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

Supporting Information

cis-Selective Synthesis of 1,3-Substituted Tetrahydro-β-Carbolines from *N,S*-Sulfonyl Acetals

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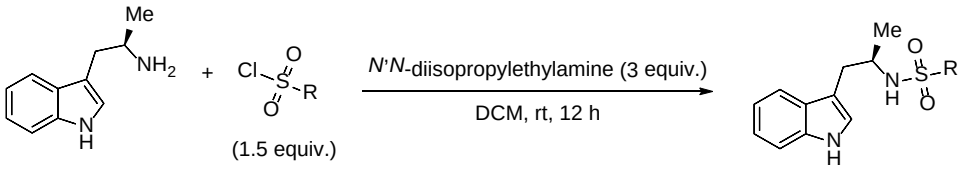
General methods

Unless otherwise indicated, all commercial reagents and solvents were used without additional purification. Anhydrous solvents were used. ^{1}H NMR spectra were recorded with a Bruker Avance 400 or 500 MHz spectrometer. Chemical shifts (in parts per million) were referenced to tetramethylsilane (δ 0) in DMSO-d_6 (δ 2.5) or $CDCl_3$ (δ 7.26) as an internal standard. ^{13}C NMR spectra were obtained with the same NMR spectrometer and were calibrated with DMSO-d_6 (δ 39.51) or $CDCl_3$ (δ 77.2). HRMS spectra were recorded on an Orbitrap Q Exactive mass spectrometer. Reactions were monitored by a walkup LCMS/UV system using 2 to 98% acetonitrile with 0.1% formic acid (or 0.01% ammonia) over 2.5 min. Flash column chromatography purifications were performed on automated systems equipped with wavelengths of 254 and 280 nm.

General sulfonylation procedure for the synthesis of *N*-sulfonamides

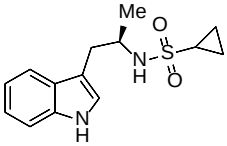


Scheme S1: General depiction of sulfonylation for the synthesis of N-sulfonamides

A 11 dram scintillation vial equipped with a Teflon-coated magnetic stir bar was charged with (*R*)-1-(1H-indol-3-yl)propan-2-amine, the appropriate sulfonyl chloride (1.5 equiv.) and dichloromethane (5.0 mL). *N*,*N*-Diisopropylethylamine (3 equiv.) was added at room temperature. The resulting solution was allowed to stir for overnight (approximately 12 h). H_2O (10 mL) was added, and the biphasic mixture was extracted with dichloromethane (10 mL) twice. The combined organic layer was dried over Na_2SO_4 and filtered. The filtrate was concentrated in vacuo, and the resulting oil was purified by silica gel column chromatography using a gradient solvent system (0 → 80% iPrOAc/Heptane) as the eluent. The pure product was thus obtained as white solid or colorless oil. To prevent decomposition during prolonged storage, all *N*-sulfonamide were kept at –20 °C.

Characterization of *N*-sulfonamides

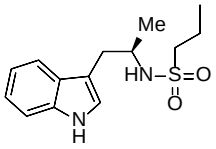
(*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)cyclopropanesulfonamide (9a)



The title compound was prepared from (*R*)-1-(1H-indol-3-yl)propan-2-amine (300 mg, 1.74 mmol) and cyclopropanesulfonyl chloride (366 mg, 2.61 mmol) according to the general sulfonylation procedure and was obtained as a white solid (477 mg, 98% yield); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.09 (s, 1H), 7.62 (ddt, *J* = 7.8, 1.3, 0.8 Hz, 1H), 7.37 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.21 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H), 7.16 – 7.08 (m, 2H), 4.15 (d, *J* = 7.3 Hz, 1H), 3.88 (hept, *J* = 6.6 Hz, 1H), 3.05 – 2.90 (m, 2H), 2.09 (tt, *J* = 8.0, 4.9

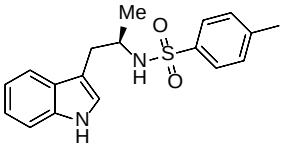
Hz, 1H), 1.32 (d, *J* = 6.5 Hz, 3H), 1.05 (ddt, *J* = 9.7, 6.7, 4.9 Hz, 1H), 0.97 – 0.89 (m, 1H), 0.74 (dddd, *J* = 9.0, 8.0, 6.6, 4.9 Hz, 1H), 0.62 (dddd, *J* = 9.2, 8.0, 6.7, 4.9 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 136.37, 127.58, 123.04, 122.36, 119.75, 118.93, 111.64, 111.24, 50.37, 33.54, 30.70, 22.55, 5.63, 5.12; **HRMS (**ESI) *m/z* calcd for $C_{14}H_{19}O_2N_2S$ $[M+H]^+$ 279.1167, found 279.1153.

(*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)propane-1-sulfonamide (27a)



The title compound was prepared from (*R*)-1-(1H-indol-3-yl)propan-2-amine (300 mg, 1.74 mmol) and propane-1-sulfonyl chloride (372 mg, 2.61 mmol) according to the general sulfonylation procedure and was obtained as a white solid (286 mg, 59% yield); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.08 (s, 1H), 7.62 (ddt, *J* = 7.8, 1.4, 0.8 Hz, 1H), 7.38 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.21 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H), 7.14 (ddd, *J* = 8.0, 7.1, 1.1 Hz, 1H), 7.08 (d, *J* = 2.4 Hz, 1H), 4.06 (d, *J* = 7.5 Hz, 1H), 3.88 – 3.77 (m, 1H), 3.01 (ddd, *J* = 14.5, 5.8, 0.8 Hz, 1H), 2.91 (ddd, *J* = 14.5, 7.2, 0.6 Hz, 1H), 2.74 – 2.57 (m, 2H), 1.67 – 1.57 (m, 1H), 1.49 – 1.37 (m, 1H), 1.31 (d, *J* = 6.5 Hz, 3H), 0.79 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 136.35, 127.48, 123.02, 122.42, 119.84, 118.86, 111.67, 111.30, 54.97, 50.50, 33.56, 22.66, 17.18, 12.72; **HRMS (**ESI) *m/z* calcd for $C_{14}H_{21}O_2N_2S$ $[M+H]^+$ 281.1324, found 281.1310.

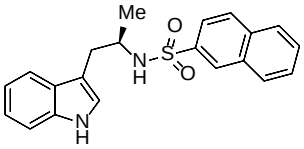
(*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)-4-methylbenzenesulfonamide (28a)



The title compound was prepared from (*R*)-1-(1H-indol-3-yl)propan-2-amine (100 mg, 0.57 mmol) and 4-methylbenzenesulfonyl chloride (164 mg, 0.86 mmol) according to the general sulfonylation procedure and was obtained as a white solid (179 mg, 95% yield); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.12 (s, 1H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.32 – 7.26 (m, 2H), 7.17 – 7.11 (m, 1H), 7.04 (d, *J* = 8.0 Hz, 2H), 6.99 (t, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 1.8 Hz, 1H), 4.68 (dd, *J* = 16.9, 6.1 Hz, 1H), 3.53 (hept, *J* = 6.5 Hz, 1H), 2.86 – 2.73 (m, 2H), 2.31 (s, 3H), 1.15 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ

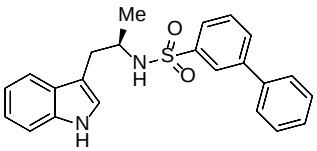
142.97, 137.01, 136.31, 129.36, 127.26, 126.75, 123.06, 121.94, 119.38, 118.65, 111.23, 111.06, 49.88, 33.04, 21.70, 21.45; **HRMS (**ESI) *m/z* calcd for $C_{18}H_{21}N_2O_2S$ $[M+H]^+$ 329.1324, found 329.1313.

(*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)naphthalene-2-sulfonamide (29a)



The title compound was prepared from (*R*)-1-(1H-indol-3-yl)propan-2-amine (100 mg, 0.57 mmol) and naphthalene-2-sulfonyl chloride (195 mg, 0.86 mmol) according to the general sulfonylation procedure and was obtained as a white solid (210 mg, >95% yield); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.27 (d, *J* = 1.6 Hz, 1H), 7.92 (s, 1H), 7.86 – 7.77 (m, 2H), 7.67 (d, *J* = 8.7 Hz, 1H), 7.63 – 7.48 (m, 3H), 7.23 – 7.17 (m, 2H), 7.03 (ddd, *J* = 8.1, 7.1, 1.1 Hz, 1H), 6.86 (d, *J* = 2.3 Hz, 1H), 6.82 (ddd, *J* = 8.0, 7.1, 1.0 Hz, 1H), 4.70 (d, *J* = 6.6 Hz, 1H), 3.63 (hept, *J* = 6.5 Hz, 1H), 2.87 – 2.75 (m, 2H), 1.18 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 136.95, 136.13, 134.57, 131.96, 129.17, 128.50, 128.12, 127.84, 127.29, 127.17, 122.92, 122.10, 121.97, 119.41, 118.46, 111.09, 50.18, 33.04, 21.90; **HRMS (**ESI) *m/z* calcd for $C_{21}H_{21}N_2O_2S$ $[M+H]^+$ 365.1324, found 365.1313.

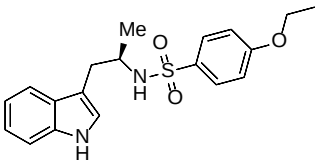
(*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)-[1,1'-biphenyl]-3-sulfonamide (30a)



The title compound was prepared from (*R*)-1-(1H-indol-3-yl)propan-2-amine (100 mg, 0.57 mmol) and [1,1'-biphenyl]-3-sulfonyl chloride (217 mg, 0.86 mmol) according to the general sulfonylation procedure and was obtained as a white solid (172 mg, 77% yield); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.94 (dt, *J* = 1.8, 0.9 Hz, 2H), 7.60 (dddd, *J* = 14.5, 7.8, 1.8, 1.1 Hz, 2H), 7.54 – 7.50 (m, 2H), 7.46 – 7.41 (m, 2H), 7.40 – 7.35 (m, 1H), 7.34 – 7.28 (m, 2H), 7.23 – 7.20 (m, 1H), 7.10 (ddd, *J* = 8.2, 7.0, 1.1 Hz, 1H), 6.96 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 6.86 (d, *J* = 2.4 Hz, 1H), 4.72 (d, *J* = 6.6 Hz, 1H), 3.61 (hept, *J* = 6.5 Hz, 1H), 2.90 – 2.75 (m, 2H), 1.18 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 141.79, 140.71, 139.18, 136.15, 130.75, 129.24, 128.96, 128.11, 127.26, 127.09, 125.34,

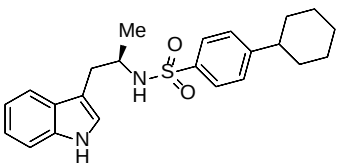
125.23, 122.98, 122.01, 119.49, 118.49, 111.23, 110.98, 50.22, 32.98, 21.78; **HRMS (**ESI) *m/z* calcd for $C_{23}H_{23}N_2O_2S$ $[M+H]^+$ 391.1480, found 391.1468.

(*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)-4-ethoxybenzenesulfonamide (31a)



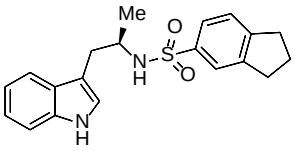
The title compound was prepared from (*R*)-1-(1H-indol-3-yl)propan-2-amine (100 mg, 0.57 mmol) and 4-ethoxybenzenesulfonyl chloride (190 mg, 0.86 mmol) according to the general sulfonylation procedure and was obtained as a white solid (198 mg, 96% yield); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.02 (s, 1H), 7.57 – 7.50 (m, 2H), 7.38 – 7.29 (m, 2H), 7.19 – 7.13 (m, 1H), 7.03 (ddd, *J* = 8.0, 7.1, 1.0 Hz, 1H), 6.94 (d, *J* = 2.3 Hz, 1H), 6.77 – 6.69 (m, 2H), 4.37 (d, *J* = 6.4 Hz, 1H), 4.02 (q, *J* = 7.0 Hz, 2H), 3.55 (hept, *J* = 6.5 Hz, 1H), 2.91 – 2.76 (m, 2H), 1.44 (t, *J* = 7.0 Hz, 3H), 1.18 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.94, 136.30, 131.49, 128.86, 127.35, 122.89, 122.15, 119.56, 118.78, 114.29, 111.30, 111.13, 63.79, 49.83, 33.06, 21.79, 14.65; **HRMS (**ESI) *m/z* calcd for $C_{19}H_{23}N_2O_3S$ $[M+H]^+$ 359.1429, found 359.1420.

(*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)-4-cyclohexylbenzenesulfonamide (32a)



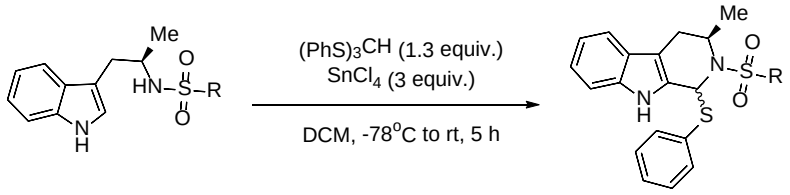
The title compound was prepared from (*R*)-1-(1H-indol-3-yl)propan-2-amine (100 mg, 0.57 mmol) and 4-cyclohexylbenzenesulfonyl chloride (223 mg, 0.86 mmol) according to the general sulfonylation procedure and was obtained as a white solid (219 mg, 96% yield); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.09 (s, 1H), 7.60 – 7.54 (m, 2H), 7.37 – 7.28 (m, 2H), 7.19 – 7.11 (m, 3H), 7.02 (ddd, *J* = 8.0, 7.1, 1.0 Hz, 1H), 6.91 (d, *J* = 2.3 Hz, 1H), 4.62 (d, *J* = 6.7 Hz, 1H), 3.57 (hept, *J* = 6.5 Hz, 1H), 2.83 (d, *J* = 6.4 Hz, 2H), 2.55 – 2.44 (m, 1H), 1.90 – 1.80 (m, 4H), 1.79 – 1.72 (m, 1H), 1.46 – 1.31 (m, 4H), 1.30 – 1.22 (m, 1H), 1.13 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 152.89, 137.51, 136.26, 127.42, 127.29, 126.96, 123.06, 122.08, 119.51, 118.72, 111.21, 111.16, 49.95, 44.40, 34.13, 34.03, 33.03, 26.66, 25.97, 21.54; **HRMS (**ESI) *m/z* calcd for $C_{23}H_{29}N_2O_2S$ $[M+H]^+$ 397.1950, found 397.1940.

(*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)-2,3-dihydro-1H-indene-5-sulfonamide (33a)



The title compound was prepared from (*R*)-1-(1H-indol-3-yl)propan-2-amine (100 mg, 0.57 mmol) and 2,3-dihydro-1H-indene-5-sulfonyl chloride (187 mg, 0.86 mmol) according to the general sulfonylation procedure and was obtained as a white solid (199 mg, 98% yield); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.02 (s, 1H), 7.52 – 7.48 (m, 1H), 7.43 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.32 (ddt, *J* = 8.2, 3.0, 0.7 Hz, 2H), 7.20 – 7.08 (m, 2H), 7.01 (ddd, *J* = 7.9, 7.1, 1.0 Hz, 1H), 6.95 (d, *J* = 2.3 Hz, 1H), 4.41 (d, *J* = 6.3 Hz, 1H), 3.57 (hept, *J* = 6.4 Hz, 1H), 2.92 – 2.80 (m, 6H), 2.08 (p, *J* = 7.5 Hz, 2H), 1.18 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 149.37, 145.16, 137.86, 136.29, 127.31, 125.10, 124.51, 122.96, 122.77, 122.13, 119.48, 118.74, 111.27, 111.11, 49.81, 33.11, 32.78, 32.54, 25.24, 21.75; **HRMS (**ESI) *m/z* calcd for $C_{20}H_{23}N_2O_2S$ $[M+H]^+$ 355.1480, found 355.1469.

General procedure for the synthesis of *N,S*-sulfonyl acetals

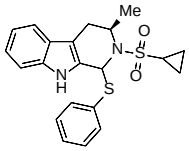


Scheme S2: General depiction for the synthesis of *N,S*-sulfonyl acetals

A 11 dram scintillation vial equipped with a Teflon-coated magnetic stir bar was charged with appropriate sulfonamide, tris(phenylthio)methane (1.3 equiv.) and dichloromethane (5.0 mL). The solution was cooled to -78°C in a dry ice/acetone bath, and Tin(IV) chloride (1.0 M in DCM) (3 equiv.) was added. The resulting solution was allowed to warm to room temperature and stir for 5 hours. Cold aq. $NaHCO_3$ (20 mL) was added, and the biphasic mixture was extracted with dichloromethane (10 mL) twice. The combined organic layer was dried over Na_2SO_4 and filtered. The filtrate was concentrated in vacuo, and the resulting oil was purified by silica gel column chromatography using a gradient solvent system (0 → 30% iPrOAc/Heptane) as the eluent. Attempts were made to purify this product via silica gel chromatography, but were proved to be unsuccessful due to the thermal instability and instability of the compound on silica gel. In the interest of completeness, *N,S*-sulfonyl acetals were characterized by ^{1}H NMR (~90% purity) and HRMS. The resulting product was thus used in subsequent step without further purification. To prevent decomposition during prolonged storage, all *N,S*-acetals were kept at –20 °C.

Characterization of *N,S*-sulfonyl acetals

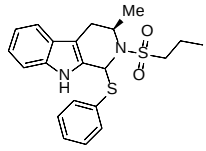
(3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (9)



The title compound was prepared from (*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)cyclopropanesulfonamide (**9a**) (50 mg, 0.18 mmol) according to the general *N,S*-sulfonyl acetal synthesis procedure and was obtained as a white solid (53 mg,

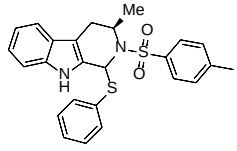
72% yield); **^{1}H NMR** (major diastereomer, ~90% purity) (400 MHz, Chloroform-*d*) δ 7.79 – 7.74 (m, 2H), 7.67 (s, 1H), 7.49 – 7.36 (m, 4H), 7.28 (d, *J* = 8.1 Hz, 1H), 7.23 – 7.18 (m, 1H), 7.12 (td, *J* = 7.5, 7.1, 1.0 Hz, 1H), 6.67 (d, *J* = 1.7 Hz, 1H), 4.60 (p, *J* = 7.2 Hz, 1H), 3.14 (ddd, *J* = 15.7, 6.3, 1.5 Hz, 1H), 2.75 (d, *J* = 15.7 Hz, 1H), 2.53 (tt, *J* = 8.0, 4.9 Hz, 1H), 1.53 (d, *J* = 7.2 Hz, 3H), 1.30 (ddd, *J* = 10.5, 4.8, 2.0 Hz, 1H), 1.23 – 1.17 (m, 1H), 1.02 – 0.96 (m, 2H); **HRMS (**ESI) *m/z* calcd for $C_{21}H_{23}N_2O_2S_2$ $[M+H]^+$ 399.1201, found 399.1187.

(3*R*)-3-methyl-1-(phenylthio)-2-(propylsulfonyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (27b)



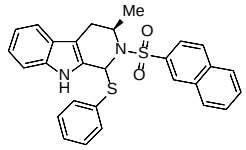
The title compound was prepared from (*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)propane-1-sulfonamide (**27a**) (51 mg, 0.18 mmol) according to the general *N,S*-sulfonyl acetal synthesis procedure and was obtained as a white solid (17 mg, 23% yield); ^{1}H NMR (major diastereomer, ~90% purity) (400 MHz, Chloroform-*d*) δ 7.74 – 7.70 (m, 2H), 7.47 (d, *J* = 7.9 Hz, 1H), 7.45 – 7.38 (m, 3H), 7.27 – 7.26 (m, 1H), 7.22 – 7.17 (m, 1H), 7.14 – 7.08 (m, 1H), 6.74 – 6.71 (m, 1H), 4.69 – 4.56 (m, 1H), 3.13 – 3.07 (m, 1H), 3.01 – 2.85 (m, 2H), 2.75 (d, *J* = 15.9 Hz, 1H), 1.90 – 1.74 (m, 2H), 1.51 (d, *J* = 7.1 Hz, 3H), 0.99 (t, *J* = 7.5 Hz, 3H); **HRMS (**ESI) *m/z* calcd for $C_{21}H_{25}N_2O_2S_2$ $[M+H]^+$ 401.1357, found 401.1337.

(3*R*)-3-methyl-1-(phenylthio)-2-tosyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (28b)



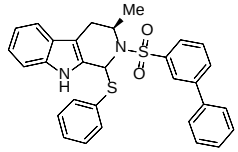
The title compound was prepared from (*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)-4-methylbenzenesulfonamide (**28a**) (1.50 g, 4.6 mmol) according to the general *N,S*-sulfonyl acetal synthesis procedure and was obtained as a white solid (1.36 g, 66% yield); **^{1}H NMR** (major diastereomer, ~90% purity) (400 MHz, Chloroform-*d*) δ 7.82 – 7.77 (m, 2H), 7.69 (d, *J* = 8.3 Hz, 2H), 7.49 – 7.38 (m, 4H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.23 – 7.17 (m, 3H), 7.11 – 7.07 (m, 1H), 6.83 (d, *J* = 1.6 Hz, 1H), 4.46 (p, *J* = 6.7 Hz, 1H), 2.67 (ddd, *J* = 15.6, 6.1, 1.5 Hz, 1H), 2.54 (d, *J* = 15.5 Hz, 1H), 2.37 (s, 3H), 1.34 (d, *J* = 7.0 Hz, 3H); **HRMS (**ESI) *m/z* calcd for $C_{25}H_{25}N_2O_2S_2$ $[M+H]^+$ 449.1357, found 449.1340.

(3*R*)-3-methyl-2-(naphthalen-2-ylsulfonyl)-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (29b)



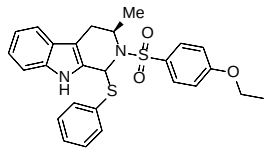
The title compound was prepared from (*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)naphthalene-2-sulfonamide (**29a**) (86 mg, 0.24 mmol) according to the general *N*,*S*-sulfonyl acetal synthesis procedure and was obtained as a white solid (63 mg, 55% yield); **^{1}H NMR** (major diastereomer, ~90% purity) (400 MHz, Chloroform-*d*) δ 8.43 (d, *J* = 1.6 Hz, 1H), 7.93 – 7.88 (m, 1H), 7.87 – 7.82 (m, 2H), 7.80 (dt, *J* = 5.9, 1.4 Hz, 3H), 7.71 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.63 – 7.56 (m, 2H), 7.49 – 7.40 (m, 3H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 7.22 – 7.16 (m, 1H), 7.10 – 7.05 (m, 1H), 6.96 – 6.90 (m, 1H), 4.53 (p, *J* = 6.8 Hz, 1H), 2.68 (ddd, *J* = 15.6, 6.1, 1.7 Hz, 1H), 2.54 (d, *J* = 15.6 Hz, 1H), 1.35 (d, *J* = 7.0 Hz, 3H); **HRMS (**ESI) *m/z* calcd for $C_{28}H_{25}N_2O_2S_2$ $[M+H]^+$ 485.1357, found 485.1338.

(3*R*)-2-([1,1'-biphenyl]-3-ylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (30b)



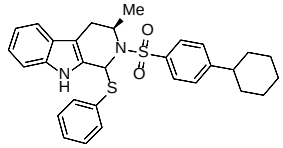
The title compound was prepared from (*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)-[1,1'-biphenyl]-3-sulfonamide (**30a**) (980 mg, 2.5 mmol) according to the general *N*,*S*-sulfonyl acetal synthesis procedure and was obtained as a white solid (487 mg, 38% yield); **^{1}H NMR** (major diastereomer, ~90% purity) (400 MHz, Chloroform-*d*) δ 8.01 (t, *J* = 1.7 Hz, 1H), 7.82 (s, 1H), 7.78 (ddt, *J* = 7.9, 3.0, 1.2 Hz, 3H), 7.71 (ddd, *J* = 7.8, 1.7, 1.1 Hz, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 1.5 Hz, 1H), 7.42 – 7.39 (m, 2H), 7.39 – 7.35 (m, 3H), 7.33 – 7.32 (m, 2H), 7.30 – 7.28 (m, 1H), 7.22 – 7.18 (m, 1H), 7.10 – 7.07 (m, 1H), 6.90 (d, *J* = 1.6 Hz, 1H), 4.54 (p, *J* = 6.8 Hz, 1H), 2.71 (ddd, *J* = 15.7, 6.2, 1.6 Hz, 1H), 2.57 (d, *J* = 15.5 Hz, 1H), 1.39 (d, *J* = 7.0 Hz, 3H); **HRMS (**ESI) *m/z* calcd for $C_{30}H_{27}N_2O_2S_2$ $[M+H]^+$ 511.1514, found 511.1497.

(3*R*)-2-((4-ethoxyphenyl)sulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (31b)



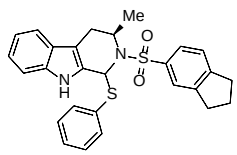
The title compound was prepared from (*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)-4-ethoxybenzenesulfonamide (**31a**) (150 mg, 0.42 mmol) according to the general *N*,*S*-sulfonyl acetal synthesis procedure and was obtained as a white solid (172 mg, 86% yield); **^{1}H NMR** (major diastereomer, ~90% purity) (400 MHz, Chloroform-*d*) δ 7.83 – 7.77 (m, 2H), 7.75 – 7.71 (m, 2H), 7.49 – 7.43 (m, 2H), 7.40 (d, *J* = 7.7 Hz, 1H), 7.28 (d, *J* = 8.1 Hz, 1H), 7.22 – 7.16 (m, 1H), 7.11 – 7.06 (m, 1H), 6.88 – 6.84 (m, 2H), 6.84 – 6.82 (m, 1H), 4.44 (p, *J* = 6.9 Hz, 1H), 4.04 (q, *J* = 7.0 Hz, 2H), 2.76 – 2.66 (m, 1H), 2.55 (d, *J* = 15.6 Hz, 1H), 1.41 (t, *J* = 7.0 Hz, 3H), 1.32 (d, *J* = 7.0 Hz, 3H); **HRMS (**ESI) *m/z* calcd for $C_{26}H_{27}N_2O_3S_2$ $[M+H]^+$ 479.1463, found 479.1444.

(3*R*)-2-((4-cyclohexylphenyl)sulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (32b)



The title compound was prepared from (*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)-4-cyclohexylbenzenesulfonamide (**32a**) (1.08 g, 2.7 mmol) according to the general *N*,*S*-sulfonyl acetal synthesis procedure and was obtained as a white solid (680 mg, 48% yield); **^{1}H NMR** (major diastereomer, ~90% purity) (400 MHz, Chloroform-*d*) δ 7.77 (dt, *J* = 5.7, 1.5 Hz, 2H), 7.73 – 7.68 (m, 2H), 7.48 – 7.37 (m, 4H), 7.29 (dt, *J* = 8.2, 0.8 Hz, 1H), 7.24 – 7.21 (m, 2H), 7.19 (ddd, *J* = 8.2, 7.1, 1.1 Hz, 1H), 7.08 (ddd, *J* = 8.0, 7.1, 1.0 Hz, 1H), 6.84 (d, *J* = 1.6 Hz, 1H), 4.45 (p, *J* = 6.4 Hz, 1H), 2.67 (ddd, *J* = 15.6, 6.1, 1.6 Hz, 1H), 2.58 – 2.54 (m, 1H), 2.54 – 2.47 (m, 1H), 1.89 – 1.69 (m, 6H), 1.37 (t, *J* = 8.1 Hz, 3H), 1.33 (d, *J* = 7.0 Hz, 3H), 1.27 – 1.19 (m, 1H); **HRMS (**ESI) *m/z* calcd for $C_{30}H_{33}N_2O_2S_2$ $[M+H]^+$ 517.1983, found 517.1970.

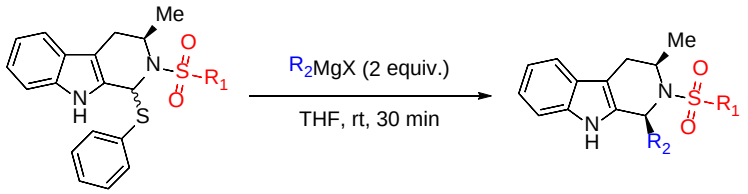
(3*R*)-2-((2,3-dihydro-1H-inden-5-yl)sulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (33b)



The title compound was prepared from (*R*)-N-(1-(1H-indol-3-yl)propan-2-yl)-2,3-dihydro-1H-indene-5-sulfonamide (**33a**) (800 mg, 2.3 mmol)

according to the general *N*,*S*-sulfonyl acetal synthesis procedure and was obtained as a white solid (624 mg, 58% yield); **^{1}H NMR** (major diastereomer, ~90% purity) (400 MHz, Chloroform-*d*) δ 7.80 – 7.77 (m, 2H), 7.67 – 7.59 (m, 1H), 7.56 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.48 – 7.36 (m, 4H), 7.30 – 7.26 (m, 1H), 7.22 – 7.15 (m, 2H), 7.08 (ddd, *J* = 8.0, 7.2, 1.0 Hz, 1H), 6.86 – 6.81 (m, 1H), 4.46 (p, *J* = 6.7 Hz, 1H), 2.87 (dt, *J* = 20.5, 7.2 Hz, 4H), 2.69 (ddd, *J* = 15.6, 6.2, 1.6 Hz, 1H), 2.54 (d, *J* = 15.6 Hz, 1H), 2.07 (p, *J* = 7.3 Hz, 2H), 1.35 (d, *J* = 7.0 Hz, 3H); **HRMS (**ESI) *m/z* calcd for $C_{27}H_{27}N_2O_2S_2$ $[M+H]^+$ 475.1514, found 475.1496.

General procedure for the synthesis of 1,3-substituted *cis*-tetrahydro-β-carbolines

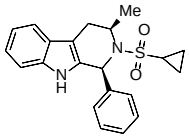


Scheme S3: General depiction of the synthesis of 1,3-substituted *cis*-tetrahydro-β-carbolines

A flame-dried 100 mL Schlenk flask equipped with a Teflon-coated magnetic stir bar under N_2 was charged with appropriate *N*,*S*-acetal and anhydrous THF (20 mL). Grignard reagent of appropriate nucleophile (2 equiv.) was added at room temperature. The resulting solution was allowed to stir for 30 minutes. H_2O (10 mL) was added, and the biphasic mixture was extracted with dichloromethane (10 mL) twice. The combined organic layer was dried over Na_2SO_4 and filtered. The filtrate was concentrated in vacuo, and the resulting oil was purified by silica gel column chromatography using a gradient solvent system (0 → 40% iPrOAc/Heptane) as the eluent. The pure product was thus obtained as white soild. To prevent decomposition during prolonged storage, all tetrahydro-β-carbolines were kept at –20 °C.

Characterization of tetrahydro-β-carbolines

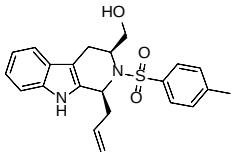
(1*S*,3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-phenyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (10)



The title compound was prepared from (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (46 mg, 0.12 mmol) and phenylmagnesium chloride (2.0 M, 0.12 mL, 0.23 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (34 mg, 80% yield); **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.91 (s, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.50 – 7.48 (m, 2H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.35 – 7.29 (m, 3H), 7.26 –

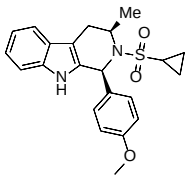
7.23 (m, 1H), 7.20 – 7.16 (m, 1H), 6.29 (s, 1H), 4.64 (p, *J* = 7.1 Hz, 1H), 3.27 (ddd, *J* = 15.8, 6.8, 1.8 Hz, 1H), 2.78 (d, *J* = 15.8 Hz, 1H), 2.12 (tt, *J* = 8.0, 4.9 Hz, 1H), 1.22 (ddd, *J* = 10.9, 6.1, 3.3 Hz, 1H), 1.19 – 1.13 (m, 1H), 1.07 (d, *J* = 7.2 Hz, 3H), 0.90 – 0.84 (m, 1H), 0.81 (tdd, *J* = 9.0, 6.5, 4.7 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 140.48, 136.29, 129.19, 128.56, 128.50, 128.05, 127.36, 122.62, 119.81, 118.46, 111.10, 107.94, 54.03, 48.70, 30.08, 26.73, 22.48, 5.59, 5.30; **HRMS (**ESI) *m/z* calcd for $C_{21}H_{23}N_2O_2S$ $[M+H]^+$ 367.1480, found 367.1473.

((1*S*,3*S*)-1-allyl-2-tosyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indol-3-yl)methanol (12)



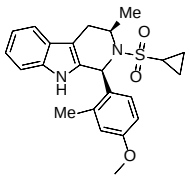
A flame-dried 100 mL Schlenk flask equipped with a Teflon-coated magnetic stir bar under N_2 was charged with ethyl (1*S*,3*S*)-1-allyl-2-tosyl -2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (120 mg, 0.27 mmol) and anhydrous THF (20 mL). Lithium borohydride (4 equiv.) was added at room temperature. The resulting solution was allowed to stir at room temperature for 15 hours. Methanol (10 mL) and H_2O (10 mL) were added, and the biphasic mixture was extracted with dichloromethane (10 mL) twice. The combined organic layer was dried over Na_2SO_4 and filtered. The filtrate was concentrated in vacuo, and the resulting oil was purified by silica gel column chromatography using a gradient solvent system (0 → 50% iPrOAc/Heptane) as the eluent to afford a white solid (83 mg, 76% yield); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.09 (s, 1H), 7.67 (d, *J* = 8.3 Hz, 2H), 7.32 (dd, *J* = 18.7, 8.0 Hz, 2H), 7.22 – 7.12 (m, 3H), 7.12 – 7.01 (m, 1H), 6.20 (dddd, *J* = 16.9, 10.3, 8.4, 5.9 Hz, 1H), 5.41 – 5.20 (m, 3H), 4.39 (q, *J* = 6.8 Hz, 1H), 3.62 (dtd, *J* = 17.4, 10.9, 4.2 Hz, 2H), 3.00 – 2.88 (m, 1H), 2.70 (dt, *J* = 14.0, 8.6 Hz, 1H), 2.61 (d, *J* = 16.0 Hz, 1H), 2.38 (ddd, *J* = 16.1, 6.8, 1.9 Hz, 1H), 2.34 (s, 3H), 2.13 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.70, 137.47, 136.00, 135.43, 131.09, 129.88, 126.78, 126.41, 122.33, 119.61, 119.43, 118.16, 111.02, 105.42, 63.59, 53.69, 51.79, 43.80, 21.47, 20.51; **HRMS (**ESI) *m/z* calcd for $C_{22}H_{25}N_2O_3S$ $[M+H]^+$ 397.1586, found 397.1572.

(1*S*,3*R*)-2-(cyclopropylsulfonyl)-1-(4-methoxyphenyl)-3-methyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (13)



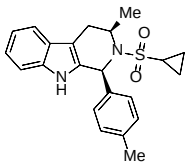
The title compound was prepared from (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (30 mg, 0.08 mmol) and 4-methoxyphenylmagnesium bromide (0.5 M, 0.3 mL, 0.15 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (25 mg, 84% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 11.03 (s, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.27 (d, *J* = 8.8 Hz, 2H), 7.14 – 7.09 (m, 1H), 7.04 – 6.99 (m, 1H), 6.93 – 6.89 (m, 2H), 6.14 (s, 1H), 4.50 (p, *J* = 7.1 Hz, 1H), 3.73 (s, 3H), 3.23 – 3.14 (m, 1H), 2.69 (d, *J* = 15.8 Hz, 1H), 2.44 (tt, *J* = 7.8, 4.9 Hz, 1H), 1.01 (qd, *J* = 8.9, 7.6, 3.6 Hz, 1H), 0.91 (d, *J* = 7.2 Hz, 3H), 0.90 – 0.85 (m, 2H), 0.77 – 0.69 (m, 1H); **^{13}C NMR** (126 MHz, DMSO) δ 158.39, 136.20, 133.24, 129.54, 129.03, 126.77, 121.30, 118.37, 117.88, 113.35, 111.13, 105.56, 54.96, 52.73, 47.79, 29.16, 25.91, 22.20, 4.76, 4.51; **HRMS (**ESI) *m/z* calcd for $C_{22}H_{25}N_2O_3S$ $[M+H]^+$ 397.1586, found 397.1571.

(1*S*,3*R*)-2-(cyclopropylsulfonyl)-1-(4-methoxy-2-methylphenyl)-3-methyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (14)



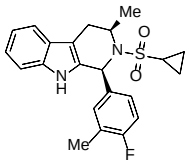
The title compound was prepared from (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (120 mg, 0.30 mmol) and 4-methoxy-2-methyl-phenylmagnesium bromide (0.5 M, 1.0 mL, 0.60 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (106 mg, 86% yield); **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.59 (s, 1H), 7.54 (d, *J* = 7.7 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 7.21 – 7.12 (m, 2H), 6.89 (d, *J* = 8.7 Hz, 1H), 6.79 (d, *J* = 2.7 Hz, 1H), 6.61 (dd, *J* = 8.6, 2.8 Hz, 1H), 6.33 (d, *J* = 1.6 Hz, 1H), 4.69 (td, *J* = 6.9, 1.0 Hz, 1H), 3.78 (s, 3H), 3.28 (ddd, *J* = 15.7, 6.9, 1.8 Hz, 1H), 2.80 (d, *J* = 15.9 Hz, 1H), 2.63 (s, 3H), 1.97 (tt, *J* = 8.1, 5.0 Hz, 1H), 1.23 (d, *J* = 7.1 Hz, 3H), 1.13 – 1.04 (m, 2H), 0.81 – 0.68 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.11, 139.08, 136.15, 131.64, 130.30, 127.46, 122.22, 119.75, 118.26, 116.29, 111.58, 111.14, 107.15, 55.19, 52.60, 48.71, 30.44, 27.19, 23.72, 20.40, 5.64, 5.34; **HRMS (**ESI) *m/z* calcd for $C_{23}H_{27}N_2O_3S$ $[M+H]^+$ 411.1742, found 411.1723.

(1*S*,3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(p-tolyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (15)



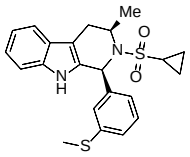
The title compound was prepared from (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (60 mg, 0.15 mmol) and *p*-tolylmagnesium bromide (1.0 M, 0.30 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (55 mg, 96% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 11.04 (s, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.26 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.13 – 7.09 (m, 1H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.15 (s, 1H), 4.51 (p, *J* = 7.1 Hz, 1H), 3.24 – 3.15 (m, 1H), 2.68 (d, *J* = 15.9 Hz, 1H), 2.44 (tt, *J* = 7.8, 5.0 Hz, 1H), 2.29 (s, 3H), 1.05 – 0.98 (m, 1H), 0.89 (d, *J* = 7.1 Hz, 3H), 0.89 – 0.84 (m, 2H), 0.72 (ddd, *J* = 10.8, 7.0, 4.3 Hz, 1H); **^{13}C NMR** (126 MHz, DMSO) δ 139.02, 137.04, 136.79, 129.98, 129.17, 128.28, 127.35, 121.89, 118.96, 118.48, 111.74, 106.15, 53.51, 48.48, 29.72, 26.49, 22.82, 21.13, 5.36, 5.10; **HRMS (**ESI) *m/z* calcd for $C_{22}H_{25}N_2O_2S$ $[M+H]^+$ 381.1637, found 381.1627.

(1*S*,3*R*)-2-(cyclopropylsulfonyl)-1-(4-fluoro-3-methylphenyl)-3-methyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (16)



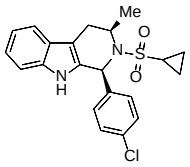
The title compound was prepared from (3R)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (60 mg, 0.15 mmol) and 4-fluoro-3-methylphenyl magnesium bromide (1.0 M, 0.30 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (58 mg, 97% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 11.04 (s, 1H), 7.49 (d, *J* = 7.8 Hz, 1H), 7.37 (d, *J* = 8.1 Hz, 1H), 7.26 (dd, *J* = 7.4, 1.9 Hz, 1H), 7.20 (ddd, *J* = 7.5, 5.0, 2.2 Hz, 1H), 7.17 – 7.09 (m, 2H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.14 (s, 1H), 4.52 (p, *J* = 7.1 Hz, 1H), 3.24 – 3.16 (m, 1H), 2.69 (d, *J* = 15.9 Hz, 1H), 2.46 (ddd, *J* = 7.8, 5.0, 2.8 Hz, 1H), 2.24 – 2.17 (m, 3H), 1.02 (tq, *J* = 10.4, 3.7 Hz, 1H), 0.92 (d, *J* = 7.1 Hz, 3H), 0.88 (ddd, *J* = 8.6, 6.3, 2.6 Hz, 2H), 0.73 (ddd, *J* = 10.8, 7.4, 3.9 Hz, 1H); **^{13}C NMR** (126 MHz, DMSO) δ 161.34, 159.49, 137.93, 136.84, 131.43, 129.69, 127.83, 127.33, 124.22, 124.08, 122.01, 119.04, 118.55, 115.21, 115.03, 111.83, 106.31, 53.19, 48.49, 40.28, 29.66, 26.44, 22.83, 14.80, 5.36, 5.09; **HRMS (**ESI) *m/z* calcd for $C_{22}H_{24}FN_2O_2S$ $[M+H]^+$ 399.1543, found 399.1528.

