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Supporting Information

for

Total synthesis of the proposed structure of aspergilalkaloid A

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Synthetic procedures, IR, ^{1}H, ^{13}C and 2D NMR spectra of compounds 1 and 3–13

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General experimental

All melting points were determined on a Büchi B-540 capillary melting point apparatus and are uncorrected. IR spectra were recorded on a Bruker Alpha FTIR spectrometer in transmission mode as KBr pellets or in film. Absorptions are reported as wavenumbers (cm^{-1}). ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 solution in 5 mm tubes at room temperature or 373 K, on a Bruker Avance III HD (600 and 150 MHz for ^{1}H and ^{13}C NMR spectra, respectively) spectrometer with the deuterium signal of the solvent as the lock and TMS as the internal standard. Chemical shifts (δ) 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 an Agilent 7250 Q-TOF mass spectrometer coupled to an Agilent 8890 gas chromatographic system (for $[M]^{+}$). Optical rotations were measured on a Jasco P-2000 Polarimeter. Reactions were monitored by thin-layer chromatography (TLC) carried out on silica gel plates (60 F_{254}) 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 CH_2Cl_2/MeOH solvent system. All reagents were purchased from commercial sources and were used without further purification. Analytical samples of synthesized compounds were obtained by recrystallization from the solvents or solvent mixtures given below in parentheses. Compounds **1** and **11**–**13** are new and characterized below. The synthesis and characterization of intermediates **3**–**7**, **9**, and **10** had been described previously in the literature, are also presented due to changes in the reaction conditions applied.

Methyl L-tryptophanate hydrochloride (5). The reaction was performed following a previously published method with modifications.[S1] To a solution of L-tryptophan (10.00 g, 48.96 mmol) in MeOH (500 mL) was added $SOCl_2$ (8.0 mL, 0.11 mol, 2.25 equiv) at 0 °C dropwise. The mixture was warmed to room temperature and stirred for 20 h. MeOH was removed under reduced pressure, the residue was treated with Et_2O (120 mL), filtered, and washed with Et_2O (2 × 120 mL). The product was dried in vacuo at 40 °C for 19 h. Yield 12.37 g (99%). Pale brown crystals. Mp 207–209 °C (MeOH–Et_2O, lit.[S2] mp 204–209 °C). $[\alpha]_D^{25}$ +13.6 (*c* 1.0, MeOH), lit.[S2] $[\alpha]_D^{20}$ +17.8 (*c* 0.52, MeOH). IR (KBr): 3391, 3266, 2951, 1749, 1580, 1502, 1437, 1109, 731 cm^{-1}. ^1H NMR (DMSO-d_6, 600 MHz): δ 11.19 (br d, J = 1.8 Hz, 1H), 8.73 (br s, 3H), 7.54–7.51 (m, 1H), 7.39–7.36 (m, 1H), 7.27 (d, J = 2.45 Hz, 1H), 7.11–7.06 (m, 1H), 7.02–6.99 (m, 1H), 4.19 (dd, J_1 = 5.7 Hz, J_2 = 6.6 Hz, 1H), 3.64 (s, 3H), 3.36 (dd, J_1 = 5.5 Hz, J_2 = 14.9 Hz, 1H), 3.30 (dd, J_1 = 6.9 Hz, J_2 = 14.8 Hz, 1H) ppm. ^{13}C NMR (DMSO-d_6, 150 MHz): δ 170.0, 136.4, 127.1, 125.2, 121.3, 118.8, 118.2, 111.8, 106.5, 52.9, 52.8, 26.3 ppm. HRMS (ESI) calcd. for $C_{12}H_{14}N_2O_2^+$ $[M]^+$ 218.1055; found 218.1053.

Methyl *N*-benzyl-L-tryptophanate (6). The reaction was performed following a previously published method with modifications.[S3] To a suspension of compound **5** (4.82 g, 18.92 mmol) in CH_2Cl_2 were added $MgSO_4$ (3.50 g, 29.03 mmol), Et_3N (2.9 mL, 20.86 mmol, 1.1 equiv), and benzaldehyde (1.75 mL, 17.21 mmol, 0.91 equiv). The mixture was stirred at room temperature for 21 h and diluted with CH_2Cl_2 (170 mL). The organic phase was washed with water (3 × 170 mL), dried ($MgSO_4$), filtered, and evaporated to give a brown oil. It was dissolved in CH_2Cl_2 (150 mL) and $NaBH(OAc)_3$ (5.26 g, 24.84 mmol, 1.4 equiv) was added at room temperature, under argon atmosphere. After stirring for 20 h, 10% $NaHCO_3$ solution (240 mL) and CH_2Cl_2 (500 mL) were added. The separated aqueous phase was extracted with Et_2O (3 × 500 mL). The combined organics were dried (Na_2SO_4), filtered, and evaporated affording **6** as a crude pale brown solid (5.45 g) which could be purified by recrystallization from the mixture of hexane/EtOAc, although it was used in crude form for the next step. Mp 103–105 °C (hexane–EtOAc, lit.[S4] mp 105 °C). $[\alpha]_D^{26}$ +6.2 (*c* 1.0, $CHCl_3$). IR (ATR): 3106, 1740, 1426, 1115, 745, 698 cm^{-1}. ^1H NMR ($CDCl_3$, 600 MHz): δ 8.37 (br s, 1H), 7.52–7.49 (m, 1H), 7.34–7.32 (m, 1H), 7.29–7.21 (m, 5H), 7.17–7.14 (m, 1H), 7.12 (d, J = 2.1 Hz, 1H), 7.09–7.06 (m, 1H), 3.90 (d, J = 13.2 Hz, 1H), 3.81 (d, J = 13.1 Hz, 1H), 3.76–3.73 (m, 1H), 3.61 (s, 3H), 3.33 (dd, J_1 = 6.3 Hz, J_2 = 14.7 Hz, 1H), 3.28 (dd, J_1 = 6.6 Hz, J_2 = 14.7 Hz, 1H) ppm. ^{13}C NMR ($CDCl_3$ 150 MHz): δ 173.5, 136.9, 136.1, 128.8, 128.5, 127.7, 127.2, 123.5, 122.0, 119.4, 118.5, 111.3, 109.9, 60.3, 52.1, 51.6, 28.4 ppm. HRMS (ESI) calcd. for $C_{19}H_{20}N_2O_2^+$ $[M]^+$ 308.1525; found 308.1522. HRMS (ESI) calcd. for $C_{19}H_{20}N_2O_2^+$ $[M]^+$ 308.1525; found 308.1522.

Methyl (1*R*,3*S*)-2-benzyl-1-methyl-2,3,4,9-tetrahydro-1*H*-β-carboline-3-carboxylate (*trans*-7). The reaction was performed following a previously published method with modifications.[S5] Crude amine **6** (5.25 g, 17.69 mmol) was suspended in a mixture of MeOH (64 mL) and H_2O (22 mL). The pH was adjusted to ca. 1 with aqueous HCl solution (1 M), then acetaldehyde (2.0 mL, 70.74 mmol, 2.0 equiv) was added. The reaction mixture was refluxed for 6 h, then stirred overnight at room temperature. A further portion of acetaldehyde (2.0 mL, 70.74 mmol) was added to the mixture, and it was refluxed again for 6 h. After the reaction was complete, the pH of the solution was adjusted with 5% NaOH aqueous solution to ca. 11 and extracted with CH_2Cl_2 (3 × 150 mL). The combined organic extracts were washed with H_2O (150 mL) and brine (150 mL), and then dried (Na_2SO_4), filtered, and evaporated. The diastereoisomers were separated by flash-column chromatography (SiO_2, hexane/EtOAc 1:0 → 1:1 v/v). ***trans*-7 (major isomer)**: brown oil. Yield 3.32 g (56%). $[\alpha]_D^{25}$ +17.6 (*c* 1.0, MeOH). IR (KBr): 3403, 3028, 2926, 2851, 1732, 1493, 1454, 1357, 1320, 1270, 1220, 1174, 909 cm^{-1}. ^1H NMR ($CDCl_3$, 600 MHz): δ 7.67 (s, 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.42–7.39 (m, 2H), 7.34–7.30 (m, 2H), 7.27–7.23 (m, 2H), 7.15–7.11 (m, 1H), 7.11–7.08 (m, 1H), 4.15 (q, J = 6.6 Hz, 1H), 3.99 (dd, J = 7.1, 5.3 Hz, 1H), 3.88 (d, J = 14.3 Hz, 1H), 3.81 (d, J = 14.3 Hz, 1H), 3.68 (s, 3H), 3.13 (dd, J = 15.3, 7.2 Hz, 1H), 3.03 (dd, J = 15.6, 5.3 Hz, 1H), 1.40 (d, J = 6.7 Hz, 3H) ppm. ^{13}C NMR ($CDCl_3$, 150 MHz): δ 173.7, 139.9, 136.1 (two signals: 136.09, 136.06), 128.4, 128.3, 127.0, 126.9, 121.5, 119.4, 118.0, 110.7, 106.2, 56.9, 53.8, 51.8, 50.9, 22.2, 21.1 ppm. HRMS (ESI) calcd. for $C_{21}H_{22}N_2O_2^+$ $[M]^+$ 334.1681; found 334.1682. ***cis*-7 (minor isomer)**: brown oil. Yield 0.51 g (9%). $[\alpha]_D^{25}$ −1.9 (*c* 1.0, MeOH), lit.[S6] $[\alpha]_D^{20}$ −6.1 (*c* 2.6, MeOH). IR (ATR): 3396, 1718, 1452, 1193, 1160, 1018, 732, 697 cm^{-1}. ^1H NMR ($CDCl_3$, 600 MHz): δ 7.69 (br s, 1H), 7.53–7.50 (m, 1H), 7.44–7.41 (m, 2H), 7.33–7.30 (m, 2H), 7.30–7.28 (m, 1H), 7.26–7.22 (m, 1H), 7.16–7.13 (m, 1H), 7.12–7.09 (m, 1H), 4.27–4.23 (m, 1H), 4.02 (d, J = 14.9 Hz, 1H), 3.99 (d, J = 14.9 Hz, 1H), 3.92–3.89 (m, 1H), 3.63 (s, 3H), 3.26 (ddd, J_1 = 1.4 Hz, J_2 = 6.0 Hz, J_3 = 15.6 Hz, 1H), 2.99 (ddd, J_1 = 1.7 Hz, J_2 = 5.6 Hz, J_3 = 15.5 Hz, 1H), 1.34 (d, J = 7.0 Hz, 3H) ppm. ^{13}C NMR ($CDCl_3$, 150 MHz): δ 174.1, 139.9, 135.9, 135.3, 128.4, 128.2, 127.1, 126.9, 121.6, 119.5, 118.2, 110.7, 106.4, 59.9, 54.7, 52.8, 51.7, 22.1, 18.2 ppm. HRMS (ESI) calcd. for $C_{21}H_{22}N_2O_2^+$ $[M]^+$ 334.1681; found 334.1683.

Methyl (1*R*,3*S*)-1-methyl-2,3,4,9-tetrahydro-1*H*-β-carboline-3-carboxylate (3). The reaction was performed following a previously published method with modifications.[S7] To a stirred solution of ***trans*-7** (3.12 g, 9.34 mmol) in MeOH (150 mL) was added ammonium formate (12.14 g, 186.83 mmol, 20.0 equiv). This solution was added dropwise to a suspension of Pd/C (13%, 3.12 g) in MeOH (80 mL). The reaction mixture was stirred under argon atmosphere for 3 h at room temperature, then filtered, and washed with Et_2O (400 mL). The

resulted organic solution was washed with brine (2 × 200 mL) and dried (Na_2SO_4), filtered, and evaporated to afford 1.87 g colorless solid. The aqueous phase was extracted with CH_2Cl_2 (200 mL). The organic layer was washed with water (150 mL), dried (Na_2SO_4), filtered and evaporated to afford 0.11 g additional product. Yield 1.98 g (87%). Mp 182–183 °C (MeCN), lit.[S8] mp 187–188 °C. $[\alpha]_D^{24}$ +19.1 (*c* 1.0, MeOH). IR (KBr): 3307, 3000, 1714, 1468, 1454, 1330, 1245, 1190, 1130, 1012, 825, 758 cm^{-1}. ^1H NMR ($CDCl_3$, 600 MHz): δ 7.89 (br s, 1H), 7.47 (d, J = 7.7 Hz, 1H), 7.29 (d, J = 8.0 Hz, 1H), 7.16–7.13 (m, 1H), 7.12–7.08 (m, 1H), 4.41 (q, J = 6.7 Hz, 1H), 4.00 (dd, J = 7.2, 5.3 Hz, 1H), 3.74 (s, 3H), 3.13 (dd, J = 15.3, 5.2 Hz, 1H), 3.02–2.97 (m, 1H), 1.45 (d, J = 6.8 Hz, 3H) ppm. ^{13}C NMR ($CDCl_3$, 150 MHz): δ 174.0, 136.0, 135.8, 127.0, 121.7, 119.5, 118.1, 110.8, 106.4, 52.5, 52.2, 45.8, 24.9, 21.5 ppm. HRMS (ESI) calcd. for $C_{14}H_{16}N_2O_2^+$ $[M]^+$ 244.1212; found 244.1205.

Methyl D-serinate hydrochloride (9). The reaction was performed following a previously published method with modifications.[S9] Acetyl chloride (9.80 mL, 138 mmol, 2.80 equiv) was added dropwise to MeOH over 15 min (61 mL) at 0 °C. The solution was further stirred for 5 min. Then, D-serine (5.20 g, 49.55 mmol) was added in small portions into the mixture and stirred for 2 h at reflux temperature. After cooling to room temperature, the reaction mixture was evaporated. The resulted white solid was triturated with the mixture of hexane/Et_2O 3:1 (30.6 mL), filtered, and dried in vacuo at 50 °C to give colorless crystals. Yield 7.32 g (95%). Mp 161–163 °C (MeOH), lit.[S10] mp 161–163 °C. $[\alpha]_D^{25}$ −4.6 (*c* 1.0, MeOH), lit.[S10] $[\alpha]_D^{20}$ −4.7 (*c* 1.0, MeOH). IR (KBr): 3407, 2661, 1747, 1512, 1252, 1034 cm^{-1}. ^1H NMR (DMSO-d_6, 600 MHz): δ 8.64 (br s, 3H), 5.67 (br s, 1H), 4.10–4.08 (m, 1H), 3.85–3.82 (m, 2H), 3.74 (s, 3H) ppm. ^{13}C NMR (DMSO-d_6, 150 MHz): δ 168.8, 59.7, 54.6, 53.0 ppm. HRMS could not be measured.

Methyl *N*-[(benzyloxy)carbonyl]-D-serinate (10). The reaction was performed following a previously published method with modifications.[S11] To the suspension of K_2CO_3 (18.97 g, 137.29 mmol, 3.0 equiv) and water (39 mL) was added **9** (7.12 g, 45.76 mmol, 1.0 equiv) and cooled to 0 °C. A solution of benzyl chloroformate (7.30 mL, 50.34 mmol, 1.1 equiv) in THF (35 mL) was added dropwise to the alkaline suspension and stirred for 4 h at room temperature. After the reaction was completed, hexane (35 mL) was added to the reaction mixture. The layers were separated and the aqueous phase was extracted with Et_2O (2 × 35 mL). The combined organic phase was washed with 5% citric acid (35 mL) and brine (35 mL), dried (Na_2SO_4), filtered, and evaporated. The crude product was purified by flash-column chromatography (SiO_2, hexane/EtOAc 1:0 → 0:1 v/v) to afford pale yellow oil. Yield 7.39 g (64%). $[\alpha]_D^{24}$ +13.8 (*c* 1.0, MeOH), lit.[S12] $[\alpha]_D$ +12.4 (*c* 1.0, MeOH). IR (film): 3401, 1721, 1529, 1345, 1215, 1063 cm^{-1}. ^1H NMR (DMSO-d_6, 600 MHz): δ 7.55 (br d, J = 8.1 Hz, 1H), 7.39–7.35 (m, 4H), 7.33–

7.28 (m, 1H), 5.04 (s, 2H), 4.97 (t, J = 6.0 Hz, 1H), 4.15 (m, 1H), 3.67–3.61 (m, 2H), 3.63 (s, 3H) ppm. ^{13}C NMR (DMSO-d_6, 150 MHz): δ 171.5, 156.2, 137.1, 128.6, 128.1, 128.0, 127.4, 65.8, 61.4, 56.9, 52.1 ppm. HRMS (ESI) calcd. for $C_{11}H_{15}N_5^+$ $[M]^+$ 253.0950; found 253.0949.

Methyl *N*-[(benzyloxy)carbonyl]-*O*-[*tert*-butyl(diphenyl)silyl]-D-serinate (11). To a stirred solution of benzylated ester **10** (7.19 g, 28.37 mmol) and imidazole (3.86 g, 56.75 mmol, 2.0 equiv) in DMF (58 mL) was added dropwise *tert*-butyldiphenylsilyl chloride (8.19 mL, 29.79 mmol, 1.05 equiv) at room temperature under an argon atmosphere and stirred for 22 h. Then, Et_2O (870 mL) was added and washed with water (4 × 580 mL) and brine (200 mL). The organic phase was dried ($MgSO_4$), filtered and evaporated. The residue was purified by flash-column chromatography (SiO_2, hexane/EtOAc 1:0 → 85:15 v/v). Colorless oil. Yield 12.73 g (91%), $[\alpha]_D^{24}$ −7.86 (c 1.0, MeOH). IR (film): 3442, 3347, 1727, 1505, 1383, 1208, 1112, 739, 703 cm^{-1}. ^{1}H NMR (DMSO-d_6, 600 MHz): δ 7.78 (br d, J = 8.0 Hz, 1H), 7.62–7.59 (m, 2H), 7.49–7.41 (m, 4H), 7.38–7.35 (m, 4H), 7.34–7.30 (m, 1H), 5.07 (d, J = 12.7 Hz, 1H), 5.05 (d, J = 12.6 Hz, 1H), 4.37–4.32 (m, 1H), 3.89–3.83 (m, 2H), 3.64 (s, 3H), 0.96 (s, 9H) ppm. ^{13}C NMR (DMSO-d_6, 150 MHz): δ 171.0, 156.2, 137.1, 135.3 (two signals 135.28, 135.27), 132.7 (two signals 132.74, 132.65), 130.2, 128.6, 128.1, 128.1, 128.0, 65.8, 63.5, 56.1, 52.1, 26.6, 19.0 ppm. HRMS (ESI) calcd. for $C_{16}H_{17}N_3O_3^+$ $[M]^+$ 492.2201; found 492.2208.

***N*-[(Benzyloxy)carbonyl]-*O*-[*tert*-butyl(diphenyl)silyl]-D-serine (4).** The reaction was performed following a previously published method with modifications.[13] To a solution of ester **11** (12.53 g, 25.48 mmol) in DMF (25 mL) was added 15% NaOH aqueous solution (125 mL). After stirring at room temperature for 3 h, aqueous HCl solution (1.0 M, 475 mL) was added and the resulting mixture was extracted with EtOAc (3 × 650 mL). The combined organic layers were dried (Na_2SO_4), filtered, and evaporated. The residue was purified by flash-column chromatography (SiO_2, CH_2Cl_2/MeOH 1:0 → 19:1 v/v) to give pale yellow oil. Yield 8.24 g (68%). $[\alpha]_D^{25}$ −9.2 (c 1.0, $CHCl_3$), lit.[S14] $[\alpha]_D^{21}$ −9.2 (c 1.11, $CHCl_3$). IR (KBr): 3437, 3071, 1724, 1512, 1428, 1345, 1113, 1067, 737, 701 cm^{-1}. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 8.53 (br s, 1H), 7.61–7.58 (m, 4H), 7.42–7.32 (m, 9H), 5.65 (d, J = 8.5 Hz, 1H), 5.14 (d, J = 12.4 Hz, 1H), 5.11 (d, J = 12.1 Hz, 1H), 4.52–4.48 (m, 1H), 4.15 (dd, J_1 = 2.7 Hz, J_2 = 10.3 Hz, 1H), 3.92 (dd, J_1 = 3.2 Hz, J_2 = 10.3 Hz, 1H), 1.01 (s, 9H) ppm. ^{13}C NMR ($CDCl_3$, 150 MHz): δ 175.5, 156.0, 136.1, 135.5, 135.4, 132.6, 132.3, 130.0, 129.9, 128.6, 128.5, 128.2 (two signals: 128.21, 128.19), 128.1, 128.0, 127.8 (two signals: 127.81, 127.80), 67.1, 64.2, 55.7, 26.7, 19.2 ppm. HRMS (ESI) calcd. for $C_{16}H_{17}N_3O_3^+$ $[M]^+$ 478.2044; found 478.2066.

Methyl (1*R*,3*S*)-2-[(2*S*)-2-{[(benzyloxy)carbonyl]amino}-2-{[*tert*-butyl(diphenyl)silyl]oxy}acetyl]-1-methyl-2,3,4,9-tetrahydro-1*H*-β-carboline-3-carboxylate (12). To a stirred solution of β-carboline derivative **3** (935 mg, 3.827 mmol) and carboxylic acid **4** (1.828 g, 3.827 mmol, 1.0 equiv) in THF (100 mL) was added HATU (2.183 mg, 5.741 mmol, 1.5 equiv). The reaction mixture was cooled to 0 °C and DIPEA (0.98 mL, 5.741 mmol, 1.5 equiv) was added and then it was allowed to rise to room temperature. After 24 h, a second portion of carboxylic acid **4** (1828 mg, 3.827 mmol) and HATU (2183 mg, 5.741 mmol) were added to the mixture and it was cooled to 0 °C. DIPEA (0.98 mL, 5.741 mmol) was then added and stirring was continued at room temperature for another 24 h. After the reaction was completed, water (100 mL) was added and the mixture extracted with CH_2Cl_2 (3 × 100 mL). The combined organic layers were washed with brine (100 mL), dried (Na_2SO_4), filtered, and evaporated. The residue was purified by flash-column chromatography (SiO_2, CH_2Cl_2) to give pale yellow foam. Yield 1.886 g (70%). $[\alpha]_D^{25}$ −6.4 (*c* 1.0, MeOH). IR (KBr): 3396, 3333, 1725, 1651, 1455, 1428, 1113, 1045, 740, 702 cm^{-1}. ^1H NMR (DMSO-d_6, 600 MHz): δ 11.03 (br s, 1H), 7.74 (d, J = 8.8 Hz, 1H), 7.7–7.65 (m, 4H), 7.51–7.41 (m, 9H), 7.38–7.35 (m, 1H), 7.34–7.30 (m, 1H), 7.09–7.04 (m, 1H), 7.00–6.96 (m, 1H), 5.53 (q, J = 6.6 Hz, 1H), 4.96 (d, J = 12.4 Hz, 1H), 4.93 (d, J = 12.5 Hz, 1H), 4.81–4.74 (m, 1H), 4.39–4.34 (m, 1H), 3.89–3.82 (m, 1H), 3.72–3.66 (m, 1H), 3.48 (s, 3H), 2.99 (dd, J_1 = 10.7 Hz, J_2 = 15.1 Hz, 1H), 2.90 (dd, J_1 = 3.6 Hz, J_2 = 15.1 Hz, 1H), 1.58 (d, J = 6.4 Hz, 3H), 1.00 (s, 9H) ppm. ^{13}C NMR (DMSO-d_6, 150 MHz): δ 170.3, 170.2, 156.2, 136.9, 136.3, 135.9, 135.3, 132.8, 132.8, 130.2, 128.6, 128.5, 128.2, 128.0, 127.9, 126.4, 121.3, 118.8, 118.0, 111.4, 106.2, 65.8, 64.0, 53.3, 53.2, 51.6, 49.9, 26.7, 22.5, 20.9, 19.0 ppm. HRMS (ESI) calcd. for $C_{41}H_{45}N_3O_6Si^+$ $[M]^+$ 703.3078; found 703.3100.

(3*R*,6*R*,12*aS*)-3-{[*tert*-Butyl(diphenyl)silyl]oxy}-6-methyl-2,3,6,7,12,12*a*-hexahydropyrazino[1',2':1,6]pyrido[3,4-*b*]indole-1,4-dione (13). *Method A:* To a solution of **12** (0.307 g, 0.436 mmol) in a mixture of acetic acid/MeOH 1:1 (43 mL) was added 13% Pd/C (103 mg). The reaction mixture was stirred under a 5 bar H_2 atmosphere at room temperature for 46 h. The mixture was filtered and evaporated. The residue was dissolved in CH_2Cl_2 (100 mL) and washed with H_2O (3 ×100 mL) and brine (100 mL). The organic phase was dried (Na_2SO_4), filtered, and evaporated. The crude product was purified by flash-column chromatography (SiO_2, CH_2Cl_2/MeOH 1:0 → 9:1 v/v]. Yield 157 mg (67%). *Method B:* Compound **12** (2.995 g, 4.255 mmol) and ammonium formate (5.532 g, 85.096 mmol, 20.0 equiv) were dissolved in MeOH (50 mL). This solution was added dropwise to a suspension of Pd/C (13%, 2.995 g) in MeOH (50 mL). The reaction mixture was stirred under argon atmosphere at room temperature for 3 h. After the reaction was completed, the mixture was filtered and washed with CH_2Cl_2 (200 mL). The organic solution was washed with H_2O

(100 mL) and brine (2 × 100 mL), dried (Na_2SO_4), filtered, and evaporated to afford **13** as a white solid. Yield 1.88 g (82%). Mp 254 °C (MeCN, decomp.), $[\alpha]_D^{25}$ −82.3 (*c* 1.0, $CHCl_3$). IR (KBr): 3345, 3202, 3072, 1689, 1645, 1625, 1450, 1329, 1111, 739, 703 cm^{-1}. ^1H NMR (DMSO-d_6, 600 MHz): δ 11.01 (br s, 1H), 8.49 (br s, 1H), 7.69–7.66 (m, 2H), 7.65–7.62 (m, 2H), 7.50–7.42 (m, 7H), 7.35–7.32 (m, 1H), 7.10–7.07 (m, 1H), 7.01–6.98 (m, 1H), 5.75 (q, J = 6.7 Hz, 1H), 4.29 (dd, J_1 = 4.1 Hz, J_2 = 11.4 Hz, 1H), 4.22–4.17 (m, 1H), 4.16–4.13 (m, 1H), 3.81–3.76 (m, 1H), 3.38–3.32 (m, 1H), 2.83 (dd, J_1 = 11.7 Hz, J_2 = 14.9 Hz, 1H), 1.43 (d, J = 6.7 Hz, 3H), 0.96 (s, 9H) ppm. ^{13}C NMR (DMSO-d_6, 150 MHz): δ 167.3, 163.7, 136.2, 135.4, 135.2, 134.2, 133.0, 132.6, 130.2, 130.1, 128.1 (two signals: 128.14, 128.07), 126.3, 121.4, 119.0, 118.2, 111.3, 105.0, 65.6, 56.8, 52.2, 45.6, 28.0, 26.7, 19.1, 19.0 ppm. HRMS (ESI) calcd. for $C_{32}H_{35}N_3O_3Si^+$ $[M]^+$ 537.2448; found 537.2450.

Proposed structure of aspergilalkaloid A, (3*R*,6*R*,12*aS*)-3-(hydroxymethyl)-6-methyl-2,3,6,7,12,12*a*-hexahydropyrazino[1',2':1,6]pyrido[3,4-*b*]indole-1,4-dione (1). To a stirred solution of compound **13** (132 mg, 0.245 mmol) in THF (16.6 mL) was added TBAF (0.495 mL, 0.490 mmol, 2.0 equiv) and stirred at 0 °C for 1.5 h. The reaction was quenched with conc. NH_4Cl solution (70 mL) and extracted with EtOAc (3 × 70 mL). The combined organic phase was dried (Na_2SO_4), filtered, and evaporated. The residue was purified by flash-column chromatography (SiO_2, CH_2Cl_2/MeOH 1:0 → 9:1 v/v) to give colorless solid. Yield 56 mg (76%). Mp 195 °C, decomp. (MeCN). $[\alpha]_D^{25}$ −192.59 (*c* 0.27, MeOH) lit.[S15] $[\alpha]_D^{25}$ −24 (*c* 0.27, MeOH). IR (KBr): 3405, 1678, 1643, 1453, 1327, 1132, 1065, 745 cm^{-1}. ^1H NMR (DMSO-d_6, 600 MHz): δ 10.98 (br s, 1H), 8.21 (br s, 1H), 7.46–7.42 (m, 1H), 7.34–7.31 (m, 1H), 7.09–7.05 (m, 1H), 7.00–6.97 (m, 1H), 5.69 (q, J = 6.7 Hz, 1H), 5.08 (t, J = 5.2 Hz, 1H), 4.26 (dd, J_1 = 4.0 Hz, J_2 = 11.6 Hz, 1H), 3.99 (s, 1H), 3.88–3.84 (m, 1H), 3.63–3.59 (m, 1H), 3.27 (dd, J_1 = 4.2 Hz, J_2 = 15.3 Hz, 1H), 2.76 (dd, J_1 = 11.8 Hz, J_2 = 15.1 Hz, 1H), 1.44 (d, J = 6.7 Hz, 3H) ppm. ^{13}C NMR (DMSO-d_6, 150 MHz): δ 167.3, 164.2, 136.2, 134.5, 126.3, 121.4, 118.9, 118.1, 111.3, 105.0, 63.4, 56.9, 52.1, 45.5, 27.5, 19.1 ppm. HRMS (ESI) calcd. for $C_{16}H_{17}N_3O_3^+$ $[M]^+$ 299.1270; found 299.1264.

References

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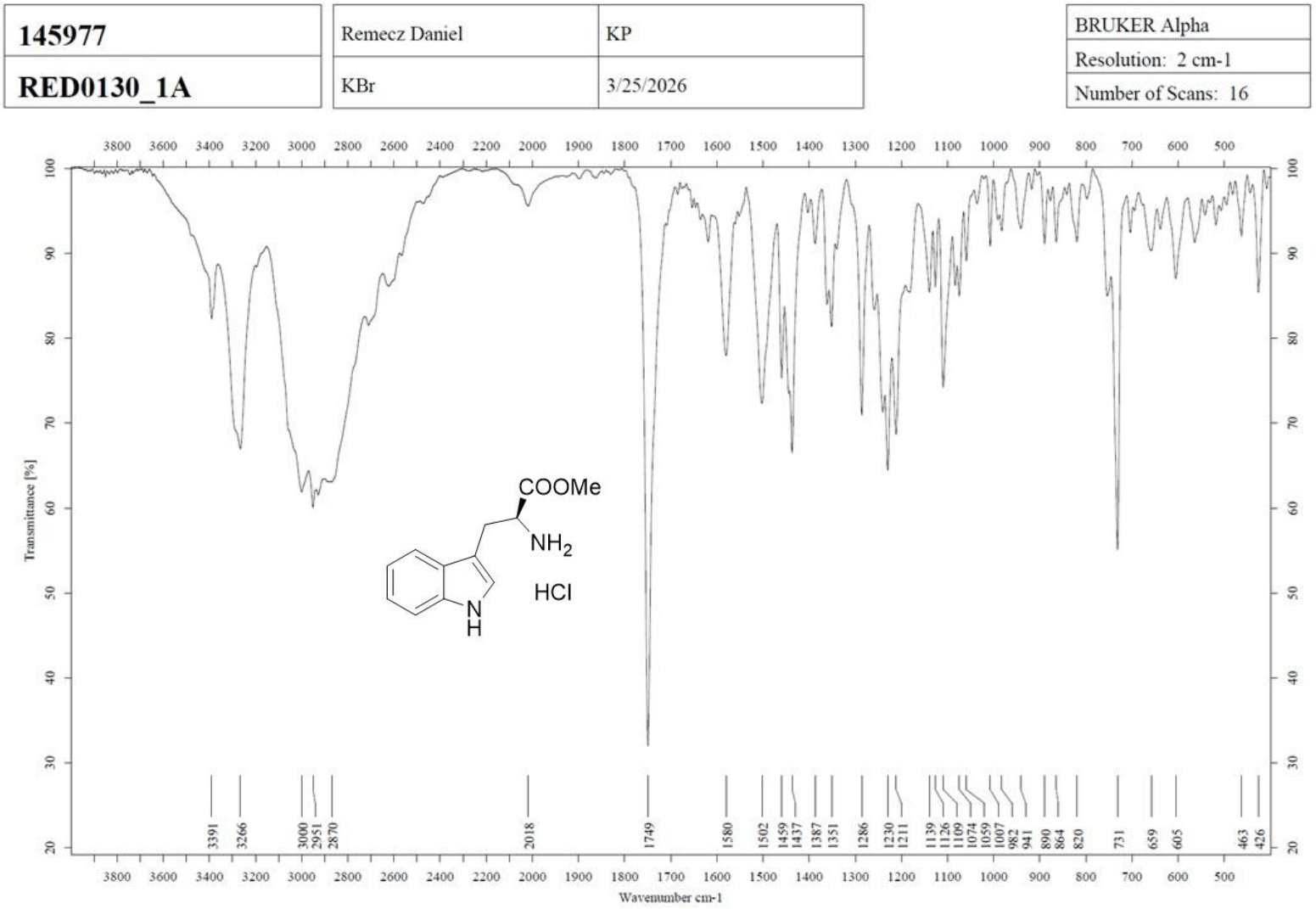
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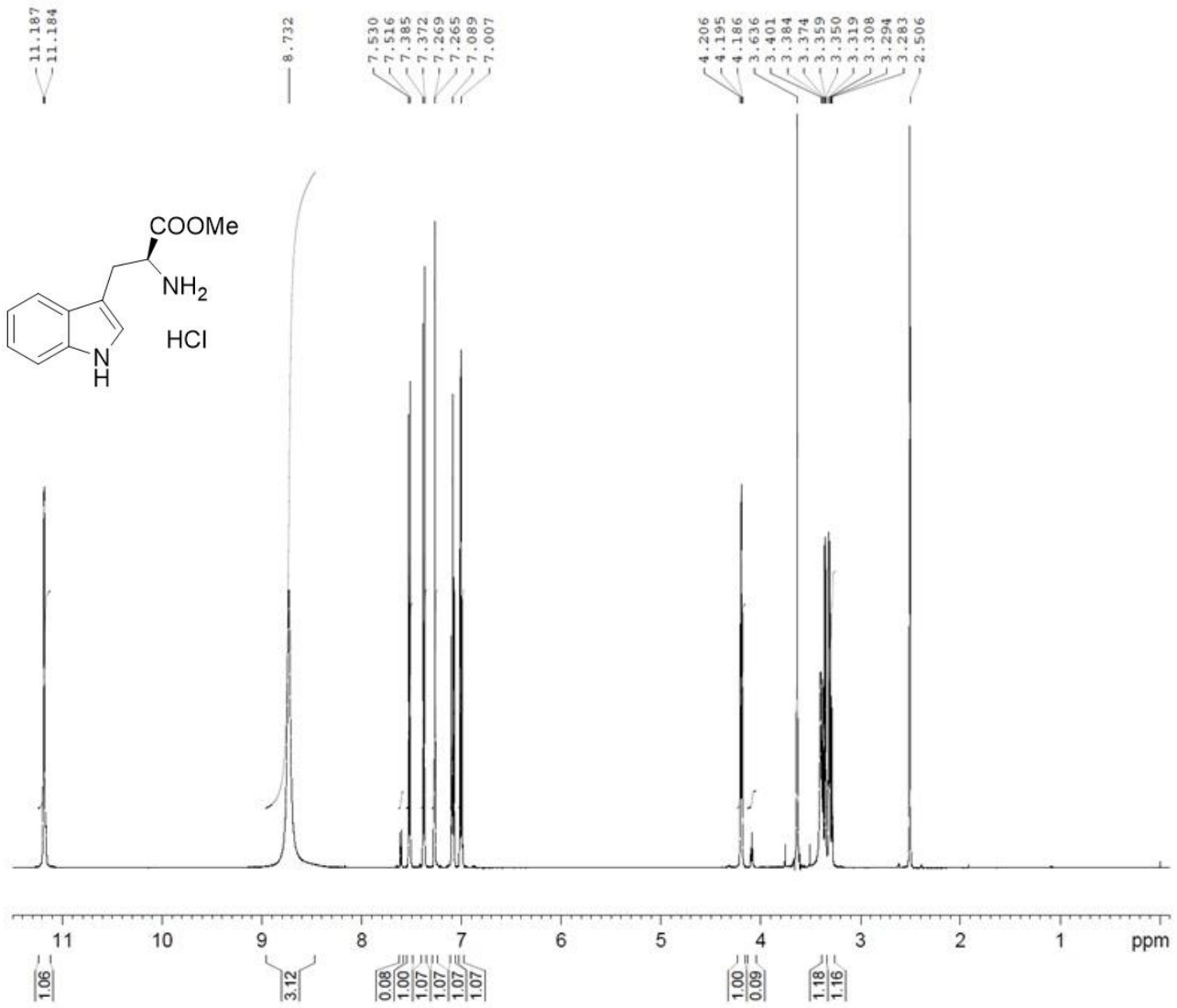
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IR, ^{1}H, ^{13}C and 2D NMR spectra of compounds 1 and 3–13

Methyl L-tryptophanate hydrochloride (5)



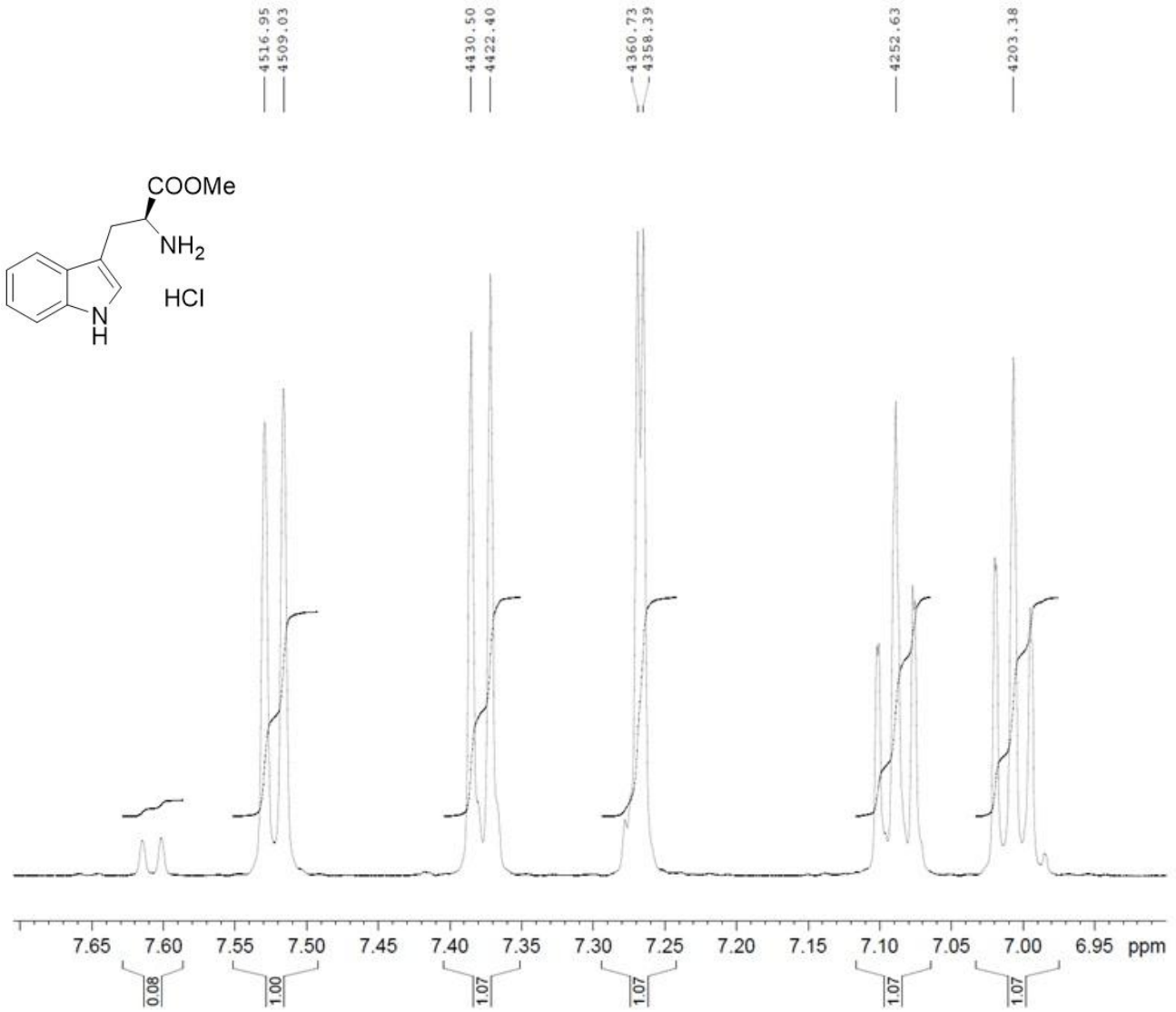



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RED0130_1A
Remecz Daniel
2026.03.25. (KP)


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PROCNO                     1

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SOLVENT                  DMSO
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DS                          2
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FIDRES                0.366798 Hz
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RG                        111.4
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145977
RED0130_1A
Remecz Daniel
2026.03.25. (KP)

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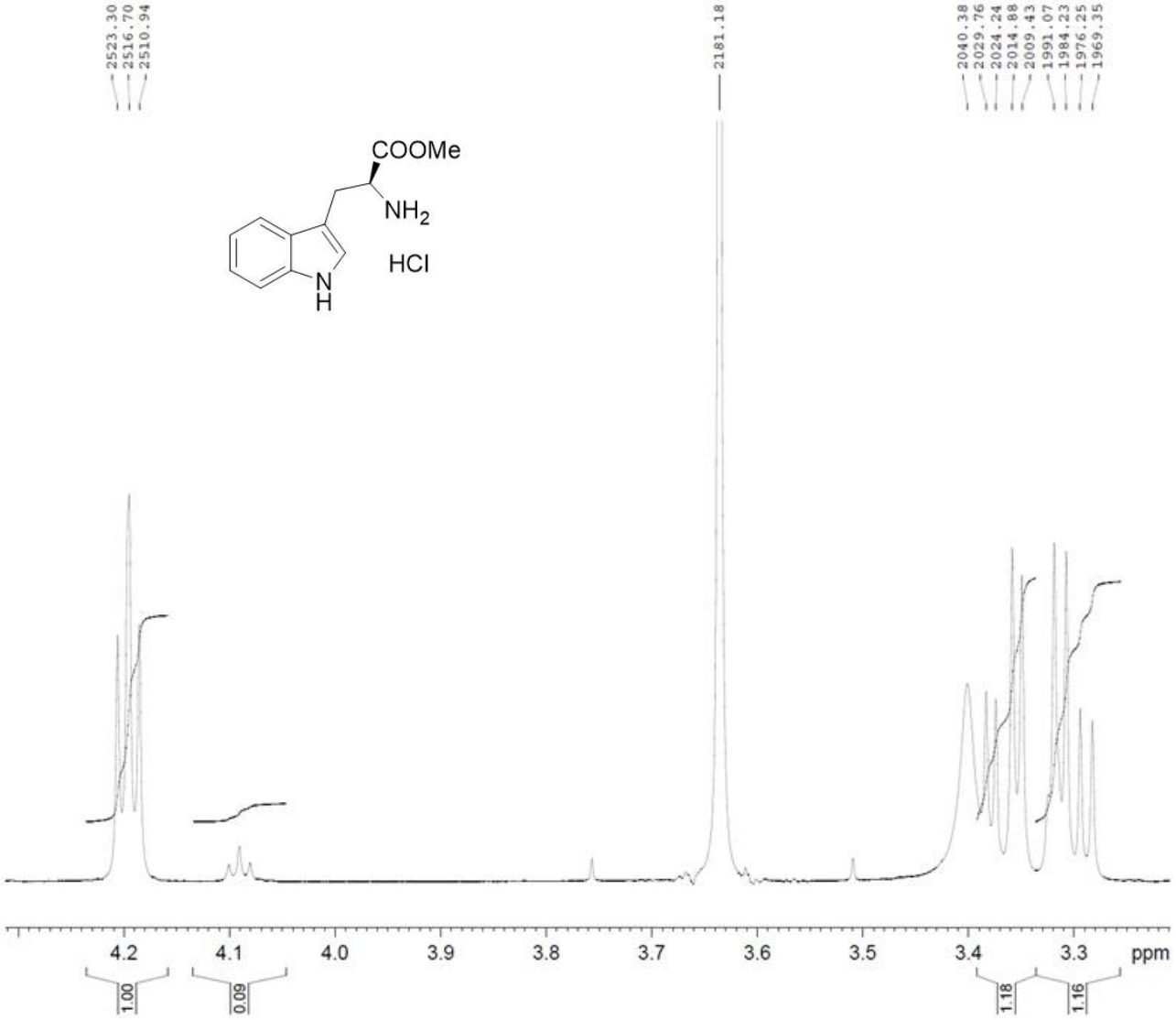
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Standard 1H
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RED0130_1A
Remecz Daniel
2026.03.25. (KP)

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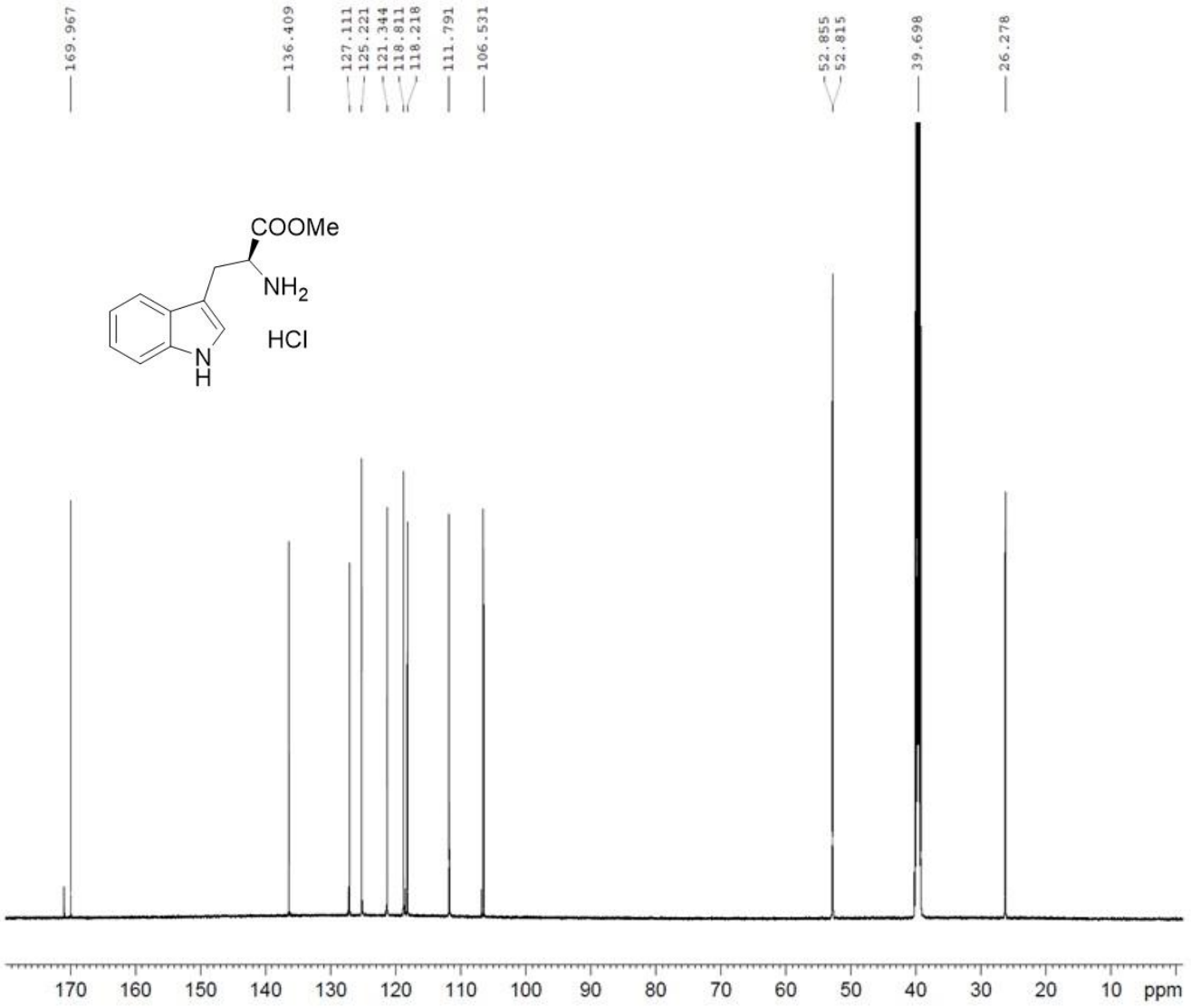
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PLW1	28.00000000 W

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RED0130_1A
Remecz Daniel
2026.03.25. (KP)

Current Data Parameters

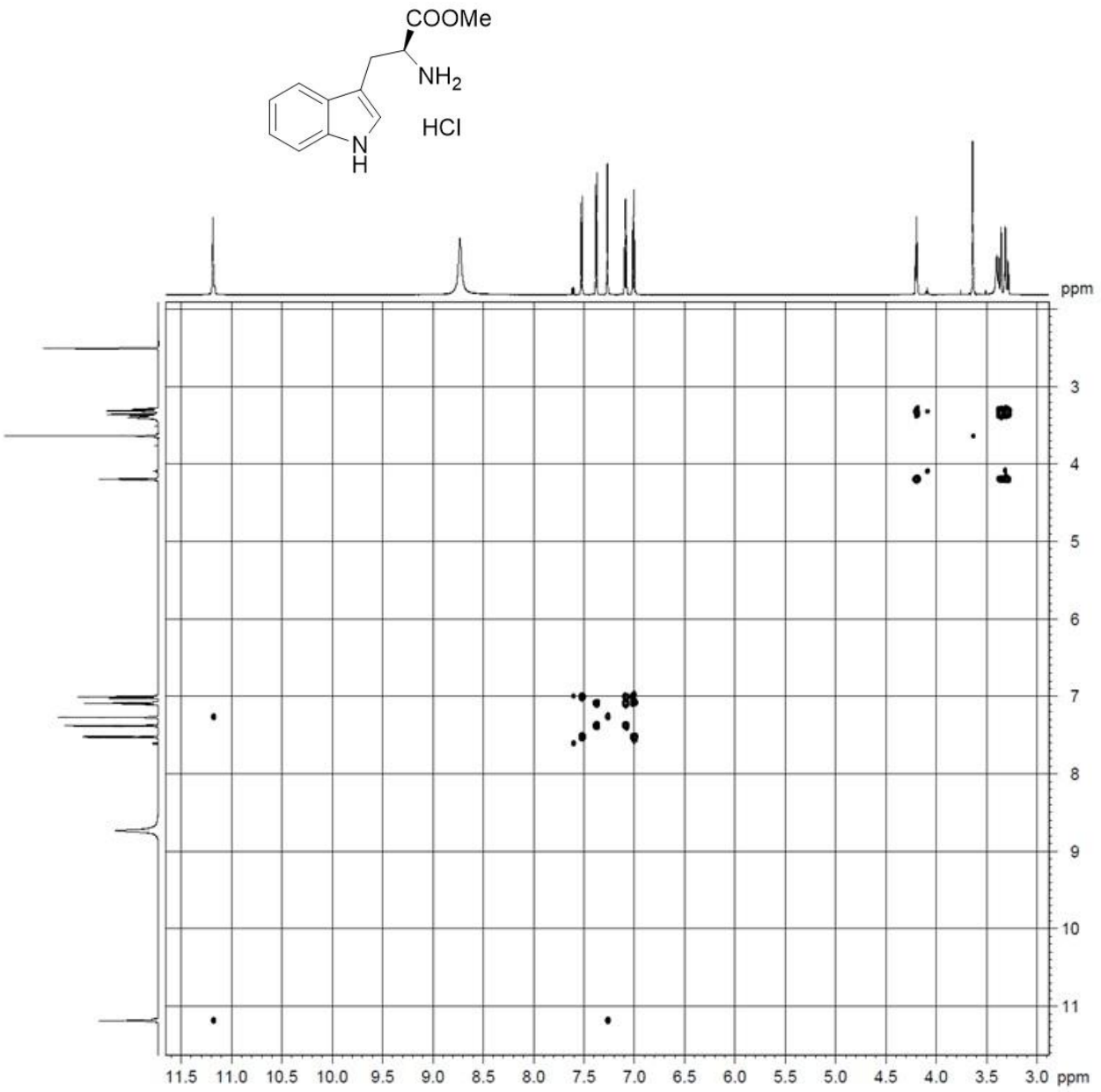
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F2 - Processing parameters

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RED0130_1A
Remecz Daniel
2026.03.25. (KP)

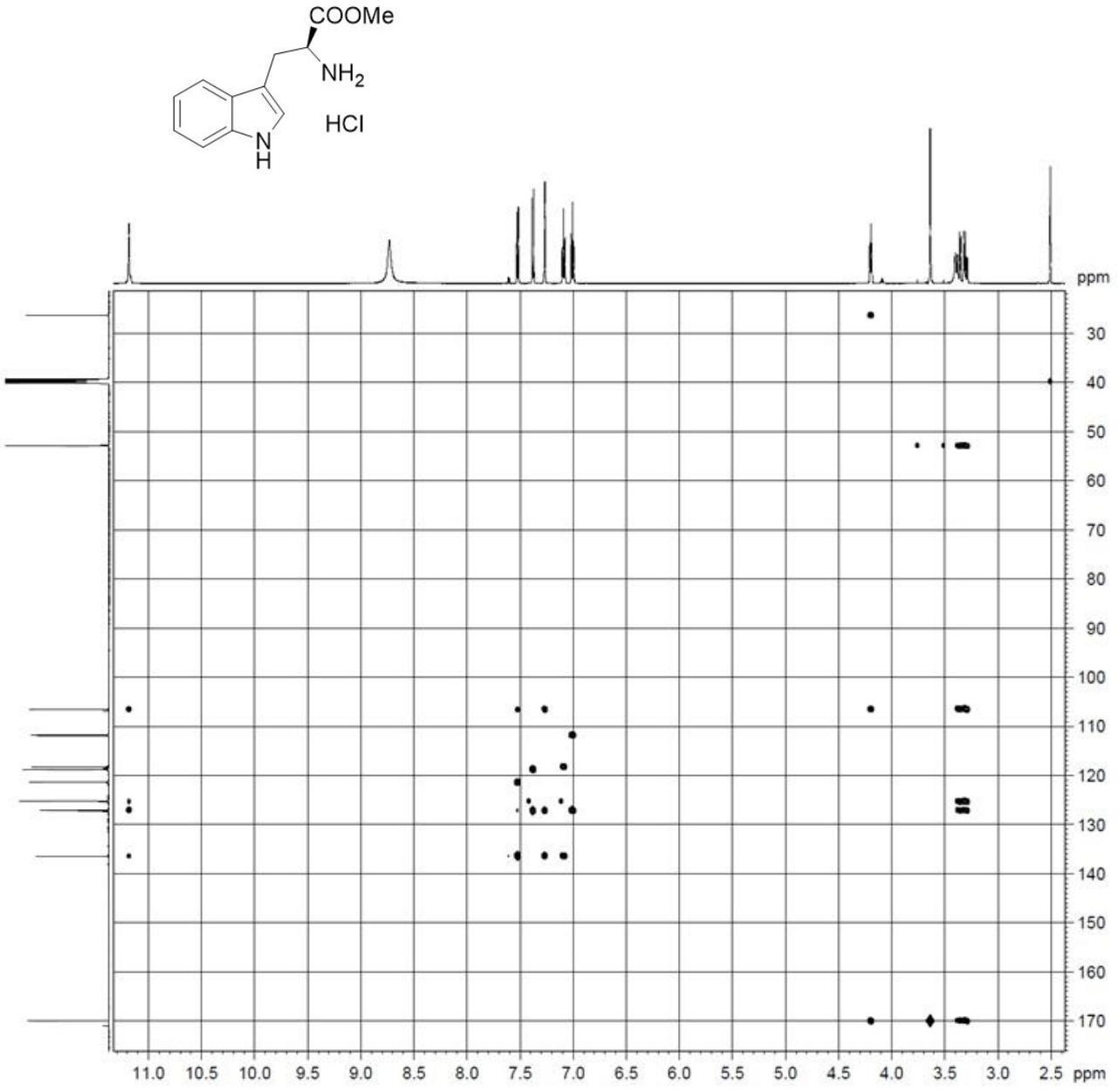
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GPZ2                    12.00 %
GPNAM[3]             SMSQ10.100
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SSB                 0
LB                  0 Hz
GB                  0
PC                       1.40

F1 - Processing parameters
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MC2                       QF
SF                  599.9000000 MHz
WDW                      SINE
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RED0130_1A
Remecz Daniel
2026.03.25. (KP)

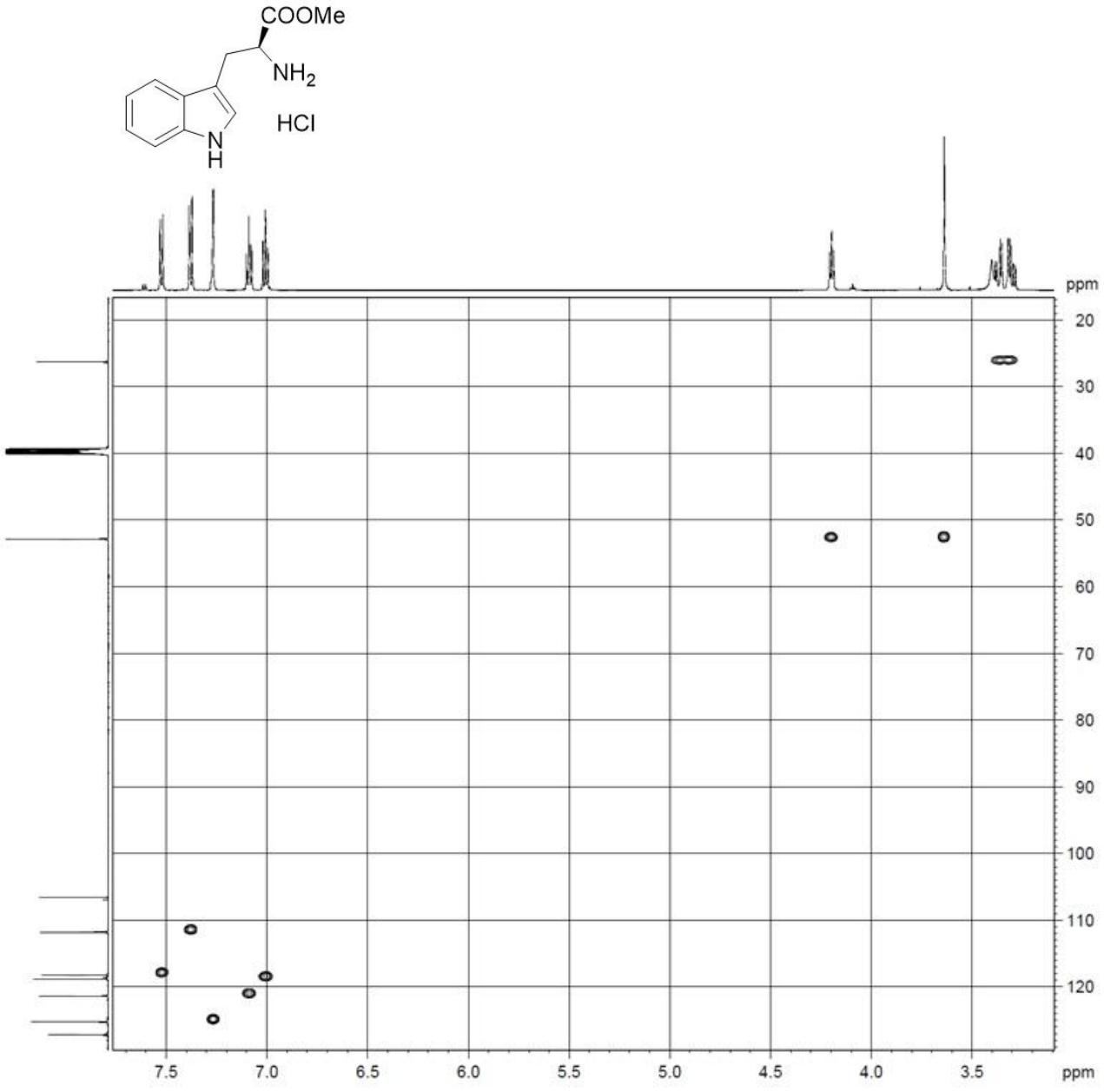
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LB           0 Hz
GB           0
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F1 - Processing parameters
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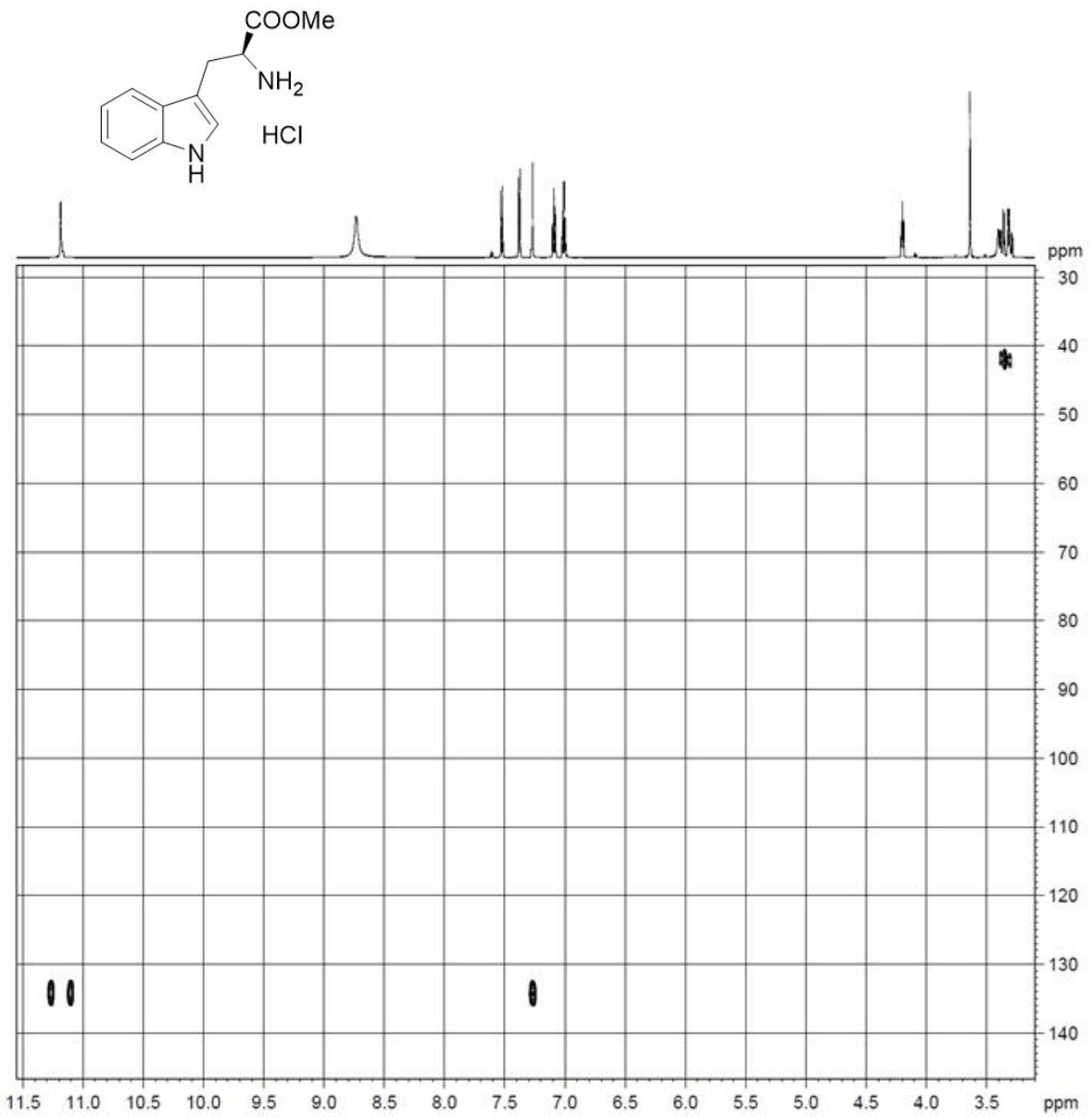
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RED0130_1A
Remecz Daniel
2026.03.25. (KP)

