Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Synthesis of novel 5-arylidenethiazolidinones with apoptotic properties *via* a three component reaction using piperidine as a bifunctional reagent

Chandramohan Bathula,[1] Sayantan Tripathi,[2] Ramprasad Srinivasan,[3] Kunal Kumar Jha,[1] Arnab Ganguly,[4] G. Chakraborty,[4] Shailja Singh,[2] Parthapratim Munshi,[1] Subhabrata Sen*,[1]

[1] Department of Chemistry, School of Natural Sciences, Shiv Nadar University, Chithera, Dadri, Gautam Budh Nagar, Uttar Pradesh 201308, India

[2] Department of Life Science, School of Natural Sciences, Shiv Nadar University, Chithera, Dadri, Gautam Budh Nagar, Uttar Pradesh 201308, India

[3] Shantani, 100 NCL Innovation Park, Dr. Homi Bhabha Road, Pune - 411 008, India

[4] Department of Biotechnology And Dr. B. C. Guha Centre for Genetic, Engineering And Biotechnology, University of Calcutta
35 Ballygunge Circular Road, Kolkata, WB 700 019, India.

Contents

Chemistry

Experimental

General

All reactions were carried out in flame-dried sealed tubes with magnetic stirring. Unless otherwise noted, all experiments were performed under argon atmosphere. All reagents were purchased from Sigma Aldrich, Acros or Alfa Aesar. Solvents were treated with 4 Å molecular sieves or sodium and distilled prior to use. Purifications of reaction products were carried out by washing with ethanol followed by recrystallization from 5% dichloromethane in methanol at rt. ^{1}H NMR and ^{13}C NMR spectra were recorded with tetramethylsilane (TMS) as internal standard at ambient temperature unless otherwise indicated Bruker 500 MHz for ^{1}H NMR and 120 MHz for ^{13}C NMR. Chemical shifts are reported in parts per million (ppm) and coupling constants are reported as Hertz (Hz). Splitting patterns are designated as singlet (s), broad singlet (bs), doublet (d), triplet (t). Splitting patterns that could not be interpreted or easily visualized are designated as multiple (m). The Mass Spectrometry analysis was done on the 6540 UHD Accurate-Mass Q-TOF LC/MS system (Agilent Technologies) equipped with Agilent 1290 LC system obtained by the Dept. of Chemistry, School of Natural Sciences, Shiv Nadar University, Uttar Pradesh 203207, India.

General procedure for synthesis of substituted (Z)-5-aryl-2-(piperidin-1-yl)thiazol-4(5H)-one and appropriate aldehydes

To a stirred solution of thiazolidine-2,4-dione (200 mg, 0.86 mmoles) in ethanol (10 mL) added piperidine (218 mg, 2.58 mmol), followed by corresponding aldehyde (0.94 mmoles) under N_2 atmosphere at room temperature, then the reaction mixture stirred at 80 °C for 12 h, allowed to cool to room temperature and the precipitate obatined was filtered and washed with ethanol and the product was recrystallized from 5% DCM:MeOH at rt to get substituted (Z)-5-aryl-2-(piperidin-1-yl)thiazol-4(5H)-one.

(Z)-5-(4-methylbenzylidene)-2-(piperidin-1-yl)thiazol-4(5H)-one (**17a**)

Following the general protocol 4-methylbenzaldehyde (227 mg, 0.94 mmoles) afforded **17a** in 209 mg (yield 85%) as white fluffy solid.^{1}H NMR (500 MHz; DMSO-d_6): δ 7.59 (s, 1H), 7.52 (d, J = 6.5 Hz, 2H), 7.32 (d, J = 6.5 Hz, 2H), 3.89 (br. s, 2H), 3.61 (br. s, 2H), 2.35 (s, 3H), 1.67

(m, 6H).^{13}C NMR (125 MHz; $CDCl_3$): δ 181.20, 174.46, 139.96, 131.40, 131.21, 129.64, 129.62, 127.04, 50.14, 49.55, 26.06, 25.36, 23.95, 21.40, HRMS (ESI-TOF) m/z: $[M + H]^+$calculated for ($C_{16}H_{19}N_2OS$) 287.1218, found 287.1242.

(Z)-5-((1H-indol-3-yl)methylene)-2-(piperidin-1-yl)thiazol-4(5H)-one (**17b**)

Following the general protocol 1H-indole-3-carbaldehyde (136 mg, 0.94 mmoles) afforded **17b** in 232 mg (yield 87%) as yellow solid.^{1}H NMR (500 MHz; DMSO-d_6): δ 7.87 (s, 1H), 7.84 (d, J = 8 Hz, 1H), 7.74 (s, 1H), 7.48 (d, J = 8 Hz, 1H), 7.24-7.21 (t, J = 7 Hz, 1H), 7.18-7.15 (t, J = 7.5 Hz, 1H), 3.88 (br. s, 2H), 3.60 (br. s, 2H), 3.36 (br. s, 1H), 1.67 (m, 6H). ^{13}C NMR (125 MHz; DMSO-d_6): δ 179.77, 172.41, 136.31, 127.23, 126.79, 122.76, 122.62, 121.55, 120.65, 118.25, 112.27, 111.02, 49.65, 48.65, 25.74, 25.11, 23.49. HRMS (ESI-TOF) m/z: $[M + H]^+$calculated for ($C_{17}H_{18}N_3OS$), 312.1171 found 312.1154.

(Z)-5-(3,4-dimethoxybenzylidene)-2-(piperidin-1-yl)thiazol-4(5H)-one (**17c**)

Following the general protocol 3,4-dimethoxybenzaldehyde (156 mg, 0.94 mmoles) afforded **17c** in 234 mg (yield 82%) as pale yellow fluffy solid.^{1}H NMR (500 MHz; $CDCl_3$): δ 7.73 (s, 1H), 7.14 (d, *J* = 6.5 Hz, 1H), 7.02 (s, 1H), 6.92-6.90 (m, 1H), 3.92 (br. s, 2H), 3.91 (s, 3H), 3.90 (s, 3H), 3.56 (br. s, 2H), 1.75 m, 6H). ^{13}C NMR (125 MHz; $CDCl_3$): δ 181.20, 174.30, 150.28, 149.04, 131.31, 127.15, 125.80, 123.45, 112.20, 111.18, 55.91, 55.88, 50.13, 49.57, 26.09, 25.36, 23.97. HRMS (ESI-TOF) m/z: $[M + H]^+$calculated for ($C_{17}H_{21}N_2O_3S$) 333.1273, found 333.1299.

(Z)-5-(4-methoxy-3-methylbenzylidene)-2-(piperidin-1-yl)thiazol-4(5H)-one (**17d**)

Following the general protocol 4-methoxy-3-methylbenzaldehyde (141 mg, 0.94 mmoles) afforded **17d** in 233 mg (yield 86%) as pale yellow solid.^{1}H NMR (500 MHz; DMSO-d_6): δ 7.54 (s, 1H), 7.48-7.46 (m, 1H), 7.41 (s, 1H), 7.07 (d, *J* = 8.5 Hz, 1H), 3.90-3.88 (t, *J* = 8.5 Hz, 2H), 3.85 (s, 3H), 3.62 (br. s, 2H), 2.20 (s, 3H), 1.68 (m, 6H). ^{13}C NMR (125 MHz; $CDCl_3$): δ 181.40, 174.47, 158.92, 131.78, 131.38, 129.44, 127.27, 126.27, 125.06, 110.00, 55.34, 50.08, 49.44, 26.04, 25.34, 23.95, 16.29 HRMS (ESI-TOF) m/z: $[M + H]^+$calculated for ($C_{17}H_{21}N_2O_2S$) 317.1324, found 313.1329.

(Z)-2-(piperidin-1-yl)-5-(2,4,5-trimethoxybenzylidene)thiazol-4(5H)-one (**17e**)

Following the general protocol 2,4,5-trimethoxybenzaldehyde (184 mg, 0.94 mmoles) afforded **17e** in 249 mg (yield 80%) as yellow solid.^{1}H NMR (300 MHz; DMSO-d_6): δ 7.83 (s, 1H), 7.01 (s, 1H), 6.79 (s, 1H), 3.89 (bs, 2H), 3.88 (s, 6H), 3.78 (s, 3H), 3.61 (s, 2H), 1.67 (m, 6H).^{13}C NMR (125 MHz; $CDCl_3$): δ 181.32, 174.18, 154.21, 151.60, 142.85, 126.27, 124.98, 114.61, 111.51, 96.54, 56.54, 56.16, 55.90, 49.95, 49.32, 25.97, 25.27, 23.89. HRMS (ESI-TOF) m/z: $[M + H]^+$calculated for ($C_{18}H_{23}N_2O_4S$) 363.1379, found 363.1397

(Z)-5-(3-hydroxy-4-methoxybenzylidene)-2-(piperidin-1-yl)thiazol-4(5H)-one (**17f**)

Following the general protocol 3-hydroxy-4-methoxybenzaldehyde (142 mg, 0.94 mmoles) afforded **17f** in 232 mg (yield 75%) as light yellow solid.^{1}H NMR (500 MHz; DMSO-d_6): δ 9.39 (br. s, 1H), 7.48 (s, 1H), 7.06 (s, 1H), 7.03 (s, 1H), 7.01 (m, 1H), 3.87 (br. s, 2H), 3.81 (s, 3H), 3.58 (br. s, 2H), 1.66 (m, 6H). ^{13}C NMR (125 MHz; DMSO-d_6): δ180.02, 173.65, 149.71, 147.21, 130.37, 126.89, 125.93, 122.99, 115.90, 112.64, 56.00, 50.11, 49.30, 26.07, 25.47, 23.79. HRMS (ESI-TOF) m/z: $[M + H]^+$calculated for ($C_{16}H_{19}N_2O_3S$) 319.116, found 319.1185

(Z)-5-(4-(dimethylamino)benzylidene)-2-(piperidin-1-yl)thiazol-4(5H)-one (**17g**)

Following the general protocol 4-(dimethylamino)benzaldehyde (140 mg, 0.94 mmoles) afforded **17g** in 230 mg (yield 85%) as dark yellow solid.^{1}H NMR (500 MHz; DMSO-d_6): 7.50 (s, 1H), 7.44 (d, J = 8.5 Hz, 2H), 6.78 (d, J = 9 Hz, 2H), 3.87-3.85 (t, J = 5 Hz, 2H), 3.57 (br. s, 2H), 2.98 (s, 6H), 1.66 (m, 6H). ^{13}C NMR (125 MHz; DMSO-d_6): δ 180.31, 173.48, 151.31, 131.66, 130.94, 122.31, 121.04, 112.34, 49.93, 49.07, 26.04, 25.43, 23.79. HRMS (ESI-TOF) m/z: $[M + H]^+$calculated for ($C_{17}H_{22}N_3OS$) 316.1484, found 316.1456

(Z)-5-(4-methoxybenzylidene)-2-(piperidin-1-yl)thiazol-4(5H)-one (**17h**)

Following the general protocol 4-methoxybenzaldehyde (127 mg, 0.94 mmoles) afforded **17h** in 228 mg (yield 88%) as fluffy solid white .^{1}H NMR (500 MHz; $CDCl_3$): δ 7.69 (s, 1H), 7.42 (d, J = 9 Hz, 2H), 6.85 (d, J = 9 Hz, 2H), 3.95-3.93 (t, J = 5.5 Hz, 2H), 3.61 (s, 3H), 3.51 (br. s, 2H), 1.70 (m, 6H).^{13}C NMR (125 MHz; $CDCl_3$): δ181.53, 174.58, 160.78, 131.60, 131.16, 126.97,

125.72, 114.58, 55.53, 50.33, 49.70, 26.25, 25.56, 24.15. HRMS (ESI-TOF) m/z: [M + H]$^+$calculated for ($C_{16}H_{19}N_2O_2S$) 303.1167, found 303.1192

(Z)-2-(piperidin-1-yl)-5-(4-propoxybenzylidene)thiazol-4(5H)-one (**17i**)

Following the general protocol 4-propoxybenzaldehyde (155 mg, 0.94 mmoles) afforded **17i** in 221 mg (yield 78%) as pale yellow solid.^{1}H NMR (500 MHz; $CDCl_3$): δ 7.73 (s, 1H), 7.45 (d, J = 8.5 Hz, 2H), 6.92 (d, J = 8.5 Hz, 2H), 3.99-3.97 (t, J = 5.5 Hz, 2H), 3.95-3.92 (t, J = 6.5 Hz, 2H), 3.55 (br. s, 2H), 1.82-1.78 (m, 2H), 1.73 (m, 6H), 1.03-1.00 (t, J = 7.5 Hz, 3H).^{13}C NMR (125 MHz; $CDCl_3$): δ181.31, 174.33, 160.15, 131.34, 131.01, 126.44, 125.22, 114.79, 69.47, 50.05, 49.41, 25.98, 25.29, 23.88, 22.30, 10.34. HRMS (ESI-TOF) m/z: [M + H]$^+$calculated for ($C_{18}H_{23}N_2O_2S$) 331.1480, found 331.1499

(Z)-5-(4-methoxy-2,3-dimethylbenzylidene)-2-(piperidin-1-yl)thiazol-4(5H)-one (**17j**)

Following the general protocol 4-methoxy-2,3-dimethylbenzaldehyde (154 mg, 0.94 mmoles) afforded **17j** in 238 mg (yield 84%) as yellow solid.^{1}H NMR (500 MHz; $CDCl_3$): δ 7.98 (s, 1H), 7.35 (d, J = 8.5 Hz, 2H), 6.74 (d, J = 8.5 Hz, 2H), 3.98-3.96 (t, J = 6 Hz, 2H), 3.81 (s, 3H), 3.50-3.48 (t, J = 6 Hz, 2H), 2.30 (s, 3H), 2.15 (s, 3H), 1.71 (m, 6H). ^{13}C NMR (125 MHz; $CDCl_3$): 180.71, 174.90, 158.34, 138.44, 130.30, 128.25, 126.51, 125.90, 125.78, 107.43, 55.36, 50.02, 49.29, 25.98, 25.31, 23.90, 16.04, 11.86. HRMS (ESI-TOF) m/z: [M + H]$^+$calculated for ($C_{18}H_{23}N_2O_2S$) 331.1480, found 331.1497

(Z)-5-(2-methylbenzylidene)-2-(piperidin-1-yl)thiazol-4(5H)-one (**17k**)

Following the general protocol 2-methylbenzaldehyde (112 mg, 0.94 mmoles) afforded **17k** in 209 mg (yield 85%) as light brown solid. ^{1}H NMR (500 MHz; DMSO-d_6): δ 7.74 (s, 1H), 7.53-7.52 (t, J = 4 Hz, 1H), 7.33 (m, 3H), 3.91-3.89 (t, J = 5.5 Hz, 2H), 3.60-3.58 (t, J = 5.5 Hz, 2H), 2.39 (s, 3H), 1.68 (m, 6H).^{13}C NMR (125 MHz; $CDCl_3$): δ 180.58, 174.77, 138.60, 133.67, 130.66, 130.02, 129.36, 128.92, 127.11, 126.11, 50.14, 49.50, 26.04, 25.34, 23.90, 19.95. HRMS (ESI-TOF) m/z: [M + H]$^+$calculated for ($C_{16}H_{19}N_2OS$) 287.1218, found 287.1248

(Z)-5-(2,5-dimethylbenzylidene)-2-(piperidin-1-yl)thiazol-4(5H)-one (**17l**)

Following the general protocol 2,5-dimethylbenzaldehyde (125 mg, 0.94 mmoles) afforded **17l** in 214 mg (yield 83%) as white fluffy solid. ^{1}H NMR (500 MHz; $CDCl_3$): δ 7.93 (s, 1H), 7.29 (s, 1H), 7.15 (d, J = 7.5 Hz, 1H), 7.05 (d, J = 7.5 Hz, 1H), 4.00-3.98 (t, J = 5.5 Hz, 2H), 3.53 (br. s, 2H), 2.36 (s, 3H), 2.34 (s, 3H), 1.73 (m, 6H).^{13}C NMR (125 MHz; $CDCl_3$): δ180.67, 174.88, 135.65, 135.62, 133.46, 130.61, 130.21, 129.57, 129.22, 127.64, 50.15, 49.51, 26.09, 25.38, 23.95, 21.03, 19.49. HRMS (ESI-TOF) m/z: $[M + H]^+$calculated for ($C_{17}H_{21}N_2OS$) 301.1375, found 301.1389

(Z)-5-(2,3-dimethoxybenzylidene)-2-(piperidin-1-yl)thiazol-4(5H)-one (**17m**)

Following the general protocol 2,3-dimethoxybenzaldehyde (156 mg, 0.94 mmoles) afforded **17m** in 238 mg (yield 82%) as brown solid. ^{1}H NMR (500 MHz; $CDCl_3$): δ 8.04 (s, 1H), 7.10-7.05 (m, 2H), 6.91-6.90 (m, 1H), 3.96-3.94 (t, J = 5.5 Hz, 2H), 3.84 (s, 3H), 3.80 (s, 3H), 3.51-3.50 (t, J = 5.5 Hz, 2H), 1.70 (m, 6H).^{13}C NMR (125 MHz; $CDCl_3$): δ180.76, 174.49, 152.83, 148.37, 129.70, 128.59, 125.99, 124.03, 120.02, 113.39, 61.37, 55.66, 49.99, 49.36, 25.94, 25.26, 23.80. HRMS (ESI-TOF) m/z: $[M + H]^+$calculated for ($C_{17}H_{21}N_2O_3S$) 333.1273, found 333.1285

(Z)-5-(benzo[d][1,3]dioxol-4-ylmethylene)-2-(piperidin-1-yl)thiazol-4(5H)-one (**17n**)

Following the general protocol benzo[d][1,3]dioxole-4-carbaldehyde (141 mg, 0.94 mmoles) afforded **17n** in 217 mg (yield 80%) as white solid.^{1}H NMR (500 MHz; $CDCl_3$): δ 7.66 (s, 1H), 6.98 (d, J = 8.5 Hz, 1H), 6.97 (s, 1H); 6.83 (d, J = 8.5 Hz, 1H); 5.99 (s, 2H), 3.98-3.96 (t, J = 6 Hz, 2H), 3.53 (br. s, 2H), 1.72 (m, 6H). ^{13}C NMR (125 MHz; $CDCl_3$): δ 181.26, 174.30, 148.87, 148.32, 131.08, 128.54, 126.13, 125.64, 108.84, 108.68, 101.71, 50.27, 49.64, 26.14, 25.46, 24.02. HRMS (ESI-TOF) m/z: $[M + H]^+$calculated for ($C_{16}H_{17}N_2O_3S$) 317.0960, found 317.0967

(Z)-5-(naphthalen-1-ylmethylene)-2-(piperidin-1-yl) thiazol-4(5H)-one (**17o**)

Following the general protocol 1-naphthaldehyde (141 mg, 0.94 mmoles) afforded **17o** in 139 mg (yield 70%) as pale brown solid. ^{1}H NMR (400 MHz; $CDCl_3$): δ 8.48 (s, 1H), 8.16 (d, J = 8 Hz, 1H), 7.86 (d, J = 7.5 Hz, 2H), 7.70 (d, J = 7 Hz, 1H), 7.57-7.48 (m, 3H), 4.01-3.99 (t, J = 6 Hz, 2H), 3.52 (br. s, 2H), 1.72 (m, 6H).^{13}C NMR (125 MHz; $CDCl_3$): δ 180.26, 174.75, 133.46, 132.18, 131.93, 131.66, 130.00, 128.60, 127.92, 126.83, 126.41, 125.74, 125.12, 123.71, 50.18,

49.53, 26.04, 25.36, 23.89. HRMS (ESI-TOF) m/z: $[M + H]^+$ calculated for ($C_{19}H_{19}N_2OS$) 323.1218, found 323.1227.

Scale up procedure of 17i:

To a stirred solution of thiazolidine-2,4-dione (16.77 g, 143.37 mmoles) in ethanol (250 mL) added piperidine (36.55 g, 430.11 mmol), followed by 4-propoxybenzaldehyde (25 g, 152.36 mmoles) under N_2 atmosphere at room temperature, then the reaction mixture stirred at 90° C for 12 h, allowed to cool to room temperature evaporated in vacuum the resulting residue purified by chromatography on silica gel to get (Z)-2-(piperidin-1-yl)-5-(4-propoxybenzylidene)thiazol-4(5H)-one (**17i**) as pale yellow solid in 29.7g (65% yield).

Target deconvolution by affinity chromatography

Loading of **17i** on the matrix

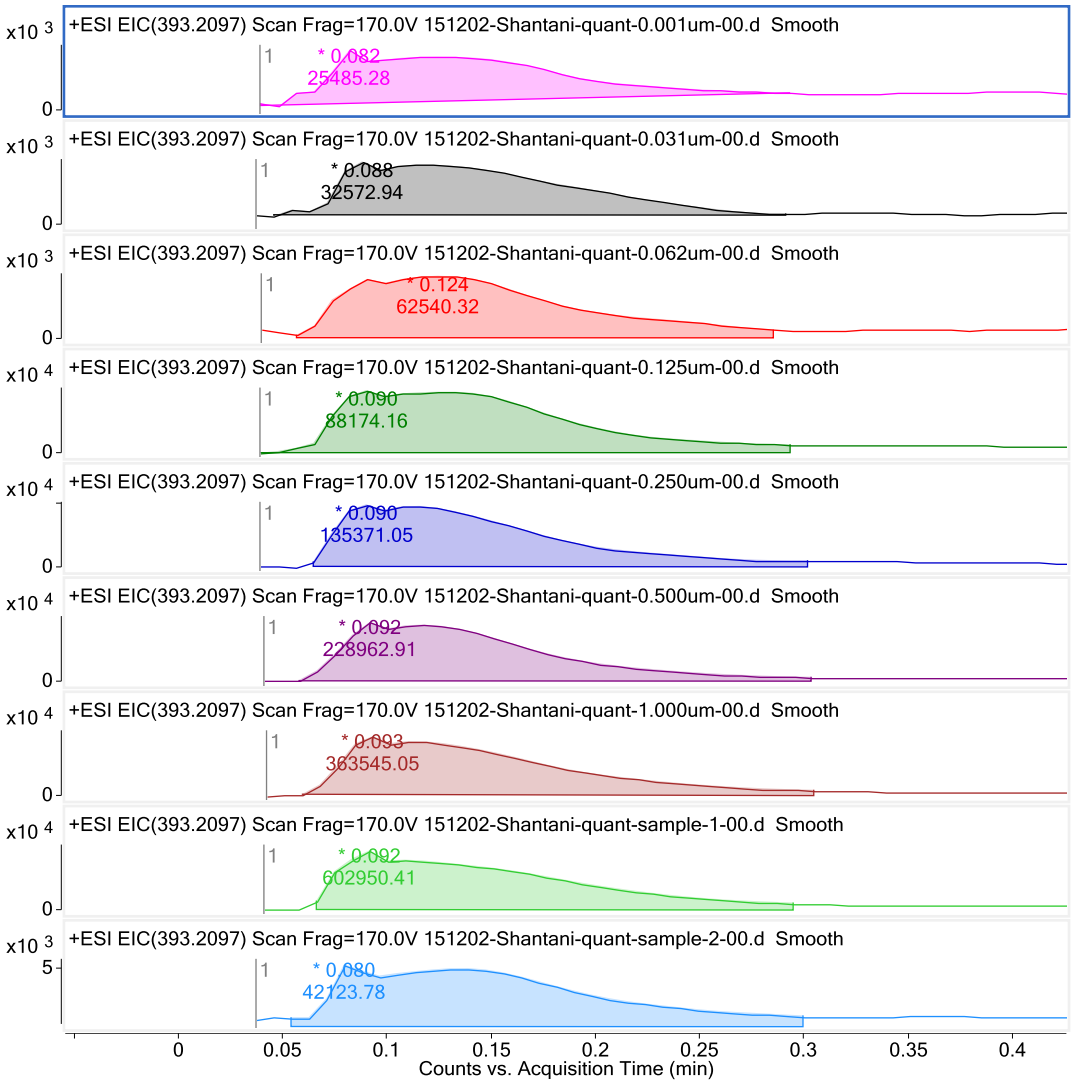


Figure 1

<u>Retention characteristics of **17i**.</u>

Coating conditions: 40% methanol or 100% chloroform

With 40% methanol:

1. 50mM **17i** stock was prepared in DMSO.
2. Matrix was pretreated with 20% Methanol for 10 minutes.
3. Working stock of 107.5 µM, **17i** solution was prepared in 10ml 40% Methanol.
4. Pretreated matrix was coated with **17i** and was felt for drying it out in the hood.
5. Next day the matrix was washed thrice with 2ml 1X TBS Ph-7.4 for 2 minutes and washes were collected.
6. After 3 washes the matrix was cut into pieces and was incubated in 3ml chloroform on shaker for 30 minutes.

7. After 30 minutes the chloroform was collected.
8. The collected chloroform was evaporated at room temperature.
9. The reduced 804µl of the chloroform was dissolved in 7ml of chloroform.
10. For analysis 4.65ul was dissolved in HPLC water and was analyzed in MS.

With 100% chloroform:

1. 50mM **17i** stock was prepared in DMSO.
2. Working stock of 107.5 µM, **17i** was prepared in 10ml 100% Chloroform.
3. Matrix was coated with 7ml **17i** solution and was left overnight for drying in a clean hood.
4. Next day the matrix was washed thrice with 2ml 1X TBS (pH 7.4) for 2 minutes and washes were collected.
5. After 3 washes the matrix was cut into pieces and was incubated in 3ml chloroform on shaker for 30 minutes.
6. After 30 minutes the chloroform was collected.
7. The collected chloroform was evaporated at room temperature.
8. The reduced 874µl of the chloroform was dissolved in 7ml of chloroform.
9. For analysis 4.65µl was dissolved in HPLC water and was analyzed in MS.

Table 1:

Standard Curve			
17i in ng/ml	**Area under the peak**		
392.5	363545.05		
196.25	228962.91		
98.125	135371.05		
49.062	88174.16		
24.53	62540.32		
12.265	32572.94		
0.392	25485.28	ng/ml	concentration factor
40% Methanol	602950.41	653.0469	**466.4620709**
100% Chloroform	42123.78	4.407462	
100% 17i was bound to 40% methanol coated mtarix.			

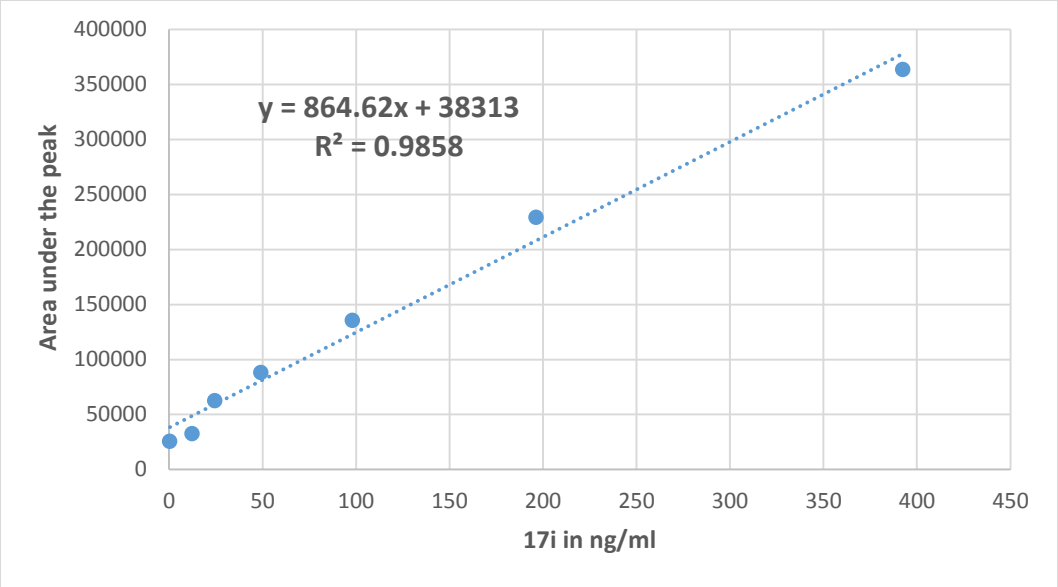


Figure 2

Validation of Target Capture Method:

This method relies on a validated hypothesis that weak-molecular interaction forces, such as pi-pi, cation-pi, hydrogen, van der waals, ionic, hydrophobic, arising from of a drug-like molecule can be used in immobilizing them over a surface that offers complementary interactions. Though interactions are weak in nature, sum of multiple weak interactions allow drug-like molecule to stay on the surface for a time that is sufficient for it to further interact with its affinity protein partners in a biological sample. Unique Polymer Technology makes available polymeric surface that offer possibilities of forming complementary weak interactions with drug-like molecules. Several examples of preparing molecule-specific affinity matrix using weak molecular interactions and capturing their protein targets using Unique Polymer Technology (UPT) has been reported in Patent Application Number (Pro. Patent Application # 201621000681) and is also available on http://www.shantani.com/UPT.php

To validate the method in one of the examples - a compound Bisindolylmaleimide-III (Bis-III) was used as the test molecule. Glycogen Synthase Kinase 3 (GSK3) is the well-established protein target of Bis-III and in the validation experiment GSK3 was captured and identified from the whole cell-lysate using the UPT method. For the purpose of illustration Bis-III, a red colored compound, was immobilized on a 1.5 ml tube using the proprietary polymeric matrix that offers possibilities of complementary weak interactions (Figure 1).

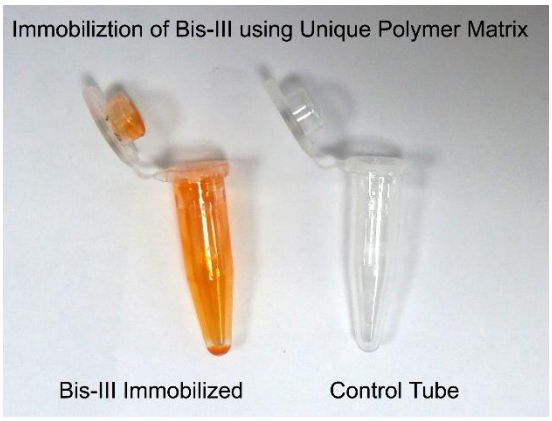


Figure 3. Immobilization of Bis-III using proprietary Matrix Surface

After immobilization of Bis-III the polymeric surface was washed for two hours and the amount of Bis-III in the washed was quantified using absorption spectrometry based method.

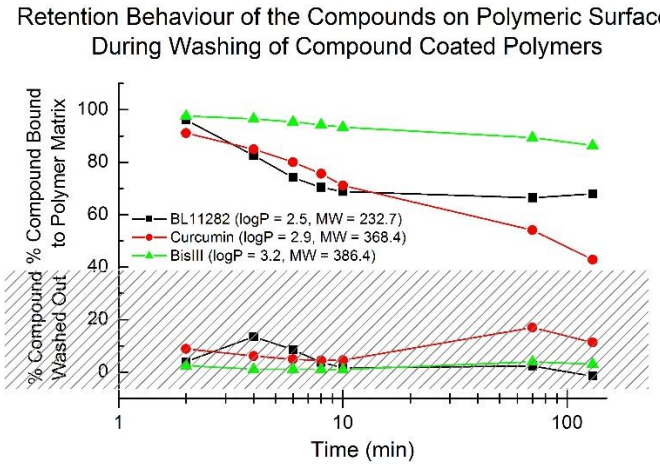


Figure 4. Retention Behavior of Bis-III on the Polymeric Surface

After confirming that >1 micromoles of Bis-III was immobilized on the polymeric surface, He-la Cell lysate was incubated with the Bis-III immobilized and Control Polymeric Matrix Chips for 2 minutes. Chips were washed and the protein bound to the chip was eluted using 2 ml elution buffer (1 mM Bis-III in TBST). Eluted proteins were acetone precipitated and captured proteins were analyzed using western blot method. The Target protein GSK3 was captured specifically on the polymeric matrix chip where Bis-III was immobilized. This confirmed the capability of the UPT in immobilizing and specifically capturing the target of the Bis-III.

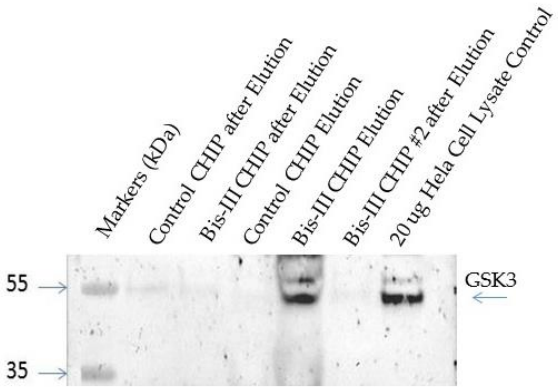
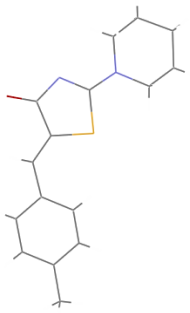
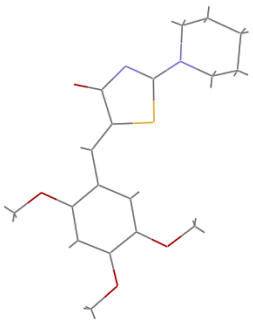


Figure 5. Specific Capture of GSK3 on CHIP where Bis-III was immobilized

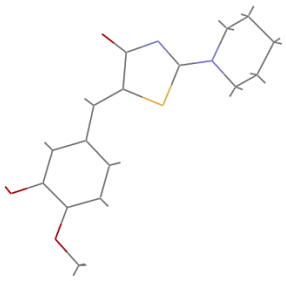
Single crystal X-Ray structures



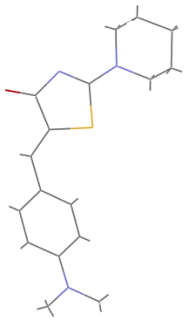
17a



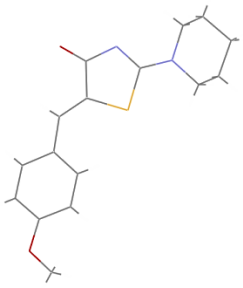
17e



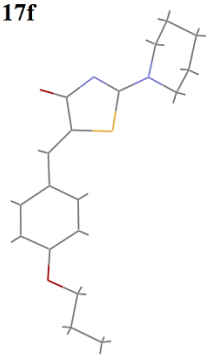
17f



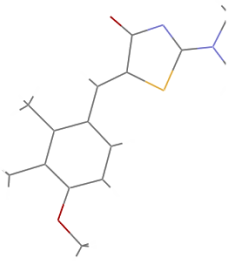
17g



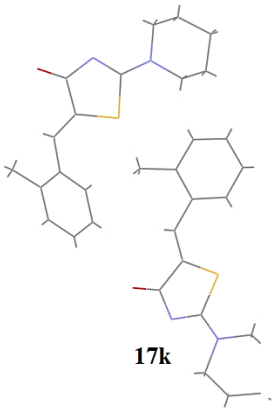
17h



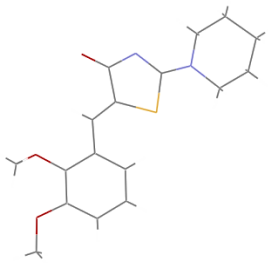
17i



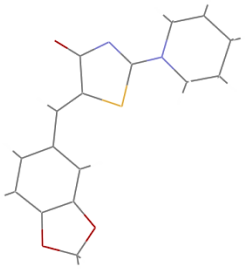
17j



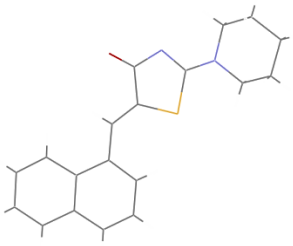
17k



17m



17n



17o

CCDCs:

CCDC 1453249-1453259

Summary of Data CCDC 1453249 (**17a**)

Compound Name:
Formula: C16 H18 N2 O1 S1
Unit Cell Parameters: a 12.5012(6) b 16.1346(7) c 7.6541(4) P21/c
---

Summary of Data CCDC 1453250 (**17e**)

Compound Name:
Formula: C18 H22 N2 O4 S1
Unit Cell Parameters: a 10.0466(4) b 7.7834(3) c 22.9774(10) P21/c
---

Summary of Data CCDC 1453251 (**17f**)

Compound Name:
Formula: C16 H18 N2 O3 S1
Unit Cell Parameters: a 7.303(3) b 16.637(5) c 12.598(5) P21/c
---

Summary of Data CCDC 1453252 (**17g**)

Compound Name:
Formula: C17 H21 N3 O1 S1
Unit Cell Parameters: a 12.7194(4) b 8.0294(3) c 16.4422(6) P21/n
---

Summary of Data CCDC 1453253 (**17h**)

Compound Name:
Formula: C16 H18 N2 O2 S1
Unit Cell Parameters: a 8.5748(3) b 16.5115(5) c 10.8532(4) P21/n
---

Summary of Data CCDC 1453254 (**17i**)

Compound Name:
Formula: C18 H22 N2 O2 S1
Unit Cell Parameters: a 14.6019(6) b 15.8336(5) c 7.5085(3) P21/c
---

Summary of Data CCDC 1453255 (**17j**)

Compound Name:
Formula: C18 H22 N2 O2 S1
Unit Cell Parameters: a 13.1879(8) b 8.2959(4) c 16.8693(10) P21/c
---

Summary of Data CCDC 1453256 (**17k**)

Compound Name:
Formula: C16 H18 N2 O1 S1
Unit Cell Parameters: a 19.808(2) b 19.648(2) c 7.5797(8) P21/c
---

Summary of Data CCDC 1453257 (**17m**)

Compound Name:
Formula: C17 H20 N2 O3 S1
Unit Cell Parameters: a 6.9066(6) b 10.3537(10) c 12.5514(13) P-1

Summary of Data CCDC 1453258 (**17n**)

Compound Name:
Formula: C16 H16 N2 O3 S1
Unit Cell Parameters: a 8.3333(6) b 16.8148(12) c 10.7927(8) P21/n
---

Summary of Data CCDC 1453259 (**17o**)

Compound Name:
Formula: C19 H18 N2 O1 S1
Unit Cell Parameters: a 19.3839(6) b 7.7880(3) c 20.9133(8) Pbca
---

					Experiment 1 : MCF 7 screening 48 hours							
Raw Data{Wavelength:595.0}												
	1	2	3	4	5	6	7	8	9	10	11	12
A	1.106	1.283	1.245	0.561	0.528	0.558	0.324	0.04	0.033	0.039	0.038	0.036
B	0.303	0.32	0.342	0.84	0.89	0.427	0.09	0.092	0.093	0.039	0.037	0.046
C	0.635	0.817	0.823	0.4	0.396	0.425	0.039	0.039	0.039	0.041	0.041	0.041
D	0.715	0.567	0.74	0.98	0.714	0.712	0.037	0.038	0.046	0.039	0.041	0.04
E	0.587	0.637	0.565	0.781	0.747	0.525	0.037	0.037	0.037	0.038	0.04	0.04
F	0.523	0.902	0.556	0.737	0.606	0.675	0.04	0.038	0.036	0.044	0.038	0.037
G	0.598	0.82	0.753	0.704	0.496	0.551	0.037	0.038	0.038	0.039	0.041	0.038
H	0.739	0.839	0.7	0.712	0.889	0.8	0.037	0.038	0.036	0.04	0.039	0.045
Compounds	**O.D1**	**O.D2**	**O.D3**	**AVG**	**CTRL-TEST**	**CTRL-TEST/CTRL**	***100**					
CONTROL	1.106	1.283	1.245	1.211	0	0	0					
DMSO	0.303	0.32	0.342	0.322	0.88966667	0.734452394	73.44					
17b	0.635	0.815	0.823	0.758	0.45366667	0.374518437	37.45±0.065					
17k	0.715	0.567	0.74	0.674	0.53733333	0.443588332	44.35±0.366					
17c	0.587	0.637	0.565	0.596	0.615	0.507705008	50.77±1.789					
17e	0.523	0.902	0.556	0.54	0.67183333	0.554623005	55.46±1.981					
17f	0.598	0.82	0.753	0.724	0.48766667	0.402586681	40.25±0.214					
17n	0.739	0.839	0.7	0.759	0.452	0.373142543	37.31±1.221					
17m	0.561	0.528	0.558	0.549	0.66233333	0.546780407	54.67±1.647					
17l	0.84	0.89	1.02	0.637	0.57466667	0.474408365	47.44±0.691					
17i	0.4	0.396	0.425	0.407	0.80433333	0.664006604	66.4±1.221					
17a	0.98	0.714	0.712	0.802	0.40933333	0.337919648	33.79±2.655					
17d	0.781	0.747	0.525	0.684	0.527	0.435057788	43.5±2.053					
17o	0.737	0.606	0.675	0.673	0.53866667	0.444689048	44.46±0.997					
17g	0.704	0.496	0.551	0.524	0.68783333	0.567831591	56.78±1.751					
17h	0.712	0.889	0.8	0.8	0.411	0.339295542	33.92±1.233					

