



## Supporting Information

for

### Studies on the syntheses of $\beta$ -carboline alkaloids brevicarine and brevicolline

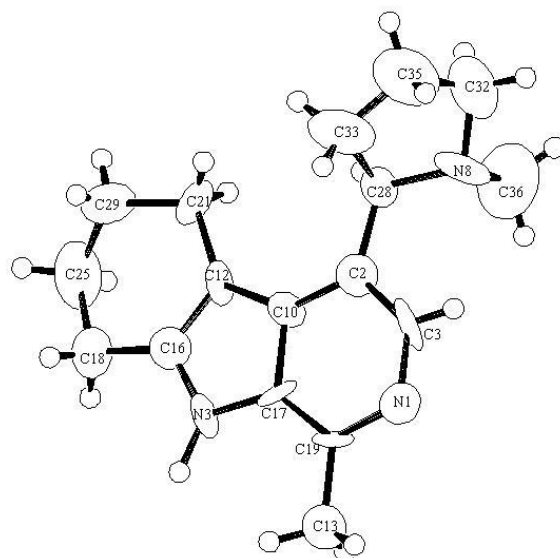
Benedek Batizi, Patrik Pollák, András Dancsó, Péter Keglevich, Gyula Simig, Balázs Volk and Mátyás Milen

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**ORTEP diagram of compound 31, synthetic procedures, IR,  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$  and 2D NMR spectra of compounds 2, 5, 6, 24–28 and 30–32**

**Content:**

|                                                                                                                                   |     |
|-----------------------------------------------------------------------------------------------------------------------------------|-----|
| <b>Figure S1.</b> X-ray structure (ORTEP diagram) of compound <b>31</b> .....                                                     | S2  |
| Experimental section of compounds <b>2, 5, 6, 24–28</b> and <b>30–32</b> .....                                                    | S3  |
| References.....                                                                                                                   | S12 |
| IR, $^1\text{H}$ , $^{13}\text{C}$ , $^{19}\text{F}$ and 2D NMR spectra of compounds <b>2, 5, 6, 24–28</b> and <b>30–32</b> ..... | S13 |



**Figure S1.** X-ray structure (ORTEP diagram) of compound **31**

# Experimental

## General

All melting points were determined on a Büchi B-540 capillary melting point apparatus and are uncorrected. IR spectra were obtained on a Bruker Alpha FT-IR spectrometer in transmission mode in KBr pellets, film or attenuated total reflection (ATR).  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded in  $\text{DMSO}-d_6$  solution in 5 mm tubes at room temperature, on a Bruker Avance III HD (600, 150 and 564 MHz for  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  NMR spectra, respectively) spectrometer with the deuterium signal of the solvent as the lock and TMS as the internal standard. Chemical shifts ( $\delta$ ) and coupling constants ( $J$ ) are given in ppm and in Hz, respectively. The following abbreviations are used to designate multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. Mass spectra were recorded on a Bruker O-TOF MAXIS Impact mass spectrometer coupled to a Dionex Ultimate 3000 RS HPLC system with a diode array detector. High-resolution mass spectra (HRMS) were recorded on a Bruker Q-TOF MAXIS Impact mass spectrometer coupled with a Waters I-Class UPLC system with a diode array detector (for  $[\text{M}+\text{H}]^+$ ) or on an Agilent 7250 Q-TOF mass spectrometer coupled to an Agilent 8890 gas chromatographic system (for  $[\text{M}]^+$ ). The single crystal X-ray diffraction measurements were carried out on a Rigaku R-Axis Spider instrument with image plate detector. Single-crystal X-ray structure of compound **31** has been uploaded to the CCDC database (CCDC number: 2410549). Reactions were monitored by thin-layer chromatography (TLC) carried out on silica gel plates (60 F<sub>254</sub>) using UV light as visualizing agent. Purifications by flash column chromatography were carried out using Merck 107736 silica gel 60 H using a hexane–EtOAc or DCM–MeOH solvent system. All reagents were purchased from commercial sources and used without further purification. Analytical samples of synthesized compounds were obtained by recrystallization from the solvents or solvent mixtures given below in

parentheses. Compounds **2**, **5**, **6** are described in the literature, while compounds **24–28**, **30–32** are new and characterized below.

## Procedures

### ***N*-Methyl-4-(1-methyl-9*H*- $\beta$ -carbolin-4-yl)butan-1-amine (2)**

Compound **26** (61 mg, 0.22 mmol) was dissolved in dry THF (5.0 mL) and  $\text{BH}_3 \cdot \text{SMe}_2$  (66  $\mu\text{L}$ , 0.87 mmol) reagent was added. The mixture was heated to reflux and reacted for 5 hours. After that, the mixture was cooled to room temperature and 37 wt % aqueous HCl solution (3.0 mL) was added. The mixture was heated to reflux and reacted for 1 hour. The mixture was poured onto ice and treated with 10 wt % aqueous NaOH until pH 7. It was extracted with DCM ( $3 \times 15$  mL). The combined organic layer was dried over  $\text{Na}_2\text{SO}_4$  and concentrated in vacuo to give a colorless oil (44 mg, 60 %). IR (ATR): 3142, 3059, 1620, 1455, 1323, 1293, 735  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR ( $\text{DMSO-}d_6$ , 600 MHz):  $\delta$  11.57 (br s, 1H), 8.13 (m, 1H), 7.99 (s, 1H), 7.61 (m, 1H), 7.53 (m, 1H), 7.25 (m, 1H), 3.11 (t,  $J = 7.6$  Hz, 2H), 2.72 (s, 3H), 2.50 (m, 2H), 2.25 (s, 3H), 1.75 (m, 2H), 1.55 (m, 2H) ppm.  $^{13}\text{C}$  NMR ( $\text{DMSO-}d_6$ , 150 MHz):  $\delta$  140.5, 140.1, 137.7, 134.5, 129.0, 127.3, 125.1, 123.3, 121.1, 119.6, 112.1, 51.5, 36.4, 30.8, 29.3, 27.5, 20.4 ppm. HRMS (ESI) calcd. for  $\text{C}_{17}\text{H}_{21}\text{N}_3^+ [\text{M}]^+$  267.1735; found 267.1728.

### ***N*-Methyl-4-(1-methyl-9*H*- $\beta$ -carbolin-4-yl)butan-1-amine dihydrochloride (2 · 2 HCl)**

Brevicarine dihydrochloride salt was obtained by the addition of cc. HCl to an ethanolic solution of brevicarine (**2**) to give colorless crystals. Mp 192–195 °C (EtOH). (lit. S1 mp. 195–196 °C). IR (ATR): 3385, 3187, 2765, 2468, 1620, 1452, 1407, 1329, 1060, 765, 734  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR ( $\text{DMSO-}d_6$ , 600 MHz):  $\delta$  11.70 (br s, 1H), 8.56 (br s, 2H), 8.13 (m, 1H), 8.03 (s, 1H), 7.64 (m, 1H), 7.55 (m, 1H), 7.27 (m, 1H), 3.17 (t,  $J = 7.1$  Hz, 2H), 2.91 (t,  $J = 7.4$  Hz, 2H), 2.74 (s, 3H), 2.50 (s, 3H), 1.79 (m, 2H), 1.72 (m, 2H) ppm.  $^{13}\text{C}$  NMR ( $\text{DMSO-}d_6$ , 150 MHz):  $\delta$  140.6, 140.3, 137.4, 134.5, 128.4, 127.6, 125.3, 123.4, 121.0, 119.7, 112.2, 48.3, 32.6, 30.2, 26.3, 25.4, 20.2 ppm.

## 2-[4-(1-Methyl-9H- $\beta$ -carbolin-4-yl)but-3-yn-1-yl]-1H-isoindole-1,3-(2H)-dione (5)<sup>S2</sup>

Compound **3** (422 mg, 1.28 mmol) was dissolved in EtOAc (25.0 mL). Reagent **4** (636 mg, 3.19 mmol), TEA (0.71 mL, 5.11 mmol), CuI (29.2 mg, 0.15 mmol) and Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> (90 mg, 0.13 mmol) were added under argon atmosphere. The mixture was heated to 60 °C and reacted for 3 hours. After that, it was concentrated in vacuo and the residue was purified by silica gel column chromatography (hexane–EtOAc) to give yellow crystals (458 mg, 93%). Mp 245–248 °C (EtOAc) (lit. S2 mp. 245–248 °C (*n*-hexane–DCM)). IR (KBr): 3473, 3186, 2926, 2243, 1716, 1396, 1339, 1295, 1031, 721 cm<sup>-1</sup> (newly measured and in agreement with lit. S2). <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz):  $\delta$  11.85 (s, 1H), 8.29 (d, *J* = 7.6 Hz, 1H), 8.24 (br s, 1H), 7.90 (m, 2H), 7.84 (m, 2H), 7.60 (d, *J* = 8.8 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.01 (t, *J* = 7.6 Hz, 1H), 3.97 (t, *J* = 6.6 Hz, 2H), 3.10 (t, *J* = 7.0 Hz, 2H), 2.77 (s, 3H). <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 150 MHz):  $\delta$  168.3, 142.1, 141.1, 140.3, 135.0, 132.0, 128.9, 126.6, 123.7, 122.5, 122.2, 120.9, 120.1, 119.9, 112.5, 93.3, 78.7, 46.2, 36.9, 19.3, 9.1. HRMS (ESI) calcd. for C<sub>24</sub>H<sub>18</sub>N<sub>3</sub>O<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup> 380.1394; found: 380.1396.

## 4-(1-Methyl-9H- $\beta$ -carbolin-4-yl)but-3-yn-1-amine (6)<sup>S2</sup>

Compound **5** (286 mg, 0.75 mmol) was dissolved in 40 wt % aqueous MeNH<sub>2</sub> (4.72 mL, 54.50 mmol) solution and stirred at room temperature for 30 minutes. After that, 20 wt % aqueous NaOH (1.65 mL) was added and reacted with stirring at room temperature for 2 hours. Afterwards, brine (10 mL) was added. The combined aqueous phase was washed with DCM (3  $\times$  10 mL). The combined organic layer was dried over NaSO<sub>4</sub> and concentrated in vacuo. The crude product was purified by silica gel column chromatography (DCM–15 wt % NH<sub>3</sub> in MeOH) to give pale yellow crystals (147 mg, 78%). Mp 166–168 °C (EtOH–H<sub>2</sub>O). (lit. S2 mp. 166–168 °C). IR (KBr): 3131, 2987, 1620, 1593, 1421, 1296, 905, 747 cm<sup>-1</sup> (newly measured and in agreement with lit. S2). <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz):  $\delta$  11.78 (br s, 1H), 8.53 (d, *J* = 7.9 Hz, 1H), 8.26 (s, 1H), 7.64 (d, *J* = 8.2 Hz, 1H), 7.59 (m, 1H), 7.28 (t, *J* = 7.7 Hz, 1H), 2.92

(t,  $J = 6.9$  Hz, 2H), 2.78 (s, 3H), 2.71 (t,  $J = 6.8$  Hz, 2H) ppm.  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 150 MHz):  $\delta$  141.8, 140.8, 140.7, 134.0, 128.4, 126.3, 122.5, 121.0, 119.7, 112.2, 110.2, 95.3, 78.0, 41.6, 24.5, 20.6 ppm. HRMS (ESI) calcd. for  $\text{C}_{16}\text{H}_{16}\text{N}_3^+$   $[\text{M}+\text{H}]^+$  250.1339; found: 250.1343.

#### **2-[4-(1-Methyl-9H- $\beta$ -carbolin-4-yl)butyl]-1H-isoindole-1,3(2H)-dione (24)**

In a 22-mL autoclave, compound **5** (488 mg, 1.29 mmol) was dissolved in a mixture of EtOAc–MeOH (1:1, 15.0 mL), and 10 wt % Pd/C (150 mg, 0.141 mmol) was added. The autoclave was purged with argon gas. After that, it was washed with hydrogen gas three times and the starting pressure was adjusted to 20 bar. The mixture was reacted at room temperature while stirring for 16 hours. After the reaction was complete, the mixture was filtered through celite and the filter pad was washed with EtOAc–MeOH (1:1,  $3 \times 10$  mL). It was concentrated in vacuo and the residue was purified by silica gel column chromatography (hexane–EtOAc) to give yellow crystals (353 mg, 72%). Mp 107–110 °C (EtOH). IR (KBr): 3377, 1706, 1620, 1396, 1030, 718  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (DMSO- $d_6$ , 600 MHz):  $\delta$  11.56 (br s, 1H), 8.04 (m, 1H), 7.99 (s, 1H), 7.83 (m, 2H), 7.82 (m, 2H), 7.60 (m, 1H), 7.49 (m, 1H), 7.15 (m, 1H), 3.62 (t,  $J = 6.4$  Hz, 2H), 3.13 (t,  $J = 6.9$  Hz, 2H), 2.71 (s, 3H), 1.76 (m, 2H), 1.75 (m, 2H) ppm.  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 150 MHz):  $\delta$  168.2, 140.5, 140.3, 137.7, 134.6, 131.7, 128.5, 127.3, 125.0, 123.2, 123.1, 121.0, 119.5, 112.2, 48.8, 37.5, 30.3, 28.0, 26.8, 20.4 ppm. HRMS (ESI) calcd. for  $\text{C}_{24}\text{H}_{22}\text{N}_3\text{O}_2^+$   $[\text{M}+\text{H}]^+$  384.1707; found: 384.1713.

#### **4-(1-Methyl-9H- $\beta$ -carbolin-4-yl)butan-1-amine (25)**

Method A: Compound **24** (337 mg, 0.88 mmol) was dissolved in 40 wt % aqueous  $\text{MeNH}_2$  (7.0 mL, 66.7 mmol) solution and stirred at room temperature for 30 minutes. After that, 20 wt % aqueous NaOH (7.0 mL) was added, and the mixture was reacted at room temperature for 2 hours. Afterwards, brine (100.0 mL) was added, and the combined aqueous phases were extracted with DCM ( $3 \times 150$  mL). The combined organic layer was dried over  $\text{Na}_2\text{SO}_4$  and

concentrated in vacuo. The crude product was purified by silica gel column chromatography (DCM–15 wt % NH<sub>3</sub> in MeOH) to give pale yellow crystals (182 mg, 82%).

**Method B:** In a 22-mL autoclave, compound **6** (185 mg, 0.74 mmol) was dissolved in EtOH (15.0 mL) and 10 wt % Pd/C (77 mg, 0.07 mmol) was added. The autoclave was purged with argon gas. After that, it was washed with hydrogen gas three times and the starting pressure was adjusted to 20 bar. The mixture was reacted at room temperature for 16 hours. After the reaction was complete, the mixture was filtered through celite, and the filter pad was washed with EtOH (3 × 10 mL). It was concentrated in vacuo and the residue was purified by silica gel column chromatography (DCM–15 wt % NH<sub>3</sub> in MeOH) to give pale yellow crystals (165 mg, 88%). Mp 101–103 °C (MeCN). IR (ATR): 3058, 2923, 2859, 1620, 1570, 1507, 1455, 1394, 1323, 1293, 1030 cm<sup>-1</sup>. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz):  $\delta$  11.57 (s, 1H), 8.11 (d, *J* = 8.0 Hz, 1H), 7.99 (s, 1H), 7.61 (d, *J* = 8.2 Hz, 1H), 7.53 (t, *J* = 8.1 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 1H), 3.11 (t, *J* = 7.6 Hz, 2H), 2.72 (s, 3H), 2.58 (t, *J* = 7.0 Hz, 2H), 1.75 (m, 2H), 1.50 (m, 2H) ppm. <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 150 MHz):  $\delta$  140.5, 140.1, 137.7, 134.5, 129.0, 127.3, 125.1, 123.3, 121.1, 119.6, 112.1, 41.6, 33.1, 30.7, 27.2, 20.4 ppm. HRMS (ESI) calcd. for C<sub>16</sub>H<sub>19</sub>N<sub>3</sub><sup>+</sup> [M]<sup>+</sup> 253.1573; found 253.1570.

#### ***N*-[4-(1-Methyl-9*H*- $\beta$ -carbolin-4-yl)butyl]formamide (**26**)**

**Method A:** Compound **25** (80 mg, 0.32 mmol) was dissolved in toluene (5.0 mL) and formic acid (15.0  $\mu$ L, 0.38 mmol) was added. The mixture was heated to reflux and reacted for 16 hours. After concentration in vacuo, the residue was dissolved in EtOAc (10.0 mL), washed with 10 wt % aqueous NaHCO<sub>3</sub> solution (10.0 mL). The aqueous phase was extracted with EtOAc (2 × 15 mL). The combined organic layer was dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated in vacuo to give colorless crystals. The crude product was purified by preparative TLC (DCM–MeOH) to give colorless crystals (61 mg, 69%).

**Method B:** Compound **28** (10.0 mg, 0.03 mmol) was dissolved in dry THF (10.0 mL) and cooled to 0 °C. Under argon atmosphere, LiAlH<sub>4</sub> (3.50 mg, 0.09 mmol) was added slowly. After that, the mixture was heated to reflux and stirred for 1 hour. The reaction cooled to 0 °C and the excess reagent was hydrolyzed by carefully adding water (4 × 10 mL) and 15 wt % NaOH solution (10.0 mL). The mixture was stirred for 20 minutes and additional THF (30.0 mL) was added and filtered through celite, and the filter pad was washed with THF (50.0 mL). The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated in vacuo to give a yellow oil. The crude product was purified by preparative TLC (DCM–MeOH) to give colorless crystals (4.4 mg, 51%). Mp 121–123 °C (MeCN). IR (KBr): 3472, 1665, 1564, 1508, 1381, 907, 731 cm<sup>-1</sup>. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz): δ 11.58 (br s, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 8.01 (br s, 1H), 8.00 (s, 1H), 7.97 (s, 1H), 7.62 (m, 1H), 7.53 (t, *J* = 7.7 Hz, 1H), 7.26 (t, *J* = 7.6 Hz, 1H), 3.13 (m, 2H), 3.12 (m, 2H) 2.72 (s, 3H), 1.73 (m, 2H), 1.56 (m, 2H) ppm. <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 150 MHz): δ 161.1, 140.5, 140.2, 137.7, 134.5, 128.8, 127.4, 125.1, 123.3, 121.1, 119.6, 112.1, 37.1, 30.4, 29.1, 27.0, 20.4 ppm. HRMS (ESI) calcd. for C<sub>17</sub>H<sub>19</sub>N<sub>3</sub>O<sup>+</sup> [M]<sup>+</sup> 281.1528; found 281.1523.

***N,N*-Dimethyl-4-(1-methyl-9*H*-β-carbolin-4-yl)butan-1-amine (27)**

Compound **25** (165 mg, 0.65 mmol) was dissolved in formic acid (2.33 mL, 61.7 mmol) and 35 wt % aqueous CH<sub>2</sub>O solution (102 μL, 1.30 mmol) was added. The mixture was heated to 90 °C and reacted for 5 hours. The mixture was added to 10 wt % aqueous NaHCO<sub>3</sub> (47.0 mL) and extracted with DCM (3 × 25 mL). The combined organic layer was dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated in vacuo. The residue was purified by silica gel column chromatography (DCM–MeOH) to give pale yellow crystals (118 mg, 65%). Mp 189–192 °C (EtOH). (lit. S1 mp. 128–129 °C (benzene)). IR (film): 3422, 2940, 1664, 1622, 1458, 1325, 736 cm<sup>-1</sup>. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz): δ 11.62 (br s, 1H), 8.16 (m, 1H), 8.01 (s, 1H), 7.62 (m, 1H), 7.53 (m, 1H), 7.26 (m, 1H), 3.13 (t, *J* = 7.6 Hz, 2H), 2.73 (s, 3H), 2.51 (m, 2H), 2.30 (s, 6H), 1.75 (m, 2H), 1.64

(m, 2H) ppm.  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 150 MHz):  $\delta$  140.5, 140.2, 137.7, 134.5, 128.8, 127.4, 125.1, 123.4, 121.1, 119.6, 112.1, 58.1, 48.8, 44.4, 30.5, 27.1, 26.0, 20.4 ppm. HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{23}\text{N}_3^+ [\text{M}]^+$  281.1892; found: 281.1891.

#### **Ethyl [4-(1-methyl-9H- $\beta$ -carbolin-4-yl)butyl]carbamate (28)**

Compound **25** (20.0 mg, 0.08 mmol) was dissolved in  $\text{CHCl}_3$  (1.0 mL) and cooled to 0 °C. While stirring, ethyl chloroformate (7.50  $\mu\text{L}$ , 0.08 mmol) and 4.0 M aqueous solution of NaOH (20.0  $\mu\text{L}$ , 0.08 mmol) was added. The mixture was reacted for 3 hours at room temperature, then washed with water (5.0 mL). The aqueous phase was extracted with DCM ( $3 \times 15$  mL). The combined organic layers were dried over  $\text{Na}_2\text{SO}_4$  and concentrated in vacuo to give brown oil. The crude product was purified by silica gel column chromatography (DCM–MeOH) to give yellow crystals (20 mg, 78%). Mp 155–157 °C (MeCN). IR (KBr): 3420, 1694, 1662, 1540, 1457, 1411, 1325, 739  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (DMSO- $d_6$ , 600 MHz):  $\delta$  11.58 (br s, 1H), 8.09 (m, 1H), 8.00 (s, 1H), 7.62 (m, 1H), 7.53 (m, 1H), 7.25 (m, 1H), 7.09 (br t,  $J = 5.4$  Hz, 1H), 3.94 (q,  $J = 7.1$  Hz, 2H), 3.11 (t,  $J = 7.5$  Hz, 2H) 3.02 (q,  $J = 6.4$  Hz, 2H), 2.73 (s, 3H), 1.72 (m, 2H), 1.55 (m, 2H), 1.12 (t,  $J = 7.1$  Hz, 3H) ppm.  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 150 MHz):  $\delta$  156.5, 140.5, 140.1, 137.7, 134.5, 128.8, 127.4, 125.1, 123.3, 121.1, 119.6, 112.1, 59.6, 40.2, 30.5, 29.6, 26.9, 20.4, 14.9 ppm. HRMS (ESI) calcd. for  $\text{C}_{19}\text{H}_{23}\text{N}_3\text{O}_2^+ [\text{M}]^+$  325.1782; found 325.1777.

#### **1-Methyl-4-(1-methyl-1H-pyrrol-2-yl)-9H- $\beta$ -carboline (30)**

Compound **3** (500 mg, 1.50 mmol) was dissolved in 1,2-dimethoxyethane solvent (150.0 mL). 2.0 M aqueous solution of  $\text{Na}_2\text{CO}_3$  (80.0 mL) and reagent **29** (625 mg, 3.0 mmol) was added. The mixture was heated under argon atmosphere to 50 °C and stirred at this temperature for 5 minutes.  $\text{Pd}(\text{PPh}_3)_4$  (15 mg, 0.01 mmol) was added, the mixture was heated to reflux and reacted for 1 hour. After the reaction was complete, it was concentrated in vacuo and extracted with DCM ( $3 \times 200$  mL). The combined organic layer was dried over  $\text{Na}_2\text{SO}_4$  and concentrated in

vacuo. The crude product was purified by silica gel column chromatography (DCM–MeOH) to give pale yellow crystals (396 mg, 99%). Mp 216–218 °C (EtOH). IR (KBr): 3158, 1618, 1381, 1318, 711  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (DMSO- $d_6$ , 600 MHz):  $\delta$  11.75 (br s, 1H), 8.09 (s, 1H), 7.62 (d,  $J$  = 8.2 Hz, 1H), 7.50 (t,  $J$  = 7.4 Hz, 1H), 7.15 (d,  $J$  = 7.9 Hz, 1H), 7.09 (t,  $J$  = 7.3 Hz, 1H), 7.04 (s, 1H), 6.24 (m, 1H), 6.19 (m, 1H), 3.32 (s, 3H), 2.82 (s, 3H) ppm.  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 150 MHz):  $\delta$  142.0, 140.7, 138.8, 134.2, 129.5, 128.0, 126.5, 123.5, 122.0, 120.9, 120.1, 119.6, 112.3, 109.2, 107.8, 34.0, 20.6 ppm. HRMS (ESI) calcd. for  $\text{C}_{17}\text{H}_{16}\text{N}_3^+$   $[\text{M}+\text{H}]^+$  262.1339; found 262.1343.

### **1-Methyl-4-(1-methylpyrrolidin-2-yl)-6,7,8,9-tetrahydro-5H- $\beta$ -carboline (31)**

In a 22-mL autoclave, compound **30** (48.0 mg, 0.18 mmol) was dissolved in a mixture of MeOH–H<sub>2</sub>O (4:1, 10 mL) and 37 wt % aqueous HCl solution (46  $\mu\text{L}$ , 0.55 mmol),  $\text{PtO}_2 \cdot \text{H}_2\text{O}$  (90 mg, 0.29 mmol) was added at room temperature. The autoclave was purged with argon gas. After that, it was washed with hydrogen gas three times and the starting pressure was adjusted to 15 bar. The mixture was reacted at room temperature for 24 hours. After the reaction was complete, the mixture was filtered through celite and the filter pad was washed with MeOH (4  $\times$  15 mL). It was concentrated in vacuo, the residue was dissolved in DCM (50 mL), washed with 10 wt % aqueous  $\text{NaHCO}_3$  (10 mL) and extracted with DCM (2  $\times$  20 mL). The combined organic layer was dried over  $\text{Na}_2\text{SO}_4$  and concentrated in vacuo to give yellow crystals (45 mg, 91%). An analytical sample was recrystallized from MeCN. Mp 242–245 °C (MeCN). (lit. S3 mp. 234–237 °C (acetone)). IR (KBr): 3429, 3045, 2930, 2843, 1559, 1444, 1312, 1049  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (DMSO- $d_6$ , 600 MHz):  $\delta$  11.03 (br s, 1H), 7.96 (s, 1H), 3.52 (t,  $J$  = 8.3 Hz, 1H), 3.18 (t,  $J$  = 8.0 Hz, 1H), 2.90 (m, 1H), 2.79 (m, 1H), 2.74 (m, 2H), 2.54 (s, 3H), 2.22 (m, 1H), 2.20 (m, 1H), 2.11 (s, 3H), 1.83 (m, 1H), 1.83 (m, 1H), 1.82 (m, 1H), 1.78 (m, 1H), 1.76 (m, 1H), 1.76 (m, 1H), 1.60 (m, 1H) ppm.  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 150 MHz):  $\delta$  139.7, 138.2, 135.2, 131.1,

129.6, 127.5, 108.2, 66.6, 56.7, 40.8, 35.8, 23.9, 23.6, 23.4, 22.4, 22.2, 20.0 ppm. HRMS (ESI) calcd. for  $C_{17}H_{23}N_3^+$   $[M]^+$  269.1885; found 269.1885.

**1-Methyl-4-[1-methyl-5-(2,2,2-trifluoroethyl)-1*H*-pyrrol-2-yl]-9*H*- $\beta$ -carboline** (32)

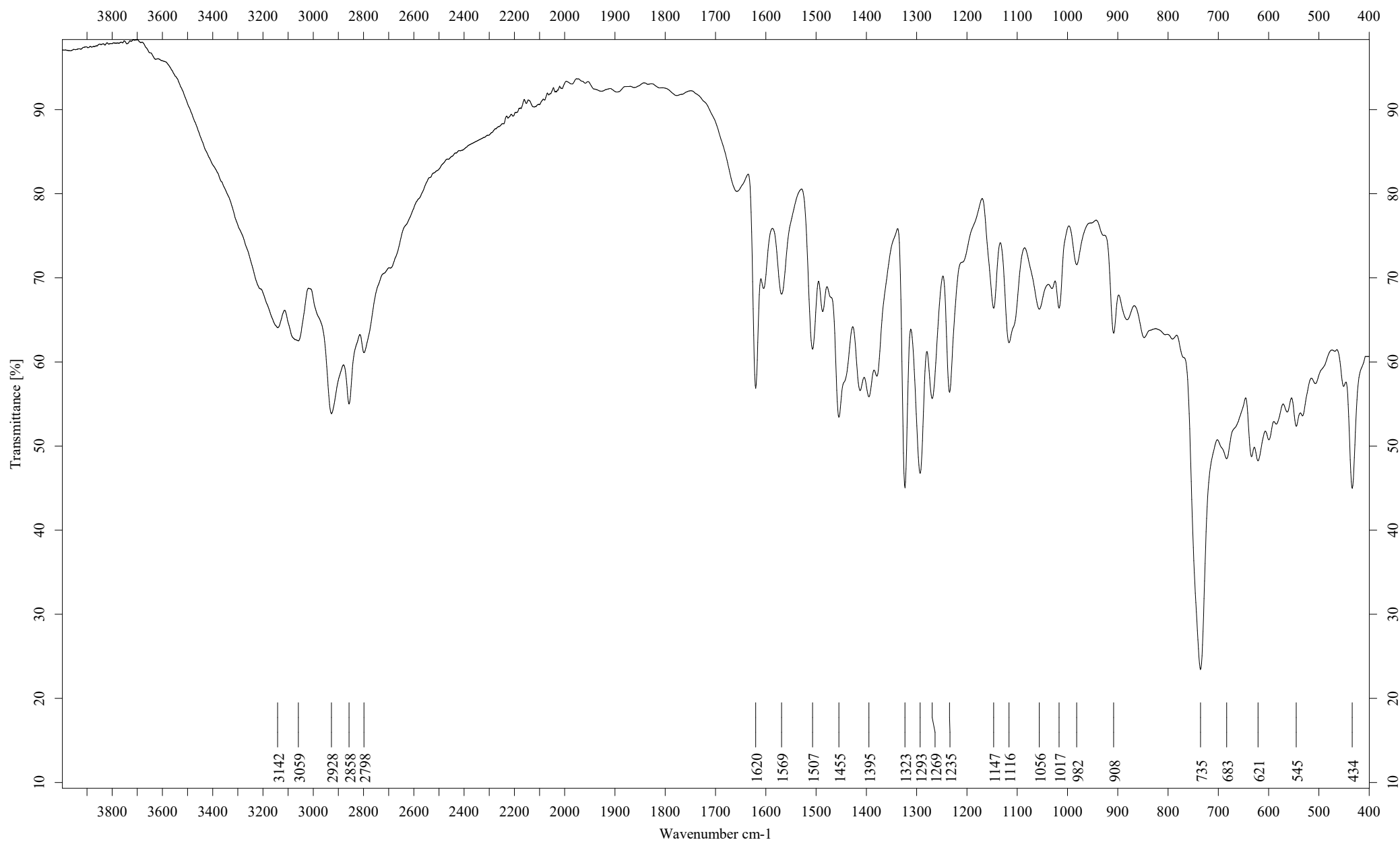
Compound **30** (196 mg, 0.75 mmol) was dissolved in TFA (10.0 mL, 130.0 mmol) and  $NaCNBH_3$  (800 mg, 12.7 mmol) was added. The mixture was stirred at room temperature for 2 hours, it was poured onto ice and treated with 10 wt % aqueous  $NaHCO_3$  solution (100.0 mL) until pH 7. It was extracted with DCM ( $3 \times 200$  mL). The combined organic layer was dried over  $Na_2SO_4$  and concentrated in vacuo. The crude product was purified by silica gel column chromatography (DCM–MeOH) to give yellow crystals (68 mg, 36%). Mp 246–248 °C (MeCN). IR (KBr): 1621, 1457, 1254, 1137, 1071, 739  $cm^{-1}$ .  $^1H$  NMR (DMSO- $d_6$ , 600 MHz):  $\delta$  11.78 (br s, 1H), 8.09 (s, 1H), 7.62 (m, 1H), 7.50 (m, 1H), 7.08 (m, 1H), 7.05 (m, 1H), 6.31 (d,  $J = 3.5$  Hz, 1H), 6.19 (d,  $J = 3.5$  Hz, 1H), 3.90 (d,  $J = 11.1$  Hz, 1H), 3.87 (d,  $J = 11.1$  Hz, 1H), 3.24 (s, 3H), 2.82 (s, 3H) ppm.  $^{13}C$  NMR (DMSO- $d_6$ , 150 MHz):  $\delta$  142.2, 140.8, 138.7, 134.1, 130.9, 128.1, 126.5, 126.2, 122.8, 121.9, 120.8, 120.1, 119.6, 112.3, 110.2, 108.4, 31.3, 30.9, 20.6 ppm.  $^{19}F$  NMR (DMSO- $d_6$ , 564 MHz):  $\delta$  -64.5 ppm. HRMS (ESI) calcd. for  $C_{19}H_{17}F_3N_3^+$   $[M+H]^+$  344.1369; found: 344.1374.

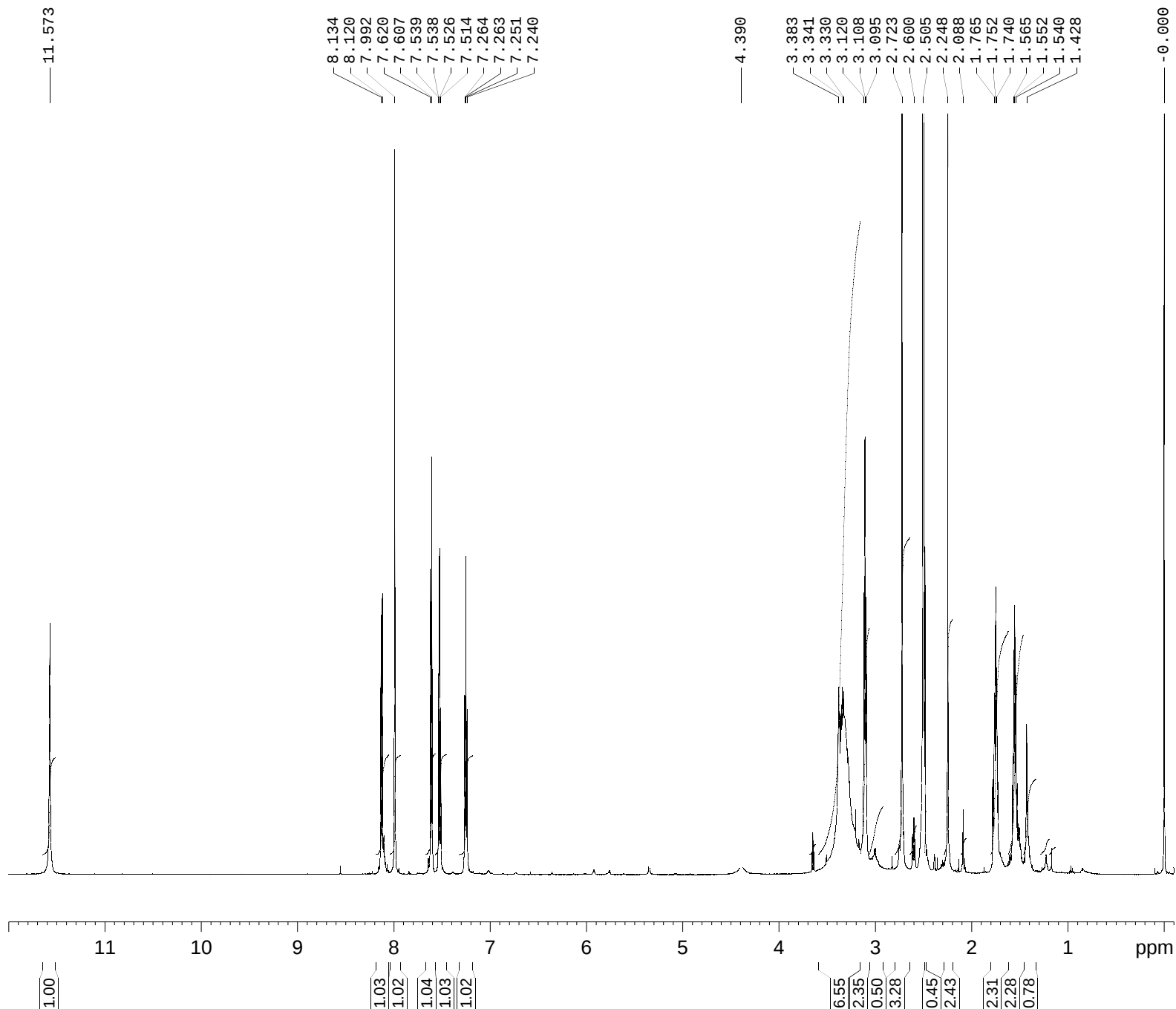
## References

- S1. Terent'eva, I. V.; Lazur'evskii, G. V.; Shirshova, T. I. *Chem. Nat. Compd.*, **1969**, 5, 330–334. doi: 10.1007/BF00595071
- S2. Szabó, T.; Görür, F. L.; Horváth, S.; Volk, B.; Milen, M. *Synthesis*, **2022**, 54, 3867–3873. doi: 10.1055/s-0041-1737830
- S3. Lazurjevski, G.; Terentjeva, I. *Heterocycles*, **1976**, 4, 1783–1816.

|                |           |
|----------------|-----------|
| Batizi Benedek | KP        |
| Gyemant ATR    | 10/3/2024 |

|                     |
|---------------------|
| BRUKER Alpha        |
| Resolution: 2 cm-1  |
| Number of Scans: 32 |





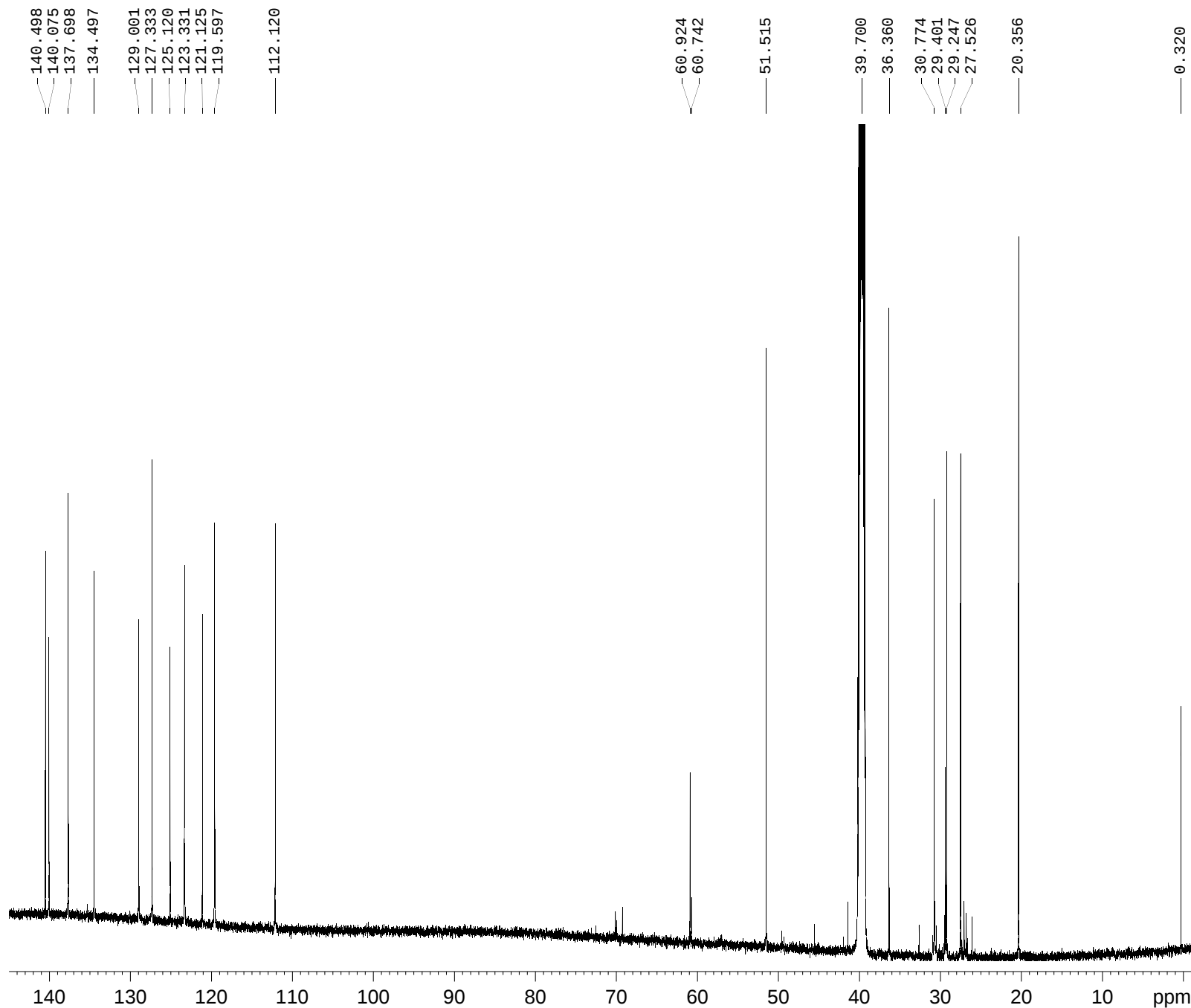
Standard 1H  
143648  
BAB0325\_1A  
Batizi Benedek  
2024.10.03. (KP)

Current Data Parameters  
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EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
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PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 2.7262976 sec  
RG 196.07  
DW 41.600 usec  
DE 25.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 600.0037050 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W

F2 - Processing parameters  
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SF 600.0000020 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





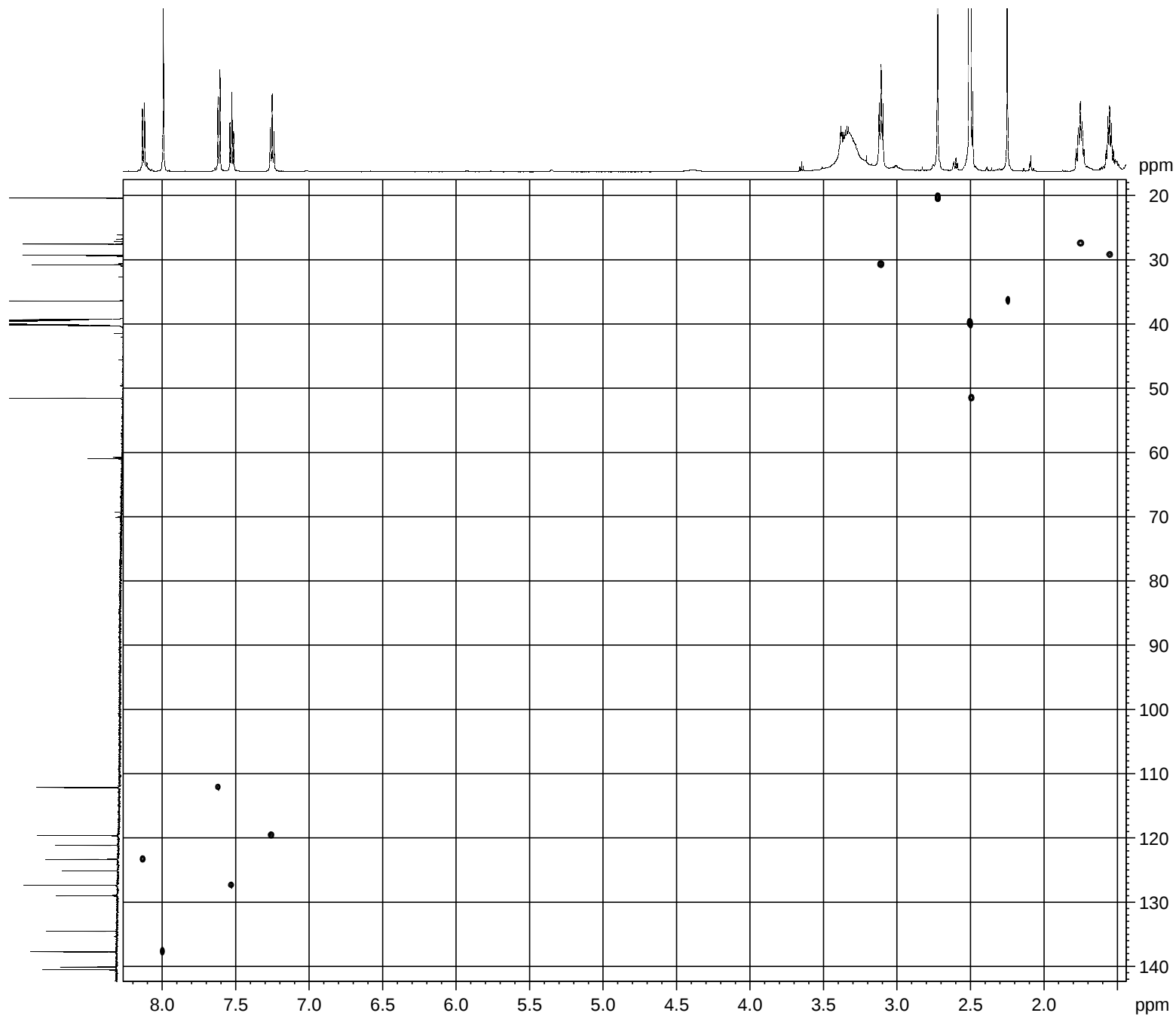
Standard 13C  
143648  
BAB0325\_1A  
Batizi Benedek  
2024.10.03. (KP)