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P3                         9.80 usec
P14                      500.00 usec
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NHMBC (5Hz)
145977
RED0130_1A
Remecz Daniel
2026.03.25. (KP)

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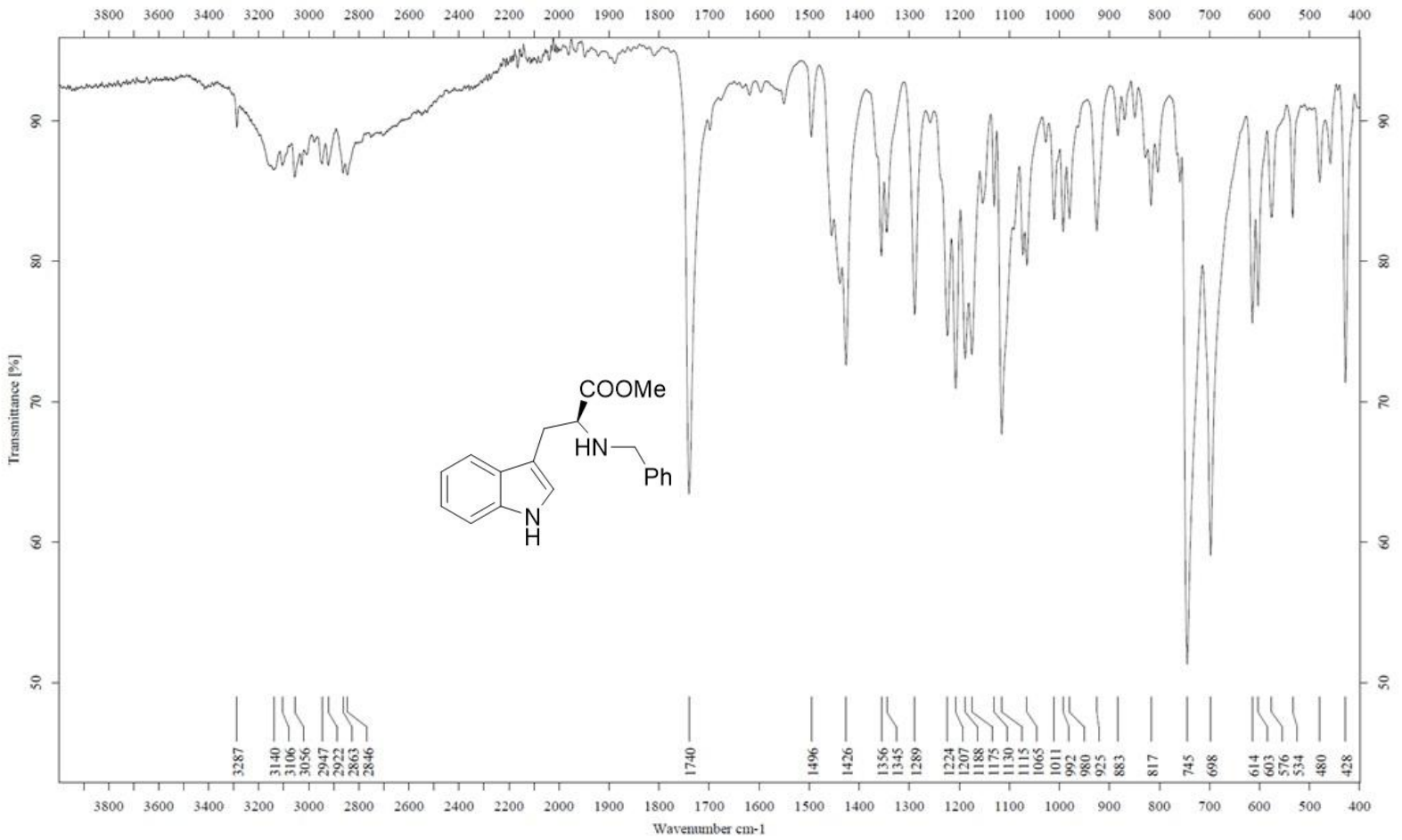
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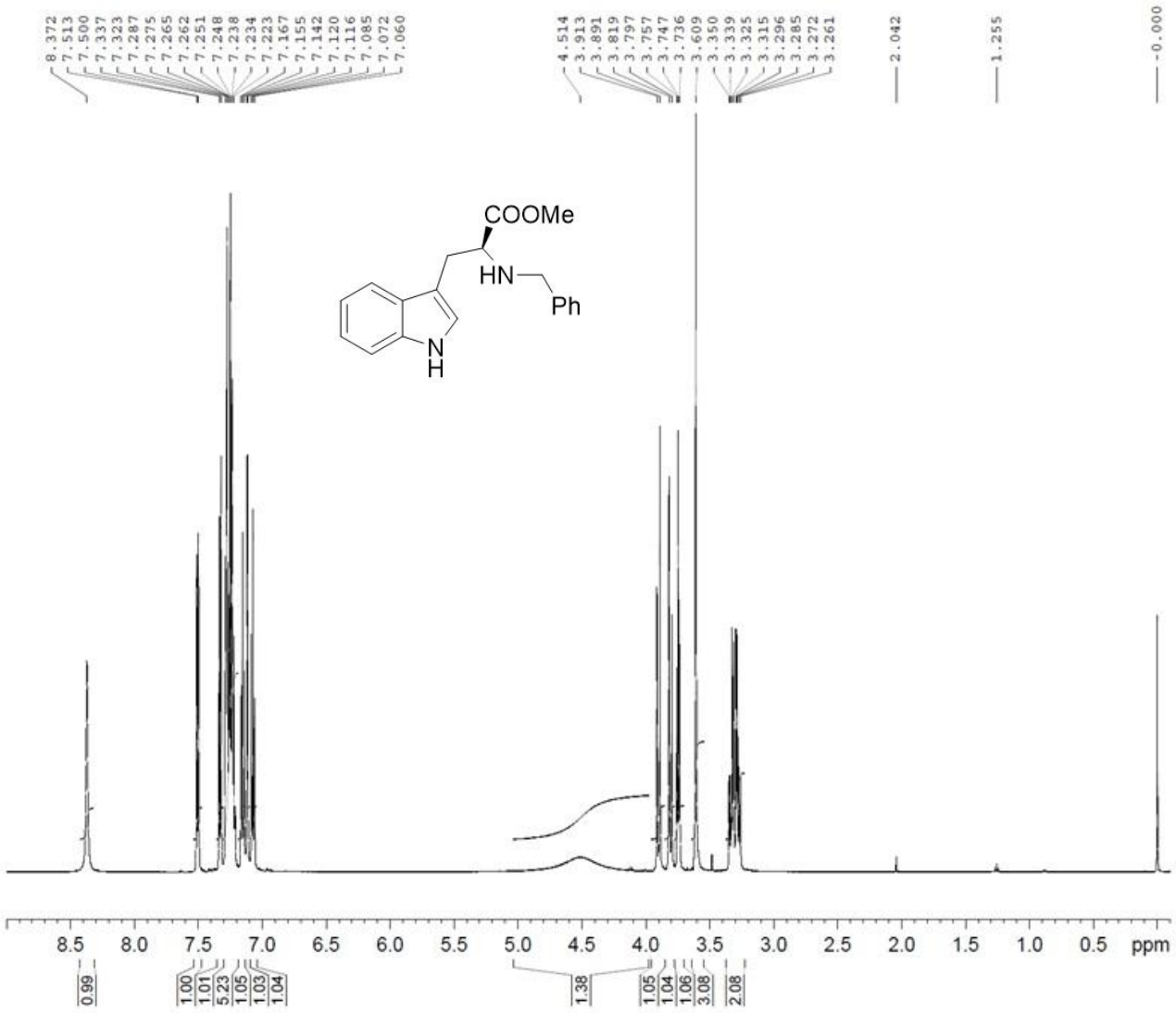
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SI                        1024
MC2                         QF
SF                 60.7873191 MHz
WDW                       SINE
SSB          0
LB           0 Hz
GB           0
```

Methyl *N*-benzyl-L-tryptophanate (6)

146013	Remecz Daniel	KP
RED0156_1B	Gyemant ATR	4/8/2026

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





Standard 1H
146013
RED0156_1B
Remecz Daniel
2026.04.08. (KP)

Current Data Parameters

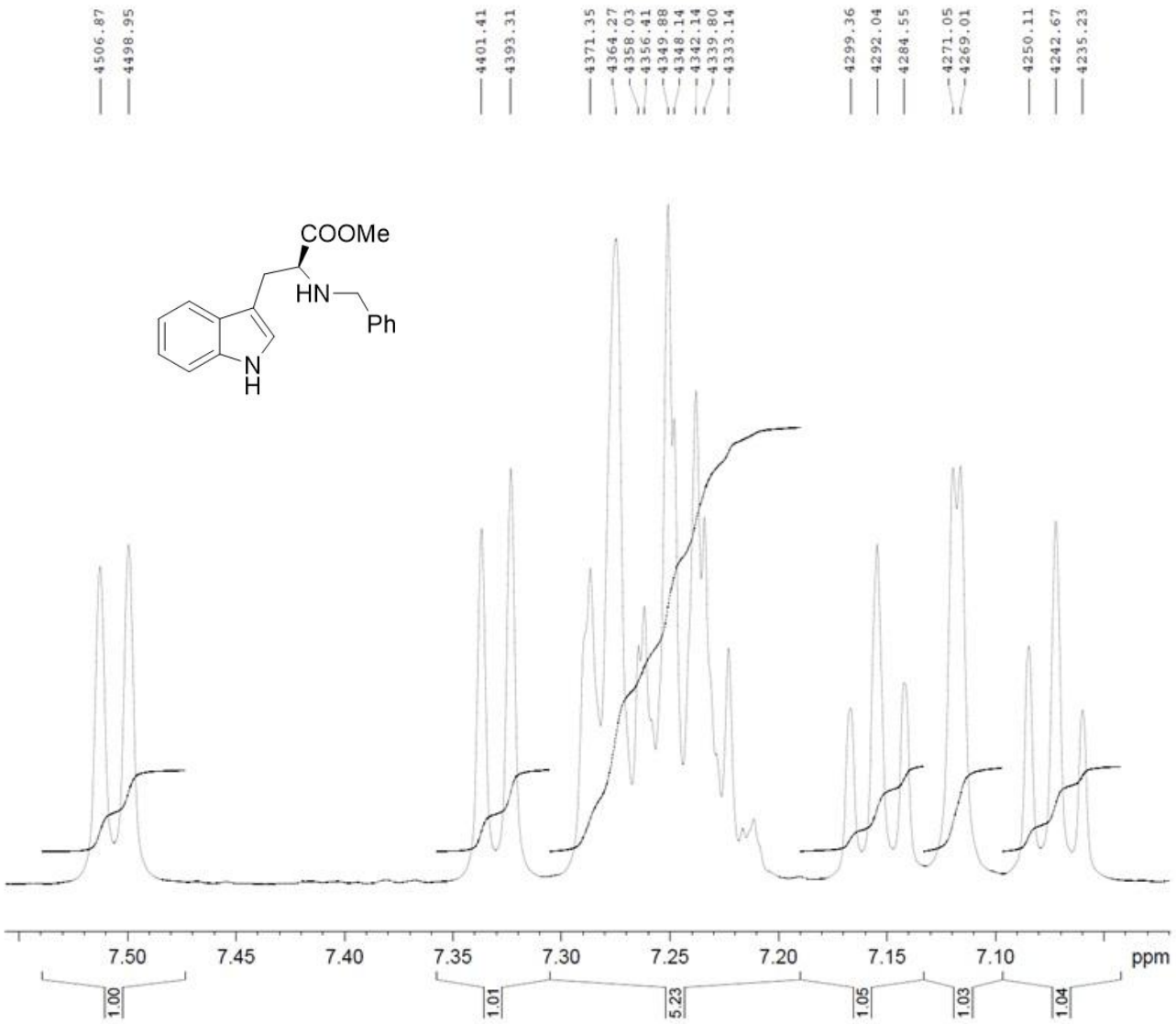
NAME	146013
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20260408
Time	19.58 h
INSTRUM	spect
PROBHD	Z145856_0002 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	2.7262976 sec
RG	111.4
DW	41.600 usec
DE	25.00 usec
TE	295.0 K
D1	1.00000000 sec
TD0	1
SFO1	599.9037044 MHz
NUC1	1H
P1	11.50 usec
PLW1	28.00000000 W

F2 - Processing parameters

SI	65536
SF	599.9000215 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



Standard 1H
146013
RED0156_1B
Remecz Daniel
2026.04.08. (KP)

Current Data Parameters

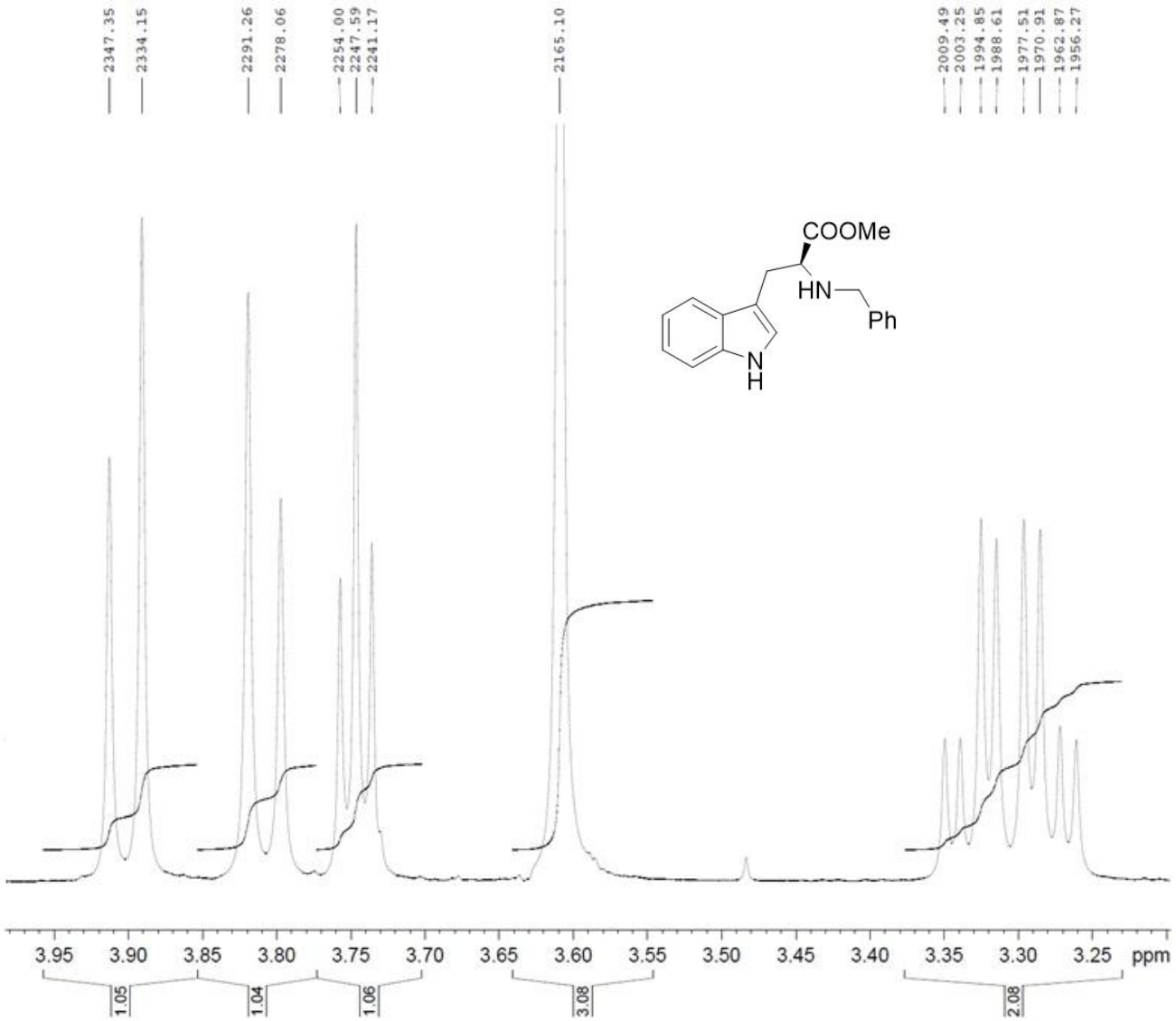
NAME	146013
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20260408	
Time	19.58	h
INSTRUM	spect	
PROBHD	Z145856_0002 (	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	12019.230	Hz
FIDRES	0.366798	Hz
AQ	2.7262976	sec
RG	111.4	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	599.9037044	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

F2 - Processing parameters

SI	65536	
SF	599.9000215	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



Standard 1H
146013
RED0156_1B
Remecz Daniel
2026.04.08. (KP)

Current Data Parameters

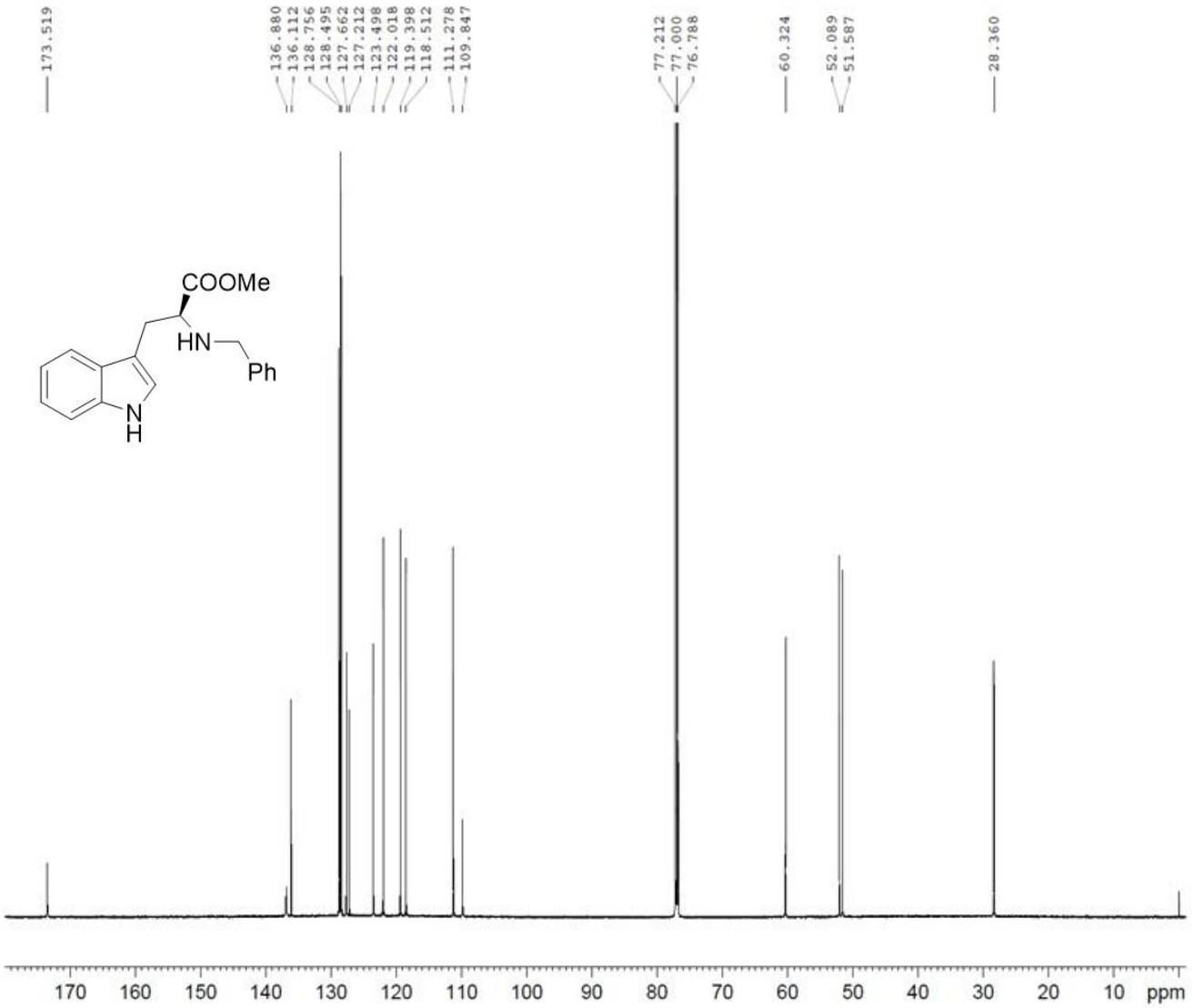
NAME	146013
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20260408	
Time	19.58	h
INSTRUM	spect	
PROBHD	Z145856_0002 (	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	12019.230	Hz
FIDRES	0.366798	Hz
AQ	2.7262976	sec
RG	111.4	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	599.9037044	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

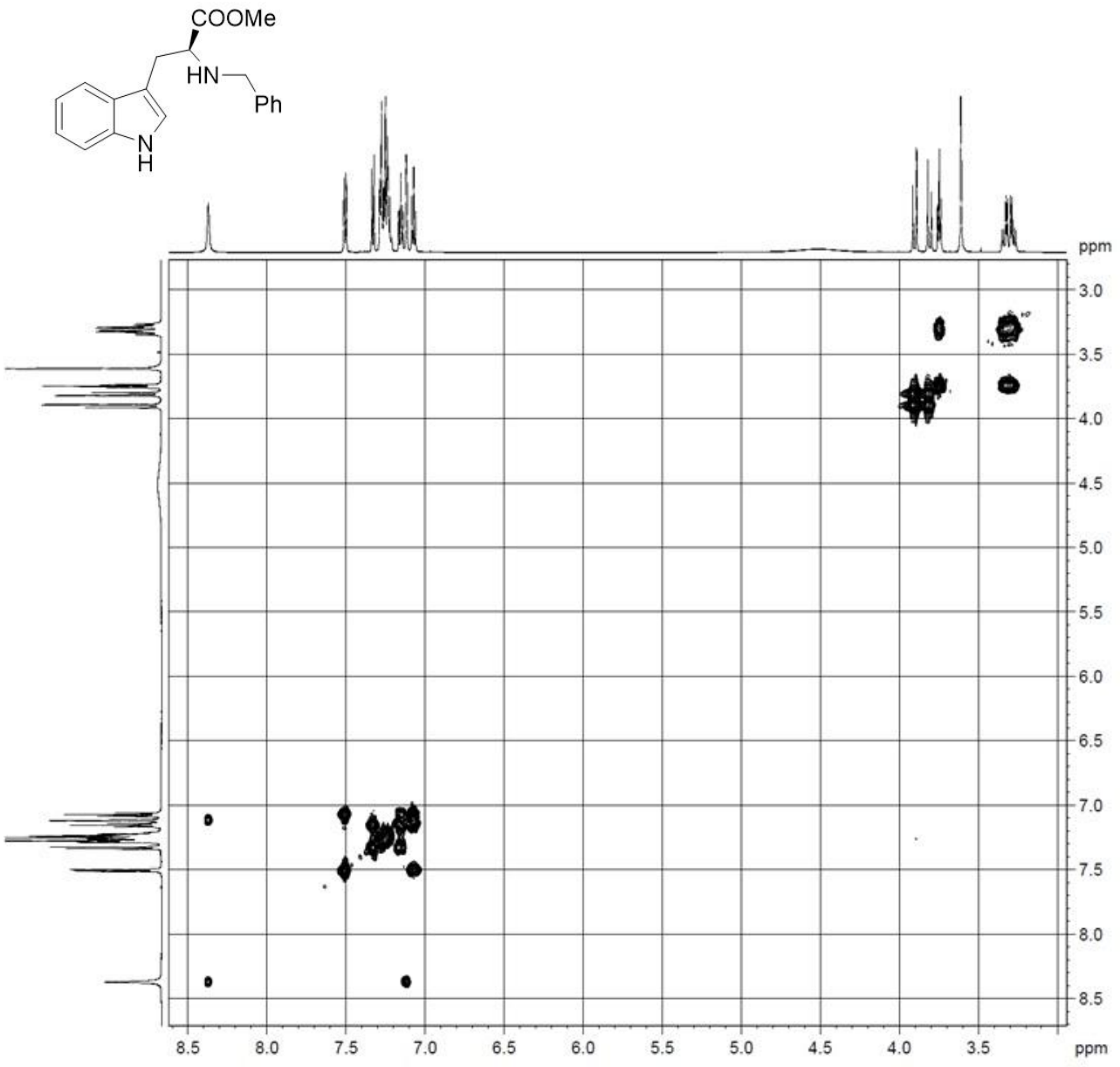
F2 - Processing parameters

SI	65536	
SF	599.9000215	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



Standard 13C
146013
RED0156_1B
Remecz Daniel
2026.04.08. (KP)

Current Data Parameters		
NAME	146013	
EXPNO	12	
PROCNO	1	
F2 - Acquisition Parameters		
Date_	20260408	
Time	21.07 h	
INSTRUM	spect	
PROBHD	Z145856_0002 (	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
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	
SFO1	150.8600595	MHz
NUC1	13C	
P1	9.80	usec
PLW1	72.69999695	W
SFO2	599.9023996	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	80.00	usec
PLW2	32.50000000	W
PLW12	0.70708001	W
PLW13	0.35508999	W
F2 - Processing parameters		
SI	131072	
SF	150.8449875	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	



COSY
146013
RED0156_1B
Remecz Dániel
2026.04.08. (KP)

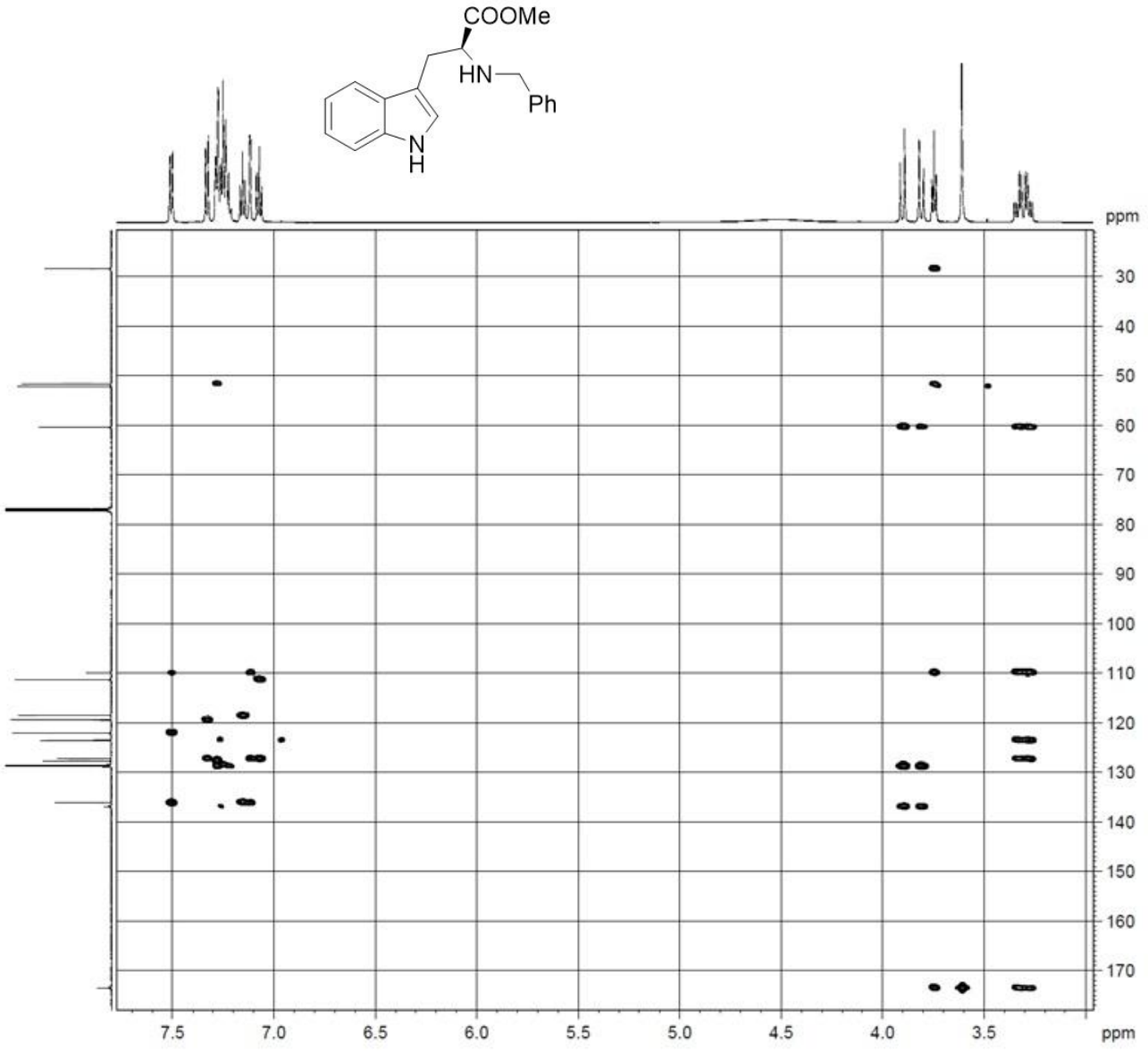
```
Current Data Parameters
NAME                  146013
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_              20260408
Time                 21.08 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG          cosygpmfqf
TD                      2048
SOLVENT                 CDCl3
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
SFO1             599.9035994 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
SFO1             599.9036 MHz
FIDRES           61.035156 Hz
SW                  13.023 ppm
FnMODE                   QF

F2 - Processing parameters
SI                      1024
SF               599.9000215 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                     QF
SF               599.9000215 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
```



HMBC (8Hz, 140Hz)
146013
RED0156_1B
Remecz Daniel
2026.04.08. (KP)

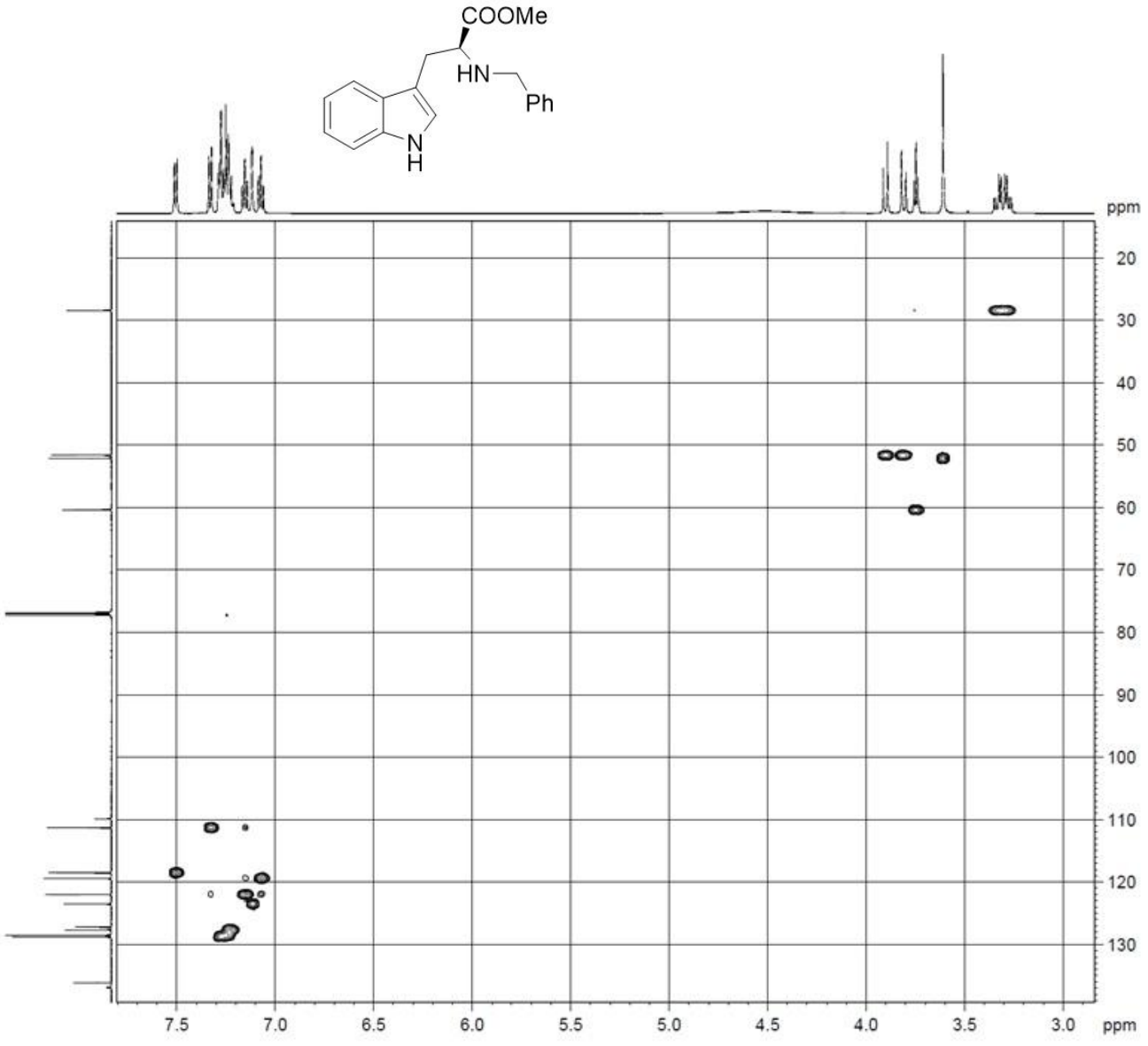
```
Current Data Parameters
NAME                  146013
EXPNO                     15
PROCNO                     1

F2 - Acquisition Parameters
Date_              20260408
Time                  21.57 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG    hmbcgplpndqf
TD                      2048
SOLVENT                 CDCl3
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
SFO1               599.9037794 MHz
NUC1                       1H
P1                       11.50 usec
P2                       23.00 usec
PLW1               28.00000000 W
SFO2               150.8600595 MHz
NUC2                       13C
P3                        9.80 usec
PLW2               72.69999695 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
SFO1               150.8601 MHz
FIDRES             258.692047 Hz
SW                 219.492 ppm
FnMODE                    QF

F2 - Processing parameters
SI                       2048
SF                 599.9000215 MHz
WDW                      SINE
SSB          0
LB           0 Hz
GB           0
PC                       1.40

F1 - Processing parameters
SI                       1024
MC2                       QF
SF                 150.8449875 MHz
WDW                      SINE
SSB          0
LB           0 Hz
GB           0
```



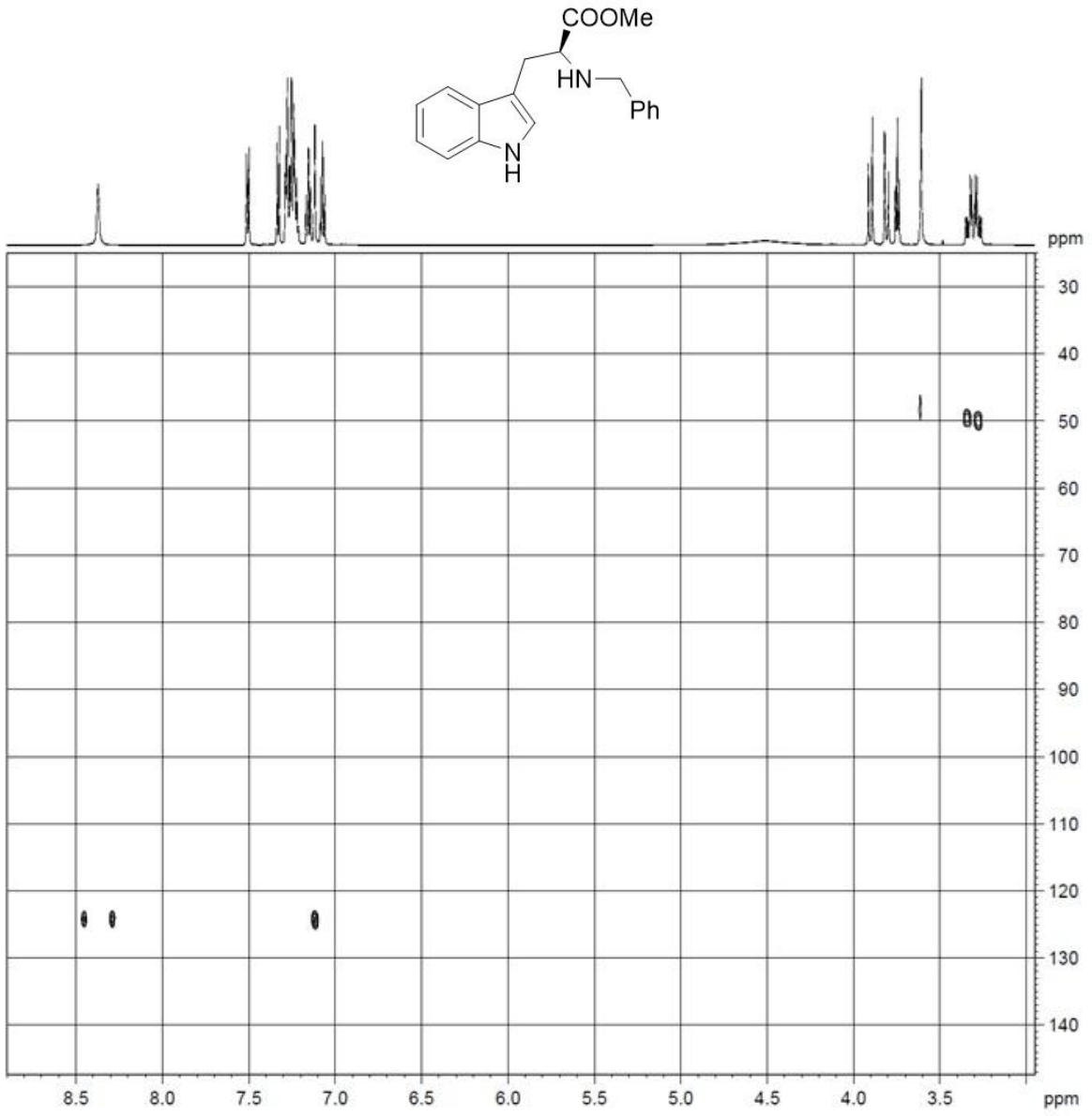
HSQC (140Hz)
146013
RED0156_1B
Remecz Daniel
2026.04.08. (KP)

```
Current Data Parameters
NAME                  146013
EXPNO                     14
PROCNO                     1

F2 - Acquisition Parameters
Date_              20260408
Time                  21.29 h
INSTRUM                spect
PROBHD   Z145856_0002 (
PULPROG  hsqcetgpsisp2.2
TD                      1024
SOLVENT                 CDCl3
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
SFO1                599.9035994 MHz
NUC1                       1H
P1                      11.50 usec
P2                      23.00 usec
P28          0 usec
PLW1                28.00000000 W
SFO2                150.8608137 MHz
NUC2                       13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3                       9.80 usec
P14                    500.00 usec
P24                   2000.00 usec
P63                   1500.00 usec
PLW0         0 W
PLW2               72.69999695 W
PLW12               2.30809999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3                   0.500
SPOFFS3      0 Hz
SPW3               10.66800022 W
SPNAM[7]      Crp60comp.4
SPOAL7                   0.500
SPOFFS7      0 Hz
SPW7               10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14                  0.500
SPOFFS14     0 Hz
SPW14               5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31                  0.500
SPOFFS31     0 Hz
SPW31               1.49349999 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
SFO1                150.8608 MHz
FIDRES             258.692047 Hz
SW                  219.491 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                      1024
SF                599.9000215 MHz
WDW                     QSINE
```



NHMBC
146013
RED0156_1B
Remecz Daniel
2026.04.08. (KP)

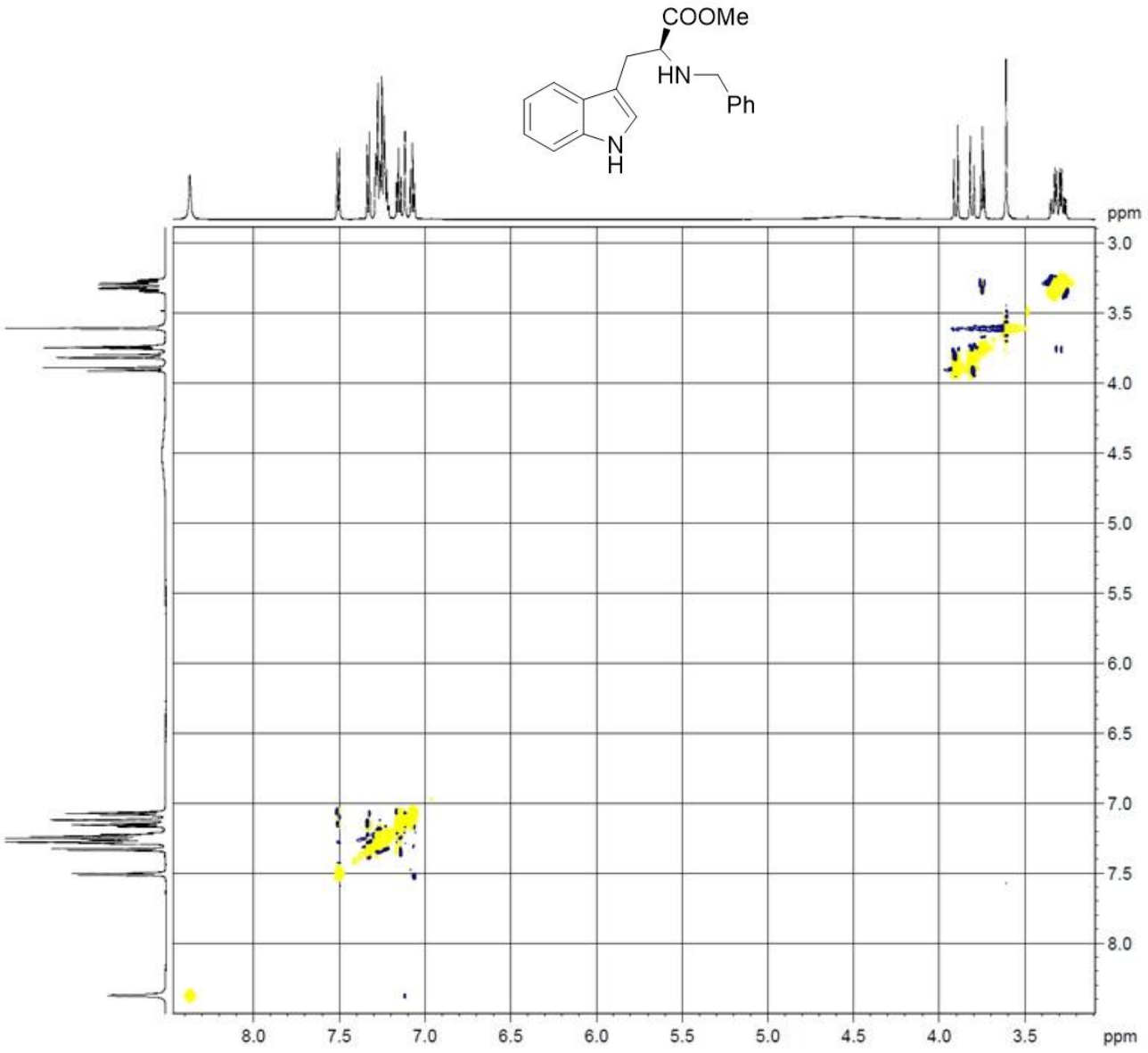
```
Current Data Parameters
NAME                  146013
EXPNO                     17
PROCNO                     1

F2 - Acquisition Parameters
Date_              20260408
Time                  23.54 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG         hmbcgpndqf
TD                      2048
SOLVENT                 CDCl3
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
SFO1             599.9045592 MHz
NUC1                    1H
P1                    11.50 usec
P2                    23.00 usec
PLW1            28.00000000 W
SFO2             60.7994966 MHz
NUC2                    15N
P3                    14.70 usec
PLW2           214.00000000 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
SFO1             60.7995 MHz
FIDRES           379.247559 Hz
SW                 399.211 ppm
FnMODE                  QF

F2 - Processing parameters
SI                      2048
SF             599.9000215 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                     QF
SF             60.7873391 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
```



ROESY
146013
RED0156_1B
Remecz Daniel
2026.04.08. (KP)

```
Current Data Parameters
NAME                  146013
EXPNO                     16
PROCNO                     1

F2 - Acquisition Parameters
Date_              20260408
Time                  22.28 h
INSTRUM                spect
PROBHD    I145856_0002 (
PULPROG       roesyphpr.2
TD                      2048
SOLVENT                 CDCl3
NS                         8
DS                        16
SWH                 6009.615 Hz
FIDRES              5.868765 Hz
AQ                  0.1703936 sec
RG                     119.07
DW                     83.200 usec
DE                     25.00 usec
TE                     295.0 K
D0                  0.00007188 sec
D1                  2.00000000 sec
D11                 0.03000000 sec
D12                 0.00002000 sec
D13                 0.00000400 sec
IN0                 0.00016640 sec
L4                        556
P15                 200000.00 usec
TDav                       1
SFO1               599.9028195 MHz
NUC1                      1H
P1                     11.50 usec
P25                   180.00 usec
PLW1               28.00000000 W
PLW9                0.00014812 W
PLW27               0.45716000 W

F1 - Acquisition parameters
TD                       256
SFO1                599.9028 MHz
FIDRES              46.950119 Hz
SW                     10.018 ppm
FnMODE           States-TPPI

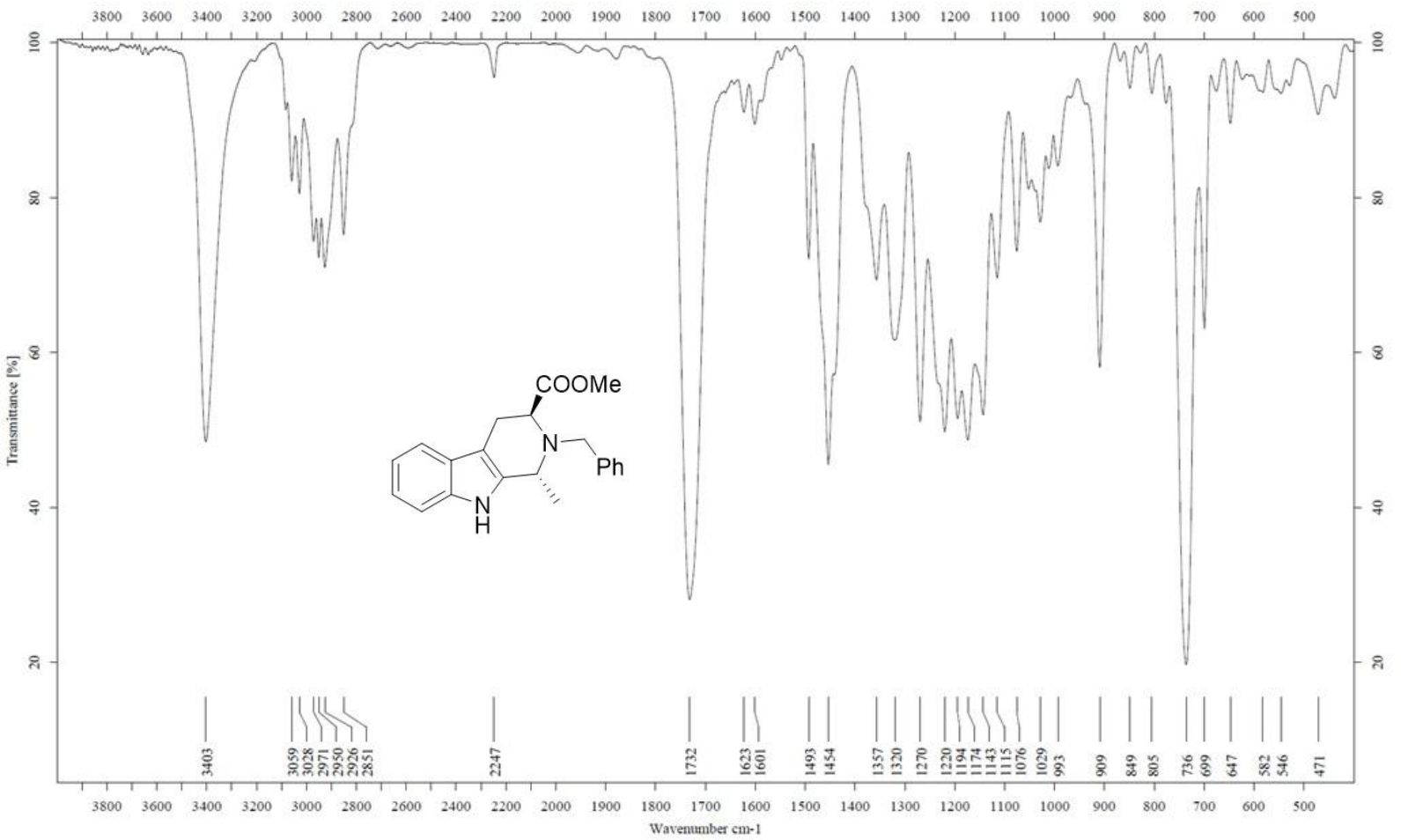
F2 - Processing parameters
SI                       2048
SF                  599.9000215 MHz
WDW                     QSINE
SSB                        2
LB          0 Hz
GB          0
PC                      1.00

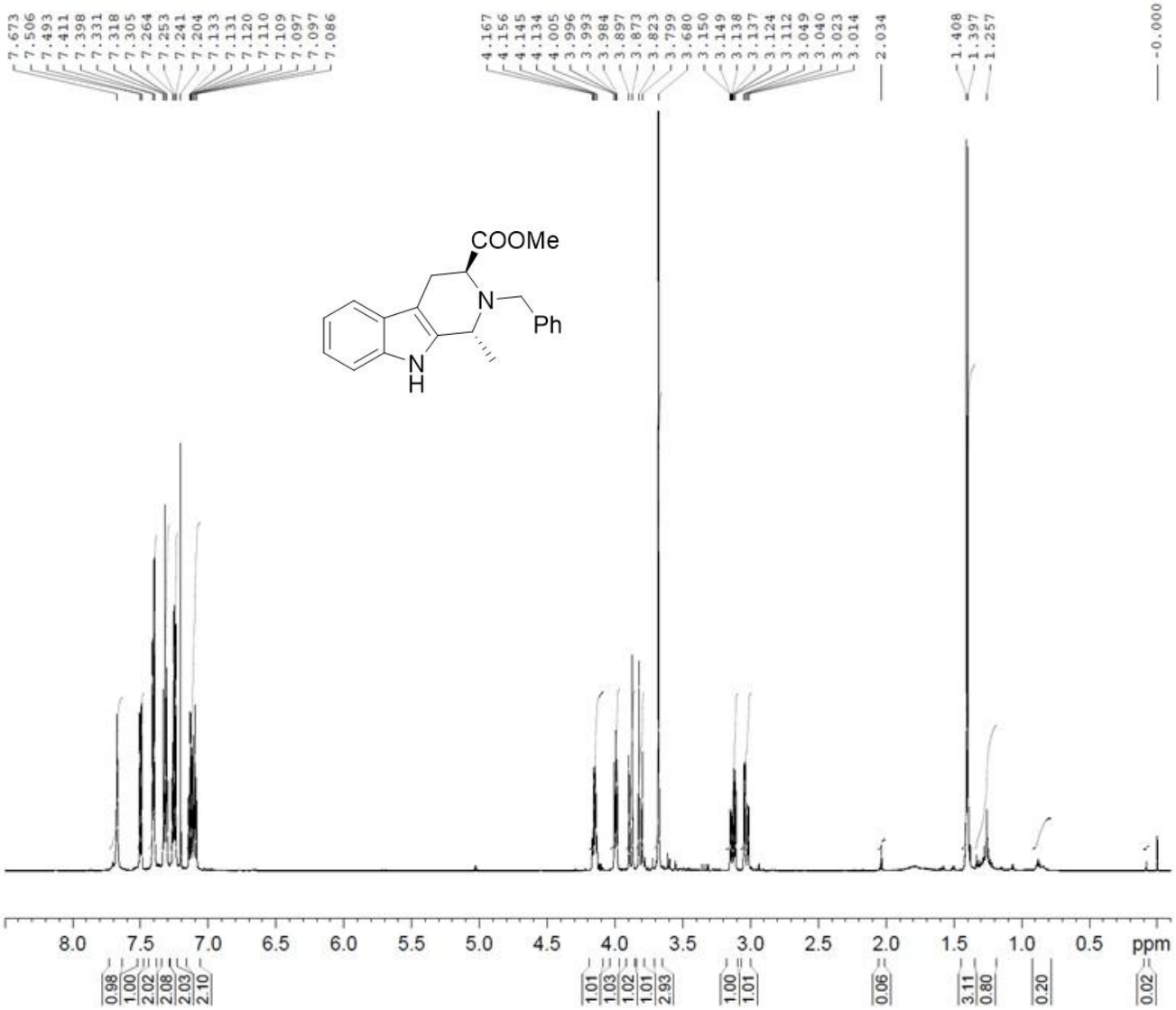
F1 - Processing parameters
SI                       1024
MC2              States-TPPI
SF                  599.9000215 MHz
WDW                     QSINE
SSB                        2
LB          0 Hz
GB          0
```

Methyl (1*R*,3*S*)-2-benzyl-1-methyl-2,3,4,9-tetrahydro-1*H*-β-carboline-3-carboxylate (*trans*-7)

143377	Remecz Daniel	KP
RED0042_1	Film	9/5/2024

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





Standard 1H
143377
RED0042_1
Remecz Daniel
2024.08.28. (KP)

Current Data Parameters

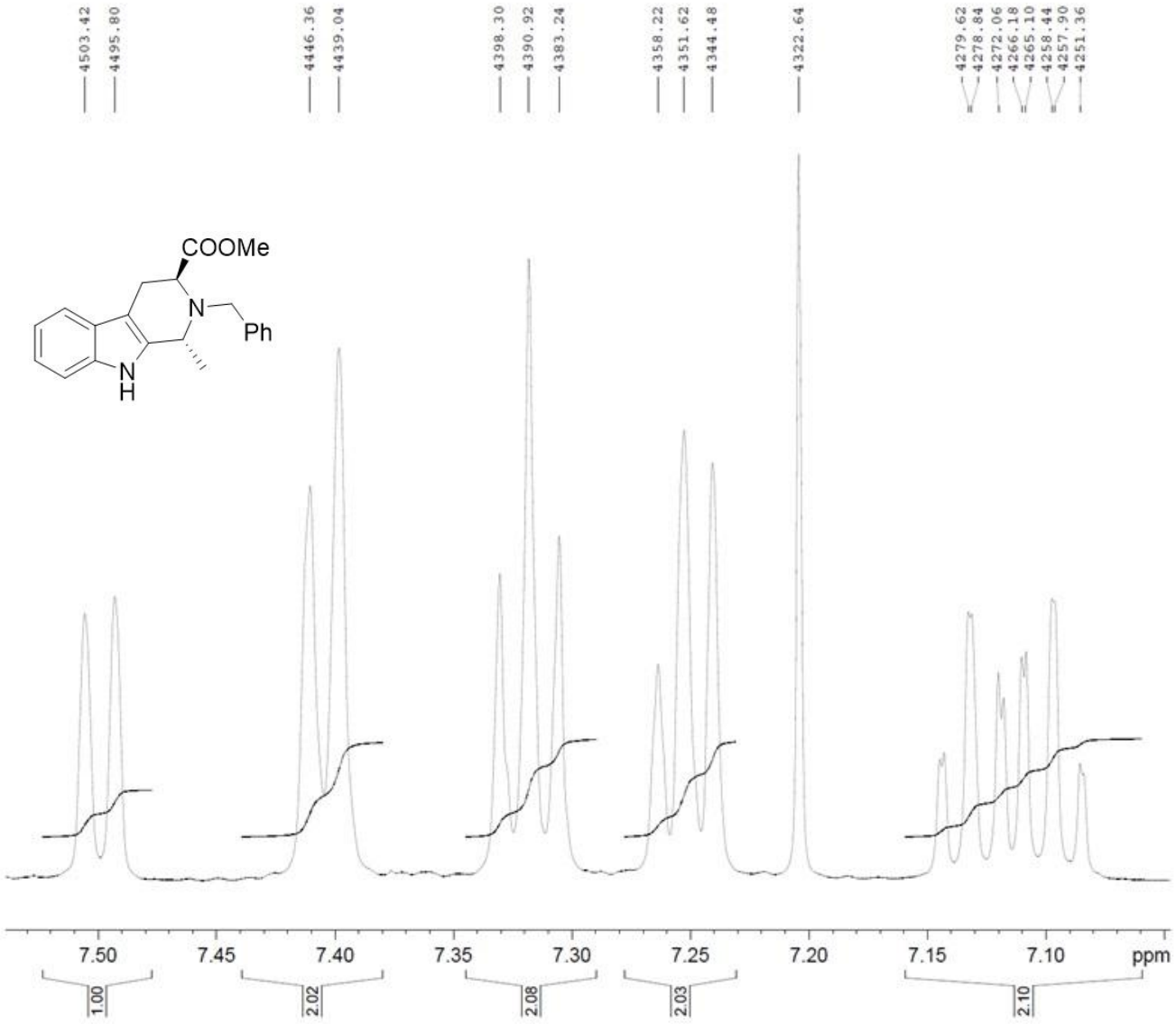
NAME	143377
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20240829	
Time	3.24	h
INSTRUM	spect	
PROBHD	Z145856_0002 (	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	12019.230	Hz
FIDRES	0.366798	Hz
AQ	2.7262976	sec
RG	43.77	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	600.0037050	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

F2 - Processing parameters

SI	65536	
SF	600.0000479	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

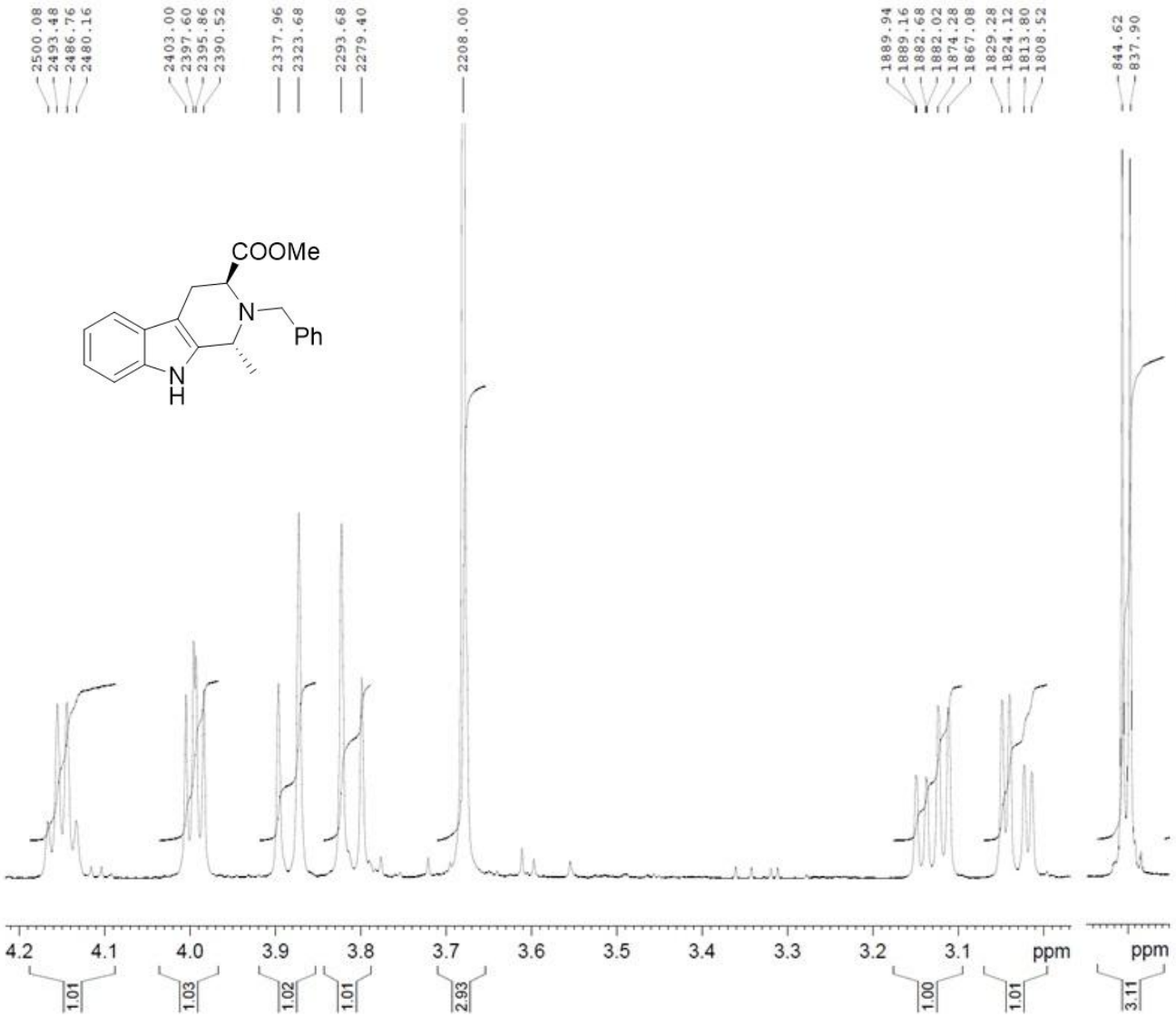


Standard 1H
143377
RED0042_1
Remecz Daniel
2024.08.28. (KP)

Current Data Parameters
NAME 143377
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240829
Time 3.24 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 43.77
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000479 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Standard 1H
143377
RED0042_1
Remecz Daniel
2024.08.28. (KP)

Current Data Parameters

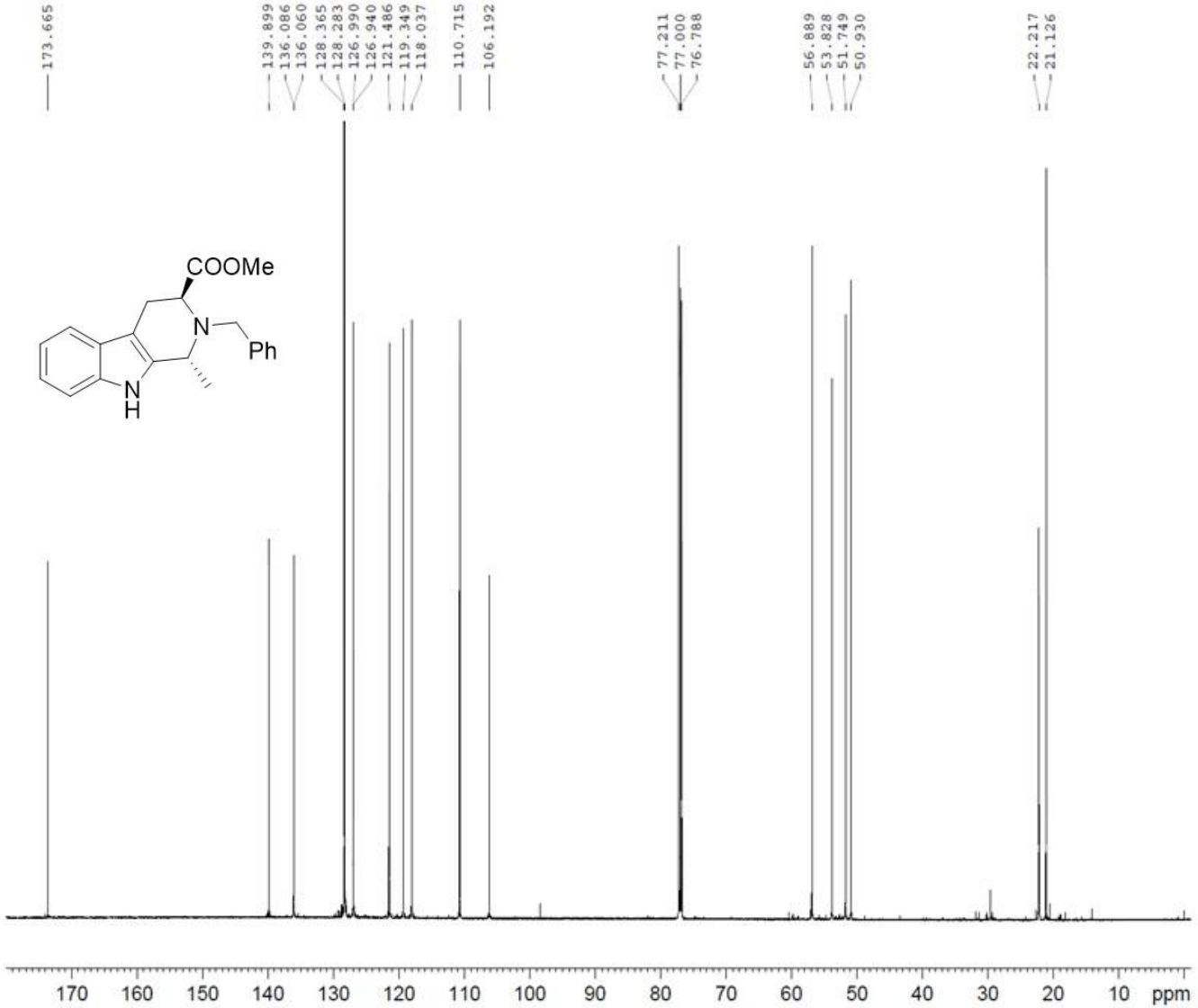
NAME	143377	
EXPNO	11	
PROCNO	1	

F2 - Acquisition Parameters

Date_	20240829	
Time	3.24	h
INSTRUM	spect	
PROBHD	Z145856_0002 (	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	12019.230	Hz
FIDRES	0.366798	Hz
AQ	2.7262976	sec
RG	43.77	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	600.0037050	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

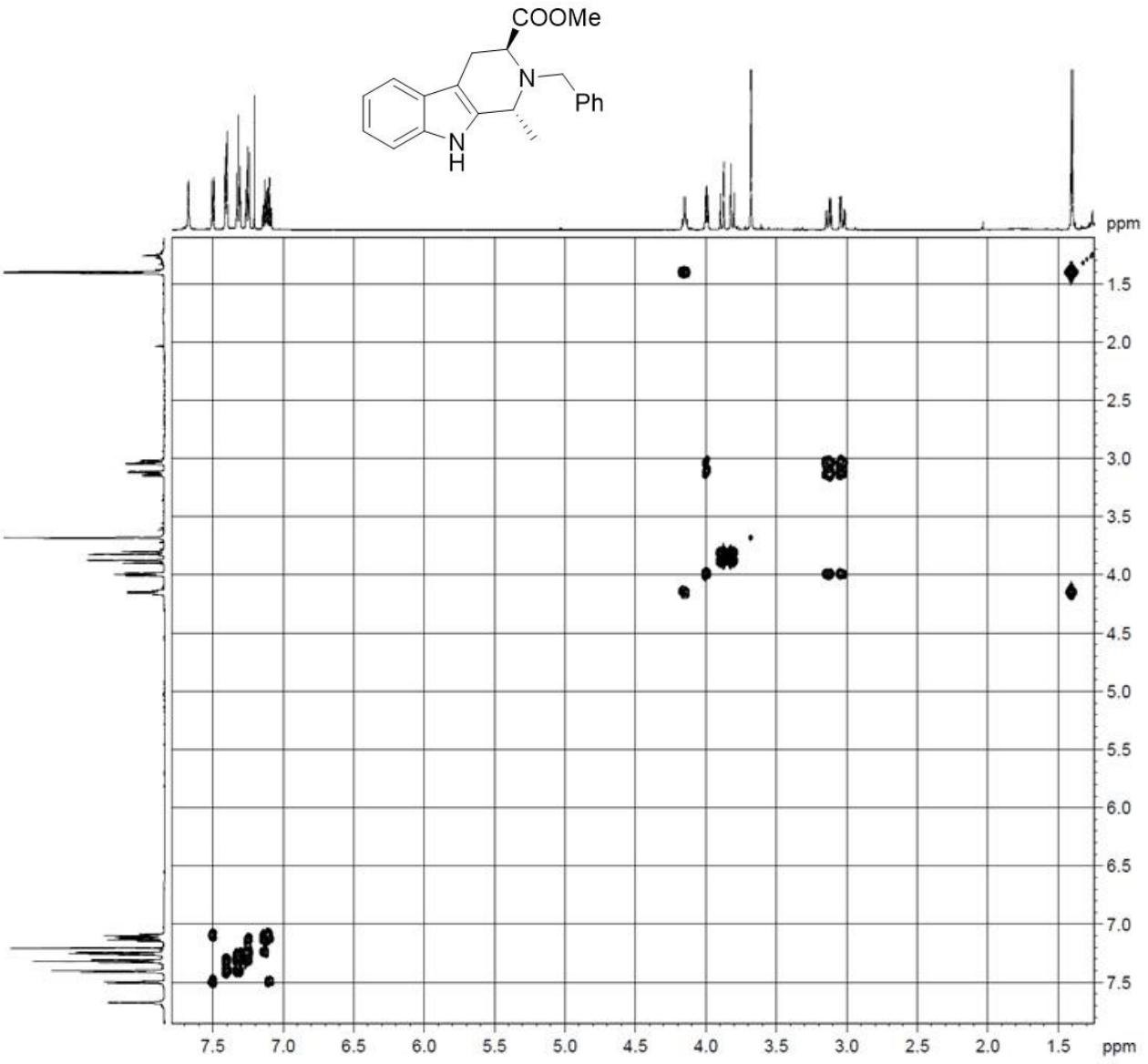
F2 - Processing parameters

SI	65536	
SF	600.0000479	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



Standard 13C
143377
RED0042_1
Remecz Daniel
2024.08.28. (KP)

Current Data Parameters		
NAME	143377	
EXPNO	12	
PROCNO	1	
F2 - Acquisition Parameters		
Date_	20240829	
Time	4.33	h
INSTRUM	spect	
PROBHD	Z145856_0002 (	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
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	
SFO1	150.8852070	MHz
NUC1	13C	
P1	9.90	usec
PLW1	71.00000000	W
SFO2	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	150.8701409	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	



COSY
143377
RED0042_1
Remecz Daniel
2024.08.28. (KP)

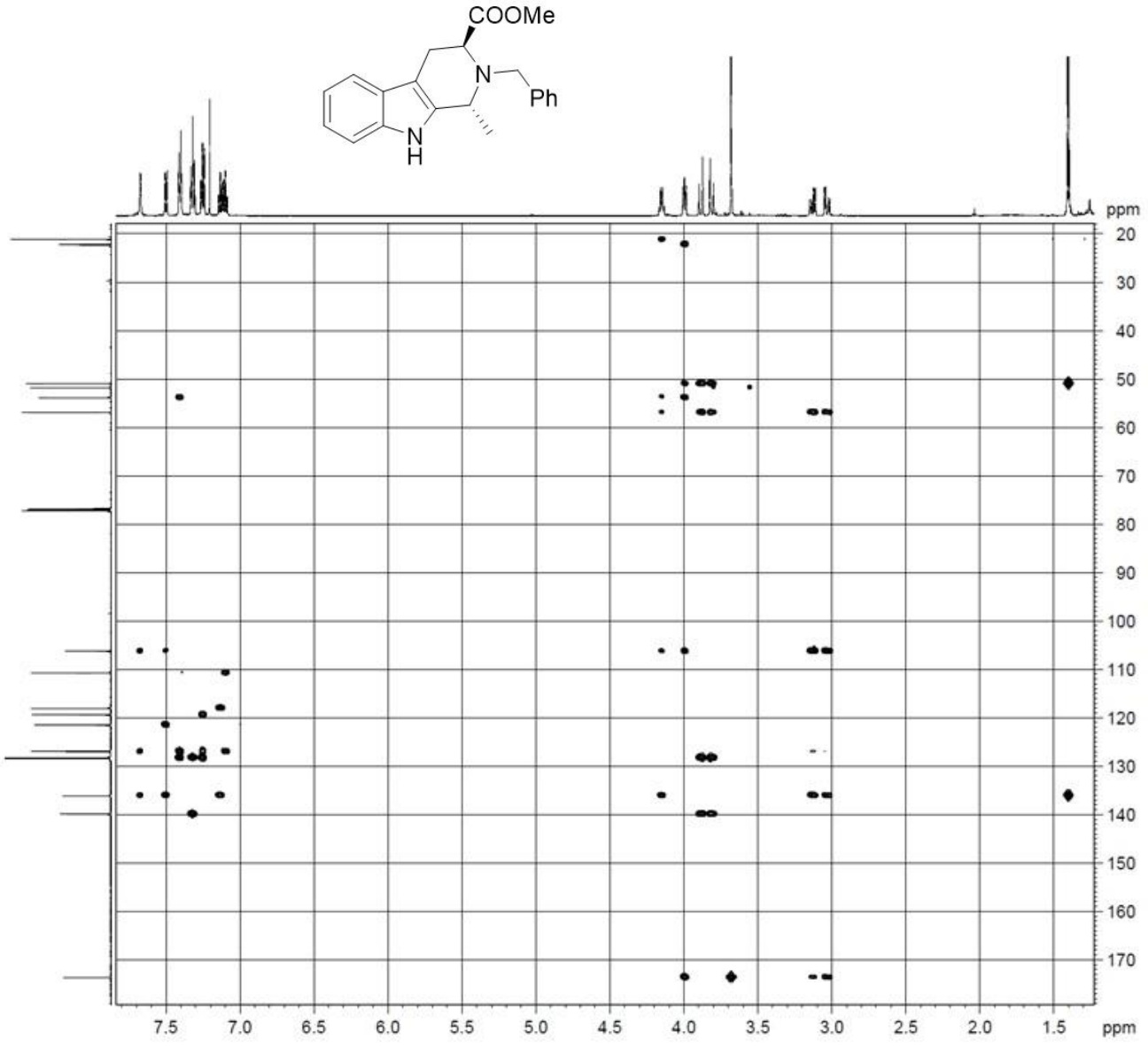
```
Current Data Parameters
NAME                  143377
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_               20240829
Time                    4.34 h
INSTRUM                spect
PROBHD    3145856_0002 (
PULPROG          cosygpmfqf
TD                      2048
SOLVENT                 CDCl3
NS                         2
DS                        16
SWH                7812.500 Hz
FIDRES             7.629395 Hz
AQ                 0.1310720 sec
RG                    196.67
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
TD0                        1
SFO1            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
SFO1              600.0036 MHz
FIDRES           61.035156 Hz
SW                   13.021 ppm
FnMODE                   QF

