

An Unprecedented, One-pot Chemocontrolled Entry to Thioxoimidazolidinones and Aminoimidazolones: Synthesis of a Kinase Inhibitor Leucettamine B

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General experimental methods:

Methanol, dichloromethane and acetone were distilled before use. All reactions were performed under an inert atmosphere with unpurified reagents and dry solvents. Analytical thin-layer chromatography (TLC) was performed using 0.25 mm silica gel coated plates. Flash chromatography was performed using the indicated solvent and silica gel 60 (230-400 mesh). All the microwave experiments were performed in CEM microwave reactor under optimized reaction conditions of power and pressure. ^1H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were recorded on a 300 MHz spectrometer. Chemical shifts are reported in parts per million (ppm) on the scale from an internal standard.

3-benzyl-5-((2-(cyclohex-1-en-1-yl)ethyl)amino)-5-phenyl-2-thioxoimidazolidin-4-one 5{2,2,2}

^1H NMR (300 MHz, CDCl_3) δ 7.81 (s, 1H), 7.58 – 7.50 (m, 2H), 7.47 – 7.36 (m, 5H), 7.34 – 7.25 (m, 4H), 5.41 (s, 1H), 5.11 (d, J = 14.5 Hz, 1H), 4.99 (d, J = 14.5 Hz, 1H), 2.68 – 2.51 (m, 1H), 2.43 (d, J = 6.5 Hz, 1H), 2.09 (t, J = 6.6 Hz, 3H), 1.97 (s, 2H), 1.81 (s, 2H), 1.59 – 1.54 (m, 4H); ^{13}C NMR (75 MHz, CDCl_3) δ 182.8, 172.9, 136.5, 135.6, 134.5, 129.6, 129.1, 128.6, 128.4, 127.8, 125.6, 123.5, 80.0, 44.6, 40.3, 37.9, 27.9, 25.2, 22.8, 22.3; MS (ESI) m/z : 406 (MH^+); HRMS (ESI, m/z) calcd for $\text{C}_{24}\text{H}_{27}\text{N}_3\text{OS}$ [MH^+]: 406.1948; Found 406.2061 ($\text{M}+\text{H}$).

3-benzyl-5-((2-(cyclohex-1-en-1-yl)ethyl)amino)-5-isobutyl-2-thioxoimidazolidin-4-one 5{5,2,2}

^1H NMR (300 MHz, CDCl_3) δ 7.55 – 7.44 (m, 2H), 7.39 – 7.23 (m, 3H), 6.96 (s, 1H), 5.37 (s, 1H), 5.03 (s, 2H), 2.50 – 2.21 (m, 2H), 1.98 (d, J = 6.6 Hz, 4H), 1.75 (d, J = 6.6 Hz, 4H), 1.71 – 1.49 (m, 7H), 0.92 (d, J = 6.5 Hz, 3H), 0.81 (d, J = 6.5 Hz, 3H);

^{13}C NMR (75 MHz, CDCl_3) δ 183.1, 175.3, 136.1, 134.8, 129.3, 128.8, 128.2, 123.8, 78.9, 45.9, 44.8, 40.1, 38.2, 28.2, 25.5, 24.4, 24.2, 23.7, 23.2, 22.7; MS (ESI) m/z : 386 (MH^+); HRMS (ESI, m/z) calcd for $\text{C}_{22}\text{H}_{31}\text{N}_3\text{OS}$ [MH^+]: 386.2261; Found 386.2265 ($\text{M}+\text{H}$).

5-isobutyl-5-((4-methoxybenzyl)amino)-3-phenethyl-2-thioxoimidazolidin-4-one
5{5,4,3}

^1H NMR (300 MHz, CDCl_3) δ 7.56 (s, 1H), 7.32 – 7.27 (m, 5H), 7.19 (d, J = 8.0 Hz, 2H), 6.84 (d, J = 8.0 Hz, 2H), 4.10 – 4.04 (m, 2H), 3.79 (s, 3H), 3.42 (d, J = 12.0 Hz, 1H), 3.24 (d, J = 12.0 Hz, 1H), 3.07 (t, J = 7.2 Hz, 2H), 1.99 (s, 1H), 1.73 (s, 2H), 1.70 – 1.57 (m, 1H), 0.94 (d, J = 6.1 Hz, 3H), 0.88 (d, J = 6.0 Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 182.6, 174.6, 158.9, 137.5, 130.6, 129.4, 129.1, 128.5, 126.7, 113.8, 78.5, 55.2, 46.0, 45.6, 42.0, 33.6, 24.1, 23.8, 23.6; MS (ESI) m/z : 412 (MH^+); HRMS (ESI, m/z) calcd for $\text{C}_{23}\text{H}_{29}\text{N}_3\text{O}_2\text{S}$ [MNa^+]: 434.1878; Found 434.1881 ($\text{M}+\text{Na}$).

5-isobutyl-3-isopropyl-5-((4-methoxybenzyl)amino)-2-thioxoimidazolidin-4-one
5{5,3,3}

^1H NMR (300 MHz, CDCl_3) δ 7.43 (s, 1H), 7.20 (d, J = 8.4 Hz, 2H), 6.85 (d, J = 8.4 Hz, 2H), 4.97 – 4.93 (m, 1H), 3.79 (s, 3H), 3.53 (d, J = 11.8 Hz, 1H), 3.49 (d, J = 11.8 Hz, 1H), 2.06 (s, 1H), 1.84 – 1.63 (m, 3H), 1.48 (J = 6.2 Hz, 6H), 0.96 (d, J = 6.2 Hz, 2H), 0.91 (d, J = 6.2 Hz, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 183.7, 175.4, 159.3, 131.0, 129.8, 114.3, 77.6, 55.6, 47.9, 46.2, 46.1, 24.4, 24.3, 23.9, 19.7, 19.3; MS (ESI) m/z : 350 (MH^+); HRMS (ESI, m/z) calcd for $\text{C}_{18}\text{H}_{27}\text{N}_3\text{O}_2\text{S}$ [MNa^+]: 372.1722; Found 372.1724 ($\text{M}+\text{Na}$).

3-benzyl-5-((2-(cyclohex-1-en-1-yl)ethyl)amino)-5-methyl-2-thioxoimidazolidin-4-one
5{3,2,2}

^1H NMR (300 MHz, CDCl_3) δ 7.46 (d, J = 7.2 Hz, 2H), 7.30 – 7.26 (m 3H), 5.37 (s,

1H), 5.03 (d, $J = 14.6$ Hz, 1H), 4.95 (d, $J = 14.6$ Hz, 1H) 2.46 (d, $J = 6.6$ Hz, 1H), 2.30 – 2.27 (m, 1H), 2.00 – 1.95 (m, 4H), 1.75 (s, 3H), 1.63 – 1.44 (m, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 182.3, 174.6, 135.7, 134.2, 128.6, 128.5, 127.9, 123.5, 75.4, 4.4, 40.4, 37.5, 27.8, 25.1, 23.6, 22.7, 22.3; MS (ESI) m/z : 344 (MH^+); HRMS (ESI, m/z) calcd for $\text{C}_{19}\text{H}_{25}\text{N}_3\text{OS}$ [MH^+]: 344.1791; Found 344.1794 ($\text{M}+\text{H}$).

3-benzyl-5-isopropyl-5-((4-methoxybenzyl) amino)-2-thioxoimidazolidin-4-one 5{4,2,3}

^1H NMR (300 MHz, CDCl_3) δ 7.59 (s, 1H), 7.52 (dd, $J = 7.7, 1.7$ Hz, 2H), 7.38 – 7.25 (m, 3H), 7.15 (d, $J = 8.6$ Hz, 2H), 6.86 – 6.80 (m, 2H), δ 5.10 (d, $J = 16.5$ Hz, 1H), δ 4.97 (d, $J = 16.5$ Hz, 1H), 3.81 (s, 3H), 3.52 (d, $J = 12.1$ Hz, 1H), 3.40 (d, $J = 12.1$ Hz, 1H), 2.16 – 2.02 (m, 1H) 1.04 (d, $J = 6.9$ Hz, 3H), 0.81 (d, $J = 6.9$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 183.8, 175.4, 159.3, 136.1, 131.1, 129.7, 129.3, 128.8, 128.3, 114.2, 82.1, 55.6, 46.8, 44.8, 3.5, 16.8, 16.5; MS (ESI) m/z : 384 (MH^+); HRMS (ESI, m/z) calcd for $\text{C}_{21}\text{H}_{25}\text{N}_3\text{O}_2\text{S}$ [MH^+]: 384.1740; Found 384.1742 ($\text{M}+\text{H}$).

3,5-diisopropyl-5-((3-methoxypropyl)amino)-2-thioxoimidazolidin-4-one 5{4,3,4}

^1H NMR (300 MHz, CDCl_3) δ 7.56 (s, 1H), 4.92– 4.86 (m, 1H), 3.43 (t, $J = 6.0$ Hz, 2H), 3.31 (s, 3H), 2.62 – 2.44 (m, 2H), 2.05 – 2.02 (m, 1H), 1.70 (m, 2H), 1.45 (d, $J = 7.0$ Hz, 6H), 1.01 (d, $J = 6.7$ Hz, 3H), 0.86 (d, $J = 6.7$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 183.9, 175.4, 80.4, 71.3, 58.6, 47.3, 40.4, 35.0, 29.7, 19.2, 18.9, 16.2, 16.1; MS (ESI) m/z : 288 (MH^+); HRMS (ESI, m/z) calcd for $\text{C}_{13}\text{H}_{25}\text{N}_3\text{O}_2\text{S}$ [MH^+]: 288.1740; Found 288.1740 ($\text{M}+\text{H}$).

3,5-diisopropyl-5-((3-phenylpropyl)amino)-2-thioxoimidazolidin-4-one 5{4,3,5}

^1H NMR (300 MHz, Acetone) δ 7.33 – 7.09 (m, 5H), 5.01 – 4.86 (m, 1 H) 2.84 (s, 1H), 2.66 (t, $J = 7.4$ Hz, 2H), 2.43 (t, $J = 6.4$ Hz, 2H), 2.12 – 2.01 (m, 3H), 1.74 (d, $J = 7.3$ Hz, 2H), 1.39 (d, $J = 7.0$ Hz, 6H), 1.06 (d, $J = 6.9$ Hz, 3H), 0.86 (d, $J = 6.9$ Hz,

3H); ^{13}C NMR (75 MHz, Acetone) δ 205.2, 204.9, 183.5, 175.2, 142.2, 128.3, 128.1, 125.5, 110.0, 80.3, 46.3, 41.7, 34.7, 33.1, 31.8, 29.7, 29.4, 29.1, 28.9, 28.6, 28.4, 28.1, 18.4, 18.16, 15.79, 15.4; MS (ESI) m/z : 334 (MH^+); HRMS (ESI, m/z) calcd for $\text{C}_{18}\text{H}_{27}\text{N}_3\text{OS}$ [MH^+]: 333.1875; Found 333.1875 ($\text{M}+\text{H}$).

(Z)-4-benzylidene-1-butyl-2-(butylamino)-1H-imidazol-5(4H)-one 6{1,1,13}

^1H NMR (300 MHz, CDCl_3) δ 8.08 (d, $J = 7.5$ Hz, 2H), 7.37 (t, $J = 7.8$ Hz, 2H), 7.28 – 7.23 (m, 1H), 6.70 (s, 1H), 4.52 (s, 1H), 3.62 – 3.53 (m, 4H), 1.76 – 1.31 (m, 8H), 1.00 (t, $J = 7.2$ Hz, 3H), 0.95 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 170.4, 157.4, 139.3, 135.7, 130.8, 128.4, 128.0, 116.6, 41.8, 39.0, 31.7, 31.0, 20.1, 20.0, 13.8, 13.7; MS (FB^+): m/z 300; HRMS (EI): calcd for $\text{C}_{18}\text{H}_{25}\text{N}_3\text{O}$ 299.1998; Found 299.1975.

(Z)-4-benzylidene-1-butyl-2-(cyclopentylamino)-1H-imidazol-5(4H)-one 6{1,1,6}

^1H NMR (300 MHz, CDCl_3) δ 8.10 (d, $J = 7.5$ Hz, 2H), 7.39 (t, $J = 7.8$ Hz, 2H), 7.3 – 7.28 (m, 1H), 6.68 (s, 1H), 4.58 (d, $J = 6.9$ Hz, 1H), 4.56 – 4.46 (m, 1H), 3.55 (t, $J = 6.9$ Hz, 2H), 2.25–2.15 (m, 2H), 1.80 – 1.52 (m, 8H), 1.35 (sext, $J = 6.6$ Hz, 2H), 0.94 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 170.4, 157.0, 139.5, 135.8, 130.8, 128.4, 127.9, 116.6, 53.8, 38.9, 33.5, 31.0, 23.9, 20.1, 13.7; MS (EI): m/z 311; HRMS (EI): calcd for $\text{C}_{19}\text{H}_{25}\text{N}_3\text{O}$ 311.1998; Found 311.2009.

(Z)-2-(benzylamino)-4-benzylidene-1-butyl-1H-imidazol-5(4H)-one 6{1,1,7}

^1H NMR (300 MHz, CDCl_3) δ 8.10 (d, $J = 7.5$ Hz, 2H), 7.45 – 7.26 (m, 8H), 6.74 (s, 1H), 4.92 (s, 1H), 4.81 (s, 2H), 3.55 (t, $J = 6.9$ Hz, 2H), 1.58 (quint, $J = 7.2$ Hz, 2H), 1.35 (sext, $J = 7.8$ Hz, 2H), 0.93 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 170.4, 157.4, 138.6, 137.7, 135.5, 130.9, 128.9, 128.5, 128.2, 128.1, 128.0, 117.4, 47.2, 39.1, 31.0, 20.0, 13.7; MS (EI): m/z 333; HRMS (EI): calcd for $\text{C}_{21}\text{H}_{23}\text{N}_3\text{O}$ 333.1841; Found 333.1837.

(Z)-4-benzylidene-1-butyl-2-((2-(cyclohex-1-en-1-yl)ethyl)amino)-1H-imidazol-5(4H)-one **6{1,1,2}**

¹H NMR (300 MHz, CDCl₃) δ 8.1 (d, *J* = 7.5 Hz, 2H), 7.37 (t, *J* = 7.2 Hz, 2H), 7.27 – 7.22 (m, 1H), 6.70 (s, 1H), 5.57 (s, 1H), 4.59 (s, 1H), 3.65 (m, 2H), 3.52 (t, *J* = 7.2 Hz, 2H), 2.35 (t, *J* = 6.6 Hz, 2H), 2.09 – 1.91 (m, 4H), 1.69 – 1.51 (m, 6H), 1.36 (sext, *J* = 7.2 Hz, 2H), 0.94 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 170.3, 157.2, 139.4, 135.7, 134.7, 130.8, 128.4, 127.9, 124.8, 116.8, 38.9, 38.8, 37.4, 30.9, 27.6, 25.4, 22.8, 22.4, 20.1, 13.7; MS (EI): *m/z* 351; HRMS(EI): calcd for C₂₂H₂₉N₃O 351.2311; Found 351.2316.

(Z)-4-benzylidene-1-butyl-2-((2-(pyridin-2-yl)ethyl)amino)-1H-imidazol-5(4H)-one **6{1,1,8}**

¹H NMR (300 MHz, CDCl₃) δ 8.48 (d, *J* = 7.5 Hz, 1H), 8.10 (d, *J* = 7.2 Hz, 2H), 7.66 (dt, *J* = 1.8, 7.8 Hz, 1H), 7.37 (t, *J* = 7.8 Hz, 2H), 7.27 – 7.17 (m, 3H), 6.67 (s, 1H), 3.98 (t, *J* = 7.2 Hz, 2H), 3.58 (t, *J* = 7.5 Hz, 2H), 3.16 (t, *J* = 7.2 Hz, 2H), 1.59 (quint, *J* = 7.2 Hz, 2H), 1.36 (sext, *J* = 7.8 Hz, 2H), 0.93 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 170.4, 160.0, 157.8, 148.7, 139.4, 137.2, 135.9, 130.7, 128.4, 127.8, 123.9, 122.0, 115.8, 41.0, 39.1, 35.5, 30.8, 20.1, 13.7; MS (EI): *m/z* 348; HRMS(EI): calcd for C₂₁H₂₄N₄O 348.1950; Found 348.1949.

(Z)-4-benzylidene-2-((2-morpholinoethyl)amino)-1-phenyl-1H-imidazol-5(4H)-one **6{1,7,9}**

¹H NMR (300 MHz, CDCl₃) δ 8.15 (d, *J* = 7.4 Hz, 2H), 7.55 (d, *J* = 7.4 Hz, 2H), 7.49 (d, *J* = 7.0 Hz, 2H), 7.41 (t, *J* = 7.4 Hz, 2H), 7.31– 7.28 (m, 2H), 6.81 (s, 1H), 5.57 (s, 1H), 3.65 (t, *J* = 8.2 Hz, 2H), 3.56 (s, 4H), 2.61 (t, *J* = 8.2 Hz, 2H), 2.44 (s, 4H); ¹³C NMR (75 MHz, CDCl₃) δ 169.6, 156.5, 139.4, 136.3, 132.4, 131.2, 130.5, 129.4, 128.8, 128.5, 127.4, 117.6, 67.3, 56.3, 53.3, 37.9; MS (ESI) *m/z*: 377 (MH⁺); HRMS

(ESI, m/z) calcd for $C_{22}H_{24}N_4O_2$ [MH^+]: 376.1899; Found 376.1899 ($M+H$).

(Z)-4-benzylidene-1-(4-methoxyphenyl)-2-(phenethylamino)-1H-imidazol-5(4H)-one 6{1,5,10}

1H NMR (300 MHz, $CDCl_3$) δ 8.19 (d, $J = 7.4$ Hz, 2H), 7.45 (t, $J = 7.5$ Hz, 2H), 7.40 – 7.28 (m, 4H), 7.28 – 7.19 (m, 2H), 7.16 – 7.08 (m, 2H), 6.98– 6.90 (m, 2H), 6.83 (s, 1H), 4.54 (s, 1H), 3.85 (s, 3H), 3.84 (t, $J = 7.0$ Hz, 2H), 3.03 (t, $J = 7.0$ Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.4, 160.4, 156.8, 139.4, 138.7, 136.1, 131.3, 129.2, 129.1, 129.1, 128.8, 128.5, 127.1, 124.3, 117.7, 115.7, 77.9, 77.4, 77.6, 56.2, 43.3, 35.7; MS (ESI) m/z : 398 (MH^+); HRMS (ESI, m/z) calcd for $C_{25}H_{23}N_3O_2$ [MH^+]: 397.1790; Found 397.1790 ($M+H$).

(Z)-1-benzyl-2-((2-(cyclohex-1-en-1-yl)ethyl)amino)-4-(2-methylpropylidene)-1H-imidazol-5(4H)-one 6{5,2,2}

1H NMR (300 MHz, $CDCl_3$) δ 7.37 – 7.30 (m, 3H), 7.26 – 7.21 (m, 2H), 5.98 (d, $J = 9.9$ Hz, 1H), 5.23 (s, 1H), 4.75 (s, 2H), 3.54 (t, $J = 6.1$ Hz, 2H), 3.23 – 3.05 (m, 1H), 2.11 (t, $J = 6.1$ Hz, 2H), 1.85 (m, 4H), 1.59 – 1.41 (m, 4H), 1.11 (d, $J = 7.0$ Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.8, 156.2, 139.2, 135.6, 134.5, 130.3, 129.3, 128.4, 127.1, 124.5, 42.9, 39.1, 37.6, 27.7, 27.1, 25.5, 23.1, 22.8, 22.5; MS (ESI) m/z : 352 (MH^+); HRMS (ESI, m/z) calcd for $C_{22}H_{29}N_3O$ [MH^+]: 352.2389; Found 352.2391 ($M+H$).

(Z)-1-benzyl-4-(2-methylpropylidene)-2-morpholino-1H-imidazol-5(4H)-one 6{5,2,9}

1H NMR (300 MHz, $CDCl_3$) δ 7.39 – 7.27 (m, 3H), 7.22 – 7.16 (m, 2H), 6.14 (d, $J = 9.8$ Hz, 1H), 4.80 (s, 2H), 3.64 – 3.61 (m, 4H), 3.31 – 3.26 (m, 4H), 3.15 – 3.11 (m, 1H), 1.14 (d, $J = 6.7$ Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.7, 159.8, 138.2, 136.4, 134.7, 129.3, 129.4, 128.9, 128.1, 126.6, 66.5, 48.3, 46.3, 27.5, 22.7; MS (ESI)

m/z : 314 (MH^+); HRMS (ESI, m/z) calcd for $C_{18}H_{23}N_3O_2$ [MH^+]: 314.1863; Found 314.1868 ($M+H$).

(Z)-2-((3,3-diphenylpropyl)amino)-1-(3-methoxypropyl)-4-(2-methylpropylidene)-1H-imidazol-5(4H)-one 6{5,6,11}

1H NMR (300 MHz, $CDCl_3$) δ 7.30 – 7.23 (m, 8H), 7.19 – 7.04 (m, 2H), 5.87 (d, J = 9.7 Hz, 1H), 5.74 (s, 1H), 4.07 (t, J = 7.7 Hz, 1H), 3.49 – 3.45 (m, 4H), 3.37 (t, J = 6.6 Hz, 3H), 3.32 (s, 3H), 3.24 – 3.04 (m, 1H), 2.45 – 2.40 (m, 2H), 1.89 – 1.76 (m, 2H), 1.14 (d, J = 6.7 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.1, 156.9, 144.6, 144.5, 139.1, 129.1, 129.6, 129.1, 128.2, 128.1, 126.8, 68.6, 58.7, 49.4, 49.2, 40.9, 35.7, 35.6, 28.6, 27.1, 22.9; MS (ESI) m/z : 420 (MH^+); HRMS (ESI, m/z) calcd for $C_{26}H_{33}N_3O_2$ [MH^+]: 420.2651; Found 420.2648 ($M+H$).

(Z)-1-(3-methoxypropyl)-4-(2-methylpropylidene)-2-(piperidin-1-yl)-1H-imidazol-5(4H)-one 6{5,6,12}

1H NMR (300 MHz, $CDCl_3$) δ 5.94 (d, J = 9.2 Hz, 1H), 3.61 (t, J = 7.4 Hz, 2H), 3.42 (t, J = 7.4 Hz, 2H), 3.30 (s, 7H), 3.15 – 3.08 (m, 1H), 1.95 (t, J = 7.4, 2H), 1.65 (s, 6H), 1.06 (d, J = 6.7 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.51, 160.50, 132.38, 69.80, 58.69, 49.06, 40.20, 29.69, 28.63, 26.93, 25.38, 24.29, 22.39; MS (ESI) m/z : 294 (MH^+); HRMS (ESI, m/z) calcd for $C_{16}H_{12}N_4O_2$ [MH^+]: 294.2176; Found 294.2186 ($M+H$).

(Z)-1-isopropyl-2-((4-methoxybenzyl)amino)-4-(2-methylpropylidene)-1H-imidazol-5(4H)-one 6{5,3,3}

1H NMR (300 MHz, $CDCl_3$) δ 7.26 (d, J = 8.5 Hz, 2H), 6.85 (d, J = 8.5 Hz, 2H), 5.76 (d, J = 9.7 Hz, 1H), 4.55 (s, 2H), 4.29 – 4.13 (m, 1H), 3.77 (s, 3H), 3.18 – 2.95 (m, 1H), 1.38 (d, J = 7.0 Hz, 6H), 1.07 (d, J = 6.6 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.1, 159.1, 130.3, 129.2, 129.1, 128.3, 114.4, 114.6, 55.2, 45.9, 43.8, 26.7, 22.4,

20.2; MS (ESI) m/z : 316 (MH^+); HRMS (ESI, m/z) calcd for $C_{18}H_{25}N_3O_2$ [MH^+]: 316.2025; Found 316.2023 ($M+H$).

(Z)-2-((4-methoxybenzyl)amino)-4-(2-methylpropylidene)-1-phenethyl-1H-imidazol-5(4H)-one 6{5,4,3}

1H NMR (300 MHz, $CDCl_3$) δ 7.28 – 7.18 (m, 3H), 7.16 – 7.09 (m, 4H), 6.89 (d, J = 7.2 Hz, 2H), 5.92 (d, J = 9.8 Hz, 1H), 4.27 (s, 2H), 3.82 (s, 3H), 3.72 (t, J = 6.6 Hz, 2H), 3.18 – 3.05 (m, 1H), 2.87 (t, J = 6.6 Hz, 2H), 1.11 (d, J = 6.6 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6, 138.8, 129.9, 129.4, 129.1, 127.5, 114.3, 55.7, 46.0, 42.1, 35.6, 27.2, 23.3, 22.9; MS (ESI) m/z : 378 (MH^+); HRMS (ESI, m/z) calcd for $C_{23}H_{27}N_3O_2$ [MH^+]: 378.2181; Found 378.2182 ($M+H$).

2-((4-methoxybenzyl)amino)-1-phenyl-4-(propan-2-ylidene)-1H-imidazol-5(4H)-one 6{4,7,3}

1H NMR (300 MHz, $CDCl_3$) δ 7.55 – 7.40 (m, 3H), 7.33 – 7.22 (m, 4H), 6.94 – 6.84 (m, 3H), 4.56 (s, 2H), 4.37 (s, 1H), 3.79 (s, 3H), 2.35 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.3, 159.1, 152.1, 137.3, 135.2, 132.1, 130.1, 129.3, 128.8, 127.3, 119.7, 114.2, 114.0, 113.9, 55.2, 45.1, 21.8, 18.9; MS (ESI) m/z : 336 (MH^+); HRMS (ESI, m/z) calcd for $C_{20}H_{21}N_3O_2$ [MH^+]: 336.1707; Found 336.1709 ($M+H$).

1-benzyl-2-((4-methoxybenzyl)amino)-4-(propan-2-ylidene)-1H-imidazol-5(4H)-one 6{4,2,3}

1H NMR (300 MHz, $CDCl_3$) δ 7.35 – 7.25 (m, 3H), 7.19 (dd, J = 6.8, 2.1 Hz, 2H), 7.03 (d, J = 6.8 Hz, 2H), 6.80 (dd, J = 6.8, 2.1 Hz, 2H), 4.71 (s, 2H), 4.44 (s, 2H), 3.82 (s, 3H), 2.35 (s, 3H), 2.16 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.3, 159.4, 153.5, 137.5, 135.8, 135.6, 130.3, 129.5, 129.3, 128.4, 127.3, 114.3, 77.9, 77.5, 77.1, 60.8, 55.6, 45.4, 42.7, 22.1, 21.4, 19.3, 14.6; MS (ESI) m/z : 350 (MH^+); HRMS (ESI, m/z) calcd for $C_{21}H_{23}N_3O_2$ [MH^+]: 350.1868; Found 350.1870 ($M+H$).

3-Benzyl-2-isobutylimino-5-phenyl-2,3-dihydro-imidazol-4-one 7{2,2,1}

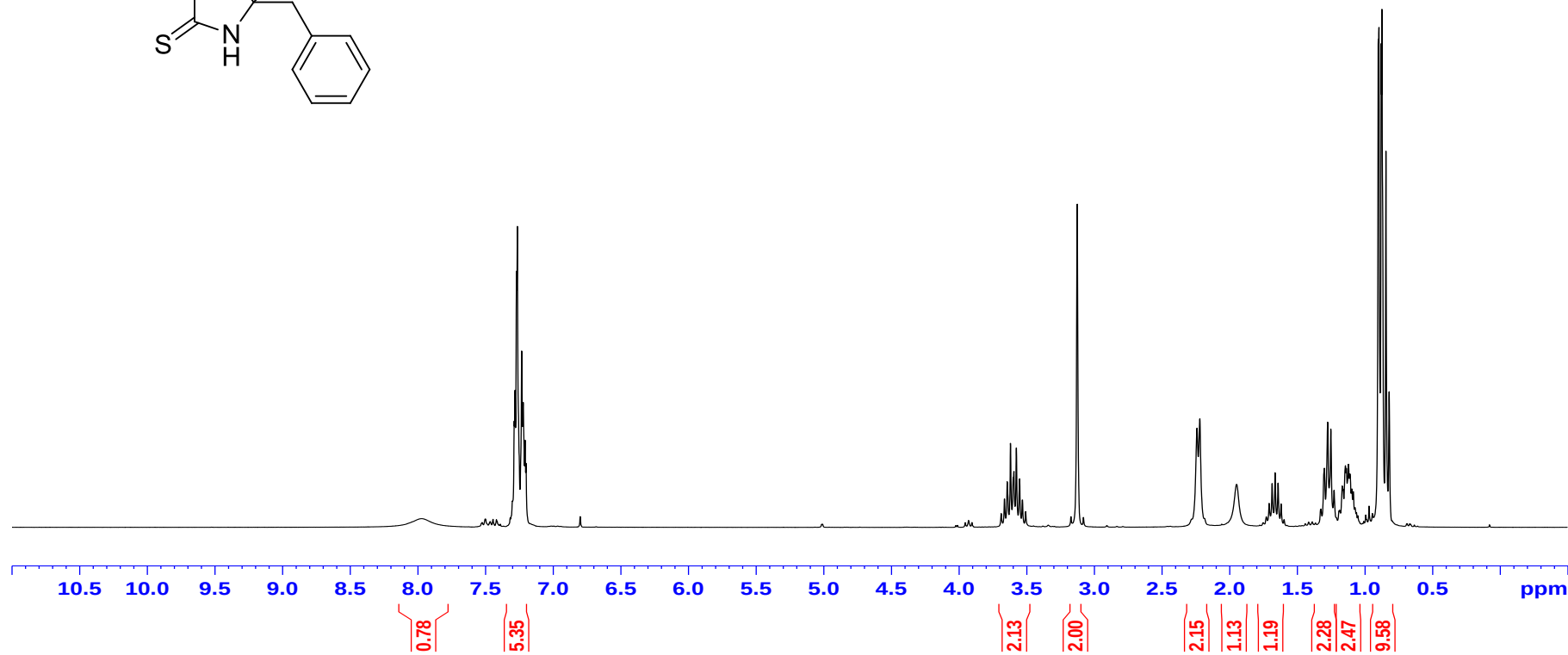
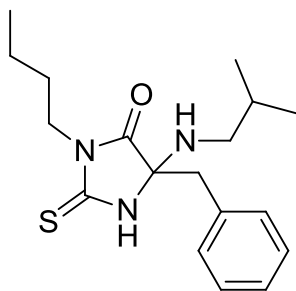
^1H NMR (300 MHz, CDCl_3) δ 8.57 (d, $J = 7.2$ Hz, 2H), 7.63 – 7.24 (m, 8H), 4.91 (s, 2H), 3.86 (d, $J = 6.6$ Hz, 2H), 2.00 (sept, $J = 6.6$ Hz, 1H), 0.97 (d, $J = 6.6$ Hz, 6H); ^{13}C NMR (75 MHz, CDCl_3): δ 165.1, 165.0, 154.0, 136.6, 133.7, 130.3, 129.4, 128.9, 128.7, 128.5, 127.7, 57.5, 43.2, 30.3, 20.7; MS (EI): m/z 319; HRMS (EI): calcd for $\text{C}_{20}\text{H}_{21}\text{N}_3\text{O}$ 319.1685; Found 319.168.

3-Benzyl-2-butylimino-5-phenyl-2,3-dihydro-imidazol-4-one 7{2,2,13}

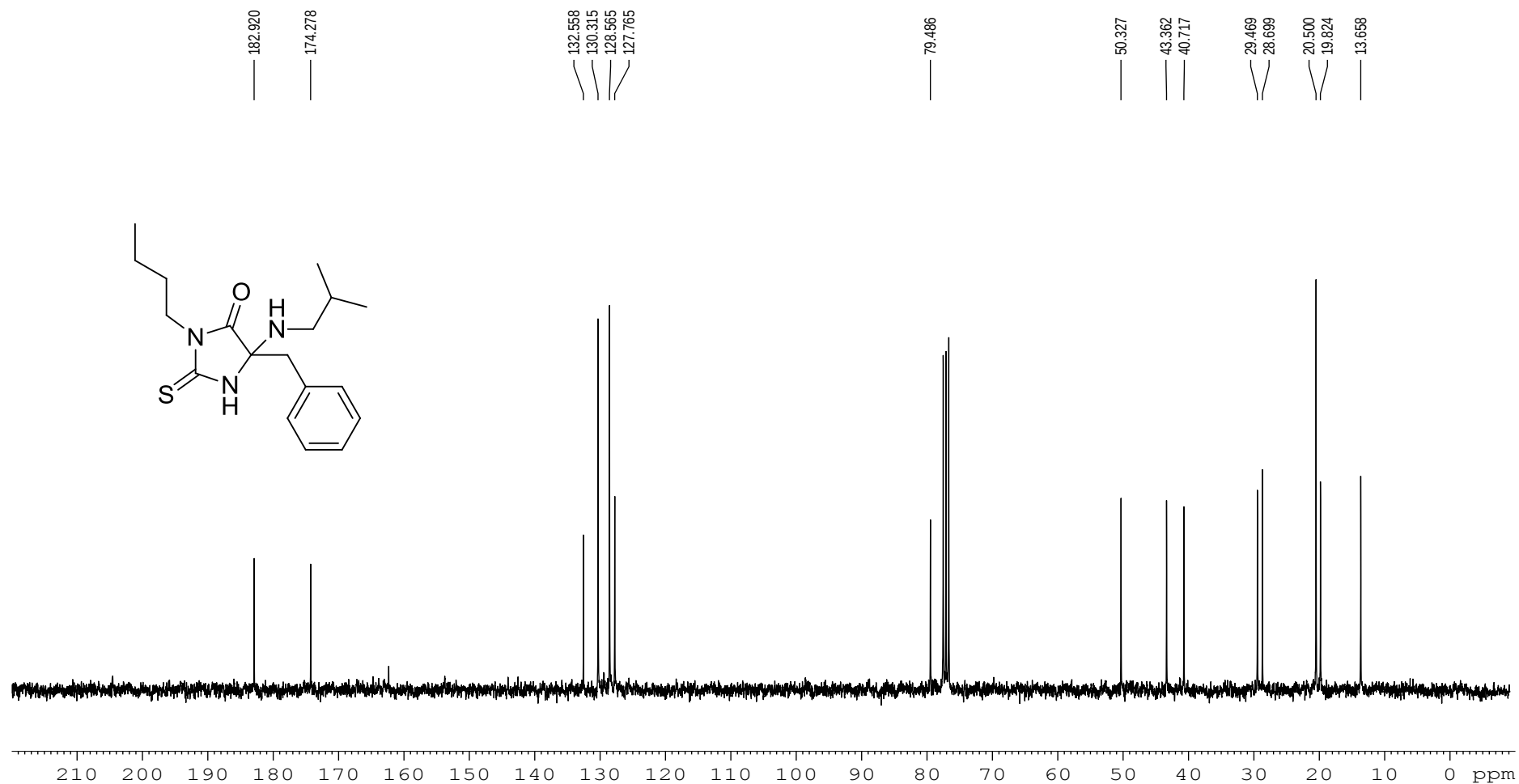
^1H NMR (300 MHz, CDCl_3) δ 8.57 (d, $J = 6.6$ Hz, 2H), 7.62 – 7.57 (m, 1H), 7.52 – 7.43 (m, 4H), 7.34 – 7.26 (m, 3H), 4.9 (s, 2H), 4.04 (t, $J = 6.9$ Hz, 2H), 1.70 (quin, $J = 6.9$ Hz, 2H), 1.41 (sext, $J = 7.2$ Hz, 2H), 0.96 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 165.1, 165.05, 154.05, 136.6, 133.7, 130.3, 129.4, 128.9, 128.7, 128.5, 127.7, 49.6, 43.1, 33.5, 20.5, 13.9; MS (EI): m/z 319; HRMS (EI): calcd for $\text{C}_{20}\text{H}_{21}\text{N}_3\text{O}$ 319.1685; Found 319.1689.

3-Benzyl-5-phenyl-2-(2-pyridin-2-yl-ethylimino)-2,3-dihydro-imidazol-4-one 7{2,2,8}

^1H NMR (300 MHz, CDCl_3) δ 8.53 (d, $J = 6.6$ Hz, 2H), 7.60–7.45 (m, 4H), 7.37 – 7.25 (m, 6H), 7.09 – 7.04 (m, 2H), 4.85 (s, 2H), 4.44 (t, $J = 6.9$ Hz, 2H), 3.19 (t, $J = 6.9$ Hz, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 165.1, 165.0, 159.9, 154.6, 149.3, 136.5, 136.1, 133.8, 130.3, 129.2, 128.9, 138.7, 128.5, 127.7, 123.6, 121.3, 49.6, 43.1, 40.0; MS (EI): m/z 368; HRMS (EI): calcd for $\text{C}_{23}\text{H}_{24}\text{N}_4\text{O}$ 368.1637; Found 368.1643.



^1H NMR spectrum (300 MHz) of compound 5{1,1,1} in CDCl_3

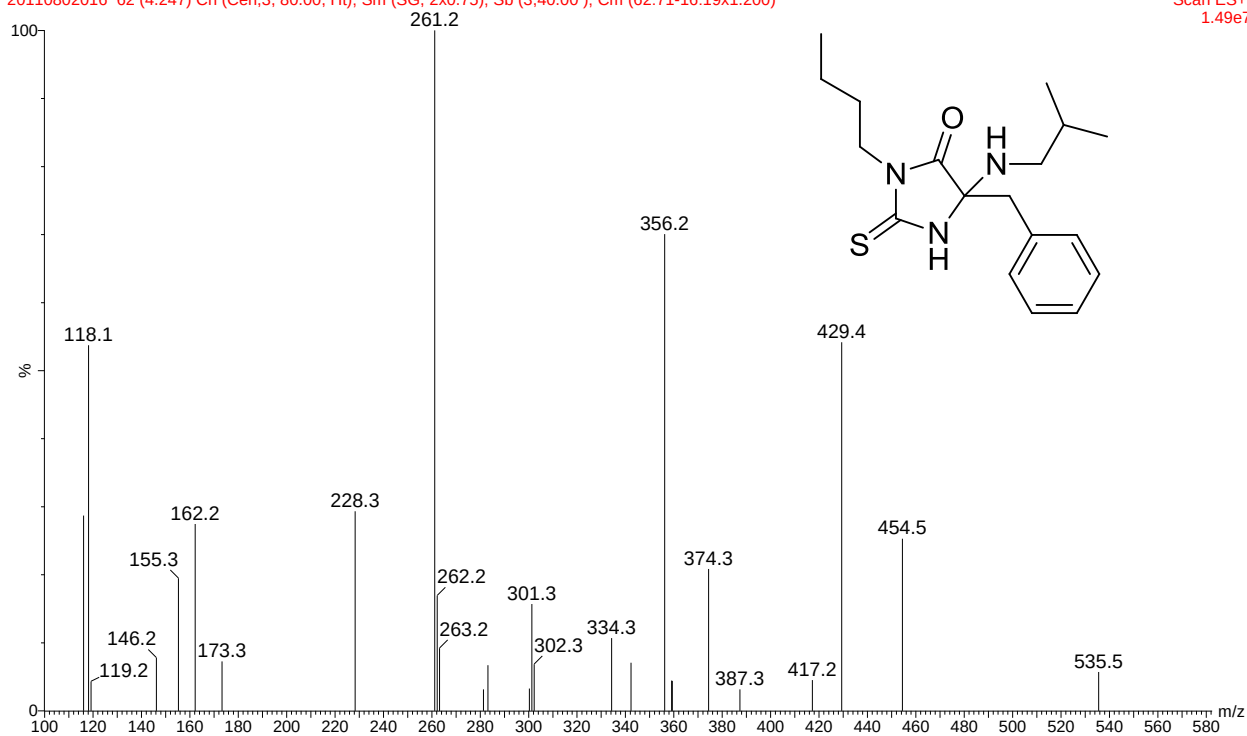


^{13}C spectrum (75 MHz) of compound 5{1,1,1} in CDCl_3

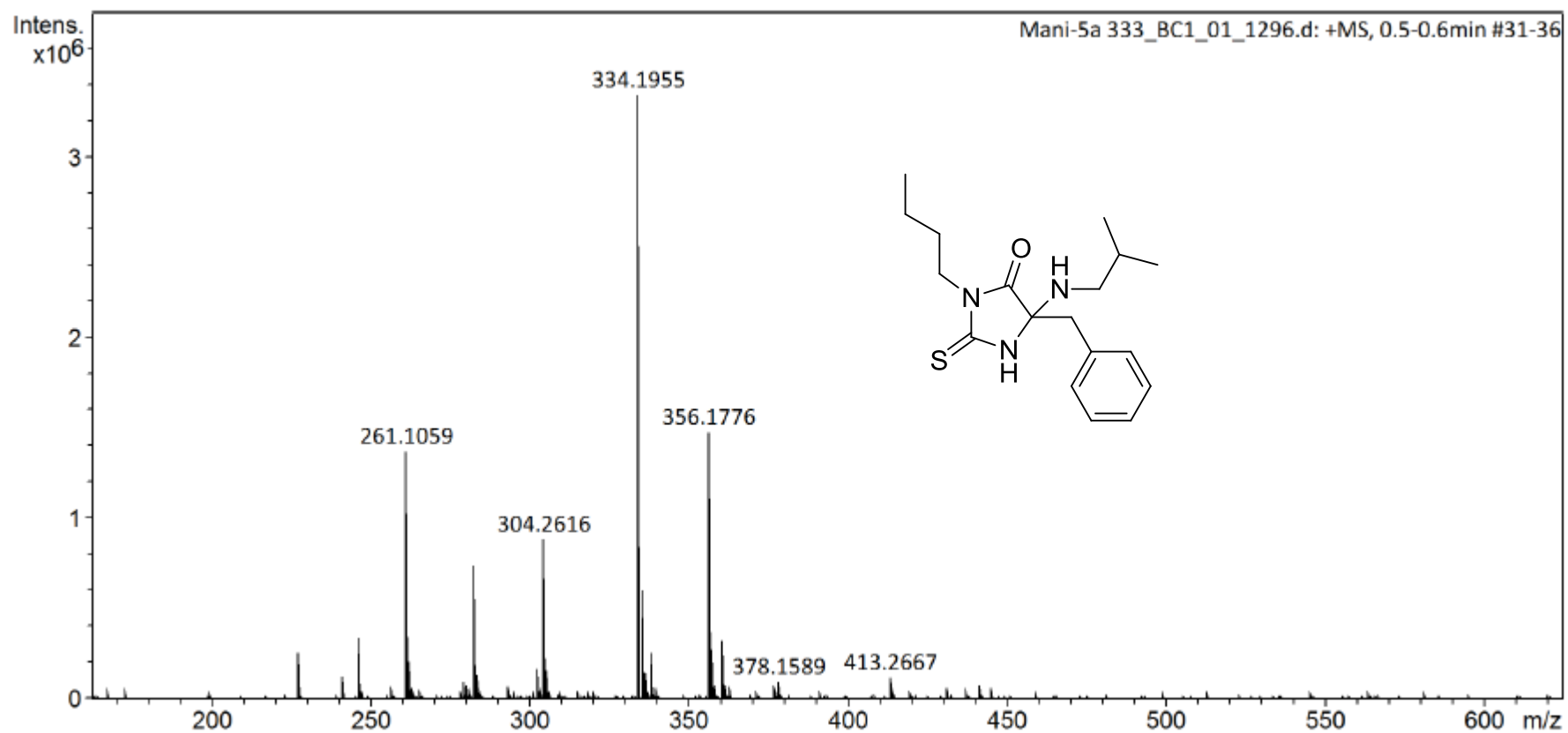
Main-Hg1

20110802016 62 (4.247) Cn (Cen,3, 80.00, Ht); Sm (SG, 2x0.75); Sb (3,40.00); Cm (62:71-16:19x1.200)

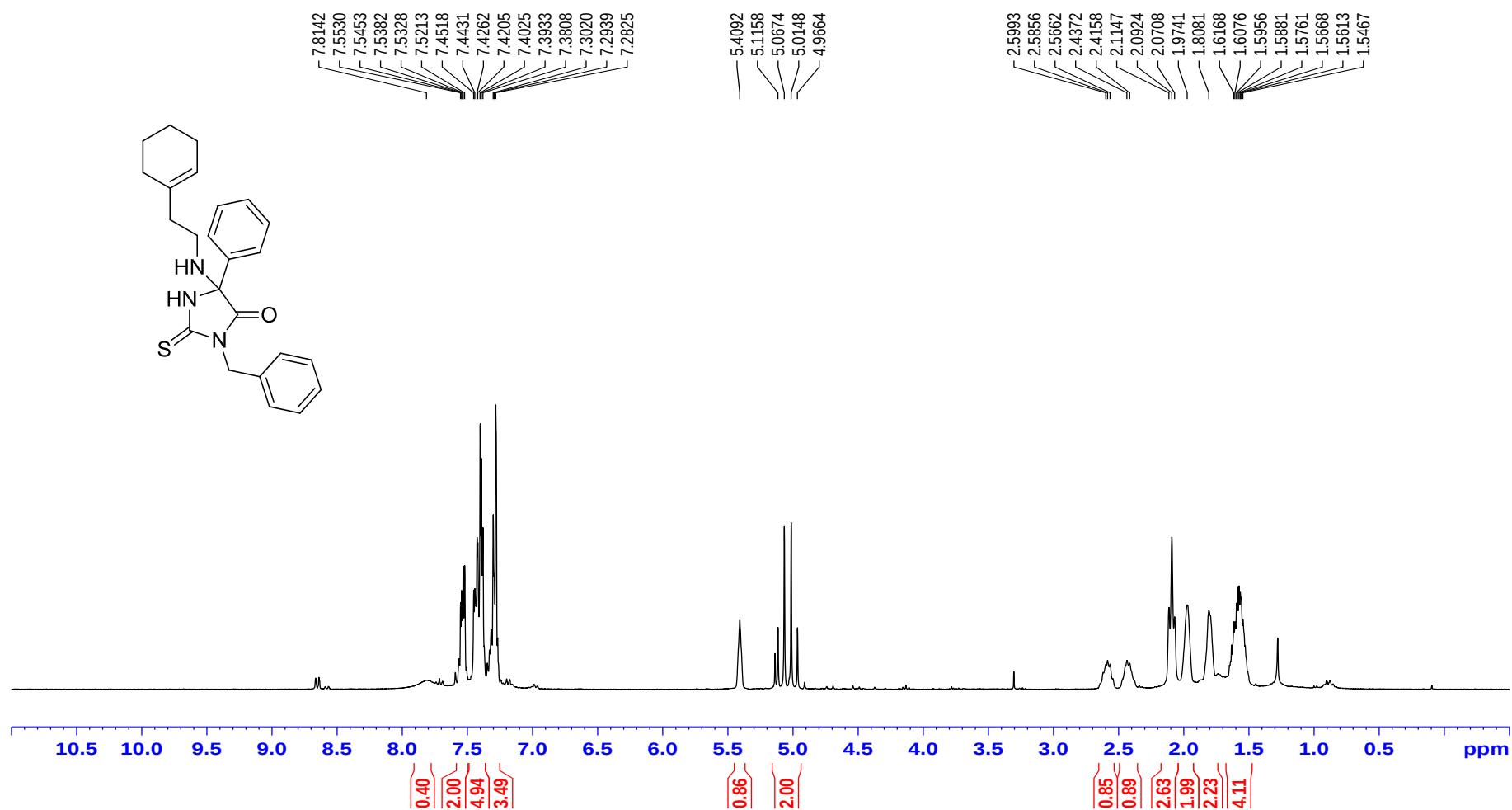
Scan ES+
1.49e7



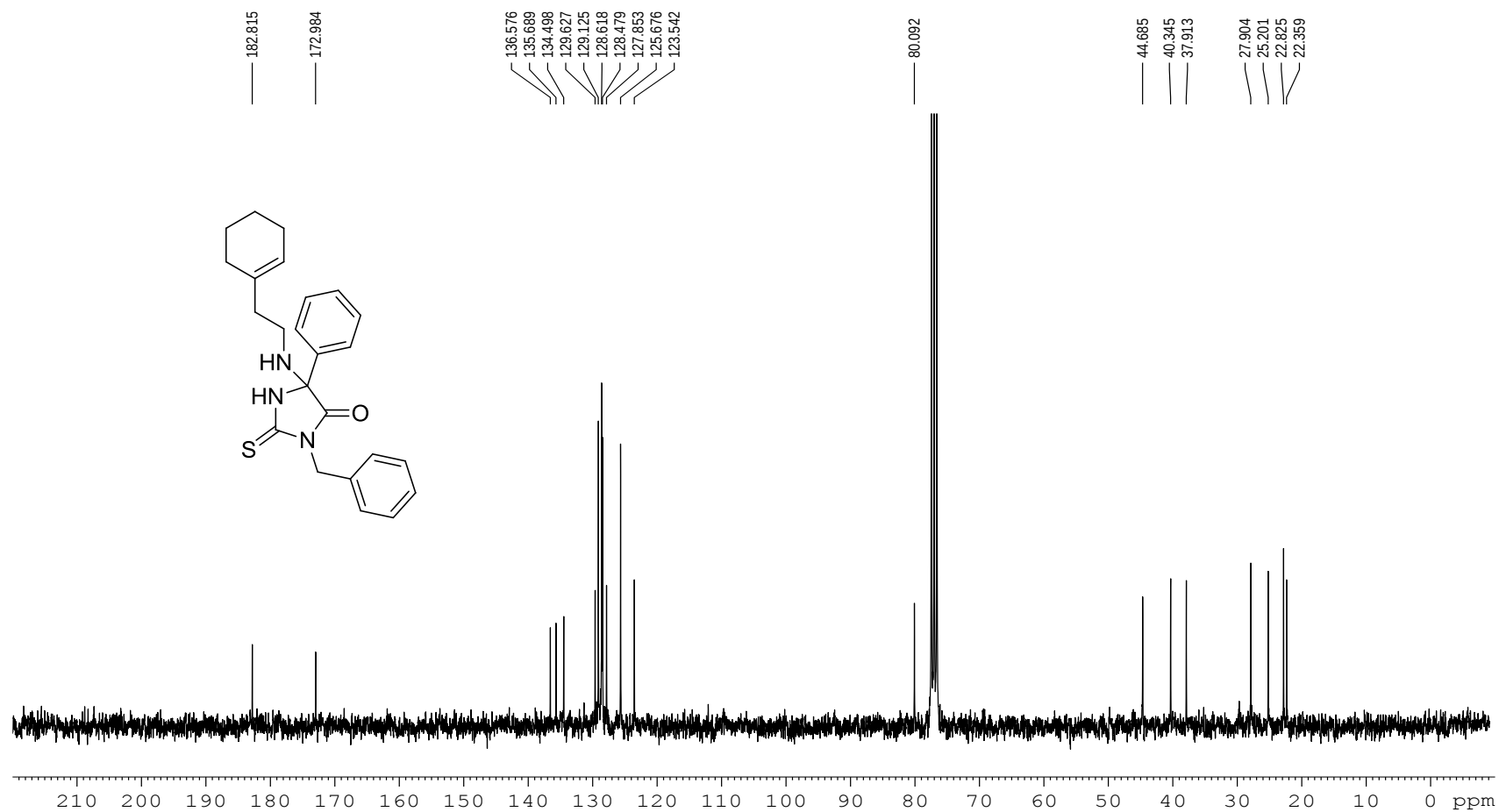
ESI Mass spectrum of compound 5{1,1,1}



HRMS Mass (ESI) spectrum of compound 5{1,1,1}

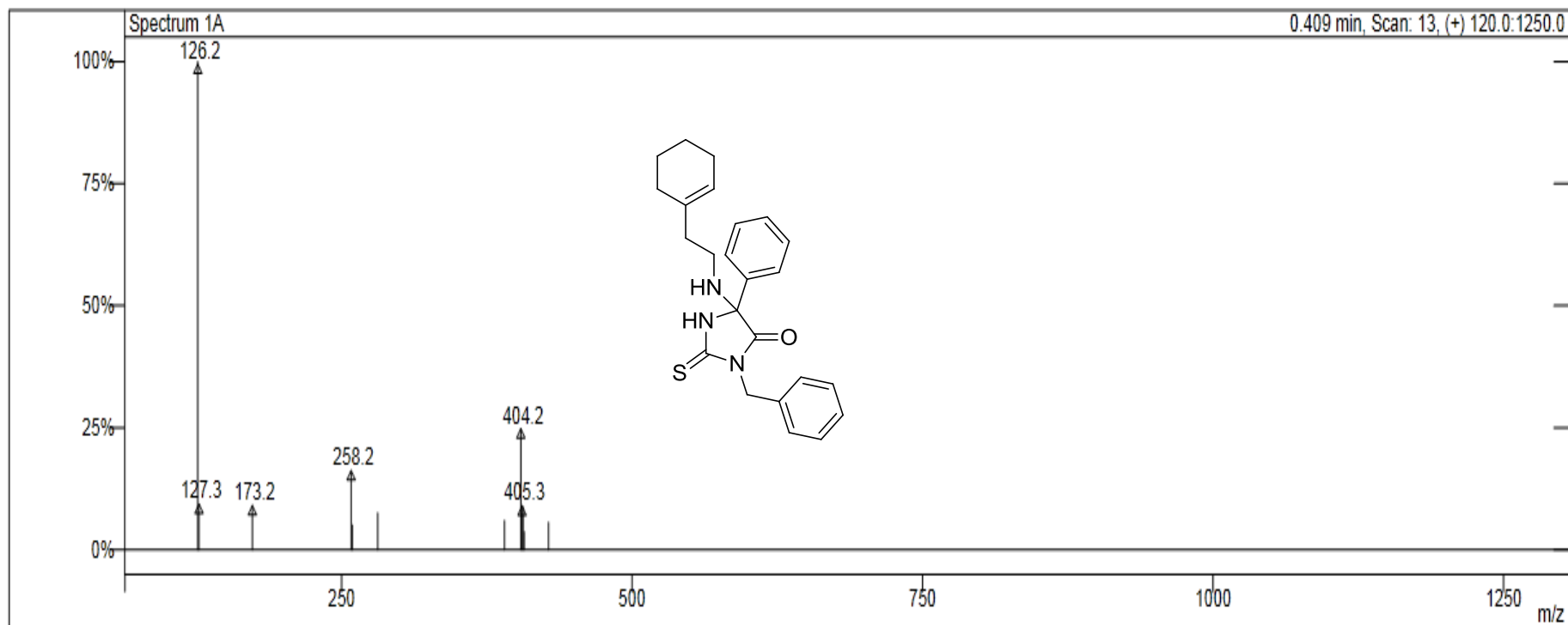


¹H NMR spectrum (300 MHz) of compound 5{2,2,2} in CDCl₃

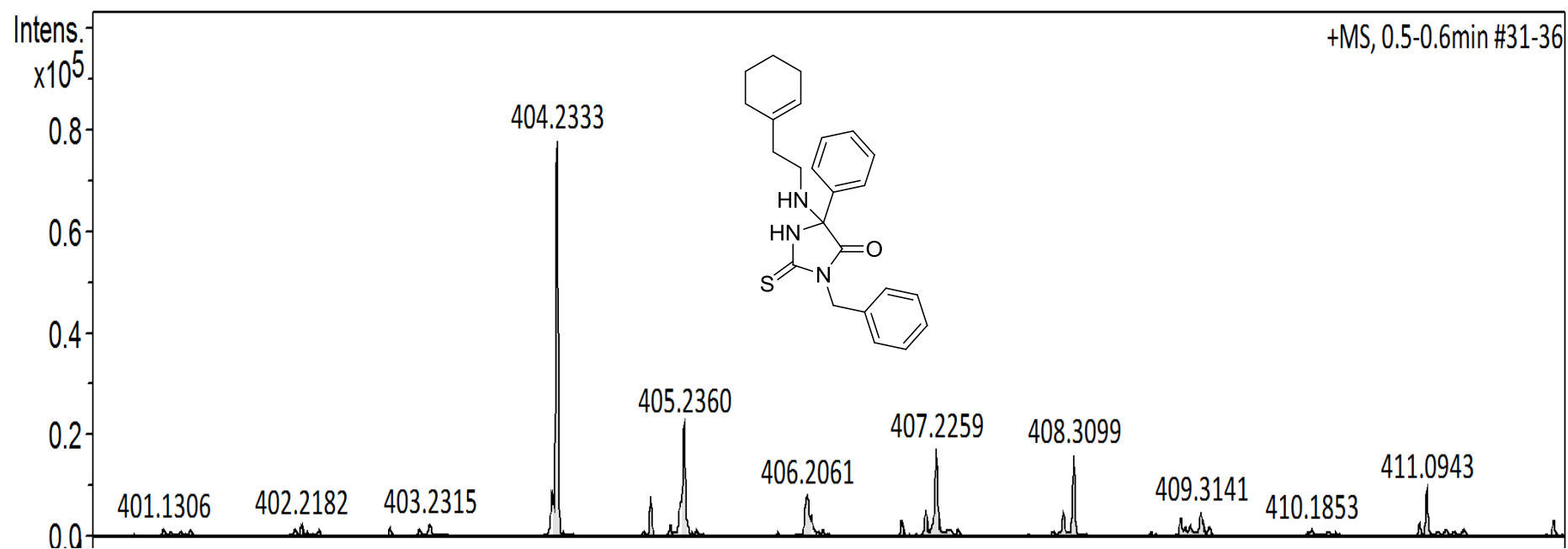


¹³C spectrum (75 MHz) of compound 5{2,2,2} in CDCl₃

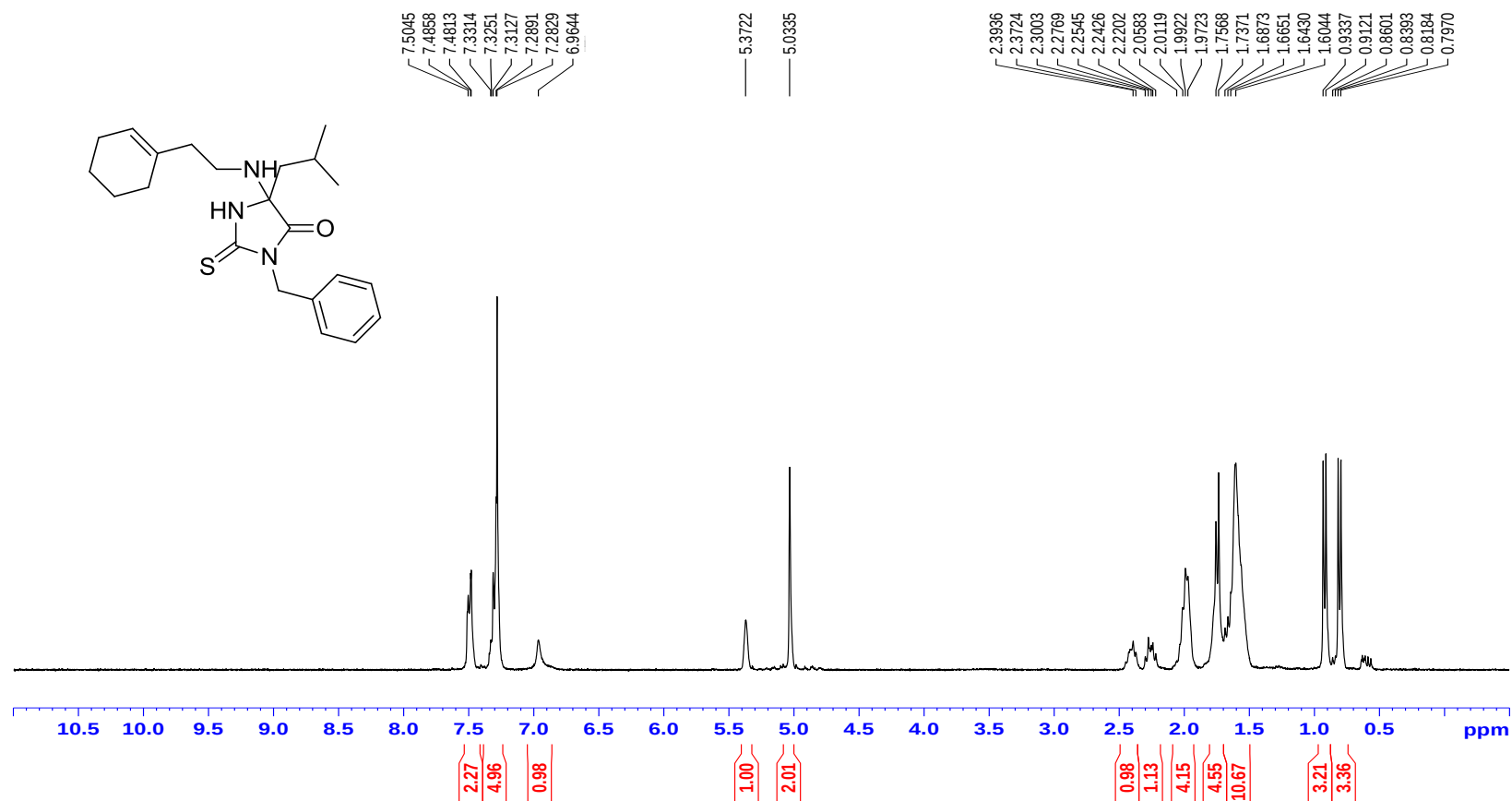
Scan 13 from c:\service\direct\20140415\2014-04-15_mani-5b.xms