Current Data Parameters  
NAME 143648  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
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Time 18.04 h  
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PROBHD Z145856\_0002 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 4096  
DS 4  
SWH 36231.883 Hz  
FIDRES 1.105709 Hz  
AQ 0.9043968 sec  
RG 196.07  
DW 13.800 usec  
DE 18.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 150.8852070 MHz  
NUC1 13C  
P1 9.90 usec  
PLW1 71.00000000 W  
SF02 600.0024000 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 32.90000153 W  
PLW12 0.70370001 W  
PLW13 0.35339001 W

F2 - Processing parameters  
SI 131072  
SF 150.8701598 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





HSQC (140Hz)  
143648  
BAB0325\_1A  
Batizi Benedek  
2024.10.03. (KP)

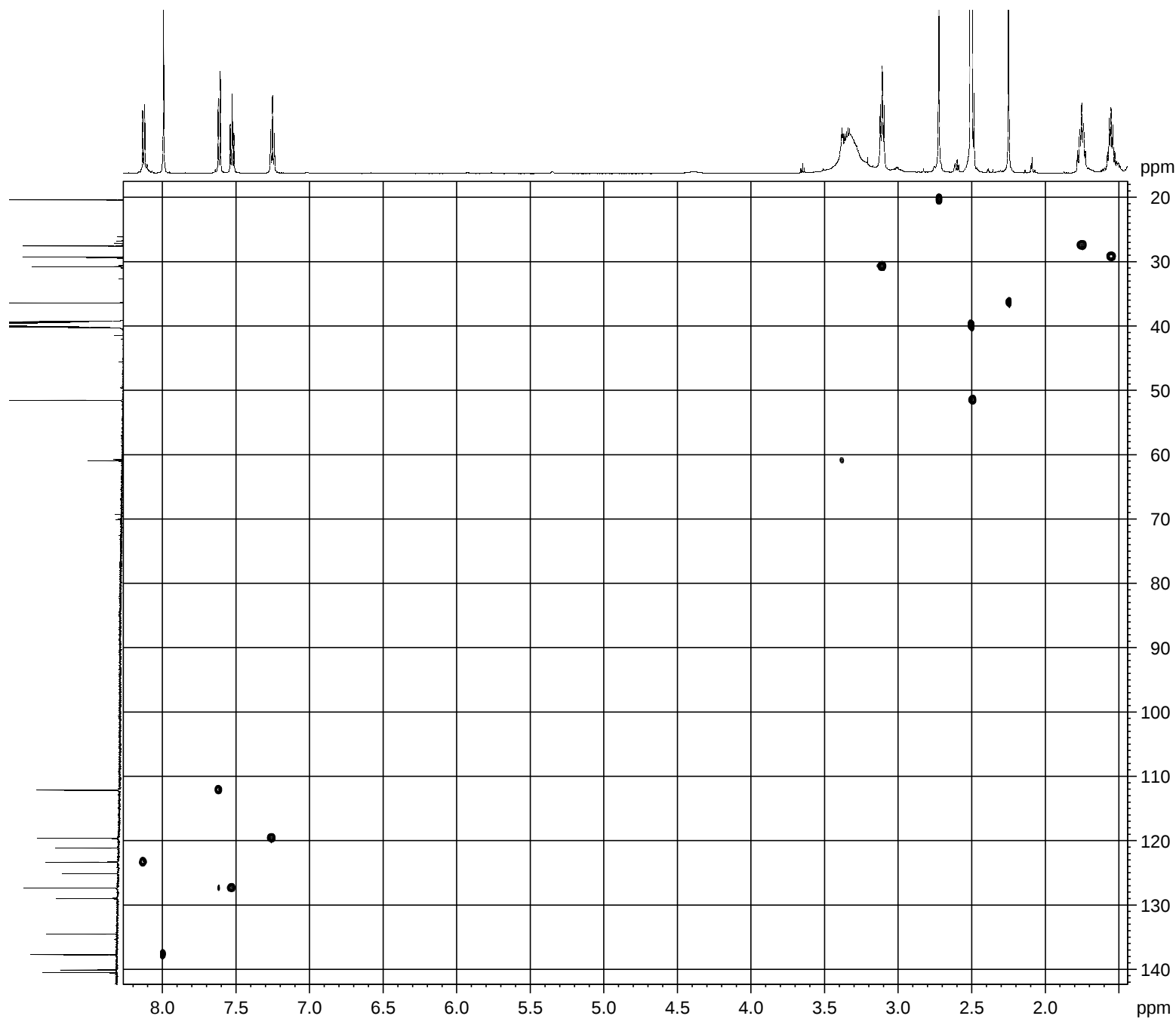
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EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
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PULPROG hsqcetgpsisp2.2  
TD 2048  
SOLVENT DMSO  
NS 8  
DS 32  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST17 -0.5000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D4 0.00178571 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
P28 0 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
CPDPRG2 bi\_p5m4sp\_4sp.2  
P3 9.90 usec  
P14 500.00 usec  
P24 2000.00 usec  
P63 1500.00 usec  
PLW0 0 W  
PLW2 71.00000000 W  
PLW12 2.30040002 W  
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SPOFFS3 0 Hz  
SPW3 10.63199997 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 10.63199997 W  
SPNAM[14] Crp42, 1.5, 20.2  
SPOAL14 0.500  
SPOFFS14 0 Hz  
SPW14 5.95400000 W  
SPNAM[31] Crp42, 1.5, 20.2  
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SPOFFS31 0 Hz  
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GPZ1 80.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 20.10 %  
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GPZ3 11.00 %  
GPNAM[4] SMSQ10.100  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 600.000020 MHz  
WDW QSINE





HSQC (140Hz)  
143648  
BAB0325\_1A  
Batizi Benedek  
2024.10.03. (KP)

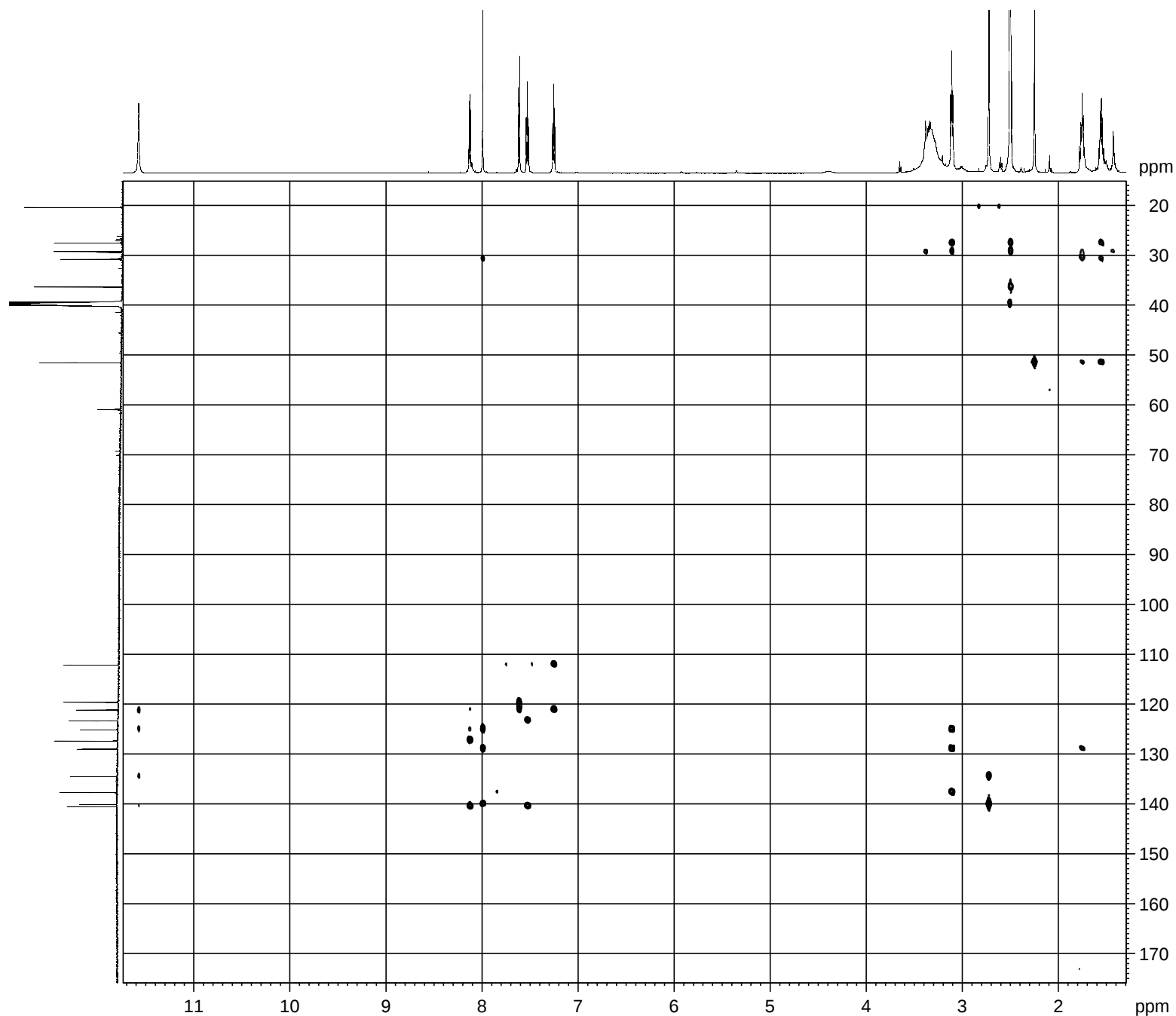
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EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
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PULPROG hsqcetgpsisp2.2  
TD 2048  
SOLVENT DMSO  
NS 8  
DS 32  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST17 -0.5000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D4 0.00178571 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
P28 0 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
CPDPRG2 bi\_p5m4sp\_4sp.2  
P3 9.90 usec  
P14 500.00 usec  
P24 2000.00 usec  
P63 1500.00 usec  
PLW0 0 W  
PLW2 71.00000000 W  
PLW12 2.30040002 W  
SPNAM[3] Crp60, 0.5, 20.1  
SPOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 10.63199997 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 10.63199997 W  
SPNAM[14] Crp42, 1.5, 20.2  
SPOAL14 0.500  
SPOFFS14 0 Hz  
SPW14 5.95400000 W  
SPNAM[31] Crp42, 1.5, 20.2  
SPOAL31 0.500  
SPOFFS31 0 Hz  
SPW31 1.48850000 W  
GPNAM[1] SMSQ10.100  
GPZ1 80.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 20.10 %  
GPNAM[3] SMSQ10.100  
GPZ3 11.00 %  
GPNAM[4] SMSQ10.100  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 600.000020 MHz  
WDW QSINE





HMBC (8Hz, 140Hz)  
143648  
BAB0325\_1A  
Batizi Benedek  
2024.10.03. (KP)

Current Data Parameters  
NAME 143648  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20241003  
Time 19.24 h  
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PROBHD Z145856\_0002 (  
PULPROG hmbcgp1pndqf  
TD 2048  
SOLVENT DMSO  
NS 8  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D2 0.00357143 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00001510 sec  
T0av 1  
SF01 600.0037800 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
P3 9.90 usec  
PLW2 71.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 50.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.10 %  
P16 1000.00 usec

F1 - Acquisition parameters  
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SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE QF

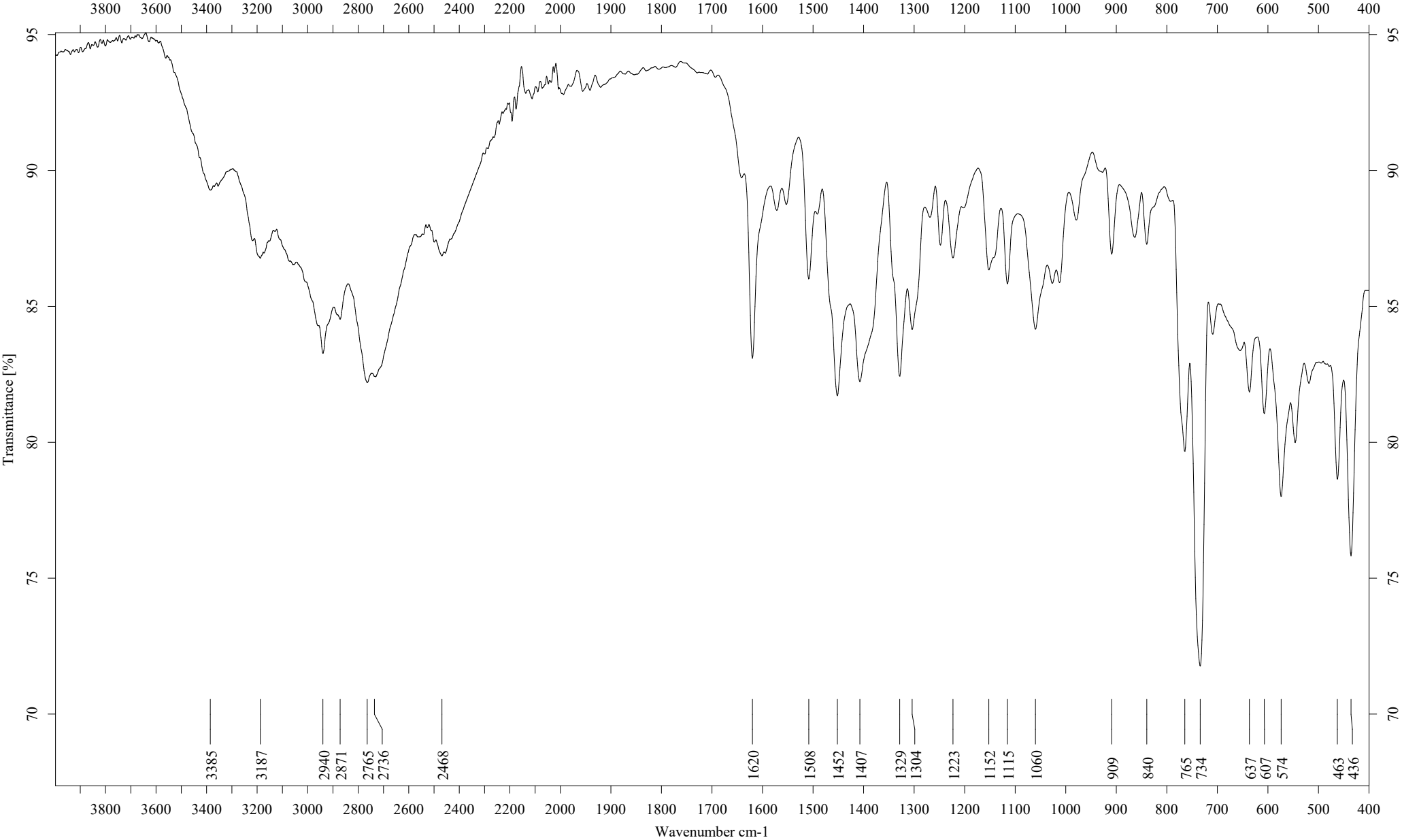
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SSB 0  
LB 0 Hz  
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PC 1.40

F1 - Processing parameters  
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MC2 QF  
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WDW SINE  
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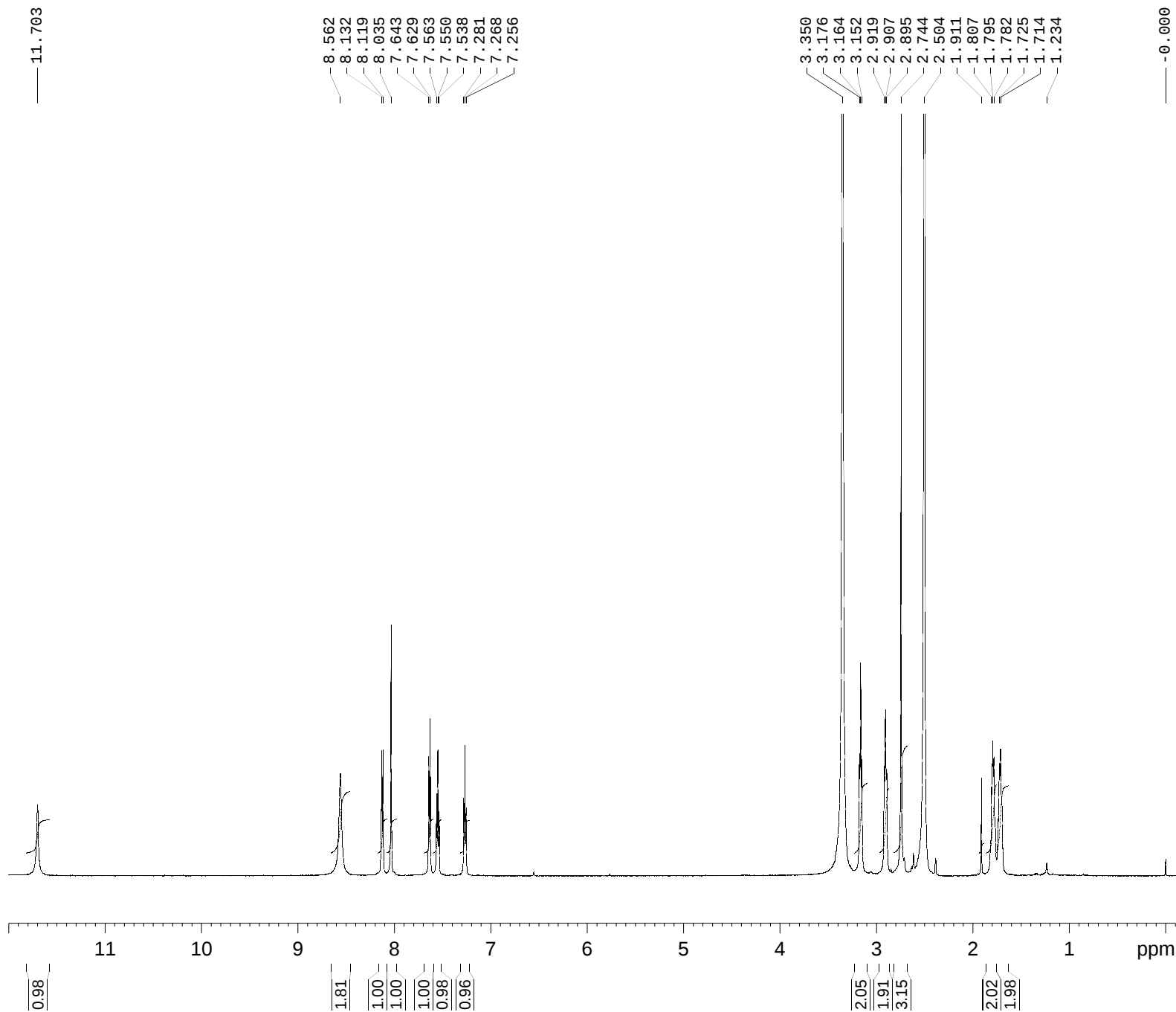
2 · 2 HCl

|                |           |
|----------------|-----------|
| Batizi Benedek | KP        |
| Gyemant ATR    | 11/8/2024 |

|                     |
|---------------------|
| BRUKER Alpha        |
| Resolution: 2 cm-1  |
| Number of Scans: 32 |



# 2 · 2 HCl



Standard 1H  
143819  
BAB0352\_1  
Batizi Benedek  
2024.11.08. (KP)

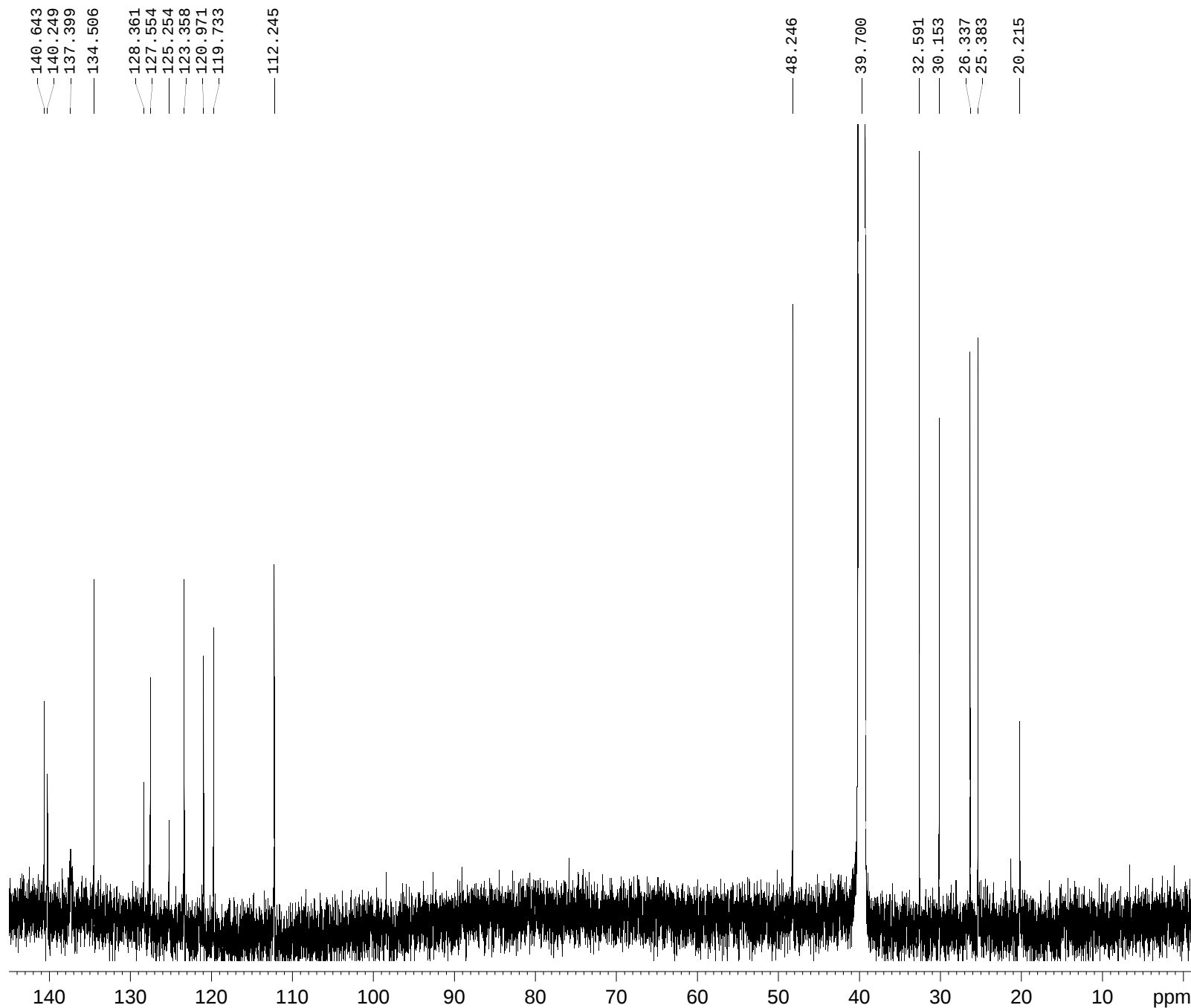
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EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
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PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 2.7262976 sec  
RG 196.07  
DW 41.600 usec  
DE 25.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 600.0037050 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W

F2 - Processing parameters  
SI 65536  
SF 600.0000023 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



# 2 · 2 HCl



Standard 13C  
143819  
BAB0352\_1  
Batizi Benedek  
2024.11.08. (KP)

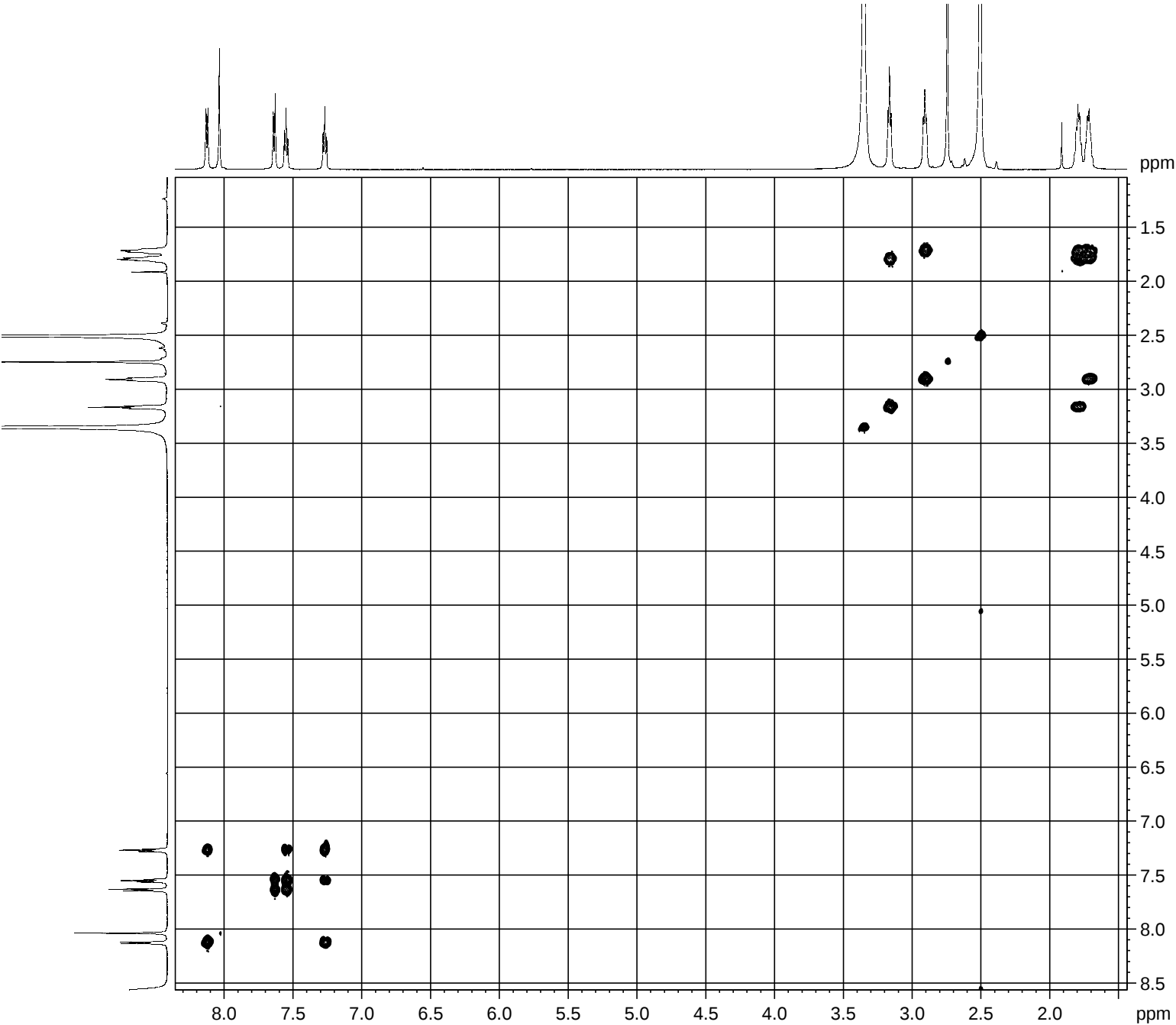
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NAME 143819  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
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PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
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SWH 36231.883 Hz  
FIDRES 1.105709 Hz  
AQ 0.9043968 sec  
RG 196.07  
DW 13.800 usec  
DE 18.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 150.8852070 MHz  
NUC1 13C  
P1 9.90 usec  
PLW1 71.00000000 W  
SF02 600.0024000 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 32.90000153 W  
PLW12 0.70370001 W  
PLW13 0.35339001 W

F2 - Processing parameters  
SI 131072  
SF 150.8701599 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



2 · 2 HCl



COSY  
143819  
BAB0352\_1  
Batizi Benedek  
2024.11.08. (KP)

Current Data Parameters  
NAME 143819  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20241109  
Time 3.26 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG cosygpmfqr  
TD 2048  
SOLVENT DMSO  
NS 2  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
D0 0.00000300 sec  
D1 2.00000000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00012800 sec  
TDav 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 16.00 %  
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GPZ2 12.00 %  
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GPZ3 40.00 %  
P16 1000.00 usec

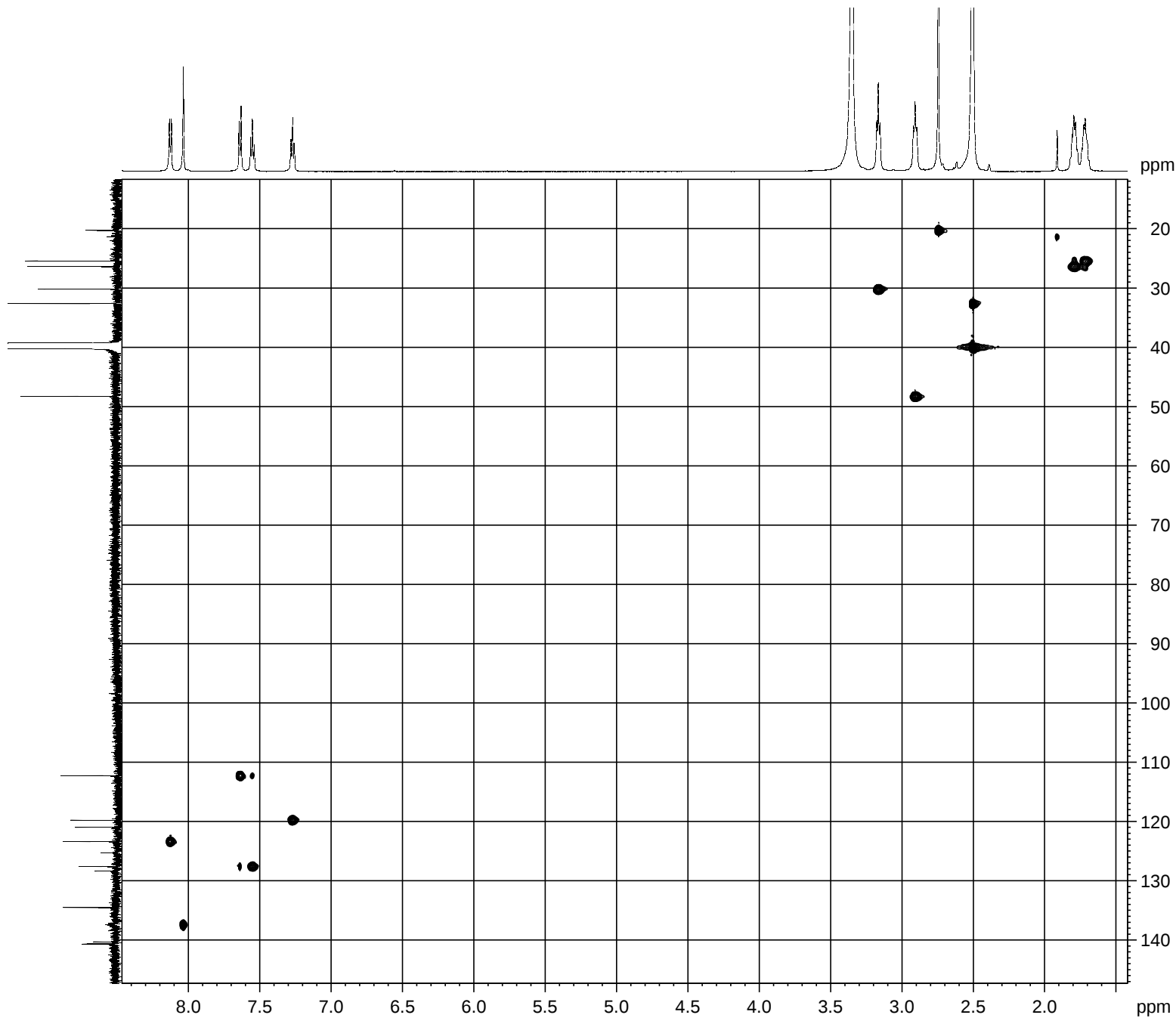
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SF01 600.0036 MHz  
FIDRES 61.035156 Hz  
SW 13.021 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 600.0000023 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 600.0000023 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



2 · 2 HCl



HSQC (140Hz)  
143819  
BAB0352\_1  
Batizi Benedek  
2024.11.08. (KP)

Current Data Parameters  
NAME 143819  
EXPNO 14  
PROCNO 1

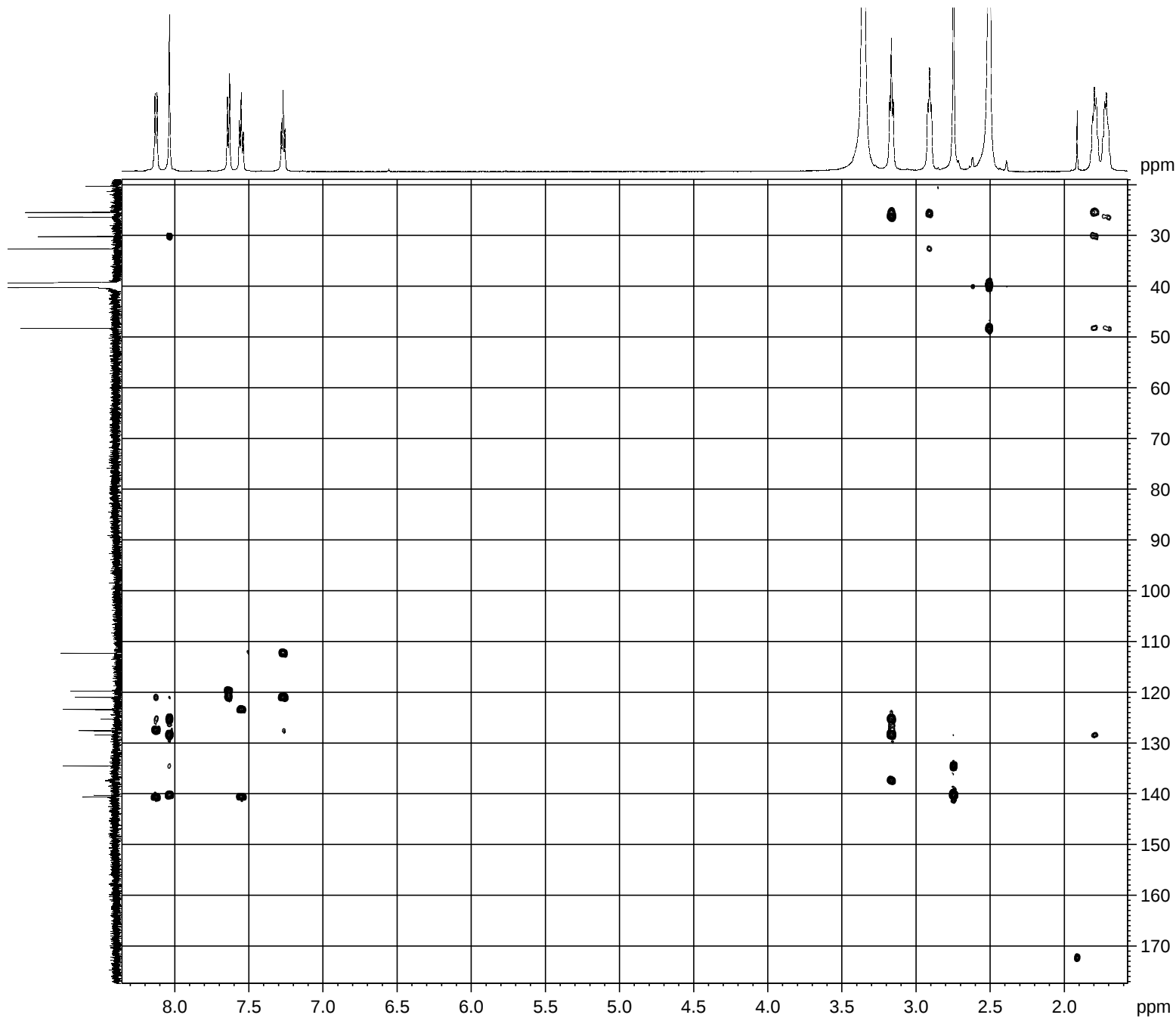
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PULPROG hsqcetgpsisp2.2  
TD 2048  
SOLVENT DMSO  
NS 4  
DS 32  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST17 -0.5000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D4 0.00178571 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
P28 0 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
CPDPRG2 bi\_p5m4sp\_4sp.2  
P3 9.90 usec  
P14 500.00 usec  
P24 2000.00 usec  
P63 1500.00 usec  
PLW0 0 W  
PLW2 71.00000000 W  
PLW12 2.30040002 W  
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SPOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 10.63199997 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 10.63199997 W  
SPNAM[14] Crp42, 1.5, 20.2  
SPOAL14 0.500  
SPOFFS14 0 Hz  
SPW14 5.95400000 W  
SPNAM[31] Crp42, 1.5, 20.2  
SPOAL31 0.500  
SPOFFS31 0 Hz  
SPW31 1.48850000 W  
GPNAM[1] SMSQ10.100  
GPZ1 80.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 20.10 %  
GPNAM[3] SMSQ10.100  
GPZ3 11.00 %  
GPNAM[4] SMSQ10.100  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 600.000023 MHz  
WDW QSINE



2 · 2 HCl



HMBC (8Hz, 140Hz)  
143819  
BAB0352\_1  
Batizi Benedek  
2024.11.08. (KP)

Current Data Parameters  
NAME 143819  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20241109  
Time 4.16 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgp1pndqf  
TD 2048  
SOLVENT DMSO  
NS 4  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D2 0.00357143 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00001510 sec  
TDav 1  
SF01 600.0037800 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
P3 9.90 usec  
PLW2 71.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 50.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.10 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE QF

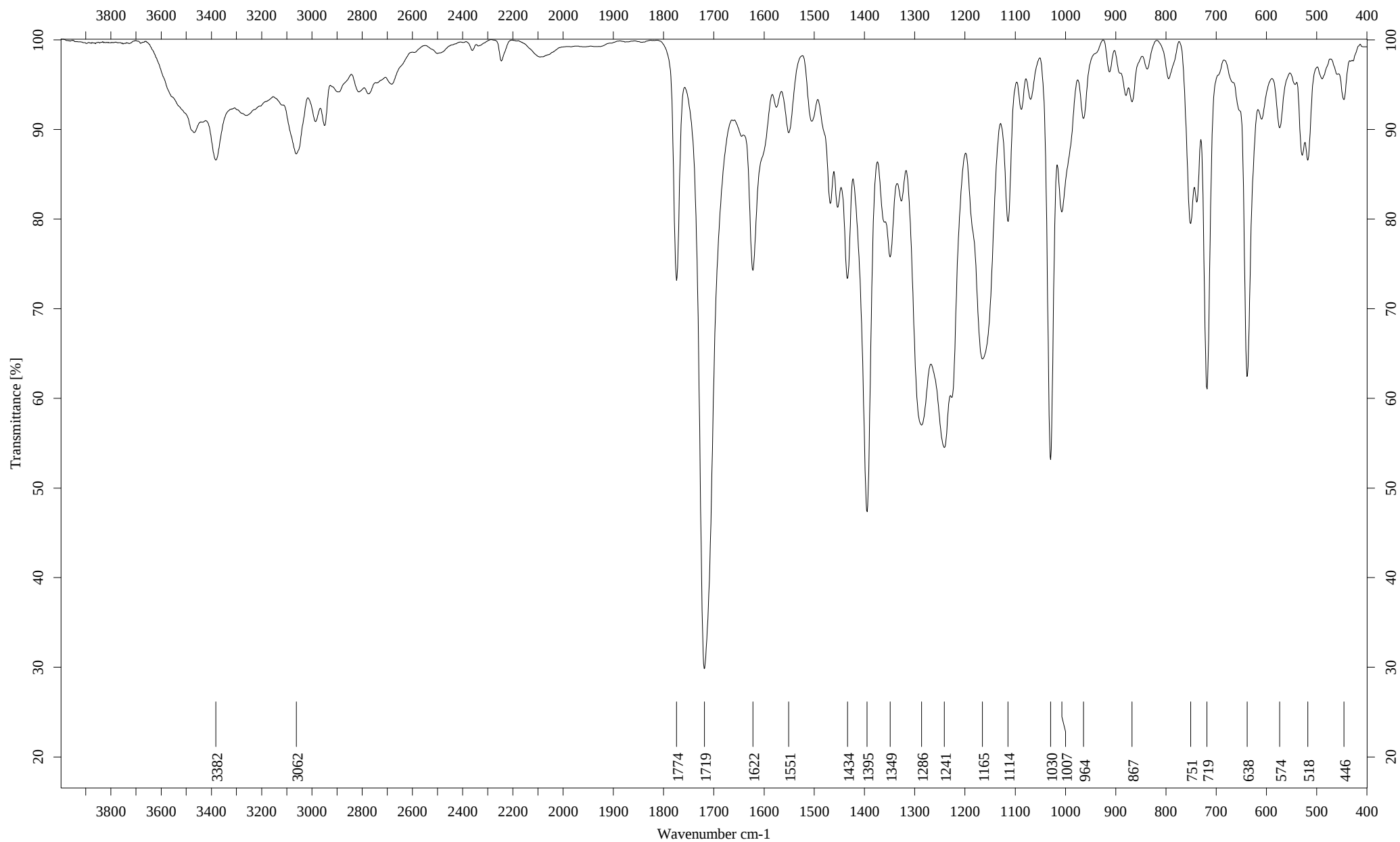
F2 - Processing parameters  
SI 2048  
SF 600.0000023 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

