Supporting Information

To accompany

New Zileuton-Hydroxycinnamic Acid Hybrids: Synthesis and Structure-Activity Relationship towards 5-Lipoxygenase Inhibition

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3-Phenylpropyl 1-benzothiophene-2-carboxylate (6)

Following our general procedure esterification with thianaphtene-2-carboxylic acid (**3**) (500 mg, 2.81 mmol, 1 eq), Na_2CO_3 (356 mg, 3.36 mmol, 1.2 eq), and 1-bromo-3-phenylpropane (0.51 mL, 3.36 mmol, 1.2 eq) compound **6** was obtained as a yellow oil after flash chromatography (8% EtOAc/Hex), yield = 20%, Rf = 0.46 (10% EtOAc/Hex). ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.07 (s, 1H, H3), 7.92-7.88 (t, 2H, J = 7.0 Hz, H4, H7), 7.51-7.22 (m, 7H, H5, H6, H2′, H3′, H4′, H5′, H6′), 4.41-4.38 (t, 2H, J = 7.0 Hz, $OCH_2CH_2CH_2C$), 2.85-2.82 (t, 2H, J =7.0 Hz, $CH_2CH_2CH_2C$), 2.19-2.12 (quint., 2H, J = 7.0 Hz, $CH_2CH_2CH_2C$). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 162.81 (C=O), 142.24 (C7a), 141.06 (C3a), 138.74 (C2), 133.70 (C1′), 130.48 (C3′, C5′), 128.51 (C2′, C6′), 128.48 (C4′), 126.93 (C6), 126.09 (C5), 125.55 (C7), 124.91 (C4), 122.77 (C2), 64.78 ($OCH_2CH_2CH_2C$), 32.19 ($OCH_2CH_2CH_2C$), 30.24 ($OCH_2CH_2CH_2C$). HRMS *m*/*z* calc. for $C_{18}H_{16}O_2S$ + (H^+): 297.0944; found: 297.0945.

4-Phenylbutyl 1-benzothiophene-2-carboxylate (7)

Following our general procedure esterification with thianaphtene-2-carboxylic acid (**3**) (250 mg, 1.40 mmol, 1 eq), Na_2CO_3 (178 mg, 1.68 mmol, 1.2 eq), and 1-bromo-4-phenylbutane (358 mg, 1.68 mmol, 1.2 eq) compound **7** was obtained as a yellow solid after flash chromatography (8% EtOAc/Hex), yield = 62%, Rf = 0,61 (10% EtOAc/Hex), m.p.= 56-57°C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.08 (s, 1H, H3), 7.91-7.88 (t, 2H, J = 7.0 Hz, H4, H7), 7.50-7.20 (m, 7H, H5, H6, H2′, H3′, H4′, H5′, H6′), 4.41-4.38 (t, 2H, J = 6.0 Hz, $OCH_2CH_2CH_2CH_2$), 2.75-2.71 (t, 2H, J =7.0 Hz, $CH_2CH_2CH_2CH_2C$), 1.87-1.82 (m, 4H, $CH_2CH_2CH_2CH_2C$). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm) : 162.87 (C=O), 142.22 (C7a), 141.98 (C3a), 138.74 (C2), 133.78 (C1′), 130.42 (C3′, C5′), 128.43 (C2′, C6′), 128.39 (C4′), 126.90 (C6), 125.89 (C5), 125.53 (C4), 124.89 (C7), 122.76 (C3), 65.43 ($CH_2CH_2CH_2CH_2C$), 35.46 ($CH_2CH_2CH_2CH_2C$), 28.27 ($CH_2CH_2CH_2CH_2C$), 27.74 ($CH_2CH_2CH_2CH_2C$). HRMS *m*/*z* calc. for $C_{19}H_{18}O_2S$ + (H^+): 311.1100; found: 311.1098.

2-(*p*-Methoxyphenyl)ethyl 1-benzothiophene-2-carboxylate (8)

Following our general procedure esterification with thianaphtene-2-carboxylic acid (**3**) (250 mg, 1.40 mmol, 1 eq), Na_2CO_3 (178 mg, 1.68 mmol, 1.2 eq), and 4-methoxyphenethylbromide (361 mg, 1.68 mmol, 1.2 eq) compound **8** was obtained as a pink solid after flash chromatography (10% EtOAc/Hex), yield = 76%, Rf = 0,48 (10% EtOAc/Hex), m.p.= 98-99°C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.07 (s, 1H, H3), 7.91-7.89 (m, 2H, H4, H7), 7.50-7.41 (m, 2H, H5, H6), 7.28-7.24 (m, 2H, H2′, H6′), 6.91-6.89 (d, 2H, J = 8.0 Hz, H3′, H5′) 4.56-4.52 (t, 2H, J = 7.0 Hz, OCH_2CH_2C), 3.82 (s, 3H, OCH_3), 3.08-3.05 (t, 2H, J = 7.0 Hz, OCH_2CH_2C).^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 162.72 (C=O), 158.42 (C4′), 142.25 (C7a), 138.72 (C3a), 133.64 (C2), 130.53 (C1′), 130.01 (C2′, C6′), 129.67 (C6), 126.94 (C5), 125.56 (C4), 124.90 (C7), 122.77 (C3), 114.01 (C3′, C5′), 66.26 (OCH_2CH_2C), 55.27 (OCH_3), 34.35 (OCH_2CH_2C). HRMS *m*/*z* calc. for $C_{18}H_{16}O_3S$ + (Na^+): 335.0712; found: 335.0705.

2-(*p*-Hydroxyphenyl)ethyl 1-benzothiophene-2-carboxylate (9)

Following our general procedure esterification with thianaphtene-2-carboxylic acid (**3**) (184 mg, 1.00 mmol, 1 eq),

Na_2CO_3 (127 mg, 1.20 mmol, 1.2 eq), and 4-hydroxyphenethylbromide (250 mg, 1.2 mmol, 1.2 eq) compound **9** was obtained as an orange solid after flash chromatography (15% EtOAc/Hex), yield = 57%, Rf = 0,40 (10% EtOAc/Hex), m.p.= 142-143°C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm) : 8.07 (s, 1H, H3), 7.91-7.89 (m, 2H, H4, H7), 7.50-7.41 (m, 2H, H5, H6), 7.20-7.18 (d, 2H, J=8.0 Hz, H2′, H6′), 6.84-6.80 (m, 2H, H3′, H5′), 4.55-4.51 (t, 2H, J = 7.0 Hz, $OC\underline{H_2}CH_2$), 3.06-3.03 (t, 2H, $CH_2C\underline{H_2}C$). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 162.81 (C=O), 154.45 (C4′), 142.26 (C7a), 138.70 (C3a), 133.55 (C2), 133.55 (C1′), 130.59 (C2′, C6′), 130.20 (C6), 129.69 (C5), 126.96 (C4), 125.57 (C7), 124.91 (C3), 115.46 (C3′, C5′), 66.28 ($\underline{C}H_2CH_2C$), 34.34 ($CH_2\underline{C}H_2C$). HRMS *m*/*z* calc. for $C_{17}H_{14}O_3S$ + (NH_4^+): 316.4; found: 316.1006.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(*m*-methoxyphenyl)-2-propen-1-one (12)

Following our general procedure for the aldol condensation in the presence of sodium ethoxide with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1 eq), sodium ethoxide (97 mg, 1.42 mg, 1 eq) and 3-methoxybenzaldehyde (232 mg, 1.70 mmol, 1.2 eq) compound **12** was obtained as a yellow solid after flash chromatography (8% EtOAc), yield = 17%, Rf = 0.27 (10% EtOAc), m.p. = 124-125°C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.13 (s, 1H, H3), 7.96-7.92 (m, 2H, H4, H7), 7.91-7.87 (d, 1H, J=16 Hz, CH=C$\underline{H}$C), 7.57-7.53 (d, 1H, J=16 Hz, COC$\underline{H}$=CH), 7.51-7.28 (m, 4H, H5, H6, H2′, H6′), 7.21 (s, 1H, H5′), 7.03-7.00 (m, 1H, H4′), 3.90 (s, 3H, OCH_3). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 183.42 (C=O), 160.00 (C3′), 145.17 (C7a), 144.34 (C2), 142.73 (COCH=$\underline{C}$H), 139.28 (C3a), 136.04 (C1′), 130.02 (C5′), 128.92 (C6), 127.46 (C5), 126.00 (C4), 125.06 (C7), 123.03 (CO$\underline{C}$H=CH), 121.43 (C3), 121.22 (C6′), 116.49 (C4′), 113.65 (C2′), 55.41 (OCH_3). HRMS *m*/*z* calc. for $C_{18}H_{14}O_2S$ + (H^+): 295.0787; found: 295.078.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(*m*-hydroxyphenyl)-2-propen-1-one (15)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 3-hydroxybenzaldehyde (145 mg, 1.18 mmol, 1 eq) under reflux for 20 h, compound **15** was obtained as a yellow solid after flash chromatography (18% EtOAc/Hex), yield = 18 %, Rf = 0.60 (30% EtOAc/Hex), m.p. =197-199°C. ^{1}H-NMR (400 MHz, DMSO-d6, 25°C); δ (ppm): 9.67 (s, 1H, OH - D_2O exchange), 8.78 (s, 1H, H3), 8.10-8.04 (m, 2H, H4, H7), 7.98-7.94 (d, 1H, J=16 Hz, CH=C$\underline{H}$C), 7.72-7.68 (d, 1H, J=16 Hz, COC$\underline{H}$=CH), 7.58-7.49 (m, 2H, H2′, H5′), 7.37-7.27 (m, 3H, H5, H6, H6′), 6.93-6.90 (m, 1H, H4′). ^{13}C-NMR (101 MHz, DMSO-d6, 25°C); δ (ppm): 183.62 (C=O), 158.25 (C3′), 145.48 (C7a), 144.25 (C2), 142.32 (COCH=$\underline{C}$H), 139.86 (C3a), 136.24 (C1′), 131.58 (C5′), 130.38 (C6), 128.28 (C5), 126.86 (C4), 125.79 (C7), 123.65 (CO$\underline{C}$H=CH), 121.79 (C3), 120.51 (C6′), 118.51 (C4′), 115.89 (C2′). HRMS *m*/*z* calc. for $C_{17}H_{12}O_2S$ + (H^+): 281.0631; found: 281.062.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(*p*-hydroxyphenyl)-2-propen-1-one (16)

Following our base-catalyzed aldol condensation general procedure with 2-Acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 4-hydroxybenzaldehyde (144 mg, 1.18 mmol, 1 eq) under reflux for 6h, compound **16** was obtained as a yellow solid after flash chromatography (40% EtOAc/Hex), yield = 28%, Rf = 0,18 (50% EtOAc/Hex),

m.p.= 179-180°C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm) : 8.13 (s, 1H, H3), 7.96-7.92 (m, 2H, H4, H7), 7.91-7.87 (d, 1H, J=16 Hz, CH=C<u>H</u>C), 7.64-7.62 (d, 2H, J=8.6 Hz, H5, H6), 7.52-7.45 (m, 2H, H2', H6'), 7.47-7.43 (d, 1H, J=16 Hz, COC<u>H</u>=CH), 6.94-6.92 (d, 2H, J=8.6 Hz, H3', H5'), 5.39 (s, 1H, OH). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 183.58 (C=O), 158.07 (C4'), 145.39 (C7a), 144.21 (C2), 142.63 (COCH=<u>C</u>H), 139.32 (C3a), 130.65 (C1'), 128.65 (C2', C6'), 127.64 (C6), 127.31 (C5), 125.90 (C4, C7)), 123.01 (COCH=<u>C</u>H), 118.90 (C3), 116.05 (C3', C5'). HRMS *m*/*z* calc. for $C_{17}H_{12}O_2S$ + (H^+): 281.0631; found: 281.0628.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(3-hydroxy-4-methoxyphenyl)-2-propen-1-one (17)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 3-hydroxy-4-methoxybenzaldehyde (180 mg, 1.18 mmol, 1 eq) under reflux for 10h, compound **17** was obtained as a yellow solid after flash chromatography (28% EtOAc/Hex), yield = 47%, Rf = 0.50 (40% EtOAc/Hex), m.p. = 158-159°C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.11 (s, 1H, H3), 7.96-7.91 (m, 2H, H4, H7), 7.86-7.82 (d, 1H, J = 15 Hz, CH=C<u>H</u>C), 7.51-7.42 (m, 2H, H_{ar}), 7.45-7.41 (d, 1H, J=15 Hz, COC<u>H</u>=CH), 7.36-7.35 (d, 1H, J = 2.0 Hz H6'), 7.29 (s, 1H, H5), 7.21-7.18 (m, 1H, H6), 6.93-6.90 (d, 1H, J = 8.0 Hz, H2'), 5.73 (s, 1H, OH), 3.98 (s, 3H, OC<u>H</u>$_3$). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 183.39 (C=O), 149.03 (C7a), 145.98 (C2), 145.45 (C3'), 144.33 (C4'), 142.62 (COCH=<u>C</u>H), 139.34 (C3a), 128.56 (C1'), 128.34 (C6), 127.29 (C5), 125.93 (C4), 124.98 (C7), 123.11 (CO<u>C</u>H=CH), 122.99 (C3), 119.34 (C2'), 112.97 (C3'), 110.61 (C6'), 56.07 (OCH_3). HRMS *m*/*z* calc. for $C_{18}H_{14}O_3S$ + (H^+): 311.0736; found: 311.0729.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(4-hydroxy-3-methoxyphenyl)-2-propen-1-one (18)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 4-hydroxy-3-methoxybenzaldehyde (180 mg, 1.18 mmol, 1 eq) under reflux for 9h, compound **18** was obtained as a yellow solid after flash chromatography (30% EtOAc/Hex), yield = 29%, Rf = 0,29 (40% EtOAc/Hex), m.p. = 113-114°C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.13 (s, 1H, H3), 7.96-7.91 (t, 2H, J=8.0 Hz H4, H7), 7.88-7.85 (d, 1H, J=15 Hz, CH=C<u>H</u>C), 7.52-7.42 (m, 2H, H5, H6), 7.43-7.40 (d, 1H, J=15 Hz, COC<u>H</u>=CH), 7.31-7.30 (d, 1H, J=2.0 Hz H6'), 7.18 (d, 1H, J=2.0 Hz, H2'), 7.01-6.99 (d, 1H, J=8.0 Hz, H5'), 6.0 (s, 1H, OH), 4.02 (s, 3H, OC<u>H</u>$_3$). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 183.39 (C=O), 148.52 (C7a), 146.84 (C3'), 145.44 (C2), 144.76 (C4'), 142.60 (COCH=<u>C</u>H), 139.32 (C3a), 128.45 (C1'), 127.28 (C6), 125.87 (C5), 125.00 (C4), 123.50 (C7), 123.01 (CO<u>C</u>H=CH), 118.76 (C3, C6'), 114.95 (C5'), 110.29 (C6'). HRMS *m*/*z* calc. for $C_{18}H_{14}O_3S$ + (H^+): 311.0736; found: 311.0736.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(3,4-dimethoxyphenyl)-2-propen-1-one (19)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (500 mg, 2.84 mmol, 1.2 eq) and 3,4-dimethoxybenzaldehyde (394 mg, 2.37 mmol, 1 eq) under reflux for 22.5 h, compound **19** was obtained as a yellow solid after flash chromatography (18% EtOAc/Hex), yield = 23 %, Rf = 0.24 (20% EtOAc/Hex), m.p. =127-128°C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.13 (s, 1H, H3), 7.96-7.91 (m, 2H, H4,

H7), 7.89-7.86 (d, 1H, J=15 Hz, CH=CHC), 7.52-7.42 (m, 2H, H5, H6), 7.45-7.41 (d, 1H, J=15 Hz, COCH=CH), 7.32-7.28 (m, 1H, H6′), 7.22-7.21 (d, 1H, J=2 Hz, H2′), 6.95-6.93 (d, 1H, J=8 Hz, H5′), 4.00 (s, 3H, OCH$_3$), 3.97 (s, 3H, OCH$_3$). ^{13}C-NMR (101 MHz, CDCl$_3$, 25°C); δ (ppm): 183.38 (C=O), 151.68 (C7a), 149.32 (C3′), 145.43 (C4′), 144.60 (C2), 142.61 (COCH=CH), 139.32 (C3a), 138.48 (C1′), 127.65 (C6), 127.30 (C5), 125.88 (C4), 125.00 (C7), 123.41 (COCH=CH), 123.01 (C3), 119.00 (C2′), 111.18 (C3′) , 110.28 (C6′), 56.04 (OCH$_3$). HRMS *m*/*z* calc. for $C_{19}H_{16}O_3S$ + (H^+): 325.0893; found: 325.0883.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(3,5-dimethoxyphenyl)-2-propen-1-one (20)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 3,5-dimethoxybenzaldehyde (197 mg, 1.18 mmol, 1 eq) under reflux for 8 h, compound **20** was obtained as a yellow solid after flash chromatography (12% EtOAc/Hex), yield = 15 %, Rf = 0,62 (20% EtOAc/Hex), m.p. =113-114°C. ^{1}H-NMR (400 MHz, CDCl$_3$, 25°C); δ (ppm): 8.13 (s, 1H, H3), 7.96-7.93 (t, 2H, J=8 Hz, H4, H7), 7.91-7.85 (d, 1H, J=16 Hz, CH=CHC), 7.53-7.49 (d, 1H, J=16 Hz, COCH=CH), 7.53-7.91-7.43 (m, 2H, H5, H6), 6.84-6.83 (d, 2H, J = 2 Hz, H2′, H6′), 6.58-6.57 (t, 1H, J=2 Hz, H4′), 3.88 (s, 6H, OCH$_3$). ^{13}C-NMR (101 MHz, CDCl$_3$, 25°C); δ (ppm): 183.40 (C=O), 161.12 (C3′, C5′), 145.13 (C7a), 144.43 (C2), 142.73 (COCH=CH), 139.27 (C3a), 136.54 (C1′), 128.94 (C6), 127.47 (C5), 126.00 (C4), 125.06 (C7), 123.02 (COCH=CH), 121.62 (C3), 106.51 (C2′, C6′), 102.94 (C4′), 55.53 (OCH$_3$). HRMS *m*/*z* calc. for $C_{19}H_{16}O_3S$ + (H^+): 325.0893; found: 325.0885.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(2,3-dimethoxyphenyl)-2-propen-1-one (21)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 2,3-dimethoxybenzaldehyde (197 mg, 1.18 mmol, 1 eq) under reflux for 14.5 h, compound **21** was obtained as a yellow solid after flash chromatography (10 % EtOAc/Hex), yield = 14 %, Rf = 0.19 (10 % EtOAc/Hex), m.p. =86-87°C. ^{1}H-NMR (400 MHz, CDCl$_3$, 25°C); δ (ppm): 8.22-8.18 (d, 1H, J = 16 Hz, CH=CHC), 8.11 (s, 1H, H3), 7.95-7.90 (t, 2H, J = 9 Hz, H4, H7), 7.67-7.63 (d, 1H, J = 16 Hz, COCH=CH), 7.51-7.42 (m, 2H, H5, H6), 7.34-7.32 (d, 1H, J = 8 Hz, H6′), 7.16-7.12 (t, 1H, J = 8 Hz, H5′), 7.02-7.00 (d, 1H, J = 8 Hz, H4′), 3.94 (s, 3H, OCH$_3$), 3.92 (s, 3H, OCH$_3$). ^{13}C-NMR (101 MHz, CDCl$_3$, 25°C); δ (ppm): 183.79 (C=O), 153.28 (C7a), 149.16 (C3′), 145.34 (C2′), 142.68 (C2), 139.35 (COCH=CH), 139.31 (C3a), 128.87 (C6), 128.84 (C5), 127.37 (C4), 125.98 (C7), 125.01 (COCH=CH), 124.25 (C3), 122.72 (C5′), 119. 82 (C6′), 114.44 (C4′), 61.39 (OCH$_3$), 55.94 (OCH$_3$). HRMS *m*/*z* calc. for $C_{19}H_{16}O_3S$ + (H^+): 325.0893; found: 325.0886.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(2,4-dimethoxyphenyl)-2-propen-1-one (22)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 2,4-dimethoxybenzaldehyde (197 mg, 1.18 mmol, 1 eq) under reflux for 14.5 h, compound **22** was obtained as a yellow solid after flash chromatography (15 % EtOAc/^{1}H-NMR (400 MHz, CDCl$_3$, 25°C); δ (ppm Hex), yield = 45 %, Rf = 0.45 (20% EtOAc/Hex), m.p. = 98-100°C.): 8.17-8.13 (d, 1H, J = 16 Hz, CH=CHC), 8.08 (s, 1H, H3), 7.94-7.90 (t, 2H, J = 8 Hz, H4, H7), 7.63-7.60 (m, 1H, H5), 7.61-7.57 (d, 1H, J = 16 Hz, CH=CHC), 7.49-

7.41 (m, 1H, H6′), 6.59-6.56 (m, 1H, H5′$_r$), 6.51-6.50 (d, 1H, J = 2 Hz, H3′), 3.95 (s, 3H, OC$\underline{H}_3$), 3.86 (s, 3H, OC$\underline{H}_3$). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 184.02 (C=O), 163.27 (C4′), 160.65 (C7a), 145.87 (C2′), 142.50 (C2), 140.20 (COCH=$\underline{C}$H), 139.41 (C3a), 131.32 (C6′), 128.14 (C6), 127.05 (C5), 125.81 (C4), 124.86 (C7), 122.96 (COCH=$\underline{C}$H), 119.47 (C3), 116.94 (C1′), 105.53 (C5′), 98.48 (C3′), 55.61 (OCH_3), 55.53 (OCH_3). LC-MS *m*/*z* calc. for $C_{19}H_{16}O_3S$ + (H^+): 325.0893; found: 325.089.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(2,5-dimethoxyphenyl)-2-propen-1-one (23)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (250 mg, 1.42 mmol, 1.2 eq) and 2,5-dimethoxybenzaldehyde (197 mg, 1.18 mmol, 1 eq) under reflux for 13 h, compound **23** was obtained as a brown solid after flash chromatography (7-10 % EtOAc/Hex), quantitative yield, Rf = 0.22 (10% EtOAc/Hex), m.p.= 95-97 °C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.17-8.13 (d, 1H, J=16 Hz, CH=C$\underline{H}$C), 8.08 (s, 1H, H3), 7.94-7.90 (t, 2H, J = 8 Hz, H4, H7), 7.63-7.60 (m, 1H, H6′), 7.61-7.57 (d, 1H, J = 16 Hz, COC$\underline{H}$=CH), 7.49-7.41 (m, 2H, H5, H6), 6.59-6.56 (m, 1H, H3′), 6.51-6.50 (d, 1H, J = 2 Hz, H4′), 3.95 (s, 3H, OC$\underline{H}_3$), 3.86 (s, 3H, OC$\underline{H}_3$). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 183.94 (C=O), 153.56 (C5′), 153.55 (C2′), 145.46 (C7a), 142.64 (C2), 139.85 (COCH=$\underline{C}$H), 139.33 (C3a), 128.67 (C6), 127.27 (C5), 125.93 (C4), 124.96 (C7), 124.29 (CO$\underline{C}$H=CH), 122.99 (C3), 122.22 (C3′), 117.45 (C1′), 114.09 (C4′), 112.52 (C6′), 56.16 (OCH_3), 55.90 (OCH_3). LC-MS *m*/*z* calc. for $C_{19}H_{16}O_3S$ + (H^+): 325.0893; found: 325.0883.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(2,6-dimethoxyphenyl)-2-propen-1-one (24)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 2,6-dimethoxybenzaldehyde (196 mg, 1.18 mmol, 1 eq), under reflux for 7.5h, compound **24** was obtained as a yellow solid after flash chromatography (18% EtOAc/Hex), yield = 36%, Rf = 0,25 (20% EtOAc/Hex), m.p. = 175-176 °C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.40-8.36 (d, 1H, J=16 Hz, CH=C$\underline{H}$C), 8.07-8.01 (d, 1H, J = 16 Hz, COC$\underline{H}$=CH), 8.05 (s, 1H, H3), 7.95-7.91 (t, 2H, J = 9 Hz, H4, H7), 7.50-7.41 (m, 2H, H5, H6), 7.36-7.32 (t, 1H, J=8 Hz, H4′), 6.38-6.62 (d, 2H, J = 8 Hz, H3′, H5′), 3.98 (s, 6H, OC$\underline{H}_3$). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 185.11 (C=O), 160.57 (C7a), 146.05 (C2′, C6′), 142.53 (C2), 139.43 (COCH=$\underline{C}$H), 135.48 (C3a), 131.79 (C4′), 128.20 (C6), 126.98 (C5), 125.80 (C4), 124.80 (C7), 124.01 (CO$\underline{C}$H=CH), 122.97 (C3), 112.78 (C1′), 103.79 (C3′, C5′), 55.94 (OCH_3). HRMS *m*/*z* calc. for $C_{19}H_{16}O_3S$ + (H^+): 325.0893; found: 325.0885.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(3,4,5-trimethoxyphenyl)-2-propen-1-one (26)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 3,4,5-trimethoxybenzaldehyde (232 mg, 1.18 mmol, 1 eq) under reflux for 14 h, compound **26** was obtained as a yellow solid after flash chromatography (18% EtOAc/Hex), yield = 12 %, Rf = 0,20 (20% EtOAc/Hex), m.p. =125-127°C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.14 (s, 1H, H3), 7.97-7.92 (t, 2H, J = 9 Hz, H4, H7), 7.86-7.82 (d, 1H, J = 16 Hz, CH=C$\underline{H}$C), 7.53-7.43 (m, 2H, H5, H6) 7.46-7.42 (d, 1H, J = 16 Hz, COC$\underline{H}$=CH), 6.93 (s, 2H, H2′, H6′), 3.97 (s, 6H, O-C$\underline{H}_3$), 3.94 (s, 3H, O-C$\underline{H}_3$). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ

(ppm): 183.30 (C=O), 153.54 (C7a), 145.22 (C3'), 144.61 (C5'), 142.68 (COCH=CH), 140.72 (C3a), 139.28 (C4'), 130.12 (C1'), 128.73 (C6), 127.42 (C5), 125.93 (C4), 125.06 (C7), 123.03 (COCH=CH), 120.37 (C3), 105.88 (C2', C6'), 61.04 (OCH_3), 56.30 (OCH_3). HRMS *m*/*z* calc. for $C_{20}H_{18}O_4S$ + (H^+): 355.0999; found: 355.0989.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(2,4,6-trimethoxyphenyl)-2-propen-1-one (27)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 2,4,6-trimethoxybenzaldehyde (232 mg, 1.18 mmol, 1 eq) under reflux for 7 h, compound **27** was obtained as a yellow solid after flash chromatography (25% EtOAc/Hex), yield = 36 %, Rf = 0.41 (30% EtOAc/Hex), m.p. =145-147°C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.38-8.34 (d, 1H, J=16 Hz, CH=CHC), 8.04 (s, 1H, H3), 7.94-7.87 (d, 1H, J=16 Hz, COCH=CH), 7.92 (s, 2H, H4, H7), 7.48-7.40 (m, 2H, H5, H6), 6.17 (s, 2H, H3', H5'), 3.96 (s, 6H, OCH_3), 3.89 (s, 3H, OCH_3). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 185.04 (C=O), 163.40 (C4'), 161.94 (C2', C6'), 146.40 (C7a), 142.40 (C2), 139.49 (COCH=CH), 135.72 (C3a), 127.71 (C6), 126.79 (C5), 125.69 (C4), 124.72 (C7), 122.93 (COCH=CH), 121.04 (C3), 106.47 (C1'), 90.57 (C3', C5'), 55.88 (OCH_3), 55.44 (OCH_3). HRMS *m*/*z* calc. for $C_{20}H_{18}O_4S$ + (H^+): 355.0999; found: 355.099.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(4-hydroxy-3,5-dimethoxyphenyl)-2-propen-1-one (28)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 4-hydroxy-3,5-methoxybenzaldehyde (215 mg, 1.18 mmol, 1 eq) under reflux for 10h, compound **28** was obtained as a yellow solid after flash chromatography (30% EtOAc/Hex), yield = 11%, Rf = 0.26 (50% EtOAc/Hex), m.p. = 69-70°C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.13 (s, 1H, H3), 7.96-7.91 (m, 2H, H4, H7), 7.85-7.81 (d, 1H, J = 15 Hz, CH=CHC), 7.51-7.28 (m, 2H, H5, H6), 7.42-7.38 (d, 1H, J=15 Hz, COCH=CH), 6.94 (s, 2H, H2', H6'), 5.9 (s, 1H, OH), 4.00 (s, 6H, OCH_3). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 183.26, (CO) 147.32 (C3', C5'), 145.39 (C7a), 145.00 (C2), 142.61 (COCH=CH), 139.31 (C3a), 137.79 (C4'), 128.51 (C1'), 127.31 (C6), 126.18 (C5), 125.87 (C4), 125.01 (C7), 123.00 (COCH=CH), 118.99 (C3), 105.74 (C2', C6'), 56.46 (OCH_3). HRMS *m*/*z* calc. for $C_{19}H_{16}O_4S$ + (H^+): 341.0842; found: 341.0842.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(4-hydroxy-3,5-dimethylphenyl)-2-propen-1-one (29)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 4-hydroxy-3,5-dimethylbenzaldehyde (178 mg, 1.18 mmol, 1 eq) under reflux for 7.5h, compound **29** was obtained as a yellow solid after flash chromatography (18% EtOAc/Hex), yield = 16%, Rf = 0,51 (30% EtOAc/Hex), m.p. = 178-179°C. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C); δ (ppm): 8.12 (s, 1H, H3), 7.95-7.82 (t, 2H, J = 9 Hz, H4, H7), 7.85-7.82 (d, 1H, J = 15 Hz, CH=CHC), 7.51-7.28 (m, 4H, H5, H6, H2', H6'), 7.45-7.41 (d, 1H, J = 15 Hz, COCH=CH), 5.15 (s, 1H, OH), 2.33 (s, 6H, OCH_3). ^{13}C-NMR (101 MHz, $CDCl_3$, 25°C); δ (ppm): 183.52 (C=O), 155.07 (C4'), 145.60 (C7a), 144.83 (C2), 142.59 (COCH=CH), 139.37 (C3a), 129.57 (C2', C6'), 128.40 (C1'), 127.22 (C6), 126.87 (C5), 125.86 (C4), 124.96 (C7), 123.73 (COCH=CH), 122.99 (C3), 118.35 (C3', C5'), 15.91 (CH_3). HRMS *m*/*z* calc. for $C_{19}H_{16}O_2S$ + (H^+): 309.0944; found: 309.0933.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(4-hydroxy-2,6-dimethoxyphenyl)-2-propen-1-one (30)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 4-hydroxy-2,6-dimethoxybenzaldehyde (215 mg, 1.18 mmol, 1 eq), under reflux for 15 hr, compound **30** was obtained as a yellow solid after flash chromatography (40% EtOAc/Hex), yield = 66%, Rf = 0,38 (60% EtOAc/Hex), m.p. = 195-197 ˚C. ^{1}H-NMR (400 MHz, DMSO-d6 25°C); δ (ppm): 10.40 (s, 1H, OH), 8.35 (s, 1H, H3), 8.17-8.13 (d, 1H, J = 15 Hz, CH=C<u>H</u>C), 8.09-8.05 (t, 2H, J = 8 Hz, H4, H7), 7.89-7.85 (d, 1H, J = 15 Hz, COC<u>H</u>=CH), 7.53-7.48 (m, 2H, H5, H6), 6.19 (s, 2H, H3', H5'), 3.32 (s, 6H, OC<u>H</u>$_3$). ^{13}C-NMR (101 MHz, DMSO-d6, 25°C); δ (ppm): 184.14 (C=O), 163.07 (C2', C6', C4'), 162.38 (C7a), 146.34 (C2), 141.89 (COCH=<u>C</u>H), 139.97 (C3a), 135.75 (C6), 129.07 (C5), 127.77 (C4), 126.71 (C7), 125.56 (CO<u>C</u>H=CH), 118.84 (C3), 104.19 (C1'), 92.71 (C3', C5'), 56.38 (OCH$_3$). HRMS *m*/*z* calc. for $C_{19}H_{16}O_4S$ + (H^+): 341.0842; found: 341.0836.

(*E*)-1-(1-Benzothiophen-2-yl)-3-(3-hydroxy-4,5-dimethoxyphenyl)-2-propen-1-one (31)

Following our base-catalyzed aldol condensation general procedure with 2-acetylbenzothiophene (**10**) (250 mg, 1.42 mmol, 1.2 eq) and 5-hydroxy-3,4-dimethoxybenzaldehyde (215 mg, 1.18 mmol, 1 eq) under reflux for 15 h, compound **31** was obtained as a yellow solid after flash chromatography (20 % EtOAc/Hex), yield = 41 %, Rf = 0.29 (30 % EtOAc/Hex), m.p. = 158-160˚C. ^{1}H-NMR (400 MHz, DMSO, 25°C); δ (ppm): 9.37 (s, 1H, OH), 8.73 (s, 1H, H3), 8.10-8.8.05 (m, 2H, H4, H7), 7.90-7.86 (d, 1H, J = 16 Hz, CH=C<u>H</u>C), 7.67-7.63 (d, 1H, J = 16 Hz, COC<u>H</u>=CH), 7.58-7.49 (m, 2H, H5, H6), 7.14-7.13 (d, 1H, J = 2 Hz, H2'), 7.01-7.00 (d, 1H, J = 2 Hz, H6'), 3.89 (s, 3H, OC<u>H</u>$_3$), 3.75 (s, 3H, OC<u>H</u>$_3$). ^{13}C-NMR (101 MHz, DMSO, 25°C); δ (ppm): 183.50 (C=O), 153.88 (C7a), 151.15 (C5'), 145.70 (C3'), 144.51 (C2), 142.29 (COCH=<u>C</u>H), 139.84 (C3'), 139.46 (C3a), 131.20 (C1'), 130.36 (C6), 128.21 (C5), 126.77 (C4), 125.79 (C7), 123.65 (CO<u>C</u>H=CH), 120.78 (C3), 111.52 (C2'), 104.60 (C6'), 60.58 (OCH3), 56.52 (OCH3). HRMS *m*/*z* calc. for $C_{19}H_{16}O_4S$ + (H^+): 341.0842; found: 341.0835.

1-Hydroxy-1-((E)-3-(4-hydroxy-3-methoxyphenyl)acryloyl)urea (35)

Following our general procedure for the peptide coupling of hydroxyl urea (**32**) (195 mg, 2.57 mmol, 1 eq) with 4-hydroxy-3-methoxycinnamic acid (500 mg, 2.57 mmol, 1 eq), TEA (537 µL, 3.85 mmol, 1.5 eq), and BOP (1136 mg, 2.57 mmol, 1 eq), compound **35** was obtained as a light yellow solid after flash chromatography (70% EtOAc/Hex), yield = 38 %, Rf = 0.24 (80 % EtOAc/Hex), m.p. = 150-152˚C. ^{1}H-NMR (400 MHz, DMSO-d6, 25°C); δ (ppm): 9.69 (s, 1H, OH - D_2O exchange), 9.58 (s, 1H, OH - D_2O exchange), 7.69-7.65 (d, 1H, J = 16 Hz, C<u>H</u>=CHCO), 7.36-7.35 (d, 1H, J = 2 Hz, H2), 7.19-7.16 (m, 1H, H6), 6.83-6.81 (d, 1H, J = 8 Hz, H5$_r$), 6.58-6.54 (d, 1H, J = 16 Hz, CH=C<u>H</u>CO), 6.49 (s, 2H, NH_2 - D_2O exchange), 3.83 (s, 3H, OCH$_3$). ^{13}C-NMR (101 MHz, DMSO-d6, 25°C); δ (ppm): 166.64 (C=O), 159.97 (NCON), 150.19 (C3), 148.42 (C4), 146.89 (C<u>C</u>H=CH), 125.94 (C1), 123.92 (C6), 116.03 (CCH=<u>C</u>H)), 111.99 (C5), 111.85 (C2), 56.18 (OCH$_3$). HRMS *m*/*z* calc. for $C_{11}H_{12}N_2O_5$ + (Na^+): 275.0644; found: 275.0640.

1-Hydroxy-1-((E)-3-(3,4-dimethoxyphenyl)acryloyl)urea (36)

Following our general procedure for the peptide coupling of hydroxyl urea (**32**) (183 mg, 2.4 mmol, 2 eq) with 3,4-

dimethoxycinnamic acid (250 mg, 1.2 mmol, 1 eq), TEA (334 µL, 2.4 mmol, 2 eq), and BOP (530 mg, 1.2 mmol, 1 eq), compound **36** was obtained as a white solid after filtering through celite, quantitative yield, Rf = 0.49 (50% EtOAc/Hex), m.p. = 195-197°C. ^{1}H-NMR (400 MHz, DMSO-d6, 25°C); δ (ppm) : 9.67 (s, 1H, OH - D_2O exchange), 7.72-7.68 (d, 1H, J = 16 Hz, CC<u>H</u>=CH), 7.39-7.38 (d, 1H, J = 2 Hz, H2), 7.31-7.29 (d, 1H, J = 8 Hz, $H6_r$), 7.02-7.00 (d, 1H, J = 8 Hz, H5), 6.67-6.63 (d, 1H, J = 16 Hz, CCH=C<u>H</u>), 6.52 (s, 2H, NH_2 - D_2O exchange), 3.82 (s, 3H, OCH_3), 3.81 (s, 3H, OCH_3). ^{13}C-NMR (101 MHz, DMSO-d6, 25°C); δ (ppm): 166.51 (C=O), 159.95 (NCON), 151.75 (C3), 149.45 (C4), 146.50 (C<u>C</u>H=CH), 127.20 (C1), 123.75 (C6), 113.15 CCH=<u>C</u>H), 112.02 (C5), 110.94 (C2), 56.11 (CH_3), 56.07 (OCH_3). HRMS *m*/*z* calc. for $C_{12}H_{14}N_2O_5$ + (Na^+): 289.0795; found: 289.0778.

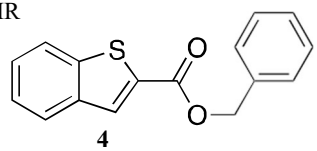
1-Hydroxy-1-((E)-3-(4-hydroxy-3,5-dimethoxyphenyl)acryloyl)urea (37)

Following our general procedure for the peptide coupling of hydroxyl urea (**32**) (85 mg, 1.12 mmol, 1 eq) with 4-hydroxy-3,5-dimethoxycinnamic acid (250 mg, 1.12 mmol, 1 eq), TEA (234 µL, 1.68 mmol, 1.5 eq), and BOP (495 mg, 1.12 mmol, 1 eq), compound **37** was obtained as a light yellow solid after flash chromatography (75% EtOAc/Hex), yield = 23 %, Rf = 0.15 (80 % EtOAc/Hex), m.p. = 164-166°C. ^{1}H-NMR (400 MHz, DMSO-d6, 25°C) ; δ (ppm) : 9.59 (s, 1H, OH - D_2O exchange), 9.05 (s, 1H, OH - D_2O exchange), 7.69-7.65 (d, 1H, J = 16 Hz, CC<u>H</u>=CH), 7.08 (s, 2H, NH_2 - D_2O exchange), 6.64-6.60 (d, 1H, J = 16 Hz, CCH=C<u>H</u>), 6.49 (s, 2H, H2, H6), 3.81 (s, 6H, OCH_3). ^{13}C-NMR (101 MHz, DMSO-d6, 25°C); δ (ppm): 166.61 (C=O), 159.96 (NCON), 148.51 (C3, C5), 147.20 (C<u>C</u>H=CH), 139.17 (C4), 124.75 (C1), 112.44 (CCH=<u>C</u>H), 106.93 (C2, C6), 56.58 (OCH_3). HRMS *m*/*z* calc. for $C_{12}H_{14}N_2O_6$ + (Na^+):305.0732; found:305.0744.

1-(3-Phenylpropanoyl)-1-hydroxyurea (40)

Following our general procedure for hydroxyurea analogs synthesis with acyl chlorides, hydroxyurea (**32**) (245 mg, 3.23 mmol), DMAP (394 mg, 3.23 mmol), and hydrocinnamoyl chloride (500 mg, 3.23 mmol) compound **40** was obtained as a white solid after flash chromatography, yield = 65 %, Rf = 0.25 (50 % EtOAc/Hex), m.p. = 79-81°C.^{1}H-NMR (400 MHz, DMSO-d6, 25°C); δ (ppm): 9.55 (s, 1H, OH - D_2O exchange), 7.31-7.25 (m, 4H, H2, H3, H5, H6), 7.22-7.19 (m, 1H, H4), 6.49 (s, 2H, NH_2 – D_2O exchange), 2.90-2.87 (t, 2H, J = 7 Hz, CC<u>H$_2$</u>CH_2), 2.78-2.74 (t, 2H, J = 7 Hz, CCH_2C<u>H$_2$</u>). ^{13}C-NMR (101 MHz, DMSO-d6, 25°C); δ (ppm): 172.09 (C=O), 159.95 (NCON), 140.70 (C1), 128.83 (C3, C5), 128.73 (C2, C6), 126.63 (C4), 33.25 (C<u>C</u>H_2CH_2), 30.28 (CCH_2<u>C</u>H_2),. LC-MS *m*/*z* calc. for $C_{10}H_{12}N_2O_3$ + (Na^+): 231.0740; found: 231.0745.

^{1}H NMR



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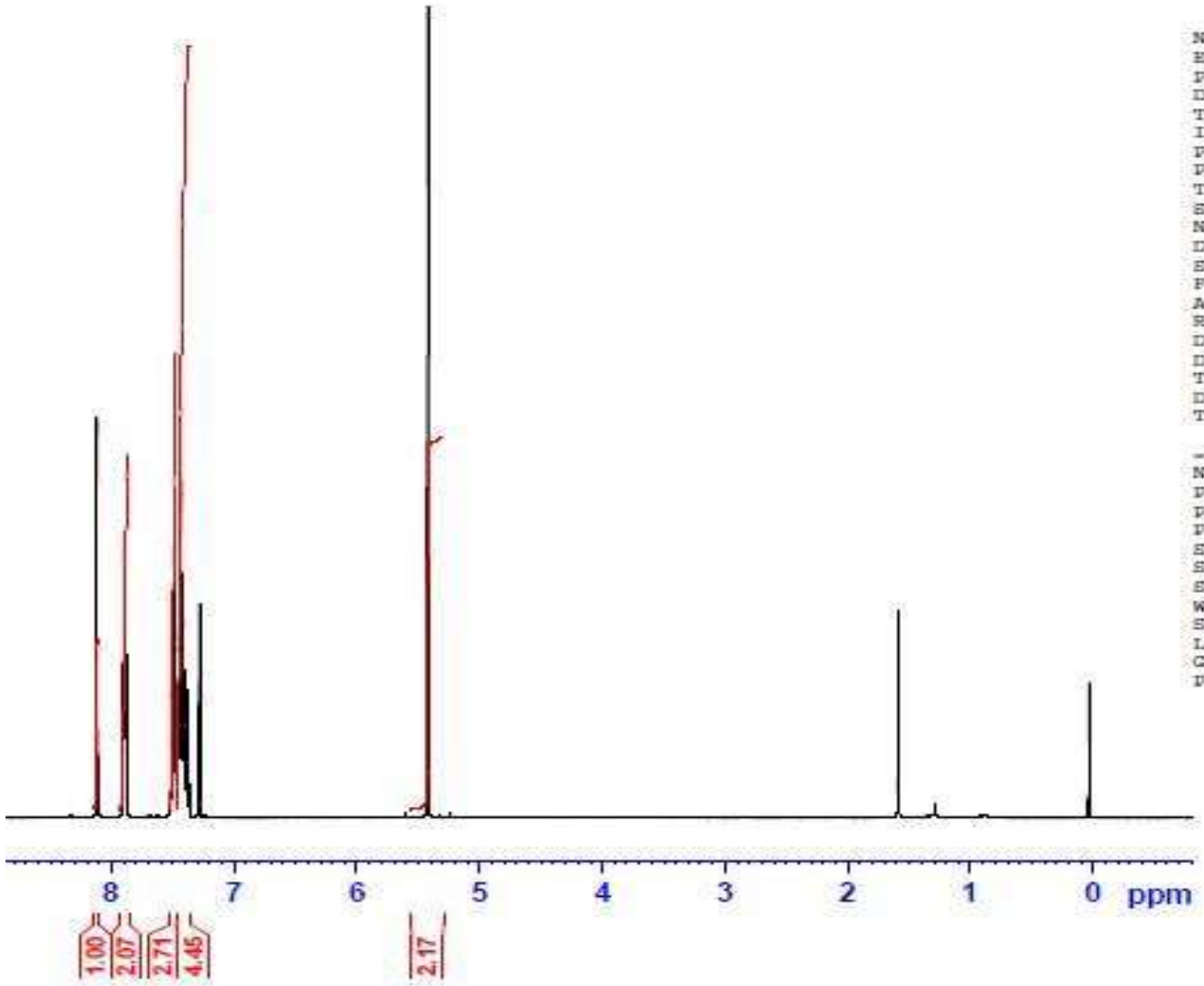

BRUKER

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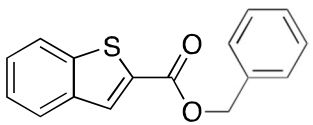
^{13}C NMR



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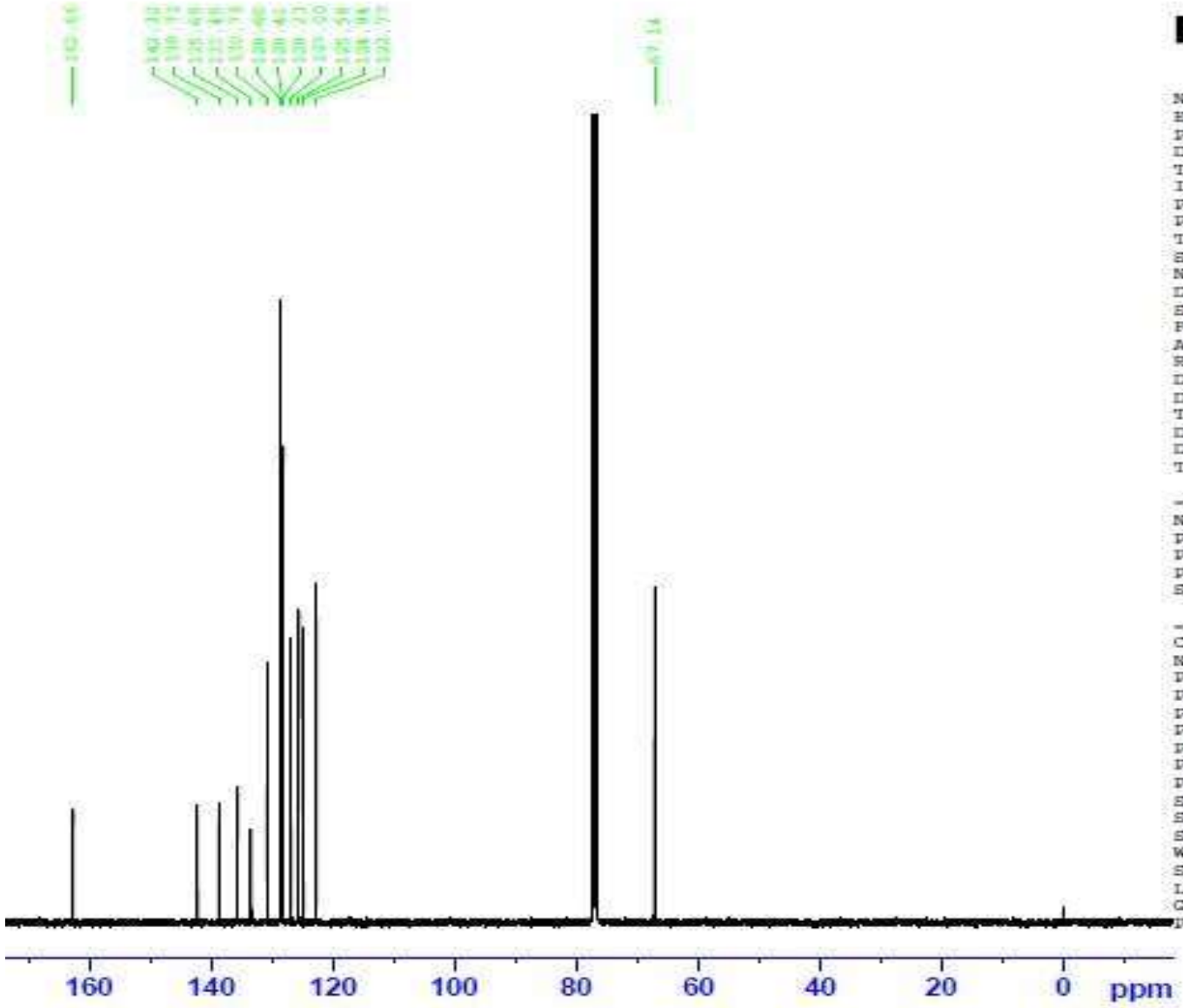

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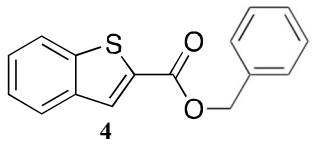

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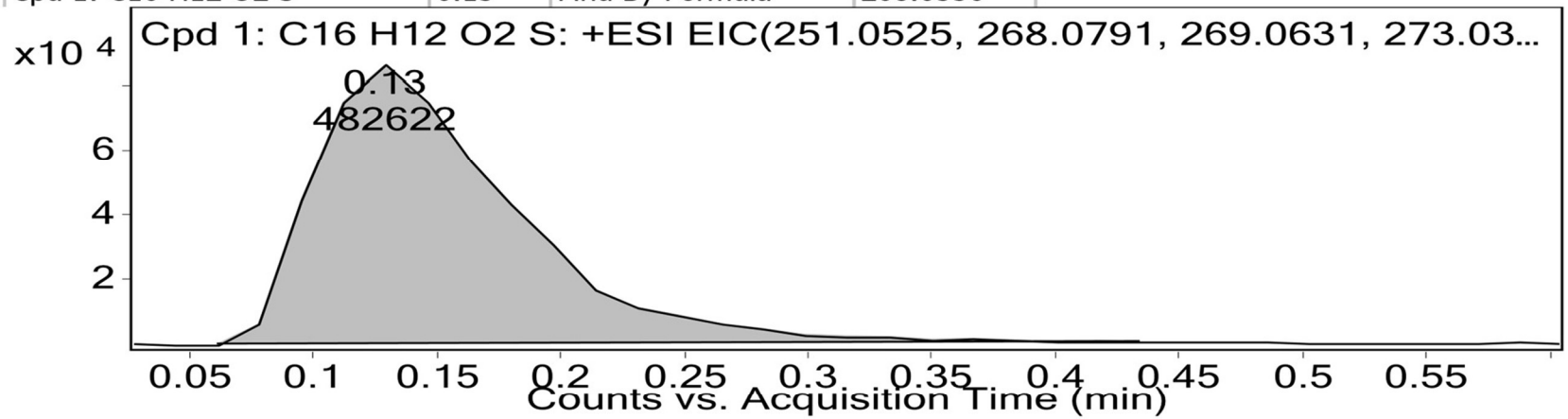
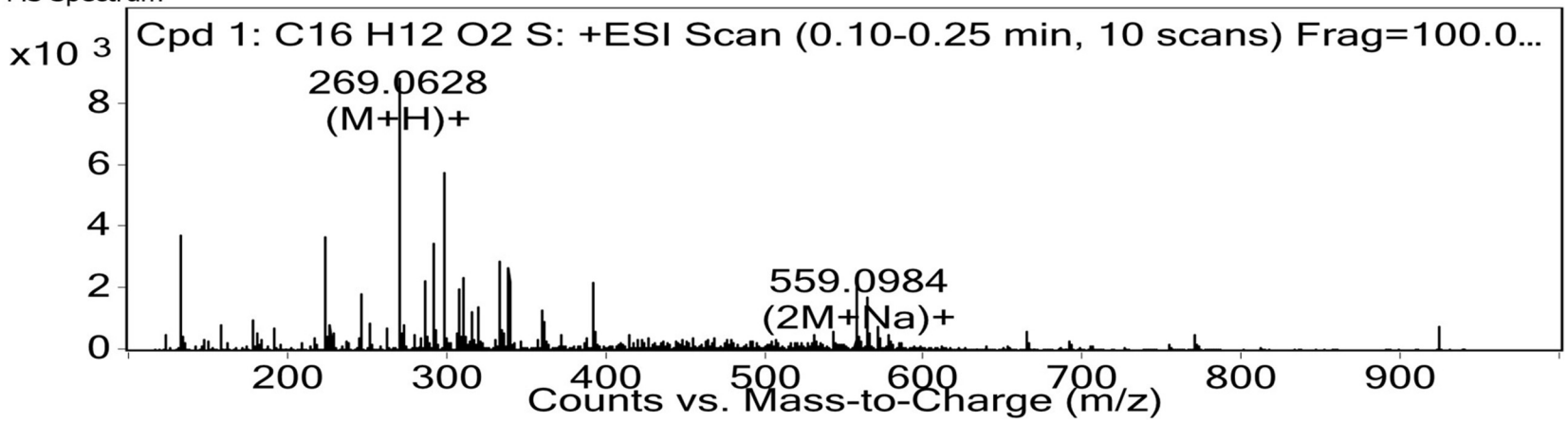
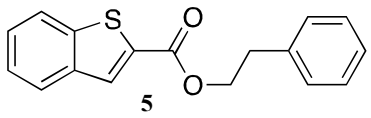


MS Spectrum



^{1}H NMR



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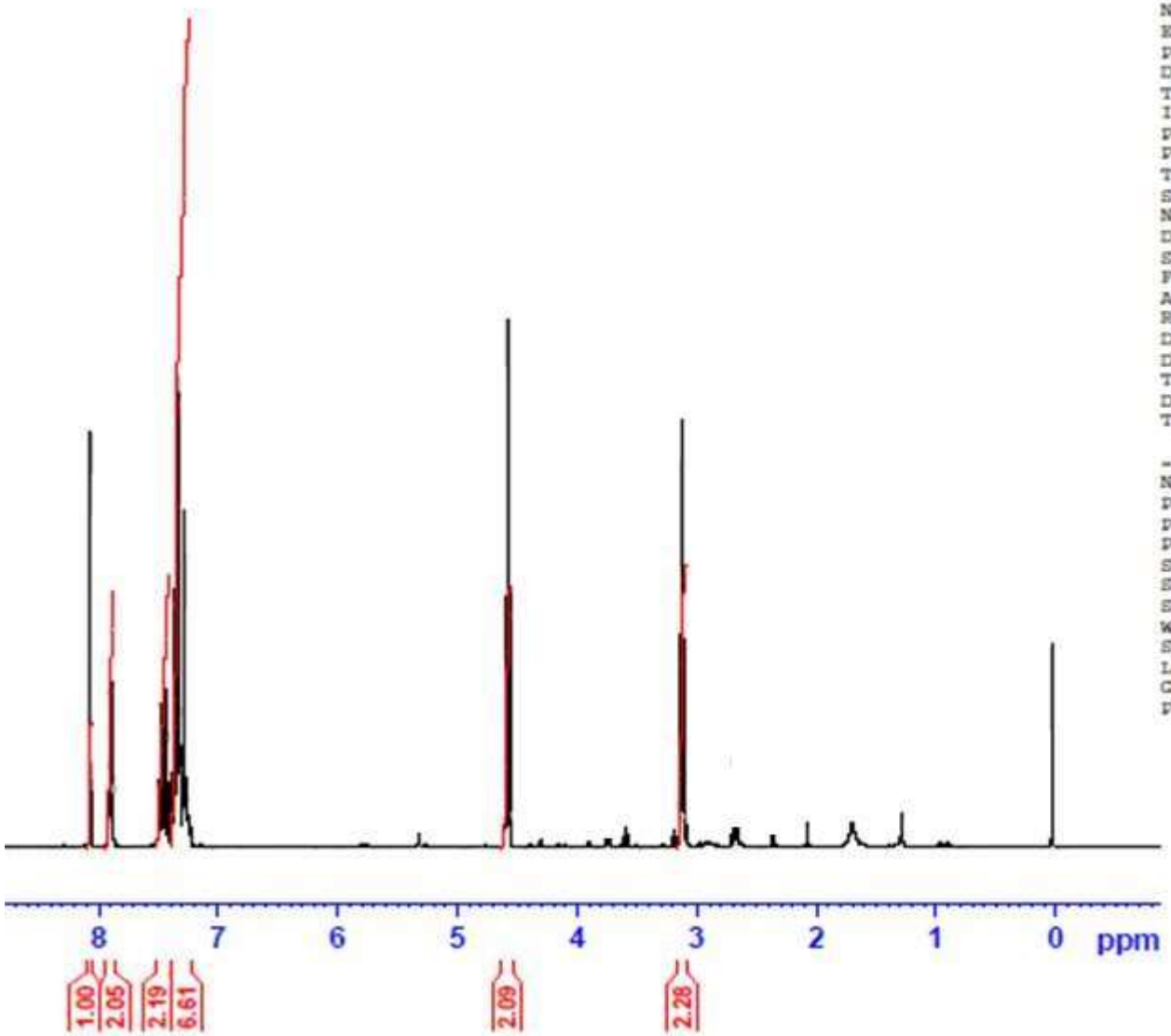
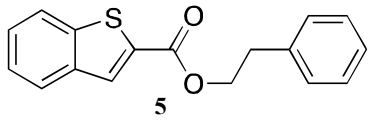



```
NAME          Audrey Isabelle
EXPNO                       1
PROCNO                      1
Date_              20181017
Time                   15.59
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                      90.5
DW                    60.800 usec
DE                     6.50 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      14.07 usec
PL1                      0.30 dB
PL1W            11.25229836 W
SFO1            400.1324710 MHz
SI                      32768
SF              400.1300000 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```

^{13}C NMR



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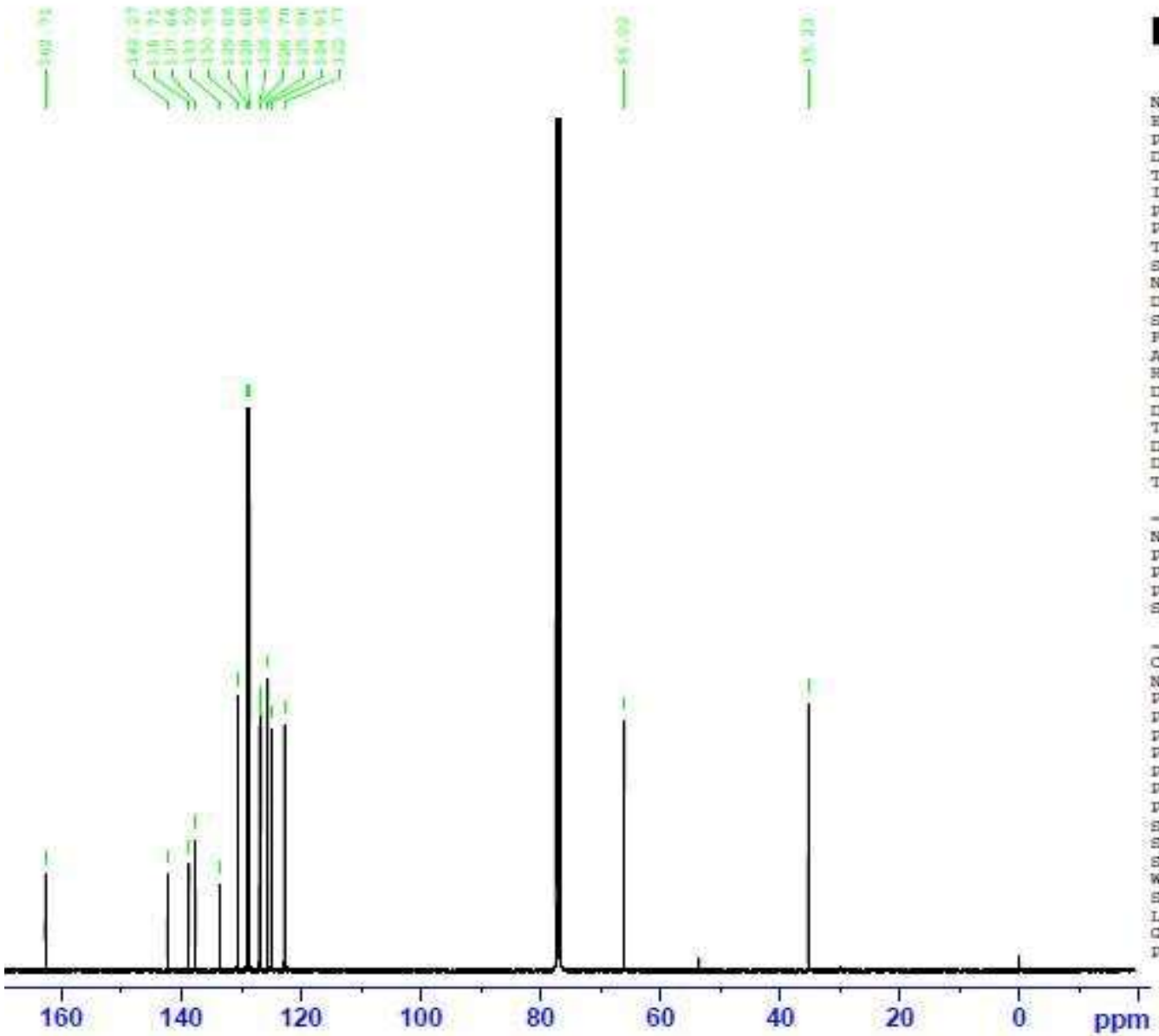
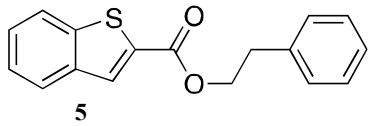


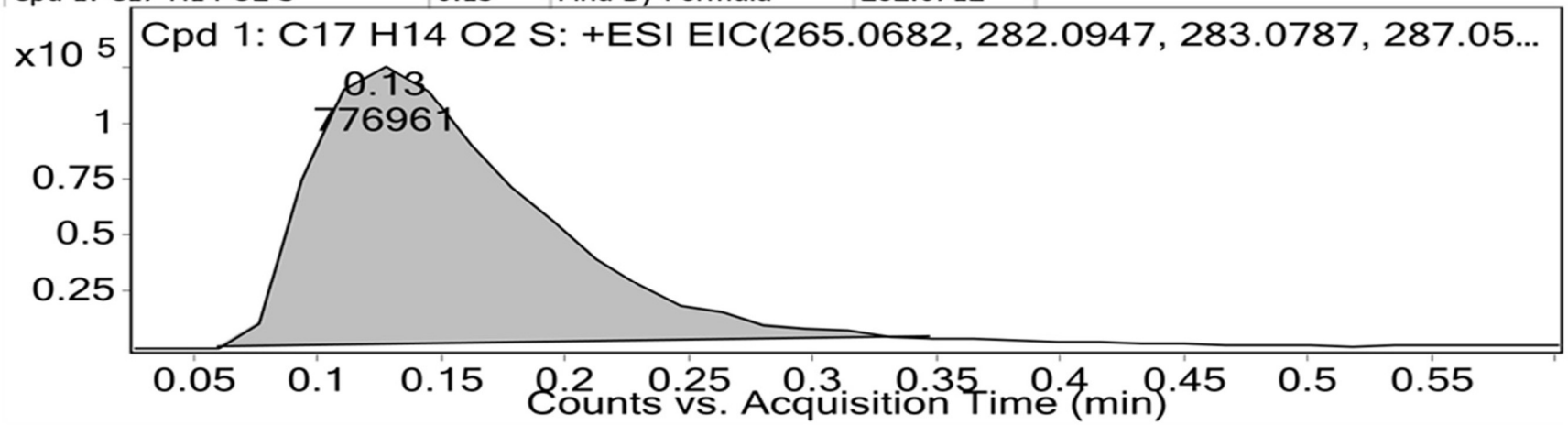