(1*S*,3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(3-(methylthio)phenyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (17)



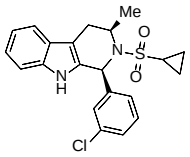
The title compound was prepared from (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (60 mg, 0.15 mmol) and 3-thioanisolemagnesium bromide (0.5 M, 0.60 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (55 mg, 89% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 11.06 (s, 1H), 7.49 (d, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.32 (t, *J* = 7.8 Hz, 1H), 7.29 (s, 1H), 7.20 (d, *J* = 8.0 Hz, 1H), 7.16 – 7.10 (m, 2H), 7.05 – 7.01 (m, 1H), 6.15 (s, 1H), 4.53 (p, *J* = 7.1 Hz, 1H), 3.24 – 3.17 (m, 1H), 2.69 (d, *J* = 15.9 Hz, 1H), 2.49 – 2.45 (m, 1H), 2.42 (s, 3H), 1.02 (ddp, *J* = 13.1, 8.1, 4.4 Hz, 1H), 0.91 (d, *J* = 7.2 Hz, 3H), 0.88 (dq, *J* = 10.5, 3.8, 3.3 Hz, 2H), 0.73 (ddd, *J* = 10.8, 7.0, 4.1 Hz, 1H); **^{13}C NMR** (126 MHz, DMSO) δ 142.79, 138.40, 136.81, 129.44, 129.35, 127.29, 125.95, 125.28, 124.91, 122.04, 119.04, 118.56, 111.78, 106.34, 53.57, 48.56, 29.66, 26.43, 22.79, 15.20, 5.37, 5.09; **HRMS (**ESI) *m/z* calcd for $C_{22}H_{25}N_2O_2S_2$ $[M+H]^+$ 413.1357, found 413.1346.

(1*S*,3*R*)-1-(4-chlorophenyl)-2-(cyclopropylsulfonyl)-3-methyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (18)



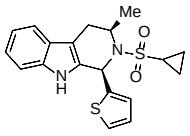
The title compound was prepared from (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (60 mg, 0.15 mmol) and 3-chlorophenylmagnesium bromide (0.5 M, 0.60 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (56 mg, 93% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 11.05 (s, 1H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.46 – 7.41 (m, 2H), 7.41 – 7.36 (m, 3H), 7.15 – 7.10 (m, 1H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.17 (s, 1H), 4.53 (p, *J* = 7.1 Hz, 1H), 3.24 – 3.17 (m, 1H), 2.69 (d, *J* = 15.9 Hz, 1H), 2.50 – 2.45 (m, 1H), 1.02 (dq, *J* = 9.4, 4.5 Hz, 1H), 0.95 – 0.89 (m, 2H), 0.89 (d, *J* = 7.2 Hz, 3H), 0.77 – 0.71 (m, 1H); **^{13}C NMR** (126 MHz, DMSO) δ 141.12, 136.83, 132.54, 130.20, 129.27, 128.66, 127.31, 122.08, 119.08, 118.58, 111.82, 106.42, 53.13, 48.54, 29.66, 26.39, 22.80, 5.38, 5.10; **HRMS (**ESI) *m/z* calcd for $C_{21}H_{22}ClN_2O_2S$ $[M+H]^+$ 401.1091, found 401.1077.

(1*S*,3*R*)-1-(3-chlorophenyl)-2-(cyclopropylsulfonyl)-3-methyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (19)



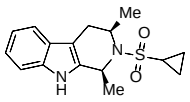
The title compound was prepared from (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (60 mg, 0.15 mmol) and 3-chlorophenylmagnesium bromide (0.5 M, 0.60 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (59 mg, 98% yield); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.08 (s, 1H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.40 (dt, *J* = 8.5, 3.9 Hz, 4H), 7.34 (d, *J* = 7.2 Hz, 1H), 7.16 – 7.12 (m, 1H), 7.03 (t, *J* = 7.3 Hz, 1H), 6.18 (s, 1H), 4.54 (p, *J* = 7.1 Hz, 1H), 3.24 – 3.18 (m, 1H), 2.70 (d, *J* = 16.0 Hz, 1H), 2.55 – 2.51 (m, 1H), 1.06 – 1.00 (m, 1H), 0.95 – 0.90 (m, 2H), 0.89 (d, *J* = 7.1 Hz, 3H), 0.74 (ddd, *J* = 11.2, 7.6, 4.3 Hz, 1H); **^{13}C NMR** (126 MHz, DMSO) δ 144.69, 136.84, 133.33, 130.66, 128.93, 128.03, 127.97, 127.27, 126.97, 122.16, 119.13, 118.64, 111.87, 106.54, 53.24, 48.58, 29.61, 26.35, 22.80, 5.39, 5.09; **HRMS (**ESI) *m/z* calcd for $C_{21}H_{22}ClN_2O_2S$ $[M+H]^+$ 401.1091, found 401.1076.

(1*R*,3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(thiophen-2-yl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (20)



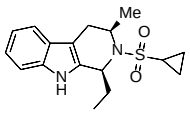
The title compound was prepared from (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (60 mg, 0.15 mmol) and 2-thienylmagnesium bromide (1.0 M, 0.30 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (51 mg, 91% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 11.12 (s, 1H), 7.50 (dd, *J* = 13.9, 6.4 Hz, 2H), 7.37 (d, *J* = 8.1 Hz, 1H), 7.12 (t, *J* = 7.5 Hz, 1H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.98 – 6.94 (m, 1H), 6.92 (d, *J* = 3.5 Hz, 1H), 6.38 (s, 1H), 4.54 (p, *J* = 7.0 Hz, 1H), 3.18 – 3.11 (m, 1H), 2.72 (d, *J* = 15.7 Hz, 1H), 2.55 (tt, *J* = 7.6, 5.2 Hz, 1H), 1.08 (d, *J* = 7.1 Hz, 3H), 1.05 – 0.99 (m, 1H), 0.96 – 0.89 (m, 2H), 0.81 (tt, *J* = 7.2, 3.0 Hz, 1H); **^{13}C NMR** (126 MHz, DMSO) δ 146.36, 136.81, 129.68, 127.10, 126.88, 126.85, 126.83, 122.08, 119.07, 118.59, 111.87, 105.85, 50.34, 48.48, 30.02, 26.66, 22.11, 5.38, 5.12; **HRMS (**ESI) *m/z* calcd for $C_{19}H_{21}N_2O_2S_2$ $[M+H]^+$ 373.1044, found 373.1033.

(1*S*,3*R*)-2-(cyclopropylsulfonyl)-1,3-dimethyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (21)



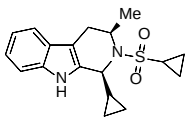
The title compound was prepared from (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (60 mg, 0.15 mmol) and methylmagnesium bromide (1.4 M, 0.22 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (43 mg, 94% yield); ^{1}H NMR (500 MHz, DMSO-*d*6) δ 10.98 (s, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.15 – 7.02 (m, 1H), 6.98 (td, *J* = 0.9, 7.6 Hz, 1H), 5.08 – 5.00 (m, 1H), 4.49 (p, *J* = 6.9 Hz, 1H), 2.98 (ddd, *J* = 1.6, 6.0, 15.3 Hz, 1H), 2.69 (d, *J* = 15.3 Hz, 1H), 2.62 (tt, *J* = 5.0, 7.8 Hz, 1H), 1.61 (d, *J* = 6.9 Hz, 3H), 1.25 (d, *J* = 7.0 Hz, 3H), 1.03 – 0.85 (m, 4H). **^{13}C NMR** (126 MHz, DMSO) δ 136.12, 132.71, 126.80, 120.91, 118.36, 117.65, 110.93, 103.40, 58.97, 47.52, 29.36, 26.30, 23.32, 22.12, 4.59, 4.50. **HRMS (**ESI) *m/z* calcd for $C_{16}H_{21}N_2O_2S$ $[M+H]^+$ 305.1324, found 305.1316.

(1*S*,3*R*)-2-(cyclopropylsulfonyl)-1-ethyl-3-methyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (22)



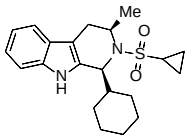
The title compound was prepared from (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (60 mg, 0.15 mmol) and ethylmagnesium bromide (1.0 M, 0.30 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (46 mg, 96% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.88 (s, 1H), 7.43 – 7.39 (m, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.06 (t, *J* = 7.1 Hz, 1H), 6.97 (t, *J* = 7.4 Hz, 1H), 4.86 (dd, *J* = 9.7, 4.8 Hz, 1H), 4.51 (p, *J* = 7.0 Hz, 1H), 3.13 – 3.07 (m, 1H), 2.65 (d, *J* = 15.6 Hz, 1H), 2.50 – 2.46 (m, 1H), 2.10 – 2.00 (m, 1H), 1.77 (ddq, *J* = 14.7, 10.1, 7.4 Hz, 1H), 1.28 (d, *J* = 7.1 Hz, 3H), 1.10 (t, *J* = 7.4 Hz, 3H), 0.99 (ddt, *J* = 9.6, 6.5, 4.8 Hz, 1H), 0.93 – 0.82 (m, 2H), 0.77 (ddt, *J* = 8.8, 7.0, 4.3 Hz, 1H); **^{13}C NMR** (126 MHz, DMSO) δ 136.22, 132.68, 126.95, 121.03, 118.44, 117.77, 111.11, 103.40, 53.29, 47.57, 29.68, 29.08, 25.88, 22.27, 11.30, 5.04, 4.46; **HRMS (**ESI) *m/z* calcd for $C_{17}H_{23}N_2O_2S$ $[M+H]^+$ 319.1480, found 319.1466.

(1*S*,3*R*)-1-cyclopropyl-2-(cyclopropylsulfonyl)-3-methyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (23)



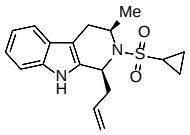
The title compound was prepared from (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (60 mg, 0.15 mmol) and cyclopropylmagnesium bromide (1.0 M, 0.30 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (37 mg, 75% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.67 (s, 1H), 7.40 (dd, *J* = 16.6, 7.9 Hz, 2H), 7.10 – 7.05 (m, 1H), 6.98 (t, *J* = 7.2 Hz, 1H), 4.50 (p, *J* = 7.0 Hz, 1H), 4.19 – 4.13 (m, 1H), 3.08 – 3.00 (m, 1H), 2.68 (d, *J* = 15.5 Hz, 1H), 2.50 – 2.45 (m, 1H), 1.38 (d, *J* = 7.1 Hz, 3H), 1.32 – 1.23 (m, 1H), 1.01 – 0.94 (m, 1H), 0.93 – 0.86 (m, 2H), 0.82 (ddd, *J* = 12.2, 8.4, 4.2 Hz, 2H), 0.76 (dq, *J* = 9.1, 4.6 Hz, 1H), 0.73 – 0.66 (m, 1H), 0.60 – 0.53 (m, 1H); **^{13}C NMR** (126 MHz, DMSO) δ 136.87, 132.44, 127.25, 121.59, 118.88, 118.23, 111.78, 104.21, 57.28, 47.89, 30.07, 26.70, 22.52, 18.81, 6.18, 5.34, 5.14, 4.10; **HRMS (**ESI) *m/z* calcd for $C_{18}H_{23}N_2O_2S$ $[M+H]^+$ 331.1480, found 331.1464.

(1*S*,3*R*)-1-cyclohexyl-2-(cyclopropylsulfonyl)-3-methyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (24)



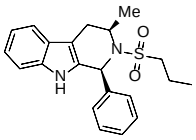
The title compound was prepared from (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (60 mg, 0.15 mmol) and cyclohexylmagnesium bromide (2.0 M, 0.15 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (51 mg, 91% yield); **^{1}H NMR** (500 MHz, DMSO-*d6*) δ 10.78 (s, 1H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.08 – 7.00 (m, 1H), 6.99 – 6.94 (m, 1H), 4.53 (d, *J* = 10.1 Hz, 1H), 4.33 (ddq, *J* = 3.5, 7.0, 10.7 Hz, 1H), 3.29 – 3.21 (m, 1H), 2.59 (dd, *J* = 3.7, 15.7 Hz, 1H), 2.21 – 2.13 (m, 2H), 1.81 (dd, *J* = 8.2, 16.7 Hz, 2H), 1.70 (dt, *J* = 7.0, 14.2 Hz, 2H), 1.64 – 1.58 (m, 1H), 1.42 (d, *J* = 6.9 Hz, 3H), 1.22 – 1.03 (m, 4H), 0.87 (ddt, *J* = 4.3, 7.2, 9.5 Hz, 1H), 0.78 – 0.67 (m, 2H), 0.52 – 0.43 (m, 1H). **^{13}C NMR** (126 MHz, DMSO) δ 135.72, 133.28, 126.25, 120.77, 118.31, 117.53, 111.09, 104.35, 57.67, 48.07, 42.56, 30.47, 30.43, 28.00, 26.11, 25.79, 25.46, 25.40, 23.74, 4.30, 4.05. **HRMS (**ESI) *m/z* calcd for $C_{21}H_{29}N_2O_2S$ $[M+H]^+$ 373.1950, found 373.1939.

(1*S*,3*R*)-1-allyl-2-(cyclopropylsulfonyl)-3-methyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (25)



A 11-dram scintillation vial equipped with a Teflon-coated magnetic stir bar was charged with (3*R*)-2-(cyclopropylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**9**) (60 mg, 0.15 mmol), allyltrimethylsilane (2 equiv.) and dichloromethane (5.0 mL). The solution was cooled to -78^{o}C in a dry ice/acetone bath, and Tin(IV) chloride (1.0 M in DCM) (2 equiv.) was added. The resulting solution was allowed to warm to room temperature and stir for 3 hours. Cold aq. $NaHCO_3$ (20 mL) was added, and the biphasic mixture was extracted with dichloromethane (10 mL) twice. The combined organic layer was dried over Na_2SO_4 and filtered. The filtrate was concentrated in vacuo, and the resulting oil was purified by silica gel column chromatography using a gradient solvent system (0 → 30% iPrOAc/Heptane) as the eluent to afford a white solid (24 mg, 48% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.83 (s, 1H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.05 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 6.99 – 6.90 (m, 1H), 6.00 (dddd, *J* = 16.8, 10.4, 7.7, 6.3 Hz, 1H), 5.13 – 5.10 (m, 1H), 5.09 – 5.04 (m, 2H), 4.46 (p, *J* = 7.0 Hz, 1H), 3.04 (ddd, *J* = 15.6, 6.5, 1.9 Hz, 1H), 2.80 (dddd, *J* = 13.1, 6.6, 4.0, 1.5 Hz, 1H), 2.63 (d, *J* = 15.5 Hz, 1H), 2.61 – 2.48 (m, 2H), 1.27 (d, *J* = 7.2 Hz, 3H), 0.96 (tdt, *J* = 9.7, 6.7, 3.7 Hz, 1H), 0.92 – 0.82 (m, 2H), 0.77 (ddt, *J* = 12.8, 8.5, 3.4 Hz, 1H); **^{13}C NMR** (126 MHz, DMSO) δ 136.25, 135.54, 131.84, 126.88, 121.16, 118.50, 117.81, 117.29, 111.19, 103.90, 51.54, 47.52, 41.30, 29.30, 25.96, 22.25, 4.97, 4.58; **HRMS (**ESI) *m/z* calcd for $C_{18}H_{23}N_2O_2S$ $[M+H]^+$ 331.1480, found 331.1466.

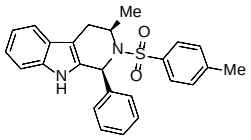
(1*S*,3*R*)-3-methyl-1-phenyl-2-(propylsulfonyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (27)



The title compound was prepared from (3*R*)-3-methyl-1-(phenylthio)-2-(propylsulfonyl)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**27b**) (60 mg, 0.15 mmol) and phenylmagnesium chloride (2.0 M, 0.15 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (44 mg, 80% yield); **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.93 (s, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.50 – 7.45 (m, 2H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.34 – 7.28 (m, 3H), 7.28 – 7.24 (m, 1H), 7.21 – 7.16 (m, 1H), 6.23 (s, 1H), 4.62 (p, *J* = 7.1 Hz, 1H), 3.17 (ddd, *J* = 15.9, 6.8, 1.7 Hz, 1H), 2.83 (t, *J* = 7.8 Hz, 2H), 2.79 (d, *J* = 15.9 Hz, 1H), 1.90 – 1.67 (m, 2H), 1.07 (d, *J* = 7.2 Hz, 3H), 0.95 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 140.42, 136.30, 129.22, 128.62, 128.50, 128.08,

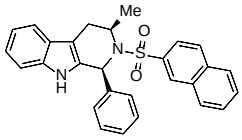
127.30, 122.67, 119.84, 118.48, 111.14, 107.80, 54.49, 53.79, 48.31, 26.59, 22.52, 17.14, 13.18; **HRMS** (ESI) *m/z* calcd for $C_{21}H_{25}N_2O_2S$ $[M+H]^+$ 369.1637, found 369.1627.

(1*S*,3*R*)-3-methyl-1-phenyl-2-tosyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (28)



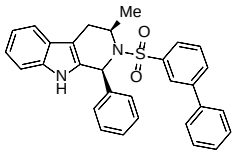
The title compound was prepared from (3*R*)-3-methyl-1-(phenylthio)-2-tosyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (28b) (67 mg, 0.15 mmol) and phenylmagnesium chloride (2.0 M, 0.15 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (52 mg, 83% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.97 (s, 1H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.42 – 7.36 (m, 4H), 7.31 (td, *J* = 7.7, 7.3, 3.9 Hz, 3H), 7.24 (d, *J* = 8.2 Hz, 2H), 7.09 – 7.05 (m, 1H), 6.94 (t, *J* = 7.5 Hz, 1H), 6.38 (s, 1H), 4.47 (p, *J* = 7.0 Hz, 1H), 2.43 (d, *J* = 15.6 Hz, 1H), 2.38 – 2.32 (m, 1H), 2.26 (s, 3H), 0.87 (d, *J* = 7.1 Hz, 3H); **^{13}C NMR** (126 MHz, DMSO) δ 143.61, 141.94, 137.79, 136.68, 130.16, 129.37, 128.72, 128.48, 128.03, 127.07, 121.87, 118.92, 118.33, 111.71, 105.85, 53.99, 48.46, 24.97, 22.60, 21.34; **HRMS** (ESI) *m/z* calcd for $C_{25}H_{25}N_2O_2S$ $[M+H]^+$ 417.1637, found 417.1625.

(1*S*,3*R*)-3-methyl-2-(naphthalen-2-ylsulfonyl)-1-phenyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b] indole (29)



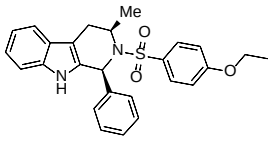
The title compound was prepared from (3*R*)-3-methyl-2-(naphthalen-2-ylsulfonyl)-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**29b**) (73 mg, 0.15 mmol) and phenylmagnesium chloride (2.0 M, 0.15 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (59 mg, 87% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.99 (s, 1H), 8.55 (s, 1H), 8.10 – 8.06 (m, 1H), 7.92 (d, *J* = 8.7 Hz, 2H), 7.68 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.63 (pd, *J* = 6.9, 1.3 Hz, 2H), 7.45 (d, *J* = 7.6 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 7.21 (d, *J* = 7.8 Hz, 1H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.88 (t, *J* = 7.4 Hz, 1H), 6.52 (s, 1H), 4.57 (p, *J* = 7.0 Hz, 1H), 2.41 (d, *J* = 15.7 Hz, 1H), 2.28 (dd, *J* = 15.7, 6.7 Hz, 1H), 0.90 (d, *J* = 7.1 Hz, 3H); **^{13}C NMR** (126 MHz, DMSO) δ 141.87, 137.56, 136.66, 134.58, 132.08, 129.81, 129.65, 129.40, 128.76, 128.53, 128.21, 128.10, 126.91, 122.26, 121.87, 118.90, 118.27, 111.69, 105.84, 54.22, 48.59, 25.11, 22.56; **HRMS** (ESI) *m/z* calcd for $C_{28}H_{25}N_2O_2S$ $[M+H]^+$ 453.1637, found 453.1623.

(1*S*,3*R*)-2-([1,1'-biphenyl]-3-ylsulfonyl)-3-methyl-1-phenyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (30)



The title compound was prepared from (3*R*)-2-([1,1'-biphenyl]-3-ylsulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (30b) (77 mg, 0.15 mmol) and phenylmagnesium chloride (2.0 M, 0.15 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (26 mg, 36% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 11.12 (s, 1H), 7.83 – 7.80 (m, 1H), 7.78 (d, *J* = 7.9 Hz, 1H), 7.75 (t, *J* = 1.7 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.45 – 7.37 (m, 5H), 7.35 – 7.27 (m, 3H), 7.22 (t, *J* = 7.7 Hz, 2H), 7.18 – 7.16 (m, 2H), 7.13 – 7.09 (m, 1H), 6.94 (t, *J* = 7.4 Hz, 1H), 6.56 (s, 1H), 4.52 (p, *J* = 7.1 Hz, 1H), 2.45 (d, *J* = 15.9 Hz, 1H), 2.39 – 2.31 (m, 1H), 0.88 (d, *J* = 7.1 Hz, 3H); **^{13}C NMR** (126 MHz, DMSO) δ 141.27, 141.15, 140.84, 138.13, 136.20, 131.04, 129.78, 128.77, 128.73, 128.19, 127.94, 127.75, 127.51, 126.62, 126.49, 125.43, 123.89, 121.47, 118.49, 117.78, 111.13, 105.39, 53.77, 47.95, 24.38, 22.11; **HRMS** (ESI) *m/z* calcd for $C_{30}H_{27}N_2O_2S$ $[M+H]^+$ 479.1793, found 479.1785.

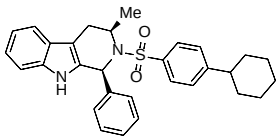
(1*S*,3*R*)-2-((4-ethoxyphenyl)sulfonyl)-3-methyl-1-phenyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (31)



The title compound was prepared from (3*R*)-2-((4-ethoxyphenyl)sulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (31b) (72 mg, 0.15 mmol) and phenylmagnesium chloride (2.0 M, 0.15 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (53 mg, 76% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 11.00 (s, 1H), 7.71 – 7.64 (m, 2H), 7.42 – 7.36 (m, 4H), 7.31 (t, *J* = 7.7 Hz, 3H), 7.09 – 7.04 (m, 1H), 6.96 – 6.89 (m, 3H), 6.37 (s, 1H), 4.45 (p, *J* = 7.0 Hz, 1H), 4.02 – 3.91 (m, 2H), 2.43 (d, *J* = 15.5 Hz, 1H), 2.36 (dd, *J* = 15.9, 6.4 Hz, 1H), 1.24 (t, *J* = 7.0 Hz, 3H), 0.86 (d, *J* = 7.1 Hz, 3H); **^{13}C NMR** (126 MHz, DMSO) δ 162.08, 142.01, 136.69, 131.94, 129.42, 129.22, 128.70, 128.43, 127.99, 127.02, 121.84, 118.89, 118.31, 115.15, 111.69, 105.85, 64.09, 53.89, 48.38, 24.98, 22.60, 14.76; **HRMS** (ESI) *m/z* calcd for $C_{26}H_{27}N_2O_3S$ $[M+H]^+$ 447.1742, found 447.1724.

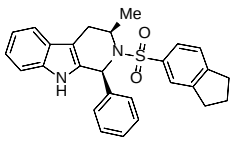
(1*S*,3*R*)-2-((4-cyclohexylphenyl)sulfonyl)-3-methyl-1-phenyl-2,3,4,9-tetrahydro-1H-pyrido[3

,4-b]indole (32)



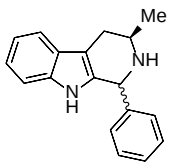
The title compound was prepared from (3*R*)-2-((4-cyclohexylphenyl)-sulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (32b) (78 mg, 0.15 mmol) and phenylmagnesium chloride (2.0 M, 0.15 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (65 mg, 89% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.95 (s, 1H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.42 – 7.35 (m, 4H), 7.33 – 7.29 (m, 2H), 7.24 (dd, *J* = 12.0, 8.1 Hz, 3H), 7.08 – 7.04 (m, 1H), 6.92 (t, *J* = 7.4 Hz, 1H), 6.37 (s, 1H), 4.45 (p, *J* = 7.0 Hz, 1H), 2.43 (tt, *J* = 8.4, 4.4 Hz, 1H), 2.39 (d, *J* = 16.0 Hz, 1H), 2.36 – 2.30 (m, 1H), 1.70 (d, *J* = 11.3 Hz, 2H), 1.64 (d, *J* = 12.6 Hz, 1H), 1.57 (d, *J* = 11.0 Hz, 2H), 1.32 – 1.11 (m, 5H), 0.86 (d, *J* = 7.1 Hz, 3H); **^{13}C NMR** (126 MHz, DMSO) δ 152.63, 141.29, 137.14, 136.08, 128.77, 128.13, 127.79, 127.43, 127.21, 126.55, 126.42, 121.23, 118.26, 117.62, 111.05, 105.27, 53.44, 47.90, 43.22, 33.23, 33.17, 25.92, 25.25, 24.35, 22.13; **HRMS** (ESI) *m/z* calcd for $C_{30}H_{33}N_2O_2S$ $[M+H]^+$ 485.2263, found 485.2250.

(1*S*,3*R*)-2-((2,3-dihydro-1H-inden-5-yl)sulfonyl)-3-methyl-1-phenyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (33)



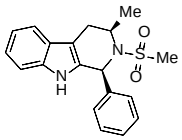
The title compound was prepared from (3*R*)-2-((2,3-dihydro-1H-inden-5-yl)sulfonyl)-3-methyl-1-(phenylthio)-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (33b) (71 mg, 0.15 mmol) and phenylmagnesium chloride (2.0 M, 0.15 mL, 0.30 mmol) according to the general 1,3-substituted *cis*-tetrahydro-β-carbolines synthesis procedure and was obtained as a white solid (60 mg, 91% yield); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 10.97 (s, 1H), 7.54 – 7.50 (m, 1H), 7.48 (s, 1H), 7.42 – 7.36 (m, 4H), 7.34 – 7.29 (m, 2H), 7.25 (dd, *J* = 13.2, 7.9 Hz, 2H), 7.10 – 7.05 (m, 1H), 6.94 (t, *J* = 7.4 Hz, 1H), 6.38 (s, 1H), 4.44 (p, *J* = 7.0 Hz, 1H), 2.81 – 2.69 (m, 3H), 2.55 – 2.51 (m, 1H), 2.38 (d, *J* = 15.4 Hz, 1H), 2.36 – 2.29 (m, 1H), 1.95 – 1.74 (m, 2H), 0.87 (d, *J* = 7.1 Hz, 3H); **^{13}C NMR** (126 MHz, DMSO) δ 149.31, 144.93, 141.46, 137.80, 136.26, 129.10, 128.27, 127.93, 127.56, 126.60, 124.86, 124.71, 122.40, 121.43, 118.45, 117.81, 111.18, 105.56, 53.69, 48.02, 32.14, 31.85, 24.79, 24.57, 22.39； **HRMS** (ESI) *m/z* calcd for $C_{27}H_{27}N_2O_2S$ $[M+H]^+$ 443.1793, found 443.1774.

(*R*)-3-methyl-1-phenyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (34)



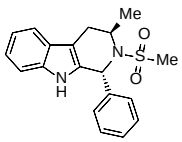
A 100-mL round bottom flask equipped with a Teflon-coated magnetic stir bar was charged with (*R*)-1-(1H-indol-3-yl)propan-2-amine (300 mg, 1.74 mmol), benzaldehyde (1 equiv.) and toluene (20.0 mL). Acetic acid (2 equiv.) was added. The resulting solution was heated to reflux at 80 ^{o}C and stirred for 15 hours. Cold aq. $NaHCO_3$ (20 mL) was added, and the biphasic mixture was extracted with dichloromethane (10 mL) twice. The combined organic layer was dried over Na_2SO_4 and filtered. The filtrate was concentrated in vacuo, and the resulting oil was purified by silica gel column chromatography using a gradient solvent system (0 → 90% iPrOAc/Heptane) as the eluent to afford colorless oil (283 mg, 62% yield) which consisted of a mixture of 5:2 (*cis*:*trans)* diastereoisomers; **^{1}H NMR** (major diastereomer) (400 MHz, Chloroform-*d*) δ 8.00 (s, 1H), 7.50 – 7.46 (m, 1H), 7.27 – 7.17 (m, 5H), 7.09 – 7.07 (m, 1H), 7.04 – 6.99 (m, 2H), 5.05 (s, 1H), 3.24 – 3.17 (m, 1H), 2.87 – 2.82 (m, 1H), 2.55 – 2.43 (m, 1H), 1.25 (d, *J* = 6.4 Hz, 3H); **HRMS** (ESI) *m/z* calcd for $C_{18}H_{19}N_2$ $[M+H]^+$ 263.1548, found 263.1534.

(1*S*,3*R*)-3-methyl-2-(methylsulfonyl)-1-phenyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (35)



The title compound was prepared from (*R*)-3-methyl-1-phenyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (34) (283 mg, 1.08 mmol) and methanesulfonyl chloride (186 mg, 1.62 mmol) according to the general sulfonylation procedure and was obtained as a white solid (142 mg, 54% yield based on the quantity of (1*S*,3*R*)-3-methyl-1-phenyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 11.09 (s, 1H), 7.49 (d, *J* = 7.8 Hz, 1H), 7.40 – 7.33 (m, 5H), 7.31 – 7.27 (m, 1H), 7.15 – 7.11 (m, 1H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.16 (s, 1H), 4.54 (p, *J* = 7.1 Hz, 1H), 3.25 – 3.14 (m, 1H), 2.90 (s, 3H), 2.66 (d, *J* = 16.1 Hz, 1H), 0.88 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR** (126 MHz, DMSO) δ 141.81, 136.84, 129.51, 128.64, 128.34, 127.95, 127.27, 122.01, 119.02, 118.52, 111.77, 106.07, 53.37, 48.23, 25.74, 22.74; **HRMS (**ESI) *m/z* calcd for $C_{19}H_{21}N_2O_2S$ $[M+H]^+$ 341.1324, found 341.1313.

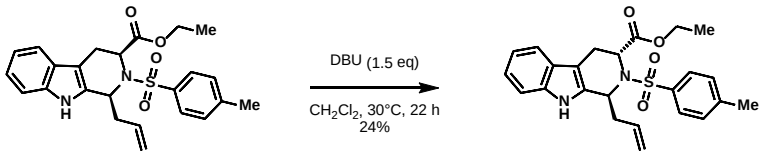
(1*R*,3*R*)-3-methyl-2-(methylsulfonyl)-1-phenyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (36)



The title compound was prepared from (3*R*)-3-methyl-1-phenyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (**34**) (283 mg, 1.08 mmol) and methanesulfonyl chloride (186 mg, 1.62 mmol) according to the general sulfonylation procedure and was obtained as a white solid (99 mg, 94% yield based on the quantity of (1*R*,3*R*)-3-methyl-1-phenyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole); **^{1}H NMR** (500 MHz, DMSO-d_6) δ 7.47 (d, *J* = 7.8 Hz, 1H), 7.37 (t, *J* = 7.3 Hz, 2H), 7.35 – 7.29 (m, 2H), 7.24 (d, *J* = 7.2 Hz, 2H), 7.12 – 7.06 (m, 1H), 7.04 – 6.98 (m, 1H), 6.13 (s, 1H), 3.78 (dq, *J* = 14.1, 7.0 Hz, 1H), 2.98 – 2.87 (m, 2H), 2.84 (s, 3H), 1.44 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR** (126 MHz, DMSO) δ 140.61, 136.78, 132.19, 128.89, 128.67, 128.35, 126.72, 121.80, 119.10, 118.45, 111.74, 108.40, 57.70, 50.29, 43.27, 28.56, 20.25; **HRMS (**ESI) *m/z* calcd for $C_{19}H_{21}N_2O_2S$ $[M+H]^+$ 341.1324, found 341.1314.

Epimerization of

ethyl(1S,3S)-1-allyl-2-tosyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylate (11) to ethyl(1S,3R)-1-allyl-2-tosyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylate (11b)



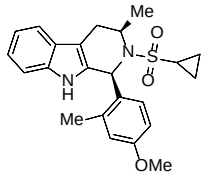
11 **11b**

To a vial containing ethyl (1S,3S)-1-allyl-2-tosyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylate (**11**) (12.5 mg, 0.0285 mmol, 1 eq) was added a solution of DBU (6.5 mg, 0.043 mmol, 1.5 eq) in methylene chloride (0.28 mL, 0.1 M). The reaction was heated at 30°C for 22 h at which point 2 mL water was added. The solution was extracted twice with methylene chloride (2 mL each), dried through sodium sulfate and concentrated. Analysis of the crude reaction mixture by NMR spectroscopy revealed compounds 11 and 11b in a ratio of approximately 3 to 1. The crude reaction was purified by silica column chromatography using an isopropyl acetate/heptanes gradient to give ethyl (1S,3R)-1-allyl-2-tosyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylate (**11b**) (3.0 mg, 24% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (d, J = 8.3 Hz, 2H), 7.75 (bs, 1H), 7.43 (d, J = 8.4 Hz, 1H), 7.29-7.24 (m, 1H), 7.21 (d, J = 7.8 Hz, 2H), 7.15 (ddd, J = 8.2, 7.1, 1.3 Hz, 1H), 7.08

(ddd, J = 8.1, 7.1, 1.1 Hz, 1H), 5.58 (ddt, J = 17.2, 10.3, 7.1 Hz, 1H), 5.08 (t, J = 6.2 Hz, 1H), 5.01 – 4.86 (m, 2H), 4.59 (dd, J = 8.0, 4.7 Hz, 1H), 4.19 (q, J = 7.1 Hz, 2H), 3.30 (ddd, J = 15.9, 8.0, 1.2 Hz, 1H), 3.07 (ddd, J = 15.9, 4.6, 0.9 Hz, 1H), 2.66 (t, J = 6.9 Hz, 2H), 2.36 (s, 3H), 1.28 – 1.17 (m, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 170.6, 143.8, 138.1, 136.2, 133.2, 133.1, 129.4, 127.7, 126.6, 122.3, 119.9, 119.1, 118.4, 111.0, 108.0, 61.7, 56.8, 55.0, 39.7, 24.2, 21.6, 14.2. **LRMS** (ESI) Calculated for $C_{24}H_{27}N_2O_4$ $(M+H)^+$: 439.2 Found: 439.1.

X-Ray Crystallography Methods and Results

(1*S*,3*R*)-2-(cyclopropylsulfonyl)-1-(4-methoxy-2-methylphenyl)-3-methyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (14)



X-ray quality crystals were grown by the slow evaporation of a saturated 1,2-dichloroethane/ethanol/methanol solution. A yellow plate 0.080 x 0.080 x 0.040 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using and scans. Crystal-to-detector distance was 50 mm and exposure time was 10 seconds per frame using a scan width of 1.0°. Data collection was 100.0% complete to 25.000° in θ. A total of 42376 reflections were collected covering the indices, -11<=*h*<=10, -13<=*k*<=13, -23<=*l*<=23. 3784 reflections were found to be symmetry independent, with an R_{int} of 0.0450. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be P 21 21 21 (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT-2014) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014. Absolute stereochemistry was unambiguously determined to be *R* at C11 and *S* at C1, respectively.

Table S1. Crystal data and structure refinement for **14**.

CCDC	1900975	
Empirical formula	C23 H26 N2 O3 S	
Formula weight	410.52	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 9.2149(3) Å	α= 90°.
	b = 11.3488(4) Å	β= 90°.
	c = 19.7251(7) Å	γ = 90°.
Volume	2062.81(12) $Å^3$	
Z	4	
Density (calculated)	1.322 Mg/m^3	
Absorption coefficient	0.184 mm^{-1}	
F(000)	872	
Crystal size	0.080 x 0.080 x 0.040 mm^3	
Theta range for data collection	2.065 to 25.367°.	
Index ranges	-11<=h<=10, -13<=k<=13, -23<=l<=23	
Reflections collected	42376	
Independent reflections	3784 [R(int) = 0.0450]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.928 and 0.842	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3784 / 0 / 265	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0342, wR2 = 0.0826	
R indices (all data)	R1 = 0.0364, wR2 = 0.0843	
Absolute structure parameter	-0.03(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.377 and -0.230 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **14**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3143(3)	3338(2)	7561(1)	17(1)
C(2)	2466(3)	3234(2)	6875(1)	17(1)
C(3)	1188(3)	2453(2)	6020(1)	20(1)
C(4)	376(3)	1729(2)	5595(1)	26(1)
C(5)	-199(3)	2232(3)	5012(1)	28(1)
C(6)	43(3)	3412(3)	4852(1)	30(1)
C(7)	840(3)	4134(2)	5282(1)	25(1)
C(8)	1413(3)	3657(2)	5878(1)	20(1)
C(9)	2227(3)	4139(2)	6438(1)	19(1)
C(10)	2770(3)	5370(2)	6553(1)	24(1)
C(11)	3321(3)	5541(2)	7285(1)	21(1)
C(12)	2137(3)	5988(2)	7759(2)	28(1)
C(13)	6144(3)	4016(2)	6607(1)	24(1)
C(14)	7686(3)	4177(3)	6370(1)	32(1)
C(15)	6531(4)	5001(3)	6132(2)	33(1)
C(16)	2024(3)	3341(2)	8129(1)	18(1)
C(17)	551(3)	3335(2)	7981(1)	21(1)
C(18)	-518(3)	3422(2)	8474(1)	23(1)
C(19)	-88(3)	3507(2)	9144(1)	21(1)
C(20)	1374(3)	3475(2)	9314(1)	22(1)
C(21)	2443(3)	3381(2)	8822(1)	20(1)
C(22)	4004(3)	3360(2)	9037(1)	23(1)
C(23)	-2528(3)	3793(3)	9511(2)	28(1)
N(1)	4023(2)	4450(2)	7565(1)	17(1)
N(2)	1848(2)	2207(2)	6631(1)	19(1)
O(1)	6215(2)	3299(2)	7840(1)	22(1)
O(2)	6424(2)	5431(2)	7628(1)	26(1)
O(3)	-1033(2)	3643(2)	9680(1)	27(1)
S(1)	5773(1)	4316(1)	7460(1)	18(1)

Table S3. Bond lengths [Å] and angles [°] for **14**.

