

One-Pot Synthesis of 4-Arylidene Imidazolin-5-ones by Reaction of Amino Acid Esters with Isocyanates and α -Bromoketones

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Characterization Data

(S)-methyl 3-(3,4-dimethoxyphenyl)-2-(3-phenethylthioureido)propanoate (3b)

Yellow oil, (84%, 141 mg); ^1H NMR (600 MHz, acetone- d_6) δ 7.35 - 7.30 (m, 1H), 7.29 - 7.24 (m, 2H), 7.23 - 7.18 (m, 2H), 6.94 (d, J = 3.7 Hz, 1H), 6.82 (d, J = 4.0 Hz, 1H), 6.74 (s, 1H), 6.66 (d, J = 5.3 Hz, 1H), 5.39 (s, 1H), 3.87 (t, J = 6.3 Hz, 1H), 3.77 (m, 2H), 3.78, 3.76 (s, 3H), 3.75 (s, 3H), 3.69 (s, 3H), 3.18 (dd, J = 9.3 Hz, J = 3.8 Hz, 1H), 3.02 (dd, J = 9.3 Hz, J = 4.1 Hz, 1H), 2.88 (t, J = 4.9 Hz, 2H); ^{13}C NMR (151 MHz, CDCl_3) δ 183.3, 173.5, 149.0, 148.8, 137.7, 128.5, 128.4, 128.3, 126.5, 121.5, 112.4, 77.1, 76.9, 60.4, 58.8, 55.9, 55.7, 37.3, 36.8, 34.8, 33.2; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{21}\text{H}_{26}\text{N}_2\text{O}_4\text{S}$ 403.1692, Found 403.1686; $[\alpha]^{27}_{\text{D}} = +146.62$ (c = 0.09, CH_2Cl_2); HPLC analysis: 10% *i*-PrOH / Hexane, 0.5 mL min $^{-1}$, 254 nm; 99% ee: t_{R} = 33.7 min; IR (cm $^{-1}$, neat): 3342, 2924, 2834, 1512.

(S)-methyl 2-(3-cyclohexylureido)-3-(3,4-dimethoxyphenyl)propanoate (3k)

White solid, (88%, 134 mg); mp 149 – 151 °C; ^1H NMR (400 MHz, CDCl_3) δ 6.73 (d, J = 8.0 Hz, 1H), 6.62 (s, 1H), 6.60 (d, J = 7.6 Hz, 1H), 5.08 (d, J = 8.0 Hz, 1H), 4.76 (d, J = 8.0 Hz, 1H), 4.68 (dd, J = 13.9 Hz, J = 6.0 Hz, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 3.68 (s, 3H), 3.42 (m, 1H), 2.99 (dd, J = 13.9 Hz, J = 6.0 Hz, 1H), 2.93 (dd, J = 13.9 Hz, J = 6.0 Hz, 1H), 1.83 (m, 2H), 1.59 (m, 3H), 1.27 (m, 2H), 1.06 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 173.6, 156.7, 148.7, 147.9, 128.8, 121.3, 112.5, 111.1, 55.8, 55.7, 54.1, 52.1, 49.1, 38.1, 33.8, 33.7, 25.5, 24.8; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{19}\text{H}_{29}\text{N}_2\text{O}_5$ 365.2076, Found 365.2071; $[\alpha]^{27}_{\text{D}} = +51.28$ (c = 0.019, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min $^{-1}$, 254 nm; 99% ee: t_{R} = 13.4 min; IR (cm $^{-1}$, neat): 3322, 2929, 2851, 1572.

(S)-methyl 3-(3,4-dimethoxyphenyl)-2-(3-phenylselenoureido)propanoate (3h)

Yellow oil, (85%, 150 mg); ^1H NMR (600 MHz, acetone- d_6) δ 9.52 (s, 1H), 7.36 (t, J = 7.7 Hz, 2H), 7.26 - 7.21 (m, 3H), 6.84 (d, J = 8.1 Hz, 2H), 6.77 (s, 1H), 6.68 (d, J = 8.1 Hz, 2H), 5.54 (s, 1H), 3.77 (s, 3H), 3.73 (s, 3H), 3.72 (s, 3H), 3.30 (dd, J = 14.1 Hz, J = 5.7 Hz, 1H), 3.12 (dd, J = 14.1 Hz, J = 6.5 Hz, 1H); ^{13}C NMR (151 MHz, acetone- d_6) δ 179.9, 171.5, 149.3, 148.5, 137.4, 129.5, 128.5, 126.3, 124.5, 124.5, 124.4, 121.3, 113.0, 111.9, 60.8, 55.2, 55.1, 51.7, 36.5; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{19}\text{H}_{22}\text{N}_2\text{O}_4\text{Se}$ 423.0823, Found 423.0858; $[\alpha]^{27}_{\text{D}} = +60.35$ (c = 0.10, CH_2Cl_2); HPLC

analysis: 15% *i*-PrOH / Hexane, 0.3 mL min⁻¹, 254 nm); 99% ee: *t*_R = 13.6 min.; IR (cm⁻¹, neat): 3331, 2951, 1737, 1463.

5-(benzo[d][1,3]dioxol-5-ylmethyl)-3-methyl-2-thioxoimidazolidin-4-one (6g)

Pale Yellow solid, (85%, 94 mg); mp 165 – 167 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.29 (s, 1H), 6.76 (d, *J* = 7.9 Hz, 1H), 6.69 – 6.62 (m, 2H), 5.95 (s, 2H), 4.24 (dd, *J* = 9.3 Hz, *J* = 3.9 Hz, 1H), 3.23 (dd, *J* = 14.1 Hz, *J* = 3.9 Hz, 1H), 3.20 (s, 3H), 2.76 (dd, *J* = 14.1 Hz, *J* = 9.3 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 184.1, 173.2, 148.2, 147.1, 128.4, 122.2, 109.2, 108.7, 101.2, 60.8, 37.3, 27.5; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₂H₁₃N₂O₃S 265.0647, Found 265.0642; IR (cm⁻¹, neat): 3202, 2915, 2849, 1500.

5-(3,4-dimethoxybenzyl)-3-(3-phenylpropyl)-2-selenoxoimidazolidin-4-one (6c)

Yellow solid, (87%, 157 mg); mp 160 – 162 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.90 (s, 1H), 7.22 (m, 5H), 6.72 (m, 3H), 4.05 (dd, *J* = 8.6 Hz, *J* = 3.8 Hz, 1H), 3.86 (s, 3H), 3.85 (m, 2H), 3.77 (s, 3H), 3.20 (dd, *J* = 14.2 Hz, *J* = 3.9 Hz, 1H), 2.80 (dd, *J* = 14.1 Hz, *J* = 8.3 Hz, 1H), 2.57 (t, *J* = 6.8 Hz, 1H), 1.88 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 184.5, 172.7, 149.0, 148.5, 140.8, 128.3, 128.2, 128.2, 128.1, 126.2, 125.9, 121.5, 112.4, 111.4, 111.3, 61.5, 56.0, 55.8, 42.4, 36.2, 32.8, 28.7; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₁H₂₅N₂O₃Se 433.1030, Found 433.1018; IR (cm⁻¹, neat): 3288, 2931, 2850, 1515.

3-cyclohexyl-5-(3,4-dimethoxybenzyl)imidazolidine-2,4-dione (6k)

White solid, (78%, 108 mg); mp 155 – 157 °C; ¹H NMR (400 MHz, CD₃OD) δ 6.83 (d, *J* = 8.4 Hz, 1H), 6.79 (s, 1H), 6.71 (d, *J* = 8.4 Hz, 1H), 4.23 (s, 1H), 3.79 (s, 3H), 3.77 (s, 3H), 3.58 (t, *J* = 11.1 Hz, 1H), 3.45 (t, *J* = 11.1 Hz, 1H), 3.30 (s, 1H), 1.86 (m, 2H), 1.71 (m, 2H), 1.59 (m, 1H), 1.31 (m, 3H), 1.17 (m, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 173.0, 149.1, 148.3, 127.5, 121.4, 112.2, 111.4, 57.6, 55.9, 55.8, 51.3, 37.6, 32.8, 32.2, 29.2, 29.0, 25.7, 25.1, 24.9, 24.7, 24.4; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₈H₂₅N₂O₄ 333.1814, Found 333.1814; IR (cm⁻¹, neat): 3330, 2927, 2852, 1706.

(Z)-5-(3,4-dimethoxybenzylidene)-3-(3-phenylpropyl)-2-selenoxoimidazolidin-4-one (8b)

Yellow solid, (80%, 144 mg); mp 130 – 132 °C; ¹H NMR (600 MHz, acetone-*d*₆) δ 7.41 (d, *J* = 6.8 Hz, 1H), 7.32 (s, 1H), 7.28 - 7.25 (m, 3H), 7.19 - 7.14 (m, 1H), 7.06 -

6.96 (m, 2H), 6.73(s, 1H), 4.01 (t, $J = 7.4$ Hz, 2H), 3.89 (s, 3H), 3.87 (s, 3H), 2.79 (s, 2H), 2.70 (d, $J = 8.1$ Hz, 1H); ^{13}C NMR (151 MHz, acetone- d_6) δ 151.2, 149.6, 141.3, 128.2, 128.2, 126.2, 125.8, 125.7, 123.9, 113.4, 111.8, 111.2, 55.4, 55.2, 55.1, 42.2, 32.8, 32.7; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{21}\text{H}_{23}\text{N}_2\text{O}_3\text{Se}$ 431.0874, Found 431.0868; IR (cm^{-1} , neat): 3272, 2927, 2850, 1516.

((S, Z)-methyl 3-(3,4-dimethoxyphenyl)-2-(2-(phenethylimino)-4-phenyl-thiazol-3(2H)-yl)propanoate (5b)

Yellow oil, (79%, 166 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.31 (m, 3H), 7.14 (m, 3H), 6.98 (d, $J = 6.7$ Hz, 2H), 6.86 (d, $J = 6.0$ Hz, 1H), 6.80 (m, 2H), 6.73 (d, $J = 8.6$ Hz, 1H), 5.60 (s, 1H), 3.98 (m, 2H), 3.83 (s, 3H), 3.81 (m, 1H), 3.79 (s, 3H), 3.68 (s, 3H), 3.28 (dd, $J = 13.6$ Hz, $J = 5.5$ Hz, 1H), 3.11 (dd, $J = 13.6$ Hz, $J = 5.5$ Hz, 1H), 2.77 (t, $J = 7.3$ Hz, 2H); ^{13}C NMR (101 MHz, Chloroform- d) δ 173.3, 161.2, 148.6, 147.5, 140.7, 138.6, 131.6, 131.1, 128.9, 128.8, 128.7, 128.4, 128.4, 128.3, 126.2, 121.6, 112.6, 111.0, 94.8, 69.2, 55.8, 55.8, 52.0, 46.5, 39.9, 33.2, 29.7; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_4\text{S}$ 503.2005, Found 503.2003; $[\alpha]^{27}_{\text{D}} = -150.22$ ($c = 0.11$, CH_2Cl_2); HPLC analysis: 10% *i*-PrOH / Hexane, 0.3 mL min^{-1} , 254 nm); 86% ee: $t_{\text{R}} = 34.0$ min; IR (cm^{-1} , neat): 3026, 2834, 1741, 1613.

(S, Z)-methyl 3-(3,4-dimethoxyphenyl)-2-(4-phenyl-2-((3-phenylpropyl) imino)-1,3-selenazol-3(2H)-yl)propanoate (5c)

Yellow oil, (75%, 177 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.36 (m, 3H), 7.26 (m, 2H), 7.19 (m, 2H), 7.12 (m, 1H), 6.97 (d, $J = 6.8$ Hz, 2H), 6.81 (d, $J = 6.4$ Hz, 2H), 6.69 (d, $J = 8.8$ Hz, 1H), 6.80 (m, 2H), 6.06 (s, 1H), 3.86 (m, 1H), 3.82 (s, 3H), 3.81 (m, 1H), 3.78 (s, 3H), 3.67 (m, 2H), 3.28 (dd, $J = 13.6$ Hz, $J = 5.6$ Hz, 1H), 3.10 (dd, $J = 13.6$ Hz, $J = 5.6$ Hz, 1H), 2.39 (m, 2H), 1.77 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 172.9, 161.0, 148.6, 147.5, 141.8, 141.3, 133.4, 130.8, 128.8, 128.8, 128.5, 128.2, 128.1, 125.7, 121.6, 112.6, 111.0, 94.5, 72.7, 55.8, 51.9, 46.0, 39.8, 32.7, 29.0; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{30}\text{H}_{33}\text{N}_2\text{O}_4\text{Se}$ 565.1606, Found 565.1609; $[\alpha]^{27}_{\text{D}} = -160.04$ ($c = 0.16$, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min^{-1} , 254 nm); 99% ee: $t_{\text{R}} = 30.9$ min.; IR (cm^{-1} , neat): 3025, 2949, 1741, 1613.

(S, Z)-methyl 3-(3,4-dimethoxyphenyl)-2-(2-((4-methoxyphenyl)imino)-4-phenylthiazol-3(2H)-yl)propanoate (5d)

(85%, 178 mg), Yellow oil; ¹H NMR (400 MHz, Acetone-*d*₆) δ 7.31 (m, 3H), 6.98 (d, *J* = 9.0 Hz, 2H), 6.86 (d, *J* = 9.0 Hz, 2H), 6.80 (m, 2H), 6.73 (d, *J* = 8.6 Hz, 1H), 5.60 (s, 1H), 3.98 (m, 2H), 3.83 (s, 3H), 3.81 (m, 1H), 3.79 (s, 3H), 3.68 (s, 3H), 3.28 (dd, *J* = 13.6 Hz, *J* = 5.5 Hz, 1H), 3.11 (dd, *J* = 13.6 Hz, *J* = 5.5 Hz, 1H), 2.77 (t, *J* = 7.3 Hz, 2H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 173.3, 161.2, 148.6, 147.5, 140.7, 138.6, 131.6, 131.1, 128.9, 128.8, 128.7, 128.4, 128.4, 128.3, 126.2, 121.6, 112.6, 111.0, 94.8, 69.2, 55.8, 55.8, 52.0, 46.5, 39.9, 33.2, 29.7; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₉H₃₀N₂O₄S 505.1797, Found 505.1804; [α]_D²⁷ = - 57.52 (*c* = 0.001, CH₂Cl₂); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min⁻¹, 254 nm); 99% ee: *t*_R = 32.3 min.; IR (cm⁻¹, neat): 2996, 2833, 1613, 1503.

((S, Z)-methyl 3-(3,4-dimethoxyphenyl)-2-(2-(phenethylimino)-4-phenyl-thiazol-3(2H)-yl)propanoate (5e)

(89%, 193 mg), Yellow solid; mp 128 – 130 °C; ¹H NMR (400 MHz, acetone-*d*₆) δ 7.93 (d, *J* = 9.0 Hz, 2H), 7.38 (m, 4H), 7.01 (dd, *J* = 8.4 Hz, *J* = 1.1 Hz, 2H), 6.85 (d, *J* = 9.0 Hz, 1H), 6.62 (dd, *J* = 8.0 Hz, *J* = 2.0 Hz, 1H), 6.54 (d, *J* = 2.0 Hz, 1H), 6.34 (s, 1H), 3.96 (dd, *J* = 10.2 Hz, *J* = 4.8 Hz, 1H), 3.87 (s, 3H), 3.85 (s, 3H), 3.77 (dd, *J* = 13.8 Hz, *J* = 10.2 Hz, 1H), 3.61 (s, 3H), 3.40 (d, *J* = 11.8 Hz, 2H), 3.21 (dd, *J* = 13.8 Hz, *J* = 4.7 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 174.6, 157.5, 150.3, 148.8, 148.1, 147.5, 147.1, 130.4, 129.6, 129.5, 129.1, 128.4, 123.9, 123.6, 123.1, 121.8, 121.3, 121.1, 112.8, 111.1, 93.0, 61.0, 56.0, 55.7, 53.5, 43.7, 34.0; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₇H₂₆N₃O₆S 520.1542, Found 520.1542; [α]_D²⁷ = - 380.22 (*c* = 0.005, CH₂Cl₂); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min⁻¹, 254 nm); 99% ee: *t*_R = 34.0 min.; IR (cm⁻¹, neat): 2919, 2851, 1707, 1590.

(S, Z)-methyl 3-(3,4-dimethoxyphenyl)-2-(4-phenyl-2-(phenylimino)-1,3-selenazol-3(2H)-yl)propanoate (5f)

Yellow oil, (80%, 174 mg); ¹H NMR (400 MHz, acetone-*d*₆) δ 7.38 (m, 3H), 7.30 (t, *J* = 8.3 Hz, 2H), 7.08 (m, 3H), 6.79 (d, *J* = 8.0 Hz, 3H), 6.57 (d, *J* = 2.0 Hz, 1H), 6.53 (dd, *J* = 8.0 Hz, *J* = 2.0 Hz, 1H), 6.08 (s, 1H), 4.61 (dd, *J* = 11.0 Hz, *J* = 3.9 Hz, 1H), 3.82 (s, 3H), 3.80 (s, 3H), 3.79 (m, 1H), 3.66 (s, 3H), 3.14 (dd, *J* = 13.9 Hz, *J* = 3.9 Hz,

1H); ^{13}C NMR (101 MHz, CDCl_3) δ 170.6, 156.2, 152.0, 148.8, 147.7, 141.7, 132.7, 130.1, 129.6, 129.1, 128.8, 128.3, 123.6, 121.4, 120.6, 112.2, 111.2, 93.9, 61.2, 56.0, 55.6, 52.5, 32.5; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{27}\text{H}_{27}\text{N}_2\text{O}_4\text{Se}$ 523.1136, Found 522.1131; $[\alpha]^{27}_{\text{D}} = -503.50$ ($c = 0.064$, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min^{-1} , 254 nm); 99% ee: $t_{\text{R}} = 21.8$ min.; IR (cm^{-1} , neat): 3027, 2834, 1617, 1582.

(S, Z)-methyl 3-(3,4-dimethoxyphenyl)-2-(2-(phenylimino)-4-(ptolyl)thiazol-3(2H)-yl)propanoate (5g)

(75%, 153 mg), Yellow oil; ^1H NMR (400 MHz, acetone- d_6) δ 7.35 (t, $J = 8.0$ Hz, 2H), 7.09 (m, 5H), 6.79 (d, $J = 7.8$ Hz, 1H), 6.69 (d, $J = 7.8$ Hz, 2H), 6.53 (d, $J = 8.2$ Hz, 2H), 5.77 (s, 1H), 4.69 (dd, $J = 11.1$ Hz, $J = 4.0$ Hz, 1H), 3.84 (dd, $J = 11.1$ Hz, $J = 2.0$ Hz, 1H), 3.81 (s, 3H), 3.80 (s, 3H), 3.62 (s, 3H), 3.16 (dd, $J = 13.9$ Hz, $J = 4.0$ Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 170.5, 156.4, 150.5, 148.8, 147.7, 140.4, 139.0, 130.1, 129.3, 129.0, 122.9, 121.4, 121.3, 121.3, 112.1, 111.2, 94.6, 60.2, 56.0, 55.5, 52.6, 32.4, 21.3; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{28}\text{H}_{29}\text{N}_2\text{O}_4\text{S}$ 489.1848, Found 489.1847; $[\alpha]^{27}_{\text{D}} = -335.87$ ($c = 0.023$, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min^{-1} , 254 nm); 99% ee: $t_{\text{R}} = 31.6$ min.; IR (cm^{-1} , neat): 2998, 2870, 1617, 1582.

(S, Z)-methyl 3-(3,4-dimethoxyphenyl)-2-(4-(4-nitrophenyl)-2-((3-phenylpropyl)imino)-1,3-selenazol-3(2H)-yl)propanoate (5h)

Brown oil, (78%, 199 mg); ^1H NMR (400 MHz, acetone- d_6) δ 8.22 (d, $J = 8.9$ Hz, 2H), 7.63 (d, $J = 8.9$ Hz, 1H), 7.16 (t, $J = 6.8$ Hz, 2H), 7.08 (t, $J = 6.8$ Hz, 1H), 7.02 (d, $J = 7.6$ Hz, 2H), 6.91 (m, 2H), 6.86 (d, $J = 8.2$ Hz, 1H), 6.79 (m, 3H), 6.52 (s, 1H), 4.75 (m, 1H), 3.78 (d, $J = 5.7$ Hz, 3H), 3.72 (d, $J = 4.6$ Hz, 3H), 3.67 (s, 3H), 3.24 (dd, $J = 5.1$ Hz, $J = 2.6$ Hz, 1H), 3.20 (dd, $J = 5.1$ Hz, $J = 2.6$ Hz, 1H), 3.03 (m, 2H), 2.41 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 170.4, 149.1, 148.5, 129.3, 128.2, 128.1, 126.8, 125.8, 123.8, 121.6, 121.3, 112.6, 112.2, 111.4, 111.0, 55.8, 55.8, 55.7, 53.6, 52.8, 36.8, 29.7, 28.9; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{30}\text{H}_{32}\text{N}_3\text{O}_6\text{Se}$ 610.1456, Found 610.1456; $[\alpha]^{27}_{\text{D}} = -93.14$ ($c = 0.015$, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH / Hexane, 1.5 mL min^{-1} , 254 nm); 99% ee: $t_{\text{R}} = 42.3$ min.; IR (cm^{-1} , neat): 2952, 2850, 1723, 1516.

(S, Z)-methyl 3-(benzo[d][1,3]dioxol-5-yl)-2-(4-(4-bromophenyl)-2-

(phenylimino)thiazol-3(2H)-yl)propanoate (5i)

Yellow oil, (84%, 199 mg); ^1H NMR (400 MHz, acetone- d_6) δ 7.55 (d, J = 8.6 Hz, 2H), 7.35 (t, J = 8.1 Hz, 2H), 7.06 (m, 3H), 6.85 (d, J = 8.1 Hz, 2H), 6.71 (d, J = 7.8 Hz, 1H), 6.51 (d, J = 7.5 Hz, 1H), 6.48 (s, 1H), 6.00 (d, J = 8.4 Hz, 2H), 5.89 (s, 1H), 4.72 (dd, J = 11.1 Hz, J = 4.0 Hz, 1H), 4.81 (dd, J = 14.0 Hz, J = 11.1 Hz, 1H), 3.80 (s, 3H), 3.17 (dd, J = 14.0 Hz, J = 4.0 Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 190.3, 170.1, 156.2, 150.3, 147.6, 146.3, 139.0, 131.7, 130.5, 129.9, 123.5, 122.4, 121.2, 109.7, 108.4, 108.3, 102.1, 100.9, 95.9, 77.3, 77.0, 76.7, 60.3, 52.7, 32.6, 29.7; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{26}\text{H}_{22}\text{BrN}_2\text{O}_4\text{S}$ 537.0484, Found 537.0483; $[\alpha]^{27}_{\text{D}} = -356.81$ (c = 0.021, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min $^{-1}$, 254 nm; 99% ee: t_{R} = 32.2 min.; IR (cm $^{-1}$, neat): 2916, 2850, 1585, 1487.

(S, Z)-methyl 2-(2-(allylimino)-4-phenylthiazol-3(2H)-yl)-3-(benzo[d][1,3]-dioxol-5-yl)propanoate (5j)

Yellow oil, (88%, 155 mg); ^1H NMR (400 MHz, Acetone- d_6) δ 7.46 – 7.37 (m, 5H), 6.82 (s, 1H), 6.76 – 6.70 (m, 2H), 5.96 (s, 3H), 5.83 – 5.72 (m, 1H), 5.03 (dd, J = 10.4 Hz, J = 1.5 Hz, 1H), 4.85 (dd, J = 17.3 Hz, J = 1.6 Hz, 1H), 4.40 (dd, J = 16.2 Hz, J = 5.1 Hz, 1H), 4.23 (dd, J = 16.2 Hz, J = 5.1 Hz, 1H), 3.82 (dd, J = 7.8 Hz, J = 5.6 Hz, 1H), 3.63 (s, 3H), 3.15 (dd, J = 13.4 Hz, J = 5.6 Hz, 1H), 2.96 (dd, J = 13.4 Hz, J = 5.6 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform- d) δ 173.0, 161.3, 147.3, 146.0, 140.7, 132.9, 132.2, 131.6, 129.1, 128.8, 128.7, 128.5, 122.5, 116.4, 110.2, 107.9, 100.7, 95.3, 69.1, 53.5, 51.9, 47.4, 39.9; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{23}\text{H}_{23}\text{N}_2\text{O}_4\text{S}$ 423.1379, Found 423.1372; $[\alpha]^{27}_{\text{D}} = -151.69$ (c = 0.20, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min $^{-1}$, 254 nm; 99% ee: t_{R} = 21.9 min.; IR (cm $^{-1}$, neat): 2987, 2897, 1614, 1380.

(S, Z)-methyl 3-(benzo[d][1,3]dioxol-5-yl)-2-(4-(4-nitrophenyl)-2-(phenyl-imino)-1,3-selenazol-3(2H)-yl)propanoate (5k)

Yellow oil, (74%, 171 mg); ^1H NMR (600 MHz, CD_3OD) δ 7.36 (t, J = 7.9 Hz, 2H), 7.2 (t, J = 7.8 Hz, 1H), 7.12 - 7.07 (m, 2H), 7.02 (d, J = 7.8 Hz, 2H), 6.90 (d, J = 7.9 Hz, 1H), 6.70 (d, J = 19.6 Hz, 1H), 6.65 (d, J = 7.8 Hz, 1H), 6.42 (d, J = 7.9 Hz, 1H), 6.32 (s, 1H), 6.22 (s, 1H), 5.95 (s, 1H), 5.91 (s, 1H), 5.86 (d, J = 5.5 Hz, 1H), 4.62 (d, J = 7.7 Hz, 1H), 3.84 (s, 3H), 3.73 (dd, J = 23.5 Hz, J = 10.7 Hz, 1H); ^{13}C NMR (151 MHz, CD_3OD) δ 170.5, 156.9, 152.0, 147.7, 139.7, 138.6, 130.9, 129.4, 128.8, 124.5,

123.4, 122.3, 122.0, 120.1, 109.3, 109.0, 107.7, 107.7, 100.9, 100.8, 96.9, 61.1, 60.5, 51.7, 39.1, 32.2; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{26}H_{22}N_3O_6Se$ 552.0674, Found 552.0675; $[\alpha]^{27}_D = -236.46$ ($c = 0.04$, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min⁻¹, 254 nm); 99% ee: $t_R = 31.6$ min.; IR (cm⁻¹, neat): 2917, 2850, 1740, 1586.

(S, Z)-methyl 3-(benzo[d][1,3]dioxol-5-yl)-2-((3-phenylpropyl)imino)-4-(p-tolyl)-1,3-selenazol-3(2H)-yl)propanoate (5l)

Yellow oil, (82%, 192 mg); ¹H NMR (400 MHz, Acetone-*d*₆) δ 7.24 – 7.20 (m, 4H), 7.18 (d, $J = 7.4$ Hz, 2H), 7.12 (t, $J = 7.2$ Hz, 1H), 7.02 (d, $J = 8.2$ Hz, 2H), 6.83 (s, 1H), 6.74 (d, $J = 7.4$ Hz, 1H), 6.68 (d, $J = 8.2$ Hz, 1H), 6.23 (s, 1H), 5.89 (s, 2H), 3.84 – 3.74 (m, 1H), 3.73 – 3.67 (m, 2H), 3.64 (s, 3H), 3.19 (dd, $J = 13.4$ Hz, $J = 5.5$ Hz, 1H), 3.02 (dd, $J = 13.4$ Hz, $J = 5.5$ Hz, 1H), 2.46–2.39 (m, 2H), 2.37 (s, 3H), 1.86 – 1.73 (m, 2H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 172.8, 161.2, 147.3, 146.0, 142.0, 141.4, 138.7, 132.0, 129.4, 129.2, 128.9, 128.8, 128.2, 128.1, 125.6, 122.5, 110.0, 108.0, 100.7, 94.1, 72.4, 52.0, 45.9, 39.9, 32.7, 29.0, 21.3; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{30}H_{31}N_2O_4Se$ 563.1449, Found 563.1454; $[\alpha]^{27}_D = -186.41$ ($c = 0.06$, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min⁻¹, 254 nm); 99% ee: $t_R = 21.4$ min.; IR (cm⁻¹, neat): 3024, 2918, 1600, 1486.

(S, Z)-methyl 3-(3,4-dimethoxyphenyl)-2-(5-methyl-4-phenyl-2-(phenylimino)thiazol-3(2H)-yl)propanoate (5m)

Yellow oil, (82%, 192 mg); ¹H NMR (400 MHz, Chloroform-*d*) δ 7.42 - 7.28 (m, 4H), 7.27 - 7.20 (m, 1H), 7.18 - 7.04 (m, 4H), 6.75 (d, $J = 8.2$ Hz, 2H), 6.52 (d, $J = 7.8$ Hz, 1H), 6.48 (s, 1H), 5.99 (s, 1H), 4.28 (s, 1H), 3.90 (s, 3H), 3.87 - 3.83 (m, 1H), 3.81 (s, 3H), 3.77 (s, 3H), 3.13 (dd, $J = 15.1$ Hz, $J = 3.7$ Hz, 1H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 170.4, 148.7, 147.7, 130.8, 129.9, 129.3, 128.9, 128.4, 128.3, 121.4, 112.3, 111.1, 60.8, 56.0, 55.6, 52.6, 32.6, 31.8, 29.6, 29.0, 22.6, 14.1, 12.6; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{28}H_{28}N_2O_4S$ 489.1848, Found 489.1845; $[\alpha]^{27}_D = -20.76$ ($c = 0.01$, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min⁻¹, 254 nm); 99% ee: $t_R = 28.8$ min.; IR (cm⁻¹, neat): 2949, 2834, 1745, 1489.

(S, Z)-methyl 3-(3,4-dimethoxyphenyl)-2-(5-methyl-4-phenyl-2-(phenylimino)-1,3-selenazol-3(2H)-yl)propanoate (5n)

Yellow oil, (76%, 170 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.42 - 7.28 (m, 4H), 7.27 - 7.20 (m, 1H), 7.18 - 7.04 (m, 4H), 6.75 (d, $J = 8.2$ Hz, 2H), 6.52 (d, $J = 7.8$ Hz, 1H), 6.48 (s, 1H), 5.99 (s, 1H), 4.28 (s, 1H), 3.90 (s, 3H), 3.87 - 3.83 (m, 1H), 3.81 (s, 3H), 3.77 (s, 3H), 3.13 (dd, $J = 15.1$ Hz, $J = 3.7$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 170.6, 148.7, 147.6, 136.0, 131.0, 130.9, 130.4, 129.9, 129.5, 128.7, 128.4, 128.2, 123.5, 121.5, 120.8, 112.4, 111.1, 61.7, 56.0, 55.7, 52.5, 32.6, 31.8, 29.6, 29.0, 22.6, 14.9, 14.1; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{28}\text{H}_{28}\text{N}_2\text{O}_4\text{Se}$ 537.1293, Found 537.1295; $[\alpha]^{27}_{\text{D}} = -520.00$ ($c = 0.017$, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min $^{-1}$, 254 nm); 99% ee: $t_{\text{R}} = 33.8$ min.; IR (cm $^{-1}$, neat): 2948, 2834, 1743, 1514.

(S, Z)-methyl 2-(2-(cyclohexylimino)-4-phenyloxazol-3(2H)-yl)-3-(3,4-dimethoxyphenyl)propanoate (5o)

White solid, (68%, 130 mg); mp 155 – 157 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.51 - 7.46 (m, 4H), 7.32 - 7.25 (m, 3H), 7.07, 7.05 (t, $J = 7.4$ Hz, 1H), 6.89 - 6.83 (m, 1H), 6.80 (d, $J = 8.1$ Hz, 1H), 6.69 (s, 1H), 6.53 (d, $J = 8.1$ Hz, 1H), 6.05 (d, $J = 8.1$ Hz, 1H), 4.63 (dd, $J = 12.8$ Hz, $J = 6.9$ Hz, 1H), 3.78 (s, 3H), 3.76 (s, 3H), 3.71 (s, 3H), 3.06 (dd, $J = 13.9$ Hz, $J = 5.2$ Hz, 1H), 2.96 (dd, $J = 14.0$ Hz, $J = 7.0$ Hz, 1H); ^{13}C NMR (151 MHz, CDCl_3) δ 171.7, 155.8, 152.3, 148.9, 148.2, 137.7, 136.2, 130.0, 129.5, 129.4, 128.8, 127.5, 123.8, 120.9, 120.0, 111.9, 111.2, 55.8, 55.75, 54.4, 52.4, 37.0, 29.6; $[\alpha]^{27}_{\text{D}} = -285.72$ ($c = 0.023$, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min $^{-1}$, 254 nm); 99% ee: $t_{\text{R}} = 13.7$ min.; IR (cm $^{-1}$, neat): 2916, 2849, 1734, 1346.

(S,Z)-methyl 3-(3,4-dimethoxyphenyl)-2-(4,5-diphenyl-2-(phenylimino) thiazol-3(2H)-yl)propanoate (5p)

White solid; 76% (170 mg); mp 105 – 107 °C; ^1H NMR (400 MHz, acetone- d_6) δ 7.50 - 7.36 (m, 5H), 7.21 - 7.02 (m, 5H), 6.92 - 6.83 (m, 3H), 6.66 (d, $J = 2.0$ Hz, 1H), 6.62 (dd, $J = 8.1$ Hz, $J = 7.0$ Hz, 1H), 5.92 (s, 1H), 4.43 (dd, $J = 11.0$ Hz, $J = 3.9$ Hz, 1H), 3.91 (dd, $J = 13.9$ Hz, $J = 11.0$ Hz, 1H), 3.81 (s, 3H), 3.79 (s, 3H), 3.71 (s, 3H), 3.40 (q, $J = 7.0$ Hz, 1H), 3.17 (dd, $J = 13.9$ Hz, $J = 4.0$ Hz, 1H); ^{13}C NMR (151 MHz, acetone- d_6) δ 169.5, 154.7, 151.0, 149.5, 148.4, 135.6, 132.1, 131.1, 130.2, 130.2, 129.3, 128.8, 128.6, 128.2, 127.5, 126.8, 123.0, 121.5, 121.23, 113.1, 112.1, 109.8, 65.2, 60.4, 55.4, 54.9, 51.8, 32.1, 14.7; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{33}\text{H}_{31}\text{N}_2\text{O}_4\text{S}$ 551.2005, Found 551.2008; $[\alpha]^{27}_{\text{D}} = -699.63$ ($c = 0.068$, CH_2Cl_2); HPLC analysis: 15% *i*-PrOH /

Hexane, 0.3 mL min⁻¹, 254 nm); 99% ee: t_R = 16.5 min.; IR (cm⁻¹, neat): 2916, 2849, 1734, 1346.

4-(3,4-dimethoxybenzyl)-2-((2-oxo-2-phenylethyl)thio)-1-phenethyl-1H-imidazol-5(4H)-one (7b)

Yellow oil, (56%, 114 mg); ¹H NMR (600 MHz, acetone-*d*₆) δ 8.08 (d, *J* = 7.0 Hz, 1H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.27 (t, *J* = 7.6 Hz, 2H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.15 (d, *J* = 7.4 Hz, 2H), 6.80 (d, *J* = 2.0 Hz, 1H), 6.70 (d, *J* = 8.2 Hz, 1H), 6.65 (dd, *J* = 8.2 Hz, *J* = 4.3 Hz, 1H), 4.86 (s, 2H), 4.15 (dd, *J* = 7.3 Hz, *J* = 2.0 Hz, 1H), 3.70 (s, 6H), 3.65 (dd, *J* = 14.8 Hz, *J* = 7.1 Hz, 1H), 3.52 (dd, *J* = 14.8 Hz, *J* = 7.1 Hz, 1H), 3.01 (dd, *J* = 13.8 Hz, *J* = 4.3 Hz, 1H), 2.73 (dd, *J* = 13.8 Hz, *J* = 4.3 Hz, 1H), 2.68 (t, *J* = 7.7 Hz, 2H); ¹³C NMR (151 MHz, acetone-*d*₆) δ 192.3, 180.3, 160.5, 148.9, 148.2, 137.9, 136.0, 133.4, 129.3, 128.7, 128.7, 128.4, 128.3, 126.5, 121.8, 113.5, 111.5, 69.3, 55.2, 55.1, 41.5, 37.8, 36.6, 34.4; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₈H₂₉N₂O₄S 489.1848, Found 489.1807; IR (cm⁻¹, neat): 3337, 2919, 2850, 1727.

4-(3,4-dimethoxybenzyl)-2-((2-oxo-2-phenylethyl)selenanyl)-1-(3-phenyl-propyl)-1H-imidazol-5(4H)-one (7c)

Yellow oil, (65%, 149 mg); ¹H NMR (400 MHz, CDCl₃) δ 8.06 (d, *J* = 7.0 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 8.1 Hz, 2H), 7.25 (t, *J* = 7.1 Hz, 2H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 6.7 Hz, 2H), 6.74 (d, *J* = 2.0 Hz, 1H), 6.70 (dd, *J* = 8.2 Hz, *J* = 2.0 Hz, 1H), 6.61 (d, *J* = 8.2 Hz, 1H), 4.78 (s, 2H), 4.37 (dd, *J* = 6.3 Hz, *J* = 4.4 Hz, 1H), 3.85 (m, 1H), 3.76 (s, 3H), 3.67 (s, 3H), 3.54 – 3.37 (m, 2H), 3.30 – 3.20 (m, 2H), 2.98 (dd, *J* = 13.9 Hz, *J* = 6.3 Hz, 1H), 2.44 – 2.35 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 194.1, 148.3, 147.8, 140.4, 135.1, 133.9, 128.8, 128.7, 128.6, 128.4, 128.3, 128.2, 128.2, 126.0, 121.8, 112.9, 110.7, 77.4, 77.0, 76.7, 70.3, 65.8, 55.7, 55.6, 40.9, 36.5, 34.0, 32.6, 30.1, 15.2; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₉H₃₁N₂O₄Se 551.1449, Found 551.1447; IR (cm⁻¹, neat): 3336, 2931, 2835, 1724.

4-(3,4-dimethoxybenzyl)-1-(4-methoxyphenyl)-2-((2-oxo-2-phenylethyl) thio)-1H-imidazol-5(4H)-one (7d)

Yellow oil, (78%, 160 mg); ¹H NMR (400 MHz, CDCl₃) δ 7.98 (d, *J* = 7.2 Hz, 2H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.7 Hz, 2H), 6.83 (dd, *J* = 17.4 Hz, *J* = 9.0 Hz, 4H),

6.73 (s, 1H), 6.27 (s, 1H), 4.62 (d, $J = 3.4$ Hz, 1H), 4.41 (dd, $J = 5.9$ Hz, $J = 4.6$ Hz, 1H), 3.80 (s, 3H), 3.73 (s, 3H), 3.71 (s, 3H), 3.21 (dd, $J = 13.8$ Hz, $J = 4.3$ Hz, 1H), 3.03 (dd, $J = 13.8$ Hz, $J = 4.3$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 192.6, 180.0, 160.2, 148.4, 147.9, 135.3, 133.9, 128.9, 128.8, 128.8, 128.7, 128.7, 128.6, 128.5, 128.5, 128.1, 127.6, 124.0, 122.0, 114.8, 113.0, 110.8, 69.5, 58.2, 56.0, 55.9, 55.8, 55.5, 55.4, 39.0, 36.9; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{27}\text{H}_{27}\text{N}_2\text{O}_5\text{S}$ 491.1641, Found 491.1644; IR (cm^{-1} , neat): 3337, 2932, 2837, 1513.

4-(3,4-dimethoxybenzyl)-2-((2-(4-nitrophenyl)-2-oxoethyl)thio)-1-phenyl-1H-imidazol-5(4H)-one (7e)

Yellow solid, (72%, 165 mg); mp 162 – 164 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.59 (d, $J = 8.4$ Hz, 2H), 8.40 (d, $J = 8.5$ Hz, 2H), 7.55 (m, 3H), 7.26 (s, 1H), 7.16 (d, $J = 2.0$ Hz, 1H), 6.96 (d, $J = 8.1$ Hz, 1H), 6.83 (d, $J = 8.1$ Hz, 3H), 5.77 (d, $J = 17.7$ Hz, 1H), 5.56 (d, $J = 17.7$ Hz, 1H), 5.04 (s, 1H), 3.93 (dd, $J = 15.2$ Hz, $J = 5.2$ Hz, 1H), 3.88 (s, 3H), 3.82 (s, 3H), 3.46 (d, $J = 16.2$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 189.5, 174.2, 170.8, 151.3, 149.0, 149.0, 137.6, 131.8, 130.7, 130.6, 130.1, 129.1, 128.5, 128.1, 127.3, 124.3, 124.0, 122.2, 113.7, 111.2, 63.7, 56.4, 56.1, 56.0, 46.3, 35.6, 30.1, 29.7; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{26}\text{H}_{24}\text{N}_3\text{O}_6\text{S}$ 506.1386, Found 506.1384; IR (cm^{-1} , neat): 3102, 2916, 2849, 1558.

4-(3,4-dimethoxybenzyl)-2-((2-oxo-2-(p-tolyl)ethyl)thio)-1-phenyl-1H-imidazol-5(4H)-one (7f)

Brown solid, (67%, 133 mg); mp 135 – 137 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.91 (d, $J = 8.2$ Hz, 2H), 7.38 (m, 3H), 7.28 (d, $J = 8.0$ Hz, 2H), 6.94 (m, 2H), 6.76 (s, 1H), 6.71 (s, 2H), 4.47 (dd, $J = 6.2$ Hz, $J = 4.4$ Hz, 1H), 3.84 (s, 3H), 3.74 (s, 3H), 3.27 (dd, $J = 13.7$ Hz, $J = 4.3$ Hz, 1H), 3.07 (dd, $J = 13.7$ Hz, $J = 4.3$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 192.1, 179.8, 161.7, 148.4, 147.9, 144.9, 132.9, 131.7, 129.5, 129.5, 129.3, 128.6, 128.2, 127.3, 122.0, 113.0, 110.8, 69.6, 55.9, 55.8, 39.0, 36.9, 21.7; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{27}\text{H}_{27}\text{N}_2\text{O}_4\text{S}$ 475.1692, Found 475.1698; IR (cm^{-1} , neat): 3326, 2917, 2834, 1741.

4-(benzo[d][1,3]dioxol-5-ylmethyl)-2-((2-(4-bromophenyl)-2-oxoethyl)thio)-1-phenyl-1H-imidazol-5(4H)-one (7g)

Orange solid; (78%, 193 mg); mp 100 – 102 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.94 (d, *J* = 8.5 Hz, 2H), 7.76 (d, *J* = 8.6 Hz, 2H), 7.48 (m, 3H), 7.06 (d, *J* = 6.6 Hz, 2H), 6.70 (d, *J* = 7.9 Hz, 1H), 6.65 (d, *J* = 1.6 Hz, 1H), 6.54 (dd, *J* = 7.9 Hz, *J* = 1.7 Hz, 1H), 5.94 (dd, *J* = 11.4 Hz, *J* = 1.0 Hz, 2H), 4.76 (q, *J* = 17.1 Hz, 1H), 4.50 (dd, *J* = 7.0 Hz, *J* = 4.3 Hz, 1H), 3.03 (dd, *J* = 13.8 Hz, *J* = 4.4 Hz, 1H), 2.81 (dd, *J* = 13.8 Hz, *J* = 7.2 Hz, 1H); ¹³C NMR (101 MHz, DMSO-*d*₆) δ 194.2, 179.7, 168.3, 162.9, 155.8, 149.4, 148.0, 146.2, 136.2, 135.2, 130.8, 129.8, 126.9, 124.1, 123.3, 110.7, 110.3, 108.6, 108.4, 102.0, 101.2, 69.3, 57.6, 55.3, 44.5; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₅H₂₀BrN₂O₄S 523.0327, Found 523.0163; IR (cm⁻¹, neat): 3102, 2916, 2849, 1517.

1-allyl-4-(benzo[d][1,3]dioxol-5-ylmethyl)-2-((2-oxo-2-phenylethyl)thio)-1H-imidazol-5(4H)-one (7h)

Yellow oil, (82%, 140 mg); ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, *J* = 7.2 Hz, 2H), 7.68 (t, *J* = 8.5 Hz, 1H), 7.57 (t, *J* = 8.0 Hz, 2H), 6.89 (dd, *J* = 8.0 Hz, *J* = 1.7 Hz, 1H), 6.84 (d, *J* = 1.9 Hz, 1H), 6.69 (d, *J* = 7.9 Hz, 1H), 5.89 (s, 2H), 5.67 (dd, *J* = 47.2 Hz, *J* = 17.1 Hz, 2H), 5.40 (m, 1H), 5.19 (d, *J* = 10.3 Hz, 1H), 4.86 (m, 2H), 4.31 (dd, *J* = 16.4 Hz, *J* = 5.4 Hz, 1H), 4.02 (dd, *J* = 16.4 Hz, *J* = 5.8 Hz, 1H), 3.82 (dd, *J* = 14.4 Hz, *J* = 4.9 Hz, 1H), 3.32 (dd, *J* = 14.4 Hz, *J* = 4.9 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 190.7, 173.6, 171.2, 147.8, 147.4, 135.2, 134.0, 133.3, 130.4, 129.5, 129.2, 128.9, 128.8, 127.3, 125.4, 123.7, 122.6, 120.6, 118.0, 110.3, 109.7, 108.5, 108.5, 101.1, 101.1, 63.0, 46.72, 43.6, 35.1; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₂H₂₁N₂O₄S 409.1222, Found 409.1213; IR (cm⁻¹, neat): 2898, 1777, 1711, 1489.

4-(3,4-dimethoxybenzyl)-2-((1-oxo-1-phenylpropan-2-yl)thio)-1-phenyl-1H-imidazol-5(4H)-one (7i)

Yellow solid, 80% (159 mg); mp 132 – 134 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.04 (dd, *J* = 18.2 Hz, *J* = 7.7 Hz, 2H), 7.65 - 7.58 (m, 1H), 7.52 - 7.45 (m, 2H), 7.40 – 7.34 (m, 3H), 6.96 - 6.88 (m, 2H), 6.82 - 6.70 (m, 2H), 6.63 - 6.59 (m, 1H), 5.63 (s, 1H), 4.51 (s, 1H), 3.87, 3.81 (s, 3H), 3.77 (s, 3H), 3.29 (dd, *J* = 15.1 Hz, *J* = 7.7 Hz, 1H), 3.12 (dd, *J* = 13.8 Hz, *J* = 5.7 Hz, 1H), 1.61 (t, *J* = 6.9 Hz, 3H); ¹³C NMR (151 MHz, CDCl₃) δ 197.3, 148.5, 148.4, 148.0, 147.8, 133.7, 129.4, 129.3, 128.8, 128.7, 127.2, 127.2, 122.1, 121.9, 113.0, 112.7, 110.8, 110.7, 55.9, 55.8, 55.7, 37.0, 36.9, 18.5; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₇H₂₆N₂O₄S 475.1692, Found 475.1685; IR (cm⁻¹, neat): 3063, 2931, 2834, 1740.

1-cyclohexyl-4-(3,4-dimethoxybenzyl)-2-(2-oxo-2-phenylethoxy)-1H-imidazol-5(4H)-one (7k)

Yellow solid, (48%, 90 mg); mp 145 – 147 °C; ¹H NMR (600 MHz, acetone-*d*₆) δ 8.00 (d, *J* = 7.3 Hz, 2H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 2H), 6.85 (s, 1H), 6.78 (dd, *J* = 17.7 Hz, *J* = 8.2 Hz, 2H), 5.15 (d, *J* = 18.4 Hz, 1H), 4.78 (d, *J* = 18.4 Hz, 1H), 4.36 (t, *J* = 4.4 Hz, 1H), 3.75 (s, 3H), 3.73 (s, 3H), 3.48 (s, 1H), 3.24 (dd, *J* = 14.5 Hz, *J* = 4.4 Hz, 1H), 3.01 (dd, *J* = 14.5 Hz, *J* = 4.7 Hz, 1H), 2.99 (m, 1H), 2.99 (m, 1H), 1.99 (m, 1H), 1.83 (m, 2H), 1.77 (m, 1H), 1.41 (m, 1H), 1.14 (m, 3H); ¹³C NMR (151 MHz, acetone *d*₆) δ 193.9, 172.2, 156.9, 149.2, 148.6, 134.9, 133.6, 128.7, 127.8, 127.8, 122.0, 113.8, 113.4, 111.9, 55.2, 55.2, 50.9, 47.4, 34.0, 33.6, 25.6, 25.5, 25.0; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₆H₃₁N₂O₅ 451.2233, Found 451.2230; IR (cm⁻¹, neat): 2927, 2853, 1707, 1448.

4-(3,4-bis(allyloxy)benzyl)-2-((2-oxo-2-phenylethyl)selenanyl)-1-phenyl-1H-imidazol-5(4H)-one (7l)

Yellow solid, (73%, 164 mg); mp 76 – 78 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.03 (d, *J* = 7.0 Hz, 2H), 7.57 (q, *J* = 6.7 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.37 - 7.32 (m, 3H), 6.90 - 6.84 (m, 2H), 6.80 (d, *J* = 1.8 Hz, 1H), 6.76 - 6.70 (m, 2H), 6.09 - 5.91 (m, 2H), 5.33 (q, *J* = 17.3 Hz, 2H), 5.18 (q, *J* = 10.5 Hz, 2H), 4.70 (s, 2H), 4.55 (d, *J* = 5.3 Hz, 2H), 4.51 (dd, *J* = 5.6 Hz, *J* = 4.3 Hz, 2H), 4.47 – 4.44 (m, 2H), 3.28 (dd, *J* = 13.8 Hz, *J* = 4.4 Hz, 1H), 3.10 (dd, *J* = 13.8 Hz, *J* = 5.7 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 191.7, 168.8, 161.7, 150.9, 148.7, 136.1, 135.4, 133.9, 132.3, 129.6, 129.2, 128.9, 128.3, 127.3, 127.2, 126.6, 125.4, 113.6, 110.7, 55.8, 55.4, 38.8; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₃₀H₂₉N₂O₄S 561.1293, Found 561.1297; IR (cm⁻¹, neat): 3059, 2919, 2851, 1420.

(Z)-4-(3,4-dimethoxybenzylidene)-2-((2-(4-nitrophenyl)-2-oxoethyl)selenanyl)-1-(3-phenylpropyl)-1H-imidazol-5(4H)-one (9b)

Red solid, (69%, 171 mg); mp 153 – 155 °C; ¹H NMR (400 MHz, acetone-*d*₆) δ 8.33 (d, *J* = 8.5 Hz, 2H), 8.21 (d, *J* = 8.8 Hz, 2H), 7.31 - 7.28 (m, 5H), 7.24 (m, 1H), 7.16 (d, *J* = 8.3 Hz, 2H), 6.73 (s, 1H), 6.18 (s, 1H), 4.01 (s, 3H), 3.92 (s, 3H), 3.89 (d, *J* = 7.6 Hz, 2H), 2.85 - 2.73 (m, 2H), 2.14 - 2.09 (m, 2H); ¹³C NMR (151 MHz, Chloroform-

d) δ 185.7, 163.5, 154.8, 150.4, 149.5, 149.3, 144.6, 140.3, 128.6, 128.4, 128.0, 126.3, 126.2, 123.9, 123.6, 123.0, 114.2, 111.7, 111.4, 56.0, 56.0, 39.1, 32.6, 29.1; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{29}H_{28}N_3O_6Se$ 594.1143, Found 594.1145; IR (cm^{-1} , neat): 2917, 2849, 1594, 1414.

(Z)-4-(benzo[d][1,3]dioxol-5-ylmethylene)-2-((2-(4-nitrophenyl)-2-oxoethyl)selanyl)-1-phenyl-1H-imidazol-5(4H)-one (9c)

Yellow solid, (67%, 150 mg); mp 78 – 80 °C; 1H NMR (400 MHz, $DMSO-d_6$) δ 8.32 (m, 5H), 7.69 (s, 1H), 7.55 (m, 3H), 7.42 (d, $J = 7.1$ Hz, 2H), 7.23 (s, 1H), 7.00 (d, $J = 8.2$ Hz, 1H), 6.86 (s, 1H), 6.80 (d, $J = 8.1$ Hz, 1H), 6.09 (s, 1H), 5.97 (s, 1H), 4.94 (d, $J = 12.2$ Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 192.7, 168.4, 158.6, 150.7, 149.8, 148.0, 139.9, 136.4, 132.6, 130.1, 129.8, 129.6, 129.5, 129.3, 129.2, 128.8, 128.5, 126.9, 126.1, 126.0, 124.2, 124.0, 110.2, 108.6, 101.6, 33.0; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{25}H_{18}N_3O_6Se$ 536.0361, Found 536.0357; IR (cm^{-1} , neat): 2923, 2854, 1717, 1489.

(Z)-4-(benzo[d][1,3]dioxol-5-ylmethylene)-2-((2-oxo-2-(p-tolyl)ethyl)selanyl)-1-(3-phenylpropyl)-1H-imidazol-5(4H)-one (9d)

Yellow solid, (73%, 167 mg); mp: 140 – 142 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.99 (t, $J = 8.0$ Hz, 2H), 7.40 (d, $J = 8.4$ Hz, 1H), 7.28 (t, $J = 8.0$ Hz, 3H), 7.19 (d, $J = 7.3$ Hz, 3H), 6.88 (s, 1H), 6.76 (d, $J = 8.1$ Hz, 1H), 6.01 (s, 2H), 4.91 (s, 2H), 3.62 (t, $J = 7.4$ Hz, 2H), 2.67 (t, $J = 7.7$ Hz, 2H), 2.43 (s, 3H), 2.01 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.6, 169.5, 159.6, 149.4, 148.0, 145.0, 140.6, 137.2, 132.7, 129.6, 128.9, 128.8, 128.5, 128.3, 128.3, 128.2, 126.1, 124.9, 110.9, 108.5, 101.5, 41.4, 34.3, 33.0, 30.6, 29.7, 21.8; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{29}H_{27}N_2O_4Se$ 547.1136, Found 547.1138; IR (cm^{-1} , neat): 2916, 2849, 1705, 1482.

(Z)-4-(3,4-dimethoxybenzylidene)-2-((2-oxo-2-phenylethyl)selanyl)-1-(3-phenylpropyl)-1H-imidazol-5(4H)-one (9e)

Yellow solid, (68%, 156 mg); mp 145 – 147 °C; 1H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, $J = 7.1$ Hz, 3H), 7.63 (t, $J = 7.5$ Hz, 1H), 7.54 – 7.41 (m, 3H), 7.31- 7.16 (m, 5H), 6.93 (s, 1H), 6.79 (d, $J = 8.4$ Hz, 1H), 4.93 (s, 2H), 3.91 (s, 3H), 3.83 (s, 3H), 3.64 (t, $J = 7.5$ Hz, 2H), 2.68 (t, $J = 7.8$ Hz, 2H), 2.08 – 1.97 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.6, 169.5, 159.1, 151.0, 148.8, 140.6, 137.0, 135.1, 134.0, 128.9, 128.6, 128.5, 128.3,

127.4, 126.8, 126.1, 125.3, 113.7, 110.8, 55.9, 55.6, 41.4, 34.0, 33.0, 30.6; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{29}H_{29}N_2O_4Se$ 549.1293, Found 549.1290; IR (cm^{-1} , neat): 2921, 2850, 1704, 1511.

(Z)-4-(3,4-dimethoxybenzylidene)-2-((1-oxo-1-phenylpropan-2-yl)thio)-1-phenyl-1H-imidazol-5(4H)-one (9f)

Yellow solid, (74%, 146 mg); mp 150 – 152 °C; 1H NMR (400 MHz, Chloroform- d) δ 8.09 (d, $J = 7.1$ Hz, 2H), 7.88 (d, $J = 2.0$ Hz, 3H), 7.63 (t, $J = 7.4$ Hz, 1H), 7.57 - 7.40 (m, 7H), 7.32 (d, $J = 6.9$ Hz, 2H), 7.03 (s, 1H), 6.68 (d, $J = 8.4$ Hz, 1H), 5.82 (q, $J = 7.2$ Hz, 1H), 3.94 (m, 1H), 3.92 (s, 6H), 1.78 (d, $J = 7.2$ Hz, 3H); ^{13}C NMR (101 MHz, Chloroform- d) δ 196.4, 168.7, 161.5, 150.9, 148.7, 136.2, 134.5, 133.7, 132.2, 129.5, 129.1, 128.9, 128.7, 127.3, 127.2, 126.4, 125.4, 113.9, 110.9, 55.9, 55.7, 45.5, 18.3; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{27}H_{24}N_2O_4S$ 473.1535, Found 473.1534; IR (cm^{-1} , neat): 3059, 2916, 2849, 1593.

(Z)-4-(3,4-dimethoxybenzylidene)-2-((1-oxo-1-phenylpropan-2-yl)selenanyl)-1-phenyl-1H-imidazol-5(4H)-one (9g)

Yellow solid, (79%, 172 mg); mp 86 – 88 °C; 1H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, $J = 1.8$ Hz, 1H), 8.10 (d, $J = 7.4$ Hz, 2H), 7.62 - 7.57 (m, 2H), 7.50 - 7.43 (m, 5H), 7.30 (dd, $J = 7.6$ Hz, $J = 1.5$ Hz, 2H), 7.26 (d, $J = 0.7$ Hz, 1H), 7.08 (s, 1H), 6.90 (d, $J = 8.4$ Hz, 1H), 5.93 (q, $J = 7.0$ Hz, 1H), 4.00 (m, 1H), 3.96 (s, 3H), 3.92 (s, 3H), 1.96 (d, $J = 7.0$ Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.4, 168.5, 159.2, 151.2, 148.9, 136.5, 134.3, 133.8, 132.6, 129.6, 129.3, 128.9, 128.6, 127.4, 127.0, 126.9, 126.9, 125.9, 113.6, 110.9, 55.9, 55.6, 42.4, 19.1; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{27}H_{25}N_2O_4Se$ 521.0980, Found 521.0980; IR (cm^{-1} , neat): 3059, 2919, 2851, 1420.

(Z)-4-(3,4-dimethoxybenzylidene)-2-((2-oxo-2-phenylethyl)selenanyl)-1-phenyl-1H-imidazol-5(4H)-one (9h)

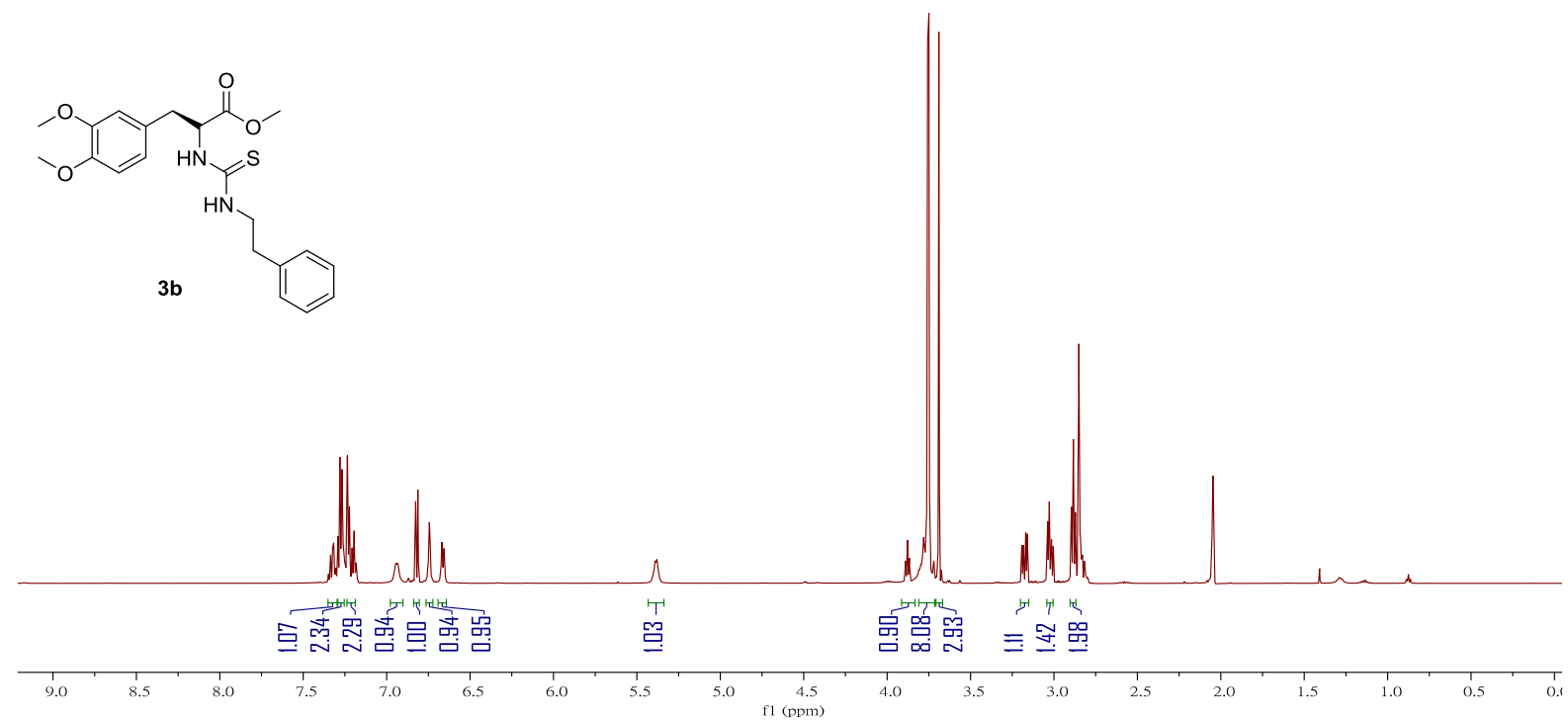
Yellow solid, (72%, 152 mg); mp: 150 – 152 °C; 1H NMR (400 MHz, $CDCl_3$) δ 8.62 (s, 1H), 8.44 (s, 1H), 8.35 (d, $J = 7.3$ Hz, 2H), 7.74 (d, $J = 8.8$ Hz, 1H), 7.65 (m, 4H), 7.54 (t, $J = 7.6$ Hz, 2H), 7.48 - 7.42 (m, 2H), 6.92 (d, $J = 8.5$ Hz, 1H), 5.85 (s, 2H), 3.98 (s, 3H), 3.91 (s, 3H); ^{13}C NMR (151 MHz, DMSO- d_6) δ 193.9, 168.1, 160.0, 151.2, 148.8, 136.5, 135.7, 134.2, 133.2, 130.1, 129.9, 129.4, 128.9, 127.8, 127.1, 127.0, 124.8, 114.2, 111.7, 55.9, 55.4, 35.5; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{26}H_{22}N_2O_4Se$ 507.0823, Found 507.0828; IR (cm^{-1} , neat): 3065, 2927, 1718, 1449.

(Z)-4-(3,4-dimethoxybenzylidene)-2-((2-oxo-1,2-diphenylethyl)thio)-1-phenyl-1H-imidazol-5(4H)-one (9i)

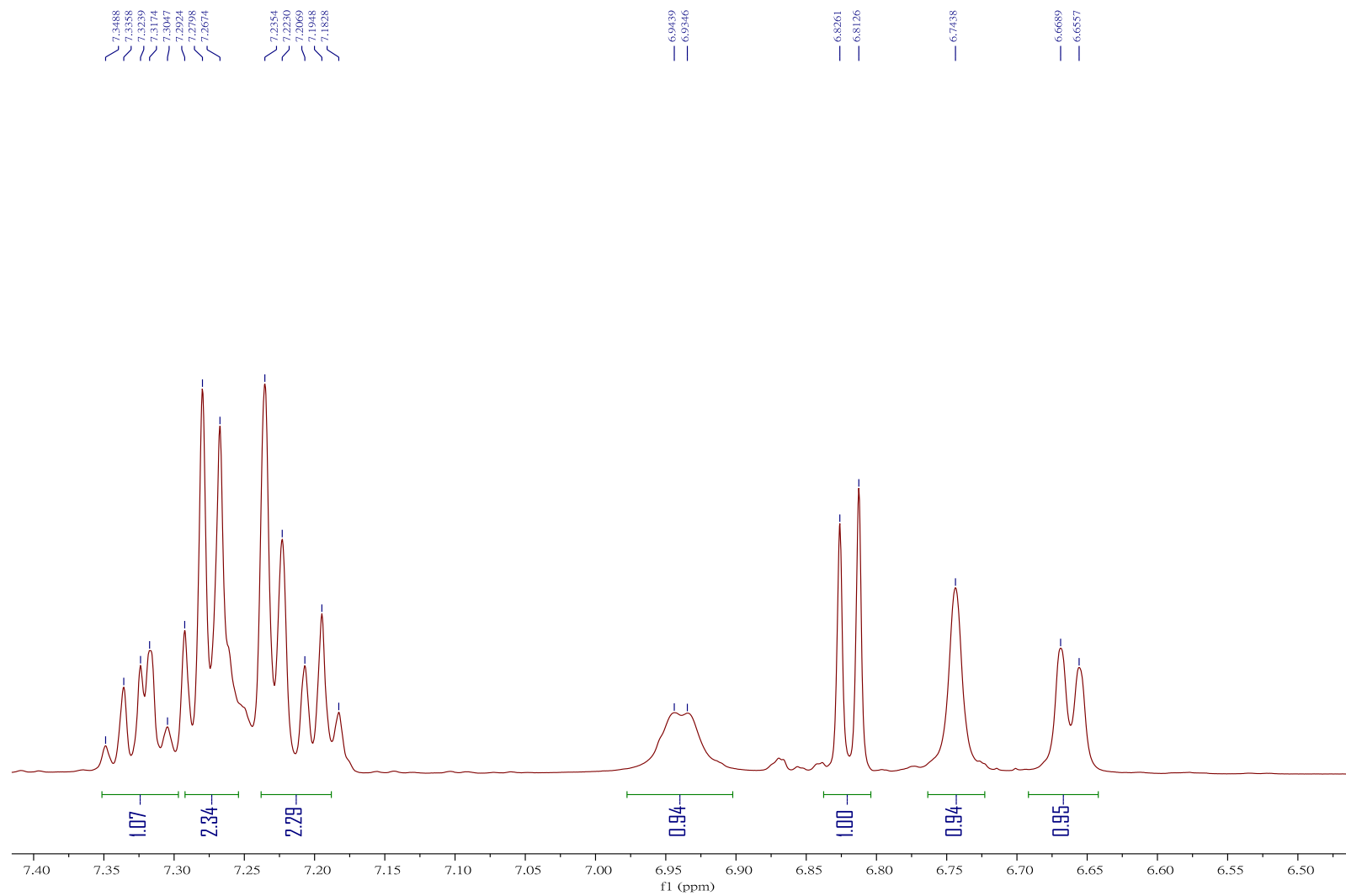
Yellow solid, (76%, 170 mg); mp 86 – 88 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.10 (d, *J* = 8.6 Hz, 1H), 7.91 (d, *J* = 8.7 Hz, 1H), 7.61 - 7.56, 7.56 (m, 2H), 7.51 – 7.45 (m, 6H), 7.43 (d, *J* = 7.4 Hz, 1H), 7.39 - 7.35 (m, 3H), 7.33 - 7.29 (m, 2H), 6.96 (q, *J* = 8.6 Hz, 2H), 6.29 (d, *J* = 8.6 Hz, 1H), 3.97 – 3.90 (m, 1H), 3.85 (s, 3H), 3.80 (s, 3H); ¹³C NMR (151 MHz, acetone) δ 193.7, 193.4, 179.3, 160.3, 148.9, 148.9, 135.6, 134.6, 134.5, 133.4, 132.5, 132.5, 129.2, 129.2, 129.0, 129.0, 128.9, 128.87, 128.8, 128.7, 128.6, 128.5, 127.3, 122.1, 113.7, 113.4, 111.5, 69.8, 69.5, 55.3, 55.1, 36.8, 36.7, 14.7; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₃₂H₂₇N₂O₄S 535.1692, Found 535.1693; IR (cm⁻¹, neat): 3059, 2919, 2851, 1420.

(Z)-4-(3,4-bis(allyloxy)benzylidene)-2-(2-oxo-2-(p-tolyl)ethoxy)-1-phenyl-1H-imidazol-5(4H)-one (9j)

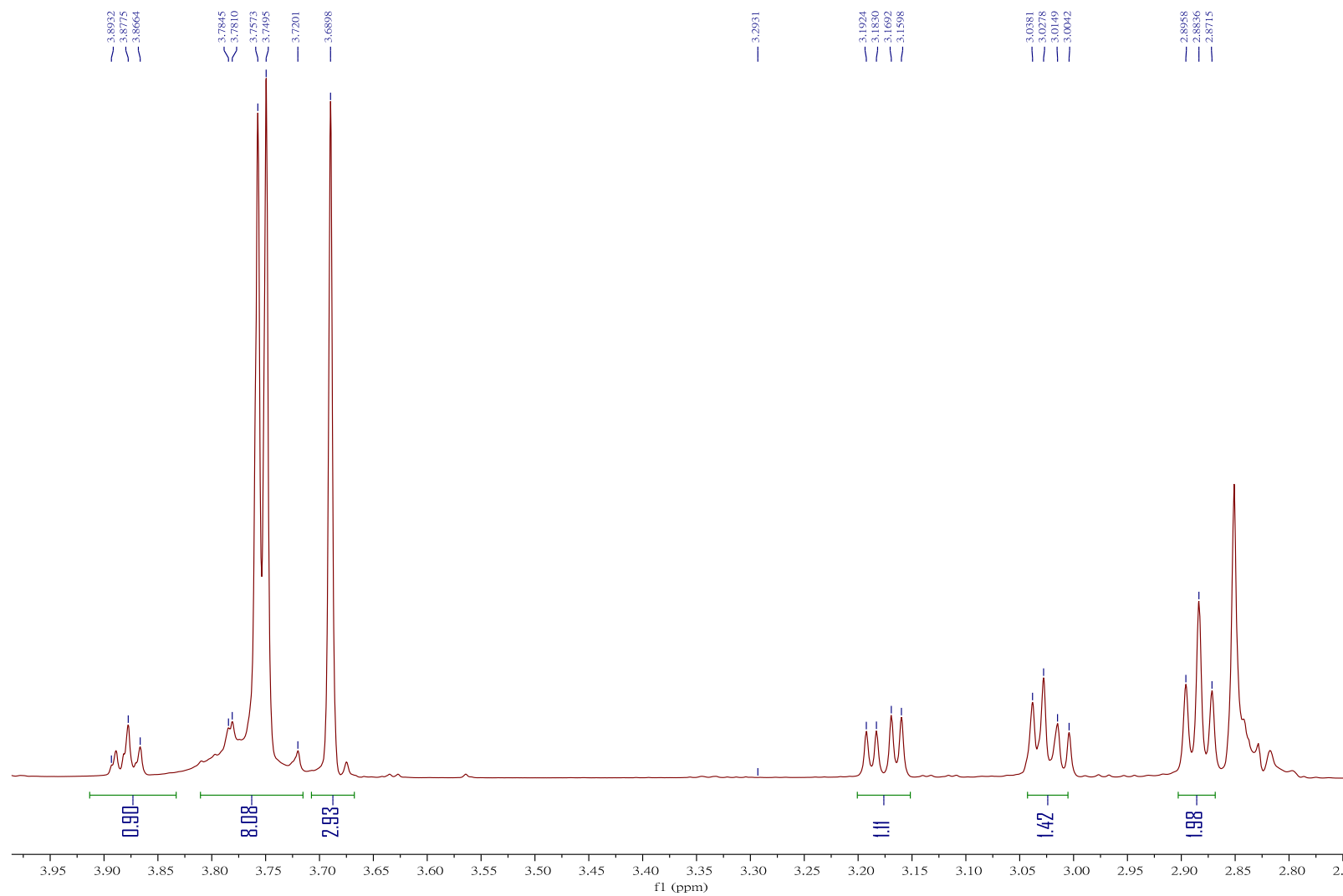
Yellow solid, (64%, 130 mg); mp 94 – 96 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.55 - 7.45 (m, 5H), 7.38 (q, *J* = 7.2 Hz, 1H), 7.28 - 7.24 (m, 1H), 7.15 (d, *J* = 8.6 Hz, 2H), 6.98 (s, 1H), 6.73 - 6.68 (m, 2H), 6.63 (d, *J* = 8.6 Hz, 1H), 6.04 - 5.92 (m, 2H), 5.35 (d, *J* = 7.9 Hz, 2H), 5.25 (d, *J* = 10.4 Hz, 2H), 4.98 (s, 2H), 4.44 - 4.42 (m, 4H), 2.37 (s, 3H); ¹³C NMR (101 MHz, cdcl₃) δ 191.1, 162.5, 155.2, 148.6, 148.1, 144.8, 132.9, 131.7, 131.6, 129.2, 129.0, 128.9, 128.4, 128.2, 127.7, 126.0, 125.06, 122.21, 120.0, 117.8, 117.7, 114.5, 113.4, 113.3, 69.7, 69.6, 48.6, 29.6, 21.7; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₃₁H₂₈N₂O₅S 509.2076, Found 509.2071; IR (cm⁻¹, neat): 3059, 2919, 2851, 1420.



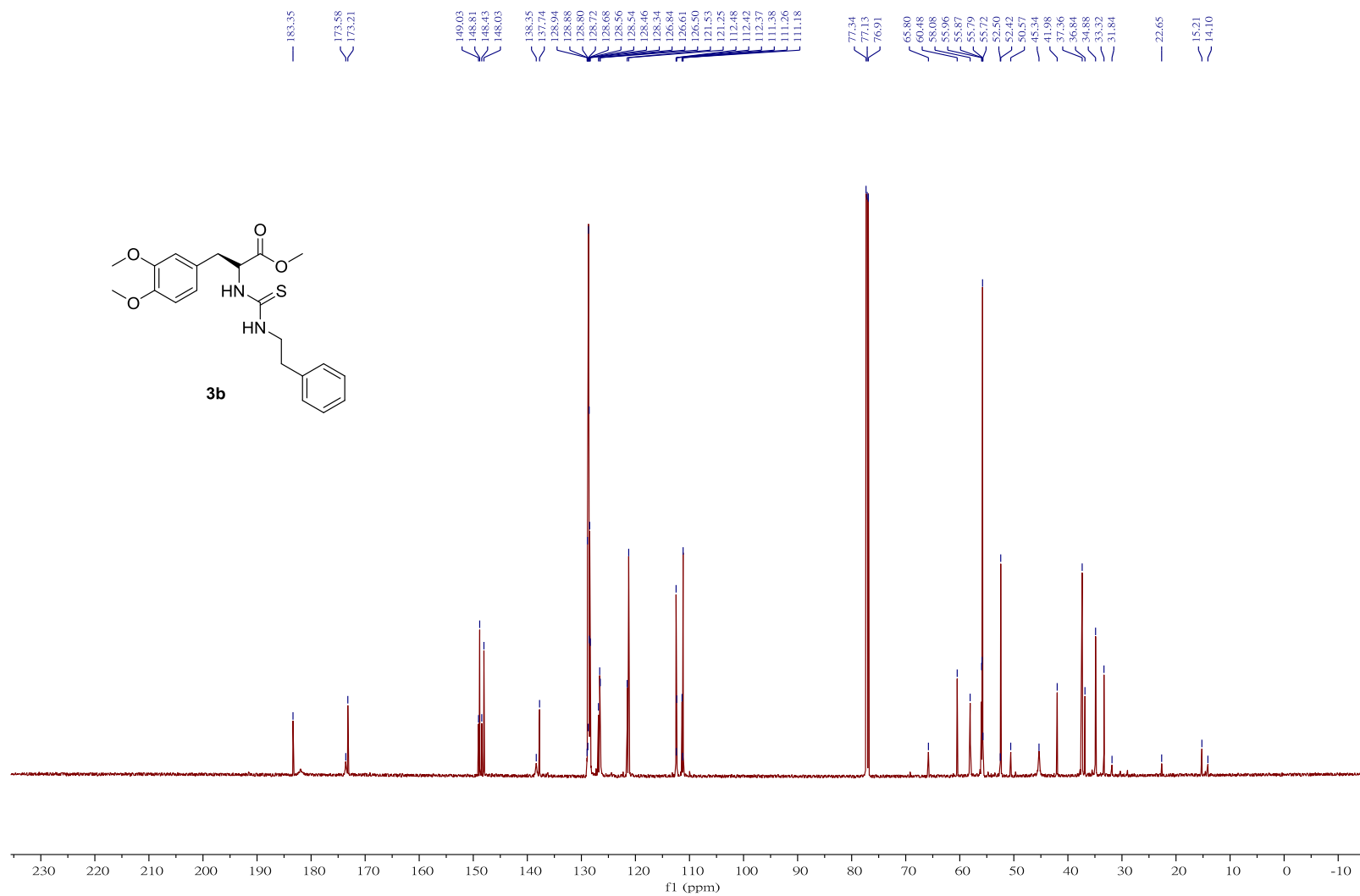
¹H NMR Spectrum (400 MHz) of compound **3b** in acetone-*d*₆



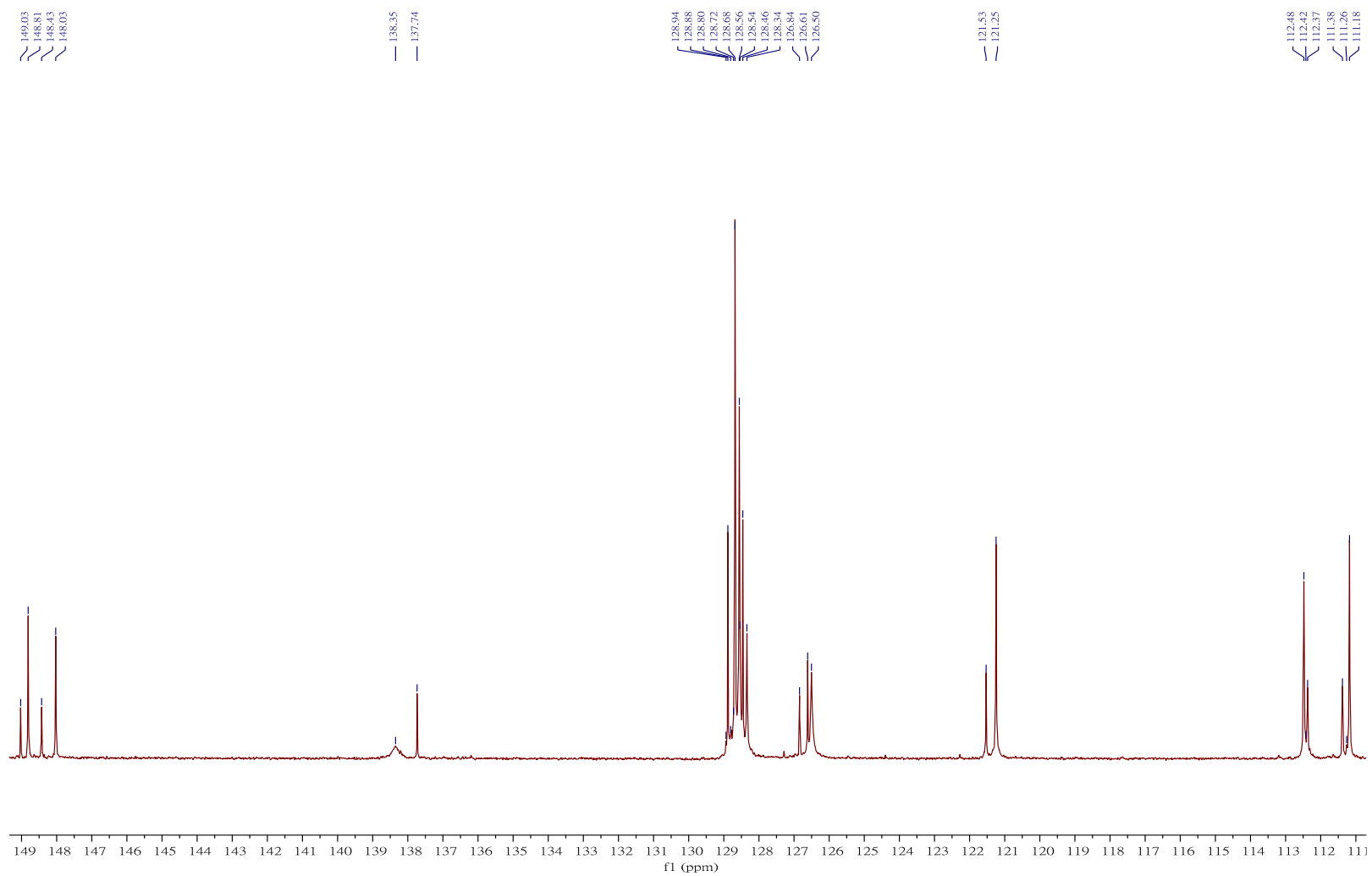
Expansion of ^1H NMR Spectrum (400 MHz) of compound **3b** in acetone- d_6



Expansion of ^1H NMR Spectrum (400 MHz) of compound **3b** in acetone- d_6



¹³C NMR Spectrum (101 MHz) of compound **3b** in CDCl₃



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **3b** in CDCl_3

Display Report

Analysis Info

Analysis Name D:\Data\ncu service\data\2018\20180814\L121-1_RC5_01_19434.d

Method Small molecule.m

Sample Name L121-1

Comment

Acquisition Date 8/14/2018 12:24:07 PM

Operator NCTU

Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type ESI

Focus Active

Scan Begin 50 m/z

Scan End 1500 m/z

Ion Polarity

Set Capillary

Set End Plate Offset

Set Charging Voltage

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Positive

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0 nA

Set Nebulizer

Set Dry Heater

Set Dry Gas

Set Divert Valve

Set APCI Heater

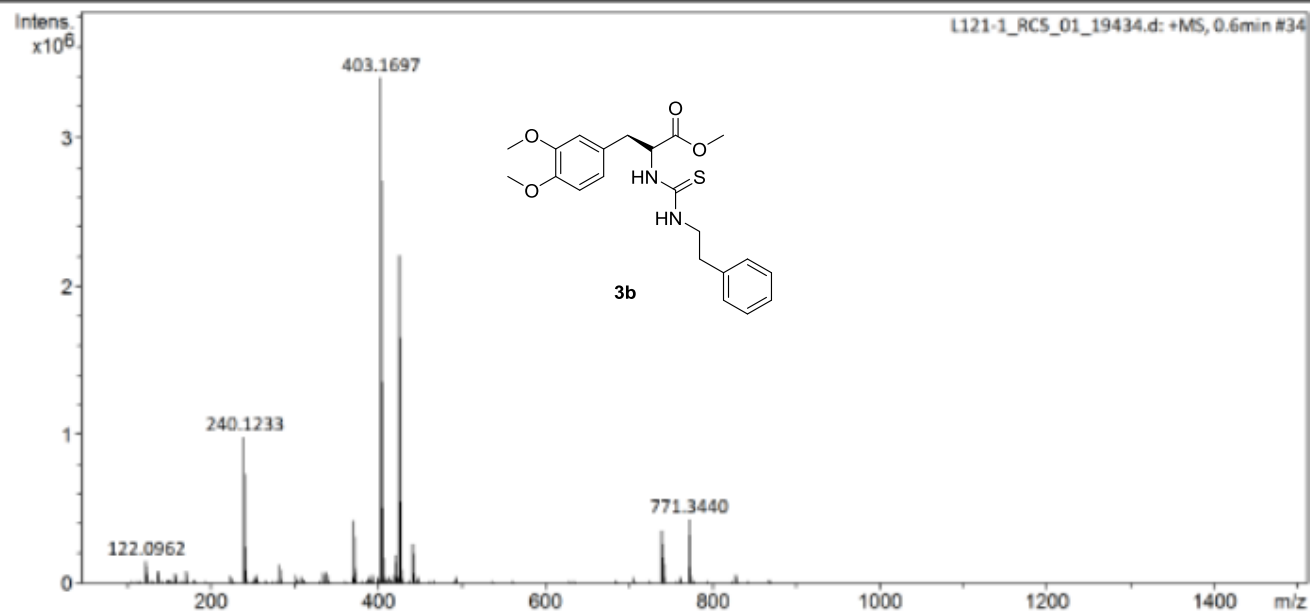
1.0 Bar

200 °C

6.0 l/min

Waste

0 °C



HRMS of compound **3b**

CSM: Linda Series: 0053 Report Name: modified System: Sys 1

Chromaster System Manager Report

Analyzed Date and Time: 2017/11/17 12:09 下午
Reported Date and Time: 2018/09/11 11:37:53 上午

Processed Date and Time: 2018/09/11 11:35 上午

Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0053\

Processing Method: L130_ee

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Series: 0053

Application(data): Linda

Vial Number: 1

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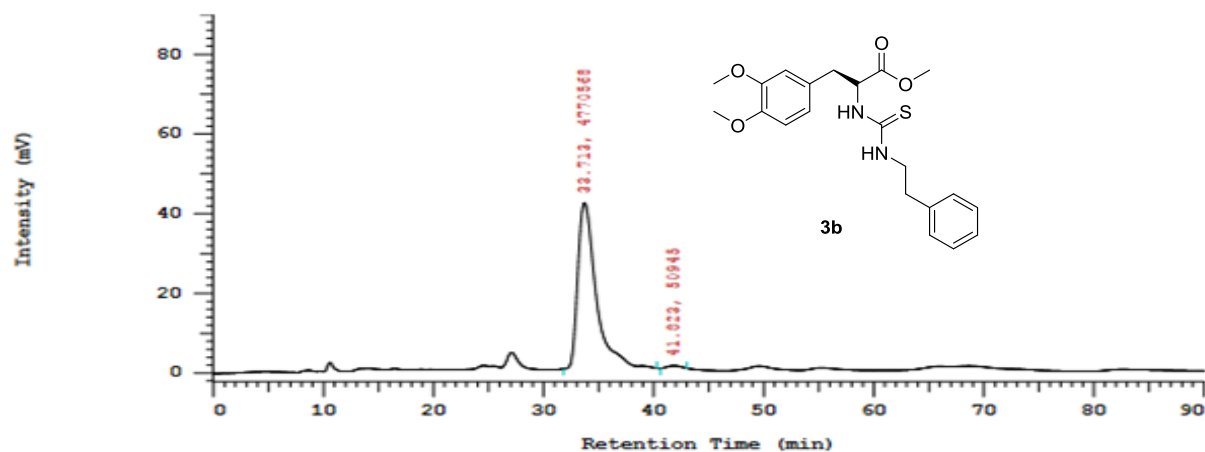
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Injection from this vial: 1 of 1

Volume: 20.0 ul

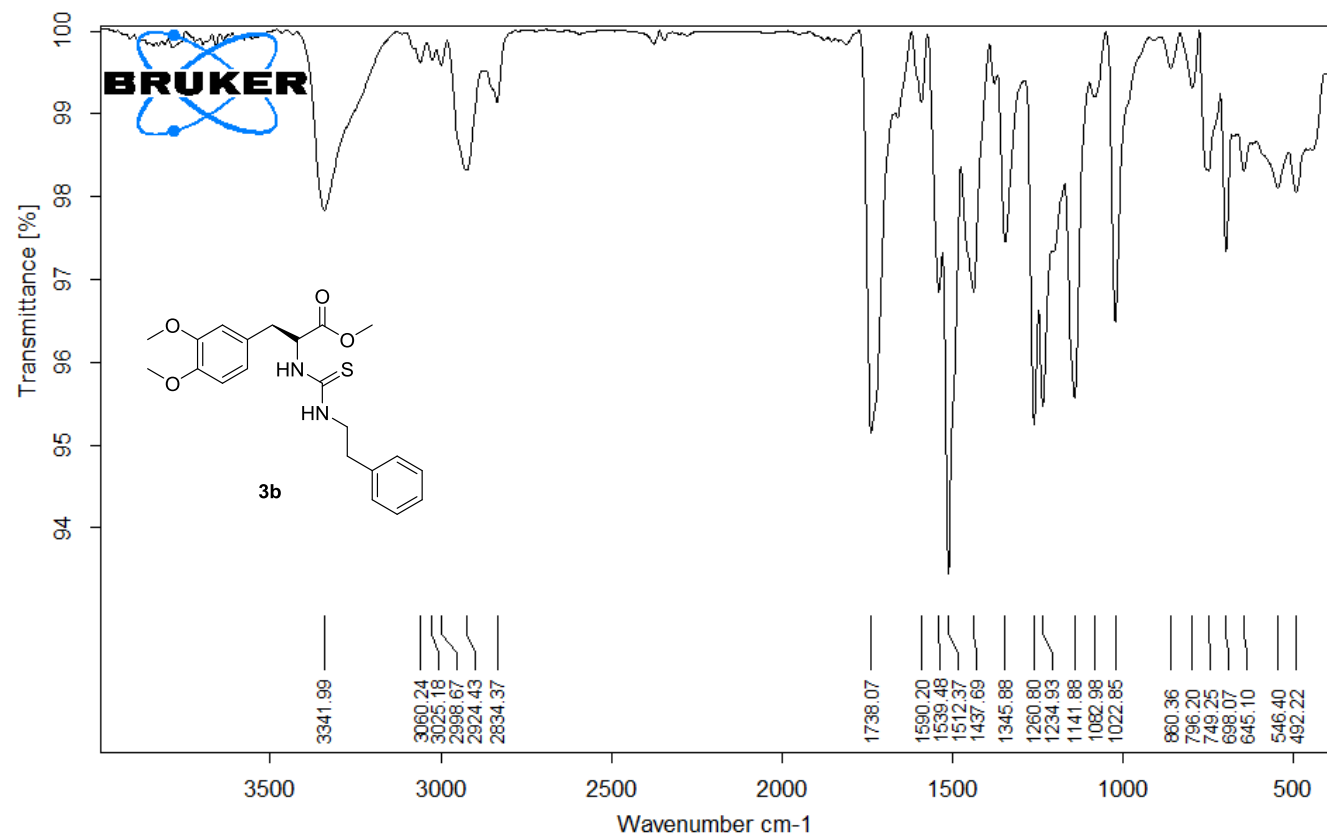
Sample Description:

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.5
mL/min , Daicel
Chiral OD, IPA 1,
Hex 10

Chiral HPLC of compound **3b**



D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L121-I.1

MIR_TR_DTGS_L121-I

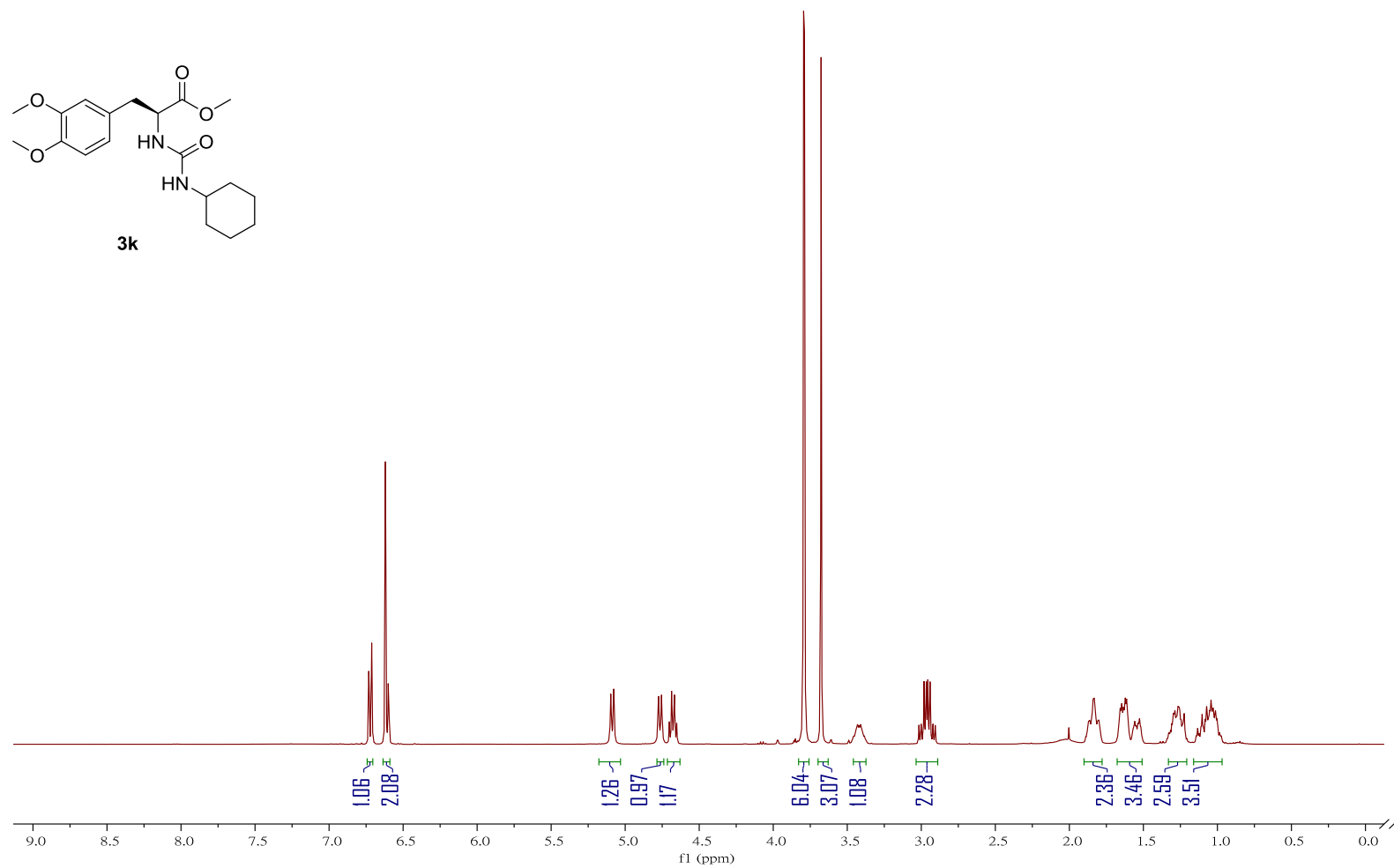
Instrument type and / or accessory

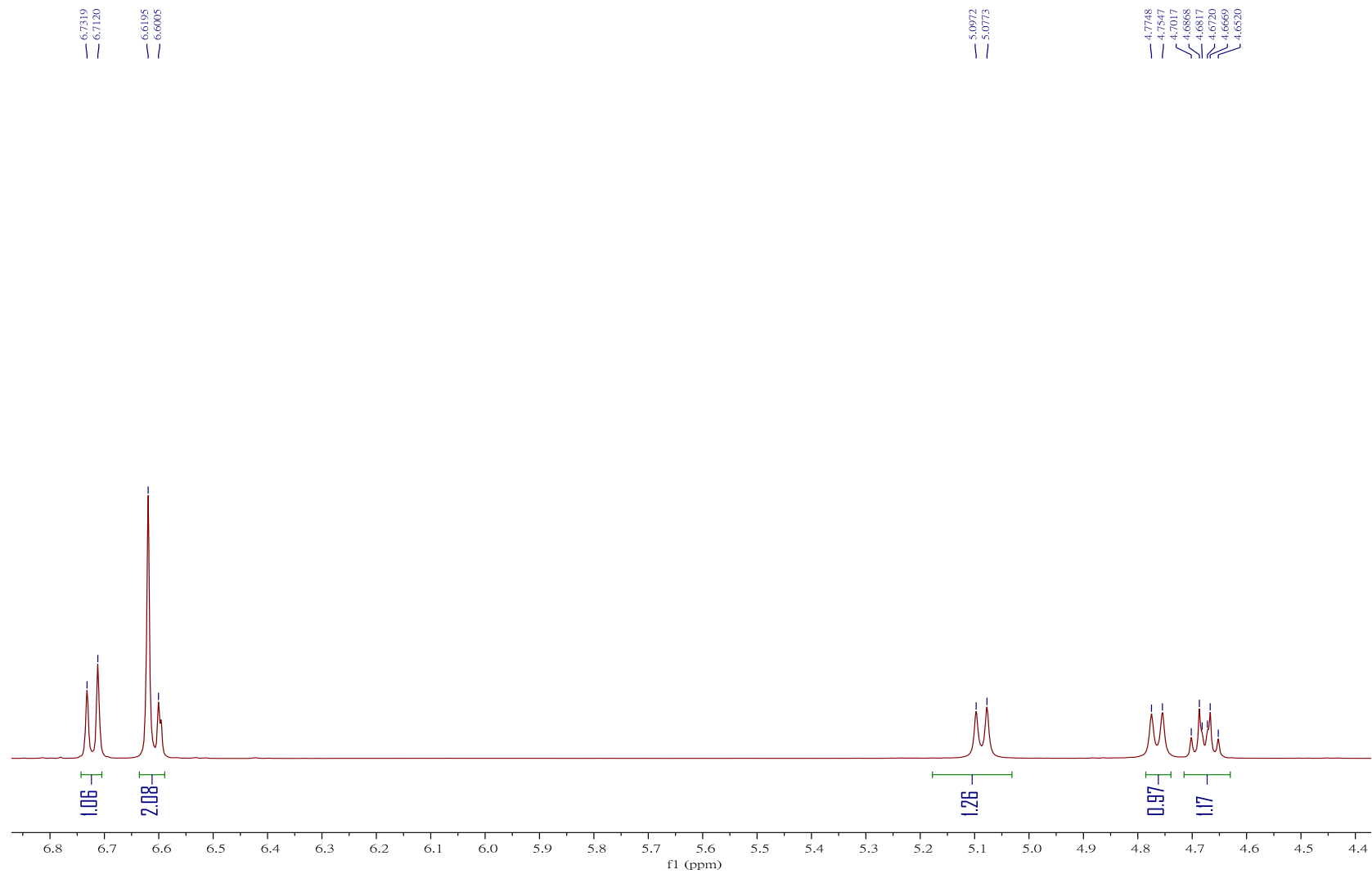
9/4/2018

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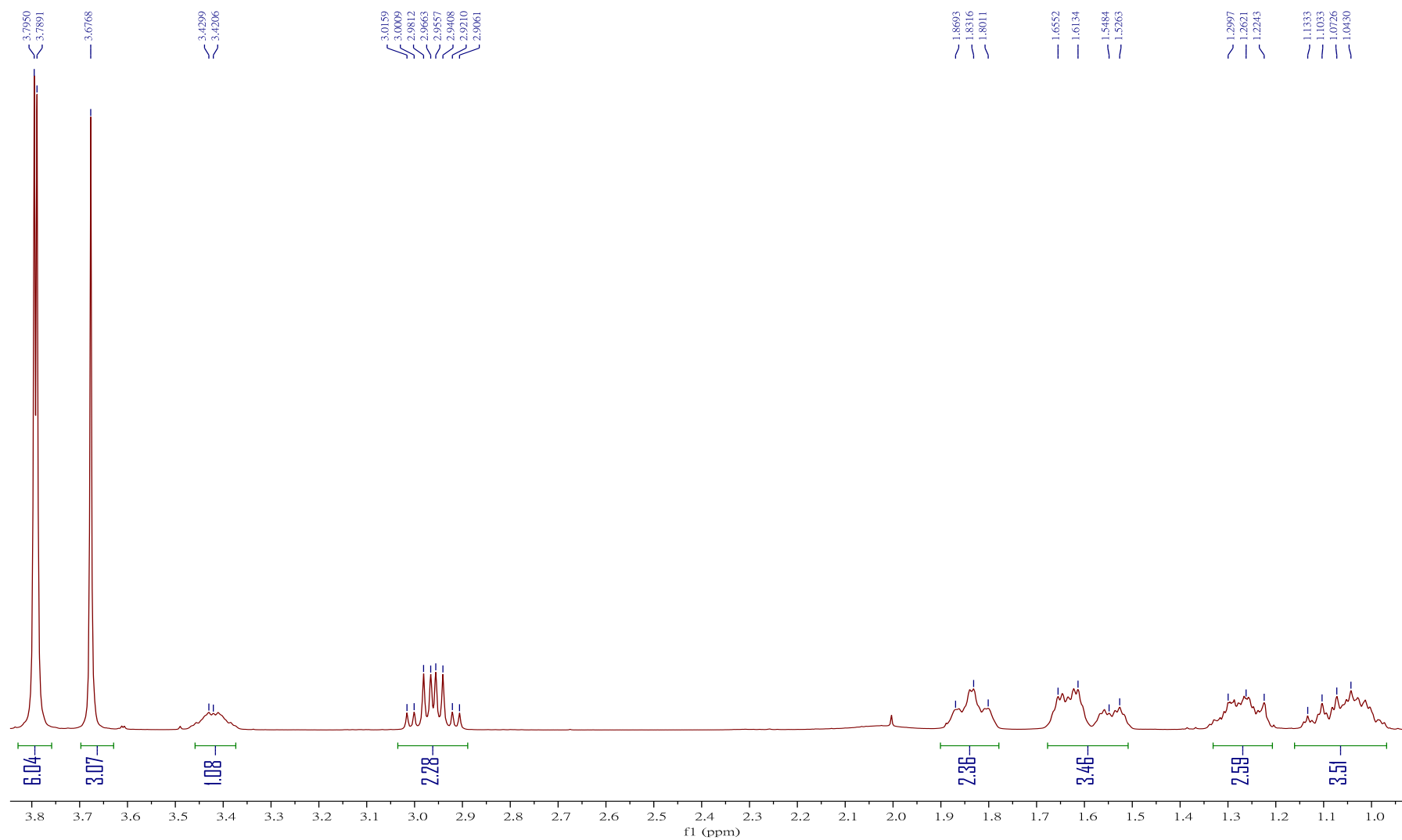
FT-IR Spectrum of compound **3b**

PROTON_01
L140-d_CDC13

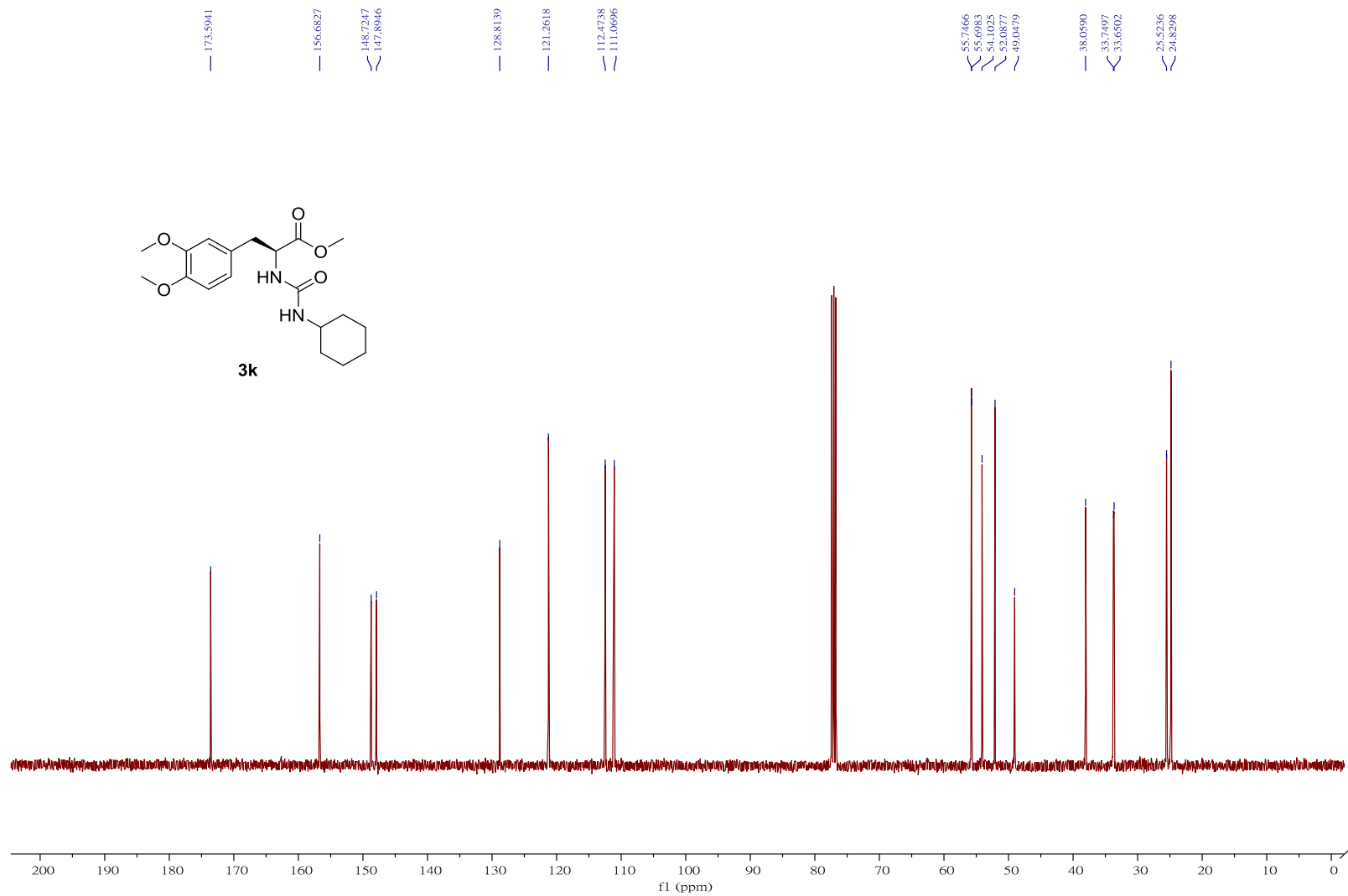


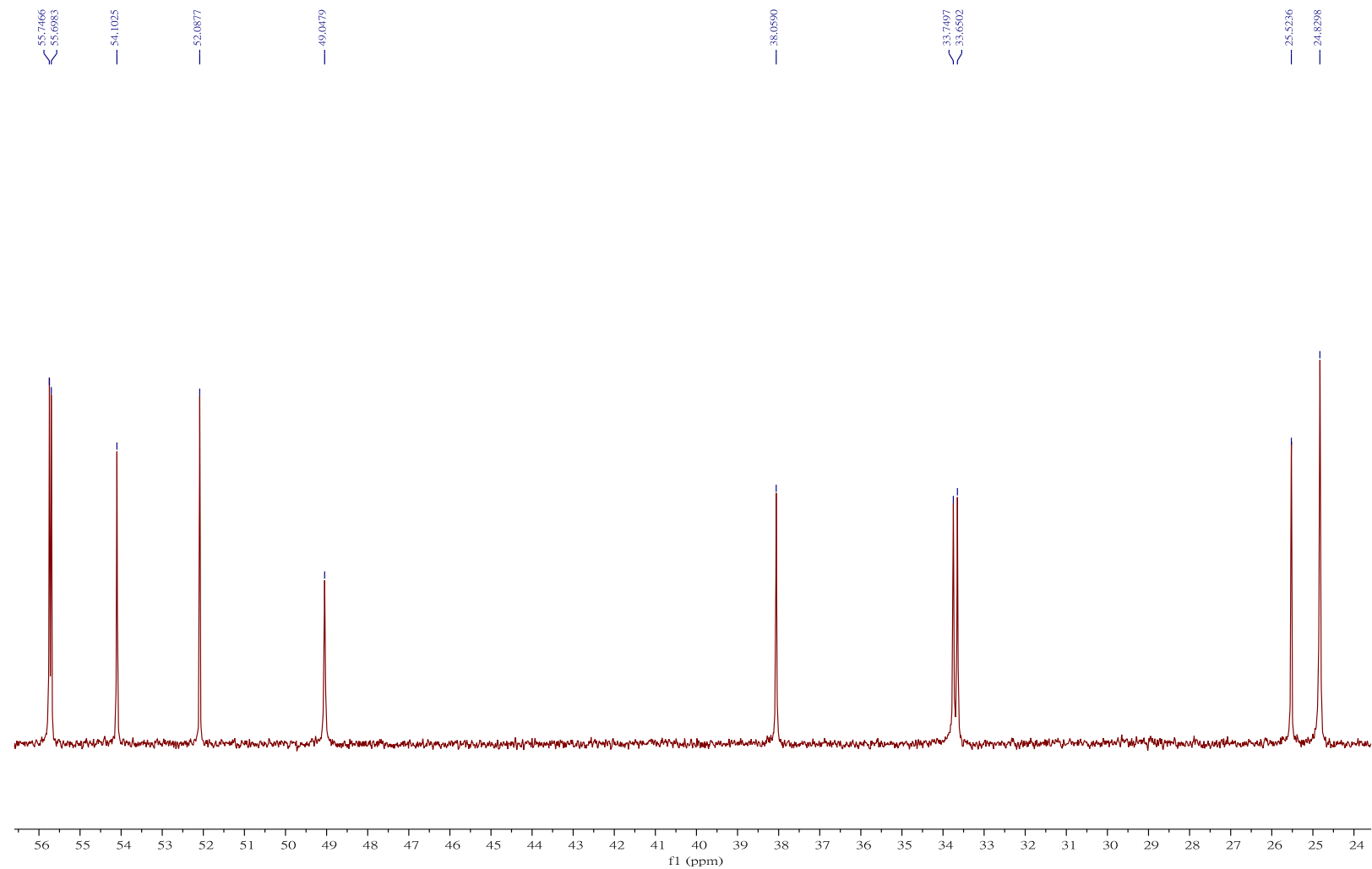


Expansion of ¹H NMR Spectrum (400 MHz) of compound **3k** in CDCl₃



Expansion of ¹H NMR Spectrum (400 MHz) of compound **3k** in CDCl₃



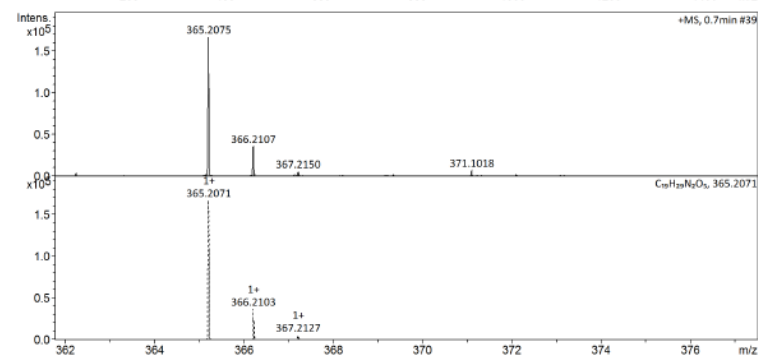
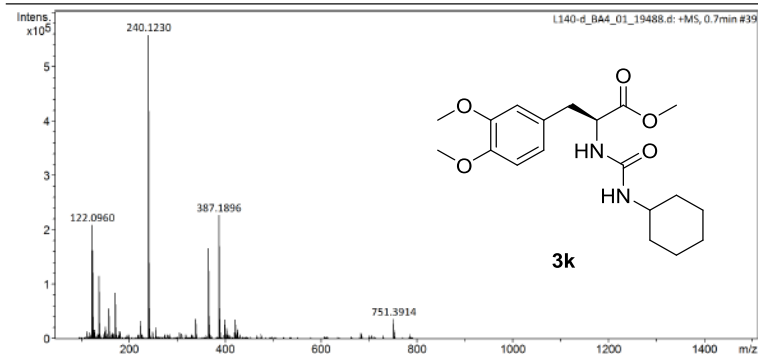


Expansion of ¹³C NMR Spectrum (101 MHz) of compound **3k** in CDCl₃

Display Report

Analysis Info		Acquisition Date	8/17/2018 12:10:08 PM	
Analysis Name	D:\Data\NCTU SERVICE\Data\2018\20180817-2\L140-d_BA4_01_19488.d	Operator	NCTU	
Method	Small molecule.m	Instrument	impact HD	1819090.00164
Sample Name	L140-d			
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



HRMS of compound **3k**

CSM: Linda Series: 0168 Report Name: modified System: Sys 1

Chromaster System Manager Report

Analyzed Date and Time: 2018/09/15 10:33 上午
Reported Date and Time: 2018/09/17 10:23:03 上午

Processed Date and Time: 2018/09/17 10:22 上午

Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0168\

Processing Method: L140-d_ee

System (acquisition): Sys 1

Series: 0168

Application(data): Linda

Vial Number: 1

Sample Name: UNKNOWN001

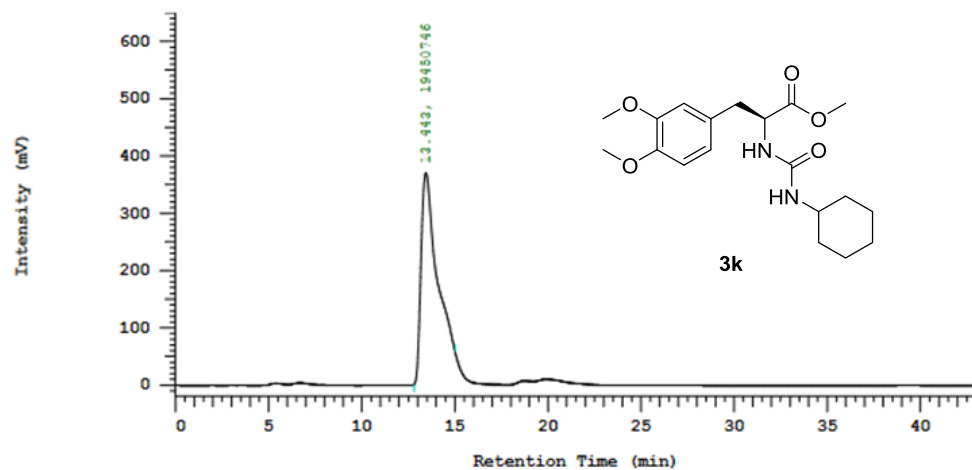
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 10.0 ul

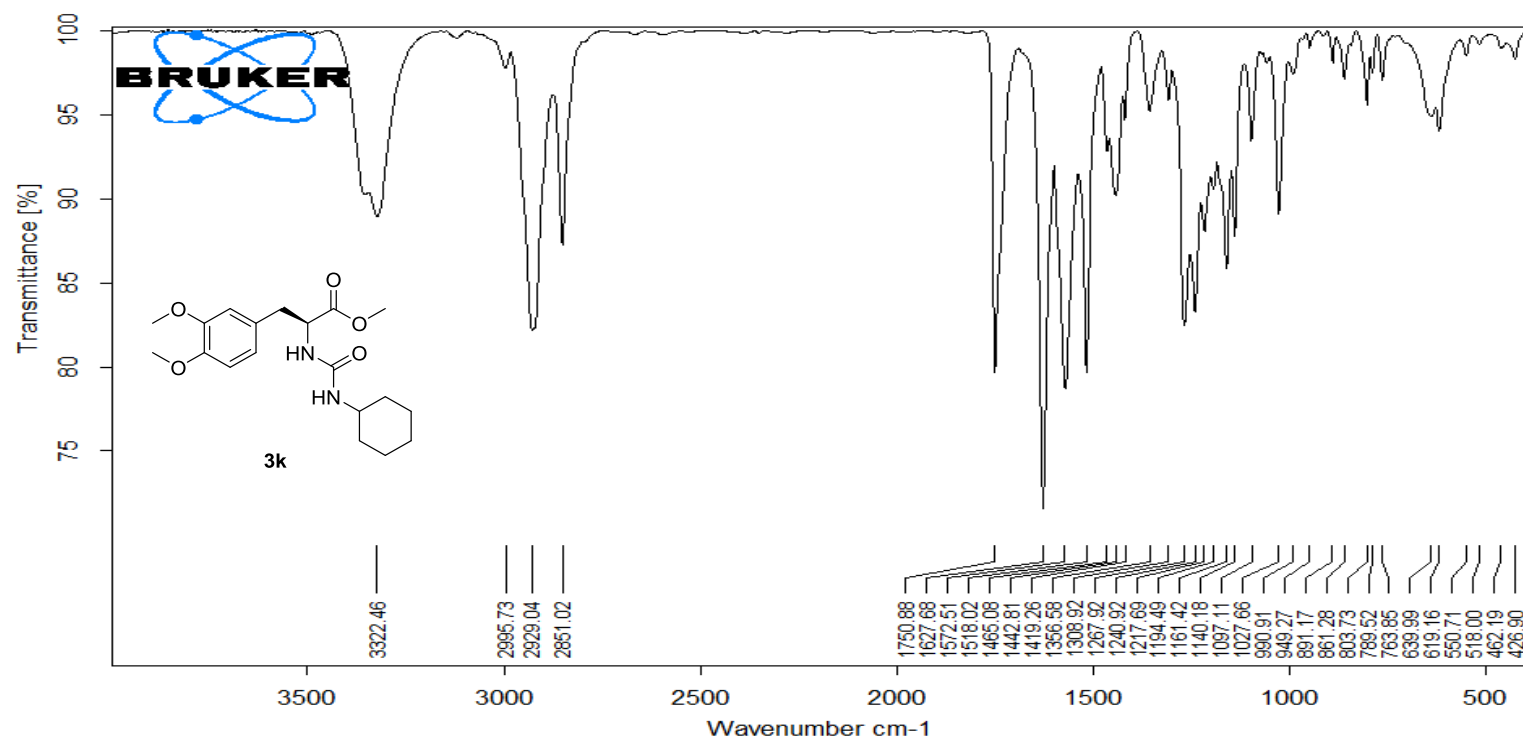
Sample Description:

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound 3k



D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L140-d.1

MIR_TR_DTGS_L140-d

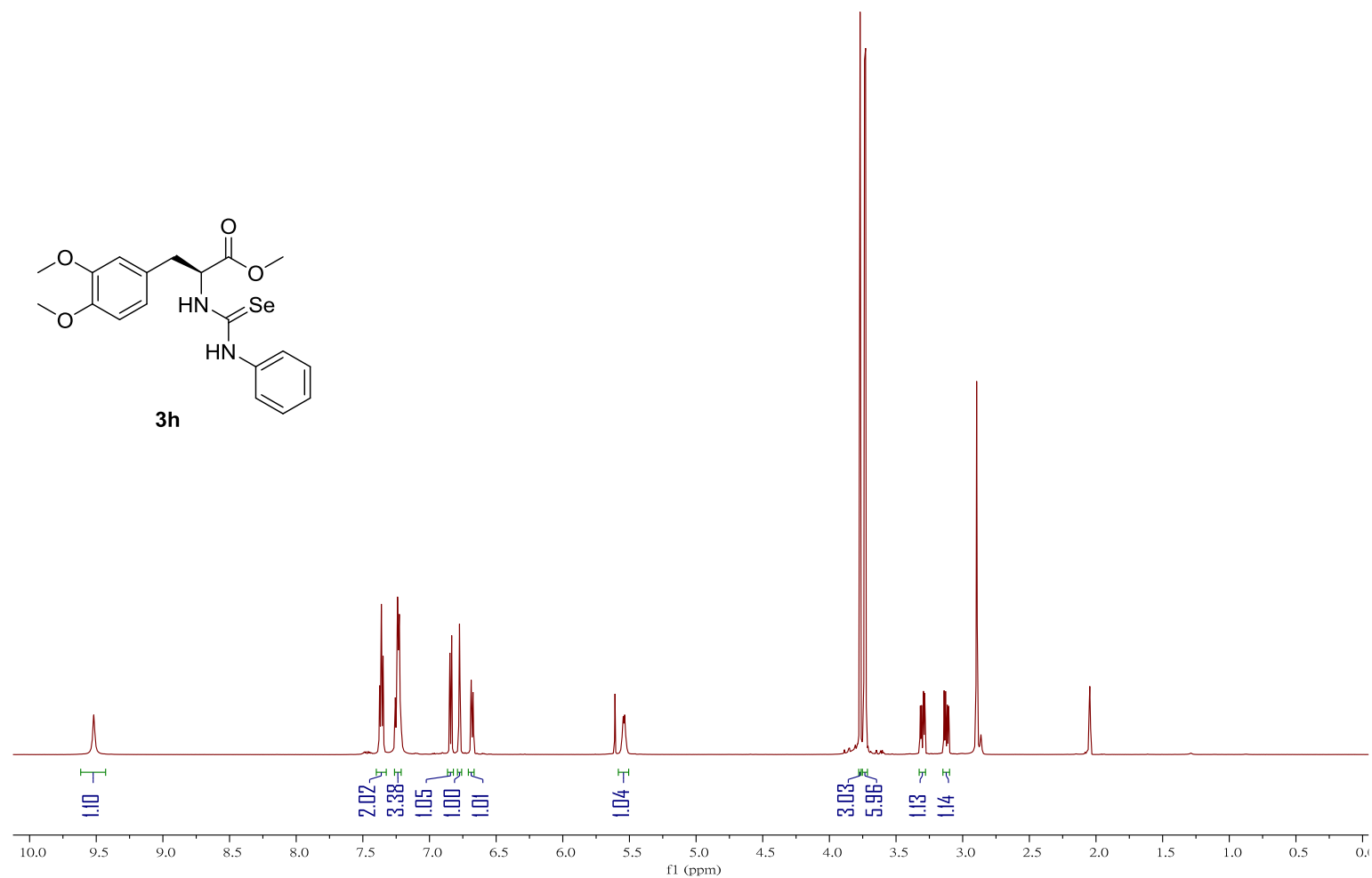
Instrument type and / or accessory

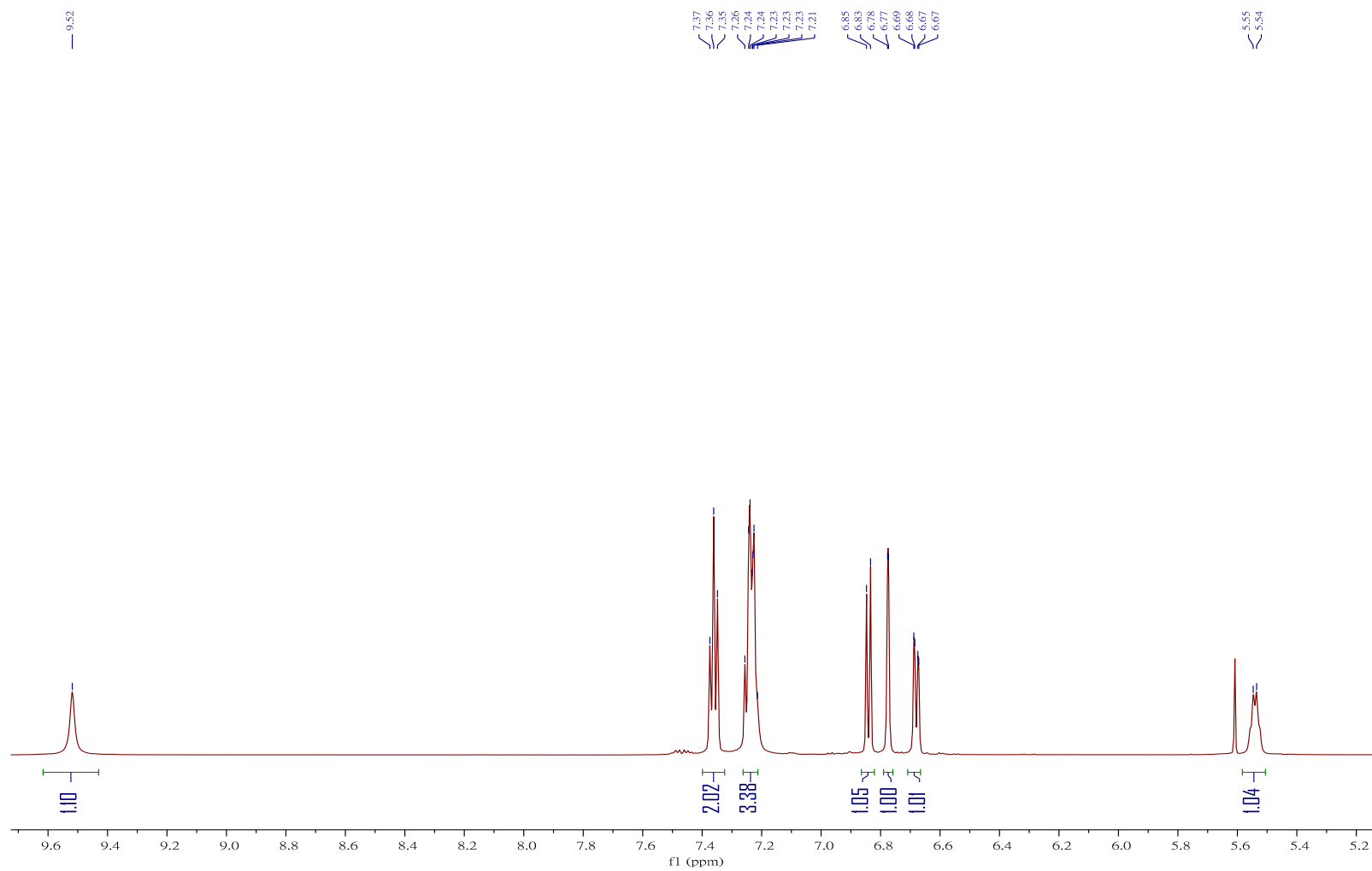
9/4/2018

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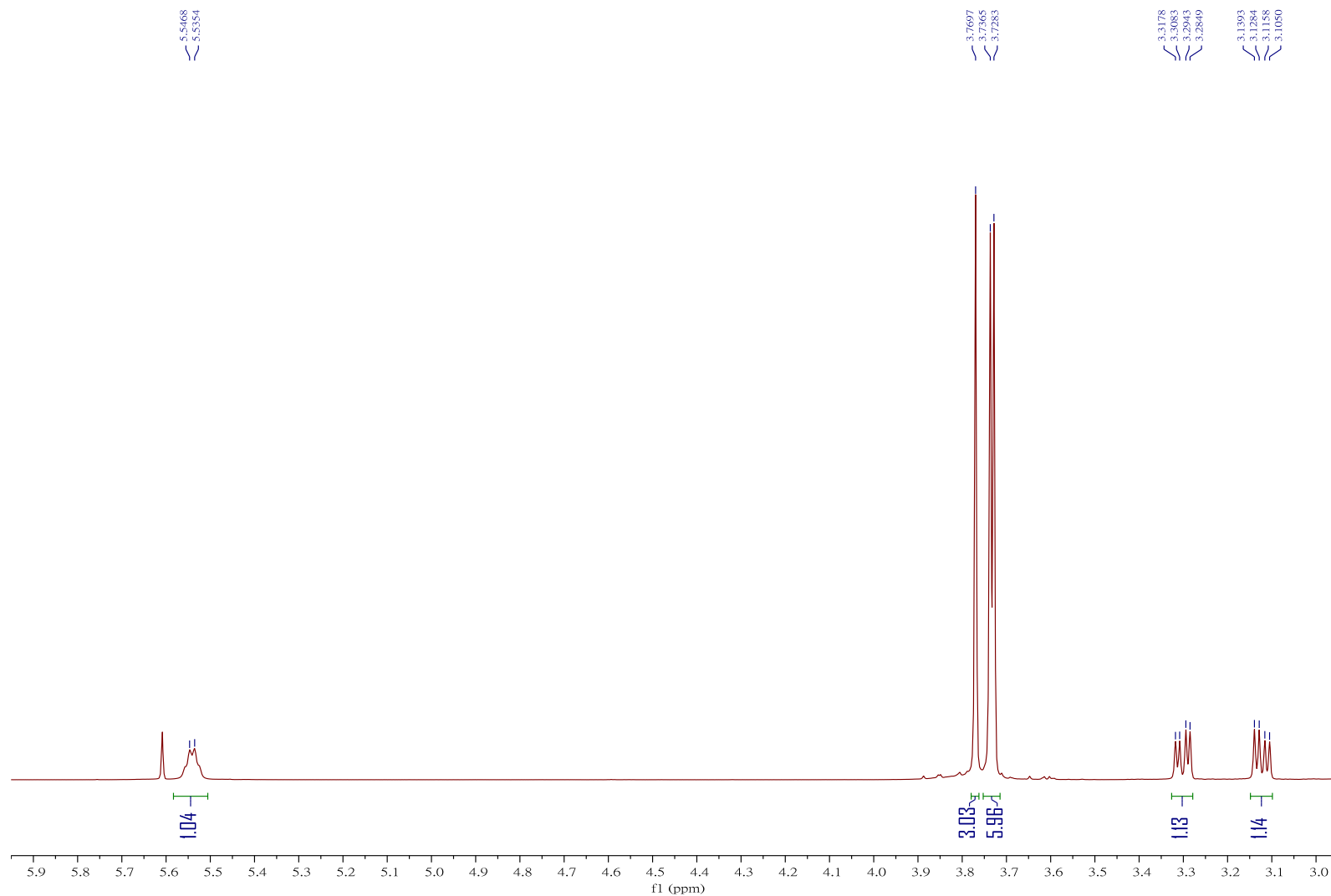
FT-IR Spectrum of compound **3k**

PROTON_01
L322-p_Wash_dAce

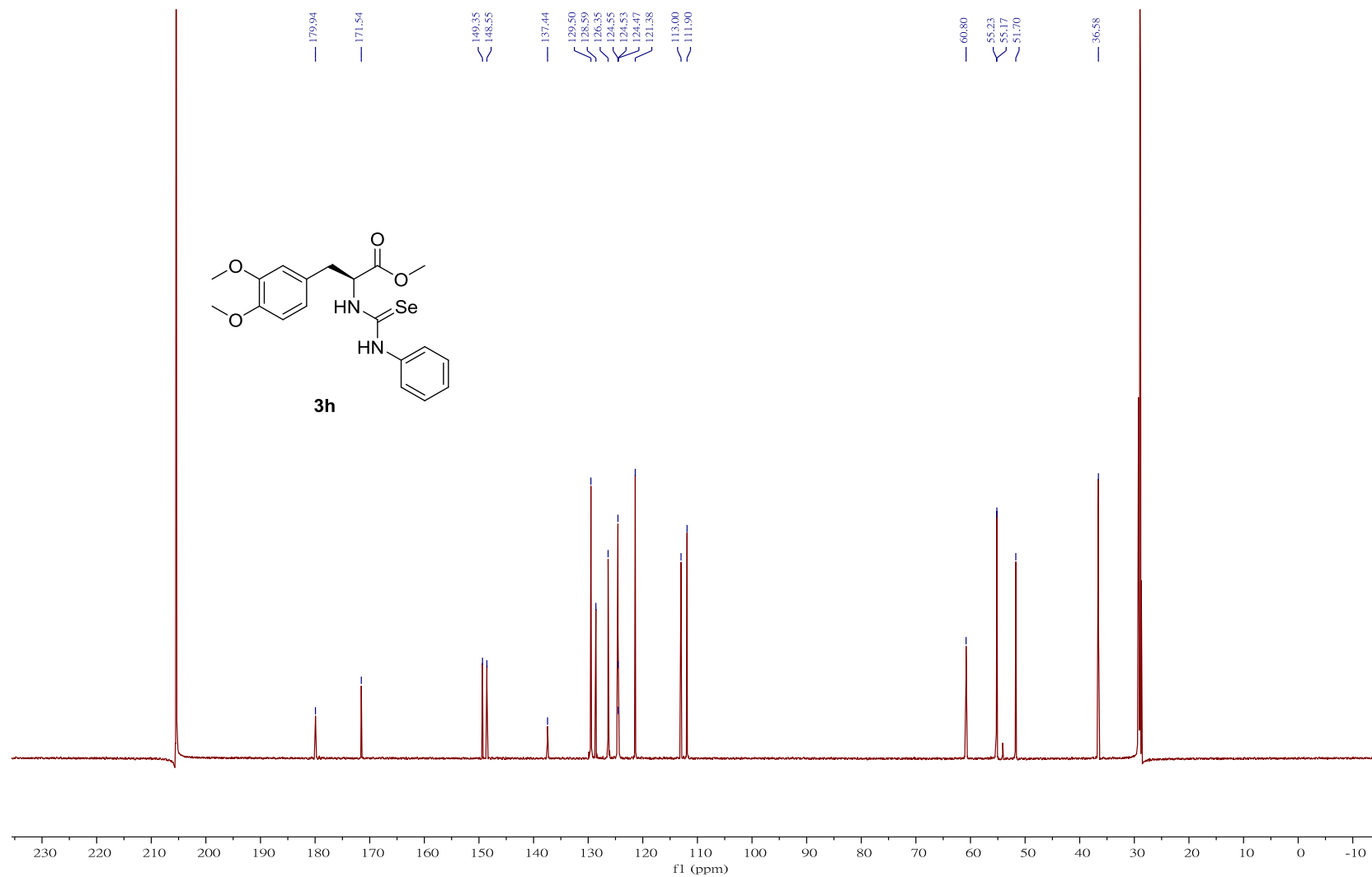




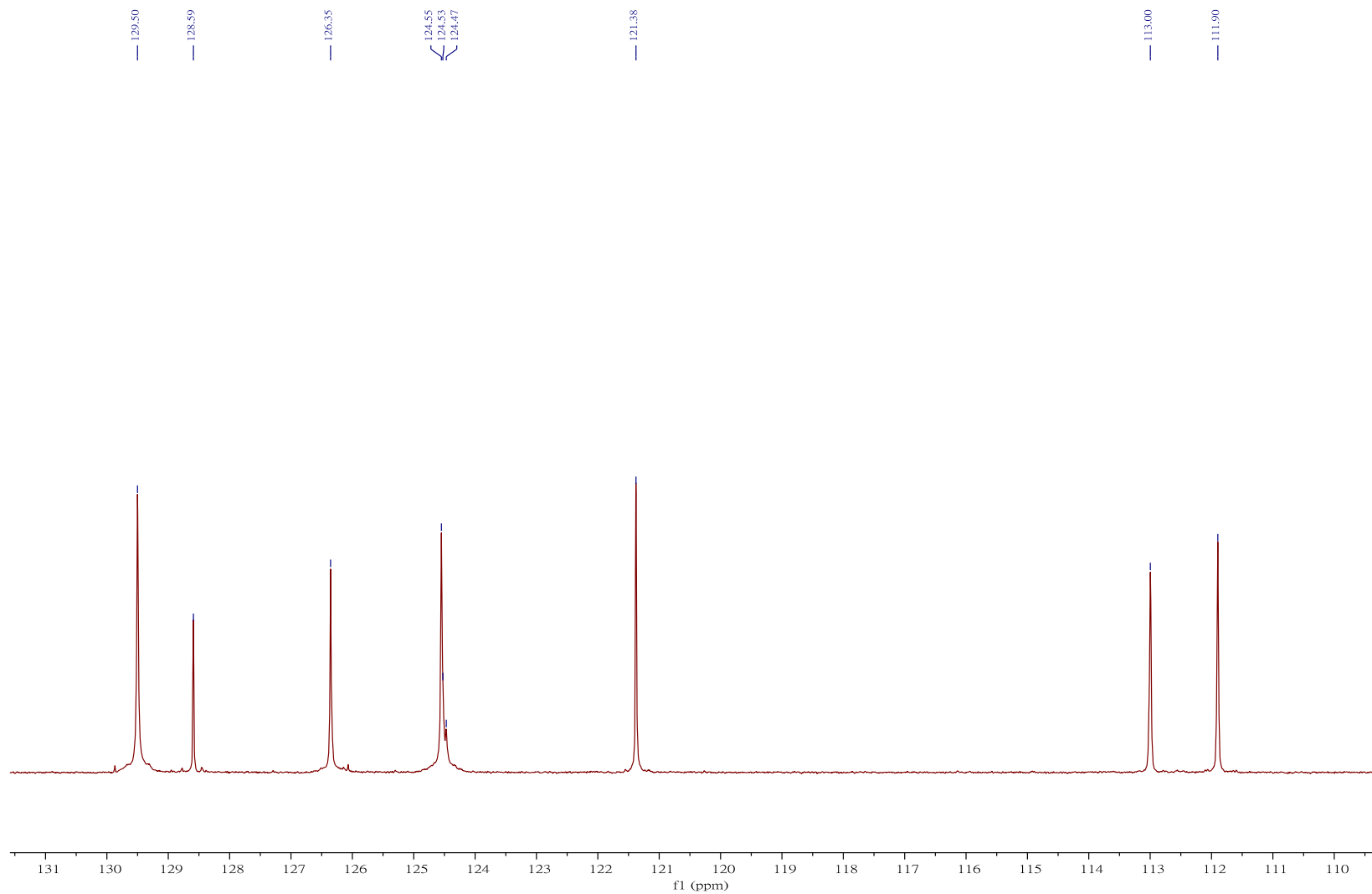
Expansion of ^1H NMR Spectrum (400 MHz) of compound **3h** in acetone- d_6



Expansion of ¹H NMR Spectrum (400 MHz) of compound **3h** in acetone-*d*₆



¹³C NMR Spectrum (101 MHz) of compound **3h** in acetone-*d*₆

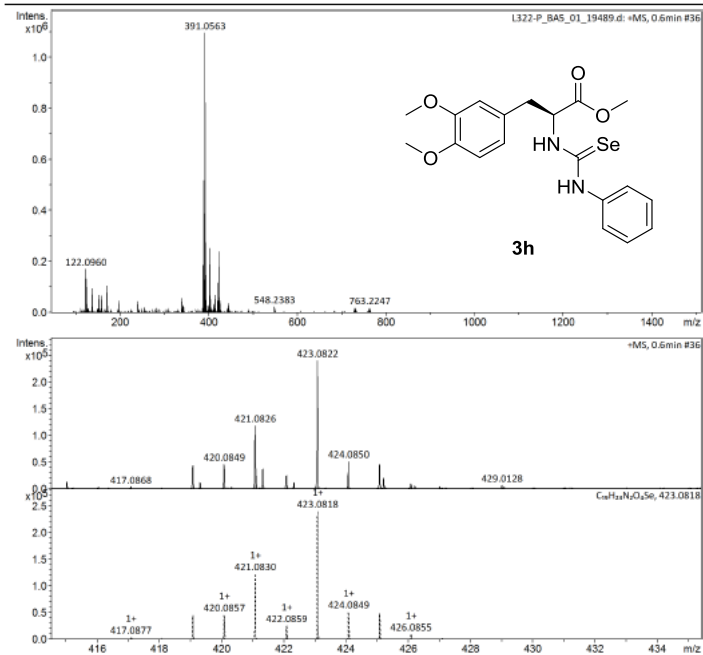


Expansion of ¹³C NMR Spectrum (101 MHz) of compound **3h** in acetone-*d*₆

Display Report

Analysis Info		Acquisition Date	8/17/2018 12:14:25 PM
Analysis Name	D:\Data\NCTU SERVICE\Data\2018\20180817-2\L322-P_BA5_01_19489.d	Operator	NCTU
Method	Small molecule.m	Instrument	Impact HD
Sample Name	L322-P		1819896.00164
Comment			

Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
Focus	Active	Set Capillary	4500 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1500 m/z	Set Charging Voltage	2000 V
		Set Corona	0 nA
		Set Nebulizer	1.0 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	6.0 l/min
		Set Divert Valve	Waste
		Set APCI Heater	0 °C



HRMS of compound **3h**

CSM: Linda Series: 0169 Report Name: modified System: Sys 1

Chromaster System Manager Report

Analyzed Date and Time: 2018/09/17 09:15 上午
Reported Date and Time: 2018/09/17 10:21:16 上午

Processed Date and Time: 2018/09/17 10:20 上午

Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0169\

Processing Method: L322_ee

System (acquisition): Sys 1

Series: 0169

Application(data): Linda

Vial Number: 1

Sample Name: UNKNOWN001

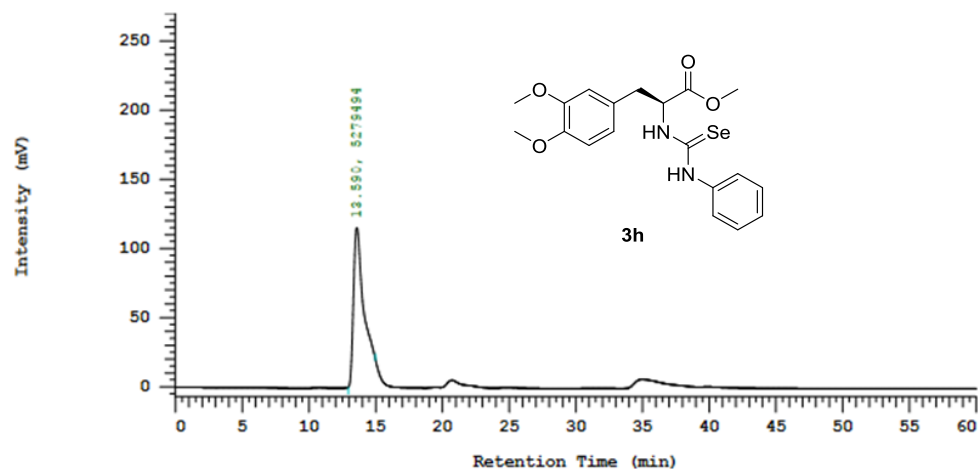
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 10.0 ul

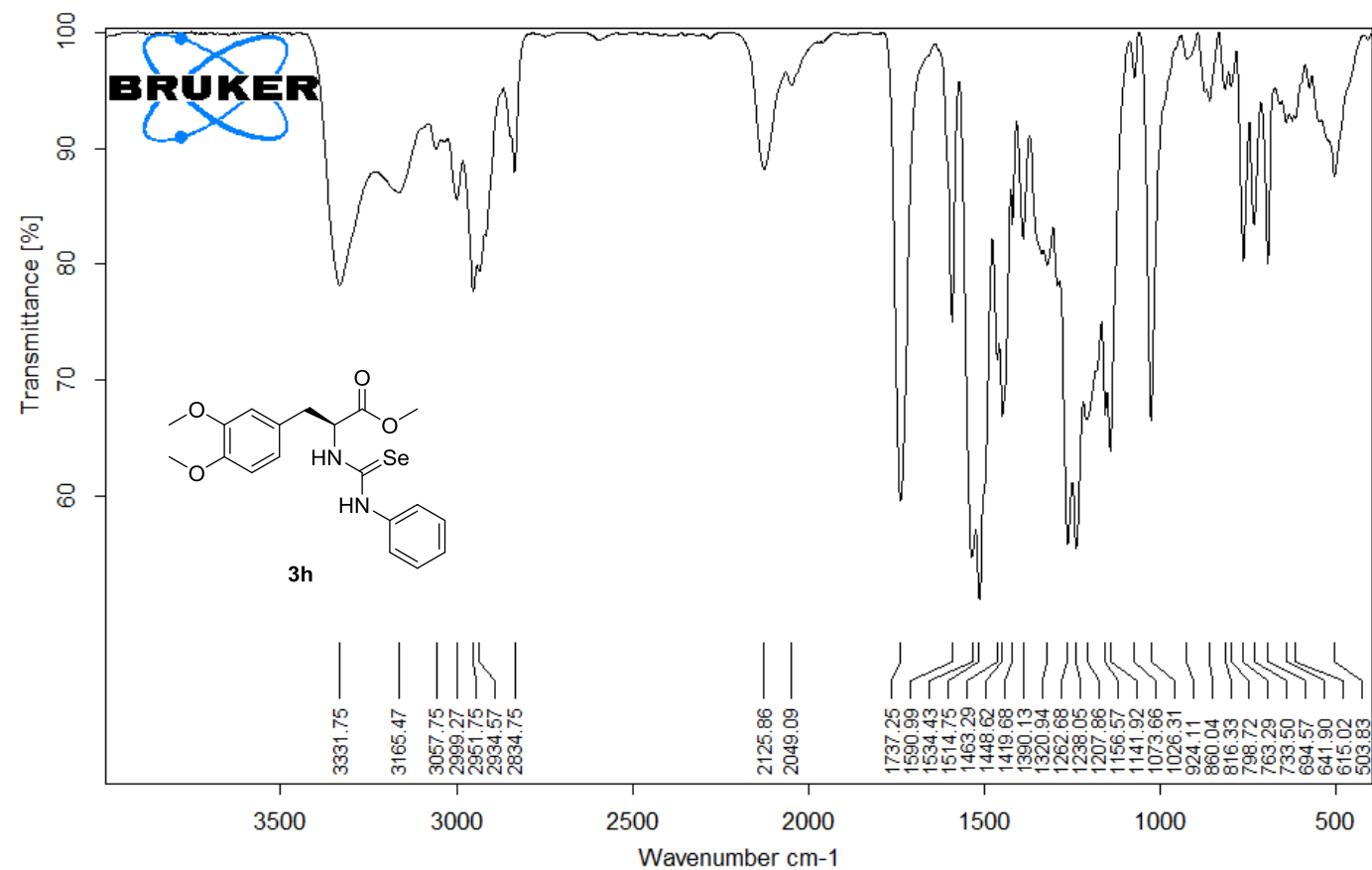
Sample Description:

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound **3h**



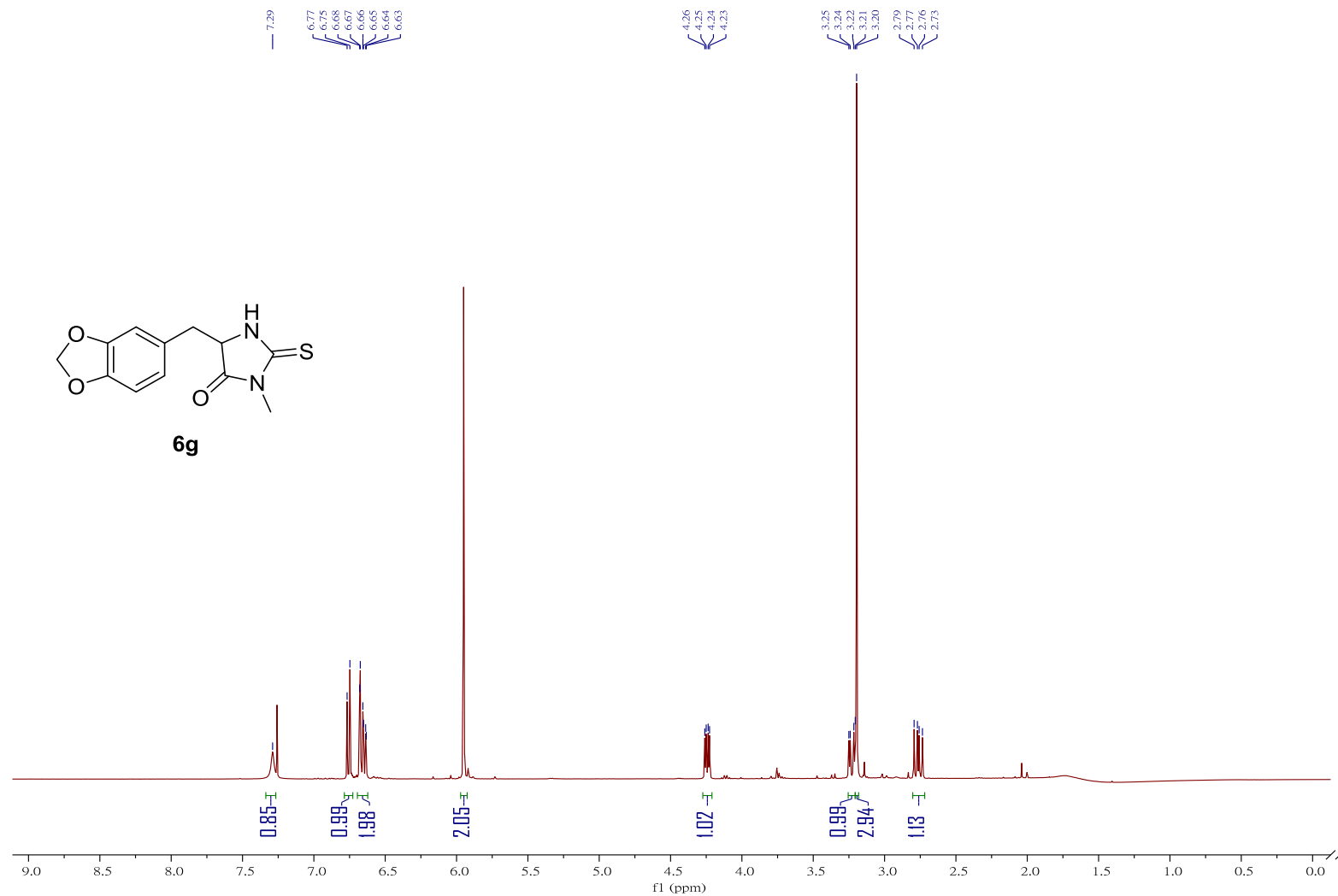
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L322.0