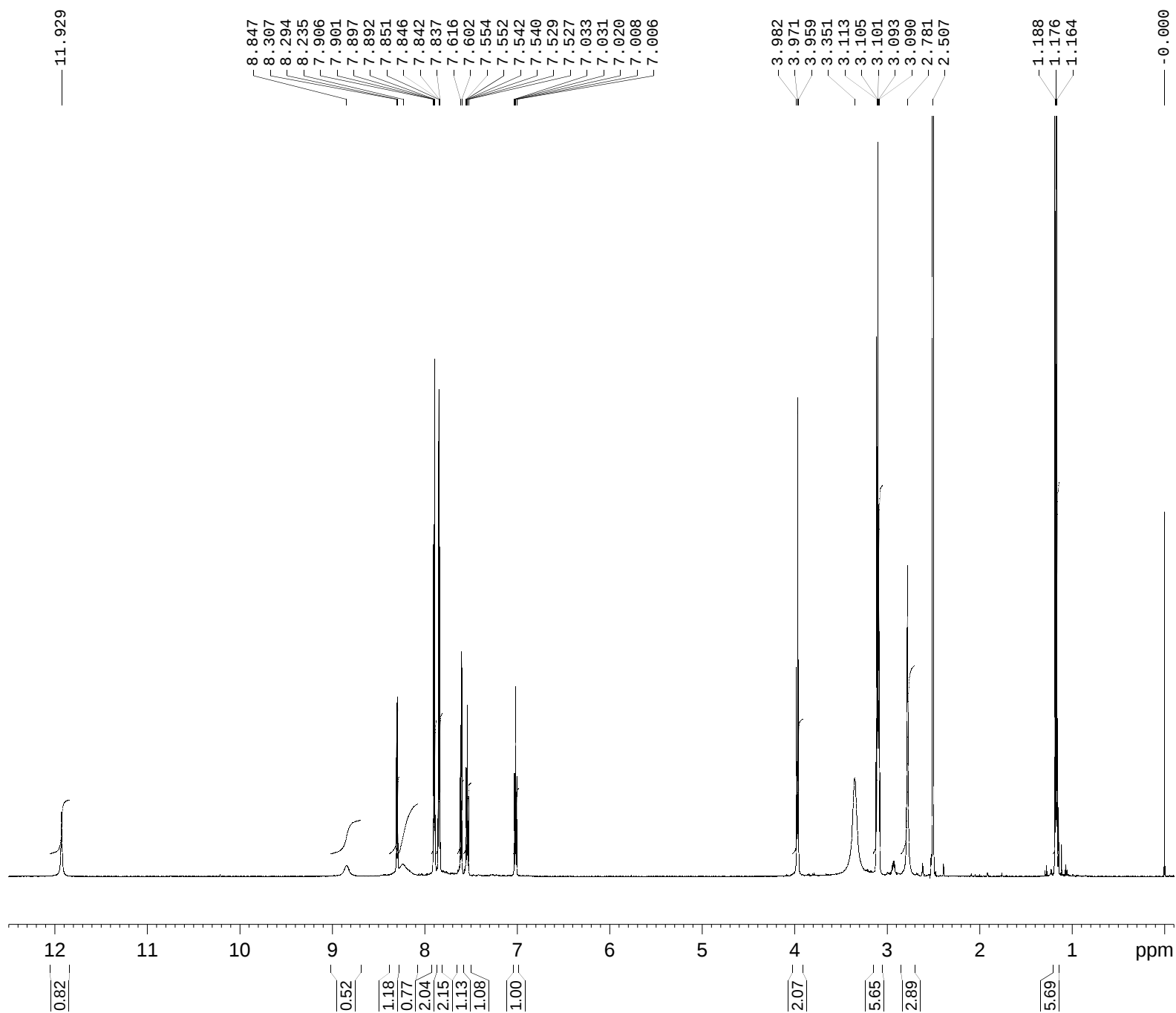
F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 150.8701599 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



|                |             |
|----------------|-------------|
| Batizi Benedek | MM          |
| KBr            | 2023.01.26. |

|                     |
|---------------------|
| BRUKER Alpha        |
| Resolution: 2 cm-1  |
| Number of Scans: 16 |





Standard 1H  
140379  
BAB0025\_1  
Batizi Benedek  
2023.01.25. (KP)

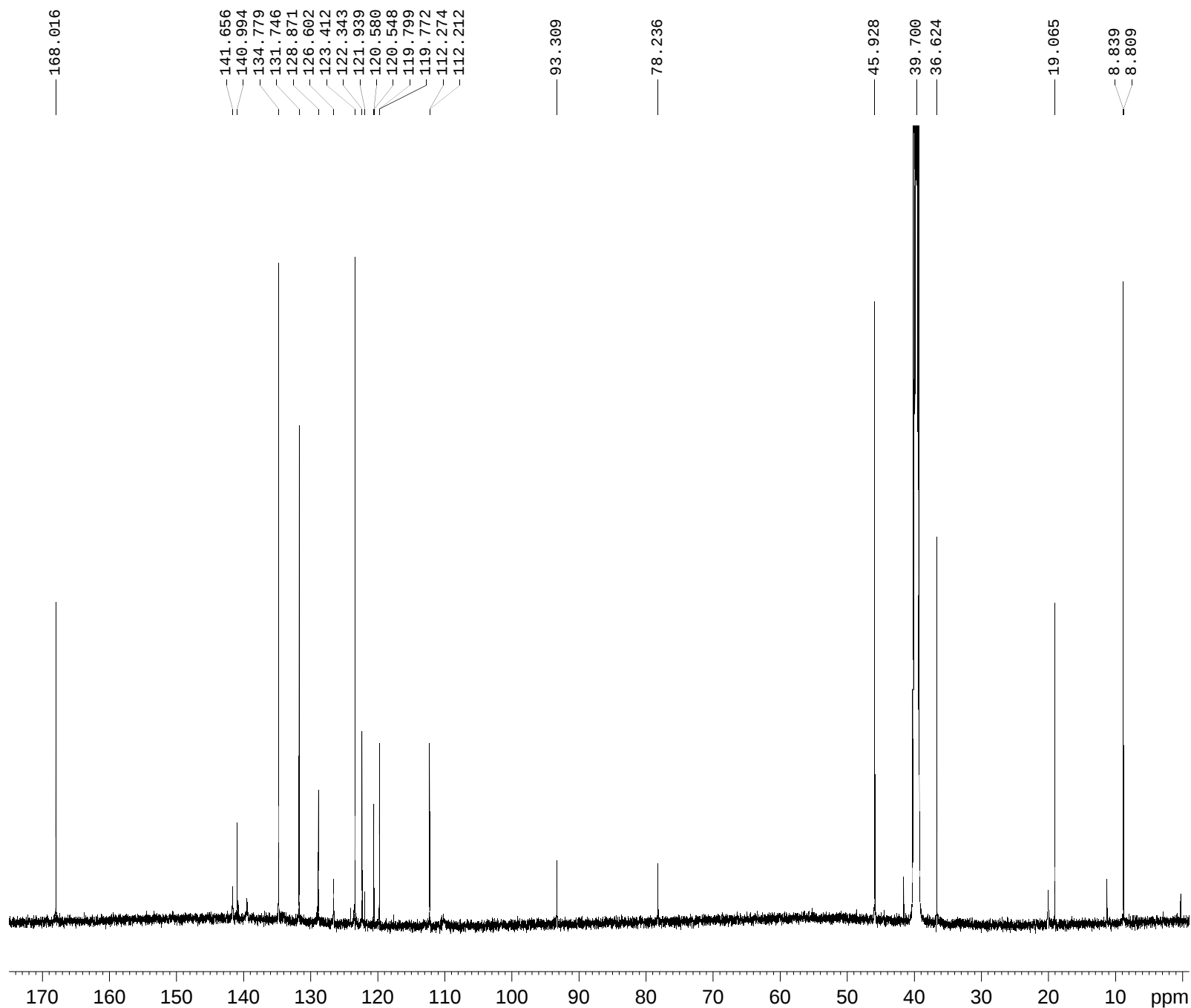
Current Data Parameters  
NAME 140379  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230125  
Time 21.23 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 2.7262976 sec  
RG 196.07  
DW 41.600 usec  
DE 25.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 600.0537053 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W

F2 - Processing parameters  
SI 65536  
SF 600.0500008 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



5



Standard 13C  
140379  
BAB0025\_1  
Batizi Benedek  
2023.01.25. (KP)

Current Data Parameters  
NAME 140379  
EXPNO 12  
PROCNO 1

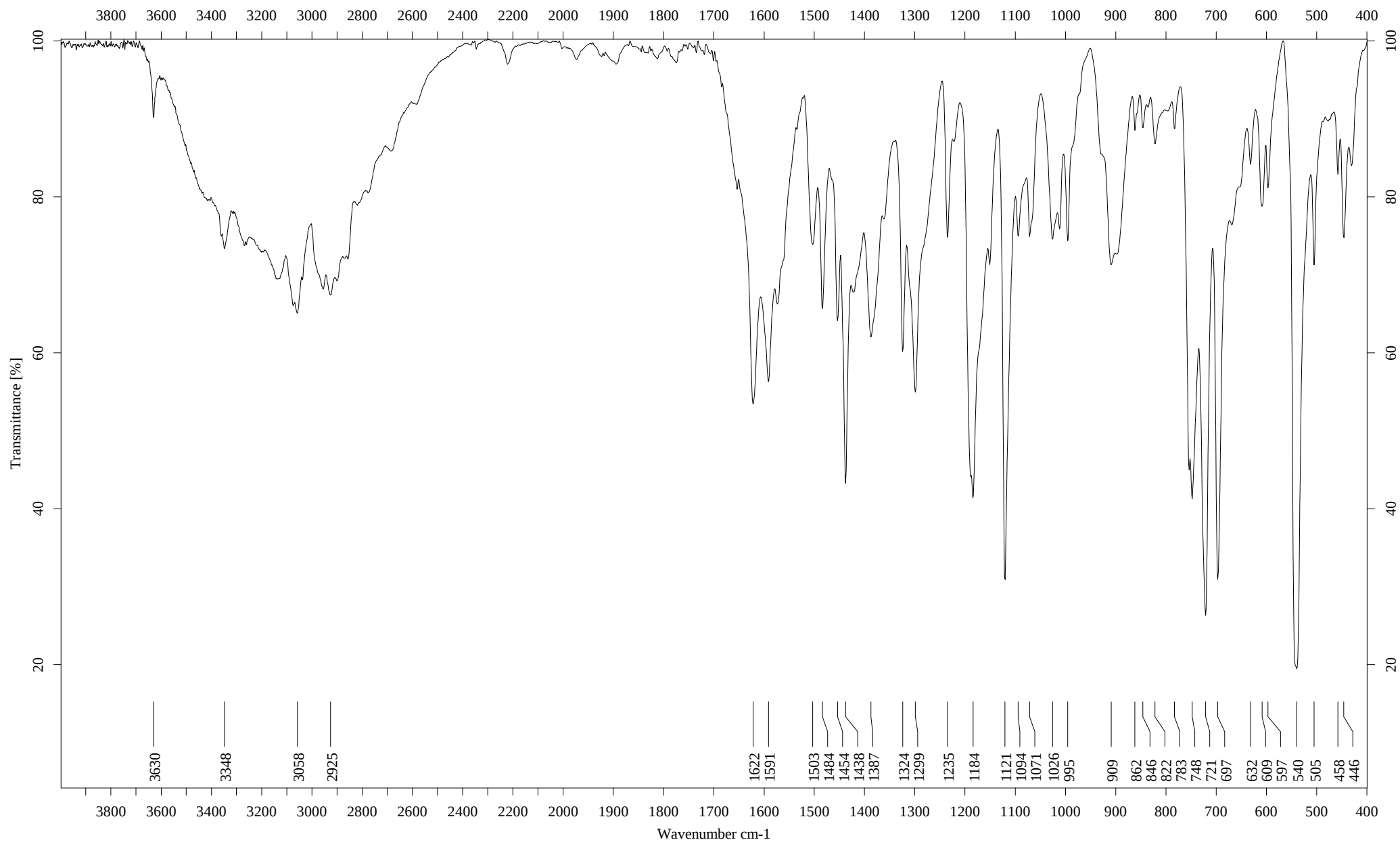
F2 - Acquisition Parameters  
Date\_ 20230125  
Time 22.32 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 2048  
DS 4  
SWH 36231.883 Hz  
FIDRES 1.105709 Hz  
AQ 0.9043968 sec  
RG 196.07  
DW 13.800 usec  
DE 18.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 150.8977808 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 70.48699951 W  
SF02 600.0524002 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 29.46299934 W  
PLW12 0.66293001 W  
PLW13 0.33292001 W

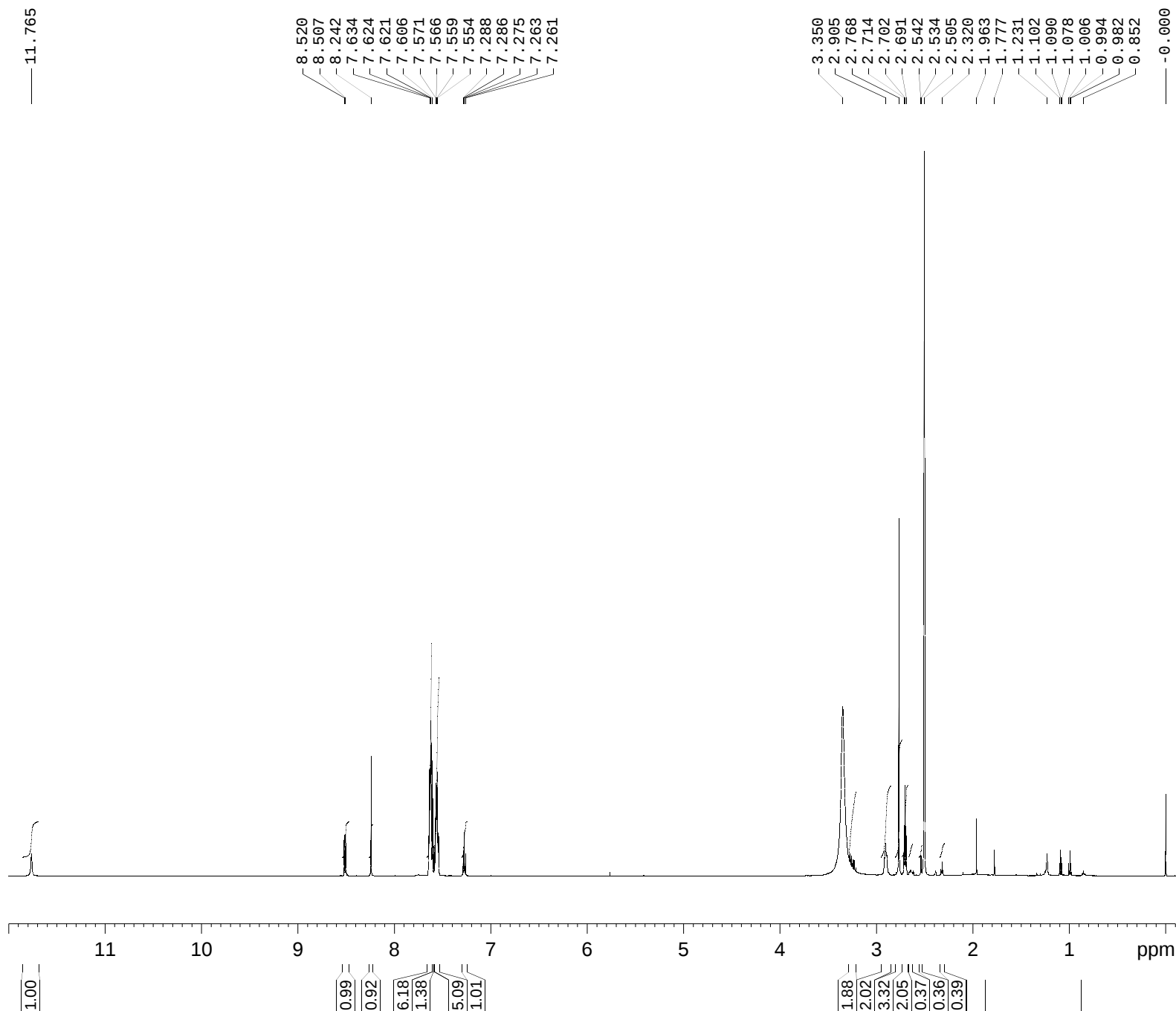
F2 - Processing parameters  
SI 32768  
SF 150.8827330 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



|                |             |
|----------------|-------------|
| Batizi Benedek | KP          |
| KBr            | 2023.10.31. |

|                     |
|---------------------|
| BRUKER Alpha        |
| Resolution: 2 cm-1  |
| Number of Scans: 16 |





Standard 1H  
142090  
BAB0103\_1  
Batizi Benedek  
2023.10.31. (DA)

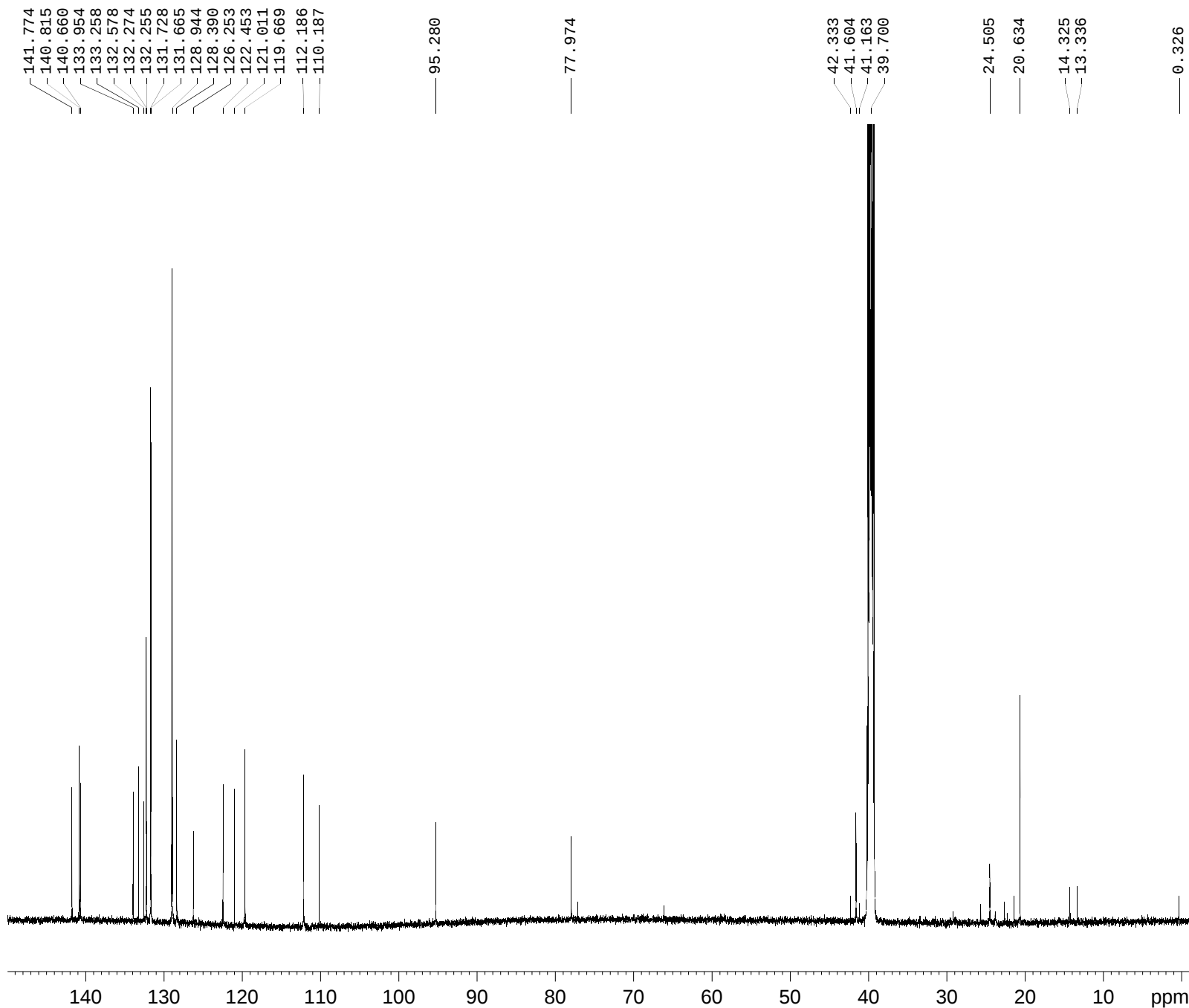
Current Data Parameters  
NAME 142090  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231031  
Time 18.18 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 2.7262976 sec  
RG 196.07  
DW 41.600 usec  
DE 25.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 600.0037050 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W

F2 - Processing parameters  
SI 65536  
SF 600.0000029 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



6



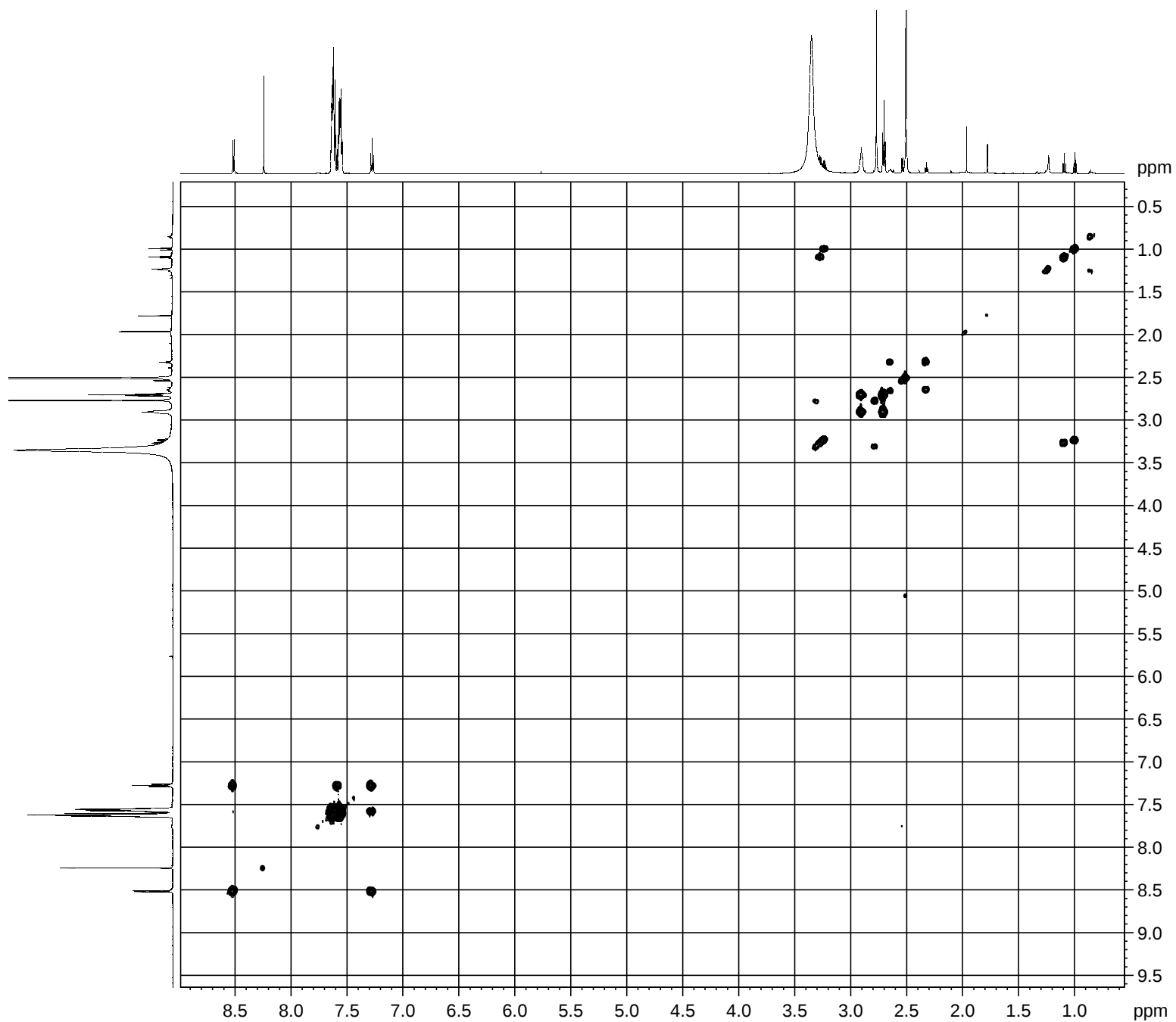
Standard 13C  
142090  
BAB0103\_1  
Batizi Benedek  
2023.10.31. (DA)

Current Data Parameters  
NAME 142090  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231031  
Time 20.33 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 4096  
DS 4  
SWH 36231.883 Hz  
FIDRES 1.105709 Hz  
AQ 0.9043968 sec  
RG 196.07  
DW 13.800 usec  
DE 18.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 150.8852070 MHz  
NUC1 13C  
P1 9.90 usec  
PLW1 80.09999847 W  
SF02 600.0024000 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 35.00000000 W  
PLW12 0.74861997 W  
PLW13 0.37595001 W

F2 - Processing parameters  
SI 32768  
SF 150.8701593 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





COSY  
142090  
BAB0103\_1  
Batizi Benedek  
2023.10.31. (DA)

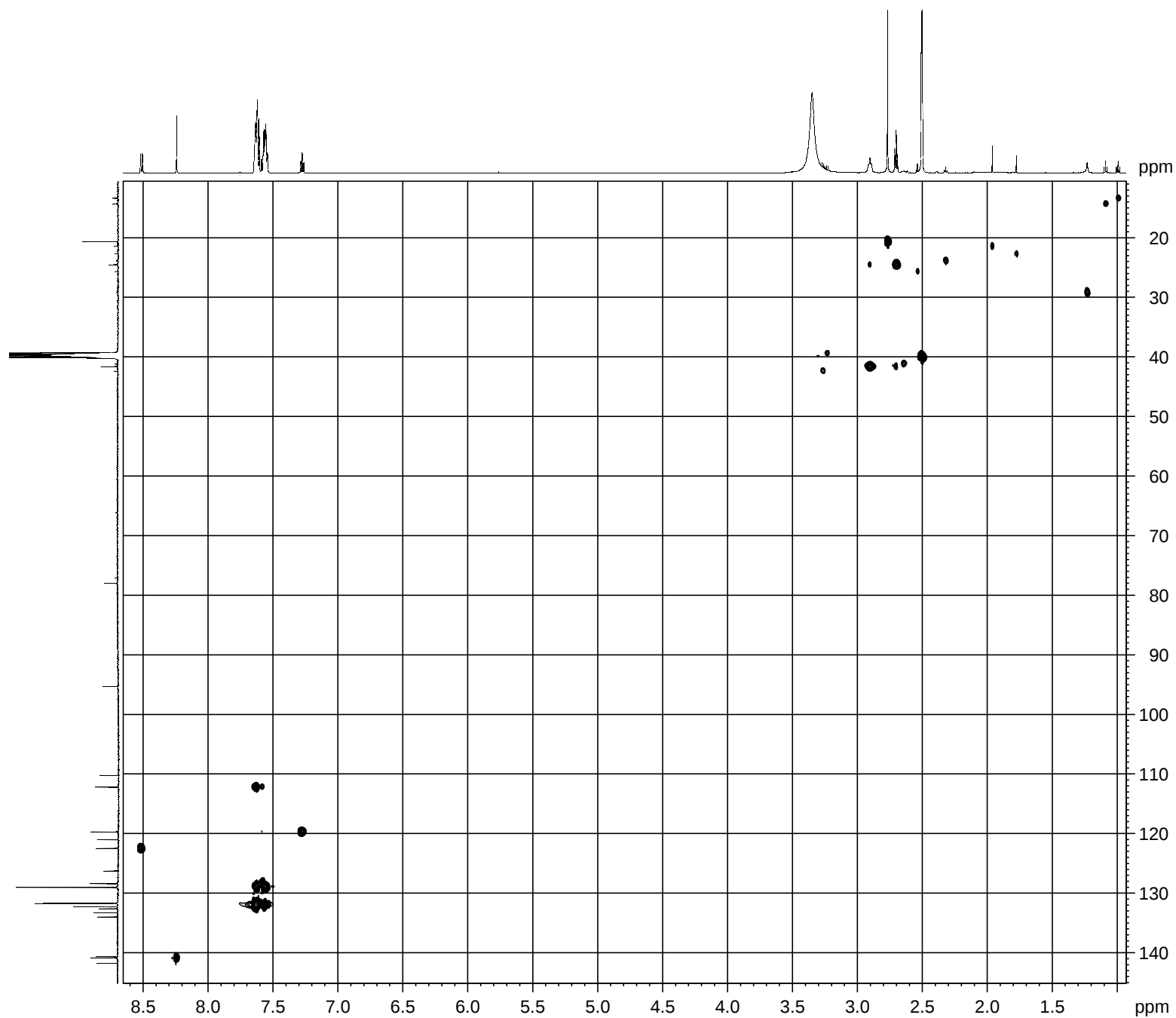
Current Data Parameters  
NAME 142090  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231031  
Time 20.35 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG cosygpmfqr  
TD 2048  
SOLVENT DMSO  
NS 2  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
D0 0.00000300 sec  
D1 2.00000000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00012800 sec  
TDav 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 16.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 12.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 600.0036 MHz  
FIDRES 61.035156 Hz  
SW 13.021 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 600.0000029 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 600.0000029 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



HSQC (140 Hz)  
142090  
BAB0103\_1  
Batizi Benedek  
2023.10.31. (DA)

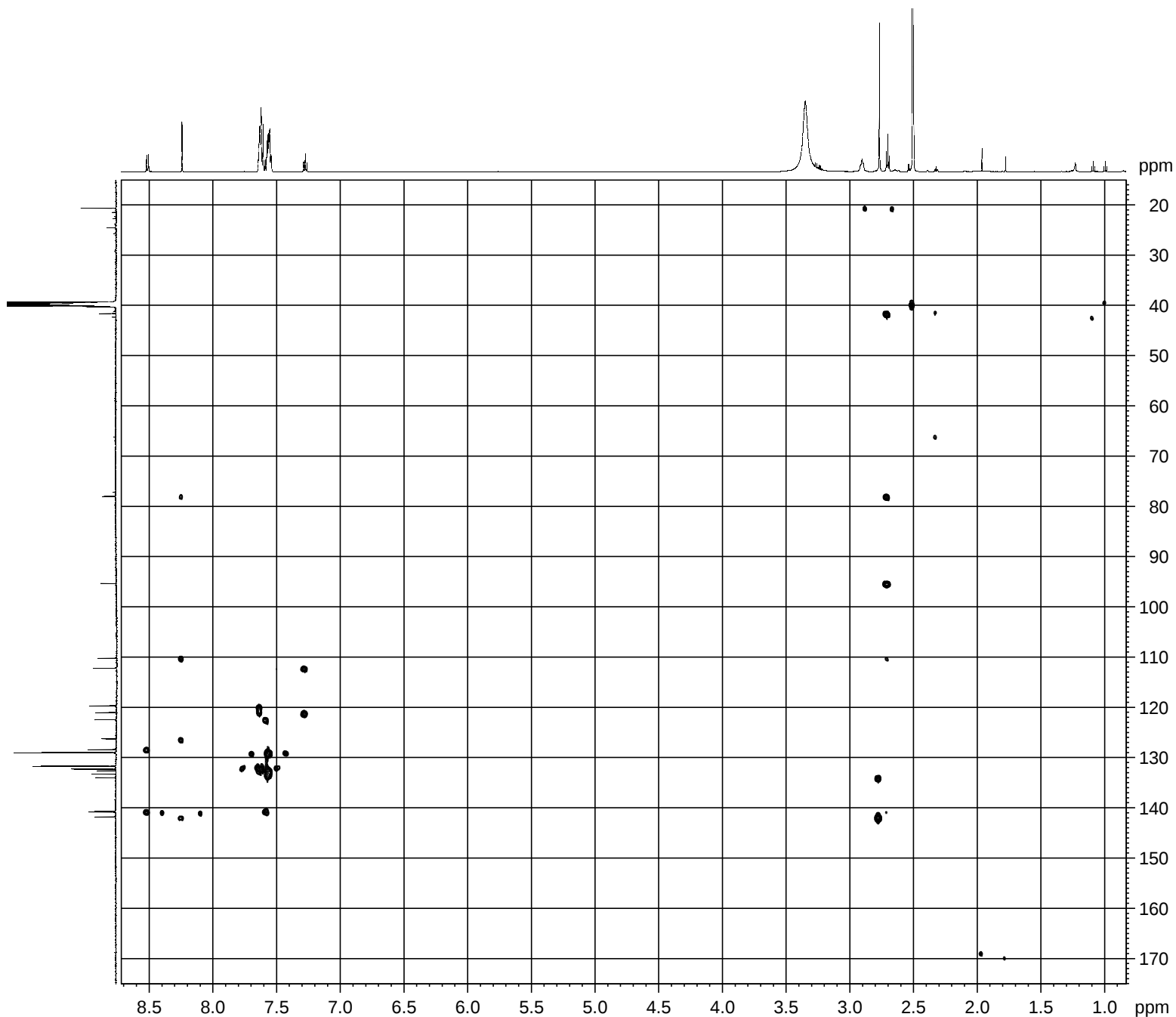
Current Data Parameters  
NAME 142090  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231031  
Time 20.56 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hsqcetgpsisp2.2  
TD 2048  
SOLVENT DMSO  
NS 4  
DS 32  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST17 -0.5000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D4 0.00178571 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
P28 0 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
CPDPRG2 bi\_p5m4sp\_4sp.2  
P3 9.90 usec  
P14 500.00 usec  
P24 2000.00 usec  
P63 1500.00 usec  
PLW0 0 W  
PLW2 80.09999847 W  
PLW12 2.59520006 W  
SPNAM[3] Crp60, 0.5, 20.1  
SPOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 11.99499989 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 11.99499989 W  
SPNAM[14] Crp42, 1.5, 20.2  
SPOAL14 0.500  
SPOFFS14 0 Hz  
SPW14 6.71710014 W  
SPNAM[31] Crp42, 1.5, 20.2  
SPOAL31 0.500  
SPOFFS31 0 Hz  
SPW31 1.67929995 W  
GPNAM[1] SMSQ10.100  
GPZ1 80.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 20.10 %  
GPNAM[3] SMSQ10.100  
GPZ3 11.00 %  
GPNAM[4] SMSQ10.100  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 600.000029 MHz  
WDW QSINE





HMBC (8 Hz, 140 Hz)  
142090  
BAB0103\_1  
Batizi Benedek  
2023.10.31. (DA)

Current Data Parameters  
NAME 142090  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231031  
Time 21.25 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgp1pndqf  
TD 2048  
SOLVENT DMSO  
NS 4  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D2 0.00357143 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0037800 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
P3 9.90 usec  
PLW2 80.09999847 W  
GPNAM[1] SMSQ10.100  
GPZ1 50.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.10 %  
P16 1000.00 usec

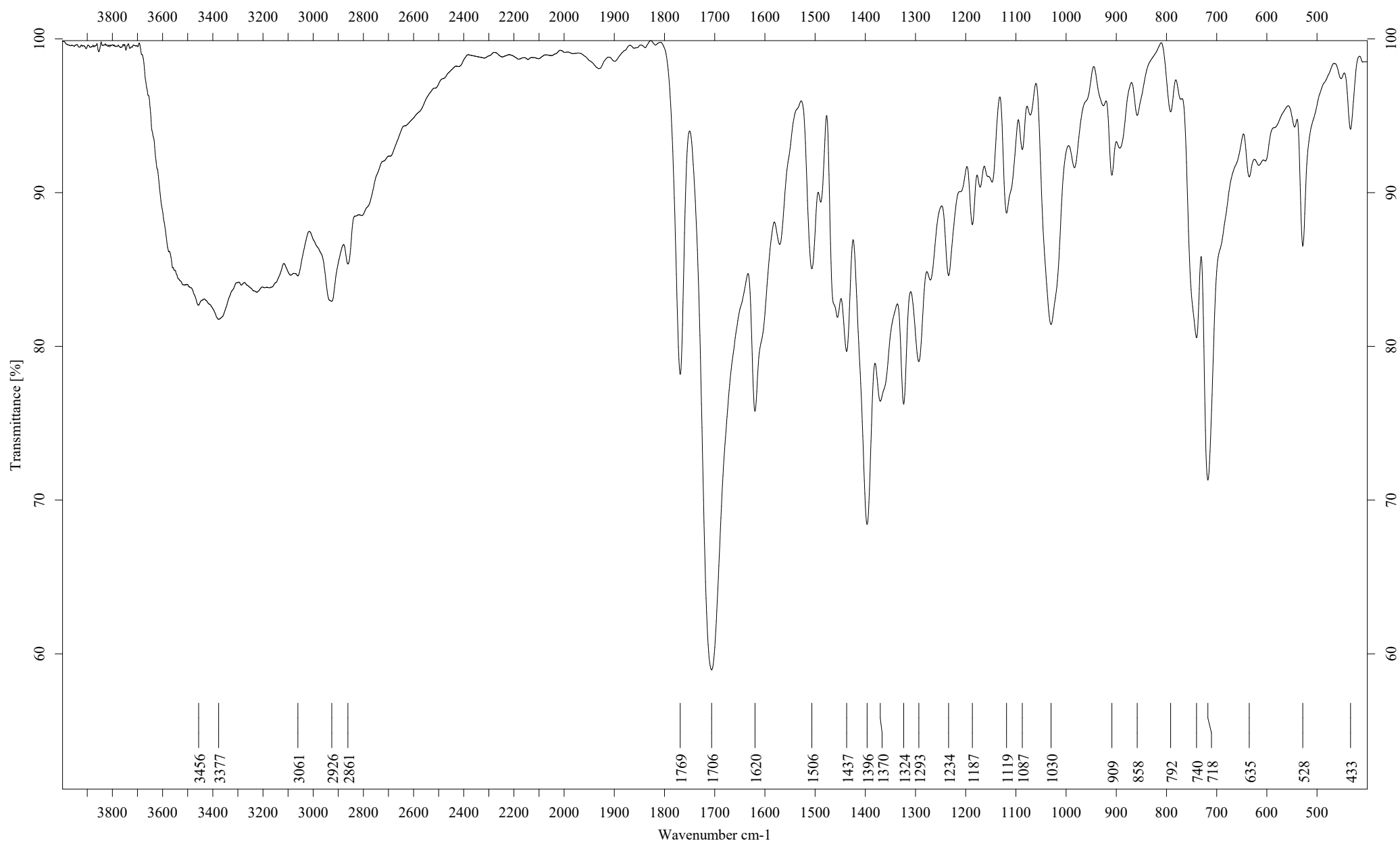
F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE QF

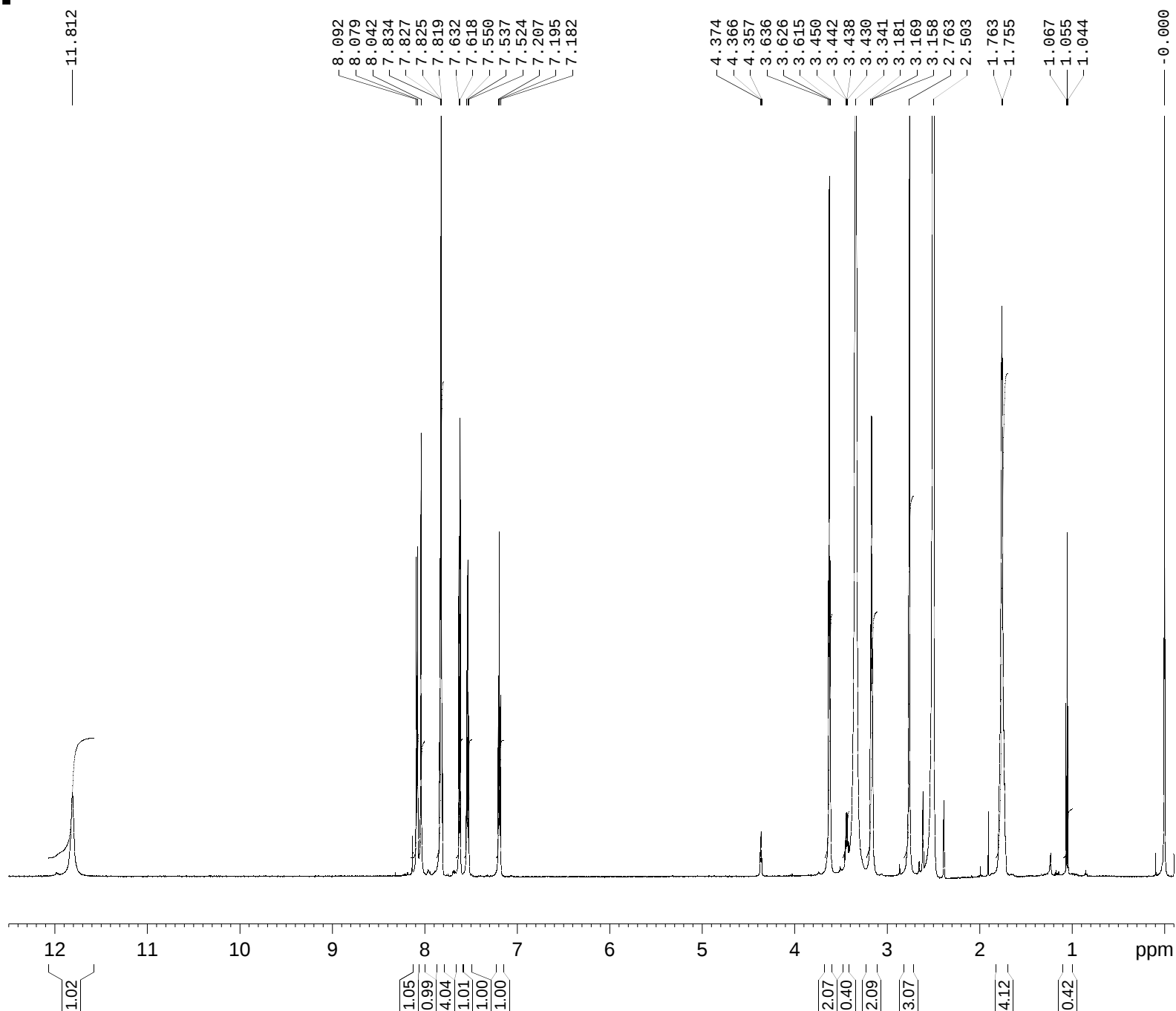
F2 - Processing parameters  
SI 2048  
SF 600.0000000 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 150.8701200 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

|                |          |
|----------------|----------|
| Batizi Benedek | KP       |
| KBr            | 8/2/2024 |

|                     |
|---------------------|
| BRUKER Alpha        |
| Resolution: 2 cm-1  |
| Number of Scans: 16 |





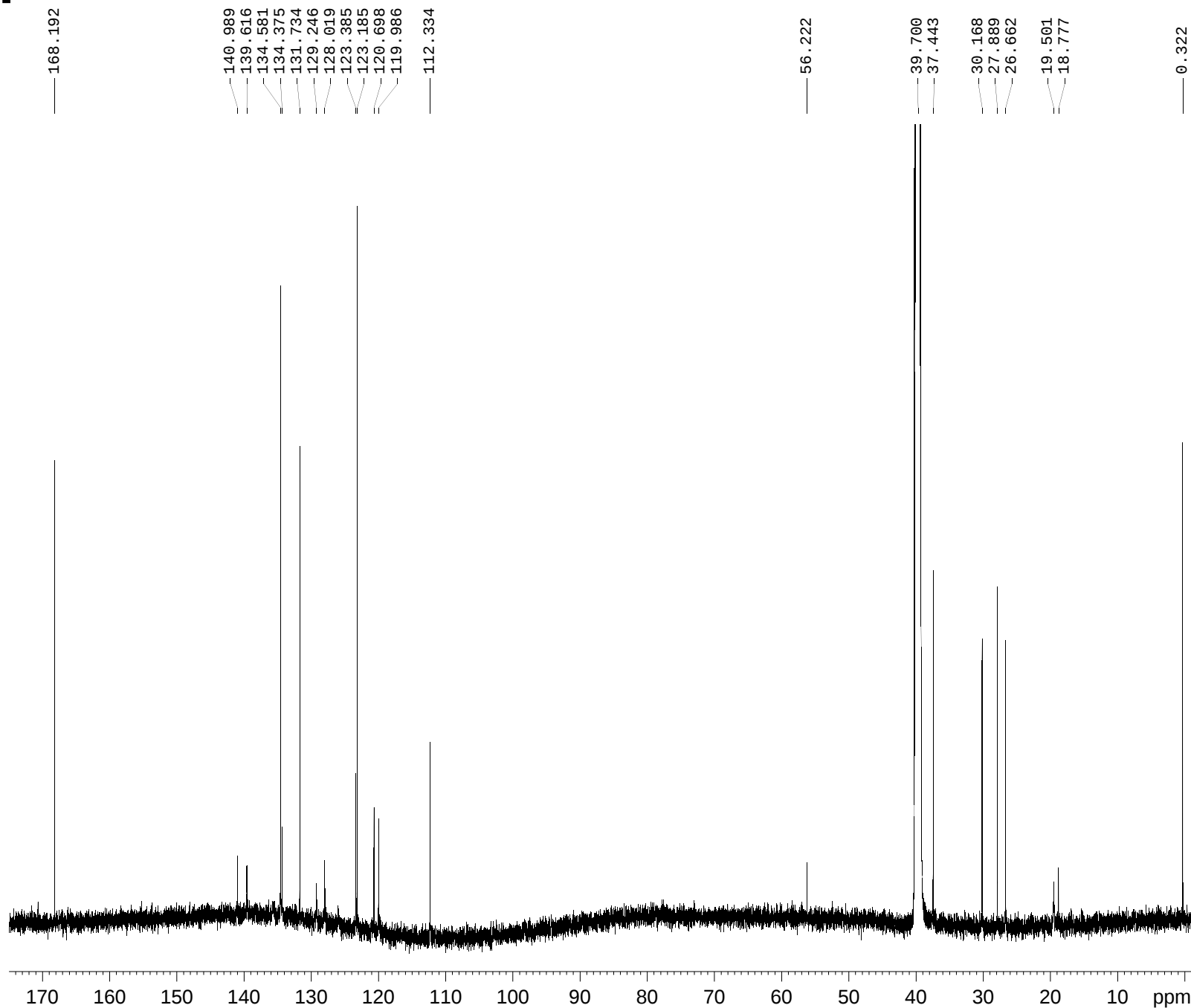
Standard 1H  
143668  
BAB0334\_1  
Batizi Benedek  
2024.10.07. (KP)