C(1)-C(2)	1.495(3)	C(14)-C(15)	1.492(4)
C(1)-N(1)	1.499(3)	C(14)-H(14A)	0.9900
C(1)-C(16)	1.522(4)	C(14)-H(14B)	0.9900
C(1)-H(1)	1.0000	C(15)-H(15A)	0.9900
C(2)-C(9)	1.359(4)	C(15)-H(15B)	0.9900
C(2)-N(2)	1.384(3)	C(16)-C(17)	1.388(4)
C(3)-N(2)	1.378(3)	C(16)-C(21)	1.421(4)
C(3)-C(4)	1.391(4)	C(17)-C(18)	1.388(4)
C(3)-C(8)	1.411(4)	C(17)-H(17)	0.9500
C(4)-C(5)	1.389(4)	C(18)-C(19)	1.384(4)
C(4)-H(4)	0.9500	C(18)-H(18)	0.9500
C(5)-C(6)	1.394(4)	C(19)-O(3)	1.378(3)
C(5)-H(5)	0.9500	C(19)-C(20)	1.389(4)
C(6)-C(7)	1.389(4)	C(20)-C(21)	1.388(4)
C(6)-H(6)	0.9500	C(20)-H(20)	0.9500
C(7)-C(8)	1.397(4)	C(21)-C(22)	1.500(4)
C(7)-H(7)	0.9500	C(22)-H(22A)	0.9800
C(8)-C(9)	1.442(4)	C(22)-H(22B)	0.9800
C(9)-C(10)	1.501(4)	C(22)-H(22C)	0.9800
C(10)-C(11)	1.543(4)	C(23)-O(3)	1.428(3)
C(10)-H(10A)	0.9900	C(23)-H(23A)	0.9800
C(10)-H(10B)	0.9900	C(23)-H(23B)	0.9800
C(11)-N(1)	1.503(3)	C(23)-H(23C)	0.9800
C(11)-C(12)	1.523(4)	N(1)-S(1)	1.633(2)
C(11)-H(11)	1.0000	N(2)-H(2)	0.8800
C(12)-H(12A)	0.9800	O(1)-S(1)	1.4349(19)
C(12)-H(12B)	0.9800	O(2)-S(1)	1.4384(18)
C(12)-H(12C)	0.9800	N(1)-C(1)-H(1)	108.6
C(13)-C(15)	1.501(4)	C(16)-C(1)-H(1)	108.6
C(13)-C(14)	1.507(4)	N(1)-C(1)-C(16)	111.1(2)
C(13)-S(1)	1.751(3)	C(2)-C(1)-H(1)	108.6
C(13)-H(13)	1.0000	C(2)-C(1)-C(16)	112.5(2)
C(2)-C(1)-N(1)	107.3(2)	C(9)-C(2)-N(2)	110.4(2)
		C(9)-C(2)-C(1)	125.7(2)
		N(2)-C(2)-C(1)	123.6(2)

N(2)-C(3)-C(4)	130.1(2)	H(12A)-C(12)-H(12C)	109.5
N(2)-C(3)-C(8)	107.8(2)	H(12B)-C(12)-H(12C)	109.5
C(4)-C(3)-C(8)	122.1(2)	C(15)-C(13)-C(14)	59.49(19)
C(5)-C(4)-C(3)	117.5(3)	C(15)-C(13)-S(1)	120.1(2)
C(5)-C(4)-H(4)	121.3	C(14)-C(13)-S(1)	117.3(2)
C(3)-C(4)-H(4)	121.3	C(15)-C(13)-H(13)	116.0
C(4)-C(5)-C(6)	121.4(3)	C(14)-C(13)-H(13)	116.0
C(4)-C(5)-H(5)	119.3	S(1)-C(13)-H(13)	116.0
C(6)-C(5)-H(5)	119.3	C(15)-C(14)-C(13)	60.07(19)
C(7)-C(6)-C(5)	120.9(3)	C(15)-C(14)-H(14A)	117.8
C(7)-C(6)-H(6)	119.6	C(13)-C(14)-H(14A)	117.8
C(5)-C(6)-H(6)	119.6	C(15)-C(14)-H(14B)	117.8
C(6)-C(7)-C(8)	119.0(3)	C(13)-C(14)-H(14B)	117.8
C(6)-C(7)-H(7)	120.5	H(14A)-C(14)-H(14B)	114.9
C(8)-C(7)-H(7)	120.5	C(14)-C(15)-C(13)	60.44(19)
C(7)-C(8)-C(3)	119.2(3)	C(14)-C(15)-H(15A)	117.7
C(7)-C(8)-C(9)	133.9(3)	C(13)-C(15)-H(15A)	117.7
C(3)-C(8)-C(9)	106.9(2)	C(14)-C(15)-H(15B)	117.7
C(2)-C(9)-C(8)	106.5(2)	C(13)-C(15)-H(15B)	117.7
C(2)-C(9)-C(10)	123.5(2)	H(15A)-C(15)-H(15B)	114.8
C(8)-C(9)-C(10)	129.9(2)	C(17)-C(16)-C(21)	117.9(2)
C(9)-C(10)-C(11)	111.7(2)	C(17)-C(16)-C(1)	120.5(2)
C(9)-C(10)-H(10A)	109.3	C(21)-C(16)-C(1)	121.6(2)
C(11)-C(10)-H(10A)	109.3	C(18)-C(17)-C(16)	123.2(2)
C(9)-C(10)-H(10B)	109.3	C(18)-C(17)-H(17)	118.4
C(11)-C(10)-H(10B)	109.3	C(16)-C(17)-H(17)	118.4
H(10A)-C(10)-H(10B)	107.9	C(19)-C(18)-C(17)	118.1(3)
N(1)-C(11)-C(12)	110.9(2)	C(19)-C(18)-H(18)	120.9
N(1)-C(11)-C(10)	112.4(2)	C(17)-C(18)-H(18)	120.9
C(12)-C(11)-C(10)	112.4(2)	O(3)-C(19)-C(18)	124.1(2)
N(1)-C(11)-H(11)	106.9	O(3)-C(19)-C(20)	115.5(2)
C(12)-C(11)-H(11)	106.9	C(18)-C(19)-C(20)	120.4(2)
C(10)-C(11)-H(11)	106.9	C(21)-C(20)-C(19)	121.5(2)
C(11)-C(12)-H(12A)	109.5	C(21)-C(20)-H(20)	119.3
C(11)-C(12)-H(12B)	109.5	C(19)-C(20)-H(20)	119.3
H(12A)-C(12)-H(12B)	109.5	C(20)-C(21)-C(16)	118.9(2)
C(11)-C(12)-H(12C)	109.5	C(20)-C(21)-C(22)	119.0(2)

C(16)-C(21)-C(22)	122.1(2)	C(1)-N(1)-C(11)	117.32(19)
C(21)-C(22)-H(22A)	109.5	C(1)-N(1)-S(1)	117.04(15)
C(21)-C(22)-H(22B)	109.5	C(11)-N(1)-S(1)	117.07(16)
H(22A)-C(22)-H(22B)	109.5	C(3)-N(2)-C(2)	108.4(2)
C(21)-C(22)-H(22C)	109.5	C(3)-N(2)-H(2)	125.8
H(22A)-C(22)-H(22C)	109.5	C(2)-N(2)-H(2)	125.8
H(22B)-C(22)-H(22C)	109.5	C(19)-O(3)-C(23)	116.3(2)
O(3)-C(23)-H(23A)	109.5	O(1)-S(1)-O(2)	117.94(11)
O(3)-C(23)-H(23B)	109.5	O(1)-S(1)-N(1)	106.79(11)
H(23A)-C(23)-H(23B)	109.5	O(2)-S(1)-N(1)	107.51(11)
O(3)-C(23)-H(23C)	109.5	O(1)-S(1)-C(13)	106.88(12)
H(23A)-C(23)-H(23C)	109.5	O(2)-S(1)-C(13)	108.08(13)
H(23B)-C(23)-H(23C)	109.5	N(1)-S(1)-C(13)	109.46(12)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **14**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	17(1)	14(1)	21(1)	0(1)	-4(1)	-1(1)
C(2)	14(1)	17(1)	21(1)	-2(1)	0(1)	0(1)
C(3)	16(1)	23(1)	20(1)	-1(1)	1(1)	2(1)
C(4)	28(2)	24(2)	25(1)	-4(1)	-2(1)	1(1)
C(5)	23(2)	39(2)	22(1)	-10(1)	-4(1)	3(1)
C(6)	25(2)	42(2)	22(1)	3(1)	-4(1)	8(1)
C(7)	23(2)	28(2)	23(1)	5(1)	1(1)	3(1)
C(8)	14(1)	24(1)	21(1)	1(1)	3(1)	2(1)
C(9)	14(1)	21(1)	22(1)	1(1)	2(1)	1(1)
C(10)	22(2)	19(1)	31(1)	5(1)	-5(1)	-1(1)
C(11)	18(1)	14(1)	31(1)	2(1)	-2(1)	1(1)
C(12)	25(2)	19(1)	40(2)	-1(1)	5(1)	3(1)
C(13)	24(2)	25(1)	23(1)	-1(1)	1(1)	1(1)
C(14)	26(2)	41(2)	29(1)	3(1)	7(1)	4(1)
C(15)	33(2)	37(2)	28(1)	7(1)	5(1)	-2(1)
C(16)	19(1)	15(1)	21(1)	1(1)	-2(1)	-1(1)
C(17)	21(1)	21(1)	19(1)	1(1)	-3(1)	-3(1)
C(18)	17(1)	21(1)	29(1)	1(1)	-1(1)	-1(1)
C(19)	22(2)	18(1)	23(1)	0(1)	4(1)	-2(1)
C(20)	25(2)	21(1)	19(1)	-1(1)	-4(1)	-1(1)
C(21)	21(1)	17(1)	22(1)	0(1)	-3(1)	0(1)
C(22)	20(2)	27(1)	21(1)	-1(1)	-1(1)	0(1)
C(23)	19(2)	38(2)	29(1)	-1(1)	3(1)	0(1)
N(1)	15(1)	14(1)	22(1)	0(1)	-2(1)	-1(1)
N(2)	23(1)	15(1)	20(1)	0(1)	-4(1)	0(1)
O(1)	18(1)	23(1)	26(1)	1(1)	-4(1)	2(1)
O(2)	18(1)	23(1)	36(1)	-6(1)	-4(1)	-2(1)
O(3)	21(1)	37(1)	23(1)	0(1)	2(1)	2(1)
S(1)	15(1)	17(1)	21(1)	-2(1)	-1(1)	0(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **14**.

	x	y	z	U(eq)
H(1)	3812	2655	7630	21
H(4)	221	922	5700	31
H(5)	-769	1762	4716	34
H(6)	-342	3727	4444	36
H(7)	993	4940	5173	30
H(10A)	1977	5936	6462	29
H(10B)	3569	5538	6232	29
H(11)	4087	6164	7268	25
H(12A)	1262	5508	7702	42
H(12B)	1916	6812	7651	42
H(12C)	2474	5932	8229	42
H(13)	5602	3340	6402	29
H(14A)	8402	4479	6701	38
H(14B)	8075	3601	6040	38
H(15A)	6209	4935	5655	40
H(15B)	6535	5813	6316	40
H(17)	261	3269	7521	25
H(18)	-1517	3423	8355	27
H(20)	1649	3518	9778	26
H(22A)	4435	4139	8965	34
H(22B)	4532	2774	8768	34
H(22C)	4066	3152	9518	34
H(23A)	-2641	4493	9224	42
H(23B)	-3097	3892	9927	42
H(23C)	-2873	3097	9265	42
H(2)	1873	1515	6831	23

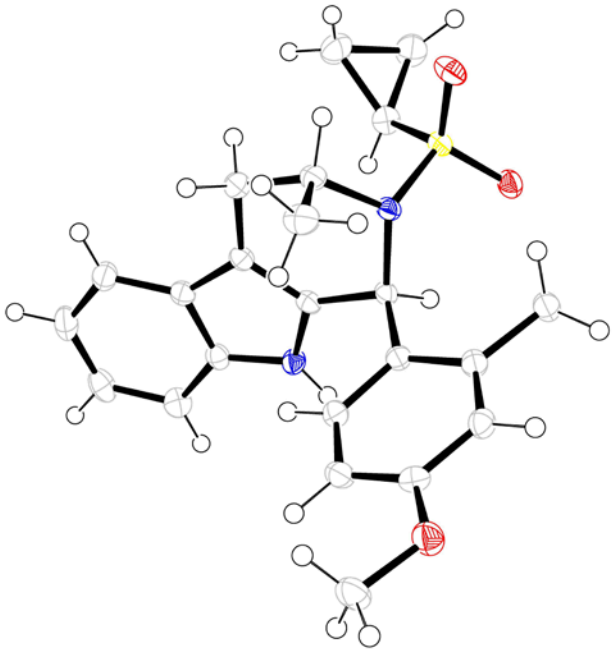
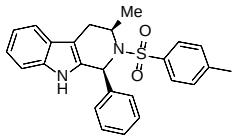


Figure S1. X-ray crystal structure of **14** with 50% probability ellipsoids.

(1*S*,3*R*)-3-methyl-1-phenyl-2-tosyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (28)



X-ray quality crystals were grown from a saturated 1,2-dichloroethane/ethanol/methanol solution followed by the slow vapor diffusion of diisopropyl ether to deposit the crystal diffracted. A colorless prism 0.070 x 0.030 x 0.030 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using and scans. Crystal-to-detector distance was 50 mm and exposure time was 20 seconds per frame using a scan width of 1.0°. Data collection was 100.0% complete to 25.000° in θ. A total of 26438 reflections were collected covering the indices, -10<=*h*<=10, -14<=*k*<=14, -22<=*l*<=22. 3817 reflections were found to be symmetry independent, with an R_{int} of 0.0602. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be P 21 21 21 (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT-2014) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014. Absolute stereochemistry was unambiguously determined to be *R* at C1 and *S* at C11, respectively.

Table S6. Crystal data and structure refinement for **28**.

CCDC ID	1900974	
Empirical formula	C25 H24 N2 O2 S	
Formula weight	416.52	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 9.0518(4) Å	α= 90°.
	b = 12.1315(5) Å	β= 90°.
	c = 18.9731(8) Å	γ = 90°.
Volume	2083.47(15) $Å^3$	
Z	4	
Density (calculated)	1.328 Mg/m^3	
Absorption coefficient	0.180 mm^{-1}	
F(000)	880	
Crystal size	0.070 x 0.030 x 0.030 mm^3	
Theta range for data collection	1.993 to 25.377°.	
Index ranges	-10<=h<=10, -14<=k<=14, -22<=l<=22	
Reflections collected	26438	
Independent reflections	3817 [R(int) = 0.0602]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.928 and 0.851	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3817 / 0 / 273	
Goodness-of-fit on F^2	1.081	
Final R indices [I>2sigma(I)]	R1 = 0.0403, wR2 = 0.0889	
R indices (all data)	R1 = 0.0472, wR2 = 0.0922	
Absolute structure parameter	0.04(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.255 and -0.290 $e.Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **28**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6266(4)	4514(3)	3074(2)	19(1)
C(2)	6141(4)	5525(2)	3546(2)	19(1)
C(3)	6867(4)	5289(3)	4241(2)	18(1)
C(4)	7543(4)	6004(3)	4750(2)	18(1)
C(5)	7737(4)	7154(3)	4805(2)	21(1)
C(6)	8497(4)	7568(3)	5376(2)	24(1)
C(7)	9041(4)	6881(3)	5908(2)	22(1)
C(8)	8855(4)	5748(3)	5876(2)	21(1)
C(9)	8117(4)	5329(3)	5288(2)	17(1)
C(10)	7032(4)	4246(3)	4486(2)	17(1)
C(11)	6411(4)	3214(2)	4167(2)	16(1)
C(12)	7792(4)	4369(3)	2749(2)	23(1)
C(13)	7496(4)	2259(3)	4132(2)	17(1)
C(14)	8995(4)	2426(3)	3992(2)	21(1)
C(15)	9961(4)	1542(3)	3958(2)	25(1)
C(16)	9457(4)	476(3)	4081(2)	26(1)
C(17)	7977(4)	304(3)	4226(2)	25(1)
C(18)	7007(4)	1192(3)	4248(2)	21(1)
C(19)	2905(4)	4076(3)	3255(2)	19(1)
C(20)	2634(4)	4696(3)	2656(2)	24(1)
C(21)	1768(4)	5637(3)	2706(2)	26(1)
C(22)	1137(4)	5951(3)	3341(2)	25(1)
C(23)	1380(4)	5287(3)	3930(2)	25(1)
C(24)	2274(4)	4370(3)	3896(2)	22(1)
C(25)	218(4)	6986(3)	3387(2)	33(1)
N(1)	5777(3)	3503(2)	3461(1)	18(1)
N(2)	7804(3)	4249(2)	5112(1)	18(1)
O(1)	3801(3)	2166(2)	3731(1)	24(1)
O(2)	4304(3)	2668(2)	2491(1)	24(1)
S(1)	4197(1)	2987(1)	3217(1)	19(1)

Table S8. Bond lengths [Å] and angles [°] for **28**.

C(1)-N(1)	1.497(4)	C(13)-C(14)	1.397(5)
C(1)-C(12)	1.523(5)	C(14)-C(15)	1.385(5)
C(1)-C(2)	1.524(4)	C(14)-H(14)	0.9500
C(1)-H(1)	1.0000	C(15)-C(16)	1.391(5)
C(2)-C(3)	1.500(4)	C(15)-H(15)	0.9500
C(2)-H(2A)	0.9900	C(16)-C(17)	1.383(5)
C(2)-H(2B)	0.9900	C(16)-H(16)	0.9500
C(3)-C(10)	1.356(4)	C(17)-C(18)	1.390(5)
C(3)-C(4)	1.435(5)	C(17)-H(17)	0.9500
C(4)-C(9)	1.409(5)	C(18)-H(18)	0.9500
C(4)-C(5)	1.410(4)	C(19)-C(20)	1.386(5)
C(5)-C(6)	1.379(5)	C(19)-C(24)	1.391(5)
C(5)-H(5)	0.9500	C(19)-S(1)	1.765(3)
C(6)-C(7)	1.398(5)	C(20)-C(21)	1.388(5)
C(6)-H(6)	0.9500	C(20)-H(20)	0.9500
C(7)-C(8)	1.387(4)	C(21)-C(22)	1.388(5)
C(7)-H(7)	0.9500	C(21)-H(21)	0.9500
C(8)-C(9)	1.396(4)	C(22)-C(23)	1.395(5)
C(8)-H(8)	0.9500	C(22)-C(25)	1.508(5)
C(9)-N(2)	1.382(4)	C(23)-C(24)	1.378(5)
C(10)-N(2)	1.379(4)	C(23)-H(23)	0.9500
C(10)-C(11)	1.499(4)	C(24)-H(24)	0.9500
C(11)-N(1)	1.499(4)	C(25)-H(25A)	0.9800
C(11)-C(13)	1.521(4)	C(25)-H(25B)	0.9800
C(11)-H(11)	1.0000	C(25)-H(25C)	0.9800
C(12)-H(12A)	0.9800	N(1)-S(1)	1.629(3)
C(12)-H(12B)	0.9800	N(2)-H(2)	0.8800
C(12)-H(12C)	0.9800	O(1)-S(1)	1.439(2)
C(13)-C(18)	1.387(4)	O(2)-S(1)	1.433(2)

N(1)-C(1)-C(12)	111.9(3)	C(2)-C(1)-H(1)	106.9
N(1)-C(1)-C(2)	110.4(3)	C(3)-C(2)-C(1)	109.3(3)
C(12)-C(1)-C(2)	113.5(3)	C(3)-C(2)-H(2A)	109.8
N(1)-C(1)-H(1)	106.9	C(1)-C(2)-H(2A)	109.8
C(12)-C(1)-H(1)	106.9	C(3)-C(2)-H(2B)	109.8

C(1)-C(2)-H(2B)	109.8	H(12B)-C(12)-H(12C)	109.5
H(2A)-C(2)-H(2B)	108.3	C(18)-C(13)-C(14)	118.4(3)
C(10)-C(3)-C(4)	106.7(3)	C(18)-C(13)-C(11)	119.9(3)
C(10)-C(3)-C(2)	121.8(3)	C(14)-C(13)-C(11)	121.7(3)
C(4)-C(3)-C(2)	131.5(3)	C(15)-C(14)-C(13)	120.6(3)
C(9)-C(4)-C(5)	118.4(3)	C(15)-C(14)-H(14)	119.7
C(9)-C(4)-C(3)	107.1(3)	C(13)-C(14)-H(14)	119.7
C(5)-C(4)-C(3)	134.5(3)	C(14)-C(15)-C(16)	120.3(3)
C(6)-C(5)-C(4)	118.7(3)	C(14)-C(15)-H(15)	119.8
C(6)-C(5)-H(5)	120.7	C(16)-C(15)-H(15)	119.8
C(4)-C(5)-H(5)	120.7	C(17)-C(16)-C(15)	119.4(3)
C(5)-C(6)-C(7)	121.8(3)	C(17)-C(16)-H(16)	120.3
C(5)-C(6)-H(6)	119.1	C(15)-C(16)-H(16)	120.3
C(7)-C(6)-H(6)	119.1	C(16)-C(17)-C(18)	120.1(3)
C(8)-C(7)-C(6)	121.1(3)	C(16)-C(17)-H(17)	120.0
C(8)-C(7)-H(7)	119.4	C(18)-C(17)-H(17)	120.0
C(6)-C(7)-H(7)	119.4	C(13)-C(18)-C(17)	121.1(3)
C(7)-C(8)-C(9)	117.0(3)	C(13)-C(18)-H(18)	119.4
C(7)-C(8)-H(8)	121.5	C(17)-C(18)-H(18)	119.4
C(9)-C(8)-H(8)	121.5	C(20)-C(19)-C(24)	120.4(3)
N(2)-C(9)-C(8)	129.5(3)	C(20)-C(19)-S(1)	119.4(3)
N(2)-C(9)-C(4)	107.5(3)	C(24)-C(19)-S(1)	120.0(3)
C(8)-C(9)-C(4)	123.0(3)	C(19)-C(20)-C(21)	119.4(3)
C(3)-C(10)-N(2)	110.4(3)	C(19)-C(20)-H(20)	120.3
C(3)-C(10)-C(11)	126.8(3)	C(21)-C(20)-H(20)	120.3
N(2)-C(10)-C(11)	122.6(3)	C(20)-C(21)-C(22)	121.2(3)
N(1)-C(11)-C(10)	108.0(2)	C(20)-C(21)-H(21)	119.4
N(1)-C(11)-C(13)	112.7(2)	C(22)-C(21)-H(21)	119.4
C(10)-C(11)-C(13)	114.3(3)	C(21)-C(22)-C(23)	118.2(3)
N(1)-C(11)-H(11)	107.2	C(21)-C(22)-C(25)	120.3(3)
C(10)-C(11)-H(11)	107.2	C(23)-C(22)-C(25)	121.5(3)
C(13)-C(11)-H(11)	107.2	C(24)-C(23)-C(22)	121.5(3)
C(1)-C(12)-H(12A)	109.5	C(24)-C(23)-H(23)	119.3
C(1)-C(12)-H(12B)	109.5	C(22)-C(23)-H(23)	119.3
H(12A)-C(12)-H(12B)	109.5	C(23)-C(24)-C(19)	119.3(3)
C(1)-C(12)-H(12C)	109.5	C(23)-C(24)-H(24)	120.3
H(12A)-C(12)-H(12C)	109.5	C(19)-C(24)-H(24)	120.3

C(22)-C(25)-H(25A)	109.5	C(10)-N(2)-C(9)	108.3(3)
C(22)-C(25)-H(25B)	109.5	C(10)-N(2)-H(2)	125.8
H(25A)-C(25)-H(25B)	109.5	C(9)-N(2)-H(2)	125.8
C(22)-C(25)-H(25C)	109.5	O(2)-S(1)-O(1)	118.74(14)
H(25A)-C(25)-H(25C)	109.5	O(2)-S(1)-N(1)	108.52(14)
H(25B)-C(25)-H(25C)	109.5	O(1)-S(1)-N(1)	106.97(14)
C(1)-N(1)-C(11)	121.1(3)	O(2)-S(1)-C(19)	106.62(15)
C(1)-N(1)-S(1)	115.8(2)	O(1)-S(1)-C(19)	108.96(15)
C(11)-N(1)-S(1)	120.0(2)	N(1)-S(1)-C(19)	106.43(14)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2$x 10^3)for **28**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

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

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **28**.

	x	y	z	U(eq)
H(1)	5558	4624	2675	22
H(2A)	6627	6163	3318	23
H(2B)	5088	5710	3621	23
H(5)	7353	7635	4454	25
H(6)	8654	8341	5410	29
H(7)	9547	7196	6298	27
H(8)	9214	5277	6238	25
H(11)	5570	2974	4473	20
H(12A)	8539	4362	3122	35
H(12B)	7991	4980	2425	35
H(12C)	7827	3671	2489	35
H(14)	9355	3153	3919	26
H(15)	10972	1665	3850	30
H(16)	10123	-129	4065	32
H(17)	7623	-421	4311	30
H(18)	5991	1064	4344	25
H(20)	3037	4480	2214	28
H(21)	1604	6074	2297	31
H(23)	918	5472	4364	30
H(24)	2458	3943	4307	26
H(25A)	-772	6802	3560	50
H(25B)	140	7322	2919	50
H(25C)	688	7507	3712	50
H(2)	8053	3663	5358	21

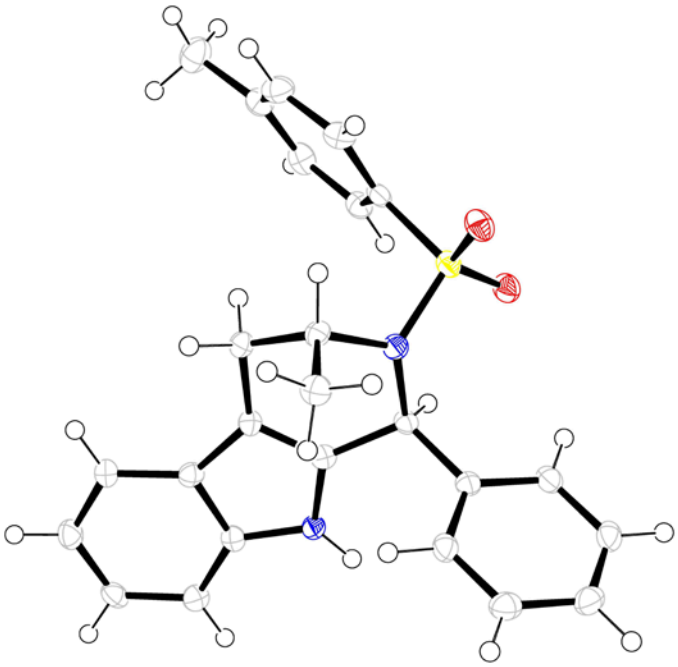


Figure S2. X-ray crystal structure of **28** with 50% probability ellipsoids.

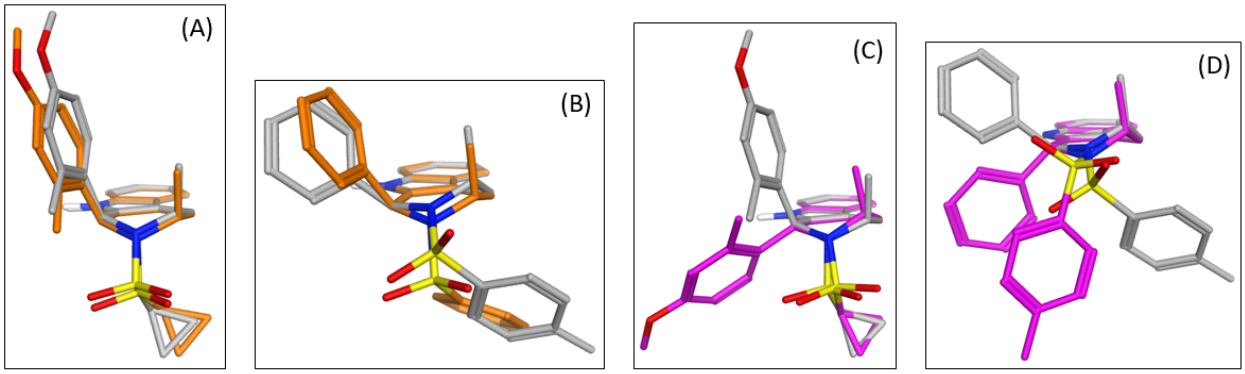
Quantum chemical calculations

The energies of cis and trans isomers of compounds **14** and **28** were calculated using the using the m062x basis set (1) within Gaussian09 (2). The X-ray structures of each were subjected to optimization within the QM package followed by heat of formation calculations *in vacuo* and in THF using the default solvation model in Gaussian. To check the energetics of the X-ray structures, each structure was also minimized using the default MMFF94 forcefield in MOE (3) and resubmitted to Gaussian for energy calculations. The resulting heats of formation were identical, indicating the optimization procedure within the QM calculations had allowed the X-ray and molecular mechanics minimized conformations to settle into the same minimum energy conformation. The chirality of the 3-aryl groups was then switched to generate a *trans*-1,3-disubstitution on the piperidine ring, followed by minimization in MOE to relieve any steric contacts. Heats of formation were then calculated on the QM-optimized versions of these isomers *in vacuo* and THF. Results are shown in Table S1. The *cis*-cyclopropyl analog **14** proved to be 3.6 - 4 kcal/mol more stable than the *trans* version, both *in vacuo* and in THF, consistent with the NMR and X-ray structure findings. The *cis*-tolyl analog **28** showed the *cis* and *trans* isomers to be essentially equienergetic. A steric contact between the SO2 oxygens and the pendant 3-aryl ring in the *trans* version of **28** was offset by an aryl-aryl stacking stabilization produced by the QM geometry optimization algorithm, coupled with a slight change in the sulfonyl nitrogen hybridization.

Table S11. Energetics of *cis* and *trans* isomers of compounds **14** and **28** after QM geometry optimization

Conformer	Energy, kcal/mol			
	Compound **14**		Compound **28**	
	In vacuo	In THF	*In vacuo*	In THF
cis-3-aryl, Xray	-1019606.426		-1019497.471	
cis-3-aryl, Xray, minimized in MOE	-1019606.426	-1019615.467	-1019497.471	-1019506.201
trans-3-aryl, minimized in MOE	-1019602.401	-1019611.895	-1019498.689	-1019506.869
Δ *cis-trans*	4.02	3.57	-1.22	-0.67

Figure S3. Conformations of Xray and QM-optimized structures used in the energy calculations



Cpd 14
X-ray
QM optimized

Cpd 28
X-ray
QM optimized

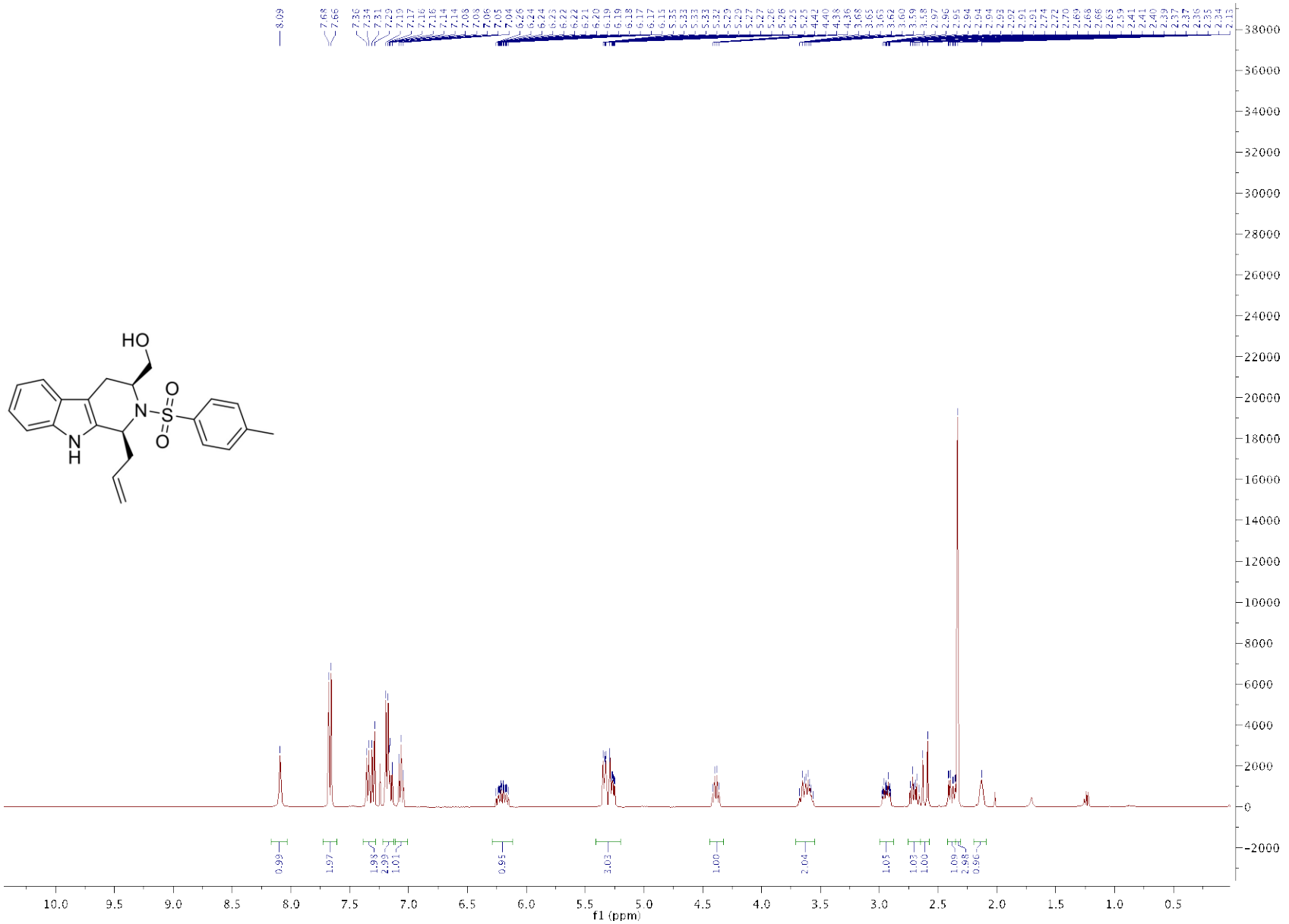
Cpd 14
X-ray
trans 3-aryl isomer,
QM optimized

Cpd 28
X-ray
trans 3-aryl isomer,
QM optimized

(1) Y. Zhao and D. G. Truhlar, "The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals," *Theor. Chem. Acc.*, 120 (2008) 215-41.

(2) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian* 09 (Gaussian, Inc., Wallingford CT, 2009).

(3) Version 2018.0101, available from Chemical Computing Group (http://www.chemcomp.com), was used for the modeling and minimizations.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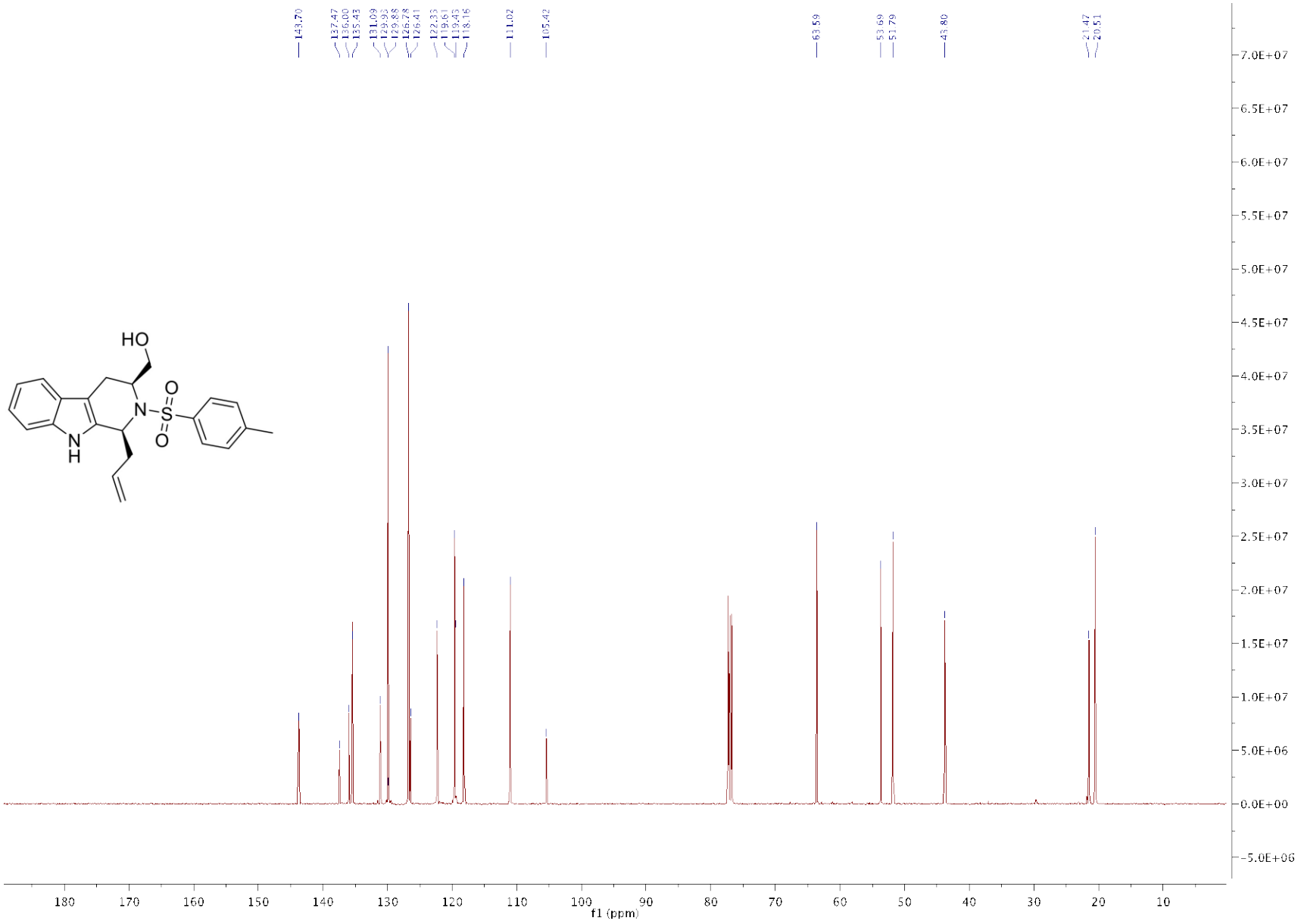
N
S
O
O
N
H
f1 (ppm)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63.59
53.69
51.79
43.80
21.47
20.51
HO
N
S
O
O
N
H
7.0E+07
6.5E+07
6.0E+07
5.5E+07
5.0E+07
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
-5.0E+06
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60
50
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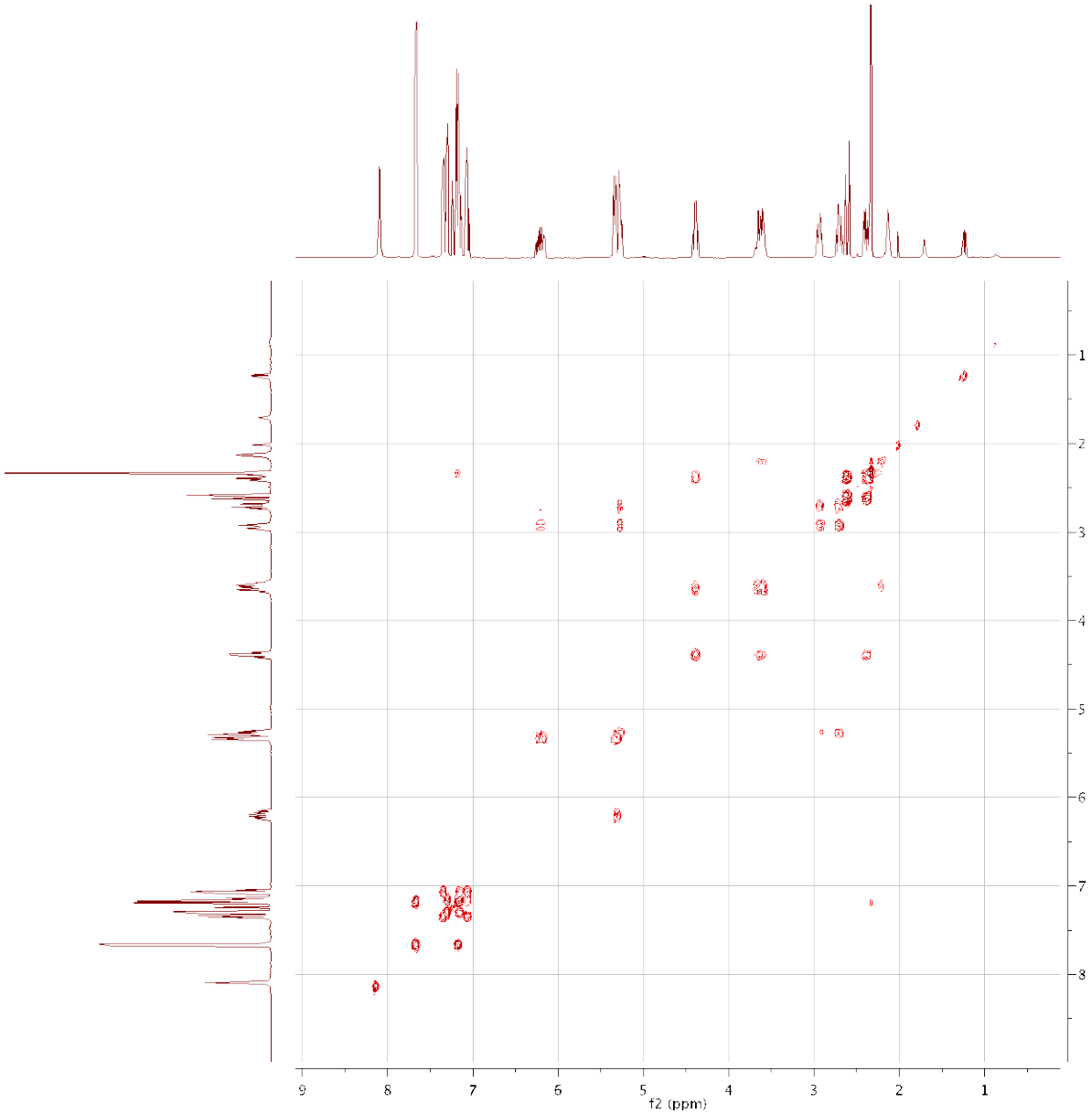
f1 (ppm)



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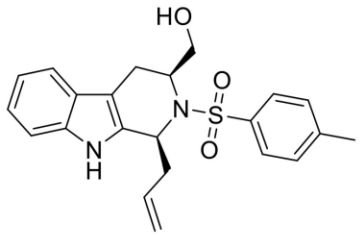