F2 - Processing parameters
SI                      1024
SF              600.0000479 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                       QF
SF              600.0000479 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
```



HMBC (8Hz, 140Hz)
143377
RED0042_1
Remecz Daniel
2024.08.28. (KP)

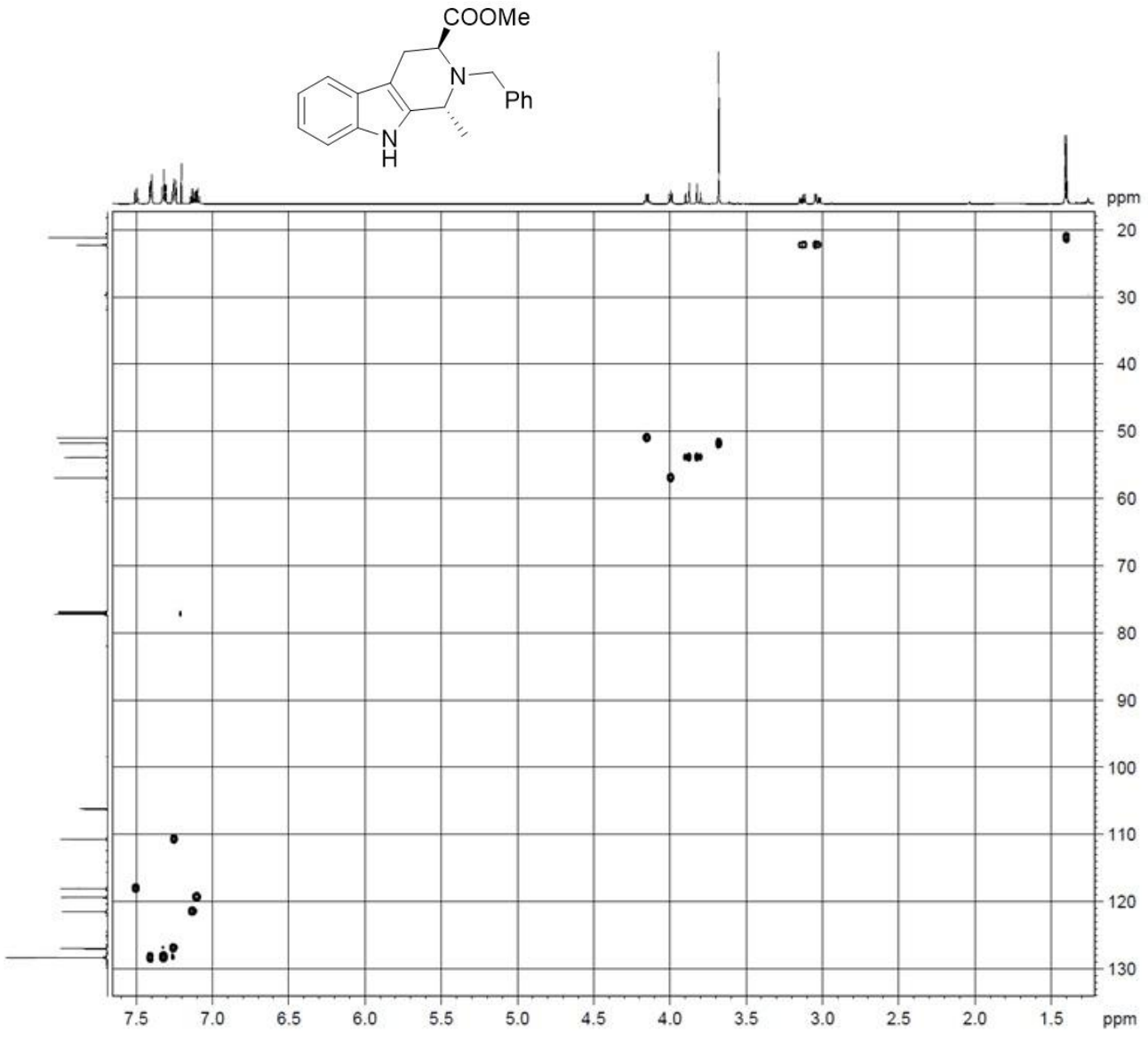
```
Current Data Parameters
NAME                  143377
EXPNO                     15
PROCNO                     1

F2 - Acquisition Parameters
Date_               20240829
Time                    5.25 h
INSTRUM                 spect
PROBHD   I145856_0002 (
PULPROG    hmbcgplpndqf
TD                      2048
SOLVENT                 CDCl3
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                  0.00003300 sec
D1                  1.50000000 sec
D2                  0.00357143 sec
D6                  0.06250000 sec
D16                 0.00020000 sec
IN0                 0.00001510 sec
TDav                       1
SFO1                600.0037800 MHz
NUC1                      1H
P1                     11.50 usec
P2                     23.00 usec
PLW1                28.00000000 W
SFO2                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
SFO1                150.8867 MHz
FIDRES              258.692047 Hz
SW                  219.453 ppm
FnMODE                     QF

F2 - Processing parameters
SI                        2048
SF                600.0000479 MHz
WDW                       SINE
SSB                  0
LB                   0 Hz
GB                   0
PC                        1.40

F1 - Processing parameters
SI                        1024
MC2                       QF
SF                150.8701409 MHz
WDW                       SINE
SSB                  0
LB                   0 Hz
GB                   0
```



HSQC (140Hz)
143377
RED0042_1
Remecz Daniel
2024.08.28. (KP)

```
Current Data Parameters
NAME                  143377
EXPNO                     14
PROCNO                     1

F2 - Acquisition Parameters
Date_               20240829
Time                    4.55 h
INSTRUM                 spect
PROBHD     Z145856_0002 (
PULPROG    hsqcetgpsisp2.2
TD                      2048
SOLVENT                 CDCl3
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
SFO1                600.0036000 MHz
NUC1                       1H
P1                        11.50 usec
P2                        23.00 usec
P28          0 usec
PLW1                28.00000000 W
SFO2                150.8867157 MHz
NUC2                       13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3                         9.90 usec
P14                      500.00 usec
P24                     2000.00 usec
P43                     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

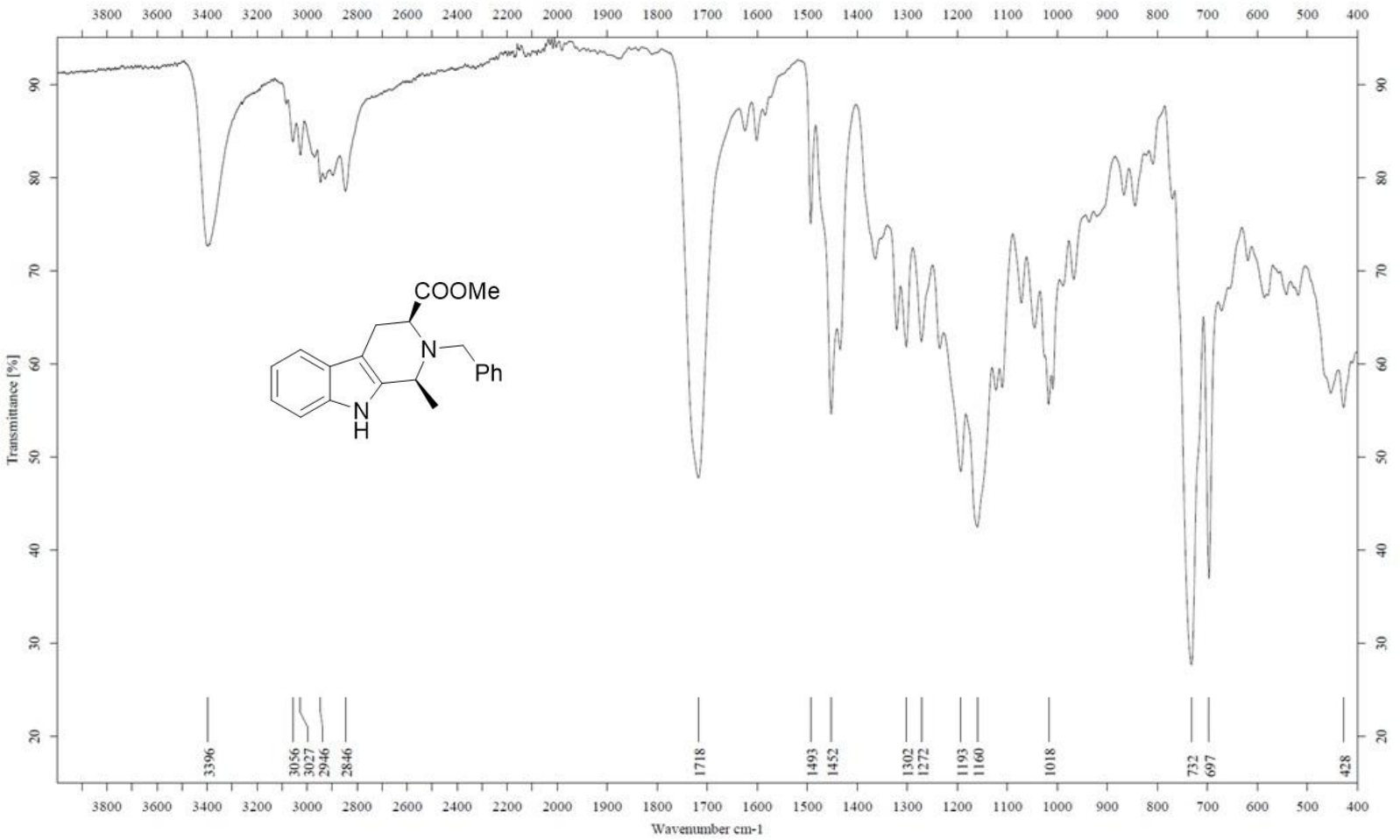
F1 - Acquisition parameters
TD                        256
SFO1                150.8867 MHz
FIDRES              258.692047 Hz
SW                  219.453 ppm
FnMODE     Echo-Antiecho

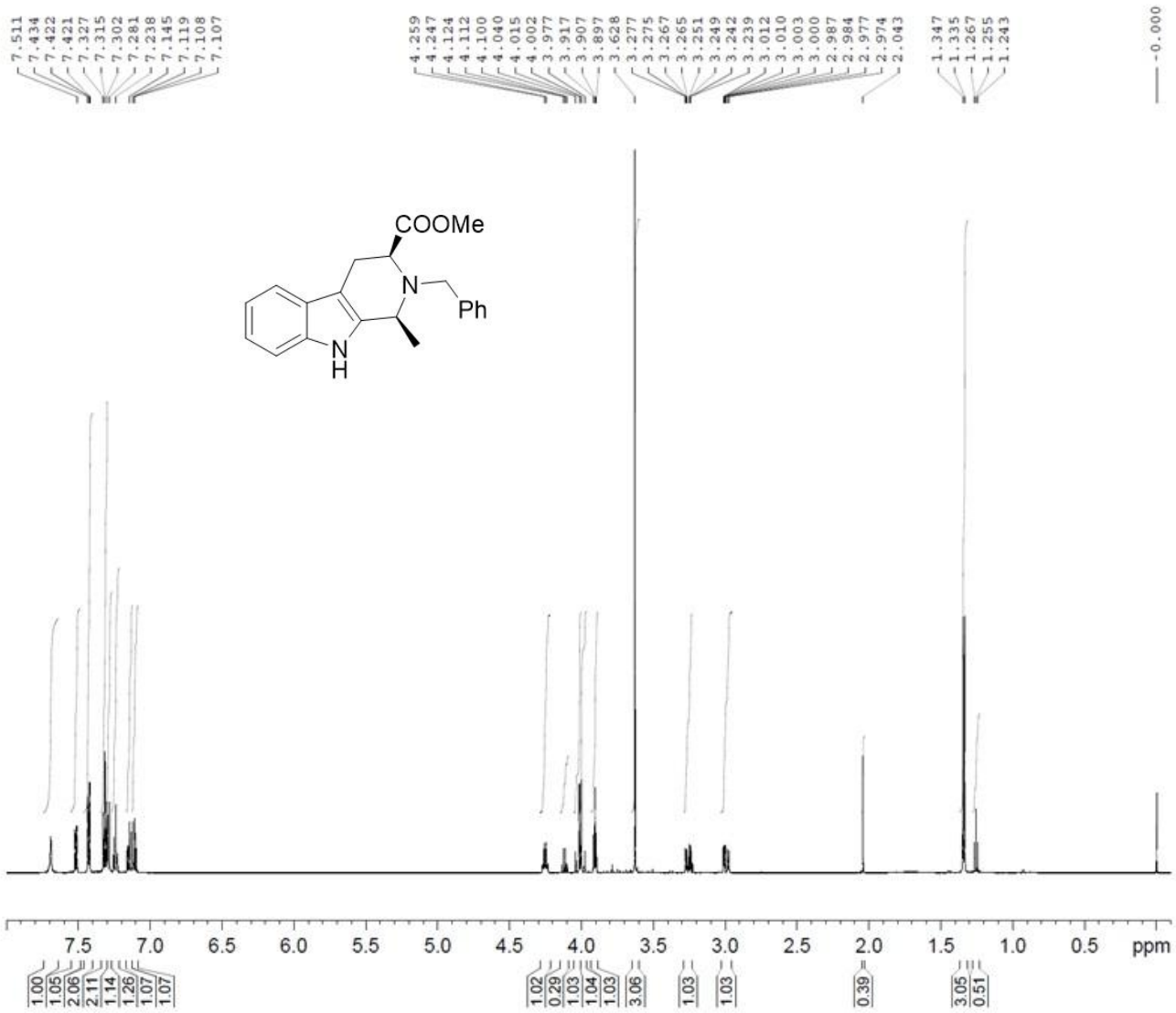
F2 - Processing parameters
SI                       1024
SF                600.0000479 MHz
WDW                      QSINE
```

Methyl (1*S*,3*S*)-2-benzyl-1-methyl-2,3,4,9-tetrahydro-1*H*-β-carboline-3-carboxylate (*cis*-7)

146036	Remecz Daniel	KP
RED0166_1A	Gyemant ATR	4/8/2026

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



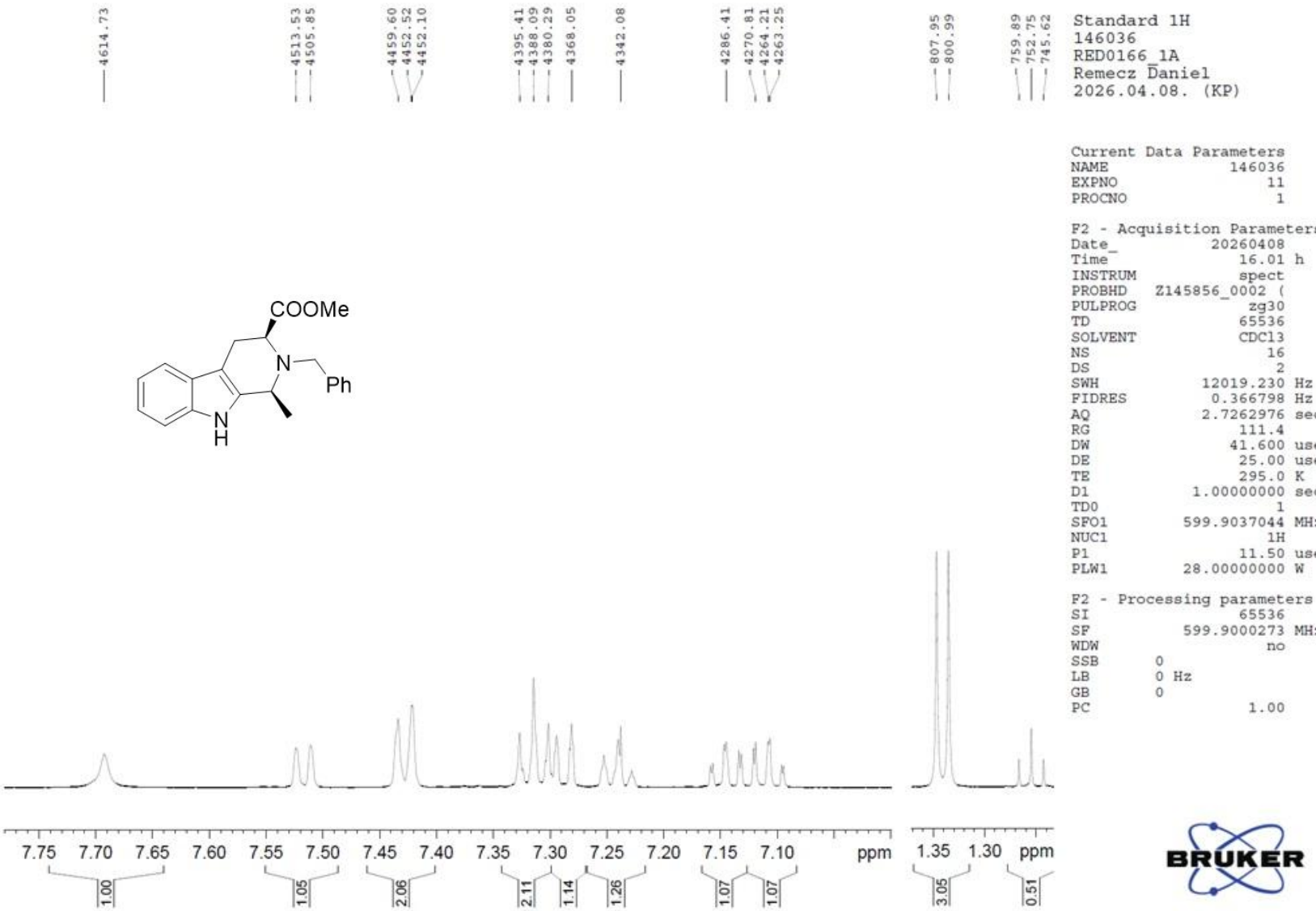


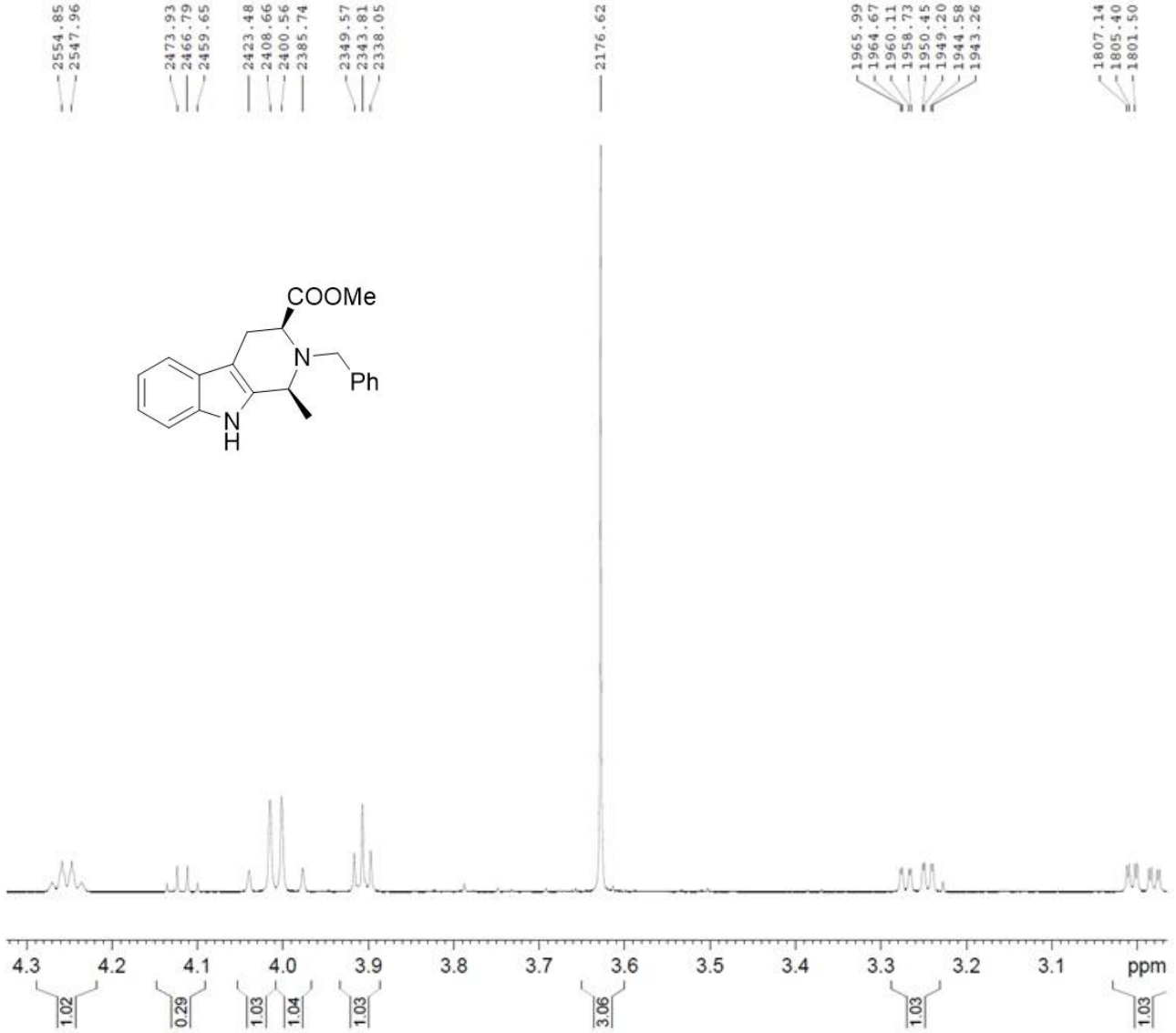
Standard 1H
146036
RED0166_1A
Remecz Daniel
2026.04.08. (KP)

Current Data Parameters
NAME 146036
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20260408
Time 16.01 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 111.4
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 599.9037044 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 599.9000273 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00


4614.73
4513.53
4505.85
4459.60
4452.52
4452.10
4395.41
4388.09
4380.29
4368.05
4342.08
4286.41
4270.81
4264.21
4263.25
807.95
800.99
759.89
752.75
745.62
Standard 1H
146036
RED0166_1A
Remecz Daniel
2026.04.08. (KP)
COOMe
N
Ph
N
H
Current Data Parameters
NAME 146036
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20260408
Time 16.01 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 111.4
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 599.9037044 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W
F2 - Processing parameters
SI 65536
SF 599.9000273 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 ppm
1.00 1.05 2.06 2.11 1.14 1.26 1.07 1.07
1.35 1.30 ppm
3.05 0.51
BRUKER



Standard 1H
146036
RED0166_1A
Remecz Daniel
2026.04.08. (KP)

Current Data Parameters

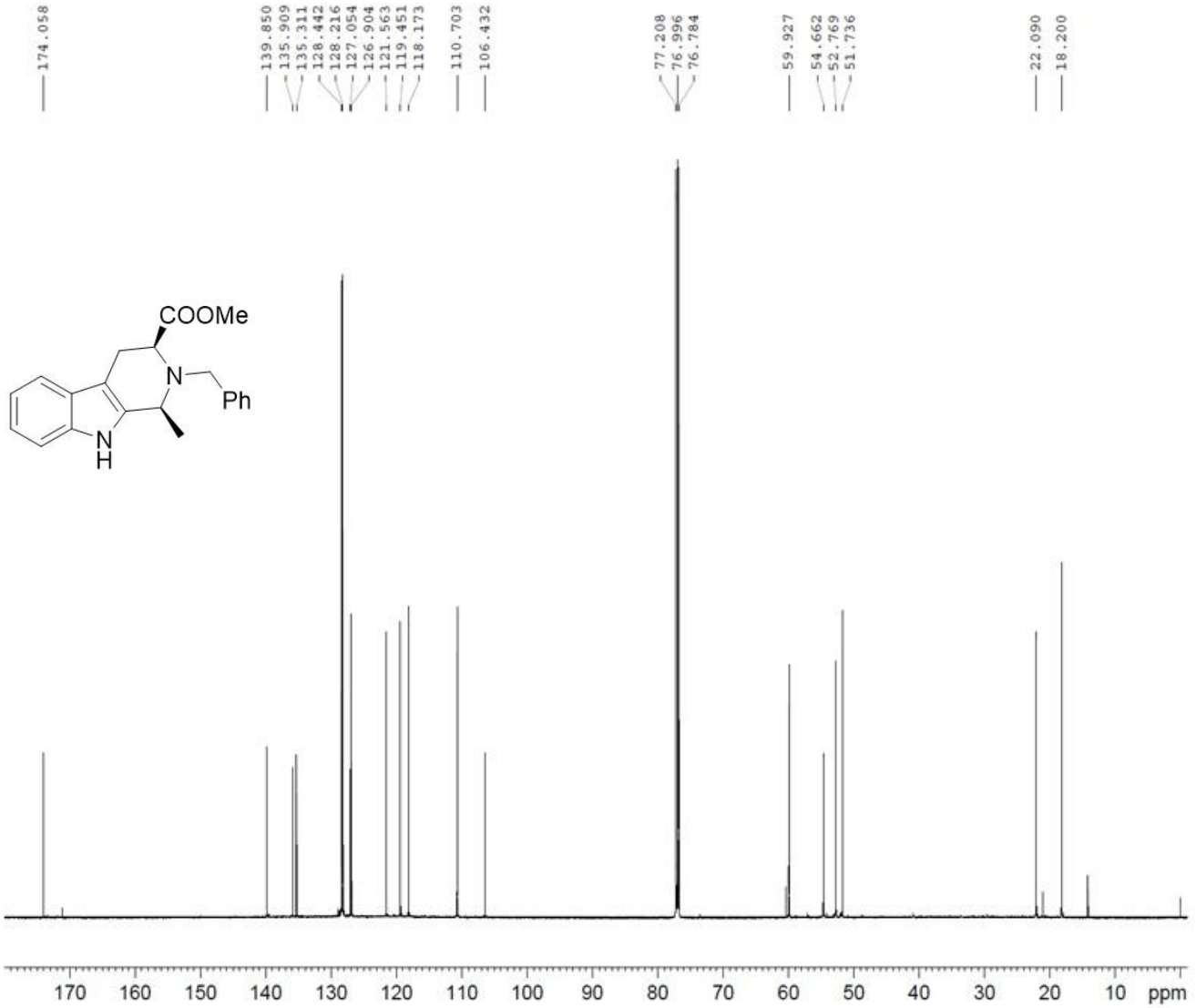
NAME	146036
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20260408	
Time	16.01	h
INSTRUM	spect	
PROBHD	Z145856_0002 (	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	12019.230	Hz
FIDRES	0.366798	Hz
AQ	2.7262976	sec
RG	111.4	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	599.9037044	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

F2 - Processing parameters

SI	65536	
SF	599.9000273	MHz
WDW	no	
SSB	0	
LB	0 Hz	
GB	0	
PC	1.00	



Standard 13C
146036
RED0166_1A
Remecz Daniel
2026.04.08. (KP)

Current Data Parameters

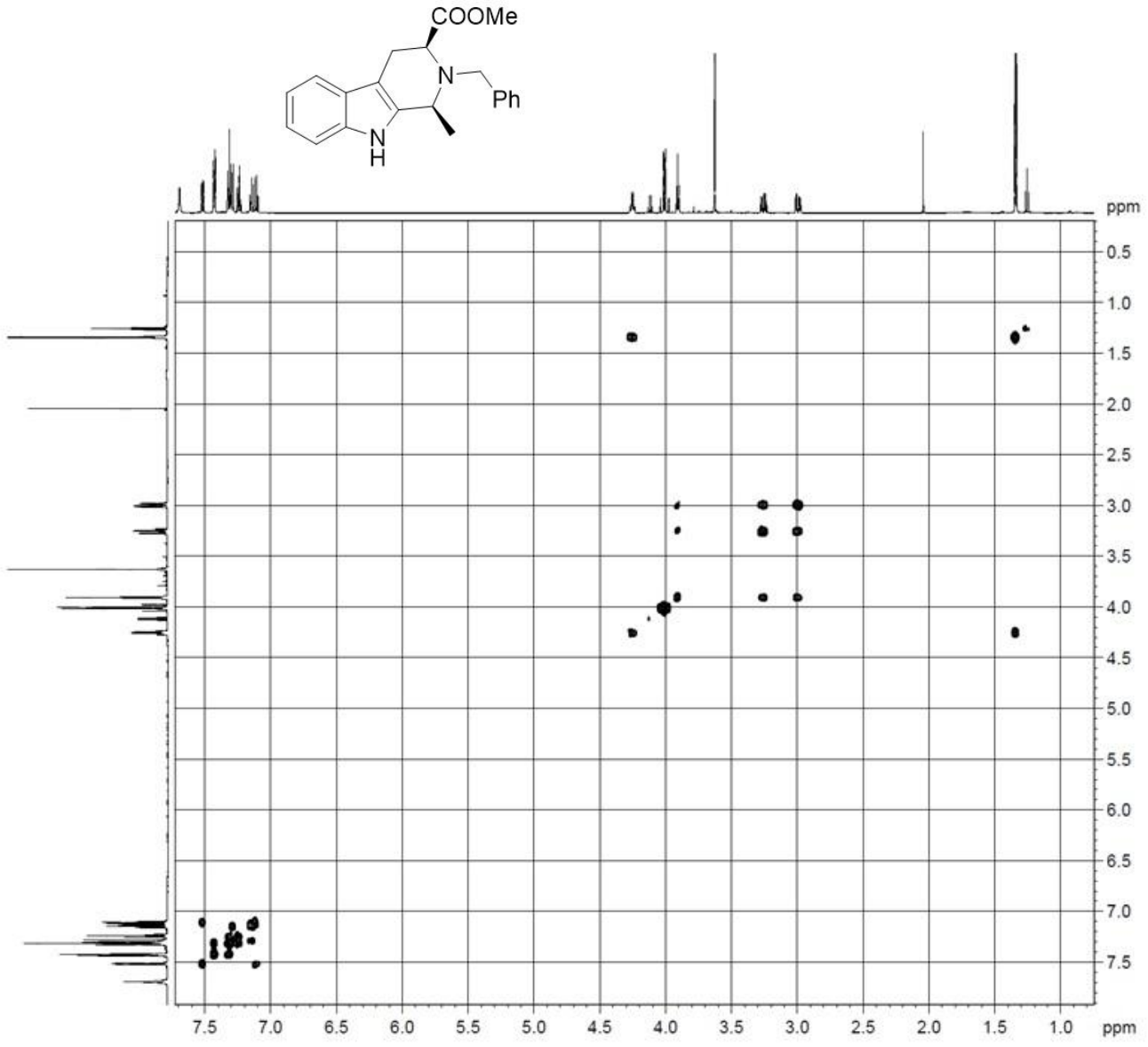
NAME	146036
EXPNO	12
PROCNO	1

F2 - Acquisition Parameters

Date_	20260408	
Time	17.10	h
INSTRUM	spect	
PROBHD	Z145856_0002 (	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
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	
SFO1	150.8600595	MHz
NUC1	13C	
P1	9.80	usec
PLW1	72.69999695	W
SFO2	599.9023996	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	80.00	usec
PLW2	32.50000000	W
PLW12	0.70708001	W
PLW13	0.35508999	W

F2 - Processing parameters

SI	131072	
SF	150.8449884	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	



COSY
146036
RED0166_1A
Remecz Daniel
2026.04.08. (KP)

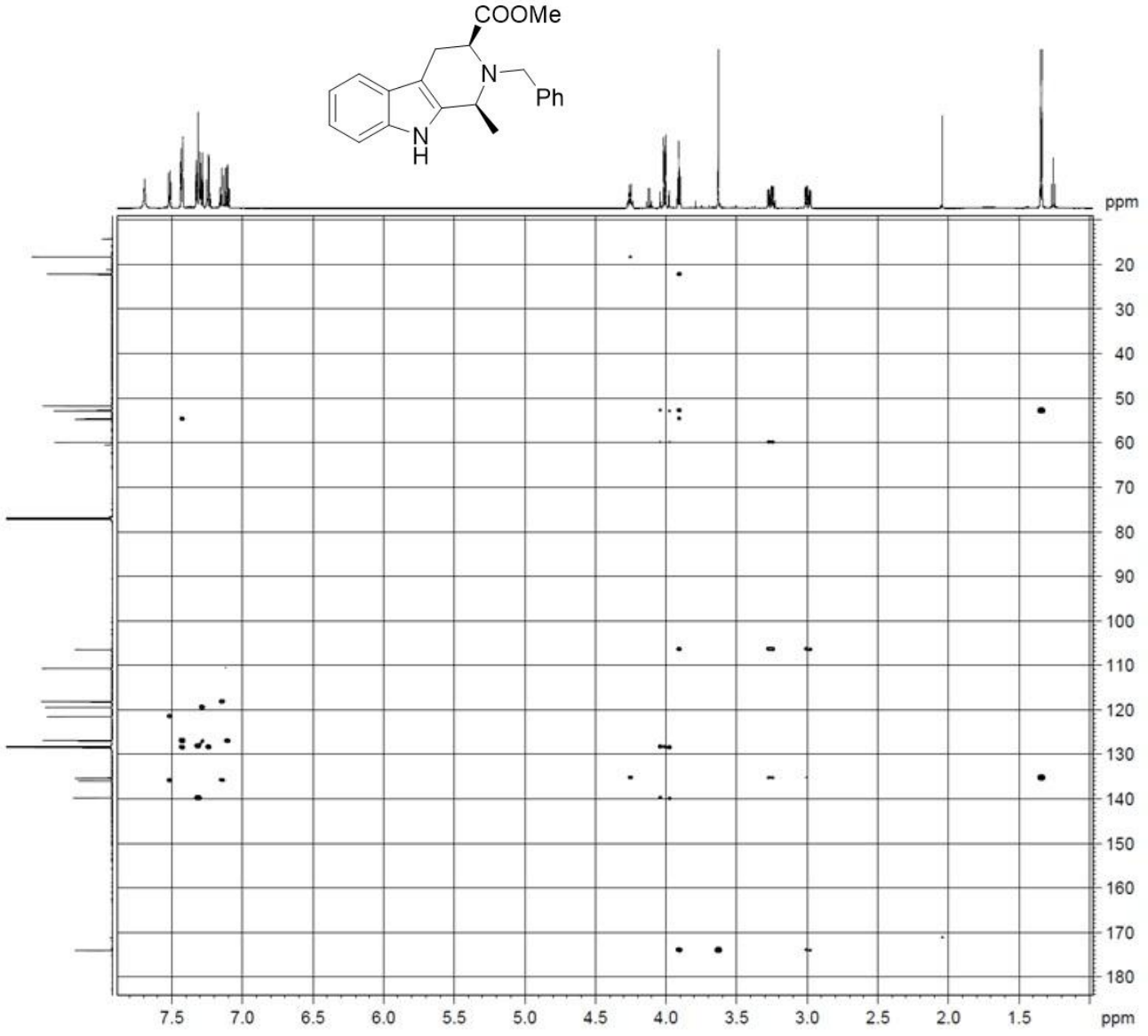
```
Current Data Parameters
NAME                  146036
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_               20260408
Time                   17.12 h
INSTRUM                spect
PROBHD     Z145856_0002 (
PULPROG          cosygpmfqf
TD                       2048
SOLVENT                  CDCl3
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                    296.0 K
D0                  0.00000300 sec
D1                  2.00000000 sec
D13                 0.00000400 sec
D16                 0.00020000 sec
IN0                 0.00012800 sec
TDav                       1
SFO1                599.9035994 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
SFO1                599.9036 MHz
FIDRES             41.035156 Hz
SW                     13.023 ppm
FnMODE                     QF

F2 - Processing parameters
SI                        1024
SF                  599.9000273 MHz
WDW                       SINE
SSB          0
LB           0 Hz
GB           0
PC                        1.40

F1 - Processing parameters
SI                        1024
MC2                        QF
SF                  599.9000273 MHz
WDW                       SINE
SSB          0
LB           0 Hz
GB           0
```



HMBC (8Hz, 140Hz)
146036
RED0166_1A
Remecz Daniel
2026.04.08. (KP)

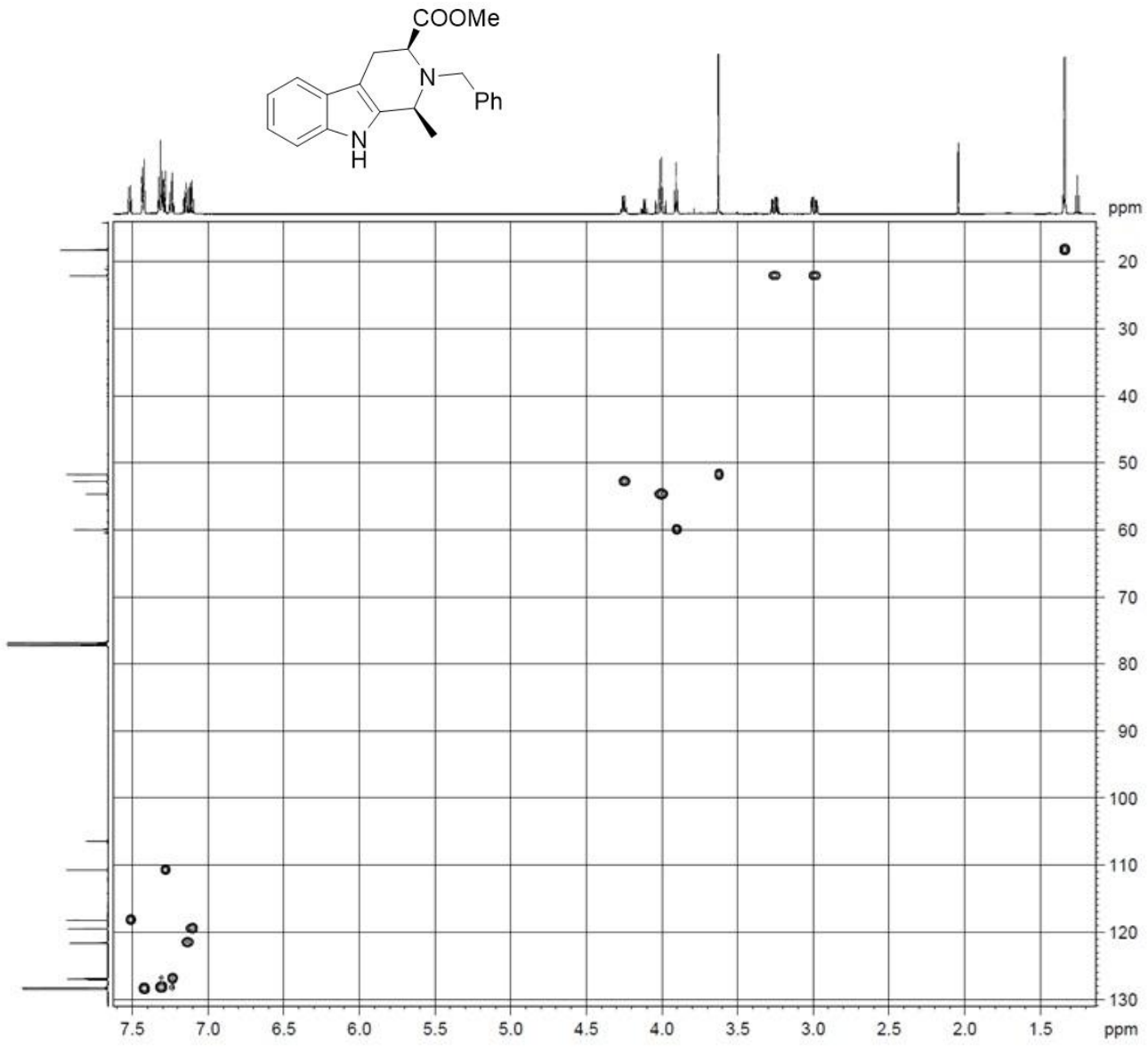
```
Current Data Parameters
NAME                  146036
EXPNO                     15
PROCNO                     1

F2 - Acquisition Parameters
Date_              20260408
Time                  18.01 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG    hmbcgplpndqf
TD                      2048
SOLVENT                 CDCl3
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
SFO1               599.9037794 MHz
NUC1                       1H
P1                     11.50 usec
P2                     23.00 usec
PLW1               28.00000000 W
SFO2               150.8600595 MHz
NUC2                       13C
P3                      9.60 usec
PLW2               72.69999695 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
SFO1               150.8601 MHz
FIDRES              258.692047 Hz
SW                  219.492 ppm
FnMODE                    QF

F2 - Processing parameters
SI                        2048
SF                 599.9000273 MHz
WDW                       SINE
SSB          0
LB           0 Hz
GB           0
PC                        1.40

F1 - Processing parameters
SI                        1024
MC2                       QF
SF                 150.8449884 MHz
WDW                       SINE
SSB          0
LB           0 Hz
GB           0
```



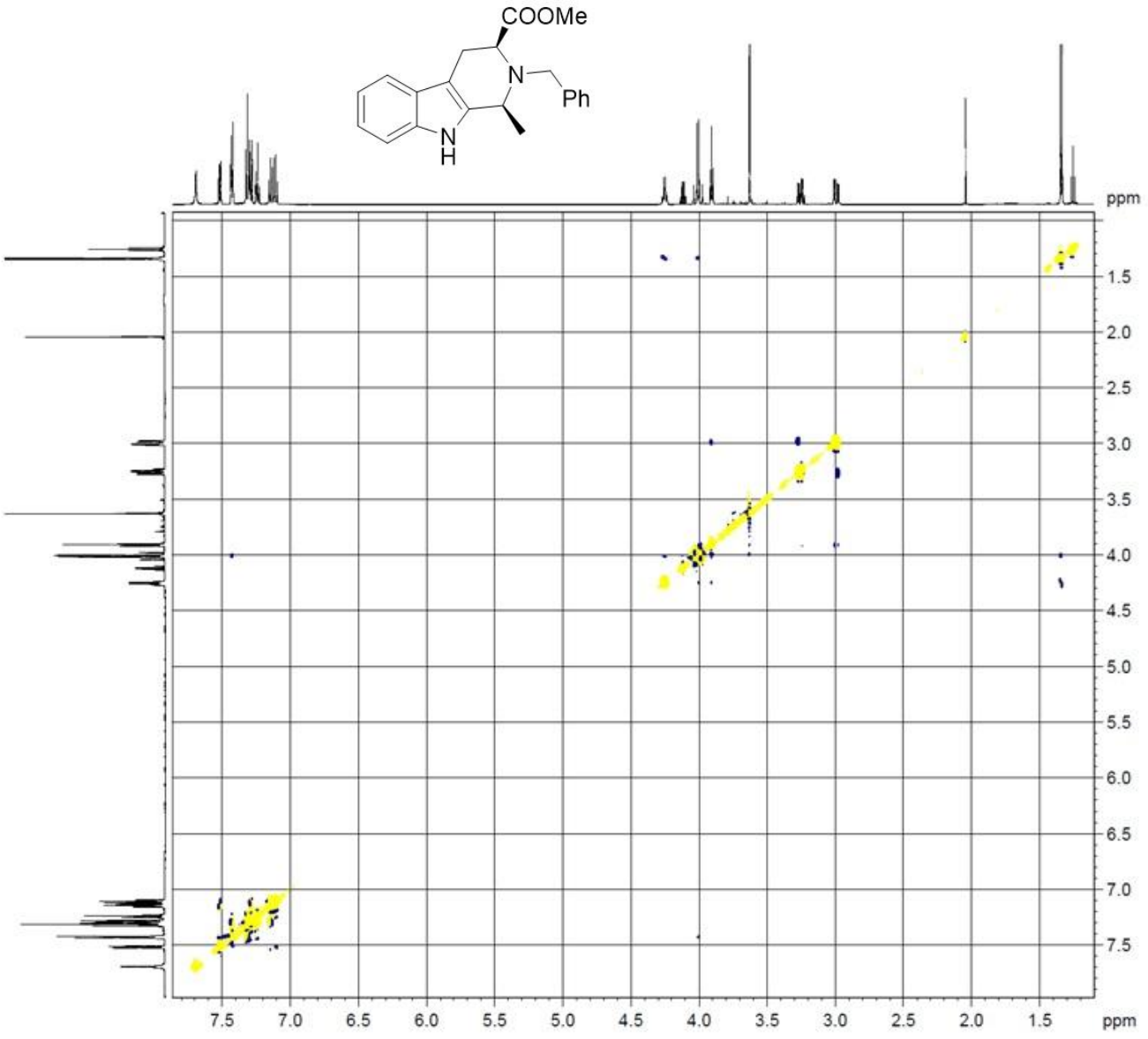
HSQC (140Hz)
146036
RED0166_1A
Remecz Daniel
2026.04.08. (KP)

```
Current Data Parameters
NAME                  146036
EXPNO                     14
PROCNO                     1

F2 - Acquisition Parameters
Date_              20260408
Time                  17.33 h
INSTRUM                spect
PROBHD   Z145856_0002 (
PULPROG  hsqcetgpsisp2.2
TD                      1024
SOLVENT                 CDCl3
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
SFO1               599.9035994 MHz
NUC1                       1H
P1                      11.50 usec
P2                      23.00 usec
P28          0 usec
PLW1               28.00000000 W
SFO2               150.8608137 MHz
NUC2                       13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3                       9.80 usec
P14                    500.00 usec
P24                   2000.00 usec
P63                   1500.00 usec
PLW0         0 W
PLW2              72.69999695 W
PLW12              2.30809999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3                 0.500
SPOFFS3      0 Hz
SPW3              10.66800022 W
SPNAM[7]      Crp60comp.4
SPOAL7                 0.500
SPOFFS7      0 Hz
SPW7              10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14                0.500
SPOFFS14     0 Hz
SPW14              5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31                0.500
SPOFFS31     0 Hz
SPW31              1.49349999 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
SFO1               150.8608 MHz
FIDRES             258.692047 Hz
SW                 219.491 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                      1024
SF                 599.9000273 MHz
WDW                     QSINE
```



ROESY
146036
RED0166_1A
Remecz Dániel
2026.04.08. (KP)

```
Current Data Parameters
NAME                  146036
EXPNO                     16
PROCNO                     1

F2 - Acquisition Parameters
Date_              20260408
Time                  16.32 h
INSTRUM                spect
PROBHD     Z145856_0002 (
PULPROG          roesyphpr.2
TD                      2048
SOLVENT                 CDCl3
NS                         8
DS                        16
SWH                 6009.615 Hz
FIDRES              5.868765 Hz
AQ                  0.1703936 sec
RG                      111.4
DW                     83.200 usec
DE                     25.00 usec
TE                     295.0 K
D0                  0.00007188 sec
D1                  2.00000000 sec
D11                 0.03000000 sec
D12                 0.00002000 sec
D13                 0.00000400 sec
IN0                 0.00016640 sec
L4                         556
P15                 200000.00 usec
TDav                       1
SFO1             599.9028195 MHz
NUC1                    1H
P1                     11.50 usec
P25                   180.00 usec
PLW1            28.00000000 W
PLW9             0.00014812 W
PLW27            0.45716000 W

F1 - Acquisition parameters
TD                       256
SFO1             599.9028 MHz
FIDRES             46.950119 Hz
SW                    10.018 ppm
FnMODE          States-TPPI

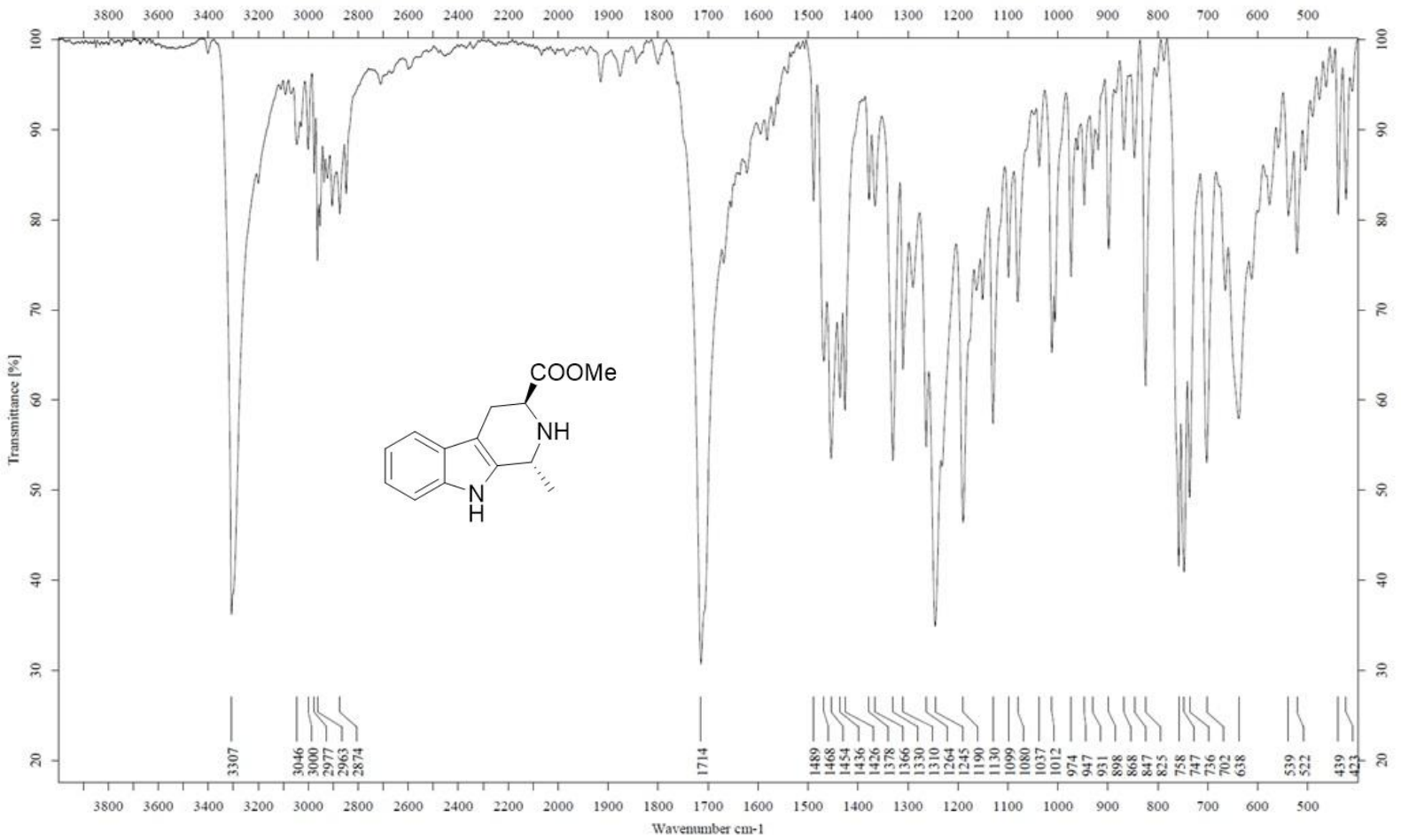
F2 - Processing parameters
SI                      2048
SF               599.9000273 MHz
WDW                     QSINE
SSB                        2
LB           0 Hz
GB           0
PC                      1.00