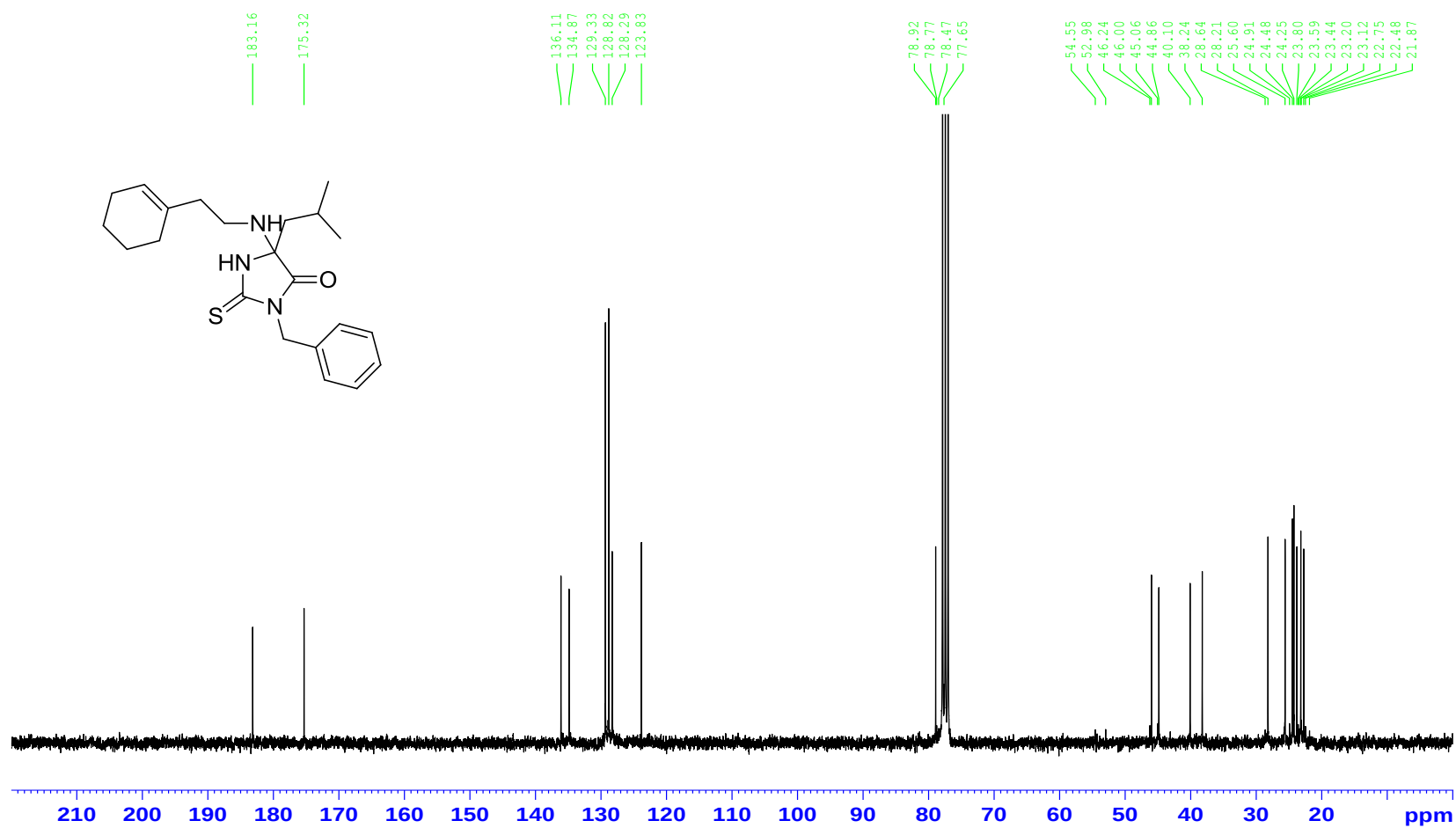
ESI Mass spectrum of compound 5{2,2,2}



HRMS Mass (ESI) spectrum of compound 5{2,2,2}

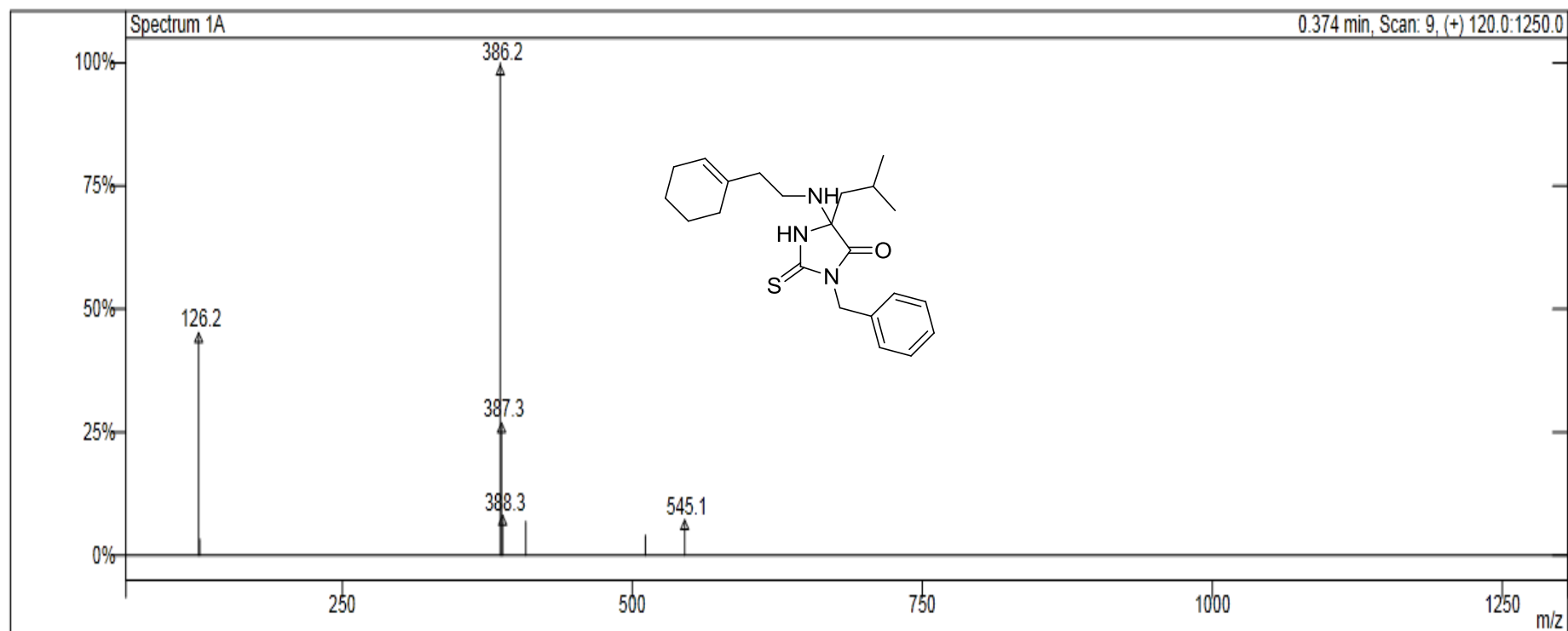


¹H NMR spectrum (300 MHz) of compound 5{5,2,2} in CDCl₃

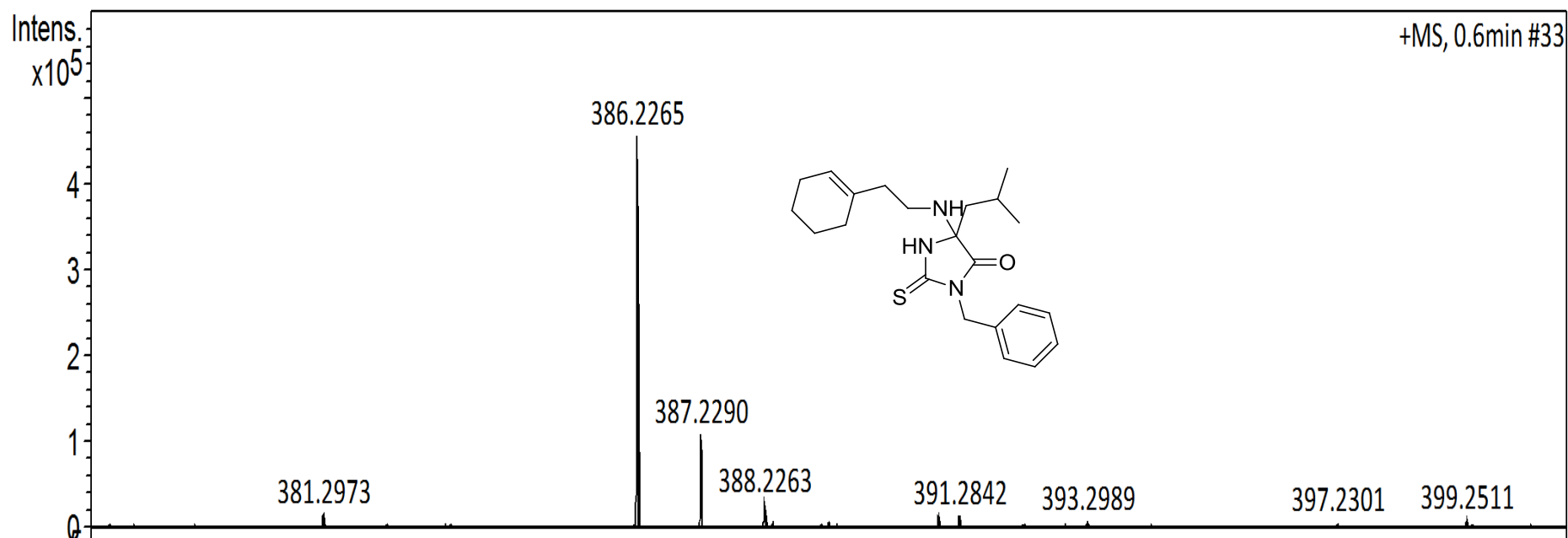


^{13}C spectrum (75 MHz) of compound 5{5,2,2} in CDCl_3

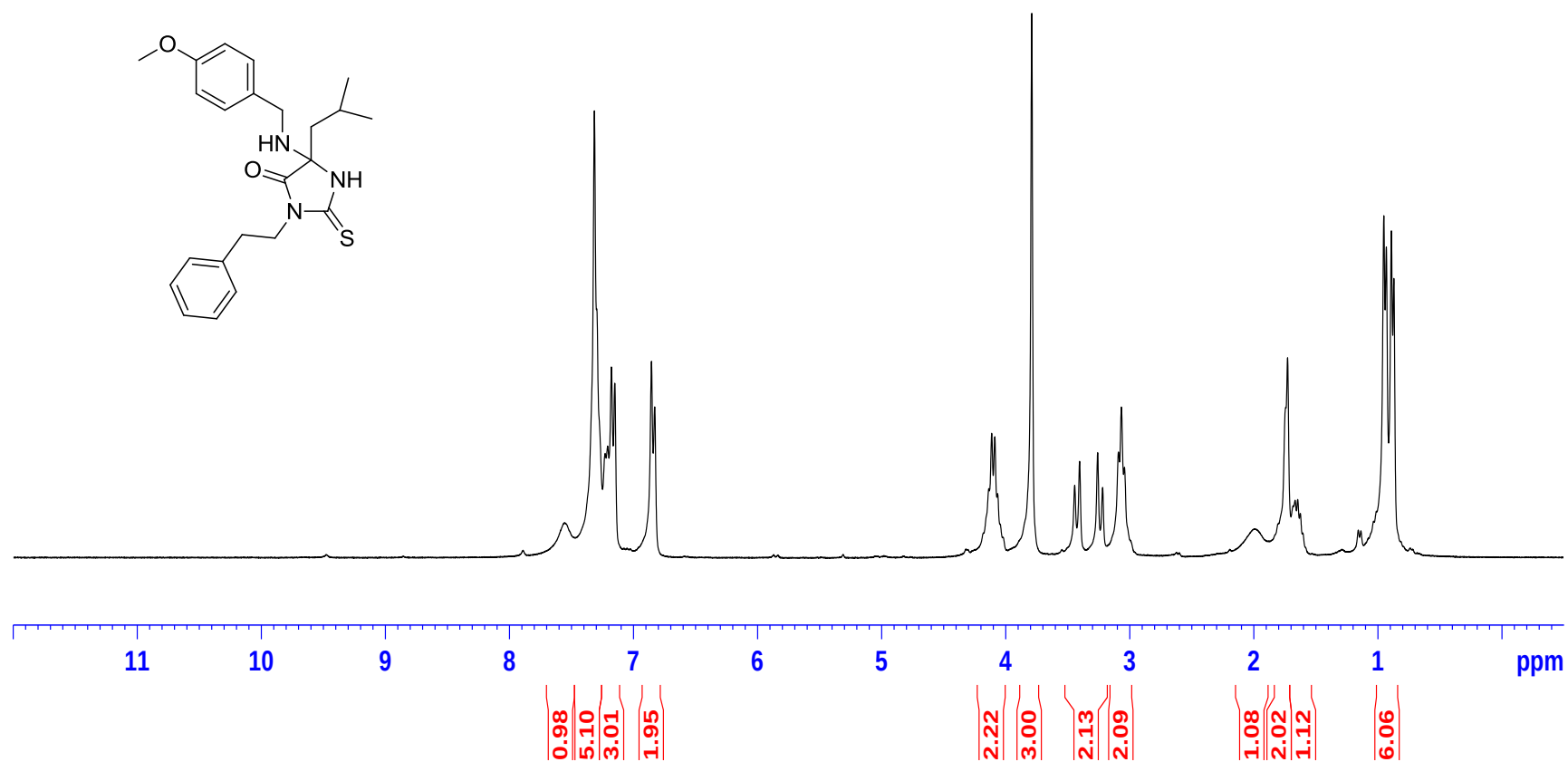
Scan 9 from c:\service\direct\20140415\2014-04-15_mani-5c.xms



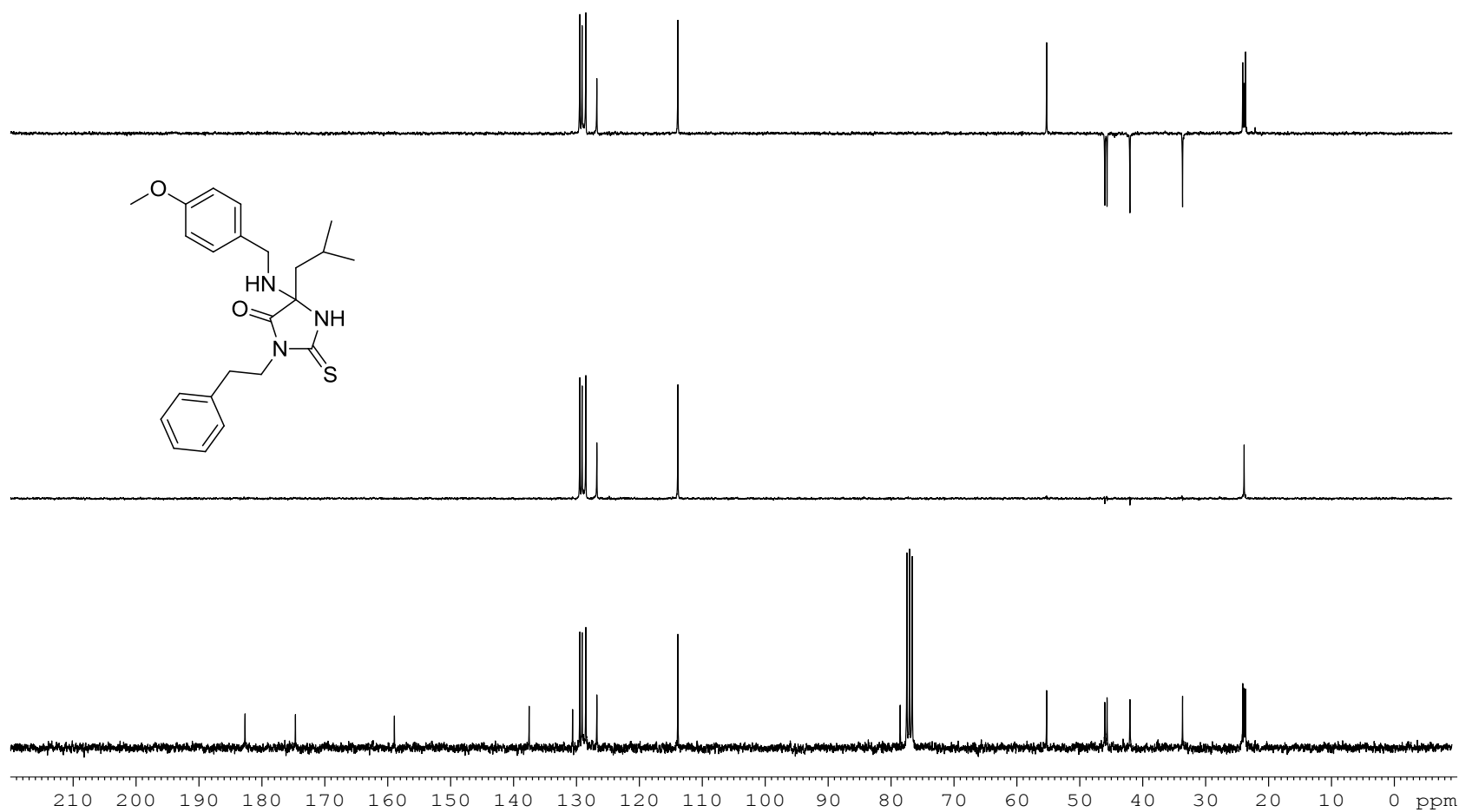
ESI Mass spectrum of compound 5{5,2,2}



HRMS Mass (ESI) spectrum of compound 5{5,2,2}



^1H NMR spectrum (300 MHz) of compound 5{5,4,3} in CDCl_3

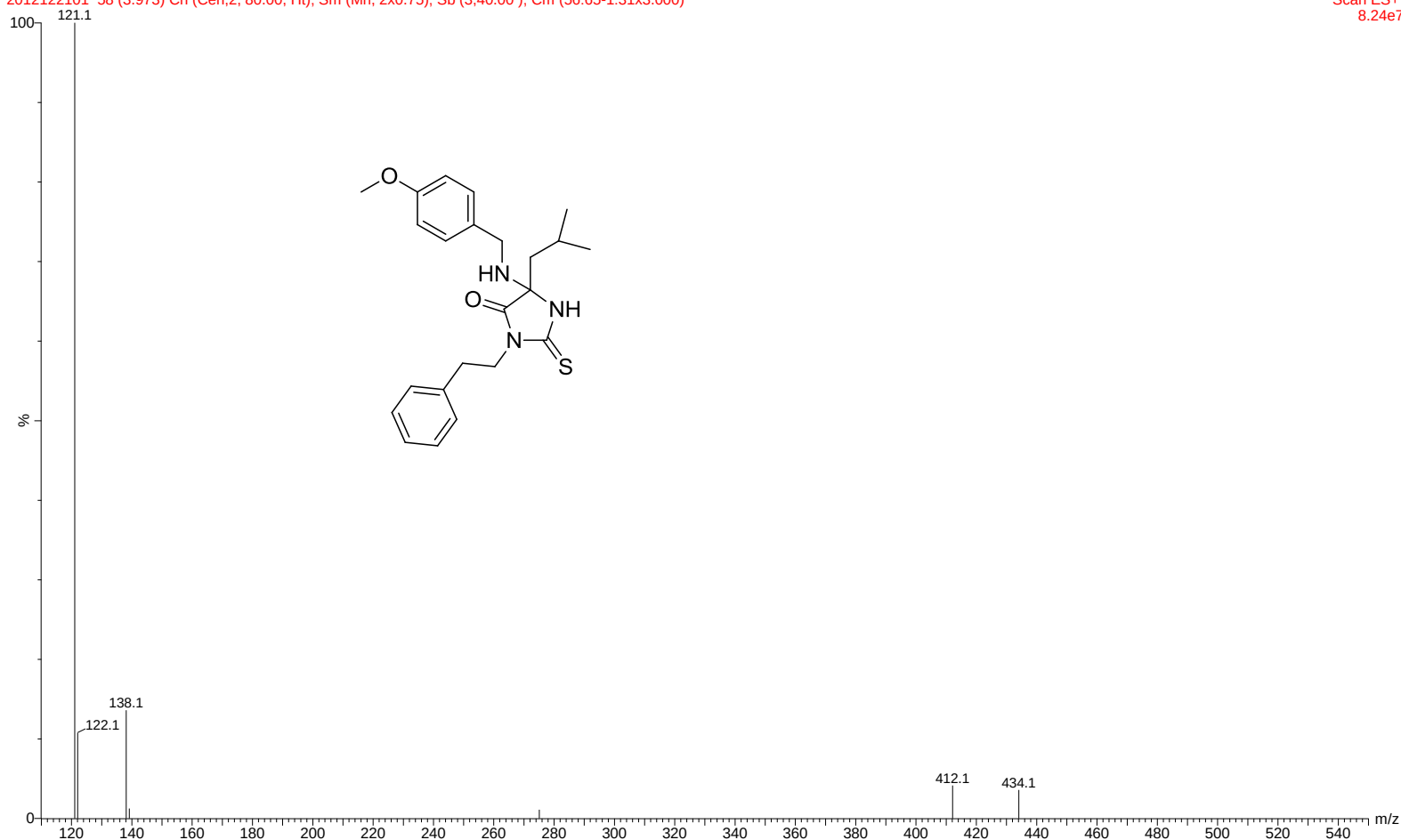


^{13}C and DEPT spectrum (75 MHz) of compound 5{5,4,3} in CDCl_3

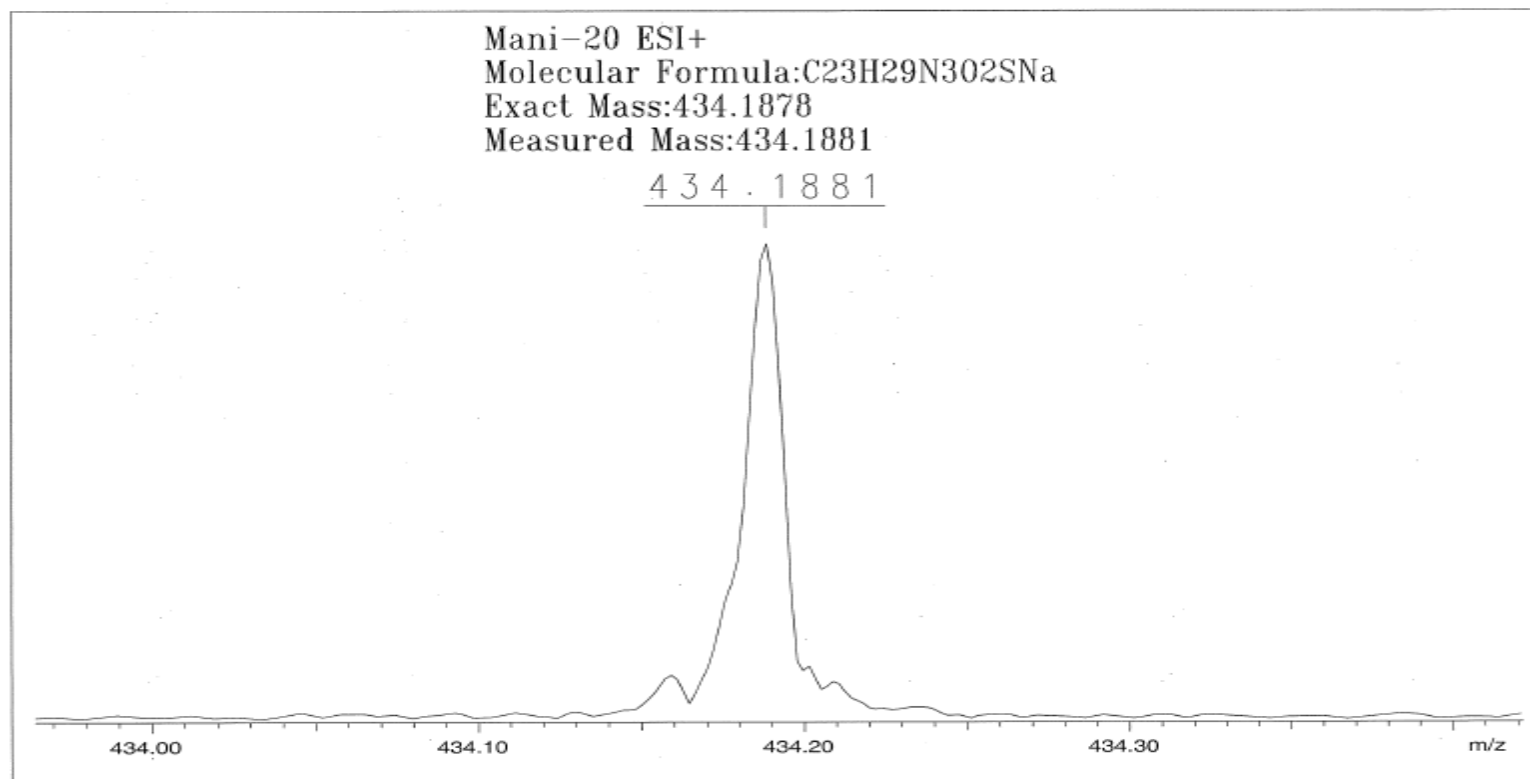
Mani-91-S1

2012122101 58 (3.973) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (56:65-1:31x3.000)

Scan ES+
8.24e7

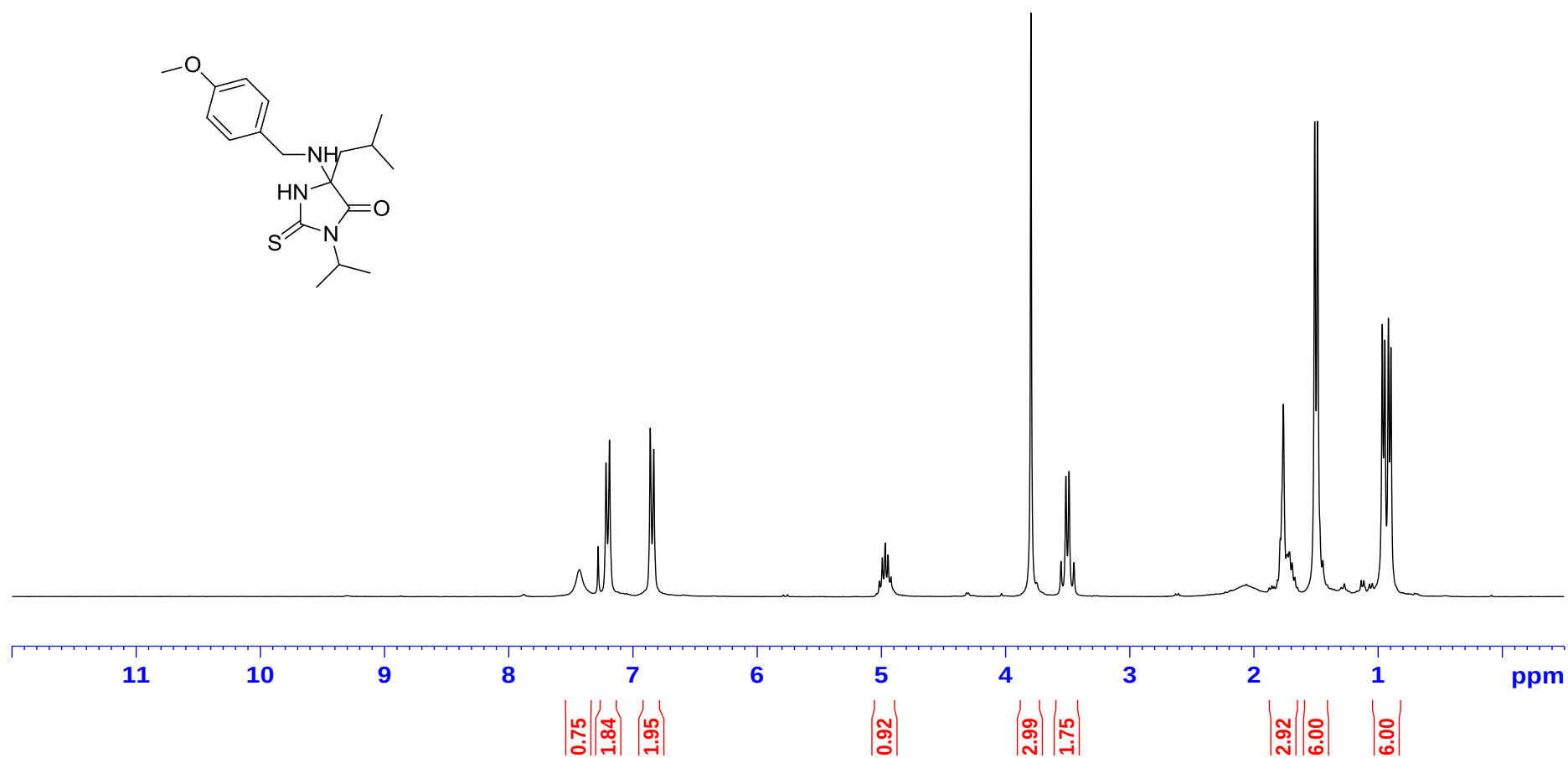


ESI Mass spectrum of compound 5{5,4,3}

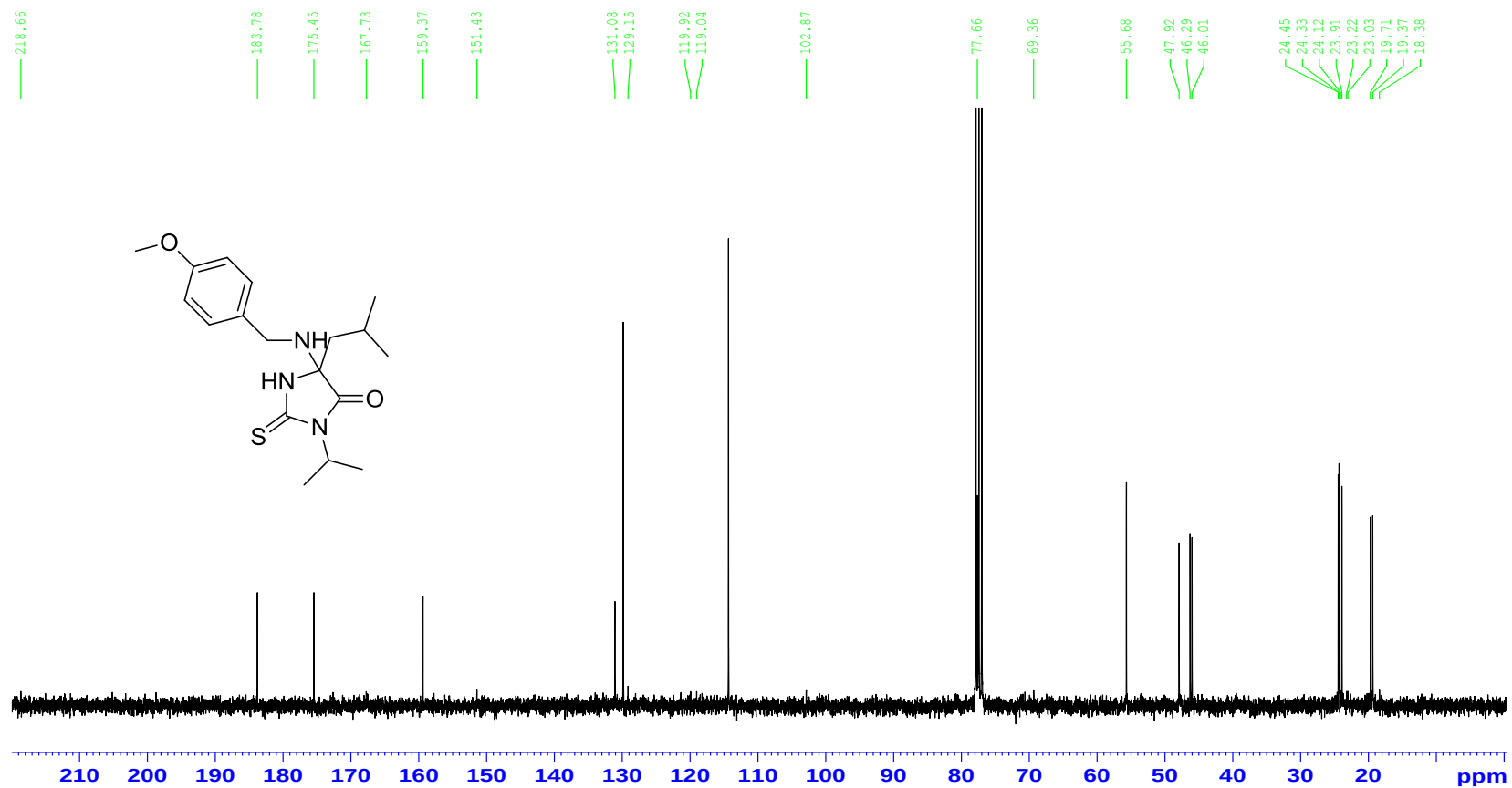


/d=/Data/yl/mani20/1/pdata/1 Administrator Tue Feb 7 14:33:30 2012

HRMS Mass (ESI) spectrum of compound 5{5,4,3}



¹H NMR spectrum (300 MHz) of compound 5{5,3,3} in CDCl₃

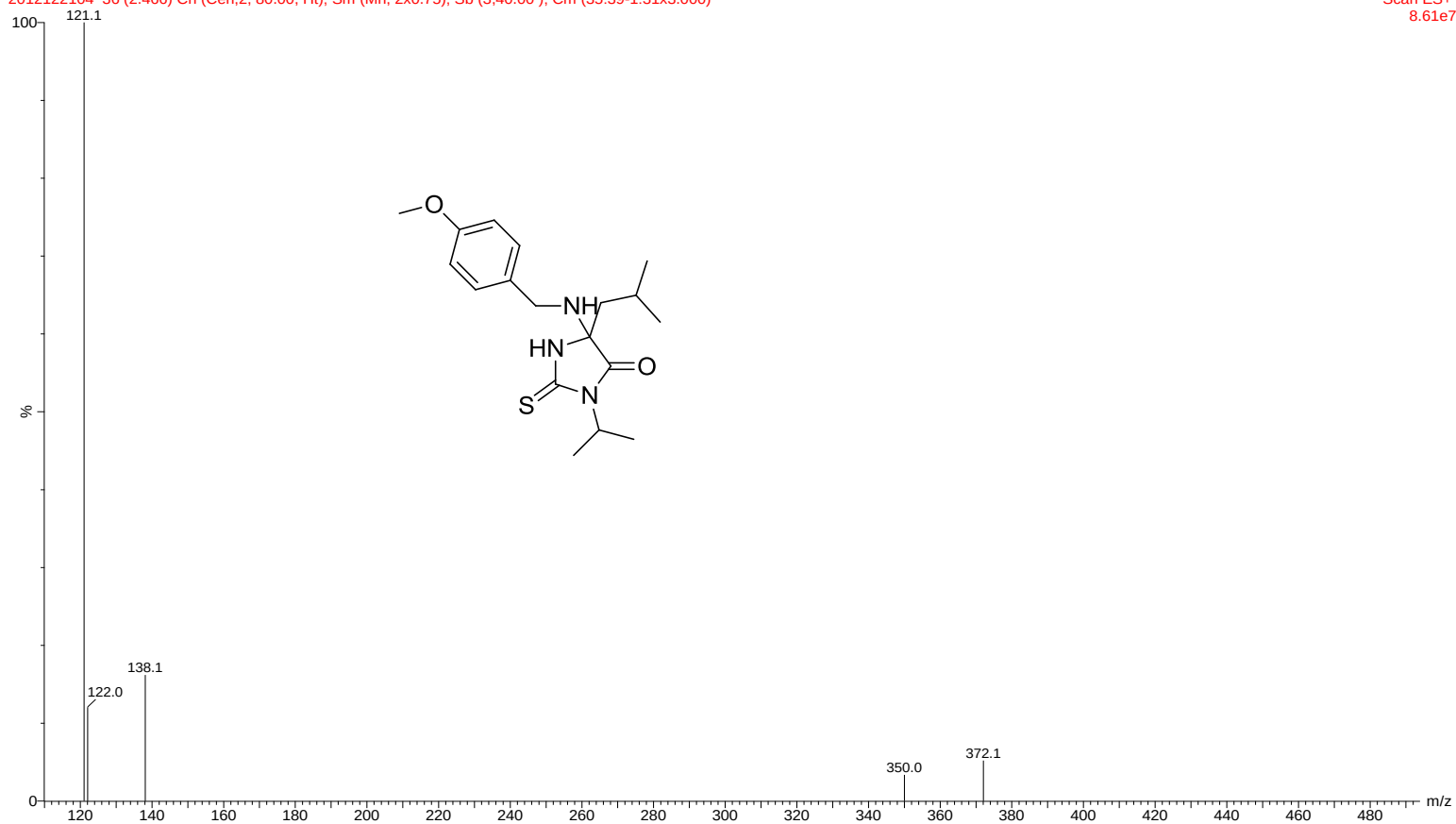


^{13}C spectrum (75 MHz) of compound 5{5,3,3} in CDCl_3

Mani-90-S1

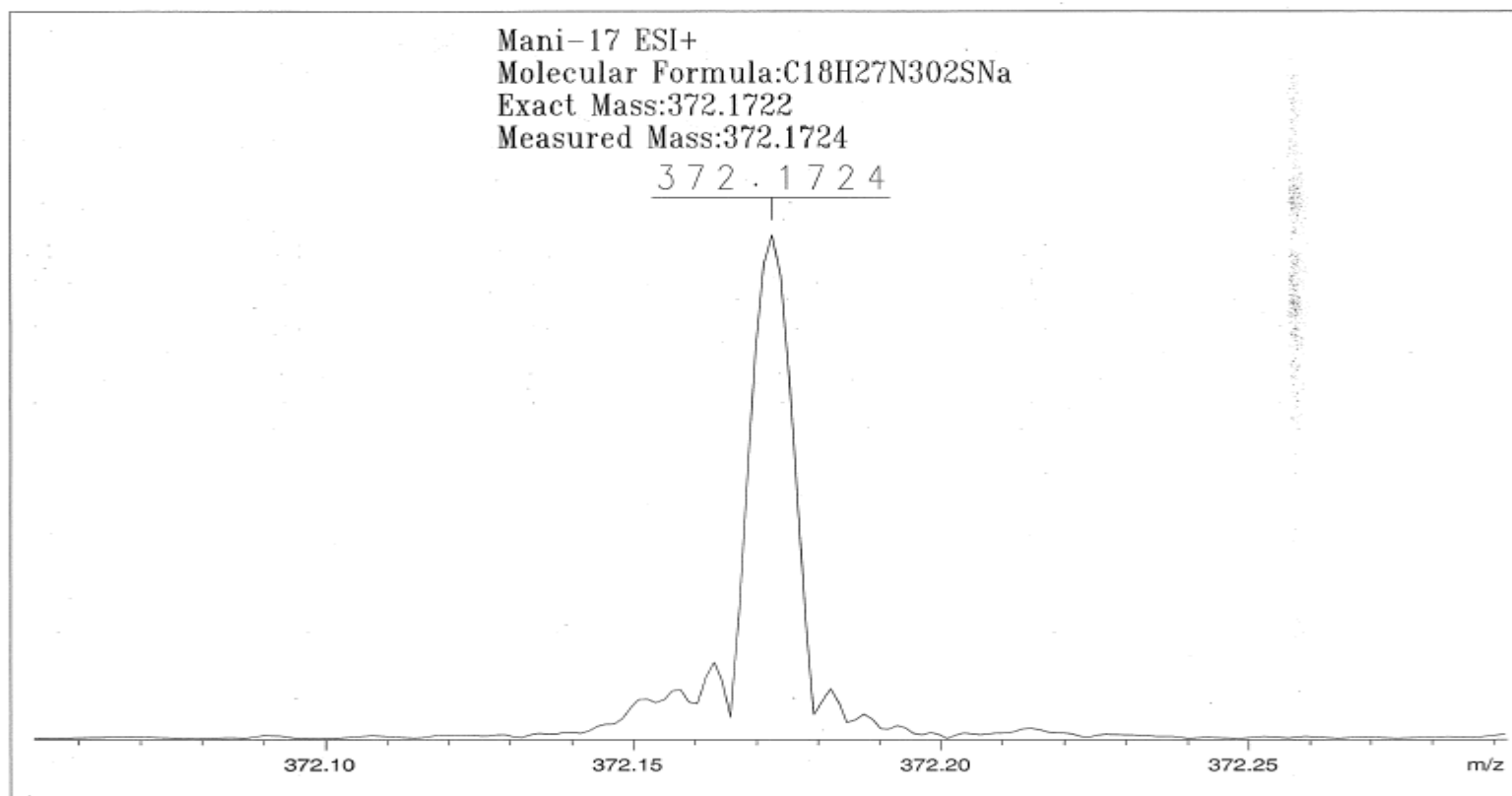
2012122104 36 (2.466) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (35:39-1:31x3.000)

Scan ES+
8.61e7



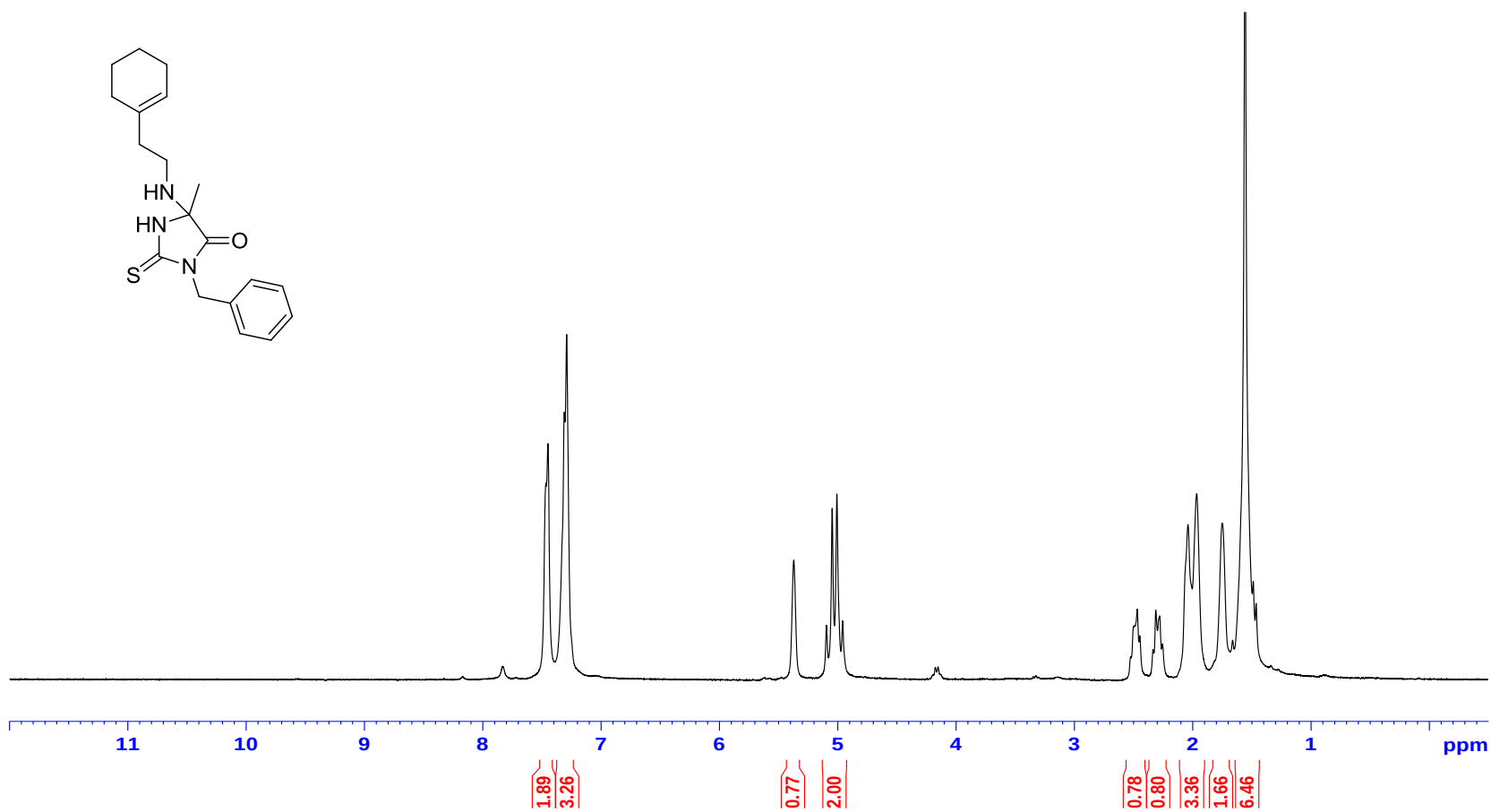
ESI Mass spectrum of compound 5{5,3,3}

S-29

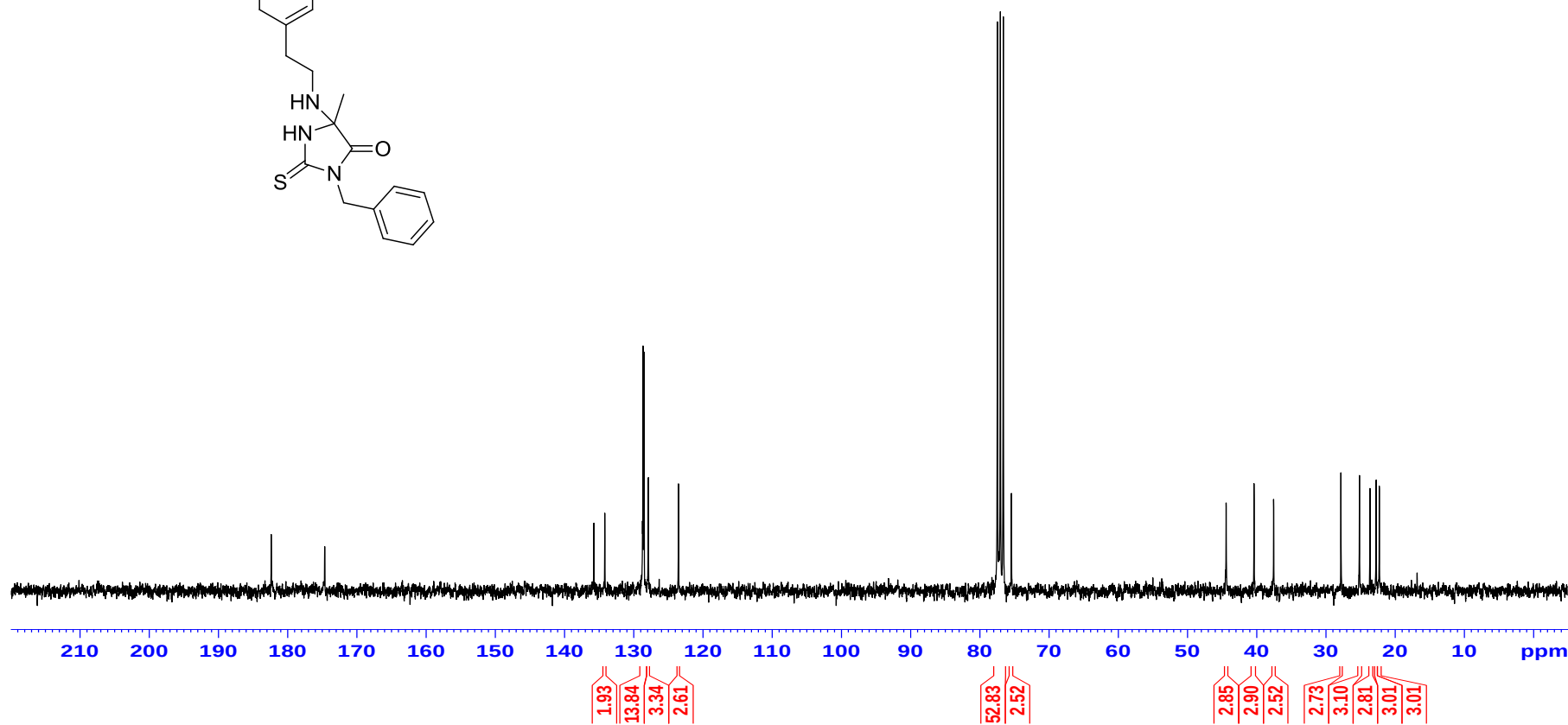
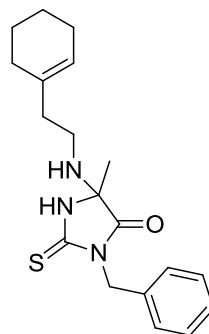


/d=/Data/yu/mani17/2/pdata/1 Administrator Tue Feb 7 16:54:31 2012

HRMS Mass (ESI) spectrum of compound 5{5,3,3}



^1H NMR spectrum (300 MHz) of compound 5{3,2,2} in CDCl_3

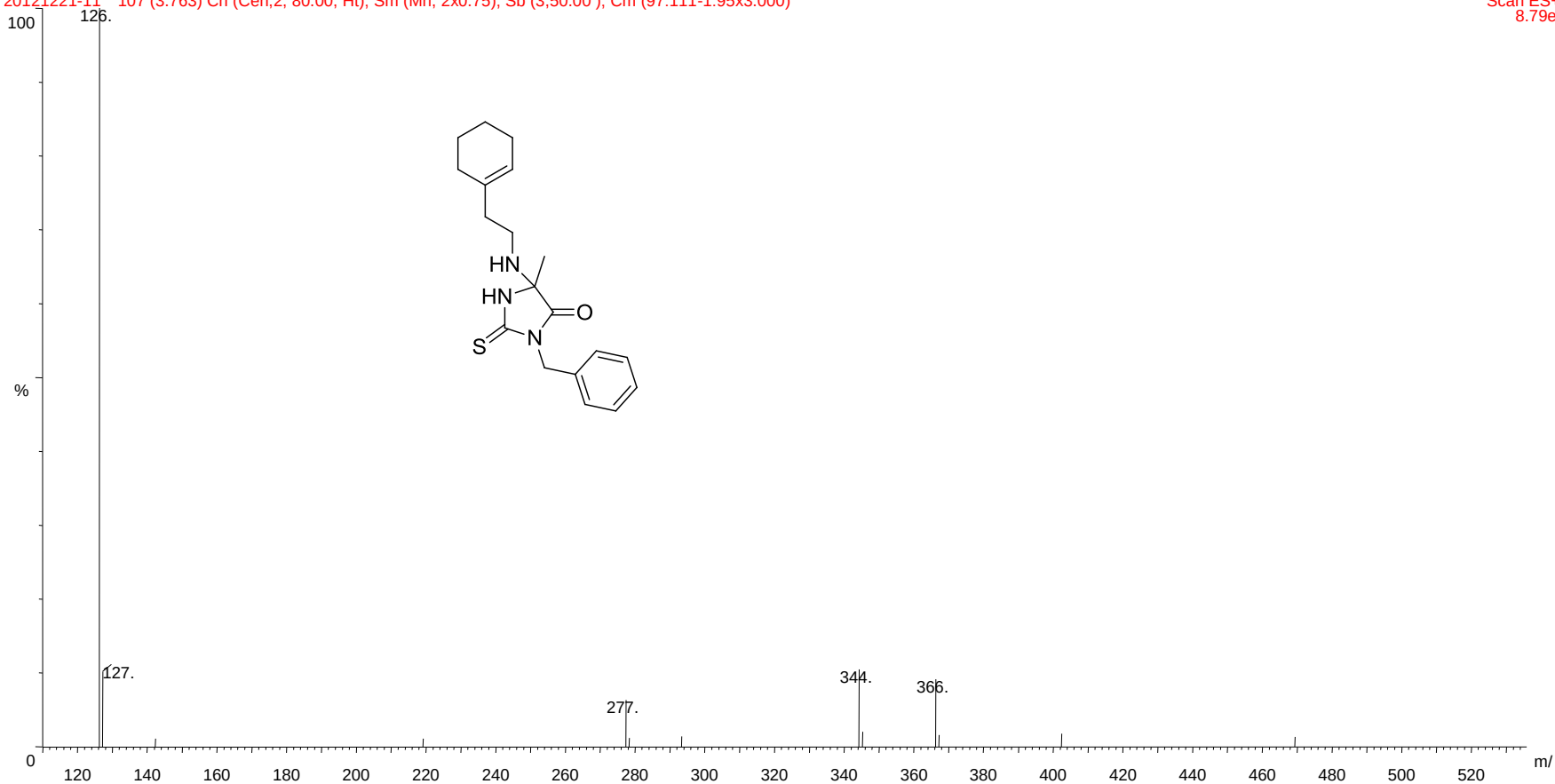


^{13}C spectrum (75 MHz) of compound **5{3,2,2}** in CDCl_3

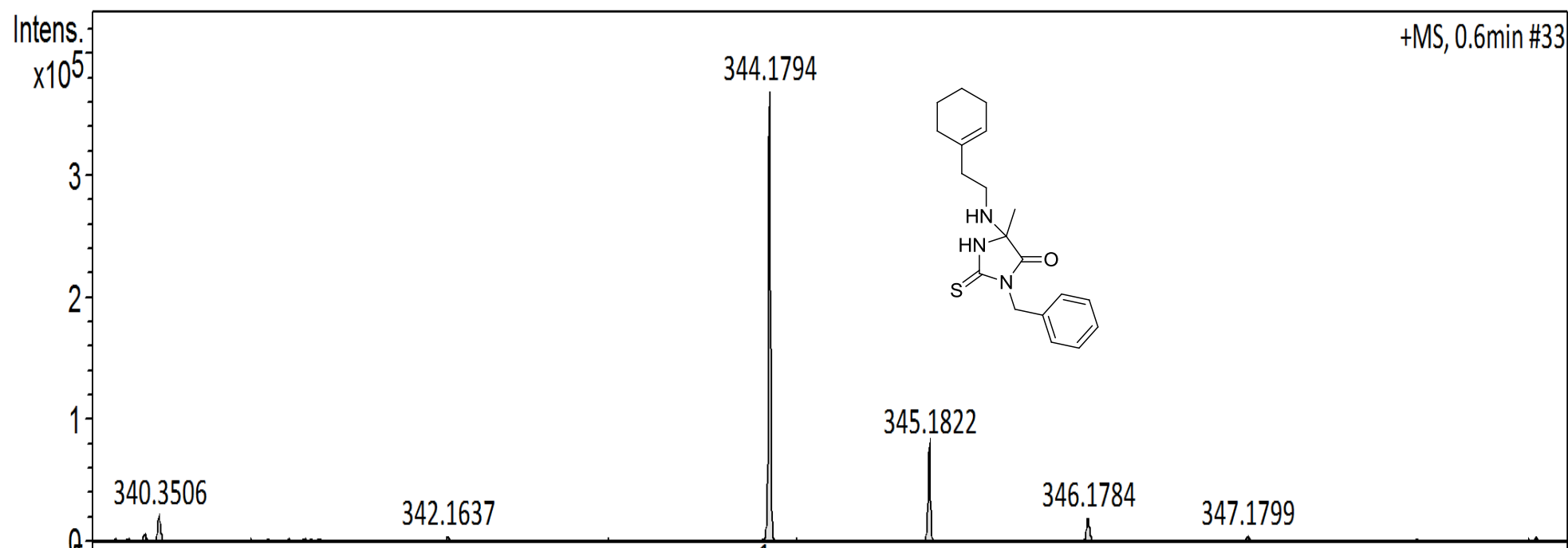
Mani-67-C

20121221-11 107 (3.763) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,50.00); Cm (97:111-1:95x3.000)