```
NAME          Audrey Isabelle
EXPNO                       4
PROCNO                      1
Date_              20181107
Time                   20.47
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      5000
DS                         4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                       203
DW                  20.800 usec
DE                   6.50 usec
TE                   298.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     9.90 usec
PL1                   -1.90 dB
PL1W          56.02249908 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz65
NUC2                     1H
PCPD2                80.00 usec
PL2                   0.30 dB
PL12                 15.40 dB
PL13                 18.40 dB
PL2W          11.25229836 W
PL12W          0.34772930 W
PL13W          0.17427748 W
SFO2         400.1316005 MHz
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

HRMS



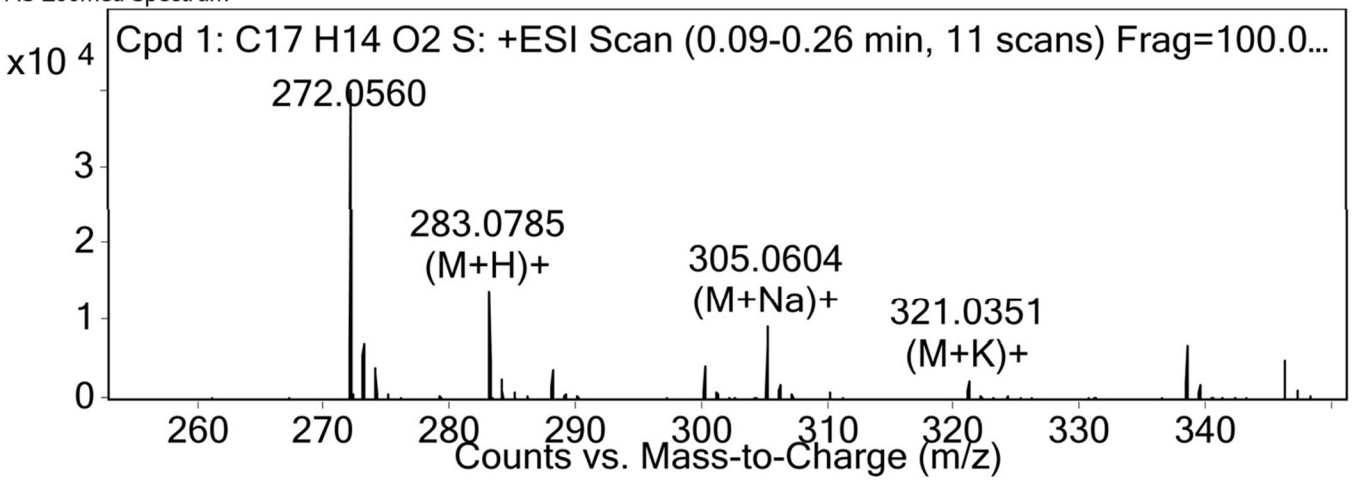
5

Compound Label	RT	Algorithm	Mass
Cpd 1: C17 H14 O2 S	0.13	Find By Formula	282.0712

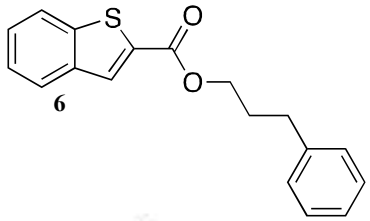


MS Spectrum

MS Zoomed Spectrum



^{1}H NMR



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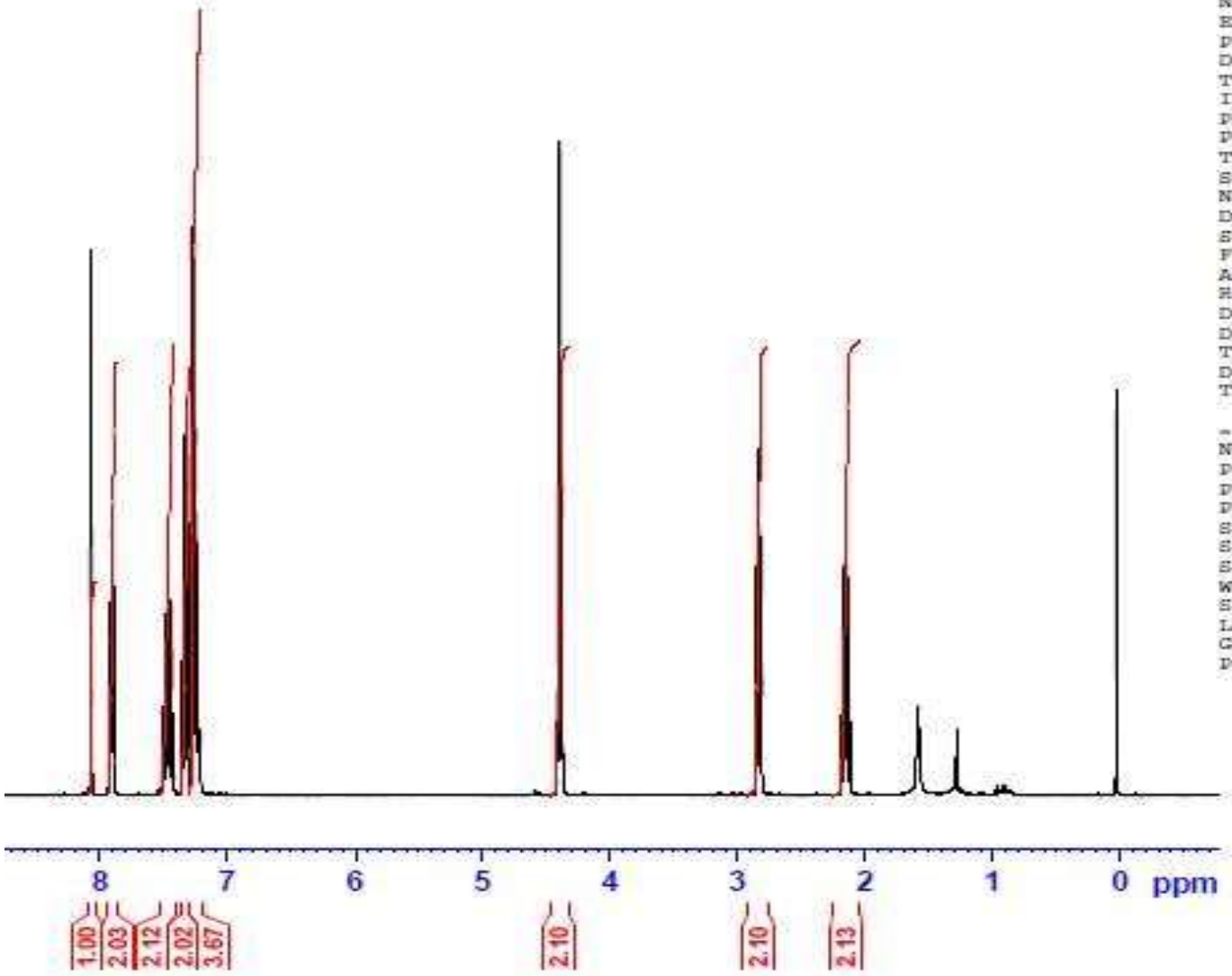
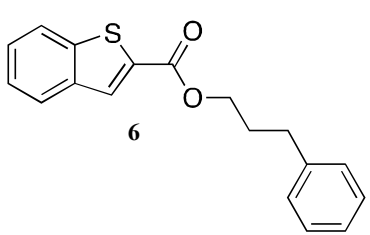


BRUKER

NAME	Audrey Isabelle
EXPNO	5
PROCNO	1
Date_	20181115
Time	13.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	101
DW	60.800 usec
DE	6.50 usec
TE	297.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