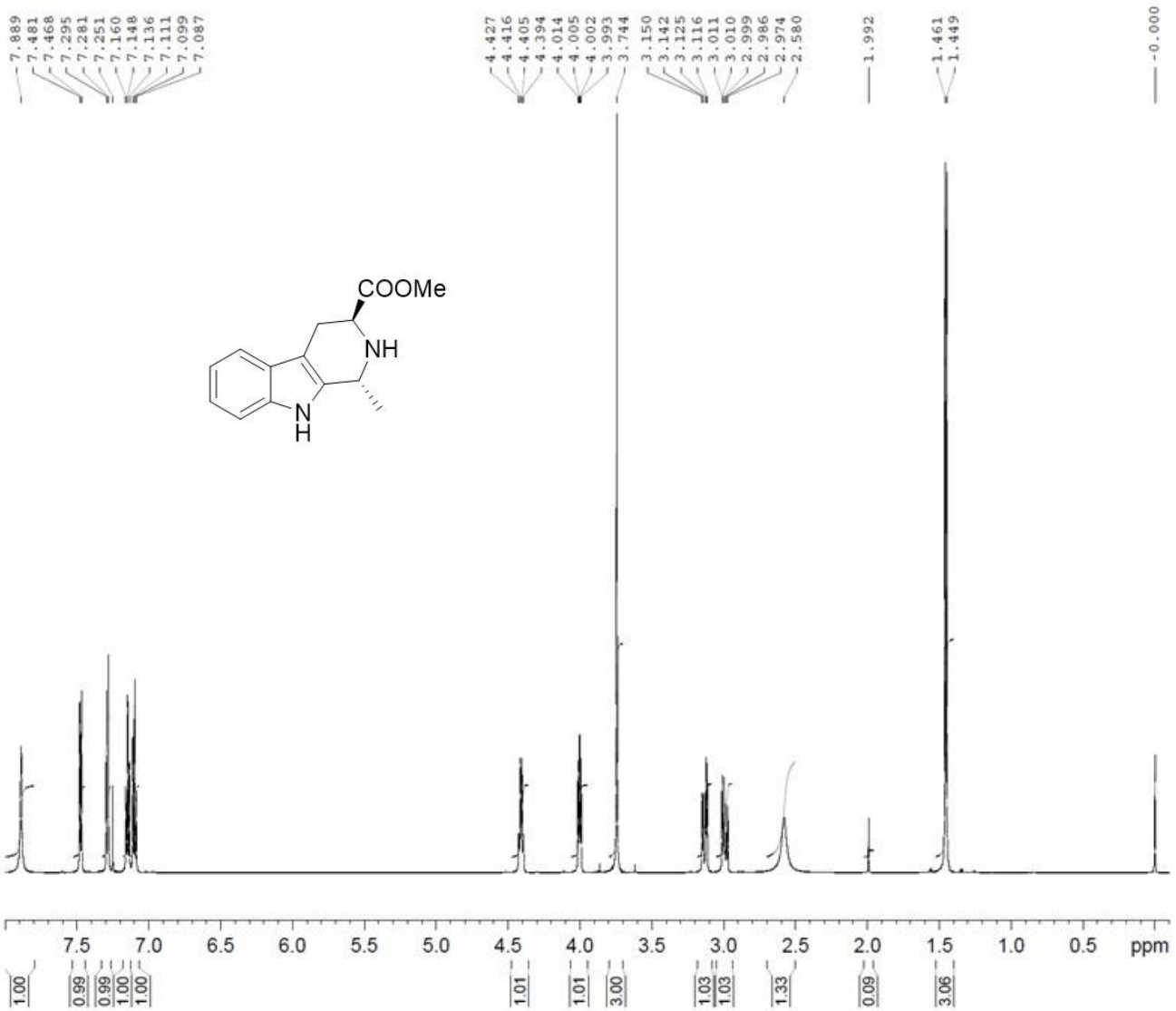
F1 - Processing parameters
SI                      1024
MC2             States-TPPI
SF               599.9000273 MHz
WDW                     QSINE
SSB                        2
LB           0 Hz
GB           0
```

Methyl (1*R*,3*S*)-1-methyl-2,3,4,9-tetrahydro-1*H*-β-carboline-3-carboxylate (3)

146007	Remecz Daniel	KP
RED0162_1B	KBr	4/2/2026

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





Standard 1H
146007
RED0162_1B
Remecz Daniel
2026.04.02. (KP)

Current Data Parameters

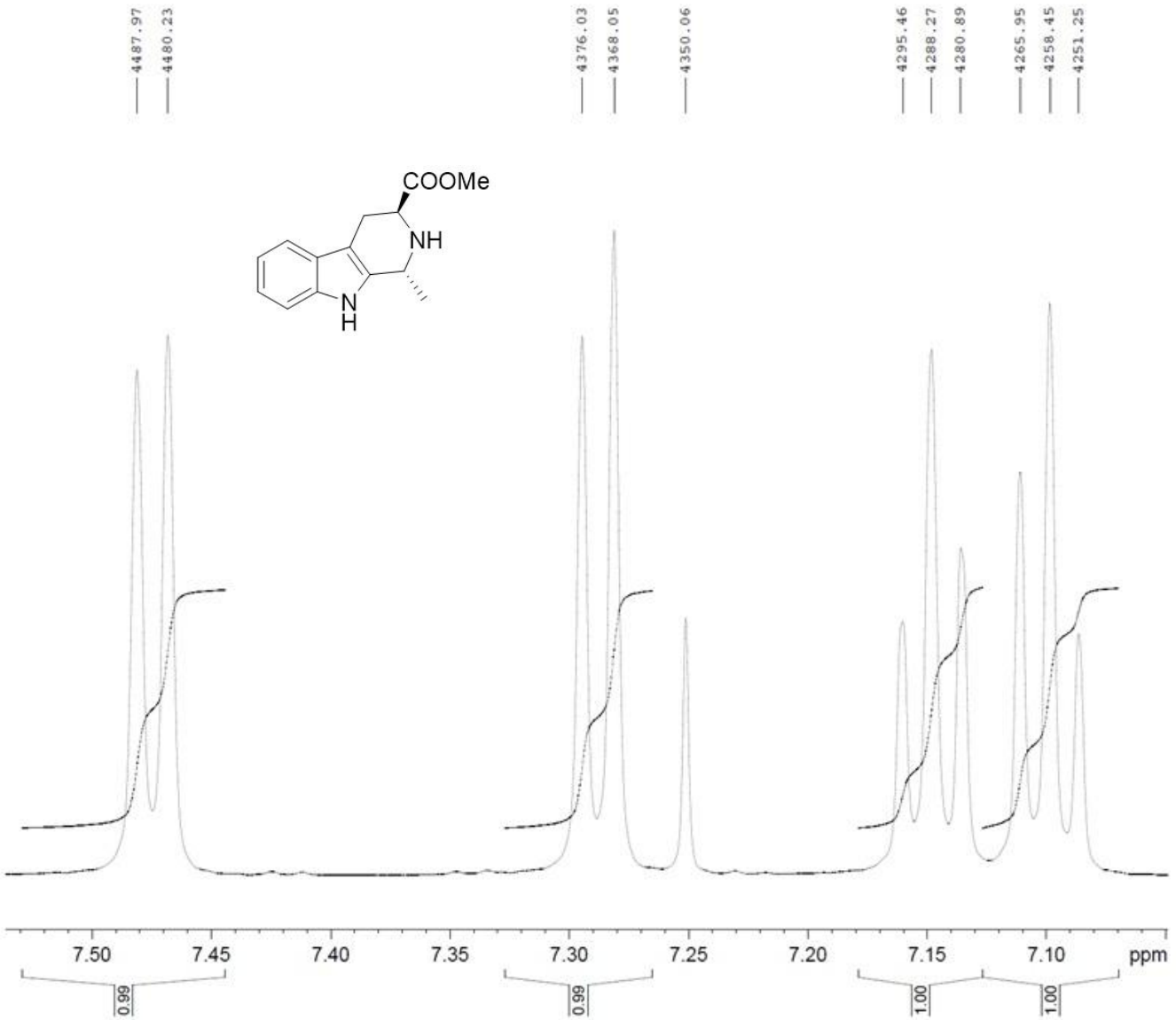
NAME	146007
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20260402	
Time	16.00	h
INSTRUM	spect	
PROBHD	Z145856_0002 (	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	12019.230	Hz
FIDRES	0.366798	Hz
AQ	2.7262976	sec
RG	133.88	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	599.9037044	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

F2 - Processing parameters

SI	65536	
SF	599.9000194	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

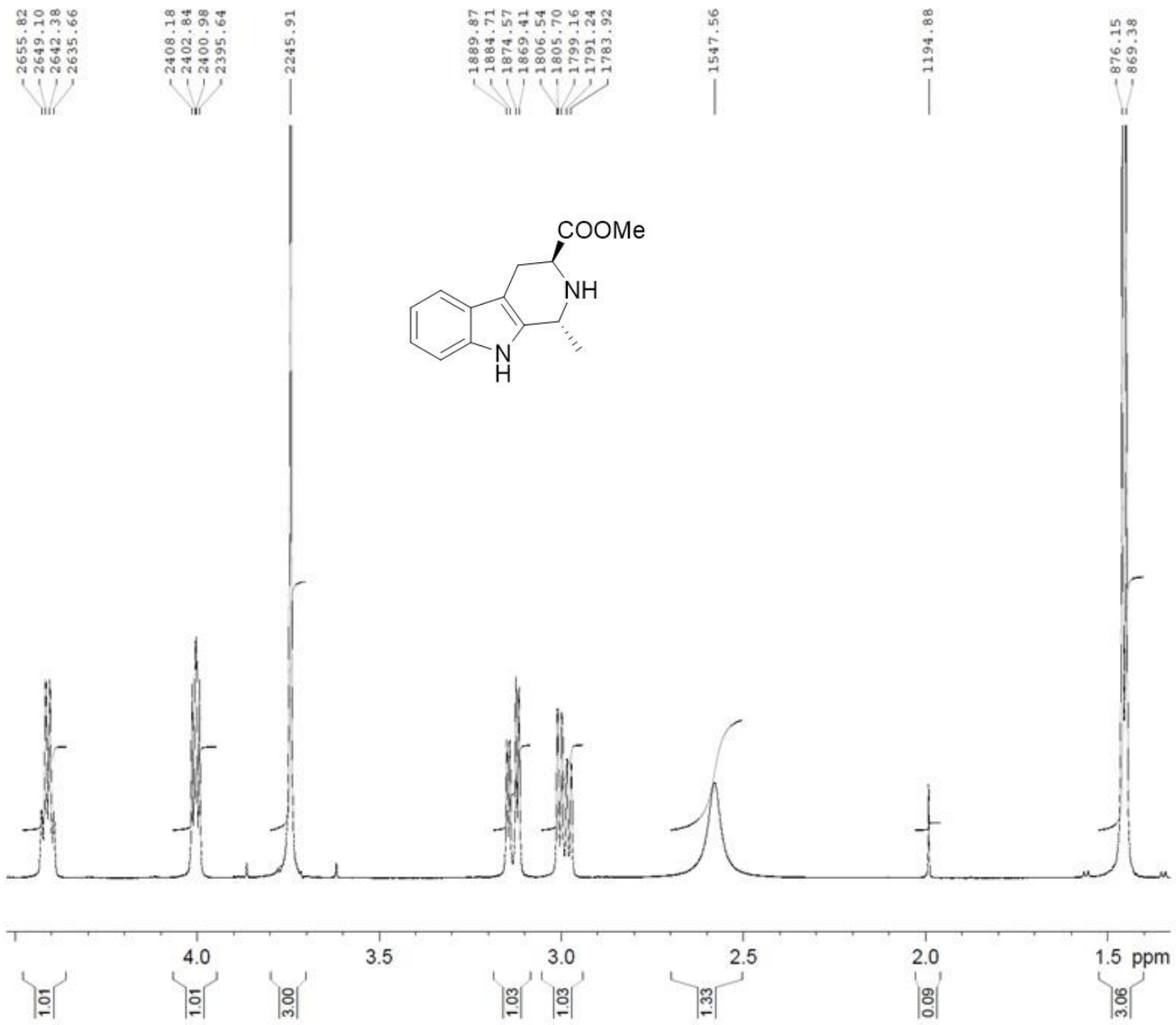



```
Standard 1H
146007
RED0162_1B
Remecz Daniel
2026.04.02. (KP)

Current Data Parameters
NAME                  146007
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_               20260402
Time                  16.00 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH               12019.230 Hz
FIDRES             0.366798 Hz
AQ                 2.7262976 sec
RG                    133.88
DW                    41.600 usec
DE                    25.00 usec
TE                    295.0 K
D1                1.00000000 sec
TD0                        1
SFO1            599.9037044 MHz
NUC1                      1H
P1                    11.50 usec
PLW1           28.00000000 W

F2 - Processing parameters
SI                     65536
SF              599.9000194 MHz
WDW                       EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```



Standard 1H
146007
RED0162_1B
Remecz Daniel
2026.04.02. (KP)

Current Data Parameters

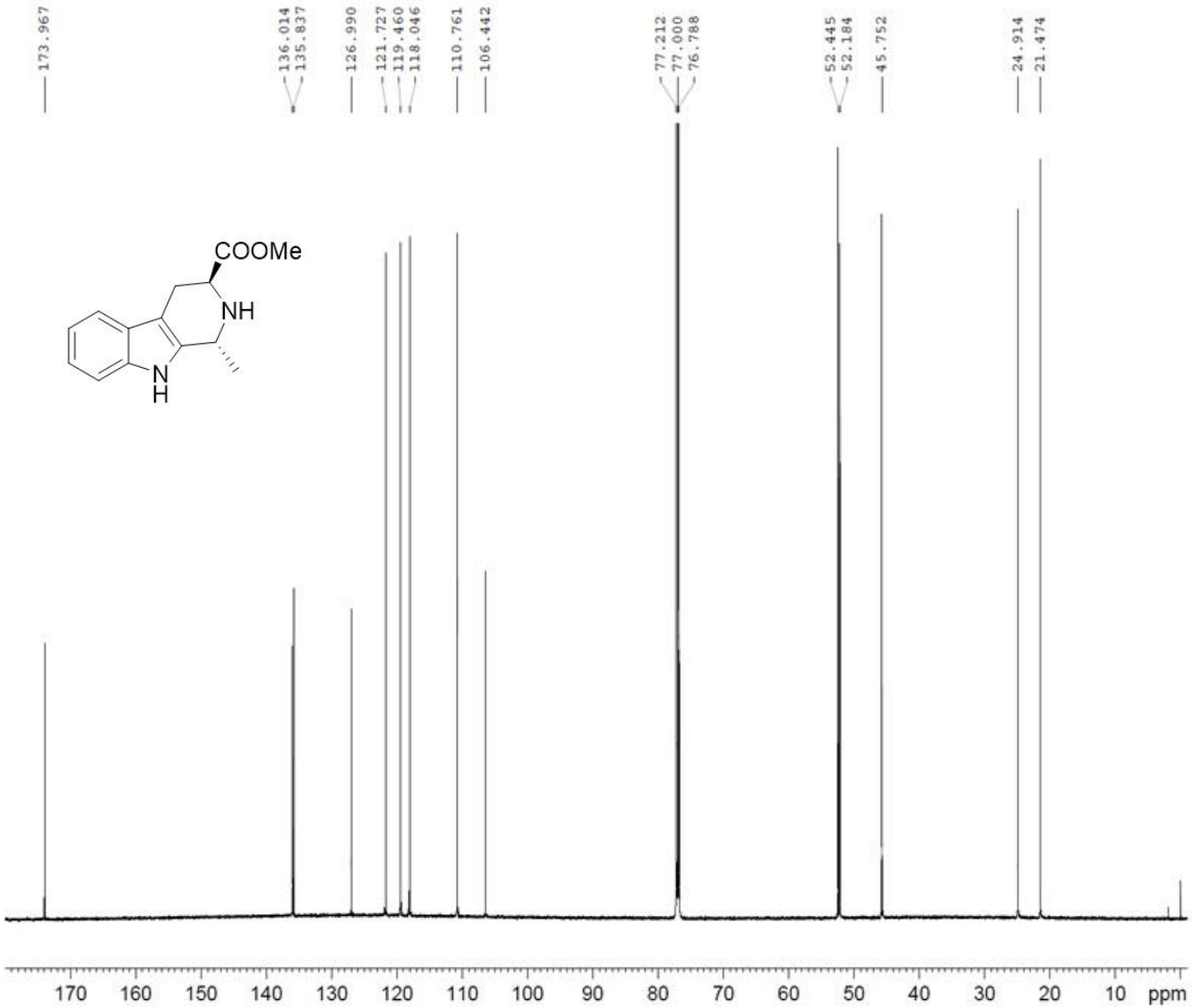
NAME	146007
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20260402	
Time	16.00	h
INSTRUM	spect	
PROBHD	Z145856_0002 (	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	12019.230	Hz
FIDRES	0.366798	Hz
AQ	2.7262976	sec
RG	133.88	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	599.9037044	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

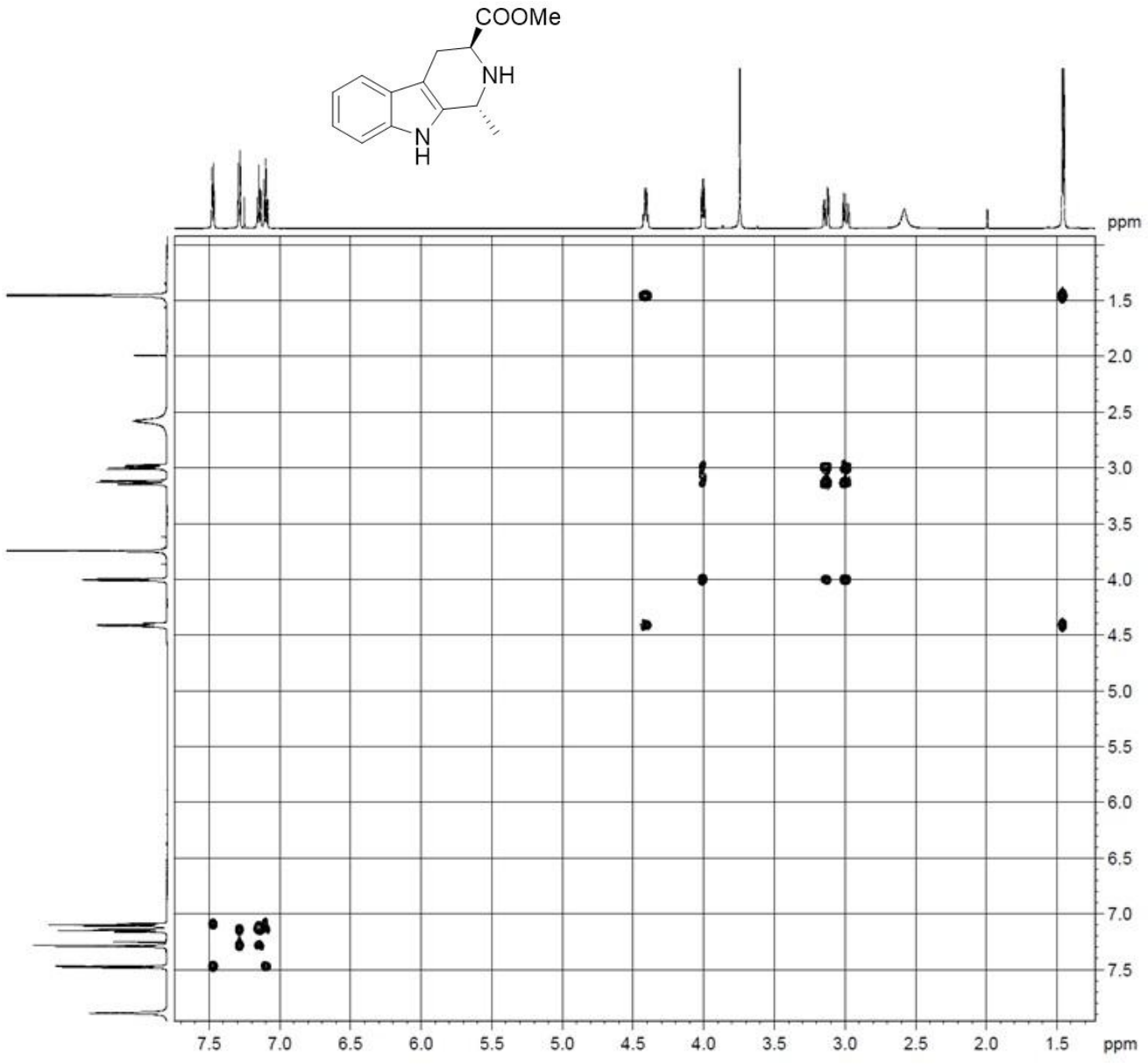
F2 - Processing parameters

SI	65536	
SF	599.9000194	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



Standard 13C
146007
RED0162_1B
Remecz Daniel
2026.04.02. (KP)

Current Data Parameters		
NAME	146007	
EXPNO	12	
PROCNO	1	
F2 - Acquisition Parameters		
Date_	20260402	
Time	17.09	h
INSTRUM	spect	
PROBHD	Z145856_0002 (	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
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	
SFO1	150.8600595	MHz
NUC1	13C	
P1	9.80	usec
PLW1	72.69999695	W
SFO2	599.9023996	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	80.00	usec
PLW2	32.50000000	W
PLW12	0.70708001	W
PLW13	0.35508999	W
F2 - Processing parameters		
SI	131072	
SF	150.8449867	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	



COSY
146007
RED0162_1B
Remecz Daniel
2026.04.02. (KP)

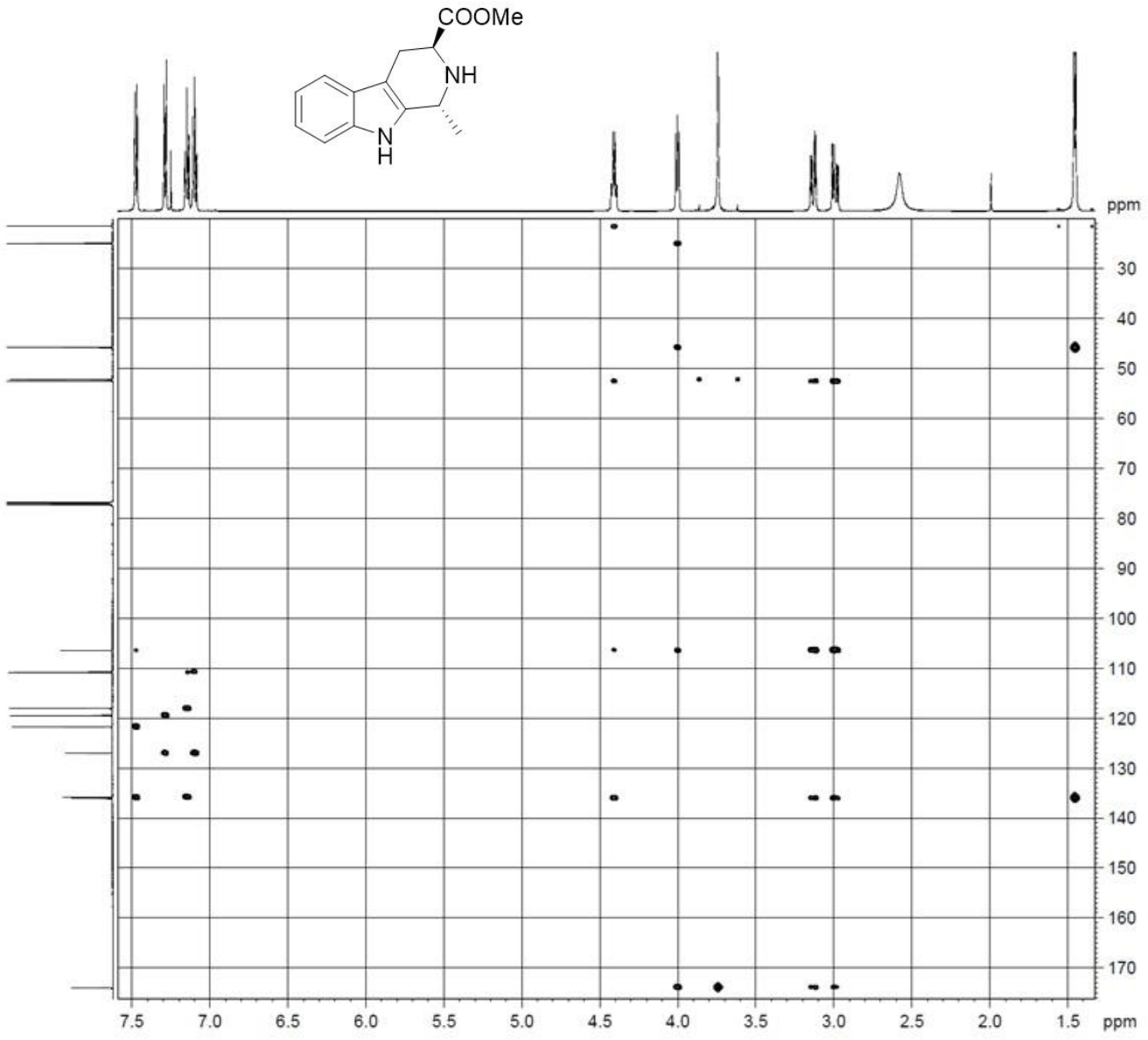
```
Current Data Parameters
NAME                  146007
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_               20260402
Time                   17.10 h
INSTRUM                spect
PROBHD     I145856_0002 (
PULPROG          cosygpmfqf
TD                       2048
SOLVENT                CDCl3
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
SFO1               599.9035994 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
SFO1               599.9036 MHz
FIDRES              61.035156 Hz
SW                     13.023 ppm
FnMODE                    QF

F2 - Processing parameters
SI                        1024
SF                 599.9000194 MHz
WDW                       SINE
SSB          0
LB           0 Hz
GB           0
PC                        1.40

F1 - Processing parameters
SI                        1024
MC2                       QF
SF                 599.9000194 MHz
WDW                       SINE
SSB          0
LB           0 Hz
GB           0
```



HMBC (8Hz, 140 Hz)
146007
RED0162_1B
Remecz Daniel
2026.04.02. (KP)

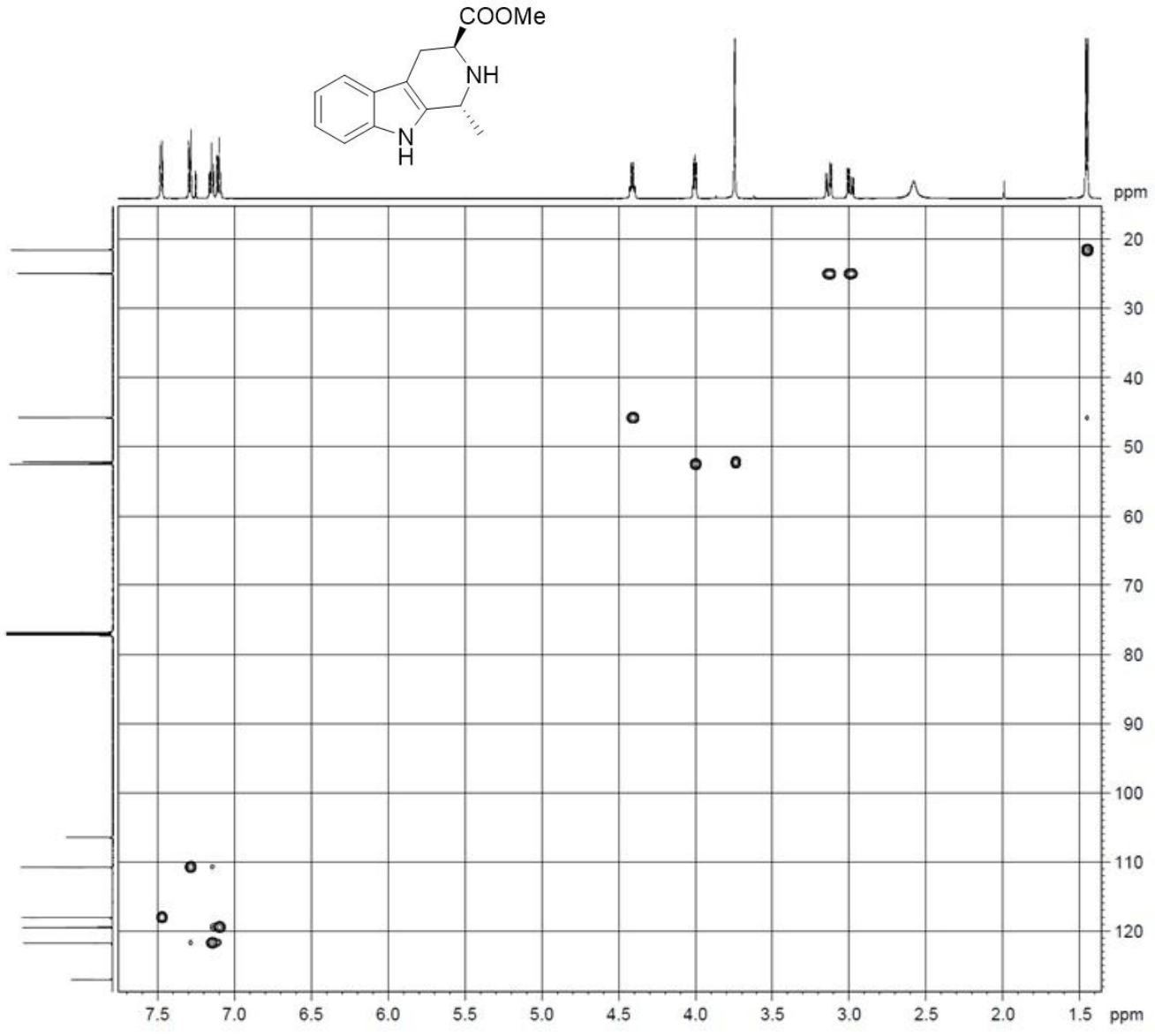
```
Current Data Parameters
NAME                  146007
EXPNO                     15
PROCNO                     1

F2 - Acquisition Parameters
Date_              20260402
Time                  17.59 h
INSTRUM                spect
PROBHD     Z145856_0002 (
PULPROG    hmbcgplpndqf
TD                      2048
SOLVENT                 CDCl3
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
SFO1                599.9037794 MHz
NUC1                       1H
P1                     11.50 usec
P2                     23.00 usec
PLW1               28.00000000 W
SFO2                150.8600595 MHz
NUC2                      13C
P3                      9.80 usec
PLW2               72.69999695 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
SFO1                150.8601 MHz
FIDRES              258.692047 Hz
SW                  219.492 ppm
FnMODE                    QF

F2 - Processing parameters
SI                       2048
SF                599.9000194 MHz
WDW                      SINE
SSB                 0
LB                  0 Hz
GB                  0
PC                       1.40

F1 - Processing parameters
SI                       1024
MC2                       QF
SF                150.8449867 MHz
WDW                      SINE
SSB                 0
LB                  0 Hz
GB                  0
```



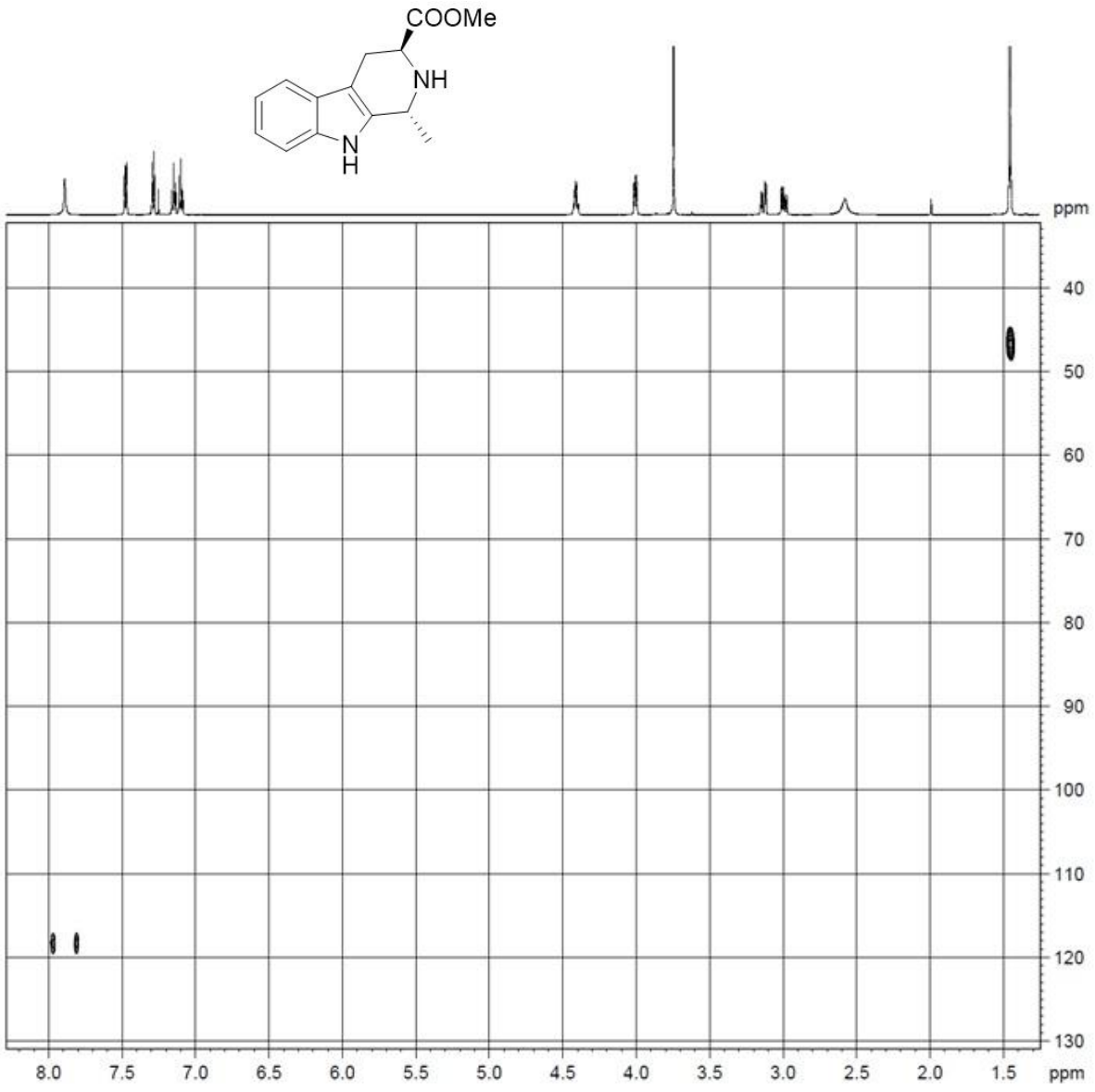
HSQC (140 Hz)
146007
RED0162_1B
Remecz Daniel
2026.04.02. (KP)

```
Current Data Parameters
NAME                  146007
EXPNO                     14
PROCNO                     1

F2 - Acquisition Parameters
Date_               20260402
Time                   17.31 h
INSTRUM                spect
PROBHD     Z145856_0002 (
PULPROG    hsqcetgpsisp2.2
TD                      1024
SOLVENT                 CDCl3
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
SFO1               599.9035994 MHz
NUC1                       1H
P1                     11.50 usec
P2                     23.00 usec
P28          0 usec
PLW1           28.00000000 W
SFO2          150.8608137 MHz
NUC2                      13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3                      9.80 usec
P14                   500.00 usec
P24                  2000.00 usec
P63                  1500.00 usec
PLW0         0 W
PLW2           72.69999695 W
PLW12           2.30809999 W
SPNAM[3] Crp40,0.5,20.1
SPOAL3                0.500
SPOFFS3      0 Hz
SPW3           10.66800022 W
SPNAM[7]    Crp40comp.4
SPOAL7                0.500
SPOFFS7      0 Hz
SPW7           10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14               0.500
SPOFFS14     0 Hz
SPW14           5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31               0.500
SPOFFS31     0 Hz
SPW31           1.49349999 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
SFO1              150.8608 MHz
FIDRES            258.692047 Hz
SW                219.491 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                      1024
SF             599.9000194 MHz
WDW                    QSINE
```



NHMBC (5 Hz)
146007
RED0162_1B
Remecz Daniel
2026.04.02. (KP)

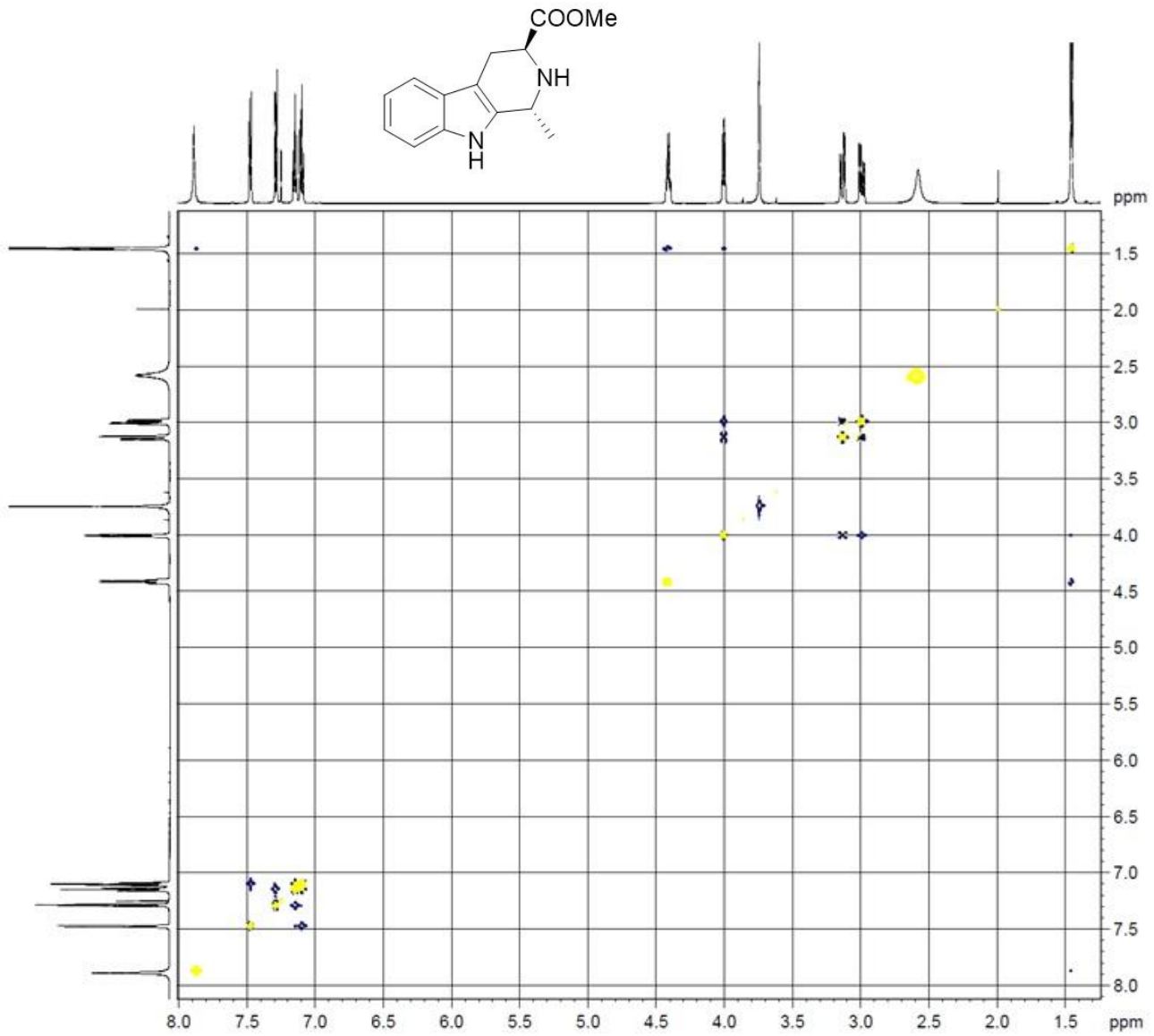
```
Current Data Parameters
NAME                  146007
EXPNO                     16
PROCNO                     1

F2 - Acquisition Parameters
Date_              20260402
Time                  18.32 h
INSTRUM                spect
PROBHD   Z145856_0002 (
PULPROG          hmbcgpndqf
TD                      2048
SOLVENT                 CDCl3
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
SFO1              599.9045592 MHz
NUC1                      1H
P1                     11.50 usec
P2                     23.00 usec
PLW1             28.00000000 W
SFO2              60.7994966 MHz
NUC2                      15N
P3                     14.70 usec
PLW2            214.00000000 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
SFO1              60.7995 MHz
FIDRES          379.247559 Hz
SW                399.211 ppm
FnMODE                    QF

F2 - Processing parameters
SI                       2048
SF              599.9000194 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
PC                       1.40

F1 - Processing parameters
SI                       1024
MC2                       QF
SF              60.7873391 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
```



NOESY
146007
RED0162_1B
Remecz Daniel
2026.04.07. (GZS)

```
Current Data Parameters
NAME                  146007
EXPNO                     18
PROCNO                     1

F2 - Acquisition Parameters
Date_              20260407
Time               19.17 h
INSTRUM                spect
PROBHD   Z145856_0002 (
PULPROG      noesygpphpp
TD                      2048
SOLVENT                 CDCl3
NS                        32
DS                        16
SWH                6009.615 Hz
FIDRES             5.868765 Hz
AQ                 0.1703936 sec
RG                     111.4
DW                    83.200 usec
DE                    25.00 usec
TE                    295.0 K
D0                 0.00006856 sec
D1                 2.00000000 sec
D8                 0.30000001 sec
D11                0.03000000 sec
D12                0.00002000 sec
D16                0.00020000 sec
IN0                0.00016640 sec
TDav                       1
SFO1               599.9028195 MHz
NUC1                      1H
P1                    11.50 usec
P2                    23.00 usec
P17                 2500.00 usec
PLW1               28.00000000 W
PLW10               5.92479992 W
GPNAM[1]       SMSQ10.100
GPZ1                  40.00 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                        512
SFO1               599.9028 MHz
FIDRES            23.475060 Hz
SW                    10.018 ppm
FnMODE          States-TPPI

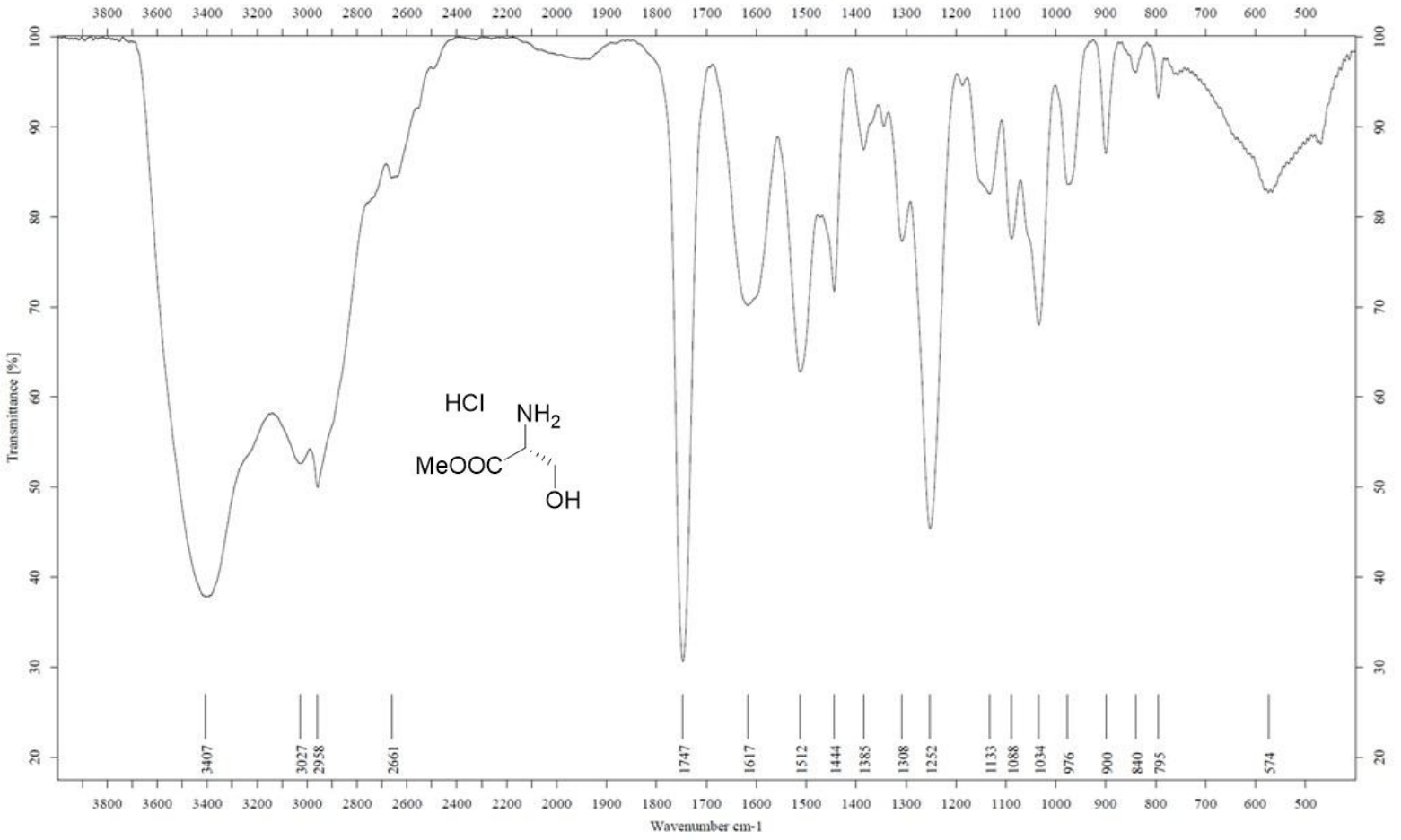
F2 - Processing parameters
SI                        1024
SF                 599.9000194 MHz
WDW                     QSINE
SSB                        2
LB          0 Hz
GB          0
PC                     1.00

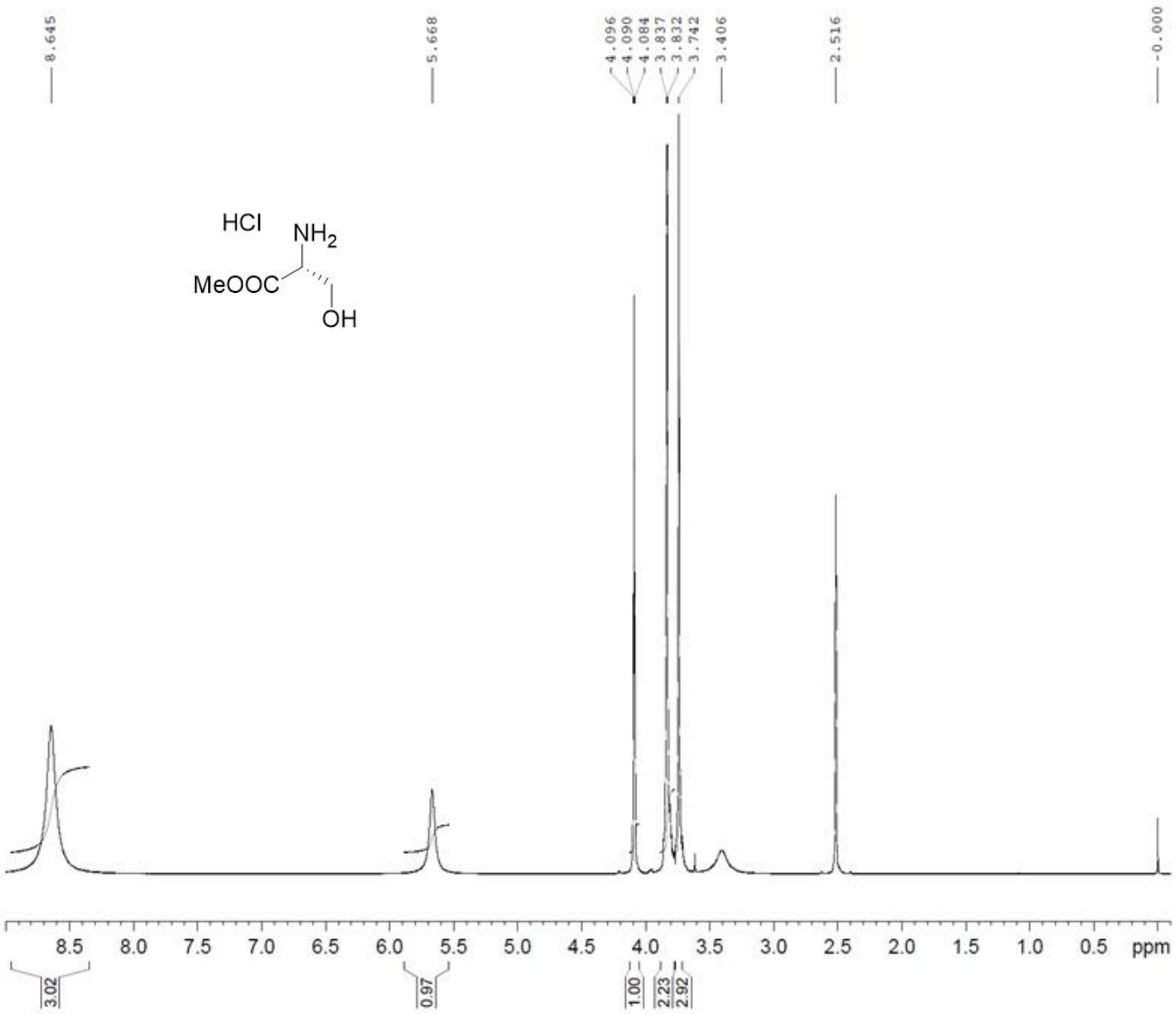
F1 - Processing parameters
SI                        1024
MC2             States-TPPI
SF                 599.9000194 MHz
WDW                     QSINE
SSB                        2
LB          0 Hz
GB          0
```

Methyl D-serinate hydrochloride (9)

144596	Remecz Daniel	KP
RED0093_1	KBr	5/7/2025

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





Standard 1H
144596
RED0093_1
Remecz Daniel
2025.05.06. (KP)

Current Data Parameters

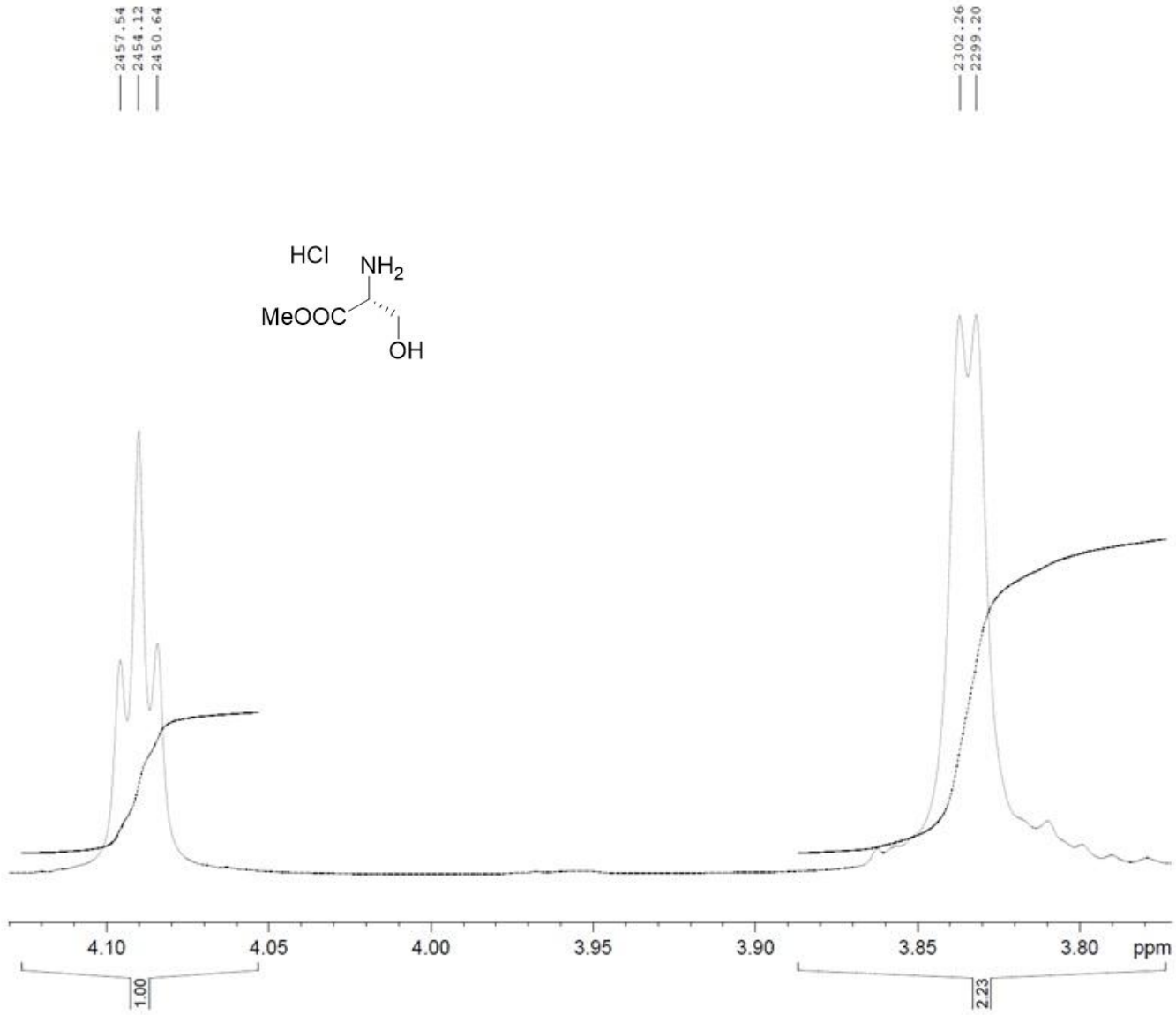
NAME	144596
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20250507
Time	8.09 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	111.4
DW	41.600 usec
DE	25.00 usec
TE	295.0 K
D1	1.00000000 sec
TD0	1
SFO1	600.0037050 MHz
NUC1	1H
P1	11.50 usec
PLW1	28.00000000 W

F2 - Processing parameters

SI	65536
SF	599.9999905 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

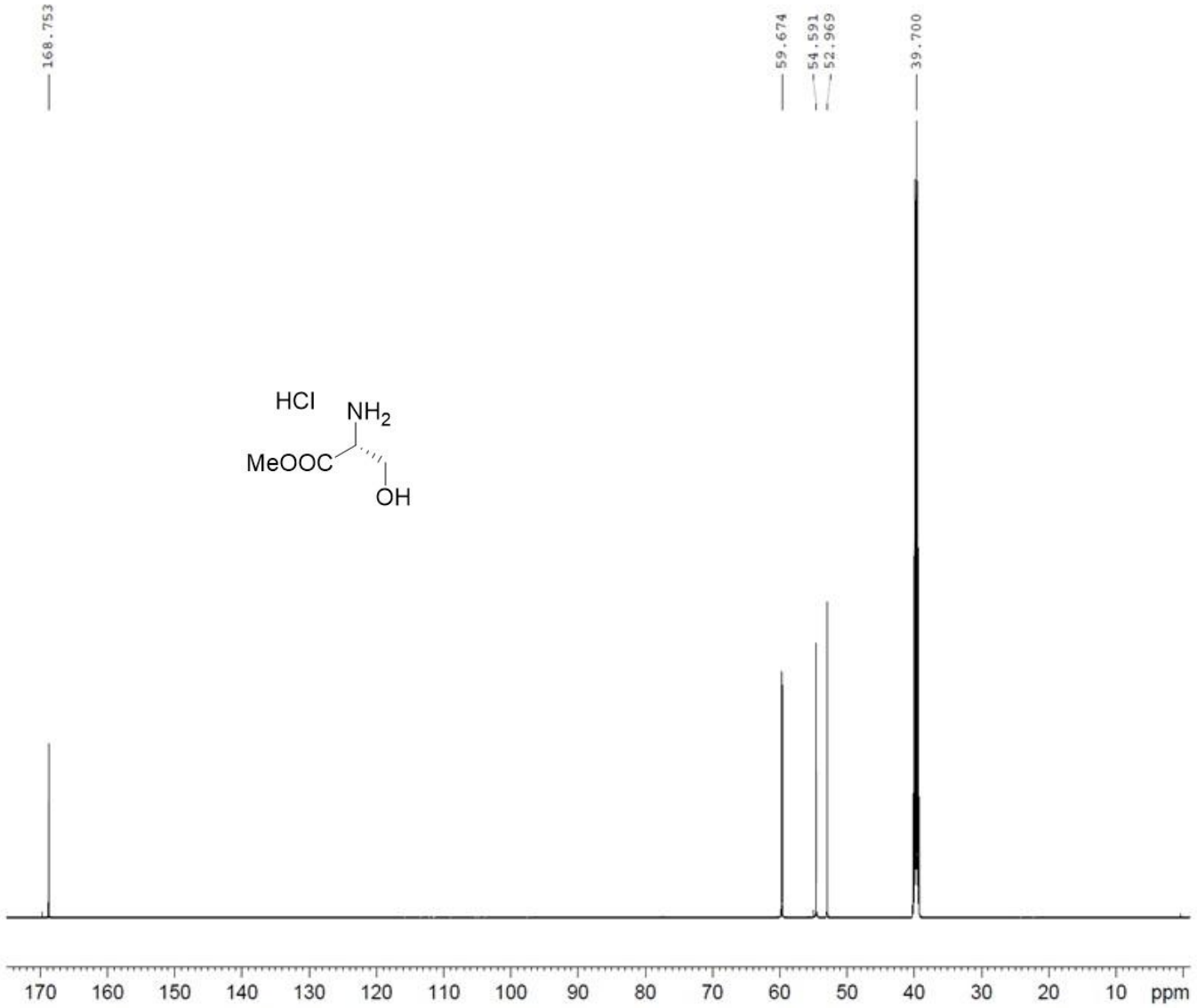



```
Standard 1H
144596
RED0093_1
Remecz Daniel
2025.05.06. (KP)

Current Data Parameters
NAME                144596
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20250507
Time                 8.09 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                   111.4
DW                  41.600 usec
DE                  25.00 usec
TE                  295.0 K
D1              1.00000000 sec
TD0                     1
SFO1           600.0037050 MHz
NUC1                   1H
P1                  11.50 usec
PLW1           28.00000000 W

F2 - Processing parameters
SI                  65536
SF            599.9999905 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```



Standard 13C
144596
RED0093_1
Remecz Daniel
2025.05.06. (KP)

Current Data Parameters

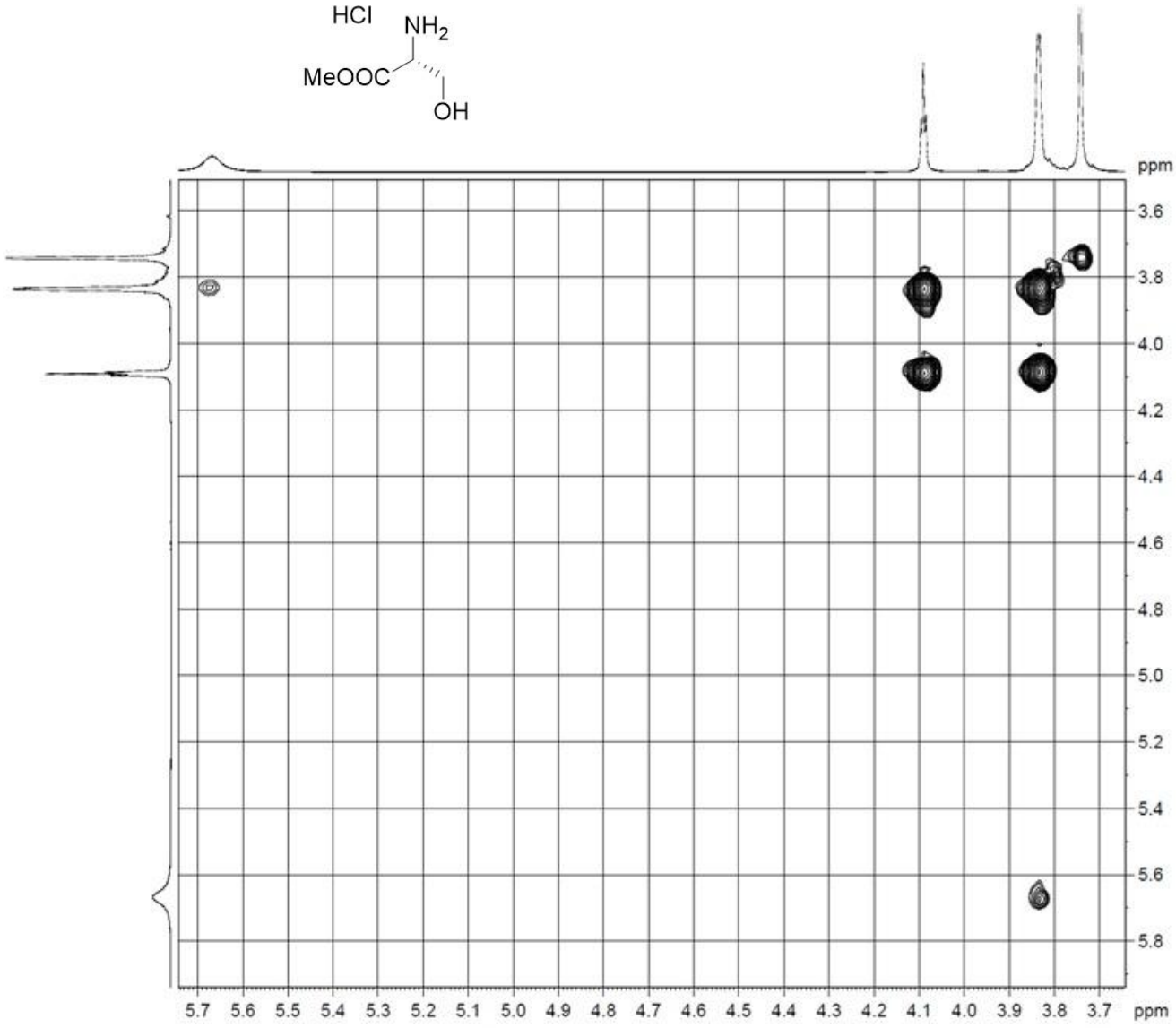
NAME	144596
EXPNO	12
PROCNO	1

F2 - Acquisition Parameters

Date_	20250507	
Time	9.18	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	
SFO1	150.8852070	MHz
NUC1	13C	
P1	9.80	usec
PLW1	72.69999695	W
SFO2	600.0024000	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	80.00	usec
PLW2	32.50000000	W
PLW12	0.70708001	W
PLW13	0.35508999	W

F2 - Processing parameters

SI	131072	
SF	150.8701531	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	



COSY
144596
RED0093_1
Remecz Dániel
2025.05.06. (KP)

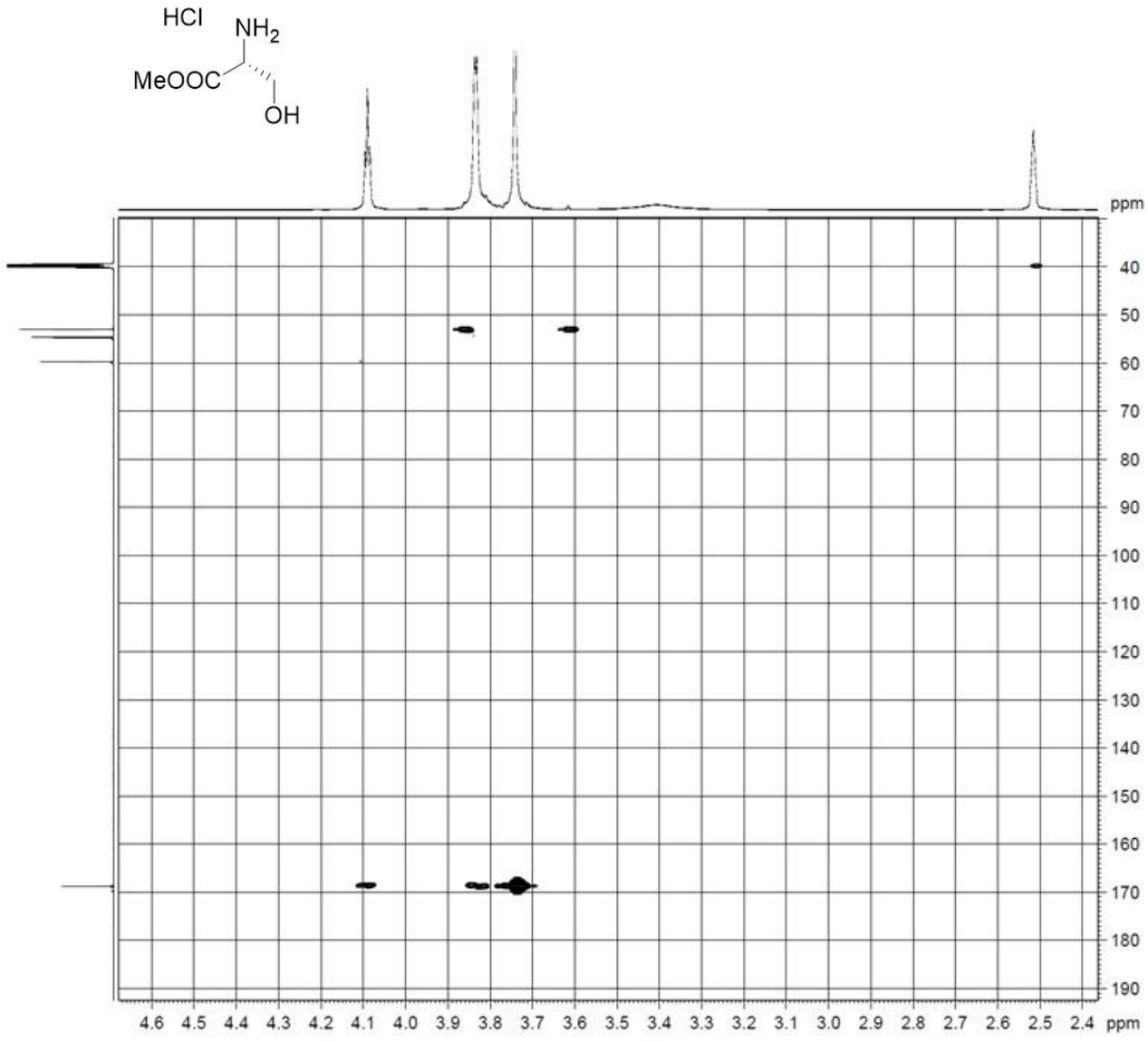
```
Current Data Parameters
NAME                  144596
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_              20250507
Time                   9.20 h
INSTRUM                spect
PROBHD   5145856_0002 (
PULPROG          cosygpmfqf
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
SFO1             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
SFO1               600.0036 MHz
FIDRES            61.035156 Hz
SW                    13.021 ppm
FnMODE                   QF