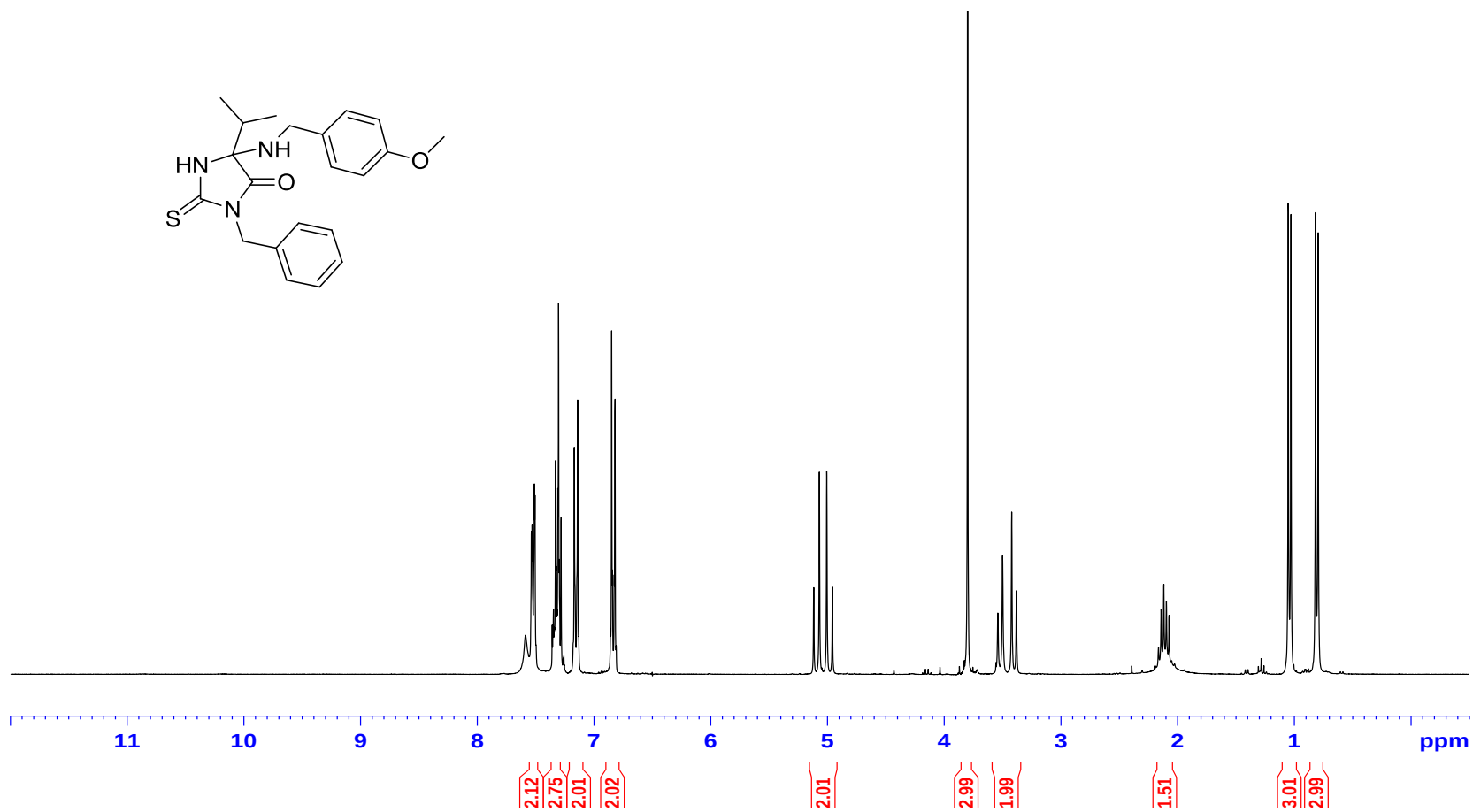
Scan ES+
8.79e7



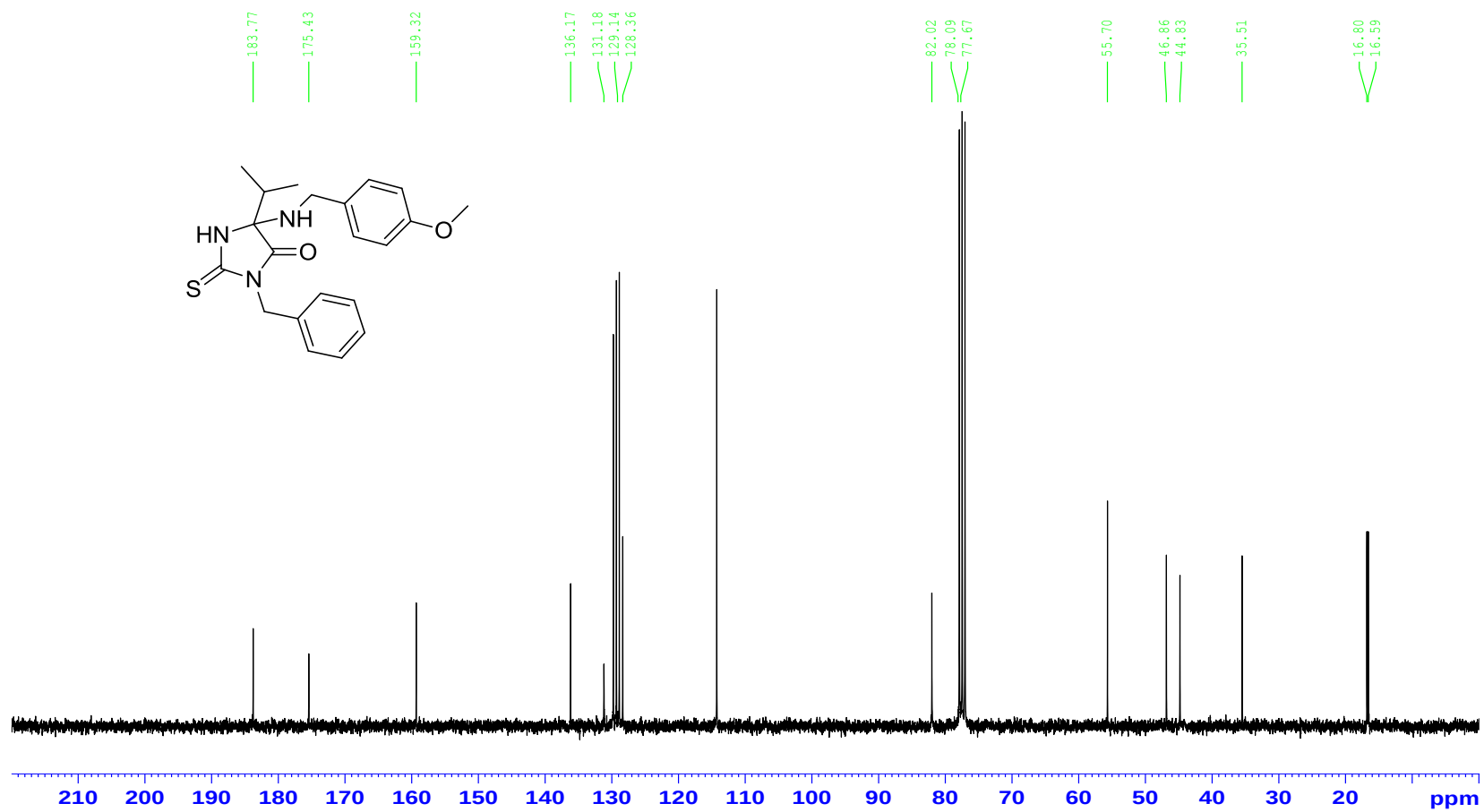
ESI Mass spectrum of compound 5{3,2,2}



HRMS Mass (ESI) spectrum of compound 5{3,2,2}



¹H NMR spectrum (300 MHz) of compound 5{4,2,3} in CDCl₃

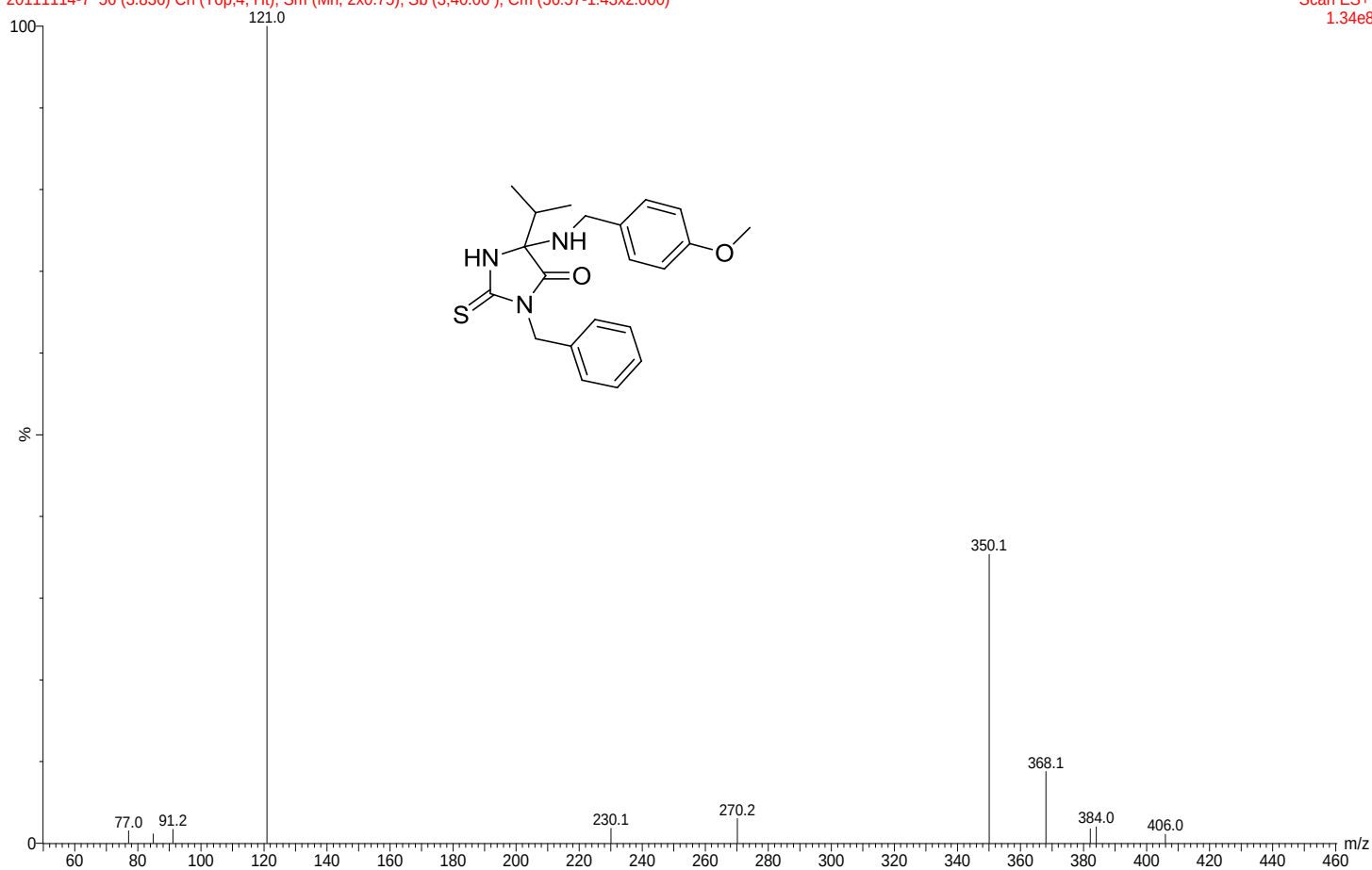


^{13}C spectrum (75 MHz) of compound 5{4,2,3} in CDCl_3

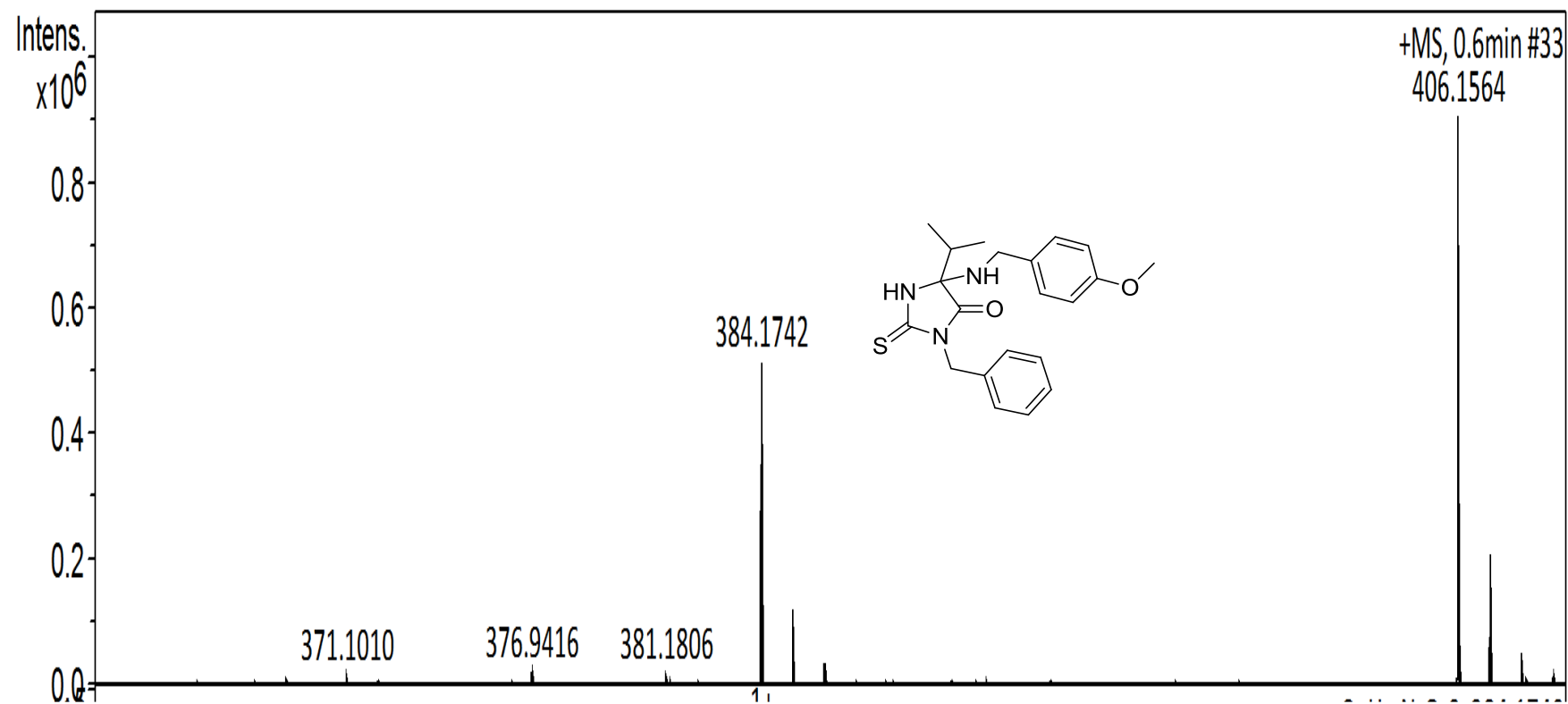
mani-v1

20111114-7 56 (3.836) Cn (Top,4, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (56:57-1:43x2.000)

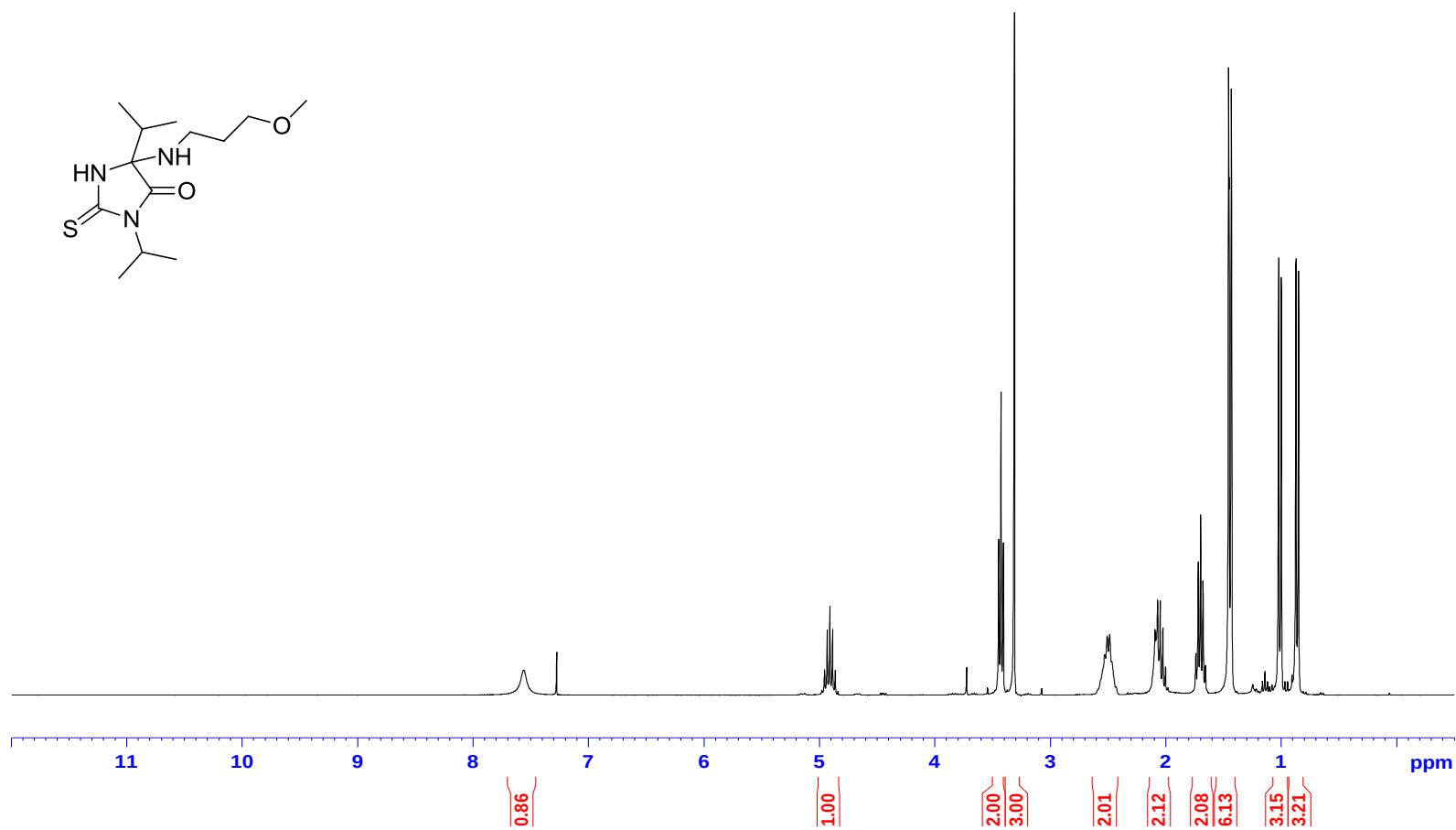
Scan ES+
1.34e8



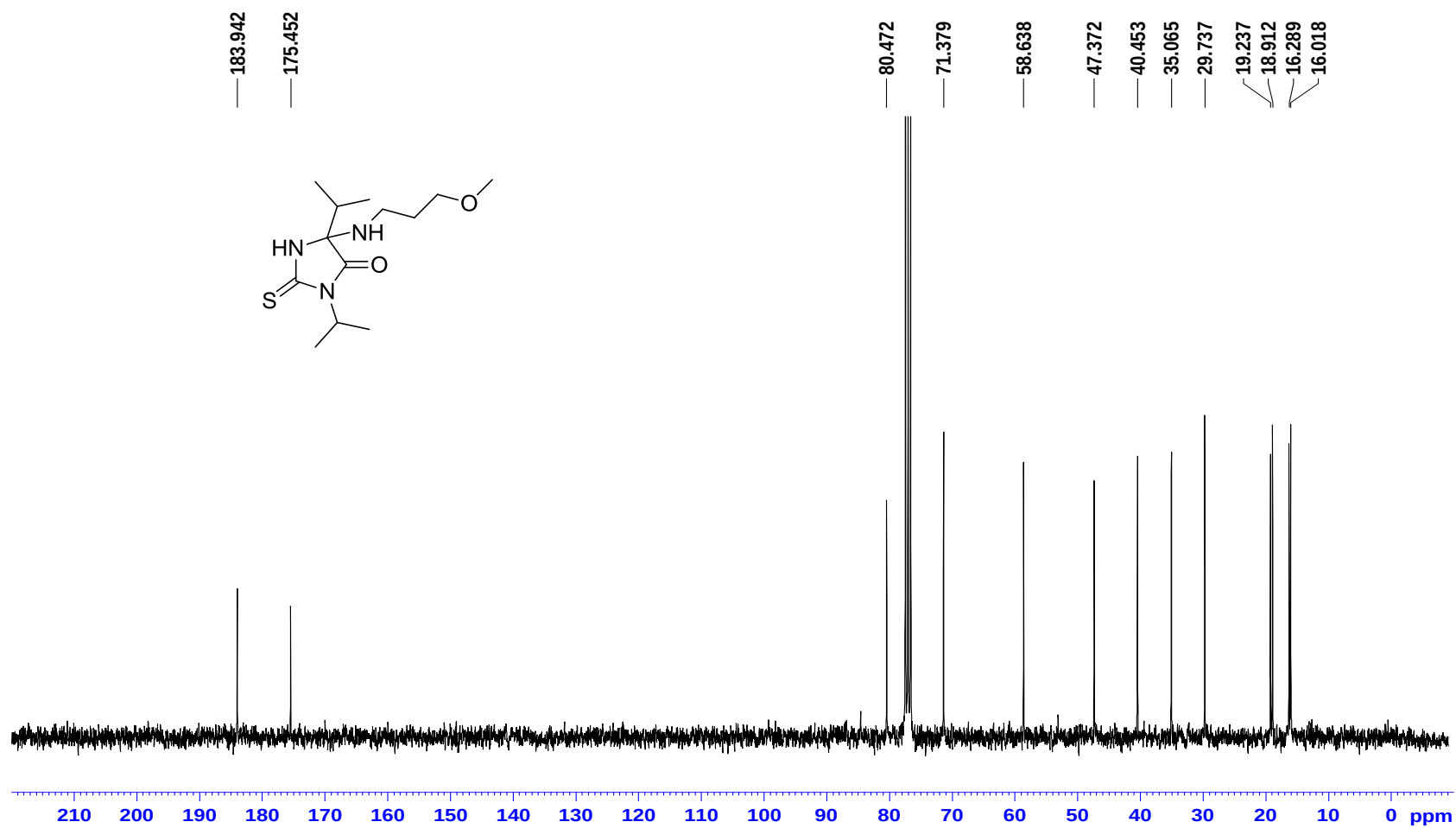
ESI Mass spectrum of compound 5{4,2,3}



HRMS Mass (ESI) spectrum of compound 5{4,2,3}



^1H NMR spectrum (300 MHz) of compound 5{4,3,4} in CDCl_3

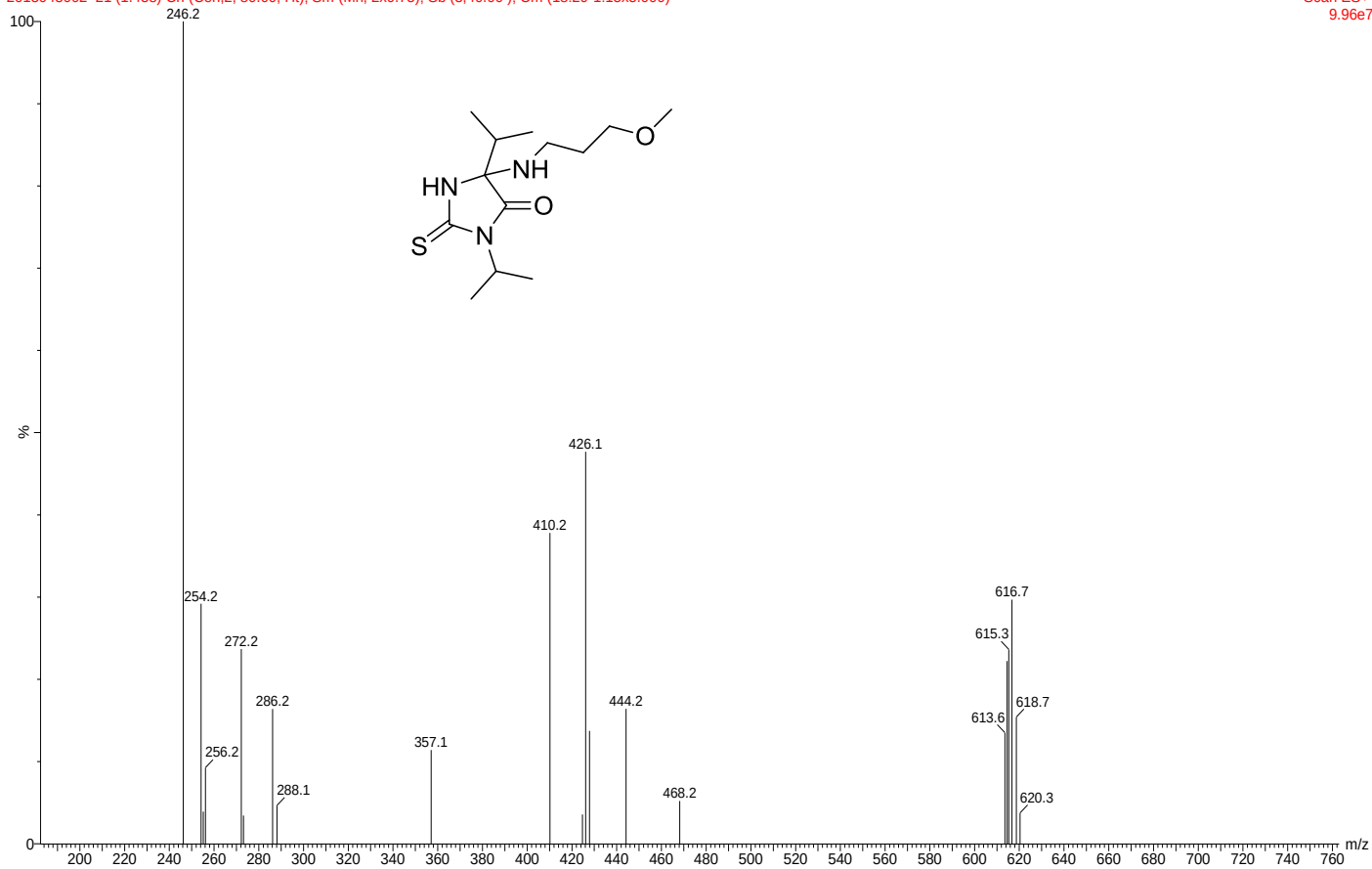


¹³C spectrum (75 MHz) of compound 5{4,3,4} in CDCl₃

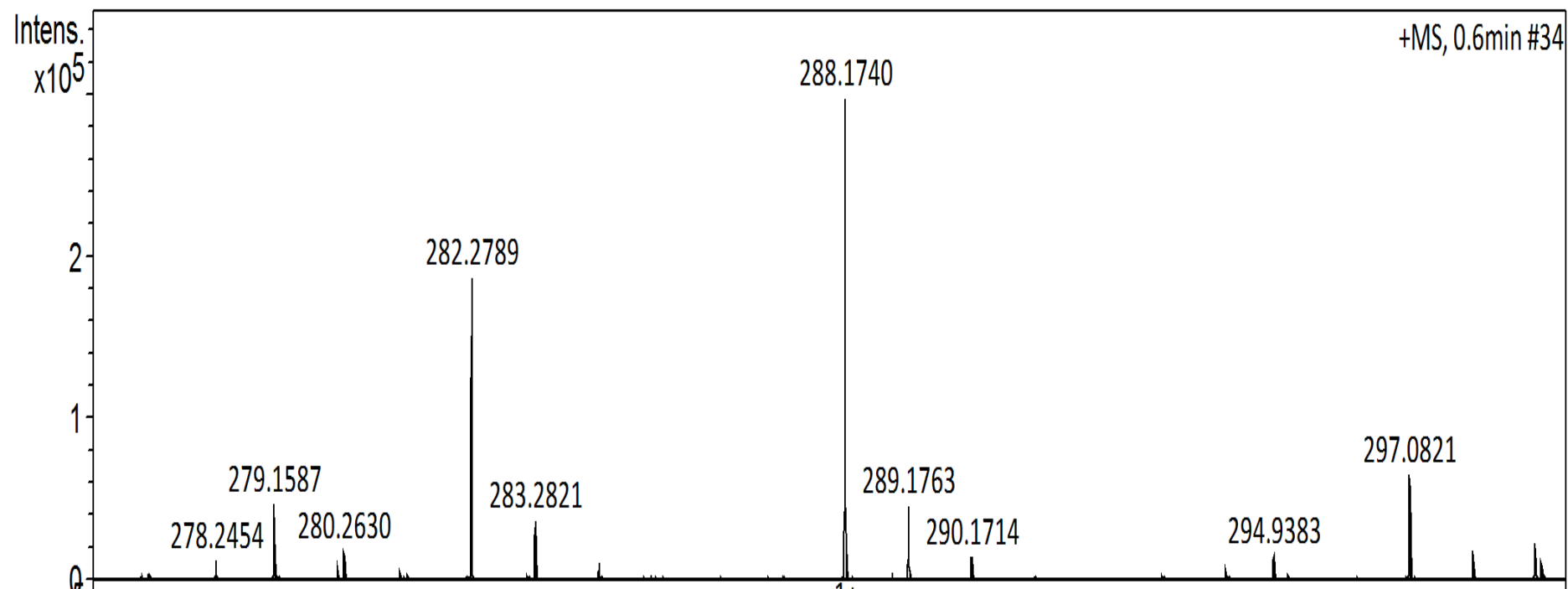
Mani-8-AI-C

2013043002 21 (1.438) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (18:29-1:15x5.000)

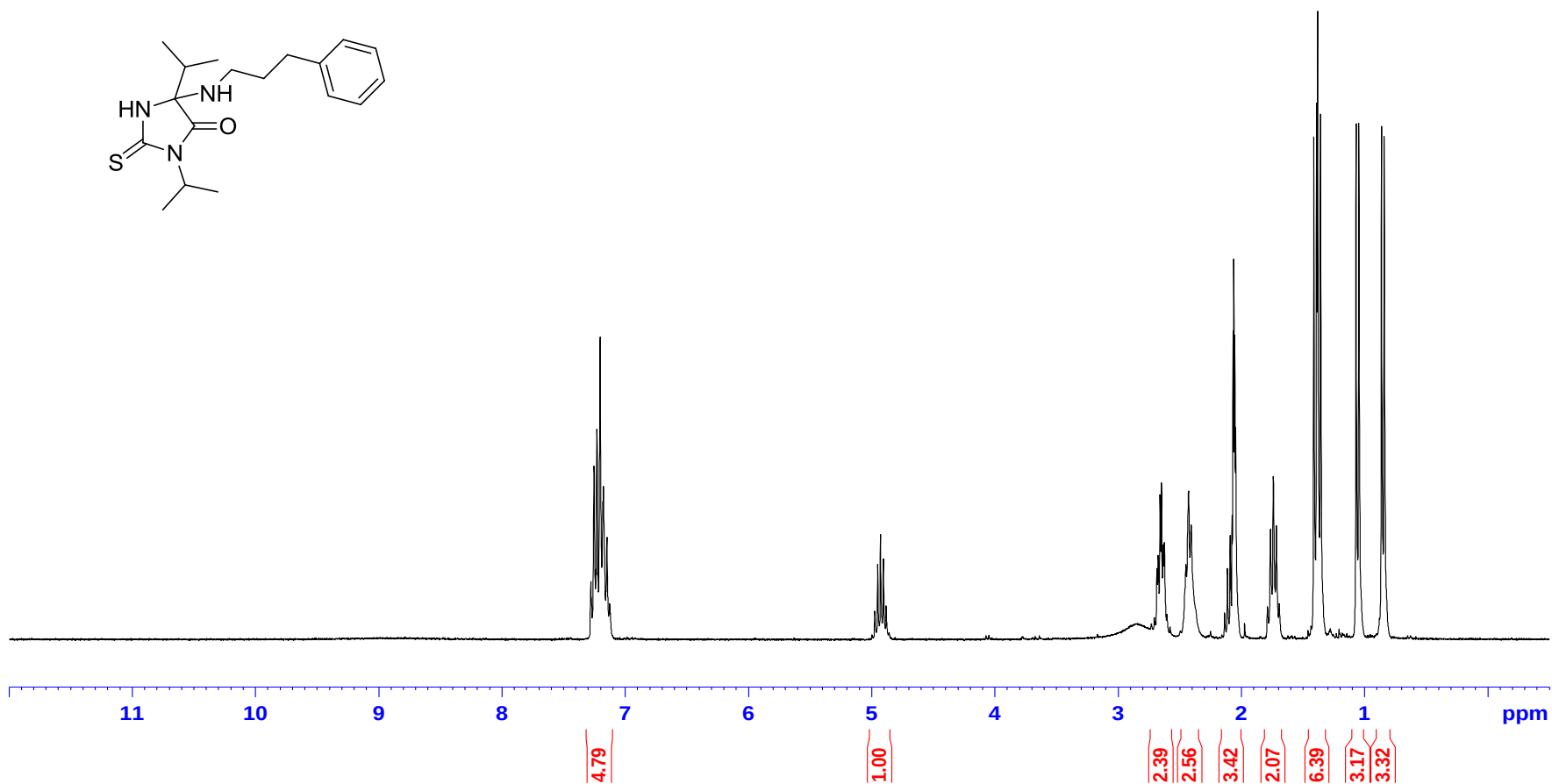
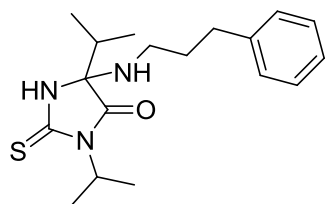
Scan ES+
9.96e7



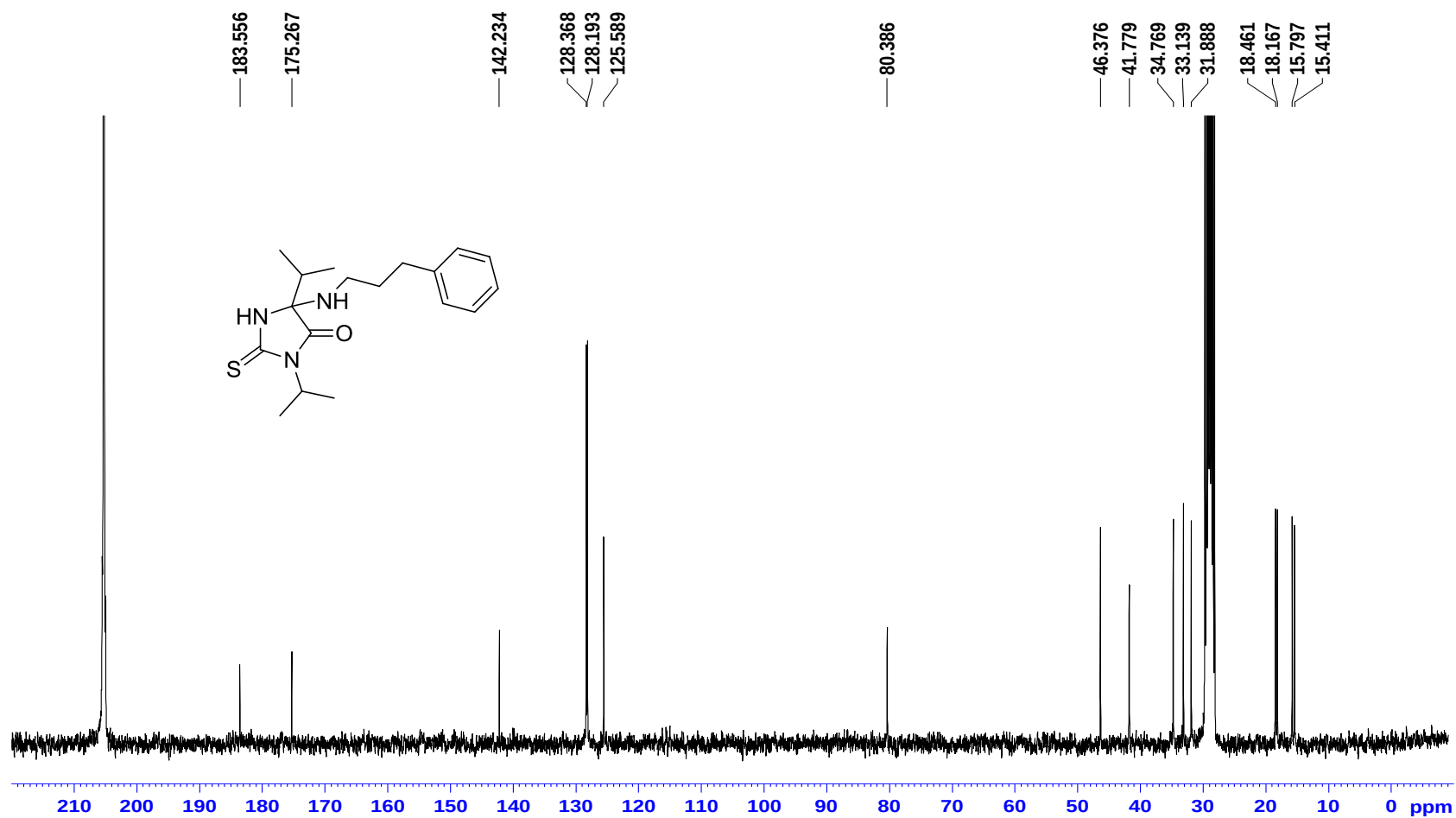
ESI Mass spectrum of compound 5{4,3,4}



HRMS Mass (ESI) spectrum of compound 5{4,3,4}



^1H NMR spectrum (300 MHz) of compound 5{4,3,4} in d-acetone

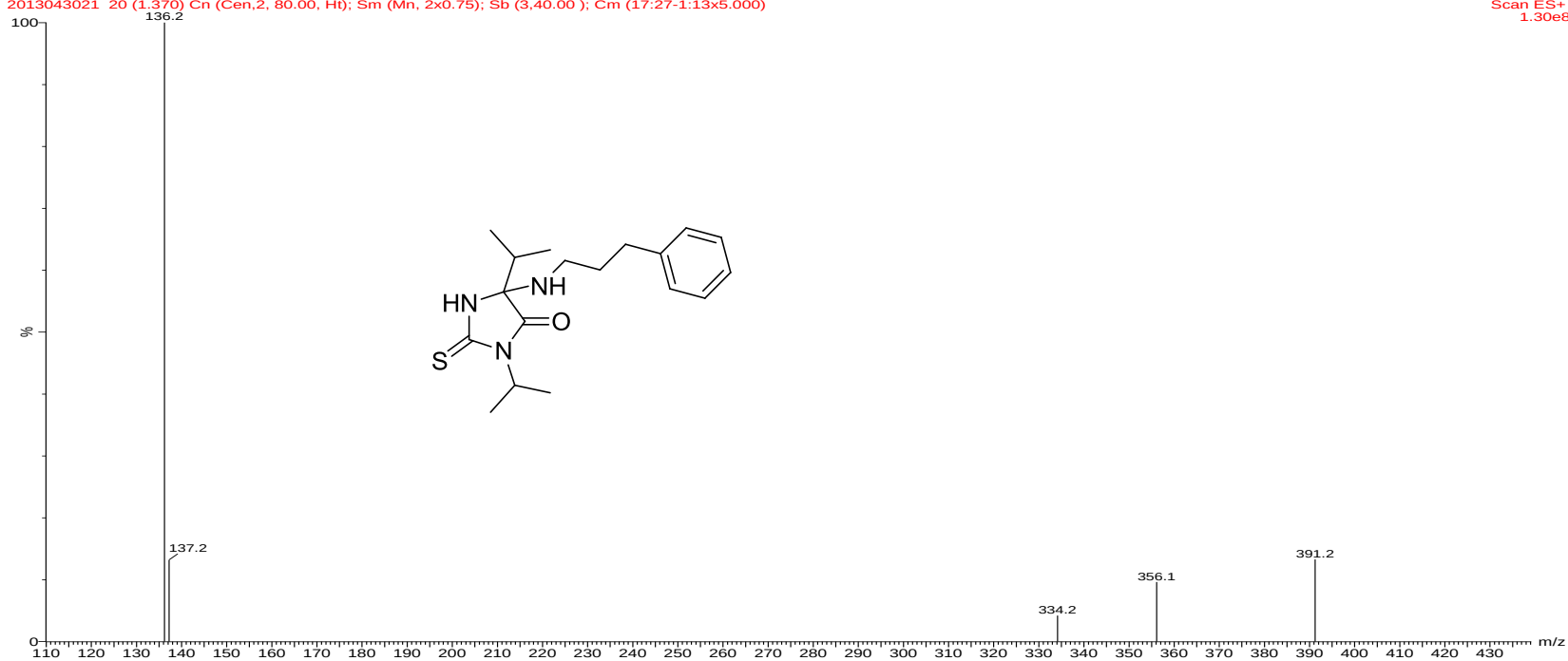


¹³C spectrum (75 MHz) of compound 5{4,3,4} in d-acetone

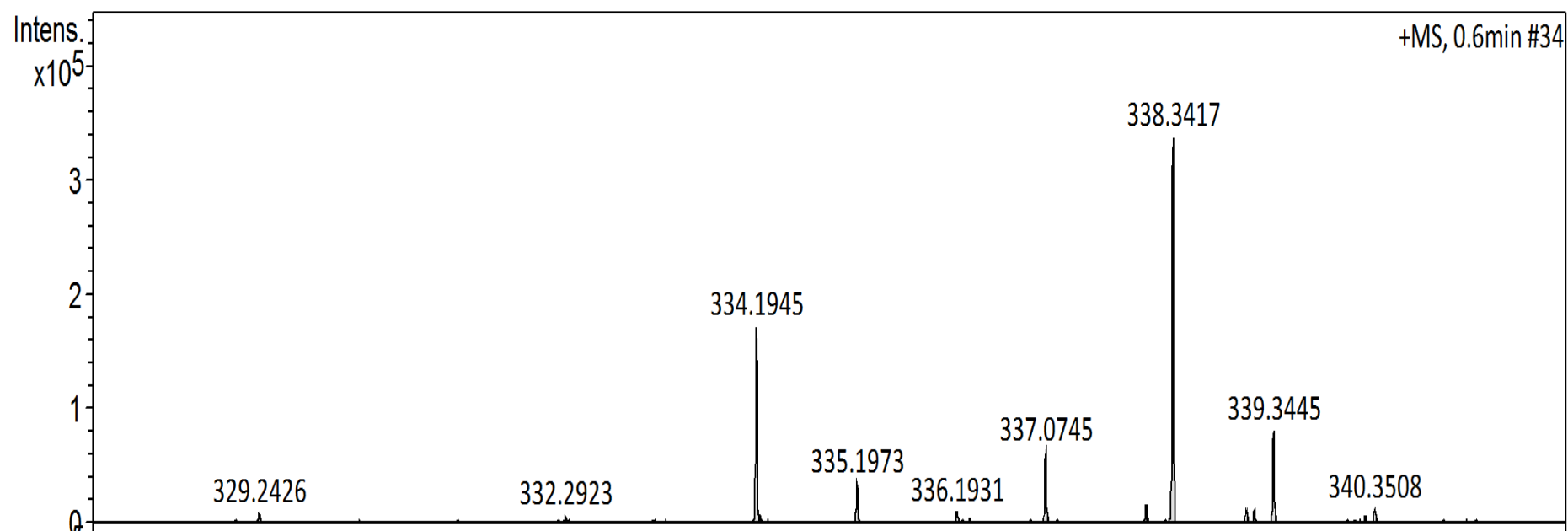
Mani-9-S1

2013043021 20 (1.370) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (17:27-1:13x5.000)

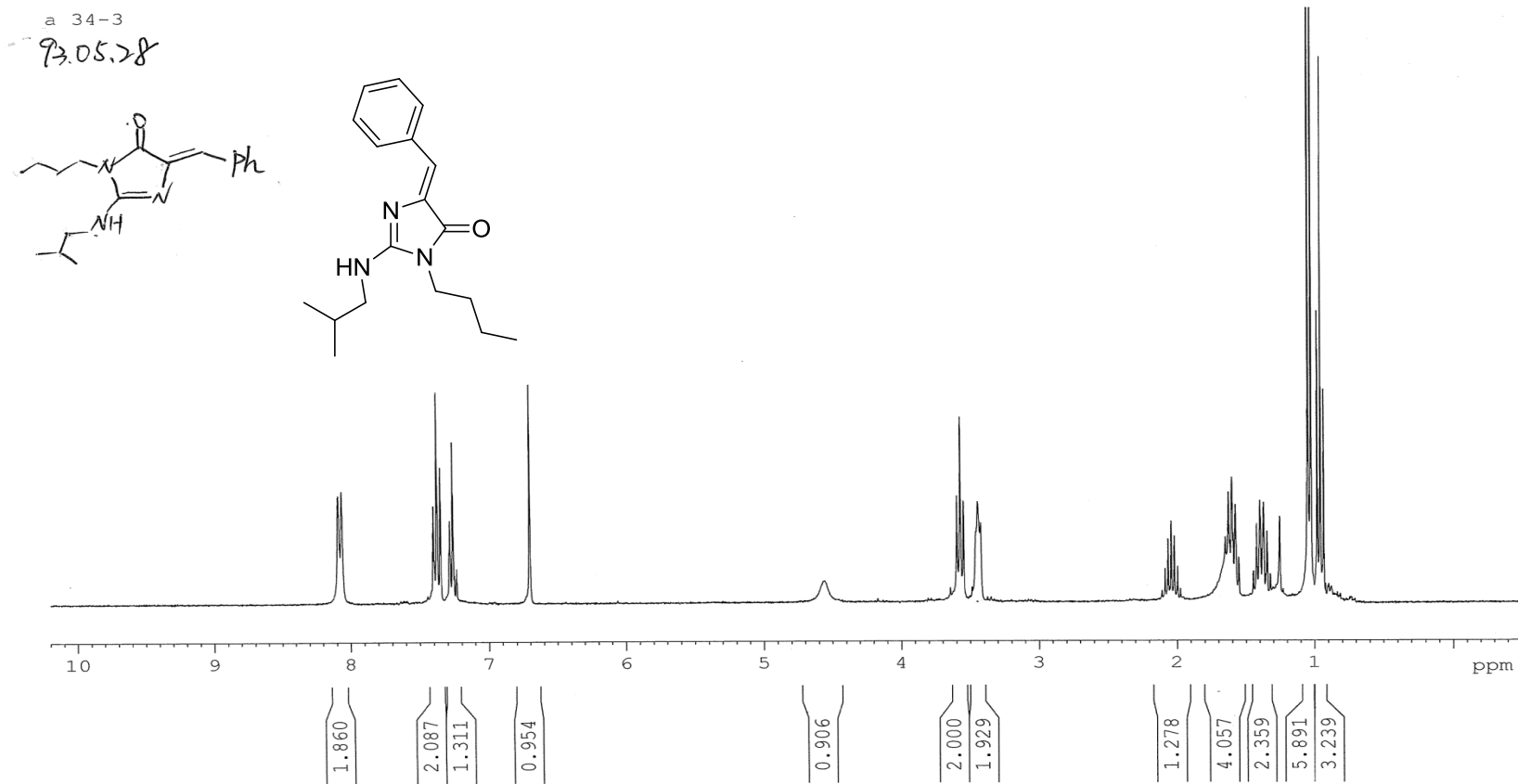
Scan ES+
1.30e8



ESI Mass spectrum of compound 5{4,3,4}

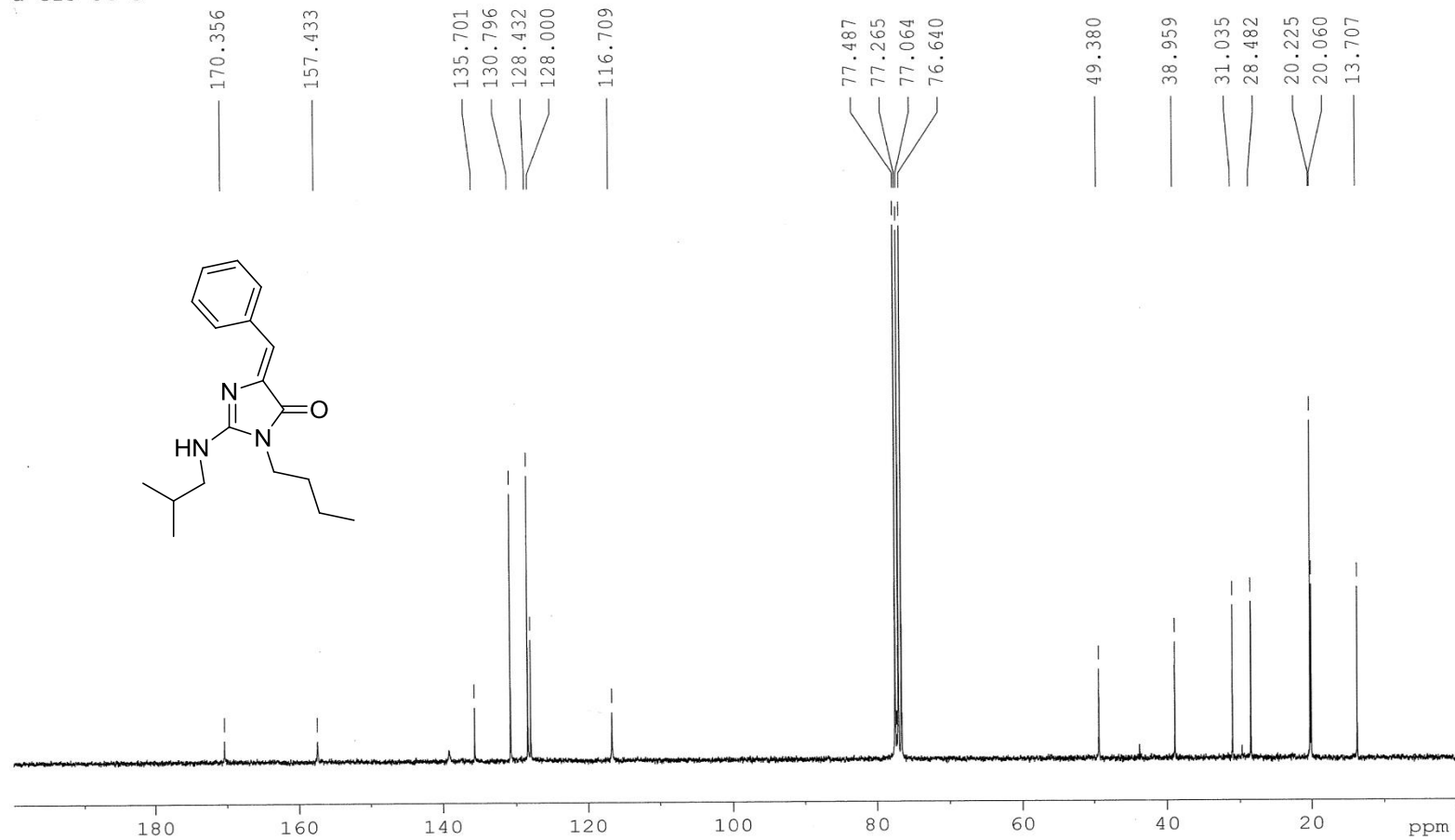


HRMS Mass (ESI) spectrum of compound 5{4,3,4}



¹H NMR spectrum (300 MHz) of compound **6{1,1,1}** in CDCl₃

a-c13 34-3

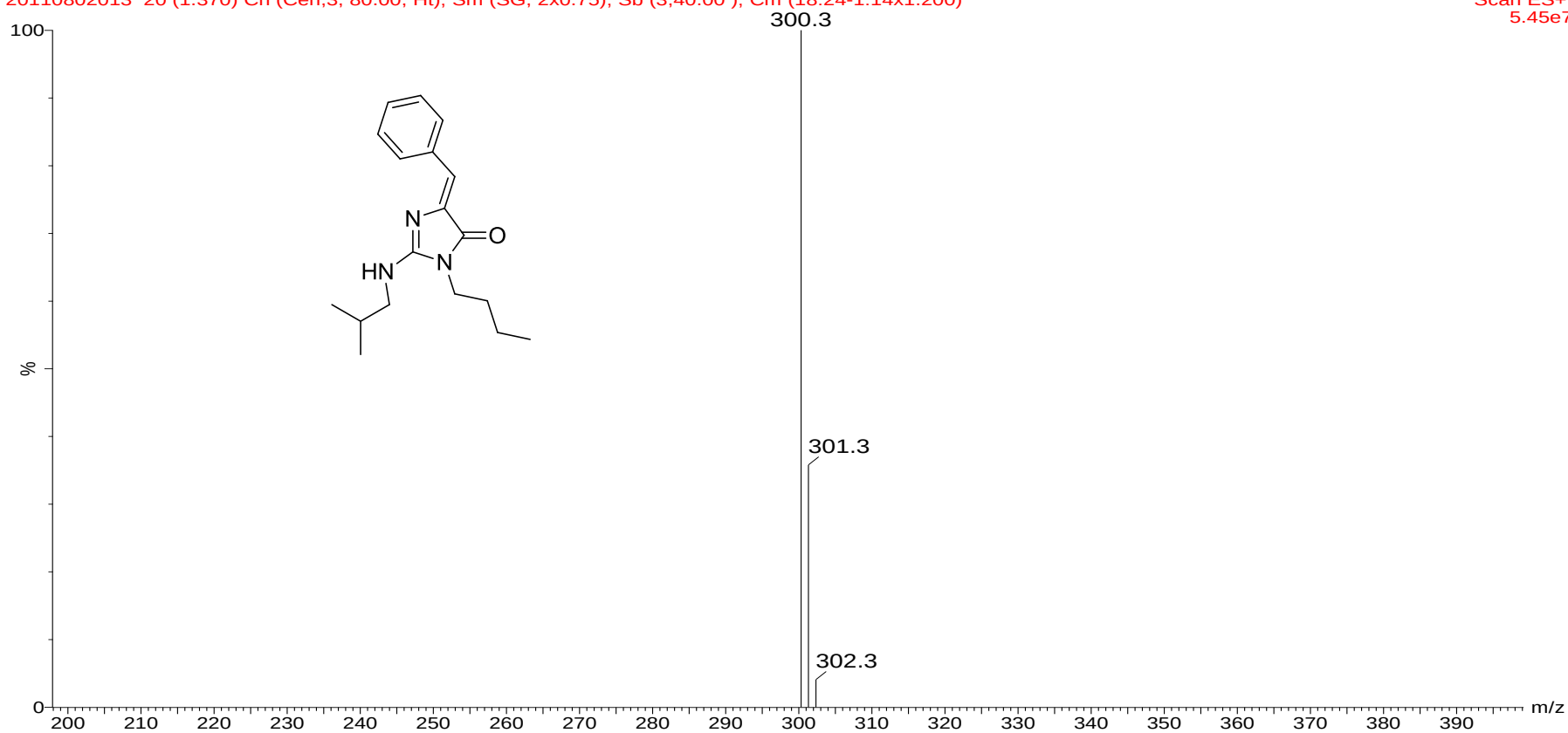


¹³C spectrum (75 MHz) of compound 6{1,1,1} in CDCl₃

Main-Hg2

20110802013 20 (1.370) Cn (Cen,3, 80.00, Ht); Sm (SG, 2x0.75); Sb (3,40.00); Cm (18:24-1:14x1.200)

Scan ES+
5.45e7



ESI Mass spectrum of compound **6{1,1,1}**

[Elemental Composition]

Data : Corp. 11084003

Date : 15-Sep-2004 12:37

Sample: a34-3 = 299.1998 m/z (2004070044)

Note : Tsai (NTHU)

Inlet : Direct

Ion Mode : EI+

RT : 1.85 min

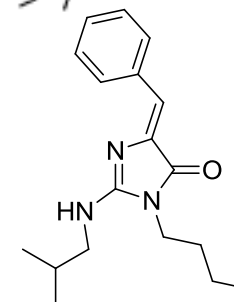
Scan#: 148

Elements : C 18/0, H 25/0, O 1/0, N 3/0

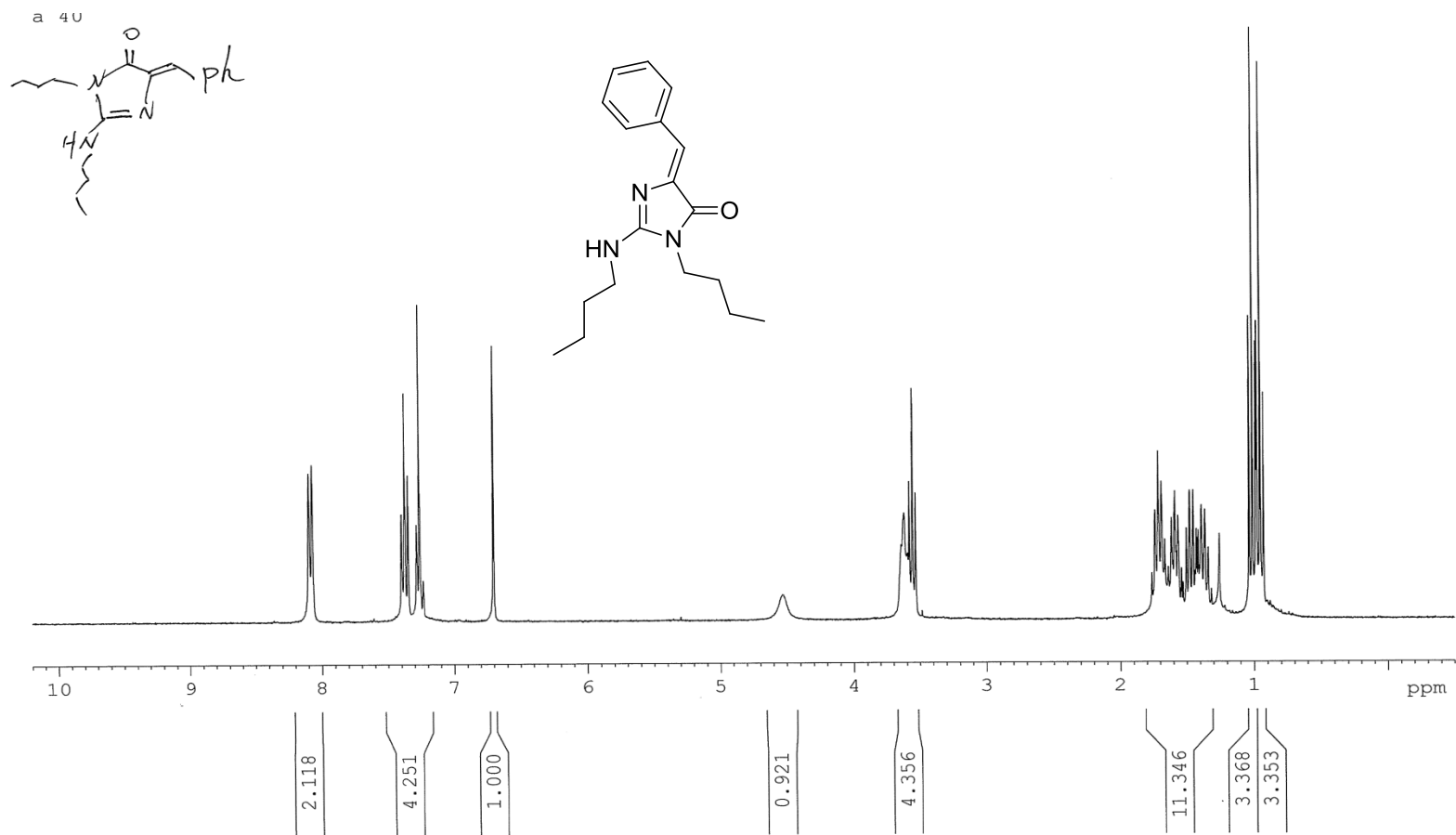
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 7mmu if m/z > 7