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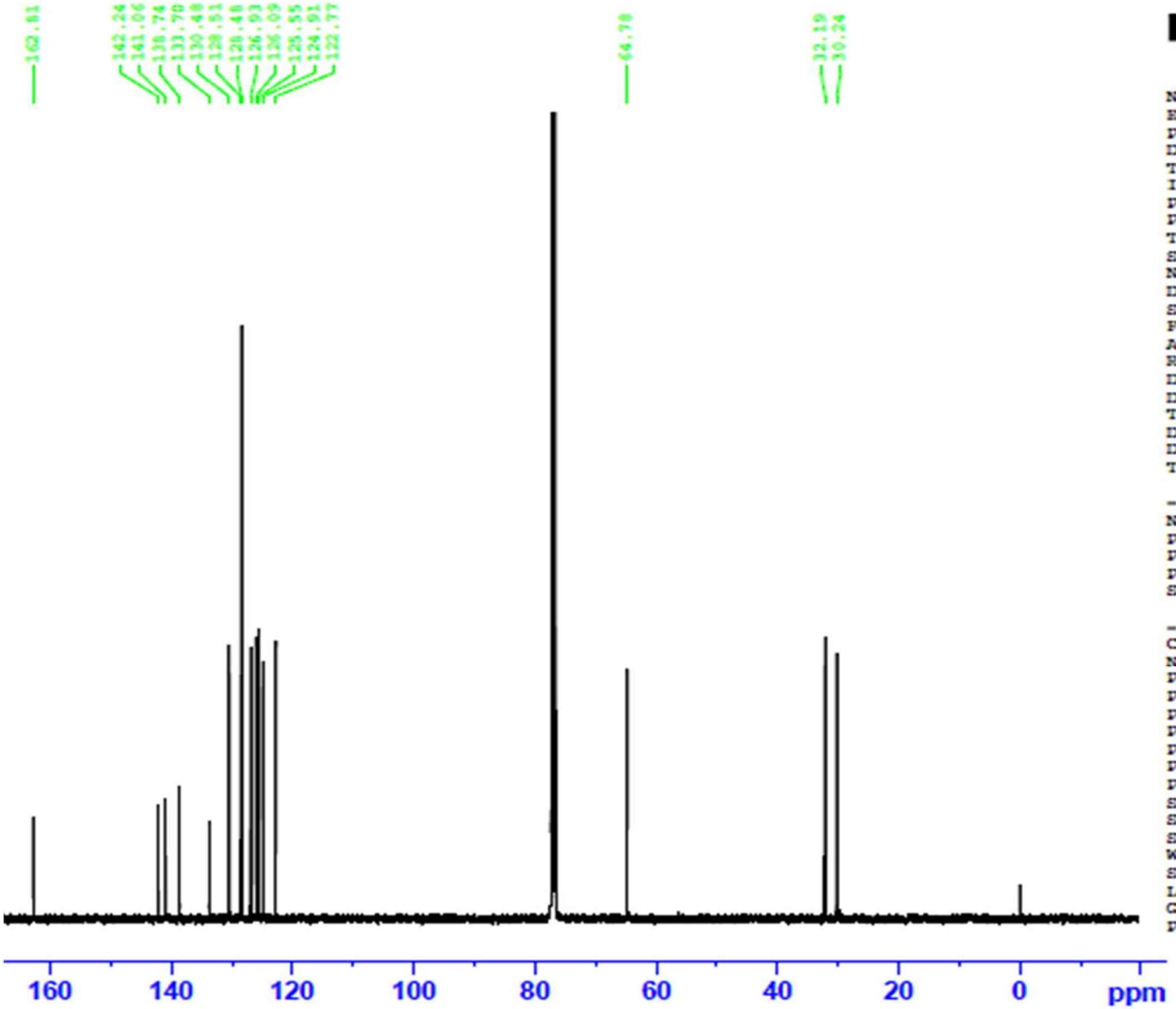
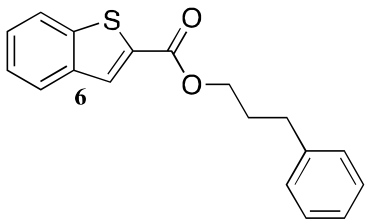
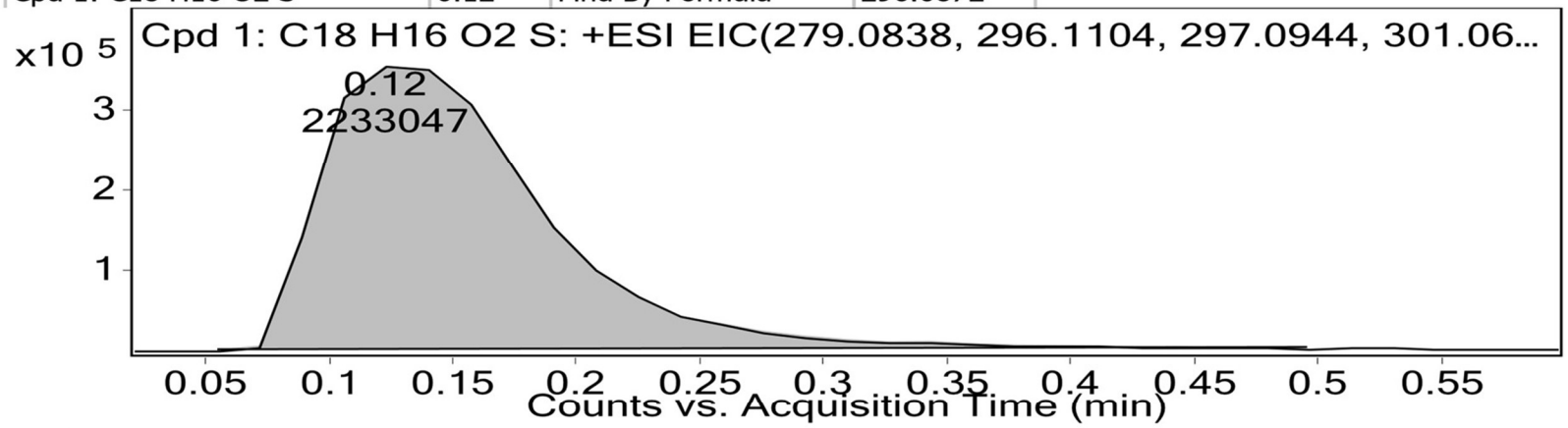



```
NAME        Audrey Isabelle
EXPNO                     6
PROCNO                    1
Date_              20181115
Time                  19.58
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT               CDCl3
NS                     5000
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      114
DW                   20.800 usec
DE                    6.50 usec
TE                   298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.90 usec
PL1                  -1.90 dB
PL1W          56.02249908 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz65
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.30 dB
PL12                 15.40 dB
PL13                 18.40 dB
PL2W          11.25229836 W
PL12W          0.34772930 W
PL13W          0.17427748 W
SFO2         400.1316005 MHz
SI                    32768
SF           100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

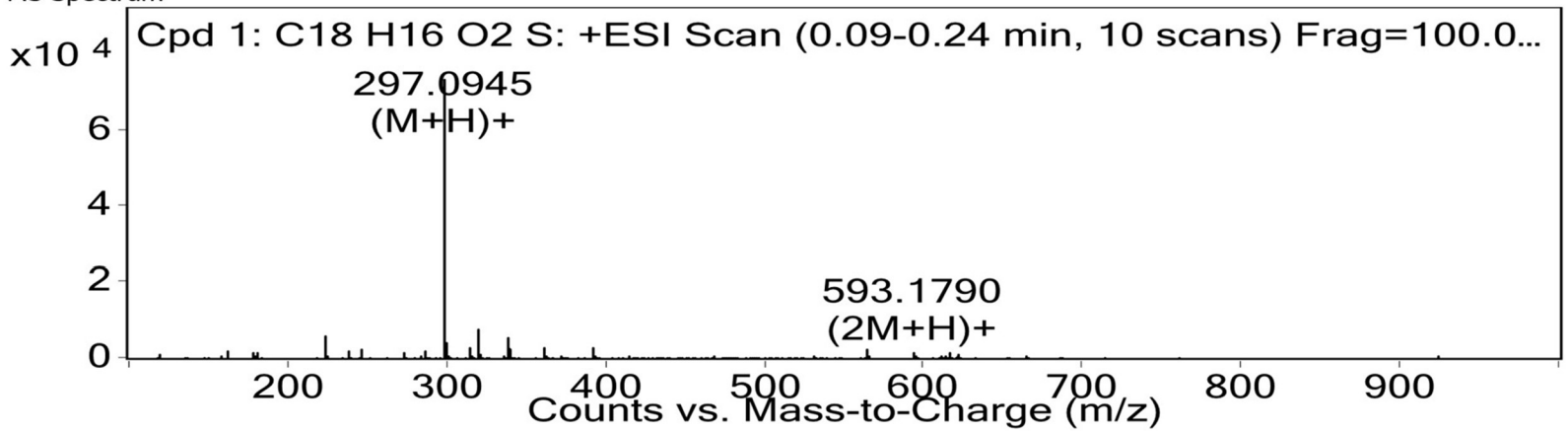
HRMS



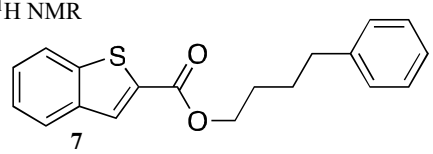
Compound Label	RT	Algorithm	Mass
Cpd 1: C18 H16 O2 S	0.12	Find By Formula	296.0872



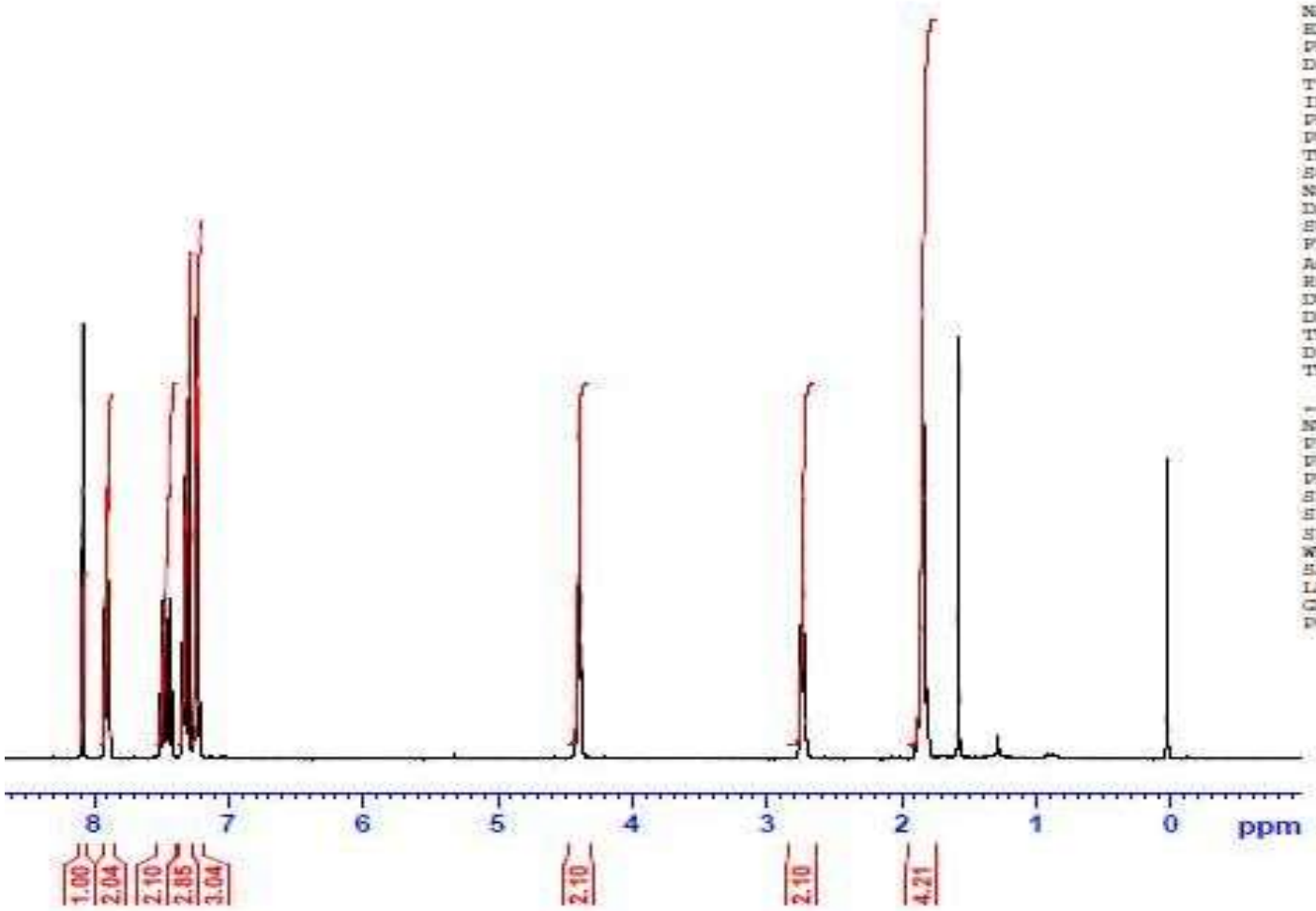
MS Spectrum



^{1}H NMR



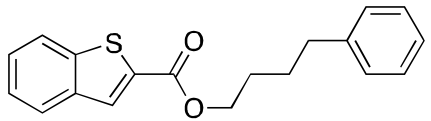
7



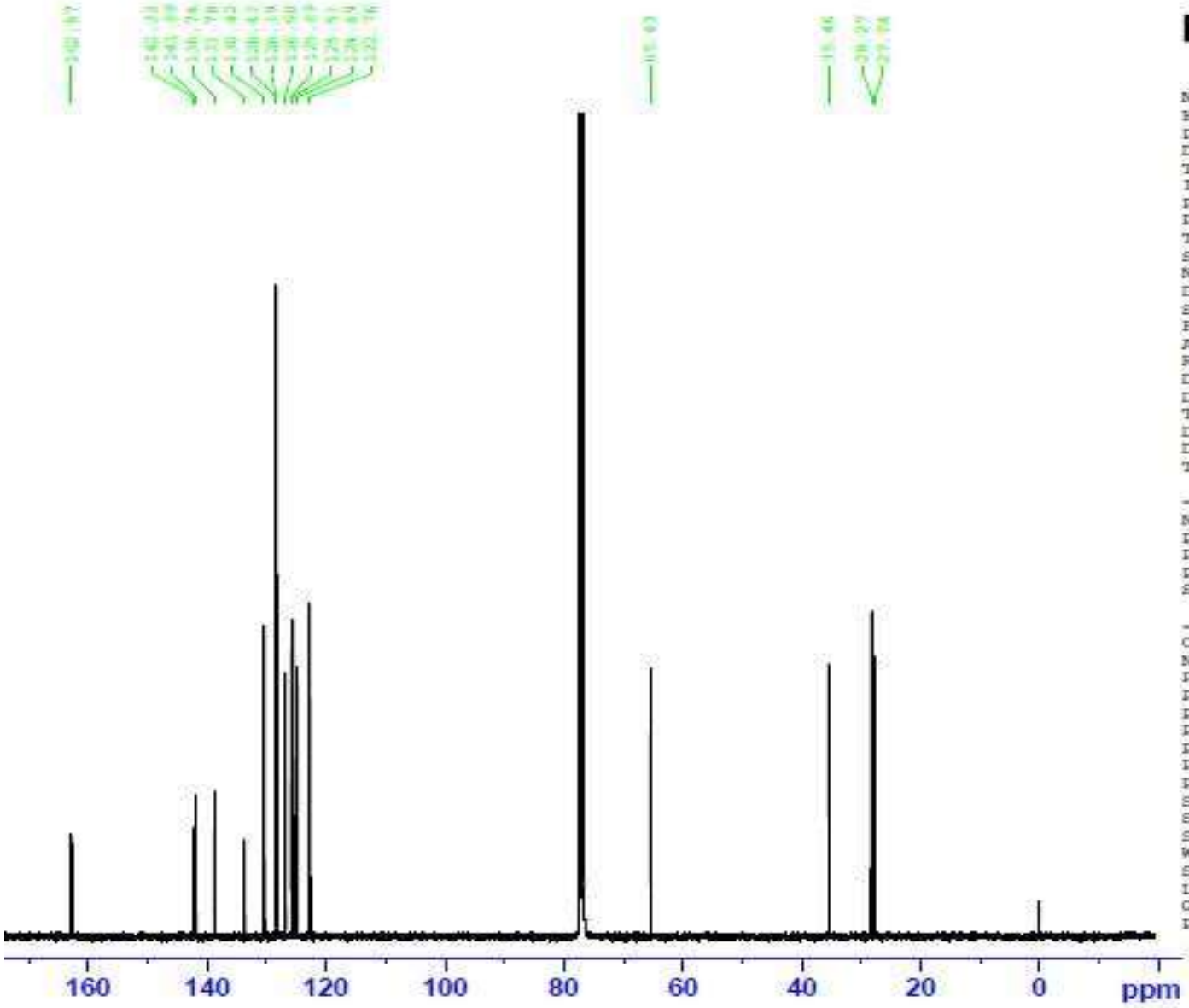
BRUKER

NAME	Audrey Isabelle	
EXPNO	10	
PROCNO	1	
Date_	20190204	
Time	15.17	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	114	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{13}C NMR



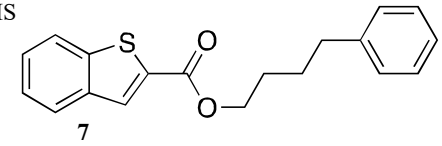
7



BRUKER

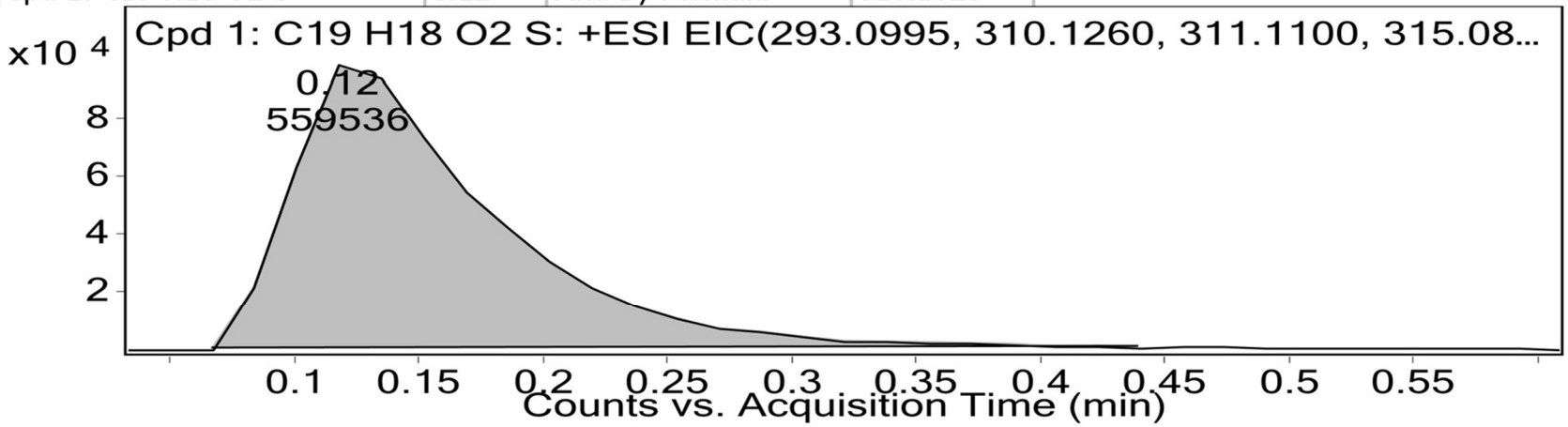
NAME	Audrey Isabelle
EXPNO	11
PROCNO	1
Date_	20190205
Time	0.51
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	10000
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

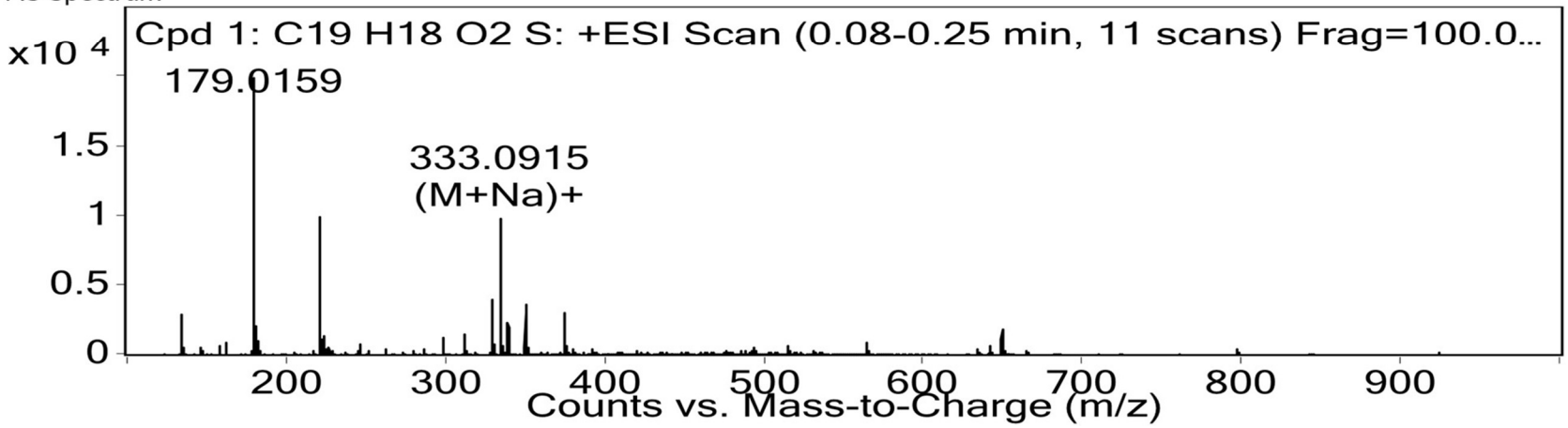


7

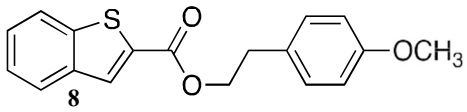
Compound Label	RT	Algorithm	Mass
Cpd 1: C19 H18 O2 S	0.12	Find By Formula	310.1023



MS Spectrum



^{1}H NMR



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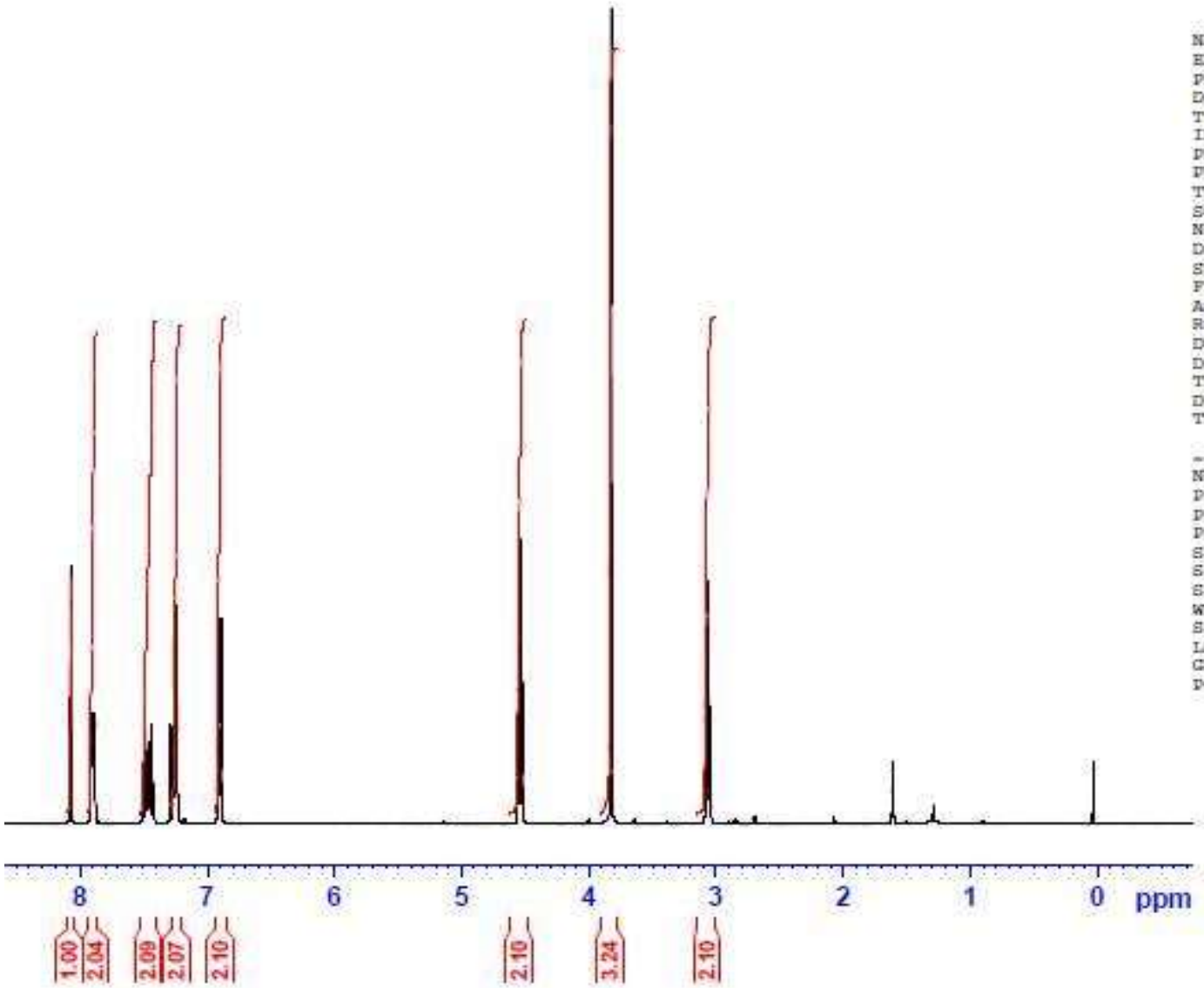
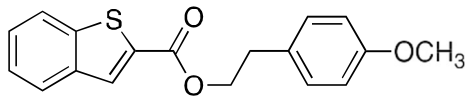


BRUKER

NAME	Audrey Isabelle	
EXPNO	12	
PROCNO	1	
Date_	20190211	
Time	10.35	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	80.6	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{13}C NMR



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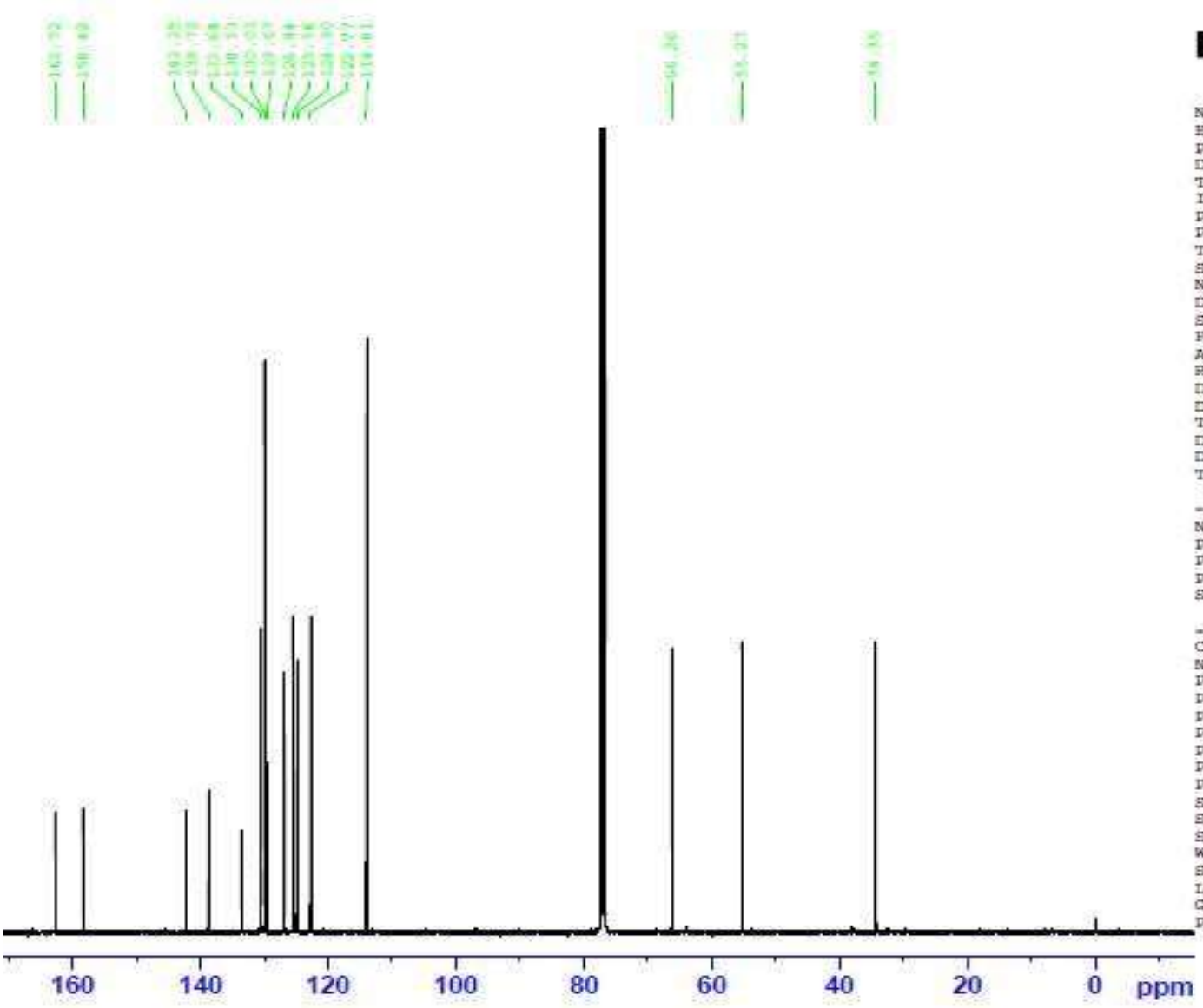
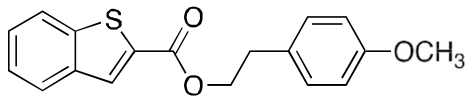


BRUKER

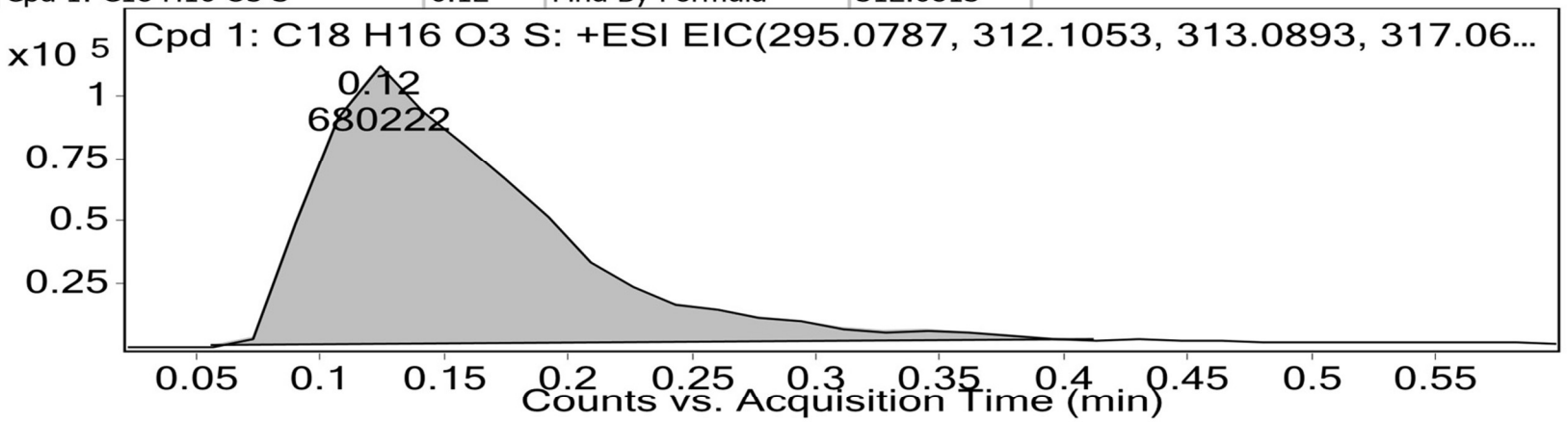
NAME	Audrey Isabelle	
EXPNO	13	
PROCNO	1	
Date_	20190211	
Time	16.02	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	5702	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS

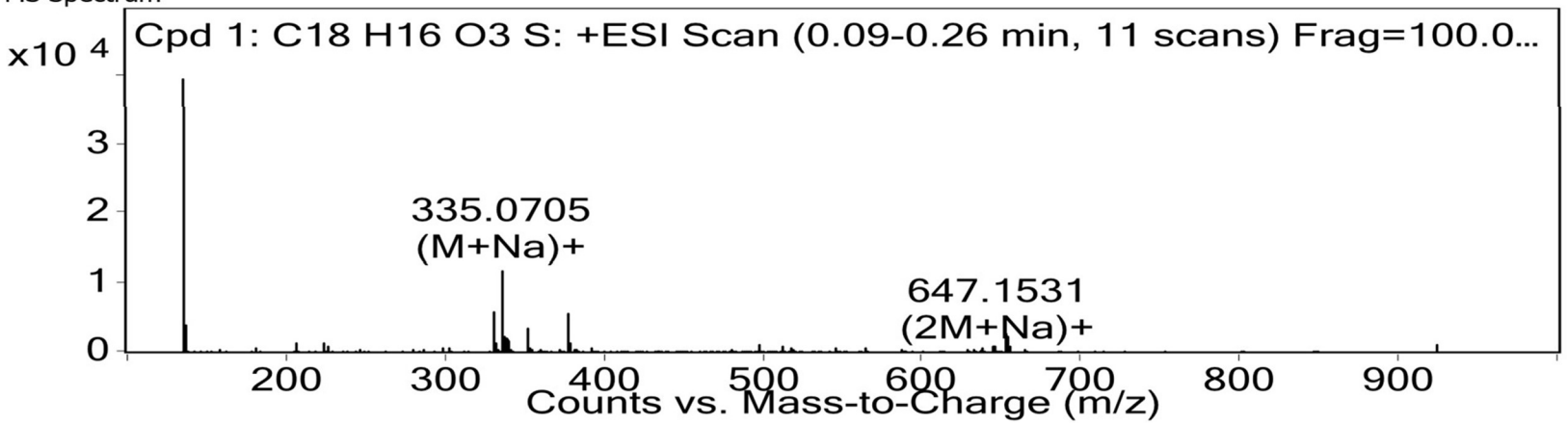


8

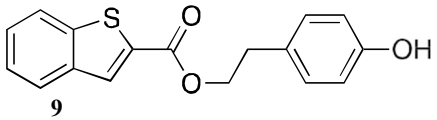
Compound Label	RT	Algorithm	Mass
Cpd 1: C18 H16 O3 S	0.12	Find By Formula	312.0813



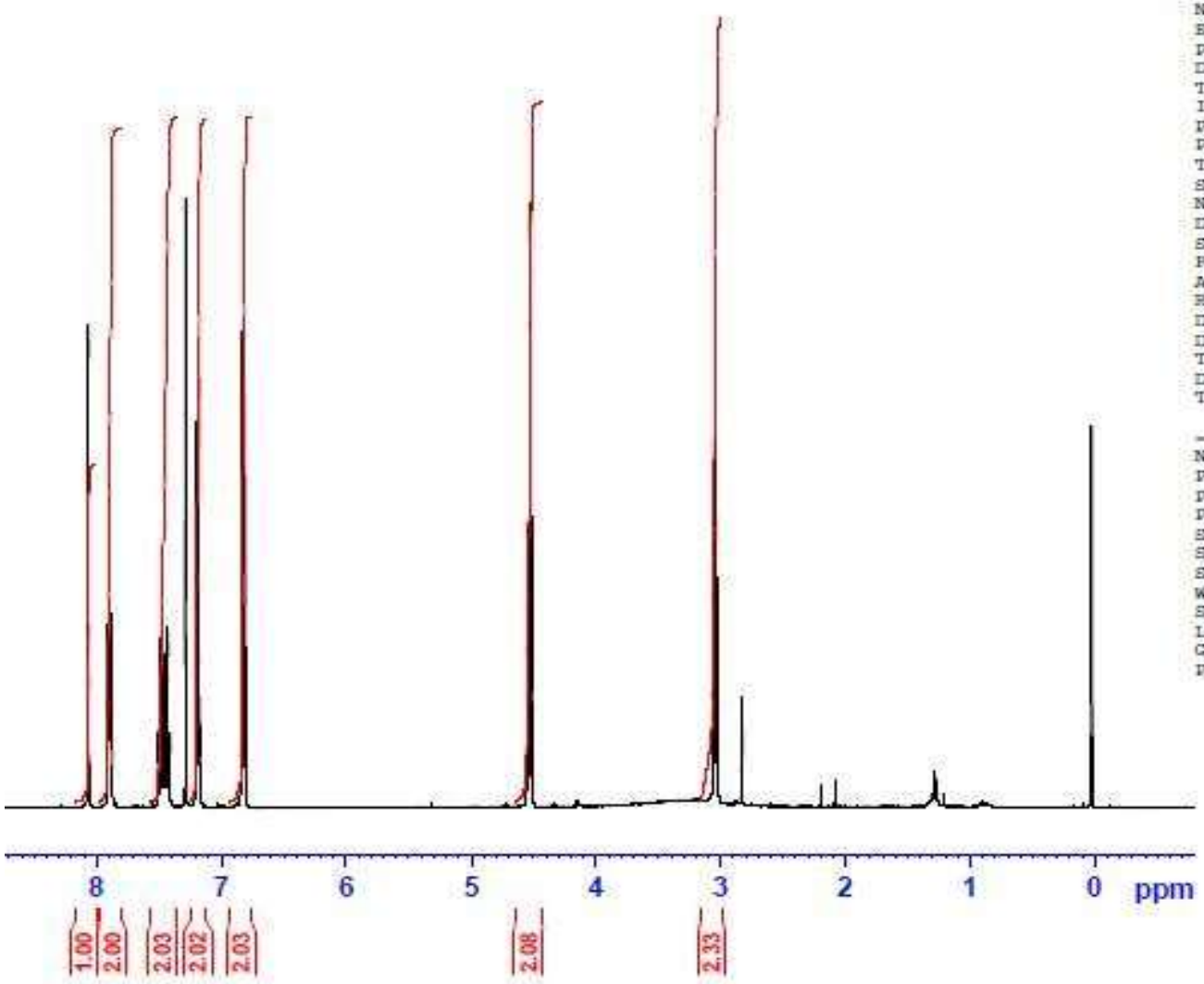
MS Spectrum



^{1}H NMR



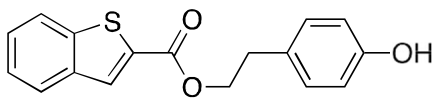
9



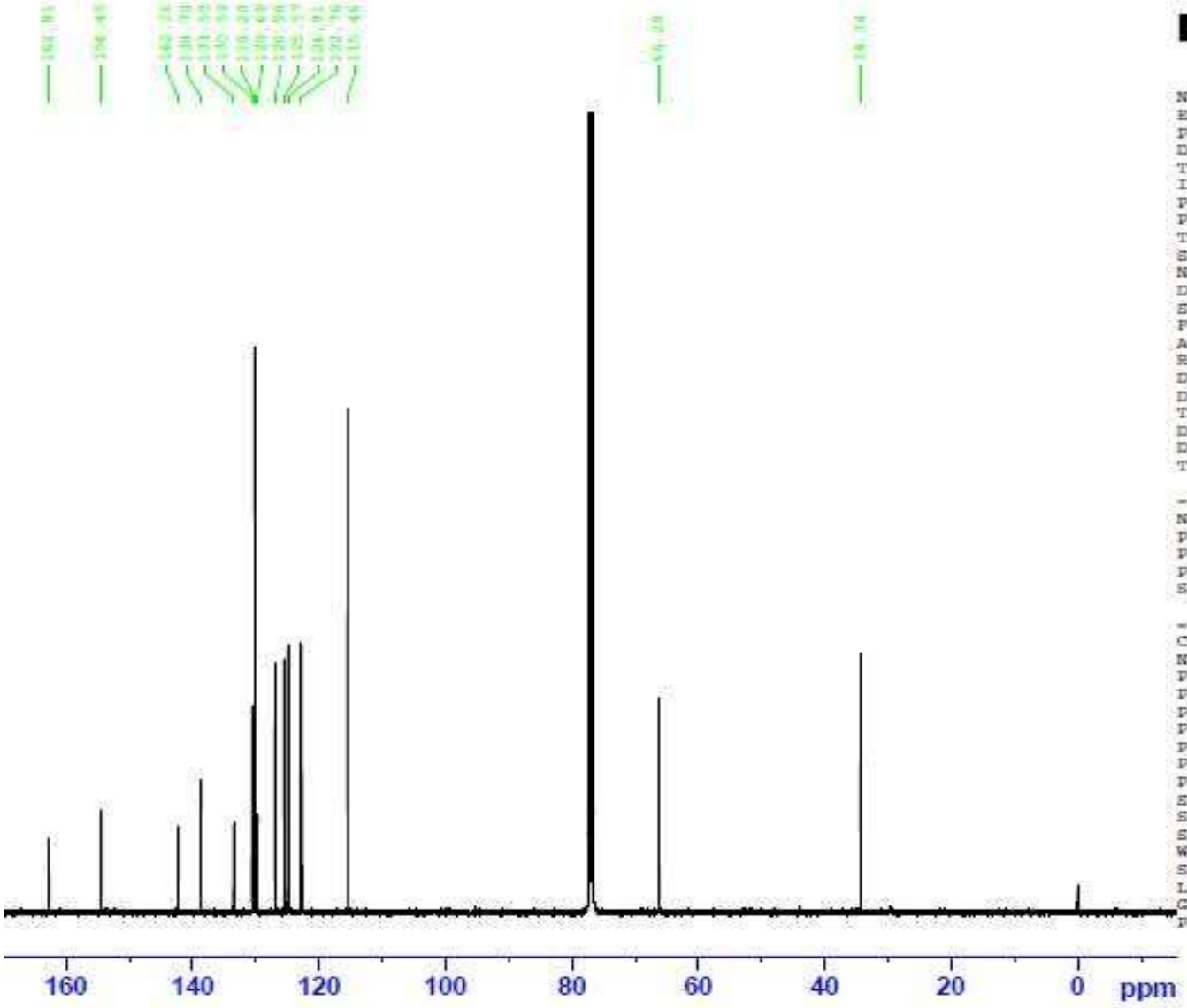
BRUKER

NAME	Audrey Isabelle
EXPNO	14
PROCNO	1
Date_	20190220
Time	15.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	128
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



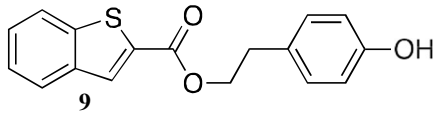
9



BRUKER

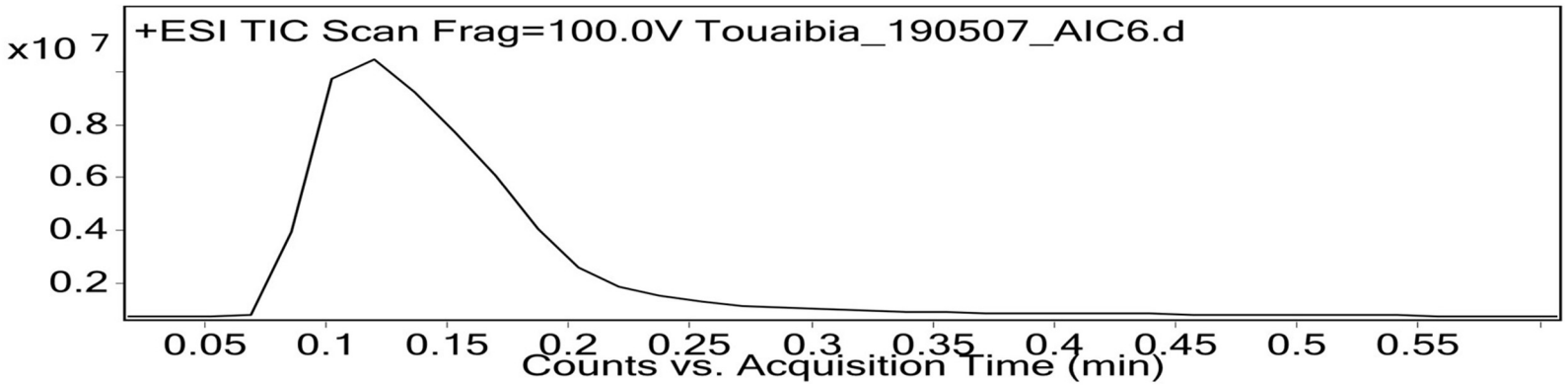
NAME	Audrey Isabelle	
EXPNO	15	
PROCNO	1	
Date_	20190221	
Time	0.51	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	10000	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS



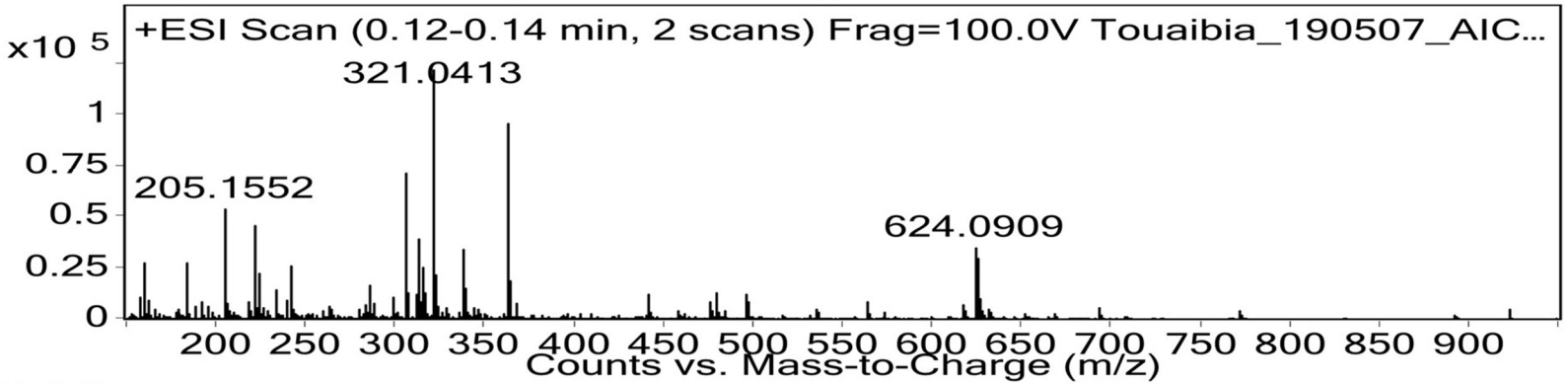
9

Fragmentor Voltage 100 **Collision Energy** 0 **Ionization Mode** Esi



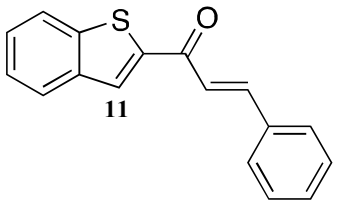
User Spectra

Fragmentor Voltage 100 **Collision Energy** 0 **Ionization Mode** Esi

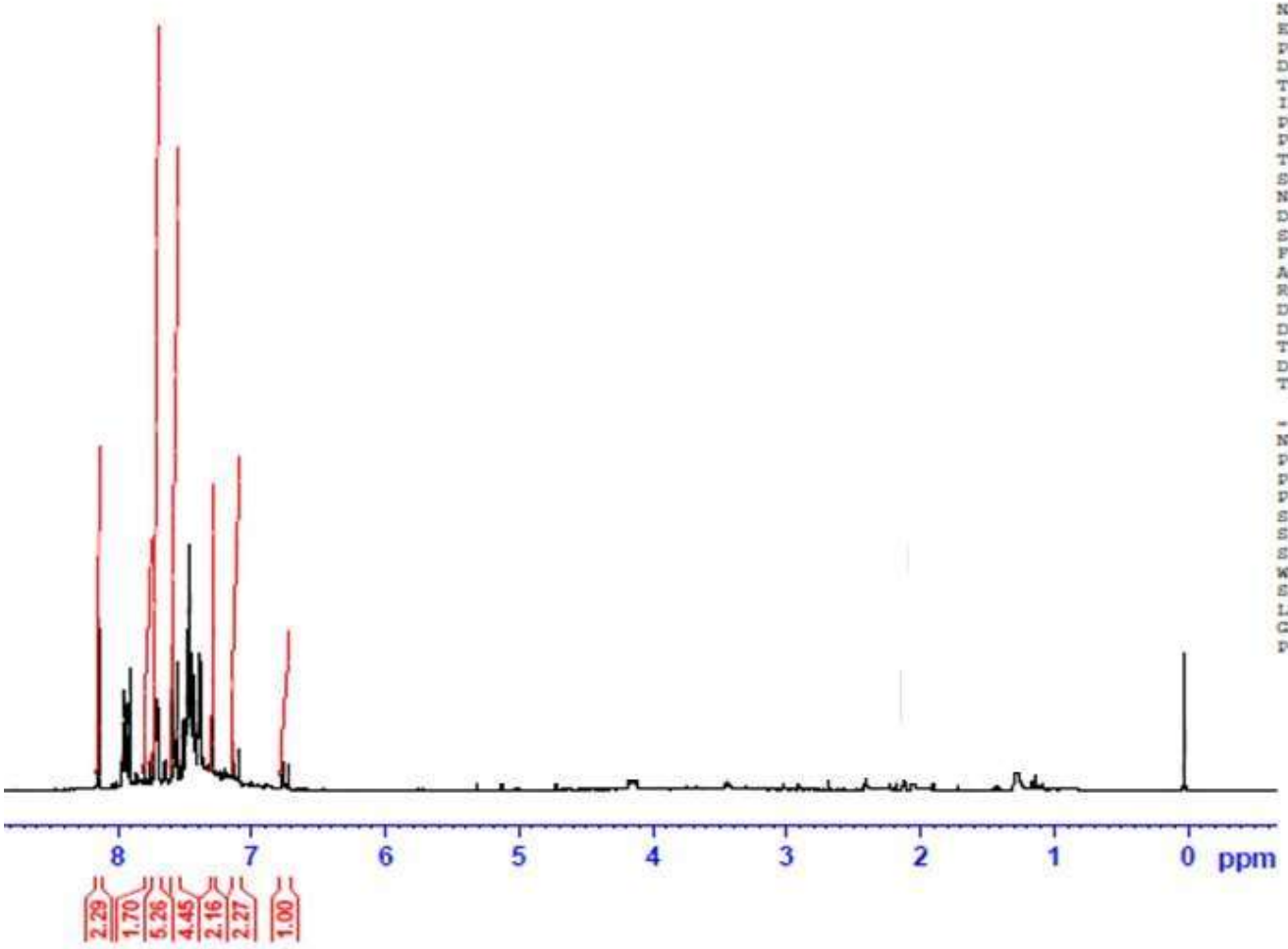


Peak List

^{1}H NMR



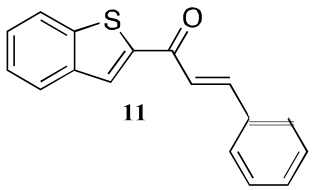
11



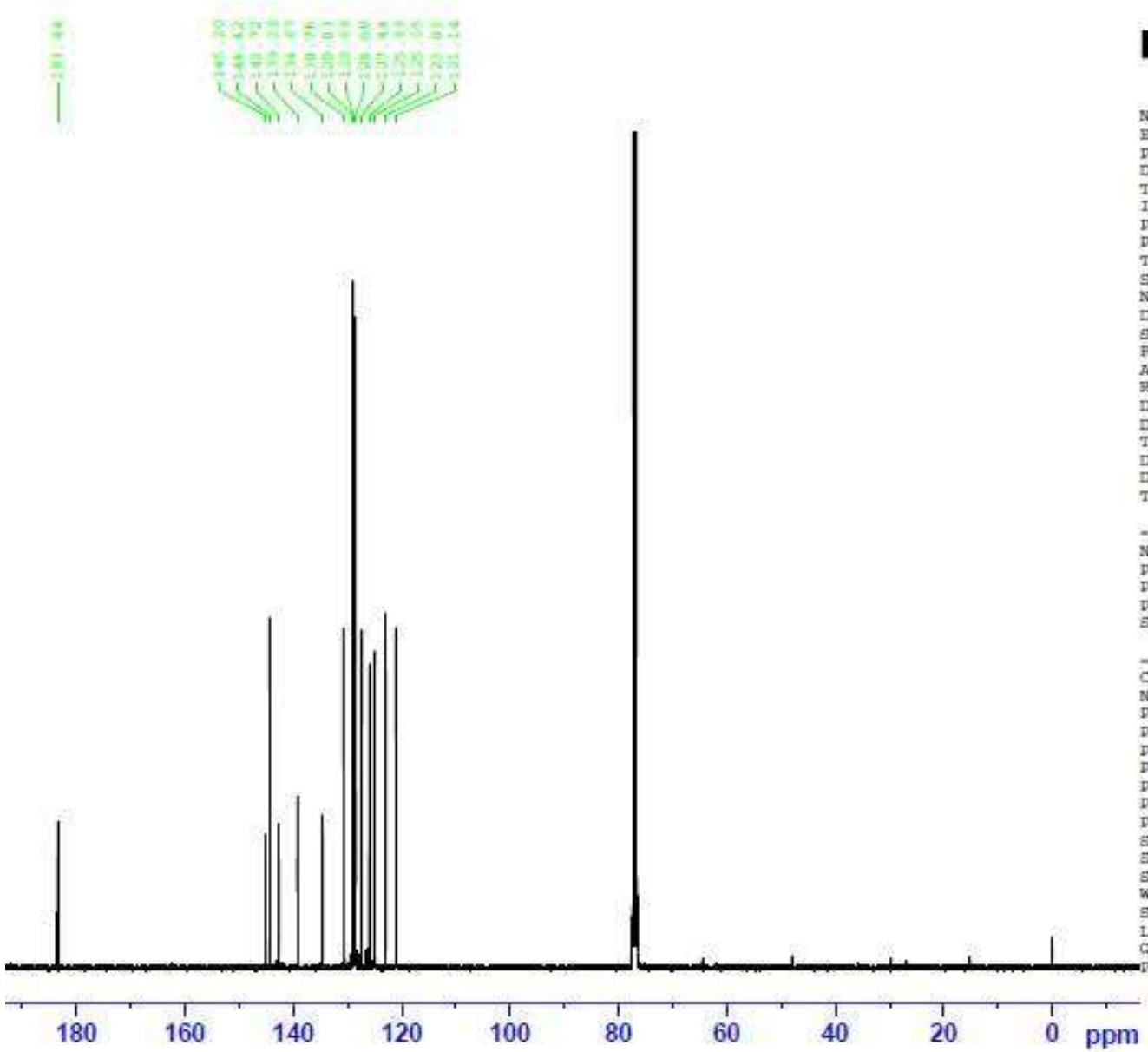
BRUKER

NAME	Audrey Isabelle	
EXPNO	47	
PROCNO	1	
Date_	20190530	
Time	14.26	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	64	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
--------	CHANNEL f1	--------
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{13}C NMR



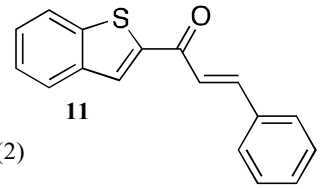
11



BRUKER

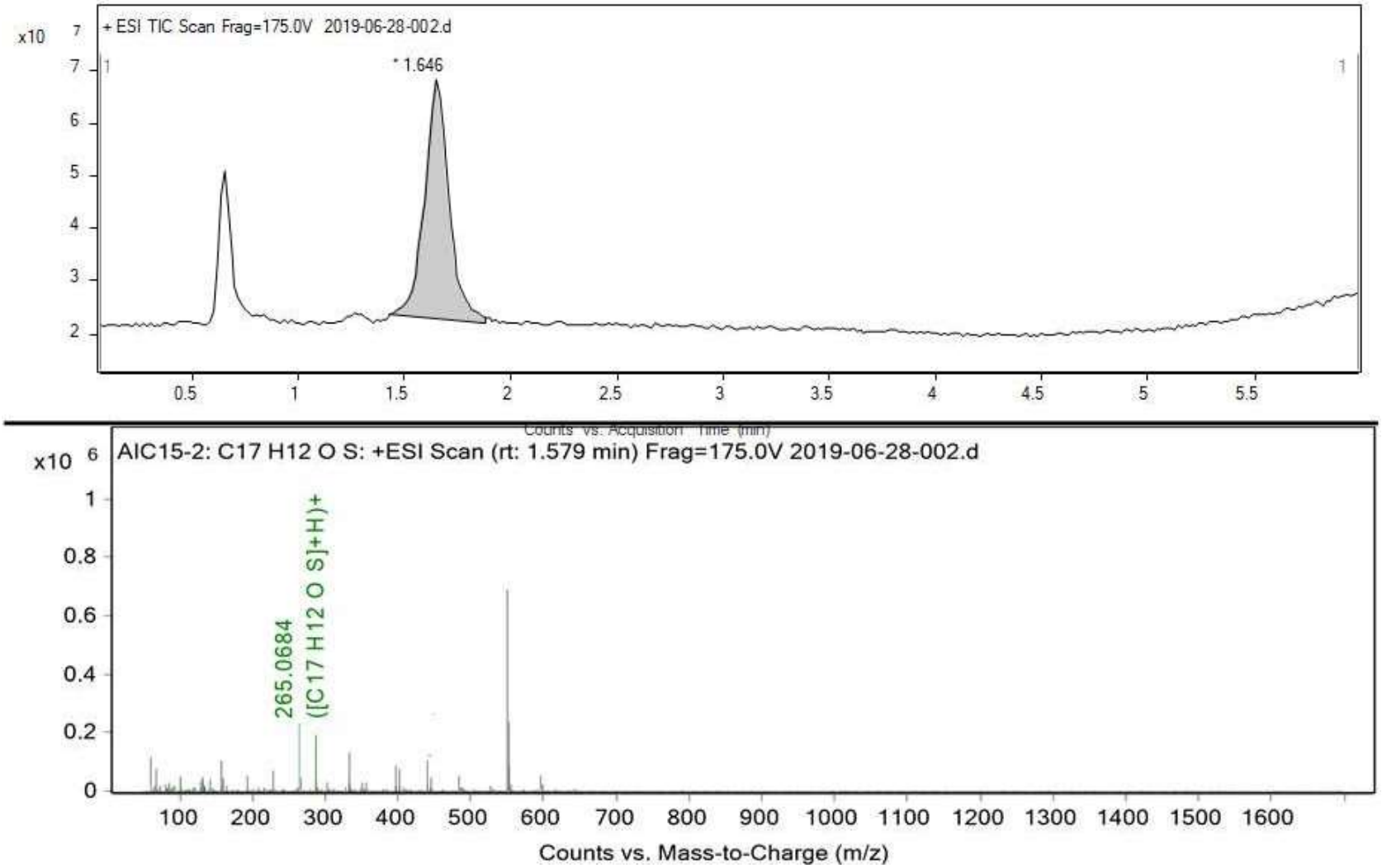
NAME	Audrey Isabelle
EXPNO	52
PROCNO	1
Date_	20190603
Time	23.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	10000
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

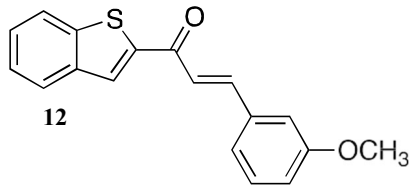


11

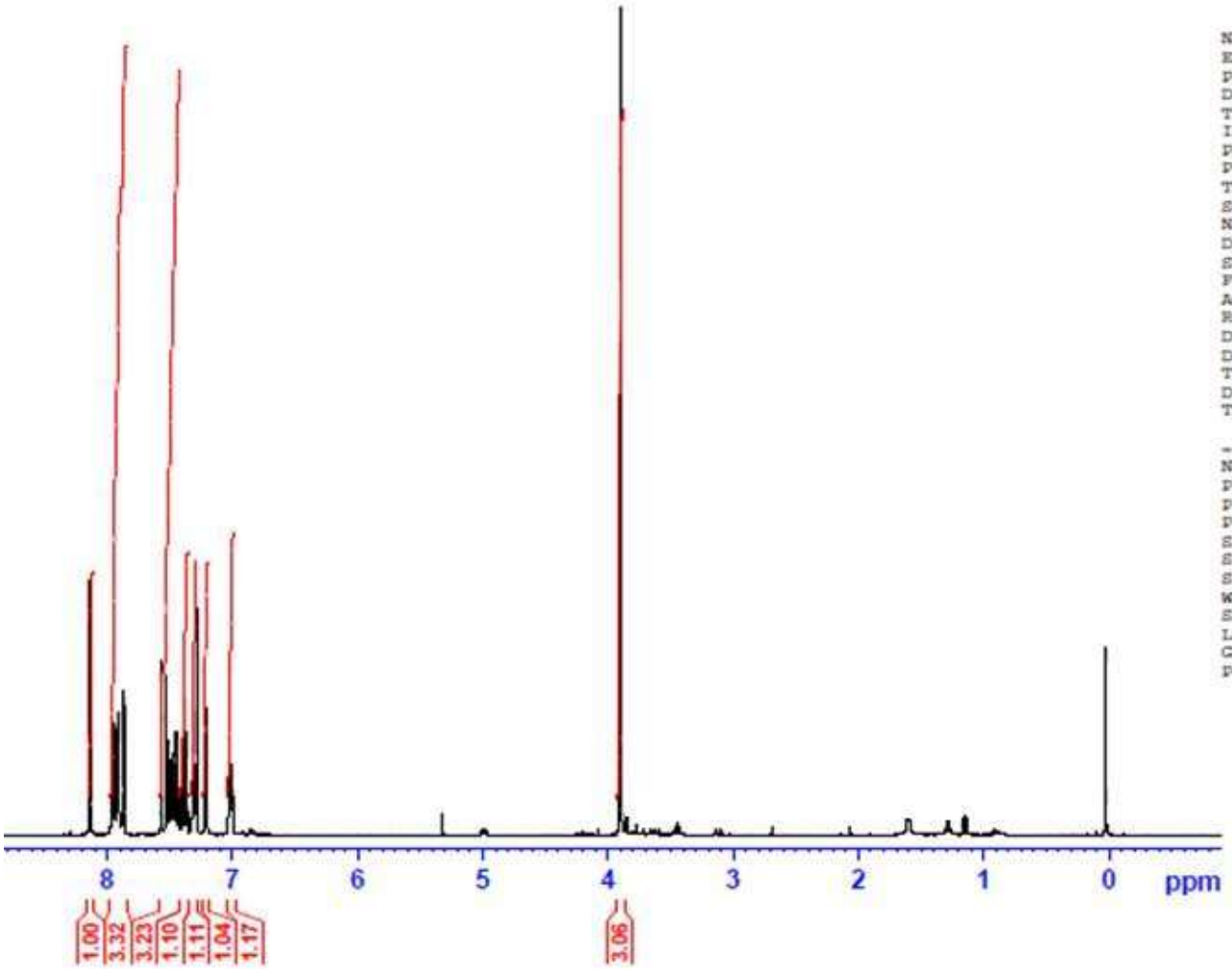
AIC 15(2)



^{1}H NMR



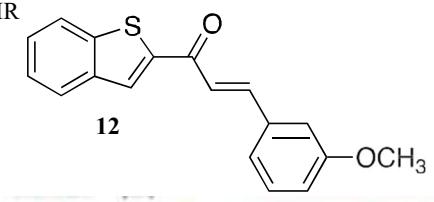
12



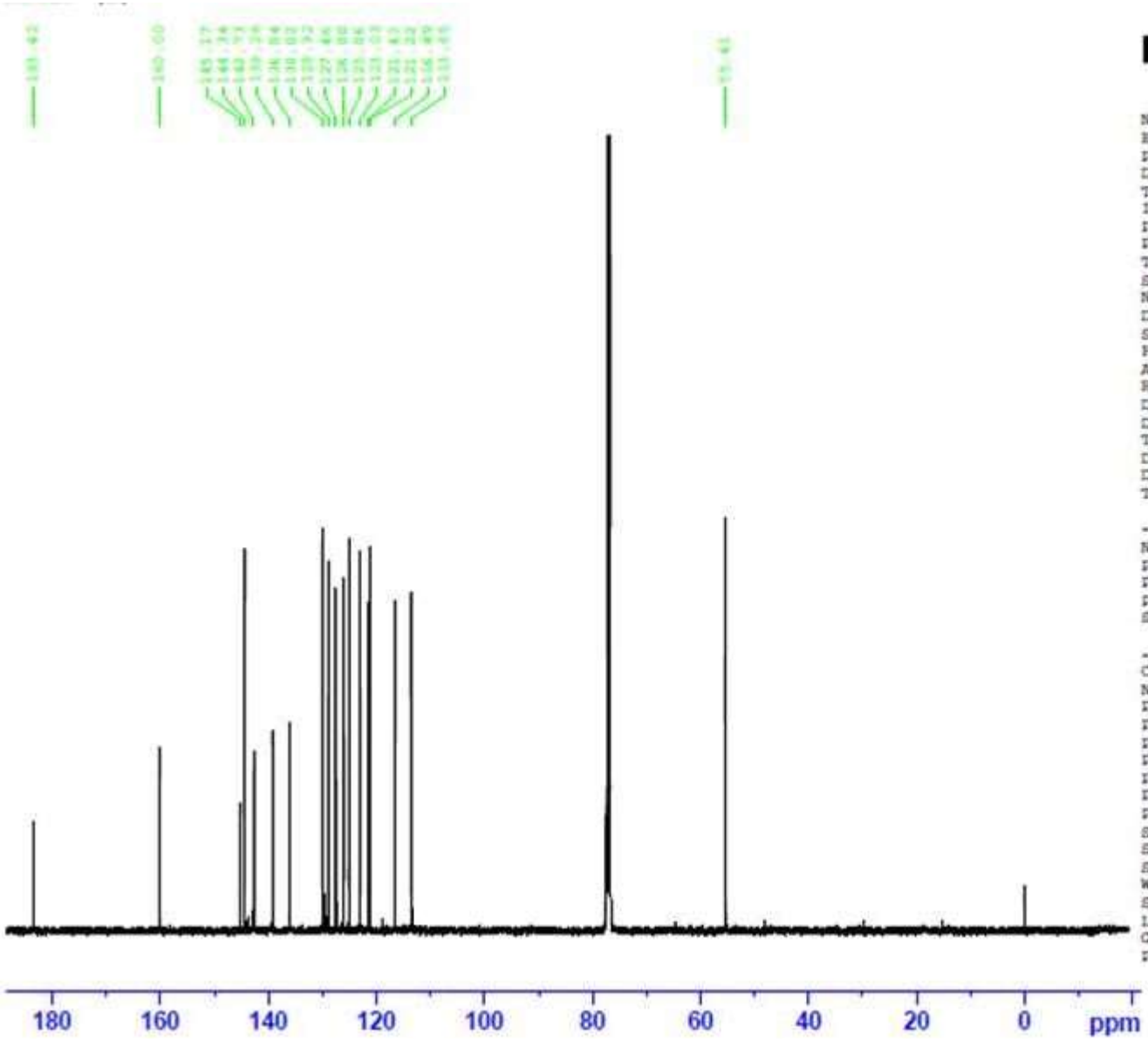
BRUKER

NAME	Audrey Isabelle	
EXPNO	54	
PROCNO	1	
Date_	20190604	
Time	16.24	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	114	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
-------- CHANNEL f1 --------		
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{13}C NMR



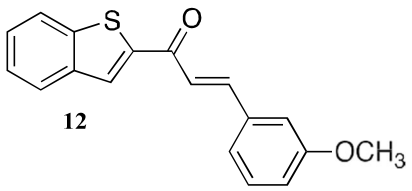
12



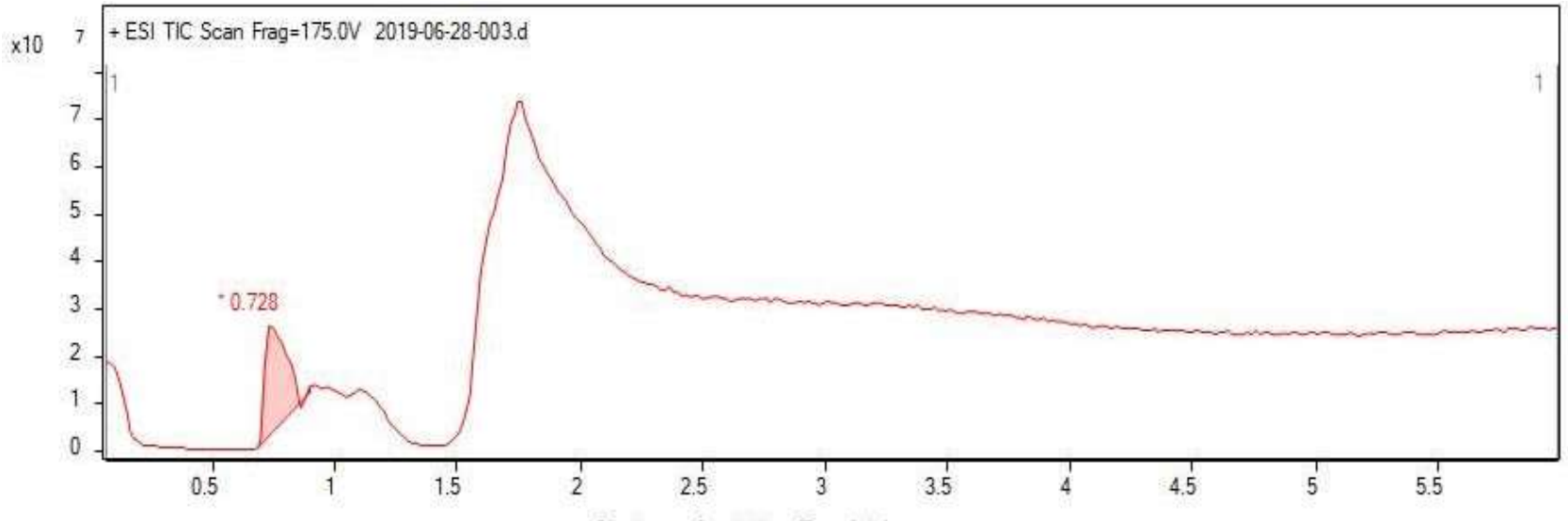
BRUKER

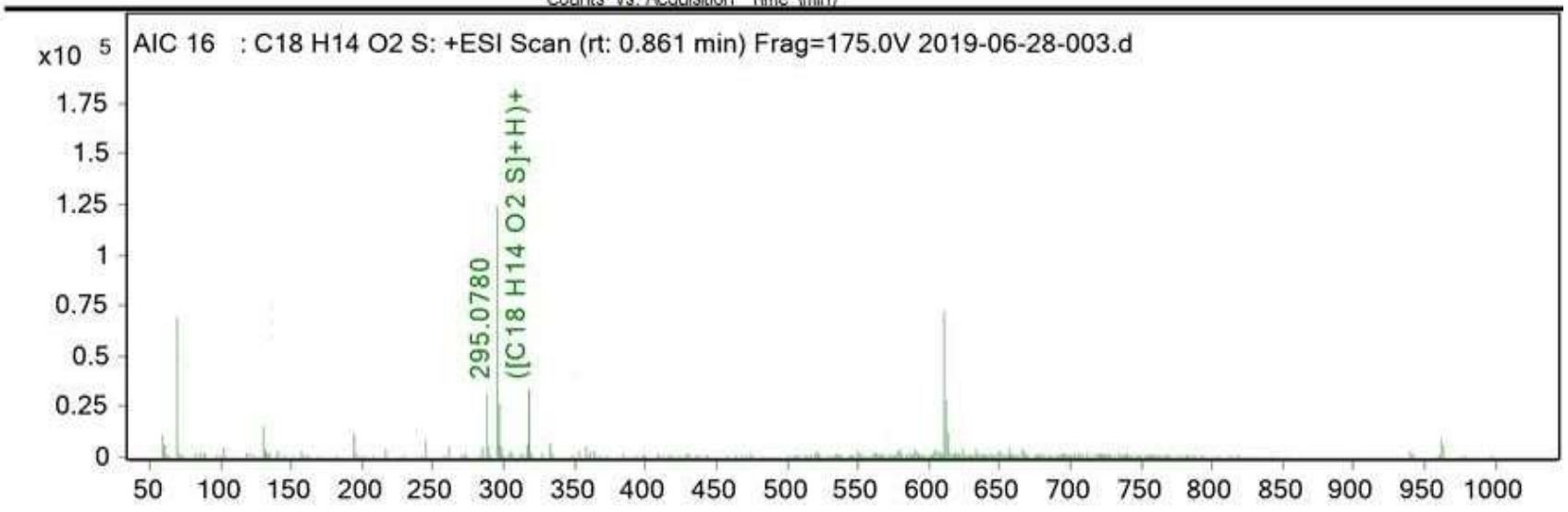
NAME	Audrey Isabelle
EXPNO	56
PROCNO	1
Date_	20190605
Time	2.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	10000
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
--------	CHANNEL f1 --------
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
--------	CHANNEL f2 --------
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

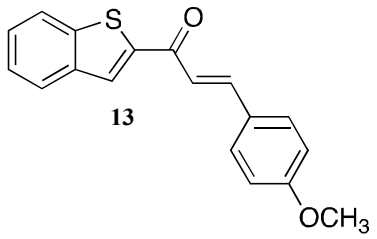

S
O
OCH3

12

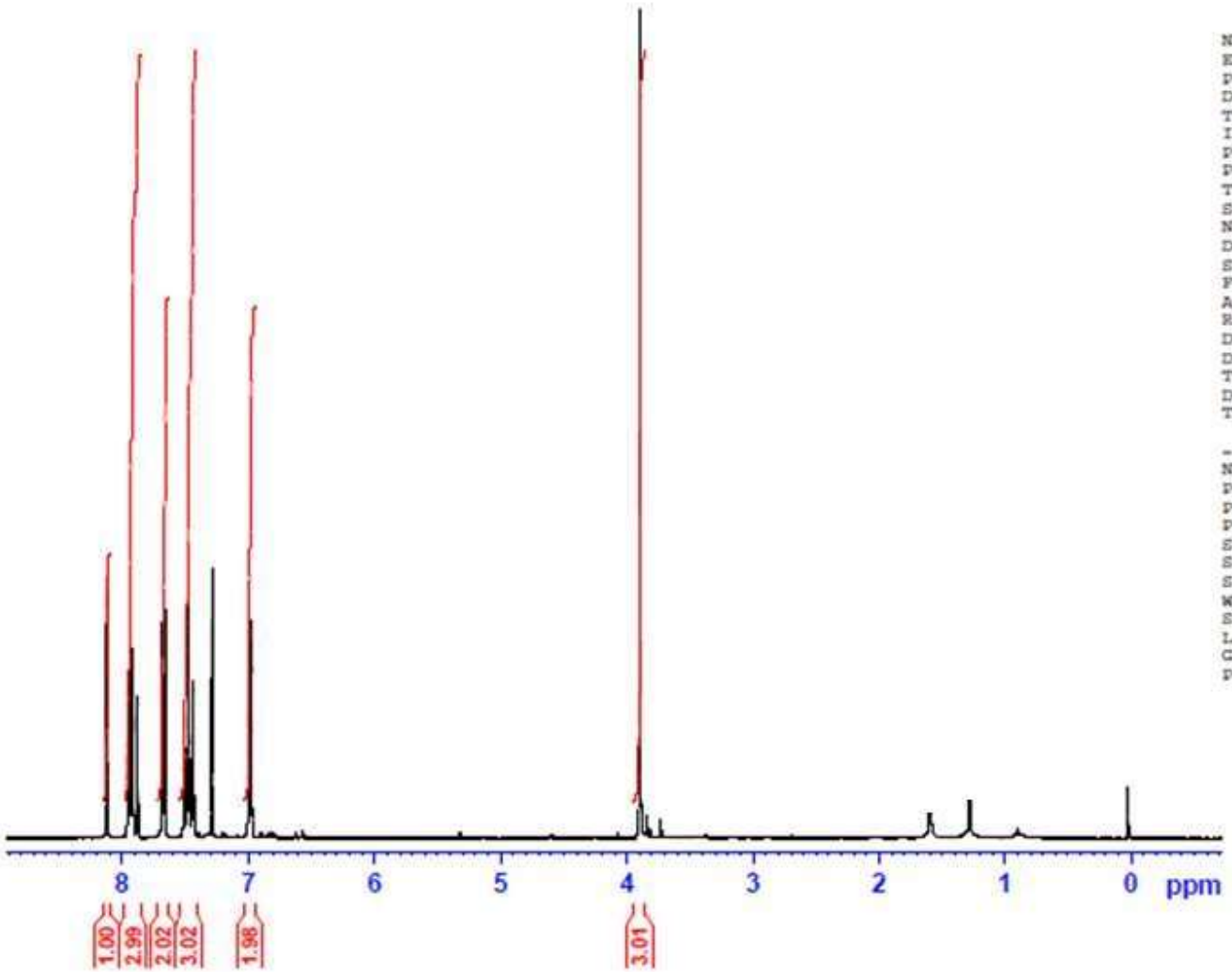

x10 7
+ ESI TIC Scan Frag=175.0V 2019-06-28-003.d
1
1
* 0.728
0 1 2 3 4 5 6 7
0.5 1 1.5 2 2.5 3 3.5 4 4.5 5 5.5
Counts vs. Acquisition Time (min)


x10 5
AIC 16 : C18 H14 O2 S: +ESI Scan (rt: 0.861 min) Frag=175.0V 2019-06-28-003.d
295.0780
([C18 H14 O2 S]+H)+
0 0.25 0.5 0.75 1 1.25 1.5 1.75
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000

^{1}H NMR



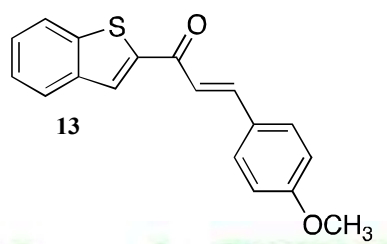
13



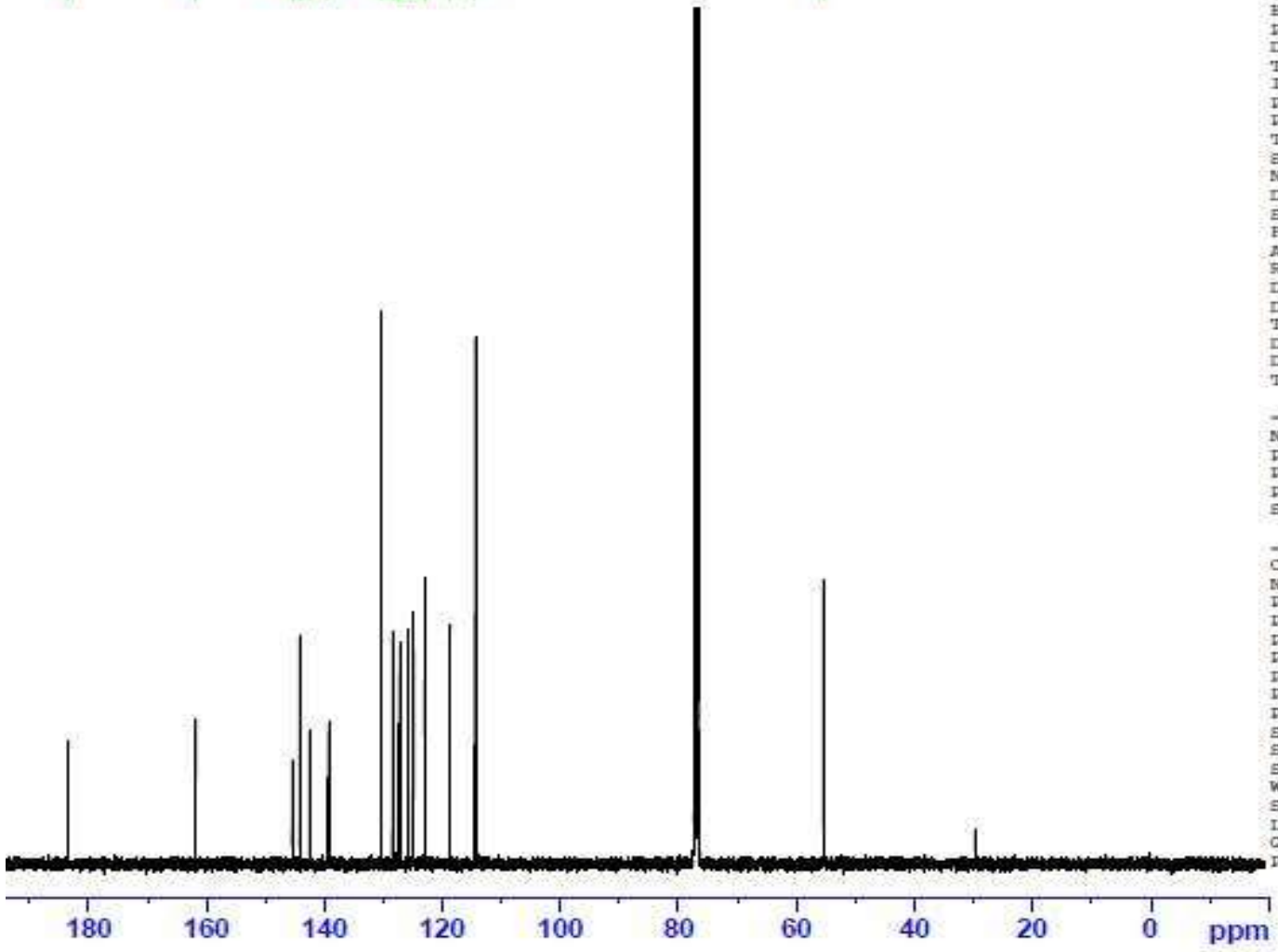
BRUKER

NAME	Audrey Isabelle	
EXPNO	30	
PROCNO	1	
Date_	20190521	
Time	13.19	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	128	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
-------- CHANNEL f1 --------		
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{13}C NMR



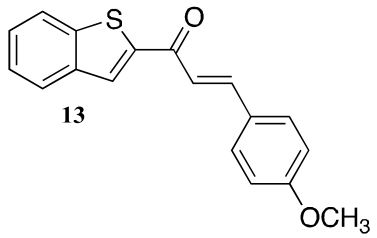
13



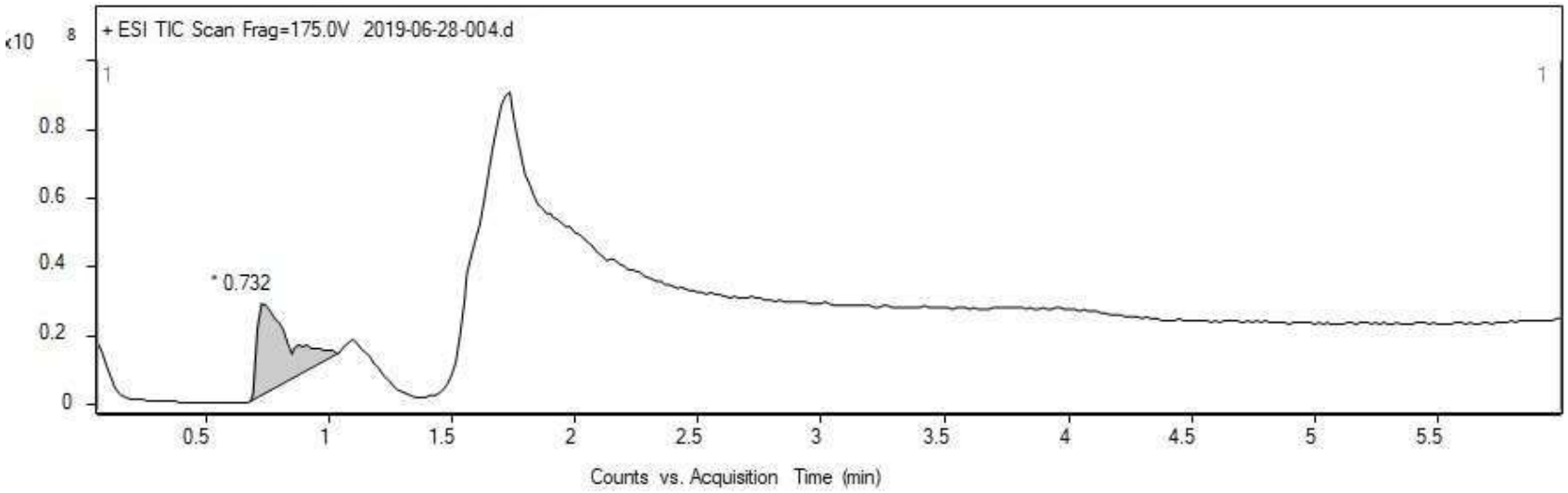
BRUKER

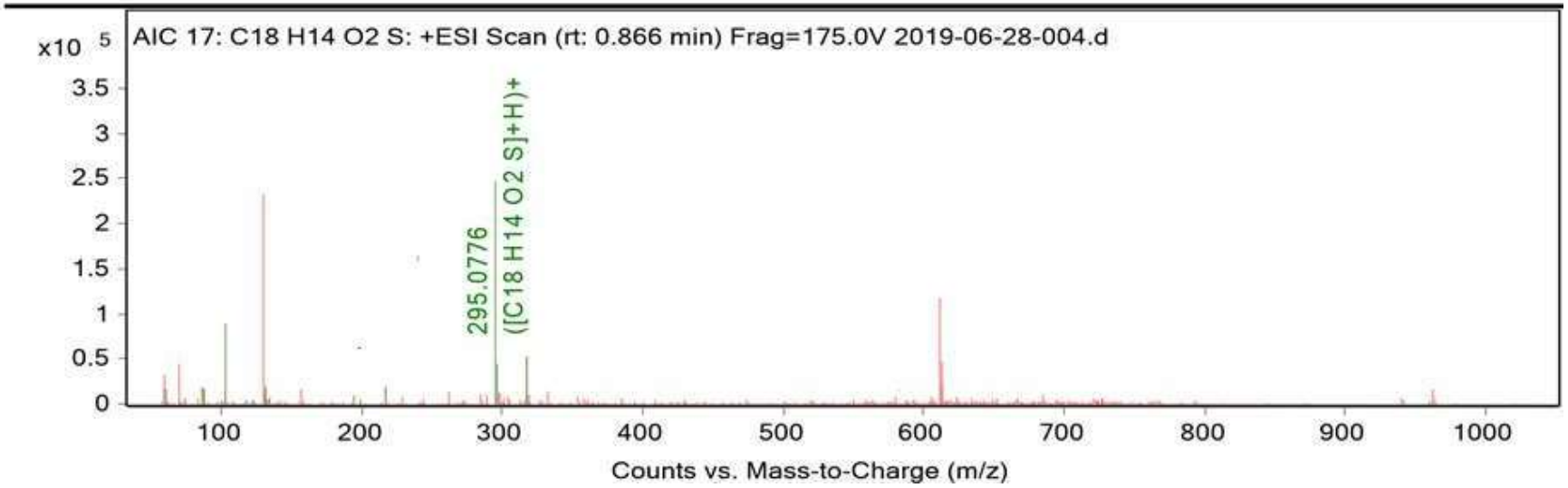
NAME	Audrey Isabelle
EXPNO	33
PROCNO	1
Date_	20190521
Time	16.41
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2829