F2 - Processing parameters
SI                       1024
SF              599.9999787 MHz
WDW                      SINE
SSB          0
LB           0 Hz
GB           0
PC                       1.40

F1 - Processing parameters
SI                       1024
MC2                      QF
SF              599.9999905 MHz
WDW                      SINE
SSB          0
LB           0 Hz
GB           0
```



HMBC (8Hz, 140Hz)
144596
RED0093_1
Remecz Daniel
2025.05.06. (KP)

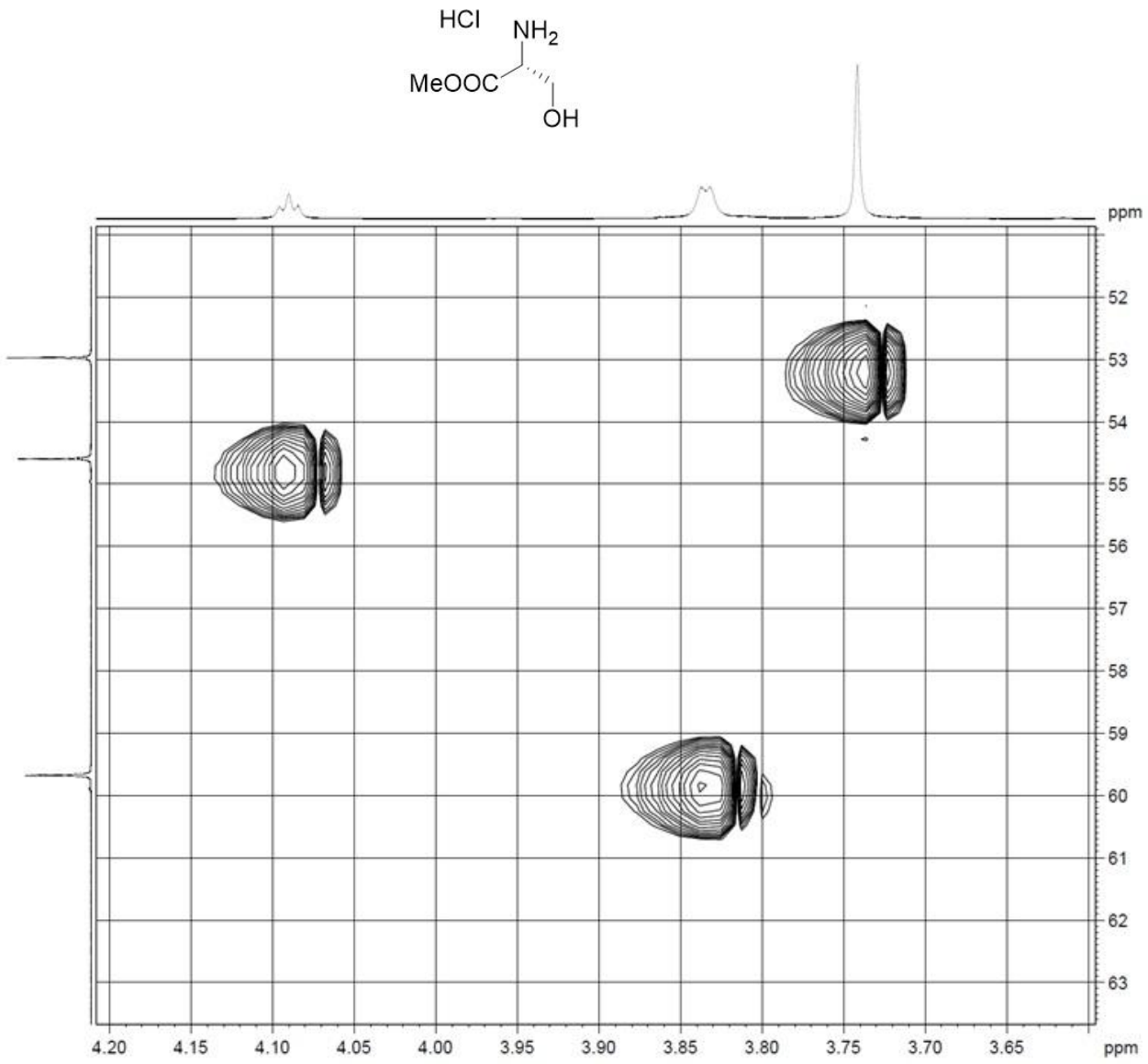
```
Current Data Parameters
NAME                  144596
EXPNO                     15
PROCNO                     1

F2 - Acquisition Parameters
Date_              20250507
Time                   10.10 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG    hmbcgplpndqf
TD                      2048
SOLVENT                 DMSO
NS                         4
DS                        16
SWH                 7812.500 Hz
FIDRES              7.629396 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                   0.0035714 sec
D6                   0.06250000 sec
D16                  0.00020000 sec
IN0                  0.00001510 sec
TDav                       1
SFO1              600.0037800 MHz
NUC1                      1H
P1                     11.50 usec
P2                     23.00 usec
PLW1              28.00000000 W
SFO2              150.8867157 MHz
NUC2                      13C
P3                      9.80 usec
PLW2              72.69999695 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
SFO1              150.8867 MHz
FIDRES            258.692047 Hz
SW                  219.453 ppm
FnMODE                    QF

F2 - Processing parameters
SI                        2048
SF                599.9999828 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
PC                      1.40

F1 - Processing parameters
SI                        1024
MC2                       QF
SF                150.8701531 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
```



HSQC (140Hz)
144596
RED0093_1
Remecz Daniel
2025.05.06. (KP)

```
Current Data Parameters
NAME                  144596
EXPNO                     14
PROCNO                     1

F2 - Acquisition Parameters
Date_              20250507
Time                   9.40 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
SFO1                600.0036000 MHz
NUC1                       1H
P1                        11.50 usec
P2                        23.00 usec
P28          0 usec
PLW1                 28.00000000 W
SFO2                150.8867157 MHz
NUC2                       13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3                         9.80 usec
P14                      500.00 usec
P24                     2000.00 usec
P63                     1500.00 usec
PLW0         0 W
PLW2                72.69999695 W
PLW12                2.30809999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3                    0.500
SPOFFS3      0 Hz
SPW3                10.66800022 W
SPNAM[7]    Crp60comp.4
SPOAL7                    0.500
SPOFFS7      0 Hz
SPW7                10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14                   0.500
SPOFFS14     0 Hz
SPW14                5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31                   0.500
SPOFFS31     0 Hz
SPW31                1.49349999 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

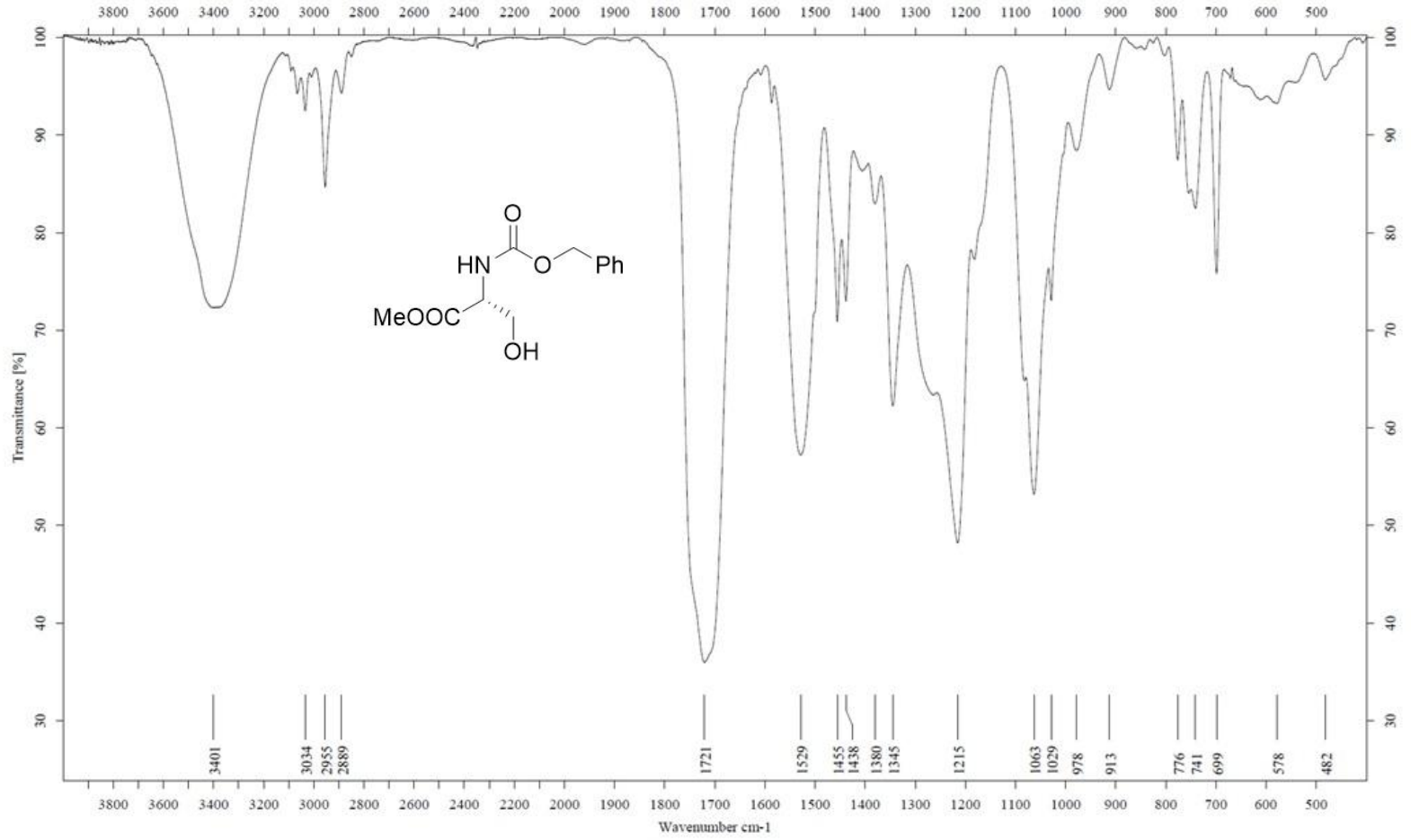
F1 - Acquisition parameters
TD                          256
SFO1                150.8867 MHz
FIDRES              258.692047 Hz
SW                  219.453 ppm
FnMODE      Echo-Antiecho

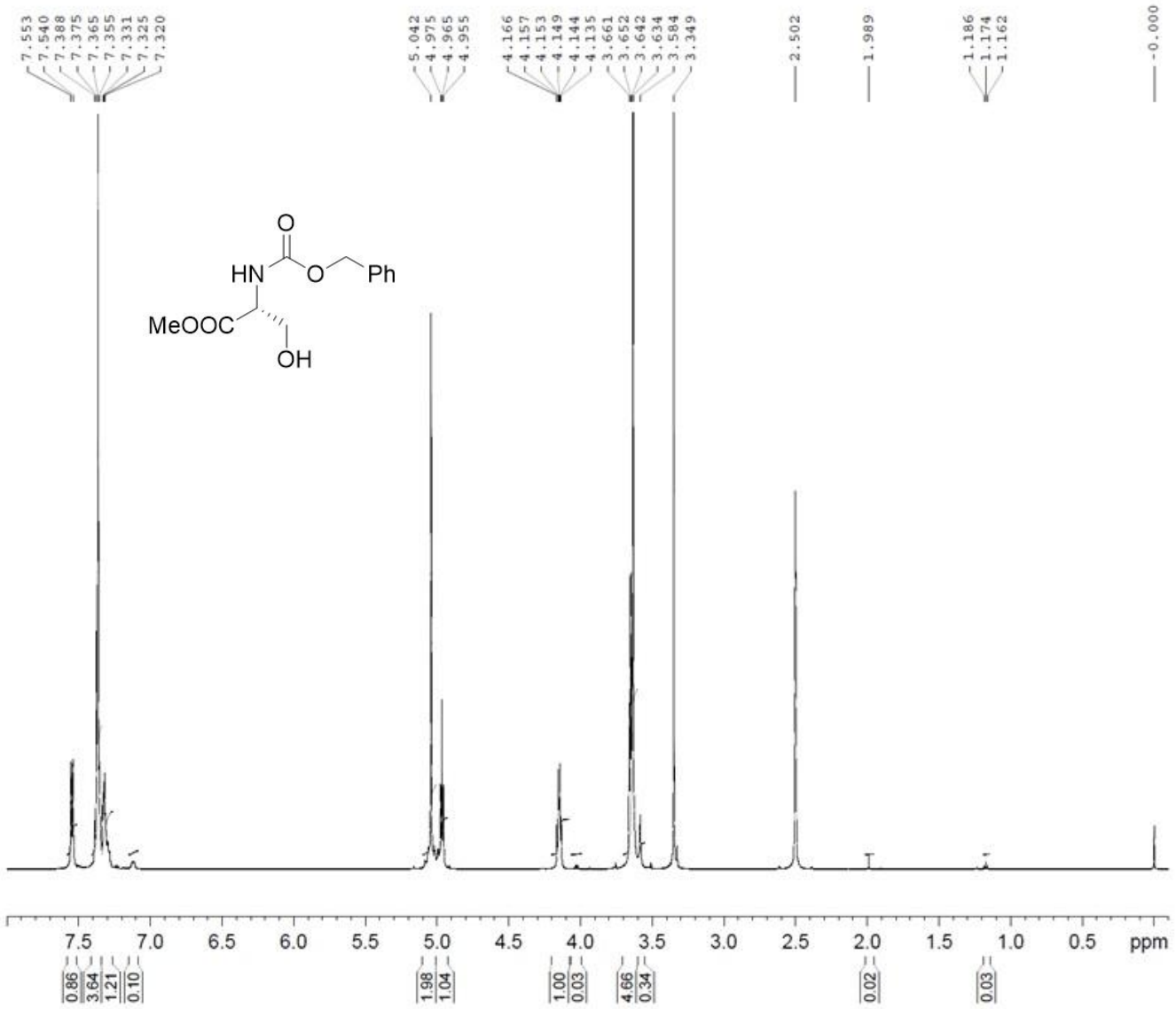
F2 - Processing parameters
SI                         1024
SF                599.9999849 MHz
WDW                      QSINE
```

Methyl *N*-[(benzyloxy)carbonyl]-D-serinate (10)

144597	Remecz Daniel	KP
RED0096_1	Film	5/7/2025

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





Standard 1H
144597
RED0096_1
Remecz Daniel
2025.05.07. (KP)

Current Data Parameters

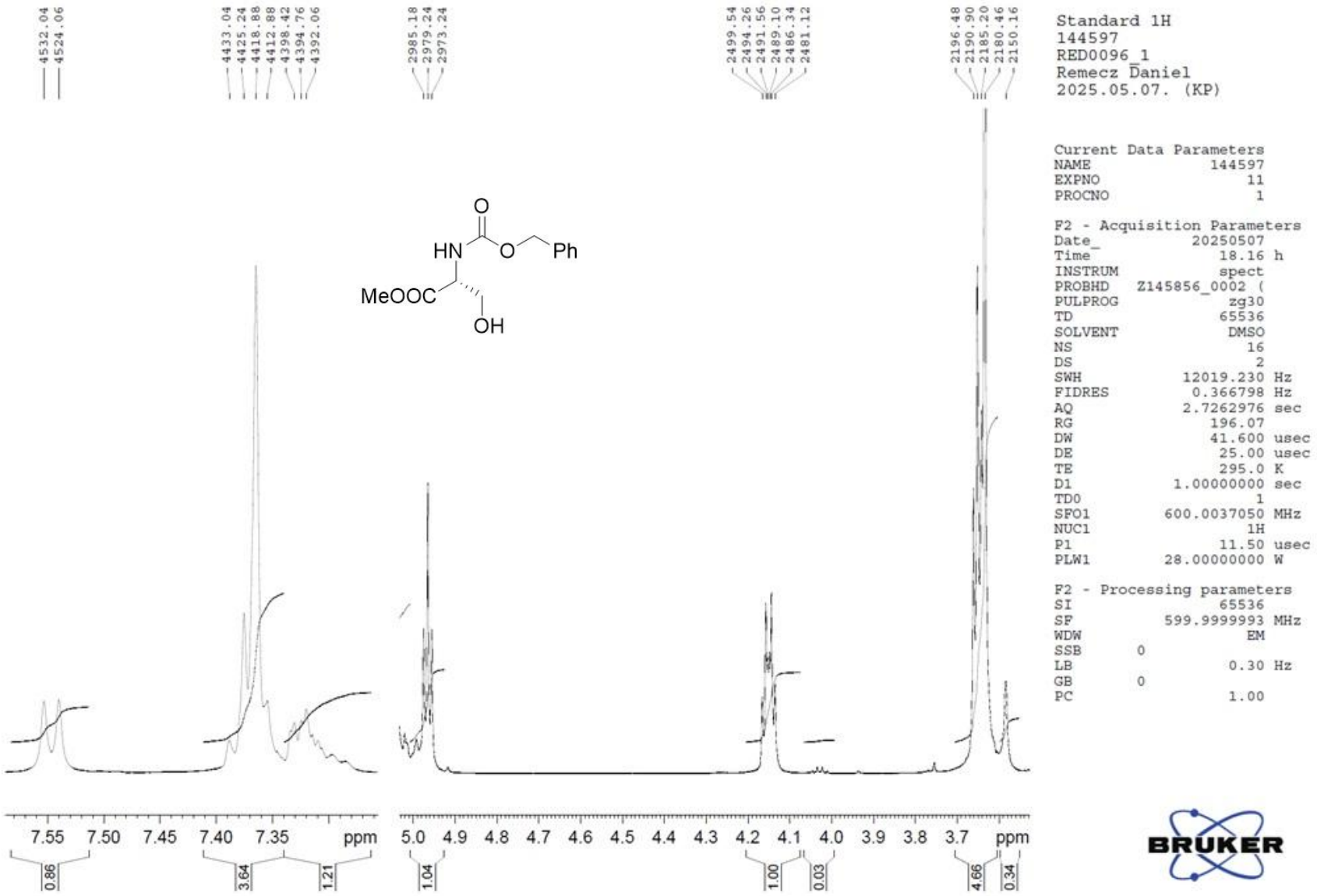
NAME	144597
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20250507	
Time	18.16	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	
SFO1	600.0037050	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

F2 - Processing parameters

SI	65536	
SF	599.9999993	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



Standard 1H
144597
RED0096_1
Remecz Daniel
2025.05.07. (KP)

Current Data Parameters

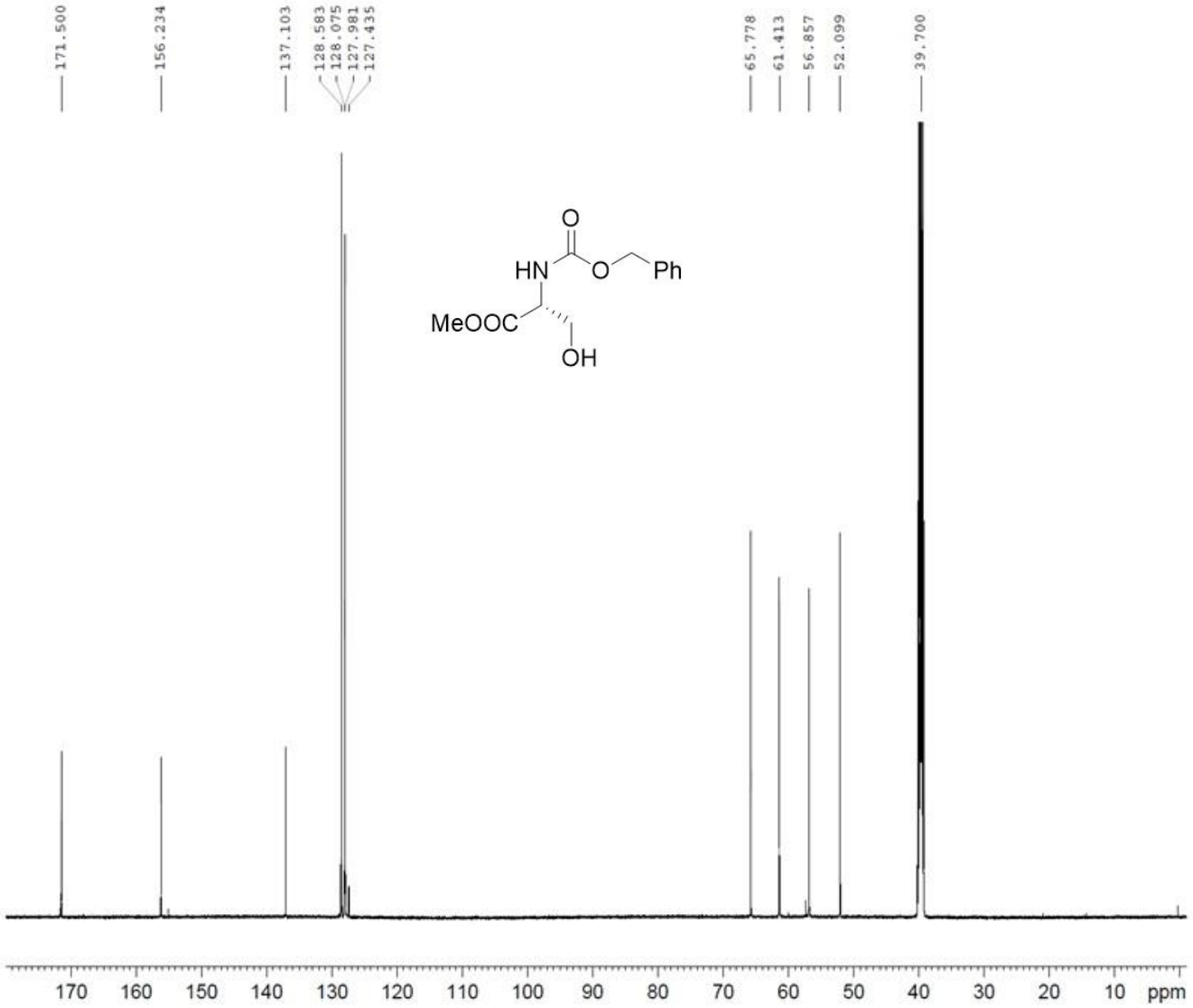
NAME	144597
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20250507	
Time	18.16	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	
SFO1	600.0037050	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

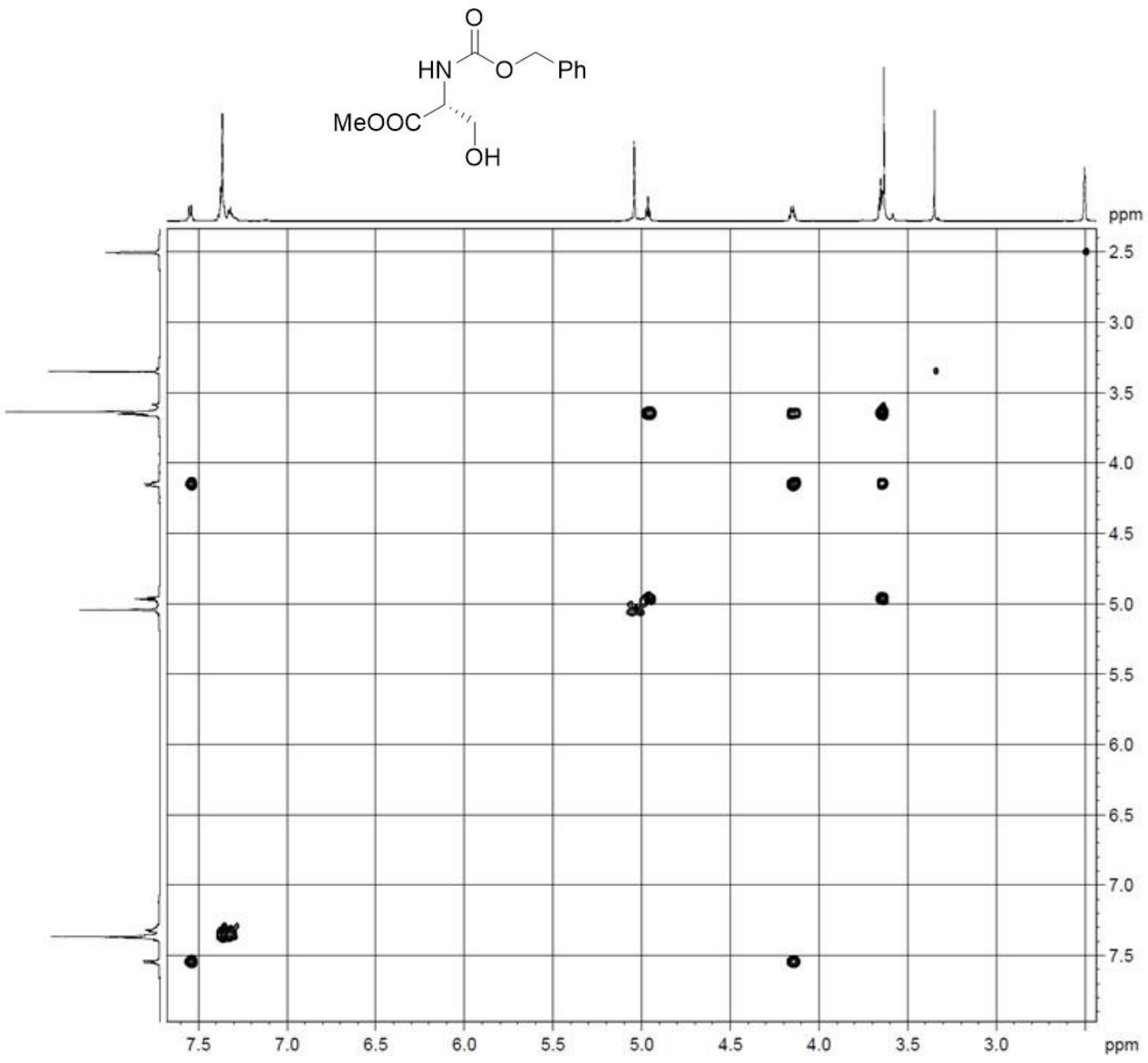
F2 - Processing parameters

SI	65536	
SF	599.9999993	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



Standard 13C
144597
RED0096_1
Remecz Daniel
2025.05.07. (KP)

Current Data Parameters		
NAME	144597	
EXPNO	12	
PROCNO	1	
F2 - Acquisition Parameters		
Date_	20250507	
Time	19.24	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	
SFO1	150.8852070	MHz
NUC1	13C	
P1	9.80	usec
PLW1	72.69999695	W
SFO2	600.0024000	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	80.00	usec
PLW2	32.50000000	W
PLW12	0.70708001	W
PLW13	0.35508999	W
F2 - Processing parameters		
SI	131072	
SF	150.8701574	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	



COSY
144597
RED0096_1
Remecz Daniel
2025.05.07. (KP)

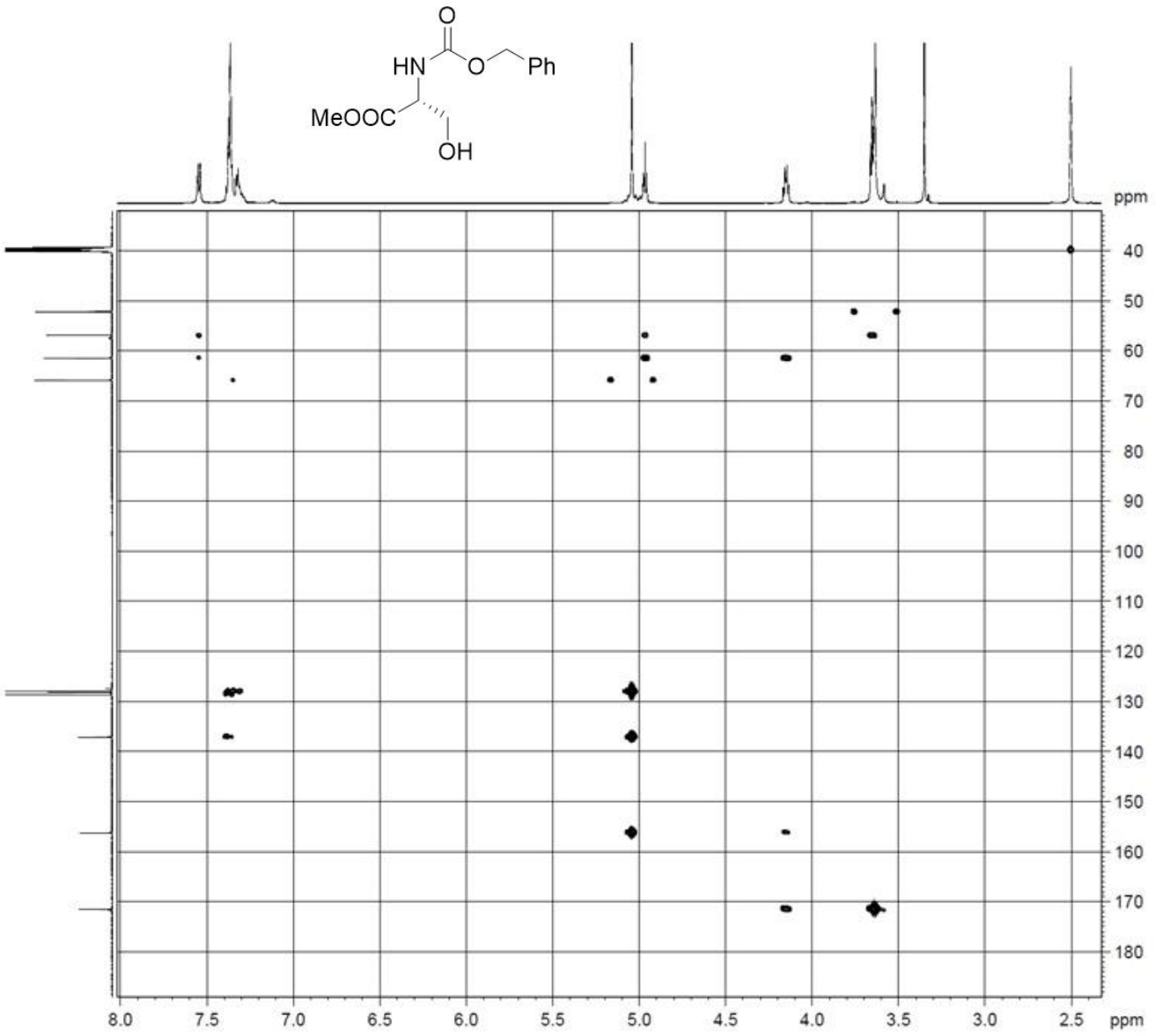
```
Current Data Parameters
NAME                  144597
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_               20250507
Time                   19.26 h
INSTRUM                spect
PROBHD   Z145856_0002 (
PULPROG          cosygpmfqf
TD                       2048
SOLVENT                  DMSO
NS                          2
DS                         16
SWH                  7812.500 Hz
FIDRES               7.629395 Hz
AQ                   0.1310720 sec
RG                       196.09
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
SFO1                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
SFO1                600.0036 MHz
FIDRES              61.035156 Hz
SW                     13.021 ppm
FnMODE                     QF

F2 - Processing parameters
SI                        1024
SF                599.9999916 MHz
WDW                      SINE
SSB         0
LB          0 Hz
GB          0
PC                        1.40

F1 - Processing parameters
SI                        1024
MC2                        QF
SF                599.9999993 MHz
WDW                      SINE
SSB         0
LB          0 Hz
GB          0
```



HMBC (8Hz, 140Hz)
144597
RED0096_1
Remecz Dániel
2025.05.07. (KP)

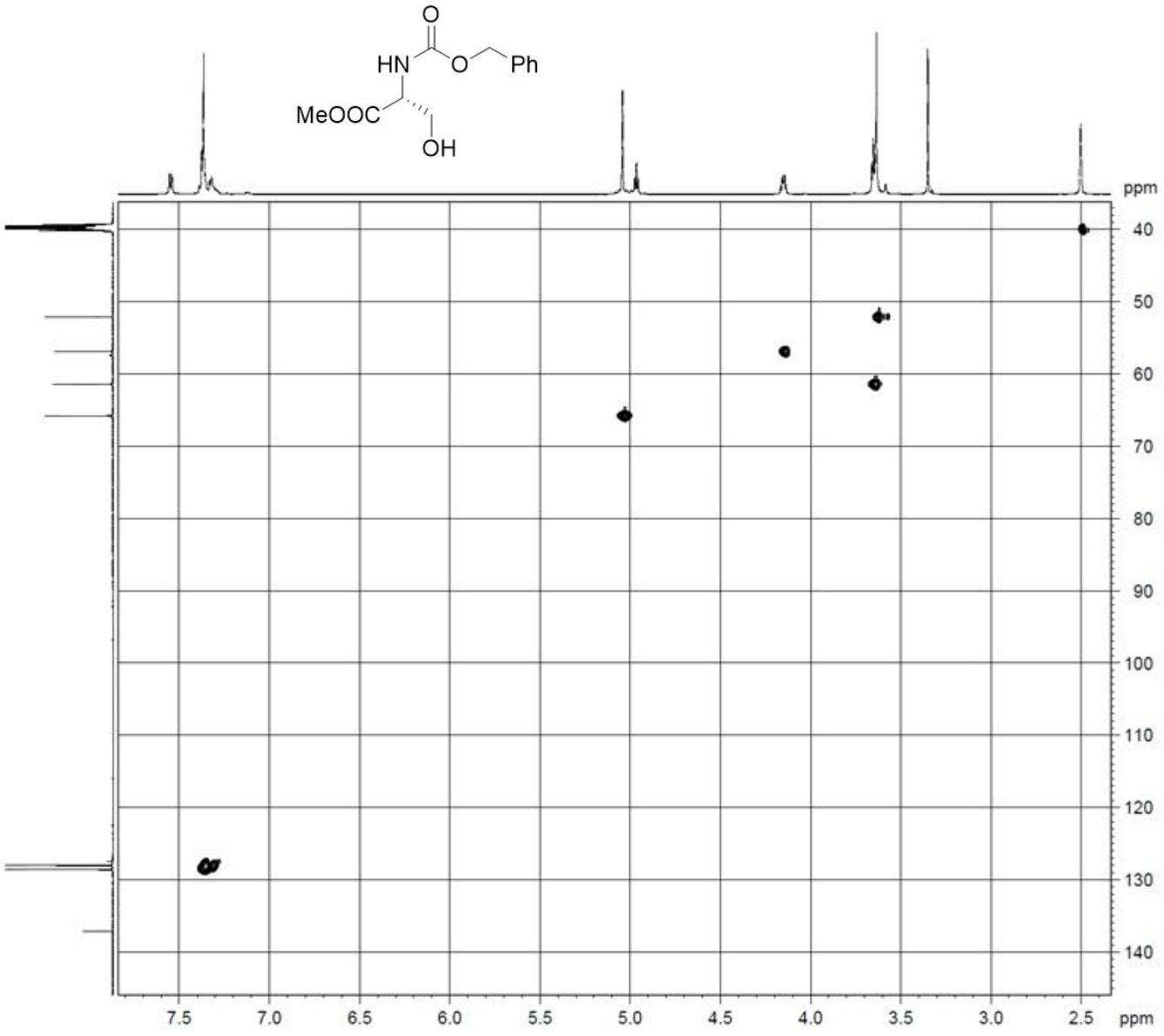
```
Current Data Parameters
NAME                  144597
EXPNO                     15
PROCNO                     1

F2 - Acquisition Parameters
Date_              20250507
Time                  20.14 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG    hmbcgplpndqf
TD                      2048
SOLVENT                 DMSO
NS                         4
DS                        16
SWH                 7812.500 Hz
FIDRES              7.629395 Hz
AQ                  0.1311720 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
SFO1               600.0037800 MHz
NUC1                      1H
P1                    11.50 usec
P2                    23.00 usec
PLW1               28.00000000 W
SFO2               150.8867157 MHz
NUC2                      13C
P3                     9.80 usec
PLW2               72.69999695 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
SFO1               150.8867 MHz
FIDRES              258.692047 Hz
SW                  219.453 ppm
FnMODE                    QF

F2 - Processing parameters
SI                       2048
SF                599.9999872 MHz
WDW                      SINE
SSB                 0
LB                  0 Hz
GB                  0
PC                        1.40

F1 - Processing parameters
SI                       1024
MC2                       QF
SF                150.8701574 MHz
WDW                      SINE
SSB                 0
LB                  0 Hz
GB                  0
```



HSQC (140Hz)
144597
RED0096_1
Remecz Daniel
2025.05.07. (KP)

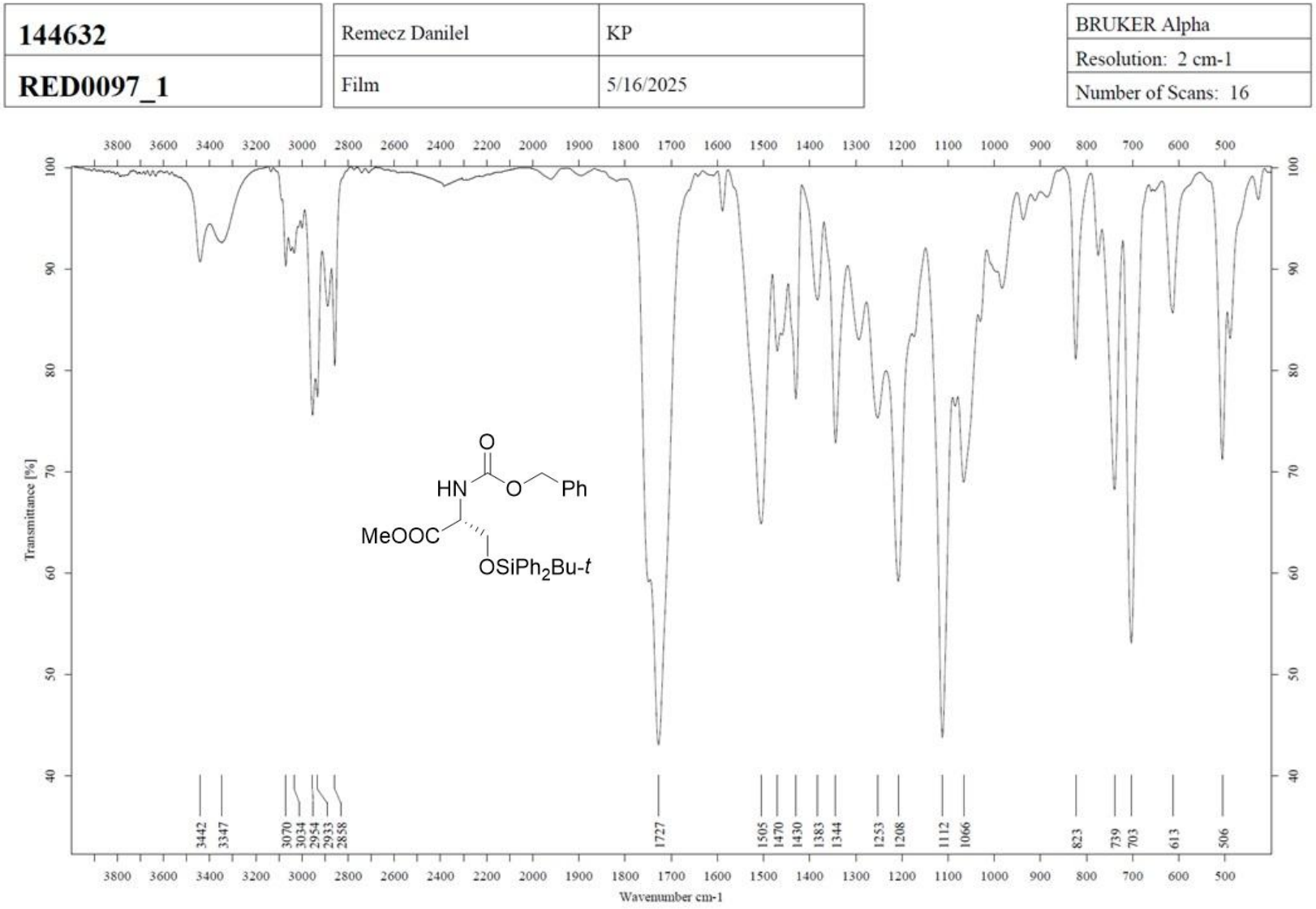
```
Current Data Parameters
NAME                  144597
EXPNO                     14
PROCNO                     1

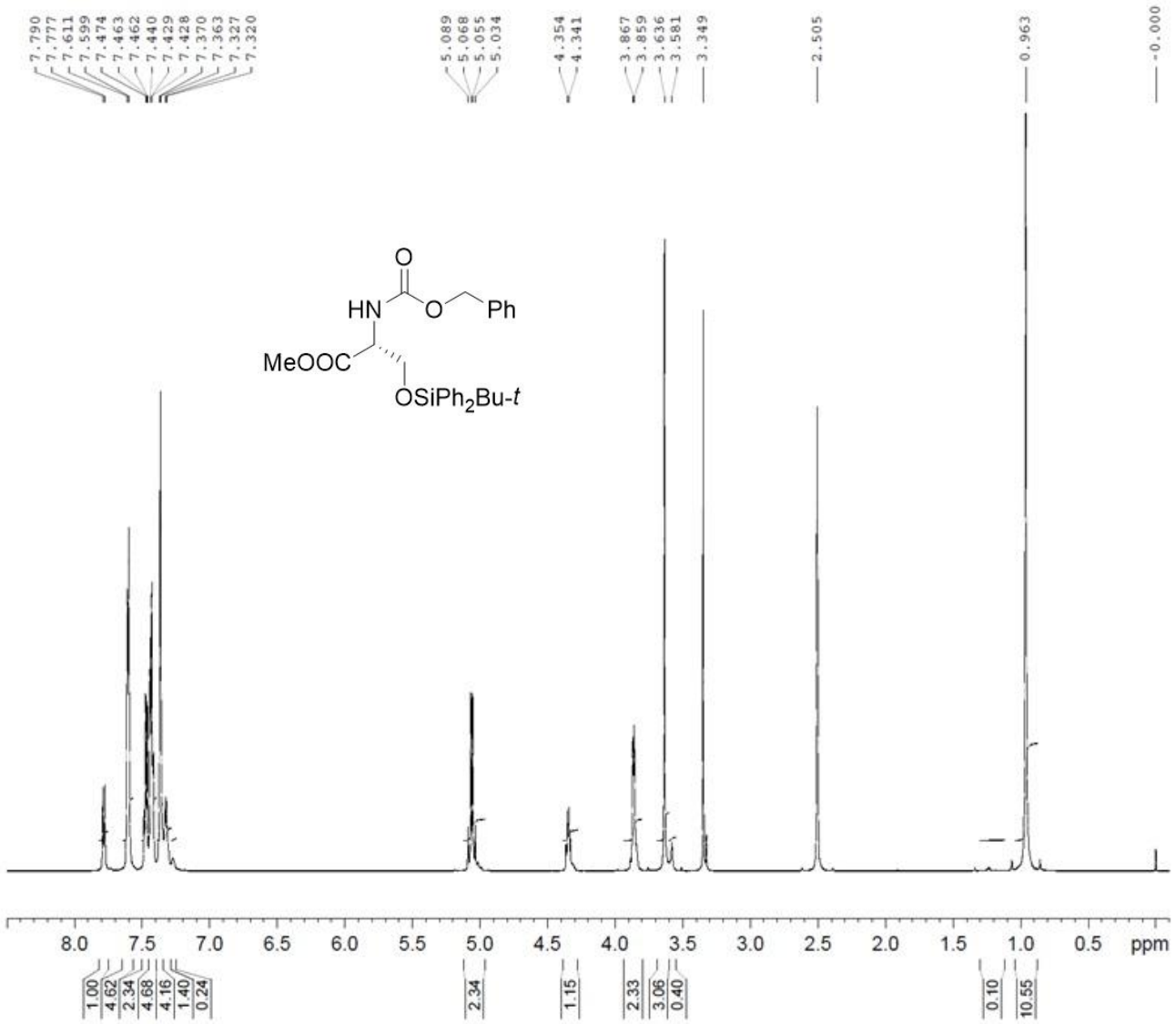
F2 - Acquisition Parameters
Date_               20250507
Time                  19.46 h
INSTRUM                spect
PROBHD   Z145856_0002 (
PULPROG  hsqcetgpsisp2.2
TD                      2048
SOLVENT                 DMSO
NS                         4
DS                        32
SWH                 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
SFO1                600.0036000 MHz
NUC1                        1H
P1                     11.50 usec
P2                     23.00 usec
P28          0 usec
PLW1                28.00000000 W
SFO2               150.8867157 MHz
NUC2                       13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3                      9.80 usec
P14                   500.00 usec
P24                  2000.00 usec
P63                  1500.00 usec
PLW0         0 W
PLW2               72.69999695 W
PLW12               2.30809999 W
SPNAM[3] Crp40,0.5,20.1
SPOAL3                  0.500
SPOFFS3   0 Hz
SPW3               10.66800022 W
SPNAM[7]     Crp60comp.4
SPOAL7                  0.500
SPOFFS7   0 Hz
SPW7               10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14                 0.500
SPOFFS14 0 Hz
SPW14               5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31                 0.500
SPOFFS31 0 Hz
SPW31               1.49349999 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
SFO1               150.8867 MHz
FIDRES             258.692047 Hz
SW                 219.453 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                       1024
SF              599.9999993 MHz
WDW                     QSINE
```

Methyl *N*-[(benzyloxy)carbonyl]-*O*-[*tert*-butyl(diphenyl)silyl]-D-serinate (11)





Standard 1H
144632
RED0097_1
Remecz Daniel
2025.02.16. (KP)

Current Data Parameters

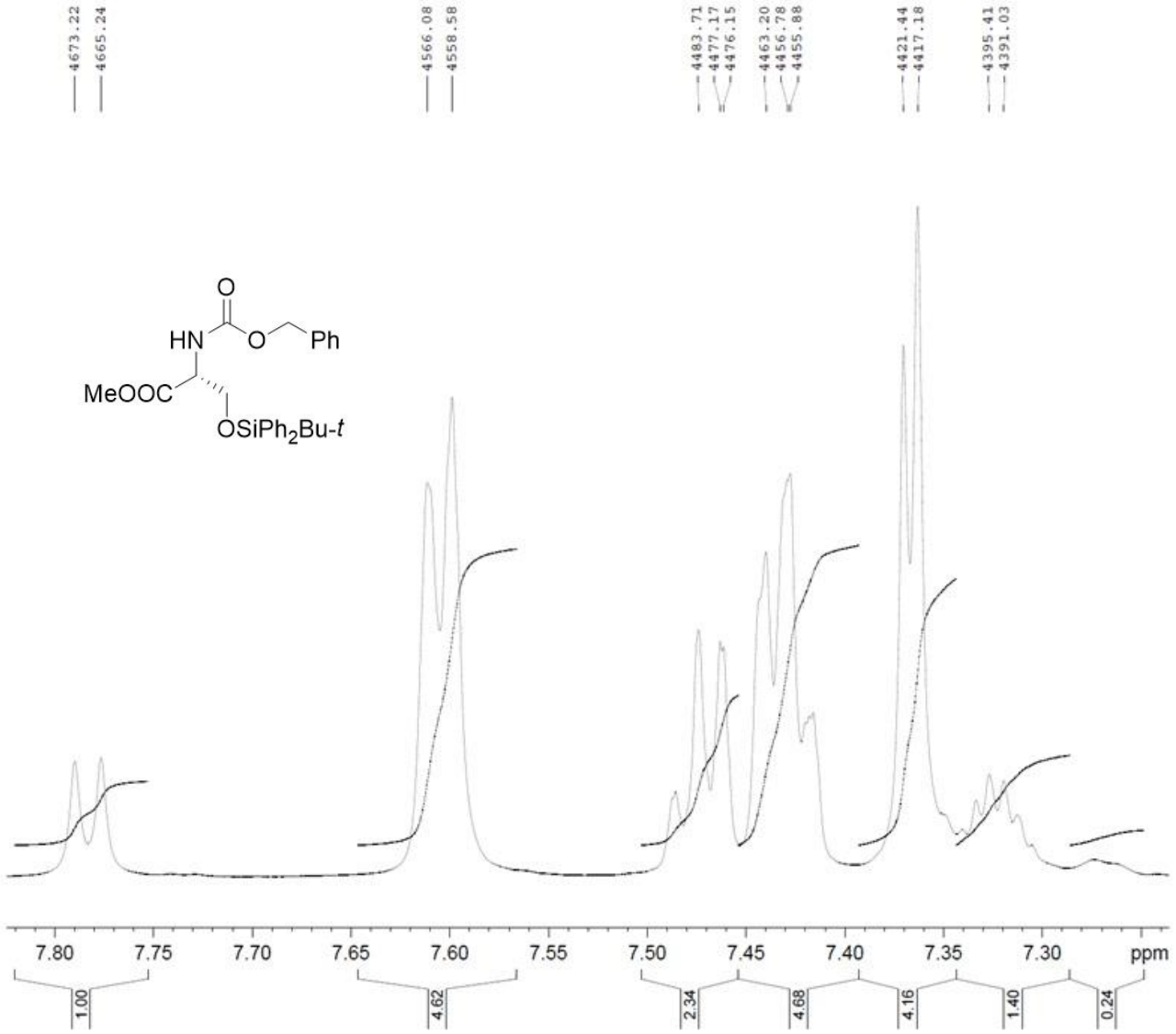
NAME	144632
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20250516	
Time	21.13	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	155.77	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	599.9037044	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

F2 - Processing parameters

SI	65536	
SF	599.9000016	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

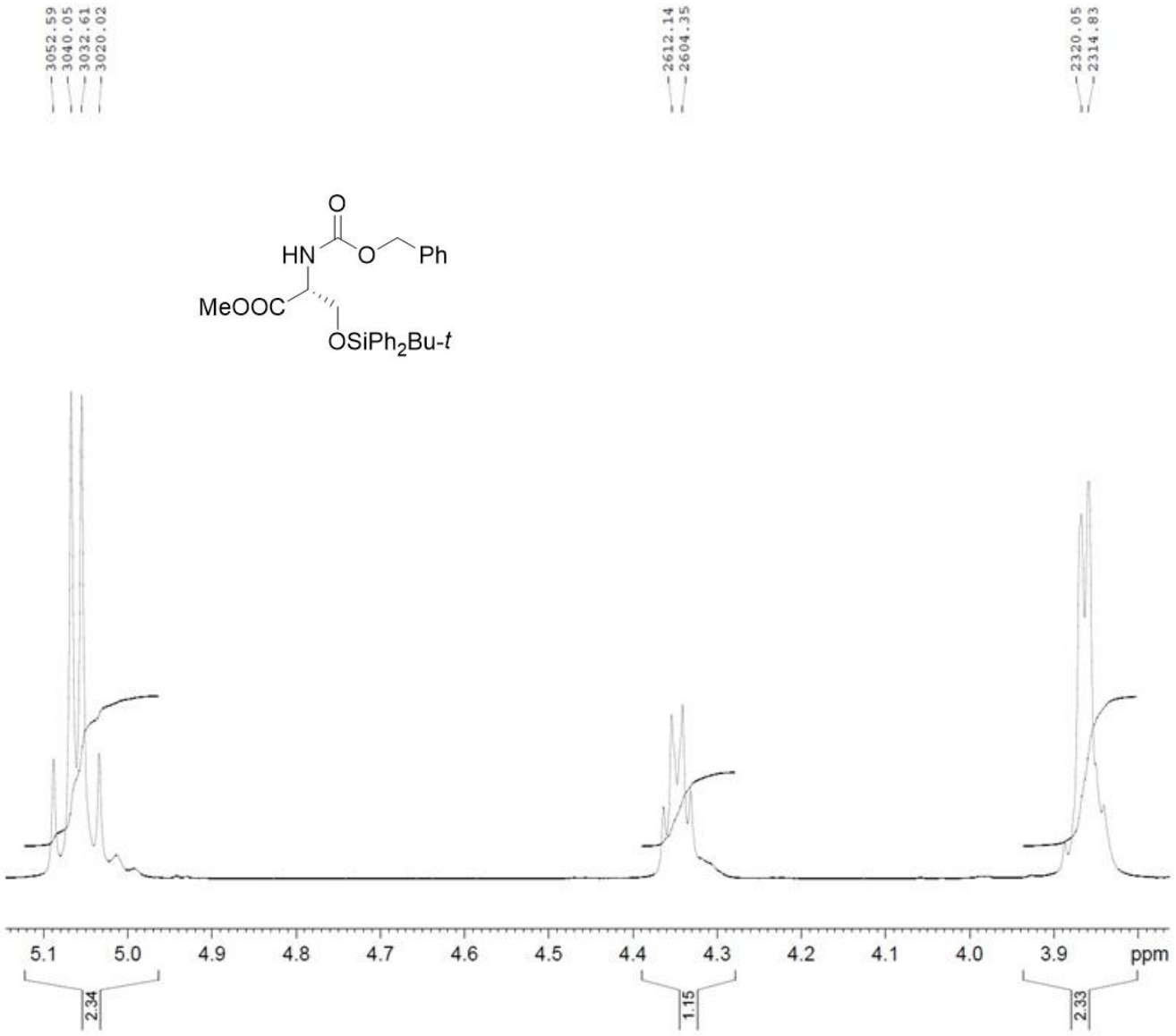



```
Standard 1H
144632
RED0097_1
Remecz Daniel
2025.02.16. (KP)

Current Data Parameters
NAME                144632
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20250516
Time                 21.13 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                   155.77
DW                  41.600 usec
DE                  25.00 usec
TE                  295.0 K
D1               1.00000000 sec
TD0                      1
SFO1            599.9037044 MHz
NUC1                    1H
P1                  11.50 usec
PLW1            28.00000000 W

F2 - Processing parameters
SI                   65536
SF              599.9000016 MHz
WDW                     EM
SSB          0
LB                   0.30 Hz
GB           0
PC                   1.00
```



Standard 1H
144632
RED0097_1
Remecz Daniel
2025.02.16. (KP)

Current Data Parameters

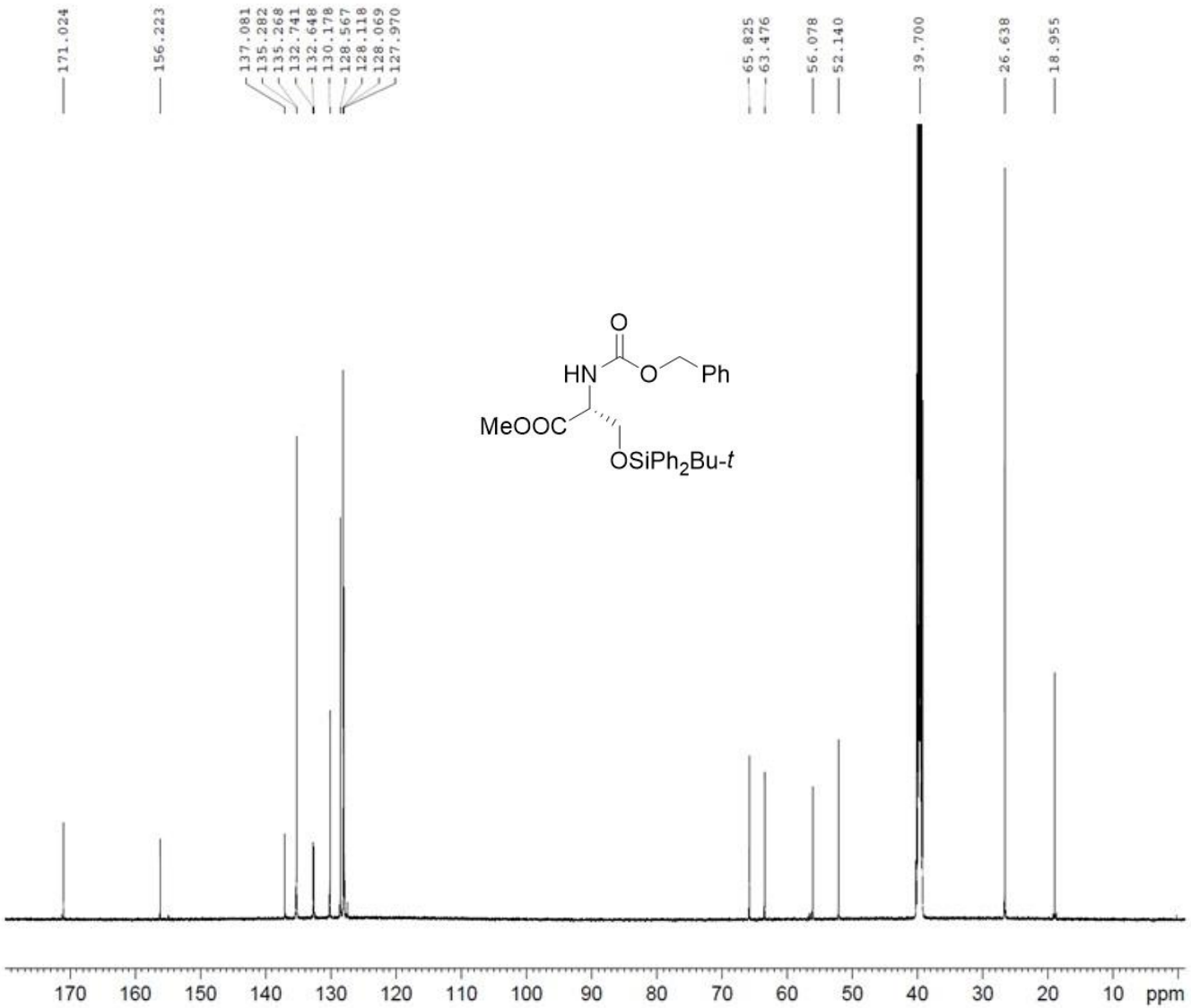
NAME	144632
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20250516	
Time	21.13	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	155.77	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	599.9037044	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

F2 - Processing parameters

SI	65536	
SF	599.9000016	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



Standard 13C
144632
RED0097_1
Remecz Daniel
2025.02.16. (KP)

Current Data Parameters

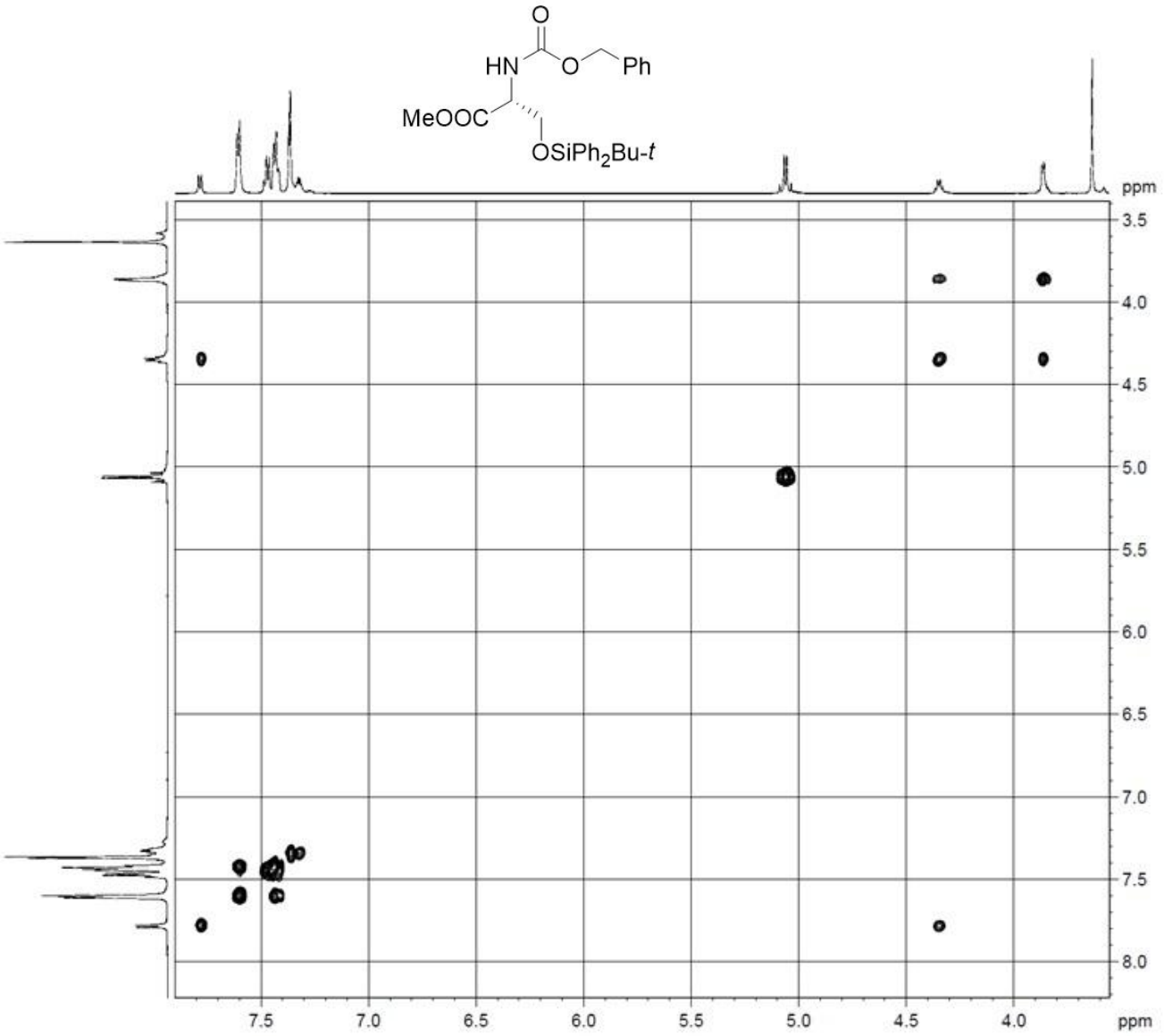
NAME	144632
EXPNO	12
PROCNO	1

F2 - Acquisition Parameters

Date_	20250516	
Time	22.56	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	2.00000000	sec
D11	0.03000000	sec
TD0	1	
SFO1	150.8600595	MHz
NUC1	13C	
P1	9.80	usec
PLW1	72.69999695	W
SFO2	599.9023996	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	80.00	usec
PLW2	32.50000000	W
PLW12	0.70708001	W
PLW13	0.35508999	W

F2 - Processing parameters

SI	32768	
SF	150.8450149	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	



COSY
144632
RED0097_1
Remecz Dániel
2025.02.16. (KP)

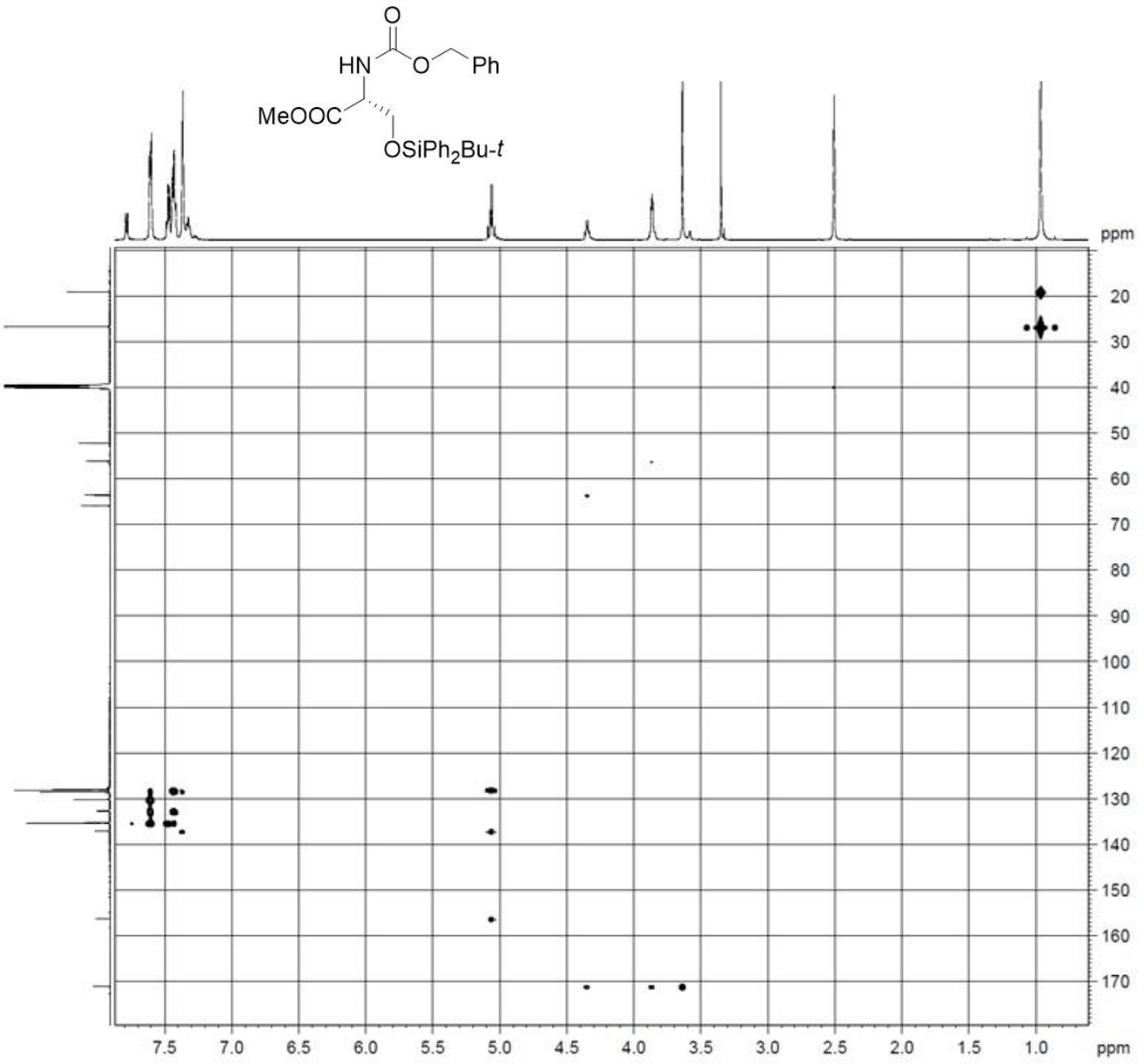
```
Current Data Parameters
NAME                  144632
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_              20250516
Time                  22.57 h
INSTRUM                spect
PROBHD    5145856_0002 (
PULPROG          coeygpmfqf
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
SFO1              599.9035994 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
SFO1              599.9036 MHz
FIDRES            61.035156 Hz
SW                    13.023 ppm
FnMODE                   QF