			Experiment 1 :MDA screening 48 hours									
Raw Data{Wavelength:595.0}												
	1	2	3	4	5	6	7	8	9	10	11	12
A	1.733	1.775	1.512	1.4	0.917	1.34	0.22	0.265	0.207	0.067	0.064	0.052
B	0.375	0.415	0.412	1.08	0.912	0.967	0.153	0.326	0.154	0.069	0.07	0.065
C	0.912	0.964	0.863	0.715	0.543	0.748	0.148	0.146	0.147	0.659	0.061	0.059
D	1.112	1.213	1.142	1.21	1.5	0.98	0.139	0.152	0.112	0.072	0.075	0.072
E	1.01	1.08	0.943	0.815	0.714	0.865	0.225	0.246	0.159	0.074	0.072	0.08
F	0.615	0.712	0.813	0.9	0.856	0.972	1.593	1.974	1.426	0.076	0.074	0.063
G	0.91	0.975	0.713	0.856	0.749	0.912	0.135	0.098	0.151	0.066	0.06	0.065
H	1.312	1.445	1.08	0.912	1.223	1.312	0.179	0.163	0.118	0.059	0.059	0.06
Compounds	**O.D1**	**O.D2**	**O.D3**	**AVG**	**CTRL-TEST**	**CTRL-TEST/CTRL**	***100**					
CONTROL	1.733	1.775	1.512	1.6733	0	0	0					
DMSO	0.375	0.415	0.412	0.4007	1.27266667	0.760557769	76.05±0.141					
17b	0.912	0.964	0.863	0.913	0.76033333	0.45438247	45.43±0.022					
17k	1.112	1.213	1.142	1.1557	0.51766667	0.30936255	30.93±0.051					
17c	1.01	1.08	0.943	1.011	0.66233333	0.395816733	39.58±0.052					
17e	0.615	0.712	0.813	0.7133	0.96	0.573705179	57.37±0.068					
17f	0.91	0.975	0.713	0.866	0.80733333	0.48247012	48.24±0.099					
17n	1.312	1.445	1.08	1.279	0.39433333	0.235657371	23.56±0.136					
17m	1.4	0.917	1.34	1.219	0.45433333	0.271513944	27.15±0.184					
17l	1.08	0.912	0.967	0.9863	0.687	0.410557769	41.05±0.263					
17i	0.715	0.543	0.748	0.6687	1.00466667	0.600398406	60.03±0.086					
17a	1.21	1.5	0.98	1.23	0.44333333	0.264940239	26.49±0.110					
17d	0.815	0.714	0.865	0.798	0.87533333	0.52310757	52.31±0.260					
17o	0.9	0.856	0.972	0.9093	0.764	0.456573705	45.65±0.076					
17g	0.856	0.749	0.912	0.839	0.83433333	0.498605578	49.86±0.058					
17h	0.912	1.223	1.312	1.149	0.52433333	0.313346614	31.33±0.082					

EC_{50} of the active compounds against MCF7 cells												
Raw Data{Wavelength:595.0}												
	1	2	3	4	5	6	7	8	9	10	11	12
A	1.312	1.139	1.21	0.039	0.037	1.191	1.045	1.127	0.036	1.467	1.491	1.114
B	0.151	0.163	0.164	0.037	0.036	0.115	0.115	0.108	0.037	0.129	0.155	0.211
C	1.09	1	1.031	0.041	0.044	0.918	0.985	1.06	0.039	1.158	0.998	1.135
D	0.823	0.876	0.891	0.038	0.042	0.835	0.941	0.879	0.036	1.073	0.953	1.057
E	0.613	0.71	0.63	0.038	0.037	0.797	0.81	0.765	0.037	0.818	0.969	1.165
F	0.492	0.456	0.571	0.04	0.038	0.694	0.712	0.68	0.039	1.34	0.821	1.075
G	0.441	0.4	0.391	0.039	0.039	0.413	0.496	0.48	0.038	0.808	1.208	0.871
H	0.251	0.283	0.321	0.039	0.037	0.312	0.38	0.29	0.043	1.175	0.88	1.237
17g	IC_{50} =3.64 μM											
	O.D1	O.D2	O.D3	AVG	CTRL-TEST	CTRL-TEST/CTRL	*100	stdev.				
CONTROL	1.312	1.139	1.21	1.220333	0	0	0	0			CONTROL	0
DMSO	0.151	0.163	0.164	0.159333	1.061	0.869435	86.94	0.007234			DMSO	86.94
1	1.09	1	1.031	1.040333	0.18	0.147501	14.75	0.04572			1	14.75
10	0.823	0.876	0.891	0.863333	0.357	0.292543	29.25	0.035726			10	29.25
20	0.613	0.71	0.63	0.651	0.569333	0.466539	46.65	0.051798			20	46.65
30	0.492	0.456	0.571	0.506333	0.714	0.585086	58.5	0.058825			30	58.5
40	0.441	0.4	0.391	0.410667	0.809667	0.66348	66.34	0.026652			40	66.34
50	0.251	0.283	0.321	0.285	0.935333	0.766457	76.64	0.035043			50	76.64
17i	IC_{50}=4.42 μM											
	O.D1	O.D2	O.D3	AVG	CTRL-TEST	CTRL-TEST/CTRL	*100	stdev.				
CONTROL	1.191	1.045	1.127	1.121	0	0	0	0				
DMSO	0.115	0.115	0.108	0.112667	1.008333	0.899494	89.94	0.004041			CONTROL	0
1	0.918	0.985	1.06	0.987667	0.133333	0.118941	11.81	0.071038			DMSO	89.94
10	0.835	0.941	0.879	0.885	0.236	0.210526	21.05	0.053254			1	11.81
20	0.797	0.81	0.765	0.790667	0.330333	0.294677	29.46	0.023159			10	21.05
30	0.694	0.712	0.68	0.695333	0.425667	0.37972	37.97	0.016042			20	29.46
40	0.413	0.496	0.48	0.463	0.658	0.586976	58.69	0.044034			30	37.97
50	0.312	0.38	0.29	0.327333	0.793667	0.707999	70.79	0.046918			40	58.69

											50	70.79
Raw Data{Wavelength:595.0}												
	1	2	3	4	5	6	7	8	9	10	11	12
A	1.351	1.265	1.31	0.037	0.037	1	1.12	1.09	0.037	1.121	0.718	0.977
B	0.172	0.125	0.113	0.037	0.037	0.137	0.133	0.123	0.038	0.115	0.108	0.104
C	1.189	1.09	0.922	0.046	0.043	0.96	0.848	0.94	0.04	1.149	1.122	1.114
D	0.998	1	1.012	0.039	0.04	0.84	0.745	0.89	0.037	1.124	1.017	1.005
E	0.977	0.912	0.92	0.04	0.04	0.78	0.712	0.695	0.037	0.713	1.214	0.834
F	0.852	0.819	0.8	0.037	0.038	0.694	0.7	0.69	0.037	1.122	1.131	0.965
G	0.612	0.718	0.632	0.043	0.039	0.534	0.497	0.484	0.041	0.977	1.341	0.968
H	0.597	0.435	0.534	0.036	0.037	0.312	0.287	0.356	0.036	0.921	1.584	0.999
17c	IC_{50}=5.11 μM											
	O.D1	O.D2	O.D3	AVG	CTRL-TEST	CTRL-TEST/CTRL	*100	stdev.				
CONTROL	1.351	1.265	1.31	1.308667	0	0	0				standard deviation	
DMSO	0.172	0.125	0.113	0.136667	1.172	0.895568	89.55	0.031182			89.55±	0.03
1	1.189	1.09	0.922	1.067	0.241667	0.184666	18.46	0.134978			18.46±	0.134
10	0.998	1	1.012	1.003333	0.305333	0.233316	23.33	0.007572			23.33±	0.07
20	0.977	0.912	0.92	0.936333	0.372333	0.284513	28.45	0.035445			28.45±	0.03
30	0.852	0.819	0.8	0.823667	0.485	0.370606	37.06	0.026312			37.06±	0.02
40	0.612	0.718	0.632	0.654	0.654667	0.500255	50.25	0.056321			50.25±	0.056
50	0.597	0.435	0.534	0.522	0.786667	0.601121	60.11	0.081664			60.11±	0.08
17d	IC_{50}= 4.635 μM											
	O.D1	O.D2	O.D3	AVG	CTRL-	CTRL-	*100	stdev.				

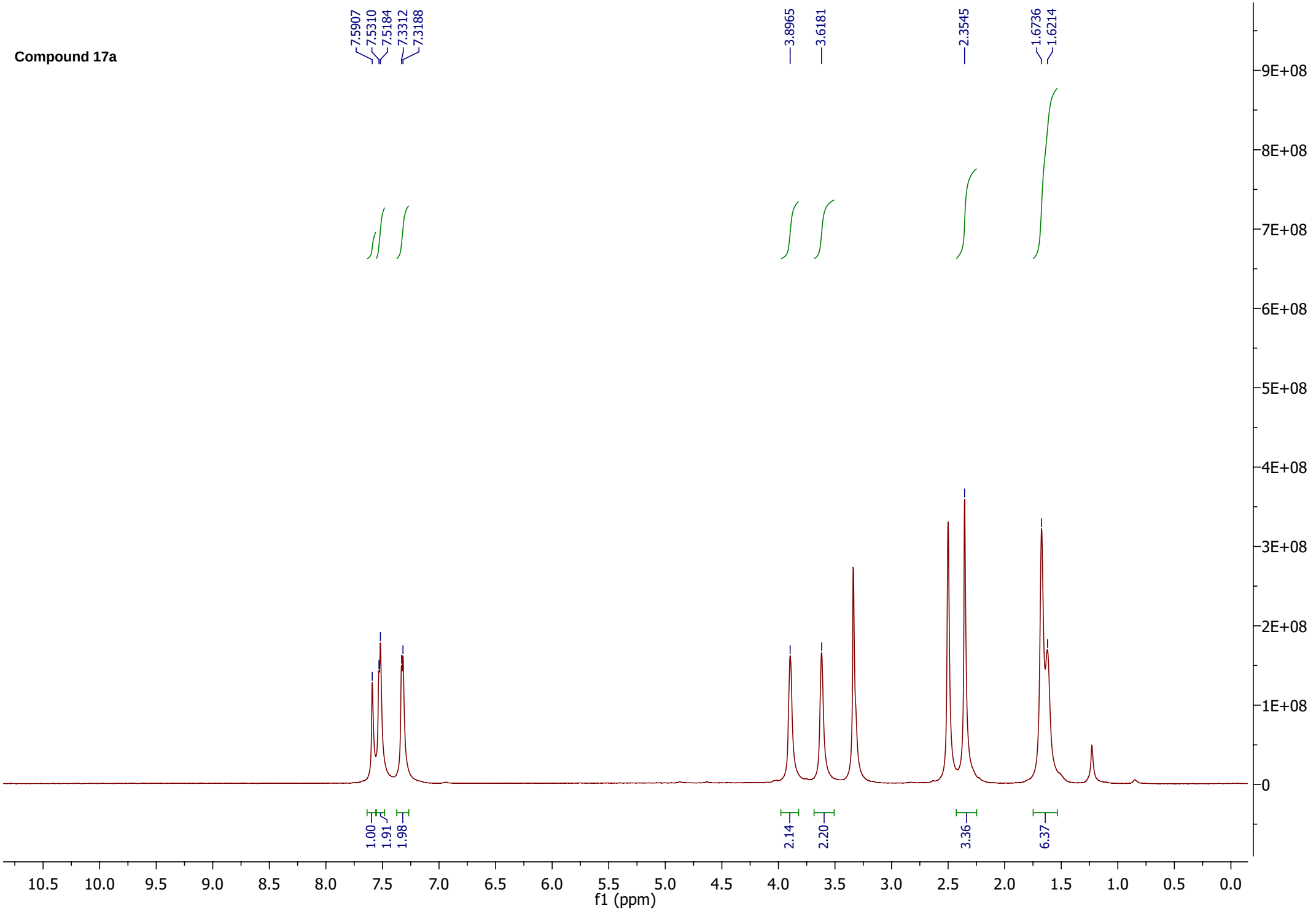
					TEST	TEST/CTRL						
CONTROL	1	1.12	1.09	1.07	0	0	0				CONTROL	0
DMSO	0.137	0.133	0.123	0.131	0.939	0.87757	87.77	0.007211			DMSO	87.77
1	0.96	0.848	0.94	0.916	0.154	0.143925	14.39	0.059733			1	14.39
10	0.84	0.745	0.89	0.825	0.245	0.228972	22.89	0.073655			10	22.89
20	0.78	0.712	0.695	0.729	0.341	0.318692	31.86	0.044978			20	31.86
30	0.694	0.7	0.69	0.694667	0.375333	0.350779	35.07	0.005033			30	35.07
40	0.534	0.497	0.484	0.505	0.565	0.528037	52.8	0.025942			40	52.8
50	0.312	0.287	0.356	0.318333	0.751667	0.702492	70.24	0.034933			50	70.24

EC_{50} of the active compounds against MDA453 cells												
Raw Data{Wavelength:595.0}												
	1	2	3	4	5	6	7	8	9	10	11	12
A	1.213	1.287	1.354	1.176	1.119	1.321	1.381	1.267	1.27	1.324	1.295	1.213
B	0.421	0.499	0.567	0.662	0.654	0.664	0.487	0.512	0.521	0.421	0.486	0.496
C	0.912	0.873	0.823	0.823	0.812	0.884	0.885	0.9	0.912	0.987	1	1.03
D	0.732	0.741	0.784	0.784	0.8	0.723	0.791	0.775	0.8	0.812	0.893	0.892
E	0.612	0.7	0.63	0.572	0.556	0.589	0.712	0.7	0.685	0.783	0.745	0.81
F	0.512	0.523	0.546	0.418	0.423	0.419	0.585	0.598	0.612	0.634	0.698	0.672
G	0.498	0.432	0.441	0.312	0.388	0.387	0.421	0.482	0.456	0.535	0.519	0.547
H	0.034	0.036	0.032	0.037	0.039	0.038	0.04	0.04	0.039	0.036	0.049	0.038
17c	IC_{50} value=3.34 μM											
	O.D1	O.D2	O.D3	AVG	CTRL-TEST	CTRL-TEST/CTRL	*100	stdev.				
control	1.213	1.287	1.354	1.284667	0	0	0	0.070529				
DMSO	0.421	0.499	0.567	0.495667	0.789	0.614167	61.41671	0.073057				
10	0.912	0.873	0.823	0.869333	0.415333	0.3233	32.33005	0.044613				
20	0.732	0.741	0.784	0.752333	0.532333	0.414375	41.43747	0.027791				
30	0.612	0.7	0.63	0.647333	0.637333	0.496108	49.61079	0.04649				
40	0.512	0.523	0.546	0.527	0.757667	0.589777	58.97769	0.017349				
50	0.498	0.432	0.441	0.457	0.827667	0.644266	64.42657	0.035791				

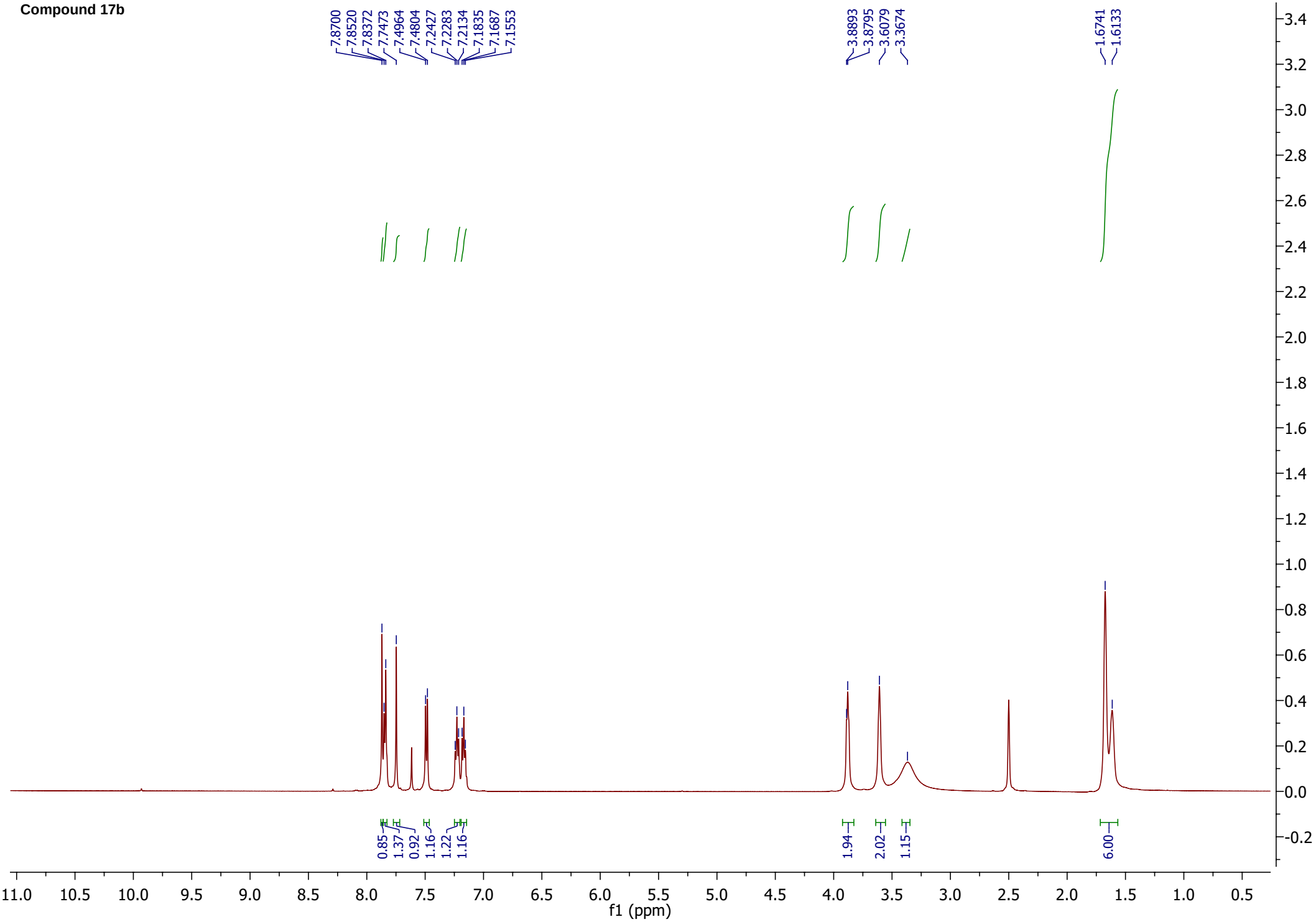
17d	IC_{50}= 3.15 μM											
	O.D1	O.D2	O.D3	AVG	CTRL-TEST	CTRL-TEST/CTRL	*100	stdev.				
control	1.176	1.119	1.321	1.205333	0	0	0	0.104146				
DMSO	0.662	0.654	0.664	0.66	0.545333	0.452434	45.24336	0.005292				
10	0.823	0.812	0.884	0.839667	0.365667	0.303374	30.33739	0.038786				
20	0.784	0.8	0.723	0.769	0.436333	0.362002	36.20022	0.040632				
30	0.572	0.556	0.589	0.572333	0.633	0.525166	52.51659	0.016503				
40	0.418	0.423	0.419	0.42	0.785333	0.651549	65.15487	0.002646				
50	0.312	0.388	0.387	0.362333	0.843	0.699392	69.93916	0.043593				
17i	IC_{50} = 3.5 μM											
	O.D1	O.D2	O.D3	AVG	CTRL-TEST	CTRL-TEST/CTRL	*100	stdev.				
control	1.381	1.267	1.27	1.306	0	0	0	0.064969				
DMSO	0.487	0.512	0.521	0.506667	0.799333	0.612047	61.2047	0.017616				
10	0.885	0.9	0.912	0.899	0.407	0.311639	31.16386	0.013528				
20	0.791	0.775	0.8	0.788667	0.517333	0.39612	39.61205	0.012662				
30	0.712	0.7	0.685	0.699	0.607	0.464778	46.47779	0.013528				
40	0.585	0.598	0.612	0.598333	0.707667	0.541858	54.18581	0.013503				
50	0.421	0.482	0.456	0.453	0.853	0.653139	65.31394	0.03061				
17g	IC_{50}= 4.06 μM											
	O.D1	O.D2	O.D3	AVG	CTRL-TEST	CTRL-TEST/CTRL	*100	stdev.				
control	1.324	1.295	1.213	1.277333	0	0	0	0.05757				
DMSO	0.421	0.486	0.496	0.467667	0.809667	0.633873	63.38727	0.040723				
10	0.987	1	1.03	1.005667	0.271667	0.212683	21.26827	0.022053				
20	0.812	0.893	0.892	0.865667	0.411667	0.322286	32.2286	0.046479				
30	0.783	0.745	0.81	0.779333	0.498	0.389875	38.98747	0.032655				
40	0.634	0.698	0.672	0.668	0.609333	0.477035	47.70355	0.032187				
50	0.535	0.519	0.547	0.533667	0.743667	0.582203	58.22025	0.014048				

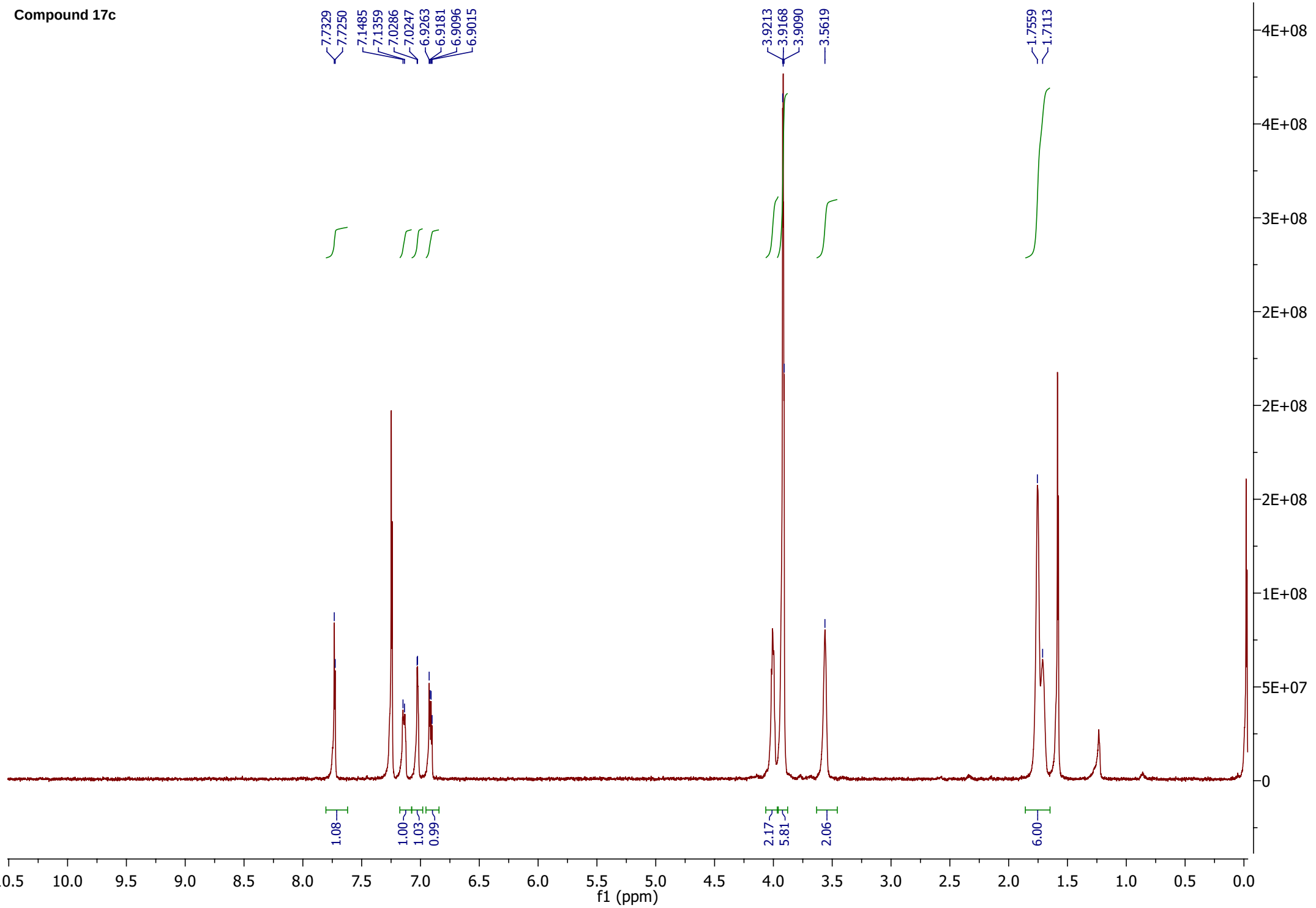
EC_{50} of Etoposide against MCF7 cells												
Raw Data{Wavelength:595.0}												
	1	2	3	4	5	6	7	8	9	10	11	12
A	1.121	1.261	1.145	0.036	0.037	0.037	0.036	0.036	0.037	0.037	0.037	0.036
B	0.551	0.665	0.519	0.037	0.038	0.037	0.037	0.037	0.037	0.037	0.037	0.037
C	0.643	0.591	0.612	0.038	0.042	0.038	0.038	0.039	0.038	0.038	0.038	0.04
D	0.534	0.567	0.5	0.036	0.037	0.038	0.038	0.037	0.037	0.054	0.039	0.037
E	0.447	0.478	0.419	0.036	0.037	0.038	0.058	0.037	0.037	0.038	0.037	0.038
F	0.317	0.345	0.301	0.037	0.038	0.038	0.049	0.039	0.038	0.038	0.036	0.039
G	0.037	0.037	0.037	0.037	0.037	0.038	0.038	0.04	0.037	0.038	0.036	0.036
H	0.036	0.041	0.037	0.037	0.037	0.037	0.036	0.037	0.038	0.036	0.037	0.037
Etoposide	IC_{50} = 2.36 μM											
	O.D1	O.D2	O.D3	AVG	CTRL-TEST	CTRL-TEST/CTRL	*100	stdev				
control	1.121	1.261	1.145	1.175667	0	0	0	0				
DMSO	0.551	0.665	0.519	0.578333	0.59733333	0.508080522	50.8	0.07674				
eto(5)	0.643	0.591	0.612	0.615333	0.56033333	0.476609016	47.66	0.02616				
eto(10)	0.534	0.567	0.5	0.533667	0.642	0.54607315	54.6	0.0335				
eto(15)	0.447	0.478	0.419	0.448	0.72766667	0.618939609	61.89	0.02951				
eto(20)	0.317	0.345	0.301	0.321	0.85466667	0.726963425	72.69	0.02227				

Cytotoxicity screening of the active compounds against COS7 cells												
Raw Data {Wavelength:595.0}												
	1	2	3	4	5	6	7	8	9	10	11	12
A	1.712	1.61	1.663	0.039	0.037	0.037	0.038	0.037	0.038	0.038	0.037	0.037
B	0.501	0.542	0.548	0.039	0.038	0.038	0.038	0.038	0.038	0.039	0.037	0.038
C	1.524	1.672	1.666	0.043	0.04	0.042	0.04	0.04	0.04	0.042	0.04	0.041
D	1.501	1.443	1.594	0.037	0.038	0.037	0.037	0.038	0.038	0.037	0.039	0.038
E	1.309	1.314	1.478	0.033	0.042	0.037	0.039	0.038	0.039	0.038	0.041	0.041
F	1.443	1.5	1.549	0.04	0.041	0.037	0.041	0.038	0.041	0.04	0.039	0.039
G	1.512	1.562	1.496	0.041	0.039	0.038	0.04	0.039	0.041	0.042	0.045	0.04
H	1.5	1.444	1.447	0.042	0.037	0.039	0.037	0.038	0.038	0.037	0.038	0.032
Compounds	**O.D1**	**O.D2**	**O.D3**	**AVG**	**CTRL-TEST**	**CTRL-TEST/CTRL**	***100**	**stdev.**				
control	1.712	1.61	1.663	1.661667	0	0	0	0.051013				
DMSO	0.501	0.542	0.548	0.530333	1.13133333	0.68084253	68.08	0.02558				
17c	1.524	1.672	1.666	1.620667	0.041	0.02467402	2.46	0.08377				
17d	1.501	1.443	1.594	1.512667	0.149	0.08966901	8.96	0.076173				
17e	1.309	1.314	1.478	1.367	0.29466667	0.177332	17.73	0.096161				
17g	1.443	1.5	1.549	1.497333	0.16433333	0.09889669	9.88	0.05305				
17i	1.512	1.562	1.496	1.523333	0.13833333	0.08324975	8.32	0.034429				
17n	1.5	1.444	1.447	1.463667	0.198	0.11915747	11.91	0.031501				

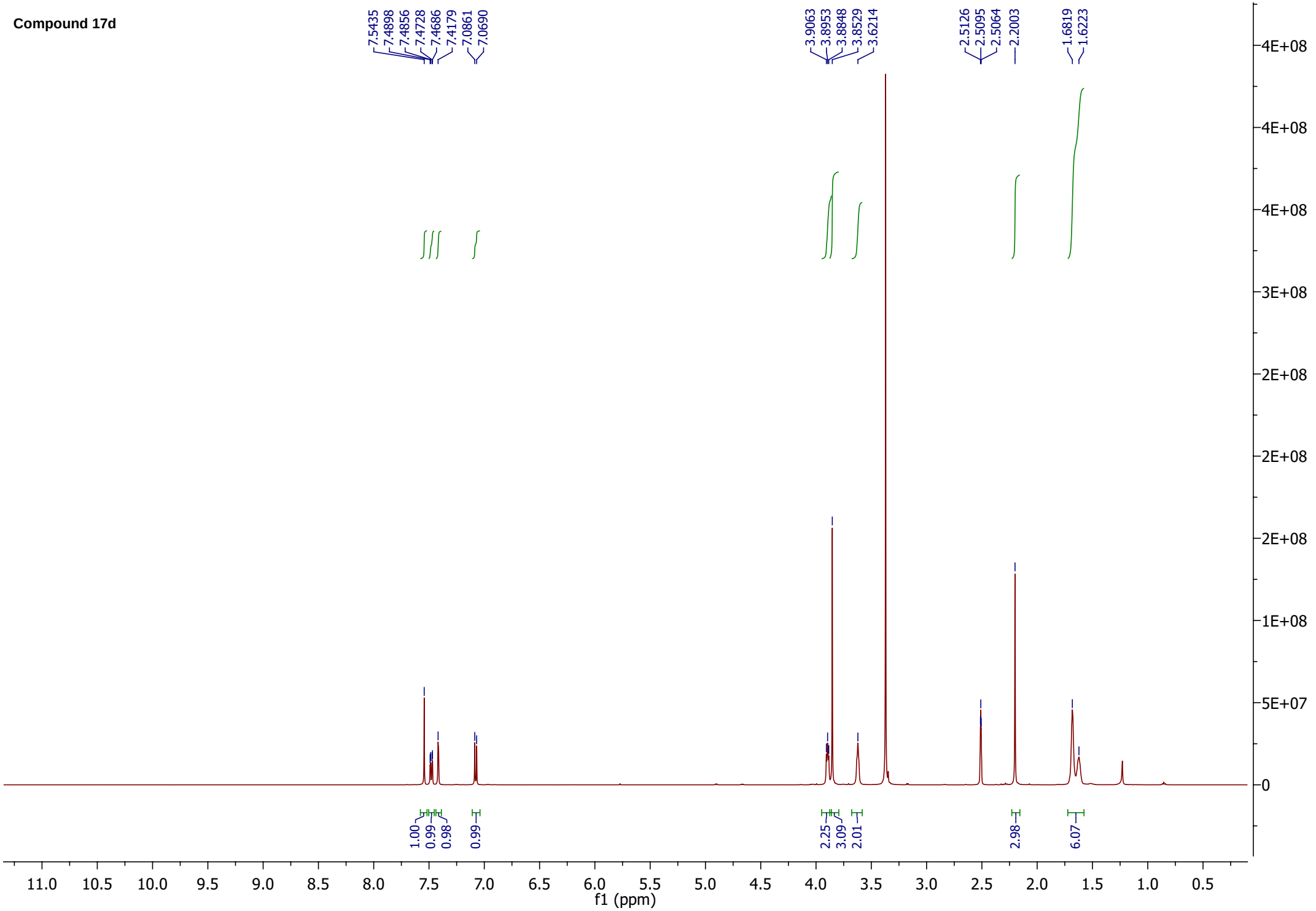

Compound 17a
7.5907
7.5310
7.5184
7.3312
7.3188
3.8965
3.6181
2.3545
1.6736
1.6214
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
1.00
1.91
1.98
2.14
2.20
3.36
6.37
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

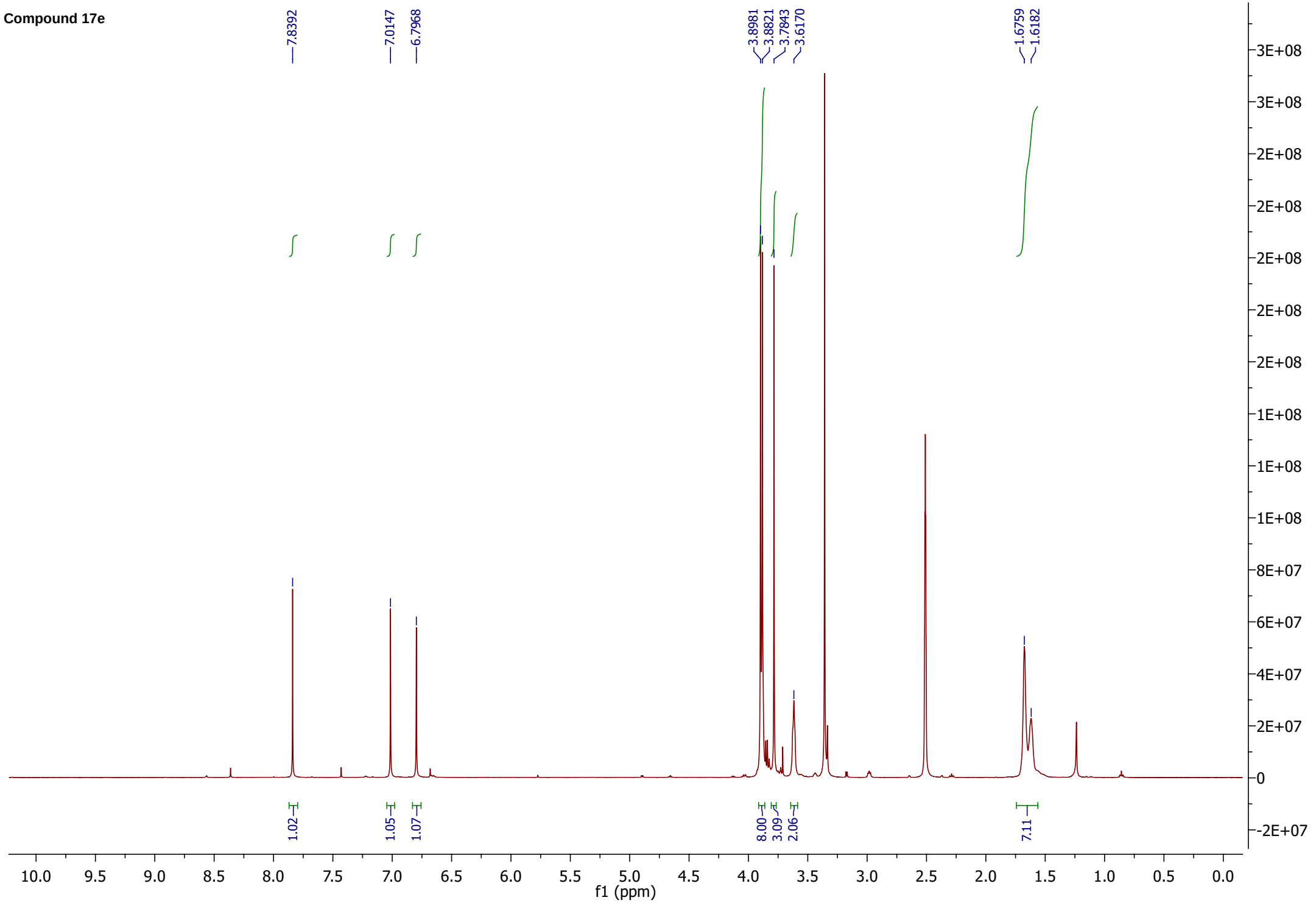
Compound 17b

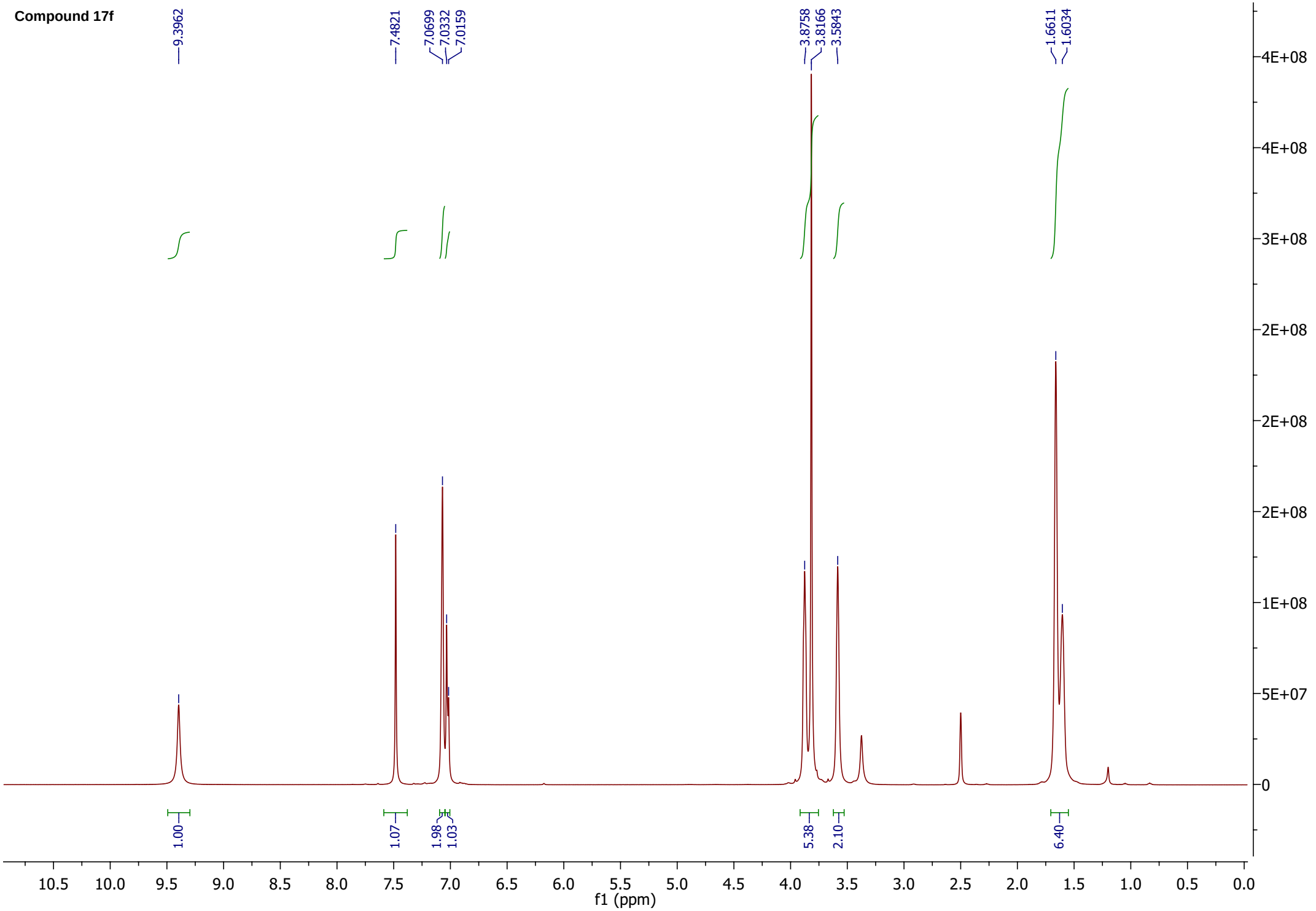



Compound 17c
7.7329
7.7250
7.1485
7.1359
7.0286
7.0247
6.9263
6.9181
6.9096
6.9015
3.9213
3.9168
3.9090
3.5619
1.7559
1.7113
1.08
1.00
1.03
0.99
2.17
5.81
2.06
6.00
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