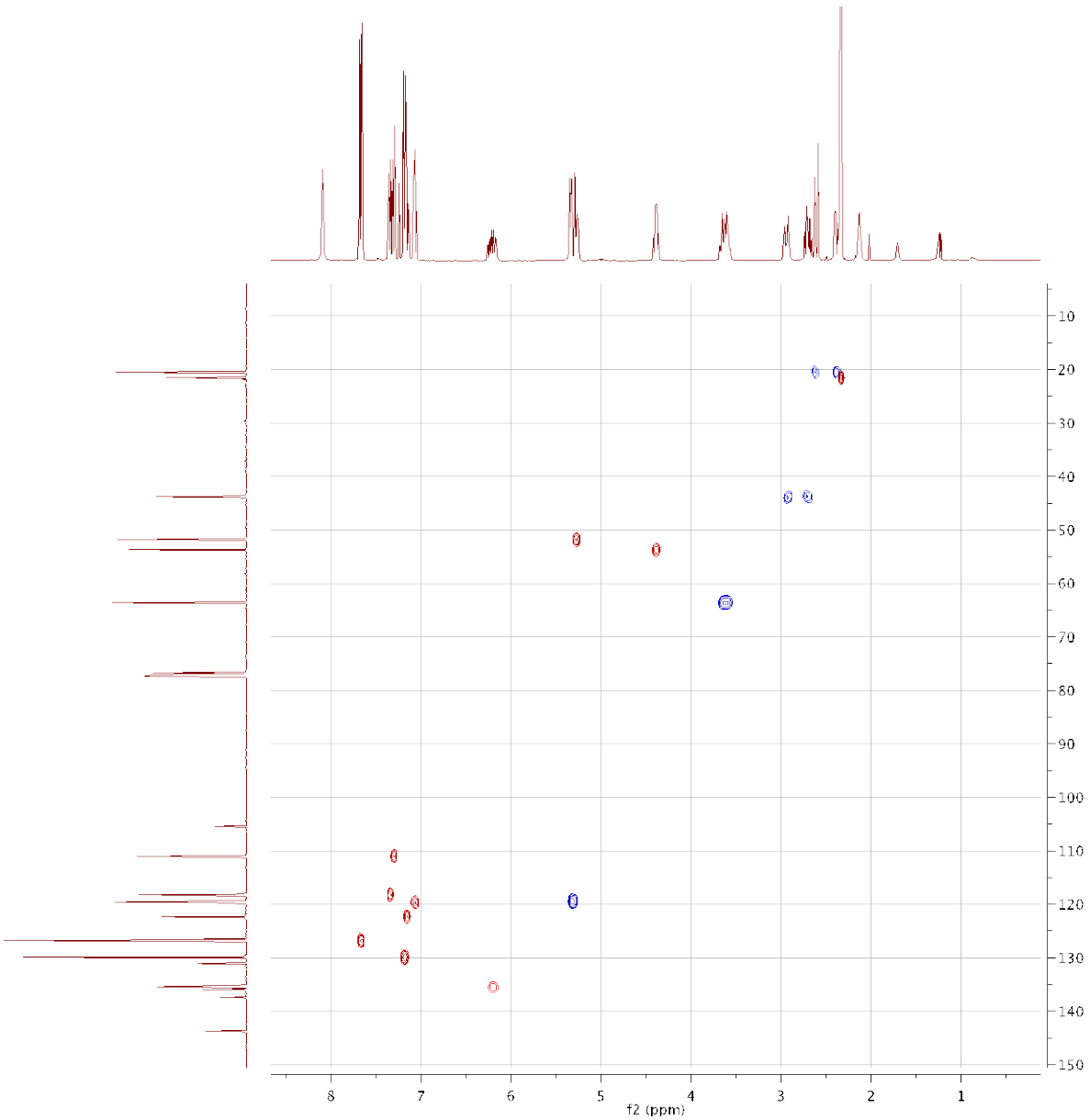

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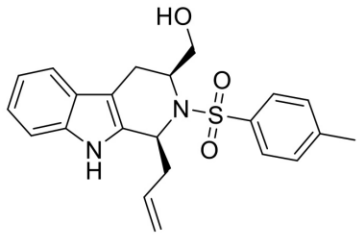
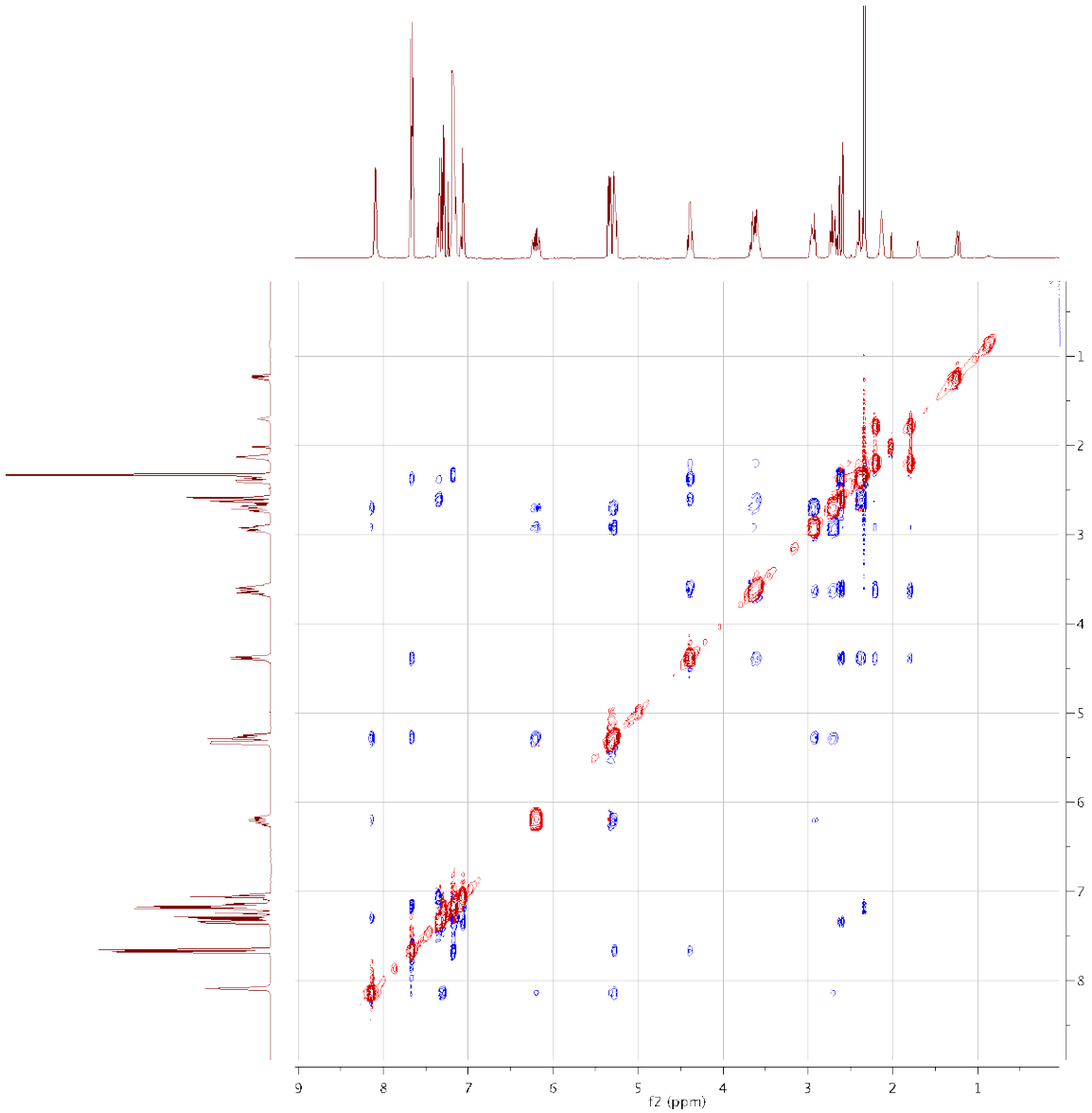
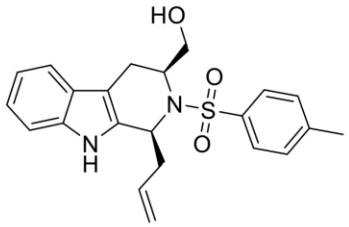
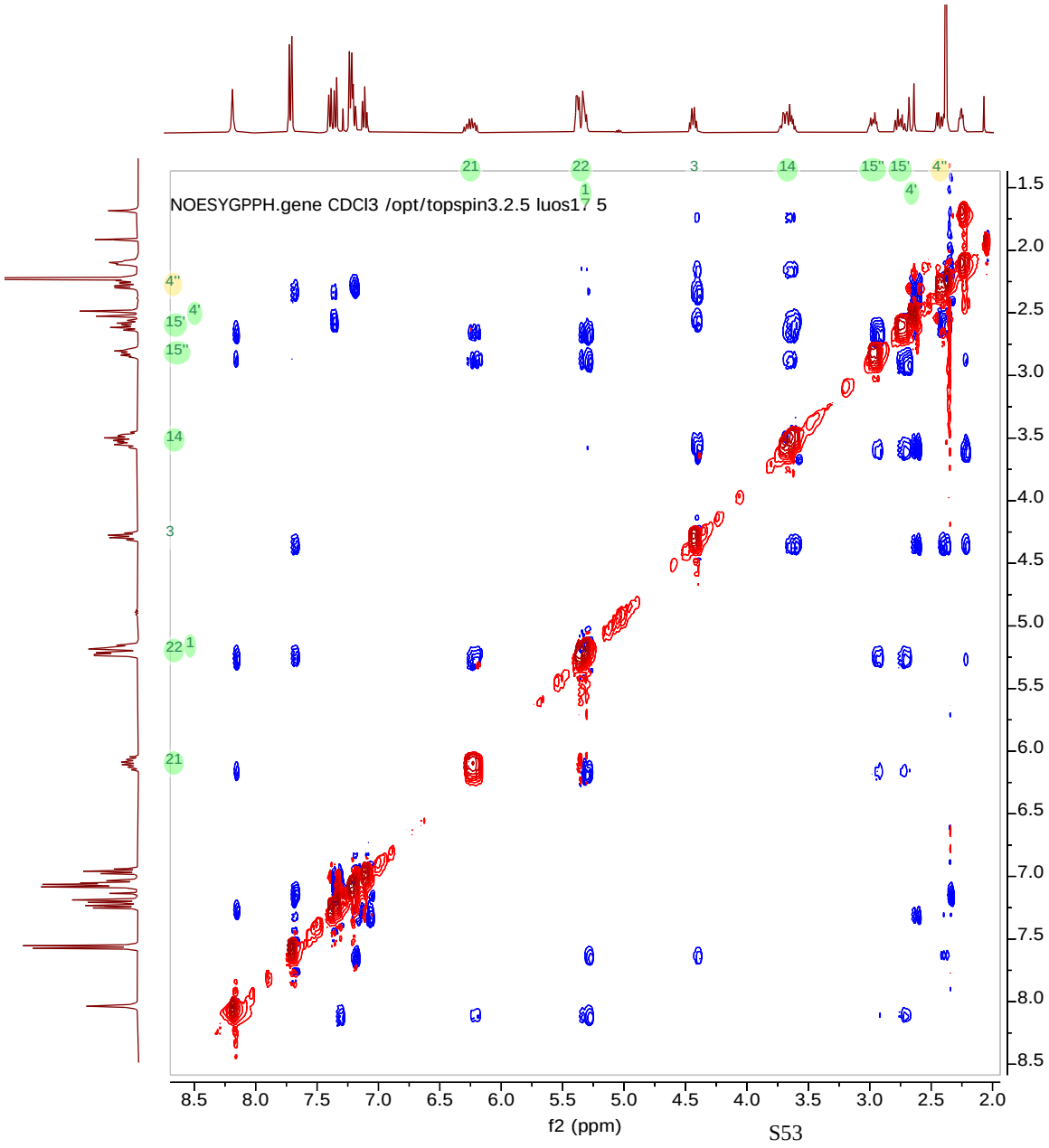
5	Pulse Sequence	hsqcedetgp
6	Number of Scans	8
7	Pulse Width	12.0000
8	Presaturation Frequency	
9	Acquisition Date	2016-08-31T19:35:43
10	Spectrometer Frequency	(400.33, 100.67)
11	Spectral Width	(3731.3, 20161.3)
12	Lowest Frequency	(-43.6, -1021.0)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



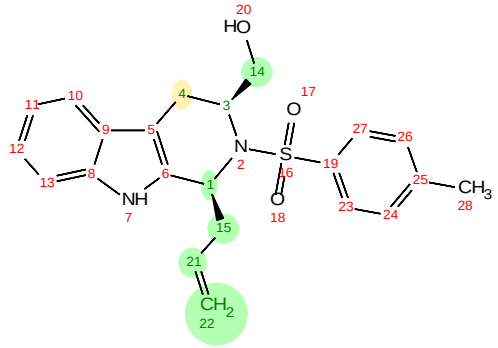


	Parameter	Value
1	Data File Name	71465-148/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	chemnmr
4	Solvent	CDCl3
5	Pulse Sequence	noesygpphpp
6	Number of Scans	64
7	Pulse Width	12.0000
8	Presaturation Frequency	
9	Acquisition Date	2016-08-31T20:18:05
10	Spectrometer Frequency	(400.33, 400.33)
11	Spectral Width	(3731.3, 3731.3)
12	Lowest Frequency	(-42.4, -42.4)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 200)
15	Spectral Size	(1024, 1024)





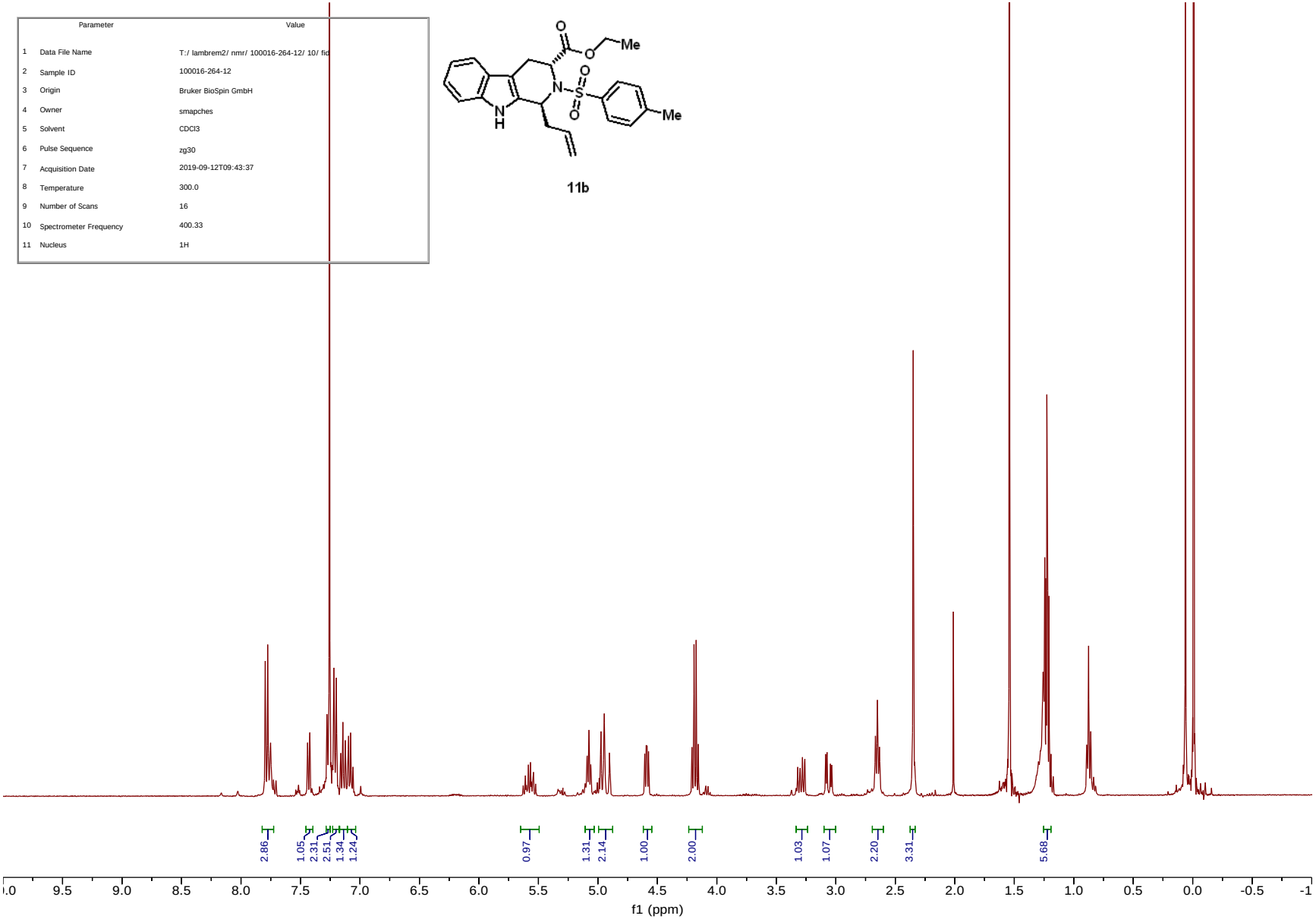
	Parameter	Value
1	Data File Name	Z:/ marzen400/ data/ luos17/ nmr/ 71465-148/ 13/ ser
2	Sample ID	71465-148
3	Origin	Bruker BioSpin GmbH
4	Owner	chemnmr
5	Solvent	CDCl3
6	Pulse Sequence	noesygpphpp
7	Acquisition Date	2016-08-31T20:18:05
8	Temperature	300.0
9	Number of Scans	64
10	Spectrometer Frequency	(400.33, 400.33)
11	Spectral Width	(3731.3, 3731.3)
12	Lowest Frequency	(-42.4, -42.4)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 200)
15	Spectral Size	(1024, 1024)
16	Digital Resolution	(3.64, 3.64)

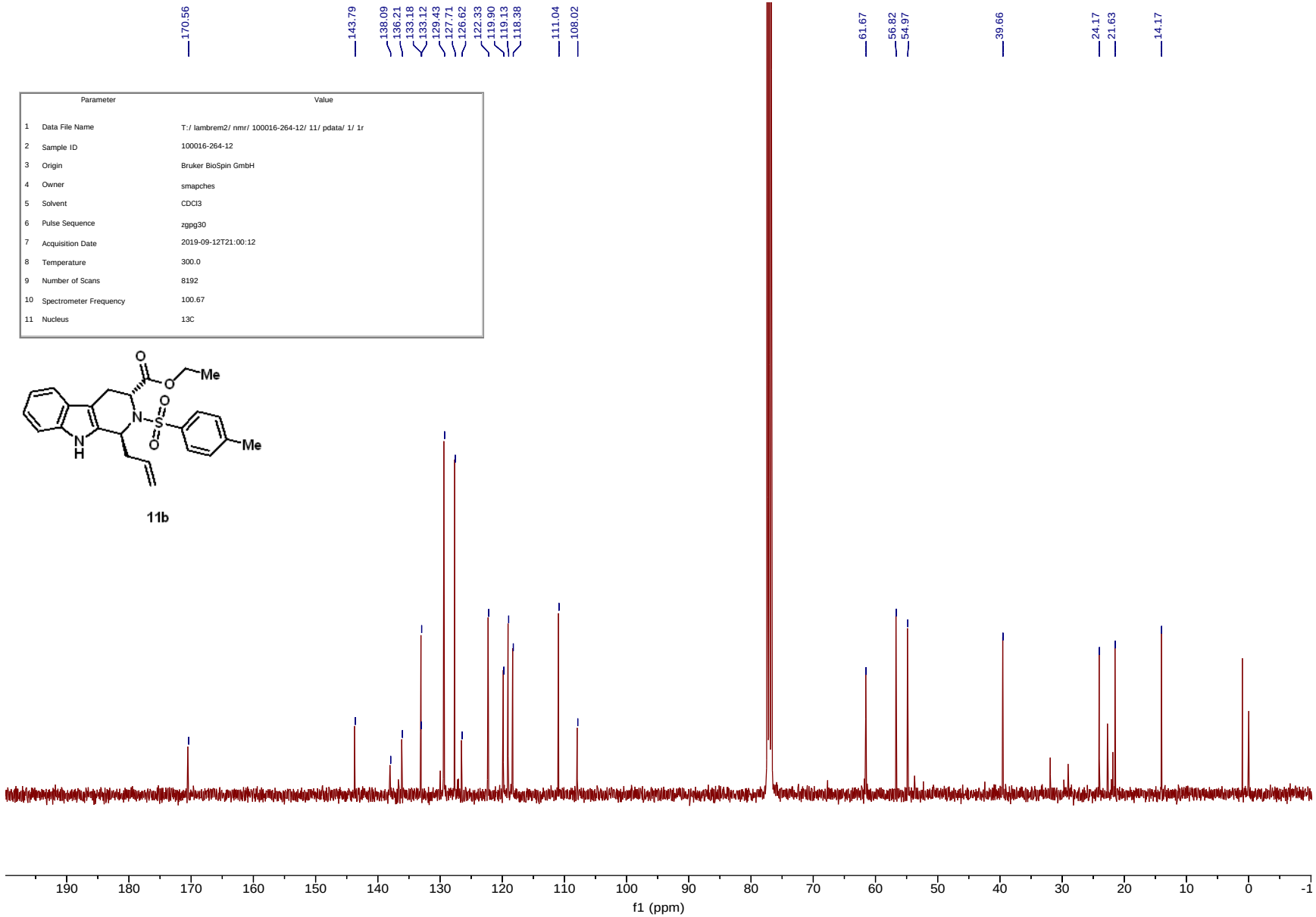


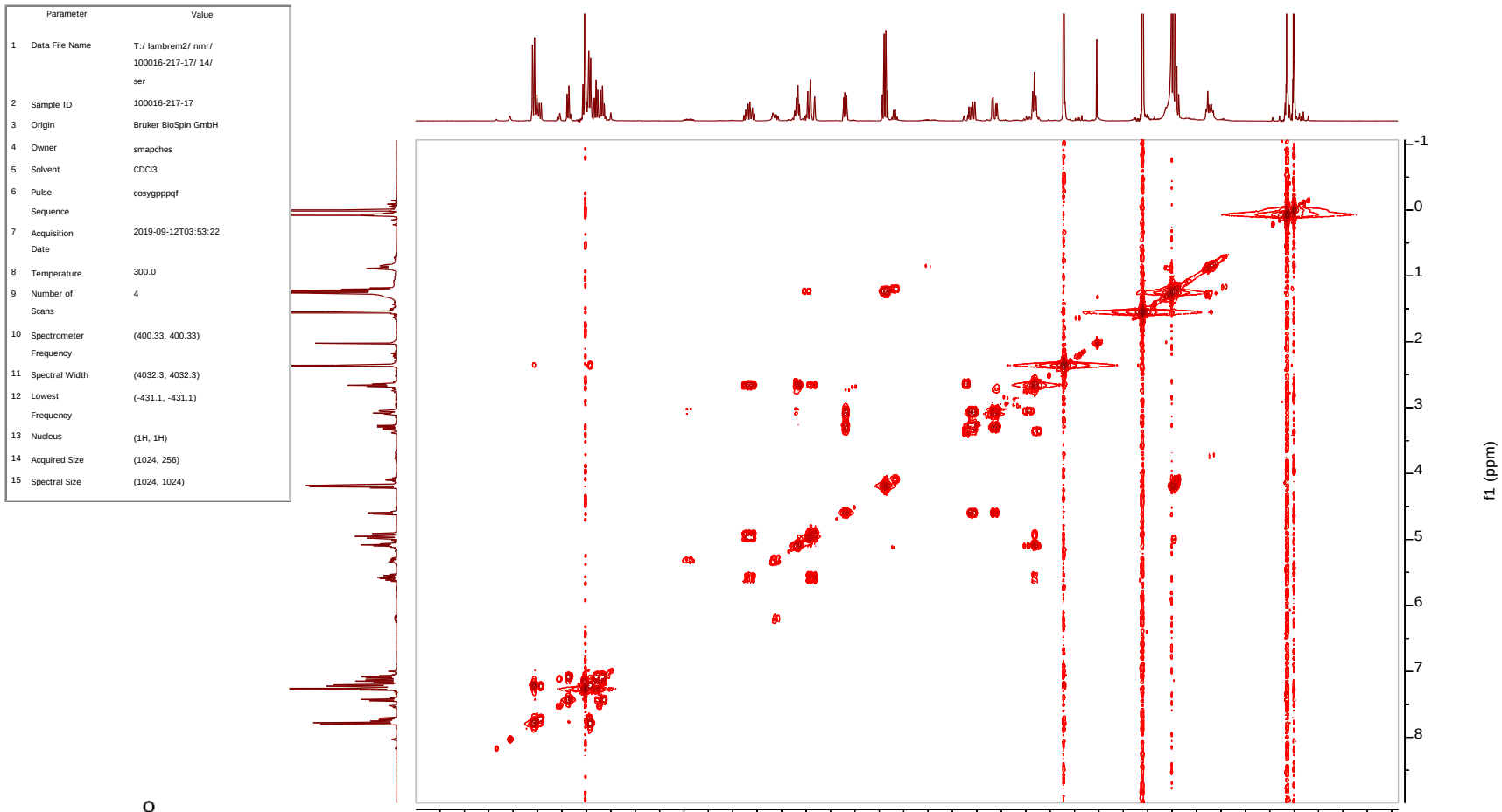
NOE observed between H14 and H15

	Parameter	Value
1	Data File Name	T:/ lambrem2/ nmr/ 100016-264-12/ 10/ fid
2	Sample ID	100016-264-12
3	Origin	Bruker BioSpin GmbH
4	Owner	smapches
5	Solvent	CDCl3
6	Pulse Sequence	zg30
7	Acquisition Date	2019-09-12T09:43:37
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	400.33
11	Nucleus	1H

11b

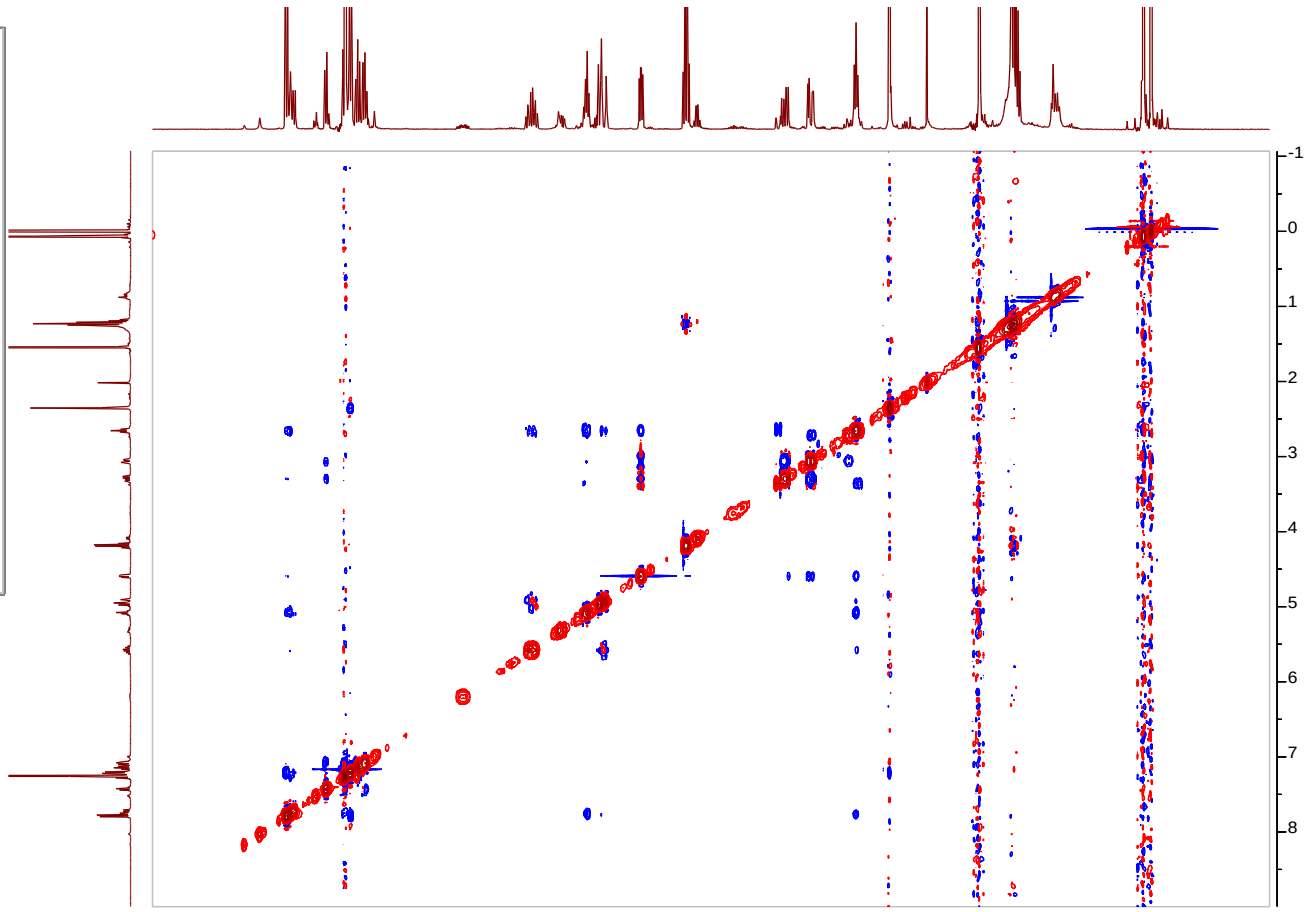


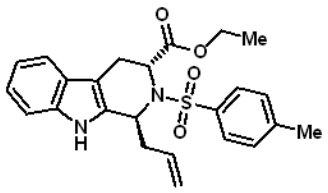

170.56
143.79
138.09
136.21
133.18
133.12
129.43
127.71
126.62
122.33
119.90
119.13
118.38
111.04
108.02
61.67
56.82
54.97
39.66
24.17
21.63
14.17
Parameter
Value
1 Data File Name
T:/ lambrem2/ nmr/ 100016-264-12/ 11/ pdata/ 1/ 1r
2 Sample ID
100016-264-12
3 Origin
Bruker BioSpin GmbH
4 Owner
smapches
5 Solvent
CDCl3
6 Pulse Sequence
zgpg30
7 Acquisition Date
2019-09-12T21:00:12
8 Temperature
300.0
9 Number of Scans
8192
10 Spectrometer Frequency
100.67
11 Nucleus
13C
Me
Me
11b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


Parameter Value
1 Data File Name T:/ lambrem2/ nmr/ 100016-217-17/ 14/ ser
2 Sample ID 100016-217-17
3 Origin Bruker BioSpin GmbH
4 Owner smapches
5 Solvent CDCl3
6 Pulse Sequence cosygpppqf
7 Acquisition Date 2019-09-12T03:53:22
8 Temperature 300.0
9 Number of Scans 4
10 Spectrometer Frequency (400.33, 400.33)
11 Spectral Width (4032.3, 4032.3)
12 Lowest Frequency (-431.1, -431.1)
13 Nucleus (1H, 1H)
14 Acquired Size (1024, 256)
15 Spectral Size (1024, 1024)
f2 (ppm)
f1 (ppm)
Me
Me
N
H
S

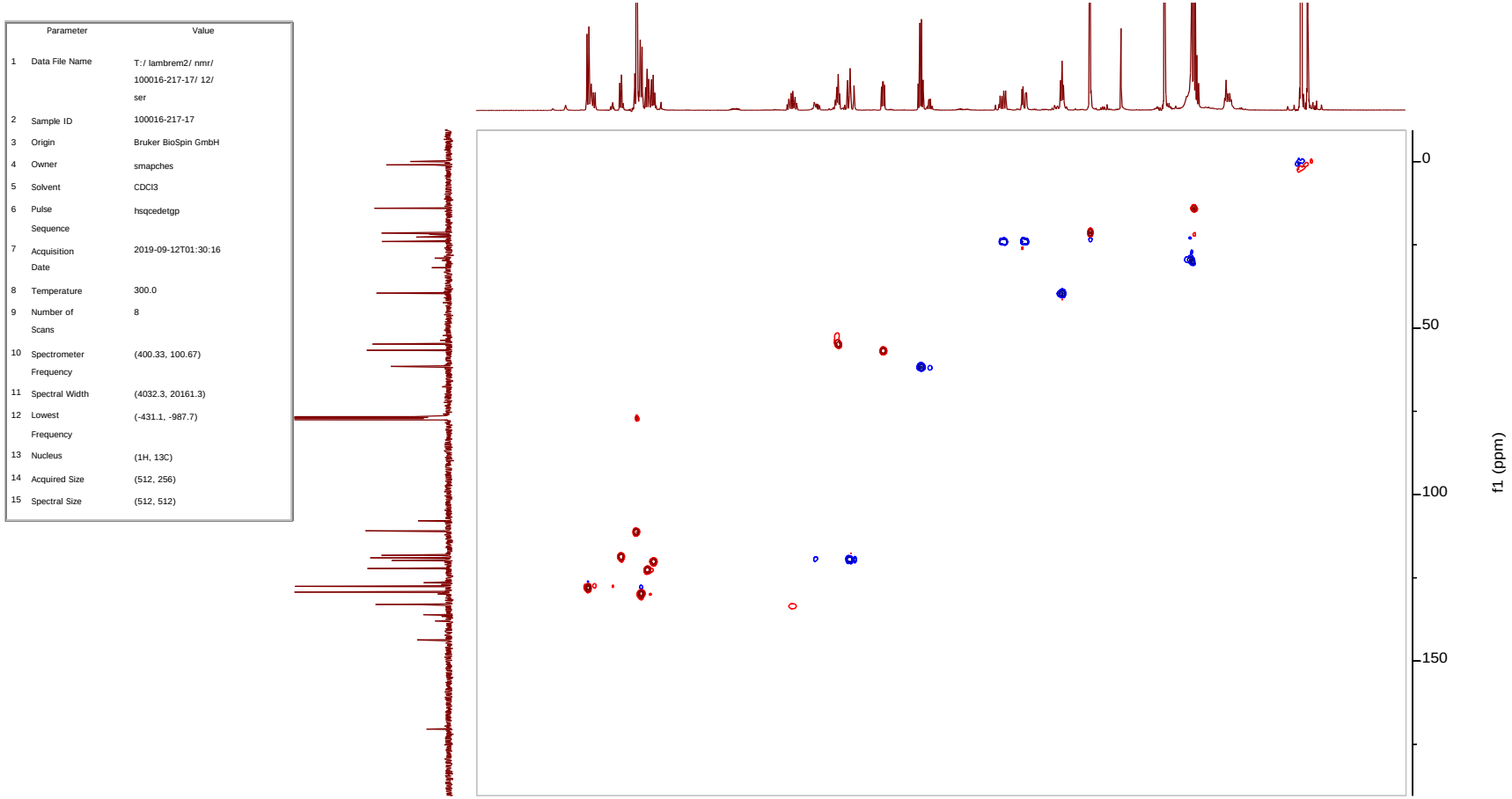
11b

	Parameter	Value
1	Data File Name	T:/ lambrem2/ nmr/ 100016-217-17/ 13/ ser
2	Sample ID	100016-217-17
3	Origin	Bruker BioSpin GmbH
4	Owner	smapches
5	Solvent	CDCl3
6	Pulse Sequence	noesygpphpp
7	Acquisition Date	2019-09-12T02:10:53
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(400.33, 400.33)
11	Spectral Width	(4032.3, 4032.3)
12	Lowest Frequency	(-431.1, -431.1)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 200)
15	Spectral Size	(1024, 1024)

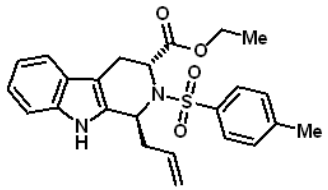




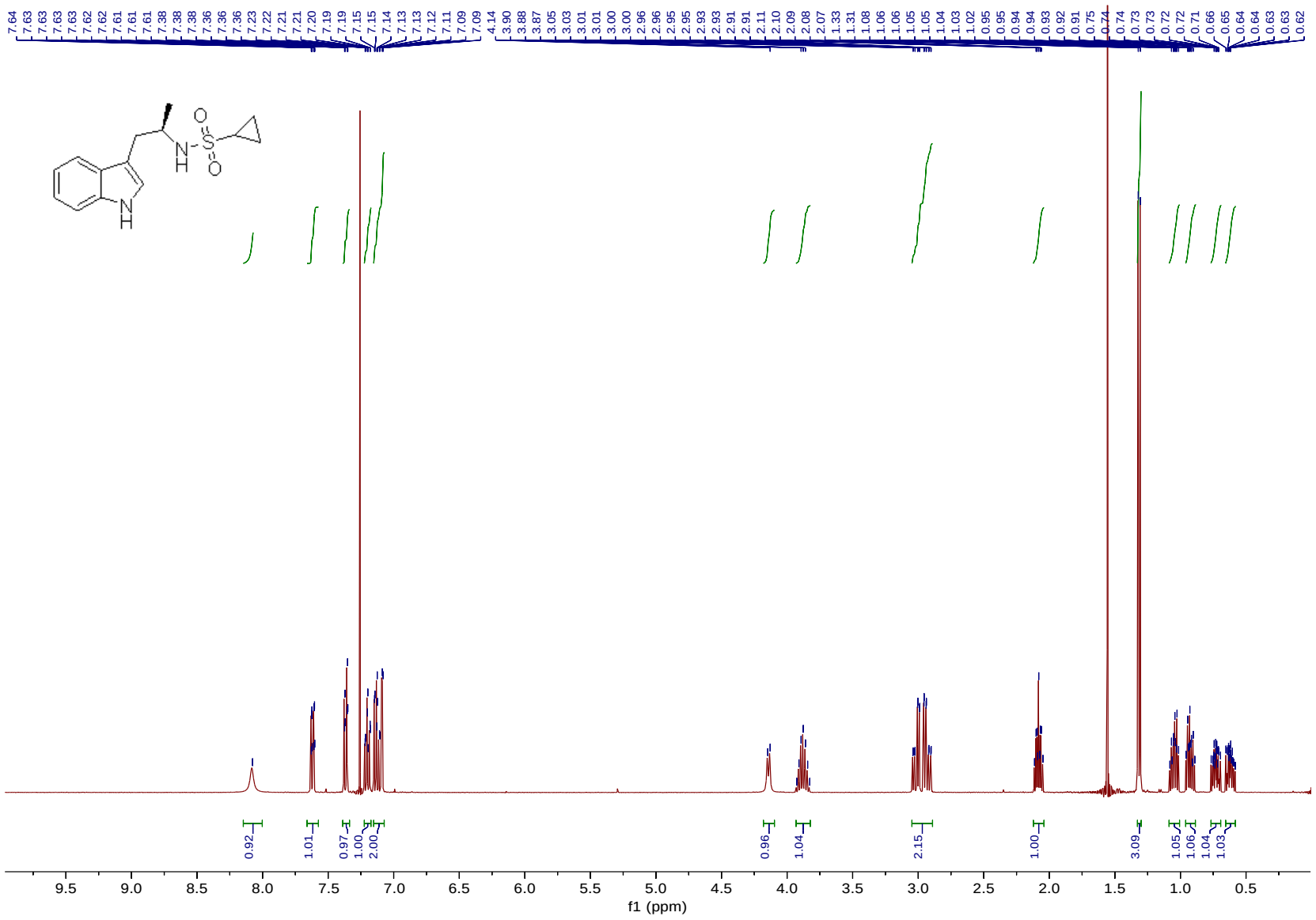
11b

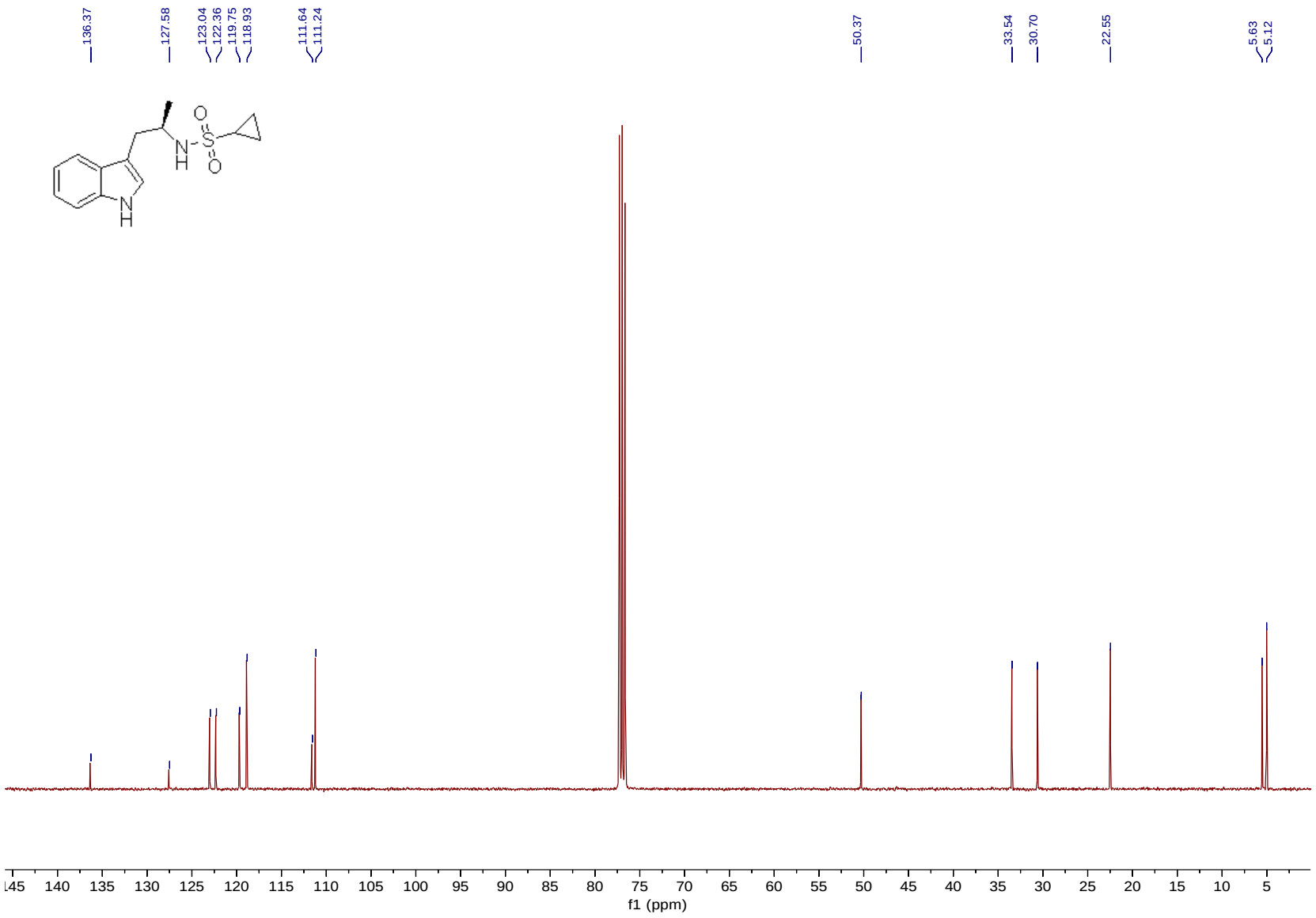


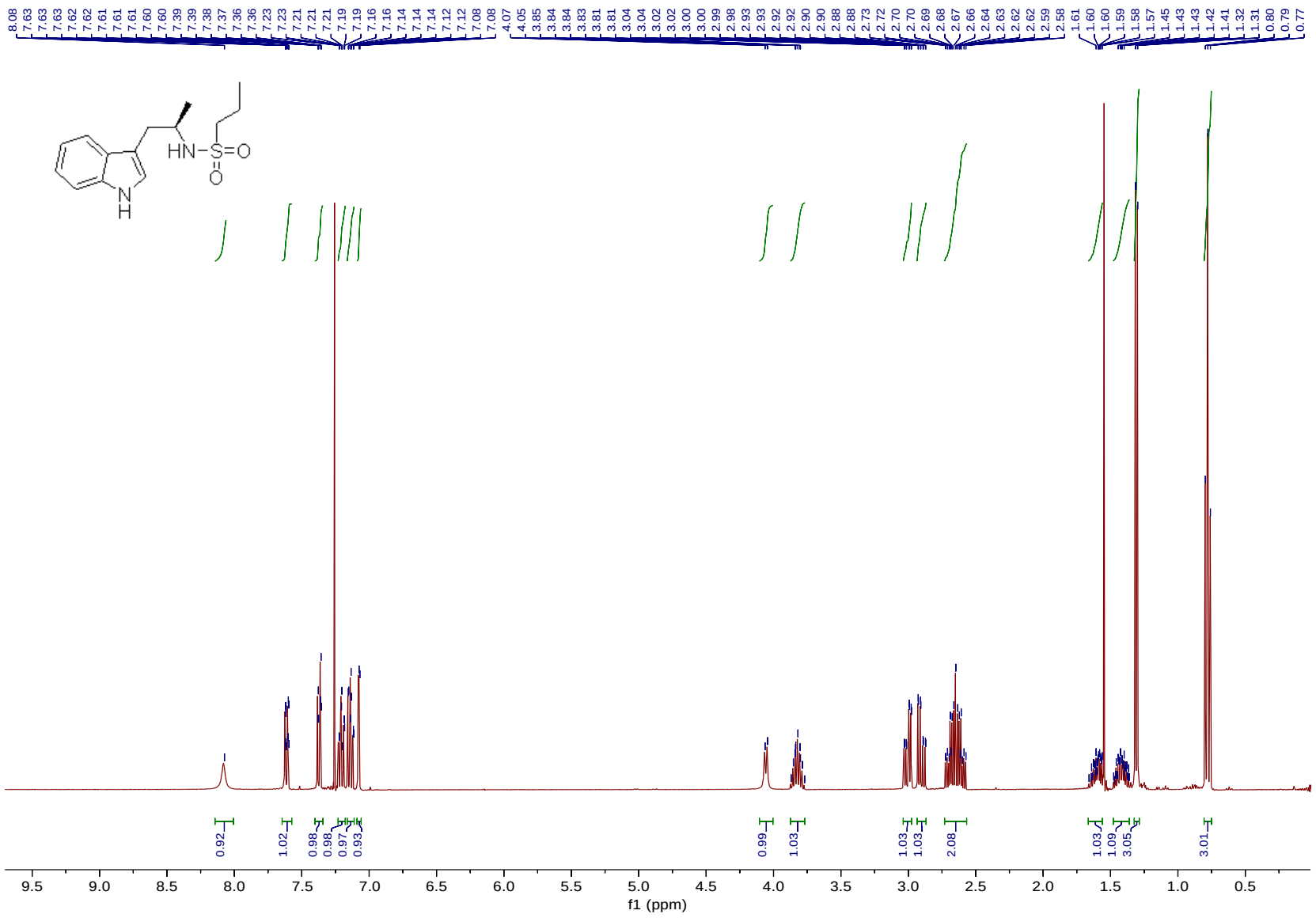
	Parameter	Value
1	Data File Name	T:/ lambrem2/ nmr/ 100016-217-17/ 12/ ser
2	Sample ID	100016-217-17
3	Origin	Bruker BioSpin GmbH
4	Owner	smapches
5	Solvent	CDCl3
6	Pulse Sequence	hsqcedetgp
7	Acquisition Date	2019-09-12T01:30:16
8	Temperature	300.0
9	Number of Scans	8
10	Spectrometer Frequency	(400.33, 100.67)
11	Spectral Width	(4032.3, 20161.3)
12	Lowest Frequency	(-431.1, -987.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