Unsaturation (U.S.) : -0.5 - 15.0

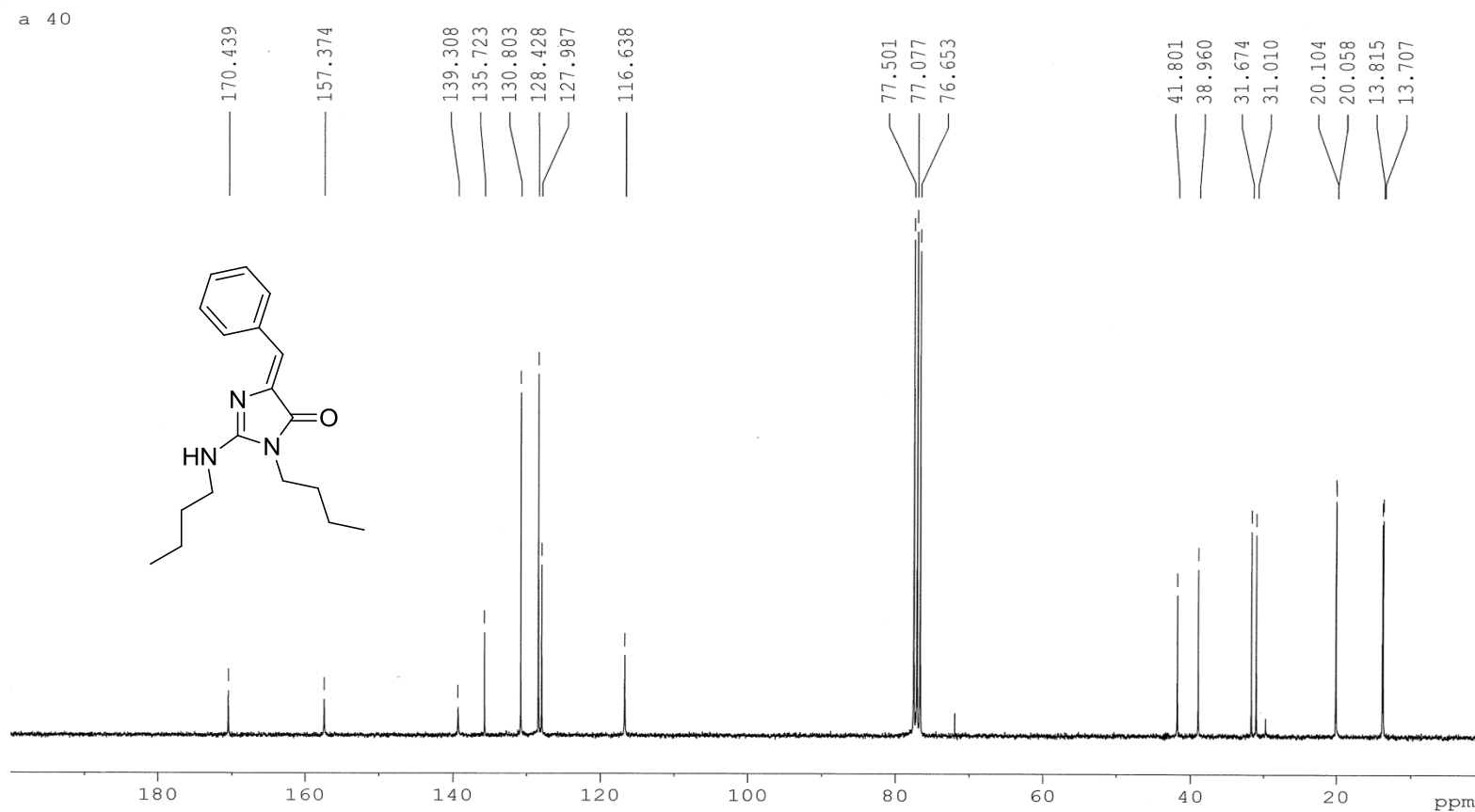
Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
299.2021	55.3	+8.0 / +2.4	8.0	C 18 H 25 O N 3
242.0621	16.7	+6.2 / +1.5	14.5	C 17 H 8 O N
202.0009	100.0	-15.9 / -3.2	14.5	C 12 O N 3
188.1018	63.9	-30.6 / -5.7	6.5	C 12 H 14 O N
		+36.3 / +6.8	7.0	C 11 H 12 O N 2
187.1261	52.6	+13.7 / +2.6	6.5	C 12 H 15 N 2



HRMS Mass (EI) spectrum of compound 6{1,1,1}



^1H NMR spectrum (300 MHz) of compound **6{1,1,13}** in CDCl_3

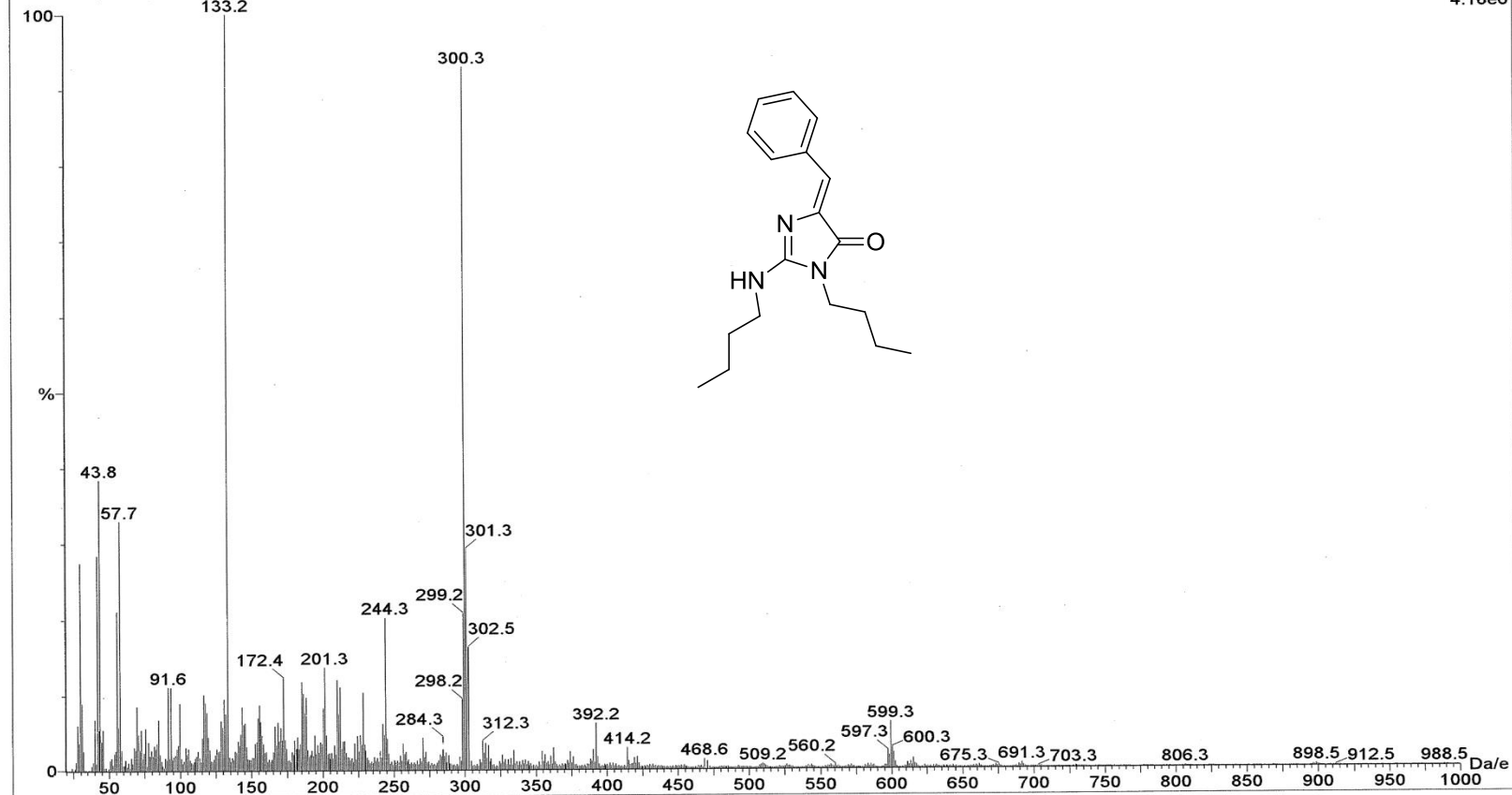


¹³C spectrum (75 MHz) of compound **6{1,1,13}** in CDCl₃

21-Jun-2004
A40A 16 (1.118) Cm (15:16)
133.2

3584 D306 a40

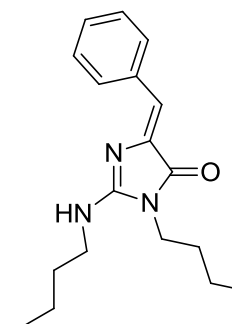
Scan FB+
4.18e6



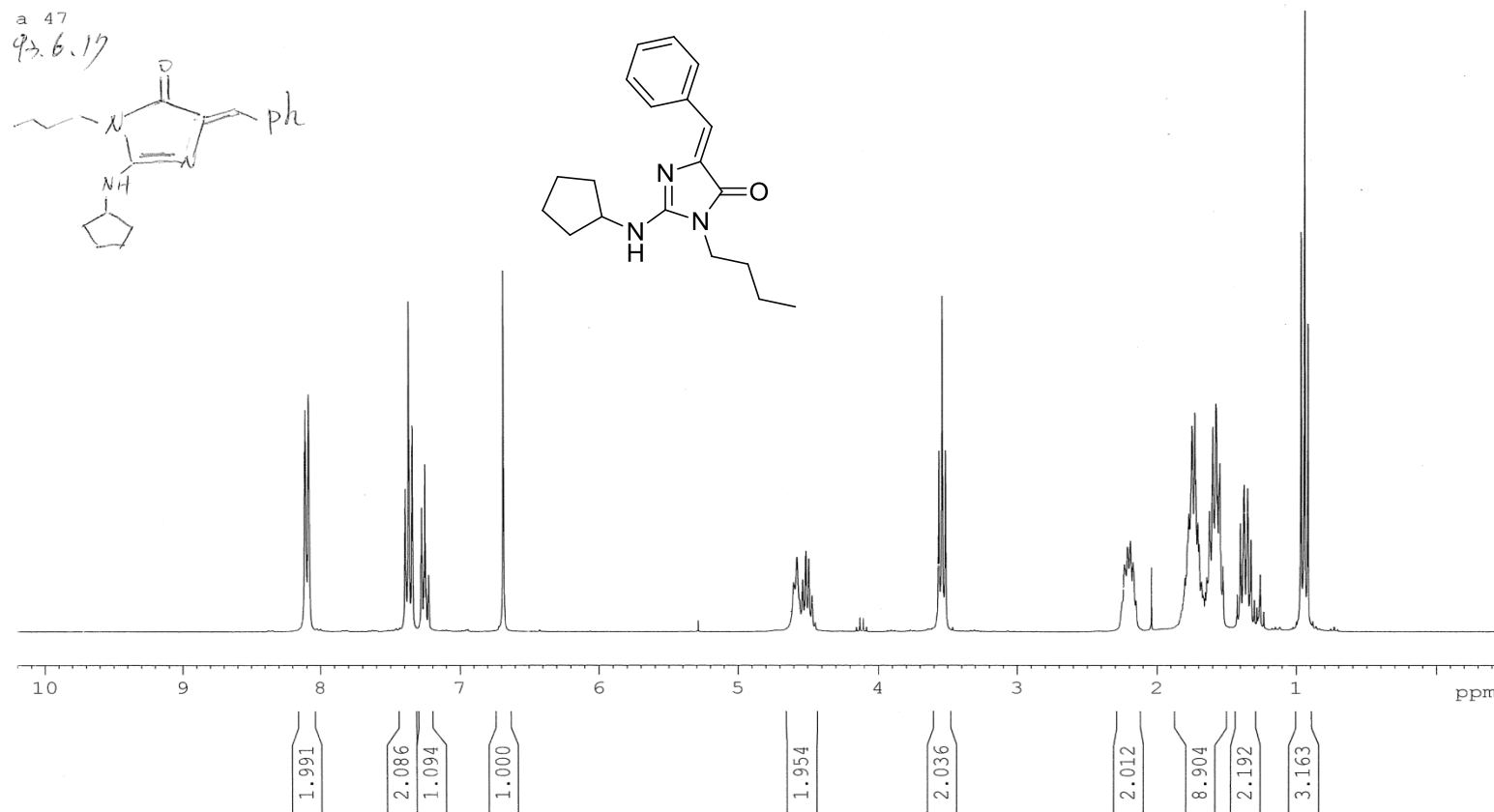
Mass spectrum of compound 6{1,1,13}

[Elemental Composition]
 Data : Corp. 11086001 Date : 15-Sep-2004 10:57
 Sample: a40 = 299.1998 m/z (2004070044)
 Note : Tsai (NTHU)
 Inlet : Direct Ion Mode : EI+
 RT : 0.82 min Scan#: 59
 Elements : C 18/0, H 25/0, O 1/0, N 3/0
 Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 9mmu if m/z > 9
 Unsaturation (U.S.) : -0.5 - 19.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
299.1975	80.8	-7.4 / -2.2	8.0	C 18 H 25 O N 3
243.1415	20.8	-33.8 / -8.2 +17.9 / +4.3	7.5 8.0	C 15 H 19 O N 2 C 14 H 17 O N 3
228.0863	64.3	-33.4 / -7.6 +21.7 / +4.9	13.0 13.5	C 18 H 12 C 17 H 10 N
201.1880	100.0	-43.0 / -8.7 +19.5 / +3.9	0.5 1.0	C 11 H 25 O N 2 C 10 H 23 O N 3
200.1653	34.7	+43.7 / +8.8	6.0	C 15 H 20
187.0139	50.5	-23.8 / -4.4 +43.5 / +8.1 -16.6 / -3.1	13.5 14.0 14.0	C 14 H 3 O C 13 H O N C 12 H N 3
185.9910	44.7	-37.8 / -7.0	14.5	C 13 O N
166.0145	27.2	-13.5 / -2.2	11.0	C 10 H 2 O N 2

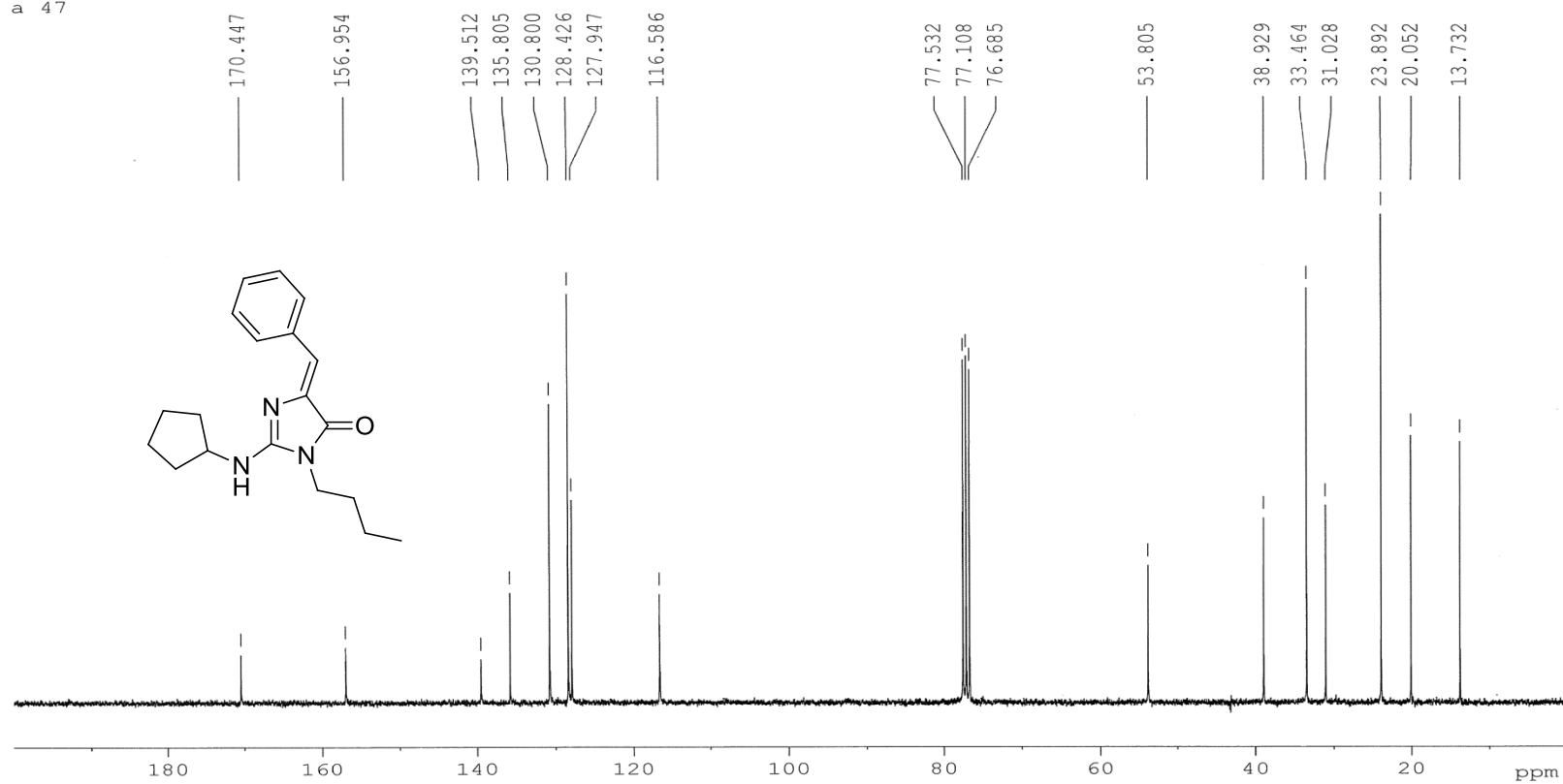


HRMS Mass (EI) spectrum of compound 6{1,1,13}



¹H NMR spectrum (300 MHz) of compound **6{1,1,6}** in CDCl₃

a 47

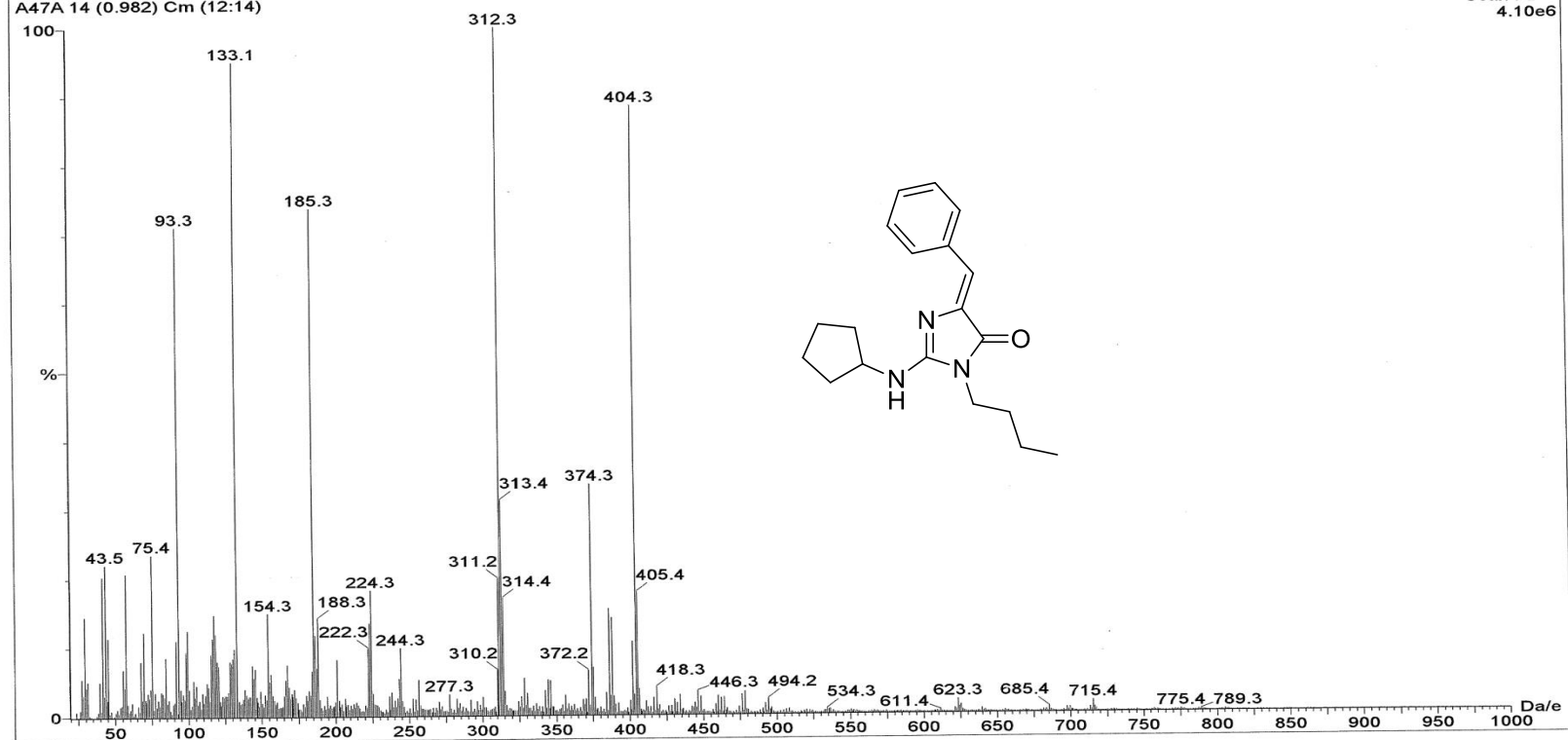


¹³C spectrum (75 MHz) of compound 6{1,1,6} in CDCl₃

27-Jun-2004
A47A 14 (0.982) Cm (12:14)

3584 D306 a47

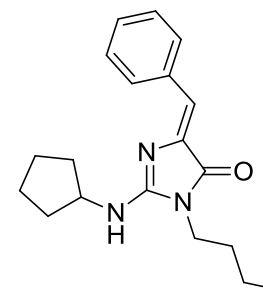
Scan FB+
4.10e6



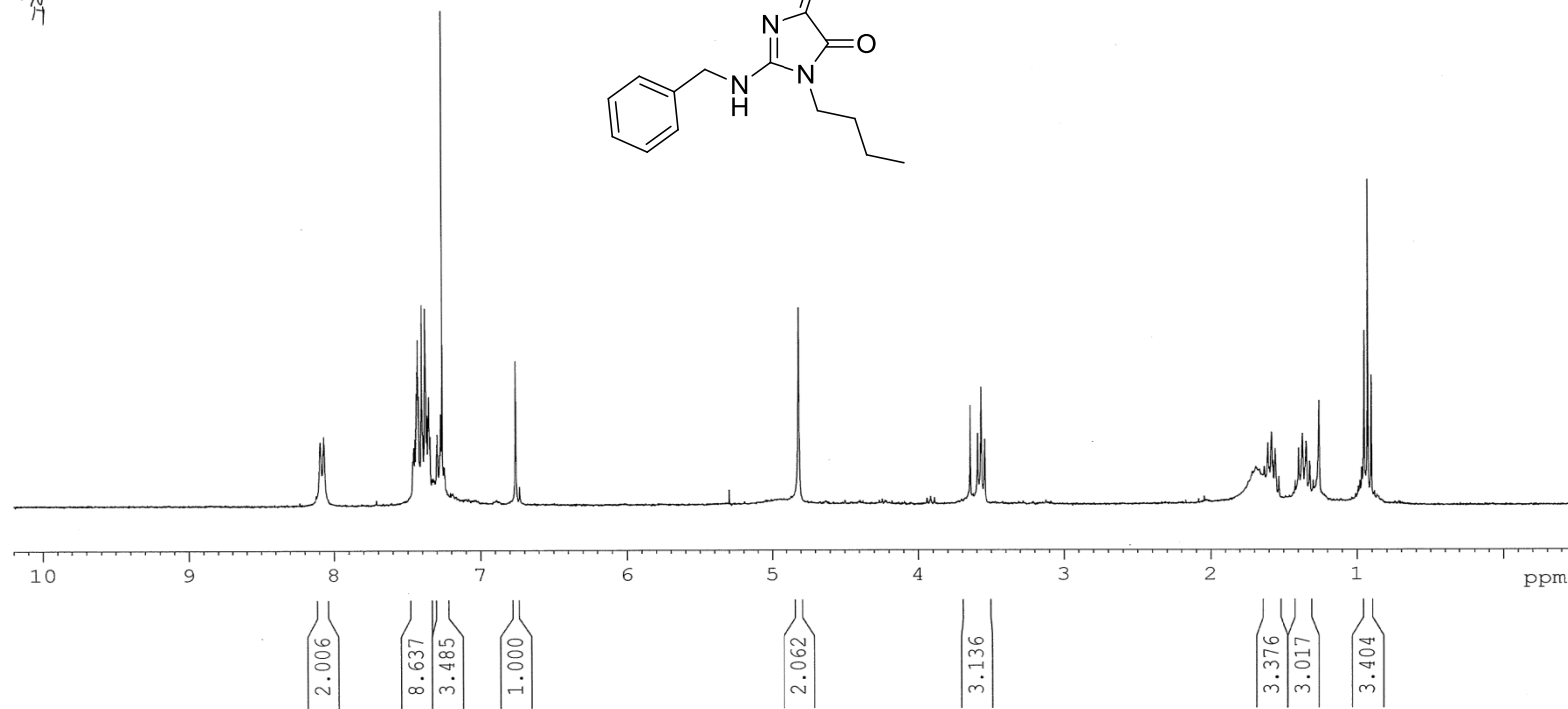
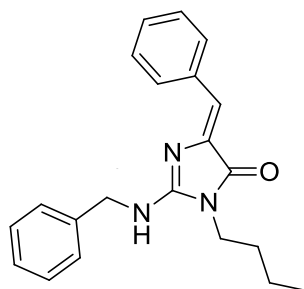
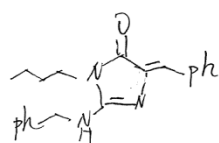
Mass spectrum of compound 6{1,1,6}

[Elemental Composition]
 Data : Corp. 11087001 Date : 15-Sep-2004 10:33
 Sample: a47 = 311.1998 m/z (2004070044)
 Note : Tsai (NTHU)
 Inlet : Direct Ion Mode : EI+
 RT : 0.63 min Scan#: 43
 Elements : C 19/0, H 25/0, O 1/0, N 3/0
 Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 10mmu if m/z > 10
 Unsaturation (U.S.) : -0.5 - 19.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
311.2009	100.0	+3.5 / +1.1	9.0	C 19 H 25 O N 3
282.1679	11.8	-18.8 / -5.3 +25.8 / +7.3	9.0 9.5	C 18 H 22 O N 2 C 17 H 20 O N 3
227.1055	12.4	-1.5 / -0.3	9.0	C 13 H 13 O N 3
201.0130	69.7	-42.3 / -8.5 +20.2 / +4.1	14.0 14.5	C 14 H 3 O N C 13 H O N 2
187.0697	53.3	-25.9 / -4.8	8.0	C 10 H 9 O N 3
186.0692	34.3	+13.3 / +2.5	8.5	C 10 H 8 O N 3

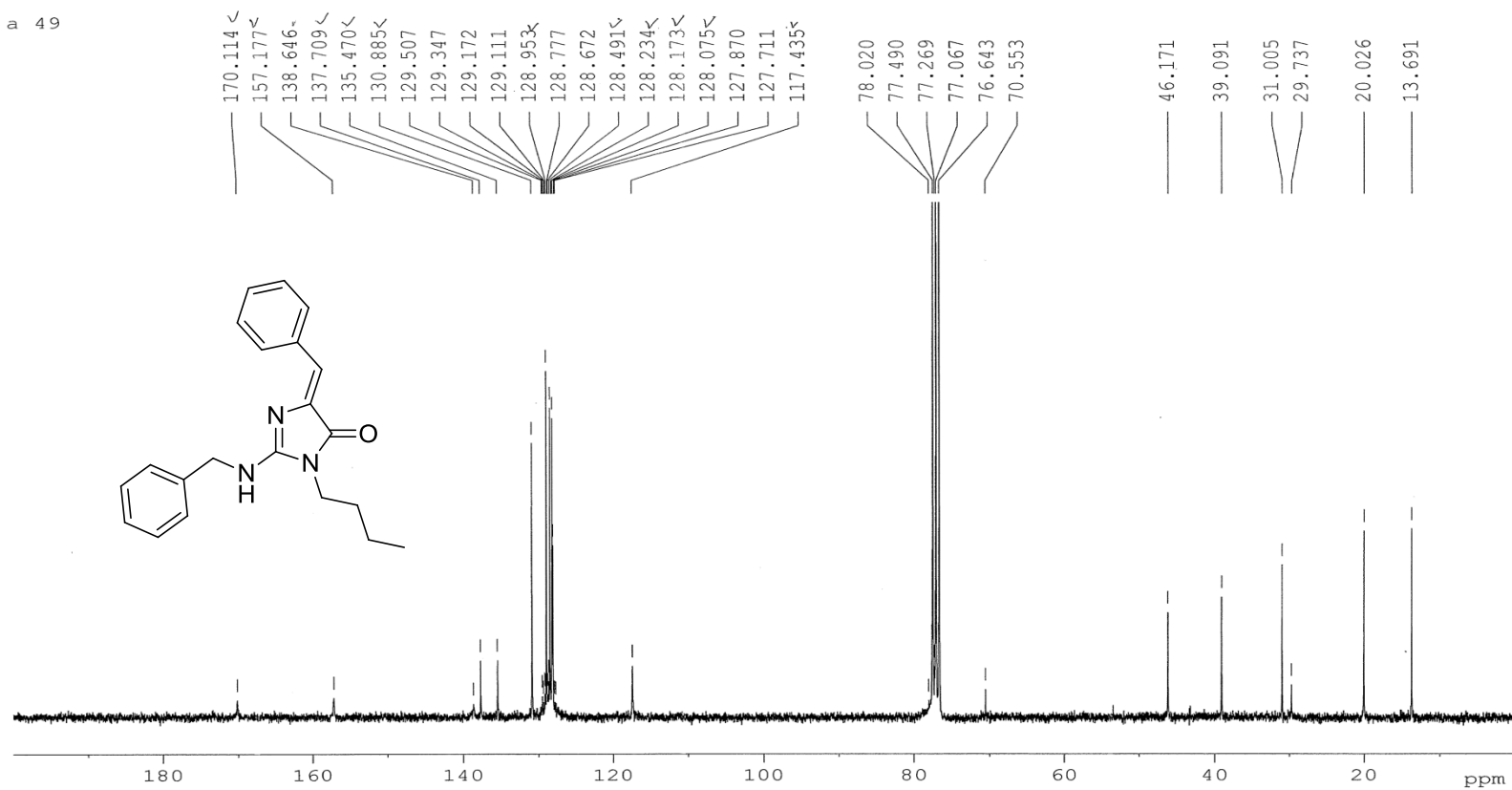


HRMS Mass (EI) spectrum of compound **6{1,1,6}**



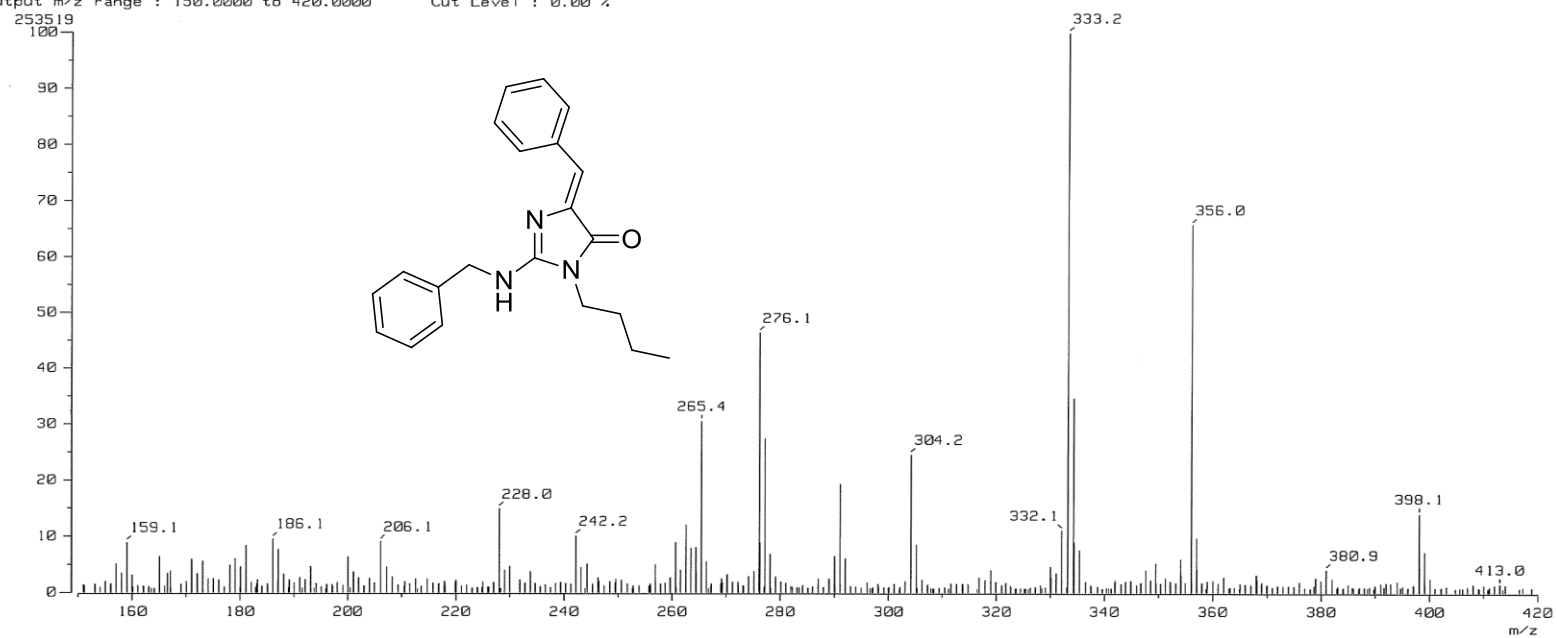
^1H NMR spectrum (300 MHz) of compound **6{1,1,7}** in CDCl_3

a 49



^{13}C spectrum (75 MHz) of compound 6{1,1,7} in CDCl_3

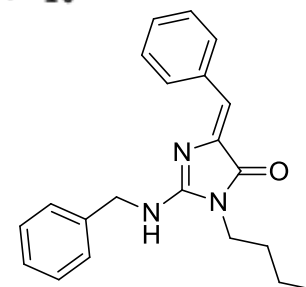
[Mass Spectrum]
Data : Corp. 11069001 Date : 14-Sep-2004 15:36
Sample: a49 = 333.1841 m/z (2004070044)
Note : Tsai (NTHU)
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 2.13 min Scan# : 135
BP : m/z 333.1837 Int. : 24.18
Output m/z range : 150.0000 to 420.0000 Cut Level : 0.00 %



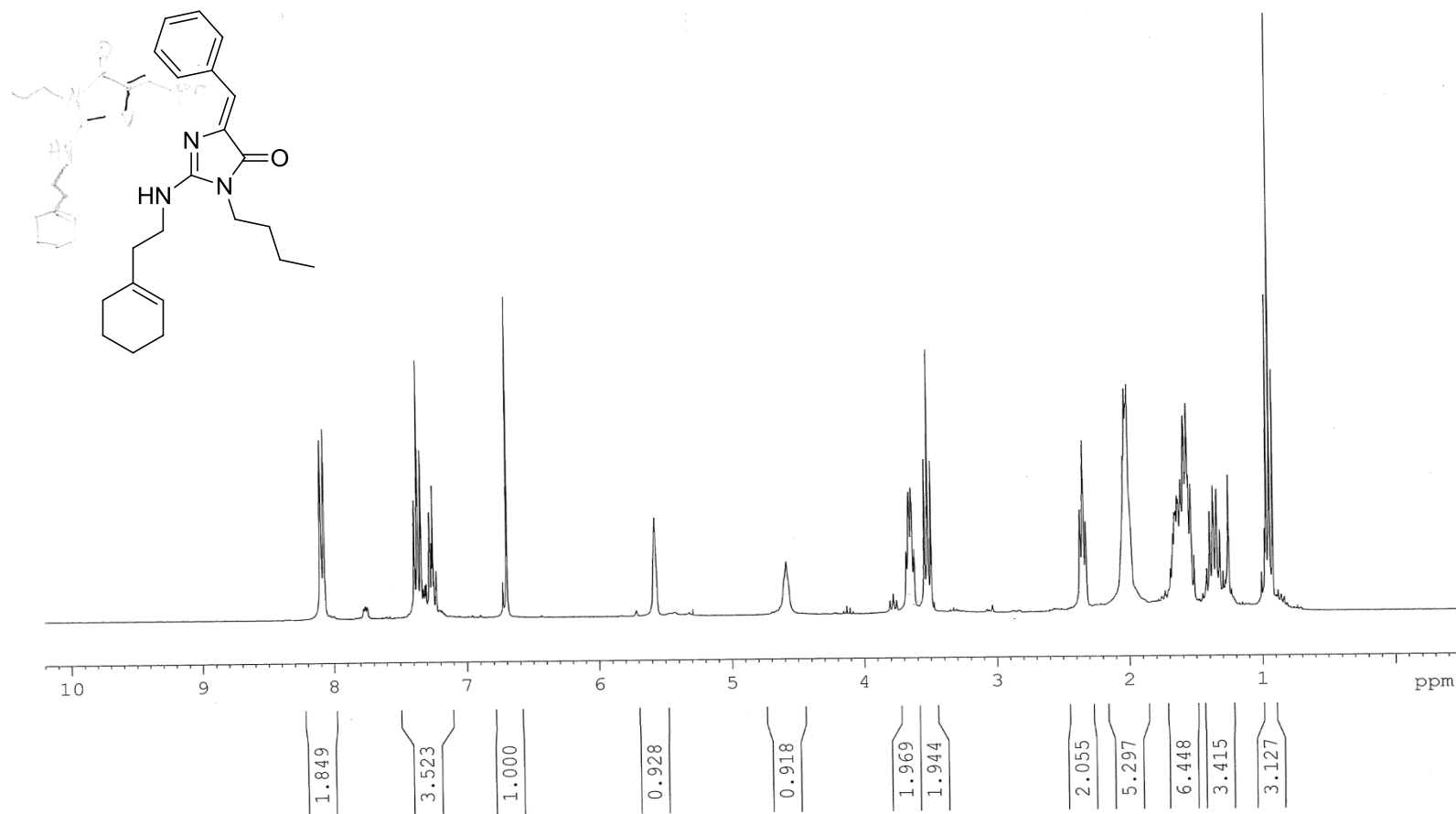
EI Mass spectrum of compound 6{1,1,7}

[Elemental Composition]
 Data : Corp. 11089001 Date : 14-Sep-2004 15:36
 Sample: a49 = 333.1841 m/z (2004070044)
 Note : Tsai (NTHU)
 Inlet : Direct Ion Mode : EI+
 RT : 2.13 min Scan#: 135
 Elements : C 21/0, H 23/0, O 1/0, N 3/0
 Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 10mmu if m/z > 10
 Unsaturation (U.S.) : -0.5 - 19.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
333.1837	100.0	-1.1 / -0.4	12.0	C 21 H 23 O N 3
304.1617	24.6	-27.6 / -8.4 +13.7 / +4.2	11.5 12.0	C 21 H 22 O N C 20 H 20 O N 2
276.1271	46.4	+3.2 / +0.9	12.0	C 18 H 16 O N 2
242.1830	10.1	+19.5 / +4.7	7.0	C 16 H 22 N 2
186.0751	9.5	-22.6 / -4.2 +45.0 / +8.4	8.0 8.5	C 11 H 10 O N 2 C 10 H 8 O N 3
159.0508	8.9	-31.8 / -5.1 +47.3 / +7.5	7.5 8.0	C 9 H 7 O N 2 C 8 H 5 O N 3

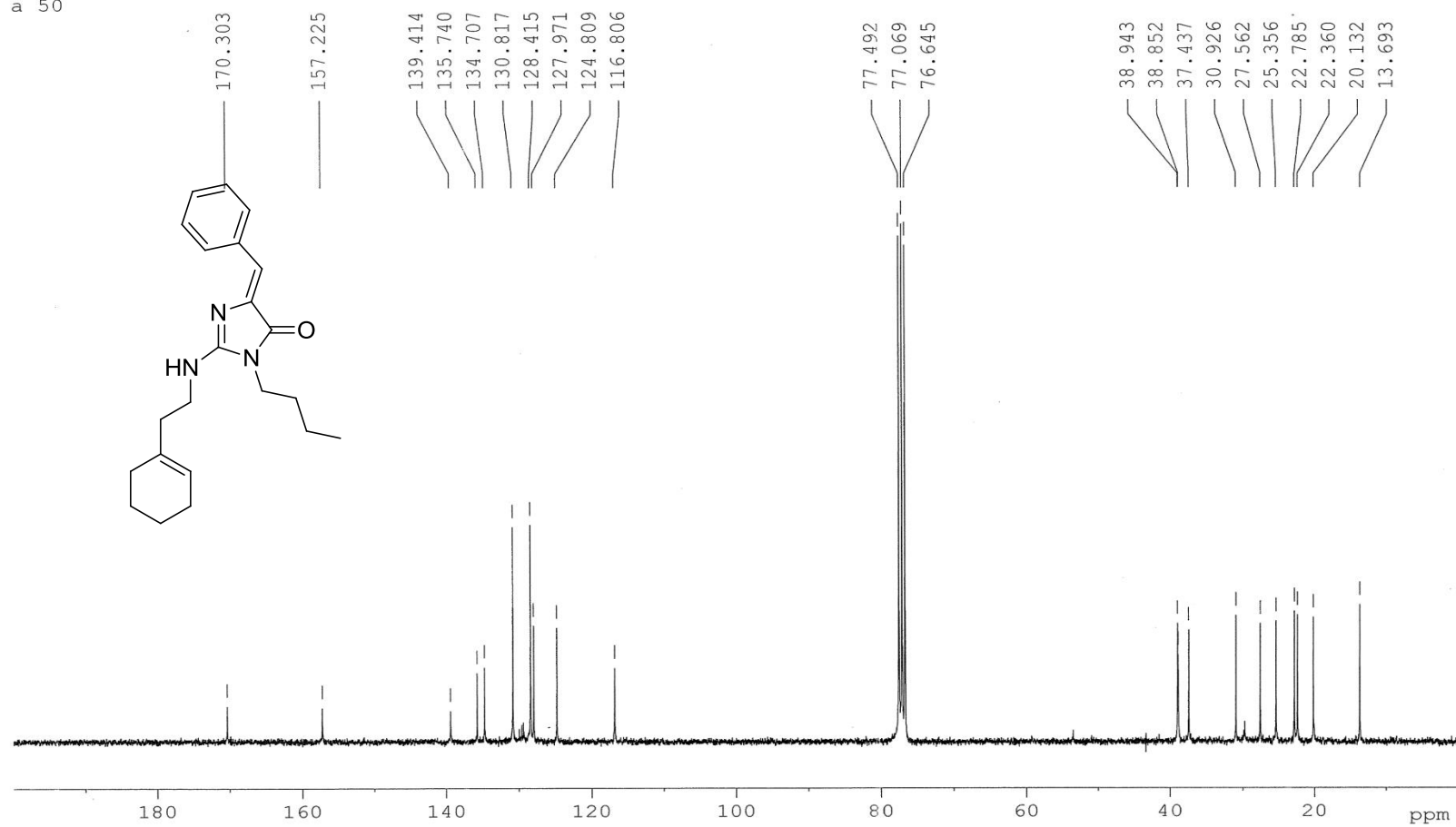


HRMS Mass (EI) spectrum of compound 6{1,1,7}

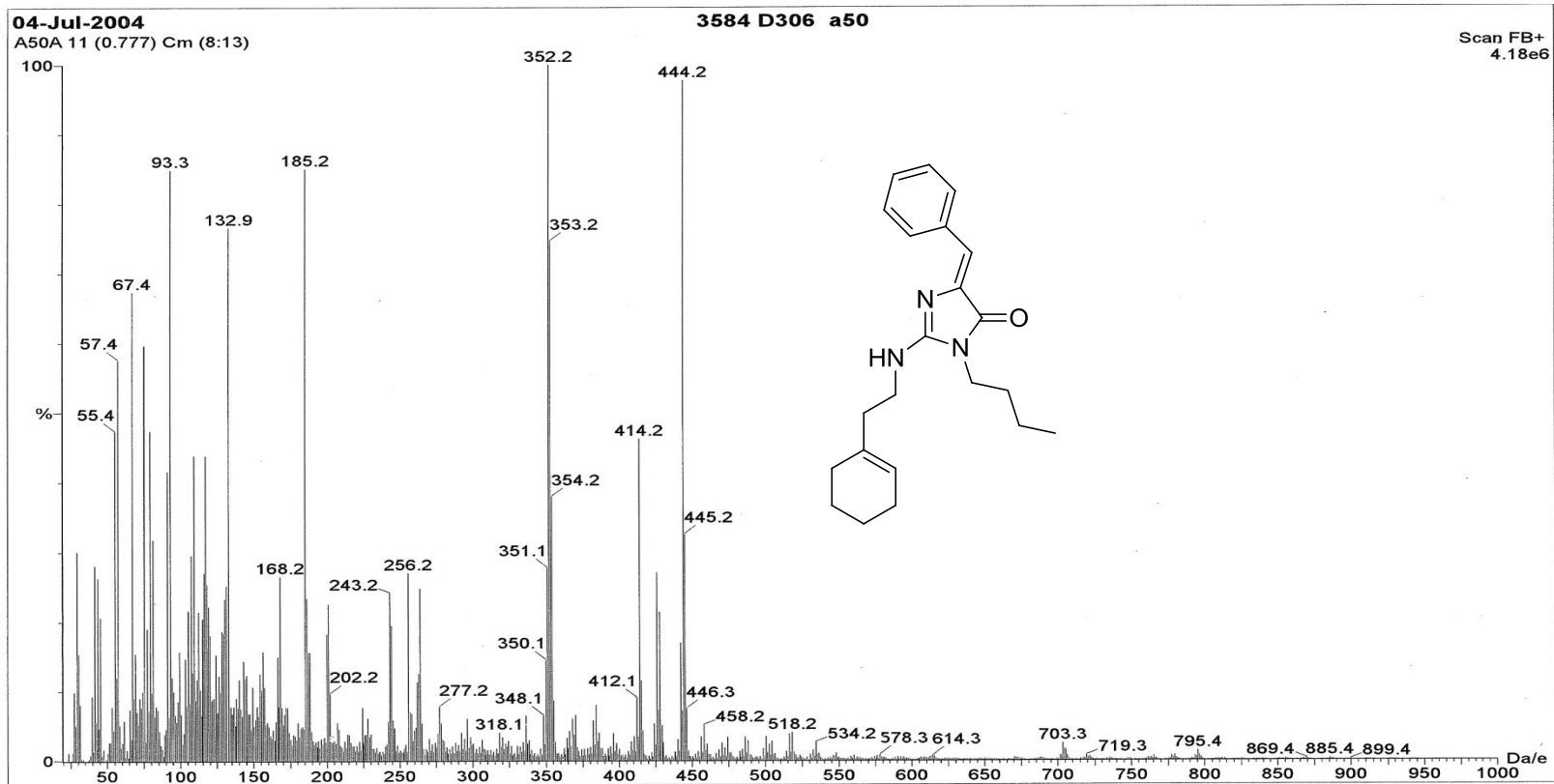


^1H NMR spectrum (300 MHz) of compound **6{1,1,2}** in CDCl_3

a 50



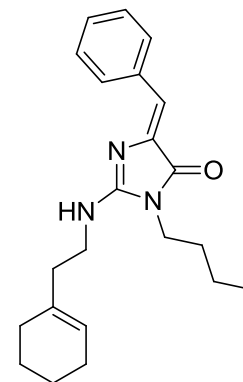
¹³C spectrum (75 MHz) of compound 6{1,1,2} in CDCl₃



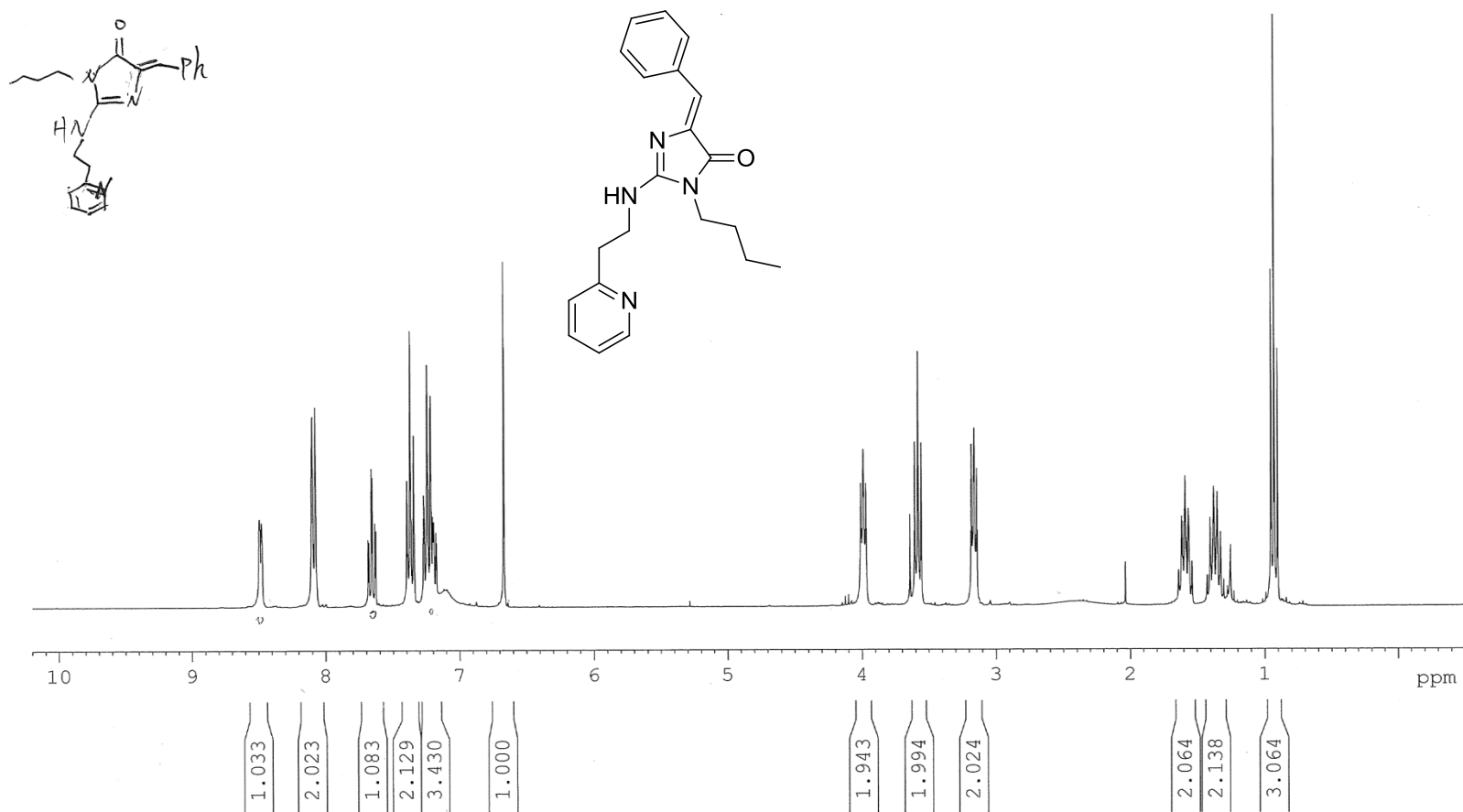
Mass spectrum of compound 6{1,1,2}

[Elemental Composition]
 Data : Corp. 11088002 Date : 14-Sep-2004 17:18
 Sample: a50 = 351.2311 m/z (2004070044)
 Note : Tsai (NTHU)
 Inlet : Direct Ion Mode : EI+
 RT : 1.13 min Scan#: 87
 Elements : C 22/0, H 29/0, O 1/0, N 3/0
 Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 10mmu if m/z > 10
 Unsaturation (U.S.) : -0.5 - 19.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
351.2316	64.5	+1.5 / +0.5	10.0	C 22 H 29 O N 3
257.1528	18.5	-0.2 / +0.0	8.0	C 15 H 19 O N 3
256.0672	93.1	-35.2 / -9.0 +13.9 / +3.6	14.5 15.0	C 18 H 10 O N C 17 H 8 O N 2
244.1351	22.7	+40.4 / +9.9 -40.7 / -9.9	12.0 7.5	C 19 H 16 C 14 H 18 O N 3
243.1399	100.0	-40.6 / -9.9 +11.2 / +2.7	7.5 8.0	C 15 H 19 O N 2 C 14 H 17 O N 3
202.0401	87.1	-8.7 / -1.7 -2.0 / -0.4	13.0 13.5	C 15 H 6 O C 13 H 4 N 3

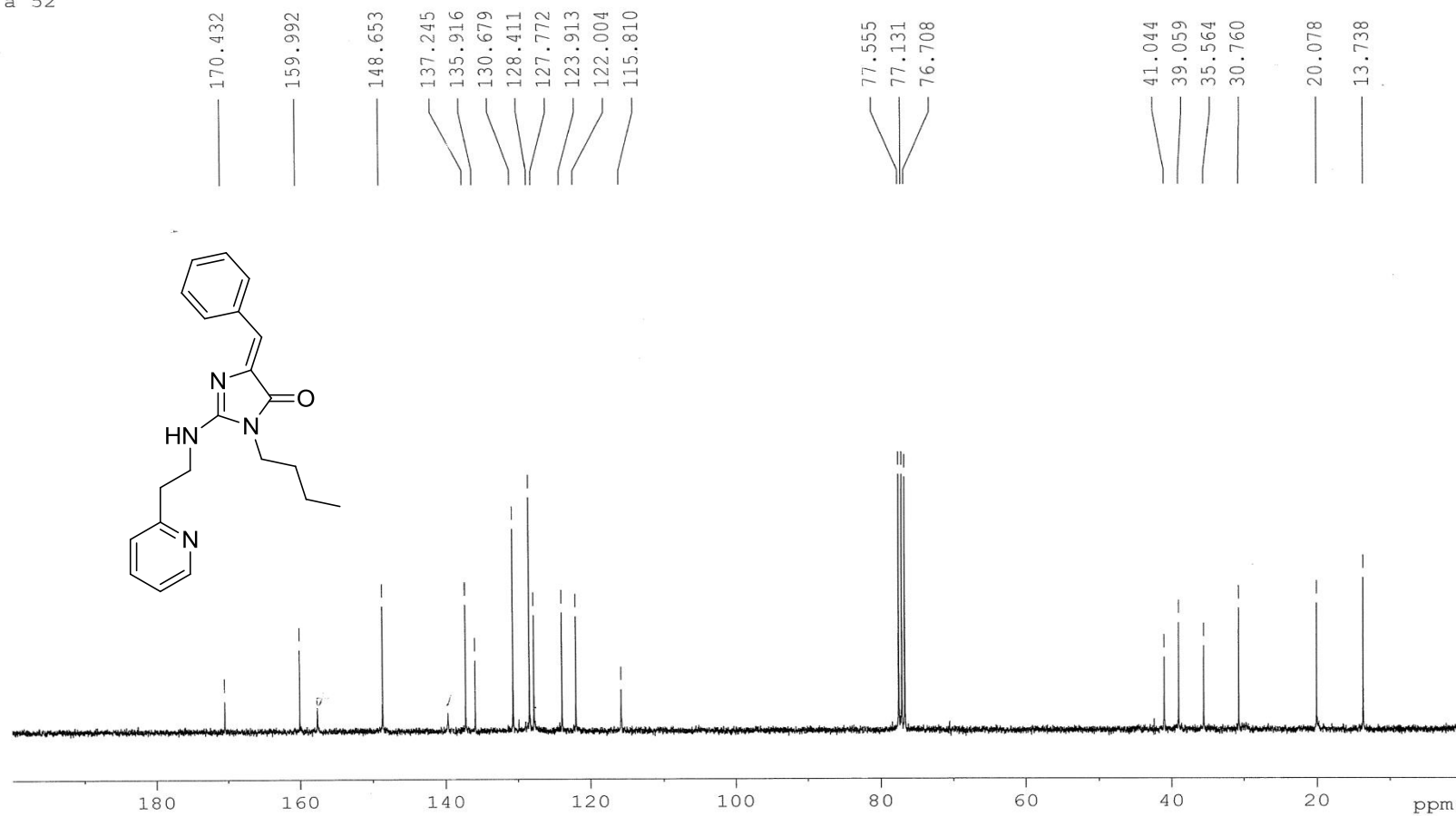


HRMS Mass (EI) spectrum of compound 6{1,1,2}

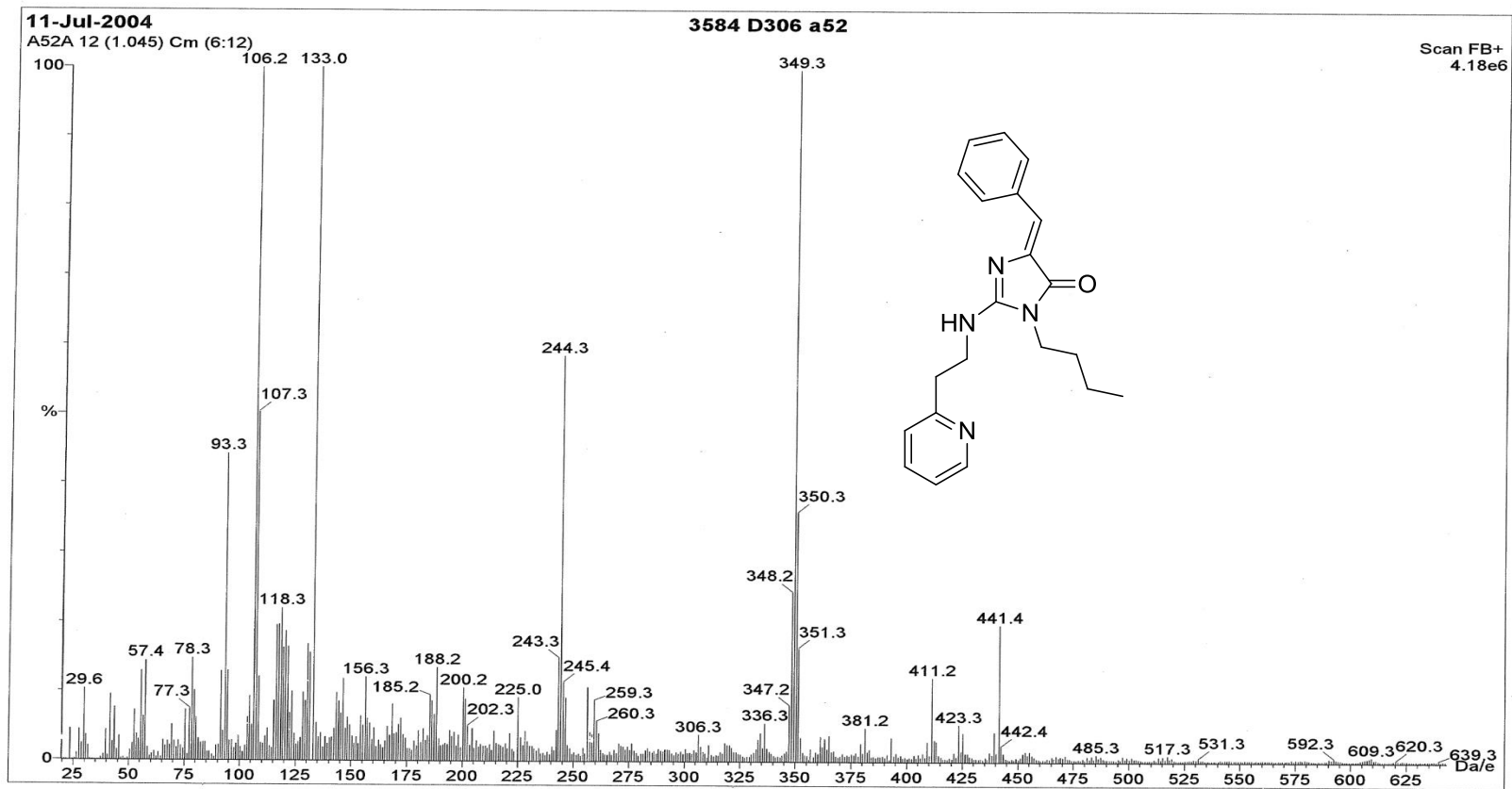


^1H NMR spectrum (300 MHz) of compound **6{1,1,8}** in CDCl_3

a 52



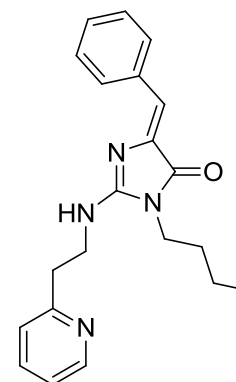
¹³C spectrum (75 MHz) of compound 6{1,1,8} in CDCl₃