Current Data Parameters  
NAME 143668  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20241007  
Time 15.44 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 128  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 2.7262976 sec  
RG 196.07  
DW 41.600 usec  
DE 25.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 600.0037050 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W

F2 - Processing parameters  
SI 65536  
SF 600.0000027 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





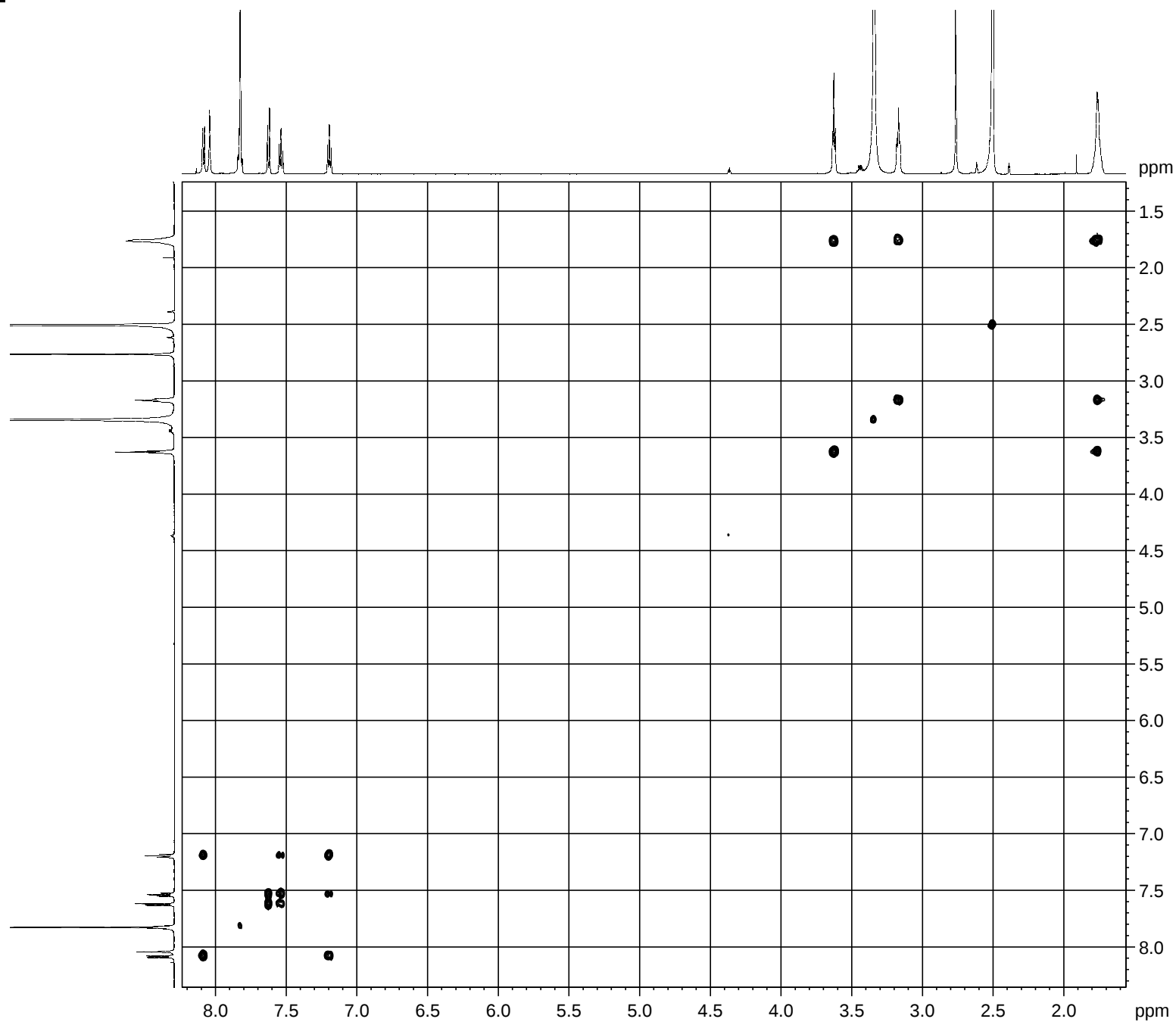
Standard  $^{13}\text{C}$   
 143668  
 BAB0334\_1  
 Batizi Benedek  
 2024.10.07. (KP)

Current Data Parameters  
 NAME 143668  
 EXPNO 12  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20241007  
 Time 20.14 h  
 INSTRUM spect  
 PROBHD Z145856\_0002 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 8192  
 DS 4  
 SWH 36231.883 Hz  
 FIDRES 1.105709 Hz  
 AQ 0.9043968 sec  
 RG 196.07  
 DW 13.800 usec  
 DE 18.00 usec  
 TE 295.0 K  
 D1 1.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SF01 150.8852070 MHz  
 NUC1  $^{13}\text{C}$   
 P1 9.90 usec  
 PLW1 71.00000000 W  
 SF02 600.0024000 MHz  
 NUC2  $^1\text{H}$   
 CPDPRG[2] waltz16  
 PCPD2 80.00 usec  
 PLW2 32.90000153 W  
 PLW12 0.70370001 W  
 PLW13 0.35339001 W

F2 - Processing parameters  
 SI 131072  
 SF 150.8701602 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





COSY  
143668  
BAB0334\_1  
Batizi Benedek  
2024.10.07. (KP)

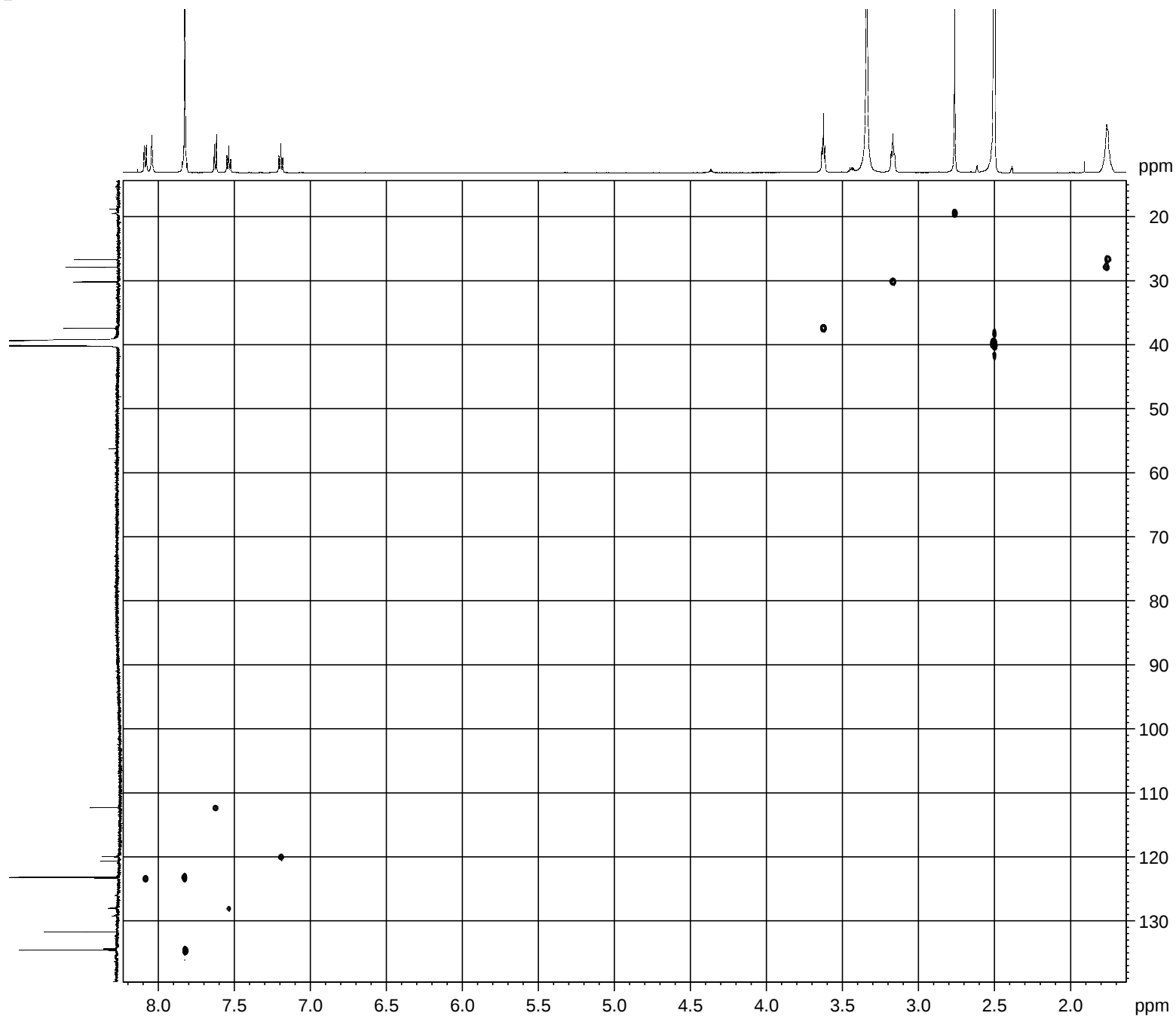
Current Data Parameters  
NAME 143668  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20241007  
Time 20.15 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG cosygpmfqr  
TD 2048  
SOLVENT DMSO  
NS 8  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
D0 0.00000300 sec  
D1 2.00000000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00012800 sec  
TDav 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 16.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 12.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 600.0036 MHz  
FIDRES 61.035156 Hz  
SW 13.021 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 600.0000027 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 600.0000027 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



HSQC (140Hz)  
143668  
BAB0334\_1  
Batizi Benedek  
2024.10.07. (KP)

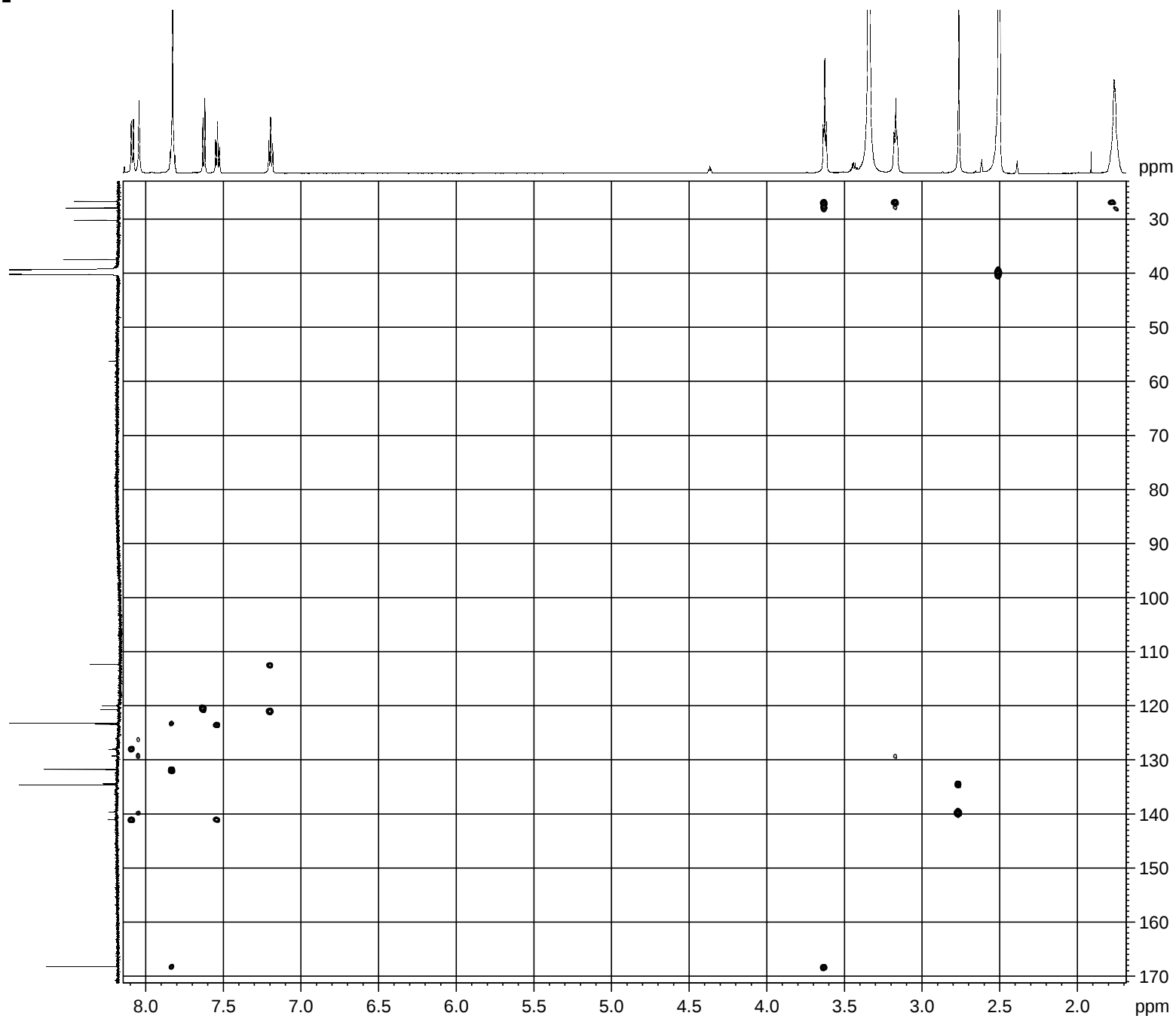
Current Data Parameters  
NAME 143668  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20241007  
Time 21.31 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hsqcetgpsisp2.2  
TD 2048  
SOLVENT DMSO  
NS 16  
DS 32  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST17 -0.5000000  
D0 0.000000000 sec  
D1 1.500000000 sec  
D4 0.00178571 sec  
D11 0.030000000 sec  
D16 0.000200000 sec  
D24 0.000890000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
P28 0 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
CPDPRG2 bi\_p5m4sp\_4sp.2  
P3 9.90 usec  
P14 500.00 usec  
P24 2000.00 usec  
P63 1500.00 usec  
PLW0 0 W  
PLW2 71.00000000 W  
PLW12 2.30040002 W  
SPNAM[3] Crp60, 0.5, 20.1  
SPOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 10.63199997 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 10.63199997 W  
SPNAM[14] Crp42, 1.5, 20.2  
SPOAL14 0.500  
SPOFFS14 0 Hz  
SPW14 5.95400000 W  
SPNAM[31] Crp42, 1.5, 20.2  
SPOAL31 0.500  
SPOFFS31 0 Hz  
SPW31 1.48850000 W  
GPNAM[1] SMSQ10.100  
GPZ1 80.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 20.10 %  
GPNAM[3] SMSQ10.100  
GPZ3 11.00 %  
GPNAM[4] SMSQ10.100  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 600.0000027 MHz  
WDW QSINE





HMBC (8Hz, 140Hz)  
143668  
BAB0334\_1  
Batizi Benedek  
2024.10.07. (KP)

Current Data Parameters  
NAME 143668  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20241007  
Time 23.26 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgp1pndqf  
TD 2048  
SOLVENT DMSO  
NS 16  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D2 0.00357143 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00001510 sec  
TDav 1  
SF01 600.0037800 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
P3 9.90 usec  
PLW2 71.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 50.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.10 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE QF

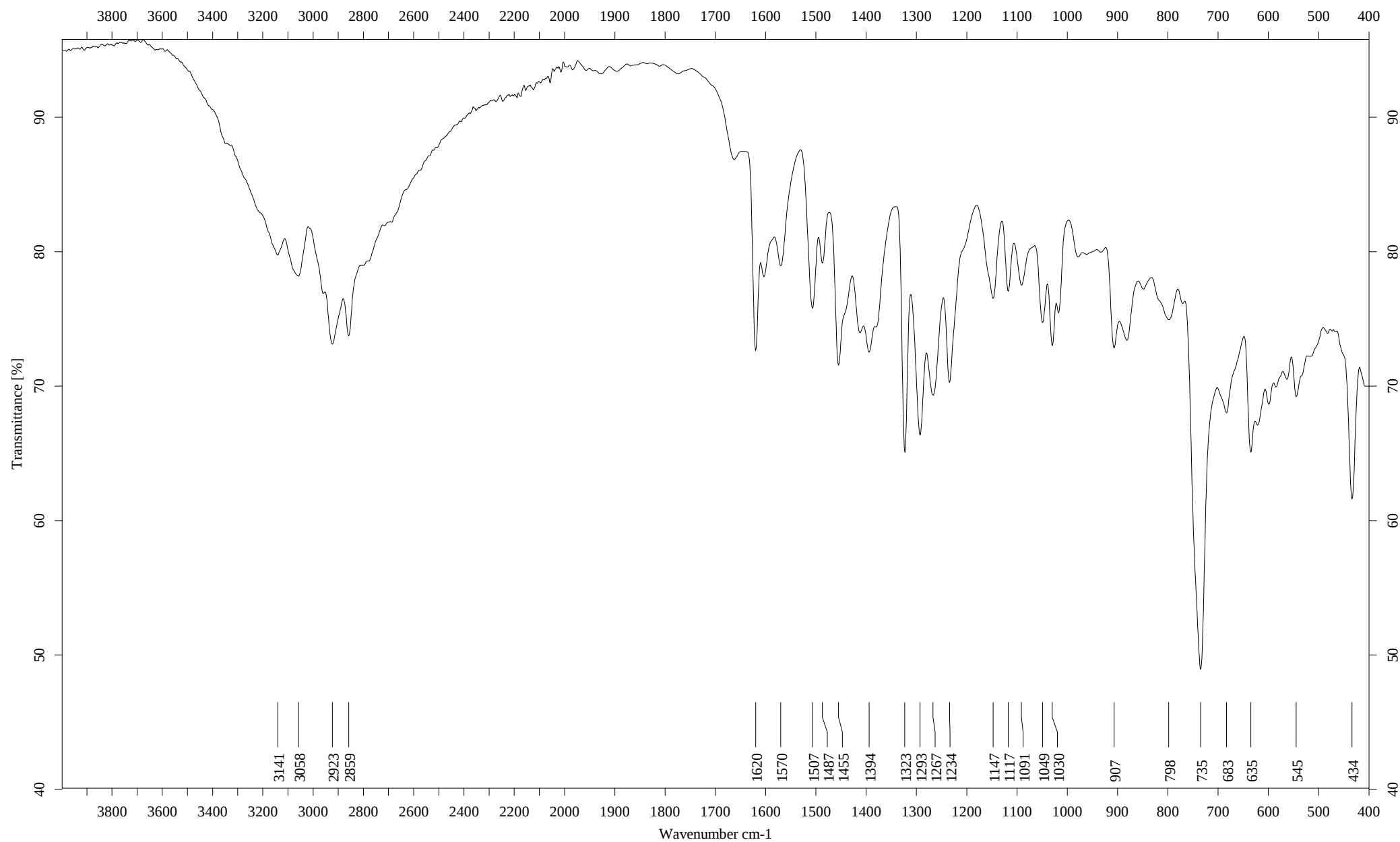
F2 - Processing parameters  
SI 2048  
SF 600.0000000 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

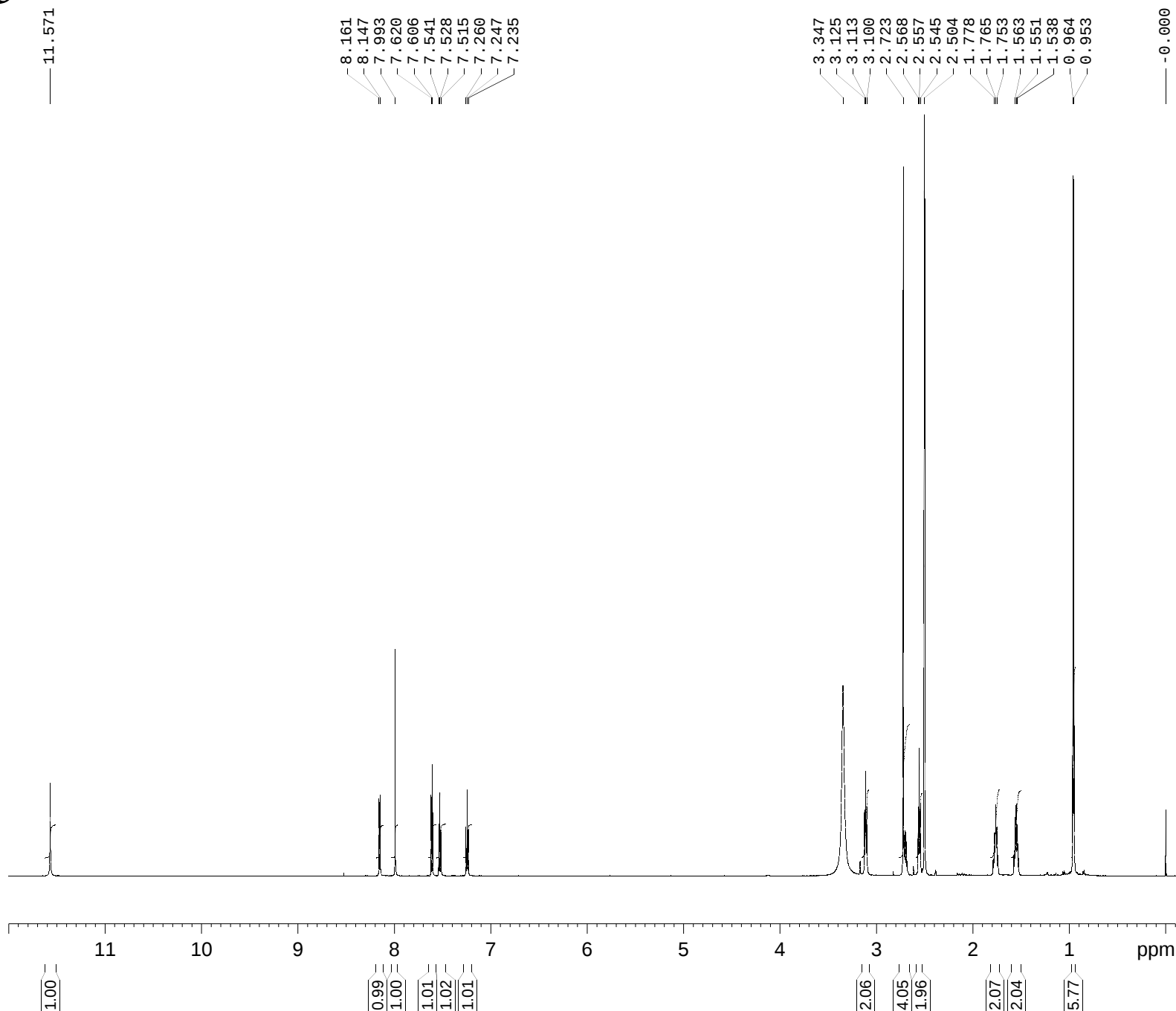
F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 150.8701200 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



|                |             |
|----------------|-------------|
| Batizi Benedek | KP          |
| Gyemant ATR    | 2023.10.17. |

|                     |
|---------------------|
| BRUKER Alpha        |
| Resolution: 2 cm-1  |
| Number of Scans: 32 |





Standard 1H  
142472  
BAB0140\_1  
Batizi Benedek  
2024.02.21. (KP)

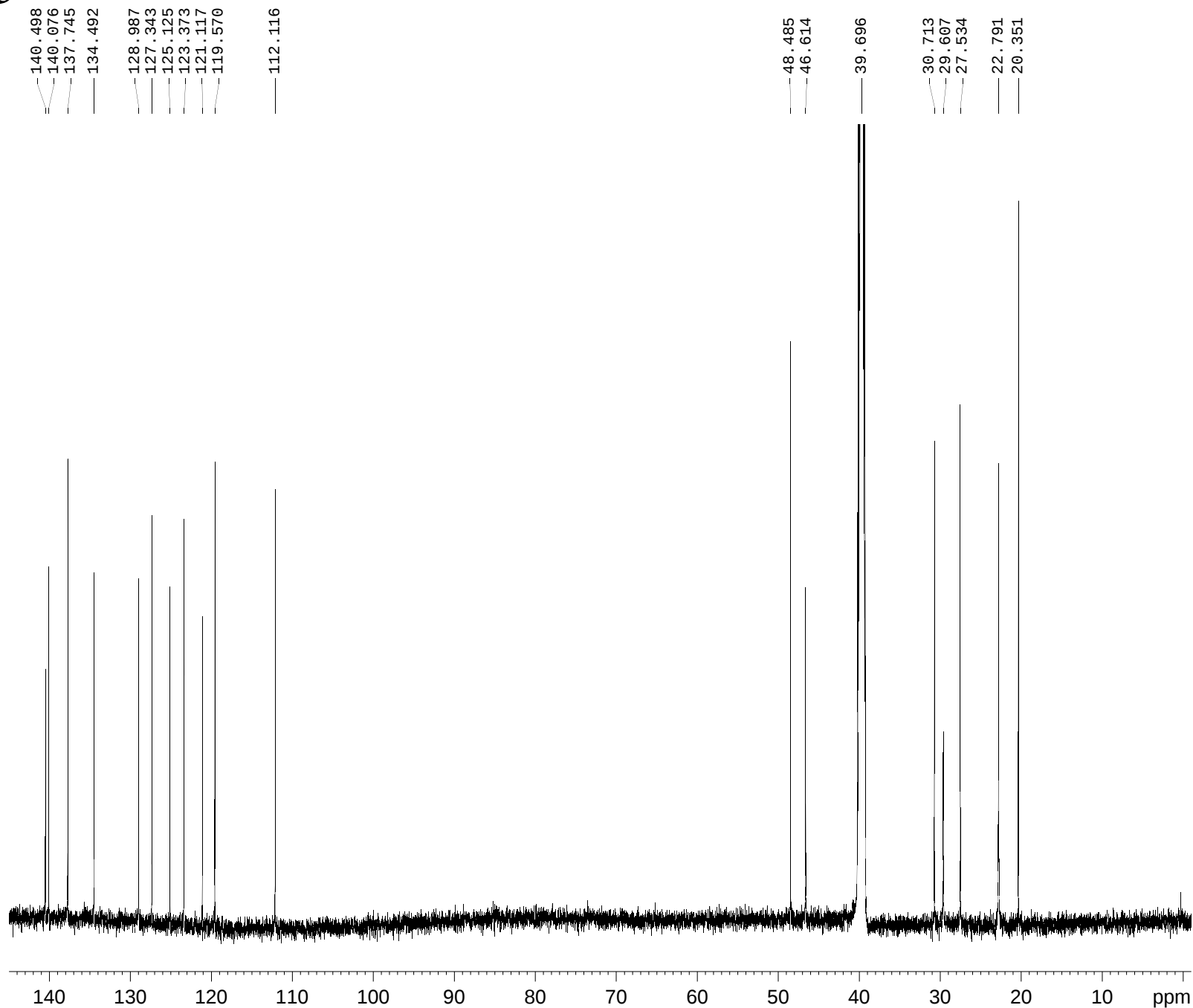
Current Data Parameters  
NAME 142472  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240221  
Time 23.04 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 2.7262976 sec  
RG 196.07  
DW 41.600 usec  
DE 25.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 600.0037050 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W

F2 - Processing parameters  
SI 65536  
SF 600.0000022 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



25



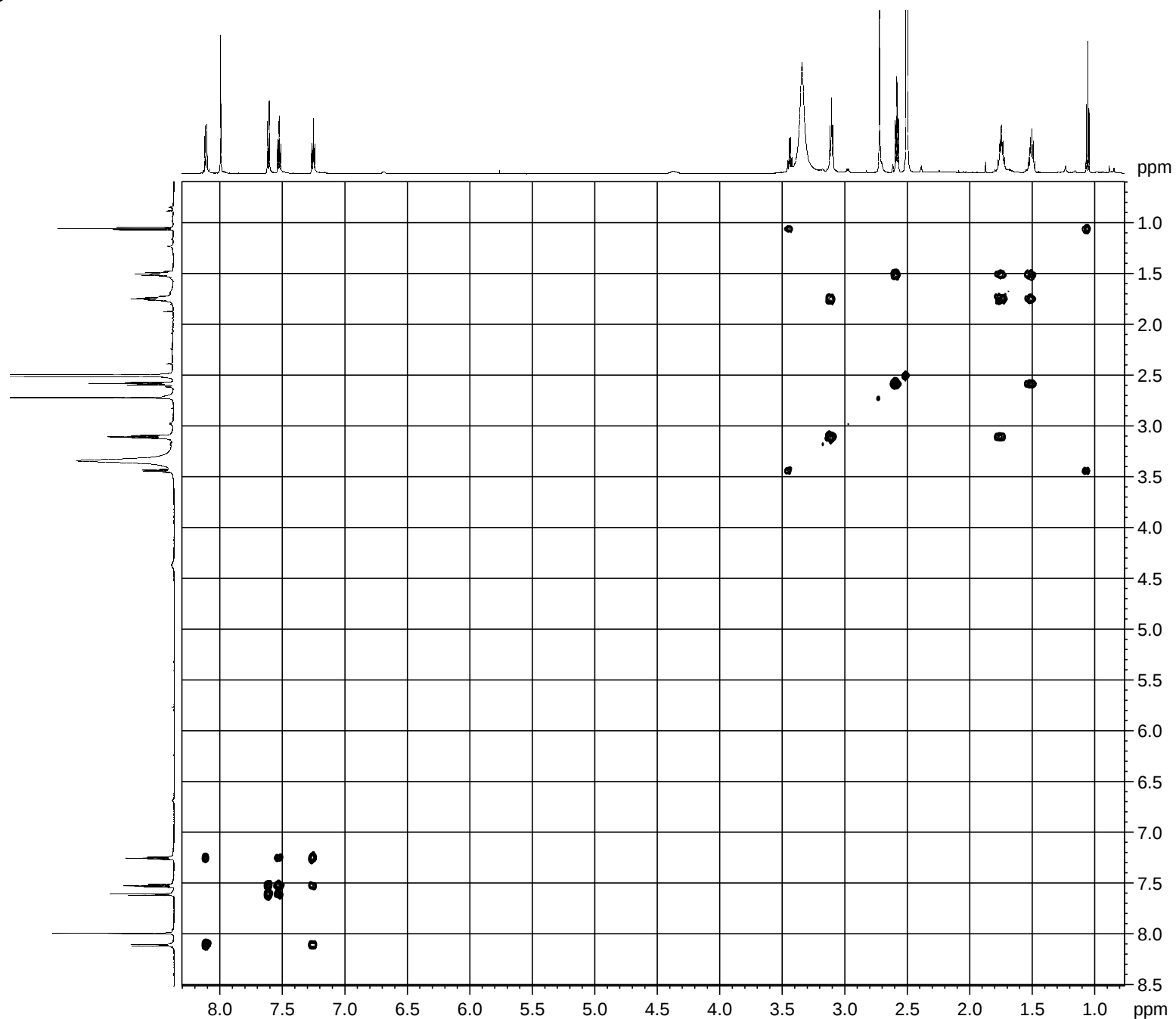
Standard 13C  
142472  
BAB0140\_1  
Batizi Benedek  
2024.02.21. (KP)

Current Data Parameters  
NAME 142472  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240222  
Time 0.13 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 2048  
DS 4  
SWH 36231.883 Hz  
FIDRES 1.105709 Hz  
AQ 0.9043968 sec  
RG 196.07  
DW 13.800 usec  
DE 18.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 150.8852070 MHz  
NUC1 13C  
P1 9.90 usec  
PLW1 71.00000000 W  
SF02 600.0024000 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 32.90000153 W  
PLW12 0.70370001 W  
PLW13 0.35339001 W

F2 - Processing parameters  
SI 32768  
SF 150.8701596 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





COSY  
142050  
BAB0085\_1  
Batizi Benedek  
2023.10.17. (KP)

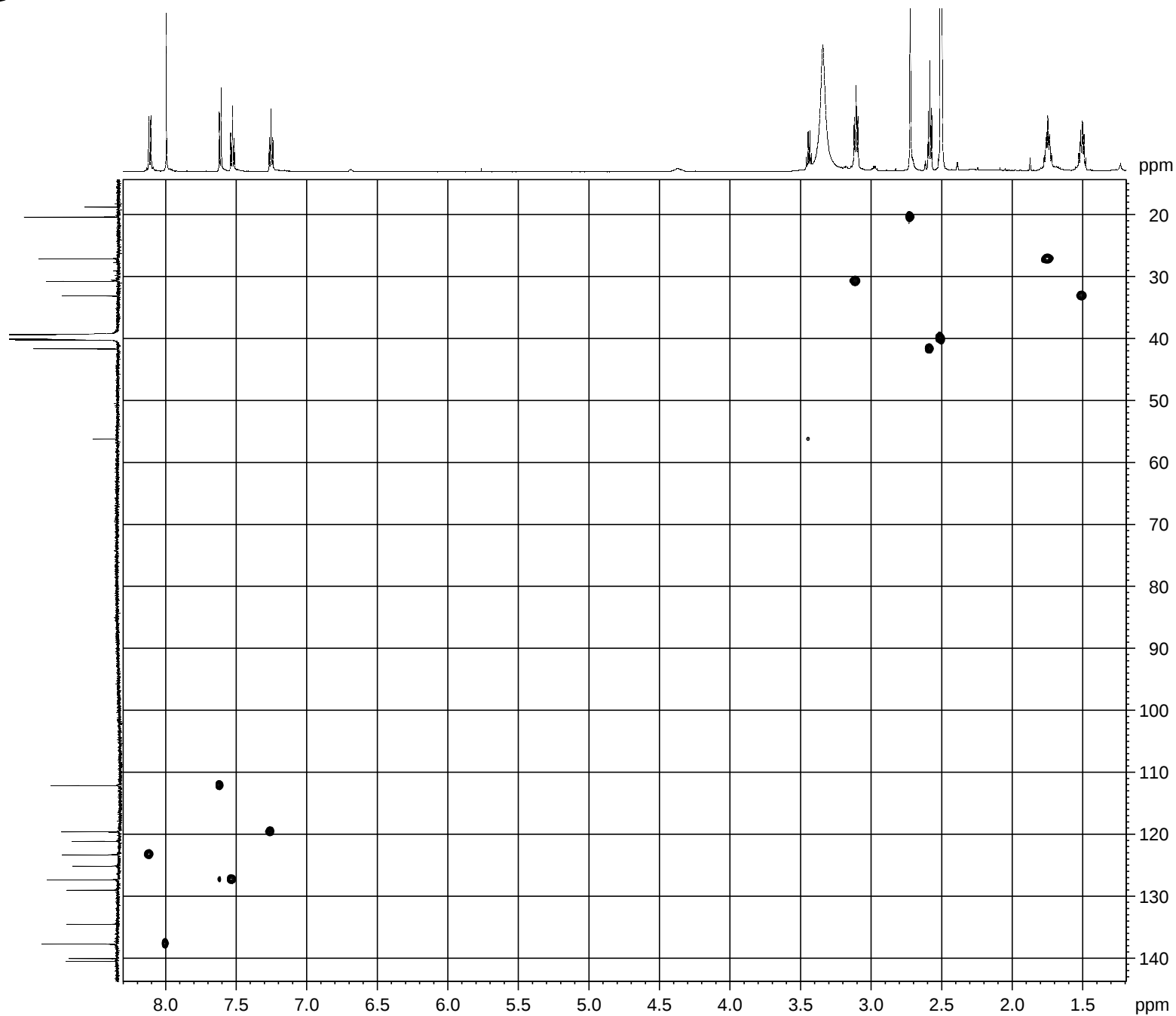
Current Data Parameters  
NAME 142050  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231017  
Time 17.42 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG cosygpmfqr  
TD 2048  
SOLVENT DMSO  
NS 8  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
D0 0.00000300 sec  
D1 2.00000000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00012800 sec  
TDav 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 16.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 12.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 600.0036 MHz  
FIDRES 61.035156 Hz  
SW 13.021 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 600.0000037 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 600.0000037 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



HSQC (140Hz)  
142050  
BAB0085\_1  
Batizi Benedek  
2023.10.17. (KP)

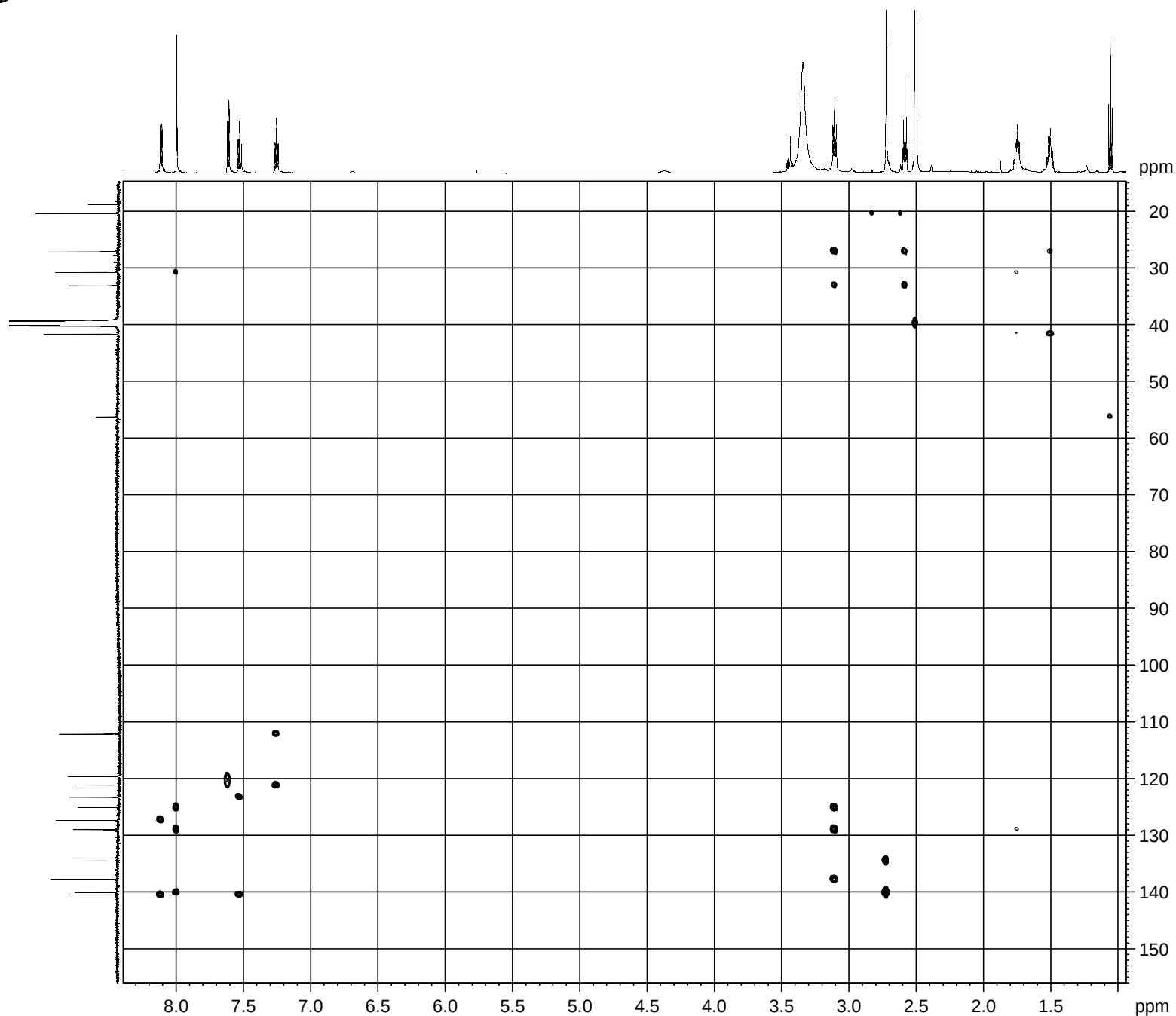
Current Data Parameters  
NAME 142050  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231017  
Time 18.57 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hsqcetgpsisp2.2  
TD 2048  
SOLVENT DMSO  
NS 16  
DS 32  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST17 -0.5000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D4 0.00178571 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
P28 0 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
CPDPRG2 bi\_p5m4sp\_4sp.2  
P3 9.90 usec  
P14 500.00 usec  
P24 2000.00 usec  
P63 1500.00 usec  
PLW0 0 W  
PLW2 80.09999847 W  
PLW12 2.59520006 W  
SPNAM[3] Crp60, 0.5, 20.1  
SPOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 11.99499989 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 11.99499989 W  
SPNAM[14] Crp42, 1.5, 20.2  
SPOAL14 0.500  
SPOFFS14 0 Hz  
SPW14 6.71710014 W  
SPNAM[31] Crp42, 1.5, 20.2  
SPOAL31 0.500  
SPOFFS31 0 Hz  
SPW31 1.67929995 W  
GPNAM[1] SMSQ10.100  
GPZ1 80.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 20.10 %  
GPNAM[3] SMSQ10.100  
GPZ3 11.00 %  
GPNAM[4] SMSQ10.100  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 600.0000037 MHz  
WDW QSI





HMBC (8Hz, 140Hz)  
142050  
BAB0085\_1  
Batizi Benedek  
2023.10.17. (KP)

