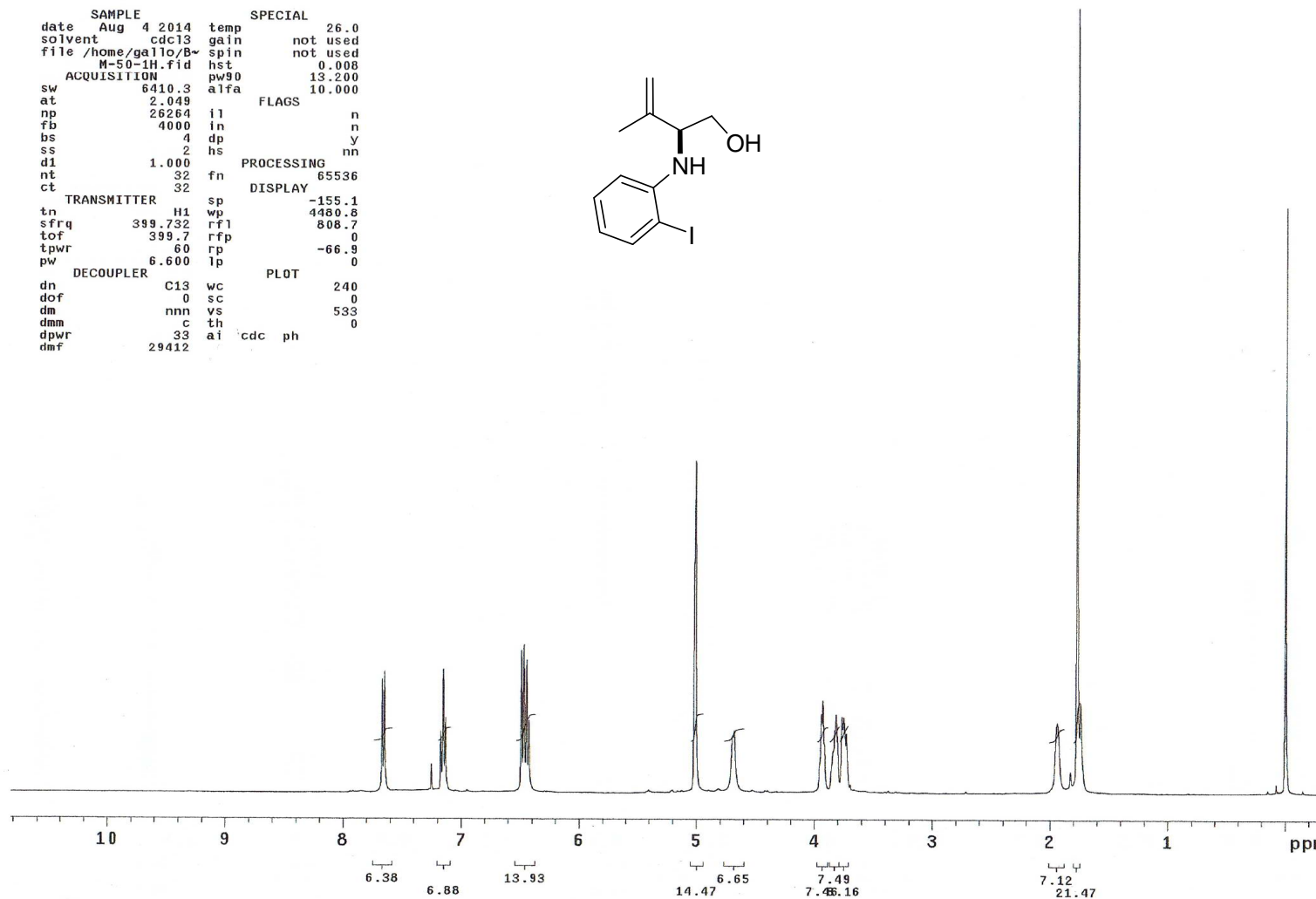
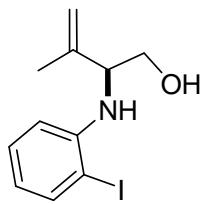
N-benzyl-4-(4-(prop-1-en-2-yl)oxazolidin-3-yl)benzamide (1i): HR-MS analysis



2-(2-iodophenylamino)-3-methylbut-3-en-1-ol (1k): ^1H NMR (400 MHz, CDCl_3)

```

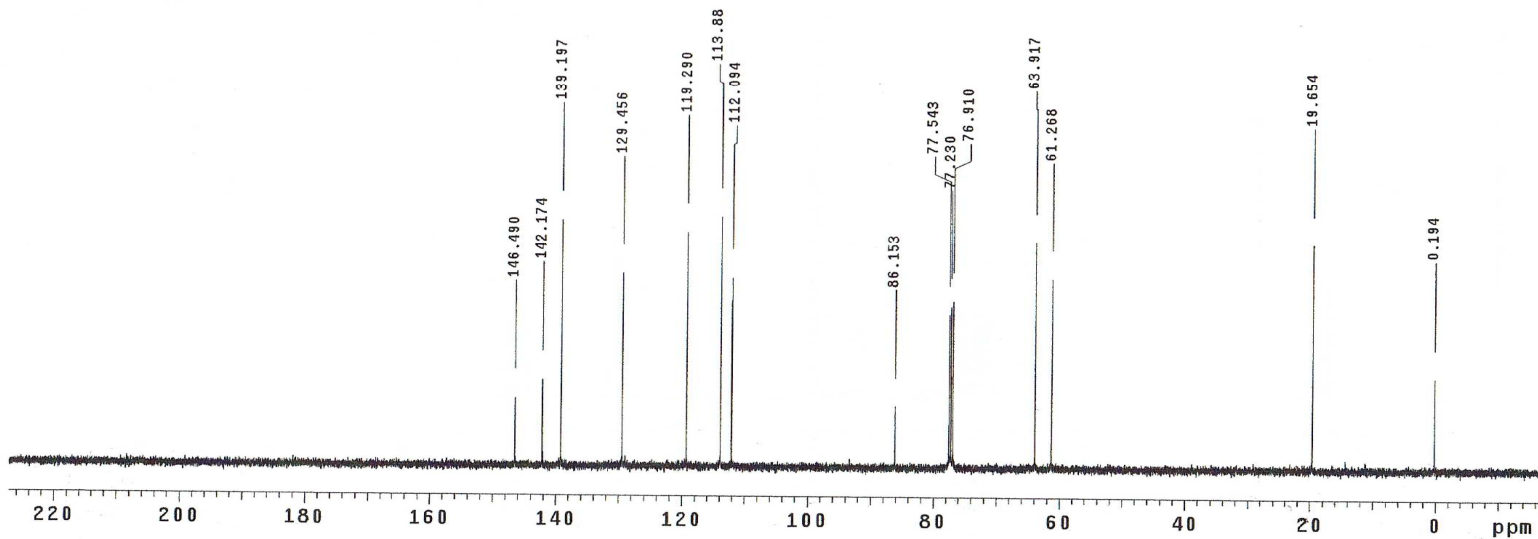
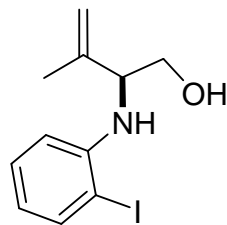
exp1 Proton
      SAMPLE
date   Aug 4 2014   temp   SPECIAL  26.0
solvent cdc13      gain   not used
file   /home/gallo/B~ spin   not used
      M-50-1H.fid  hst    0.008
ACQUISITION      pw90   13.200
sw      6410.3     alfa   10.000
at      2.049
np      26264     il     FLAGS   n
fb      4000      in     n
bs      4         dp     y
ss      2         hs     nn
d1      1.000
nt      32       fn     PROCESSING 65536
ct      32       DISPLAY
TRANSMITTER      sp     -155.1
tn      H1       wp     4480.8
sfrq    399.732 rfl    808.7
tof     399.7   rfp     0
tpwr    60      rp     -66.9
pw      6.600   lp     0
DECOUPLER C13    wc     PLOT   240
dn      0       sc     0
dm      nnn    vs     533
dmm     c      th     0
dpwr    33     ai     cdc ph
dmf     29412
    
```



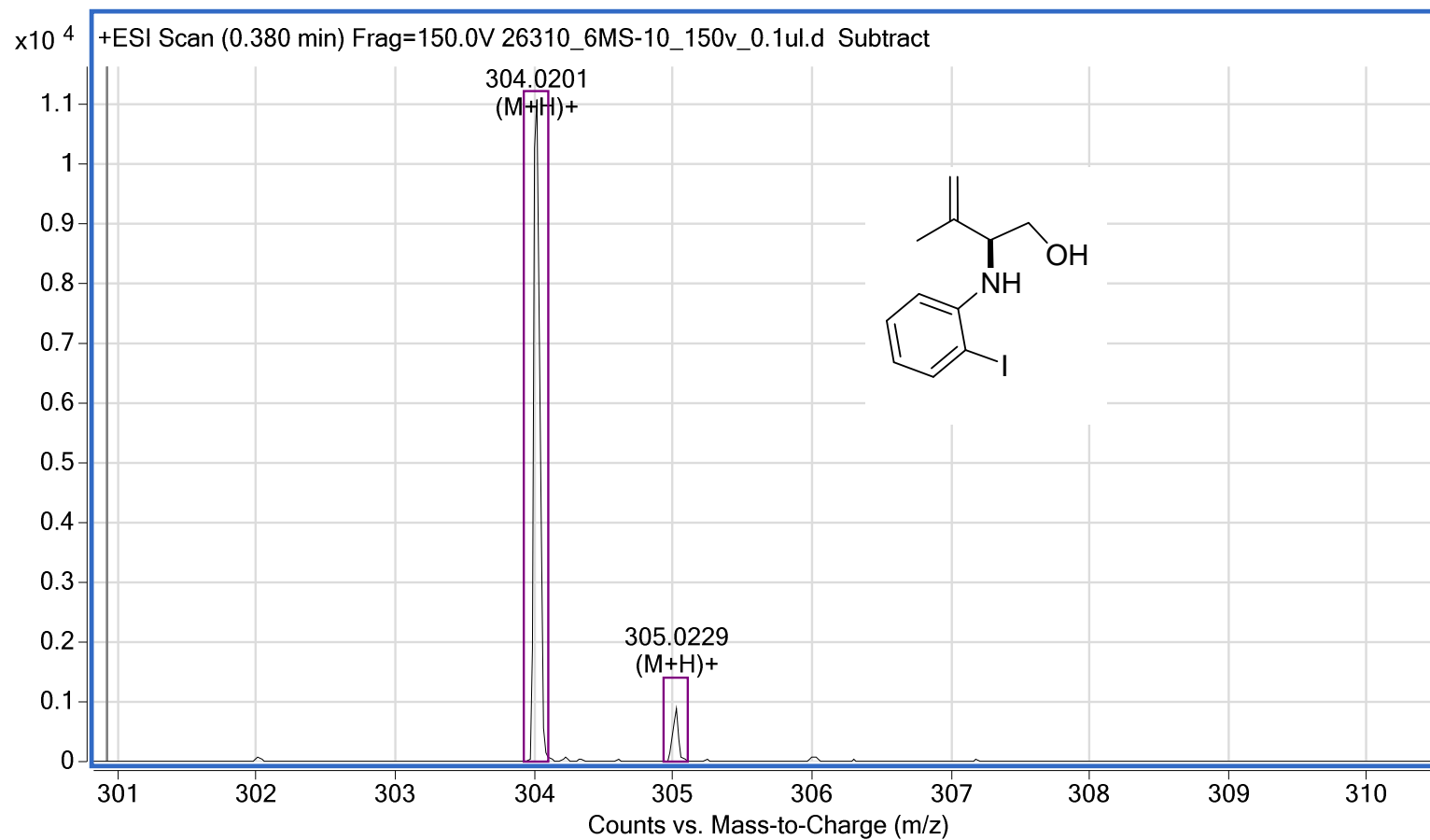
2-(2-iodophenylamino)-3-methylbut-3-en-1-ol (1k): ^{13}C NMR (100 MHz, CDCl_3)

```

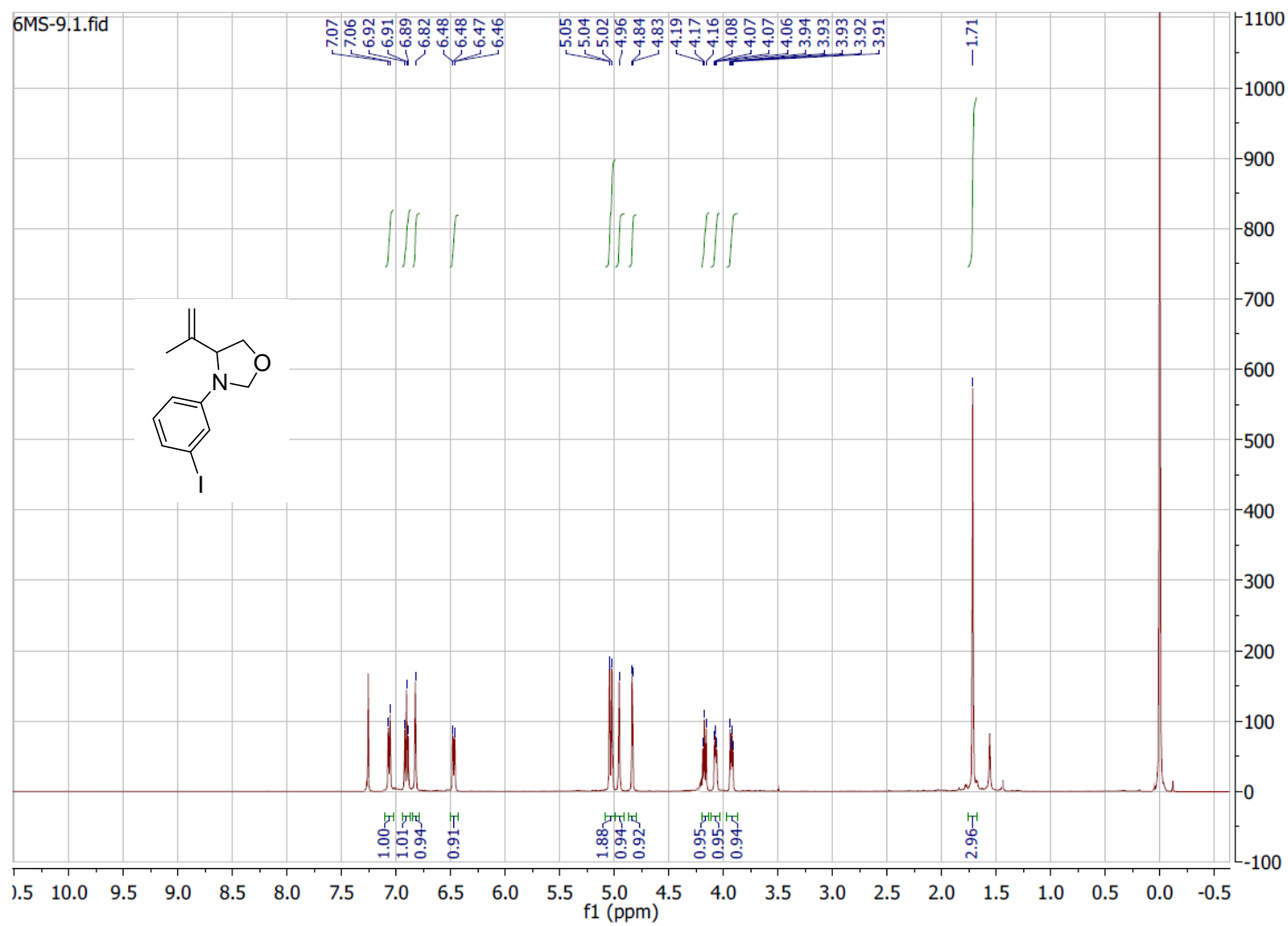
exp1 Carbon
SAMPLE
date Aug 4 2014 temp 26.0
solvent cdc13 gain 30
file exp spin not used
ACQUISITION
sw 24509.8 pw90 8.300
at 1.300 alfa 10.000
np 63750
fb 17000
bs 16
dl 1.000 dp
nt 4000
ct 304
TRANSMITTER lb 0.50
tn C13 fn not used
sfrq 100.523 DISPLAY
tof 1027.9 sp -1683.7
tpwr 55 wp 24509.1
pw 4.150 rfl 9447.0
DECOUPLER H1 rfp 7762.6
dn H1 rp 77.0
dof 0 lp 0
dm YYY PLOT
dmm w wc 240
dpwr 41 sc 0
dmf 9648 vs 23995
          th 9
          ai cdc ph
    
```