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
-------- CHANNEL f2 --------	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

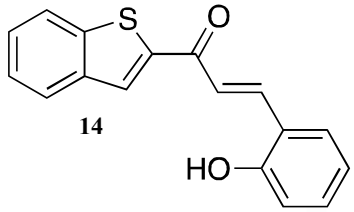

S
O
OCH3

13

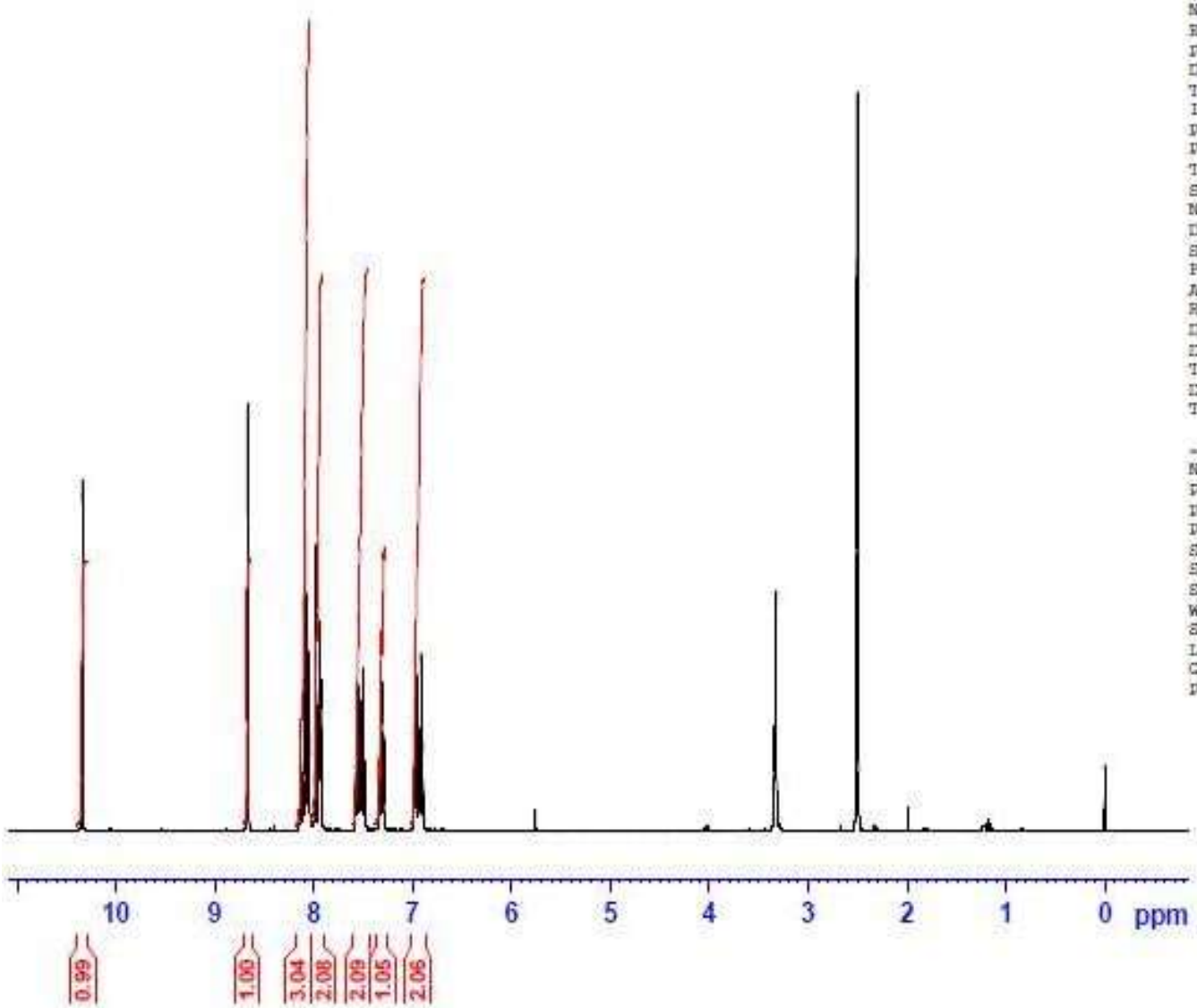

x10 8
+ ESI TIC Scan Frag=175.0V 2019-06-28-004.d
0.8
0.6
0.4
0.2
0
* 0.732
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Counts vs. Acquisition Time (min)


x10 5
AIC 17: C18 H14 O2 S: +ESI Scan (rt: 0.866 min) Frag=175.0V 2019-06-28-004.d
3.5
3
2.5
2
1.5
1
0.5
0
295.0776
([C18 H14 O2 S]+H)+
100
200
300
400
500
600
700
800
900
1000
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



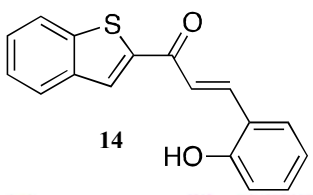
14



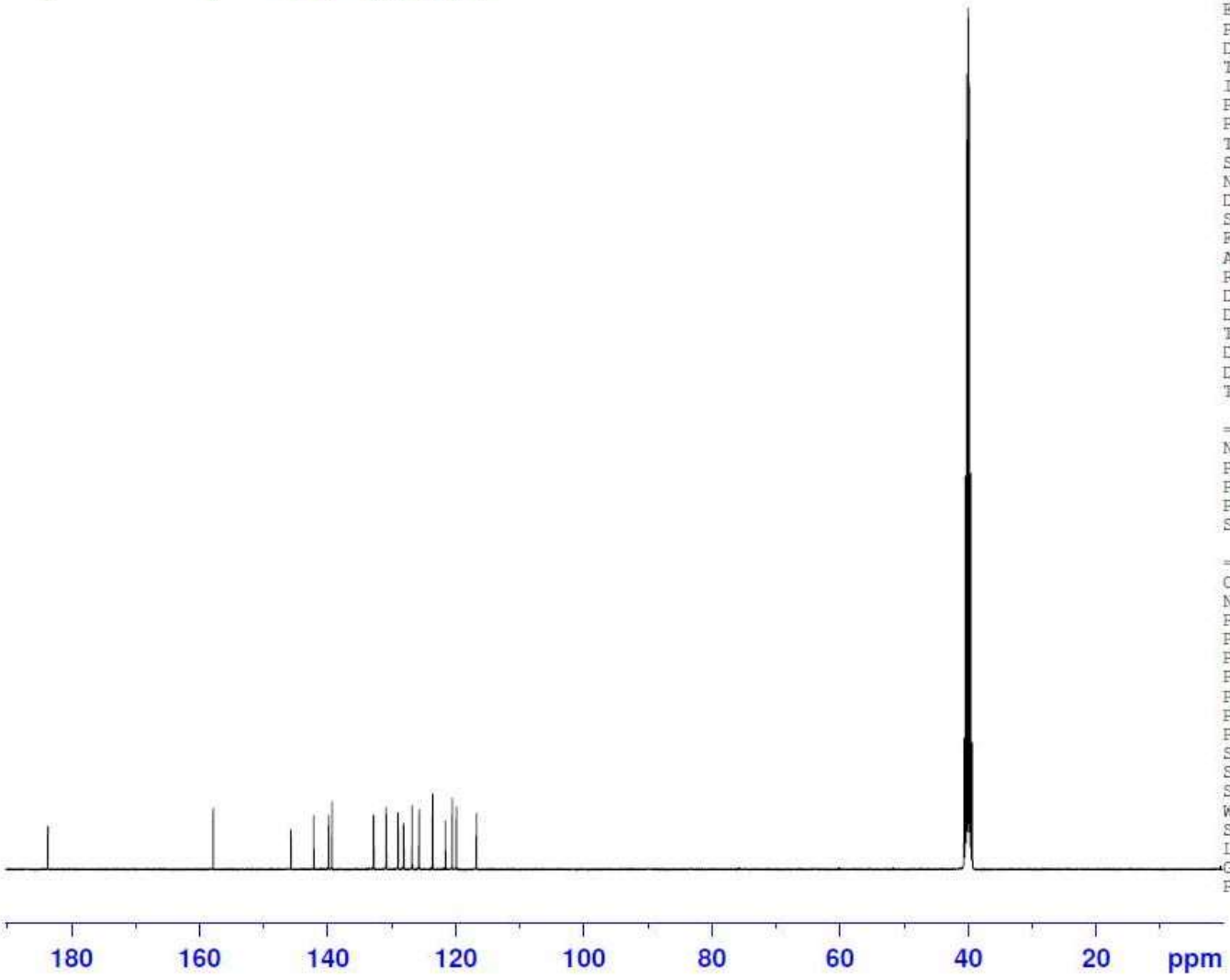
BRUKER

NAME	Audrey Isabelle
EXPNO	68
PROCNO	1
Date_	20190614
Time	10.50
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	128
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



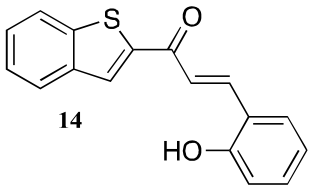
14



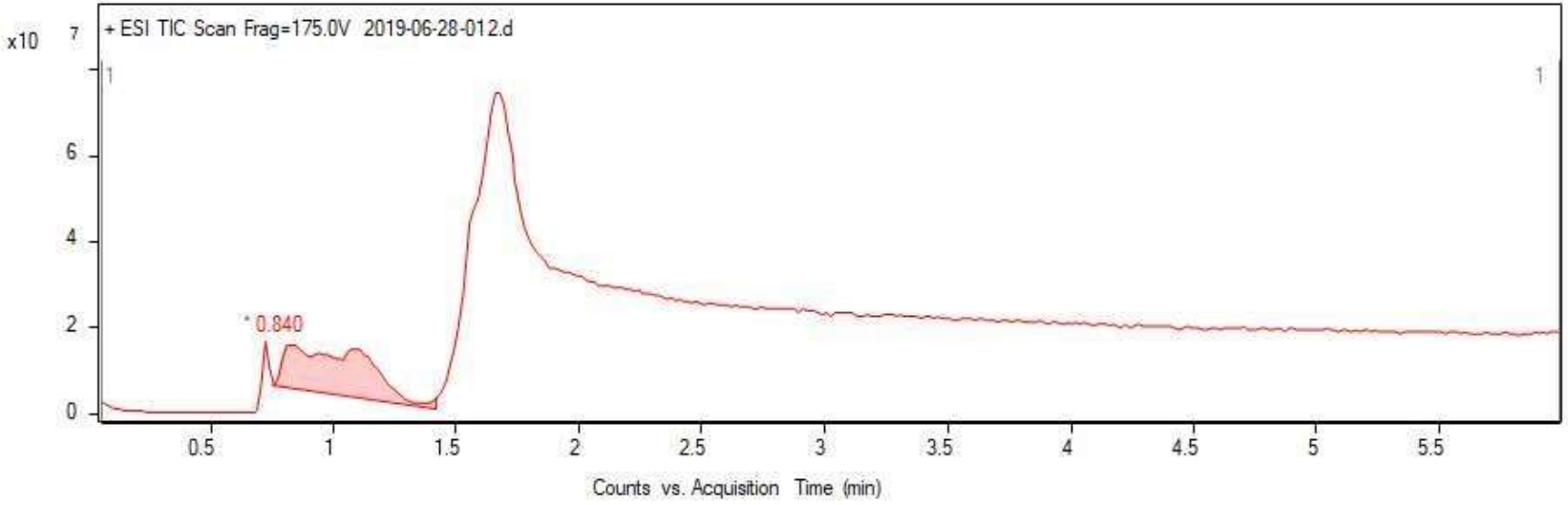
BRUKER

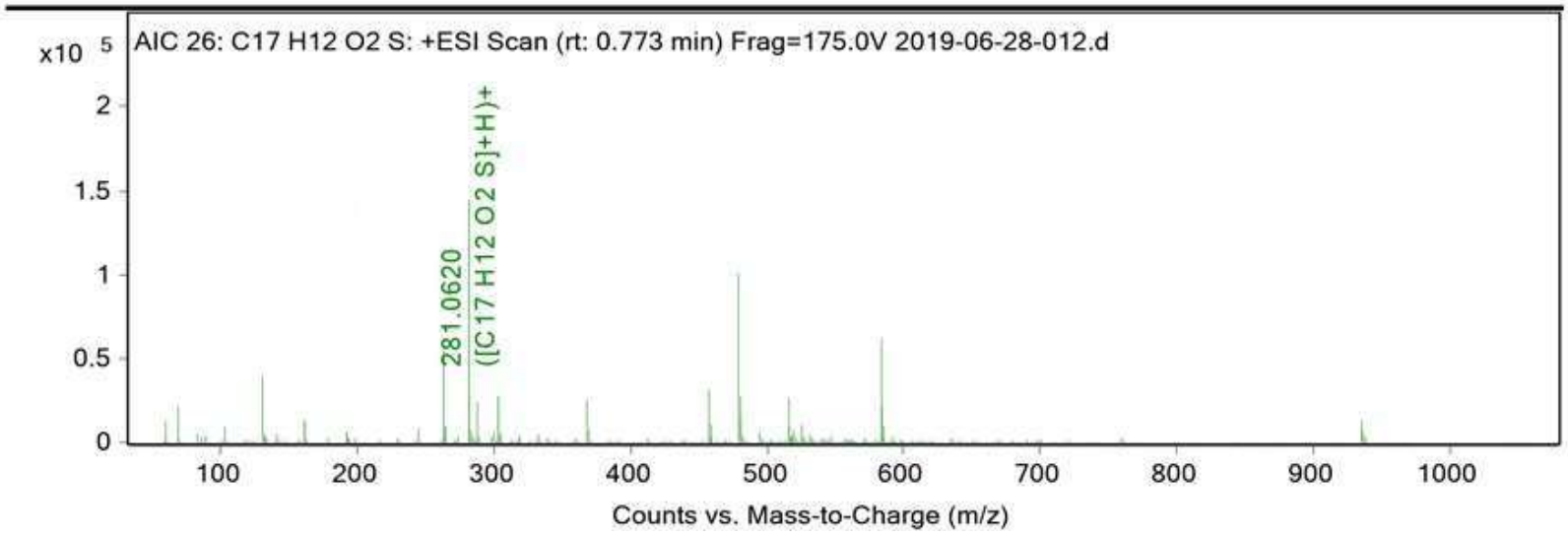
NAME	Audrey Isabelle
EXPNO	73
PROCNO	1
Date_	20190617
Time	23.34
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	10000
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

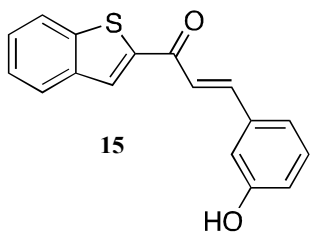

S
O
HO

14

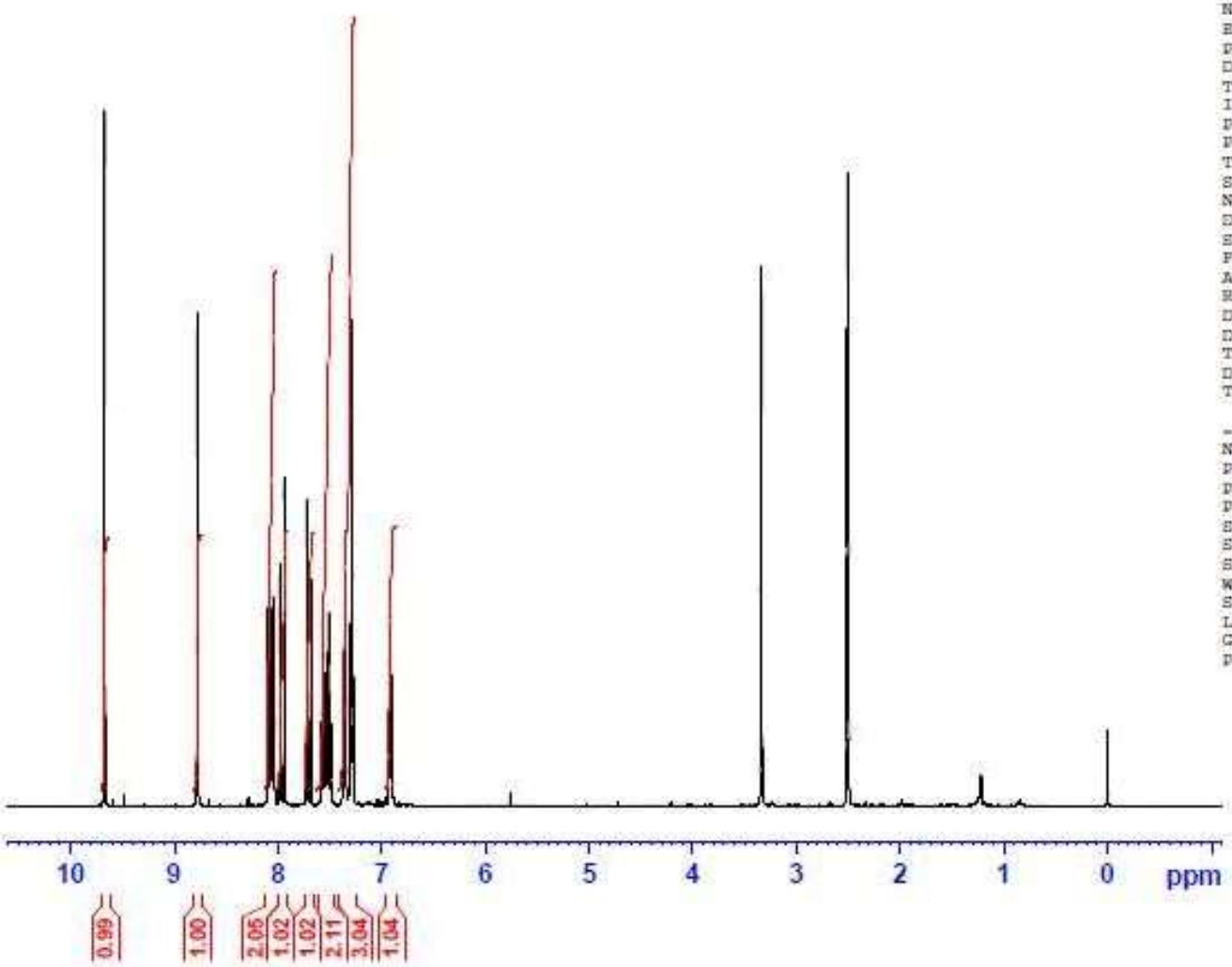

x10 7
+ ESI TIC Scan Frag=175.0V 2019-06-28-012.d
* 0.840
Counts vs. Acquisition Time (min)


x10 5
AIC 26: C17 H12 O2 S: +ESI Scan (rt: 0.773 min) Frag=175.0V 2019-06-28-012.d
281.0620
([C17 H12 O2 S]+H)+
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



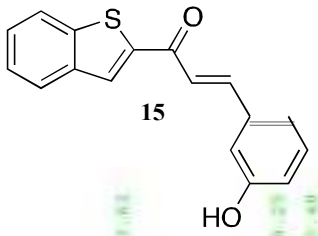
15



BRUKER

NAME	Audrey Isabelle	
EXPNO	70	
PROCNO	1	
Date_	20190614	
Time	15.50	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	DMSO	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	114	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{13}C NMR



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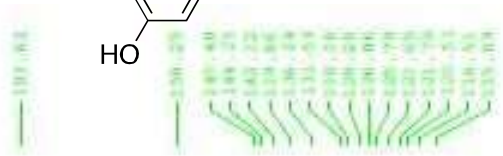
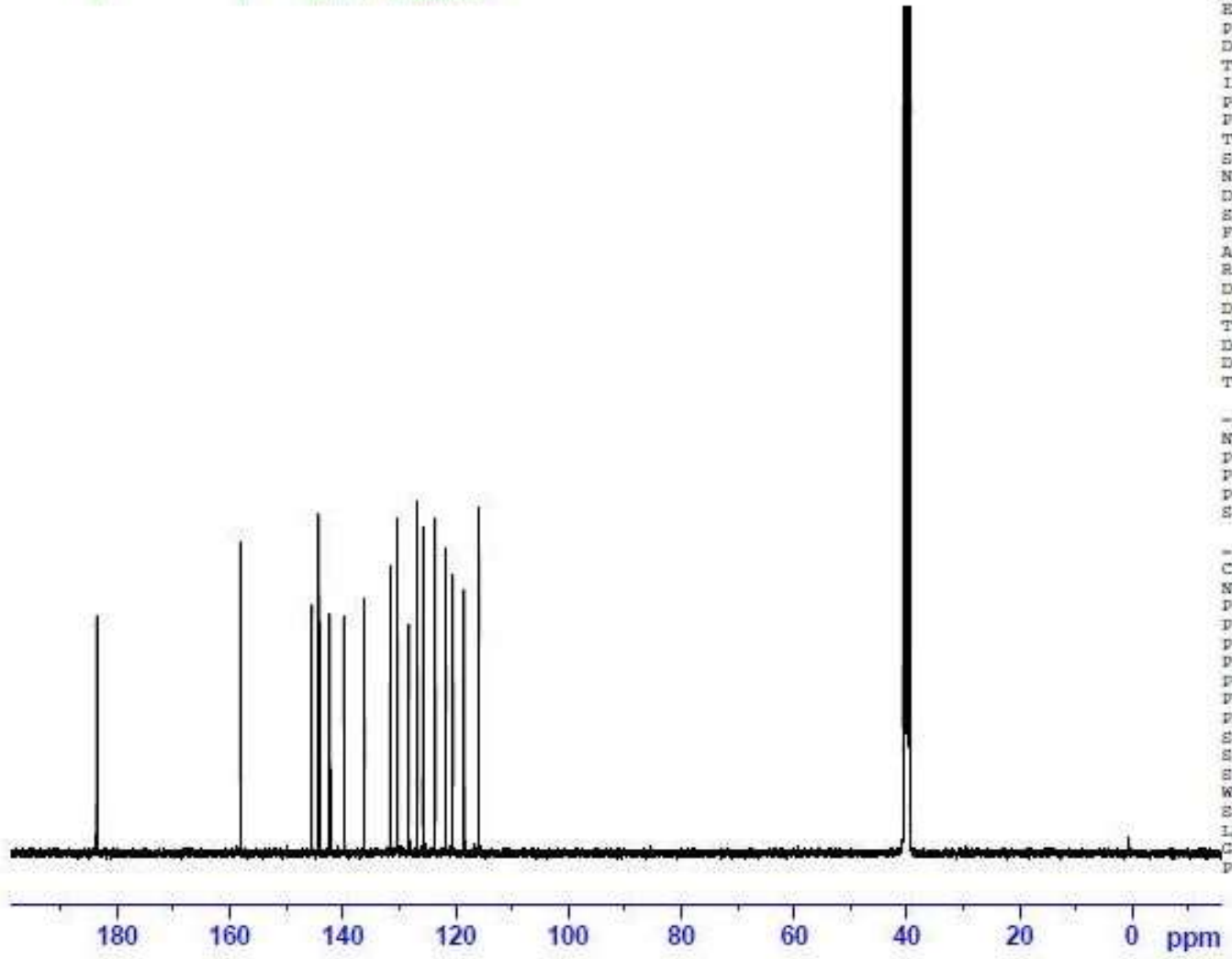
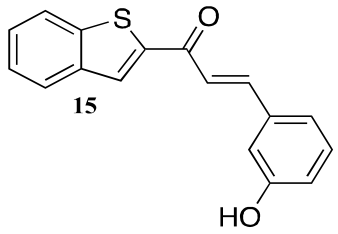




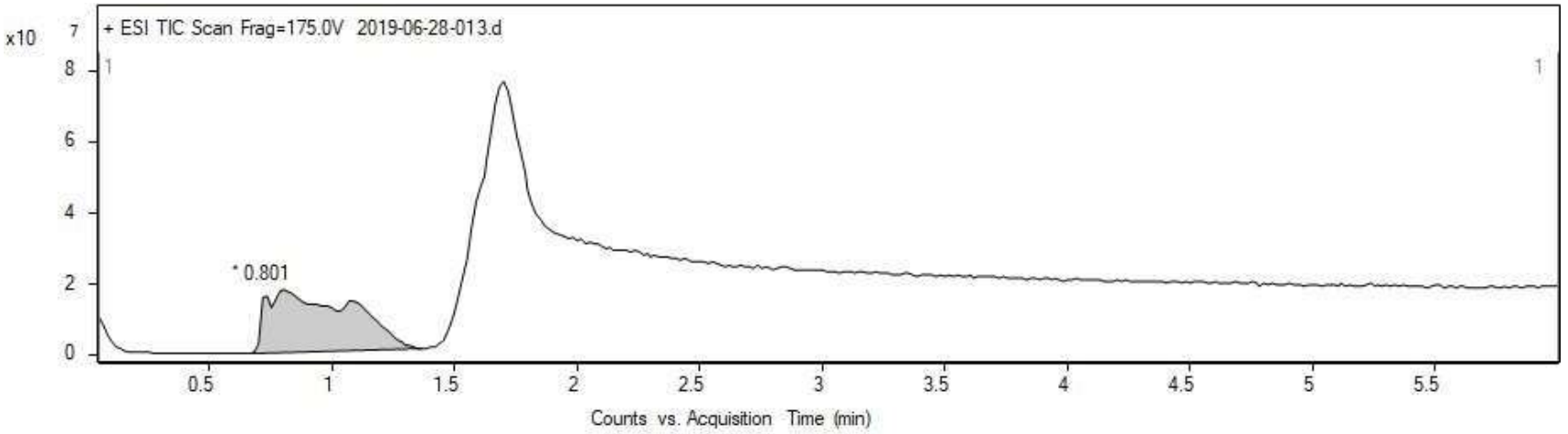
BRUKER

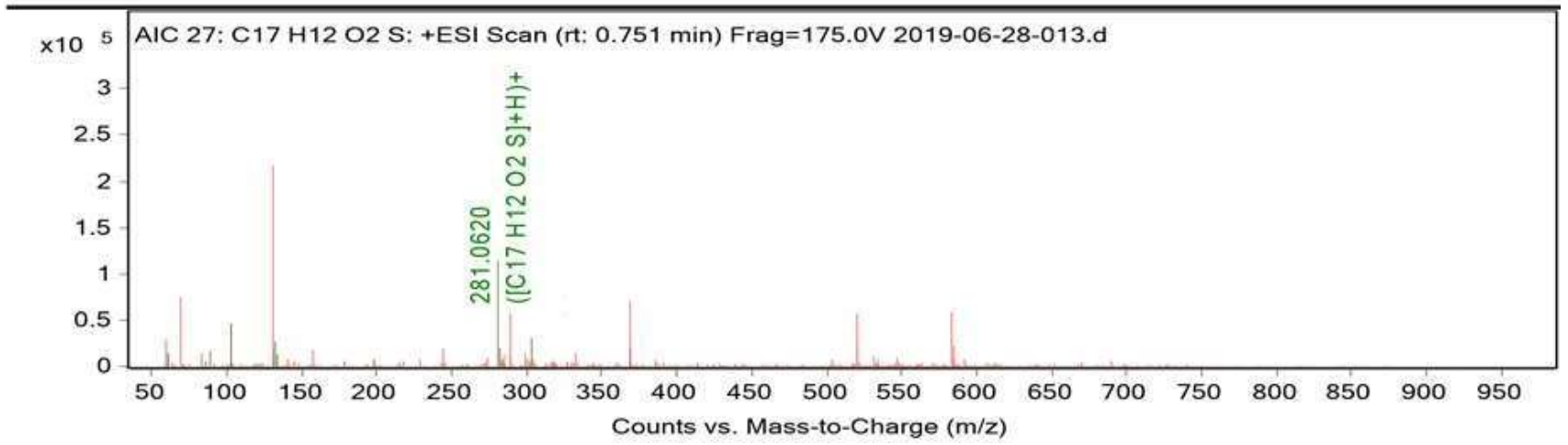
NAME	Audrey Isabelle	
EXPNO	72	
PROCNO	1	
Date_	20190615	
Time	1.49	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	DMSO	
NS	10000	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS

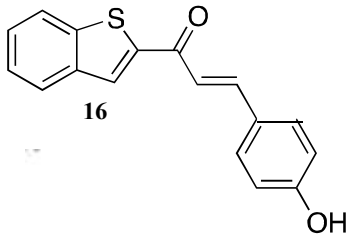

S
O
HO

15

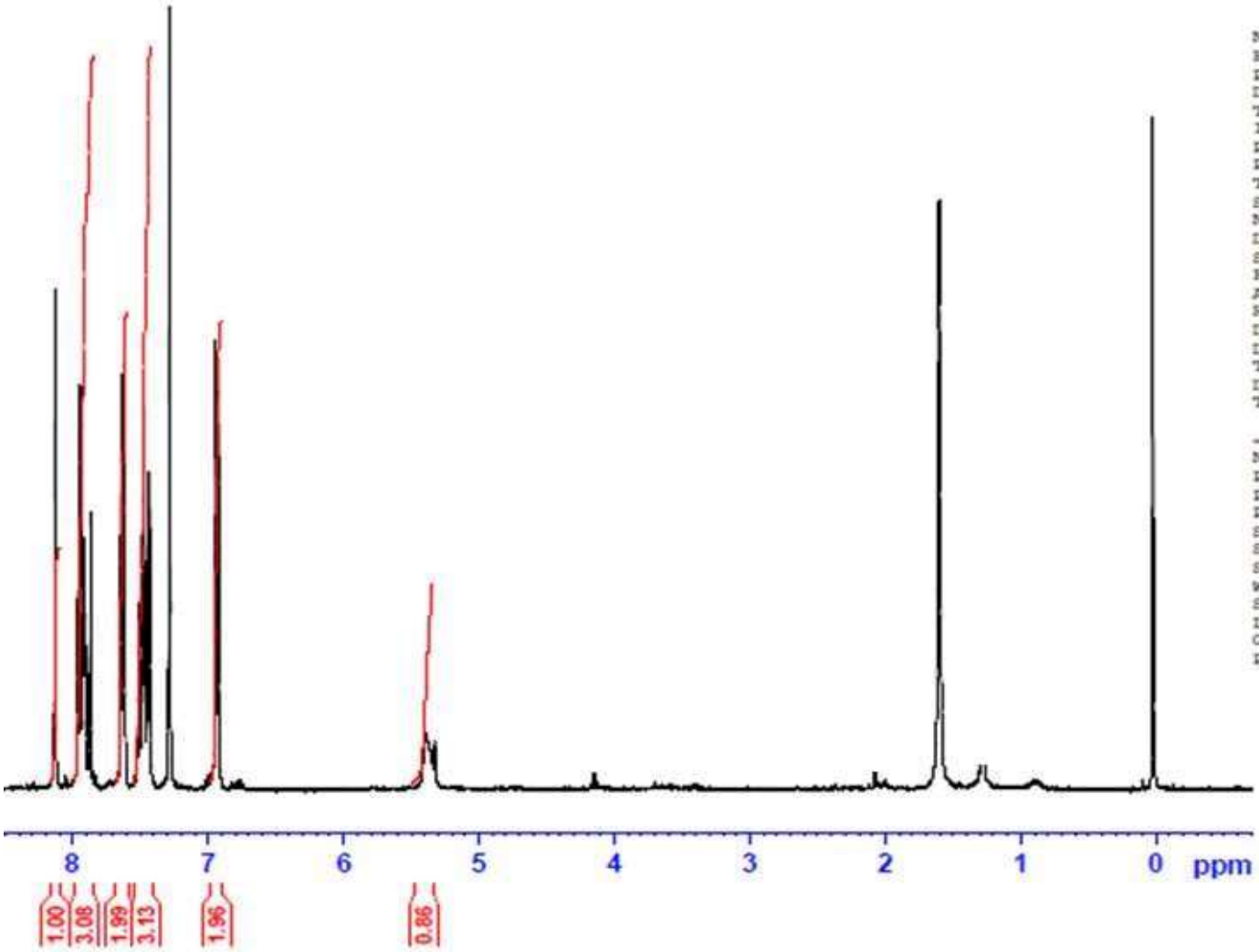

x10
7
+ ESI TIC Scan Frag=175.0V 2019-06-28-013.d
8
6
4
2
0
1
1
* 0.801
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Counts vs. Acquisition Time (min)


x10
5
AIC 27: C17 H12 O2 S: +ESI Scan (rt: 0.751 min) Frag=175.0V 2019-06-28-013.d
3
2.5
2
1.5
1
0.5
0
281.0620
([C17 H12 O2 S]+H)+
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



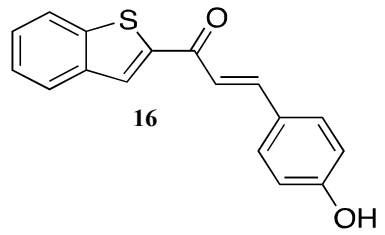
16



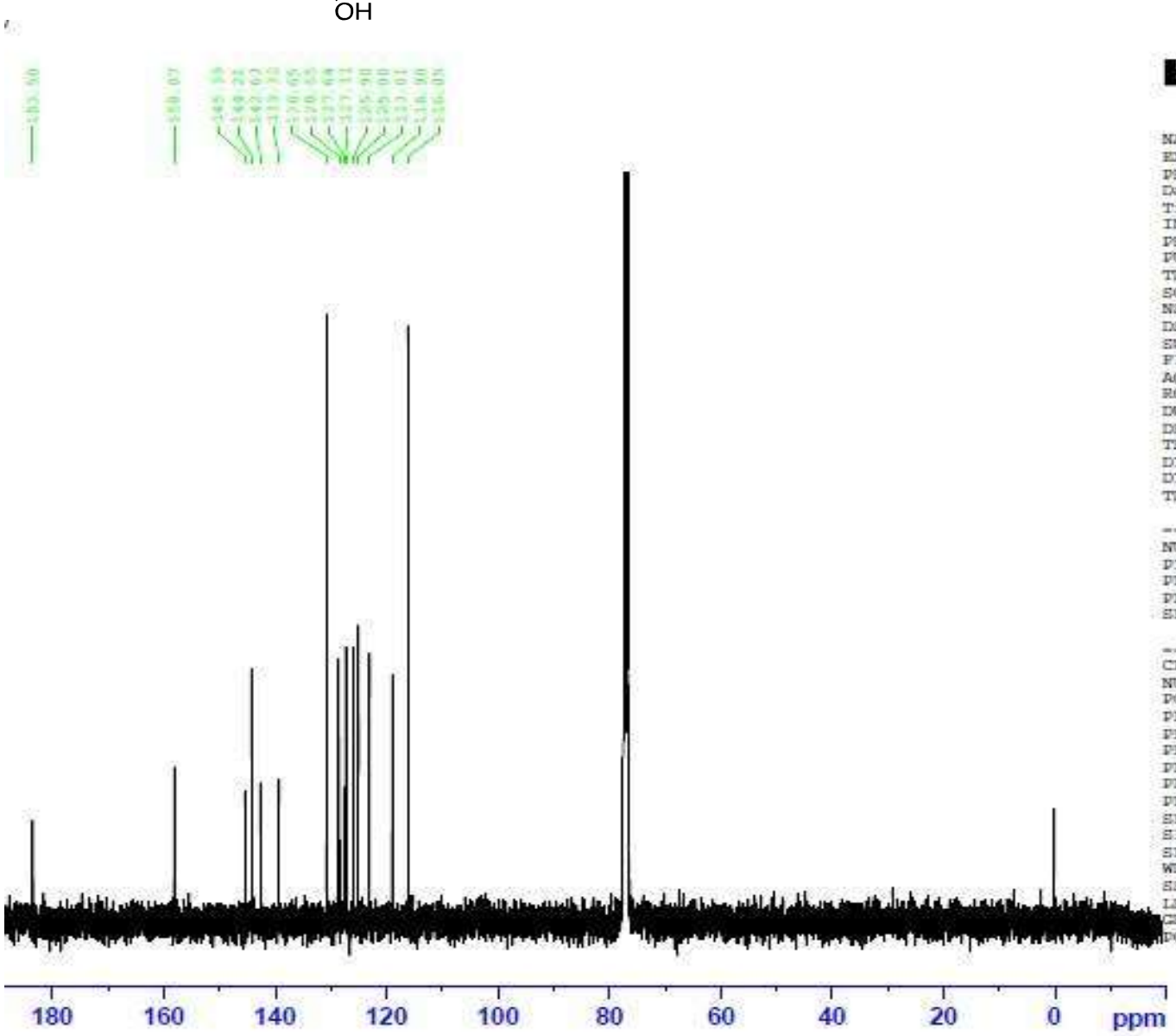
BRUKER

NAME	Audrey Isabelle	
EXPNO	16	
PROCNO	1	
Date_	20190302	
Time	11.01	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	203	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
-------- CHANNEL f1 --------		
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{13}C NMR



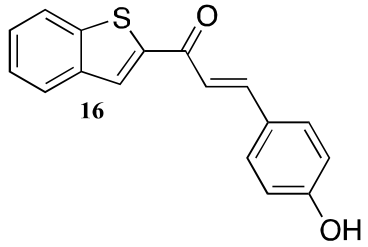
16



BRUKER

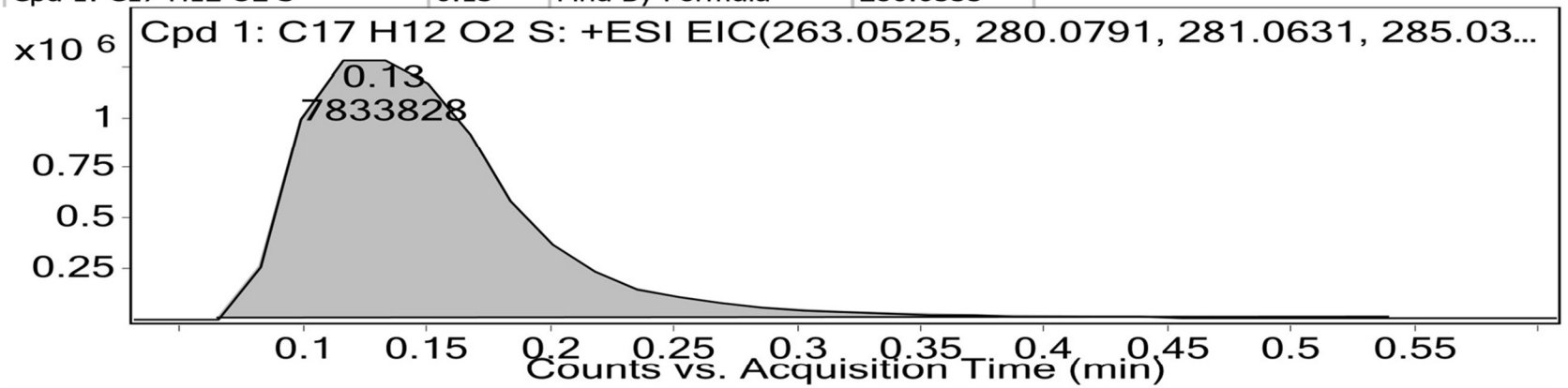
NAME	Audrey Isabelle
EXPNO	18
PROCNO	1
Date_	20190302
Time	22.40
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	12000
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

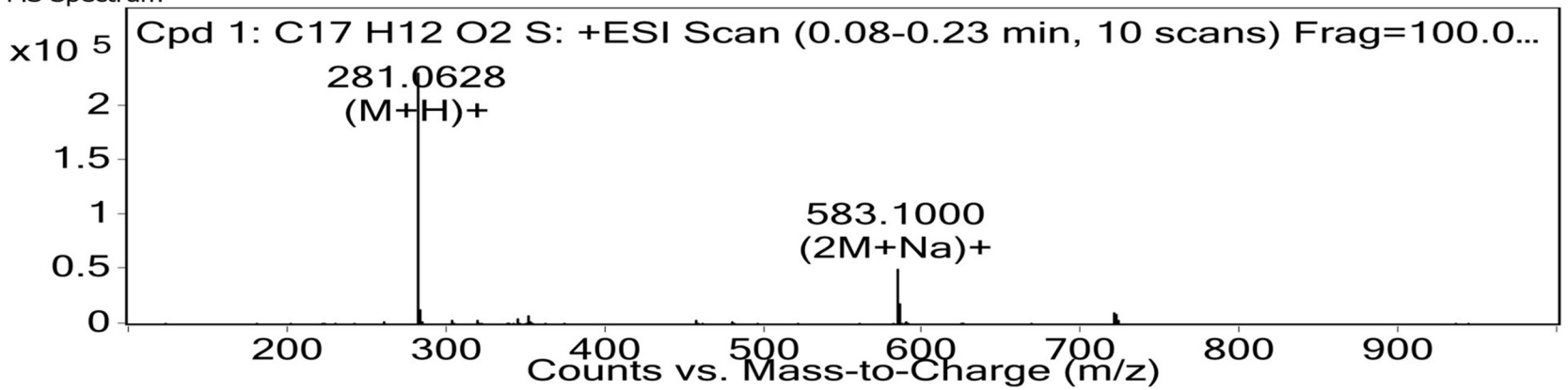


16

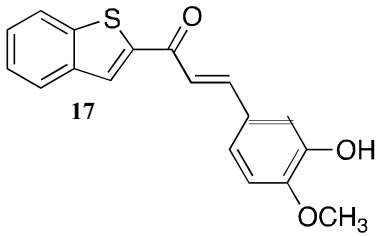
Compound Label	RT	Algorithm	Mass
Cpd 1: C17 H12 O2 S	0.13	Find By Formula	280.0555



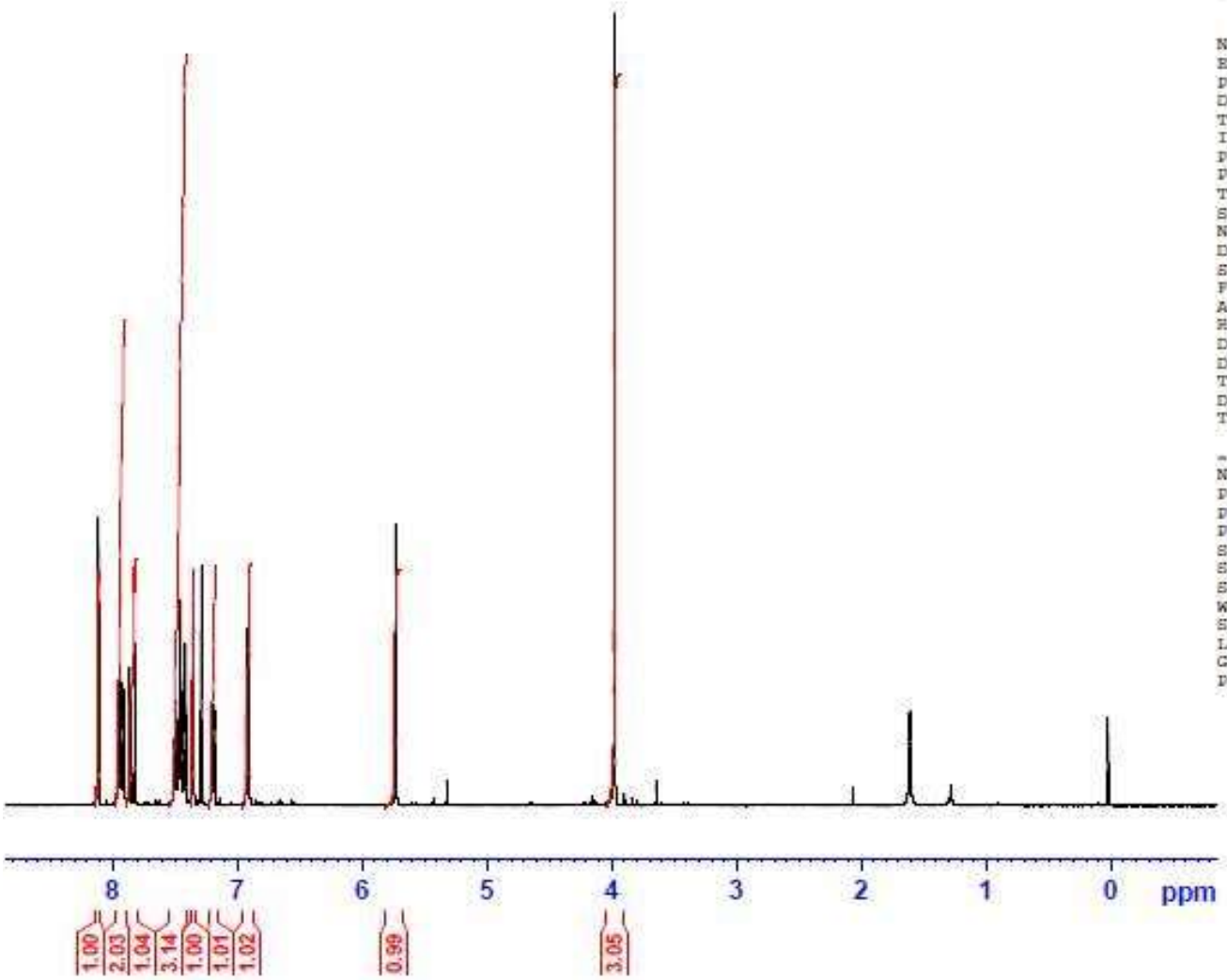
MS Spectrum



^{1}H NMR



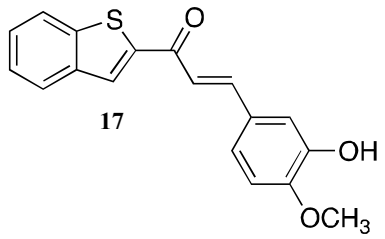
17



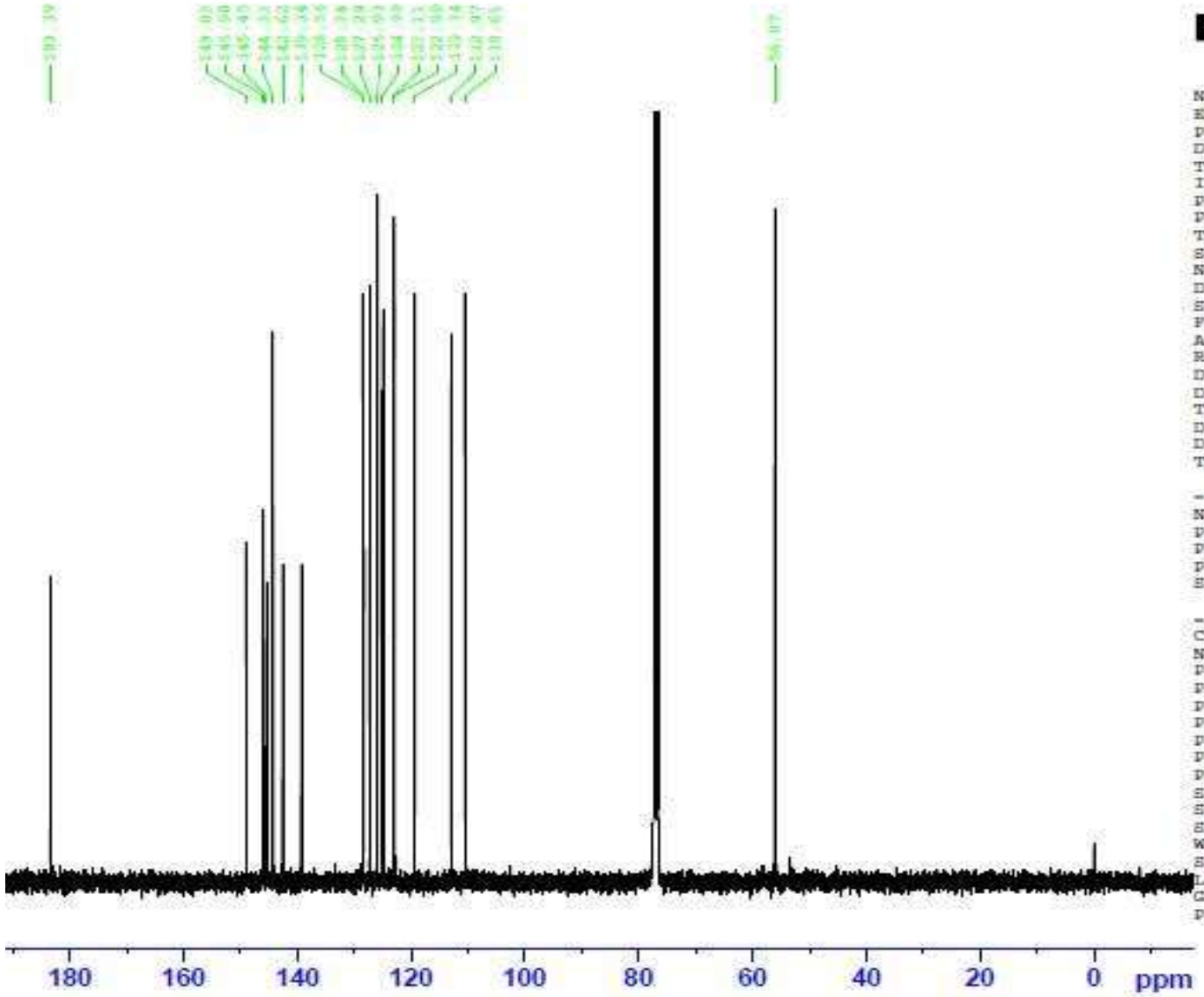
BRUKER

NAME	Audrey Isabelle
EXPNO	23
PROCNO	1
Date_	20190329
Time	9.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	128
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229636 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



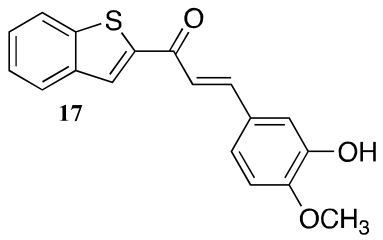
17



BRUKER

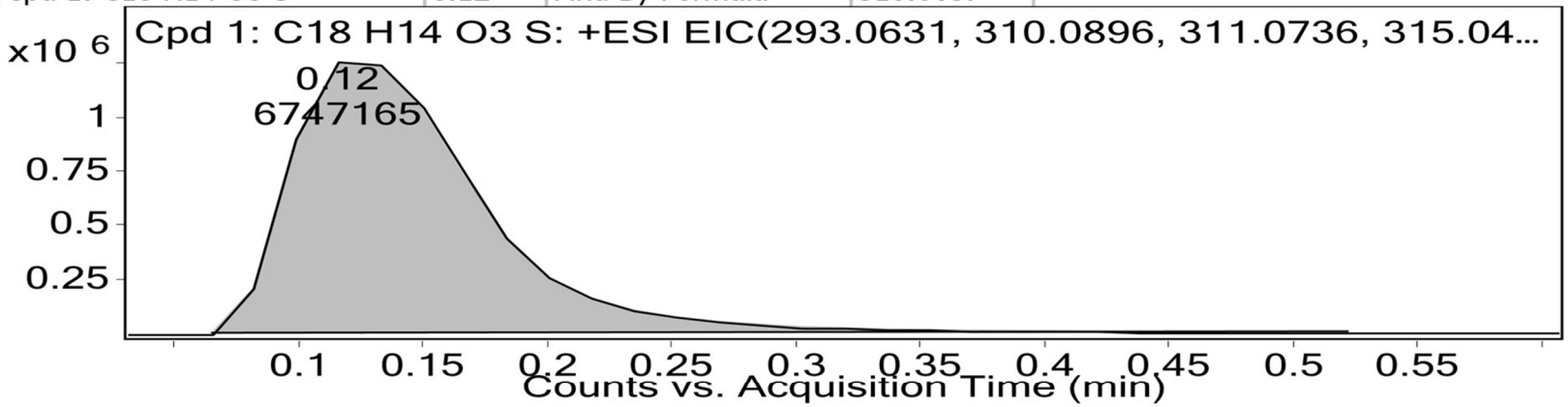
NAME	Audrey Isabelle
EXPNO	24
PROCNO	1
Date_	20190329
Time	16.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	5629
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

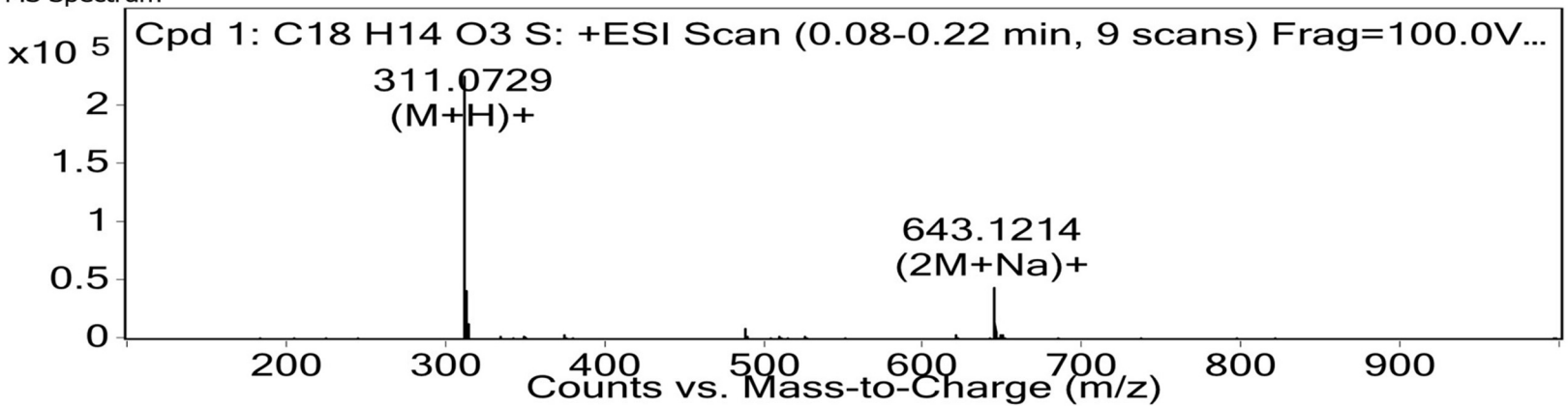


17

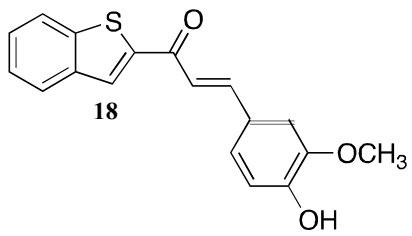
Compound Label	RT	Algorithm	Mass
Cpd 1: C18 H14 O3 S	0.12	Find By Formula	310.0657



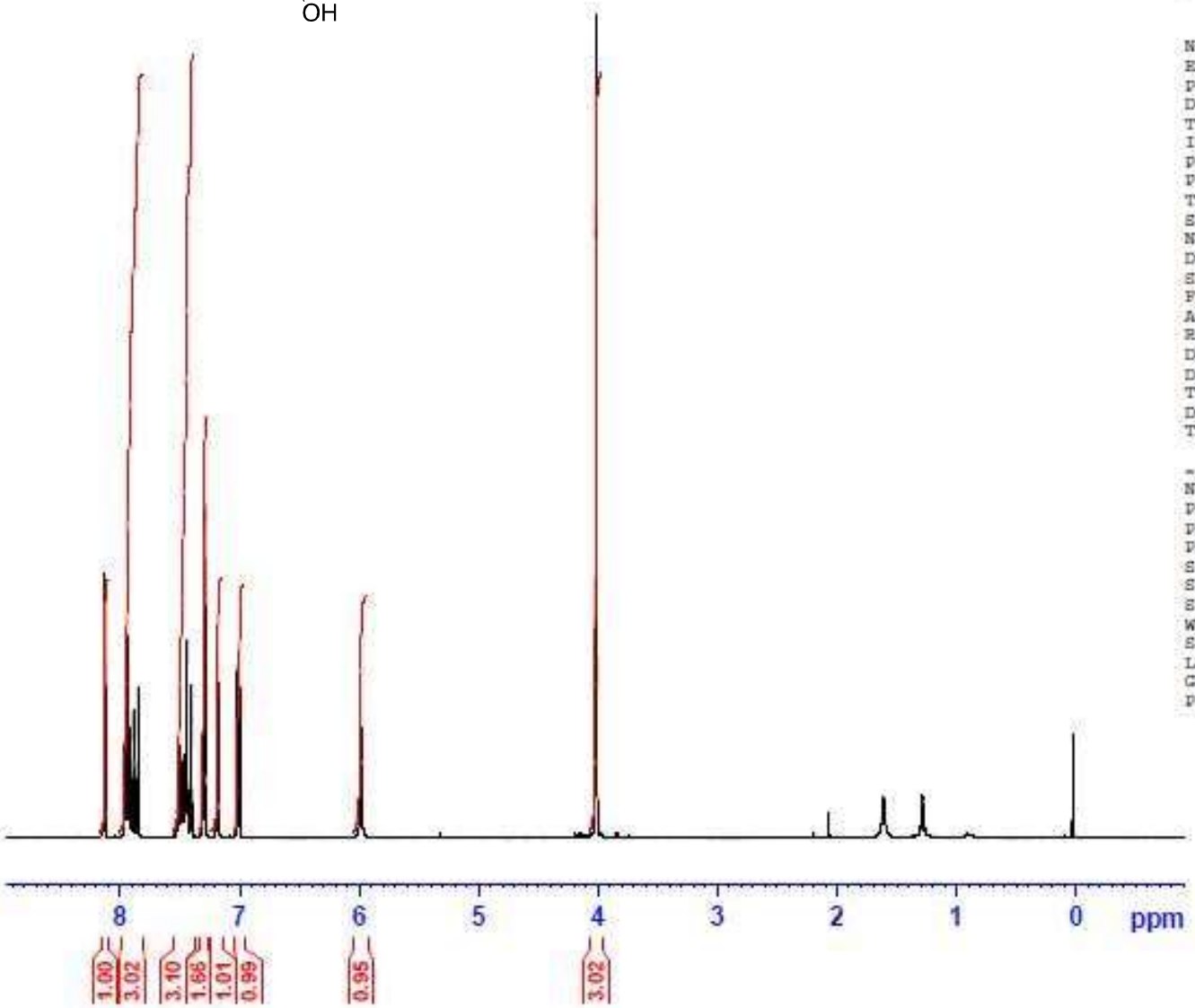
MS Spectrum



^{1}H NMR



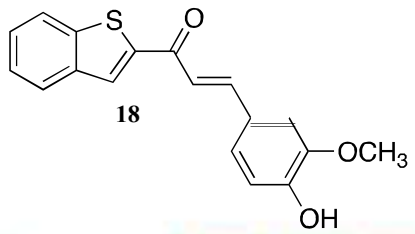
18



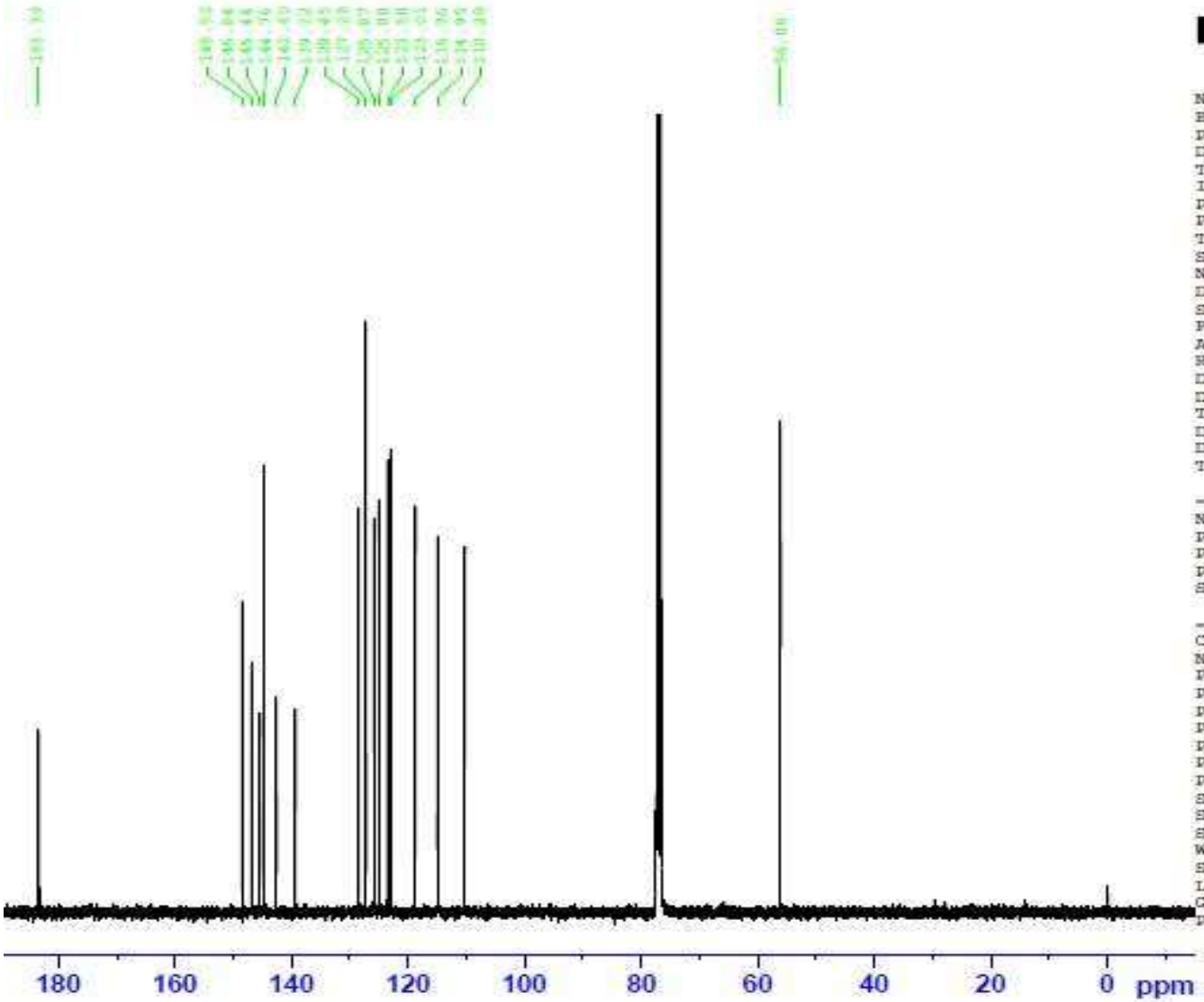
BRUKER

NAME	Audrey Isabelle
EXPNO	19
PROCNO	1
Date_	20190318
Time	9.03
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	181
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



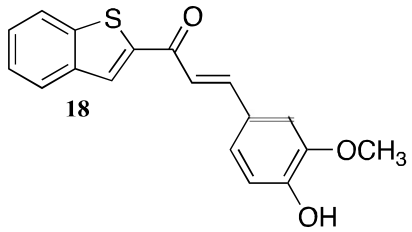
18



BRUKER

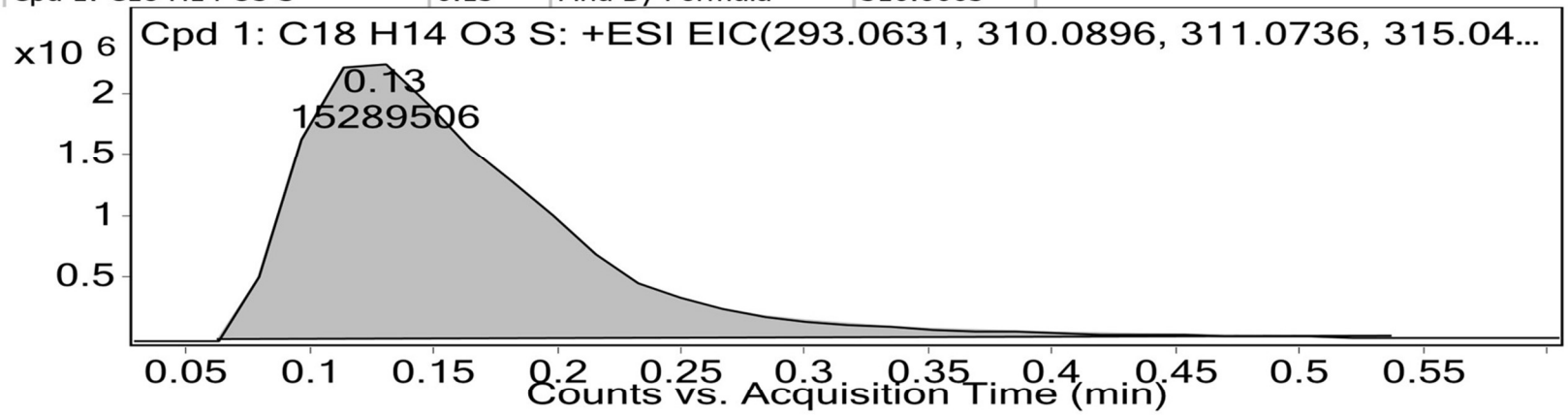
NAME	Audrey Isabelle	
EXPNO	20	
PROCNO	1	
Date_	20190318	
Time	16.27	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	7716	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
--------	CHANNEL f1	--------
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
--------	CHANNEL f2	--------
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS

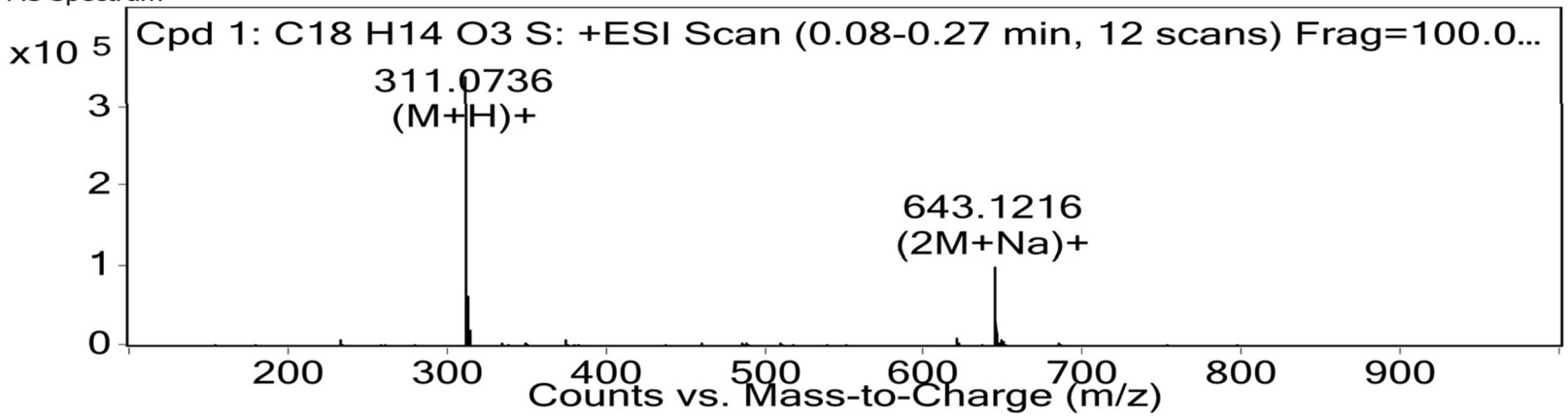


18

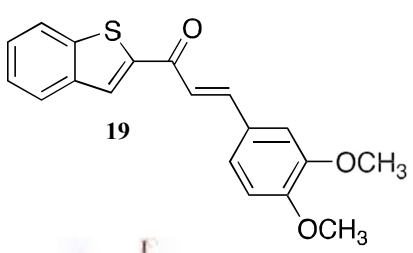
Compound Label	RT	Algorithm	Mass
Cpd 1: C18 H14 O3 S	0.13	Find By Formula	310.0663



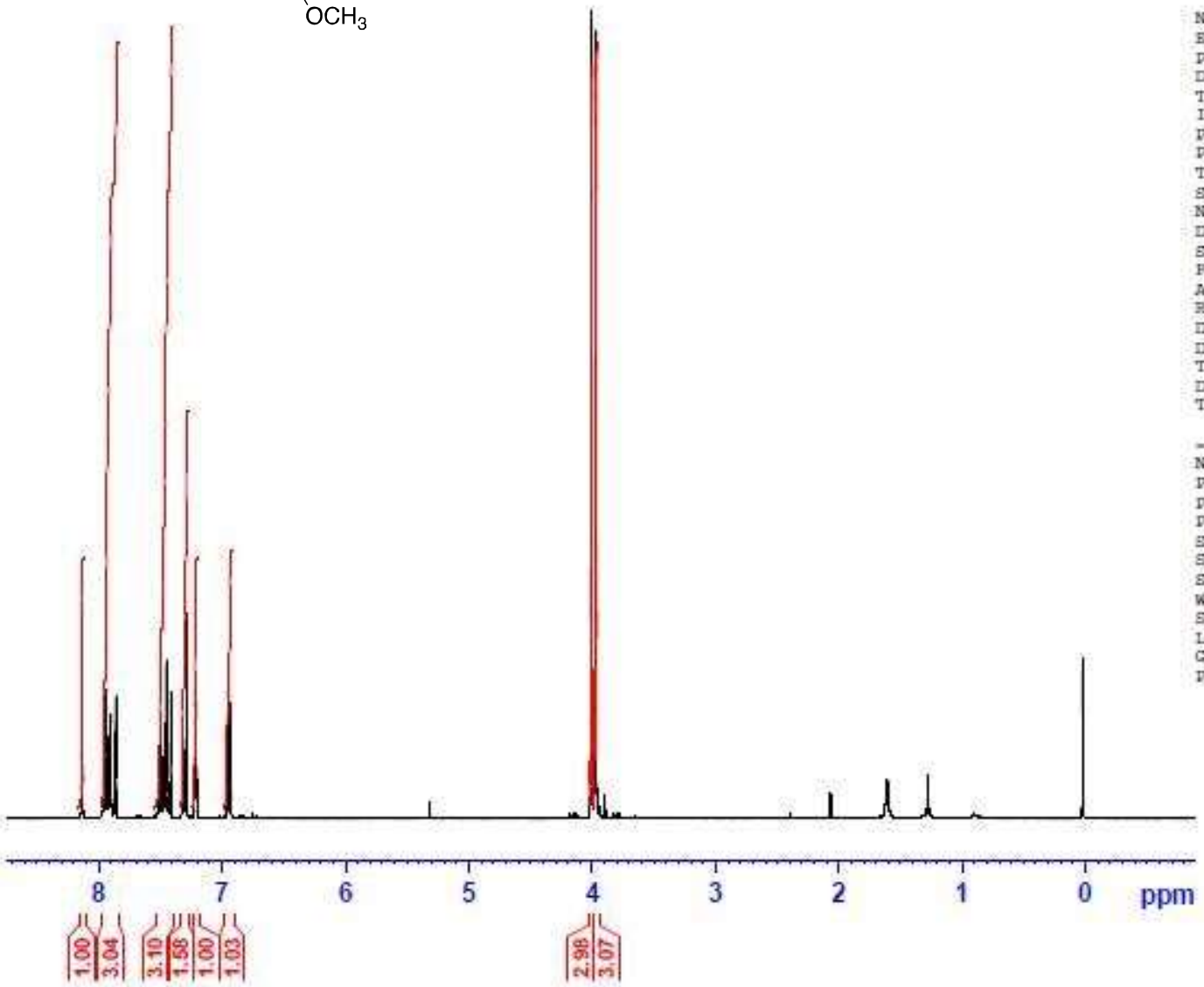
MS Spectrum



^{1}H NMR



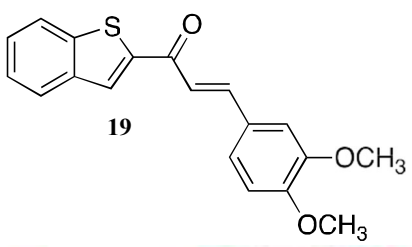
19



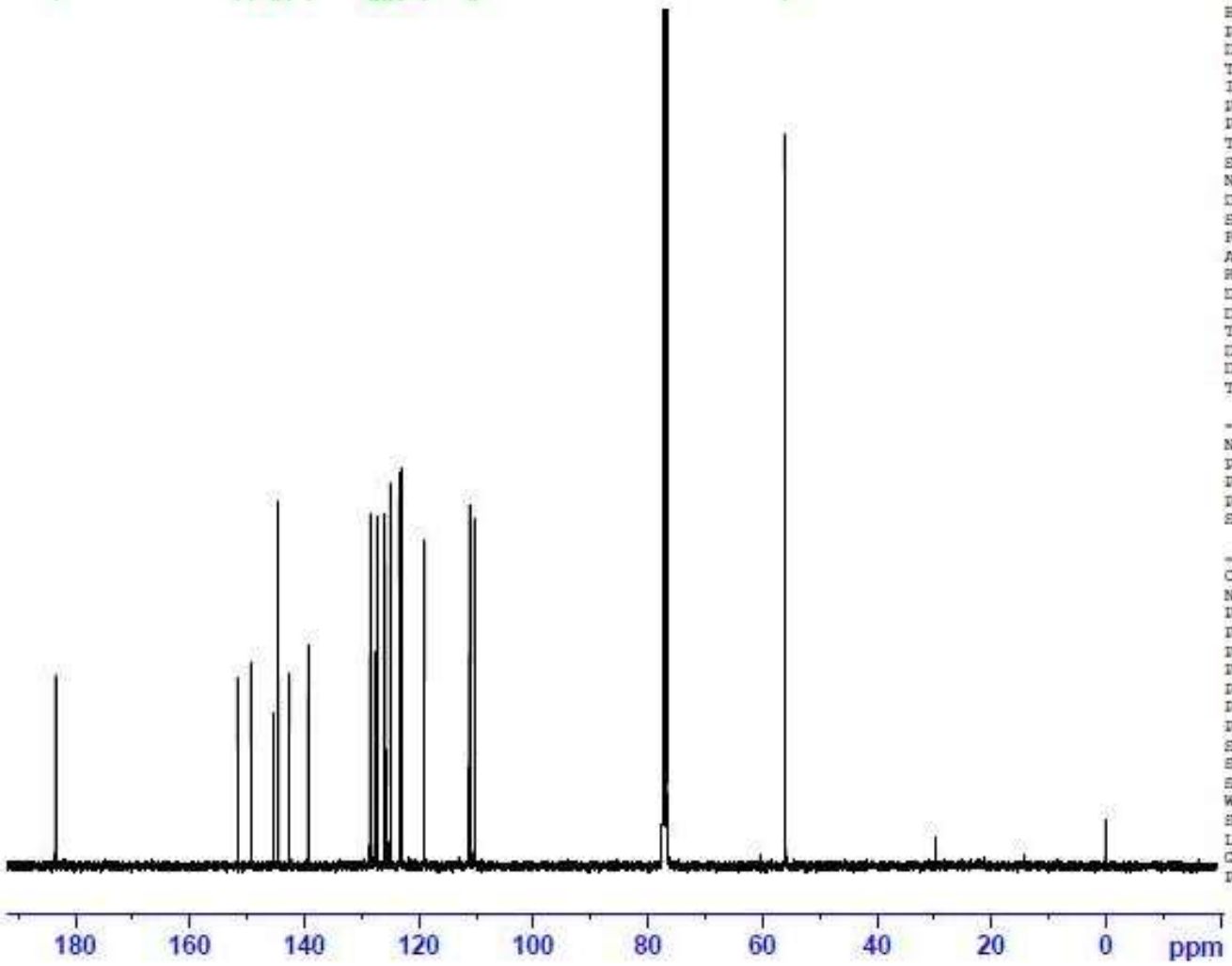
BRUKER

NAME	Audrey Isabelle
EXPNO	74
PROCNO	1
Date_	20190619
Time	8.54
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	114
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



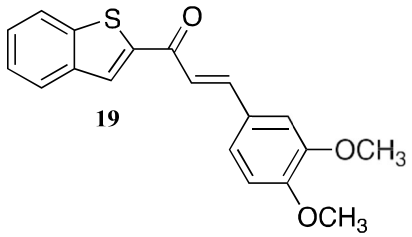
19



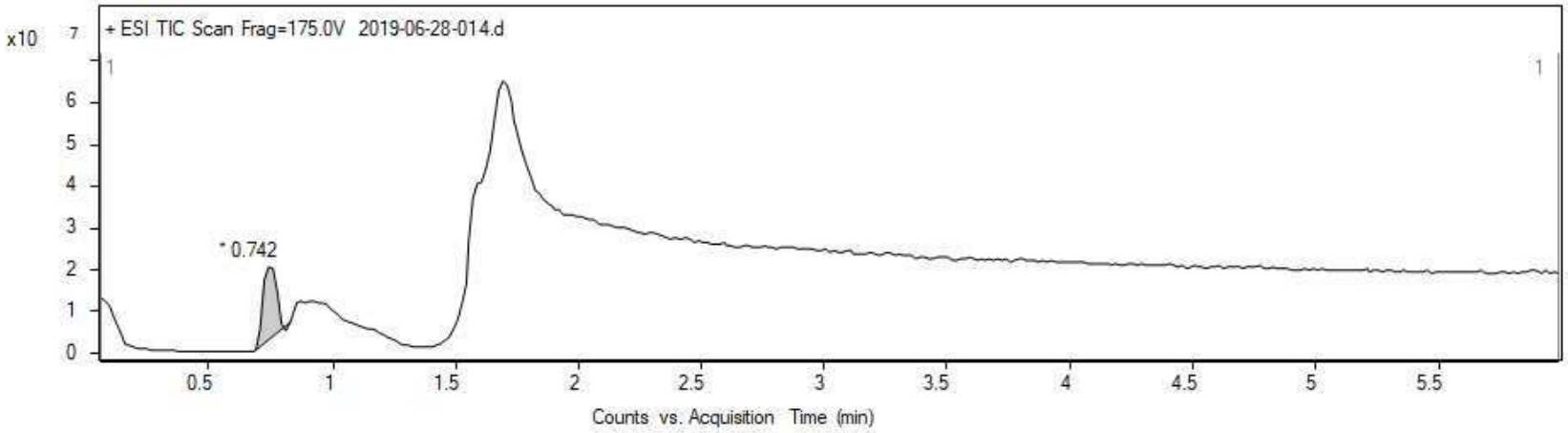
BRUKER

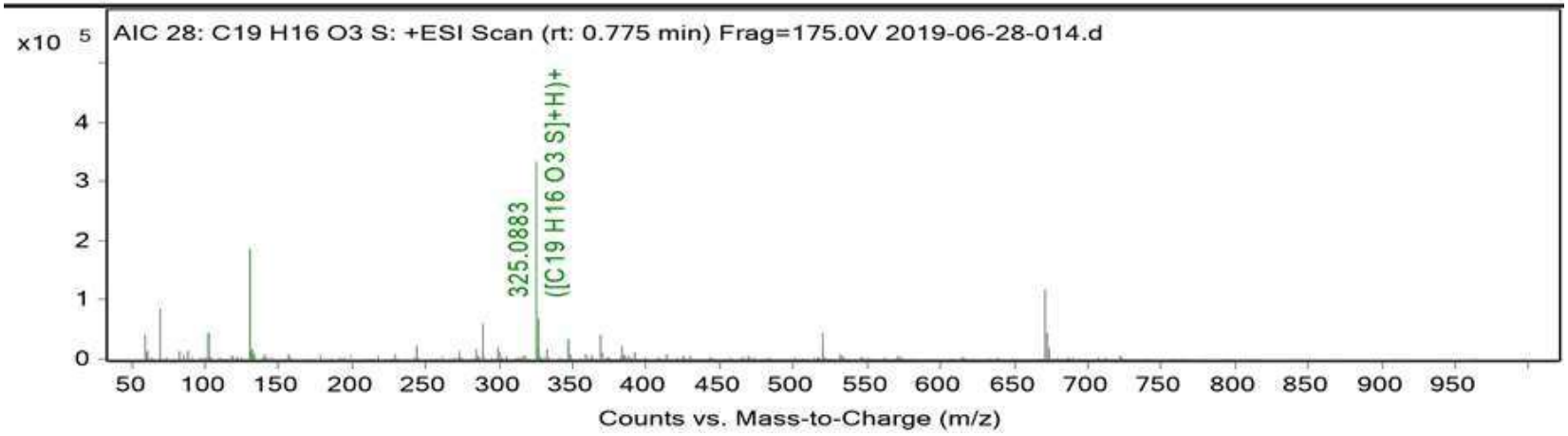
NAME	Audrey Isabelle
EXPNO	82
PROCNO	1
Date_	20190621
Time	2.09
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	10000
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

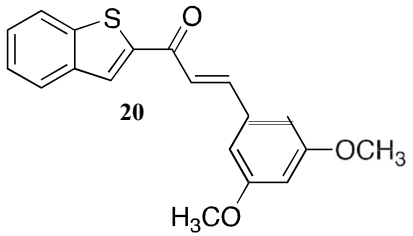

S
O
OCH3
OCH3

19

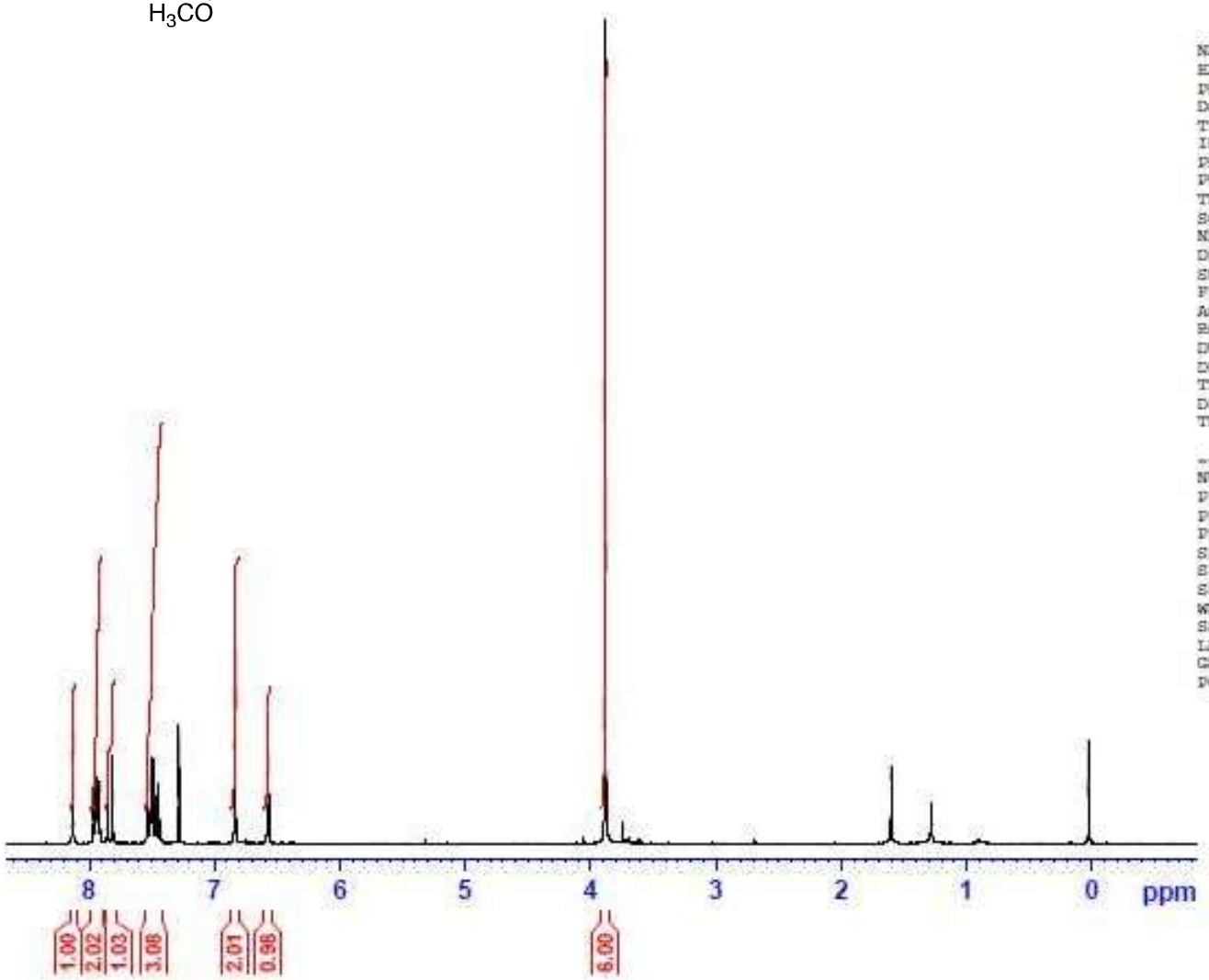

x10 7
+ ESI TIC Scan Frag=175.0V 2019-06-28-014.d
* 0.742
Counts vs. Acquisition Time (min)


x10 5
AIC 28: C19 H16 O3 S: +ESI Scan (rt: 0.775 min) Frag=175.0V 2019-06-28-014.d
325.0883
([C19 H16 O3 S]+H)+
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



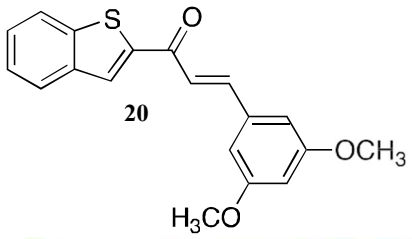
20



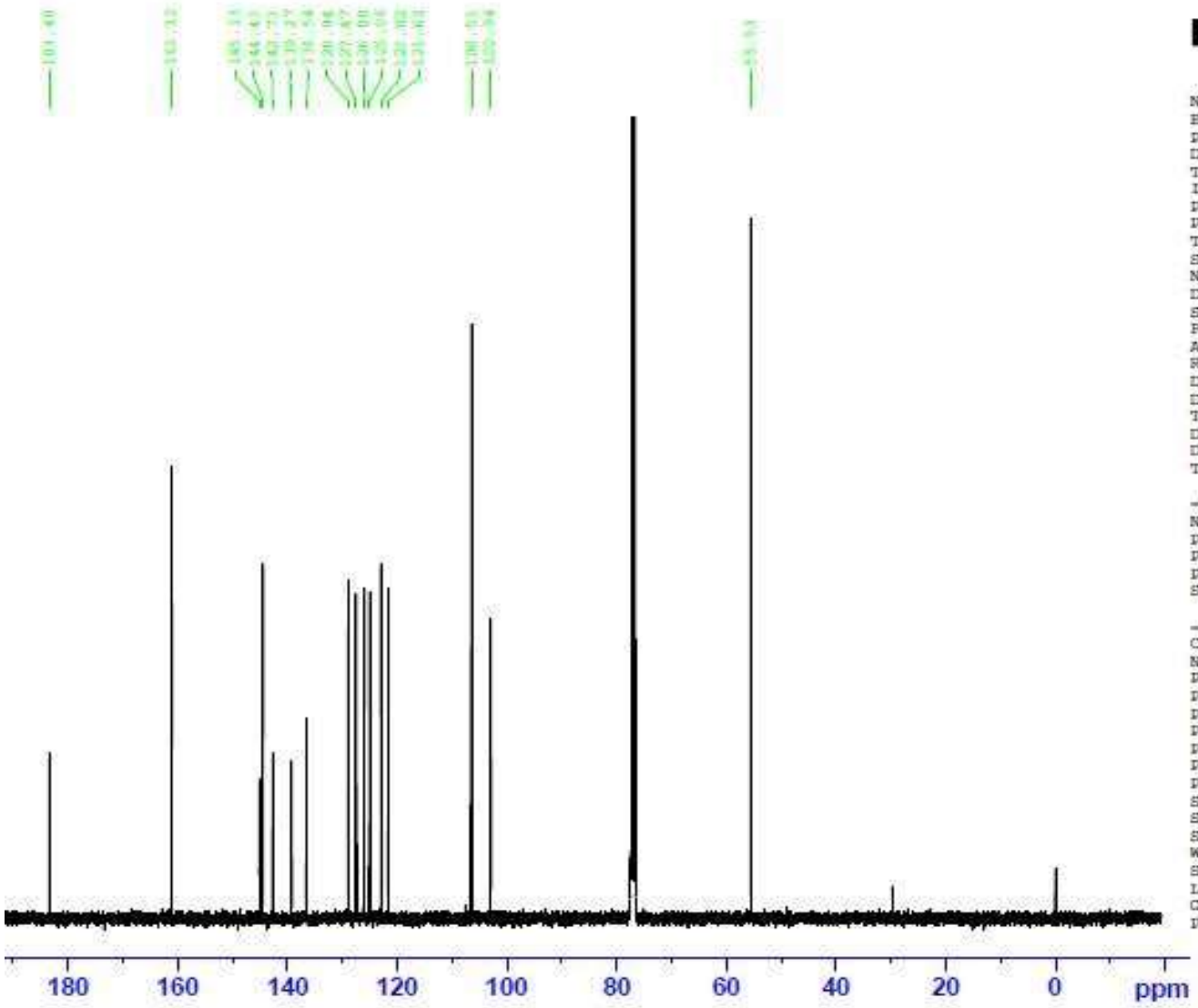
BRUKER