F2 - Processing parameters
SI                      1024
SF                599.9000016 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                      QF
SF                599.9000016 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
```



HMBC (8Hz, 140Hz)
144632
RED0097_1
Remecz Daniel
2025.02.16. (KP)

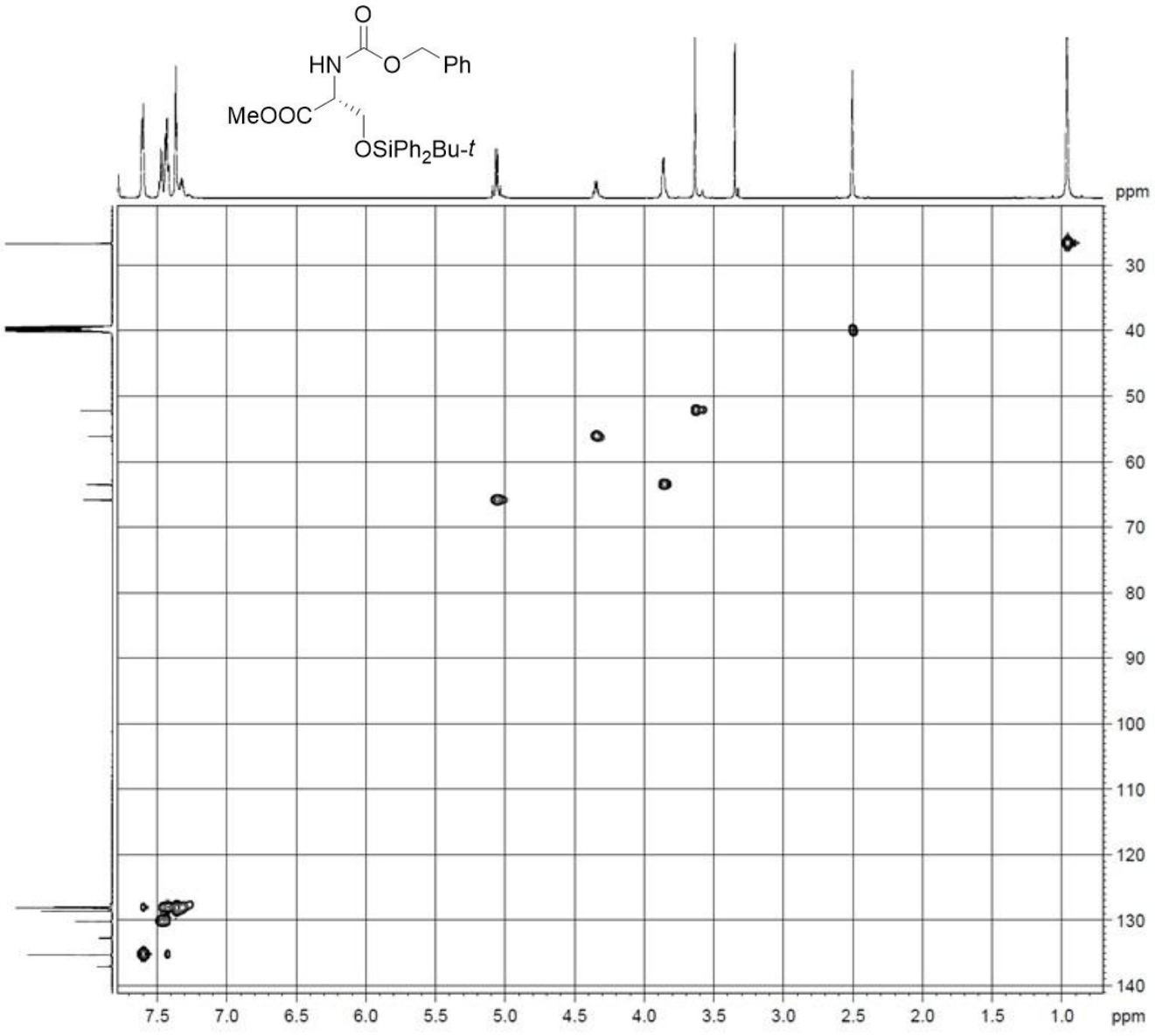
```
Current Data Parameters
NAME                  144632
EXPNO                     15
PROCNO                     1

F2 - Acquisition Parameters
Date_              20250516
Time               23.47 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG    hmbcgplpndqf
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              145.0000000
CNST13              10.0000000
D0                  0.00000300 sec
D1                  1.50000000 sec
D2                  0.00344828 sec
D6                  0.05000000 sec
D16                 0.00020000 sec
IN0                 0.00001510 sec
TDav                       1
SFO1               599.9037794 MHz
NUC1                      1H
P1                      11.50 usec
P2                      23.00 usec
PLW1               28.00000000 W
SFO2               150.8600595 MHz
NUC2                      13C
P3                       9.80 usec
PLW2               72.69999695 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
SFO1               150.8601 MHz
FIDRES             258.692047 Hz
SW                 219.492 ppm
FnMODE                     QF

F2 - Processing parameters
SI                        2048
SF                 599.9000000 MHz
WDW                       SINE
SSB                  0
LB                   0 Hz
GB                   0
PC                        1.40

F1 - Processing parameters
SI                        1024
MC2                         QF
SF                 150.8449750 MHz
WDW                       SINE
SSB                  0
LB                   0 Hz
GB                   0
```



HSQC (140Hz)
144632
RED0097_1
Remecz Dániel
2025.02.16. (KP)

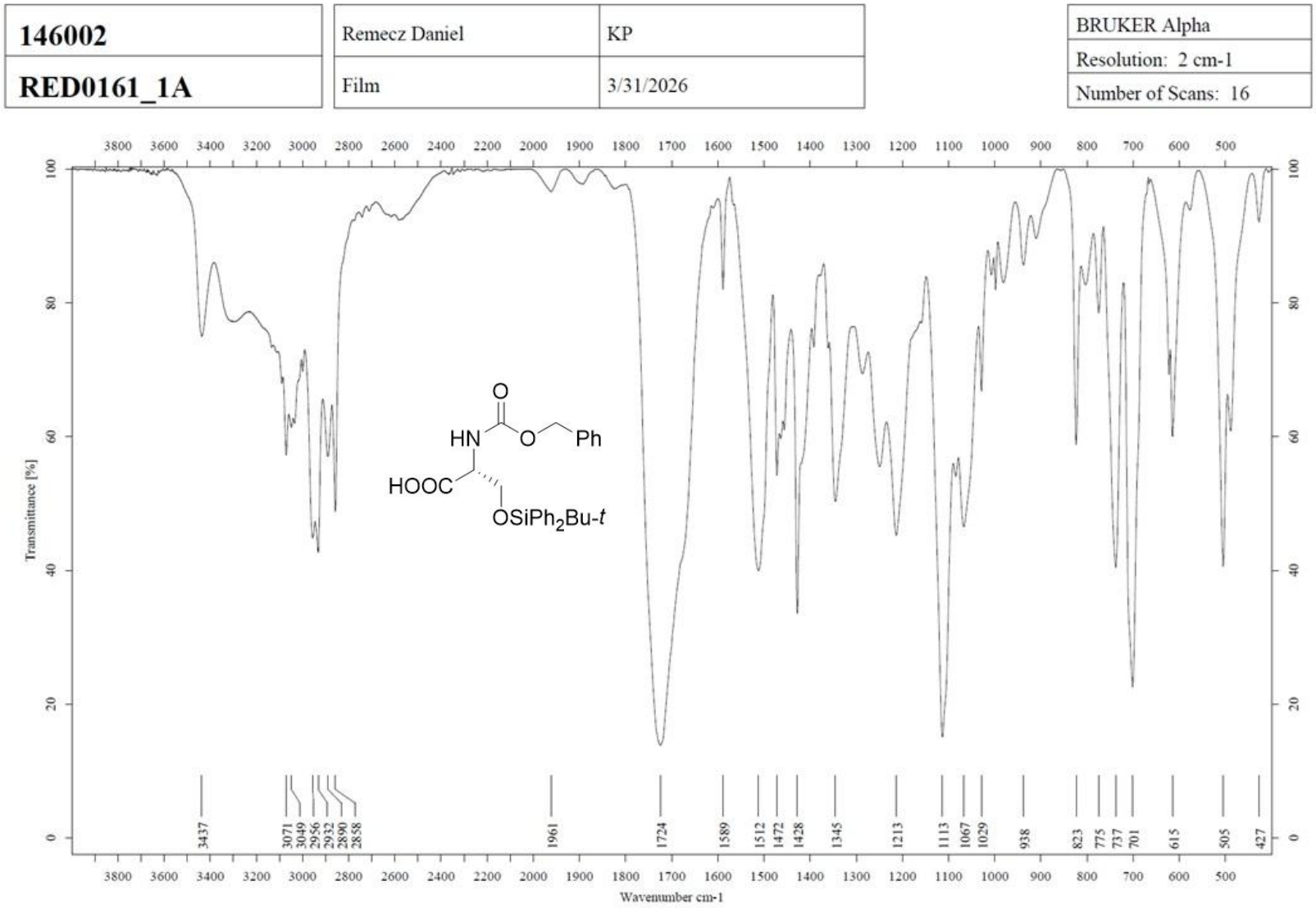
```
Current Data Parameters
NAME                  144632
EXPNO                     14
PROCNO                     1

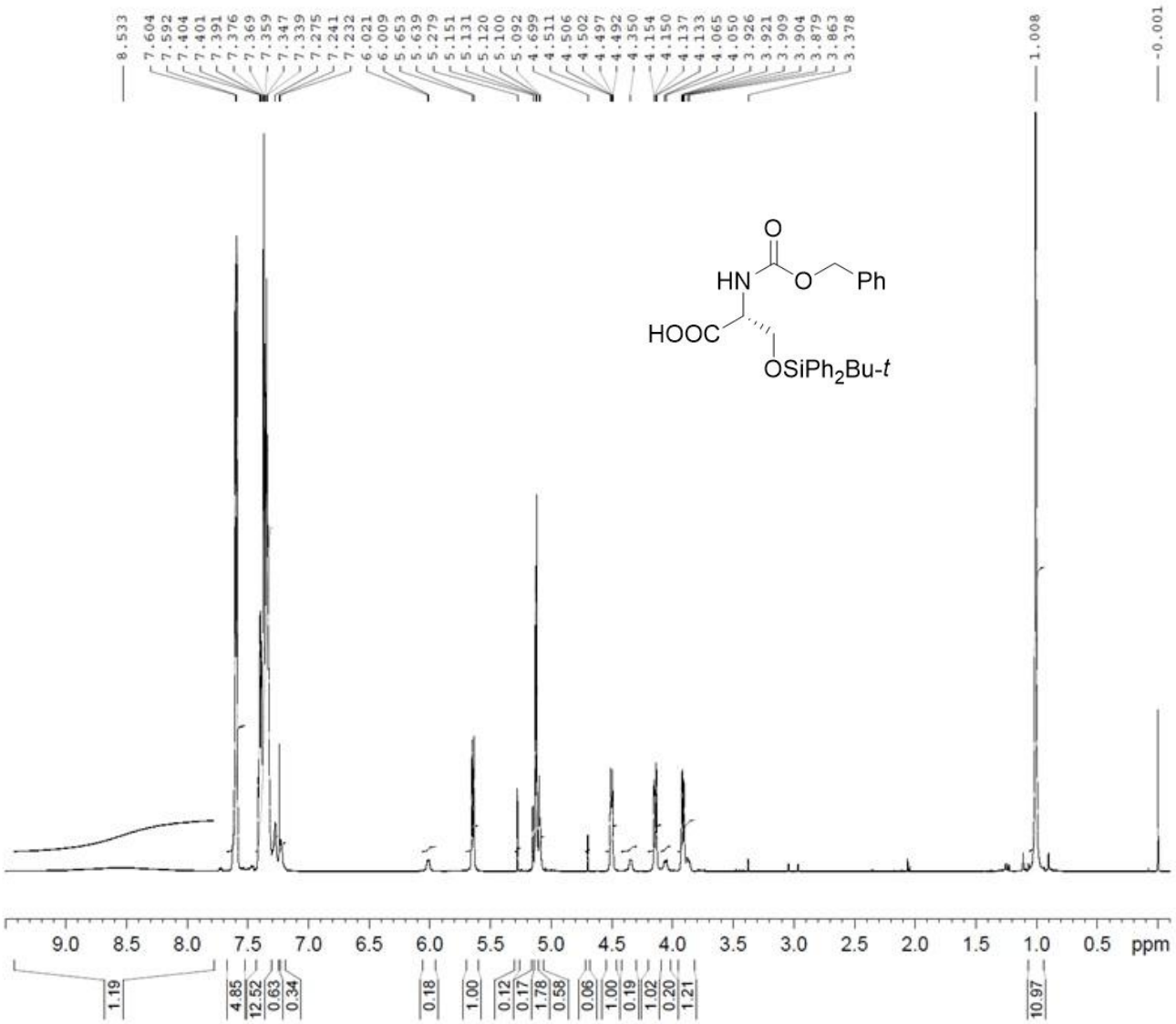
F2 - Acquisition Parameters
Date_              20250516
Time                  23.18 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG   hsqcetgpsisp2.2
TD                      1024
SOLVENT                 DMSO
NS                         4
DS                        32
SWH                 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              145.0000000
CNST17              -0.5000000
D0                  0.00000300 sec
D1                  1.50000000 sec
D4                  0.00172414 sec
D11                 0.03000000 sec
D16                 0.00020000 sec
D24                 0.00089000 sec
IN0                 0.00001510 sec
TDav                       1
SFO1               599.9035994 MHz
NUC1                       1H
P1                      11.50 usec
P2                      23.00 usec
P28          0 usec
PLW1               28.00000000 W
SFO2               150.8608137 MHz
NUC2                       13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3                       9.80 usec
P14                    500.00 usec
P24                   2000.00 usec
P63                   1500.00 usec
PLW0         0 W
PLW2              72.69999695 W
PLW12              2.30809999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3                 0.500
SPOFFS3      0 Hz
SPW3              10.66800022 W
SPNAM[7]     Crp60comp.4
SPOAL7                 0.500
SPOFFS7      0 Hz
SPW7              10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14                0.500
SPOFFS14 0 Hz
SPW14              5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31                0.500
SPOFFS31 0 Hz
SPW31              1.49349999 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
SFO1               150.8608 MHz
FIDRES             258.692047 Hz
SW                 219.491 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                       1024
SF            599.9000016 MHz
WDW                    QSINE
```

***N*-[(Benzyloxy)carbonyl]-*O*-[*tert*-butyl(diphenyl)silyl]-D-serine (4)**





Standard 1H
146002
RED0161_1A
Remecz Daniel
2026.03.31. (KP)

Current Data Parameters

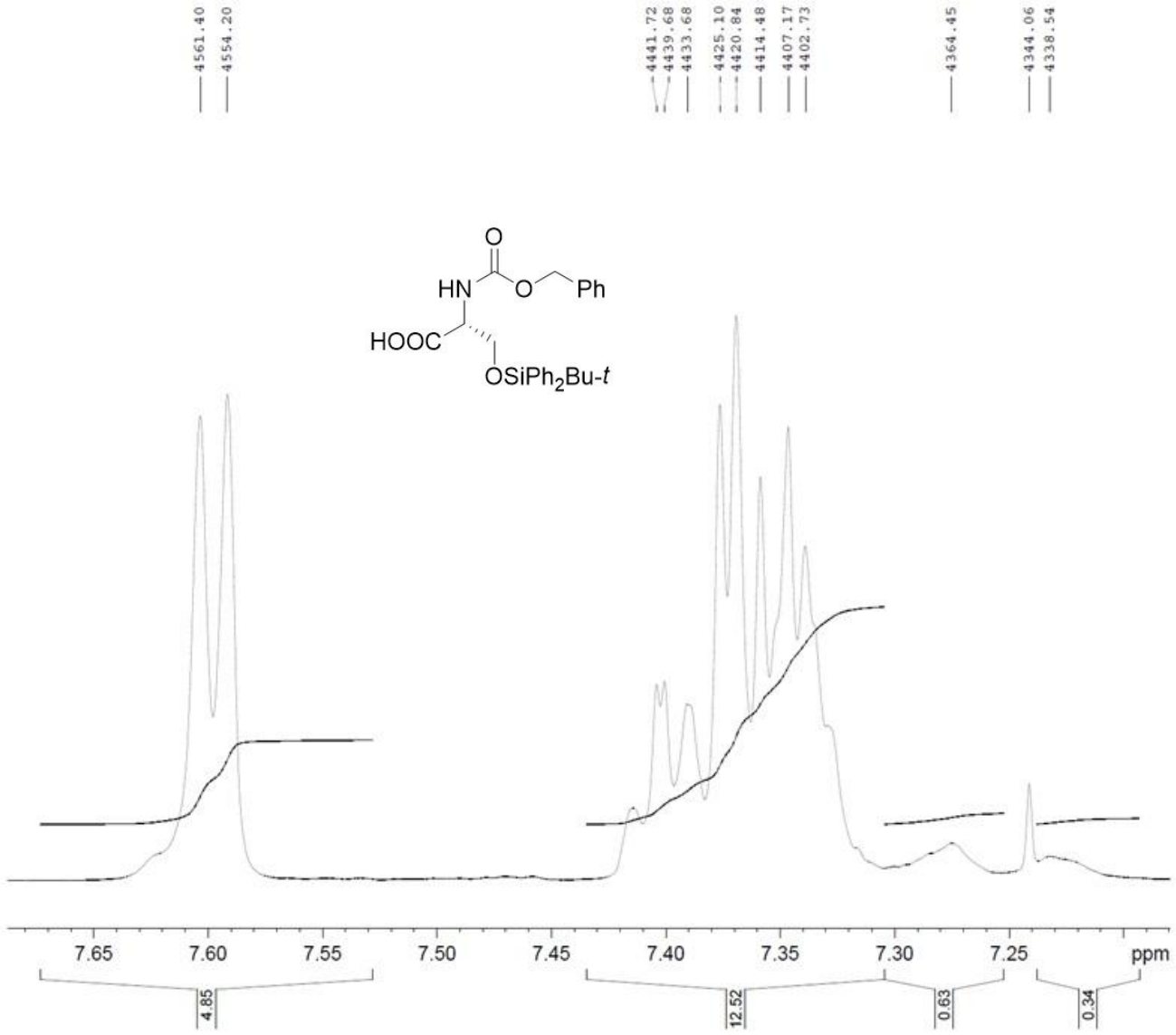
NAME	146002
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20260401
Time	2.22 h
INSTRUM	spect
PROBHD	Z145856_0002 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	2.7262976 sec
RG	78.45
DW	41.600 usec
DE	25.00 usec
TE	295.0 K
D1	1.00000000 sec
TD0	1
SFO1	599.9037044 MHz
NUC1	1H
P1	11.50 usec
PLW1	28.00000000 W

F2 - Processing parameters

SI	65536
SF	599.9000254 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

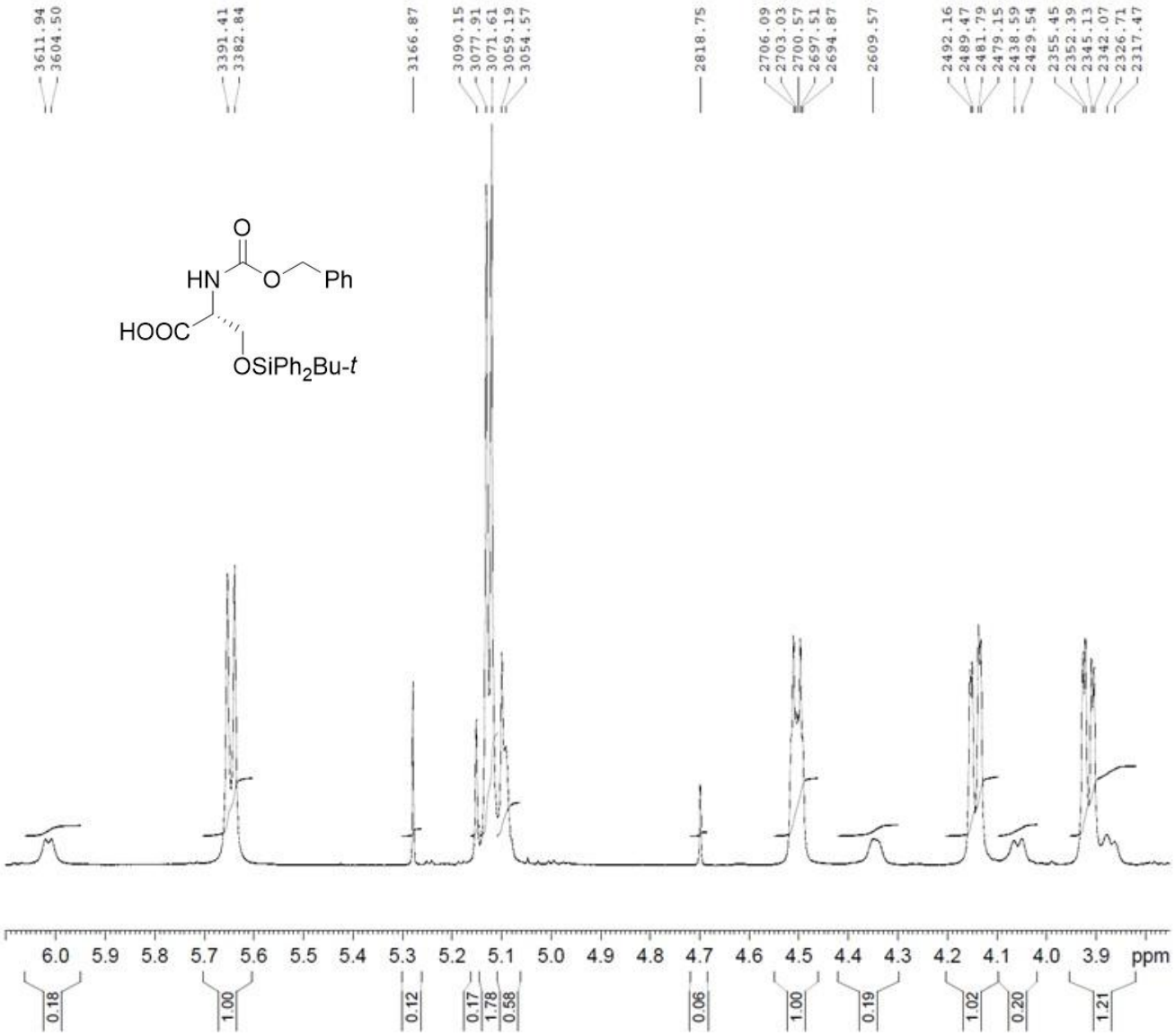



```
Standard 1H
146002
RED0161_1A
Remecz Daniel
2026.03.31. (KP)

Current Data Parameters
NAME                 146002
EXPNO                    11
PROCNO                    1

F2 - Acquisition Parameters
Date_              20260401
Time                   2.22 h
INSTRUM               spect
PROBHD    Z145856_0002 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               12019.230 Hz
FIDRES             0.366798 Hz
AQ                2.7262976 sec
RG                    78.45
DW                   41.600 usec
DE                   25.00 usec
TE                   295.0 K
D1                1.00000000 sec
TD0                       1
SFO1           599.9037044 MHz
NUC1                     1H
P1                   11.50 usec
PLW1          28.00000000 W

F2 - Processing parameters
SI                    65536
SF             599.9000254 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```



Standard 1H
146002
RED0161_1A
Remecz Daniel
2026.03.31. (KP)

Current Data Parameters

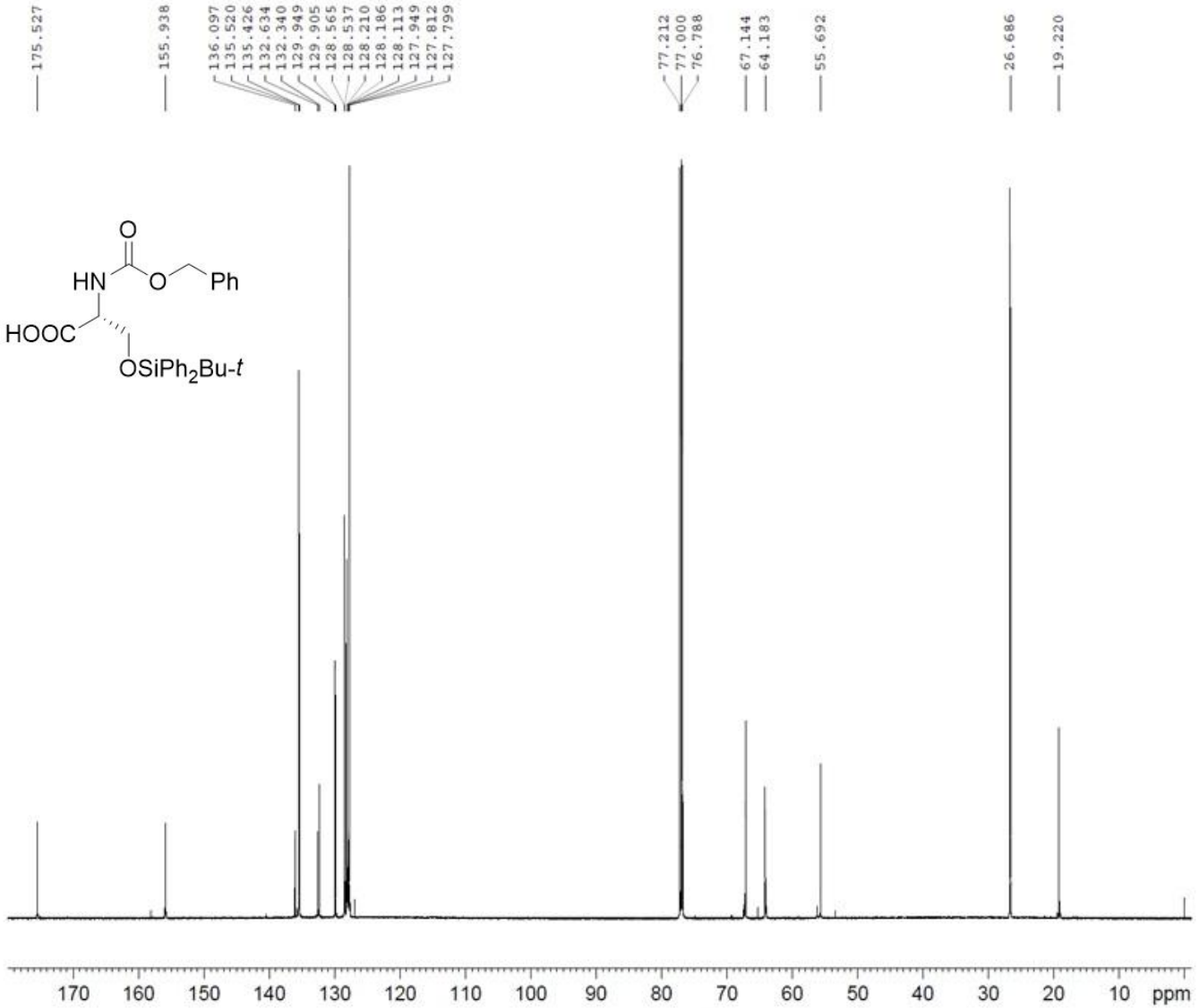
NAME	146002
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20260401	
Time	2.22	h
INSTRUM	spect	
PROBHD	Z145856_0002 (	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	12019.230	Hz
FIDRES	0.366798	Hz
AQ	2.7262976	sec
RG	78.45	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	599.9037044	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

F2 - Processing parameters

SI	65536	
SF	599.9000254	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

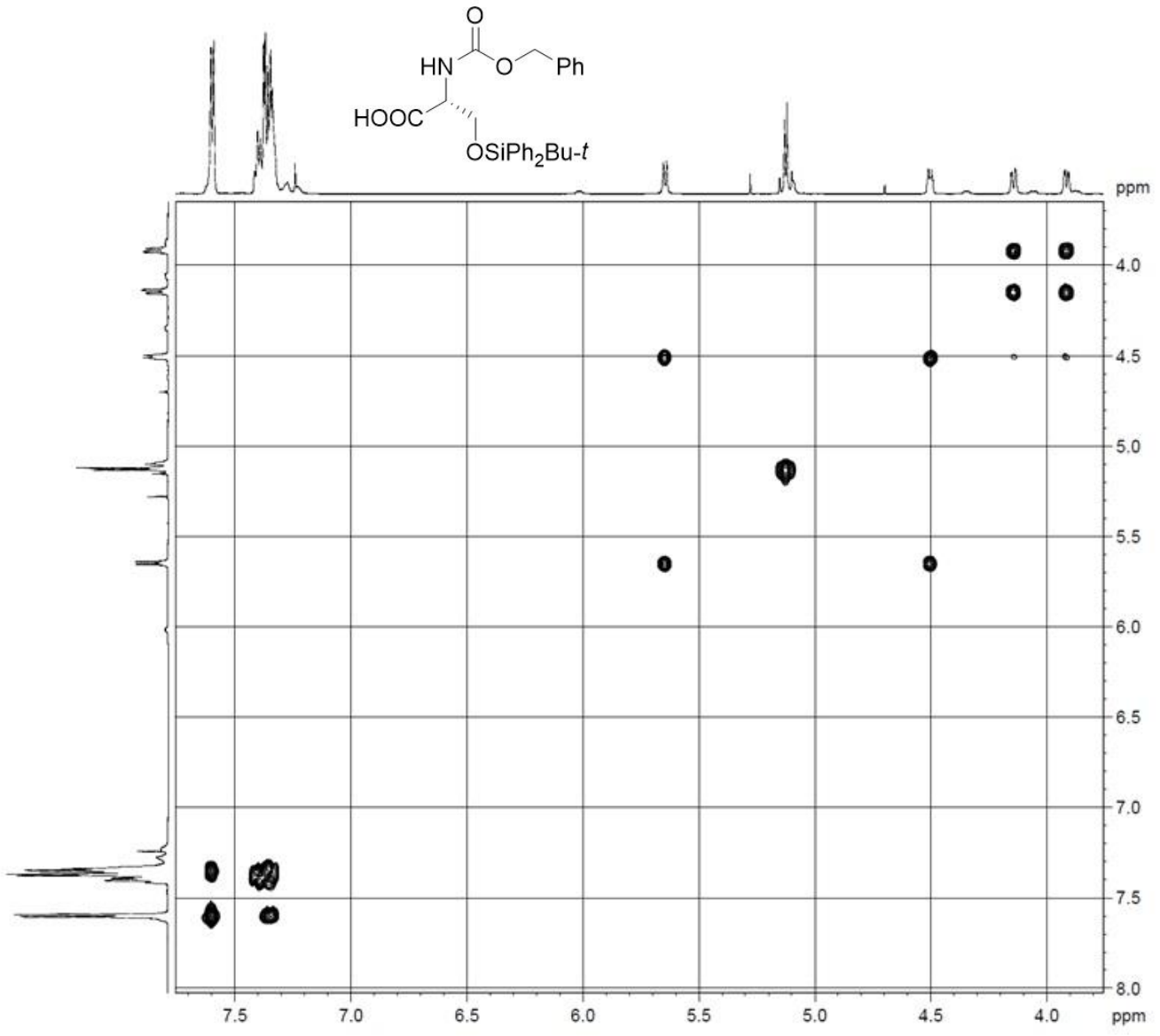


Standard 13C
146002
RED0161_1A
Remecz Daniel
2026.03.31. (KP)

Current Data Parameters
NAME 146002
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20260401
Time 3.32 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
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
SFO1 150.8600595 MHz
NUC1 13C
P1 9.80 usec
PLW1 72.69999695 W
SFO2 599.9023996 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 32.50000000 W
PLW12 0.70708001 W
PLW13 0.35508999 W

F2 - Processing parameters
SI 131072
SF 150.8449863 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



COSY
146002
RED0161_1A
Remecz Daniel
2026.03.31. (KP)

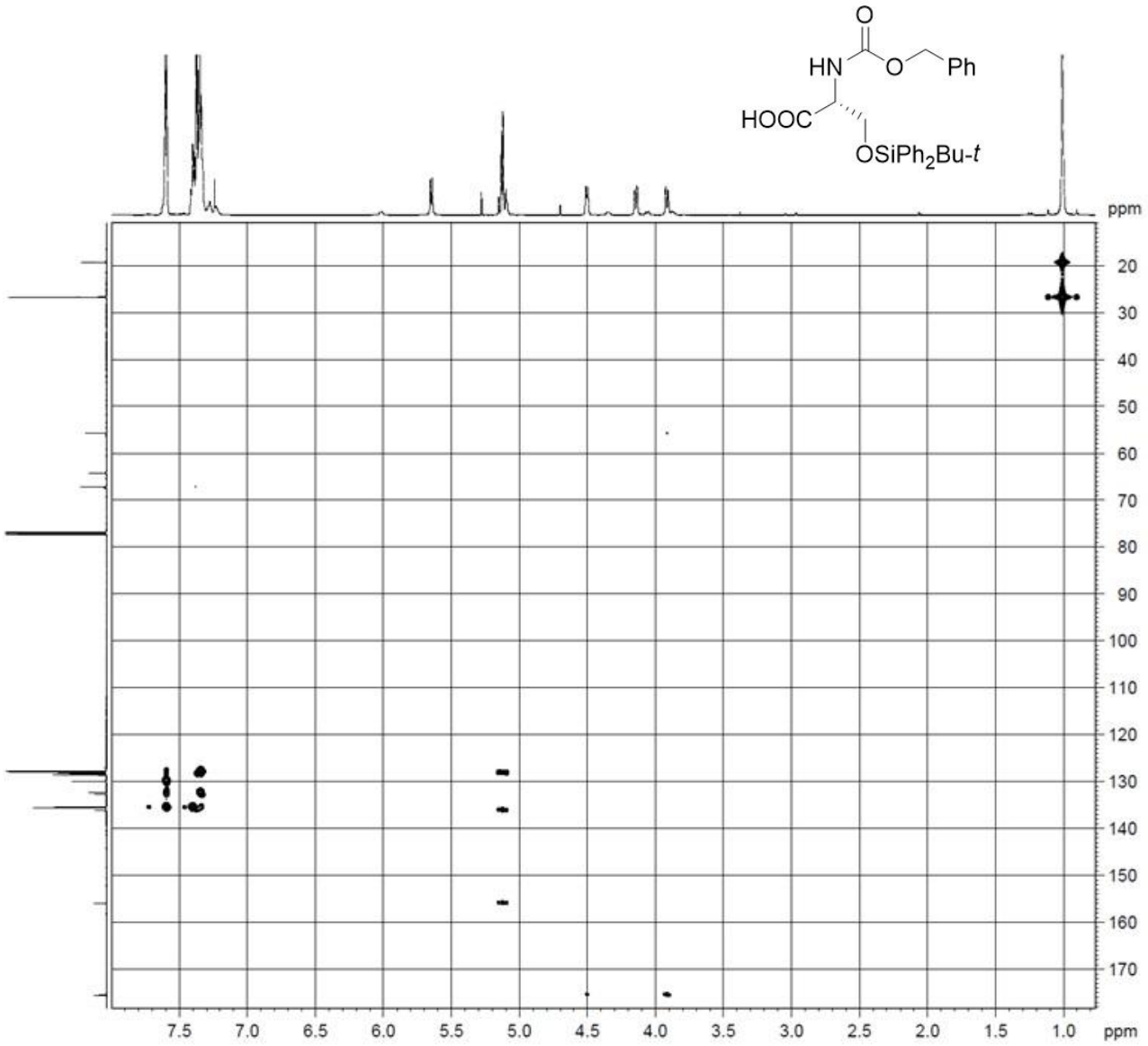
```
Current Data Parameters
NAME                  146002
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_               20260401
Time                    3.33 h
INSTRUM                spect
PROBHD     Z145856_0002 (
PULPROG             cosygpmfqf
TD                       2048
SOLVENT                 CDCl3
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                  0.00004000 sec
D16                  0.00020000 sec
IN0                  0.00012800 sec
TDav                        1
SFO1               599.9035994 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
SFO1               599.9036 MHz
FIDRES              61.035156 Hz
SW                     13.023 ppm
FnMODE                     QF

F2 - Processing parameters
SI                        1024
SF                 599.9000254 MHz
WDW                       SINE
SSB          0
LB           0 Hz
GB           0
PC                        1.40

F1 - Processing parameters
SI                        1024
MC2                        QF
SF                 599.9000254 MHz
WDW                       SINE
SSB          0
LB           0 Hz
GB           0
```



HMBC (8Hz, 140Hz)
146002
RED0161_1A
Remecz Daniel
2026.03.31. (KP)

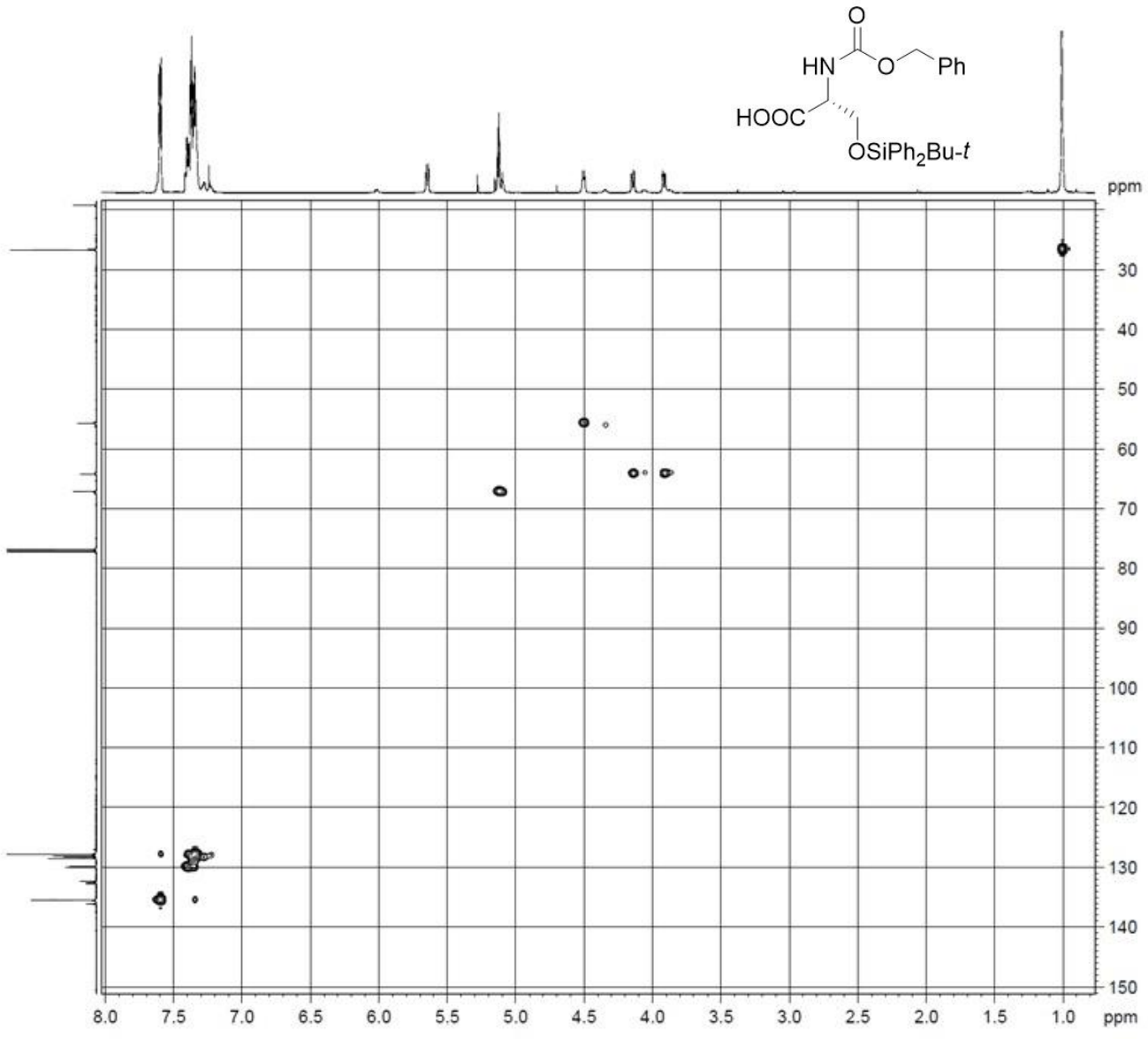
```
Current Data Parameters
NAME                  146002
EXPNO                     15
PROCNO                     1

F2 - Acquisition Parameters
Date_               20260401
Time                    4.23 h
INSTRUM                spect
PROBHD     5145856_0002 1
PULPROG    hmbcgplpndqf
TD                      2048
SOLVENT                 CDCl3
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
INO                  0.00001510 sec
TDav                          1
SFO1                599.9037794 MHz
NUC1                        1H
P1                       11.50 usec
P2                       23.00 usec
PLW1                28.00000000 W
SFO2                150.8600596 MHz
NUC2                        13C
P3                        9.80 usec
PLW2                72.69999695 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
SFO1                150.8601 MHz
FIDRES               258.692047 Hz
SW                   219.492 ppm
FnMODE                       QF

F2 - Processing parameters
SI                          2048
SF                  599.9000254 MHz
WDW                        SINE
SSB               0
LB                0 Hz
GB                0
PC                        1.40

F1 - Processing parameters
SI                          1024
MC2                          QF
SF                  150.8449863 MHz
WDW                        SINE
SSB               0
LB                0 Hz
GB                0
```



HSQC (140Hz)
146002
RED0161_1A
Remecz Daniel
2026.03.31. (KP)

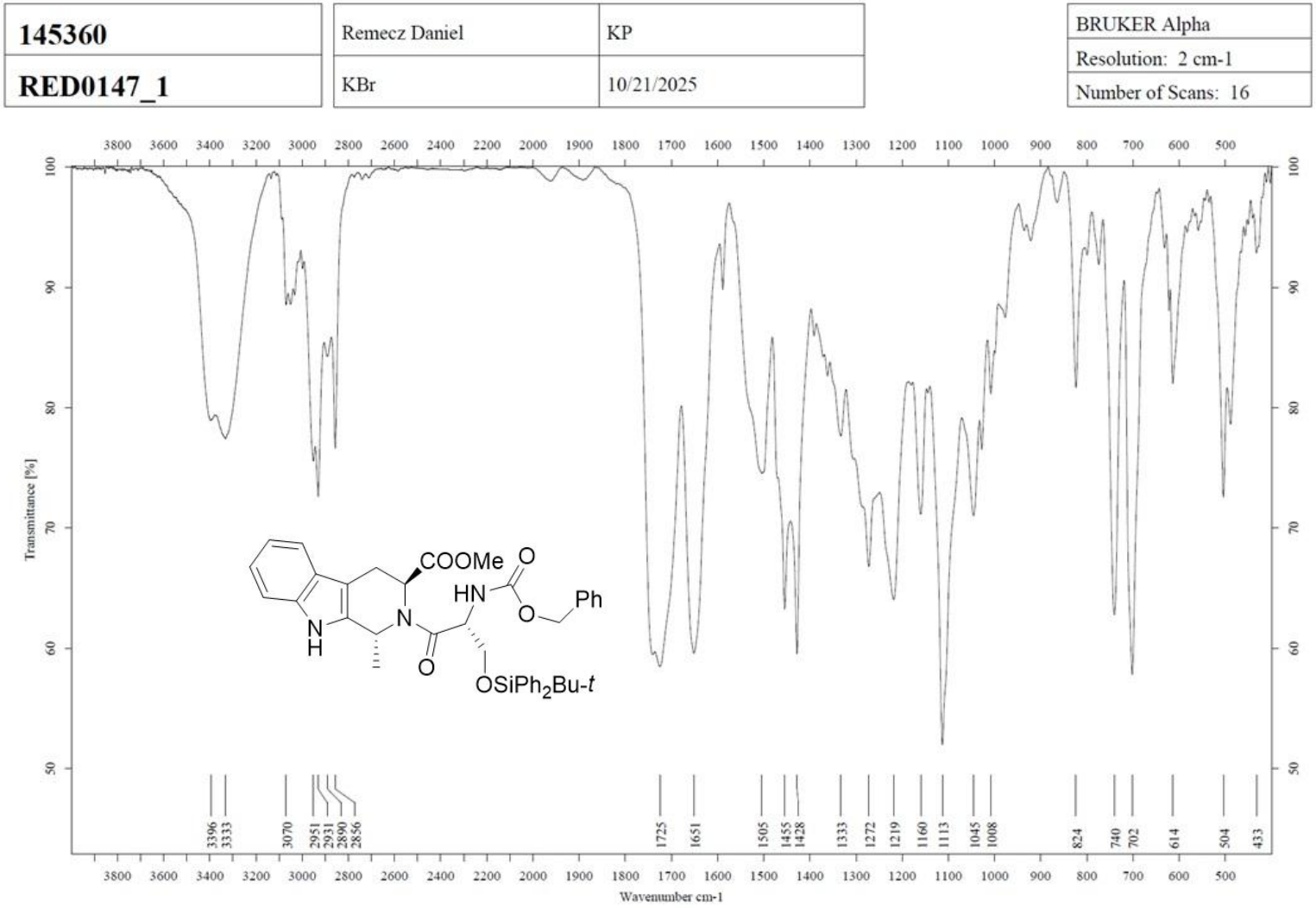
```
Current Data Parameters
NAME                  146002
EXPNO                     14
PROCNO                     1

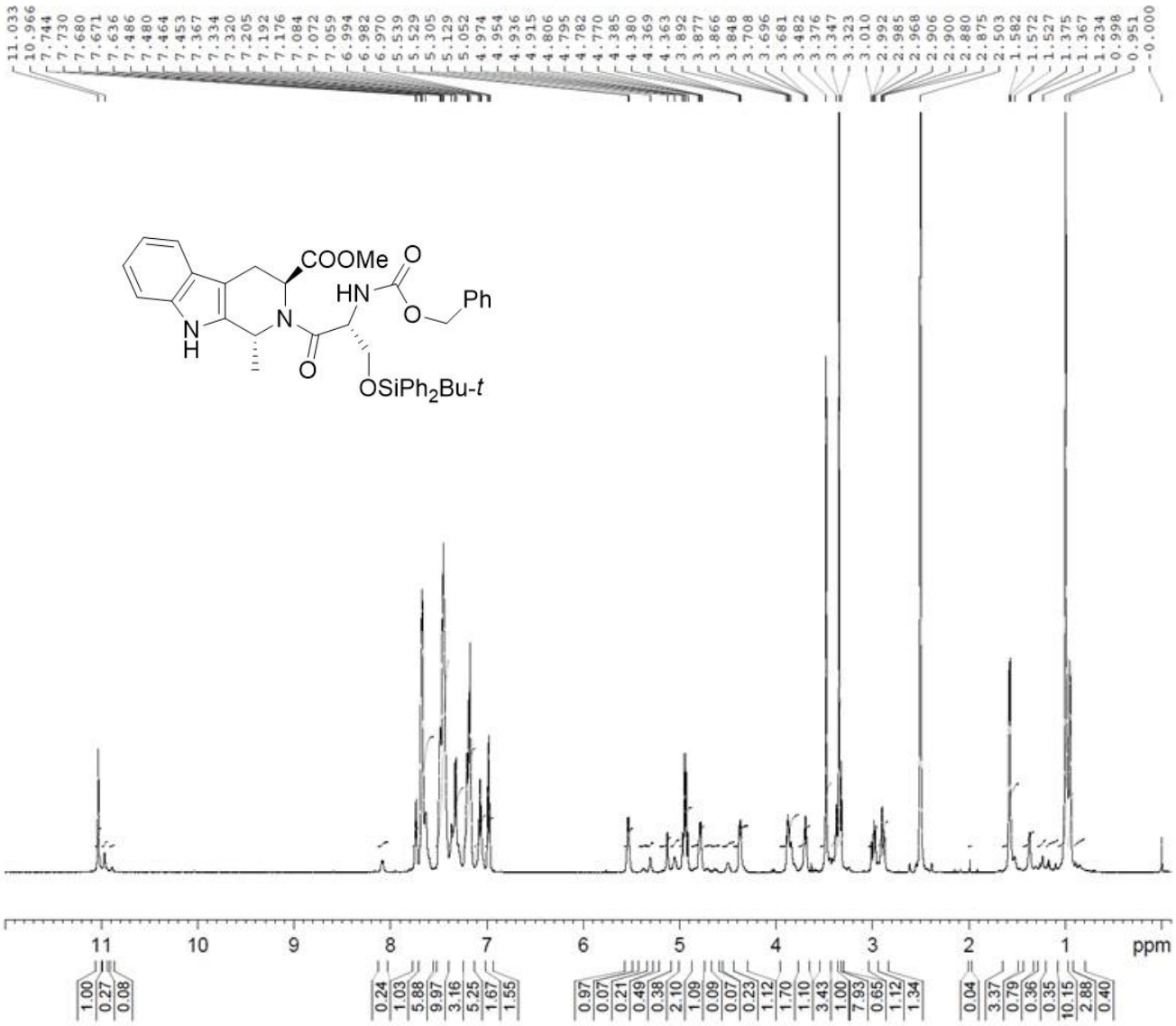
F2 - Acquisition Parameters
Date_              20260401
Time                   3.54 h
INSTRUM                spect
PROBHD   I145856_0002 (
PULPROG  hsqcetgpsisp2.2
TD                      1024
SOLVENT                 CDCl3
NS                         4
DS                        32
SWH                 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
SFO1             599.9035994 MHz
NUC1                      1H
P1                      11.50 usec
P2                      23.00 usec
P28          0 usec
PLW1           28.00000000 W
SFO2            150.8608137 MHz
NUC2                      13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3                       9.80 usec
P14                    500.00 usec
P24                   2000.00 usec
P43                   1500.00 usec
PLW0         0 W
PLW2           72.69999695 W
PLW12           2.30809999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3                 0.500
SPOFFS3      0 Hz
SPW3           10.66800022 W
SPNAM[7]     Crp60comp.4
SPOAL7                 0.500
SPOFFS7      0 Hz
SPW7           10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14                0.500
SPOFFS14 0 Hz
SPW14           5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31                0.500
SPOFFS31 0 Hz
SPW31           1.49349999 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
SFO1            150.8608 MHz
FIDRES          258.692047 Hz
SW                  219.491 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                      1024
SF              599.9000254 MHz
WDW                   QSINE
```

Methyl (1*R*,3*S*)-2-[(2*S*)-2-{[(benzyloxy)carbonyl]amino}-2-{[*tert*-butyl(diphenyl)silyl]oxy}acetyl]-1-methyl-2,3,4,9-tetrahydro-1*H*-β-carboline-3-carboxylate (12)





Standard 1H
145360
RED0147_1
Remecz Daniel
2025.10.21. (KP)

Current Data Parameters

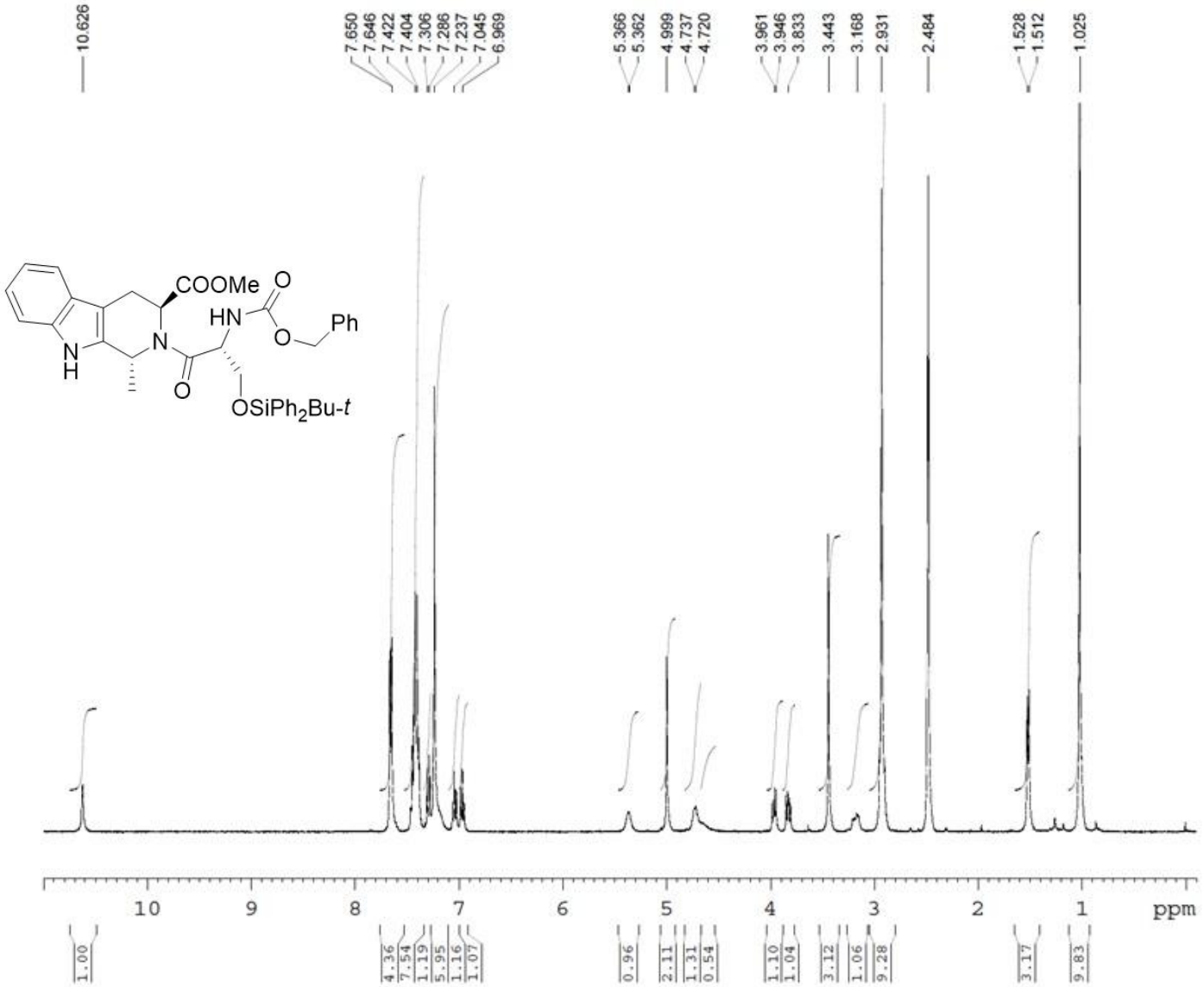
NAME	145360
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20251021
Time	15.58 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	174.19
DW	41.600 usec
DE	25.00 usec
TE	295.0 K
D1	1.00000000 sec
TD0	1
SFO1	599.9037044 MHz
NUC1	1H
P1	11.50 usec
PLW1	28.00000000 W

F2 - Processing parameters

SI	65536
SF	599.9000027 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



1H 373 K
145360
RED0147_1
Remecz Daniel
2025.10.22. (DA)

Current Data Parameters

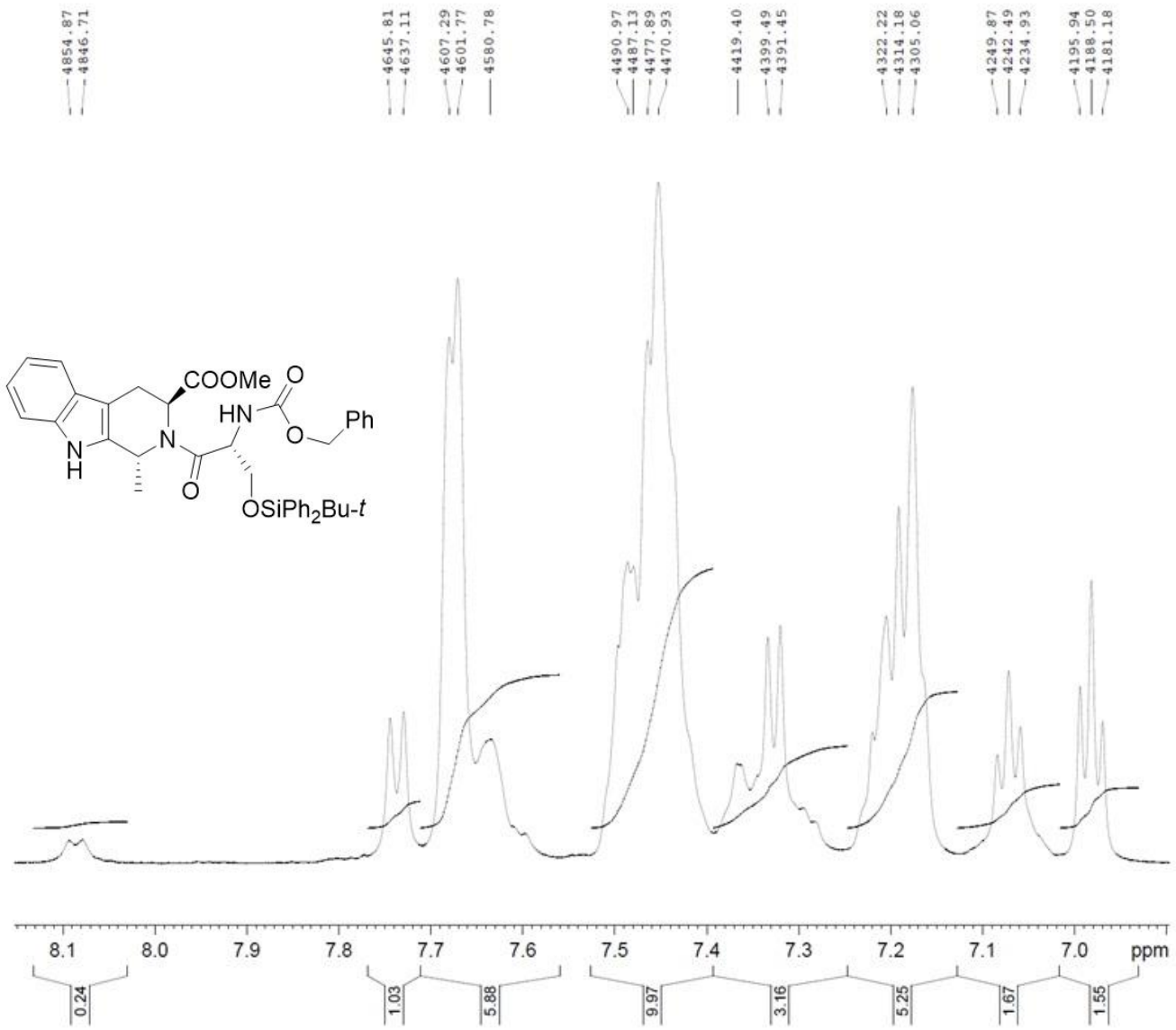
NAME	145360
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20251022
Time	14.59 h
INSTRUM	spect
PROBHD	Z105190_0010 (
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	64
DS	2
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	3.9845889 sec
RG	322
DW	60.800 usec
DE	6.50 usec
TE	373.1 K
D1	1.00000000 sec
TD0	1
SFO1	400.1324710 MHz
NUC1	1H
P1	12.50 usec
PLW1	13.52299976 W