Current Data Parameters  
NAME 142050  
EXPNO 15  
PROCNO 1

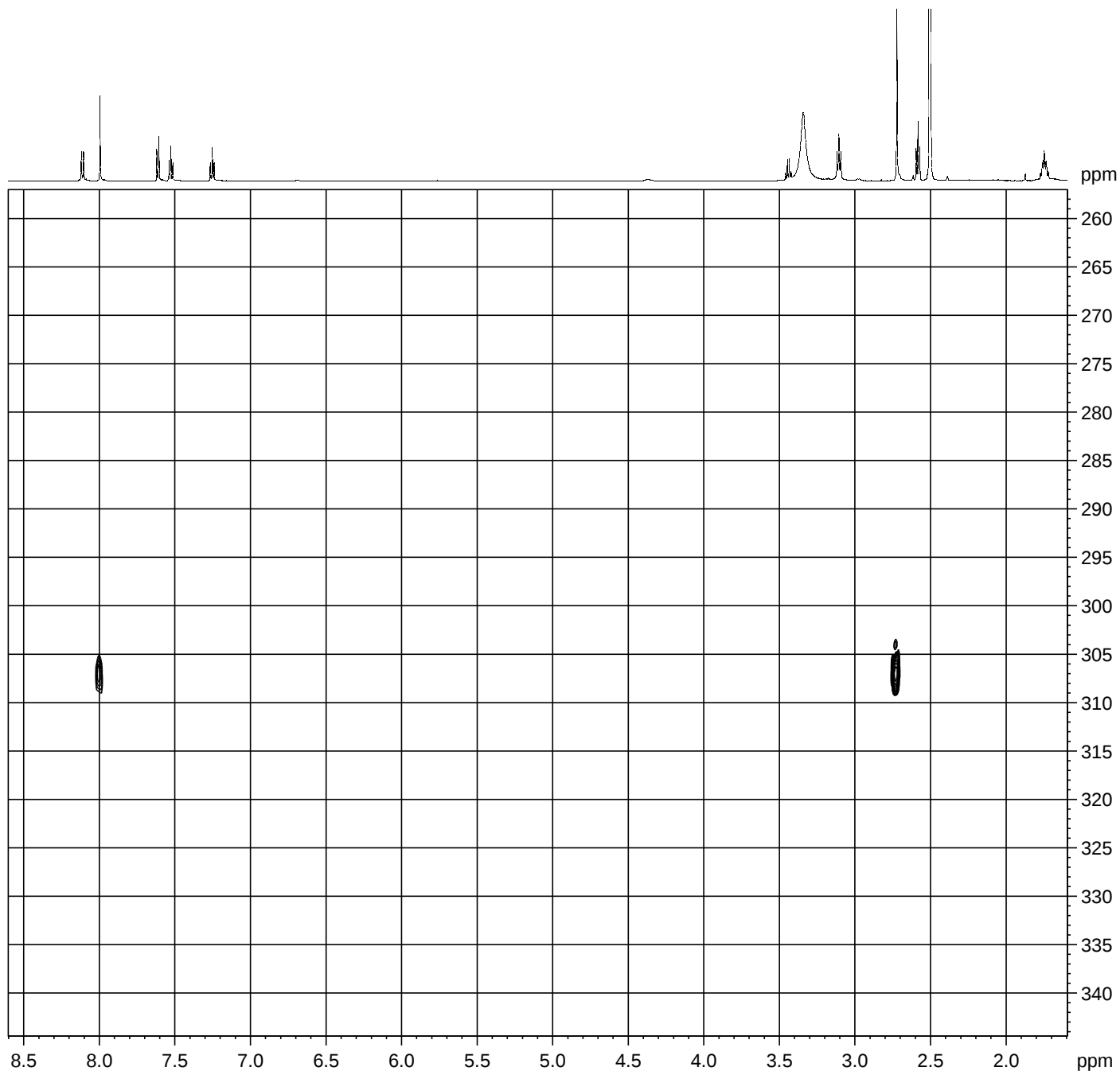
F2 - Acquisition Parameters  
Date\_ 20231017  
Time 20.52 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgp1pndqf  
TD 2048  
SOLVENT DMSO  
NS 16  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D2 0.00357143 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0037800 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
P3 9.90 usec  
PLW2 80.09999847 W  
GPNAM[1] SMSQ10.100  
GPZ1 50.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.10 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE QF

F2 - Processing parameters  
SI 2048  
SF 600.0000037 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 150.8701601 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0





NHMCB  
142050  
BAB0085\_1  
Batizi Benedek  
2023.10.17. (KP)

Current Data Parameters  
NAME 142050  
EXPNO 16  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231017  
Time 22.51 h  
INSTRUM spect  
PROBHD Z145856\_0002  
PULPROG hmbcgpndqf  
TD 2048  
SOLVENT DMSO  
NS 16  
DS 16  
SWH 9615.385 Hz  
FIDRES 9.390024 Hz  
AQ 0.1064960 sec  
RG 196.07  
DW 52.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST13 5.0000000  
D0 0.0000000 sec  
D1 2.0000000 sec  
D6 0.1000000 sec  
D16 0.0002000 sec  
IN0 0.0002060 sec  
TDav 1  
SF01 600.0045600 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.0000000 W  
SF02 60.8096315 MHz  
NUC2 15N  
P3 14.60 usec  
PLW2 236.0000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 70.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 50.10 %  
P16 1000.00 usec

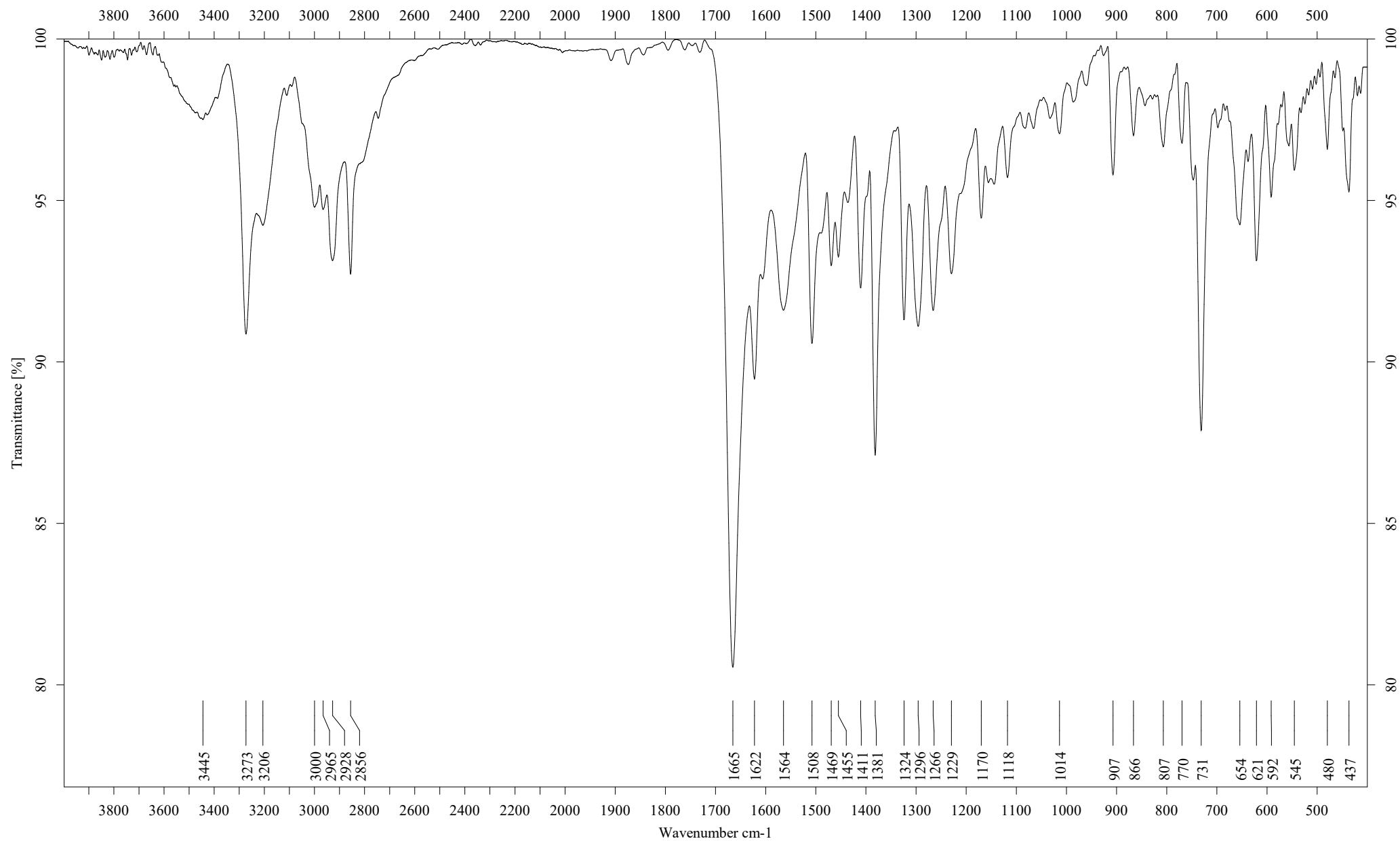
F1 - Acquisition parameters  
TD 128  
SF01 60.80963 MHz  
FIDRES 379.247559 Hz  
SW 399.145 ppm  
FnMODE QF

F2 - Processing parameters  
SI 2048  
SF 600.0000037 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 60.7974720 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

|                |            |
|----------------|------------|
| Batizi Benedek | KP         |
| KBr            | 10/25/2024 |

|                     |
|---------------------|
| BRUKER Alpha        |
| Resolution: 2 cm-1  |
| Number of Scans: 16 |



—11.579

8.103  
8.090  
7.996  
7.974  
7.622  
7.609  
7.543  
7.531  
7.518  
7.267  
7.254  
7.242

3.346  
3.174  
3.165  
3.133  
3.122  
3.111  
3.107  
2.725  
2.504  
1.911  
1.746  
1.733  
1.721  
1.574  
1.562  
1.549  
1.232  
0.853

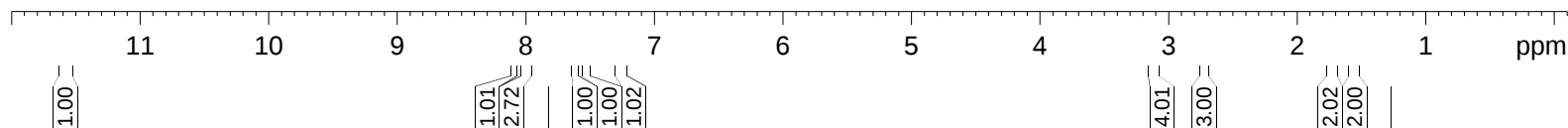
—-0.000

Standard 1H  
143759  
BAB0345\_1  
Batizi Benedek  
2024.10.25. (KP)

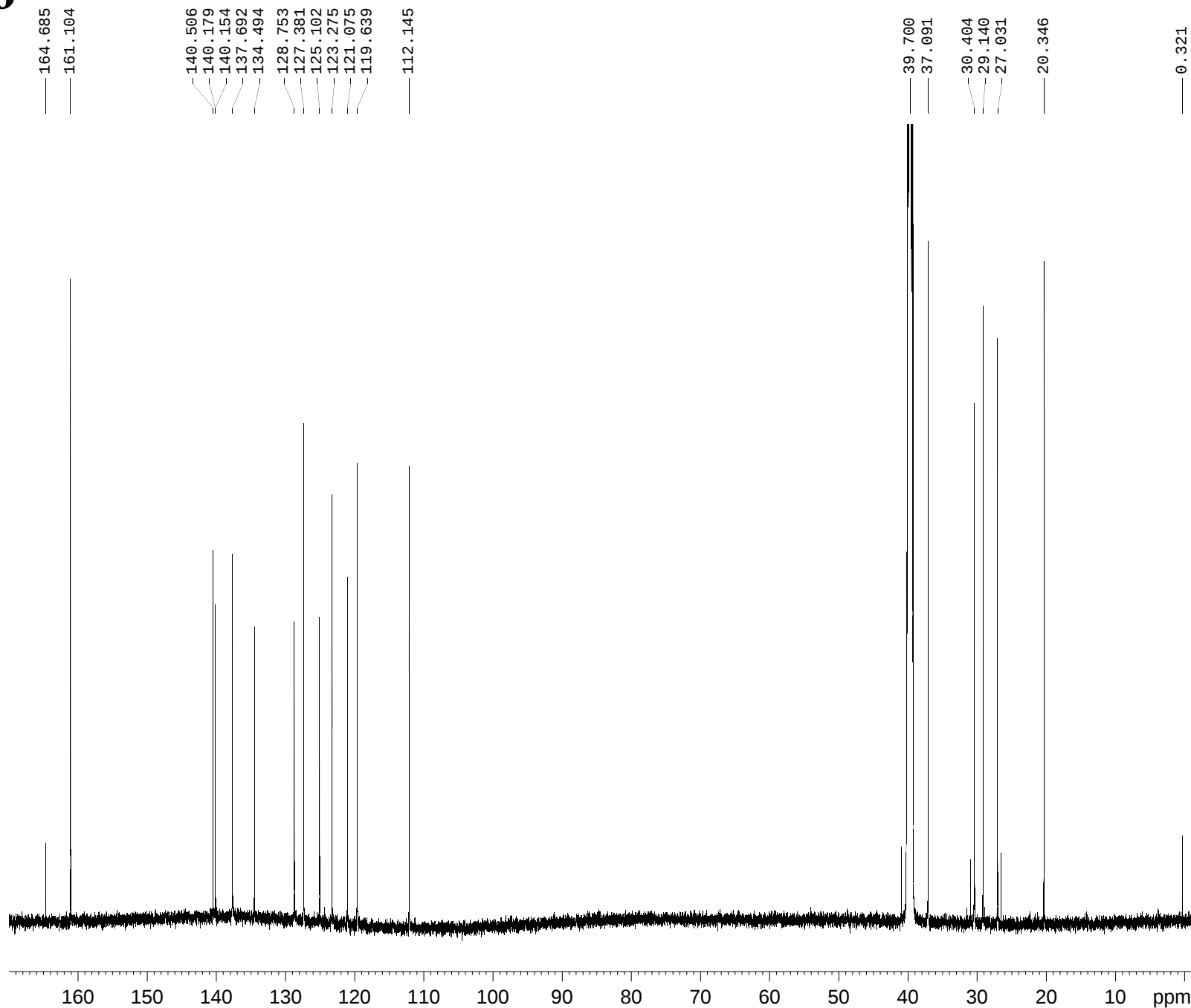
Current Data Parameters  
NAME 143759  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20241025  
Time 20.40 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 64  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 2.7262976 sec  
RG 196.07  
DW 41.600 usec  
DE 25.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 600.0037050 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W

F2 - Processing parameters  
SI 65536  
SF 600.0000025 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



26



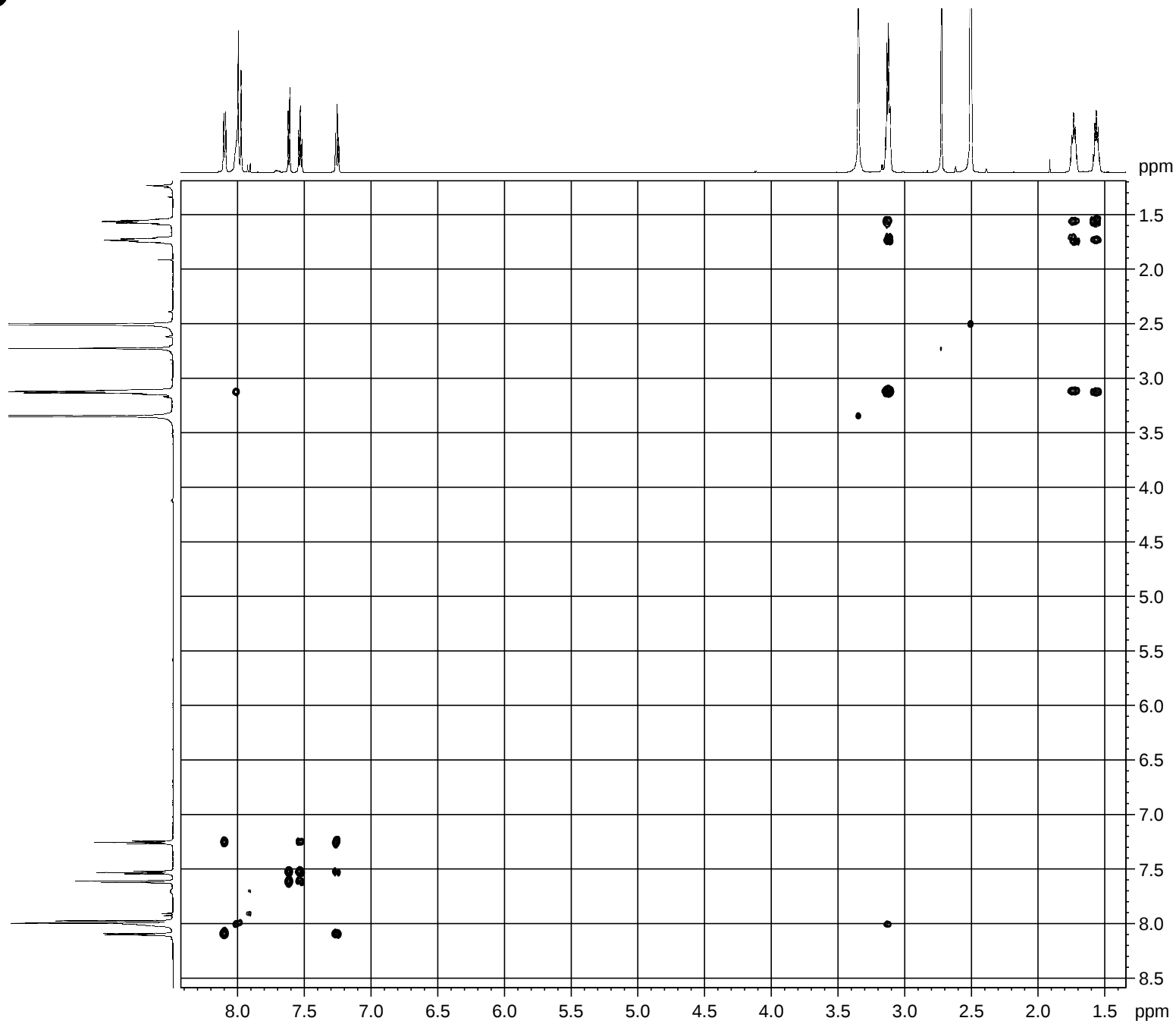
Standard 13C  
143759  
BAB0345\_1  
Batizi Benedek  
2024.10.25. (KP)

Current Data Parameters  
NAME 143759  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20241025  
Time 22.57 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 4096  
DS 4  
SWH 36231.883 Hz  
FIDRES 1.105709 Hz  
AQ 0.9043968 sec  
RG 196.07  
DW 13.800 usec  
DE 18.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 150.8852070 MHz  
NUC1 13C  
P1 9.90 usec  
PLW1 71.00000000 W  
SF02 600.0024000 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 32.90000153 W  
PLW12 0.70370001 W  
PLW13 0.35339001 W

F2 - Processing parameters  
SI 131072  
SF 150.8701601 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





COSY  
143759  
BAB0345\_1  
Batizi Benedek  
2024.10.25. (KP)

Current Data Parameters  
NAME 143759  
EXPNO 13  
PROCNO 1

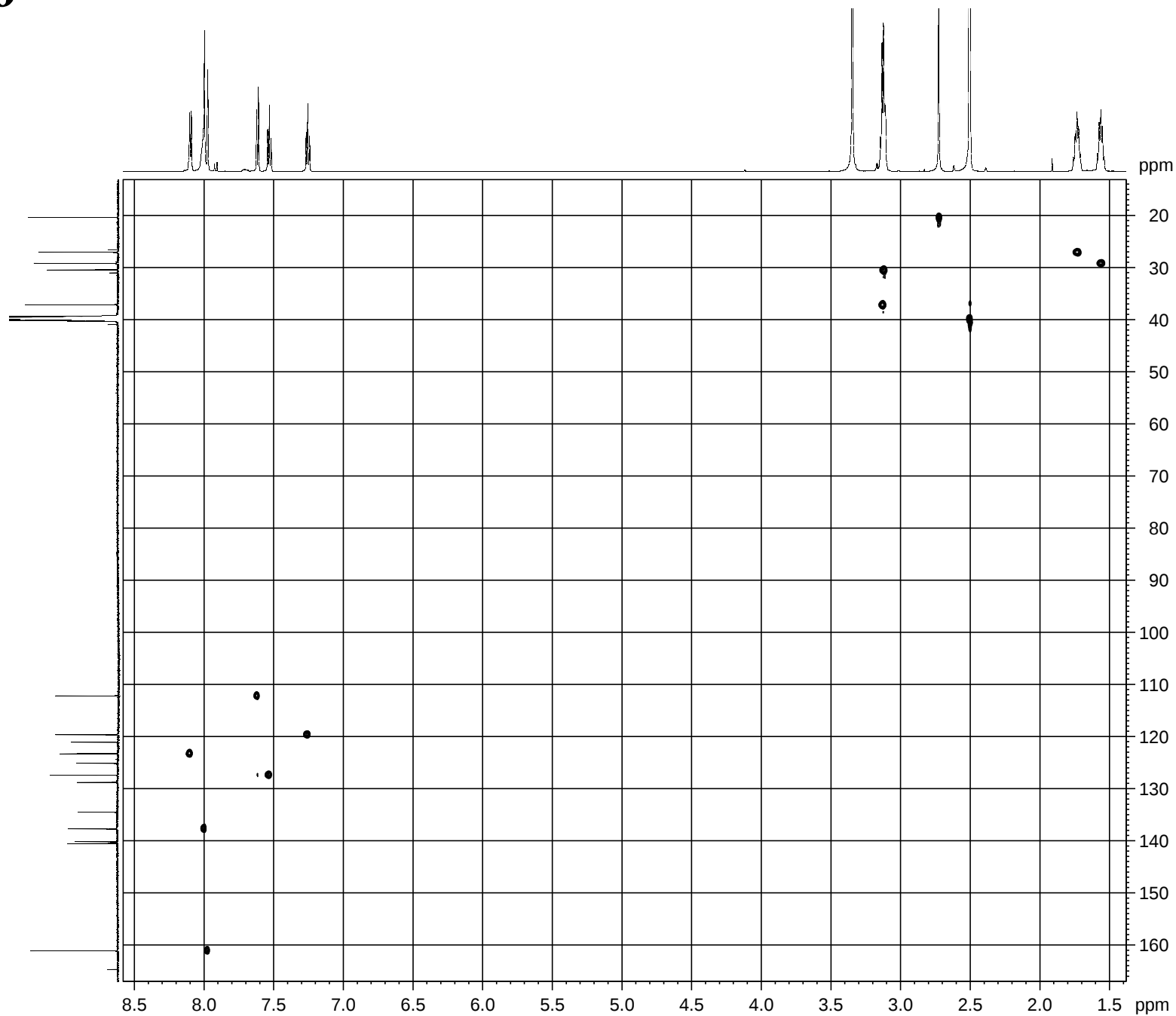
F2 - Acquisition Parameters  
Date\_ 20241025  
Time 22.59 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG cosygpmfqr  
TD 2048  
SOLVENT DMSO  
NS 4  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
D0 0.00000300 sec  
D1 2.00000000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00012800 sec  
TDav 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 16.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 12.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 600.0036 MHz  
FIDRES 61.035156 Hz  
SW 13.021 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 600.0000025 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 600.0000025 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0





HSQC (140Hz)  
143759  
BAB0345\_1  
Batizi Benedek  
2024.10.25. (KP)

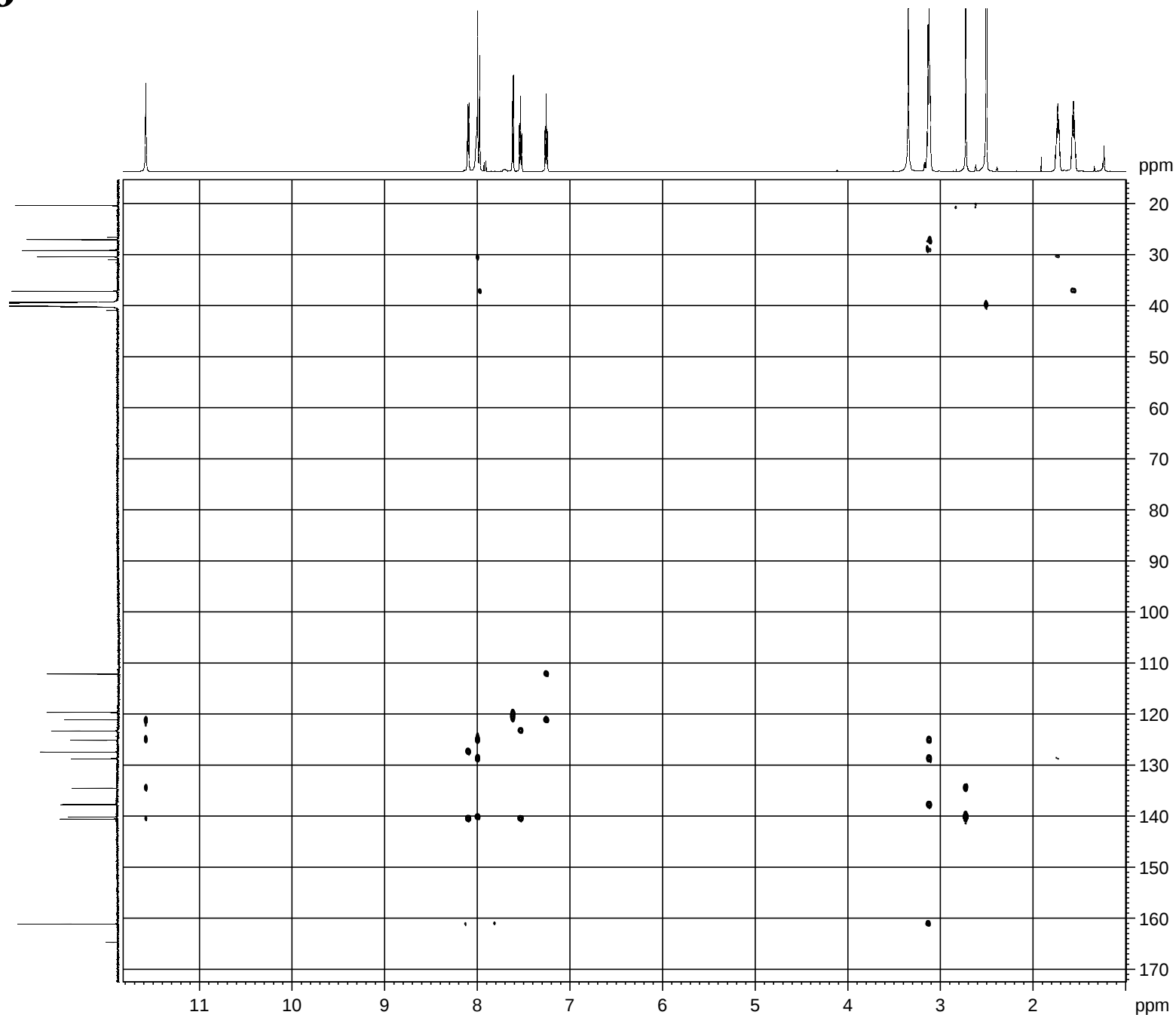
Current Data Parameters  
NAME 143759  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20241025  
Time 23.37 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hsqcetgpsisp2.2  
TD 2048  
SOLVENT DMSO  
NS 8  
DS 32  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST17 -0.5000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D4 0.00178571 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0036000 MHz  
NUC1  $^1\text{H}$   
P1 11.50 usec  
P2 23.00 usec  
P28 0 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2  $^{13}\text{C}$   
CPDPRG2 bi\_p5m4sp\_4sp.2  
P3 9.90 usec  
P14 500.00 usec  
P24 2000.00 usec  
P63 1500.00 usec  
PLW0 0 W  
PLW2 71.00000000 W  
PLW12 2.30040002 W  
SPNAM[3] Crp60, 0.5, 20.1  
SPOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 10.63199997 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 10.63199997 W  
SPNAM[14] Crp42, 1.5, 20.2  
SPOAL14 0.500  
SPOFFS14 0 Hz  
SPW14 5.95400000 W  
SPNAM[31] Crp42, 1.5, 20.2  
SPOAL31 0.500  
SPOFFS31 0 Hz  
SPW31 1.48850000 W  
GPNAM[1] SMSQ10.100  
GPZ1 80.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 20.10 %  
GPNAM[3] SMSQ10.100  
GPZ3 11.00 %  
GPNAM[4] SMSQ10.100  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FwMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 600.0000025 MHz  
WDW QSINE





HMBC (8Hz, 140Hz)  
143759  
BAB0345\_1  
Batizi Benedek  
2024.10.25. (KP)

Current Data Parameters  
NAME 143759  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20241025  
Time 0.36 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgp1pndqf  
TD 2048  
SOLVENT DMSO  
NS 8  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D2 0.00357143 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0037800 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
P3 9.90 usec  
PLW2 71.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 50.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.10 %  
P16 1000.00 usec

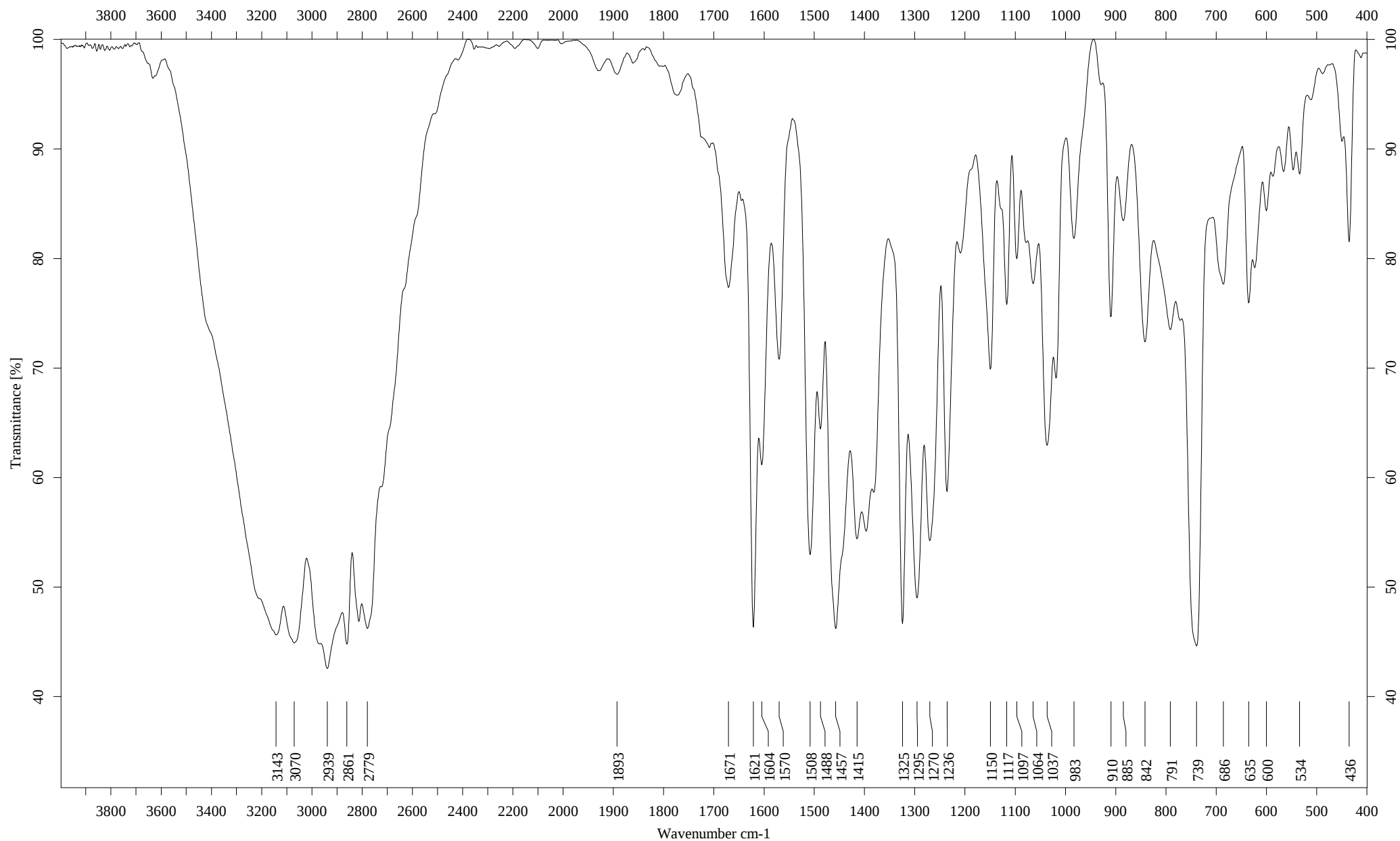
F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE QF

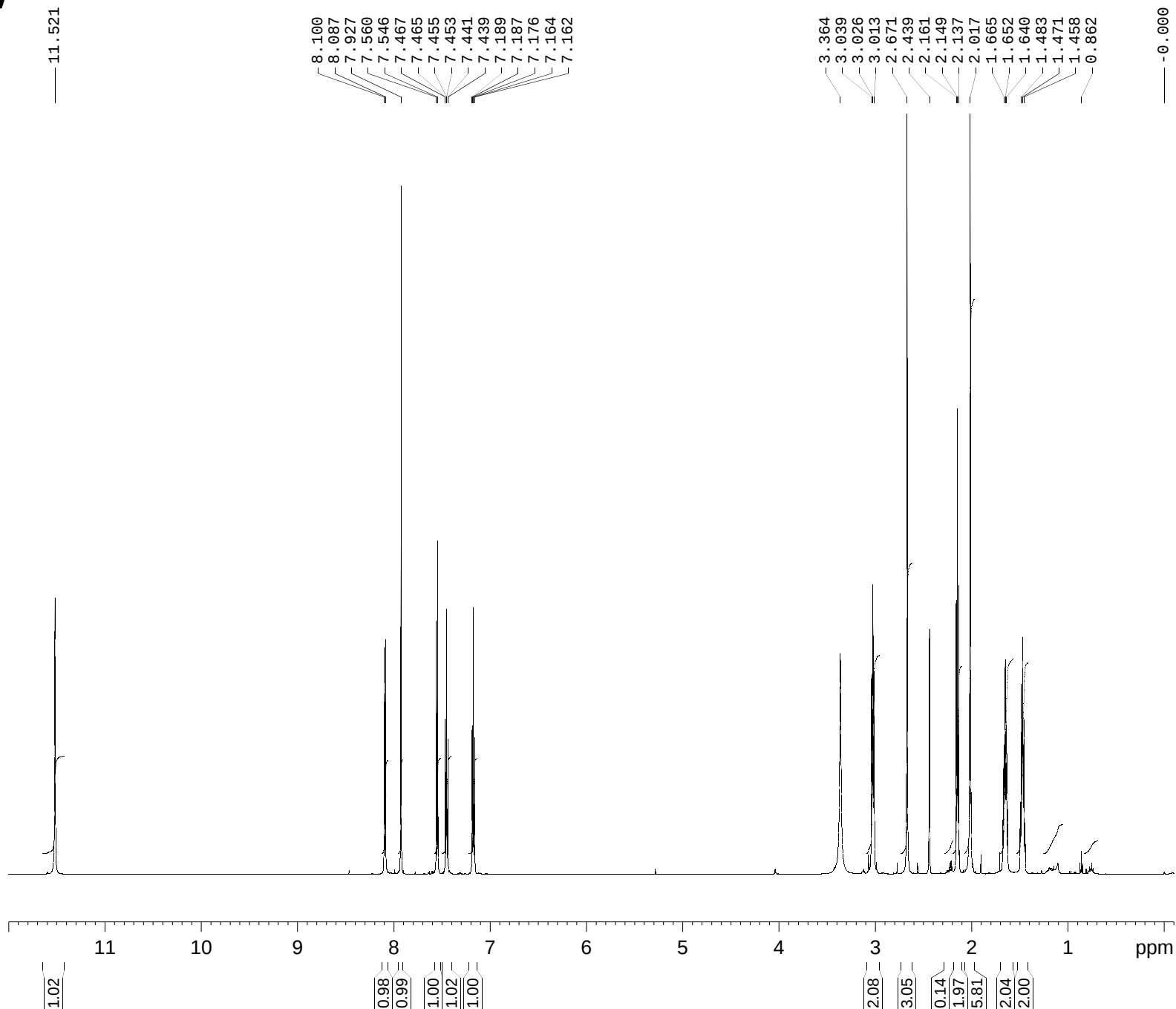
F2 - Processing parameters  
SI 2048  
SF 600.0000025 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 150.8701601 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

|                |             |
|----------------|-------------|
| Batizi Benedek | KP          |
| Film           | 2023.11.27. |

|                     |
|---------------------|
| BRUKER Alpha        |
| Resolution: 2 cm-1  |
| Number of Scans: 16 |





Standard 1H  
142221  
BAB0113\_1  
Batizi Benedek  
2023.11.27. (KP)

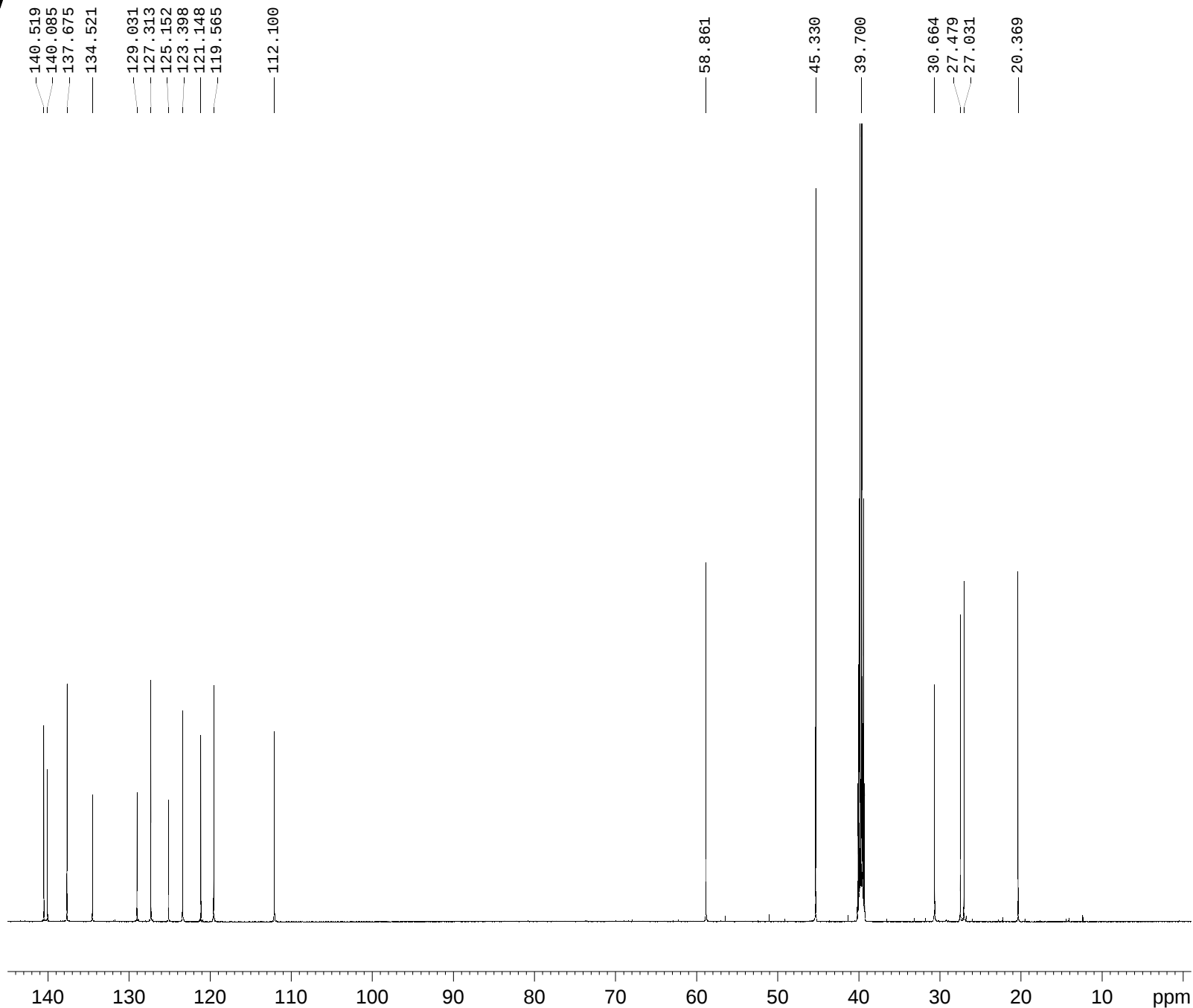
Current Data Parameters  
NAME 142221  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231127  
Time 16.11 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 2.7262976 sec  
RG 56.03  
DW 41.600 usec  
DE 25.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 600.0037050 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W

F2 - Processing parameters  
SI 65536  
SF 600.0000420 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



27



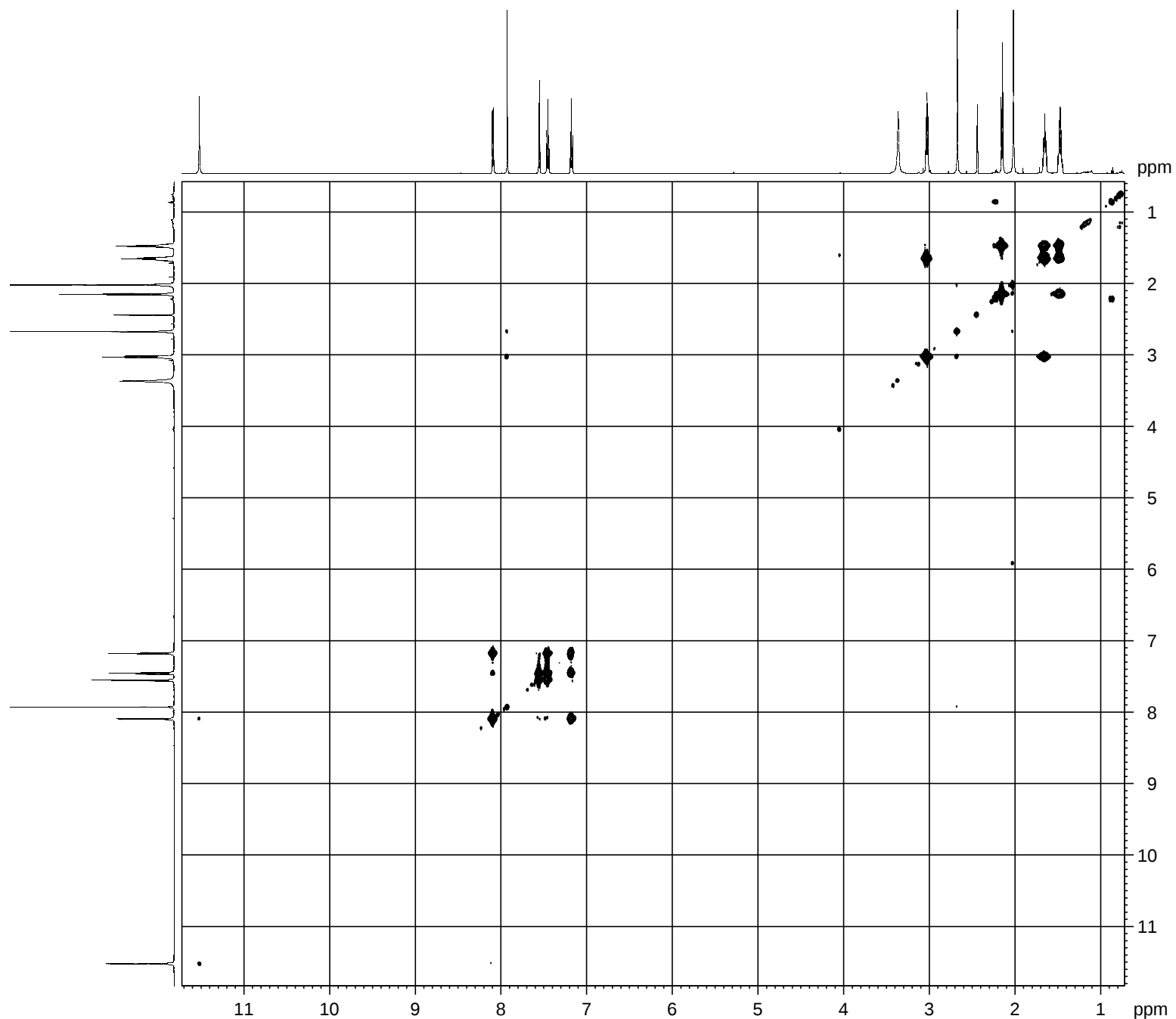
Standard 13C  
142221  
BAB0113\_1  
Batizi Benedek  
2023.11.27. (KP)

Current Data Parameters  
NAME 142221  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231127  
Time 18.07 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 2048  
DS 4  
SWH 36231.883 Hz  
FIDRES 1.105709 Hz  
AQ 0.9043968 sec  
RG 196.07  
DW 13.800 usec  
DE 18.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 150.8852070 MHz  
NUC1 13C  
P1 9.90 usec  
PLW1 80.09999847 W  
SF02 600.0024000 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 35.00000000 W  
PLW12 0.74861997 W  
PLW13 0.37595001 W