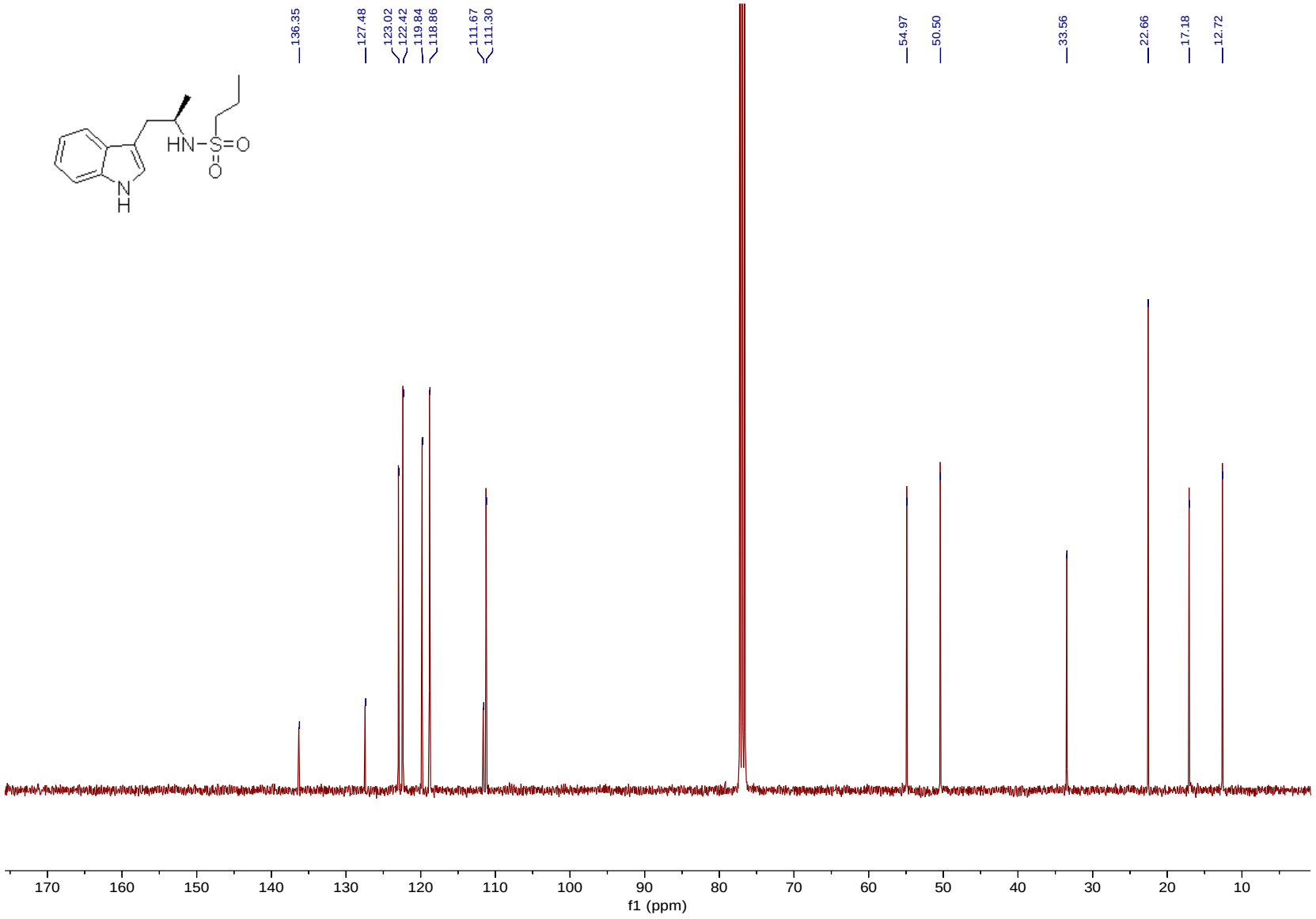


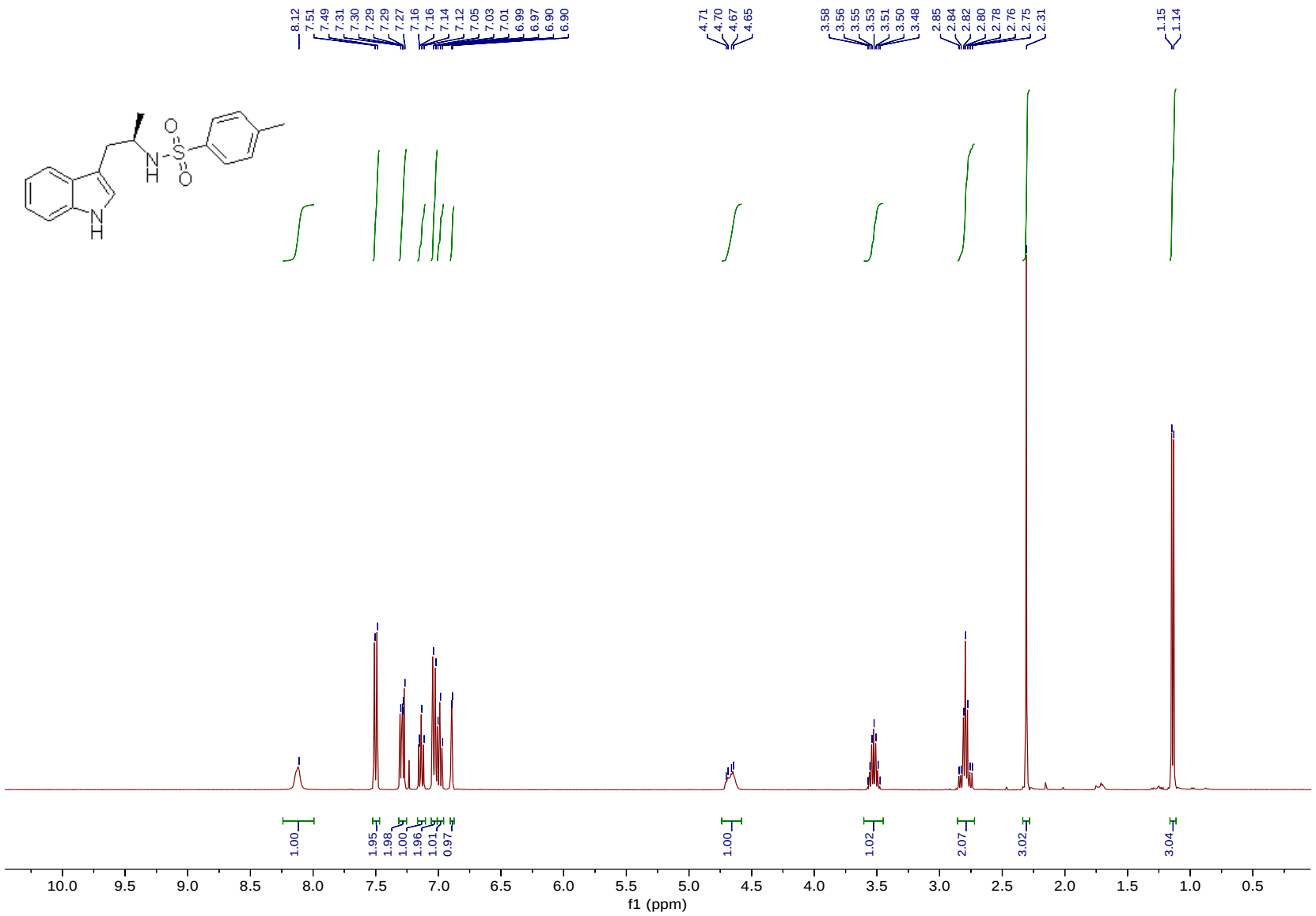
11b

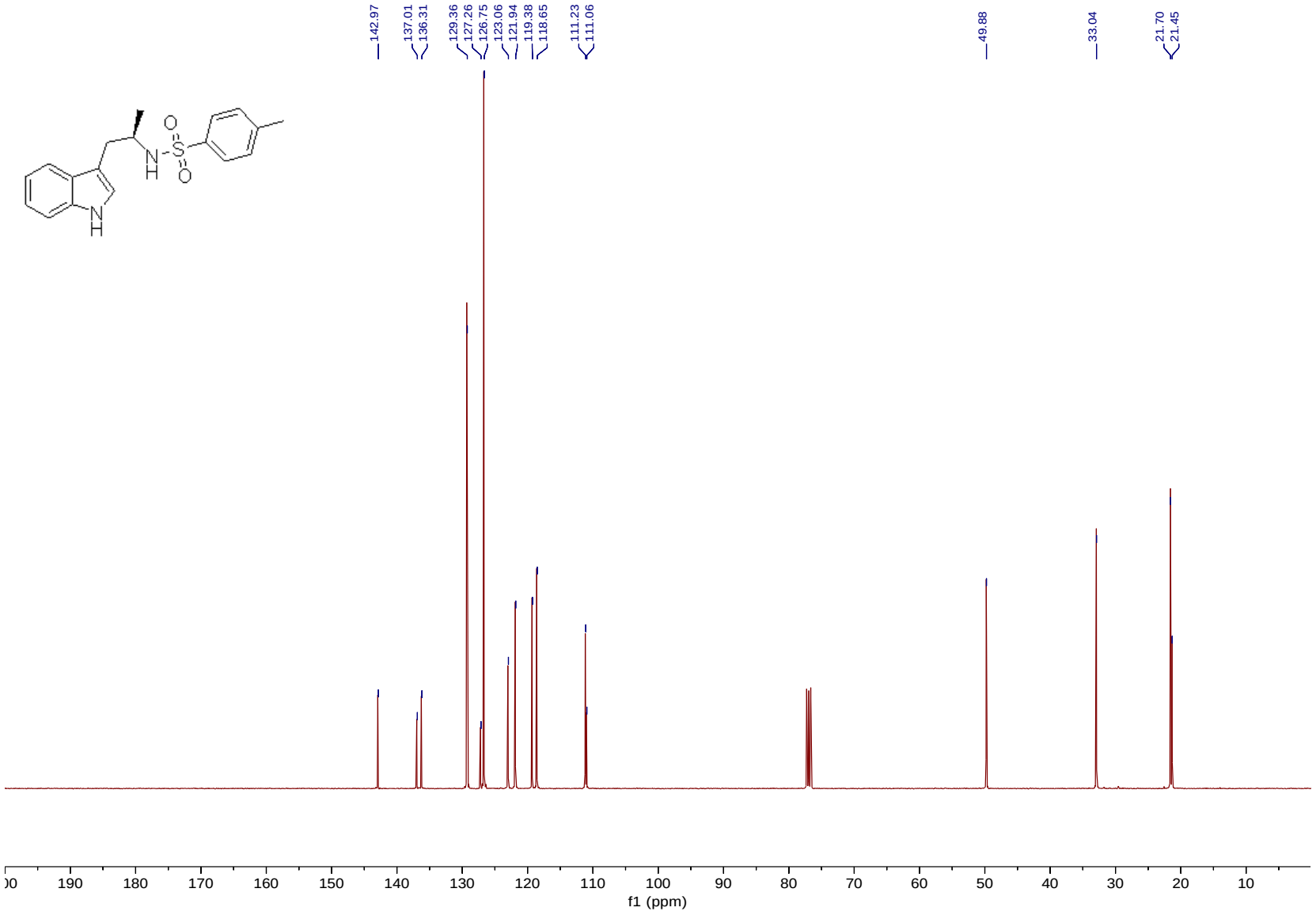

7.64 7.63 7.63 7.63 7.63 7.62 7.62 7.61 7.61 7.61 7.38 7.38 7.38 7.36 7.36 7.36 7.23 7.22 7.21 7.21 7.20 7.19 7.19 7.15 7.15 7.14 7.13 7.13 7.12 7.11 7.09 7.09
4.14 3.90 3.88 3.87 3.05 3.03 3.01 3.01 3.00 3.00 2.96 2.96 2.95 2.95 2.93 2.93 2.91 2.91 2.11 2.10 2.09 2.08 2.07 1.33 1.31 1.08 1.06 1.06 1.05 1.05 1.04 1.03 1.02 0.95 0.95 0.94 0.94 0.93 0.92 0.91 0.75 0.74 0.74 0.73 0.73 0.72 0.72 0.71 0.66 0.65 0.64 0.64 0.63 0.63 0.62
0.92 1.01 0.97 1.00 2.00 0.96 1.04 2.15 1.00 3.09 1.05 1.06 1.04 1.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

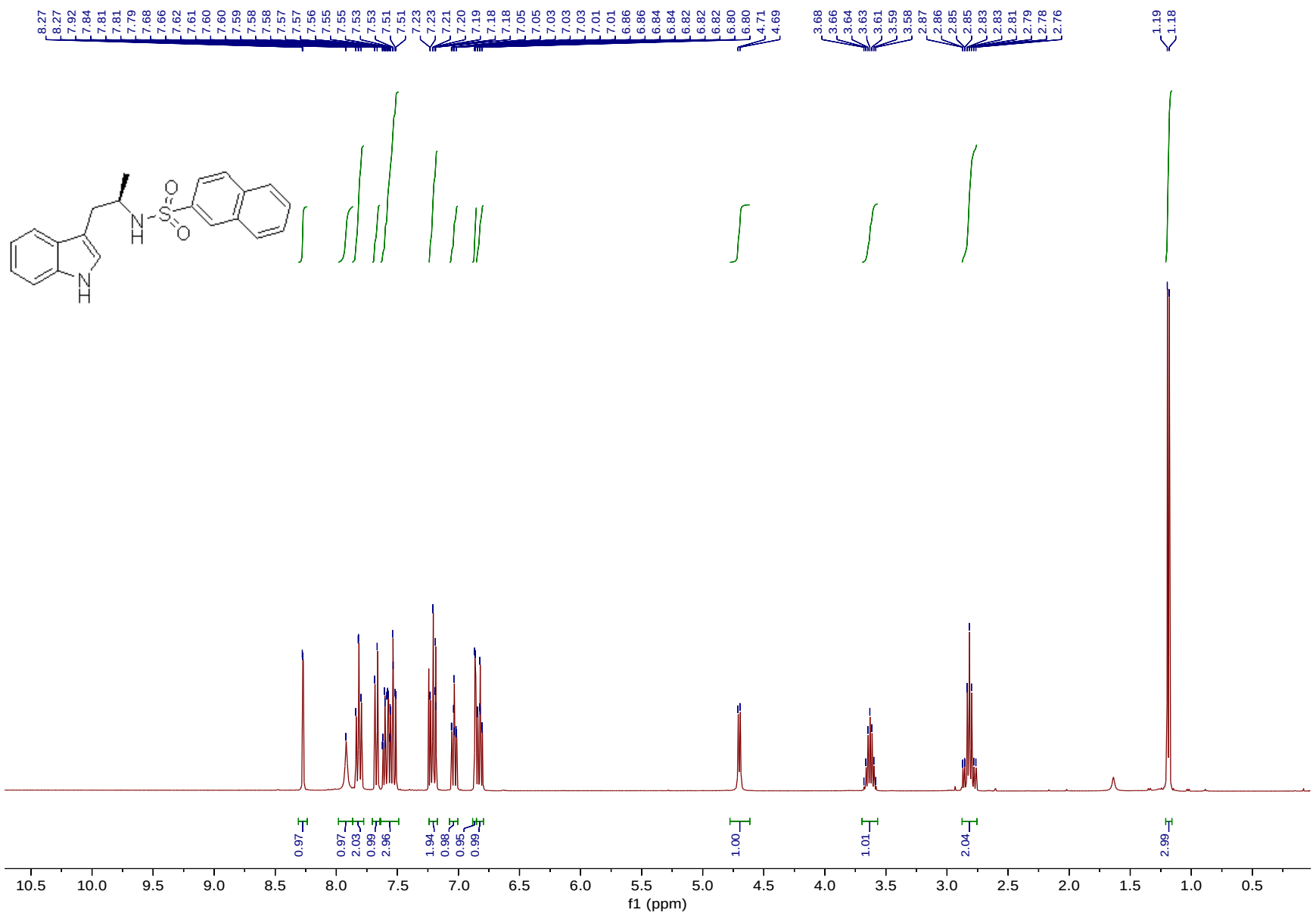

136.37
127.58
123.04
122.36
119.75
118.93
111.64
111.24
50.37
33.54
30.70
22.55
5.63
5.12
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
f1 (ppm)

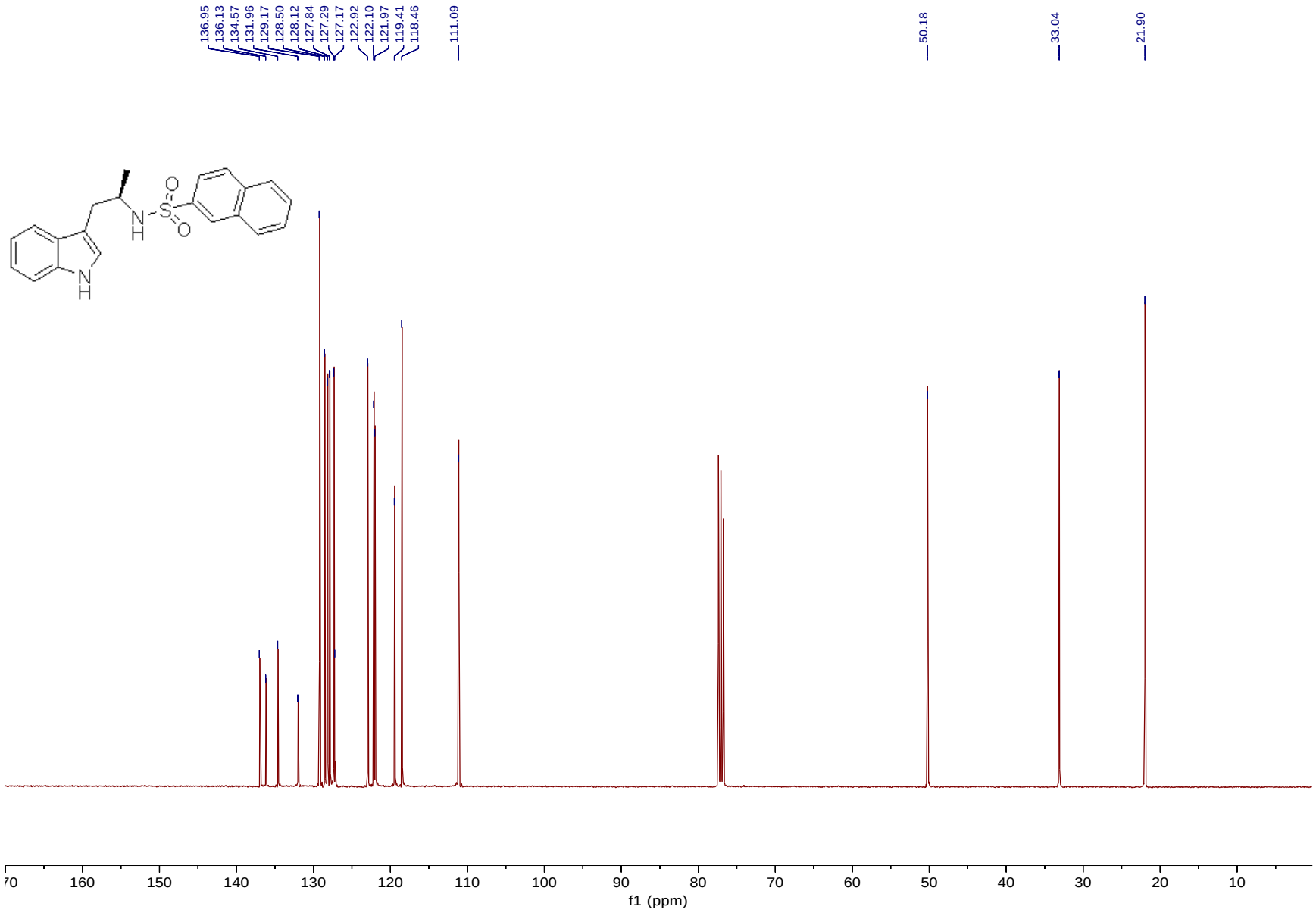

8.08 7.63 7.63 7.63 7.62 7.62 7.61 7.61 7.61 7.60 7.60 7.39 7.39 7.38 7.37 7.36 7.36 7.23 7.23 7.21 7.21 7.21 7.19 7.19 7.16 7.16 7.14 7.14 7.14 7.12 7.12 7.08 7.08
4.07 4.05 3.85 3.84 3.84 3.83 3.81 3.81 3.04 3.04 3.02 3.02 3.00 3.00 2.99 2.98 2.93 2.93 2.92 2.92 2.90 2.90 2.88 2.88 2.73 2.72 2.70 2.70 2.69 2.68 2.67 2.66 2.64 2.63 2.62 2.62 2.59 2.58
1.61 1.60 1.60 1.59 1.58 1.57 1.45 1.43 1.43 1.42 1.41 1.32 1.31 0.80 0.79 0.77
HN
S
O
O
N
H
0.92 1.02 0.98 0.98 0.97 0.93 0.99 1.03 1.03 1.03 2.08 1.03 1.09 3.05 3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

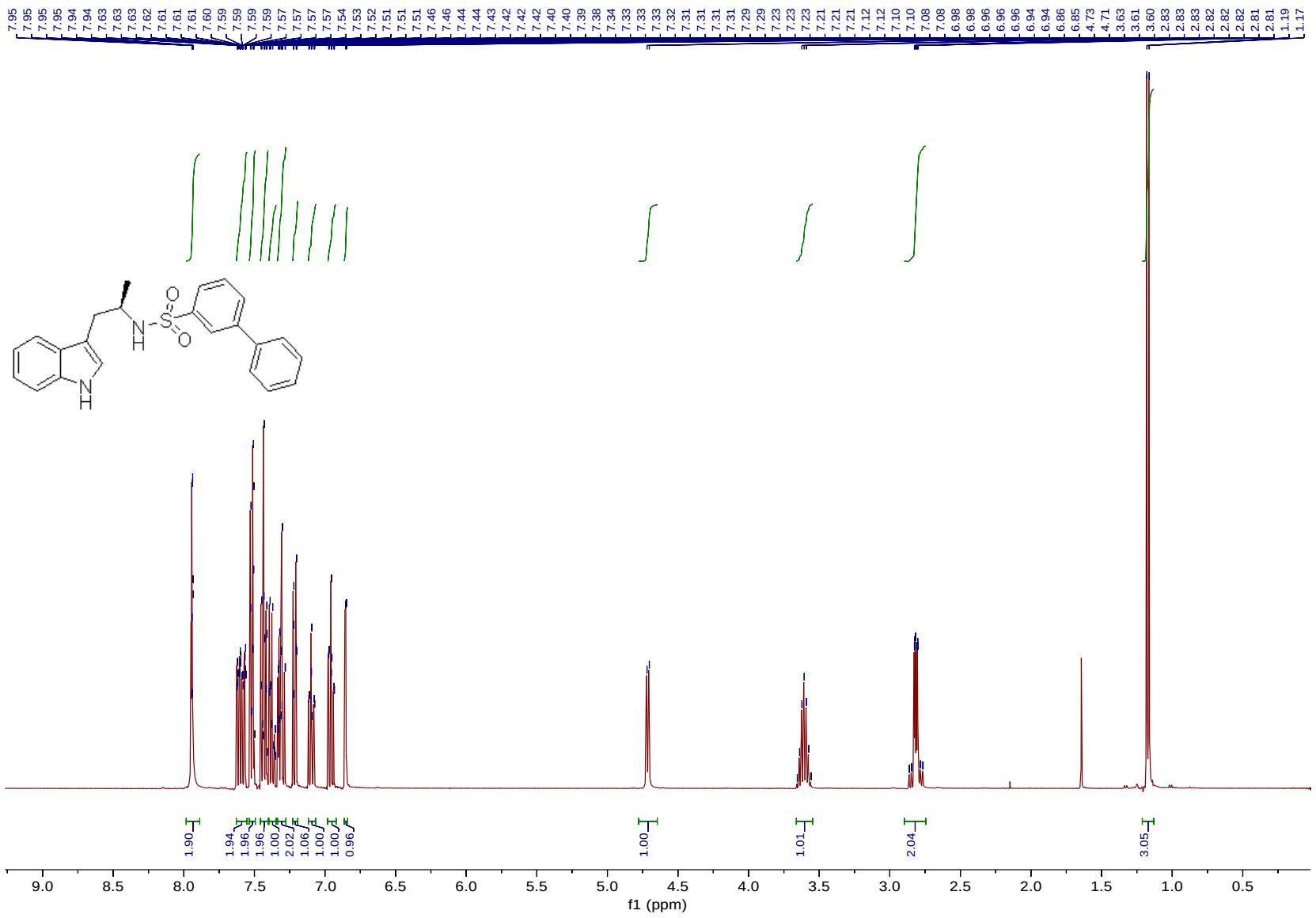

136.35
127.48
123.02
122.42
119.84
118.86
111.67
111.30
54.97
50.50
33.56
22.66
17.18
12.72
HN
S
O
O
N
H
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

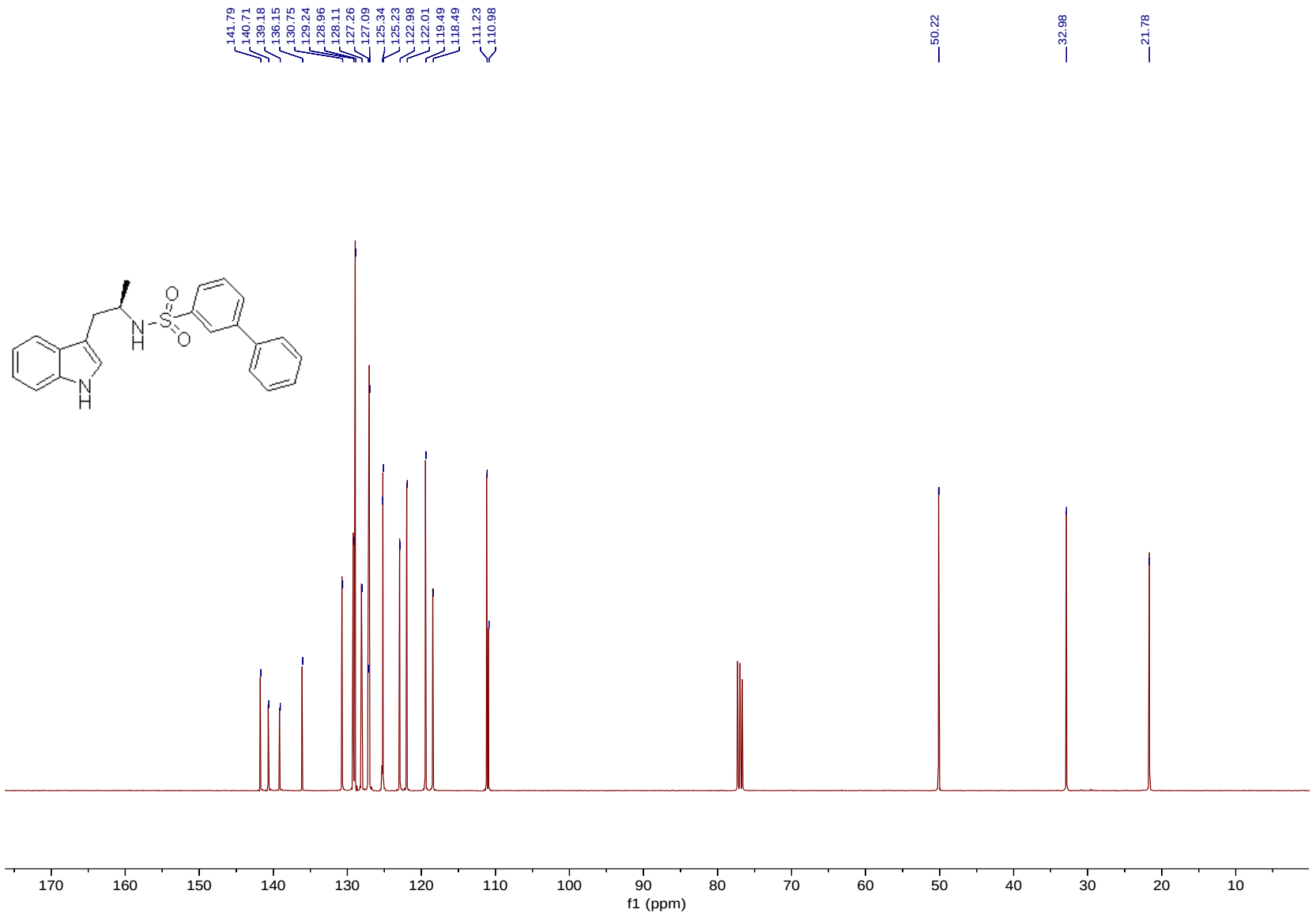

8.12
7.51
7.49
7.31
7.30
7.29
7.29
7.27
7.16
7.16
7.14
7.12
7.05
7.03
7.01
6.99
6.97
6.90
6.90
4.71
4.70
4.67
4.65
3.58
3.56
3.55
3.53
3.51
3.50
3.48
2.85
2.84
2.82
2.80
2.78
2.76
2.75
2.31
1.15
1.14
1.00
1.95
1.98
1.00
1.96
1.01
0.97
1.00
1.02
2.07
3.02
3.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

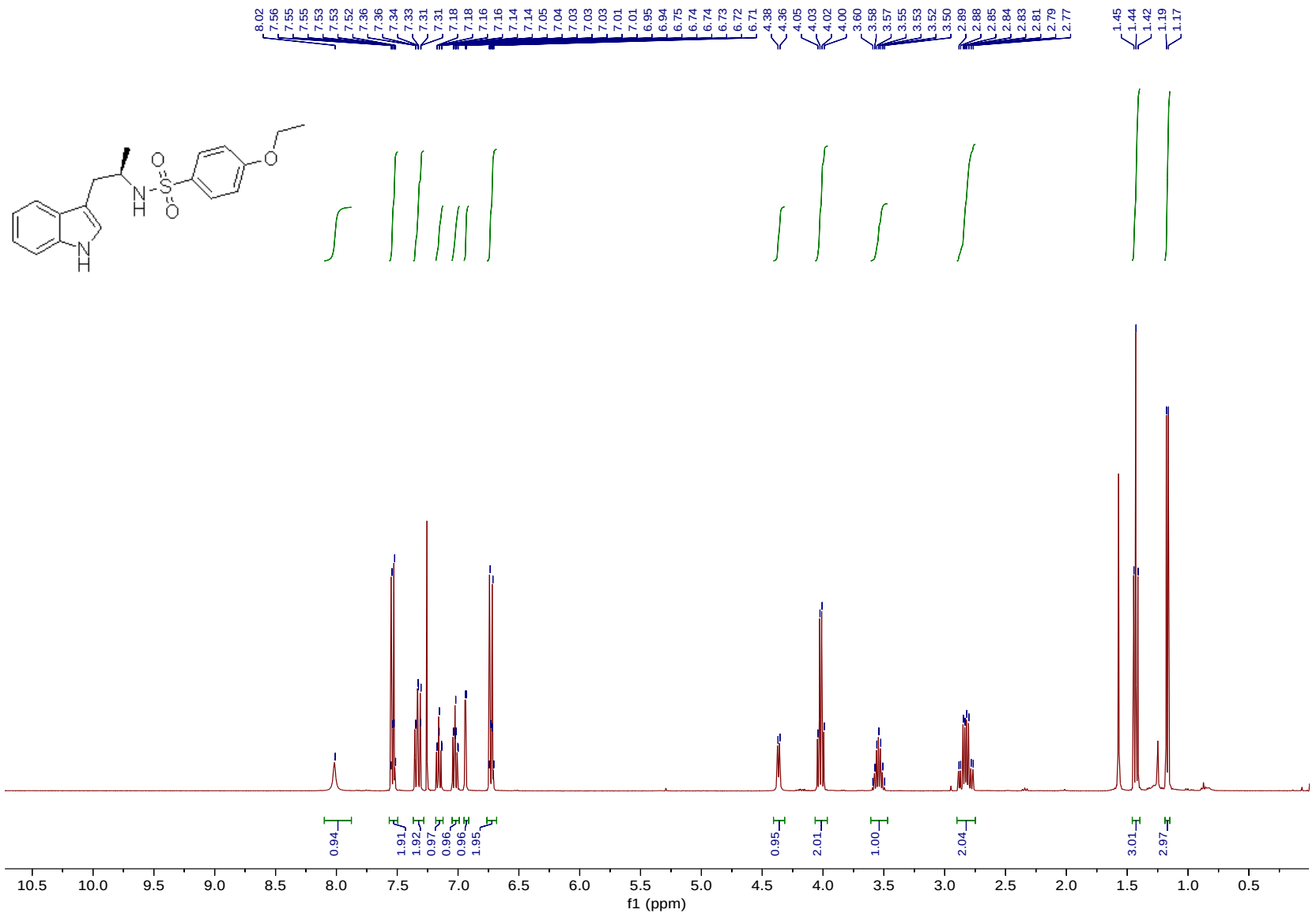

142.97
137.01
136.31
129.36
127.26
126.75
123.06
121.94
119.38
118.65
111.23
111.06
49.88
33.04
21.70
21.45
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

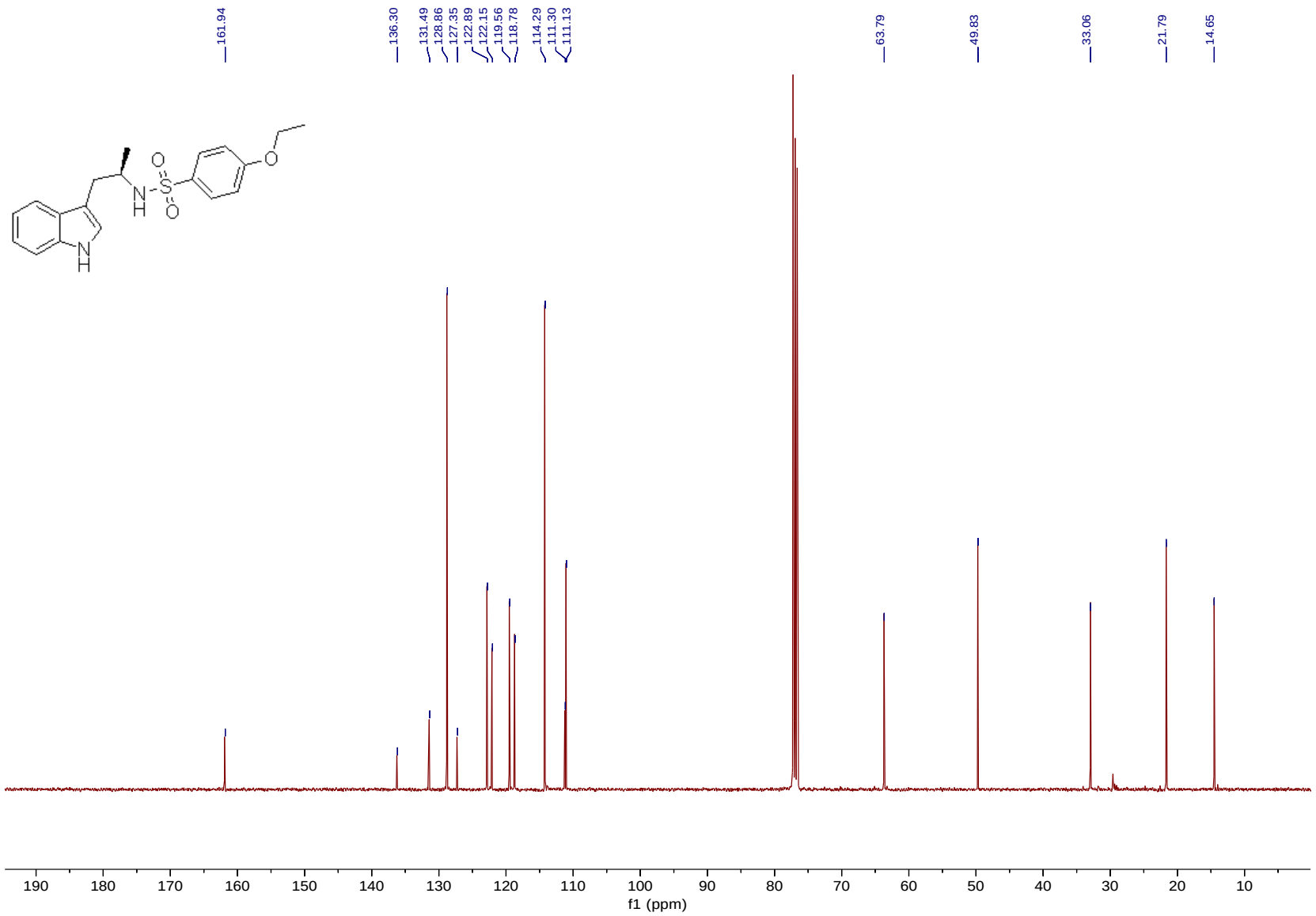

8.27 8.27 7.92 7.84 7.81 7.81 7.79 7.68 7.66 7.62 7.61 7.60 7.60 7.59 7.58 7.58 7.57 7.57 7.56 7.55 7.55 7.53 7.53 7.51 7.51 7.23 7.23 7.21 7.20 7.19 7.18 7.18 7.05 7.05 7.03 7.03 7.03 7.01 7.01 6.86 6.86 6.84 6.84 6.82 6.82 6.82 6.80 6.80 4.71 4.69 3.68 3.66 3.64 3.63 3.61 3.59 3.58 2.87 2.86 2.85 2.85 2.83 2.83 2.81 2.79 2.78 2.76 1.19 1.18
0.97 0.97 2.03 0.99 2.96 1.94 0.98 0.95 0.99 1.00 1.01 2.04 2.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