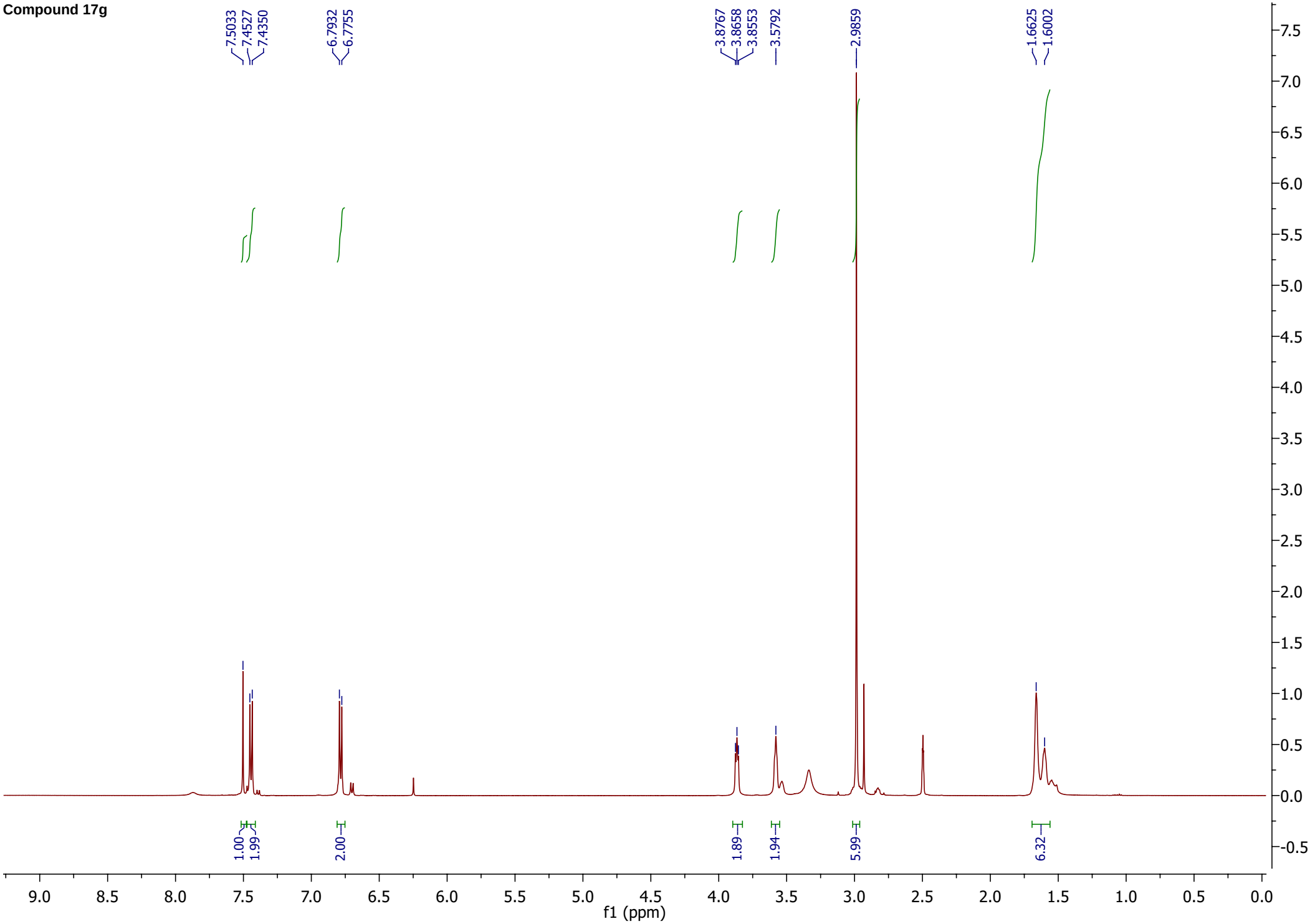
Compound 17d

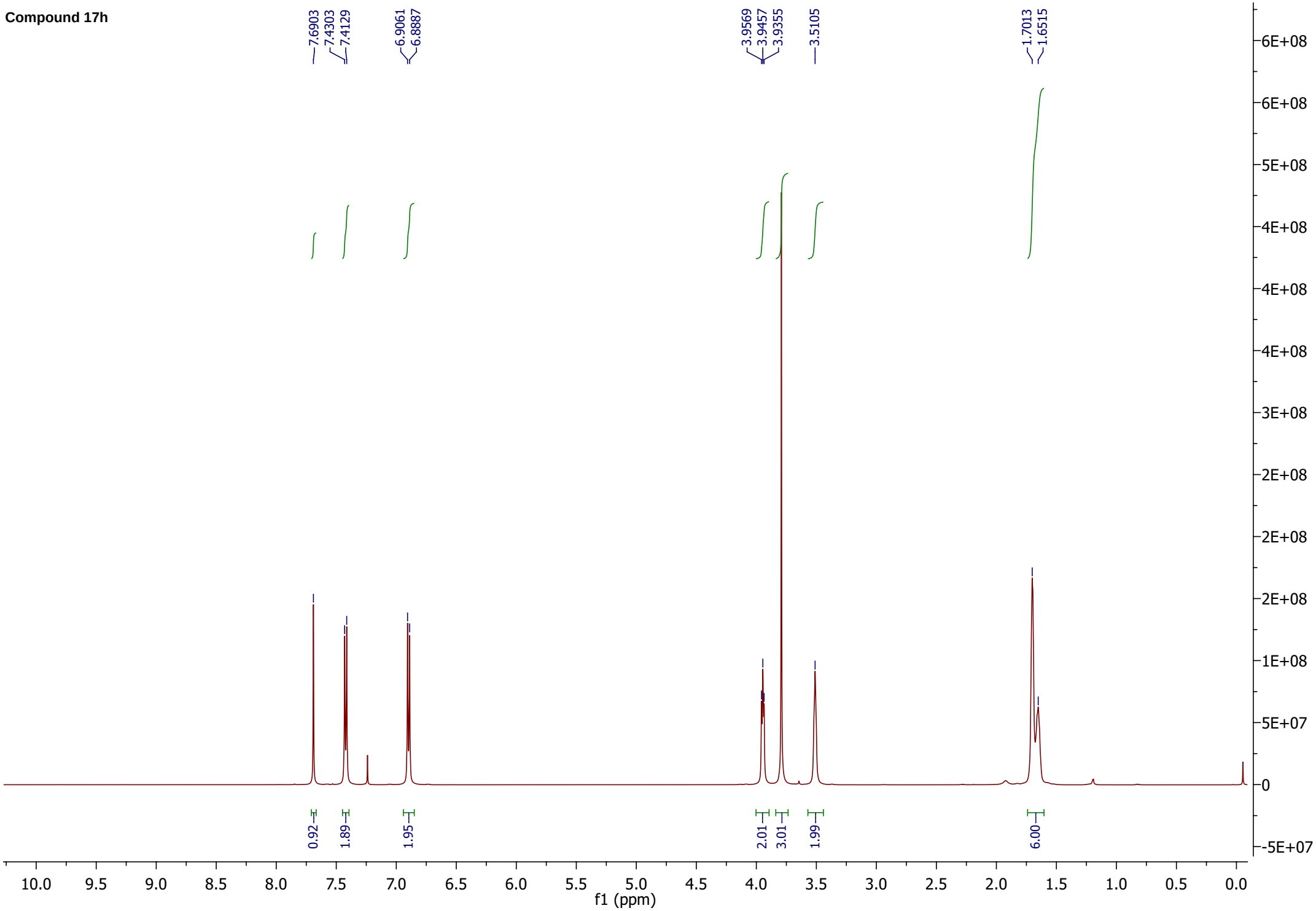



Compound 17e
7.8392
7.0147
6.7968
3.8981
3.8821
3.7843
3.6170
1.6759
1.6182
1.02
1.05
1.07
8.00
3.09
2.06
7.11
3E+08
2E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

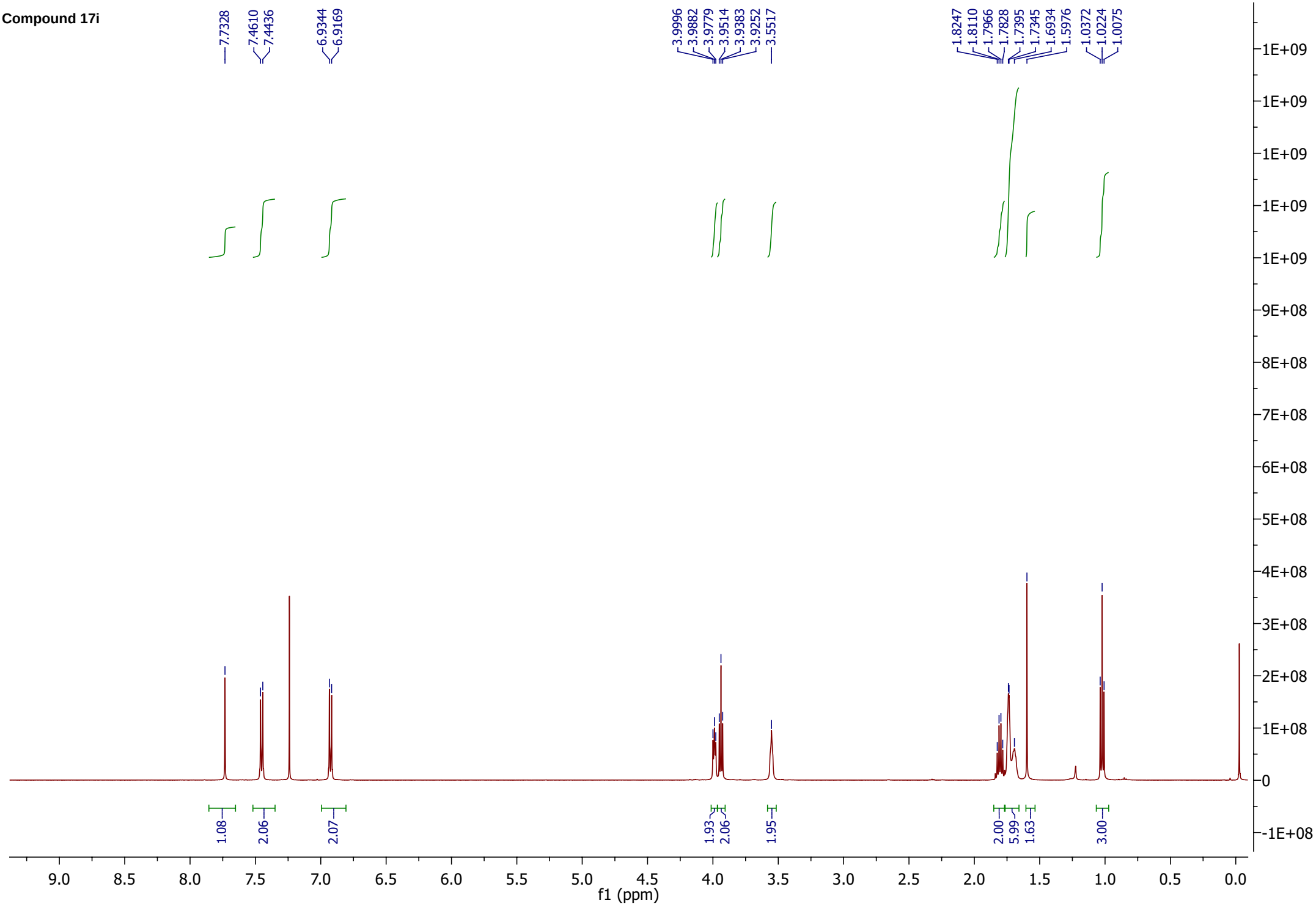

Compound 17f
9.3962
7.4821
7.0699
7.0332
7.0159
3.8758
3.8166
3.5843
1.6611
1.6034
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
1.00
1.07
1.98
1.03
5.38
2.10
6.40
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

Compound 17g

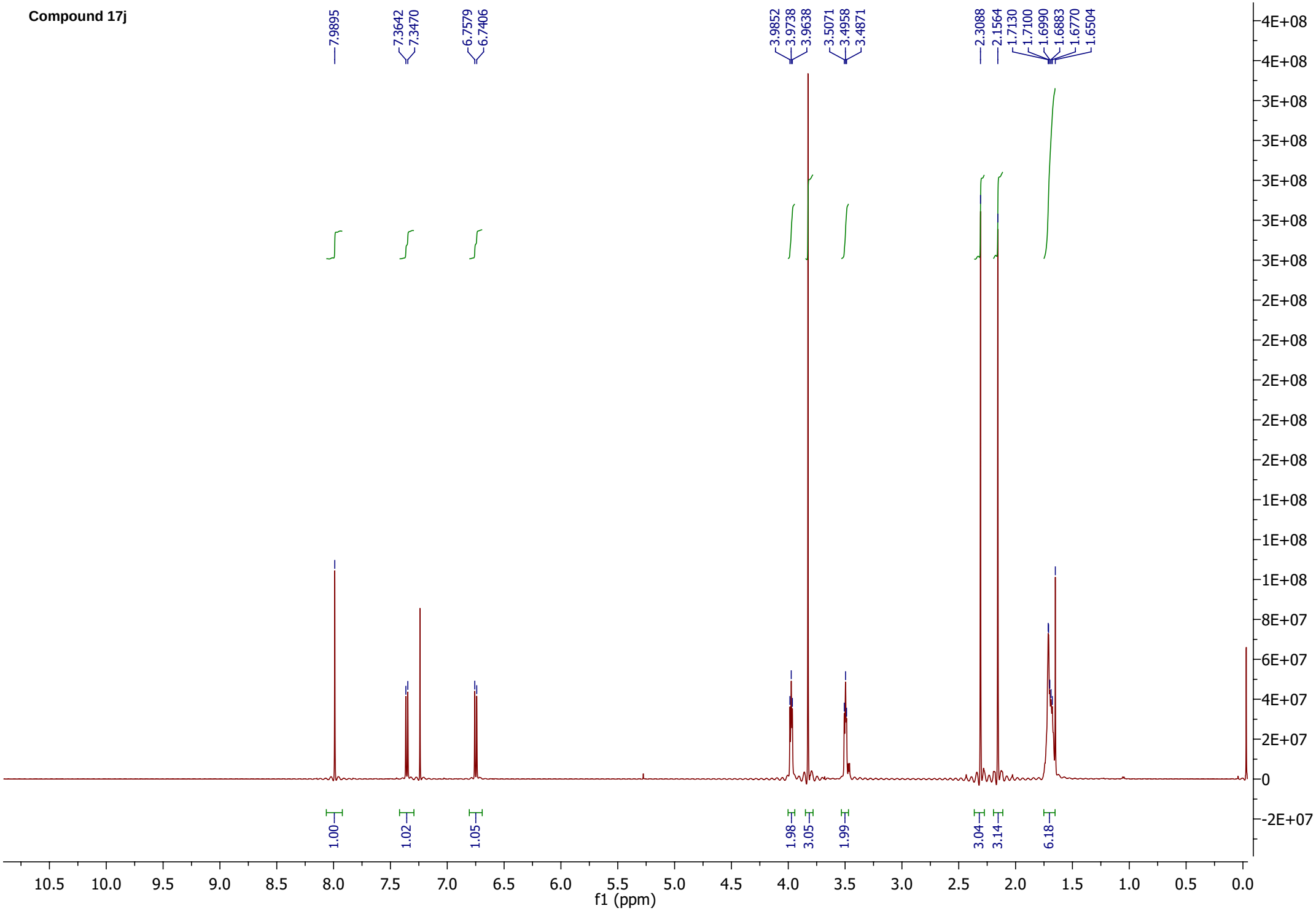


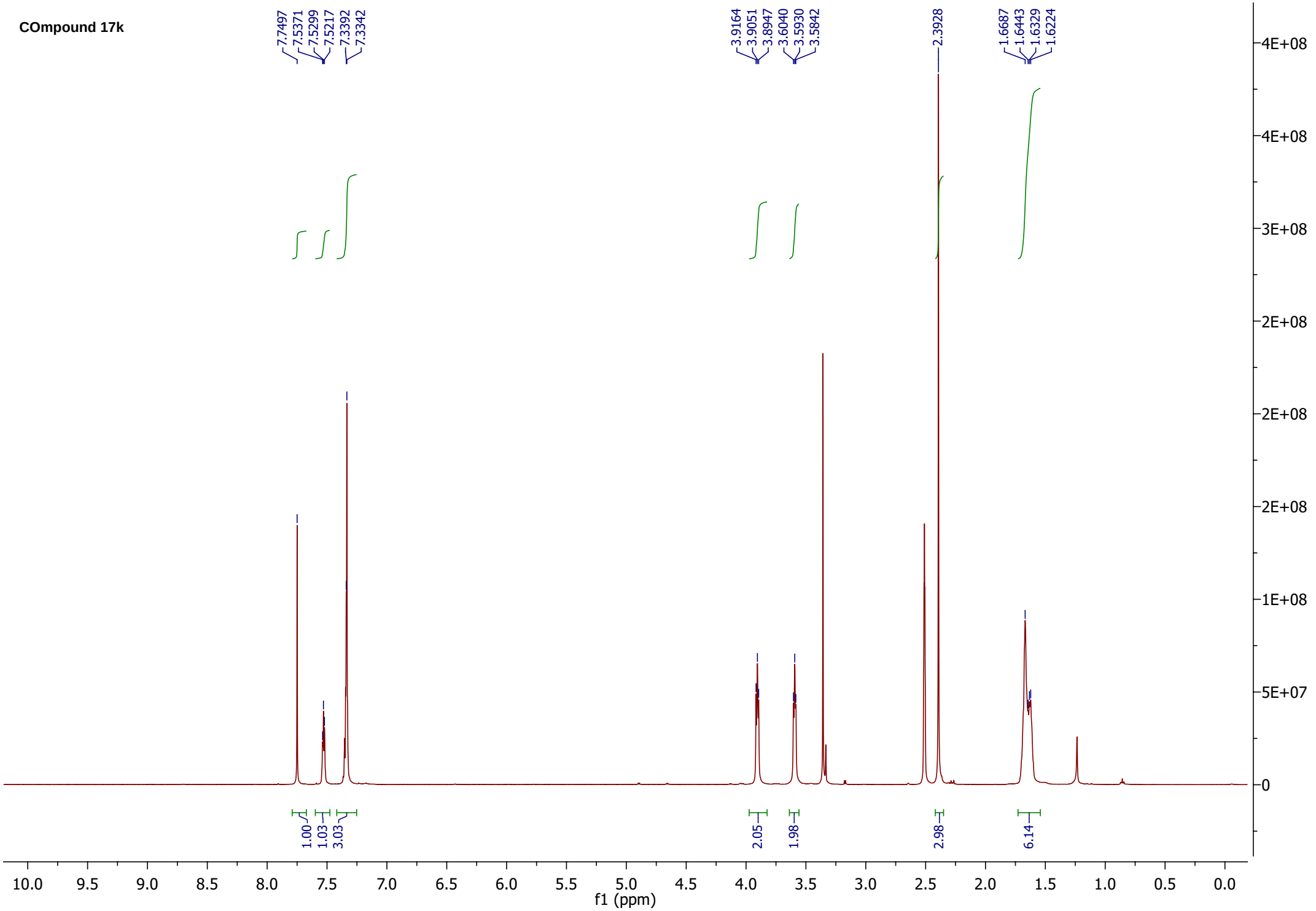

Compound 17h
7.6903
7.4303
7.4129
6.9061
6.8887
3.9569
3.9457
3.9355
3.5105
1.7013
1.6515
0.92
1.89
1.95
2.01
3.01
1.99
6.00
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

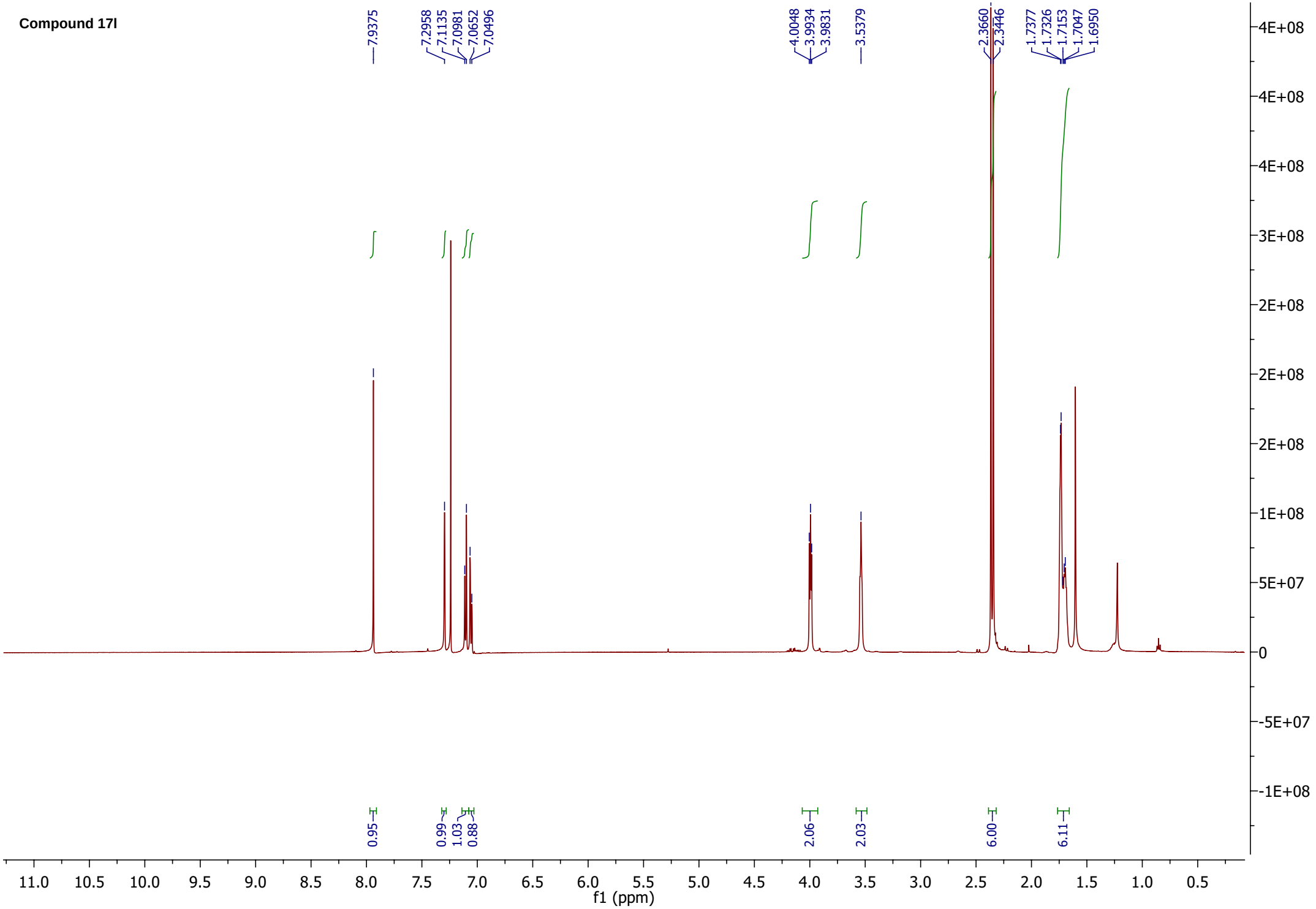
Compound 17i



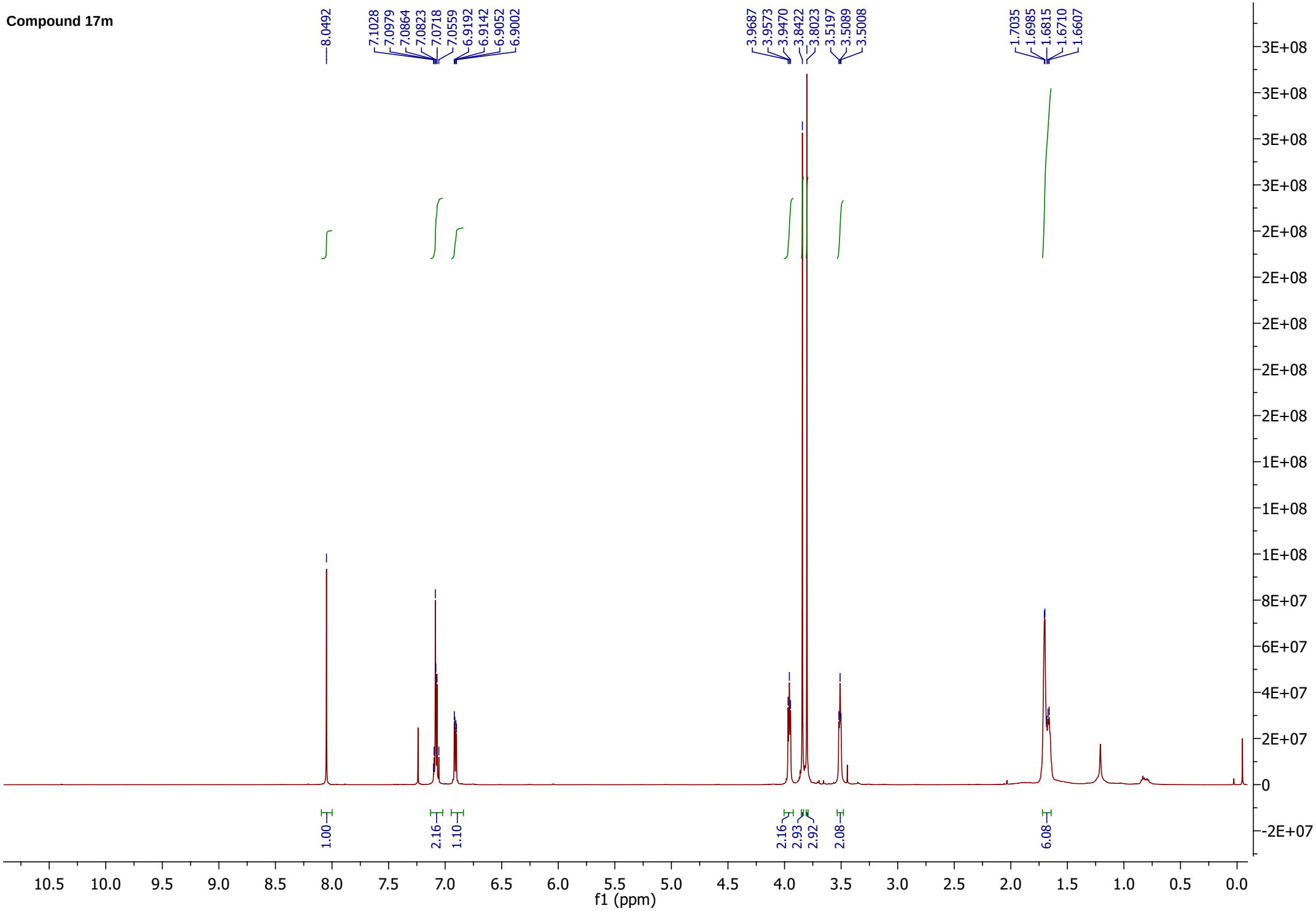
Compound 17j

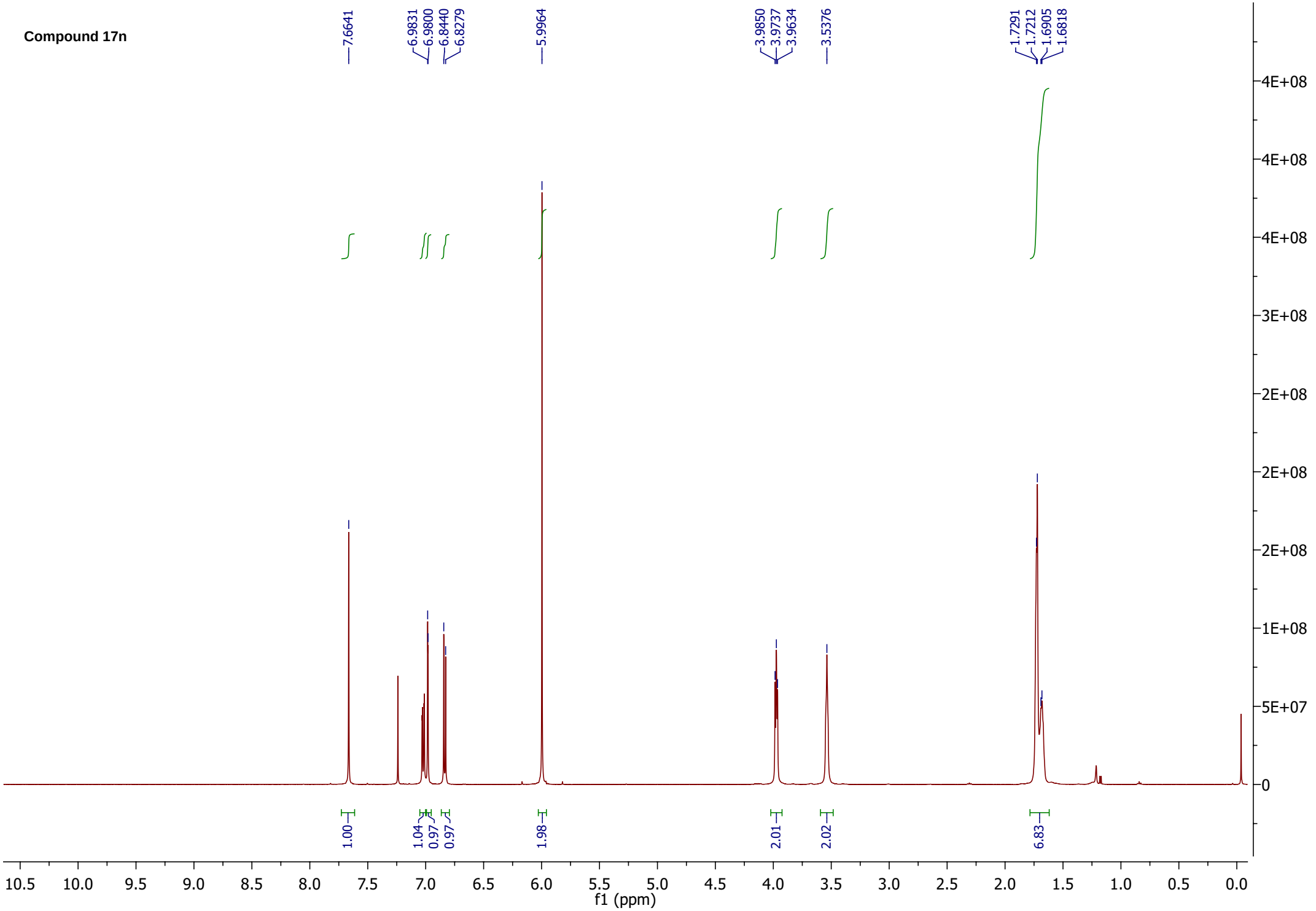



COmpound 17k
7.7497
7.5371
7.5299
7.5217
7.3392
7.3342
3.9164
3.9051
3.8947
3.6040
3.5930
3.5842
2.3928
1.6687
1.6443
1.6329
1.6224
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
1.00
1.03
3.03
2.05
1.98
2.98
6.14
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

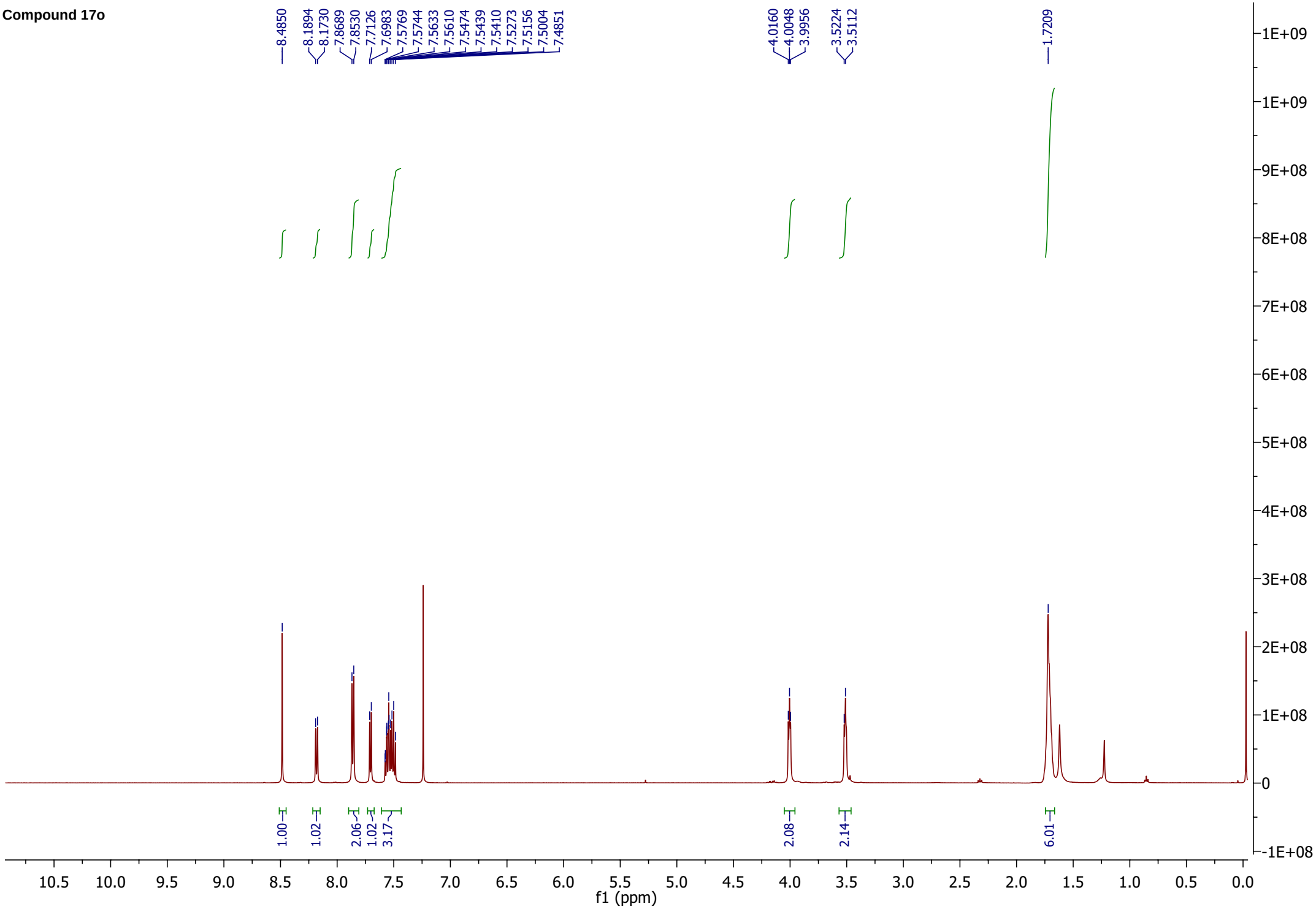

Compound 17l
7.9375
7.2958
7.1135
7.0981
7.0652
7.0496
4.0048
3.9934
3.9831
3.5379
2.3660
2.3446
1.7377
1.7326
1.7153
1.7047
1.6950
0.95
0.99
1.03
0.88
2.06
2.03
6.00
6.11
4E+08
3E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

Compound 17m

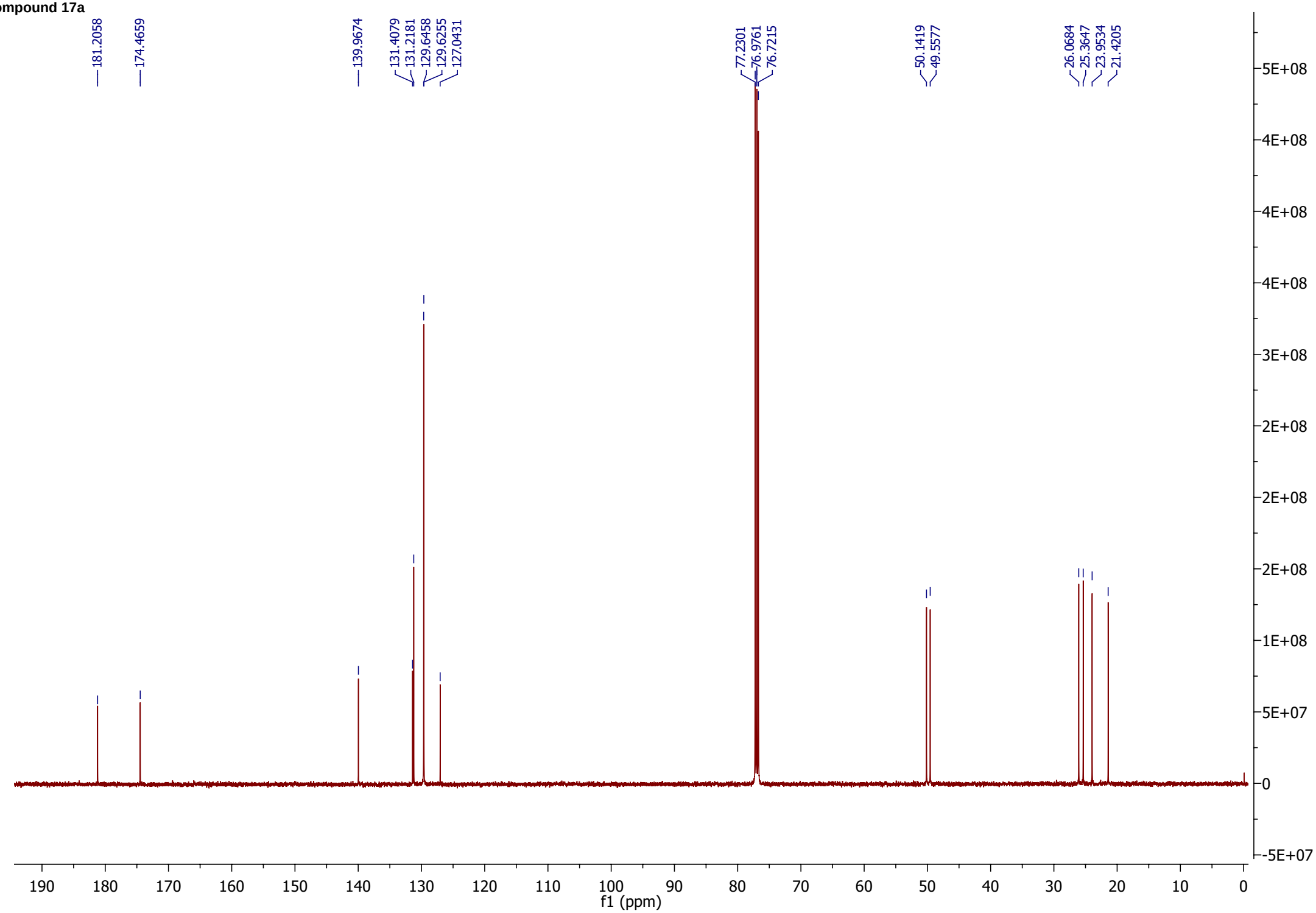



Compound 17n
7.6641
6.9831
6.9800
6.8440
6.8279
5.9964
3.9850
3.9737
3.9634
3.5376
1.7291
1.7212
1.6905
1.6818
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
1.00
1.04
0.97
0.97
1.98
2.01
2.02
6.83
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