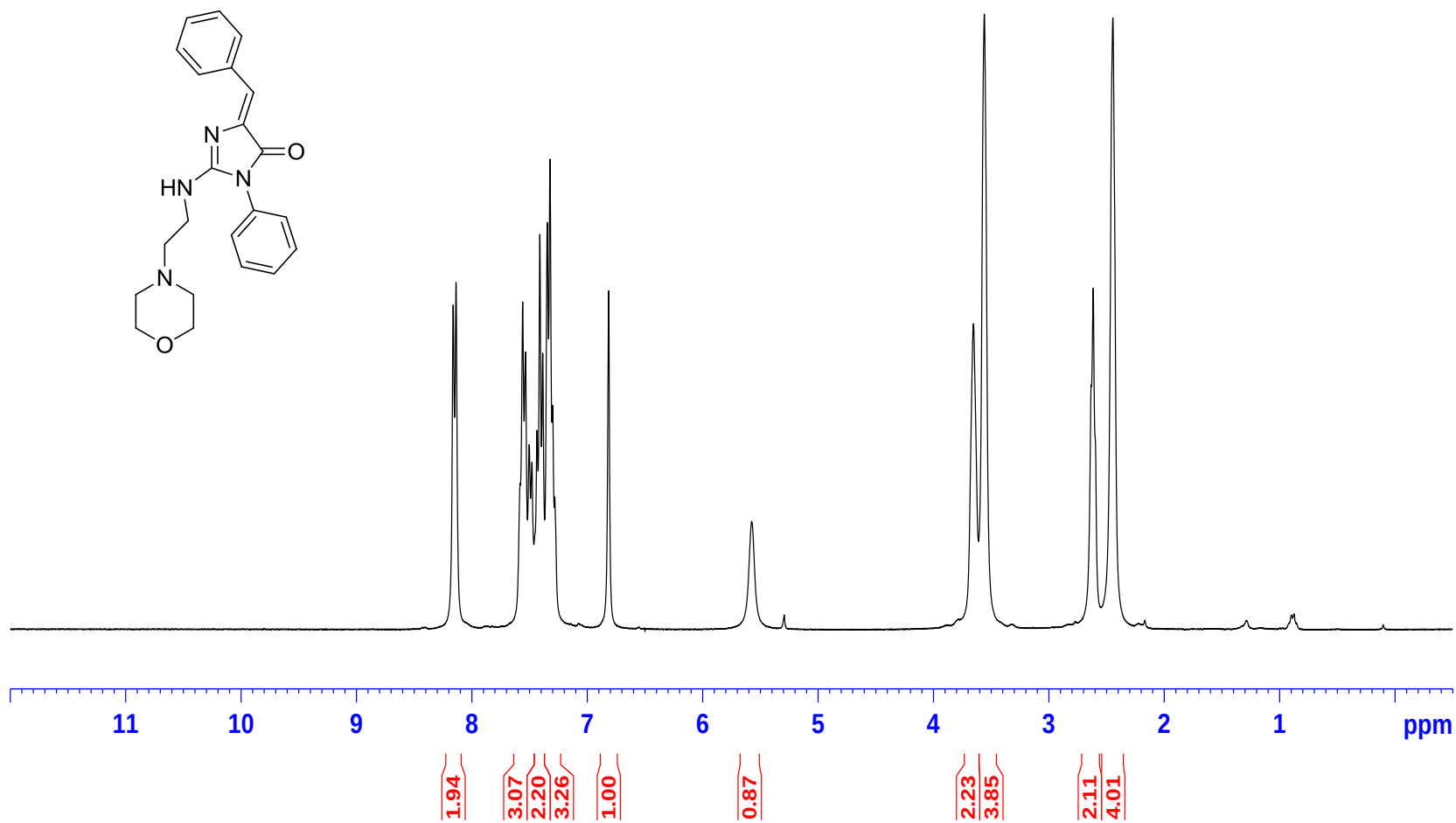
Mass spectrum of compound 6{1,1,8}

[Elemental Composition]
 Data : Corp. 11090001 Date : 14-Sep-2004 15:11
 Sample: a52 = 348.1950 m/z (2004070044)
 Note : Tsai (NTHU)
 Inlet : Direct Ion Mode : EI+
 RT : 1.30 min Scan#: 83
 Elements : C 21/0, H 24/0, O 1/0, N 4/0
 Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 10mmu if m/z > 10
 Unsaturation (U.S.) : -0.5 - 19.0

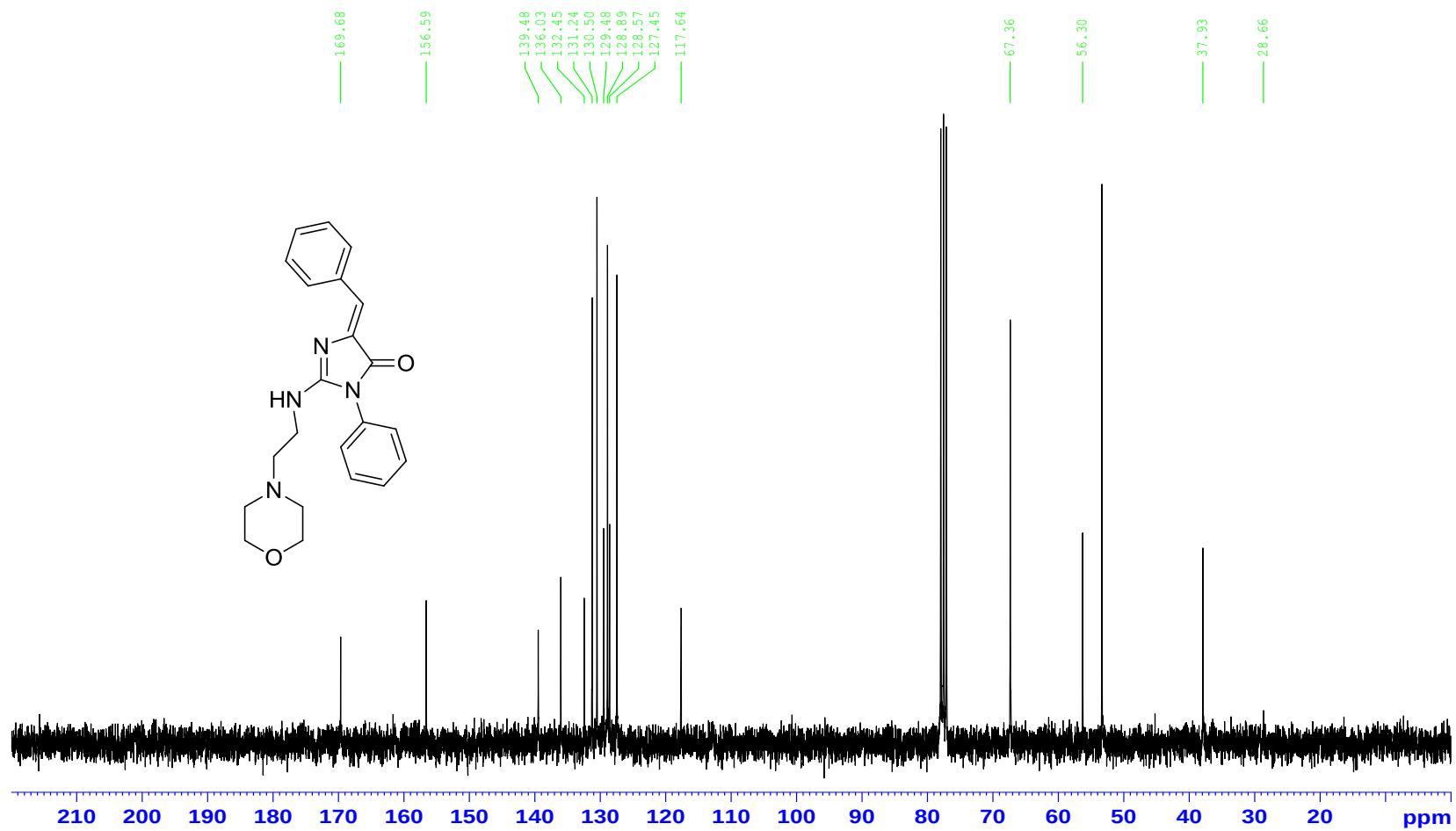
Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
348.1949	100.0	-0.5 / -0.2	12.0	C 21 H 24 O N 4
257.1386	75.7	+21.6 / +5.6 -6.4 / -1.7	12.5 8.5	C 20 H 17 C 14 H 17 O N 4
244.0748	18.9	-5.9 / -1.4 -0.4 / -0.1	13.5 14.0	C 17 H 10 O N C 15 H 8 N 4
200.0343	39.4	+40.5 / +8.1 -15.7 / -3.1 +47.2 / +9.4	14.0 14.0 14.5	C 15 H 4 O C 14 H 4 N 2 C 13 H 2 N 3
186.0599	23.6	-36.6 / -6.8 +31.0 / +5.8	8.5 9.0	C 10 H 8 O N 3 C 9 H 6 O N 4



HRMS Mass (EI) spectrum of compound 6{1,1,8}



^1H NMR spectrum (300 MHz) of compound **6{1,7,9}** in CDCl_3

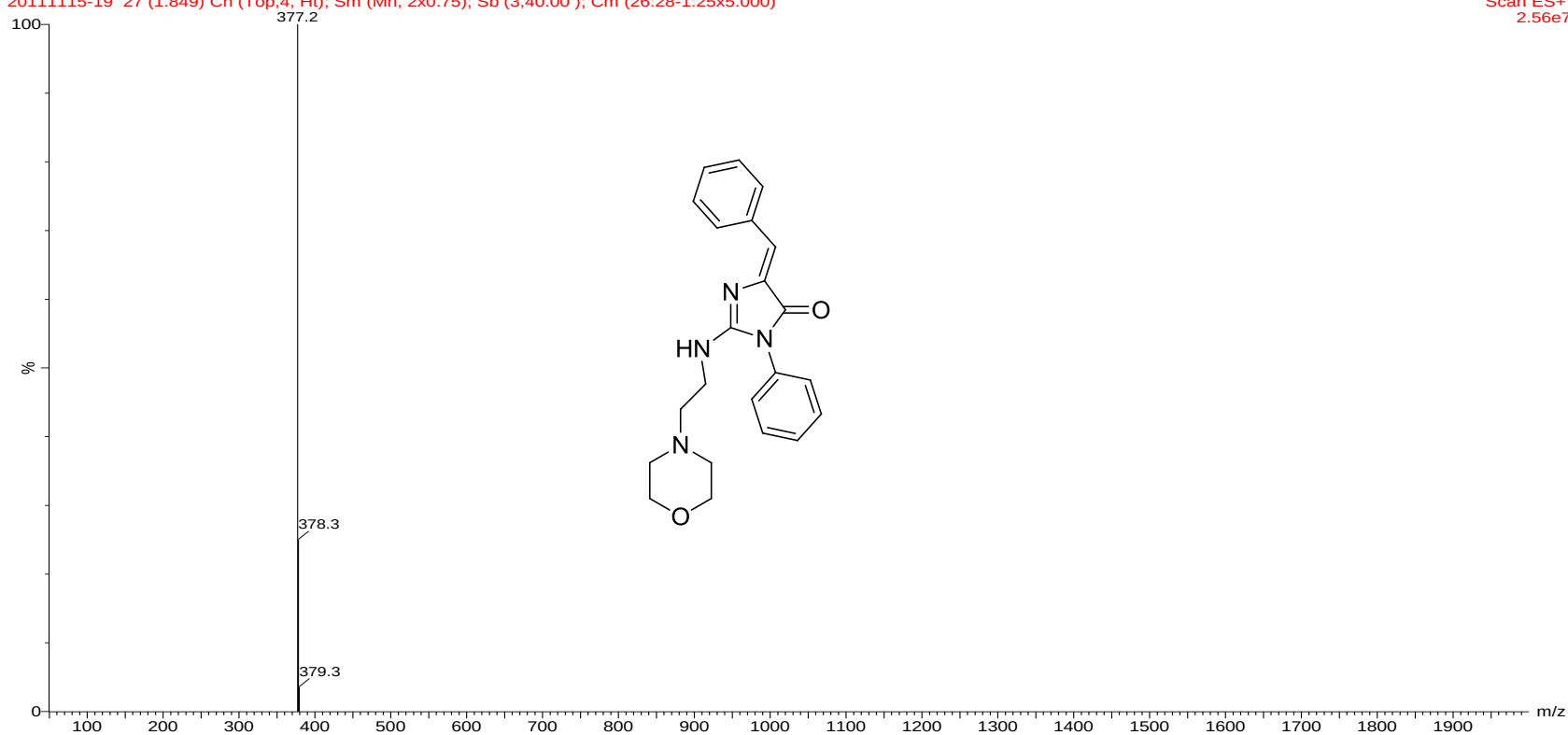


^{13}C spectrum (75 MHz) of compound **6{1,7,9}** in CDCl_3

Mani-BM

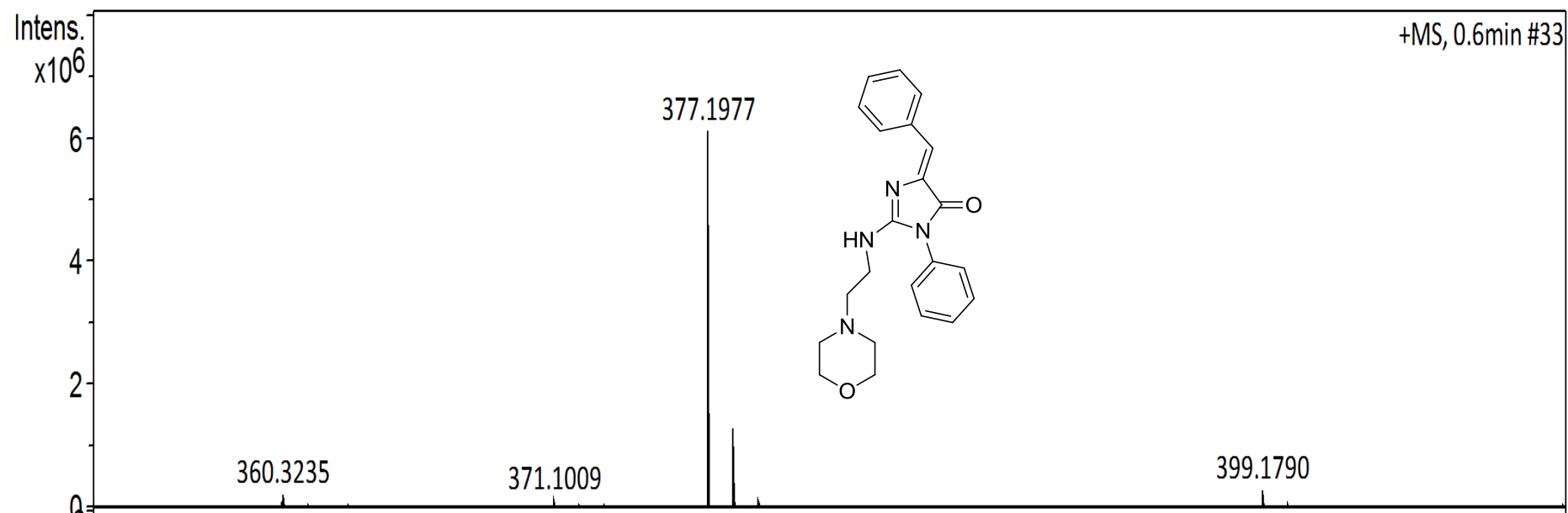
20111115-19 27 (1.849) Cn (Top,4, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (26:28-1:25x5.000)

Scan ES+
2.56e7

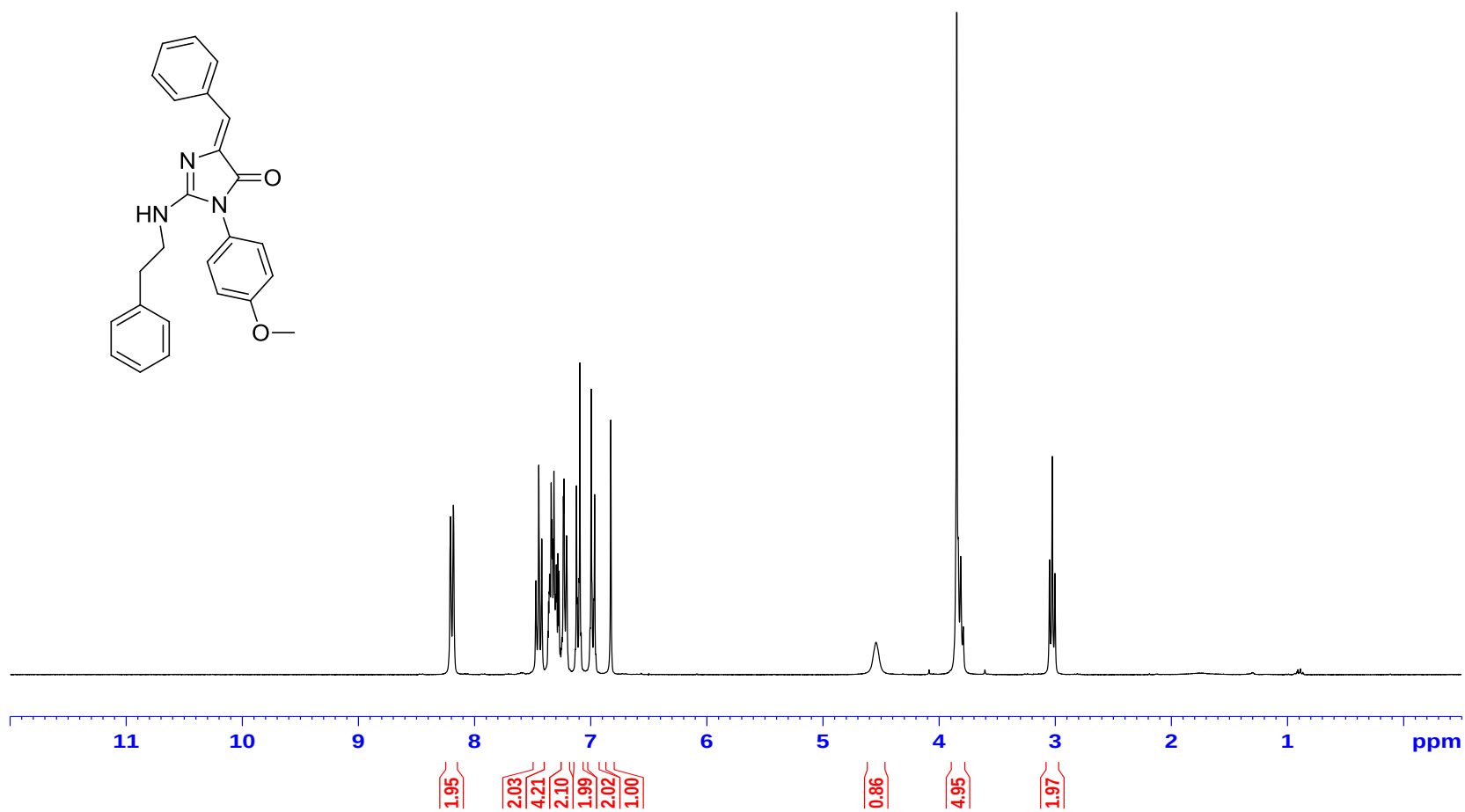


ESI Mass spectrum of compound 6{1,7,9}

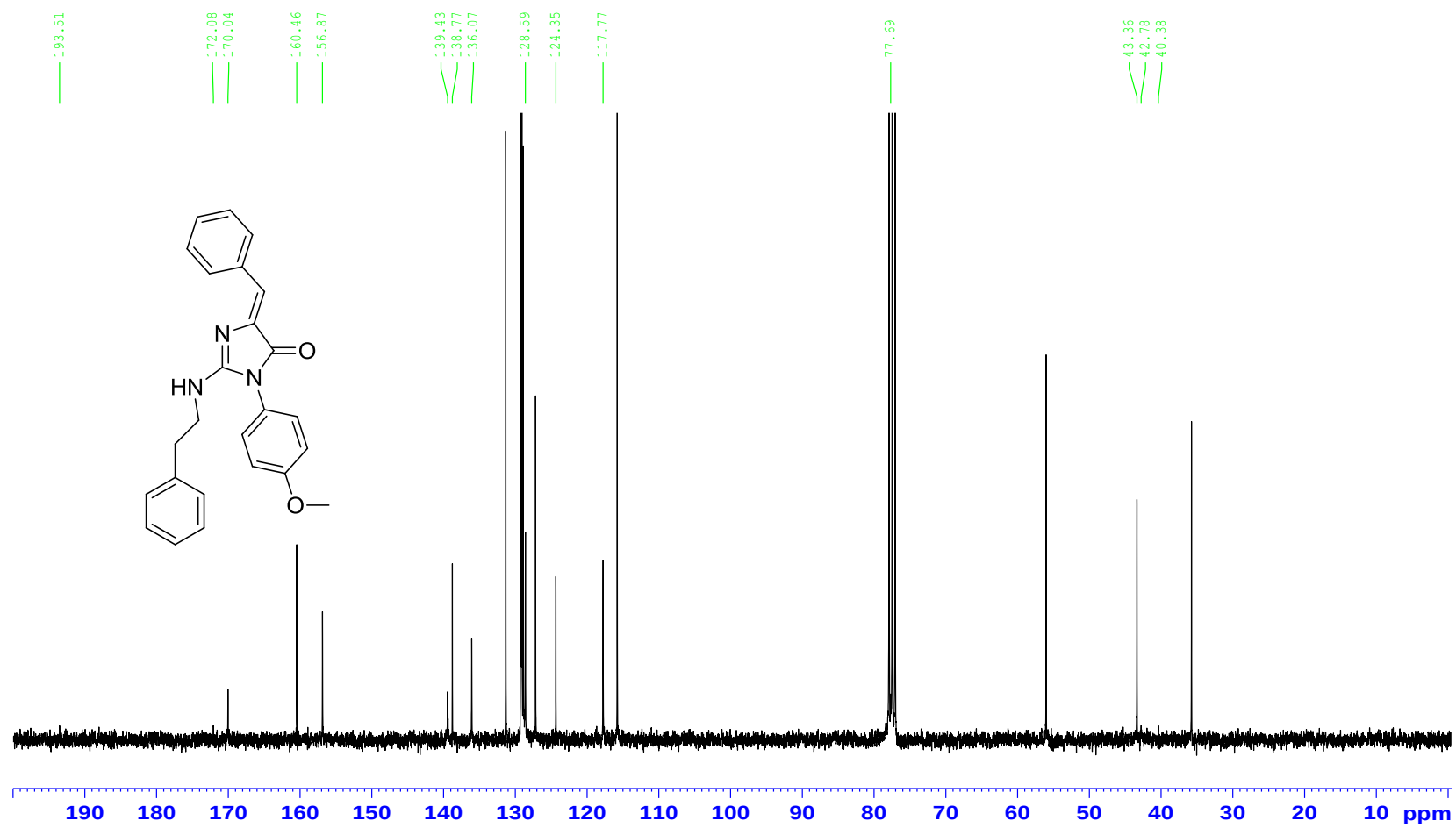
S-73



HRMS Mass (ESI) spectrum of compound **6**{1,7,9}



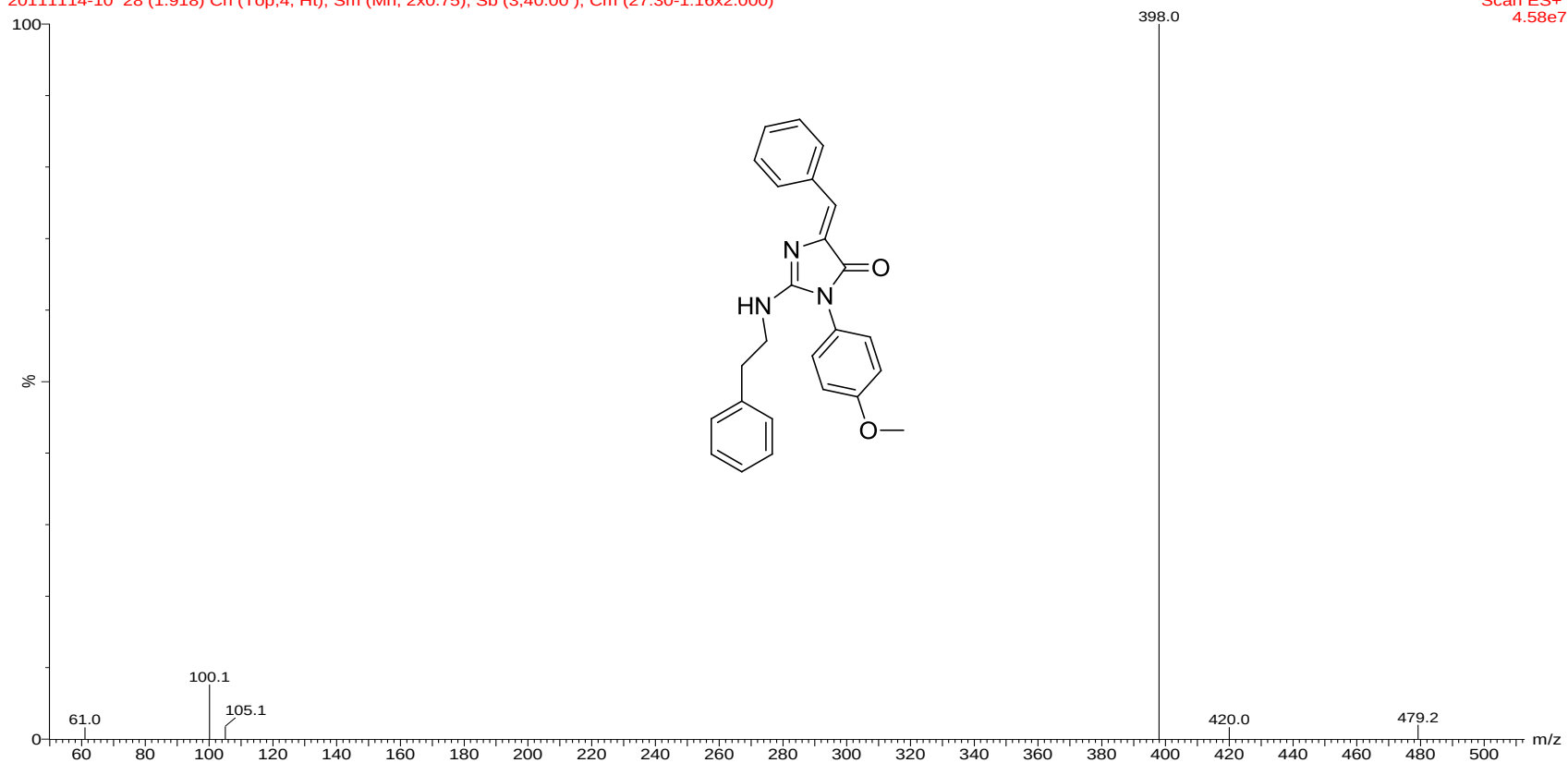
^1H NMR spectrum (300 MHz) of compound **6{1,5,10}** in CDCl_3



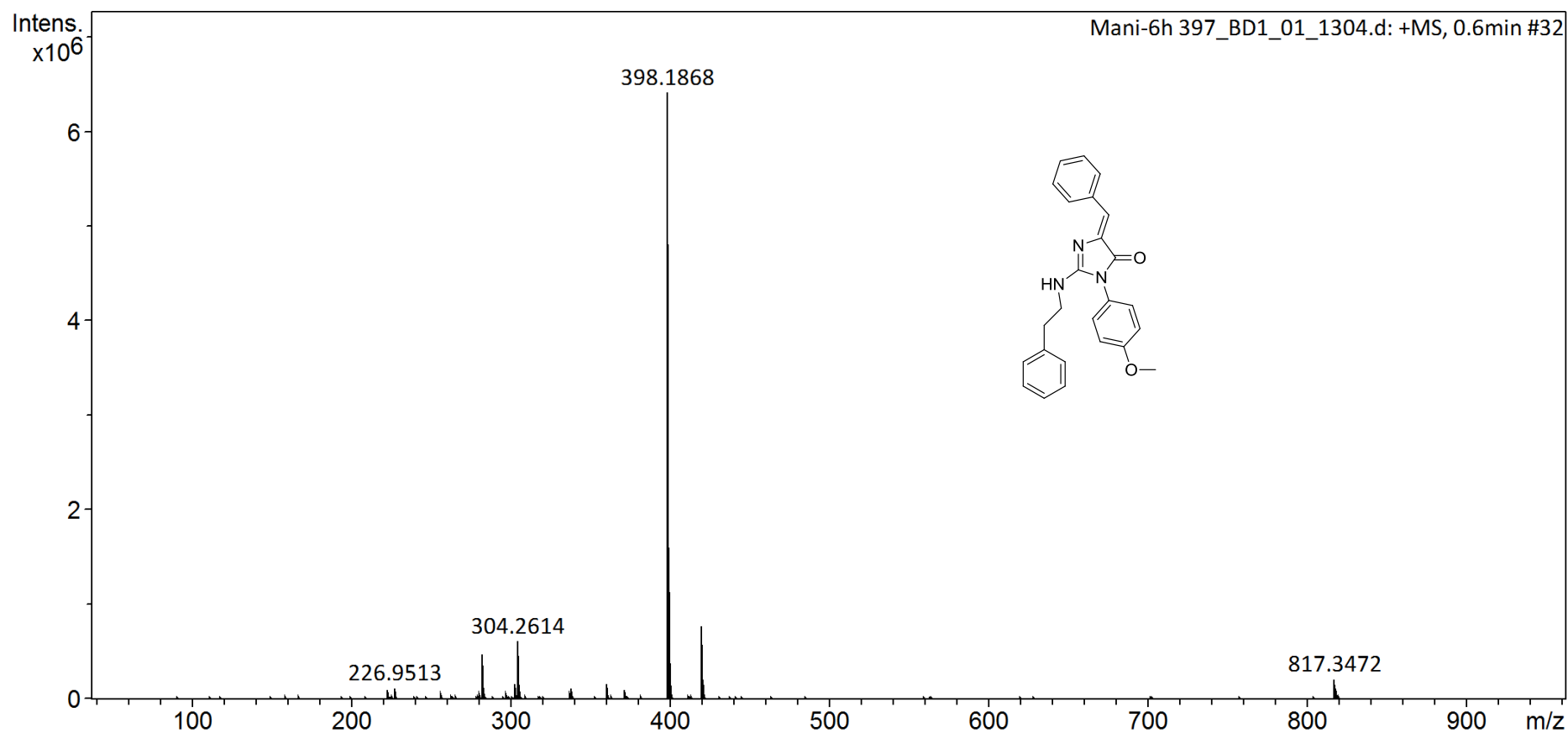
^{13}C spectrum (75 MHz) of compound **6{1,5,10}** in CDCl_3

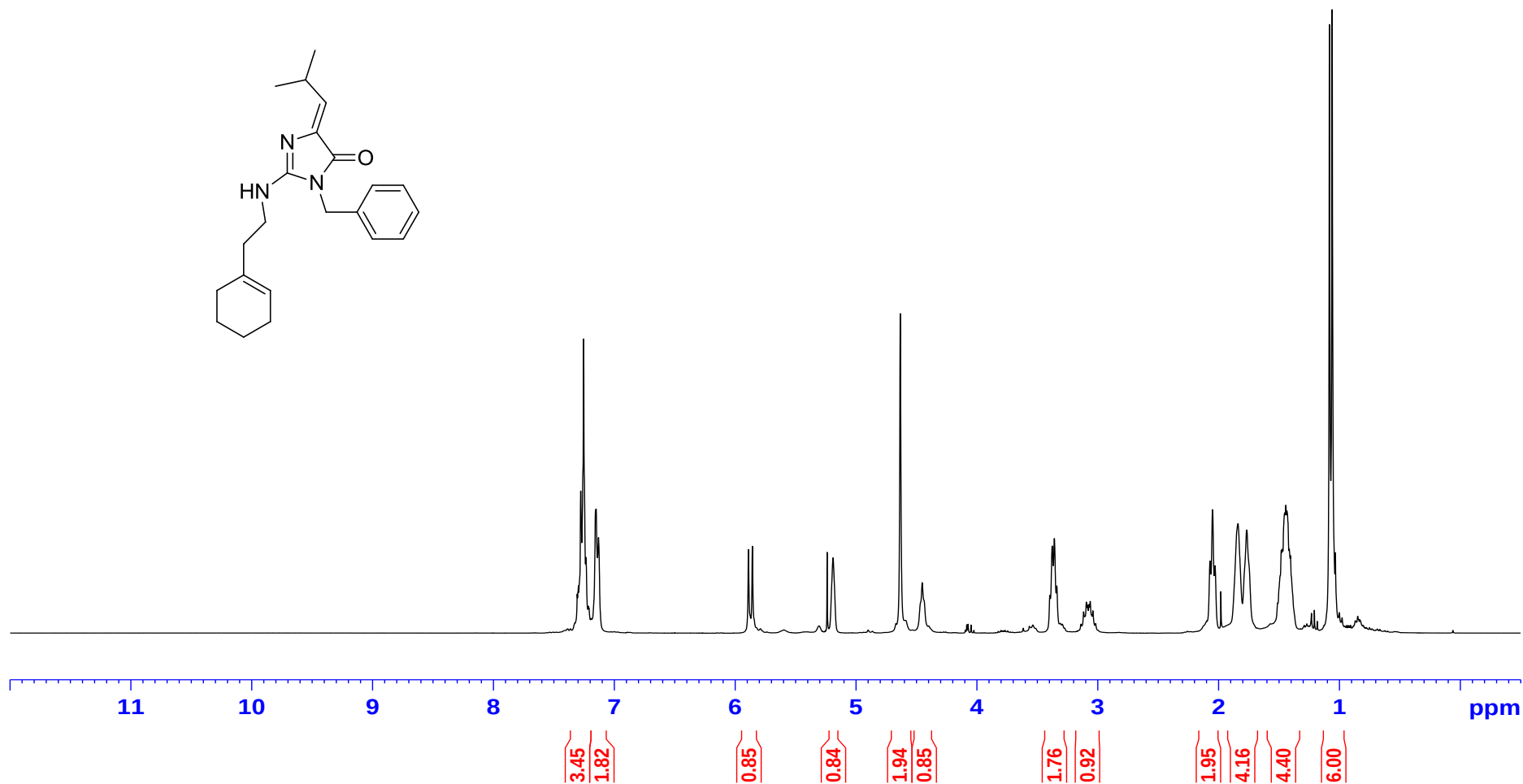
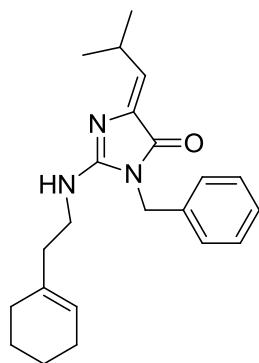
Mani-Bn

20111114-10 28 (1.918) Cn (Top,4, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (27:30-1:16x2.000)

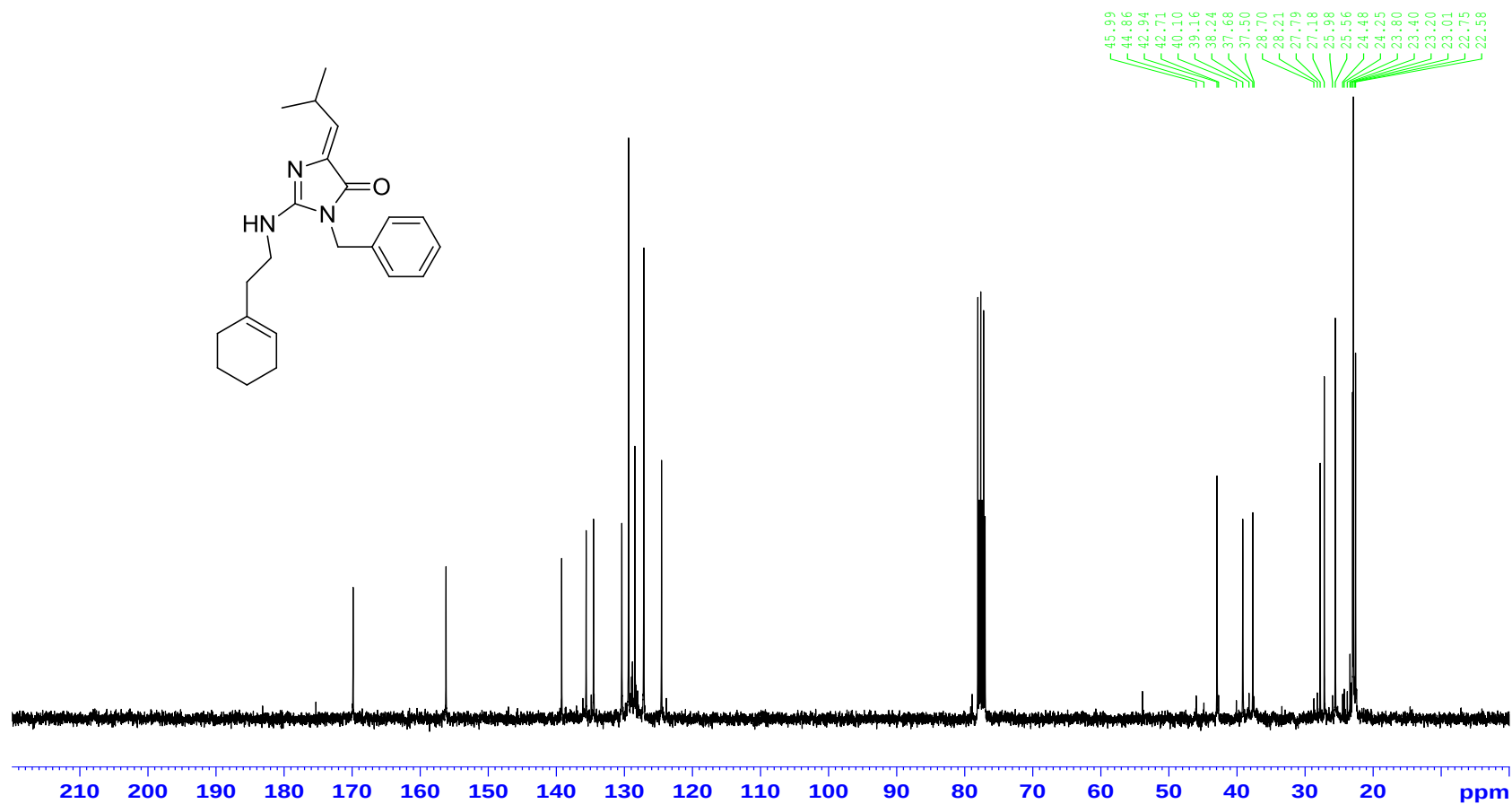


ESI Mass spectrum of compound 6{1,5,10}





^1H NMR spectrum (300 MHz) of compound **6**{5,2,2} in CDCl_3

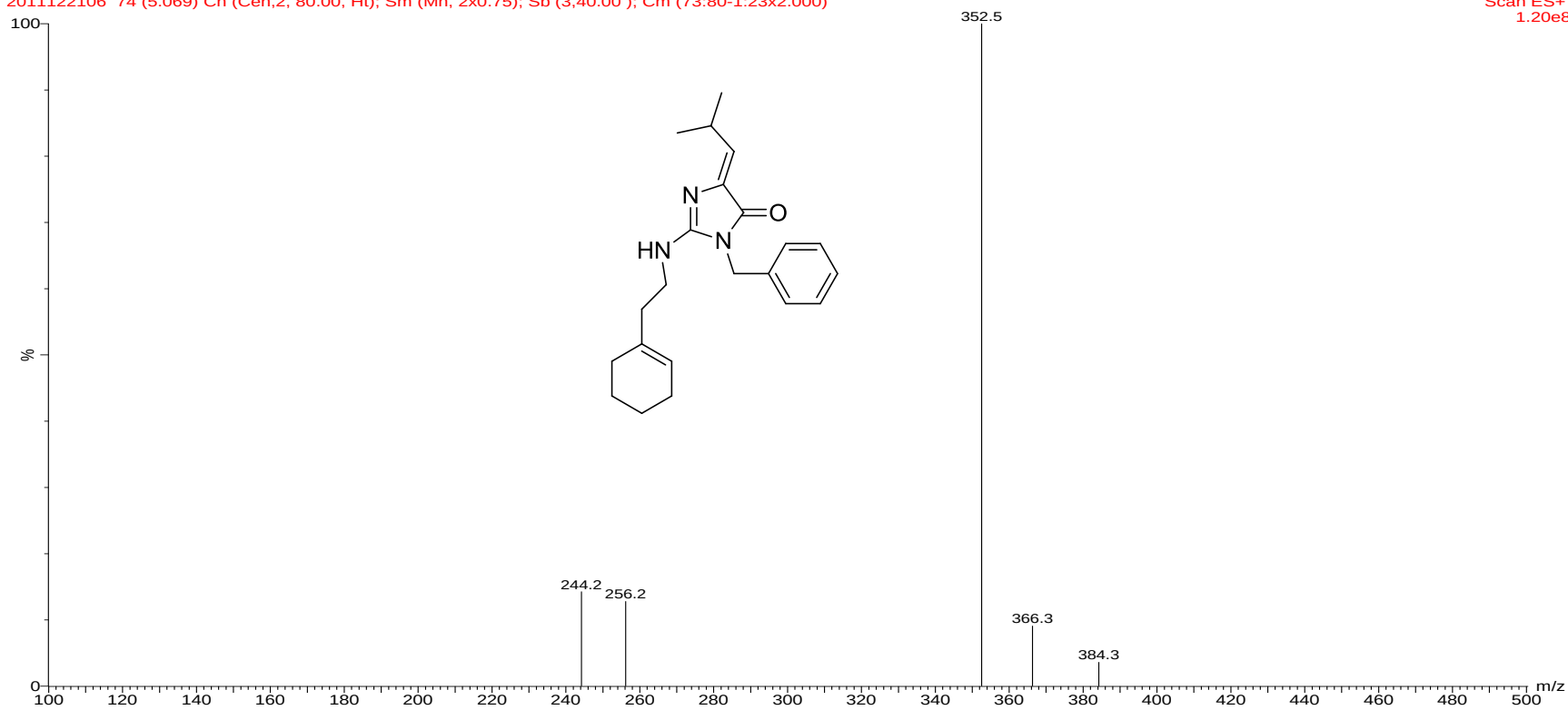


^{13}C spectrum (75 MHz) of compound **6{5,2,2}** in CDCl_3

Mani-84

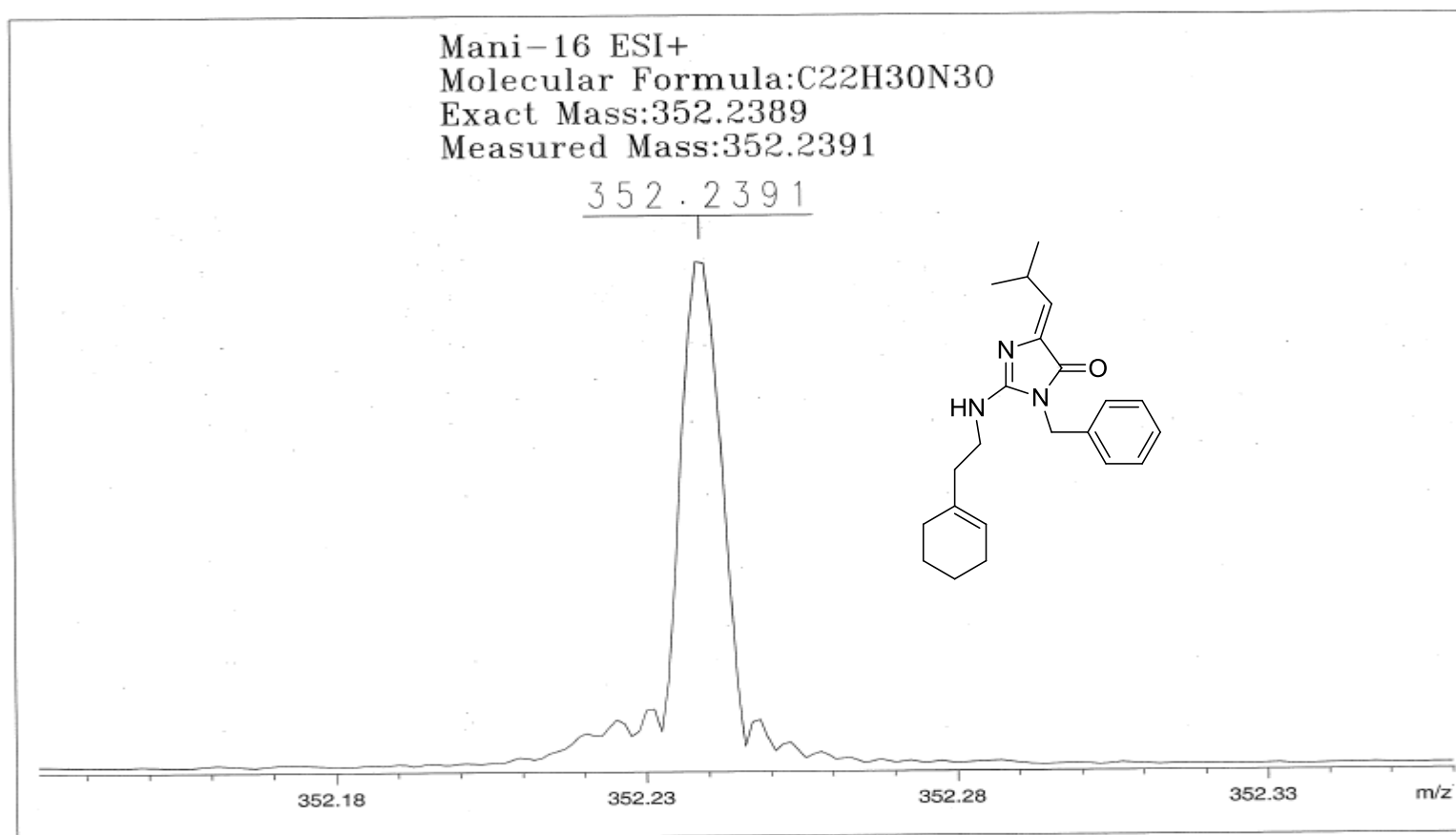
2011122106 74 (5.069) Cn (Cen.2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (73:80-1:23x2.000)

Scan ES+
1.20e8



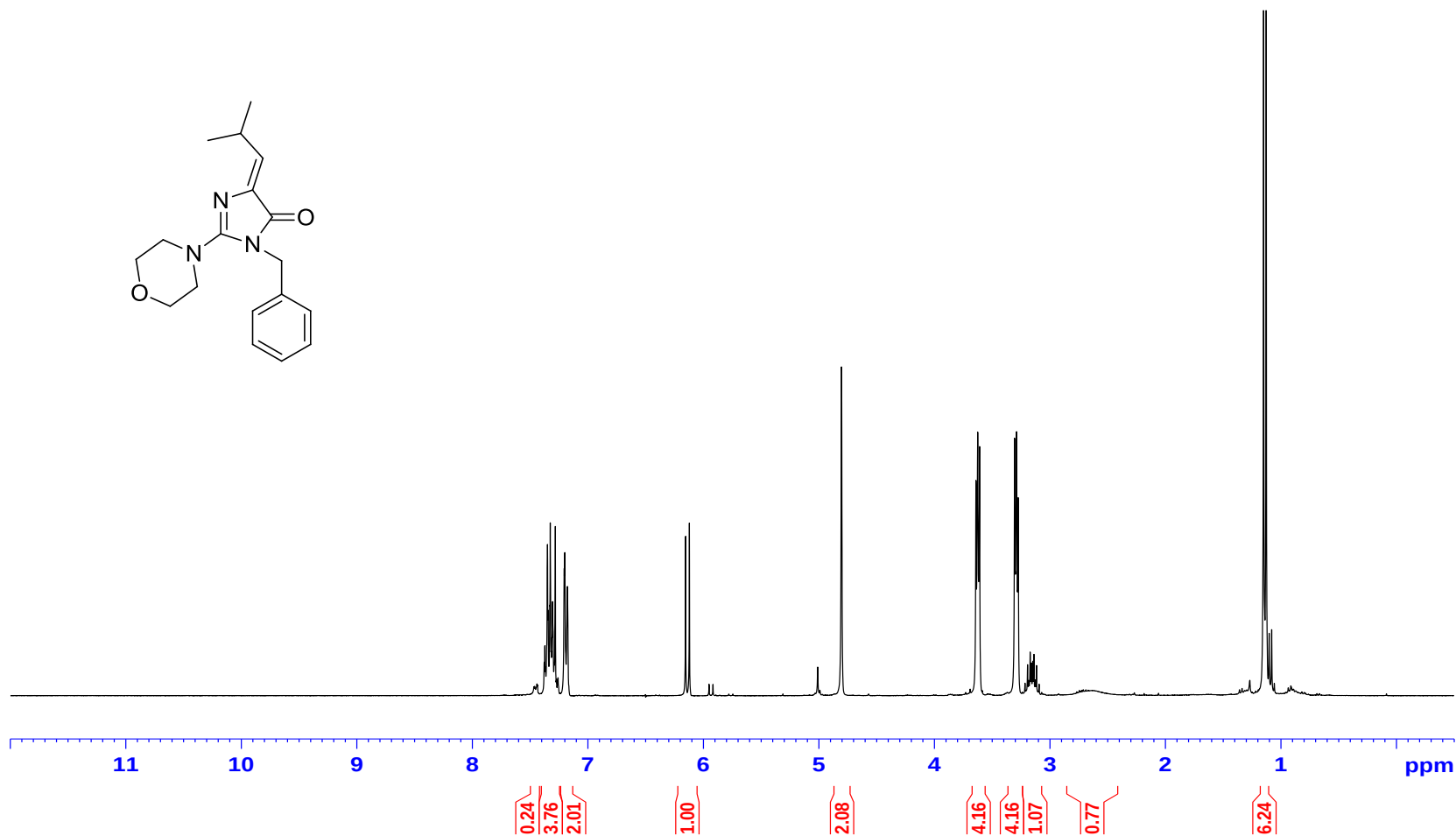
ESI Mass spectrum of compound **6{5,2,2}**