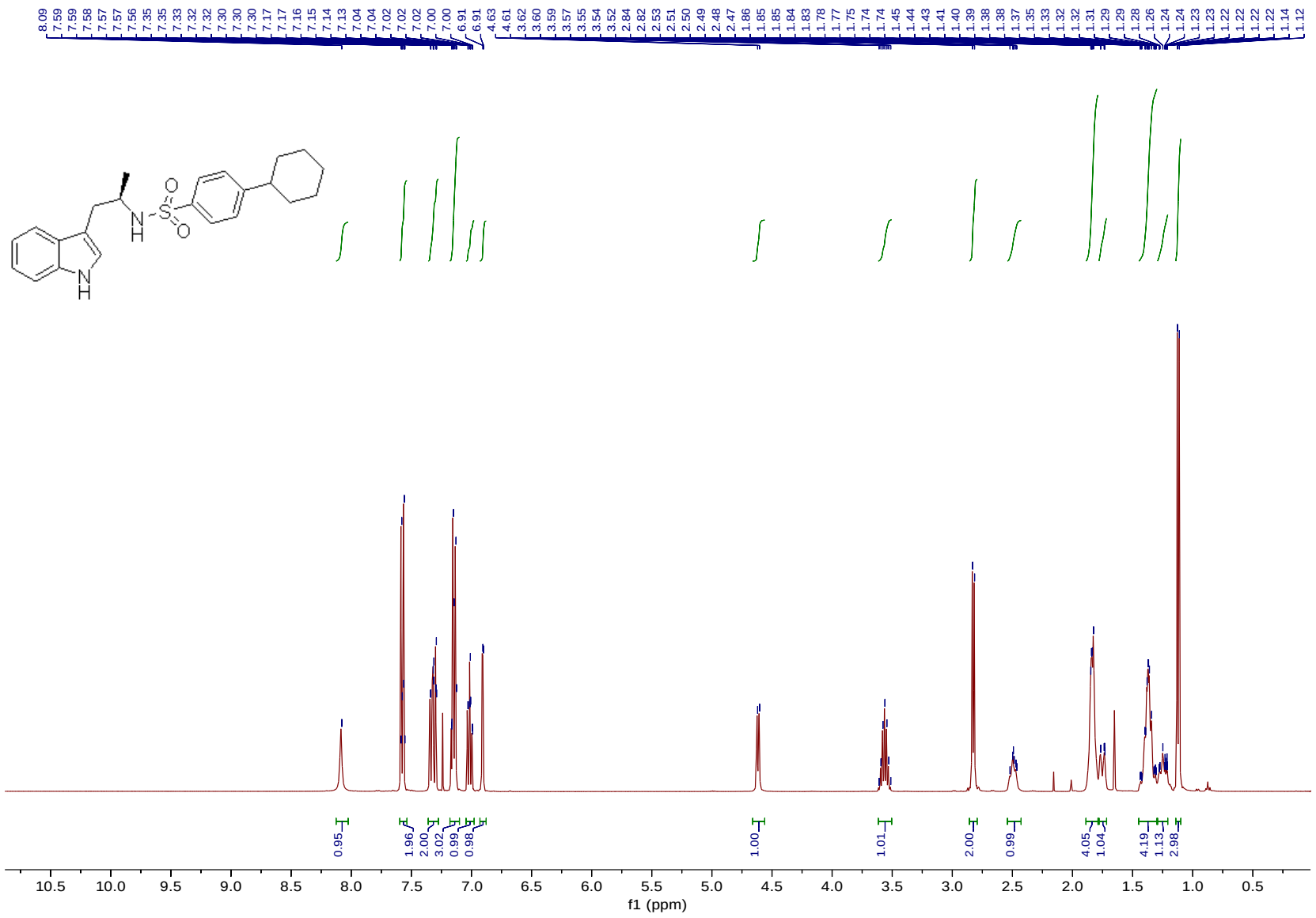

136.95
136.13
134.57
131.96
129.17
128.50
128.12
127.84
127.29
127.17
122.92
122.10
121.97
119.41
118.46
111.09
50.18
33.04
21.90
f1 (ppm)

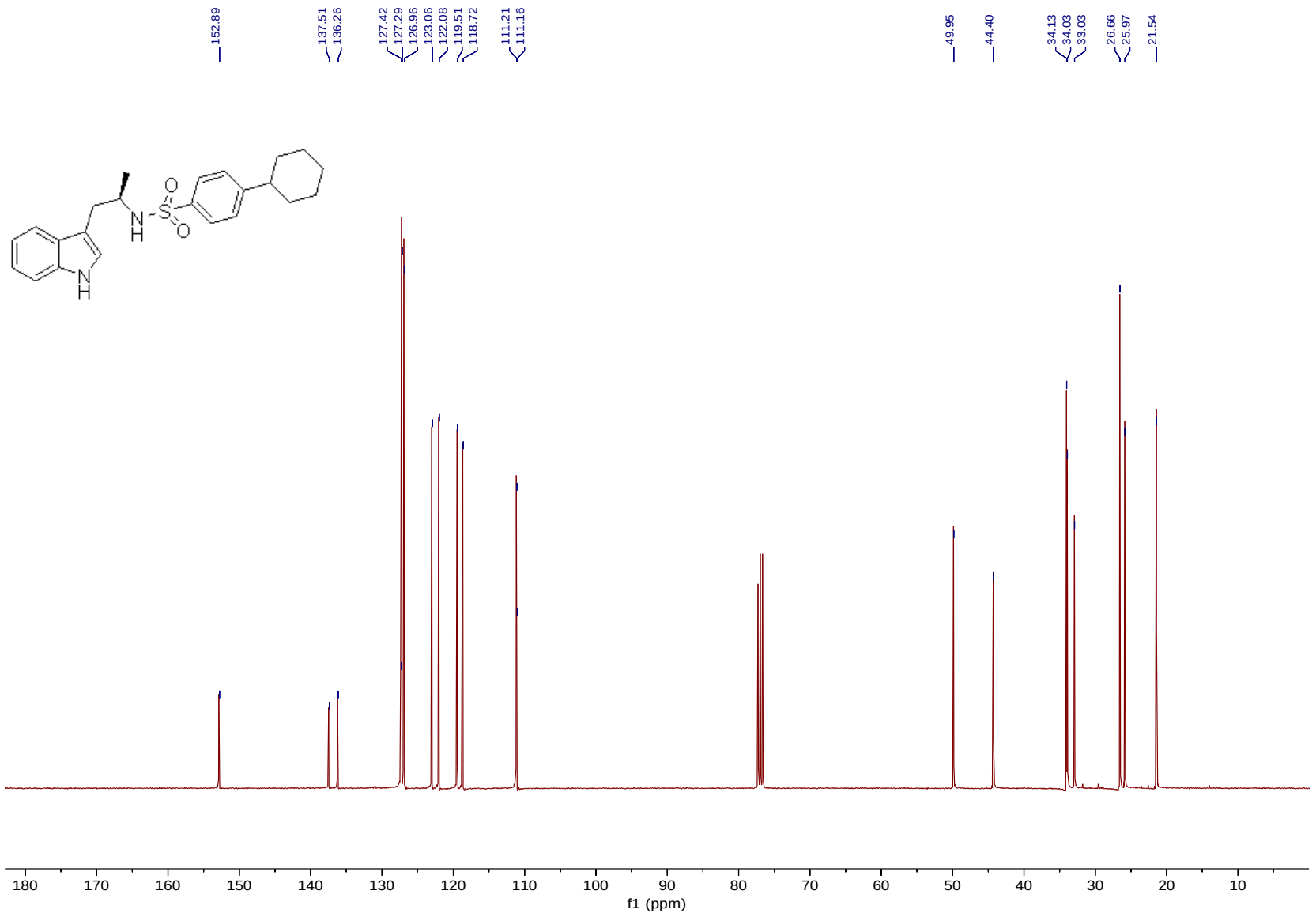

7.95 7.95 7.95 7.95 7.94 7.94 7.63 7.63 7.63 7.62 7.61 7.61 7.61 7.60 7.59 7.59 7.59 7.59 7.57 7.57 7.57 7.57 7.54 7.53 7.52 7.51 7.51 7.51 7.46 7.46 7.44 7.44 7.43 7.42 7.42 7.42 7.40 7.40 7.39 7.38 7.34 7.33 7.33 7.33 7.32 7.31 7.31 7.31 7.31 7.29 7.29 7.23 7.23 7.23 7.21 7.21 7.21 7.12 7.12 7.10 7.10 7.08 7.08 6.98 6.98 6.96 6.96 6.96 6.94 6.94 6.86 6.85 4.73 4.71 3.63 3.61 3.60 2.83 2.83 2.83 2.82 2.82 2.82 2.81 2.81 1.19 1.17
1.90
1.94
1.96
1.96
1.00
2.02
1.06
1.00
1.00
0.96
1.00
1.01
2.04
3.05
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


141.79
140.71
139.18
136.15
130.75
129.24
128.96
128.11
127.26
127.09
125.34
125.23
122.98
122.01
119.49
118.49
111.23
110.98
50.22
32.98
21.78
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.02 7.56 7.55 7.55 7.53 7.53 7.52 7.36 7.36 7.34 7.33 7.31 7.31 7.18 7.18 7.16 7.16 7.14 7.14 7.05 7.04 7.03 7.03 7.03 7.01 7.01 6.95 6.94 6.75 6.74 6.74 6.73 6.72 6.71 4.38 4.36 4.05 4.03 4.02 4.00 3.60 3.58 3.57 3.55 3.53 3.52 3.50 2.89 2.88 2.85 2.84 2.83 2.81 2.79 2.77 1.45 1.44 1.42 1.19 1.17
0.94 1.91 1.92 0.97 0.96 0.96 1.95 0.95 2.01 1.00 2.04 3.01 2.97
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


161.94
136.30
131.49
128.86
127.35
122.89
122.15
119.56
118.78
114.29
111.30
111.13
63.79
49.83
33.06
21.79
14.65
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.09 7.59 7.59 7.58 7.57 7.57 7.56 7.35 7.35 7.33 7.32 7.32 7.30 7.30 7.30 7.17 7.17 7.16 7.15 7.14 7.13 7.04 7.04 7.02 7.02 7.02 7.00 6.91 6.91 4.63 4.61 3.62 3.60 3.59 3.57 3.55 3.54 3.52 2.84 2.82 2.53 2.51 2.50 2.49 2.48 2.47 1.86 1.85 1.85 1.84 1.83 1.78 1.77 1.75 1.74 1.74 1.45 1.44 1.43 1.41 1.40 1.39 1.38 1.38 1.37 1.35 1.33 1.32 1.32 1.31 1.29 1.29 1.28 1.26 1.24 1.24 1.23 1.23 1.22 1.22 1.22 1.14 1.12
0.95 1.96 2.00 3.02 0.99 0.98 1.00 1.01 2.00 0.99 4.05 1.04 4.19 1.13 2.98
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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33.03
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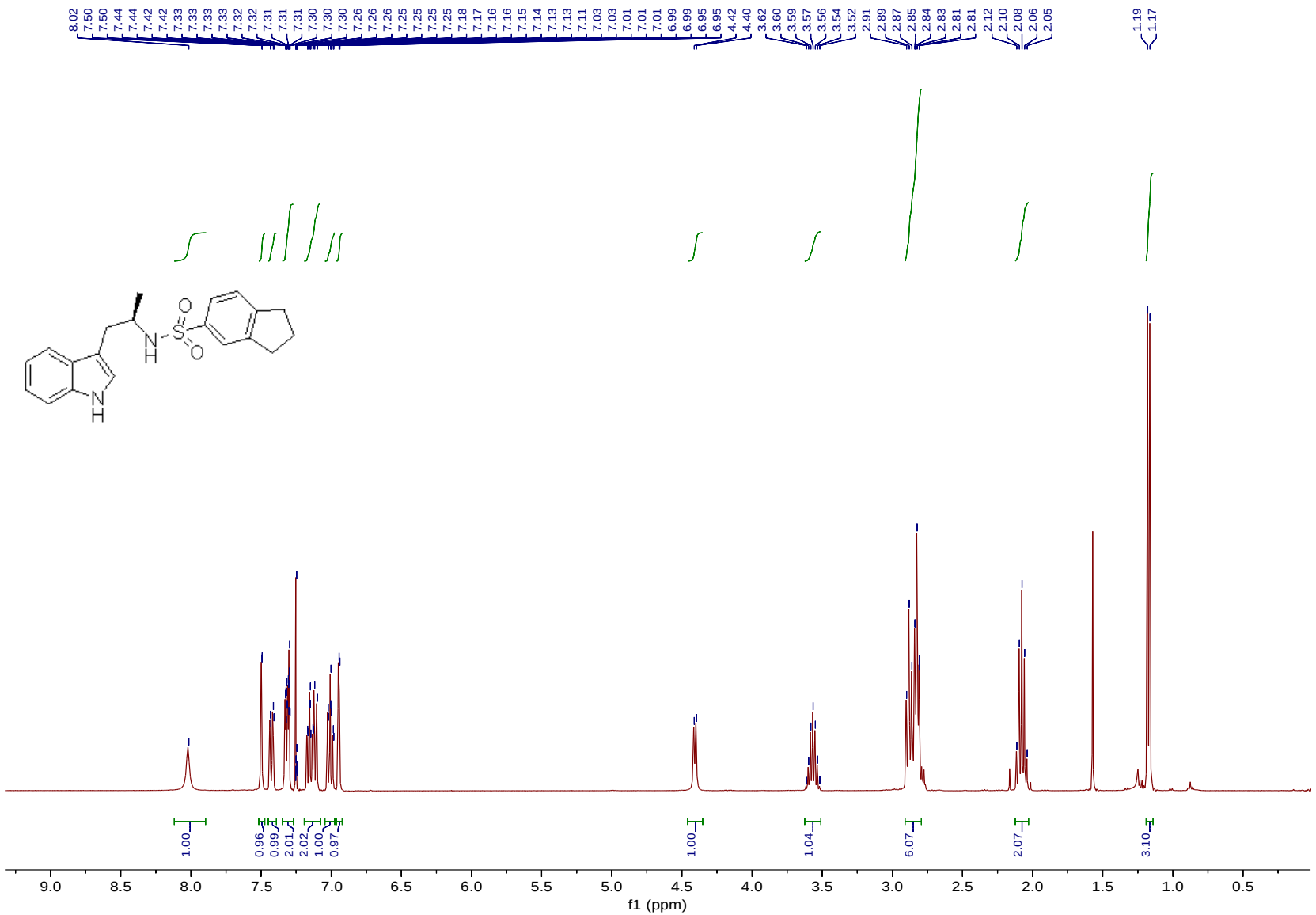
f1 (ppm)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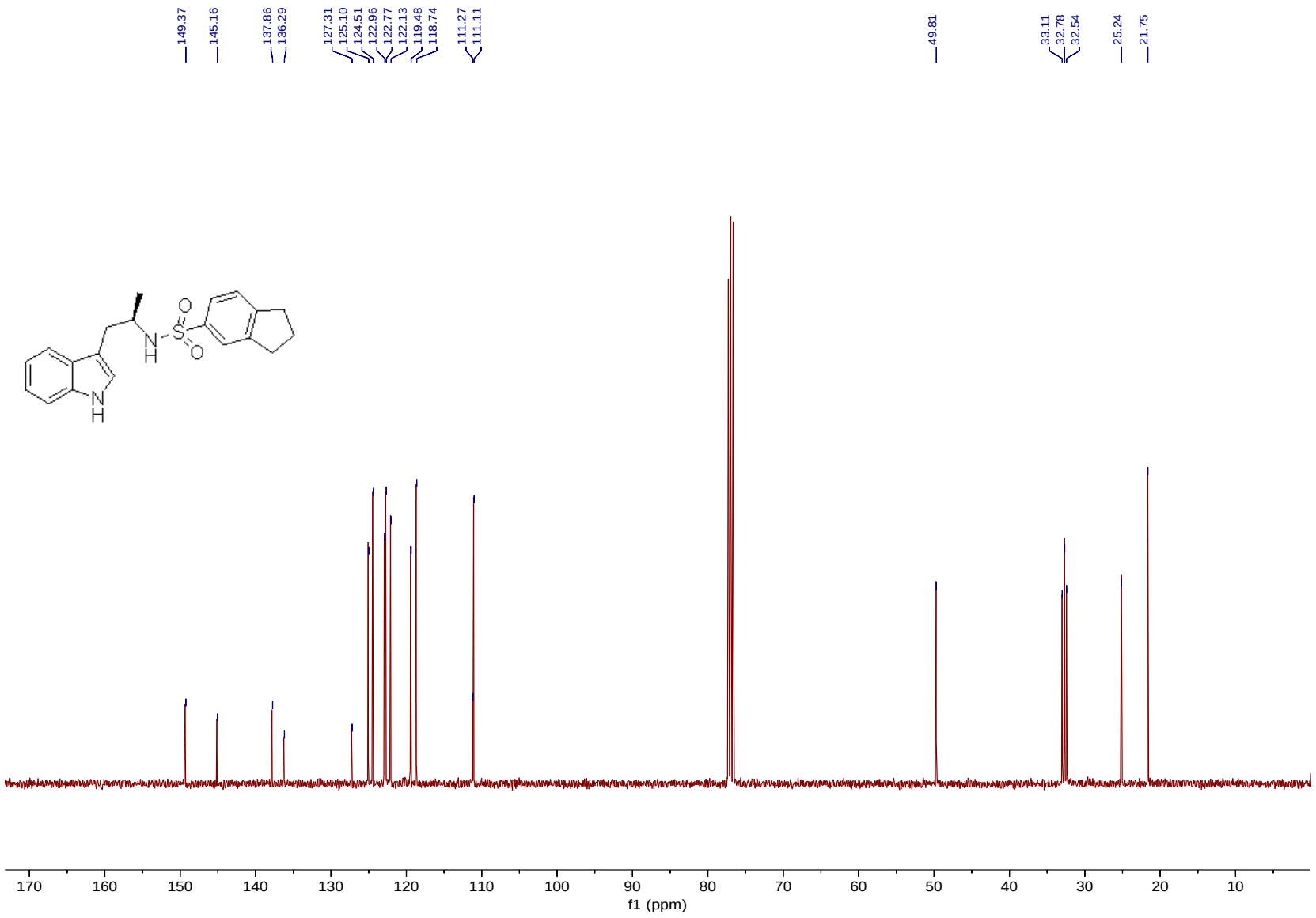
1.00 0.96 0.99 2.01 2.02 1.00 0.97 1.00 1.04 6.07 2.07 3.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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32.78
32.54
25.24
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100
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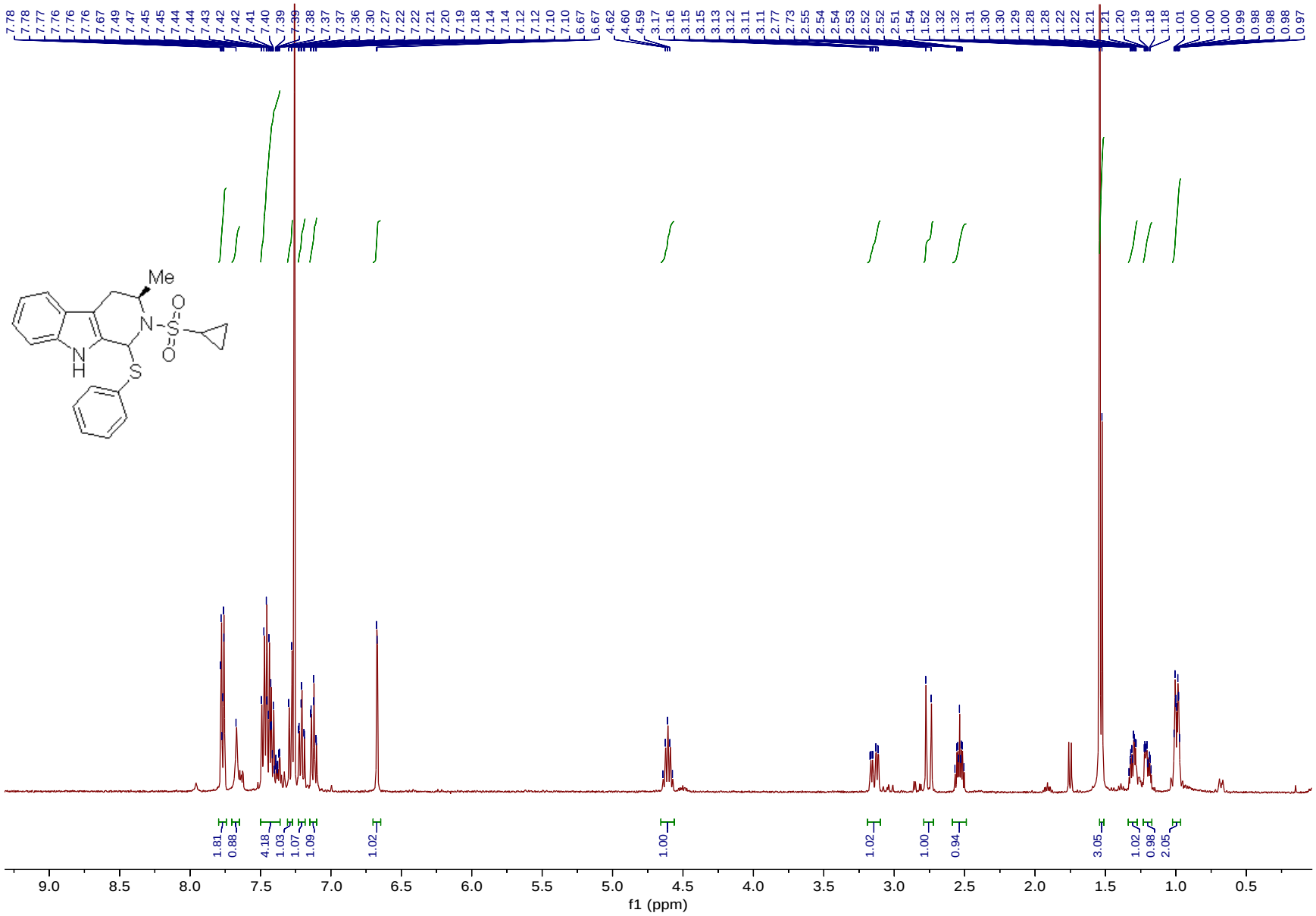
f1 (ppm)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NH
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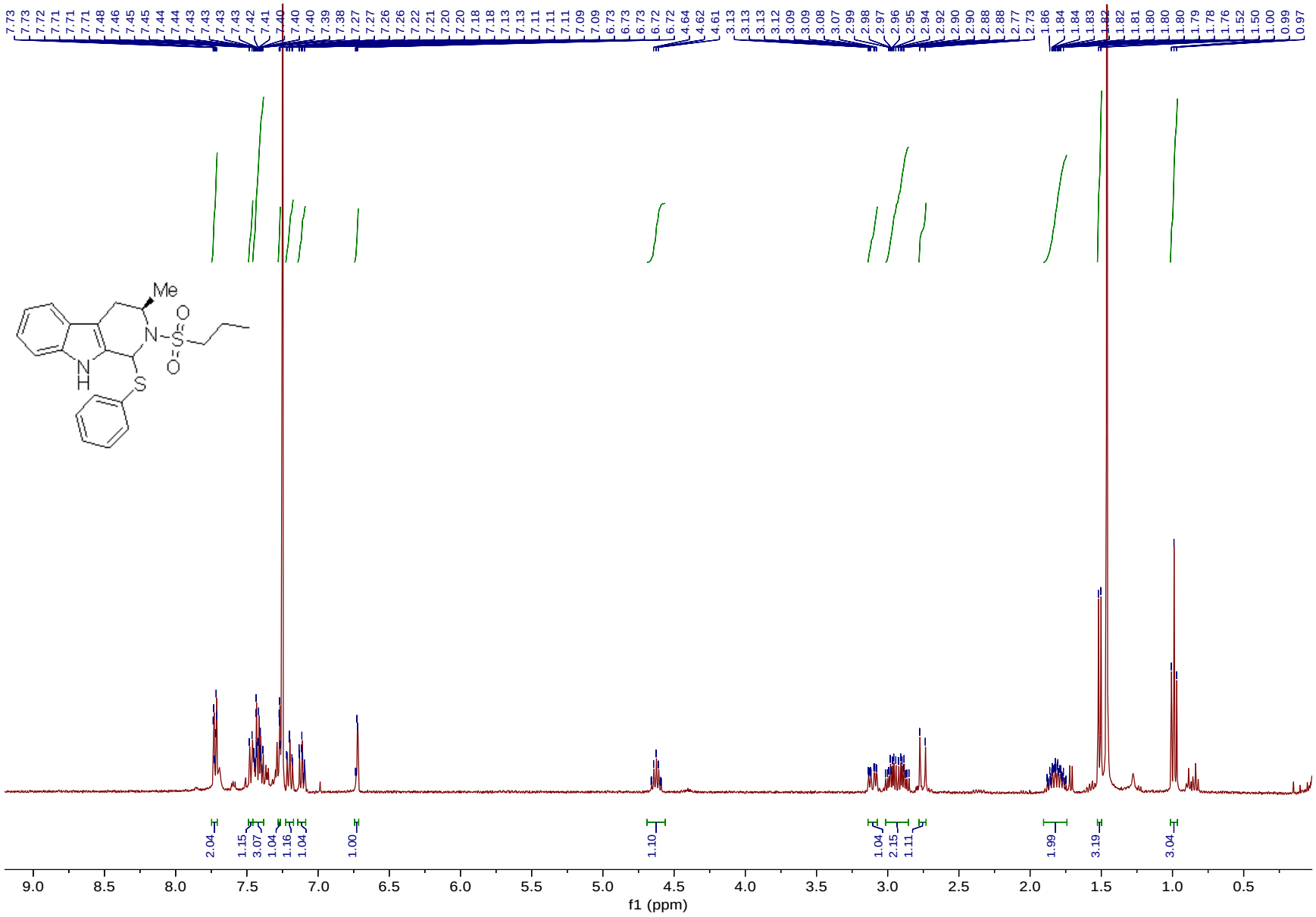
f1 (ppm)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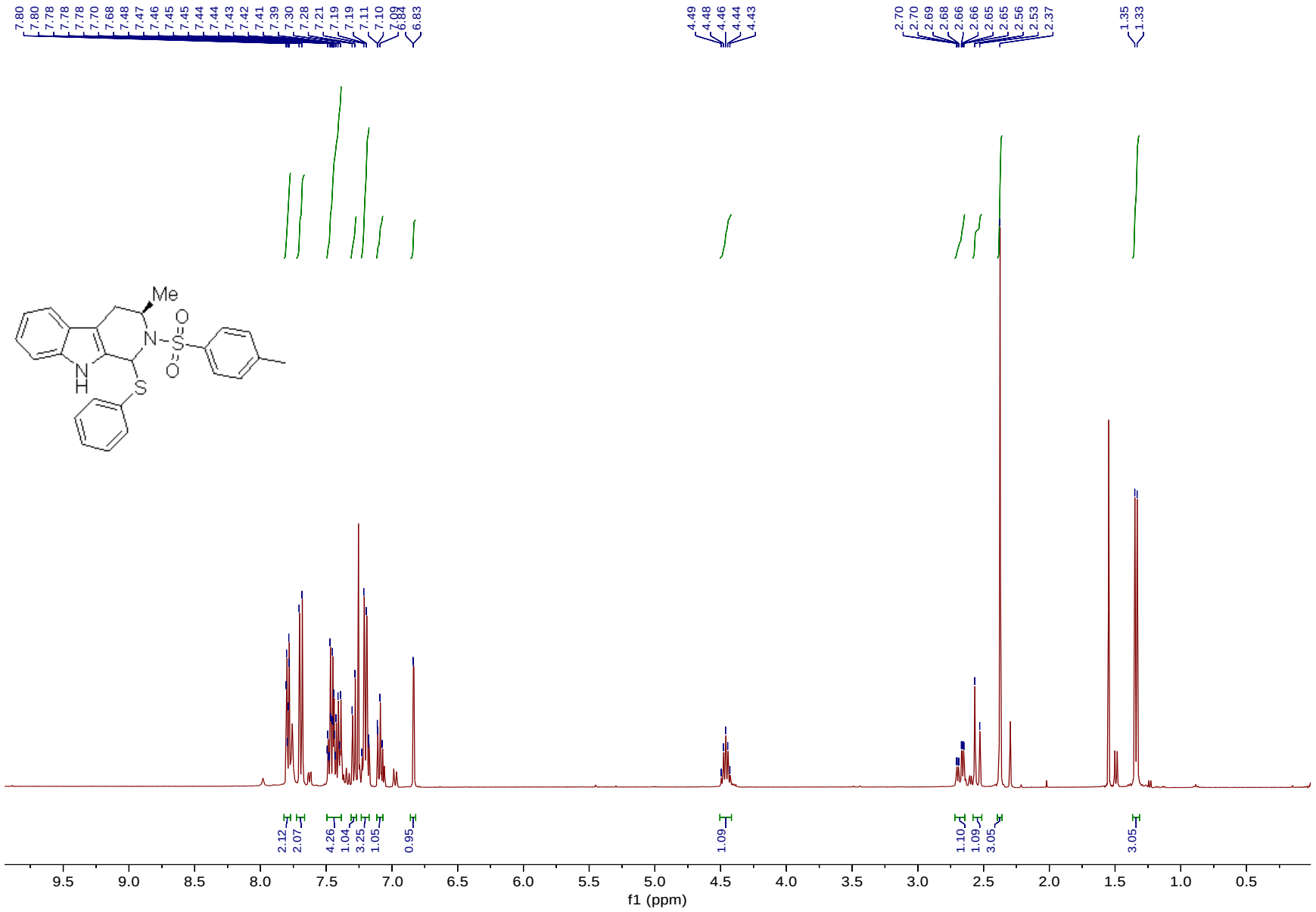
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2.68
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2.65
2.56
2.53
2.37
1.35
1.33
Me
N
S
O
O
S
N
H
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2.07
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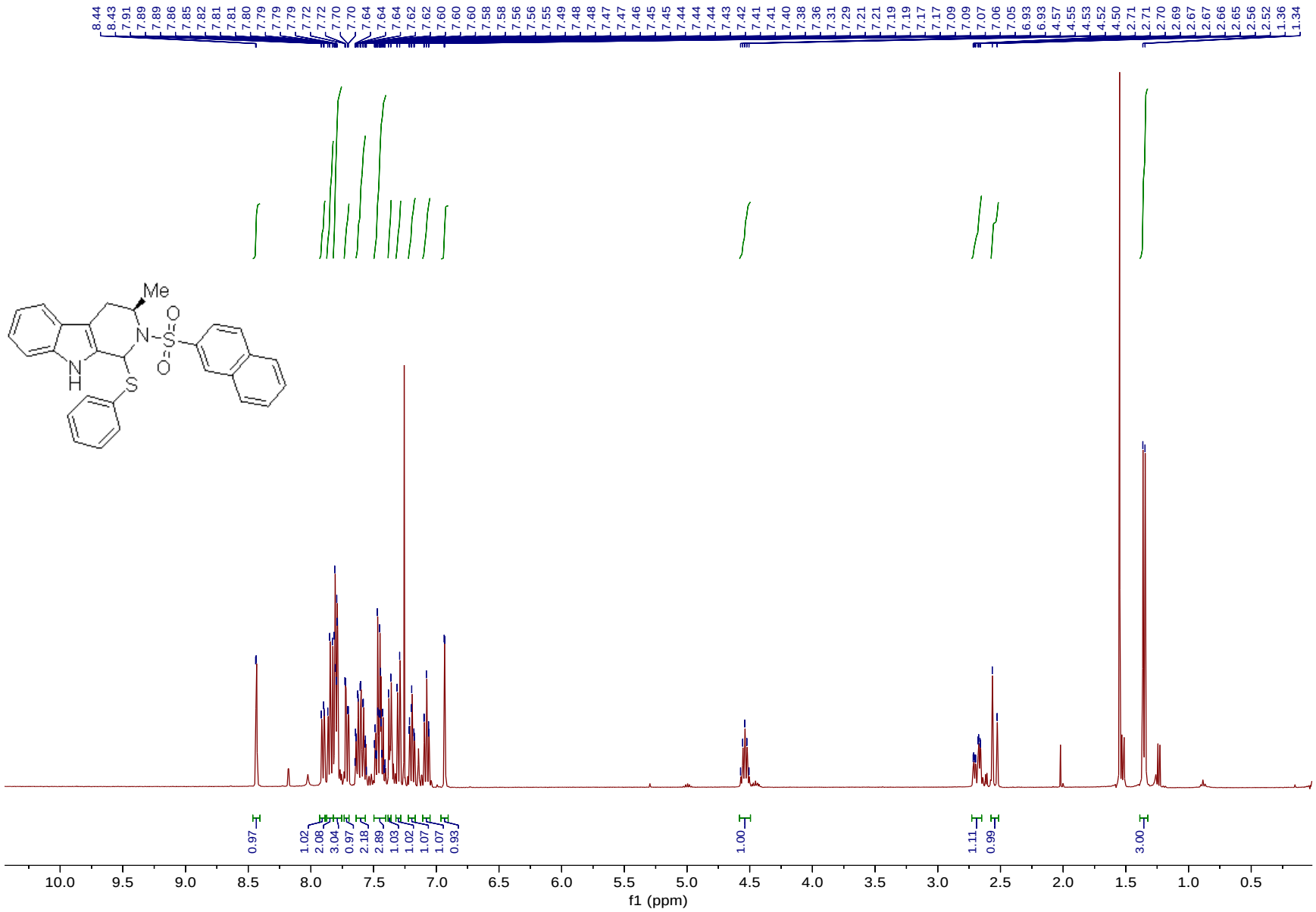
0.5
f1 (ppm)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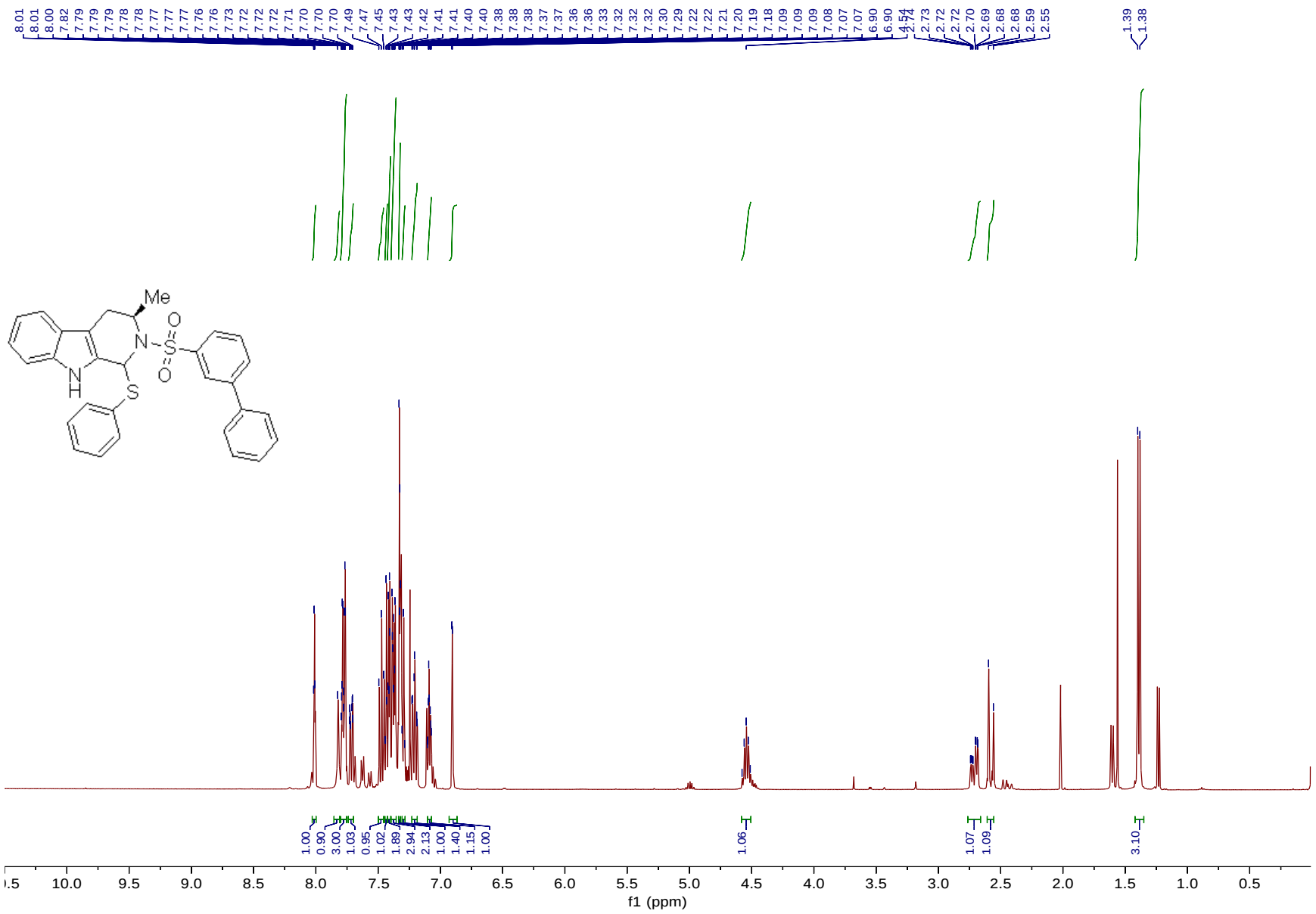
Me
O
N
S
O
N
H
S
0.97 1.02 2.08 3.04 0.97 2.18 2.89 1.03 1.02 1.07 1.07 0.93 1.00 1.11 0.99 3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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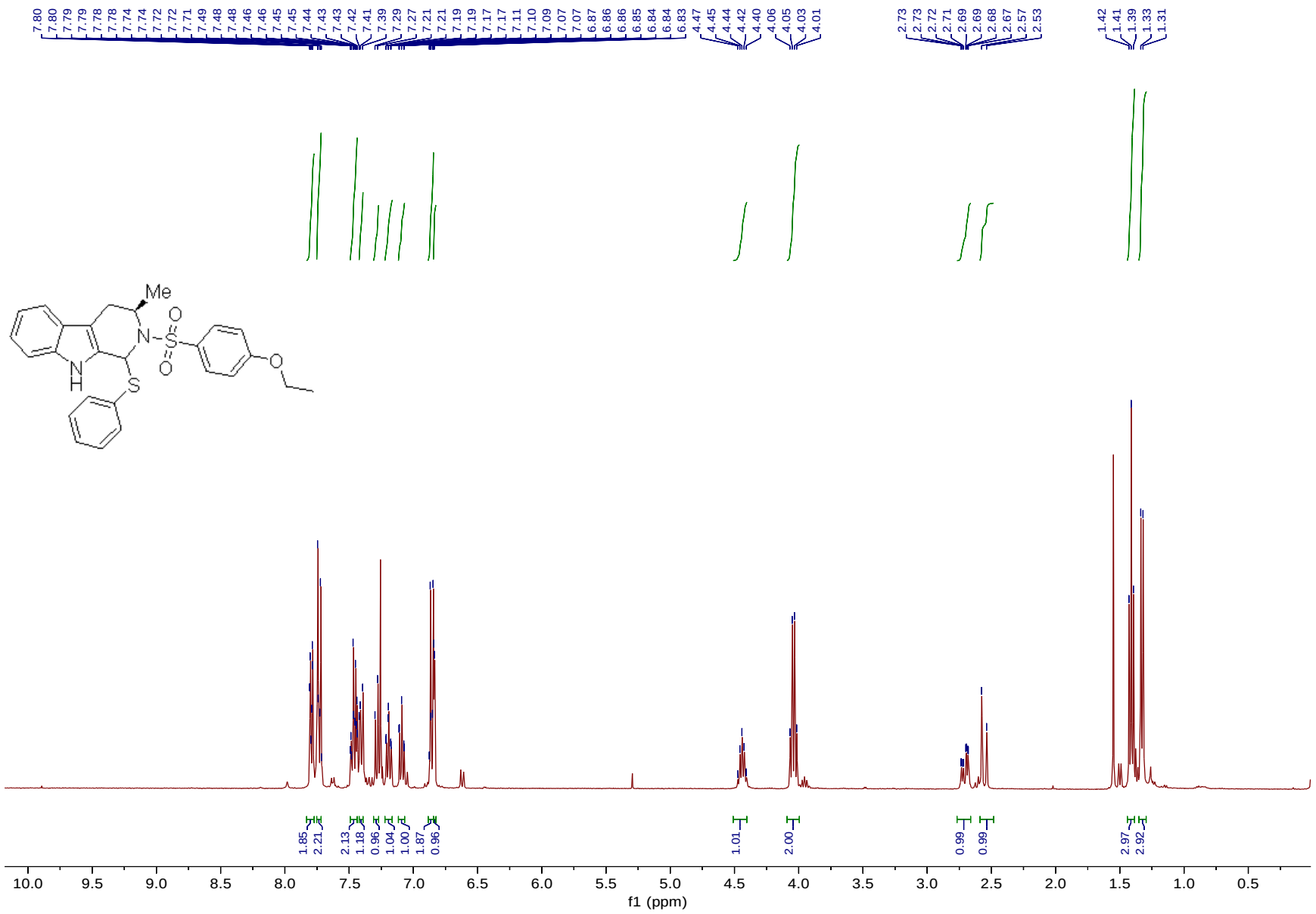
Me
N
O
S
O
N
H
S
1.00 0.90 3.00 1.03 0.95 1.02 1.89 2.94 2.13 1.00 1.40 1.15 1.00 1.06 1.07 1.09 3.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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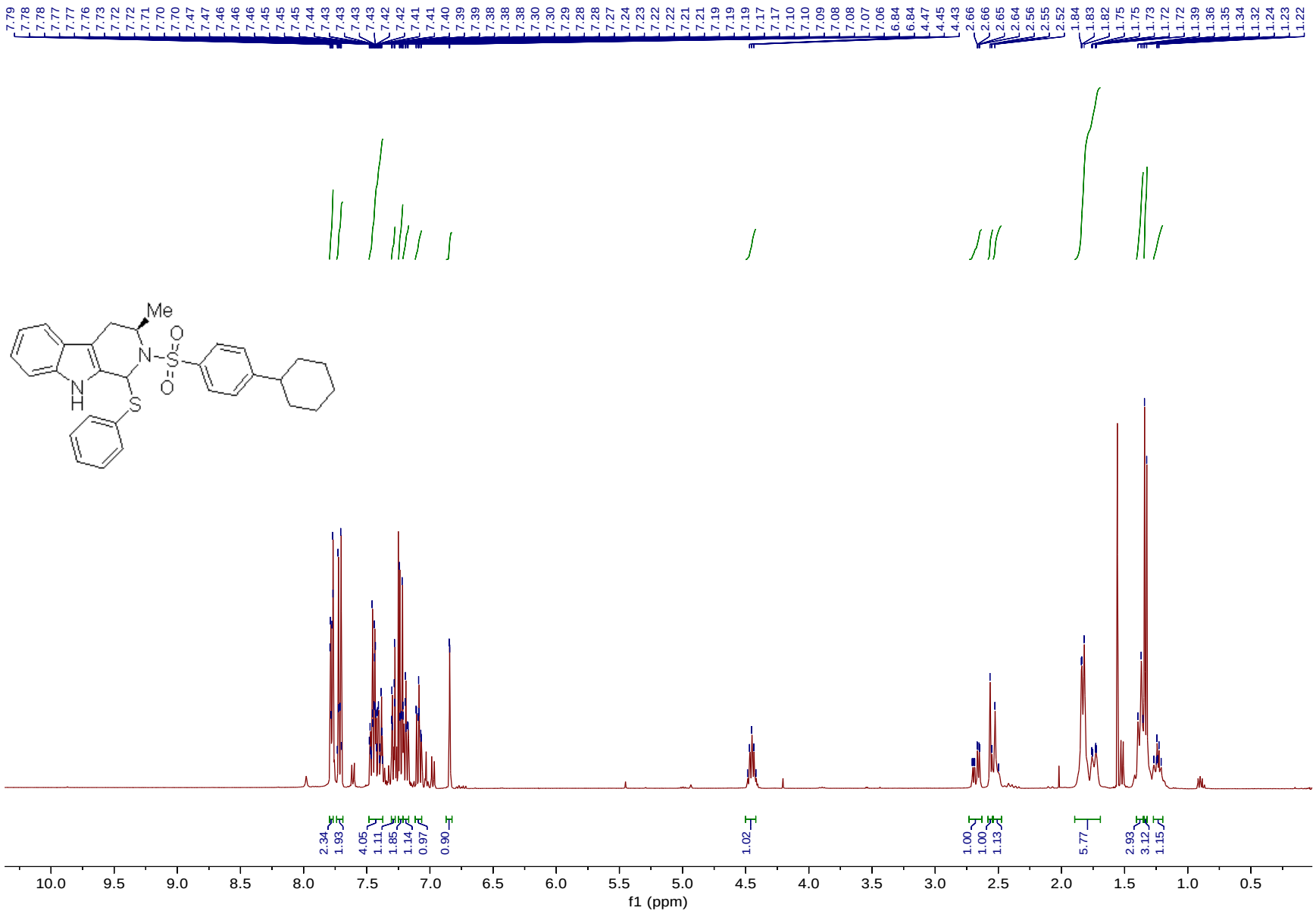
4.47 4.45 4.44 4.42 4.40 4.06 4.05 4.03 4.01
2.73 2.73 2.72 2.71 2.69 2.69 2.68 2.67 2.57 2.53
1.42 1.41 1.39 1.33 1.31
Me
O
N
S
O
O
N
H
S
1.85 2.21 2.13 1.18 0.96 1.04 1.00 1.87 0.96
1.01 2.00 0.99 0.99 2.97 2.92
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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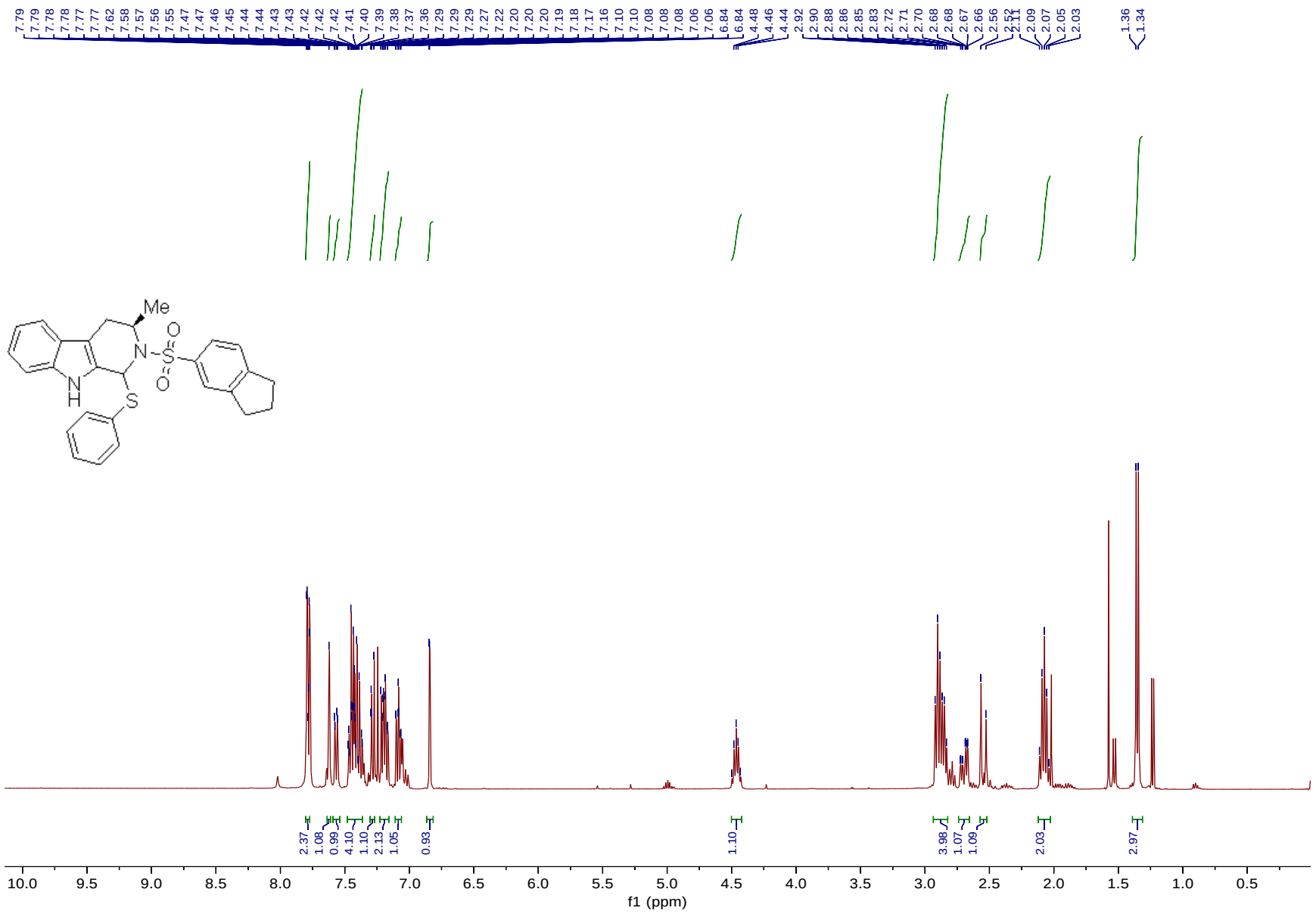
Me
N
O
S
O
N
H
S
2.34 1.93 4.05 1.11 1.85 1.14 0.97 0.90 1.02 1.00 1.00 1.13 5.77 2.93 3.12 1.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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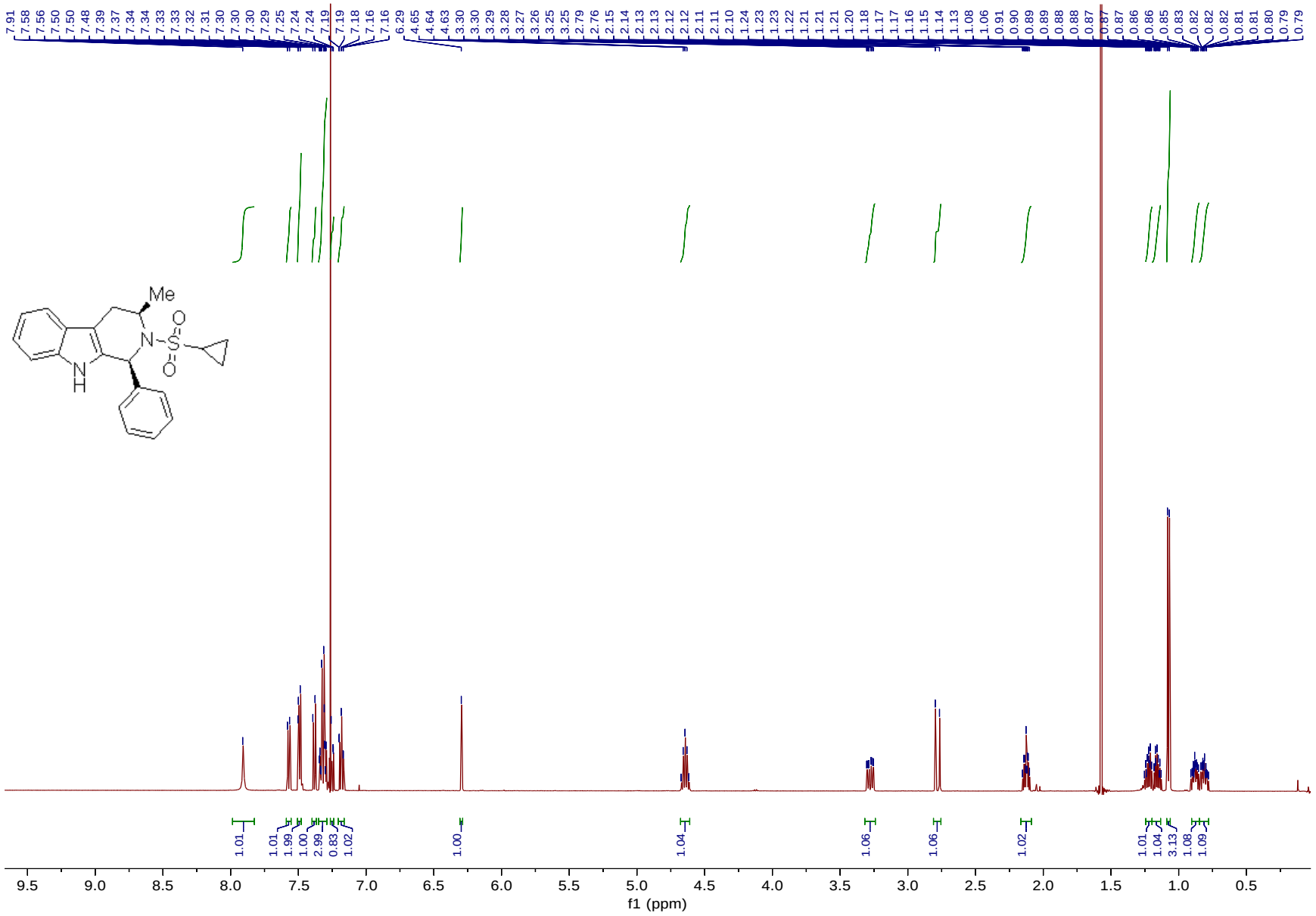
Me
O
N
S
O
N
H
S
2.37 1.08 0.99 4.10 1.10 2.13 1.05 0.93 1.10 3.98 1.07 1.09 2.03 2.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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Me
O
N
S
O
N
H
1.01 1.01 1.99 1.00 2.99 0.83 1.02 1.00 1.04 1.06 1.06 1.02 1.01 1.04 3.13 1.08 1.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
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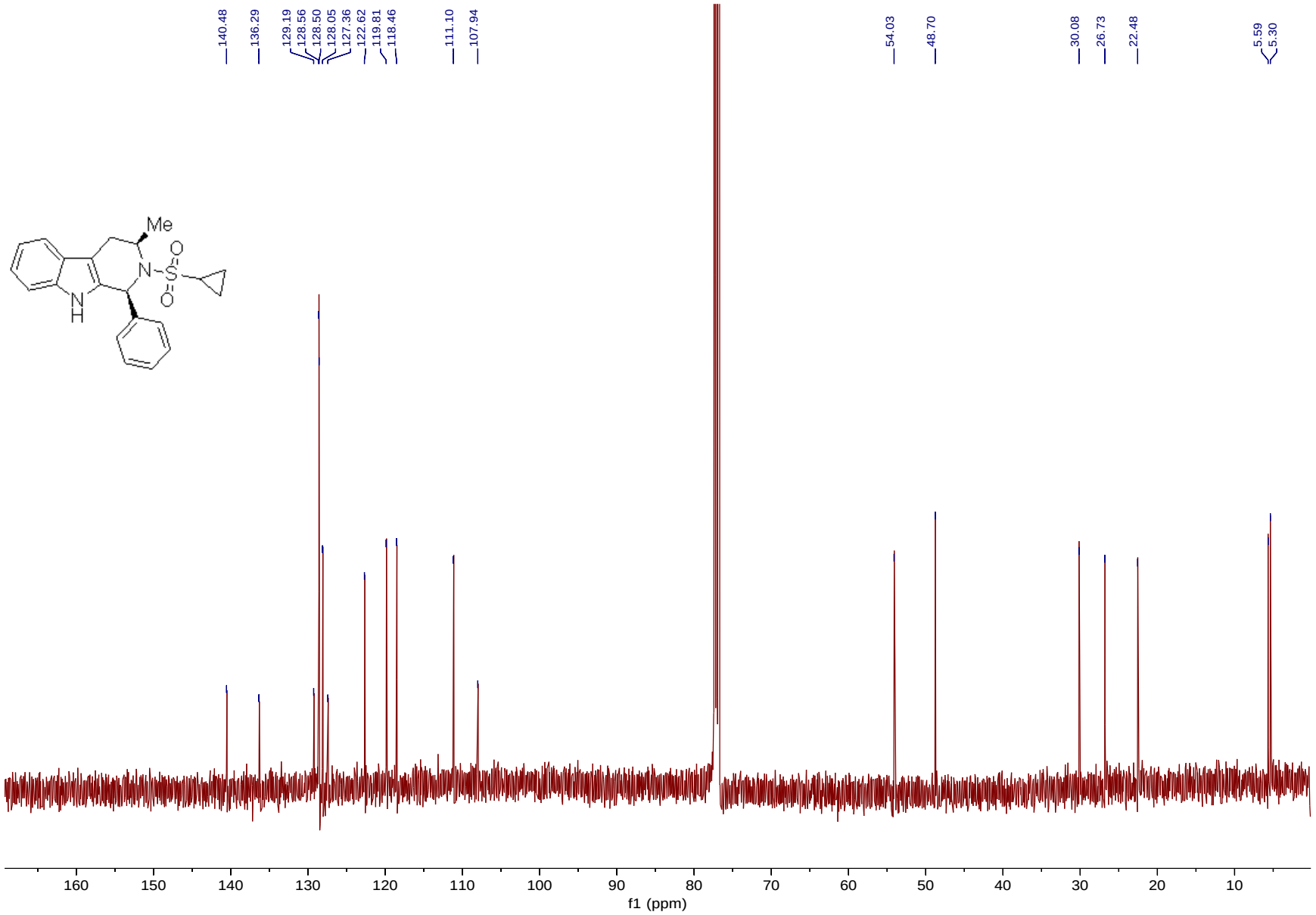
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30.08
26.73
22.48
5.59
5.30
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O
O
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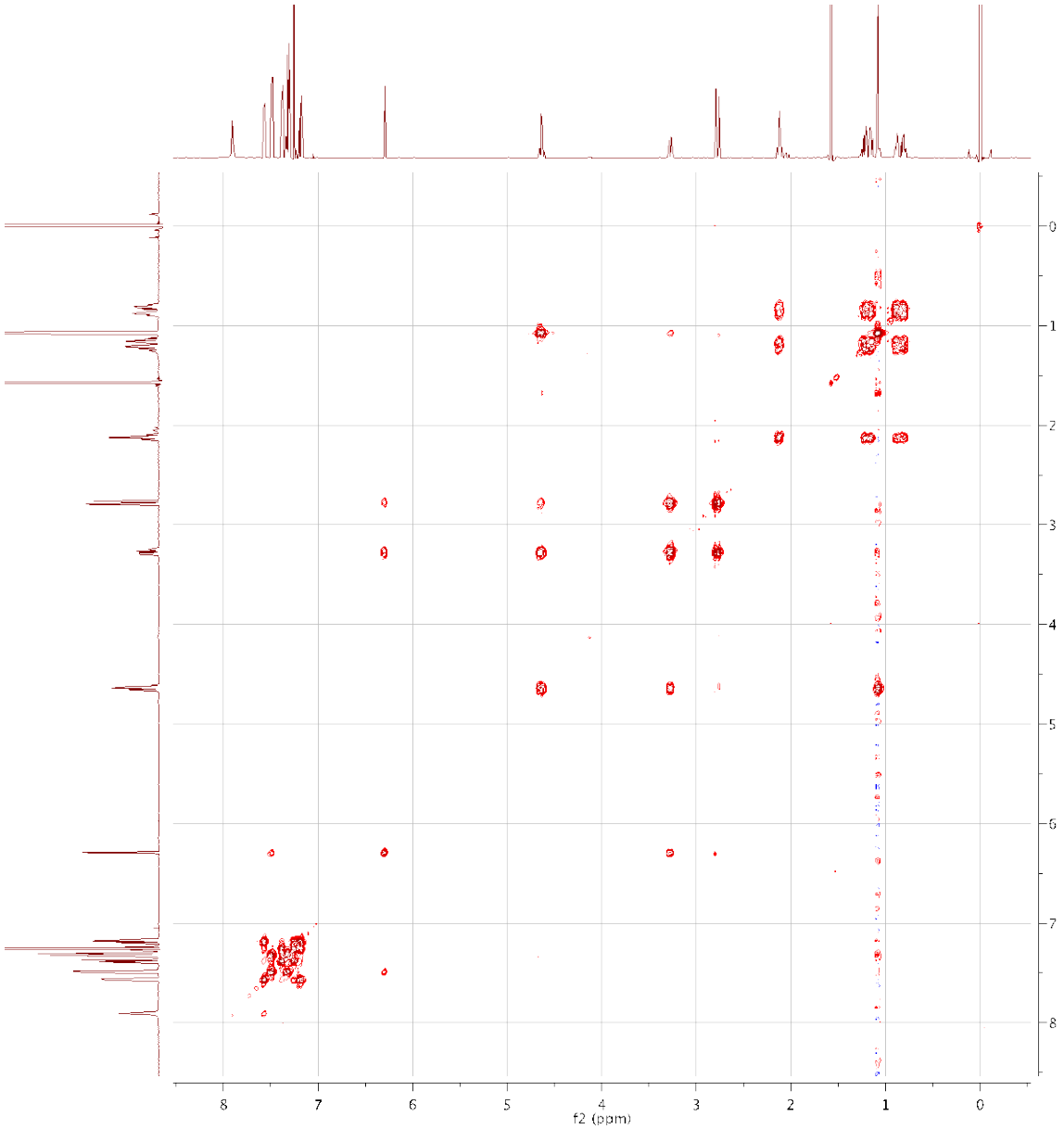
10
f1 (ppm)