MIR_TR_DTGS_L322

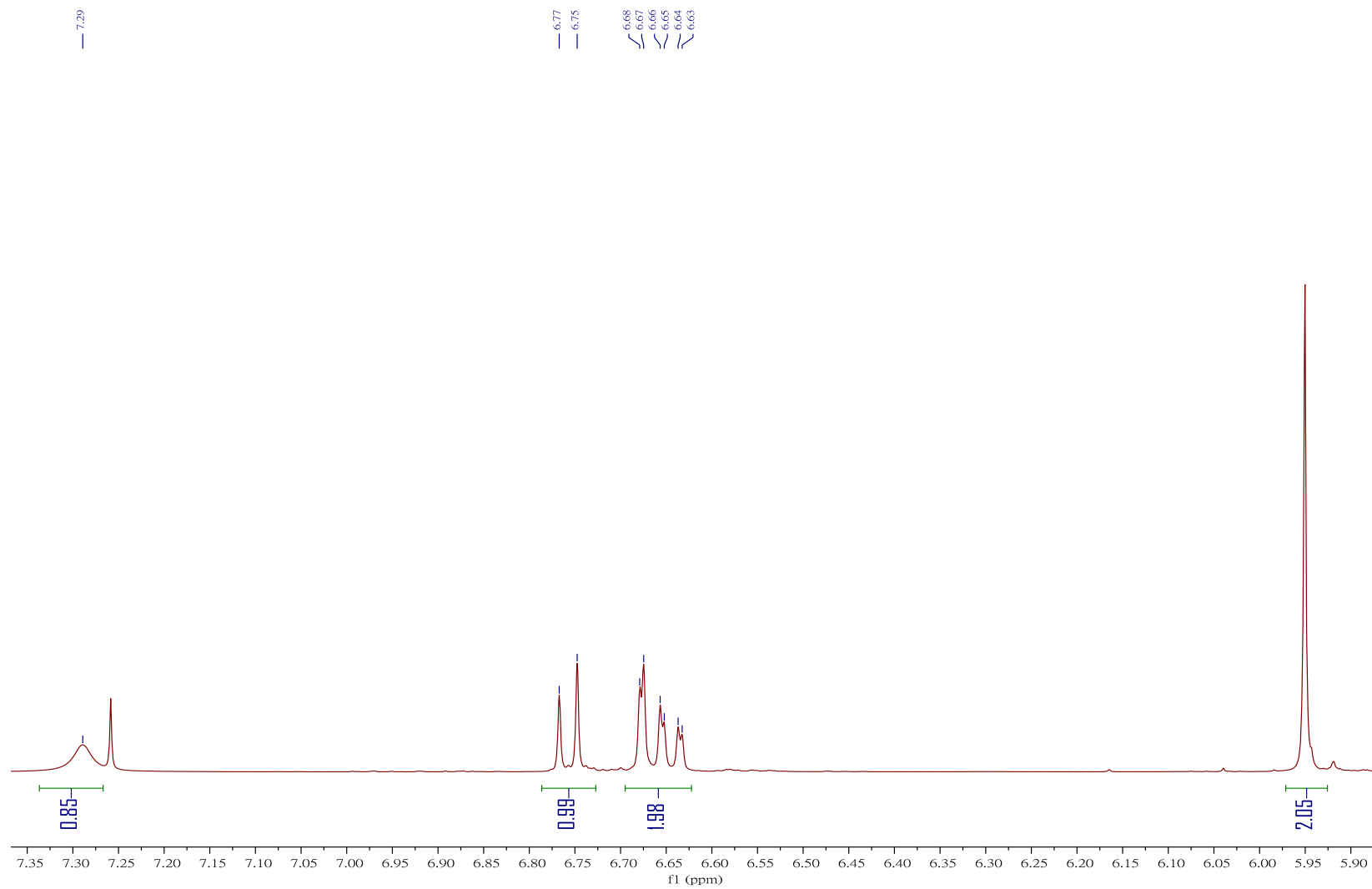
Instrument type and / or accessory

9/4/2018

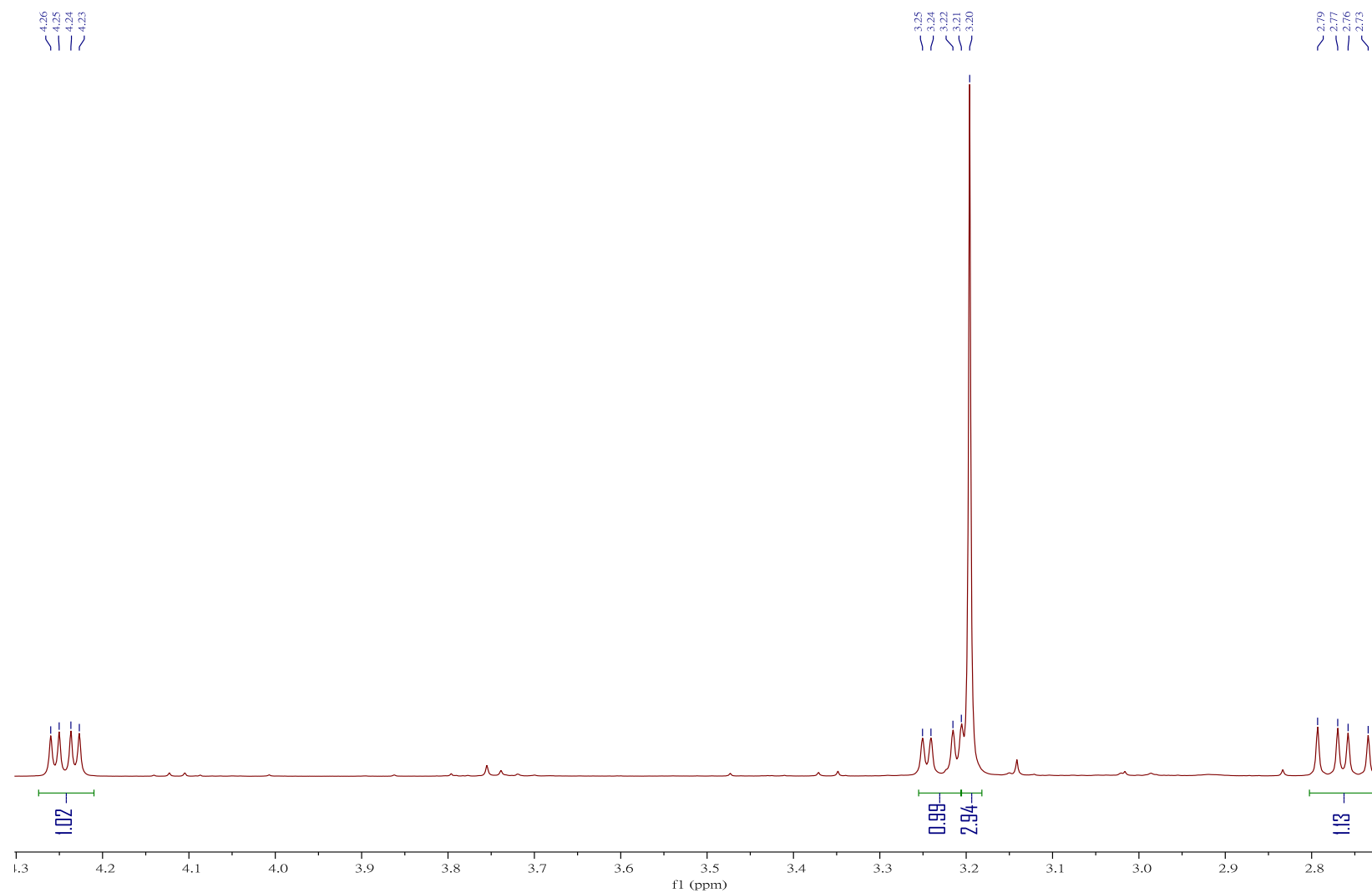
FT-IR Spectrum of compound **3h**



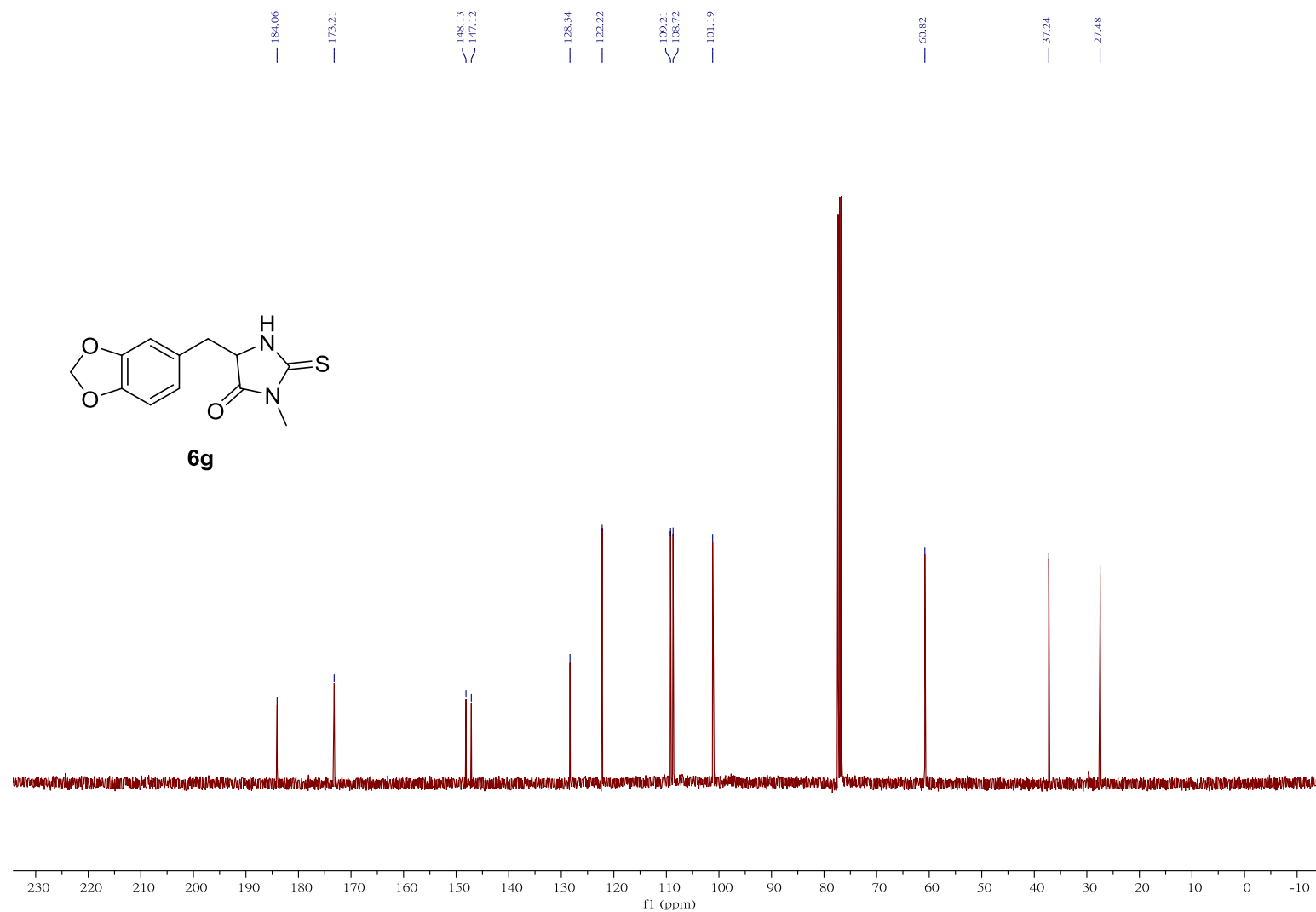
^1H NMR Spectrum (400 MHz) of compound **6g** in CDCl_3



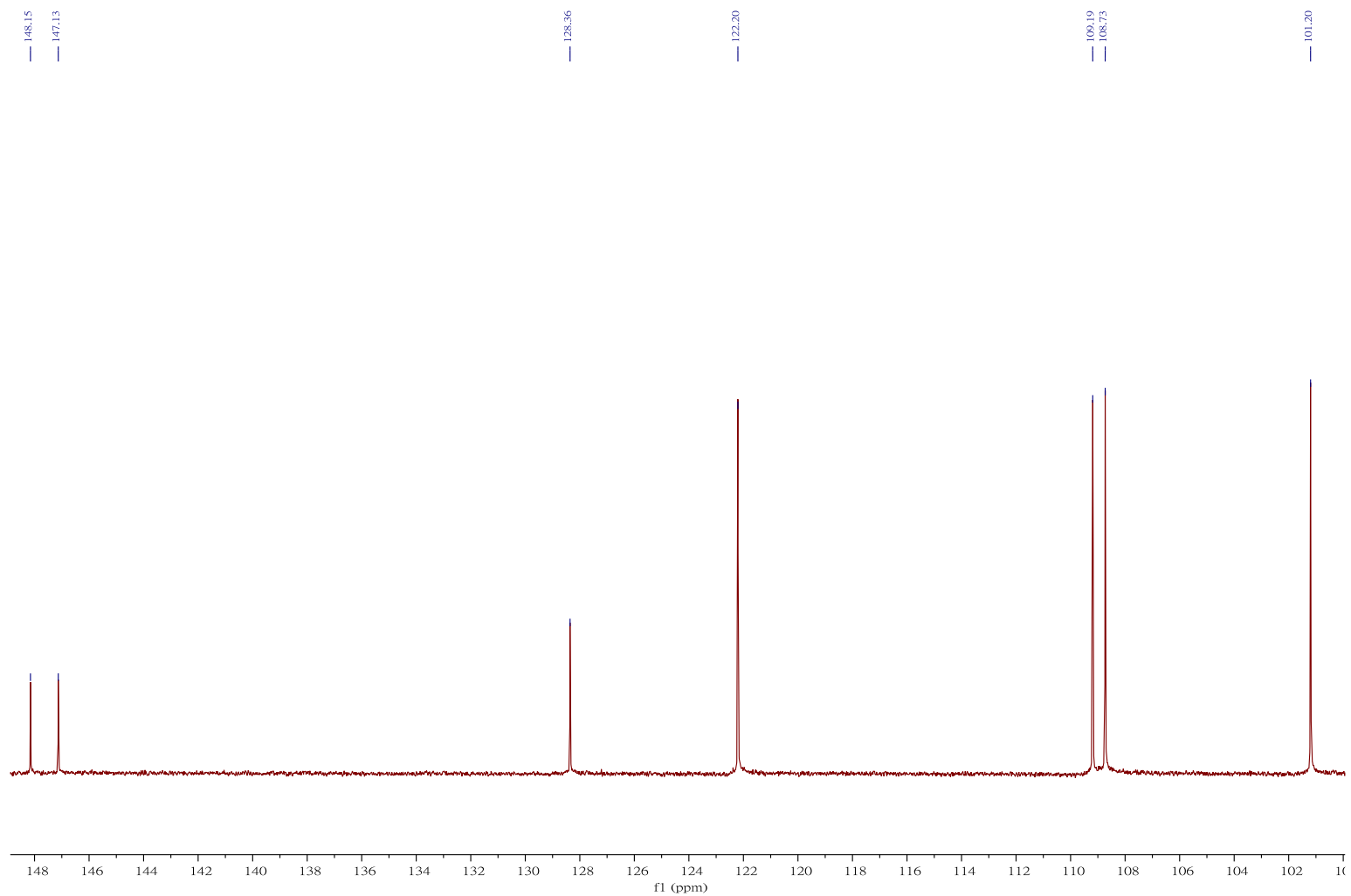
Expansion of ¹H NMR Spectrum (400 MHz) of compound **6g** in CDCl₃



Expansion of ¹H NMR Spectrum (400 MHz) of compound **6g** in CDCl₃



^{13}C NMR Spectrum (101 MHz) of compound **6g** in CDCl_3



Expansion of ¹³C NMR Spectrum (101 MHz) of compound **6g** in CDCl₃

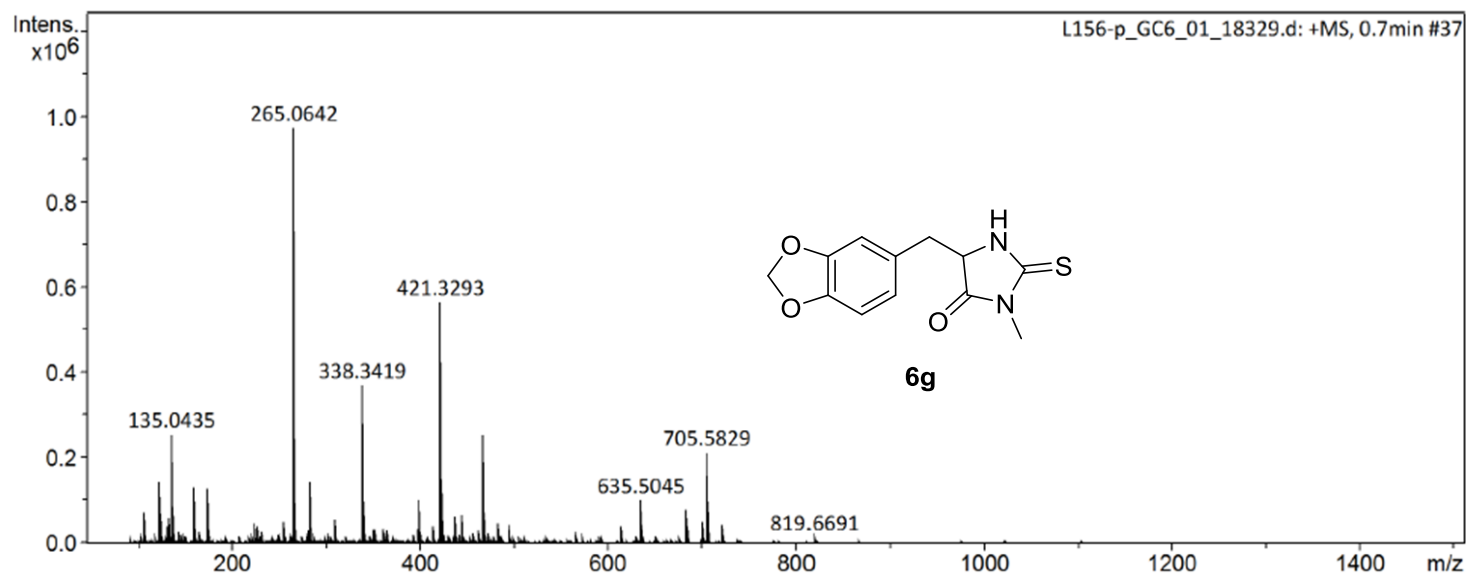
Display Report

Analysis Info

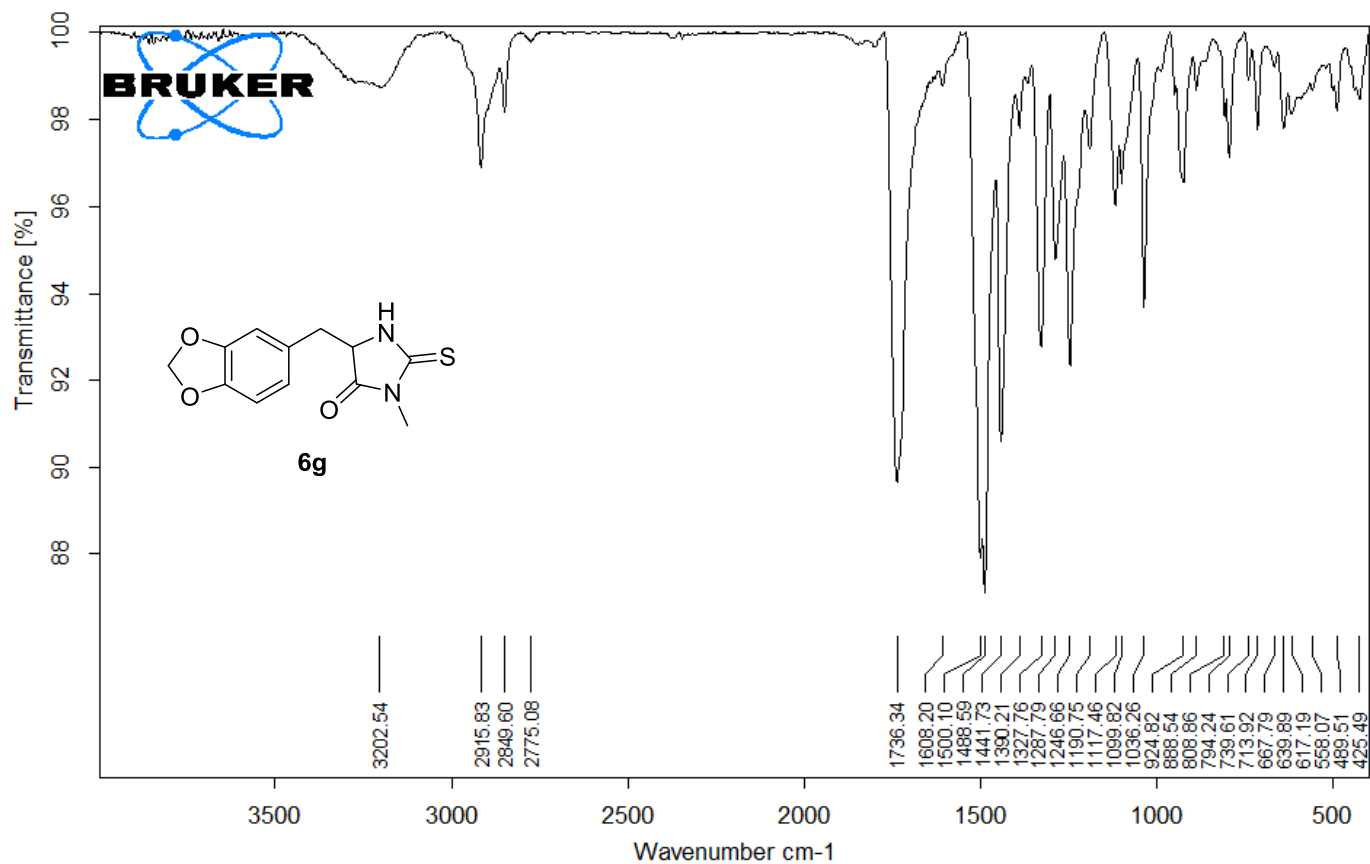
Analysis Name	D:\Data\inctu service\data\2018\20180518\L156-p_GC6_01_18329.d	Acquisition Date	5/18/2018 2:55:56 PM	
Method	Small molecule.m	Operator	NCTU	
Sample Name	L156-p	Instrument	impact HD	1819696.00164
Comment				

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



HRMS of compound **6g**



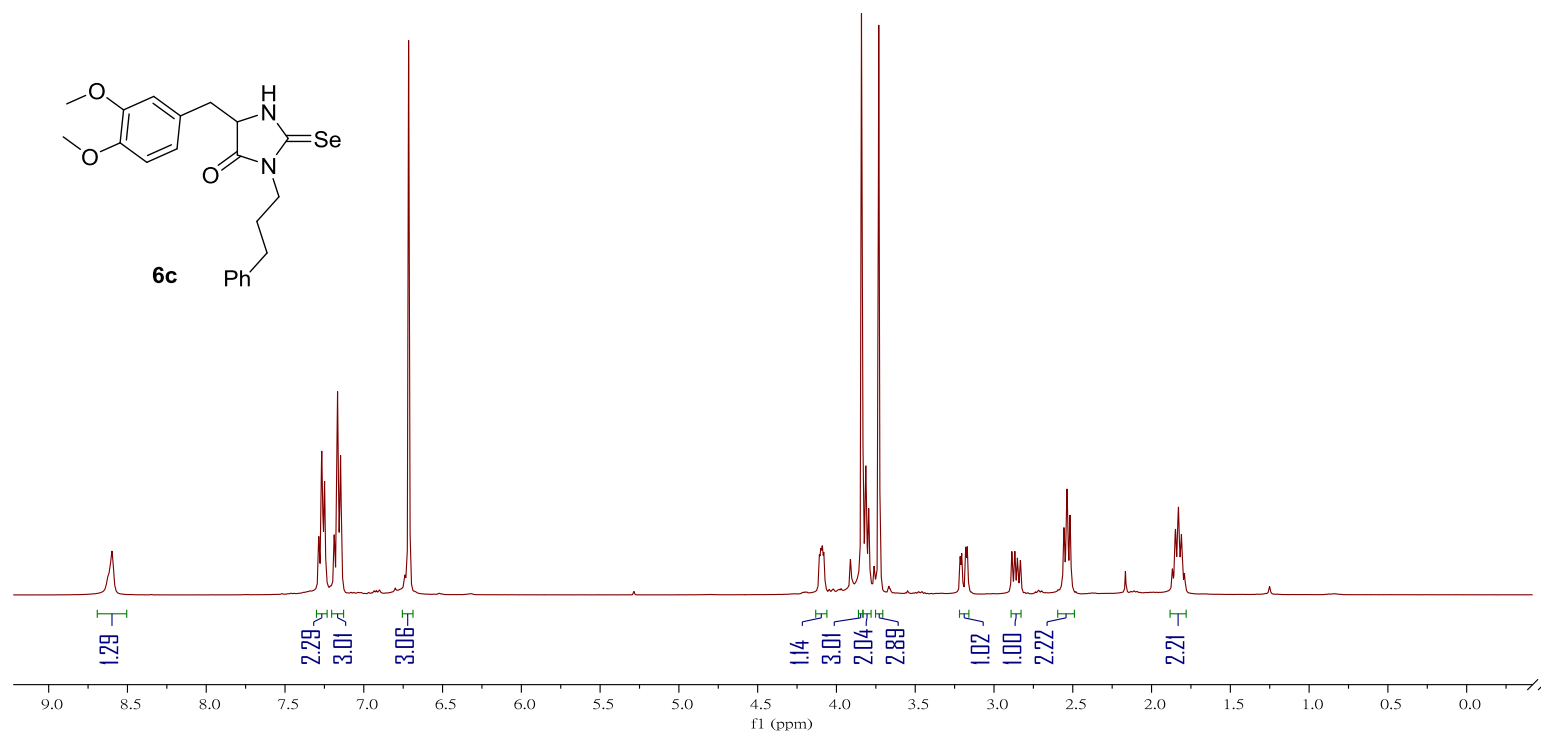
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MIR_TR_DTGS_L156

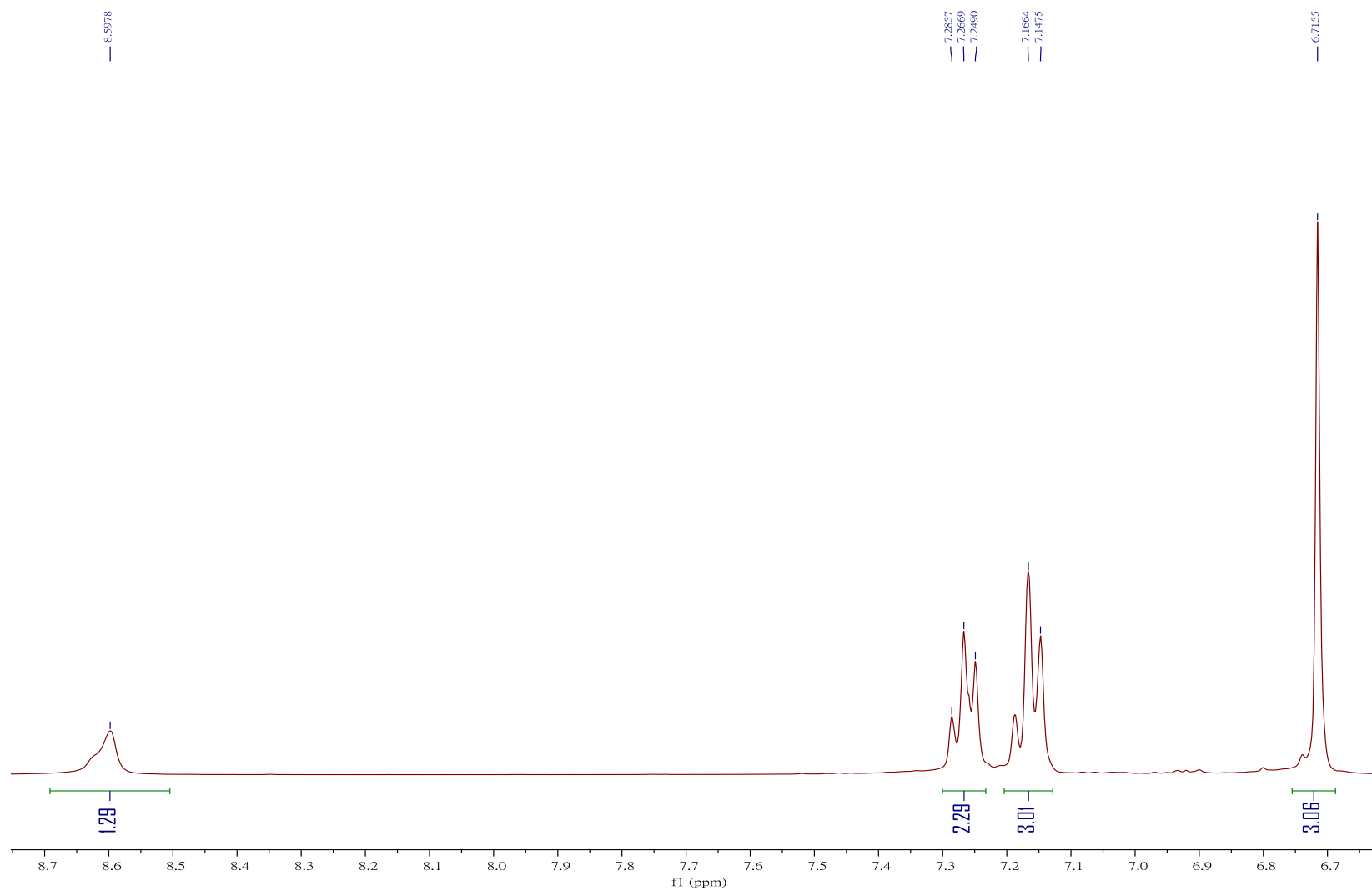
Instrument type and / or accessory

9/4/2018

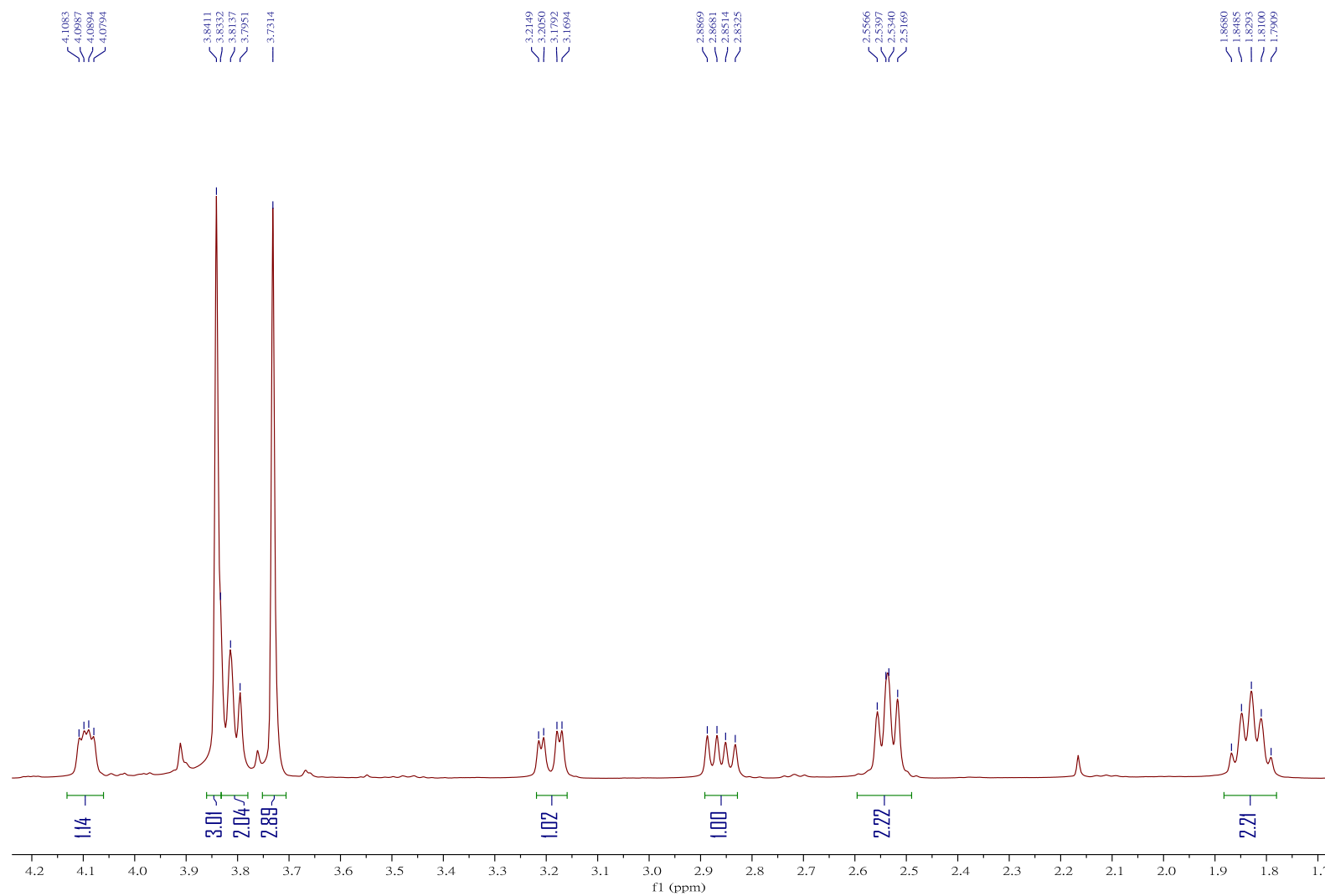
FT-IR Spectrum of compound **6g**



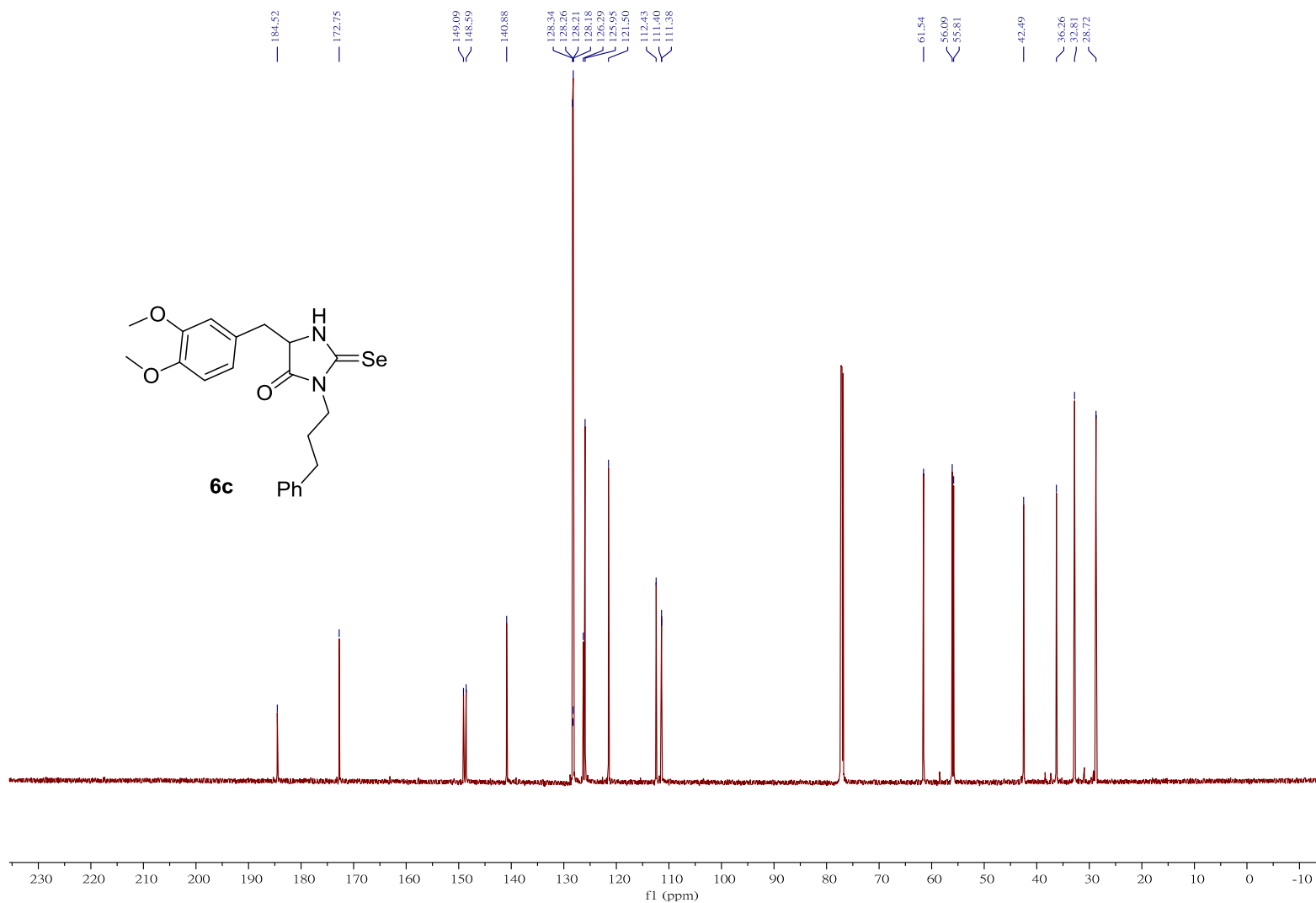
¹H NMR Spectrum (400 MHz) of compound **6c** in CDCl₃



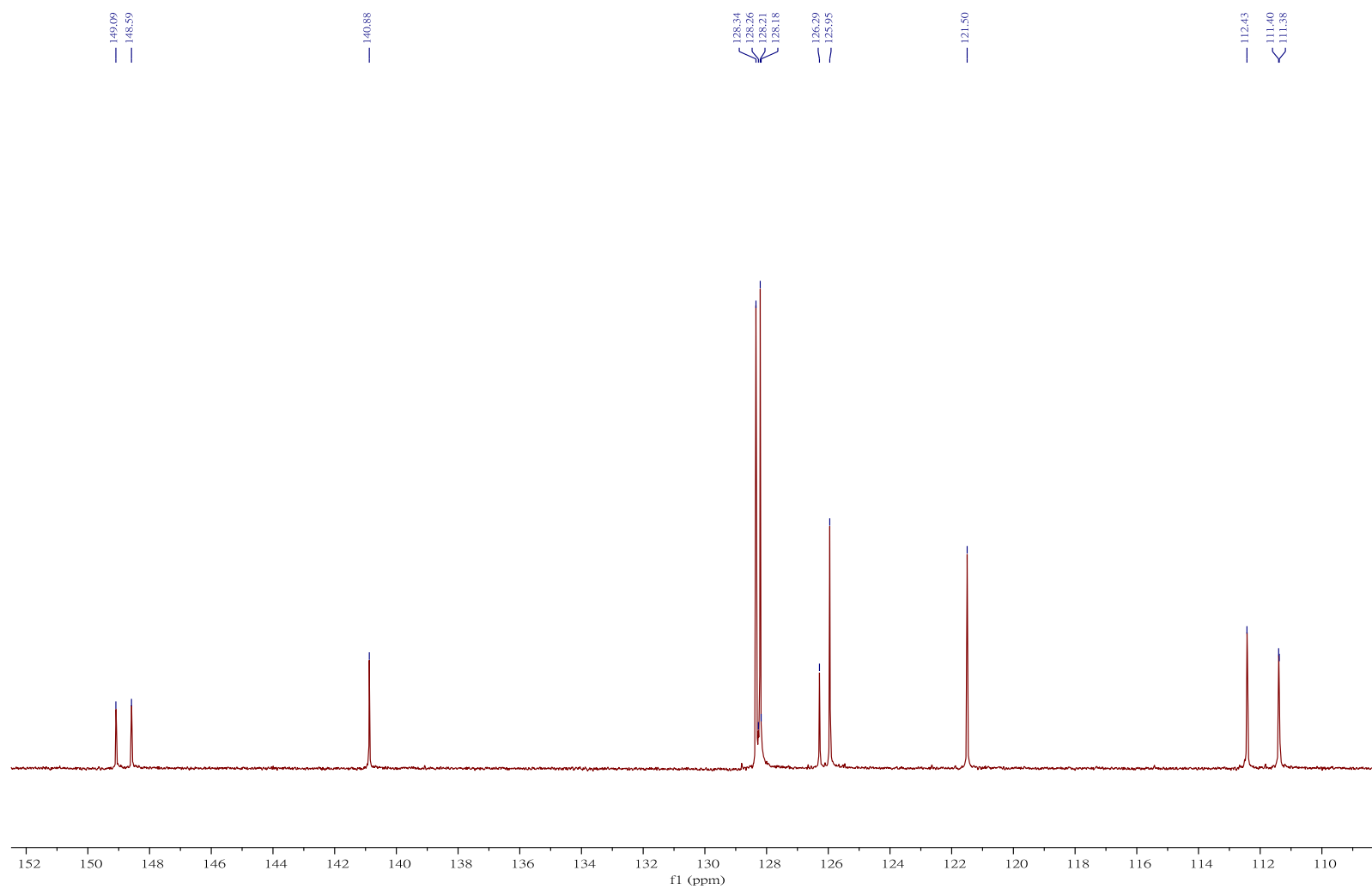
Expansion of ^1H NMR Spectrum (400 MHz) of compound **6c** in CDCl_3



Expansion of ^1H NMR Spectrum (400 MHz) of compound **6c** in CDCl_3



^{13}C NMR Spectrum (101 MHz) of compound **6c** in CDCl_3

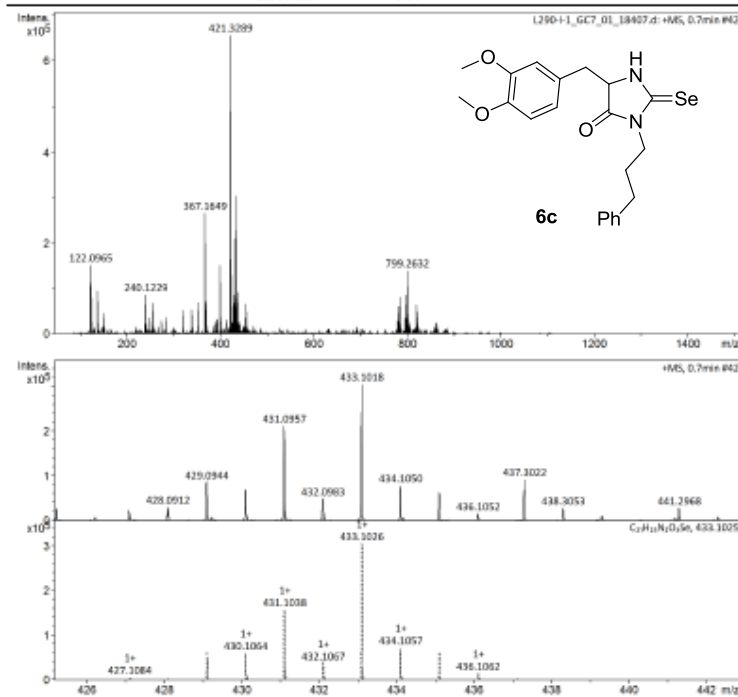


Expansion of ¹³C NMR Spectrum (101 MHz) of compound **6c** in CDCl₃

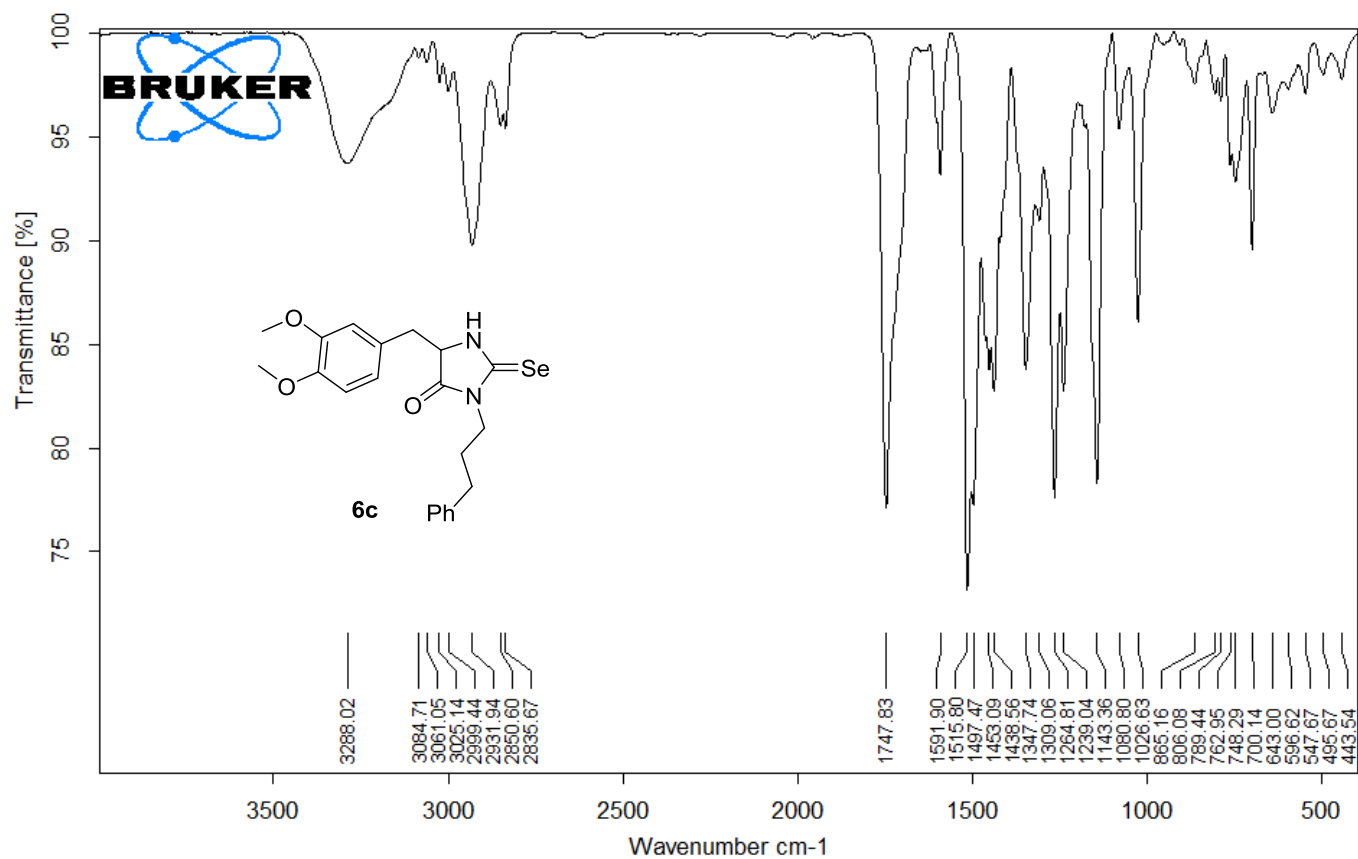
Display Report

Analysis Info		Acquisition Date	5/25/2018 12:07:12 PM
Analysis Name	H:\20181-6\20180525\L290-I-1_GC7_01_18407.d	Operator	NCTU
Method	Small molecule.m	Instrument	Impact HD
Sample Name	L290-I-1		1819696.00164
Comment			

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



HRMS of compound **6c**



D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L154.0

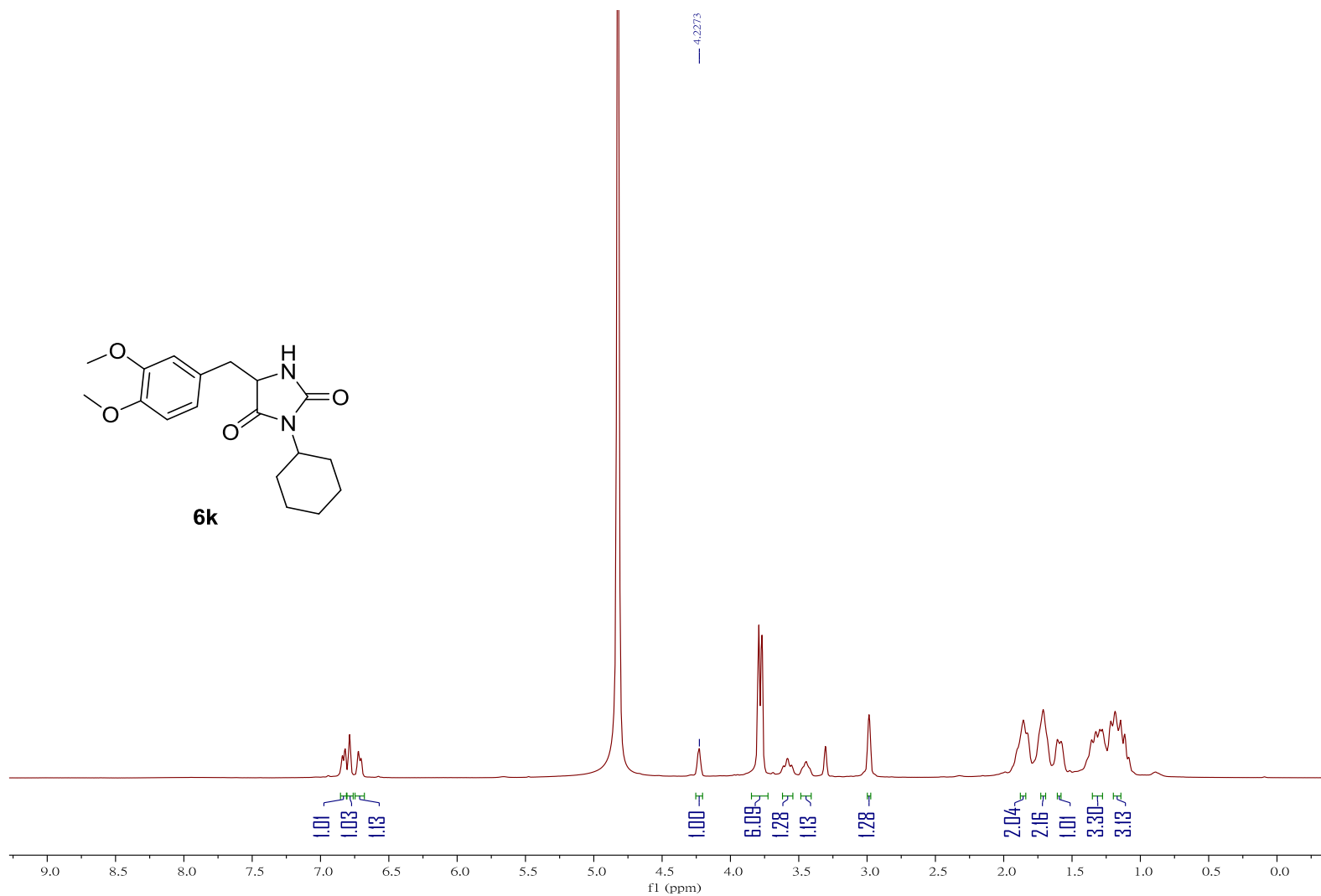
MIR_TR_DTGS_L154

Instrument type and / or accessory

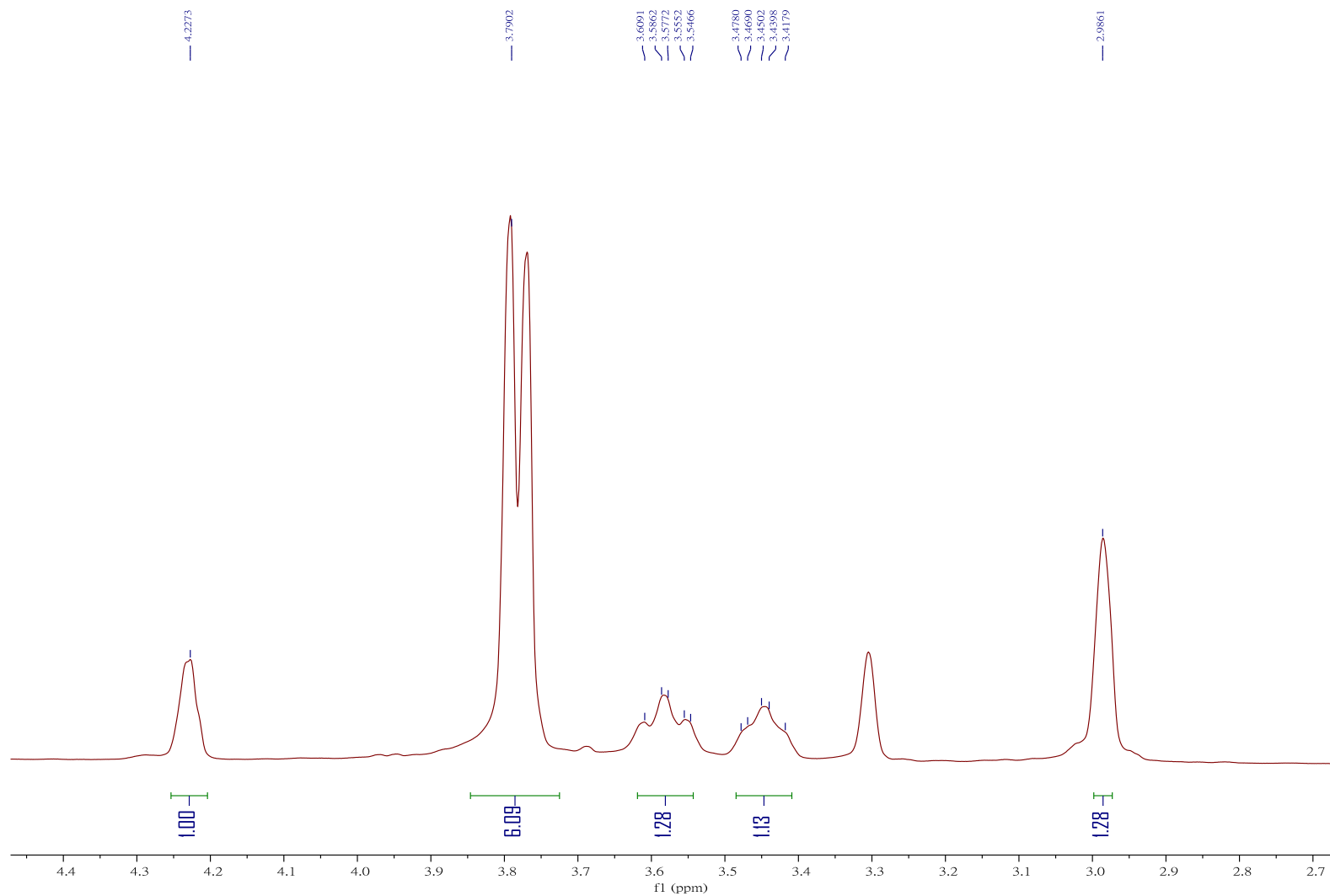
9/4/2018

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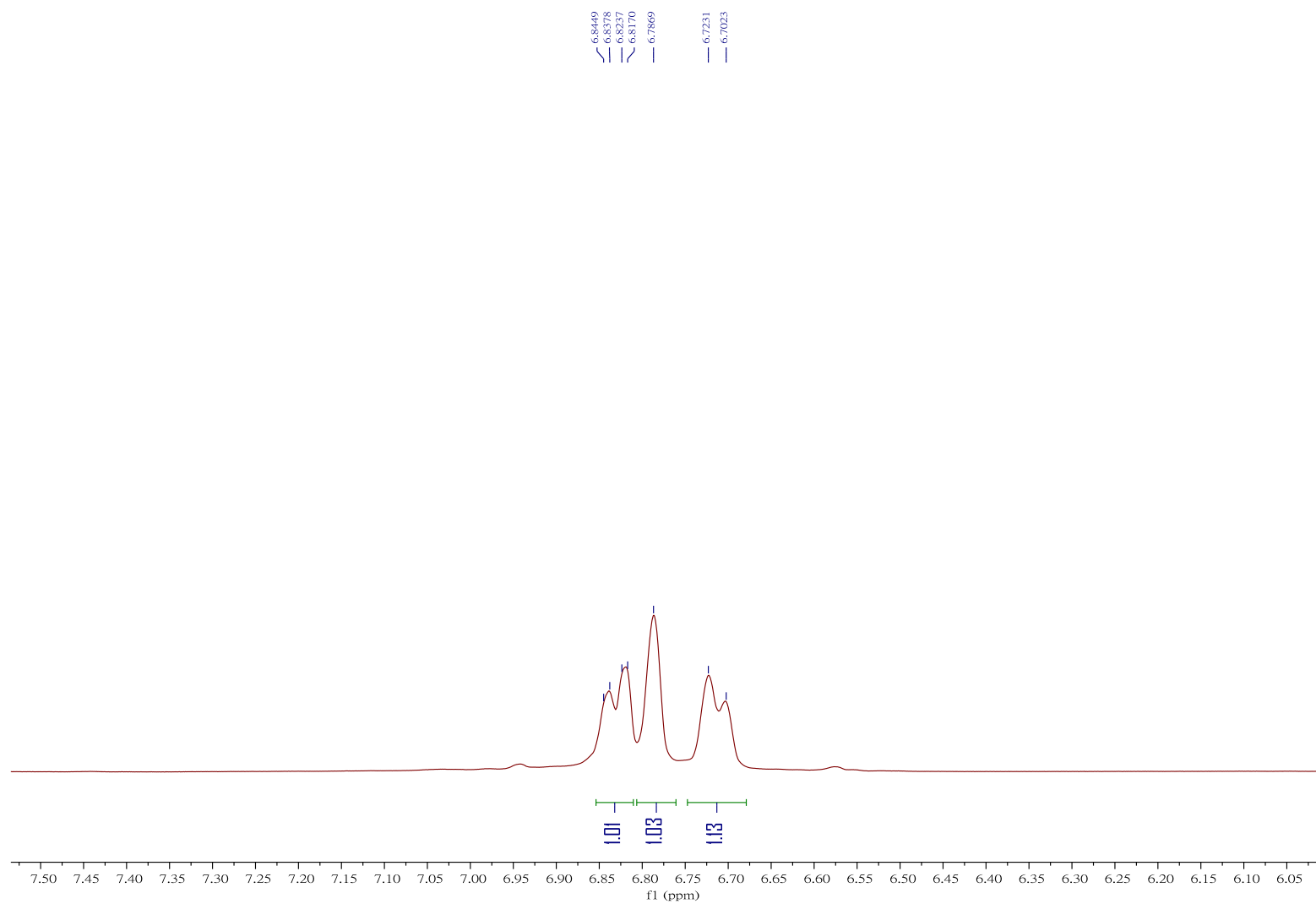
FT-IR Spectrum of compound **6c**



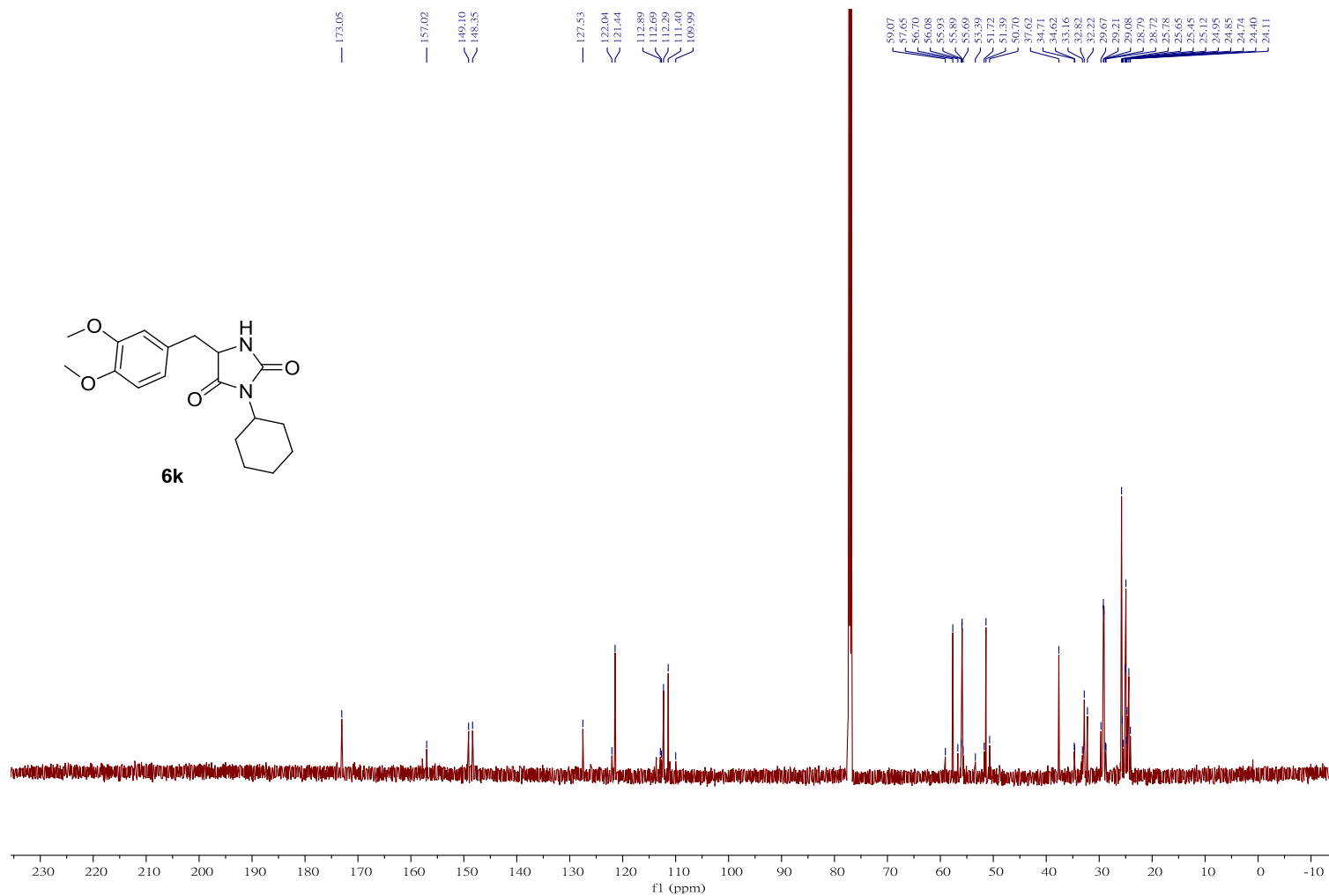
¹H NMR Spectrum (400 MHz) of compound **6k** in CD₃OD

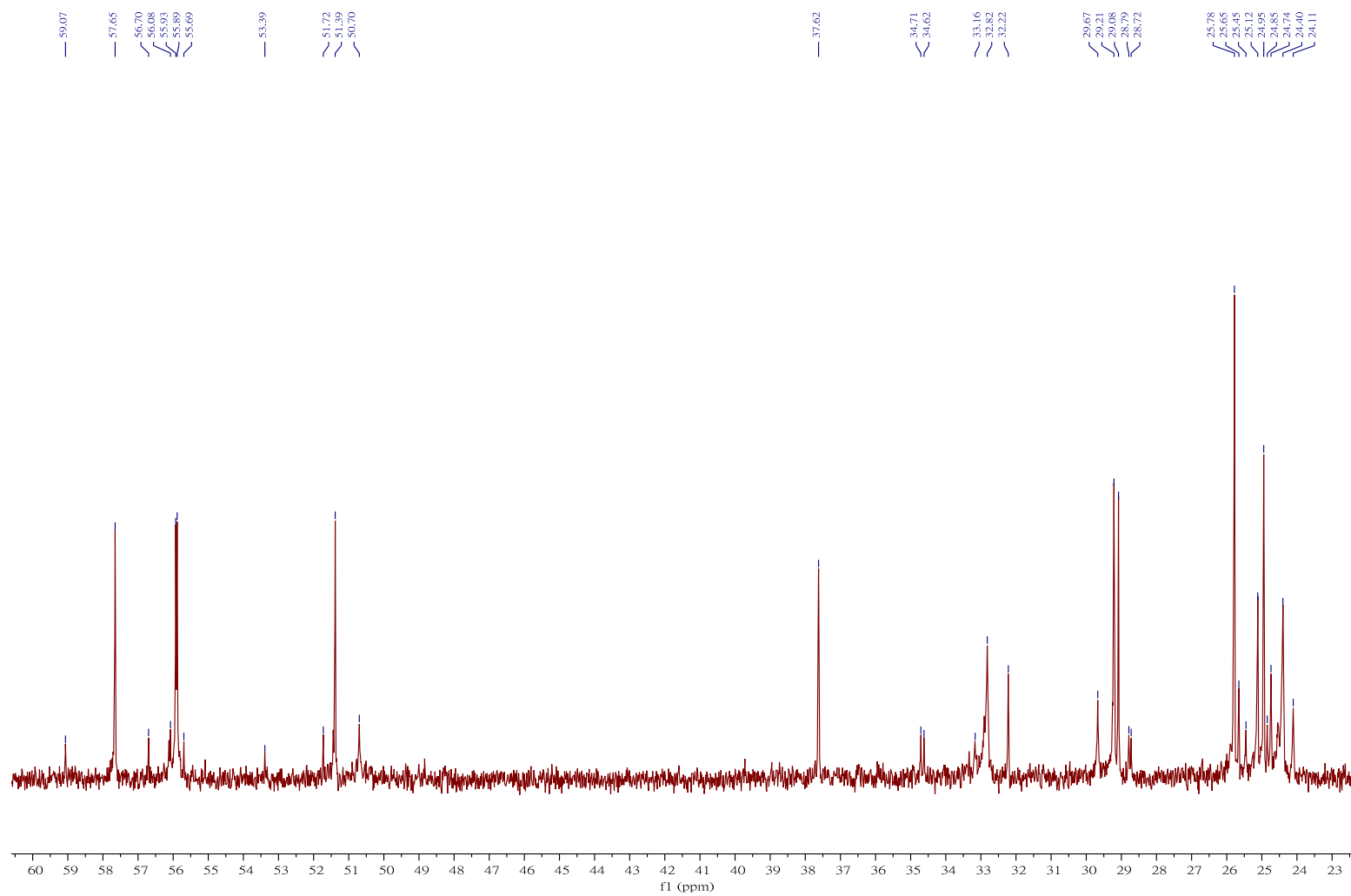


Expansion of ^1H NMR Spectrum (400 MHz) of compound **6k** in CD_3OD



Expansion of ^1H NMR Spectrum (400 MHz) of compound **6k** in CD_3OD





Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **6k** in CDCl_3

Display Report

Analysis Info

Analysis Name D:\Data\ntu service\data\2018\20180821\L298-I_GB6_01_19574.d

Method Small molecule.m

Sample Name L298-I

Comment

Acquisition Date 8/21/2018 2:31:27 PM

Operator NCTU

Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type

ESI

Ion Polarity

Positive

Set Nebulizer

1.0 Bar

Focus

Active

Set Capillary

4500 V

Set Dry Heater

200 °C

Scan Begin

50 m/z

Set End Plate Offset

-500 V

Set Dry Gas

6.0 l/min

Scan End

1500 m/z

Set Charging Voltage

2000 V

Set Divert Valve

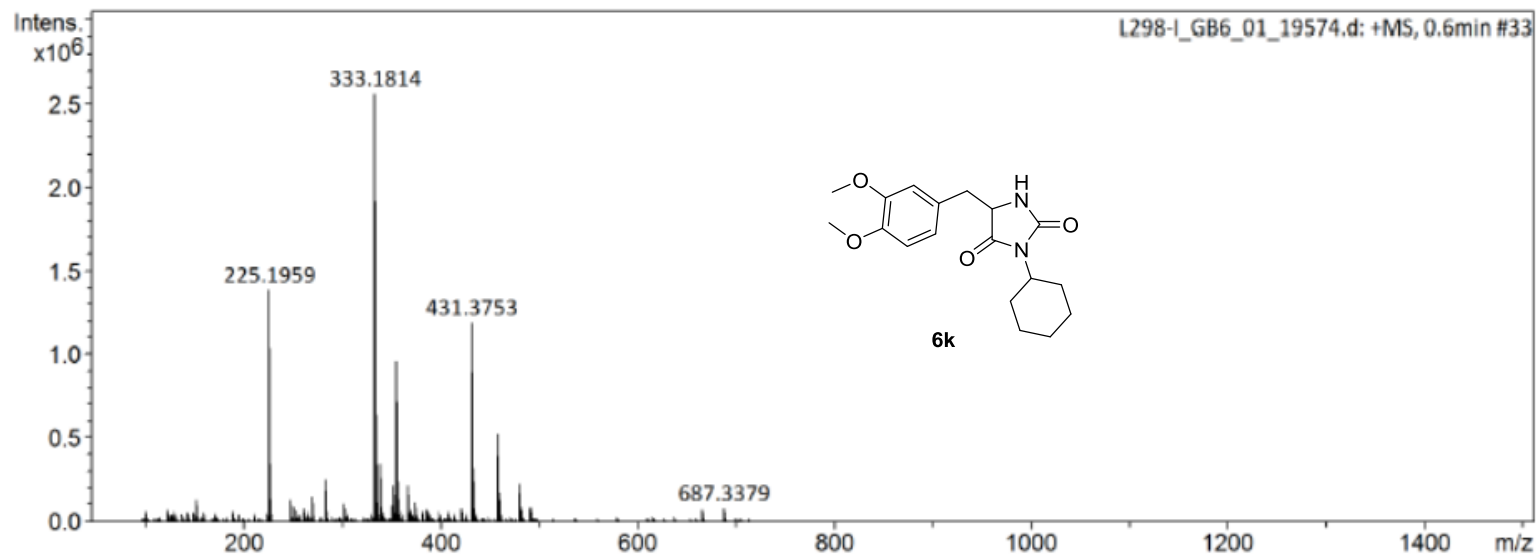
Waste

Set Corona

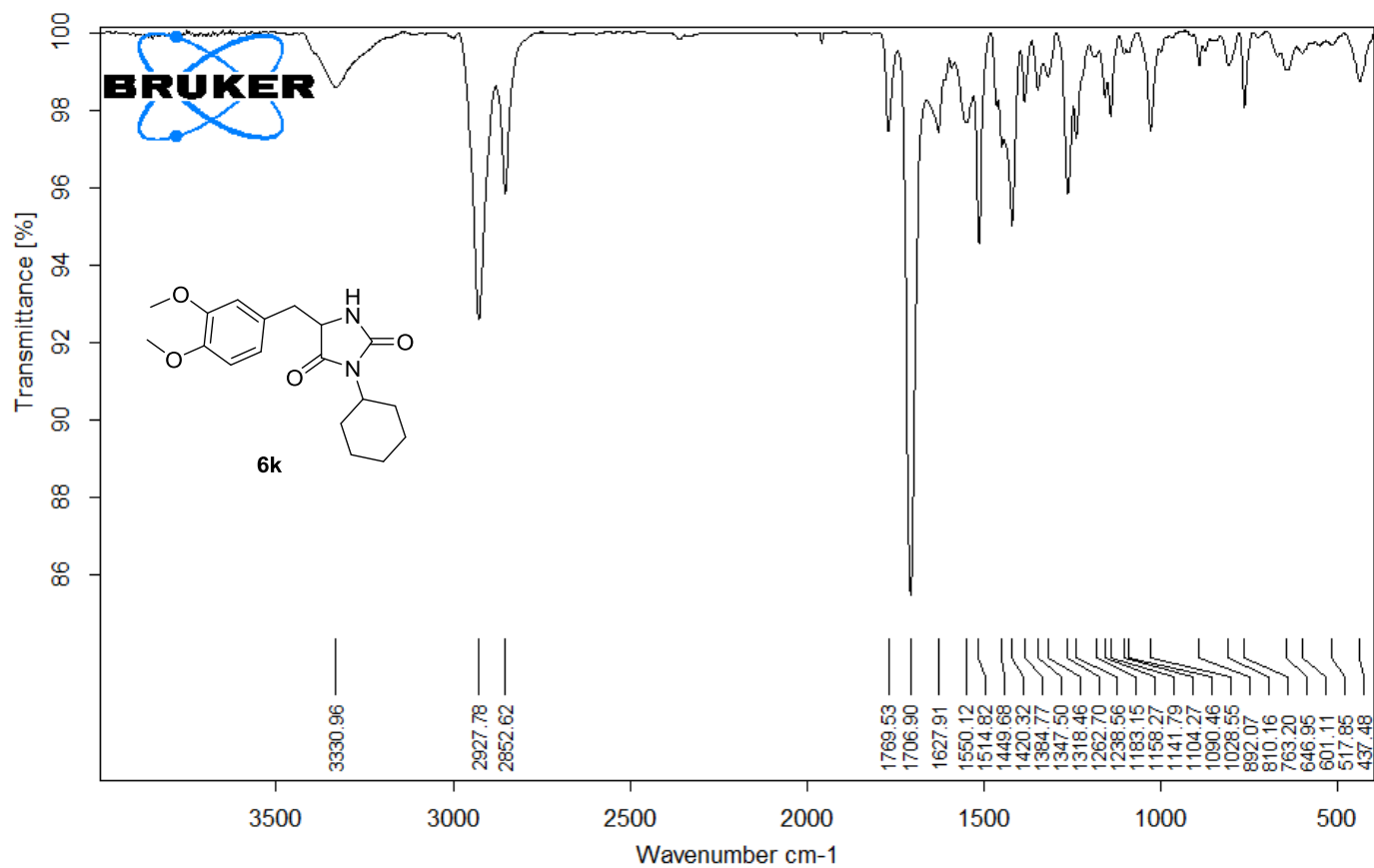
0 nA

Set APCI Heater

0 °C



HRMS of compound 6k



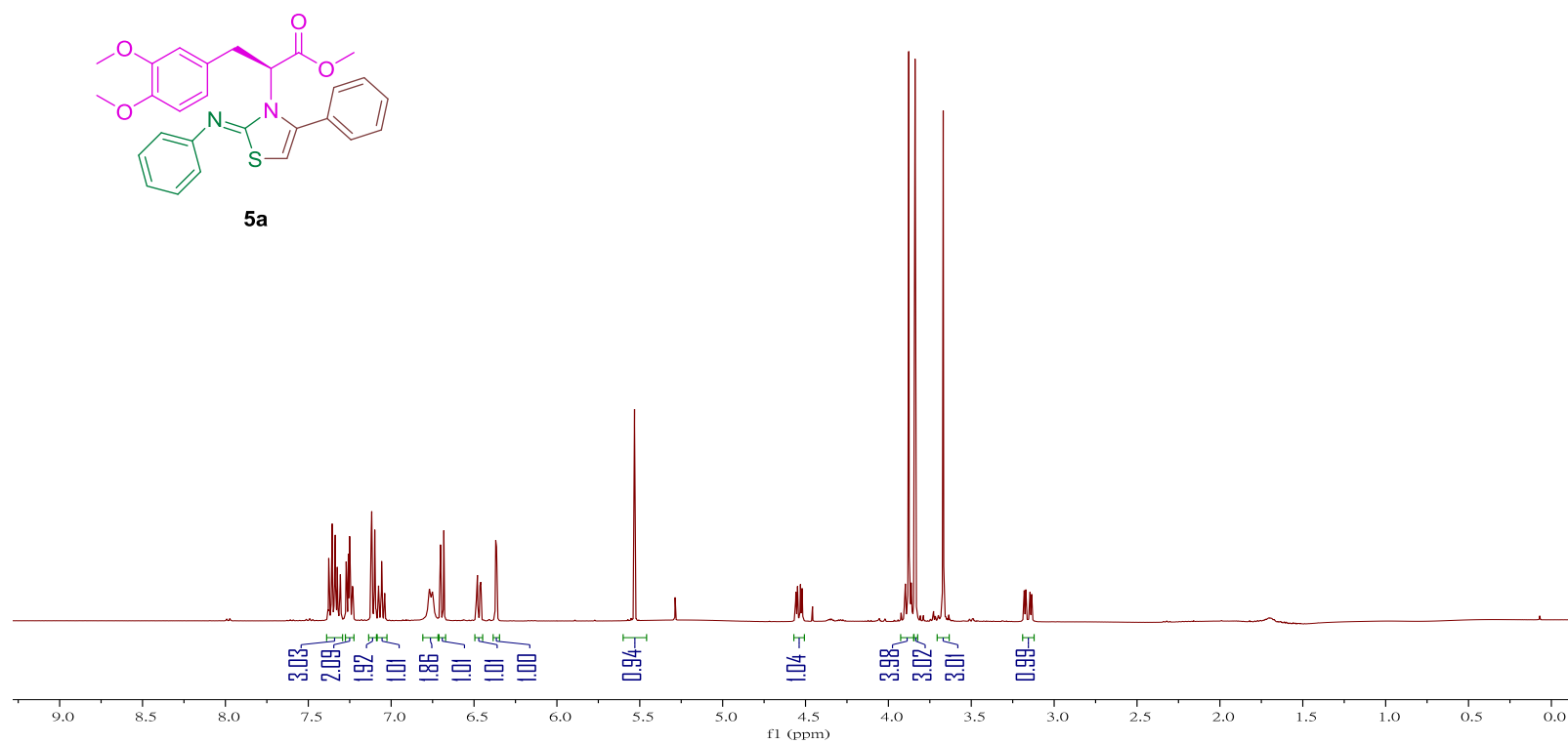
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MIR_TR_DTGS_L298-I

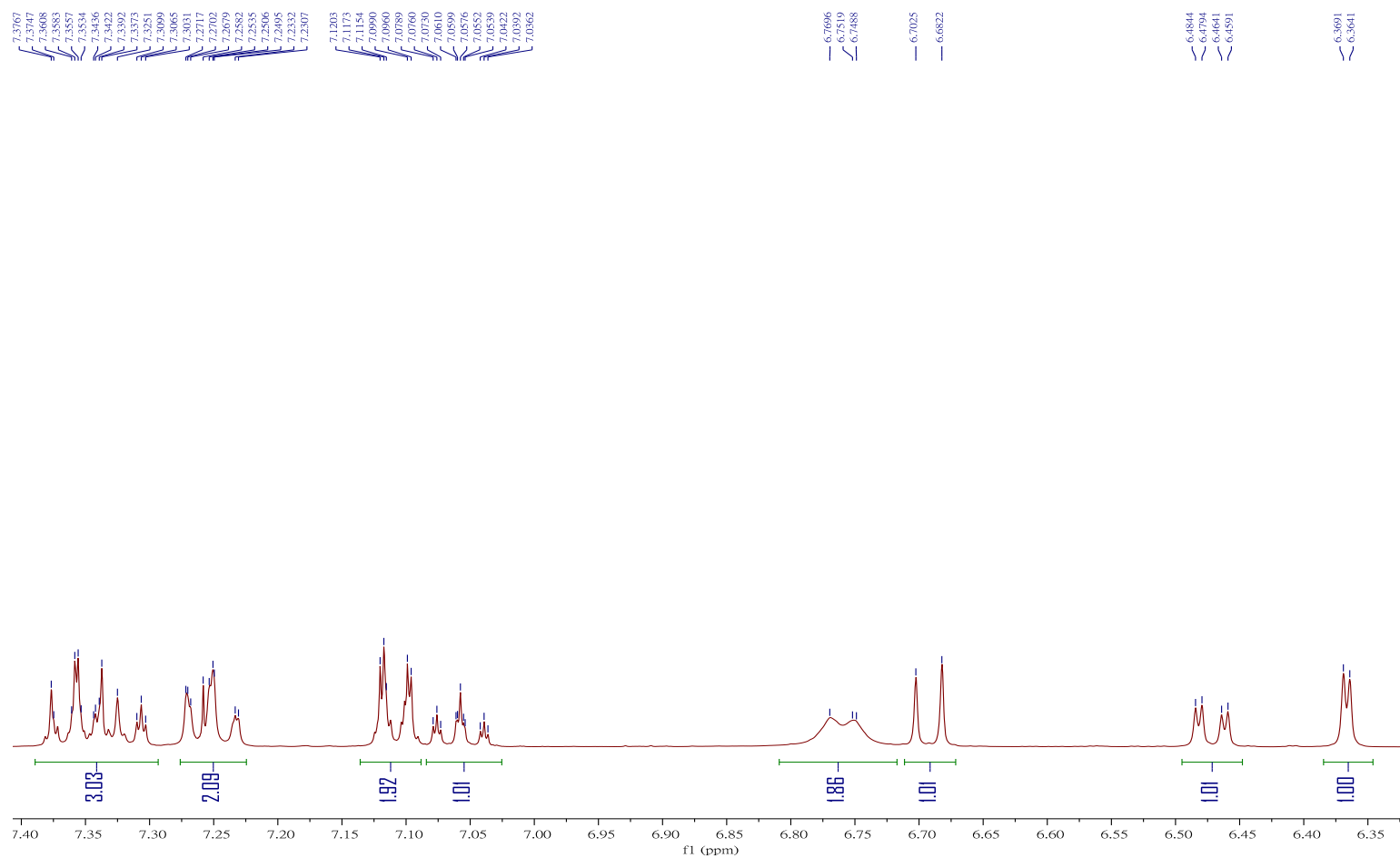
Instrument type and / or accessory

9/4/2018

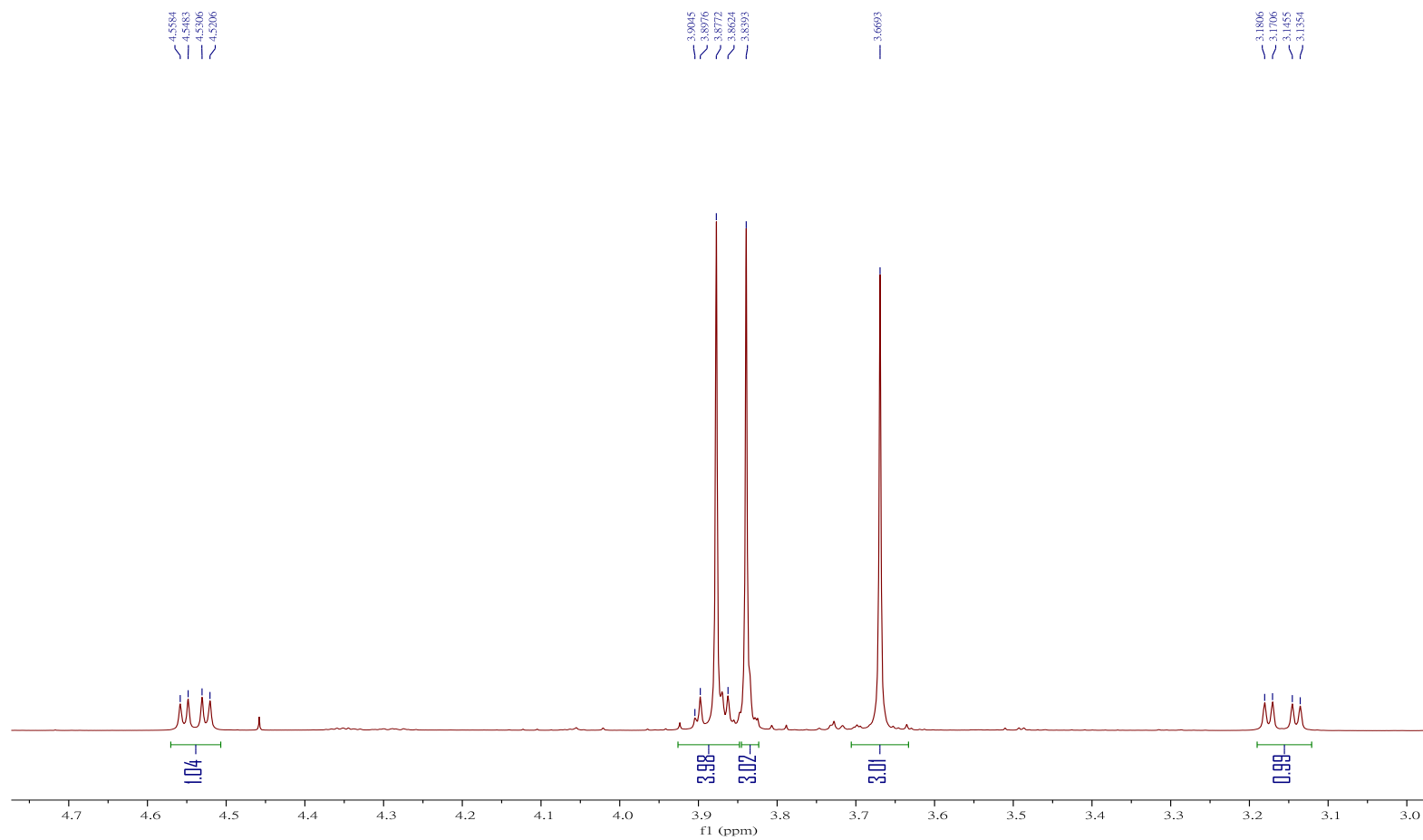
FT-IR Spectrum of compound **6k**



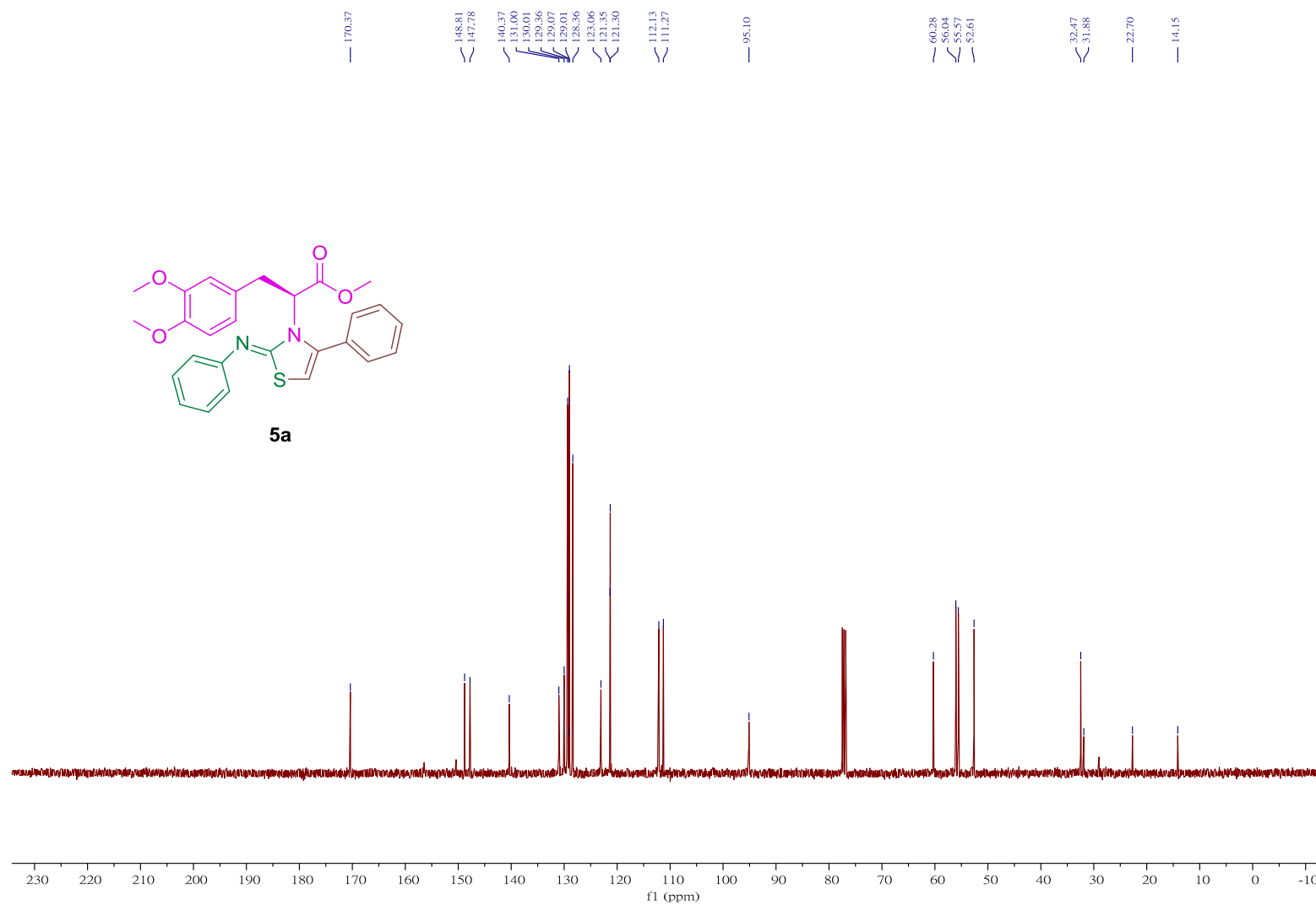
^1H NMR Spectrum (400 MHz) of compound **5a** in CDCl_3

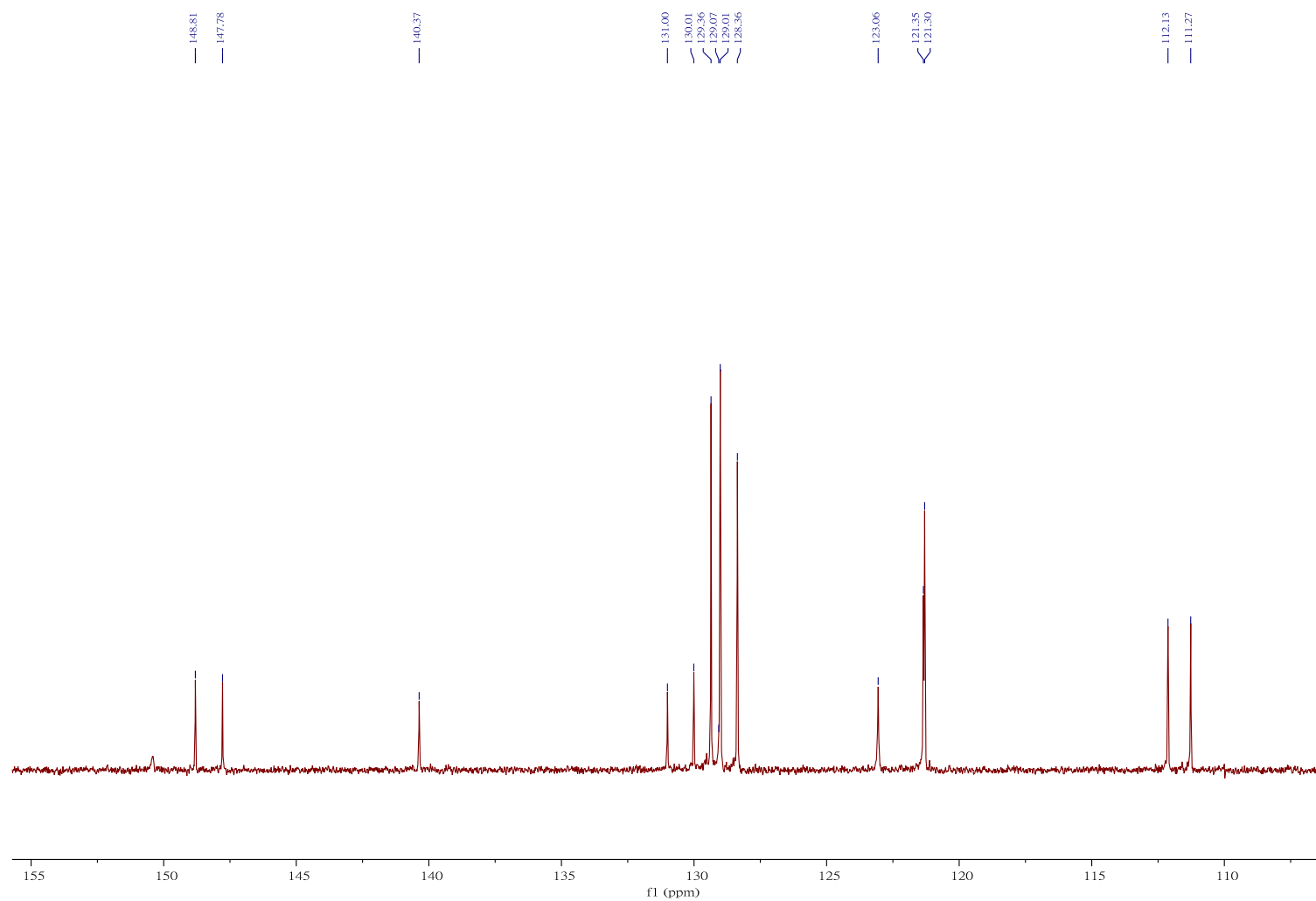


Expansion of ^1H NMR Spectrum (400 MHz) of compound **5a** in CDCl_3

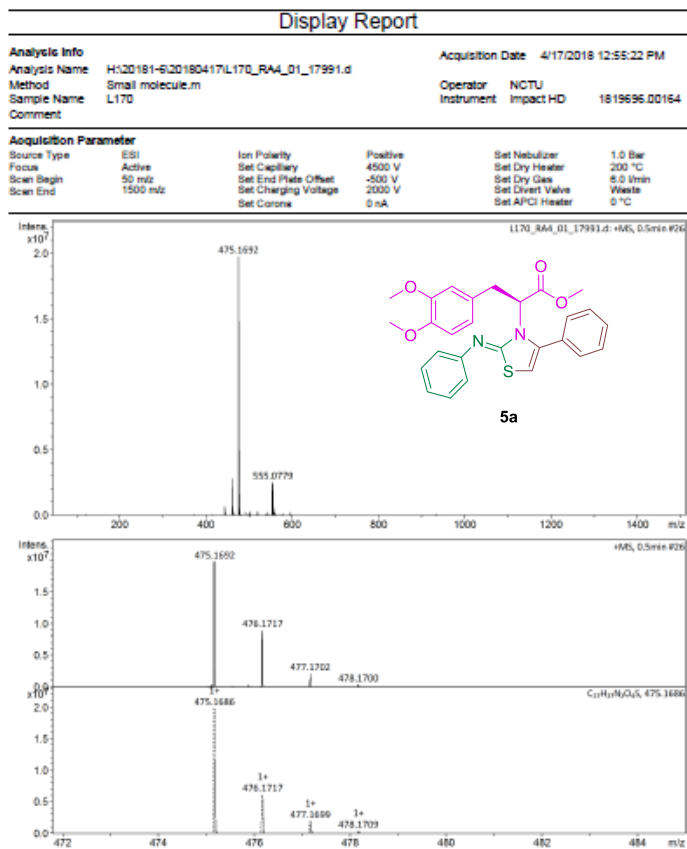


Expansion of ^1H NMR Spectrum (400 MHz) of compound **5a** in CDCl_3





Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **5a** in CDCl_3



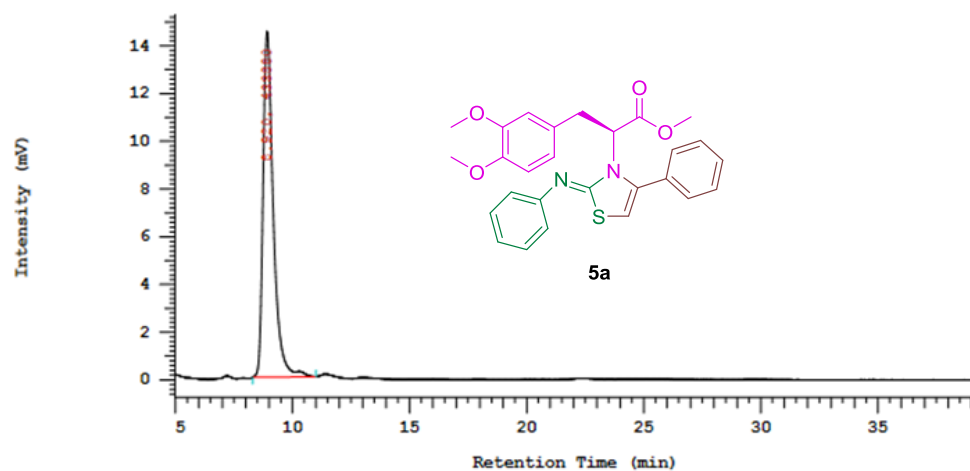
HRMS of compound **5a**

CSM: Linda Series: 0093 Report Name: modified System: Sys 1

Chromaster System Manager Report

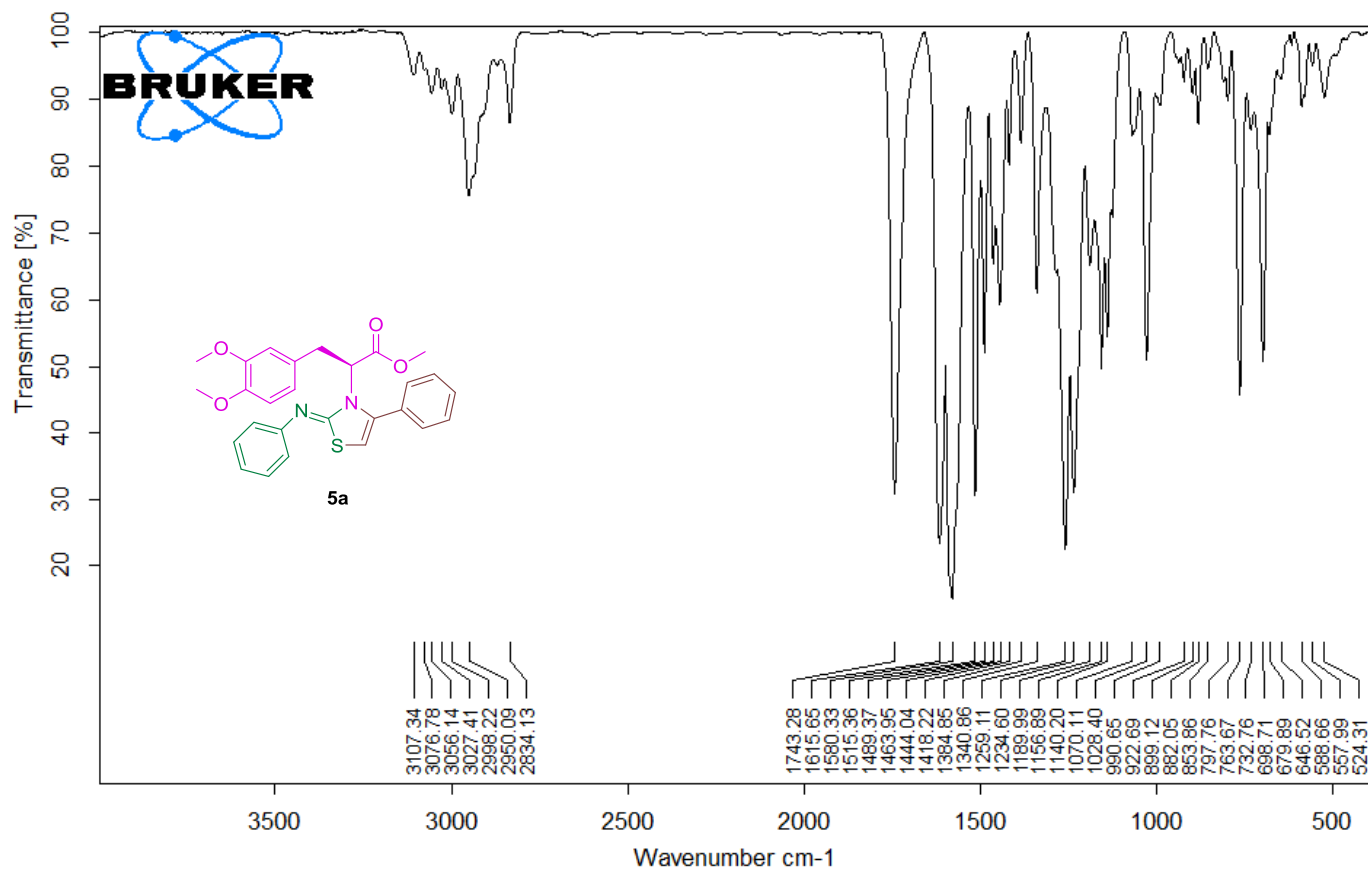
Analyzed Date and Time: 2017/12/05 02:30 下午
Reported Date and Time: 2017/12/05 04:49:13 下午
Processed Date and Time: 2017/12/05 04:48 下午
Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0093\
Processing Method: L170_ee
System (acquisition): Sys 1 Series: 0093
Application(data): Linda Vial Number: 1
Sample Name: UNKNOWN001 Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 20.0 ul
Sample Description:

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 1.0
mL/min , Daicel
Chiral OD, IPA 1, Hex
10

Chiral HPLC of compound 5a



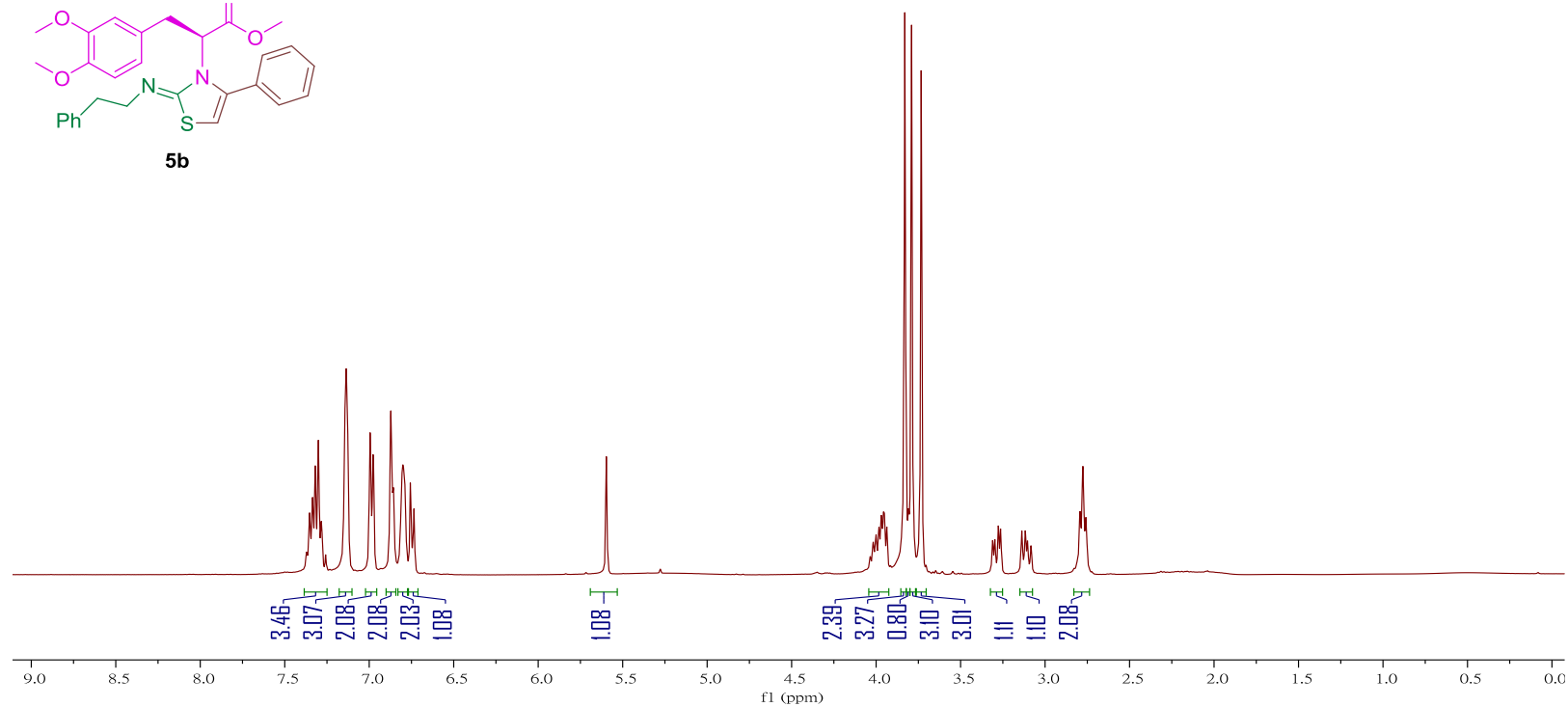
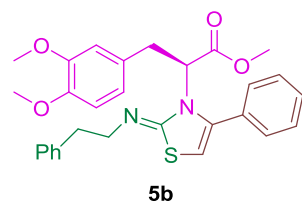
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L170.0

MIR_TR_DTGS_L170

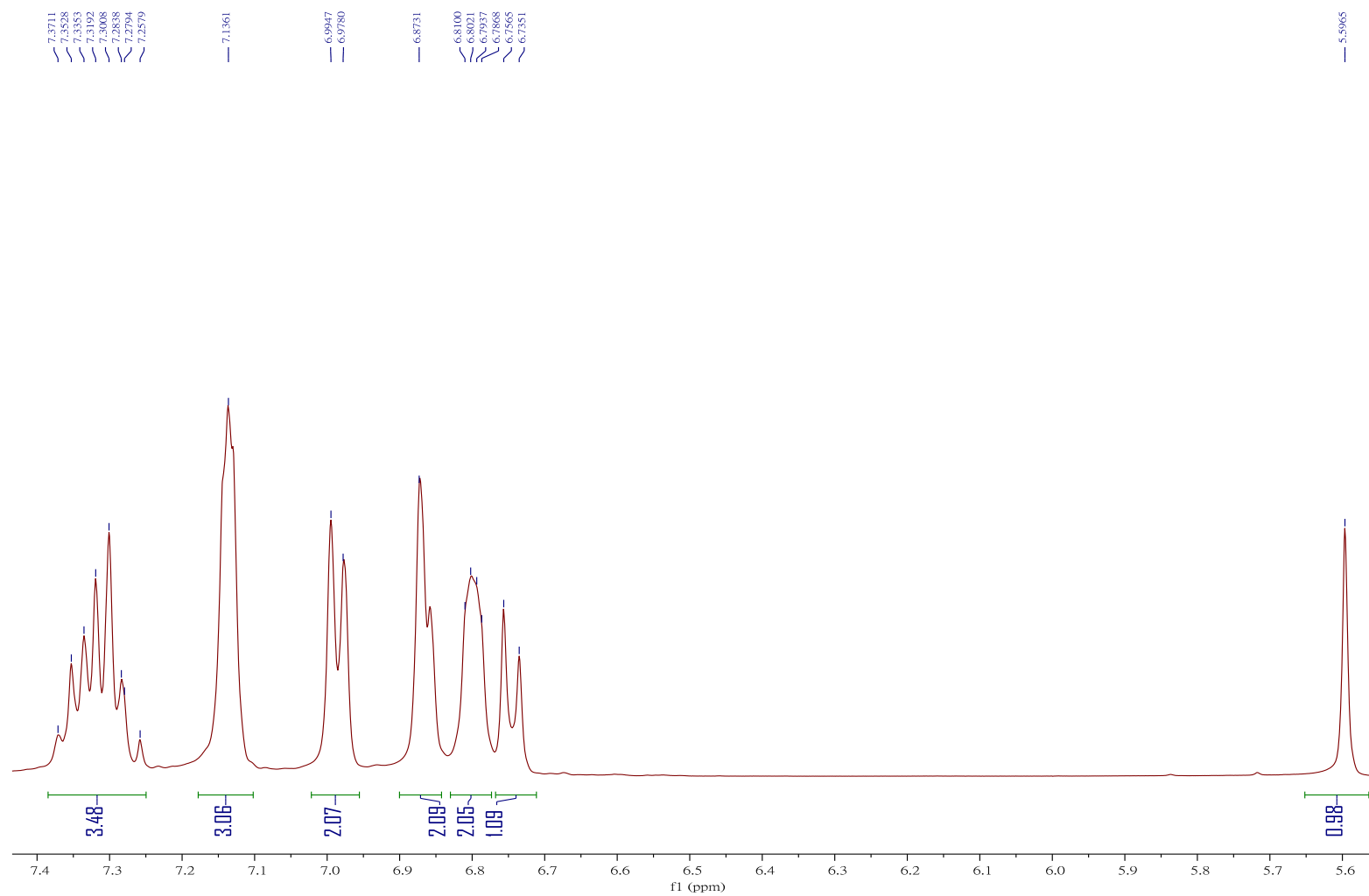
Instrument type and / or accessory

9/4/2018

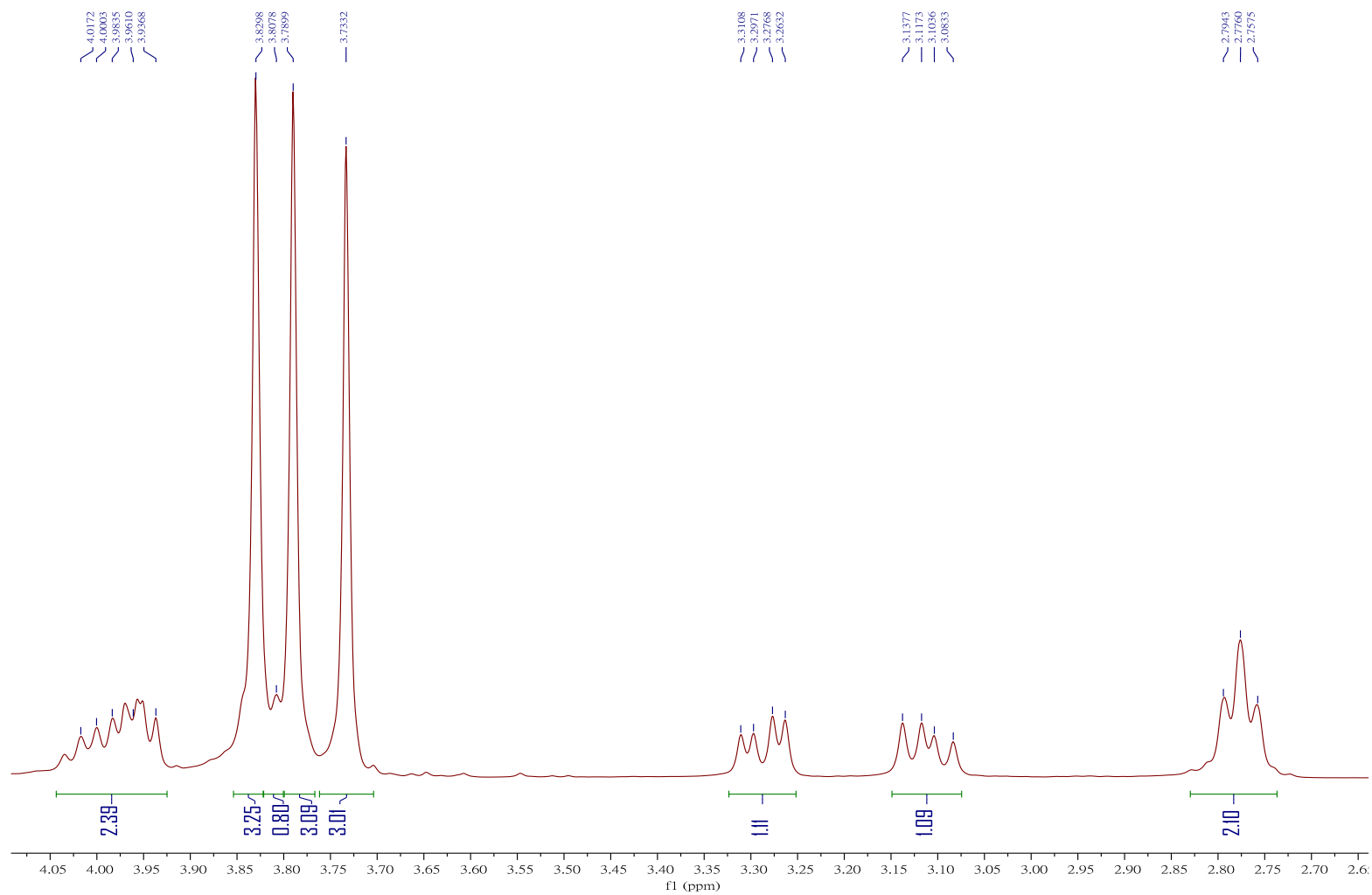
FT-IR Spectrum of compound **5a**



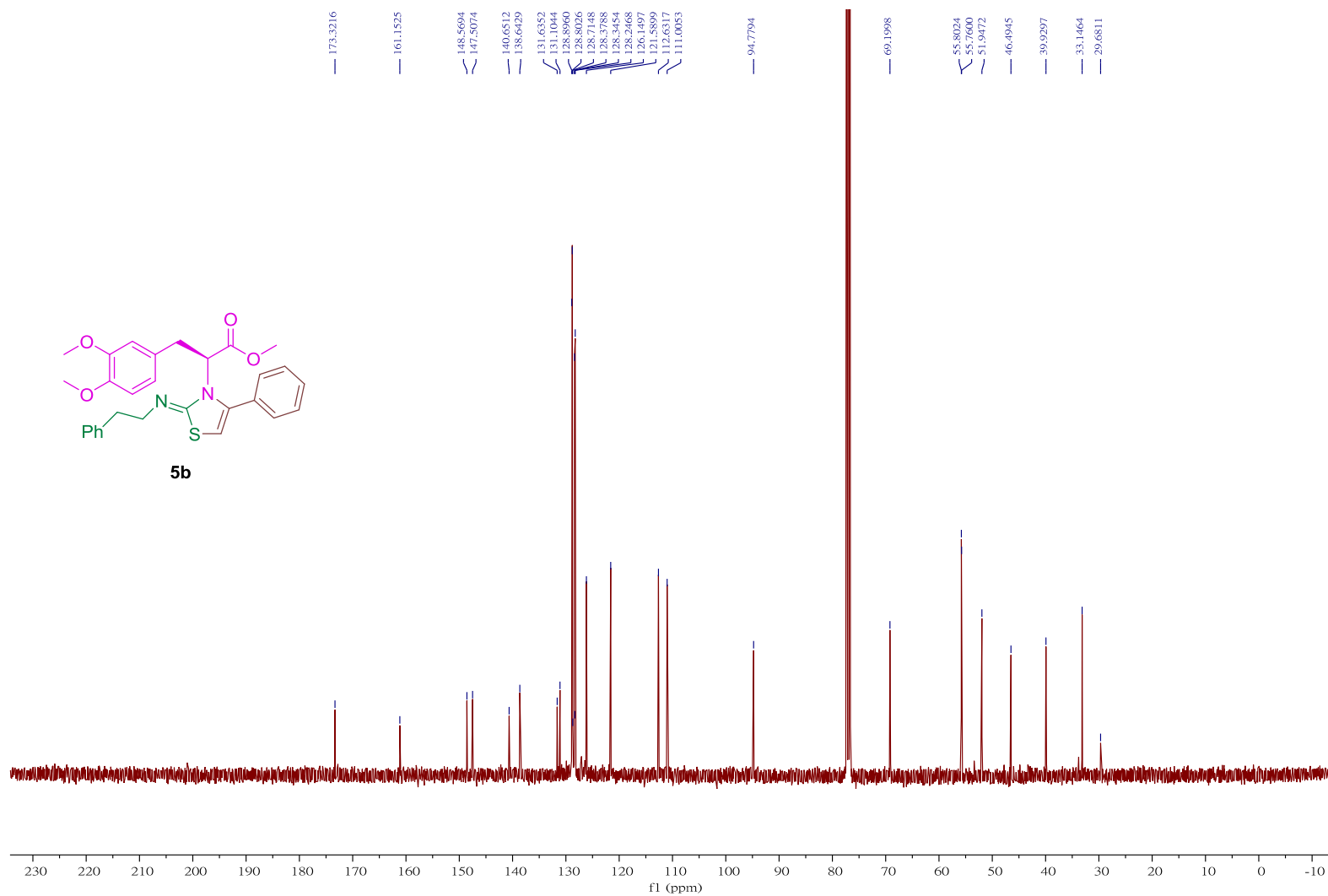
¹H NMR Spectrum (400 MHz) of compound **5b** in CDCl₃



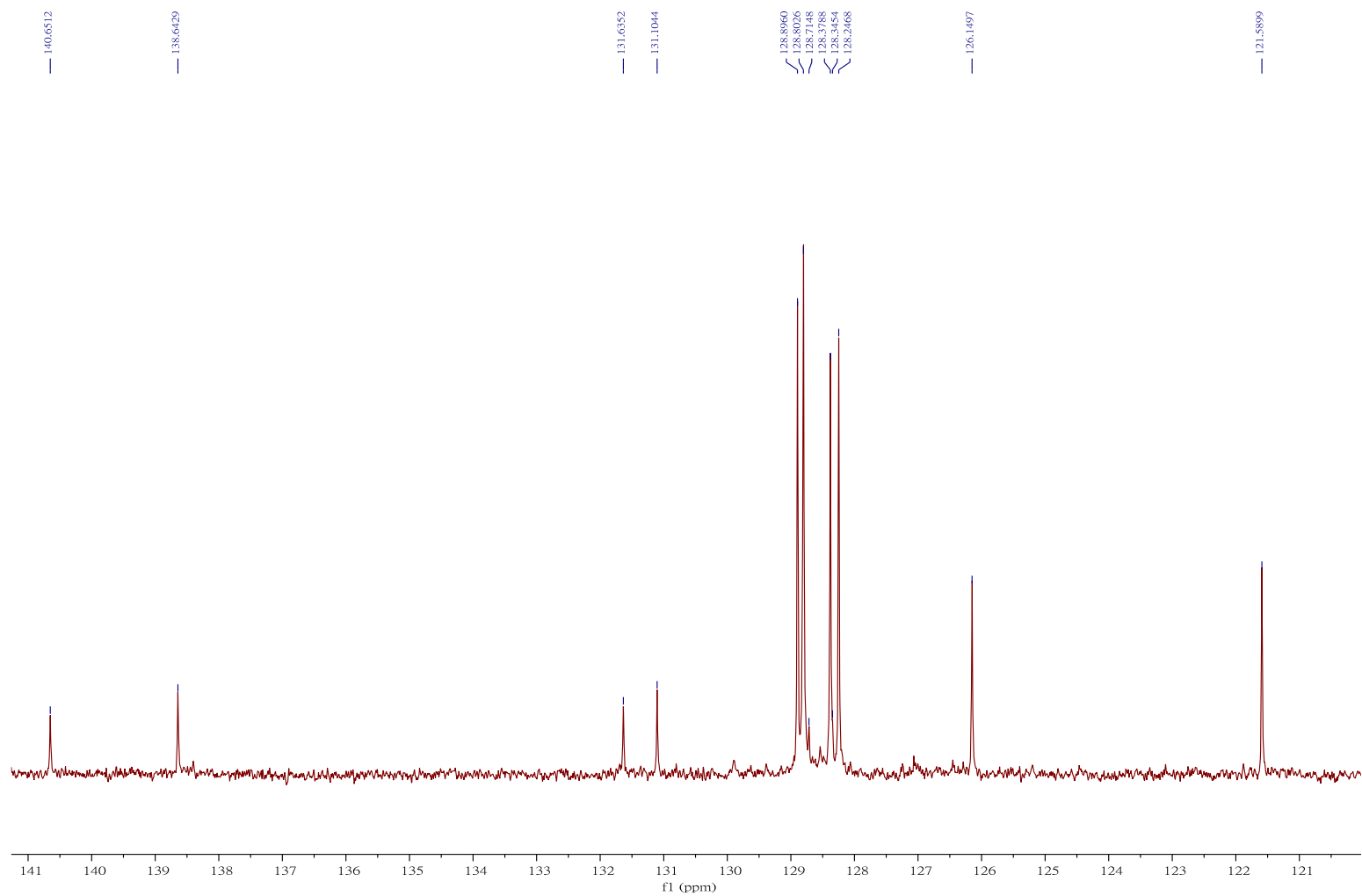
Expansion of ¹H NMR Spectrum (400 MHz) of compound **5b** in CDCl₃



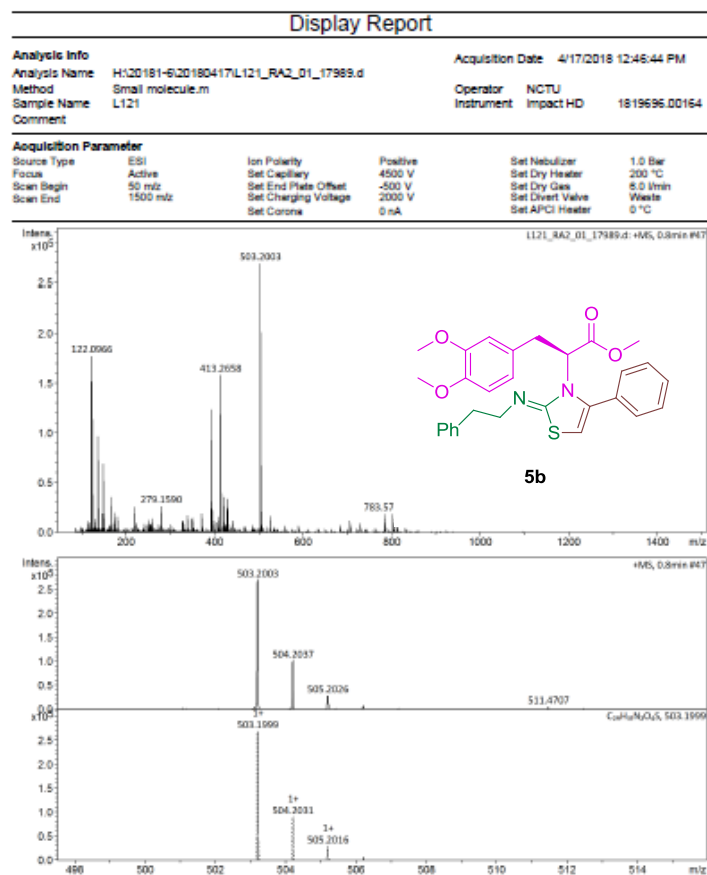
Expansion of ^1H NMR Spectrum (400 MHz) of compound **5b** in CDCl_3



^{13}C NMR Spectrum (101 MHz) of compound **5b** in CDCl_3



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **5b** in CDCl_3



HRMS of compound **5b**

CSM: Linda Series: 0033 Report Name: modified System: Sys 1

Chromaster System Manager Report

Analyzed Date and Time: 2017/11/03 01:39 下午
Reported Date and Time: 2017/11/03 04:33:51 下午

Processed Date and Time: 2017/11/03 04:05 下午

Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0033\

Processing Method: L121_ee

System (acquisition): Sys 1

Series: 0033

Application(data): Linda

Vial Number: 1

Sample Name: UNKNOWN001

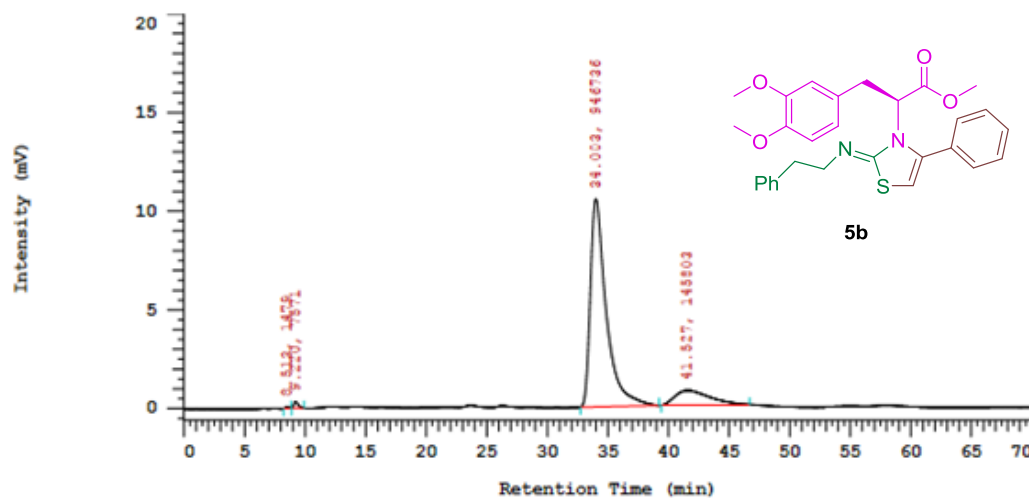
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 15.0 ul

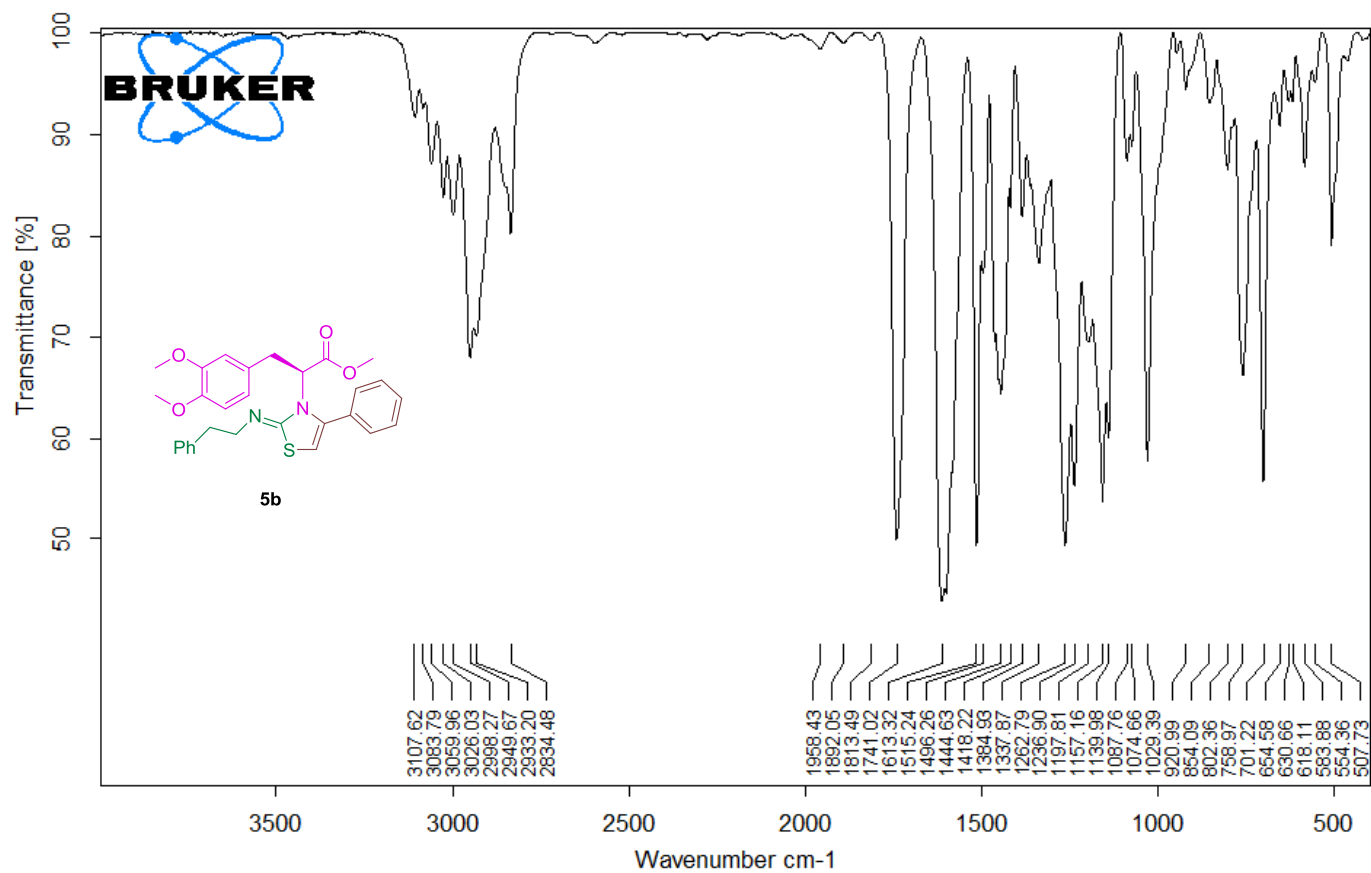
Sample Description:

Chrom Type: Chromaster Channel : 1



Method Description: flow rate:0.5 , IPA
1, Hex 10

Chiral HPLC of compound **5b**



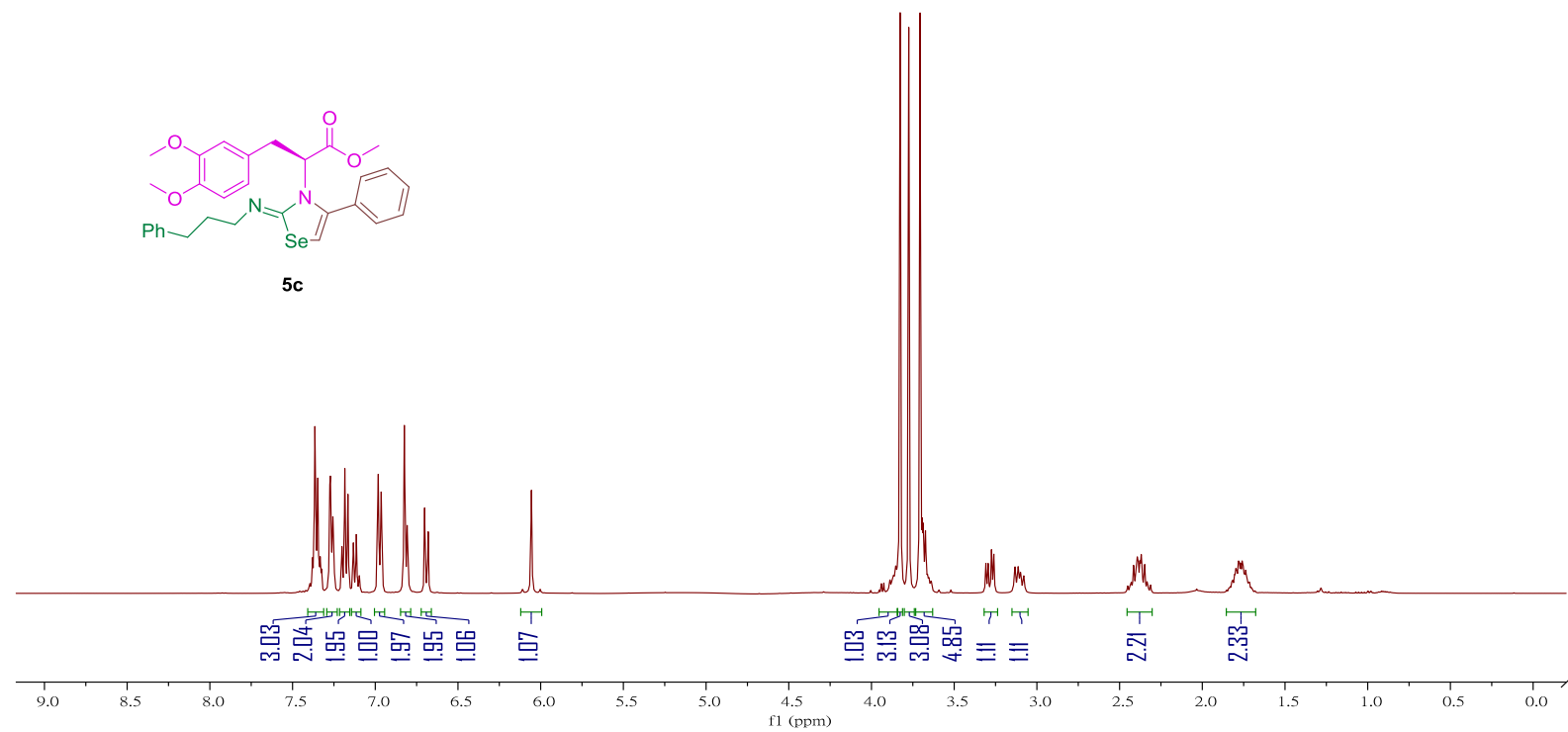
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L121.0

MIR_TR_DTGS_L121

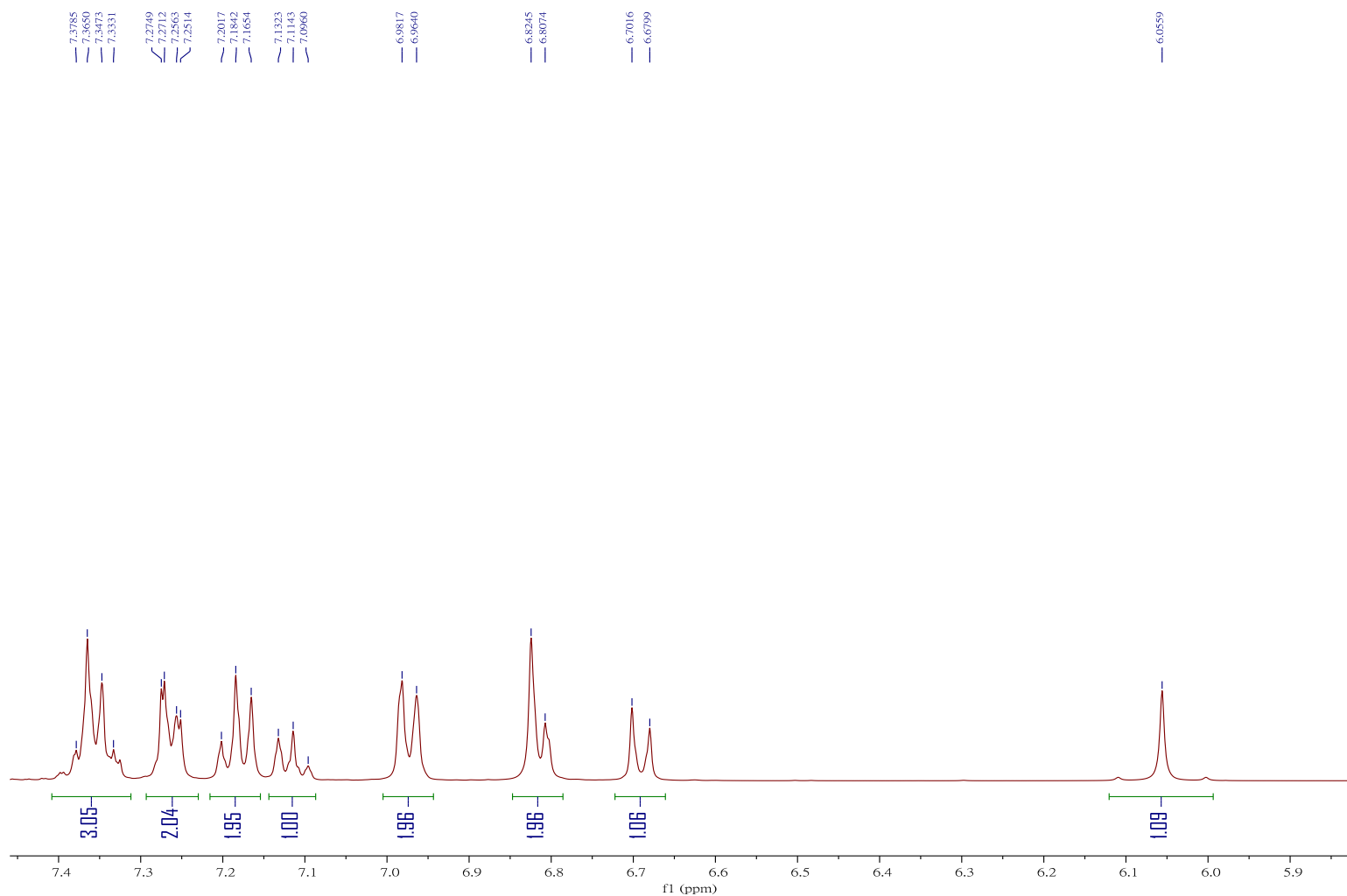
Instrument type and / or accessory

9/4/2018

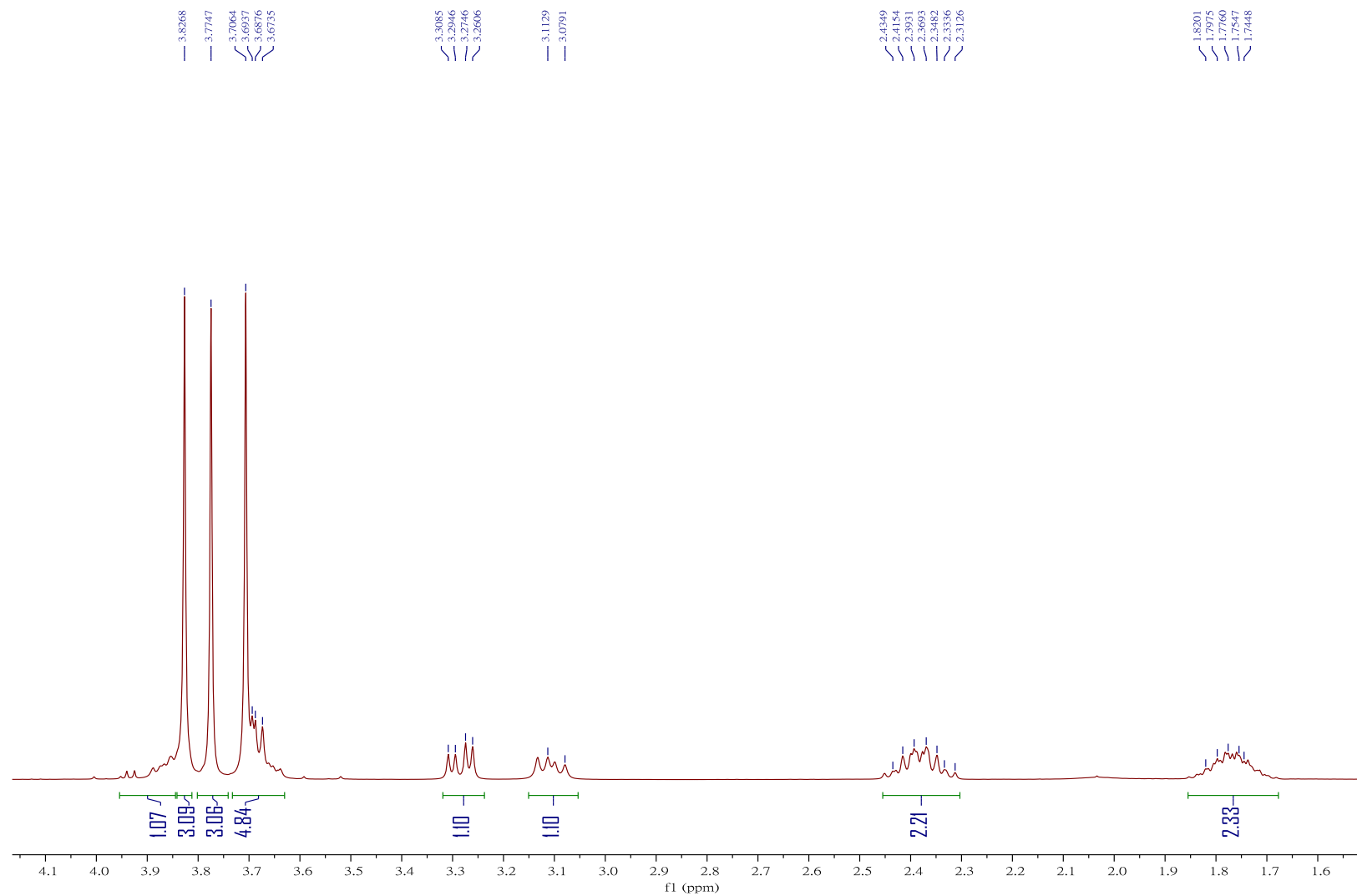
FT-IR Spectrum of compound **5b**



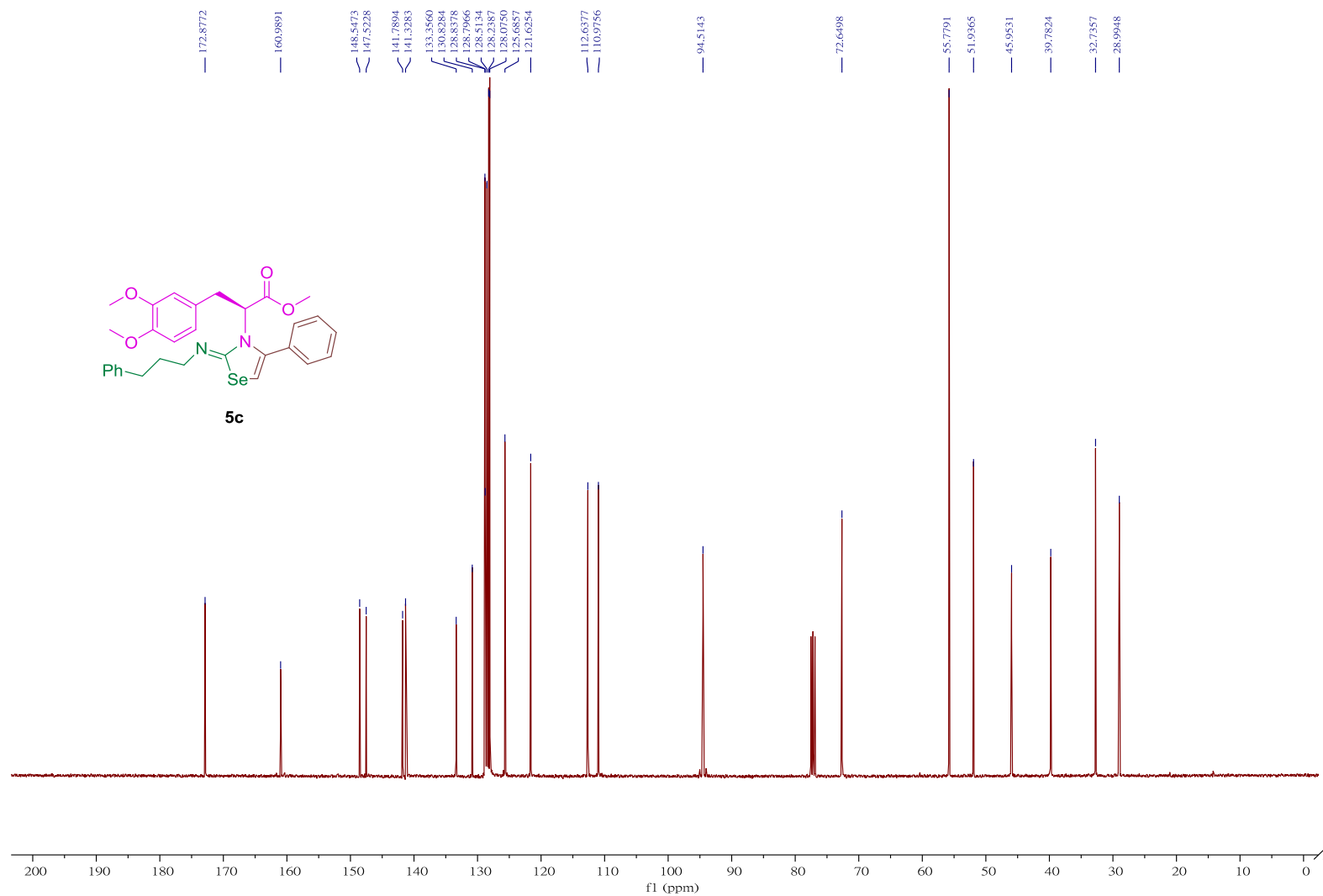
^1H NMR Spectrum (400 MHz) of compound **5c** in CDCl_3



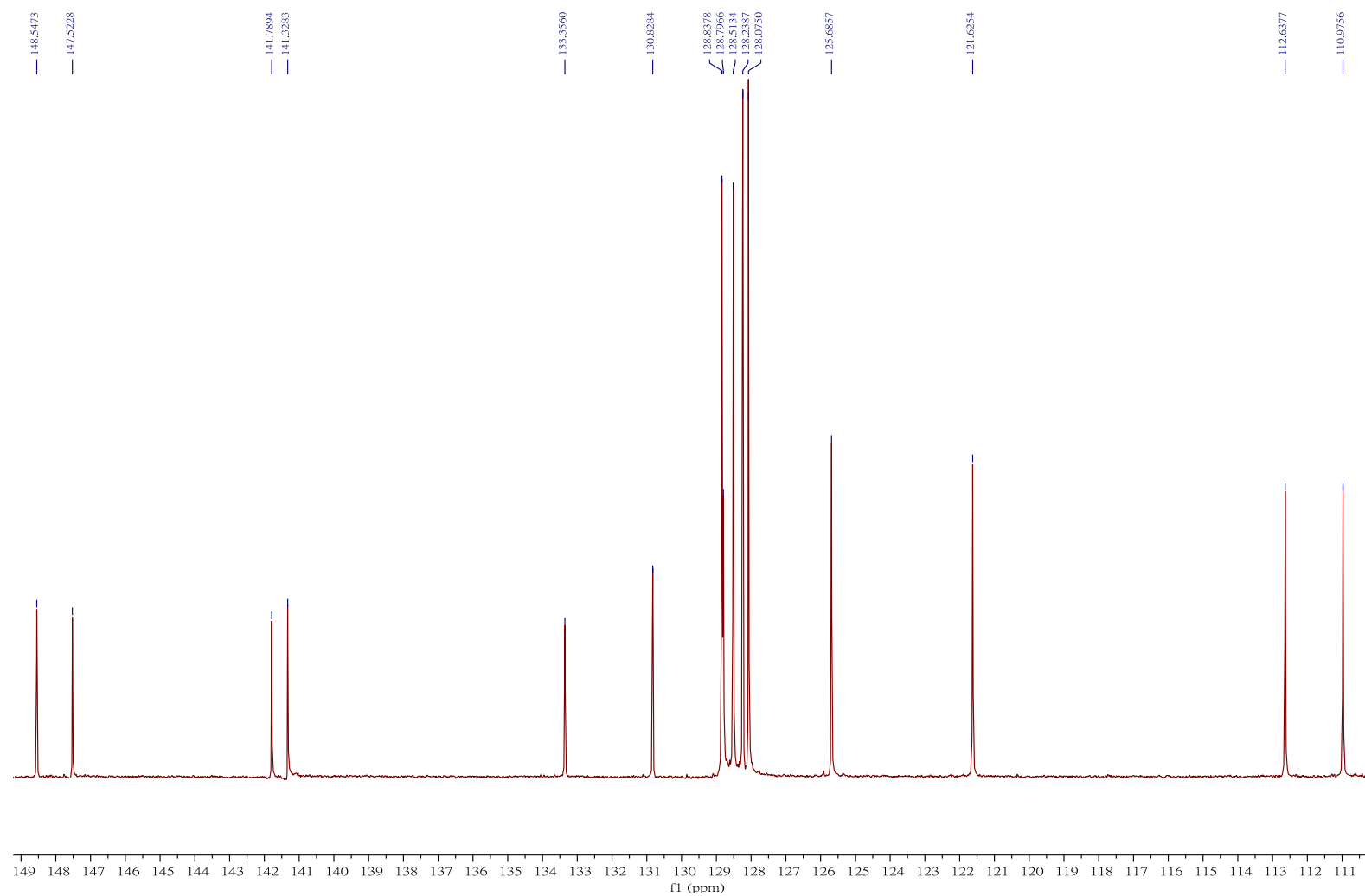
Expansion of ¹H NMR Spectrum (400 MHz) of compound **5c** in CDCl₃



Expansion of ¹H NMR Spectrum (400 MHz) of compound **5c** in CDCl₃



^{13}C NMR Spectrum (101 MHz) of compound **5c** in CDCl_3



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **5c** in CDCl_3

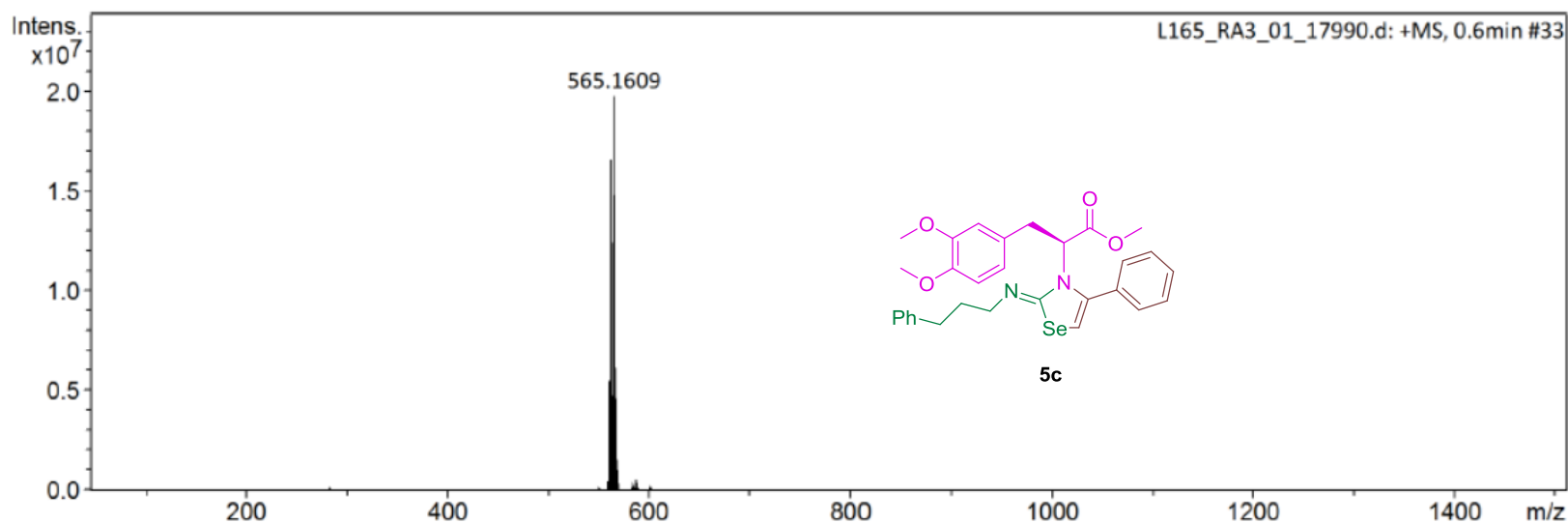
Display Report

Analysis Info

Analysis Name	D:\Data\nctu service\data\2018\20180417\L165_RA3_01_17990.d	Acquisition Date	4/17/2018 12:51:03 PM	
Method	Small molecule.m	Operator	NCTU	
Sample Name	L165	Instrument	impact HD	1819696.00164
Comment				