S-81

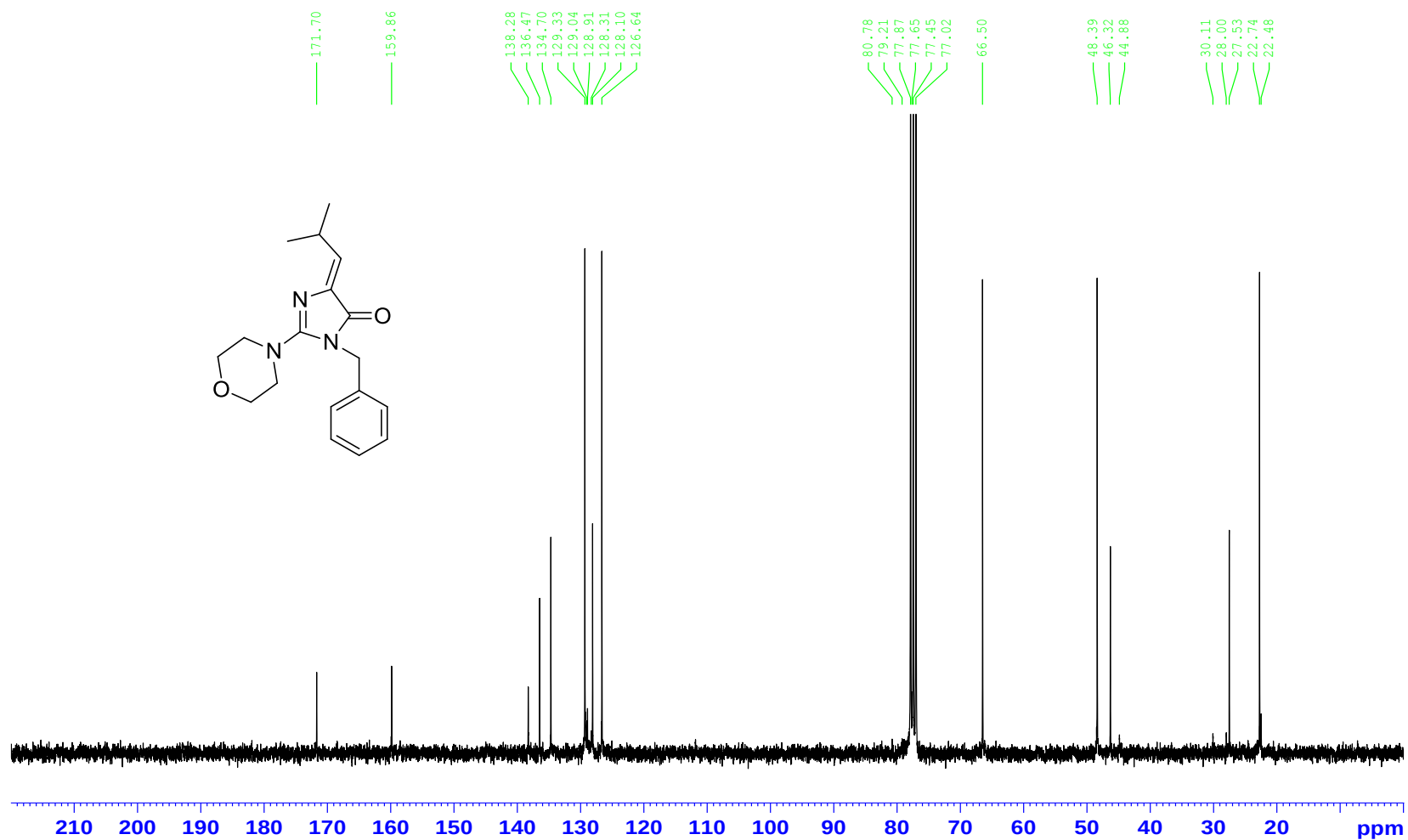


/d=/Data/yy/mani16/2/pdata/1 Administrator Tue Feb 7 16:47:57 2012

HRMS Mass (ESI) spectrum of compound 6{5,2,2}

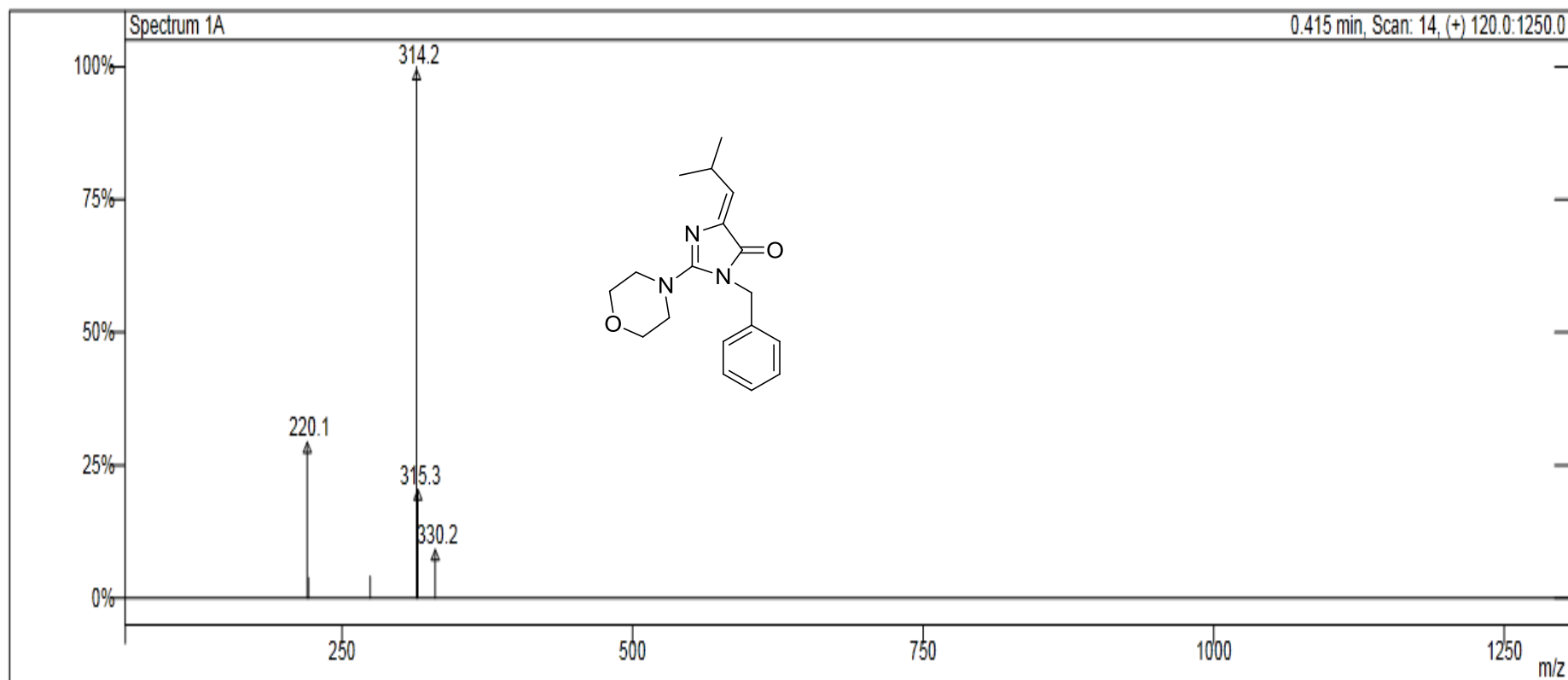


^1H NMR spectrum (300 MHz) of compound **6{5,2,9}** in CDCl_3

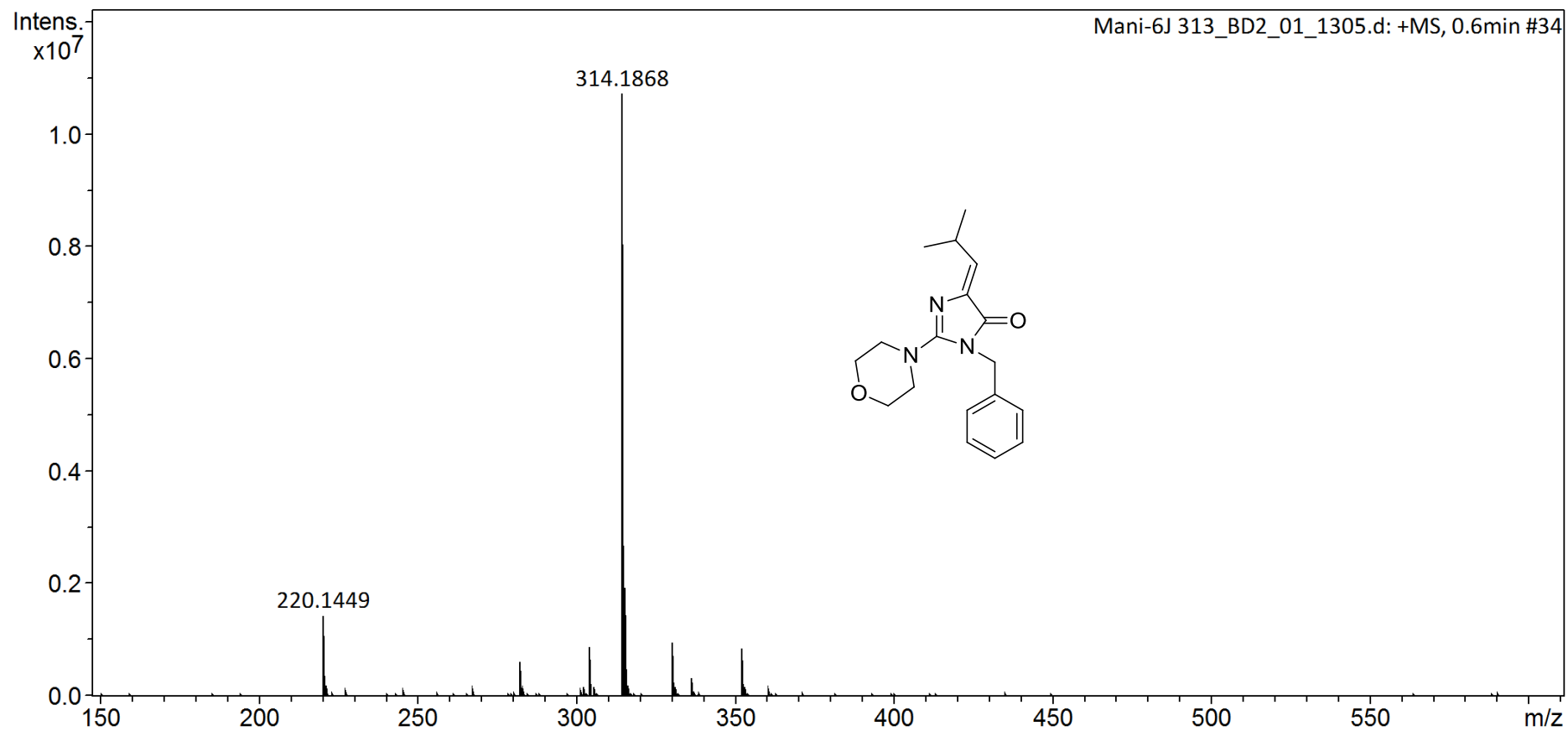


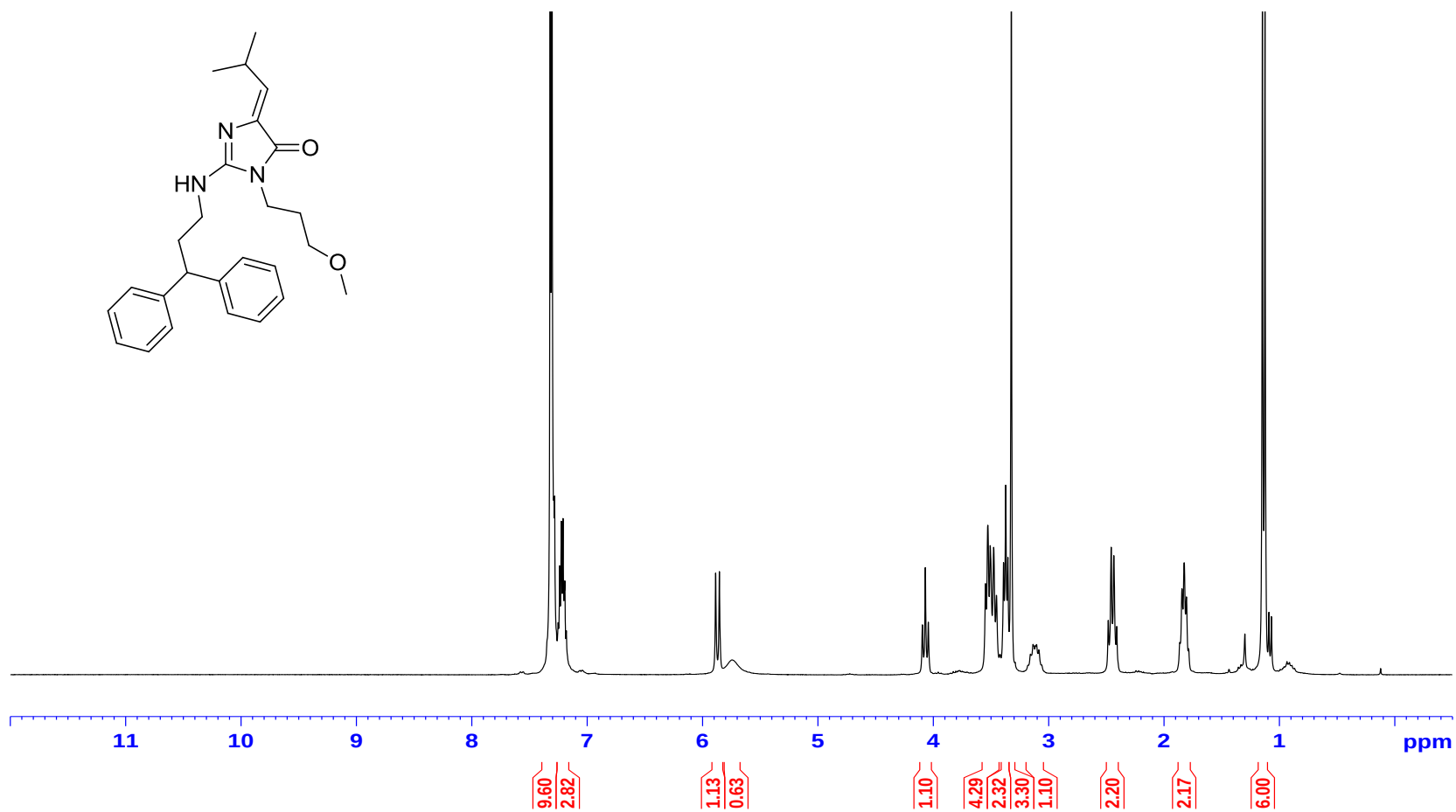
^{13}C spectrum (75 MHz) of compound **6{5,2,9}** in CDCl_3

Scan 14 from c:\service\direct\20140415\2014-04-15_mani-6j.xms

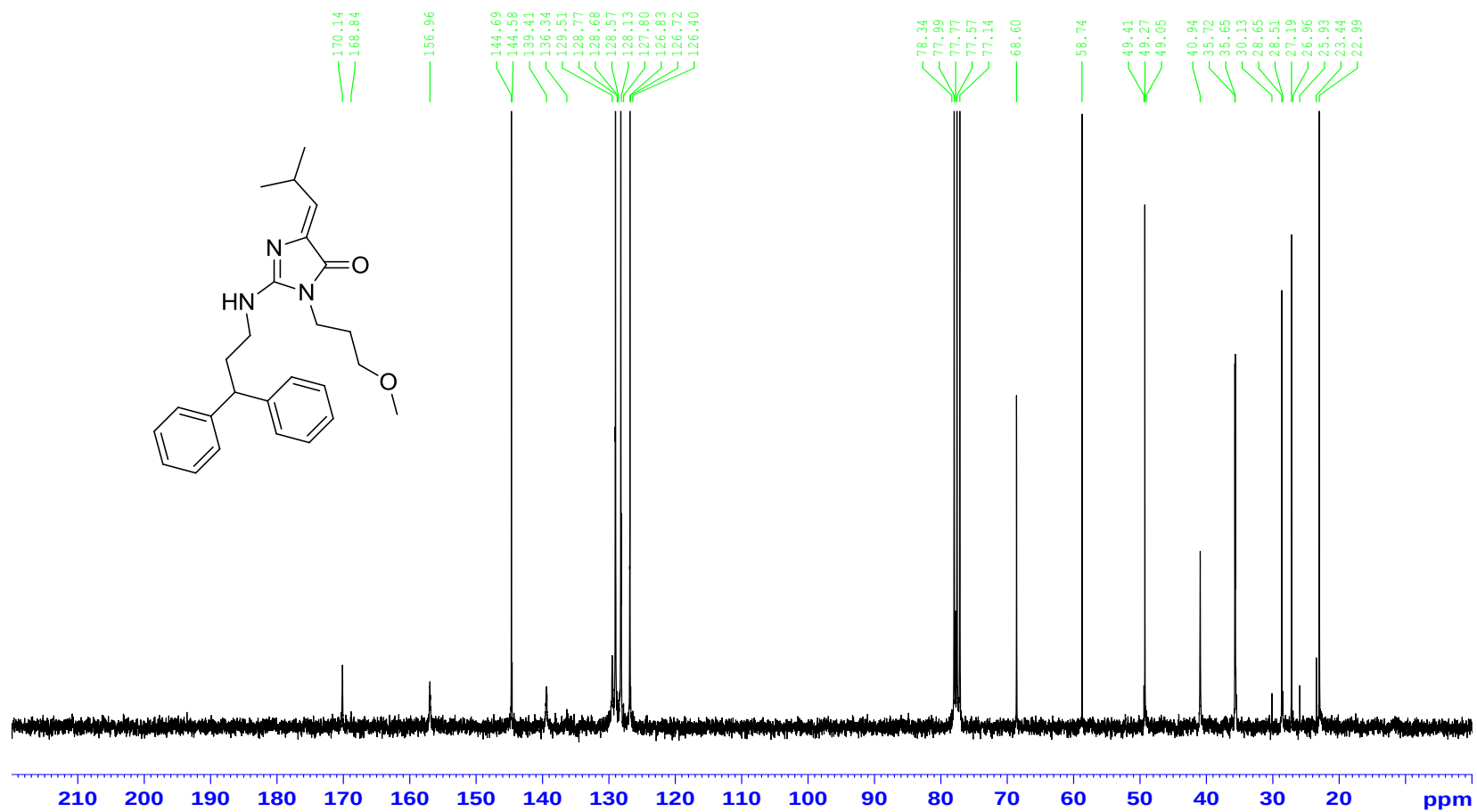


ESI Mass spectrum of compound **6{5,2,9}**





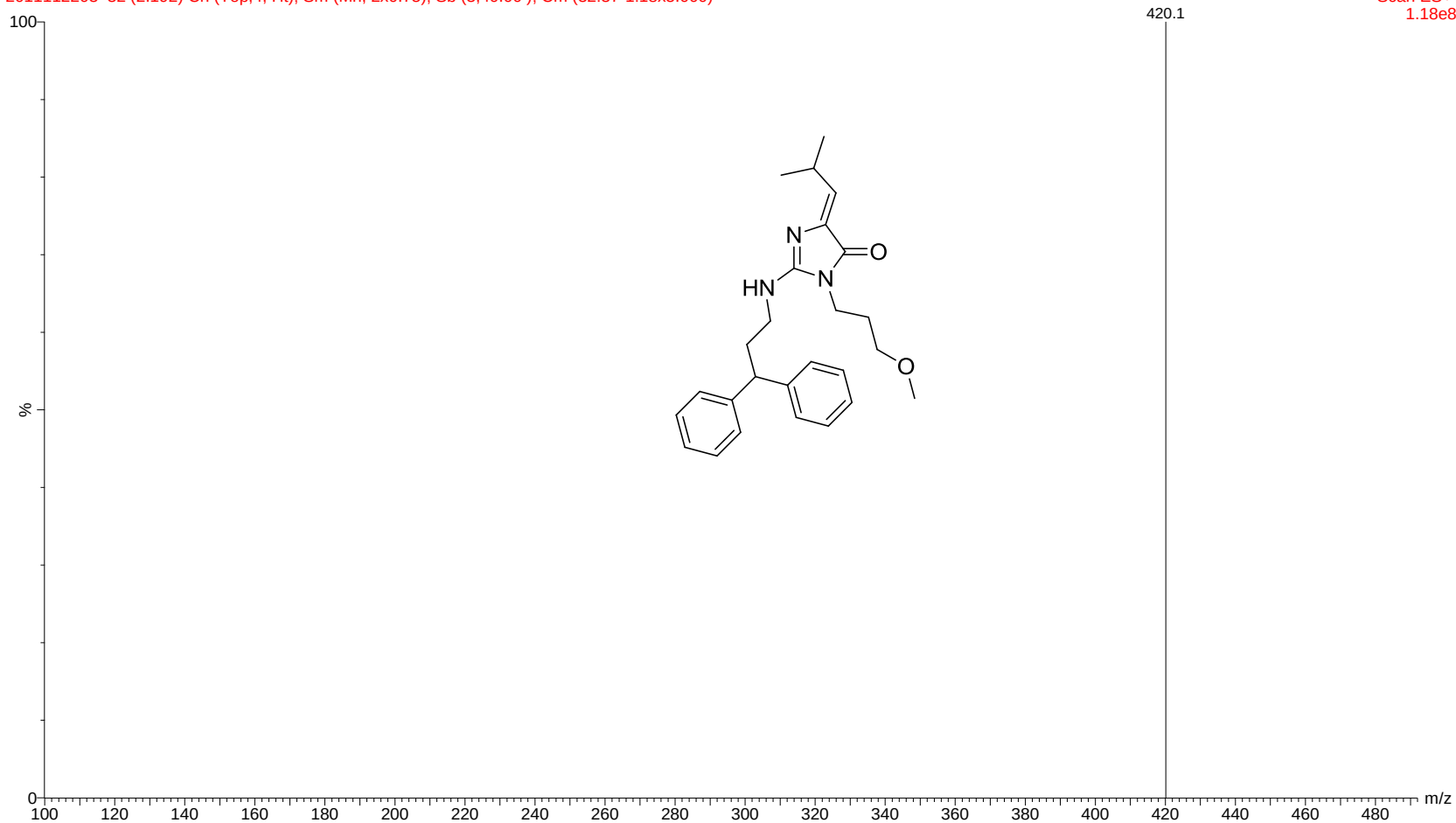
^1H NMR spectrum (300 MHz) of compound **6{5,6,11}** in CDCl_3



^{13}C spectrum (75 MHz) of compound **6{5,6,11}** in CDCl_3

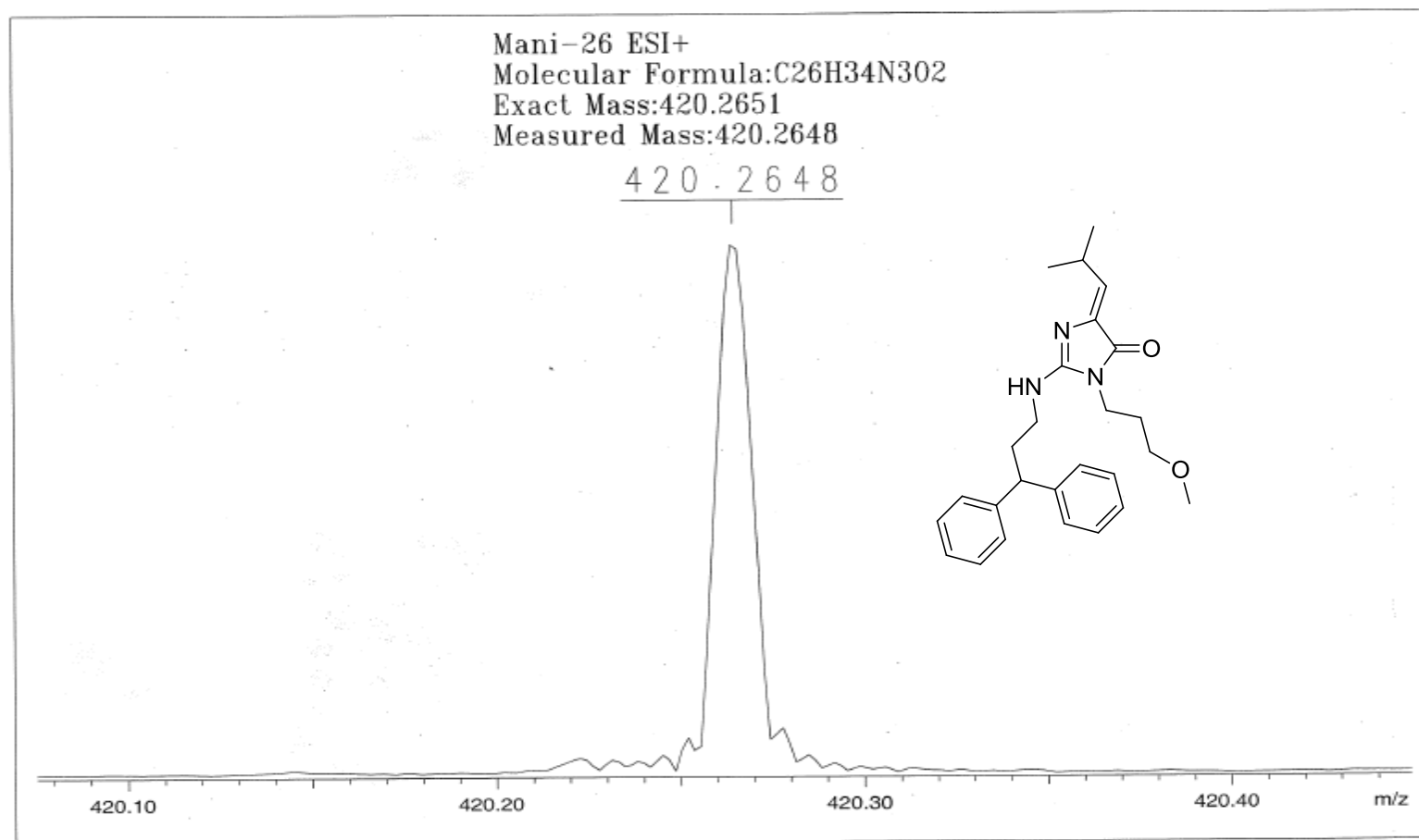
Mani-LMW

2011112203 32 (2.192) Cn (Top,4, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (32:37-1:18x5.000)



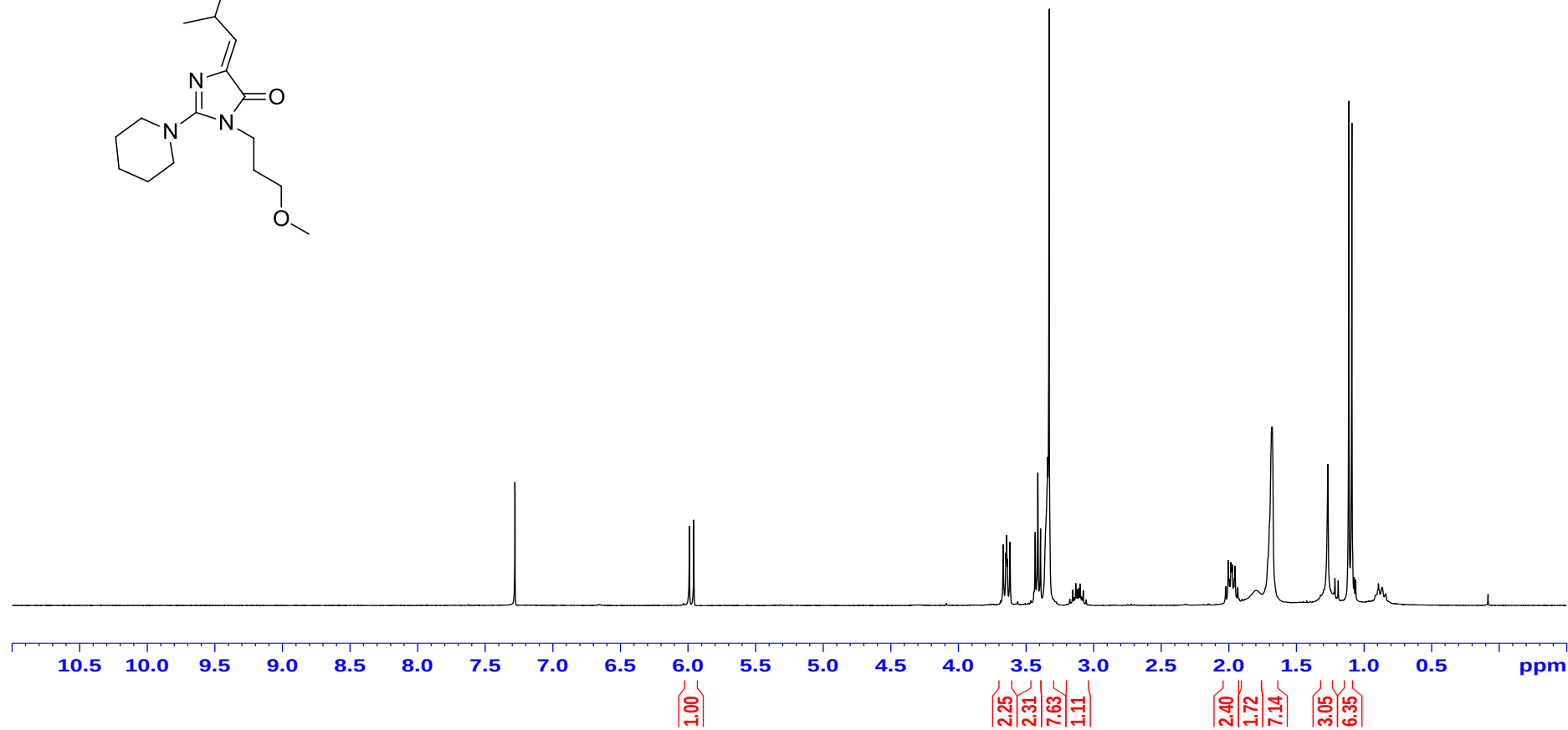
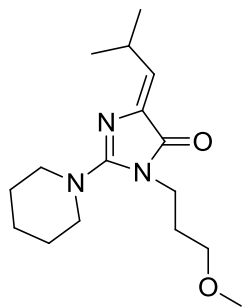
ESI Mass spectrum of compound 6{5,6,11}

S-89

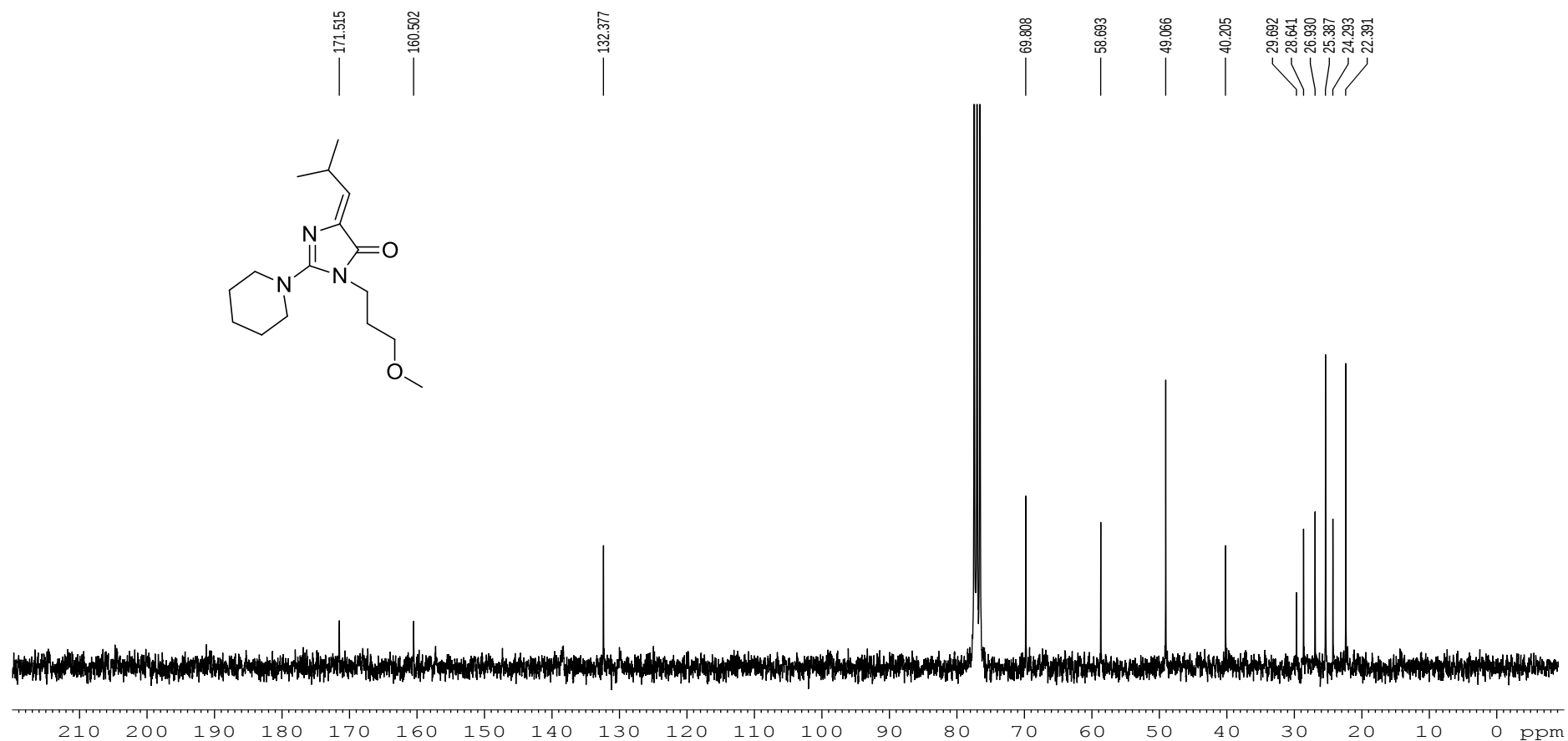


/d=/Data/yu/mani26/2/pdata/1 Administrator Tue Feb 7 15:28:58 2012

HRMS Mass (ESI) spectrum of compound **6{5,6,11}**

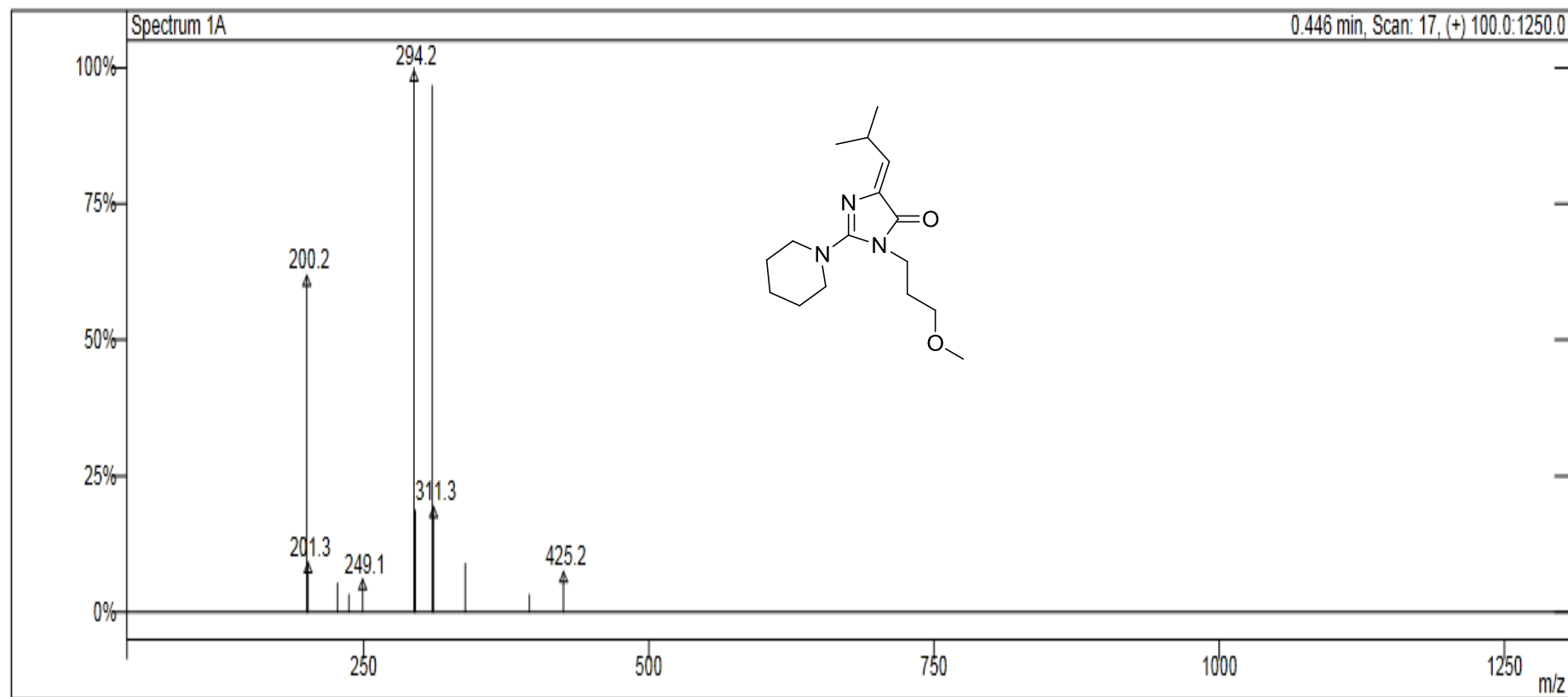


^1H NMR spectrum (300 MHz) of compound **6**{5,6,12} in CDCl_3

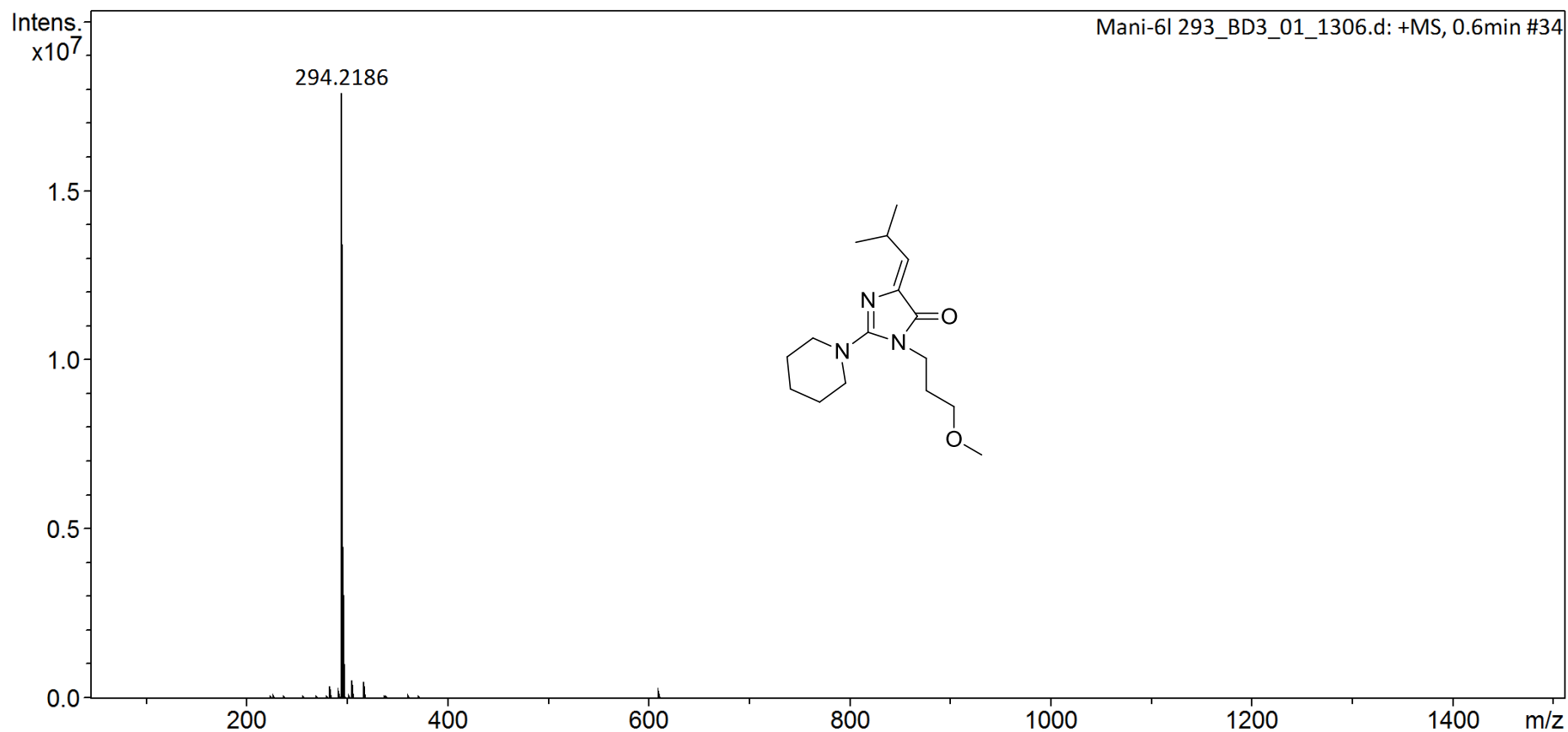


^{13}C spectrum (75 MHz) of compound **6{5,6,12}** in CDCl_3

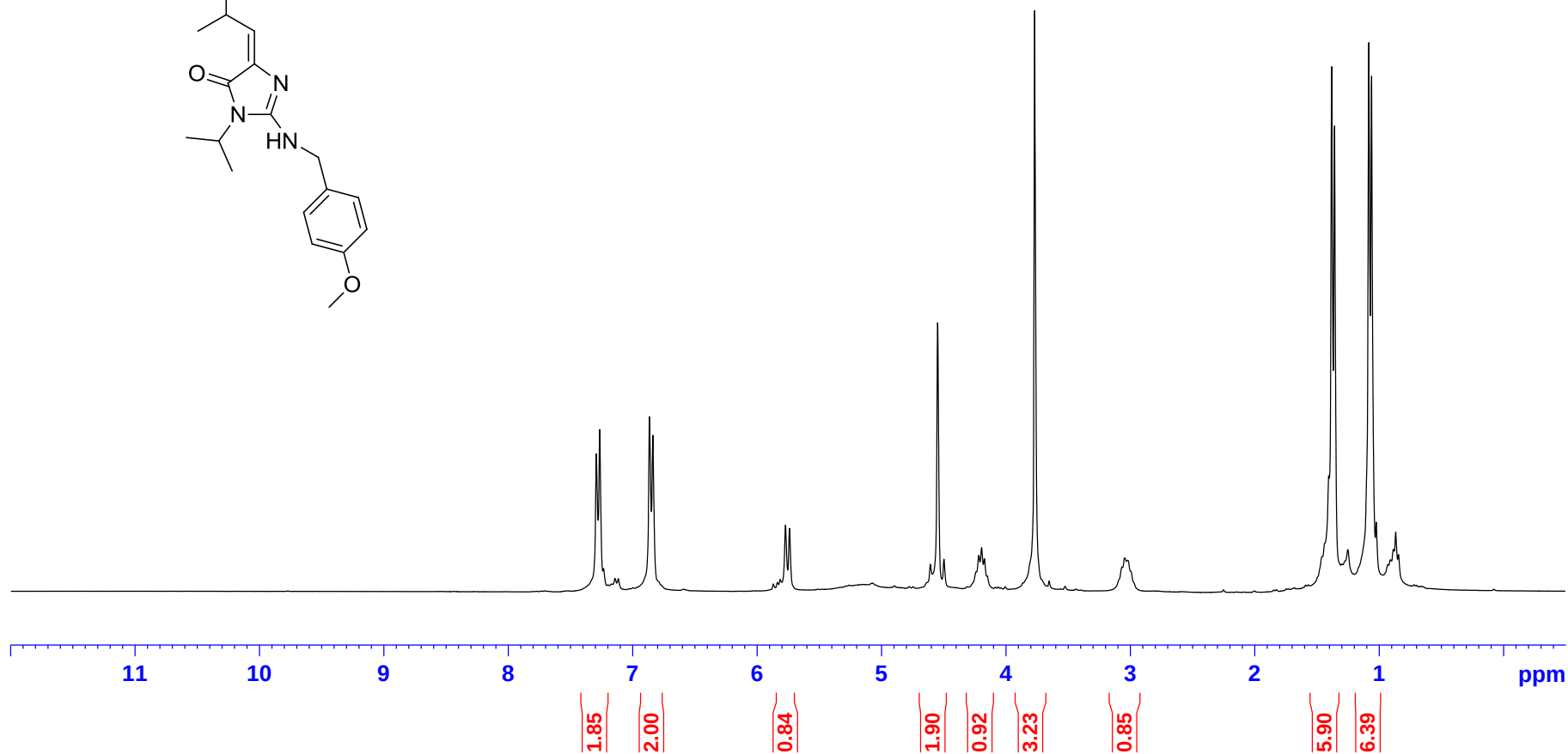
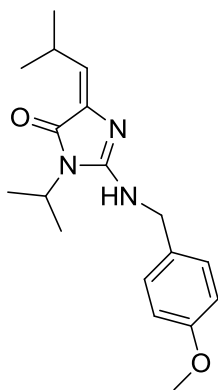
Scan 17 from c:\service\direct\20140415\vm\smal\2014-04-15_mani-6l.xms



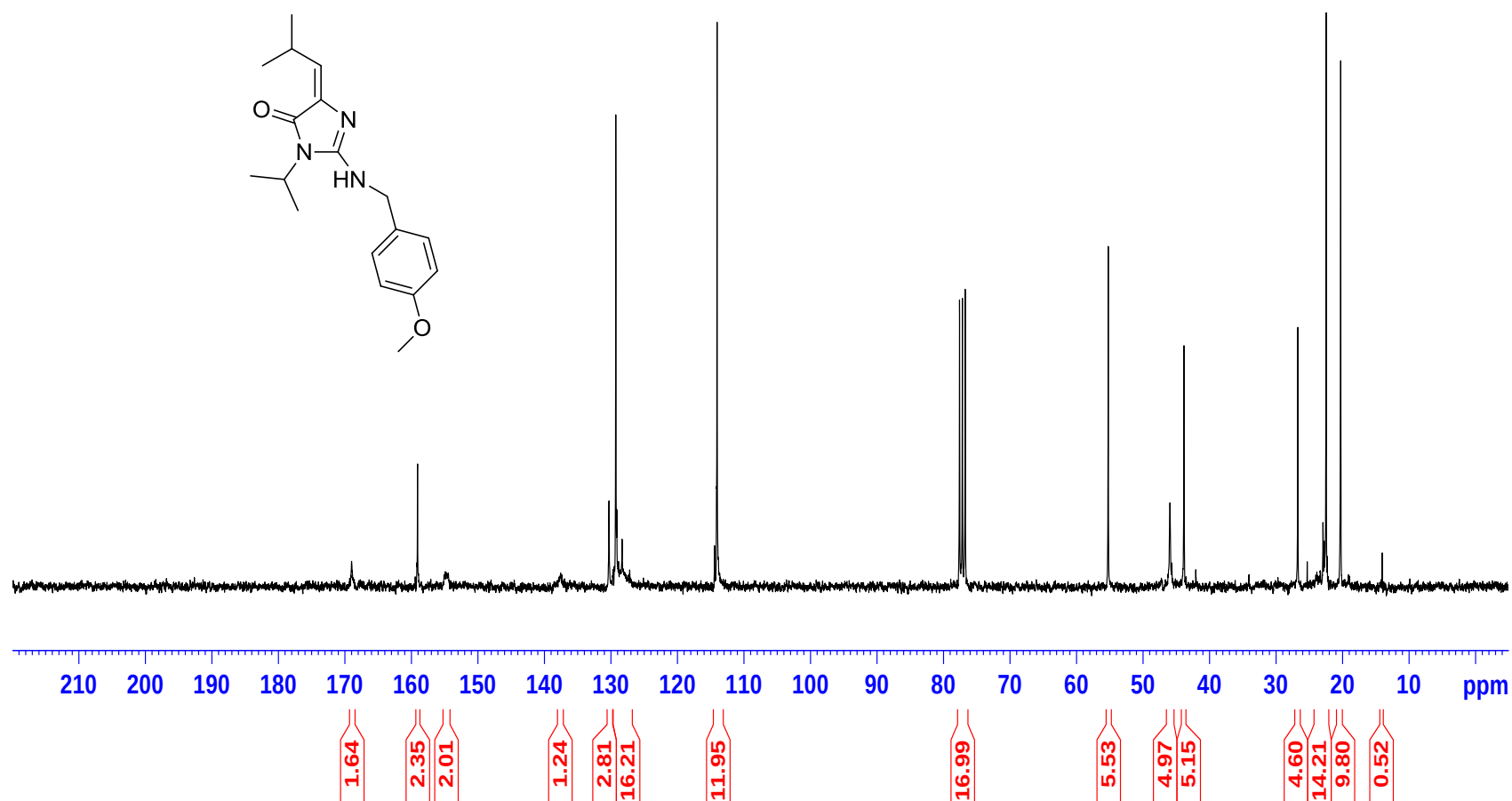
ESI Mass spectrum of compound 6{5,6,12}



HRMS Mass (ESI) spectrum of compound **6{5,6,12}**



^1H NMR spectrum (300 MHz) of compound **6{5,3,3}** in CDCl_3

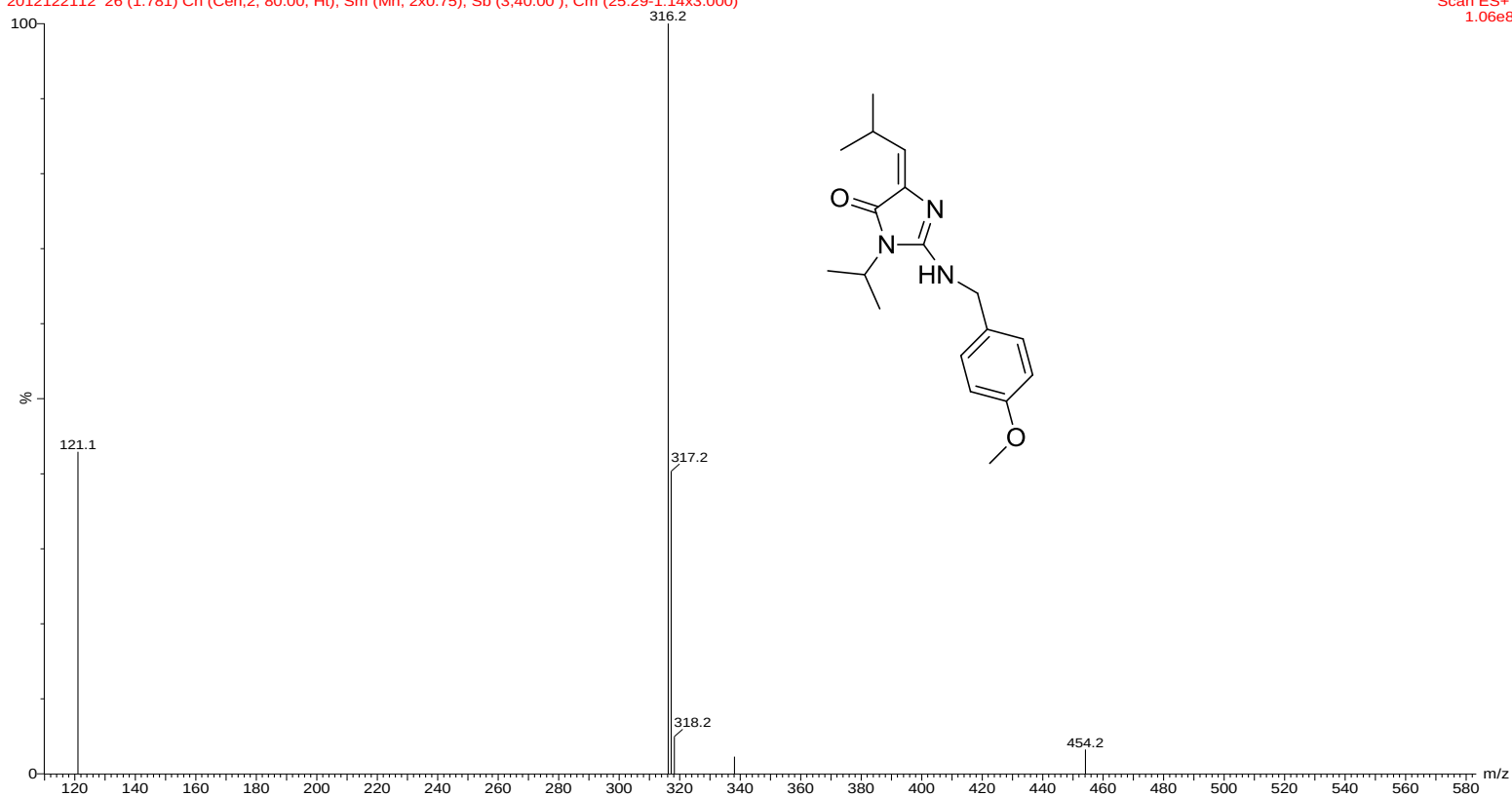


^{13}C spectrum (75 MHz) of compound **6{5,3,3}** in CDCl_3

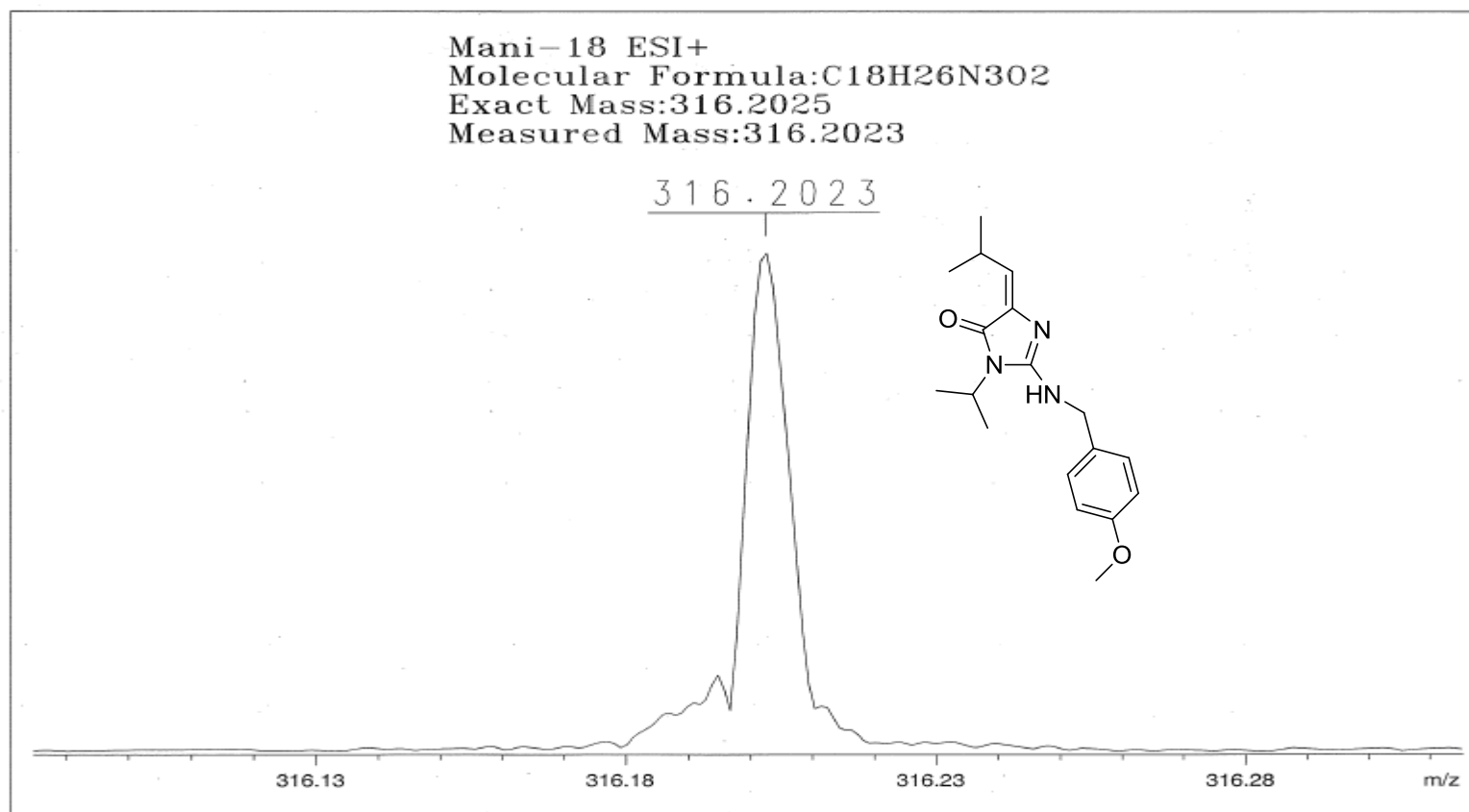
Mani-90-S2

2012122112 26 (1.781) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (25:29-1:14x3.000)

Scan ES+
1.06e8

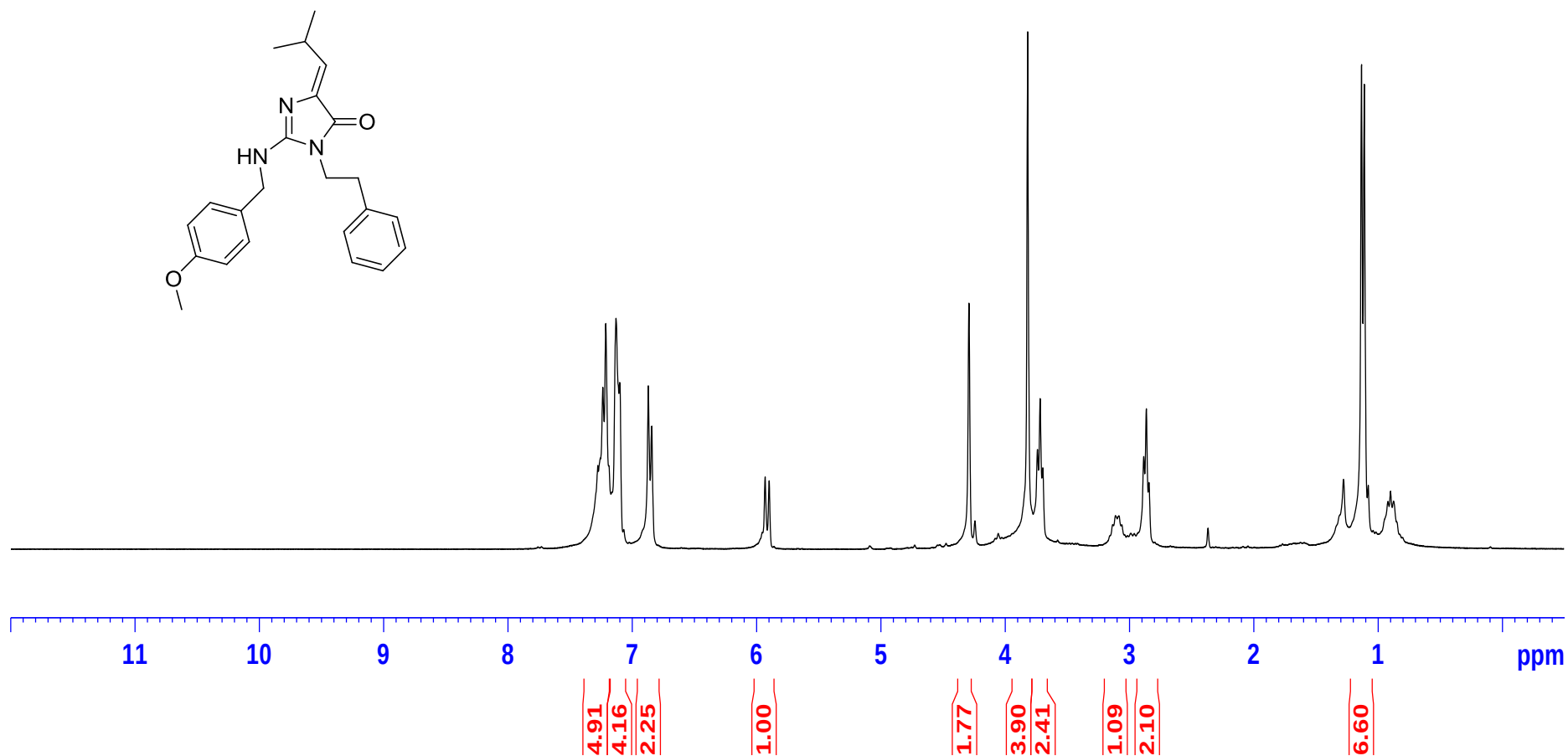


ESI Mass spectrum of compound 6{5,3,3}

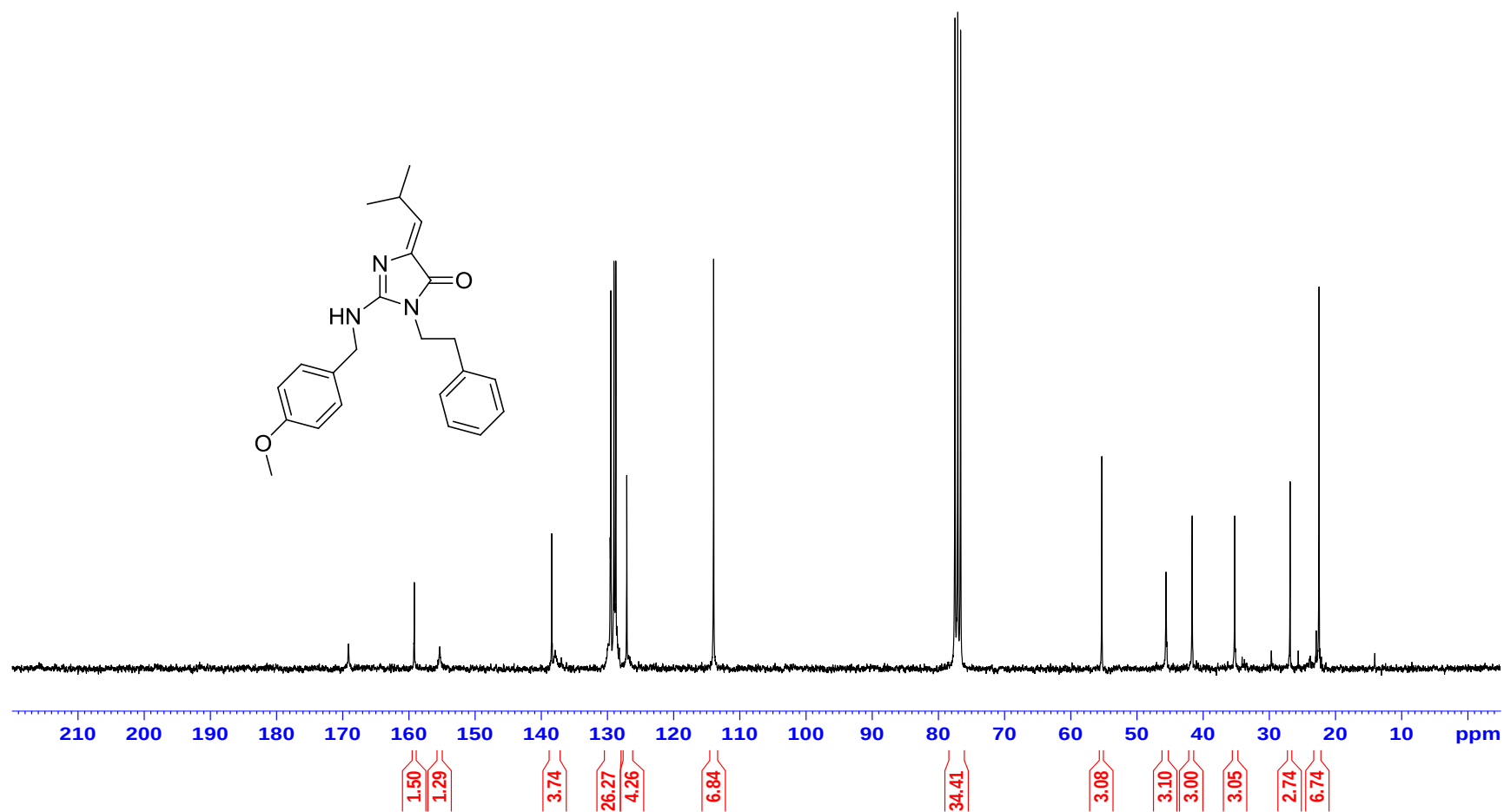


/d=/Data/yl/mani18/1/pdata/1 Administrator Tue Feb 7 17:05:33 2012

HRMS Mass (ESI) spectrum of compound 6{5,3,3}



^1H NMR spectrum (300 MHz) of compound **6{5,4,3}** in CDCl_3



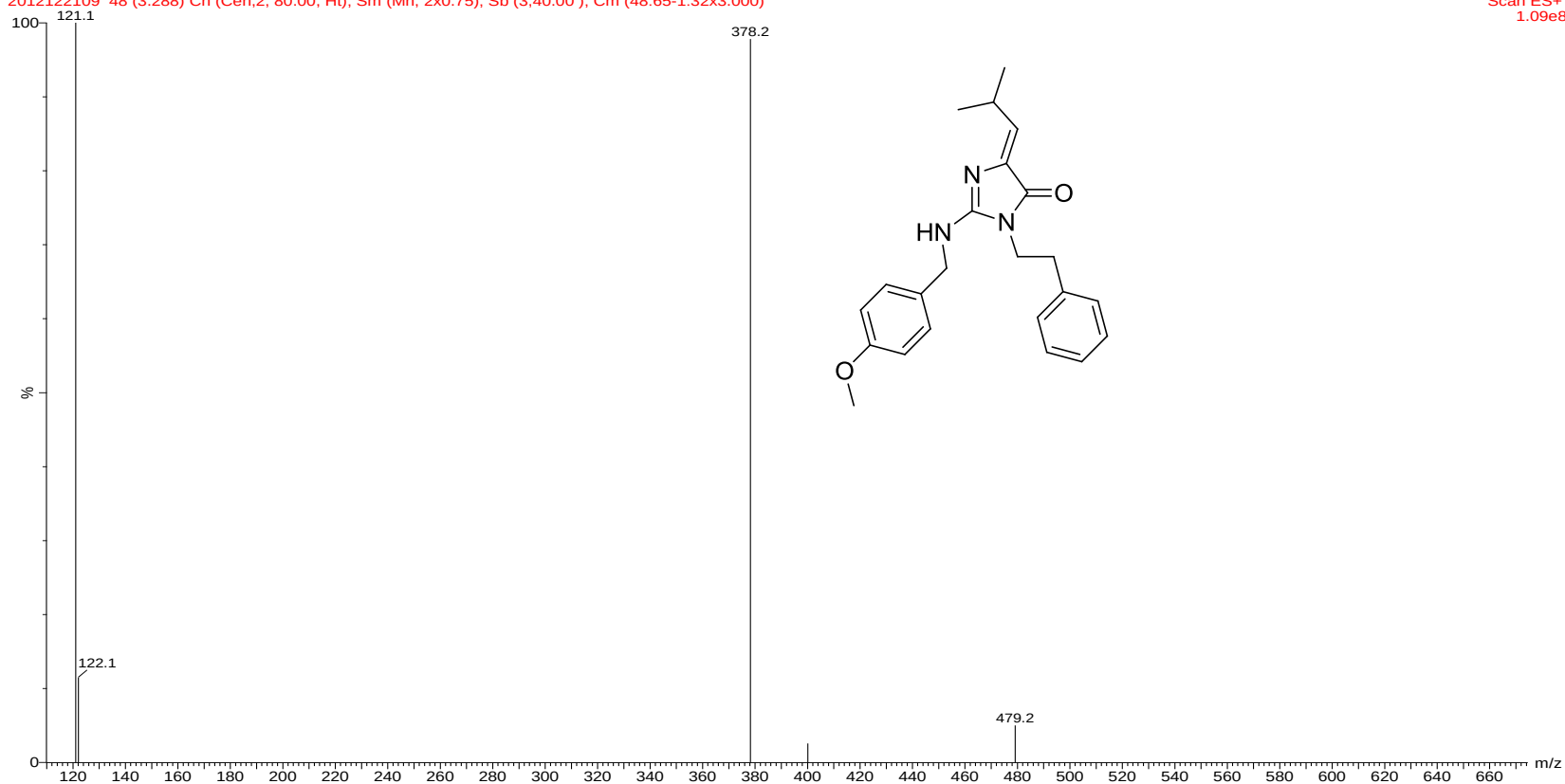
^{13}C spectrum (75 MHz) of compound **6{5,4,3}** in CDCl_3