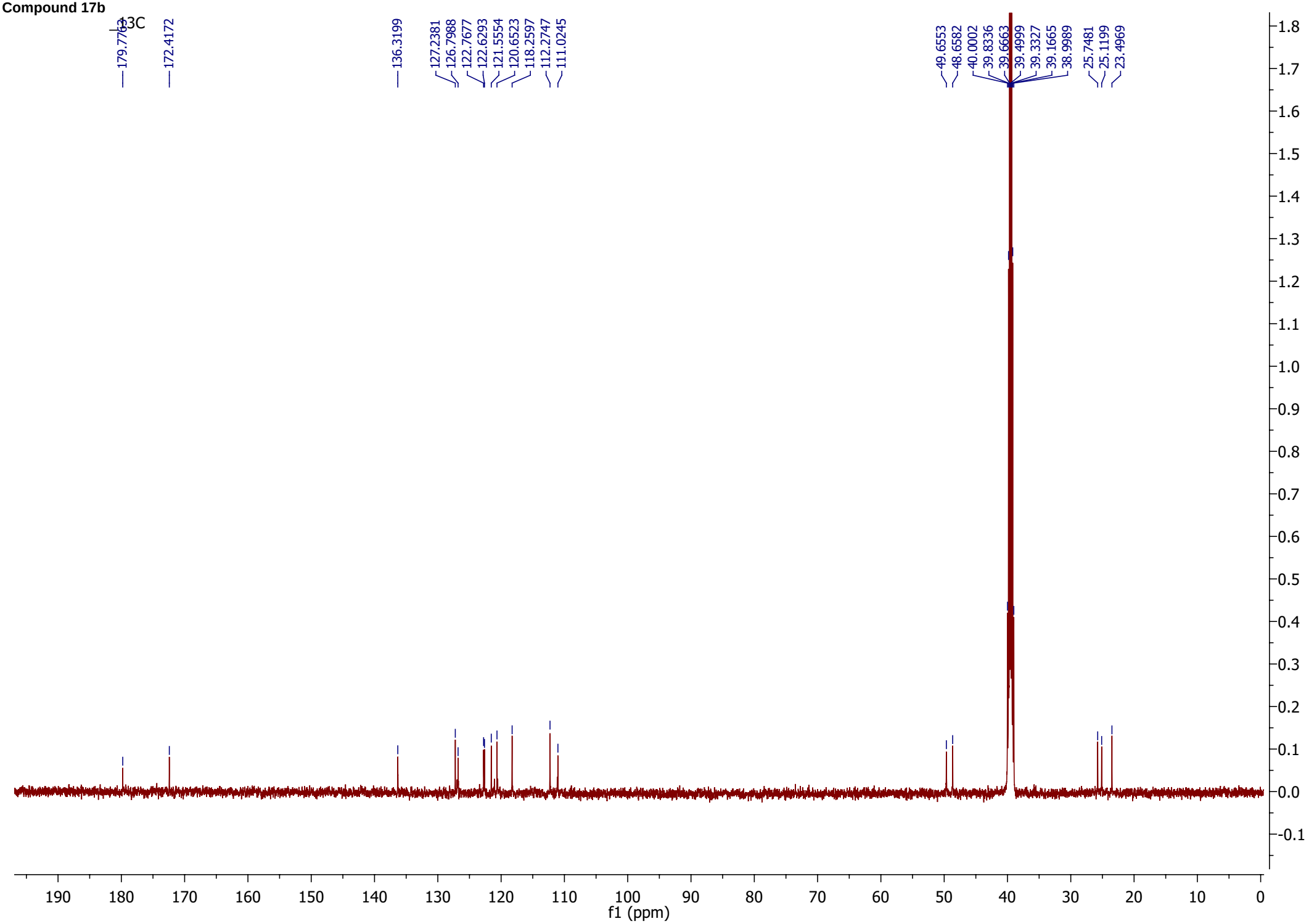
Compound 17o



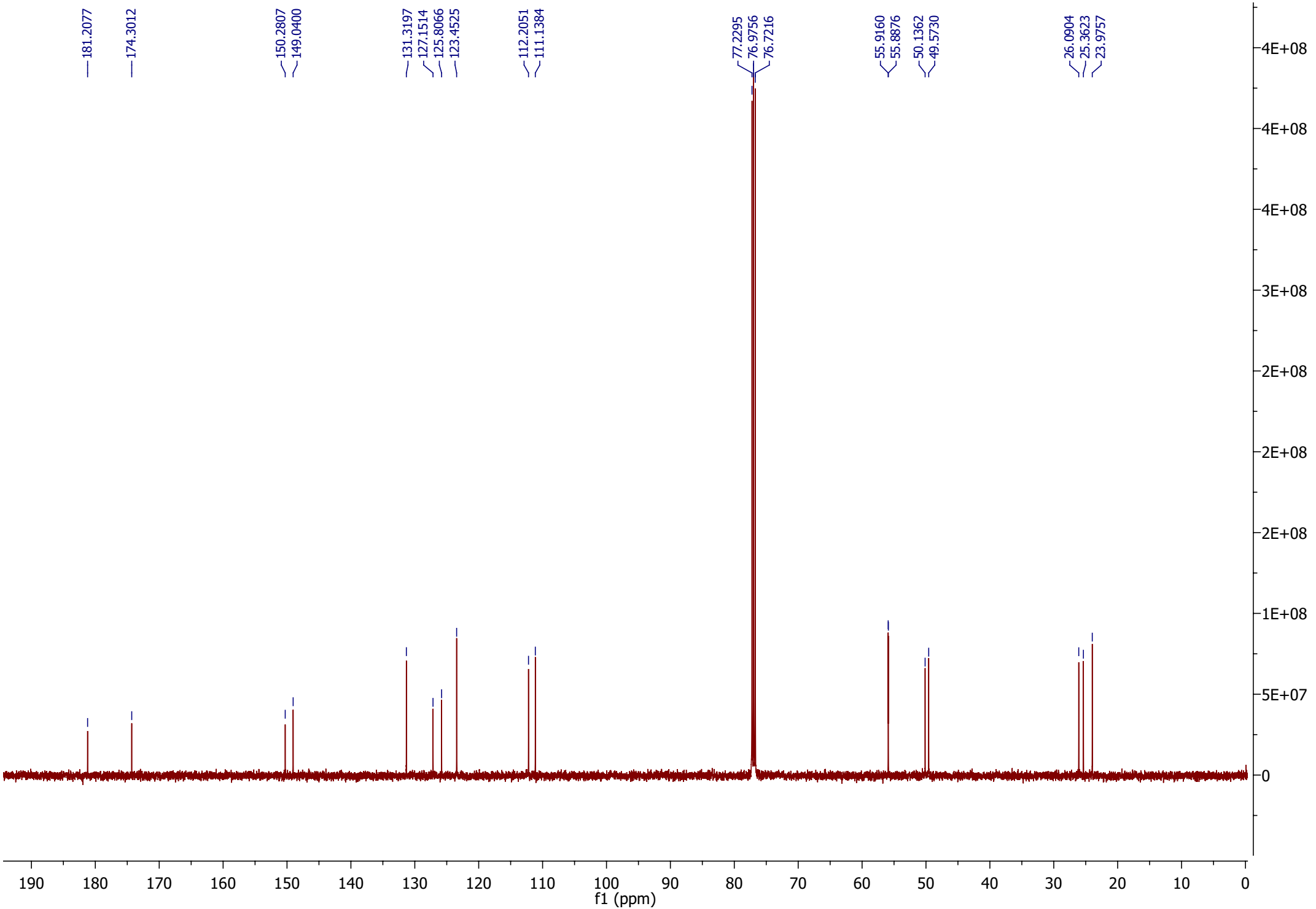
Compound 17a



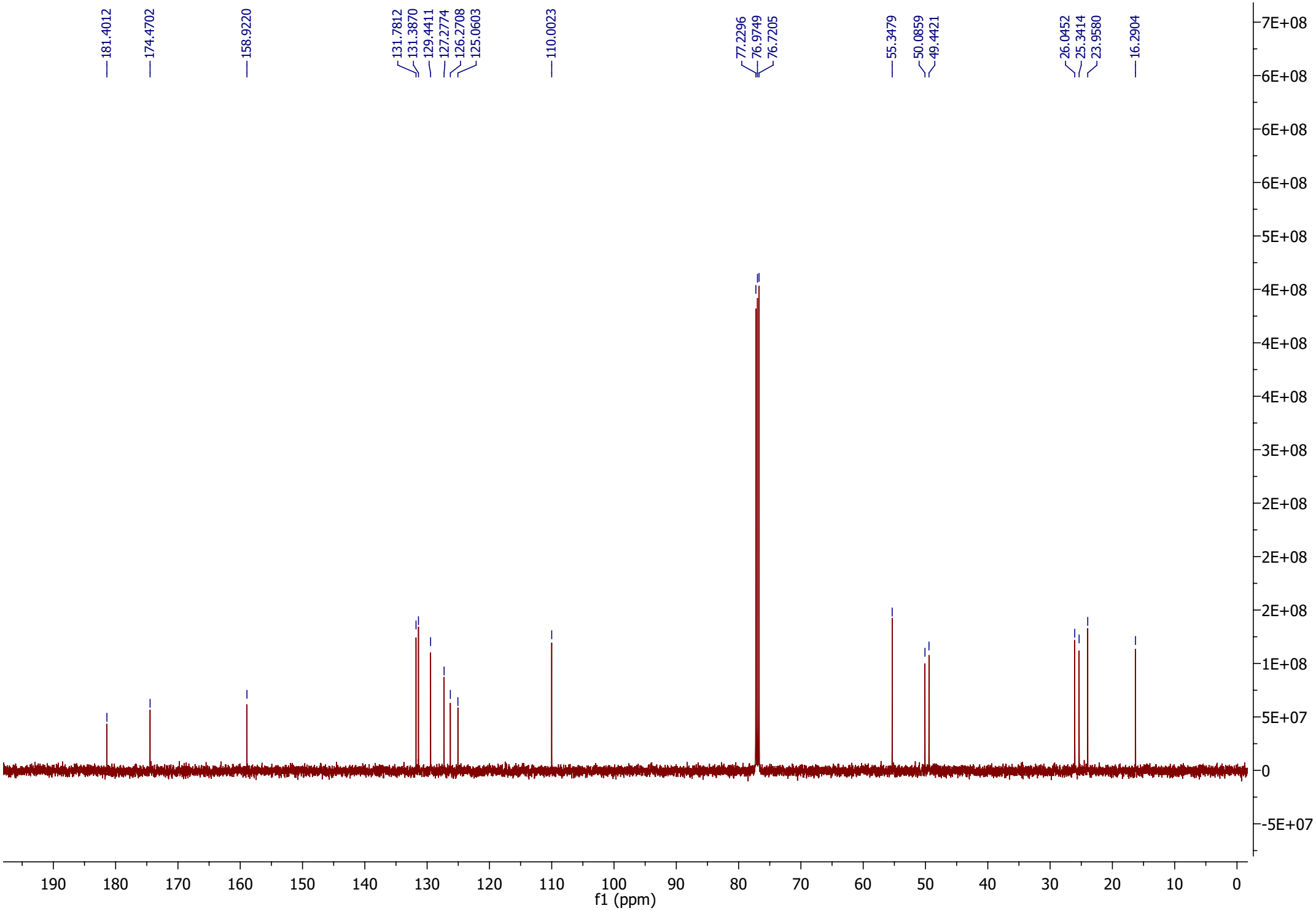
Compound 17b



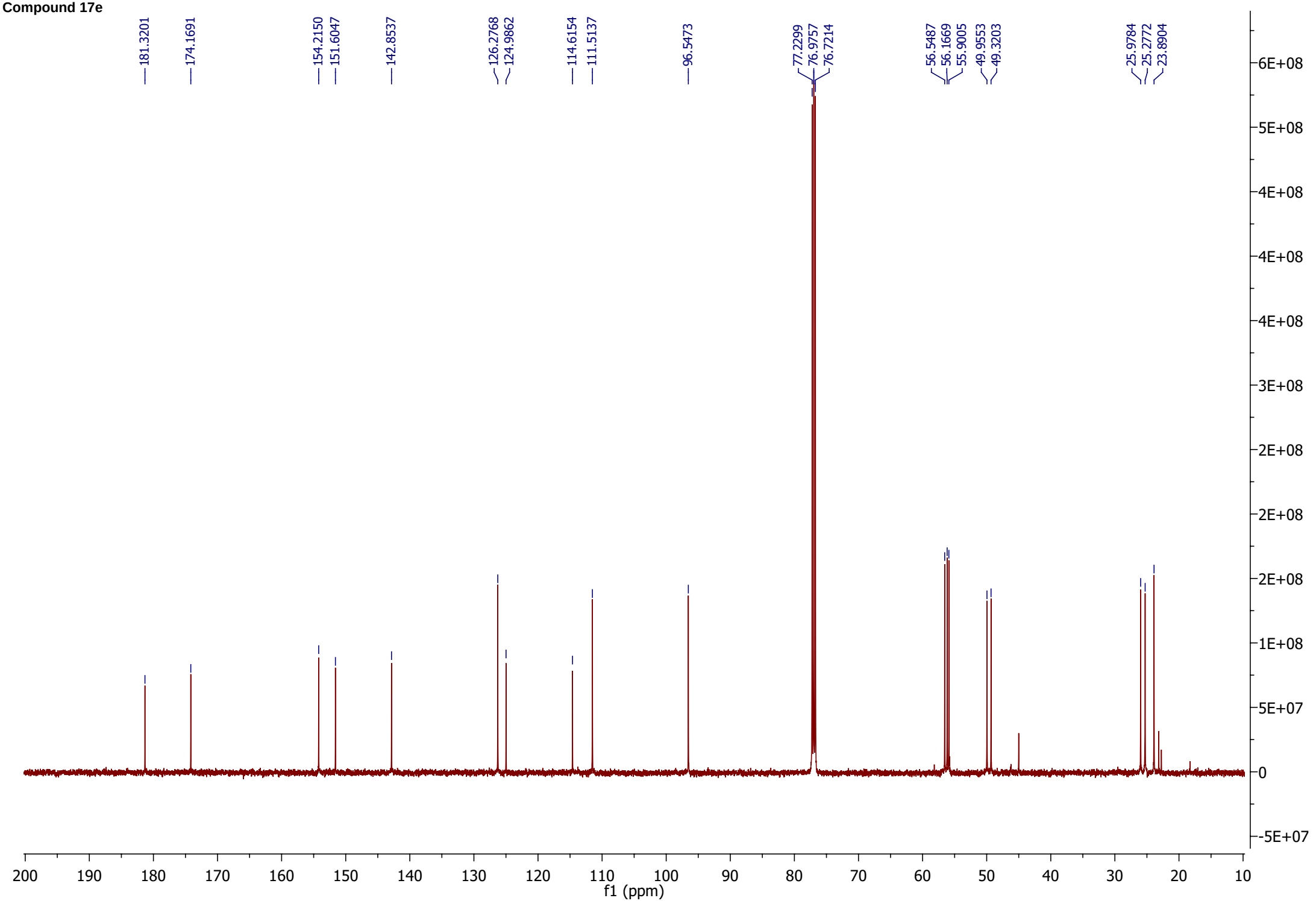
Compound 17c



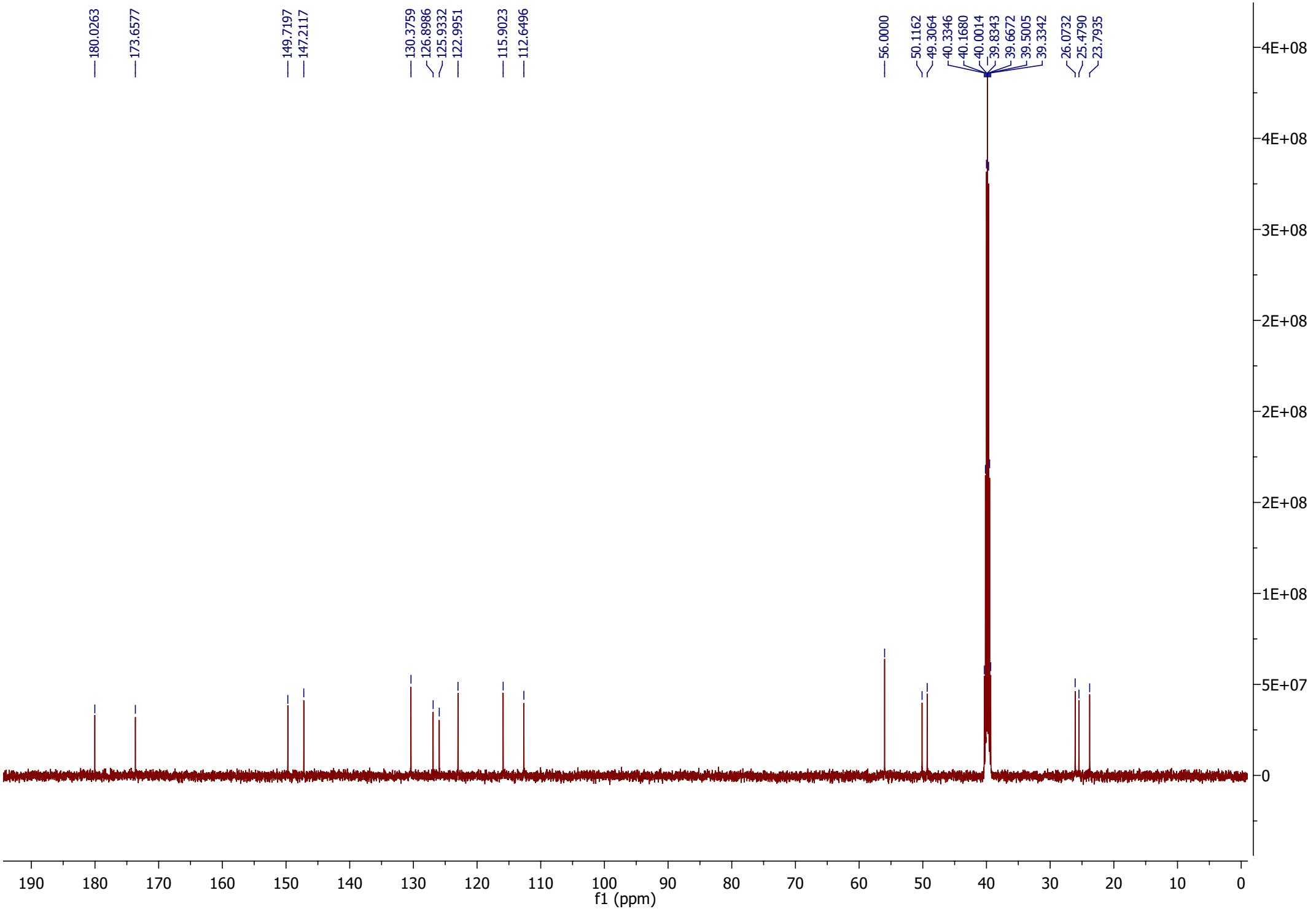
Compound 17d



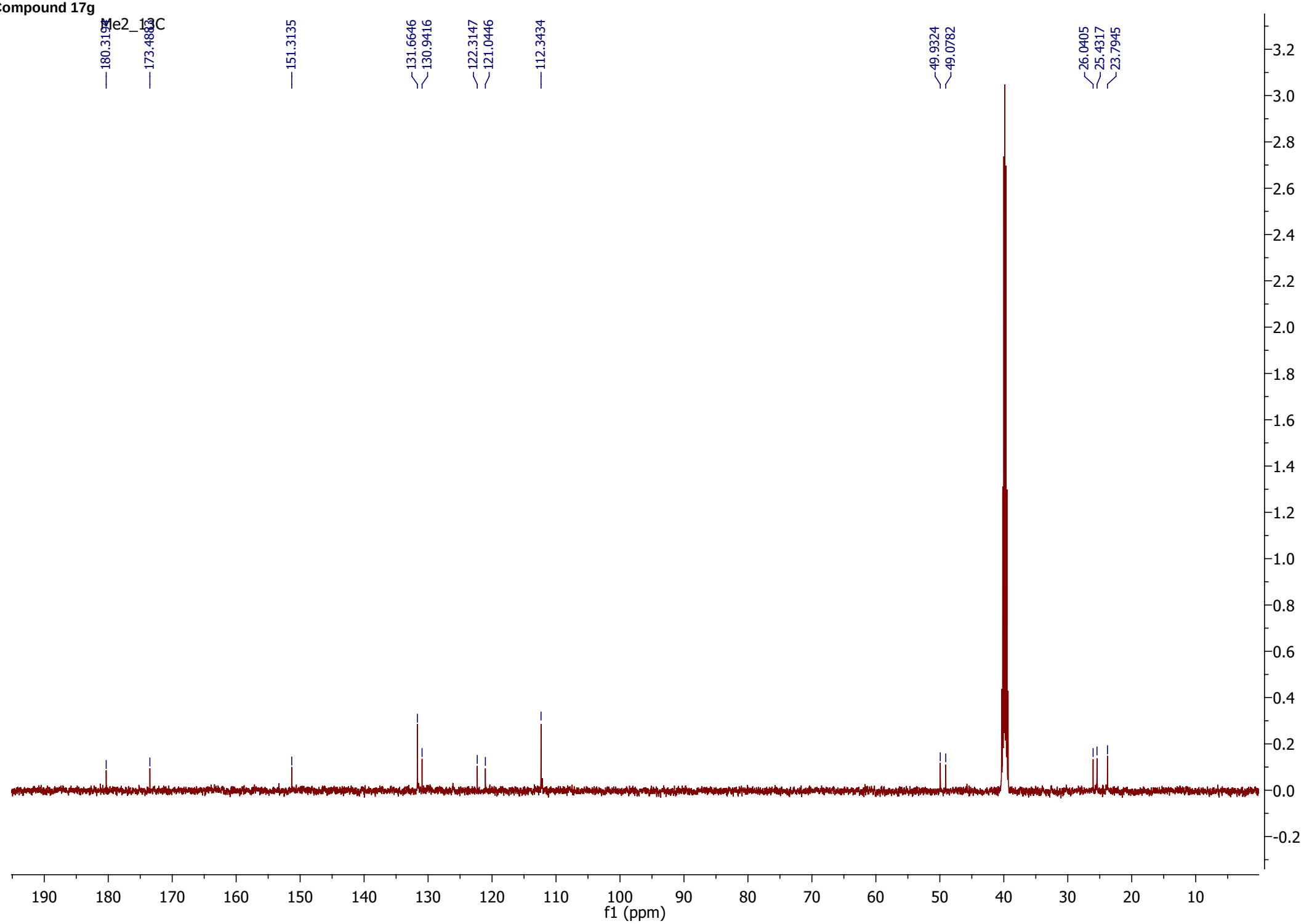
Compound 17e



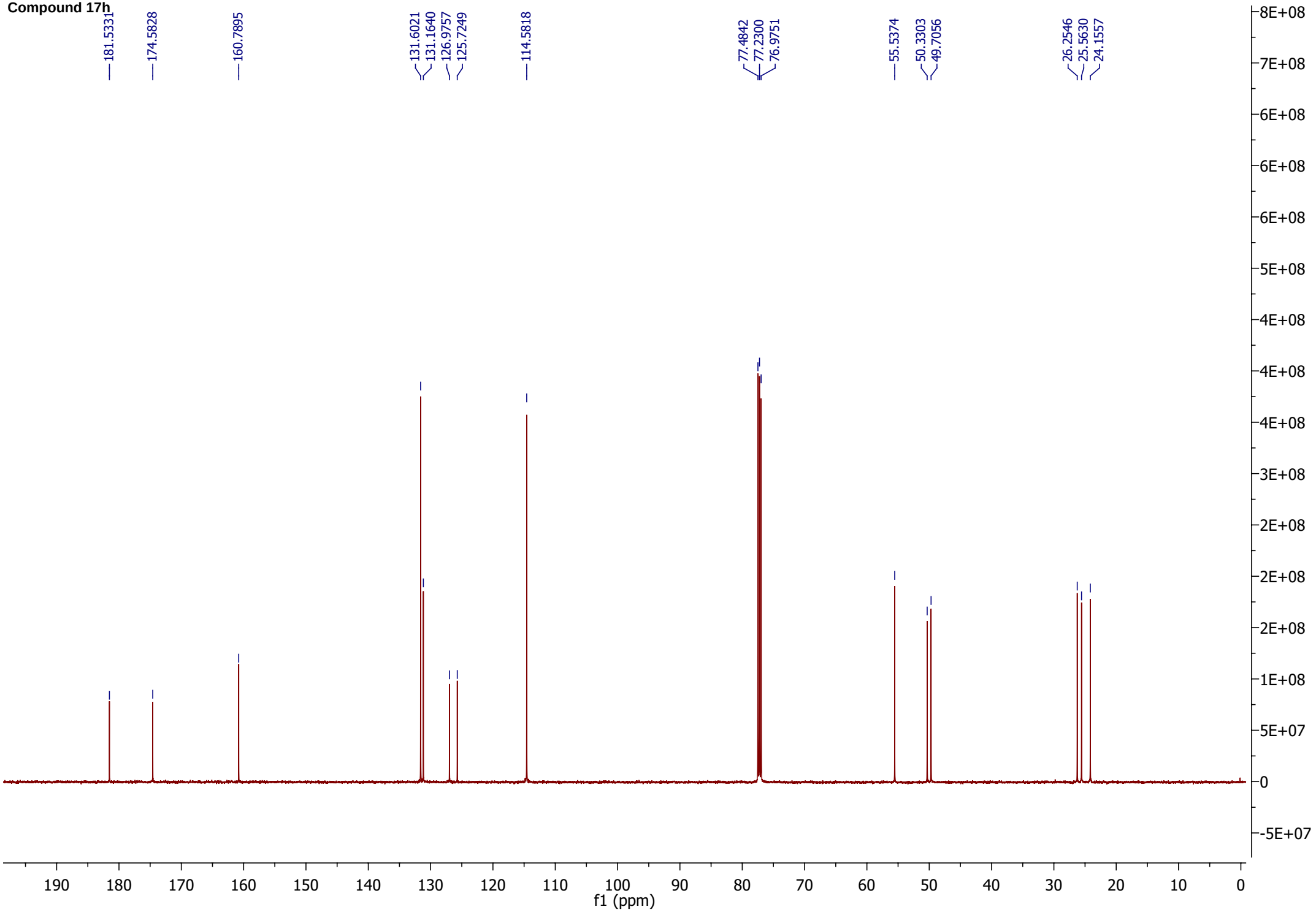
Compound 17f



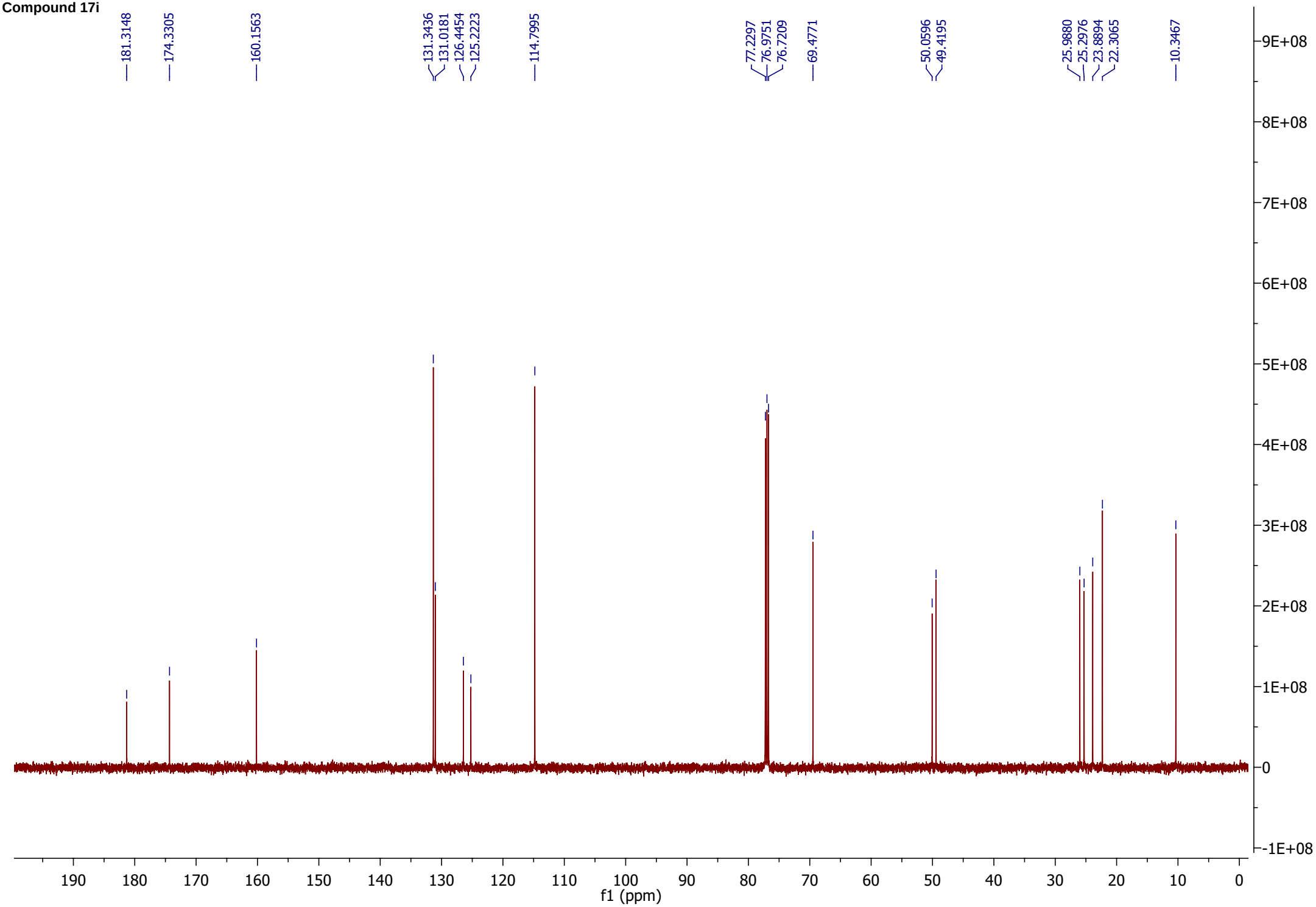
Compound 17g



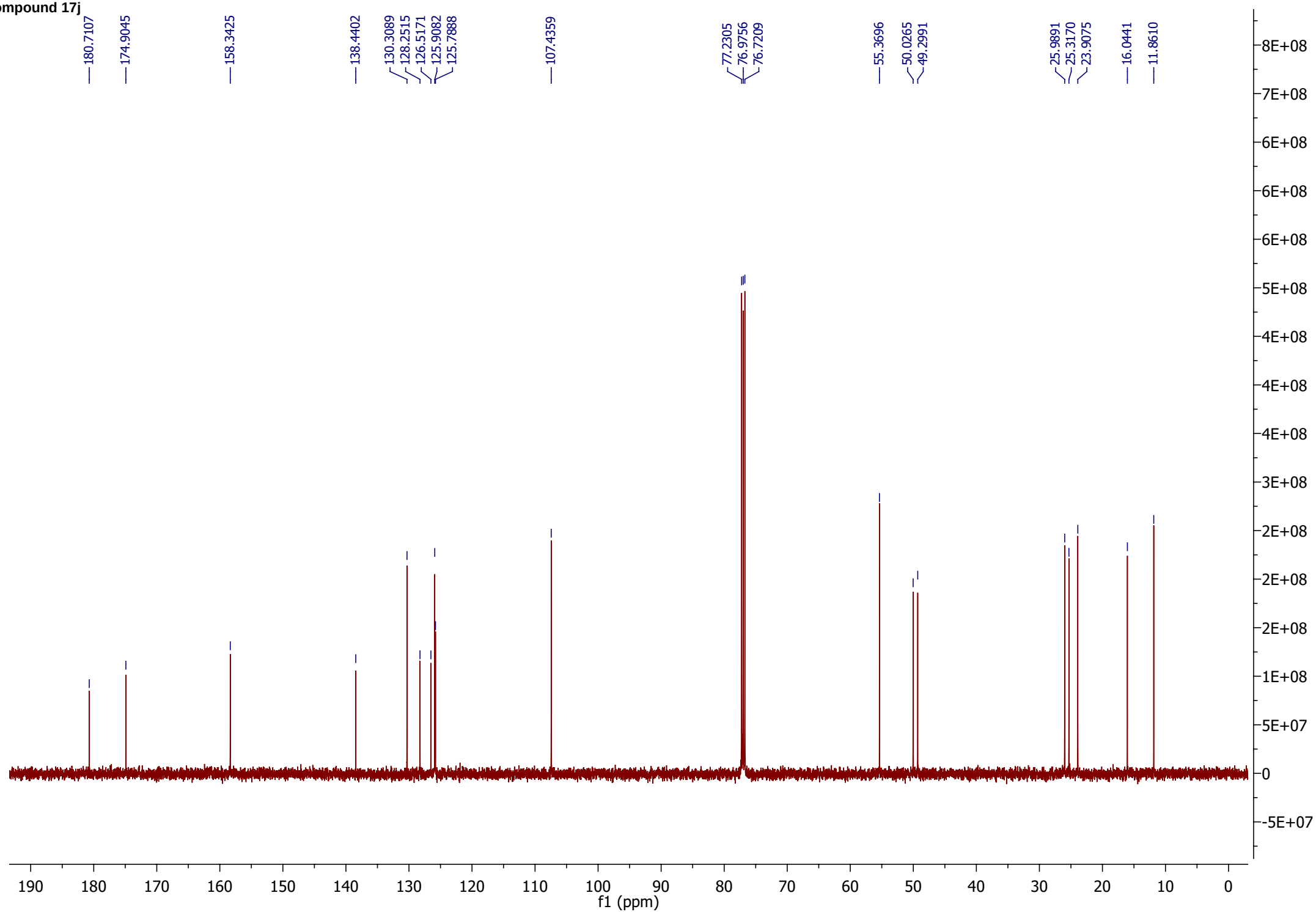
Compound 17h



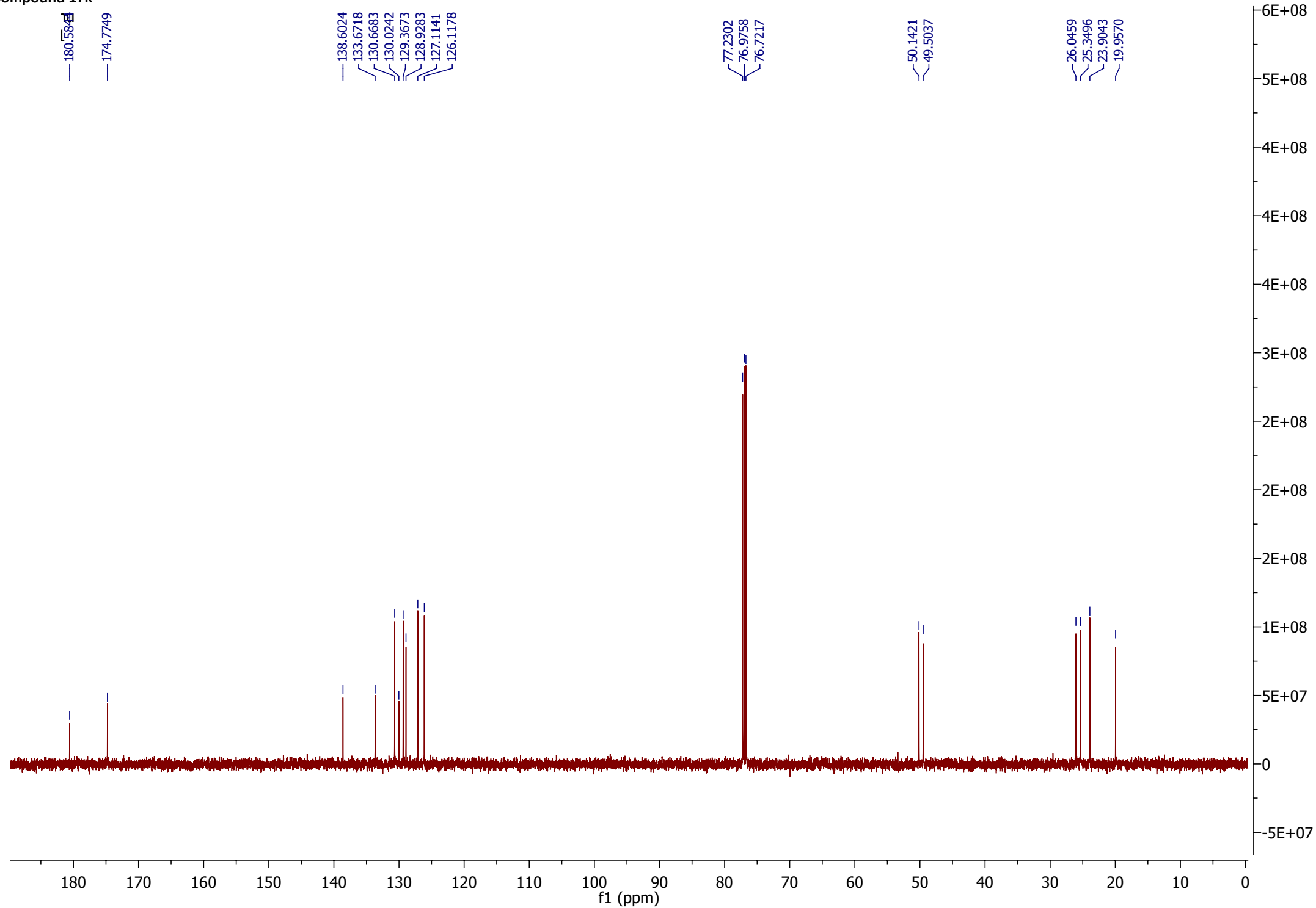
Compound 17i



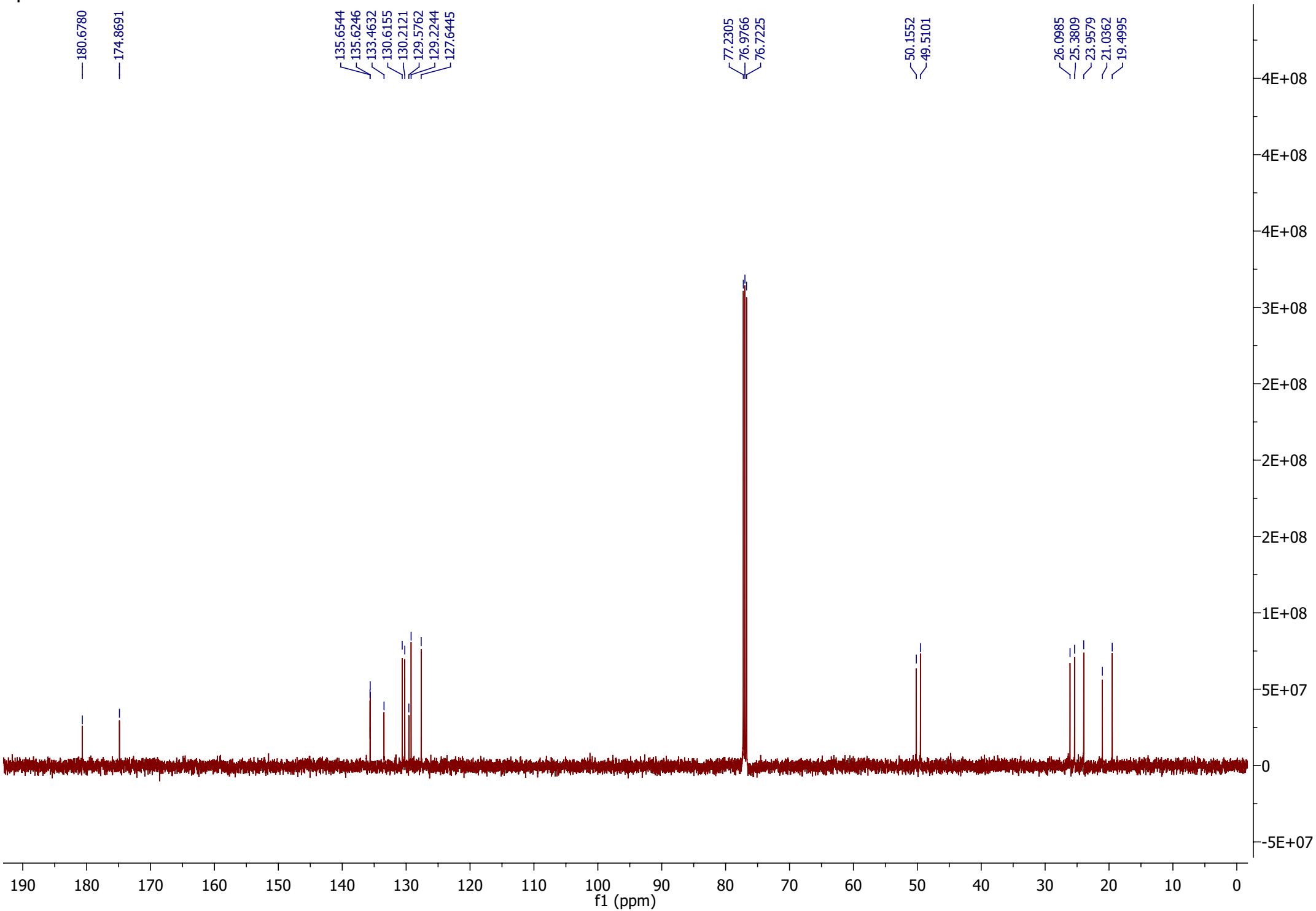
Compound 17j



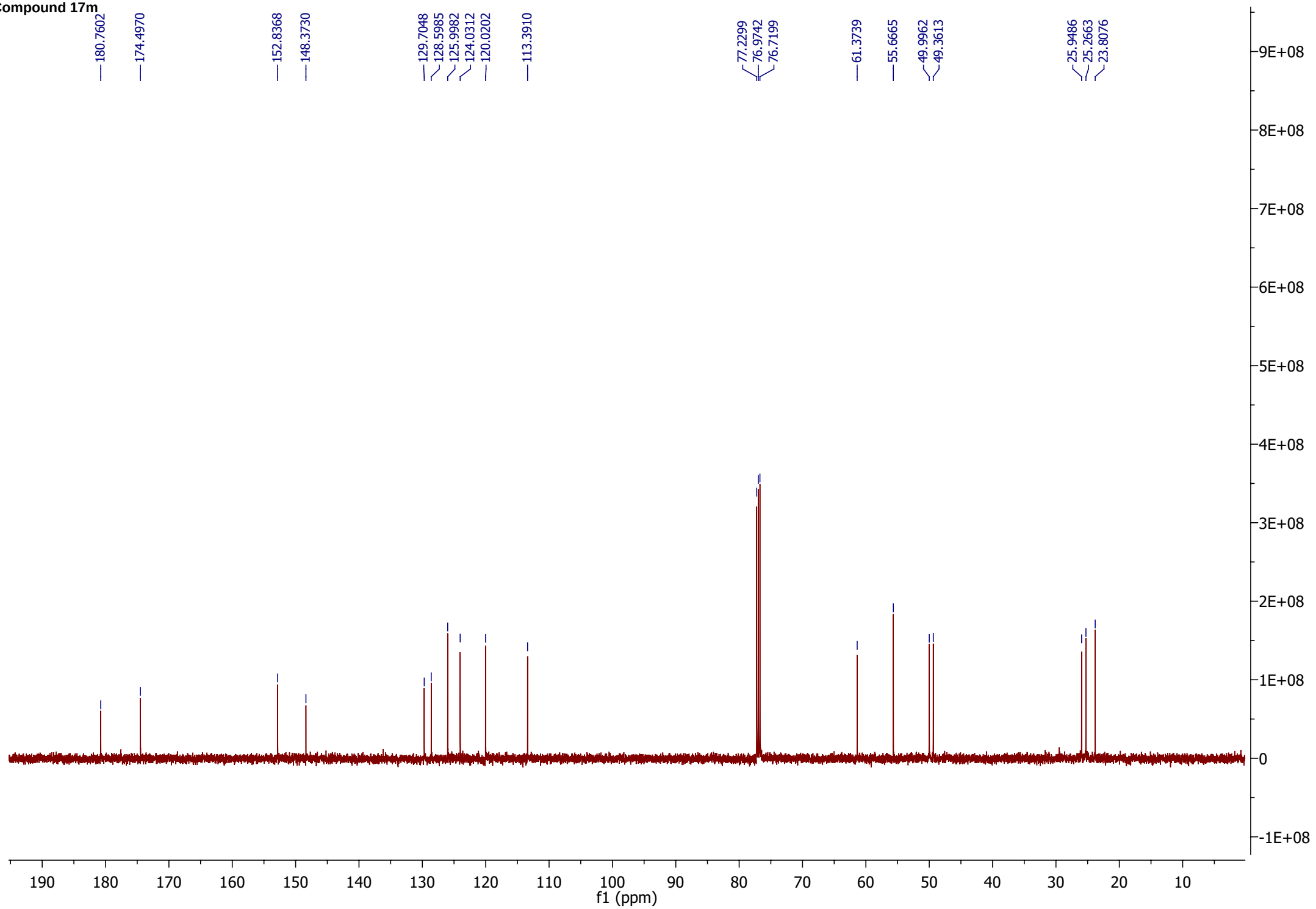
Compound 17k



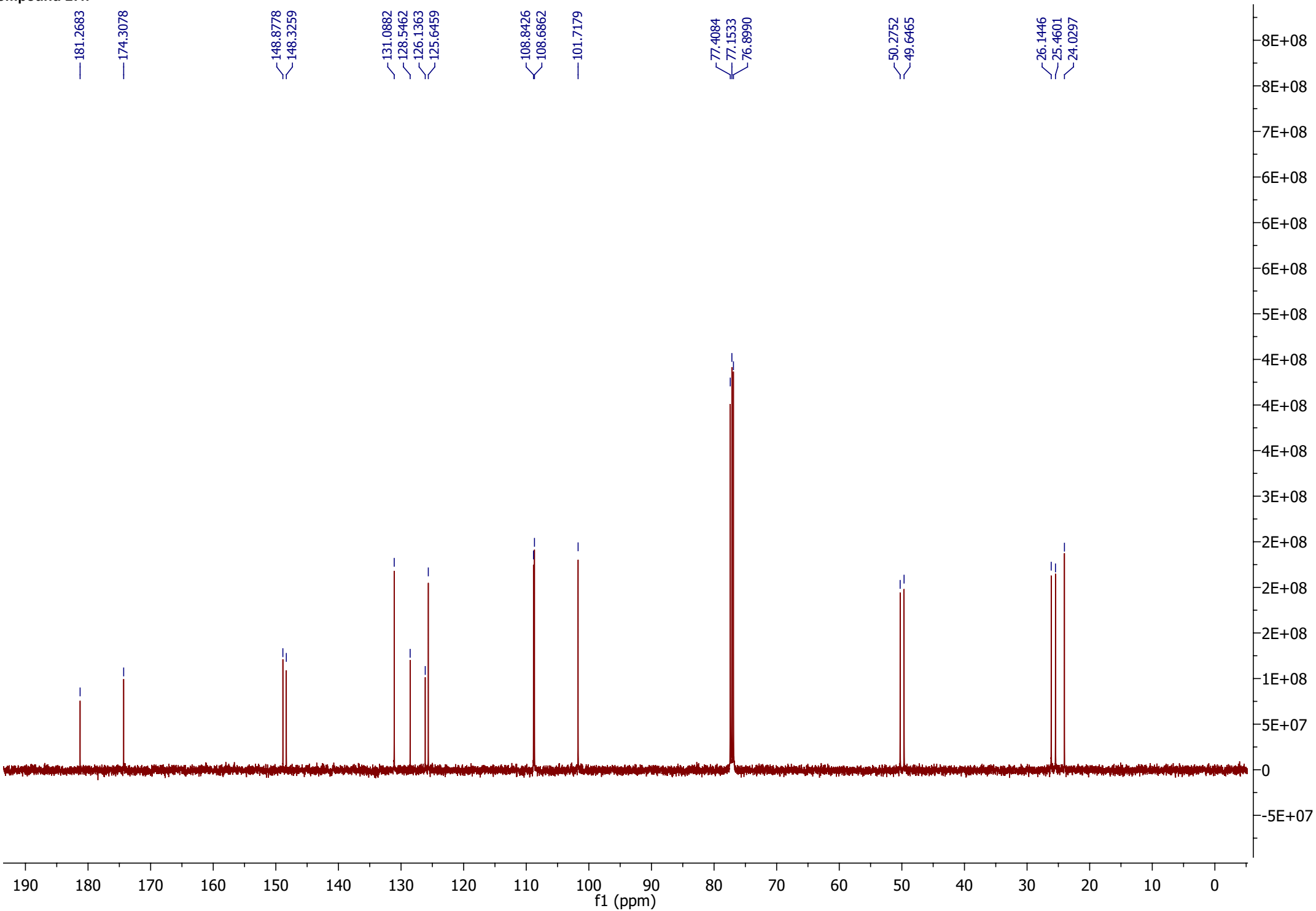
Compound 17l



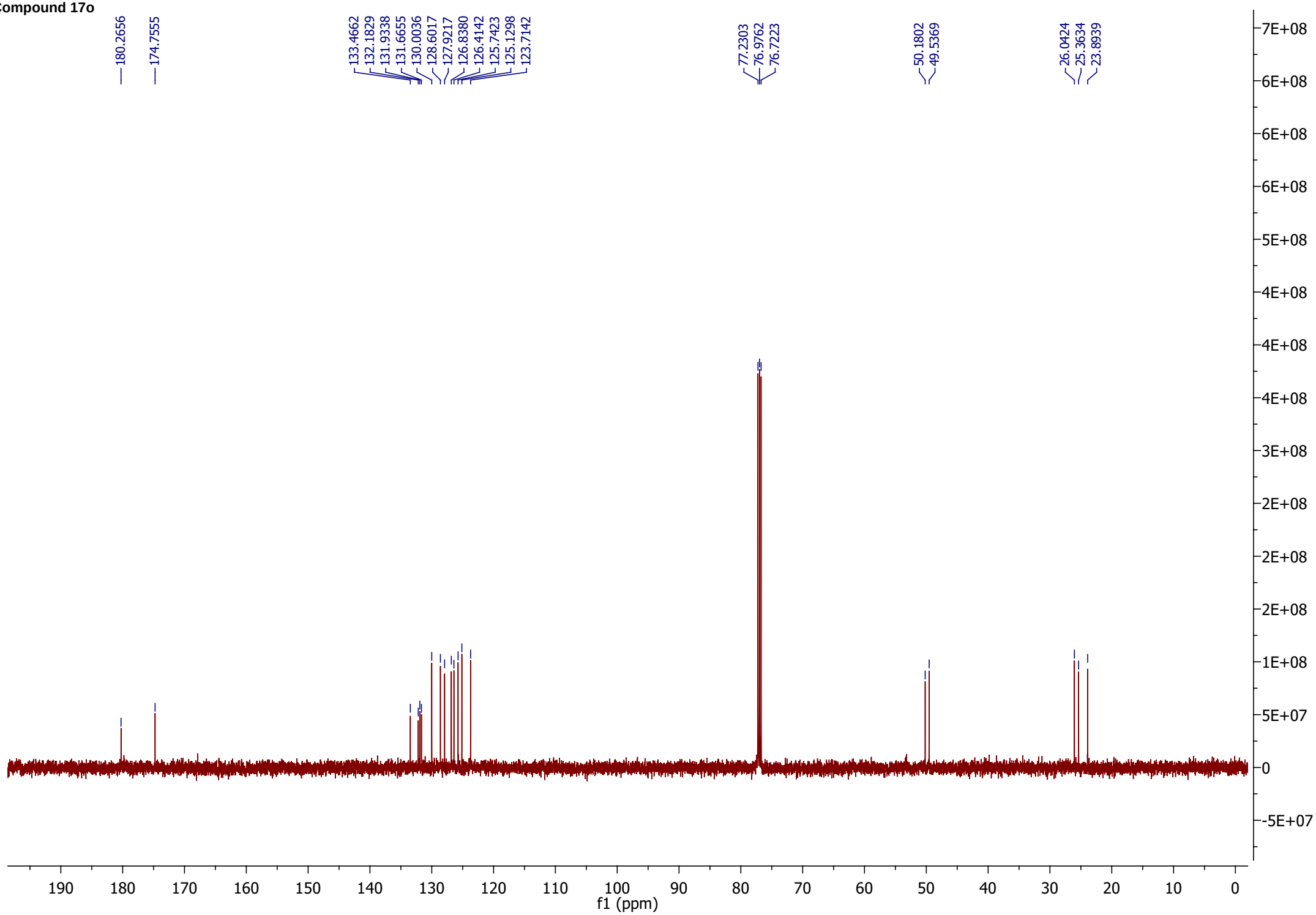
Compound 17m



Compound 17n



Compound 17o



Qualitative Analysis Report

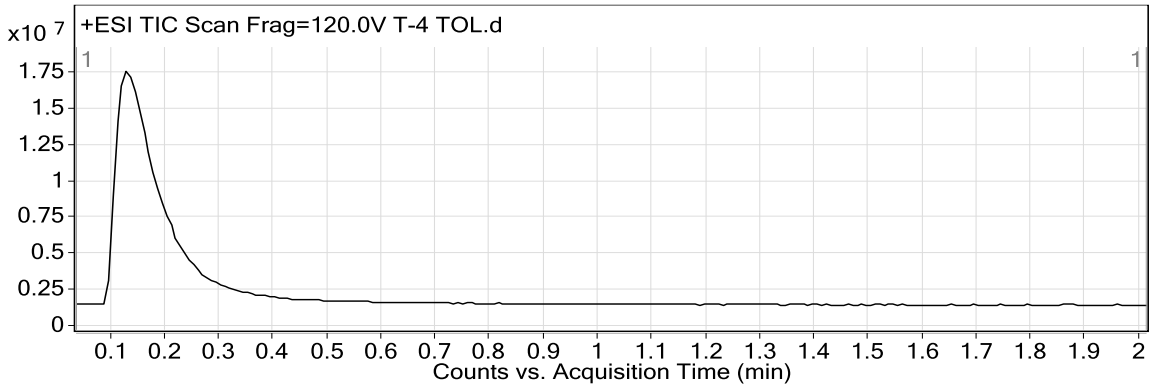
Data Filename	T-4 TOL.d	**Sample Name**	T-4 TOL
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	11/9/2015 10:07:55 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

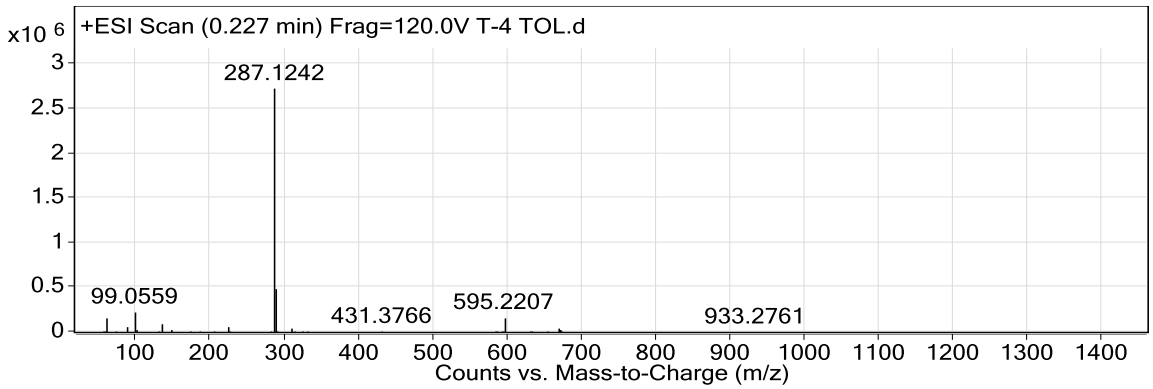
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
61.0288	1	163768.64
89.0601	1	67720.54
99.0559	1	227763.13
136.0509	1	97803.56
225.1971	1	71740.55
287.1242	1	2730979.75
288.1259	1	490584.72
289.1223	1	124862.59

595.2207	1	166091.77
596.2228	1	57091.52

--- End Of Report ---

Qualitative Analysis Report

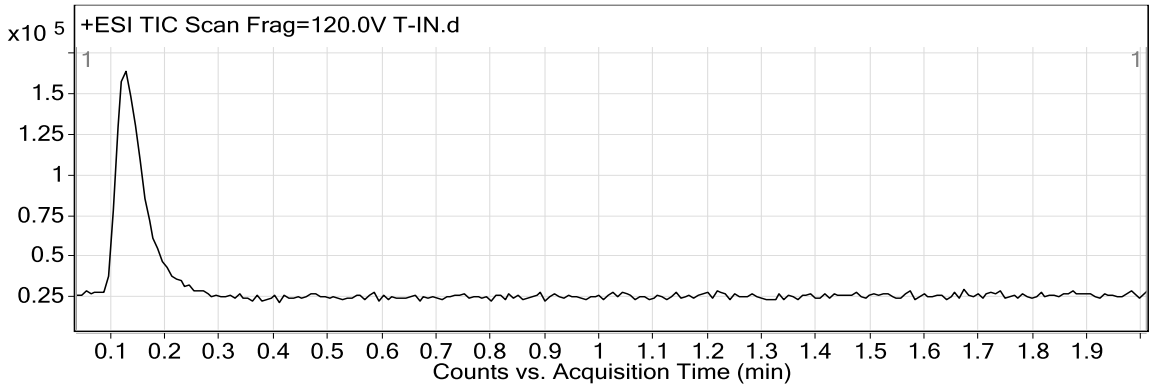
Data Filename	T-IN.d	**Sample Name**	T-IN
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	9/18/2015 4:17:45 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

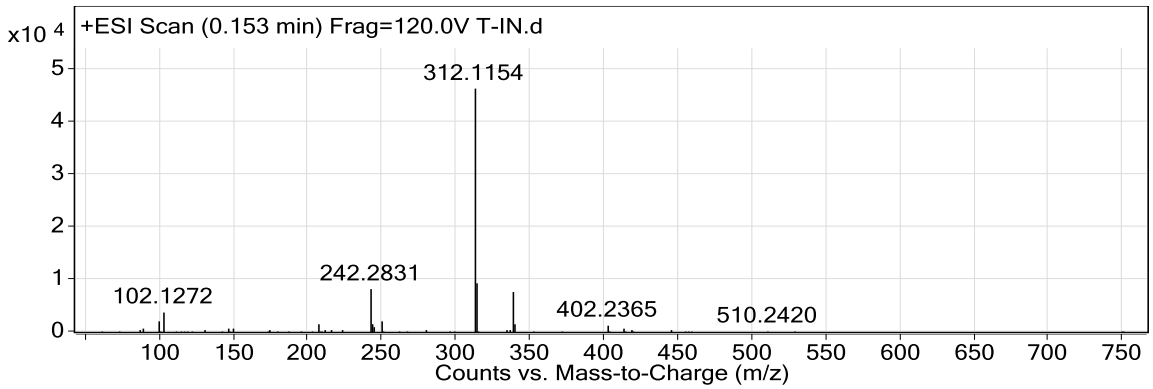
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
99.0548	1	2331.53
102.1272		3889.23
207.1609	1	1782.94
242.2831	1	8255.78
249.1698	1	2198.53
312.1154	1	46365.3
313.1178	1	9320.49
314.1151	1	2388.59

338.3397	1	7648.68
339.3454	1	1775.56

--- End Of Report ---

Qualitative Analysis Report

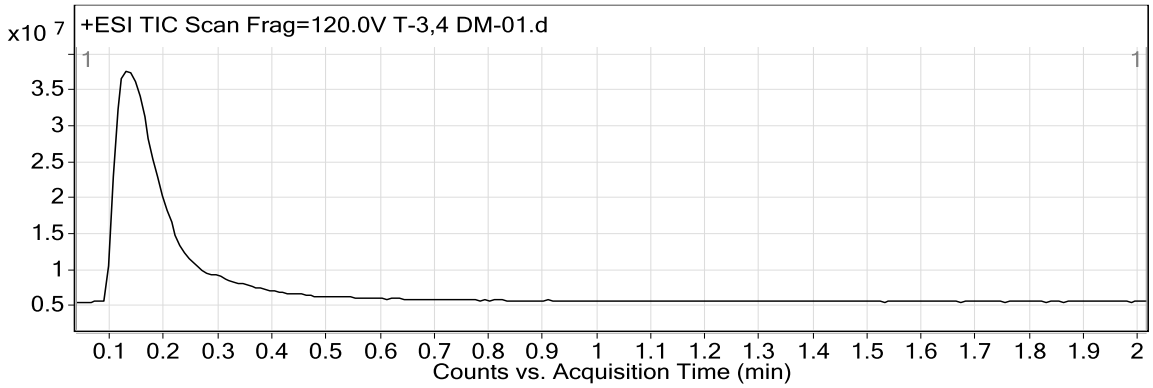
Data Filename	T-3,4 DM-01.d	**Sample Name**	T-3,4 DM-01
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	10/27/2015 3:35:20 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

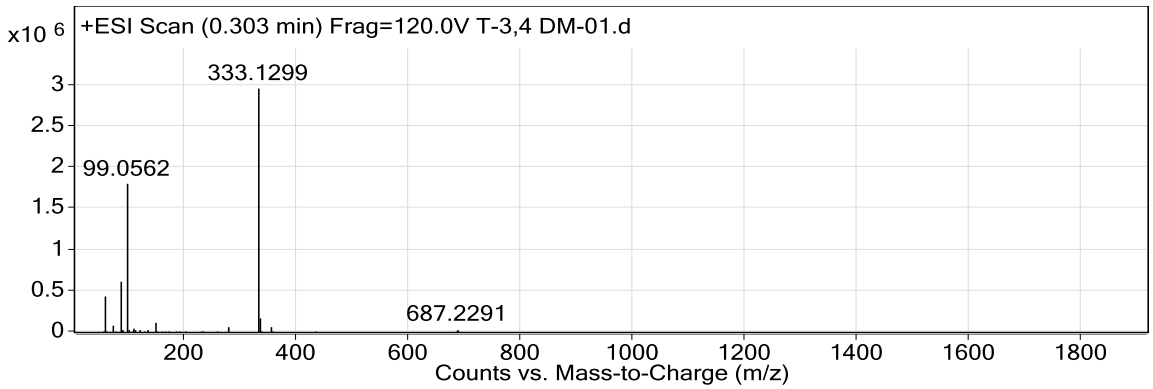
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
61.029	1	435355.22
73.0653		91127.98
89.0603	1	616620.75
99.0562	1	1802048.63
100.0589	1	73753.77
149.0238	1	131679.73
333.1299	1	2965161.5
333.2038		222337.7

334.1312	1	574944.31
335.1283	1	168838.13

--- End Of Report ---

Qualitative Analysis Report

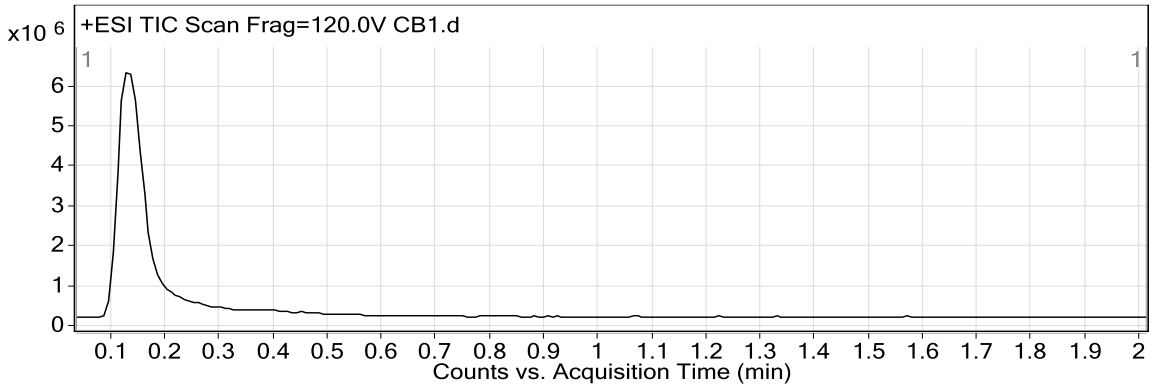
Data Filename	CB1.d	**Sample Name**	1