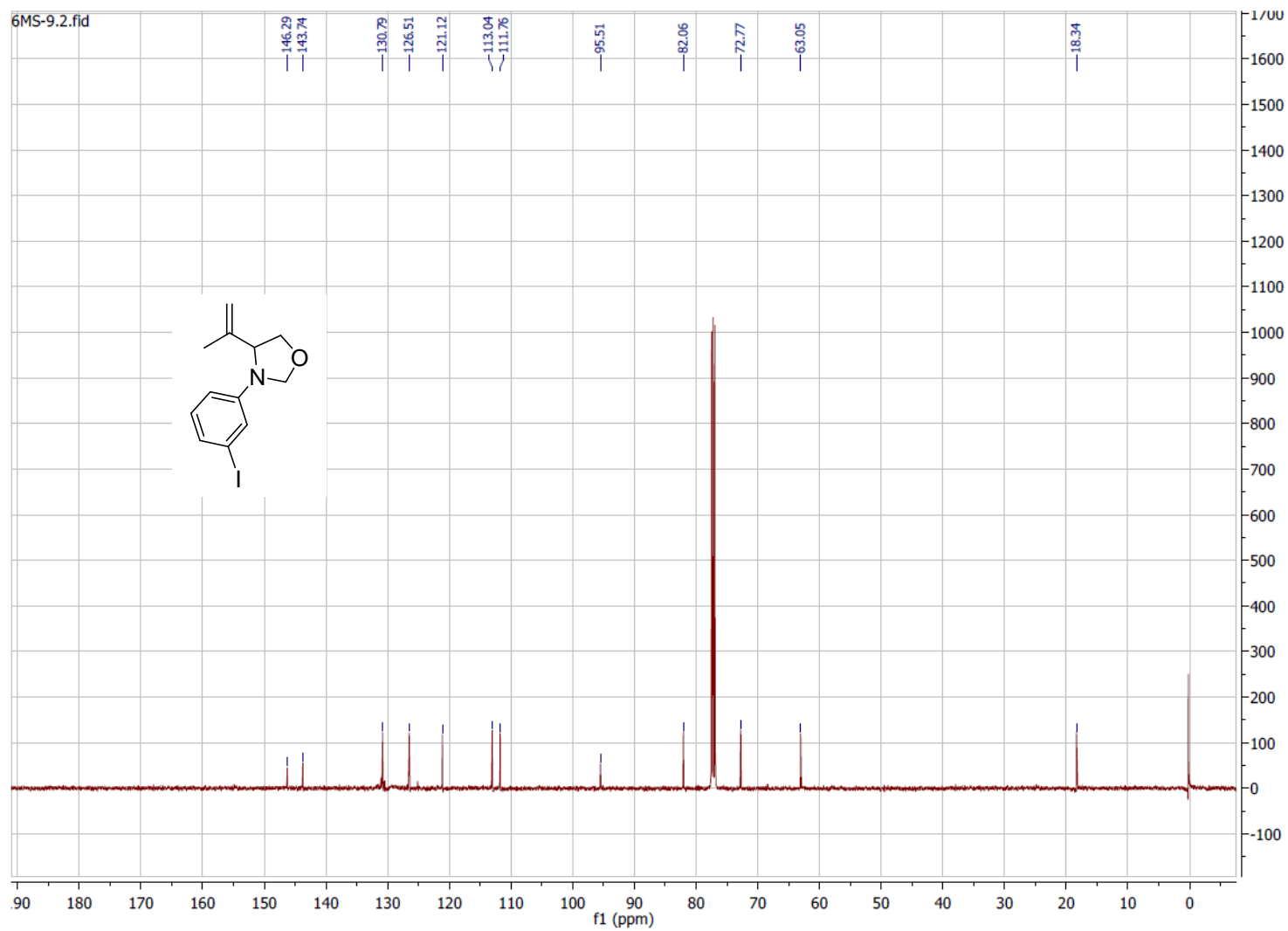
2-(2-iodophenylamino)-3-methylbut-3-en-1-ol (1k): HR-MS analysis



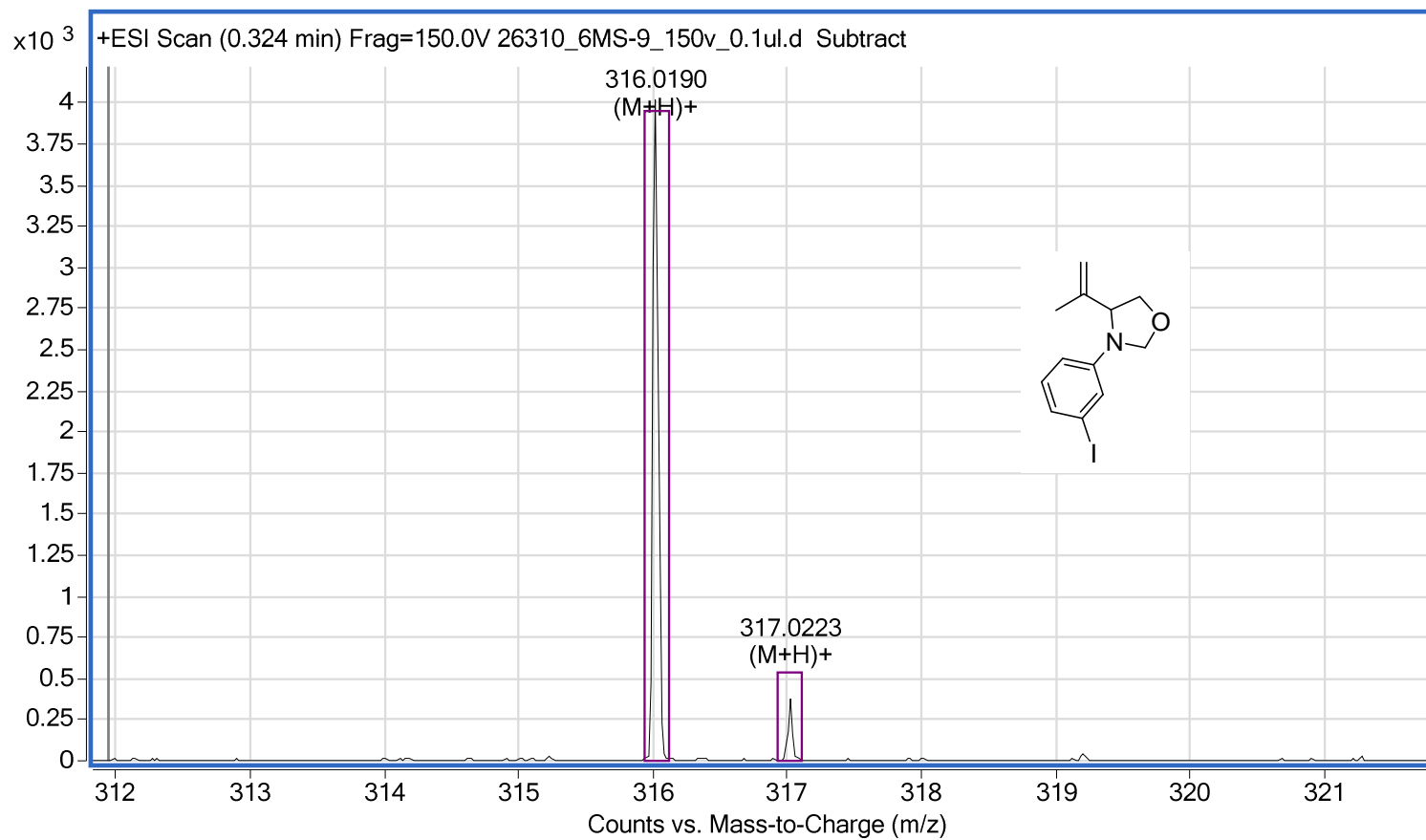
3-(3-iodophenyl)-4-(prop-1-en-2-yl)oxazolidine (11): ^1H NMR (400 MHz, CDCl_3)



3-(3-iodophenyl)-4-(prop-1-en-2-yl)oxazolidine (1): ^{13}C NMR (100 MHz, CDCl_3)



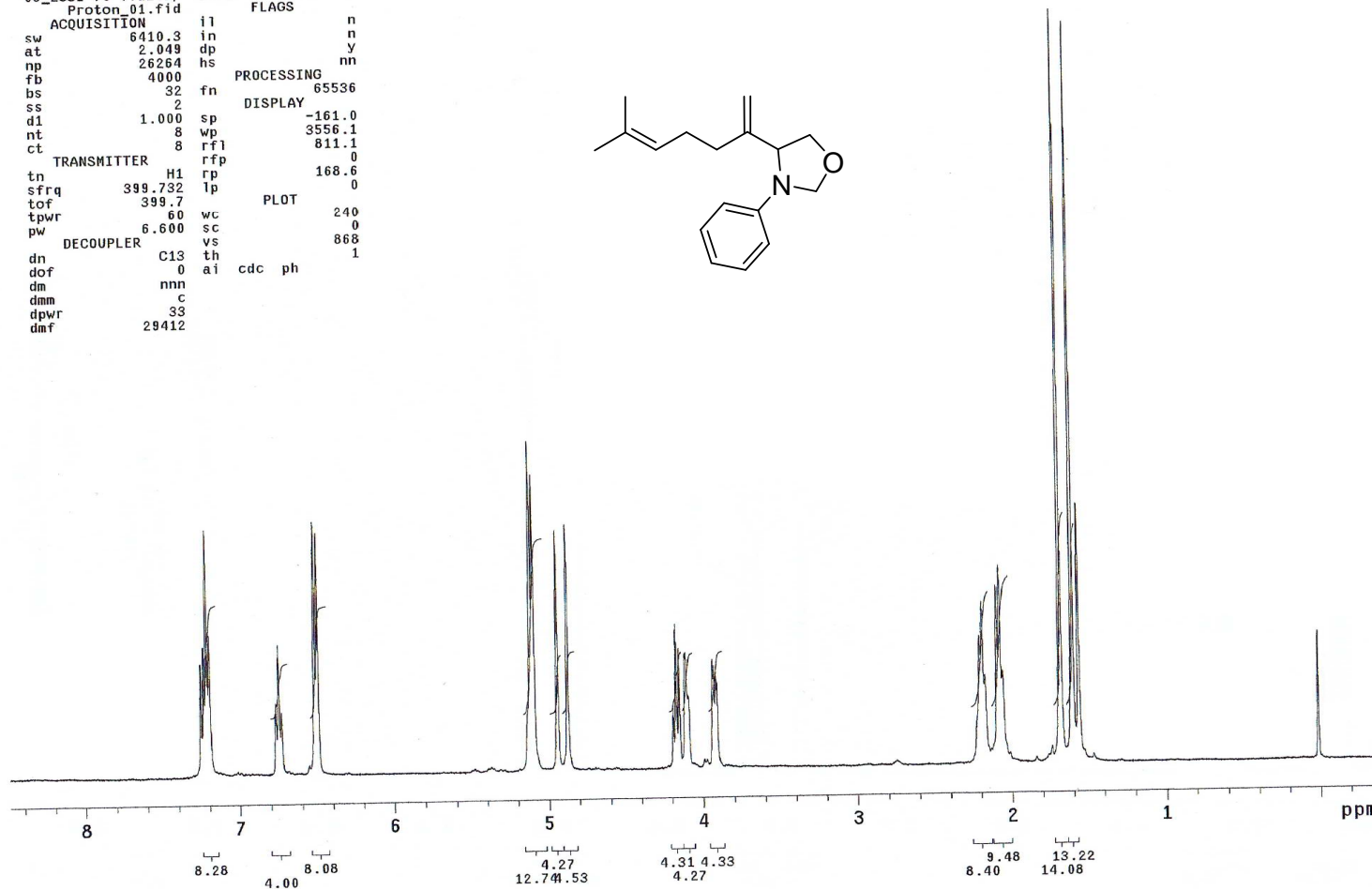
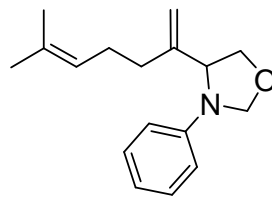
3-(3-iodophenyl)-4-(prop-1-en-2-yl)oxazolidine (11): HR-MS analysis