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



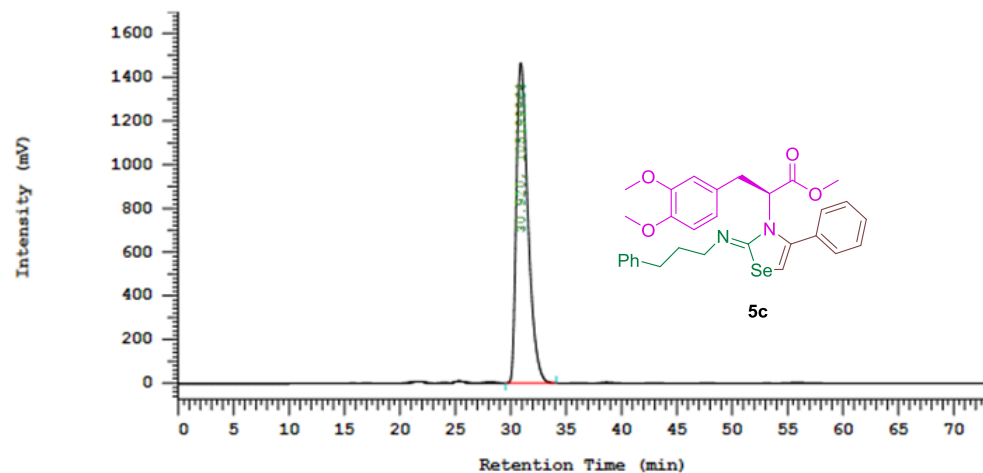
HRMS of compound **5c**

CSM: Linda Series: 0119 Report Name: modified System: Sys 1

Chromaster System Manager Report

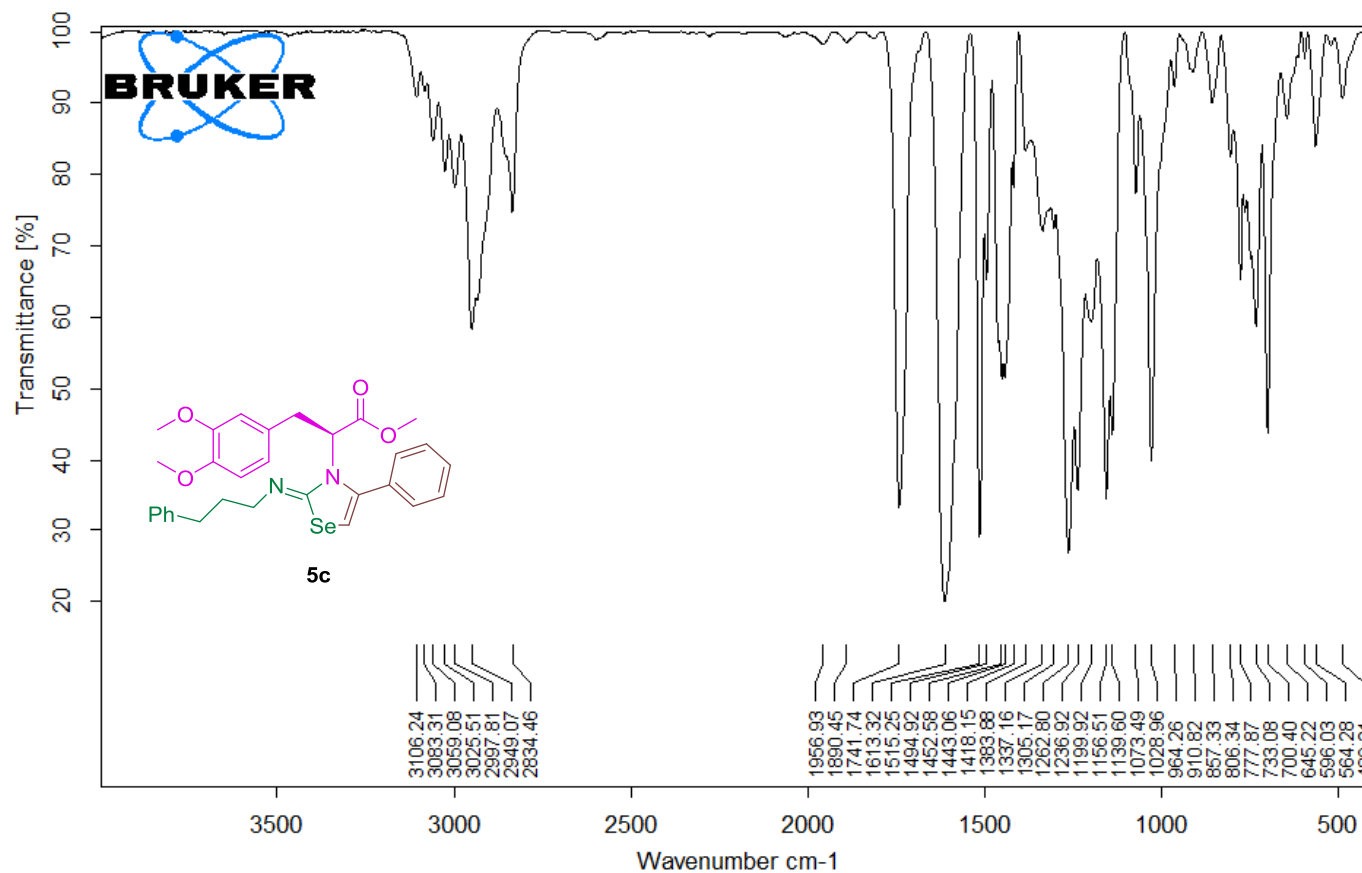
Analyzed Date and Time: 2018/09/05 08:19 上午 Reported Date and Time: 2018/09/11 09:08:01 上午
Processed Date and Time: 2018/09/11 09:07 上午
Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0119\
Processing Method: L165_ee
System (acquisition): Sys 1 Series: 0119
Application(data): Linda Vial Number: 1
Sample Name: UNKNOWN001 Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 10.0 ul
Sample Description:

Chrom Type: Chromaster Channel : 1



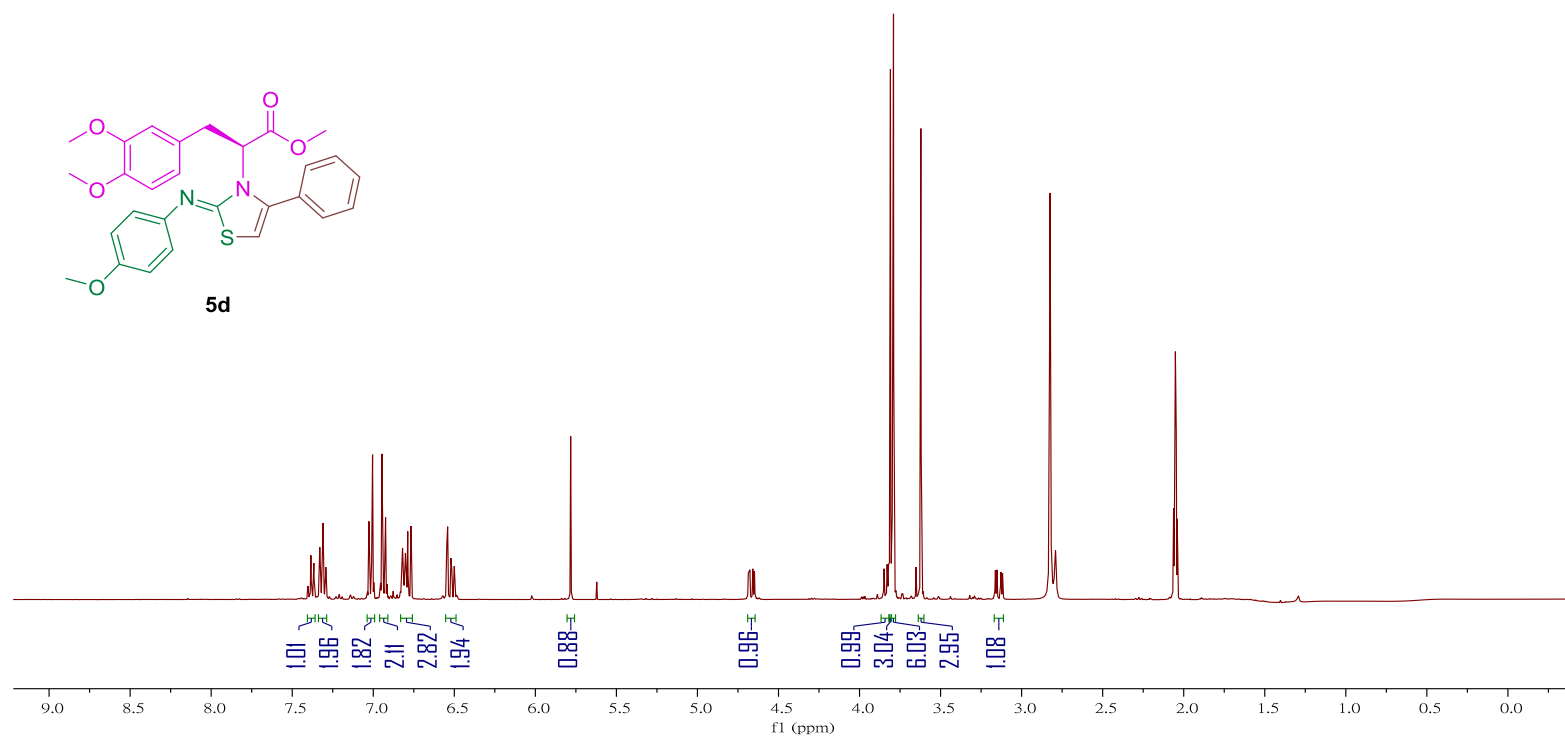
Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound **5c**

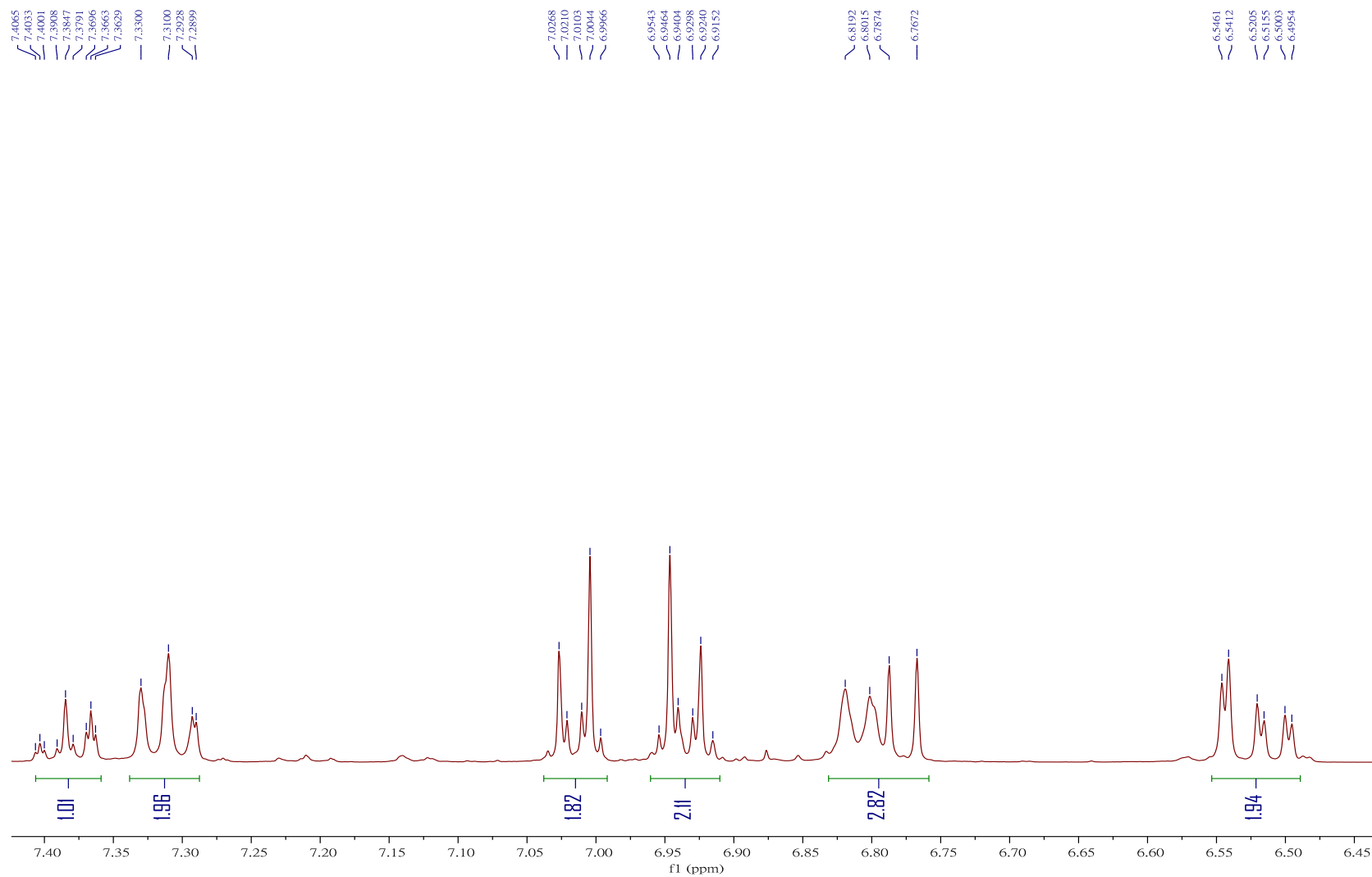


D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L165.0	MIR_TR_DTGS_L165	Instrument type and / or accessory	9/4/2018
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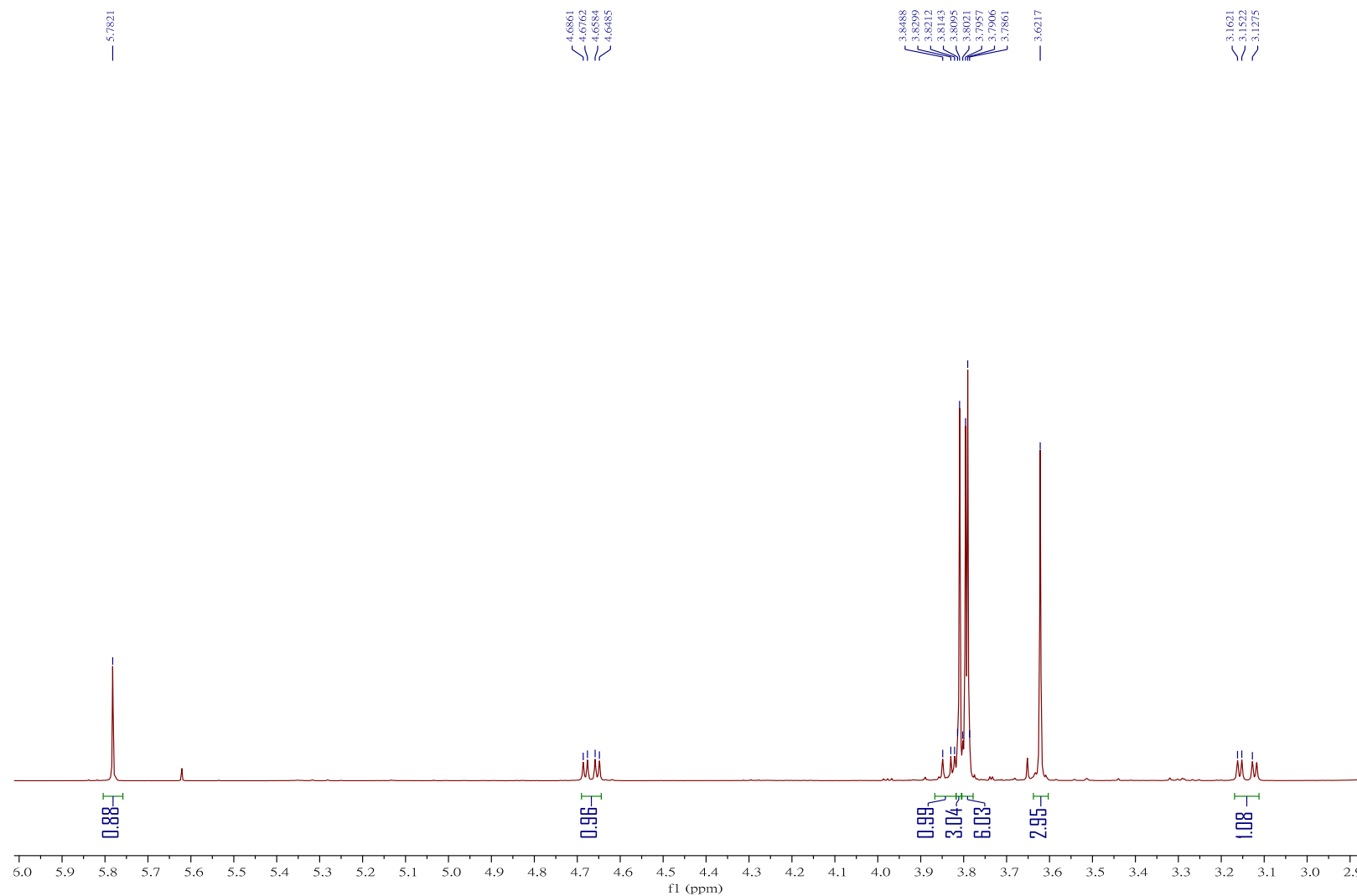
FT-IR Spectrum of compound **5c**



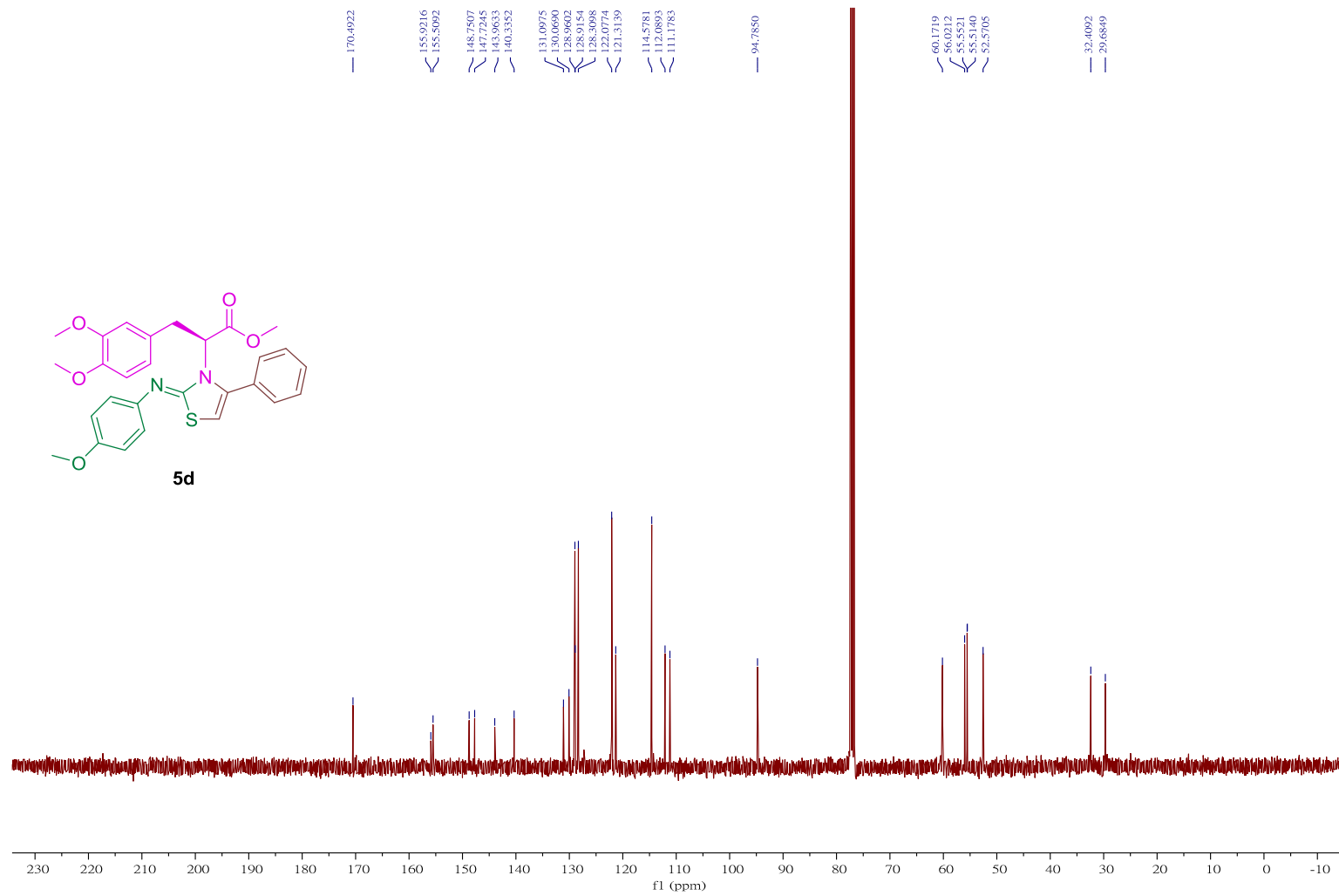
¹H NMR Spectrum (400 MHz) of compound **5d** in acetone-*d*₆



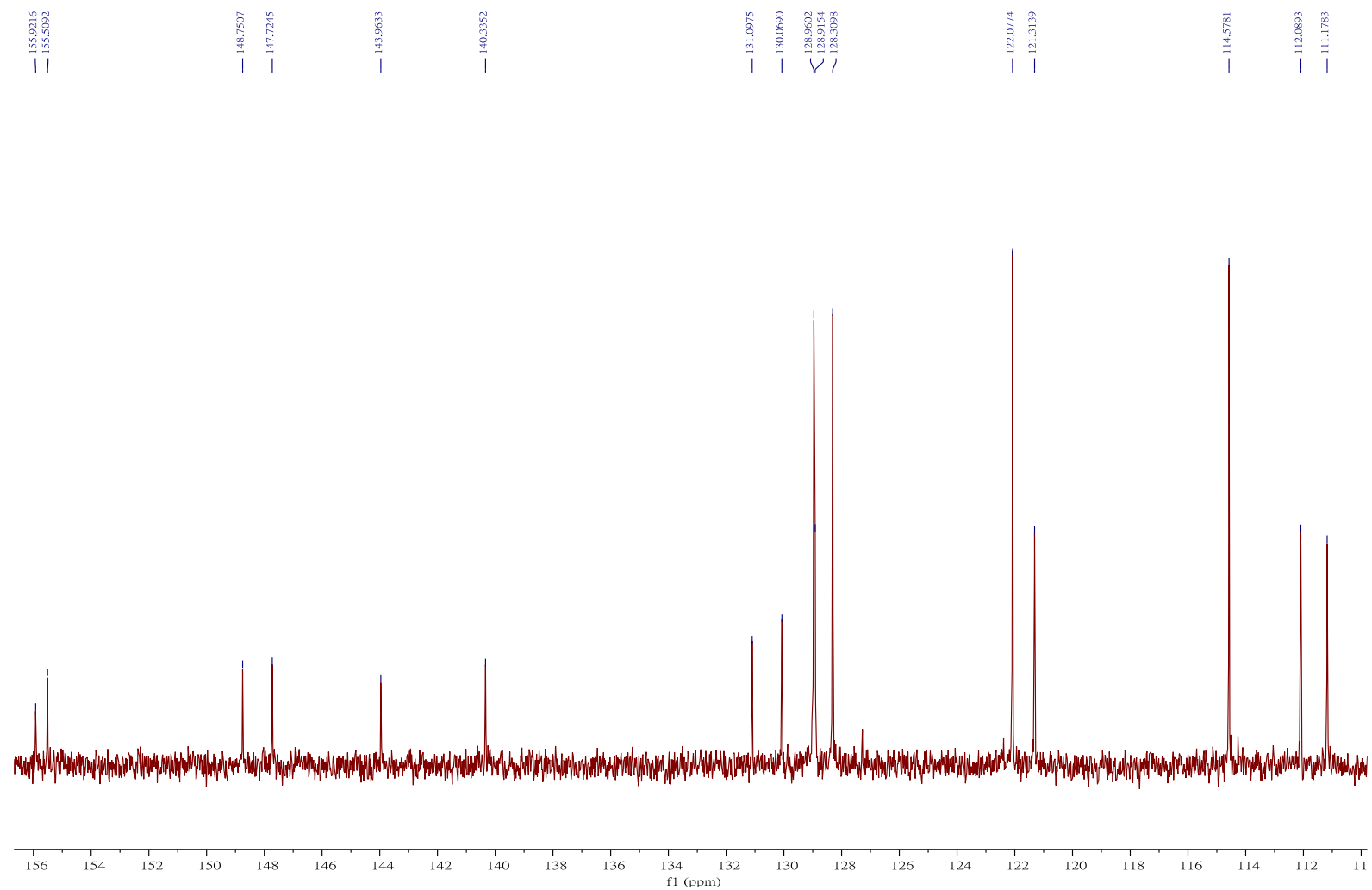
Expansion of ^1H NMR Spectrum (400 MHz) of compound **5d** in acetone- d_6



Expansion of ¹H NMR Spectrum (400 MHz) of compound **5d** in acetone-*d*₆



^{13}C NMR Spectrum (101 MHz) of compound **5d** in CDCl_3



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **5d** in CDCl_3

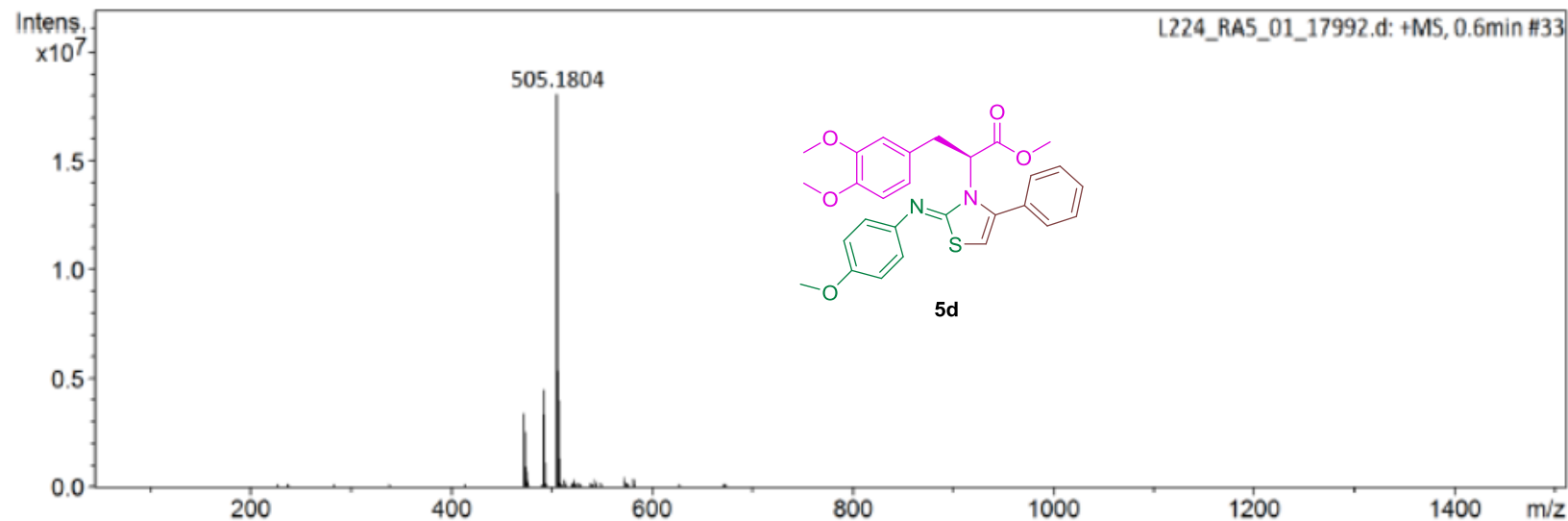
Display Report

Analysis Info

Analysis Name	D:\Data\nctu service\data\2018\20180417\L224_RA5_01_17992.d	Acquisition Date	4/17/2018 12:59:43 PM	
Method	Small molecule.m	Operator	NCTU	
Sample Name	L224	Instrument	impact HD	1819696.00164
Comment				

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



HRMS of compound 5d

Processing Method: 27d_ee

System (acquisition): Sys 1

Application(data): Linda

Sample Name: UNKNOWN001

Injection from this vial: 1 of 1

Sample Description:

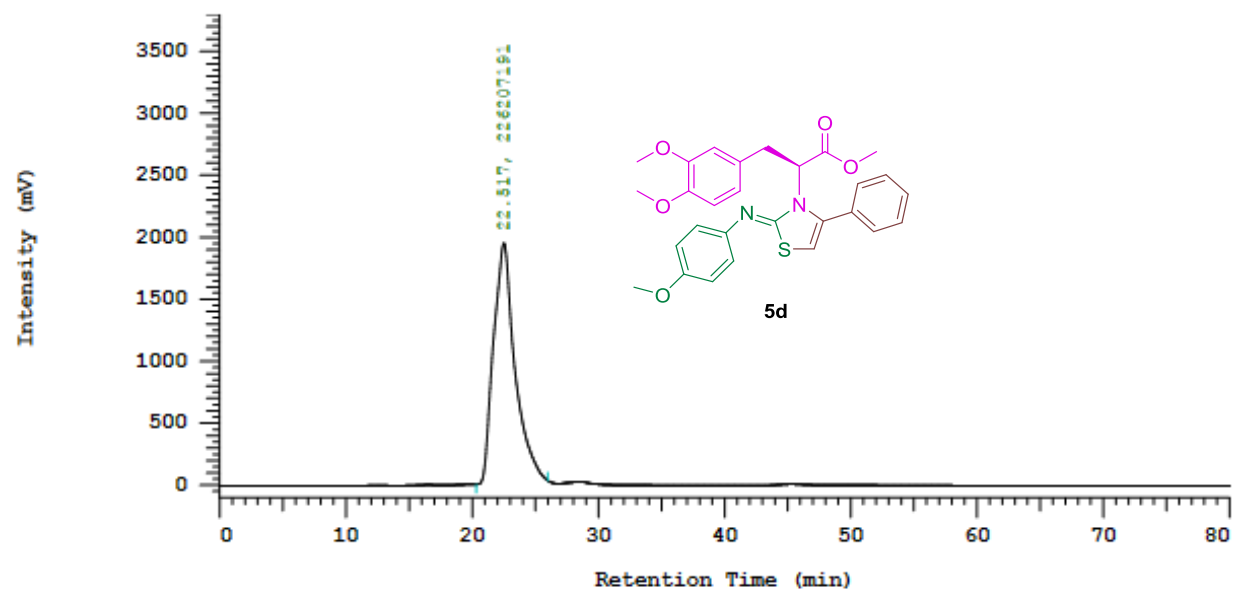
Series: 0206

Vial Number: 1

Vial Type: UNK

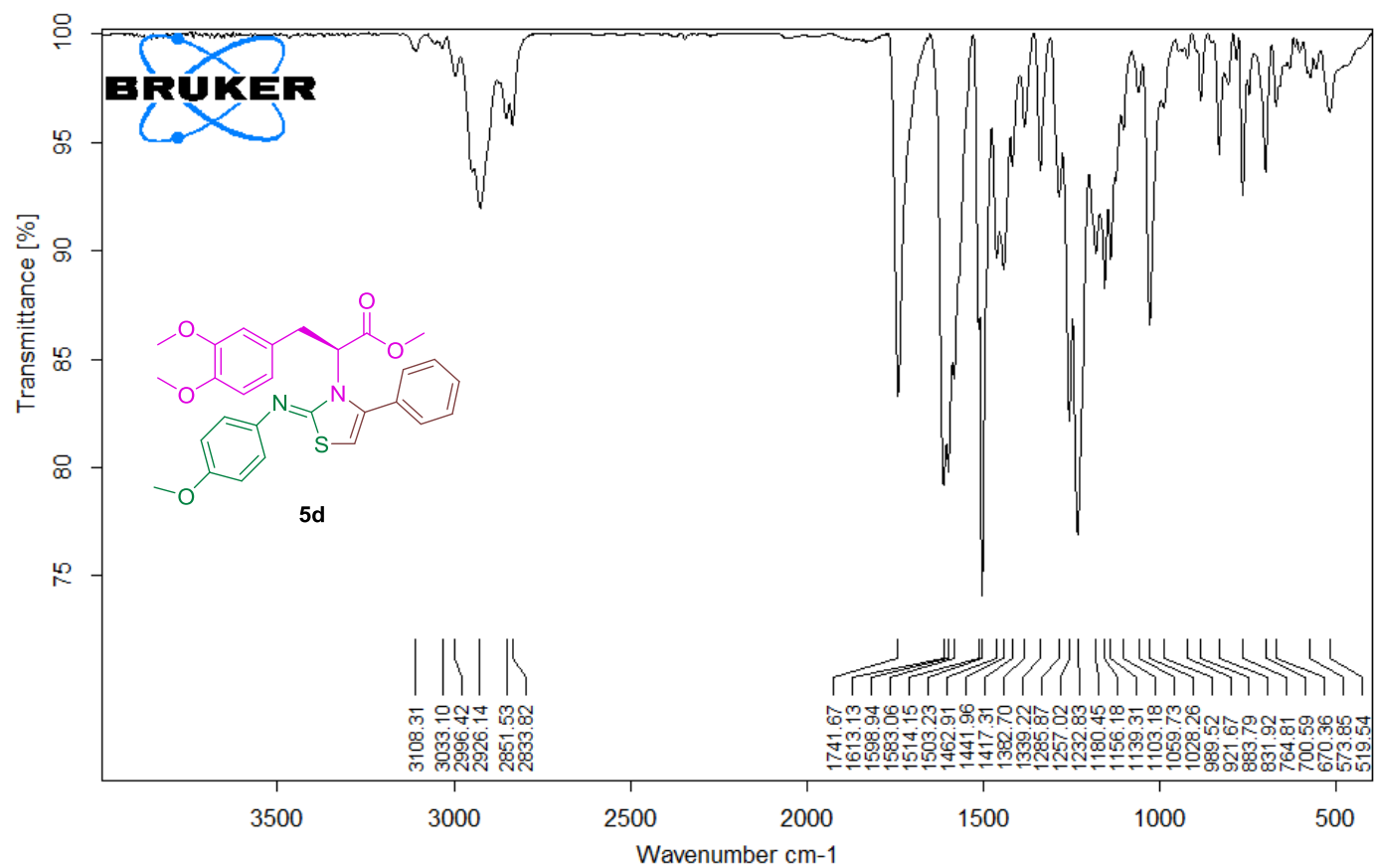
Volume: 10.0 ul

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound **5d**



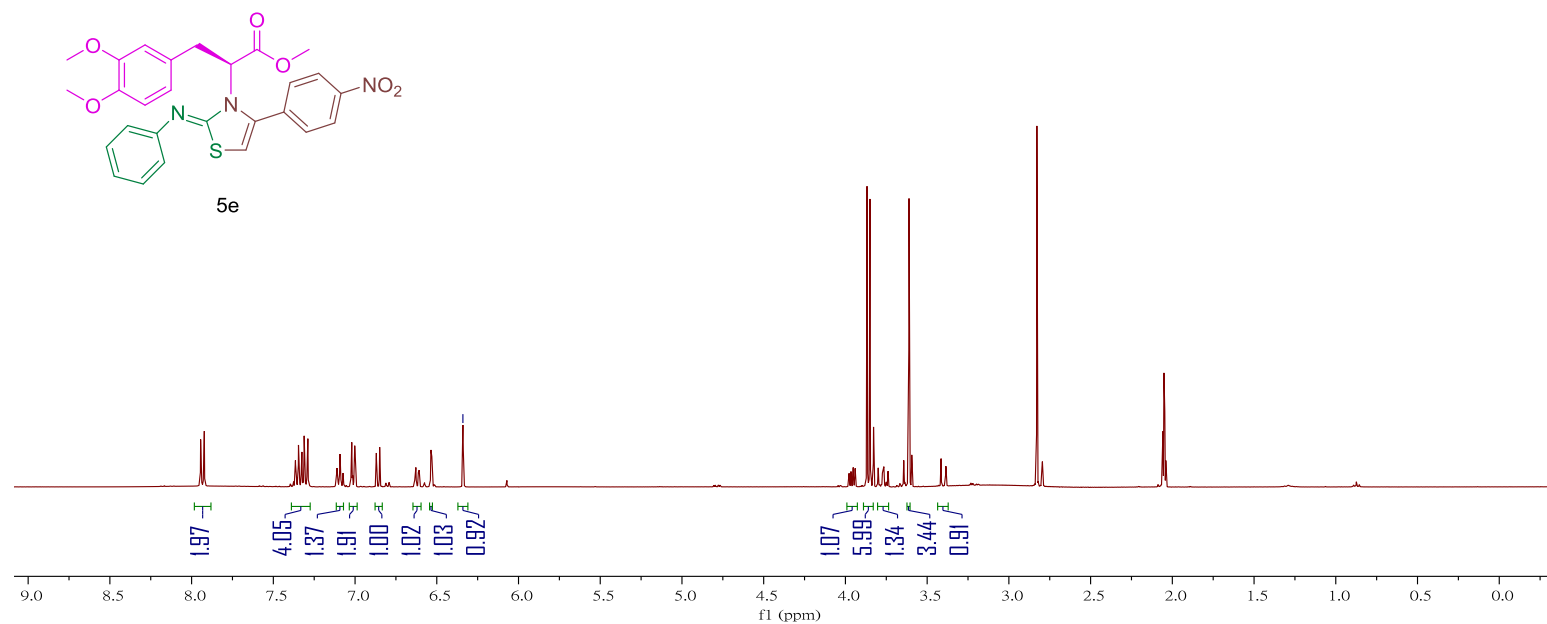
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L224.0

MIR_TR_DTGS_L224

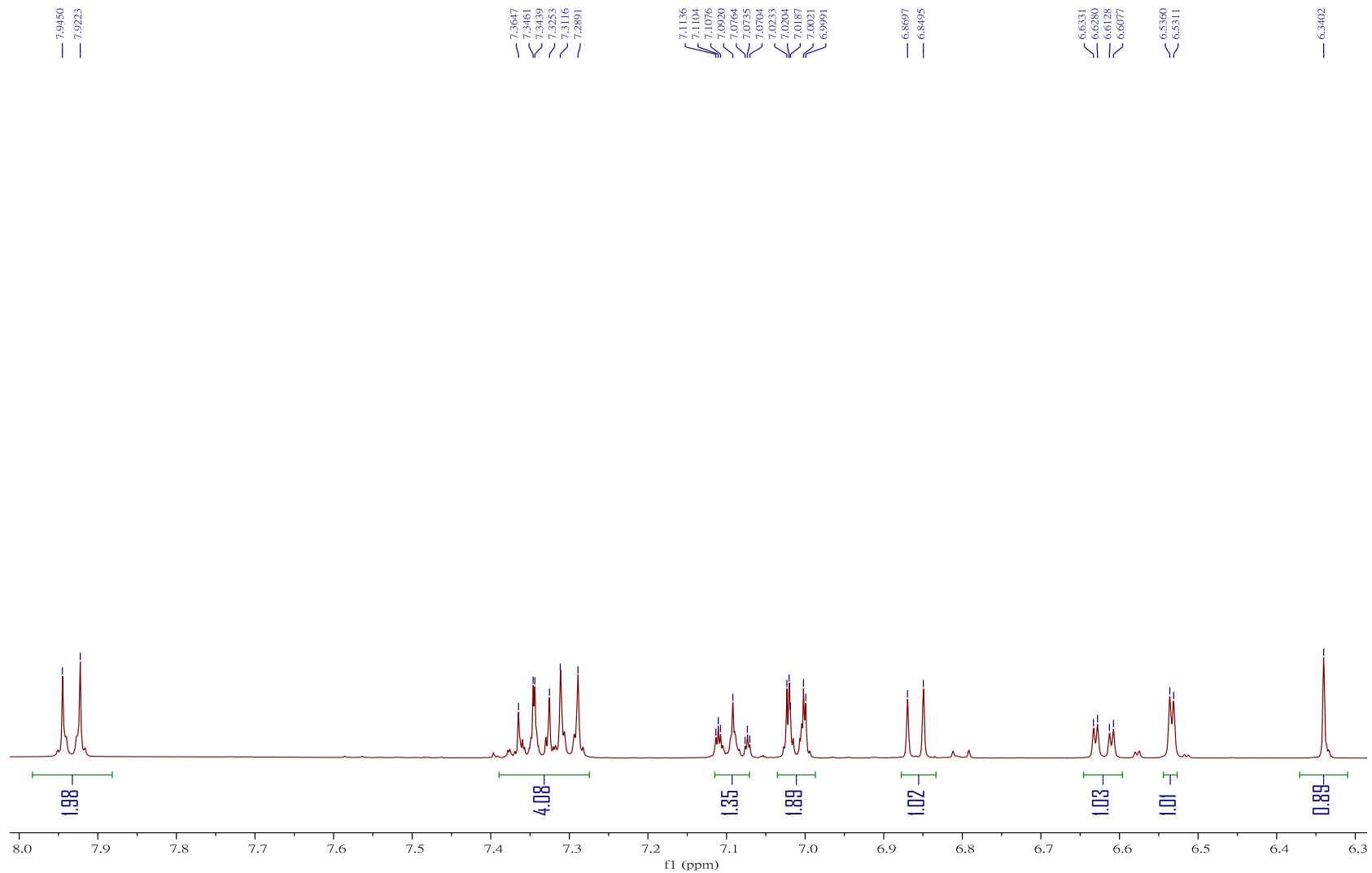
Instrument type and / or accessory

9/4/2018

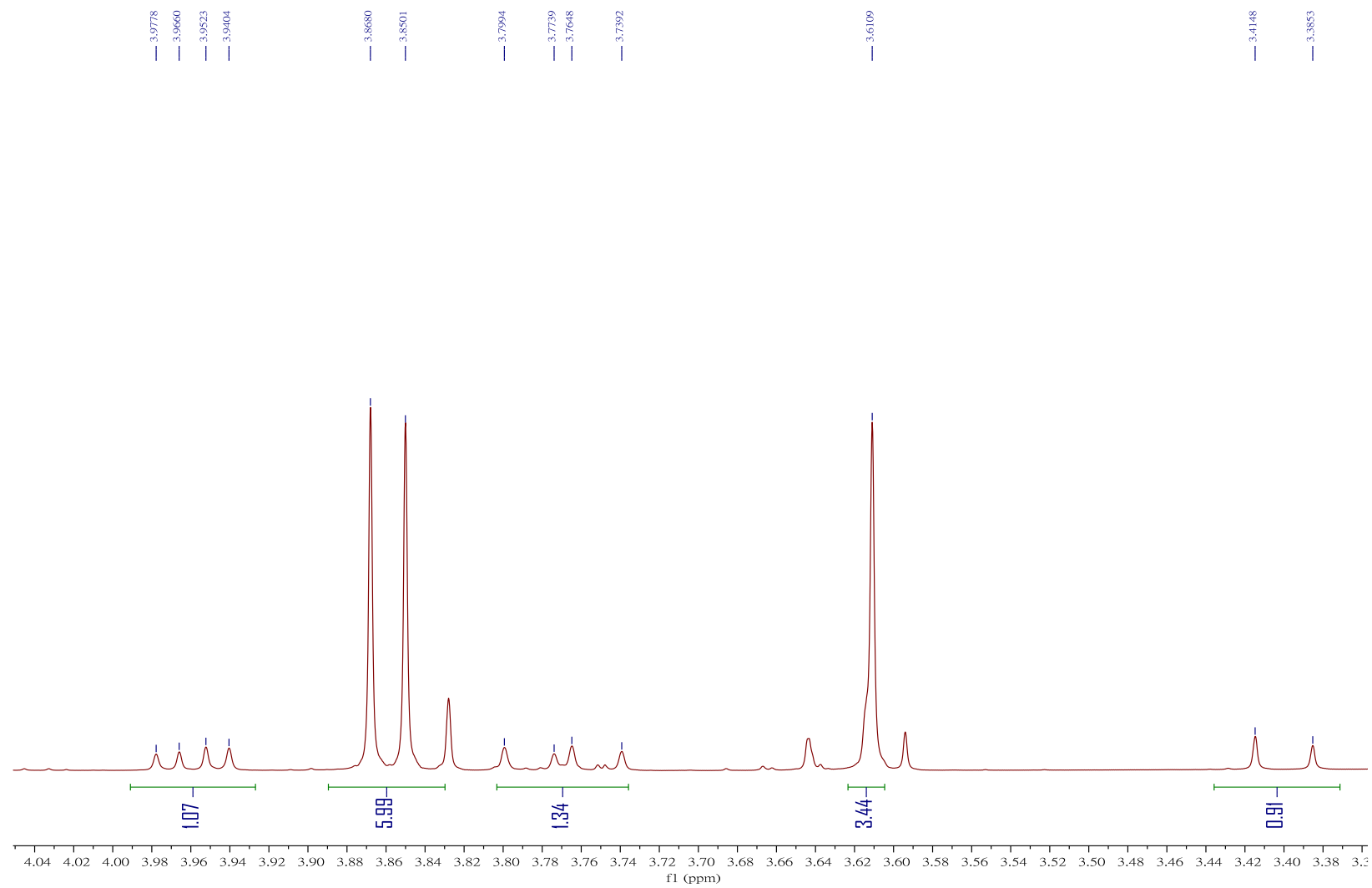
Page 1/1
FT-IR Spectrum of compound **5d**



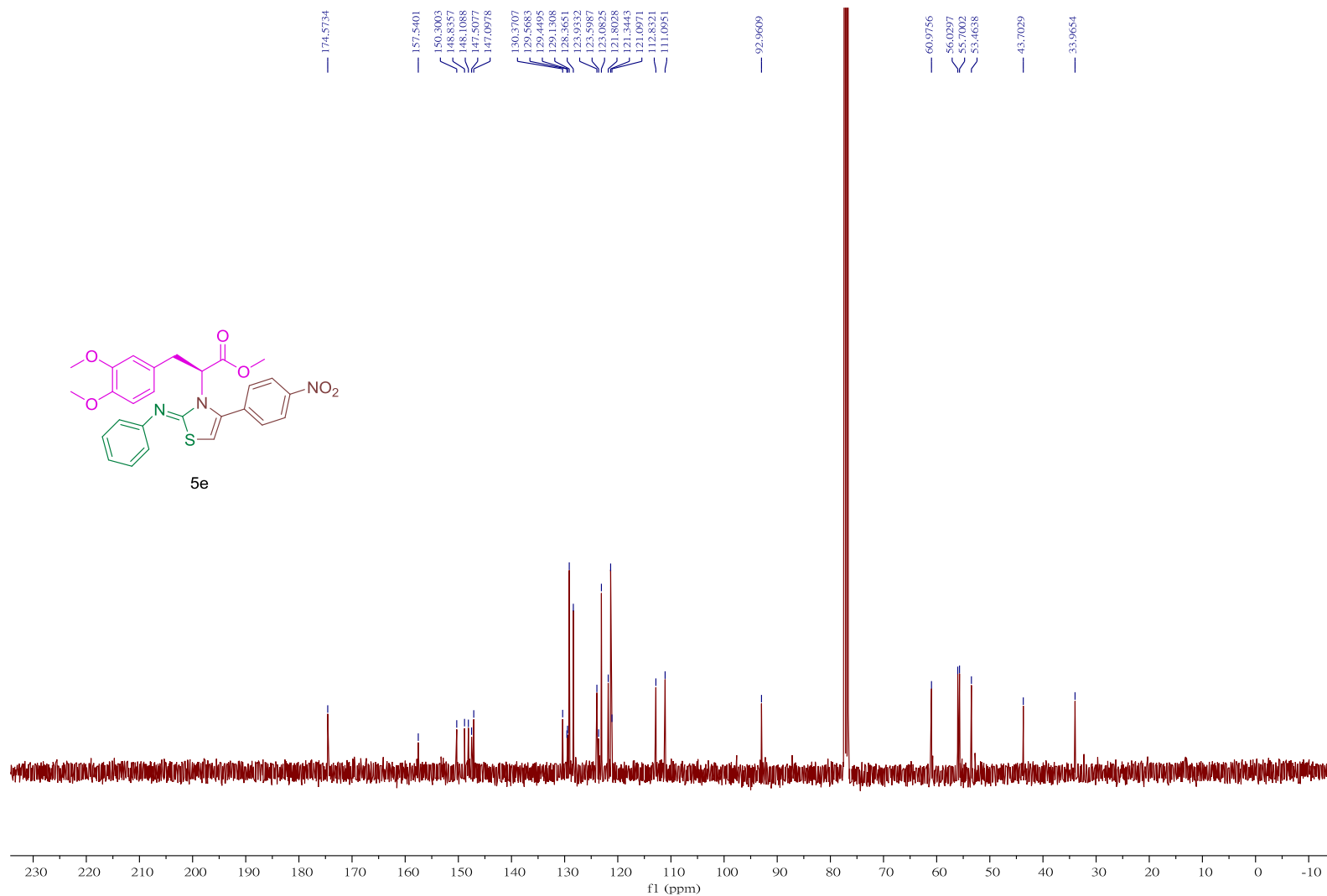
^1H NMR Spectrum (400 MHz) of compound **5e** in acetone- d_6



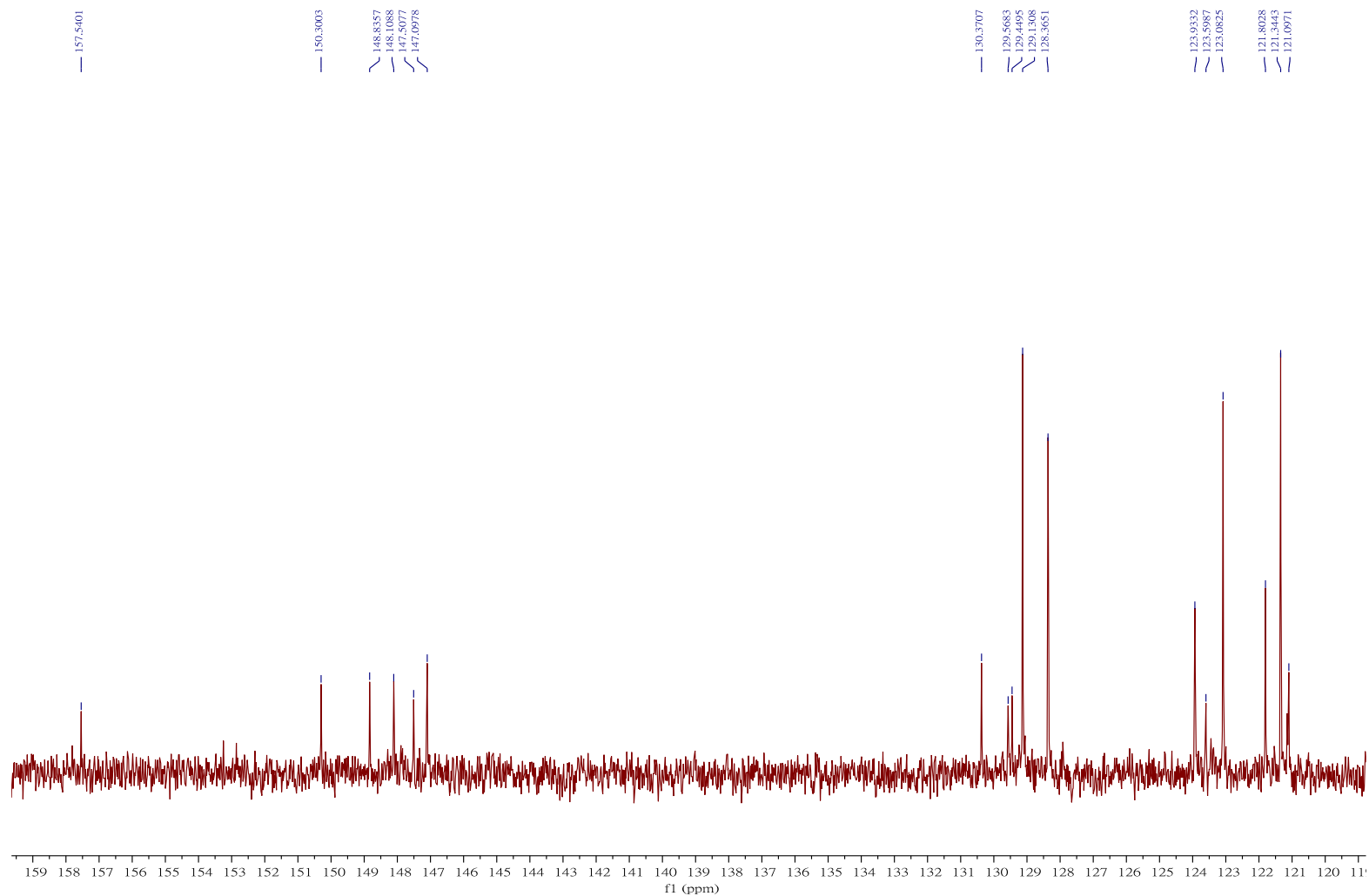
Expending ¹H NMR Spectrum (400 MHz) of compound **5e** in acetone-*d*₆



Expansion of ^1H NMR Spectrum (400 MHz) of compound **5e** in acetone- d_6



^{13}C NMR Spectrum (101 MHz) of compound **5e** in CDCl_3



Expansion of ¹³C NMR Spectrum (101 MHz) of compound **5e** in CDCl₃

Display Report

Analysis Info

Analysis Name D:\Data\nctu service\data\2018\20180417\L225_RA6_01_17993.d

Method Small molecule.m

Sample Name L225

Comment

Acquisition Date 4/17/2018 1:04:01 PM

Operator NCTU

Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type

ESI

Ion Polarity

Positive

Set Nebulizer

1.0 Bar

Focus

Active

Set Capillary

4500 V

Set Dry Heater

200 °C

Scan Begin

50 m/z

Set End Plate Offset

-500 V

Set Dry Gas

6.0 l/min

Scan End

1500 m/z

Set Charging Voltage

2000 V

Set Divert Valve

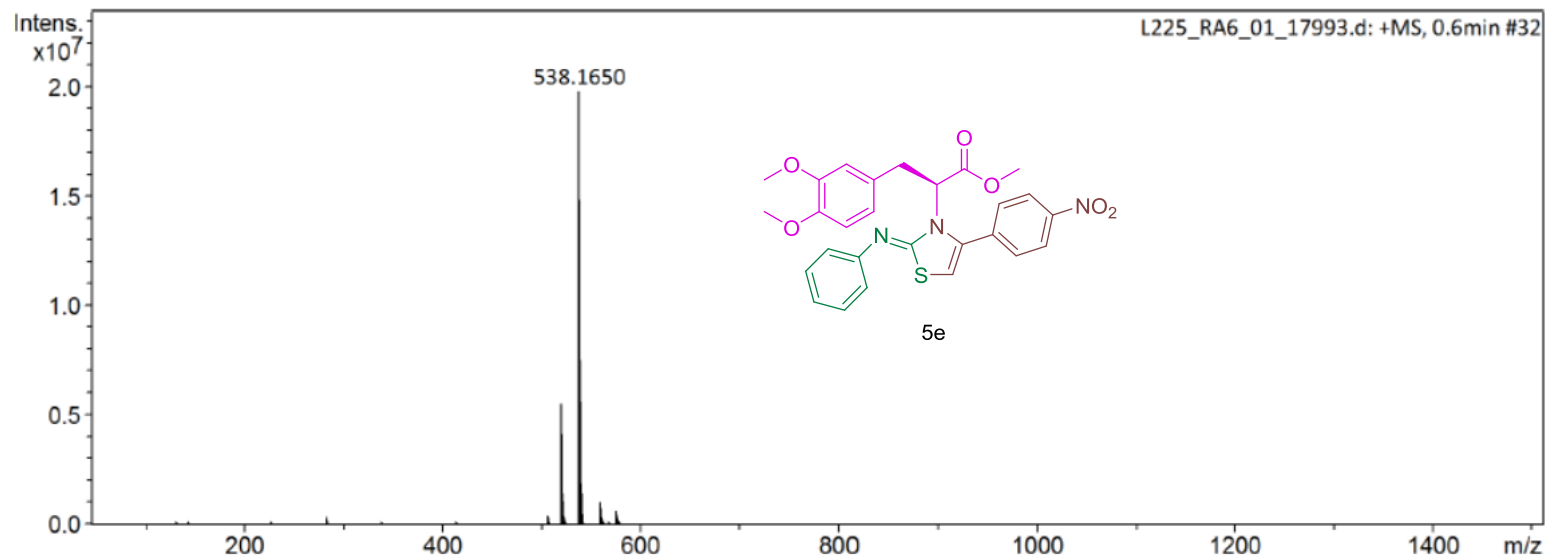
Waste

Set Corona

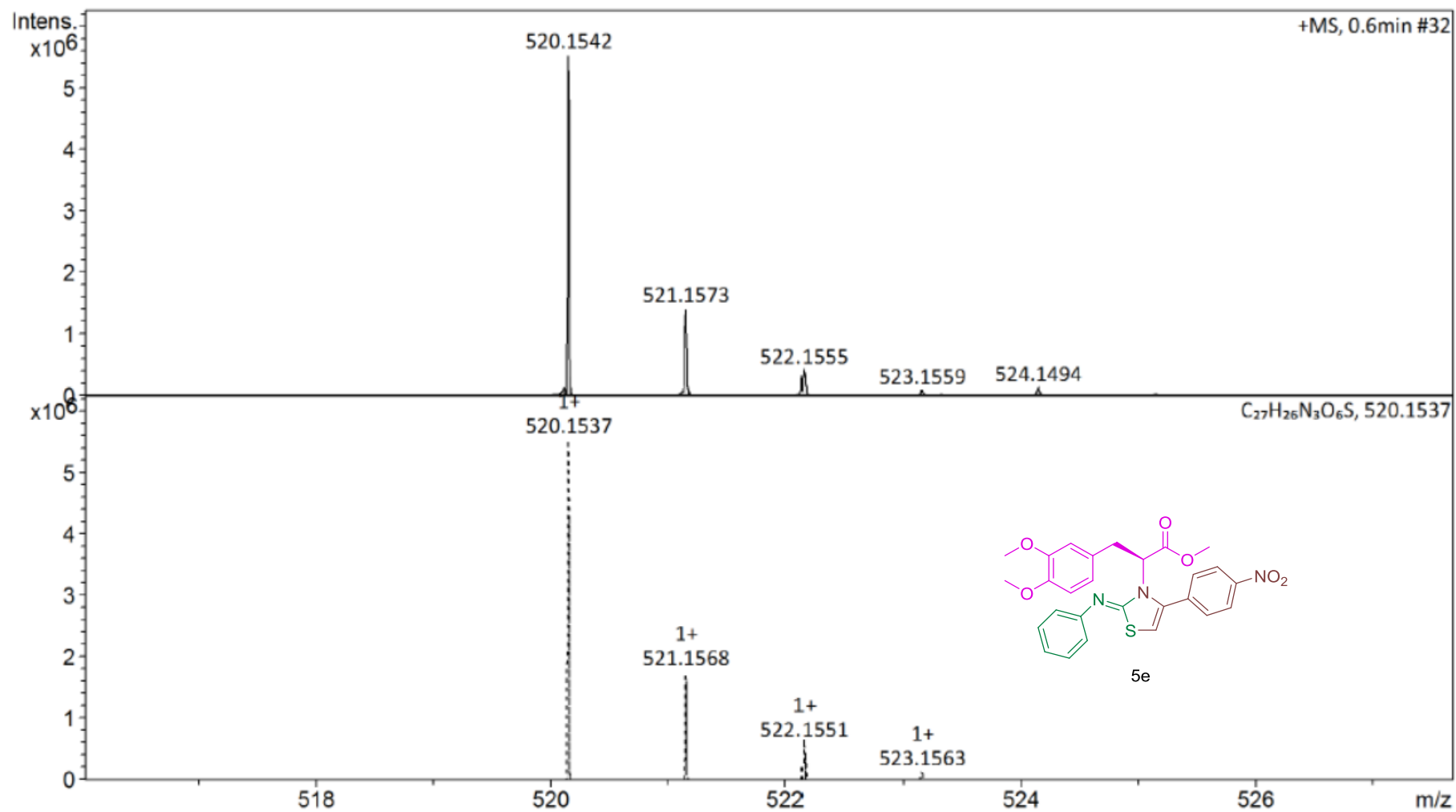
0 nA

Set APCI Heater

0 °C



HRMS of compound 5e

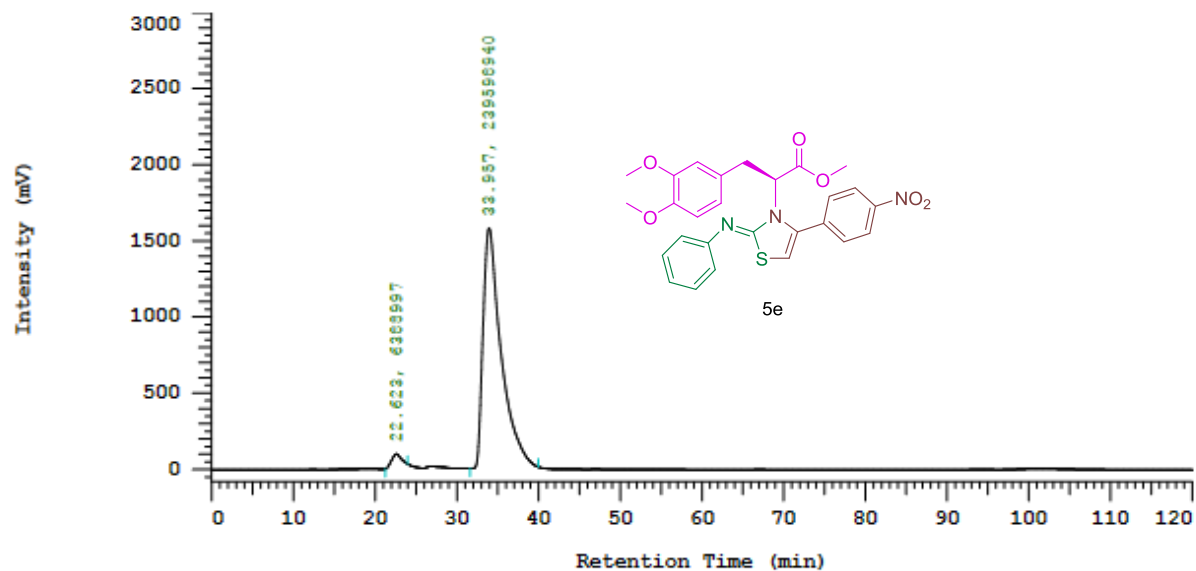


HRMS of compound 5e

Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0208\
Processing Method: 27e_ee
System (acquisition): Sys 1
Application(data): Linda
Sample Name: UNKNOWN001
Injection from this vial: 1 of 1
Sample Description:

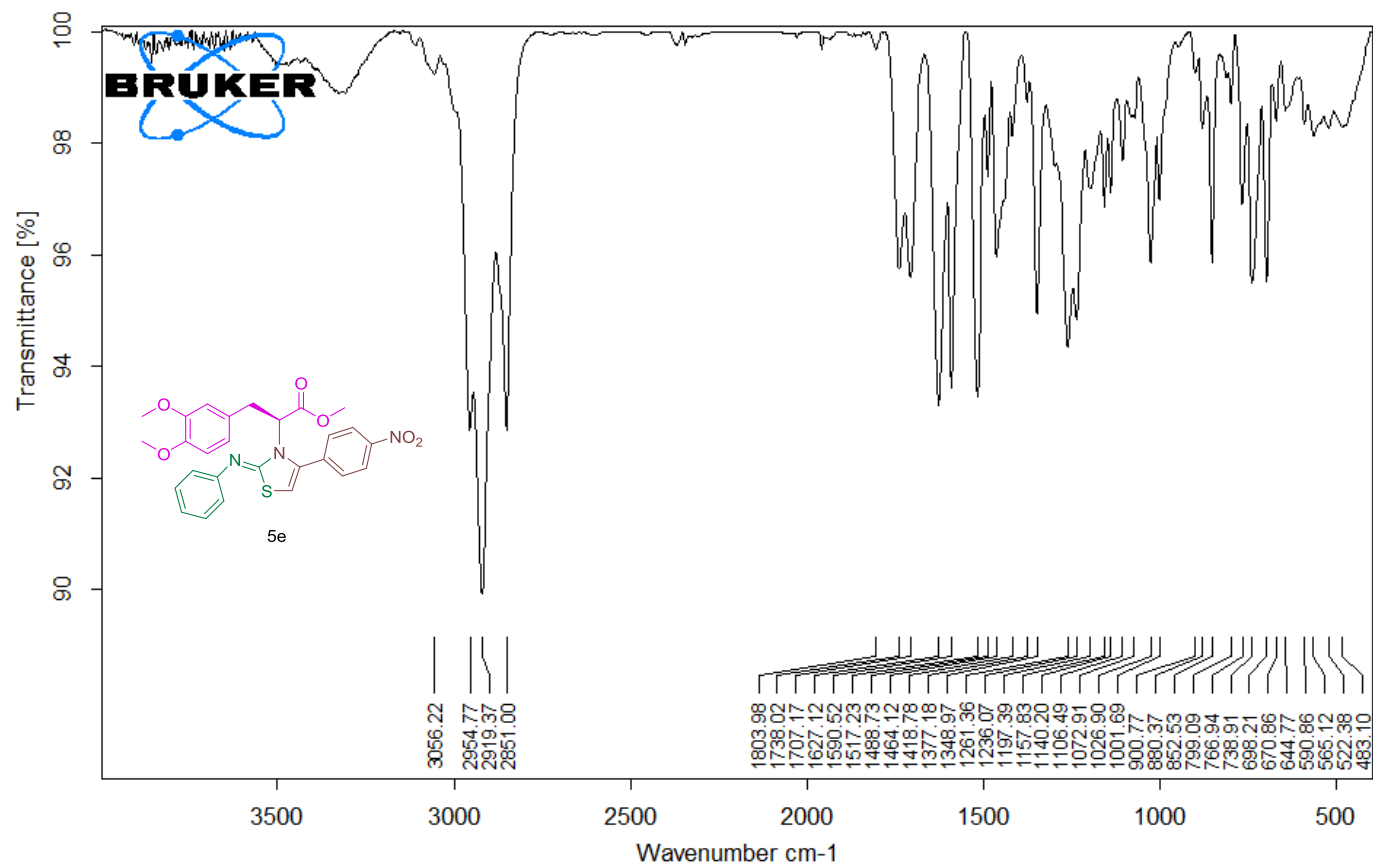
Series: 0208
Vial Number: 1
Vial Type: UNK
Volume: 10.0 ul

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound 5e



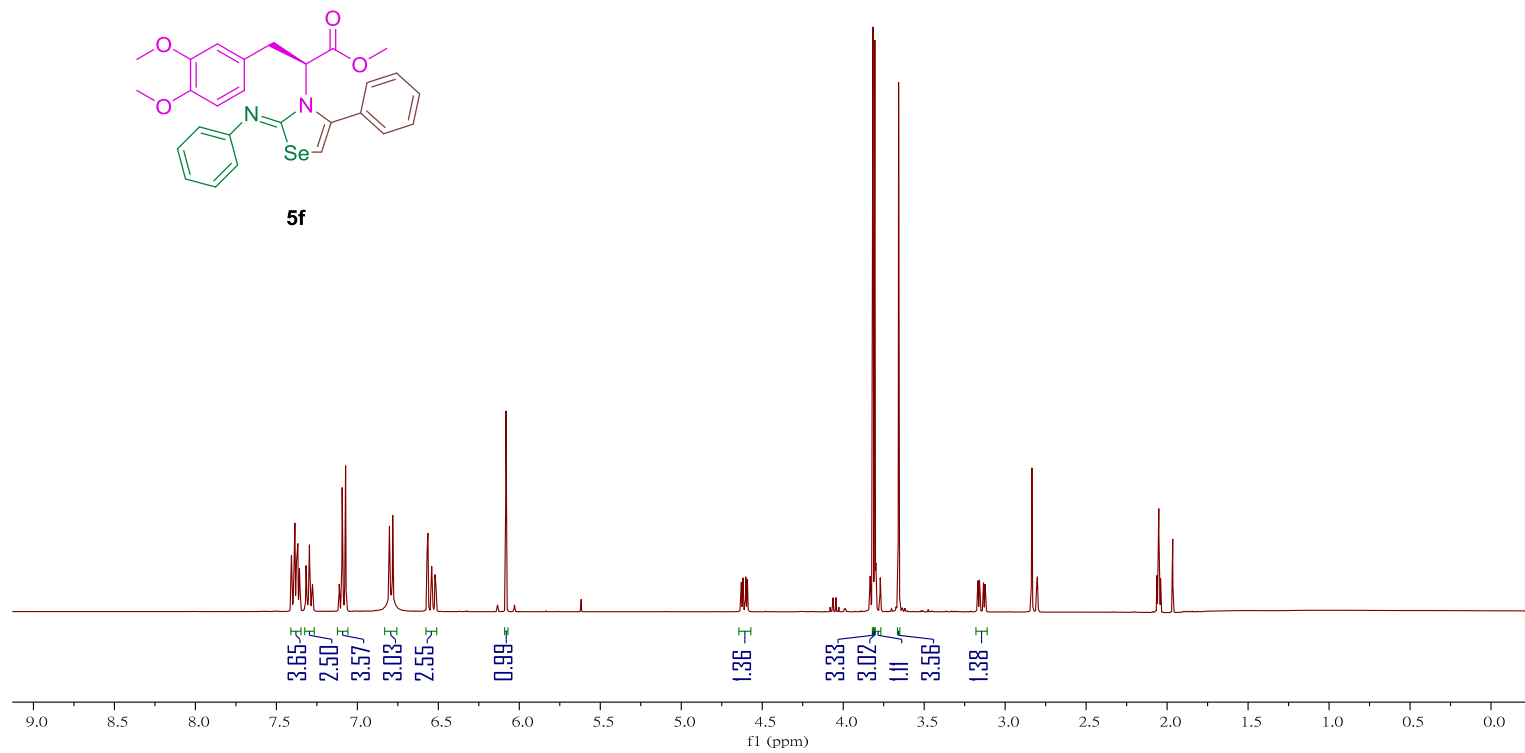
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L225.3

MIR_TR_DTGS_L225

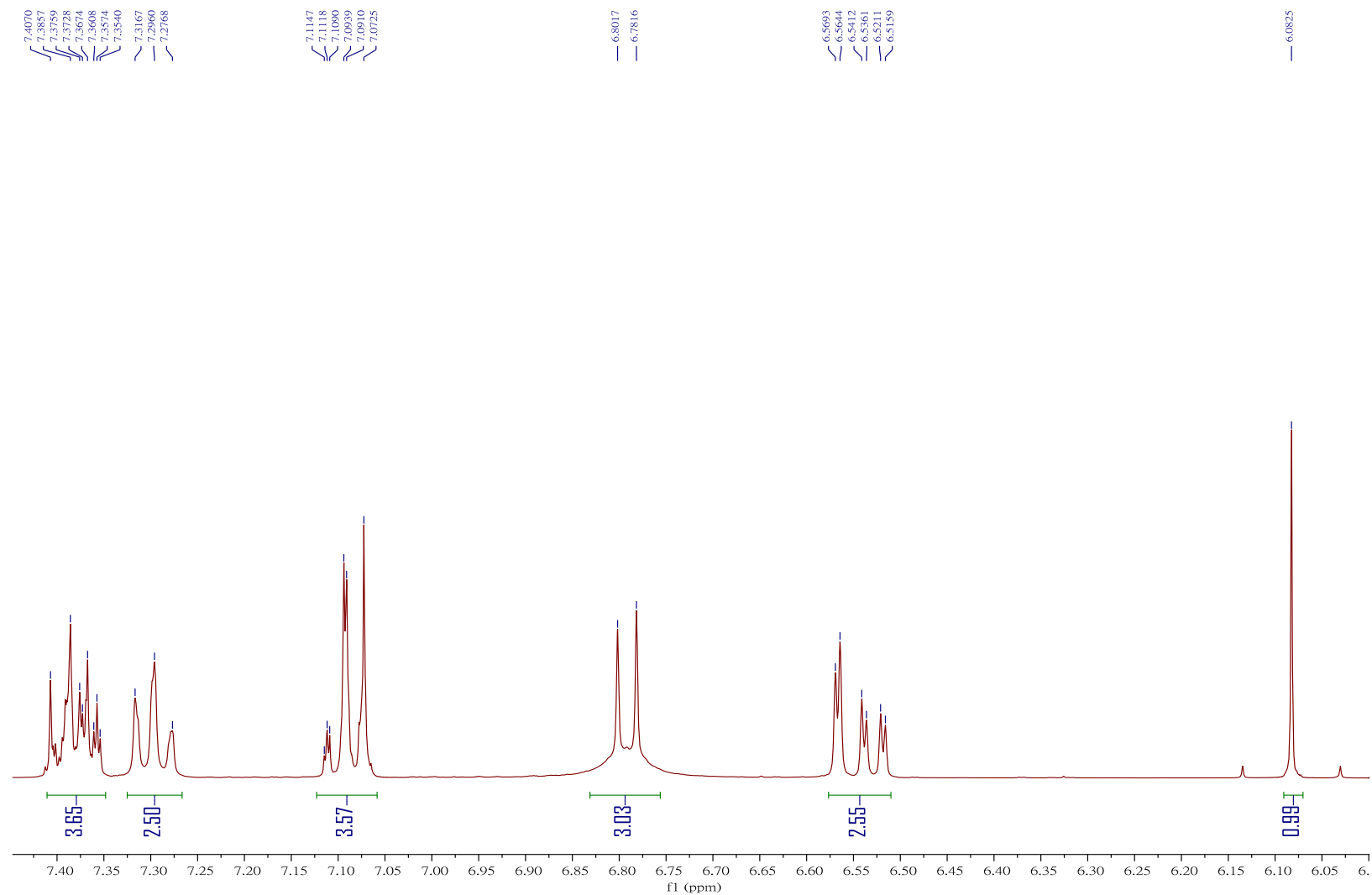
Instrument type and / or accessory

9/4/2018

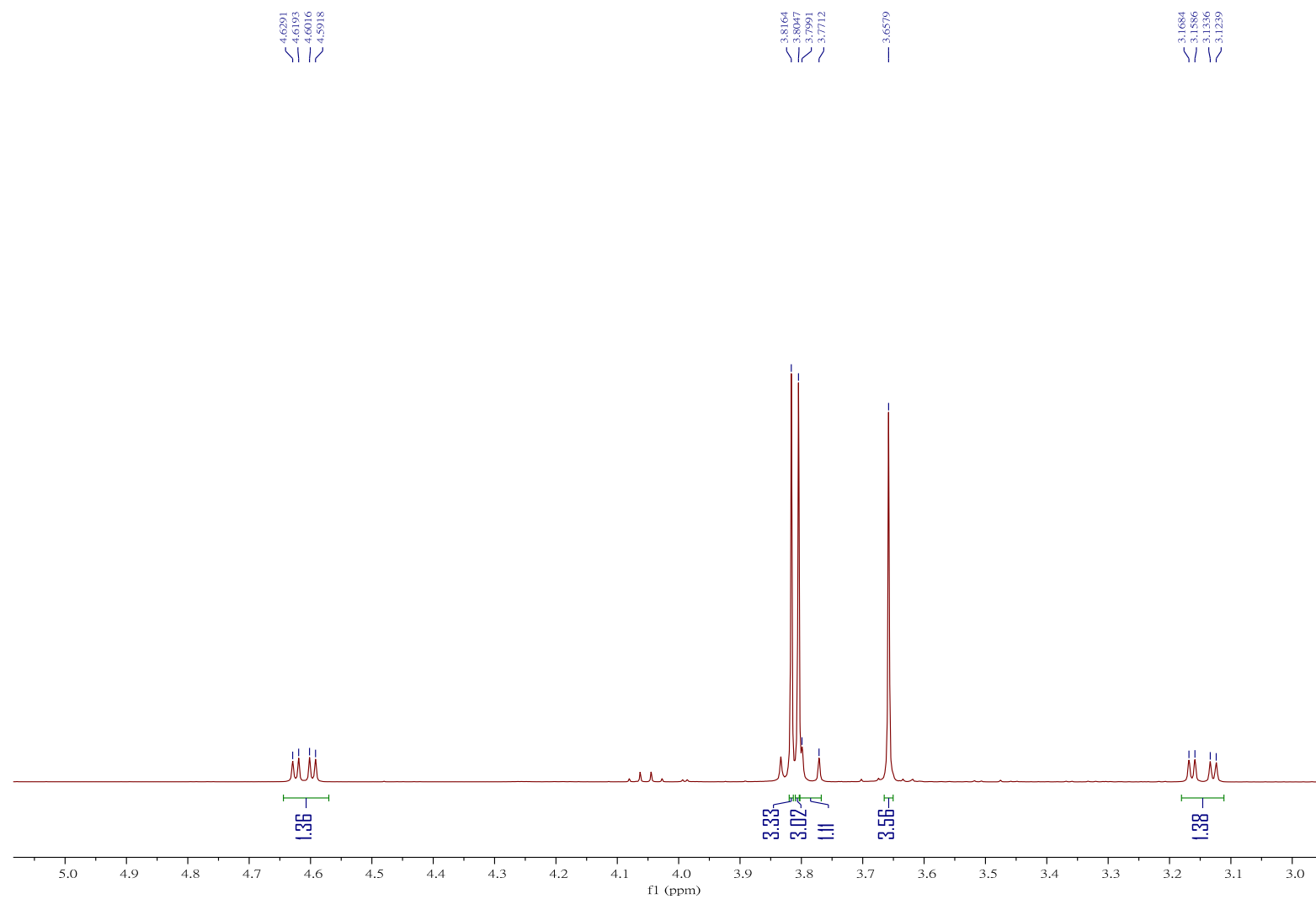
FT-IR Spectrum of compound **5e**



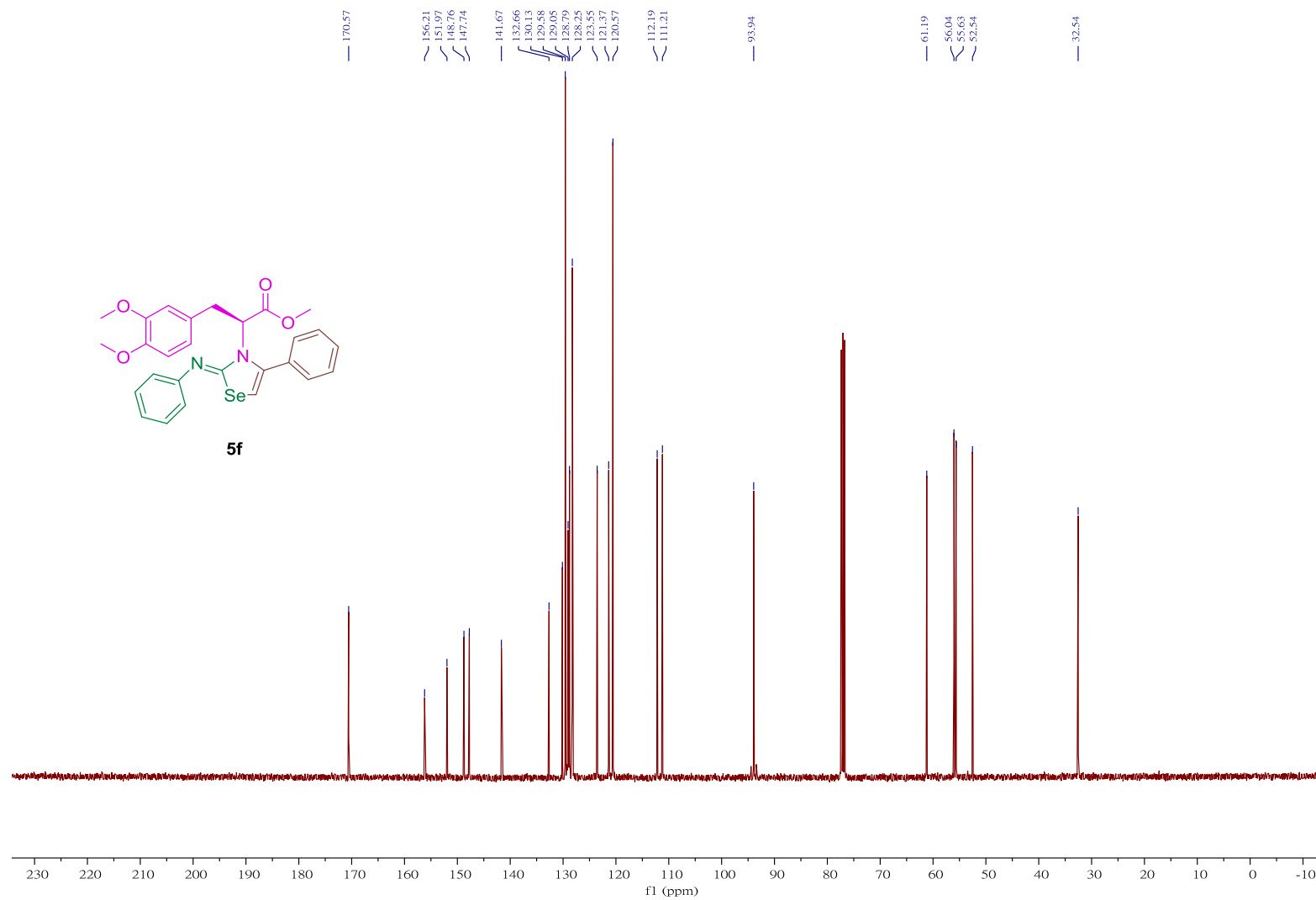
^1H NMR Spectrum (400 MHz) of compound **5f** in d_6 -Acetone



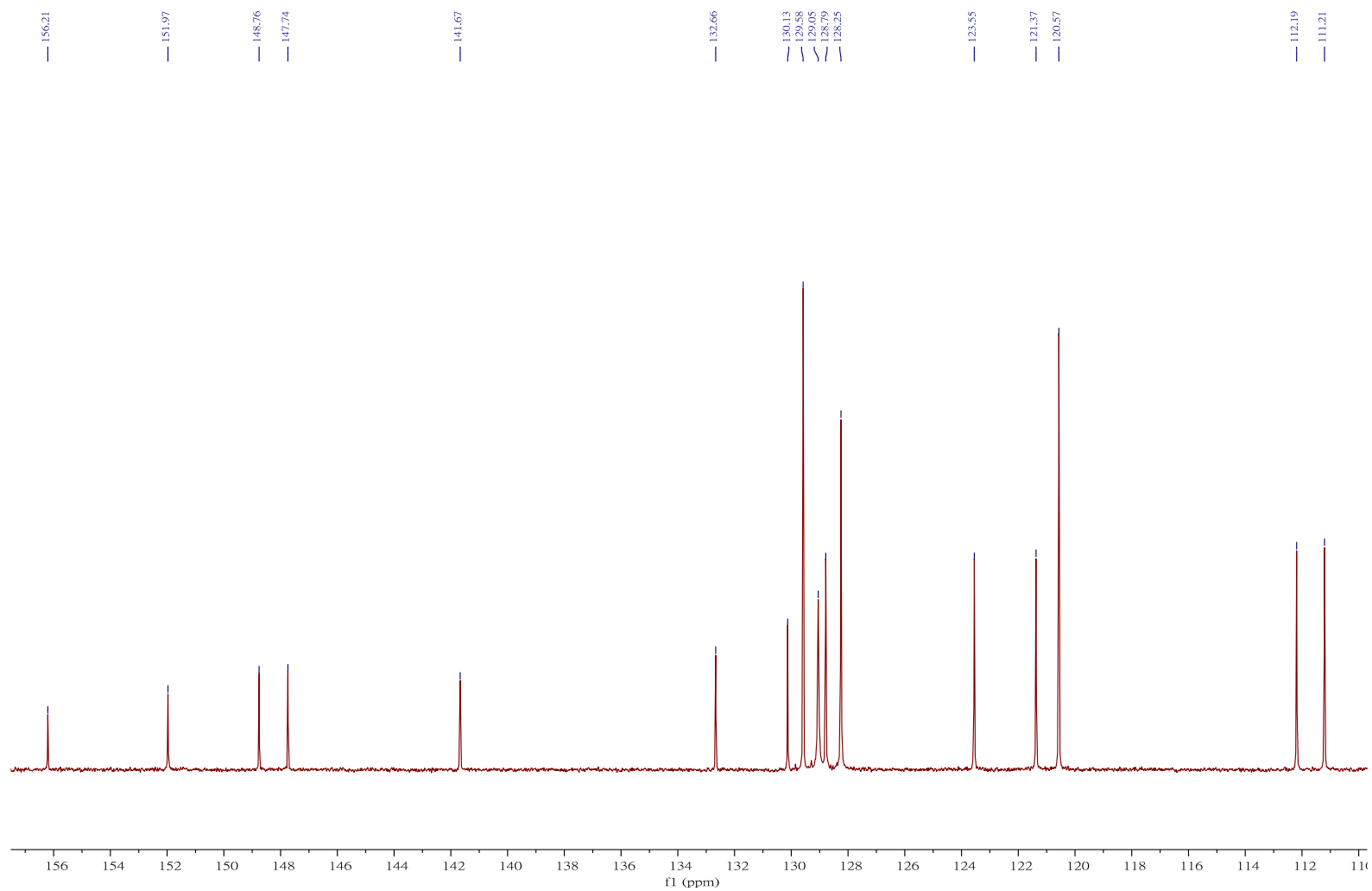
Expansion of ^1H NMR Spectrum (400 MHz) of compound **5f** in acetone- d_6



Expansion of ^1H NMR Spectrum (400 MHz) of compound **5f** in acetone- d_6



¹³C NMR Spectrum (101 MHz) of compound **5f in CDCl₃**



Expansion of ¹³C NMR Spectrum (101 MHz) of compound **27f** in CDCl₃

Display Report

Analysis Info

Analysis Name D:\Data\nctu service\data\2018\20180417\L227_RA7_01_17994.d

Method Small molecule.m

Sample Name L227

Comment

Acquisition Date 4/17/2018 1:08:21 PM

Operator NCTU

Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type ESI

Focus Active

Scan Begin 50 m/z

Scan End 1500 m/z

Ion Polarity

Positive

Set Capillary

4500 V

Set End Plate Offset

-500 V

Set Charging Voltage

2000 V

Set Corona

0 nA

Set Nebulizer

1.0 Bar

Set Dry Heater

200 °C

Set Dry Gas

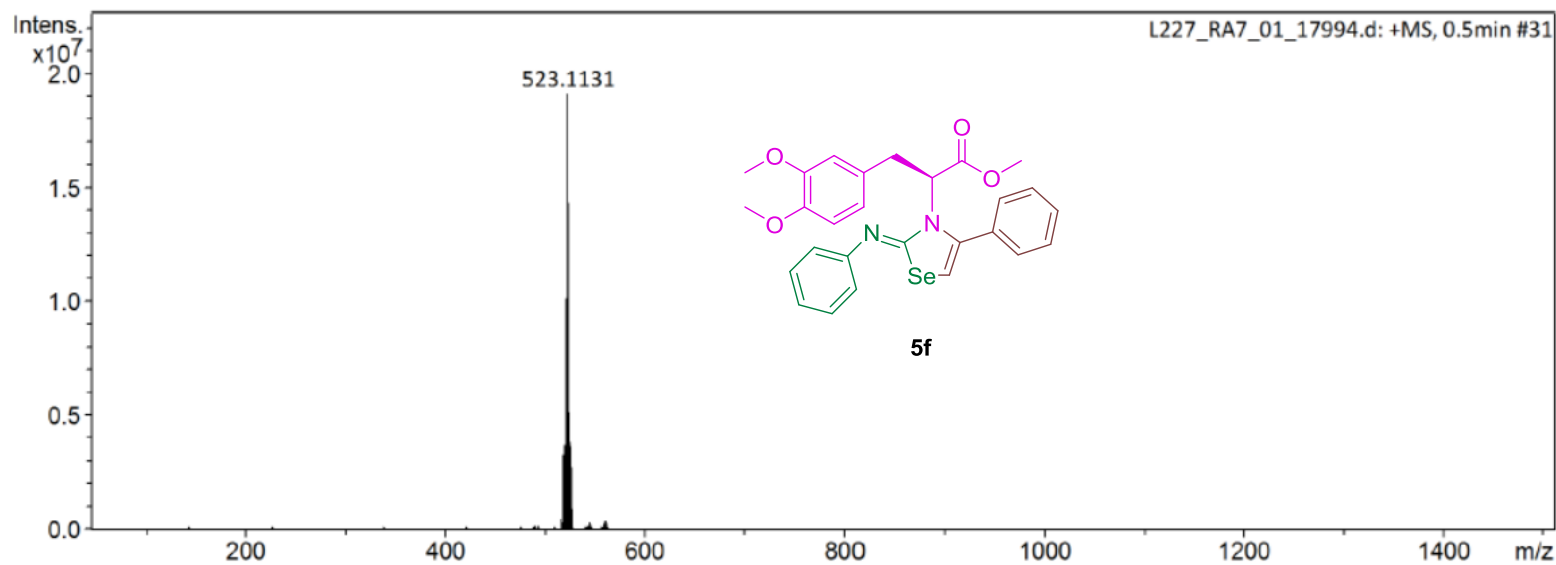
6.0 l/min

Set Divert Valve

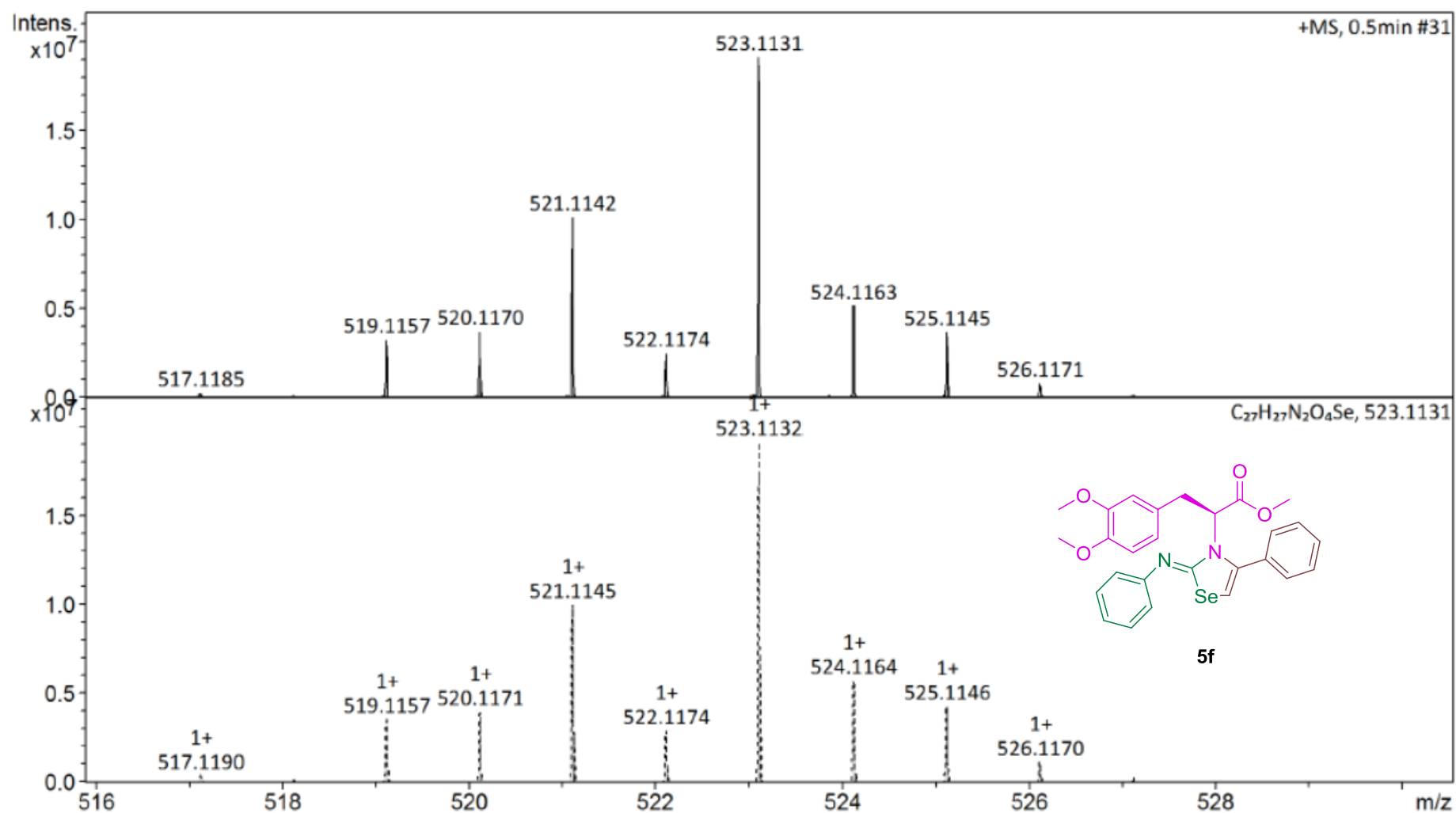
Waste

Set APCI Heater

0 °C



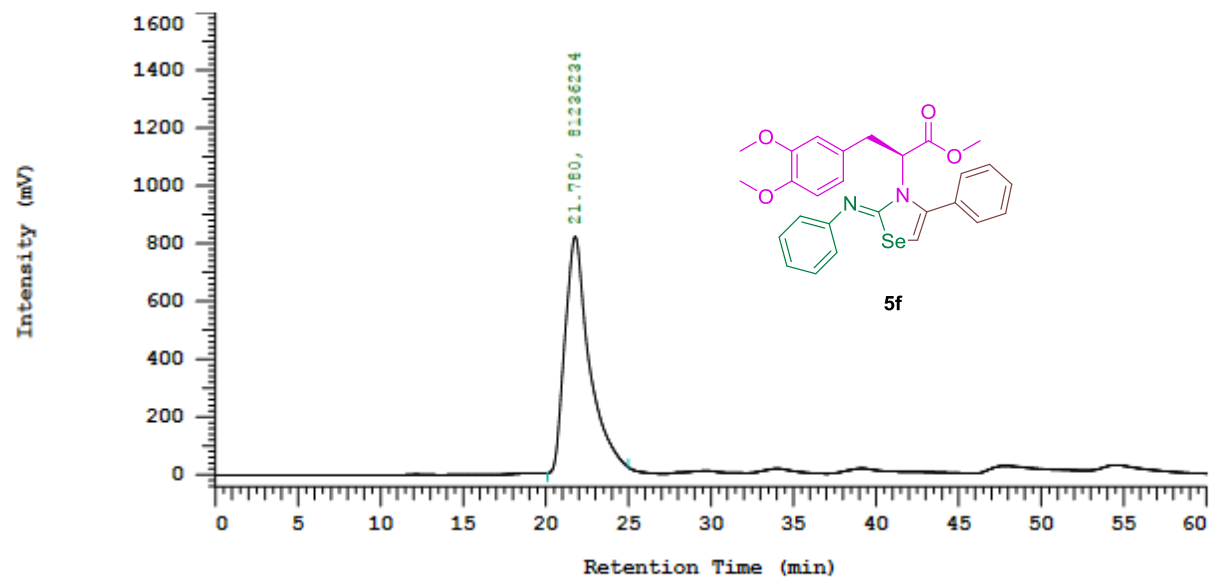
HRMS of compound **5f**



Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0213\
Processing Method: 27f_ee
System (acquisition): Sys 1
Application(data): Linda
Sample Name: UNKNOWN001
Injection from this vial: 1 of 1
Sample Description:

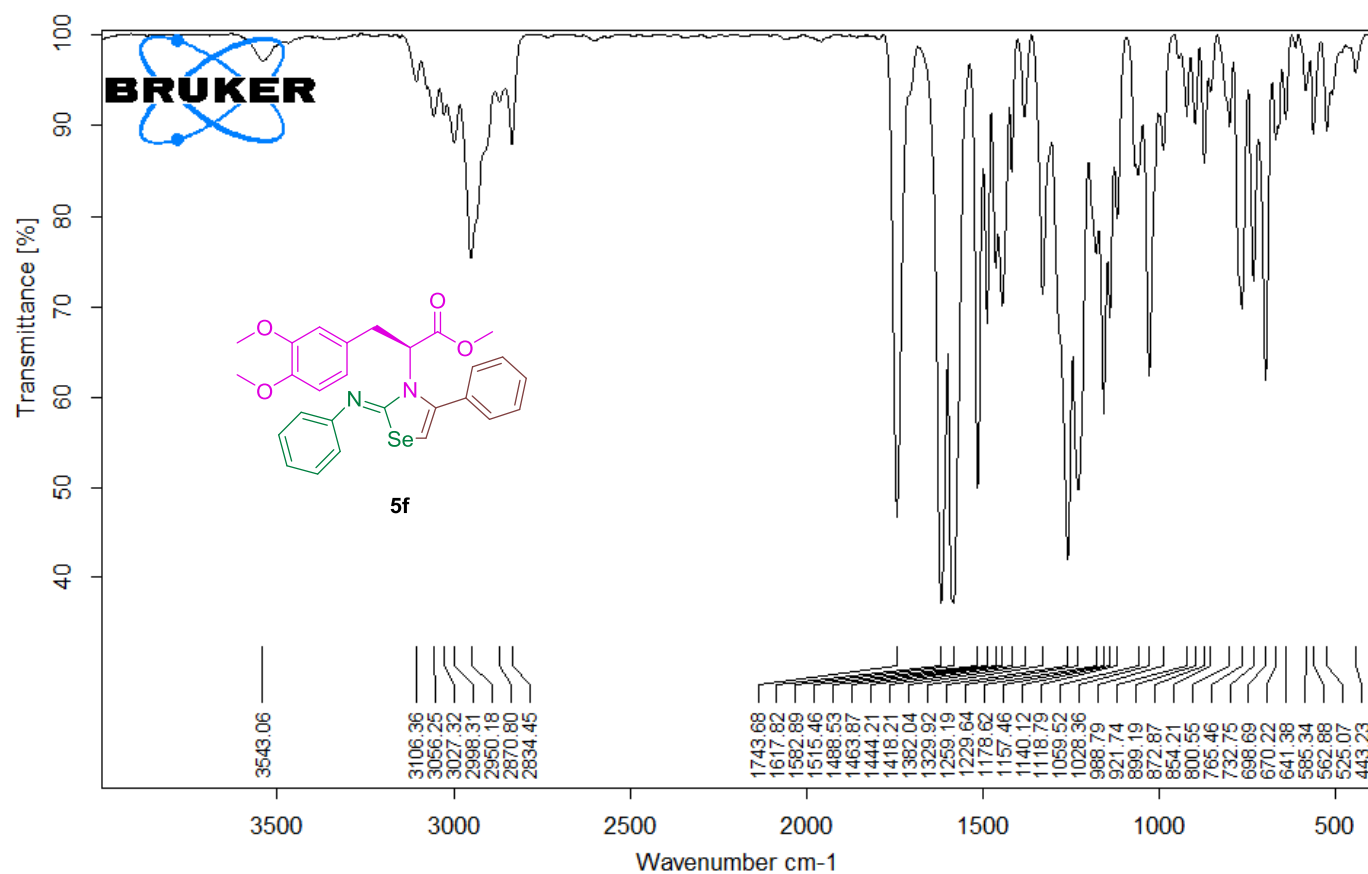
Series: 0213
Vial Number: 1
Vial Type: UNK
Volume: 10.0 ul

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound **5f**



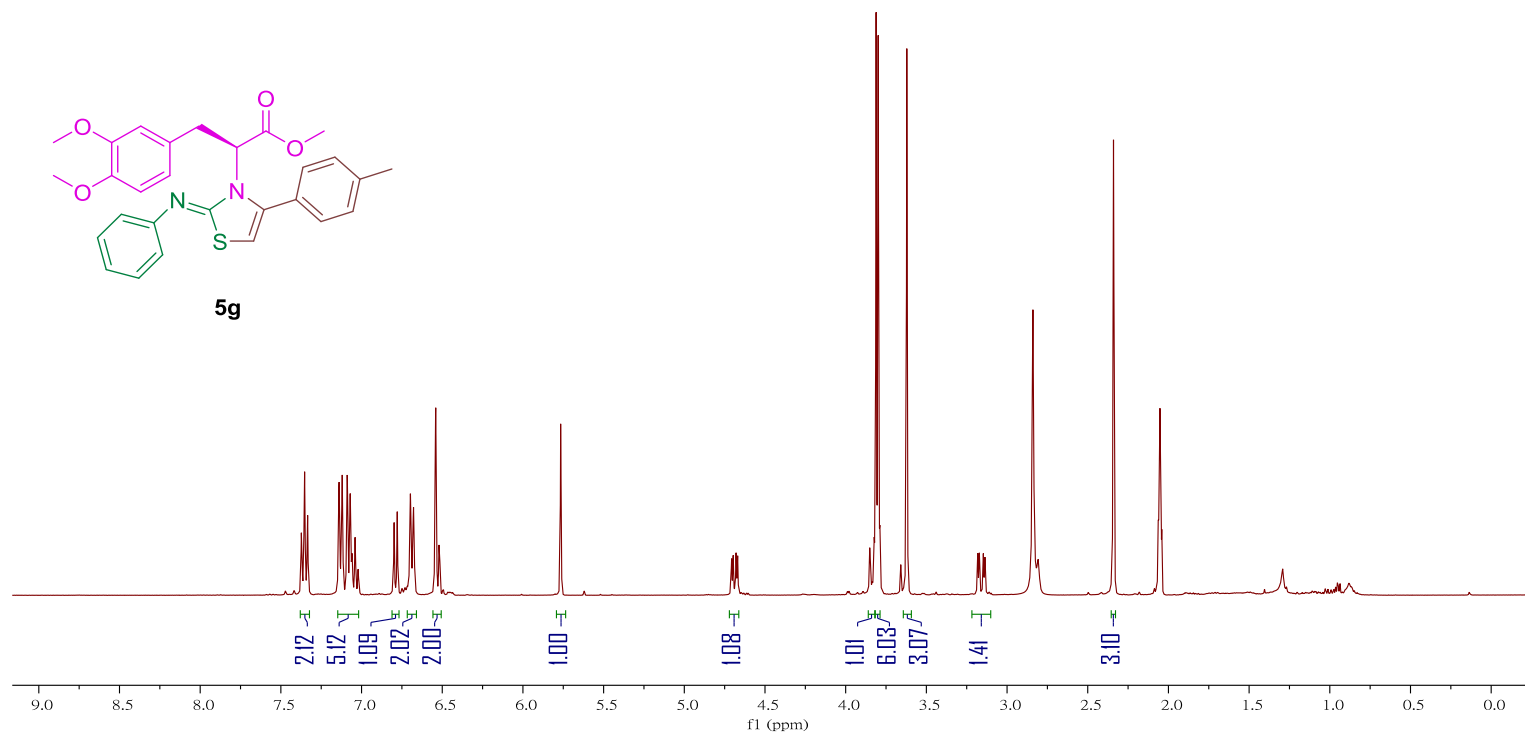
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L227.0

MIR_TR_DTGS_L227

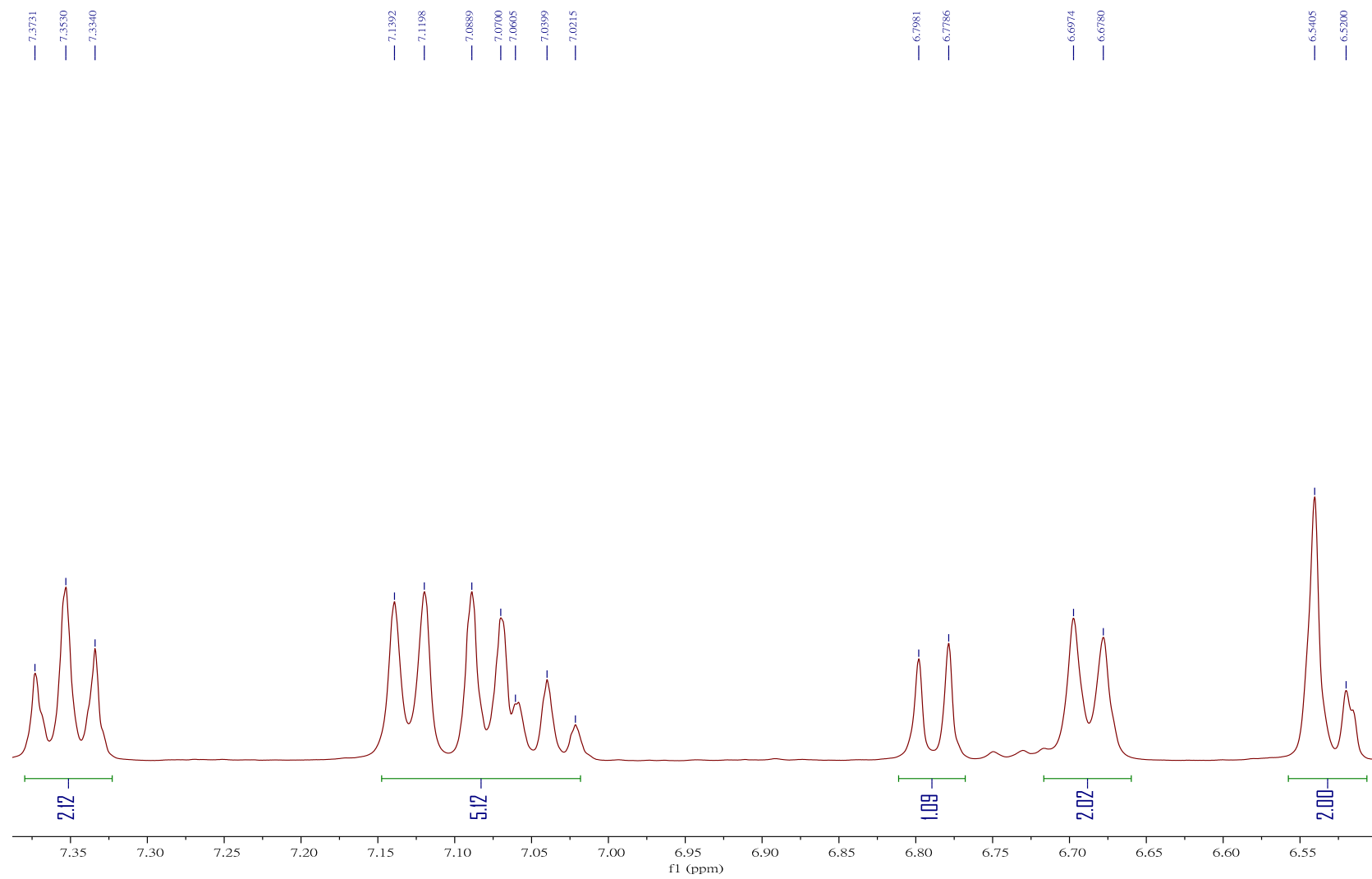
Instrument type and / or accessory

9/4/2018

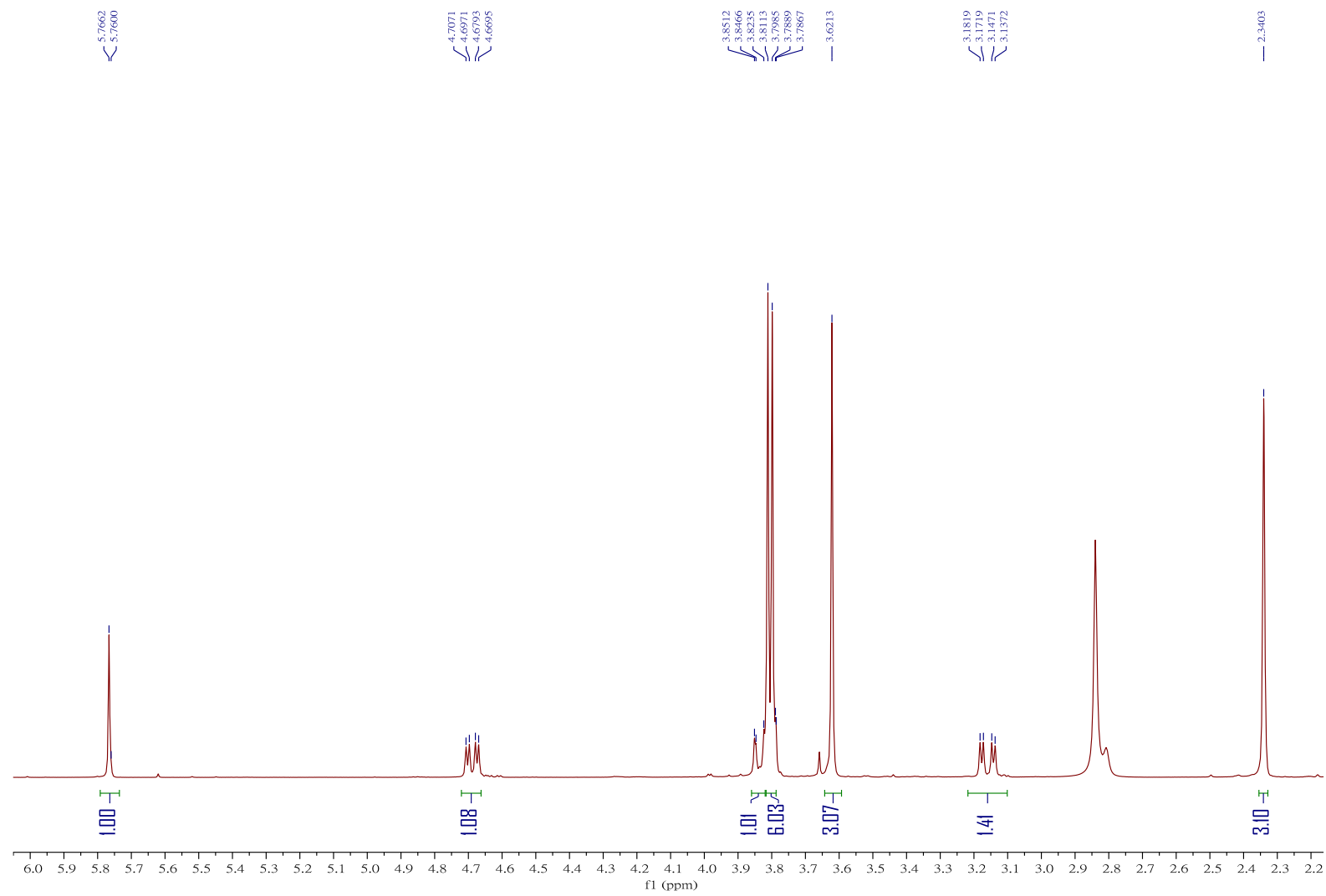
FT-IR Spectrum of compound **5f**



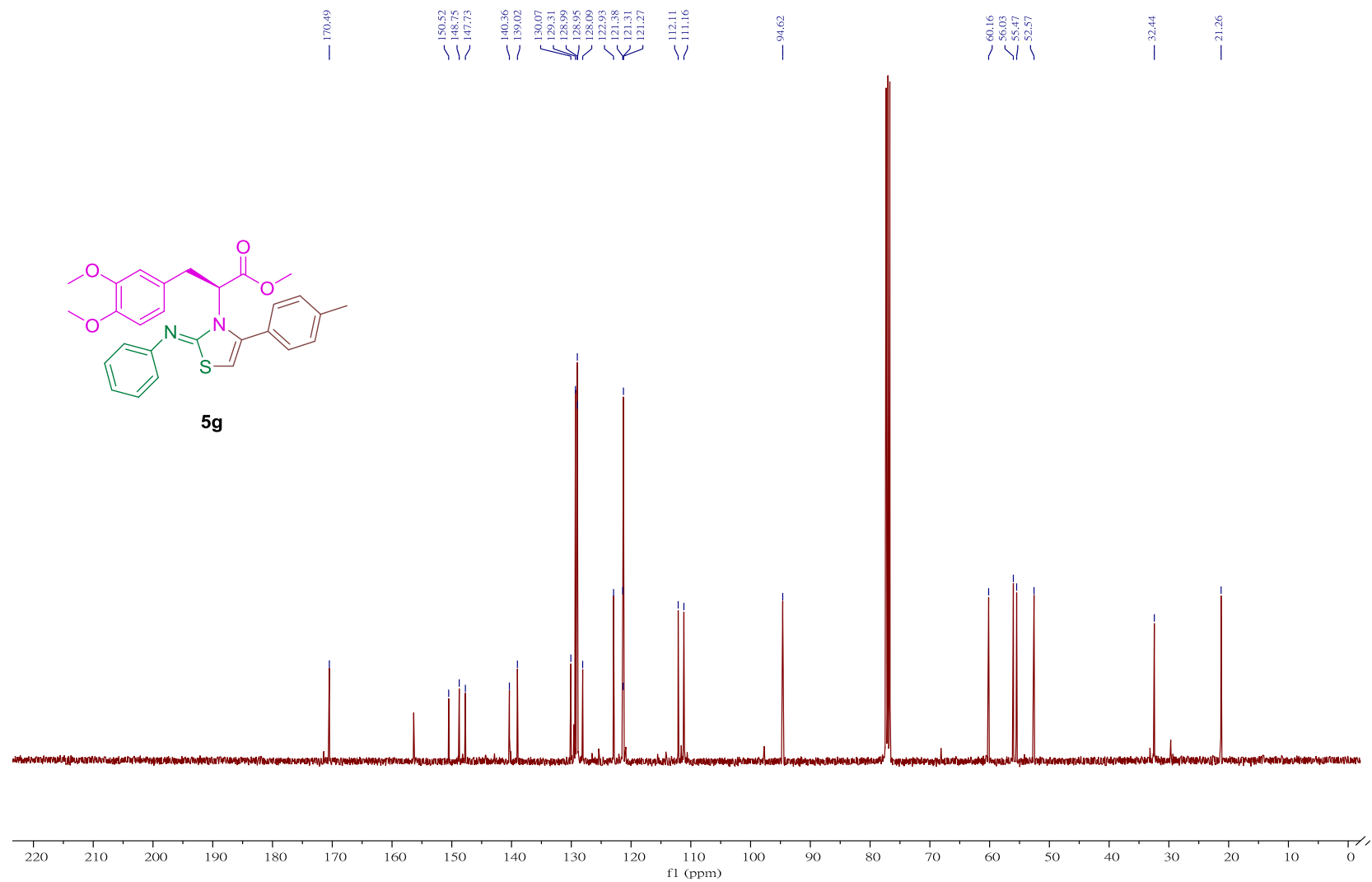
^1H NMR Spectrum (400 MHz) of compound **5g** in acetone- d_6



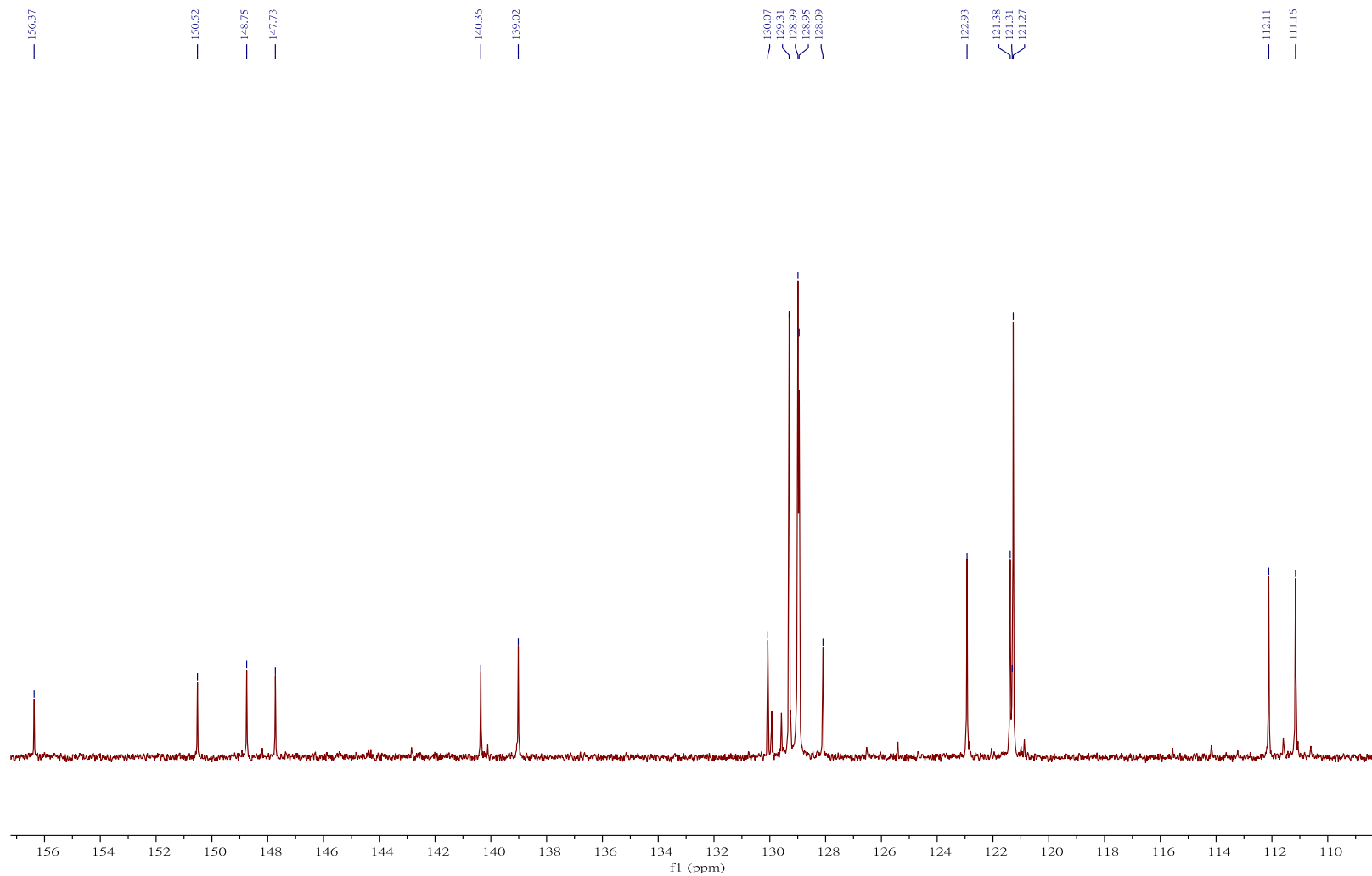
Expansion of ¹H NMR Spectrum (400 MHz) of compound **5g** in acetone-*d*₆



Expansion of ¹H NMR Spectrum (400 MHz) of compound **5g** in acetone-*d*₆



¹³C NMR Spectrum (101 MHz) of compound **5g** in CDCl₃

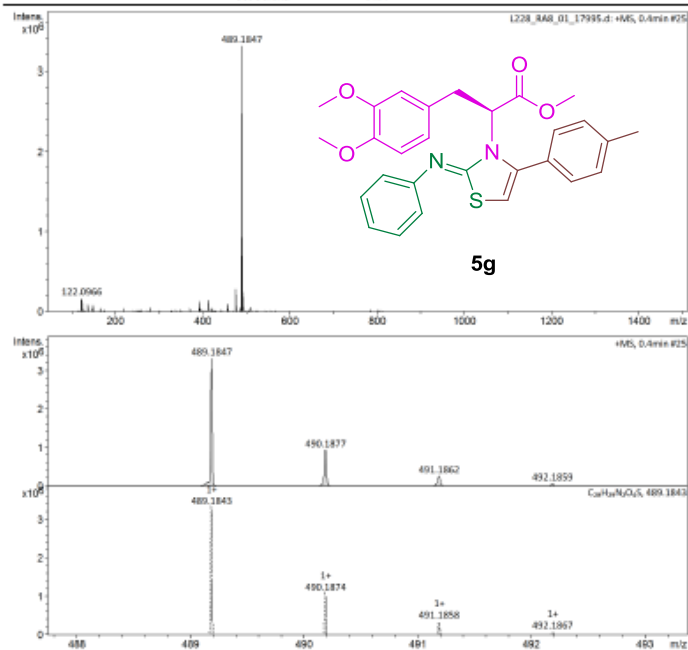


Expansion of ¹³C NMR Spectrum (101 MHz) of compound **5g** in CDCl₃

Display Report

Analysis Info		Acquisition Date	4/17/2018 1:12:40 PM	
Analysis Name	H:\20181-6\20180417\L228_RA8_01_17995.d	Operator	NCTU	
Method	Small molecule.m	Instrument	Impact HD	1819696.00164
Sample Name	L228	Comment		

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

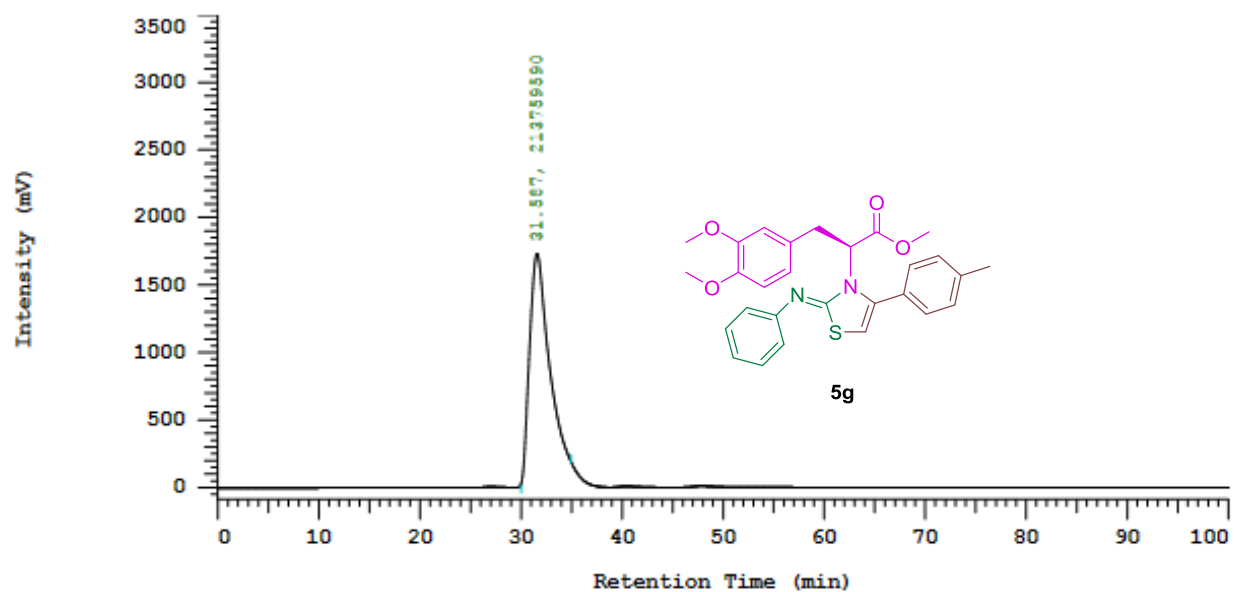


HRMS of compound **5g**

Processing Method: 27k_ee
System (acquisition): Sys 1
Application(data): Linda
Sample Name: UNKNOWN001
Injection from this vial: 1 of 1
Sample Description:

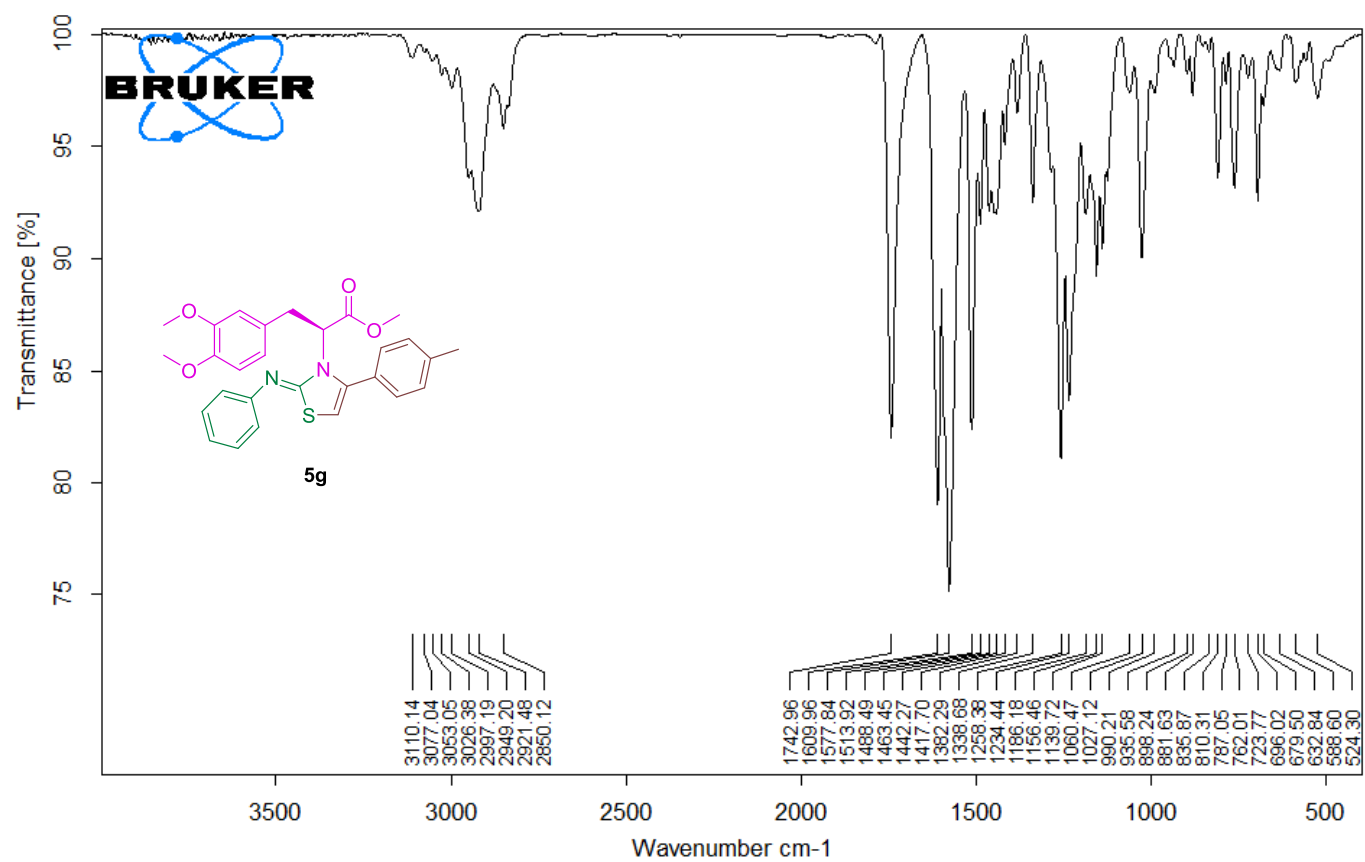
Series: 0201
Vial Number: 1
Vial Type: UNK
Volume: 10.0 ul

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound **5g**



D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L228.0

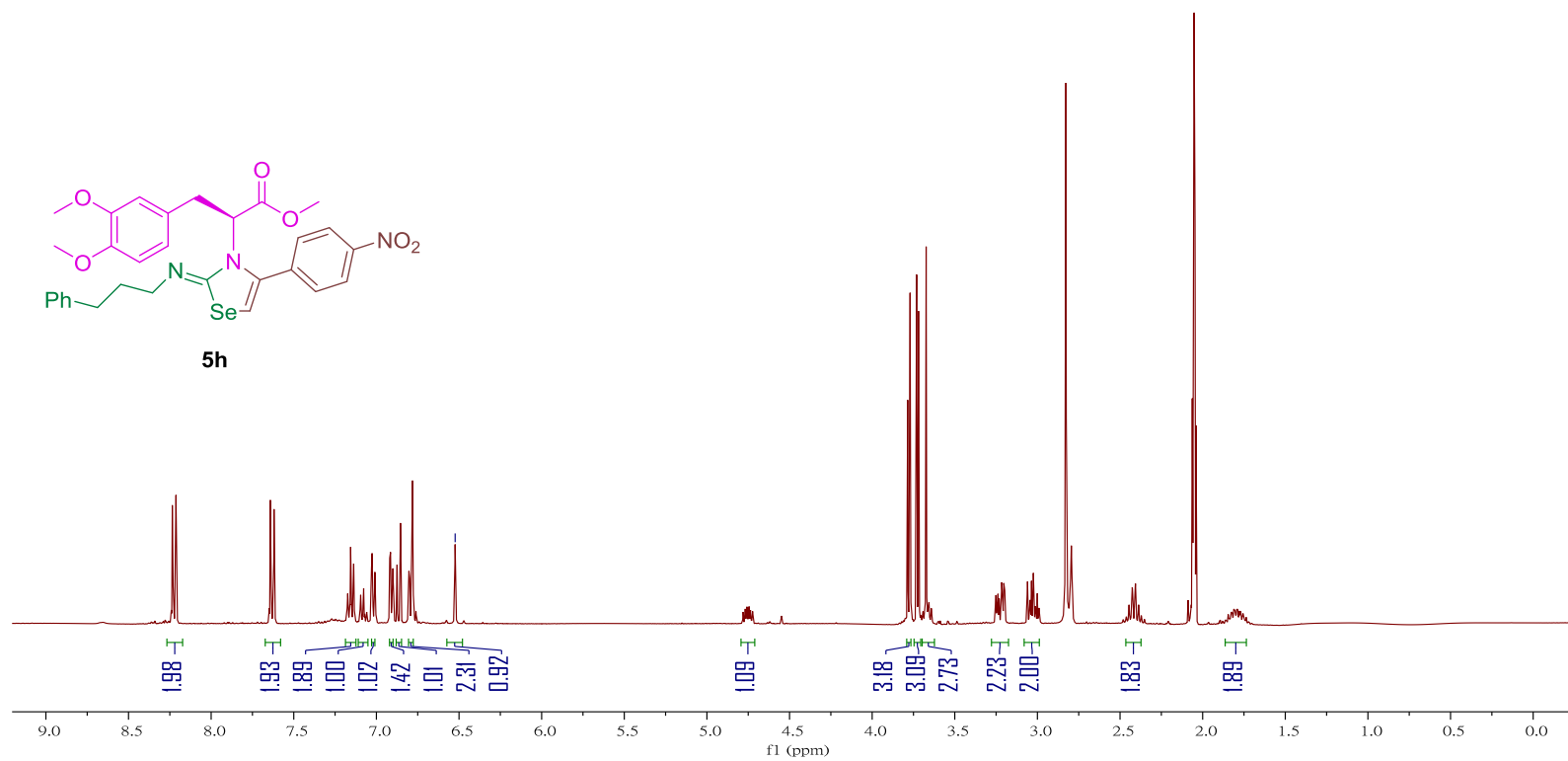
MIR_TR_DTGS_L228

Instrument type and / or accessory

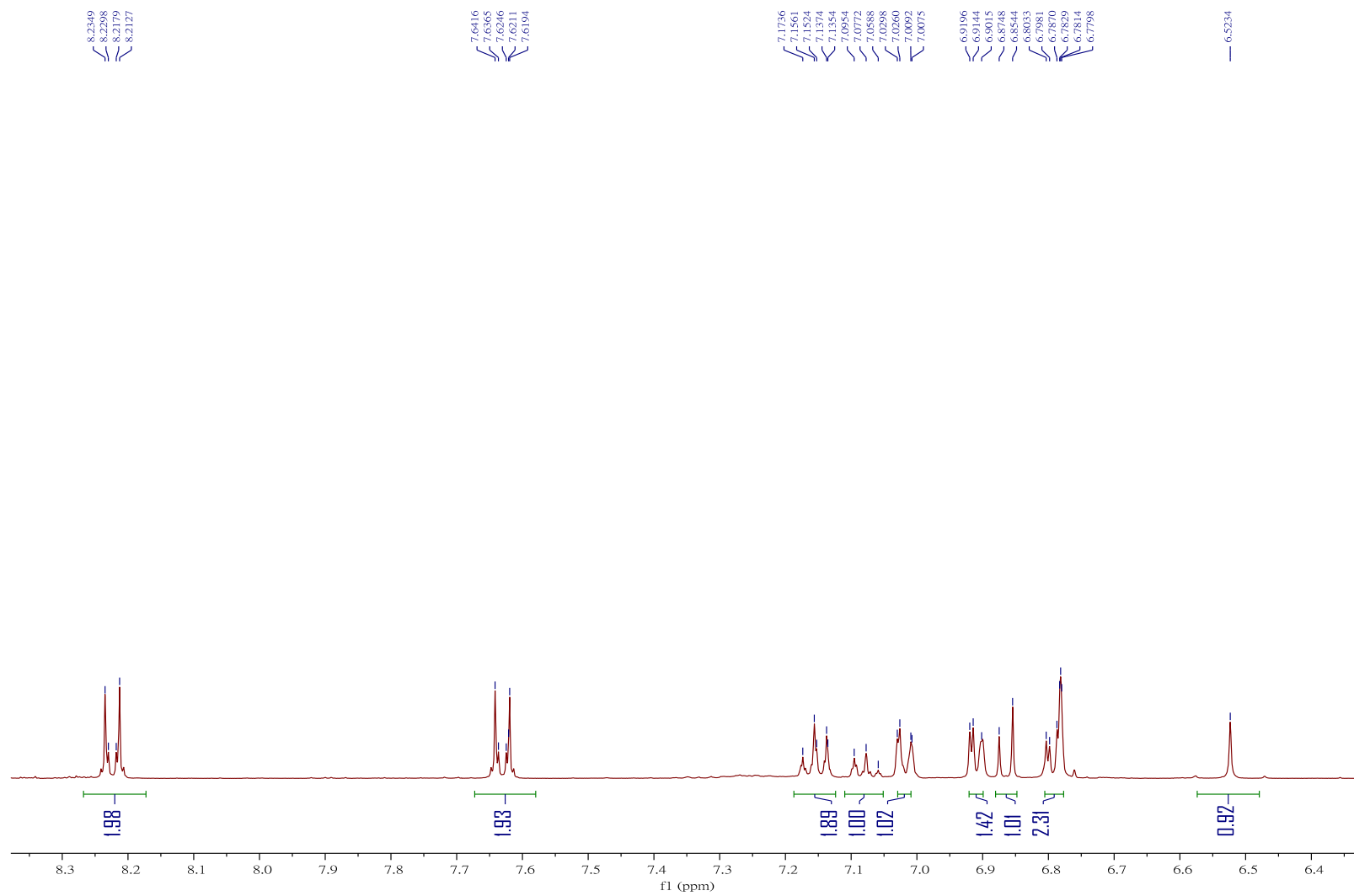
9/4/2018

Page 1/1

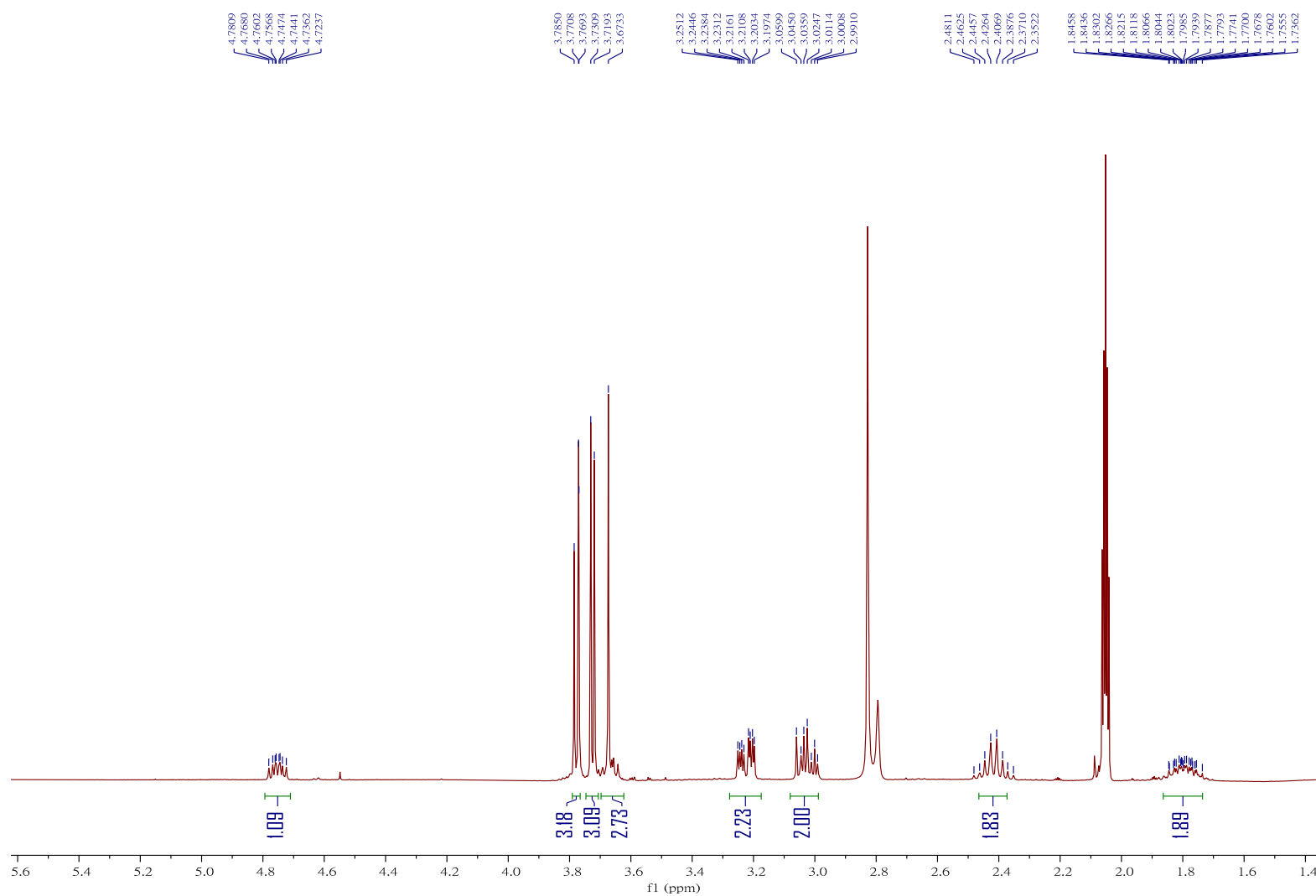
FT-IR Spectrum of compound **5g**



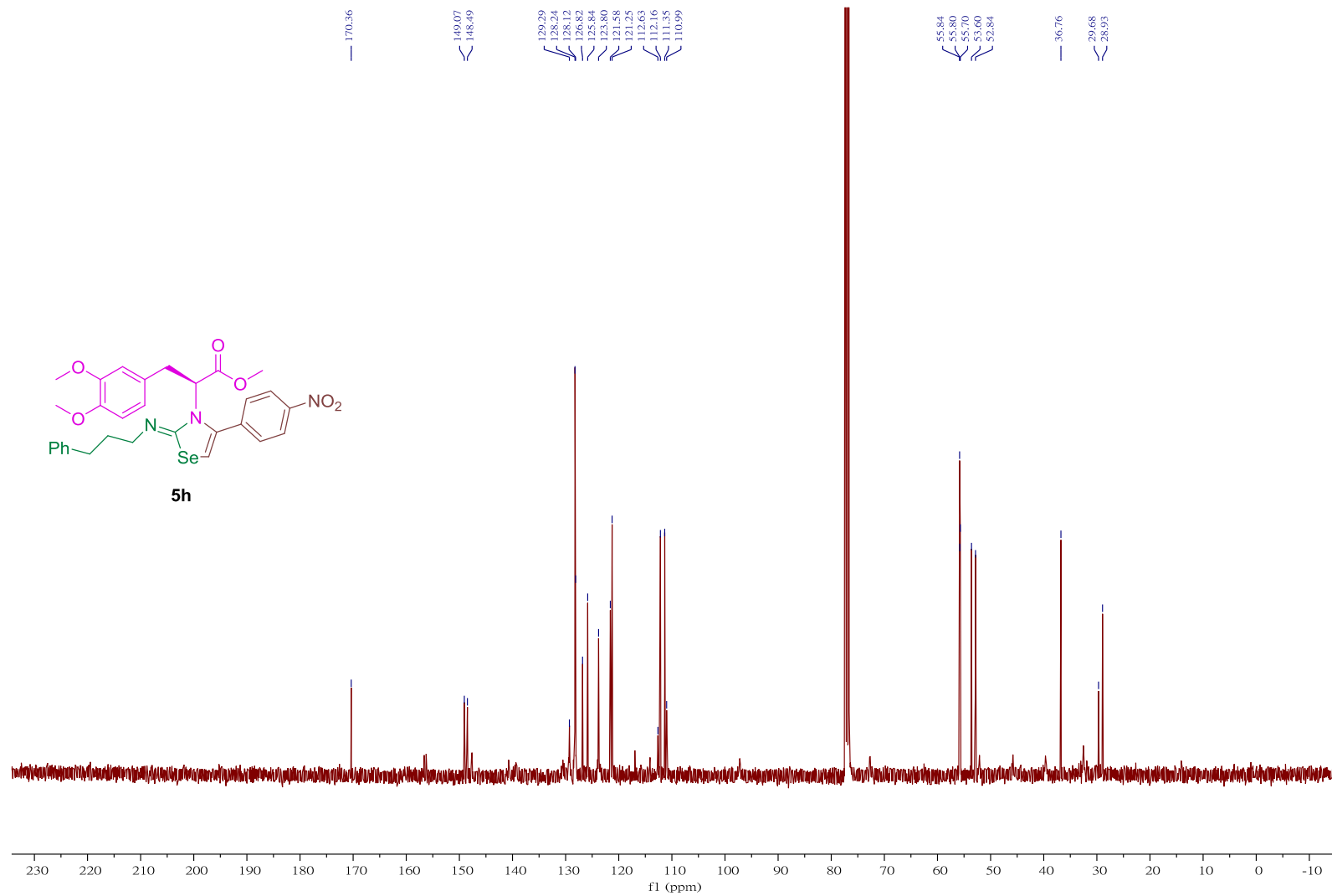
^1H NMR Spectrum (400 MHz) of compound **5h** in acetone- d_6



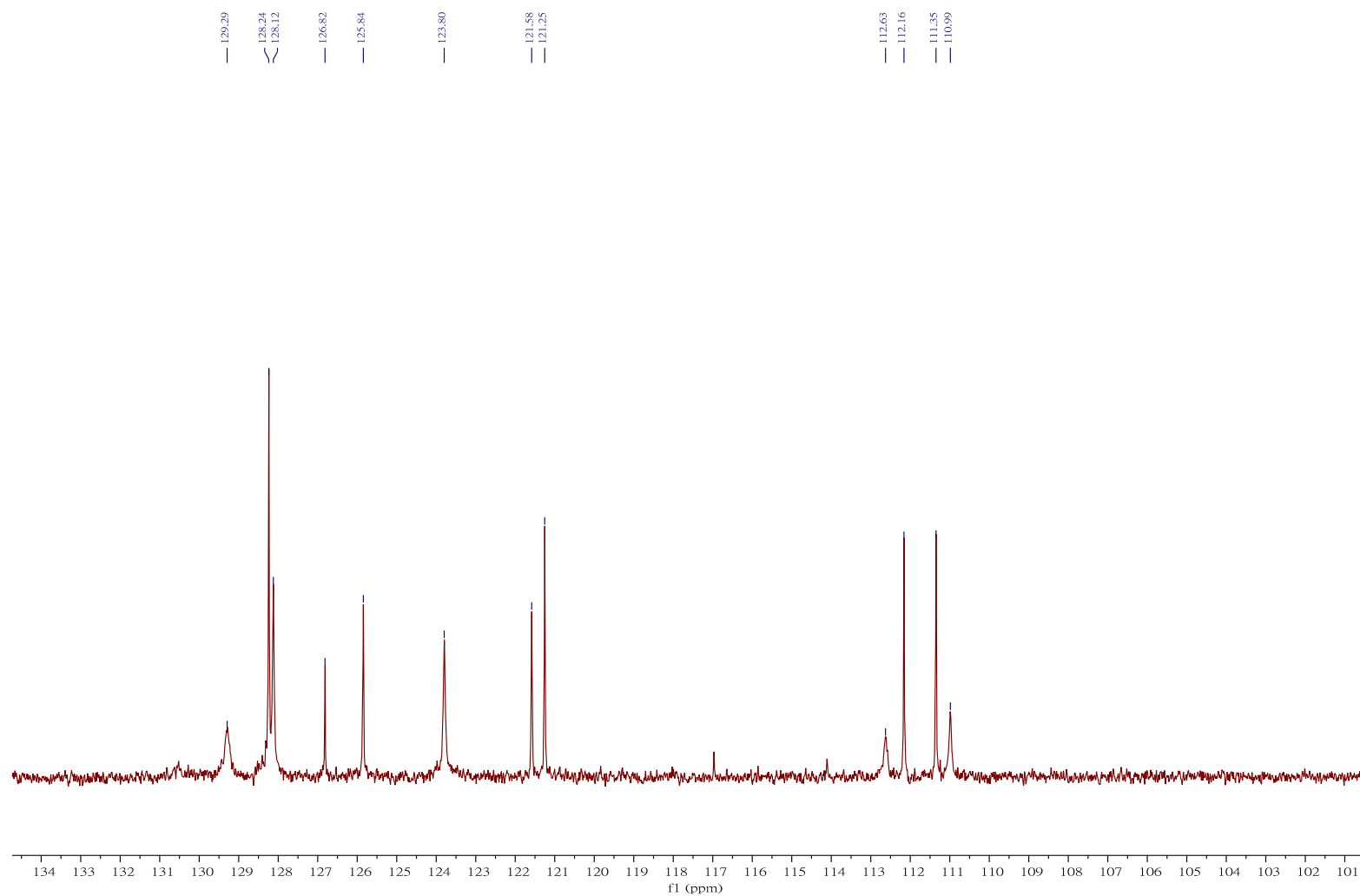
Expansion of ^1H NMR Spectrum (400 MHz) of compound **5h** in acetone- d_6