	Parameter	Value
1	Data File Name	81491772/ 13/ pdata/ 1/ 2rr
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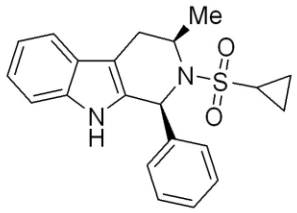
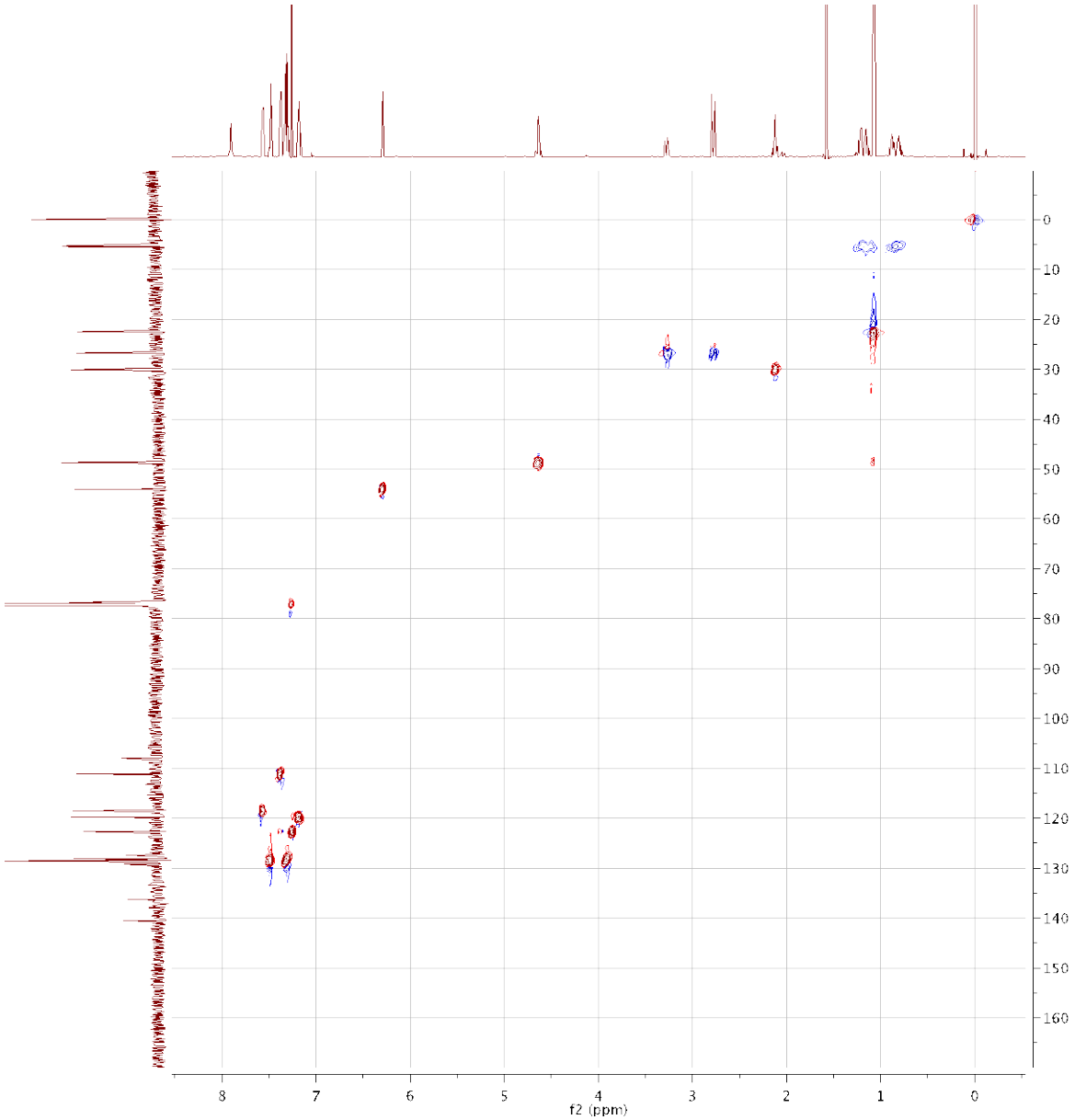
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	CDCl3
6	Pulse Sequence	cosygpmfqf
7	Acquisition Date	2015-07-09T13:52:14
8	Temperature	300.0
9	Number of Scans	4
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(4545.5, 4545.5)
12	Lowest Frequency	(-275.6, -275.6)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)





	Parameter	Value
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4	Owner	smapchemist
5	Solvent	CDCl3
6	Pulse Sequence	hsqcedetgp
7	Acquisition Date	2015-07-09T14:13:37
8	Temperature	300.0
9	Number of Scans	8
10	Spectrometer Frequency	(500.26, 125.79)
11	Spectral Width	(4545.5, 22624.4)
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13	Nucleus	(1H, 13C)
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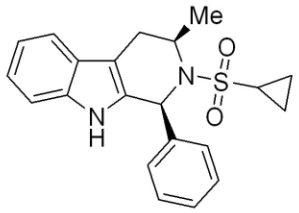

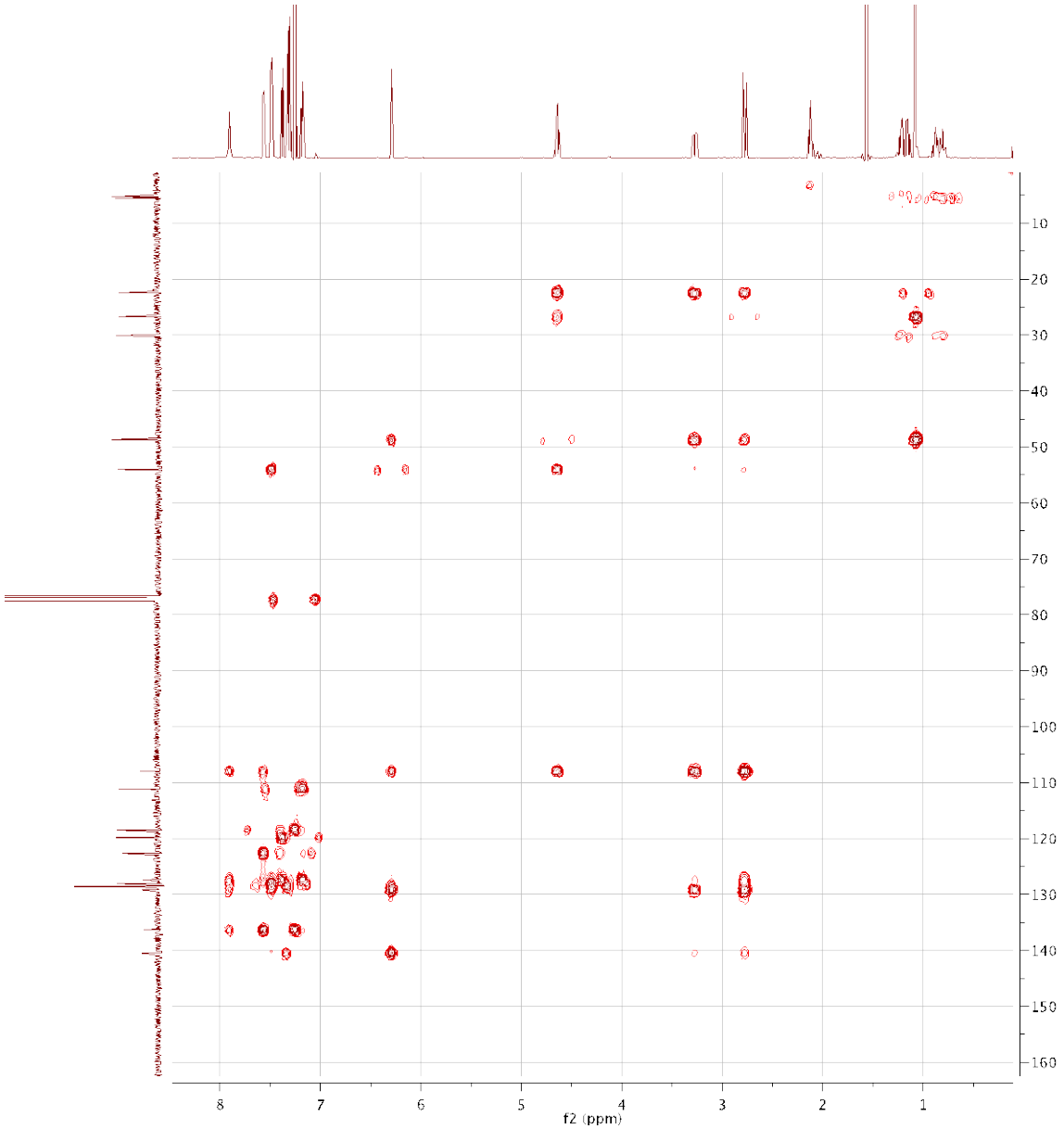

	Parameter	Value
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4	Owner	smapchemist
5	Solvent	CDCl3
6	Pulse Sequence	hmbcgplpndqf
7	Acquisition Date	2015-07-09T14:52:20
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 125.79)
11	Spectral Width	(4545.5, 30120.5)
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13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
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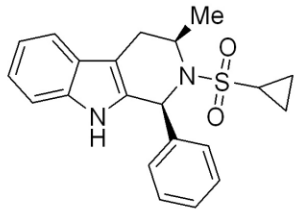

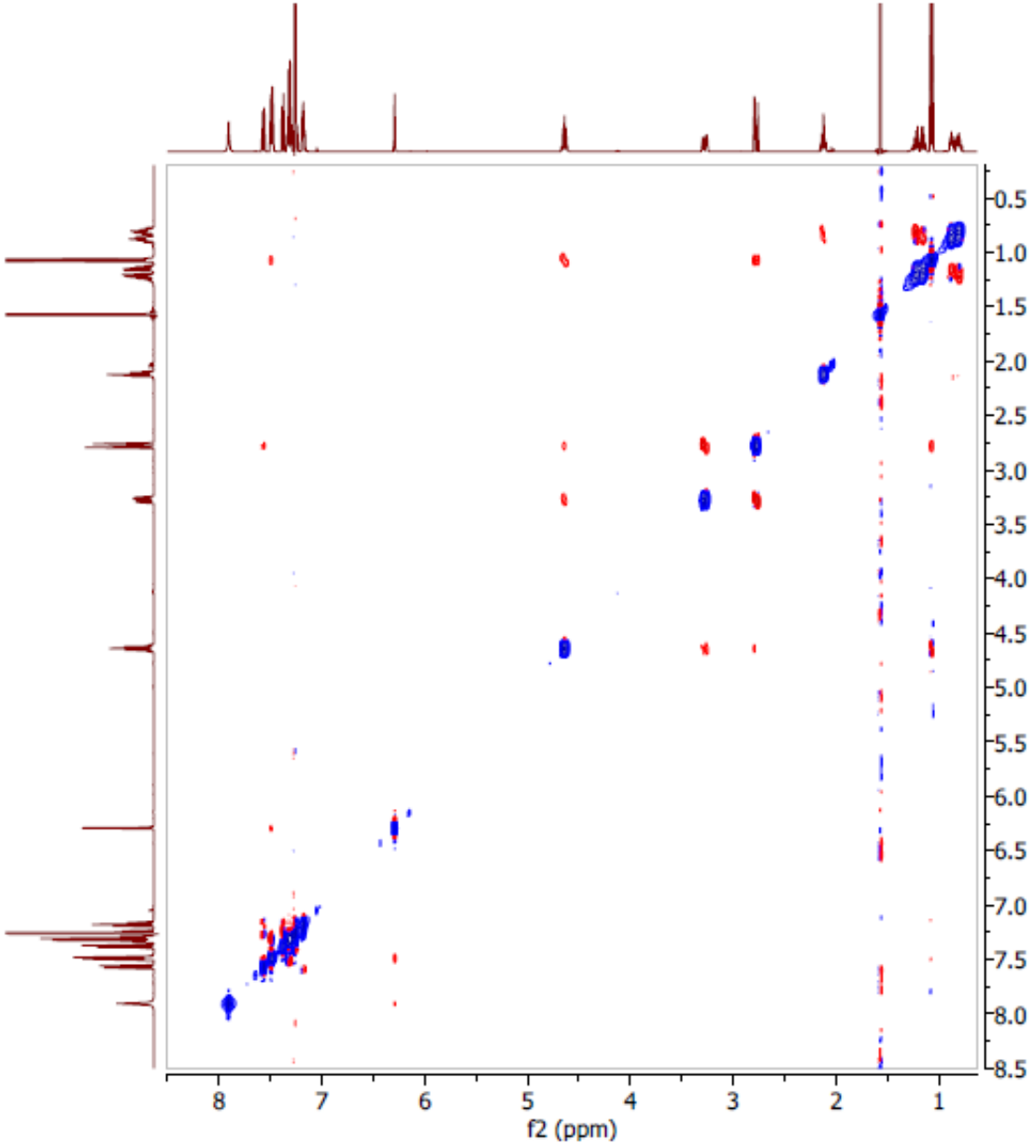

	Parameter	Value
1	Data File Name	W:/ data/ liuy55/ nmr/ 81491772/ 16/ ser
2	Sample ID	81491772
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	CDCl3
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2015-07-09T16:15:13
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(4545.5, 4545.5)
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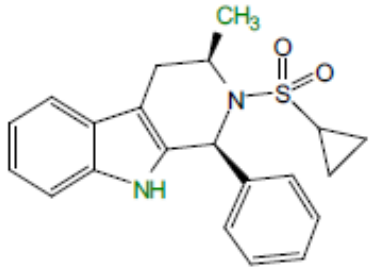
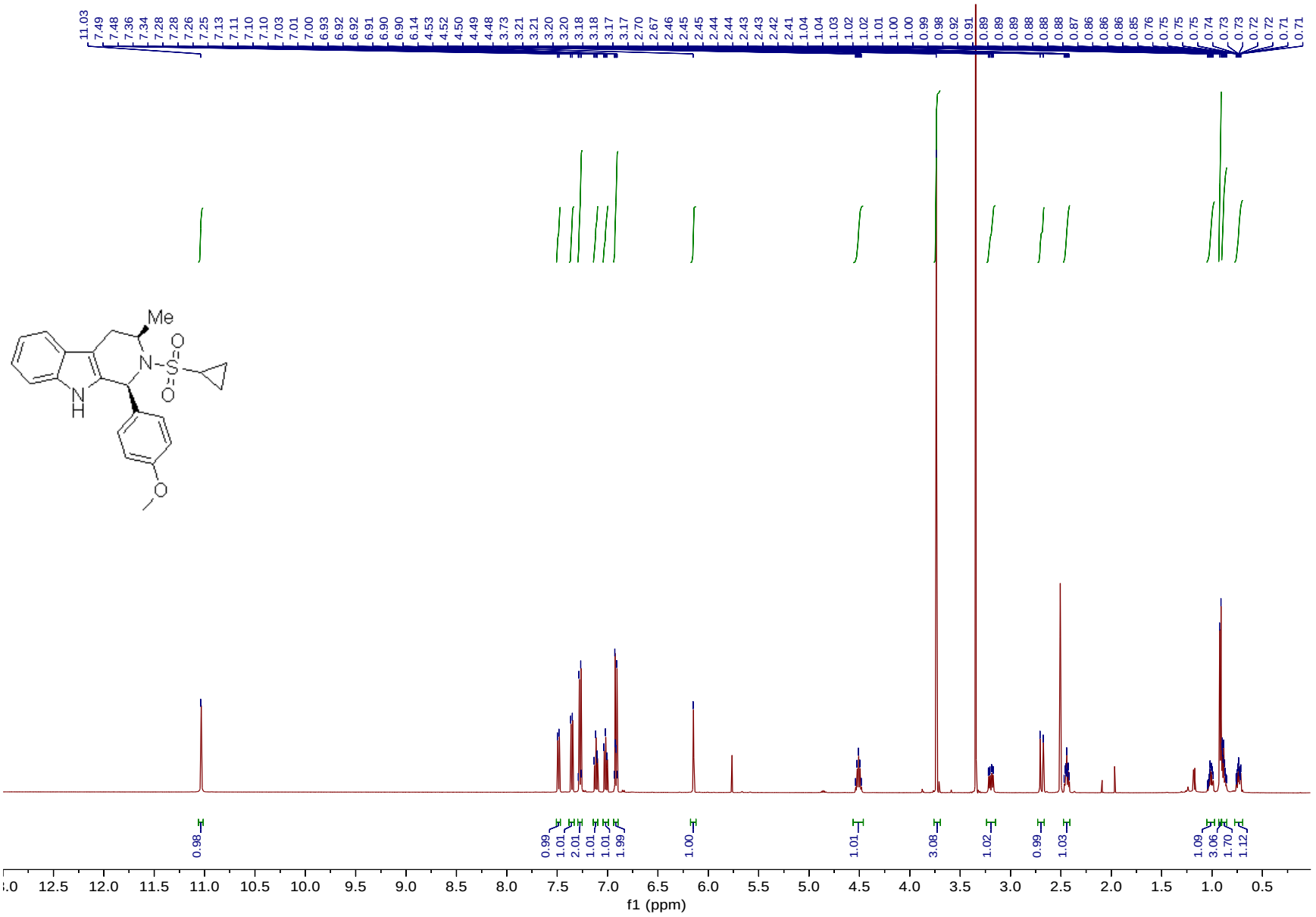
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)