4-(6-methylhepta-1,5-dien-2-yl)-3-phenyloxazolidine (2a): ¹H NMR (400 MHz, CDCl₃)

```

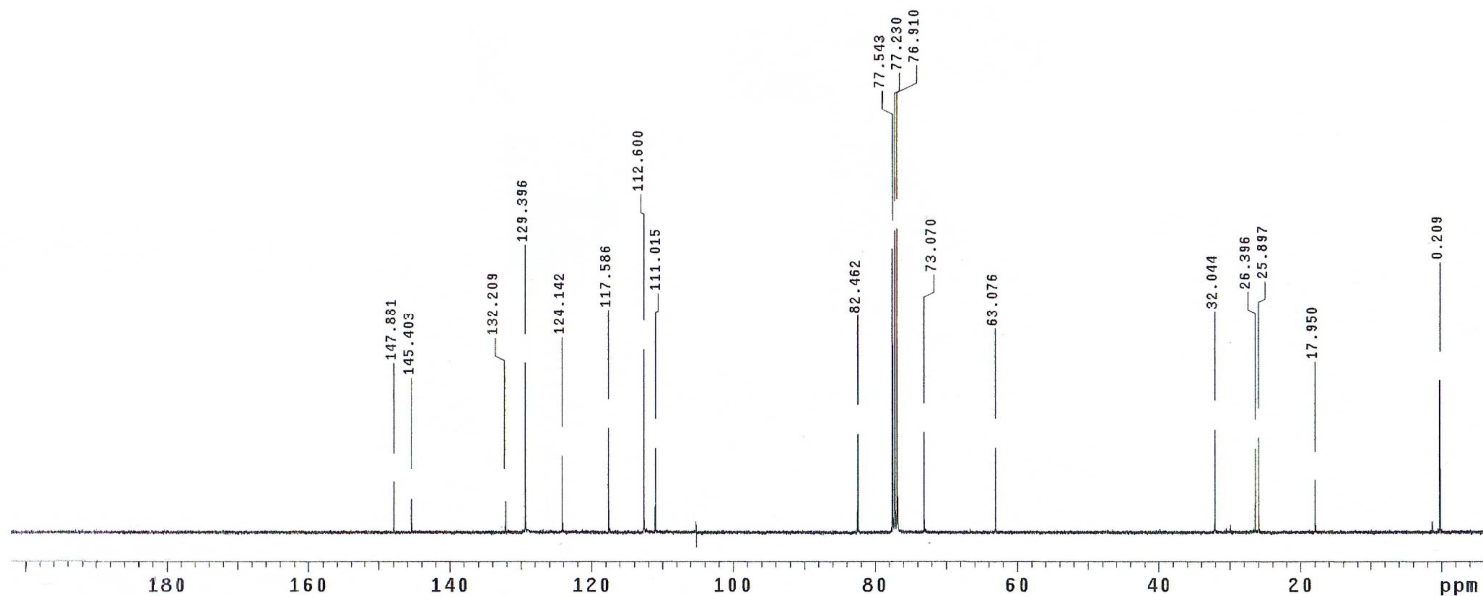
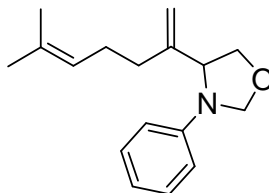
exp21 Proton
SAMPLE
date Jun 5 2015 temp 25.0
solvent cdcl3 gain not used
file /home/gallo/v~ spin not used
nmrsys/data/auto_2~ hst 0.008
015.03.31/s_201506~ pw90 13.200
05_2CSL-79-TT1201/~ alfa 10.000
Proton_01.fid
ACQUISITION
sw 6410.3 in n
at 2.049 dp n
np 26264 hs y
fb 4000
bs 32 fn PROCESSING 65536
ss 2
d1 1.000 sp DISPLAY -161.0
nt 8 wp 3556.1
ct 8 rfl 811.1
TRANSMITTER
tn H1 rfp 0
sfrq 399.732 rp 168.6
tof 399.7 lp 0
tpwr 60 wc PLOT 240
pw 6.600 vs 868
DECOUPLER C13 th 1
dn 0 ai cdc ph
dm nnn
dmm c
dpwr 33
dmf 29412
    
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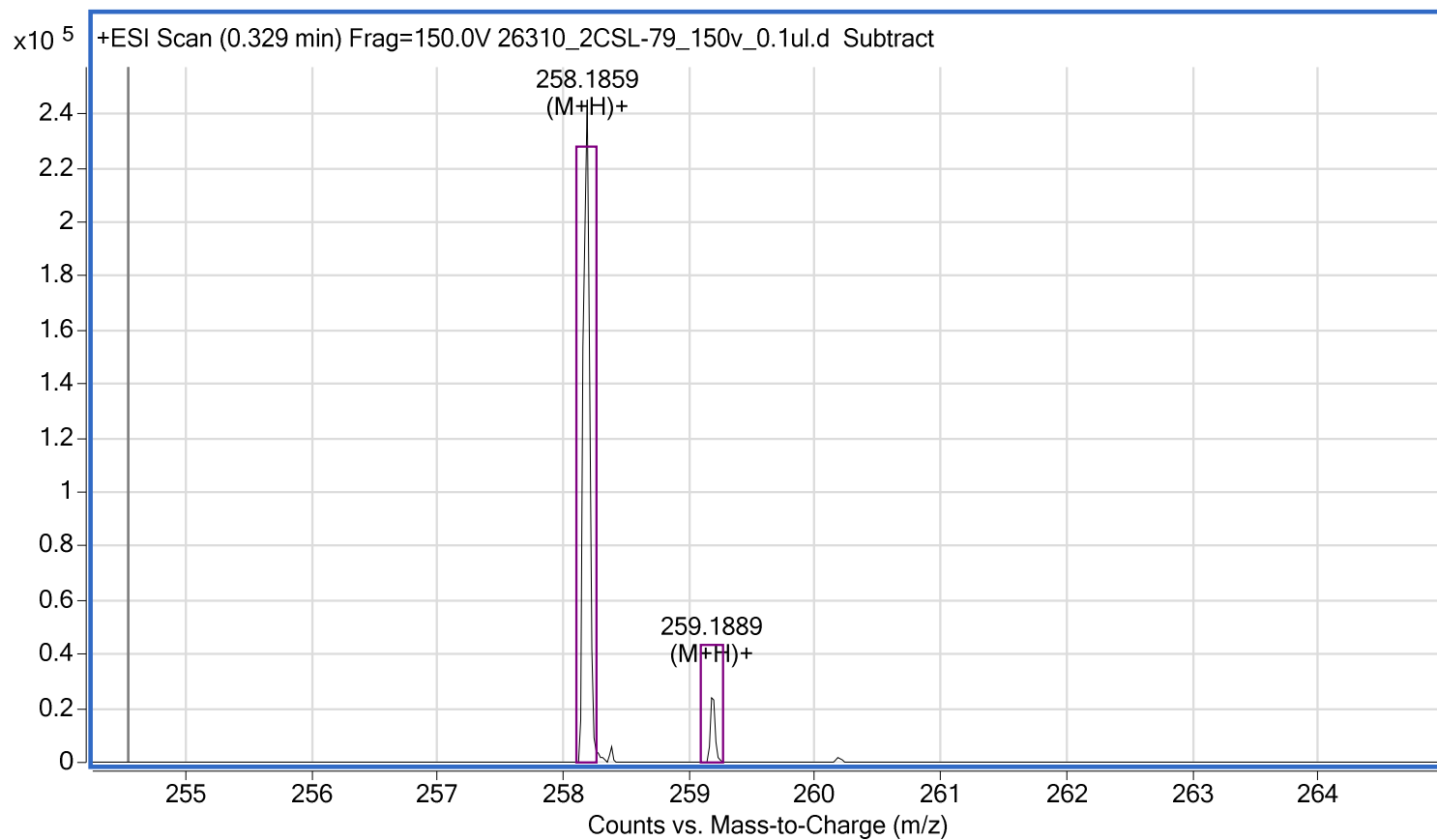
4-(6-methylhepta-1,5-dien-2-yl)-3-phenyloxazolidine (2a): ¹³C NMR (100 MHz, CDCl₃)

```

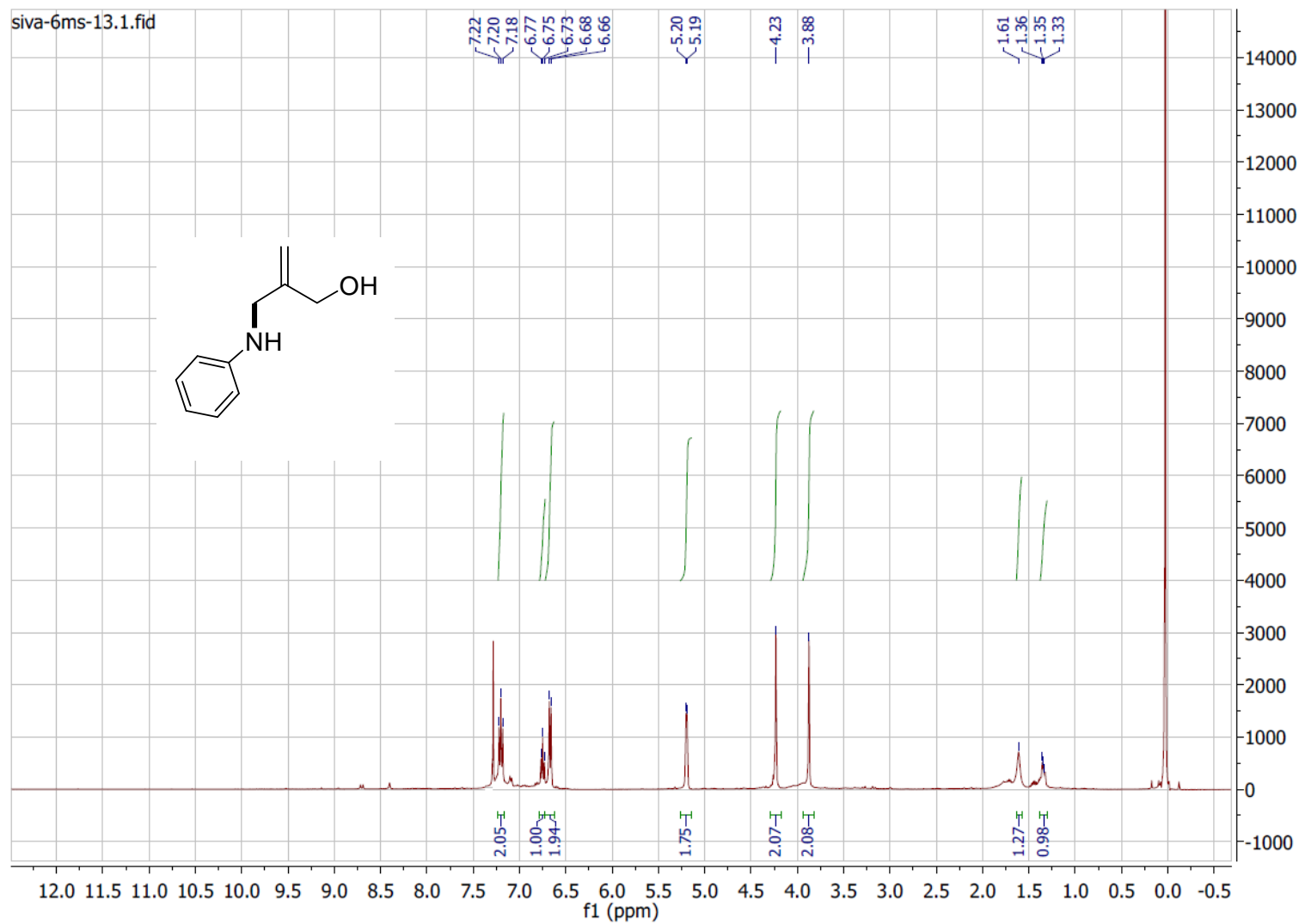
exp21 Carbon
SAMPLE
date Jun 5 2015 temp SPECIAL 25.0
solvent cdc13 gain 30
file exp spin not used
ACQUISITION
sw 24509.8 hst 0.008
at 1.300 pw90 5.300
np 63750 alfa 10.000
fb 17000 i1 n
bs 32 in n
d1 1.000 dp y
nt 10000 hs nn
ct 10000
TRANSMITTER
tn C13 lb 0.50
sfrq 100.523 fn not used
tof 1027.9 sp DISPLAY -622.3
tpwr 55 wp 20838.2
pw 4.150 rfl 9442.5
DECOUPLER
dn H1 rfp 7762.6
dof 0 rp 60.5
dm yyw lp 0
dmm w PLOT 240
dpwr 41 sc 0
dmf 9648 vs 461966
ai cdc ph 8
  