Expansion of ^1H NMR Spectrum (400 MHz) of compound **5h** in acetone- d_6



^{13}C NMR Spectrum (101 MHz) of compound **5h** in CDCl_3



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **5h** in CDCl_3

Display Report

Analysis Info

Analysis Name D:\Data\nctu service\data\2018\20180417\L190_RB1_01_17996.d

Method Small molecule.m

Sample Name L190

Comment

Acquisition Date 4/17/2018 1:17:02 PM

Operator NCTU

Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type ESI

Focus Active

Scan Begin 50 m/z

Scan End 1500 m/z

Ion Polarity

Set Capillary

Set End Plate Offset

Set Charging Voltage

Set Corona

Positive

4500 V

-500 V

2000 V

0 nA

Set Nebulizer

Set Dry Heater

Set Dry Gas

Set Divert Valve

Set APCI Heater

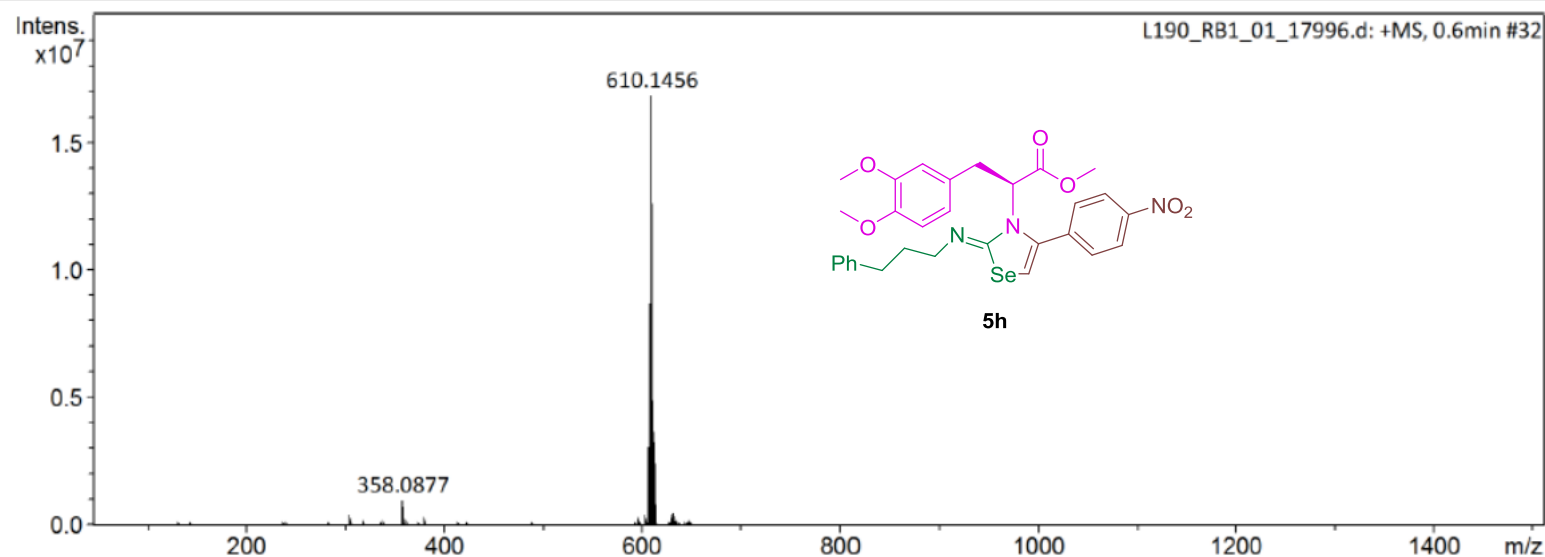
1.0 Bar

200 °C

6.0 l/min

Waste

0 °C



Processing Method: 27h_ee

System (acquisition): Sys 1

Application(data): Linda

Sample Name: UNKNOWN001

Injection from this vial: 1 of 1

Sample Description:

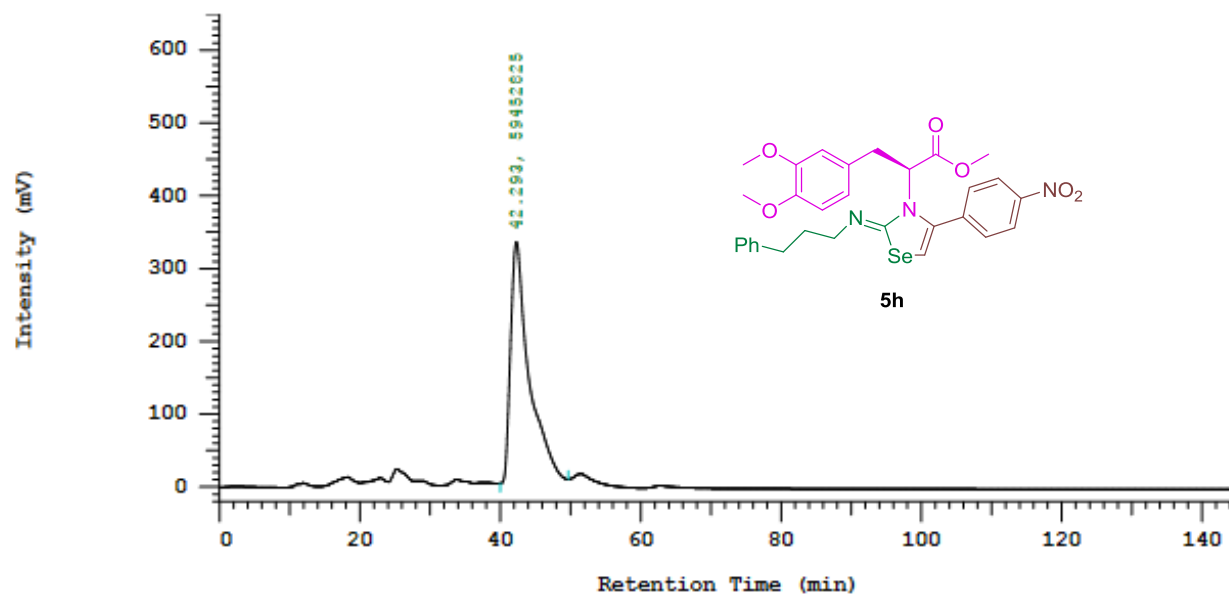
Series: 0214

Vial Number: 1

Vial Type: UNK

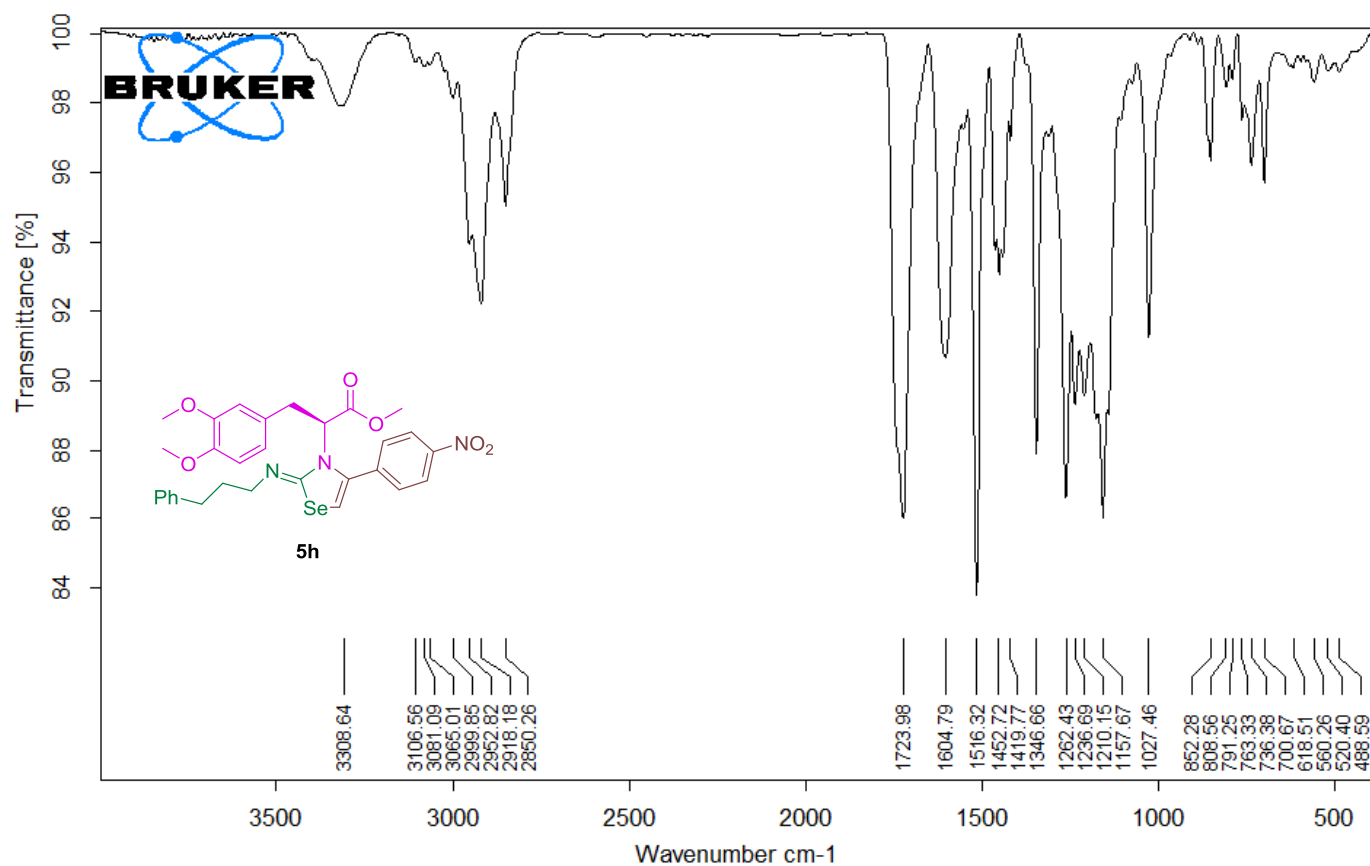
Volume: 10.0 ul

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound **5h**



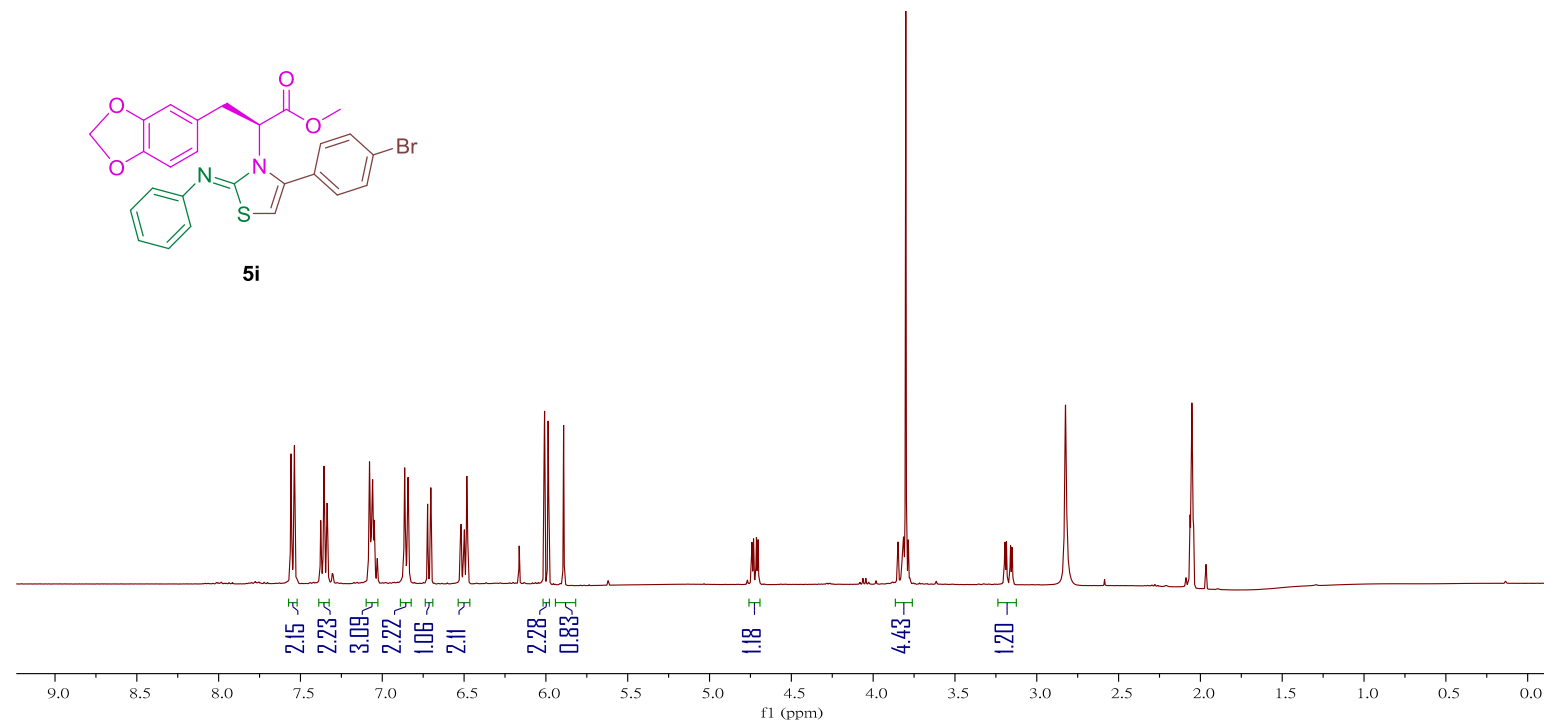
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L190.1

MIR_TR_DTGS_L190

Instrument type and / or accessory

9/4/2018

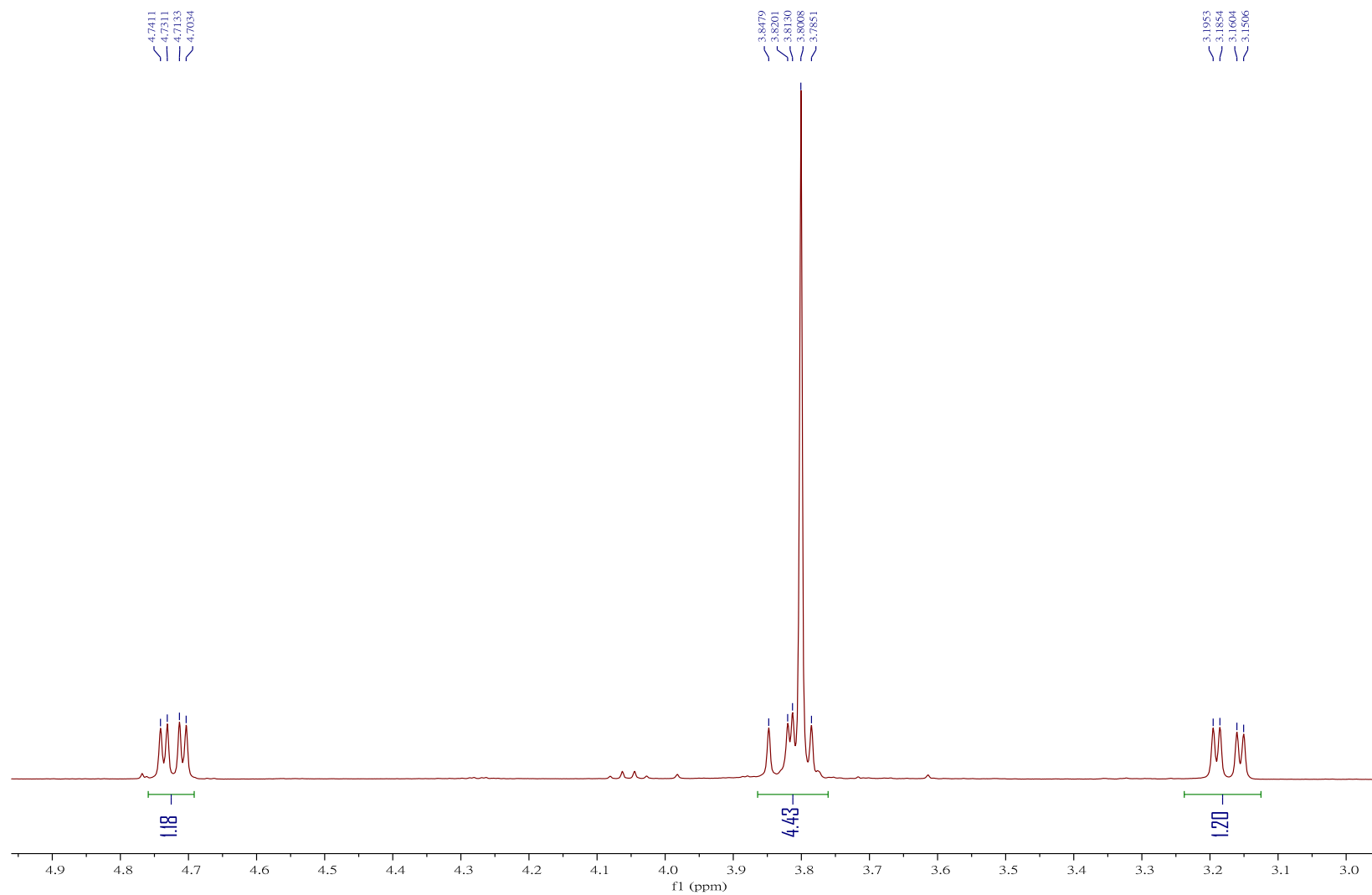
FT-IR Spectrum of compound **5h**



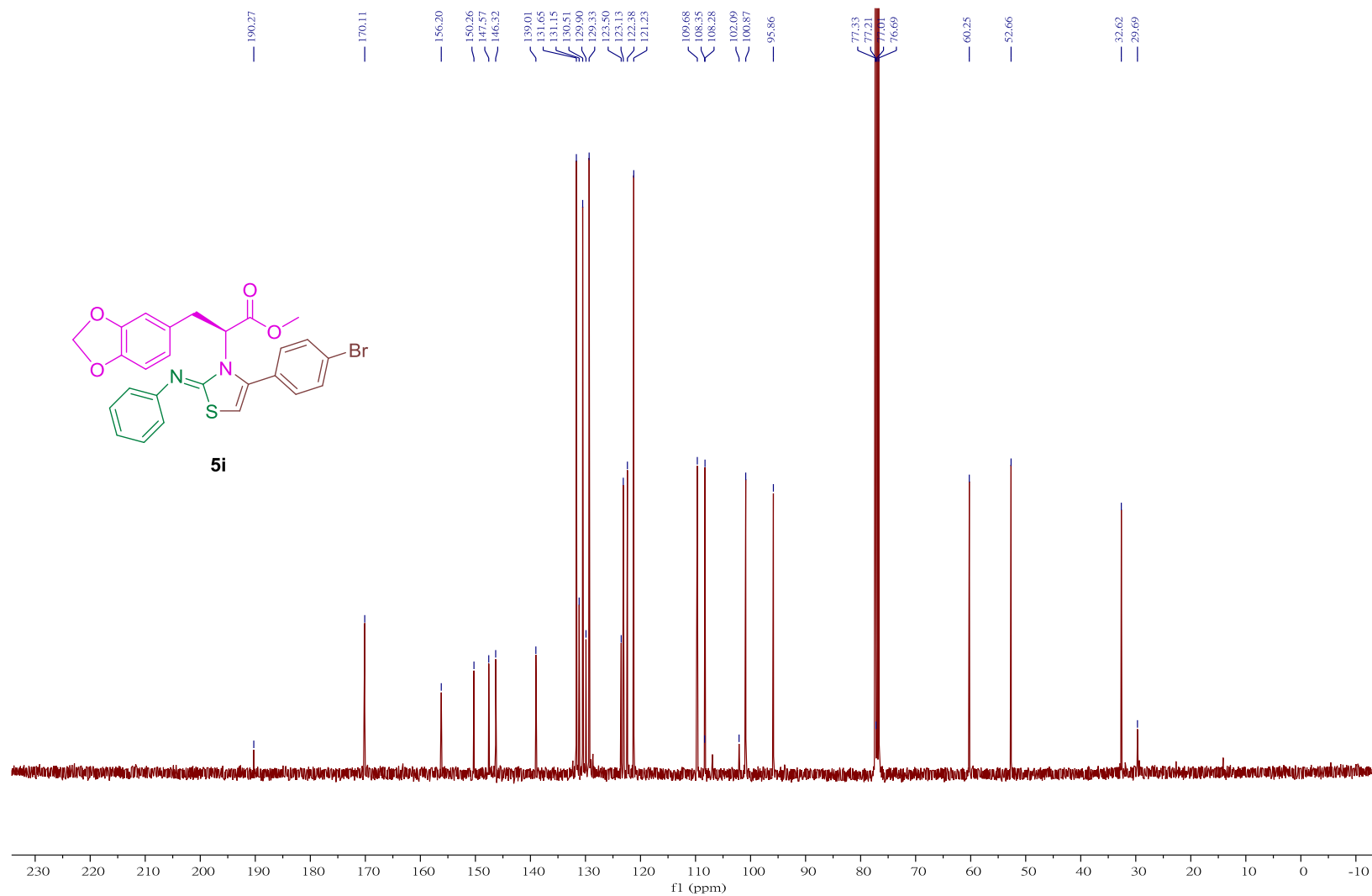
¹H NMR Spectrum (400 MHz) of compound **5i** in acetone-*d*₆



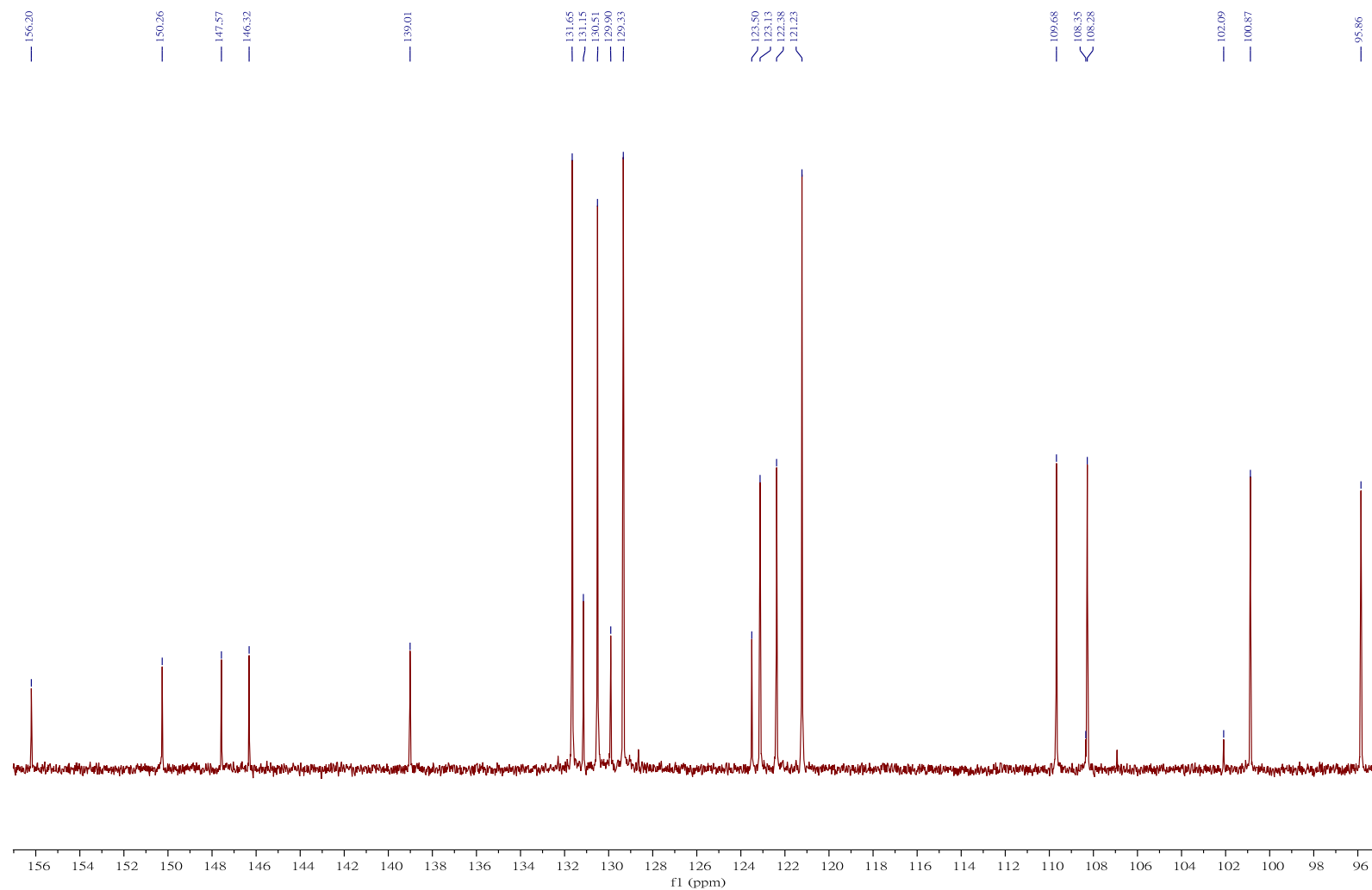
Expansion of ^1H NMR Spectrum (400 MHz) of compound **5i** in acetone- d_6



Expansion of ¹H NMR Spectrum (400 MHz) of compound **5i** in acetone-*d*₆



^{13}C NMR Spectrum (101 MHz) of compound **5i** in CDCl_3



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **5i** in CDCl_3

Display Report

Analysis Info

Analysis Name D:\Data\nctu service\data\2018\20180417\L230_RB2_01_17997.d

Method Small molecule.m

Sample Name L230

Comment

Acquisition Date 4/17/2018 1:21:21 PM

Operator NCTU

Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type

ESI

Ion Polarity

Positive

Set Nebulizer

1.0 Bar

Focus

Active

Set Capillary

4500 V

Set Dry Heater

200 °C

Scan Begin

50 m/z

Set End Plate Offset

-500 V

Set Dry Gas

6.0 l/min

Scan End

1500 m/z

Set Charging Voltage

2000 V

Set Divert Valve

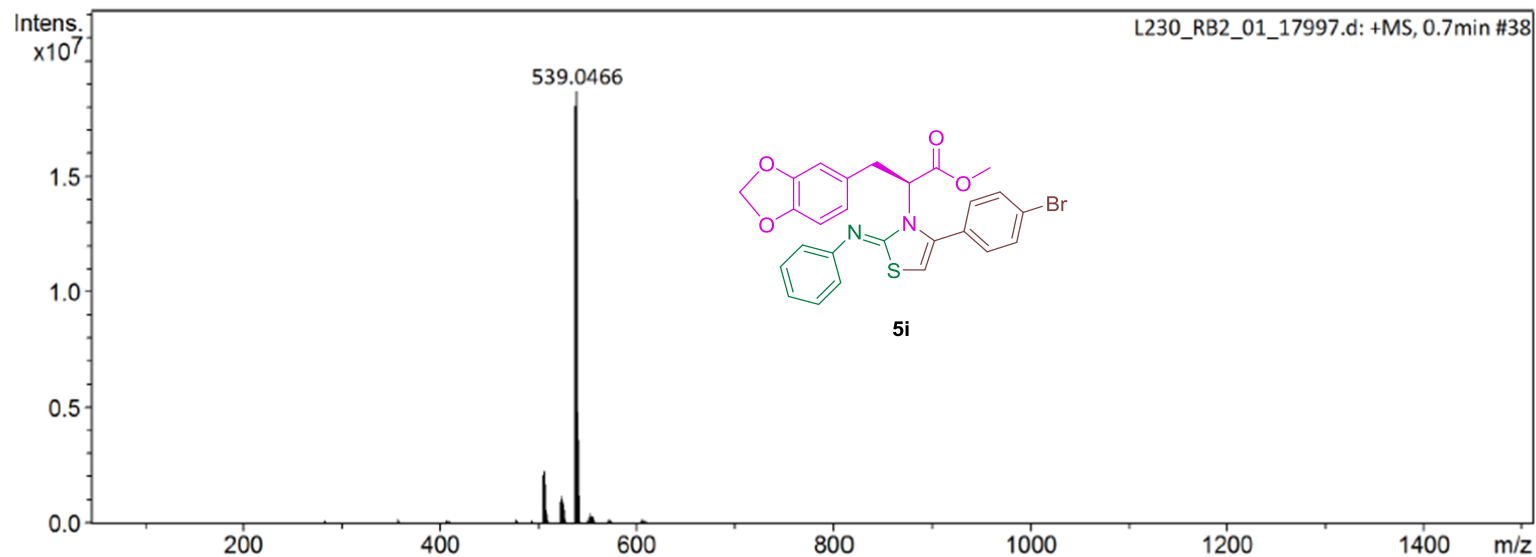
Waste

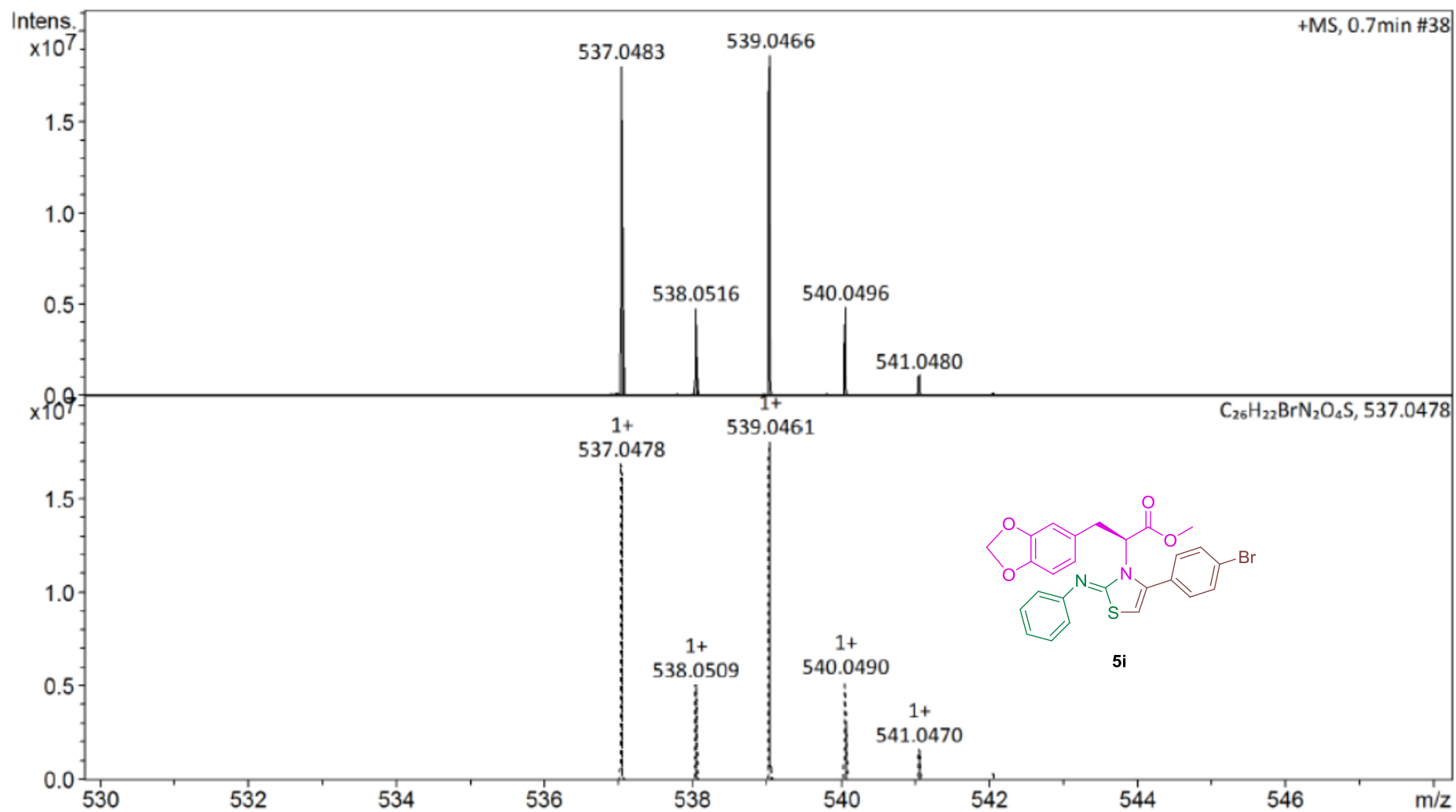
Set Corona

0 nA

Set APCI Heater

0 °C



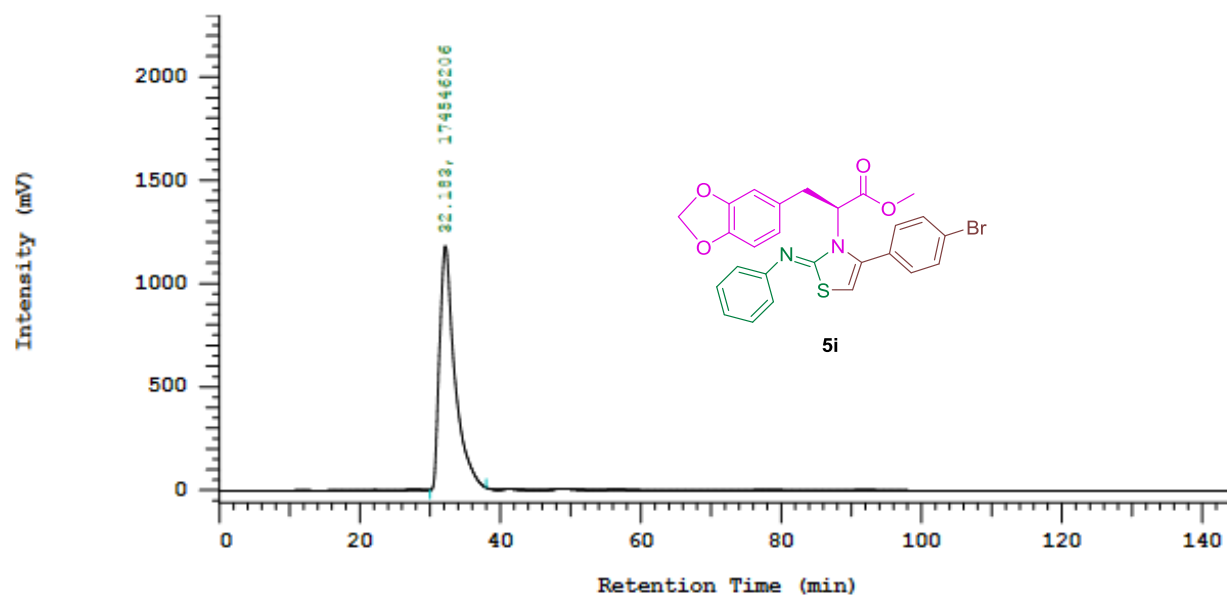


HRMS of compound **5i**

Processing Method: 27i_ee
System (acquisition): Sys 1
Application(data): Linda
Sample Name: UNKNOWN001
Injection from this vial: 1 of 1
Sample Description:

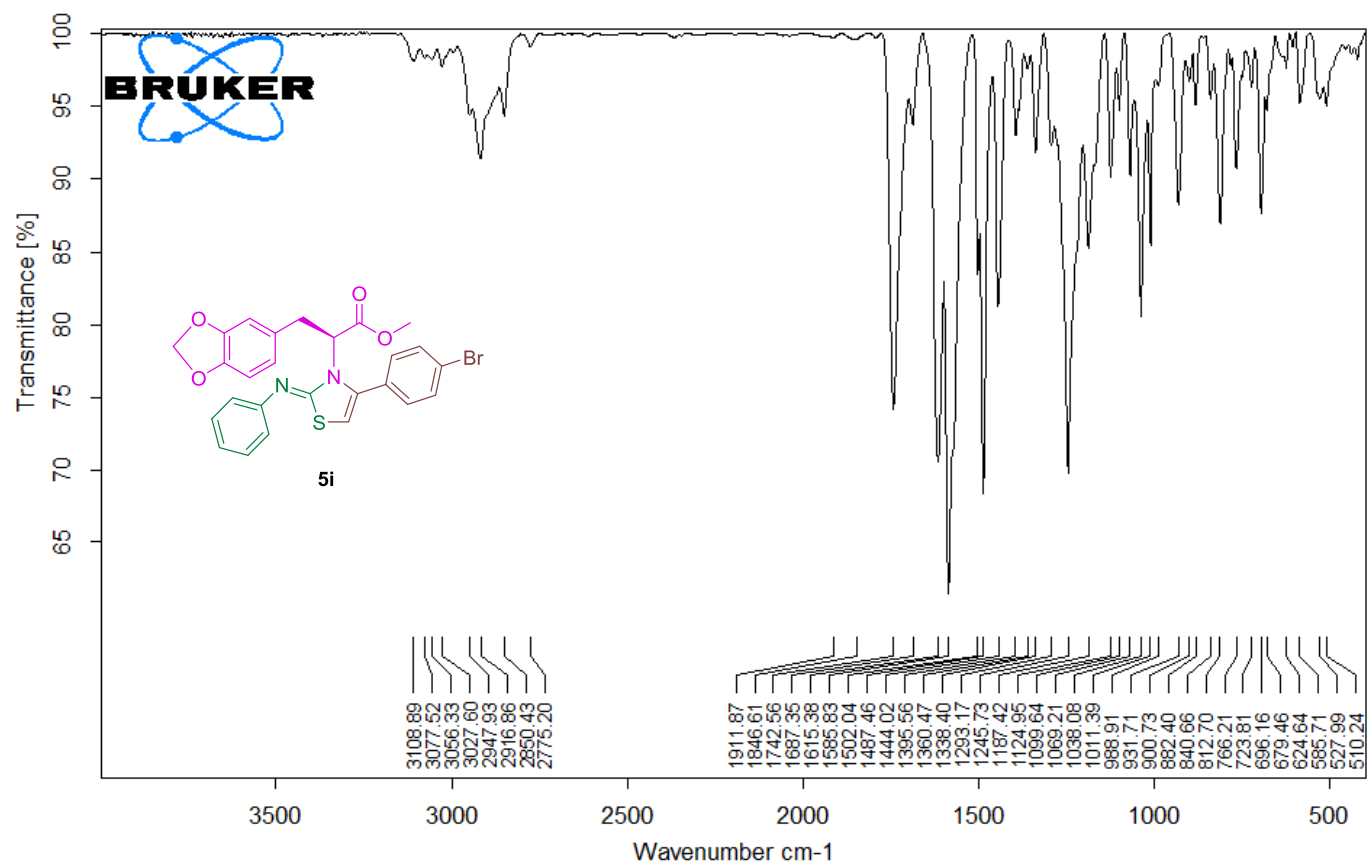
Series: 0217
Vial Number: 1
Vial Type: UNK
Volume: 10.0 ul

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound **5i**



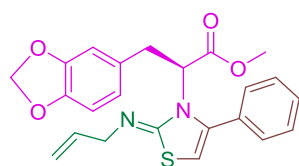
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L230.0

MIR_TR_DTGS_L230

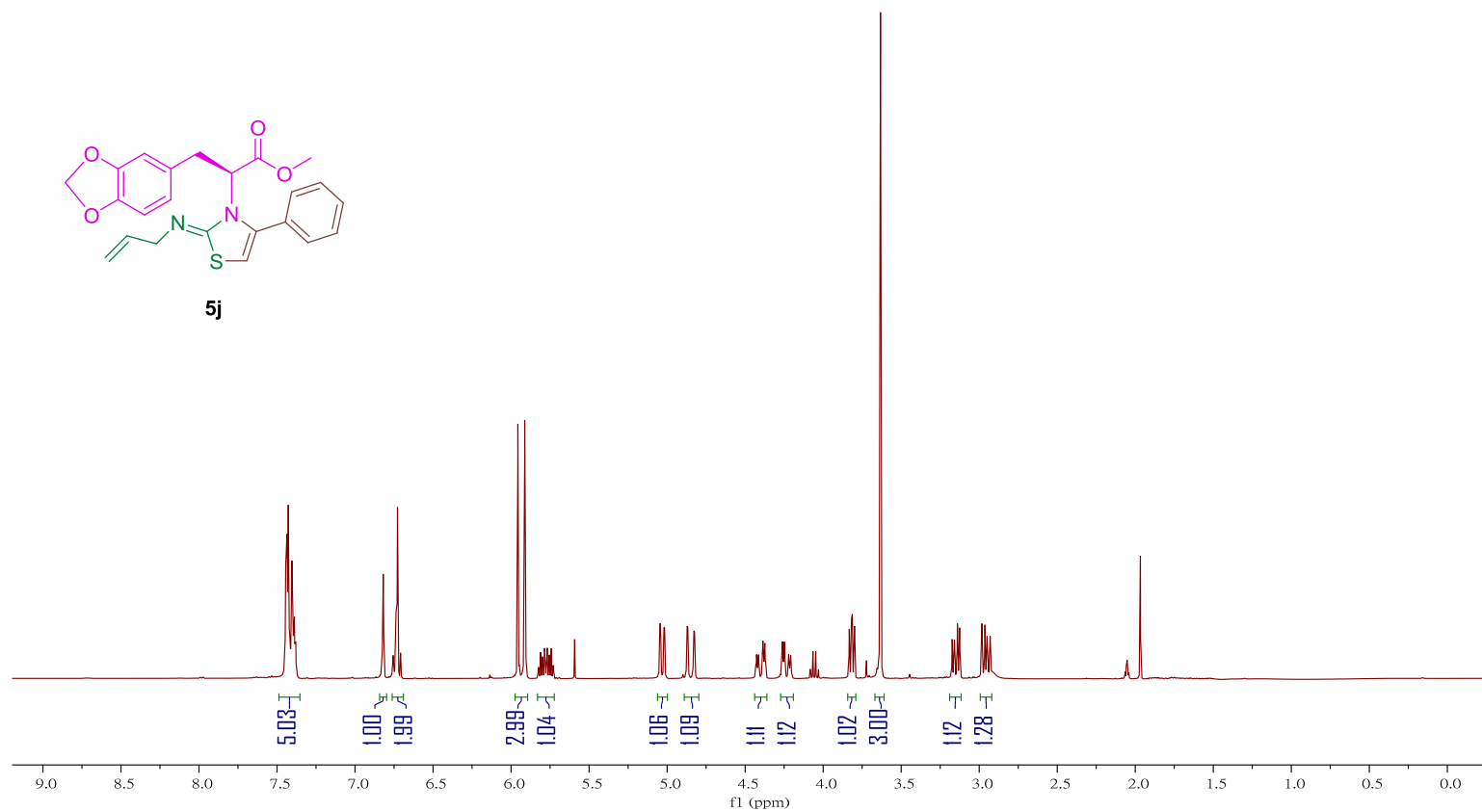
Instrument type and / or accessory

9/4/2018

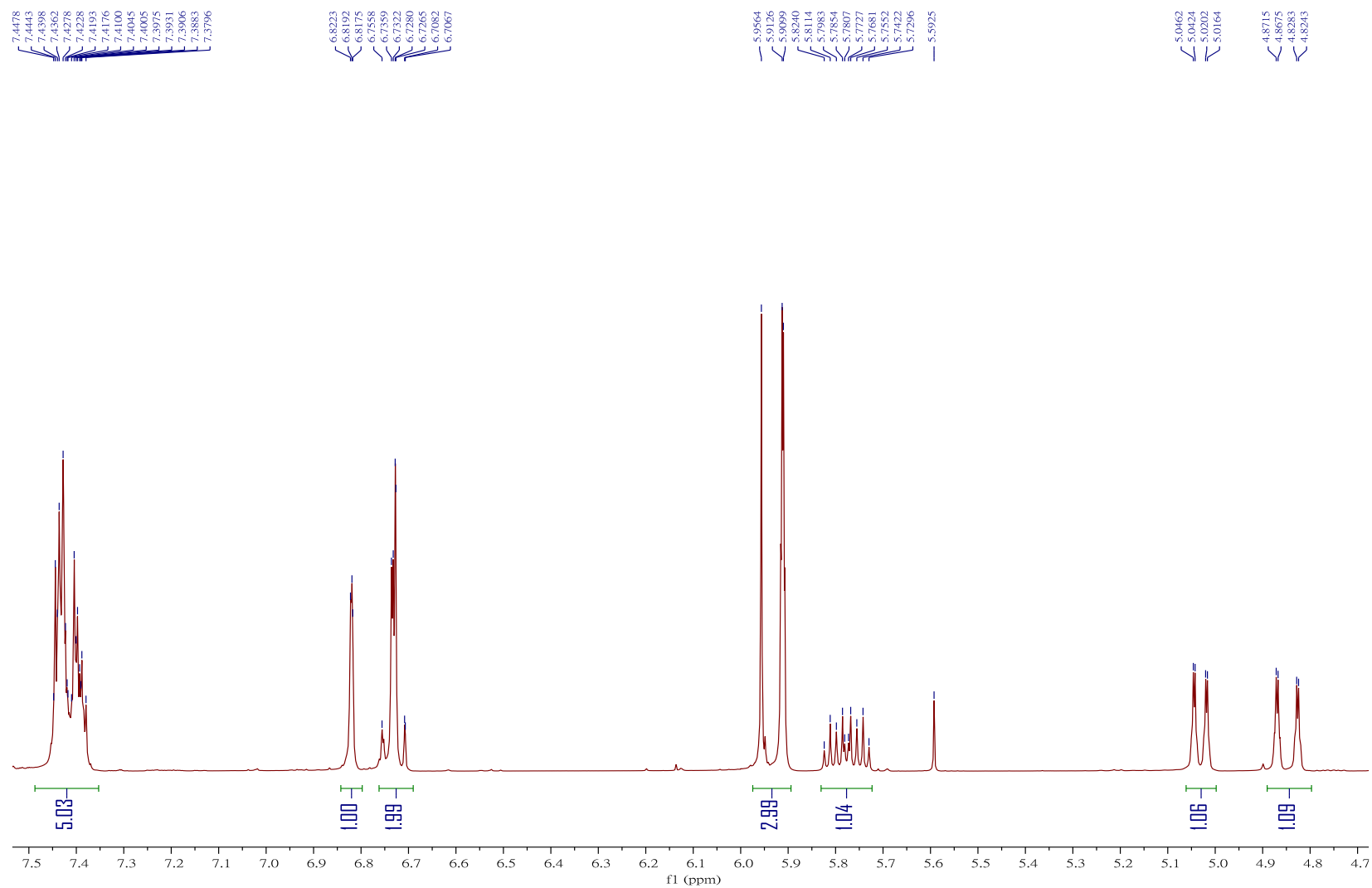
FT-IR Spectrum of compound **5i**



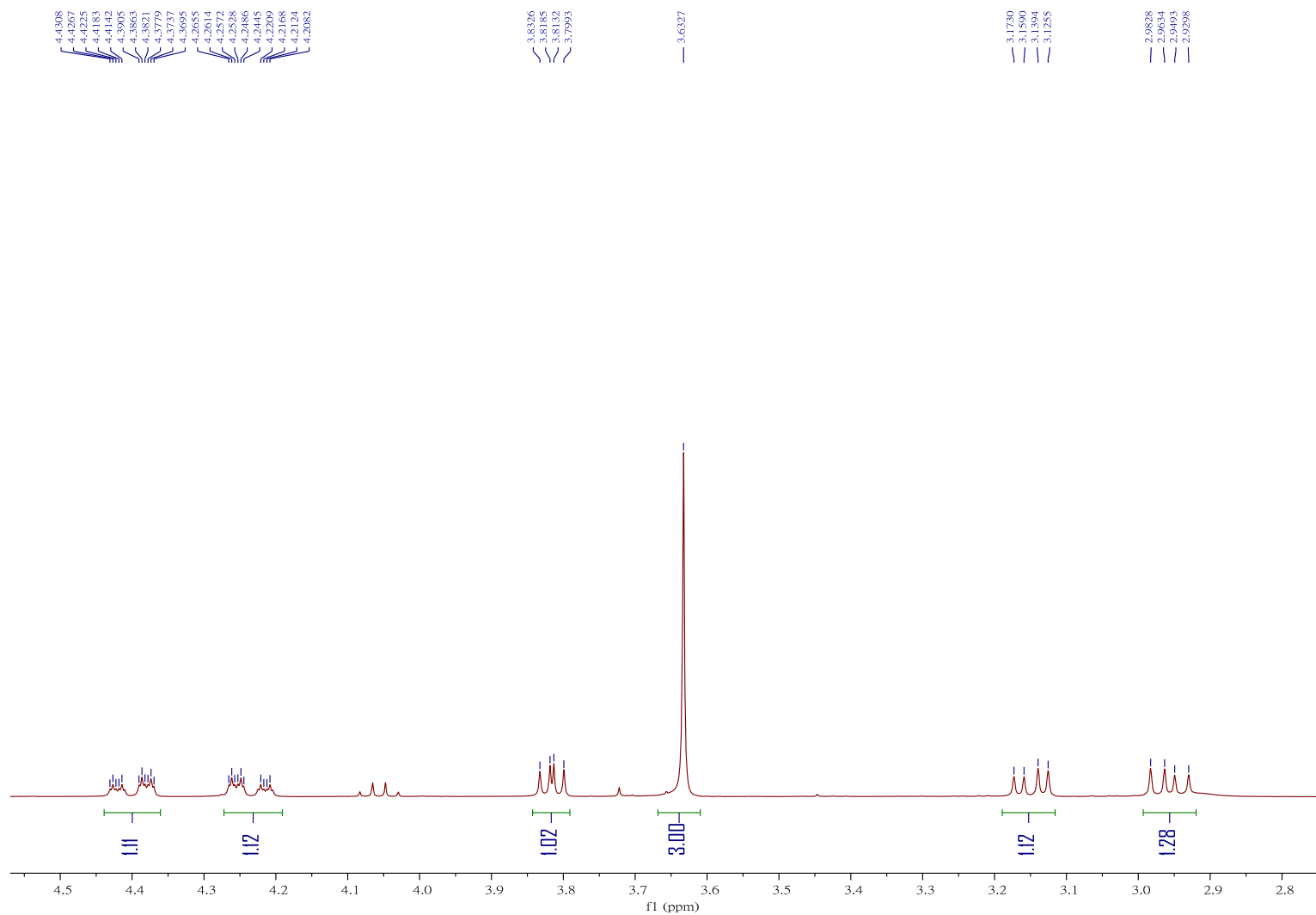
5j



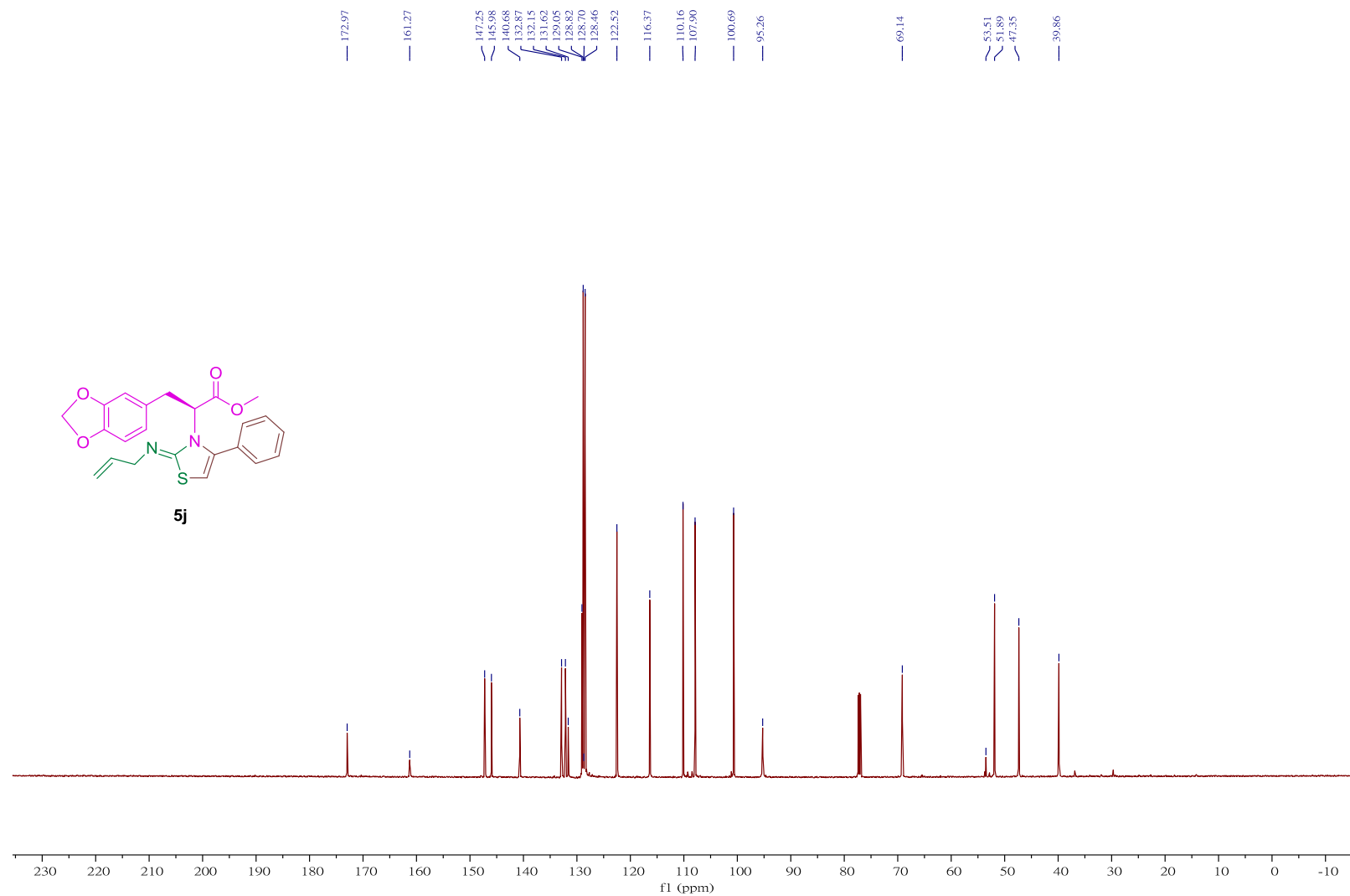
^1H NMR Spectrum (400 MHz) of compound **5j** in acetone- d_6

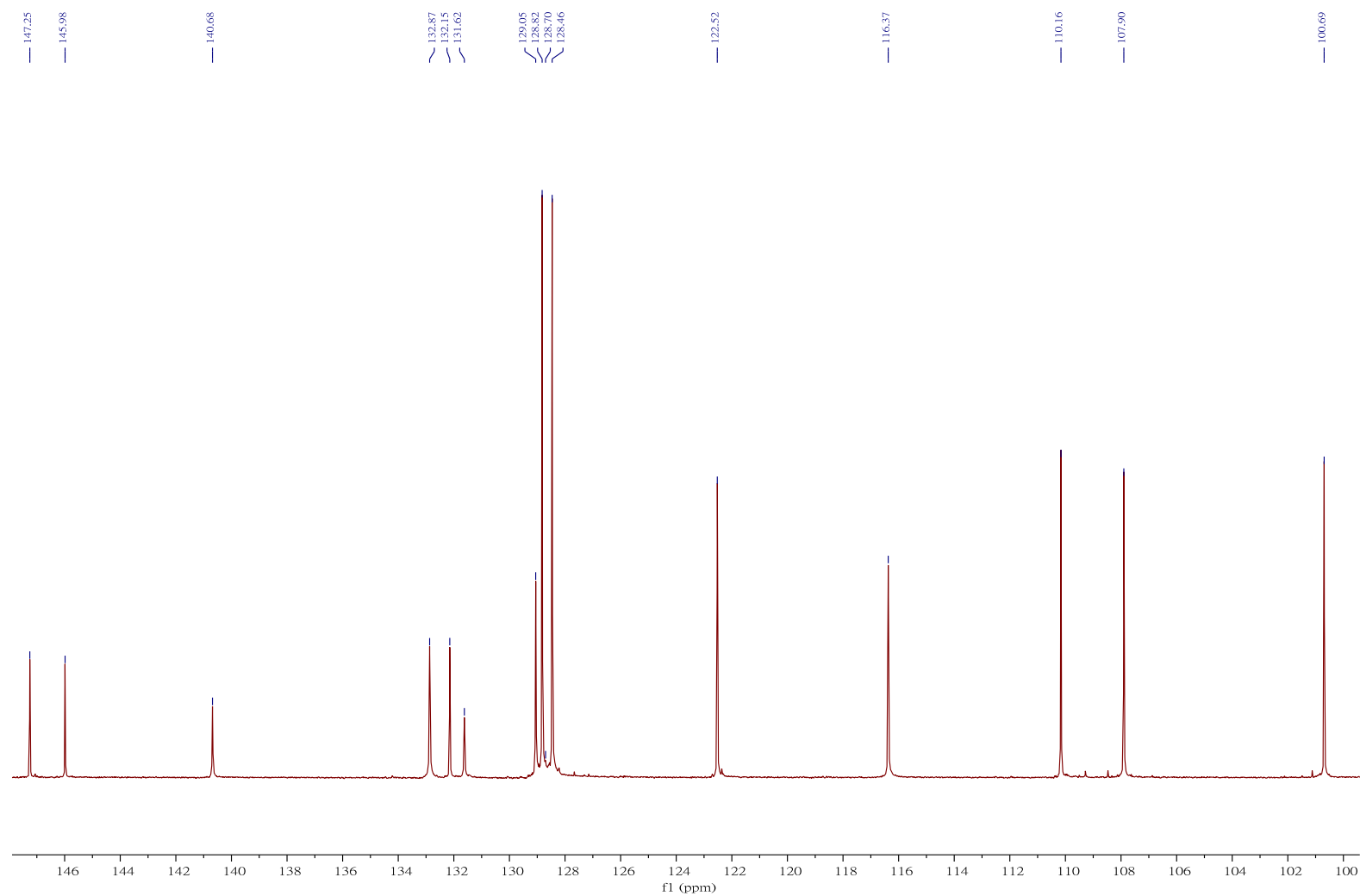


Expansion of ^1H NMR Spectrum (400 MHz) of compound **5j** in acetone- d_6



Expansion of ^1H NMR Spectrum (400 MHz) of compound **5j** in acetone- d_6



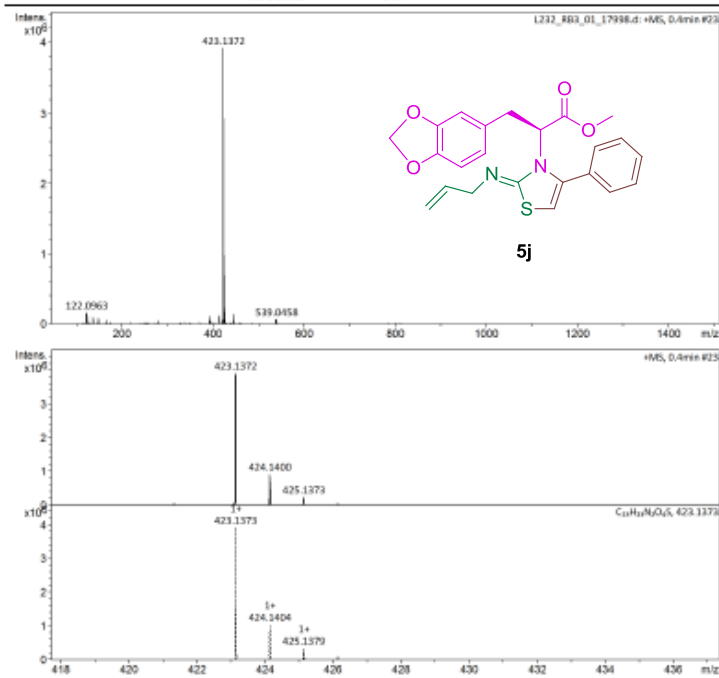


Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **5j** in CDCl_3

Display Report

Analytic Info		Acquisition Date	4/17/2018 1:25:40 PM
Analysis Name	H:\20181-6\20180417\L232_RB3_01_17998.d	Operator	NCTU
Method	Small molecule.m	Instrument	Impact HD
Sample Name	L232		1819696.00164
Comment			

Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
Focus	Active	Set Capillary	4500 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1500 m/z	Set Charging Voltage	2000 V
		Set Corona	0 nA
		Set Nebulizer	1.0 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	6.0 l/min
		Set Direct Valve	Waste
		Set APCI Heater	0 °C



HRMS of compound **5j**

CSM: Linda Series: 0118 Report Name: modified System: Sys 1

Chromaster System Manager Report

Analyzed Date and Time: 2018/09/04 08:53 下午
Reported Date and Time: 2018/09/18 02:32:58 下午

Processed Date and Time: 2018/09/18 02:32 下午

Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0118\

Processing Method: L232_ee

System (acquisition): Sys 1

Series: 0118

Application(data): Linda

Vial Number: 1

Sample Name: UNKNOWN001

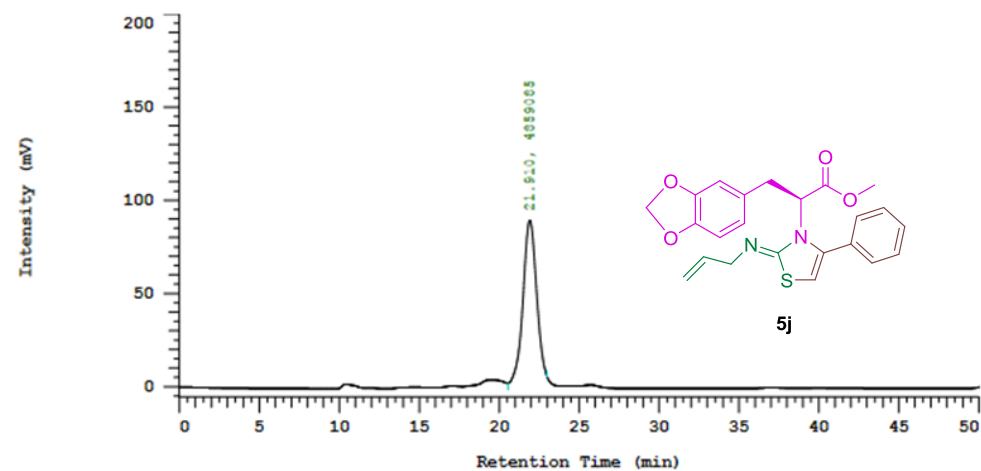
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 10.0 ul

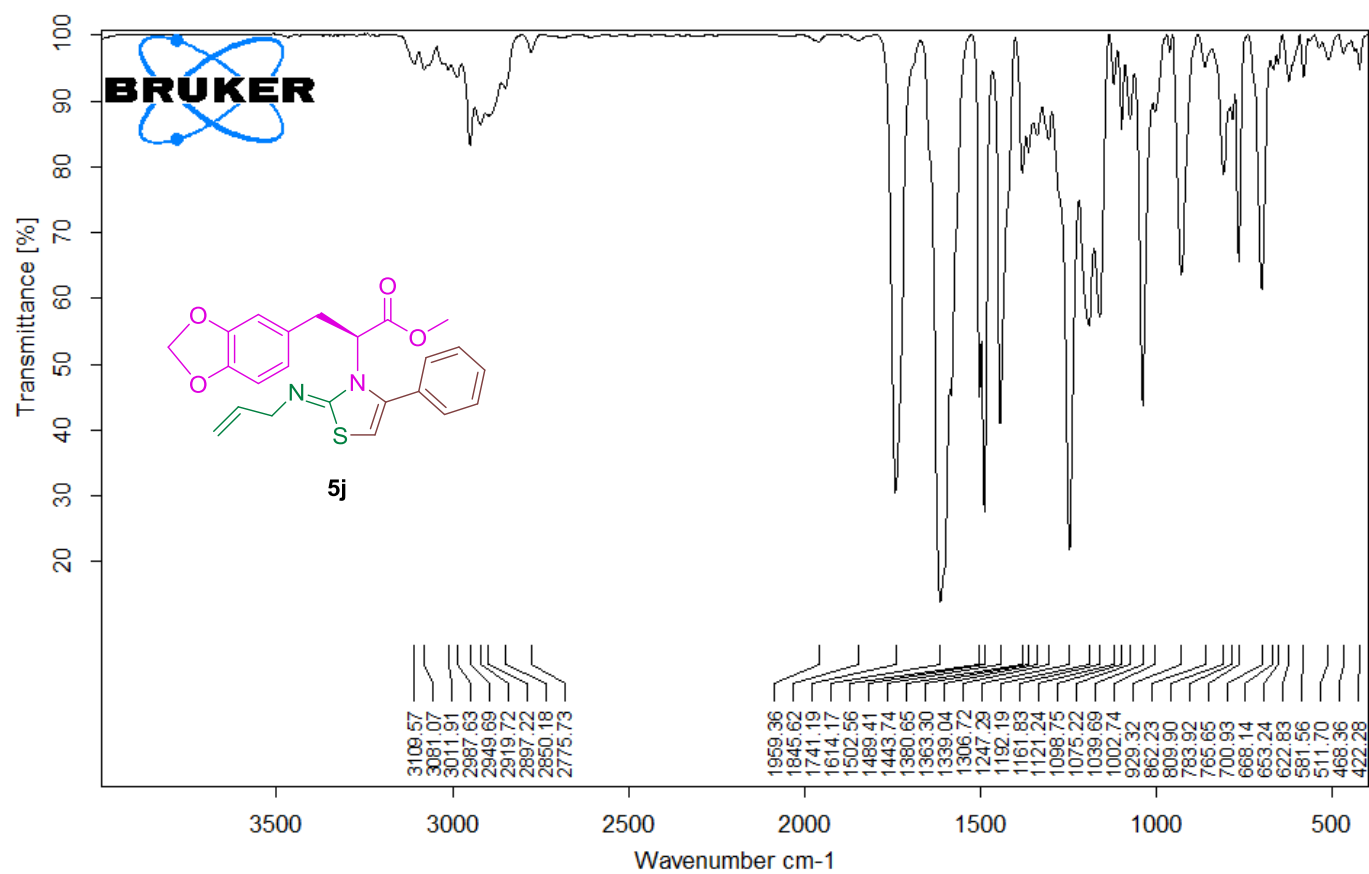
Sample Description:

Chrom Type: Chromaster Channel : 1



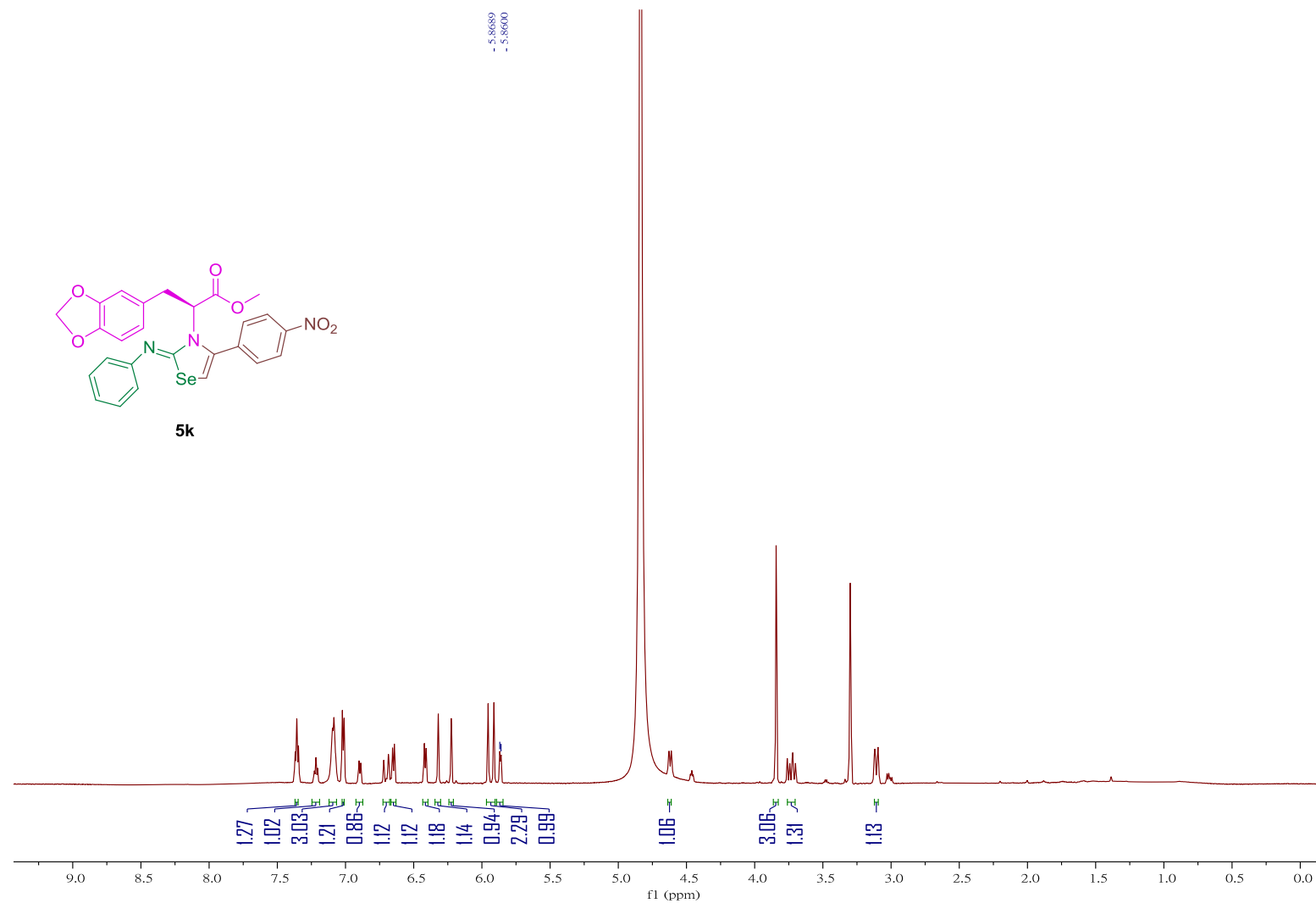
Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound 5j

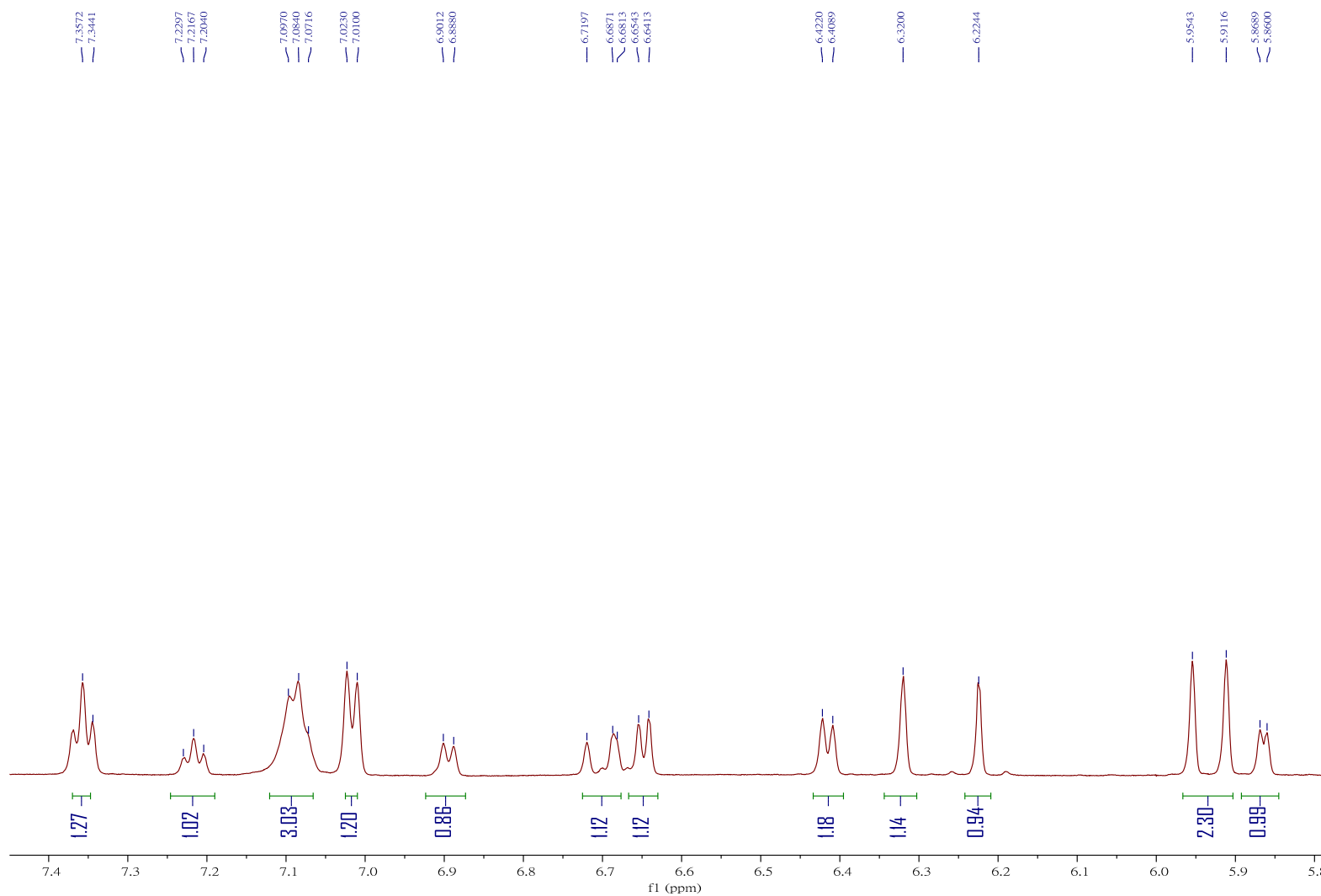


D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L232.0	MIR_TR_DTGS_L232	Instrument type and / or accessory	9/4/2018
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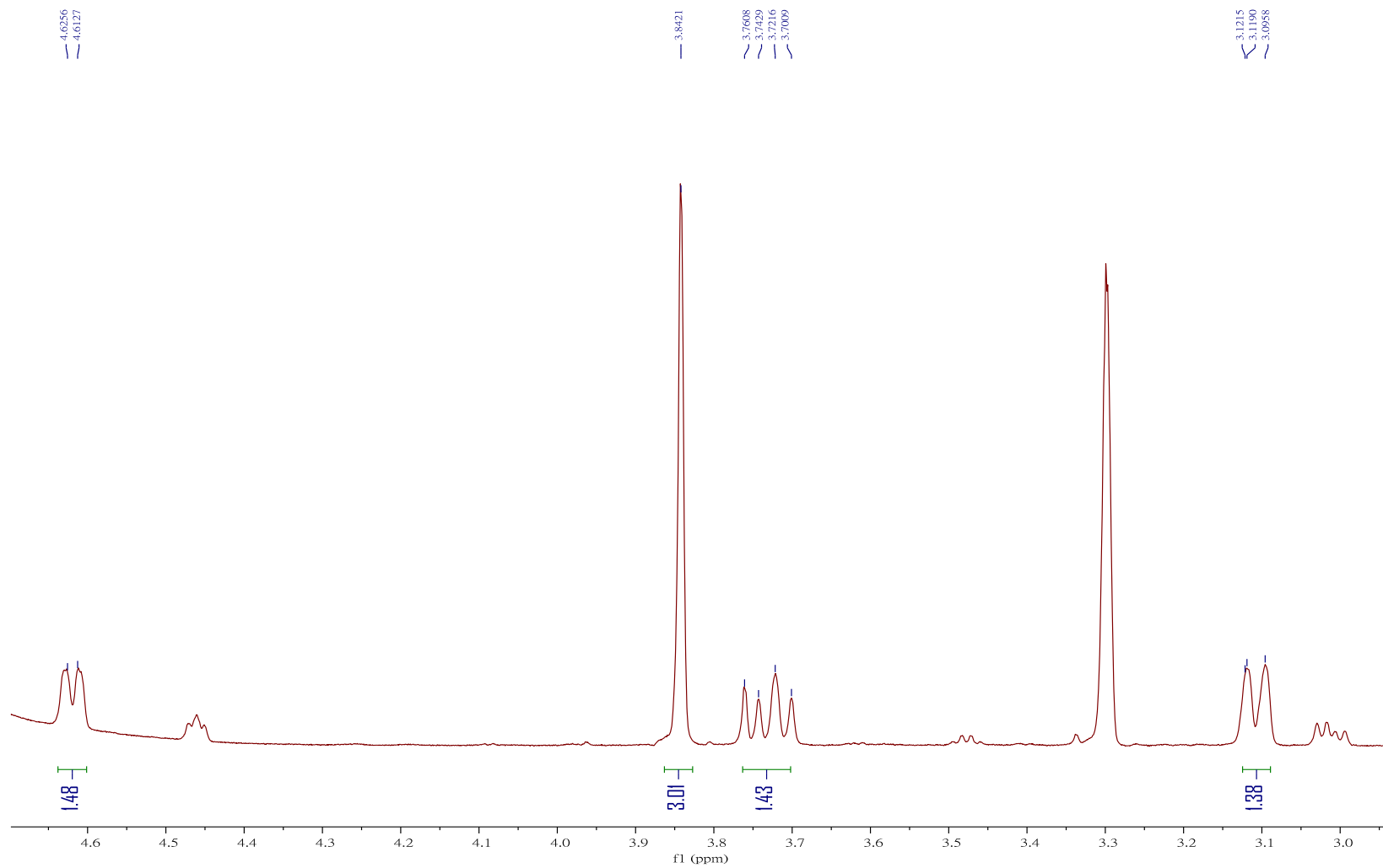
FT-IR Spectrum of compound **5j**



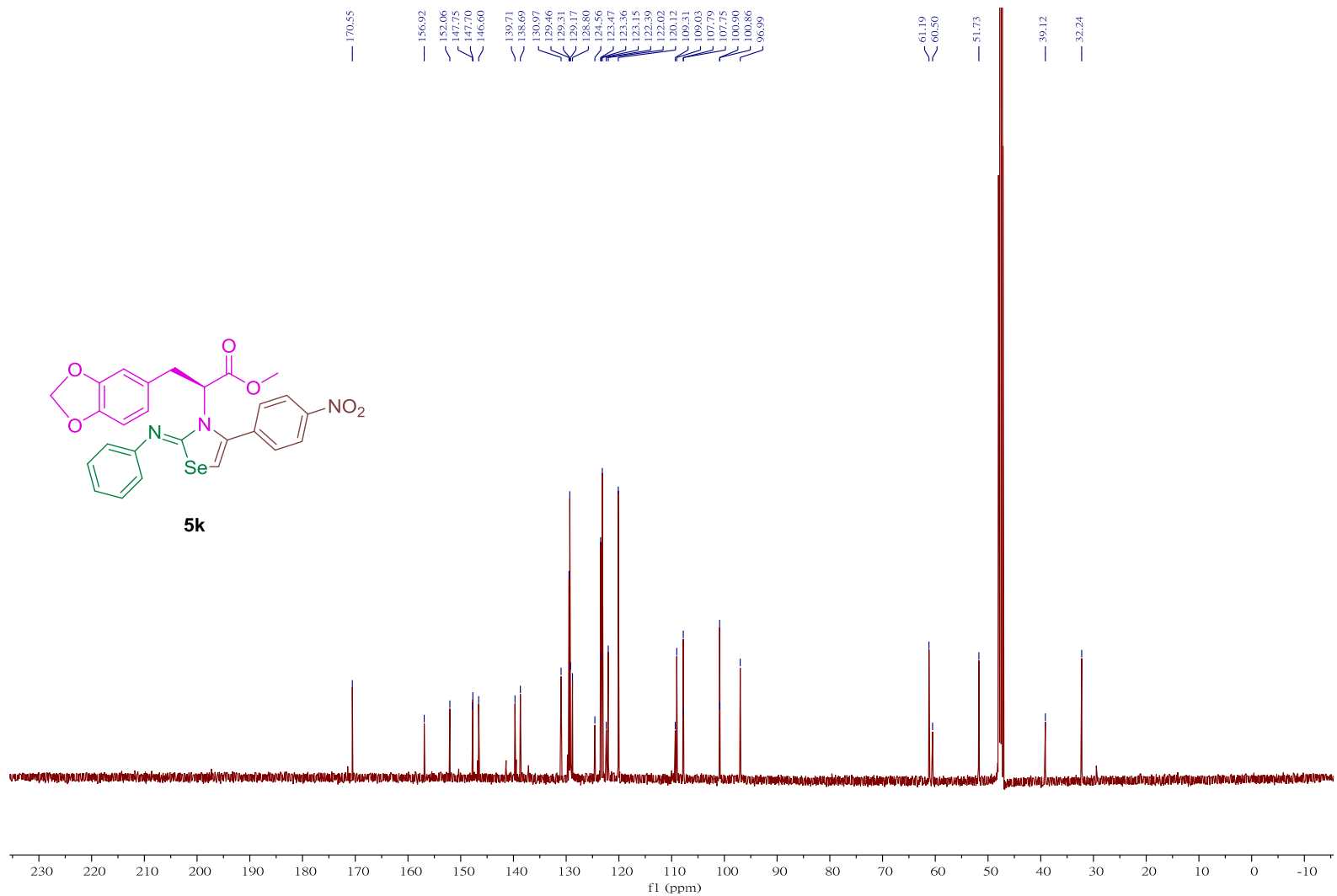
^1H NMR Spectrum (400 MHz) of compound **5k** in CD_3OD



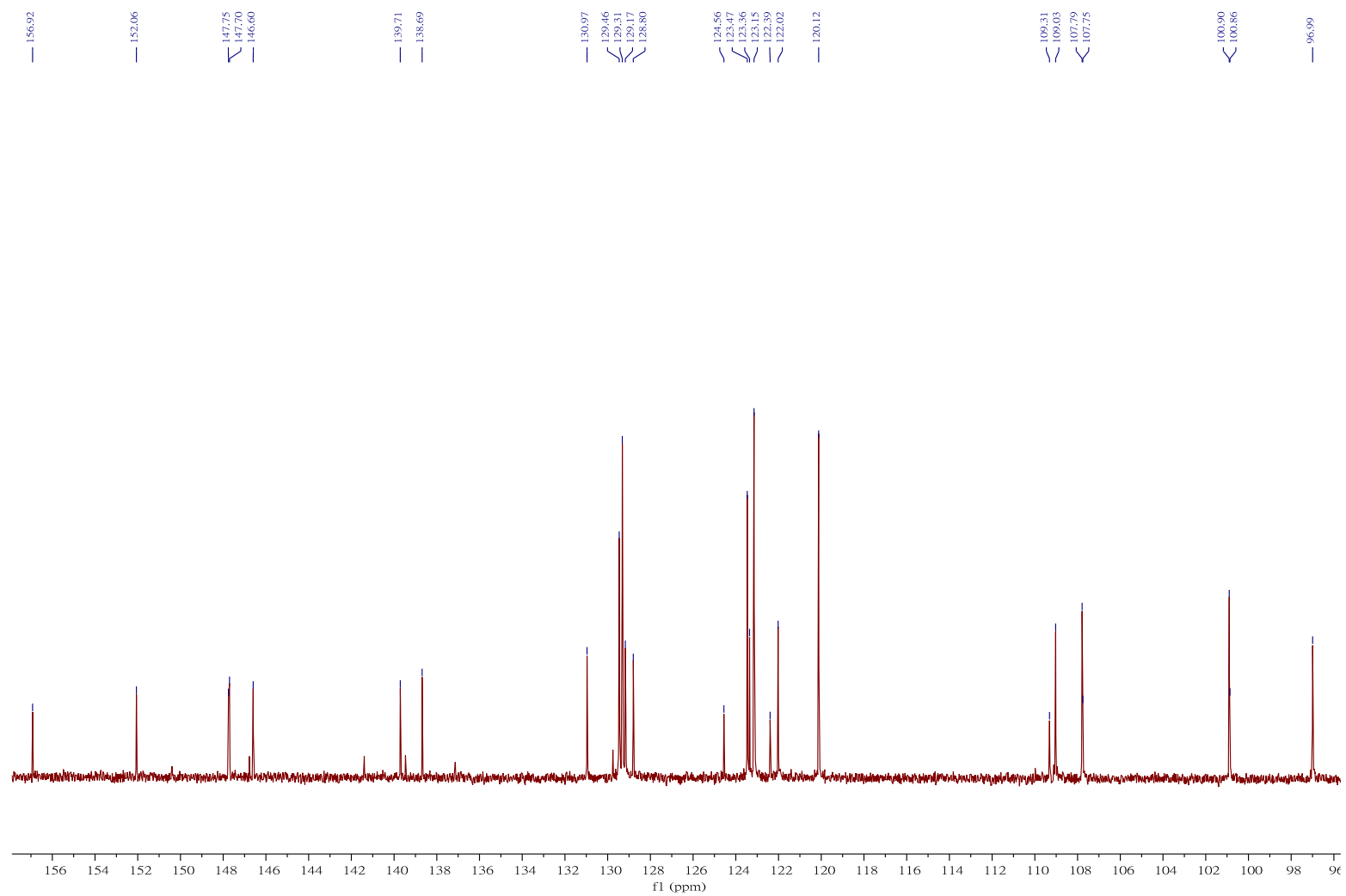
Expansion of ^1H NMR Spectrum (400 MHz) of compound **5k** in CD_3OD



Expansion of ¹H NMR Spectrum (400 MHz) of compound **5k** in CD₃OD



^{13}C NMR Spectrum (101 MHz) of compound **5k** in CDCl_3

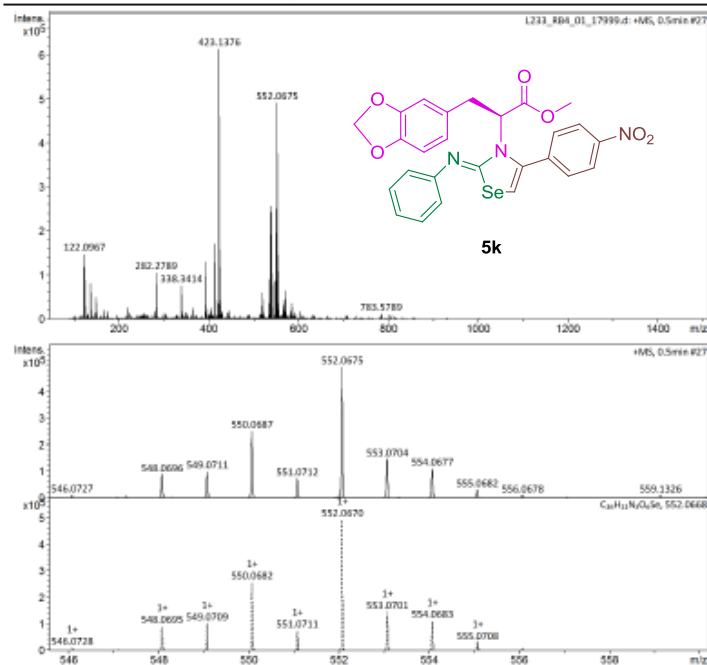


Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **5k** in CDCl_3

Display Report

Analytic Info		Acquisition Date 4/17/2018 1:29:59 PM	
Analysis Name	H:\20181-6\20180417\L233_RB4_01_17999.d	Operator	NCTU
Method	Small molecule.m	Instrument	Impact HD
Sample Name	L233		1819696.00154
Comment			

Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
Focus	Active	Set Capillary	4500 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1500 m/z	Set Charging Voltage	2000 V
		Set Corona	0 nA
		Set Nebulizer	1.0 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	8.0 l/min
		Set Divert Valve	Waste
		Set APCI Heater	0 °C



HRMS of compound **5k**

Processing Method: 27k_ee

System (acquisition): Sys 1

Application(data): Linda

Sample Name: UNKNOWN001

Injection from this vial: 1 of 1

Sample Description:

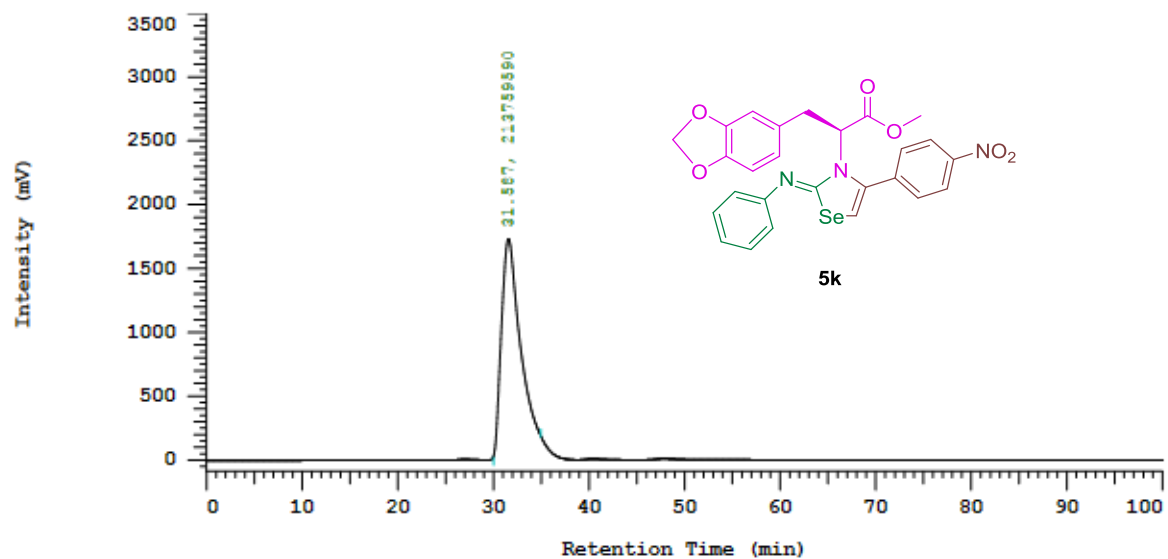
Series: 0201

Vial Number: 1

Vial Type: UNK

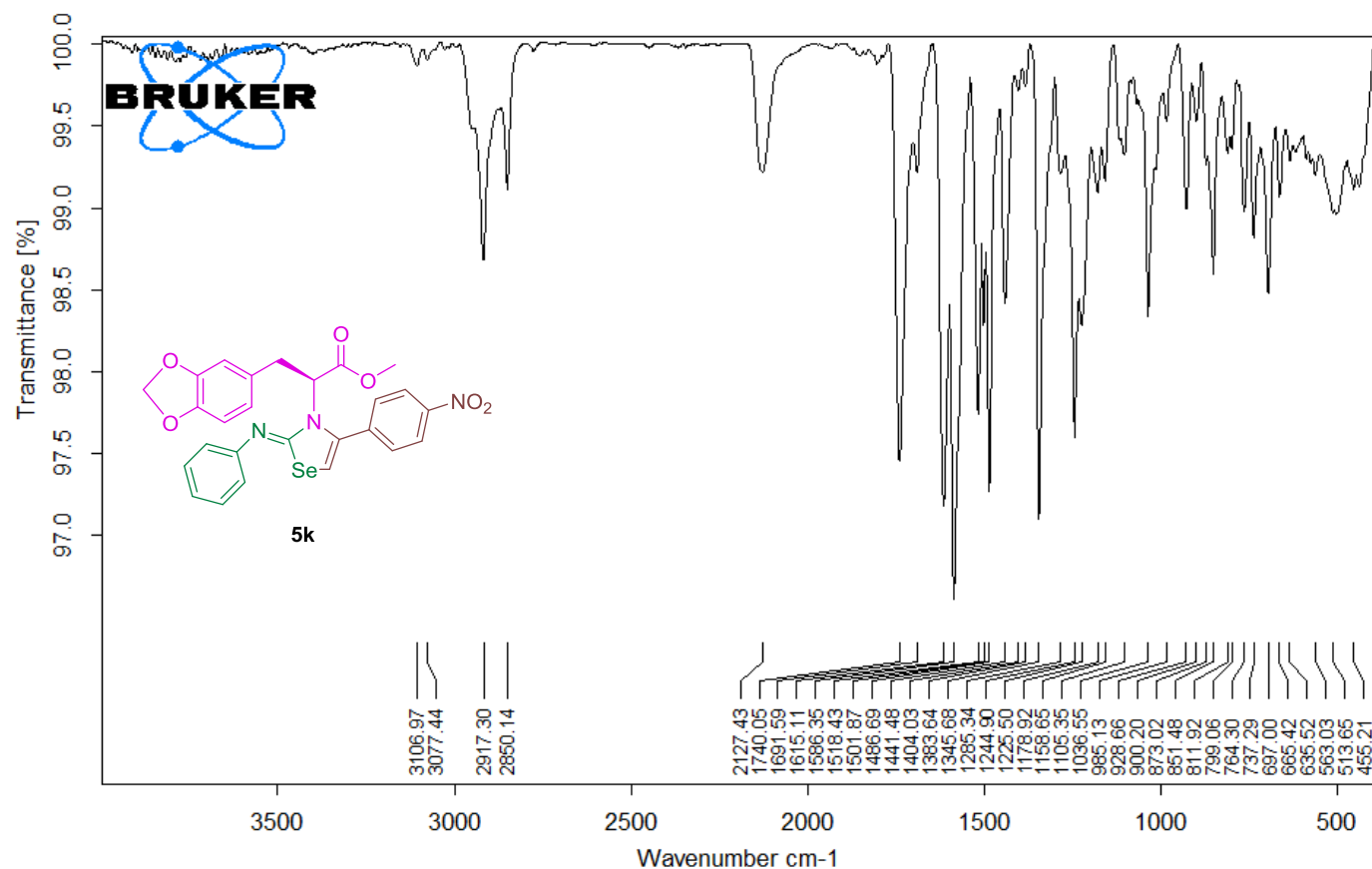
Volume: 10.0 ul

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound **5k**



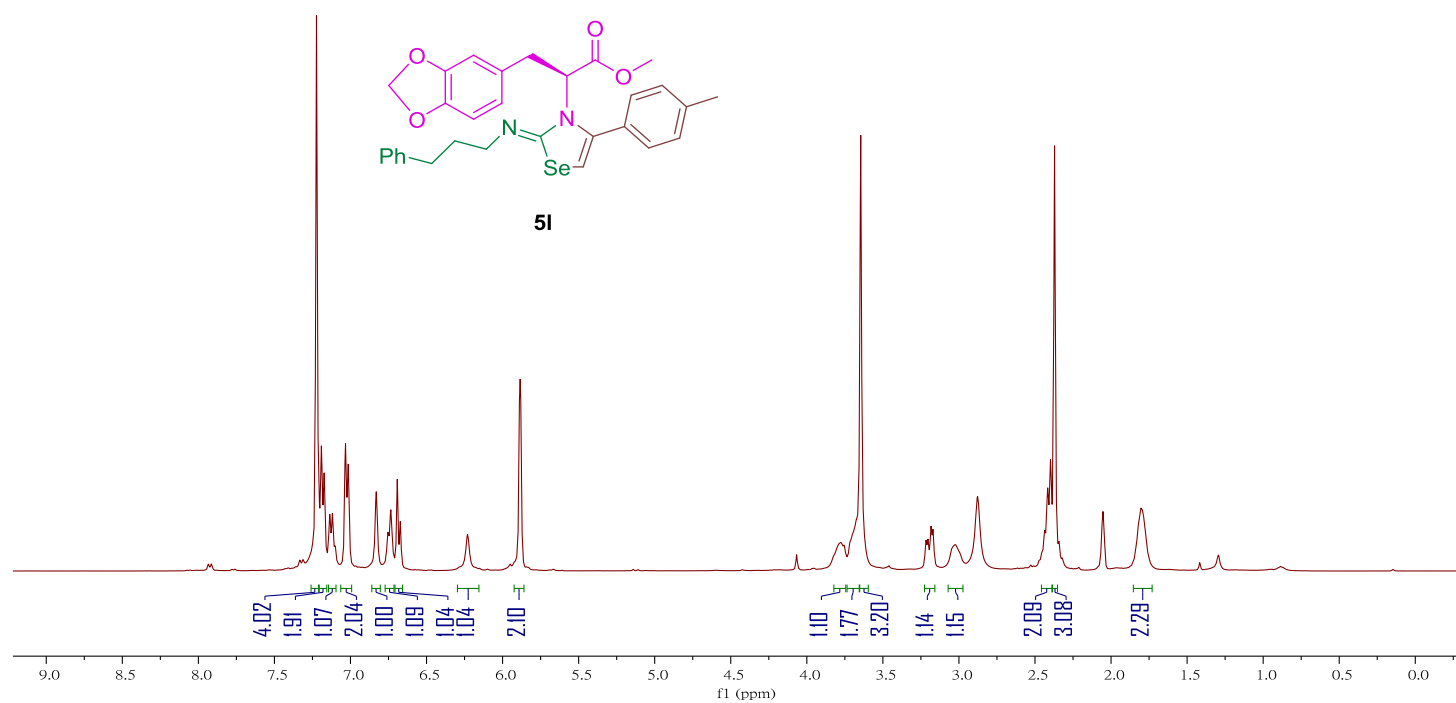
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L233.1

MIR_TR_DTGS_L233

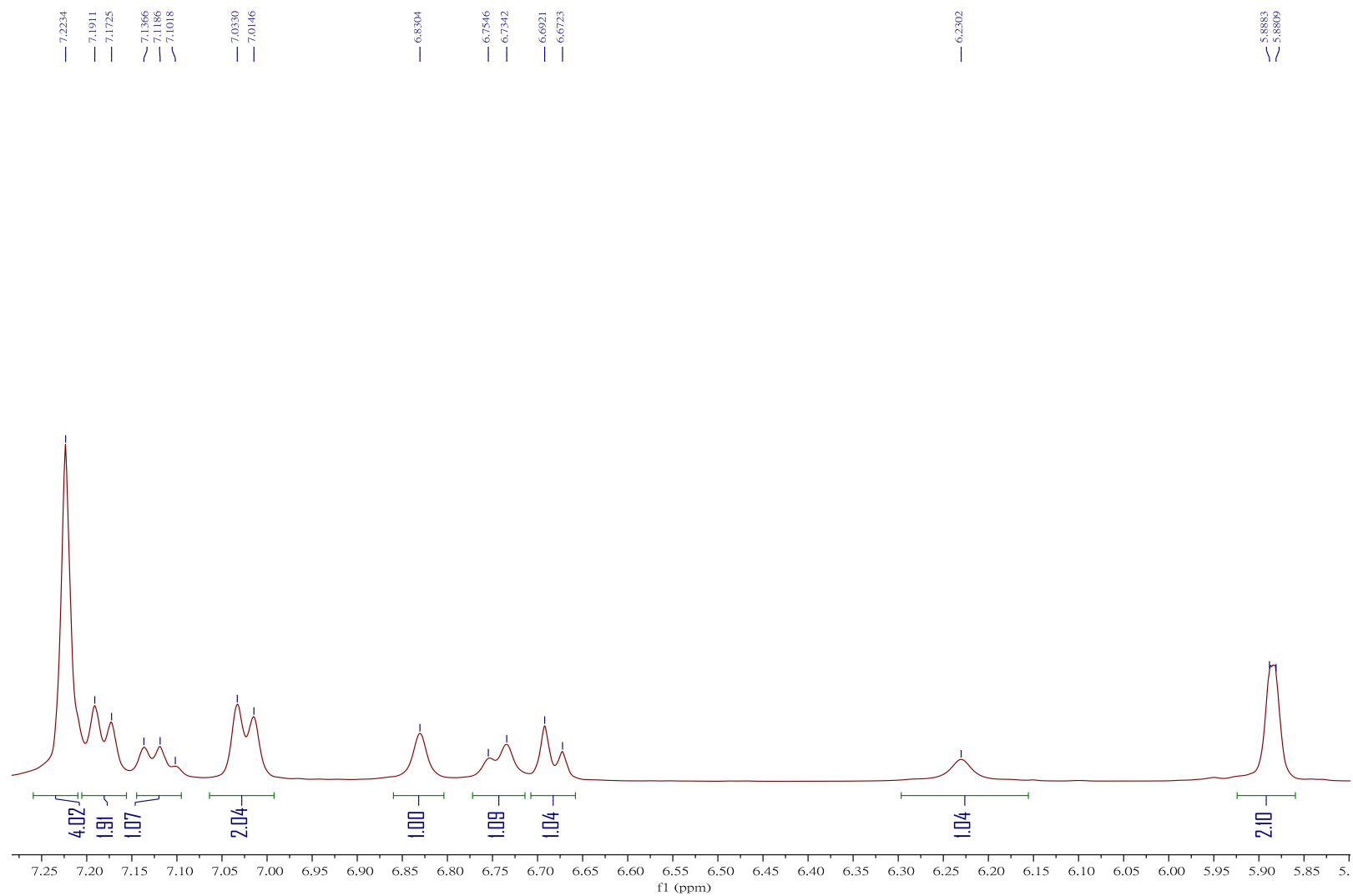
Instrument type and / or accessory

9/4/2018

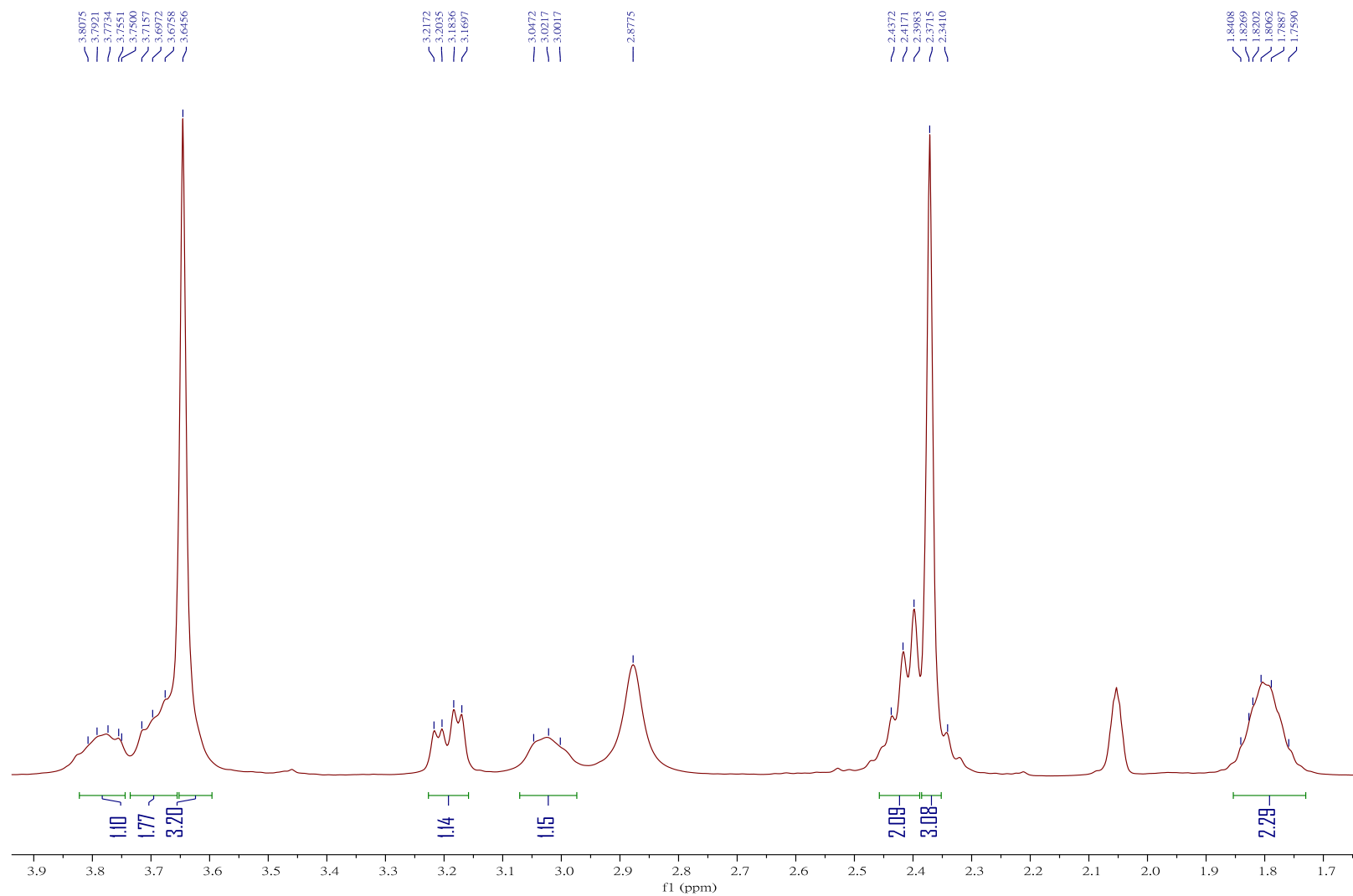
FT-IR Spectrum of compound **5k**



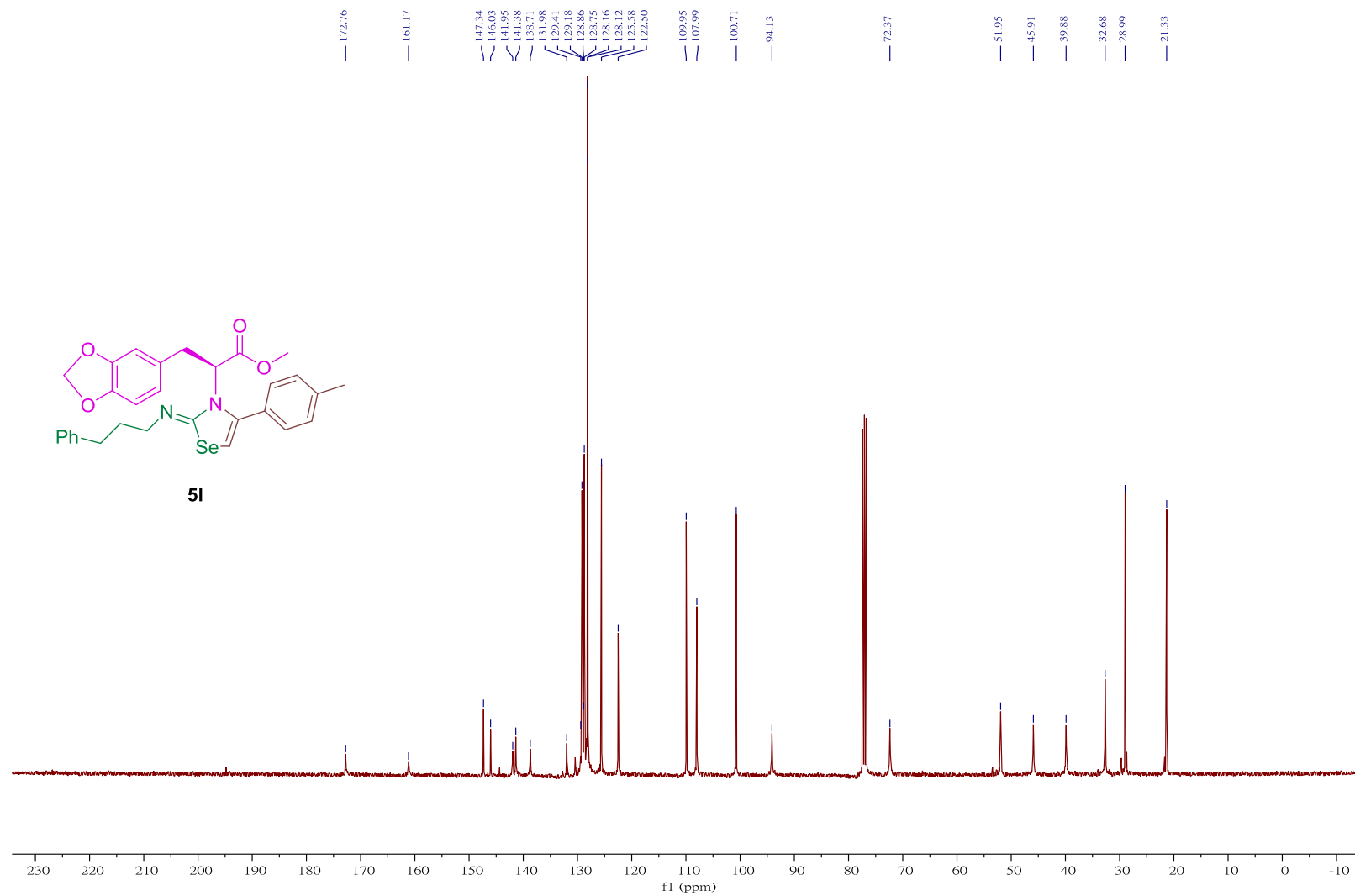
^1H NMR Spectrum (400 MHz) of compound **5l** in acetone- d_6



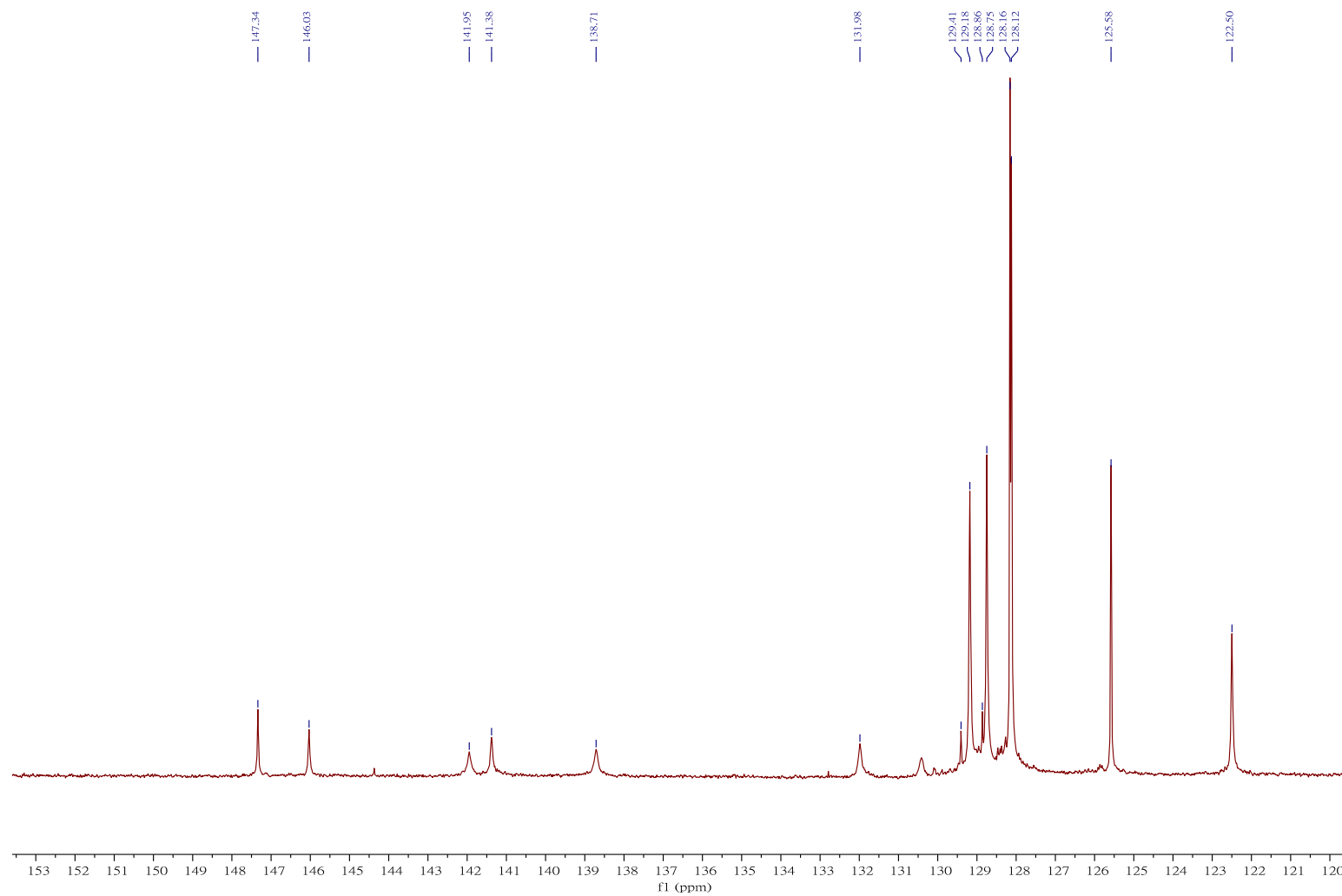
Expending ¹H NMR Spectrum (400 MHz) of compound **5l** in acetone-*d*₆



Expansion of ^1H NMR Spectrum (400 MHz) of compound **5l** in acetone- d_6



^{13}C NMR Spectrum (101 MHz) of compound **5I** in CDCl_3

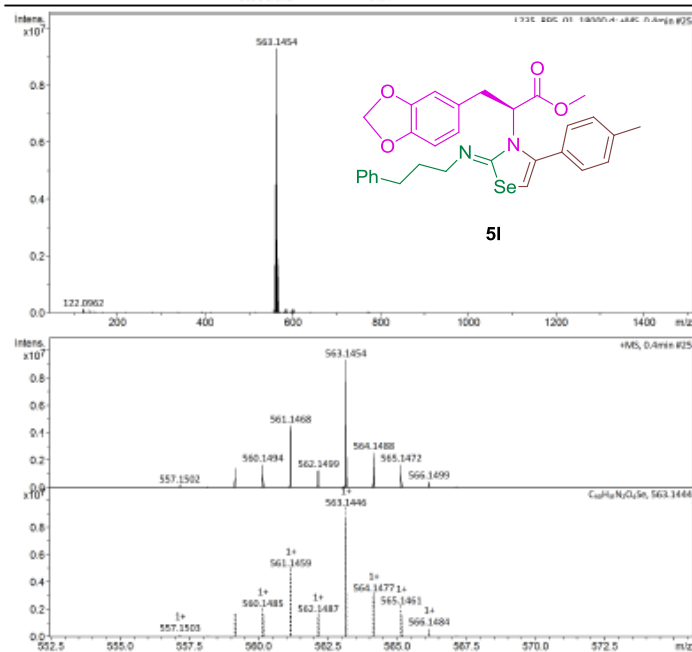


Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **5l** in CDCl_3

Display Report

Analysis Info		Acquisition Date	4/17/2018 1:34:19 PM	
Analysis Name	H:\20181-6\20180417\L235_RB5_01_18000.d	Operator	NCTU	
Method	Small molecule.m	Instrument	Impact HD	1819696.00164
Sample Name	L235			
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



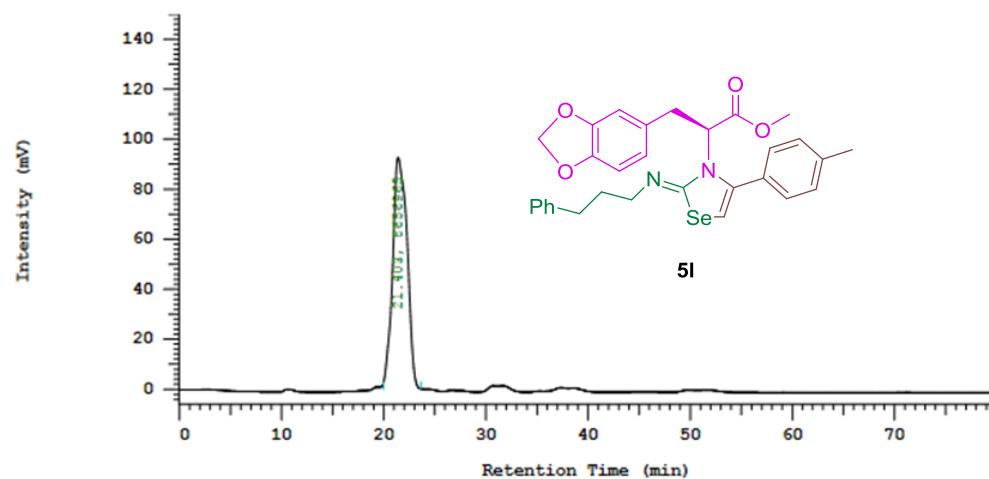
HRMS of compound **51**

CSM: Linda Series: 0125 Report Name: modified System: Sys 1

Chromaster System Manager Report

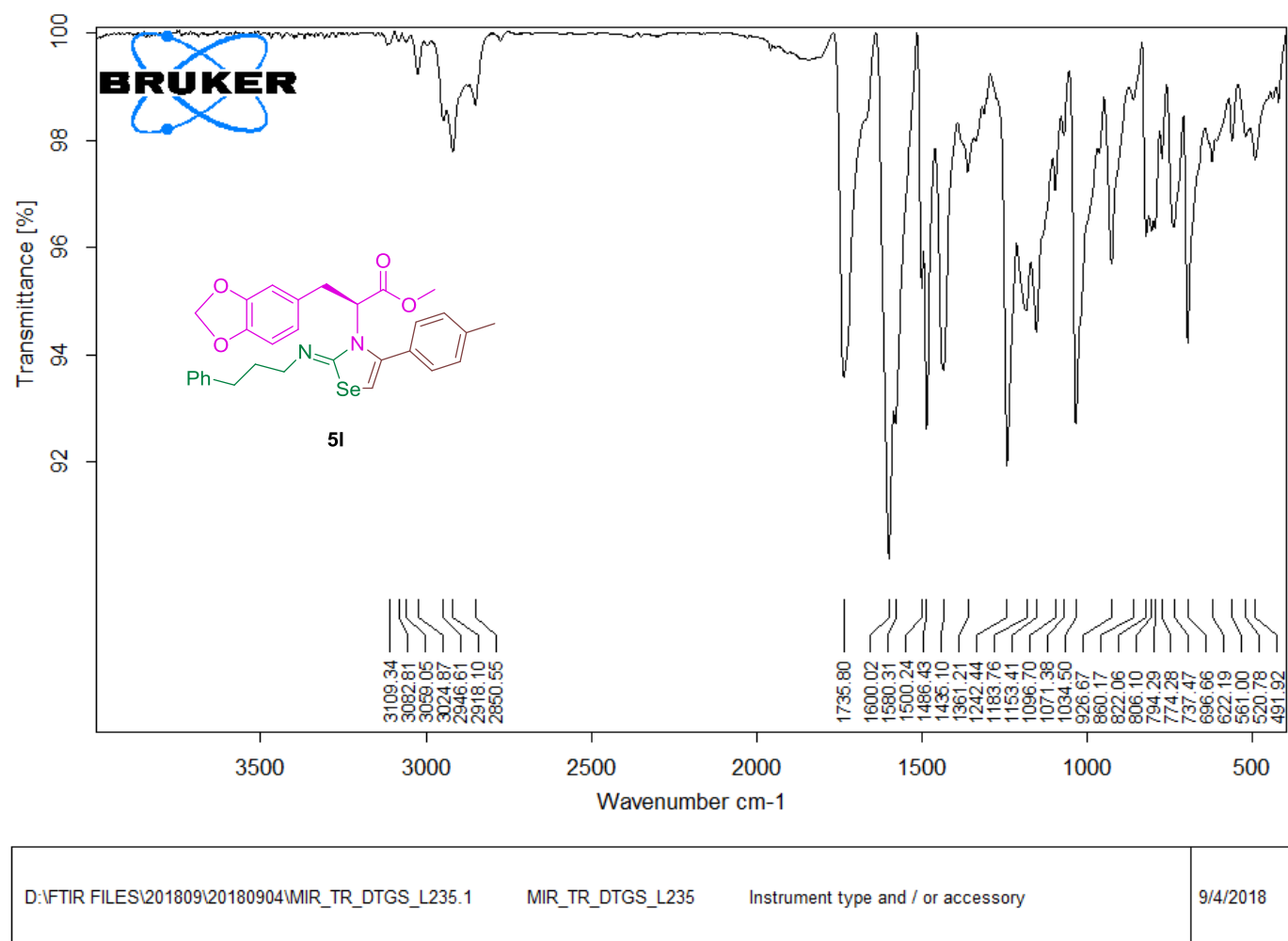
Analyzed Date and Time: 2018/09/06 08:03 下午 Reported Date and Time: 2018/09/11 12:05:13 下午
Processed Date and Time: 2018/09/11 12:04 下午
Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0125\
Processing Method: L235_ee
System (acquisition): Sys 1 Series: 0125
Application(data): Linda Vial Number: 1
Sample Name: UNKNOWN001 Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 10.0 ul
Sample Description:

Chrom Type: Chromaster Channel : 1

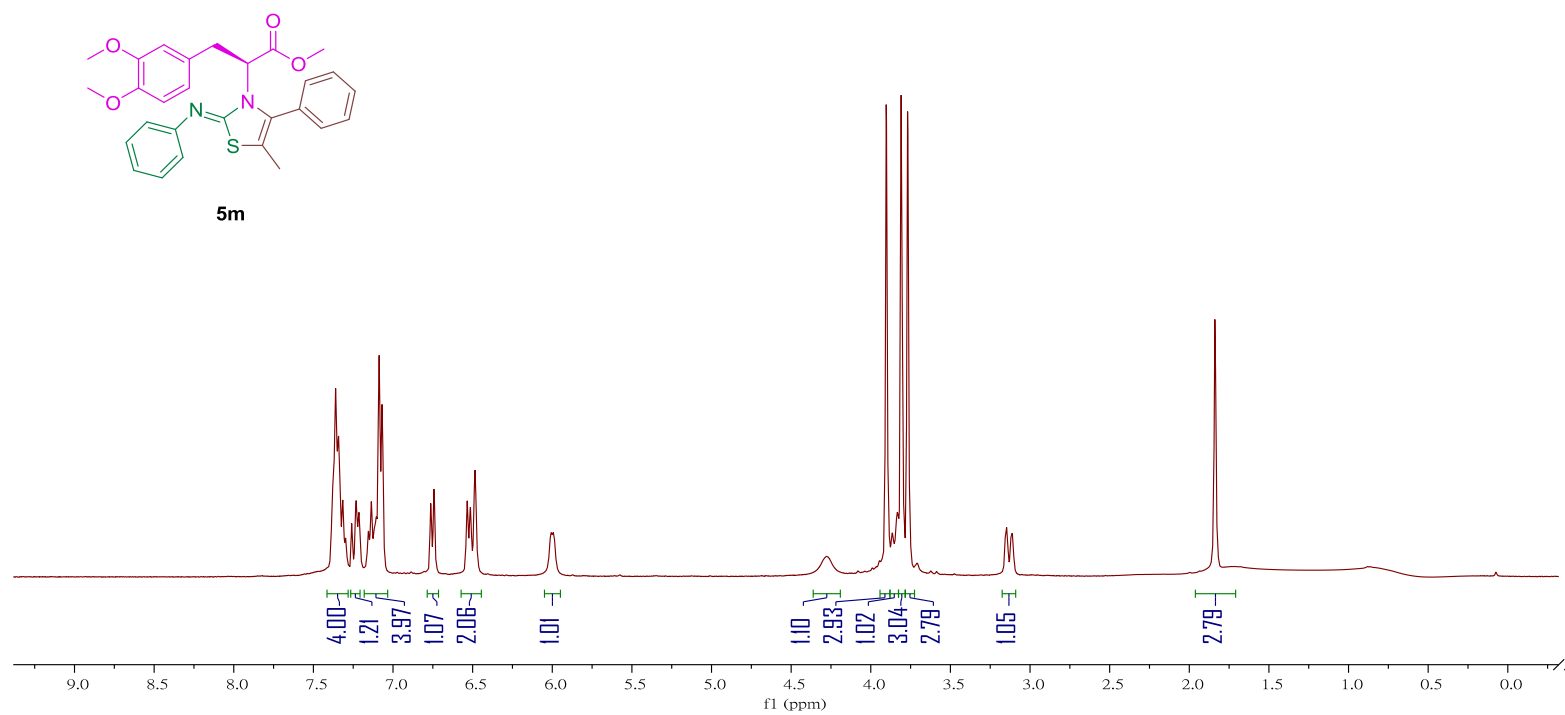


Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

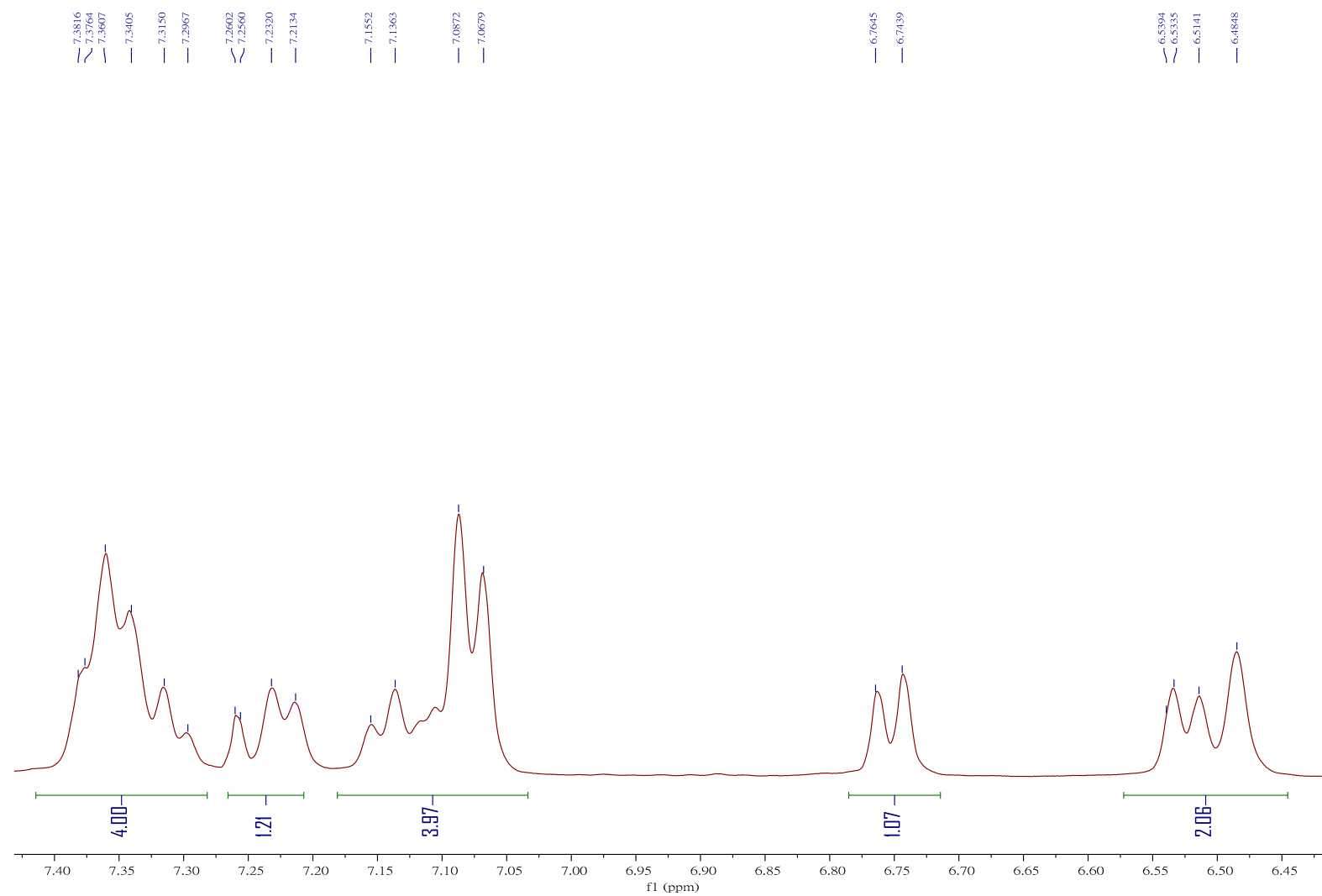
Chiral HPLC Spectrum of compound 51



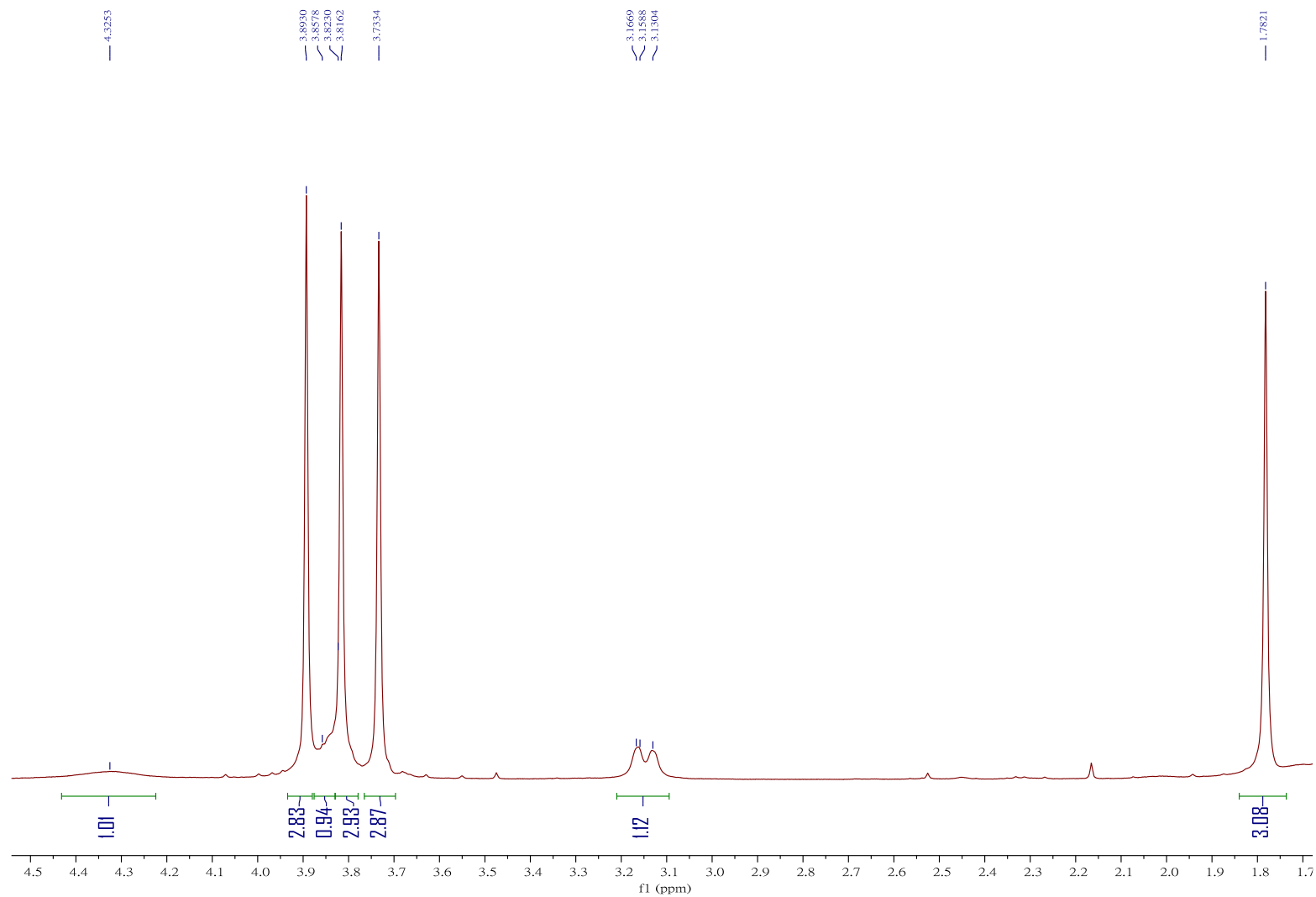
FT-IR Spectrum of compound **5l**



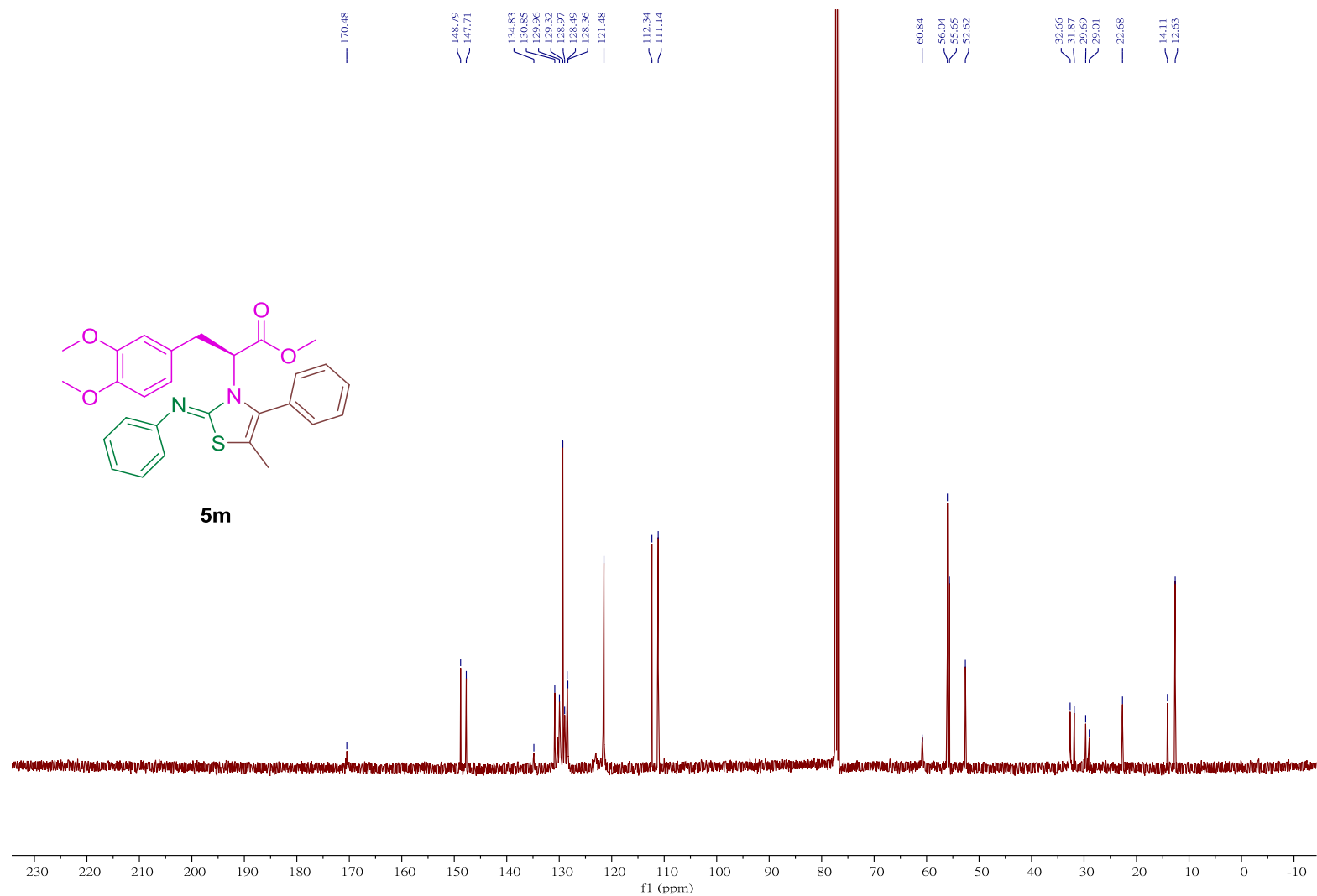
^1H NMR Spectrum (400 MHz) of compound **5m** in CDCl_3

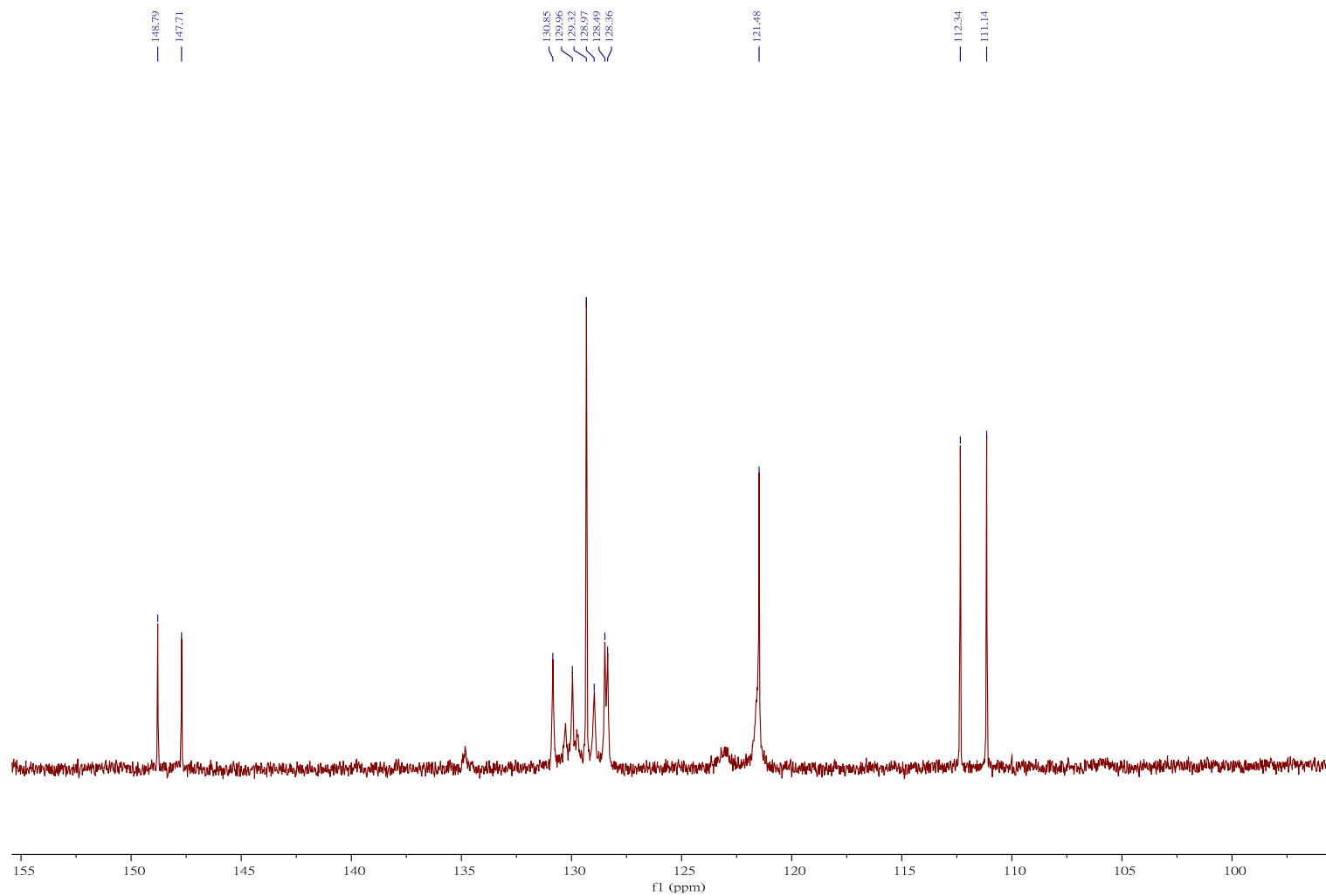


Expansion of ^1H NMR Spectrum (400 MHz) of compound **5m** in CDCl_3



Expansion of ¹H NMR Spectrum (400 MHz) of compound **5m** in CDCl₃





Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **5m** in CDCl_3

Display Report

Analysis Info

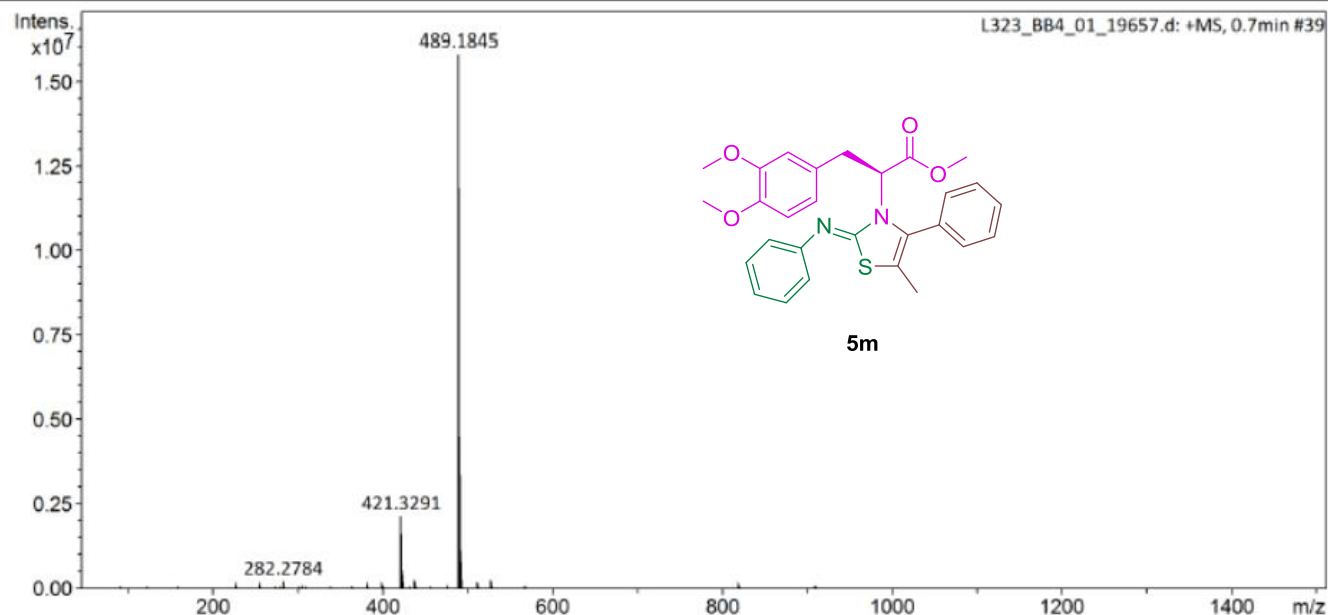
Analysis Name D:\Data\nctu service\data\2018\20180824\L323_BB4_01_19657.d
Method Small molecule.m
Sample Name L323
Comment

Acquisition Date 8/24/2018 12:59:50 PM

Operator NCTU
Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

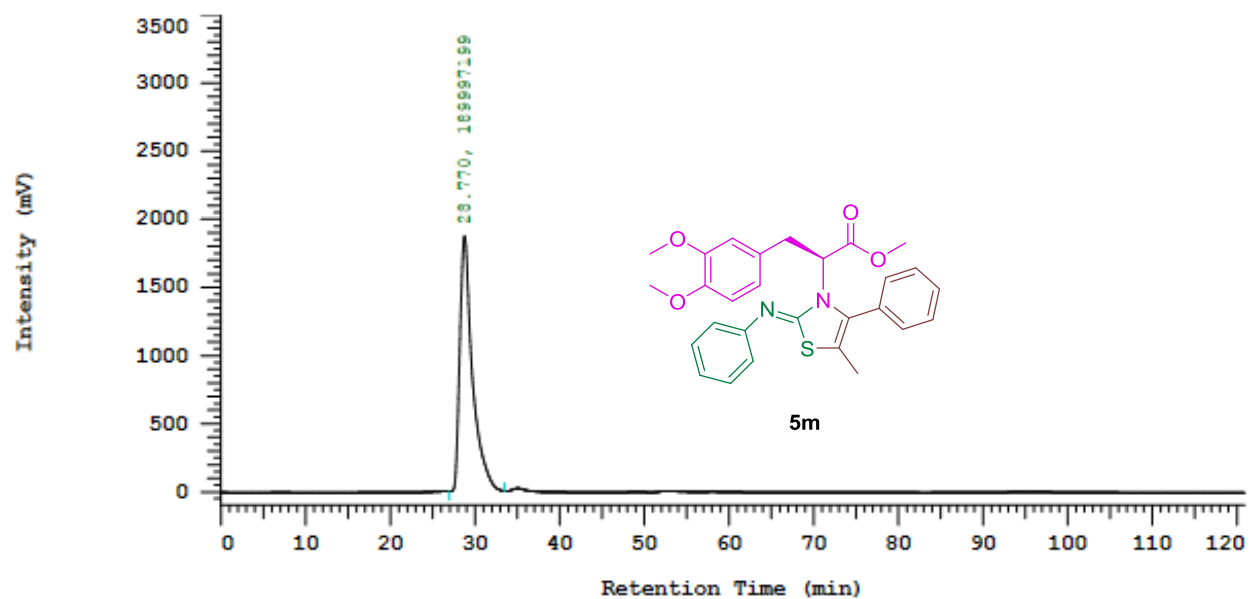


HRMS of compound **5m**

Processing Method: 27m_ee
System (acquisition): Sys 1
Application(data): Linda
Sample Name: UNKNOWN001
Injection from this vial: 1 of 1
Sample Description:

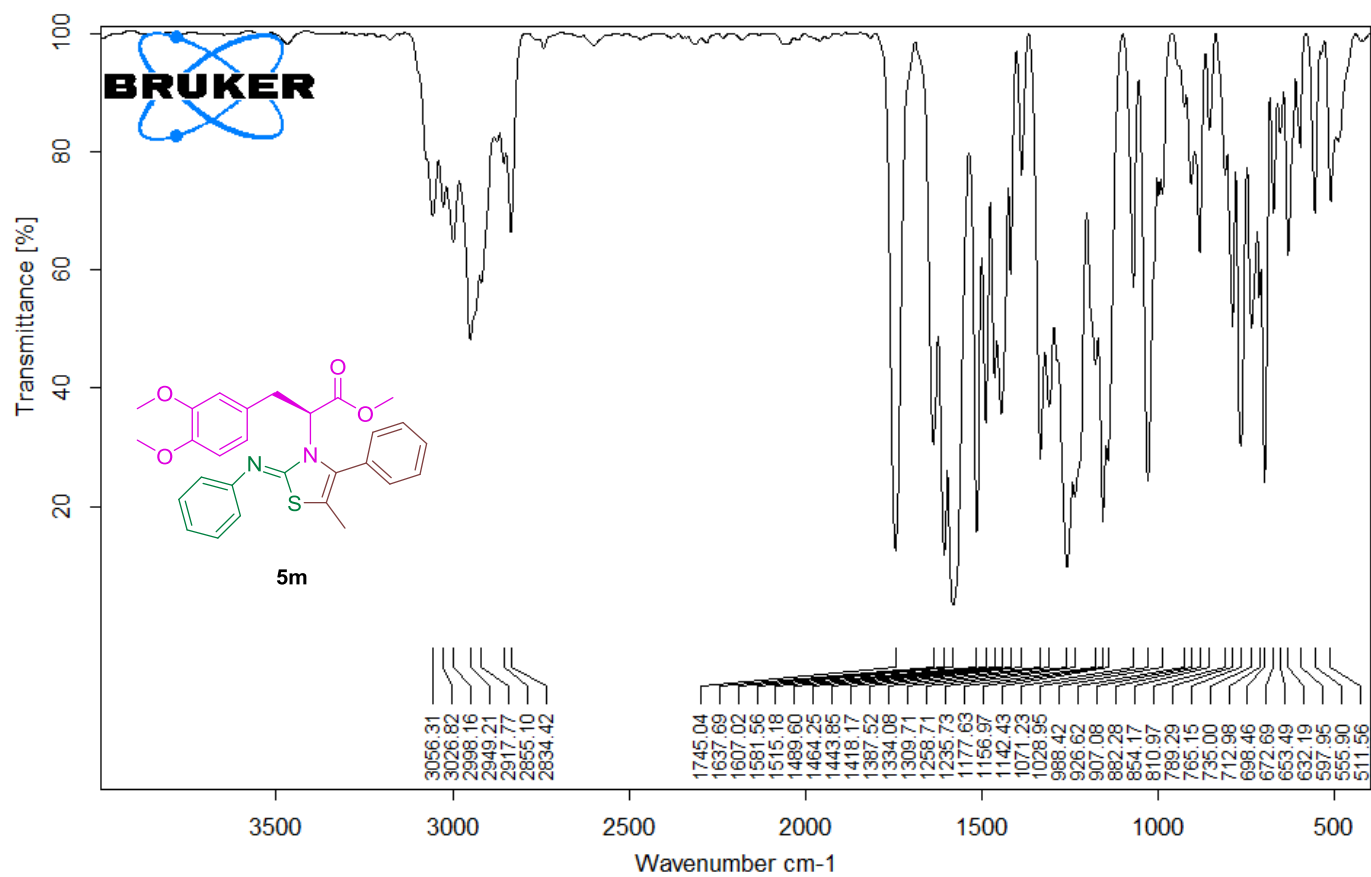
Series: 0221
Vial Number: 1
Vial Type: UNK
Volume: 10.0 ul