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	1/27/2016 9:44:07 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

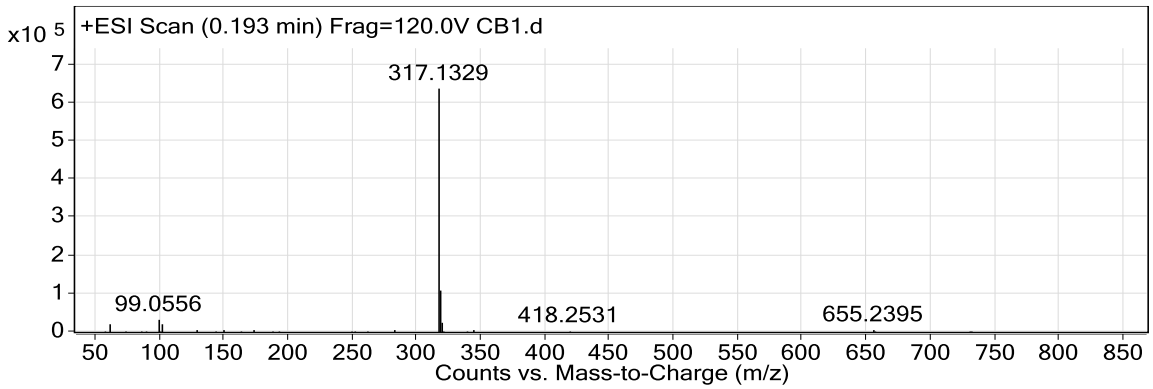
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
61.0285	1	22734.21
98.9756		11595.67
99.0556	1	33226.09
102.1281	1	21644.11
128.1182		7252.48
173.0123	1	8332.33
317.1329	1	637819.06
318.1361	1	111891.69

319.1325	1	28243.18
343.148	1	8133.93

--- End Of Report ---

Qualitative Analysis Report

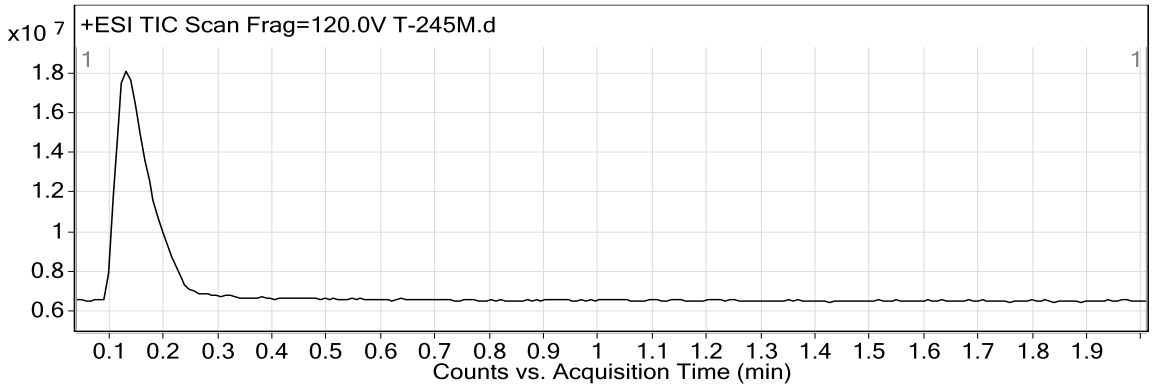
Data Filename	T-245M.d	**Sample Name**	T-245M
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	10/28/2015 9:56:22 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

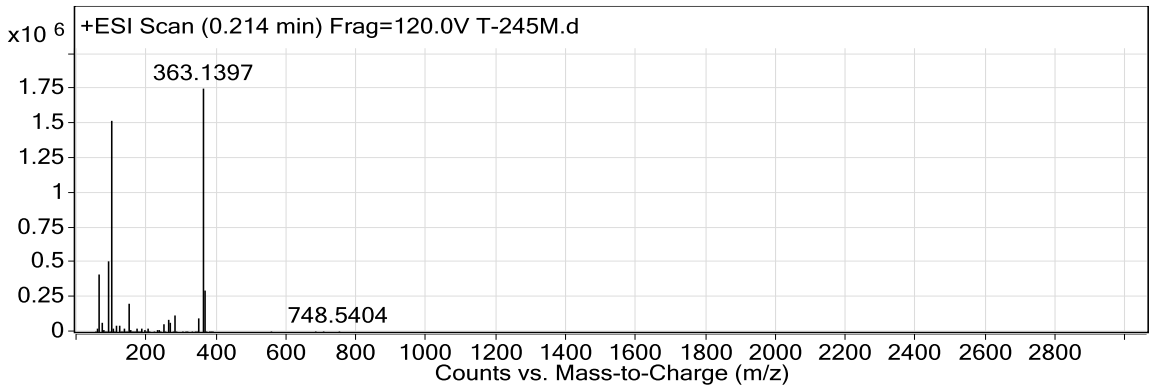
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
61.029	1	423804.97
89.0602	1	518409.72
99.056	1	1521358
149.0241	1	211558.08
264.1608	1	99208.09
279.1607	1	127013.92
346.1777	1	105325.92
363.1397	1	1756087.13

364.1428	1	300376.59
365.1395	1	91756.65

--- End Of Report ---

Qualitative Analysis Report

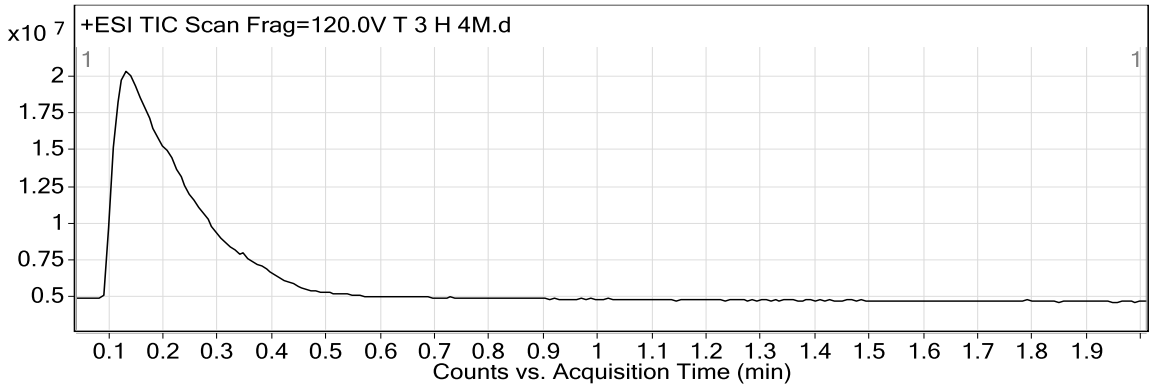
Data Filename	T 3 H 4M.d	**Sample Name**	T 3 H 4M
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	10/29/2015 9:44:03 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

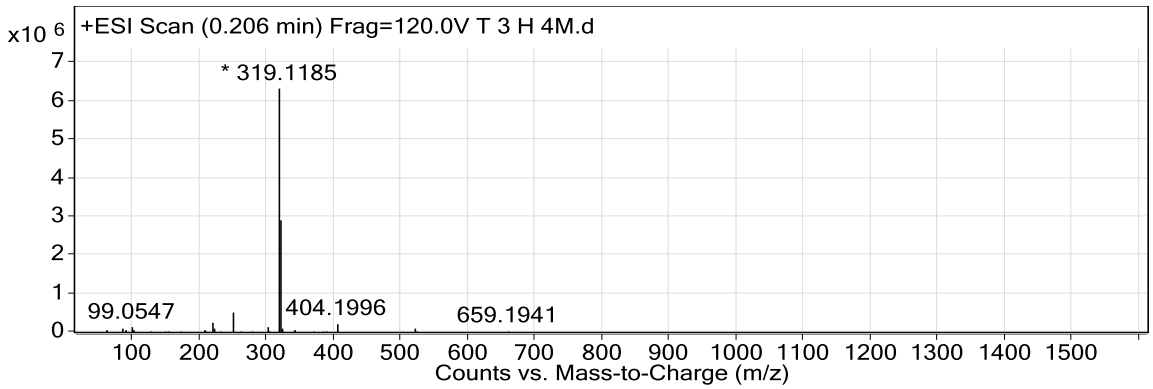
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
99.0547		134319.7
220.1333	1	259029.25
249.1706	1	517193.22
302.1495	1	140822.69
319.1185	1	6342012
320.1155	1	2931948.25
320.2038		203521.53
321.1106	1	975010.06

404.1996	1	228704.39
521.2746	1	131427.75

--- End Of Report ---

Qualitative Analysis Report

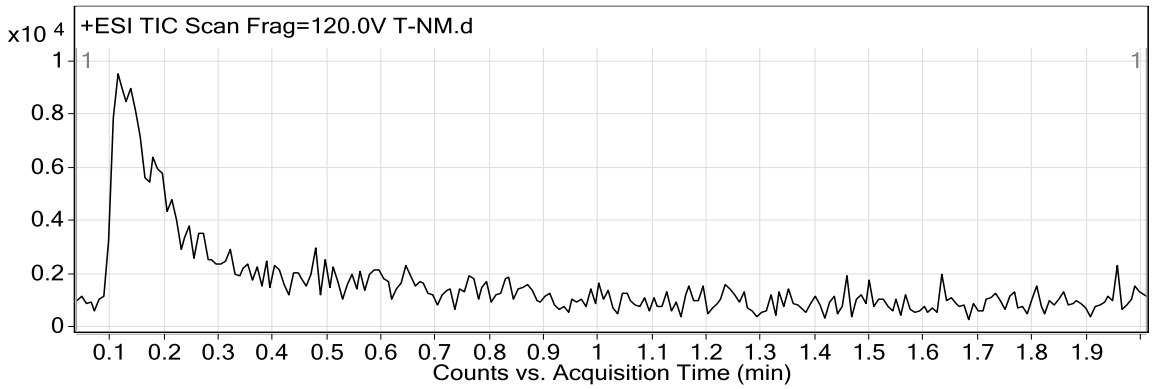
Data Filename	T-NM.d	**Sample Name**	T-NM
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	9/21/2015 10:20:37 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

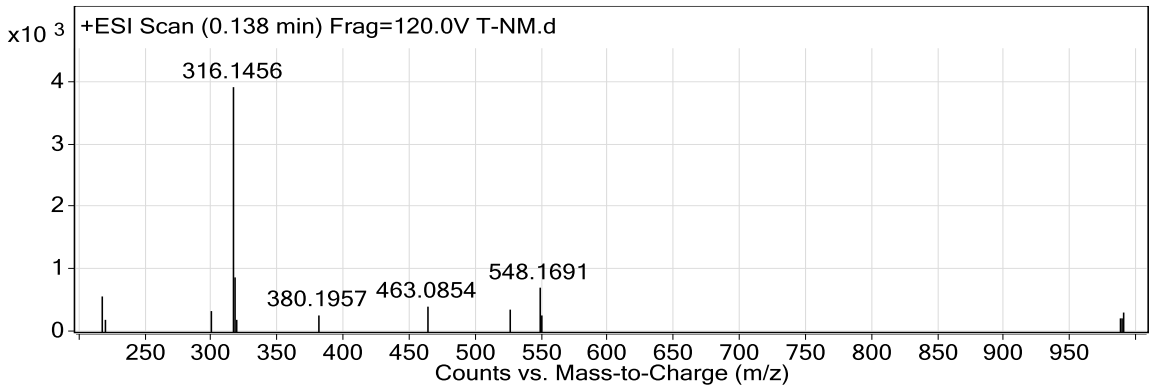
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
217.1655		581.06
299.1812		340.91
316.1456	1	3937.69
317.1468	1	879.37
380.1957		283.38
463.0854		420.82
525.0031		372.8
548.1691	1	714.45

549.1726	1	274.88
989.064		320.14

--- End Of Report ---

Qualitative Analysis Report

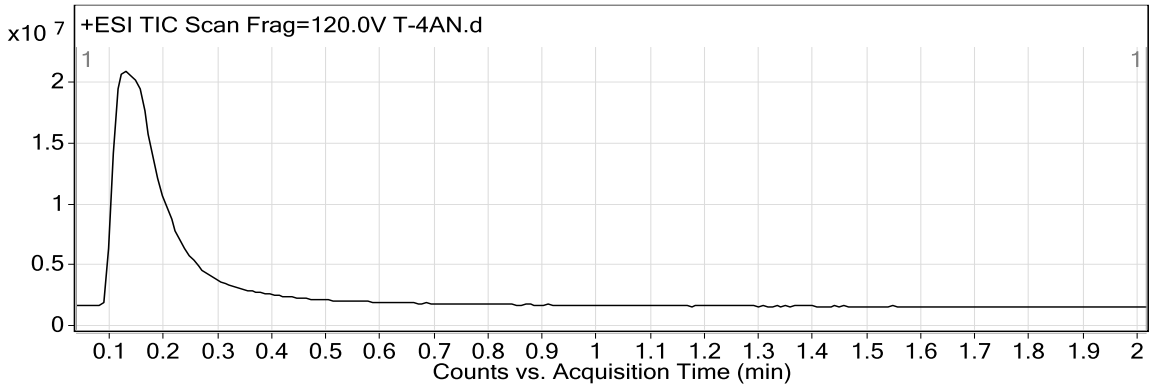
Data Filename	T-4AN.d	**Sample Name**	T-4AN
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	11/9/2015 10:05:04 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

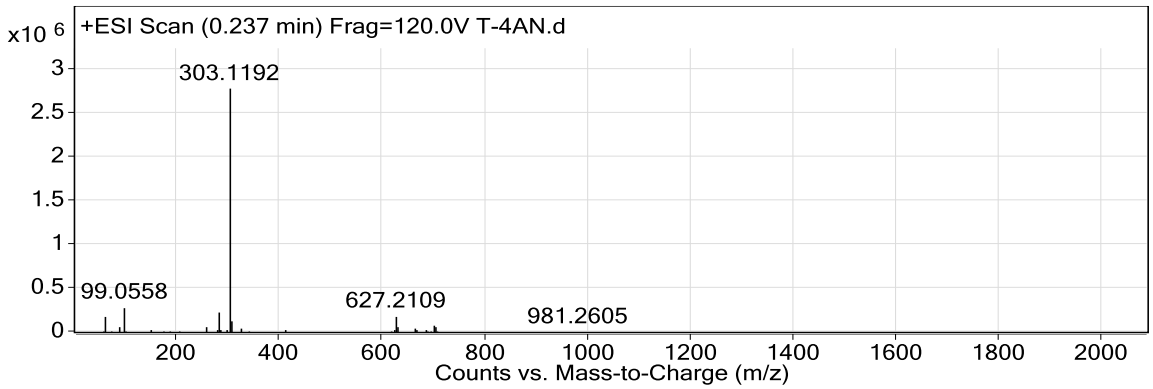
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
61.0288	1	177840.22
89.0601	1	71041.55
99.0558	1	288486.44
256.2652	1	71411.05
282.2812	1	228891.7
303.1192	1	2789945.25
304.1208	1	481535.72
305.1177	1	128030.52