F2 - Processing parameters  
SI 32768  
SF 150.8701586 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





COSY  
142221  
BAB0113\_1  
Batizi Benedek  
2023.11.27. (KP)

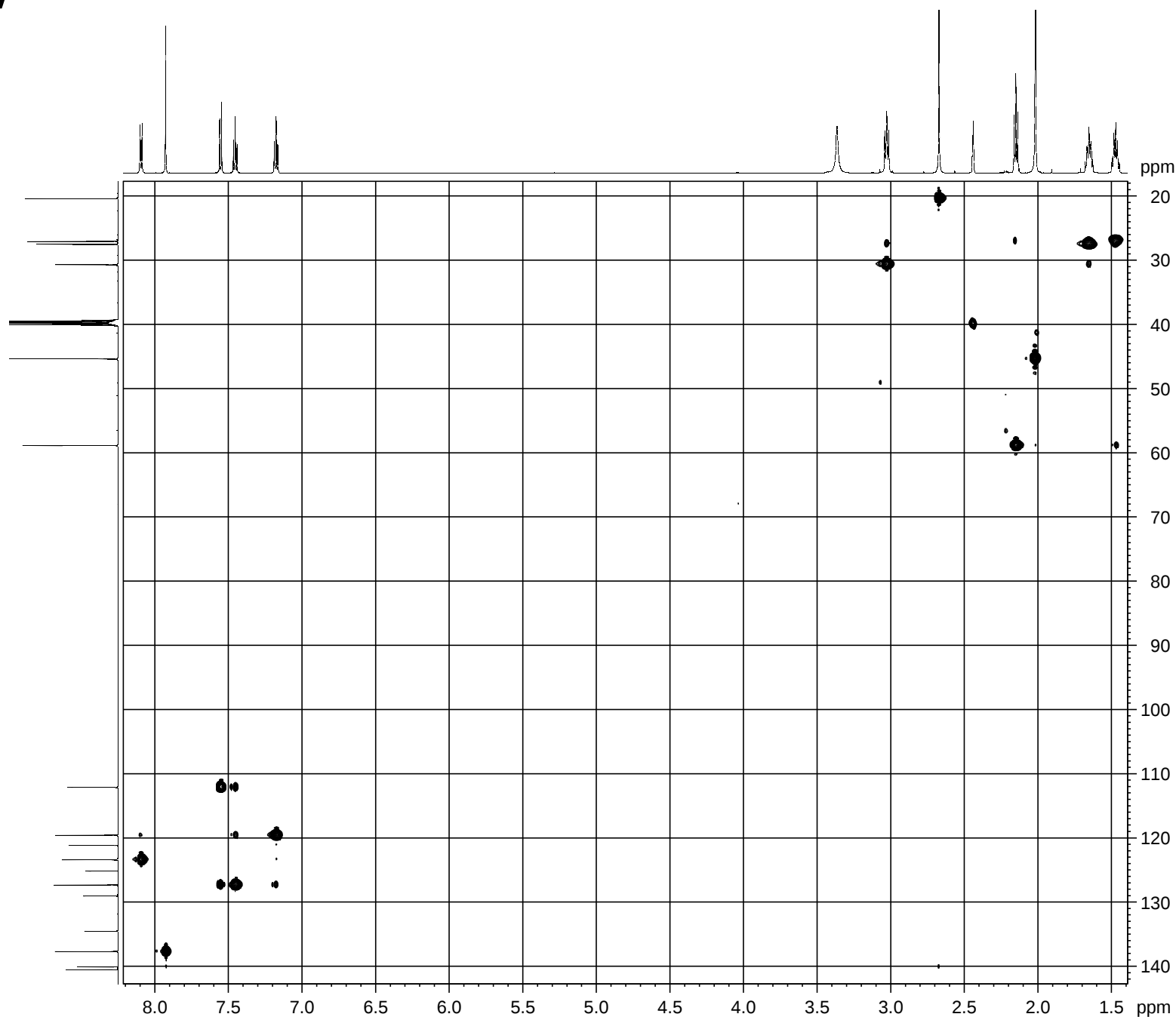
Current Data Parameters  
NAME 142221  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231127  
Time 18.08 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG cosygpmfqr  
TD 2048  
SOLVENT DMSO  
NS 2  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
D0 0.00000300 sec  
D1 2.00000000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00012800 sec  
TDav 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 16.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 12.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 600.0036 MHz  
FIDRES 61.035156 Hz  
SW 13.021 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 600.0000420 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 600.0000420 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



HSQC (140Hz)  
142221  
BAB0113\_1  
Batizi Benedek  
2023.11.27. (KP)

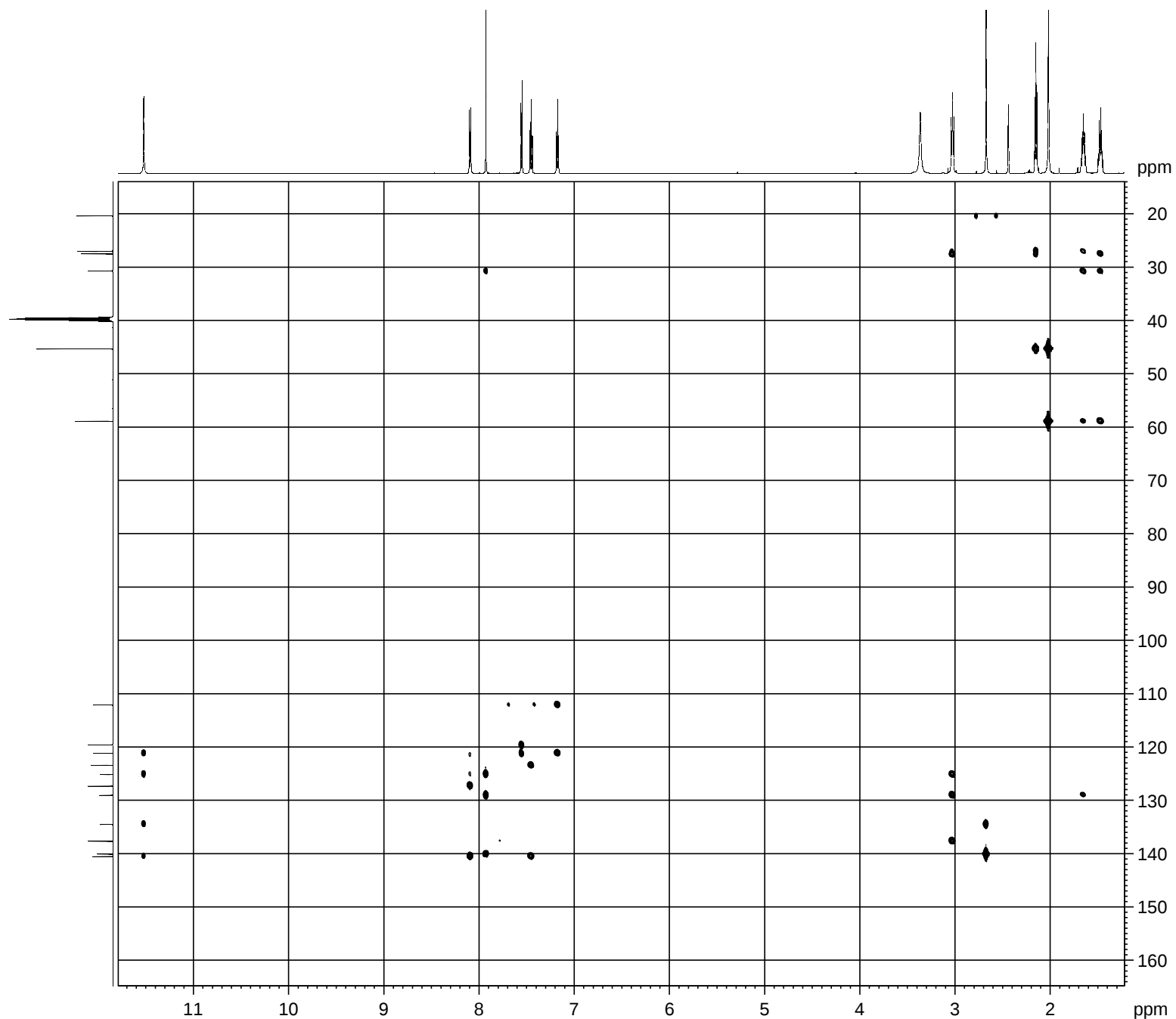
Current Data Parameters  
NAME 142221  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231127  
Time 18.29 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hsqcetgpsisp2.2  
TD 2048  
SOLVENT DMSO  
NS 4  
DS 32  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST17 -0.5000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D4 0.00178571 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
P28 0 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
CPDPRG2 bi\_p5m4sp\_4sp.2  
P3 9.90 usec  
P14 500.00 usec  
P24 2000.00 usec  
P63 1500.00 usec  
PLW0 0 W  
PLW2 80.09999847 W  
PLW12 2.59520006 W  
SPNAM[3] Crp60, 0.5, 20.1  
SPOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 11.99499989 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 11.99499989 W  
SPNAM[14] Crp42, 1.5, 20.2  
SPOAL14 0.500  
SPOFFS14 0 Hz  
SPW14 6.71710014 W  
SPNAM[31] Crp42, 1.5, 20.2  
SPOAL31 0.500  
SPOFFS31 0 Hz  
SPW31 1.67929995 W  
GPNAM[1] SMSQ10.100  
GPZ1 80.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 20.10 %  
GPNAM[3] SMSQ10.100  
GPZ3 11.00 %  
GPNAM[4] SMSQ10.100  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 600.0000420 MHz  
WDW QSINE





HMBC (8Hz, 140Hz)  
142221  
BAB0113\_1  
Batizi Benedek  
2023.11.27. (KP)

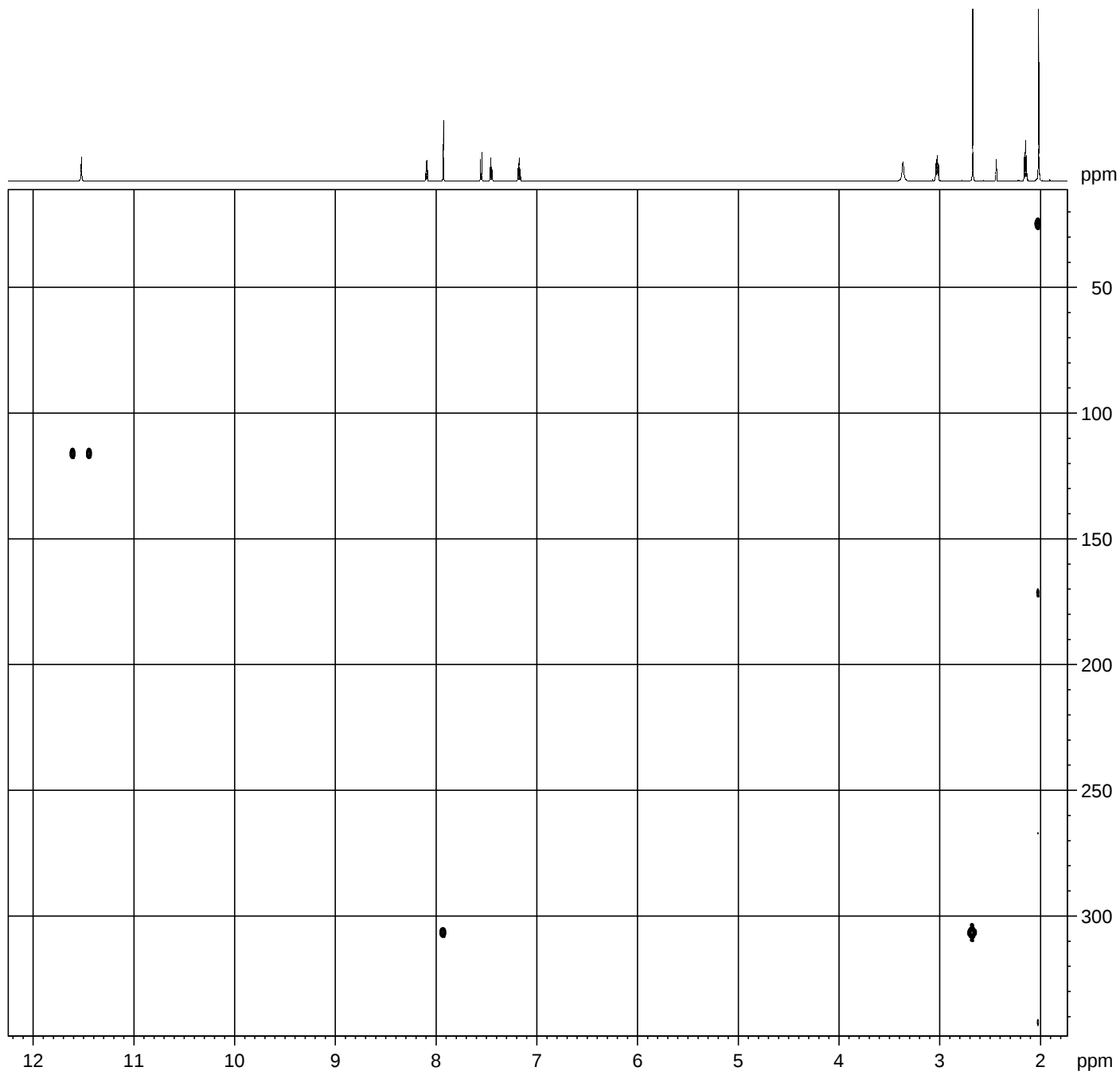
Current Data Parameters  
NAME 142221  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231127  
Time 18.58 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgp1pndqf  
TD 2048  
SOLVENT DMSO  
NS 4  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D2 0.00357143 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00001510 sec  
TDav 1  
SF01 600.0037800 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
P3 9.90 usec  
PLW2 80.09999847 W  
GPNAM[1] SMSQ10.100  
GPZ1 50.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.10 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE QF

F2 - Processing parameters  
SI 2048  
SF 600.000420 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 150.8701586 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



NHMB  
142221  
BAB0113\_1  
Batizi Benedek  
2023.11.27. (KP)

Current Data Parameters  
NAME 142221  
EXPNO 16  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231127  
Time 19.31 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgpndqf  
TD 2048  
SOLVENT DMSO  
NS 16  
DS 16  
SWH 9615.385 Hz  
FIDRES 9.390024 Hz  
AQ 0.1064960 sec  
RG 196.07  
DW 52.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST13 5.0000000  
D0 0.0000000 sec  
D1 2.0000000 sec  
D6 0.1000000 sec  
D16 0.0002000 sec  
IN0 0.0002060 sec  
TDav 1  
SF01 600.0045600 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.0000000 W  
SF02 60.8096315 MHz  
NUC2 15N  
P3 14.60 usec  
PLW2 236.0000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 70.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 50.10 %  
P16 1000.00 usec

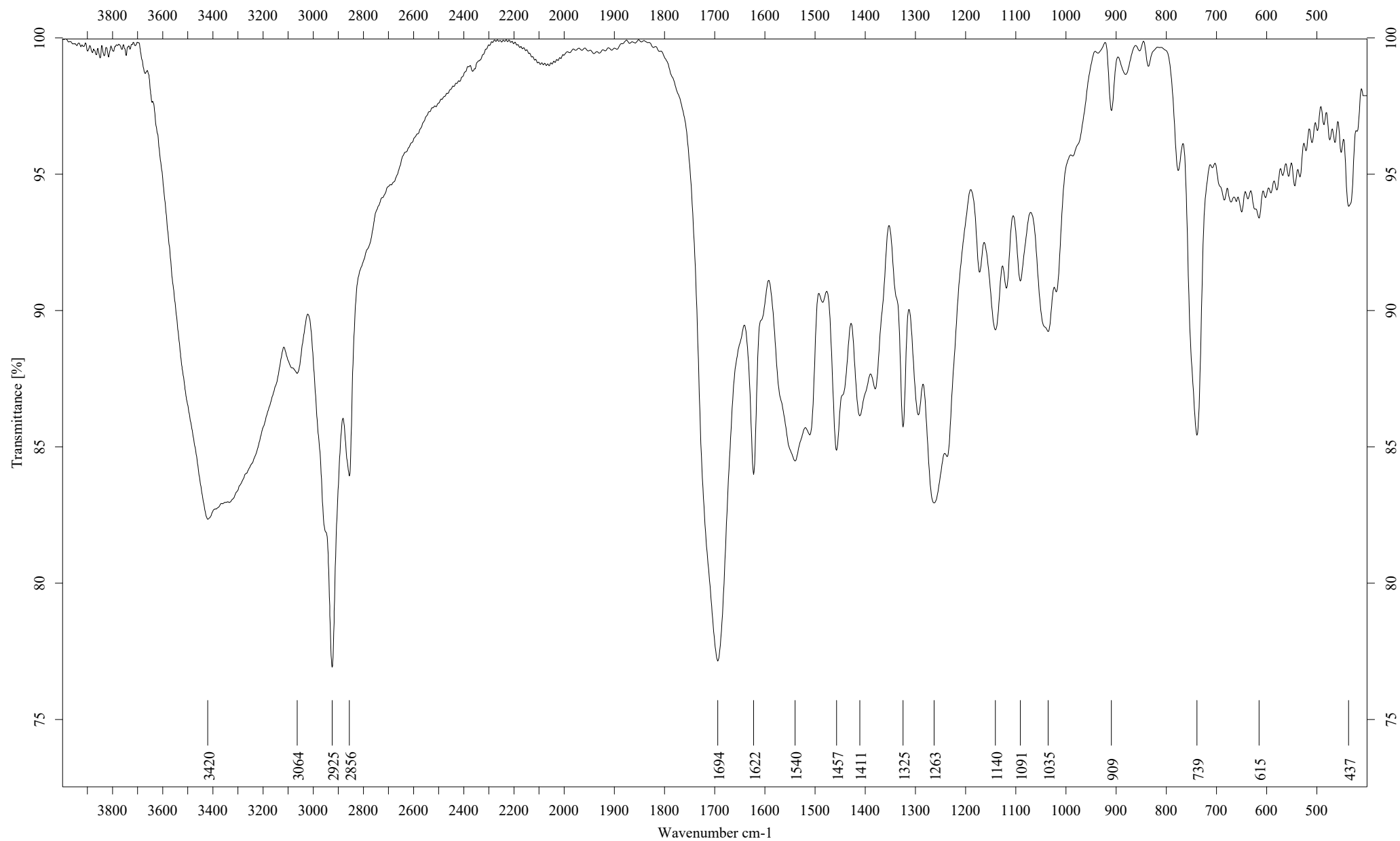
F1 - Acquisition parameters  
TD 128  
SF01 60.80963 MHz  
FIDRES 379.247559 Hz  
SW 399.145 ppm  
FnMODE QF

F2 - Processing parameters  
SI 2048  
SF 600.0000420 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 60.7974720 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

|               |          |
|---------------|----------|
| Pollak Patrik | KP       |
| KBr           | 1/3/2024 |

|                     |
|---------------------|
| BRUKER Alpha        |
| Resolution: 2 cm-1  |
| Number of Scans: 16 |



—11.582

8.096  
8.083  
7.995  
7.625  
7.612  
7.543  
7.531  
7.518  
7.262  
7.249  
7.237  
7.102  
7.093  
7.084  
6.768

3.960  
3.949  
3.937  
3.925  
3.367  
3.120  
3.107  
3.095  
3.022  
3.011  
2.729  
2.507  
1.913  
1.730  
1.718  
1.706  
1.559  
1.547  
1.534  
1.224  
1.129  
1.117  
1.105  
0.851

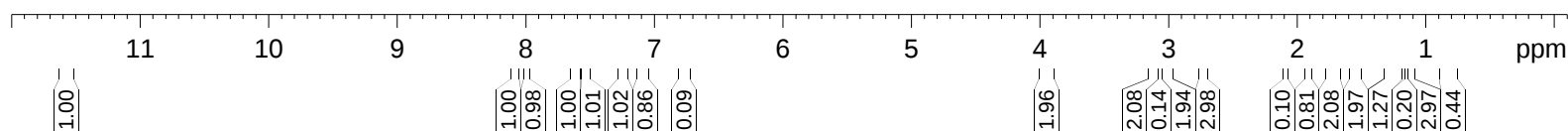
—0.000

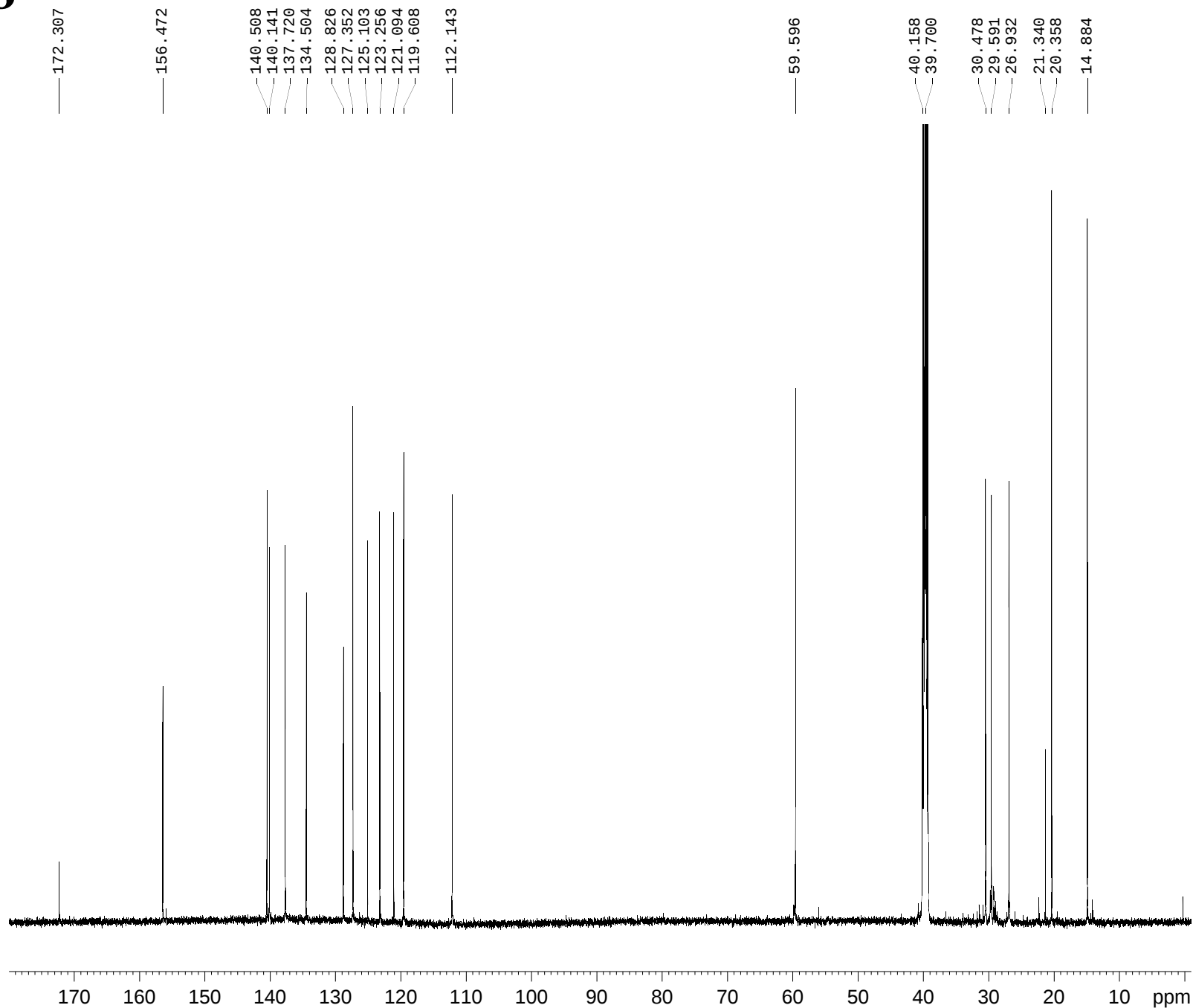
Standard 1H  
142318  
BAB0122\_1  
Pollak Patrik  
2024.01.03. (KP)

Current Data Parameters  
NAME 142318  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240103  
Time 19.41 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 2.7262976 sec  
RG 196.07  
DW 41.600 usec  
DE 25.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 600.0037050 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W

F2 - Processing parameters  
SI 65536  
SF 600.0000022 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





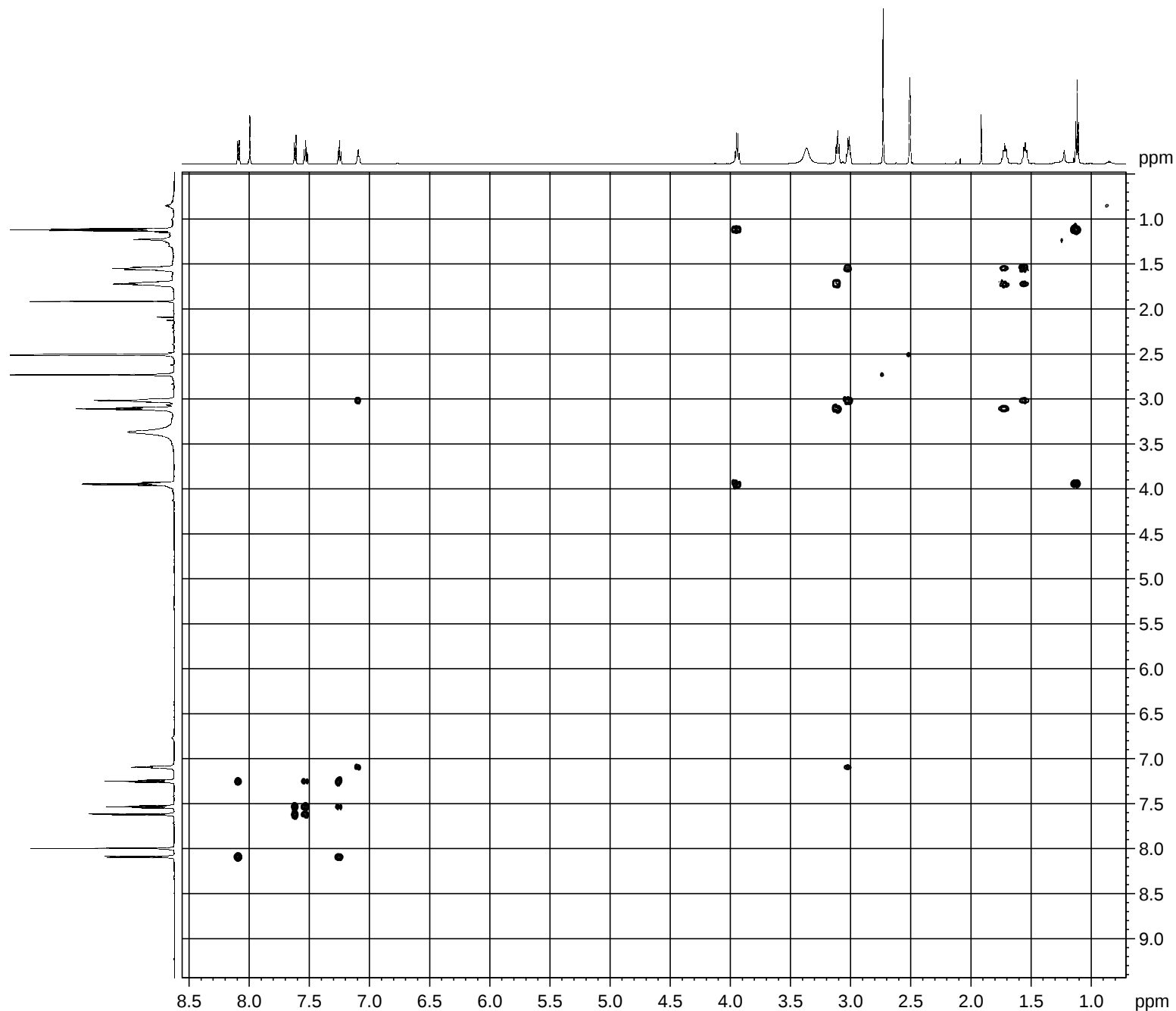
Standard 13C  
142318  
BAB0122\_1  
Pollak Patrik  
2024.01.03. (KP)

Current Data Parameters  
NAME 142318  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240103  
Time 20.49 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 2048  
DS 4  
SWH 36231.883 Hz  
FIDRES 1.105709 Hz  
AQ 0.9043968 sec  
RG 196.07  
DW 13.800 usec  
DE 18.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 150.8852070 MHz  
NUC1 13C  
P1 9.90 usec  
PLW1 80.09999847 W  
SF02 600.0024000 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 35.00000000 W  
PLW12 0.74861997 W  
PLW13 0.37595001 W

F2 - Processing parameters  
SI 32768  
SF 150.8701591 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





COSY  
142318  
BAB0122\_1  
Pollak Patrik  
2024.01.03. (KP)

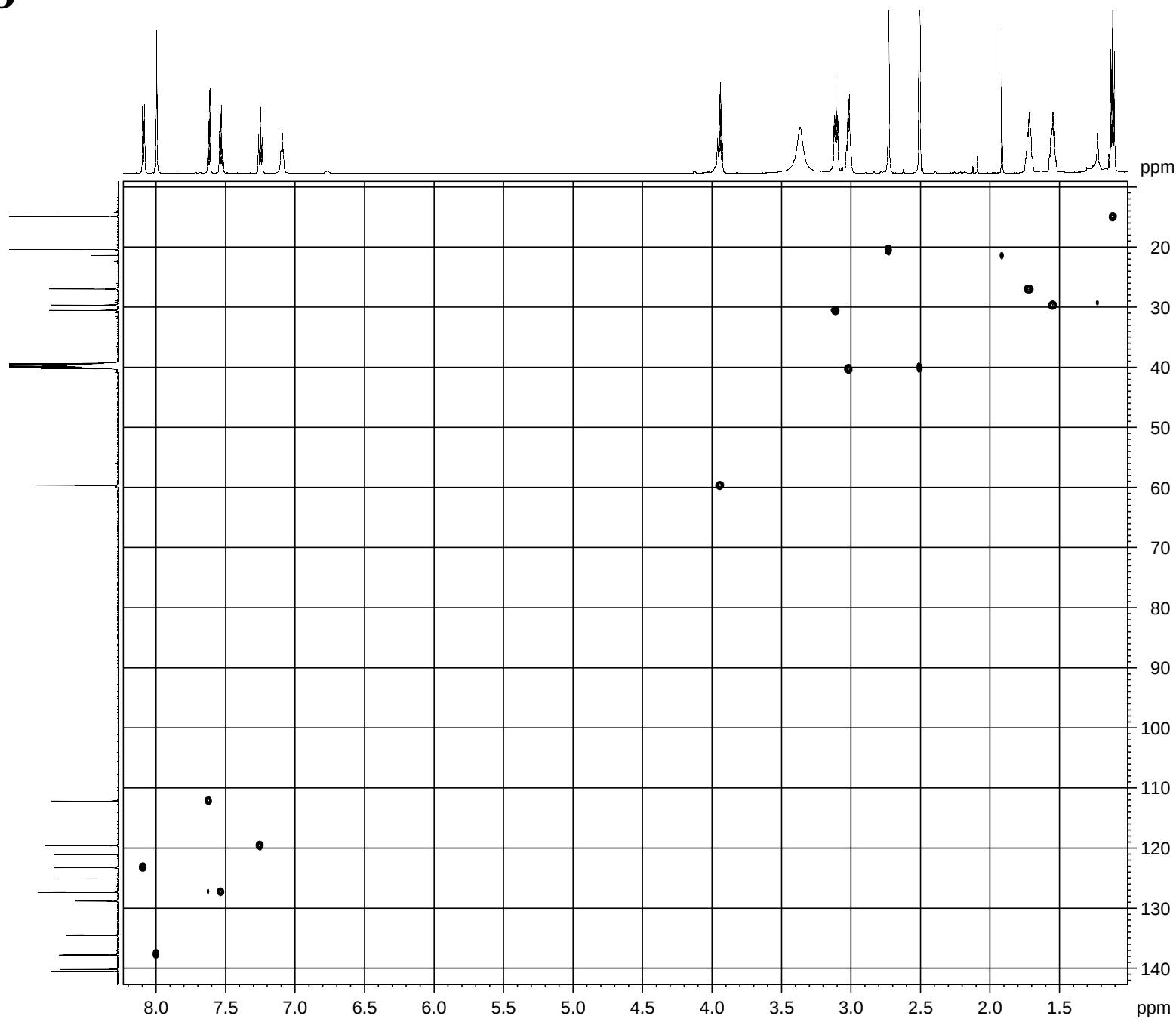
Current Data Parameters  
NAME 142318  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240103  
Time 20.51 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG cosygpmfqr  
TD 2048  
SOLVENT DMSO  
NS 2  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
D0 0.00000300 sec  
D1 2.00000000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00012800 sec  
TDav 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 16.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 12.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 600.0036 MHz  
FIDRES 61.035156 Hz  
SW 13.021 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 600.0000022 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 600.0000022 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



HSQC (140Hz)  
142318  
BAB0122\_1  
Pollak Patrik  
2024.01.03. (KP)

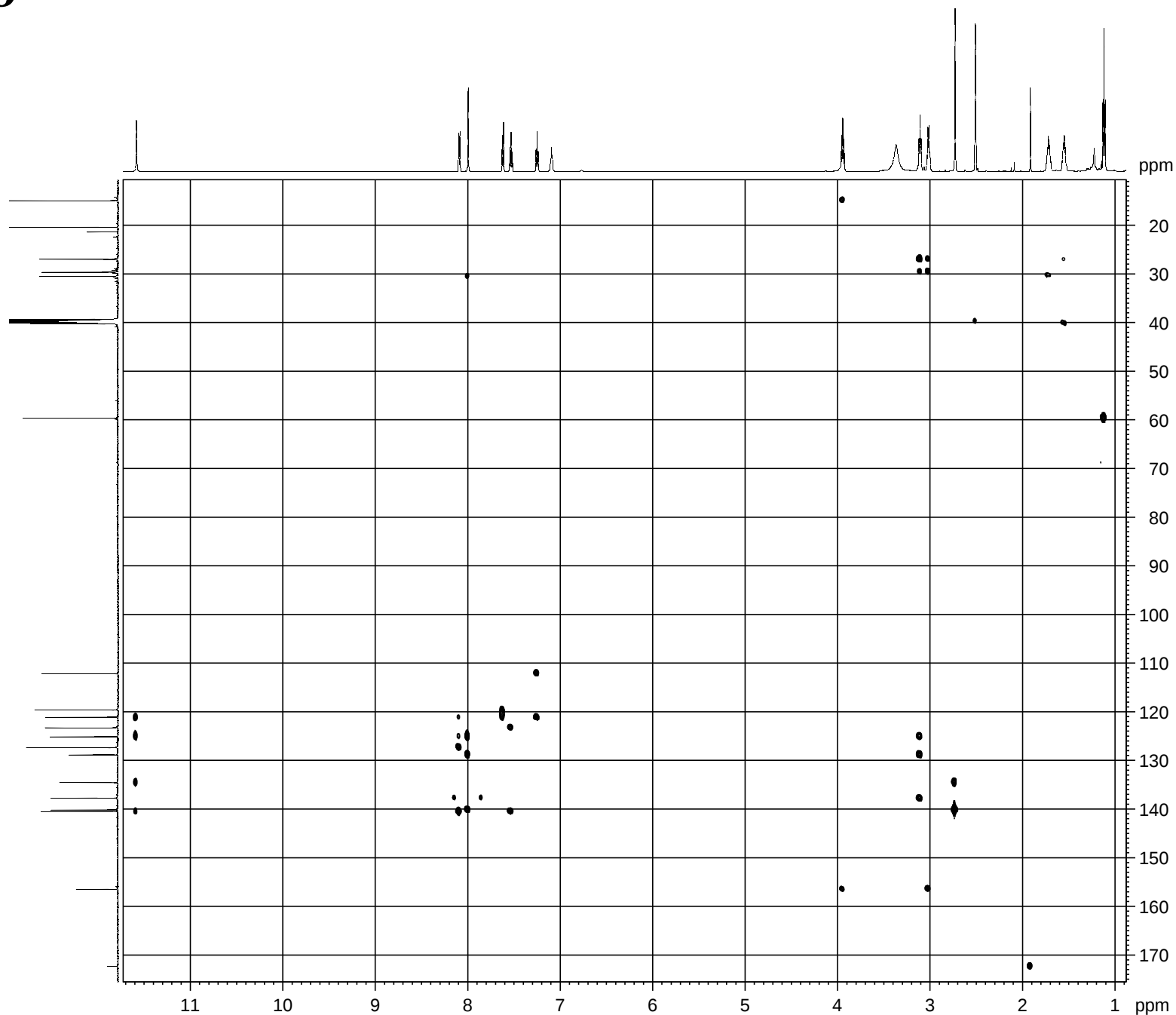
Current Data Parameters  
NAME 142318  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240103  
Time 21.11 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hsqcetgpsisp2.2  
TD 2048  
SOLVENT DMSO  
NS 4  
DS 32  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST17 -0.5000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D4 0.00178571 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.00001510 sec  
Tдав 1  
SF01 600.0036000 MHz  
NUC1  $^1\text{H}$   
P1 11.50 usec  
P2 23.00 usec  
P28 0 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2  $^{13}\text{C}$   
CPDPRG2 bi\_p5m4sp\_4sp.2  
P3 9.90 usec  
P14 500.00 usec  
P24 2000.00 usec  
P63 1500.00 usec  
PLW0 0 W  
PLW2 80.09999847 W  
PLW12 2.59520006 W  
SPNAM[3] Crp60, 0.5, 20.1  
SPOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 11.99499989 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 11.99499989 W  
SPNAM[14] Crp42, 1.5, 20.2  
SPOAL14 0.500  
SPOFFS14 0 Hz  
SPW14 6.71710014 W  
SPNAM[31] Crp42, 1.5, 20.2  
SPOAL31 0.500  
SPOFFS31 0 Hz  
SPW31 1.67929995 W  
GPNAM[1] SMSQ10.100  
GPZ1 80.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 20.10 %  
GPNAM[3] SMSQ10.100  
GPZ3 11.00 %  
GPNAM[4] SMSQ10.100  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 600.000022 MHz  
WDW QSINE





HMBC (8Hz, 140Hz)  
142318  
BAB0122\_1  
Pollak Patrik  
2024.01.03. (KP)

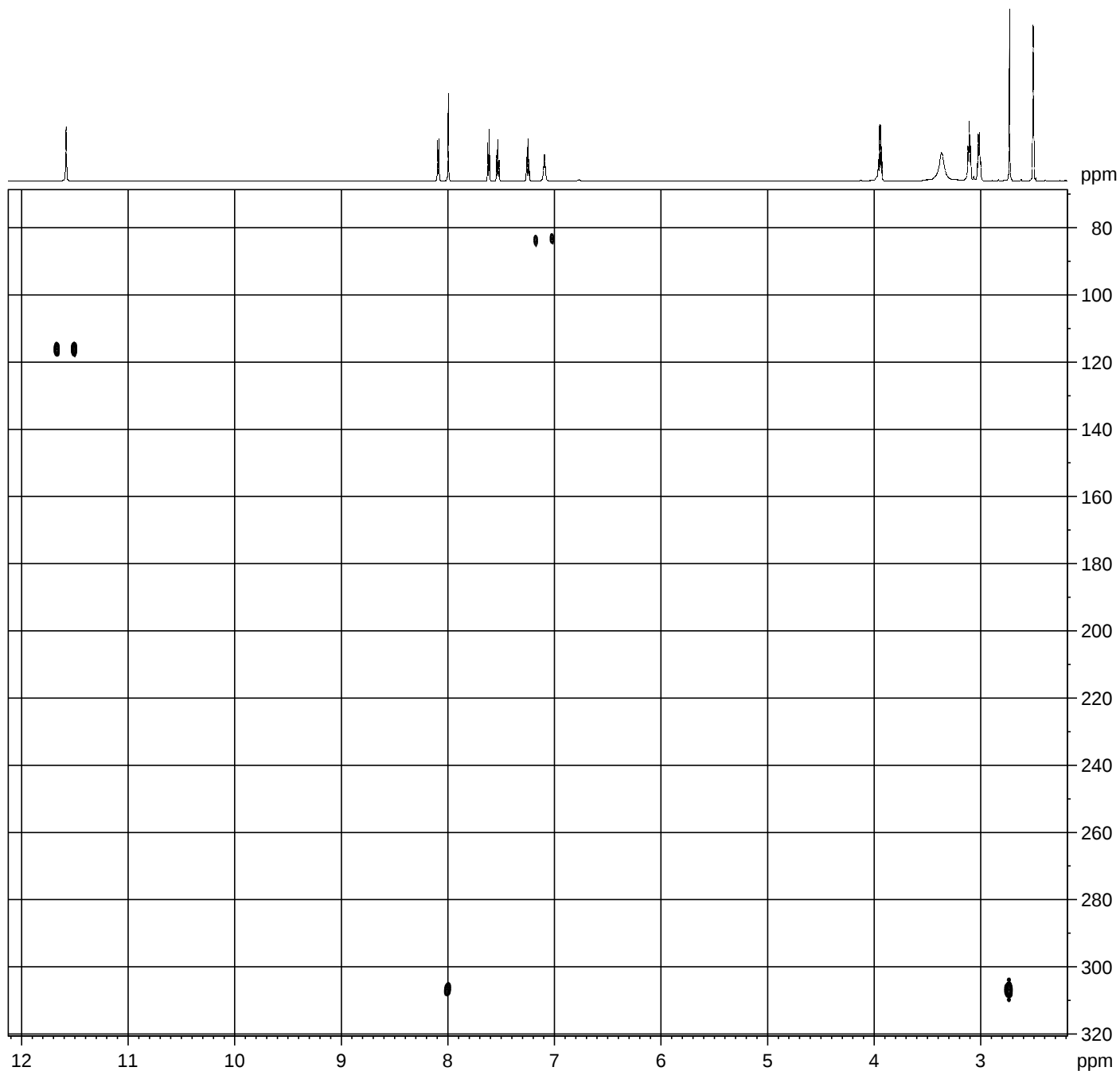
Current Data Parameters  
NAME 142318  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240103  
Time 21.41 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgp1pndqf  
TD 2048  
SOLVENT DMSO  
NS 4  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D2 0.00357143 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0037800 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
P3 9.90 usec  
PLW2 80.09999847 W  
GPNAM[1] SMSQ10.100  
GPZ1 50.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.10 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE QF

F2 - Processing parameters  
SI 2048  
SF 600.0000022 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 150.8701591 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



NHMCB  
142318  
BAB0122\_1  
Pollak Patrik  
2024.01.03. (KP)

Current Data Parameters  
NAME 142318  
EXPNO 16  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240103  
Time 22.13 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgpndqf  
TD 2048  
SOLVENT DMSO  
NS 8  
DS 16  
SWH 9615.385 Hz  
FIDRES 9.390024 Hz  
AQ 0.1064960 sec  
RG 196.07  
DW 52.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST13 5.0000000  
D0 0.00000300 sec  
D1 2.00000000 sec  
D6 0.10000000 sec  
D16 0.00020000 sec  
IN0 0.00002060 sec  
TDav 1  
SF01 600.0045600 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.00000000 W  
SF02 60.8096315 MHz  
NUC2 15N  
P3 14.60 usec  
PLW2 236.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 70.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 50.10 %  
P16 1000.00 usec