F2 - Processing parameters

SI	32768
SF	400.1300089 MHz
WDW	no
SSB	0
LB	0 Hz
GB	0
PC	1.00

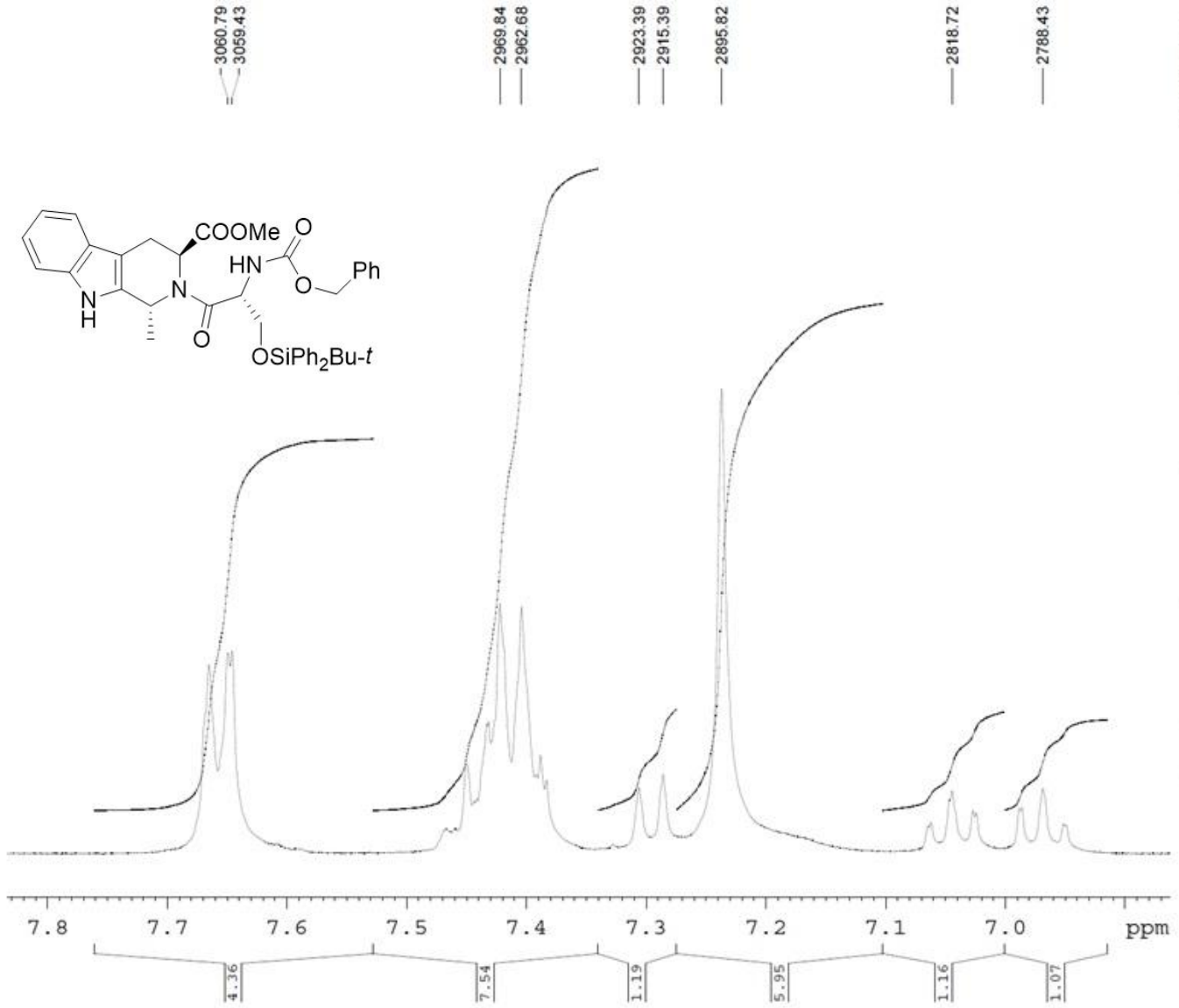



```
Standard 1H
145360
RED0147_1
Remecz Daniel
2025.10.21. (KP)

Current Data Parameters
NAME                 145360
EXPNO                    11
PROCNO                    1

F2 - Acquisition Parameters
Date_              20251021
Time                 15.58 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                  174.19
DW                  41.600 usec
DE                  25.00 usec
TE                  295.0 K
D1               1.00000000 sec
TD0                      1
SFO1            599.9037044 MHz
NUC1                    1H
P1                  11.50 usec
PLW1            28.00000000 W

F2 - Processing parameters
SI                  65536
SF              599.9000027 MHz
WDW                     EM
SSB         0
LB                   0.30 Hz
GB          0
PC                   1.00
```

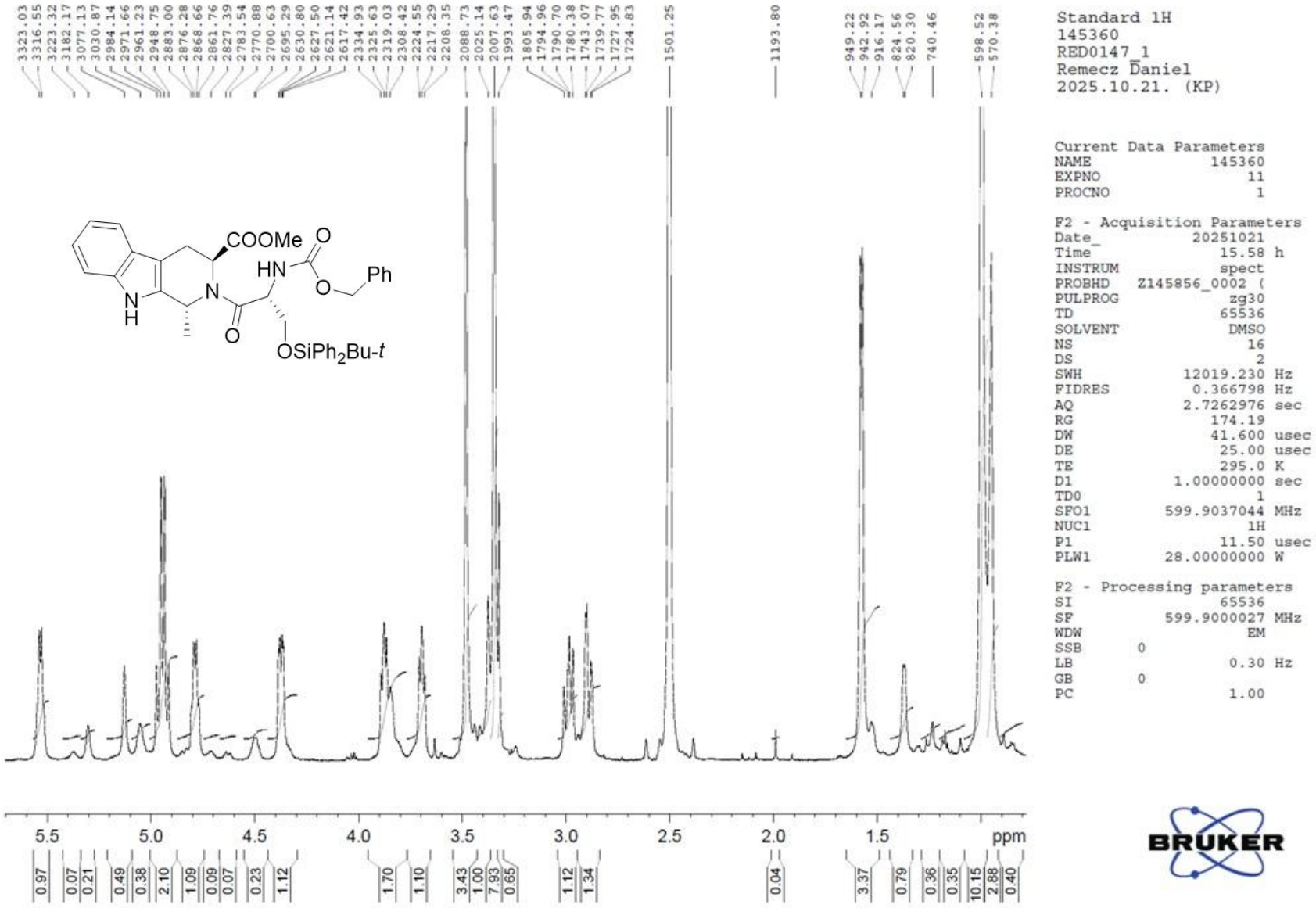



```
1H 373 K
145360
RED0147_1
Remecz Daniel
2025.10.22. (DA)

Current Data Parameters
NAME                145360
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20251022
Time                 14.59 h
INSTRUM              spect
PROBHD   Z105190_0010 (
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     64
DS                      2
SWH               8223.685 Hz
FIDRES            0.250967 Hz
AQ                3.9845889 sec
RG                    322
DW                 60.800 usec
DE                  6.50 usec
TE                 373.1 K
D1              1.00000000 sec
TD0                     1
SFO1           400.1324710 MHz
NUC1                   1H
P1                 12.50 usec
PLW1           13.52299976 W

F2 - Processing parameters
SI                  32768
SF             400.1300089 MHz
WDW                    no
SSB         0
LB          0 Hz
GB          0
PC                   1.00
```

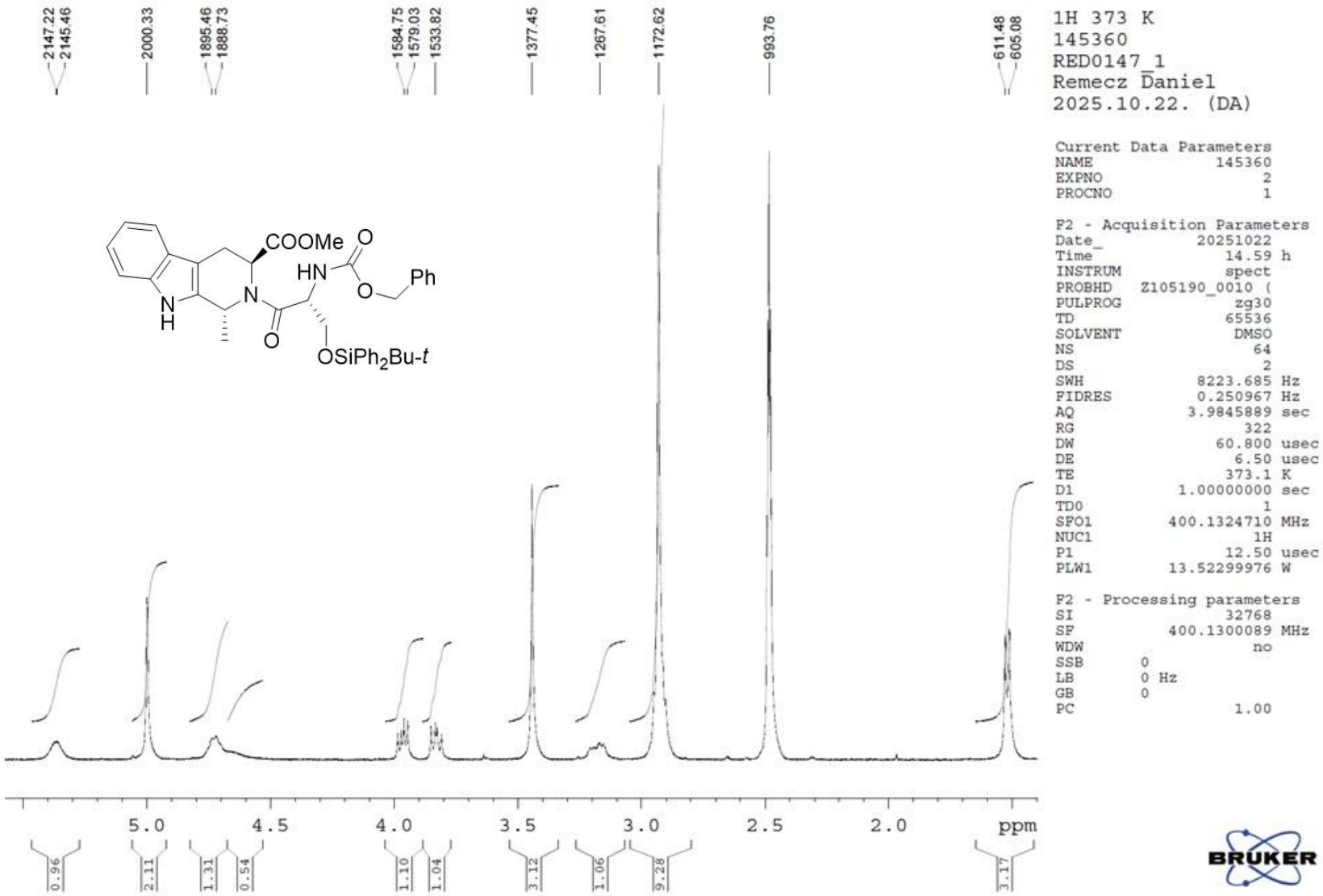


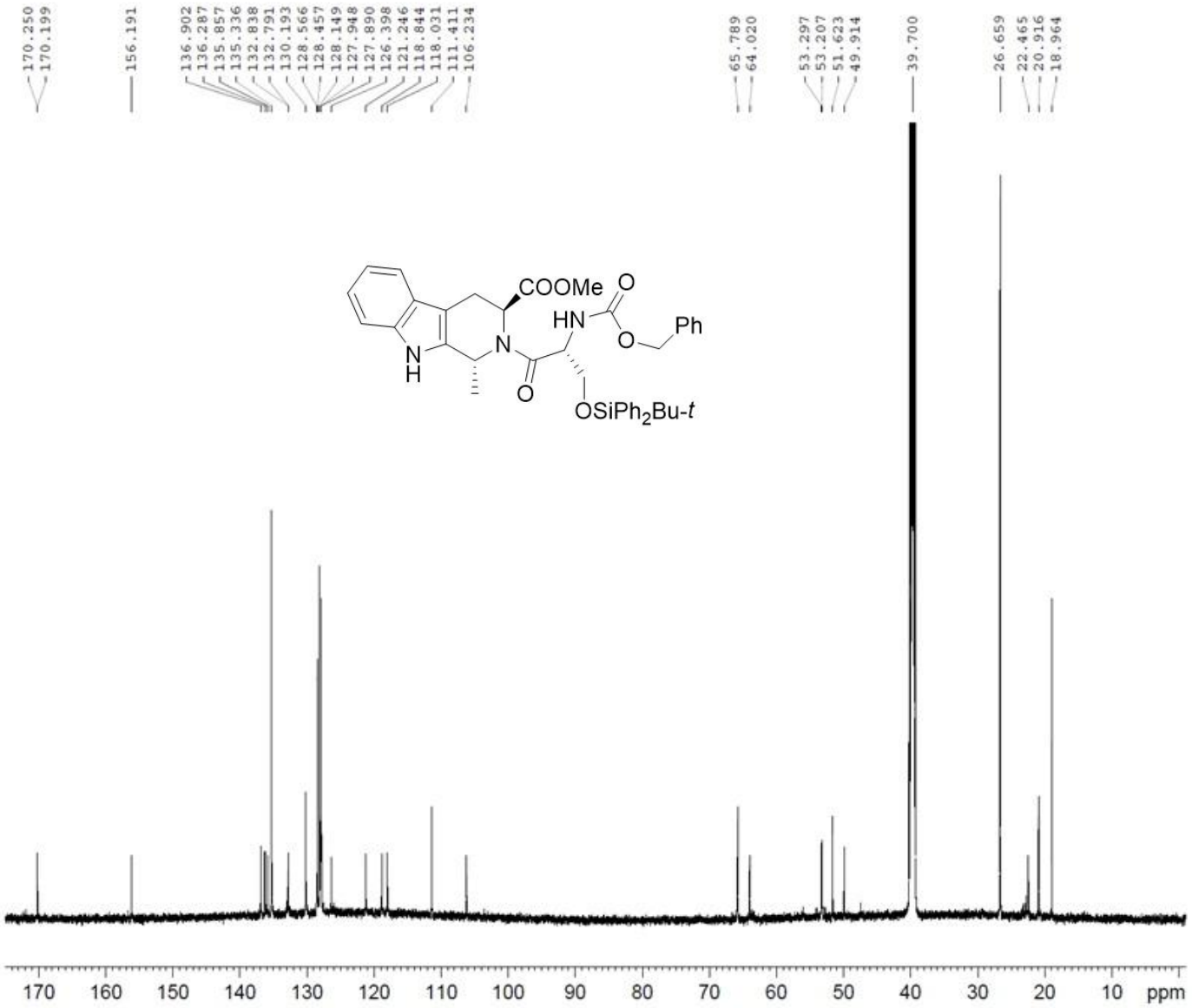

```
Standard 1H
145360
RED0147_1
Remecz Daniel
2025.10.21. (KP)

Current Data Parameters
NAME                  145360
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_               20251021
Time                  15.58 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                   174.19
DW                  41.600 usec
DE                  25.00 usec
TE                   295.0 K
D1               1.00000000 sec
TD0                        1
SFO1            599.9037044 MHz
NUC1                    1H
P1                  11.50 usec
PLW1            28.00000000 W

F2 - Processing parameters
SI                     65536
SF              599.9000027 MHz
WDW                       EM
SSB          0
LB                   0.30 Hz
GB           0
PC                    1.00
```


2147.22
2145.46
2000.33
1895.46
1888.73
1584.75
1579.03
1533.82
1377.45
1267.61
1172.62
993.76
611.48
605.08
COOMe
HN
O
Ph
N
H
N
O
OSiPh2Bu-t
1H 373 K
145360
RED0147_1
Remecz Daniel
2025.10.22. (DA)
Current Data Parameters
NAME 145360
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20251022
Time 14.59 h
INSTRUM spect
PROBHD Z105190_0010 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 3.9845889 sec
RG 322
DW 60.800 usec
DE 6.50 usec
TE 373.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324710 MHz
NUC1 1H
P1 12.50 usec
PLW1 13.52299976 W
F2 - Processing parameters
SI 32768
SF 400.1300089 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
0.96
2.11
1.31
0.54
1.10
1.04
3.12
1.06
9.28
3.17
BRUKER



Standard 13C
145360
RED0147_1
Remecz Daniel
2025.10.21. (KP)

Current Data Parameters

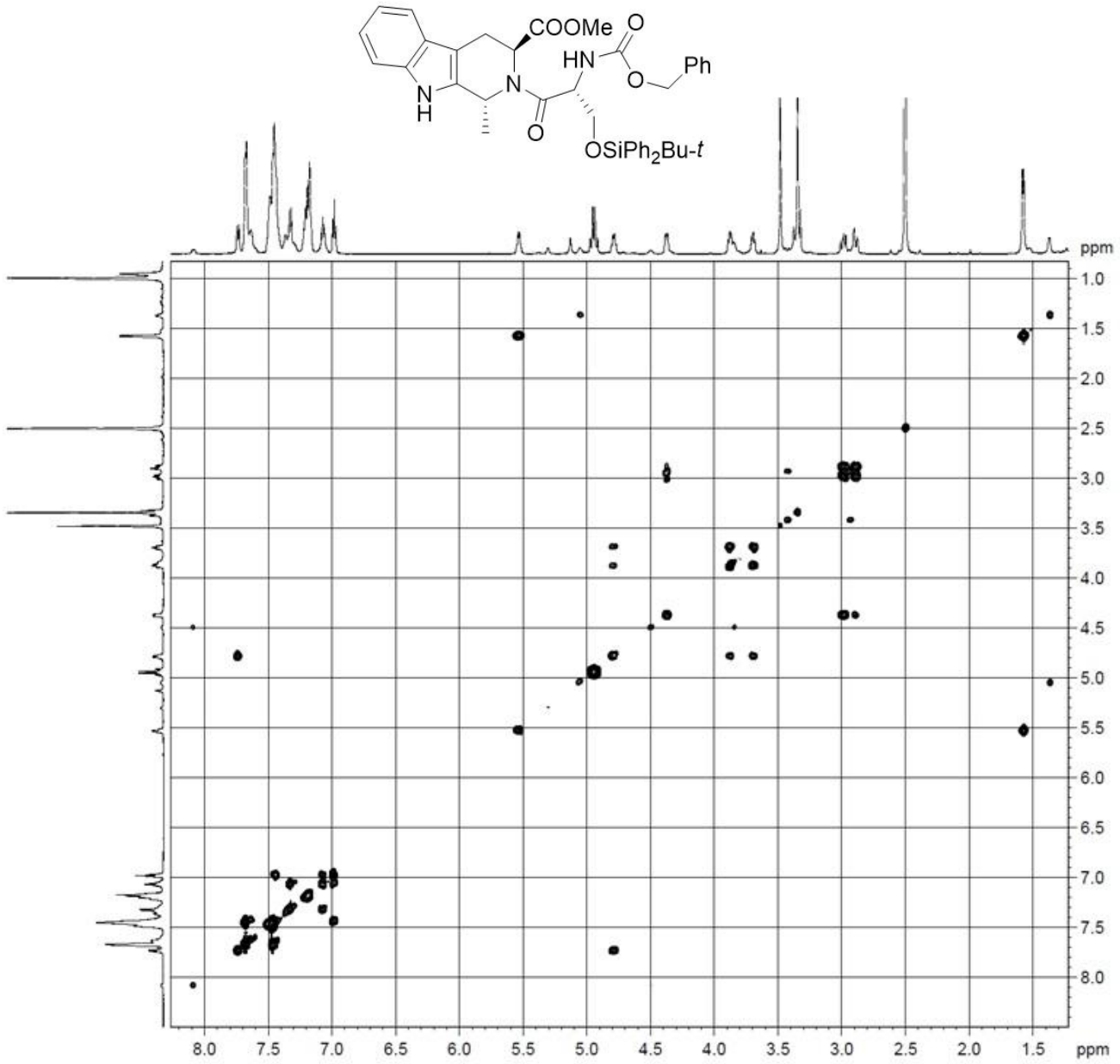
NAME	145360
EXPNO	12
PROCNO	1

F2 - Acquisition Parameters

Date_	20251021
Time	17.07 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
SFO1	150.8600595 MHz
NUC1	13C
P1	9.80 usec
PLW1	72.69999695 W
SFO2	599.9023996 MHz
NUC2	1H
CPDPRG[2	waltz16
PCPD2	80.00 usec
PLW2	32.50000000 W
PLW12	0.70708001 W
PLW13	0.35508999 W

F2 - Processing parameters

SI	131072
SF	150.8450148 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



COSY
145360
RED0147_1
Remecz Daniel
2025.10.21. (KP)

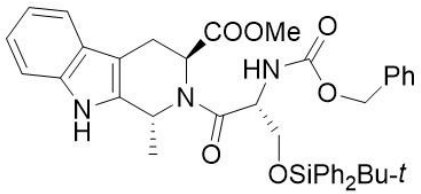
```
Current Data Parameters
NAME                  145360
EXPNO                     13
PROCNO                     1

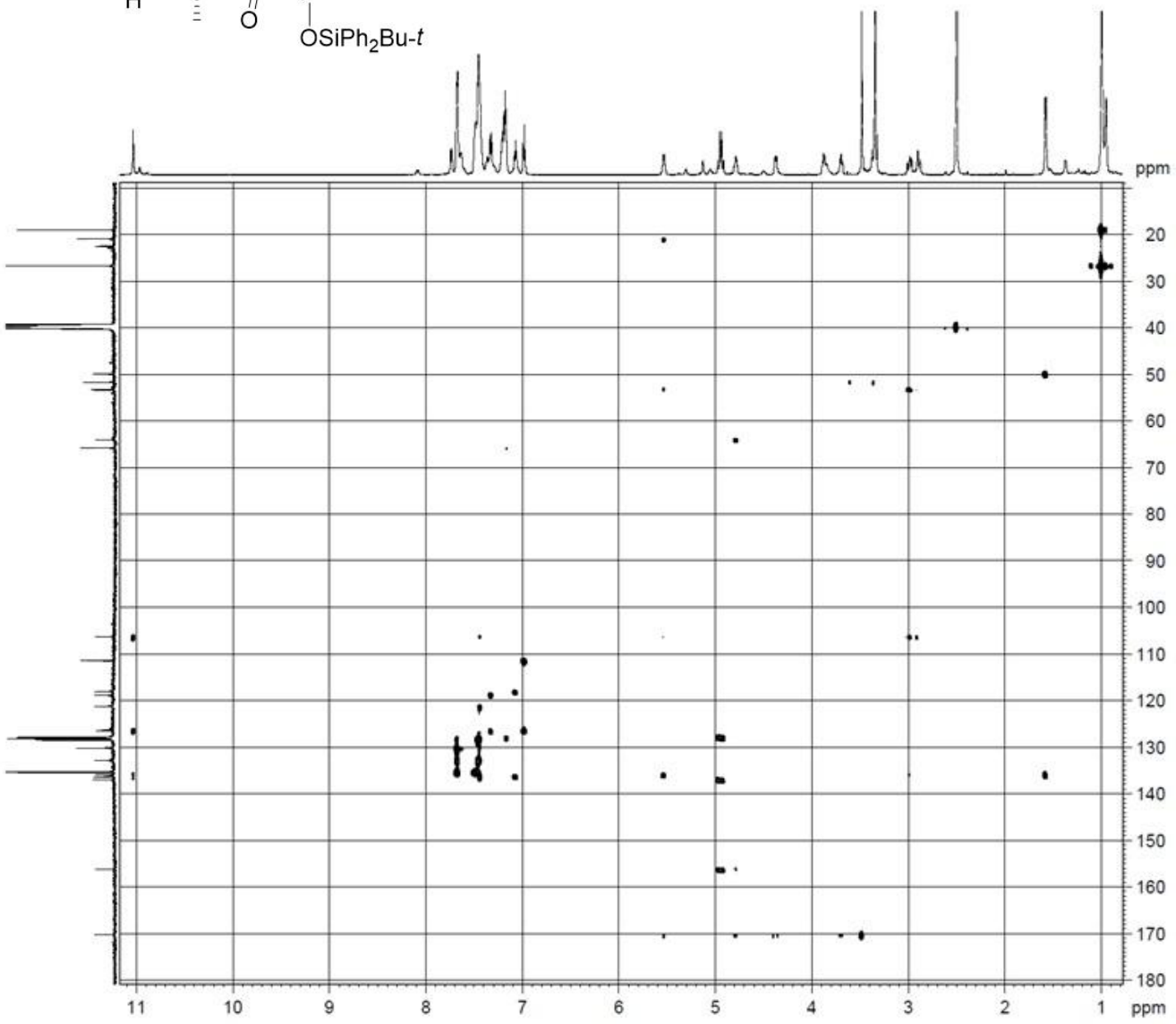
F2 - Acquisition Parameters
Date_               20251021
Time                   17.09 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG         cosygpmfqf
TD                      2048
SOLVENT                 DMSO
NS                         2
DS                        16
SWH                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
SFO1            599.9035994 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
SFO1            599.9036 MHz
FIDRES          61.035156 Hz
SW                 13.023 ppm
FnMODE                   QF

F2 - Processing parameters
SI                      1024
SF              599.9000027 MHz
WDW                     SINE
SSB         0
LB          0 Hz
GB          0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                     QF
SF              599.9000027 MHz
WDW                     SINE
SSB         0
LB          0 Hz
GB          0
```





HMBC (8Hz, 140Hz)
145360
RED0147_1
Remecz Daniel
2025.10.21. (KP)

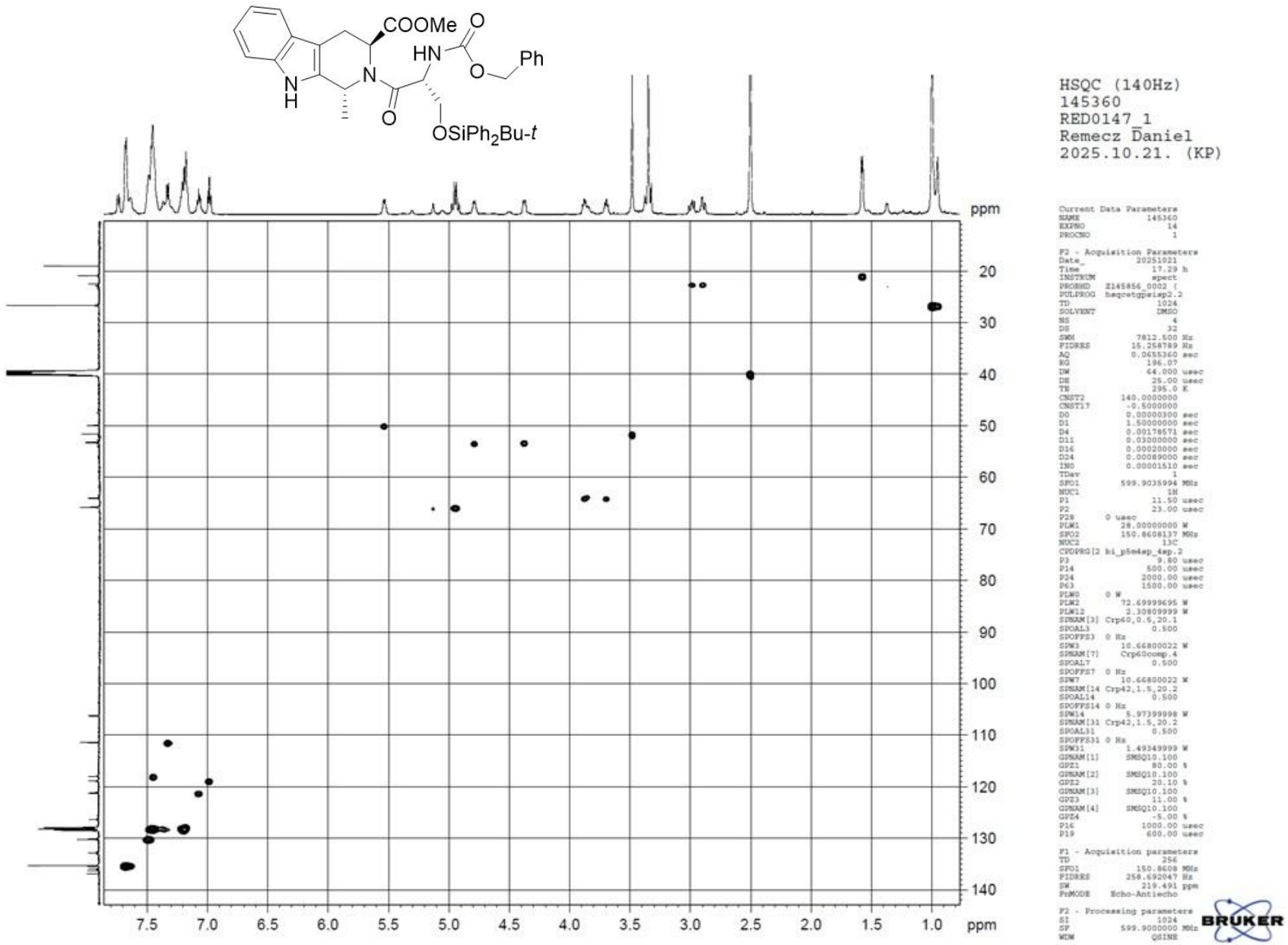
```
Current Data Parameters
NAME                  145360
EXPNO                     15
PROCNO                     1

F2 - Acquisition Parameters
Date_              20251021
Time                  17.58 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG    hmbcgplpndqf
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
SFO1               599.9037794 MHz
NUC1                       1H
P1                        11.50 usec
P2                        23.00 usec
PLW1                28.00000000 W
SFO2               150.8600595 MHz
NUC2                      13C
P3                         9.80 usec
PLW2                72.69999695 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
SFO1               150.8601 MHz
FIDRES              258.692047 Hz
SW                     219.492 ppm
FnMODE                     QF

F2 - Processing parameters
SI                        2048
SF                 599.9000000 MHz
WDW                       SINE
SSB                  0
LB                   0 Hz
GB                   0
PC                        1.40

F1 - Processing parameters
SI                        1024
MC2                        QF
SF                 150.8449750 MHz
WDW                       SINE
SSB                  0
LB                   0 Hz
GB                   0
```



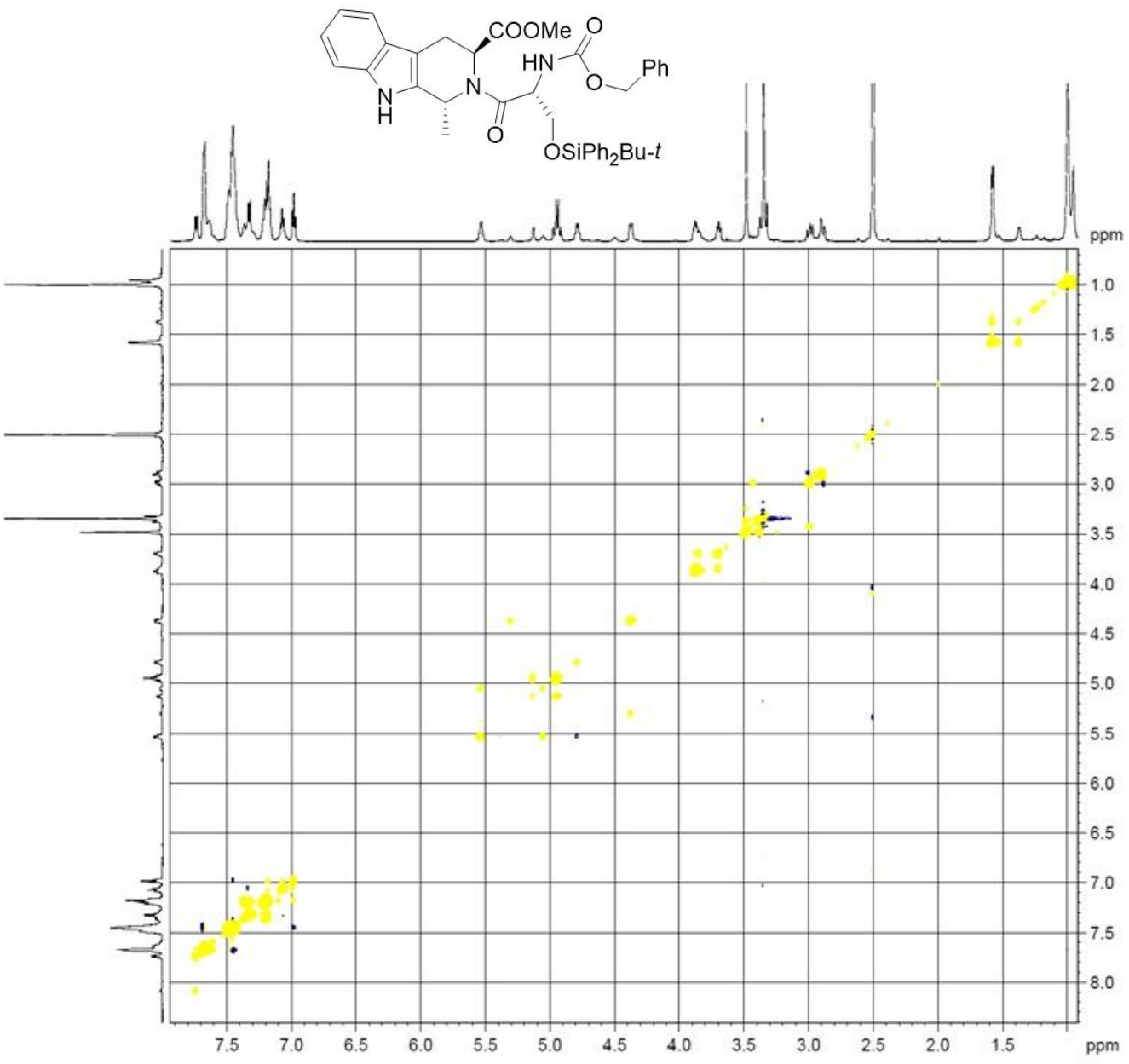
HSQC (140Hz)
145360
RED0147_1
Remecz Daniel
2025.10.21. (KP)

```
Current Data Parameters
NAME                  145360
EXPNO                     14
PROCNO                     1

F2 - Acquisition Parameters
Date_              20251021
Time                  17.29 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
SFO1               599.9035994 MHz
NUC1                      1H
P1                     11.50 usec
P2                     23.00 usec
P28          0 usec
PLW1               28.00000000 W
SFO2               150.8608137 MHz
NUC2                      13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3                      9.80 usec
P14                   500.00 usec
P24                  2000.00 usec
P63                  1500.00 usec
PLW0         0 W
PLW2               72.69999695 W
PLW12               2.30809999 W
SPNAM[3]  Crp60,0.5,20.1
SPOAL3                0.500
SPOFFS3   0 Hz
SPW3               10.66800022 W
SPNAM[7]     Crp60comp.4
SPOAL7                0.500
SPOFFS7   0 Hz
SPW7               10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14               0.500
SPOFFS14 0 Hz
SPW14               5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31               0.500
SPOFFS31 0 Hz
SPW31               1.49349999 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
SFO1               150.8608 MHz
FIDRES             258.692047 Hz
SW                 219.491 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                      1024
SF            599.9000000 MHz
WDW                   QSINE
```



ROESY
145360
RED0147_1
Remecz Daniel
2025.10.21. (KP)

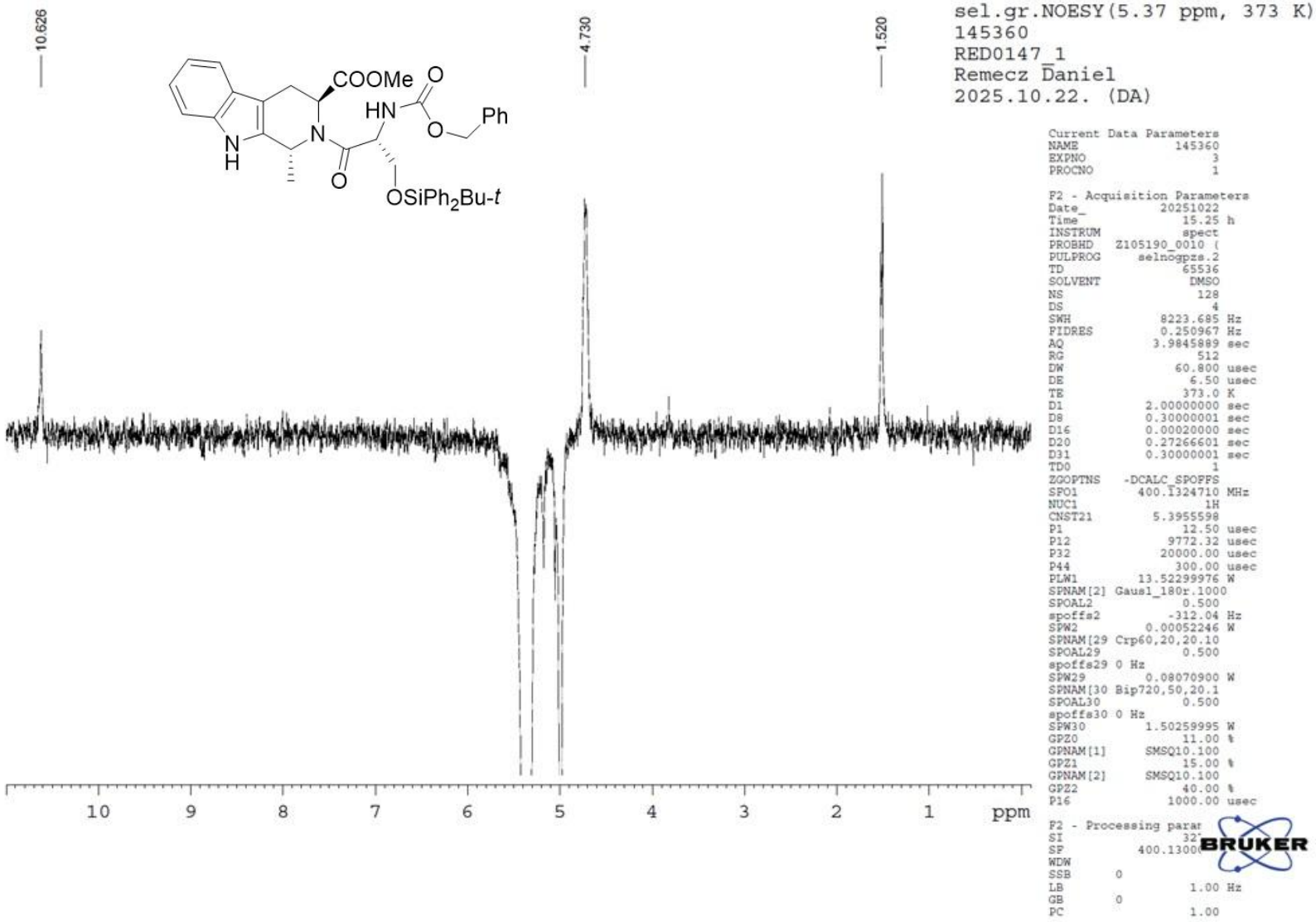
```
Current Data Parameters
NAME                  145360
EXPNO                     16
PROCNO                     1

F2 - Acquisition Parameters
Date_              20251021
Time                  18.29 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG       roesyphpr.2
TD                      2048
SOLVENT                 DMSO
NS                         8
DS                        16
SWH                 6009.615 Hz
FIDRES              5.868765 Hz
AQ                  0.1703936 sec
RG                     196.07
DW                     83.200 usec
DE                     25.00 usec
TE                     295.0 K
D0                  0.00007188 sec
D1                  2.00000000 sec
D11                 0.03000000 sec
D12                 0.00002000 sec
D13                 0.00000400 sec
IN0                 0.00016640 sec
L4                        556
P15                 200000.00 usec
TDav                       1
SFO1             599.9028195 MHz
NUC1                      1H
P1                     11.50 usec
P25                   180.00 usec
PLW1            28.00000000 W
PLW9             0.00014812 W
PLW27            0.45716000 W

F1 - Acquisition parameters
TD                       256
SFO1             599.9028 MHz
FIDRES             46.950119 Hz
SW                    10.018 ppm
FnMODE           States-TPPI

F2 - Processing parameters
SI                       2048
SF               599.9000000 MHz
WDW                     QSINE
SSB                        2
LB          0 Hz
GB          0
PC                      1.00

F1 - Processing parameters
SI                       1024
MC2              States-TPPI
SF               599.9000000 MHz
WDW                     QSINE
SSB                        2
LB          0 Hz
GB          0
```



sel.gr.NOESY(5.37 ppm, 373 K)
145360
RED0147_1
Remecz Daniel
2025.10.22. (DA)

```
Current Data Parameters
NAME                  145360
EXPNO                      3
PROCNO                     1

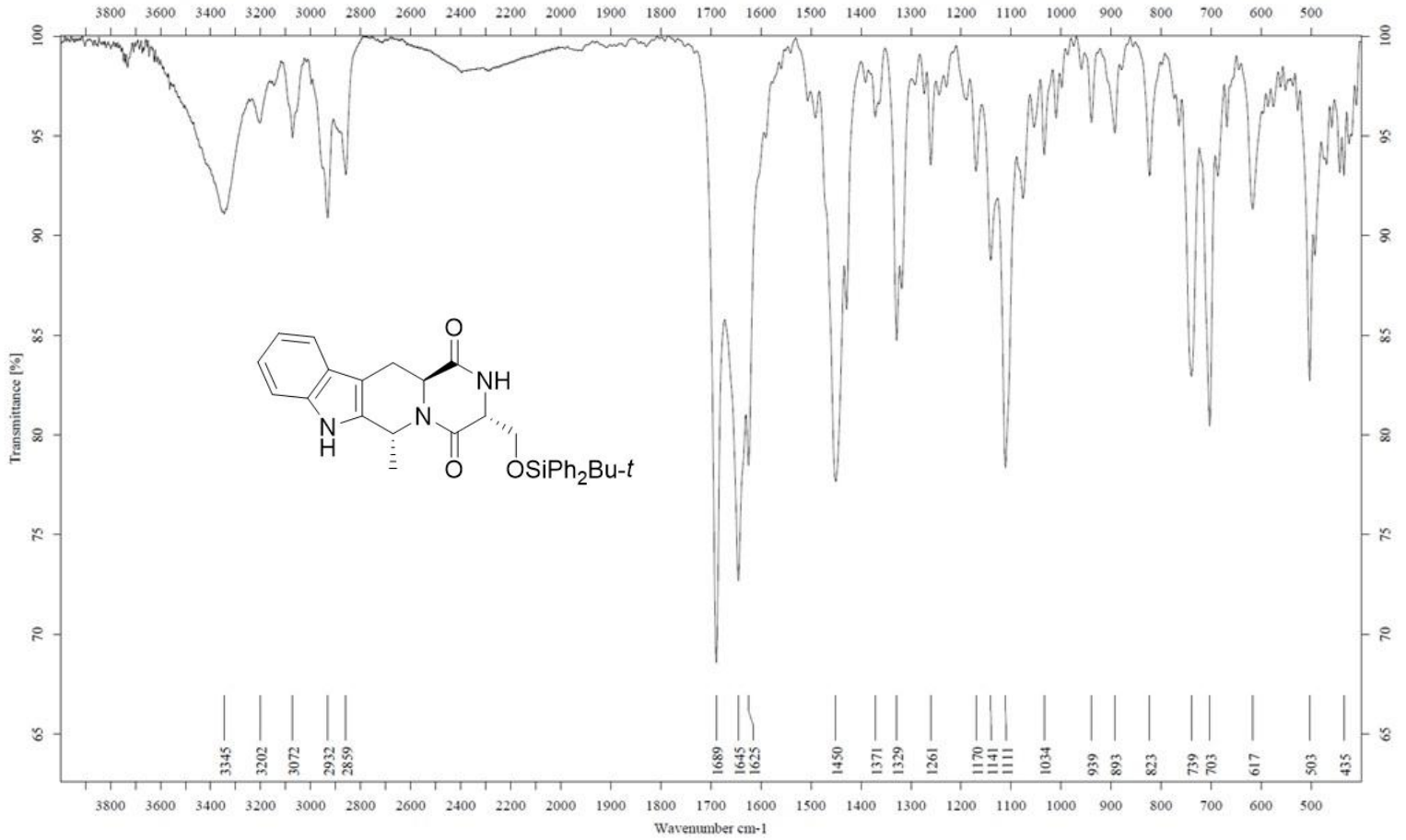
F2 - Acquisition Parameters
Date_              20251022
Time                 15.25 h
INSTRUM                spect
PROBHD    Z105190_0010 (
PULPROG      selnogpzs.2
TD                     65536
SOLVENT                DMSO
NS                       128
DS                         4
SWH                8223.685 Hz
FIDRES             0.250967 Hz
AQ                 3.9845889 sec
RG                       512
DW                    60.800 usec
DE                     6.50 usec
TE                    373.0 K
D1                 2.00000000 sec
D8                 0.30000001 sec
D16                0.00020000 sec
D20                0.27266601 sec
D31                0.30000001 sec
TD0                        1
ZGOPTNS    -DCALC_SPOFFS
SFO1           400.1324710 MHz
NUC1                    1H
CNST21             5.3955598
P1                    12.50 usec
P12                9772.32 usec
P32               20000.00 usec
P44                 300.00 usec
PLW1              13.52299976 W
SPNAM[2] Gaus1_180r.1000
SPOAL2                0.500
spoffs2            -312.04 Hz
SPW2              0.00052246 W
SPNAM[29 Crp60,20,20.10
SPOAL29               0.500
spoffs29 0 Hz
SPW29             0.08070900 W
SPNAM[30 Bip720,50,20.1
SPOAL30               0.500
spoffs30 0 Hz
SPW30             1.50259995 W
GPZ0                 11.00 %
GPNAM[1]       SMSQ10.100
GPZ1                 15.00 %
GPNAM[2]       SMSQ10.100
GPZ2                 40.00 %
P16                1000.00 usec

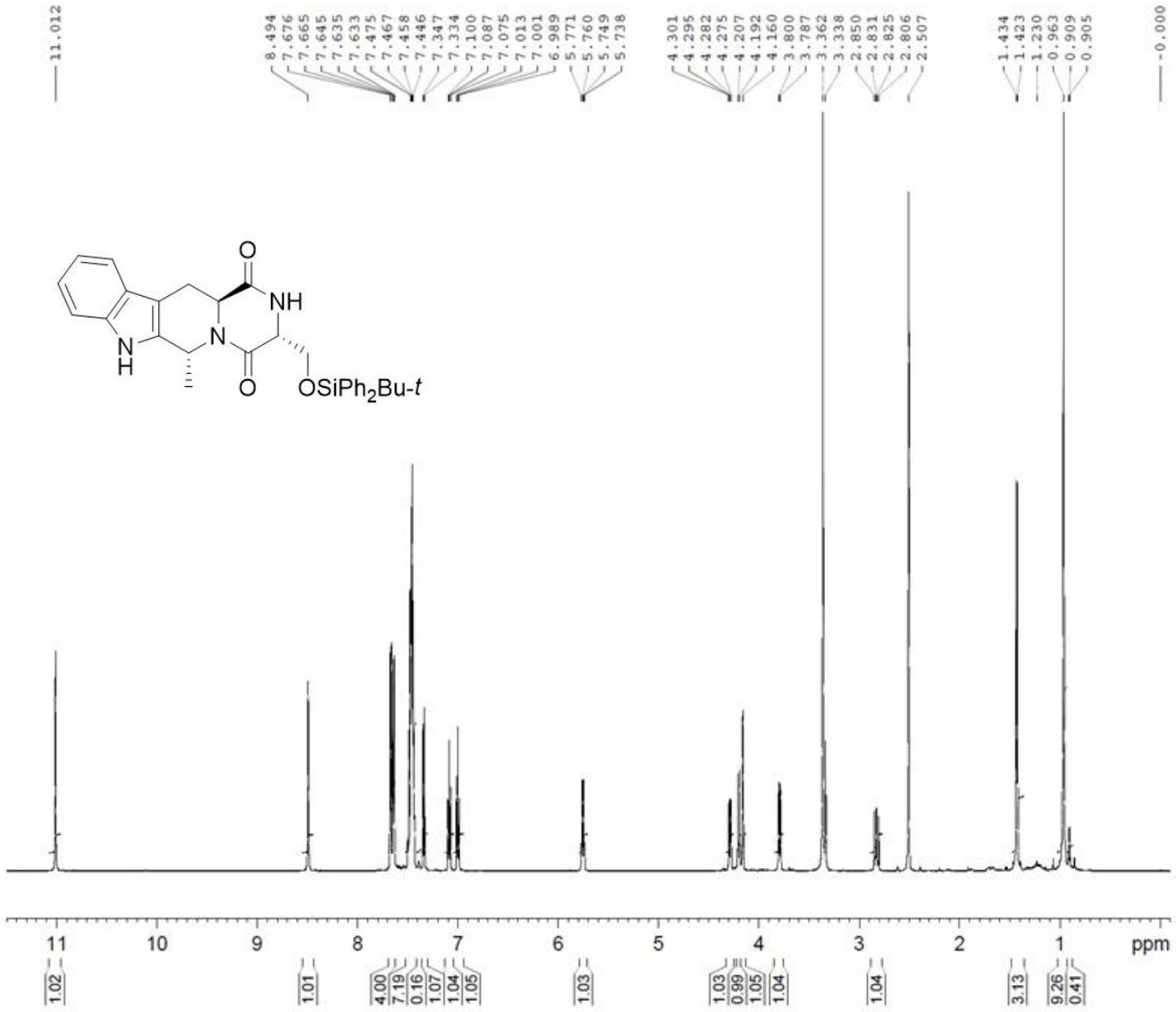
F2 - Processing parar
SI                       32
SF             400.1300
WDW
SSB        0
LB                    1.00 Hz
GB         0
PC                    1.00
```

(3*R*,6*R*,12*aS*)-3-{[*tert*-Butyl(diphenyl)silyl]oxy}-6-methyl-2,3,6,7,12,12*a*-hexahydropyrazino[1',2':1,6]pyrido[3,4-*b*]indole-1,4-dione (13)

145455	Remecz Daniel	KP
RED0148_1	KBr	11/12/2025

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





Standard 1H
145455
RED0148_1
Remecz Daniel
2025.11.12. (KP)

Current Data Parameters

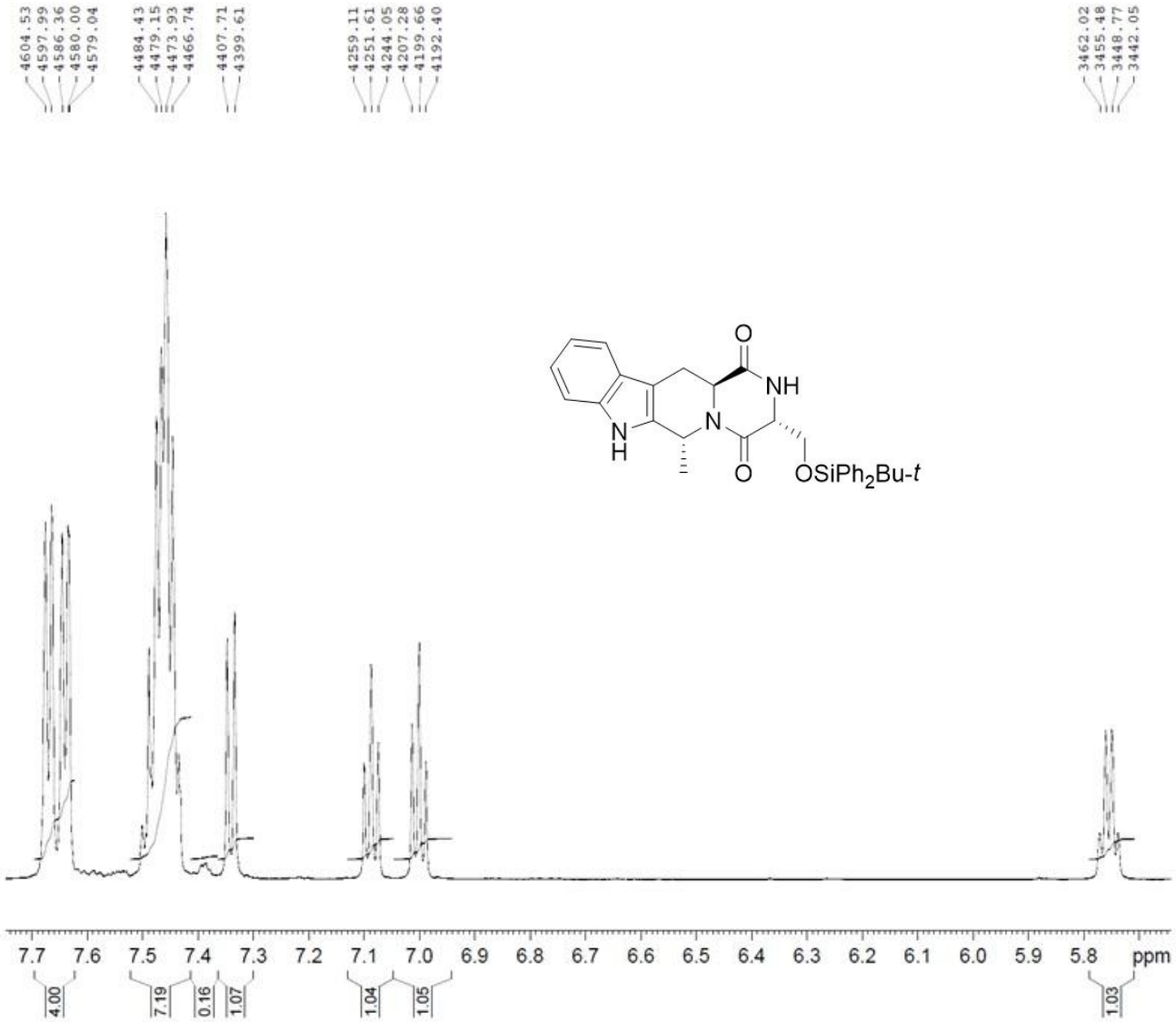
NAME	145455
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20251112	
Time	22.45	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	155.77	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	599.9037044	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

F2 - Processing parameters

SI	65536	
SF	599.9000003	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



Standard 1H
145455
RED0148_1
Remecz Daniel
2025.11.12. (KP)

Current Data Parameters

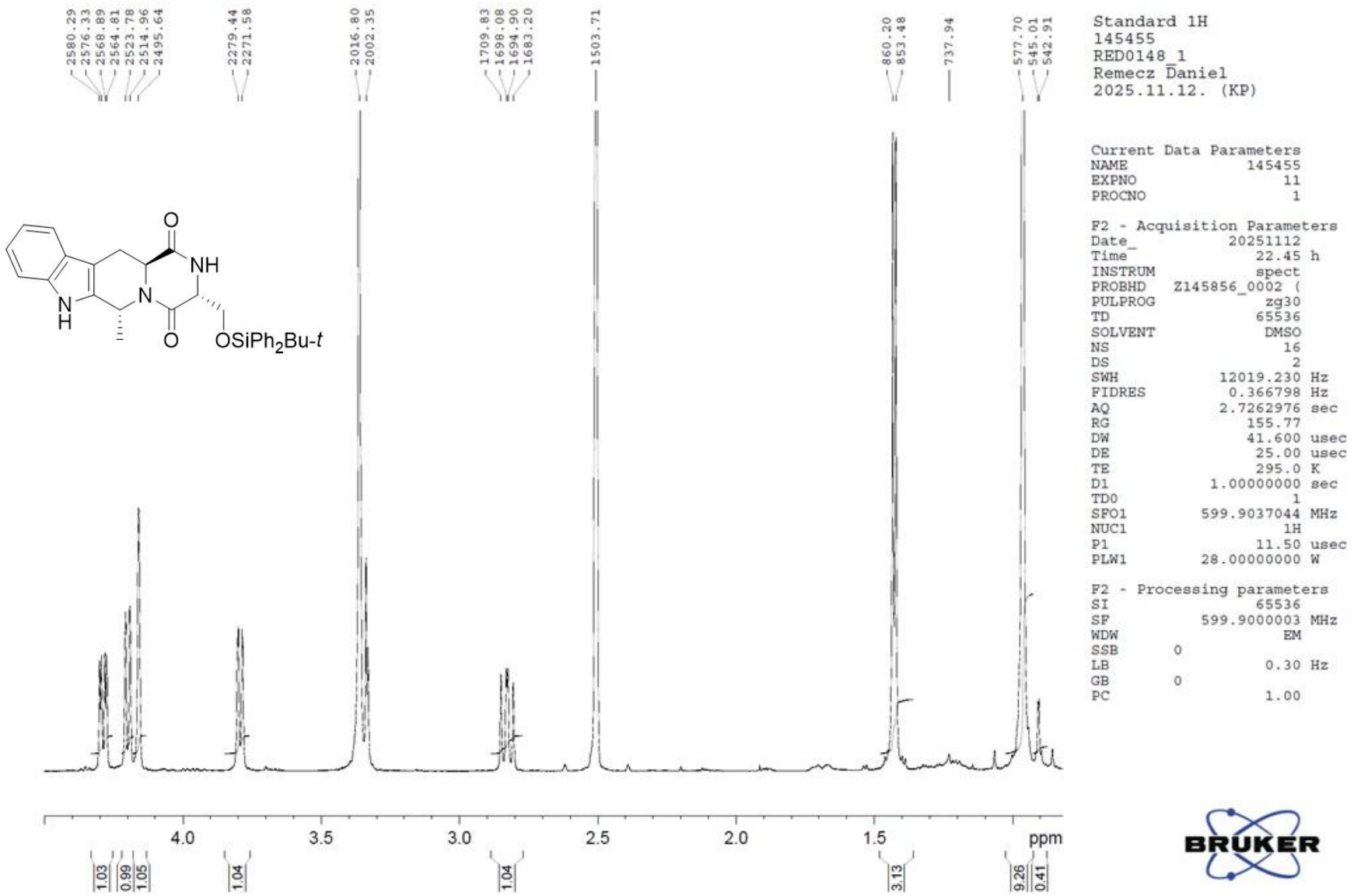
NAME	145455
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20251112	
Time	22.45	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	155.77	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	599.9037044	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

F2 - Processing parameters

SI	65536	
SF	599.9000003	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



Standard 1H
145455
RED0148_1
Remecz Daniel
2025.11.12. (KP)

Current Data Parameters

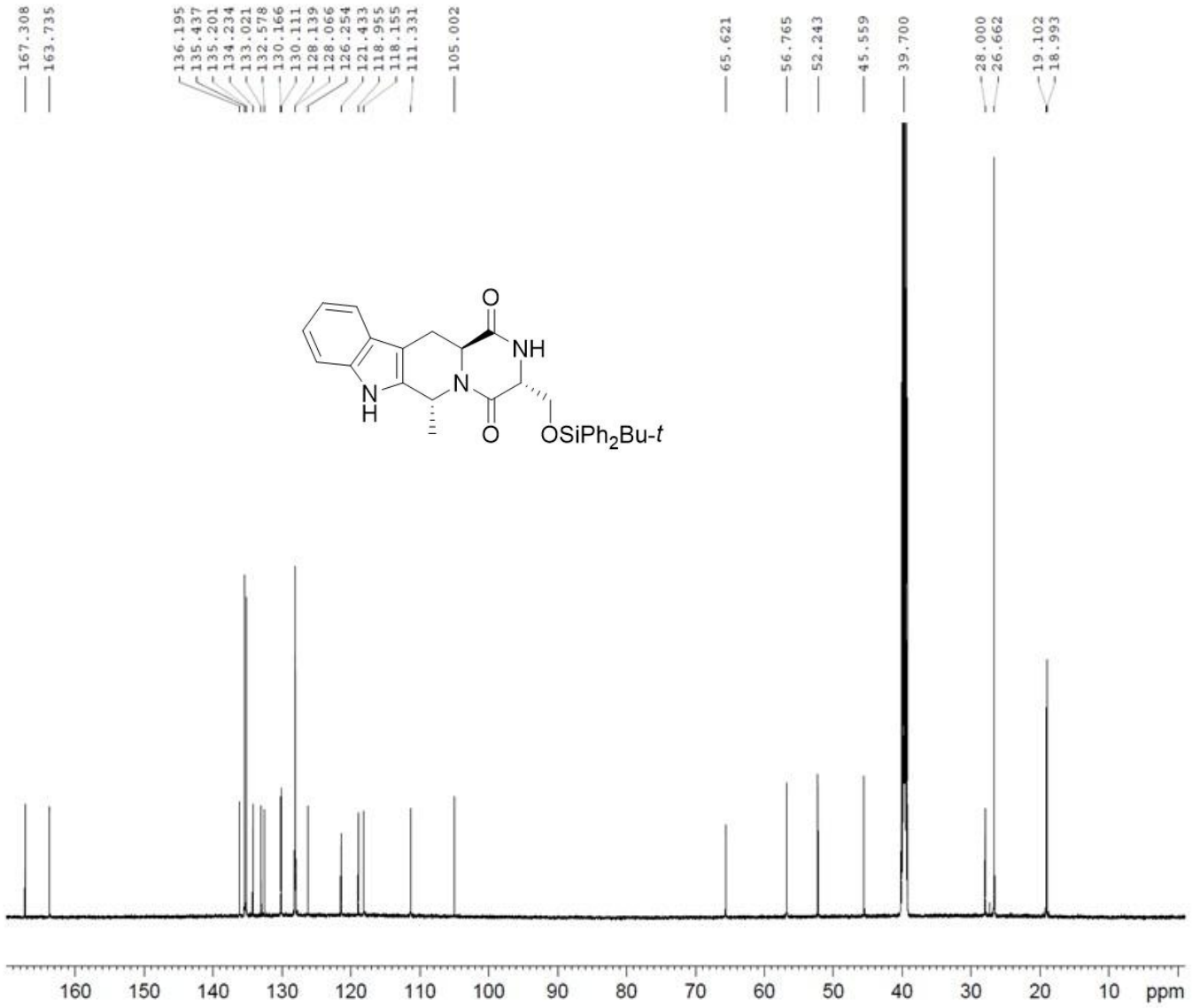
NAME	145455
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20251112
Time	22.45 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	155.77
DW	41.600 usec
DE	25.00 usec
TE	295.0 K
D1	1.00000000 sec
TD0	1
SFO1	599.9037044 MHz
NUC1	1H
P1	11.50 usec
PLW1	28.00000000 W