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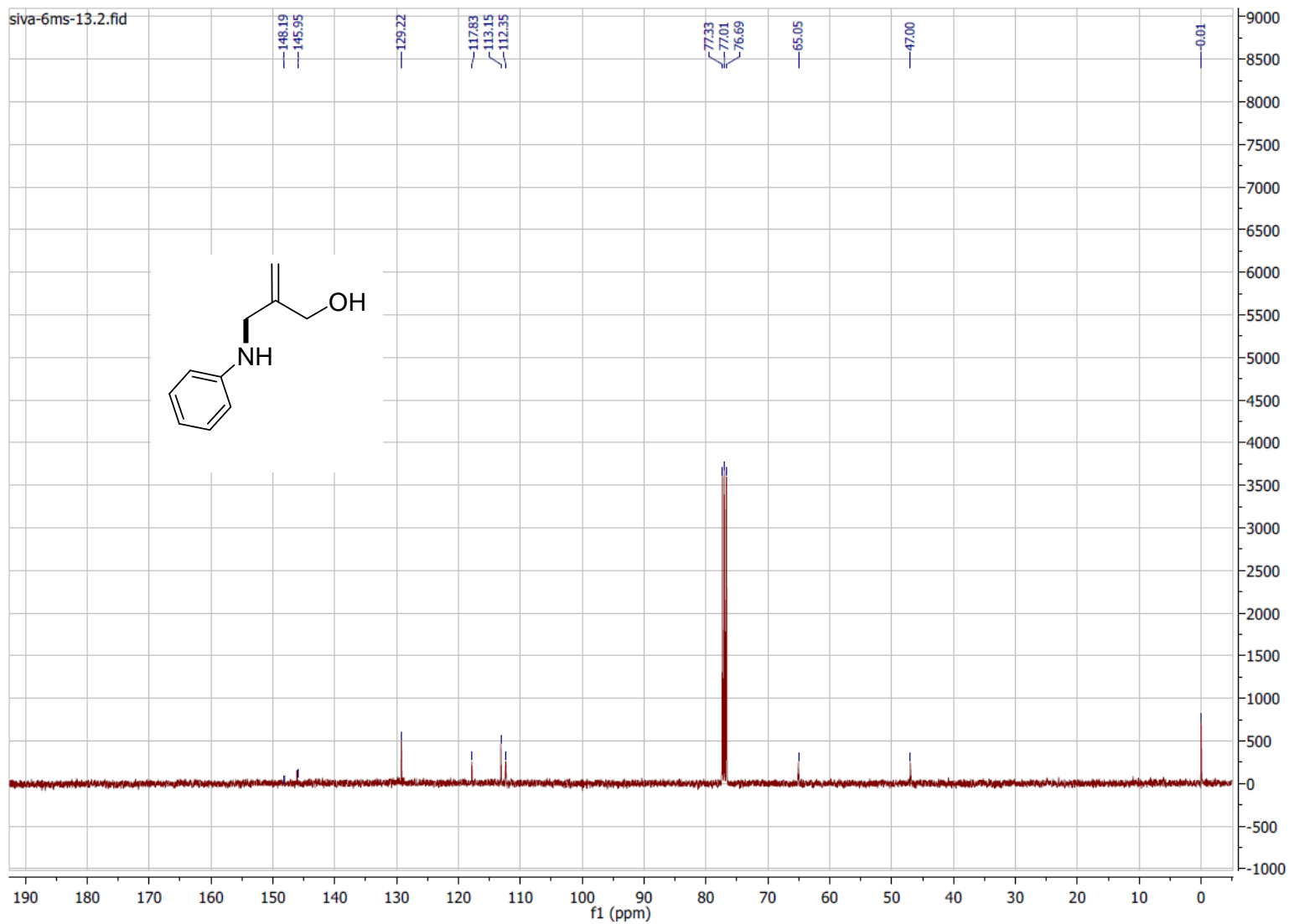
4-(6-methylhepta-1,5-dien-2-yl)-3-phenyloxazolidine (2a): HR-MS analysis



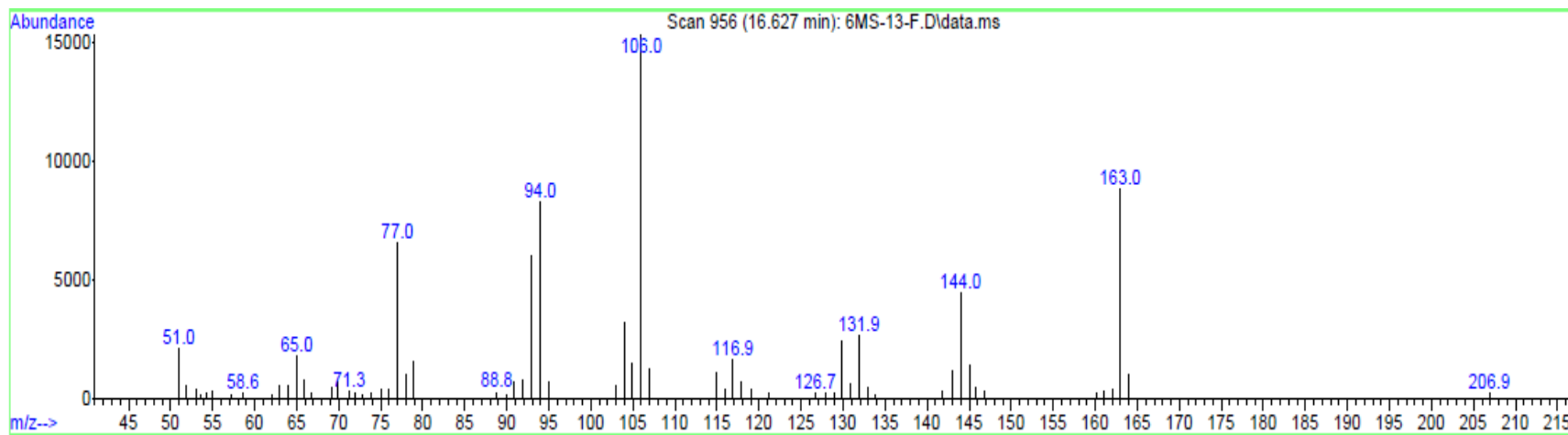
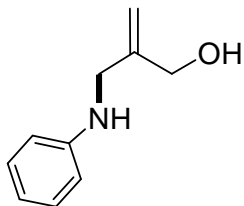
2-Phenylaminomethyl-prop-2-en-1-ol (3a): ^1H NMR (400 MHz, CDCl_3)



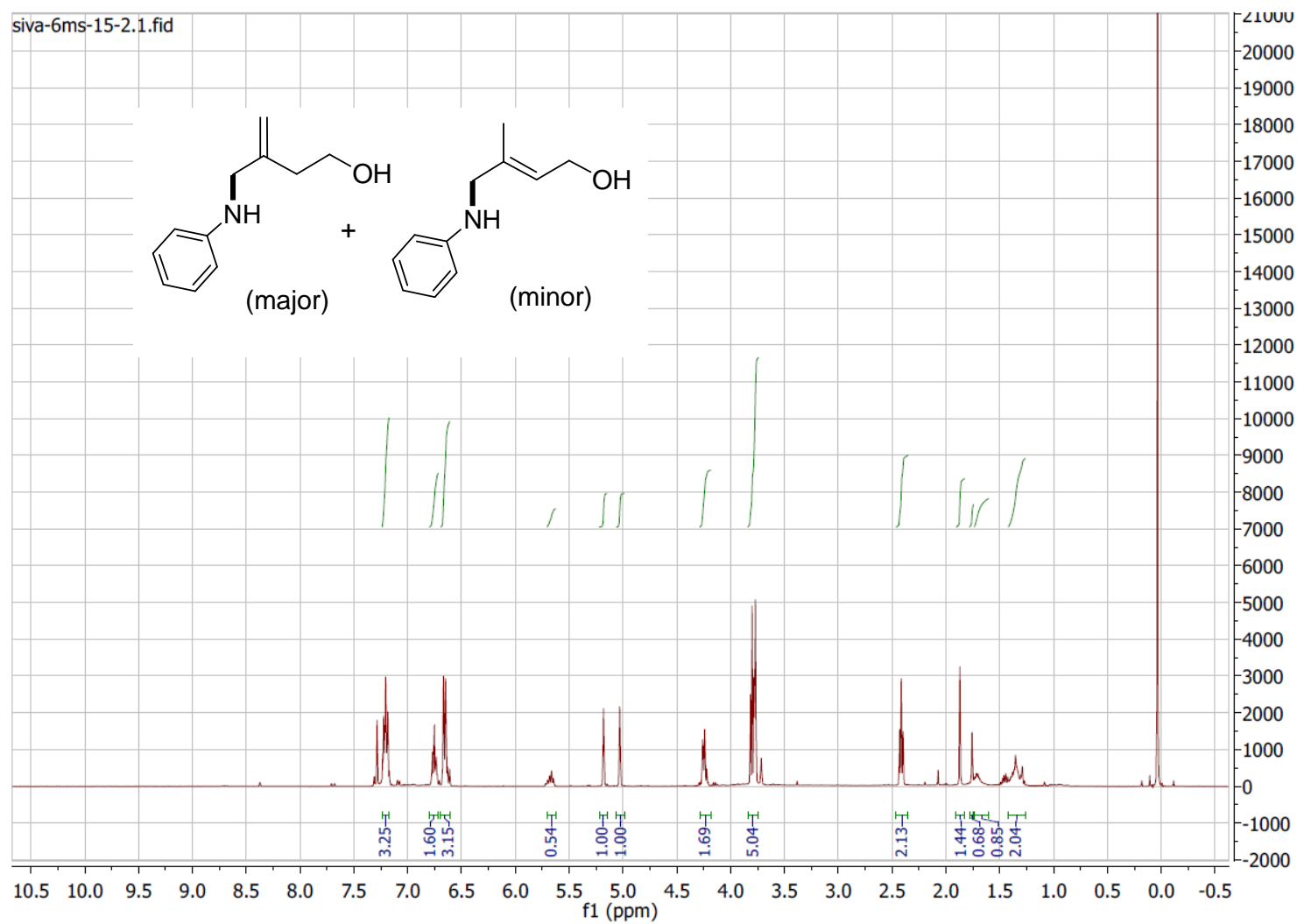
2-Phenylaminomethyl-prop-2-en-1-ol (3a): ^{13}C NMR (100 MHz, CDCl_3)