S-100

Mani-91-S2

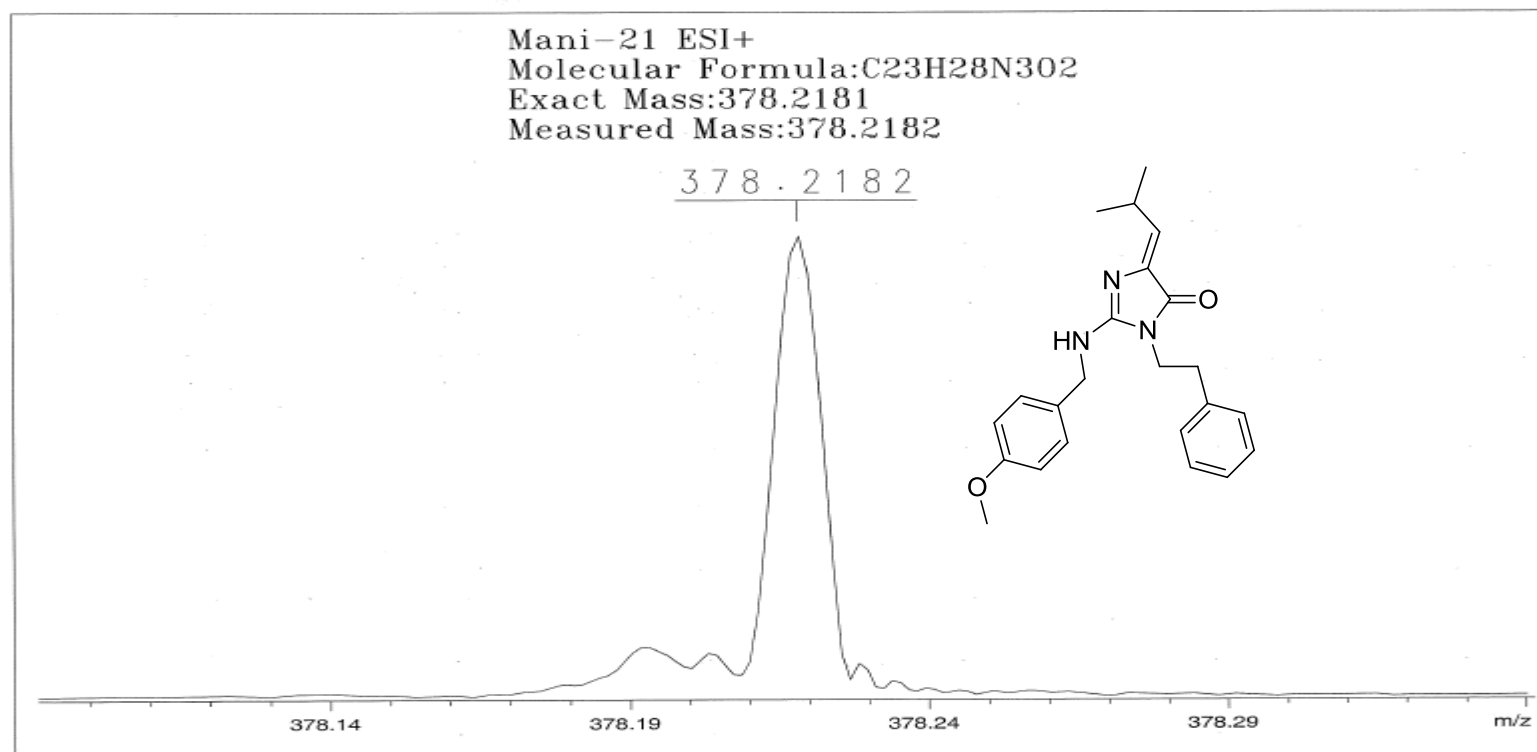
2012122109 48 (3.288) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (48:65-1:32x3.000)

Scan ES+
1.09e8



ESI Mass spectrum of compound 6{5,4,3}

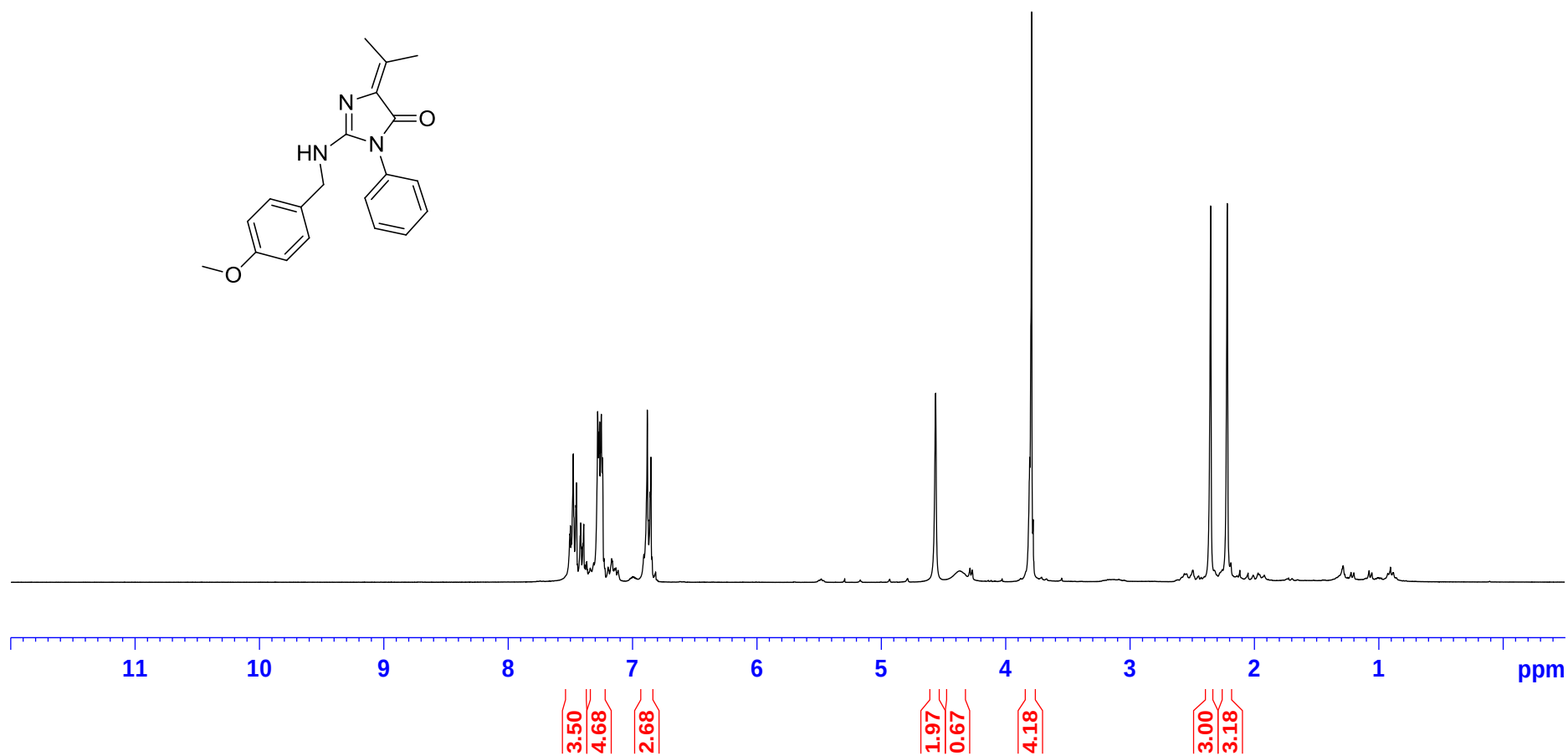
S-101



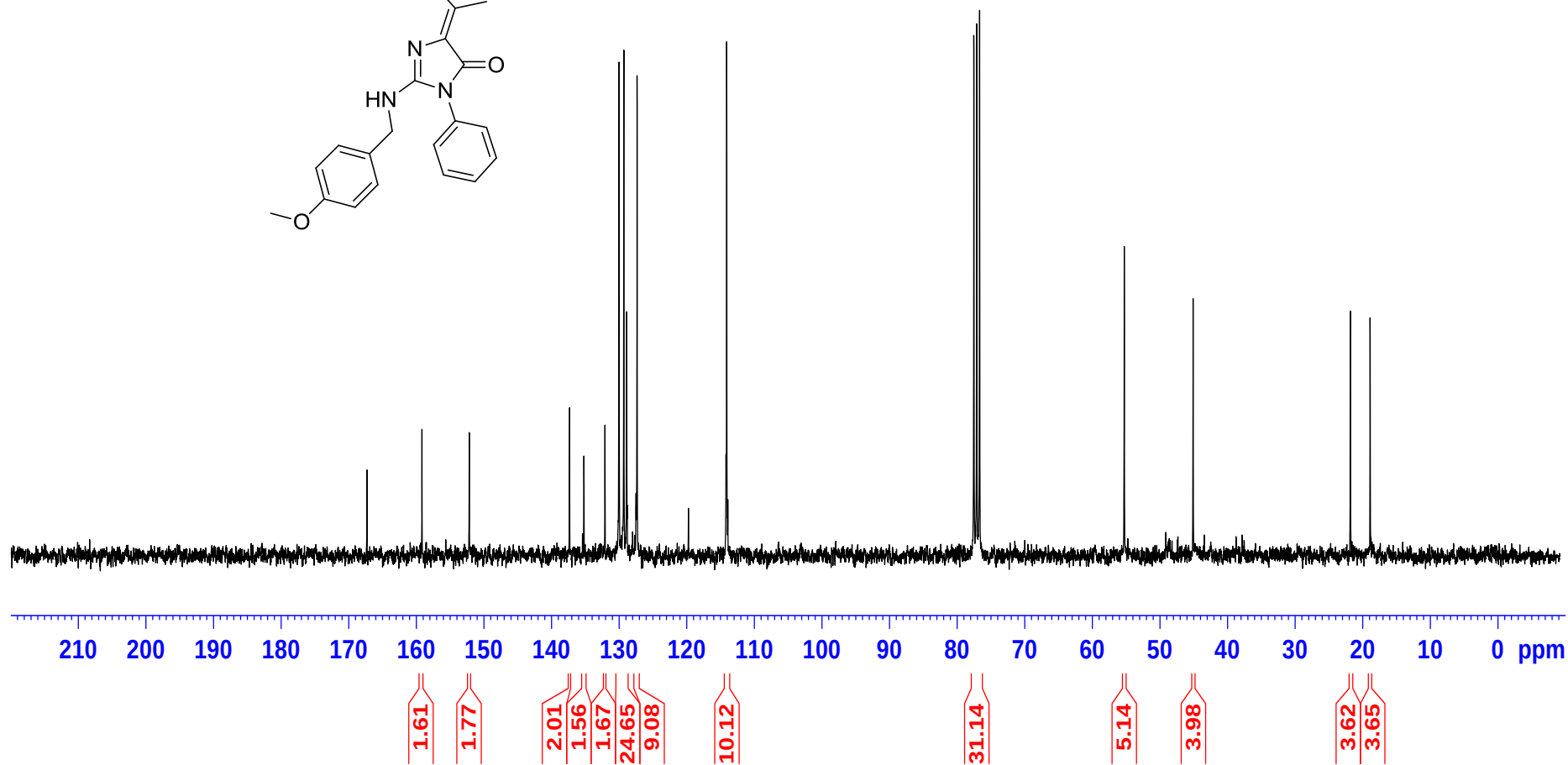
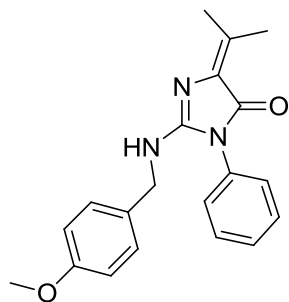
/d=/Data/yu/mani21/2/pdata/1 Administrator Tue Feb 7 14:39:56 2012

HRMS Mass (ESI) spectrum of compound 6{5,4,3}

S-102



^1H NMR spectrum (300 MHz) of compound **6{4,7,3}** in CDCl_3

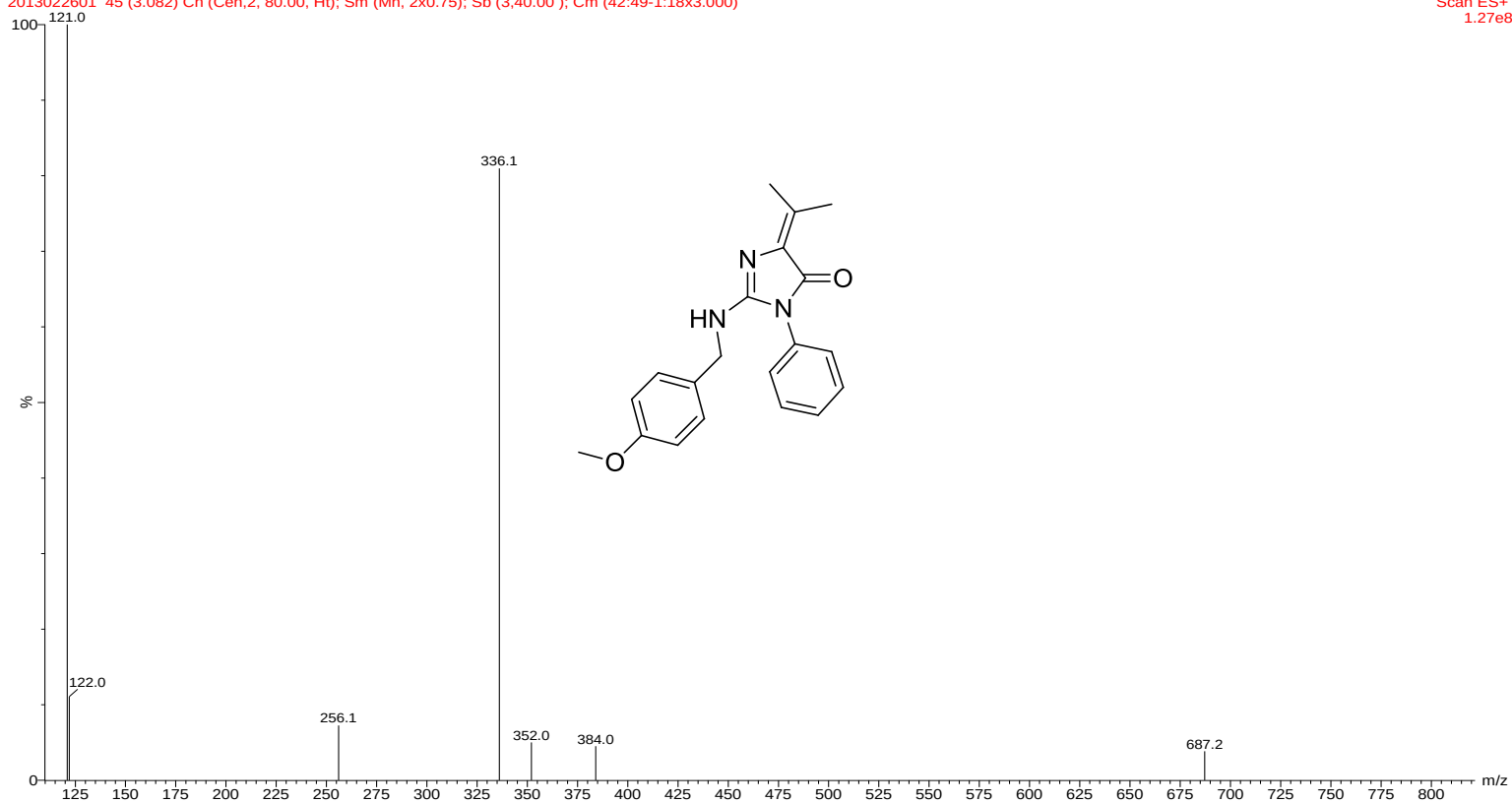


¹³C spectrum (75 MHz) of compound **6{4,7,3}** in CDCl₃

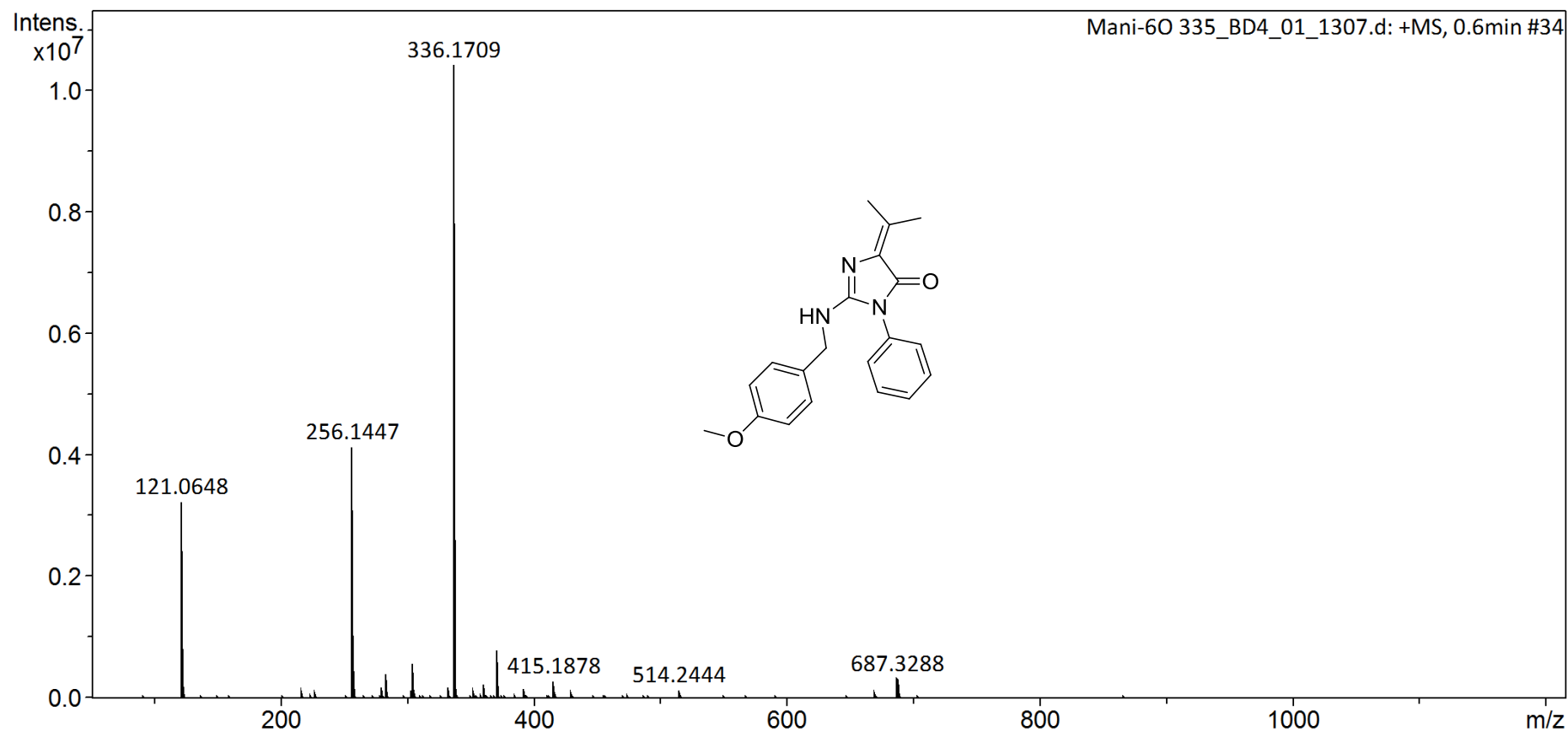
Mani-92-1-S2

2013022601 45 (3.082) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (42:49-1:18x3.000)

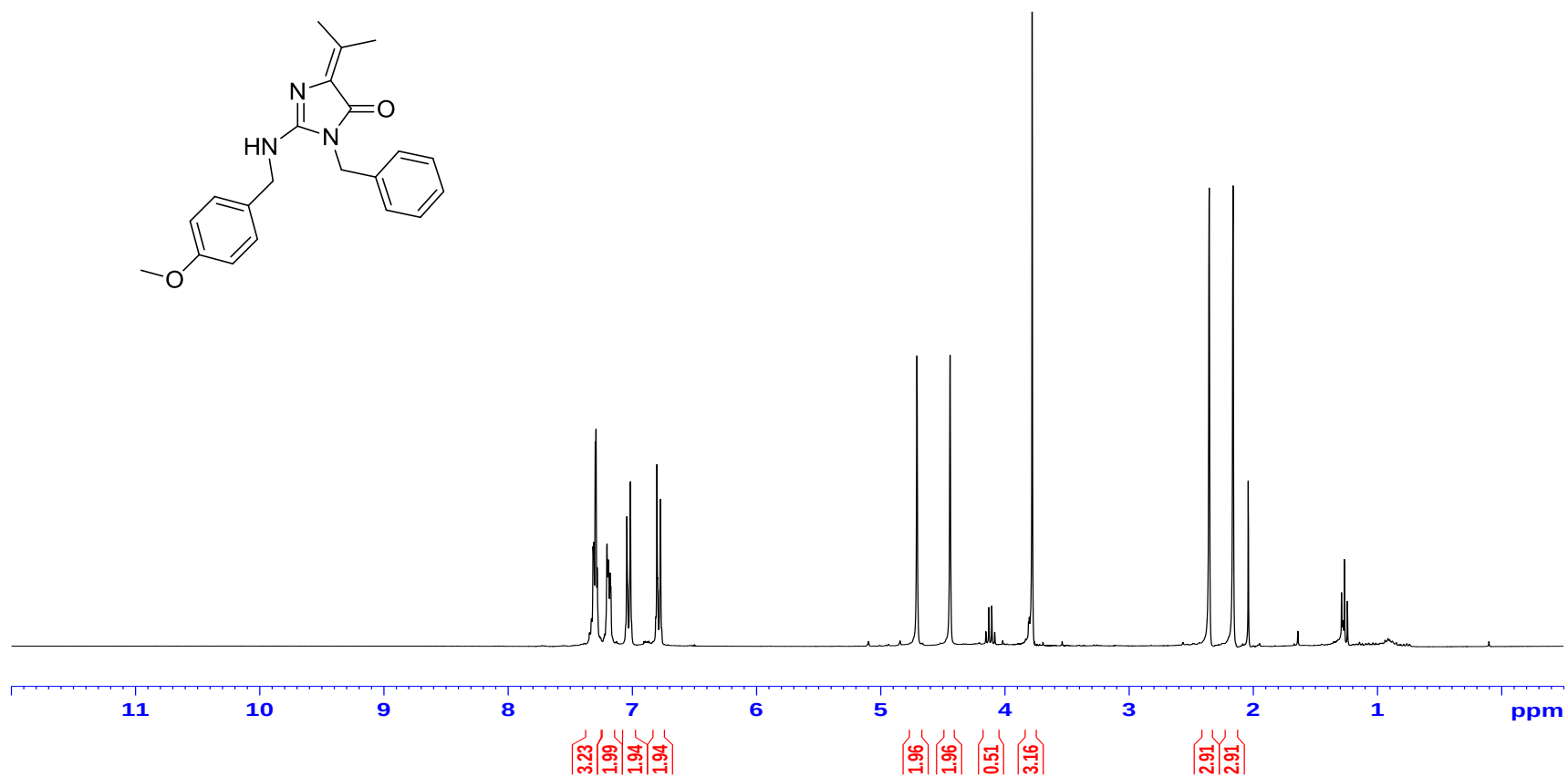
Scan ES+
1.27e8



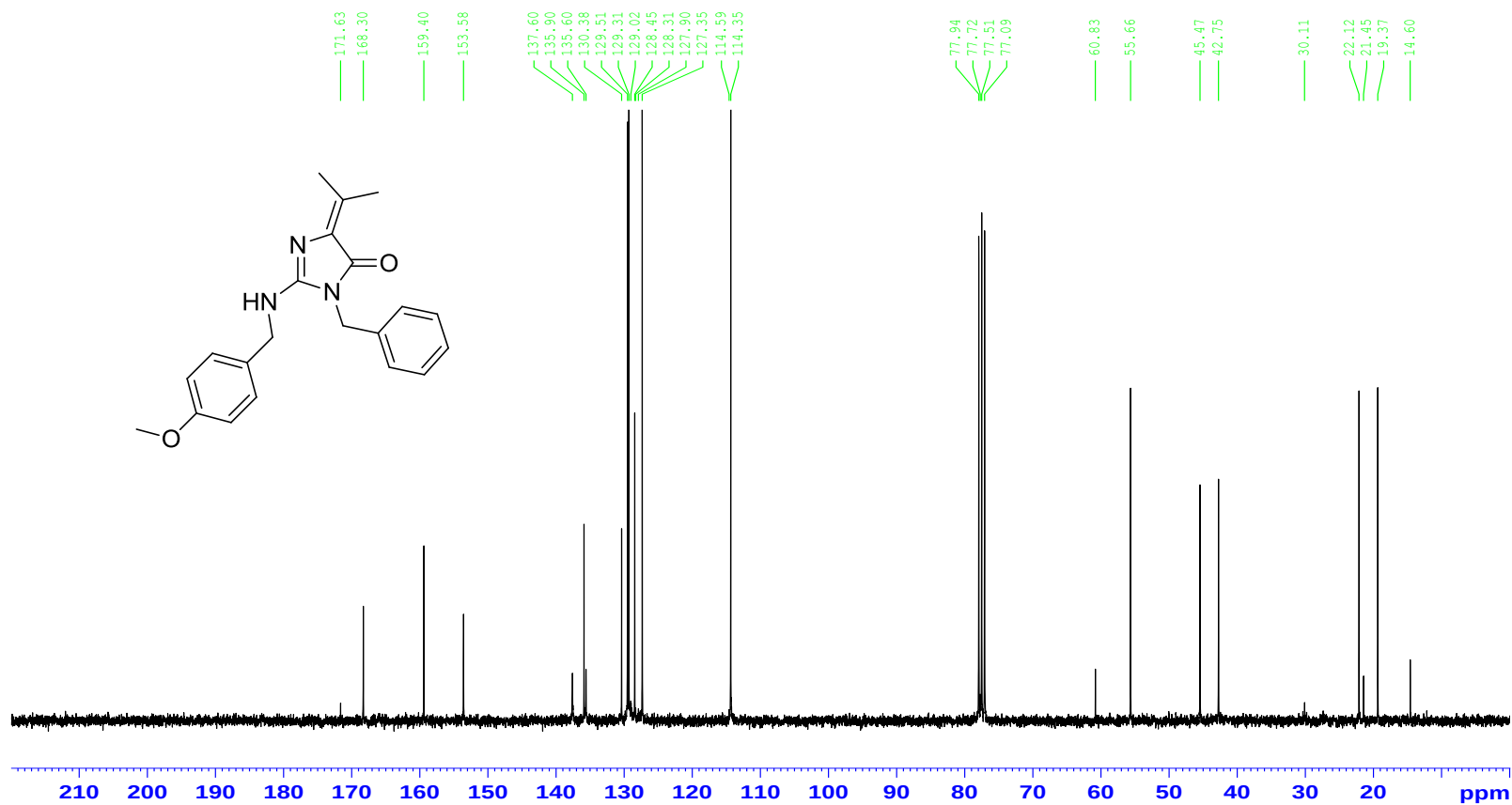
ESI Mass spectrum of compound 6{4,7,3}



HRMS Mass (ESI) spectrum of compound **6{4,7,3}**



¹H NMR spectrum (300 MHz) of compound **6{4,2,3}** in CDCl₃

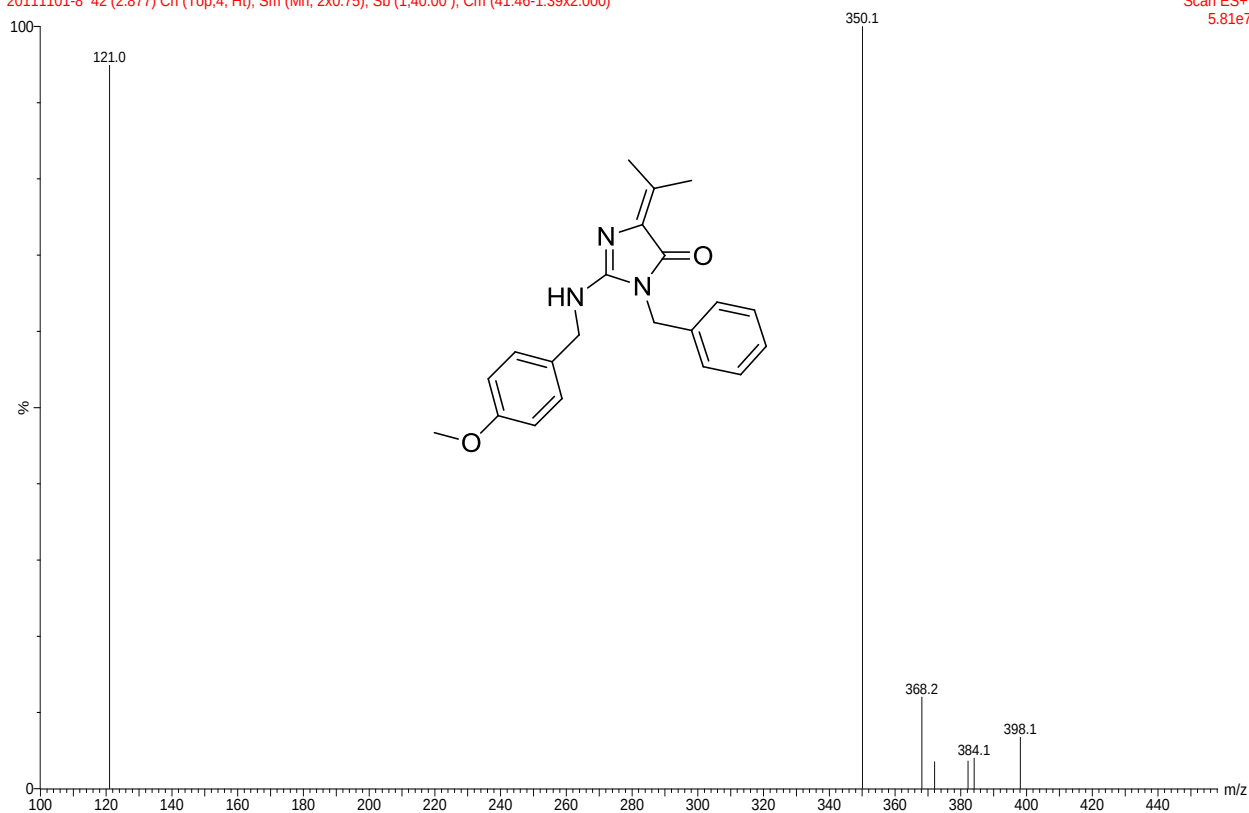


¹³C spectrum (75 MHz) of compound 6{4,2,3} in CDCl₃

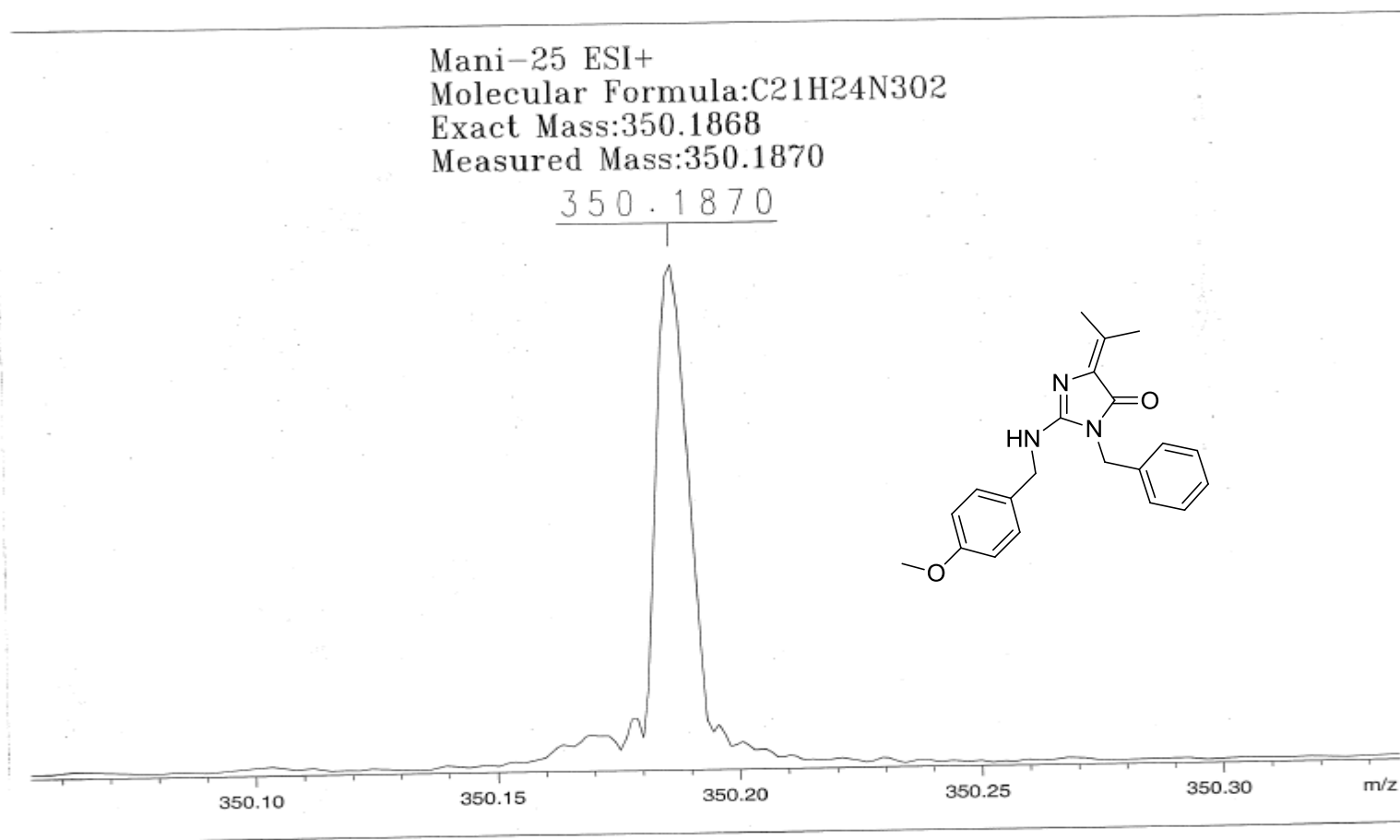
Mani-mBA-2

20111101-8 42 (2.877) Cn (Top,4, Ht); Sm (Mn, 2x0.75); Sb (1,40.00); Cm (41:46-1:39x2.000)

Scan ES+
5.81e7

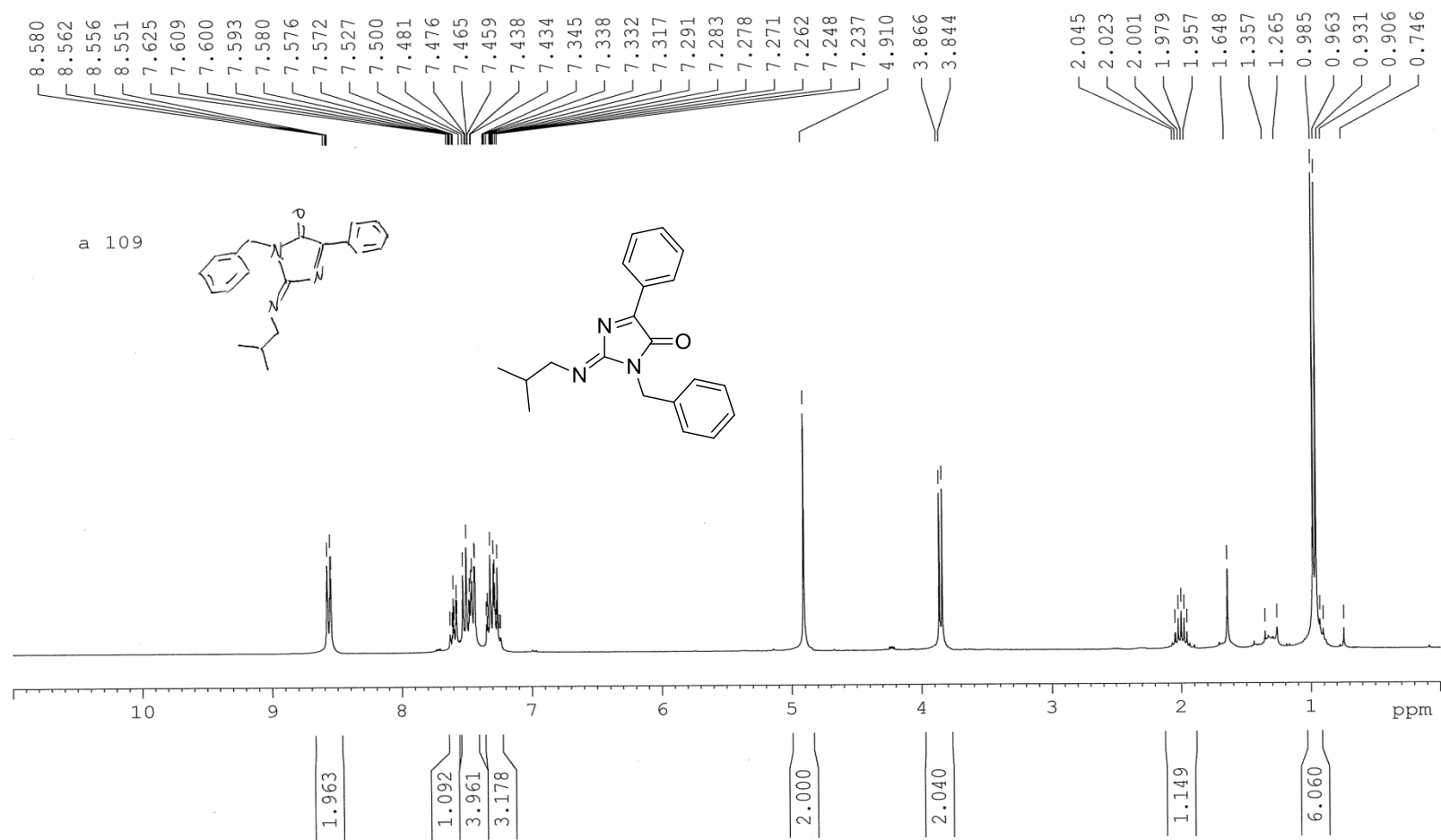


ESI Mass spectrum of compound 6{4,2,3}



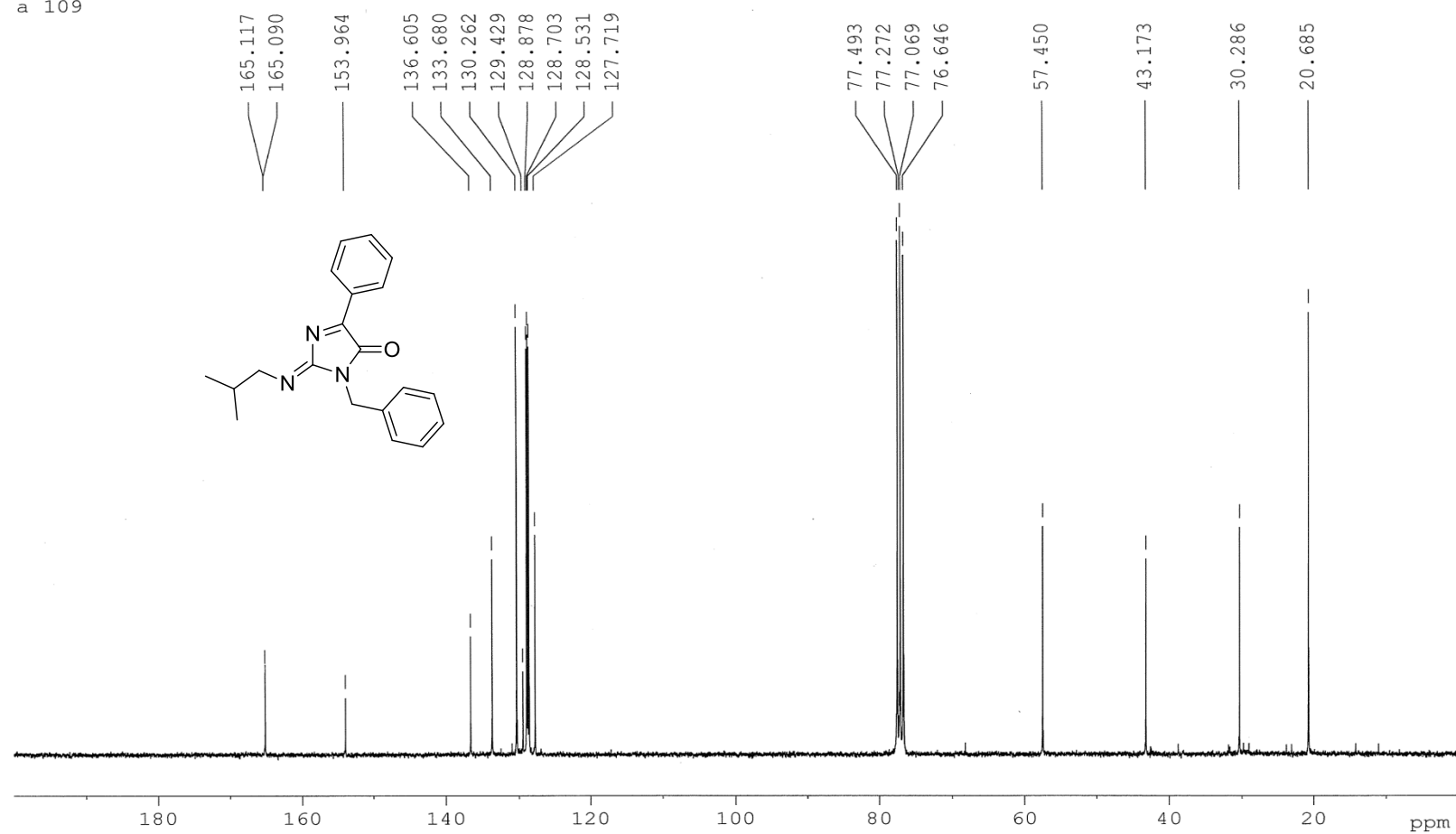
/d=/Data/yu/mani25/1/pdata/1 Administrator Tue Feb 7 15:21:45 2012

HRMS Mass (ESI) spectrum of compound 6{4,2,3}



¹H NMR spectrum (300 MHz) of compound **7{2,2,1}** in CDCl₃

a 109



¹³C spectrum (75 MHz) of compound 7{2,2,1} in CDCl₃

SPEC: 12e1lr-73
Samp: a109
Comm: FINNIGAN MAT-95XL
Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM
Oper: SCLIN
Base: 91.0
Norm: 91.0
Peak: 1000.00 mmu

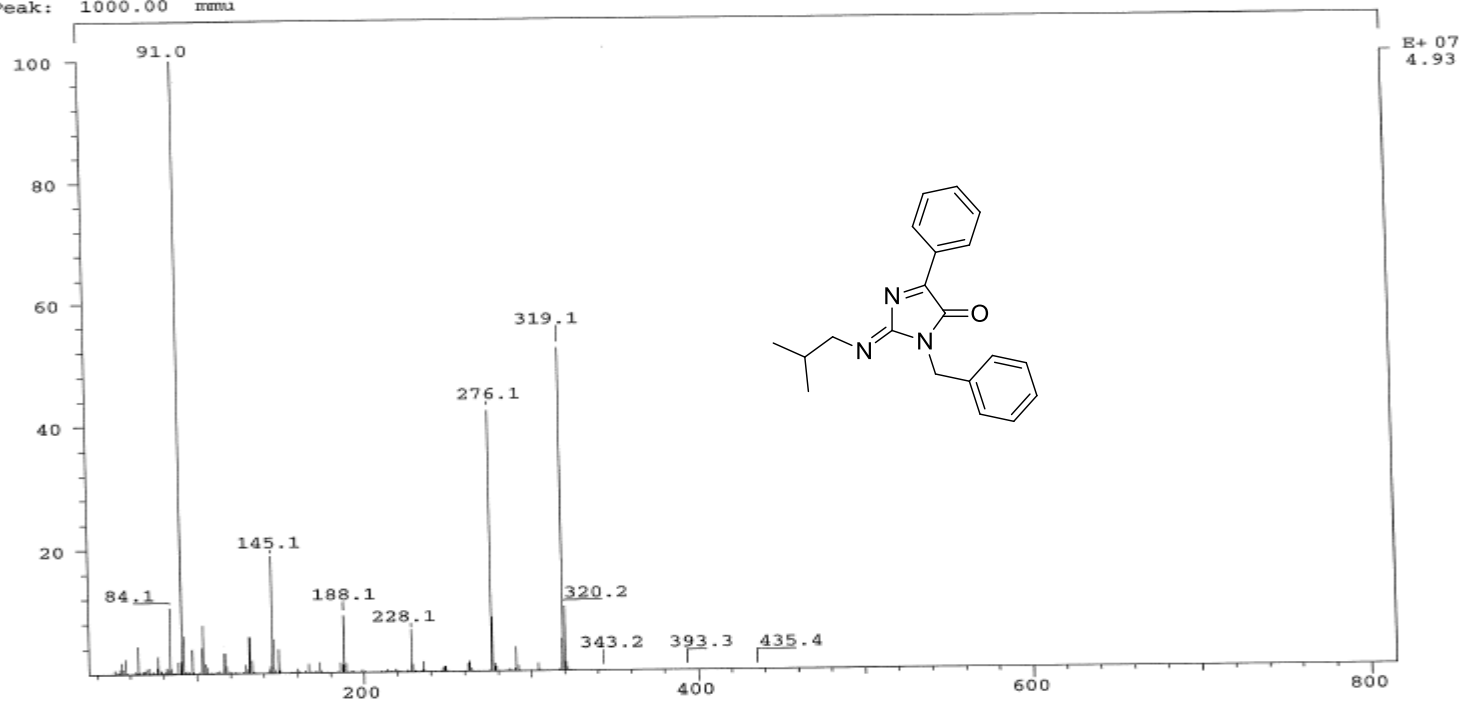
28-Dec-04

Elapse: 00:20.9
Start : 13:25:16

3
6

Inten : 49337600
RIC : 196856343

Inlet :
Masses: 50 > 800
#peaks: 397



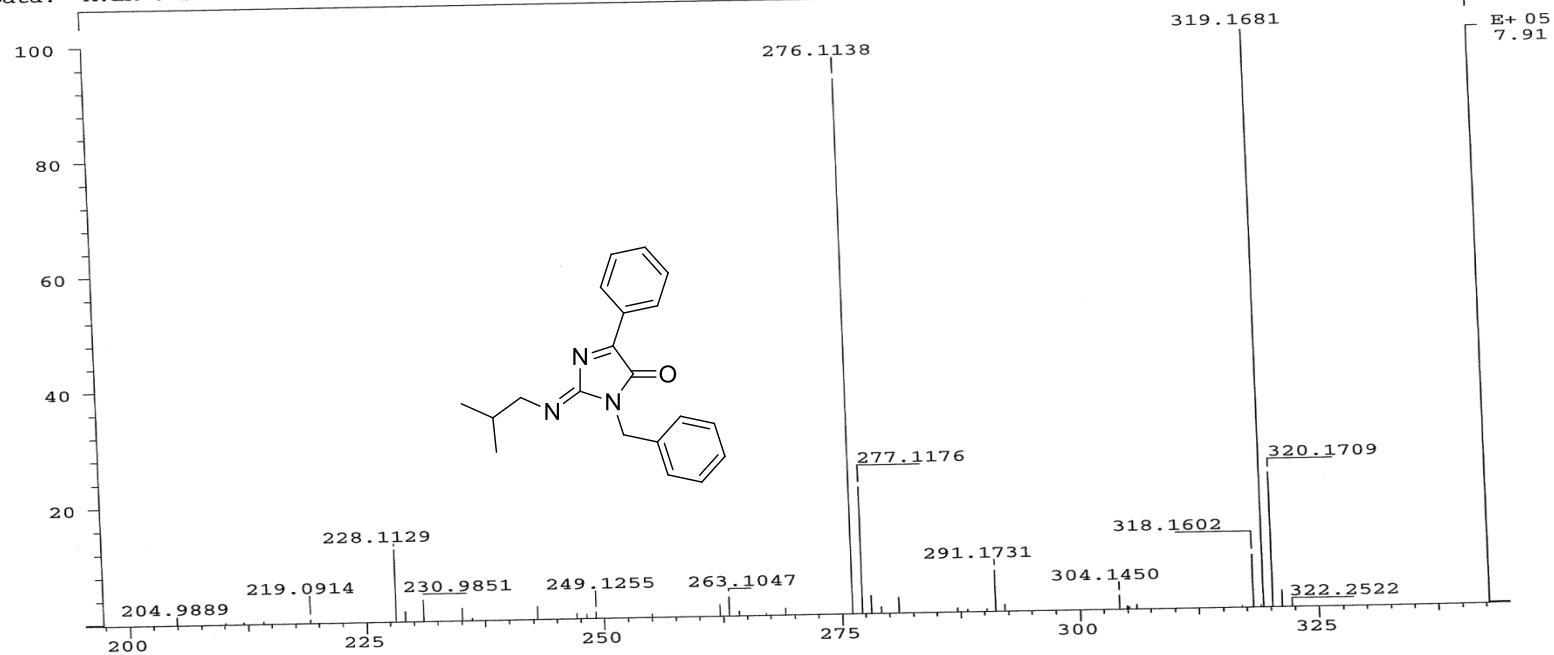
EI Mass spectrum of compound 7{2,2,1}

SPEC: 12eih-153-cl-a
 Samp: a109
 Comm: FINNIGAN MAT-95XL
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM
 Oper: SCLIN
 Base: 319.2
 Norm: 319.2
 Peak: 1000.00 mmu
 Data: AVER : Scans 1-9 from /usr/users/finnigan/data/LIN-04-12/12eih

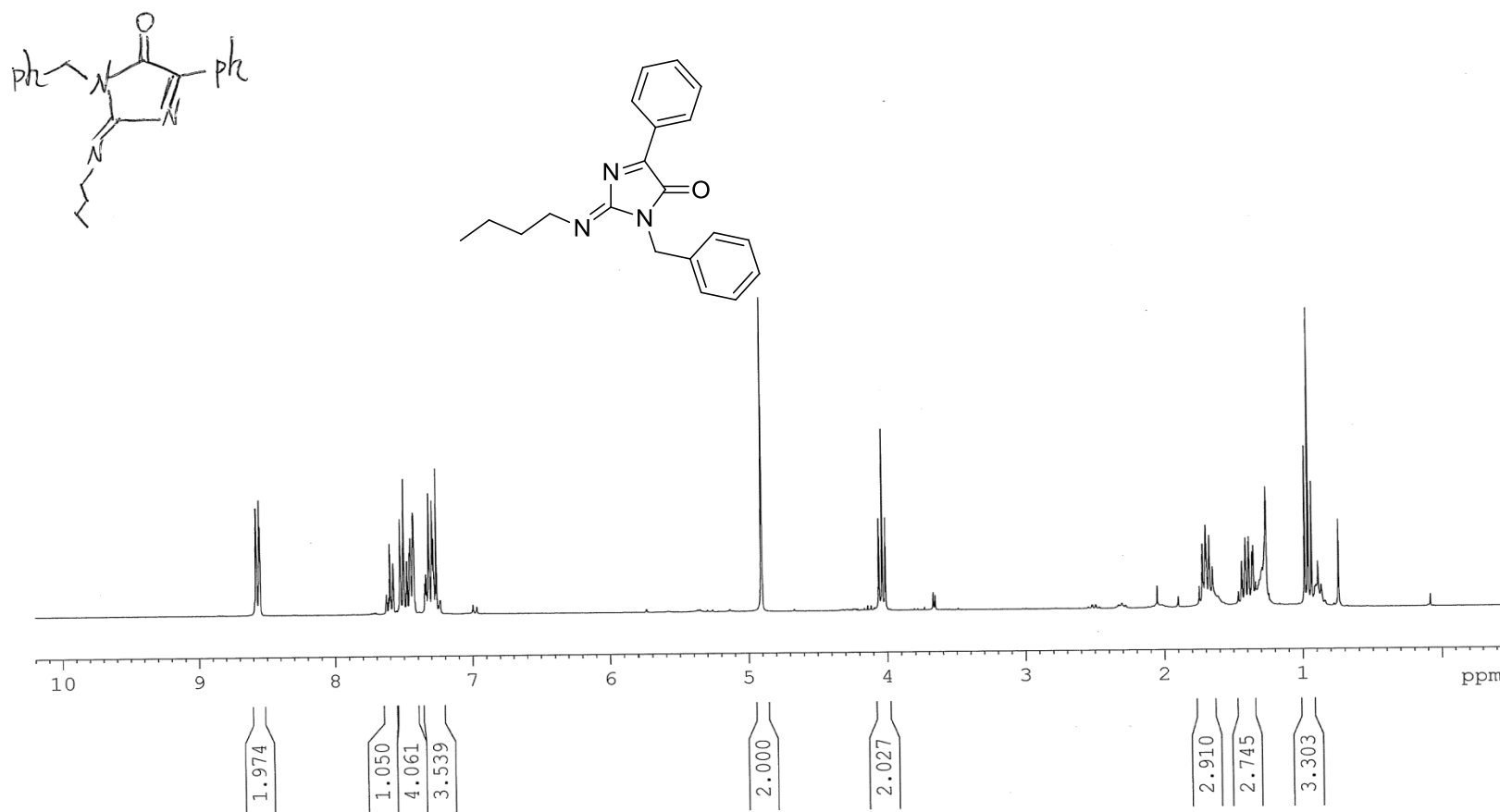
05-Jan-05 Elapse: 00:07.2
 Start : 15:51:12