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound **5m**



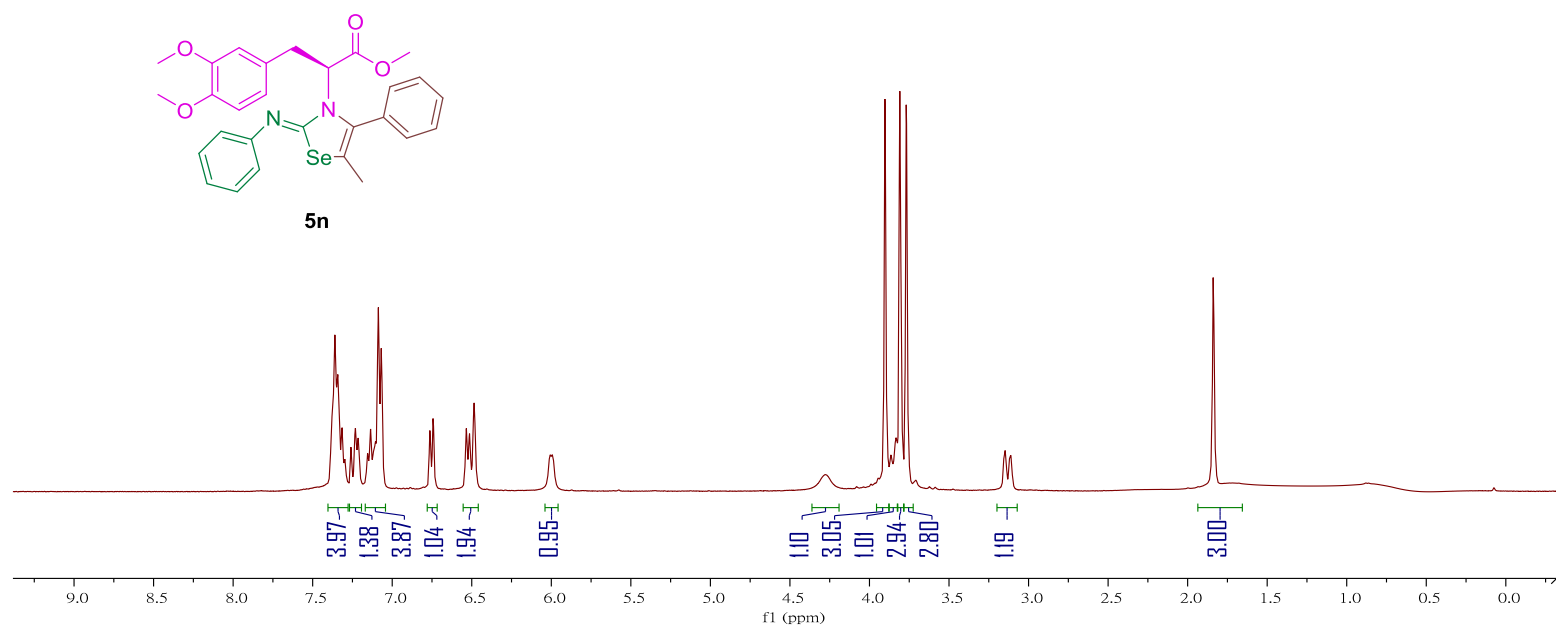
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L323.0

MIR_TR_DTGS_L323

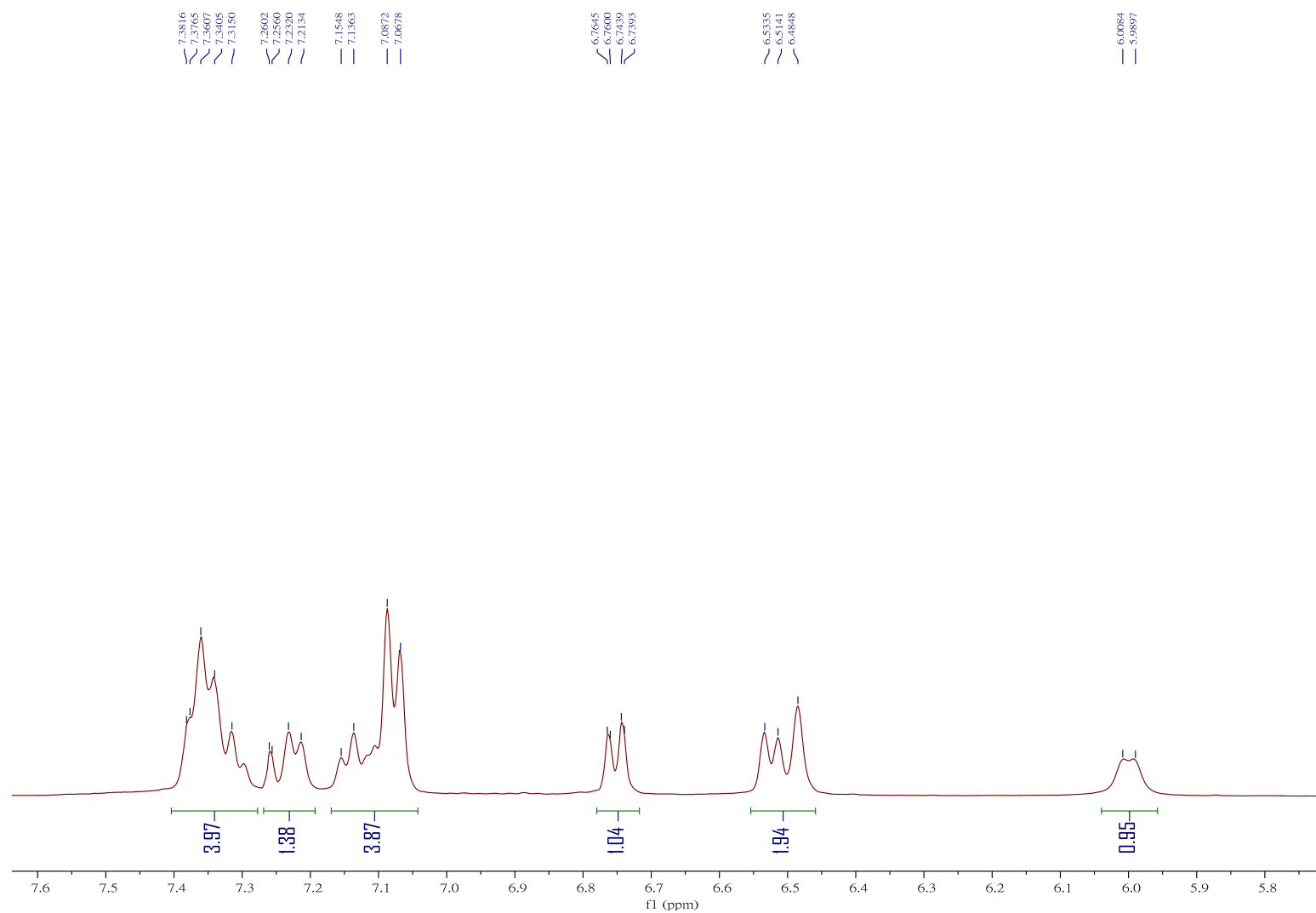
Instrument type and / or accessory

9/4/2018

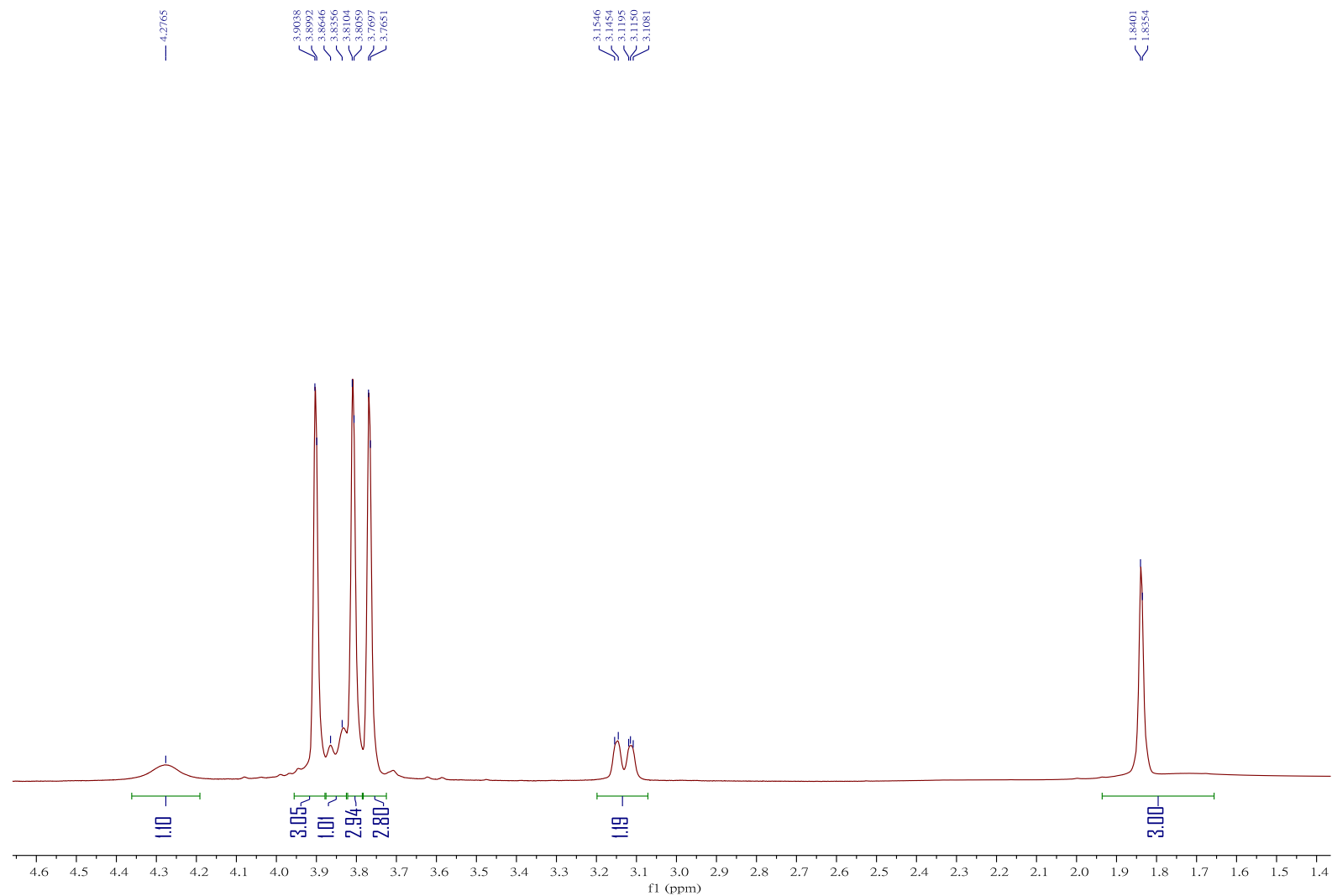
FT-IR Spectrum of compound **5m**



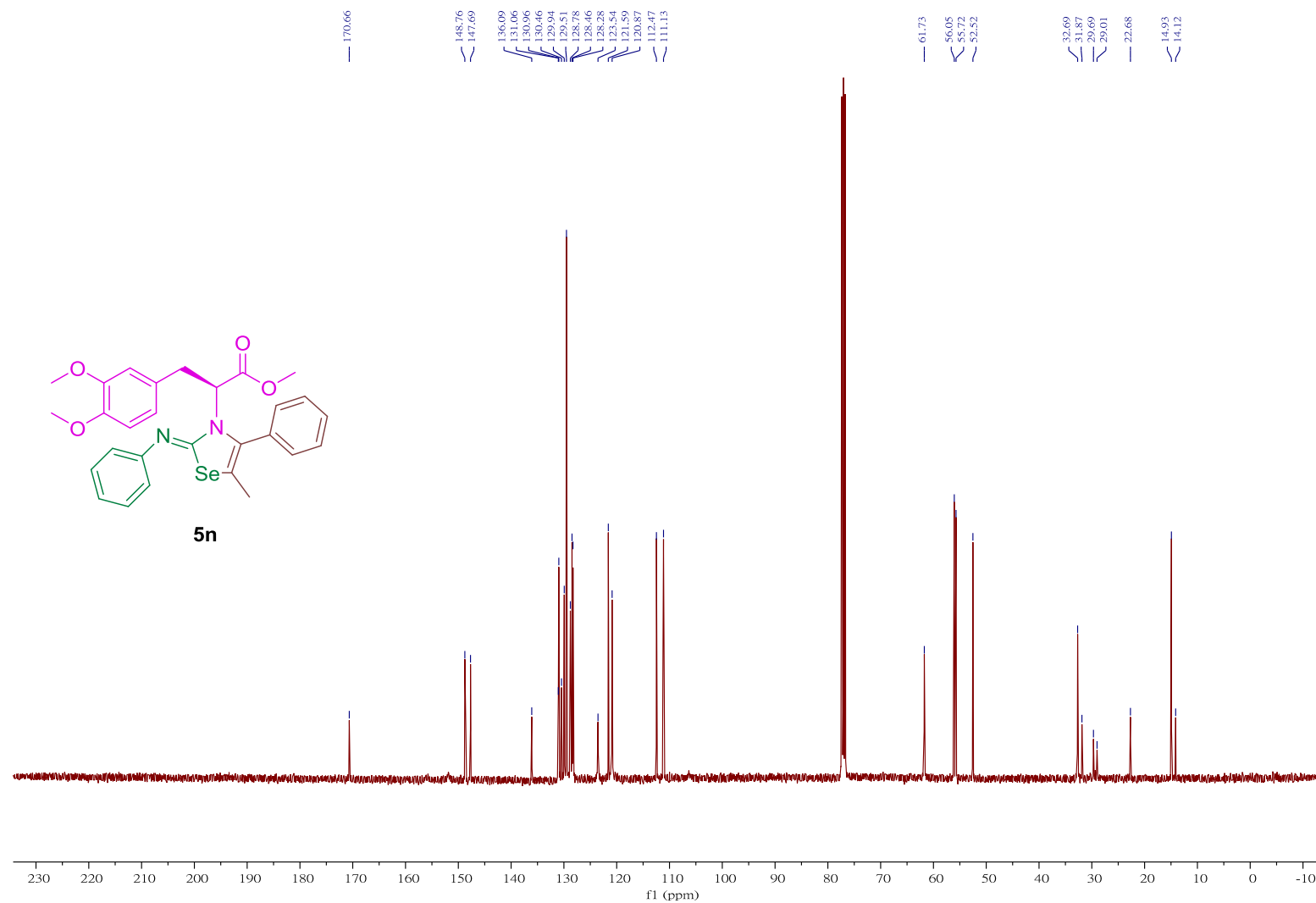
^1H NMR Spectrum (400 MHz) of compound **5n** in CDCl_3



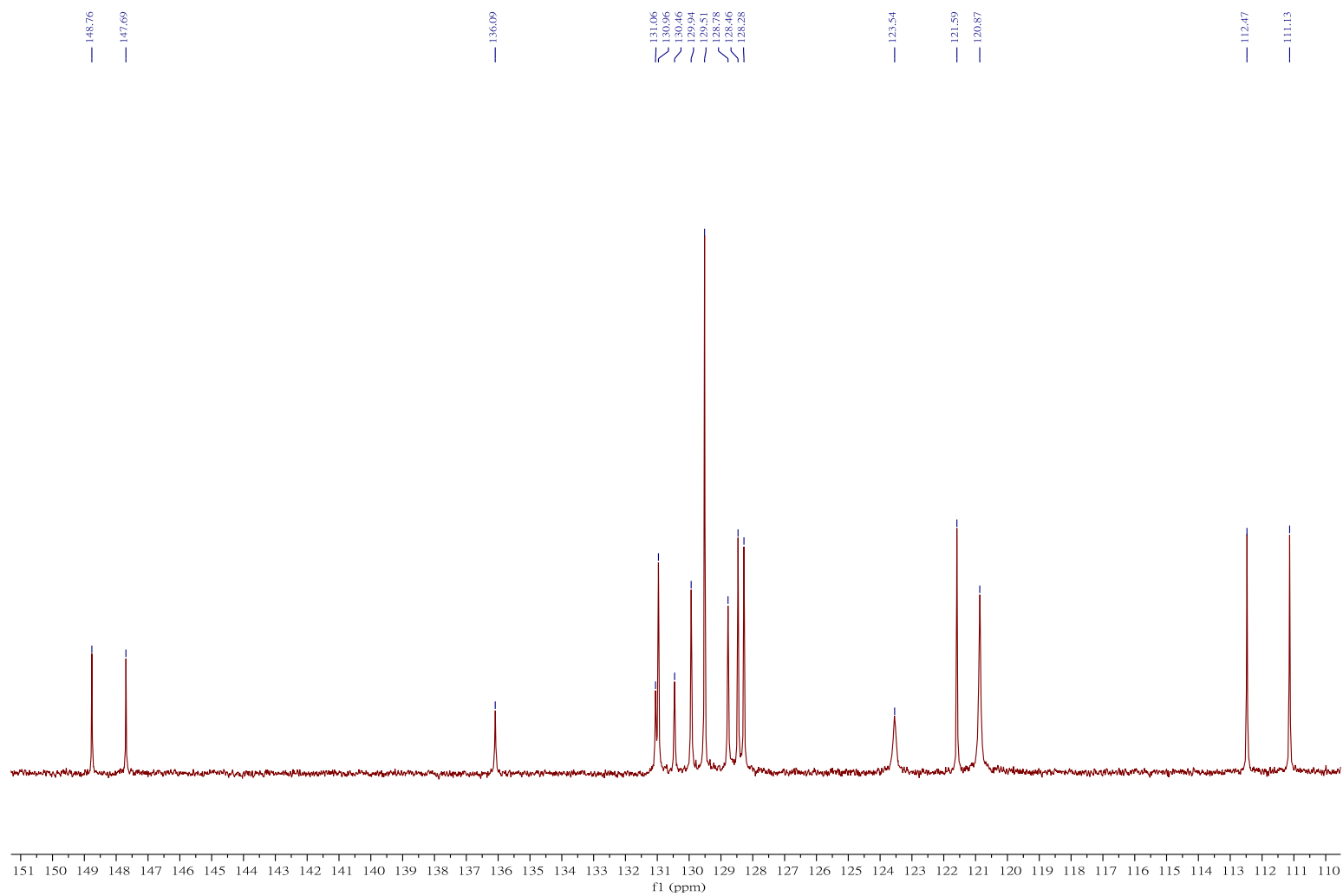
Expansion of ¹H NMR Spectrum (400 MHz) of compound **5n** in CDCl₃



Expansion of ^1H NMR Spectrum (400 MHz) of compound **5n** in CDCl_3



¹³C NMR Spectrum (101 MHz) of compound **5n** in CDCl₃



Expansion of ¹³C NMR Spectrum (101 MHz) of compound **5n** in CDCl₃

Display Report

Analysis Info

Analysis Name D:\Data\nctu service\data\2018\20180824\L324_BB5_01_19658.d
Method Small molecule.m
Sample Name L324
Comment

Acquisition Date 8/24/2018 1:04:13 PM

Operator NCTU

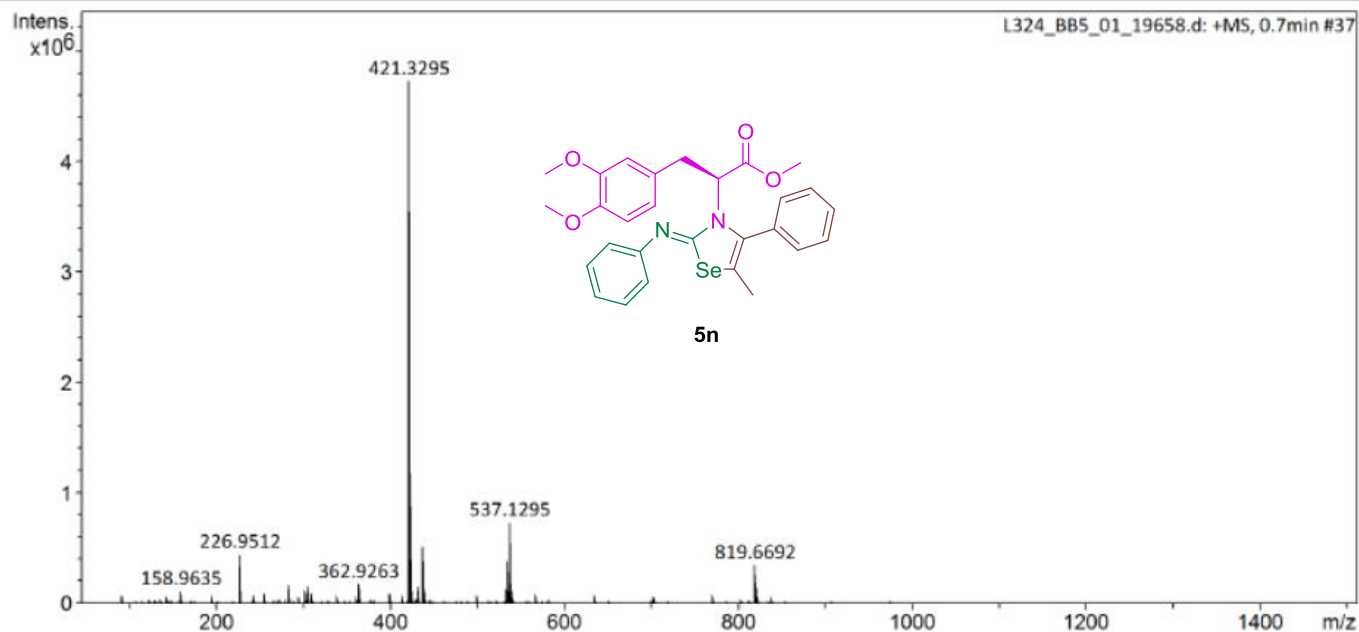
Instrument impact HD 1819696.00164

Acquisition Parameter

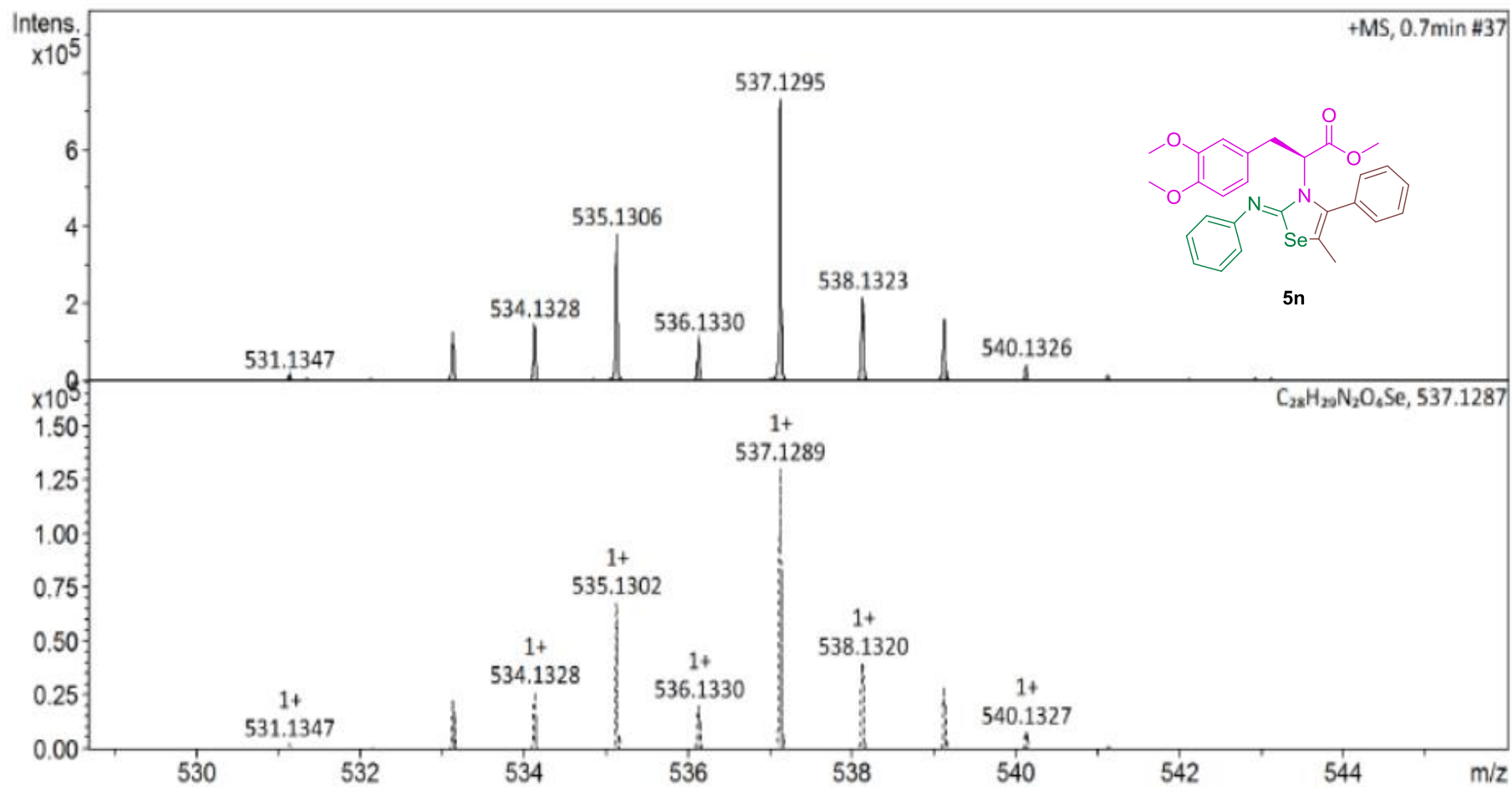
Source Type ESI
Focus Active
Scan Begin 50 m/z
Scan End 1500 m/z

Ion Polarity Positive
Set Capillary 4500 V
Set End Plate Offset -500 V
Set Charging Voltage 2000 V
Set Corona 0 nA

Set Nebulizer 1.0 Bar
Set Dry Heater 200 °C
Set Dry Gas 6.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



HRMS of compound **5n**



HRMS of compound **5n**

Processing Method: 27n_ee

System (acquisition): Sys 1

Application(data): Linda

Sample Name: UNKNOWN001

Injection from this vial: 1 of 1

Sample Description:

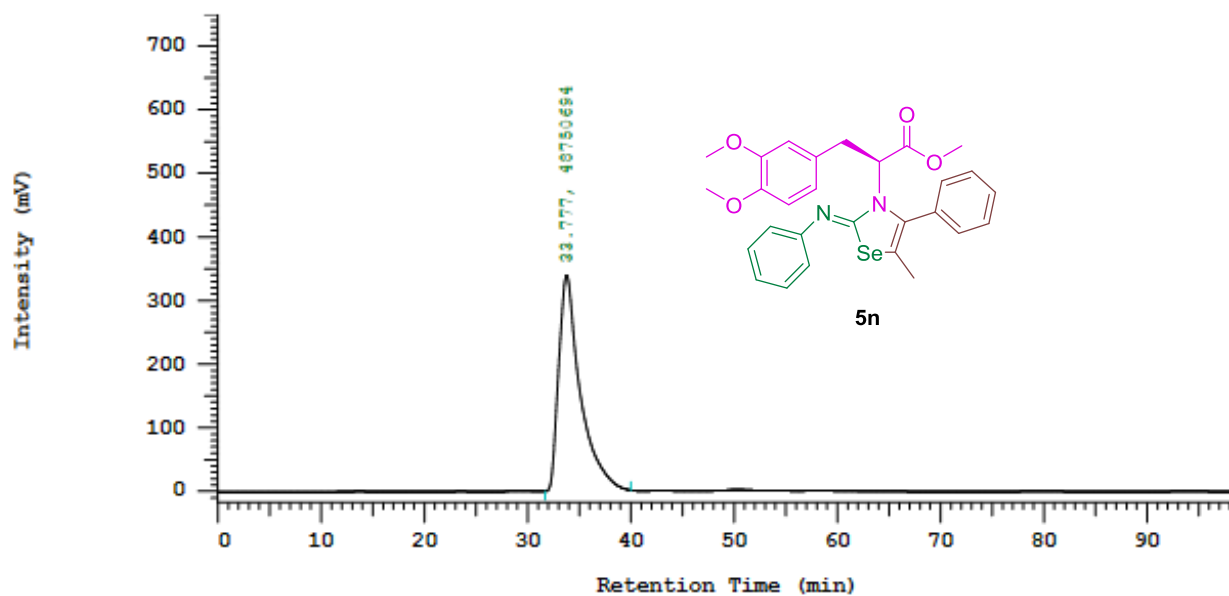
Series: 0218

Vial Number: 1

Vial Type: UNK

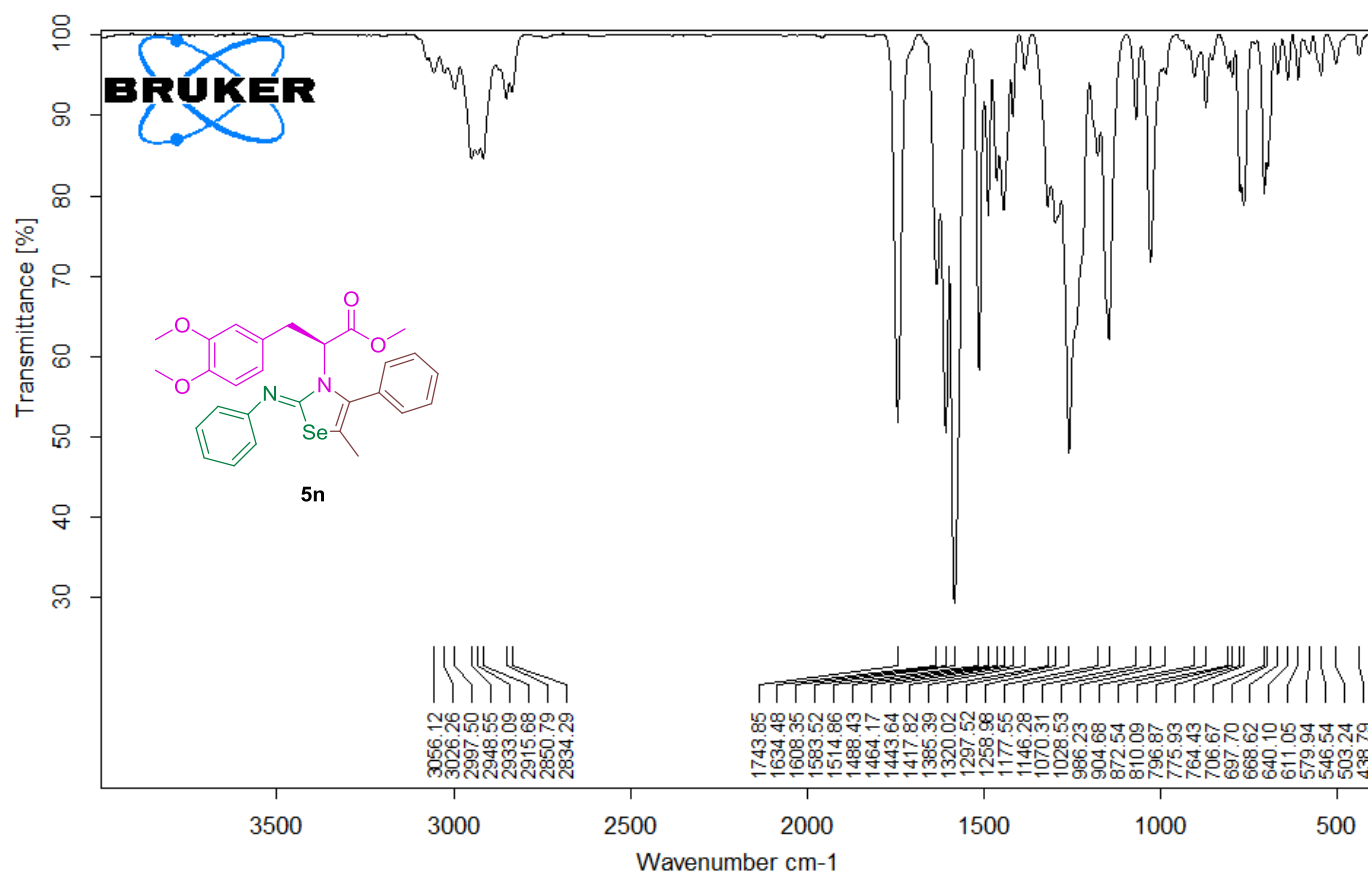
Volume: 10.0 ul

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

Chiral HPLC of compound **5n**



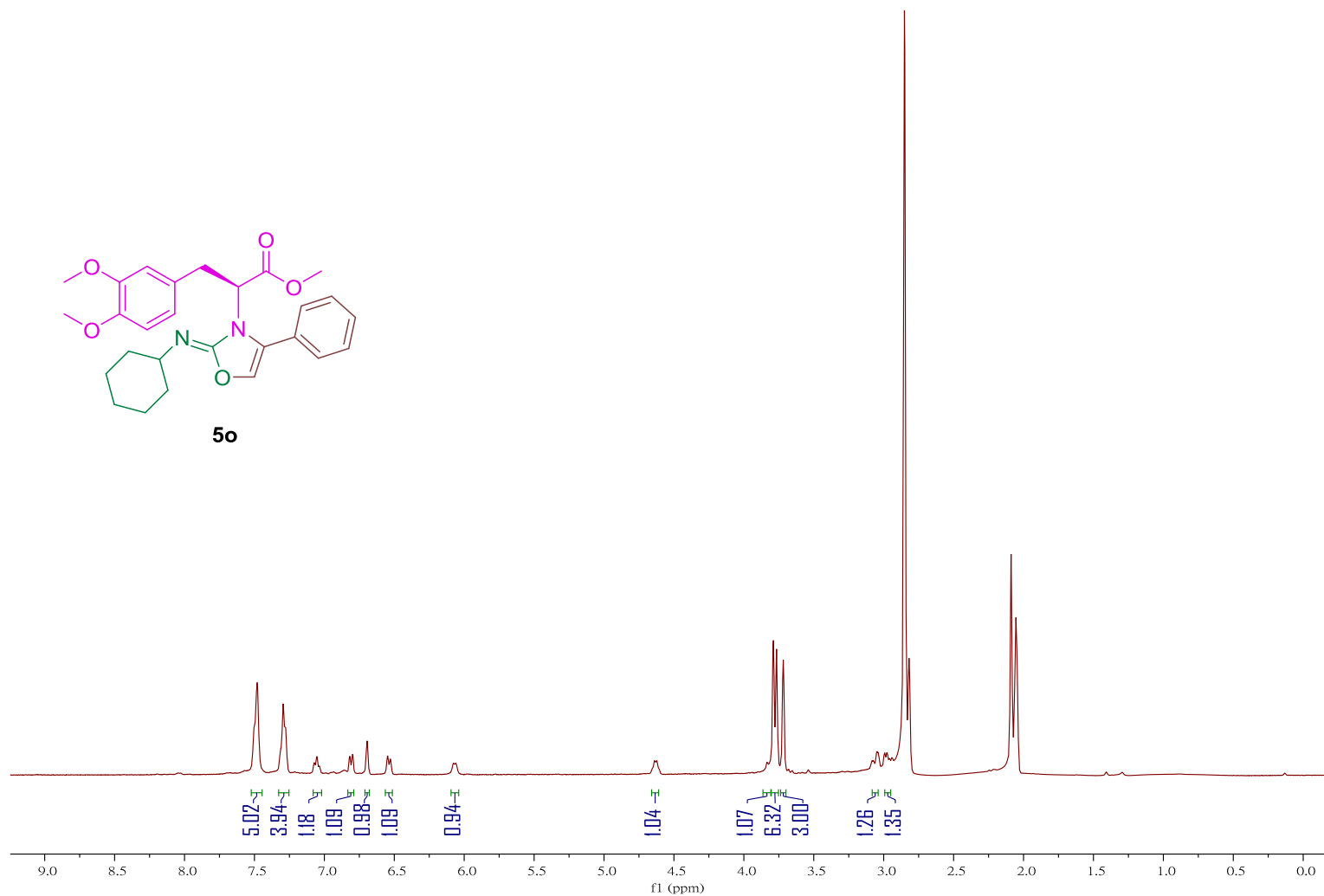
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L324.0

MIR_TR_DTGS_L324

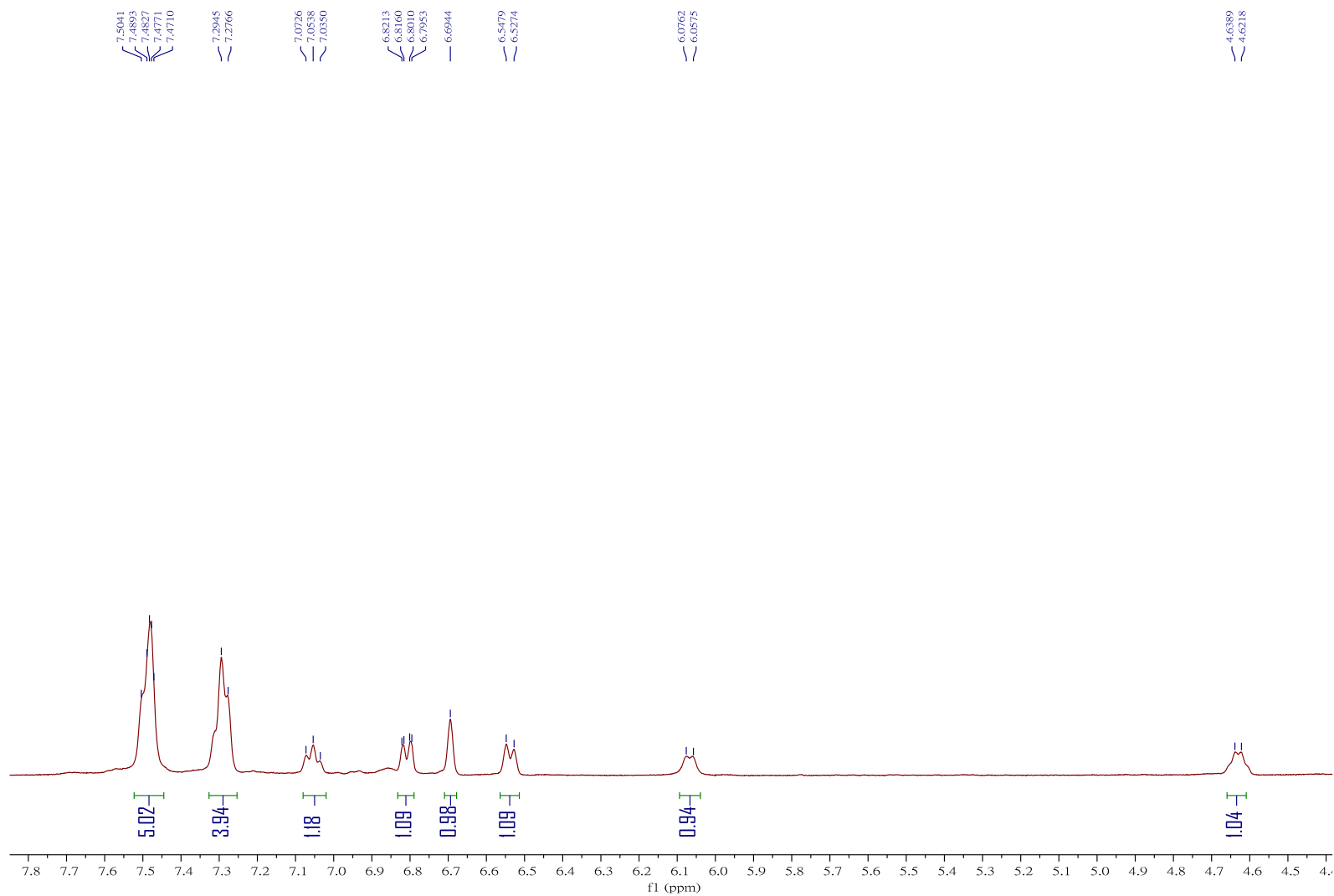
Instrument type and / or accessory

9/4/2018

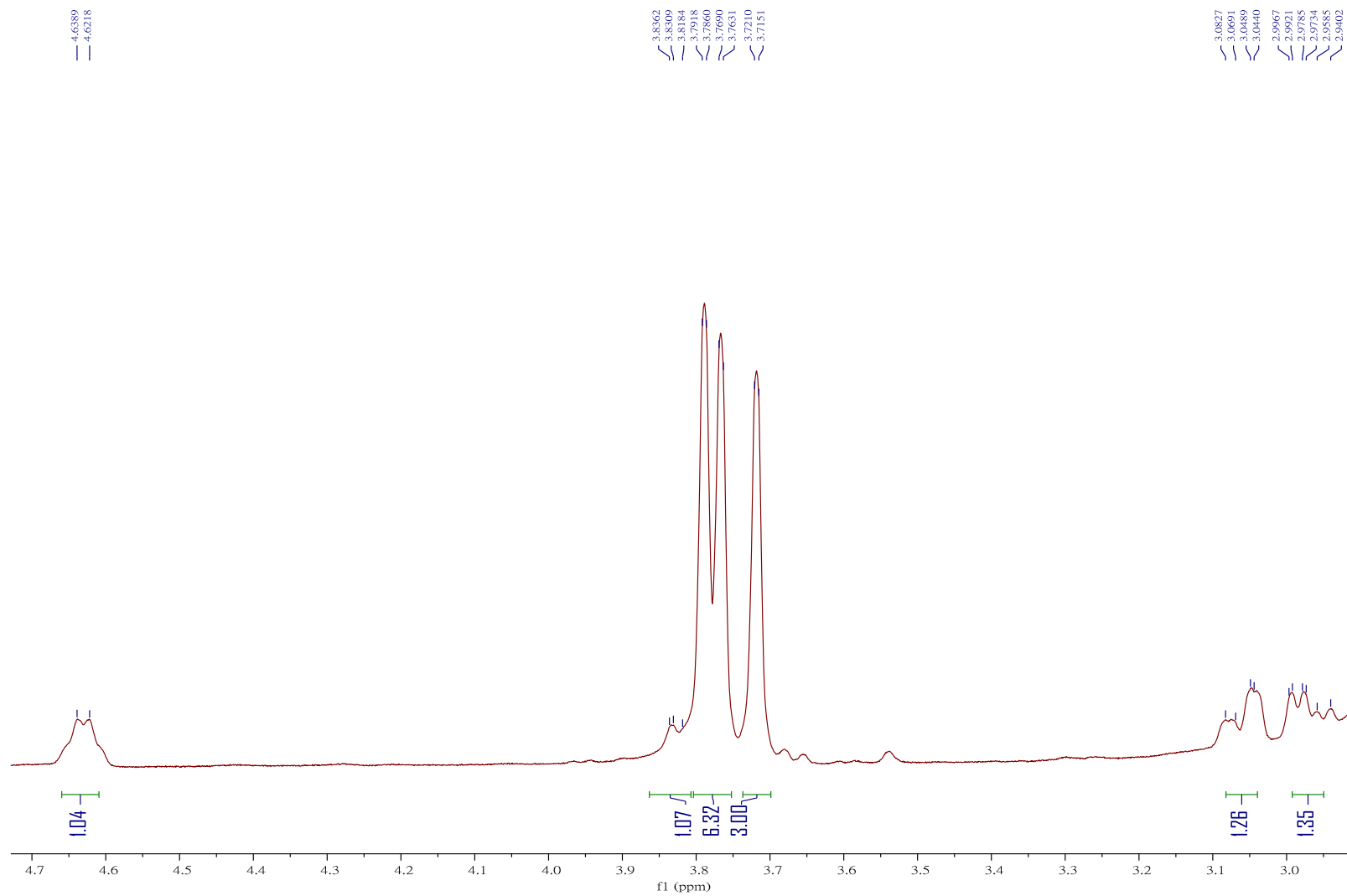
FT-IR Spectrum of compound **5n**



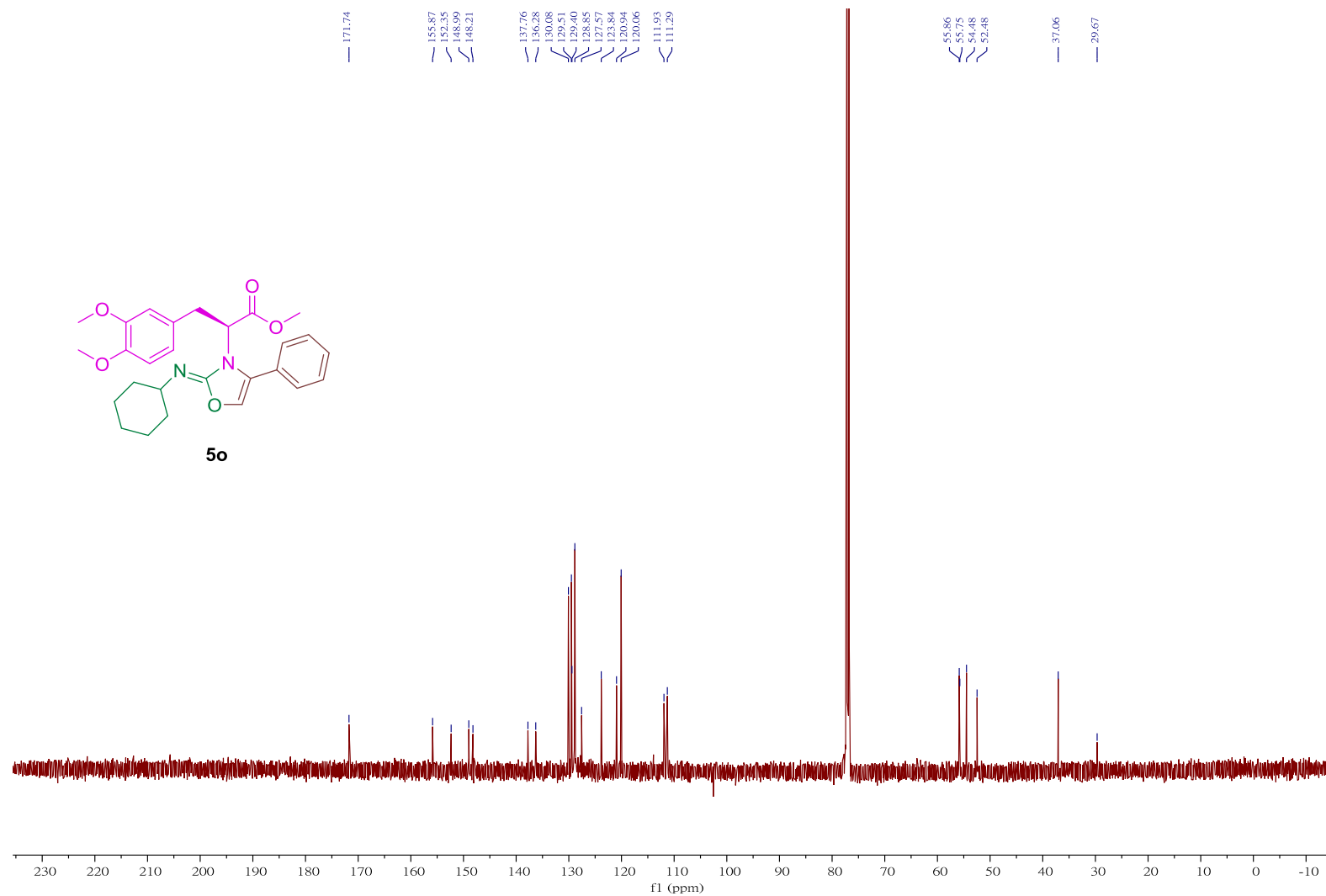
^1H NMR Spectrum (400 MHz) of compound **5o** in acetone- d_6



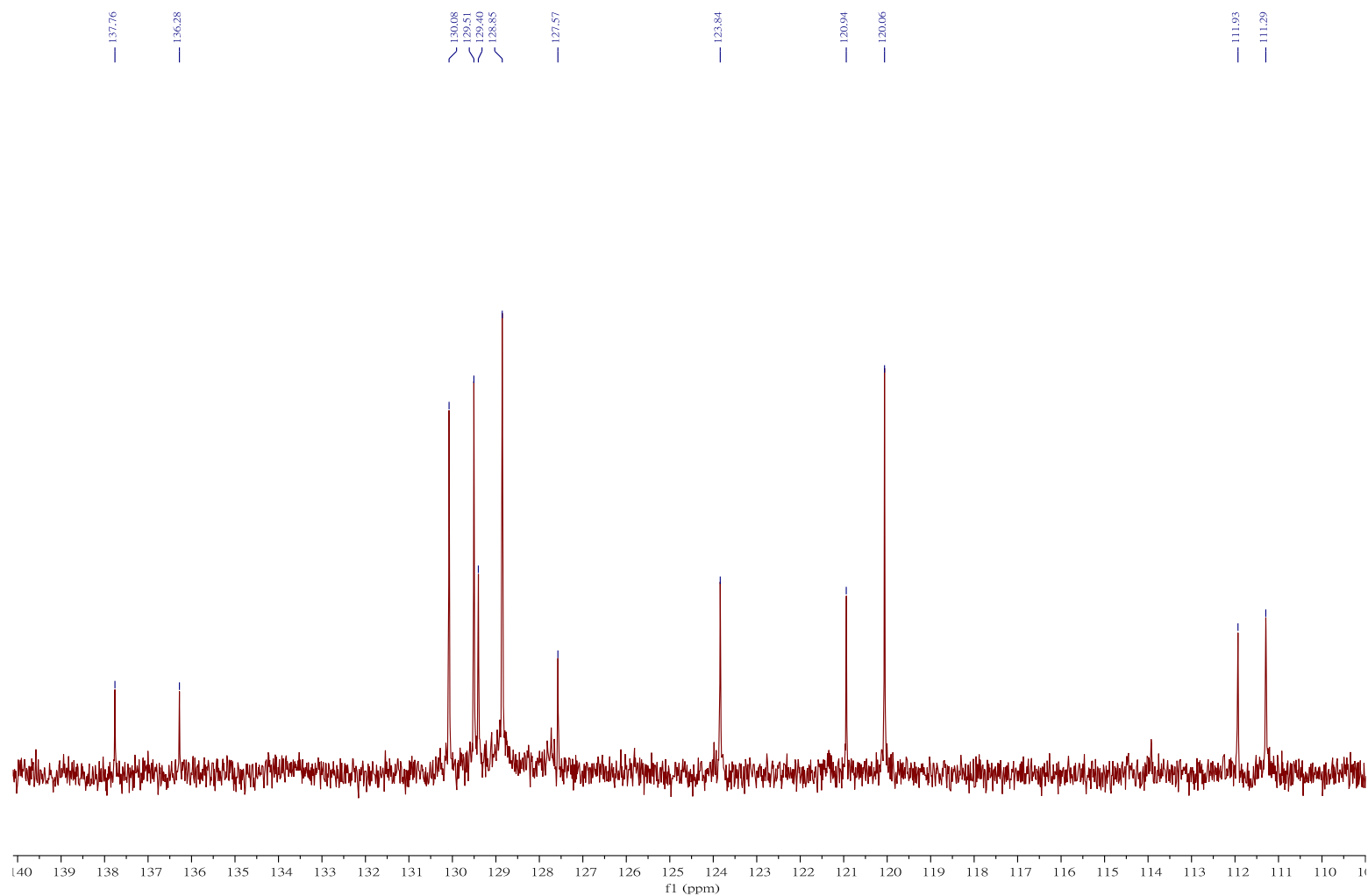
Expansion of ¹H NMR Spectrum (400 MHz) of compound **5o** in acetone-*d*₆



Expansion of ^1H NMR Spectrum (400 MHz) of compound **5o** in acetone- d_6



^{13}C NMR Spectrum (101 MHz) of compound **5o** in CDCl_3



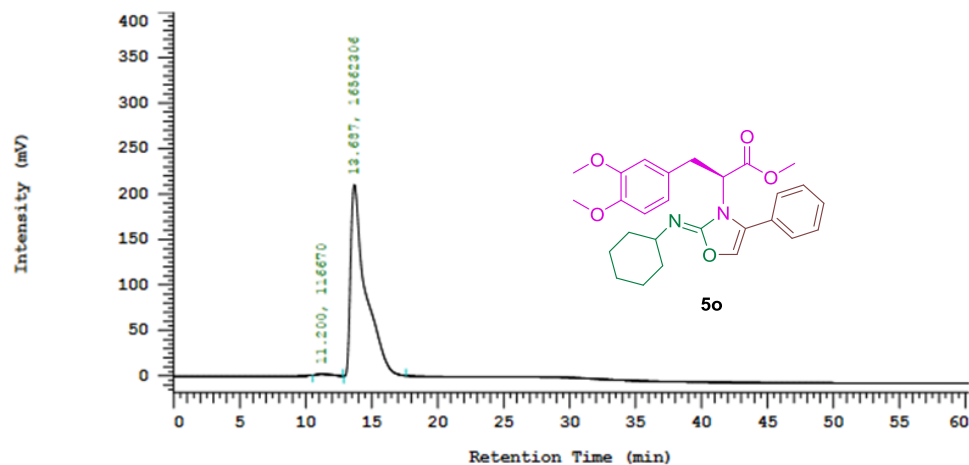
Expansion of ¹³C NMR Spectrum (101 MHz) of compound **5o** in CDCl₃

CSM: Linda Series: 0163 Report Name: modified System: Sys 1

Chromaster System Manager Report

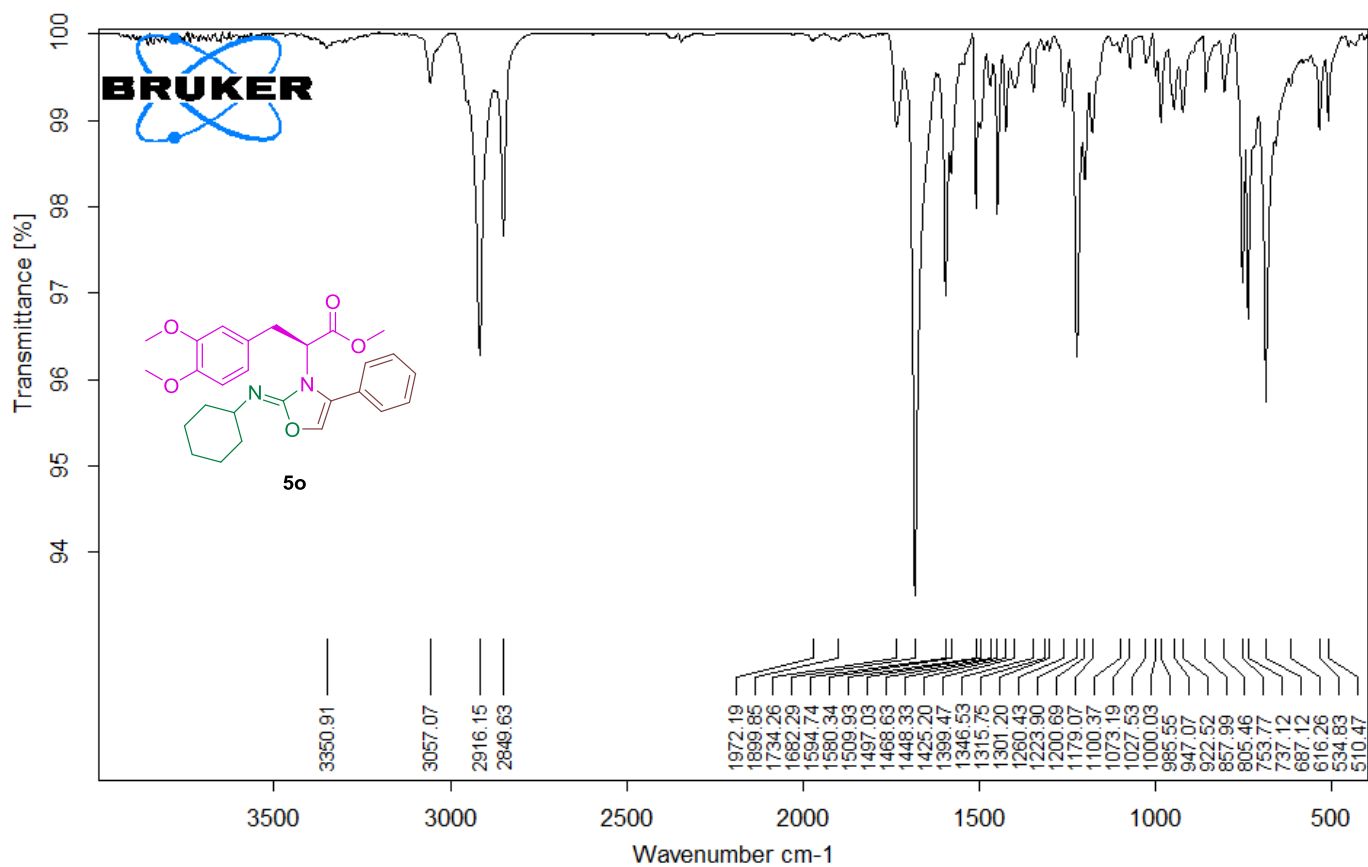
Analyzed Date and Time: 2018/09/14 08:16 下午
Reported Date and Time: 2018/09/15 08:54:50 上午
Processed Date and Time: 2018/09/15 08:54 上午
Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0163\
Processing Method: L320_ee
System (acquisition): Sys 1 Series: 0163
Application(data): Linda Vial Number: 1
Sample Name: UNKNOWN001 Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 10.0 ul
Sample Description:

Chrom Type: Chromaster Channel : 1



Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA15, Hex
85

Chiral HPLC of compound **5o**



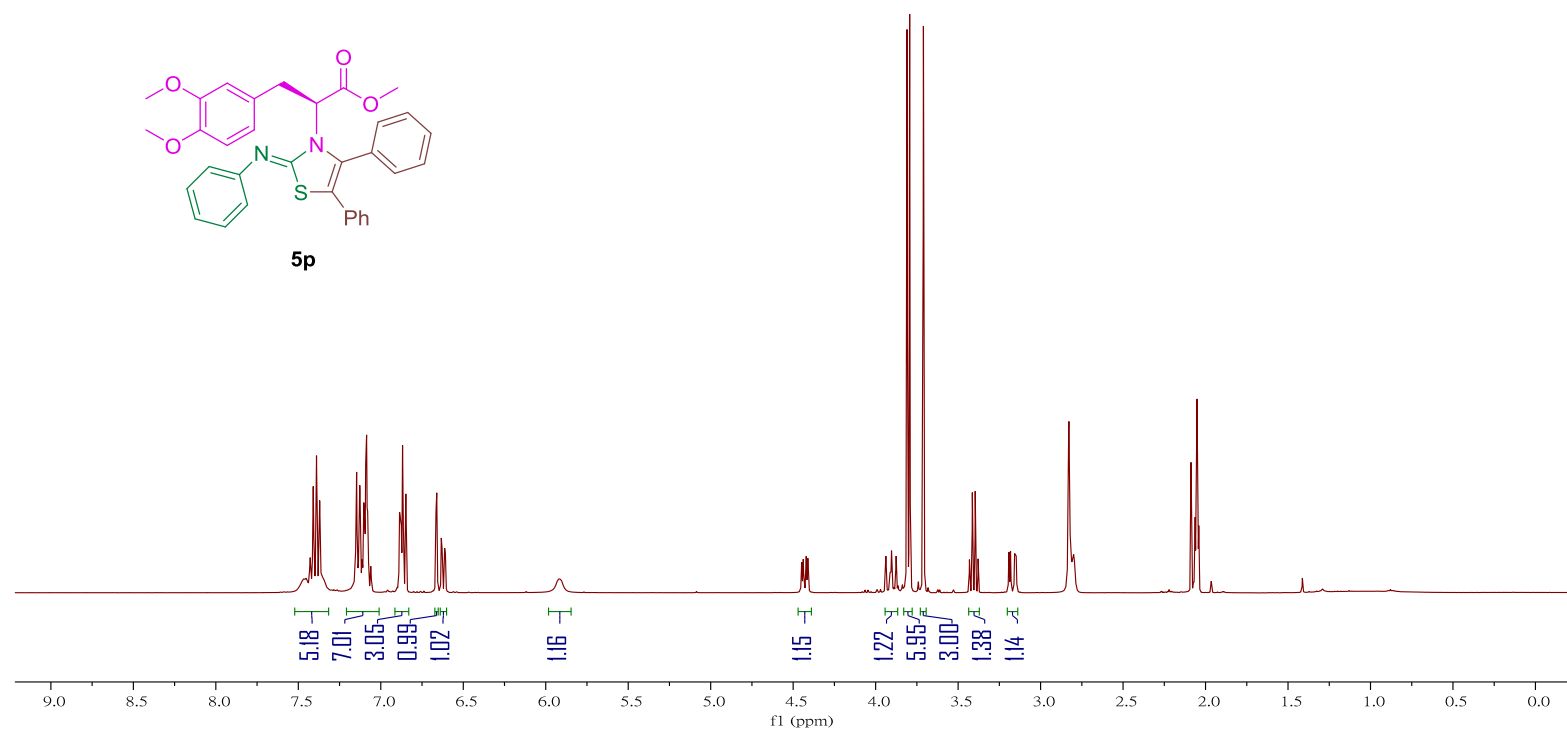
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L320.1

MIR_TR_DTGS_L320

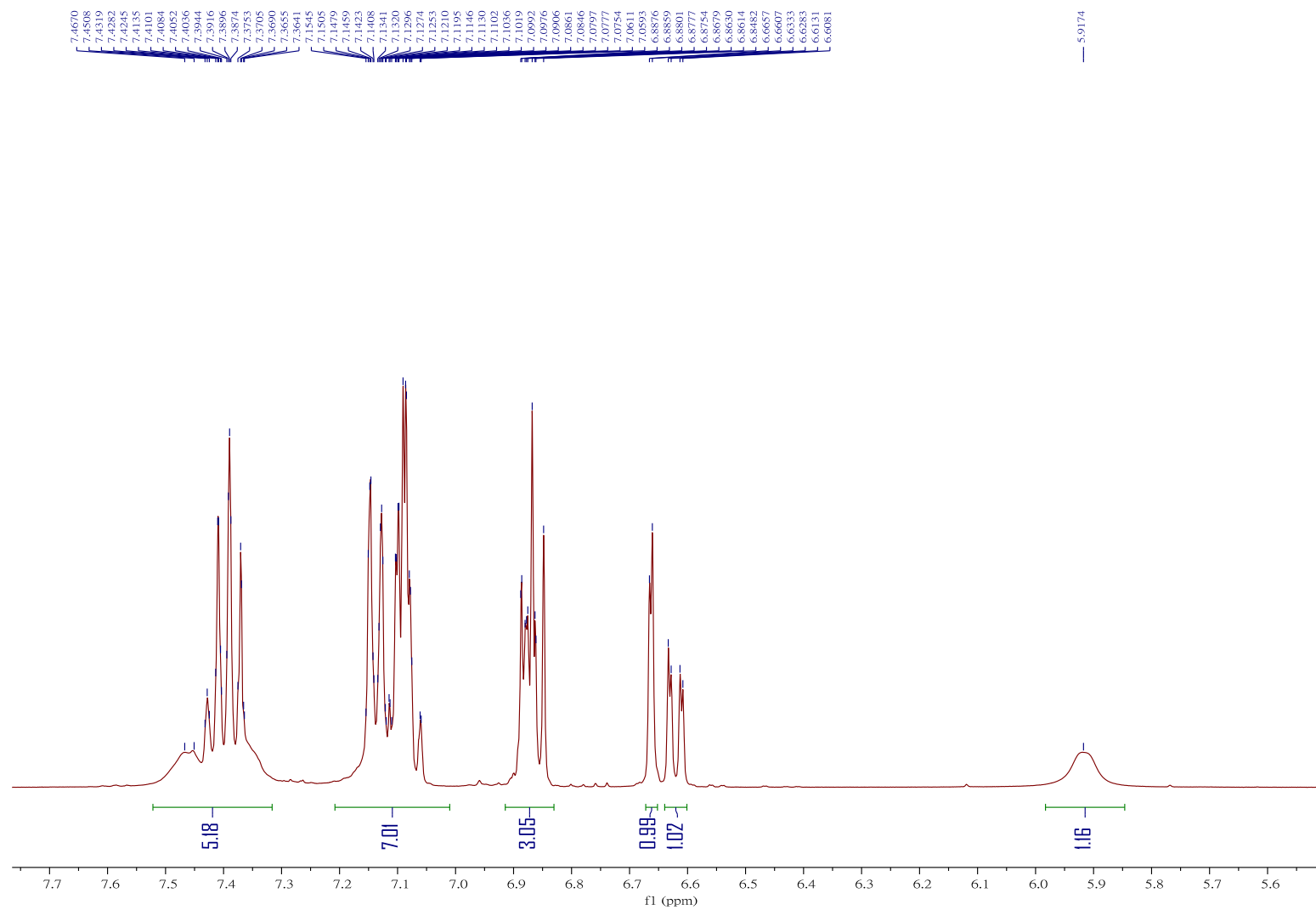
Instrument type and / or accessory

9/4/2018

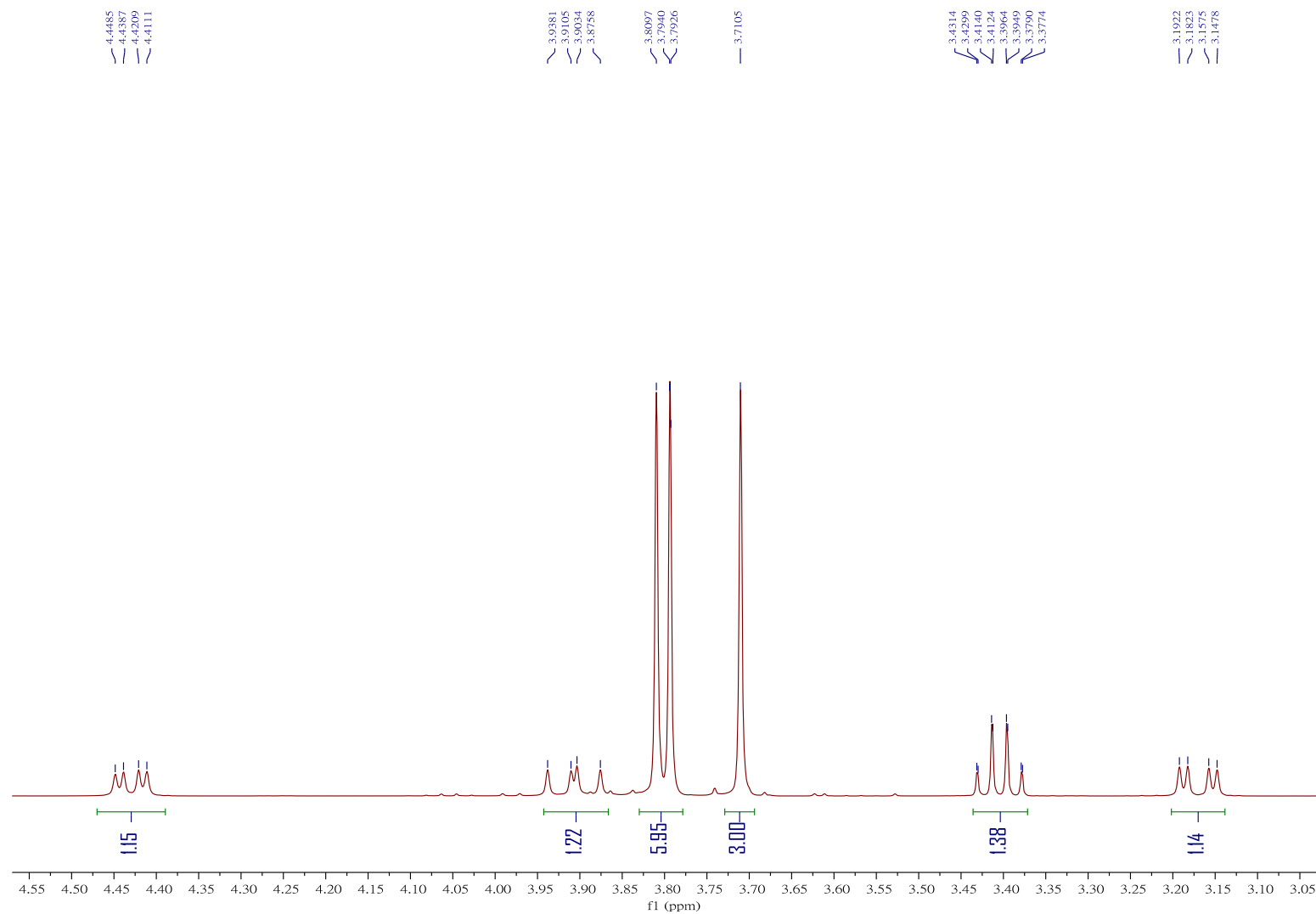
FT-IR Spectrum of compound **5o**



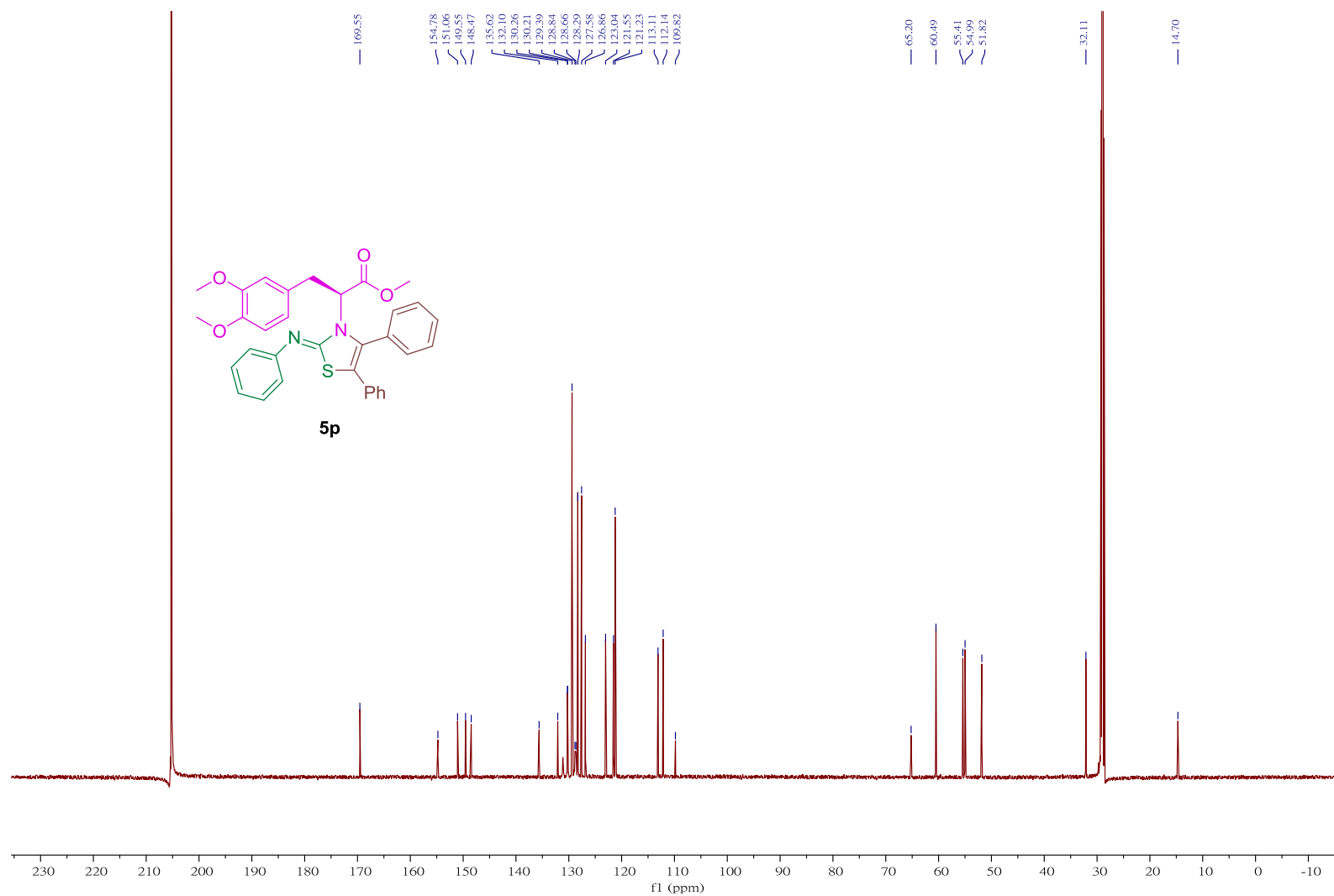
¹H NMR Spectrum (400 MHz) of compound **5p** in acetone-*d*₆



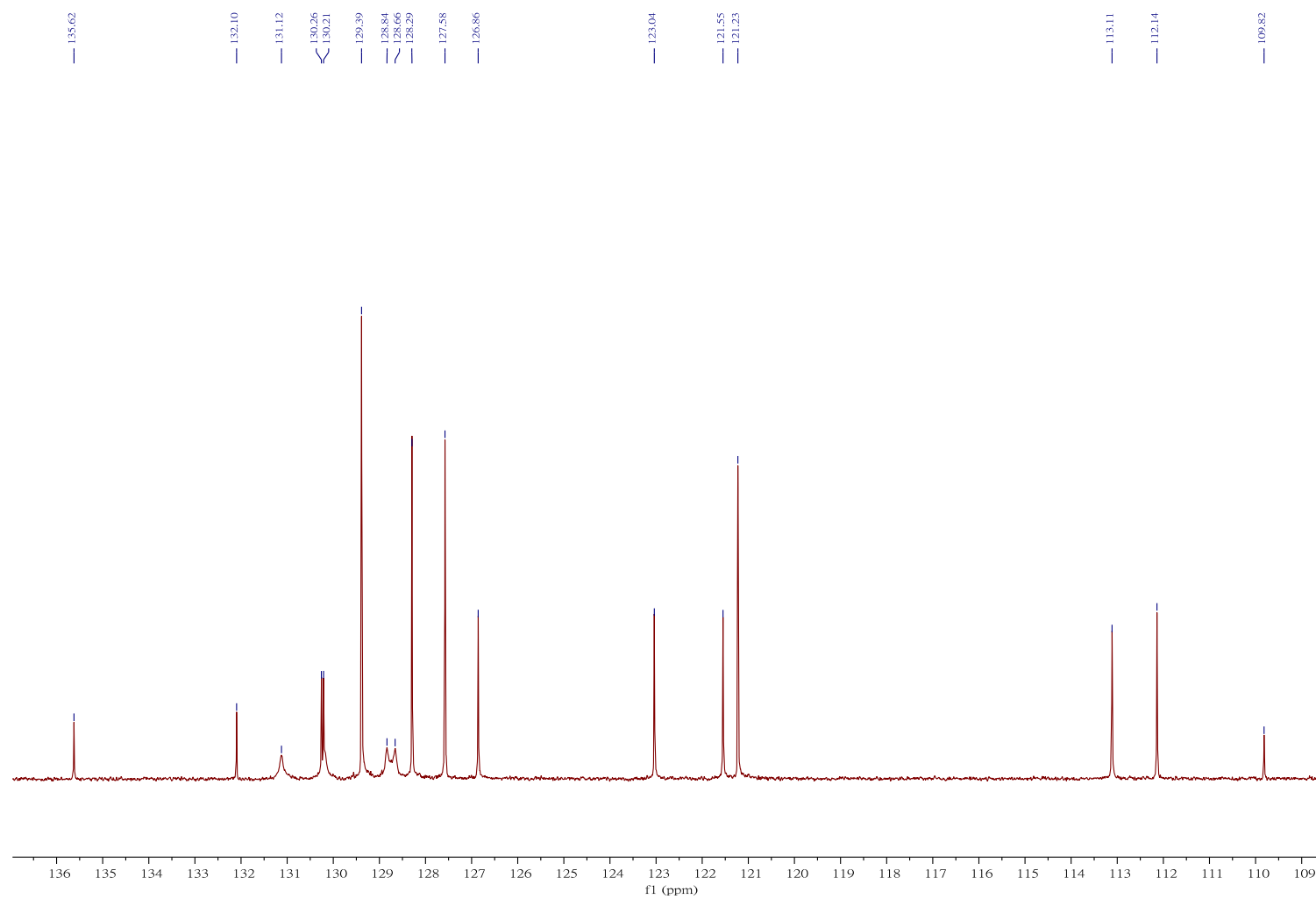
Expansion of ^1H NMR Spectrum (400 MHz) of compound **5p** in acetone- d_6



Expansion of ^1H NMR Spectrum (400 MHz) of compound **5p** in acetone- d_6



^{13}C NMR Spectrum (151 MHz) of compound **5p** in acetone- d_6

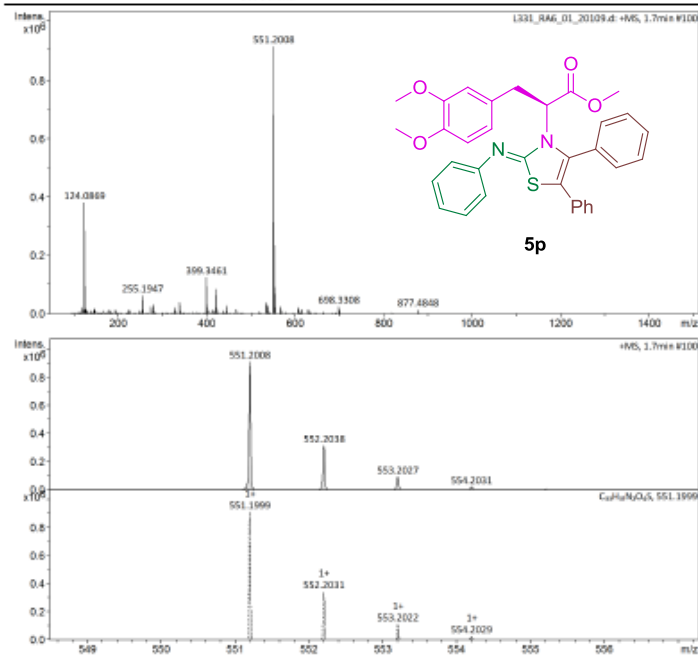


Expansion of ^{13}C NMR Spectrum (151 MHz) of compound **5p** in acetone- d_6

Display Report

Analysis Info		Acquisition Date: 9/21/2018 12:09:17 PM	
Analysis Name	D:\Data\NCTU SERVICE\Data\2018\20180921\L331_RA6_01_20109.d	Operator	NCTU
Method	Small molecule.m	Instrument	Impact HD
Sample Name	L331		1819696.00164
Comment			

Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
Focus	Active	Set Capillary	4500 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1500 m/z	Set Charging Voltage	2000 V
		Set Corona	0 nA
		Set Nebulizer	1.0 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	8.0 l/min
		Set Divert Valve	Waste
		Set APCI Heater	0 °C



HRMS of compound **5p**

Processing Method: 27r_ee

System (acquisition): Sys 1

Application(data): Linda

Sample Name: UNKNOWN001

Injection from this vial: 1 of 1

Sample Description:

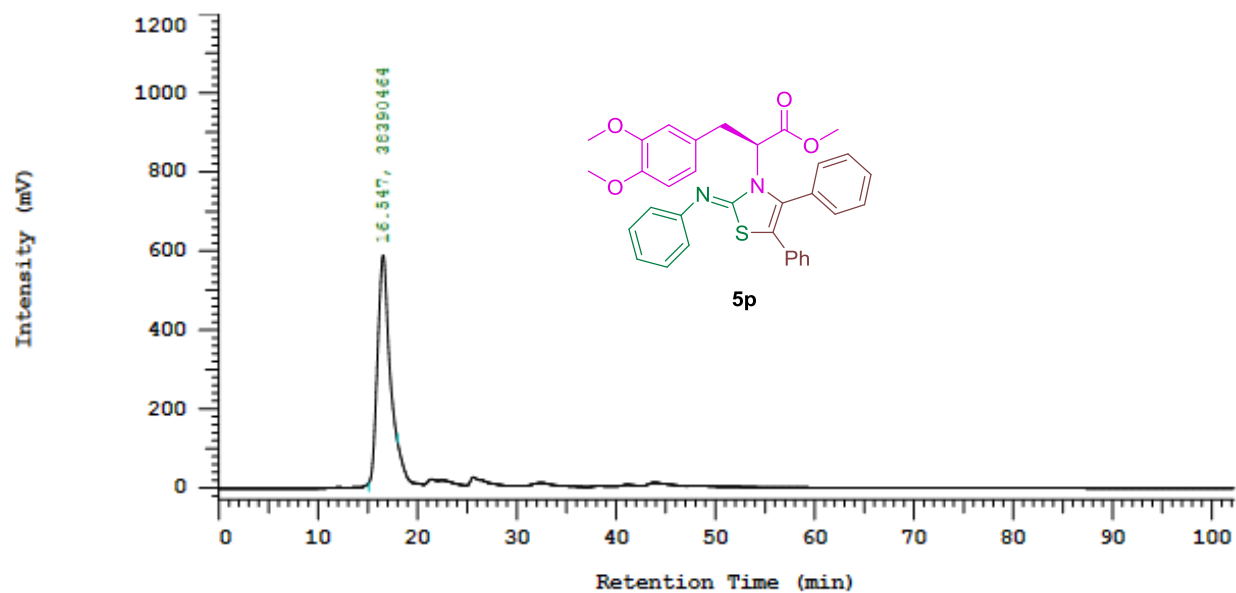
Series: 0204

Vial Number: 1

Vial Type: UNK

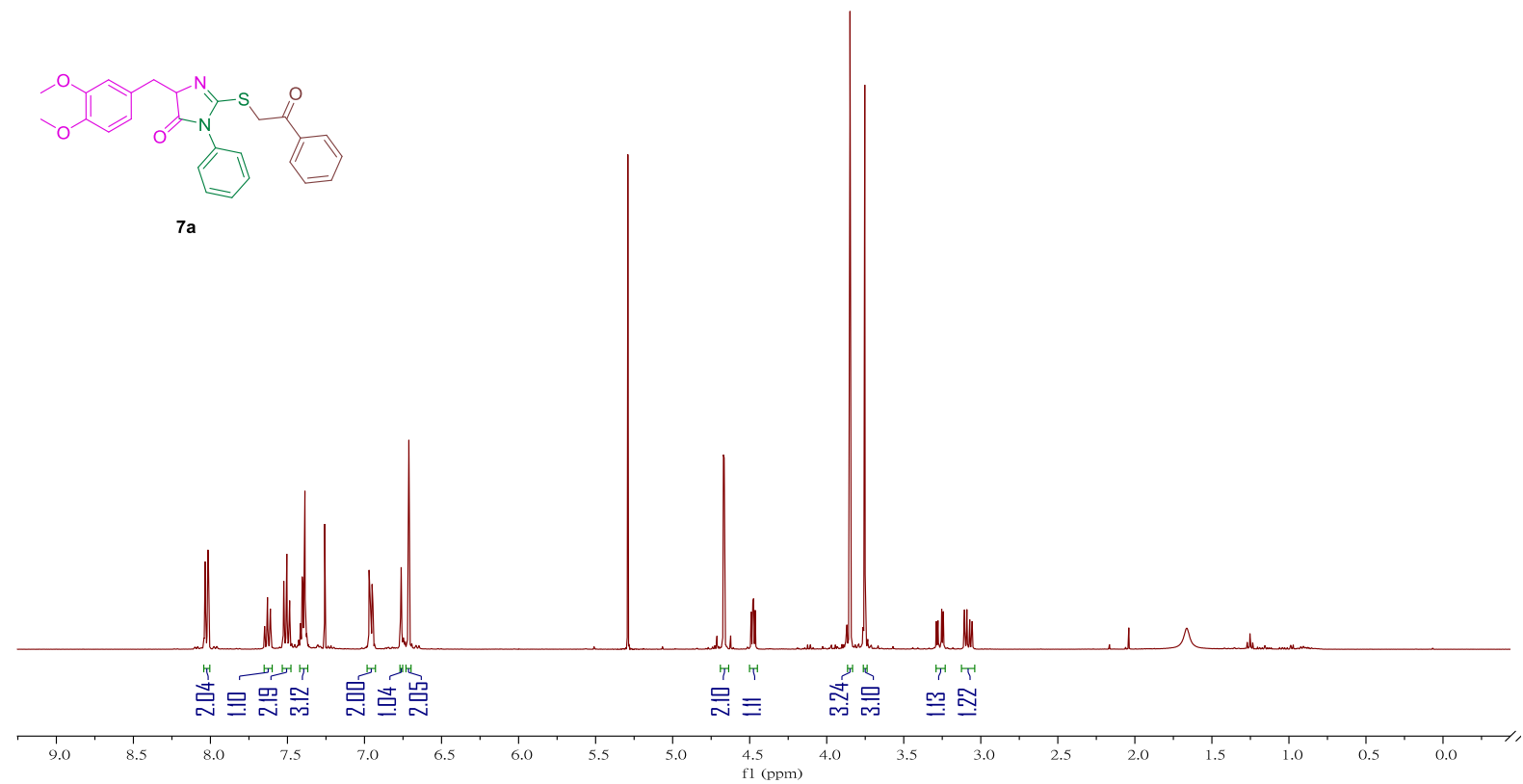
Volume: 10.0 ul

Chrom Type: Chromaster Channel : 1

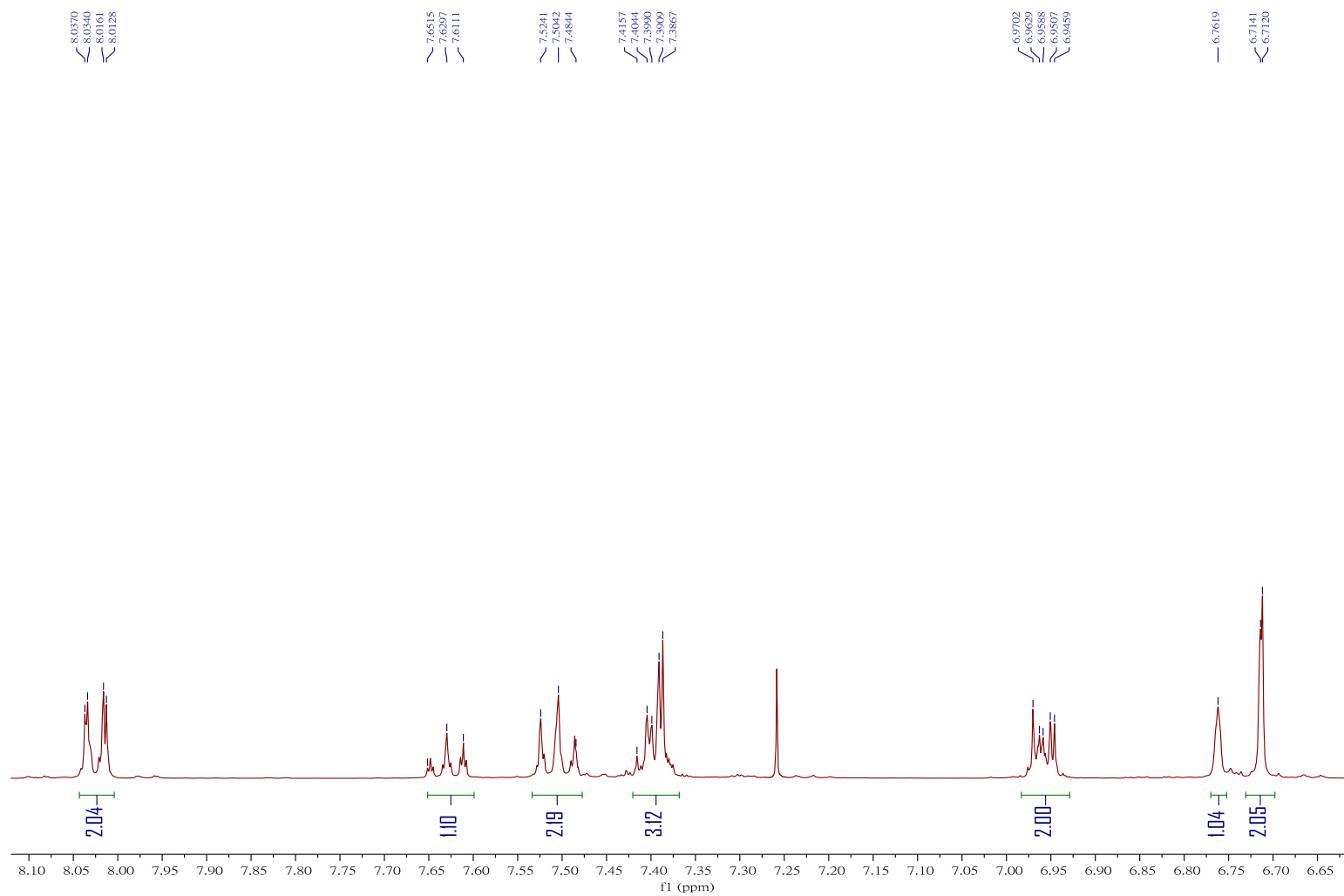


Method Description: flow rate : 0.3
mL/min , Daicel
Chiral OD, IPA 15,
Hex 85

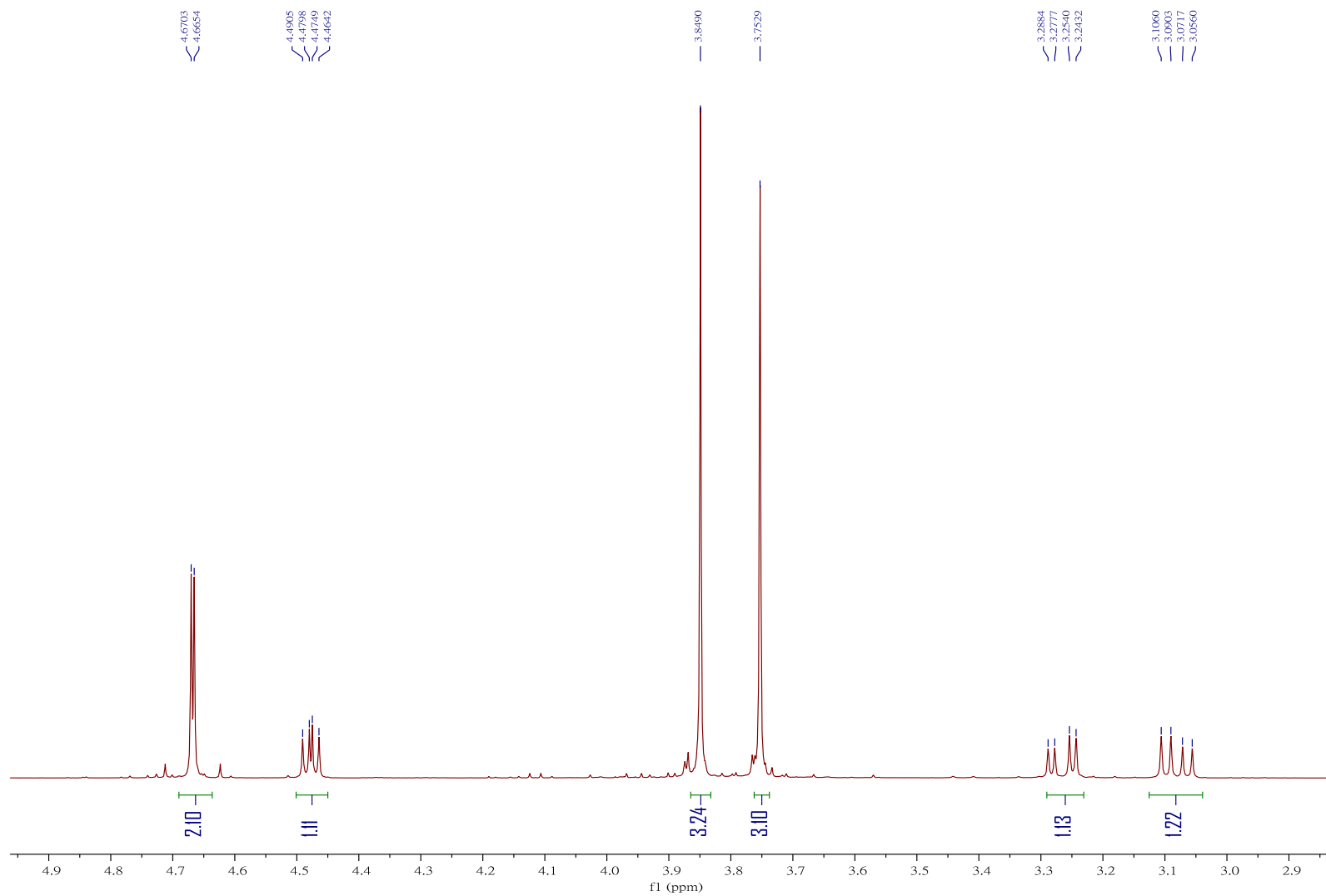
Chiral HPLC of compound 5p



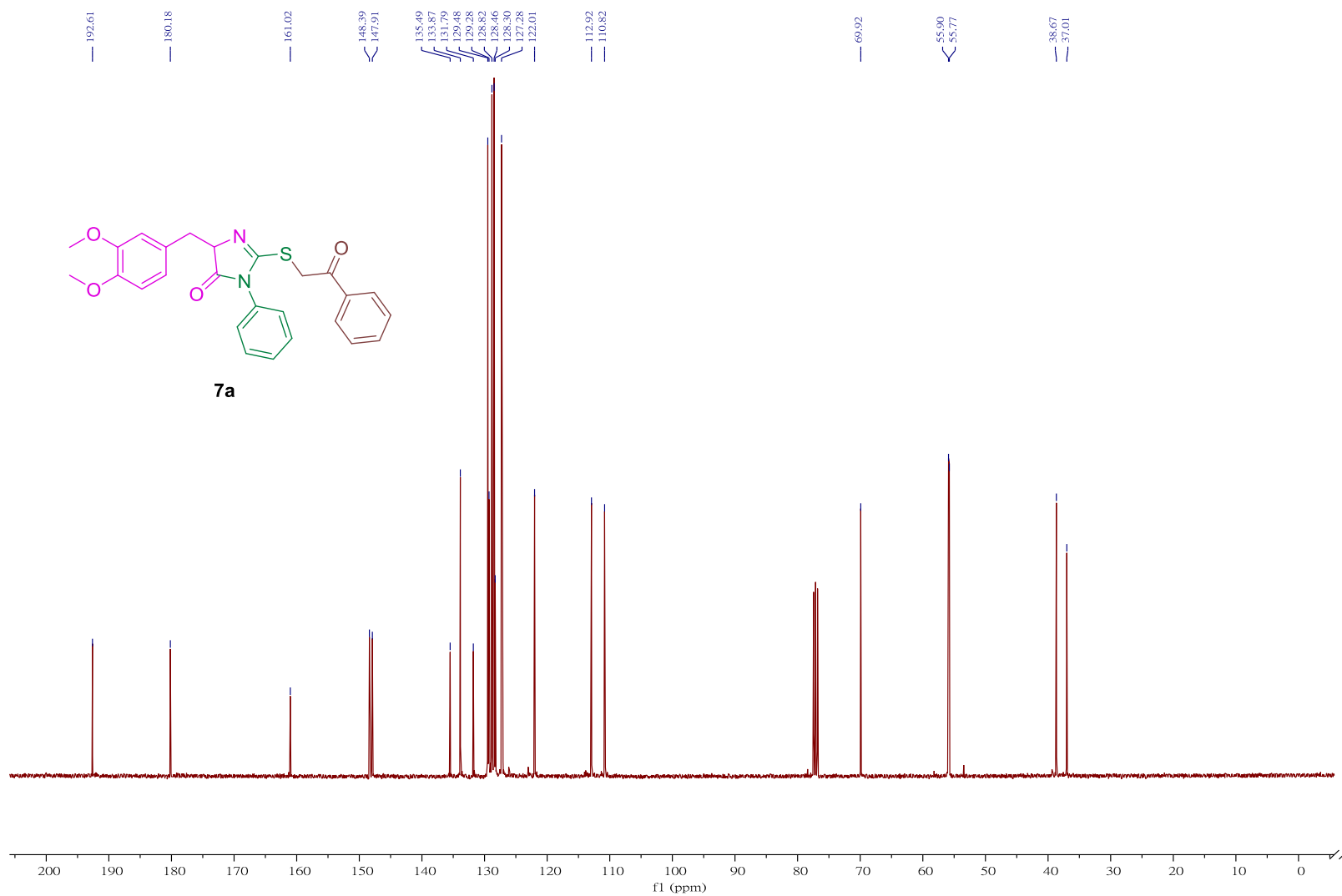
^1H NMR Spectrum (400 MHz) of compound **7a** in CDCl_3



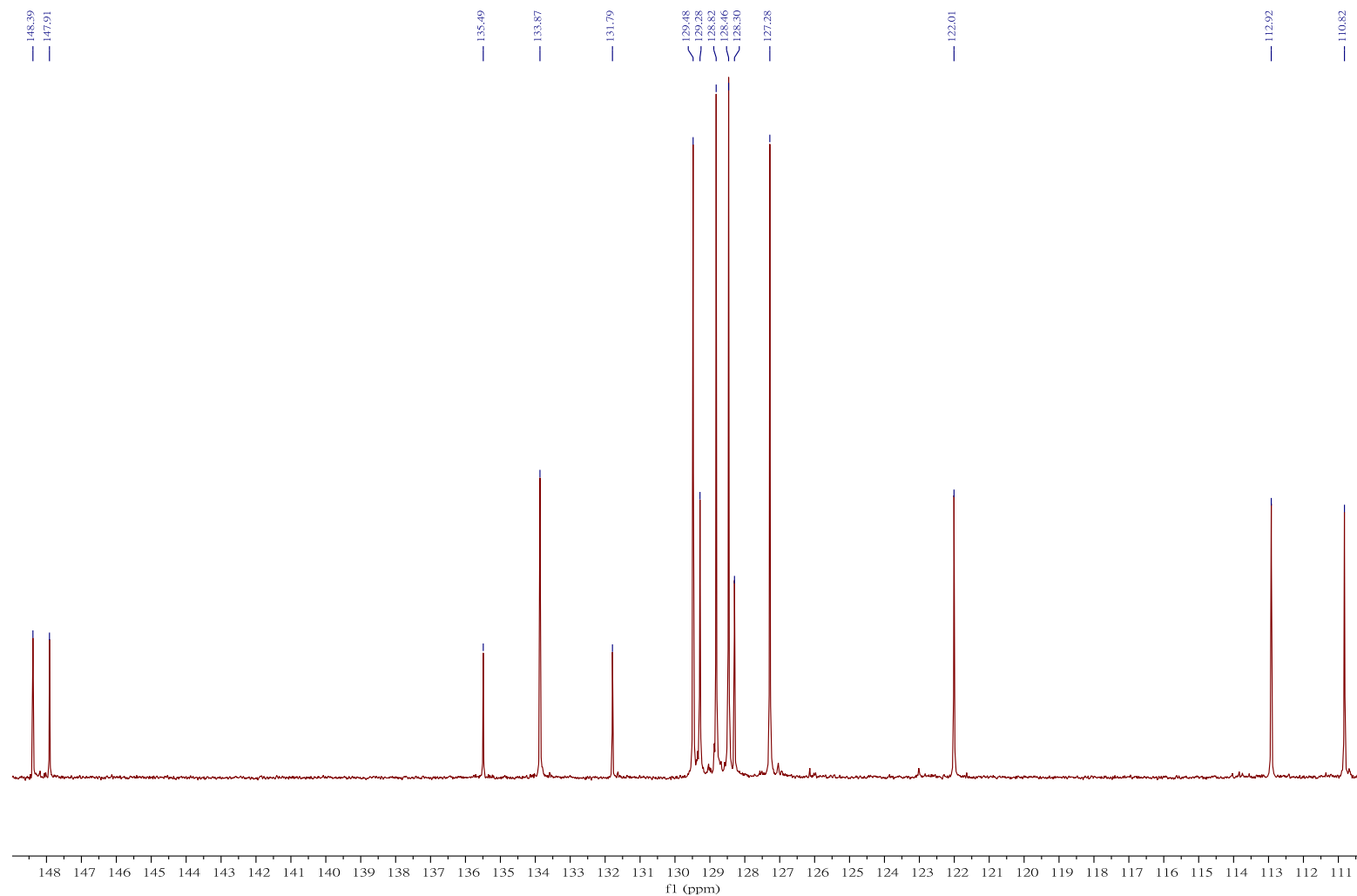
Expanding ^1H NMR Spectrum (400 MHz) of compound **7a** in CDCl_3



Expansion of ^1H NMR Spectrum (400 MHz) of compound **7a** in CDCl_3



^{13}C NMR Spectrum (101 MHz) of compound **7a** in CDCl_3



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **7a** in CDCl_3

Display Report

Analysis Info

Analysis Name D:\Data\ntcu service\data\2018\20180420\L175_RC5_01_18028.d

Method Small molecule.m

Sample Name L175

Comment

Acquisition Date 4/20/2018 12:06:25 PM

Operator NCTU

Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type

ESI

Ion Polarity

Positive

Set Nebulizer

1.0 Bar

Focus

Active

Set Capillary

4500 V

Set Dry Heater

200 °C

Scan Begin

50 m/z

Set End Plate Offset

-500 V

Set Dry Gas

6.0 l/min

Scan End

1500 m/z

Set Charging Voltage

2000 V

Set Divert Valve

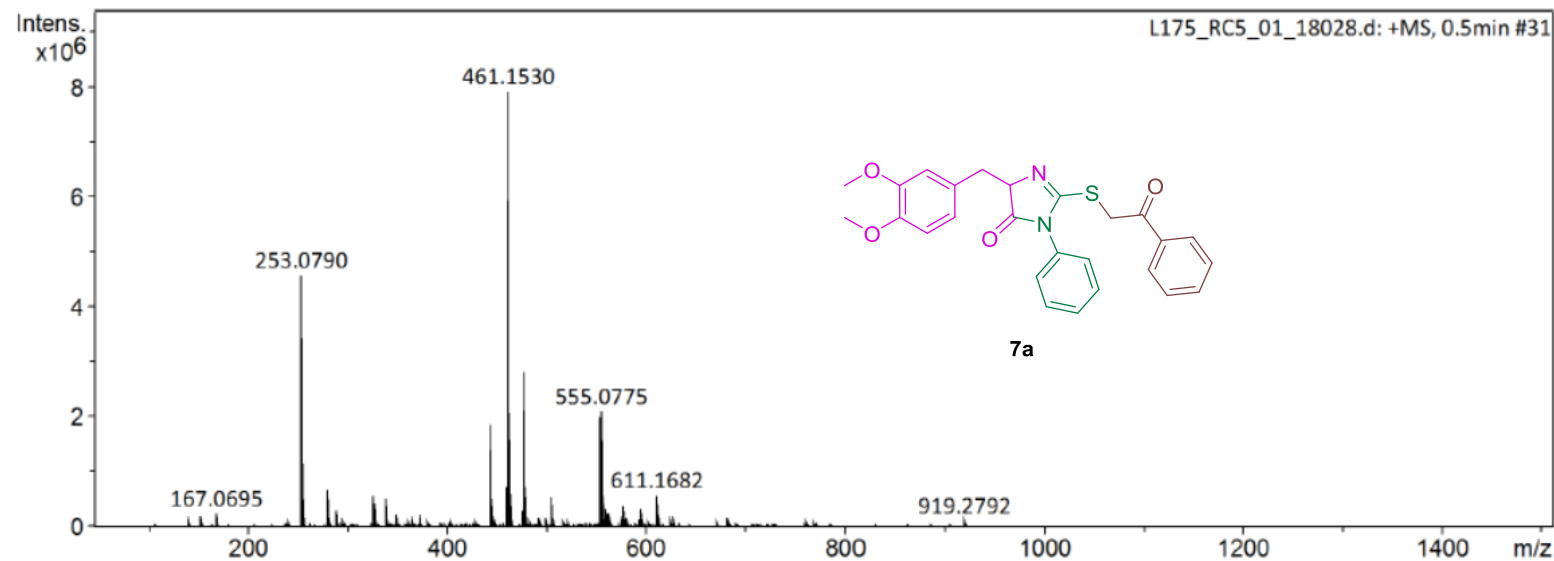
Waste

Set Corona

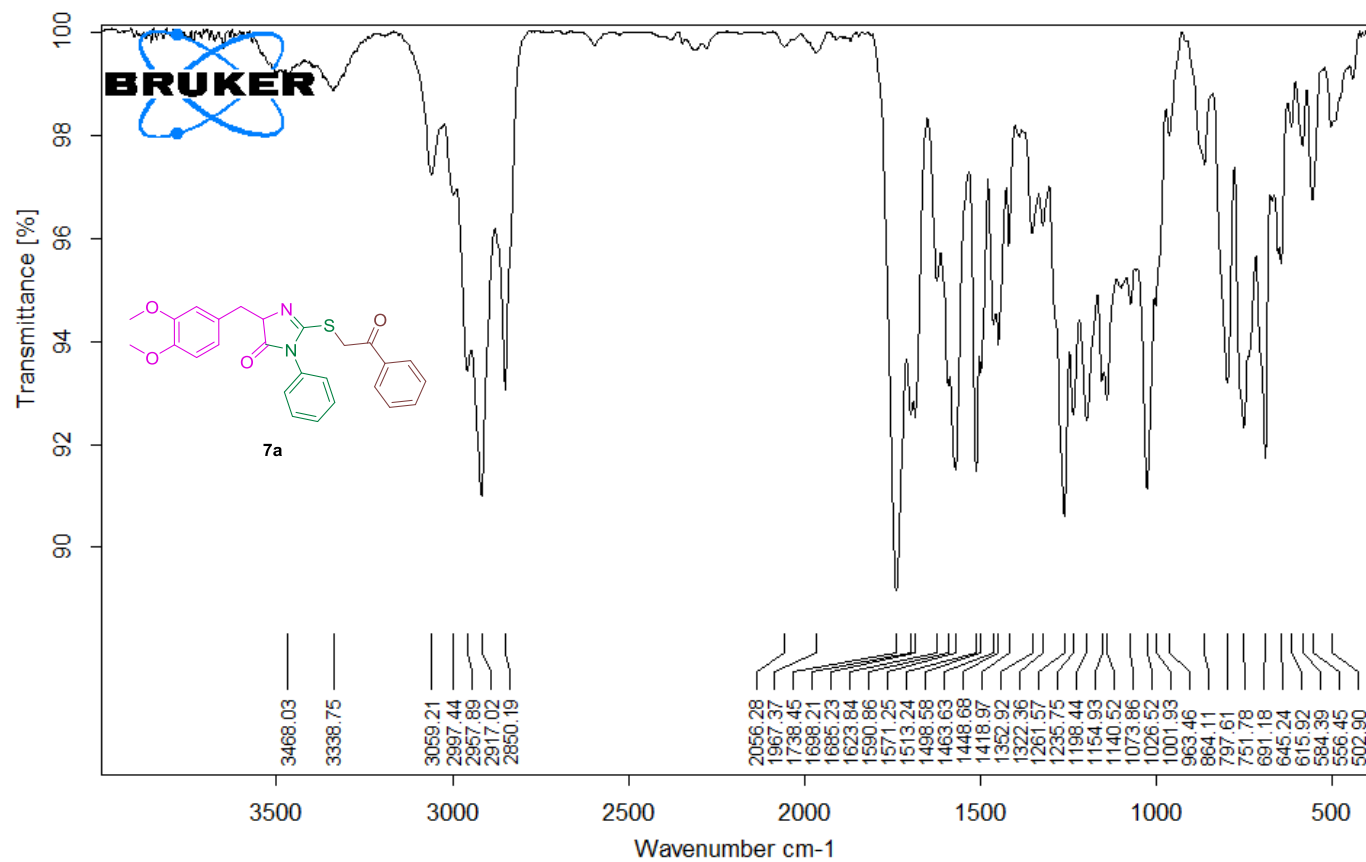
0 nA

Set APCI Heater

0 °C



HRMS of compound 7a



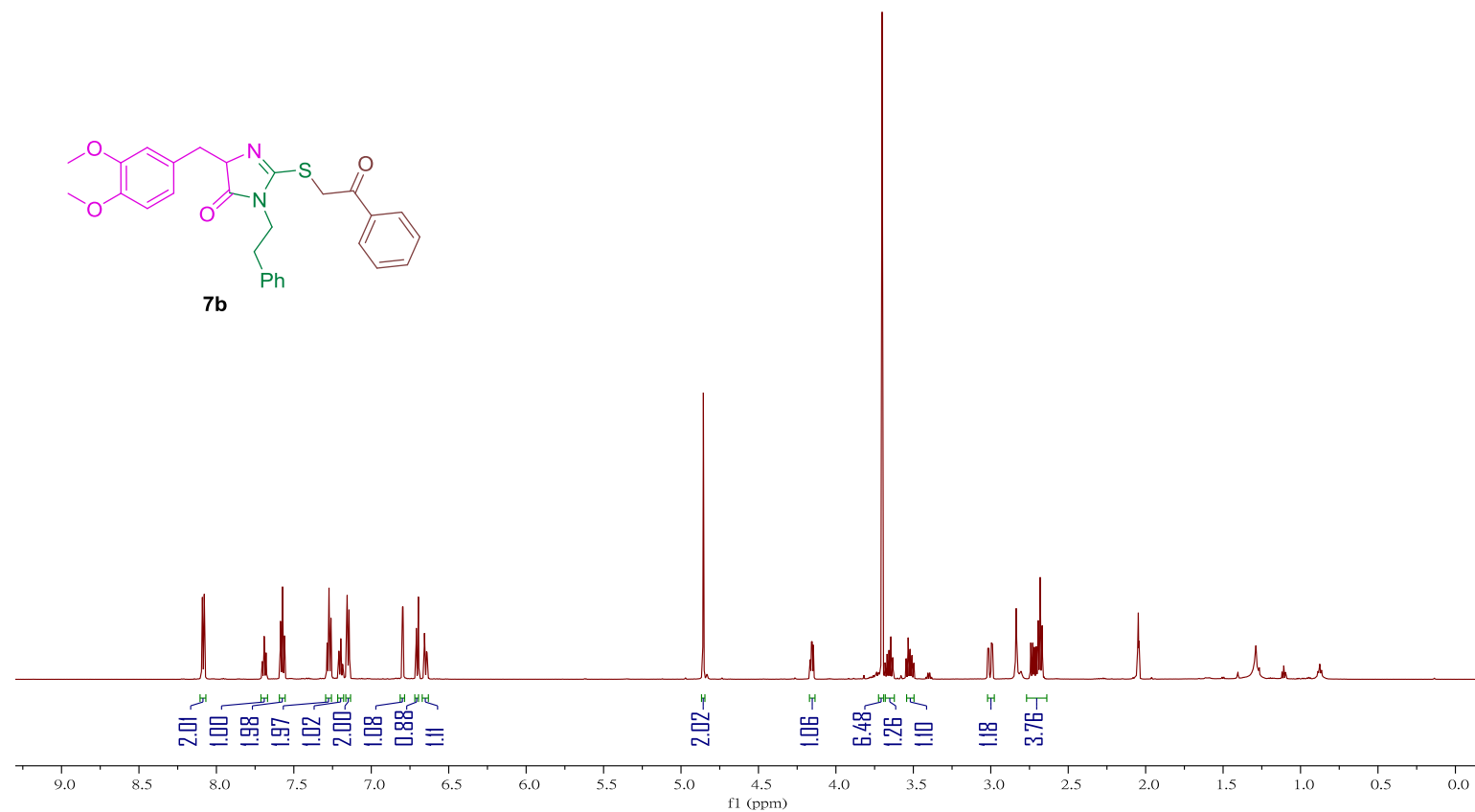
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L175.1

MIR_TR_DTGS_L175

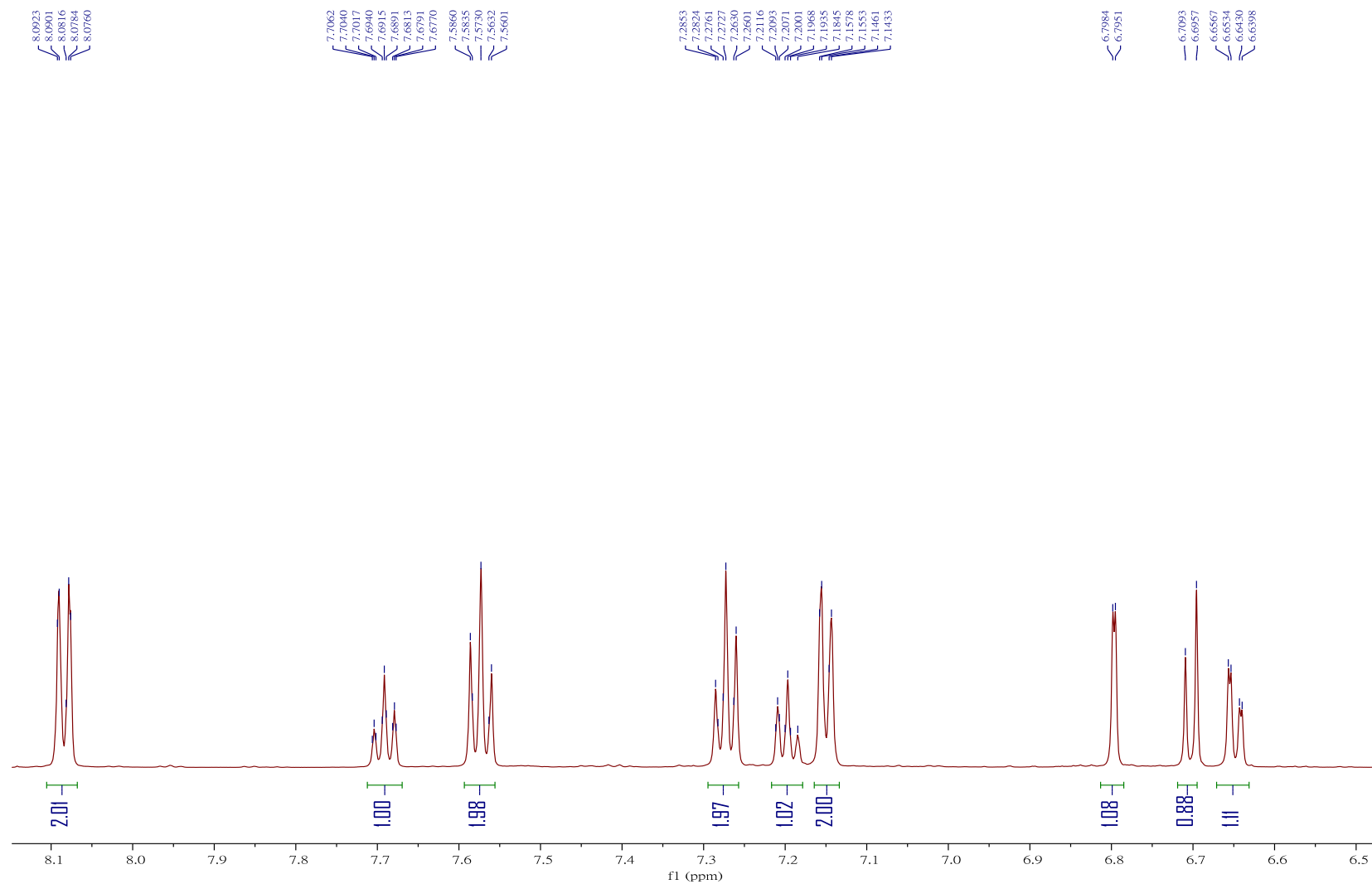
Instrument type and / or accessory

9/4/2018

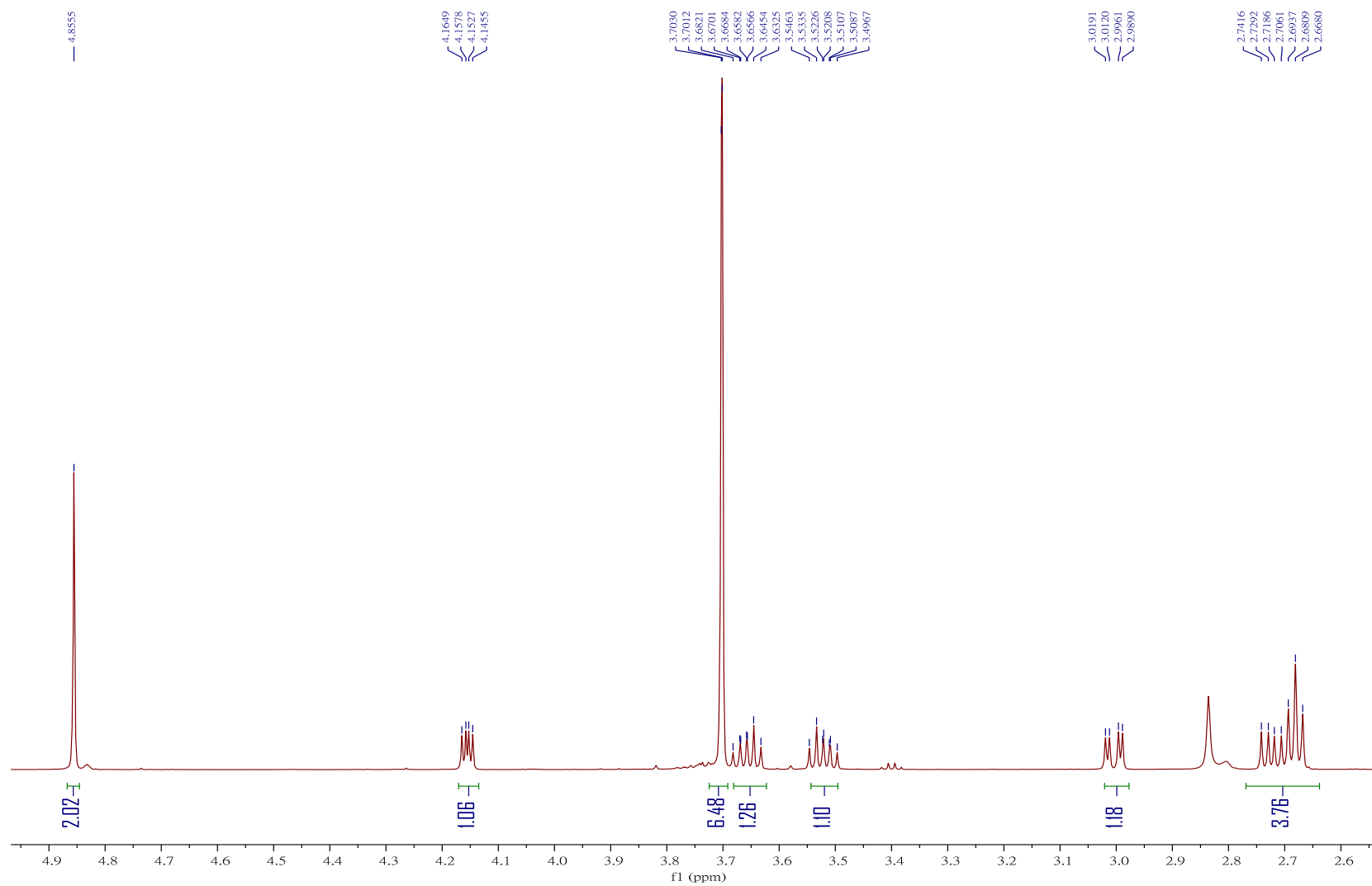
FT-IR Spectrum of compound **7a**



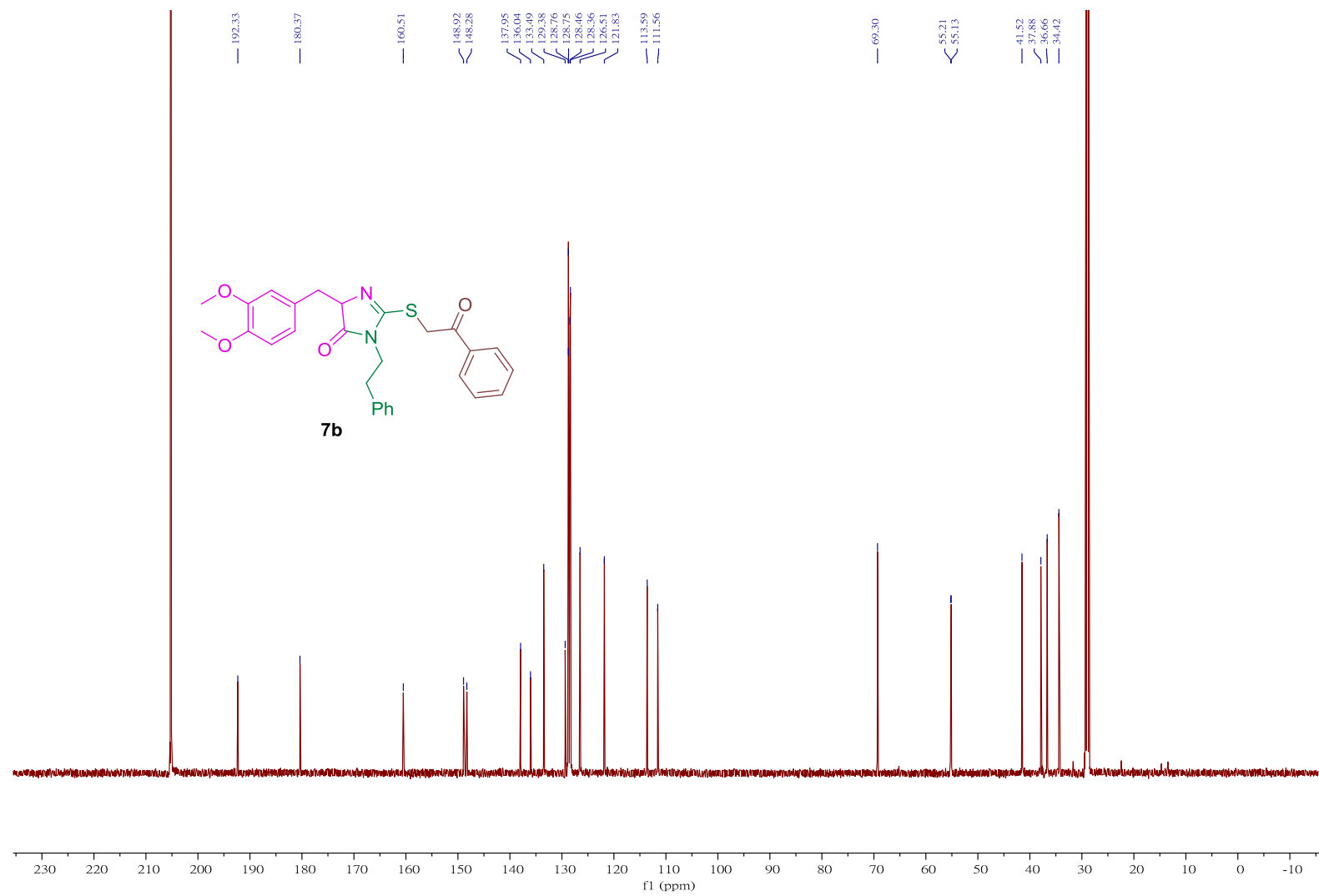
^1H NMR Spectrum (400 MHz) of compound **7b** in acetone- d_6



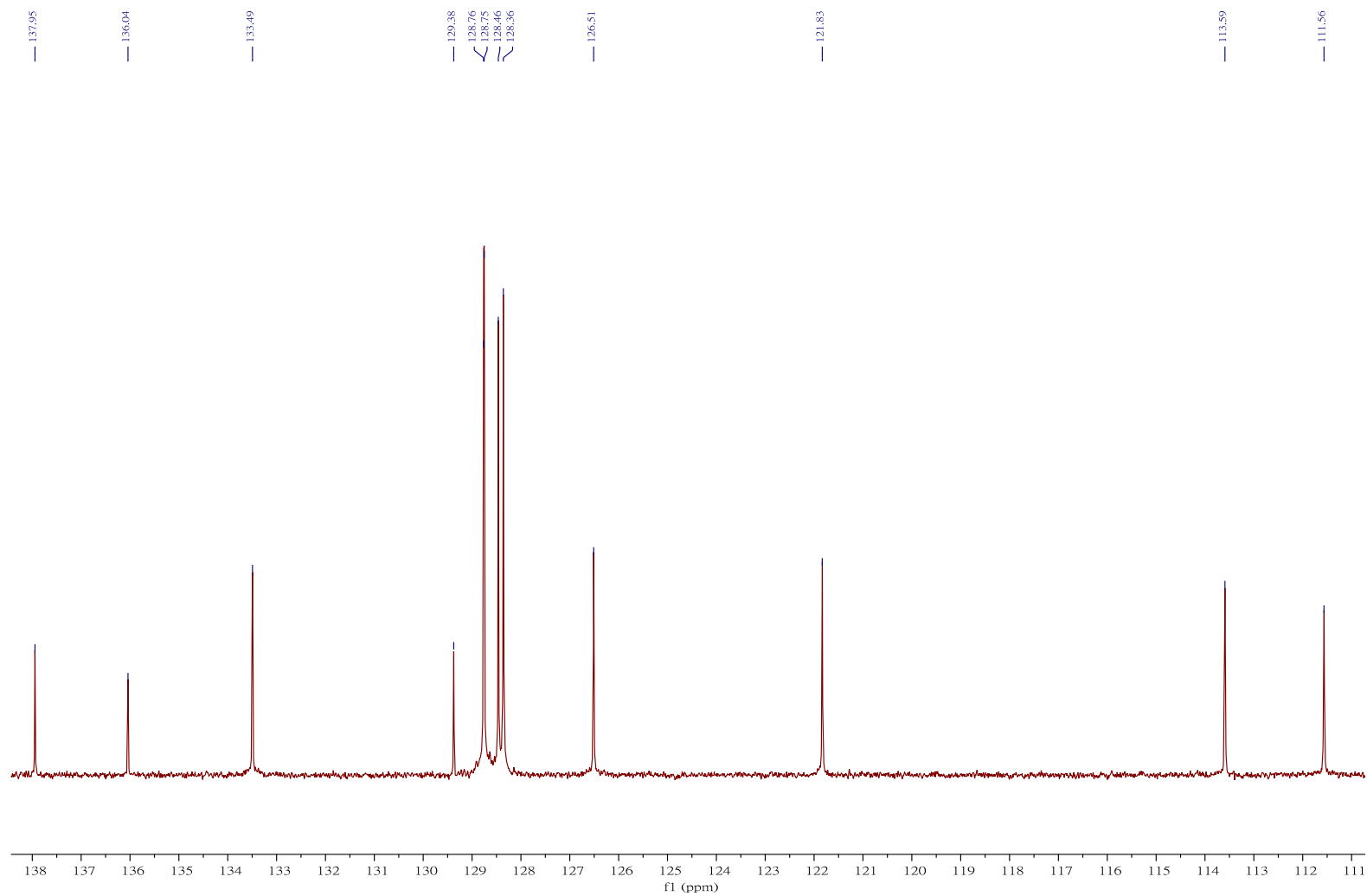
Expansion of ¹H NMR Spectrum (400 MHz) of compound **7b** in acetone-*d*₆



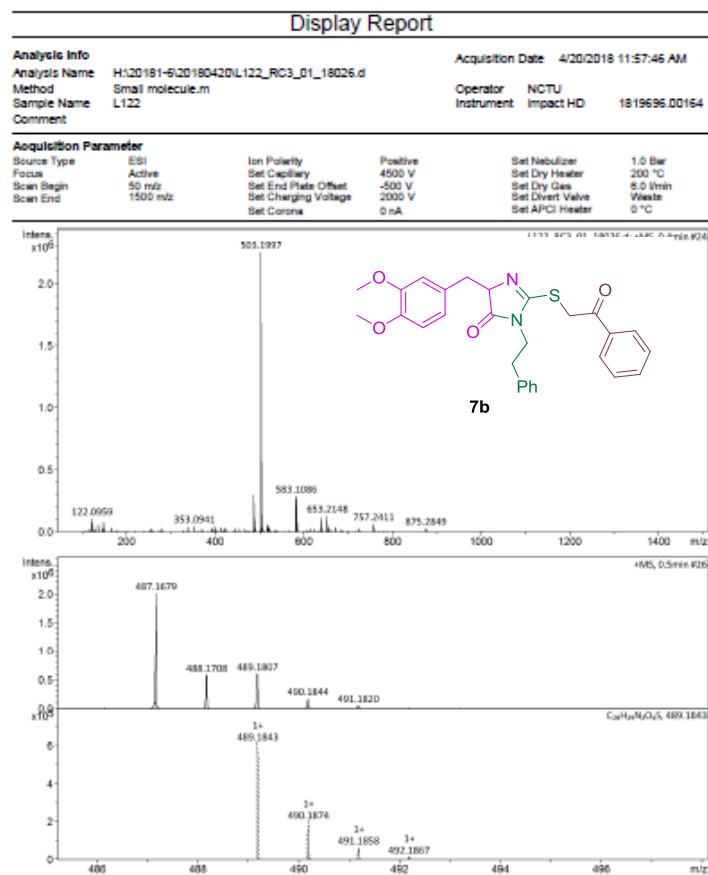
Expansion of ^1H NMR Spectrum (400 MHz) of compound **7b** in acetone- d_6



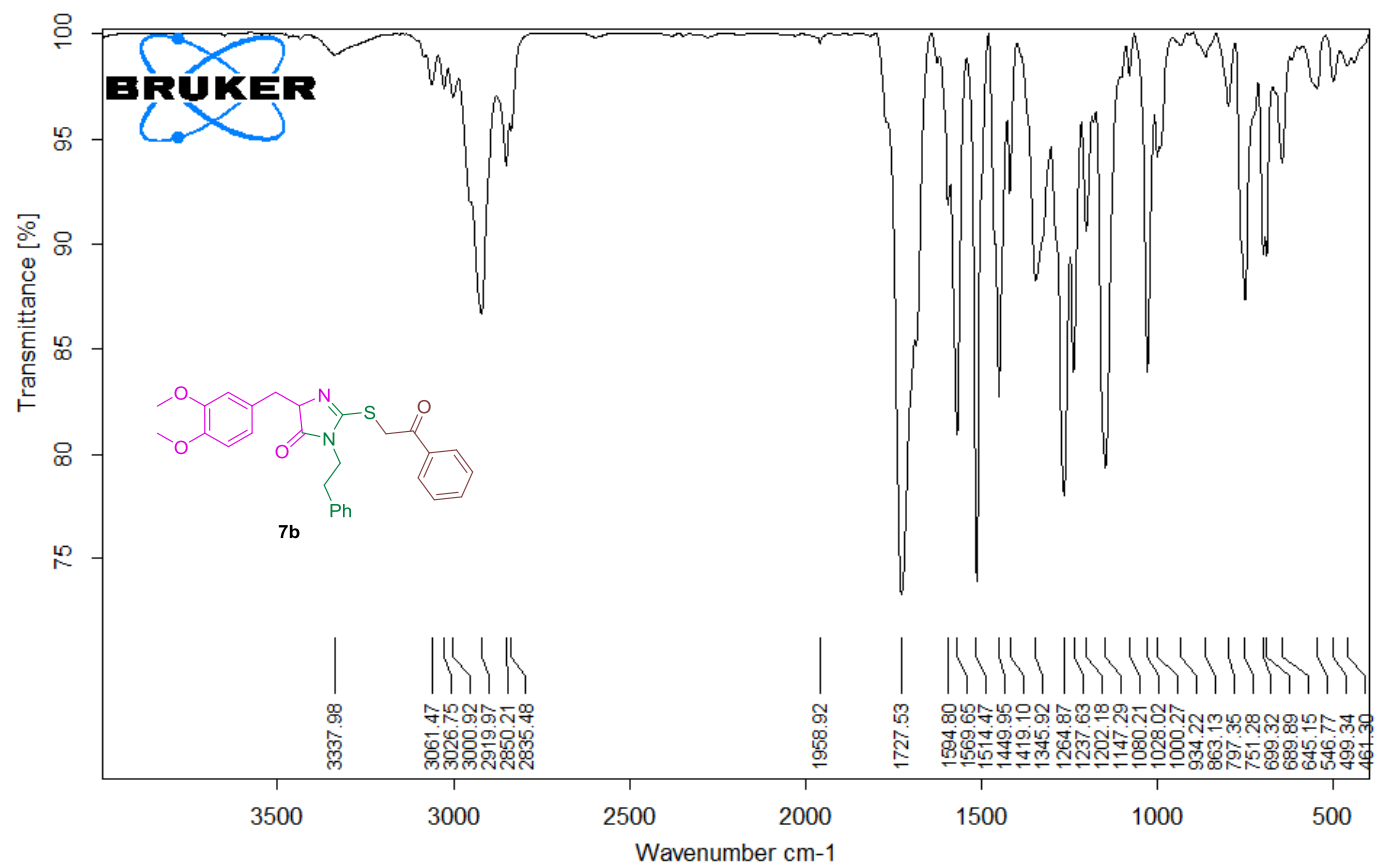
¹³C NMR Spectrum (101 MHz) of compound **7b** in acetone-*d*₆



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **7b** in acetone- d_6

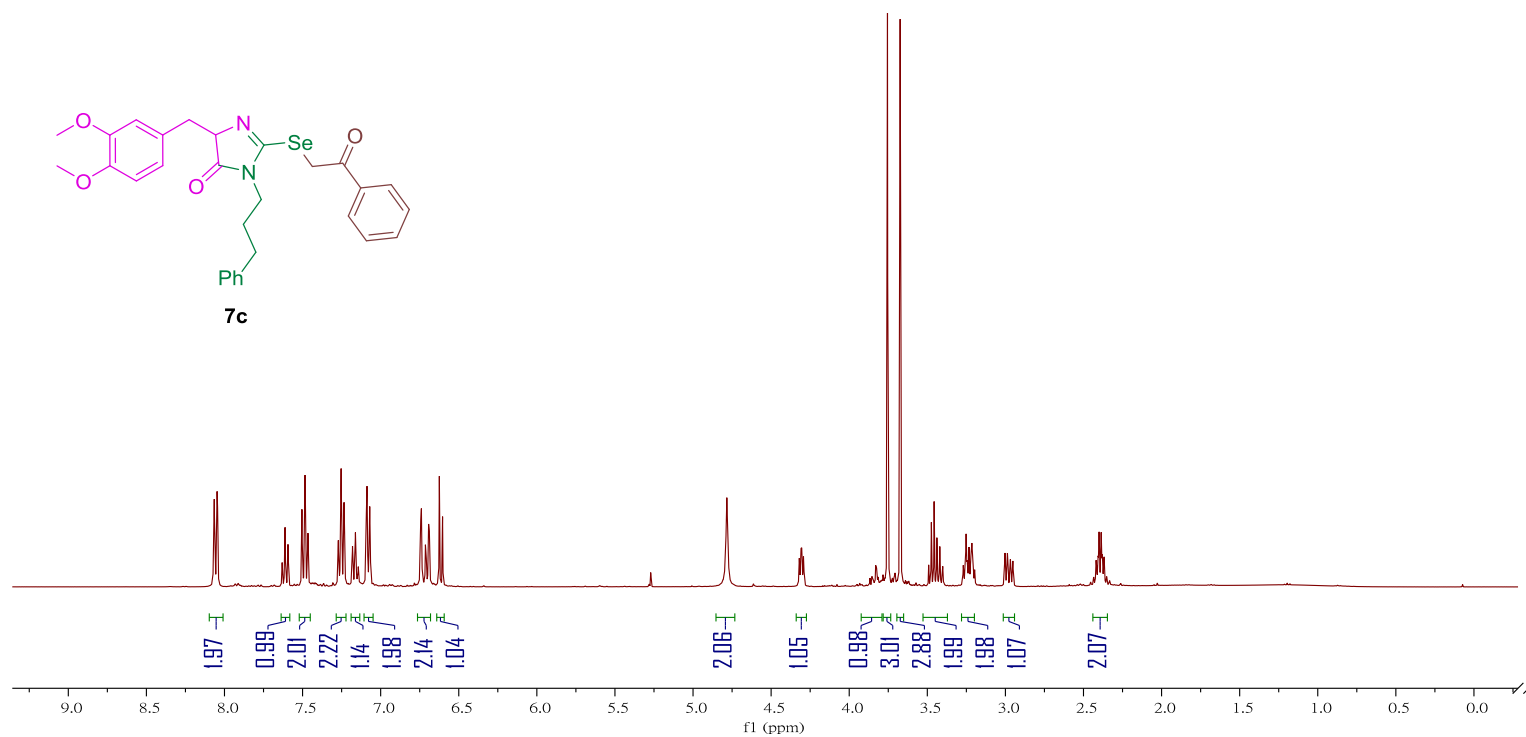


HRMS of compound **7b**

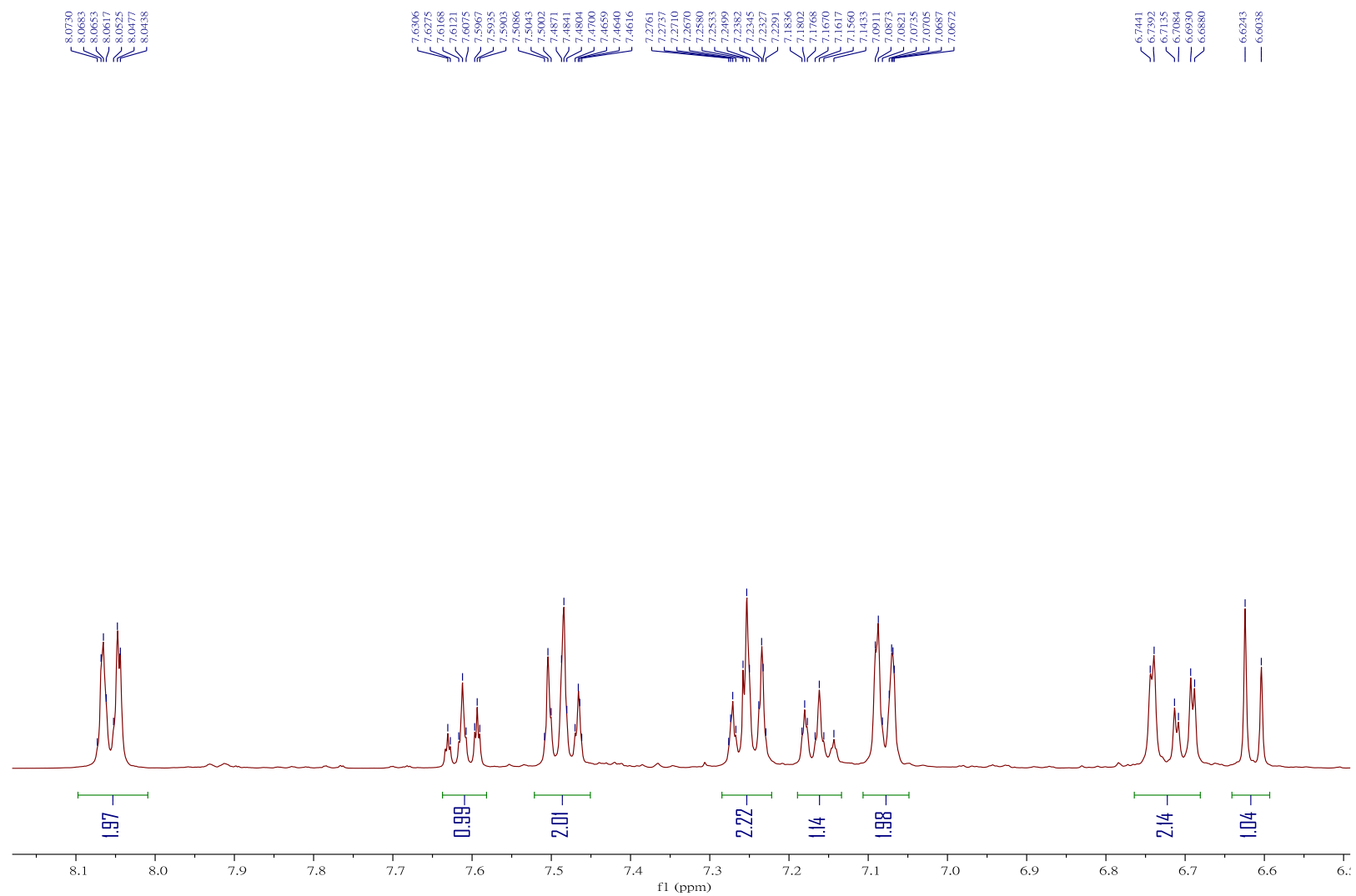


D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L122.0	MIR_TR_DTGS_L122	Instrument type and / or accessory	9/4/2018
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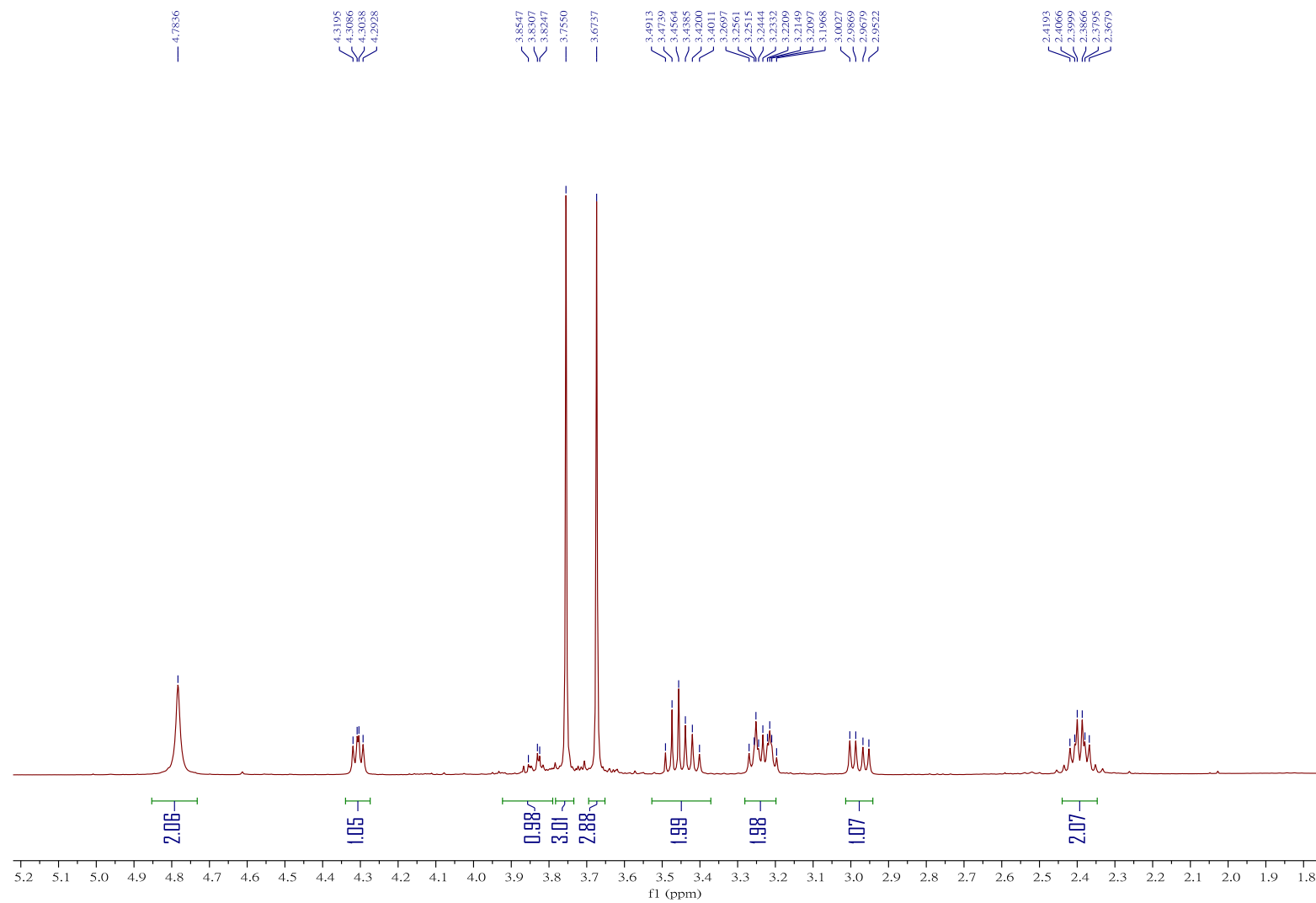
FT-IR Spectrum of compound **7b**



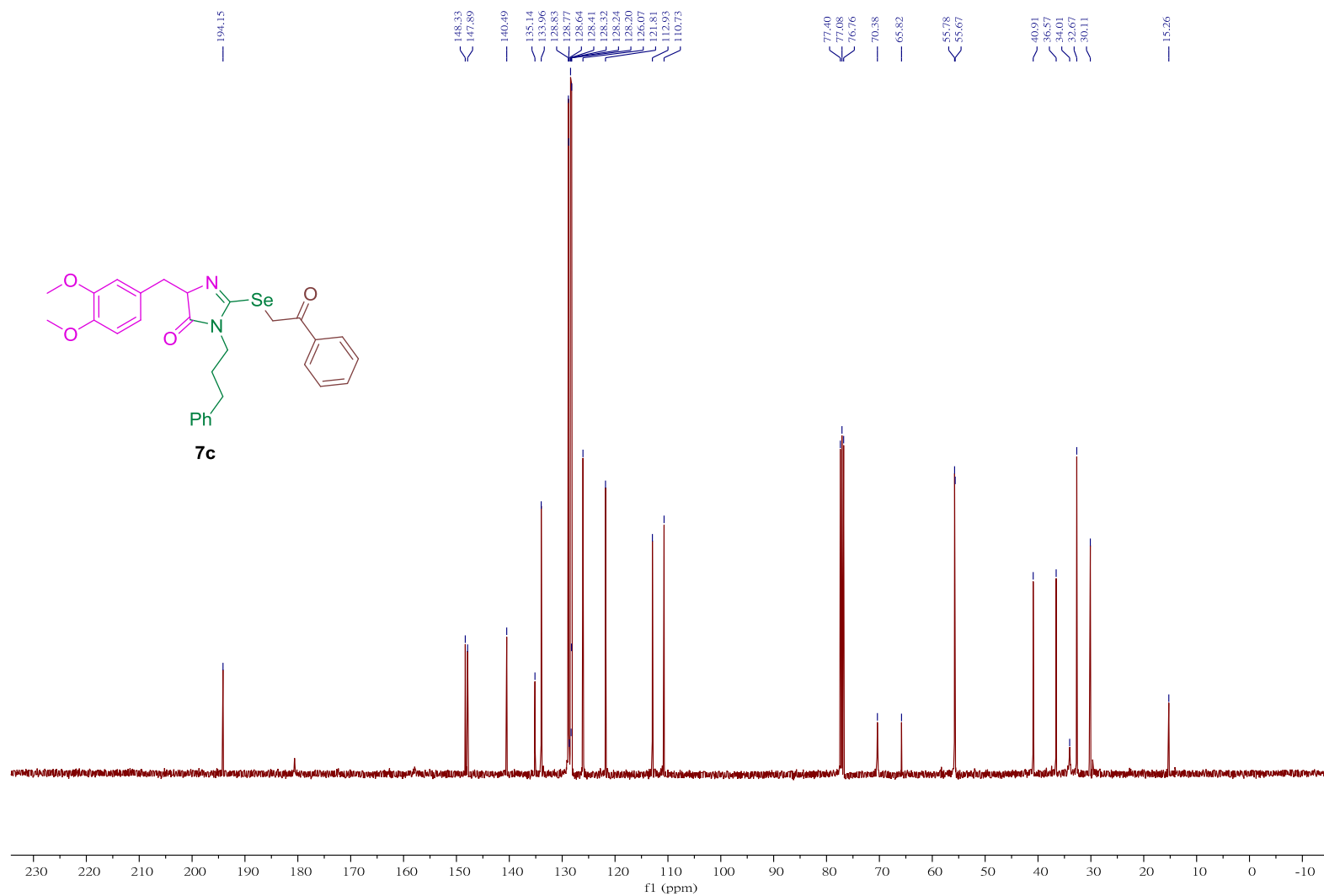
^1H NMR Spectrum (400 MHz) of compound **7c** in CDCl_3