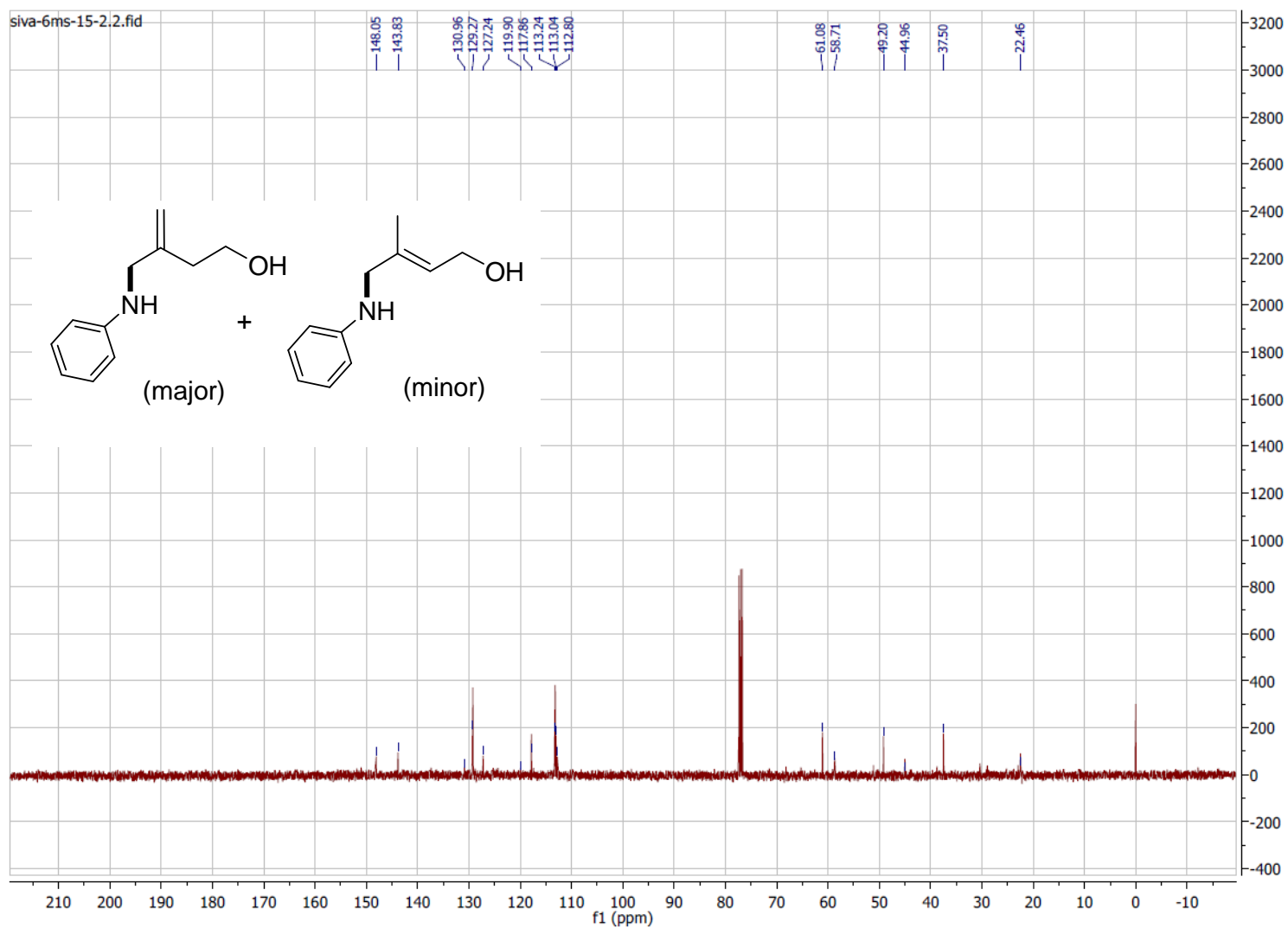
2-Phenylaminomethyl-prop-2-en-1-ol (3a): GC-MS analysis



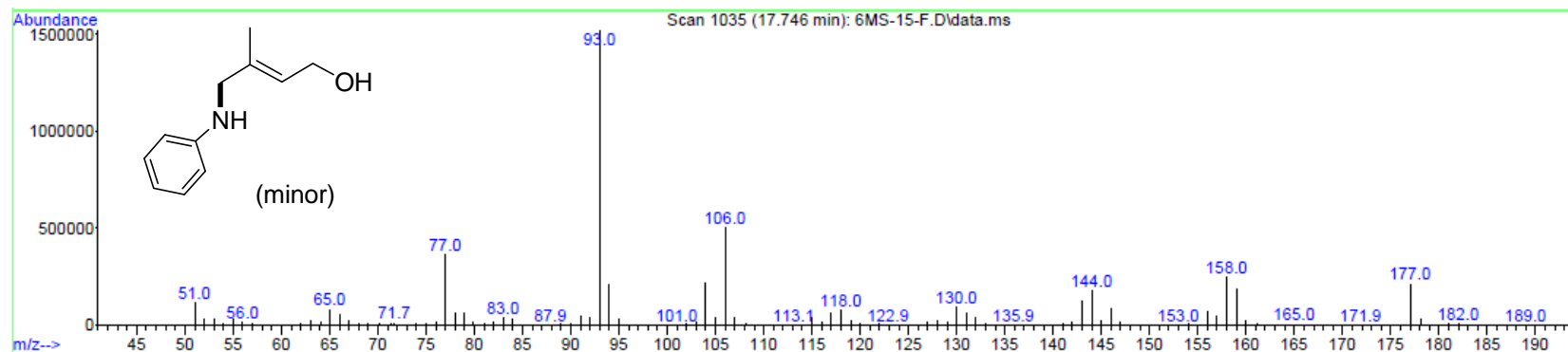
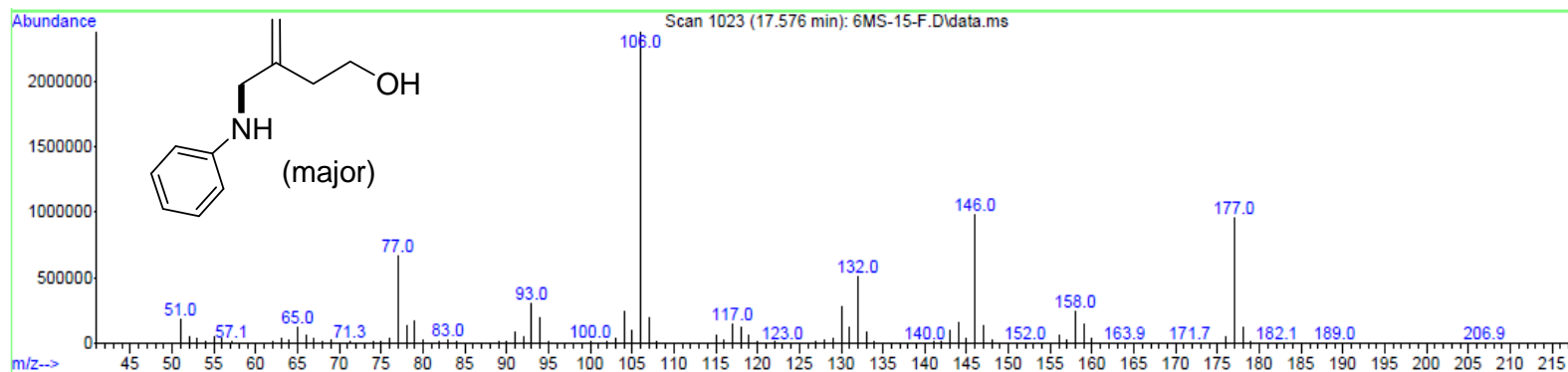
3-Phenylaminomethyl-but-3-en-1-ol and 3-Methyl-4-phenylamino-but-2-en-1-ol (4a+4a'): ^1H NMR (400 MHz, CDCl_3)



3-Phenylaminomethyl-but-3-en-1-ol and 3-Methyl-4-phenylamino-but-2-en-1-ol (4a+4a'): ^{13}C NMR (100 MHz, CDCl_3)



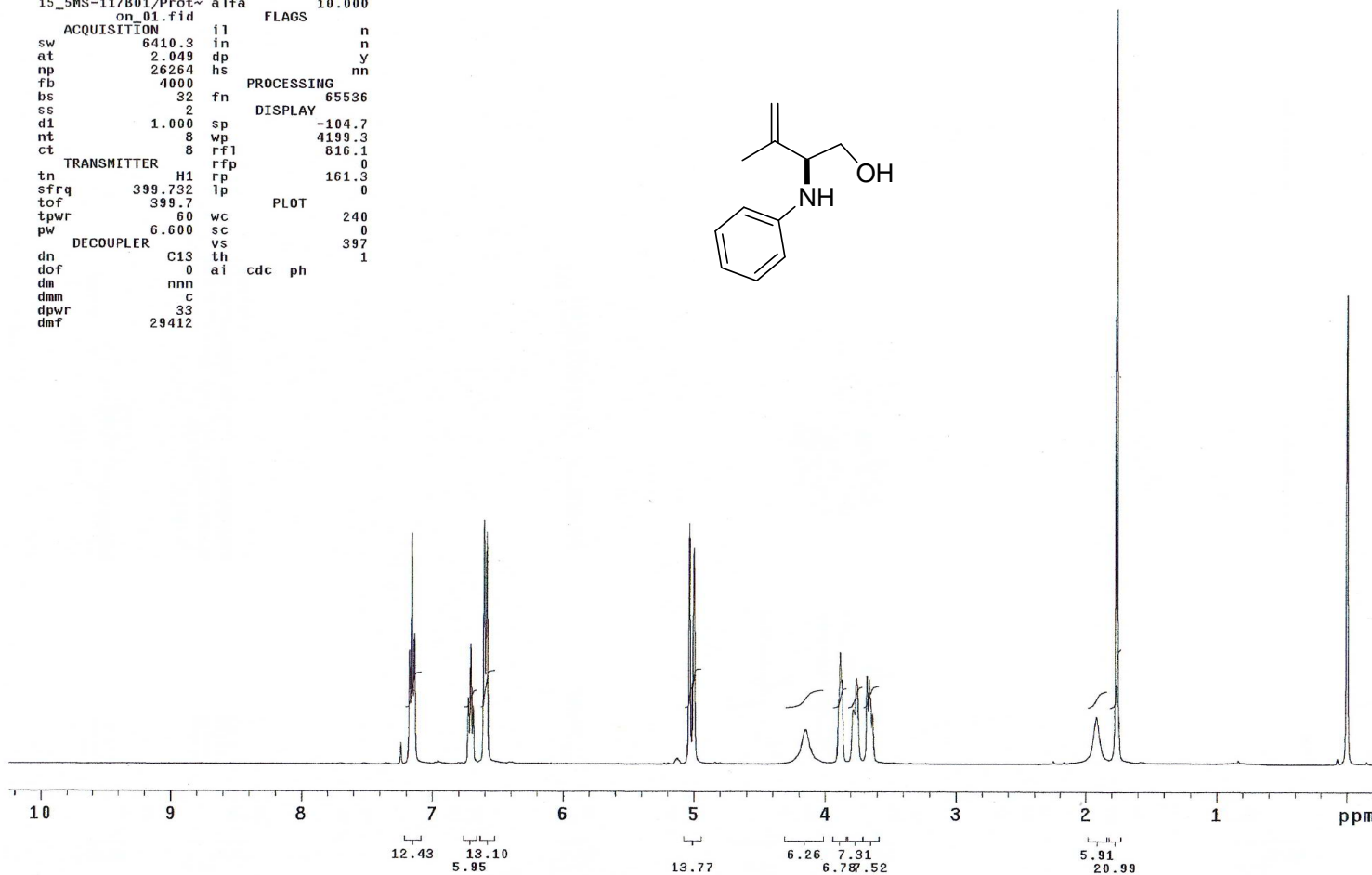
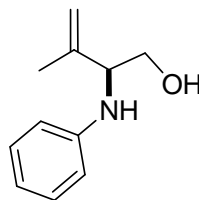
3-Phenylaminomethyl-but-3-en-1-ol and 3-Methyl-4-phenylamino-but-2-en-1-ol (4a+4a'): GC-MS analysis



3-methyl-2-(phenylamino)but-3-en-1-ol (1a'): ¹H NMR (400 MHz, CDCl₃)

exp21 Proton

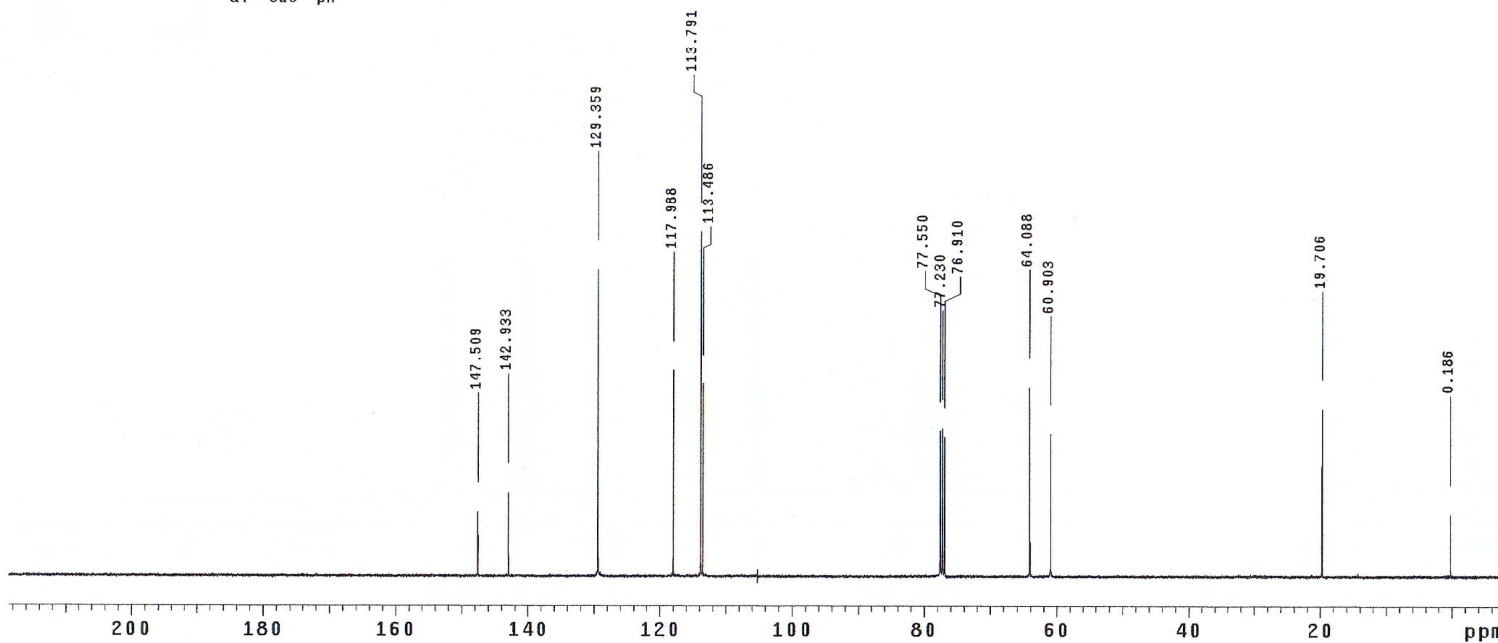
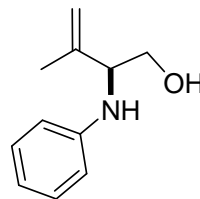
SAMPLE		SPECIAL	
date	May 15 2015	temp	25.0
solvent	cdc13	gain	not used
file	/home/gallo/v~	spin	not used
nmr	sys/data/auto_2~	hst	0.008
015.03.31/s_201505~		pw90	13.200
15_5MS-117B01/Prot~		alfa	10.000
on_01.fid		FLAGS	
ACQUISITION		PROCESSING	
sw	6410.3	il	n
at	2.049	in	n
np	26264	dp	y
fb	4000	hs	nn
bs	32	fn	65536
ss	2	DISPLAY	
d1	1.000	sp	-104.7
nt	8	wp	4199.3
ct	8	rfl	816.1
TRANSMITTER		rfp	0
tn	H1	rp	161.3
sfrq	399.732	lp	0
tof	399.7	PLOT	
tpwr	60	wc	240
pw	6.600	sc	0
DECOUPLER		vs	397
dn	C13	th	1
dof	0	ai	cdc ph
dm	nnn		
dmm	c		
dpwr	33		
dmf	29412		