```
NAME        Audrey Isabelle
EXPNO                    58
PROCNO                    1
Date_              20190607
Time                  11.29
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846367 sec
RG                      114
DW                   60.800 usec
DE                    6.50 usec
TE                   298.0 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    14.07 usec
PL1                    0.30 dB
PL1W              11.25229836 W
SFO1              400.1324710 MHz
SI                       32768
SF                400.1300000 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

^{13}C NMR



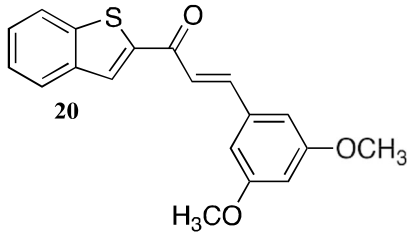
20



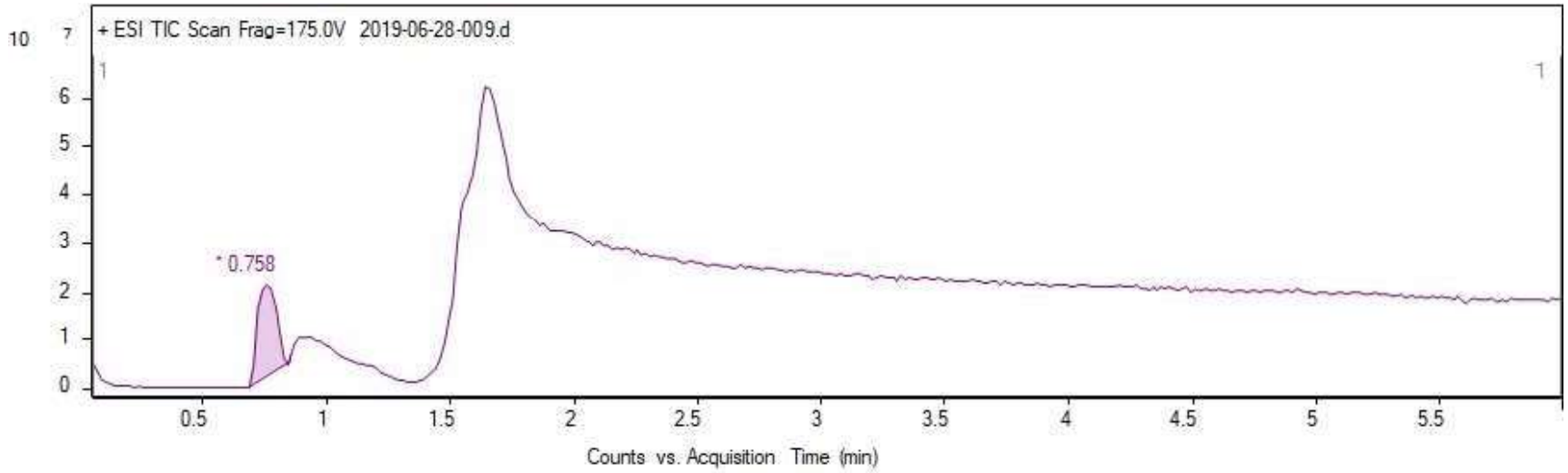
BRUKER

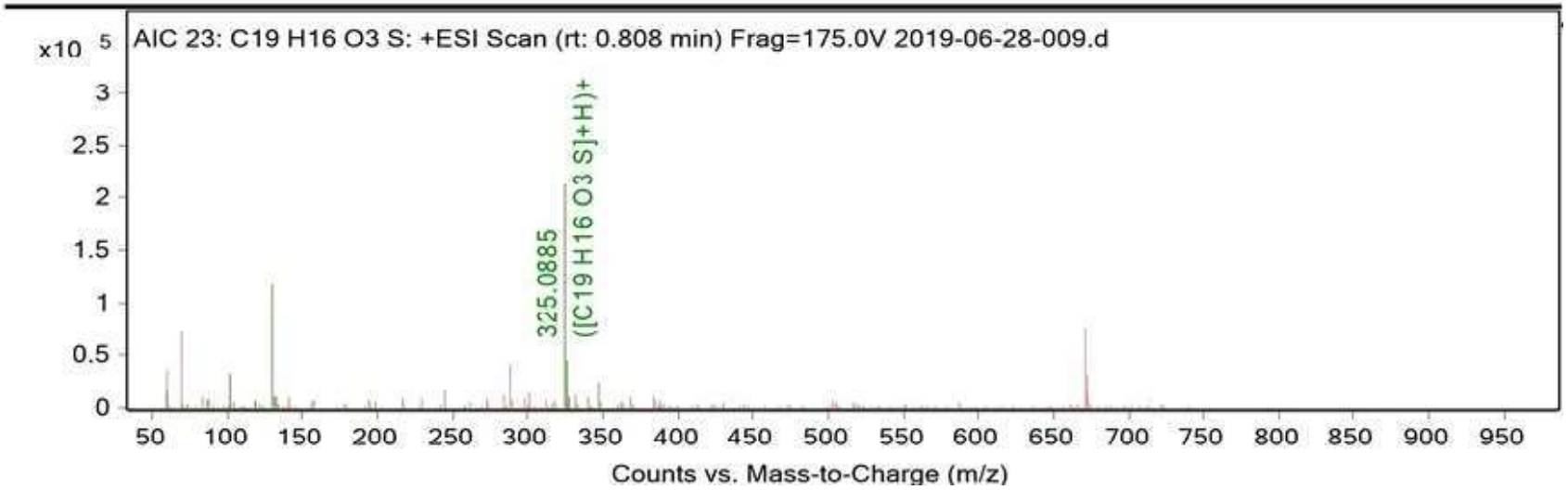
NAME	Audrey Isabelle	
EXPNO	59	
PROCNO	1	
Date_	20190607	
Time	14.39	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	3292	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
--------	CHANNEL f1	--------
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
--------	CHANNEL f2	--------
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS

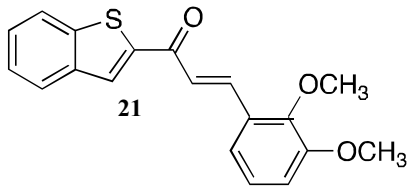

S
O
OCH3
H3CO

20

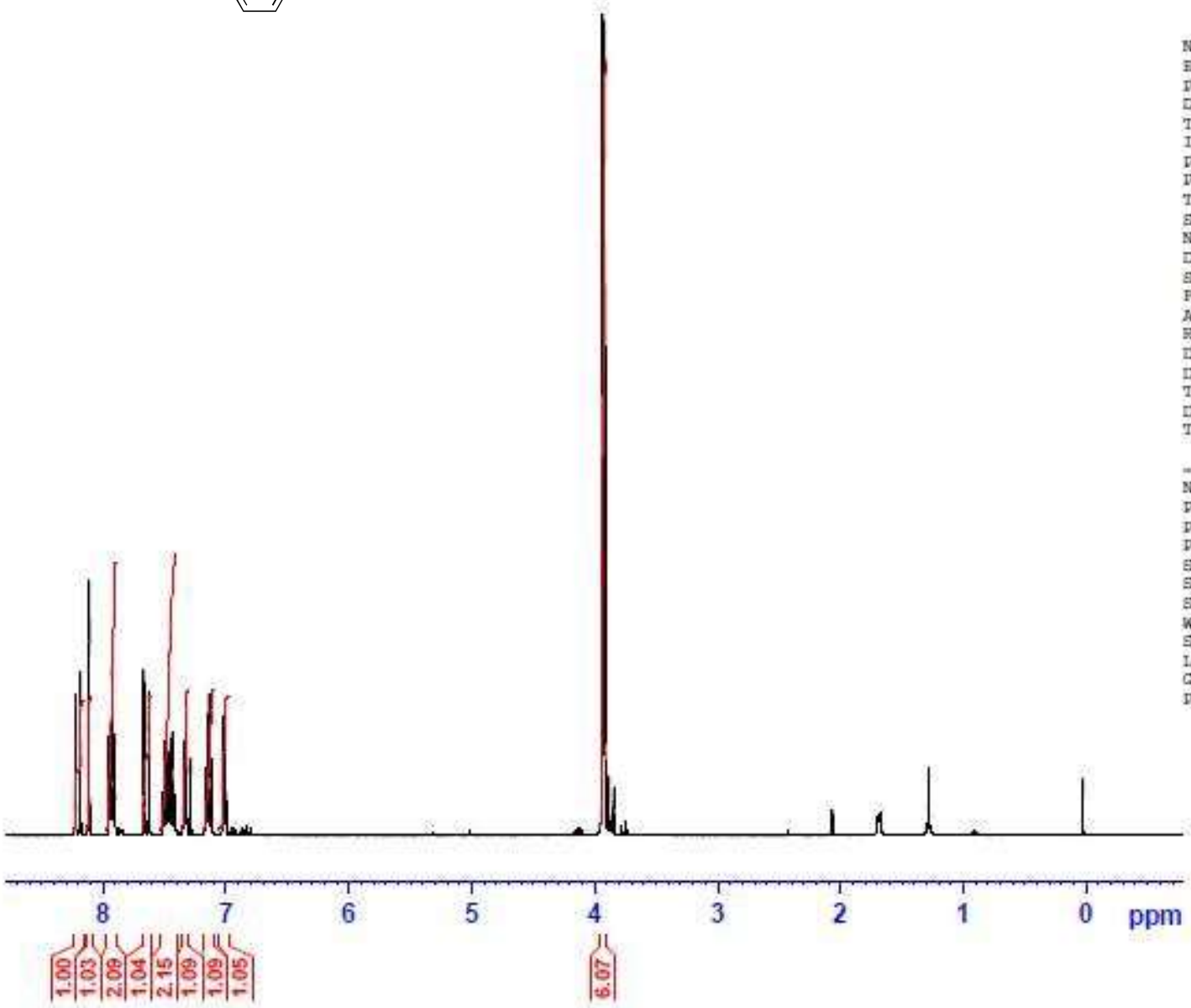

10
+ ESI TIC Scan Frag=175.0V 2019-06-28-009.d
* 0.758
Counts vs. Acquisition Time (min)


x10
AIC 23: C19 H16 O3 S: +ESI Scan (rt: 0.808 min) Frag=175.0V 2019-06-28-009.d
325.0885
([C19 H16 O3 S]+H)+
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



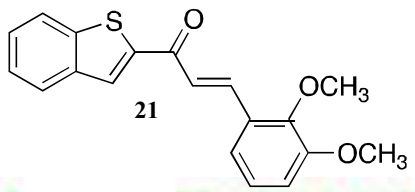
21



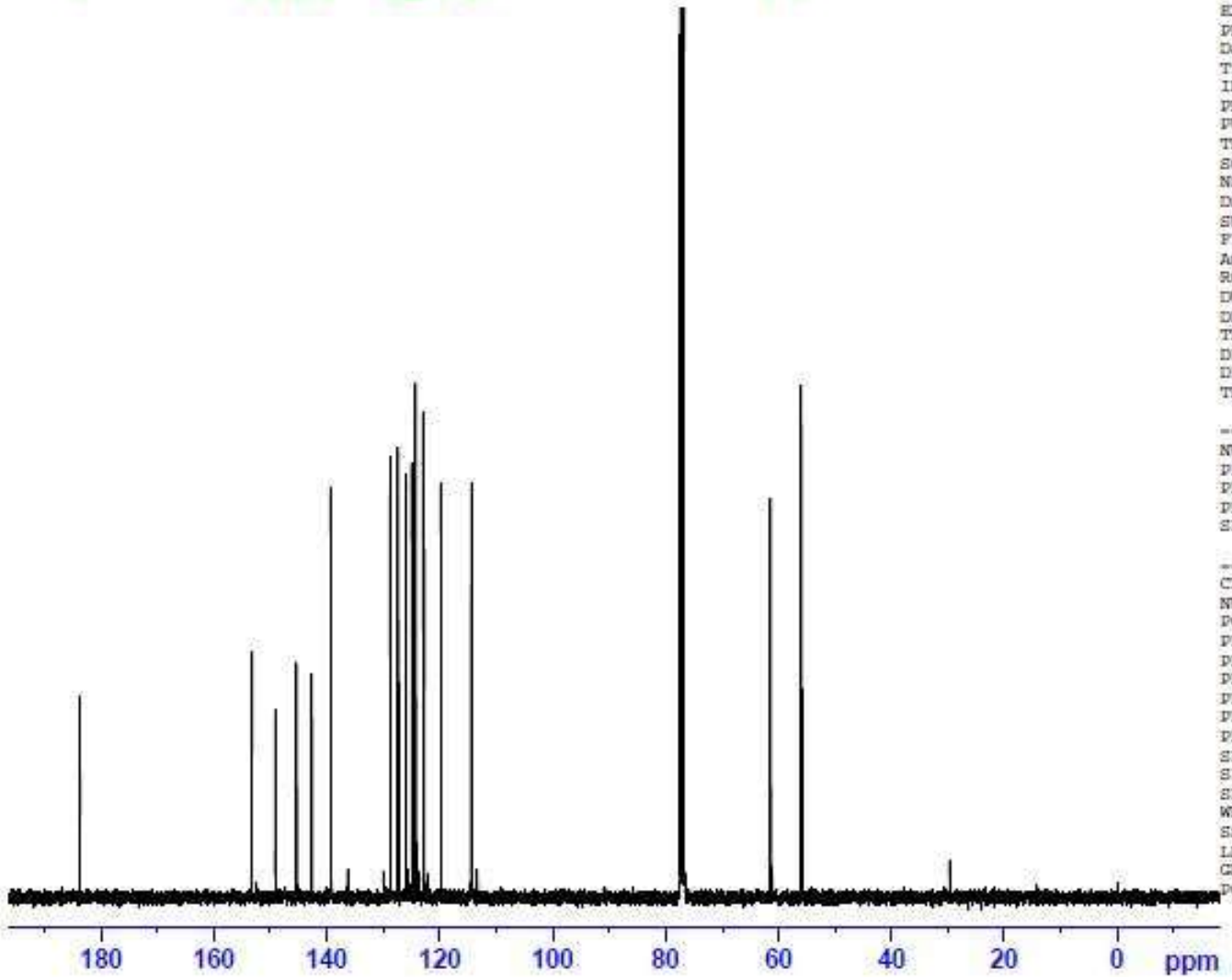
BRUKER

NAME	Audrey Isabelle
EXPNO	83
PROCNO	1
Date_	20190621
Time	8.27
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	64
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR

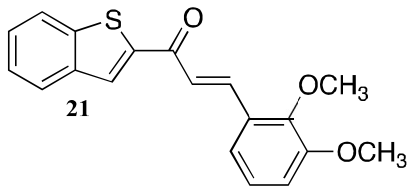


21

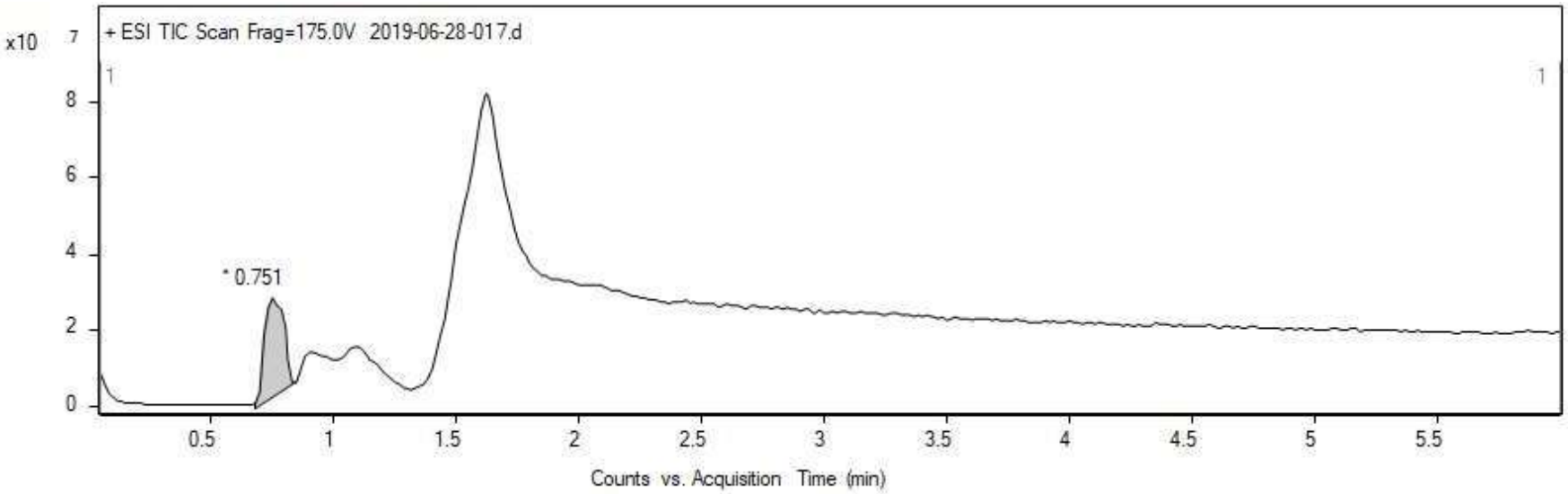


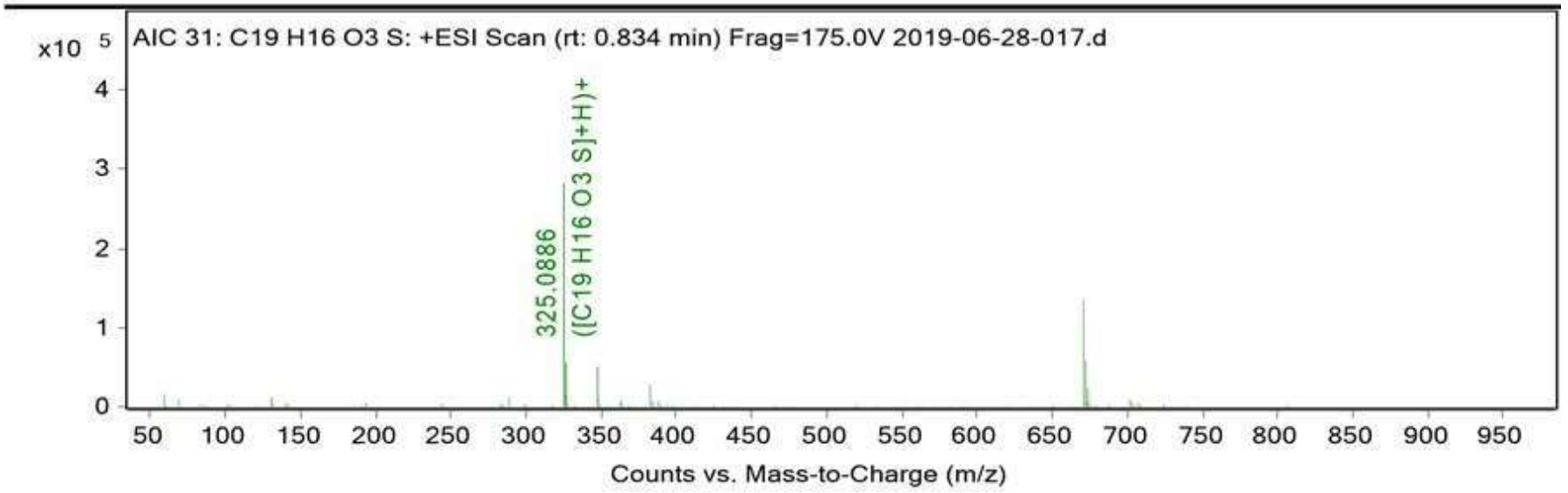
NAME	Audrey Isabelle
EXPNO	85
PROCNO	1
Date_	20190621
Time	9.49
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	637
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	297.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
--------	CHANNEL f1 --------
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
--------	CHANNEL f2 --------
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

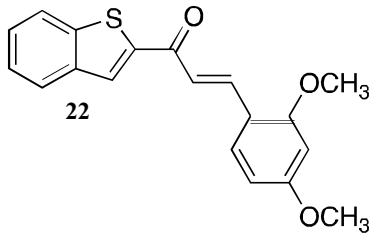

S
O
OCH3
OCH3

21

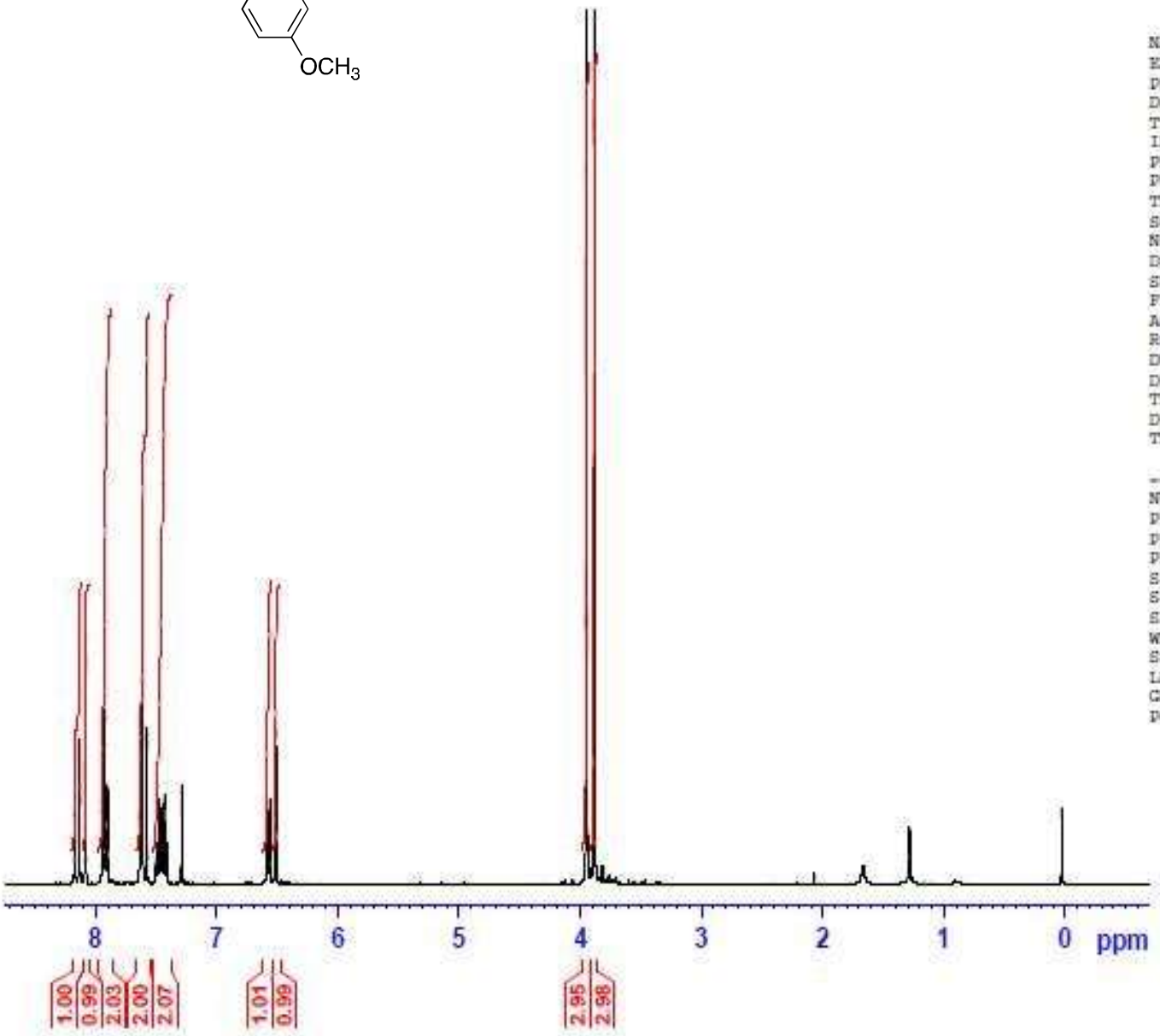

x10 7
+ ESI TIC Scan Frag=175.0V 2019-06-28-017.d
1
1
8
6
4
2
0
* 0.751
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Counts vs. Acquisition Time (min)


x10 5
AIC 31: C19 H16 O3 S: +ESI Scan (rt: 0.834 min) Frag=175.0V 2019-06-28-017.d
4
3
2
1
0
325.0886
([C19 H16 O3 S]+H)+
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



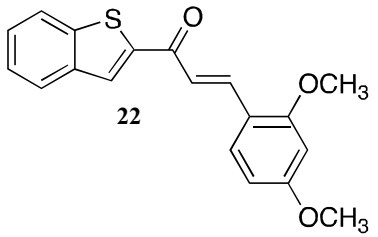
22



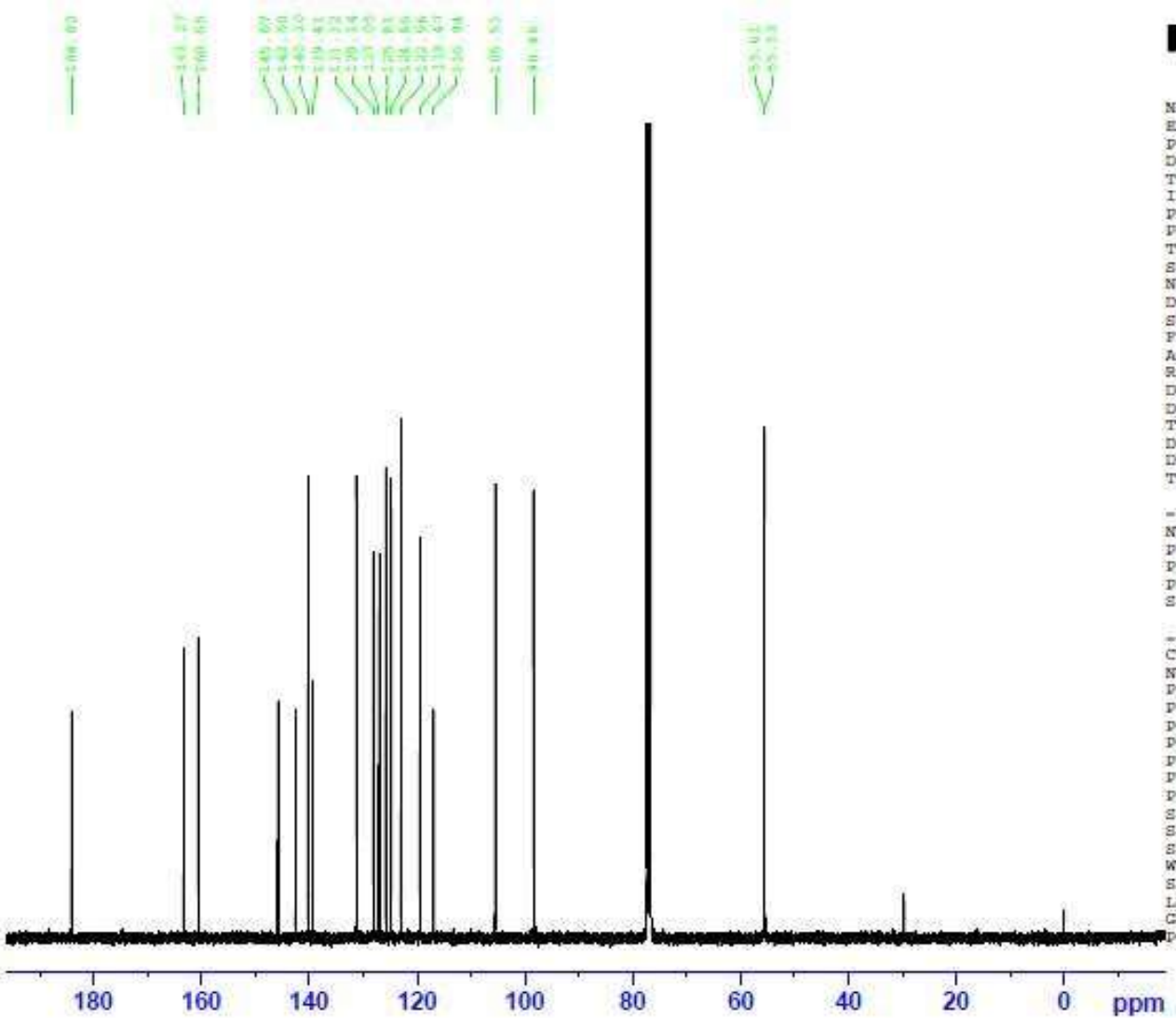
BRUKER

NAME	Audrey Isabelle
EXPNO	86
PROCNO	1
Date_	20190624
Time	9.10
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	80.6
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



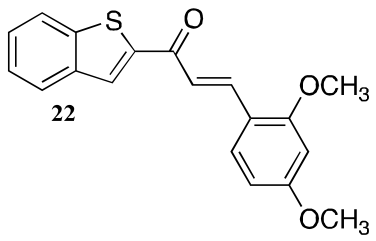
22



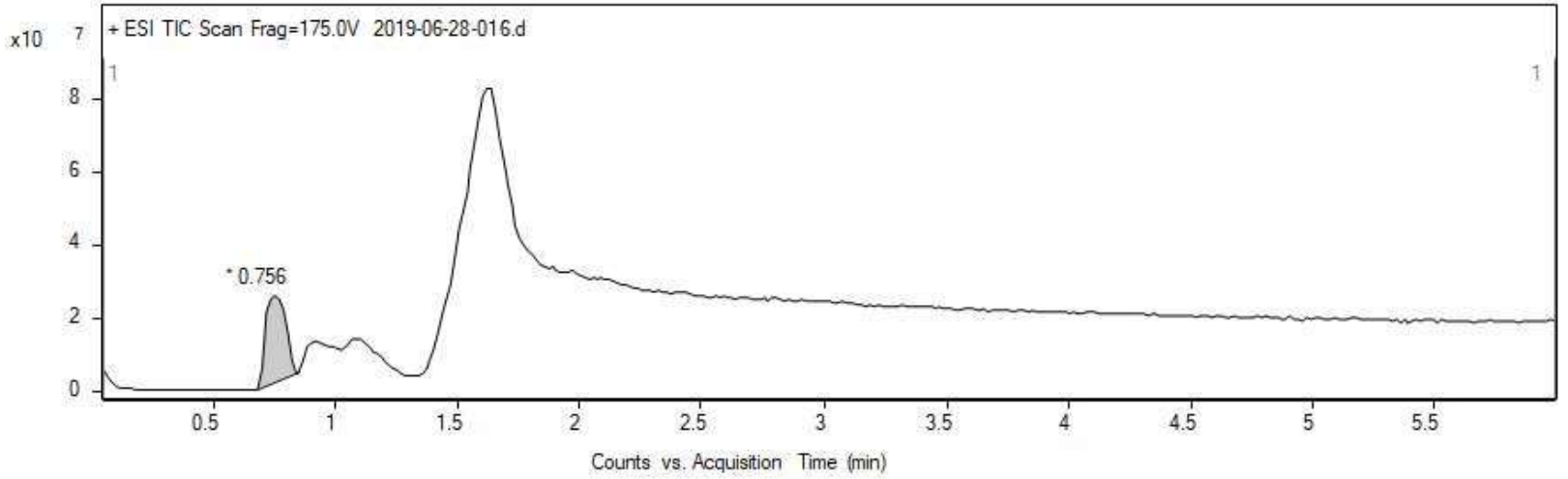
BRUKER

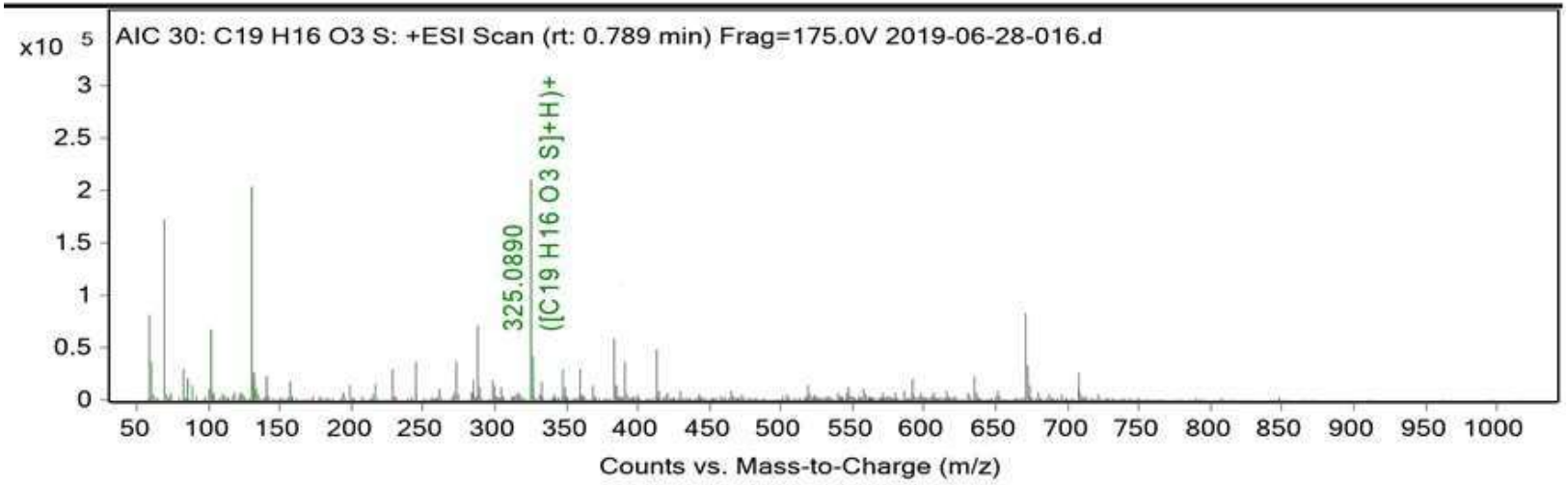
NAME	Audrey Isabelle
EXPNO	88
PROCNO	1
Date_	20190624
Time	11.07
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1836
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

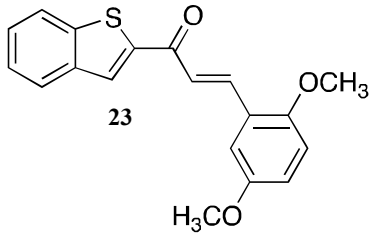

S
O
OCH3
OCH3

22

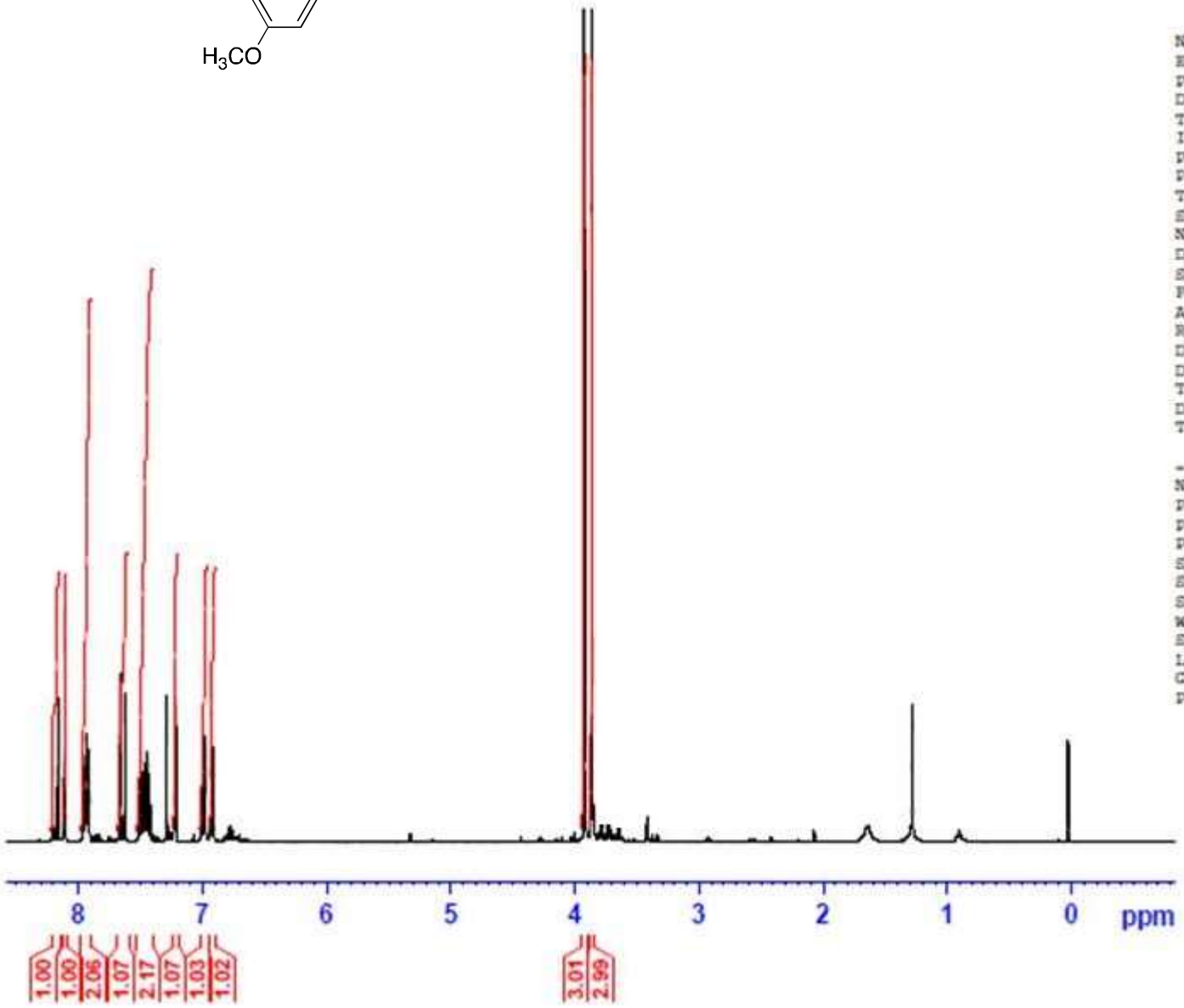

x10 7
+ ESI TIC Scan Frag=175.0V 2019-06-28-016.d
1
1
8
6
4
2
0
* 0.756
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Counts vs. Acquisition Time (min)


x10 5
AIC 30: C19 H16 O3 S: +ESI Scan (rt: 0.789 min) Frag=175.0V 2019-06-28-016.d
3
2.5
2
1.5
1
0.5
0
325.0890
([C19 H16 O3 S]+H)+
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



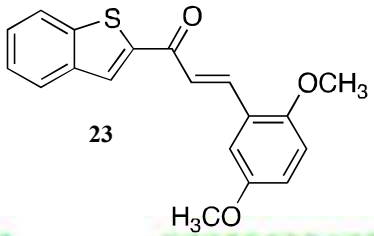
23



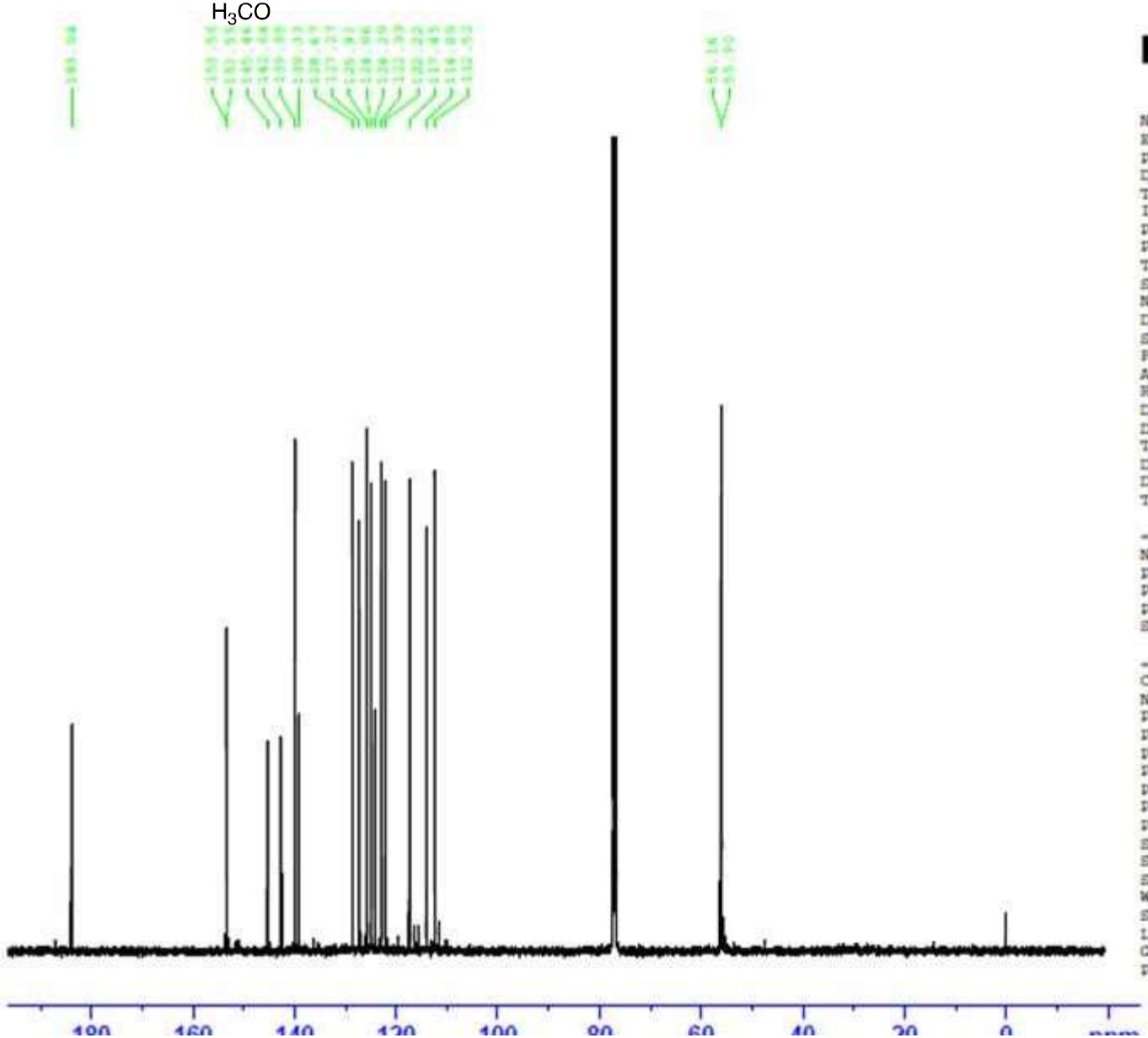
BRUKER

NAME	Audrey Isabelle
EXPNO	78
PROCNO	1
Date_	20190619
Time	15.23
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	90.5
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
--------	CHANNEL f1 --------
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



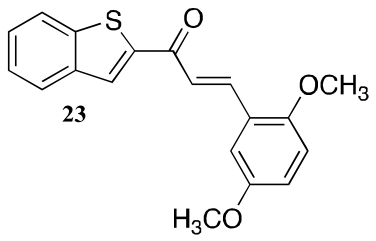
23



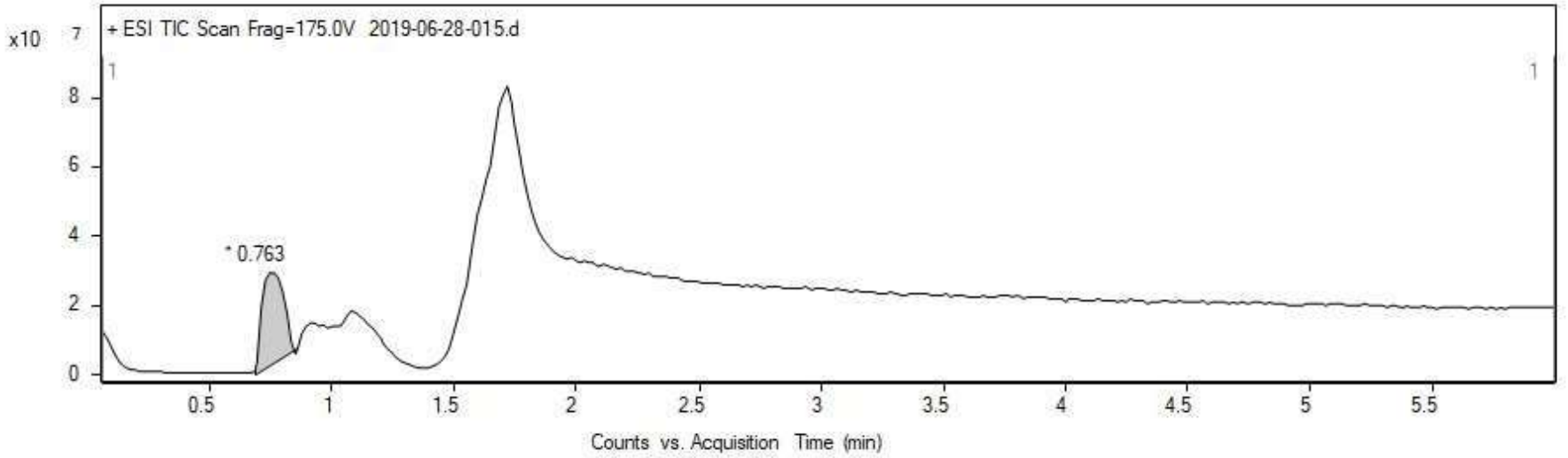
BRUKER

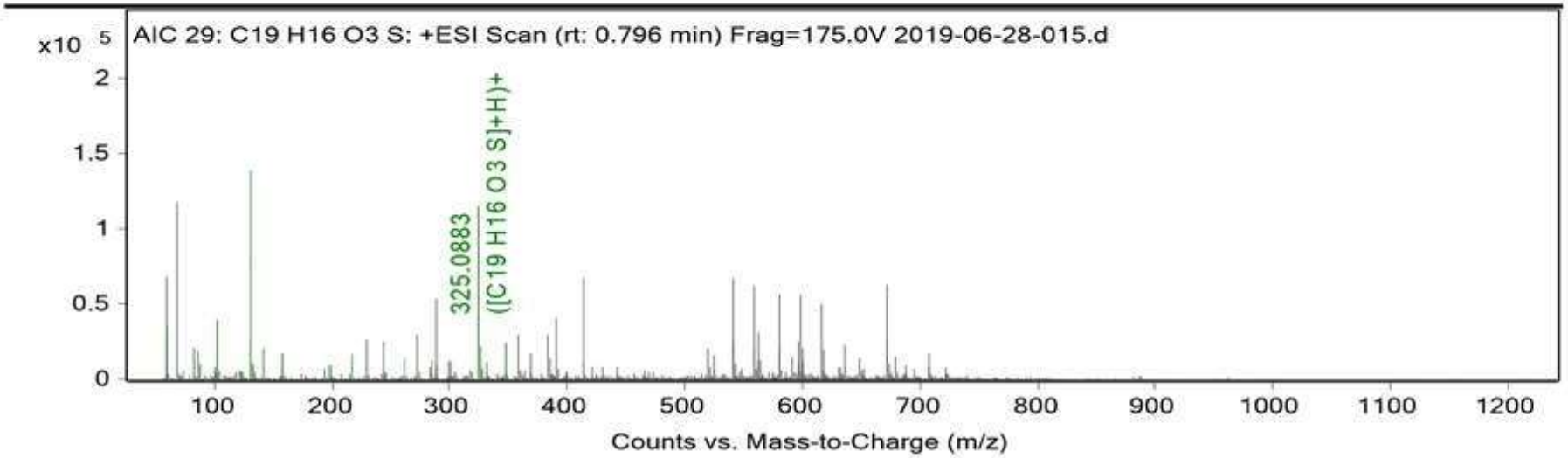
NAME	Audrey Isabelle
EXPNO	80
PROCNO	1
Date_	20190620
Time	1.06
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	10000
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
-------- CHANNEL f2 --------	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

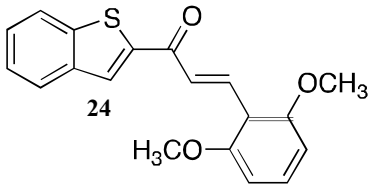

S
O
OCH3
H3CO

23

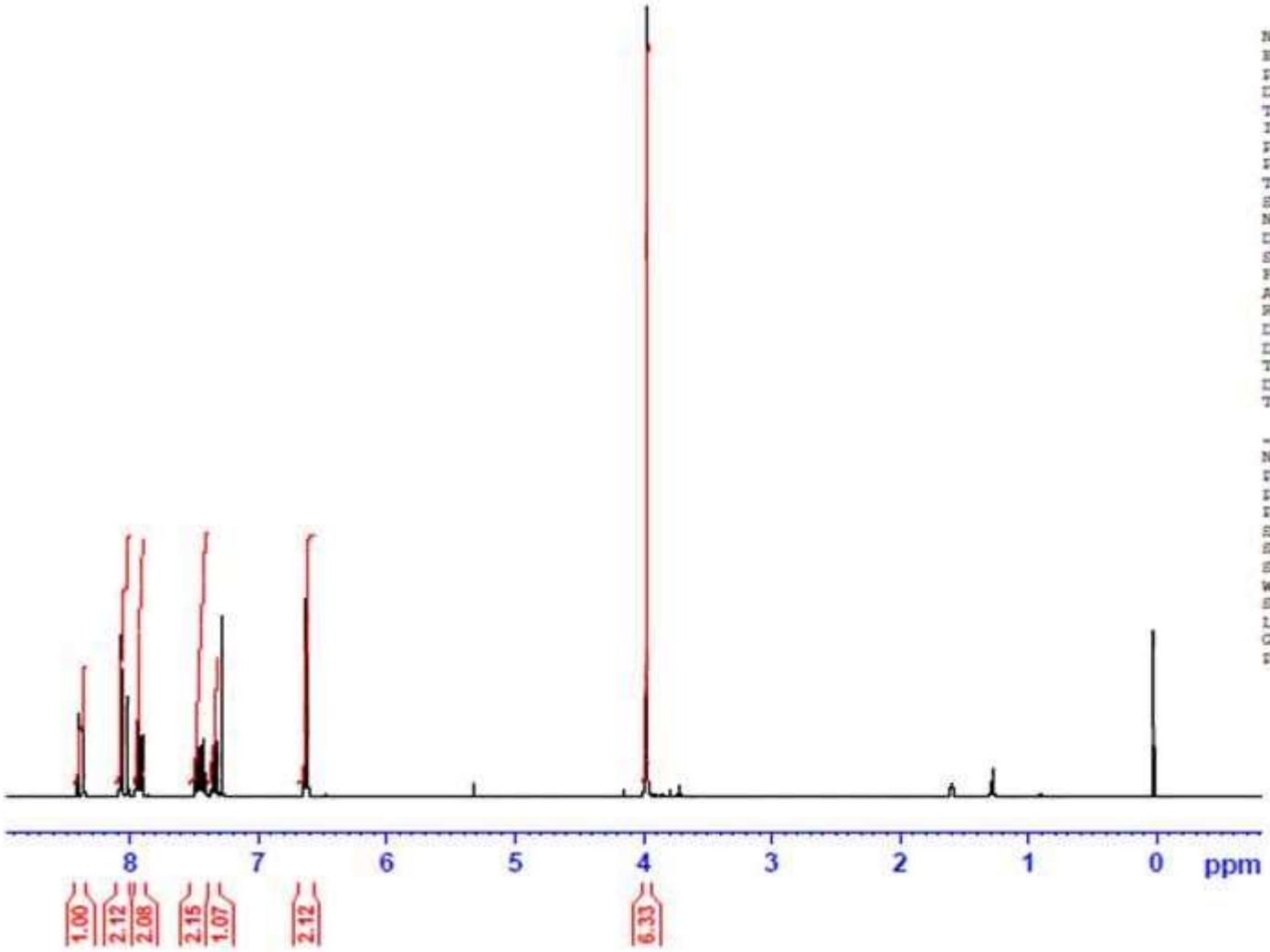

x10 7
+ ESI TIC Scan Frag=175.0V 2019-06-28-015.d
1
1
8
6
4
2
0
* 0.763
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Counts vs. Acquisition Time (min)


x10 5
AIC 29: C19 H16 O3 S: +ESI Scan (rt: 0.796 min) Frag=175.0V 2019-06-28-015.d
2
1.5
1
0.5
0
325.0883
([C19 H16 O3 S]+H)+
100
200
300
400
500
600
700
800
900
1000
1100
1200
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR

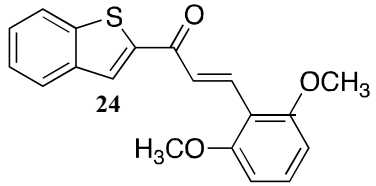


24

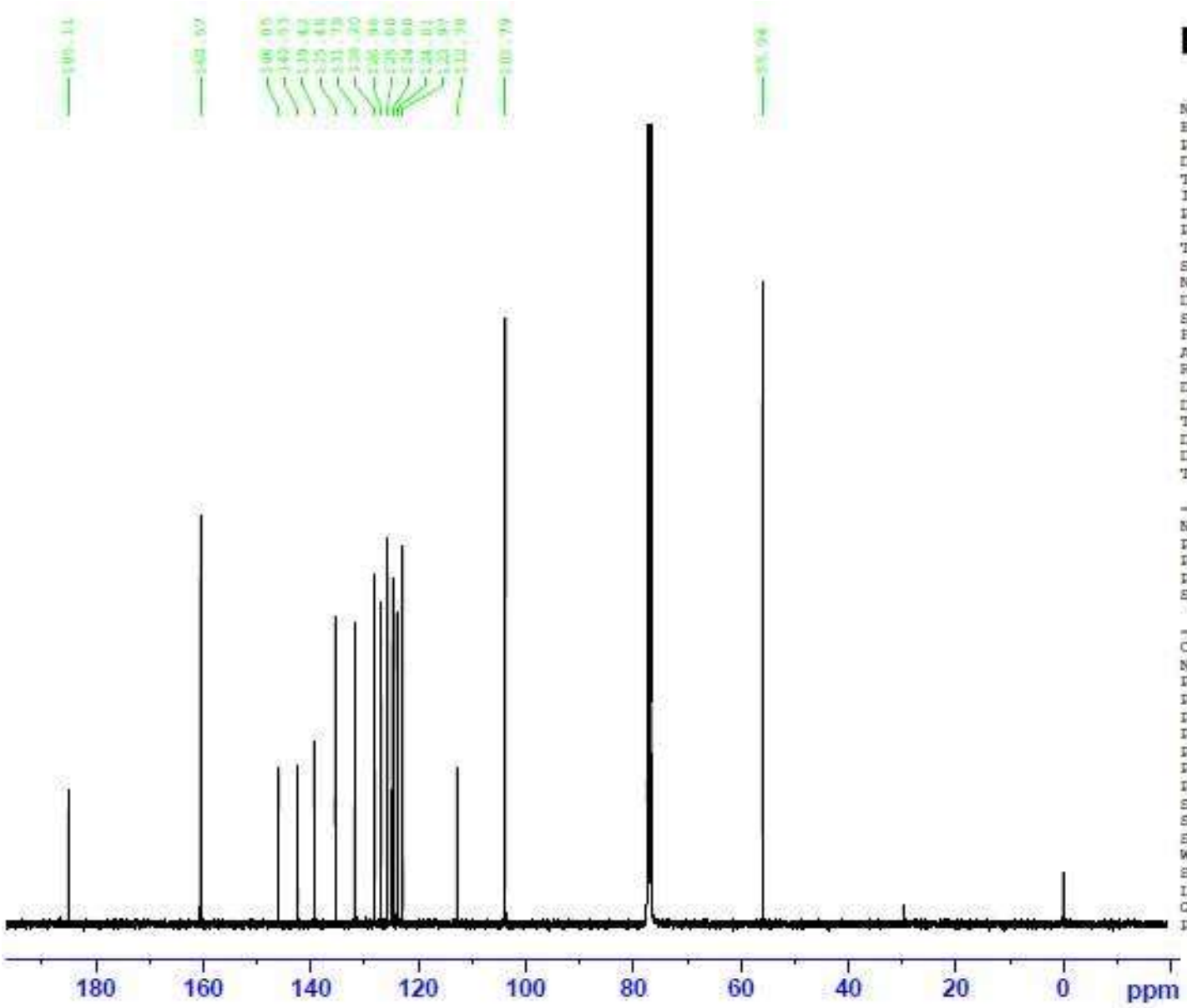



```
NAME          Audrey Isabelle
EXPNO                      38
PROCNO                      1
Date_                20190527
Time                    16.36
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9846387 sec
RG                       128
DW                    60.800 usec
DE                     6.50 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.07 usec
PL1                     0.30 dB
PL1W           11.25229836 W
SFO1           400.1324710 MHz
SI                     32768
SF             400.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

^{13}C NMR



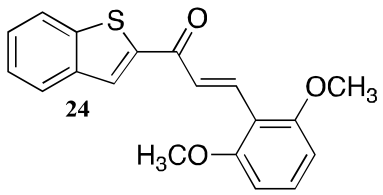
24



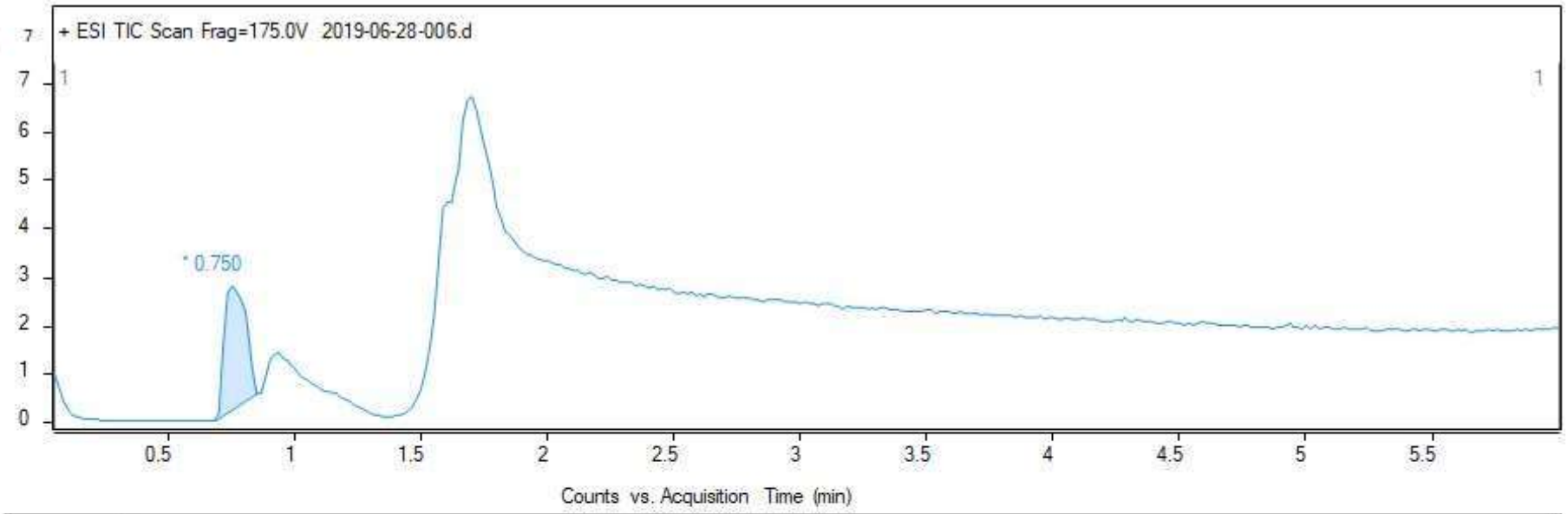
BRUKER

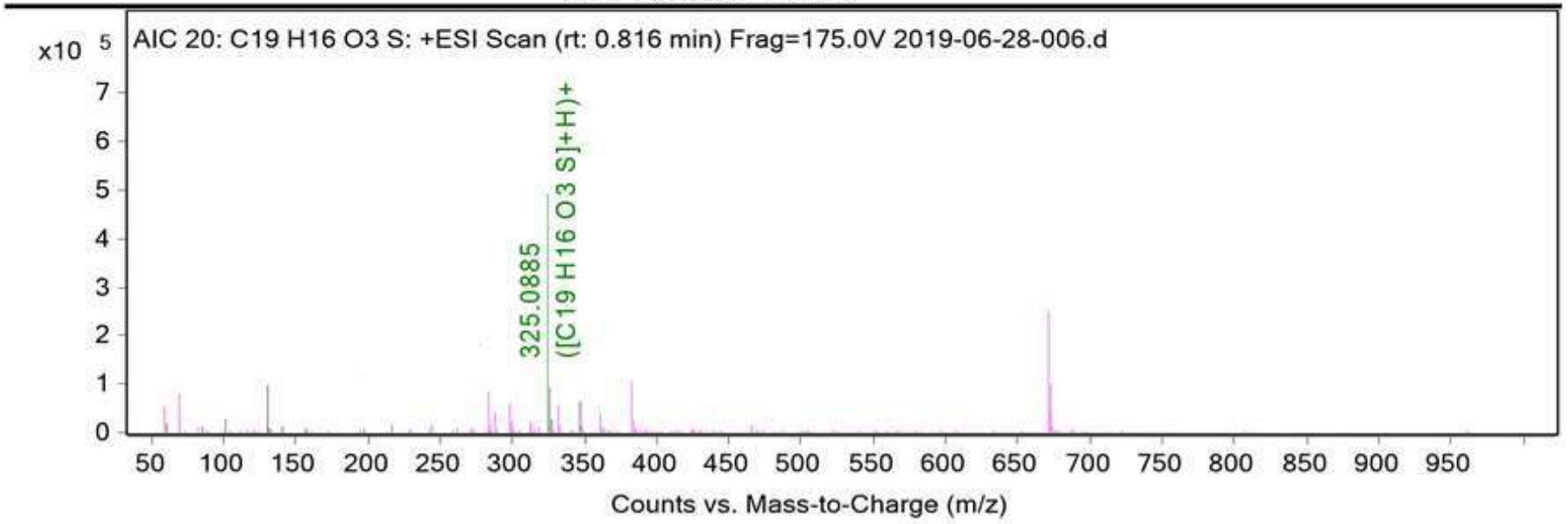
NAMR	Audrey Isabelle	
EXPNO	40	
PROCNO	1	
Date_	20190528	
Time_	2.11	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	10000	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
-------- CHANNEL f1 --------		
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
-------- CHANNEL f2 --------		
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS

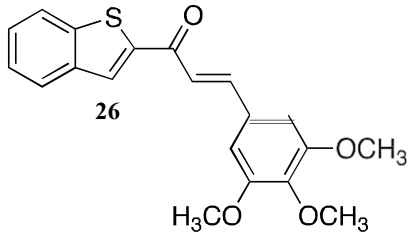

S
O
OCH3
H3CO

24

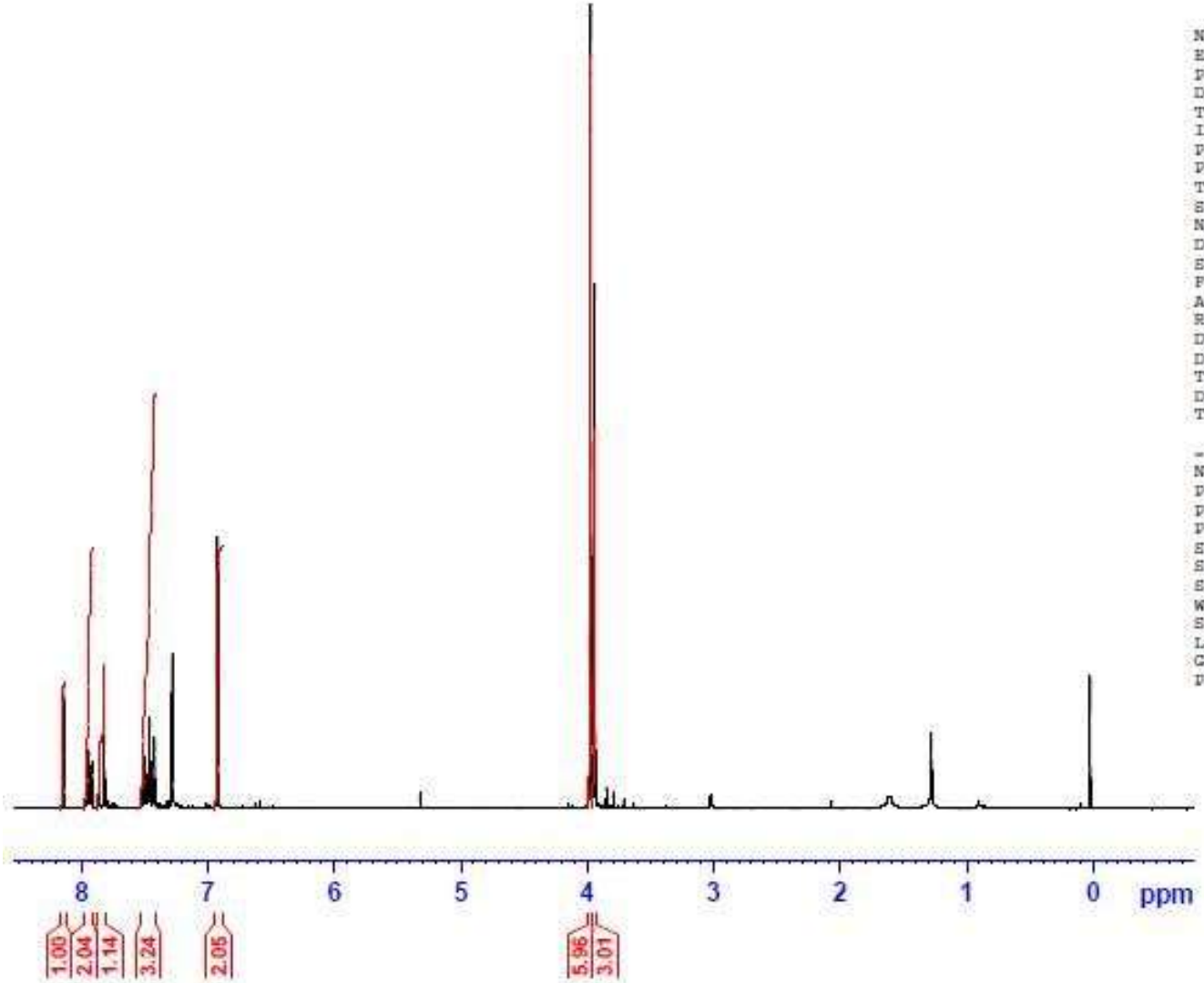

+ ESI TIC Scan Frag=175.0V 2019-06-28-006.d
* 0.750
Counts vs. Acquisition Time (min)


AIC 20: C19 H16 O3 S: +ESI Scan (rt: 0.816 min) Frag=175.0V 2019-06-28-006.d
x10
325.0885
([C19 H16 O3 S]+H)+
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



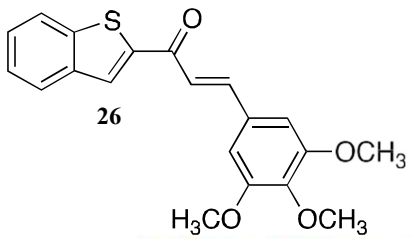
26



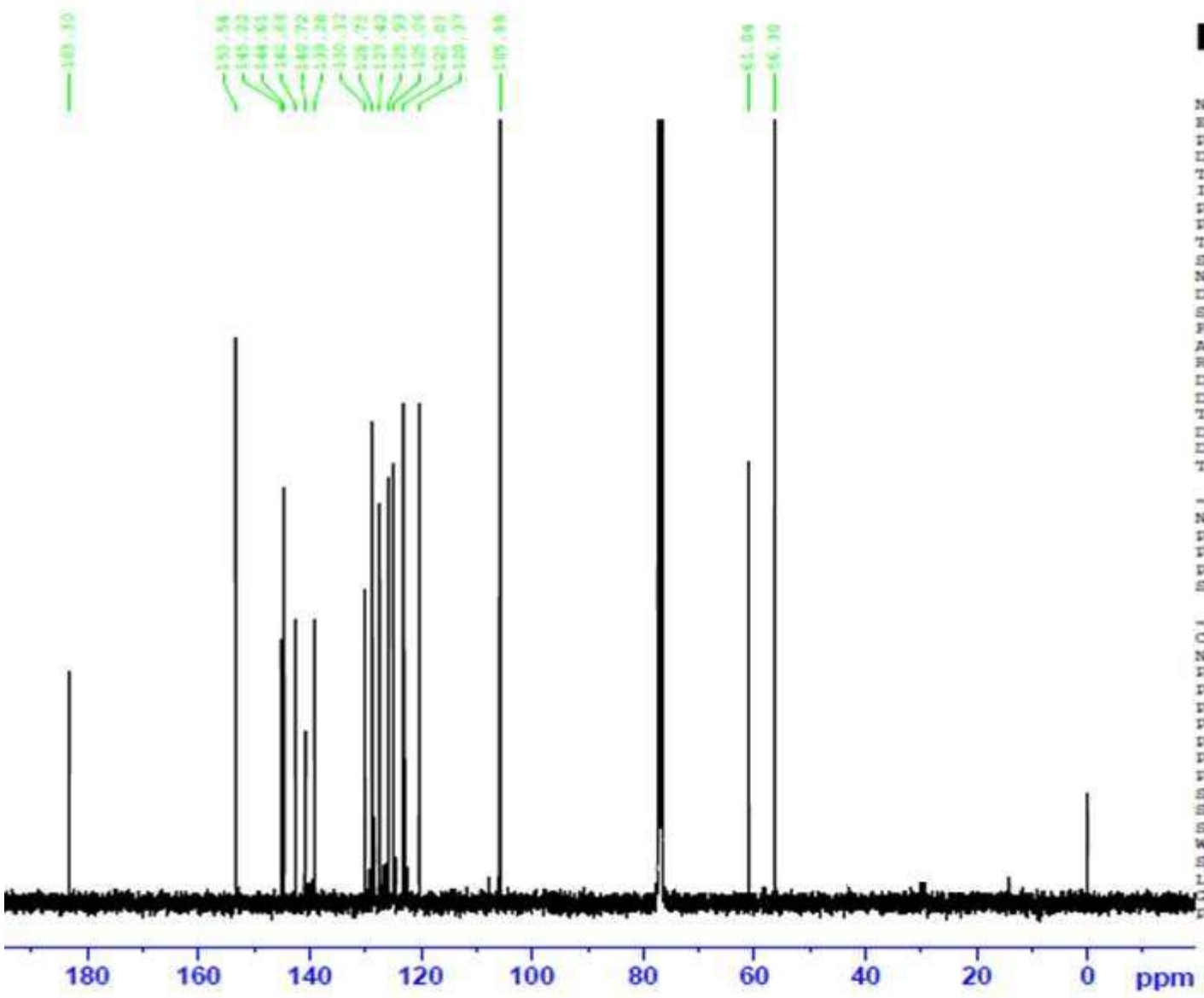
BRUKER

NAME	Audrey Isabelle
EXPNO	62
PROCNO	1
Date_	20190612
Time	8.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	114
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



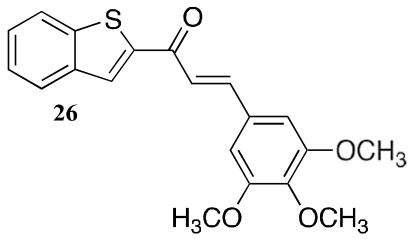
26



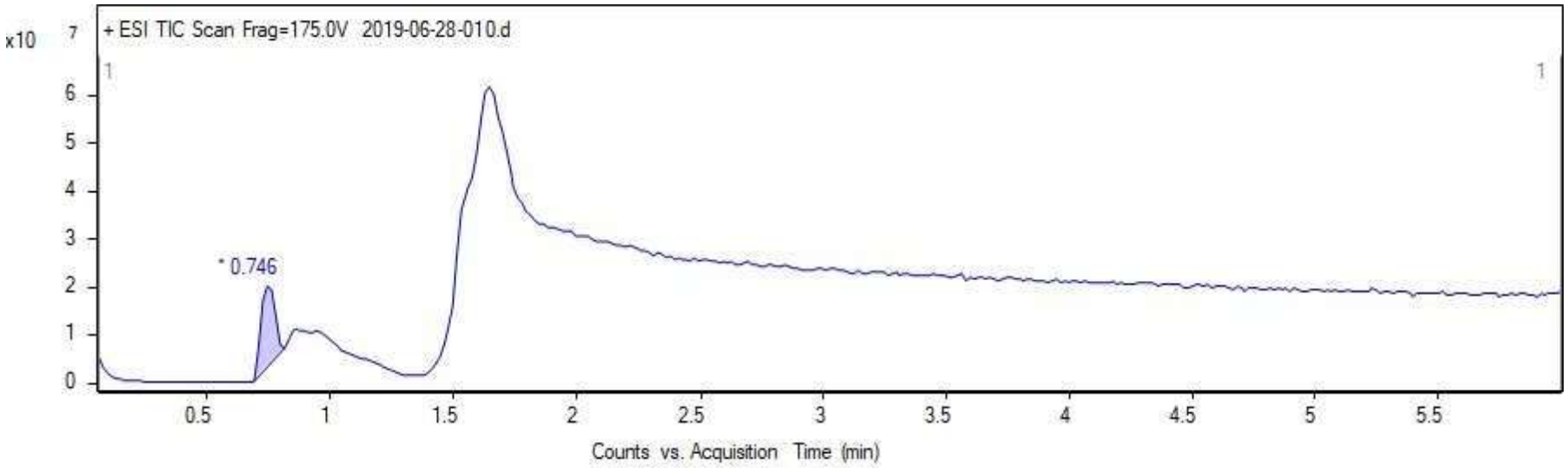
BRUKER

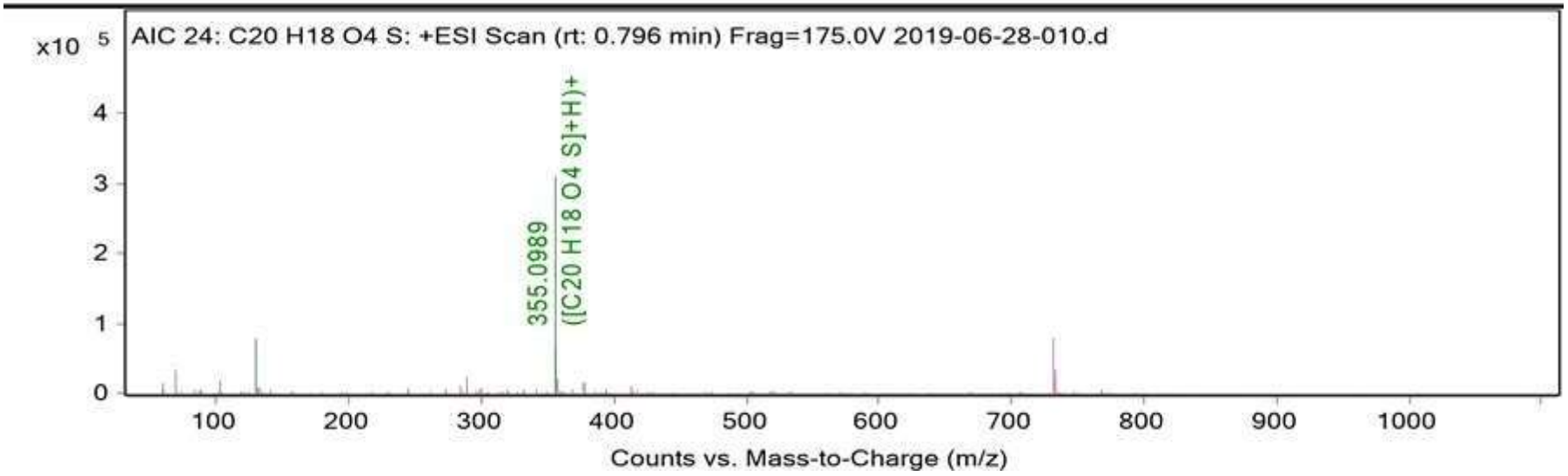
NAME	Audrey Isabelle	
EXPNO	64	
PROCNO	1	
Date_	20190612	
Time	14.36	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	5397	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS

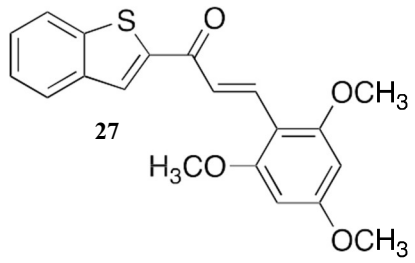

S
O
OCH3
H3CO
OCH3

26

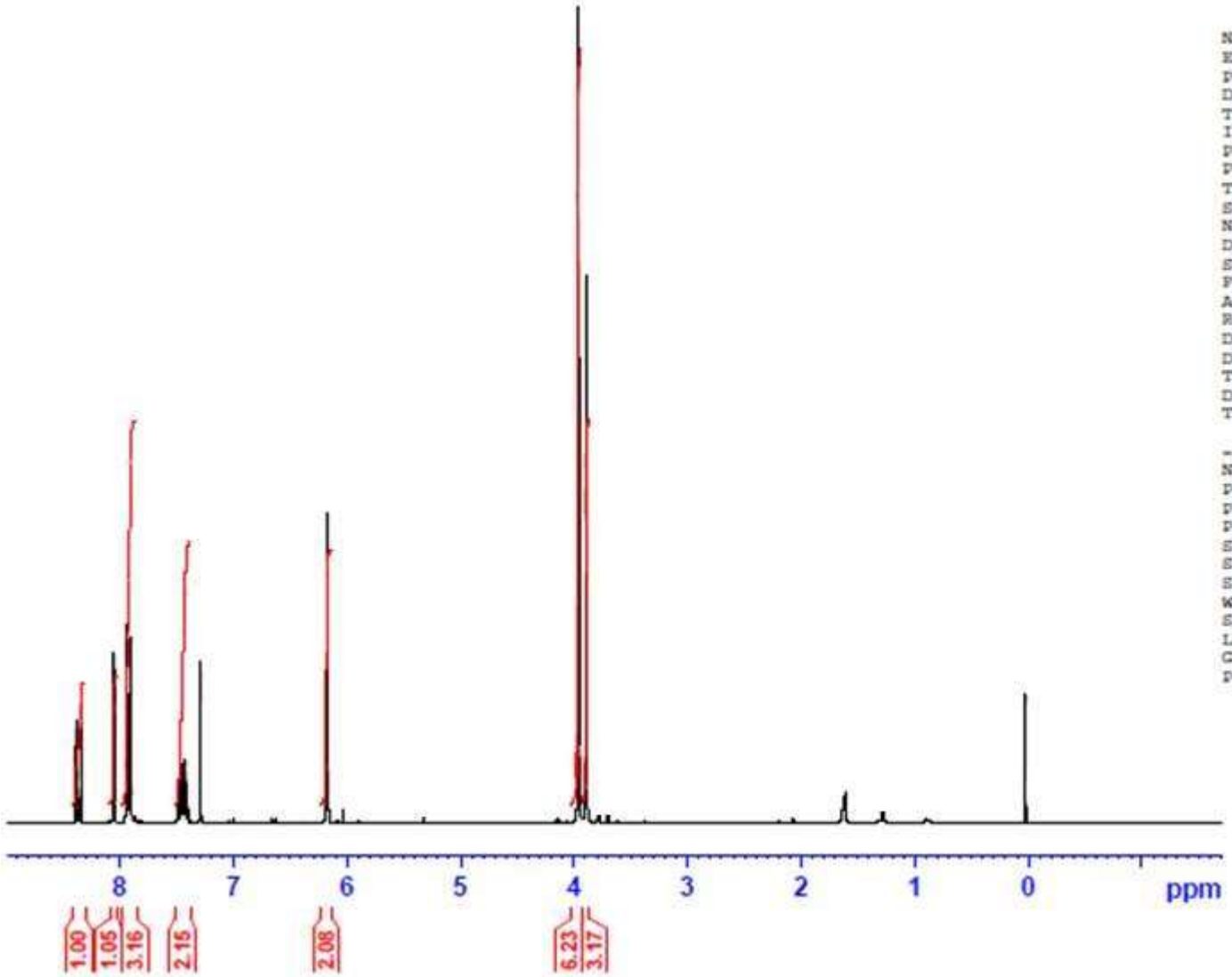

x10 7
+ ESI TIC Scan Frag=175.0V 2019-06-28-010.d
1
1
6
5
4
3
2
1
0
* 0.746
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Counts vs. Acquisition Time (min)


x10 5
AIC 24: C20 H18 O4 S: +ESI Scan (rt: 0.796 min) Frag=175.0V 2019-06-28-010.d
4
3
2
1
0
355.0989
([C20 H18 O4 S]+H)+
100
200
300
400
500
600
700
800
900
1000
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



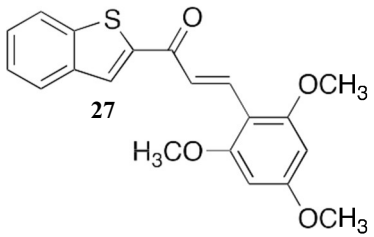
27



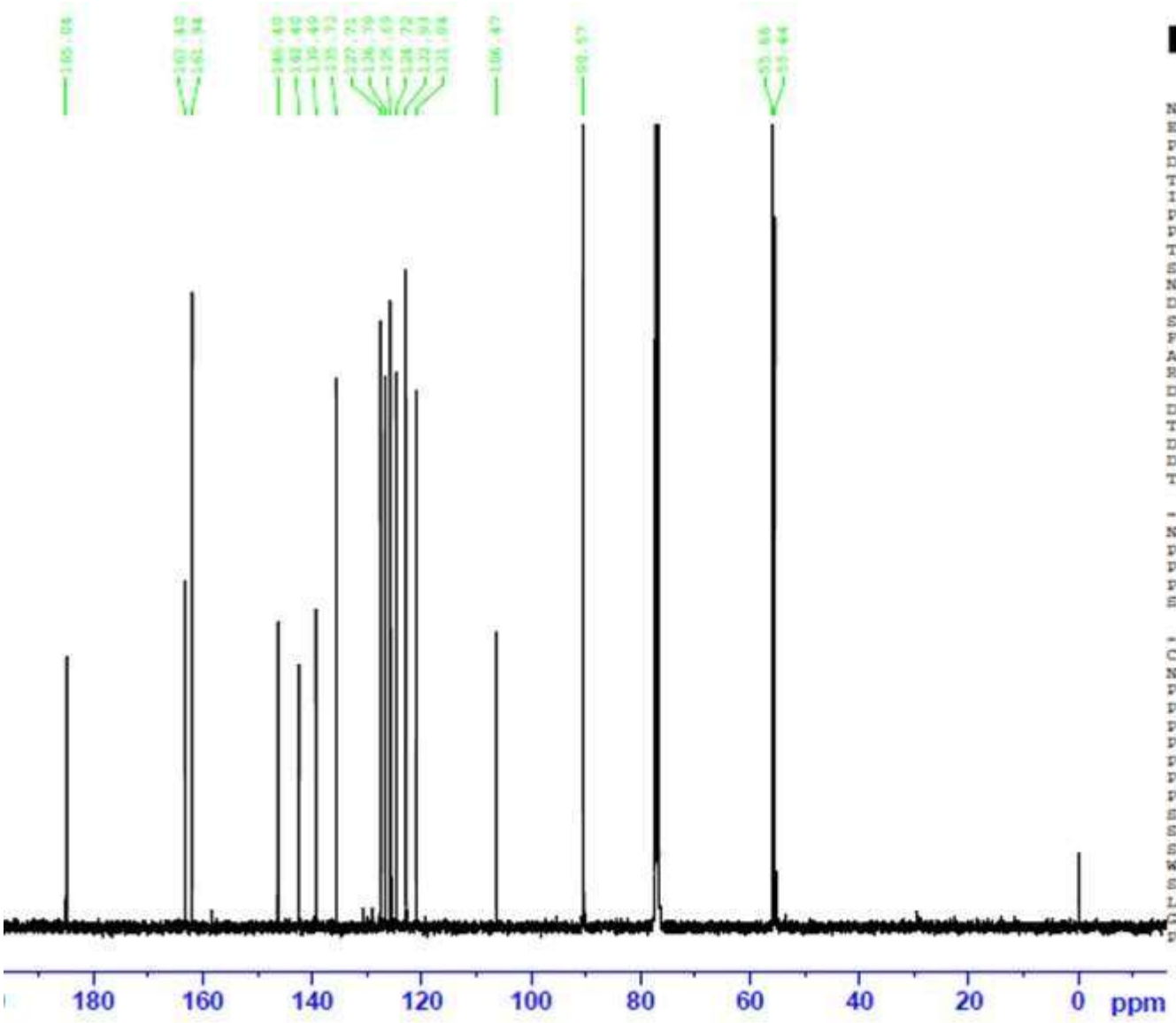
BRUKER

NAME	Audrey Isabelle	
EXPNO	65	
PROCNO	1	
Date_	20190612	
Time	14.44	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	101	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
--------	CHANNEL f1	--------
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{13}C NMR



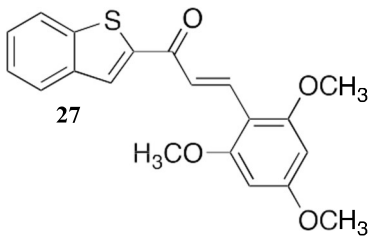
27



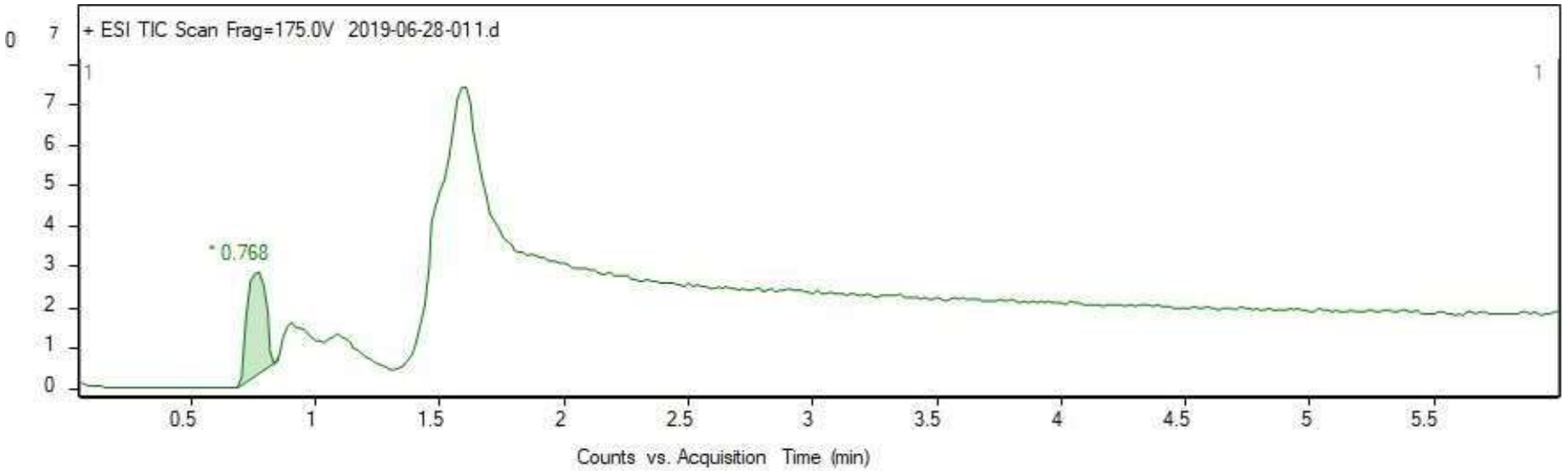
BRUKER

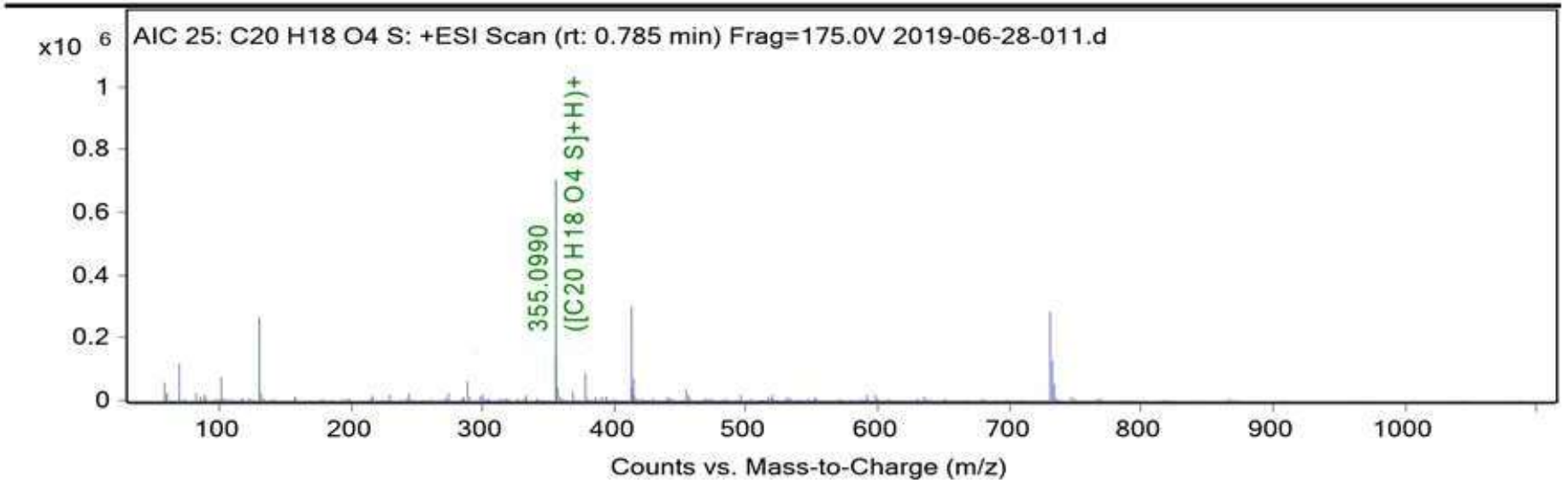
NAME	Audrey Isabelle	
EXPNO	67	
PROCNO	1	
Date_	20190613	
Time	0.49	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	10000	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
--------	CHANNEL f1	--------
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
--------	CHANNEL f2	--------
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS

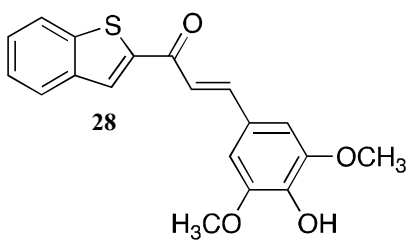

S
O
OCH3
H3CO
OCH3

27

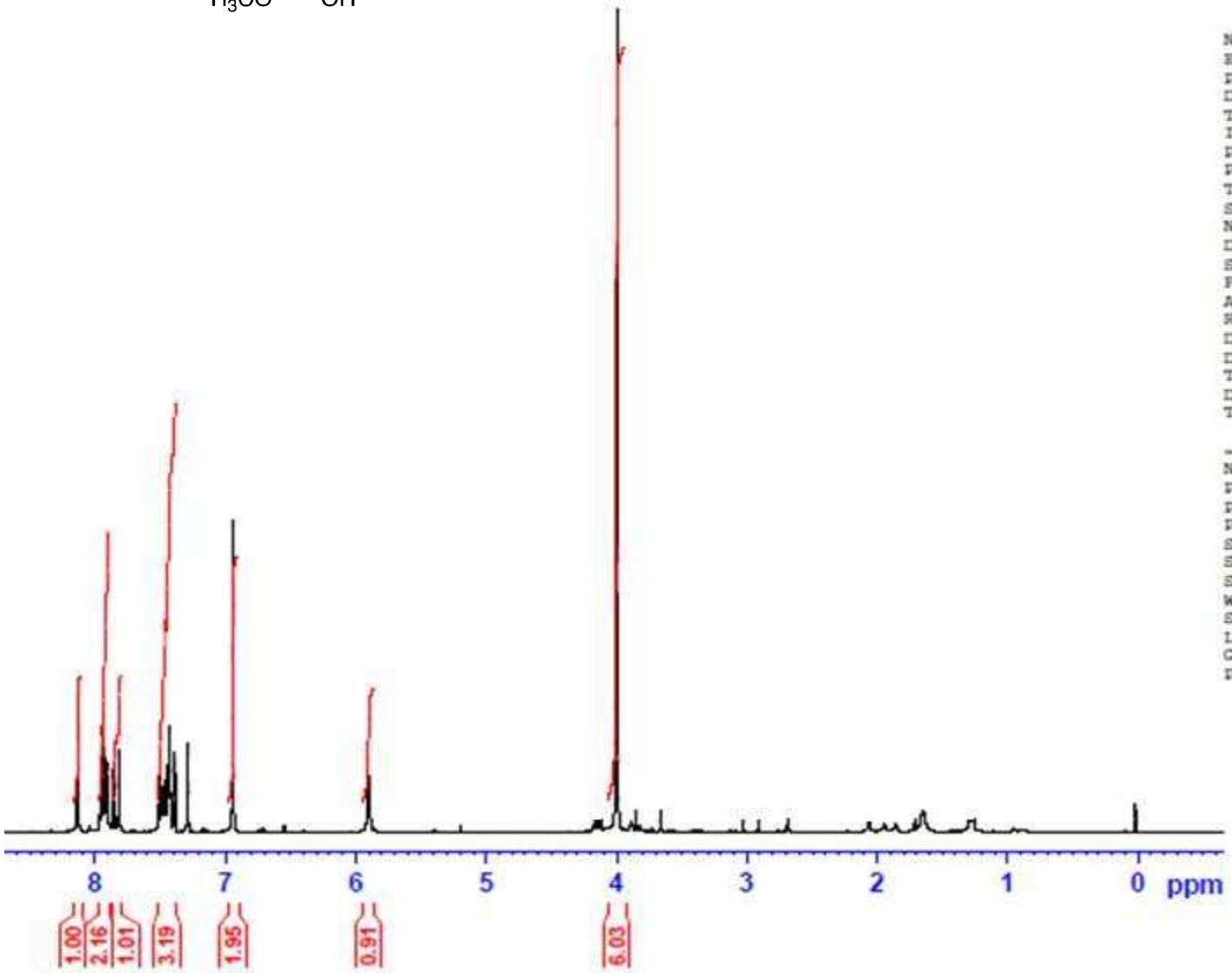

+ ESI TIC Scan Frag=175.0V 2019-06-28-011.d
* 0.768
Counts vs. Acquisition Time (min)


AIC 25: C20 H18 O4 S: +ESI Scan (rt: 0.785 min) Frag=175.0V 2019-06-28-011.d
x10 6
355.0990
([C20 H18 O4 S]+H)+
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



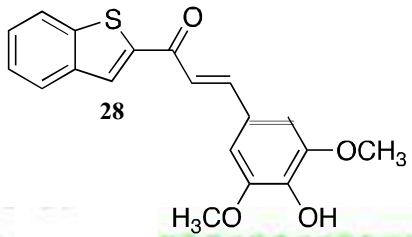
28



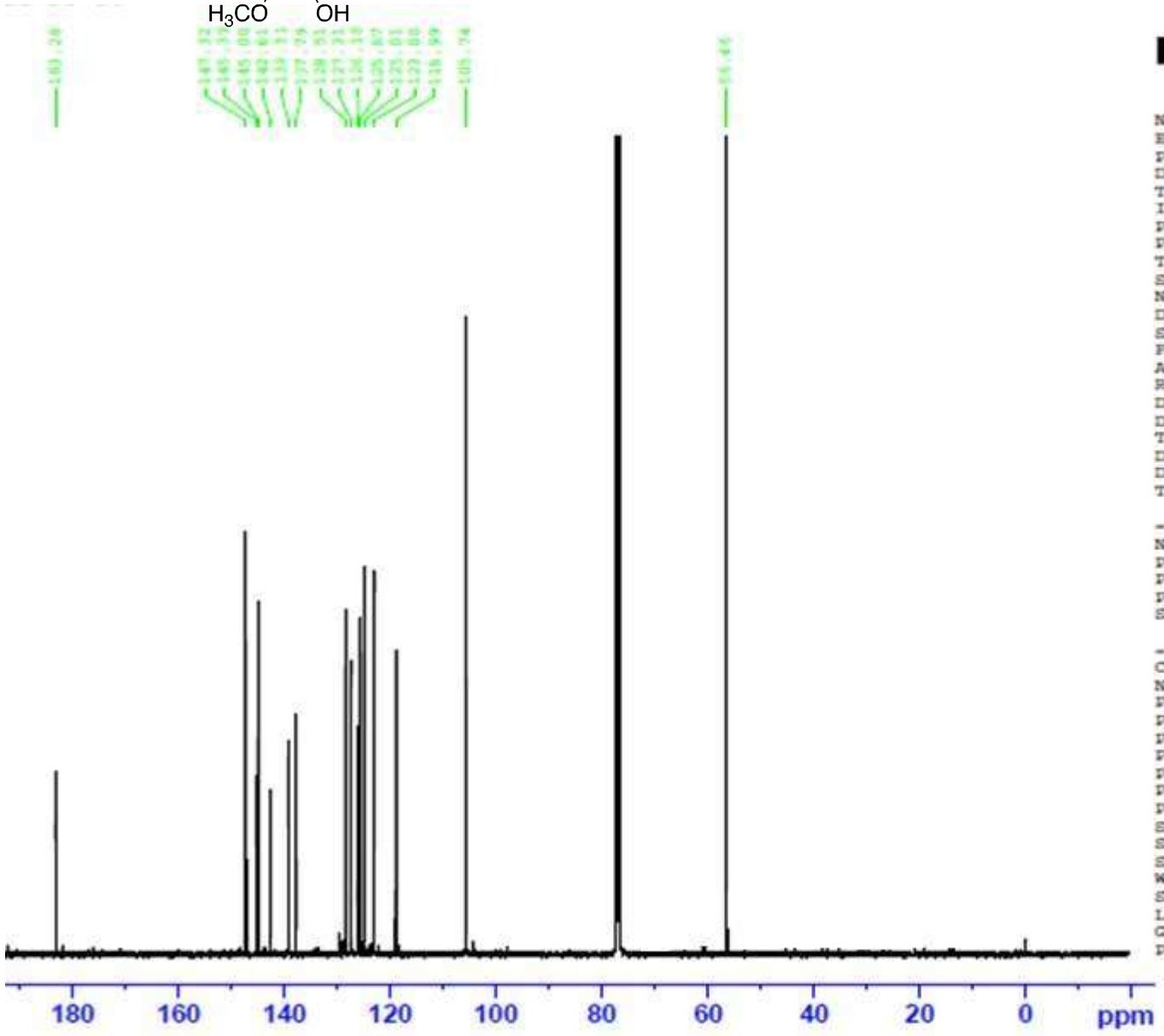
BRUKER

NAME	Audrey Isabelle	
EXPNO	21	
PROCNO	1	
Date_	20190323	
Time	10.38	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	90.5	
DW	60.800	usec
DE	6.50	usec
TE	298.0	K
D1	1.00000000	sec
TD0	1	
-------- CHANNEL f1 --------		
NUC1	1H	
P1	14.07	usec
PL1	0.30	dB
PL1W	11.25229836	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

^{13}C NMR



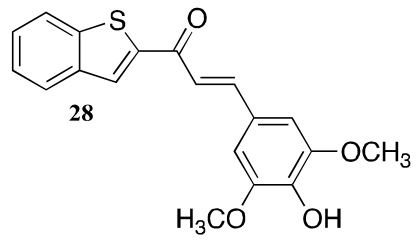
28



BRUKER

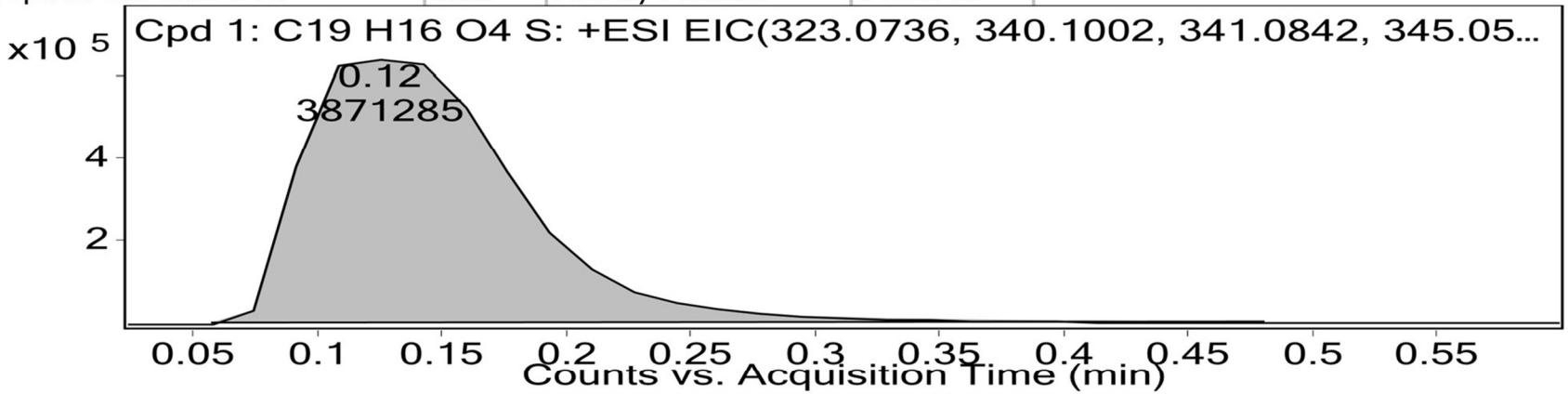
NAME	Audrey Isabelle	
EXPNO	22	
PROCNO	1	
Date_	20190323	
Time	22.11	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	12000	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
--------	CHANNEL f1	--------
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
--------	CHANNEL f2	--------
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS

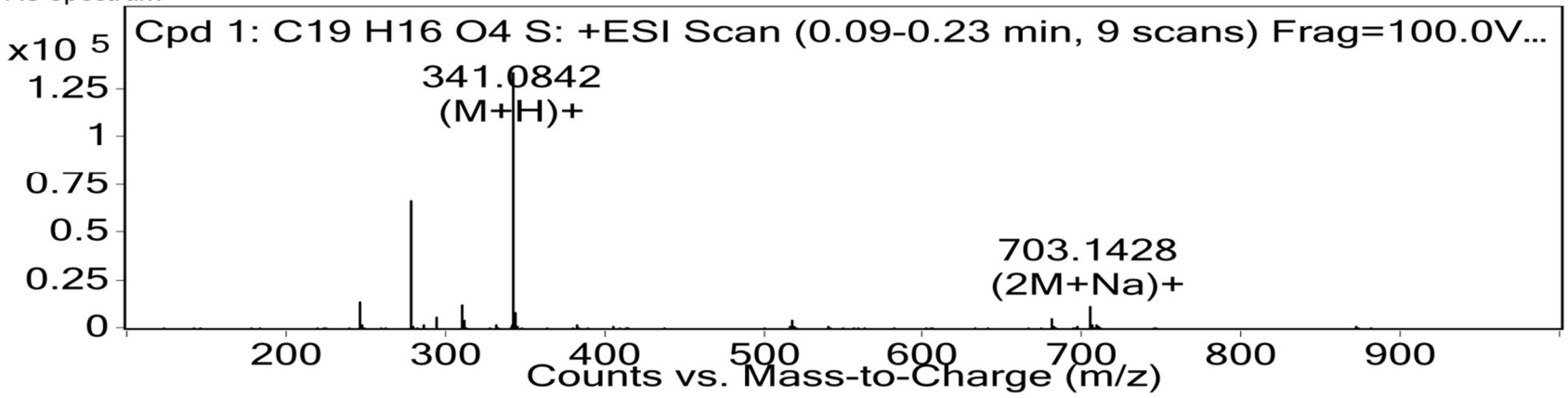


28

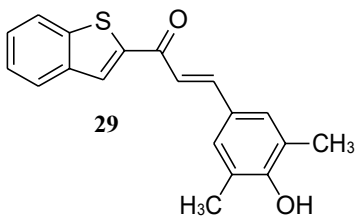
Compound Label	RT	Algorithm	Mass
Cpd 1: C19 H16 O4 S	0.12	Find By Formula	340.0769



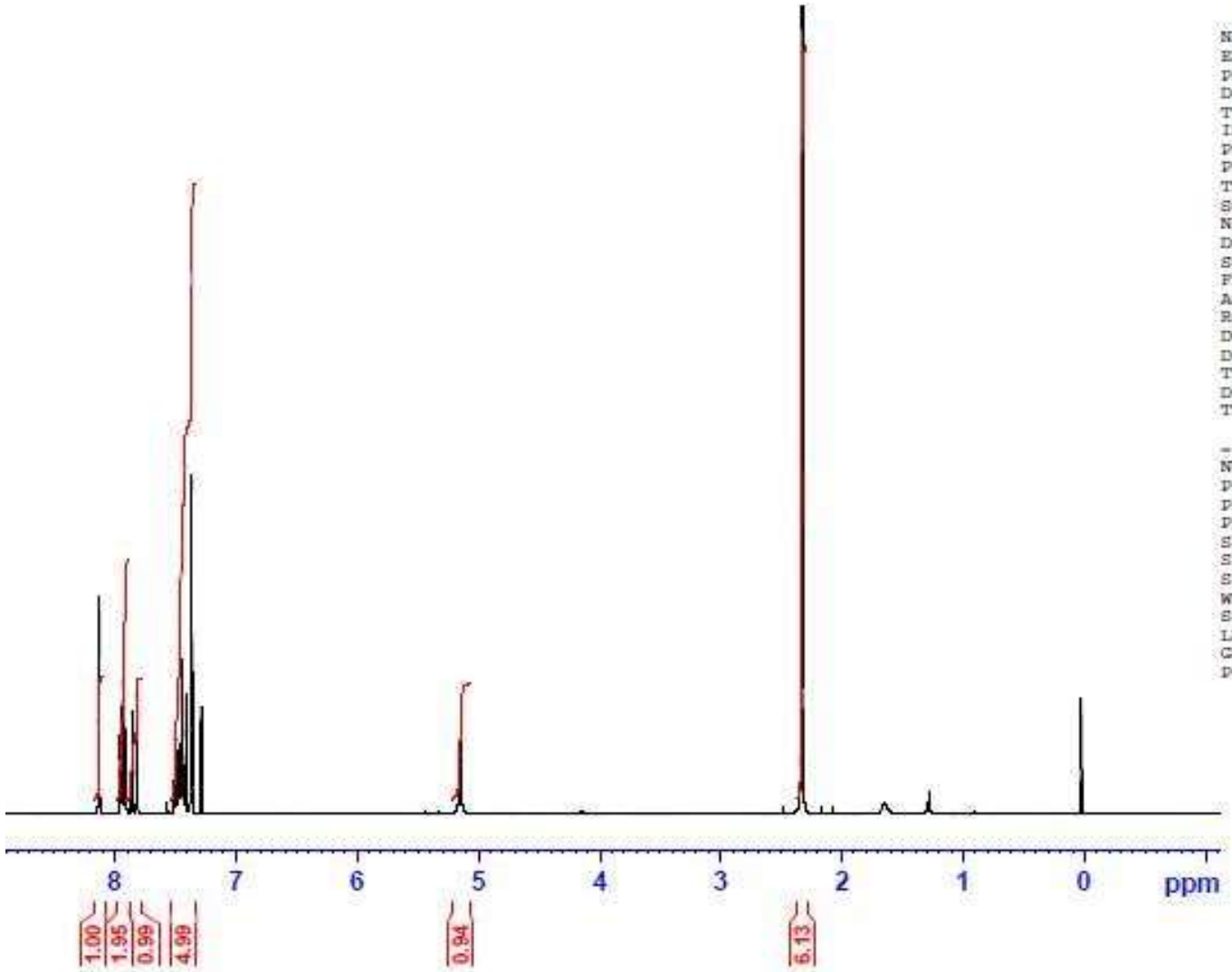
MS Spectrum



^{1}H NMR



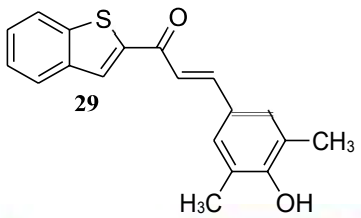
29



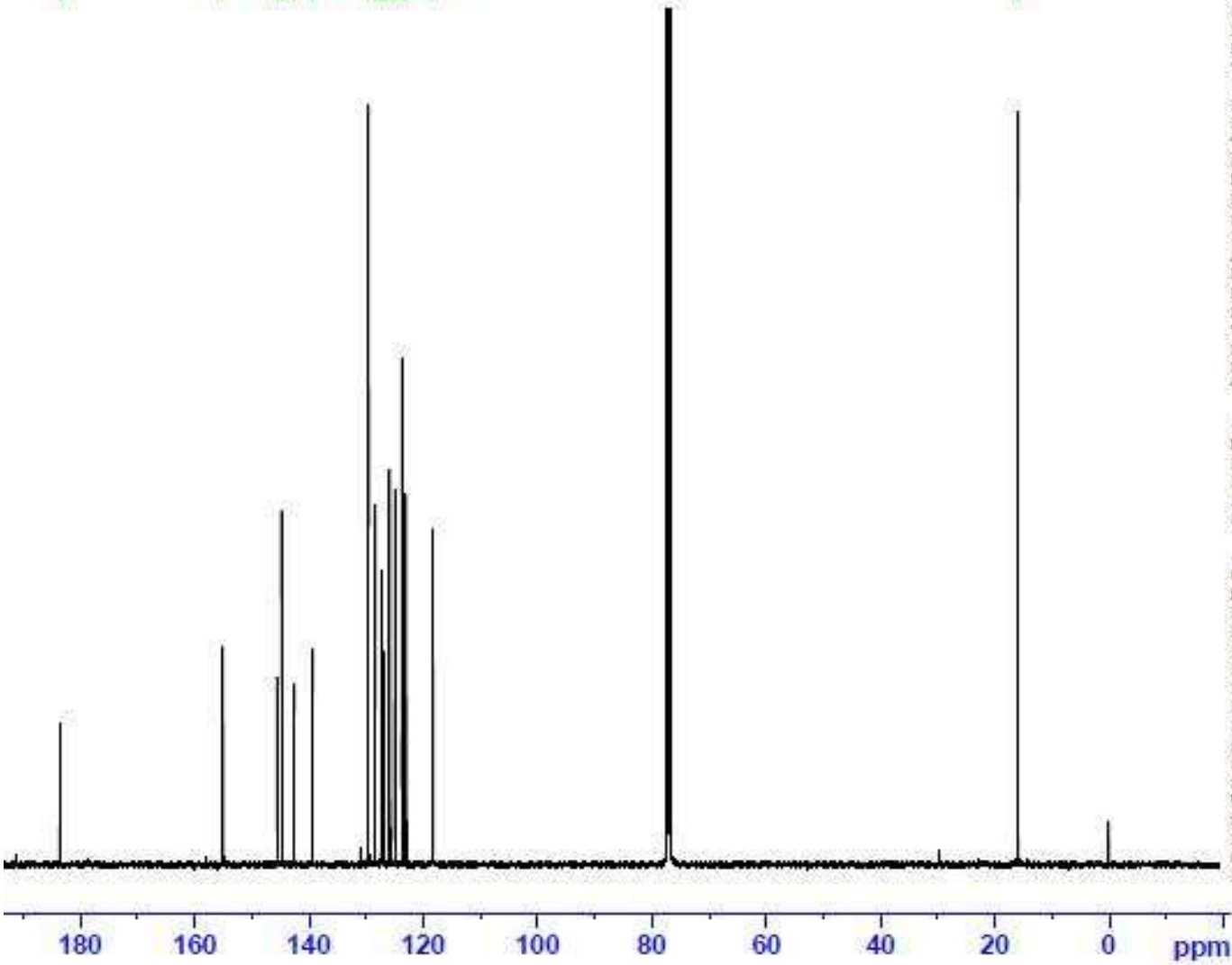
BRUKER

NAME	Audrey Isabelle
EXPNO	41
PROCNO	1
Date_	20190529
Time	9.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	101
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



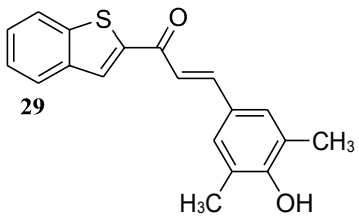
29



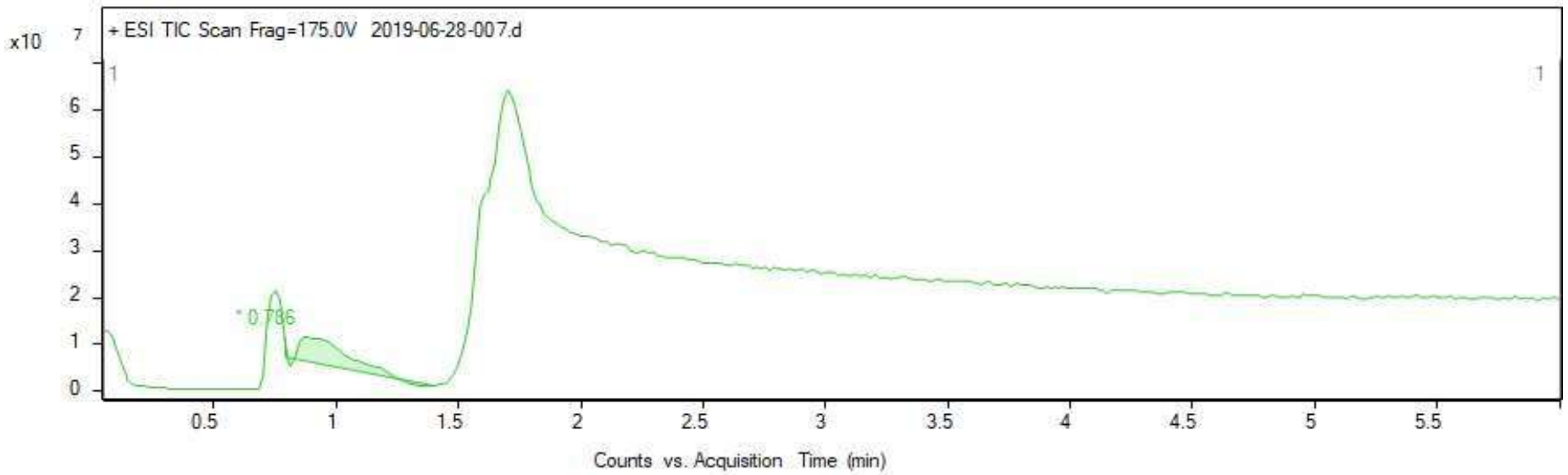
BRUKER

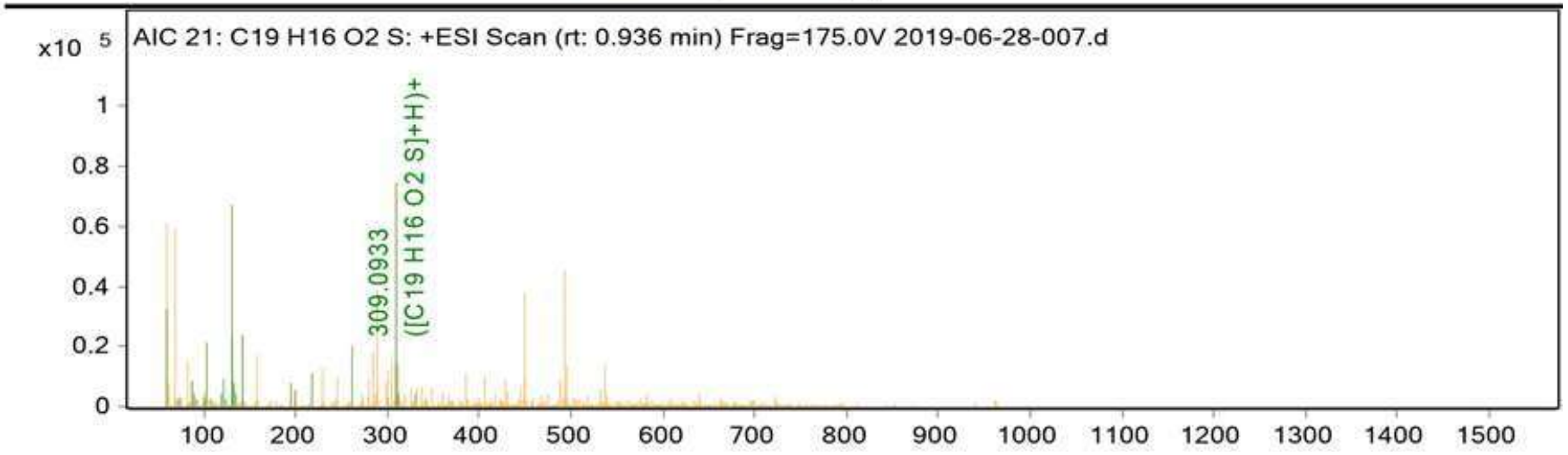
NAME	Audrey Isabelle
EXPNO	46
PROCNO	1
Date_	20190529
Time	23.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	10000
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
-------- CHANNEL f2 --------	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

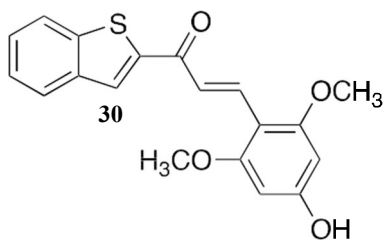

S
O
CH3
H3C
OH

29

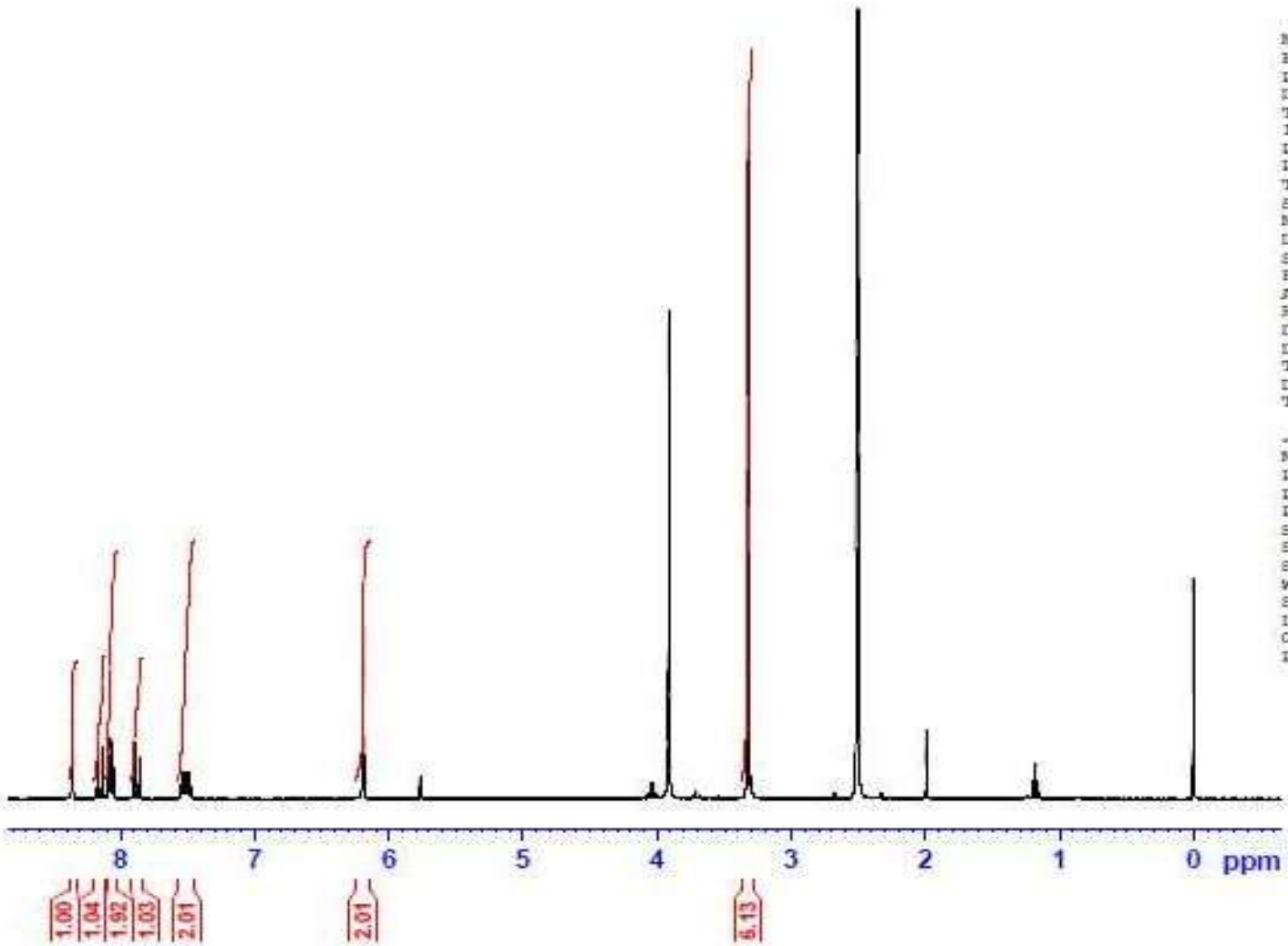

x10 7
+ ESI TIC Scan Frag=175.0V 2019-06-28-007.d
1
1
6
5
4
3
2
1
0
0.786
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Counts vs. Acquisition Time (min)


x10 5
AIC 21: C19 H16 O2 S: +ESI Scan (rt: 0.936 min) Frag=175.0V 2019-06-28-007.d
1
0.8
0.6
0.4
0.2
0
309.0933
([C19 H16 O2 S]+H)+
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500

^{1}H NMR



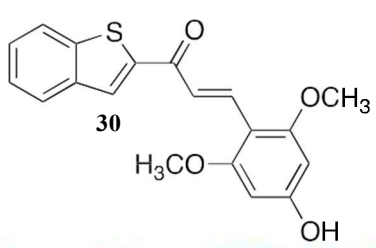
30



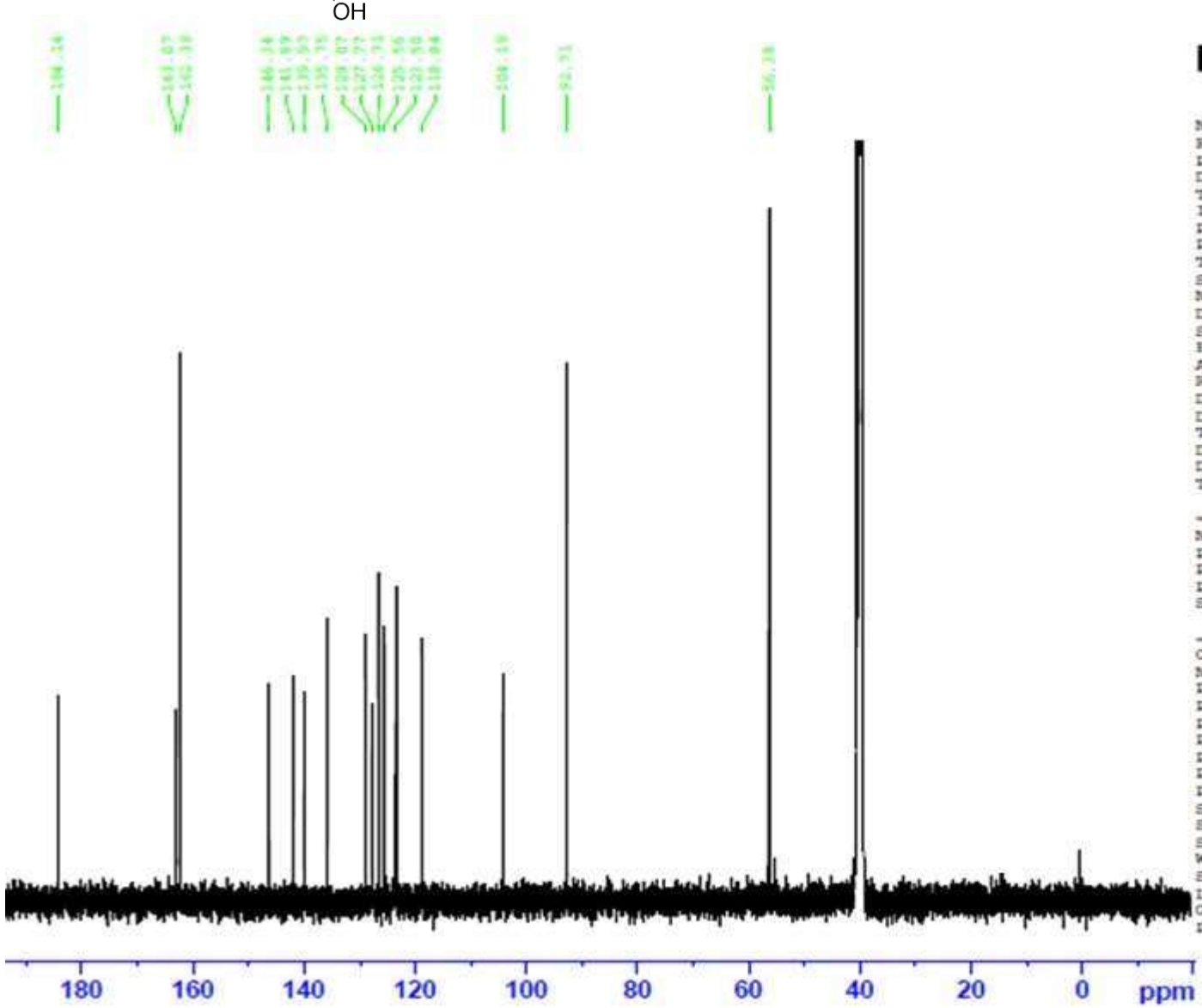
BRUKER

NAME	Audrey Isabelle
EXPNO	34
PROCNO	1
Date_	20190522
Time	13.29
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



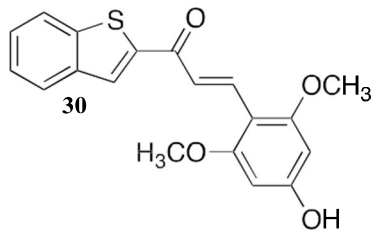
30



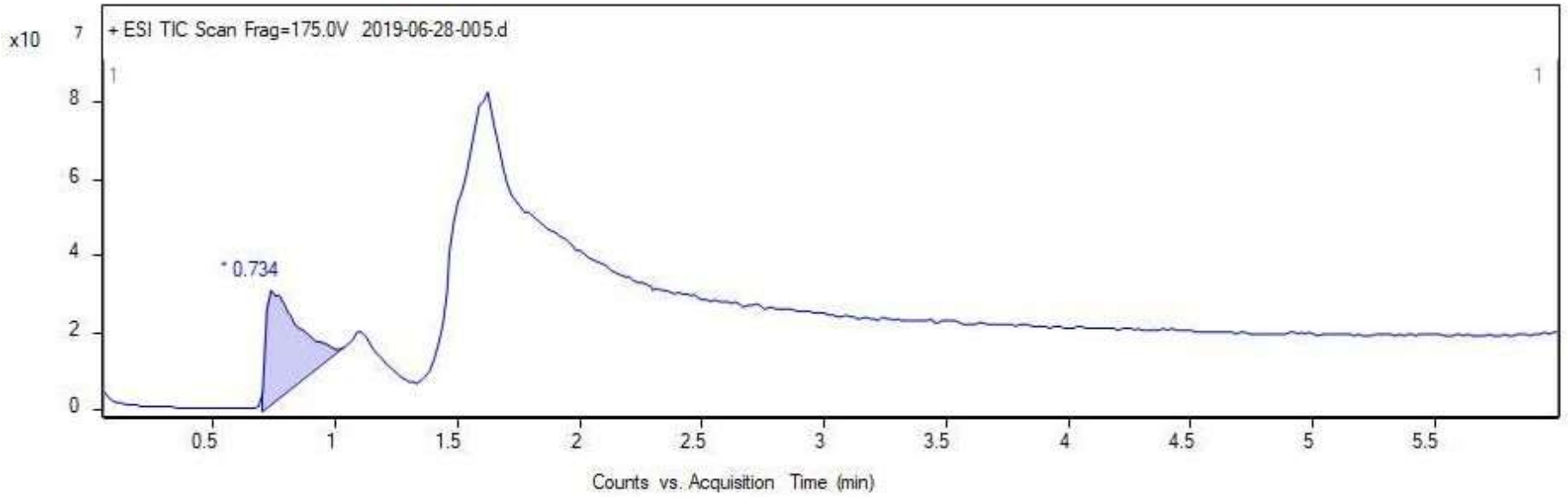
BRUKER

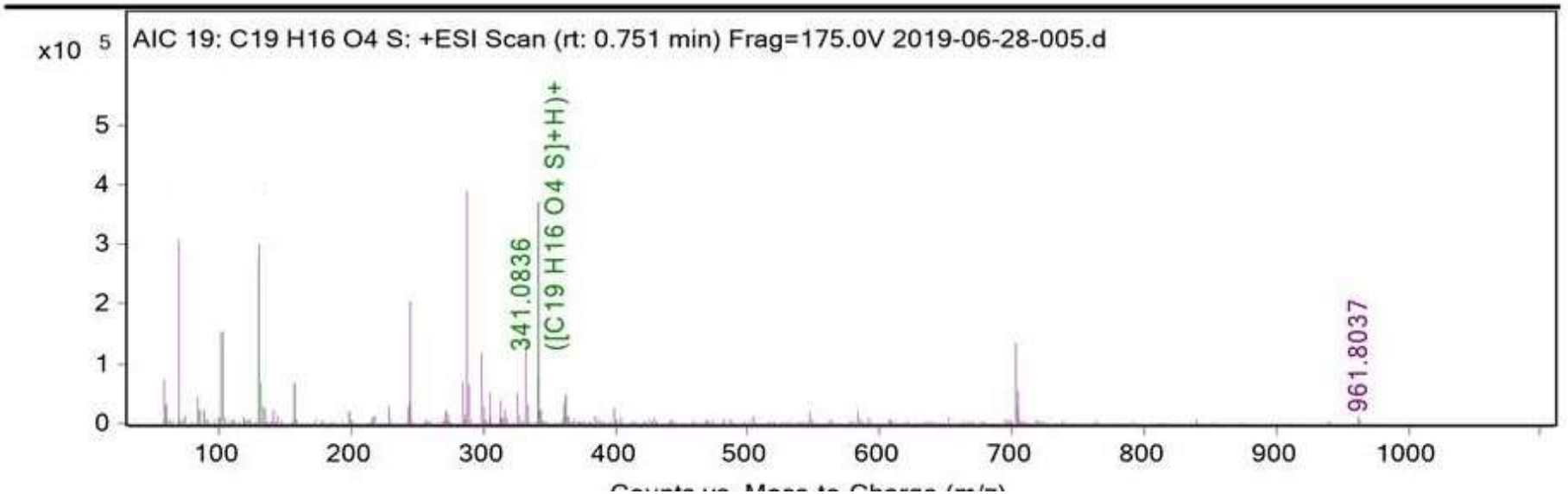
NAME	Audrey Isabelle	
EXPNO	36	
PROCNO	1	
Date_	20190523	
Time	20.37	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	DMSO	
NS	10000	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631968	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS

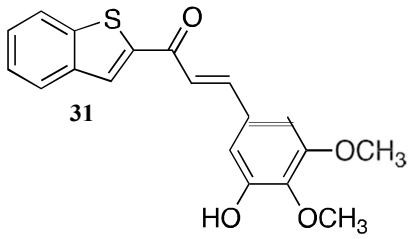

S
O
OCH3
H3CO
OH

30

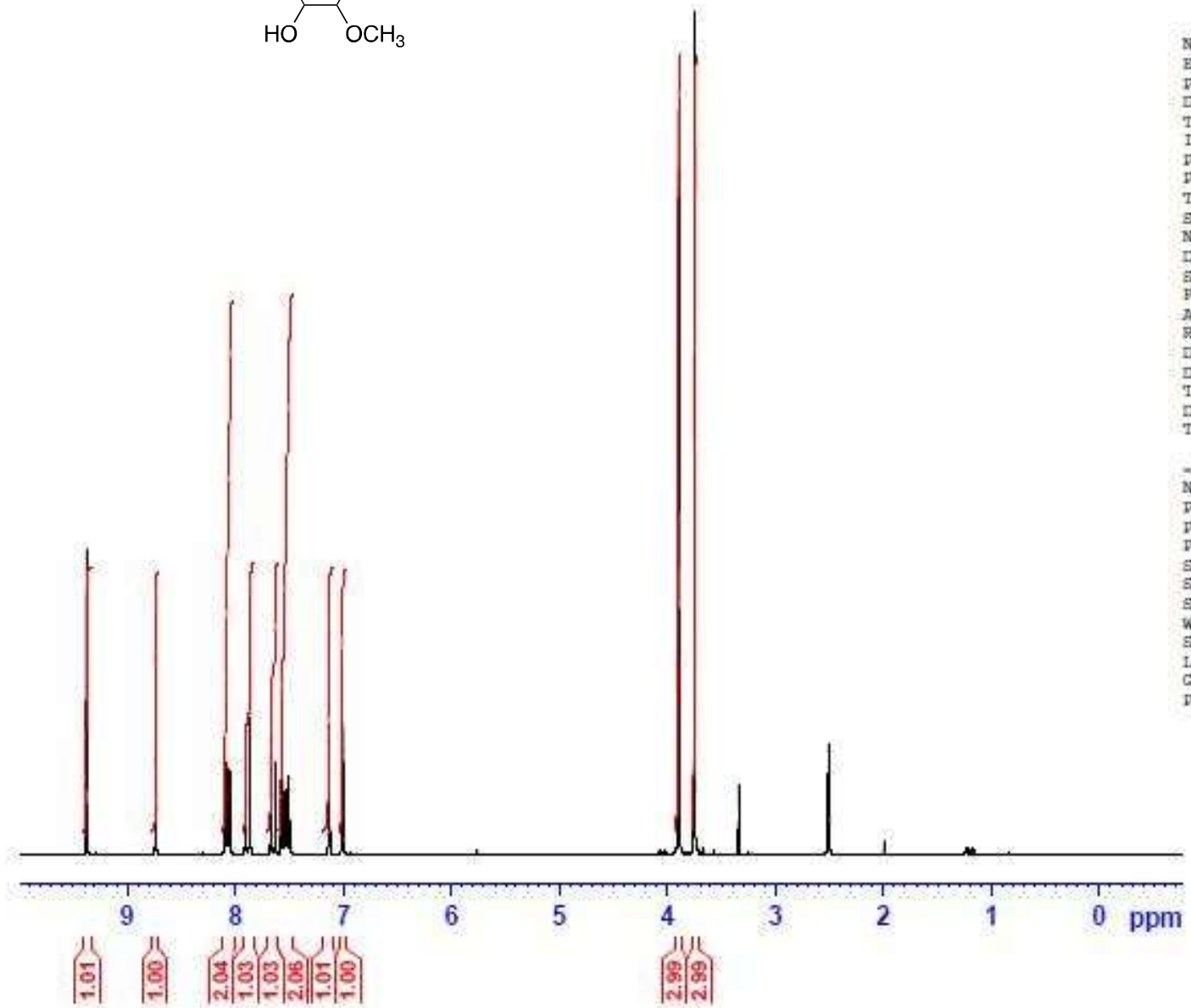

x10 7
+ ESI TIC Scan Frag=175.0V 2019-06-28-005.d
1
1
8
6
4
2
0
* 0.734
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Counts vs. Acquisition Time (min)


x10 5
AIC 19: C19 H16 O4 S: +ESI Scan (rt: 0.751 min) Frag=175.0V 2019-06-28-005.d
5
4
3
2
1
0
341.0836
([C19 H16 O4 S]+H)+
961.8037
100
200
300
400
500
600
700
800
900
1000

^{1}H NMR



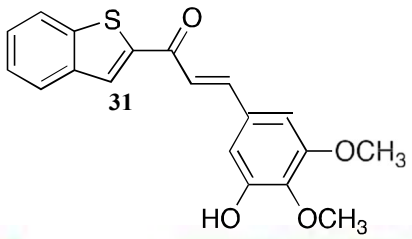
31



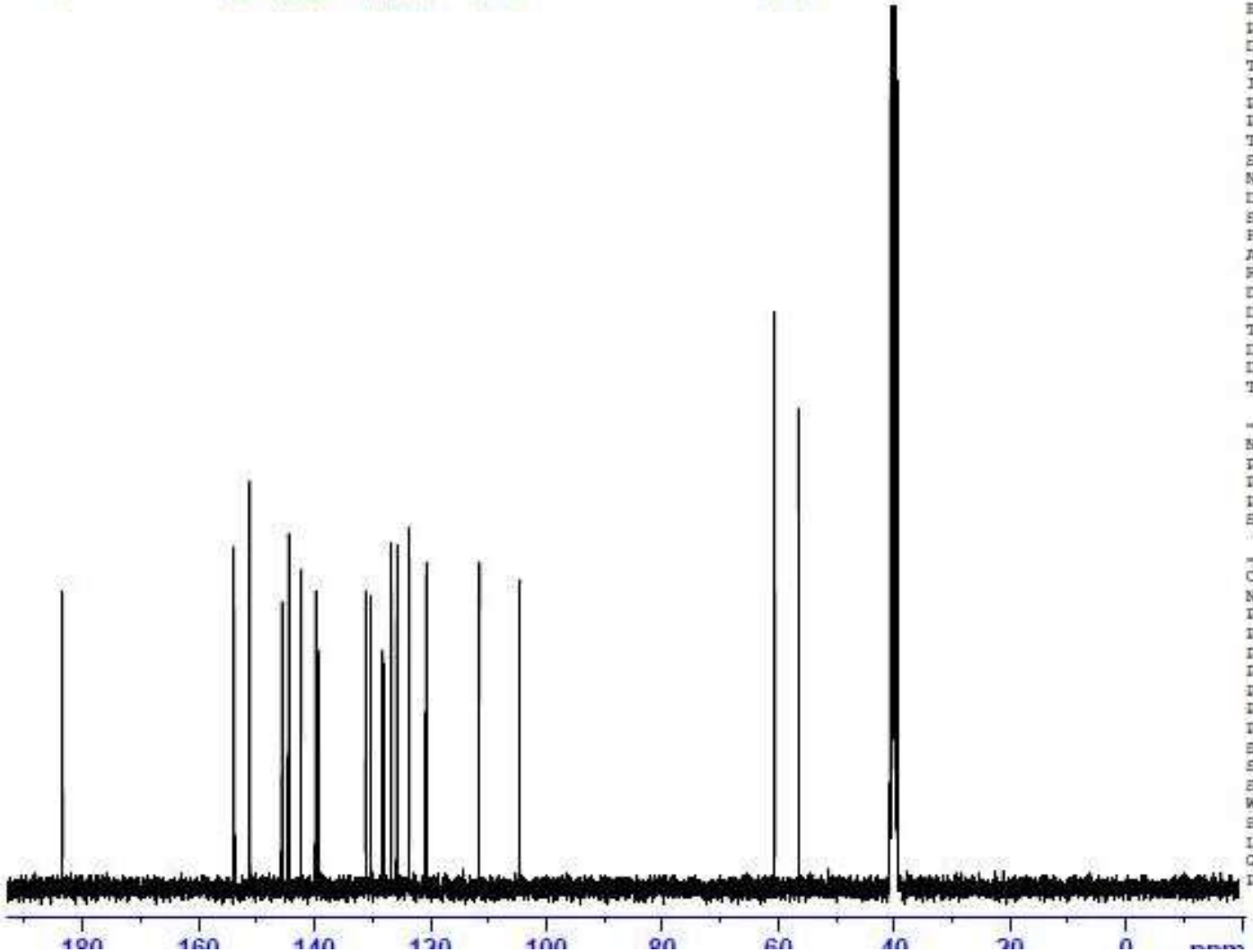
BRUKER

NAME	Audrey Isabelle
EXPNO	89
PROCNO	1
Date_	20190625
Time	8.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	101
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



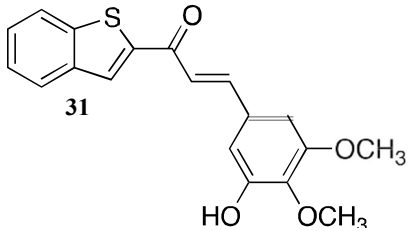
31



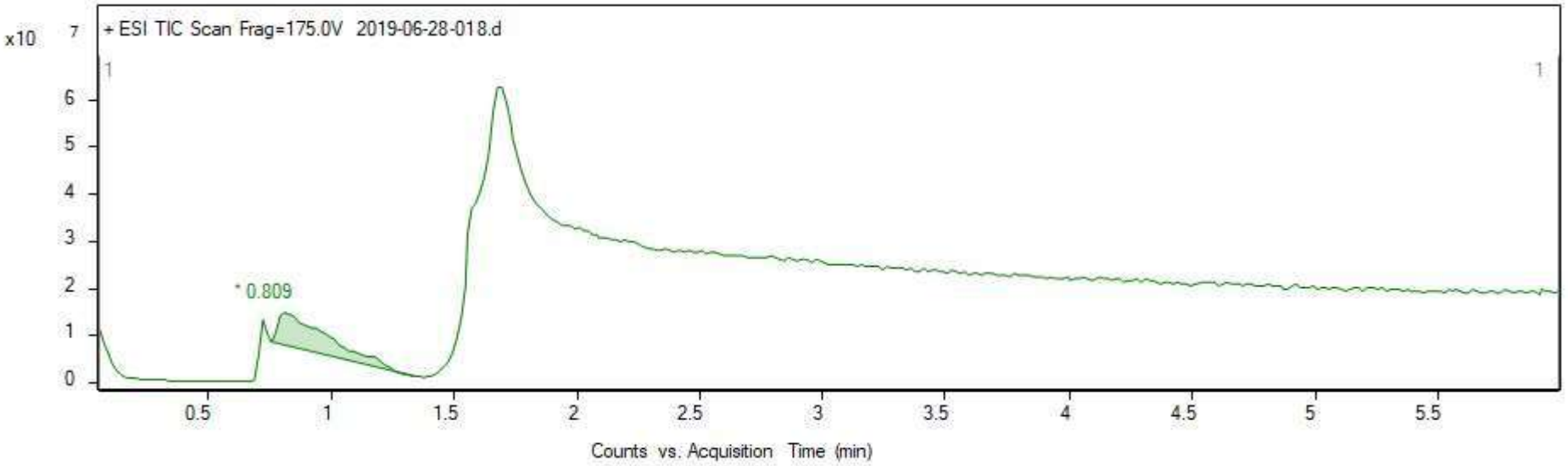
BRUKER

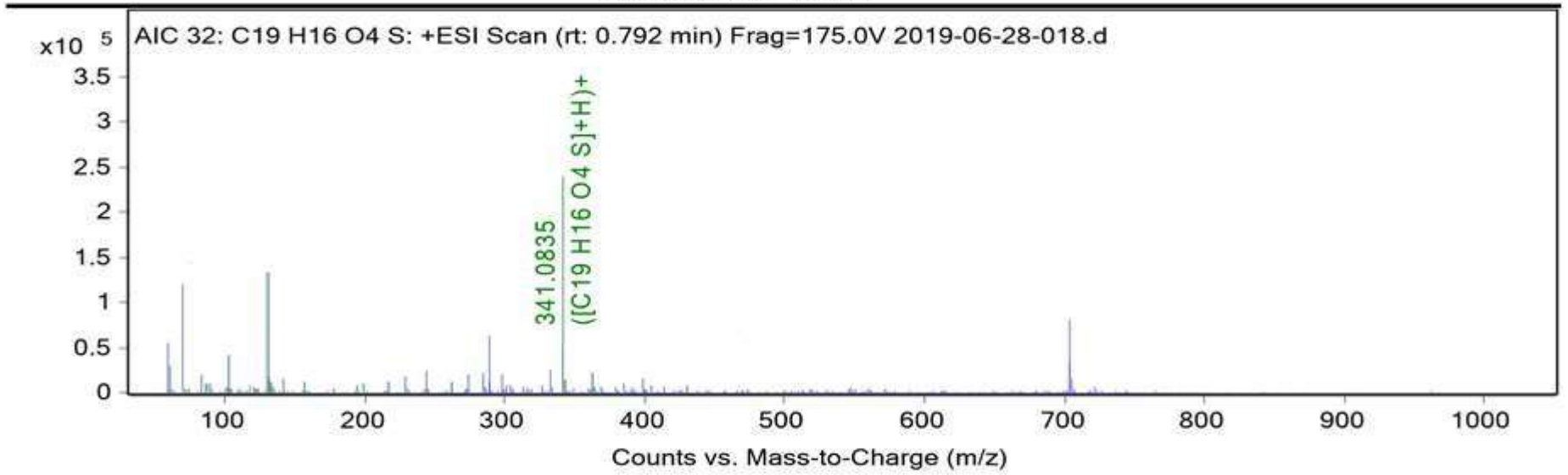
NAME	Audrey Isabelle	
EXPNO	91	
PROCNO	1	
Date_	20190625	
Time	10.03	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	DMSO	
NS	1574	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS

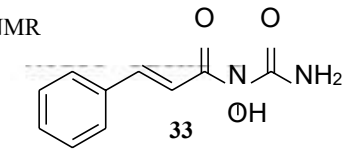

S
O
OCH3
HO
OCH3

31

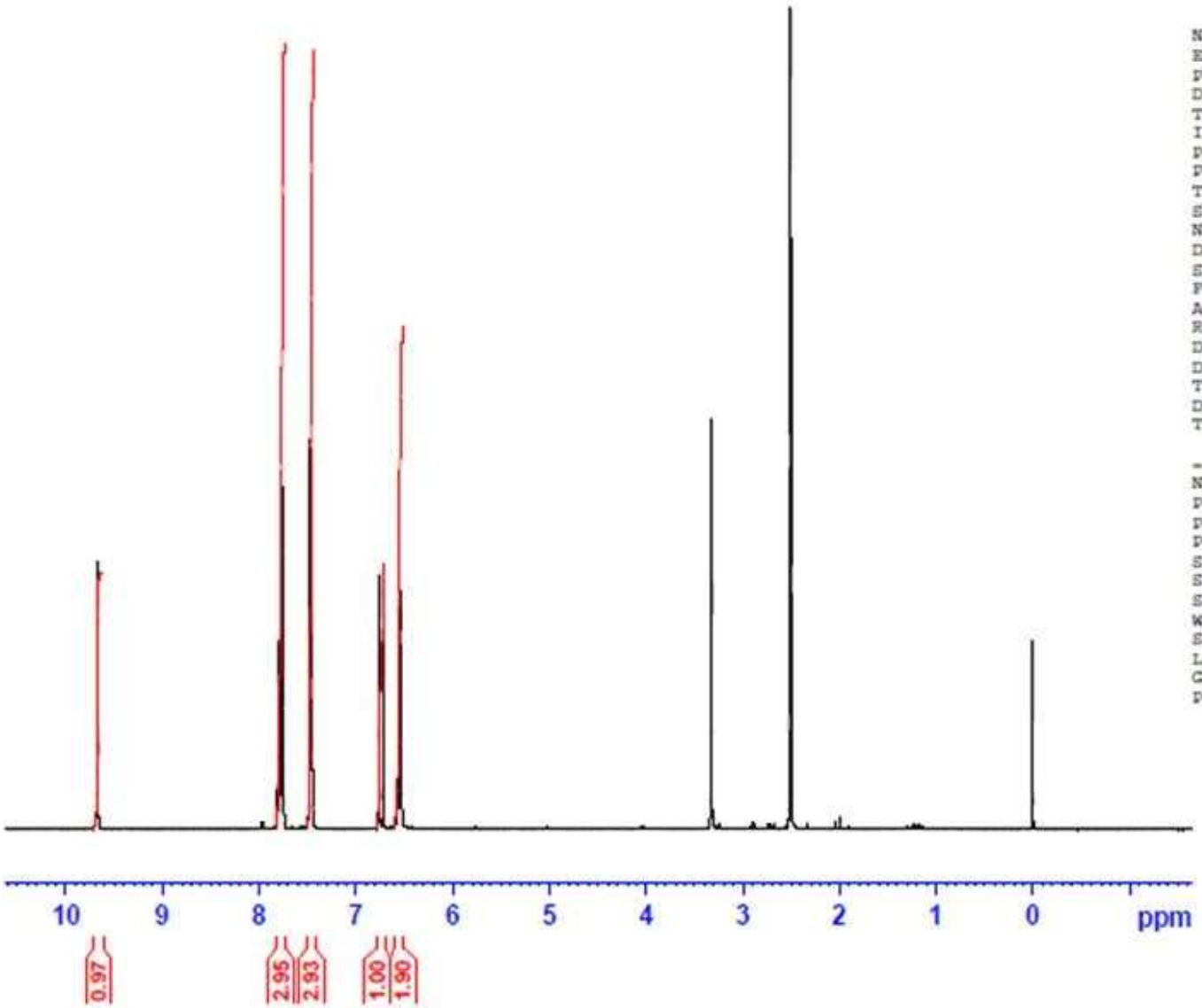

x10 7
+ ESI TIC Scan Frag=175.0V 2019-06-28-018.d
1
1
6
5
4
3
2
1
0
* 0.809
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Counts vs. Acquisition Time (min)


x10 5
AIC 32: C19 H16 O4 S: +ESI Scan (rt: 0.792 min) Frag=175.0V 2019-06-28-018.d
3.5
3
2.5
2
1.5
1
0.5
0
341.0835
([C19 H16 O4 S]+H)+
100
200
300
400
500
600
700
800
900
1000
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



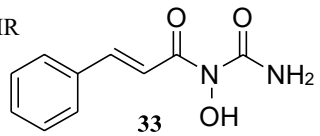
33



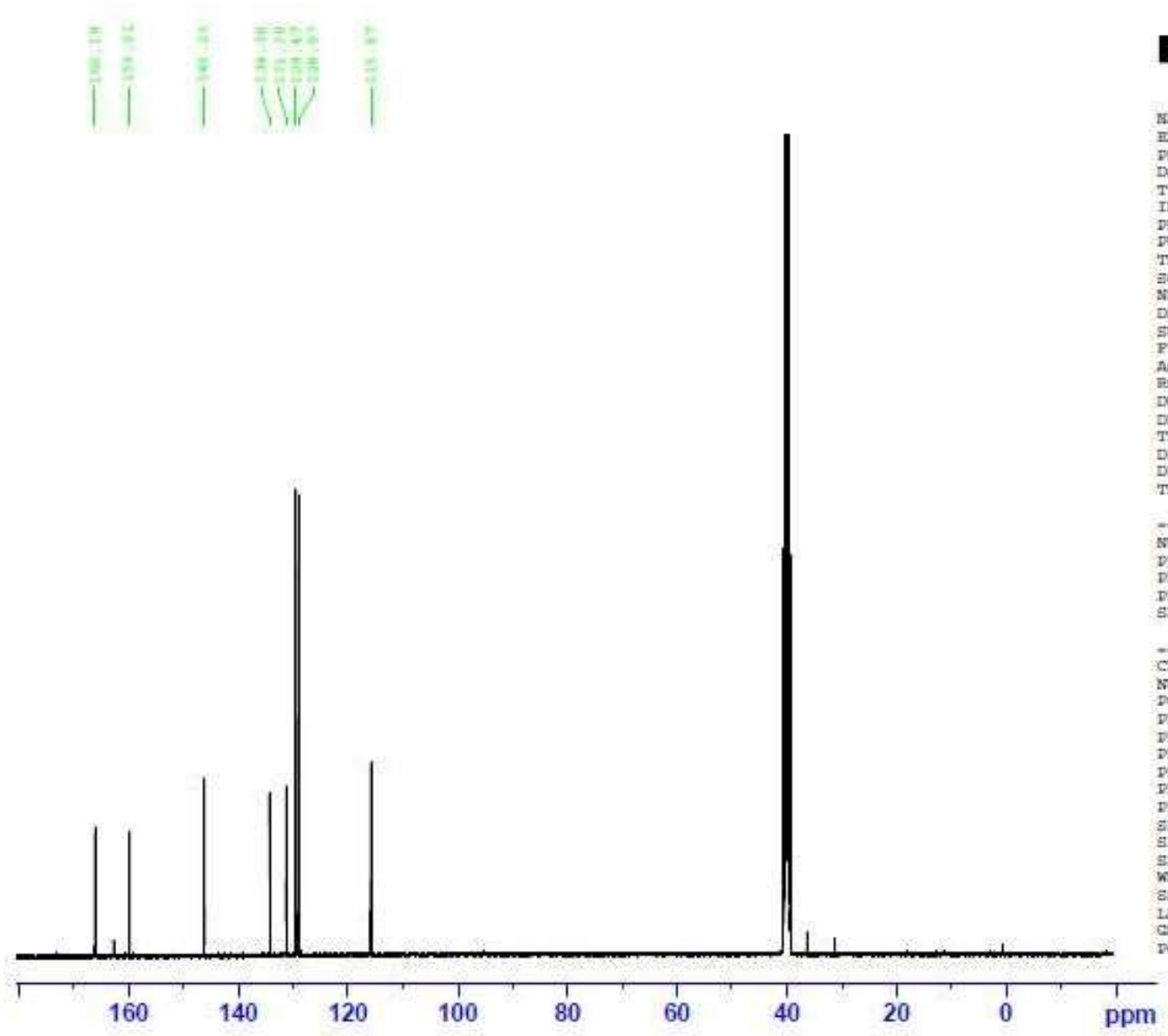
BRUKER

NAME	Moh RX
EXPNO	396
PROCNO	1
Date_	20190522
Time	13.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	128
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
-------- CHANNEL f1 --------	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



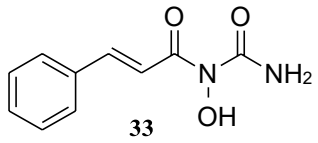
33



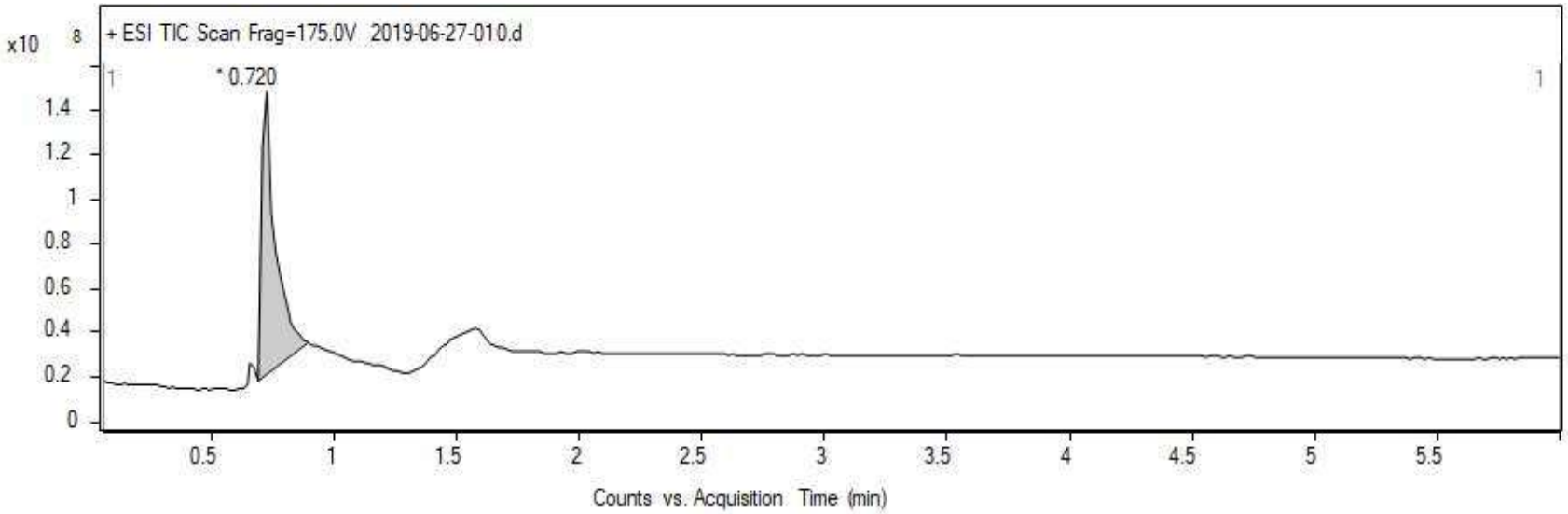
BRUKER

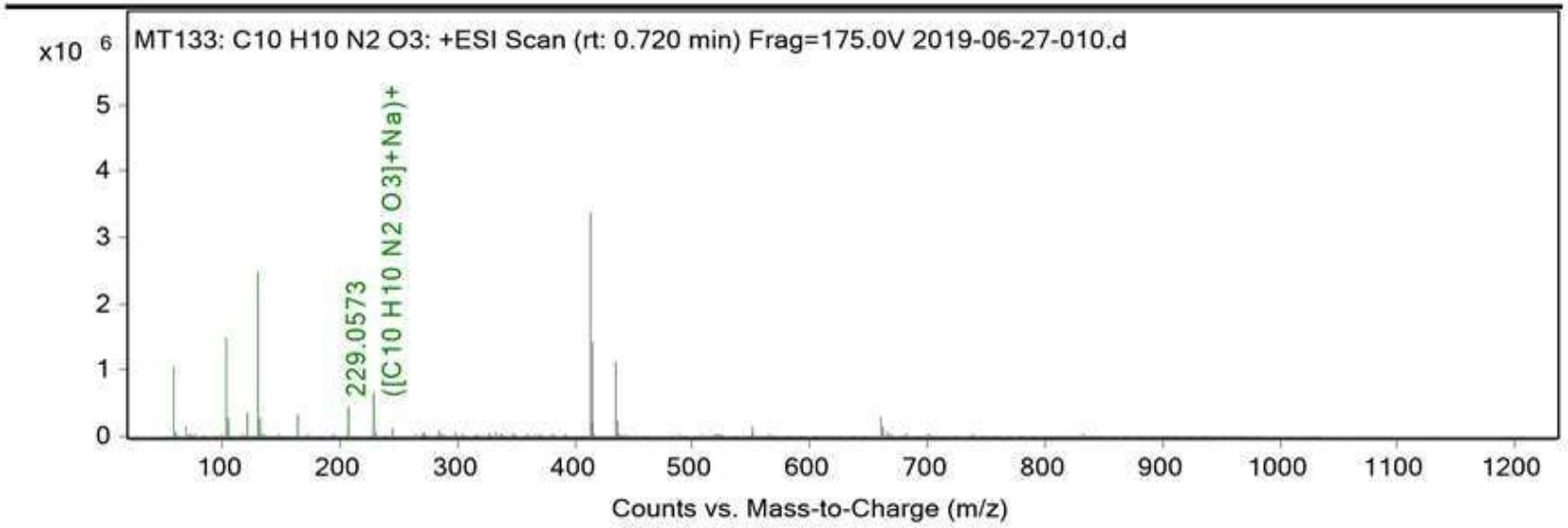
NAME	Moh RX
EXPNO	400
PROCNO	1
Date_	20190525
Time	4.14
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	12000
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631968 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

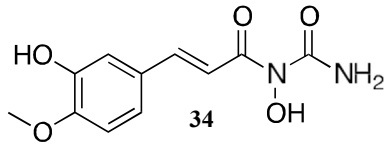

O
O
N
NH2
OH

33

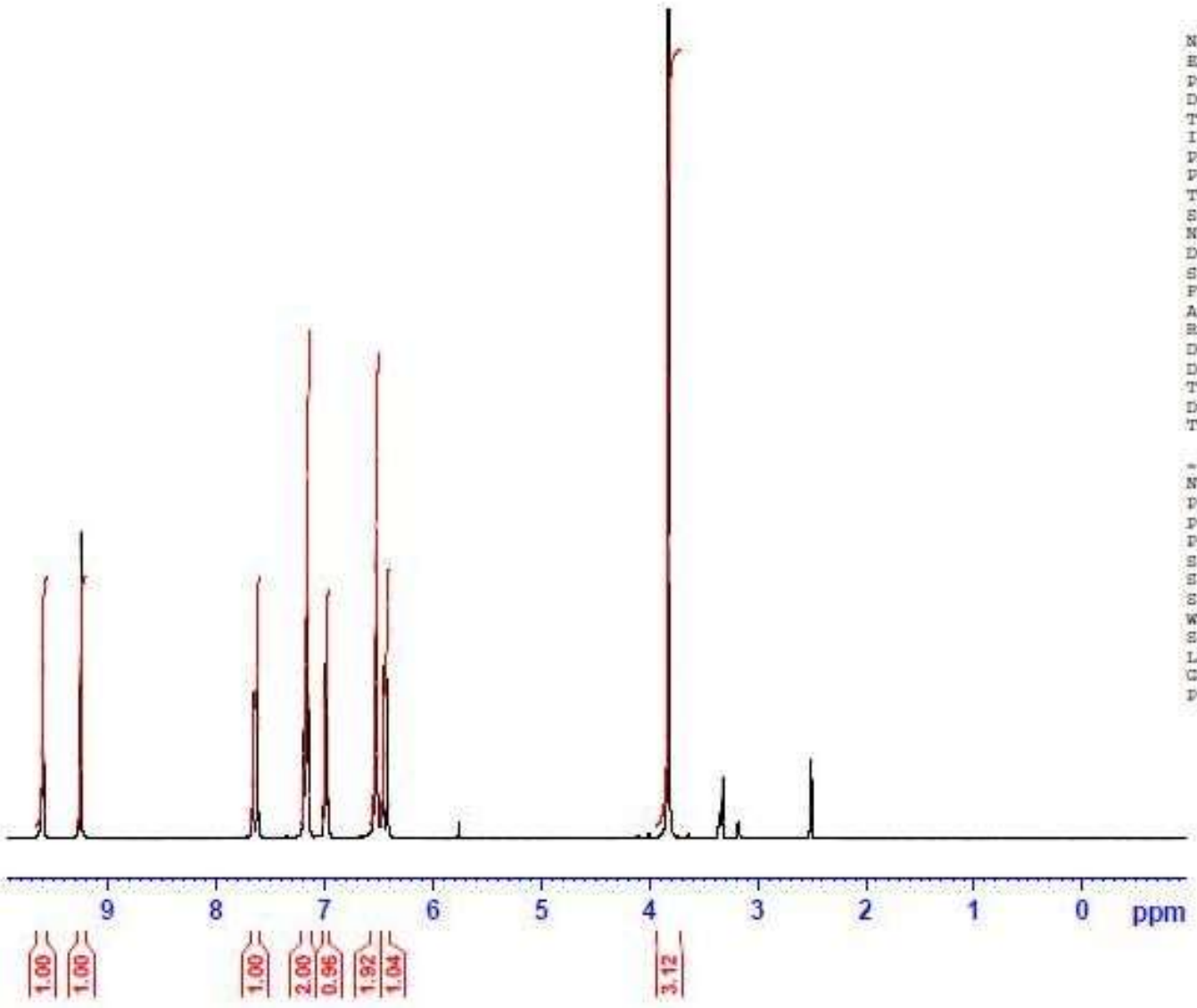

x10 8
+ ESI TIC Scan Frag=175.0V 2019-06-27-010.d
* 0.720
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Counts vs. Acquisition Time (min)


x10 6
MT133: C10 H10 N2 O3: +ESI Scan (rt: 0.720 min) Frag=175.0V 2019-06-27-010.d
229.0573
([C10 H10 N2 O3]+Na)+
5
4
3
2
1
0
100
200
300
400
500
600
700
800
900
1000
1100
1200
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



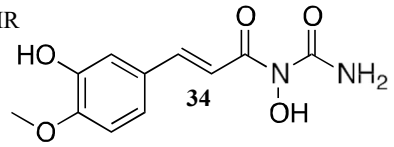
34



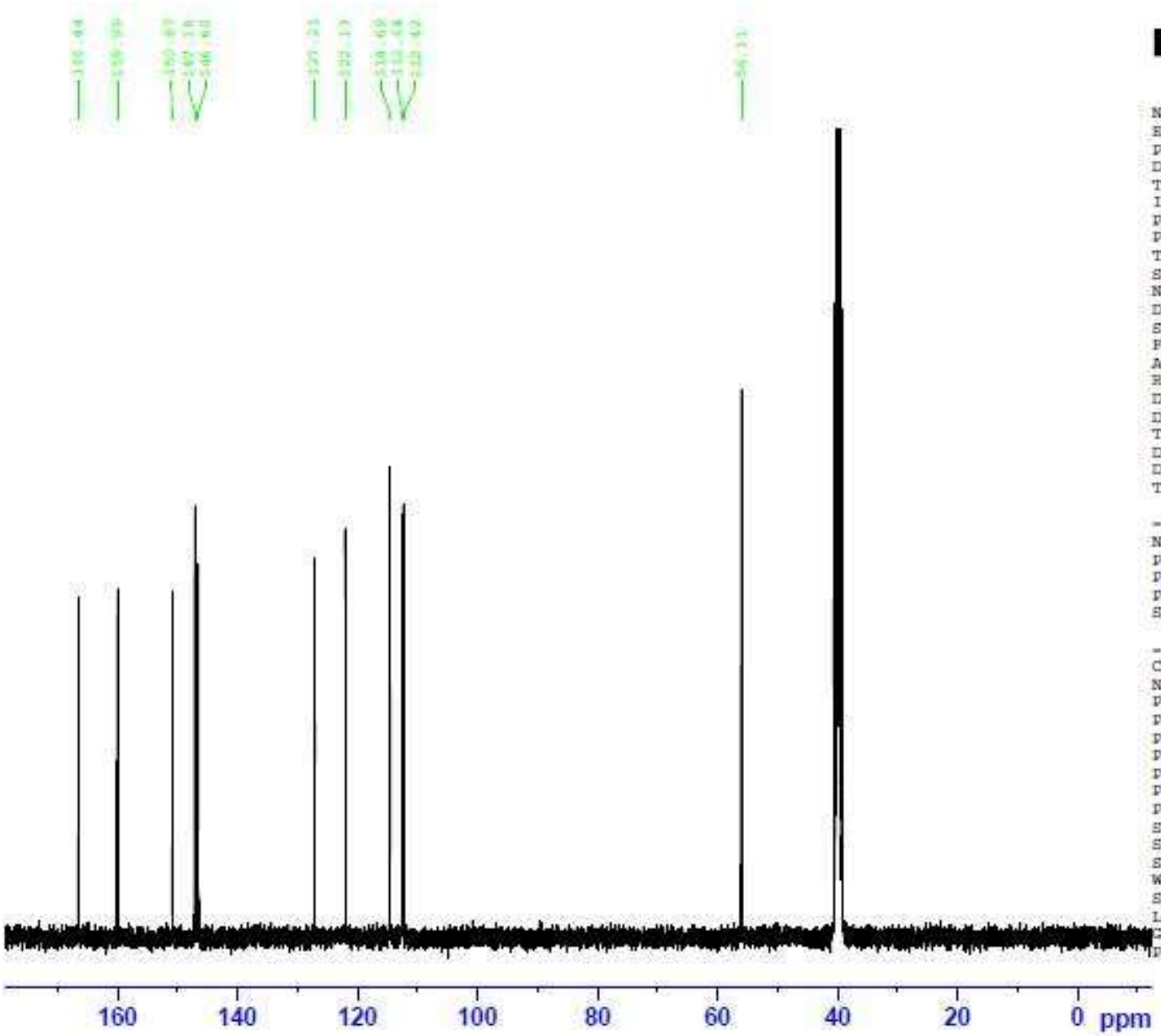
BRUKER

NAME	Audrey Isabelle
EXPNO	103
PROCNO	1
Date_	20190705
Time	7.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	101
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



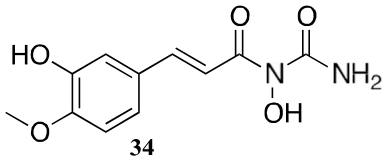
34



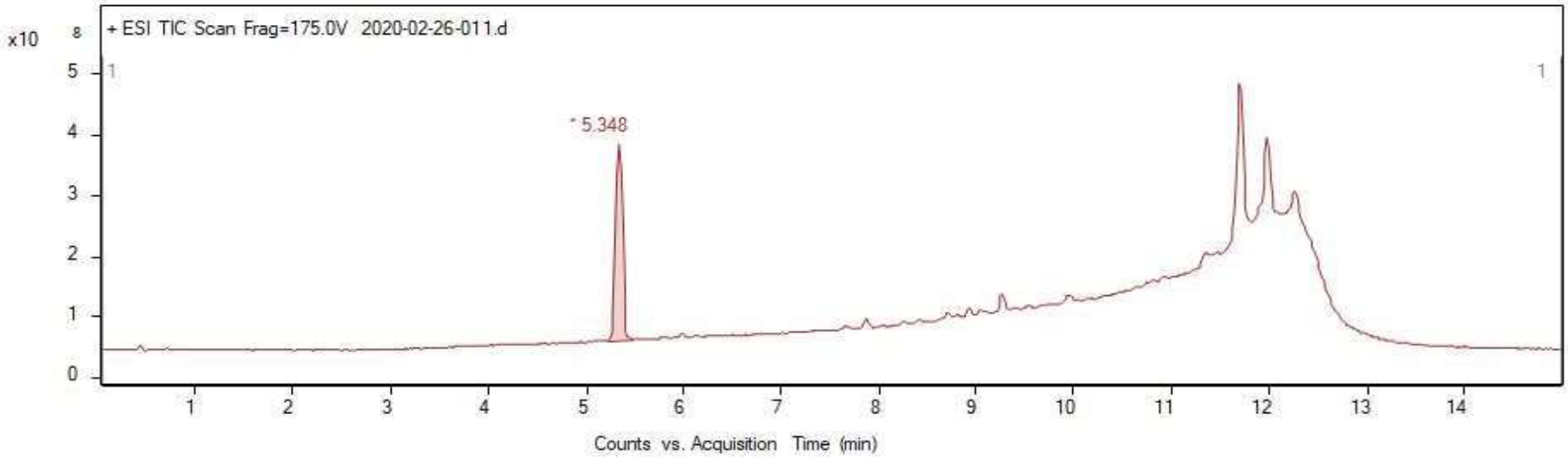
BRUKER

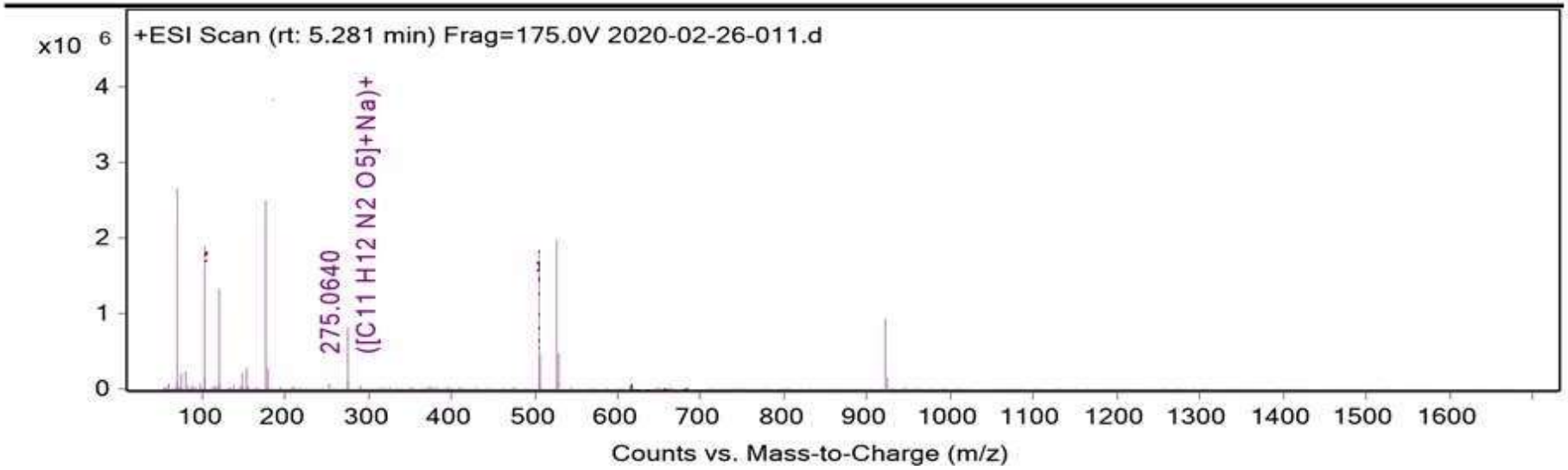
NAME	Audrey Isabelle
EXPNO	105
PROCNO	1
Date_	20190705
Time	9.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	2136
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

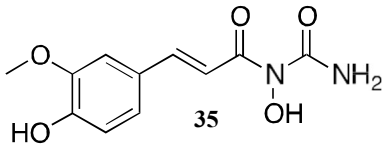

HO
O
O
N
NH2
OH
O

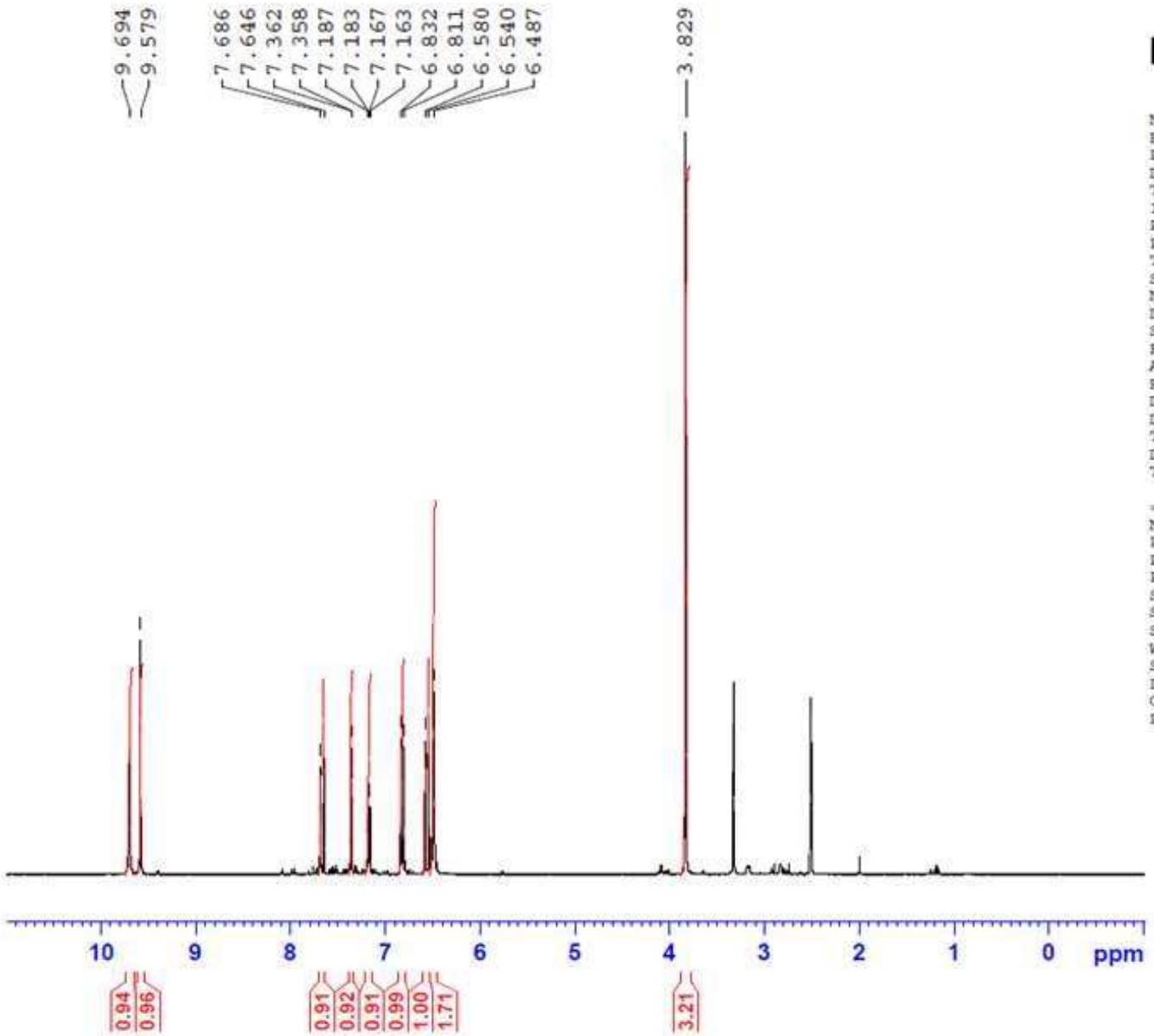
34


x10 8
+ ESI TIC Scan Frag=175.0V 2020-02-26-011.d
5.348
Counts vs. Acquisition Time (min)


x10 6
+ESI Scan (rt: 5.281 min) Frag=175.0V 2020-02-26-011.d
275.0640
([C11 H12 N2 O5]+Na)+
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR

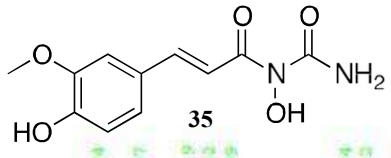




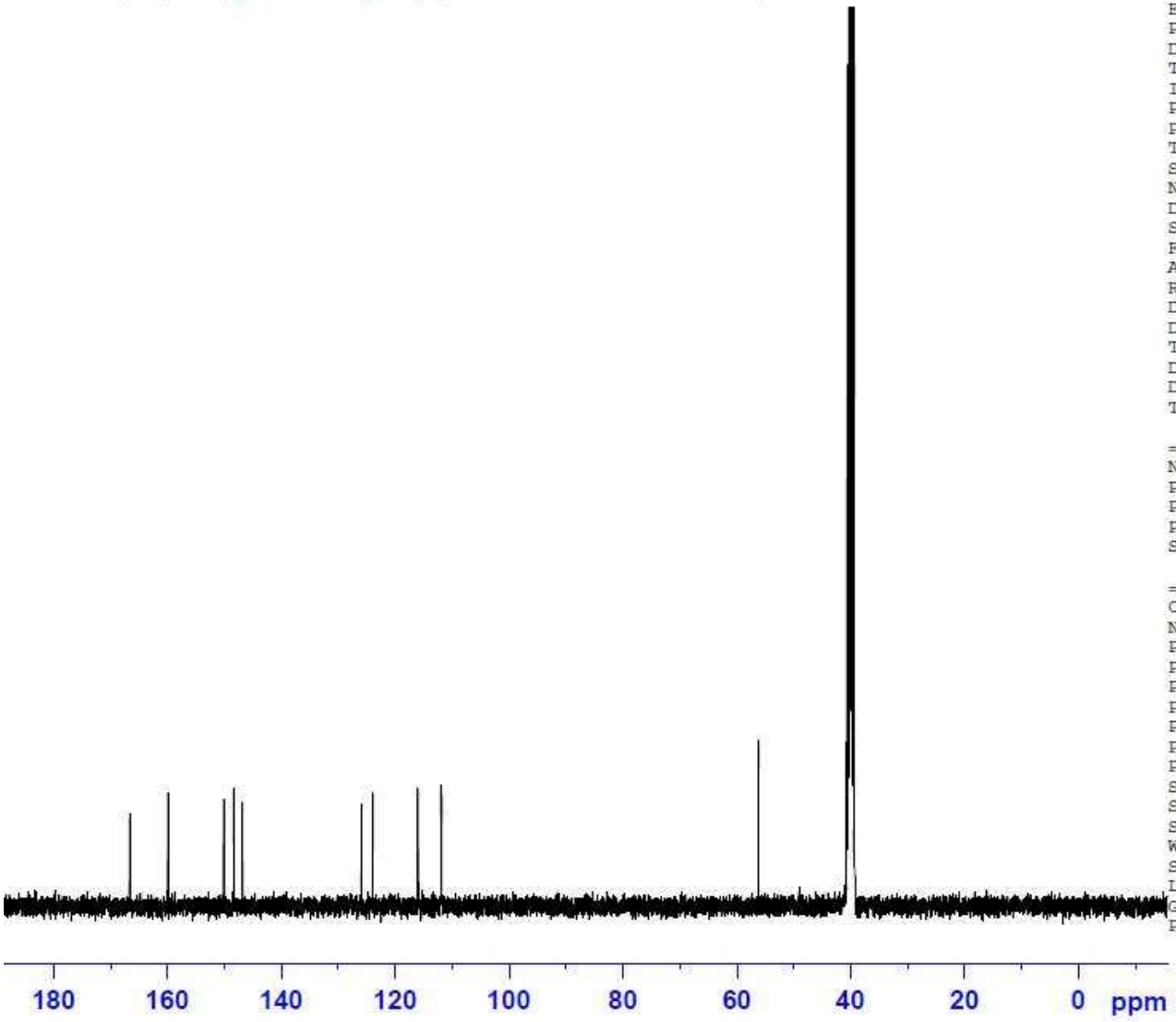
BRUKER

NAME	Audrey Isabelle
EXPNO	109
PROCNO	1
Date_	20190708
Time	8.44
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR

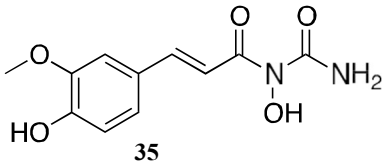


35

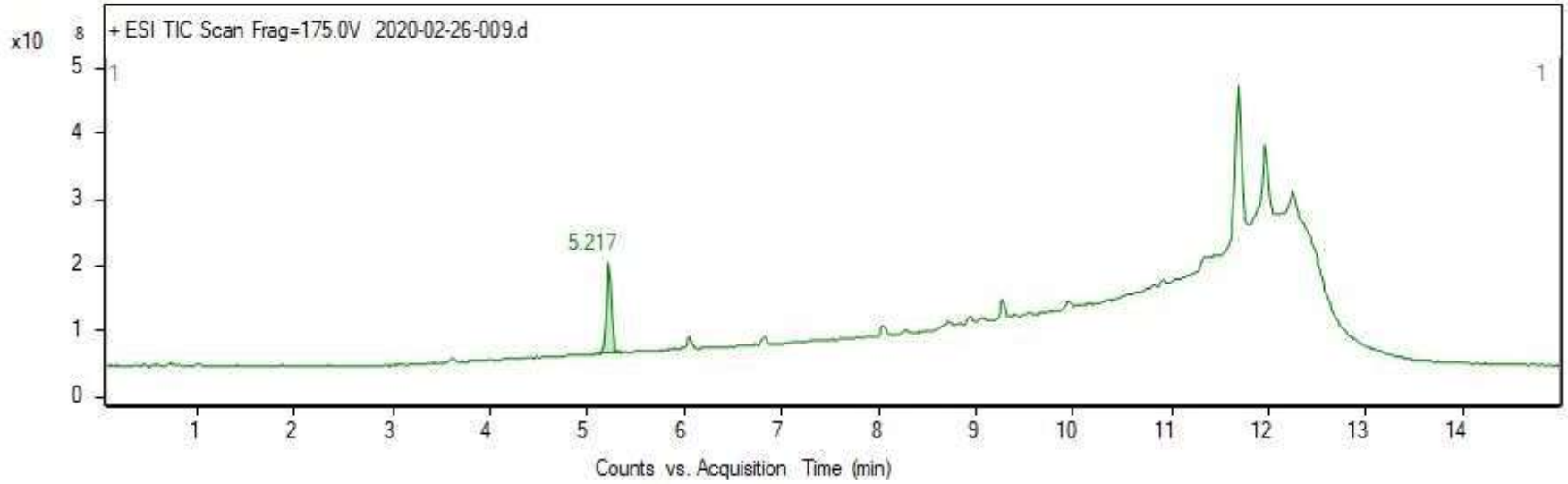


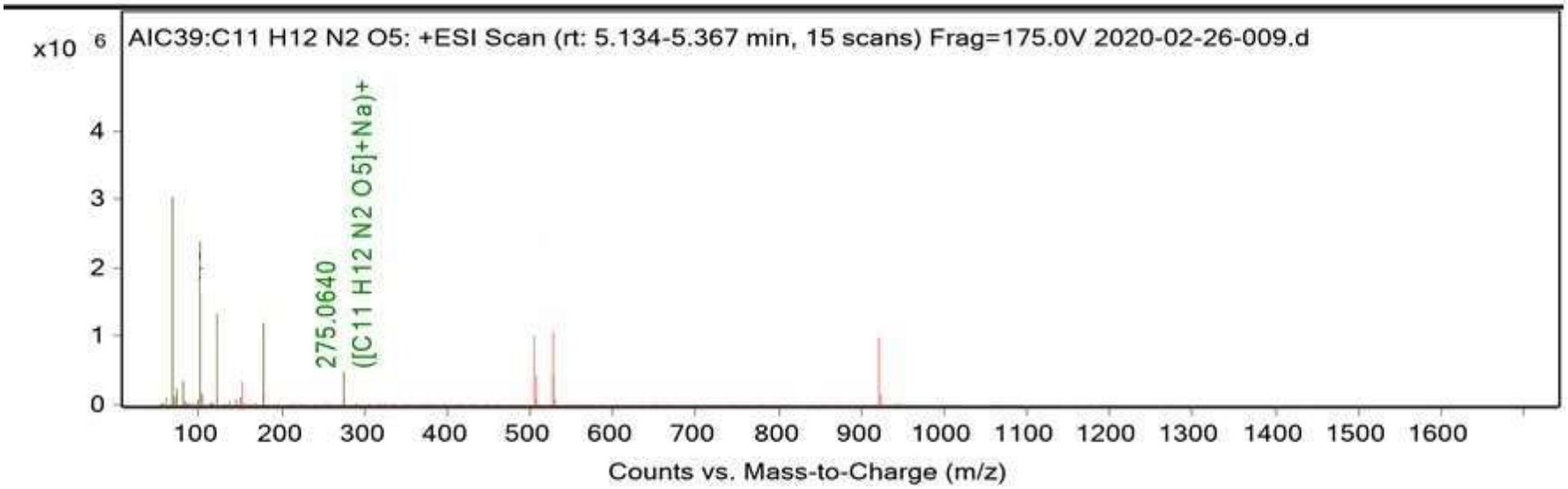