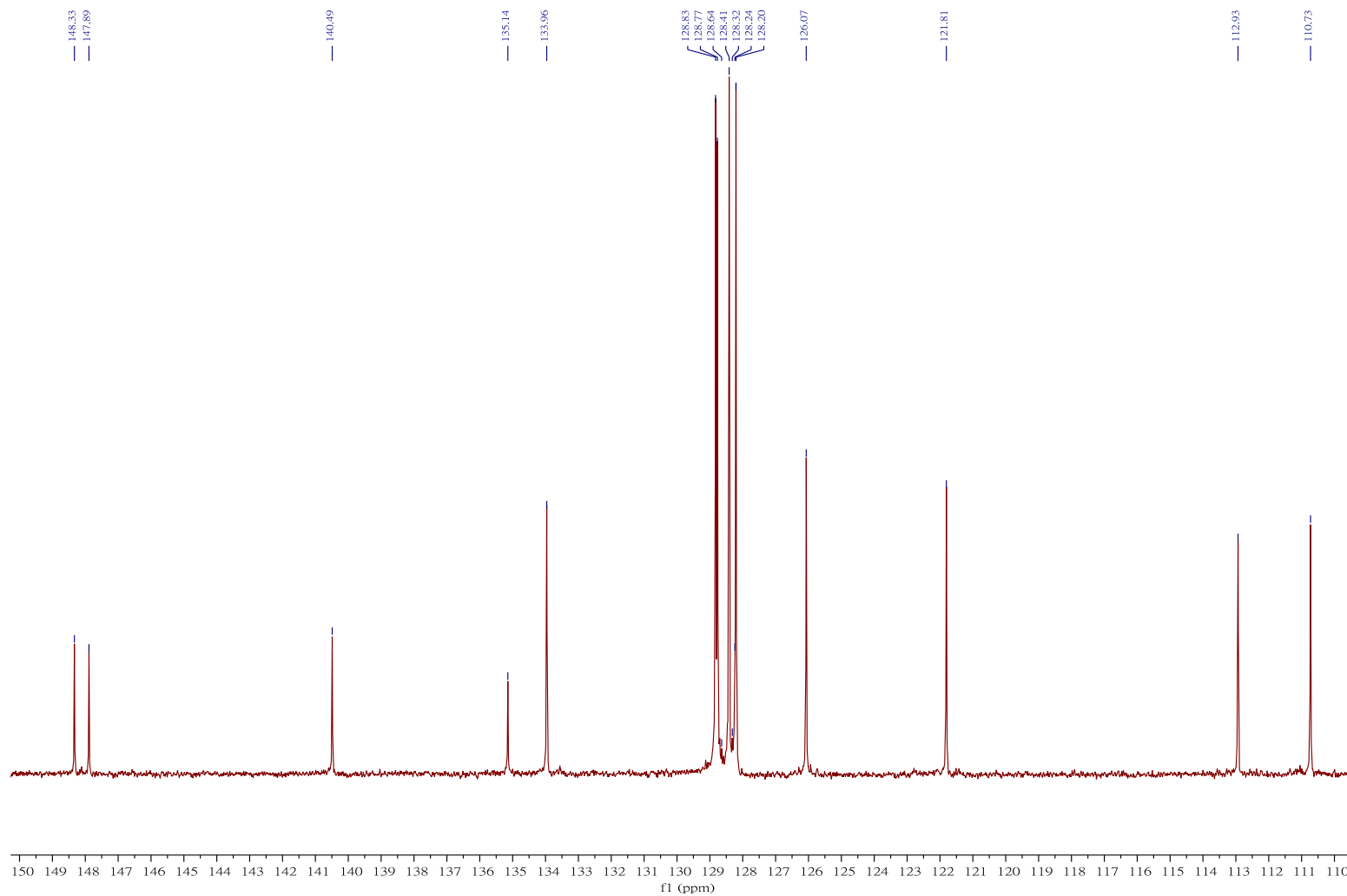
Expansion of ^1H NMR Spectrum (400 MHz) of compound **7c** in CDCl_3



Expansion of ^1H NMR Spectrum (400 MHz) of compound **7c** in CDCl_3



^{13}C NMR Spectrum (101 MHz) of compound **7c** in CDCl_3

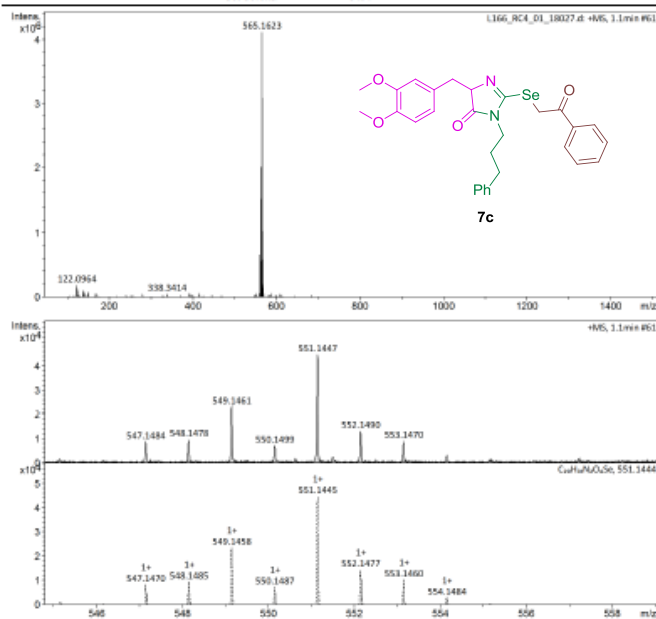


Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **7c** in CDCl_3

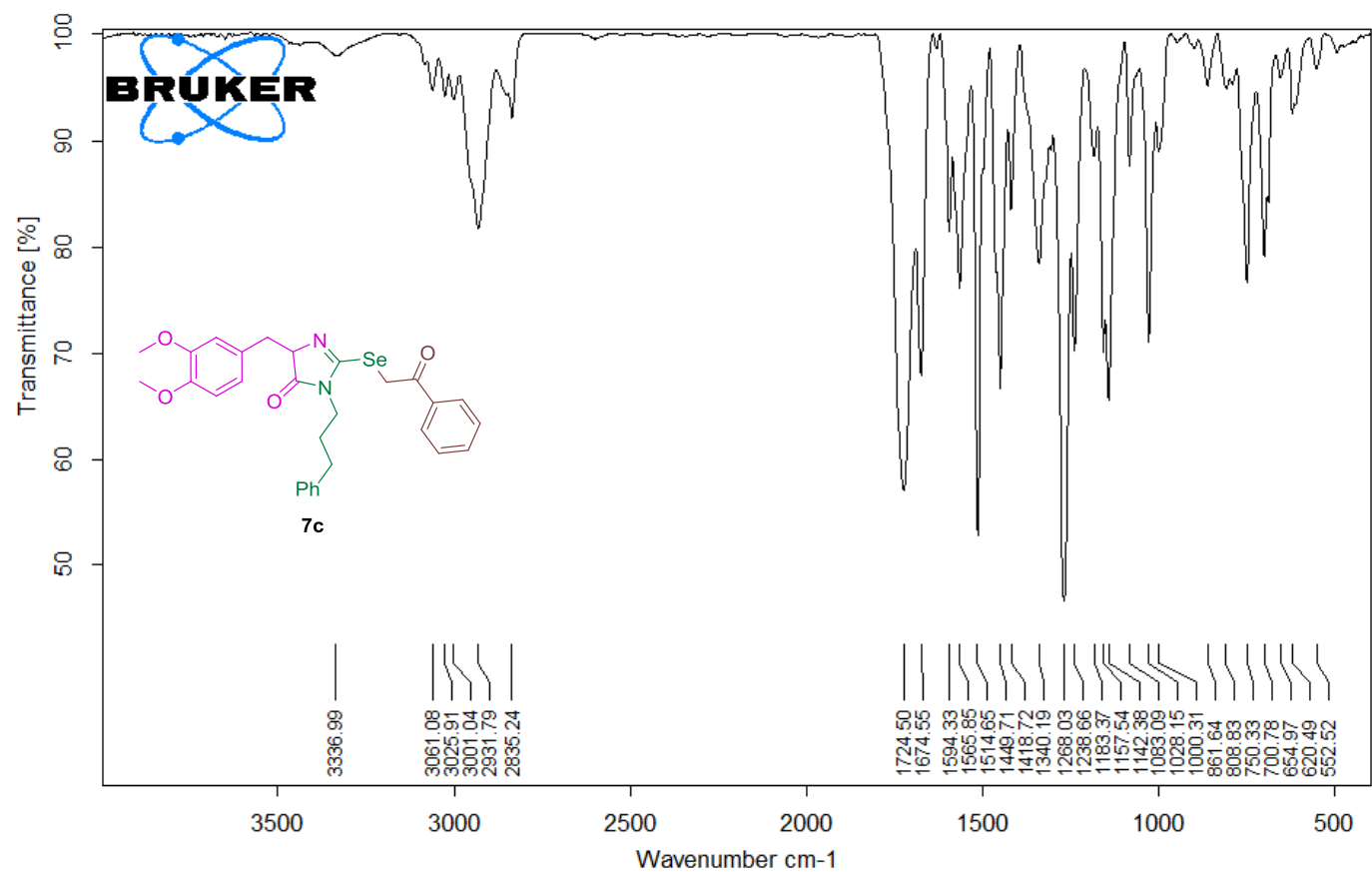
Display Report

Analysis Info		Acquisition Date	4/20/2018 12:02:06 PM	
Analysis Name	H:\20181-6\20180420\L166_RC4_01_18027.d	Operator	NCTU	
Method	Small molecule.m	Instrument	Impact HD	1819696.00164
Sample Name	L166			
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Shunt Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

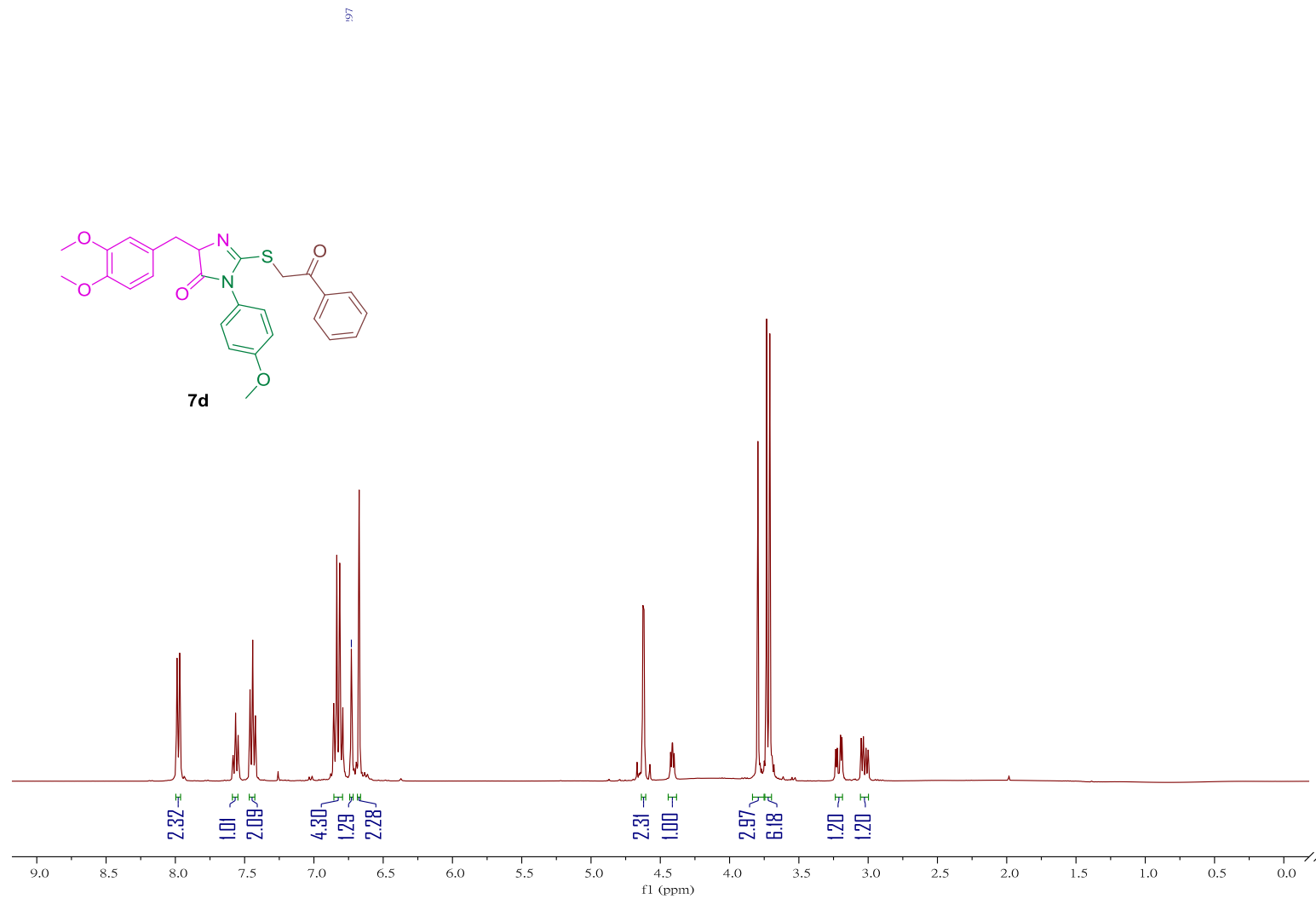


HRMS of compound **7c**

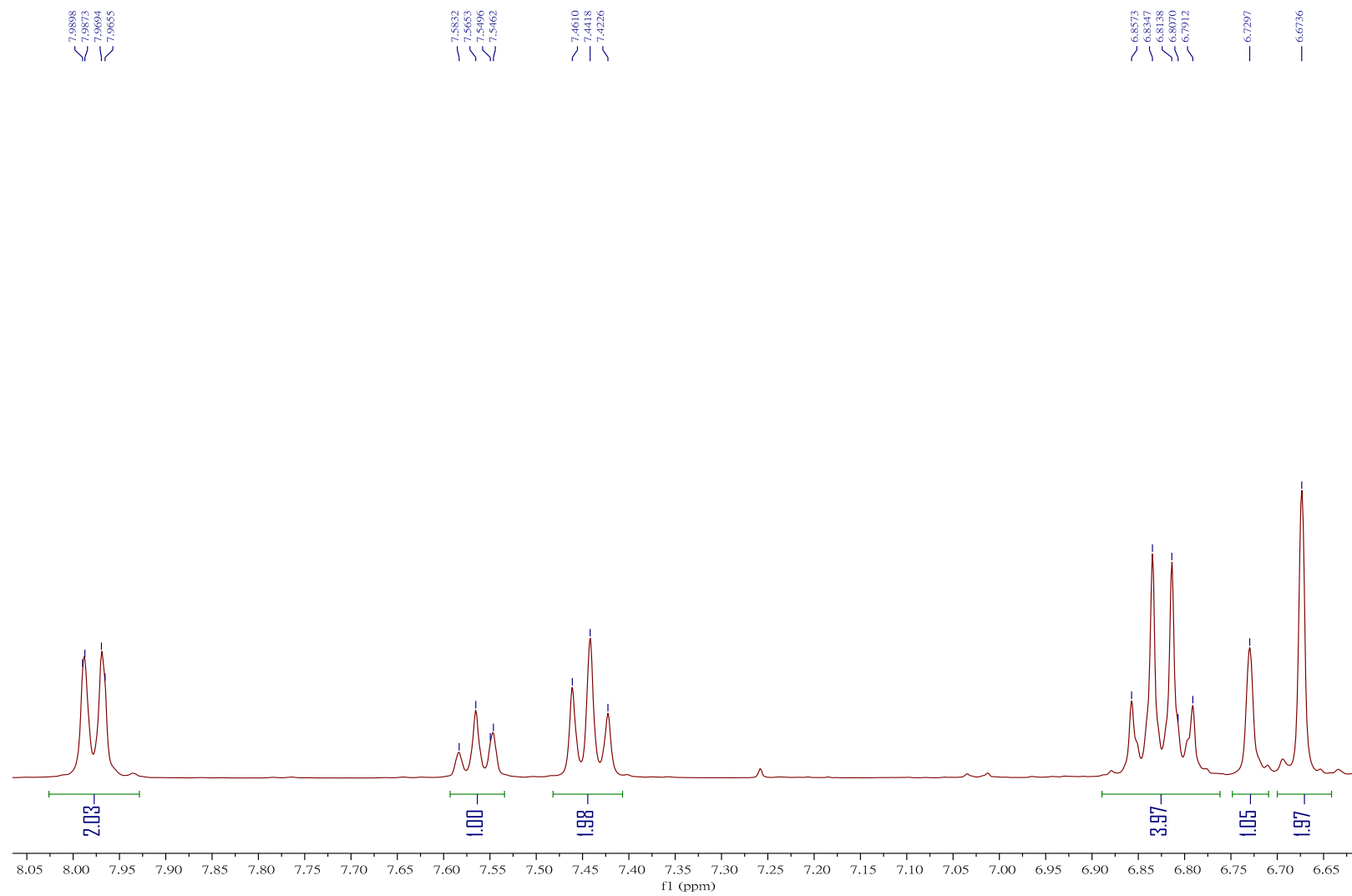


D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L166.0	MIR_TR_DTGS_L166	Instrument type and / or accessory	9/4/2018
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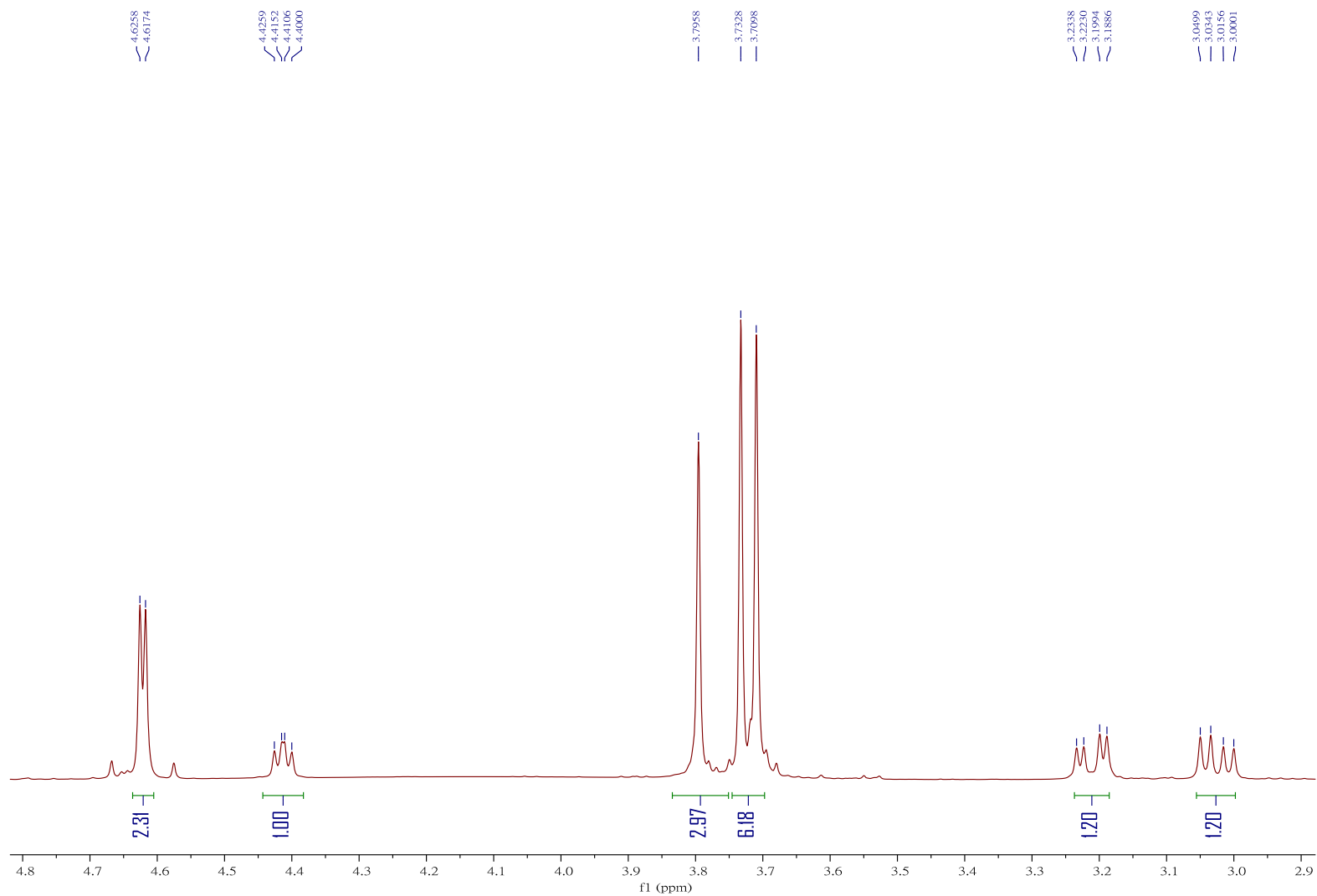
FT-IR Spectrum of compound **7c**



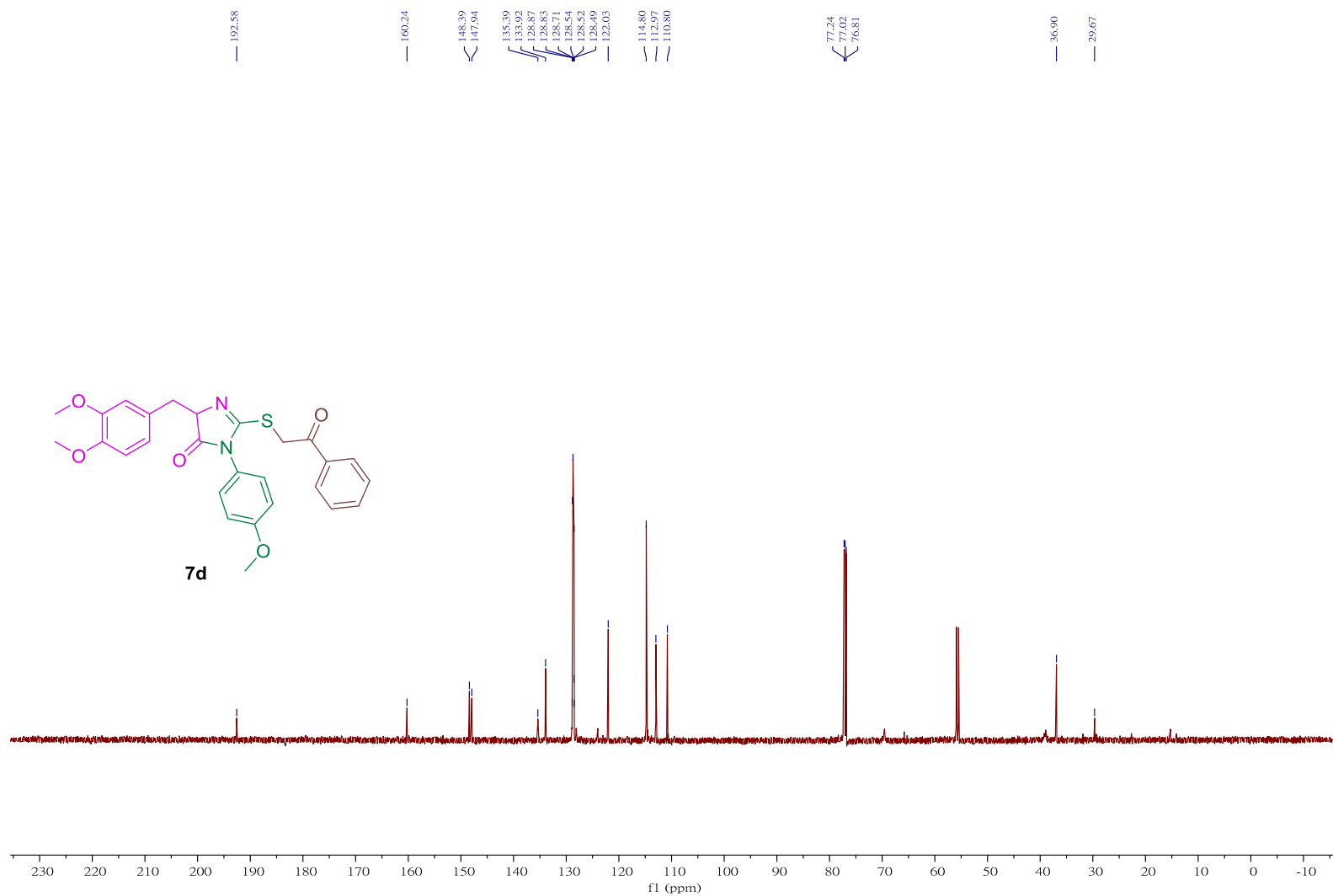
¹H NMR Spectrum (400 MHz) of compound **7d** in CDCl₃



Expansion of ^1H NMR Spectrum (400 MHz) of compound **7d** in CDCl_3



Expansion of ^1H NMR Spectrum (400 MHz) of compound **7d** in CDCl_3



^{13}C NMR Spectrum (101 MHz) of compound **7d** in CDCl_3

Display Report

Analysis Info

Analysis Name D:\Data\inctu service\data\2018\20180420\L244_RC6_01_18029.d

Method Small molecule.m

Sample Name L244

Comment

Acquisition Date 4/20/2018 12:10:45 PM

Operator NCTU

Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type ESI

Focus Active

Scan Begin 50 m/z

Scan End 1500 m/z

Ion Polarity

Set Capillary

Set End Plate Offset

Set Charging Voltage

Set Corona

Positive

4500 V

-500 V

2000 V

0 nA

Set Nebulizer

Set Dry Heater

Set Dry Gas

Set Divert Valve

Set APCI Heater

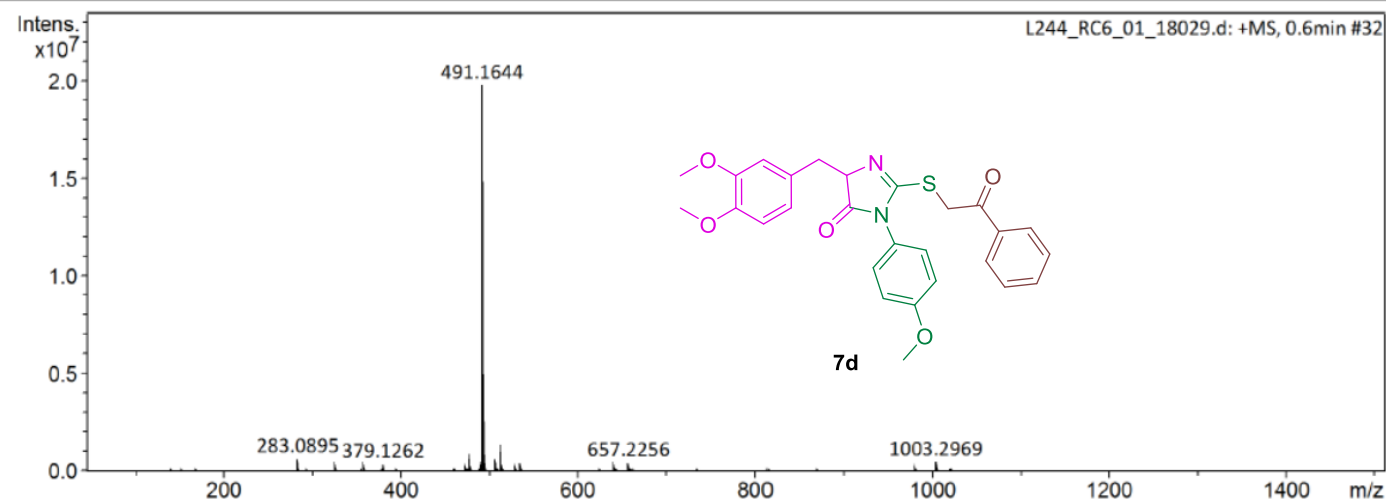
1.0 Bar

200 °C

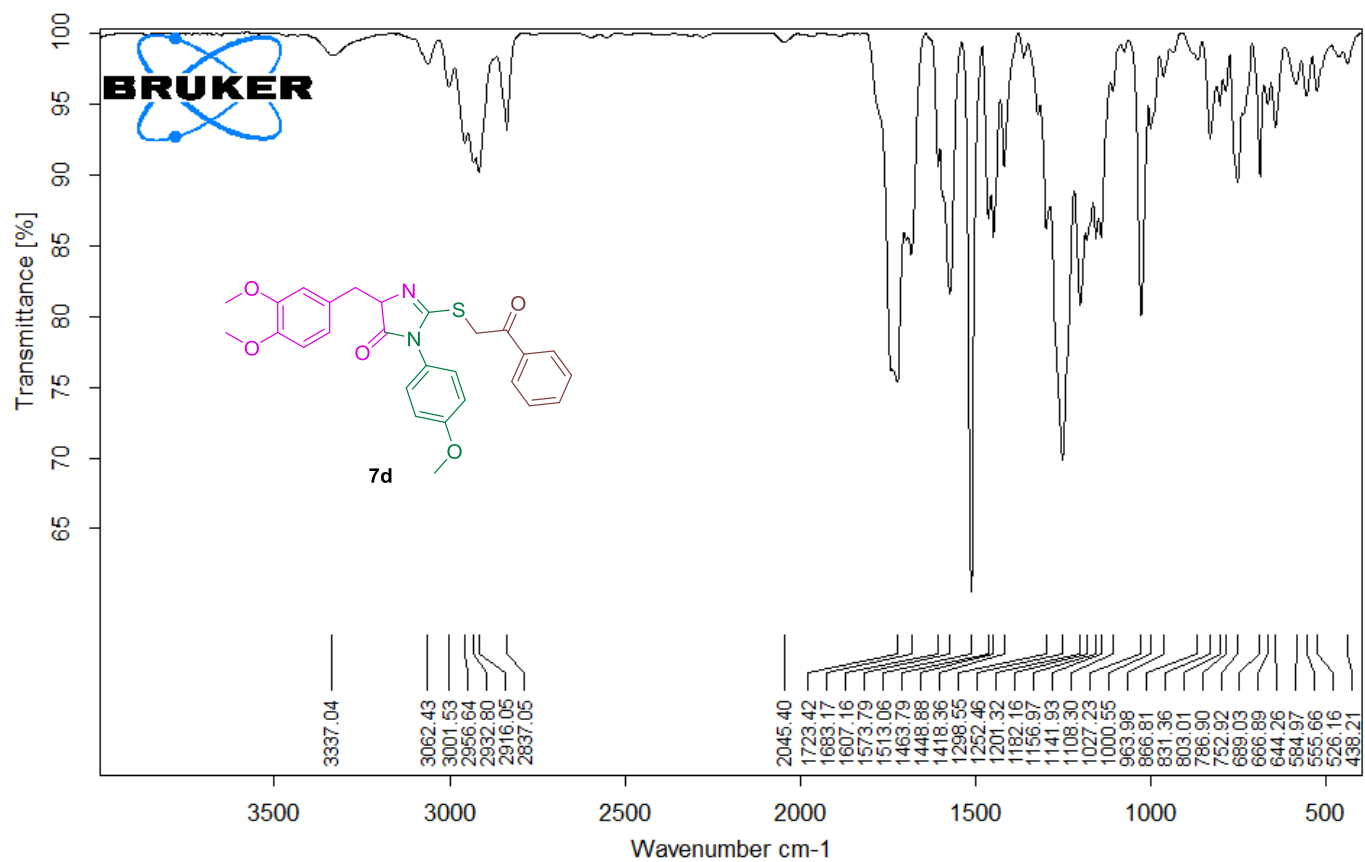
6.0 l/min

Waste

0 °C

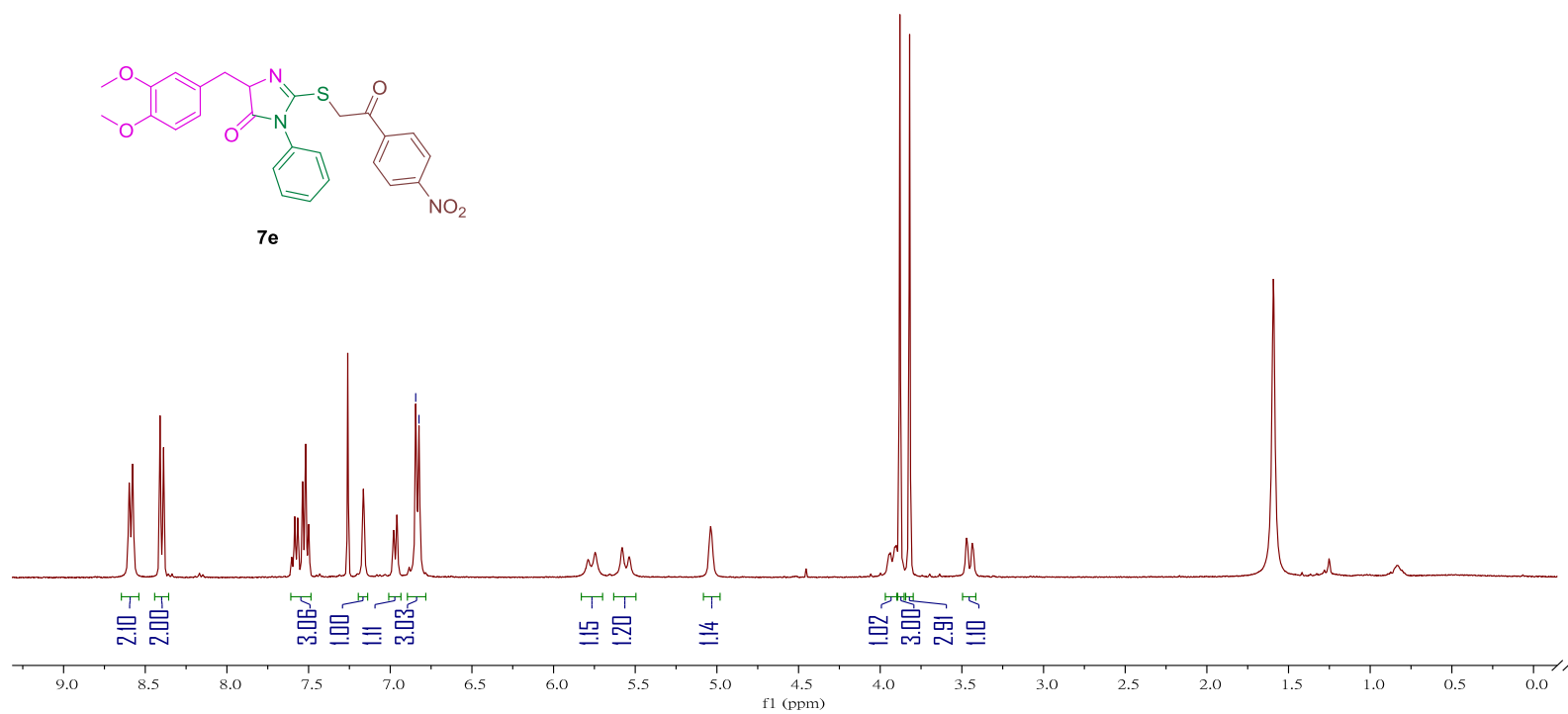


HRMS of compound **7d**

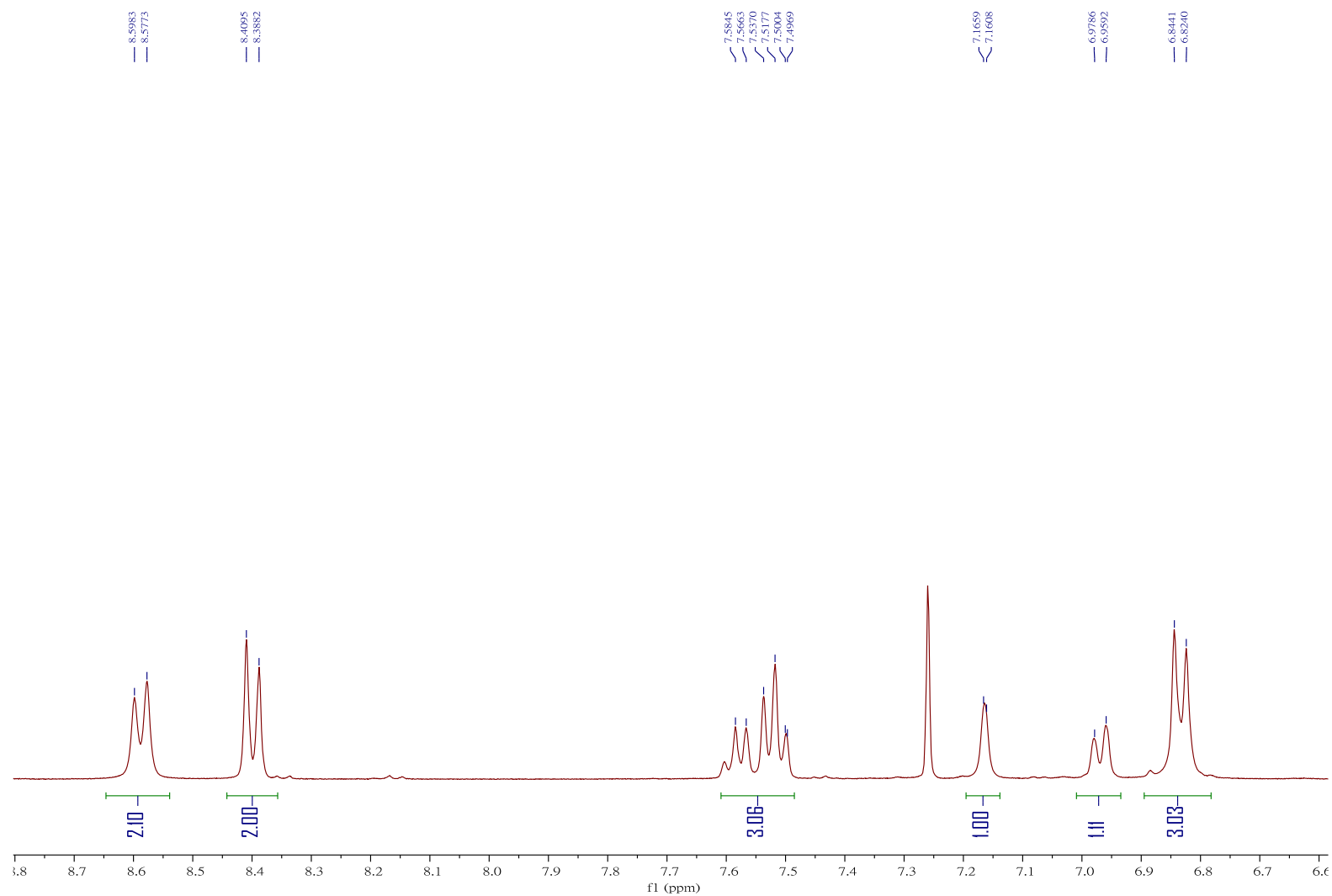


D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L244.0	MIR_TR_DTGS_L244	Instrument type and / or accessory	9/4/2018
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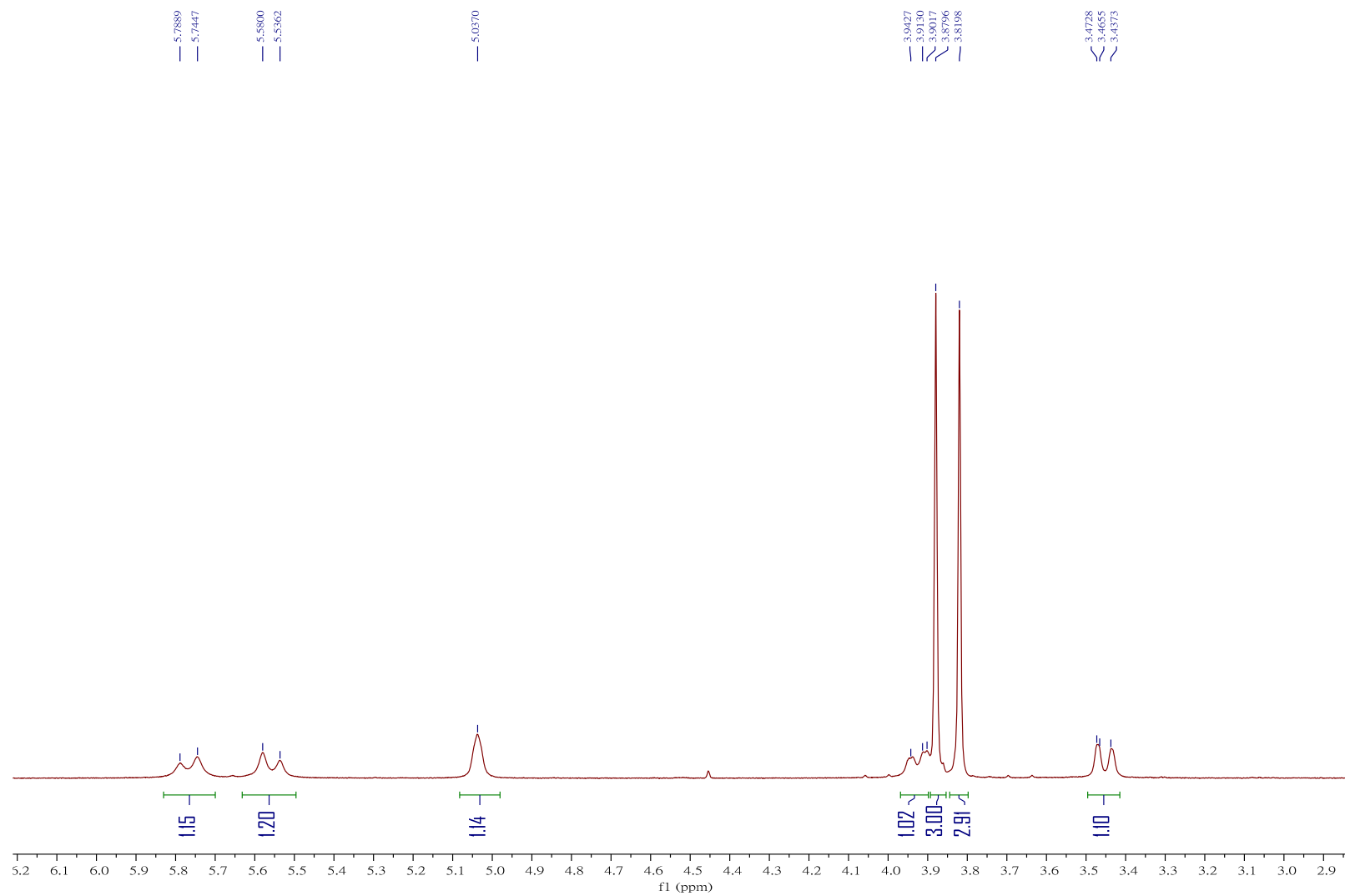
FT-IR Spectrum of compound **7d**



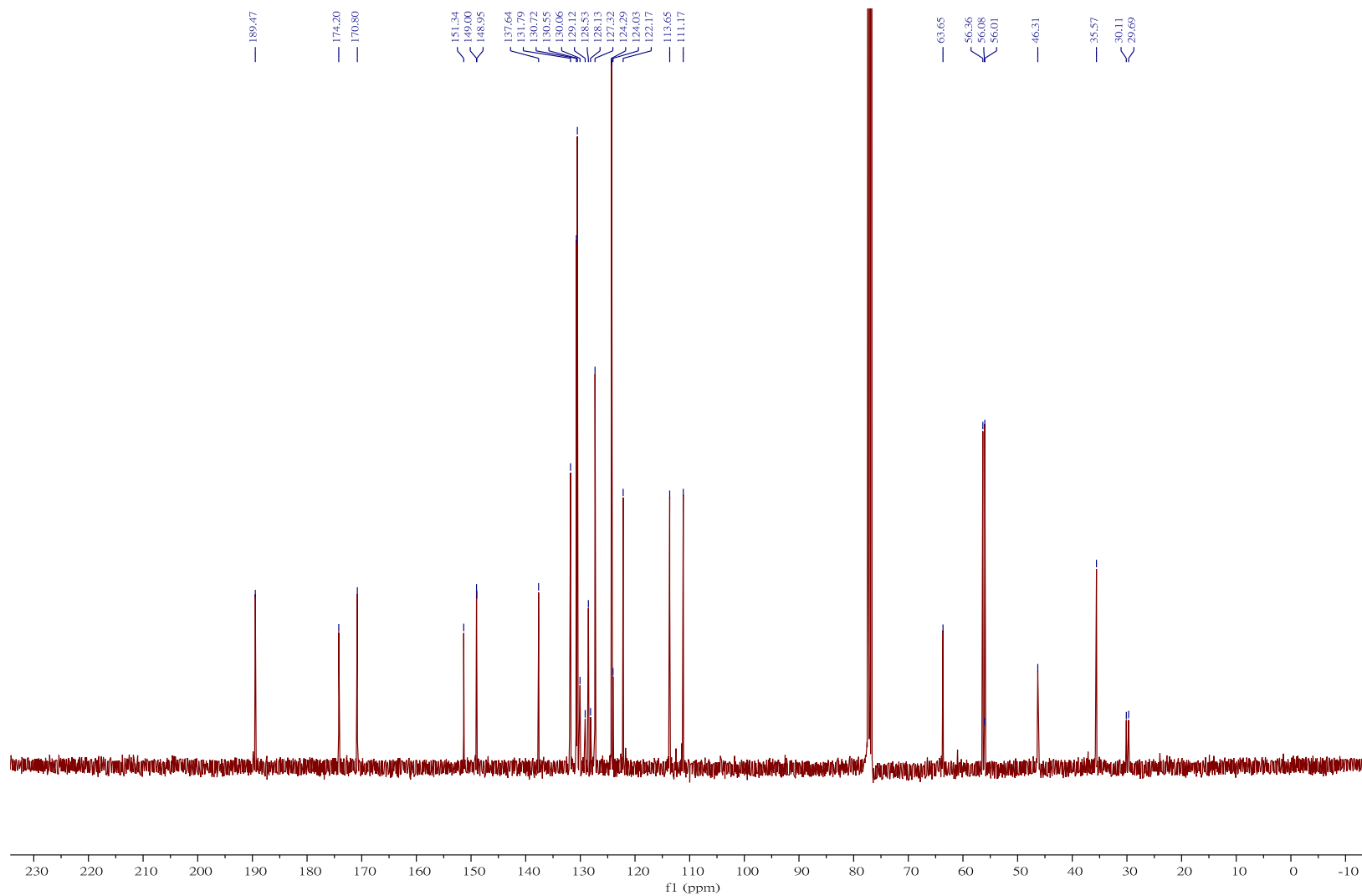
¹H NMR Spectrum (400 MHz) of compound **7e** in CDCl₃



Expansion of ¹H NMR Spectrum (400 MHz) of compound **7e** in CDCl₃



Expansion of ¹H NMR Spectrum (400 MHz) of compound **7e** in CDCl₃

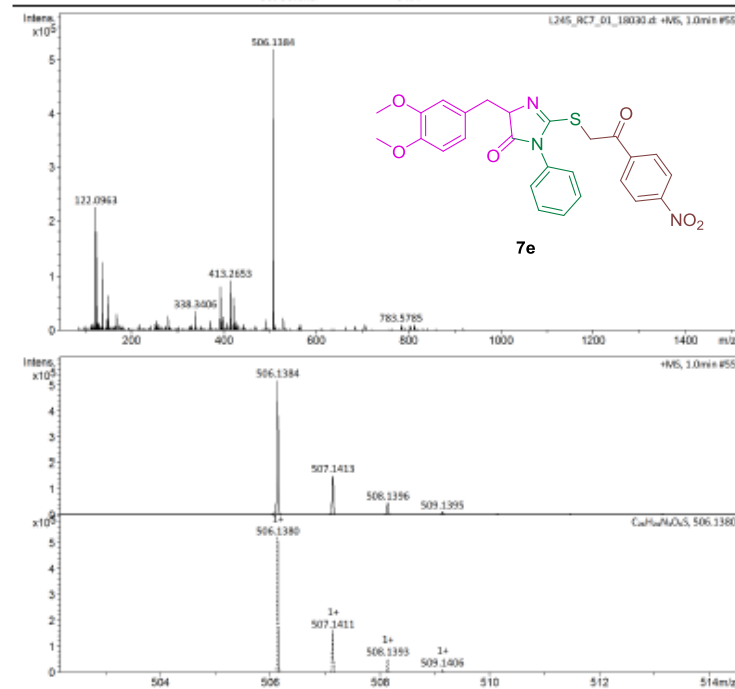


¹³C NMR Spectrum (101 MHz) of compound **7e** in CDCl₃

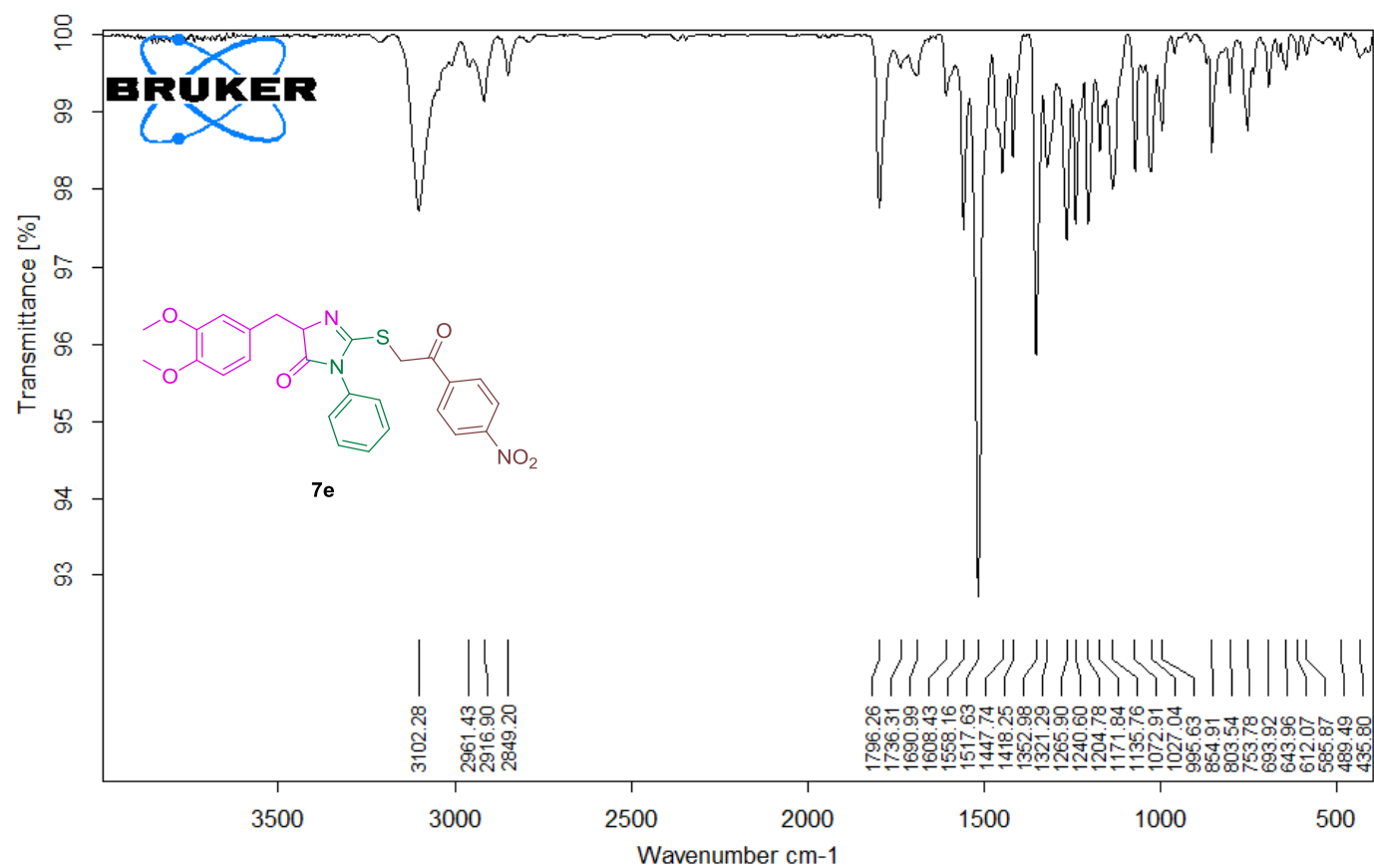
Display Report

Analysis Info		Acquisition Date: 4/20/2018 12:15:06 PM	
Analysis Name	H:\20181-6\20180420\L245_RC7_01_18030.d	Operator	NCTU
Method	Small molecule.m	Instrument	Impact HD
Sample Name	L245		1819636.00164
Comment			

Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
Focus	Active	Set Capillary	4500 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1500 m/z	Set Charging Voltage	2000 V
		Set Corona	0 nA
		Set Nebulizer	1.0 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	6.0 l/min
		Set Divert Valve	Waste
		Set AP/CI Heater	0 °C



HRMS of compound 7e



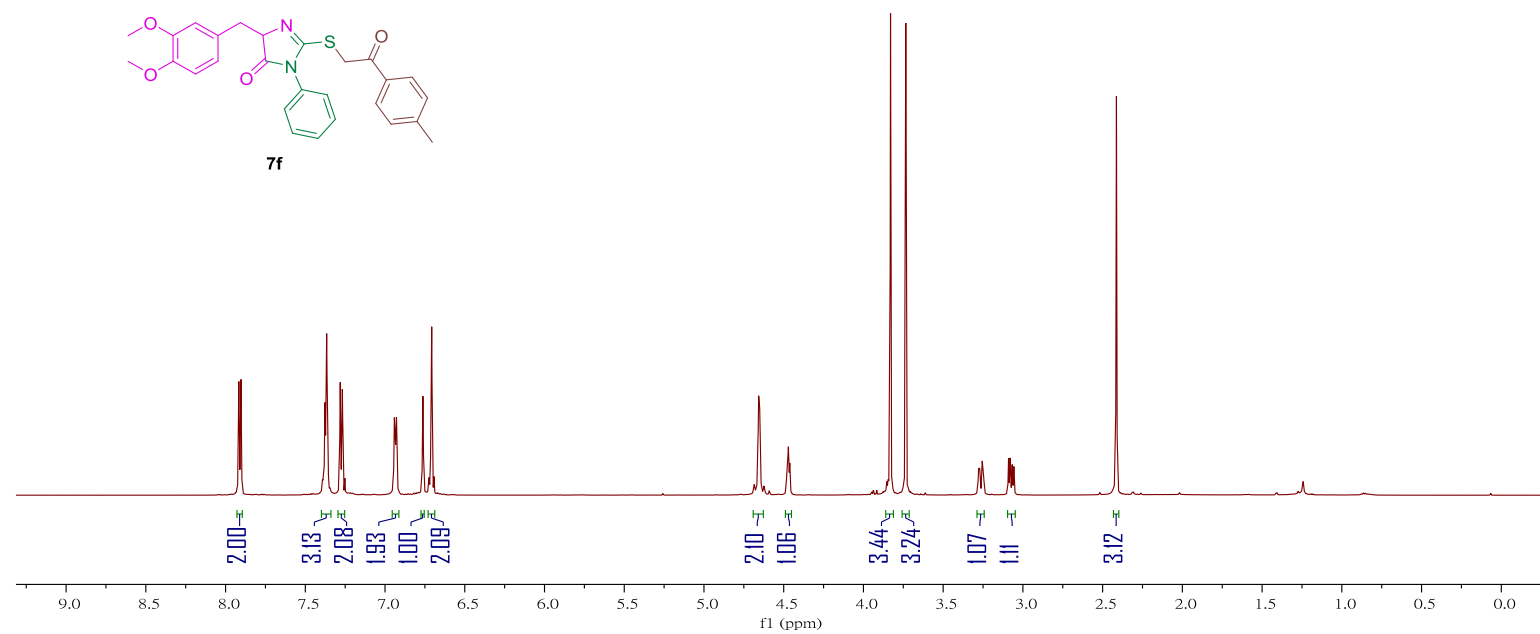
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L245.1

MIR_TR_DTGS_L245

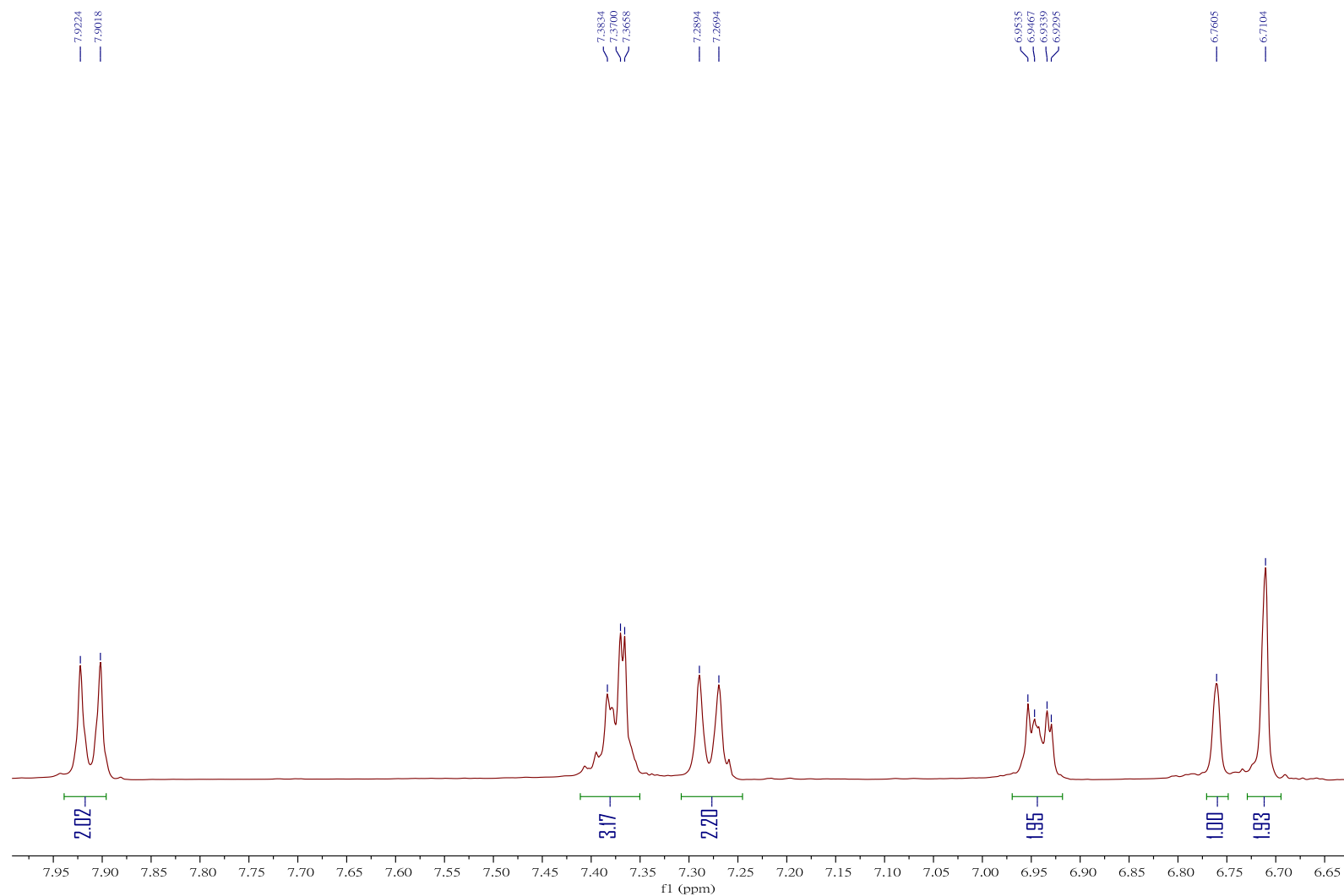
Instrument type and / or accessory

9/4/2018

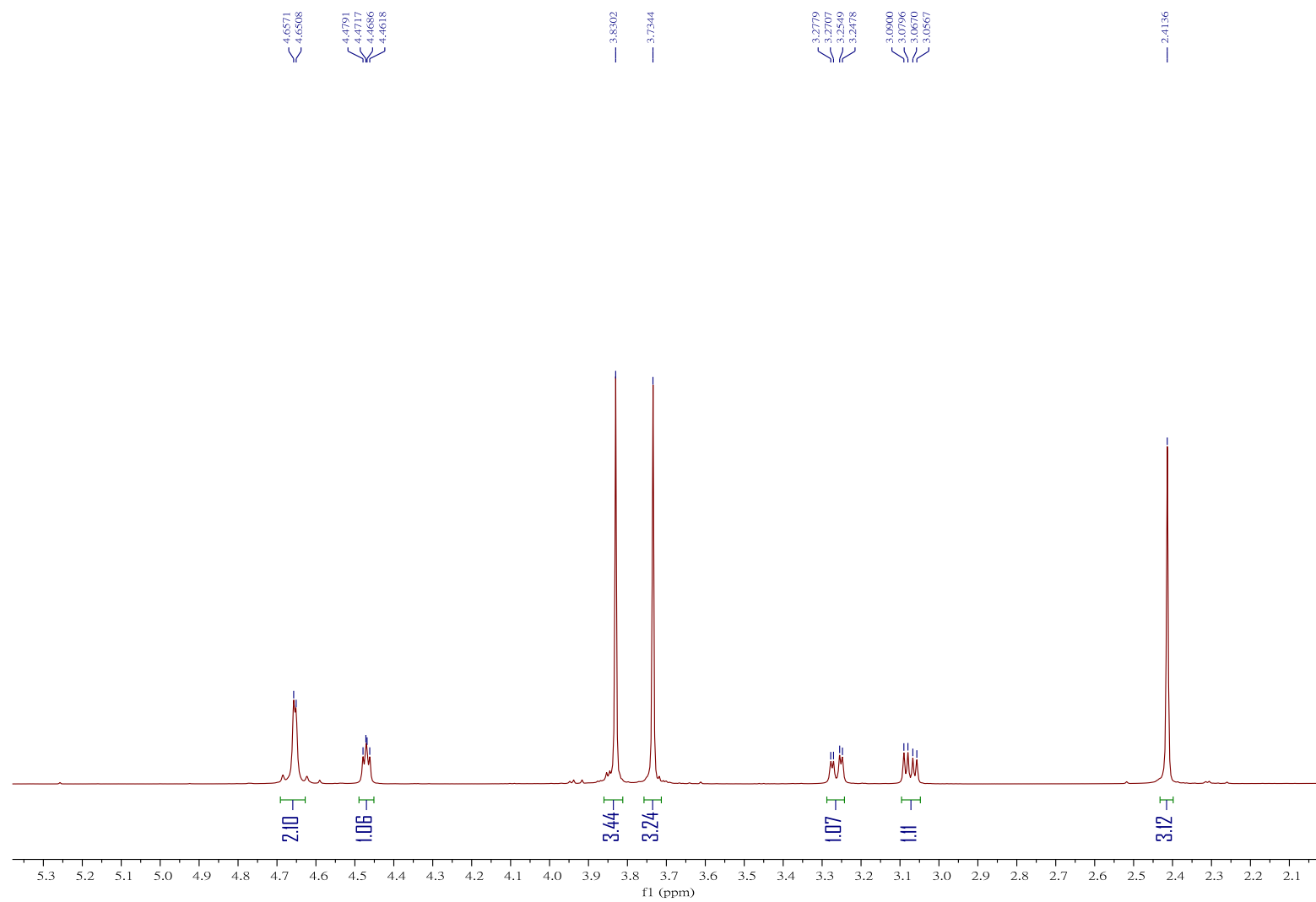
FT-IR Spectrum of compound **7e**



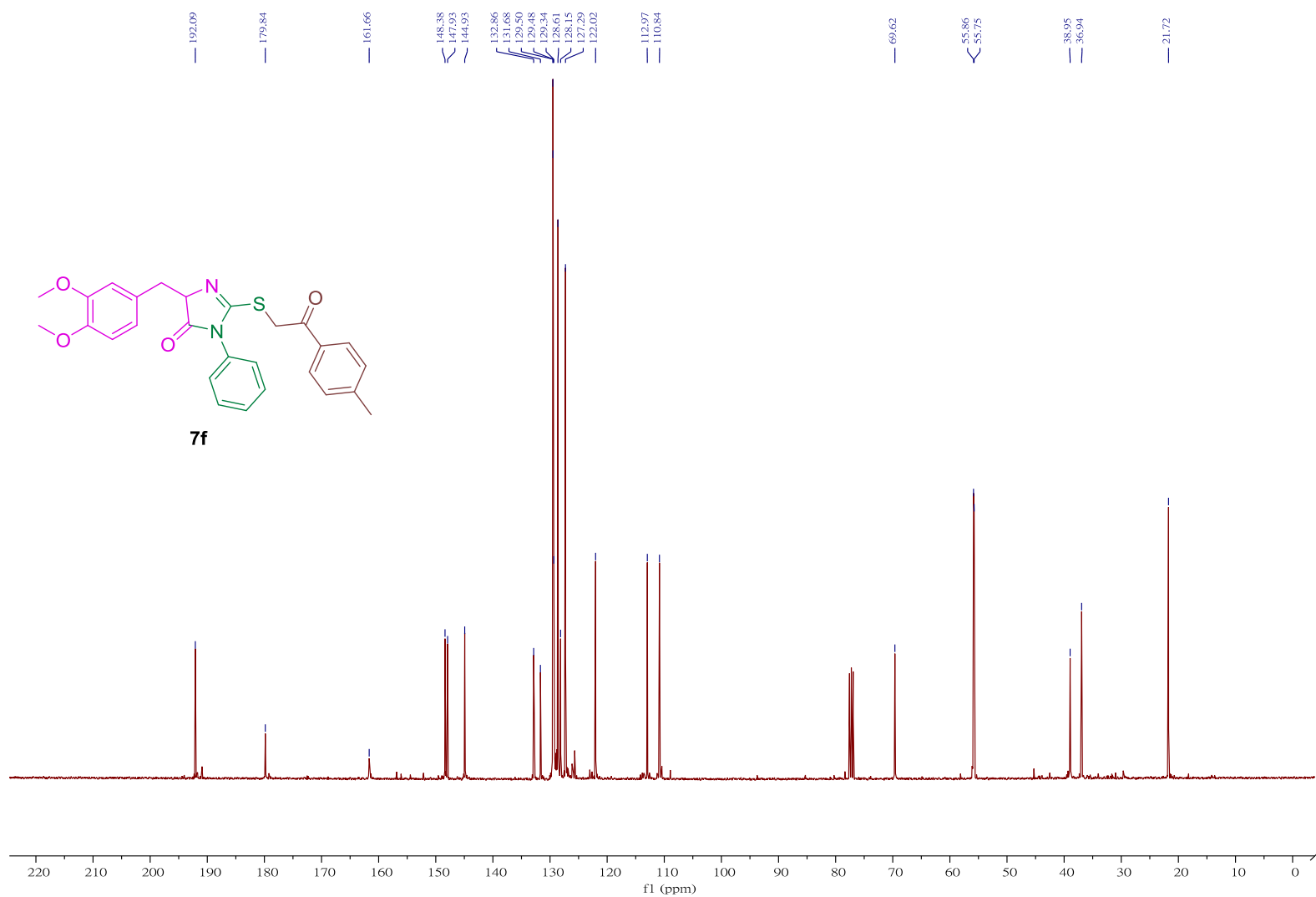
¹H NMR Spectrum (400 MHz) of compound **7f** in CDCl₃



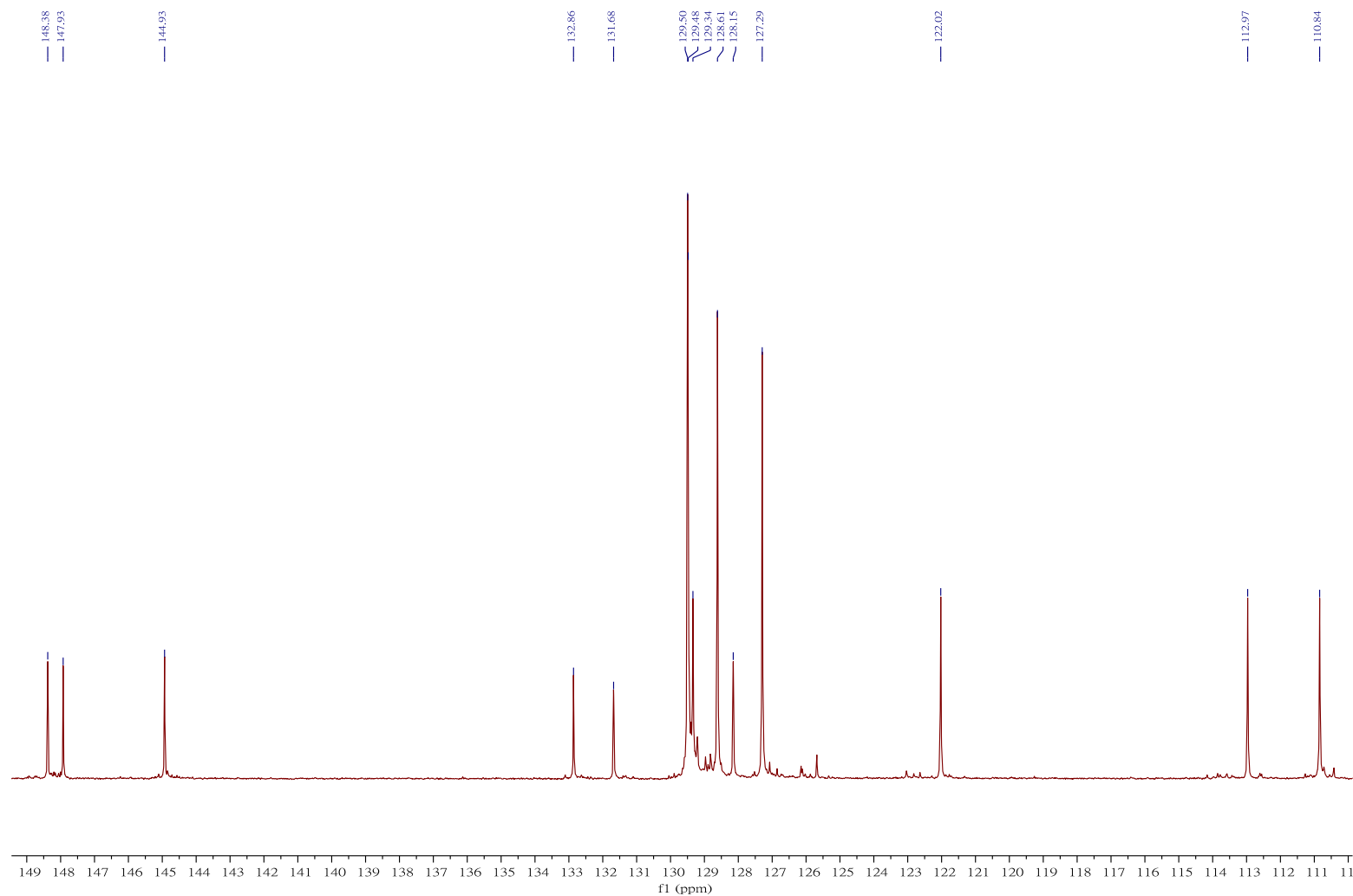
Expansion of ^1H NMR Spectrum (400 MHz) of compound **7f** in CDCl_3



Expansion of ^1H NMR Spectrum (400 MHz) of compound **7f** in CDCl_3



^{13}C NMR Spectrum (101 MHz) of compound **7f** in CDCl_3



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **7f** in CDCl_3

Display Report

Analysis Info

Analysis Name D:\Data\nctu service\data\2018\20180420\L246_RD5_01_18032.d

Method Small molecule.m

Sample Name L246

Comment

Acquisition Date 4/20/2018 12:23:47 PM

Operator NCTU

Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type ESI

Focus Active

Scan Begin 50 m/z

Scan End 1500 m/z

Ion Polarity

Set Capillary

Set End Plate Offset

Set Charging Voltage

Set Corona

Positive

4500 V

-500 V

2000 V

0 nA

Set Nebulizer

Set Dry Heater

Set Dry Gas

Set Divert Valve

Set APCI Heater

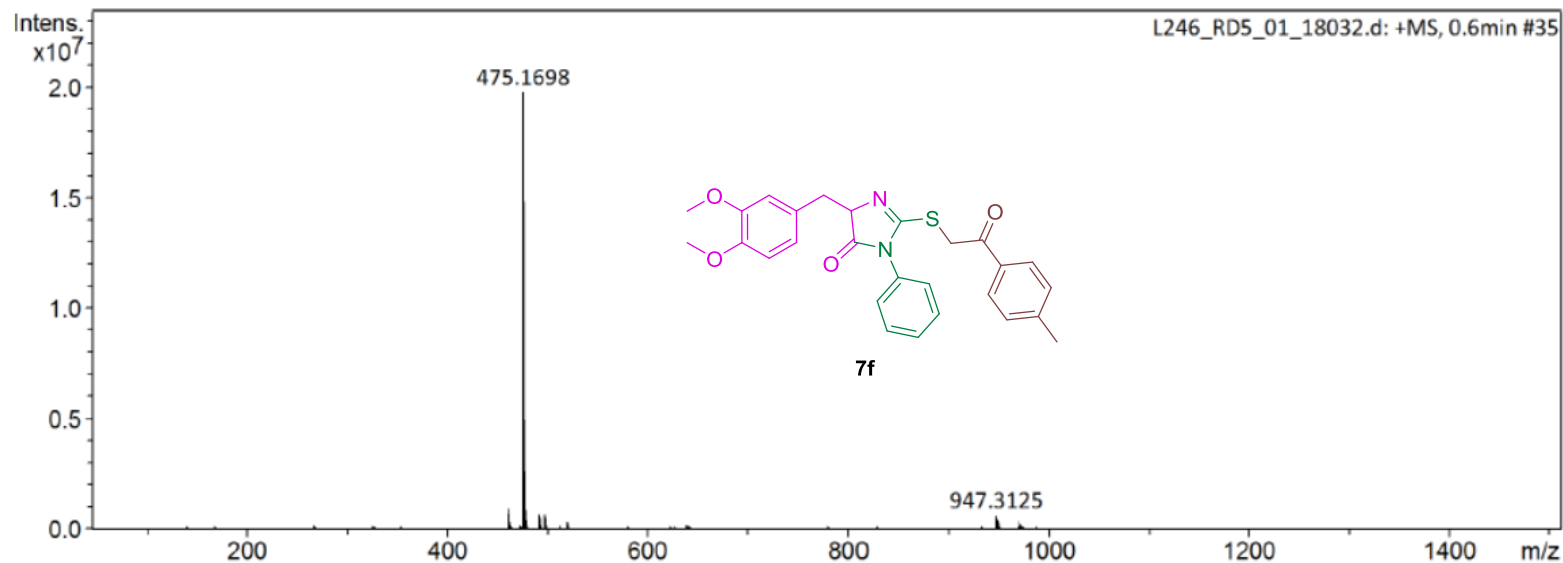
1.0 Bar

200 °C

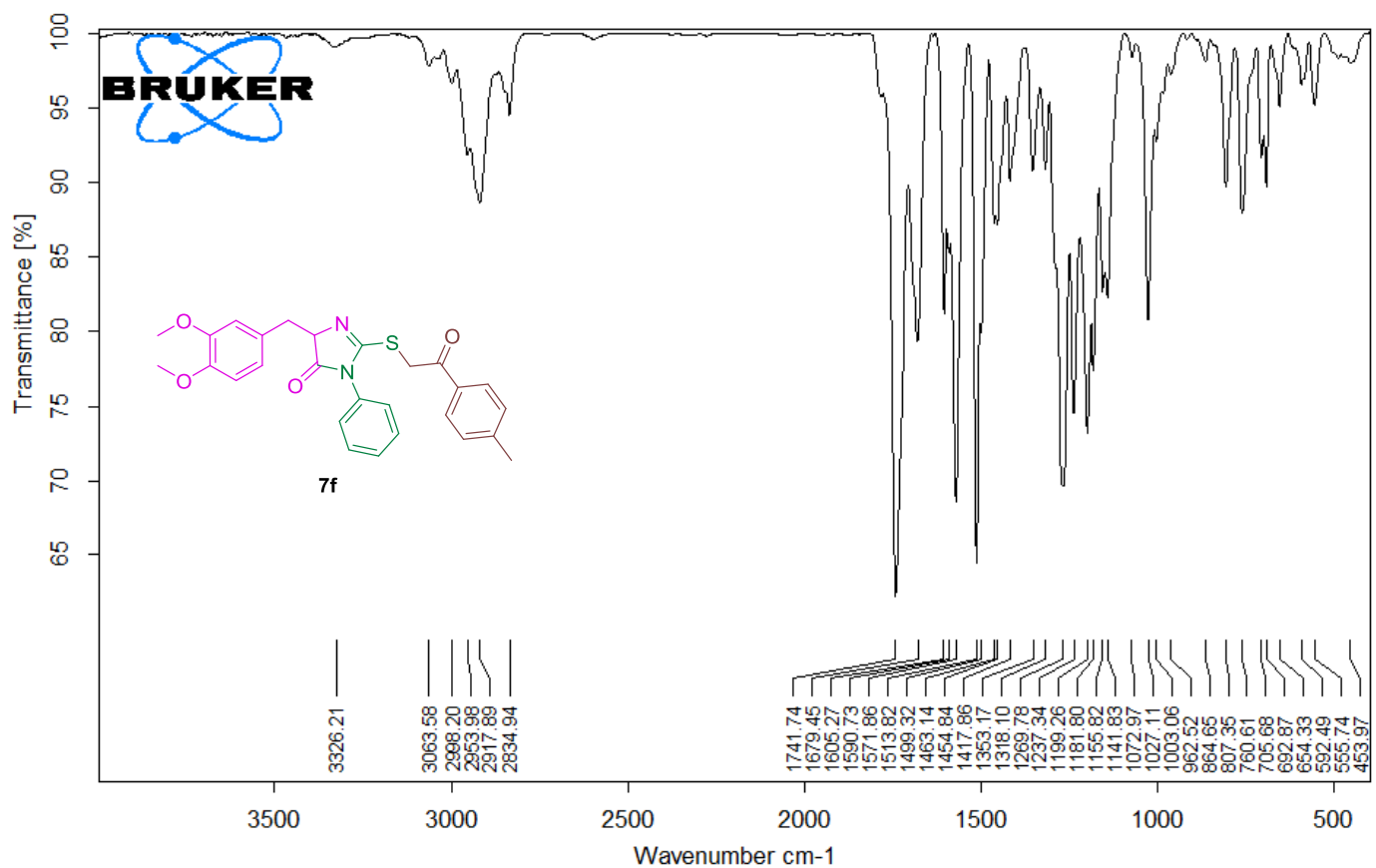
6.0 l/min

Waste

0 °C



HRMS of compound 7f



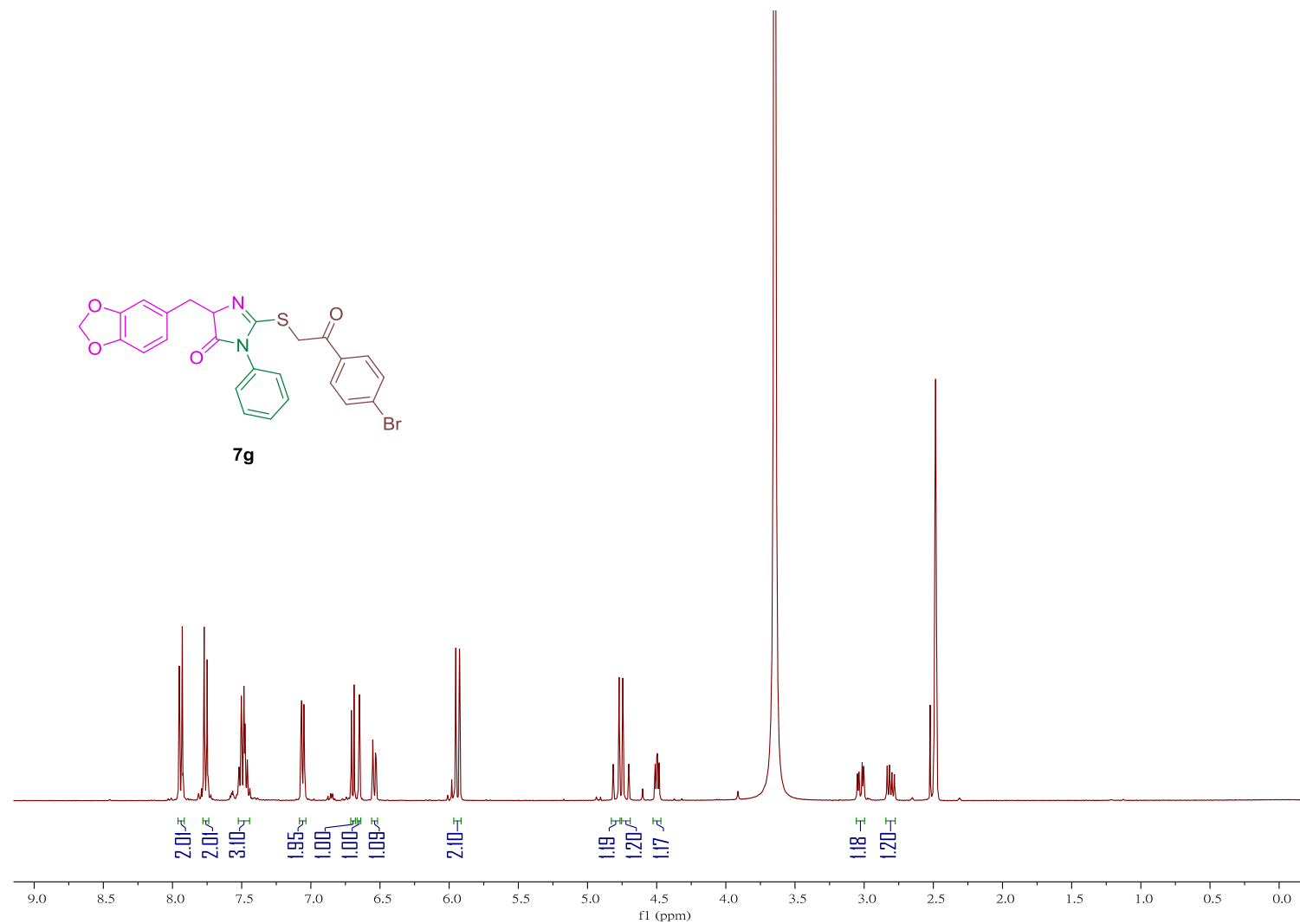
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L246.1

MIR_TR_DTGS_L246

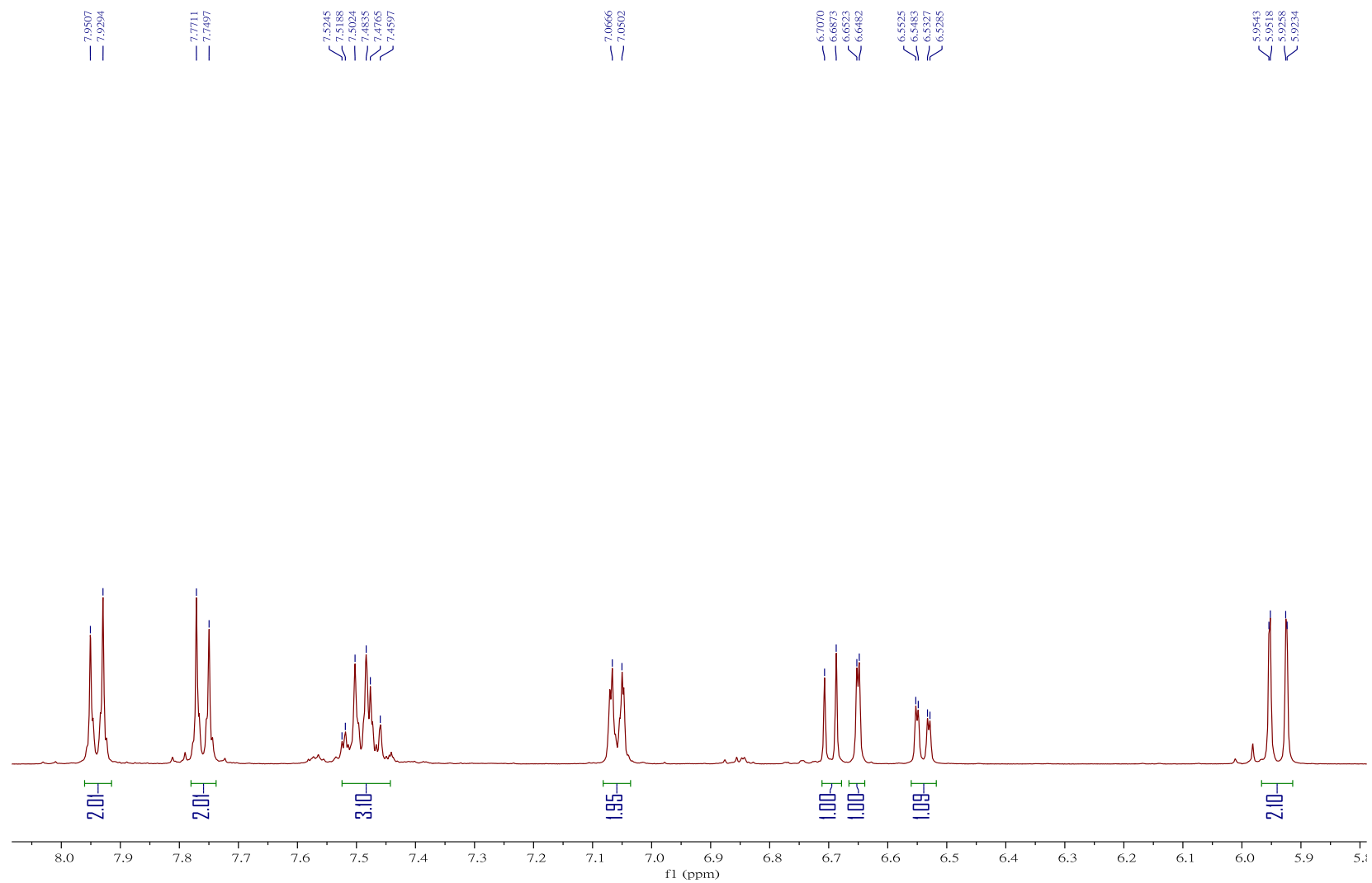
Instrument type and / or accessory

9/4/2018

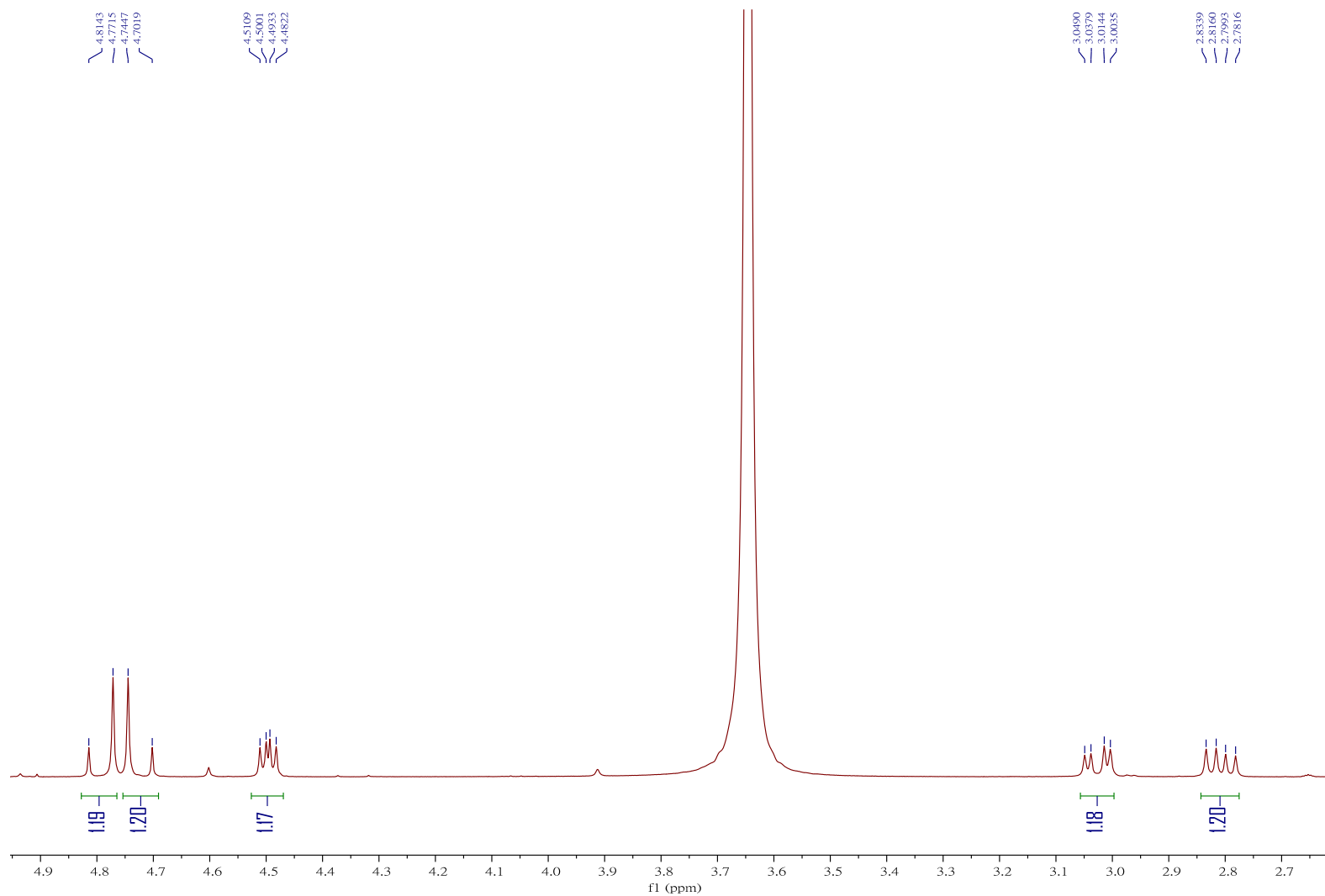
FT-IR Spectrum of compound **7f**



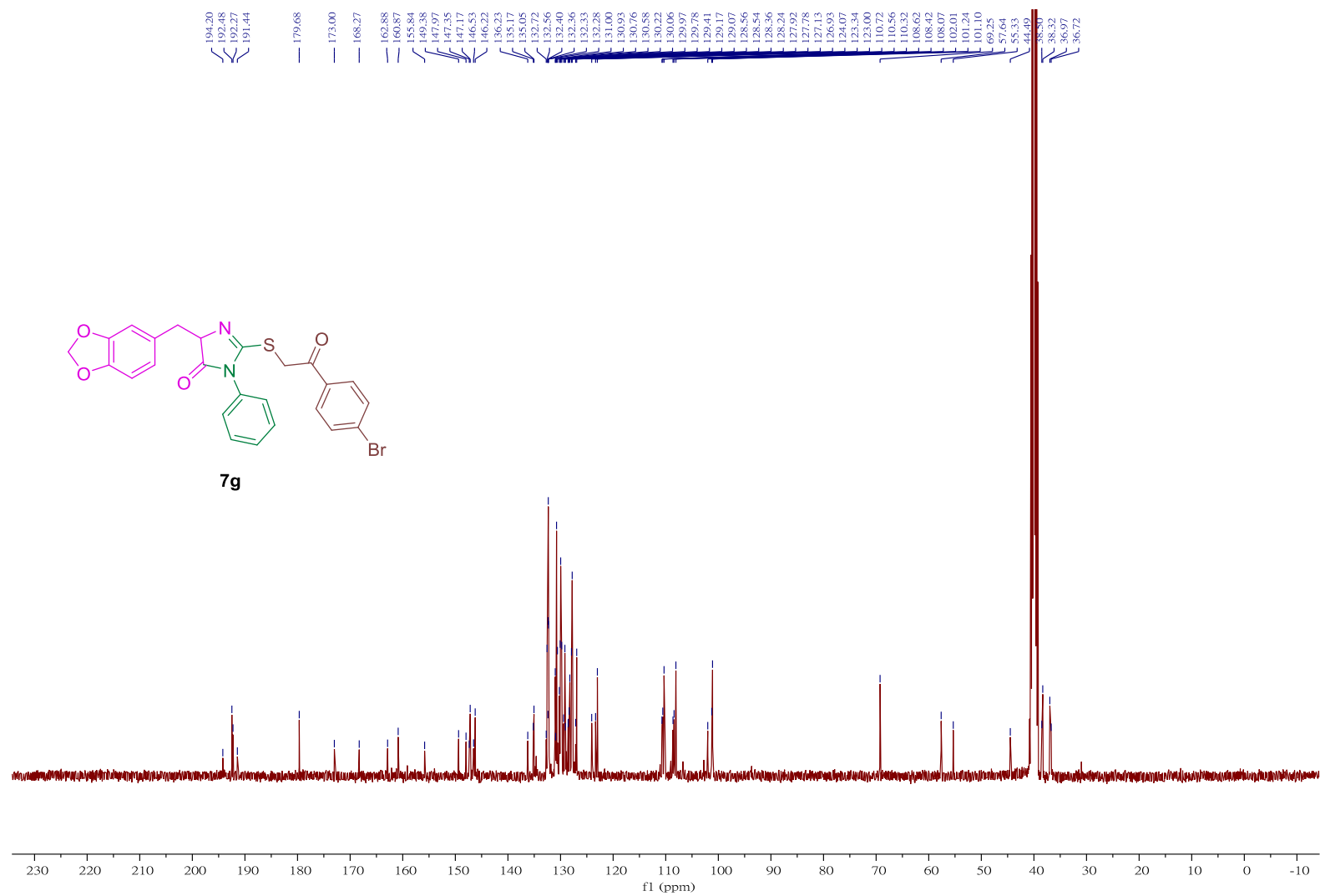
^1H NMR Spectrum (400 MHz) of compound **7g** in CDCl_3

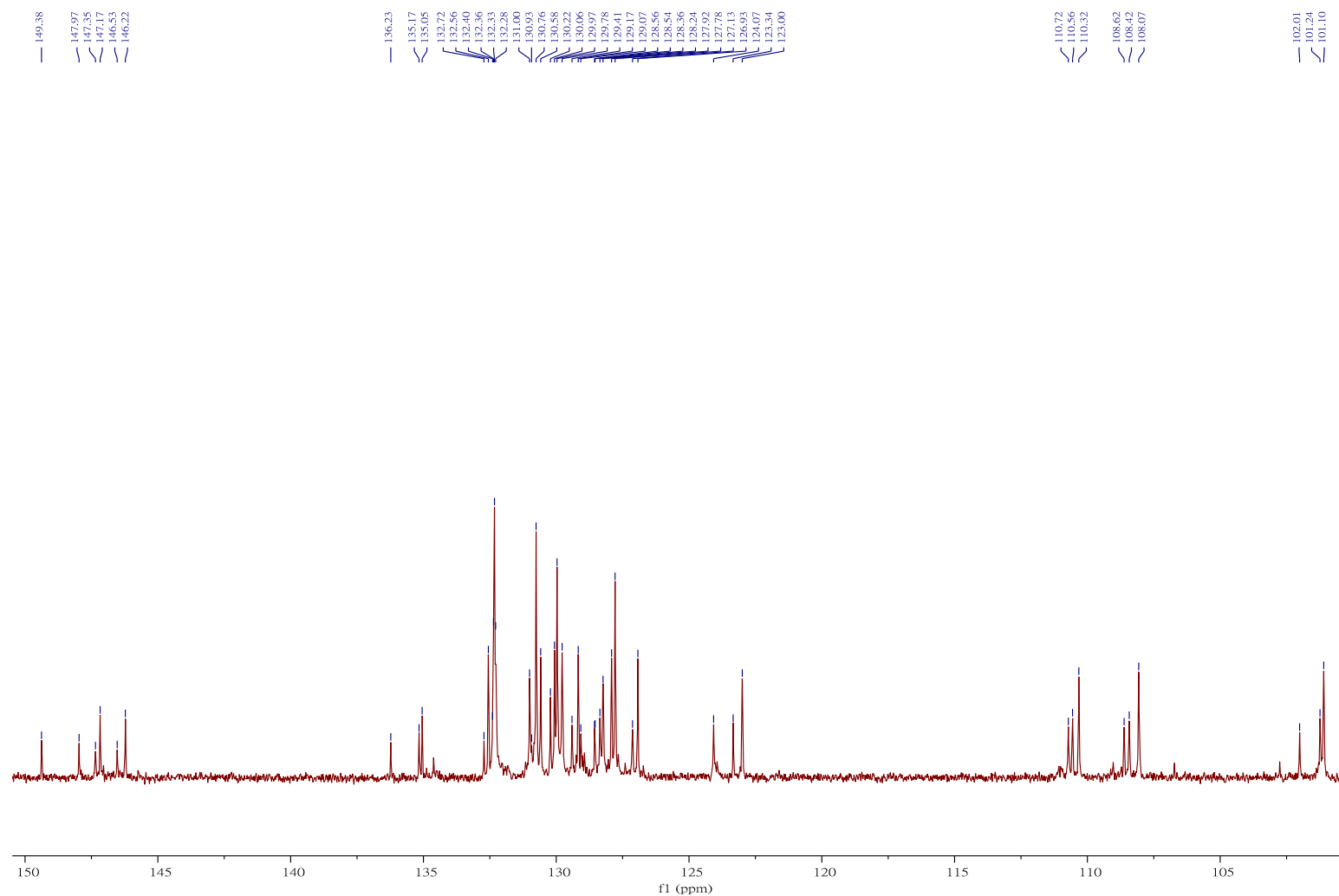


Expansion of ¹H NMR Spectrum (400 MHz) of compound **7g** in CDCl₃

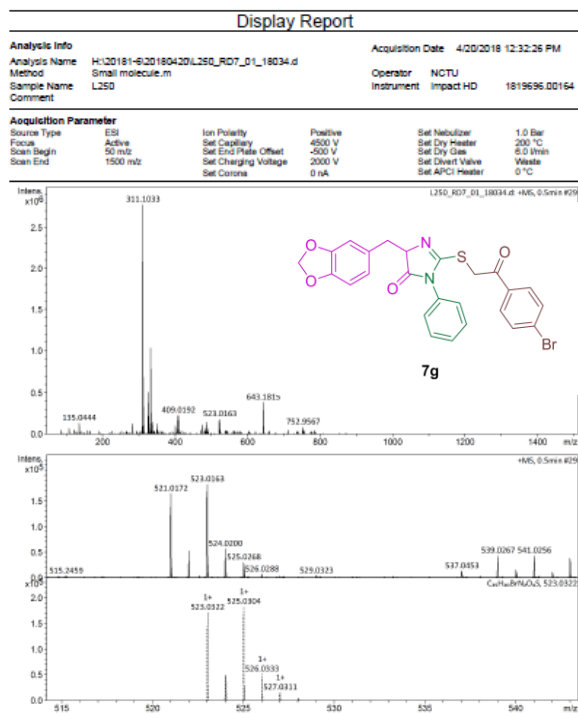


Expansion of ¹H NMR Spectrum (400 MHz) of compound **7g** in CDCl₃

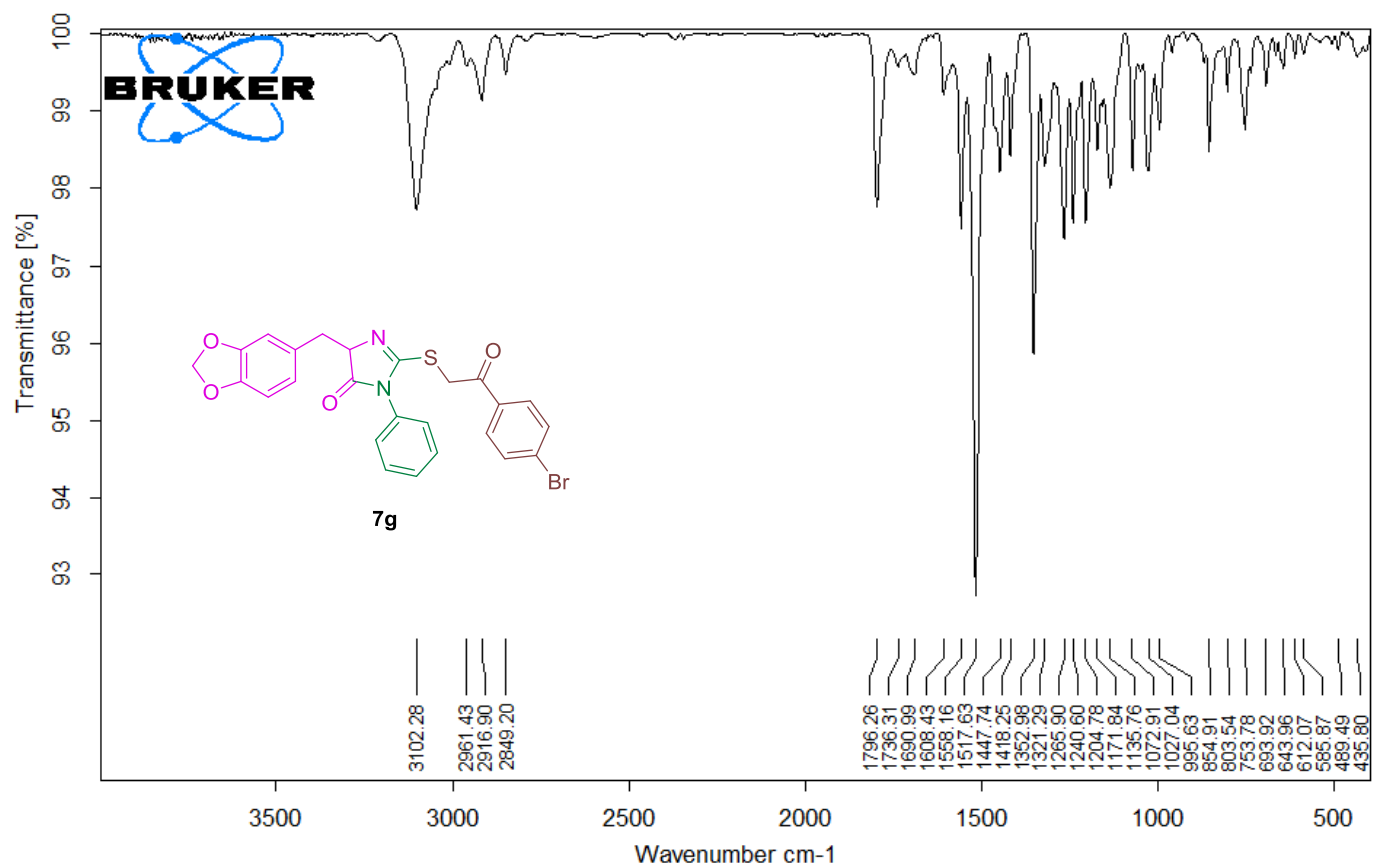




Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **7g** in $\text{DMSO-}d_6$



HRMS of compound **7g**



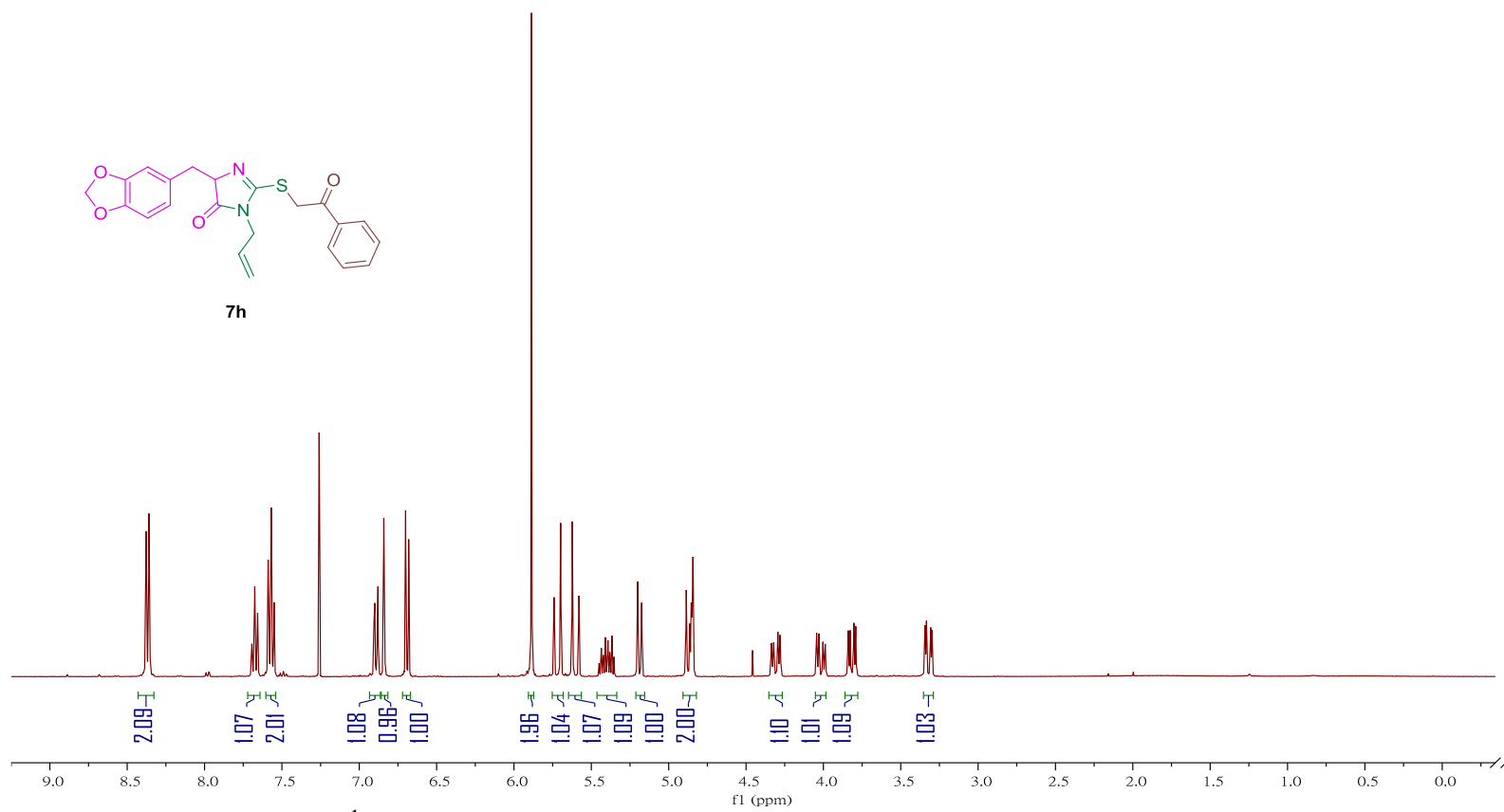
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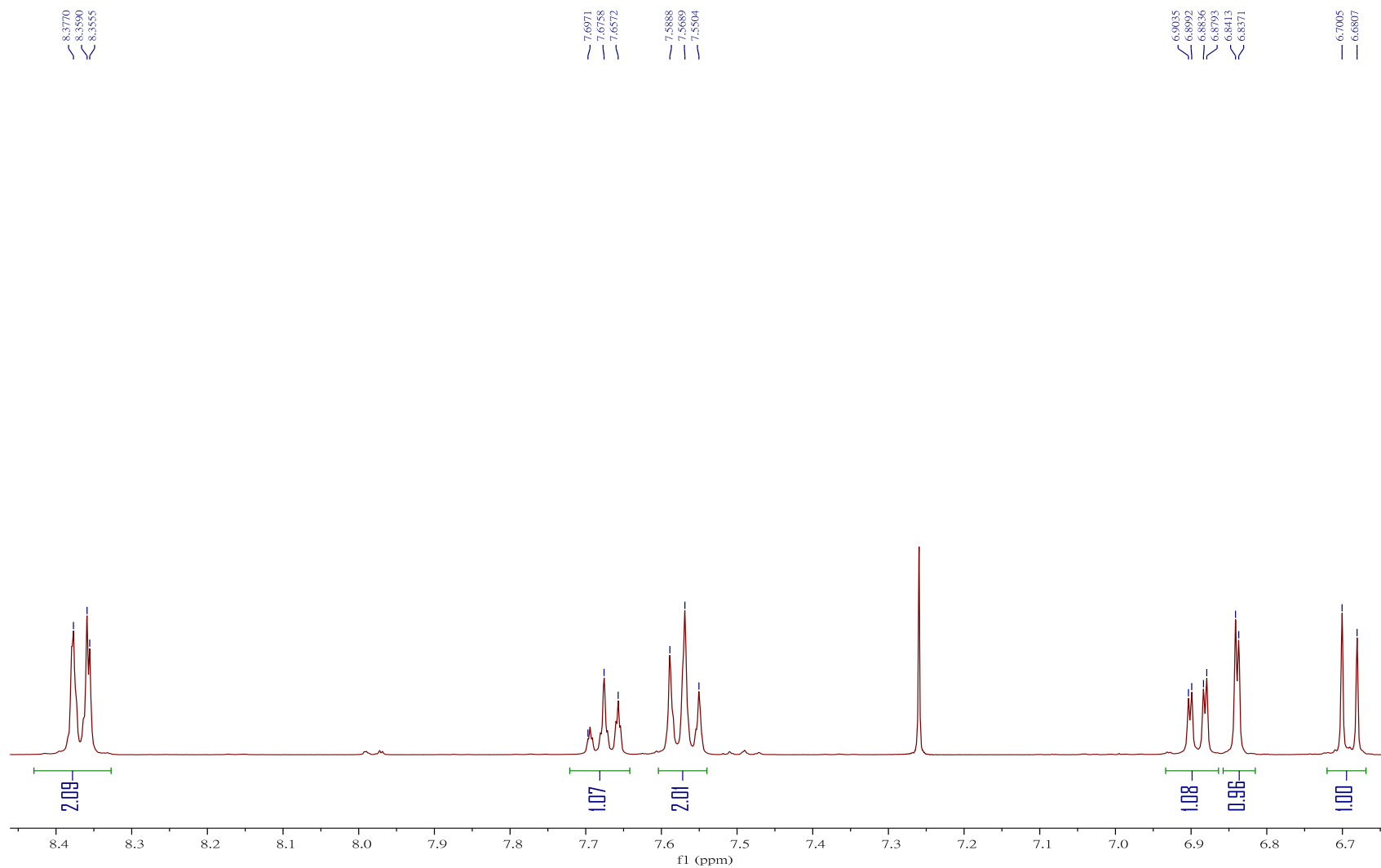
MIR_TR_DTGS_L245

Instrument type and / or accessory

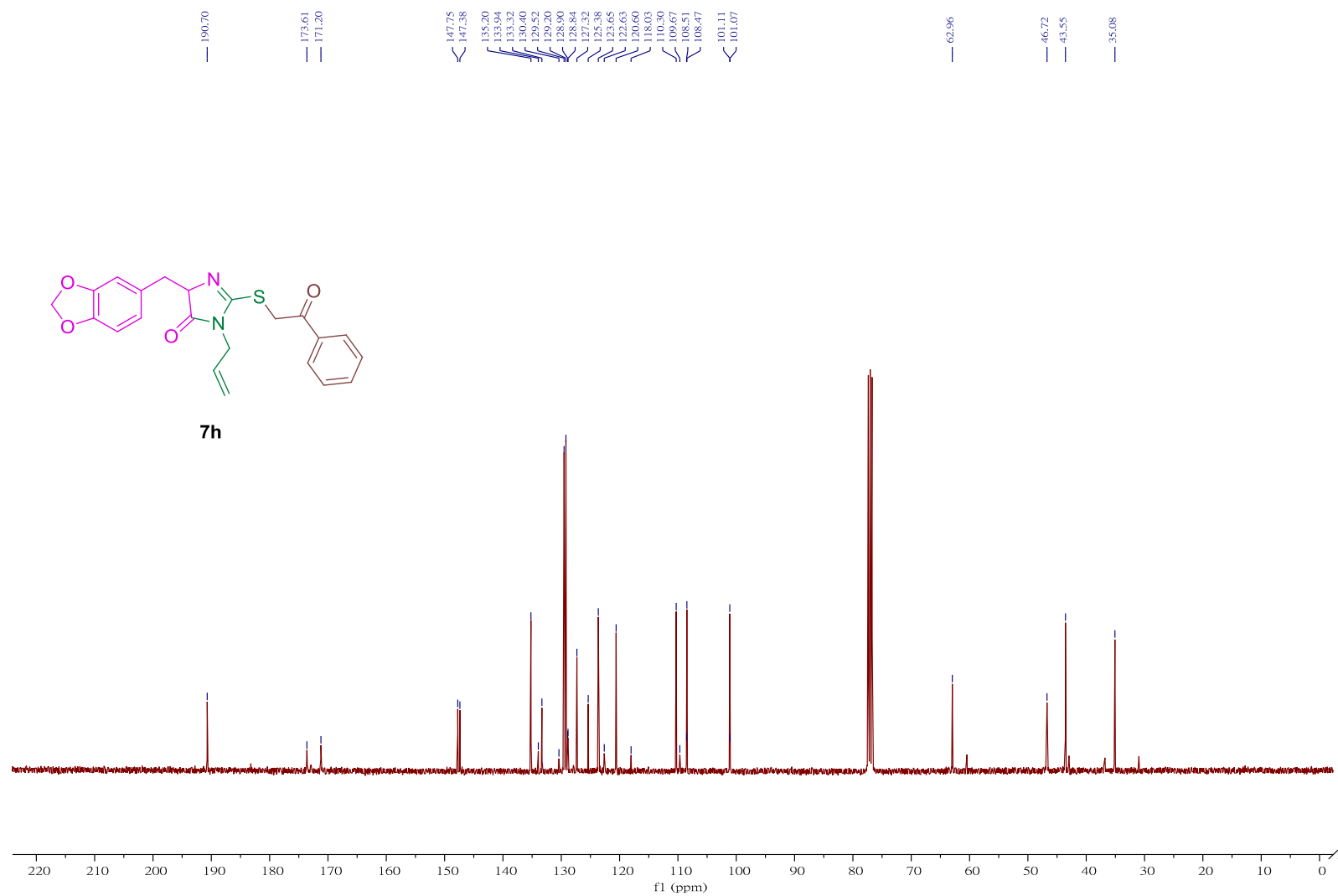
9/4/2018

FT-IR Spectrum of compound **7g**

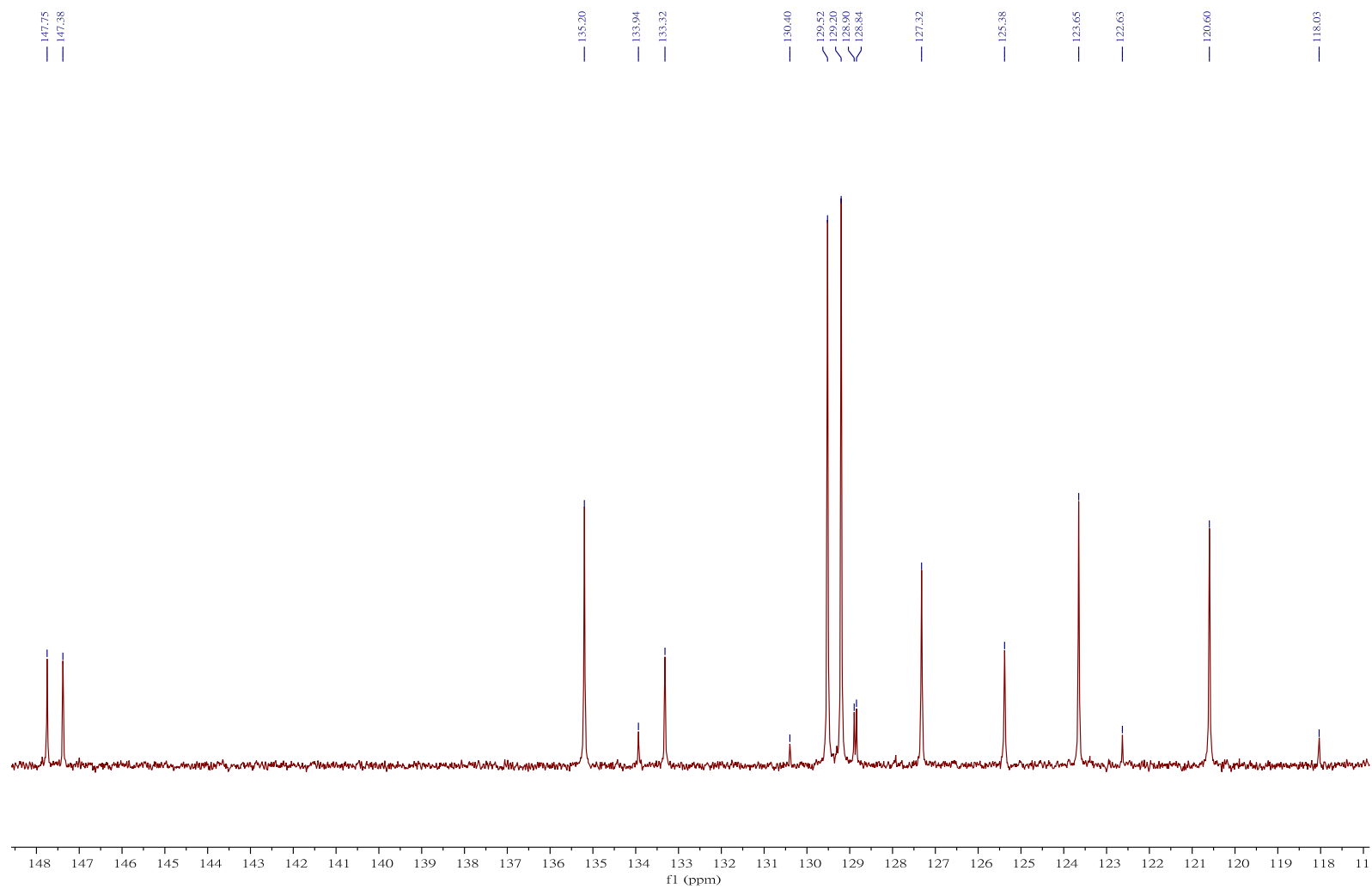




Expansion of ¹H NMR Spectrum (400 MHz) of compound **7h** in CDCl₃



¹³C NMR Spectrum (101 MHz) of compound **7h** in CDCl₃

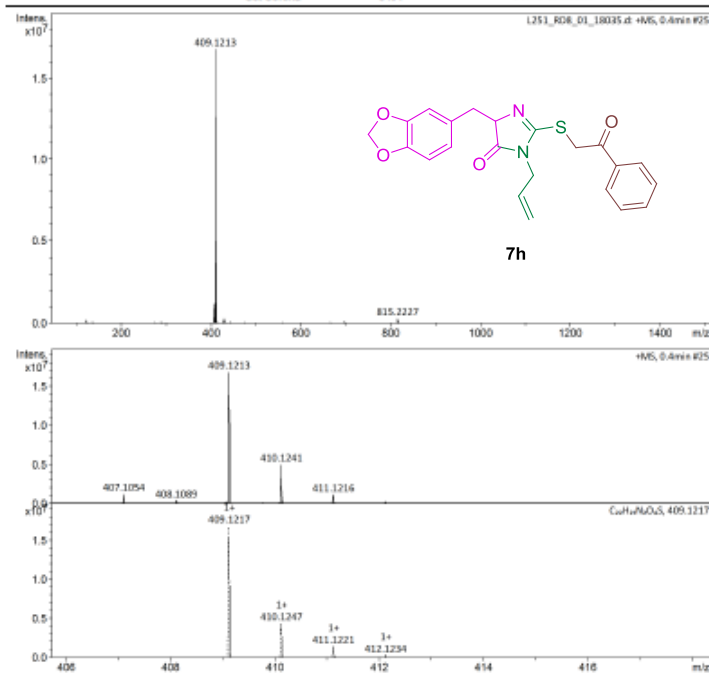


Expansion of ¹³C NMR Spectrum (101 MHz) of compound **7h** in CDCl₃

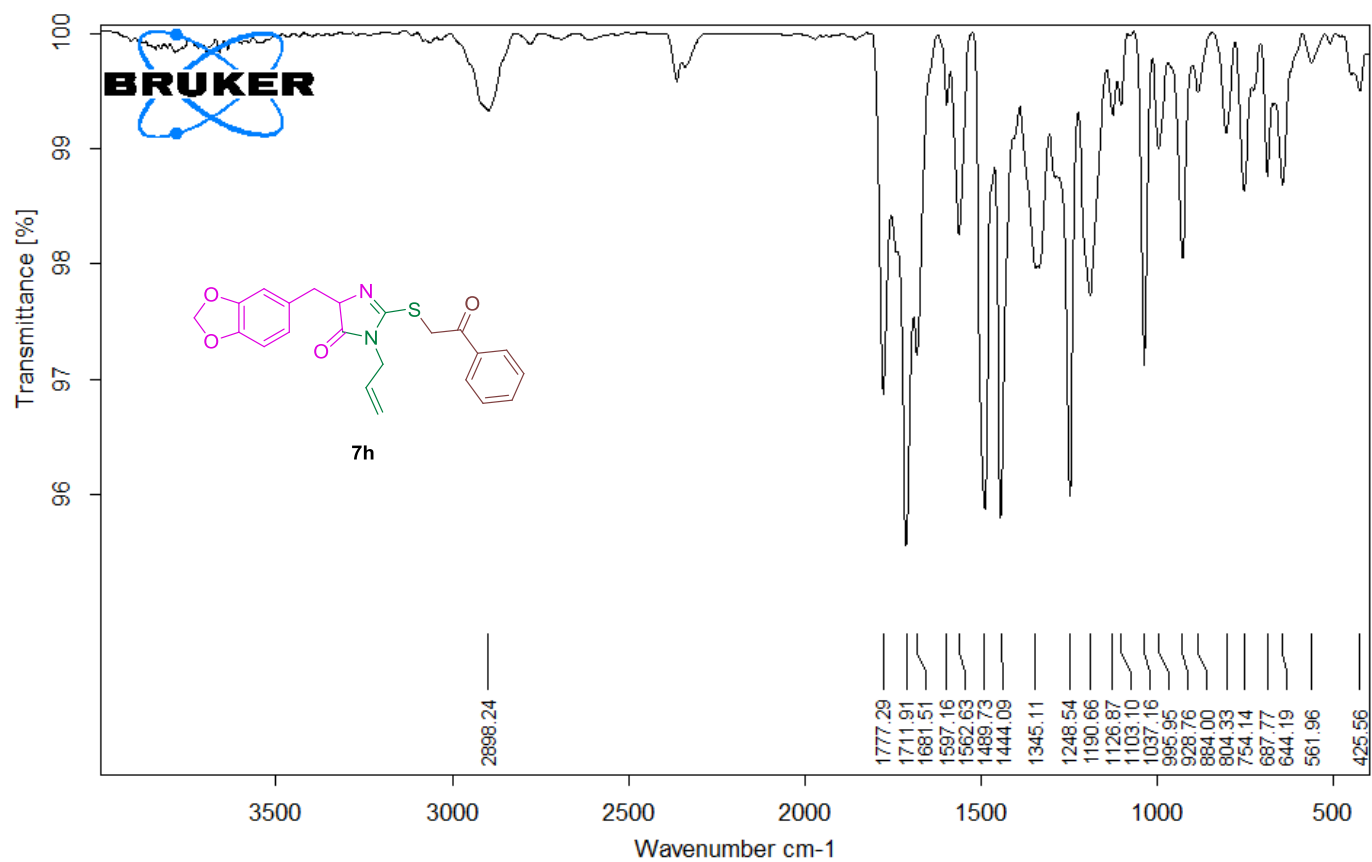
Display Report

Analysis Info		Acquisition Date 4/20/2018 12:36:47 PM	
Analysis Name	H:\20181-6\20180420\L251_RD8_01_18035.d	Operator	NCTU
Method	Small molecule.m	Instrument	Impact HD
Sample Name	L251		1819696.00154
Comment			

Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
Focus	Active	Set Capillary	4500 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1500 m/z	Set Charging Voltage	2000 V
		Set Corona	0 nA
		Set Nebulizer	1.0 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	6.0 l/min
		Set Divert Valve	Waste
		Set APCI Heater	0 °C



HRMS of compound **7h**



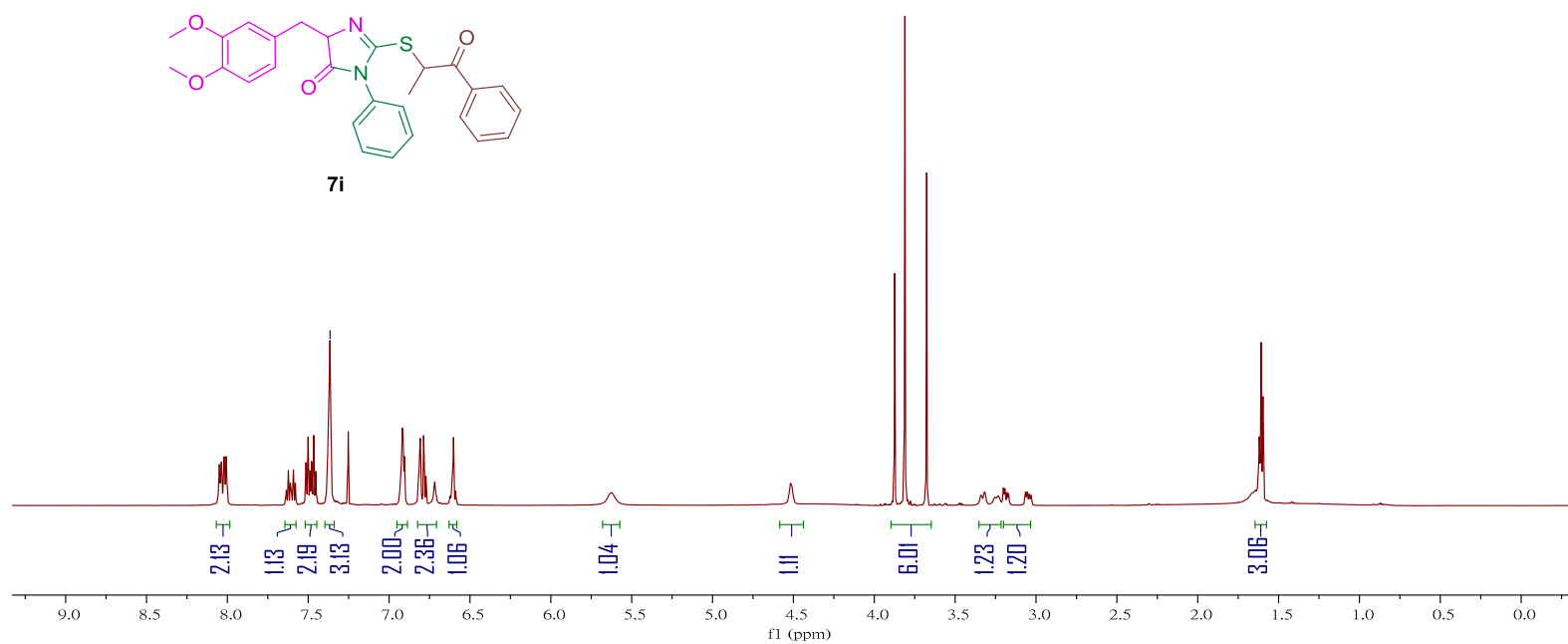
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L251.1

MIR_TR_DTGS_L251

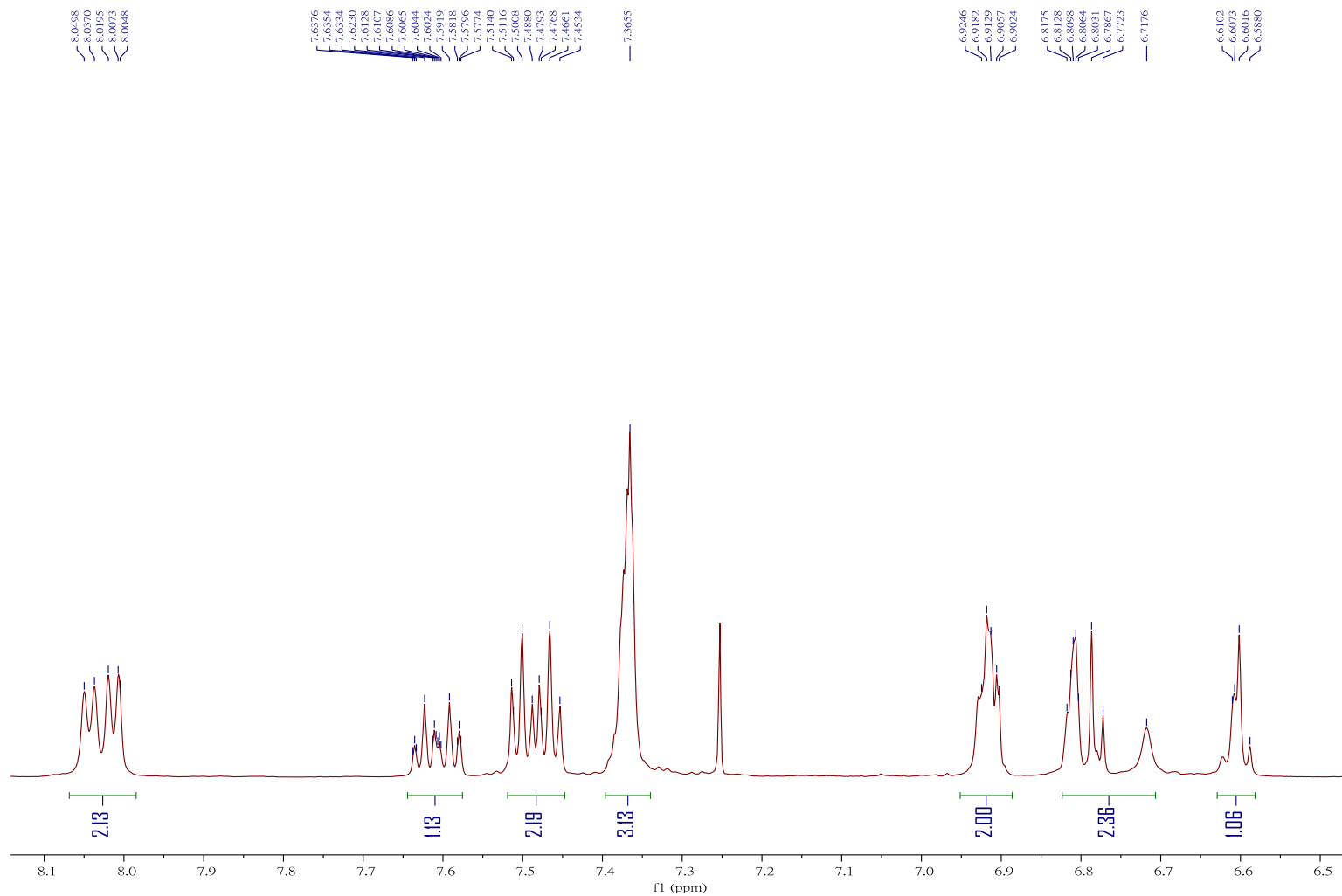
Instrument type and / or accessory

9/4/2018

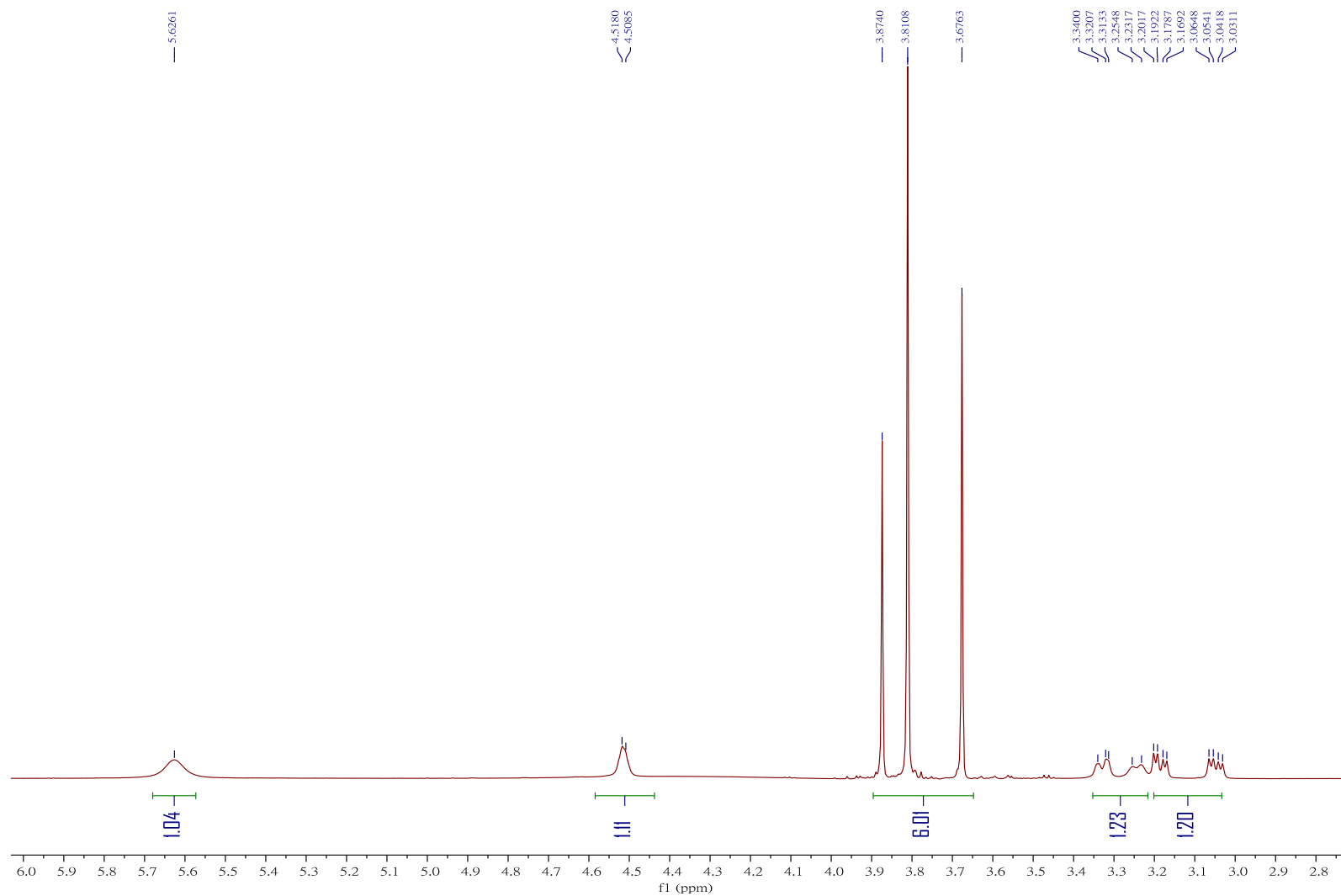
FT-IR Spectrum of compound **7h**



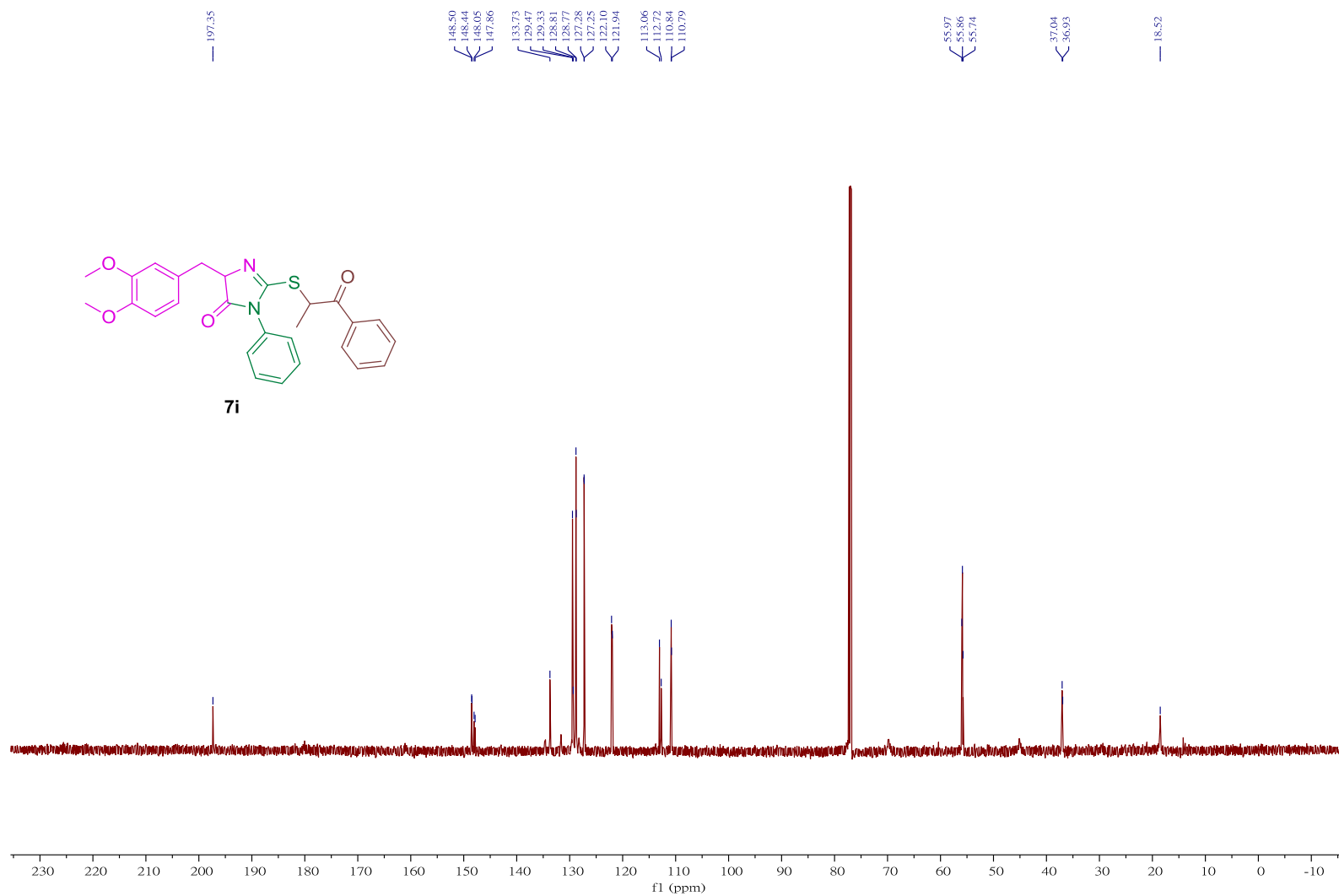
¹H NMR Spectrum (400 MHz) of compound **7i** in CDCl₃



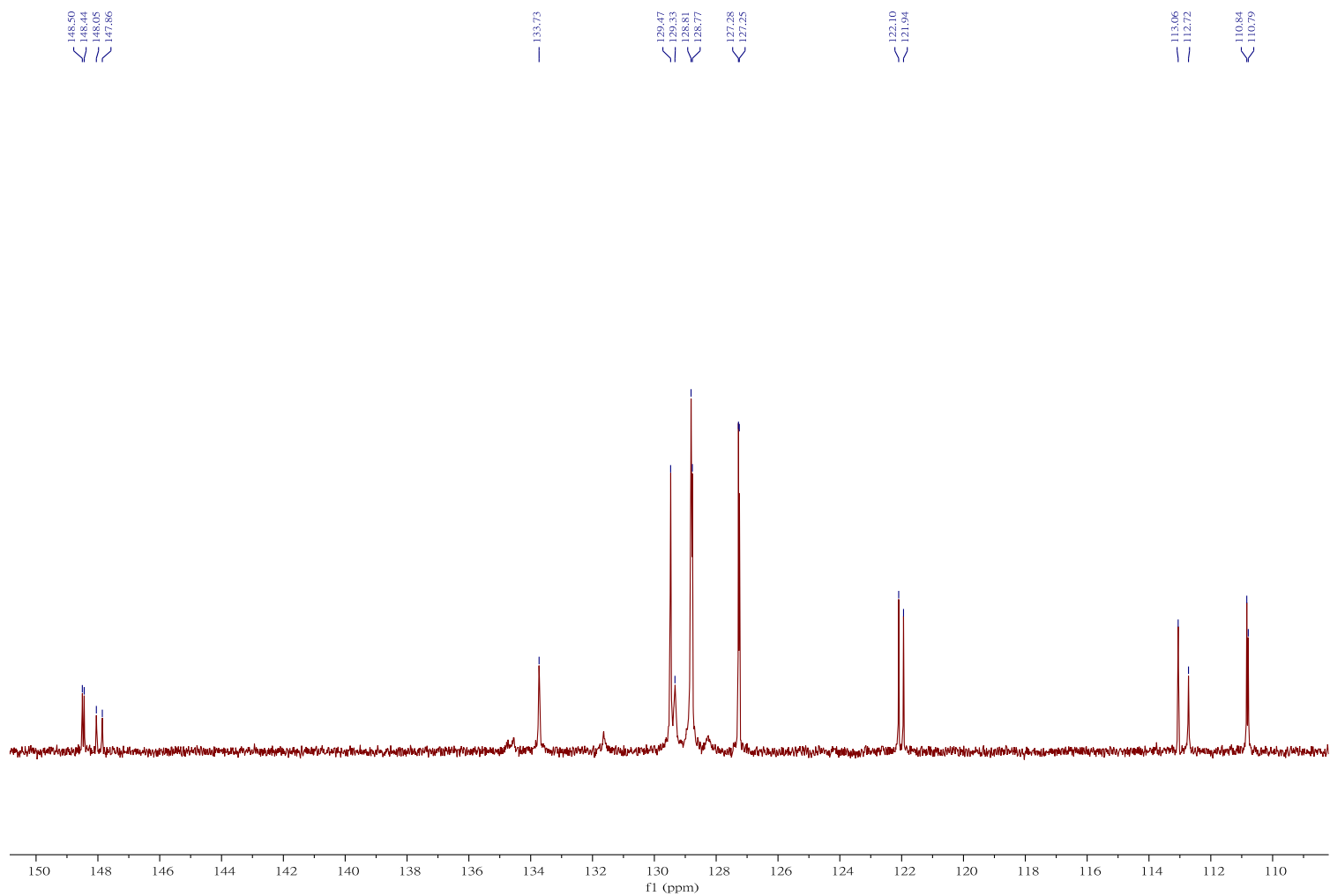
Expansion of ^1H NMR Spectrum (400 MHz) of compound **7i** in CDCl_3



Expansion of ^1H NMR Spectrum (400 MHz) of compound **7i** in CDCl_3



^{13}C NMR Spectrum (101 MHz) of compound **7i** in CDCl_3



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **7i** in CDCl_3

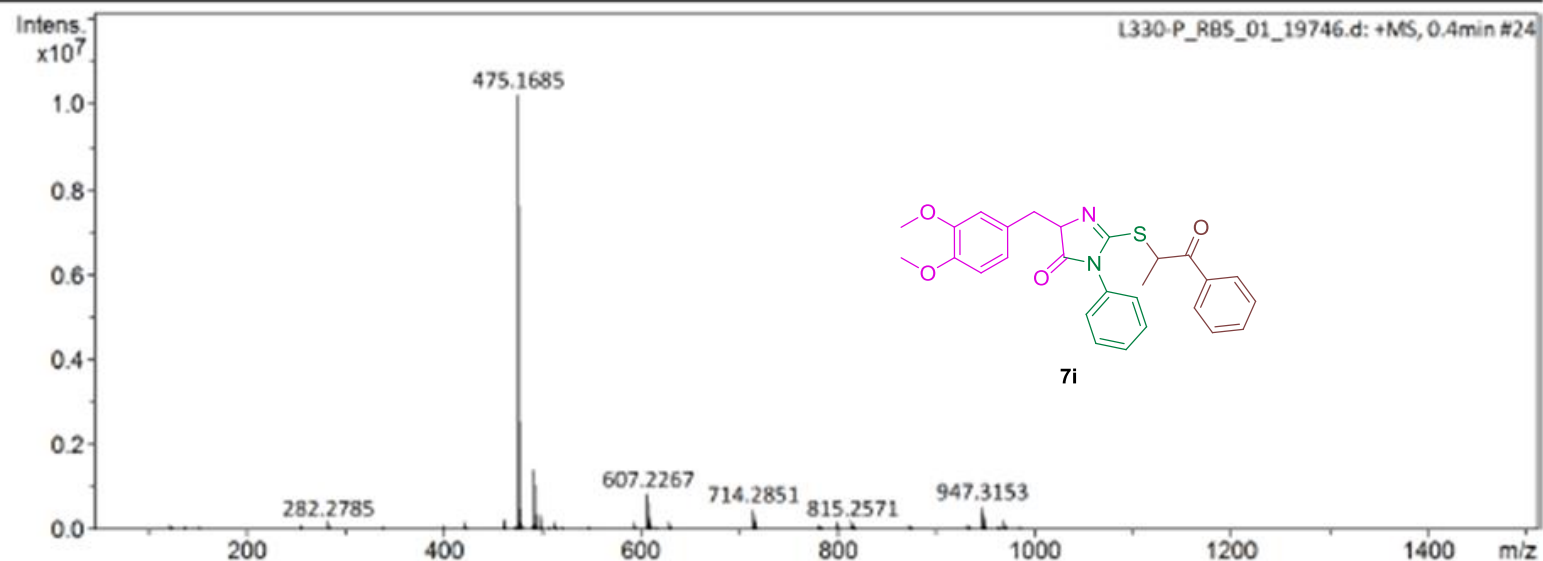
Display Report

Analysis Info

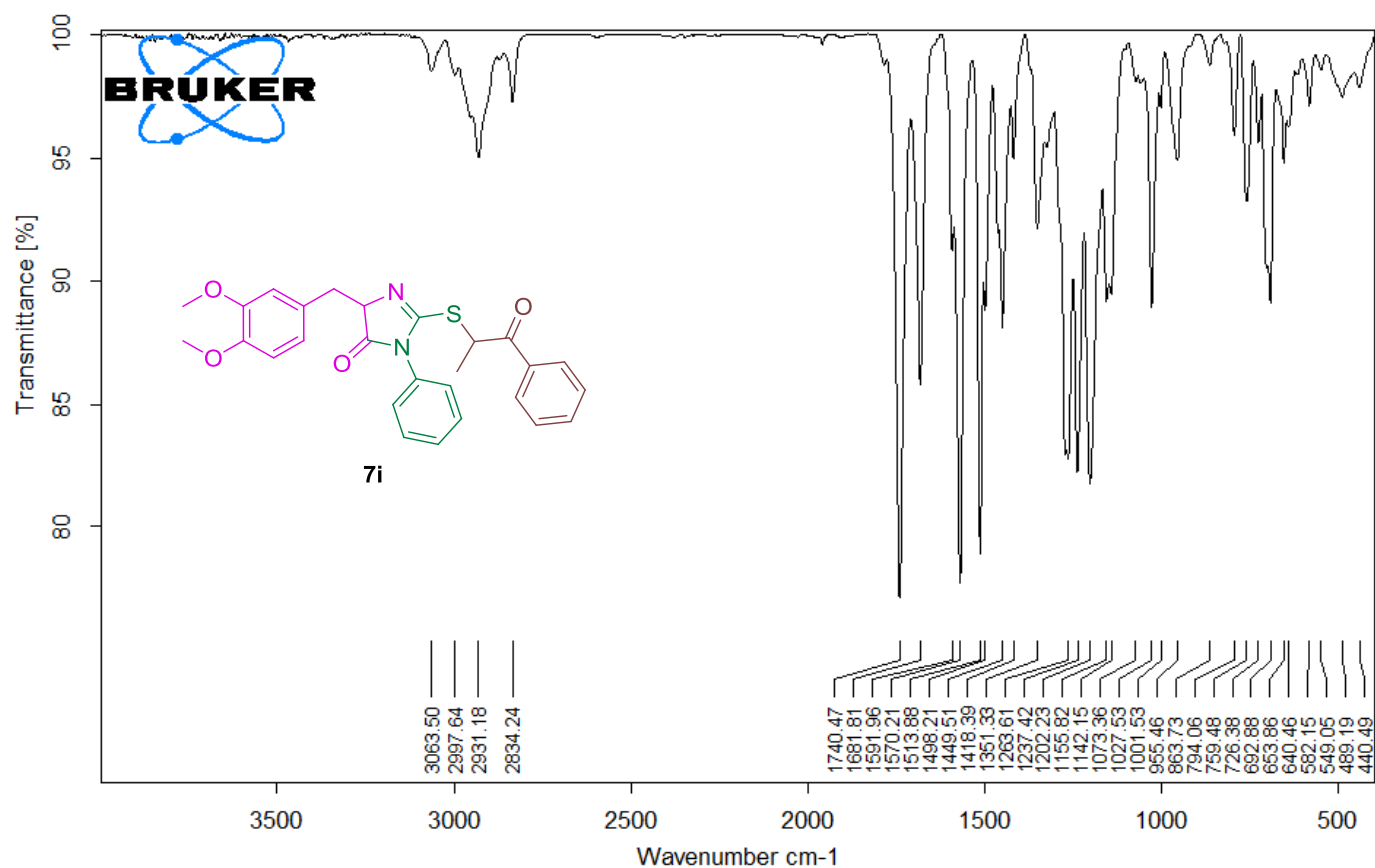
Analysis Name	D:\Data\nctu service\data\2018\20180831\L330-P_RB5_01_19746.d	Acquisition Date	8/30/2018 6:26:26 PM	
Method	Small molecule.m	Operator	NCTU	
Sample Name	L330-P	Instrument	impact HD	1819696.00164
Comment				