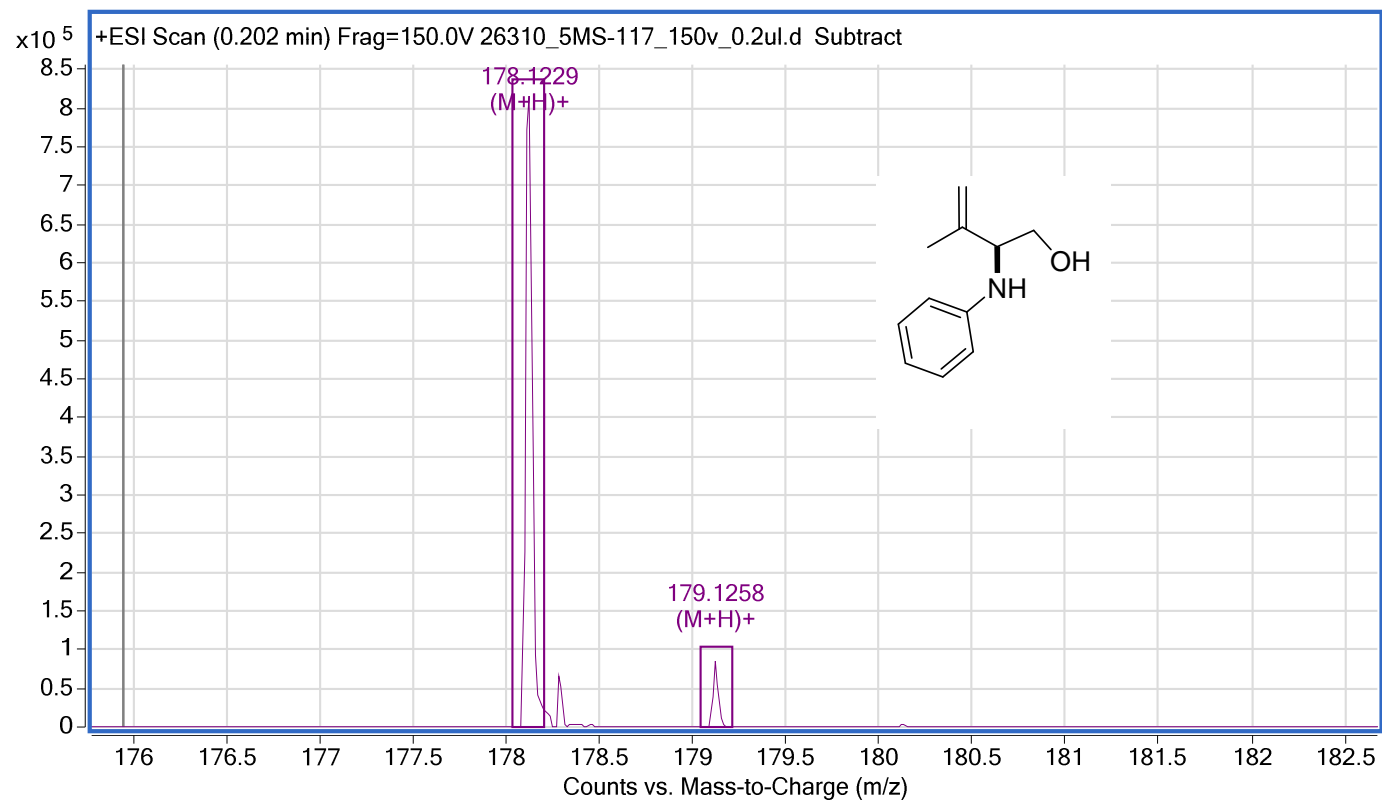
3-methyl-2-(phenylamino)but-3-en-1-ol (1a'): ^{13}C NMR (100 MHz, CDCl_3)

exp21 Carbon

SAMPLE		SPECIAL	
date	May 15 2015	temp	25.0
solvent	cdc13	gain	30
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	24509.8	pw90	8.300
at	1.300	alfa	10.000
np	63750	FLAGS	
fb	17000	il	n
bs	32	in	n
d1	1.000	dp	y
nt	5000	hs	nn
ct	2592	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	fn	not used
sfrq	100.523	DISPLAY	
tof	1027.9	sp	-894.6
tpwr	55	wp	22871.0
pw	4.150	rfl	9447.0
DECOUPLER		rfp	7752.6
dn	H1	rp	70.8
dof	0	lp	0
dm	yyy	PLOT	
dmm	w	wc	240
dpwr	41	sc	0
dmf	9648	vs	197275
		th	
		ai	cdc ph

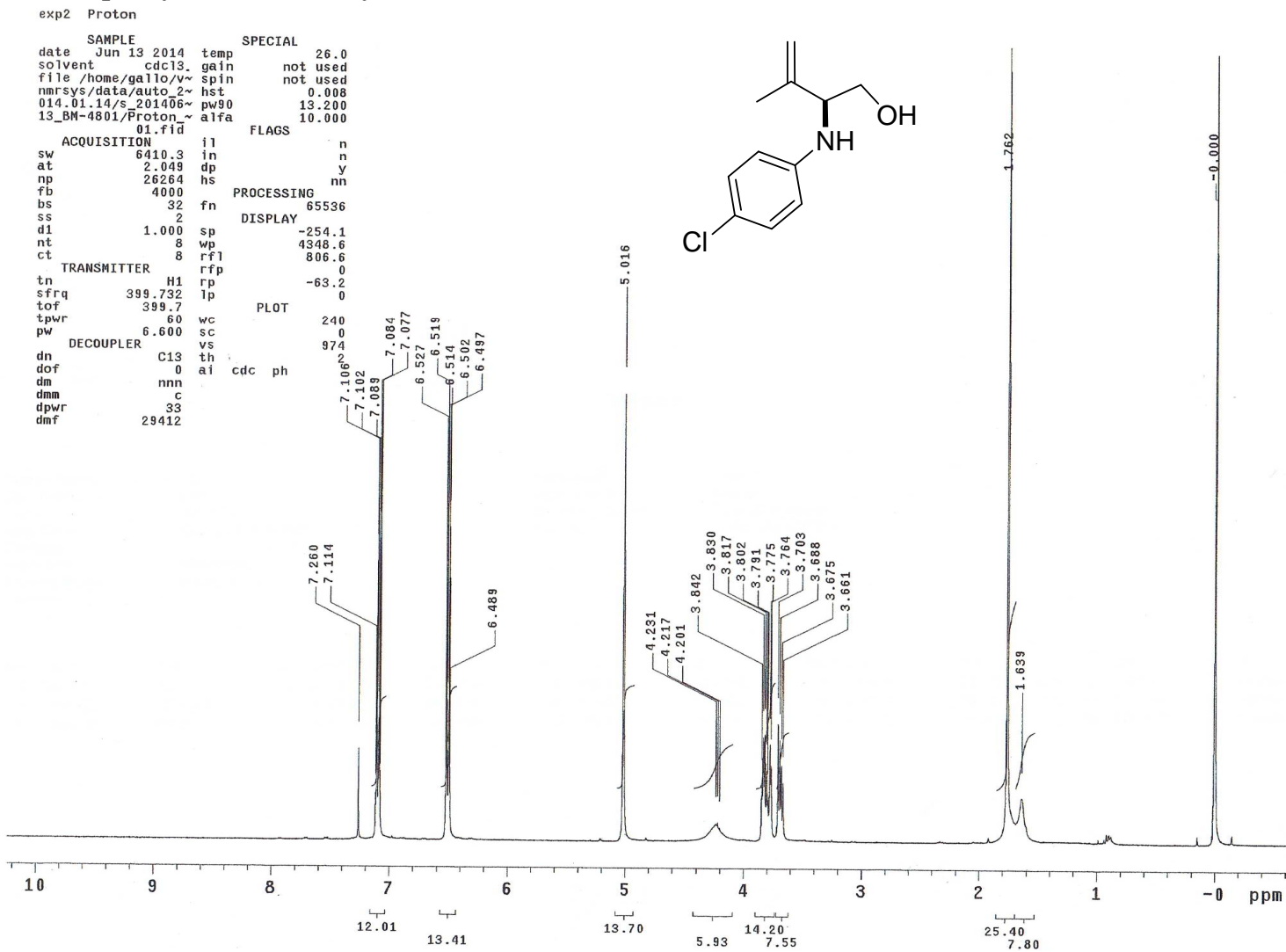


3-methyl-2-(phenylamino)but-3-en-1-ol (1a'): HR-MS analysis

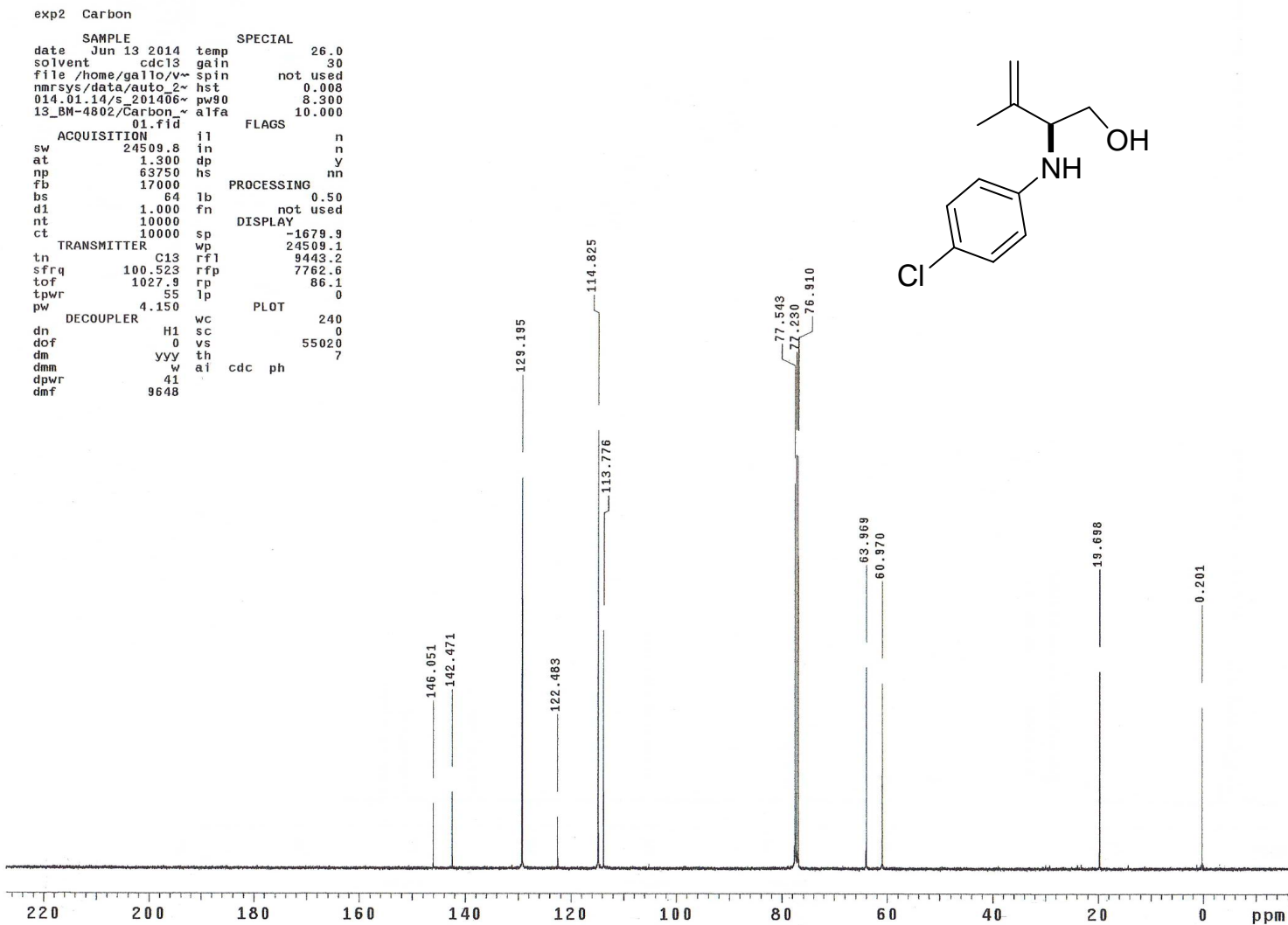


Formula (M),	Ion Formula,	Mass,	Calc Mass,	Calc m/z,	Diff (ppm),	Mass Match
C ₁₁ H ₁₅ N O,	C ₁₁ H ₁₆ N O,	177.1156,	177.1154,	178.1226,	1.4,	99.321