Inlet :
 Masses: 200 > 337
 #peaks: 199

Inten : 791261
 RIC : 2469064

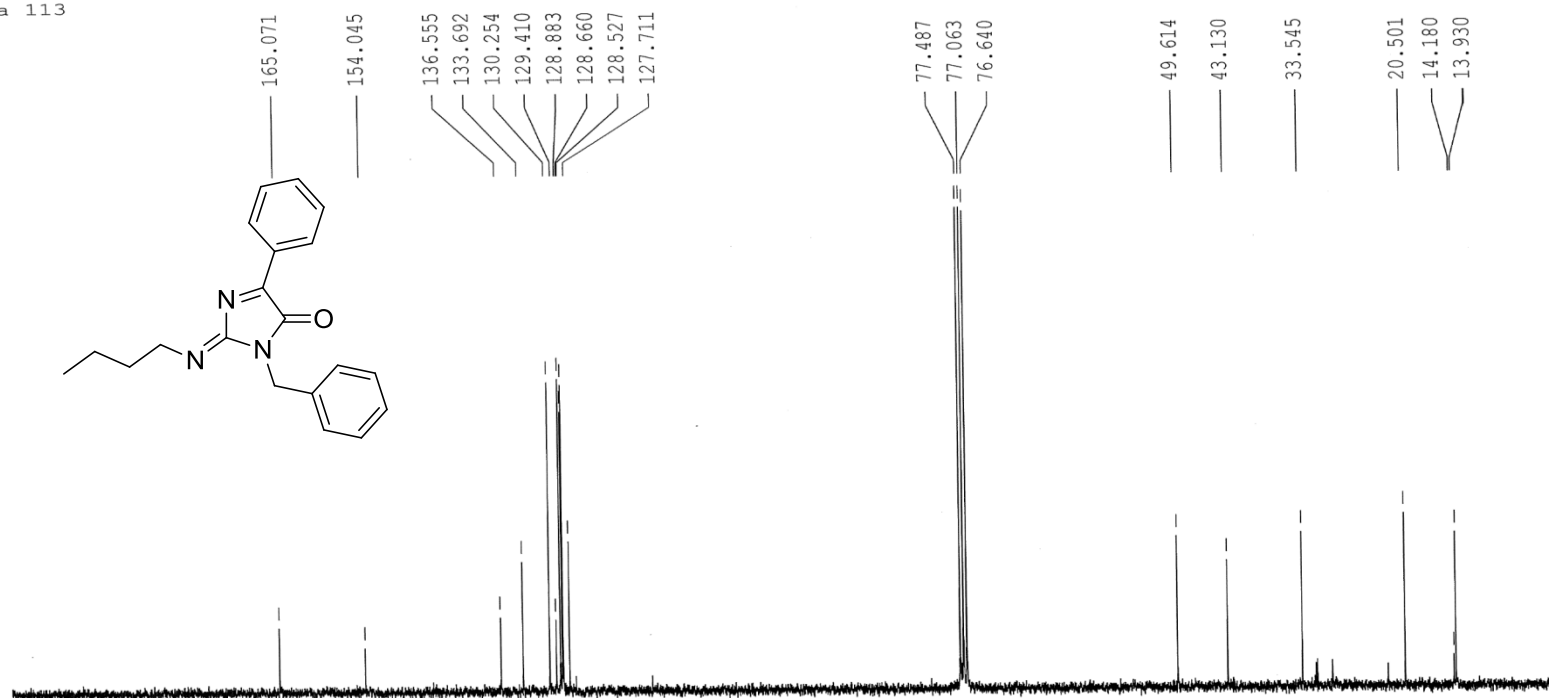


HRMS Mass (EI) spectrum of compound 7{2,2,1}



¹H NMR spectrum (300 MHz) of compound 7{2,2,13} in CDCl₃

a 113



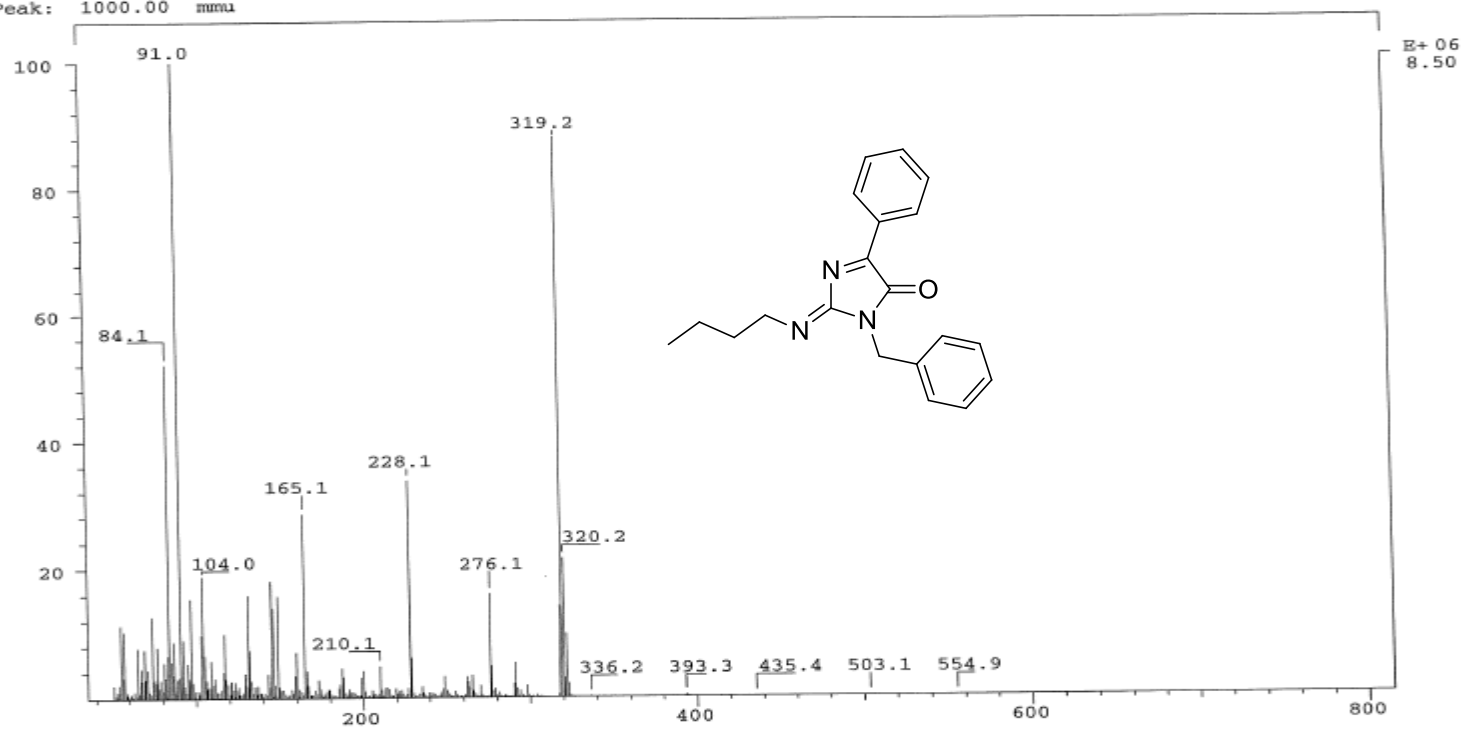
¹³C spectrum (75 MHz) of compound 7{2,2,13} in CDCl₃

SPEC: 12e1lr-74
 Samp: a113
 Comm: FINNIGAN MAT-95XL
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM
 Oper: SCLIN
 Base: 91.0
 Norm: 91.0
 Peak: 1000.00 mmu

28-Dec-04 Elapse: 00:21.6
 Start : 13:34:20

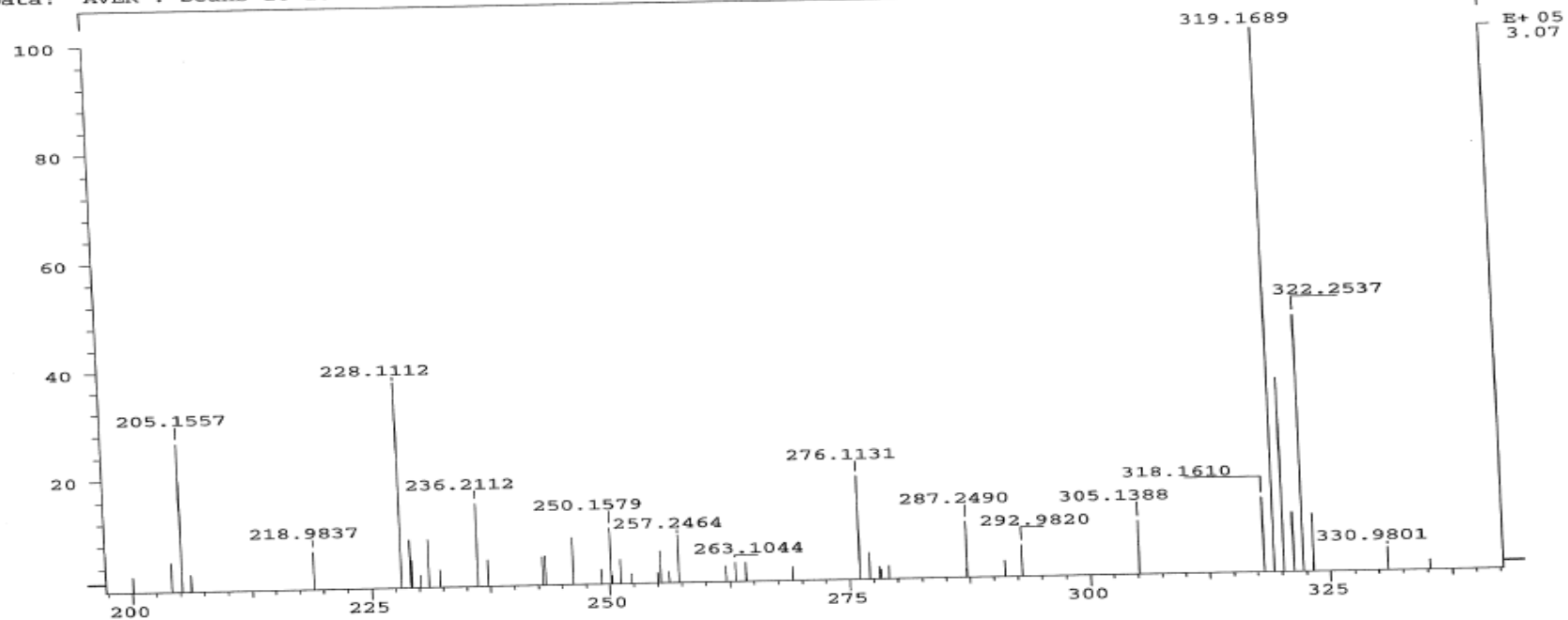
Inlet :
 Masses: 50 > 800
 #peaks: 420

Inten : 8496063
 RIC : 77683938

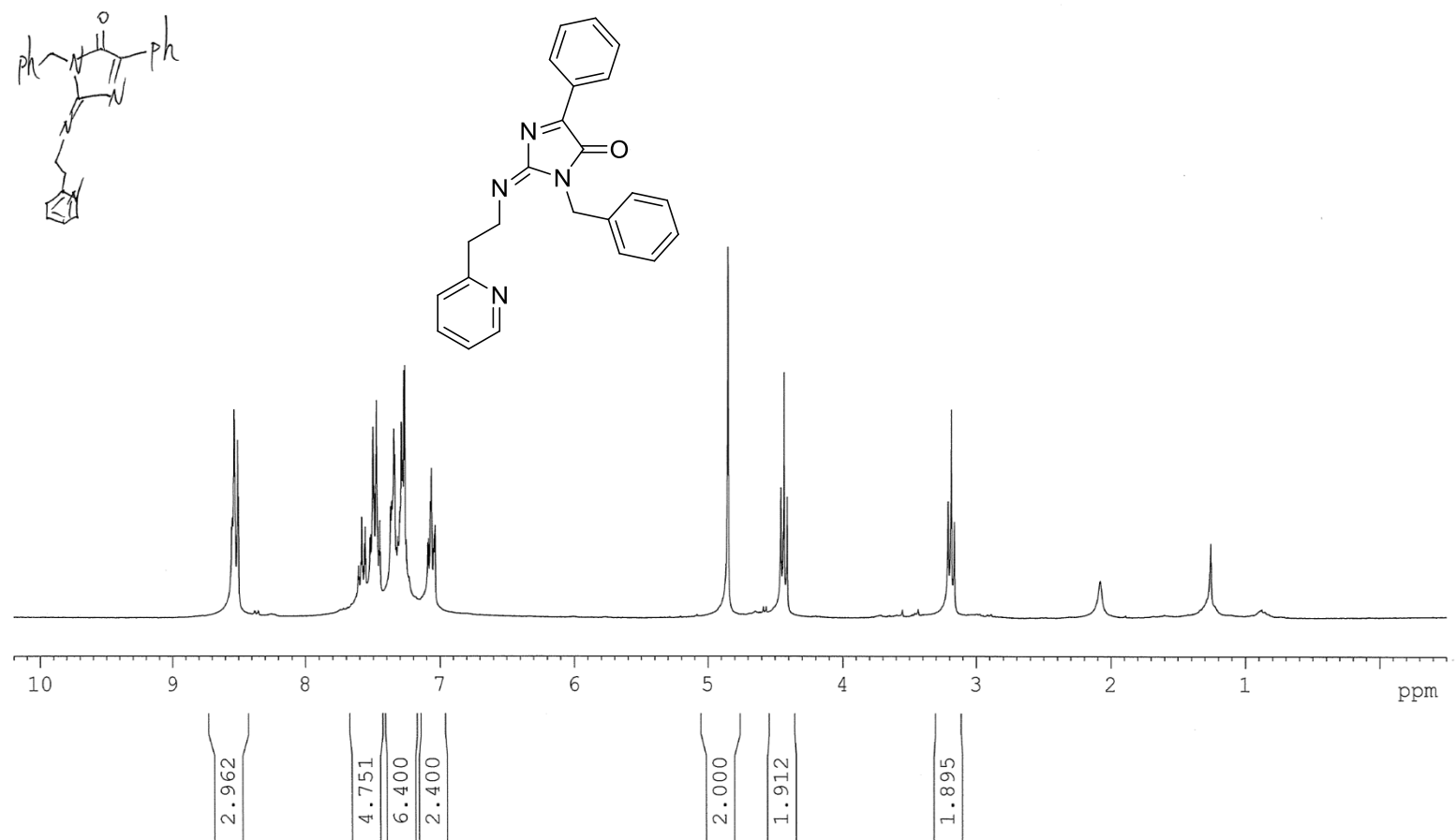


EI Mass spectrum of compound 7{2,2,13}

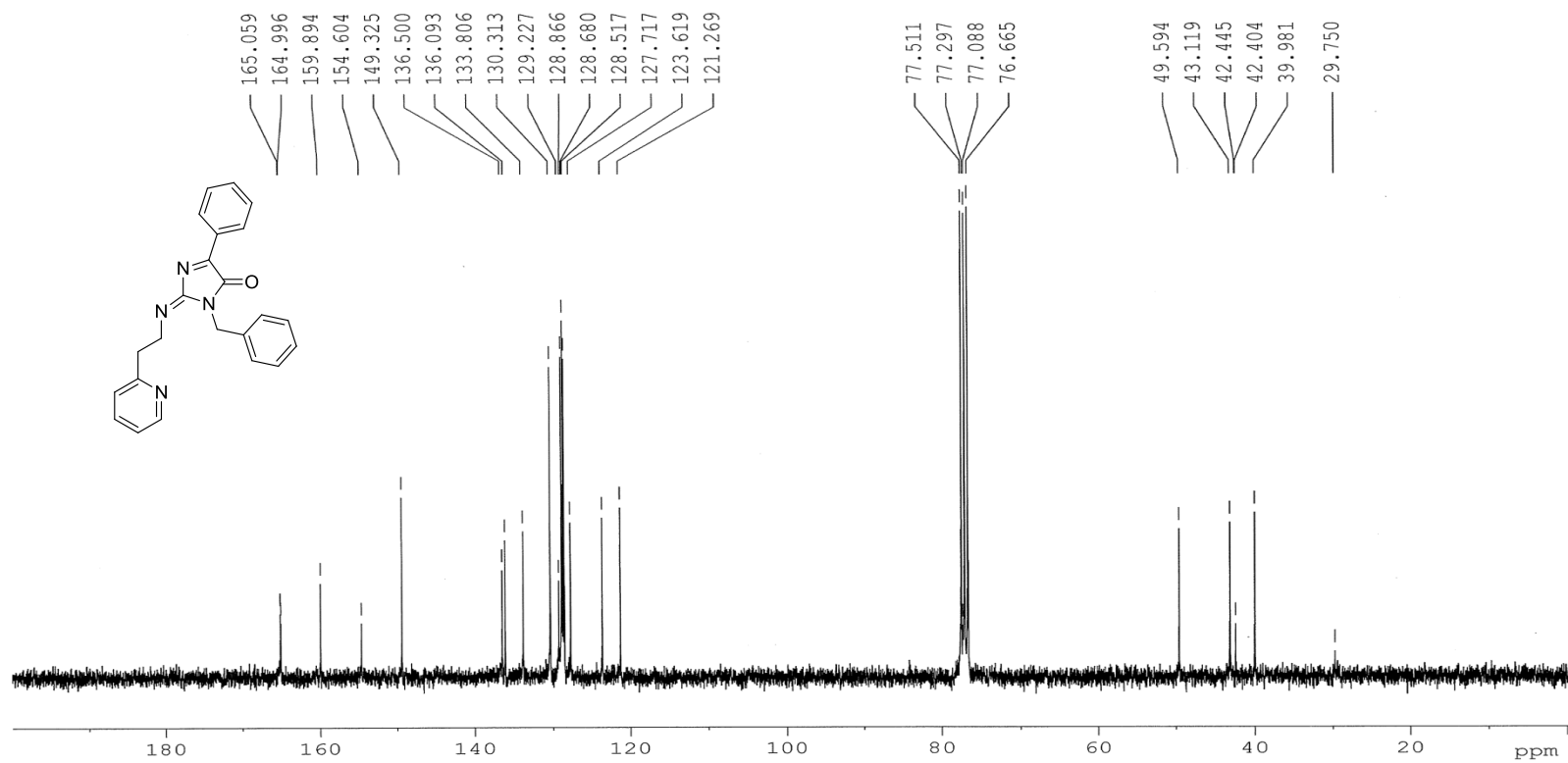
SPEC: 12eih-154-c4-a 05-Jan-05 Elapse: 00:46.8 1
 Samp: a113 Start: 15:57:15 1
 Comm: FINNIGAN MAT-95XL
 Mode: EI +VE +LMP ESCAN (EXP) UP HR NRM
 Oper: SCLIN Inlet: 200 > 339
 Base: 319.2 Inten: 307151 Masses: 506
 Norm: 319.2 RIC: 1867644 #peaks: 506
 Peak: 1000.00 mmu
 Data: AVER: Scans 16-18 from /usr/users/finnigan/data/LIN-04-12/12e



HRMS Mass (EI) spectrum of compound 7{2,2,13}



^1H NMR spectrum (300 MHz) of compound 7{2,2,8} in CDCl_3



¹³C spectrum (75 MHz) of compound 7{2,2,8} in CDCl₃

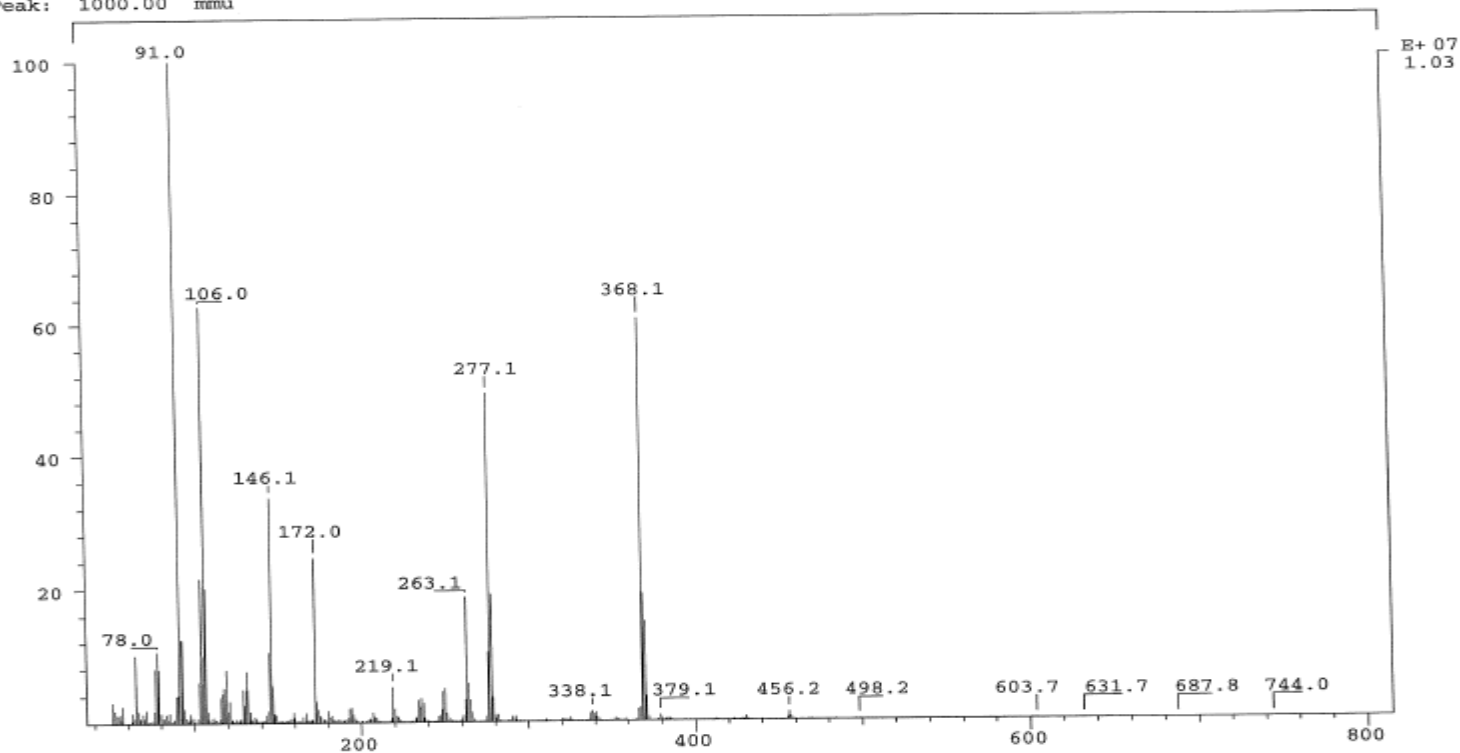
SPEC: 12e1lr-77
Samp: all4
Comm: FINNIGAN MAT-95XL
Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM
Oper: SCLIN
Base: 91.0
Norm: 91.0
Peak: 1000.00 menu

28-Dec-04 Elapse: 00:15.8
Start : 14:09:28

Inlet :
Masses: 50 > 800
#peaks: 716

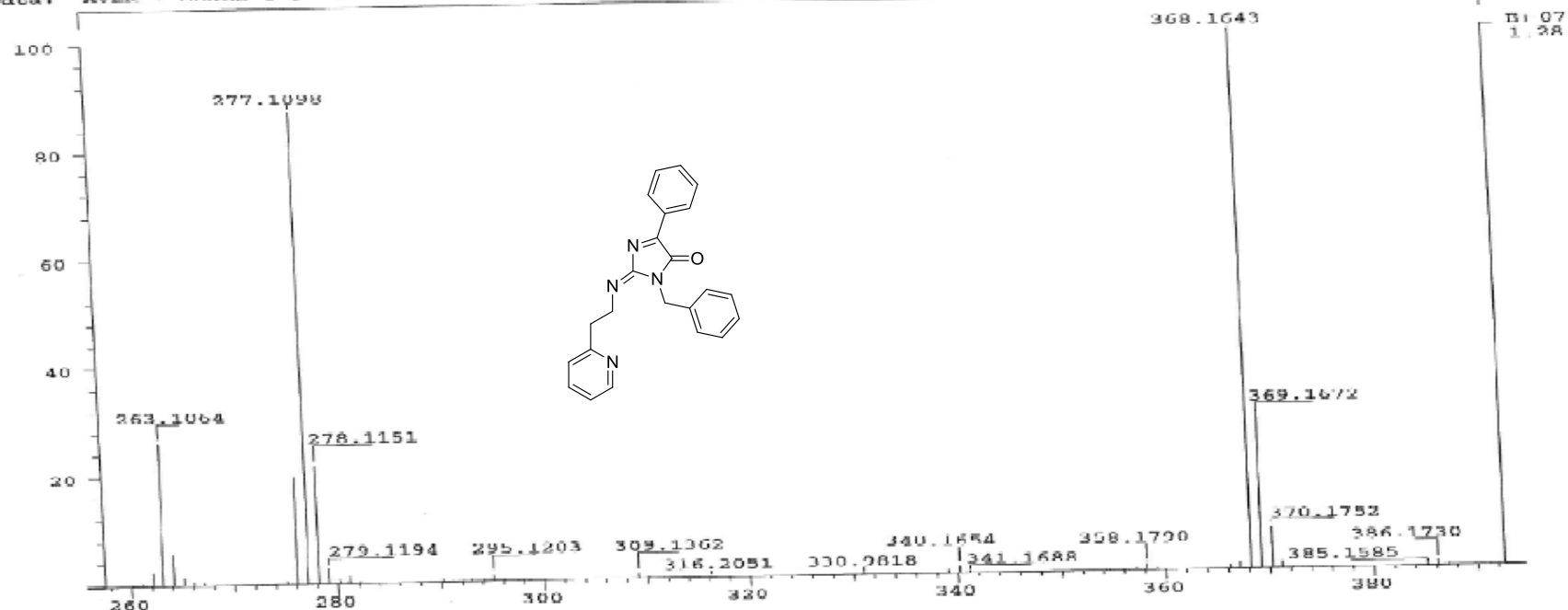
Inten : 10346948
RIC : 84053786

2
6



EI Mass spectrum of compound 7{2,2,8}

SPC: 12-11-157-04-a 05-Jan-05 Elapsed: 00:20.2 1
 Samp: 1114 Start: 14:15:19 1
 Comm: FINNIGAN MAT-95XL
 Mode: EI +VE +LMP ESCAN (EXP) UP HR NRM
 Oper: SGT:IN Inlet: 260 > 389
 Base: 269.2 Inten: 12790144 Masses: 260 > 389
 Norm: 368.2 RUC: 41420299 #peaks: 449
 Peak: 1000.00 NRM
 Data: AVLM: Status 8-9 from /usr/users/finnigan/data/LIN-04-12/12-11-157



HRMS Mass (EI) spectrum of compound 7{2,2,8}

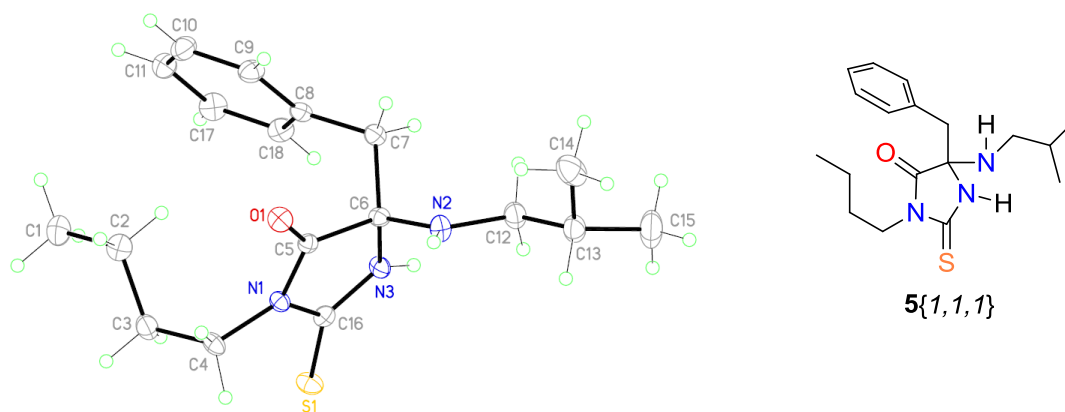


Figure 1. ORTEP representation of compounds **5{1,1,1}**

Table 1. Crystal data and structure refinement for **5{1,1,1}**

Identification code	111139lt_0m	
Empirical formula	C ₃₆ H ₅₄ N ₆ O ₂ S ₂	
Formula weight	666.97	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 2 ₁ /c 1	
Unit cell dimensions	a = 13.1619(6) Å	α = 90°.
	b = 11.2406(4) Å	β = 101.799(2)°.
	c = 25.1656(12) Å	γ = 90°.
Volume	3644.5(3) Å ³	
Z	4	
Density (calculated)	1.216 Mg/m ³	
Absorption coefficient	0.186 mm ⁻¹	
F(000)	1440	
Crystal size	0.15 x 0.05 x 0.04 mm ³	
Theta range for data collection	1.58 to 26.43°.	
Index ranges	-14 ≤ h ≤ 16, -13 ≤ k ≤ 14, -31 ≤ l ≤ 31	
Reflections collected	27897	
Independent reflections	7483 [R(int) = 0.0395]	
Completeness to theta = 26.43°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9486 and 0.9019	
Refinement method	Full-matrix least-squares on F ²	

Data / restraints / parameters	7483 / 0 / 421
Goodness-of-fit on F^2	1.064
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0458$, $wR_2 = 0.1287$
R indices (all data)	$R_1 = 0.0838$, $wR_2 = 0.1678$
Largest diff. peak and hole	0.611 and -0.973 e. $\text{\AA}^{-3}$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

for 111139LT_0m. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
S(1)	2619(1)	6968(1)	1951(1)	19(1)
S(2)	2370(1)	10509(1)	3087(1)	19(1)
O(1)	4388(1)	10907(1)	2155(1)	18(1)
O(2)	588(1)	6578(1)	2890(1)	19(1)
N(1)	3425(1)	9196(2)	1974(1)	14(1)
N(2)	4948(2)	9518(2)	3190(1)	17(1)
N(3)	4354(1)	7924(2)	2539(1)	15(1)
N(4)	1544(1)	8286(2)	3076(1)	14(1)
N(5)	625(2)	9559(2)	2506(1)	16(1)
N(6)	33(2)	7959(2)	1858(1)	17(1)
C(1)	3623(2)	9192(3)	249(1)	32(1)
C(2)	3557(2)	9726(2)	793(1)	25(1)
C(3)	2610(2)	9284(2)	994(1)	21(1)
C(4)	2577(2)	9680(2)	1566(1)	17(1)
C(5)	4253(2)	9861(2)	2238(1)	13(1)
C(6)	4934(2)	9043(2)	2654(1)	14(1)
C(7)	6045(2)	8930(2)	2554(1)	17(1)
C(8)	6108(2)	8825(2)	1964(1)	16(1)
C(9)	6402(2)	9807(2)	1693(1)	21(1)
C(10)	6485(2)	9725(2)	1154(1)	23(1)
C(11)	6278(2)	8662(2)	876(1)	23(1)
C(12)	5452(2)	8760(2)	3644(1)	21(1)
C(13)	5425(2)	9348(2)	4184(1)	24(1)
C(14)	6102(2)	10451(3)	4272(1)	32(1)
C(15)	5765(3)	8456(3)	4646(1)	38(1)
C(16)	3485(2)	8024(2)	2162(1)	14(1)
C(17)	5979(2)	7688(2)	1140(1)	23(1)
C(18)	5892(2)	7764(2)	1679(1)	20(1)
C(19)	1315(2)	8182(3)	4810(1)	35(1)
C(20)	1384(2)	7714(3)	4252(1)	27(1)
C(21)	2335(2)	8182(2)	4061(1)	23(1)

C(22)	2395(2)	7802(2)	3488(1)	17(1)
C(23)	724(2)	7624(2)	2811(1)	15(1)
C(24)	46(2)	8440(2)	2391(1)	15(1)
C(25)	-1063(2)	8563(2)	2492(1)	17(1)
C(26)	-1133(2)	8663(2)	3079(1)	16(1)
C(27)	-920(2)	9719(2)	3368(1)	21(1)
C(28)	-1024(2)	9798(2)	3902(1)	25(1)
C(29)	-1336(2)	8815(2)	4158(1)	26(1)
C(30)	1493(2)	9458(2)	2883(1)	15(1)
C(31)	-493(2)	8695(2)	1403(1)	22(1)
C(32)	-462(2)	8091(2)	866(1)	24(1)
C(33)	-841(3)	8952(3)	397(1)	38(1)
C(34)	-1106(2)	6953(2)	795(1)	31(1)
C(35)	-1435(2)	7683(2)	3345(1)	22(1)
C(36)	-1537(2)	7759(2)	3881(1)	26(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for 111139LT_0m.

S(1)-C(16)	1.656(2)
S(2)-C(30)	1.658(2)
O(1)-C(5)	1.214(3)
O(2)-C(23)	1.212(3)
N(1)-C(5)	1.375(3)
N(1)-C(16)	1.396(3)
N(1)-C(4)	1.459(3)
N(2)-C(6)	1.446(3)
N(2)-C(12)	1.471(3)
N(2)-H(2)	0.8800
N(3)-C(16)	1.333(3)
N(3)-C(6)	1.469(3)
N(3)-H(3)	0.8800
N(4)-C(23)	1.368(3)
N(4)-C(30)	1.401(3)
N(4)-C(22)	1.466(3)
N(5)-C(30)	1.332(3)
N(5)-C(24)	1.469(3)
N(5)-H(5)	0.8800
N(6)-C(24)	1.443(3)
N(6)-C(31)	1.466(3)
N(6)-H(6)	0.8800
C(1)-C(2)	1.513(4)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(3)	1.521(3)
C(2)-H(2C)	0.9900
C(2)-H(2D)	0.9900
C(3)-C(4)	1.515(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.537(3)

C(6)-C(7)	1.539(3)
C(7)-C(8)	1.511(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(18)	1.391(3)
C(8)-C(9)	1.392(3)
C(9)-C(10)	1.387(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.383(4)
C(10)-H(10)	0.9500
C(11)-C(17)	1.379(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.518(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.517(4)
C(13)-C(15)	1.530(4)
C(13)-H(13)	1.0000
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(17)-C(18)	1.388(3)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(20)	1.520(4)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.523(4)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.523(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900

C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.539(3)
C(24)-C(25)	1.537(3)
C(25)-C(26)	1.503(3)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(35)	1.389(3)
C(26)-C(27)	1.390(3)
C(27)-C(28)	1.383(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.383(4)
C(28)-H(28)	0.9500
C(29)-C(36)	1.374(4)
C(29)-H(29)	0.9500
C(31)-C(32)	1.520(3)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(34)	1.525(4)
C(32)-C(33)	1.530(4)
C(32)-H(32)	1.0000
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(36)	1.384(4)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(5)-N(1)-C(16)	111.39(18)
C(5)-N(1)-C(4)	123.64(19)
C(16)-N(1)-C(4)	124.92(19)
C(6)-N(2)-C(12)	115.31(19)
C(6)-N(2)-H(2)	122.3
C(12)-N(2)-H(2)	122.3

C(16)-N(3)-C(6)	113.88(19)
C(16)-N(3)-H(3)	123.1
C(6)-N(3)-H(3)	123.1
C(23)-N(4)-C(30)	111.46(19)
C(23)-N(4)-C(22)	123.74(19)
C(30)-N(4)-C(22)	124.72(19)
C(30)-N(5)-C(24)	113.73(19)
C(30)-N(5)-H(5)	123.1
C(24)-N(5)-H(5)	123.1
C(24)-N(6)-C(31)	115.32(19)
C(24)-N(6)-H(6)	122.3
C(31)-N(6)-H(6)	122.3
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(1)-C(2)-C(3)	111.9(2)
C(1)-C(2)-H(2C)	109.2
C(3)-C(2)-H(2C)	109.2
C(1)-C(2)-H(2D)	109.2
C(3)-C(2)-H(2D)	109.2
H(2C)-C(2)-H(2D)	107.9
C(4)-C(3)-C(2)	113.8(2)
C(4)-C(3)-H(3A)	108.8
C(2)-C(3)-H(3A)	108.8
C(4)-C(3)-H(3B)	108.8
C(2)-C(3)-H(3B)	108.8
H(3A)-C(3)-H(3B)	107.7
N(1)-C(4)-C(3)	113.09(19)
N(1)-C(4)-H(4A)	109.0
C(3)-C(4)-H(4A)	109.0
N(1)-C(4)-H(4B)	109.0
C(3)-C(4)-H(4B)	109.0
H(4A)-C(4)-H(4B)	107.8
O(1)-C(5)-N(1)	124.9(2)

O(1)-C(5)-C(6)	127.7(2)
N(1)-C(5)-C(6)	107.38(18)
N(2)-C(6)-N(3)	114.12(19)
N(2)-C(6)-C(5)	107.94(18)
N(3)-C(6)-C(5)	99.76(17)
N(2)-C(6)-C(7)	110.56(19)
N(3)-C(6)-C(7)	111.70(19)
C(5)-C(6)-C(7)	112.31(19)
C(8)-C(7)-C(6)	114.33(19)
C(8)-C(7)-H(7A)	108.7
C(6)-C(7)-H(7A)	108.7
C(8)-C(7)-H(7B)	108.7
C(6)-C(7)-H(7B)	108.7
H(7A)-C(7)-H(7B)	107.6
C(18)-C(8)-C(9)	118.5(2)
C(18)-C(8)-C(7)	121.8(2)
C(9)-C(8)-C(7)	119.8(2)
C(10)-C(9)-C(8)	120.8(2)
C(10)-C(9)-H(9)	119.6
C(8)-C(9)-H(9)	119.6
C(11)-C(10)-C(9)	120.3(2)
C(11)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9
C(17)-C(11)-C(10)	119.3(2)
C(17)-C(11)-H(11)	120.3
C(10)-C(11)-H(11)	120.3
N(2)-C(12)-C(13)	110.7(2)
N(2)-C(12)-H(12A)	109.5
C(13)-C(12)-H(12A)	109.5
N(2)-C(12)-H(12B)	109.5
C(13)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	108.1
C(14)-C(13)-C(12)	111.5(2)
C(14)-C(13)-C(15)	110.7(2)
C(12)-C(13)-C(15)	109.7(2)
C(14)-C(13)-H(13)	108.3
C(12)-C(13)-H(13)	108.3

C(15)-C(13)-H(13)	108.3
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
N(3)-C(16)-N(1)	107.52(19)
N(3)-C(16)-S(1)	126.98(18)
N(1)-C(16)-S(1)	125.50(17)
C(11)-C(17)-C(18)	120.7(2)
C(11)-C(17)-H(17)	119.6
C(18)-C(17)-H(17)	119.6
C(17)-C(18)-C(8)	120.4(2)
C(17)-C(18)-H(18)	119.8
C(8)-C(18)-H(18)	119.8
C(20)-C(19)-H(19A)	109.5
C(20)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(20)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(19)-C(20)-C(21)	112.3(2)
C(19)-C(20)-H(20A)	109.2
C(21)-C(20)-H(20A)	109.2
C(19)-C(20)-H(20B)	109.2
C(21)-C(20)-H(20B)	109.2
H(20A)-C(20)-H(20B)	107.9
C(20)-C(21)-C(22)	114.0(2)
C(20)-C(21)-H(21A)	108.8
C(22)-C(21)-H(21A)	108.8

C(20)-C(21)-H(21B)	108.8
C(22)-C(21)-H(21B)	108.8
H(21A)-C(21)-H(21B)	107.7
N(4)-C(22)-C(21)	112.70(19)
N(4)-C(22)-H(22A)	109.1
C(21)-C(22)-H(22A)	109.1
N(4)-C(22)-H(22B)	109.1
C(21)-C(22)-H(22B)	109.1
H(22A)-C(22)-H(22B)	107.8
O(2)-C(23)-N(4)	125.2(2)
O(2)-C(23)-C(24)	127.3(2)
N(4)-C(23)-C(24)	107.42(19)
N(6)-C(24)-N(5)	114.32(19)
N(6)-C(24)-C(25)	110.88(19)
N(5)-C(24)-C(25)	111.22(19)
N(6)-C(24)-C(23)	108.01(19)
N(5)-C(24)-C(23)	99.80(17)
C(25)-C(24)-C(23)	112.15(19)
C(26)-C(25)-C(24)	114.85(19)
C(26)-C(25)-H(25A)	108.6
C(24)-C(25)-H(25A)	108.6
C(26)-C(25)-H(25B)	108.6
C(24)-C(25)-H(25B)	108.6
H(25A)-C(25)-H(25B)	107.5
C(35)-C(26)-C(27)	118.2(2)
C(35)-C(26)-C(25)	119.8(2)
C(27)-C(26)-C(25)	122.0(2)
C(28)-C(27)-C(26)	120.8(2)
C(28)-C(27)-H(27)	119.6
C(26)-C(27)-H(27)	119.6
C(27)-C(28)-C(29)	120.0(2)
C(27)-C(28)-H(28)	120.0
C(29)-C(28)-H(28)	120.0
C(36)-C(29)-C(28)	119.9(2)
C(36)-C(29)-H(29)	120.0
C(28)-C(29)-H(29)	120.0
N(5)-C(30)-N(4)	107.5(2)

N(5)-C(30)-S(2)	126.94(18)
N(4)-C(30)-S(2)	125.57(17)
N(6)-C(31)-C(32)	110.3(2)
N(6)-C(31)-H(31A)	109.6
C(32)-C(31)-H(31A)	109.6
N(6)-C(31)-H(31B)	109.6
C(32)-C(31)-H(31B)	109.6
H(31A)-C(31)-H(31B)	108.1
C(31)-C(32)-C(34)	111.4(2)
C(31)-C(32)-C(33)	109.9(2)
C(34)-C(32)-C(33)	110.8(2)
C(31)-C(32)-H(32)	108.3
C(34)-C(32)-H(32)	108.3
C(33)-C(32)-H(32)	108.3
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(36)-C(35)-C(26)	121.0(2)
C(36)-C(35)-H(35)	119.5
C(26)-C(35)-H(35)	119.5
C(29)-C(36)-C(35)	120.0(2)
C(29)-C(36)-H(36)	120.0
C(35)-C(36)-H(36)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 111139LT_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	16(1)	13(1)	26(1)	-1(1)	1(1)	-2(1)
S(2)	16(1)	14(1)	25(1)	-1(1)	2(1)	-2(1)
O(1)	21(1)	11(1)	22(1)	-1(1)	3(1)	-1(1)
O(2)	22(1)	13(1)	22(1)	0(1)	1(1)	-2(1)
N(1)	13(1)	12(1)	14(1)	0(1)	1(1)	0(1)
N(2)	22(1)	15(1)	14(1)	-1(1)	2(1)	4(1)
N(3)	15(1)	12(1)	18(1)	3(1)	1(1)	1(1)
N(4)	14(1)	13(1)	14(1)	0(1)	1(1)	0(1)
N(5)	17(1)	11(1)	18(1)	2(1)	1(1)	0(1)
N(6)	21(1)	14(1)	15(1)	-1(1)	2(1)	5(1)
C(1)	30(2)	48(2)	19(1)	4(1)	5(1)	2(1)
C(2)	25(1)	28(2)	23(1)	1(1)	5(1)	-1(1)
C(3)	20(1)	23(1)	18(1)	2(1)	0(1)	0(1)
C(4)	14(1)	15(1)	20(1)	2(1)	-1(1)	4(1)
C(5)	13(1)	14(1)	13(1)	-1(1)	4(1)	1(1)
C(6)	13(1)	12(1)	17(1)	1(1)	3(1)	-1(1)
C(7)	14(1)	18(1)	17(1)	1(1)	2(1)	1(1)
C(8)	11(1)	19(1)	18(1)	1(1)	2(1)	1(1)
C(9)	19(1)	21(1)	22(1)	-4(1)	5(1)	-5(1)
C(10)	23(1)	25(1)	21(1)	0(1)	7(1)	-6(1)
C(11)	21(1)	28(1)	19(1)	0(1)	5(1)	1(1)
C(12)	22(1)	23(1)	18(1)	2(1)	2(1)	3(1)
C(13)	23(1)	34(2)	16(1)	2(1)	4(1)	7(1)
C(14)	28(2)	39(2)	26(2)	-11(1)	0(1)	3(1)
C(15)	46(2)	49(2)	19(1)	8(1)	6(1)	13(2)
C(16)	16(1)	13(1)	15(1)	-1(1)	5(1)	1(1)
C(17)	26(1)	18(1)	25(1)	-4(1)	6(1)	2(1)
C(18)	20(1)	17(1)	24(1)	1(1)	7(1)	3(1)
C(19)	31(2)	53(2)	21(1)	2(1)	5(1)	3(1)
C(20)	24(1)	36(2)	21(1)	5(1)	3(1)	-1(1)
C(21)	22(1)	25(1)	19(1)	2(1)	0(1)	1(1)
C(22)	14(1)	17(1)	20(1)	3(1)	0(1)	2(1)

C(23)	16(1)	17(1)	12(1)	-1(1)	4(1)	1(1)
C(24)	16(1)	13(1)	15(1)	0(1)	2(1)	-1(1)
C(25)	14(1)	19(1)	18(1)	-1(1)	2(1)	0(1)
C(26)	10(1)	20(1)	18(1)	0(1)	1(1)	1(1)
C(27)	21(1)	17(1)	24(1)	1(1)	6(1)	3(1)
C(28)	25(1)	26(1)	24(1)	-6(1)	5(1)	4(1)
C(29)	23(1)	38(2)	19(1)	1(1)	7(1)	4(1)
C(30)	16(1)	15(1)	14(1)	1(1)	5(1)	4(1)
C(31)	24(1)	24(1)	17(1)	1(1)	1(1)	8(1)
C(32)	22(1)	32(2)	17(1)	2(1)	4(1)	6(1)
C(33)	51(2)	44(2)	19(1)	8(1)	7(1)	8(2)
C(34)	32(2)	36(2)	23(1)	-6(1)	1(1)	1(1)
C(35)	20(1)	21(1)	26(1)	0(1)	7(1)	-6(1)
C(36)	24(1)	31(2)	25(1)	4(1)	8(1)	-5(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 111139LT_0m.

	x	y	z	U(eq)
H(2)	4674	10213	3241	21
H(3)	4561	7250	2703	18
H(5)	417	10234	2342	19
H(6)	320	7271	1810	20
H(1A)	3702	8327	286	49
H(1B)	4222	9526	126	49
H(1C)	2987	9376	-16	49
H(2C)	3524	10604	760	30
H(2D)	4191	9519	1062	30
H(3A)	1977	9573	744	25
H(3B)	2600	8404	981	25
H(4A)	2607	10560	1582	20
H(4B)	1909	9429	1652	20
H(7A)	6449	9635	2711	20
H(7B)	6375	8220	2750	20
H(9)	6547	10541	1880	25
H(10)	6686	10402	974	27
H(11)	6340	8604	508	27
H(12A)	6182	8613	3618	25
H(12B)	5092	7983	3623	25
H(13)	4694	9591	4182	29
H(14A)	6831	10223	4306	48
H(14B)	6012	10854	4605	48
H(14C)	5900	10990	3963	48
H(15A)	5309	7758	4586	57
H(15B)	5720	8829	4992	57
H(15C)	6482	8209	4655	57
H(17)	5832	6957	950	27
H(18)	5683	7086	1855	24
H(19A)	1920	7910	5077	52
H(19B)	680	7885	4910	52

H(19C)	1303	9054	4803	52
H(20A)	751	7951	3987	32
H(20B)	1409	6834	4263	32
H(21A)	2965	7900	4315	27
H(21B)	2332	9062	4078	27
H(22A)	3064	8072	3408	21
H(22B)	2378	6923	3466	21
H(25A)	-1386	9278	2298	21
H(25B)	-1472	7864	2333	21
H(27)	-699	10396	3195	25
H(28)	-882	10527	4094	30
H(29)	-1411	8869	4525	31
H(31A)	-148	9480	1418	27
H(31B)	-1223	8825	1433	27
H(32)	275	7876	865	29
H(33A)	-1560	9182	395	57
H(33B)	-805	8563	53	57
H(33C)	-400	9662	443	57
H(34A)	-886	6440	1113	46
H(34B)	-1004	6534	468	46
H(34C)	-1842	7153	759	46
H(35)	-1574	6950	3157	26
H(36)	-1746	7081	4057	32

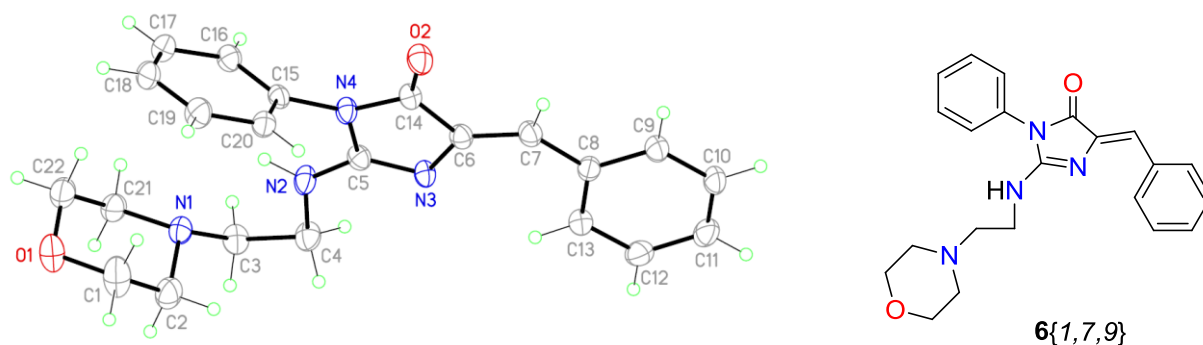


Figure 2. ORTEP representation of compounds **6{1,7,9}**

Table 1. Crystal data and structure refinement for **6{1,7,9}**

Identification code	111152lt	
Empirical formula	C ₂₂ H ₂₅ N ₄ O ₂	
Formula weight	377.46	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P c c n	
Unit cell dimensions	a = 16.1623(9) Å	α = 90°.
	b = 17.5366(11) Å	β = 90°.
	c = 13.8202(8) Å	γ = 90°.
Volume	3917.1(4) Å ³	
Z	8	
Density (calculated)	1.280 Mg/m ³	
Absorption coefficient	0.084 mm ⁻¹	
F(000)	1608	
Crystal size	0.25 x 0.20 x 0.17 mm ³	
Theta range for data collection	1.71 to 26.45°.	
Index ranges	-20 ≤ h ≤ 15, -18 ≤ k ≤ 21, -14 ≤ l ≤ 17	
Reflections collected	28744	
Independent reflections	4029 [R(int) = 0.0556]	
Completeness to theta = 26.45°	99.8 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.9486 and 0.8902
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4029 / 0 / 254
Goodness-of-fit on F^2	1.142
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0624$, $wR_2 = 0.1350$
R indices (all data)	$R_1 = 0.1011$, $wR_2 = 0.1773$
Extinction coefficient	0.029(2)
Largest diff. peak and hole	0.784 and -0.980 e. $\text{\AA}^{-3}$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

for 111152LT. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
O(1)	6779(1)	1234(1)	4253(1)	40(1)
O(2)	2930(1)	1000(1)	258(1)	30(1)
N(1)	6816(1)	860(1)	2252(1)	25(1)
N(2)	5728(1)	845(1)	831(1)	26(1)
N(3)	4994(1)	1184(1)	-572(1)	22(1)
N(4)	4279(1)	840(1)	781(1)	22(1)
C(1)	6446(2)	1732(2)	3544(2)	44(1)
C(2)	6888(2)	1645(1)	2588(2)	36(1)
C(3)	7148(1)	746(1)	1278(2)	28(1)
C(4)	6551(1)	1058(1)	521(2)	28(1)
C(5)	5043(1)	965(1)	327(2)	22(1)
C(6)	4146(1)	1222(1)	-769(2)	22(1)
C(7)	3752(1)	1409(1)	-1591(2)	24(1)
C(8)	4083(1)	1635(1)	-2532(2)	23(1)
C(9)	3533(1)	1696(1)	-3305(2)	27(1)
C(10)	3801(2)	1920(1)	-4210(2)	30(1)
C(11)	4627(2)	2085(1)	-4364(2)	33(1)
C(12)	5179(2)	2028(1)	-3605(2)	31(1)
C(13)	4917(1)	1810(1)	-2691(2)	27(1)
C(14)	3672(1)	1016(1)	116(2)	22(1)
C(15)	4162(1)	756(1)	1805(1)	21(1)
C(16)	4421(1)	106(1)	2279(2)	24(1)
C(17)	4326(1)	59(1)	3274(2)	28(1)
C(18)	3970(1)	649(1)	3783(2)	29(1)
C(19)	3709(2)	1293(1)	3300(2)	31(1)
C(20)	3808(1)	1352(1)	2308(2)	26(1)
C(21)	7175(2)	360(1)	2978(2)	30(1)
C(22)	6733(2)	465(2)	3927(2)	36(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for 111152LT.

O(1)-C(1)	1.419(3)
O(1)-C(22)	1.423(3)
O(2)-C(14)	1.216(3)
N(1)-C(21)	1.454(3)
N(1)-C(2)	1.458(3)
N(1)-C(3)	1.462(3)
N(2)-C(5)	1.325(3)
N(2)-C(4)	1.446(3)
N(2)-H(2)	0.8800
N(3)-C(5)	1.304(3)
N(3)-C(6)	1.399(3)
N(4)-C(14)	1.380(3)
N(4)-C(5)	1.401(3)
N(4)-C(15)	1.435(3)
C(1)-C(2)	1.508(4)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.525(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(6)-C(7)	1.342(3)
C(6)-C(14)	1.487(3)
C(7)-C(8)	1.460(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.394(3)
C(8)-C(13)	1.400(3)
C(9)-C(10)	1.380(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.382(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.381(3)

C(11)-H(11)	0.9500
C(12)-C(13)	1.386(3)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(15)-C(20)	1.379(3)
C(15)-C(16)	1.380(3)
C(16)-C(17)	1.386(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.377(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.379(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.385(3)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-C(22)	1.506(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900

C(1)-O(1)-C(22)	110.17(18)
C(21)-N(1)-C(2)	108.50(17)
C(21)-N(1)-C(3)	113.99(17)
C(2)-N(1)-C(3)	113.14(18)
C(5)-N(2)-C(4)	124.93(18)
C(5)-N(2)-H(2)	117.5
C(4)-N(2)-H(2)	117.5
C(5)-N(3)-C(6)	105.00(17)
C(14)-N(4)-C(5)	106.99(17)
C(14)-N(4)-C(15)	125.93(17)
C(5)-N(4)-C(15)	125.00(17)
O(1)-C(1)-C(2)	111.3(2)
O(1)-C(1)-H(1A)	109.4
C(2)-C(1)-H(1A)	109.4
O(1)-C(1)-H(1B)	109.4
C(2)-C(1)-H(1B)	109.4

H(1A)-C(1)-H(1B)	108.0
N(1)-C(2)-C(1)	109.7(2)
N(1)-C(2)-H(2A)	109.7
C(1)-C(2)-H(2A)	109.7
N(1)-C(2)-H(2B)	109.7
C(1)-C(2)-H(2B)	109.7
H(2A)-C(2)-H(2B)	108.2
N(1)-C(3)-C(4)	110.49(17)
N(1)-C(3)-H(3A)	109.6
C(4)-C(3)-H(3A)	109.6
N(1)-C(3)-H(3B)	109.6
C(4)-C(3)-H(3B)	109.6
H(3A)-C(3)-H(3B)	108.1
N(2)-C(4)-C(3)	106.62(17)
N(2)-C(4)-H(4A)	110.4
C(3)-C(4)-H(4A)	110.4
N(2)-C(4)-H(4B)	110.4
C(3)-C(4)-H(4B)	110.4
H(4A)-C(4)-H(4B)	108.6
N(3)-C(5)-N(2)	126.7(2)
N(3)-C(5)-N(4)	114.83(18)
N(2)-C(5)-N(4)	118.43(19)
C(7)-C(6)-N(3)	129.8(2)
C(7)-C(6)-C(14)	120.8(2)
N(3)-C(6)-C(14)	109.43(17)
C(6)-C(7)-C(8)	130.3(2)
C(6)-C(7)-H(7)	114.9
C(8)-C(7)-H(7)	114.9
C(9)-C(8)-C(13)	118.42(19)
C(9)-C(8)-C(7)	118.1(2)
C(13)-C(8)-C(7)	123.51(19)
C(10)-C(9)-C(8)	121.1(2)
C(10)-C(9)-H(9)	119.5
C(8)-C(9)-H(9)	119.5
C(9)-C(10)-C(11)	120.2(2)
C(9)-C(10)-H(10)	119.9
C(11)-C(10)-H(10)	119.9

C(12)-C(11)-C(10)	119.5(2)
C(12)-C(11)-H(11)	120.3
C(10)-C(11)-H(11)	120.3
C(11)-C(12)-C(13)	120.9(2)
C(11)-C(12)-H(12)	119.5
C(13)-C(12)-H(12)	119.5
C(12)-C(13)-C(8)	119.9(2)
C(12)-C(13)-H(13)	120.1
C(8)-C(13)-H(13)	120.1
O(2)-C(14)-N(4)	126.03(19)
O(2)-C(14)-C(6)	130.27(19)
N(4)-C(14)-C(6)	103.70(18)
C(20)-C(15)-C(16)	120.90(19)
C(20)-C(15)-N(4)	118.24(19)
C(16)-C(15)-N(4)	120.83(19)
C(15)-C(16)-C(17)	119.0(2)
C(15)-C(16)-H(16)	120.5
C(17)-C(16)-H(16)	120.5
C(18)-C(17)-C(16)	120.6(2)
C(18)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(17)-C(18)-C(19)	119.7(2)
C(17)-C(18)-H(18)	120.1
C(19)-C(18)-H(18)	120.1
C(18)-C(19)-C(20)	120.3(2)
C(18)-C(19)-H(19)	119.8
C(20)-C(19)-H(19)	119.8
C(15)-C(20)-C(19)	119.4(2)
C(15)-C(20)-H(20)	120.3
C(19)-C(20)-H(20)	120.3
N(1)-C(21)-C(22)	109.72(19)
N(1)-C(21)-H(21A)	109.7
C(22)-C(21)-H(21A)	109.7
N(1)-C(21)-H(21B)	109.7
C(22)-C(21)-H(21B)	109.7
H(21A)-C(21)-H(21B)	108.2
O(1)-C(22)-C(21)	111.6(2)

O(1)-C(22)-H(22A)	109.3
C(21)-C(22)-H(22A)	109.3
O(1)-C(22)-H(22B)	109.3
C(21)-C(22)-H(22B)	109.3
H(22A)-C(22)-H(22B)	108.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 111152LT. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	46(1)	49(1)	26(1)	0(1)	-7(1)	6(1)
O(2)	22(1)	44(1)	25(1)	1(1)	0(1)	-1(1)
N(1)	24(1)	28(1)	22(1)	3(1)	-2(1)	2(1)
N(2)	20(1)	39(1)	18(1)	6(1)	1(1)	0(1)
N(3)	23(1)	27(1)	16(1)	-1(1)	-1(1)	1(1)
N(4)	20(1)	30(1)	16(1)	1(1)	1(1)	1(1)
C(1)	58(2)	44(2)	31(1)	-3(1)	-8(1)	16(1)
C(2)	51(2)	27(1)	31(1)	3(1)	-6(1)	4(1)
C(3)	22(1)	36(1)	26(1)	0(1)	1(1)	4(1)
C(4)	23(1)	38(1)	24(1)	3(1)	3(1)	0(1)
C(5)	22(1)	24(1)	20(1)	-3(1)	1(1)	0(1)
C(6)	24(1)	22(1)	20(1)	-2(1)	-1(1)	1(1)
C(7)	26(1)	27(1)	21(1)	-2(1)	-1(1)	-1(1)
C(8)	32(1)	18(1)	19(1)	0(1)	-2(1)	0(1)
C(9)	32(1)	25(1)	22(1)	-1(1)	-3(1)	-1(1)
C(10)	44(2)	28(1)	18(1)	-1(1)	-5(1)	-2(1)
C(11)	51(2)	28(1)	20(1)	0(1)	4(1)	-5(1)
C(12)	35(1)	29(1)	29(1)	2(1)	4(1)	-7(1)
C(13)	32(1)	27(1)	23(1)	1(1)	-4(1)	-2(1)
C(14)	24(1)	25(1)	19(1)	-2(1)	-1(1)	1(1)
C(15)	18(1)	28(1)	16(1)	-2(1)	0(1)	-4(1)
C(16)	25(1)	27(1)	21(1)	-2(1)	1(1)	1(1)
C(17)	31(1)	29(1)	23(1)	5(1)	-1(1)	-1(1)
C(18)	34(1)	37(1)	18(1)	1(1)	3(1)	-6(1)
C(19)	38(1)	31(1)	22(1)	-4(1)	5(1)	2(1)
C(20)	32(1)	24(1)	21(1)	1(1)	-2(1)	-1(1)
C(21)	29(1)	29(1)	31(1)	7(1)	-6(1)	0(1)
C(22)	34(1)	44(2)	31(1)	11(1)	-6(1)	-6(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 111152LT.

	x	y	z	U(eq)
H(2)	5679	618	1396	31
H(1A)	6499	2265	3770	53
H(1B)	5851	1620	3455	53
H(2A)	6642	1994	2105	44
H(2B)	7479	1780	2666	44
H(3A)	7239	195	1164	33
H(3B)	7688	1009	1220	33
H(4A)	6600	1620	478	34
H(4B)	6674	837	-122	34
H(7)	3166	1392	-1555	29
H(9)	2965	1582	-3208	32
H(10)	3417	1960	-4728	36
H(11)	4813	2236	-4988	39
H(12)	5747	2141	-3711	37
H(13)	5303	1780	-2174	33
H(16)	4660	-305	1928	29
H(17)	4509	-383	3608	33
H(18)	3904	612	4464	35
H(19)	3459	1699	3650	37
H(20)	3633	1798	1976	31
H(21A)	7770	479	3059	36
H(21B)	7127	-178	2766	36
H(22A)	6145	318	3851	43
H(22B)	6982	126	4419	43