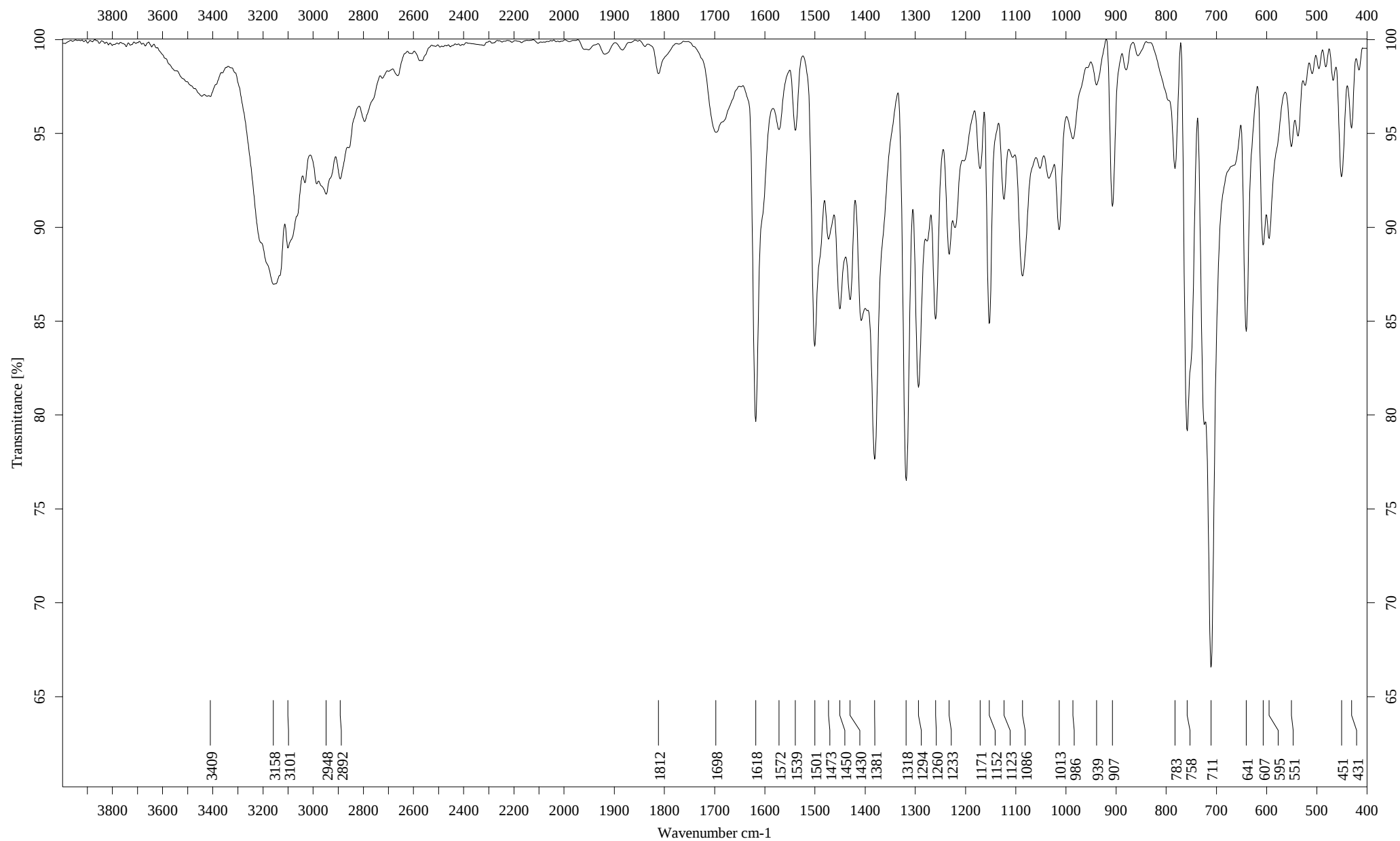
F1 - Acquisition parameters  
TD 128  
SF01 60.80963 MHz  
FIDRES 379.247559 Hz  
SW 399.145 ppm  
FnMODE QF

F2 - Processing parameters  
SI 2048  
SF 600.0000022 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 60.7974720 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

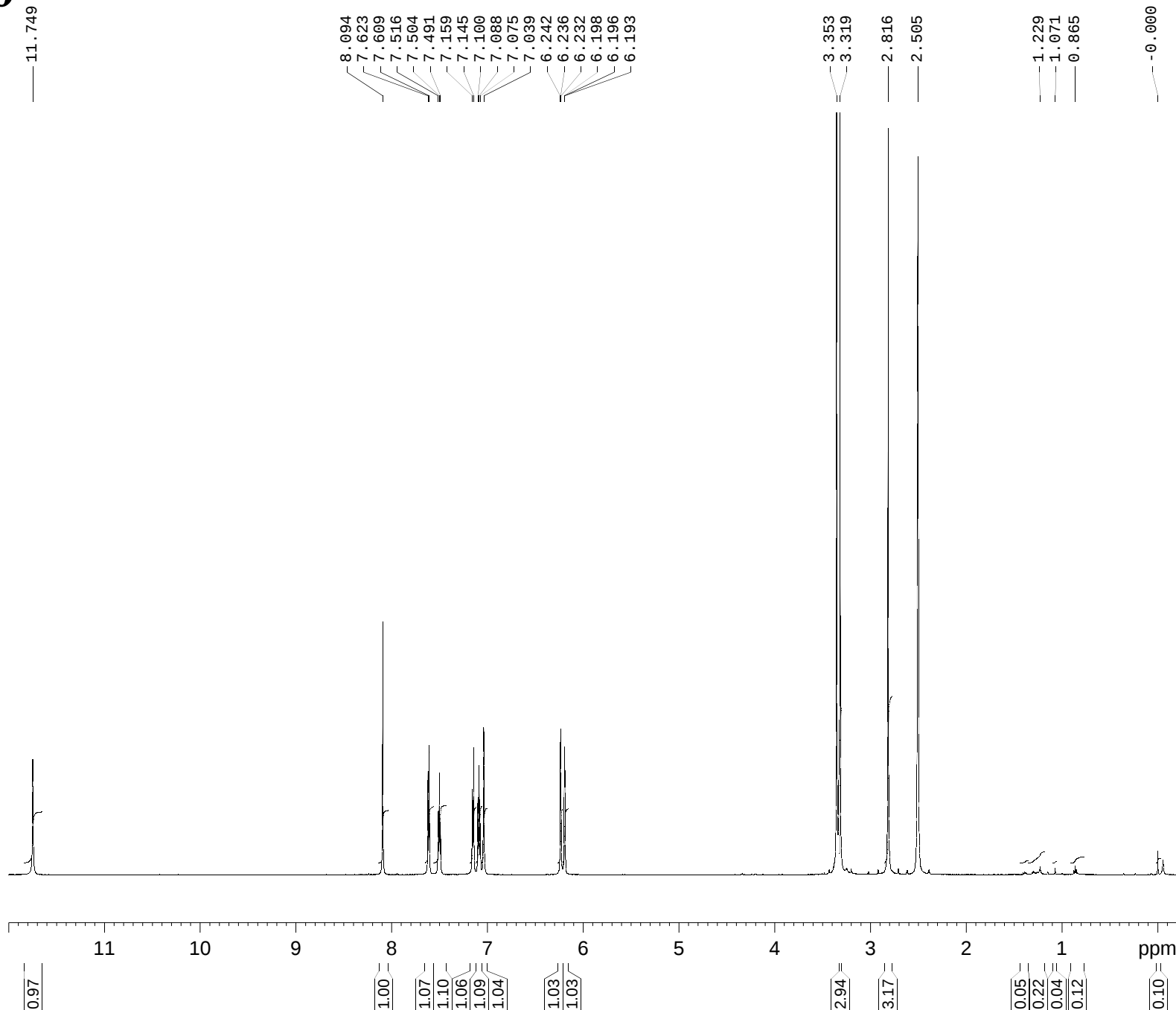
|               |             |
|---------------|-------------|
| Pollak Patrik | KP          |
| KBr           | 2023.03.08. |

|                     |
|---------------------|
| BRUKER Alpha        |
| Resolution: 2 cm-1  |
| Number of Scans: 16 |



30

11.749



Standard 1H  
140723  
BAB0035\_1  
Pollak Patrik  
2023.03.06. (DA)

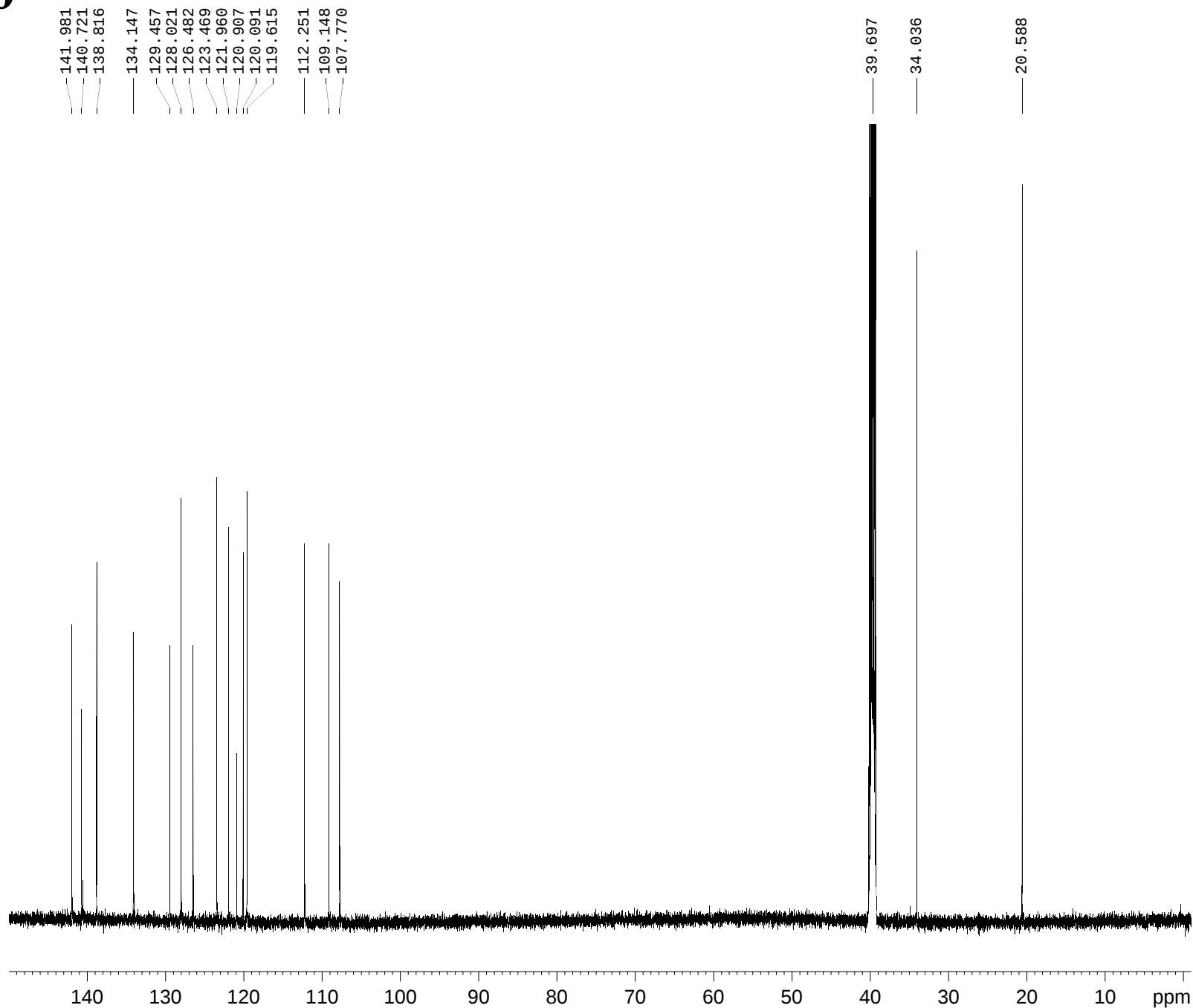
Current Data Parameters  
NAME 140723  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230307  
Time 2.58 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 2.7262976 sec  
RG 196.07  
DW 41.600 usec  
DE 25.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 600.0537053 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W

F2 - Processing parameters  
SI 65536  
SF 600.0500011 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



30



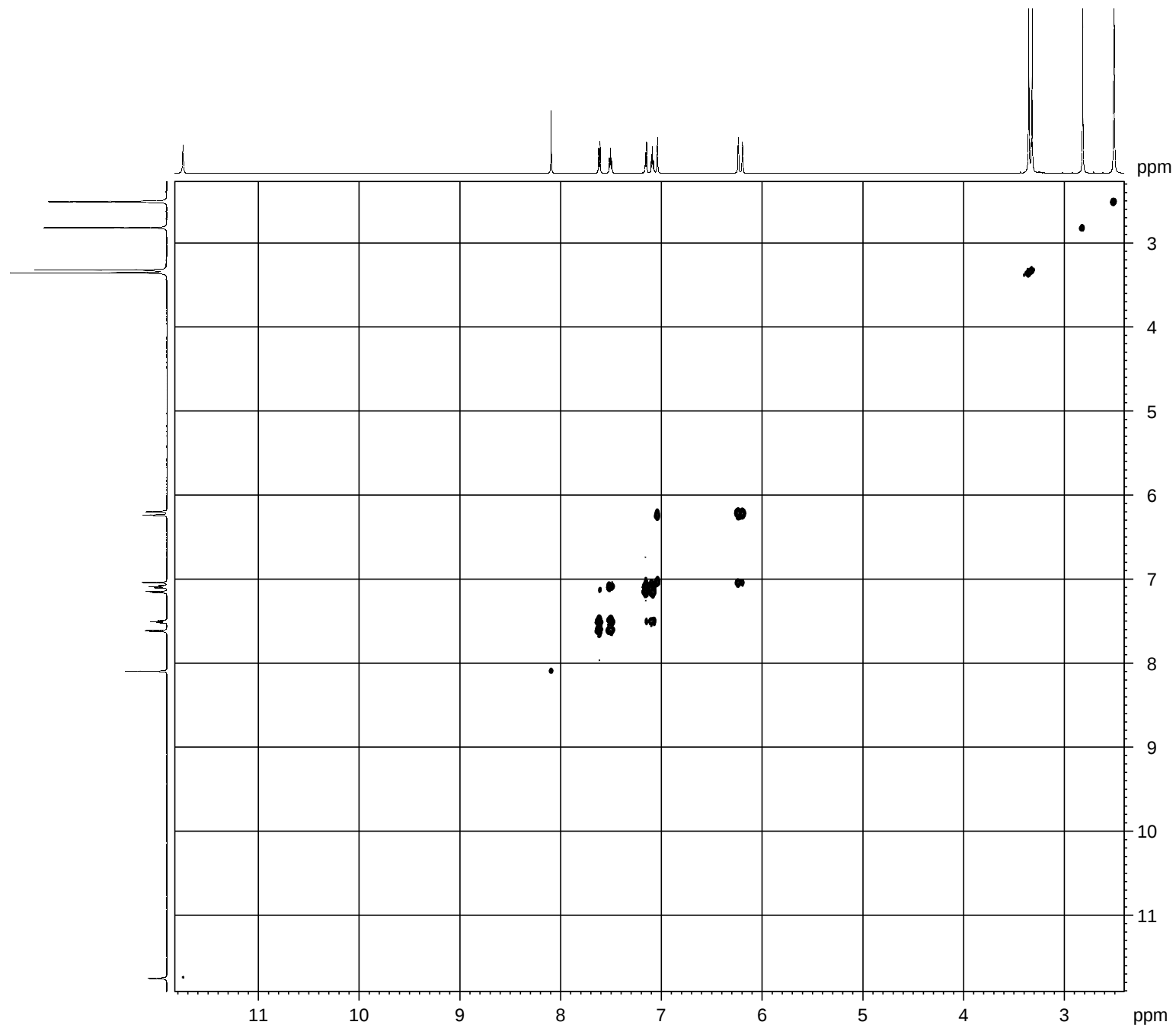
Standard 13C  
140723  
BAB0035\_1  
Pollak Patrik  
2023.03.06. (DA)

Current Data Parameters  
NAME 140723  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230307  
Time 4.10 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 2048  
DS 4  
SWH 36231.883 Hz  
FIDRES 1.105709 Hz  
AQ 0.9043968 sec  
RG 196.07  
DW 13.800 usec  
DE 18.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 150.8977808 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 70.48699951 W  
SF02 600.0524002 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 29.46299934 W  
PLW12 0.66293001 W  
PLW13 0.33292001 W

F2 - Processing parameters  
SI 32768  
SF 150.8827317 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40





COSY  
 140723  
 BAB0035\_1  
 Pollak Patrik  
 2023.03.06. (DA)

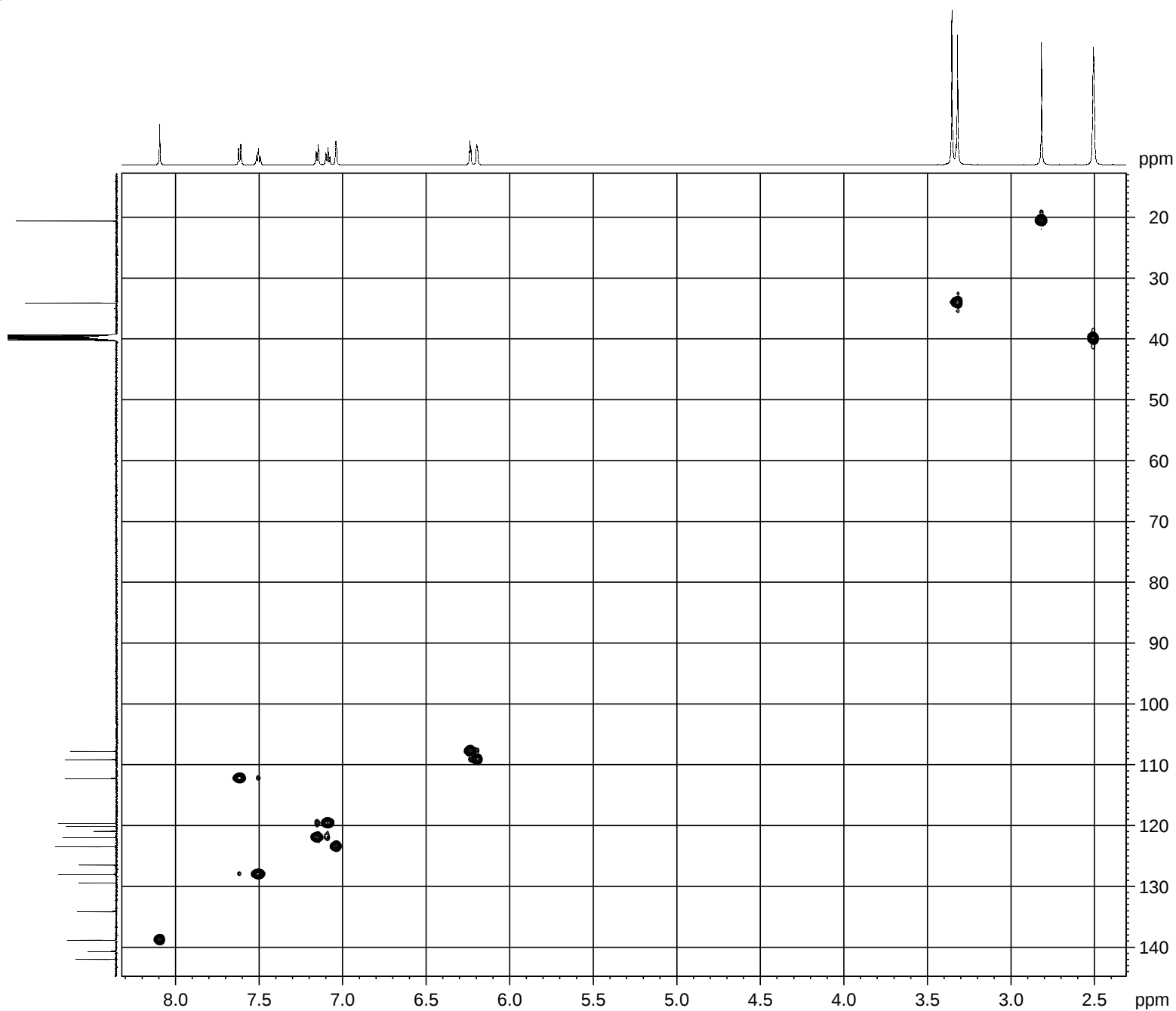
Current Data Parameters  
 NAME 140723  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230307  
 Time 4.23 h  
 INSTRUM spect  
 PROBHD Z145856\_0002 (  
 PULPROG cosygpmfqr  
 TD 2048  
 SOLVENT DMSO  
 NS 2  
 DS 16  
 SWH 7812.500 Hz  
 FIDRES 7.629395 Hz  
 AQ 0.1310720 sec  
 RG 196.07  
 DW 64.000 usec  
 DE 25.00 usec  
 TE 295.0 K  
 D0 0.00000300 sec  
 D1 2.00000000 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 IN0 0.00012800 sec  
 Tdav 1  
 SF01 600.0536003 MHz  
 NUC1 1H  
 P1 11.50 usec  
 PLW1 28.00000000 W  
 GPNAM[1] SMSQ10.100  
 GPZ1 16.00 %  
 GPNAM[2] SMSQ10.100  
 GPZ2 12.00 %  
 GPNAM[3] SMSQ10.100  
 GPZ3 40.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters  
 TD 256  
 SF01 600.0536 MHz  
 FIDRES 61.035156 Hz  
 SW 13.020 ppm  
 FnmODE QF

F2 - Processing parameters  
 SI 1024  
 SF 600.0500000 MHz  
 WDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.40

F1 - Processing parameters  
 SI 1024  
 MC2 QF  
 SF 600.0500000 MHz  
 WDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0



HSQC (140 Hz)  
140723  
BAB0035\_1  
Pollak Patrik  
2023.03.06. (DA)

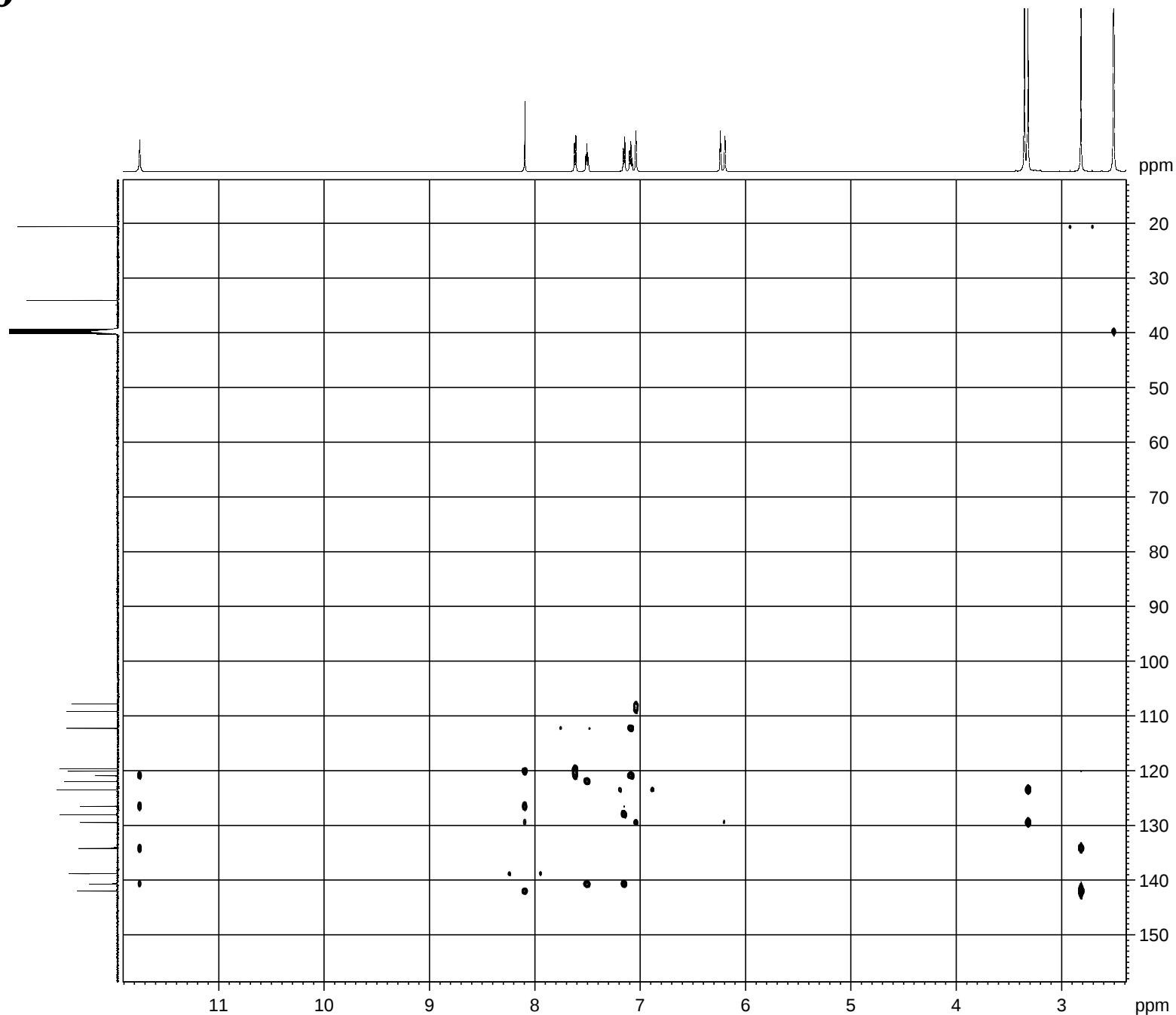
Current Data Parameters  
NAME 140723  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230307  
Time 4.49 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hsqcetgpsisp2.2  
TD 1024  
SOLVENT DMSO  
NS 4  
DS 32  
SWH 7812.500 Hz  
FIDRES 15.258789 Hz  
AQ 0.0655360 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST17 -0.5000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D4 0.00178571 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0537803 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
P28 0 usec  
PLW1 28.00000000 W  
SF02 150.8985352 MHz  
NUC2 13C  
CPDPRG2 bi\_p5m4sp\_4sp.2  
P3 10.00 usec  
P14 500.00 usec  
P24 2000.00 usec  
P63 1500.00 usec  
PLW0 0 W  
PLW2 70.48699951 W  
PLW12 2.33019996 W  
SPNAM[3] Crp60, 0.5, 20.1  
SPOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 10.77000046 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 10.77000046 W  
SPNAM[14] Crp42, 1.5, 20.2  
SPOAL14 0.500  
SPOFFS14 0 Hz  
SPW14 6.03100014 W  
SPNAM[31] Crp42, 1.5, 20.2  
SPOAL31 0.500  
SPOFFS31 0 Hz  
SPW31 1.50779998 W  
GPNAM[1] SMSQ10.100  
GPZ1 80.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 20.10 %  
GPNAM[3] SMSQ10.100  
GPZ3 11.00 %  
GPNAM[4] SMSQ10.100  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8985 MHz  
FIDRES 258.692047 Hz  
SW 219.436 ppm  
FMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 600.0500010 MHz  
WDW QSINE





HMBC (8 Hz, 140 Hz)  
140723  
BAB0035\_1  
Pollak Patrik  
2023.03.06. (DA)

Current Data Parameters  
NAME 140723  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230307  
Time 5.23 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgp1pndqf  
TD 2048  
SOLVENT DMSO  
NS 4  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D2 0.00357143 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0537803 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.00000000 W  
SF02 150.8985352 MHz  
NUC2 13C  
P3 10.00 usec  
PLW2 70.48699951 W  
GPNAM[1] SMSQ10.100  
GPZ1 50.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.10 %  
P16 1000.00 usec

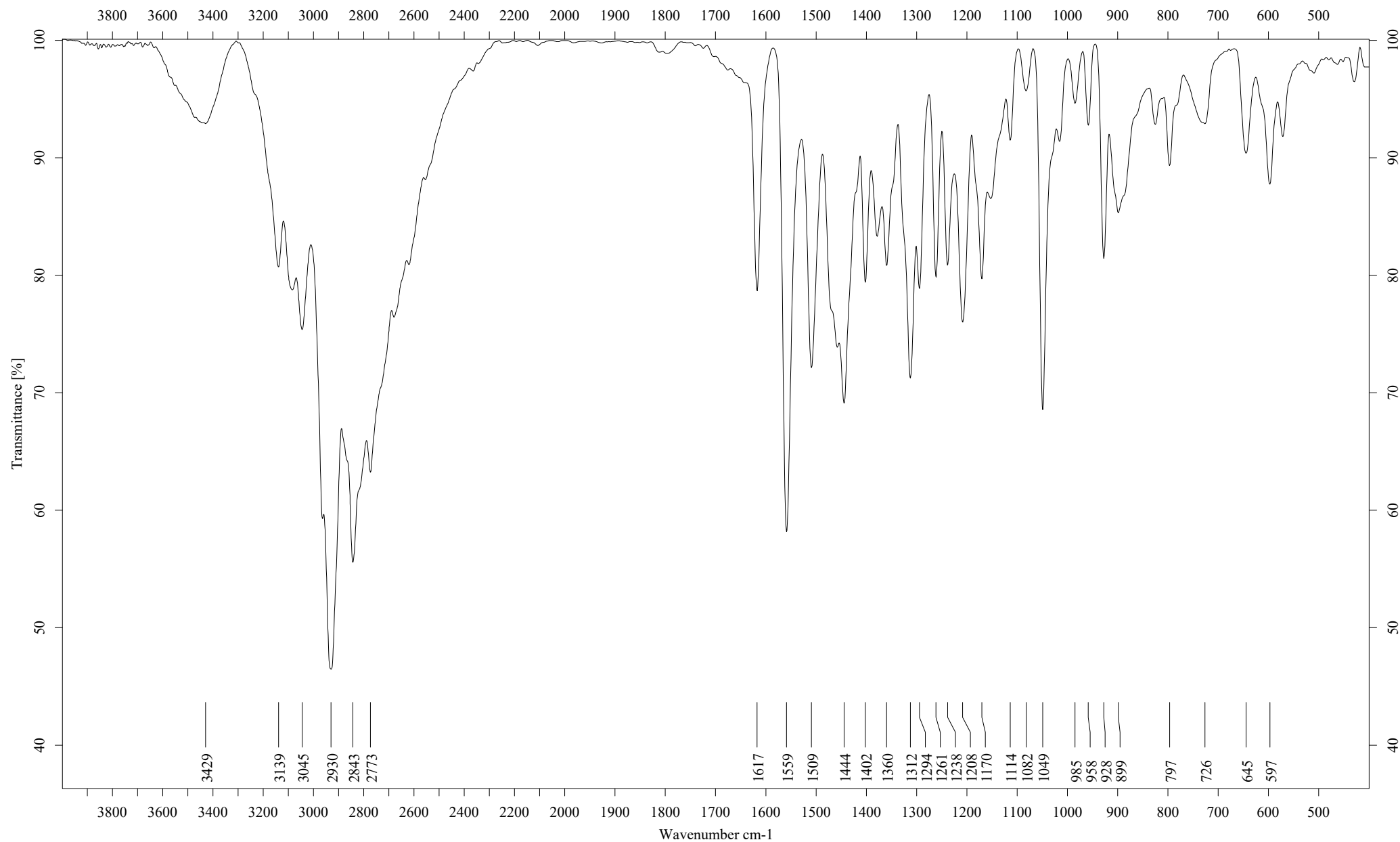
F1 - Acquisition parameters  
TD 256  
SF01 150.8985 MHz  
FIDRES 258.692047 Hz  
SW 219.436 ppm  
FnMODE QF

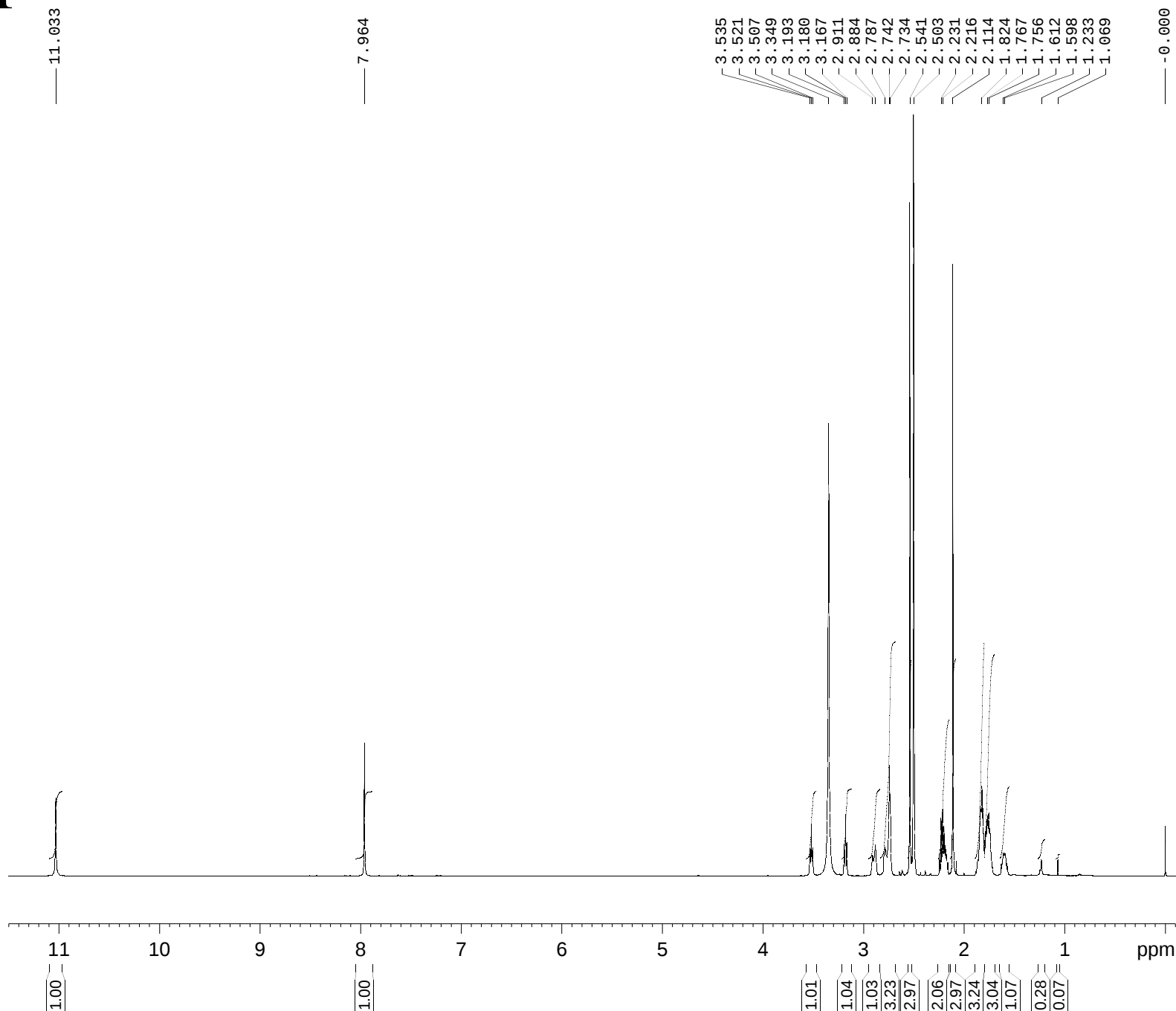
F2 - Processing parameters  
SI 2048  
SF 600.0500010 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 150.8827317 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

|               |           |
|---------------|-----------|
| Pollak Patrik | KP        |
| KBr           | 2/20/2024 |

|                     |
|---------------------|
| BRUKER Alpha        |
| Resolution: 2 cm-1  |
| Number of Scans: 16 |





Standard 1H  
142469  
BAB0141\_1  
Pollak Patrik  
2024.02.20. (KP)

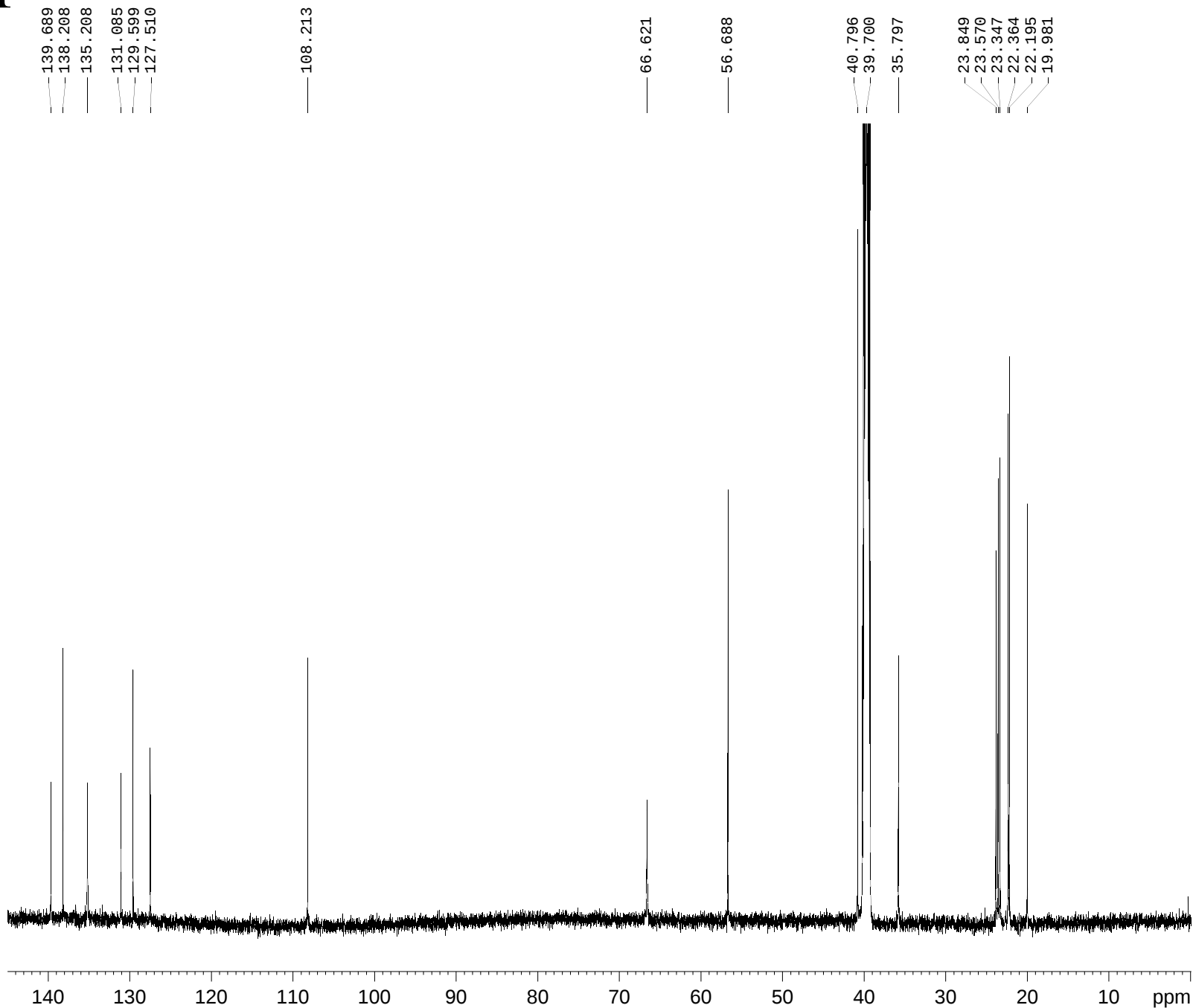
Current Data Parameters  
NAME 142469  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240220  
Time 15.56 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 2.7262976 sec  
RG 196.07  
DW 41.600 usec  
DE 25.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 600.0037050 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W

F2 - Processing parameters  
SI 65536  
SF 600.0000029 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



# 31



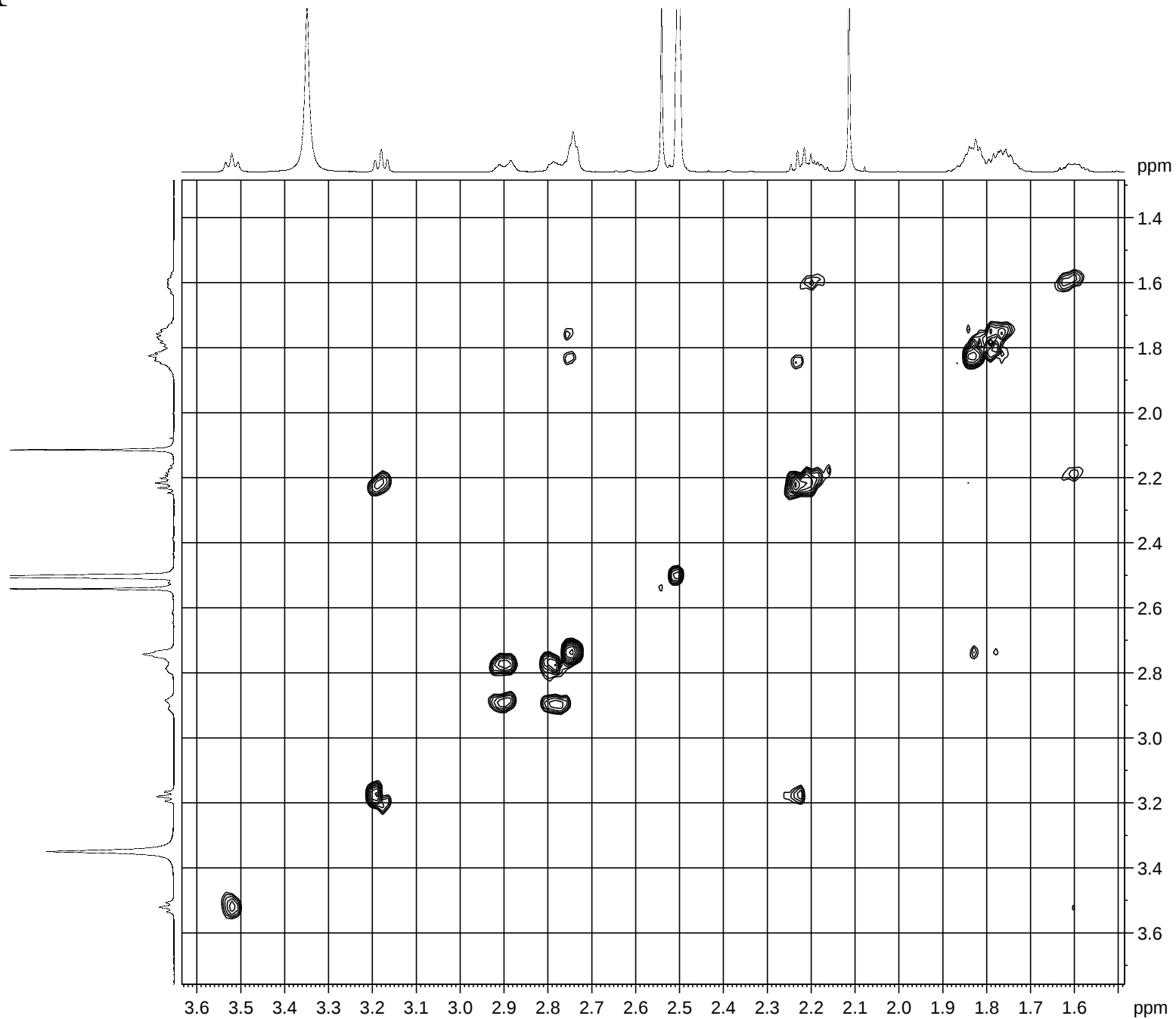
Standard 13C  
142469  
BAB0141\_1  
Pollak Patrik  
2024.02.20. (KP)

Current Data Parameters  
NAME 142469  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240220  
Time 17.05 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 2048  
DS 4  
SWH 36231.883 Hz  
FIDRES 1.105709 Hz  
AQ 0.9043968 sec  
RG 196.07  
DW 13.800 usec  
DE 18.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 150.8852070 MHz  
NUC1 13C  
P1 9.90 usec  
PLW1 71.00000000 W  
SF02 600.0024000 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 32.90000153 W  
PLW12 0.70370001 W  
PLW13 0.35339001 W

F2 - Processing parameters  
SI 32768  
SF 150.8701596 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





COSY  
 142469  
 BAB0141\_1  
 Pollak Patrik  
 2024.02.20. (KP)