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



HRMS of compound 7i



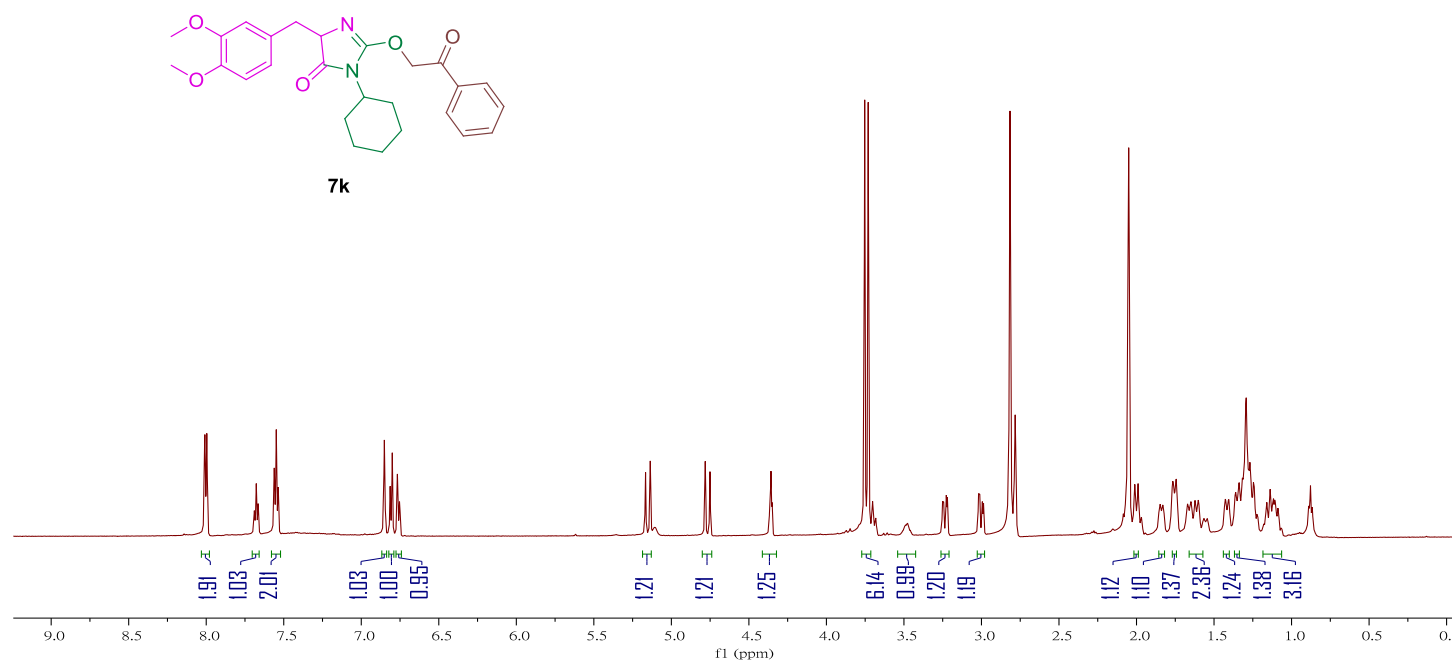
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MIR_TR_DTGS_L330

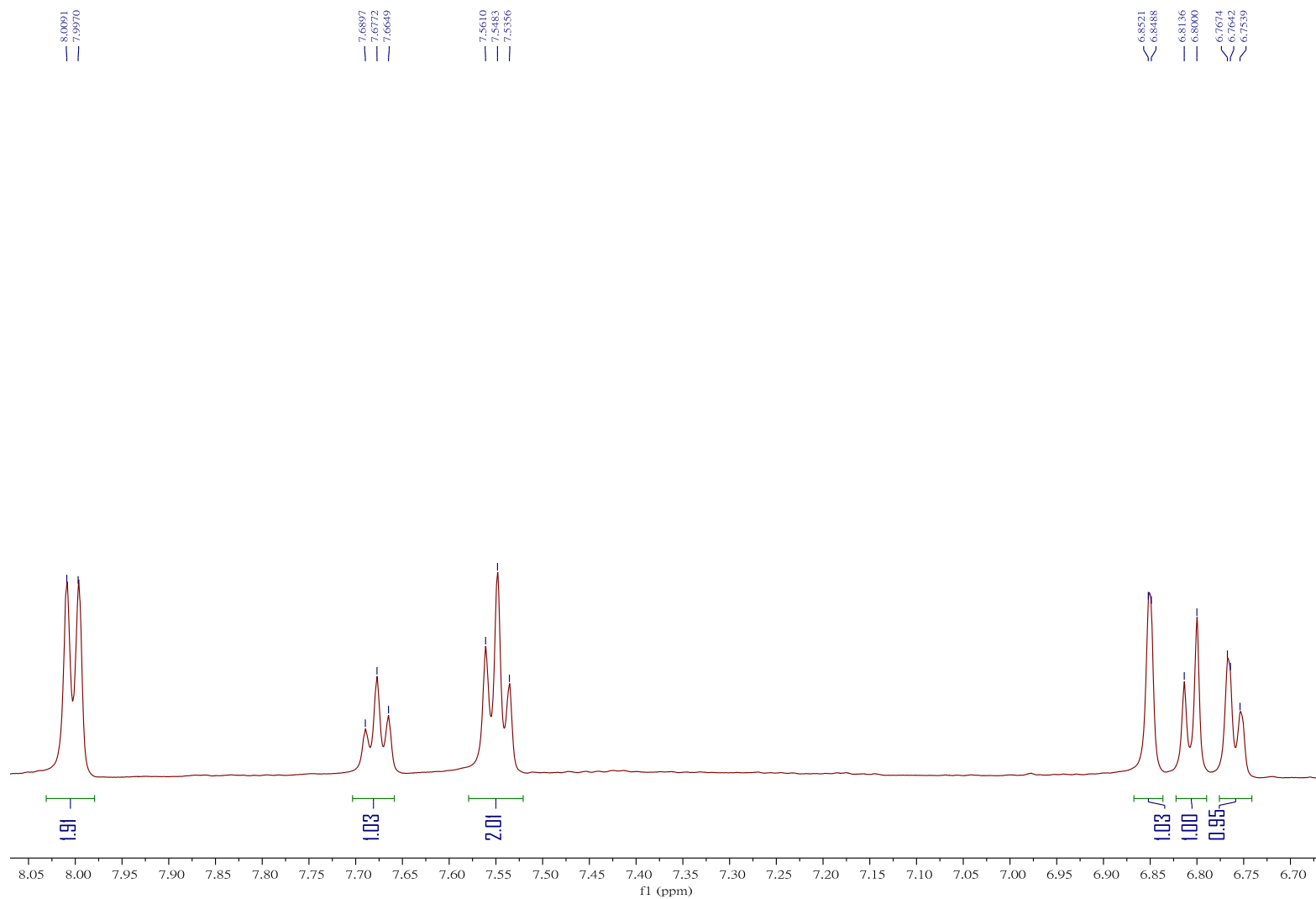
Instrument type and / or accessory

9/4/2018

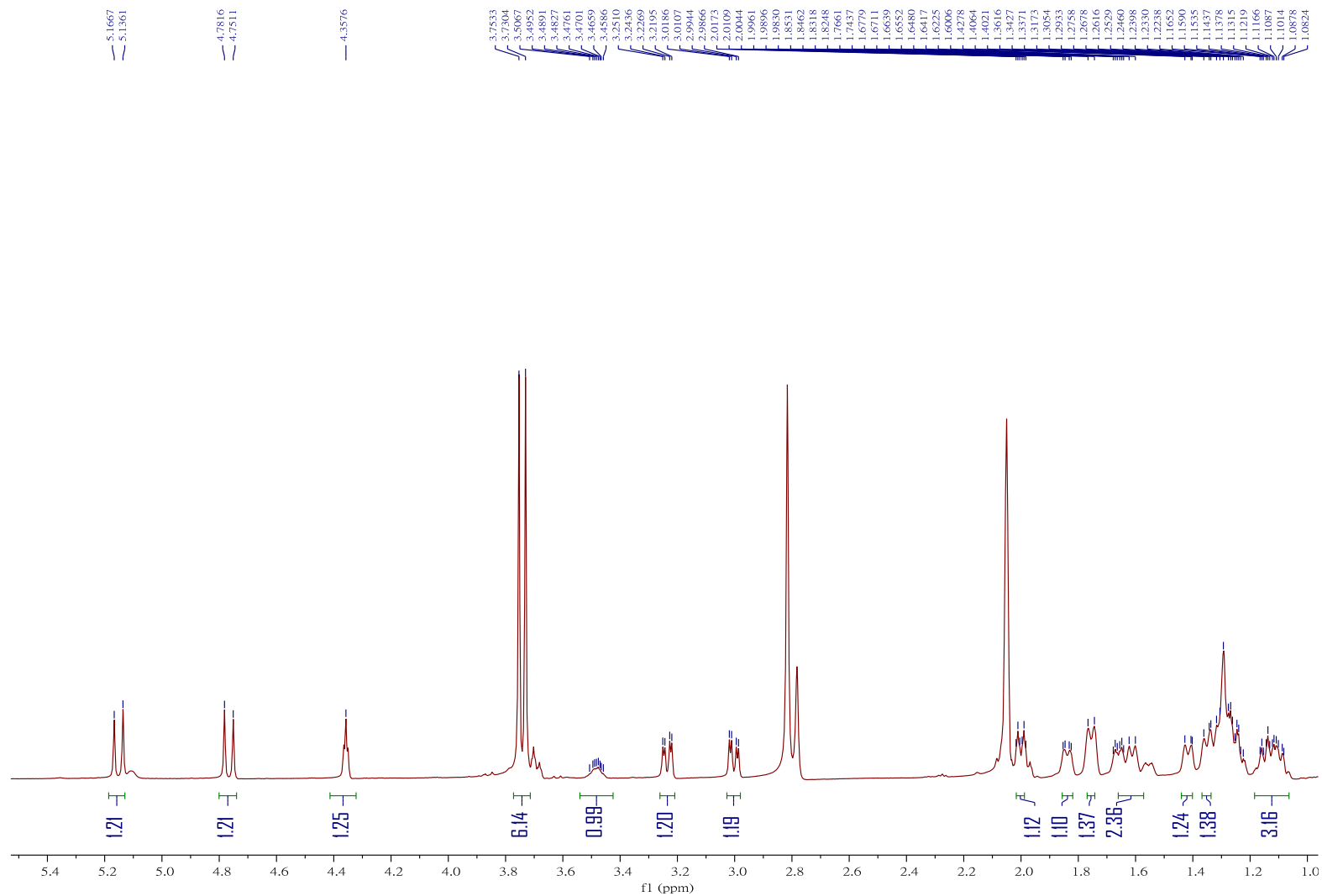
FT-IR Spectrum of compound **7i**



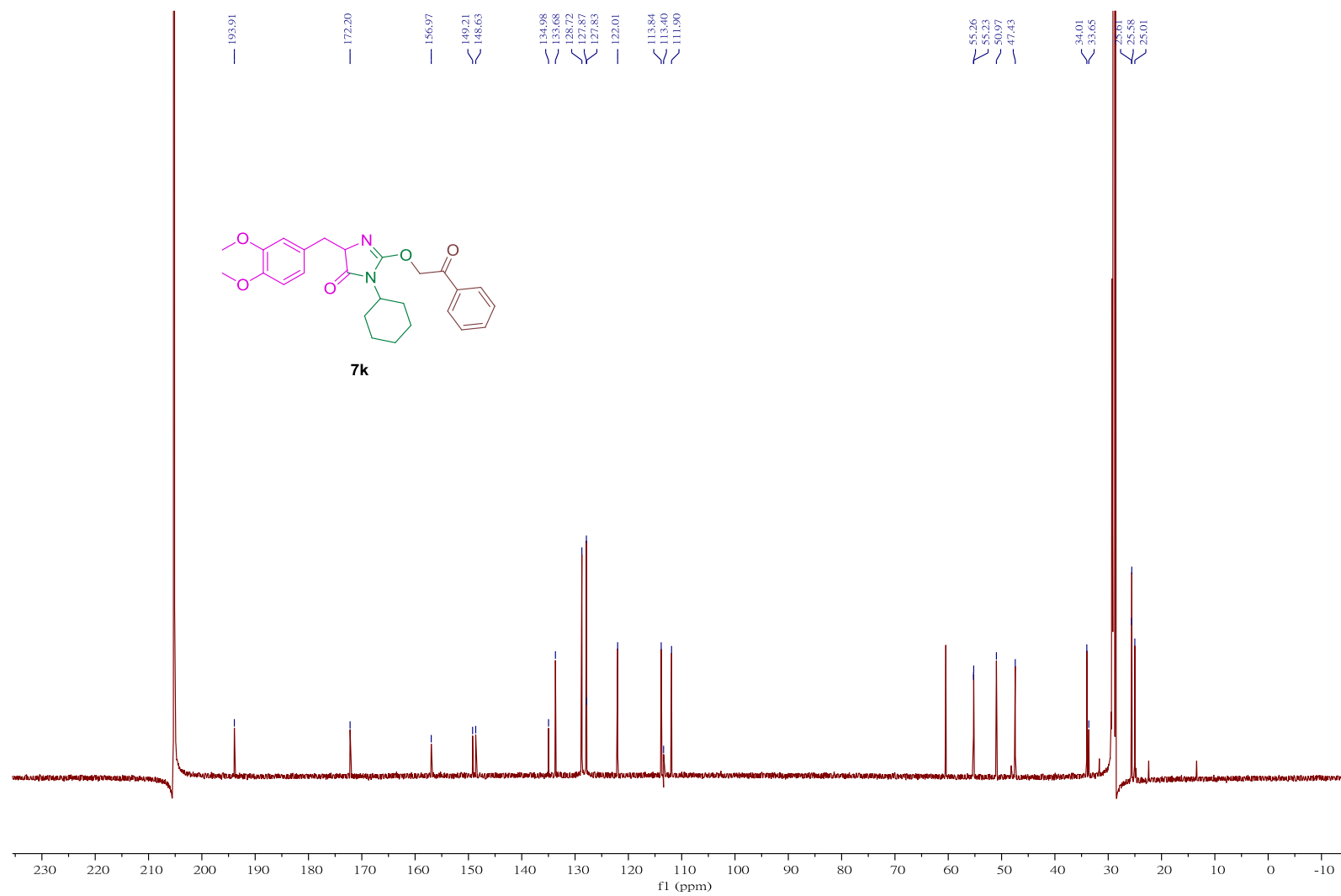
^1H NMR Spectrum (400 MHz) of compound **7k** in acetone- d_6



Expansion of ^1H NMR Spectrum (400 MHz) of compound **7k** in acetone- d_6



Expansion of ^1H NMR Spectrum (400 MHz) of compound **7k** in acetone- d_6

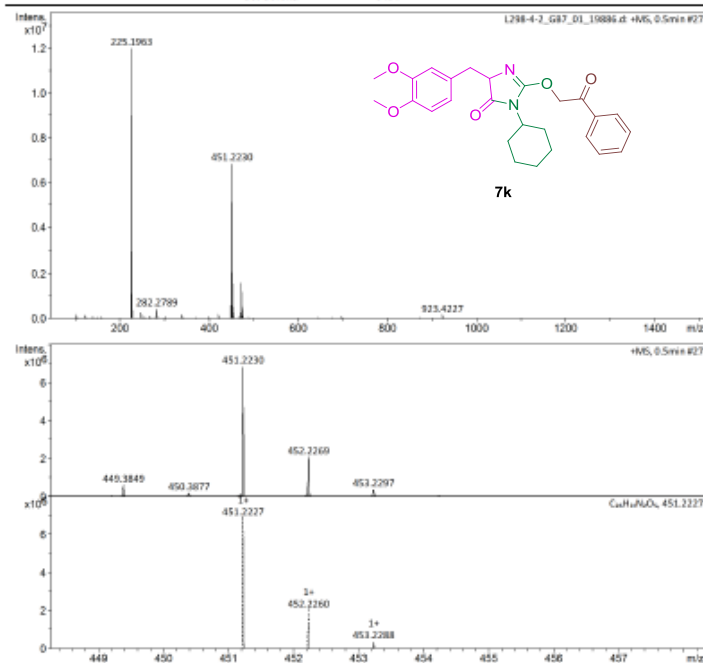


¹³C NMR Spectrum (101 MHz) of compound **7k** in acetone-*d*₆

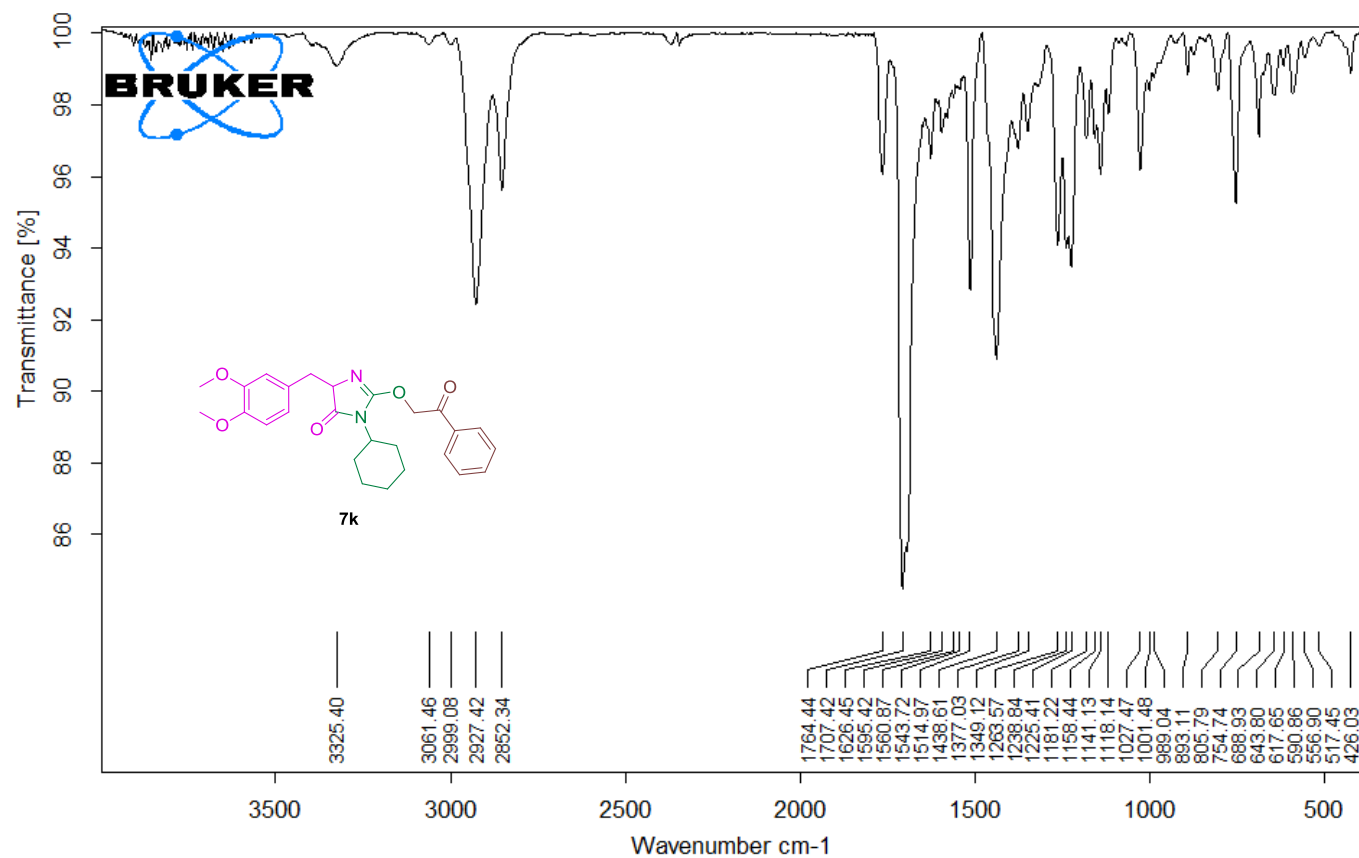
Display Report

Analysis Info		Acquisition Date 9/7/2018 12:19:23 PM	
Analysis Name	D:\Data\NCTU SERVICE\Data\2018\20180907\L298-4-2_GB7_01_19886.d	Operator	NCTU
Method	Small molecule.m	Instrument	Impact HD
Sample Name	L298-4-2		1819696.00164
Comment			

Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
Focus	Active	Set Capillary	4500 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1500 m/z	Set Charging Voltage	2000 V
		Set Corona	0 nA
		Set Nebulizer	1.0 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	6.0 l/min
		Set Divert Valve	Waste
		Set APCI Heater	0 °C



HRMS of compound **7k**



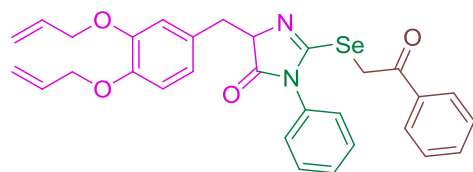
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MIR_TR_DTGS_L298

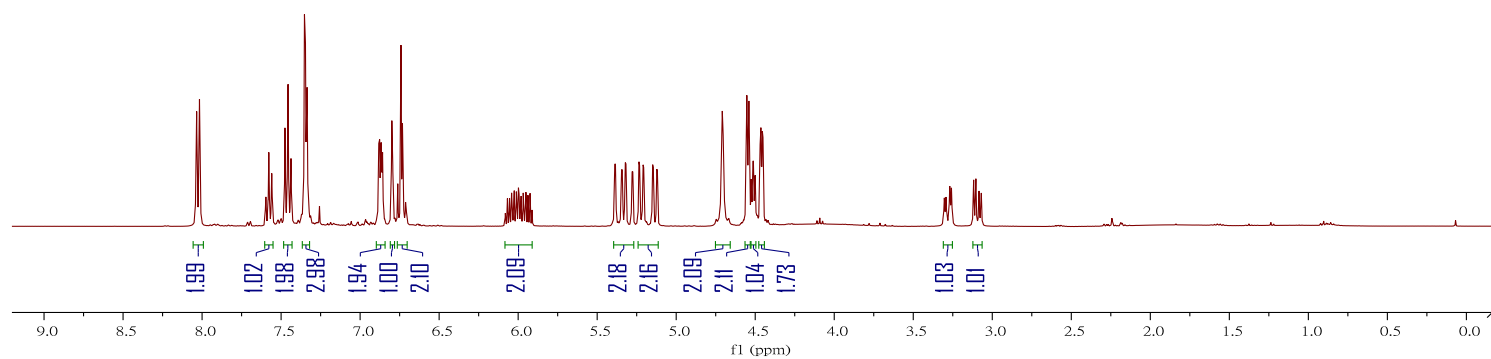
Instrument type and / or accessory

9/4/2018

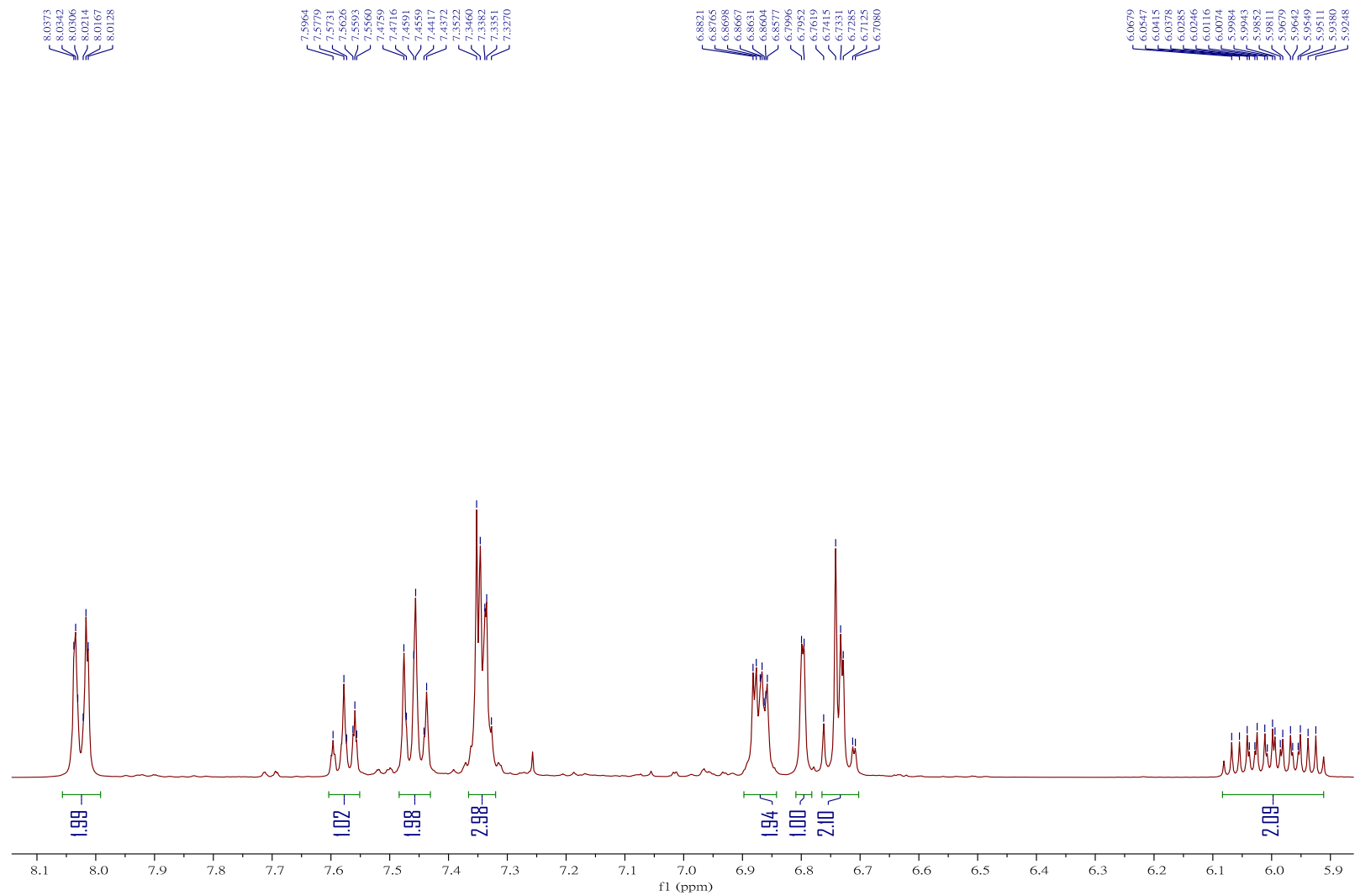
FT-IR Spectrum of compound **7k**



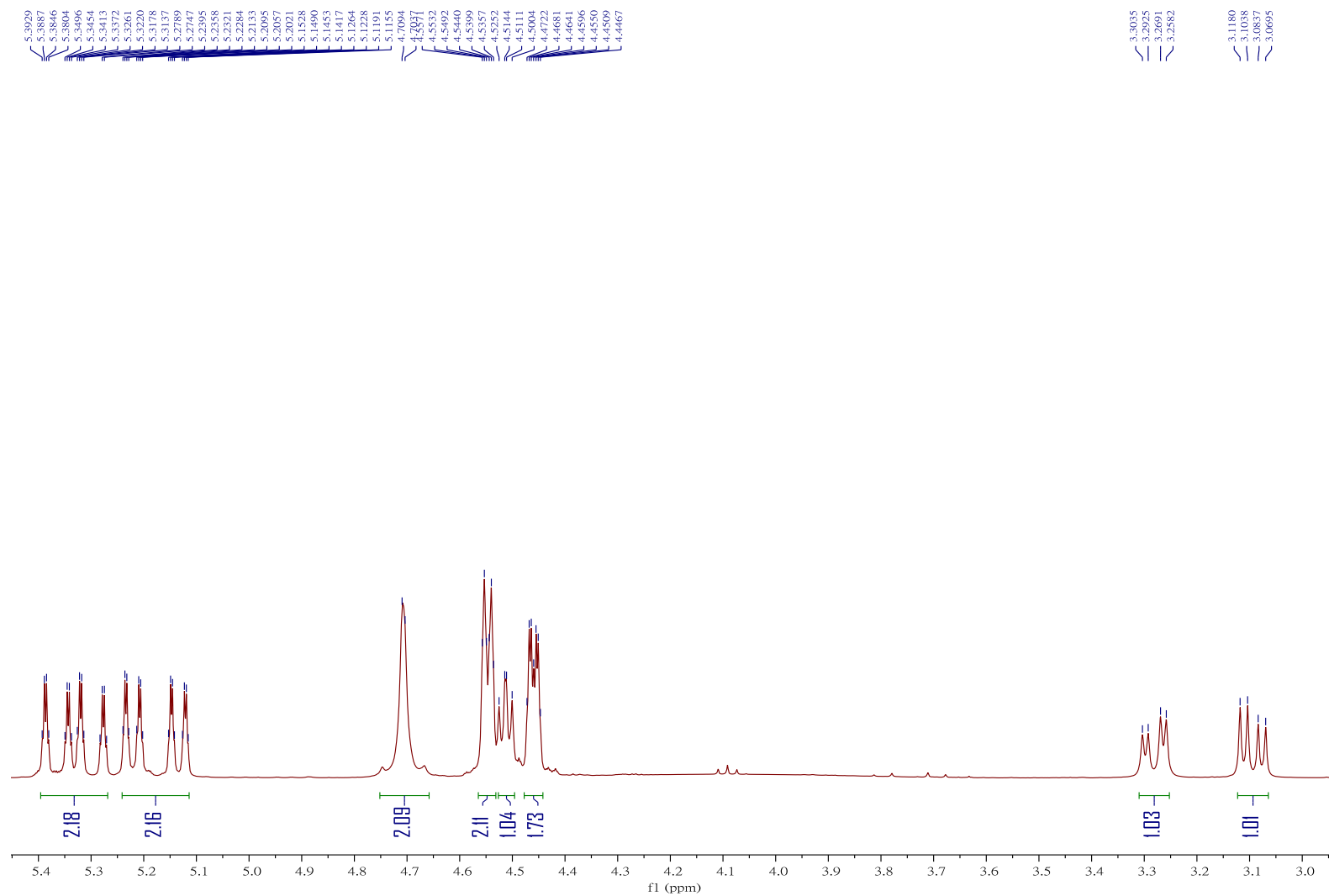
71



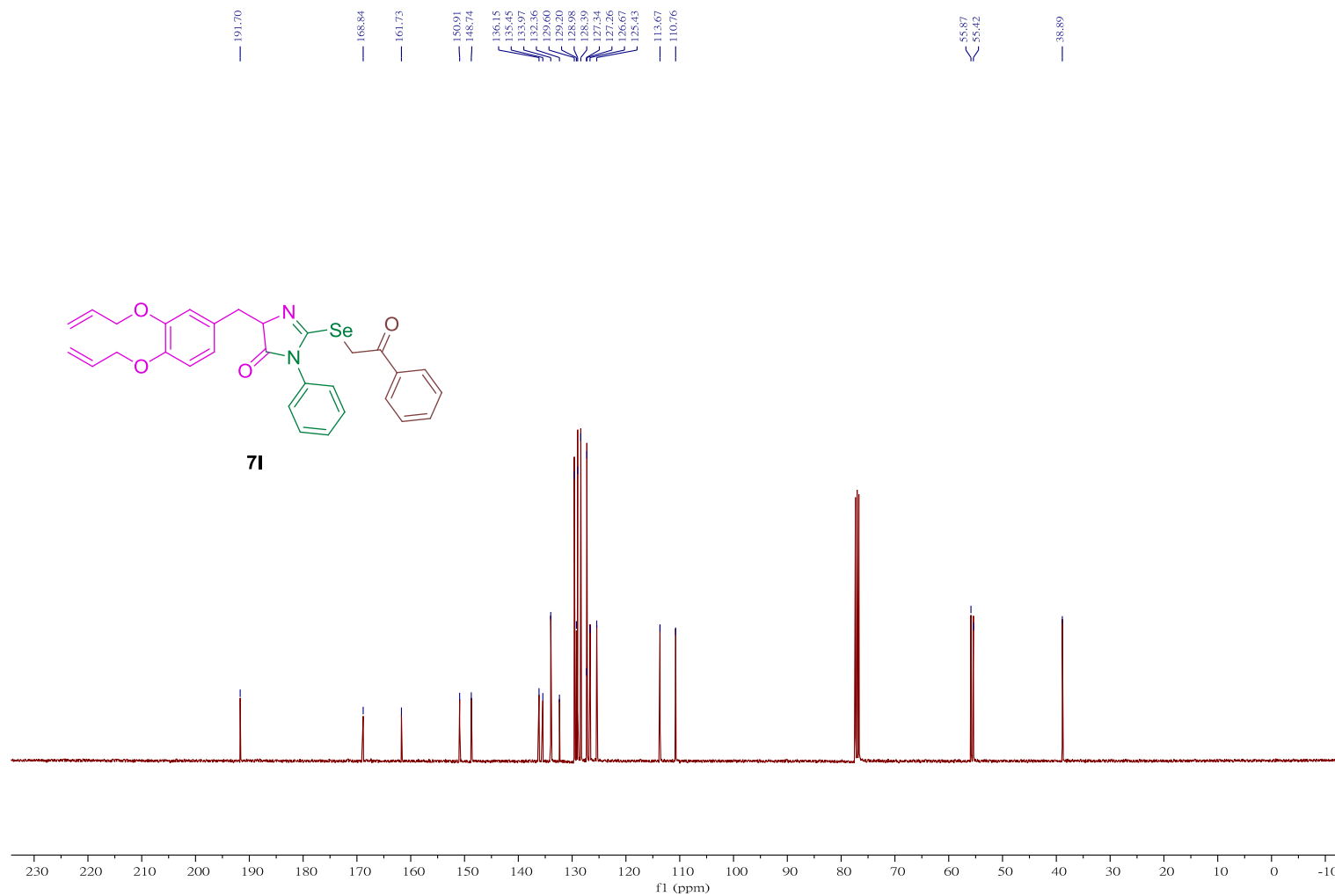
^1H NMR Spectrum (400 MHz) of compound **71** in CDCl_3

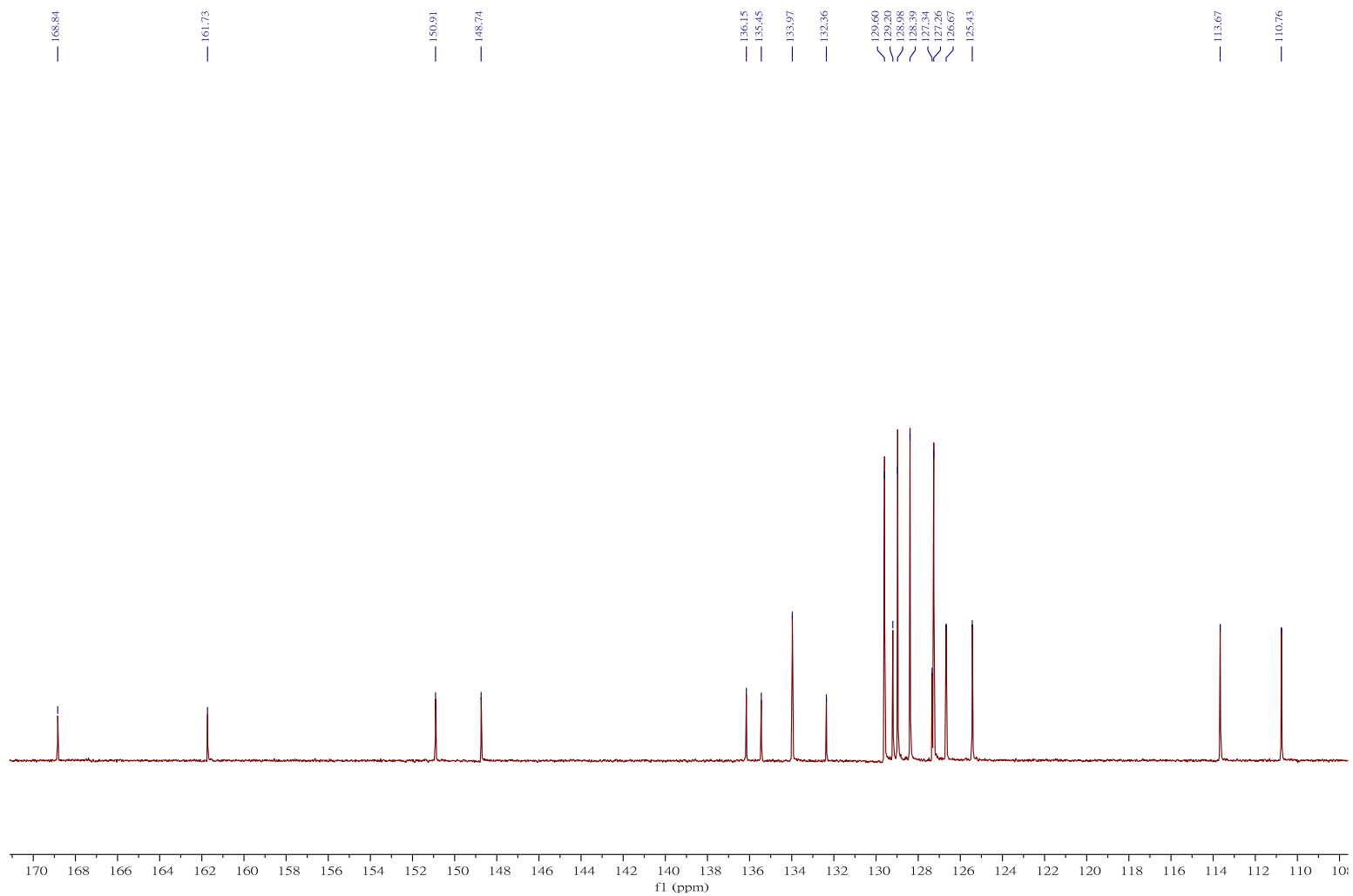


Expansion of ^1H NMR Spectrum (400 MHz) of compound **7I** in CDCl_3



Expansion of ^1H NMR Spectrum (400 MHz) of compound **7I** in CDCl_3





Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **7I** in CDCl_3

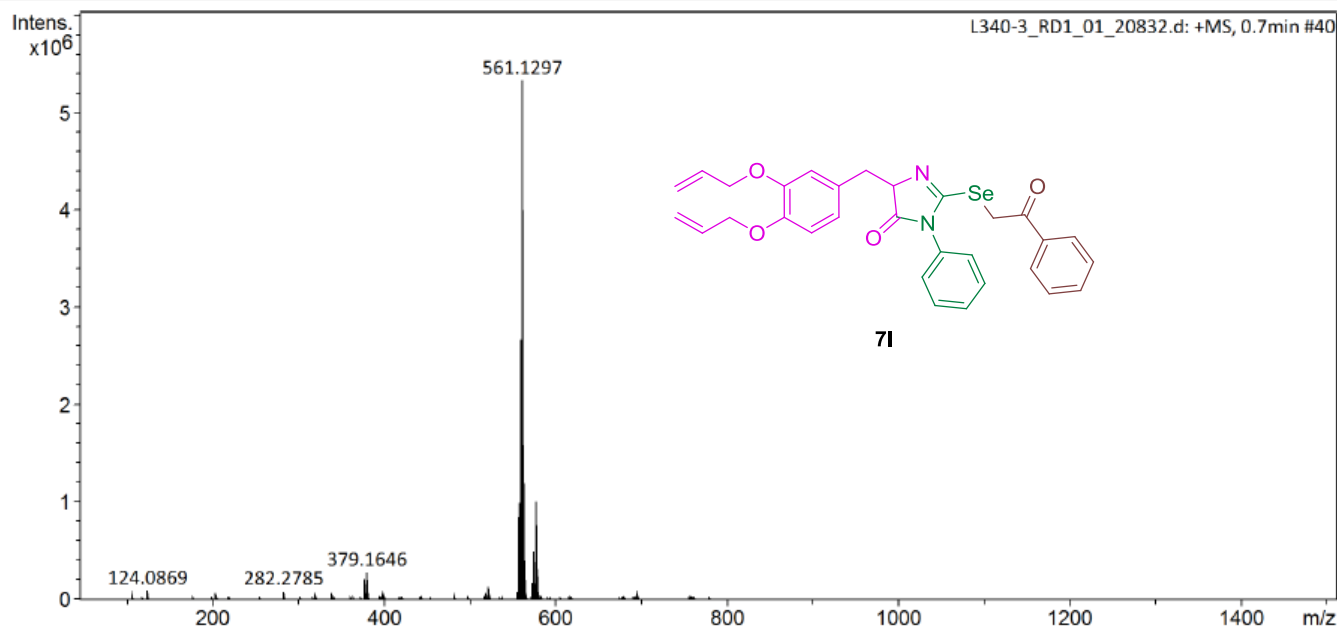
Display Report

Analysis Info

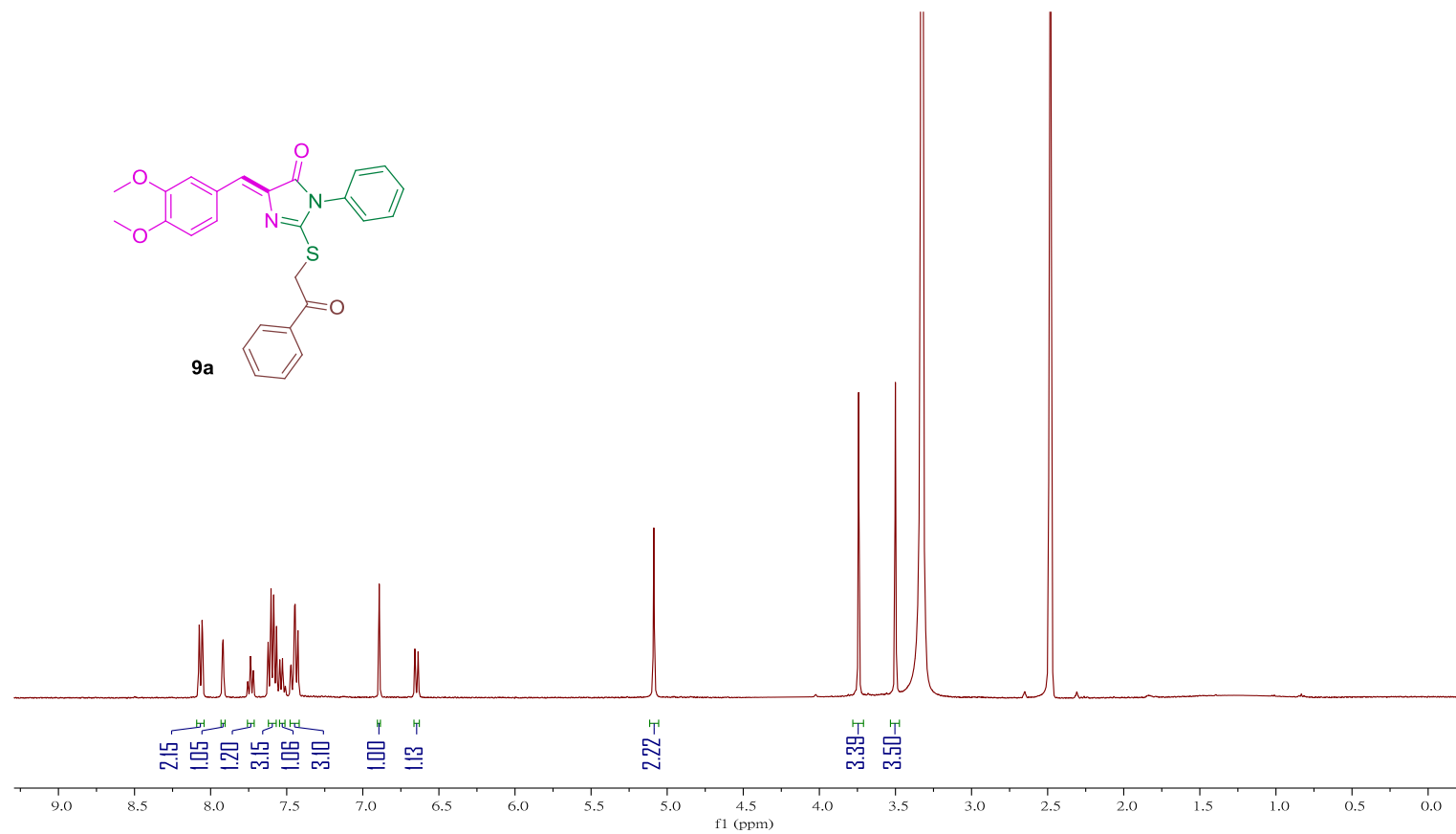
Analysis Name	D:\Data\nctu service\data\2018\20181102\L340-3_RD1_01_20832.d	Acquisition Date	11/2/2018 11:45:18 AM	
Method	Small molecule.m	Operator	NCTU	
Sample Name	L340-3	Instrument	impact HD	1819696.00164
Comment				

Acquisition Parameter

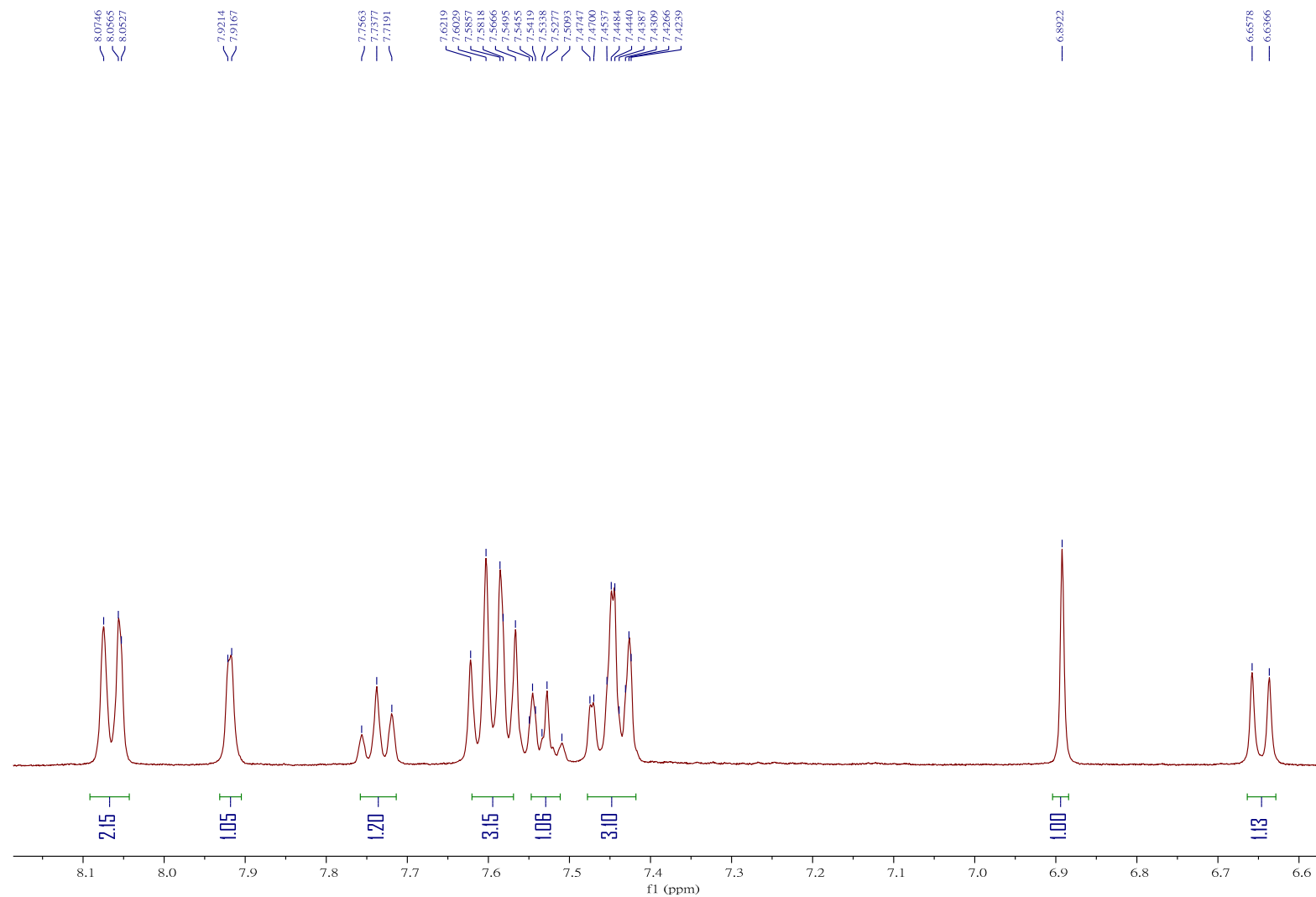
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



HRMS of compound 7I



^1H NMR Spectrum (400 MHz) of compound **9a** in $\text{DMSO}-d_6$



Expansion of ¹H NMR Spectrum (400 MHz) of compound **9a** in DMSO-*d*₆

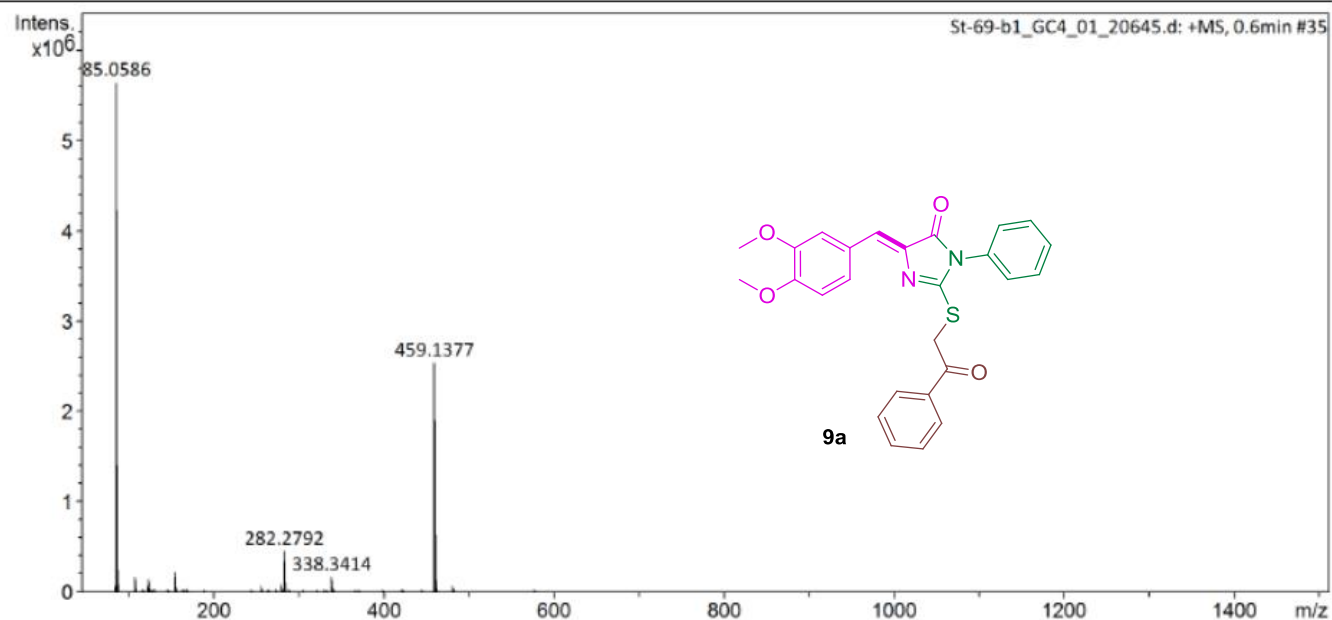
Display Report

Analysis Info

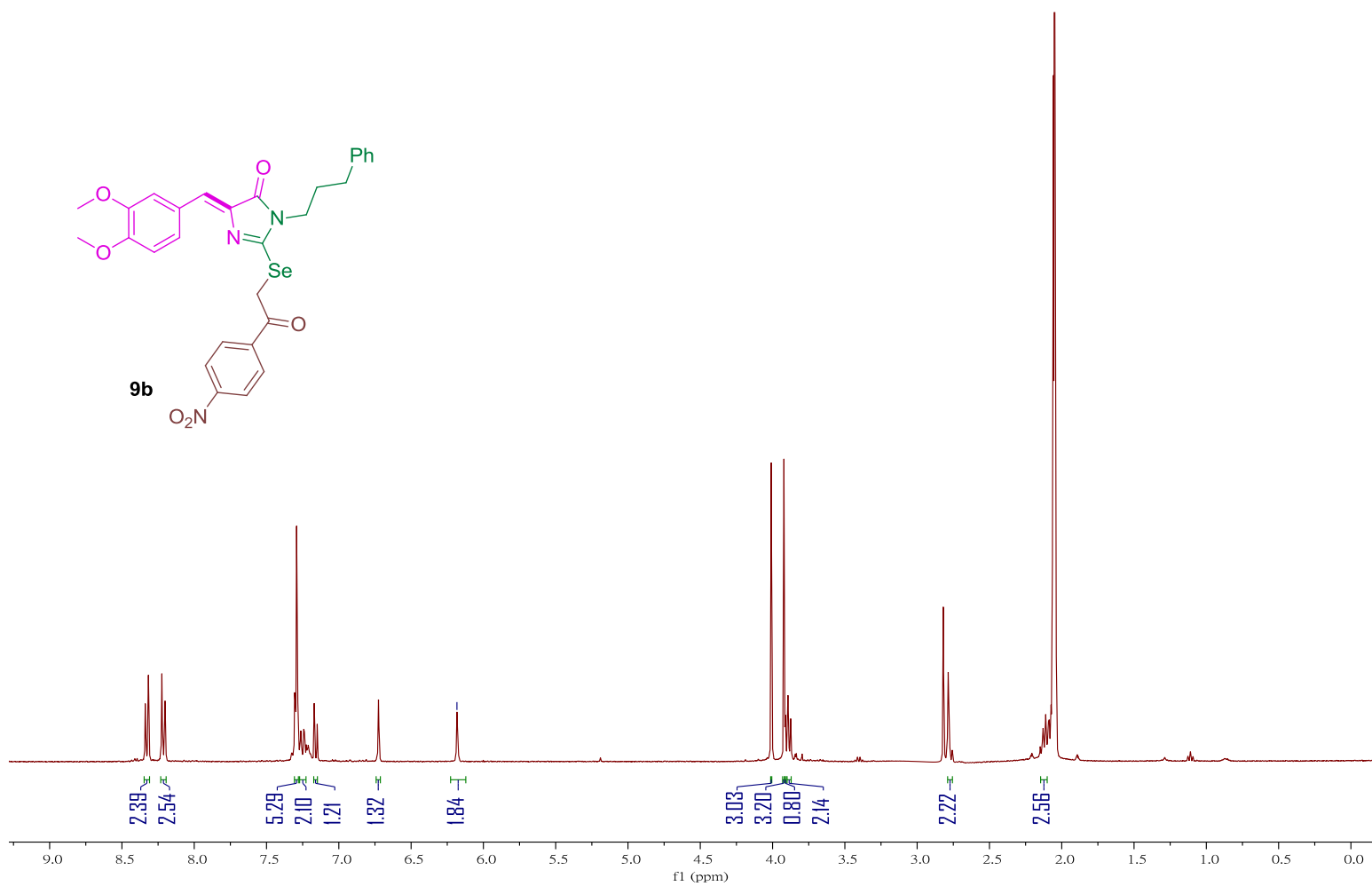
Analysis Name	D:\Data\ncu service\data\2018\20181023\St-69-b1_GC4_01_20645.d	Acquisition Date	10/23/2018 1:50:32 PM	
Method	Small molecule.m	Operator	NCTU	
Sample Name	St-69-b1	Instrument	impact HD	1819696.00164
Comment				

Acquisition Parameter

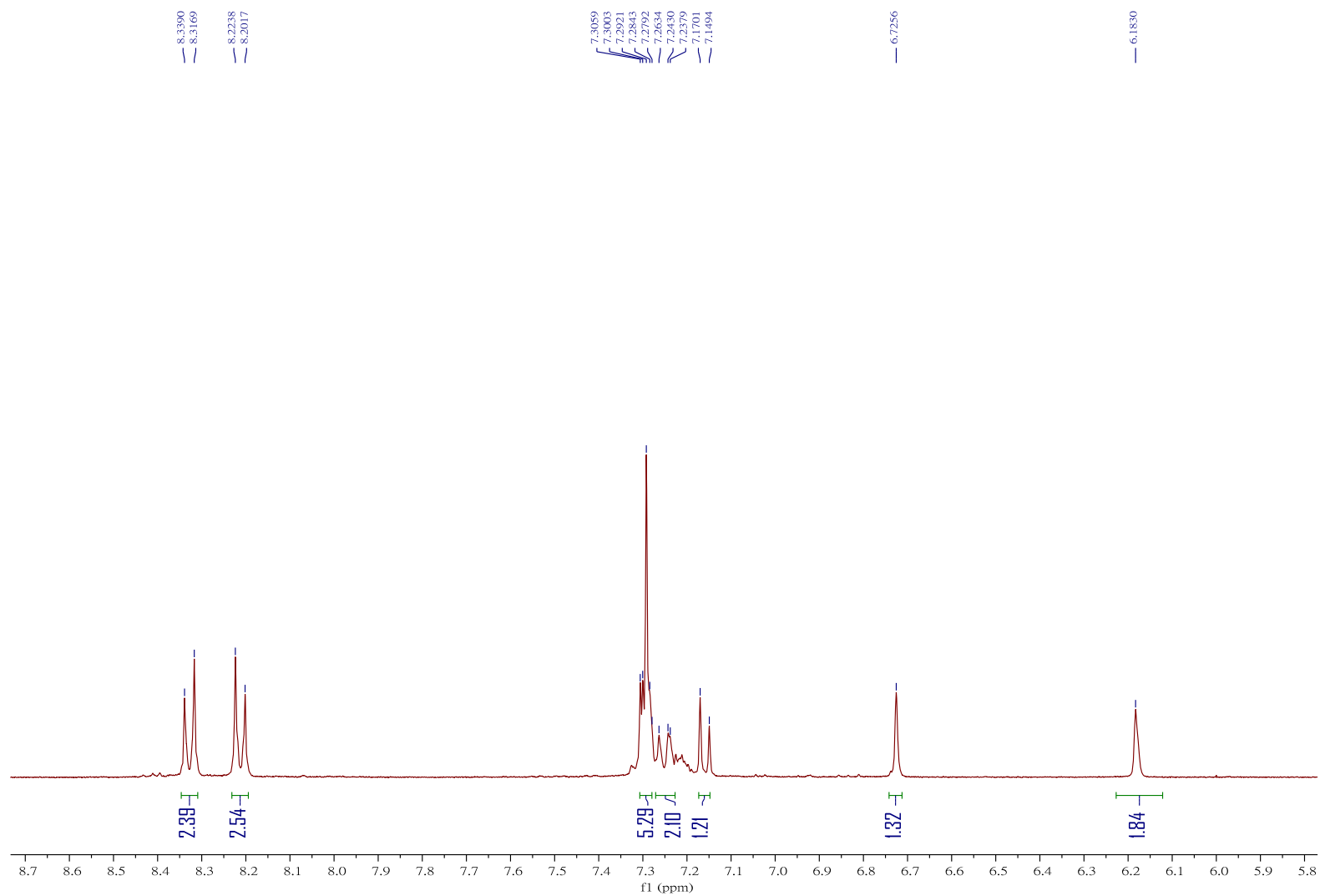
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



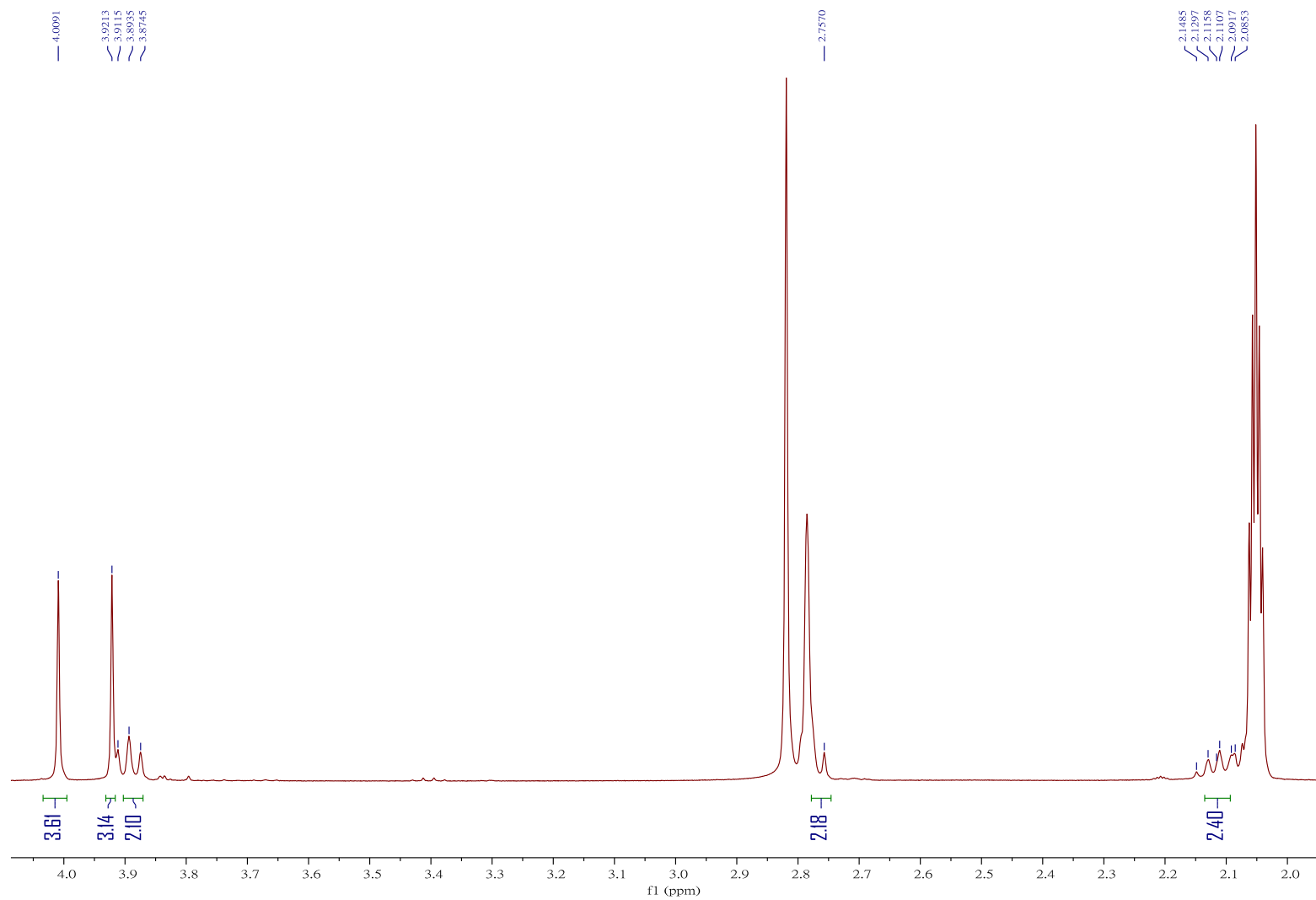
High resolution mass (ESI)⁺ spectrum of compound **9a**



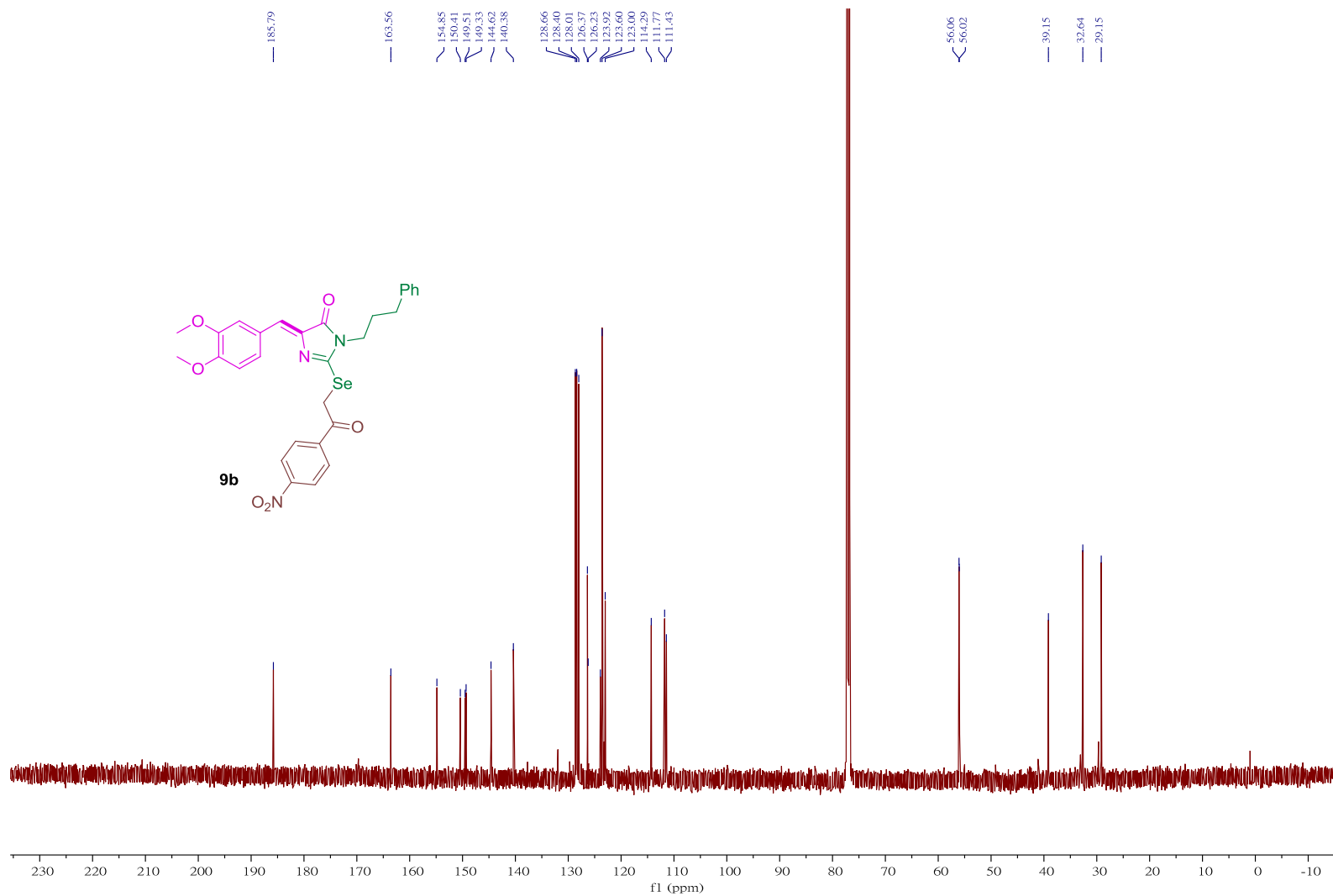
¹H NMR Spectrum (400 MHz) of compound **9b** in acetone-*d*₆

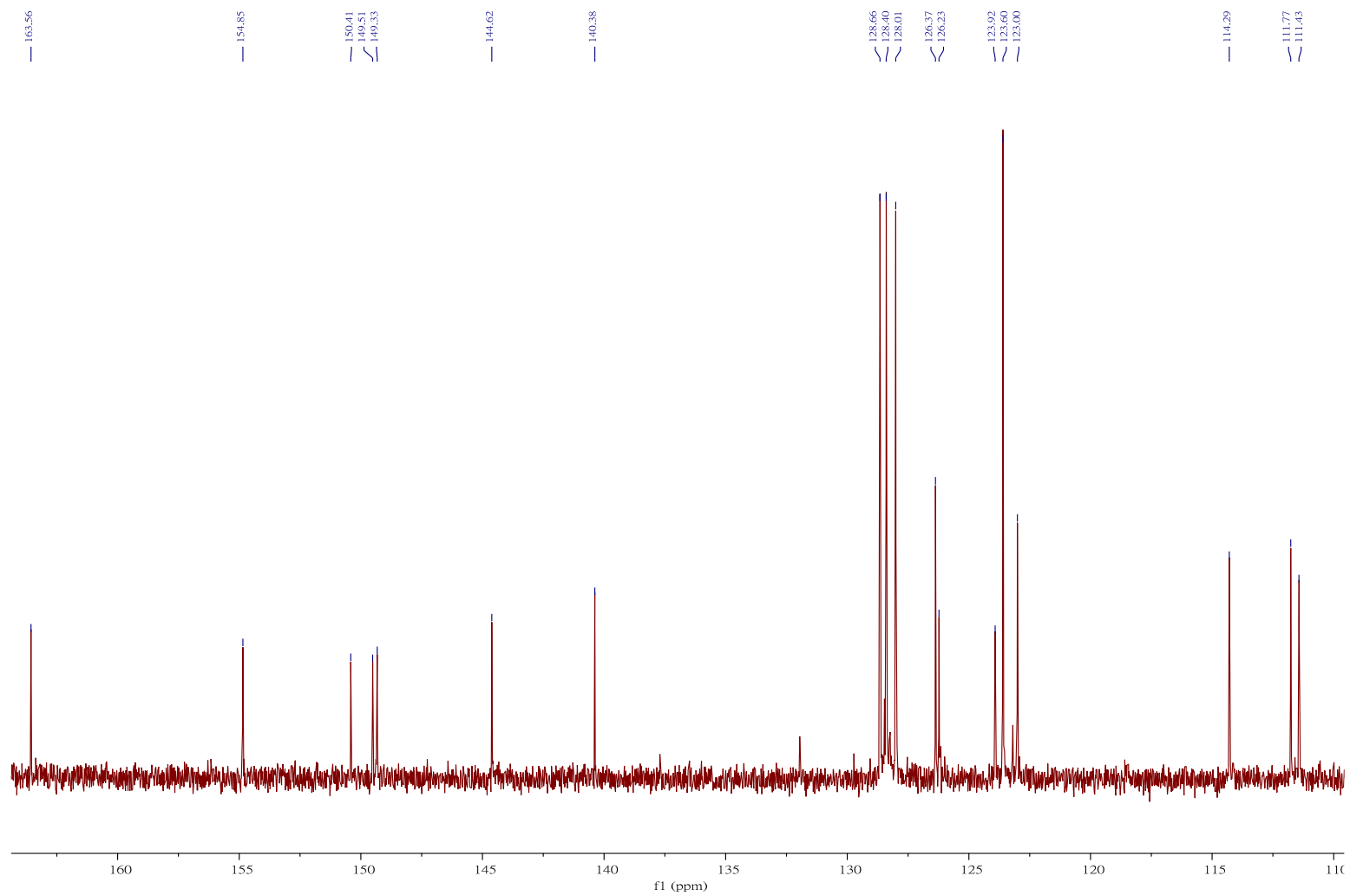


Expansion of ¹H NMR Spectrum (400 MHz) of compound **9b** in acetone-*d*₆

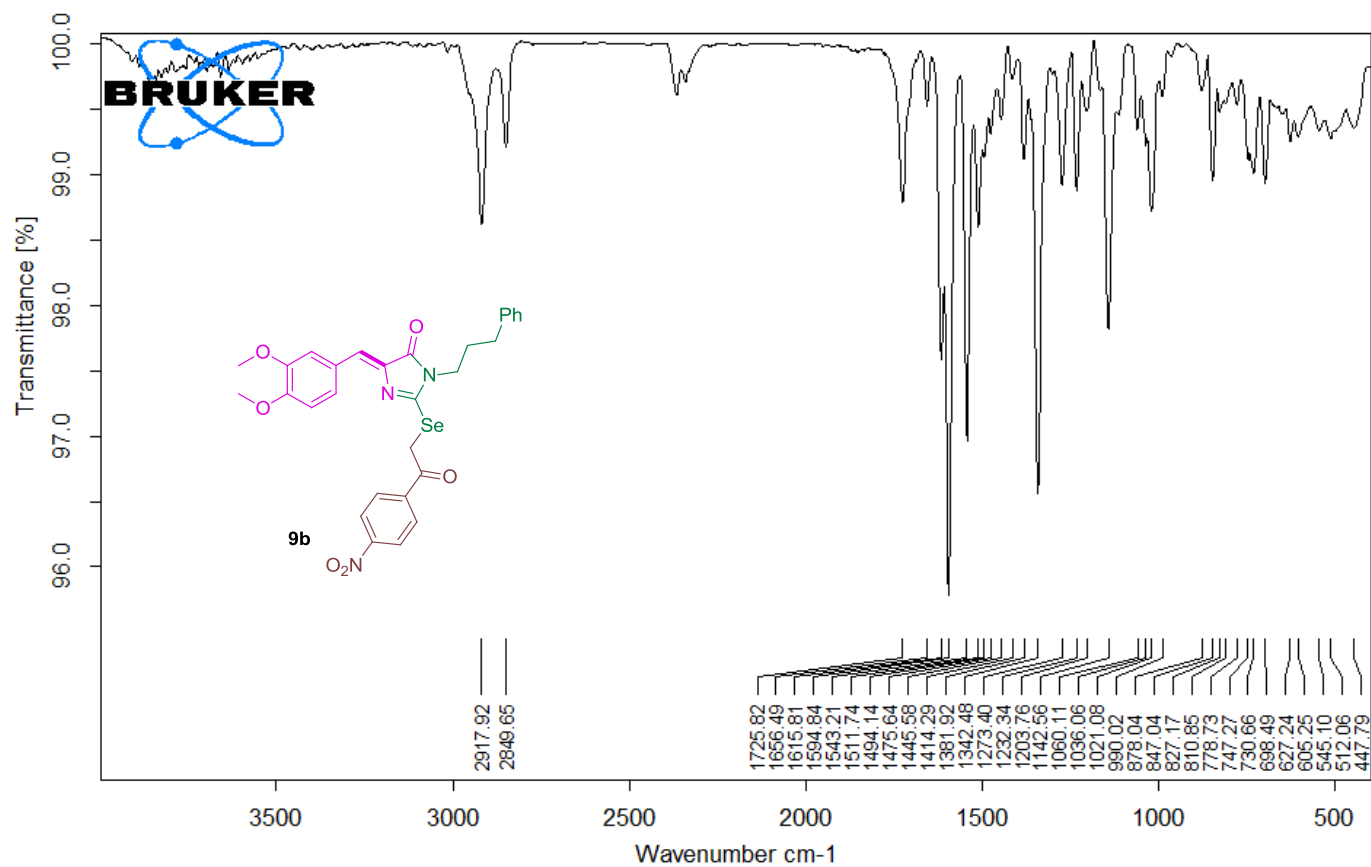


Expansion of ¹H NMR Spectrum (400 MHz) of compound **9b** in acetone-*d*₆



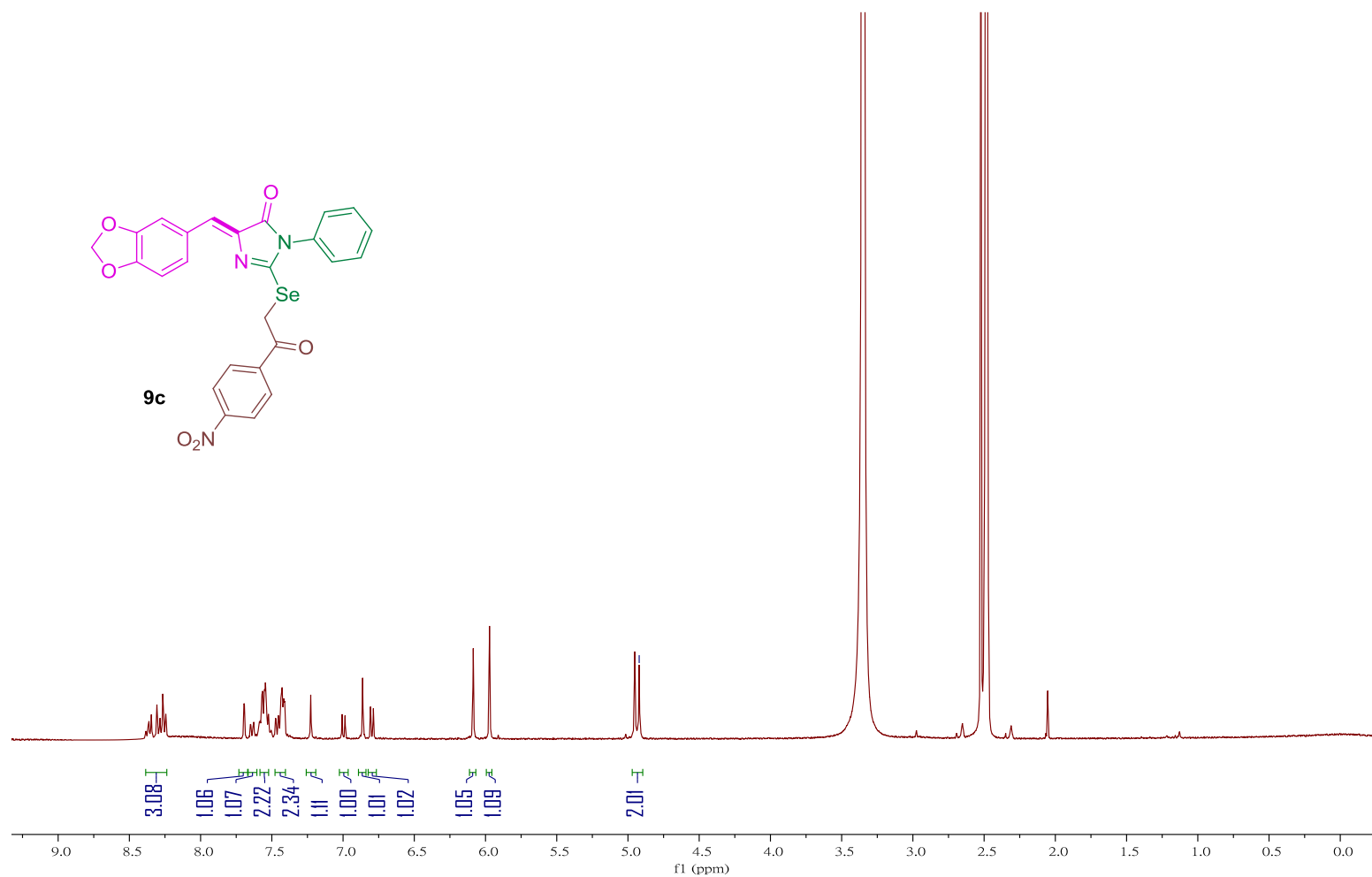


Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **9b** in CDCl_3

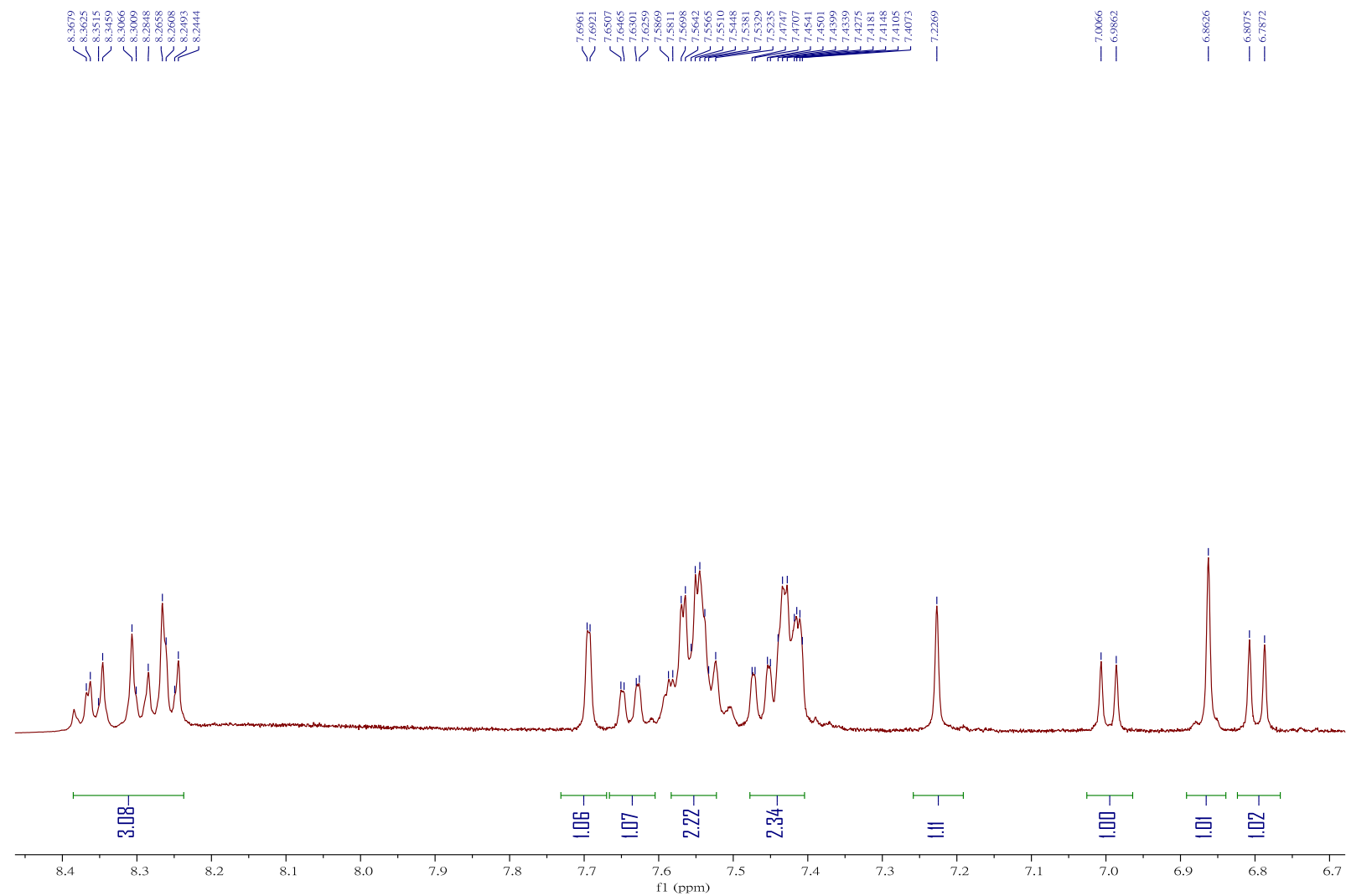


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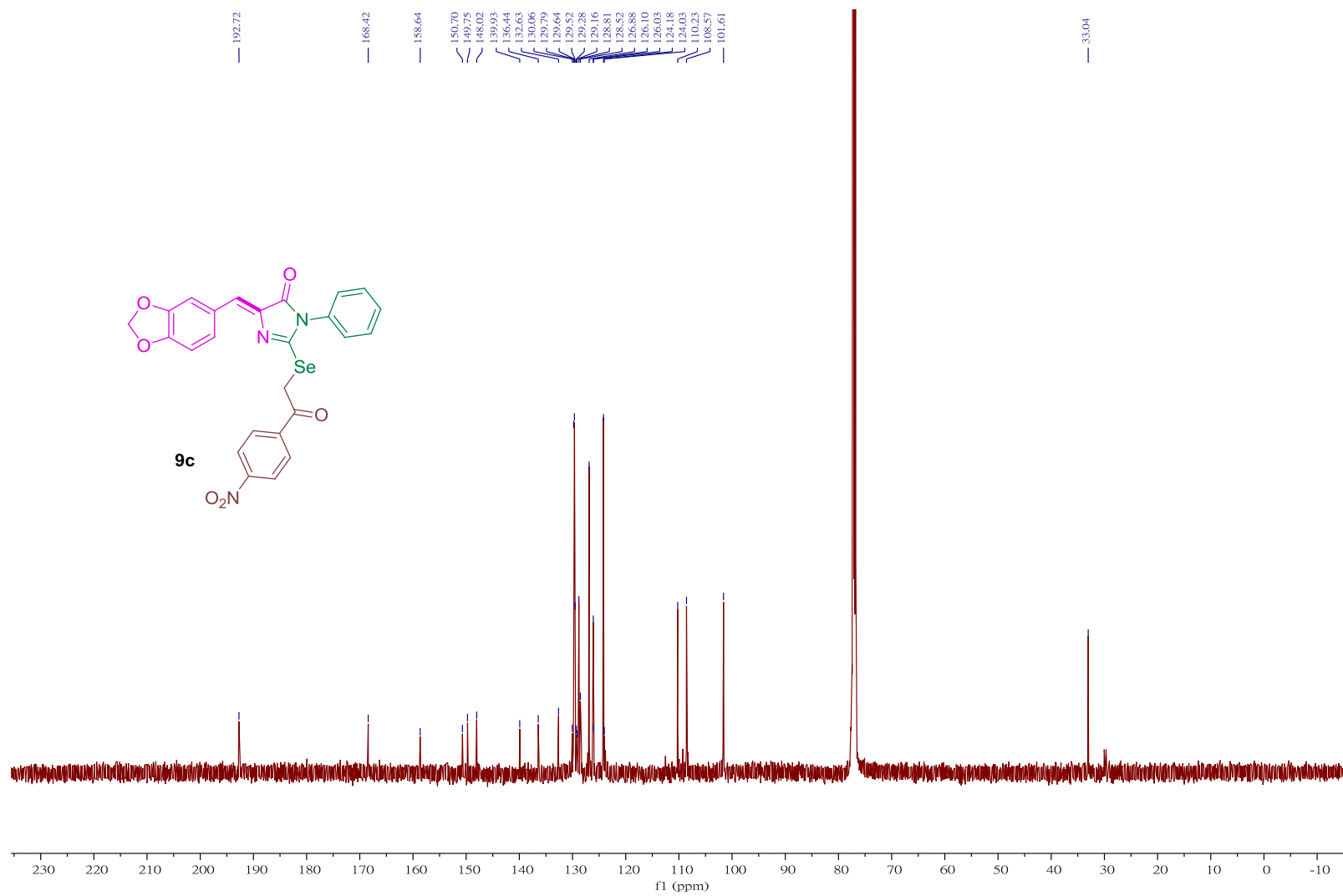
FT-IR Spectrum of compound **9b**



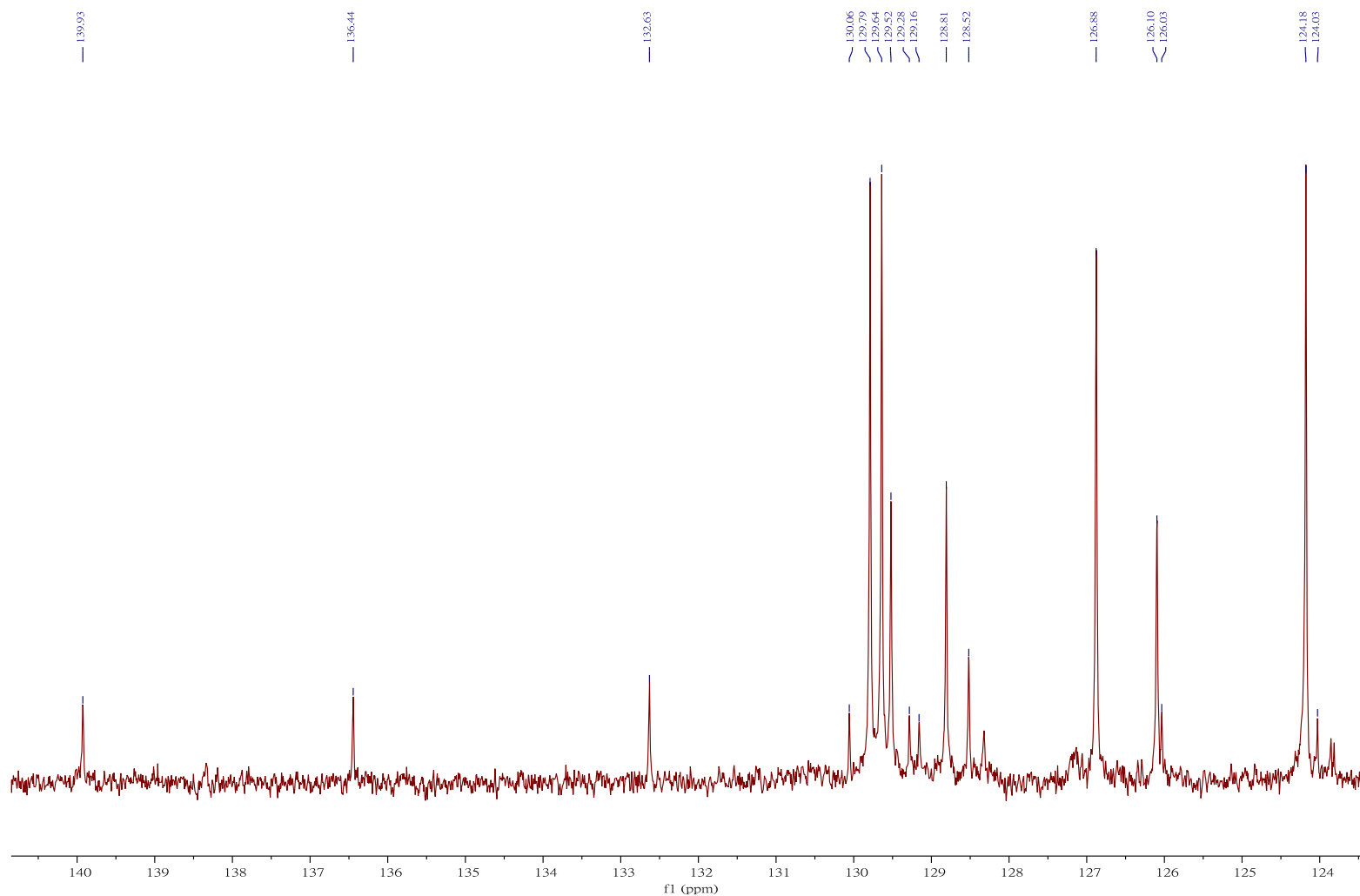
^1H NMR Spectrum (400 MHz) of compound **9c** in $\text{DMSO}-d_6$



Expansion of ^1H NMR Spectrum (400 MHz) of compound **9c** in $\text{DMSO-}d_6$



^{13}C NMR Spectrum (101 MHz) of compound **9c** in CDCl_3



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **9c** in CDCl_3

Display Report

Analysis Info

Analysis Name D:\Data\nctu service\data\2018\20180420\L252_RE1_01_18036.d

Method Small molecule.m

Sample Name L252

Comment

Acquisition Date 4/20/2018 12:41:08 PM

Operator NCTU

Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type

ESI

Ion Polarity

Positive

Set Nebulizer

1.0 Bar

Focus

Active

Set Capillary

4500 V

Set Dry Heater

200 °C

Scan Begin

50 m/z

Set End Plate Offset

-500 V

Set Dry Gas

6.0 l/min

Scan End

1500 m/z

Set Charging Voltage

2000 V

Set Divert Valve

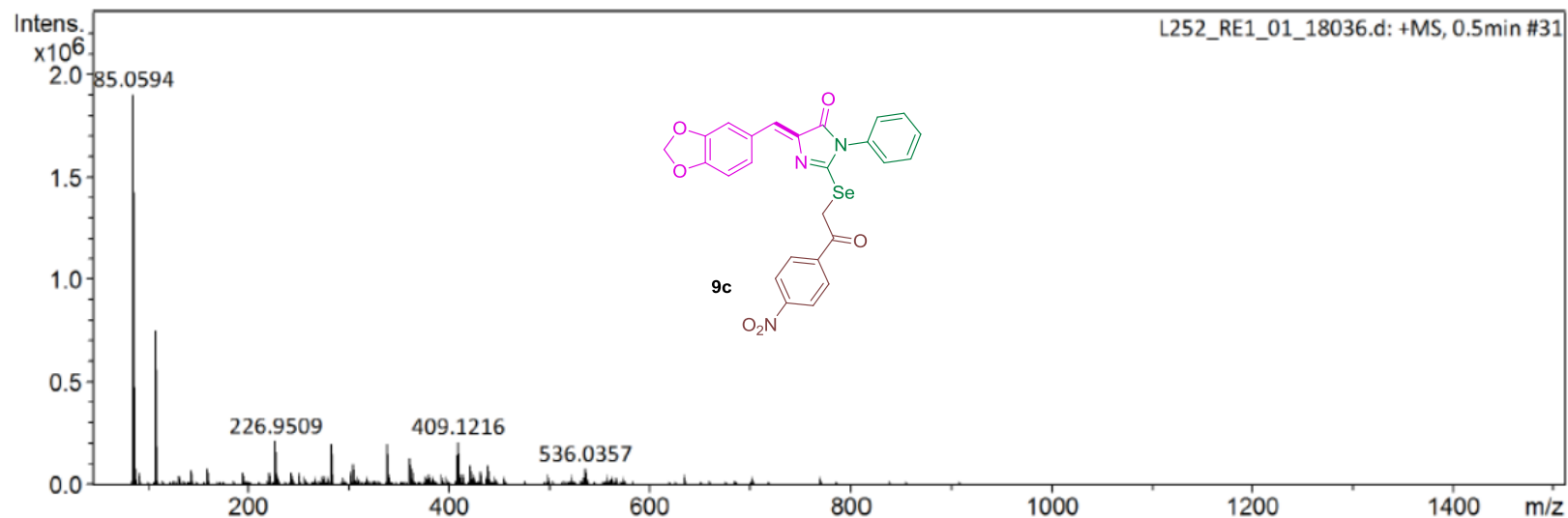
Waste

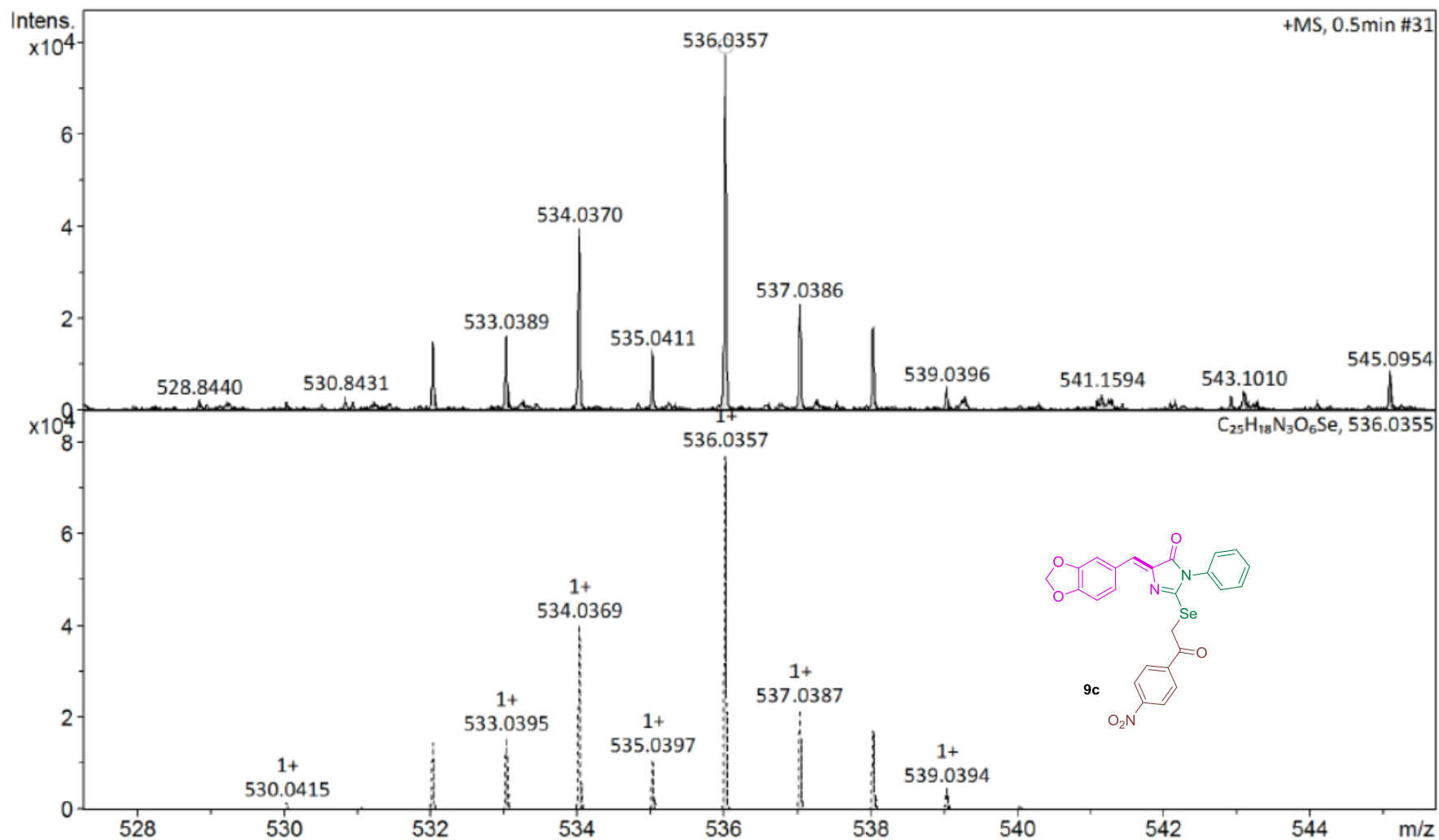
Set Corona

0 nA

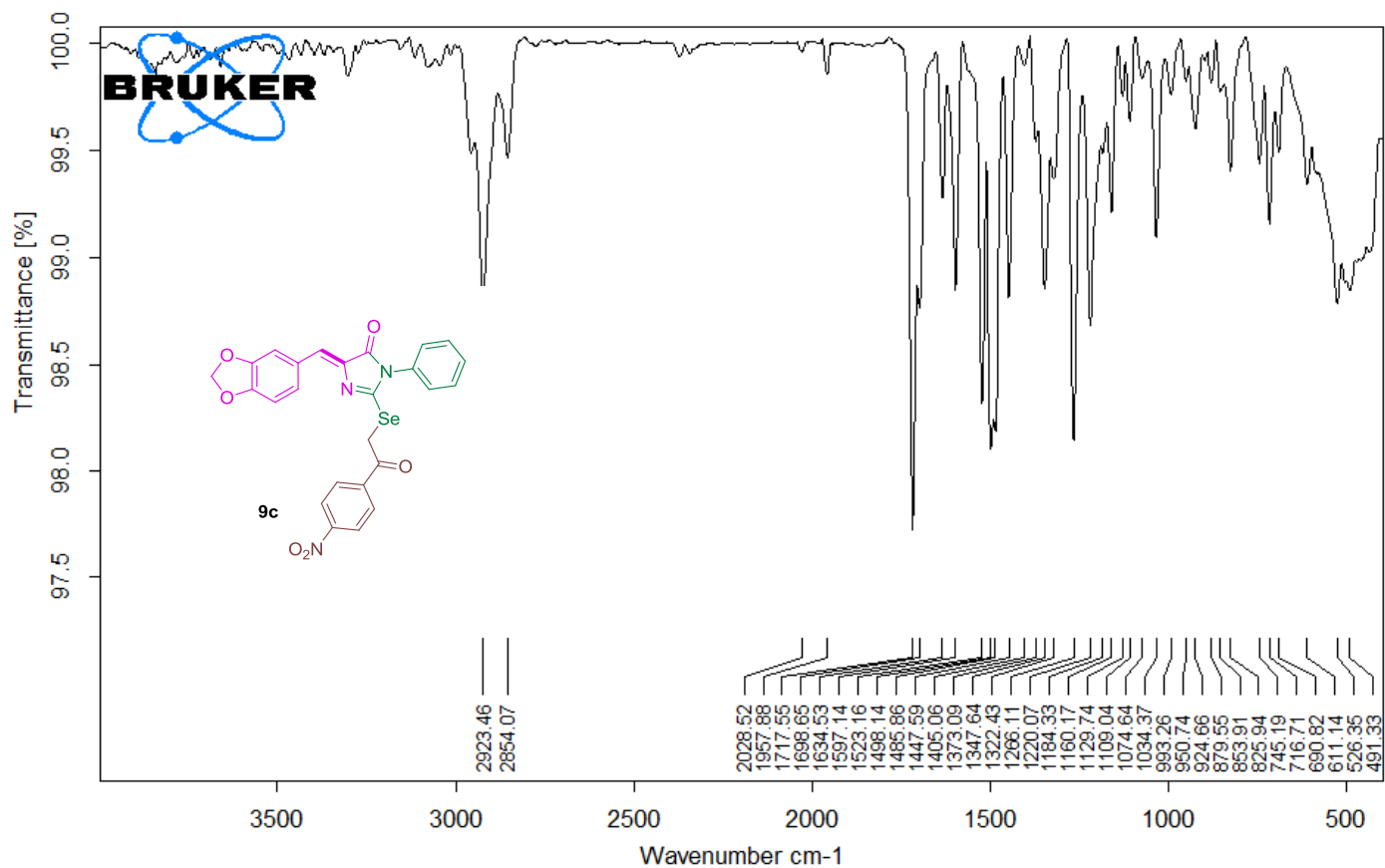
Set APCI Heater

0 °C





High resolution mass (ESI)⁺ spectrum of compound **9c**



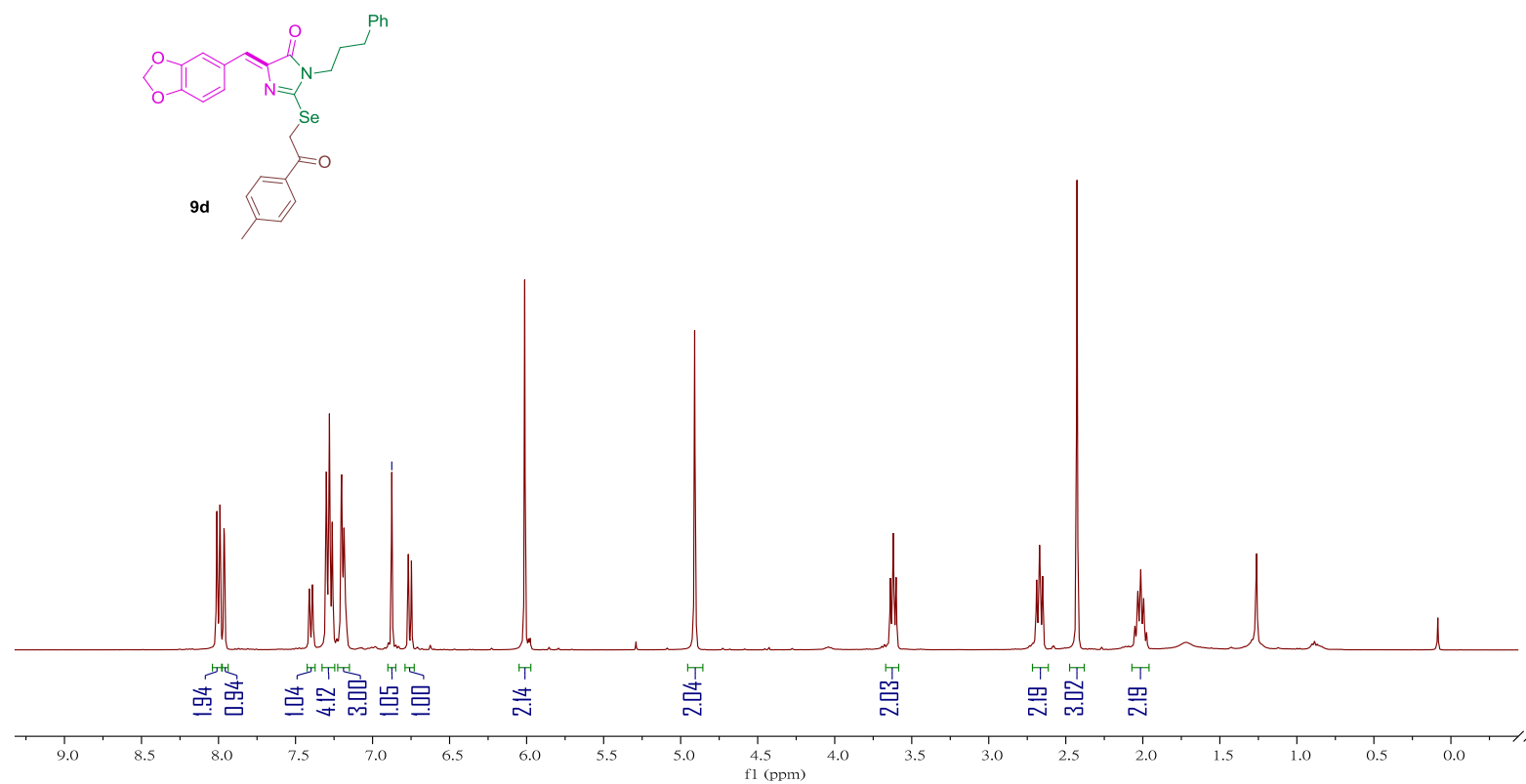
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MIR_TR_DTGS_L252

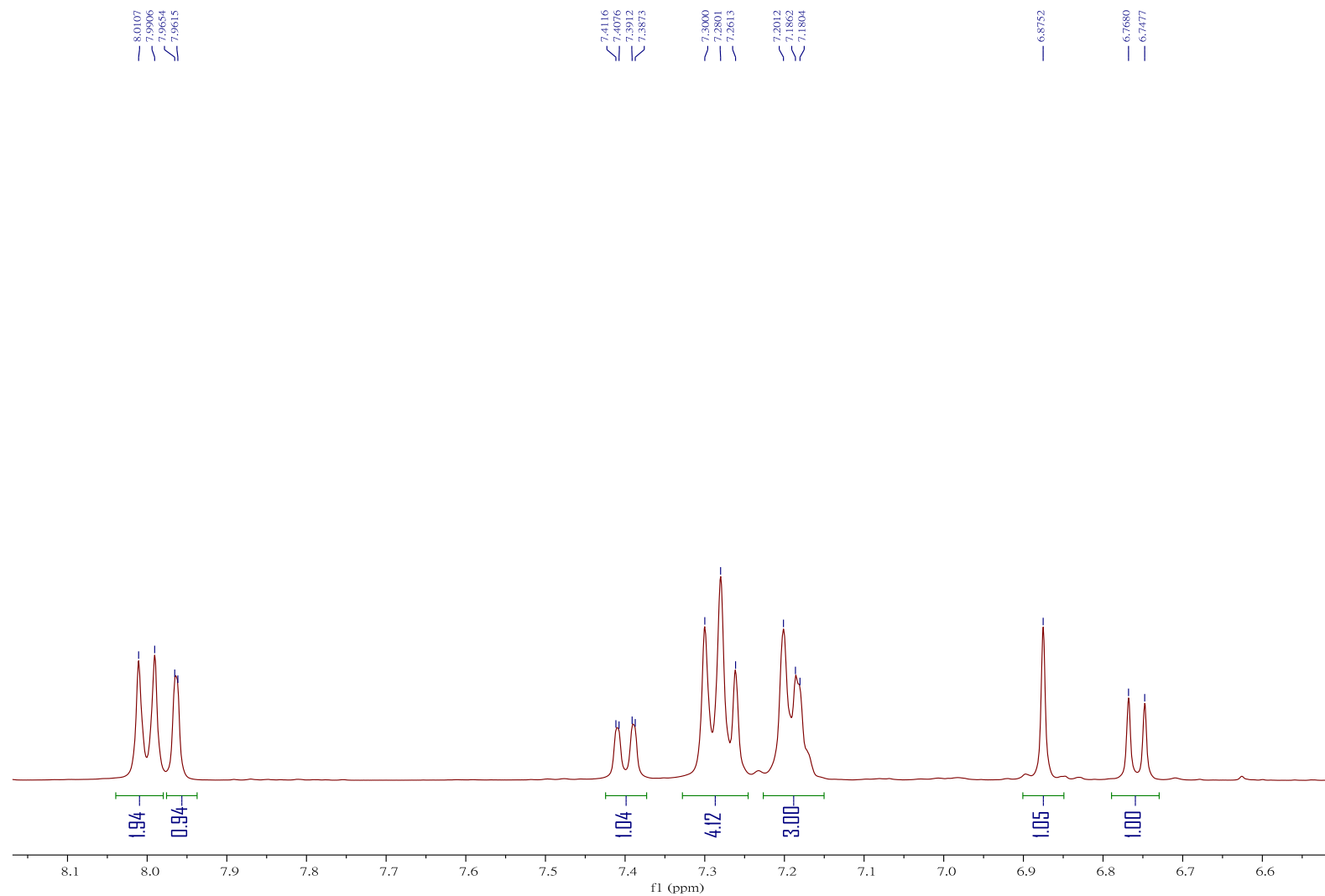
Instrument type and / or accessory

9/4/2018

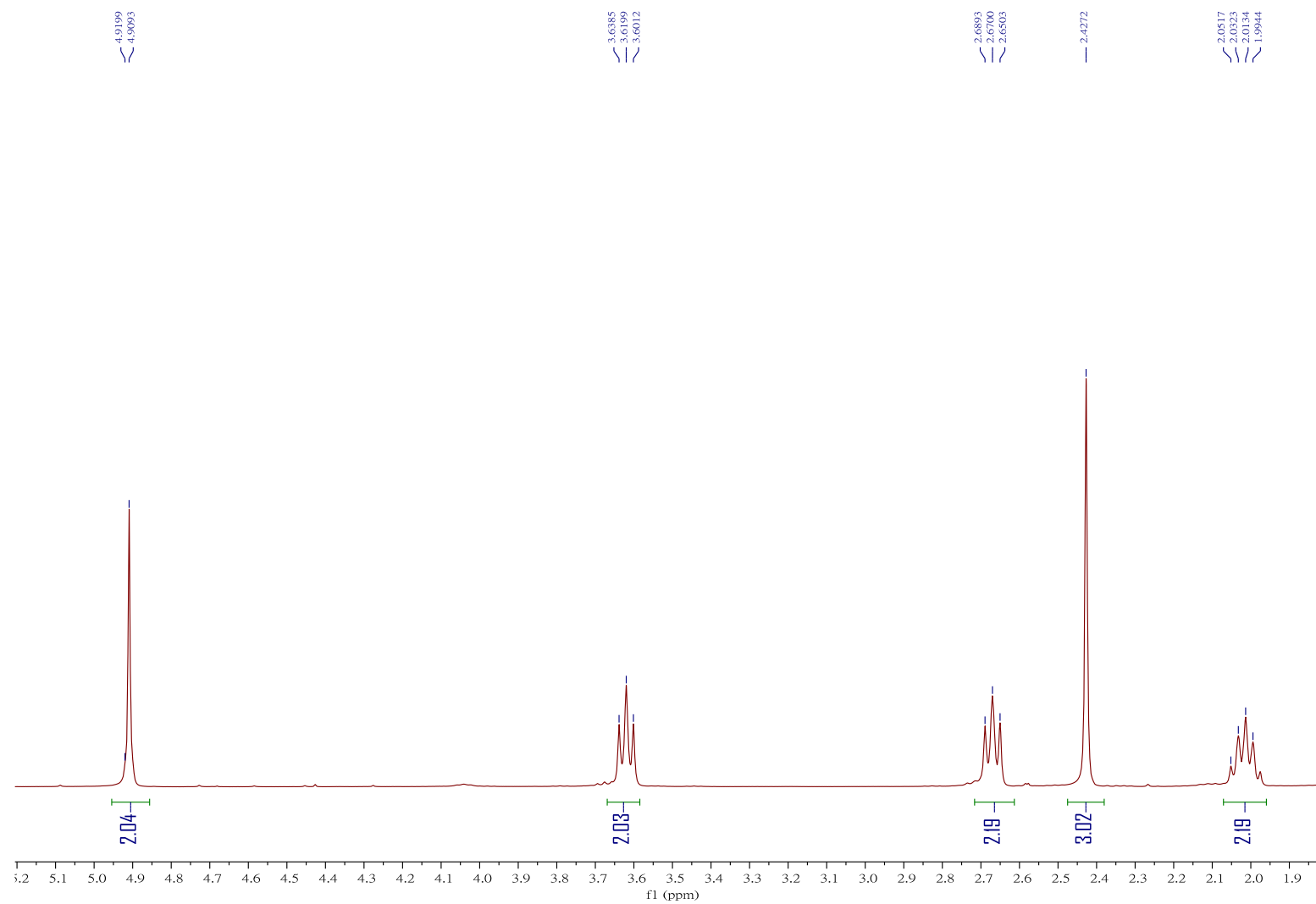
FT-IR Spectrum of compound **9c**



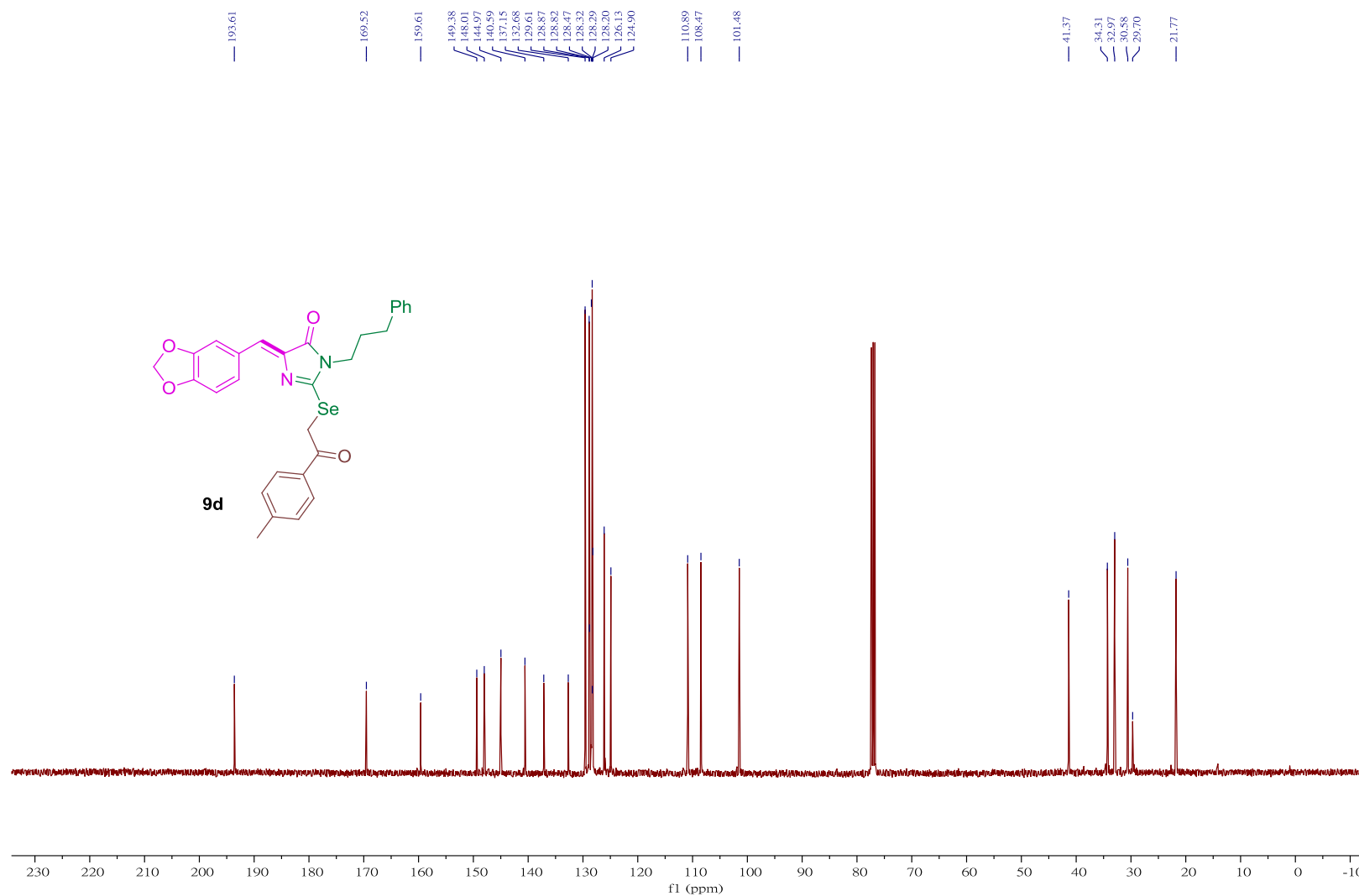
^1H NMR Spectrum (400 MHz) of compound **9d** in CDCl_3



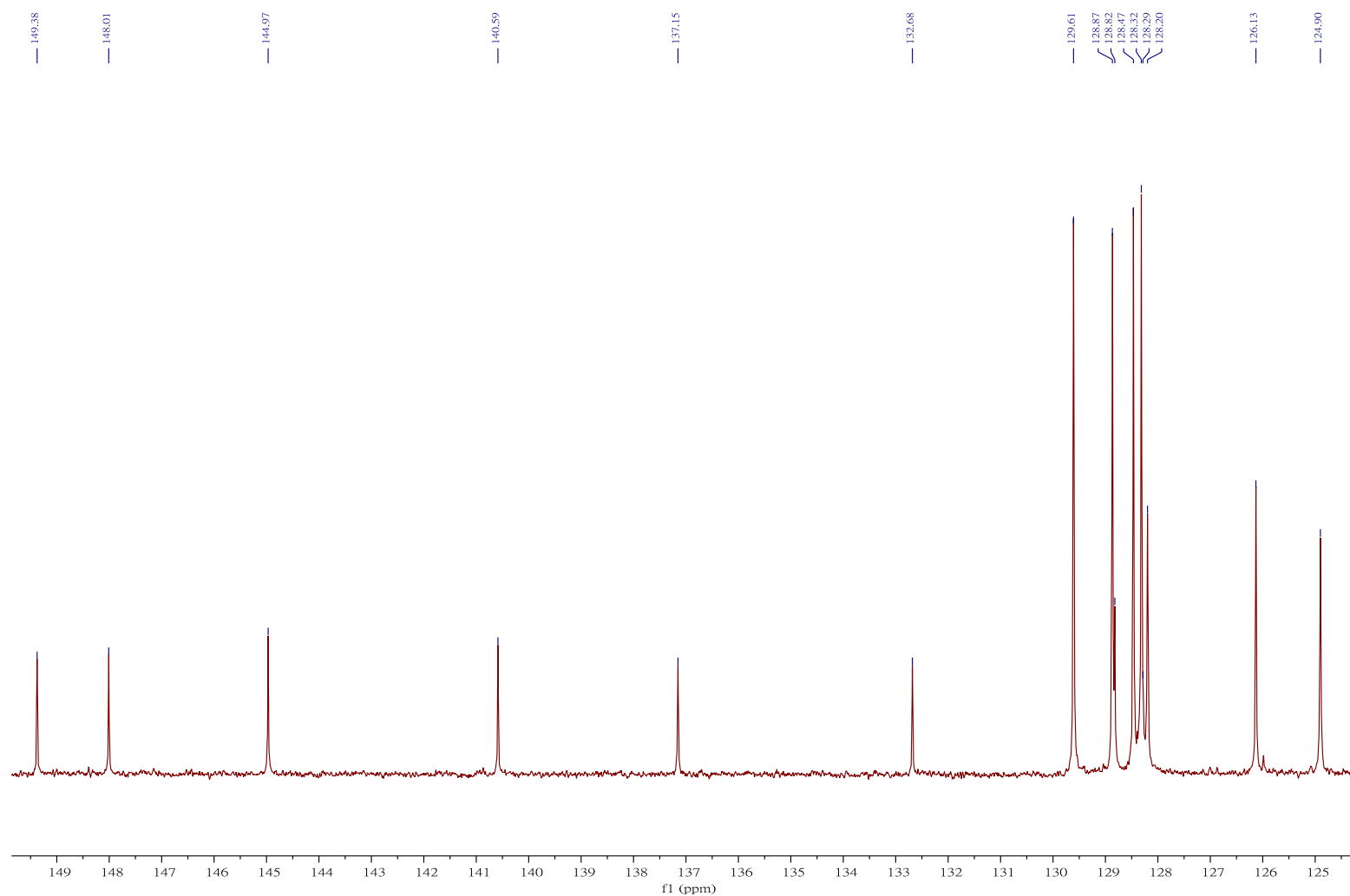
Expansion ^1H NMR Spectrum (400 MHz) of compound **9d** in CDCl_3



Expanding ¹H NMR Spectrum (400 MHz) of compound **9d** in CDCl₃



^{13}C NMR Spectrum (101 MHz) of compound **9d** in CDCl_3

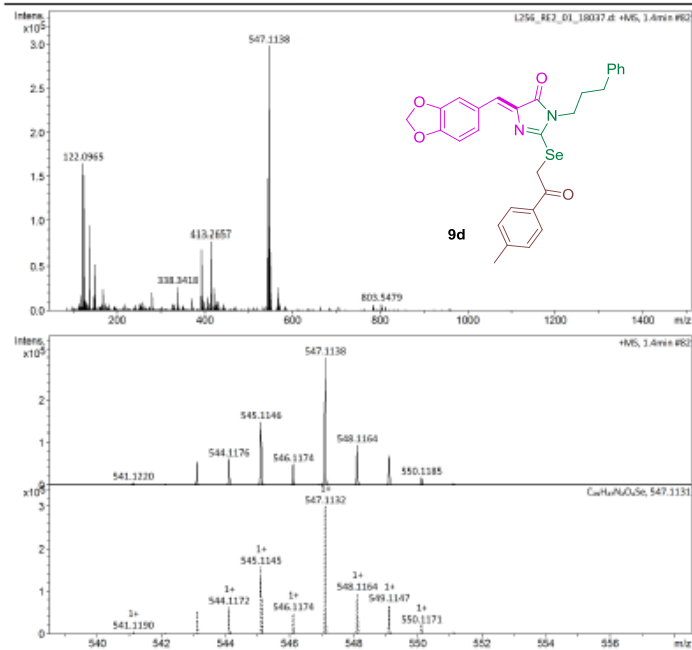


Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **9d** in CDCl_3

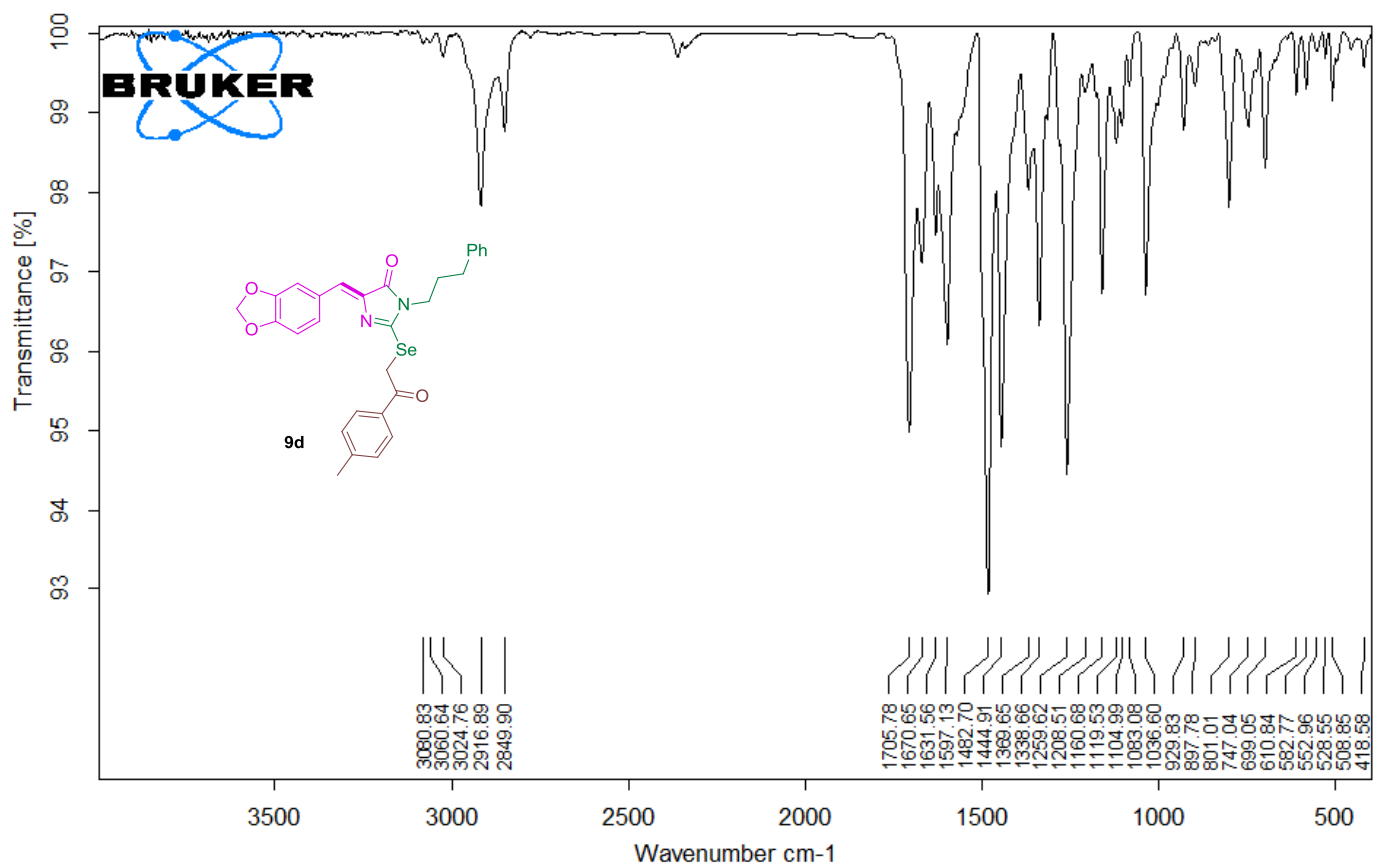
Display Report

Analysis Info		Acquisition Date	4/20/2018 12:45:27 PM	
Analysis Name	H:\20181-6\20180420\L256_RE2_01_18037.d	Operator	NCTU	
Method	Small molecule.m	Instrument	Impact HD	1819696.00164
Sample Name	L256			
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	-4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



HRMS of compound **9d**



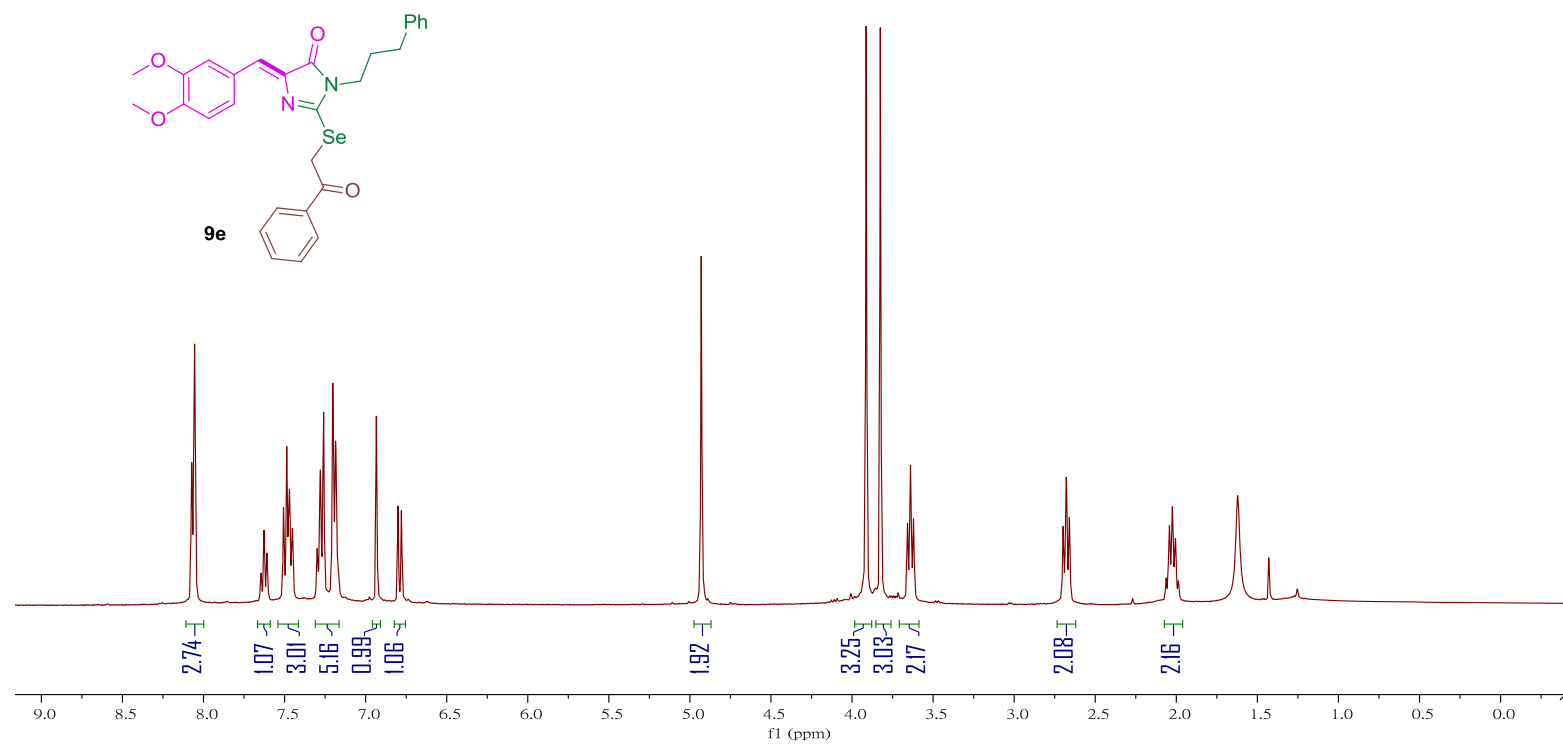
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MIR_TR_DTGS_L256

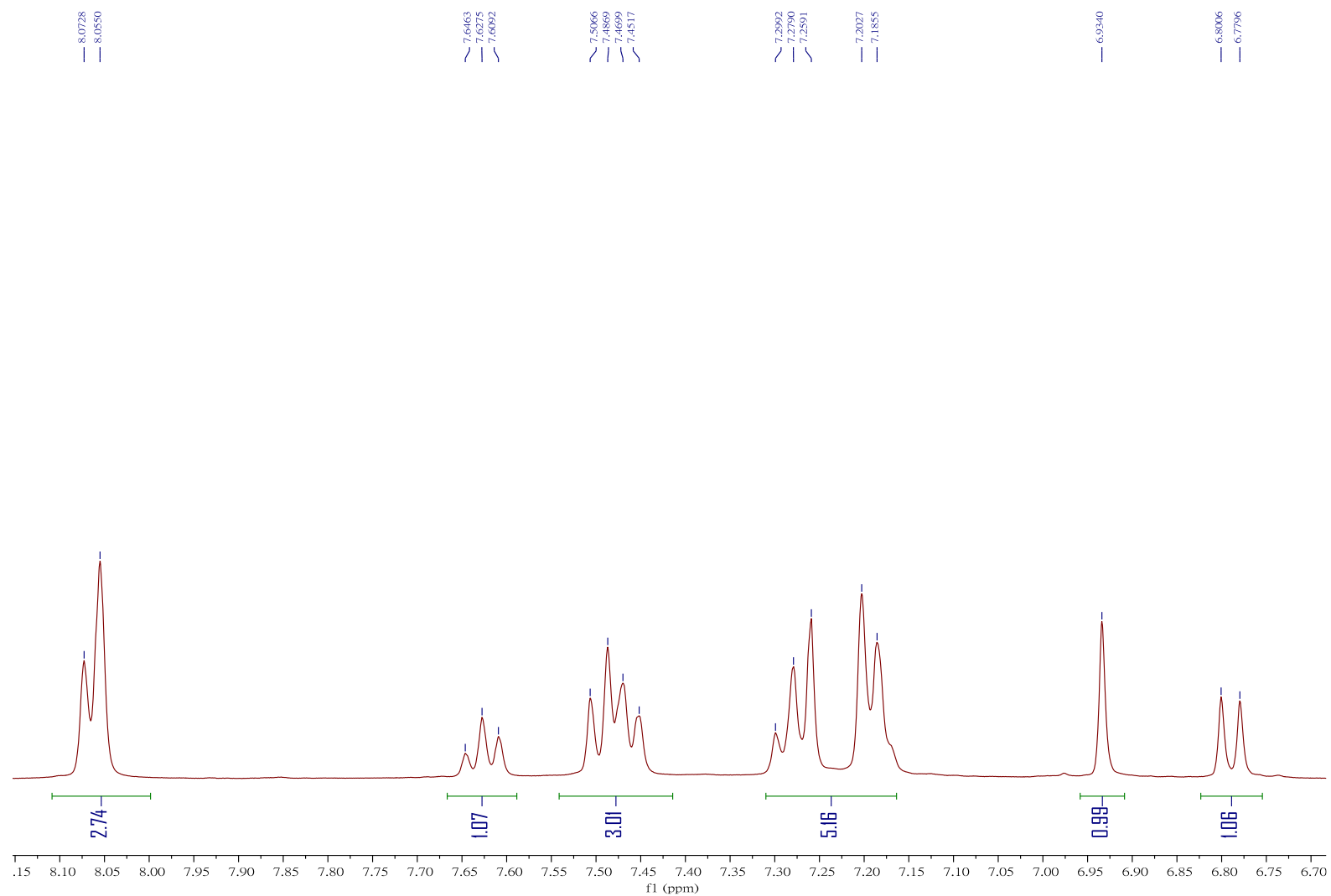
Instrument type and / or accessory

9/4/2018

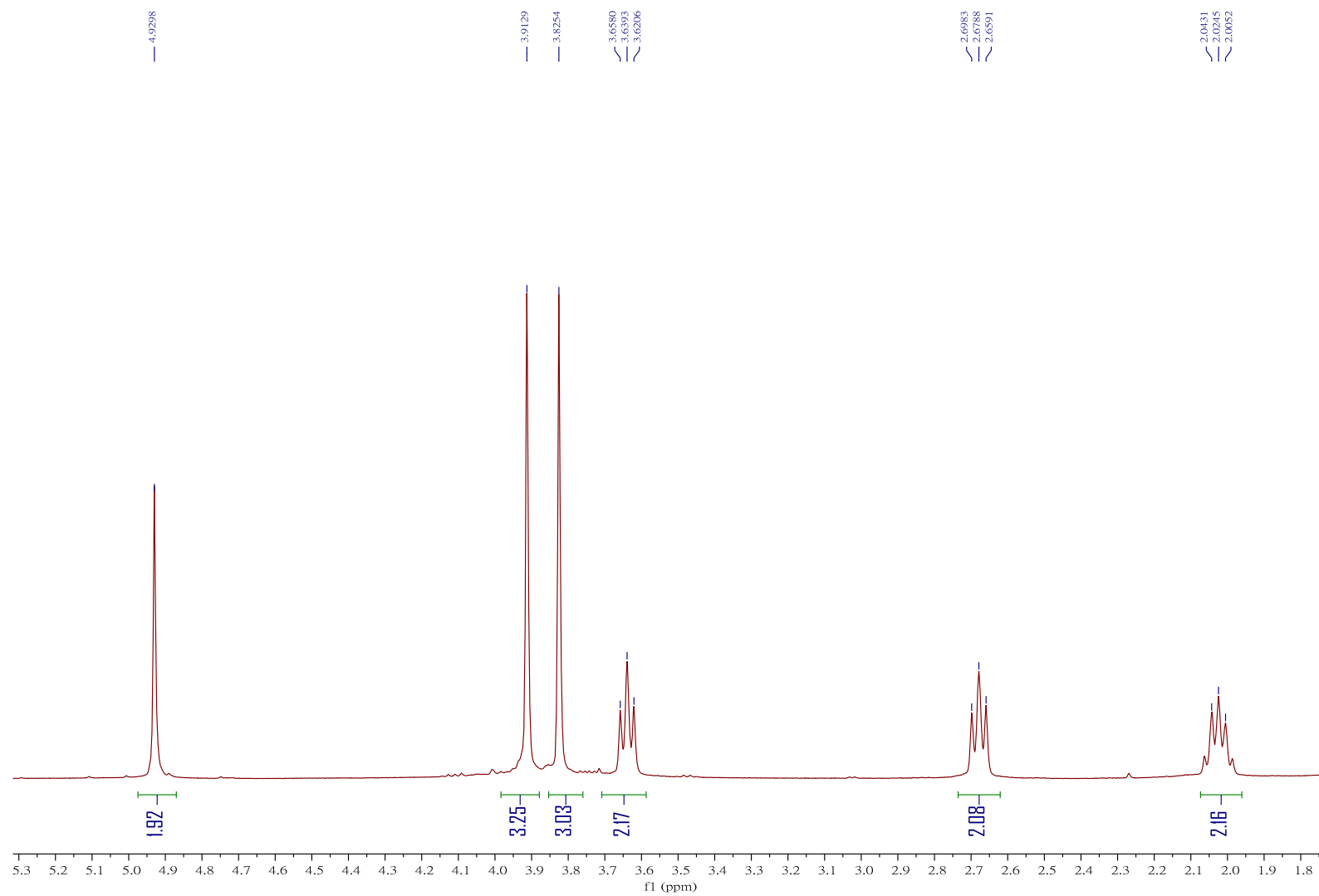
FT-IR Spectrum of compound **9d**



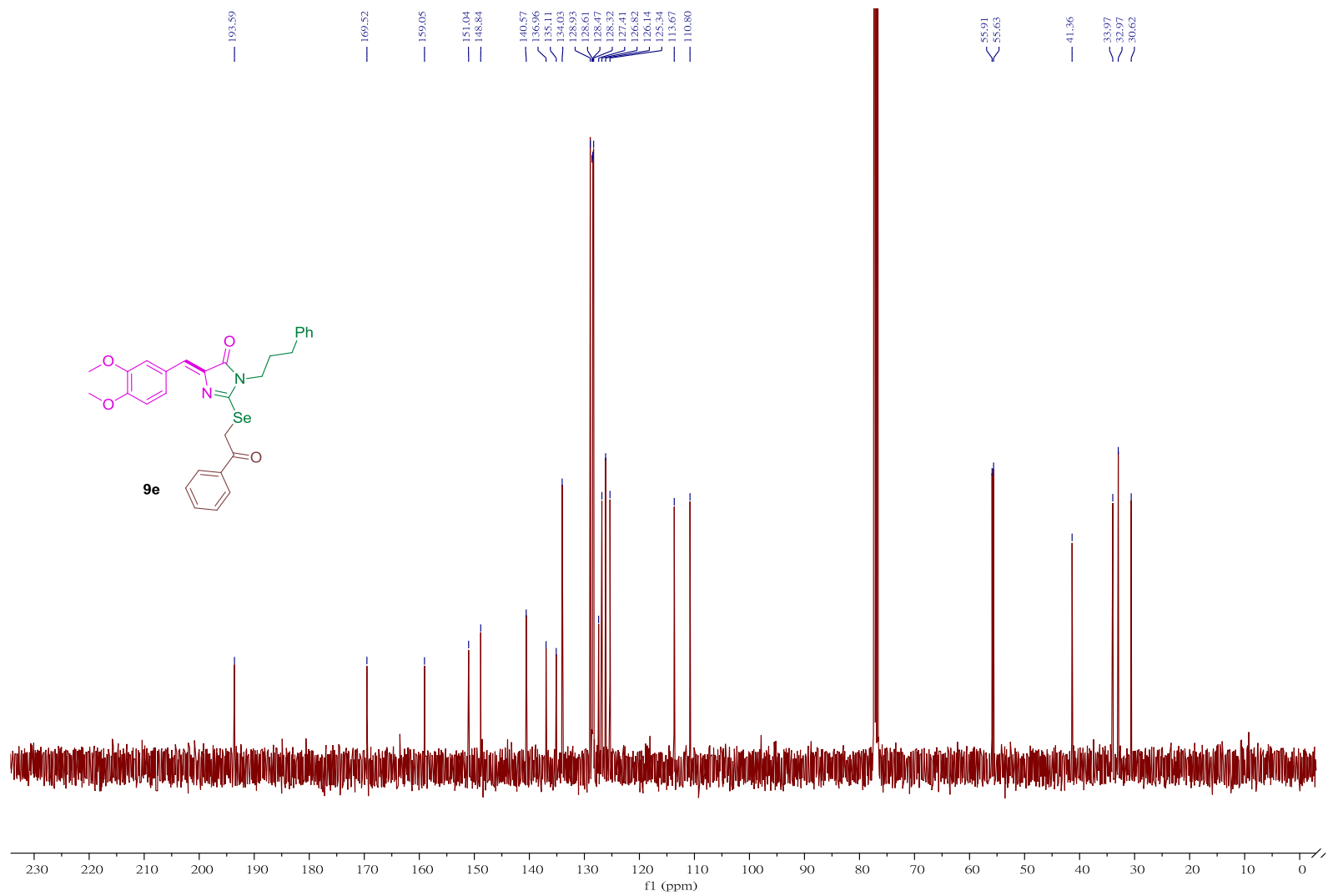
^1H NMR Spectrum (400 MHz) of compound **9e** in CDCl_3



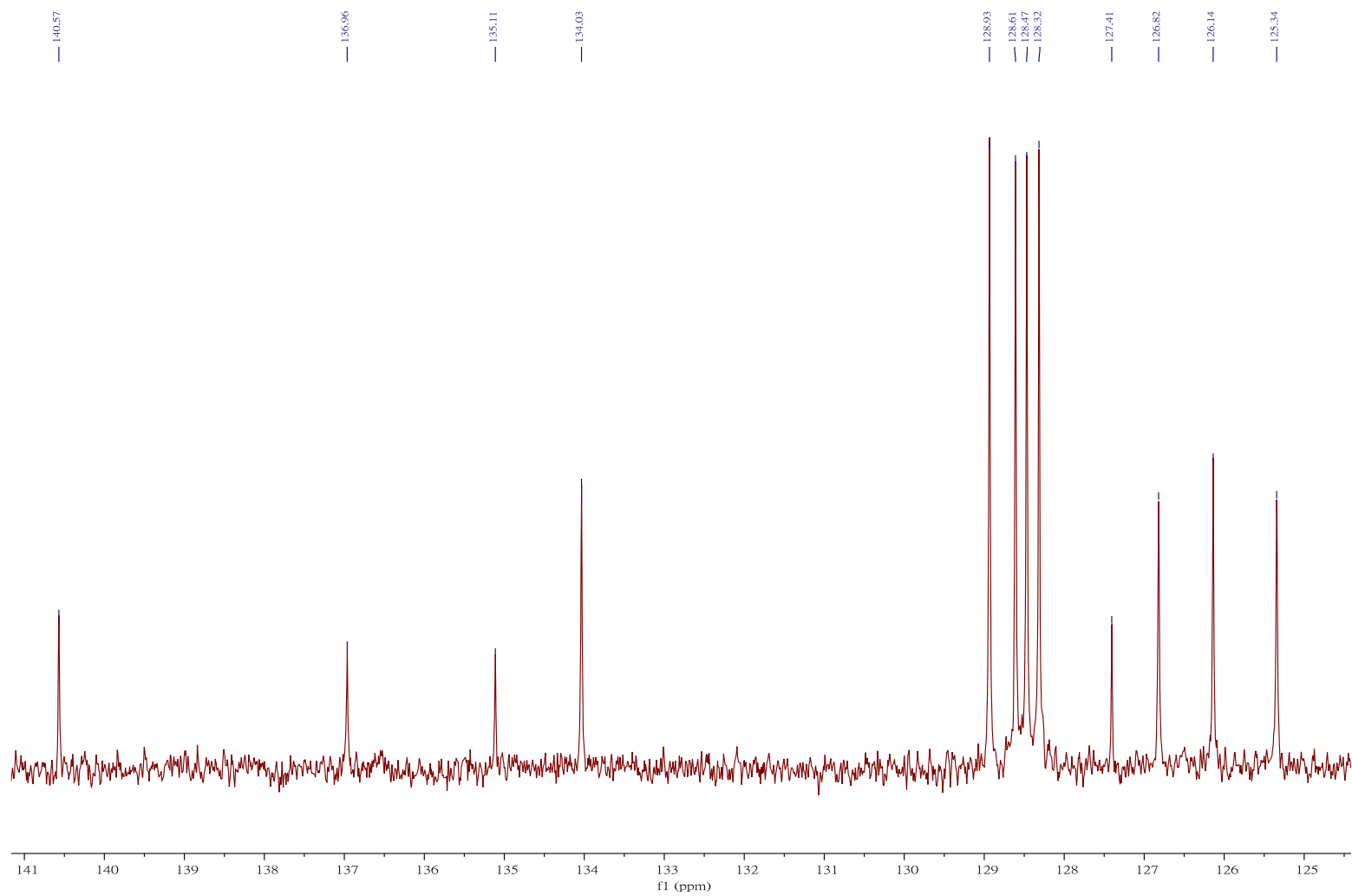
Expansion of ^1H NMR Spectrum (400 MHz) of compound **9e** in CDCl_3



Expansion of ¹H NMR Spectrum (400 MHz) of compound **9e** in CDCl₃



^{13}C NMR Spectrum (101 MHz) of compound **9e** in CDCl_3

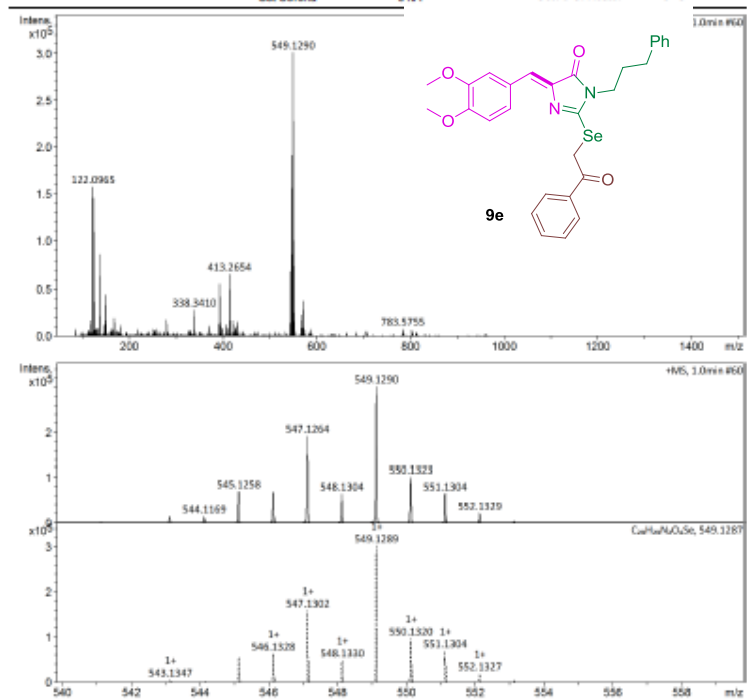


Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **9e** in CDCl_3

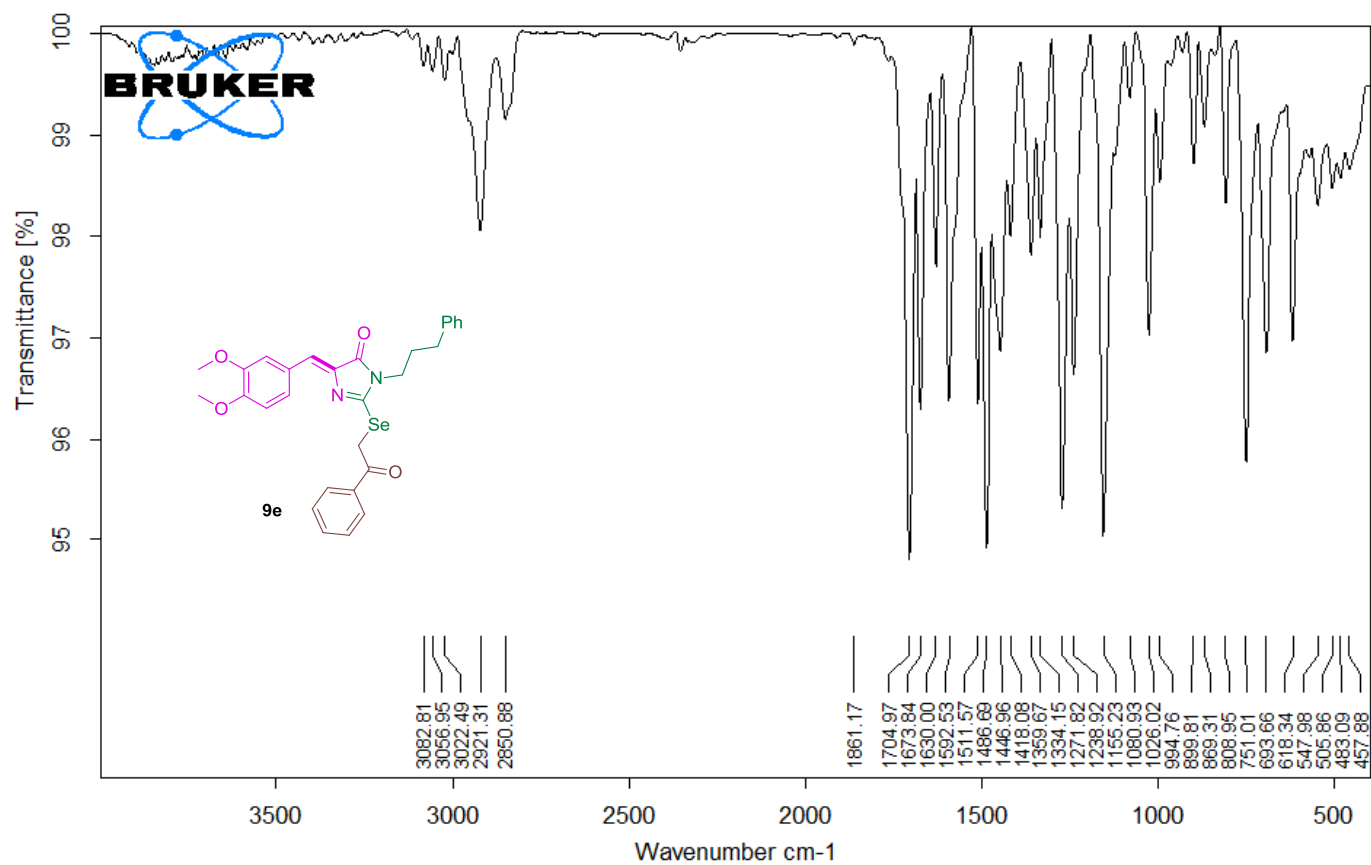
Display Report

Analysis Info		Acquisition Date	4/20/2018 12:49:46 PM	
Analysis Name	H:\20181-6\20180420\L267_RE3_01_18038.d	Operator	NCTU	
Method	Small molecule.m	Instrument	Impact HD	1819696.00164
Sample Name	L267			
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