627.2109	1	187100.38
701.1398	1	85775.02

--- End Of Report ---

Qualitative Analysis Report

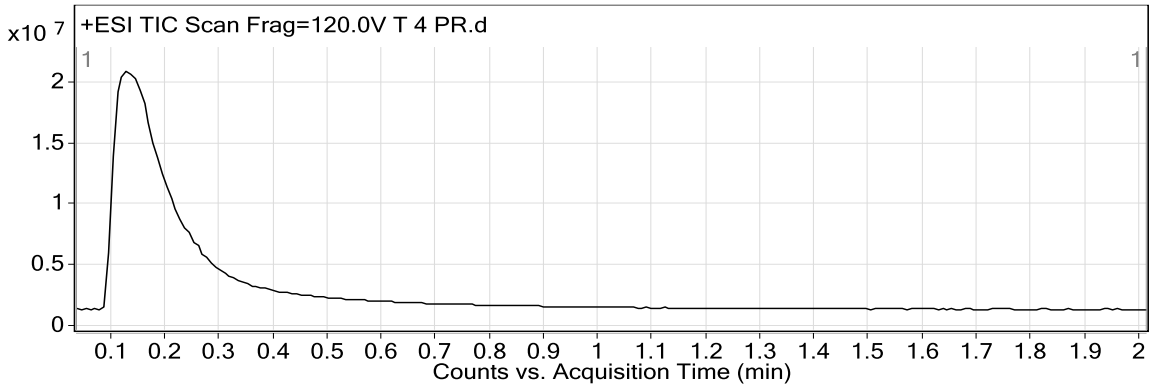
Data Filename	T 4 PR.d	**Sample Name**	T 4 PR
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	11/9/2015 10:10:48 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

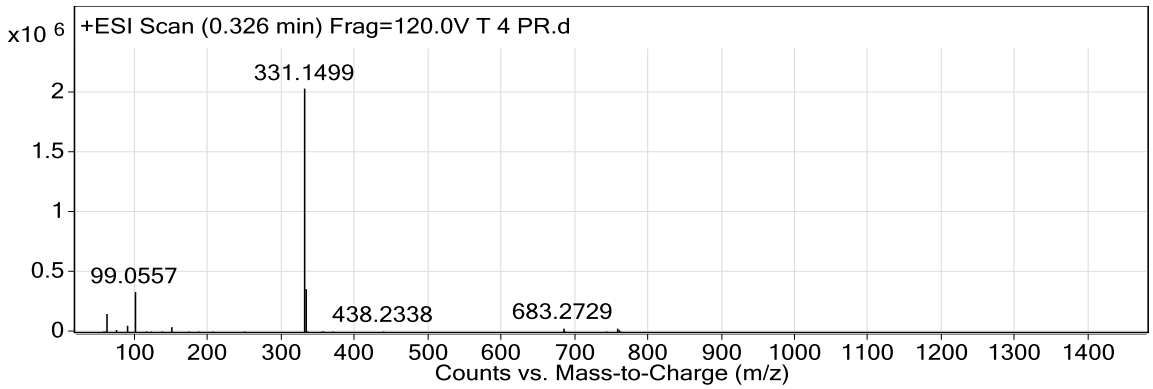
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
61.0287	1	155278.05
89.06	1	59995.7
99.0557	1	338783.25
149.0234	1	53345.82
331.1499	1	2033303.38
332.1524	1	361735.44
333.1493	1	90134.85
683.2729	1	41146.21

757.2023	1	35805.09
759.2001	1	26870.44

--- End Of Report ---

Qualitative Analysis Report

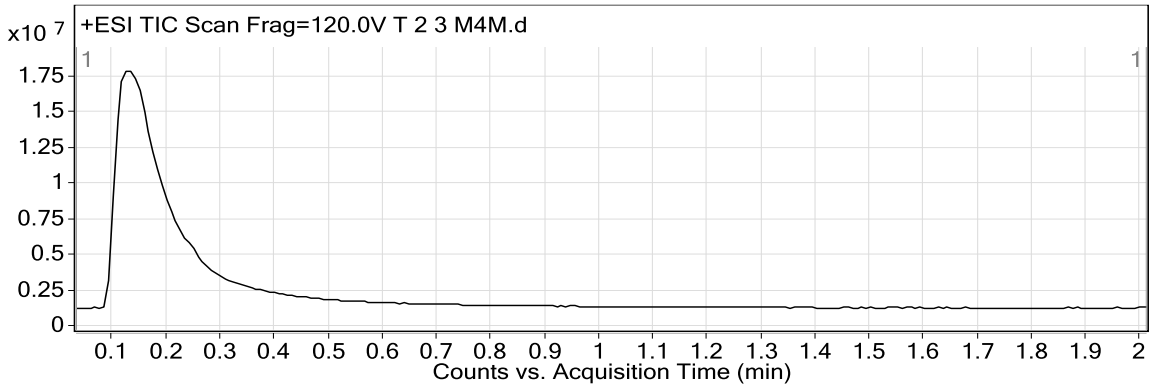
Data Filename	T 2 3 M4M.d	**Sample Name**	T 2 3 M4M
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	11/9/2015 10:16:29 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

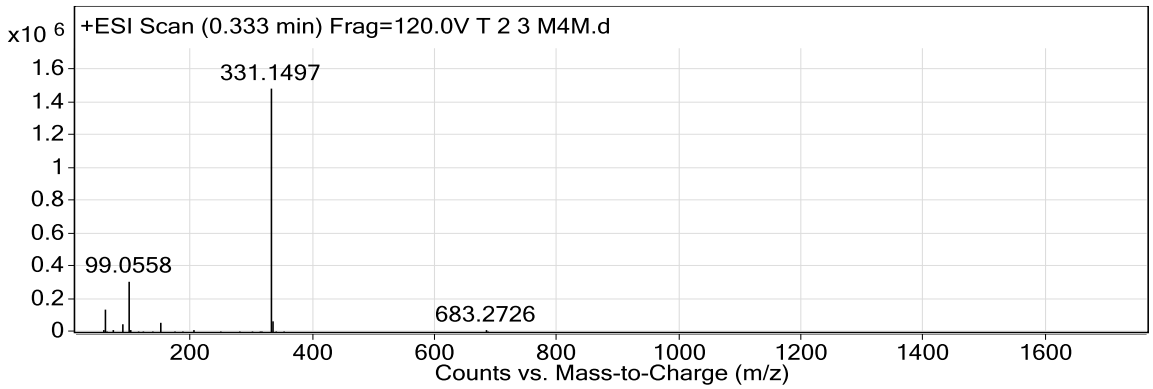
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
57.0449		15051.58
61.0287	1	139736.86
73.0651		16087.06
89.0601	1	55611.04
99.0558	1	313321.81
149.0234	1	58652.64
205.0863	1	15552.74
331.1497	1	1489850.63

332.1529	1	261858.78
333.1493	1	68640.78

--- End Of Report ---

Qualitative Analysis Report

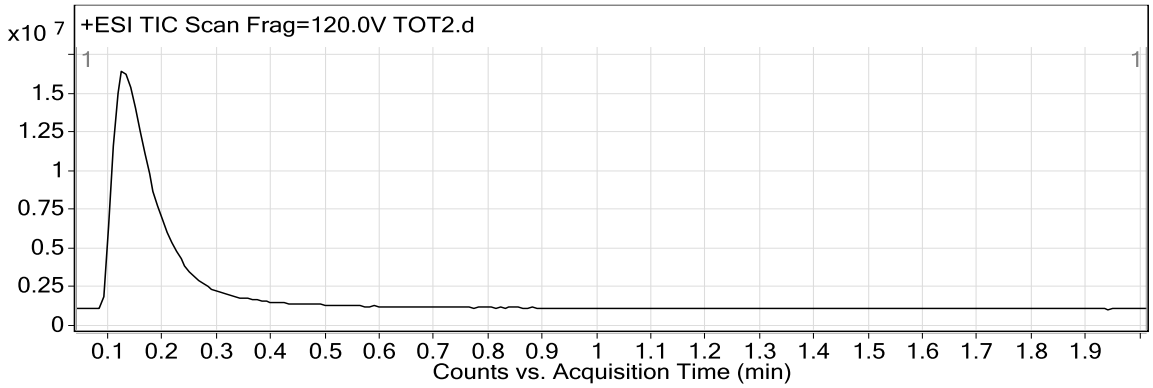
Data Filename	TOT2.d	**Sample Name**	TOT2
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	11/10/2015 3:45:32 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

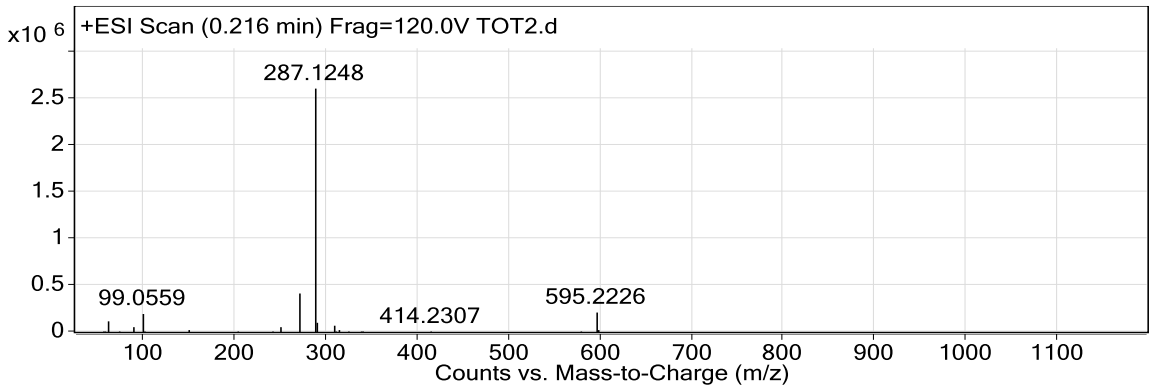
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
61.0288	1	129964.91
99.0559	1	200264.47
270.1623	1	421218.13
271.165	1	64047.27
287.1248	1	2605735.75
288.1266	1	445335.16
289.124	1	114243.35
309.1054	1	85467.14

595.2226	1	214235.7
596.2249	1	78143.38

--- End Of Report ---

Qualitative Analysis Report

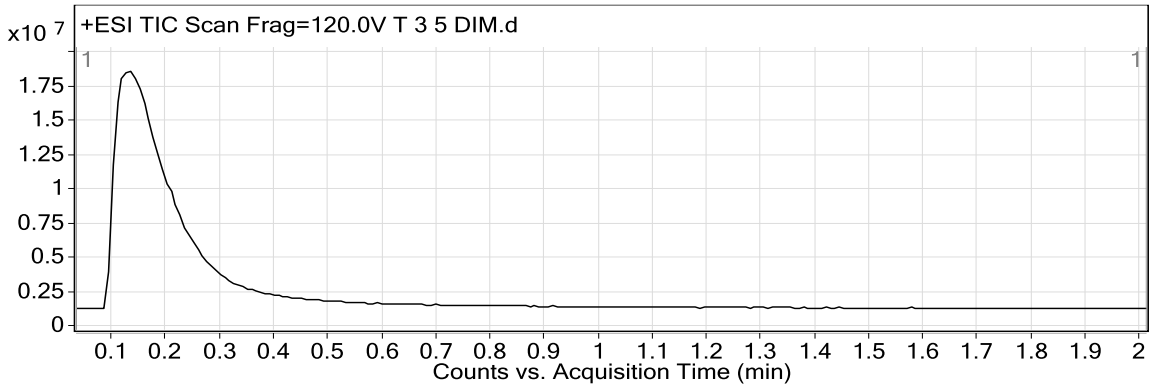
Data Filename	T 3 5 DIM.d	**Sample Name**	T 3 5 DIM
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	11/9/2015 10:13:39 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

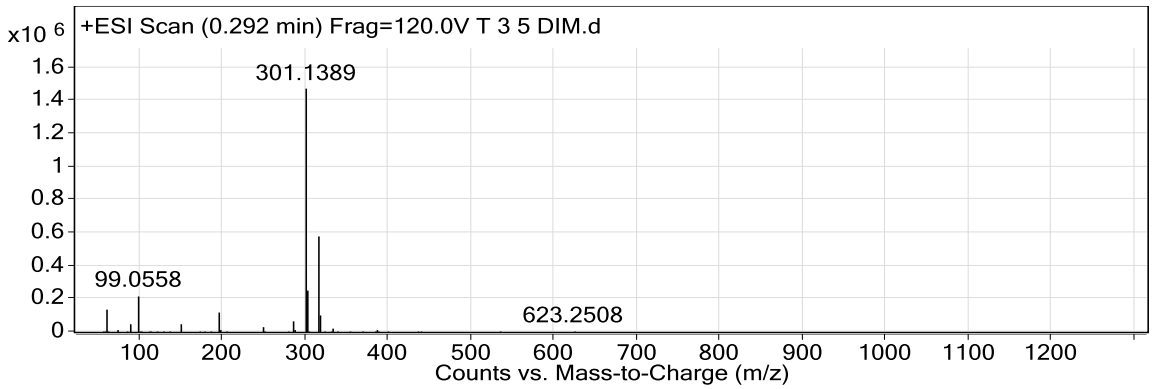
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
61.0287	1	138680.83
89.06	1	54651.77
99.0558	1	224605.72
196.1815	1	119635.35
284.1773	1	69563.63
301.1389	1	1475062.88
302.1421	1	252988.34
303.1381	1	61246.77

316.2035	1	580983.56
317.2069	1	108198.58

--- End Of Report ---

Qualitative Analysis Report

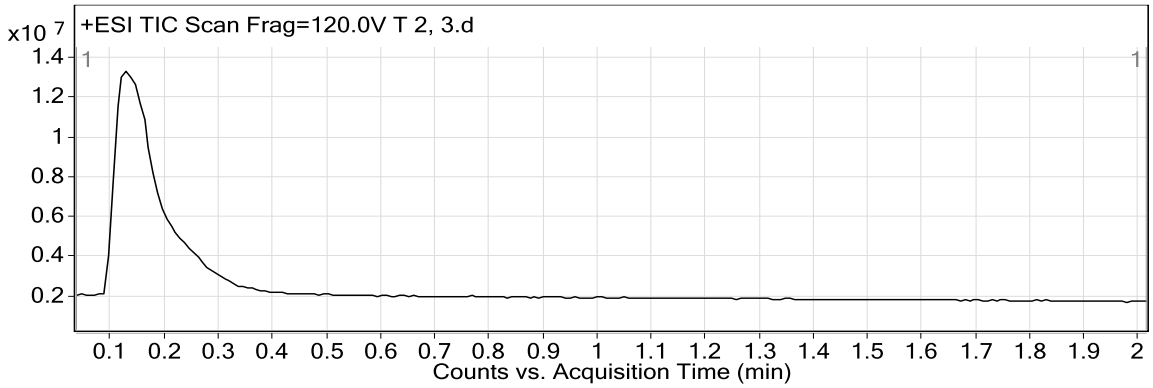
Data Filename	T 2, 3.d	**Sample Name**	T 2, 3
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	11/10/2015 9:45:20 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

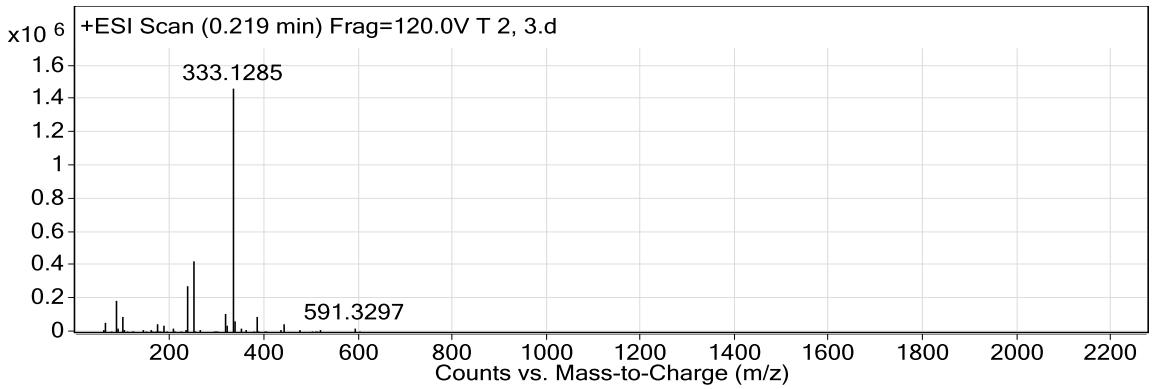
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
86.0968	1	189021.84
98.9756		94526.29
234.1501	1	284084.09
236.1654	1	161577.02
249.1721	1	431205.22
316.1691	1	116317.07
333.1285	1	1465964.38
334.1314	1	226828.02

335.1303	1	66237.14
383.2456	1	95805.5

--- End Of Report ---

Qualitative Analysis Report

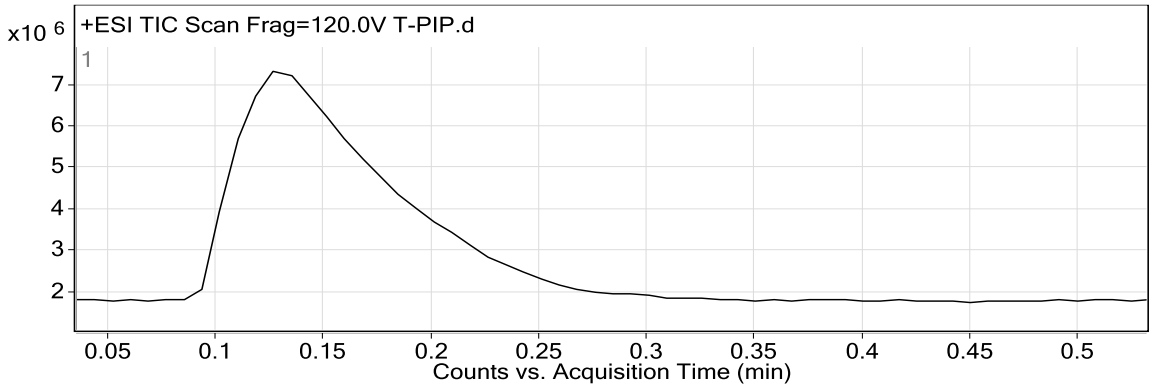
Data Filename	T-PIP.d	**Sample Name**	T-PIP
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	11/13/2015 9:36:33 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

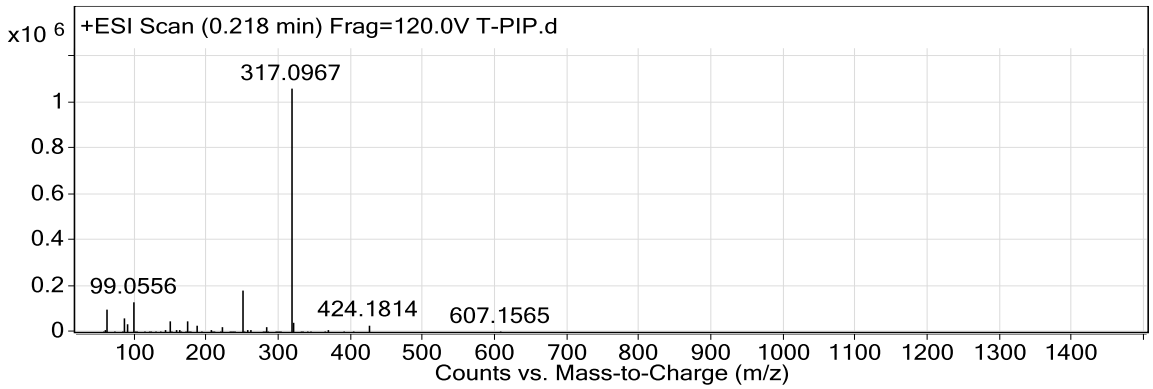
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
61.0285	1	104661.11
86.0967	1	64486.78
98.9756		81788.48
99.0556	1	132189.8
149.0233	1	49564.82
173.0124		49352.61
249.1721	1	185164.55
317.0967	1	1063203.13

318.0998	1	170020.36
319.0965	1	46153.07

--- End Of Report ---

Qualitative Analysis Report

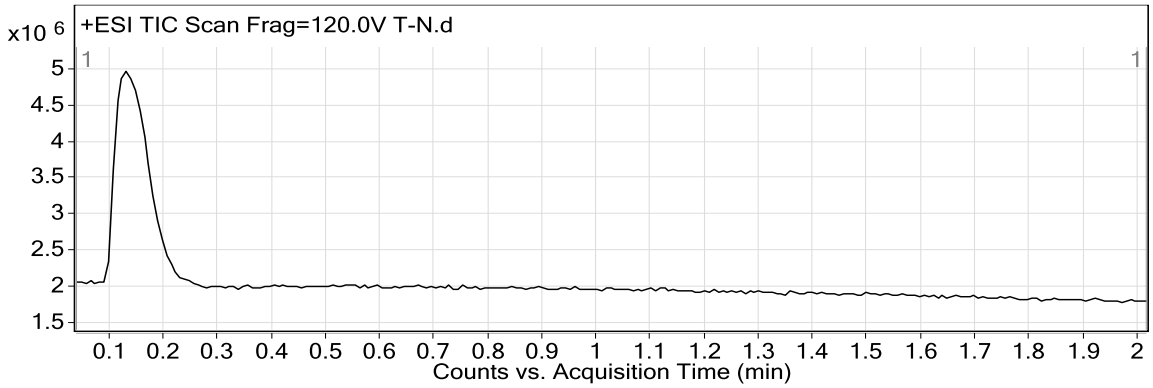
Data Filename	T-N.d	**Sample Name**	T-N
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	RAJESH UNION RUN POS.m	**Acquired Time**	11/13/2015 9:39:24 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

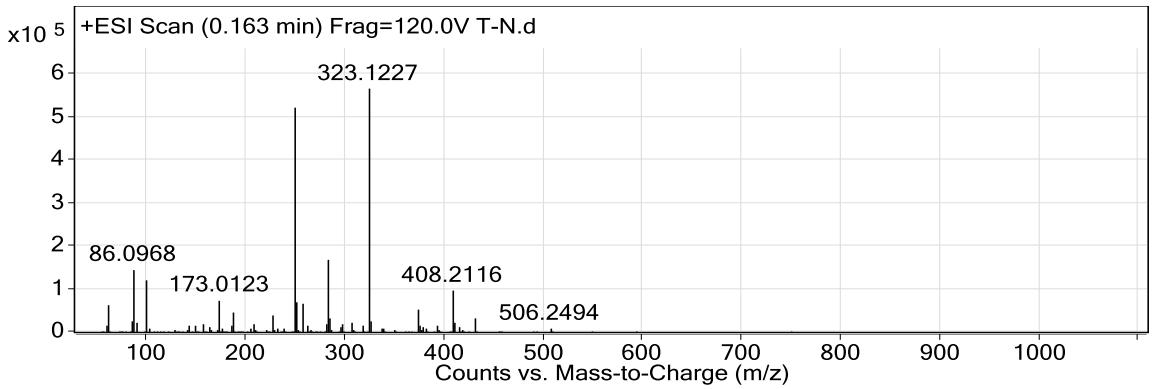
User Chromatograms

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
86.0968	1	146351.33
98.9757		123398.43
173.0123		75426.62
249.1721	1	522059.22
250.1747	1	70181.99
256.2646	1	68805.77
282.2808	1	170172.92
323.1227	1	566727.06

324.1259	1	113094.13
408.2116	1	97584.3

--- End Of Report ---

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 17o

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 17o

Bond precision: C-C = 0.0032 A Wavelength=0.71073

Cell: a=19.3839(6) b=7.7880(3) c=20.9133(8)
alpha=90 beta=90 gamma=90
Temperature: 299 K

	Calculated	Reported
Volume	3157.1(2)	3157.1(2)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C19 H18 N2 O S	C19 H18 N2 O S
Sum formula	C19 H18 N2 O S	C19 H18 N2 O S
Mr	322.41	322.41
Dx,g cm-3	1.357	1.357
Z	8	8
Mu (mm-1)	0.211	0.211
F000	1360.0	1360.0
F000’	1361.46	
h,k,lmax	23,9,25	23,9,25
Nref	2998	2998
Tmin,Tmax	0.982,0.991	0.829,0.917
Tmin’	0.932	

Correction method= # Reported T Limits: Tmin=0.829 Tmax=0.917
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.698

R(reflections)= 0.0436(2211) wR2(reflections)= 0.0956(2998)

S = 1.065 Npar= 209

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 7.521 Check

Alert level G

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ... 2 Report

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
1 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

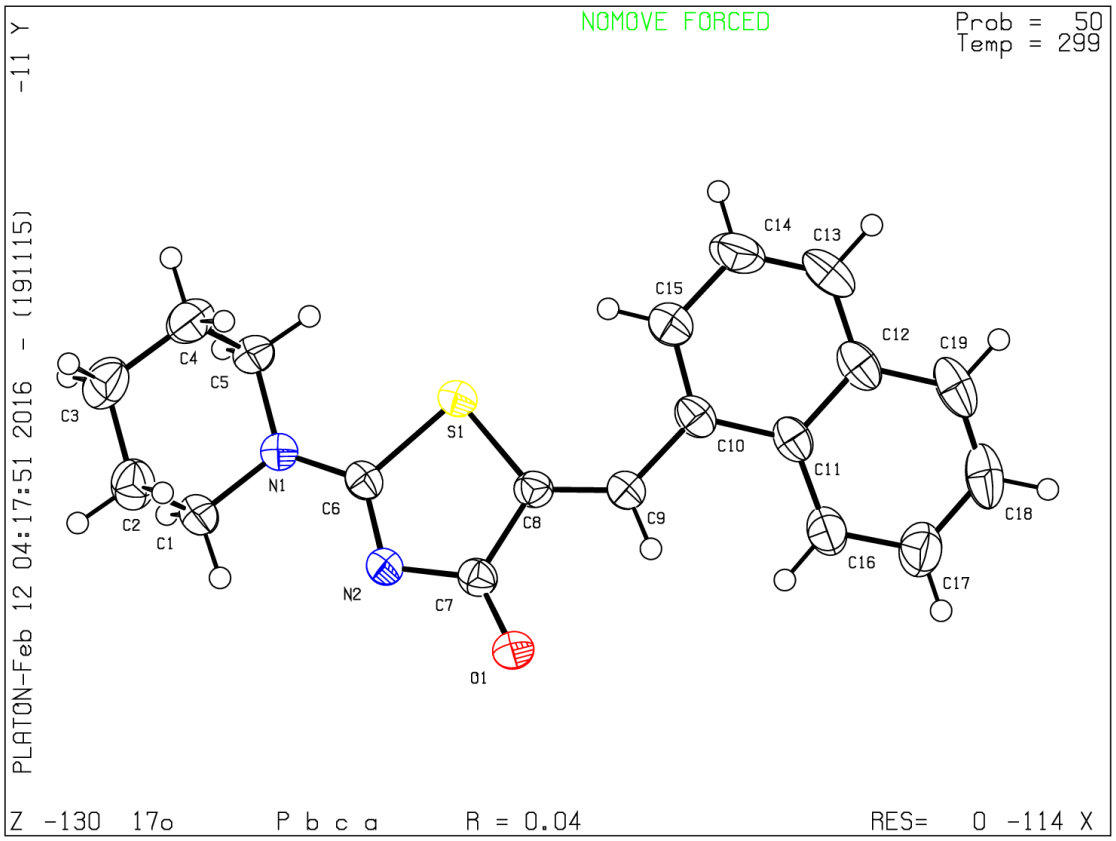
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 17o - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 17n

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 17n

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=8.3333(6) b=16.8148(12) c=10.7927(8)
alpha=90 beta=103.960(2) gamma=90
Temperature: 299 K

	Calculated	Reported
Volume	1467.64(18)	1467.64(18)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C16 H16 N2 O3 S	C16 H16 N2 O3 S
Sum formula	C16 H16 N2 O3 S	C16 H16 N2 O3 S
Mr	316.37	316.37
Dx,g cm-3	1.432	1.432
Z	4	4
Mu (mm-1)	0.235	0.235
F000	664.0	664.0
F000’	664.78	
h,k,lmax	10,20,13	10,20,13
Nref	2798	2796
Tmin,Tmax	0.963,0.976	0.779,0.894
Tmin’	0.922	

Correction method= # Reported T Limits: Tmin=0.779 Tmax=0.894
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.700

R(reflections)= 0.0403(2122) wR2(reflections)= 0.0959(2796)

S = 1.088 Npar= 200

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.692 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          2 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          2 Note
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
0 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

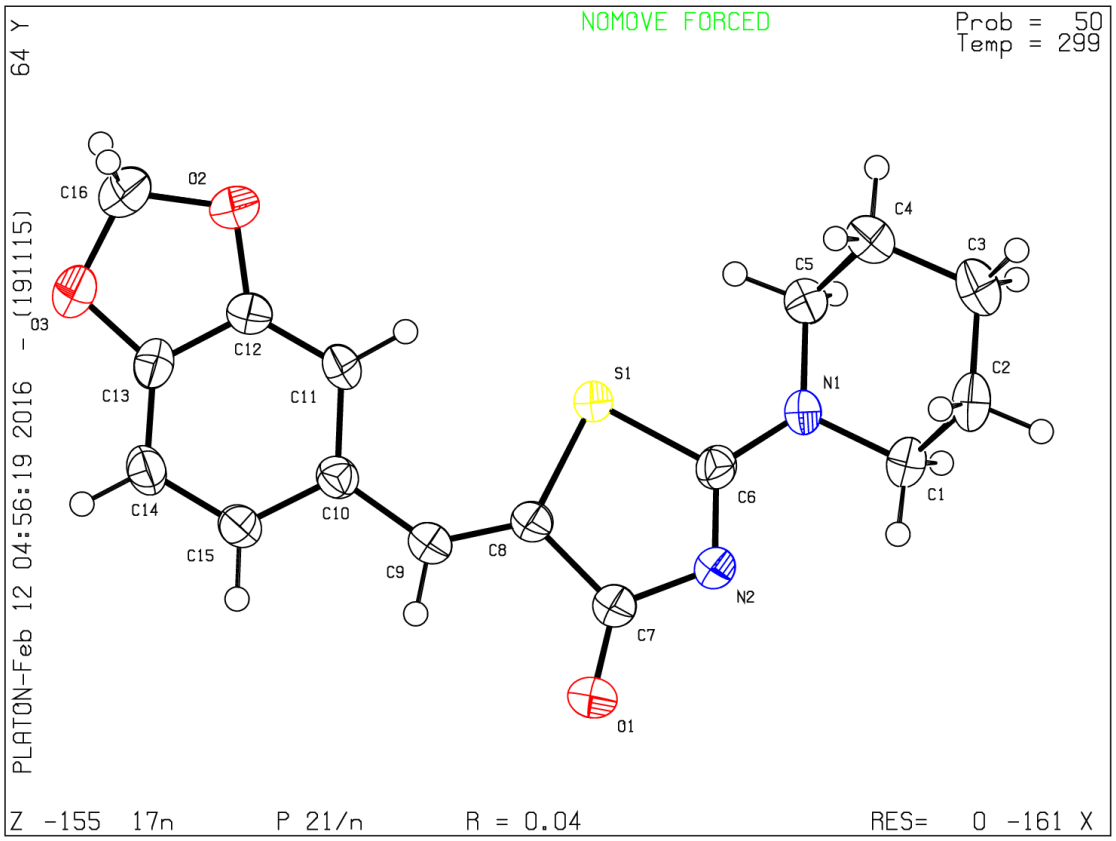
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 17n - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 17m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 17m

```
Bond precision:  C-C = 0.0030 A          Wavelength=0.71073

Cell:          a=6.9066(6)       b=10.3537(10)     c=12.5514(13)
               alpha=96.955(4)   beta=103.338(3)   gamma=100.576(3)
Temperature:   300 K
```

	Calculated	Reported
Volume	845.87(14)	845.87(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C17 H20 N2 O3 S	C17 H20 N2 O3 S
Sum formula	C17 H20 N2 O3 S	C17 H20 N2 O3 S
Mr	332.41	332.41
Dx,g cm-3	1.305	1.305
Z	2	2
Mu (mm-1)	0.207	0.207
F000	352.0	352.0
F000’	352.39	
h,k,lmax	8,12,15	8,12,15
Nref	3218	3209
Tmin,Tmax	0.937,0.963	0.799,0.841
Tmin’	0.925	

```
Correction method= # Reported T Limits: Tmin=0.799 Tmax=0.841
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 25.700

R(reflections)= 0.0389( 2735)     wR2(reflections)= 0.1122( 3209)

S = 1.038                 Npar= 211
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C3 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          7 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          3 Note
```

Alert level G

```
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........           2 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...          2 Report
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   2 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

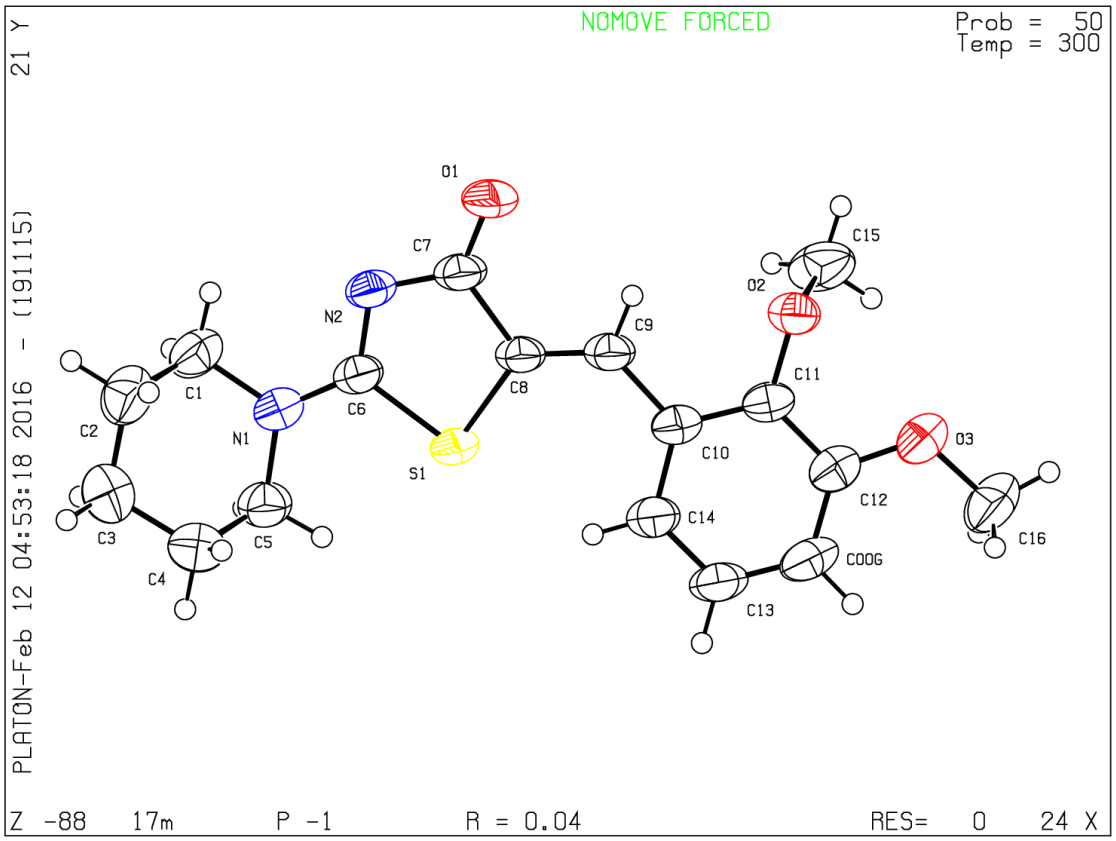
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 17m - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 17k

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 17k

```
Bond precision:  C-C = 0.0054 A          Wavelength=0.71073

Cell:            a=19.808(2)     b=19.648(2)         c=7.5797(8)
                 alpha=90        beta=95.378(4)      gamma=90
Temperature:     296 K
```

	Calculated	Reported
Volume	2936.9(5)	2937.0(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C16 H18 N2 O S	C16 H18 N2 O S
Sum formula	C16 H18 N2 O S	C16 H18 N2 O S
Mr	286.38	286.38
Dx,g cm-3	1.295	1.295
Z	8	8
Mu (mm-1)	0.218	0.218
F000	1216.0	1216.0
F000’	1217.40	
h,k,lmax	24,23,9	24,23,9
Nref	5580	5577
Tmin,Tmax	0.986,0.989	0.834,0.917
Tmin’	0.926	

```
Correction method= # Reported T Limits: Tmin=0.834 Tmax=0.917
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 25.699

R(reflections)= 0.0635( 2997)     wR2(reflections)= 0.1341( 5577)

S = 1.026                 Npar= 364
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

```
RINTA01_ALERT_3_B  The value of Rint is greater than 0.18
           Rint given   0.242
```

Alert level C

```
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00536 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     19.833 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.724 Check
```

Alert level G

```
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C16 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         10 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...          4 Report
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   3 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

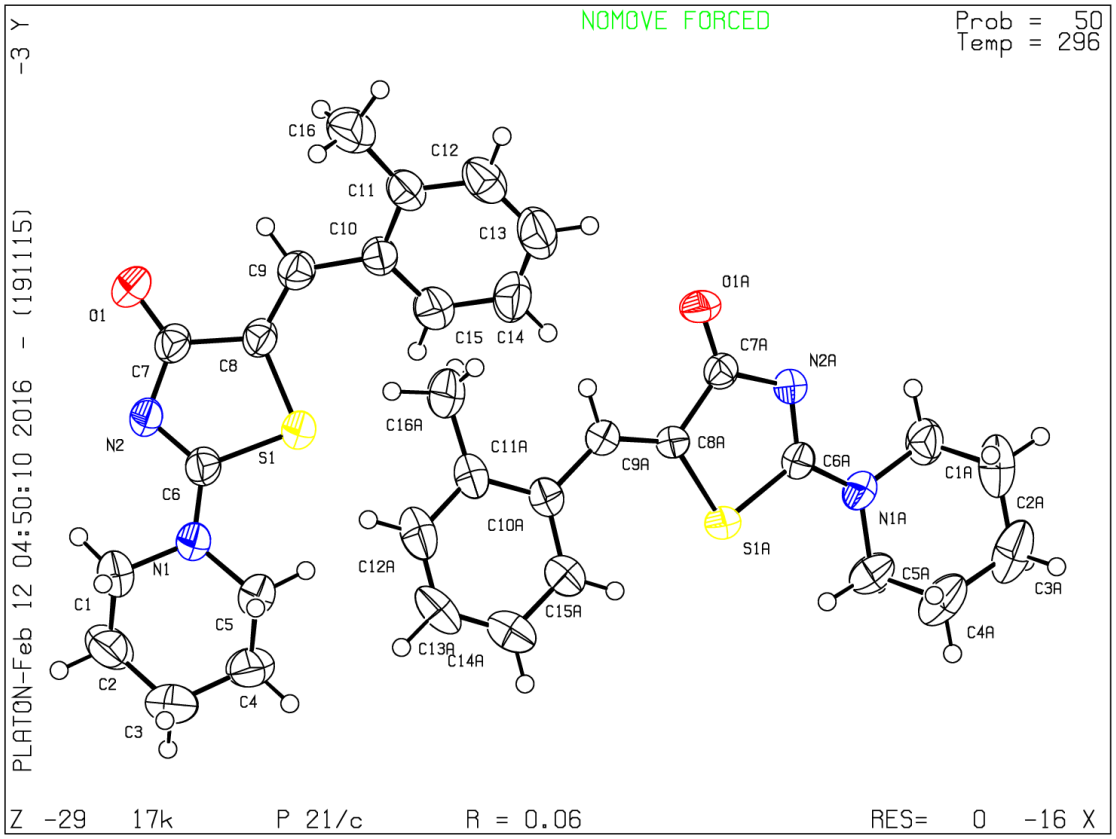
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 17k - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 17j

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 17j