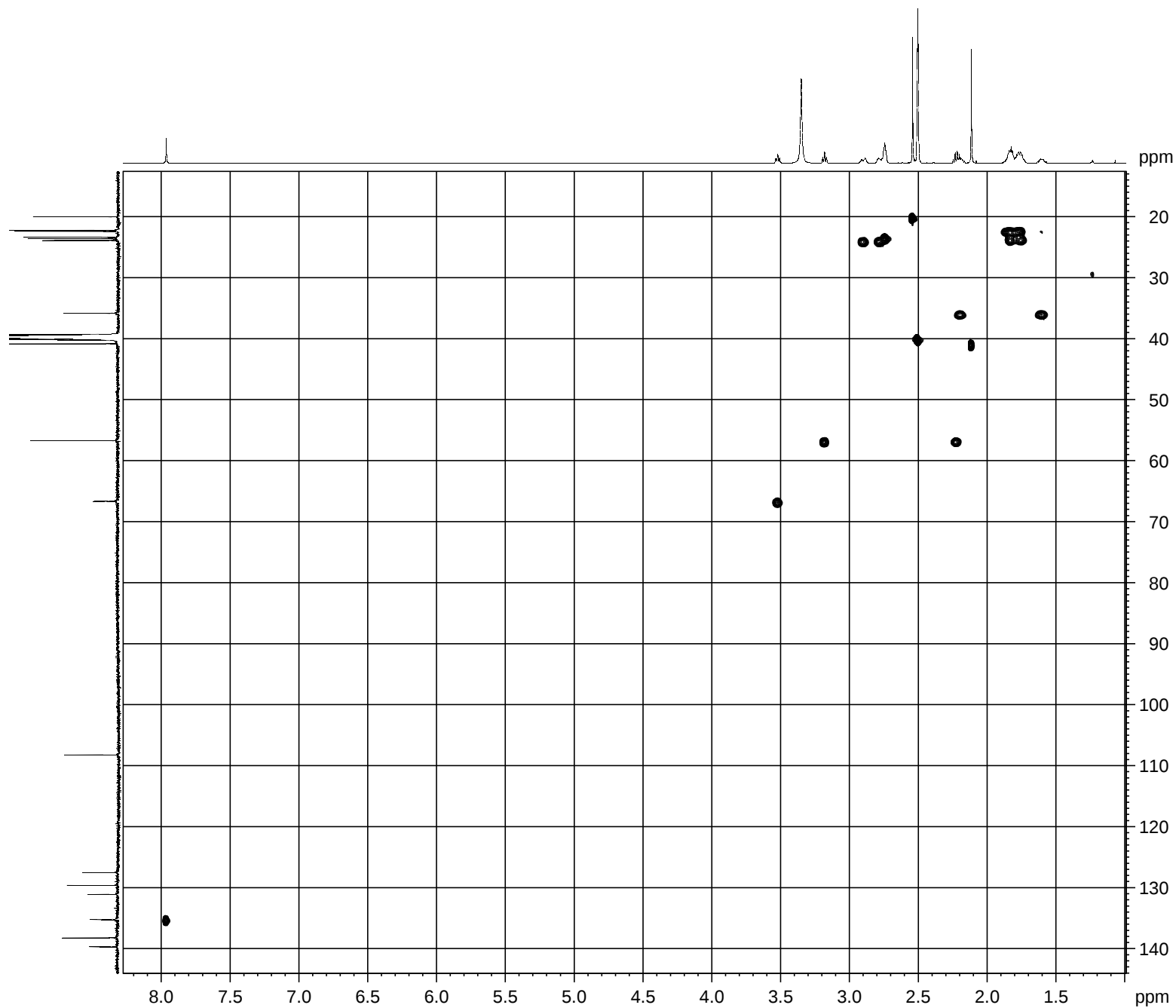
Current Data Parameters  
 NAME 142469  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20240220  
 Time 17.07 h  
 INSTRUM spect  
 PROBHD Z145856\_0002 ( )  
 PULPROG cosygpmfqr  
 TD 2048  
 SOLVENT DMSO  
 NS 2  
 DS 16  
 SWH 7812.500 Hz  
 FIDRES 7.629395 Hz  
 AQ 0.1310720 sec  
 RG 196.07  
 DW 64.000 usec  
 DE 25.00 usec  
 TE 295.0 K  
 D0 0.00000300 sec  
 D1 2.00000000 sec  
 D13 0.00000400 sec  
 D16 0.00020000 sec  
 IN0 0.00012800 sec  
 TDav 1  
 SF01 600.0036000 MHz  
 NUC1 1H  
 P1 11.50 usec  
 PLW1 28.00000000 W  
 GPNAM[1] SMSQ10.100  
 GPZ1 16.00 %  
 GPNAM[2] SMSQ10.100  
 GPZ2 12.00 %  
 GPNAM[3] SMSQ10.100  
 GPZ3 40.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters  
 TD 256  
 SF01 600.0036 MHz  
 FIDRES 61.035156 Hz  
 SW 13.021 ppm  
 FnmODE QF

F2 - Processing parameters  
 SI 1024  
 SF 600.0000029 MHz  
 WDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.40

F1 - Processing parameters  
 SI 1024  
 MC2 QF  
 SF 600.0000029 MHz  
 WDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0



HSQC (140Hz)  
142469  
BAB0141\_1  
Pollak Patrik  
2024.02.20. (KP)

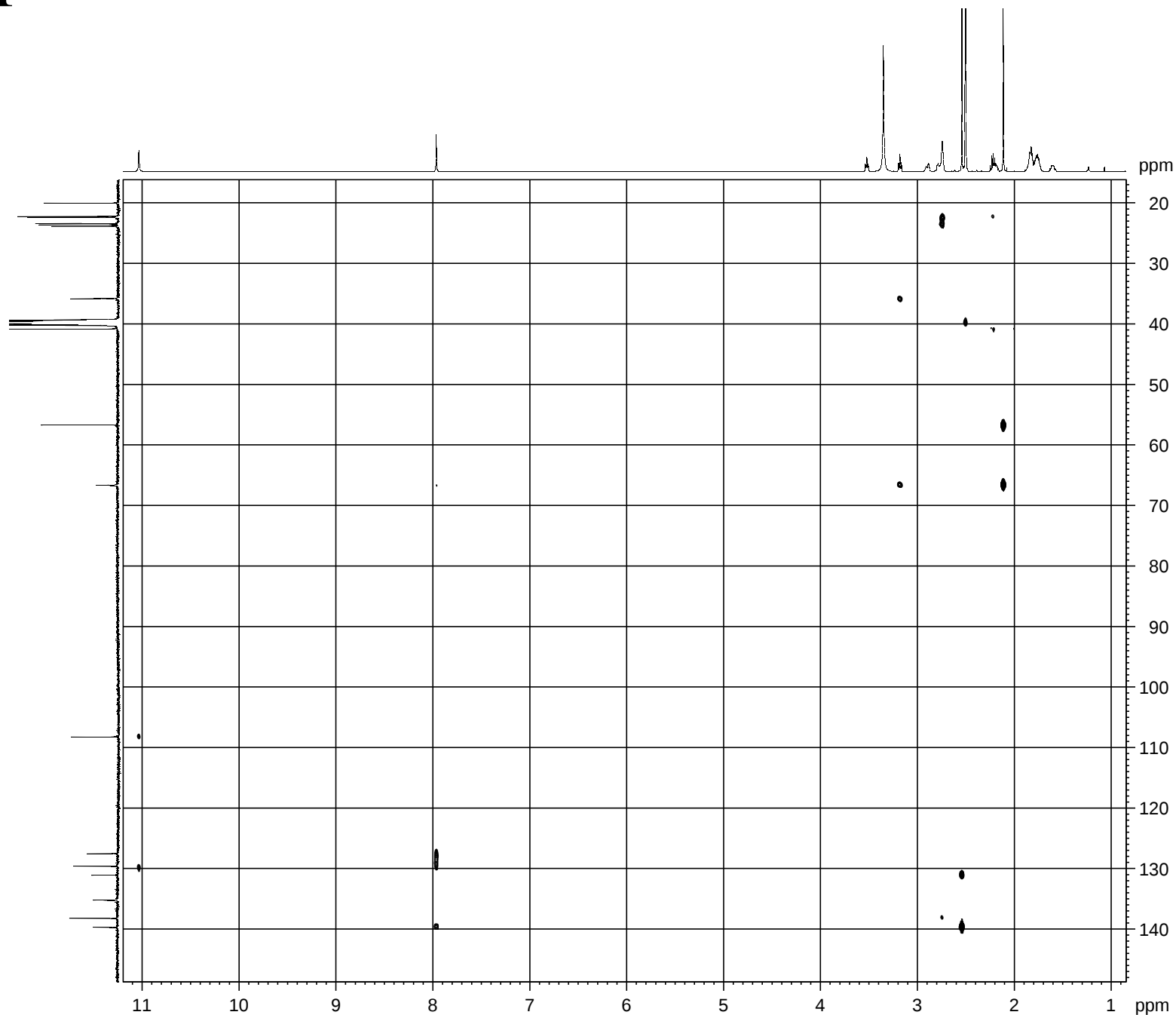
Current Data Parameters  
NAME 142469  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240220  
Time 17.27 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hsqcetgpsisp2.2  
TD 2048  
SOLVENT DMSO  
NS 4  
DS 32  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST17 -0.5000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D4 0.00178571 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0036000 MHz  
NUC1  $^1\text{H}$   
P1 11.50 usec  
P2 23.00 usec  
P28 0 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2  $^{13}\text{C}$   
CPDPRG[2] bi\_p5m4sp\_4sp.2  
P3 9.90 usec  
P14 500.00 usec  
P24 2000.00 usec  
P63 1500.00 usec  
PLW0 0 W  
PLW2 71.00000000 W  
PLW12 2.30040002 W  
SPNAM[3] Crp60, 0.5, 20.1  
SPOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 10.63199997 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 10.63199997 W  
SPNAM[14] Crp42, 1.5, 20.2  
SPOAL14 0.500  
SPOFFS14 0 Hz  
SPW14 5.95400000 W  
SPNAM[31] Crp42, 1.5, 20.2  
SPOAL31 0.500  
SPOFFS31 0 Hz  
SPW31 1.48850000 W  
GPNAM[1] SMSQ10.100  
GPZ1 80.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 20.10 %  
GPNAM[3] SMSQ10.100  
GPZ3 11.00 %  
GPNAM[4] SMSQ10.100  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 600.0000000 MHz  
WDW QSINE





HMBC (8Hz, 140Hz)  
142469  
BAB0141\_1  
Pollak Patrik  
2024.02.20. (KP)

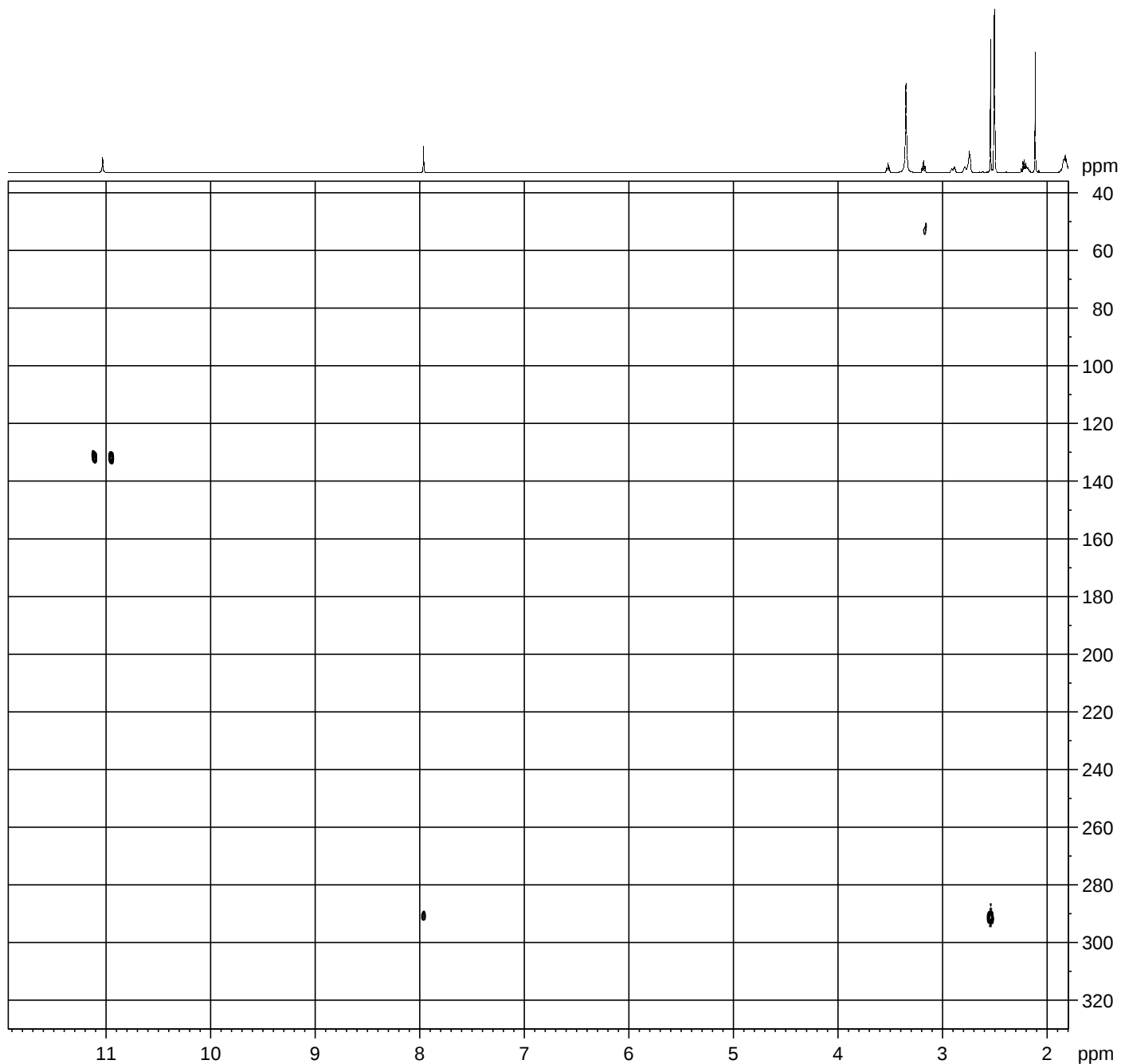
Current Data Parameters  
NAME 142469  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240220  
Time 17.57 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgp1pndqf  
TD 2048  
SOLVENT DMSO  
NS 4  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST13 8.0000000  
D0 0.00000000 sec  
D1 1.50000000 sec  
D2 0.00357143 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00001510 sec  
TDav 1  
SF01 600.0037800 MHz  
NUC1  $^1\text{H}$   
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2  $^{13}\text{C}$   
P3 9.90 usec  
PLW2 71.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 50.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.10 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE QF

F2 - Processing parameters  
SI 2048  
SF 600.0000029 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 150.8701595 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



NHBC  
142469  
BAB0141\_1  
Pollak Patrik  
2024.02.20. (KP)

Current Data Parameters  
NAME 142469  
EXPNO 16  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240220  
Time 18.29 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgpndqf  
TD 2048  
SOLVENT DMSO  
NS 8  
DS 16  
SWH 9615.385 Hz  
FIDRES 9.390024 Hz  
AQ 0.1064960 sec  
RG 196.07  
DW 52.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST13 5.0000000  
D0 0.0000000 sec  
D1 2.0000000 sec  
D6 0.1000000 sec  
D16 0.0002000 sec  
IN0 0.0002060 sec  
TDav 1  
SF01 600.0045600 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.0000000 W  
SF02 60.8096315 MHz  
NUC2 13C  
P3 15.00 usec  
PLW2 210.13999939 W  
GPNAM[1] SMSQ10.100  
GPZ1 70.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 50.10 %  
P16 1000.00 usec

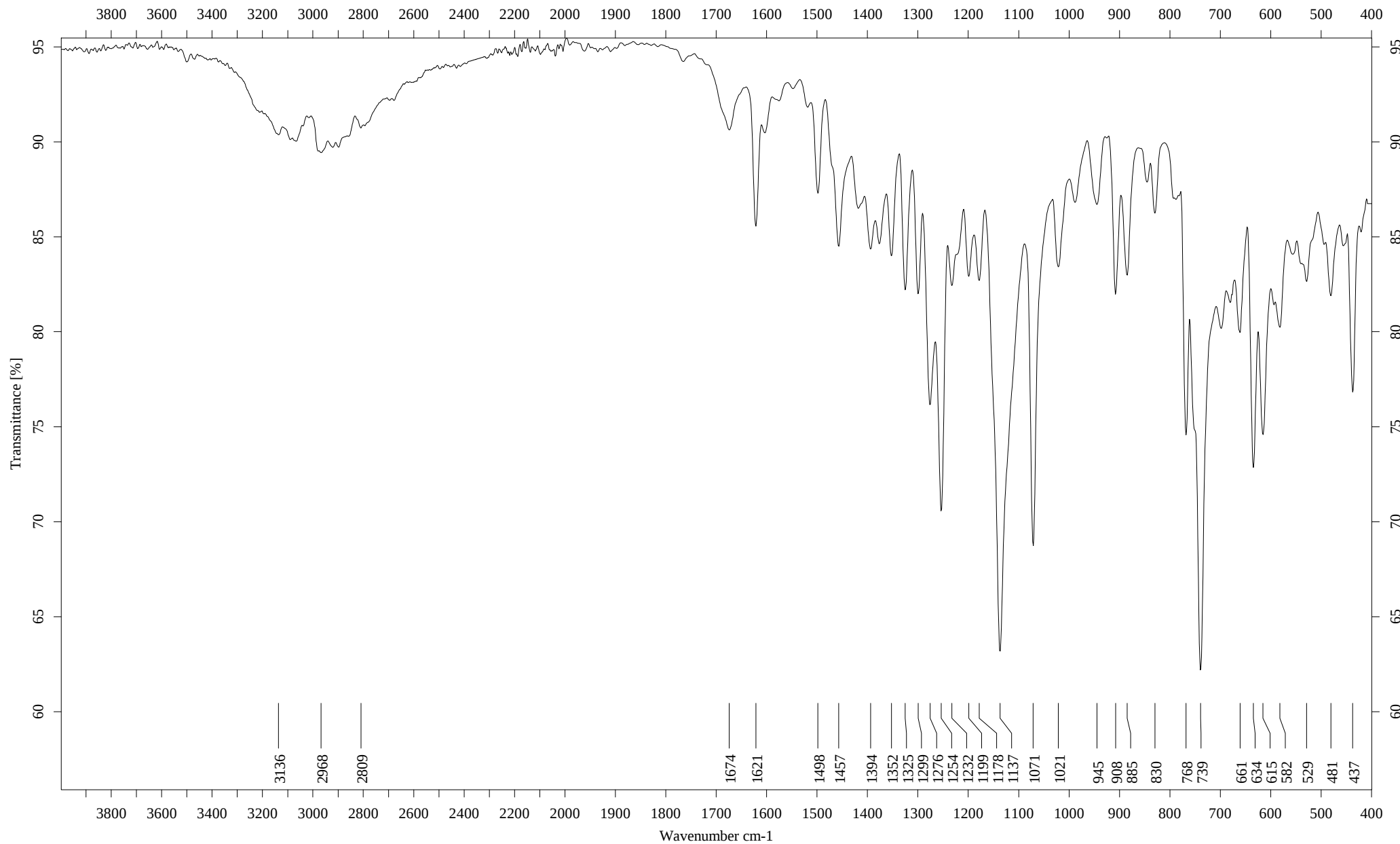
F1 - Acquisition parameters  
TD 128  
SF01 60.80963 MHz  
FIDRES 379.247559 Hz  
SW 399.145 ppm  
FnMODE QF

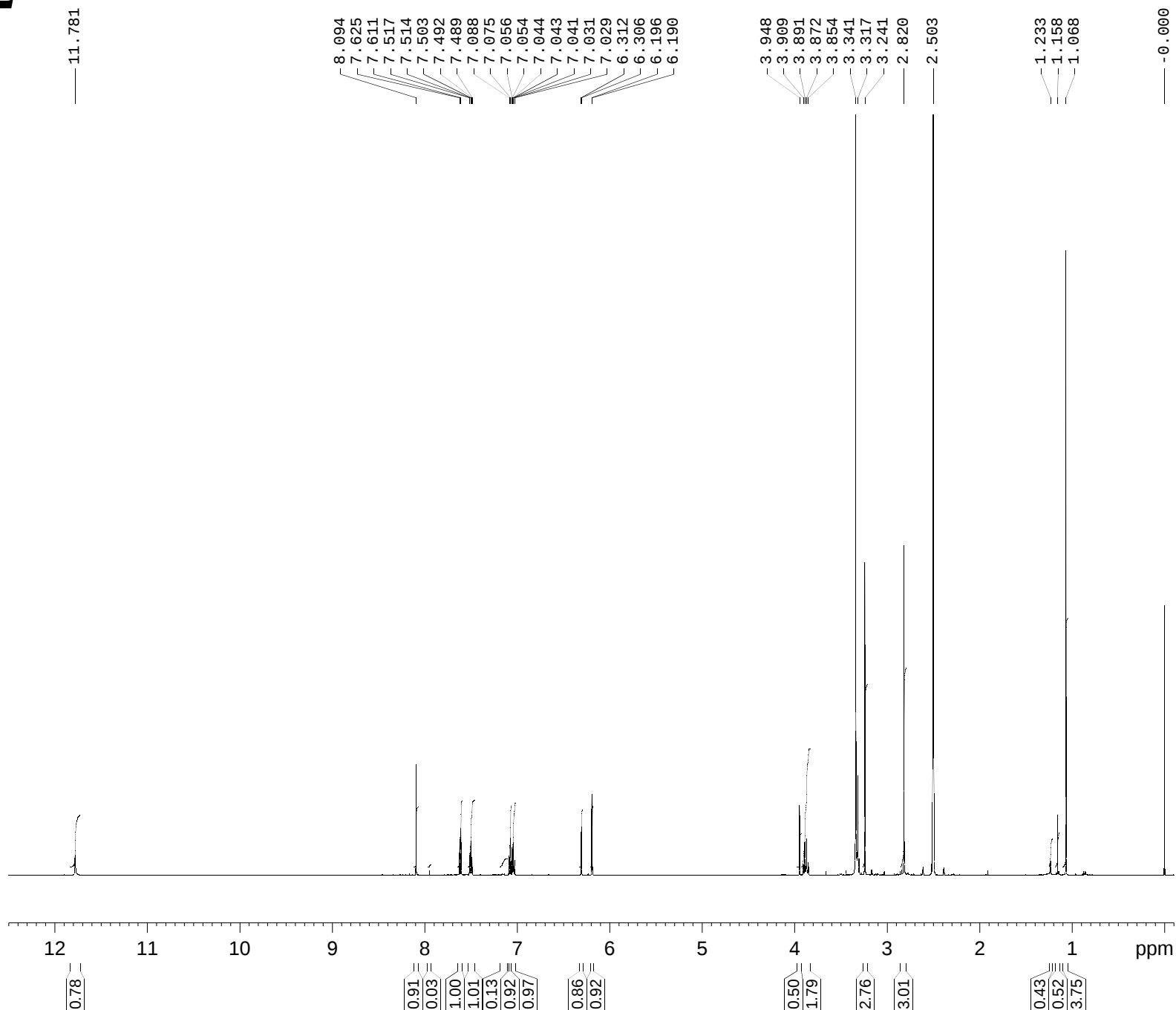
F2 - Processing parameters  
SI 2048  
SF 600.0000029 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 60.7974720 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

|               |             |
|---------------|-------------|
| Pollak Patrik | KP          |
| Gyemant ATR   | 2023.05.09. |

|                     |
|---------------------|
| BRUKER Alpha        |
| Resolution: 2 cm-1  |
| Number of Scans: 32 |





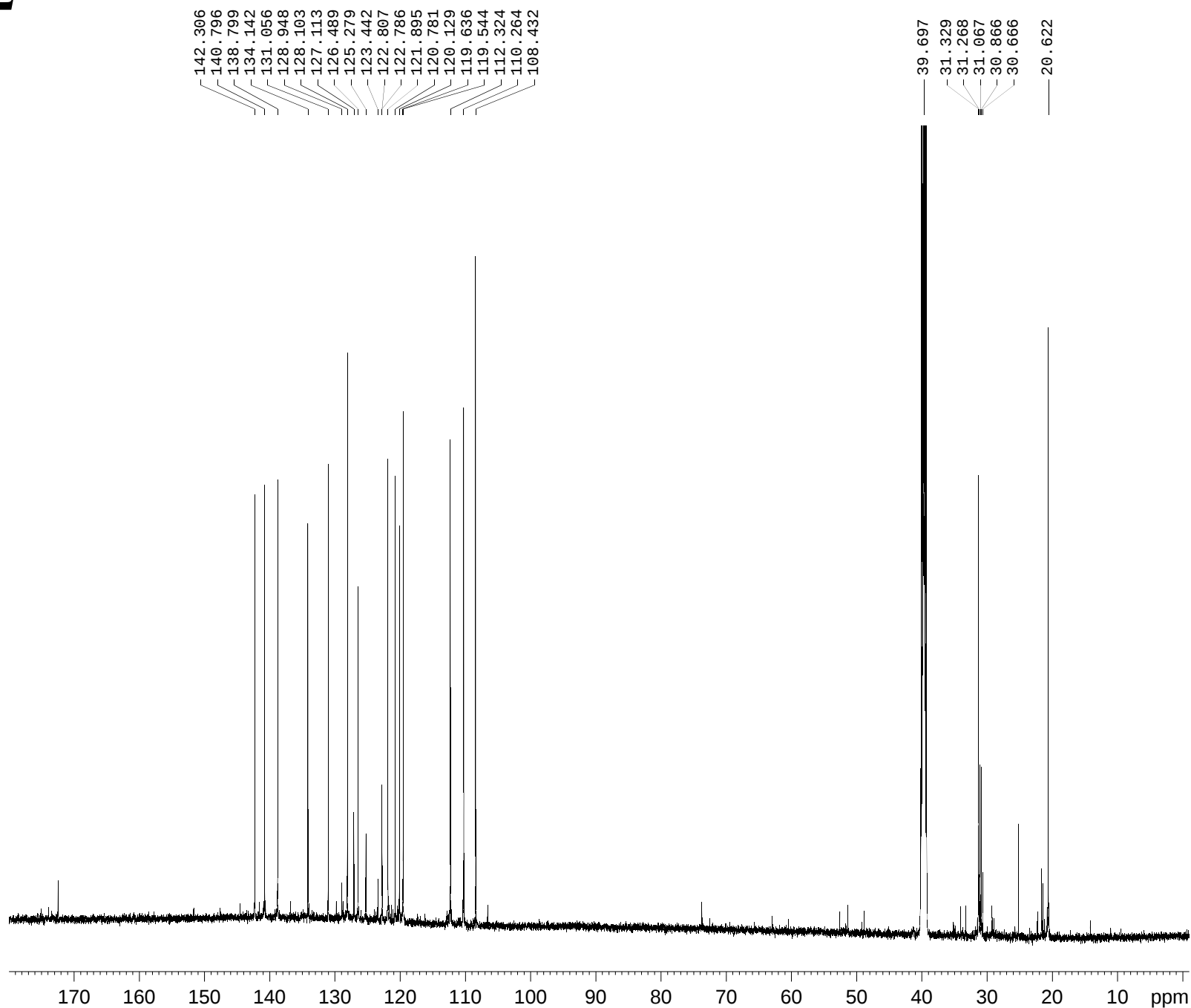
Standard 1H  
141139  
BAB0054\_1  
Pollak Patrik  
2023.05.09. (KP)

Current Data Parameters  
NAME 141139  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230509  
Time 23.18 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 64  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 2.7262976 sec  
RG 196.07  
DW 41.600 usec  
DE 25.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 600.0037050 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W

F2 - Processing parameters  
SI 65536  
SF 600.0000025 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00





Standard 13C  
141385  
BAB0054\_1B  
Pollak Patrik  
2023.06.20.(KP)

Current Data Parameters  
NAME 141385  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230621  
Time 2.31 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 2048  
DS 4  
SWH 36231.883 Hz  
FIDRES 1.105709 Hz  
AQ 0.9043968 sec  
RG 196.07  
DW 13.800 usec  
DE 18.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 150.8852070 MHz  
NUC1 13C  
P1 9.90 usec  
PLW1 80.09999847 W  
SF02 600.0024000 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 35.00000000 W  
PLW12 0.74861997 W  
PLW13 0.37595001 W

F2 - Processing parameters  
SI 32768  
SF 150.8701565 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



-64.536

19F  
141139  
BAB0054\_1  
Pollak Patrik  
2023.05.12. (DA)

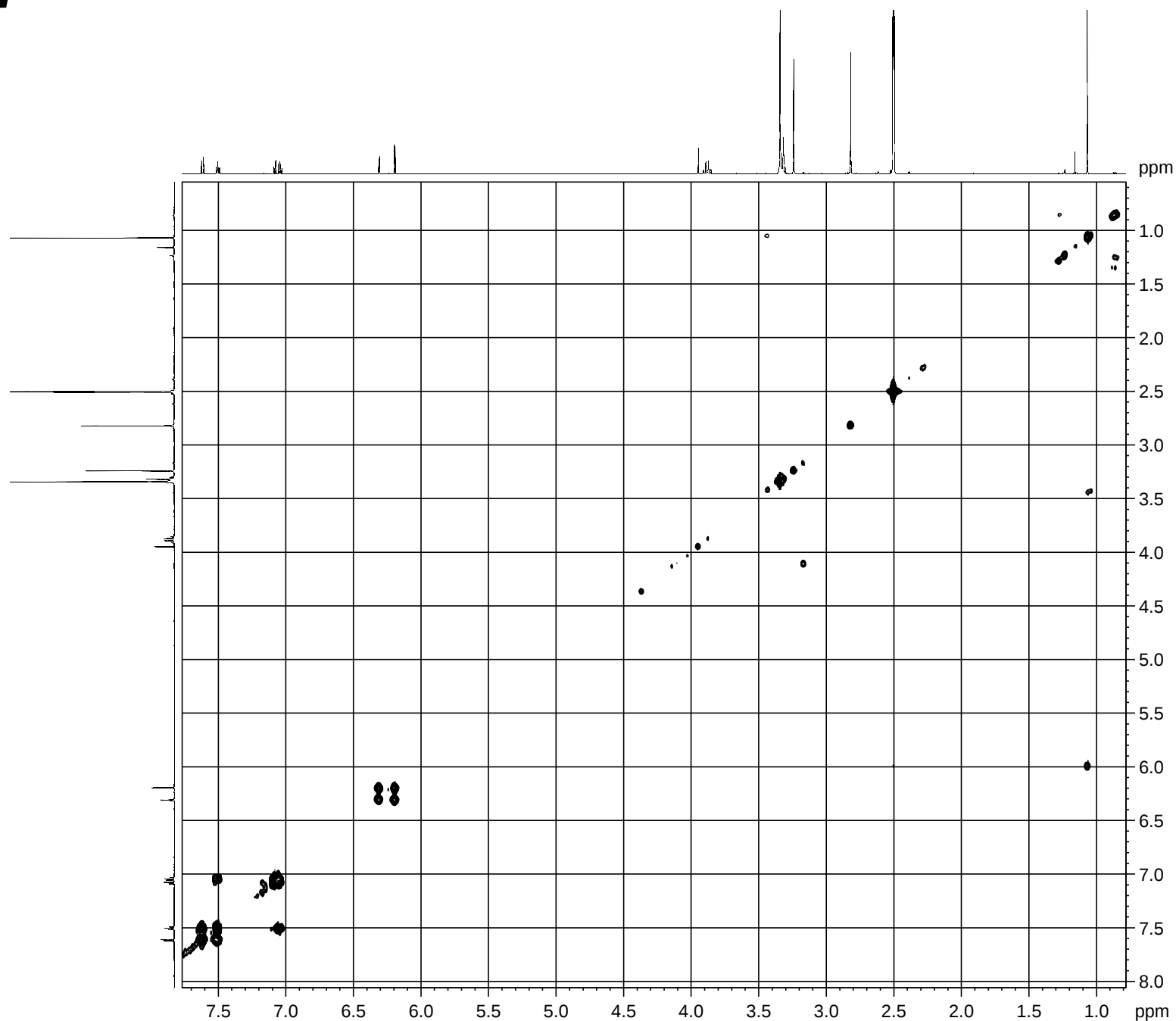
Current Data Parameters  
NAME 141139  
EXPNO 20  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230512  
Time 20.44 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG zgflqn  
TD 131072  
SOLVENT DMSO  
NS 16  
DS 4  
SWH 133928.578 Hz  
FIDRES 2.043588 Hz  
AQ 0.4893355 sec  
RG 14.01  
DW 3.733 usec  
DE 18.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 564.5076096 MHz  
NUC1 19F  
P1 14.70 usec  
PLW1 23.70000076 W

F2 - Processing parameters  
SI 65536  
SF 564.5640660 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

-5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 ppm





COSY  
141139  
BAB0054\_1  
Pollak Patrik  
2023.05.09. (KP)

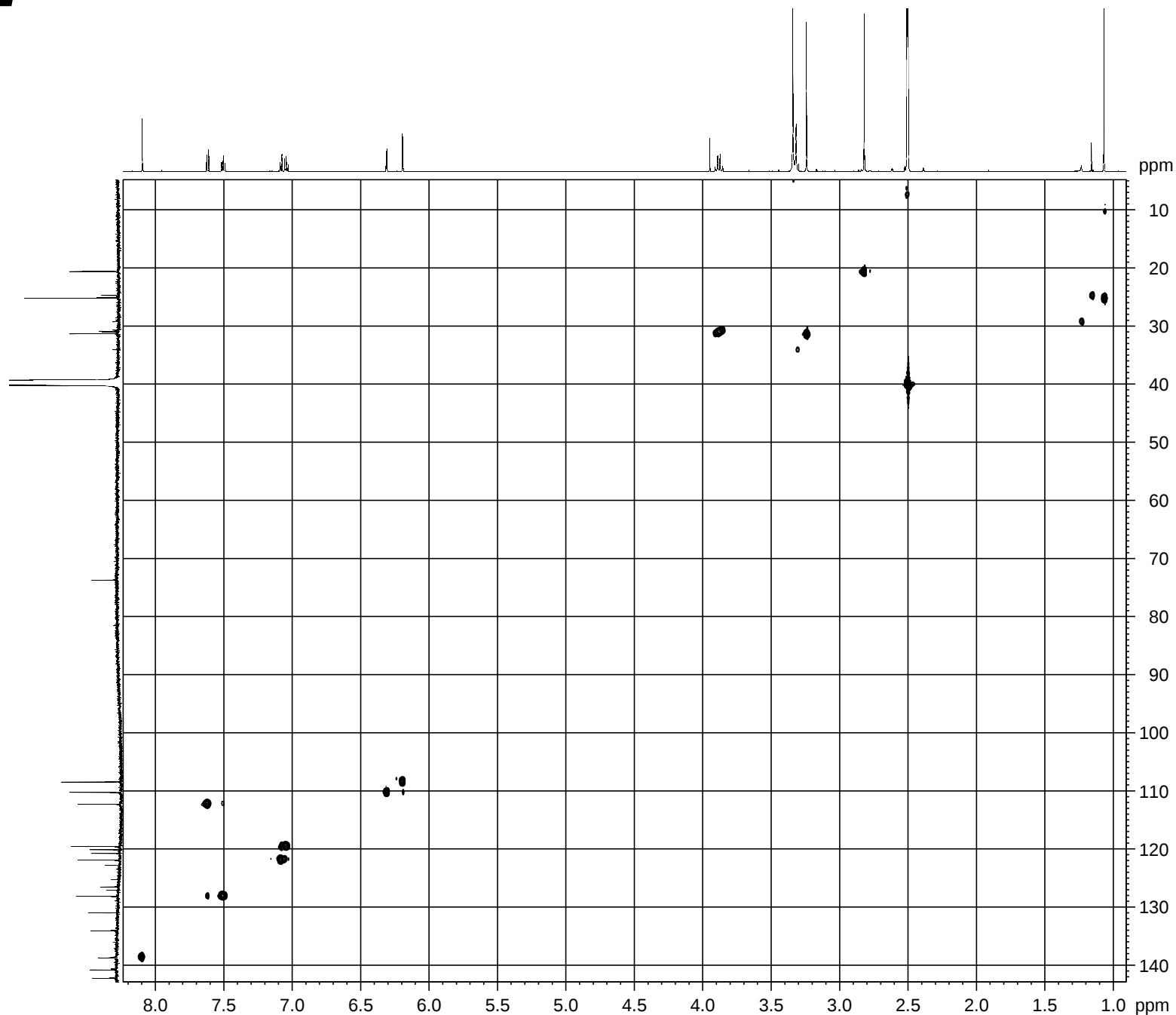
Current Data Parameters  
NAME 141139  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230510  
Time 3.49 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG cosygpmfqr  
TD 2048  
SOLVENT DMSO  
NS 16  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
D0 0.00000300 sec  
D1 2.00000000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00012800 sec  
TDav 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
PLW1 28.00000000 W  
GPNAM[1] SMSQ10.100  
GPZ1 16.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 12.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 600.0036 MHz  
FIDRES 61.035156 Hz  
SW 13.021 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 600.0000025 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 600.0000025 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0



HSQC (140Hz)  
141139  
BAB0054\_1  
Pollak Patrik  
2023.05.09. (KP)

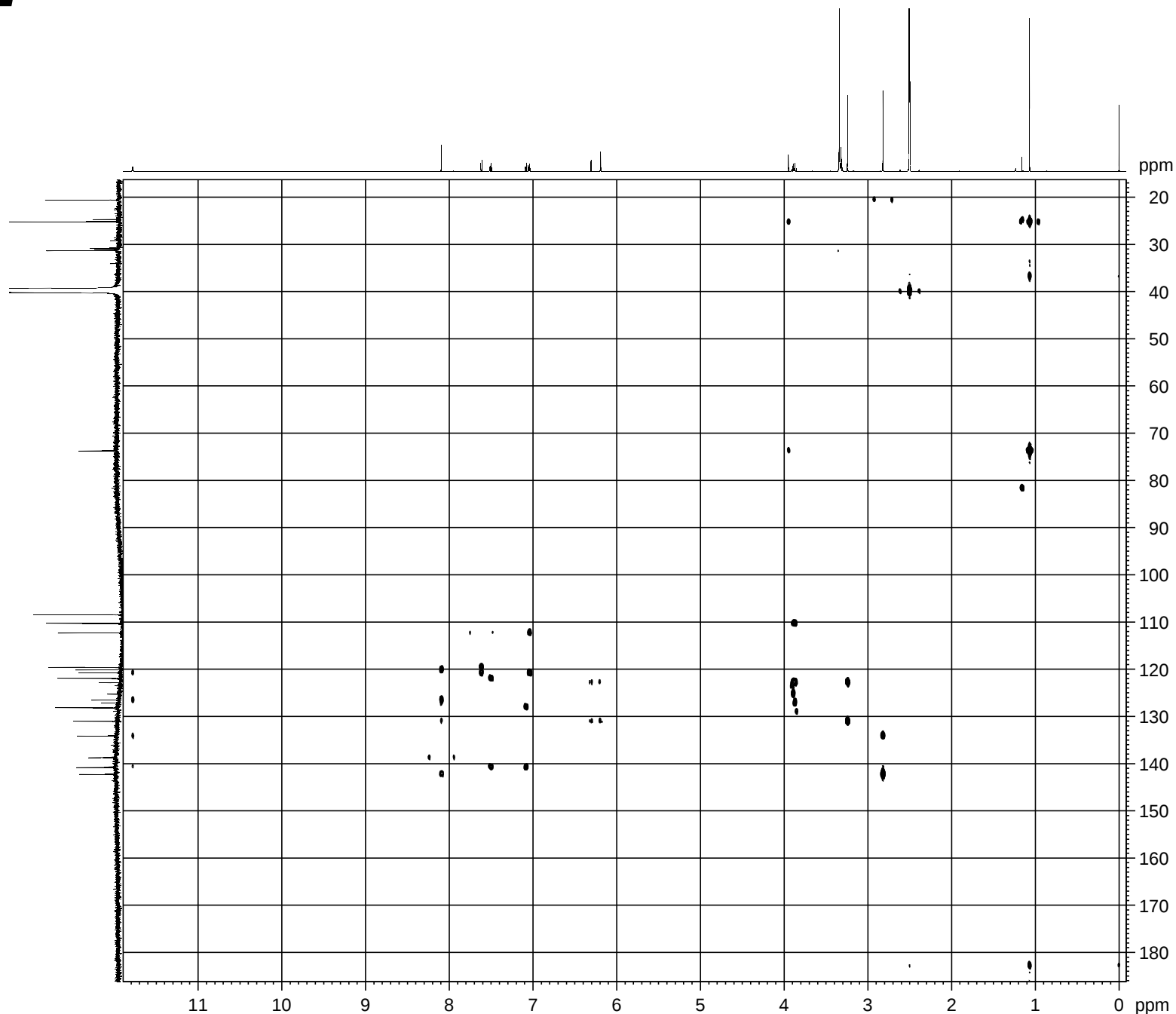
Current Data Parameters  
NAME 141139  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230510  
Time 6.18 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hsqcetgpsisp2.2  
TD 2048  
SOLVENT DMSO  
NS 8  
DS 32  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST17 -0.5000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D4 0.00178571 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.00001510 sec  
TDAV 1  
SF01 600.0036000 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
P28 0 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
CPDPRG2 bi\_p5m4sp\_4sp.2  
P3 9.90 usec  
P14 500.00 usec  
P24 2000.00 usec  
P63 1500.00 usec  
PLW0 0 W  
PLW2 80.09999847 W  
PLW12 2.59520006 W  
SPNAM[3] Crp60, 0.5, 20.1  
SPOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 11.99499989 W  
SPNAM[7] Crp60comp.4  
SPOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 11.99499989 W  
SPNAM[14] Crp42, 1.5, 20.2  
SPOAL14 0.500  
SPOFFS14 0 Hz  
SPW14 6.71710014 W  
SPNAM[31] Crp42, 1.5, 20.2  
SPOAL31 0.500  
SPOFFS31 0 Hz  
SPW31 1.67929995 W  
GPNAM[1] SMSQ10.100  
GPZ1 80.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 20.10 %  
GPNAM[3] SMSQ10.100  
GPZ3 11.00 %  
GPNAM[4] SMSQ10.100  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 600.000025 MHz  
WDW QSINE





HMBC (8Hz, 140Hz)  
141139  
BAB0054\_1  
Pollak Patrik  
2023.05.09. (KP)

Current Data Parameters  
NAME 141139  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230510  
Time 7.16 h  
INSTRUM spect  
PROBHD Z145856\_0002 (  
PULPROG hmbcgp1pndqf  
TD 2048  
SOLVENT DMSO  
NS 8  
DS 16  
SWH 7812.500 Hz  
FIDRES 7.629395 Hz  
AQ 0.1310720 sec  
RG 196.07  
DW 64.000 usec  
DE 25.00 usec  
TE 295.0 K  
CNST2 140.0000000  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D2 0.00357143 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00001510 sec  
TDav 1  
SF01 600.0037800 MHz  
NUC1 1H  
P1 11.50 usec  
P2 23.00 usec  
PLW1 28.00000000 W  
SF02 150.8867157 MHz  
NUC2 13C  
P3 9.90 usec  
PLW2 80.09999847 W  
GPNAM[1] SMSQ10.100  
GPZ1 50.00 %  
GPNAM[2] SMSQ10.100  
GPZ2 30.00 %  
GPNAM[3] SMSQ10.100  
GPZ3 40.10 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SF01 150.8867 MHz  
FIDRES 258.692047 Hz  
SW 219.453 ppm  
FnMODE QF

F2 - Processing parameters  
SI 2048  
SF 600.0000025 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 150.8701595 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