```
NAME        Audrey Isabelle
EXPNO                   111
PROCNO                    1
Date_              20190708
Time                  10.57
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                     2086
DS                        4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                      203
DW                 20.800 usec
DE                  6.50 usec
TE                  298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   9.90 usec
PL1                 -1.90 dB
PL1W         56.02249908 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz65
NUC2                    1H
PCPD2               80.00 usec
PL2                  0.30 dB
PL12                15.40 dB
PL13                18.40 dB
PL2W         11.25229836 W
PL12W         0.34772930 W
PL13W         0.17427748 W
SFO2        400.1316005 MHz
SI                  32768
SF          100.6127690 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

HRMS

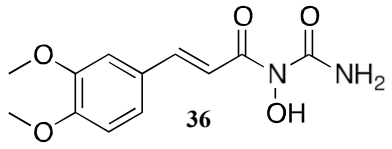

O
O
O
N
NH2
OH
HO

35

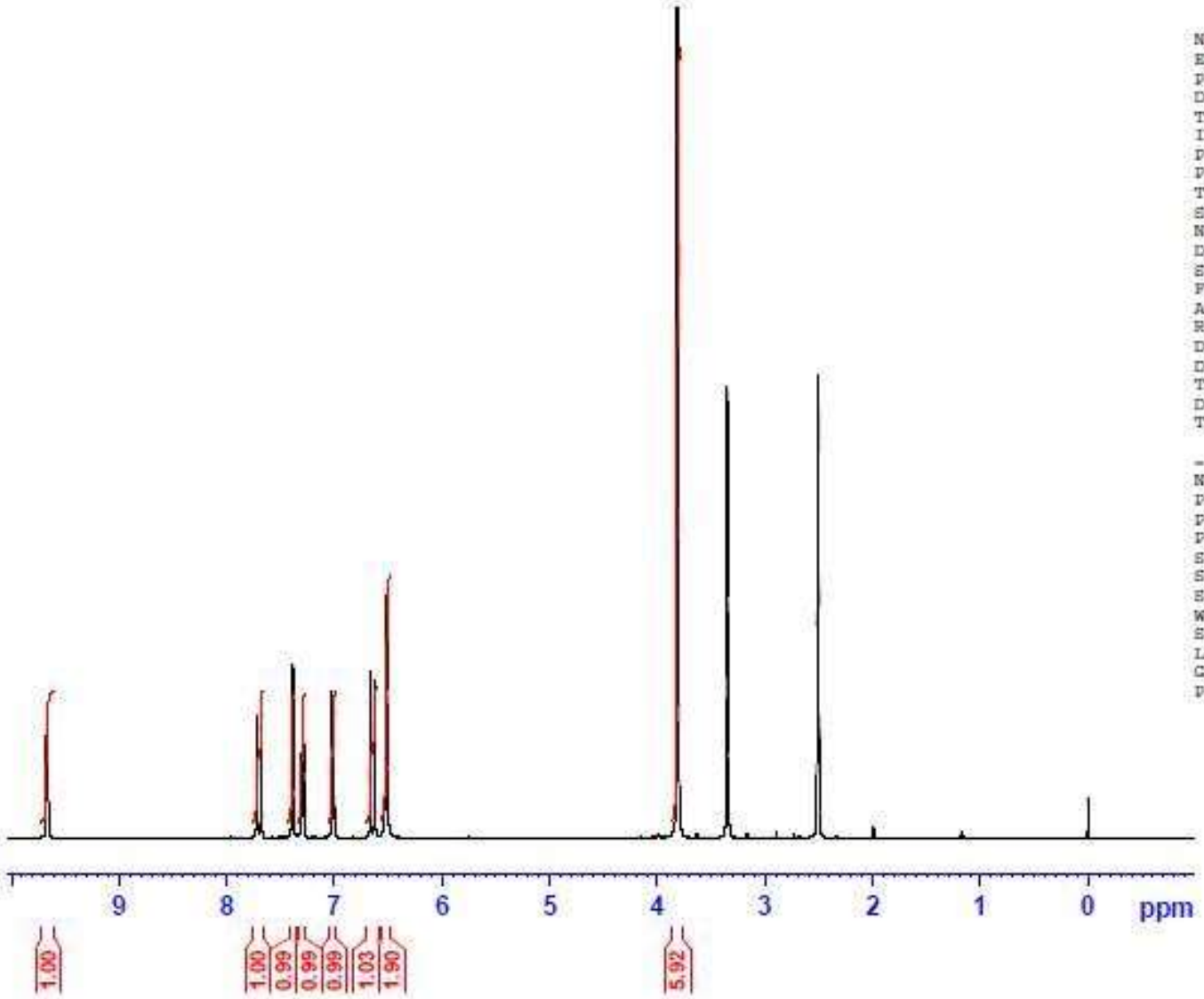

x10 8
+ ESI TIC Scan Frag=175.0V 2020-02-26-009.d
5.217
Counts vs. Acquisition Time (min)


x10 6
AIC39:C11 H12 N2 O5: +ESI Scan (rt: 5.134-5.367 min, 15 scans) Frag=175.0V 2020-02-26-009.d
275.0640
([C11 H12 N2 O5]+Na)+
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