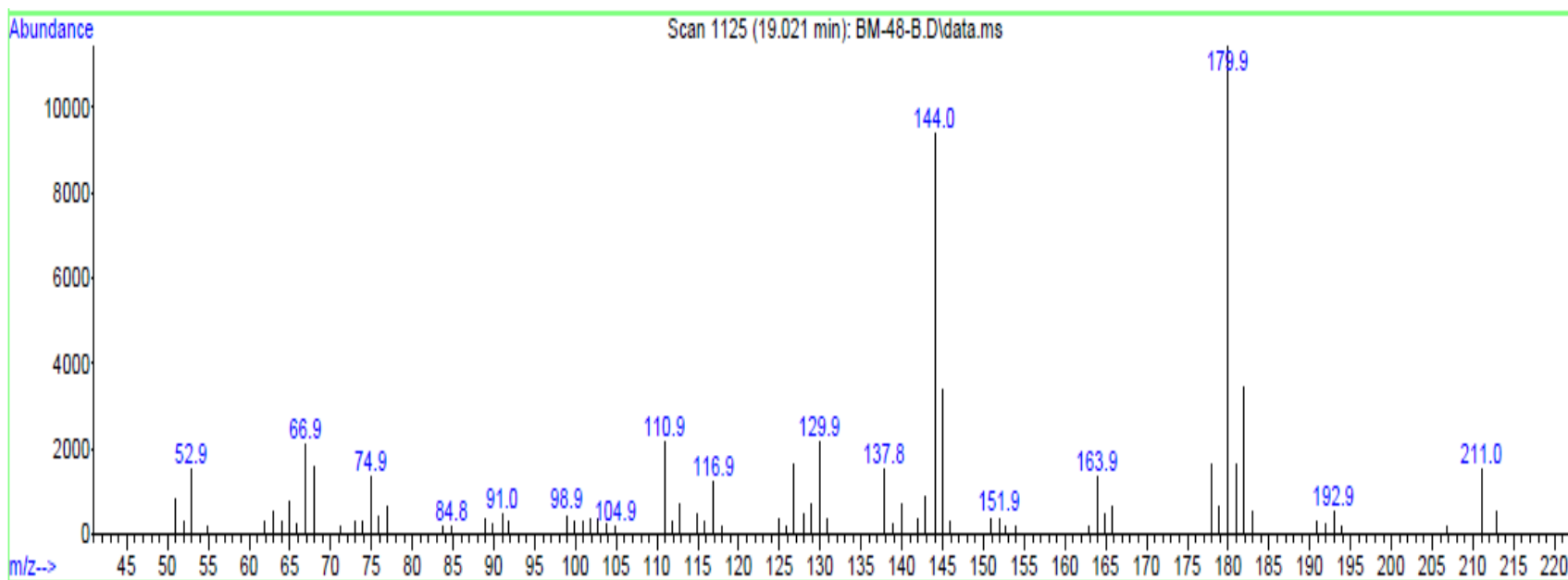
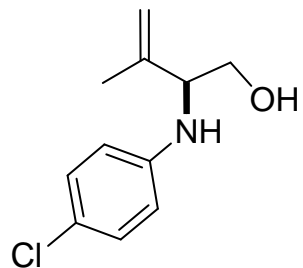
2-(4-chlorophenylamino)-3-methylbut-3-en-1-ol (1c'): ¹H NMR (400 MHz, CDCl₃)



2-(4-chlorophenylamino)-3-methylbut-3-en-1-ol (1c'): ¹³C NMR (100 MHz, CDCl₃)



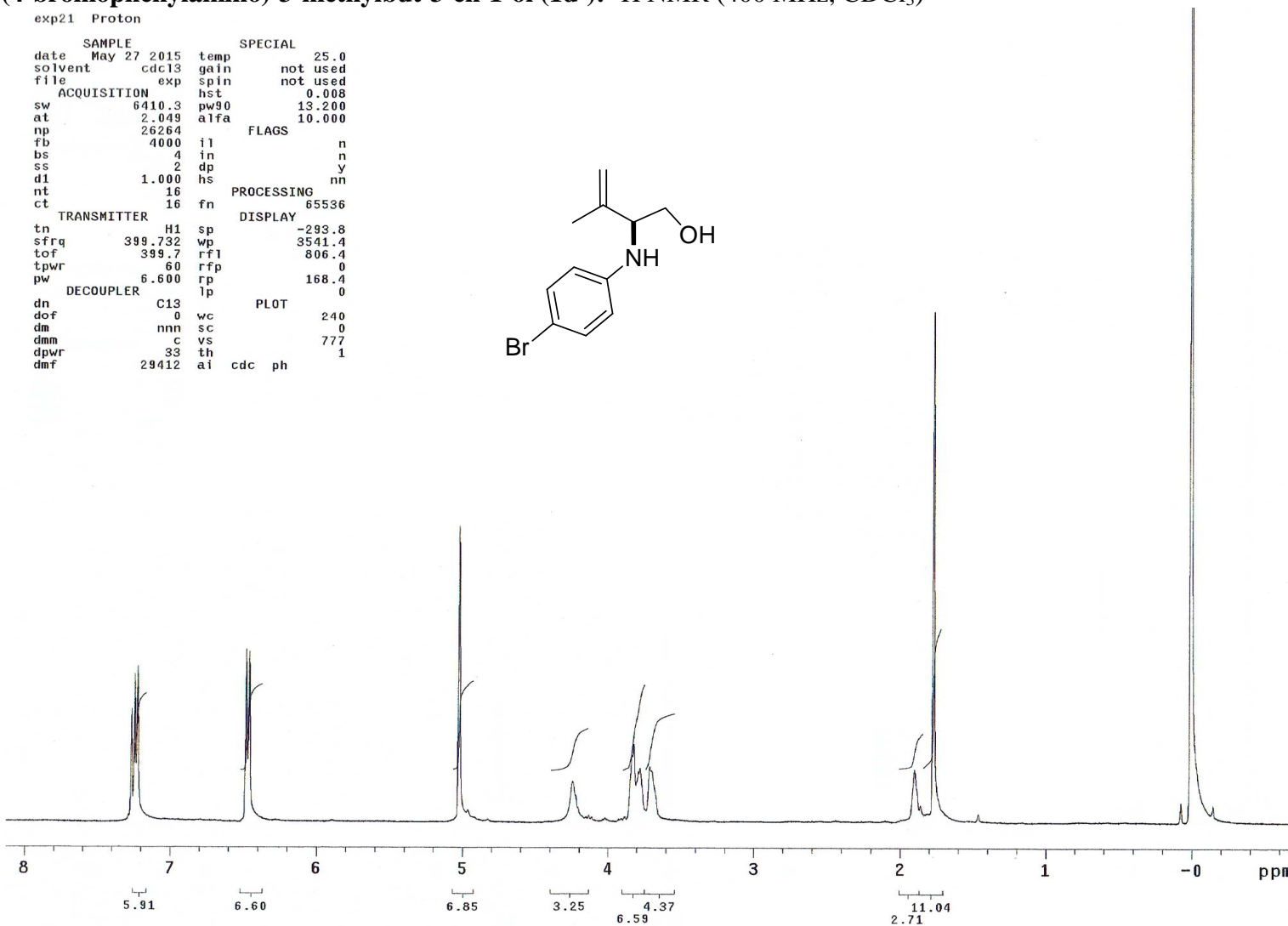
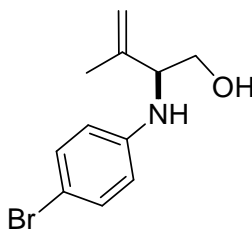
2-(4-chlorophenylamino)-3-methylbut-3-en-1-ol (1c'): GC-MS analysis



2-(4-bromophenylamino)-3-methylbut-3-en-1-ol (1d'): ¹H NMR (400 MHz, CDCl₃)

exp21 Proton

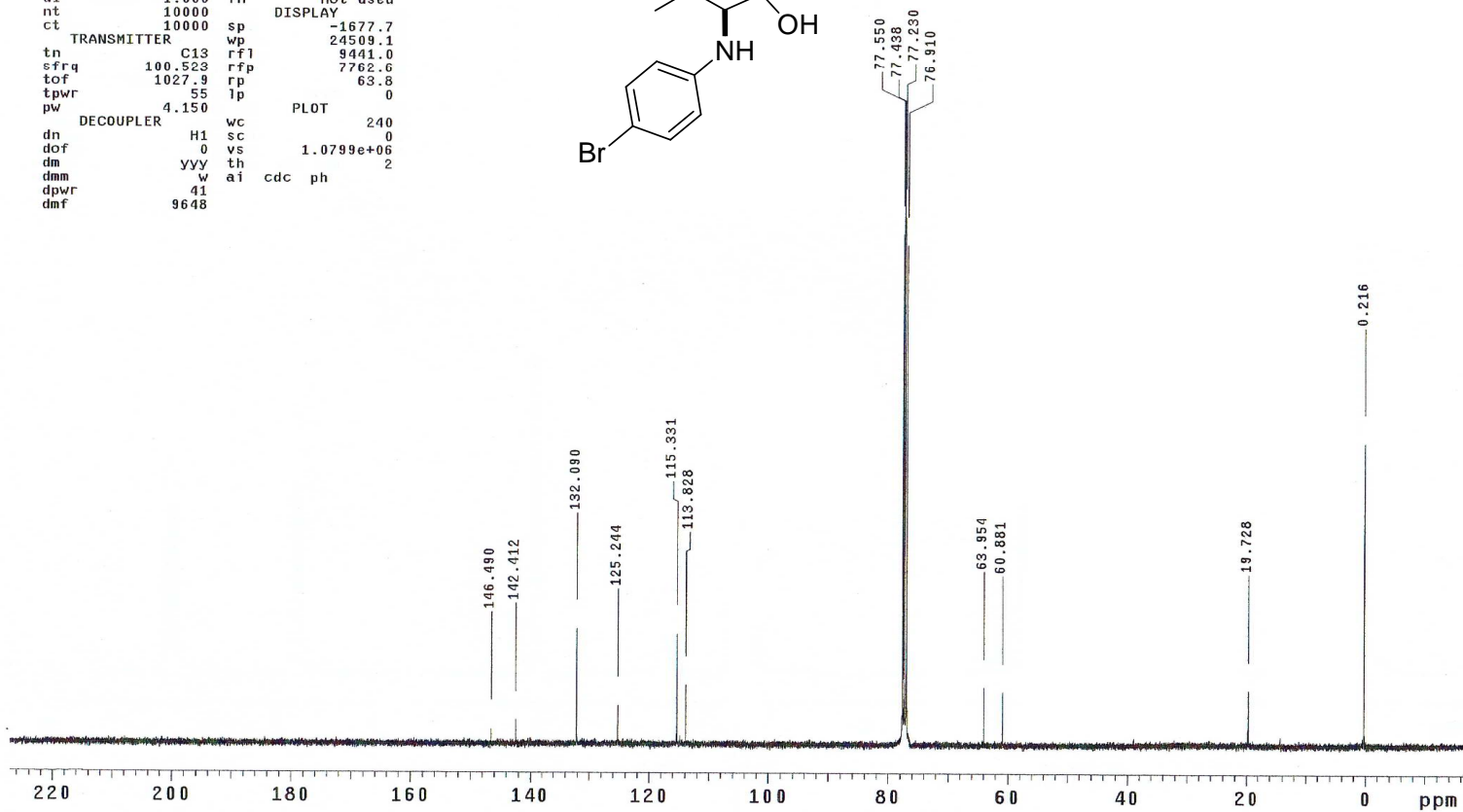
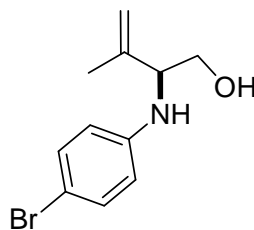
SAMPLE		SPECIAL	
date	May 27 2015	temp	25.0
solvent	cdc13	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	6410.3	pw90	13.200
at	2.049	alfa	10.000
np	26264	FLAGS	
fb	4000	il	n
bs	4	in	n
ss	2	dp	y
d1	1.000	hs	nn
nt	16	PROCESSING	
ct	16	fn	65536
TRANSMITTER		DISPLAY	
tn	H1	sp	-293.8
sfrq	399.732	wp	3541.4
tof	399.7	rfl	806.4
tpwr	60	rfp	0
pw	6.600	rp	168.4
DECOUPLER		lp	0
dn	C13	PLOT	
dof	0	wc	240
dm	nnn	sc	0
dmm	c	vs	777
dpwr	33	th	1
dmf	29412	ai	cdc ph