```
Bond precision:  C-C = 0.0031 A          Wavelength=0.71073

Cell:           a=13.1879(8)    b=8.2959(4)         c=16.8693(10)
                alpha=90        beta=111.933(2)     gamma=90
Temperature:    297 K

                Calculated                Reported
Volume          1712.01(17)               1712.01(17)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C18 H22 N2 O2 S           C18 H22 N2 O2 S
Sum formula     C18 H22 N2 O2 S           C18 H22 N2 O2 S
Mr              330.44                    330.43
Dx,g cm-3       1.282                     1.282
Z               4                         4
Mu (mm-1)       0.200                     0.200
F000            704.0                     704.0
F000'           704.76
h,k,lmax        16,10,20                  16,10,20
Nref            3249                      3241
Tmin,Tmax       0.935,0.948               0.725,0.805
Tmin'           0.887

Correction method= # Reported T Limits: Tmin=0.725 Tmax=0.805
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 25.700

R(reflections)= 0.0410( 2562)     wR2(reflections)= 0.1101( 3241)

S = 1.032                 Npar= 212
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          7 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          3 Note
```

Alert level G

```
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...          1 Report
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   1 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

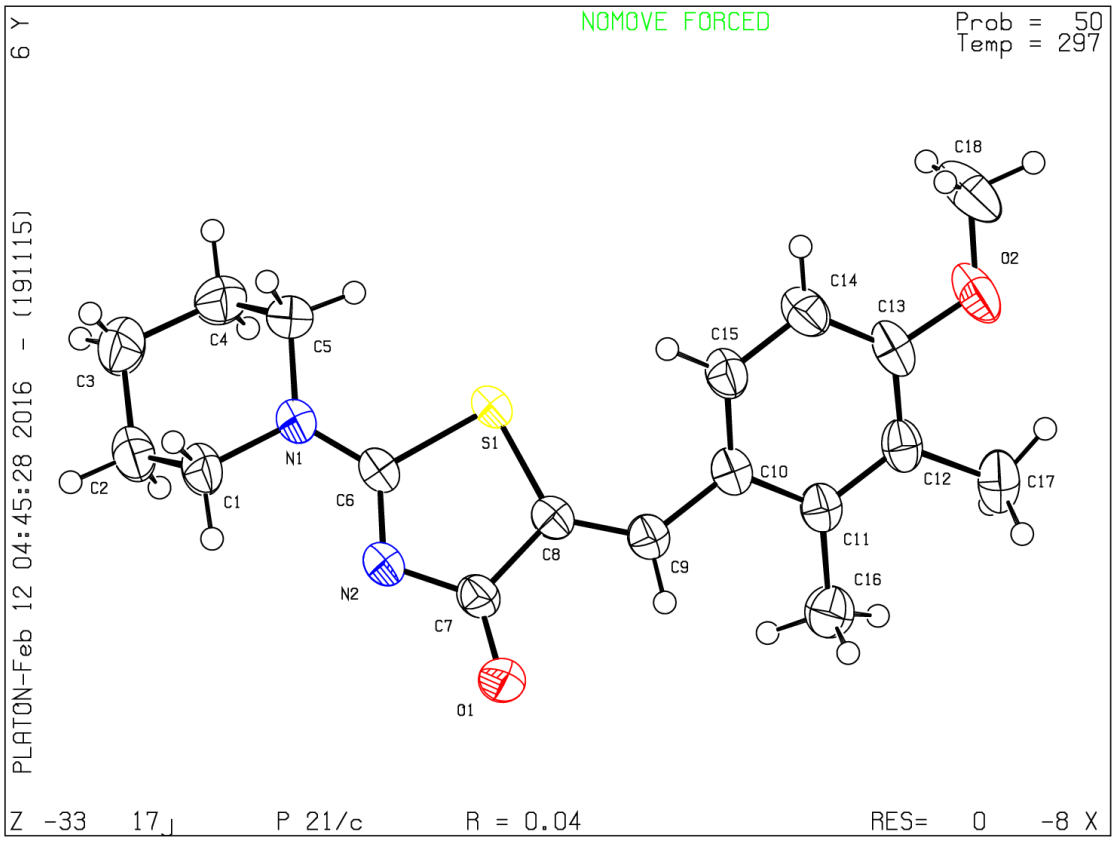
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 17j - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 17i

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 17i

Bond precision: C-C = 0.0036 A Wavelength=0.71073

Cell: a=14.6019(6) b=15.8336(5) c=7.5085(3)
alpha=90 beta=90.141(2) gamma=90
Temperature: 297 K

	Calculated	Reported
Volume	1735.97(11)	1735.96(11)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C18 H22 N2 O2 S	C18 H22 N2 O2 S
Sum formula	C18 H22 N2 O2 S	C18 H22 N2 O2 S
Mr	330.44	330.43
Dx,g cm-3	1.264	1.264
Z	4	4
Mu (mm-1)	0.197	0.197
F000	704.0	704.0
F000’	704.76	
h,k,lmax	17,19,9	17,19,9
Nref	3304	3299
Tmin,Tmax	0.951,0.979	0.811,0.865
Tmin’	0.920	

Correction method= # Reported T Limits: Tmin=0.811 Tmax=0.865
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.699

R(reflections)= 0.0472(2427) wR2(reflections)= 0.1213(3299)

S = 1.037 Npar= 210

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      5.091 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          3 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          3 Note
```

Alert level G

```
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...          3 Report
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   1 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

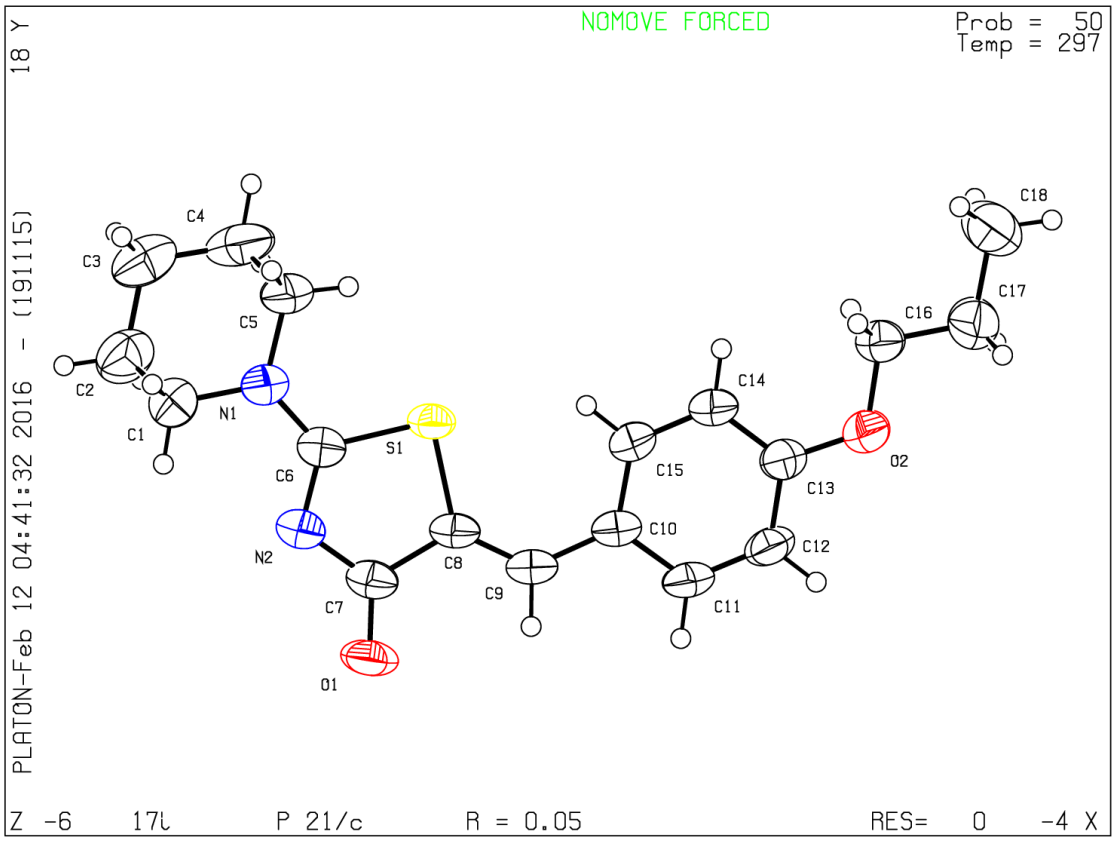
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 17i - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 17h

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 17h

Bond precision: C-C = 0.0022 A Wavelength=0.71073

Cell: a=8.5748(3) b=16.5115(5) c=10.8532(4)
alpha=90 beta=100.922(1) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	1508.79(9)	1508.79(9)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C16 H18 N2 O2 S	C16 H18 N2 O2 S
Sum formula	C16 H18 N2 O2 S	C16 H18 N2 O2 S
Mr	302.38	302.38
Dx,g cm-3	1.331	1.331
Z	4	4
Mu (mm-1)	0.220	0.220
F000	640.0	640.0
F000’	640.74	
h,k,lmax	10,20,13	10,20,13
Nref	2879	2873
Tmin,Tmax	0.922,0.972	0.753,0.850
Tmin’	0.916	

Correction method= # Reported T Limits: Tmin=0.753 Tmax=0.850
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.698

R(reflections)= 0.0333(2437) wR2(reflections)= 0.0847(2873)

S = 1.035 Npar= 192

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          5 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          2 Note
```

Alert level G

```
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...          1 Report
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   1 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

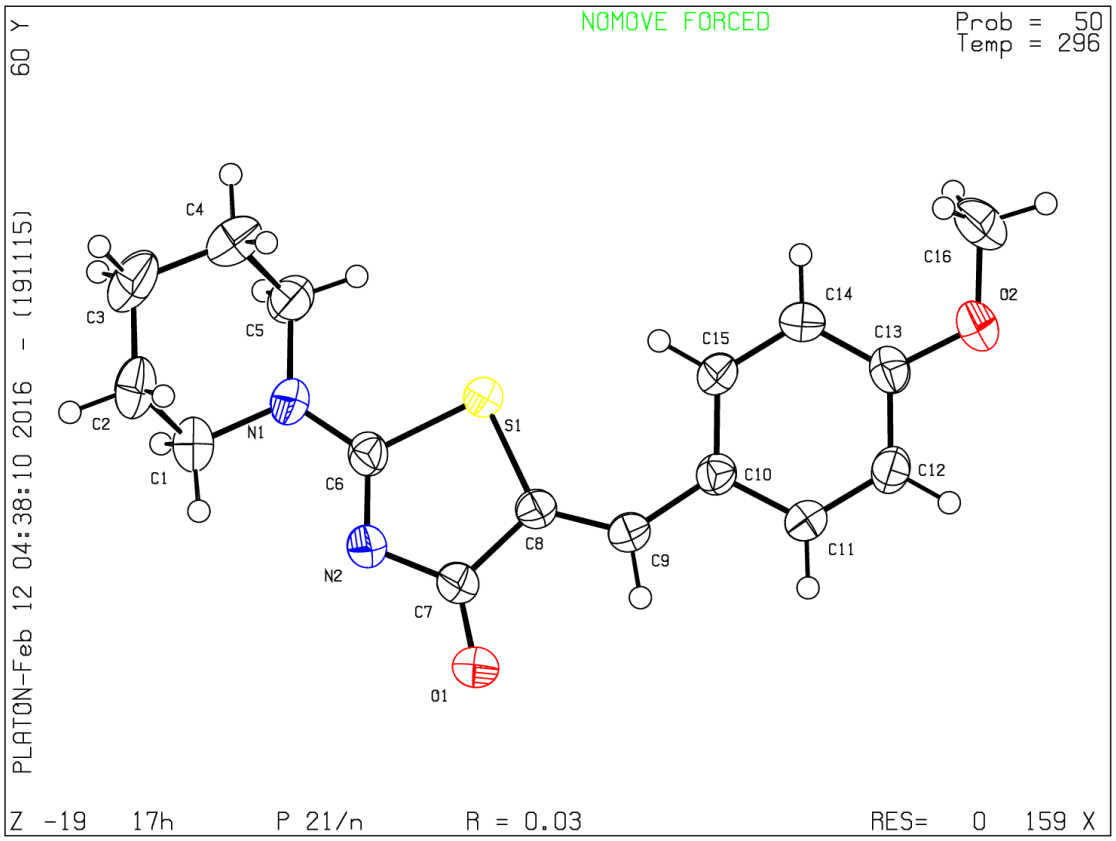
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 17h - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 17g

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 17g

```
Bond precision:  C-C = 0.0033 A          Wavelength=0.71073

Cell:           a=12.7194(4)    b=8.0294(3)         c=16.4422(6)
                alpha=90        beta=105.304(1)     gamma=90
Temperature:    298 K

                Calculated                Reported
Volume          1619.68(10)               1619.68(10)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C17 H21 N3 O S            C17 H21 N3 O S
Sum formula     C17 H21 N3 O S            C17 H21 N3 O S
Mr              315.43                    315.43
Dx,g cm-3       1.294                     1.294
Z               4                         4
Mu (mm-1)       0.205                     0.205
F000            672.0                     672.0
F000'           672.71
h,k,lmax        15,9,20                   15,9,20
Nref            3076                      3069
Tmin,Tmax       0.978,0.996               0.866,0.938
Tmin'           0.955

Correction method= # Reported T Limits: Tmin=0.866 Tmax=0.938
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 25.692

R(reflections)= 0.0438( 2543)     wR2(reflections)= 0.1167( 3069)

S = 1.029                 Npar= 202
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.541 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          7 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          5 Note
```

Alert level G

```
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...          1 Report
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   1 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

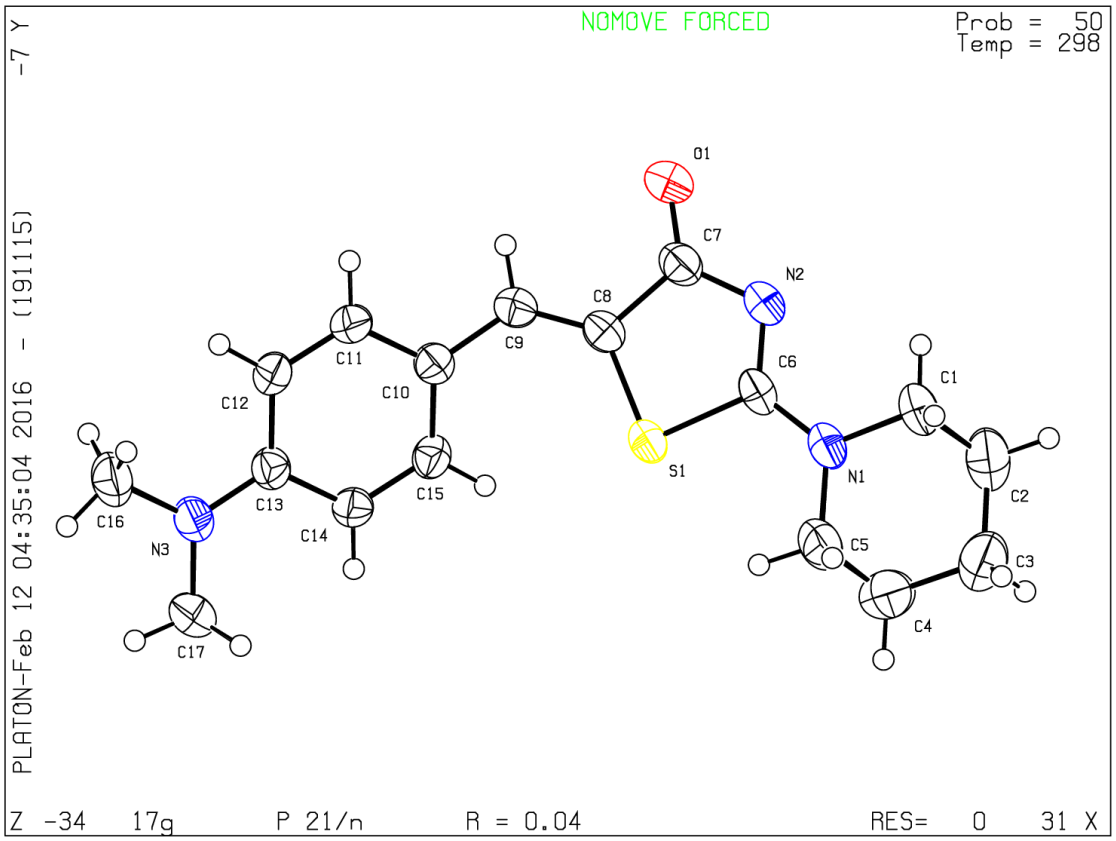
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 17g - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 17f

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 17f

Bond precision: C-C = 0.0033 A Wavelength=0.71073

Cell: a=7.303(3) b=16.637(5) c=12.598(5)
alpha=90 beta=97.725(13) gamma=90
Temperature: 297 K

	Calculated	Reported
Volume	1516.8(10)	1516.9(9)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C16 H18 N2 O3 S	C16 H18 N2 O3 S
Sum formula	C16 H18 N2 O3 S	C16 H18 N2 O3 S
Mr	318.38	318.38
Dx,g cm-3	1.394	1.394
Z	4	4
Mu (mm-1)	0.228	0.228
F000	672.0	672.0
F000’	672.78	
h,k,lmax	8,20,15	8,20,15
Nref	2880	2879
Tmin,Tmax	0.978,0.982	0.847,0.928
Tmin’	0.951	

Correction method= # Reported T Limits: Tmin=0.847 Tmax=0.928
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.697

R(reflections)= 0.0447(2127) wR2(reflections)= 0.1042(2879)

S = 1.079 Npar= 202

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.876 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          2 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          2 Note
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...          1 Report
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   2 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

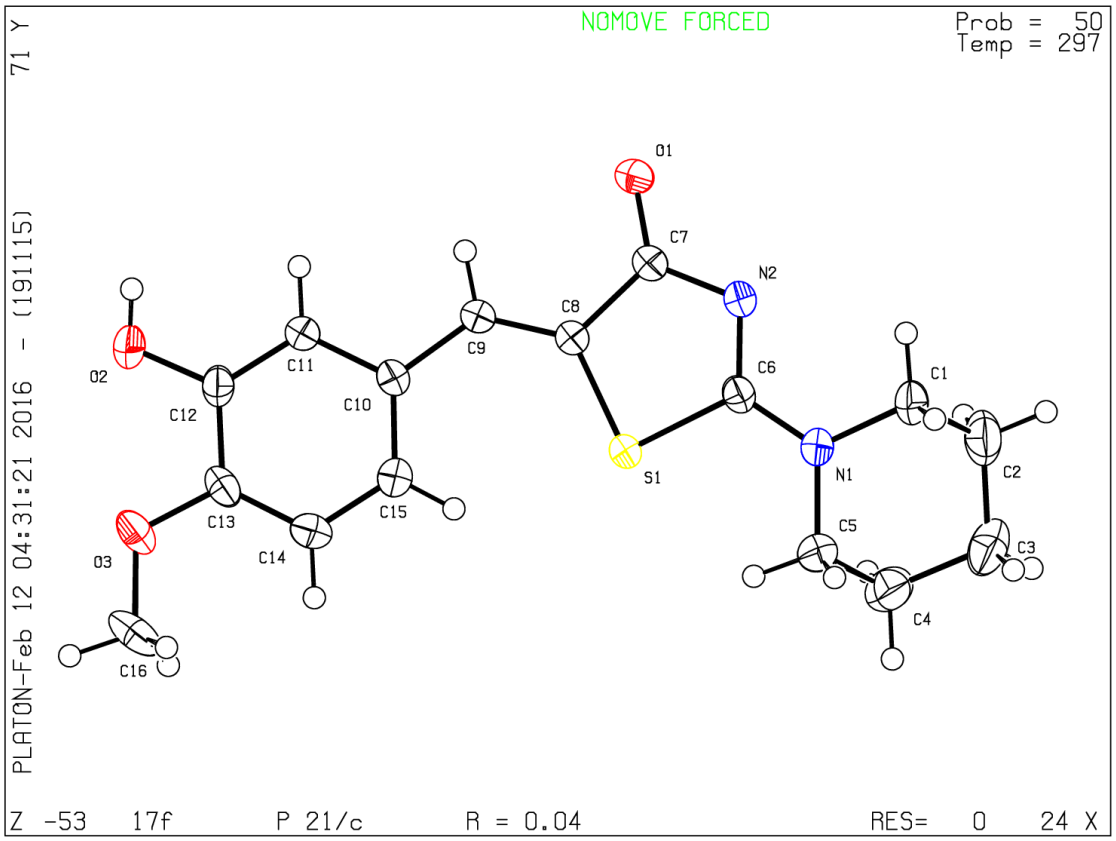
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 17f - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 17e

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 17e

```
Bond precision:  C-C = 0.0031 A          Wavelength=0.71073

Cell:           a=10.0466(4)    b=7.7834(3)       c=22.9774(10)
                alpha=90        beta=93.920(2)    gamma=90
Temperature:    297 K

                Calculated                Reported
Volume          1792.55(13)               1792.55(13)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C18 H22 N2 O4 S           C18 H22 N2 O4 S
Sum formula     C18 H22 N2 O4 S           C18 H22 N2 O4 S
Mr              362.44                    362.43
Dx,g cm-3       1.343                     1.343
Z               4                         4
Mu (mm-1)       0.206                     0.206
F000            768.0                     768.0
F000'           768.84
h,k,lmax        12,9,28                   12,9,28
Nref            3420                      3417
Tmin,Tmax       0.970,0.982               0.814,0.893
Tmin'           0.923

Correction method= # Reported T Limits: Tmin=0.814 Tmax=0.893
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 25.700

R(reflections)= 0.0420( 2616)     wR2(reflections)= 0.1066( 3417)

S = 1.023                 Npar= 230
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 3.051 Check

Alert level G

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ... 3 Report

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
1 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

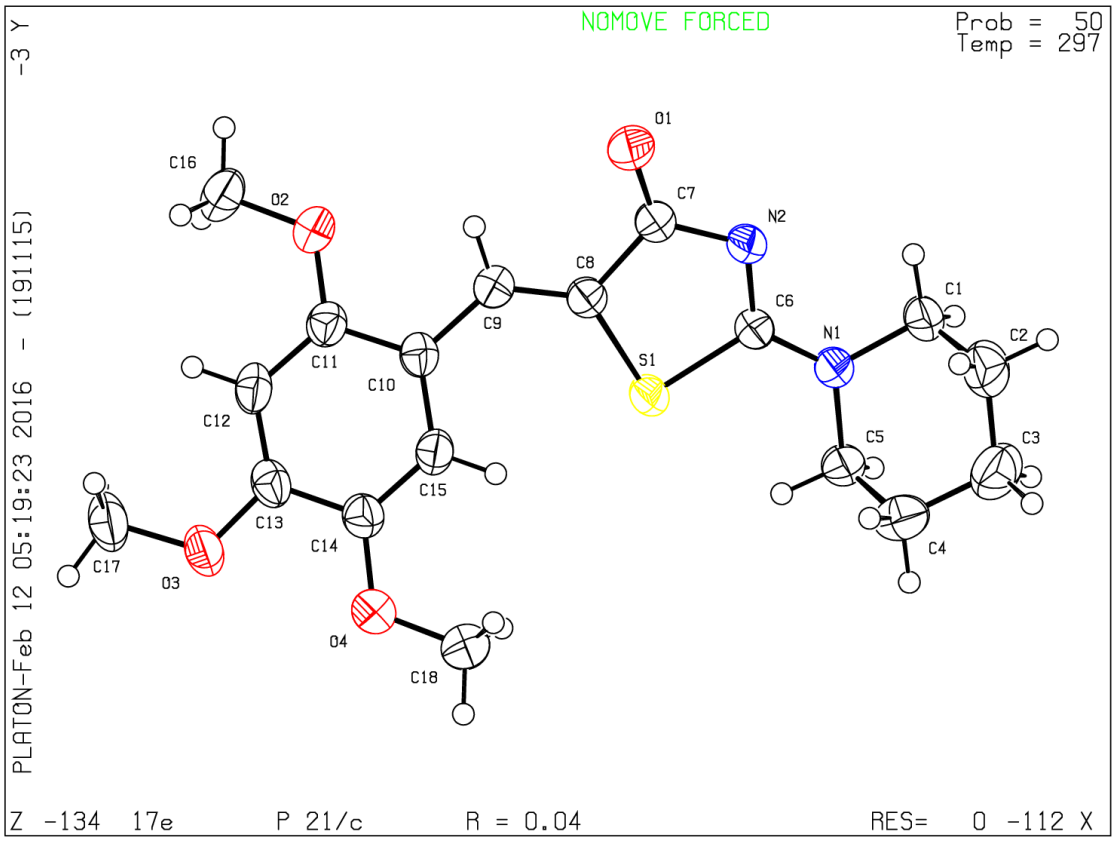
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 17e - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 17a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 17a

Bond precision: C-C = 0.0047 A Wavelength=0.71073

Cell: a=12.5012(6) b=16.1346(7) c=7.6541(4)
alpha=90 beta=106.967(2) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	1476.65(12)	1476.65(12)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C16 H18 N2 O S	C16 H18 N2 O S
Sum formula	C16 H18 N2 O S	C16 H18 N2 O S
Mr	286.38	286.38
Dx,g cm-3	1.288	1.288
Z	4	4
Mu (mm-1)	0.216	0.216
F000	608.0	608.0
F000’	608.70	
h,k,lmax	15,19,9	15,19,9
Nref	2809	2807
Tmin,Tmax	0.954,0.996	0.828,0.910
Tmin’	0.939	

Correction method= # Reported T Limits: Tmin=0.828 Tmax=0.910
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.695

R(reflections)= 0.0561(1923) wR2(reflections)= 0.1272(2807)

S = 1.092 Npar= 183

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C13 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00471 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      8.136 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.043 Check
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          1 Note
```

Alert level G

```
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...          2 Report
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   1 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

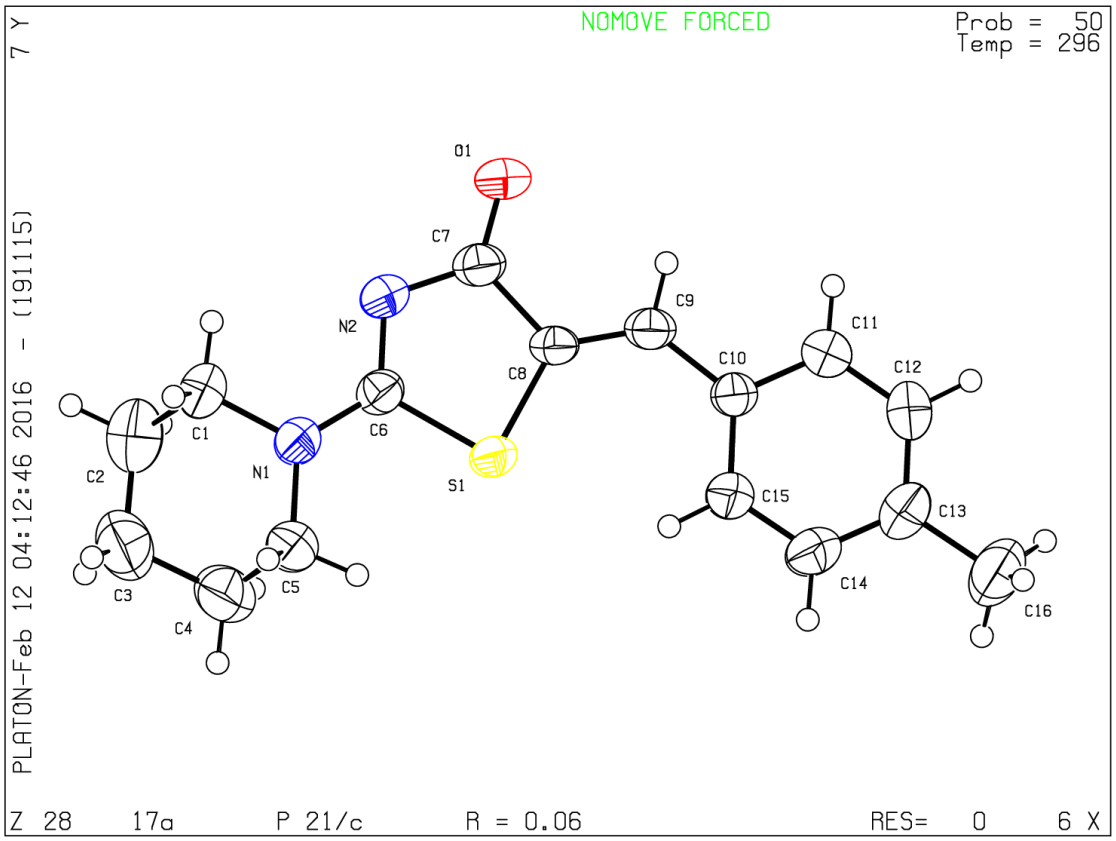
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 17a - ellipsoid plot



Contents

1. Melting Points of compound **17a**-**o**

Compounds	Melting Points
17a	152-154 °C
17b	245-247 °C
17c	198-200 °C
17d	139-141 °C
17e	240-242 °C
17f	210-212 °C
17g	228-230 °C
17h	195-197 °C
17i	155-157 °C
17j	157-159 °C
17k	137-139 °C
17l	142-144 °C
17m	165-167 °C
17n	184-186 °C
17o	210-212 °C

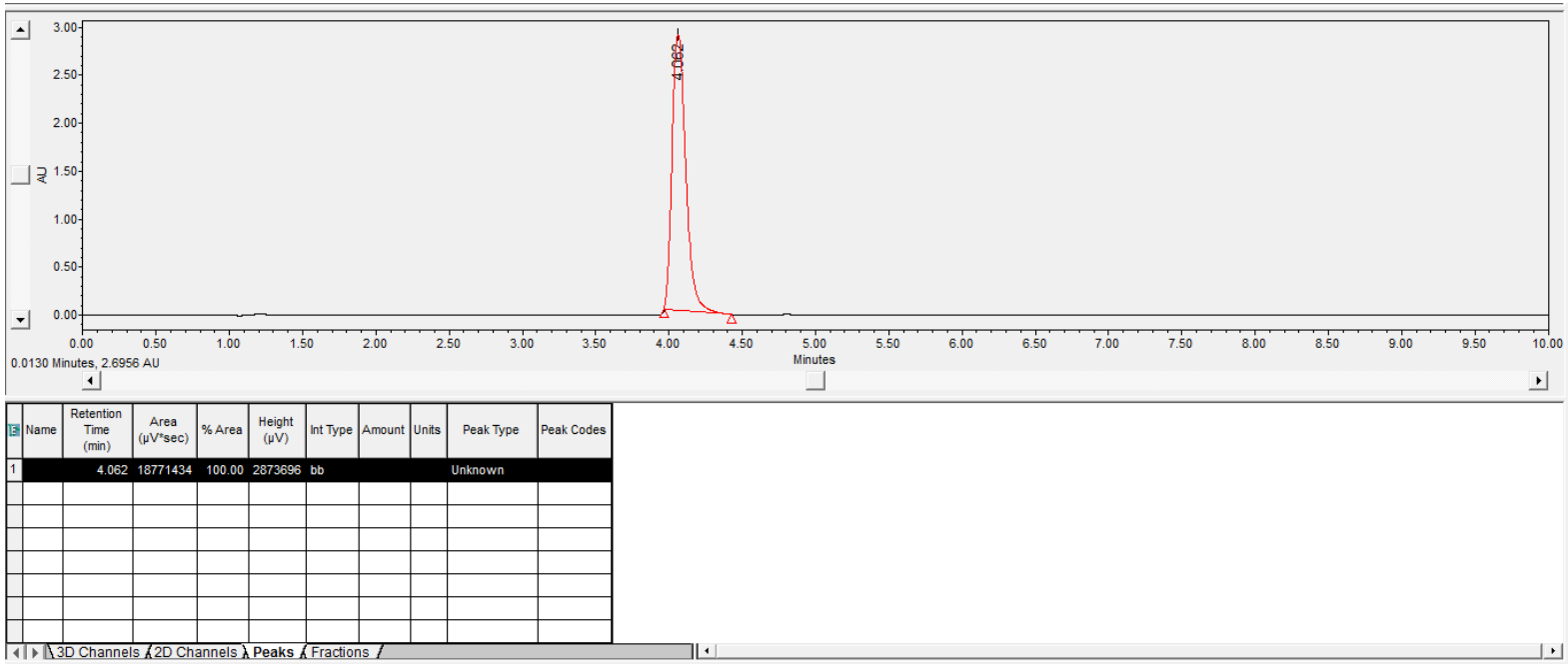
2. HPLC purity of compounds **17a**-**o**

   HPLC of samples **17a**-**o**, were executed in Waters e2695 (Separating module), equipped with 2998 PDA detector and prepared at a concentration level of 500 ppm and 10 µl is injected for the purity analysis. ACN and 0.1% Formic Acid-H_2O is used as mobile phase in ECLIPSE PLUS C18 (4.6 X 50 mm) 3.5 µM column.

Compounds	HPLC purity (%)
17a	~100
17b	~100
17c	96.6
17d	~100
17e	~100
17f	~100
17g	98.9
17h	~100
17i	~100
17j	98.2
17k	~100
17l	~100
17m	99.5
17n	99.5
17o	~100

3. HPLC spectra of compounds **17a-o**

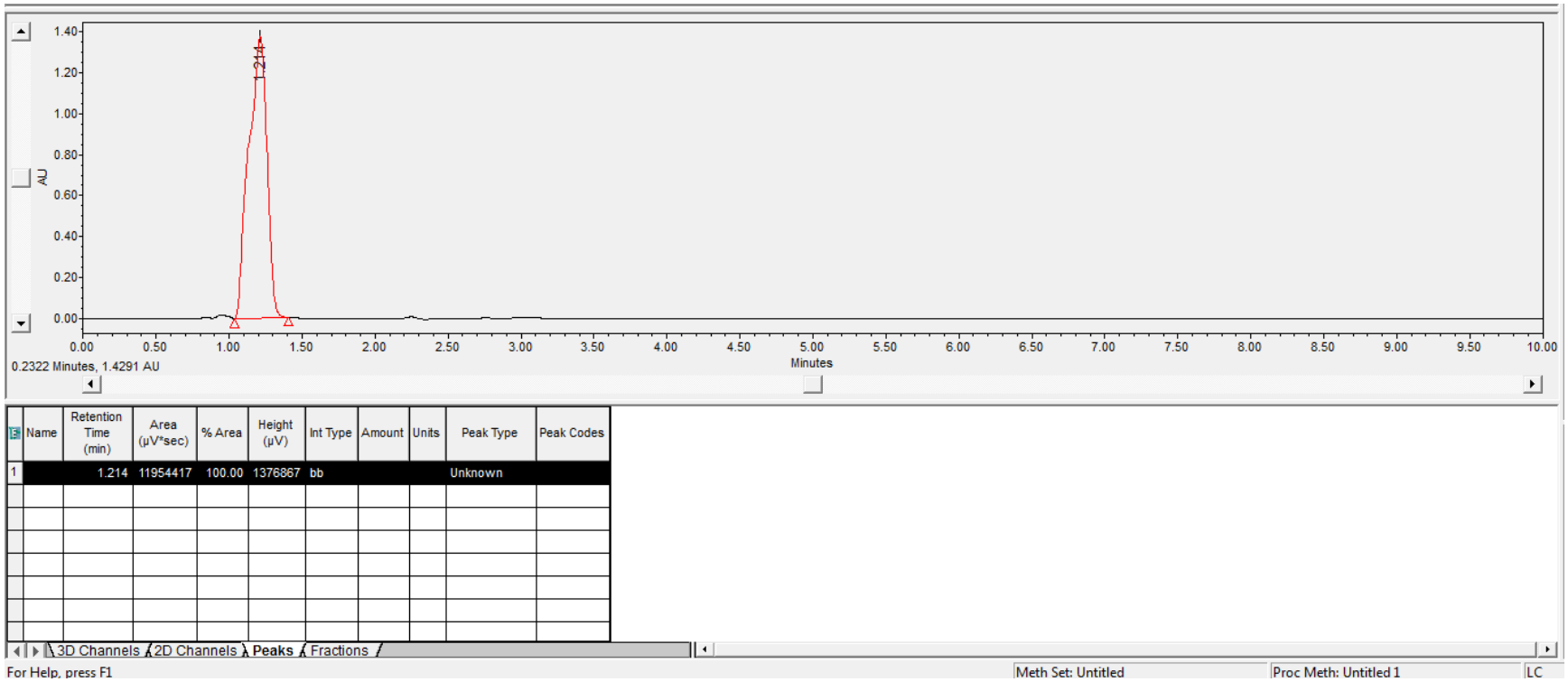
Compound **17a**



	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		4.062	18771434	100.00	2873696	bb			Unknown	

3D Channels | 2D Channels | Peaks | Fractions

Compound **17b**

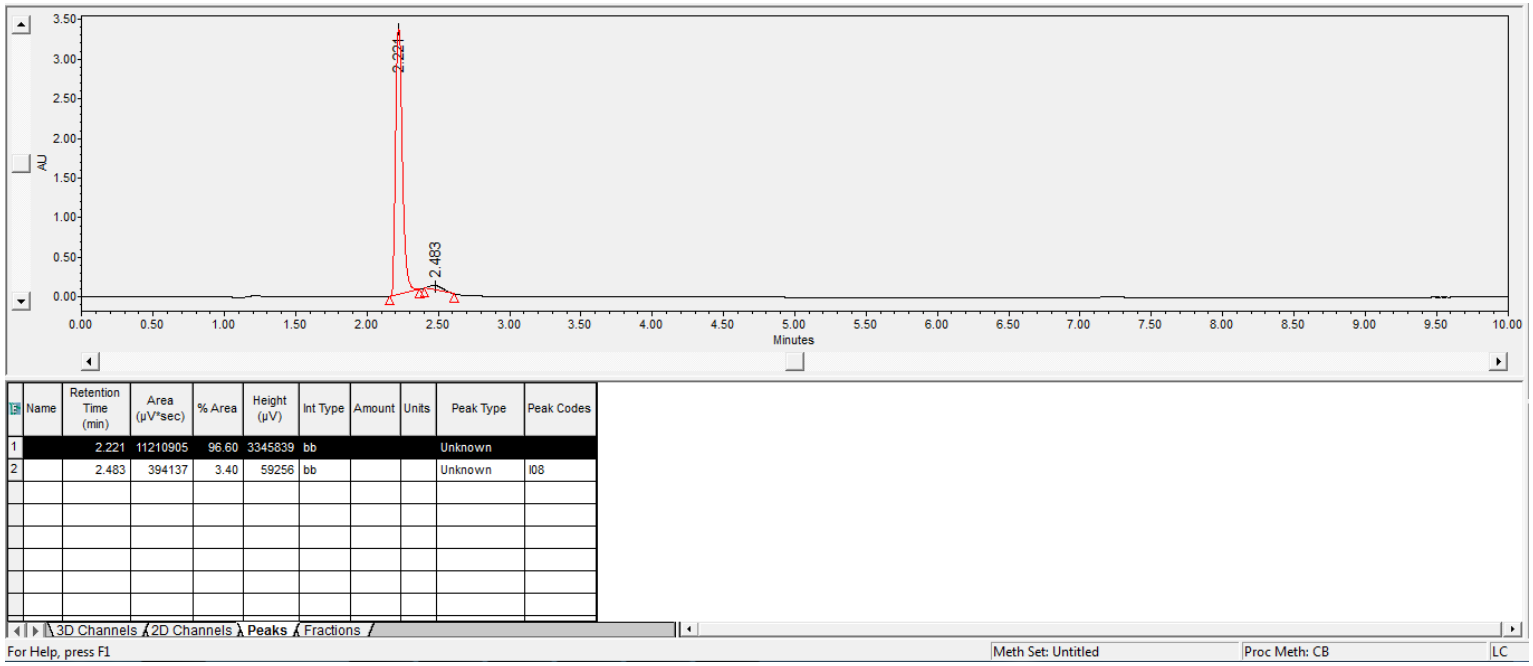


	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		1.214	11954417	100.00	1376867	bb			Unknown	