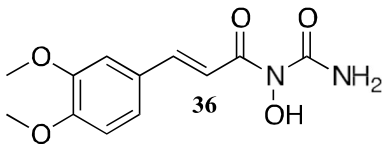
36

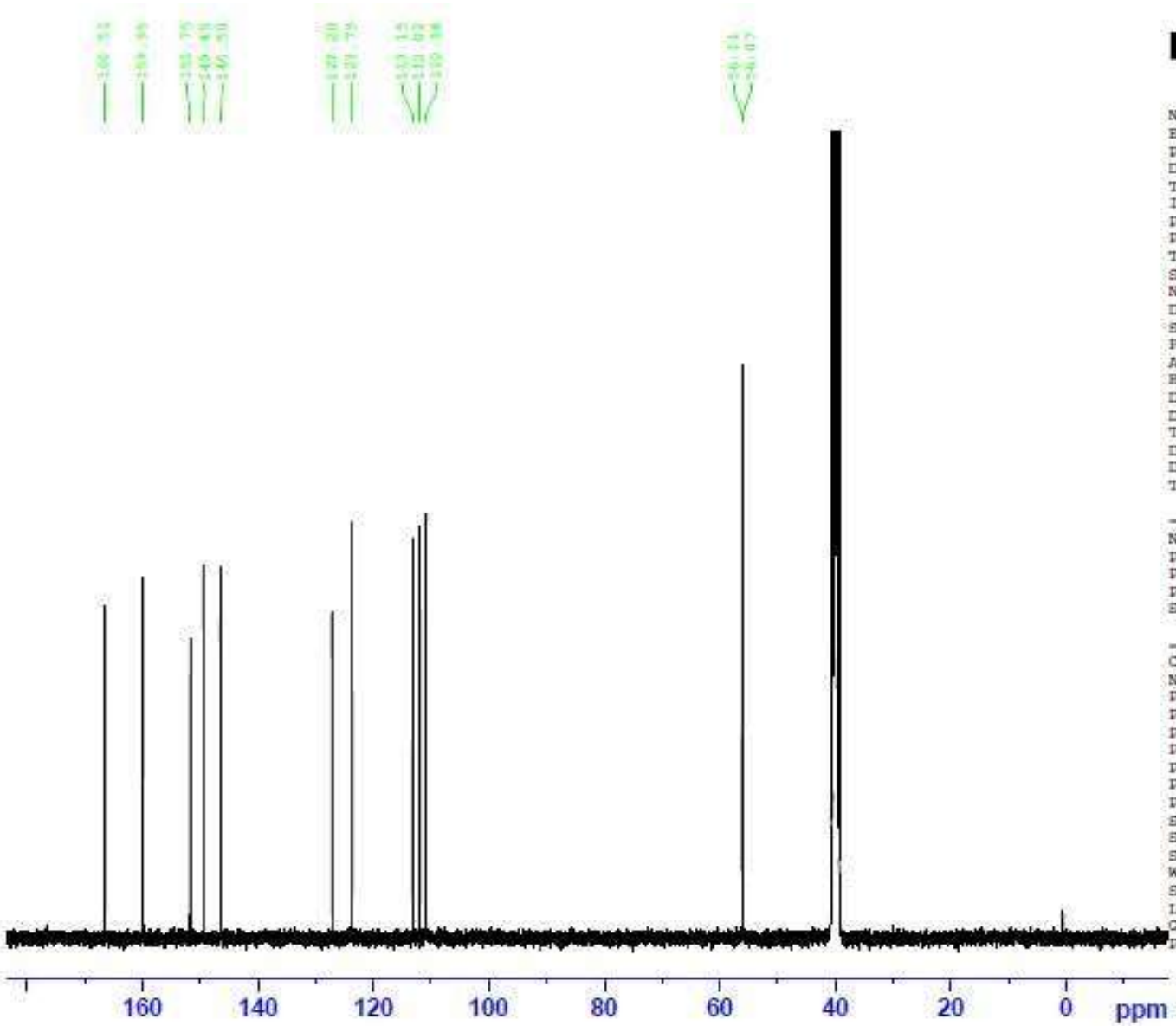


BRUKER

NAME	Audrey Isabelle
EXPNO	94
PROCNO	1
Date_	20190628
Time	16.15
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	114
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
--------	CHANNEL f1 --------
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR

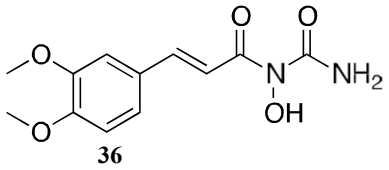




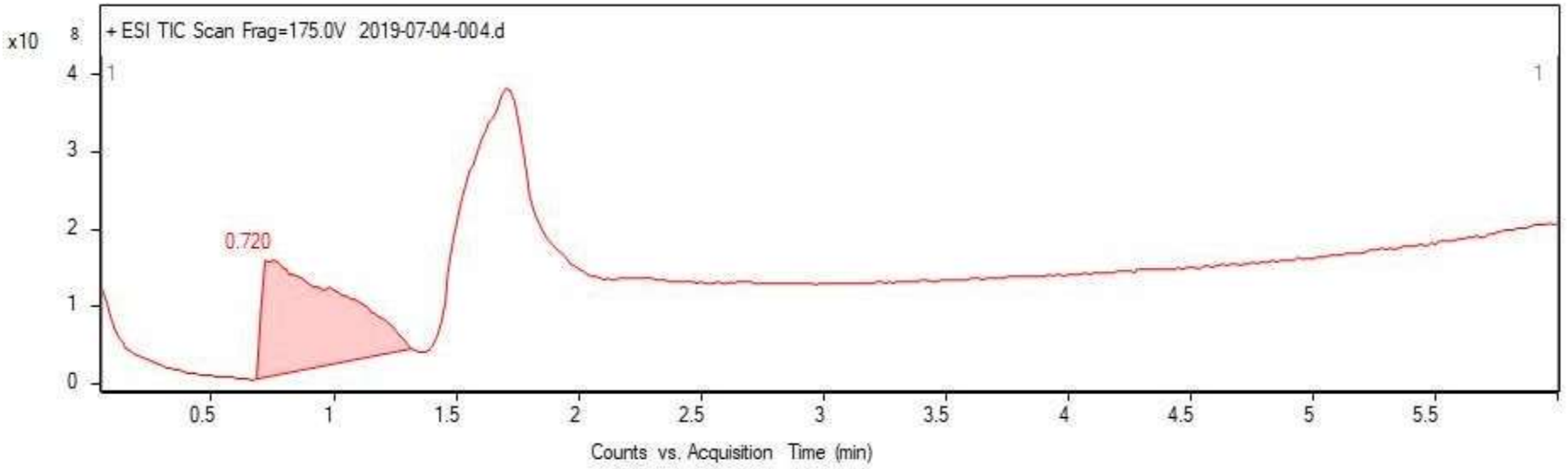
BRUKER

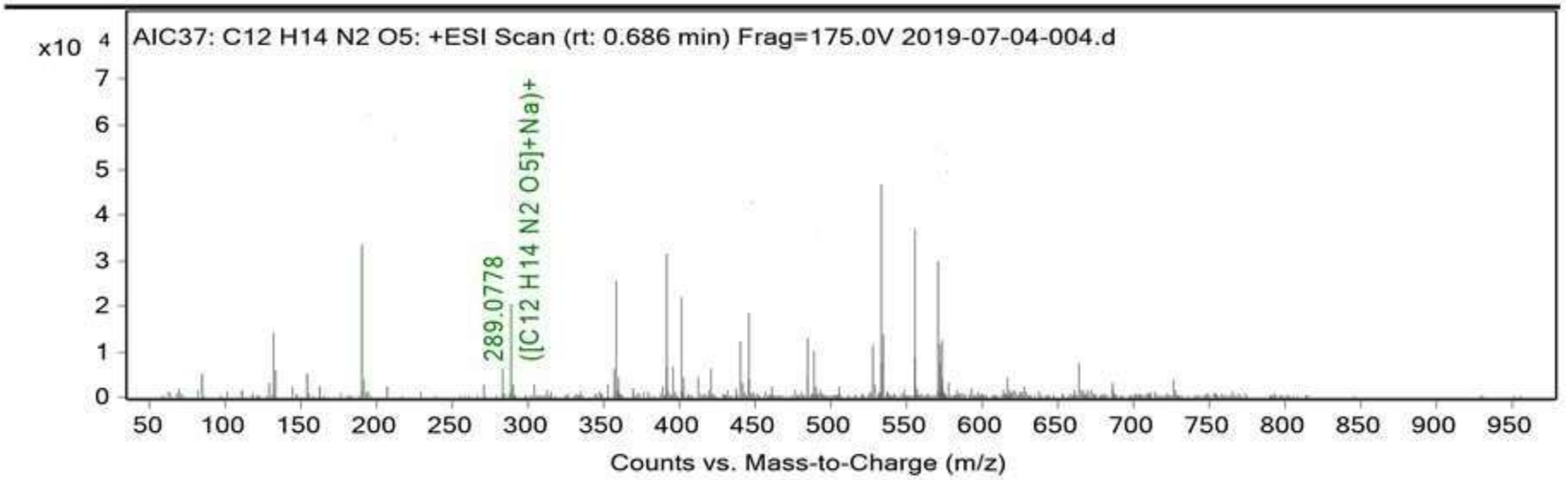
NAME	Audrey Isabelle
EXPNO	96
PROCNO	1
Date_	20190629
Time	2.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	10000
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS

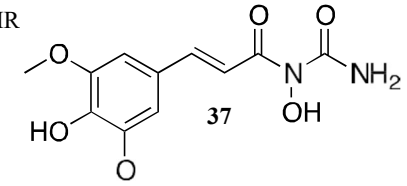

O
O
O
N
NH2
OH

36

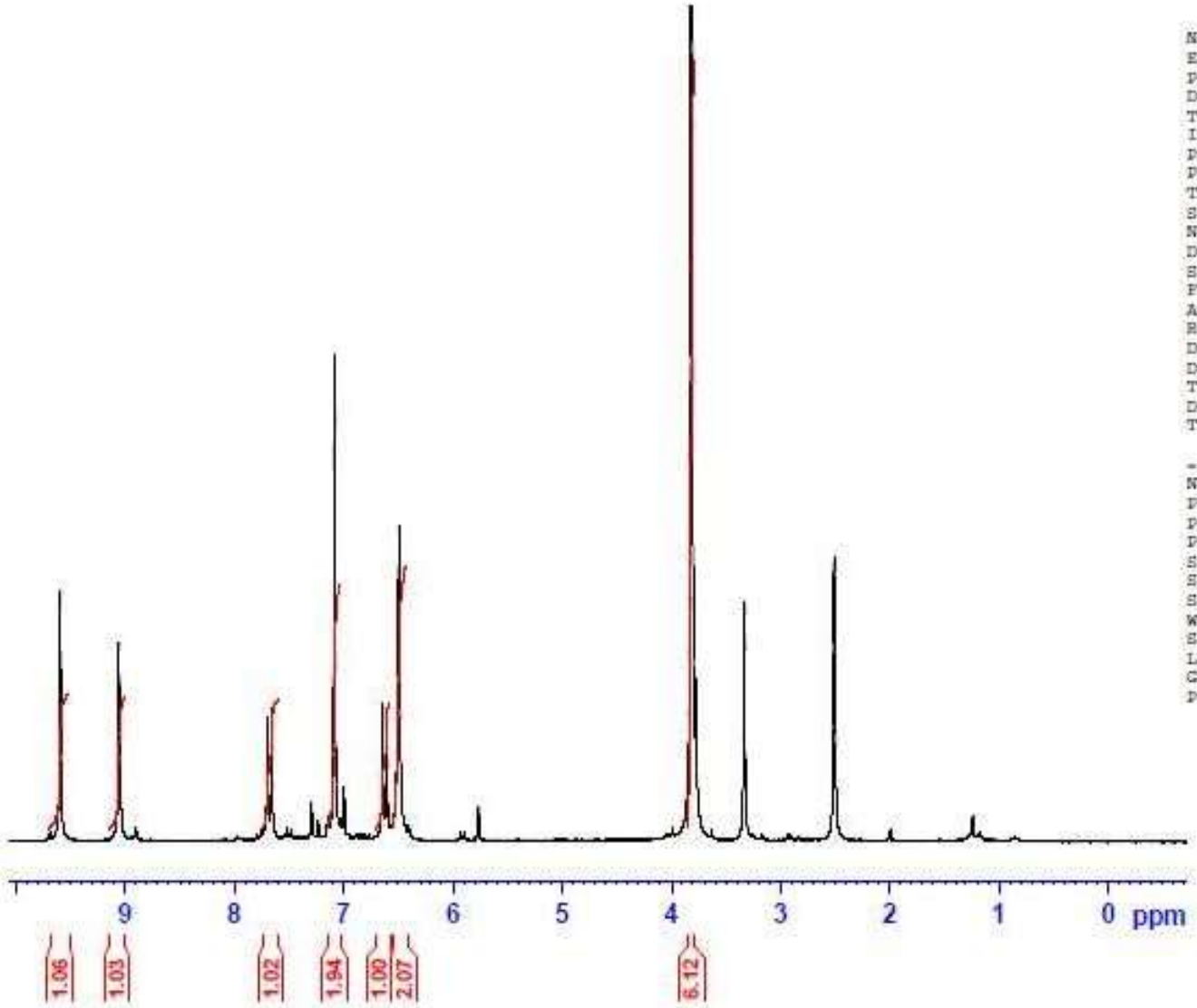

x10 8
+ ESI TIC Scan Frag=175.0V 2019-07-04-004.d
1
1
4
3
2
1
0
0.720
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Counts vs. Acquisition Time (min)


x10 4
AIC37: C12 H14 N2 O5: +ESI Scan (rt: 0.686 min) Frag=175.0V 2019-07-04-004.d
7
6
5
4
3
2
1
0
289.0778
([C12 H14 N2 O5]+Na)+
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



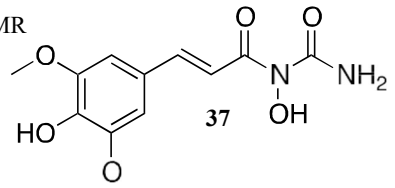
37



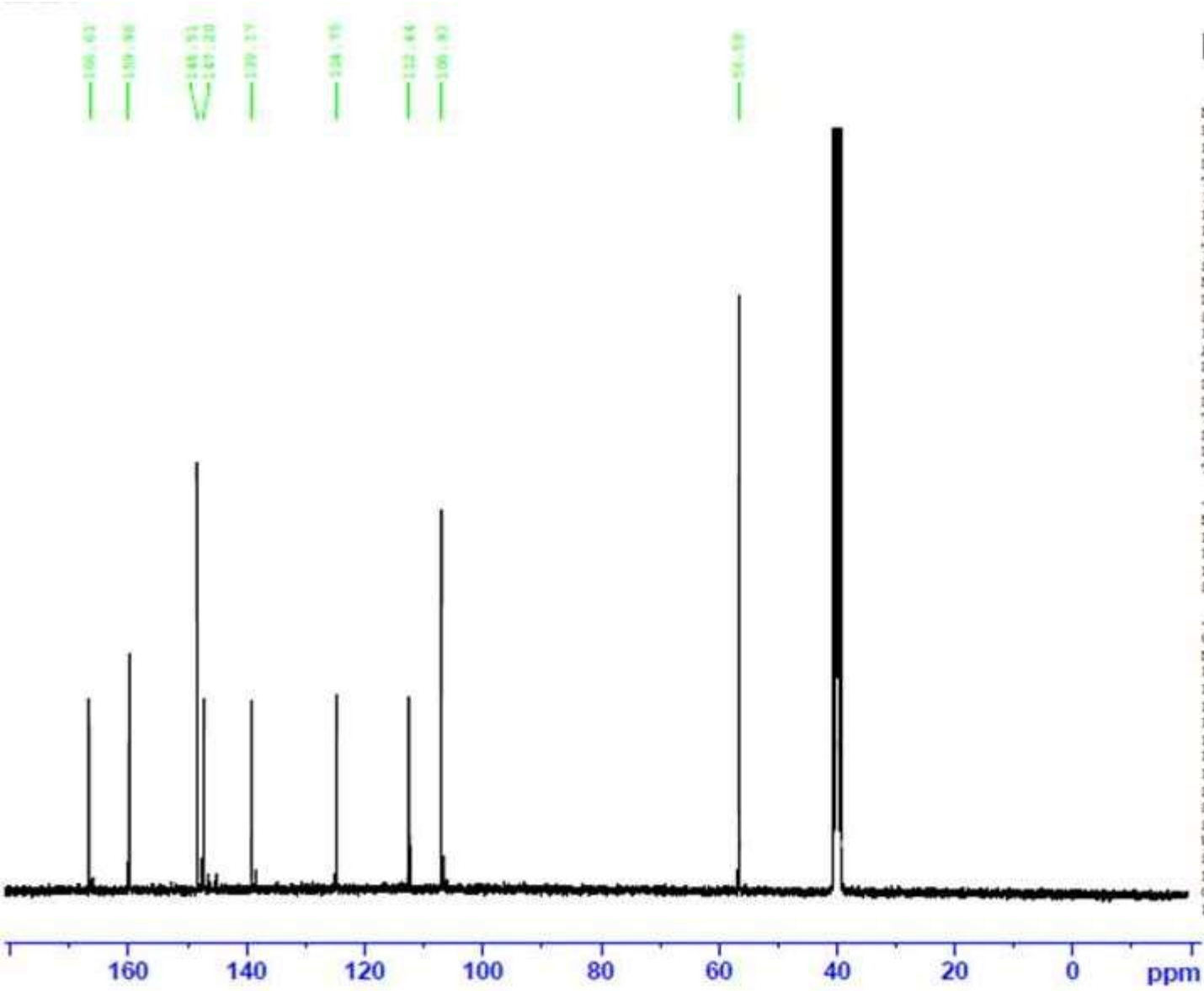
BRUKER

NAME	Audrey Isabelle
EXPNO	99
PROCNO	1
Date_	20190704
Time	8.17
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	114
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



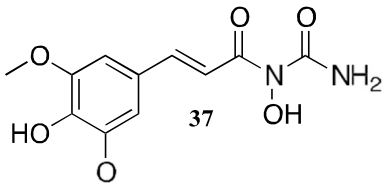
37

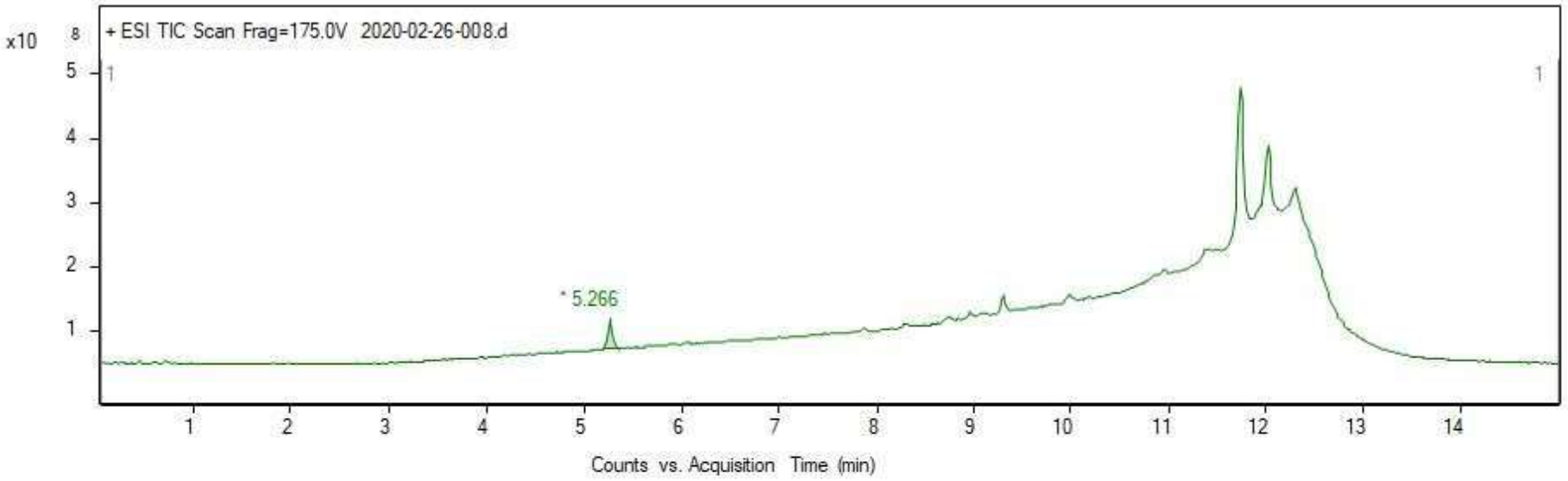


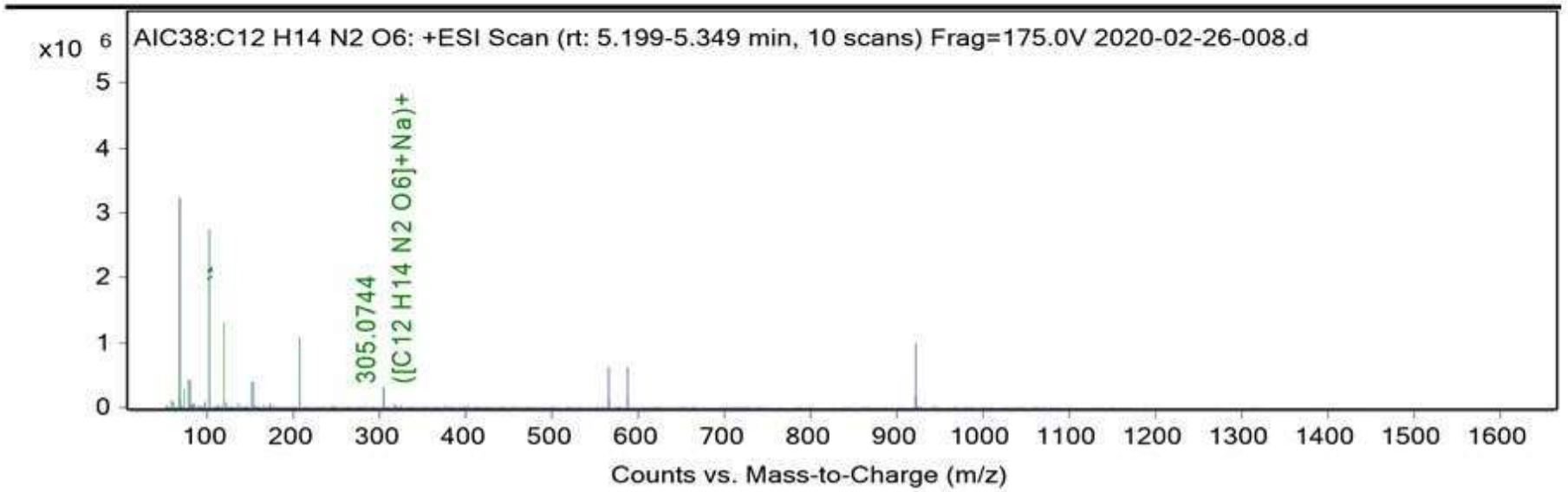
BRUKER

NAME	Audrey Isabelle	
EXPNO	102	
PROCNO	1	
Date_	20190705	
Time	0.27	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	DMSO	
NS	10000	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
--------	CHANNEL f1	--------
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
--------	CHANNEL f2	--------
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

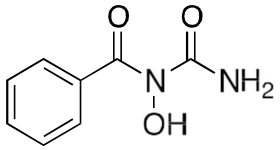
HRMS


O
O
O
N
NH2
OH
HO
O
37

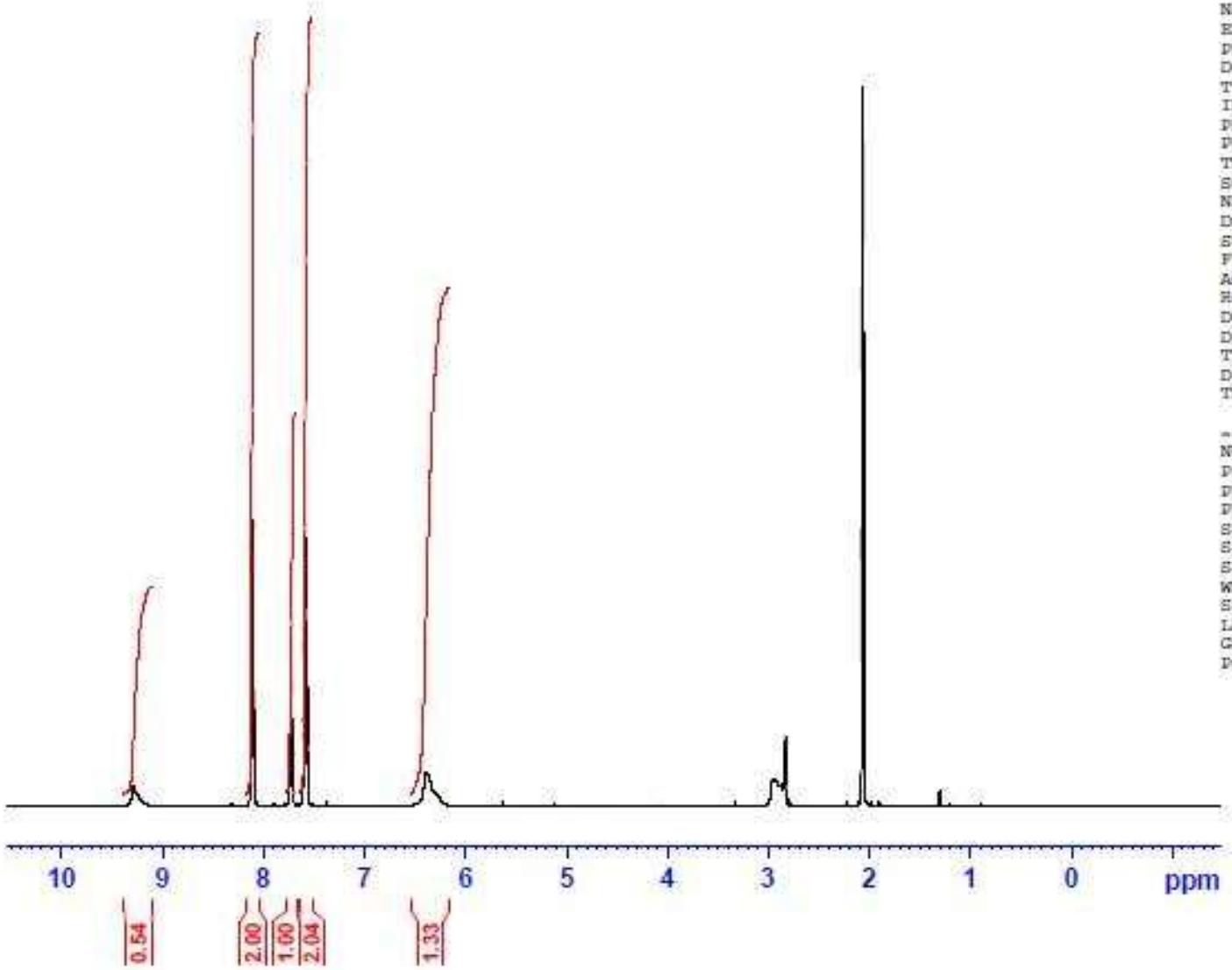

x10
8
5
4
3
2
1
+ ESI TIC Scan Frag=175.0V 2020-02-26-008.d
1
1
* 5.266
1
2
3
4
5
6
7
8
9
10
11
12
13
14
Counts vs. Acquisition Time (min)


x10
6
5
4
3
2
1
0
AIC38:C12 H14 N2 O6: +ESI Scan (rt: 5.199-5.349 min, 10 scans) Frag=175.0V 2020-02-26-008.d
305.0744
([C12 H14 N2 O6]+Na)+
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



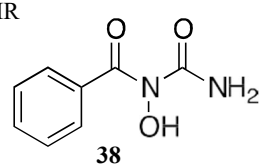
38



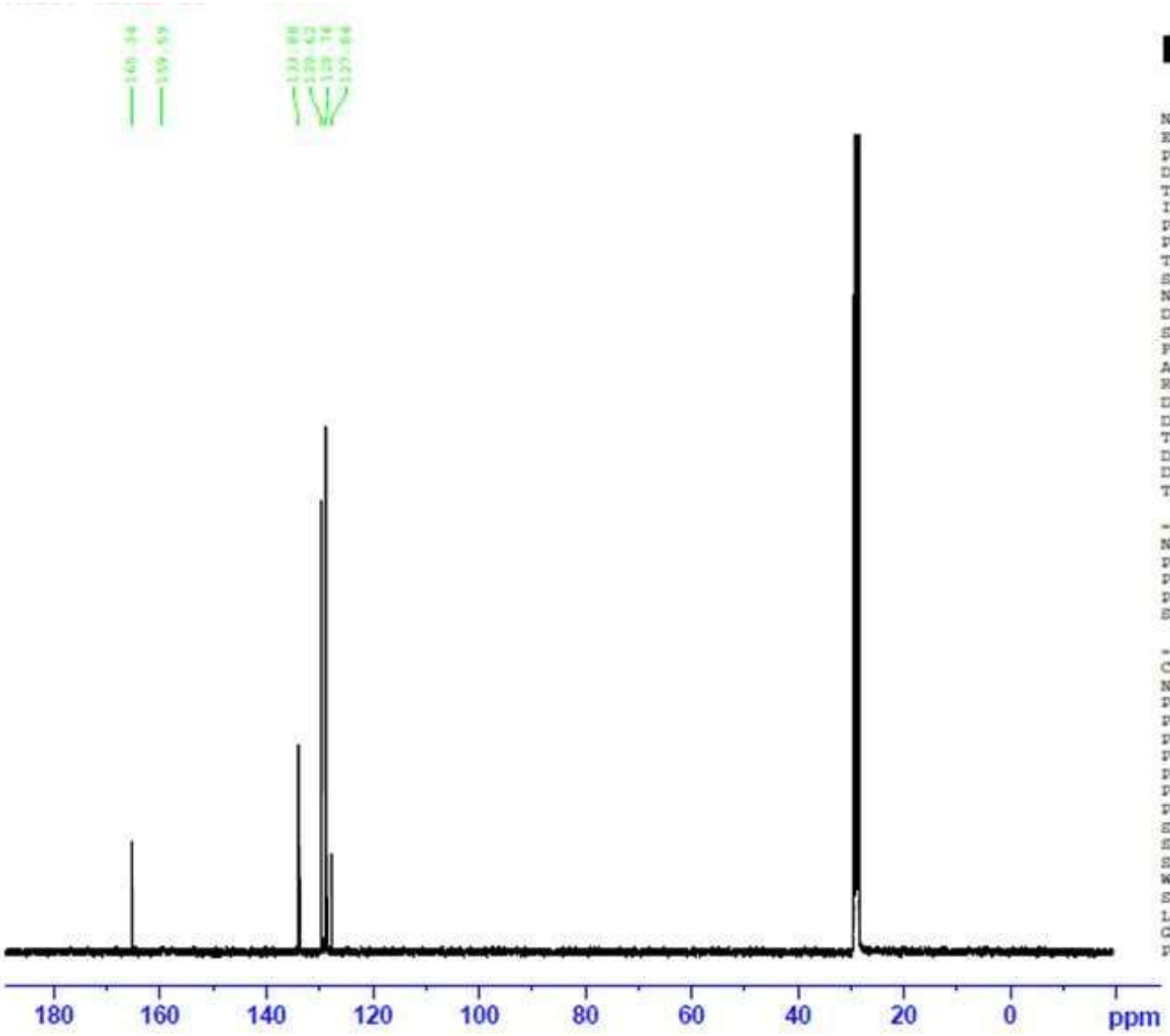
BRUKER

NAME	Moh RX
EXPNO	407
PROCNO	1
Date_	20190618
Time	8.51
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	Acetone
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	114
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



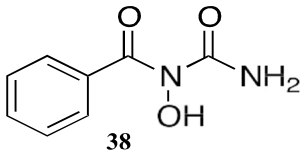
38



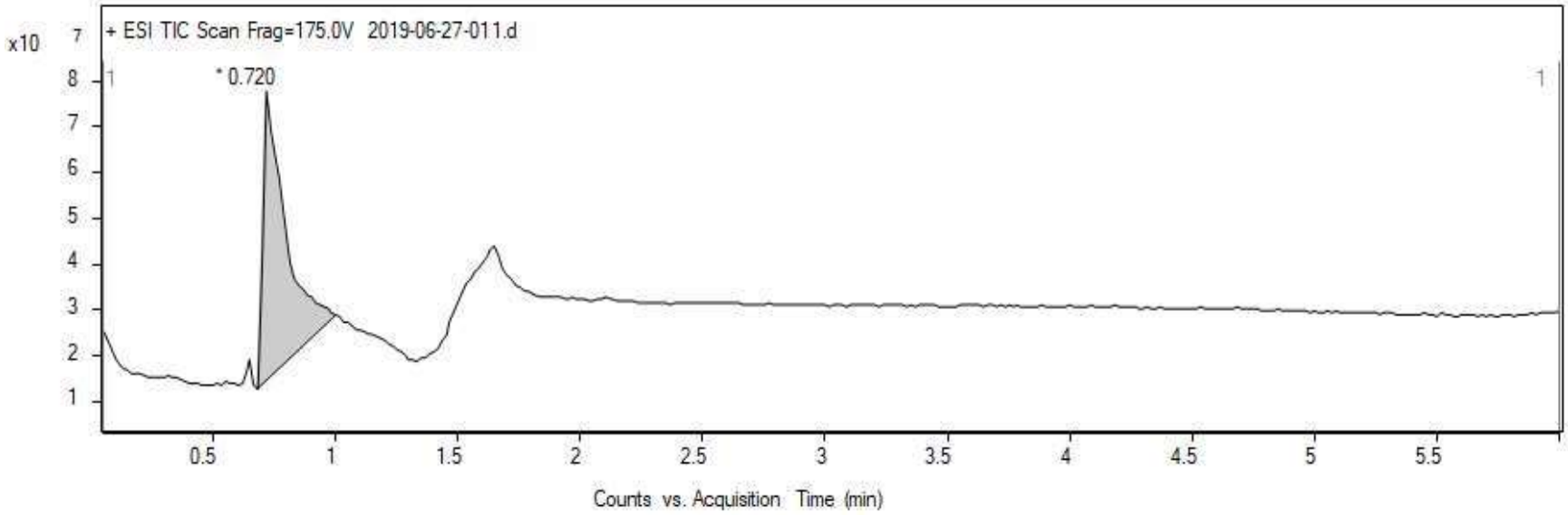
BRUKER

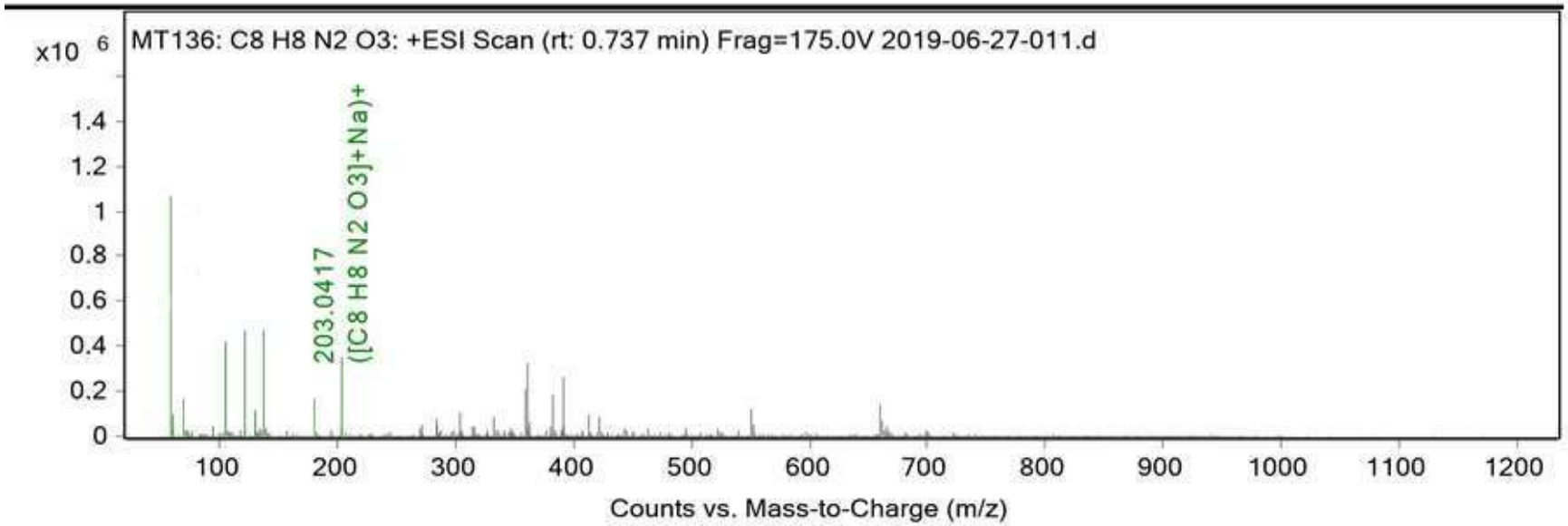
NAME	Moh RX	
EXPNO	408	
PROCNO	1	
Date_	20190618	
Time	13.47	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	Acetone	
NS	5000	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	298.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
-------- CHANNEL f1 --------		
NUC1	13C	
P1	9.90	usec
PL1	-1.90	dB
PL1W	56.02249908	W
SFO1	100.6228298	MHz
-------- CHANNEL f2 --------		
CPDPRG2	waltz65	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.30	dB
PL12	15.40	dB
PL13	18.40	dB
PL2W	11.25229836	W
PL12W	0.34772930	W
PL13W	0.17427748	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

HRMS

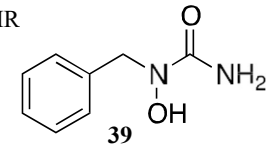

O
O
N
NH2
OH

38

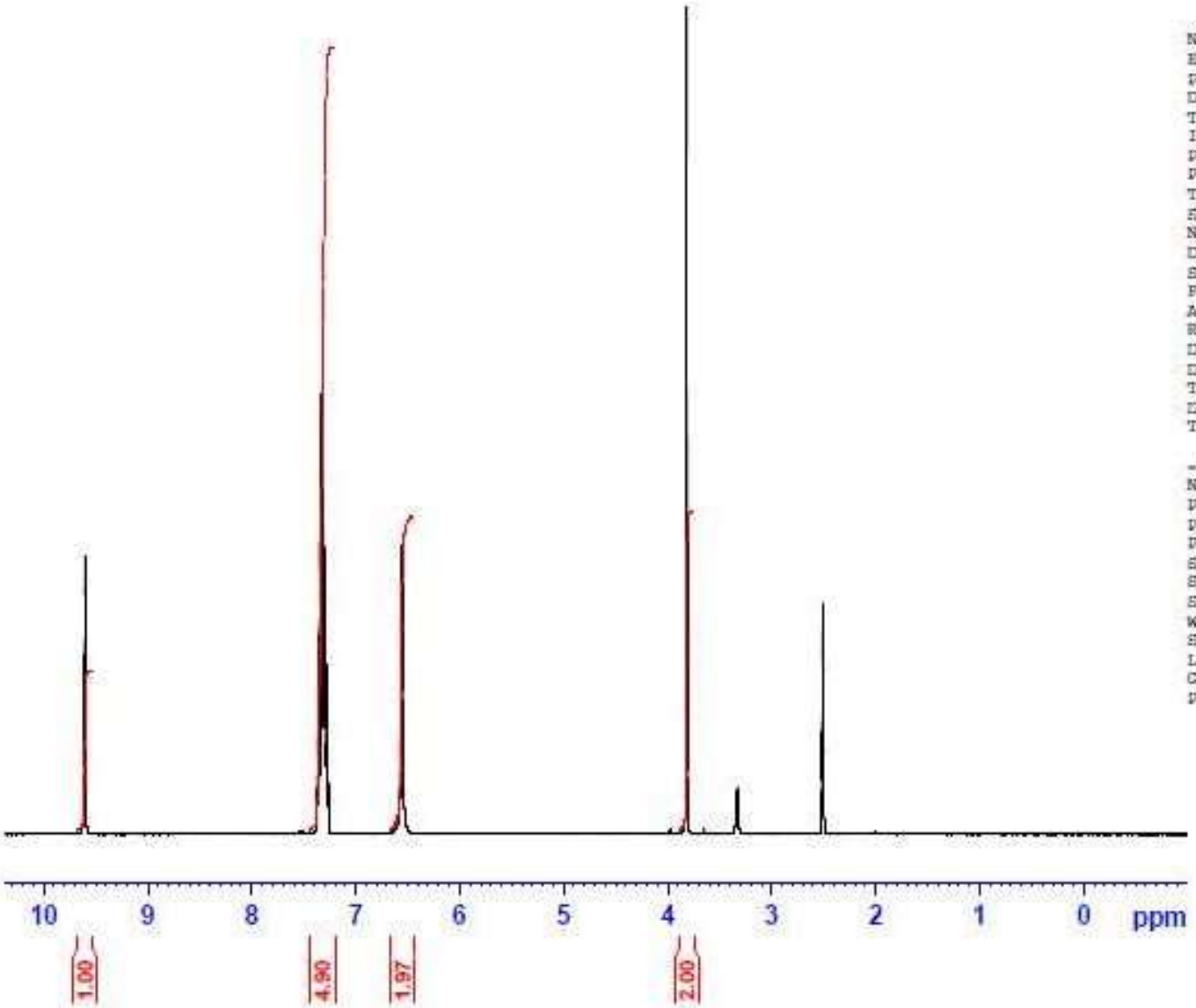

x10 7
+ ESI TIC Scan Frag=175.0V 2019-06-27-011.d
* 0.720
Counts vs. Acquisition Time (min)


x10 6
MT136: C8 H8 N2 O3: +ESI Scan (rt: 0.737 min) Frag=175.0V 2019-06-27-011.d
203.0417
([C8 H8 N2 O3]+Na)+
Counts vs. Mass-to-Charge (m/z)

^{1}H NMR



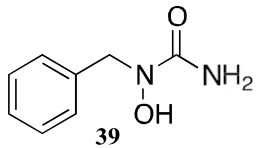
39



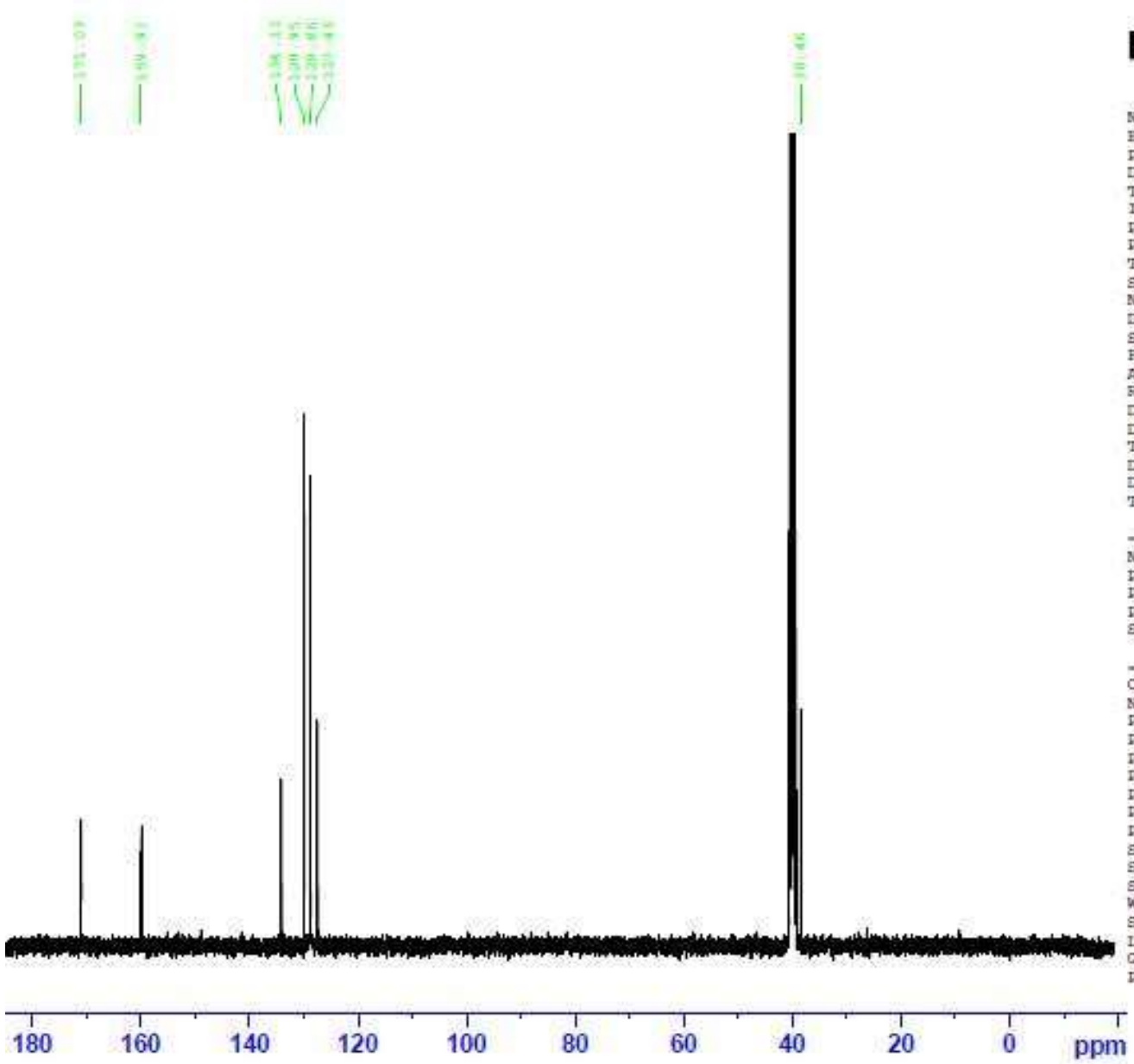
BRUKER

NAME	Moh RX
EXPNO	426
PROCNO	1
Date_	20190702
Time	10.20
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	114
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



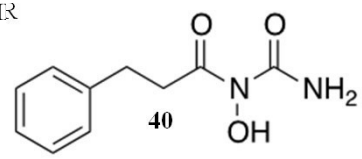
39



BRUKER

NAME	Moh RX
EXPNO	427
PROCNO	1
Date_	20190702
Time	10.54
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	530
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

^{1}H NMR



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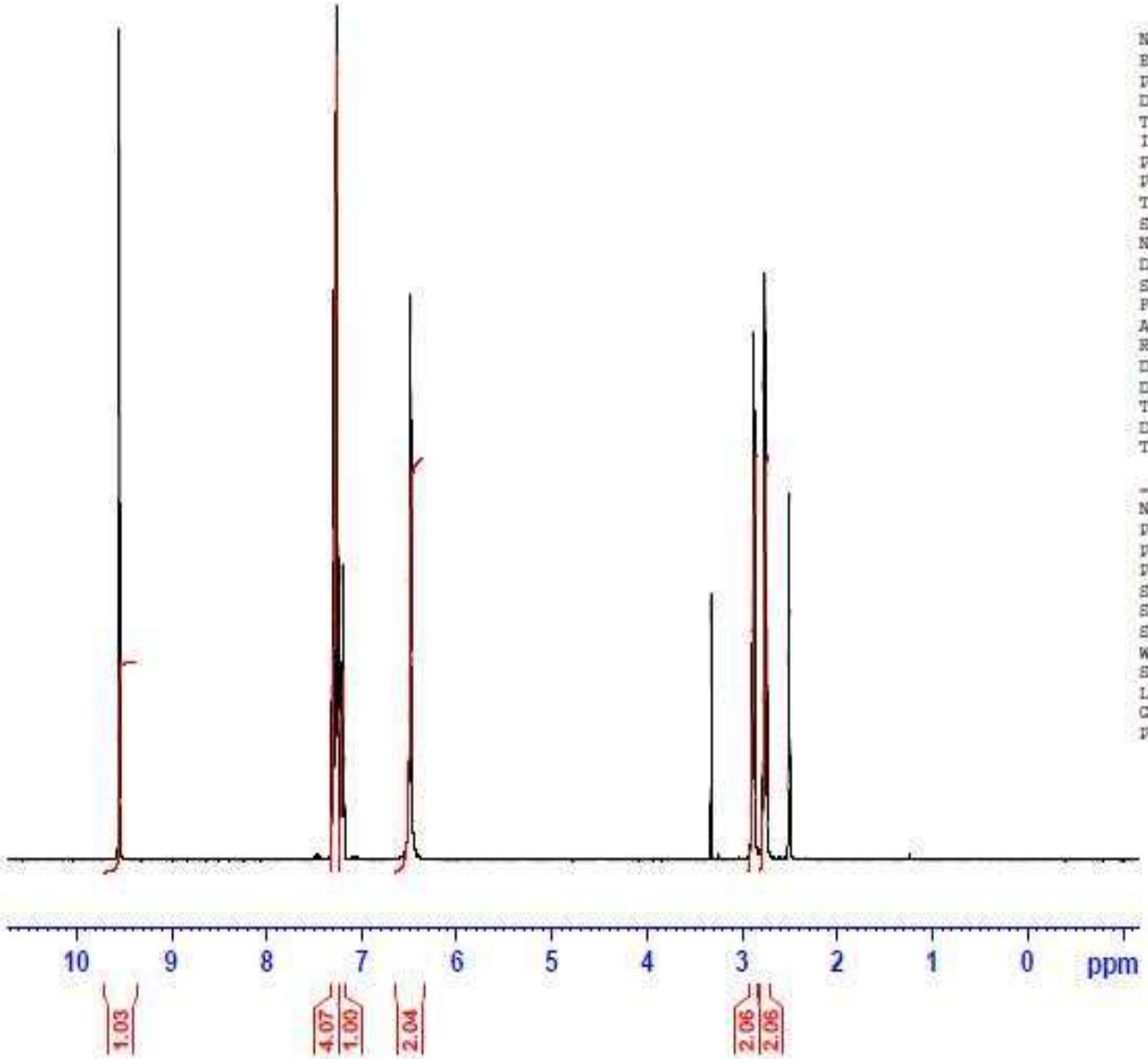
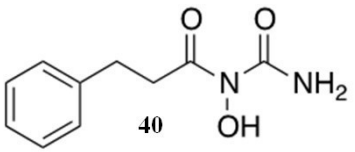


BRUKER

NAME	Moh RX
EXPNO	410
PROCNO	1
Date_	20190620
Time	8.51
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	101
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.07 usec
PL1	0.30 dB
PL1W	11.25229836 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR



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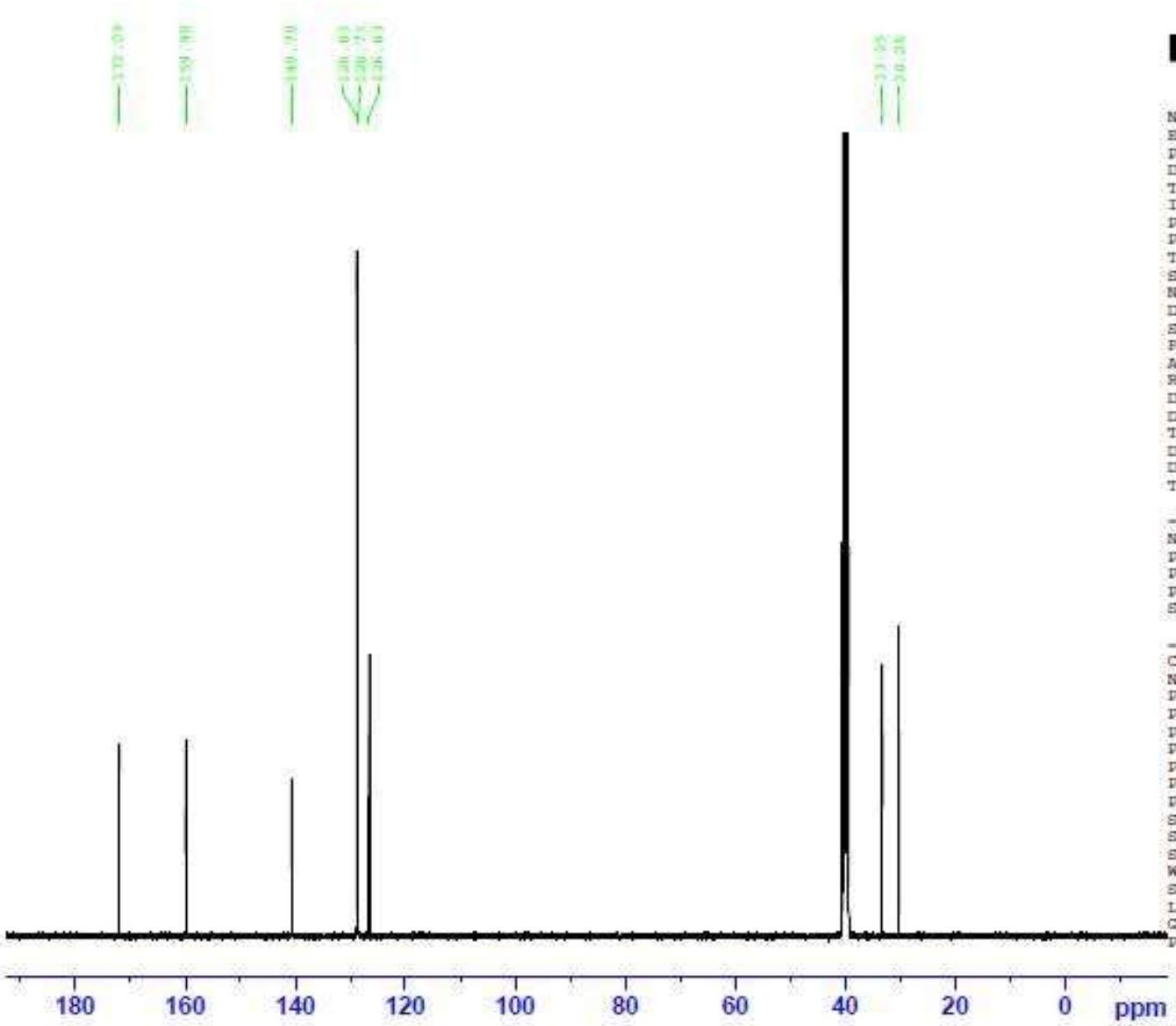
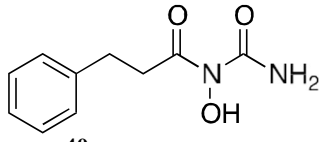


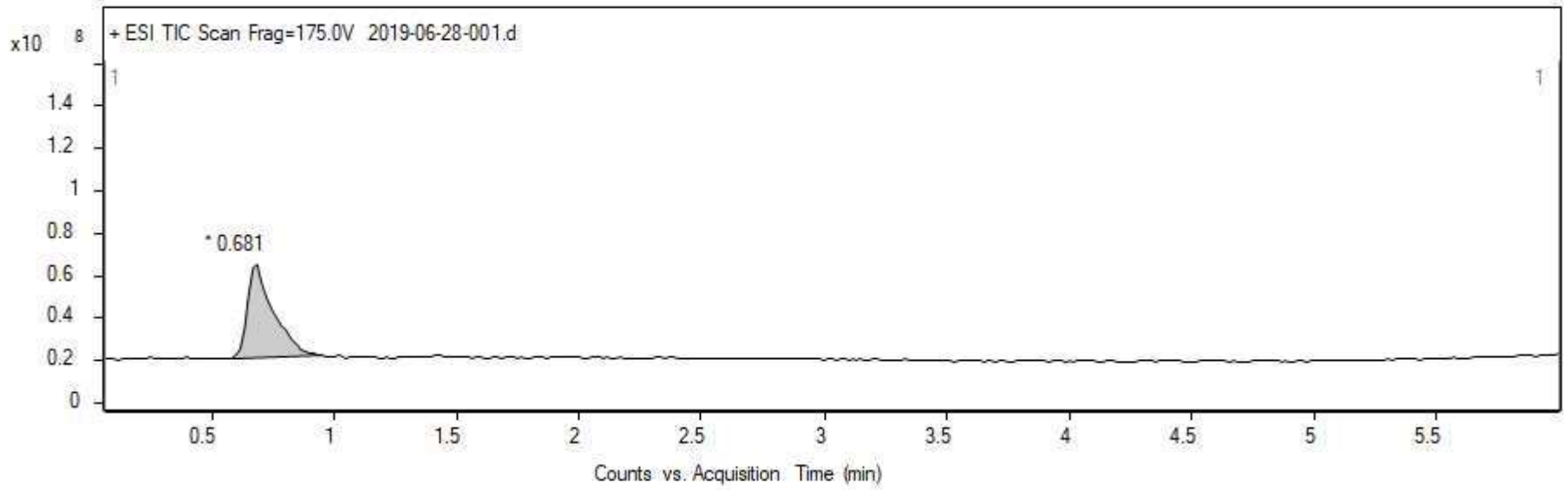
BRUKER

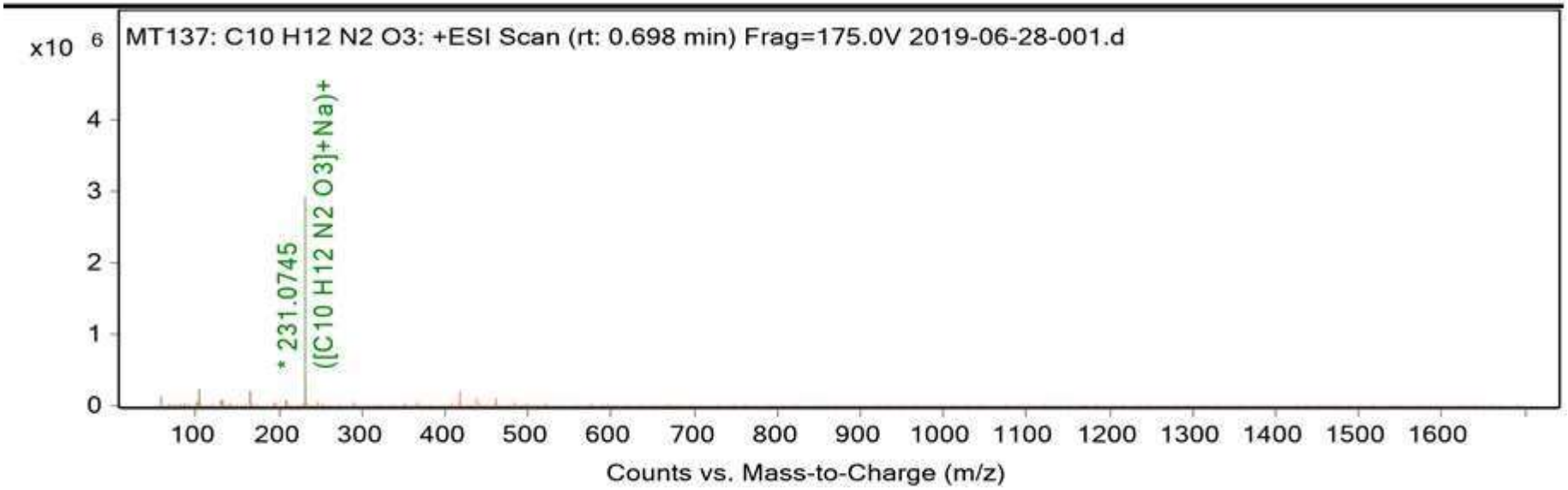
NAME	Moh RX
EXPNO	412
PROCNO	1
Date_	20190620
Time	13.39
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	4643
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.90 usec
PL1	-1.90 dB
PL1W	56.02249908 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz65
NUC2	1H
PCPD2	80.00 usec
PL2	0.30 dB
PL12	15.40 dB
PL13	18.40 dB
PL2W	11.25229836 W
PL12W	0.34772930 W
PL13W	0.17427748 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

HRMS


O
O
N
NH2
OH

40


+ ESI TIC Scan Frag=175.0V 2019-06-28-001.d
x10 8
1.4
1.2
1
0.8
0.6
0.4
0.2
0
* 0.681
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Counts vs. Acquisition Time (min)


MT137: C10 H12 N2 O3: +ESI Scan (rt: 0.698 min) Frag=175.0V 2019-06-28-001.d
x10 6
4
3
2
1
0
* 231.0745
([C10 H12 N2 O3]+Na)+
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
Counts vs. Mass-to-Charge (m/z)