HRMS of compound **9e**



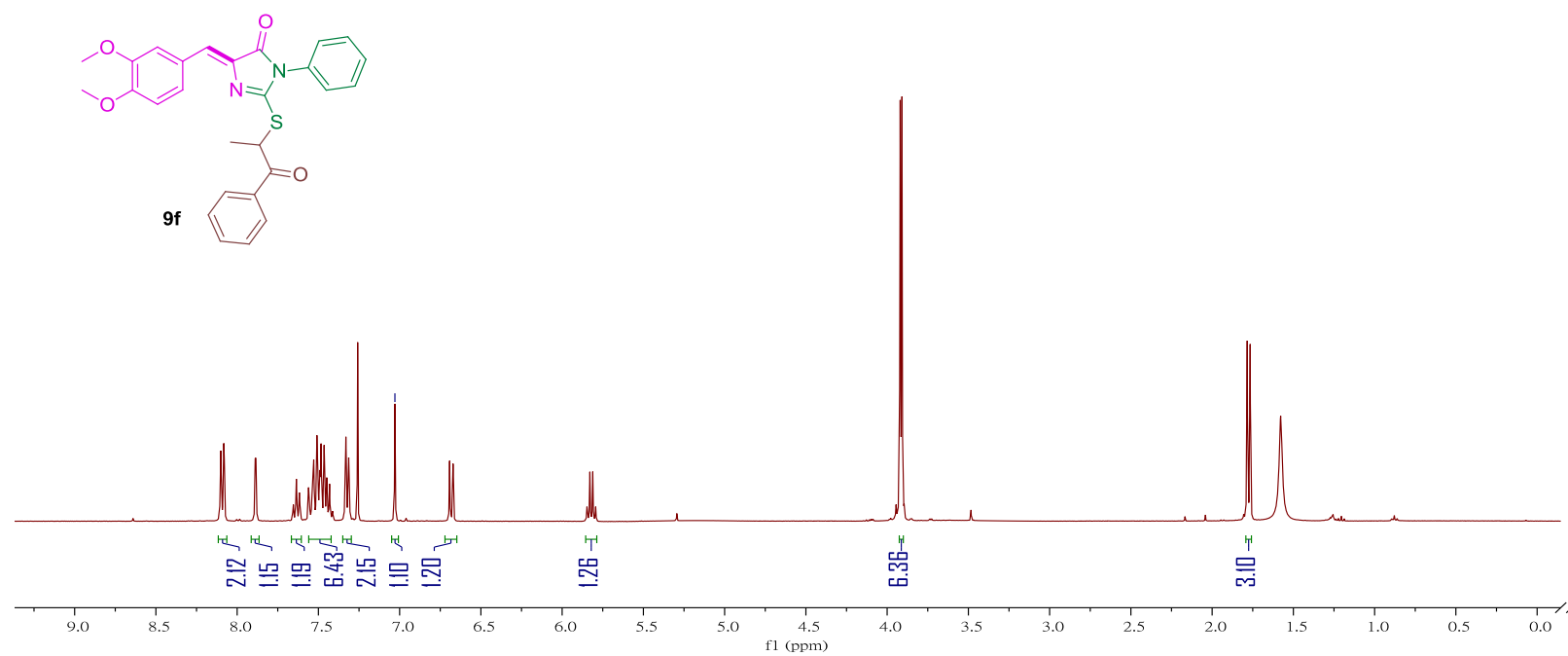
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MIR_TR_DTGS_L267

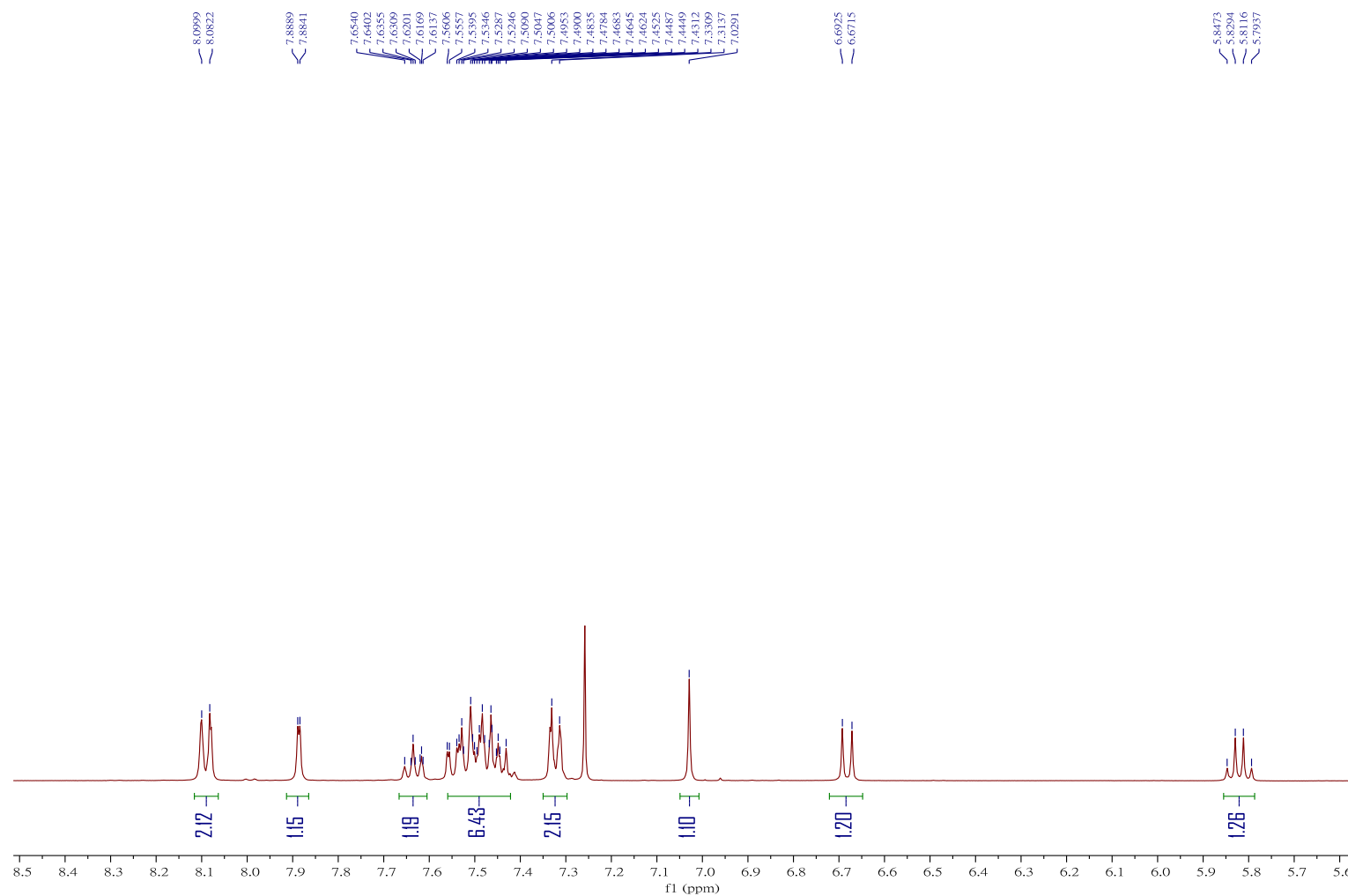
Instrument type and / or accessory

9/4/2018

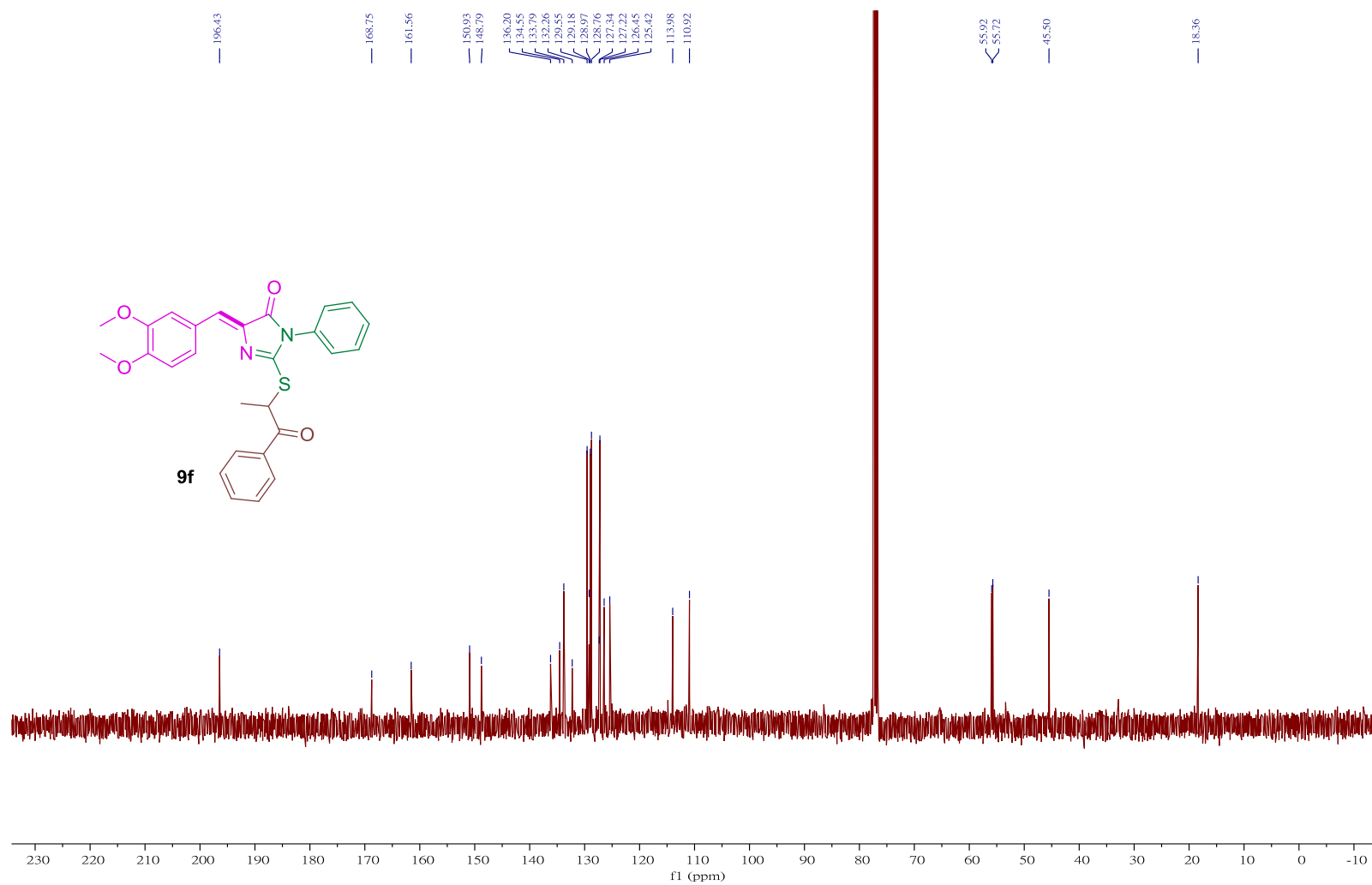
FT-IR Spectrum of compound **9e**



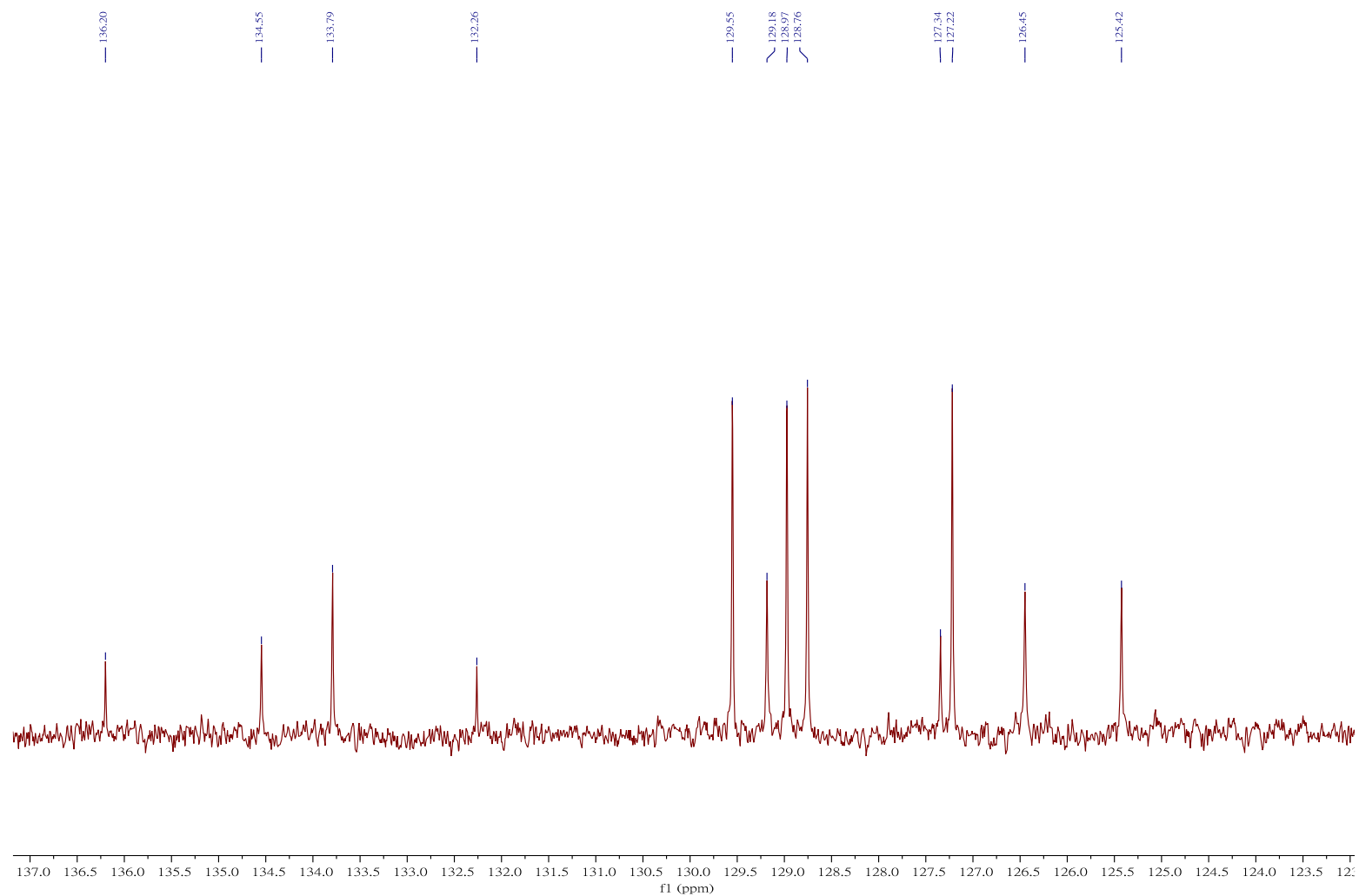
¹H NMR Spectrum (400 MHz) of compound **9f** in CDCl₃



Expansion of ¹H NMR Spectrum (400 MHz) of compound **9f** in CDCl₃



¹³C NMR Spectrum (101 MHz) of compound **9f in CDCl₃**

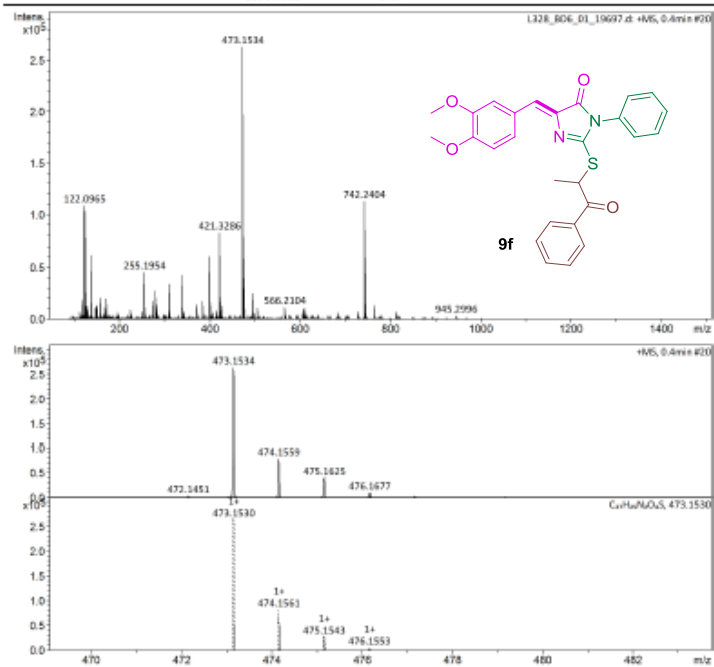


Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **9f** in CDCl_3

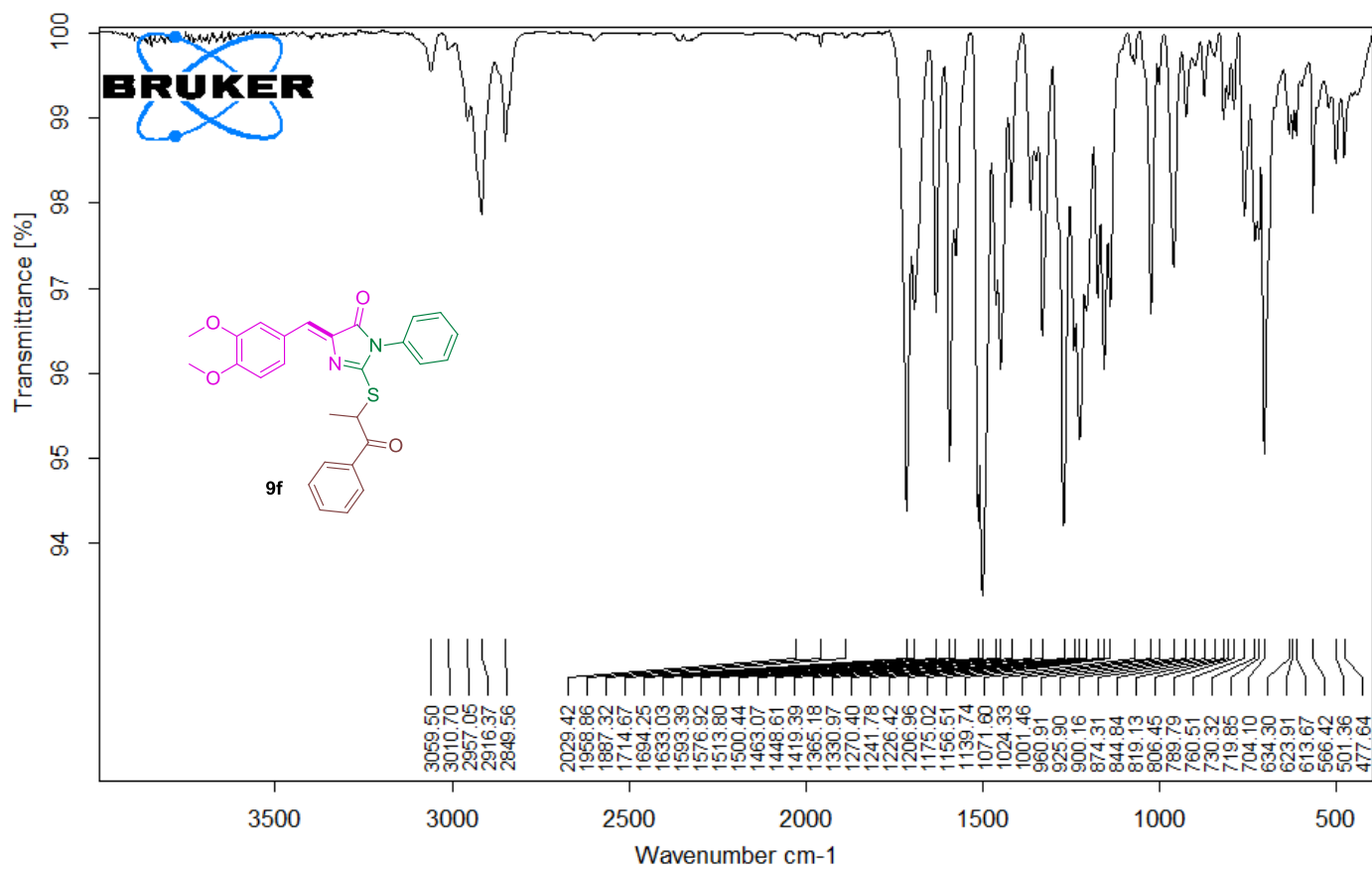
Display Report

Analysis Info		Acquisition Date	8/28/2018 2:22:16 PM	
Analysis Name	D:\Data\NCTU SERVICE\Data\2018\20180828\L328_BD6_01_19697.d	Operator	NCTU	
Method	Small molecule.m	Instrument	Impact HD	1819696.00164
Sample Name	L328			
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 L/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APC1 Heater	0 °C



HRMS of compound **9f**



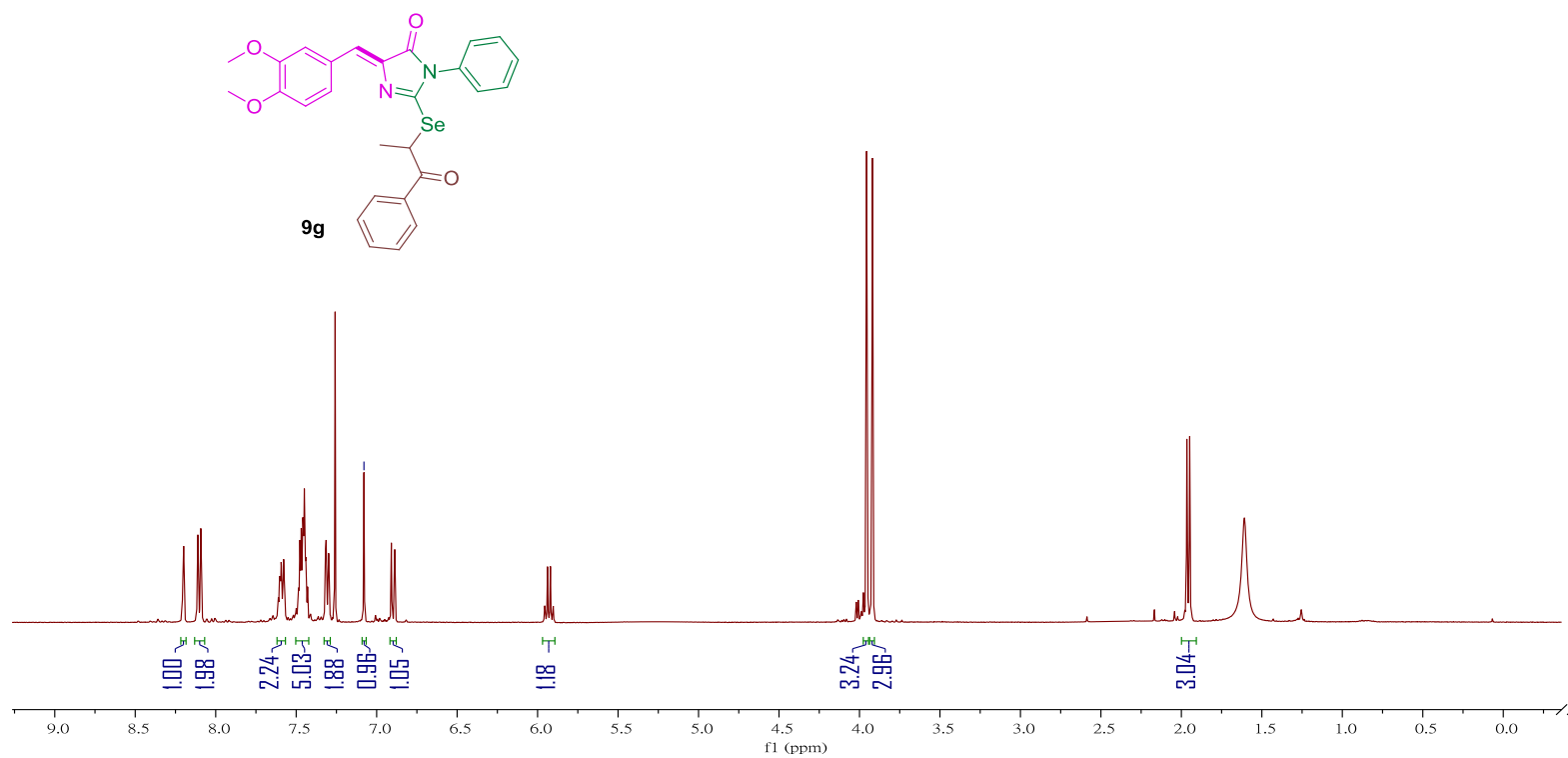
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MIR_TR_DTGS_L328

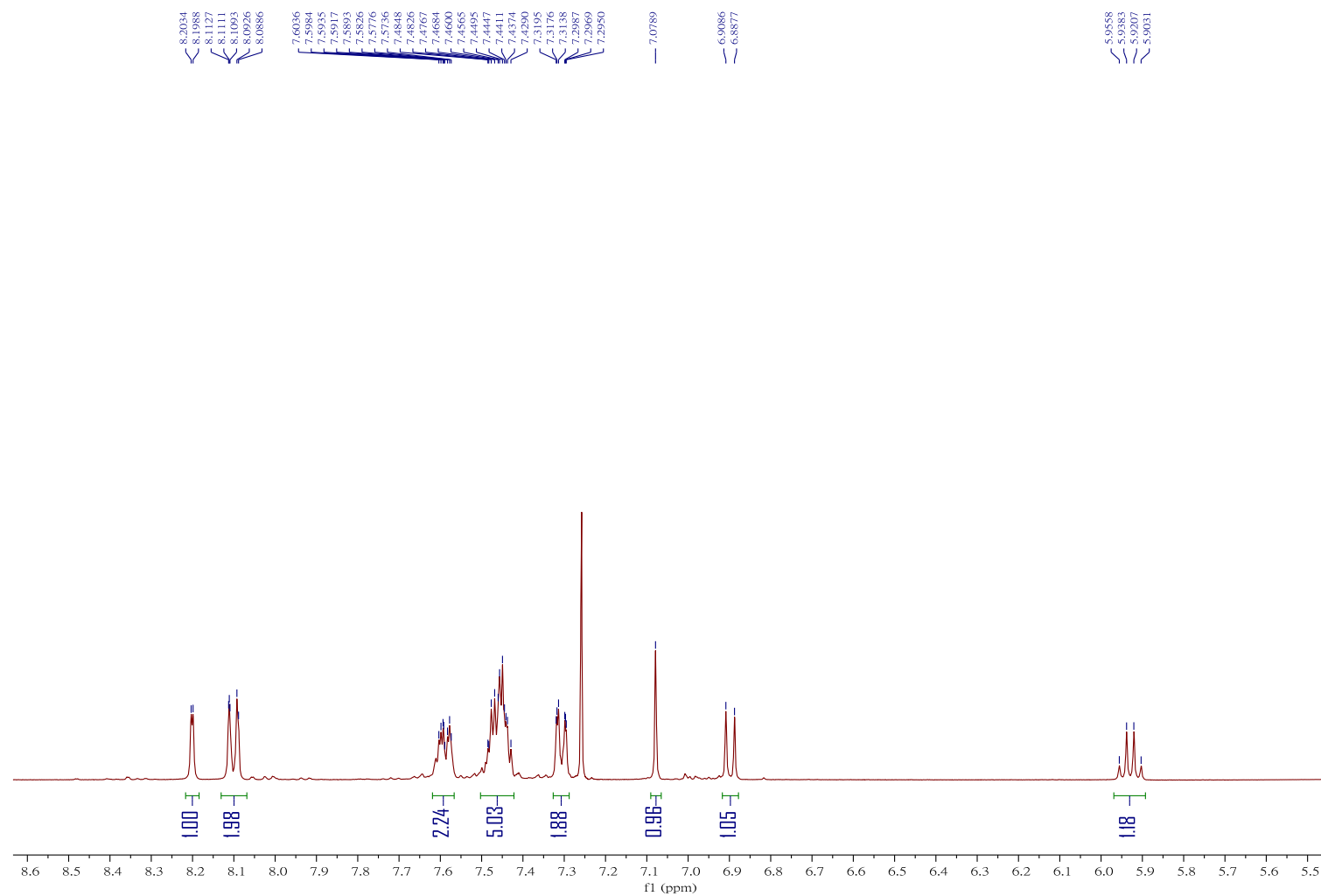
Instrument type and / or accessory

9/4/2018

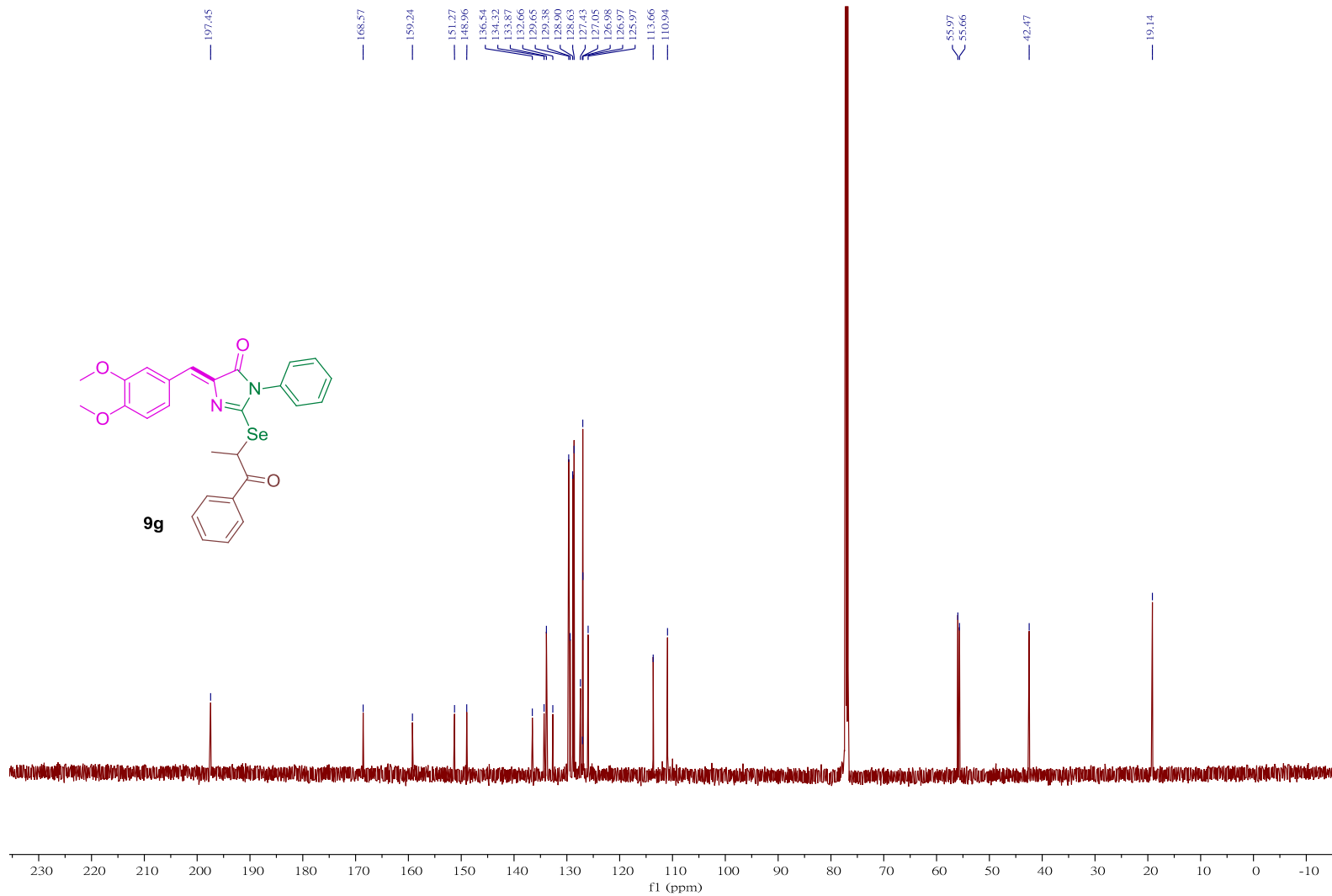
FT-IR Spectrum of compound **9f**



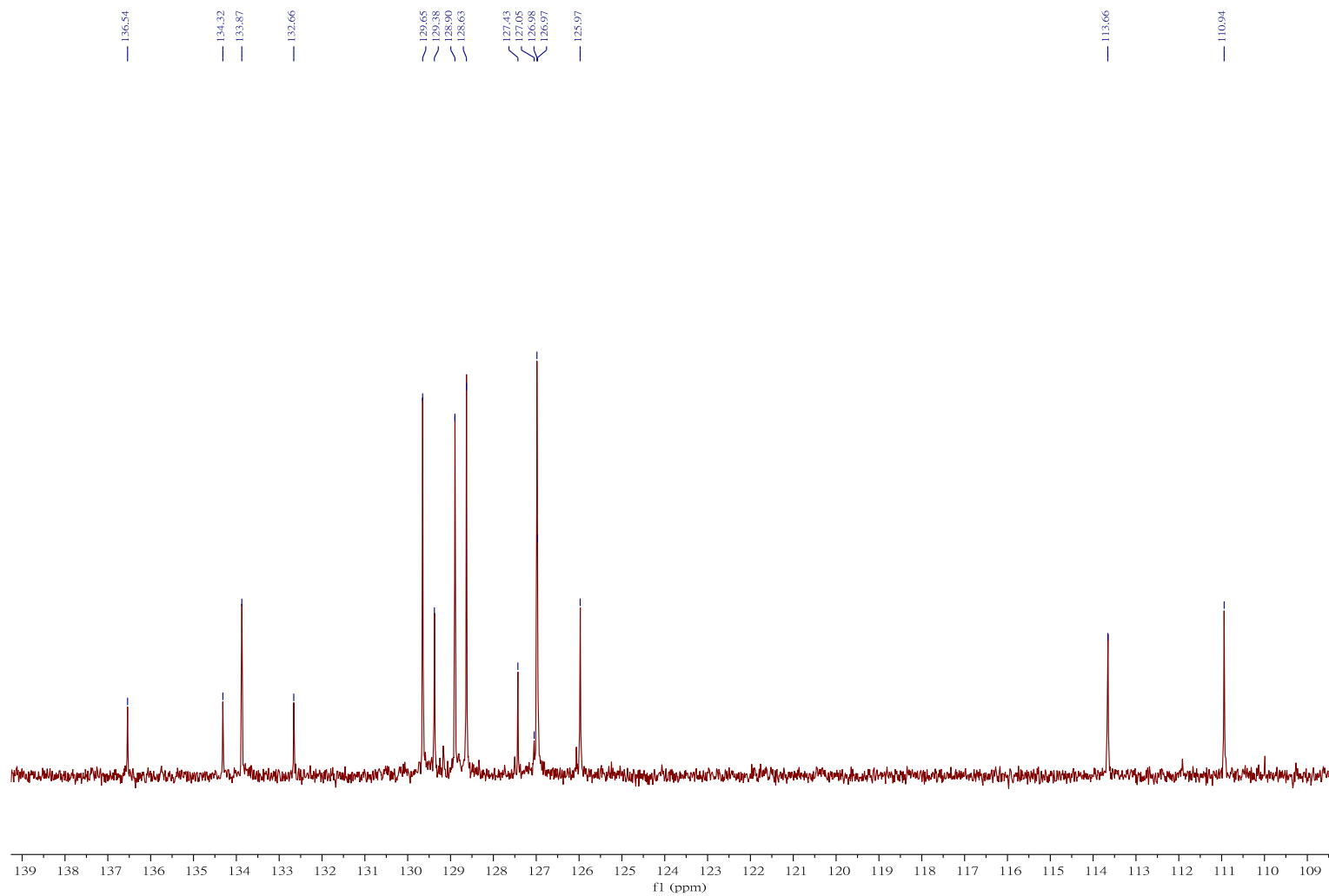
^1H NMR Spectrum (400 MHz) of compound **9g** in CDCl_3



Expansion of ¹H NMR Spectrum (400 MHz) of compound **9g** in CDCl₃



¹³C NMR Spectrum (101 MHz) of compound **9h** in CDCl₃



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **9h** in CDCl_3

Display Report

Analysis Info

Analysis Name D:\Data\ntcu service\data\2018\20180828\L329_BD7_01_19698.d

Method Small molecule.m

Sample Name L329

Comment

Acquisition Date 8/28/2018 2:26:38 PM

Operator NCTU

Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type

ESI

Ion Polarity

Positive

Set Nebulizer

1.0 Bar

Focus

Active

Set Capillary

4500 V

Set Dry Heater

200 °C

Scan Begin

50 m/z

Set End Plate Offset

-500 V

Set Dry Gas

6.0 l/min

Scan End

1500 m/z

Set Charging Voltage

2000 V

Set Divert Valve

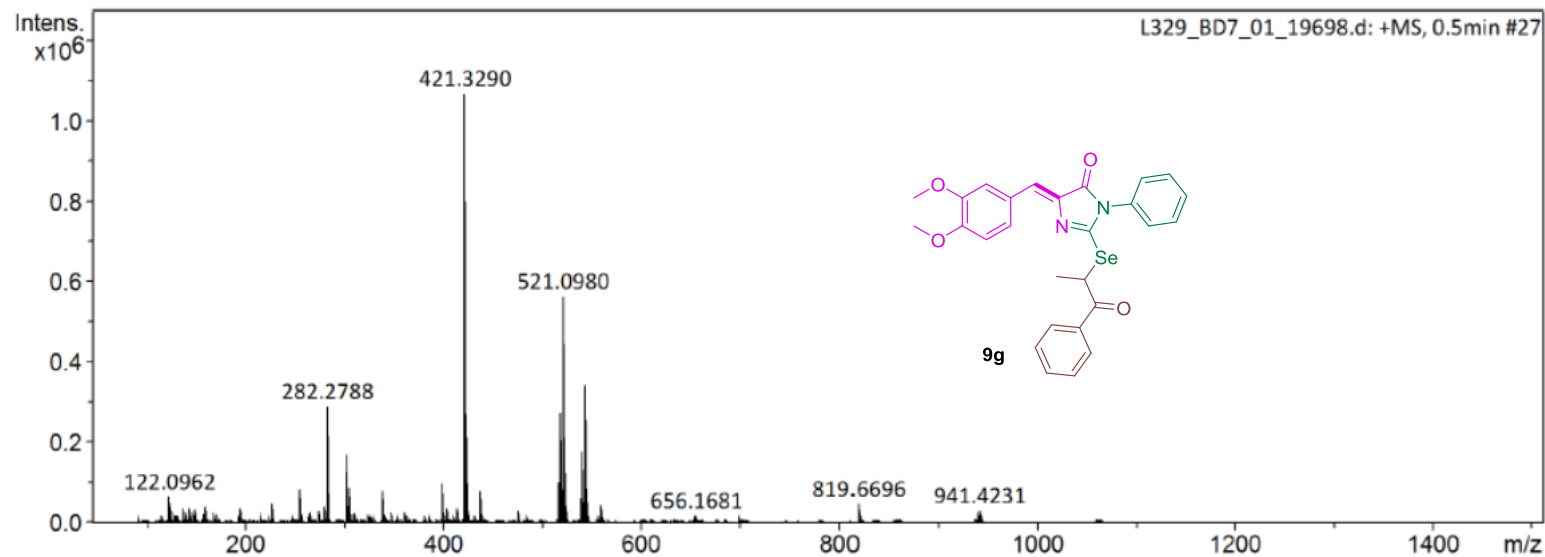
Waste

Set Corona

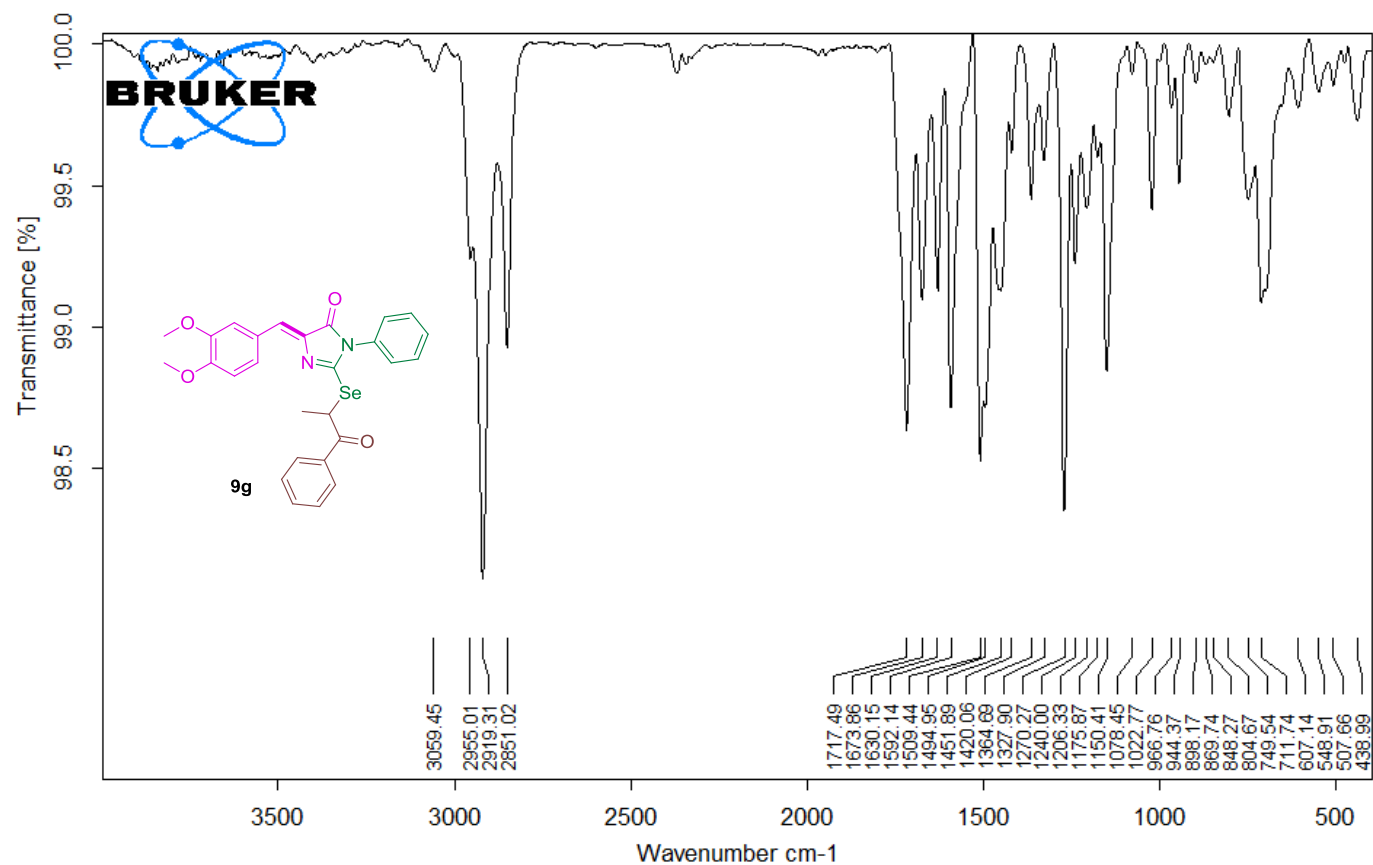
0 nA

Set APCI Heater

0 °C



HRMS of compound 9g



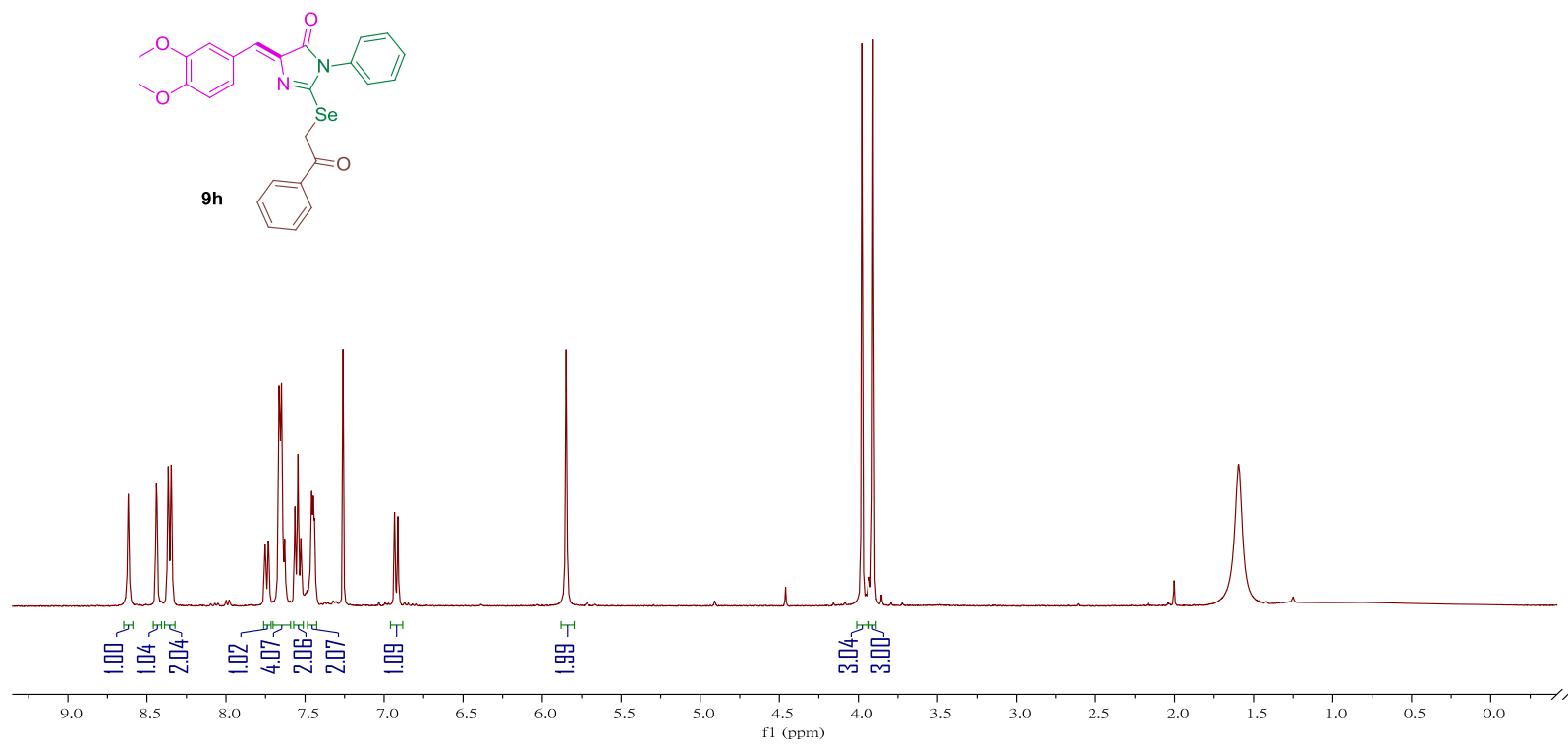
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L329.1

MIR_TR_DTGS_L329

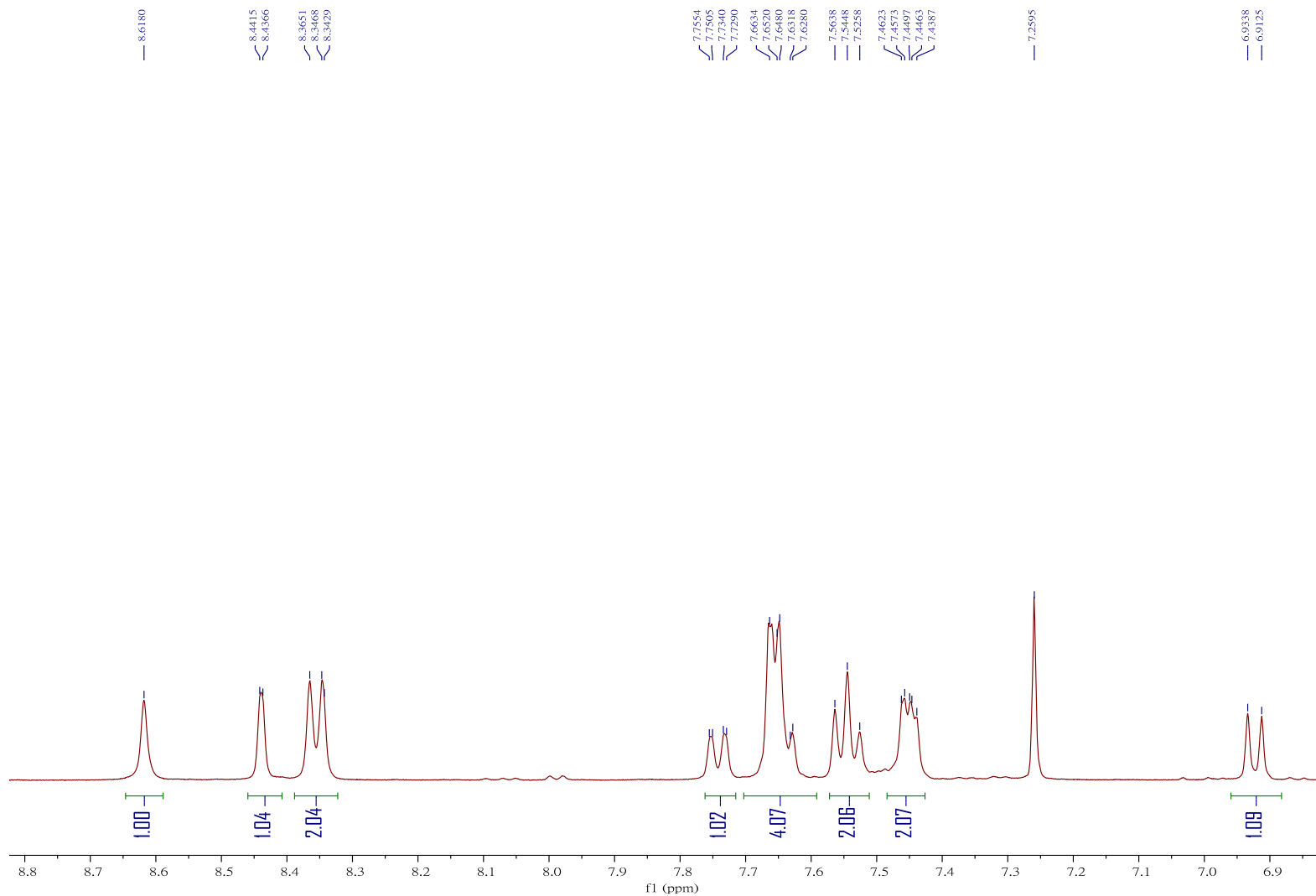
Instrument type and / or accessory

9/4/2018

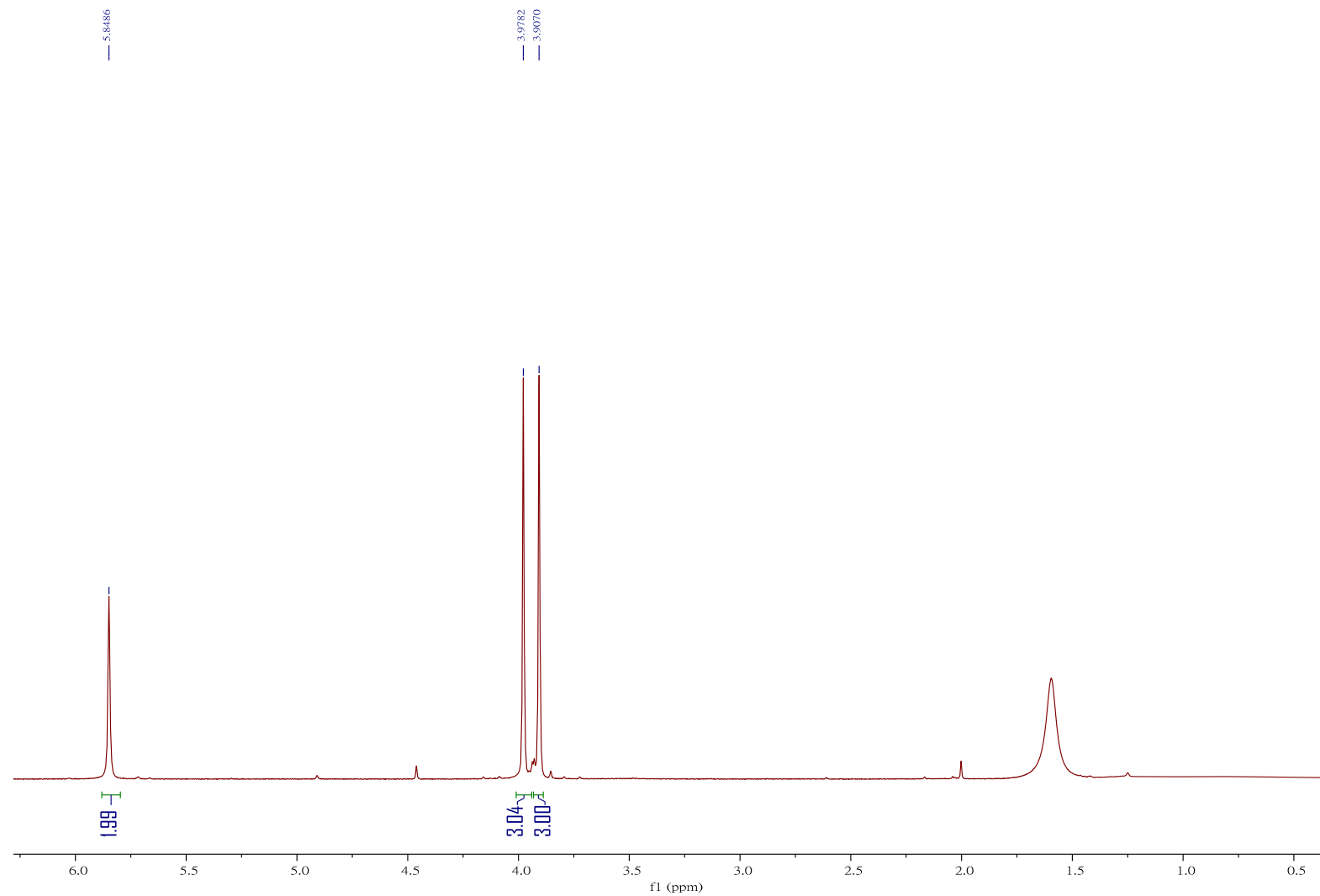
FT-IR Spectrum of compound **9g**



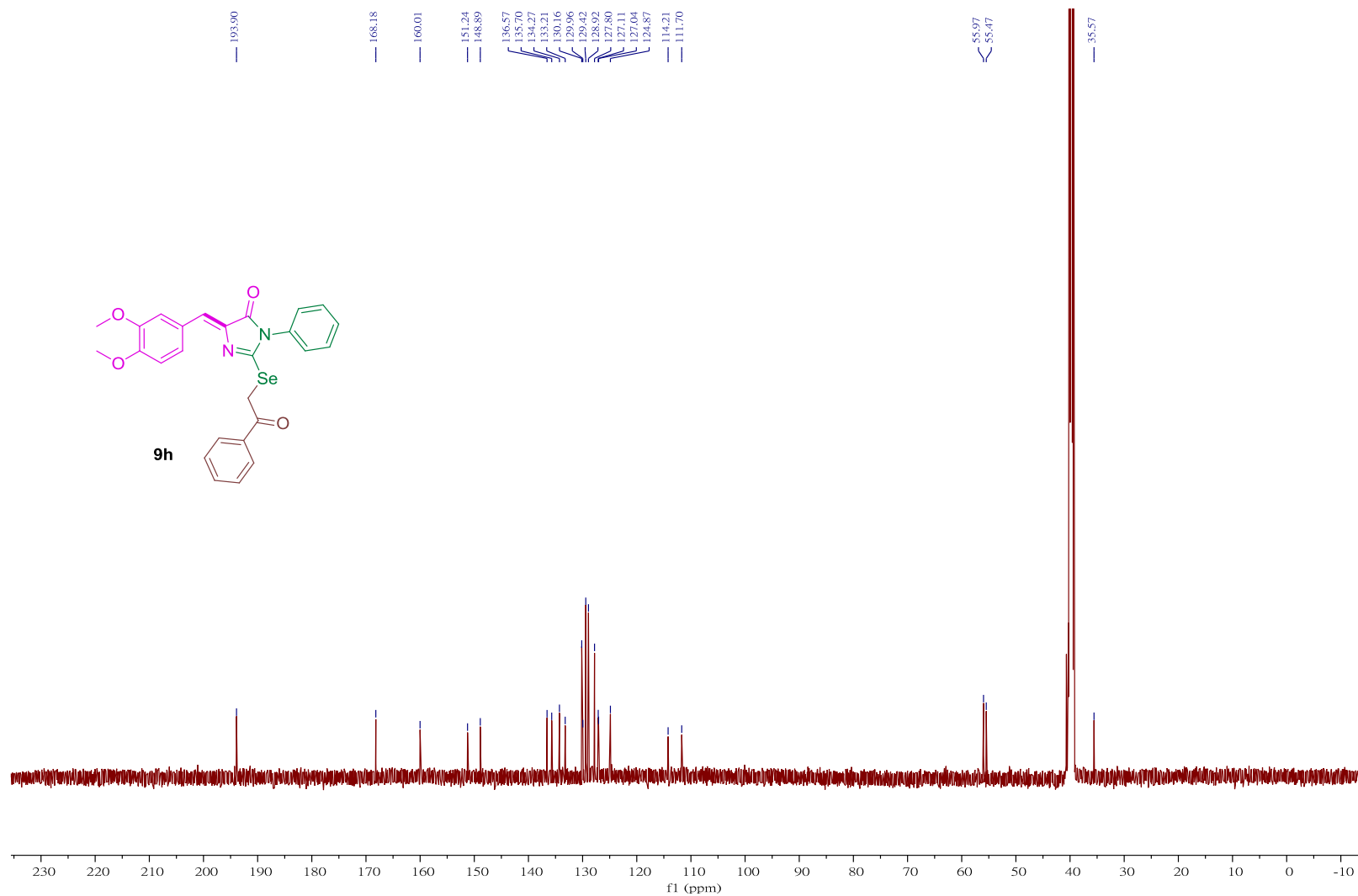
^1H NMR Spectrum (400 MHz) of compound **9h** in CDCl_3



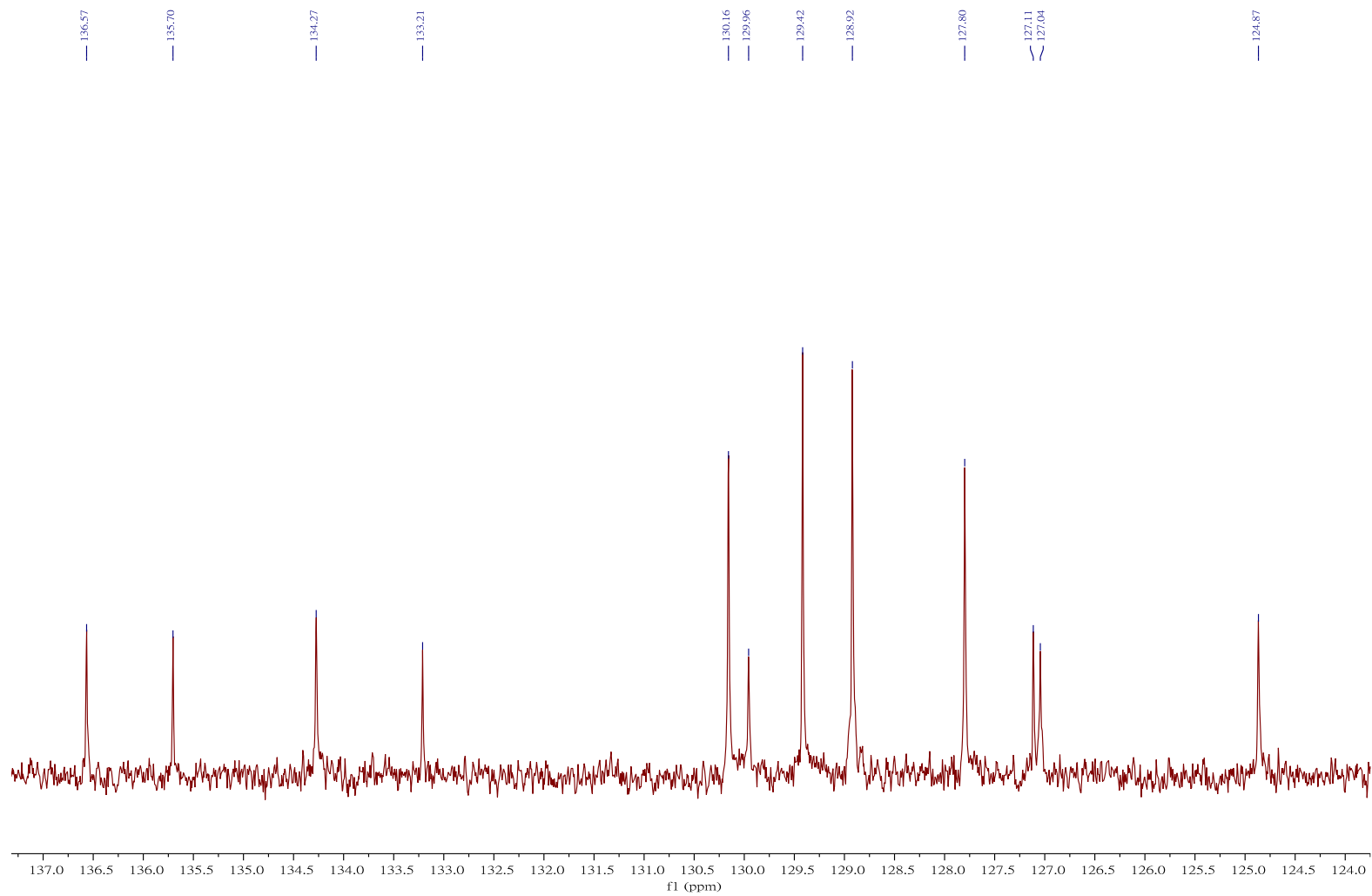
Expansion of ^1H NMR Spectrum (400 MHz) of compound **9h** in CDCl_3



Expansion of ^1H NMR Spectrum (400 MHz) of compound **9h** in CDCl_3



¹³C NMR Spectrum (101 MHz) of compound **9h** in DMSO-*d*₆



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **9h** in $\text{DMSO-}d_6$

Display Report

Analysis Info

Analysis Name D:\Data\inctu service\data\2018\20180420\L247_RC8_01_18031.d

Method Small molecule.m

Sample Name L247

Comment

Acquisition Date 4/20/2018 12:19:25 PM

Operator NCTU

Instrument impact HD 1819696.00164

Acquisition Parameter

Source Type

ESI

Ion Polarity

Positive

Set Nebulizer

1.0 Bar

Focus

Active

Set Capillary

4500 V

Set Dry Heater

200 °C

Scan Begin

50 m/z

Set End Plate Offset

-500 V

Set Dry Gas

6.0 l/min

Scan End

1500 m/z

Set Charging Voltage

2000 V

Set Divert Valve

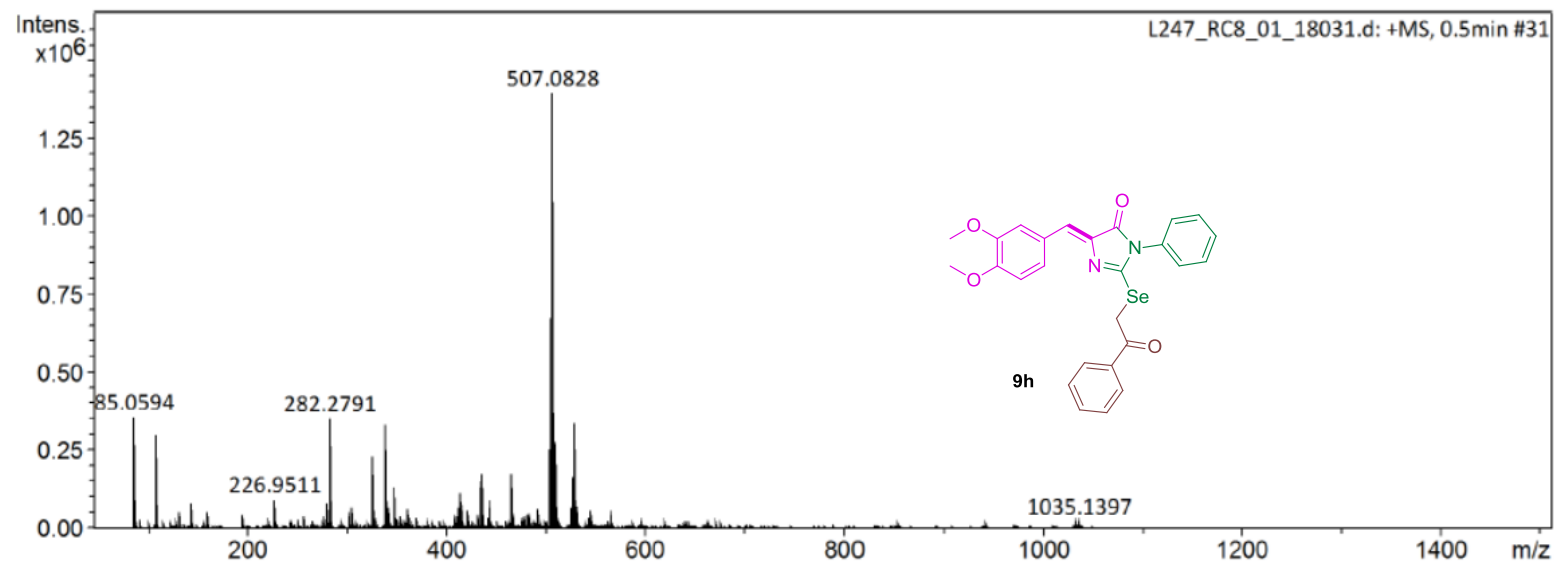
Waste

Set Corona

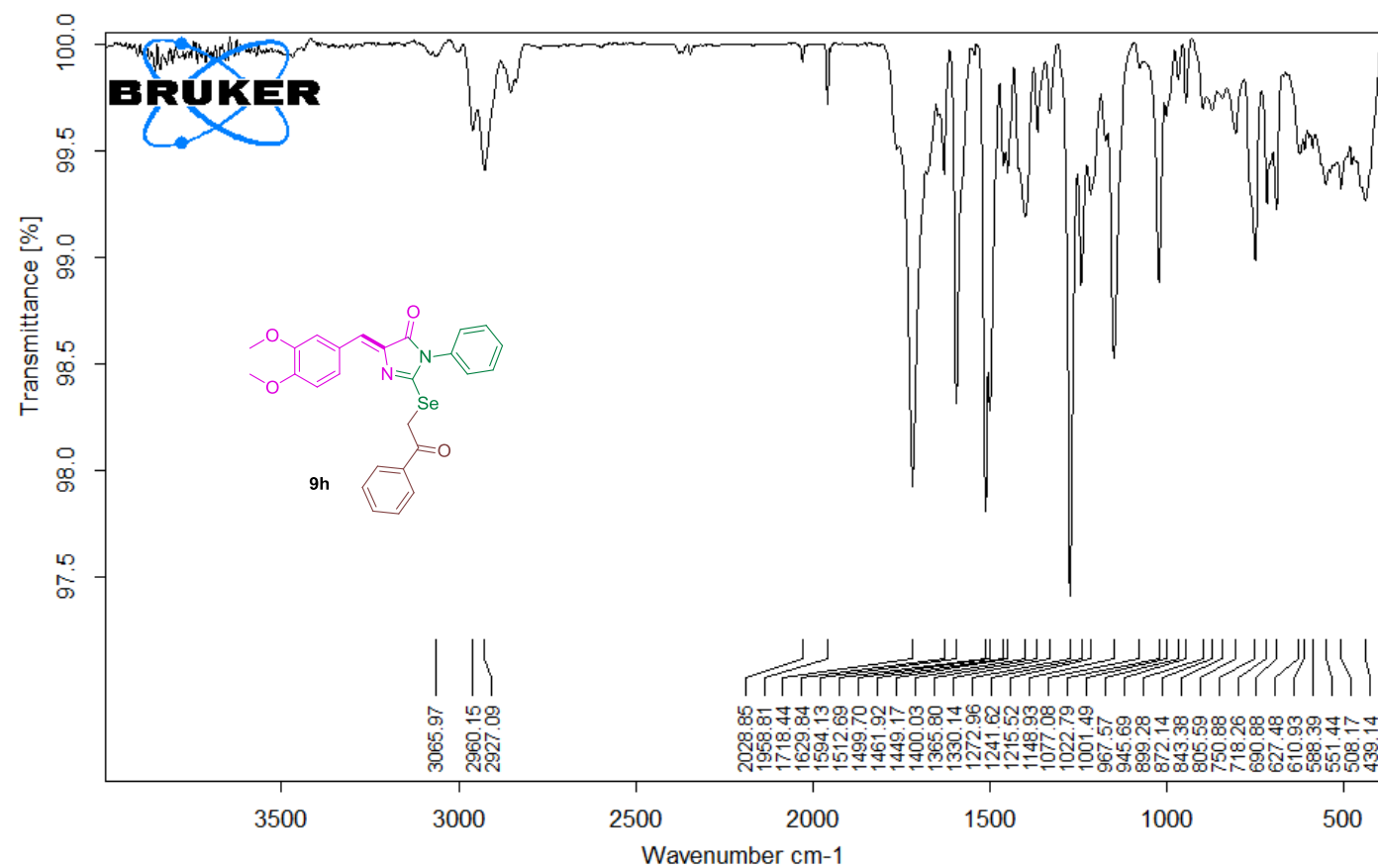
0 nA

Set APCI Heater

0 °C



HRMS of compound **9h**



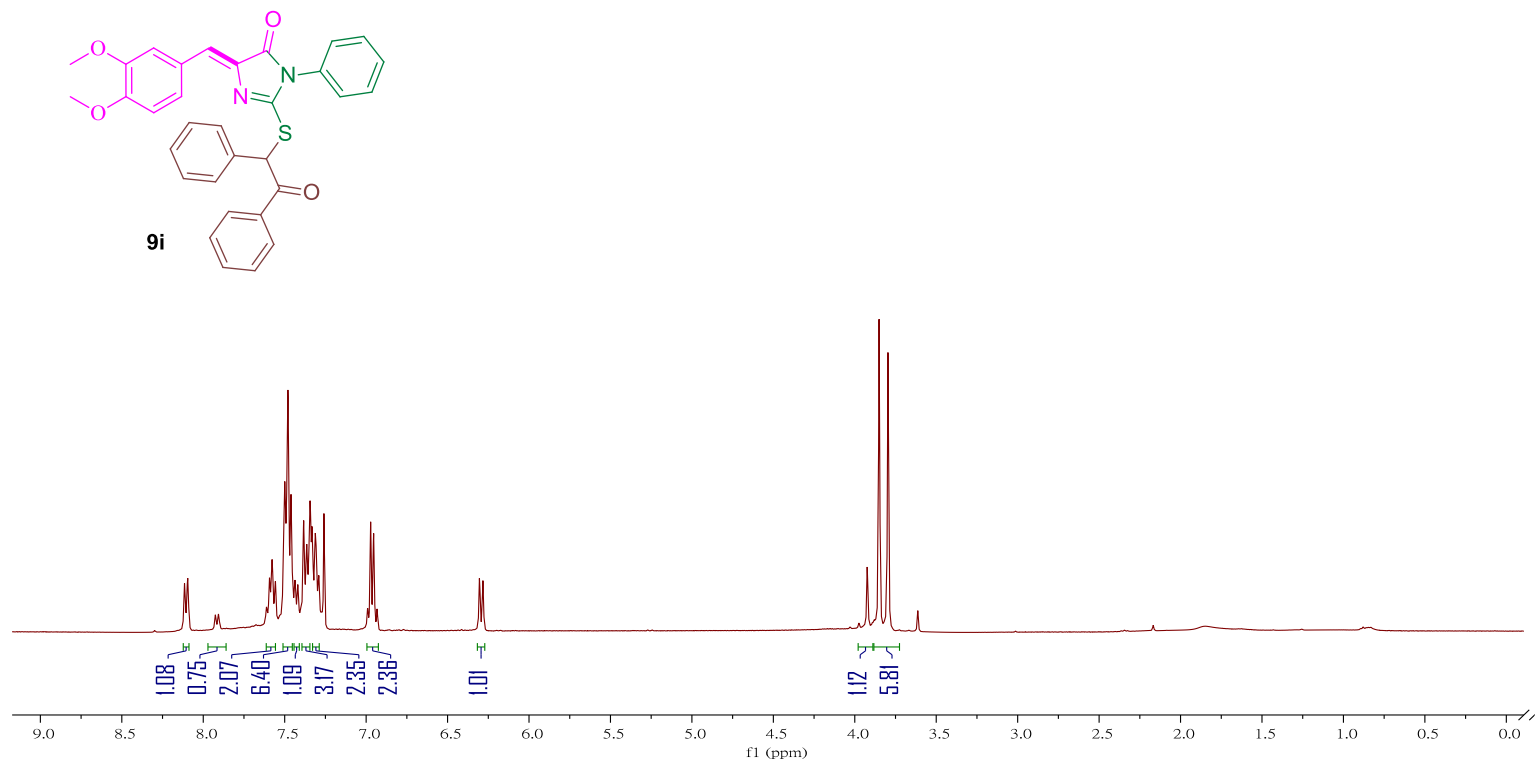
D:\FTIR FILES\201809\20180904\MIR_TR_DTGS_L247.0

MIR_TR_DTGS_L247

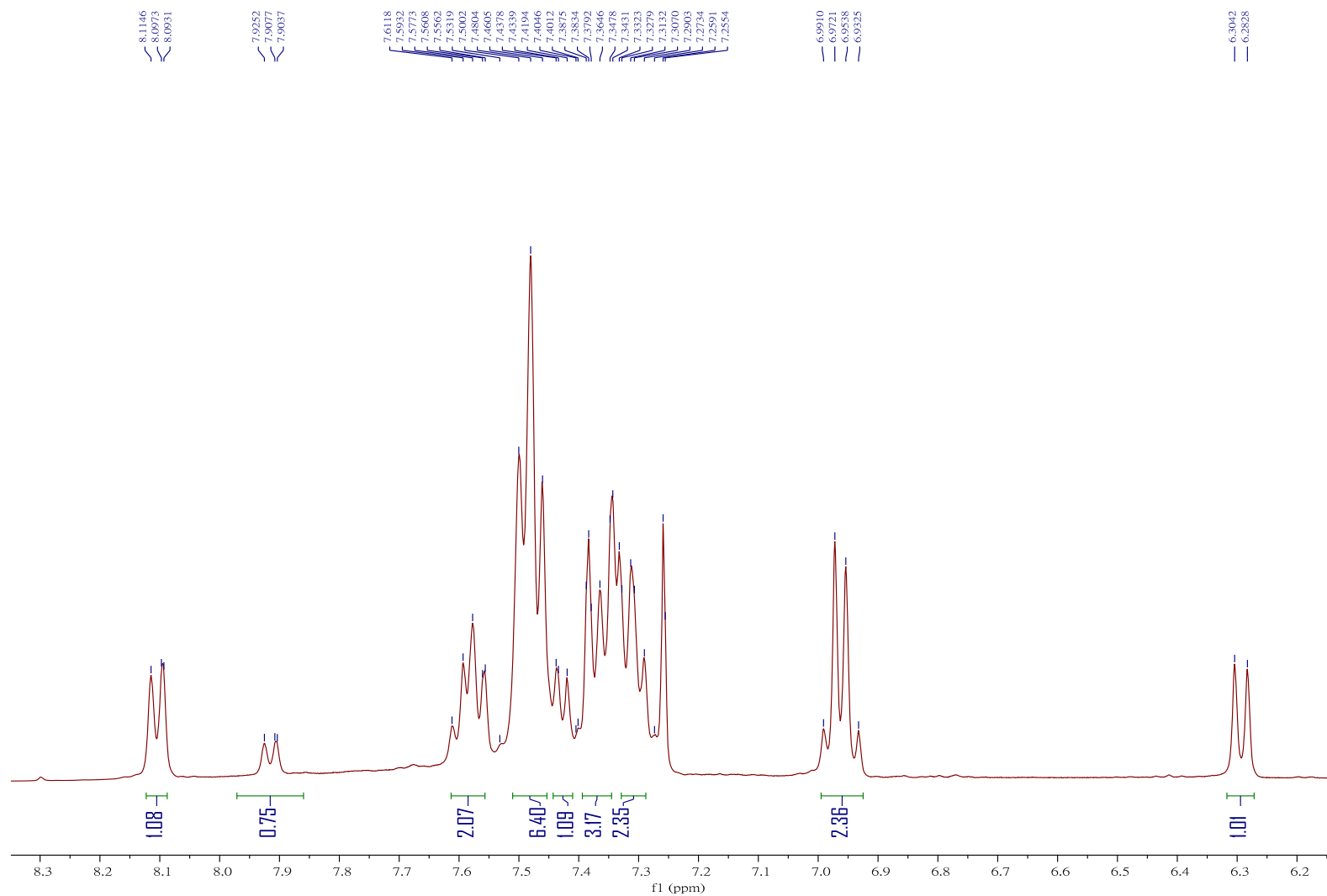
Instrument type and / or accessory

9/4/2018

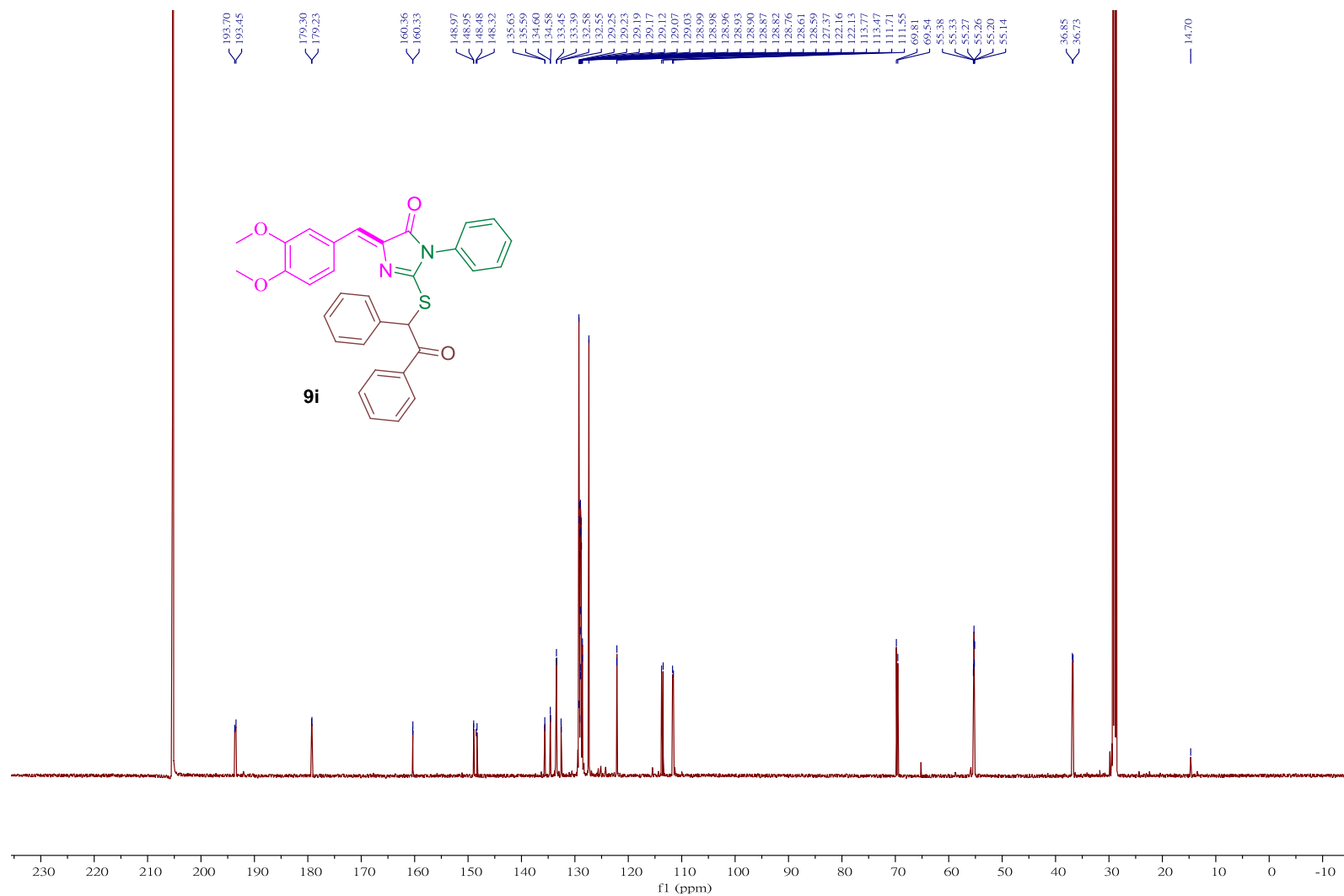
FT-IR Spectrum of compound 9h



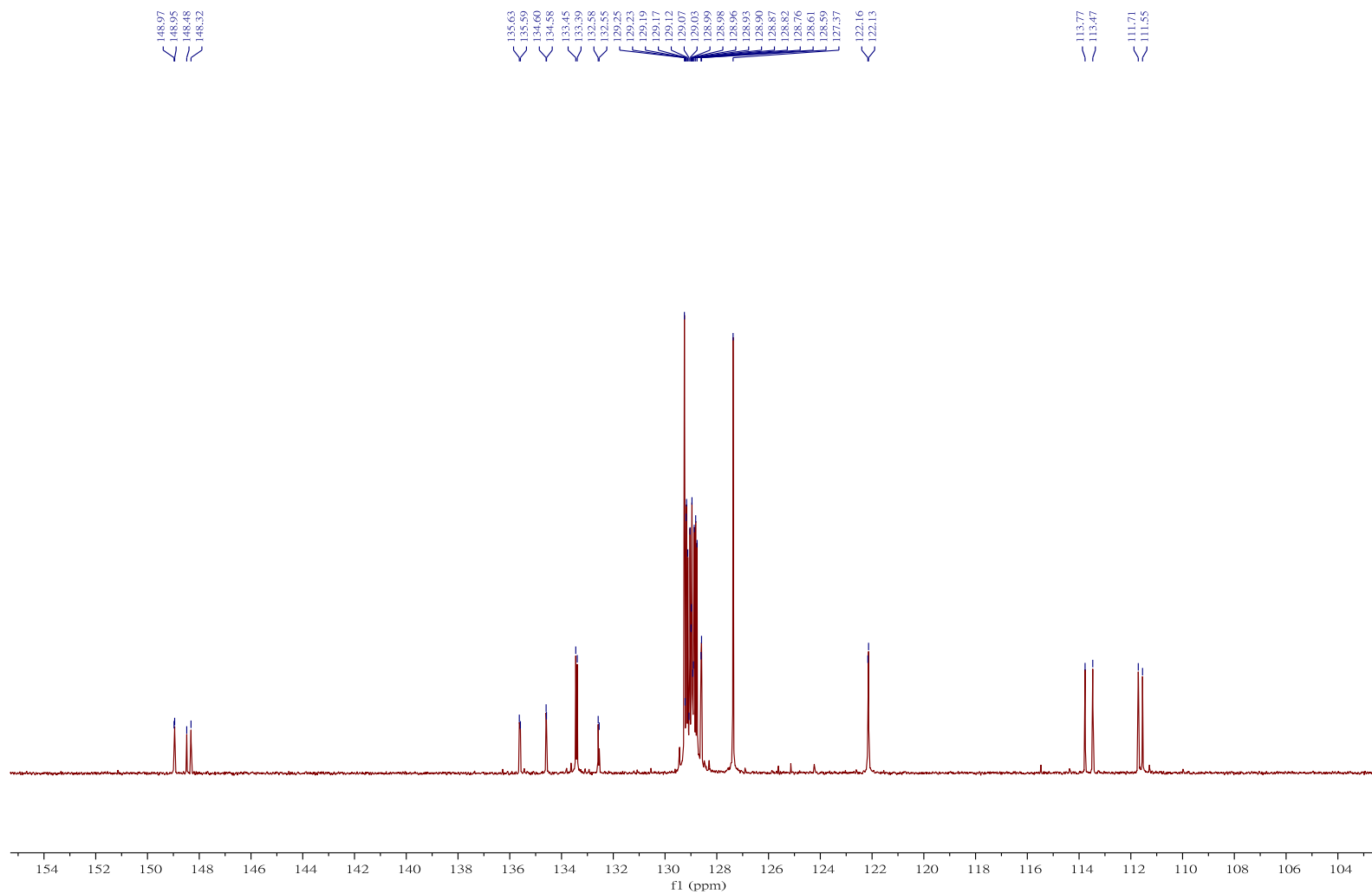
¹H NMR Spectrum (400 MHz) of compound **9i** in CDCl₃



Expansion of ¹H NMR Spectrum (400 MHz) of compound **9i** in CDCl₃



¹³C NMR Spectrum (101 MHz) of compound **9i in acetone-*d*₆**



Expansion of ^{13}C NMR Spectrum (101 MHz) of compound **9i** in acetone- d_6

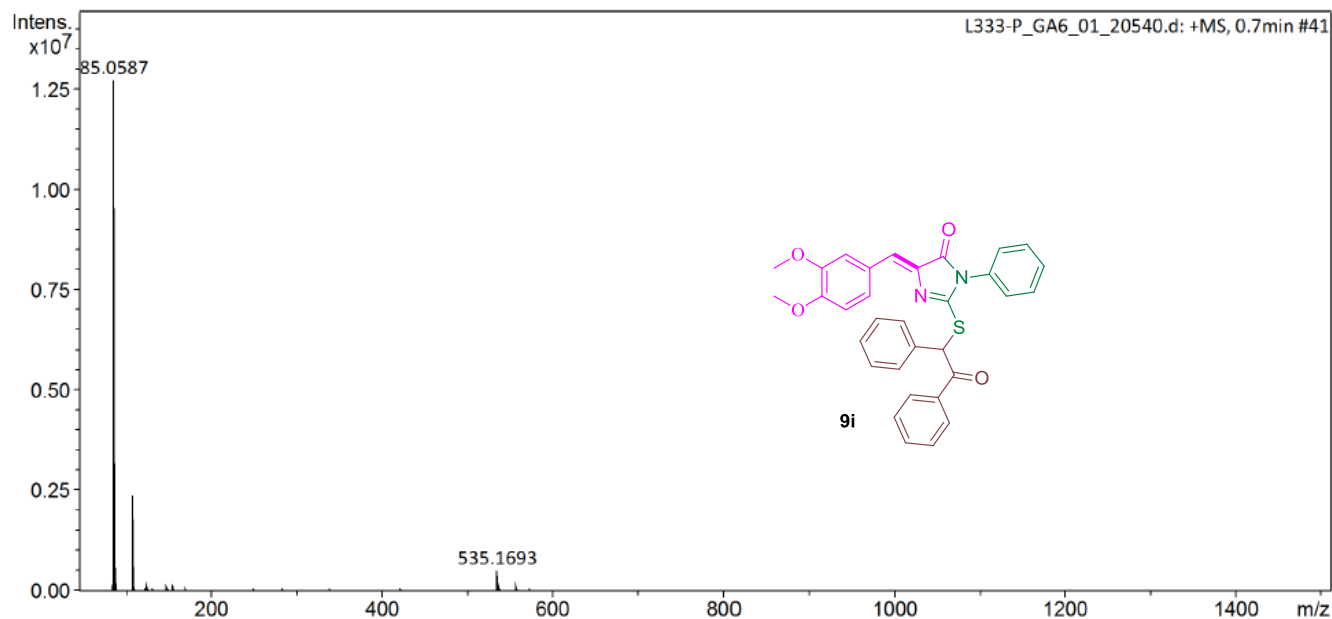
Display Report

Analysis Info

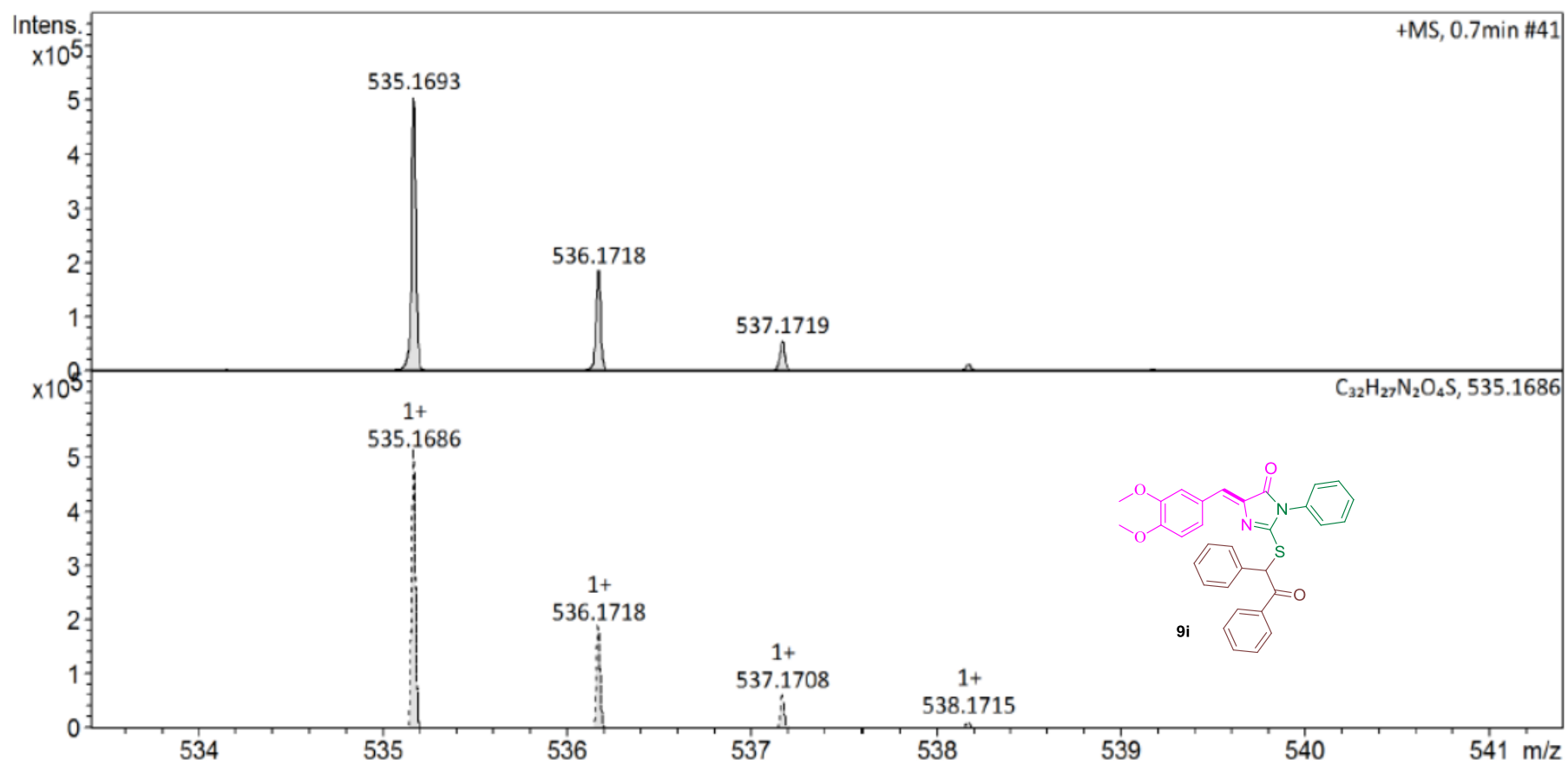
Analysis Name	D:\Data\ncu service\data\2018\20181018\L333-P_GA6_01_20540.d	Acquisition Date	10/18/2018 11:39:34 AM	
Method	Small molecule.m	Operator	NCTU	
Sample Name	L333-P	Instrument	impact HD	1819696.00164
Comment				

Acquisition Parameter

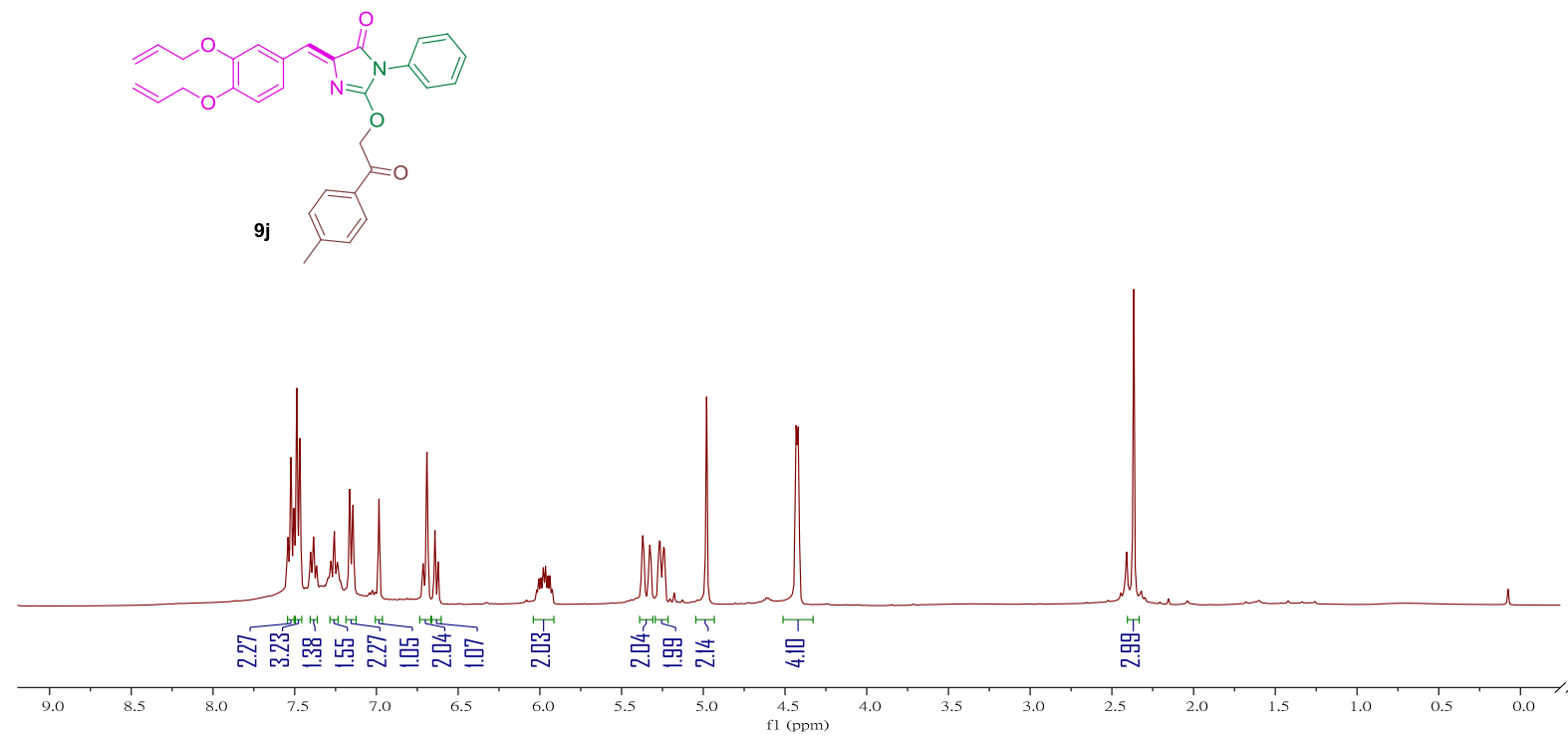
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



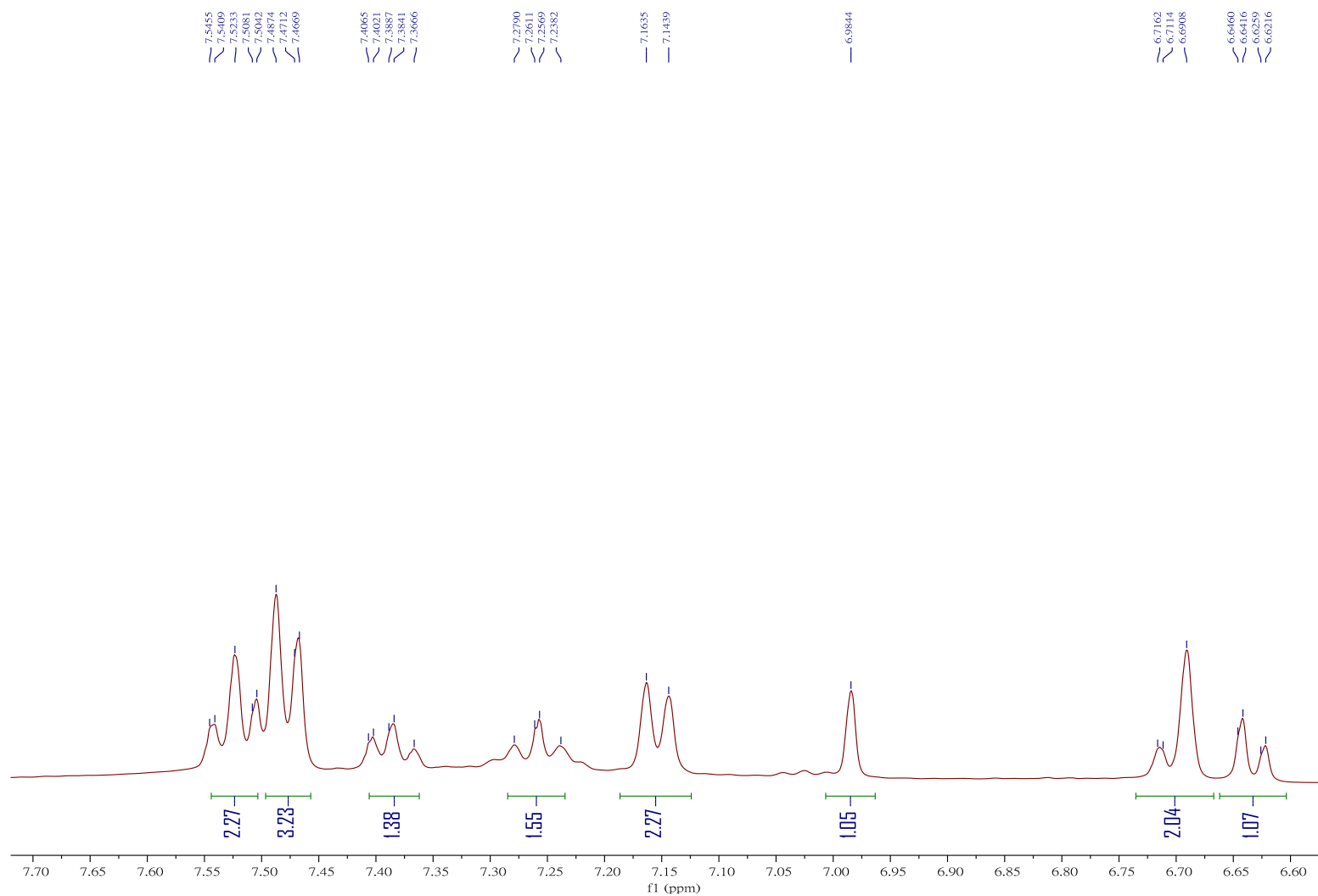
HRMS of compound **9i**



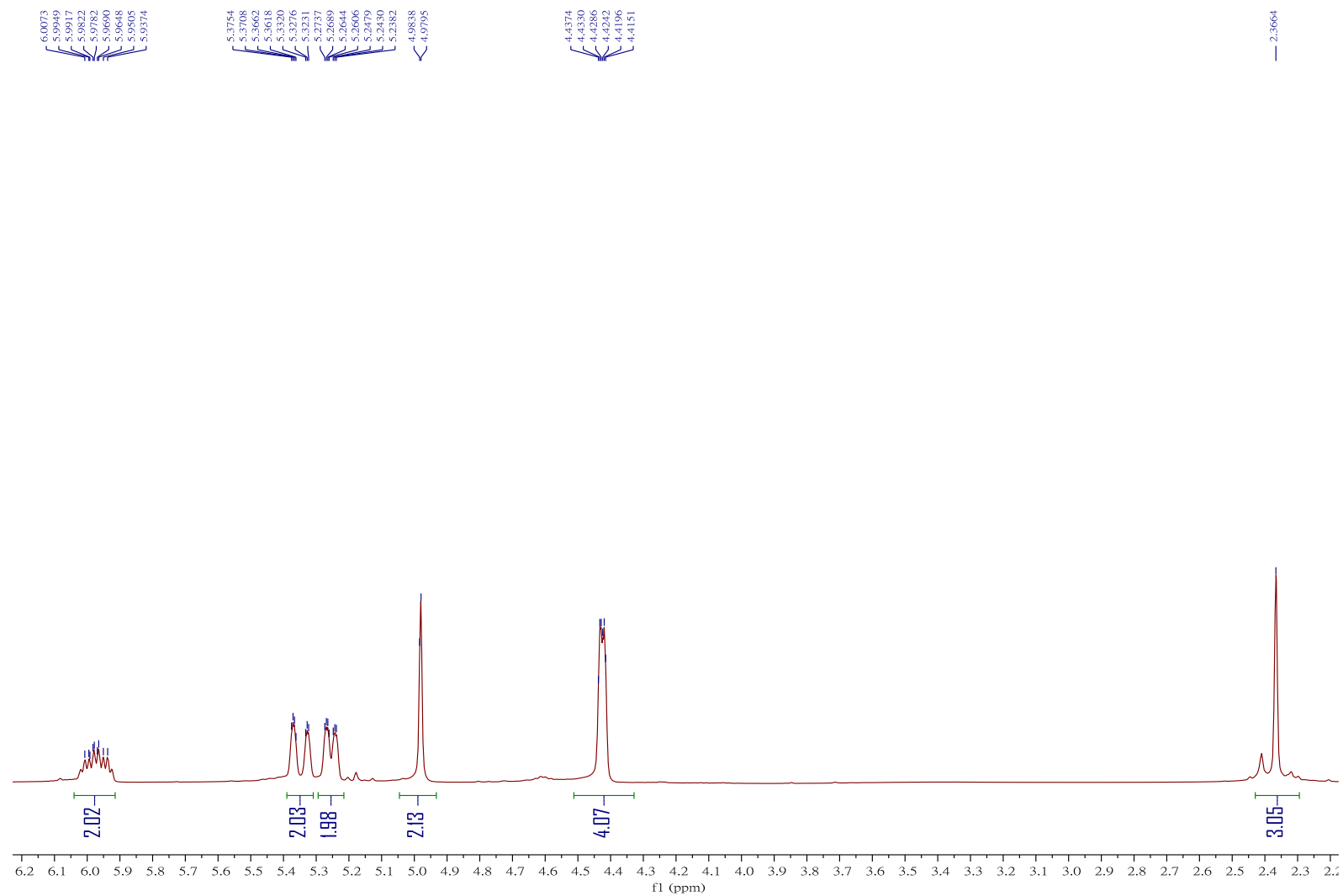
HRMS of compound **9i**



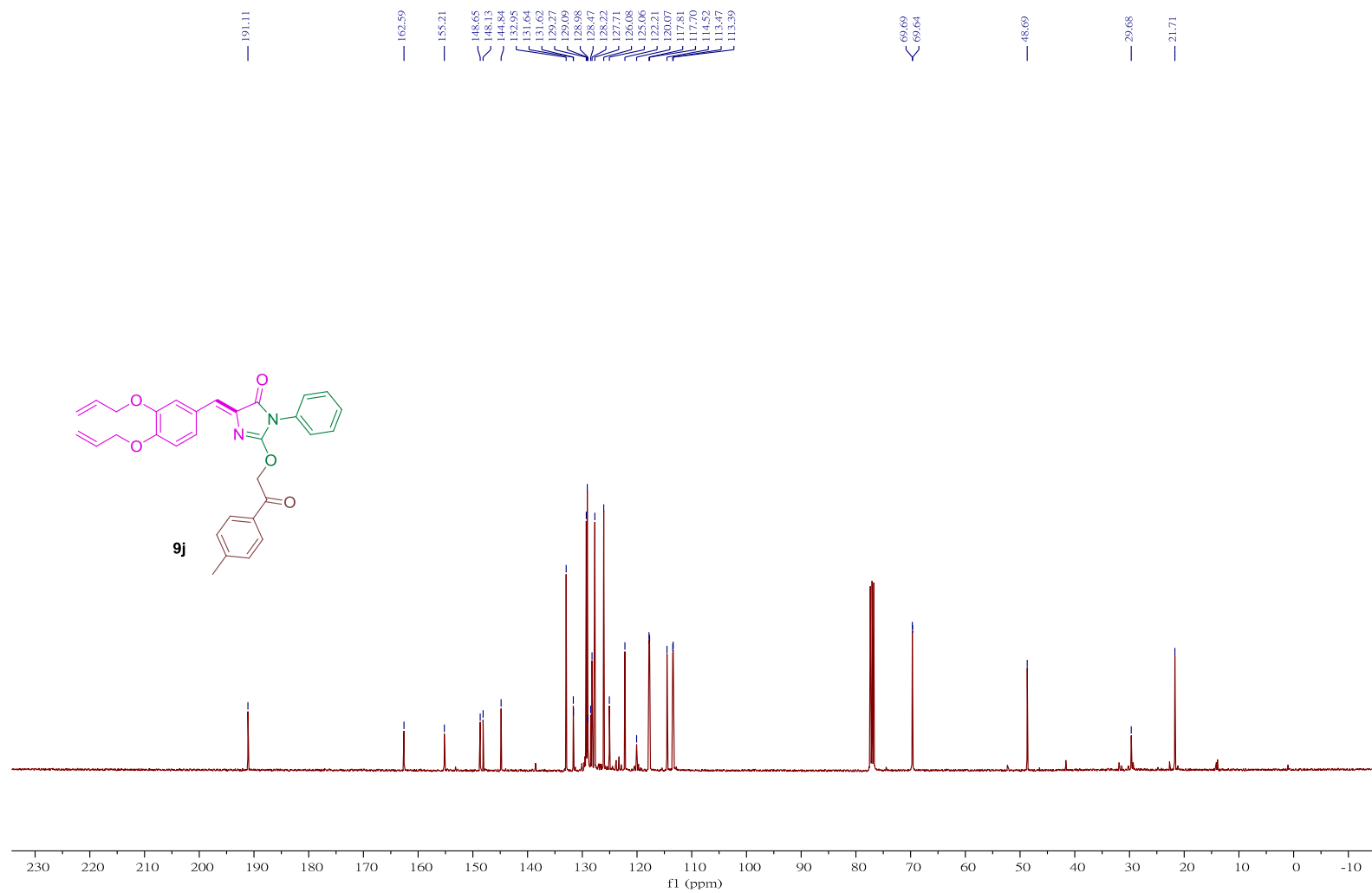
^1H NMR Spectrum (400 MHz) of compound **9j** in CDCl_3



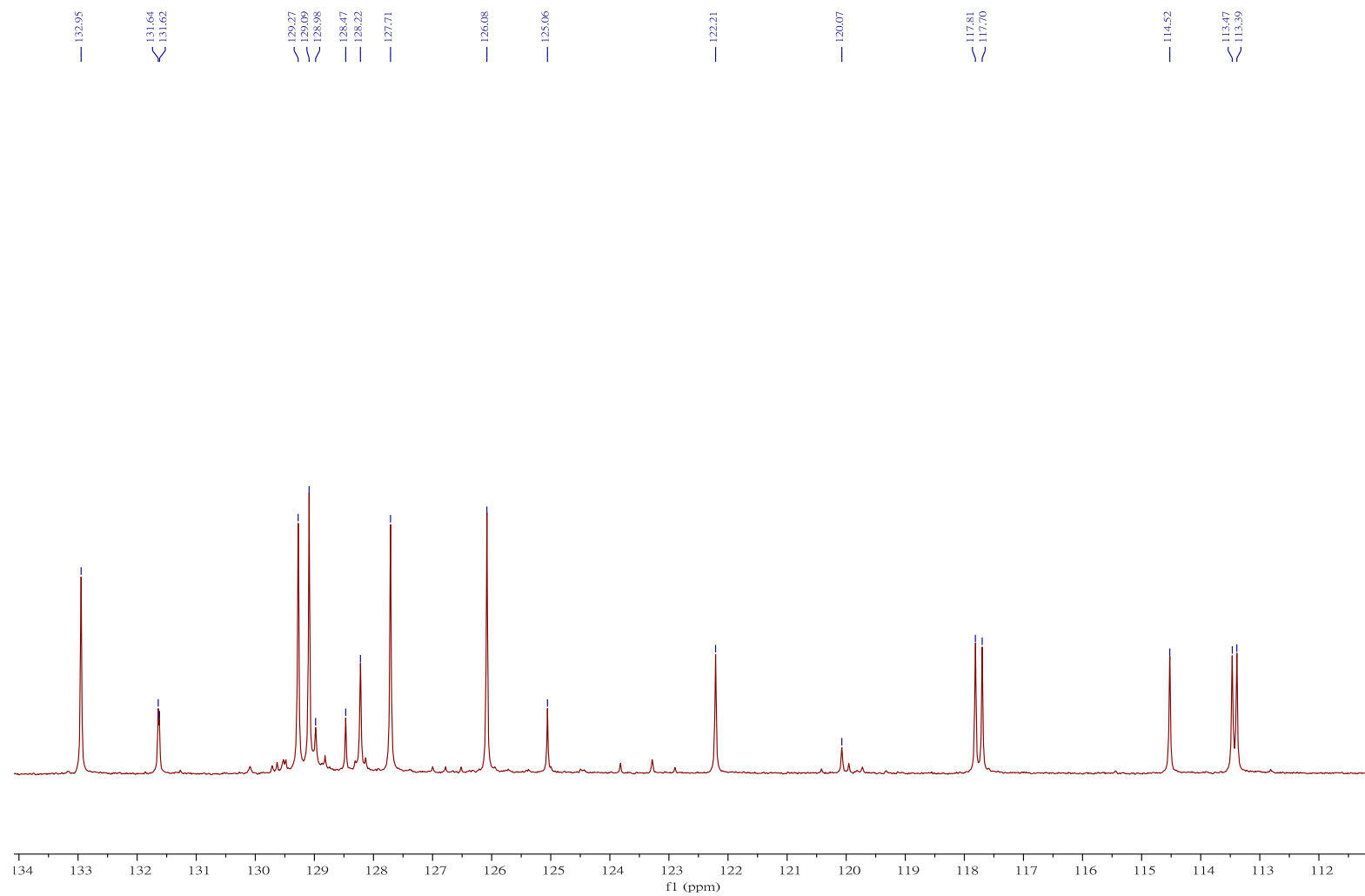
Expansion of ¹H NMR Spectrum (400 MHz) of compound **9j** in CDCl₃



Expansion of ^1H NMR Spectrum (400 MHz) of compound **9j** in CDCl_3



¹³C NMR Spectrum (101 MHz) of compound **9j in CDCl₃**



Expansion of ¹³C NMR Spectrum (101 MHz) of compound **9j** in CDCl₃

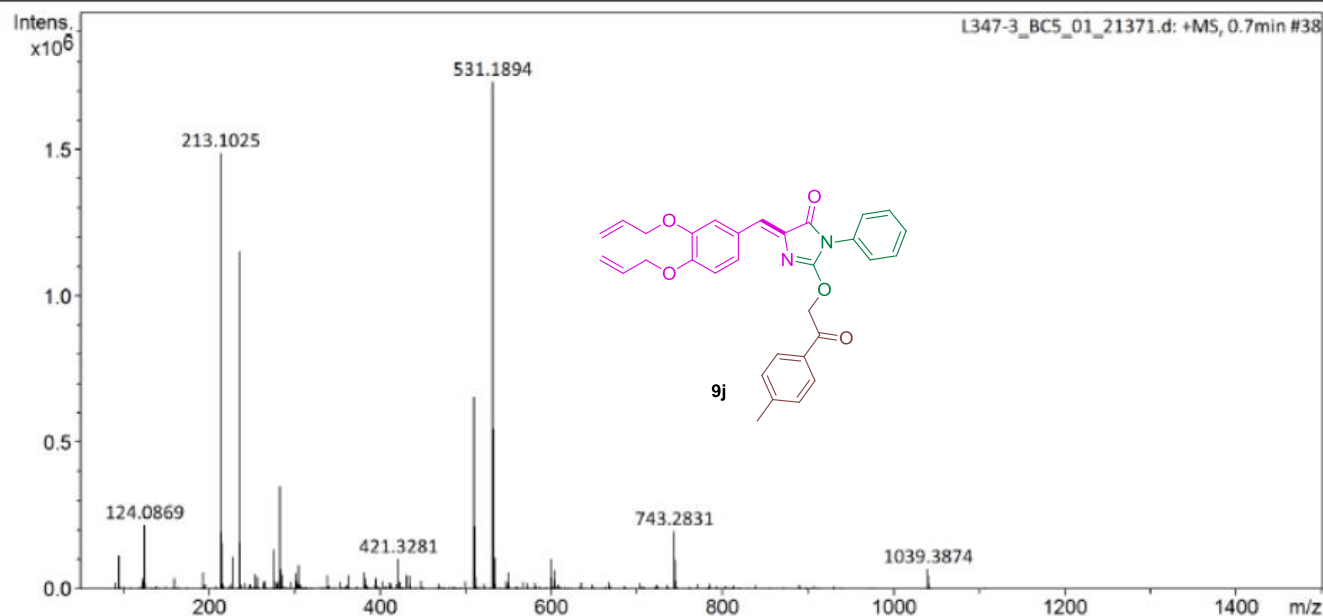
Display Report

Analysis Info

Analysis Name	D:\Data\NCTU SERVICE\Data\2018\20181130\L347-3_BC5_01_21371.d	Acquisition Date	11/30/2018 12:17:14 PM	
Method	Small molecule.m	Operator	NCTU	
Sample Name	L347-3	Instrument	impact HD	1819696.00164
Comment				

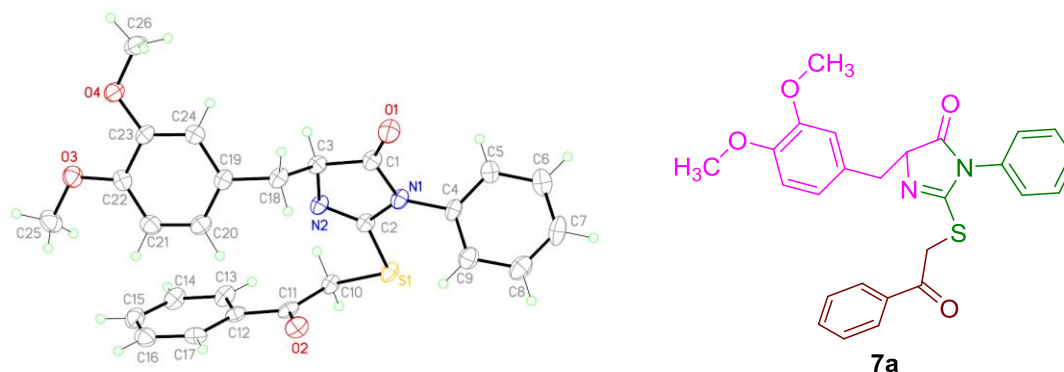
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



HRMS of compound **9j**

X-ray crystallographic data of compound 7a



ORTEP diagram of compound 7a. Atomic displacement ellipsoids are drawn at the 50% probability level

CCDC No.: 1884822

Table 1. Crystal data and structure refinement for 181208lt_0m_a.

Identification code	181208lt_0m_a	
Empirical formula	C ₂₆ H ₂₄ N ₂ O ₄ S	
Formula weight	460.53	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /c	
Unit cell dimensions	a = 14.9997(15) Å	$\alpha = 90^\circ$.
	b = 8.0616(7) Å	$\beta = 107.259(4)^\circ$.
	c = 20.034(2) Å	$\gamma = 90^\circ$.
Volume	2313.4(4) Å ³	
Z	4	
Density (calculated)	1.322 Mg/m ³	
Absorption coefficient	0.176 mm ⁻¹	
F(000)	968	
Crystal size	0.20 x 0.12 x 0.04 mm ³	
Theta range for data collection	1.422 to 26.506°.	

Index ranges	-18<=h<=18, -7<=k<=10, -25<=l<=24
Reflections collected	13728
Independent reflections	4756 [R(int) = 0.0835]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.2965
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4756 / 0 / 300
Goodness-of-fit on F ²	1.010
Final R indices [I>2sigma(I)]	R1 = 0.0760, wR2 = 0.1852
R indices (all data)	R1 = 0.0986, wR2 = 0.2052
Extinction coefficient	n/a
Largest diff. peak and hole	1.150 and -0.791 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 181208lt_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4269(2)	3016(3)	5244(2)	24(1)
C(2)	4656(2)	5252(3)	5951(1)	22(1)
C(3)	5304(2)	3047(3)	5642(1)	23(1)
C(4)	2945(2)	4884(3)	5256(2)	23(1)
C(5)	2516(2)	5167(4)	4550(1)	26(1)
C(6)	1584(2)	5620(4)	4332(2)	33(1)
C(7)	1090(2)	5803(4)	4815(2)	38(1)
C(8)	1523(2)	5504(4)	5513(2)	37(1)
C(9)	2449(2)	5034(4)	5742(2)	30(1)
C(10)	5613(2)	7552(3)	6822(1)	22(1)
C(11)	5997(2)	6431(3)	7448(1)	22(1)
C(12)	7015(2)	6546(3)	7826(1)	22(1)
C(13)	7606(2)	7658(4)	7627(2)	27(1)
C(14)	8553(2)	7666(4)	7975(2)	30(1)
C(15)	8925(2)	6567(4)	8509(2)	31(1)
C(16)	8343(2)	5477(4)	8721(2)	30(1)
C(17)	7393(2)	5484(4)	8387(1)	26(1)
C(18)	5573(2)	1511(3)	6110(1)	24(1)

C(19)	6608(2)	1467(3)	6481(1)	23(1)
C(20)	6981(2)	2114(4)	7146(2)	28(1)
C(21)	7938(2)	2119(4)	7462(2)	28(1)
C(22)	8542(2)	1472(4)	7124(1)	24(1)
C(23)	8168(2)	804(3)	6455(1)	23(1)
C(24)	7219(2)	811(3)	6139(1)	23(1)
C(25)	9897(2)	2229(4)	8042(2)	36(1)
C(26)	8456(2)	-532(5)	5483(2)	37(1)
N(1)	3906(1)	4406(3)	5484(1)	23(1)
N(2)	5459(1)	4585(3)	6051(1)	22(1)
O(1)	3836(1)	2026(3)	4825(1)	34(1)
O(2)	5498(1)	5479(3)	7648(1)	30(1)
O(3)	9495(1)	1409(3)	7395(1)	30(1)
O(4)	8817(1)	182(2)	6157(1)	28(1)
S(1)	4430(1)	7100(1)	6323(1)	24(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for 181208lt_0m_a.

C(1)-O(1)	1.201(3)
C(1)-N(1)	1.392(3)
C(1)-C(3)	1.519(4)
C(2)-N(2)	1.279(3)
C(2)-N(1)	1.408(3)
C(2)-S(1)	1.744(3)
C(3)-N(2)	1.466(3)
C(3)-C(18)	1.533(4)
C(3)-H(3)	1.0000
C(4)-C(5)	1.388(4)
C(4)-C(9)	1.394(4)
C(4)-N(1)	1.430(3)
C(5)-C(6)	1.384(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.390(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.379(5)
C(7)-H(7)	0.9500
C(8)-C(9)	1.380(4)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.515(4)
C(10)-S(1)	1.797(3)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-O(2)	1.220(3)
C(11)-C(12)	1.493(4)
C(12)-C(17)	1.393(4)
C(12)-C(13)	1.400(4)
C(13)-C(14)	1.384(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.374(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.389(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.383(4)

C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-C(19)	1.510(3)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.384(4)
C(19)-C(24)	1.400(4)
C(20)-C(21)	1.388(4)
C(20)-H(20)	0.9500
C(21)-C(22)	1.383(4)
C(21)-H(21)	0.9500
C(22)-O(3)	1.372(3)
C(22)-C(23)	1.399(4)
C(23)-C(24)	1.376(4)
C(23)-O(4)	1.378(3)
C(24)-H(24)	0.9500
C(25)-O(3)	1.420(3)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-O(4)	1.419(3)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
O(1)-C(1)-N(1)	126.2(3)
O(1)-C(1)-C(3)	129.4(2)
N(1)-C(1)-C(3)	104.4(2)
N(2)-C(2)-N(1)	115.4(2)
N(2)-C(2)-S(1)	125.9(2)
N(1)-C(2)-S(1)	118.62(18)
N(2)-C(3)-C(1)	106.0(2)
N(2)-C(3)-C(18)	111.9(2)
C(1)-C(3)-C(18)	110.5(2)
N(2)-C(3)-H(3)	109.5
C(1)-C(3)-H(3)	109.5
C(18)-C(3)-H(3)	109.5
C(5)-C(4)-C(9)	121.0(2)

C(5)-C(4)-N(1)	119.2(2)
C(9)-C(4)-N(1)	119.7(2)
C(6)-C(5)-C(4)	119.0(3)
C(6)-C(5)-H(5)	120.5
C(4)-C(5)-H(5)	120.5
C(5)-C(6)-C(7)	120.4(3)
C(5)-C(6)-H(6)	119.8
C(7)-C(6)-H(6)	119.8
C(8)-C(7)-C(6)	120.0(3)
C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0
C(7)-C(8)-C(9)	120.7(3)
C(7)-C(8)-H(8)	119.6
C(9)-C(8)-H(8)	119.6
C(8)-C(9)-C(4)	118.9(3)
C(8)-C(9)-H(9)	120.5
C(4)-C(9)-H(9)	120.5
C(11)-C(10)-S(1)	114.19(18)
C(11)-C(10)-H(10A)	108.7
S(1)-C(10)-H(10A)	108.7
C(11)-C(10)-H(10B)	108.7
S(1)-C(10)-H(10B)	108.7
H(10A)-C(10)-H(10B)	107.6
O(2)-C(11)-C(12)	120.5(2)
O(2)-C(11)-C(10)	121.9(2)
C(12)-C(11)-C(10)	117.6(2)
C(17)-C(12)-C(13)	118.9(3)
C(17)-C(12)-C(11)	118.8(2)
C(13)-C(12)-C(11)	122.3(2)
C(14)-C(13)-C(12)	120.1(3)
C(14)-C(13)-H(13)	119.9
C(12)-C(13)-H(13)	119.9
C(15)-C(14)-C(13)	120.5(3)
C(15)-C(14)-H(14)	119.7
C(13)-C(14)-H(14)	119.7
C(14)-C(15)-C(16)	119.9(3)
C(14)-C(15)-H(15)	120.0
C(16)-C(15)-H(15)	120.0

C(17)-C(16)-C(15)	120.0(3)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(12)	120.4(3)
C(16)-C(17)-H(17)	119.8
C(12)-C(17)-H(17)	119.8
C(19)-C(18)-C(3)	111.5(2)
C(19)-C(18)-H(18A)	109.3
C(3)-C(18)-H(18A)	109.3
C(19)-C(18)-H(18B)	109.3
C(3)-C(18)-H(18B)	109.3
H(18A)-C(18)-H(18B)	108.0
C(20)-C(19)-C(24)	118.5(2)
C(20)-C(19)-C(18)	121.9(2)
C(24)-C(19)-C(18)	119.6(2)
C(19)-C(20)-C(21)	120.5(2)
C(19)-C(20)-H(20)	119.7
C(21)-C(20)-H(20)	119.7
C(22)-C(21)-C(20)	120.9(3)
C(22)-C(21)-H(21)	119.5
C(20)-C(21)-H(21)	119.5
O(3)-C(22)-C(21)	125.2(2)
O(3)-C(22)-C(23)	116.1(2)
C(21)-C(22)-C(23)	118.7(2)
C(24)-C(23)-O(4)	124.7(2)
C(24)-C(23)-C(22)	120.3(2)
O(4)-C(23)-C(22)	115.0(2)
C(23)-C(24)-C(19)	120.9(3)
C(23)-C(24)-H(24)	119.5
C(19)-C(24)-H(24)	119.5
O(3)-C(25)-H(25A)	109.5
O(3)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
O(3)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
O(4)-C(26)-H(26A)	109.5
O(4)-C(26)-H(26B)	109.5

H(26A)-C(26)-H(26B)	109.5
O(4)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(1)-N(1)-C(2)	107.6(2)
C(1)-N(1)-C(4)	124.6(2)
C(2)-N(1)-C(4)	127.8(2)
C(2)-N(2)-C(3)	106.4(2)
C(22)-O(3)-C(25)	117.0(2)
C(23)-O(4)-C(26)	116.1(2)
C(2)-S(1)-C(10)	97.20(12)

Symmetry transformations used to generate equivalent atoms:

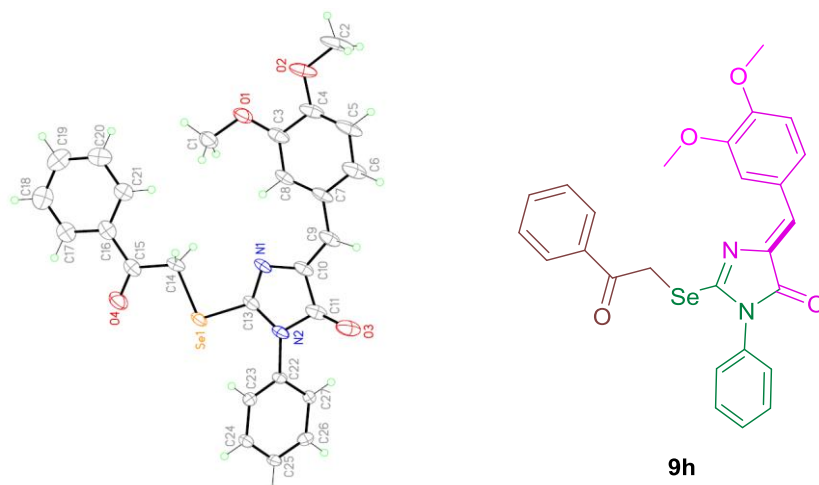
Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 181208lt_0m_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	26(1)	16(2)	31(2)	0(1)	10(1)	0(1)
C(2)	21(1)	18(2)	27(1)	-1(1)	8(1)	-1(1)
C(3)	25(1)	17(2)	28(1)	-2(1)	10(1)	-1(1)
C(4)	18(1)	16(1)	36(2)	2(1)	8(1)	1(1)
C(5)	22(1)	24(2)	32(2)	4(1)	6(1)	-4(1)
C(6)	28(2)	26(2)	42(2)	10(1)	4(1)	-4(1)
C(7)	18(1)	33(2)	60(2)	10(2)	8(1)	2(1)
C(8)	26(2)	40(2)	51(2)	-2(2)	19(1)	-2(1)
C(9)	26(2)	28(2)	37(2)	3(1)	12(1)	0(1)
C(10)	20(1)	16(1)	31(1)	-4(1)	9(1)	-2(1)
C(11)	27(1)	14(1)	31(1)	-5(1)	16(1)	-1(1)
C(12)	27(1)	16(1)	26(1)	-4(1)	13(1)	0(1)
C(13)	26(1)	20(2)	37(2)	1(1)	13(1)	-1(1)
C(14)	26(1)	24(2)	41(2)	-2(1)	14(1)	-3(1)
C(15)	26(1)	30(2)	36(2)	-6(1)	8(1)	3(1)
C(16)	38(2)	26(2)	26(1)	-1(1)	8(1)	4(1)
C(17)	35(2)	23(2)	24(1)	-3(1)	14(1)	-2(1)
C(18)	24(1)	17(1)	34(2)	0(1)	11(1)	-1(1)
C(19)	25(1)	12(1)	32(1)	2(1)	9(1)	1(1)
C(20)	32(2)	21(2)	33(2)	-3(1)	12(1)	2(1)
C(21)	35(2)	22(2)	26(1)	-3(1)	7(1)	1(1)
C(22)	27(1)	17(1)	27(1)	2(1)	5(1)	-2(1)
C(23)	26(1)	15(1)	31(1)	2(1)	12(1)	2(1)
C(24)	28(1)	14(1)	26(1)	0(1)	8(1)	-2(1)
C(25)	30(2)	42(2)	31(2)	-6(1)	2(1)	-9(1)
C(26)	31(2)	47(2)	37(2)	-12(2)	14(1)	2(1)
N(1)	20(1)	17(1)	32(1)	-3(1)	7(1)	0(1)
N(2)	21(1)	14(1)	30(1)	-1(1)	9(1)	0(1)
O(1)	30(1)	24(1)	44(1)	-11(1)	5(1)	-2(1)
O(2)	31(1)	27(1)	37(1)	2(1)	16(1)	-5(1)
O(3)	24(1)	29(1)	33(1)	-4(1)	5(1)	-3(1)
O(4)	26(1)	29(1)	31(1)	-5(1)	10(1)	0(1)
S(1)	20(1)	17(1)	35(1)	-4(1)	9(1)	2(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 181208lt_0m_a.

	x	y	z	U(eq)
H(3)	5676	3073	5303	27
H(5)	2857	5052	4222	32
H(6)	1280	5806	3850	40
H(7)	453	6135	4663	45
H(8)	1181	5622	5841	45
H(9)	2745	4816	6223	36
H(10A)	6016	7456	6512	27
H(10B)	5646	8715	6986	27
H(13)	7357	8408	7253	32
H(14)	8949	8437	7843	36
H(15)	9579	6553	8734	37
H(16)	8599	4727	9094	36
H(17)	6996	4759	8542	32
H(18A)	5226	1516	6460	29
H(18B)	5393	500	5820	29
H(20)	6577	2559	7387	34
H(21)	8183	2572	7918	34
H(24)	6974	365	5682	27
H(25A)	9712	3399	7998	54
H(25B)	10579	2147	8169	54
H(25C)	9677	1706	8406	54
H(26A)	8042	-1458	5506	56
H(26B)	8972	-939	5322	56
H(26C)	8103	307	5156	56

X-ray crystallographic data of compound 9h



ORTEP diagram of compound 9h. Atomic displacement ellipsoids are drawn at the 50% probability level

CCDC No.: 1882293

Table 1. Crystal data and structure refinement for mo_180912lt_0m_b.

Identification code	mo_180912LT_0m_b	
Empirical formula	C ₂₆ H ₂₂ N ₂ O ₄ Se	
Formula weight	505.41	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 5.0331(3) Å	$\alpha = 90^\circ$.
	b = 12.9922(8) Å	$\beta = 93.403(2)^\circ$.
	c = 17.1983(11) Å	$\gamma = 90^\circ$.
Volume	1122.63(12) Å ³	
Z	2	
Density (calculated)	1.495 Mg/m ³	
Absorption coefficient	1.709 mm ⁻¹	
F(000)	516	
Crystal size	0.20 x 0.10 x 0.09 mm ³	
Theta range for data collection	1.966 to 26.482°.	
Index ranges	-6 ≤ h ≤ 5, -16 ≤ k ≤ 16, -21 ≤ l ≤ 21	
Reflections collected	19872	
Independent reflections	4603 [R(int) = 0.0465]	

Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6698
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4603 / 217 / 355
Goodness-of-fit on F ²	1.077
Final R indices [I>2sigma(I)]	R1 = 0.0335, wR2 = 0.0644
R indices (all data)	R1 = 0.0394, wR2 = 0.0658
Absolute structure parameter	0.031(8)
Extinction coefficient	n/a
Largest diff. peak and hole	0.349 and -0.628 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_180912lt_0m_b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Se(1)	2258(1)	2815(1)	7472(1)	28(1)
O(1)	5717(5)	7873(3)	6605(2)	44(1)
O(2)	9129(7)	9253(2)	7034(2)	47(1)
O(3)	9792(8)	3516(3)	9557(2)	47(1)
O(4)	-1765(5)	2774(4)	6264(2)	40(1)
N(1)	5893(7)	4427(2)	7911(2)	24(1)
N(2)	6314(6)	3014(3)	8683(2)	24(1)
C(1)	3753(9)	7127(4)	6358(3)	43(1)
C(2)	11139(13)	10020(4)	7223(3)	63(2)
C(3)	7445(9)	7592(3)	7203(3)	33(1)
C(4)	9313(11)	8357(3)	7453(3)	35(1)
C(5)	11113(12)	8159(3)	8064(3)	47(2)
C(6)	11145(12)	7203(4)	8434(3)	44(2)
C(7)	9370(9)	6435(3)	8191(3)	30(1)
C(8)	7524(8)	6639(3)	7577(3)	28(1)
C(9)	9474(9)	5456(3)	8602(3)	33(1)
C(10)	7949(10)	4604(3)	8484(3)	26(1)
C(11)	8293(10)	3685(3)	8995(3)	31(1)
C(13)	5027(8)	3504(3)	8053(3)	25(1)

C(14)	1362(9)	3979(3)	6791(3)	27(1)
C(15)	-877(8)	3649(4)	6234(3)	28(1)
C(16)	-1966(9)	4394(3)	5642(3)	30(1)
C(17)	-4112(9)	4125(4)	5137(3)	38(1)
C(18)	-5128(11)	4797(4)	4585(3)	47(1)
C(19)	-4033(10)	5769(4)	4509(3)	45(1)
C(20)	-1877(11)	6053(4)	4994(3)	46(1)
C(21)	-859(10)	5370(4)	5561(3)	37(1)
C(22)	5970(50)	1953(12)	9015(12)	19(3)
C(23)	3565(18)	1683(6)	9277(5)	22(2)
C(24)	3158(17)	663(6)	9513(5)	26(2)
C(25)	5220(40)	-27(12)	9524(10)	25(2)
C(26)	7681(17)	251(6)	9282(5)	26(2)
C(27)	8133(15)	1258(6)	9031(5)	20(2)
C(22')	5900(50)	2005(13)	8877(13)	20(3)
C(23')	5077(17)	1806(6)	9603(5)	21(2)
C(24')	4945(17)	781(6)	9855(6)	26(2)
C(25')	5510(40)	-19(12)	9355(11)	26(3)
C(26')	6217(16)	197(6)	8619(5)	27(2)
C(27')	6416(18)	1193(6)	8357(5)	23(2)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for mo_180912lt_0m_b.

Se(1)-C(13)	1.892(4)
Se(1)-C(14)	1.949(4)
O(1)-C(3)	1.357(6)
O(1)-C(1)	1.431(6)
O(2)-C(4)	1.371(5)
O(2)-C(2)	1.443(6)
O(3)-C(11)	1.210(6)
O(4)-C(15)	1.224(7)
N(1)-C(13)	1.304(5)
N(1)-C(10)	1.405(6)
N(2)-C(22')	1.372(17)
N(2)-C(13)	1.383(6)
N(2)-C(11)	1.406(6)
N(2)-C(22)	1.506(16)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-C(8)	1.395(6)
C(3)-C(4)	1.416(6)
C(4)-C(5)	1.370(7)
C(5)-C(6)	1.395(6)
C(5)-H(5)	0.9500
C(6)-C(7)	1.388(6)
C(6)-H(6)	0.9500
C(7)-C(8)	1.389(6)
C(7)-C(9)	1.454(6)
C(8)-H(8)	0.9500
C(9)-C(10)	1.355(6)
C(9)-H(9)	0.9500
C(10)-C(11)	1.487(6)
C(14)-C(15)	1.498(6)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900

C(15)-C(16)	1.485(7)
C(16)-C(17)	1.390(6)
C(16)-C(21)	1.395(6)
C(17)-C(18)	1.366(7)
C(17)-H(17)	0.9500
C(18)-C(19)	1.387(8)
C(18)-H(18)	0.9500
C(19)-C(20)	1.379(7)
C(19)-H(19)	0.9500
C(20)-C(21)	1.393(7)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(23)	1.36(2)
C(22)-C(27)	1.414(19)
C(23)-C(24)	1.404(10)
C(23)-H(23)	0.9500
C(24)-C(25)	1.371(17)
C(24)-H(24)	0.9500
C(25)-C(26)	1.378(18)
C(25)-H(25)	0.9500
C(26)-C(27)	1.400(10)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(22')-C(23')	1.363(17)
C(22')-C(27')	1.417(19)
C(23')-C(24')	1.403(10)
C(23')-H(23')	0.9500
C(24')-C(25')	1.389(17)
C(24')-H(24')	0.9500
C(25')-C(26')	1.363(16)
C(25')-H(25')	0.9500
C(26')-C(27')	1.376(11)
C(26')-H(26')	0.9500
C(27')-H(27')	0.9500
C(13)-Se(1)-C(14)	94.99(18)
C(3)-O(1)-C(1)	116.4(4)
C(4)-O(2)-C(2)	116.3(4)

C(13)-N(1)-C(10)	105.0(4)
C(22')-N(2)-C(13)	124.0(13)
C(22')-N(2)-C(11)	127.8(13)
C(13)-N(2)-C(11)	107.6(3)
C(13)-N(2)-C(22)	131.2(11)
C(11)-N(2)-C(22)	121.2(11)
O(1)-C(1)-H(1A)	109.5
O(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
O(2)-C(2)-H(2A)	109.5
O(2)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
O(2)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
O(1)-C(3)-C(8)	126.0(4)
O(1)-C(3)-C(4)	115.2(4)
C(8)-C(3)-C(4)	118.8(5)
C(5)-C(4)-O(2)	125.7(4)
C(5)-C(4)-C(3)	119.9(4)
O(2)-C(4)-C(3)	114.4(5)
C(4)-C(5)-C(6)	120.3(4)
C(4)-C(5)-H(5)	119.8
C(6)-C(5)-H(5)	119.8
C(7)-C(6)-C(5)	120.9(5)
C(7)-C(6)-H(6)	119.6
C(5)-C(6)-H(6)	119.6
C(6)-C(7)-C(8)	118.7(4)
C(6)-C(7)-C(9)	118.6(5)
C(8)-C(7)-C(9)	122.7(4)
C(7)-C(8)-C(3)	121.3(4)
C(7)-C(8)-H(8)	119.3
C(3)-C(8)-H(8)	119.3
C(10)-C(9)-C(7)	129.7(5)
C(10)-C(9)-H(9)	115.2

C(7)-C(9)-H(9)	115.2
C(9)-C(10)-N(1)	128.7(4)
C(9)-C(10)-C(11)	121.6(5)
N(1)-C(10)-C(11)	109.8(4)
O(3)-C(11)-N(2)	126.0(4)
O(3)-C(11)-C(10)	131.5(4)
N(2)-C(11)-C(10)	102.5(4)
N(1)-C(13)-N(2)	115.1(4)
N(1)-C(13)-Se(1)	125.4(4)
N(2)-C(13)-Se(1)	119.5(3)
C(15)-C(14)-Se(1)	107.5(3)
C(15)-C(14)-H(14A)	110.2
Se(1)-C(14)-H(14A)	110.2
C(15)-C(14)-H(14B)	110.2
Se(1)-C(14)-H(14B)	110.2
H(14A)-C(14)-H(14B)	108.5
O(4)-C(15)-C(16)	120.9(4)
O(4)-C(15)-C(14)	120.1(4)
C(16)-C(15)-C(14)	119.0(4)
C(17)-C(16)-C(21)	117.8(5)
C(17)-C(16)-C(15)	120.4(4)
C(21)-C(16)-C(15)	121.8(4)
C(18)-C(17)-C(16)	121.2(5)
C(18)-C(17)-H(17)	119.4
C(16)-C(17)-H(17)	119.4
C(17)-C(18)-C(19)	120.9(5)
C(17)-C(18)-H(18)	119.6
C(19)-C(18)-H(18)	119.6
C(20)-C(19)-C(18)	119.3(5)
C(20)-C(19)-H(19)	120.4
C(18)-C(19)-H(19)	120.4
C(19)-C(20)-C(21)	119.8(5)
C(19)-C(20)-H(20)	120.1
C(21)-C(20)-H(20)	120.1
C(20)-C(21)-C(16)	121.1(5)
C(20)-C(21)-H(21)	119.5
C(16)-C(21)-H(21)	119.5
C(23)-C(22)-C(27)	121.8(12)

C(23)-C(22)-N(2)	119.1(13)
C(27)-C(22)-N(2)	119.0(14)
C(22)-C(23)-C(24)	119.1(9)
C(22)-C(23)-H(23)	120.4
C(24)-C(23)-H(23)	120.4
C(25)-C(24)-C(23)	119.9(10)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
C(24)-C(25)-C(26)	121.2(12)
C(24)-C(25)-H(25)	119.4
C(26)-C(25)-H(25)	119.4
C(25)-C(26)-C(27)	120.2(9)
C(25)-C(26)-H(26)	119.9
C(27)-C(26)-H(26)	119.9
C(26)-C(27)-C(22)	117.6(10)
C(26)-C(27)-H(27)	121.2
C(22)-C(27)-H(27)	121.2
C(23')-C(22')-N(2)	117.6(14)
C(23')-C(22')-C(27')	120.9(13)
N(2)-C(22')-C(27')	121.4(12)
C(22')-C(23')-C(24')	119.1(10)
C(22')-C(23')-H(23')	120.4
C(24')-C(23')-H(23')	120.4
C(25')-C(24')-C(23')	120.2(10)
C(25')-C(24')-H(24')	119.9
C(23')-C(24')-H(24')	119.9
C(26')-C(25')-C(24')	119.7(12)
C(26')-C(25')-H(25')	120.1
C(24')-C(25')-H(25')	120.1
C(25')-C(26')-C(27')	121.7(10)
C(25')-C(26')-H(26')	119.2
C(27')-C(26')-H(26')	119.2
C(26')-C(27')-C(22')	118.3(10)
C(26')-C(27')-H(27')	120.9
C(22')-C(27')-H(27')	120.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_180912lt_0m_b. 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}
Se(1)	20(1)	15(1)	50(1)	0(1)	5(1)	-5(1)
O(1)	34(2)	25(2)	73(2)	9(2)	4(2)	-7(2)
O(2)	76(3)	18(2)	49(2)	-3(2)	21(2)	-15(2)
O(3)	82(3)	33(2)	24(2)	-1(2)	-6(2)	-26(2)
O(4)	38(2)	30(2)	50(2)	-6(2)	0(1)	-12(2)
N(1)	23(2)	16(2)	34(2)	-5(2)	13(2)	-6(1)
N(2)	23(2)	14(2)	36(2)	-3(2)	11(2)	-4(1)
C(1)	29(3)	34(3)	66(4)	9(3)	8(3)	-4(2)
C(2)	129(6)	29(3)	34(3)	-10(2)	26(3)	-44(3)
C(3)	35(2)	19(3)	46(3)	-6(2)	20(2)	-4(2)
C(4)	59(3)	18(2)	30(3)	-10(2)	22(3)	-12(2)
C(5)	85(4)	30(2)	28(3)	-12(2)	11(3)	-36(3)
C(6)	75(4)	37(3)	20(3)	-7(2)	3(3)	-30(3)
C(7)	43(3)	22(2)	26(3)	-9(2)	16(2)	-15(2)
C(8)	31(3)	19(2)	37(3)	-9(2)	15(2)	-10(2)
C(9)	49(3)	29(2)	21(3)	-9(2)	10(2)	-20(2)
C(10)	36(3)	21(2)	23(3)	-7(2)	12(2)	-10(2)
C(11)	48(3)	22(2)	23(3)	-9(2)	13(2)	-11(2)
C(13)	17(2)	14(2)	45(3)	-5(2)	12(2)	0(2)
C(14)	30(2)	19(2)	31(3)	-1(2)	10(2)	-7(2)
C(15)	25(2)	28(2)	31(3)	-9(2)	12(2)	-3(2)
C(16)	28(2)	35(2)	27(3)	-11(2)	13(2)	-2(2)
C(17)	37(3)	38(3)	38(3)	-8(2)	7(2)	0(2)
C(18)	51(3)	51(3)	39(3)	-14(3)	1(3)	6(3)
C(19)	57(3)	50(3)	28(3)	-4(2)	9(3)	19(3)
C(20)	57(3)	37(3)	46(4)	1(2)	15(3)	0(3)
C(21)	39(3)	34(3)	39(3)	-1(2)	4(2)	-5(2)
C(22)	23(4)	10(4)	23(6)	-3(4)	2(5)	-1(4)
C(23)	21(4)	23(3)	23(4)	3(3)	1(4)	0(3)
C(24)	25(4)	26(4)	27(4)	6(3)	1(4)	-9(3)
C(25)	28(5)	18(4)	28(6)	6(4)	-4(4)	-8(4)
C(26)	29(4)	18(3)	31(4)	4(3)	0(4)	4(3)

C(27)	18(3)	19(3)	24(4)	1(3)	0(3)	-2(3)
C(22')	19(4)	17(4)	24(6)	1(4)	7(5)	0(4)
C(23')	16(4)	19(3)	28(4)	2(3)	5(4)	-2(3)
C(24')	17(4)	28(4)	33(4)	10(3)	3(4)	-6(3)
C(25')	23(5)	14(4)	40(6)	7(4)	-4(5)	-2(4)
C(26')	22(4)	18(3)	43(4)	-3(3)	-1(4)	3(3)
C(27')	19(4)	19(4)	30(5)	-3(3)	4(4)	-1(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for mo_180912lt_0m_b.

	x	y	z	U(eq)
H(1A)	4634	6516	6159	64
H(1B)	2563	7421	5944	64
H(1C)	2719	6932	6800	64
H(2A)	11099	10205	7775	95
H(2B)	10787	10633	6902	95
H(2C)	12895	9742	7121	95
H(5)	12347	8676	8236	57
H(6)	12399	7077	8858	53
H(8)	6291	6120	7409	34
H(9)	10810	5407	9014	39
H(14A)	812	4576	7102	32
H(14B)	2925	4183	6503	32
H(17)	-4885	3462	5176	45
H(18)	-6603	4597	4249	57
H(19)	-4761	6235	4128	54
H(20)	-1088	6712	4942	55
H(21)	613	5572	5898	45
H(23)	2182	2177	9300	27
H(24)	1457	452	9665	31
H(25)	4948	-709	9702	30
H(26)	9075	-242	9285	31
H(27)	9834	1467	8878	24
H(23')	4599	2353	9933	25
H(24')	4470	634	10370	31
H(25')	5397	-713	9524	31
H(26')	6584	-355	8280	33
H(27')	6887	1332	7841	27