3D Channels | 2D Channels | Peaks | Fractions

For Help, press F1 | Meth Set: Untitled | Proc Meth: Untitled 1 | LC

Compound **17c**

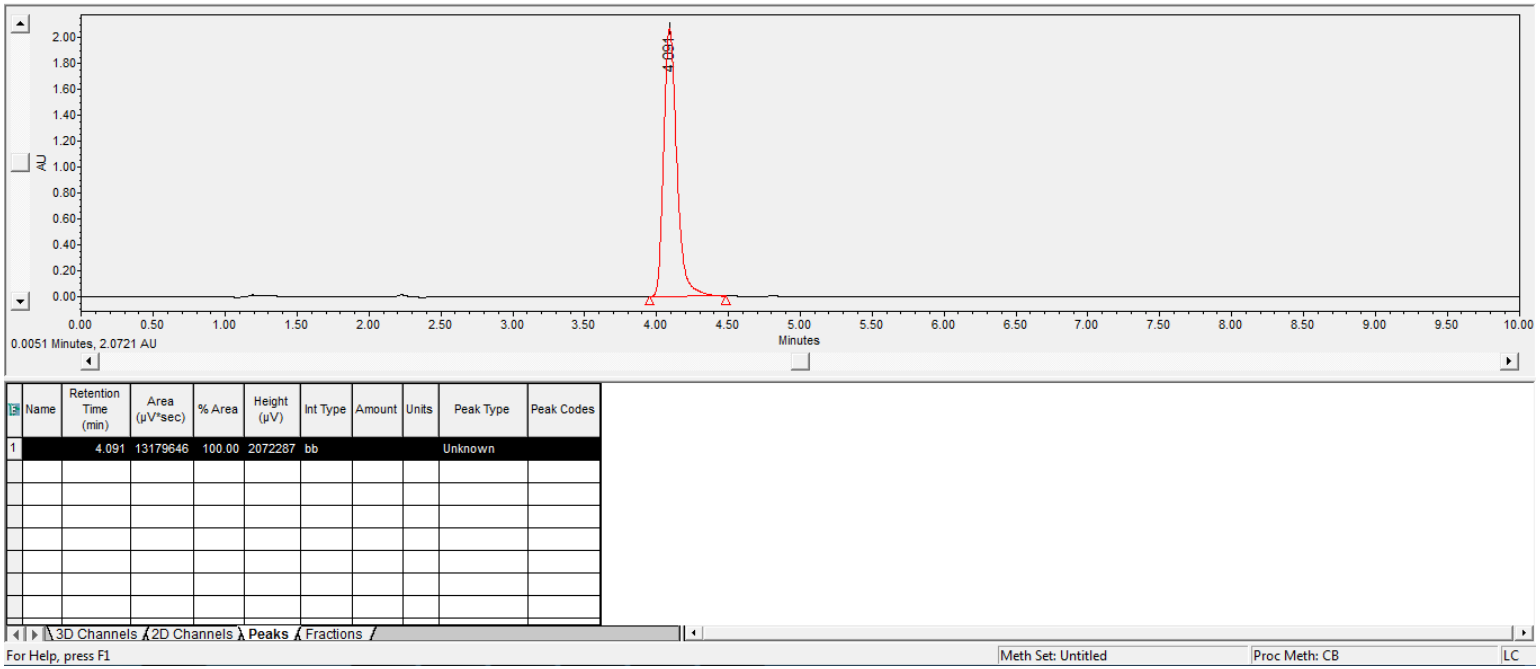


	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		2.221	11210905	96.60	3345839	bb			Unknown	
2		2.483	394137	3.40	59256	bb			Unknown	I08

3D Channels | 2D Channels | Peaks | Fractions

For Help, press F1 | Meth Set: Untitled | Proc Meth: CB | LC

Compound **17d**

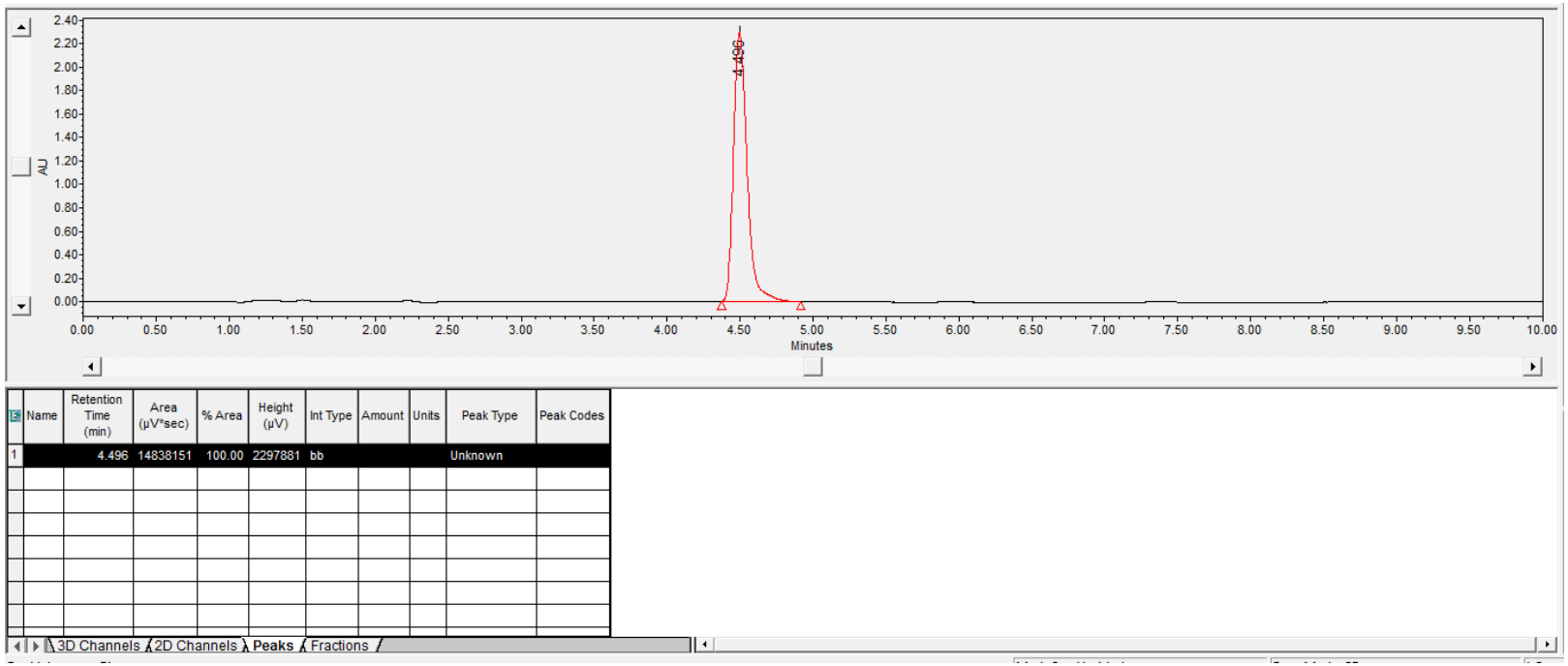


	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		4.091	13179646	100.00	2072287	bb			Unknown	

3D Channels | 2D Channels | **Peaks** | Fractions

For Help, press F1 | Meth Set: Untitled | Proc Meth: CB | LC

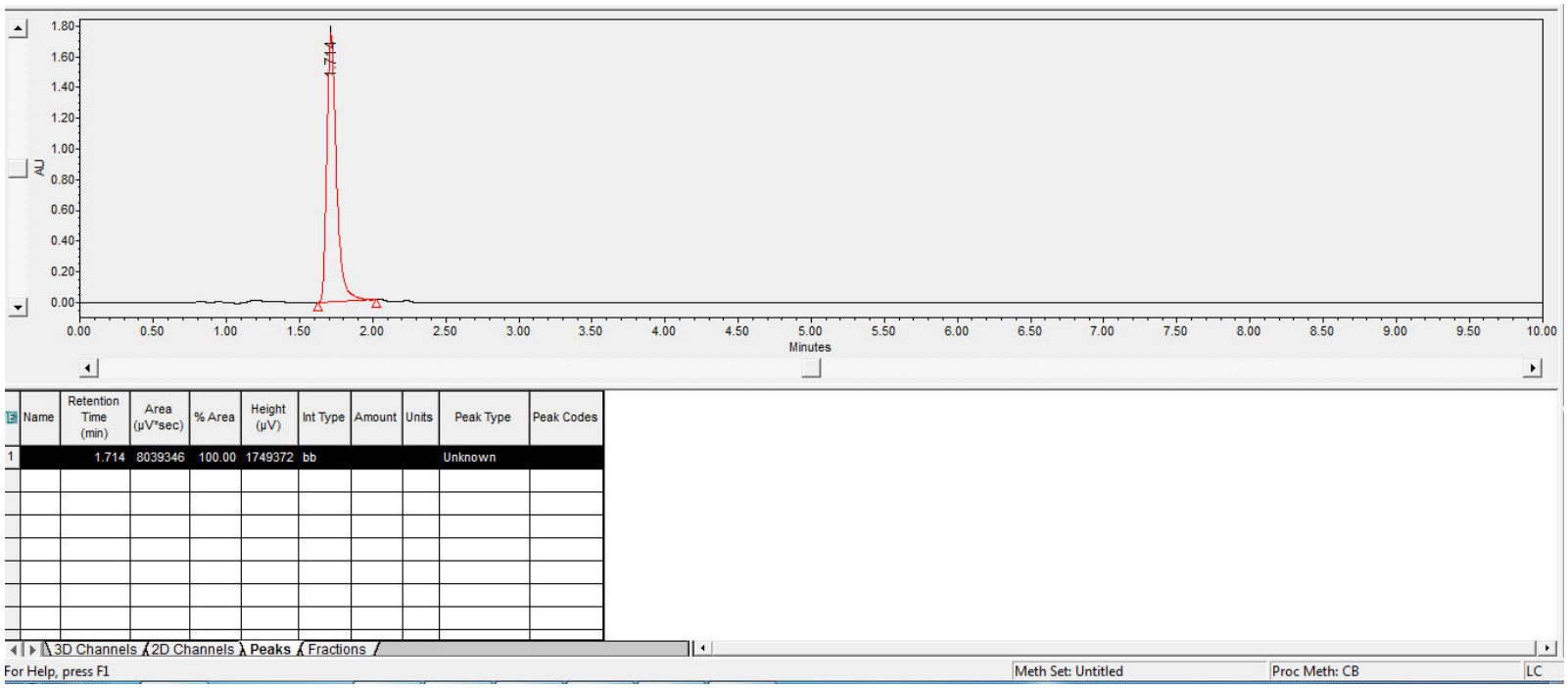
Compound **17e**



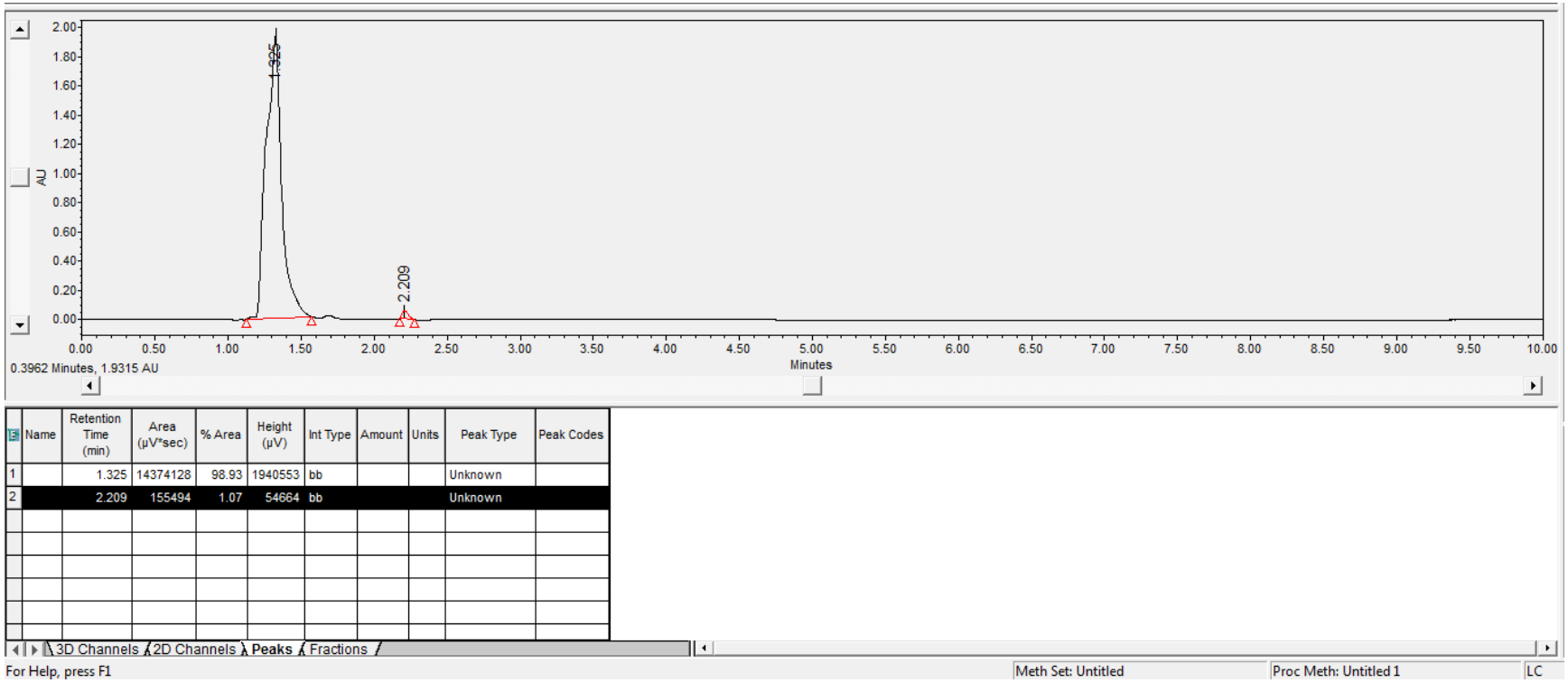
	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		4.496	14838151	100.00	2297881	bb			Unknown	

3D Channels | 2D Channels | Peaks | Fractions

Compound **17f**



Compound **17g**

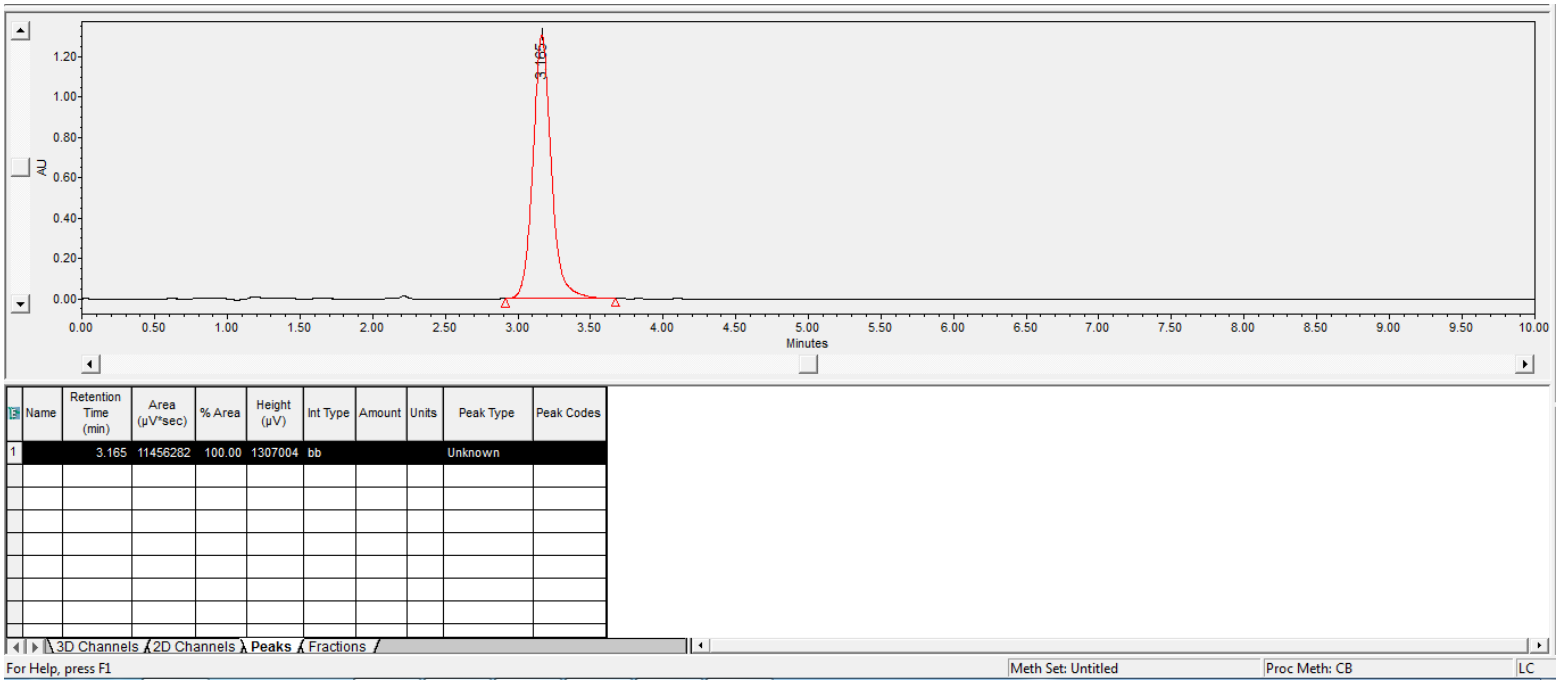


	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		1.325	14374128	98.93	1940553	bb			Unknown	
2		2.209	155494	1.07	54664	bb			Unknown	

3D Channels | 2D Channels | Peaks | Fractions

For Help, press F1 | Meth Set: Untitled | Proc Meth: Untitled 1 | LC

Compound **17h**

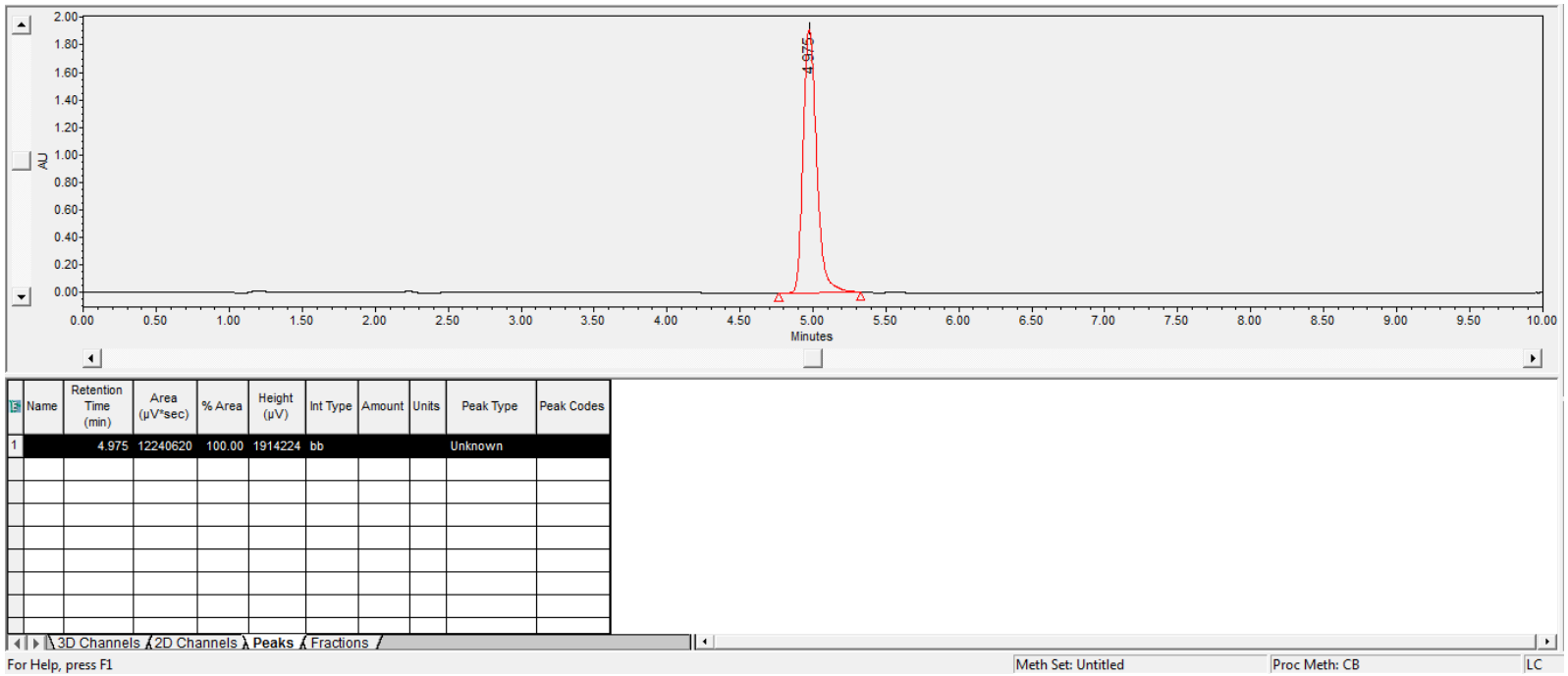


	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		3.165	11456282	100.00	1307004	bb			Unknown	

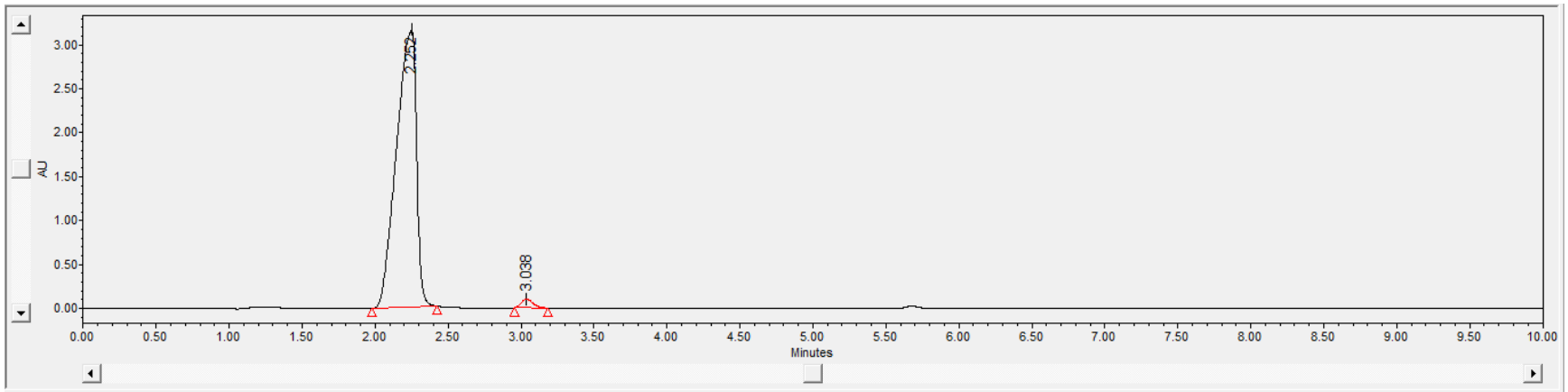
3D Channels | 2D Channels | Peaks | Fractions

For Help, press F1 | Meth Set: Untitled | Proc Meth: CB | LC

Compound **17i**



Compound **17j**

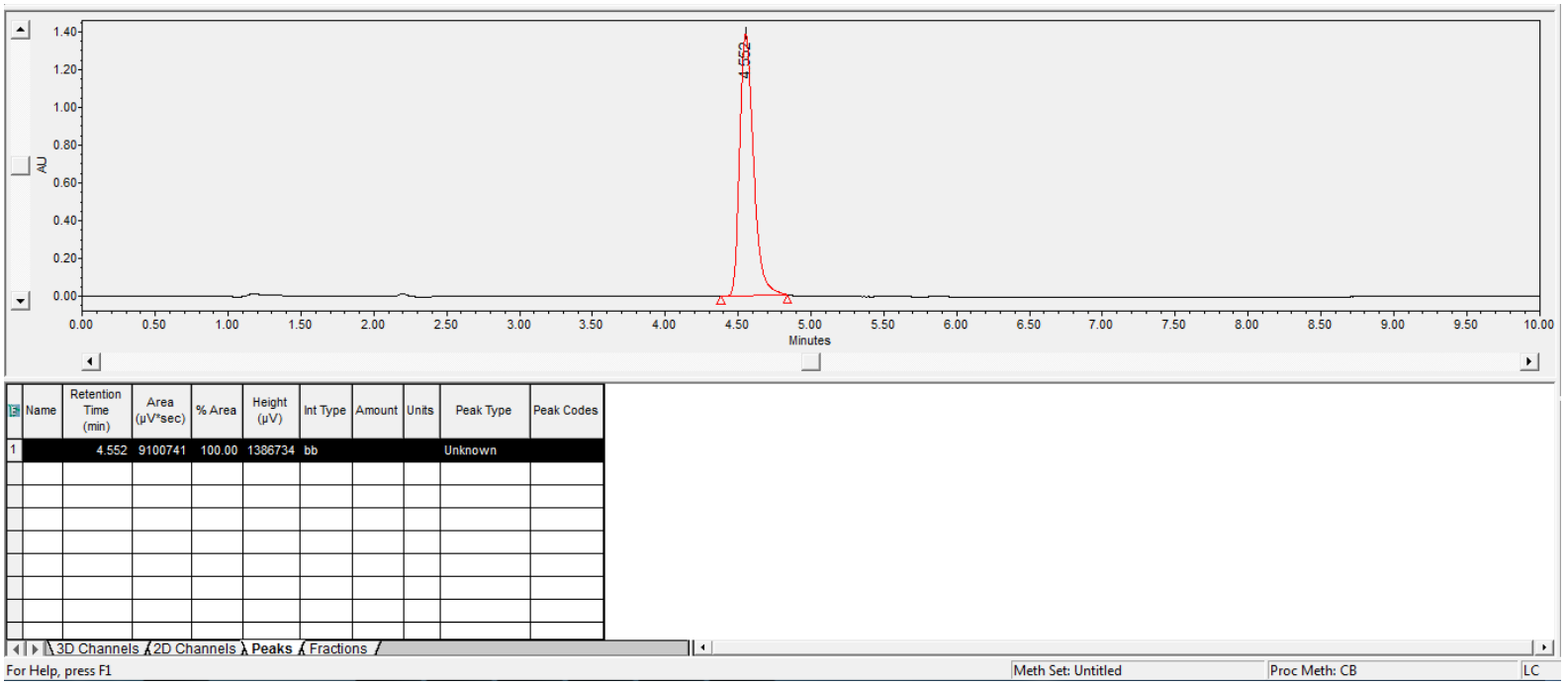


	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		2.252	29984293	98.18	3156908	bb			Unknown	
2		3.038	556599	1.82	100411	bb			Unknown	

3D Channels | 2D Channels | Peaks | Fractions

For Help, press F1 | Meth Set: Untitled | Proc Meth: Untitled 1 | LC

Compound **17k**

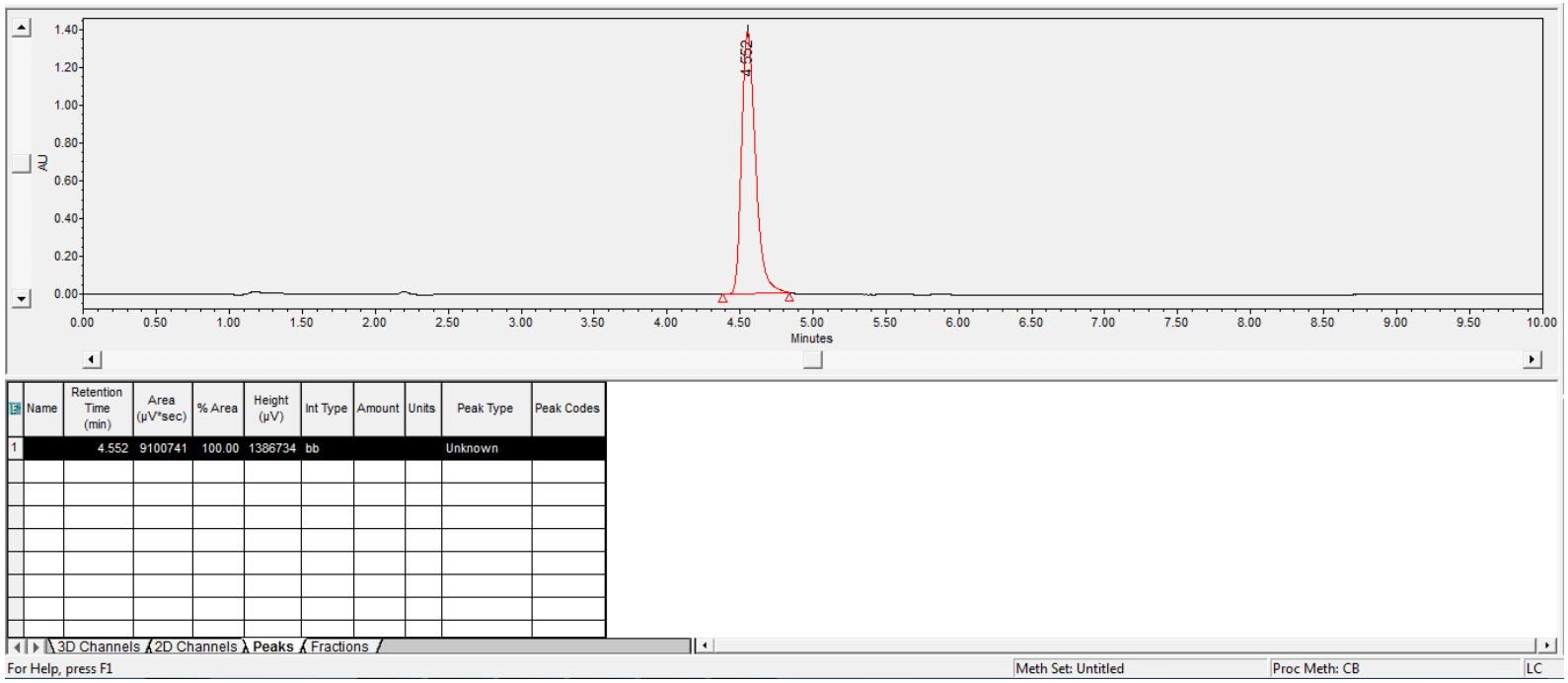


	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		4.552	9100741	100.00	1386734	bb			Unknown	

3D Channels | 2D Channels | Peaks | Fractions

For Help, press F1 | Meth Set: Untitled | Proc Meth: CB | LC

Compound **17l**

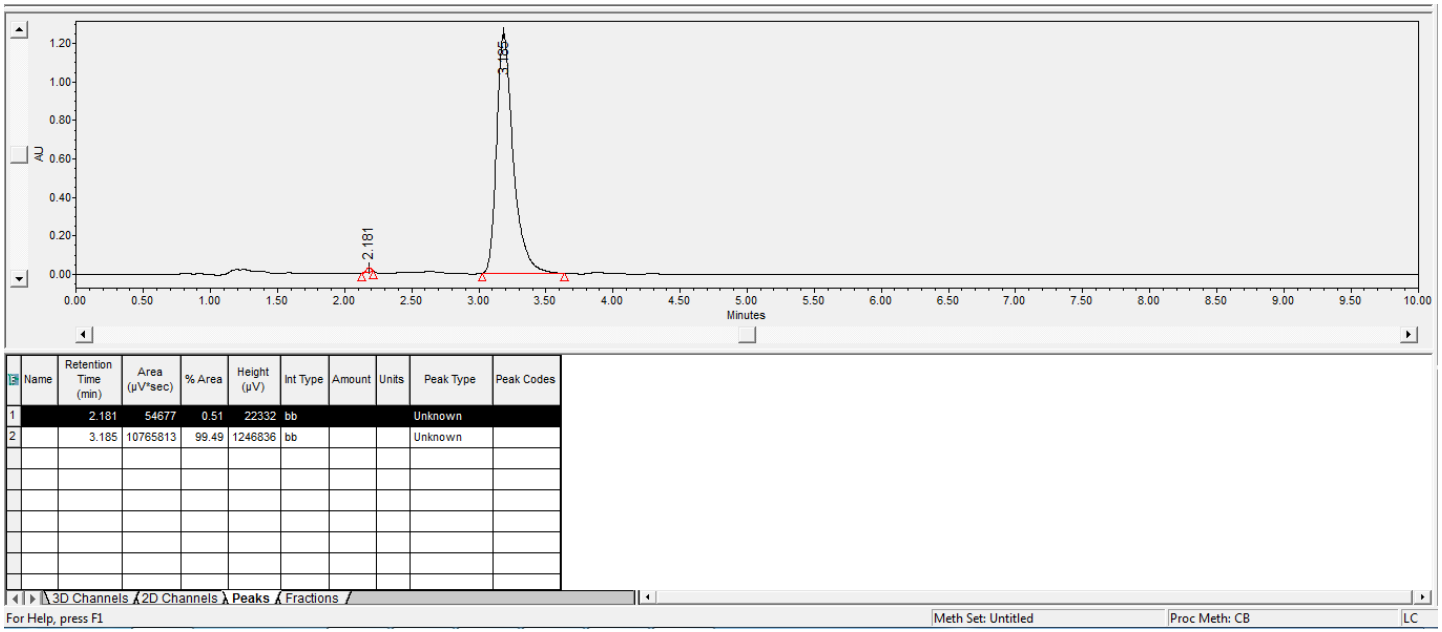


	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		4.552	9100741	100.00	1386734	bb			Unknown	

3D Channels | 2D Channels | Peaks | Fractions

For Help, press F1 | Meth Set: Untitled | Proc Meth: CB | LC

Compound **17m**

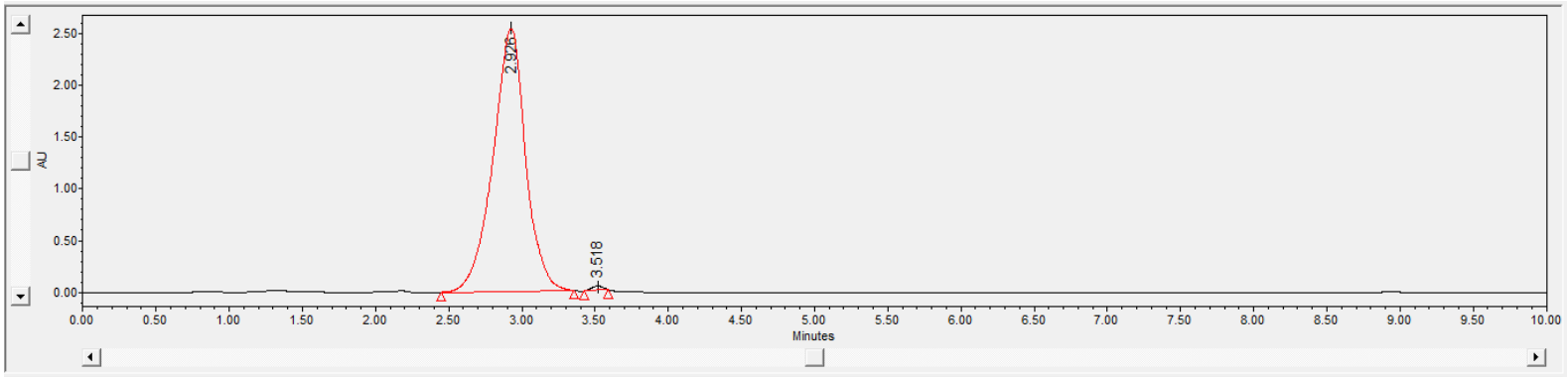


	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		2.181	54677	0.51	22332	bb			Unknown	
2		3.185	10765813	99.49	1246836	bb			Unknown	

3D Channels | 2D Channels | Peaks | Fractions

For Help, press F1 | Meth Set: Untitled | Proc Meth: CB | LC

Compound **17n**

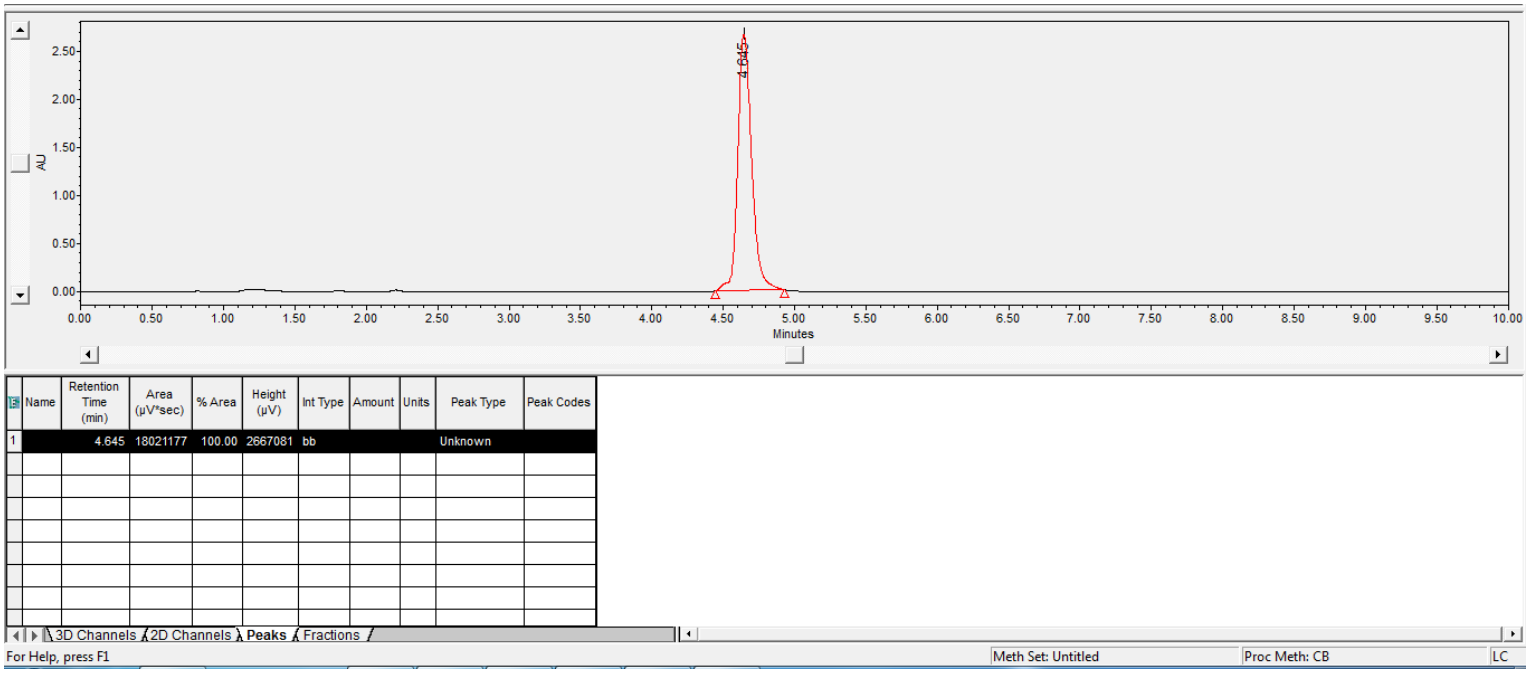


	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		2.926	39386733	99.45	2540133	bb			Unknown	
2		3.518	217143	0.55	40455	bb			Unknown	

3D Channels | 2D Channels | Peaks | Fractions

For Help, press F1 | Meth Set: Untitled | Proc Meth: CB | LC

Compound **17o**



	Name	Retention Time (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount	Units	Peak Type	Peak Codes
1		4.645	18021177	100.00	2667081	bb			Unknown	

3D Channels | 2D Channels | **Peaks** | Fractions

For Help, press F1 | Meth Set: Untitled | Proc Meth: CB | LC