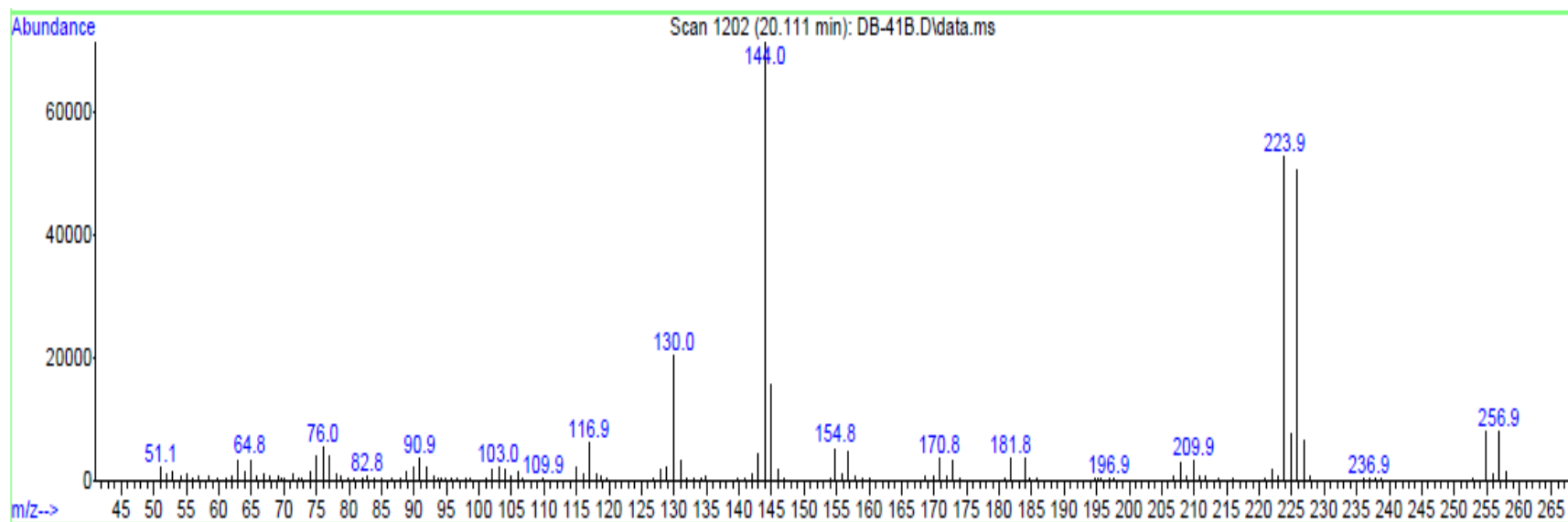
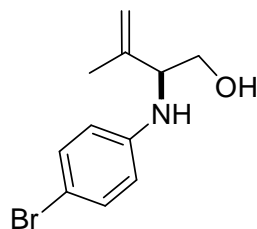
2-(4-bromophenylamino)-3-methylbut-3-en-1-ol (1d'): ¹³C NMR (100 MHz, CDCl₃)

```

exp21 Carbon
SAMPLE
date May 27 2015 temp 25.0
solvent cdc13 gain 30
file /home/gallo/v~ spin not used
nmrSYS/data/auto_2~ hst 0.008
015_03_31/s_201505~ pw90 8.300
27_DB-41B02/Carbon~ alfa 10.000
01.fid
ACQUISITION il n
sw 24509.8 in n
at 1.300 dp y
np 63750 hs nn
fb 17000
bs 64 lb 0.50
d1 1.000 fn not used
nt 10000 DISPLAY
ct 10000 sp -1677.7
TRANSMITTER wp 24509.1
tn C13 rfl 9441.0
sfrq 100.523 rfp 7762.6
tof 1027.9 rp 63.8
tpwr 55 lp 0
pw 4.150 PLOT
DECOUPLER wc 240
dn H1 sc 0
dof 0 vs 1.0799e+06
dm yyy th 2
dmm w ai cdc ph
dpwr 41
dmf 9648
    
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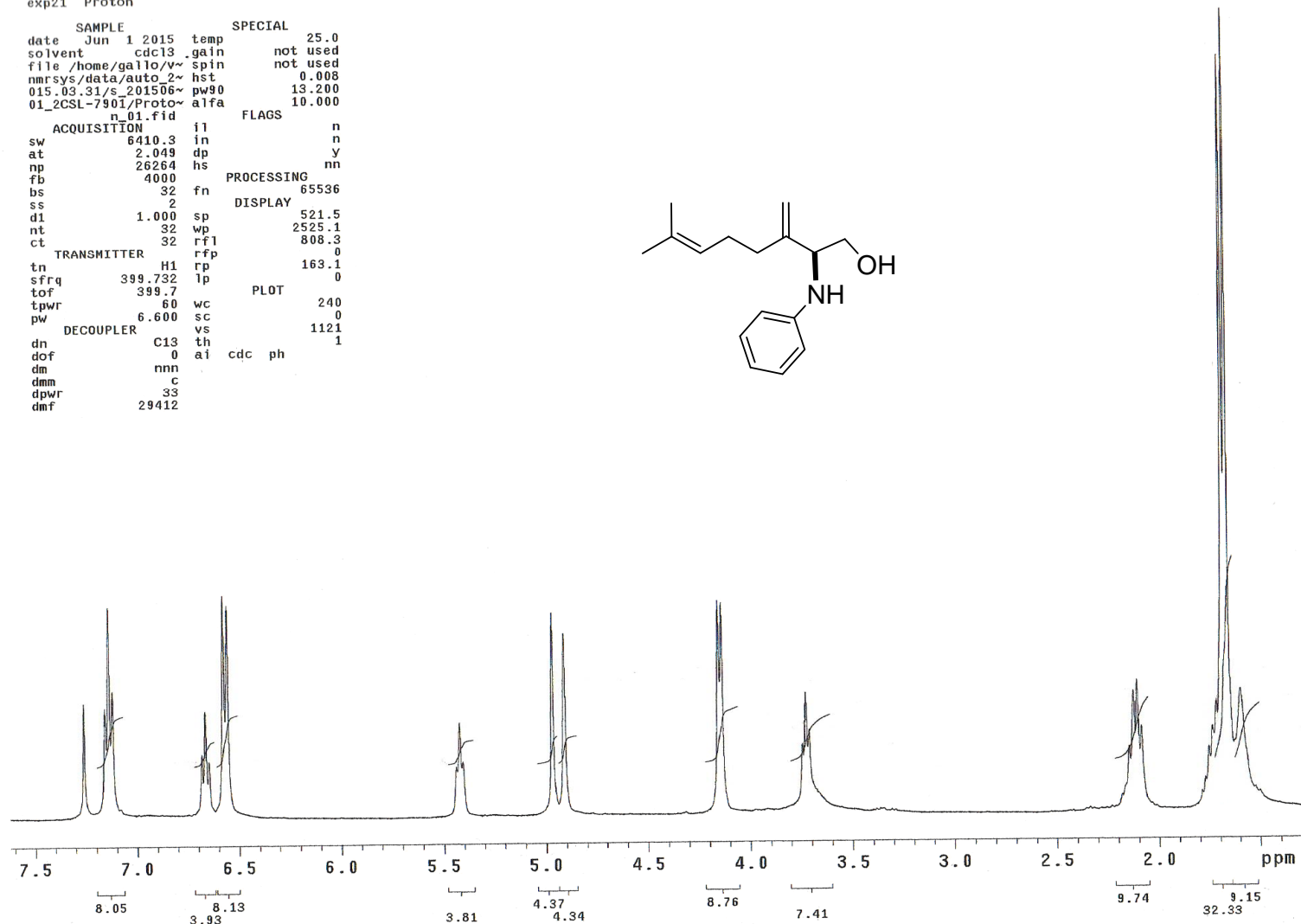
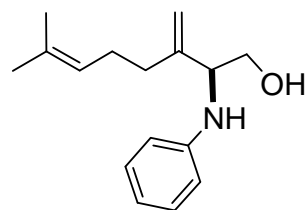
2-(4-bromophenylamino)-3-methylbut-3-en-1-ol (1d'): GC-MS analysis



7-methyl-3-methylene-2-(phenylamino)oct-6-en-1-ol (2a'): ^1H NMR (400 MHz, CDCl_3)

exp21 Proton

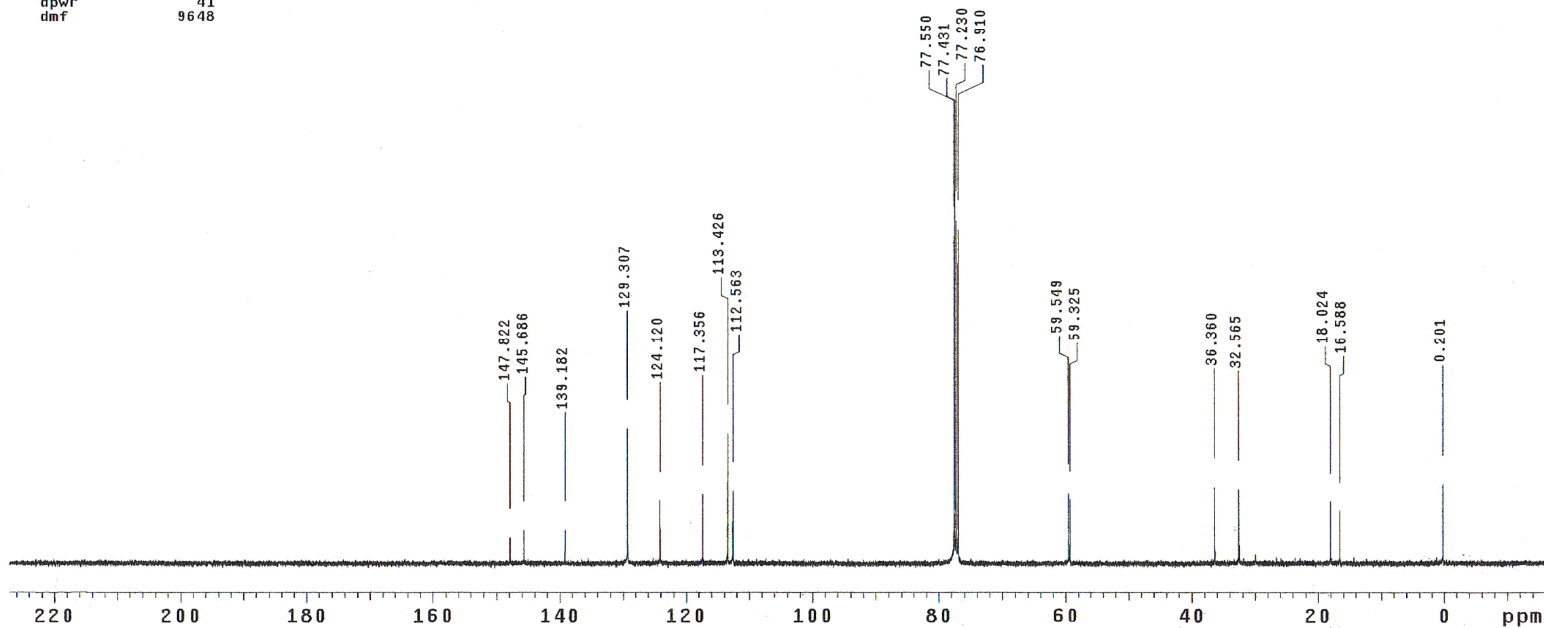
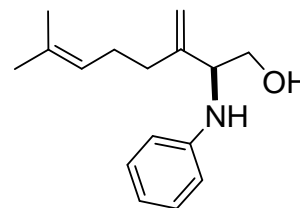
SAMPLE		SPECIAL	
date	Jun 1 2015	temp	25.0
solvent	cdcl3	gain	not used
file	/home/gallo/v*	spin	not used
nmr sys	/data/auto_2*	hst	0.008
015_03_31/s_201506*		pw90	13.200
01_2CSL-7901/Proto*		alfa	10.000
n_01.fid		FLAGS	
ACQUISITION		il	n
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	32	fn	65536
ss	2	DISPLAY	
di	1.000	sp	521.5
nt	32	wp	2525.1
ct	32	rfl	808.3
TRANSMITTER		rfp	0
tn	H1	rp	163.1
sfrq	399.732	lp	0
tof	399.7	PLOT	
tpwr	60	wc	240
pw	6.600	sc	0
DECOUPLER		vs	1121
dn	C13	th	1
dof	0	ai	cdc ph
dm	nnn		
dmm	c		
dpwr	33		
dmf	29412		



7-methyl-3-methylene-2-(phenylamino)oct-6-en-1-ol (2a'): ^{13}C NMR (100 MHz, CDCl_3)

```

exp21 Carbon
SAMPLE
date Jun 1 2015 temp 25.0
solvent cdc13 gain 30
file /home/gallo/v~ spin not used
nmr sys/data/auto_2~ hst 0.008
015_03_31/s_201506~ pw90 8.300
01_2CSL-7902/Carbo~ alfa 10.000
n_01.fid
ACQUISITION
sw 24509.8 in n
at 1.300 dp y
np 63750 hs nn
fb 17000
bs 64 lb PROCESSING 0.50
d1 1.000 fn not used
nt 10000 DISPLAY
ct 10000 sp -1679.2
TRANSMITTER wp 24509.1
tn C13 rfl 9442.5
sfrq 100.523 rfp 7762.6
tof 1027.9 rp 60.0
tpwr 55 lp 0
pw 4.150 PLOT
DECOUPLER wc 240
dn H1 sc 0
dof 0 vs 801443
dm yy th 4
dmm w ai cdc ph
dpwr 41
dmf 9648
    
```



7-methyl-3-methylene-2-(phenylamino)oct-6-en-1-ol (2a'): HR-MS analysis