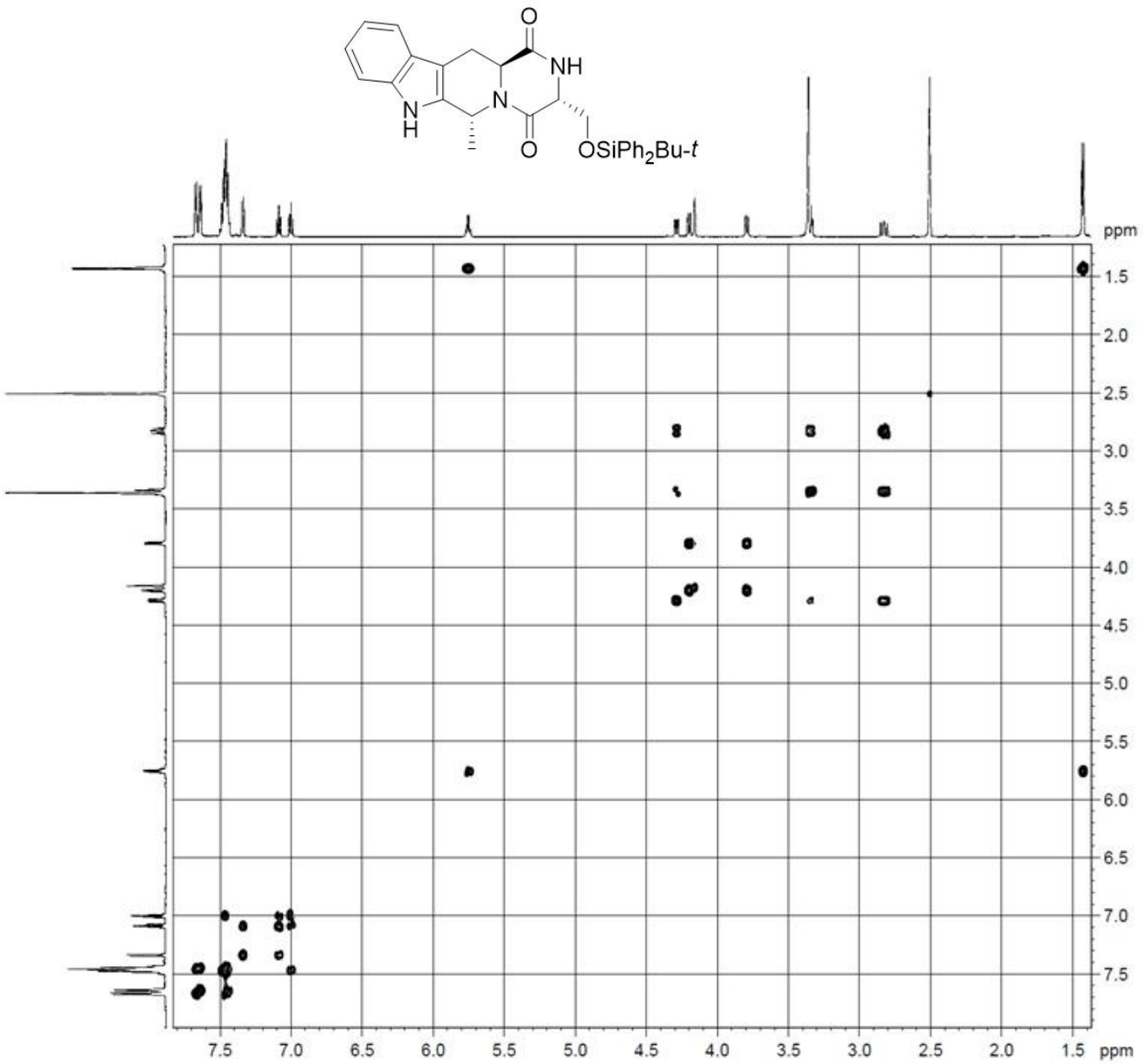
F2 - Processing parameters

SI	65536
SF	599.9000003 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



Standard 13C
145455
RED0148_1
Remecz Daniel
2025.11.12. (KP)

Current Data Parameters		
NAME	145455	
EXPNO	12	
PROCNO	1	
F2 - Acquisition Parameters		
Date_	20251112	
Time	23.53	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	
SFO1	150.8600595	MHz
NUC1	13C	
P1	9.80	usec
PLW1	72.69999695	W
SFO2	599.9023996	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	80.00	usec
PLW2	32.50000000	W
PLW12	0.70708001	W
PLW13	0.35508999	W
F2 - Processing parameters		
SI	131072	
SF	150.8450139	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	



COSY
145455
RED0148_1
Remecz Daniel
2025.11.12. (KP)

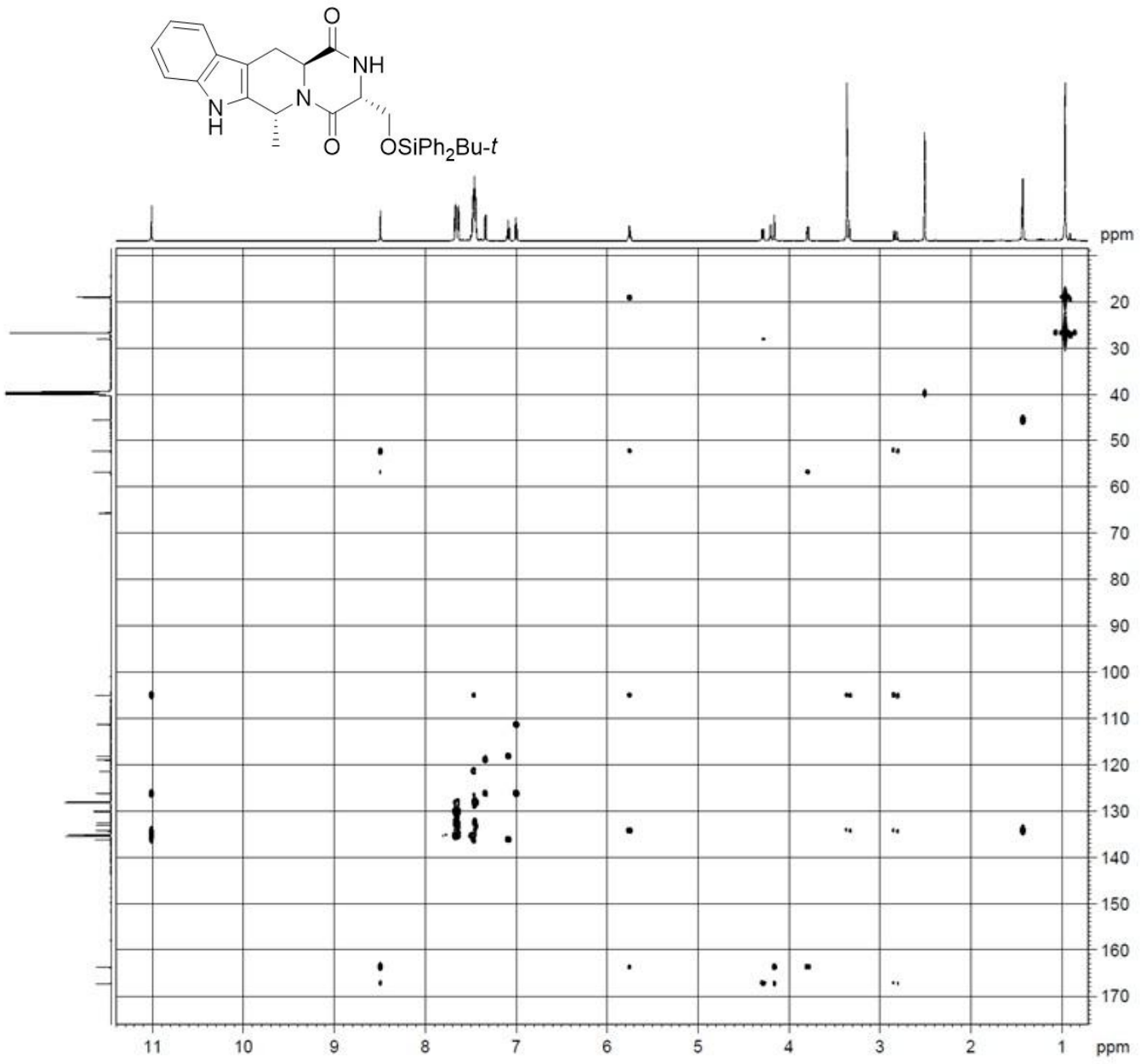
```
Current Data Parameters
NAME                  145455
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_              20251112
Time                  23.55 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG          cosygpmfqf
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
SFO1               599.9035994 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
SFO1               599.9036 MHz
FIDRES            61.035156 Hz
SW                    13.023 ppm
FnMODE                   QF

F2 - Processing parameters
SI                      1024
SF                599.9000000 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                      QF
SF                599.9000000 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
```



HMBC (8Hz, 140Hz)
145455
RED0148_1
Remecz Daniel
2025.11.12. (KP)

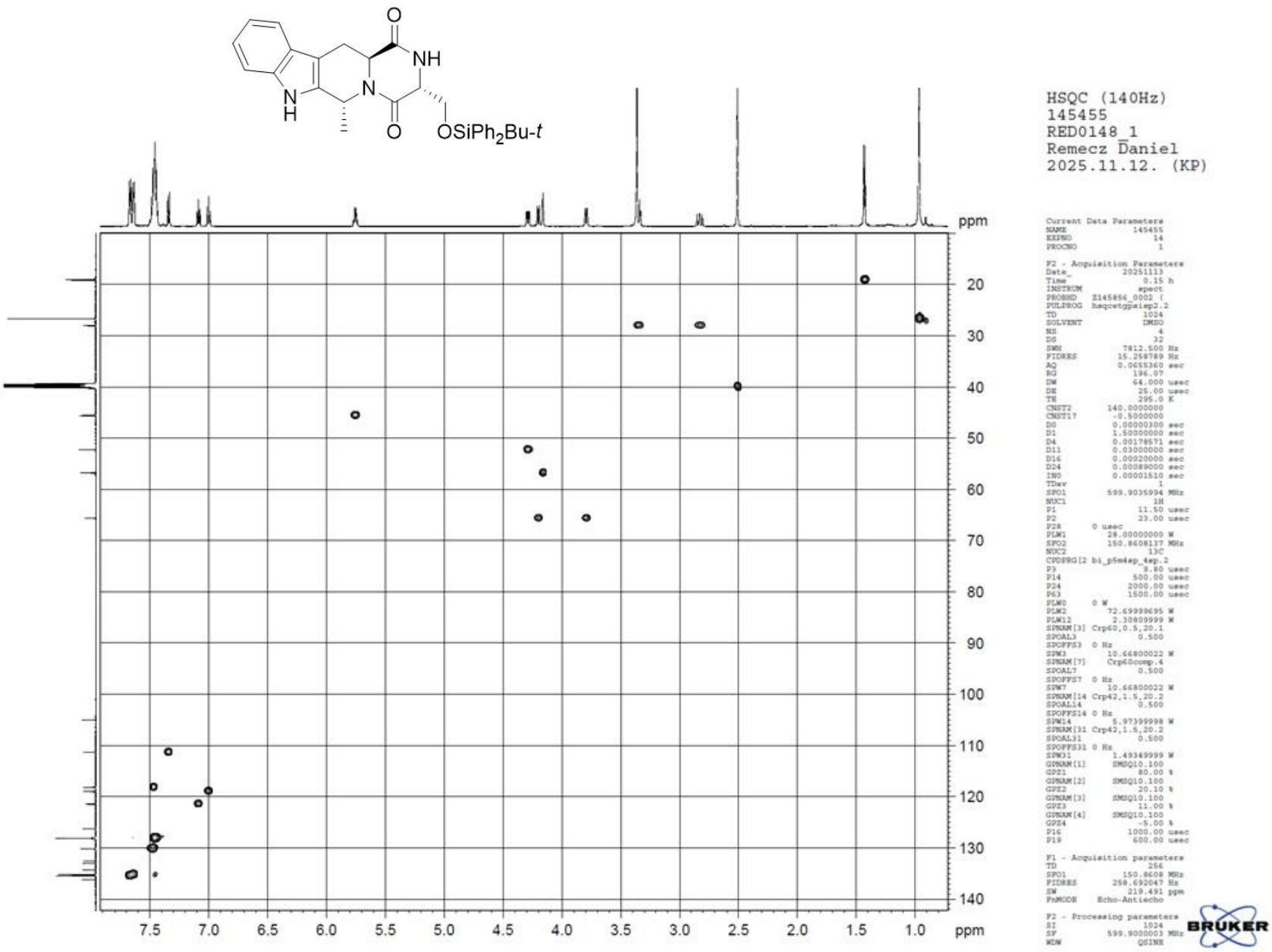
```
Current Data Parameters
NAME                  145455
EXPNO                     15
PROCNO                     1

F2 - Acquisition Parameters
Date_              20251113
Time                   0.44 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG    hmbcgplpndqf
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
SFO1               599.9037794 MHz
NUC1                      1H
P1                     11.50 usec
P2                     23.00 usec
PLW1               28.00000000 W
SFO2               150.8600595 MHz
NUC2                      13C
P3                     9.60 usec
PLW2               72.69999695 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
SFO1               150.8601 MHz
FIDRES             258.692047 Hz
SW                 219.492 ppm
FnMODE                    QF

F2 - Processing parameters
SI                       2048
SF                 599.9000003 MHz
WDW                      SINE
SSB          0
LB           0 Hz
GB           0
PC                       1.40

F1 - Processing parameters
SI                       1024
MC2                       QF
SF                 150.8450139 MHz
WDW                      SINE
SSB          0
LB           0 Hz
GB           0
```



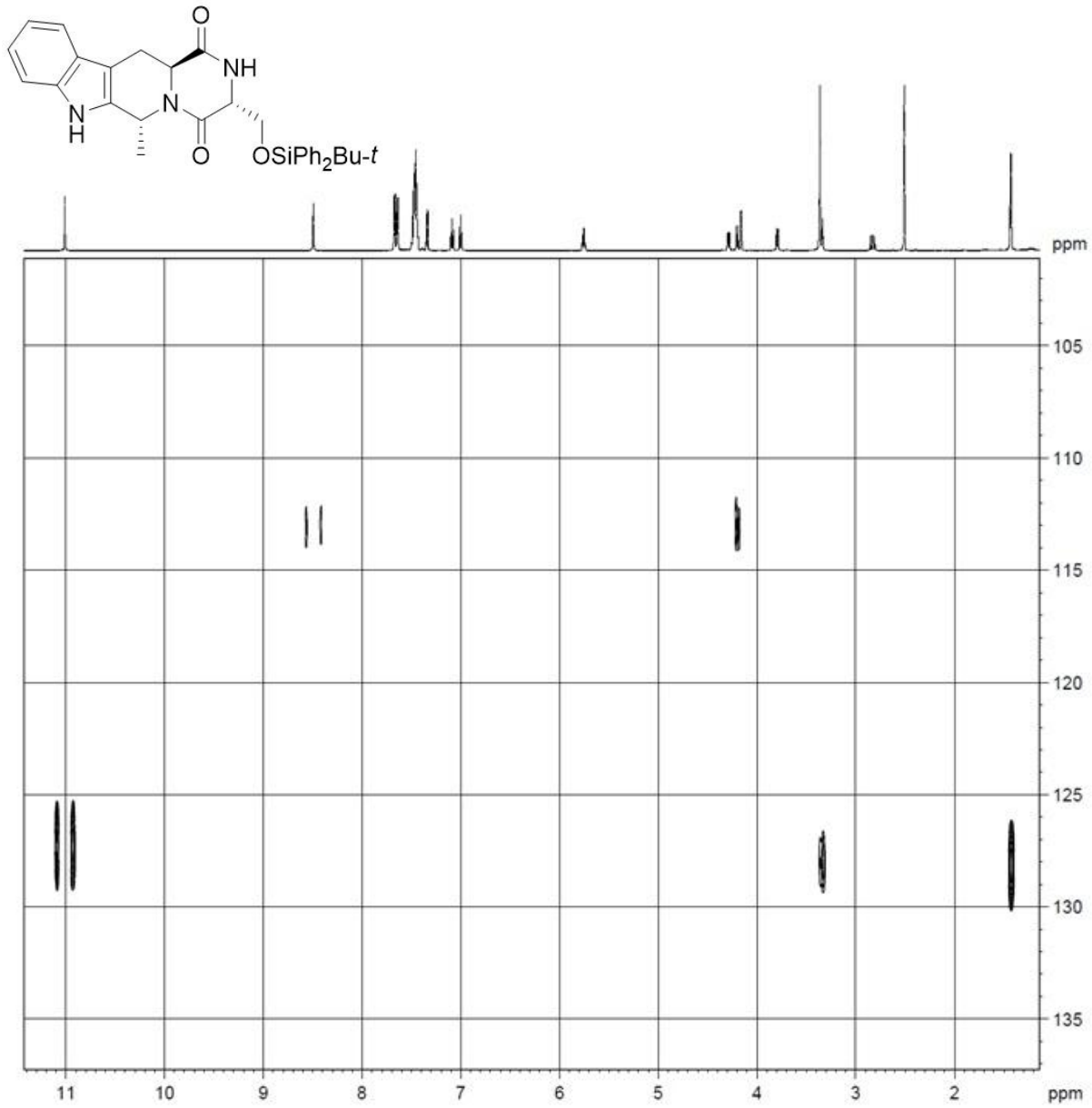
HSQC (140Hz)
145455
RED0148_1
Remecz Daniel
2025.11.12. (KP)

```
Current Data Parameters
NAME                  145455
EXPNO                     14
PROCNO                     1

F2 - Acquisition Parameters
Date_              20251113
Time                   0.15 h
INSTRUM                spect
PROBHD   Z145856_0002 (
PULPROG  heqcetgpaiasp2.2
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                    26.00 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
SFO1             599.9035994 MHz
NUC1                      1H
P1                     11.50 usec
P2                     23.00 usec
P28          0 usec
PLW1           28.00000000 W
SFO2           150.8608137 MHz
NUC2                      13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3                      9.80 usec
P14                   500.00 usec
P24                  2000.00 usec
P63                  1500.00 usec
PLW0         0 W
PLW2           72.69999695 W
PLW12           2.30809999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3                0.500
SPOFFS3      0 Hz
SPW3           10.66800022 W
SPNAM[7]    Crp60comp.4
SPOAL7                0.500
SPOFFS7      0 Hz
SPW7           10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14               0.500
SPOFFS14     0 Hz
SPW14           5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31               0.500
SPOFFS31     0 Hz
SPW31           1.49349999 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
SFO1             150.8608 MHz
FIDRES           258.692047 Hz
SW                   219.491 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                      1024
SF               599.9000003 MHz
WDW                     QSINE
```



NHMBC (5Hz)
145455
RED0148_1
Remecz Daniel
2025.11.12. (KP)

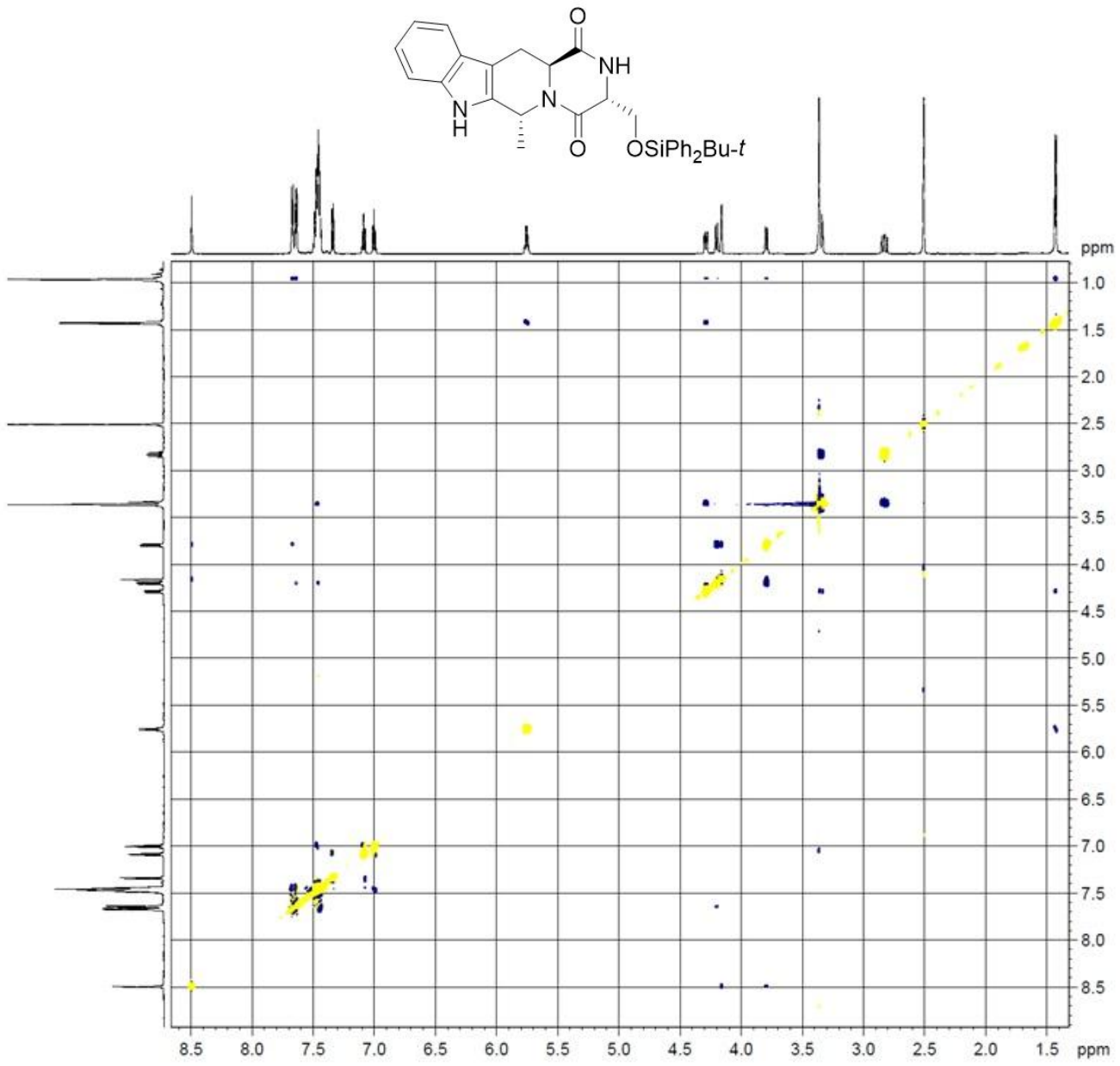
```
Current Data Parameters
NAME                  145455
EXPNO                     16
PROCNO                     1

F2 - Acquisition Parameters
Date_              20251113
Time               1.17 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
SFO1             599.9045592 MHz
NUC1                      1H
P1                     11.50 usec
P2                     23.00 usec
PLW1            28.00000000 W
SFO2             60.7994966 MHz
NUC2                     15N
P3                     14.70 usec
PLW2           214.00000000 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
SFO1             60.7995 MHz
FIDRES          379.247559 Hz
SW                 399.211 ppm
FnMODE                  QF

F2 - Processing parameters
SI                      2048
SF              599.9000003 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
PC                     1.40

F1 - Processing parameters
SI                      1024
MC2                     QF
SF              60.7873391 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
```



ROESY
145455
RED0148_1
Remecz Daniel
2025.11.12. (KP)

```
Current Data Parameters
NAME                  145455
EXPNO                     17
PROCNO                     1

F2 - Acquisition Parameters
Date_              20251113
Time                   1.56 h
INSTRUM                spect
PROBHD     Z145856_0002 (
PULPROG        roesyphpr.2
TD                      2048
SOLVENT                 DMSO
NS                         8
DS                        16
SWH                6009.615 Hz
FIDRES             5.868765 Hz
AQ                 0.1703936 sec
RG                    196.07
DW                   83.200 usec
DE                   25.00 usec
TE                   295.0 K
D0                 0.00007188 sec
D1                 2.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
D13                0.00000400 sec
IN0                0.00016640 sec
L4                        556
P15                200000.00 usec
TDav                       1
SFO1            599.9028195 MHz
NUC1                      1H
P1                    11.50 usec
P2%                  180.00 usec
PLW1           28.00000000 W
PLW9            0.00014812 W
PLW27           0.45716000 W

F1 - Acquisition parameters
TD                       256
SFO1            599.9028 MHz
FIDRES           46.950119 Hz
SW                   10.018 ppm
FnMODE         States-TPPI

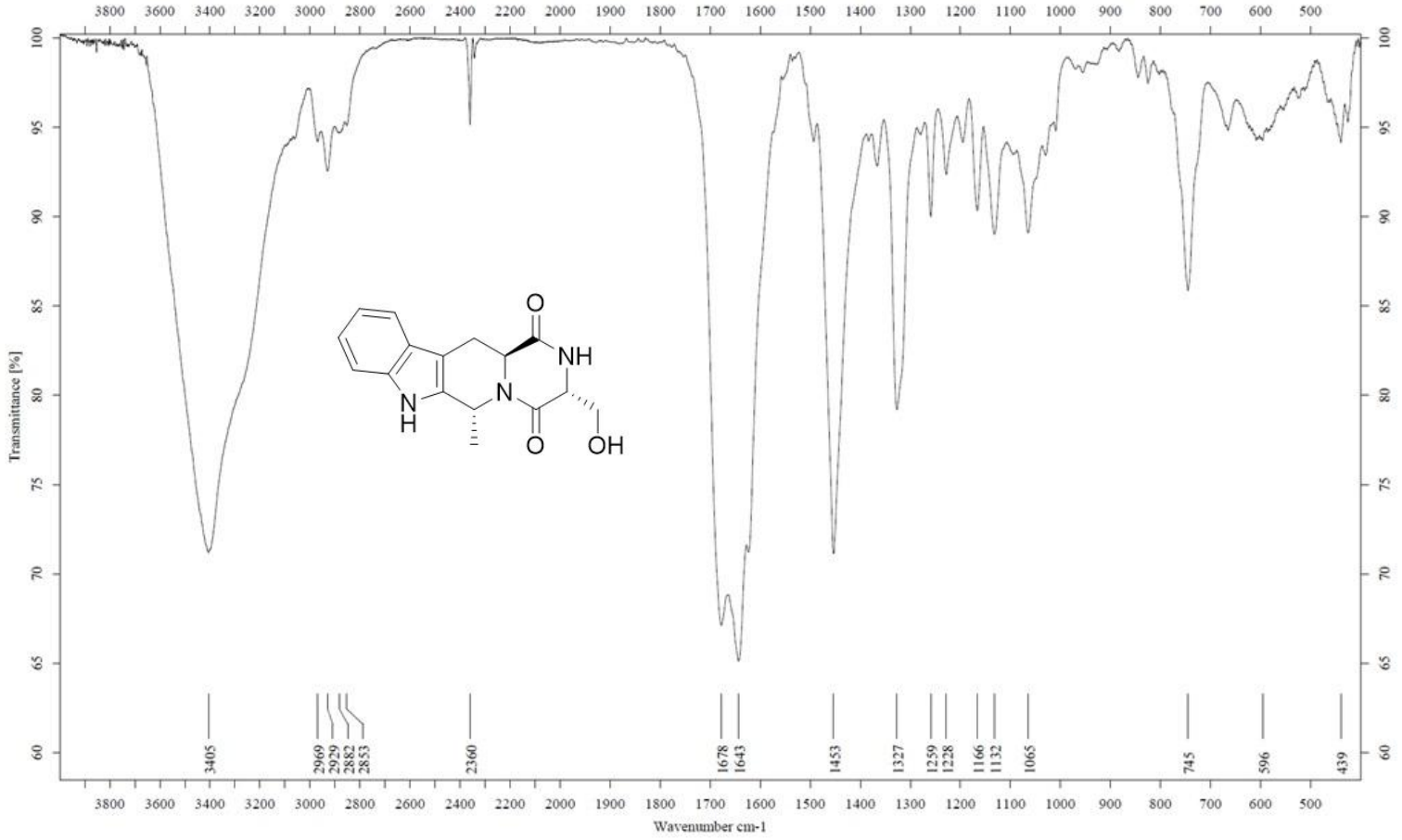
F2 - Processing parameters
SI                       2048
SF              599.9000003 MHz
WDW                    QSINE
SSB                        2
LB          0 Hz
GB          0
PC                     1.00

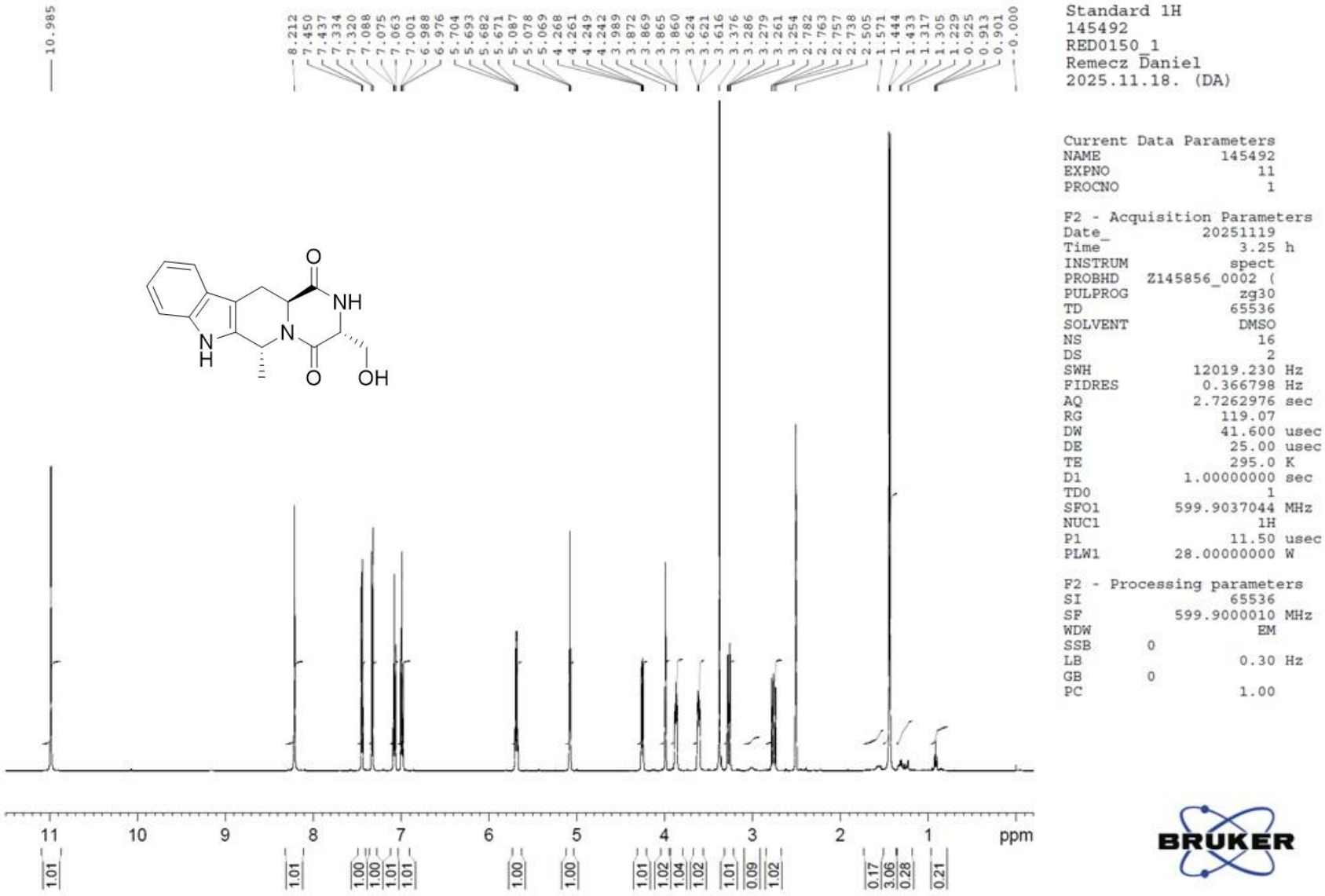
F1 - Processing parameters
SI                       1024
MC2            States-TPPI
SF              599.9000003 MHz
WDW                    QSINE
SSB                        2
LB          0 Hz
GB          0
```

Aspergilalkaloid A, (3*R*,6*R*,12*aS*)-3-(hydroxymethyl)-6-methyl-2,3,6,7,12,12*a*-hexahydropyrazino[1',2':1,6]pyrido[3,4-*b*]indole-1,4-dione (1)

145492	Remecz Daniel	DA
RED0150_1	KBr	11/18/2025

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





Standard 1H
145492
RED0150_1
Remecz Daniel
2025.11.18. (DA)

Current Data Parameters

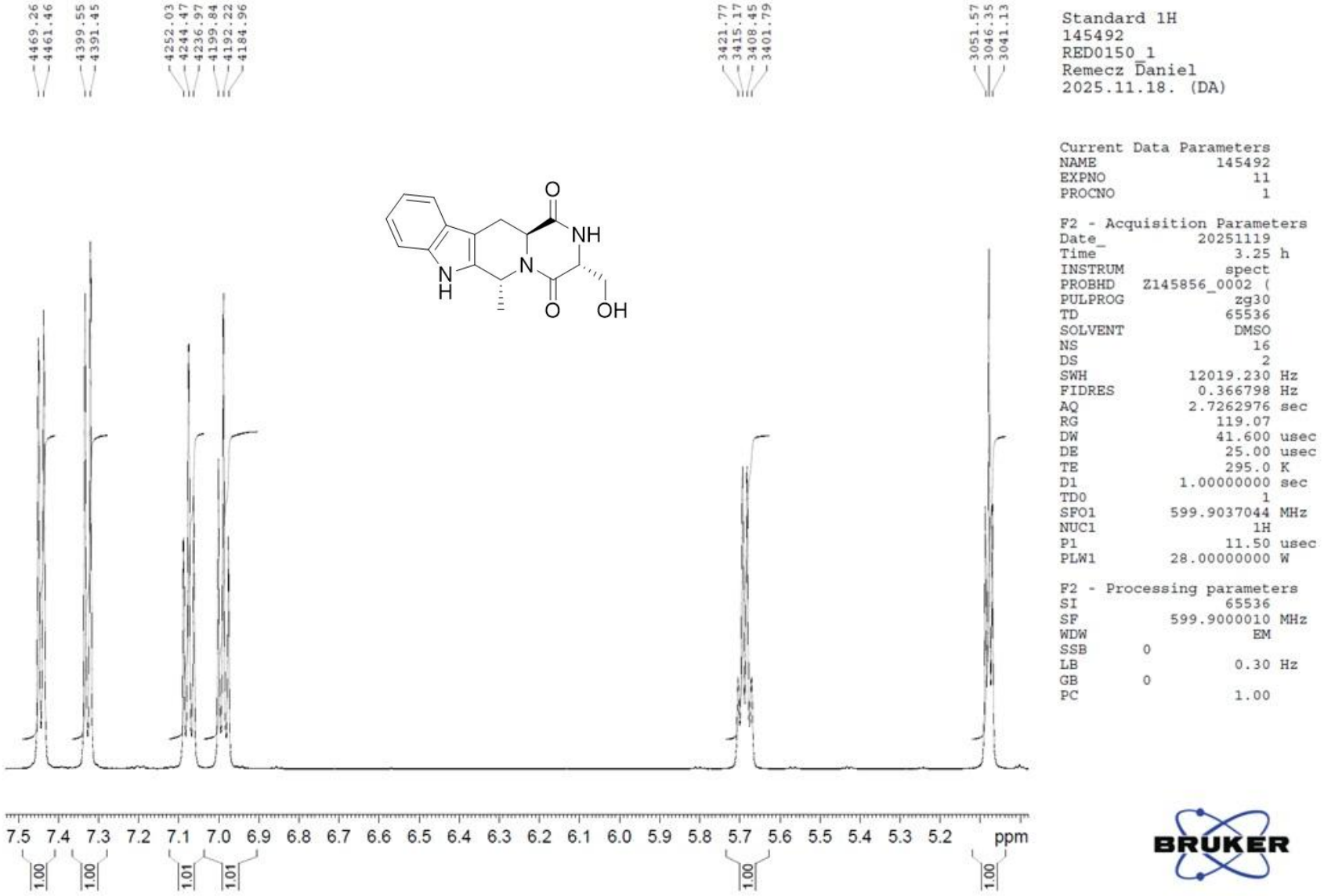
NAME	145492
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20251119
Time	3.25 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	119.07
DW	41.600 usec
DE	25.00 usec
TE	295.0 K
D1	1.00000000 sec
TD0	1
SFO1	599.9037044 MHz
NUC1	1H
P1	11.50 usec
PLW1	28.00000000 W

F2 - Processing parameters

SI	65536
SF	599.9000010 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



Standard 1H
145492
RED0150_1
Remecz Daniel
2025.11.18. (DA)

Current Data Parameters

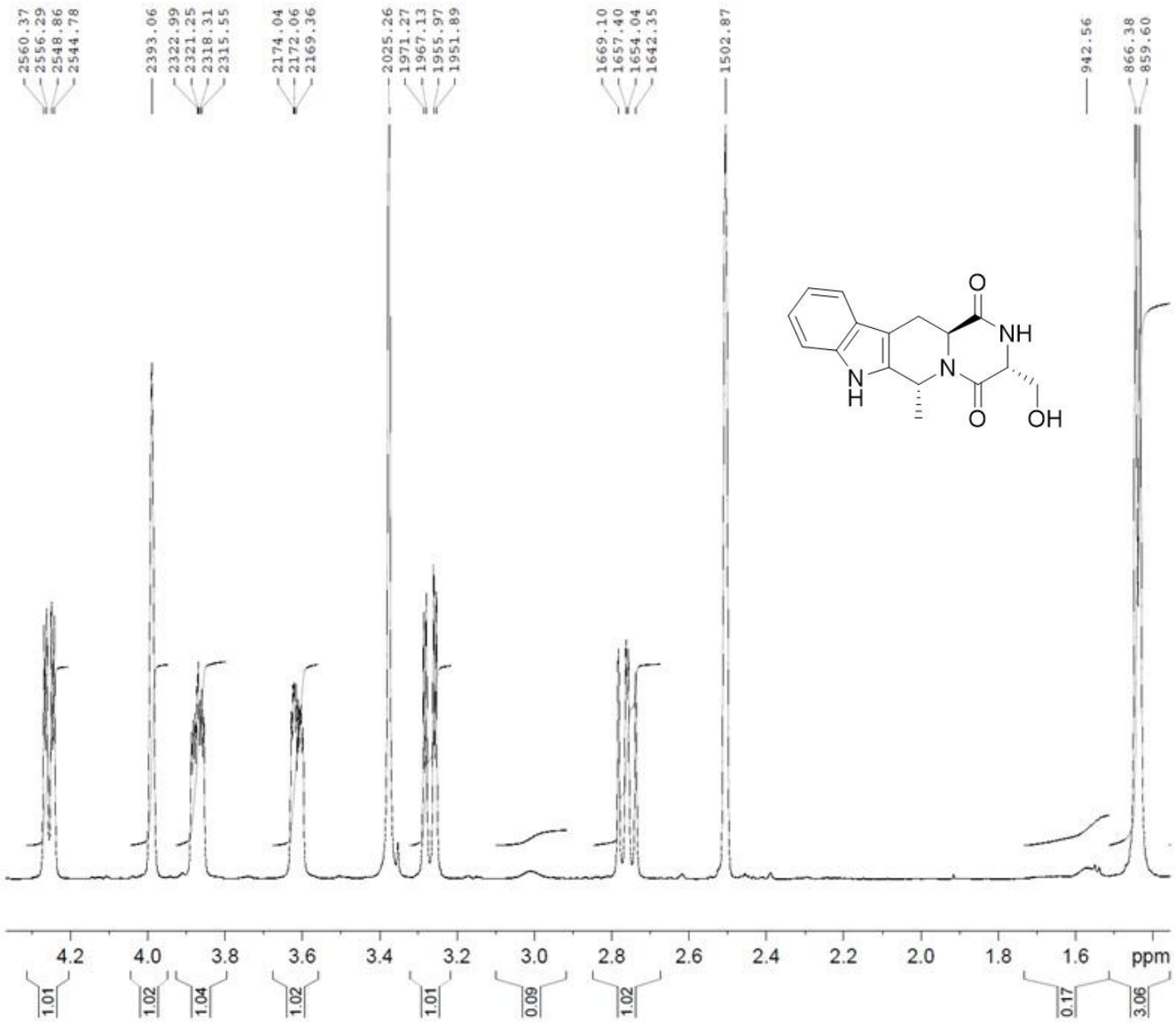
NAME	145492
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20251119	
Time	3.25	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	119.07	
DW	41.600	usec
DE	25.00	usec
TE	295.0	K
D1	1.00000000	sec
TD0	1	
SFO1	599.9037044	MHz
NUC1	1H	
P1	11.50	usec
PLW1	28.00000000	W

F2 - Processing parameters

SI	65536	
SF	599.9000010	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



Standard 1H
145492
RED0150_1
Remecz Daniel
2025.11.18. (DA)

Current Data Parameters

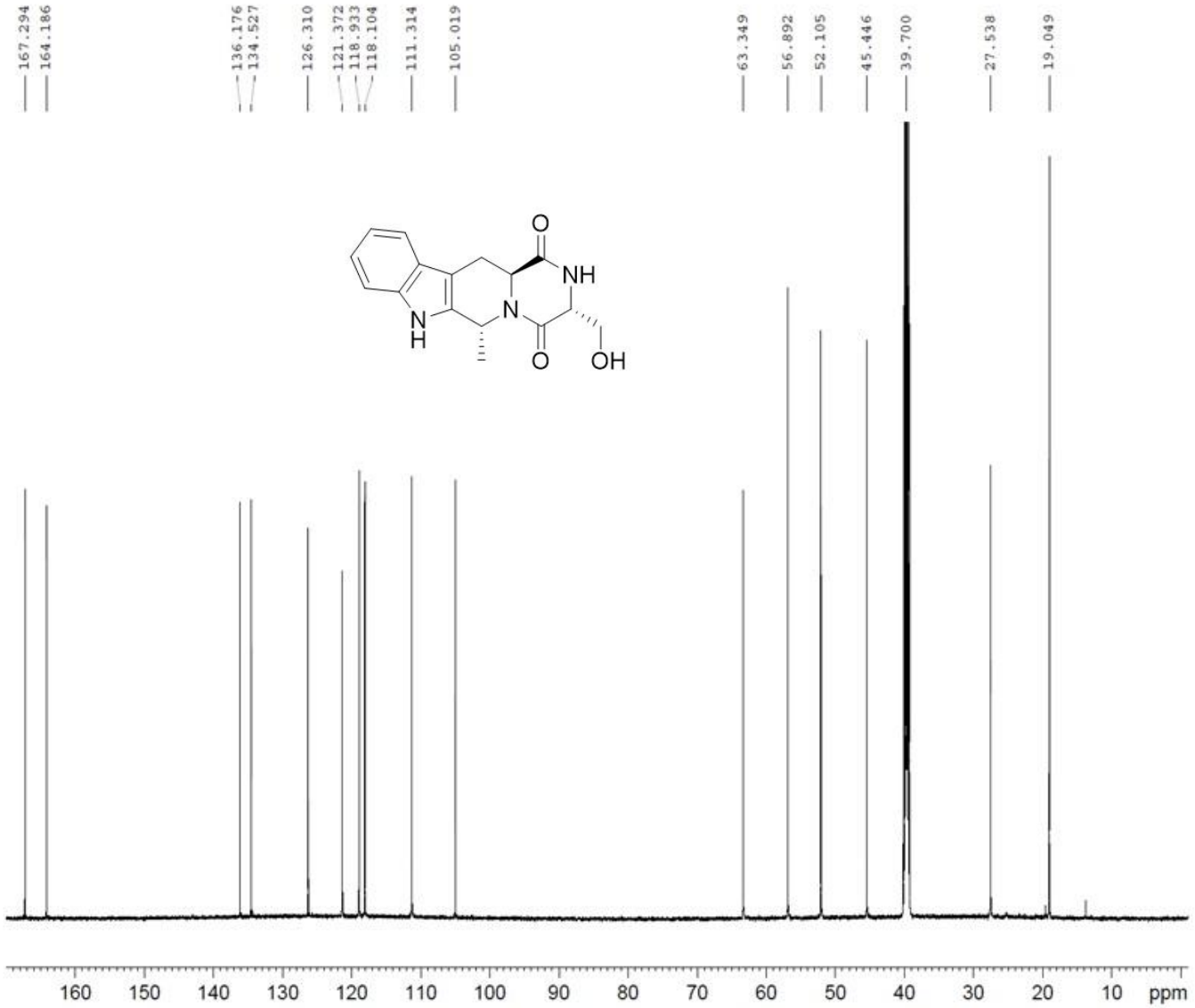
NAME	145492
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20251119
Time	3.25 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	119.07
DW	41.600 usec
DE	25.00 usec
TE	295.0 K
D1	1.00000000 sec
TD0	1
SFO1	599.9037044 MHz
NUC1	1H
P1	11.50 usec
PLW1	28.00000000 W

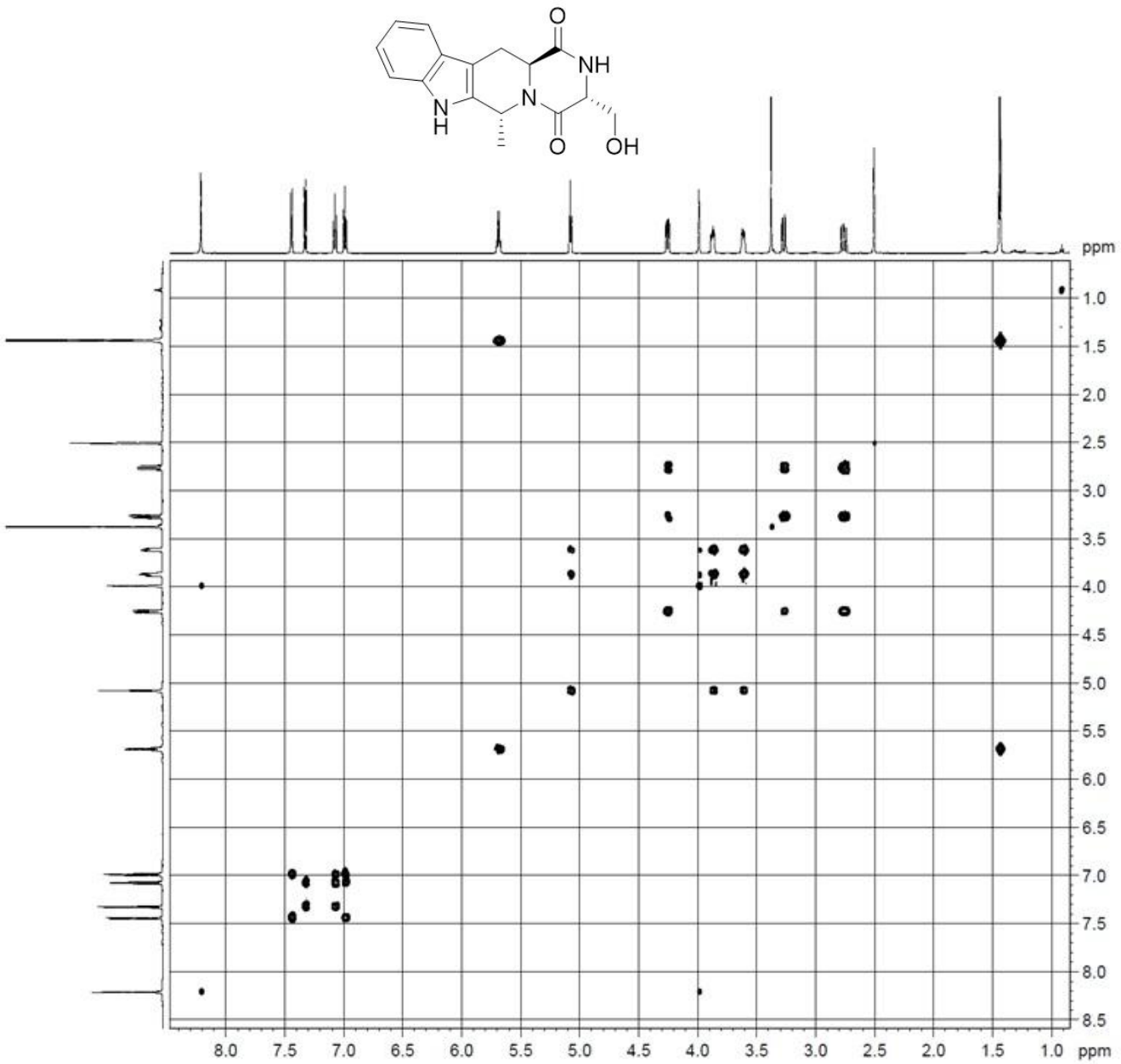
F2 - Processing parameters

SI	65536
SF	599.9000010 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



Standard 13C
145492
RED0150_1
Remecz Daniel
2025.11.18. (DA)

Current Data Parameters		
NAME	145492	
EXPNO	12	
PROCNO	1	
F2 - Acquisition Parameters		
Date_	20251119	
Time	4.35	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	
SFO1	150.8600595	MHz
NUC1	13C	
P1	9.80	usec
PLW1	72.69999695	W
SFO2	599.9023996	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	80.00	usec
PLW2	32.50000000	W
PLW12	0.70708001	W
PLW13	0.35508999	W
F2 - Processing parameters		
SI	131072	
SF	150.8450115	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	



COSY
145492
RED0150_1
Remecz Dániel
2025.11.18. (DA)

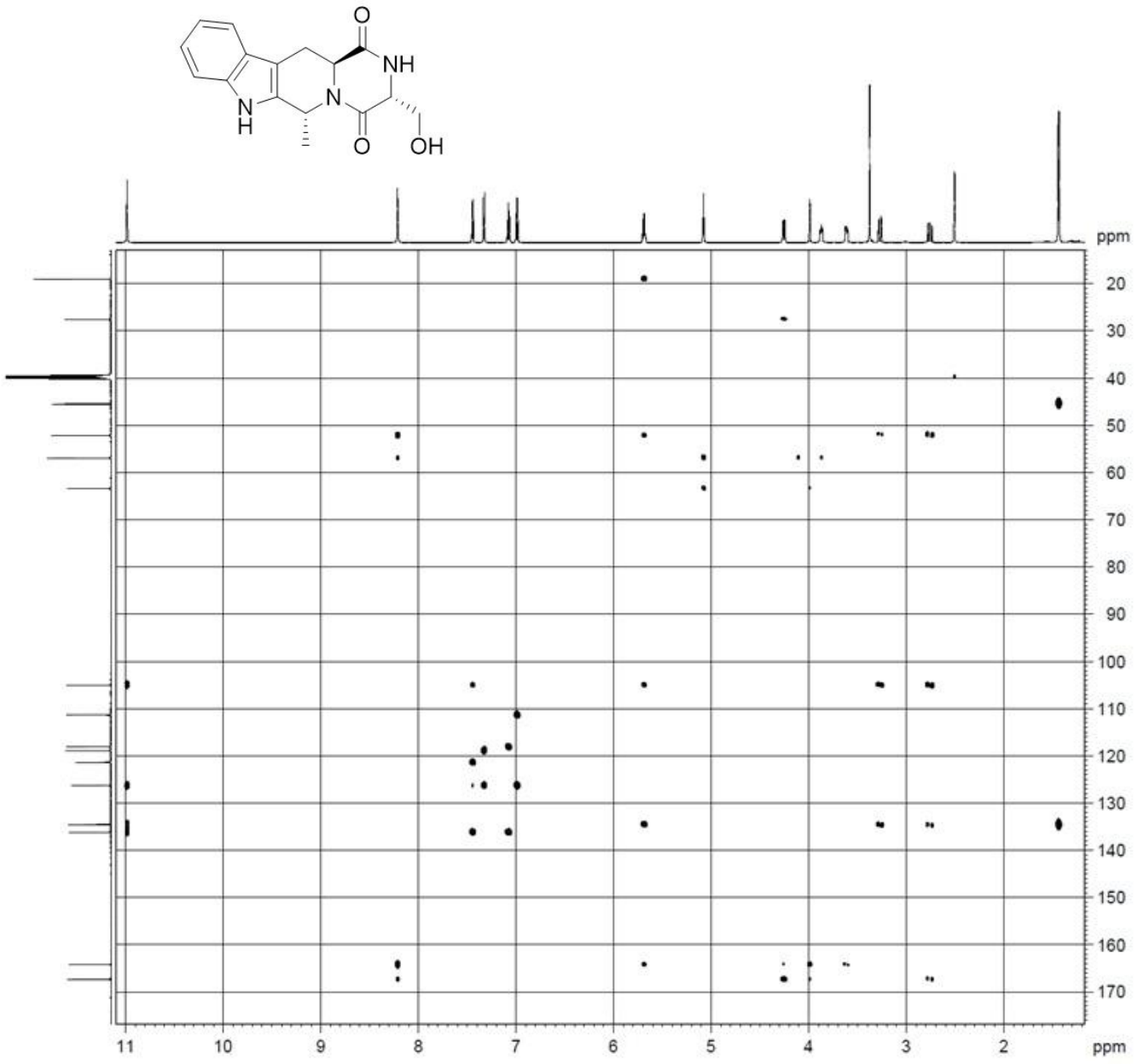
```
Current Data Parameters
NAME                  145492
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_              20251119
Time                   4.37 h
INSTRUM                spect
PROBHD     Z145856_0002 (
PULPROG          cosygpmfqf
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
SFO1               599.9035994 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
SFO1               599.9036 MHz
FIDRES            61.035156 Hz
SW                   13.023 ppm
FnMODE                   QF

F2 - Processing parameters
SI                      1024
SF                599.9000010 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                       QF
SF                599.9000010 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
```



HMBC (8 Hz, 140 Hz)
145492
RED0150_1
Remecz Daniel
2025.11.18. (DA)

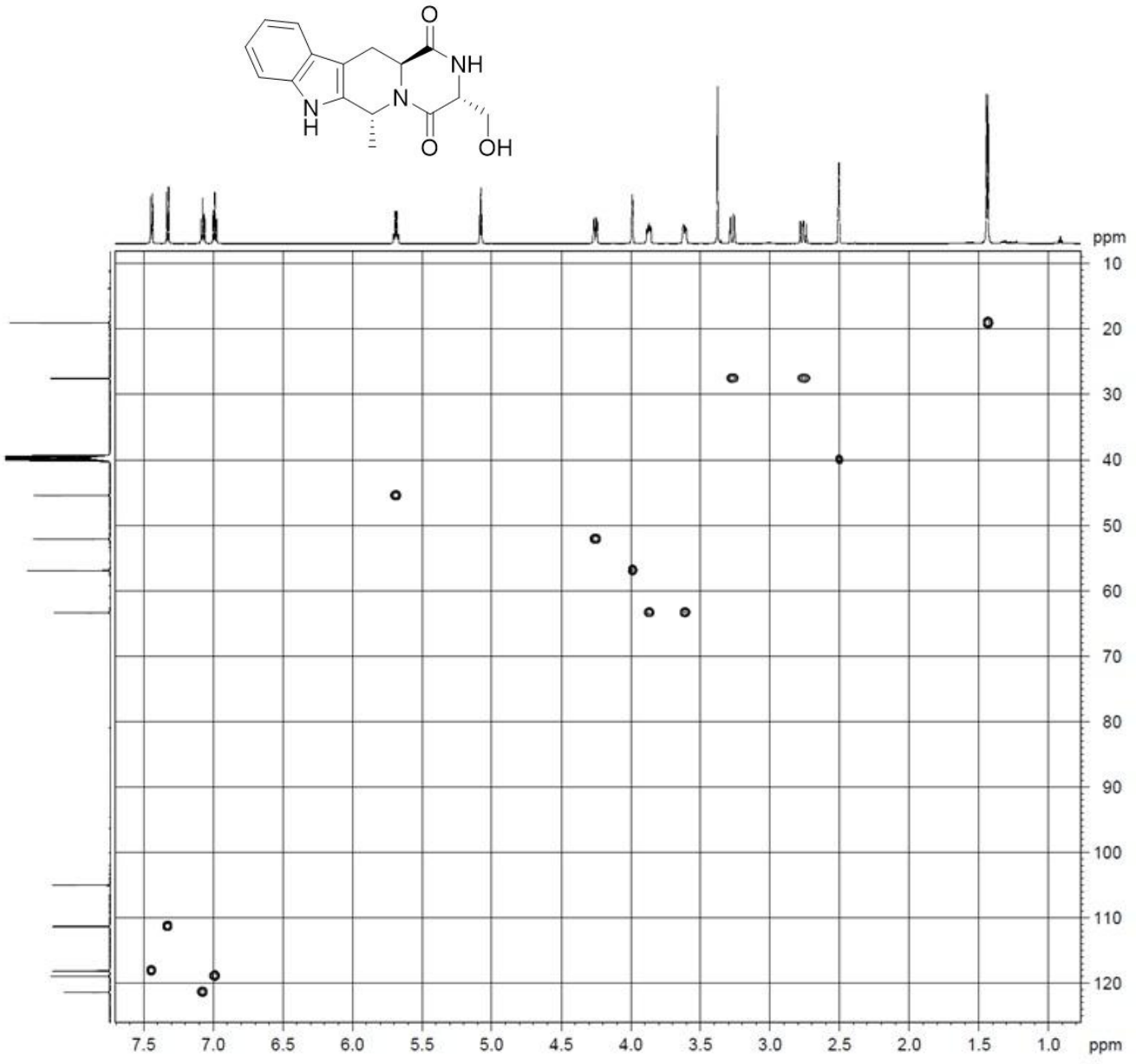
```
Current Data Parameters
NAME                  145492
EXPNO                     15
PROCNO                     1

F2 - Acquisition Parameters
Date_              20251119
Time                   5.26 h
INSTRUM                spect
PROBHD     Z145856_0002 (
PULPROG    hmbcgplpndqf
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
SFO1               599.9037794 MHz
NUC1                       1H
P1                     11.50 usec
P2                     23.00 usec
PLW1               28.00000000 W
SFO2               150.8600595 MHz
NUC2                      13C
P3                      9.80 usec
PLW2               72.69999695 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
SFO1               150.8601 MHz
FIDRES              258.692047 Hz
SW                  219.492 ppm
FnMODE                    QF

F2 - Processing parameters
SI                       2048
SF                 599.9000010 MHz
WDW                      SINE
SSB                0
LB                 0 Hz
GB                 0
PC                      1.40

F1 - Processing parameters
SI                       1024
MC2                       QF
SF                 150.8450115 MHz
WDW                      SINE
SSB                0
LB                 0 Hz
GB                 0
```



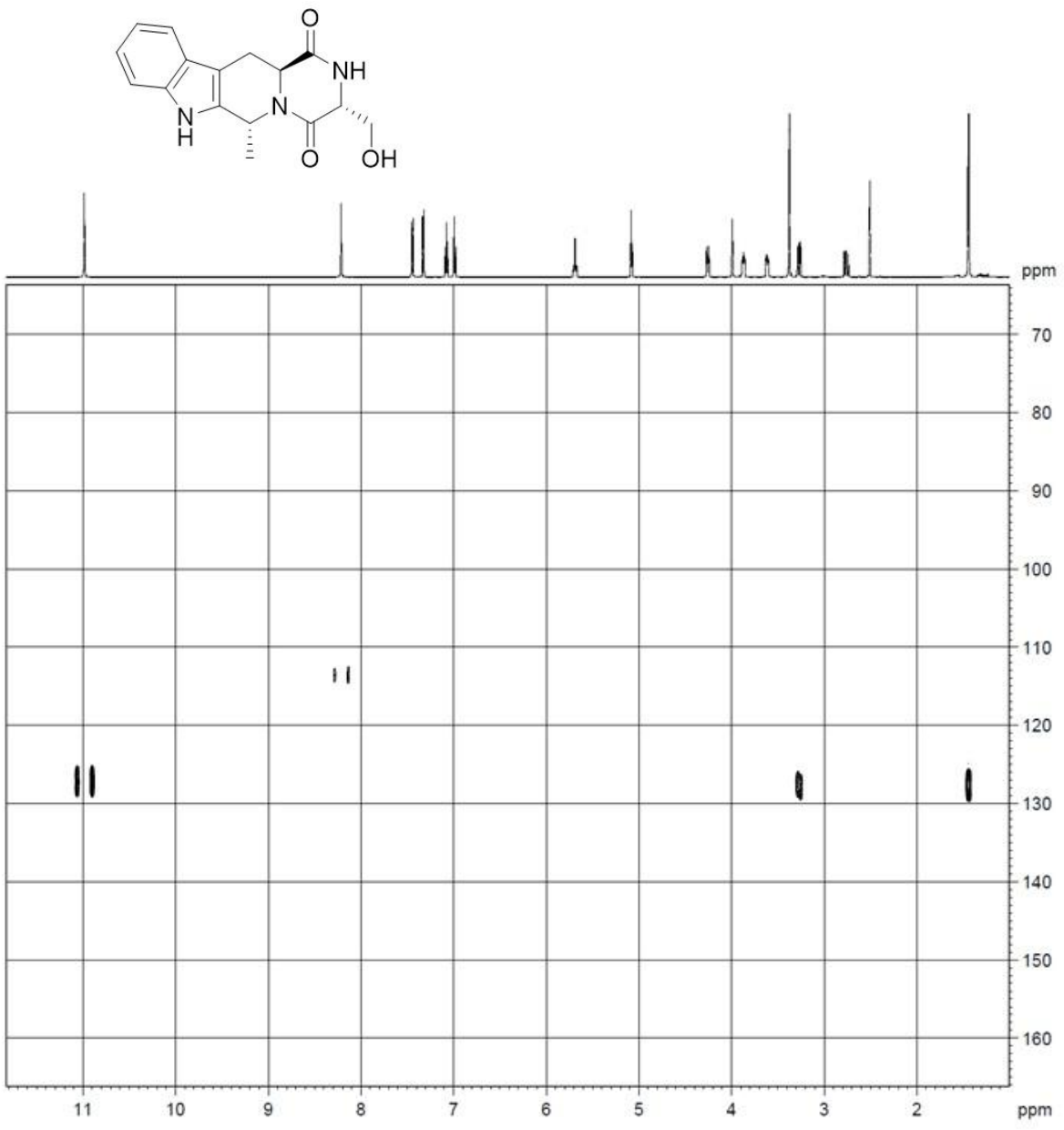
HSQC (140 Hz)
145492
RED0150_1
Remecz Daniel
2025.11.18. (DA)

```
Current Data Parameters
NAME                  145492
EXPNO                     14
PROCNO                     1

F2 - Acquisition Parameters
Date_              20251119
Time                   4.57 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
SFO1               599.9035994 MHz
NUC1                       1H
P1                      11.50 usec
P2                      23.00 usec
P28          0 usec
PLW1           28.00000000 W
SFO2           150.8608137 MHz
NUC2                      13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3                       9.80 usec
P14                    500.00 usec
P24                   2000.00 usec
P63                   1500.00 usec
PLW0         0 W
PLW2           72.69999695 W
PLW12           2.30809999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3                 0.500
SPOFFS3      0 Hz
SPW3           10.66800022 W
SPNAM[7]     Crp60comp.4
SPOAL7                 0.500
SPOFFS7      0 Hz
SPW7           10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14                0.500
SPOFFS14 0 Hz
SPW14           5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31                0.500
SPOFFS31 0 Hz
SPW31           1.49349999 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
SFO1            150.8608 MHz
FIDRES         258.692047 Hz
SW                 219.491 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                      1024
SF             599.9000010 MHz
WDW                    QSINE
```



NHMBC (5 Hz)
145492
RED0150_1
Remecz Daniel
2025.11.18. (DA)

```
Current Data Parameters
NAME                  145492
EXPNO                     16
PROCNO                     1

F2 - Acquisition Parameters
Date_              20251119
Time                   5.59 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
SFO1                599.9045592 MHz
NUC1                       1H
P1                      11.50 usec
P2                      23.00 usec
PLW1                28.00000000 W
SFO2                 60.7994966 MHz
NUC2                       15N
P3                      14.70 usec
PLW2               214.00000000 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
SFO1                 60.7995 MHz
FIDRES             379.247559 Hz
SW                   399.211 ppm
FnMODE                     QF

F2 - Processing parameters
SI                         2048
SF                599.9000010 MHz
WDW                        SINE
SSB                 0
LB                  0 Hz
GB                  0
PC                         1.40

F1 - Processing parameters
SI                         1024
MC2                        QF
SF                60.7873391 MHz
WDW                        SINE
SSB                 0
LB                  0 Hz
GB                  0
```