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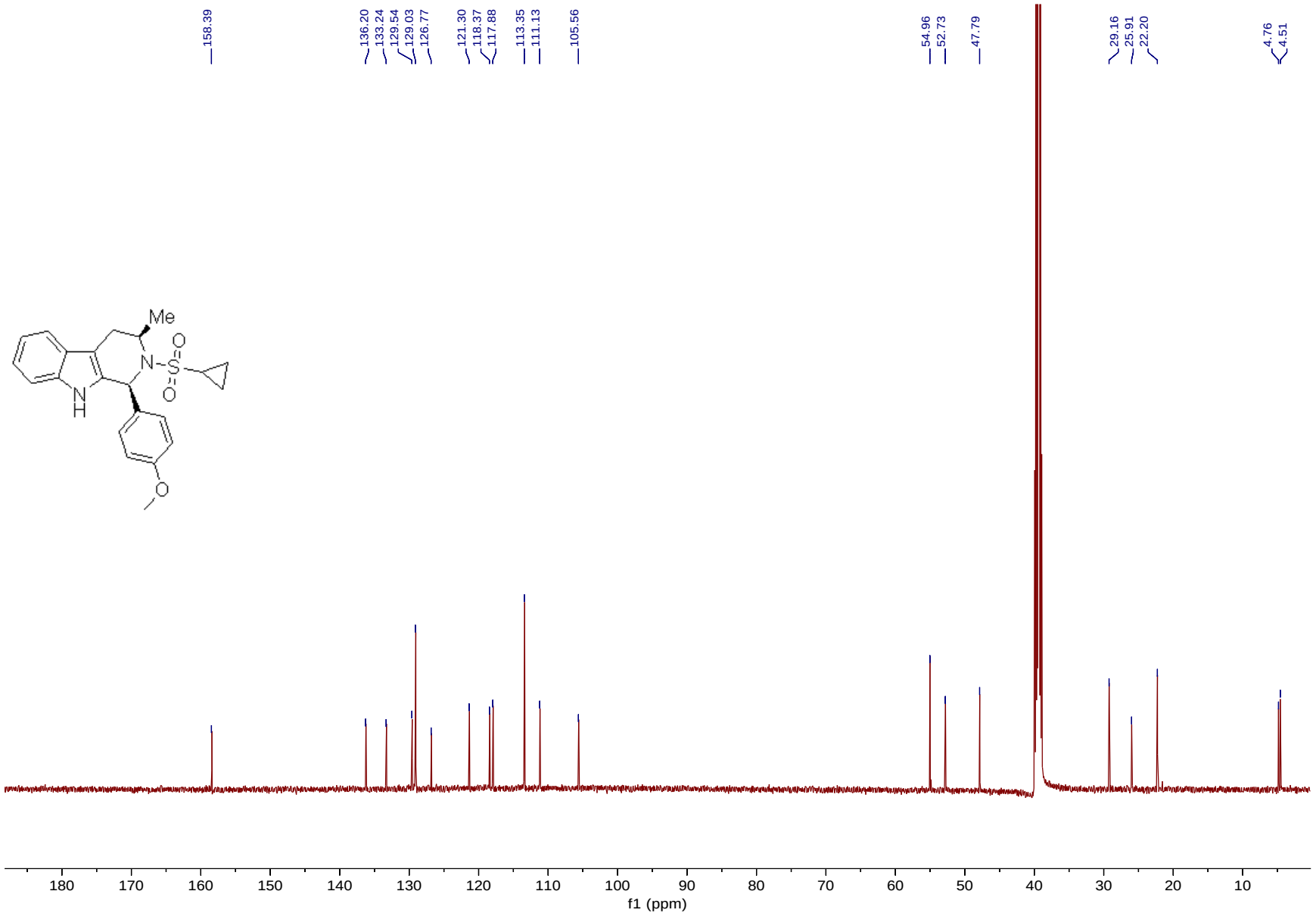
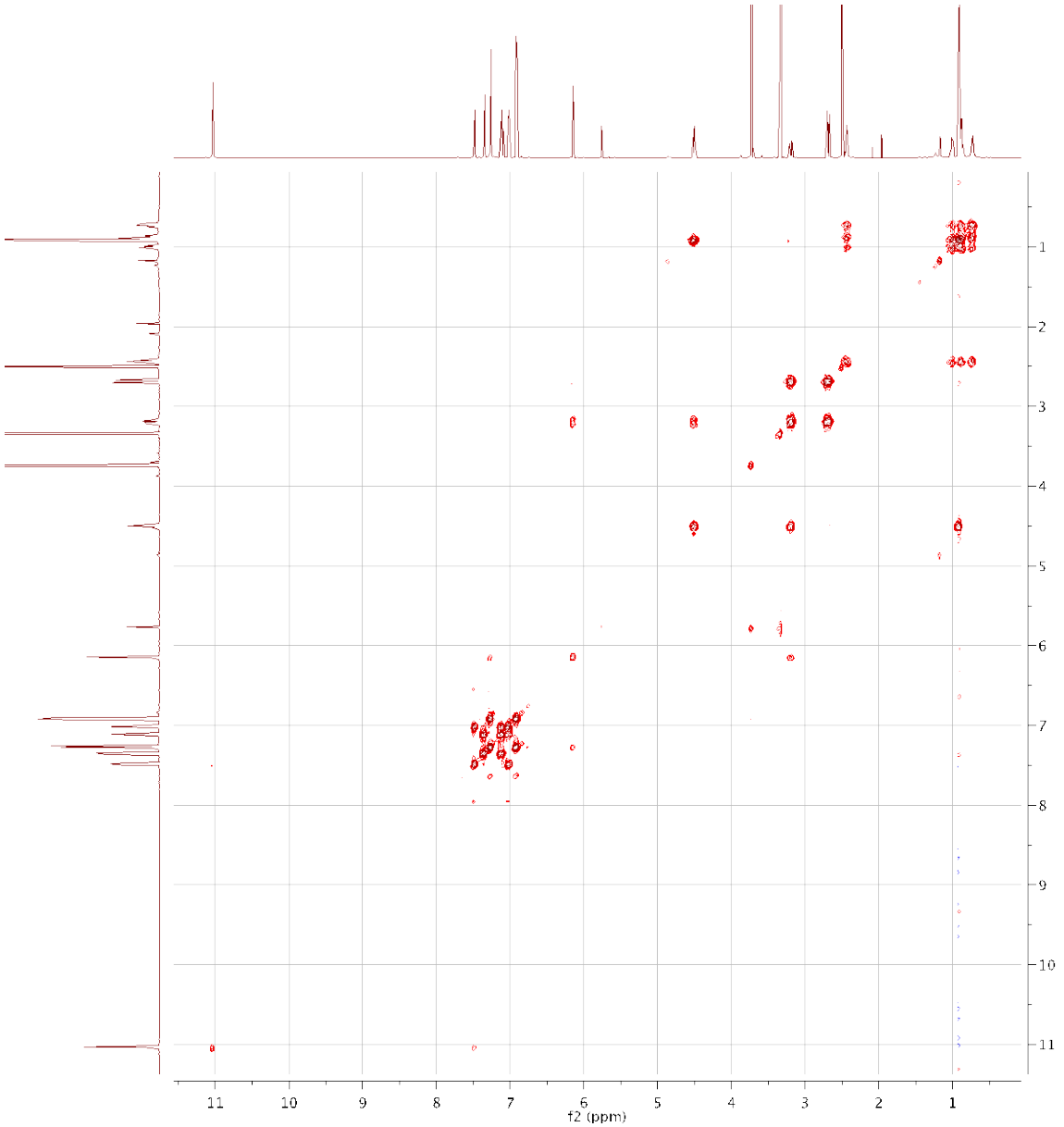
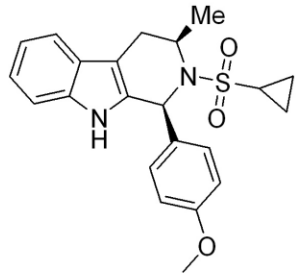
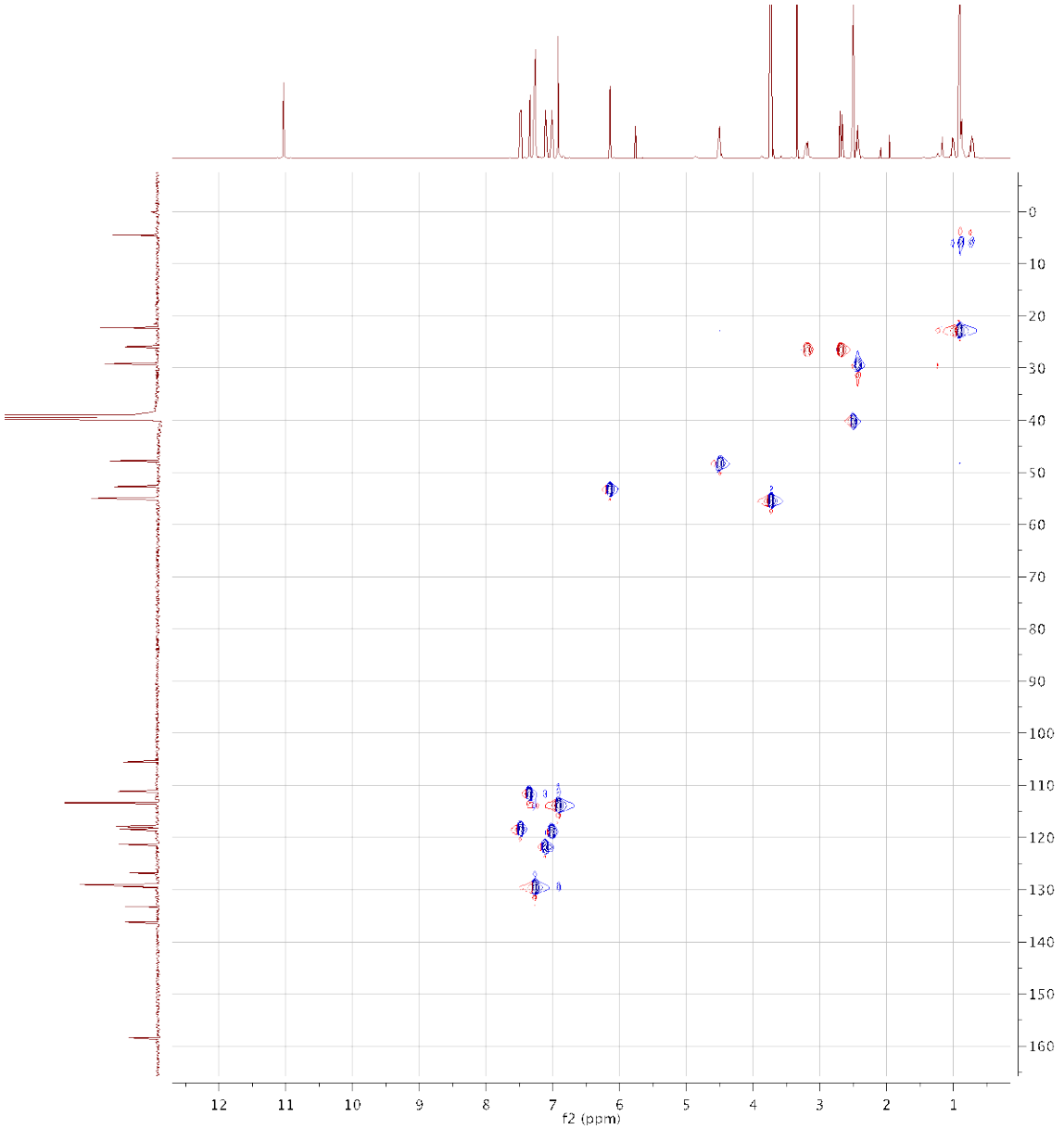
0.5
f1 (ppm)


158.39
136.20
133.24
129.54
129.03
126.77
121.30
118.37
117.88
113.35
111.13
105.56
54.96
52.73
47.79
29.16
25.91
22.20
4.76
4.51
Me
N
S
O
O
H
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

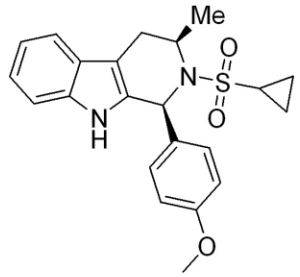


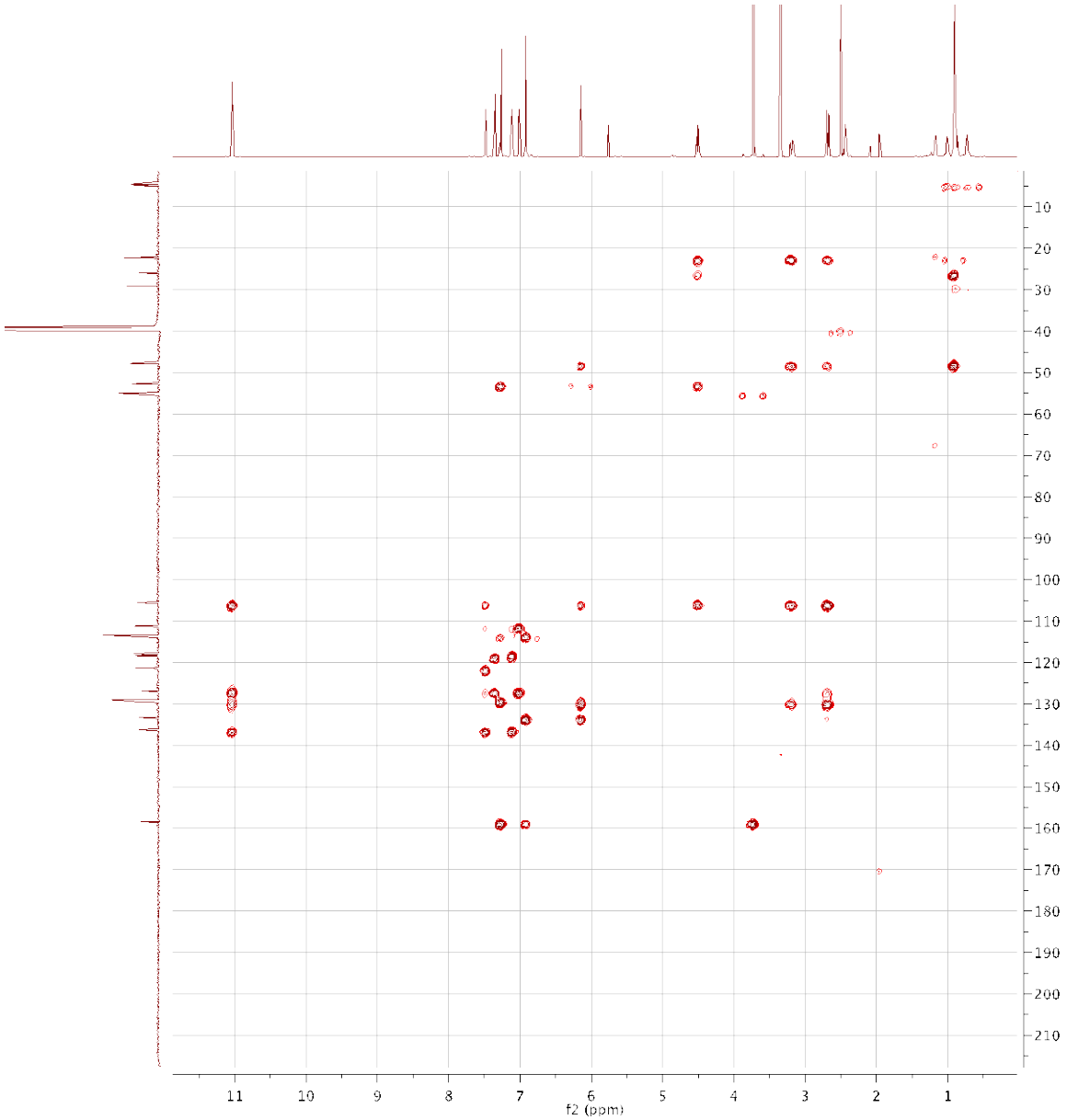
	Parameter	Value
1	Data File Name	81837682/ 13/ pdata/ 1/ 2rr
2	Sample ID	81837682
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	cosygpmfqf
7	Acquisition Date	2016-07-06T12:04:22
8	Temperature	300.0
9	Number of Scans	4
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6097.6, 6097.6)
12	Lowest Frequency	(-153.7, -153.7)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



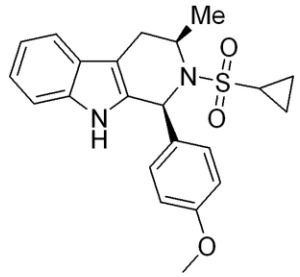


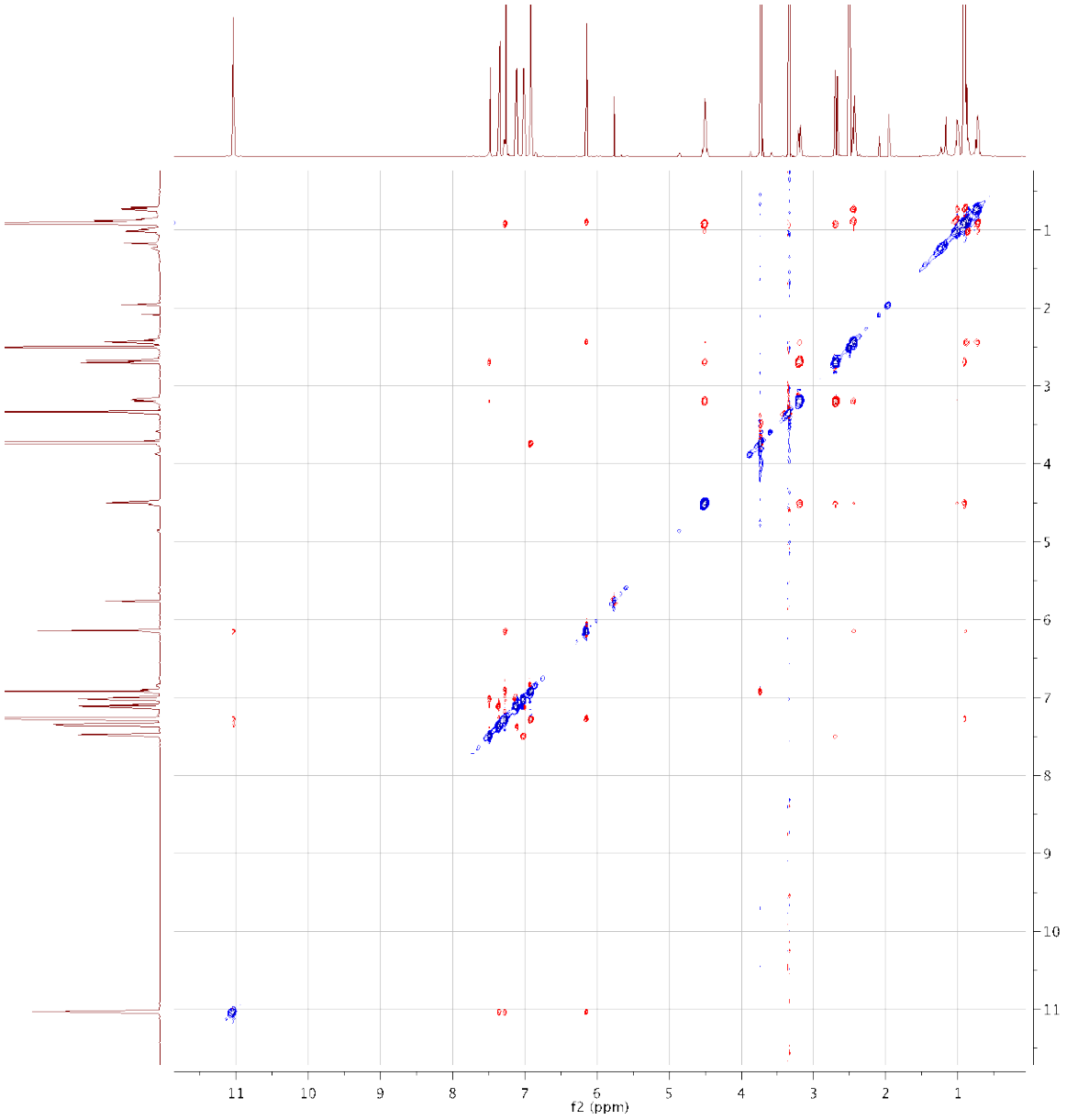
	Parameter	Value
1	Data File Name	81837682/ 14/ pdata/ 1/ 2rr
2	Sample ID	81837682
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	hsqcedetgpsisp2.2
7	Acquisition Date	2016-07-06T12:25:54
8	Temperature	300.0
9	Number of Scans	4
10	Spectrometer Frequency	(500.26, 125.79)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(1024, 1024)



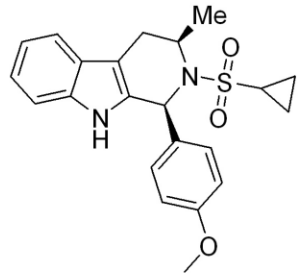


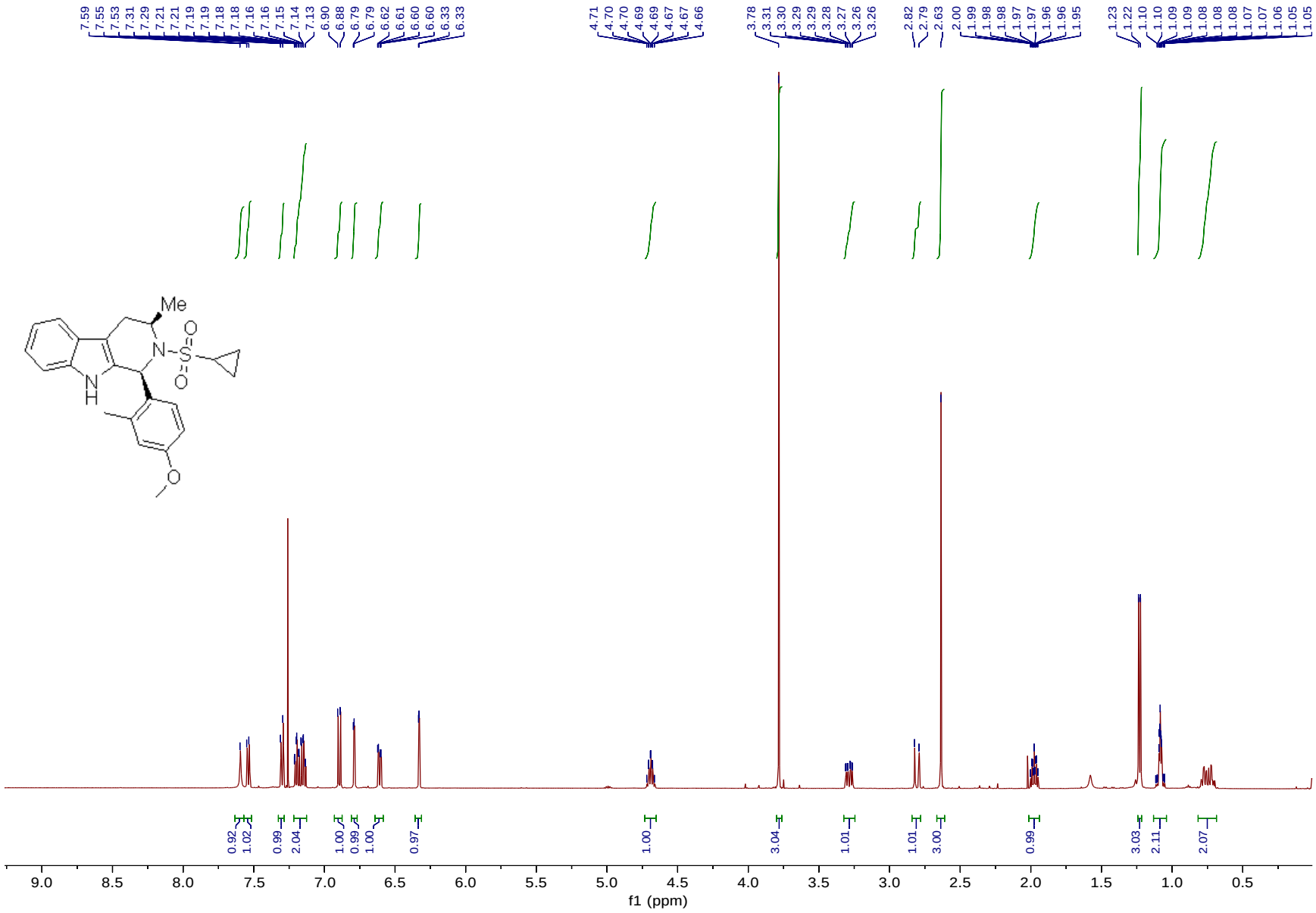
	Parameter	Value
1	Data File Name	81837682/ 15/ pdata/ 1/ 2rr
2	Sample ID	81837682
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	hmbcgplpndqf
7	Acquisition Date	2016-07-06T12:46:20
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 125.79)
11	Spectral Width	(6097.6, 30120.5)
12	Lowest Frequency	(-153.7, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(1024, 1024)

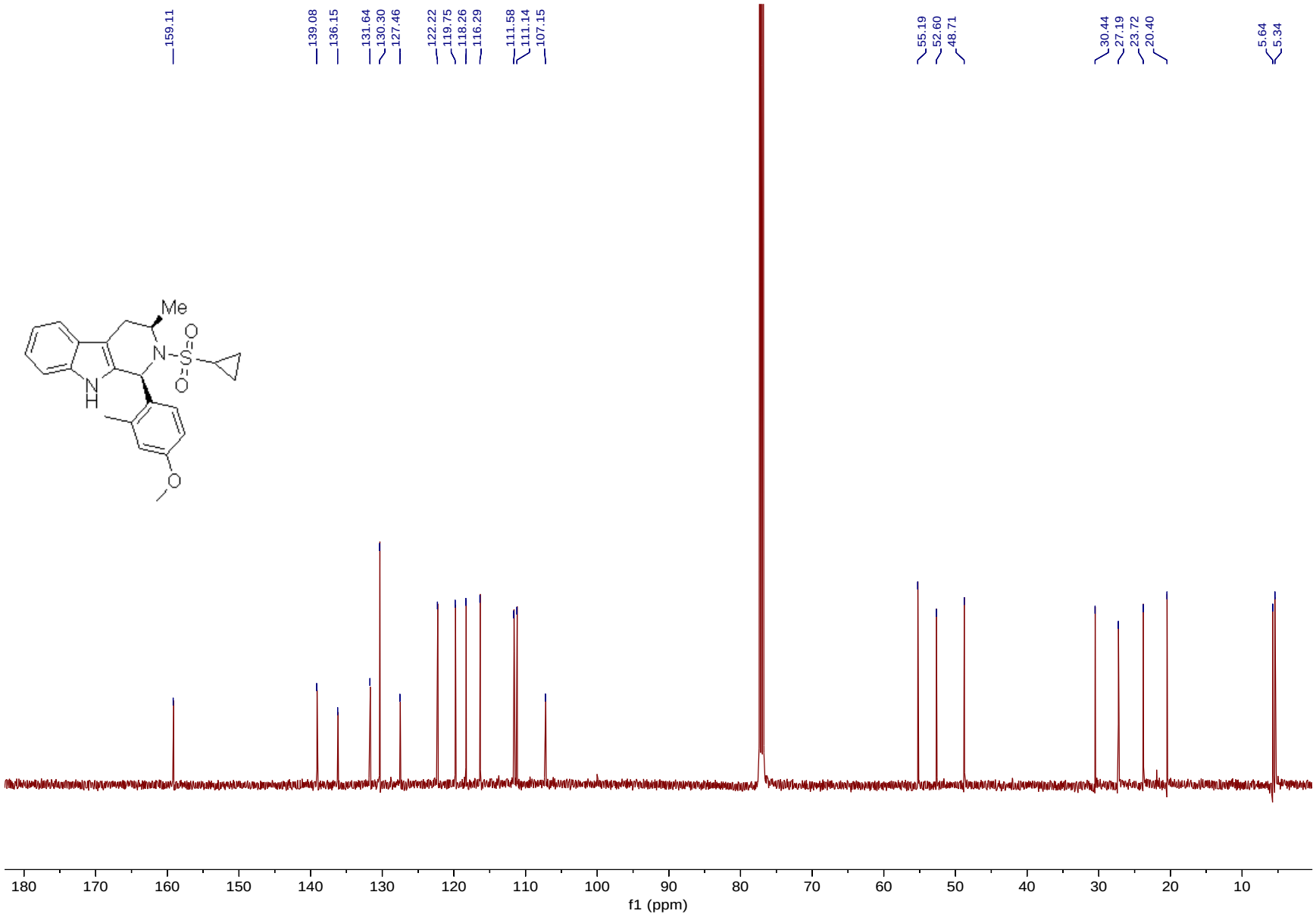




	Parameter	Value
1	Data File Name	81837682/ 16/ pdata/ 1/ 2rr
2	Sample ID	81837682
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-07-06T14:09:14
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6097.6, 6097.6)
12	Lowest Frequency	(-153.7, -153.7)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




7.59 7.55 7.53 7.31 7.29 7.21 7.21 7.19 7.19 7.18 7.18 7.16 7.16 7.15 7.14 7.13 6.90 6.88 6.79 6.79 6.62 6.61 6.60 6.60 6.33 6.33
4.71 4.70 4.70 4.69 4.69 4.67 4.67 4.66
3.78 3.31 3.30 3.29 3.29 3.28 3.27 3.26 3.26
2.82 2.79 2.63 2.00 1.99 1.98 1.98 1.97 1.97 1.96 1.96 1.95
1.23 1.22 1.10 1.10 1.09 1.09 1.08 1.08 1.08 1.07 1.07 1.06 1.05 1.05
Me
N
S
O
O
N
H
O
0.92 1.02 0.99 2.04 1.00 0.99 1.00 0.97 1.00 3.04 1.01 1.01 3.00 0.99 3.03 2.11 2.07
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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139.08
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131.64
130.30
127.46
122.22
119.75
118.26
116.29
111.58
111.14
107.15
55.19
52.60
48.71
30.44
27.19
23.72
20.40
5.64
5.34
Me
N
S
O
O
N
H
O
180
170
160
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130
120
110
100
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80
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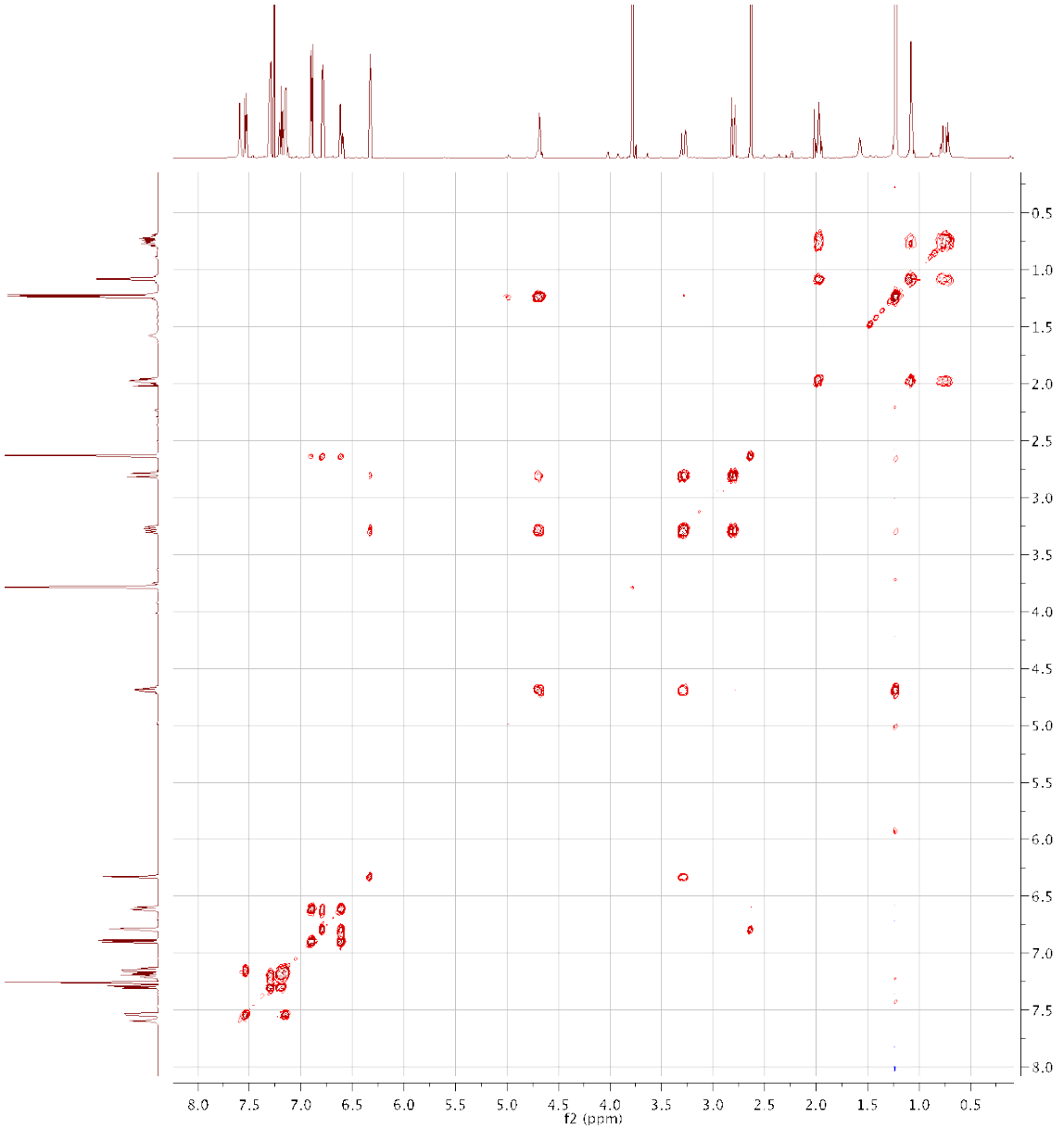
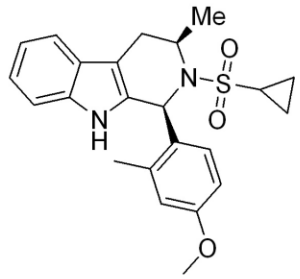
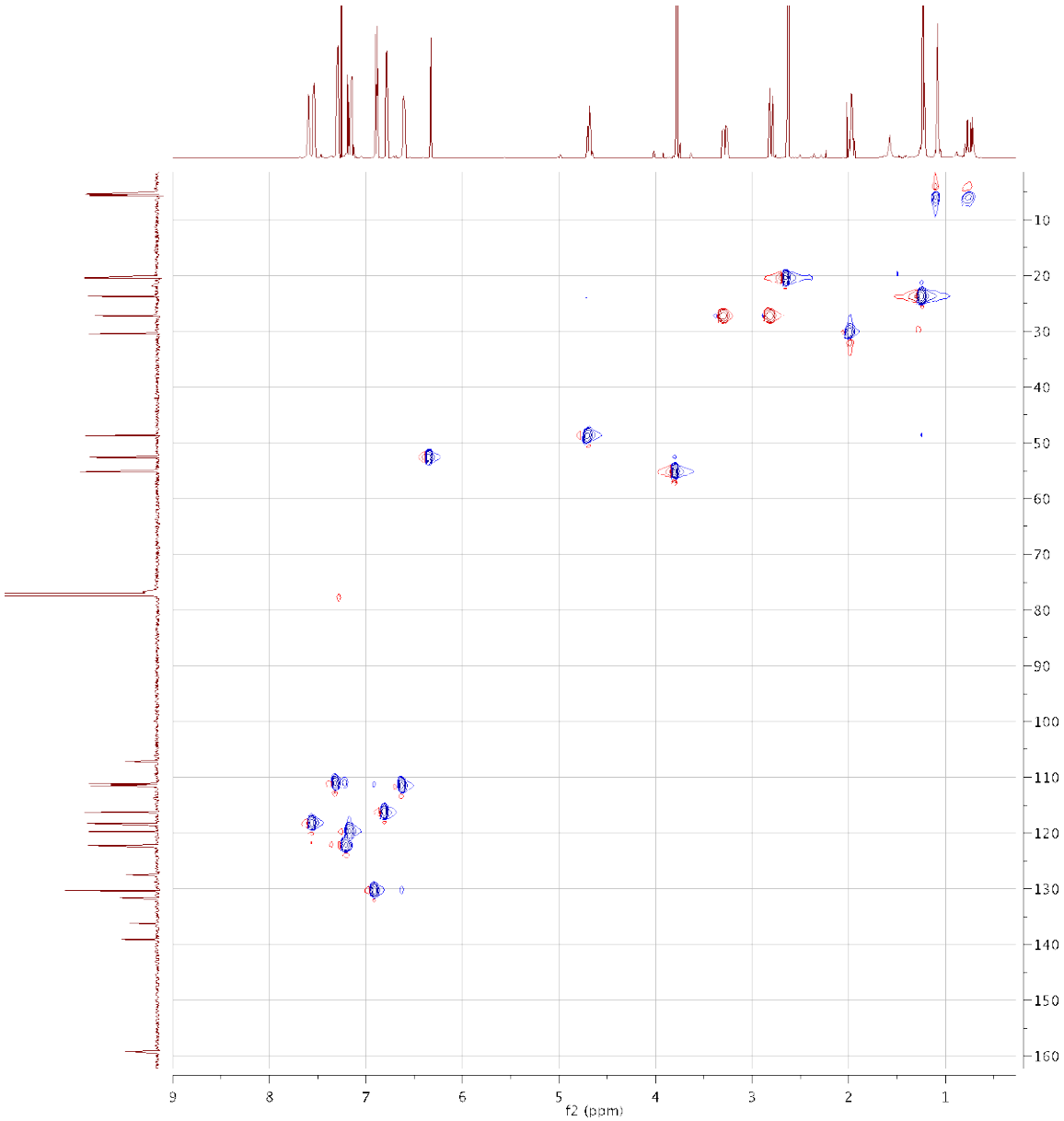
60
50
40
30
20
10
f1 (ppm)

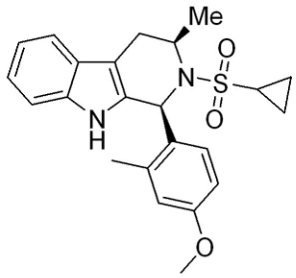


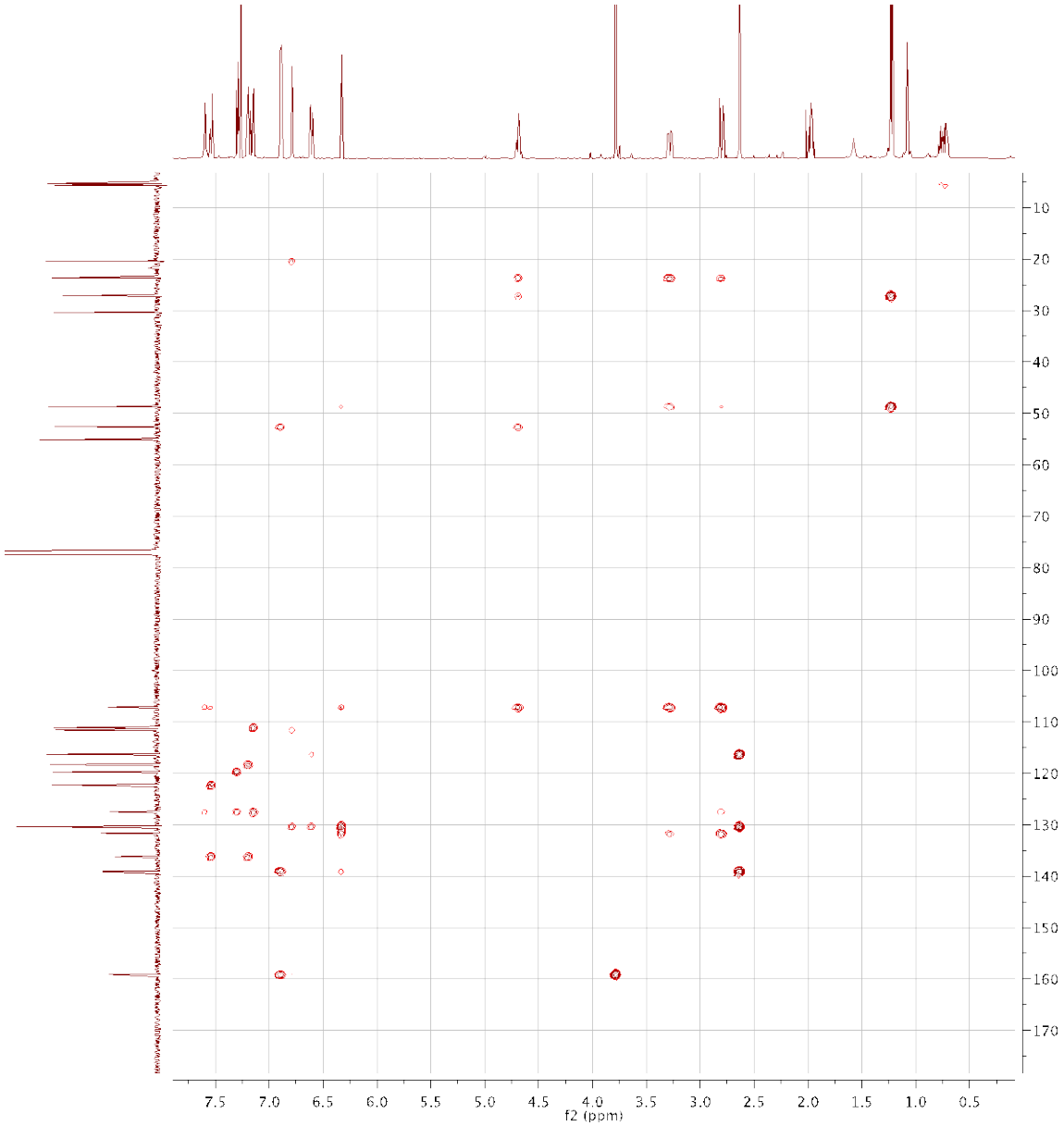
	Parameter	Value
1	Data File Name	81846848/ 13/ pdata/ 1/ 2rr
2	Sample ID	81846848
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	CDCl3
6	Pulse Sequence	cosygpmfqf
7	Acquisition Date	2016-07-18T11:12:13
8	Temperature	300.0
9	Number of Scans	4
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(4237.3, 4237.3)
12	Lowest Frequency	(-83.7, -83.7)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



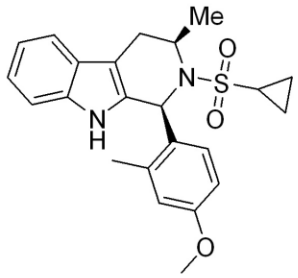


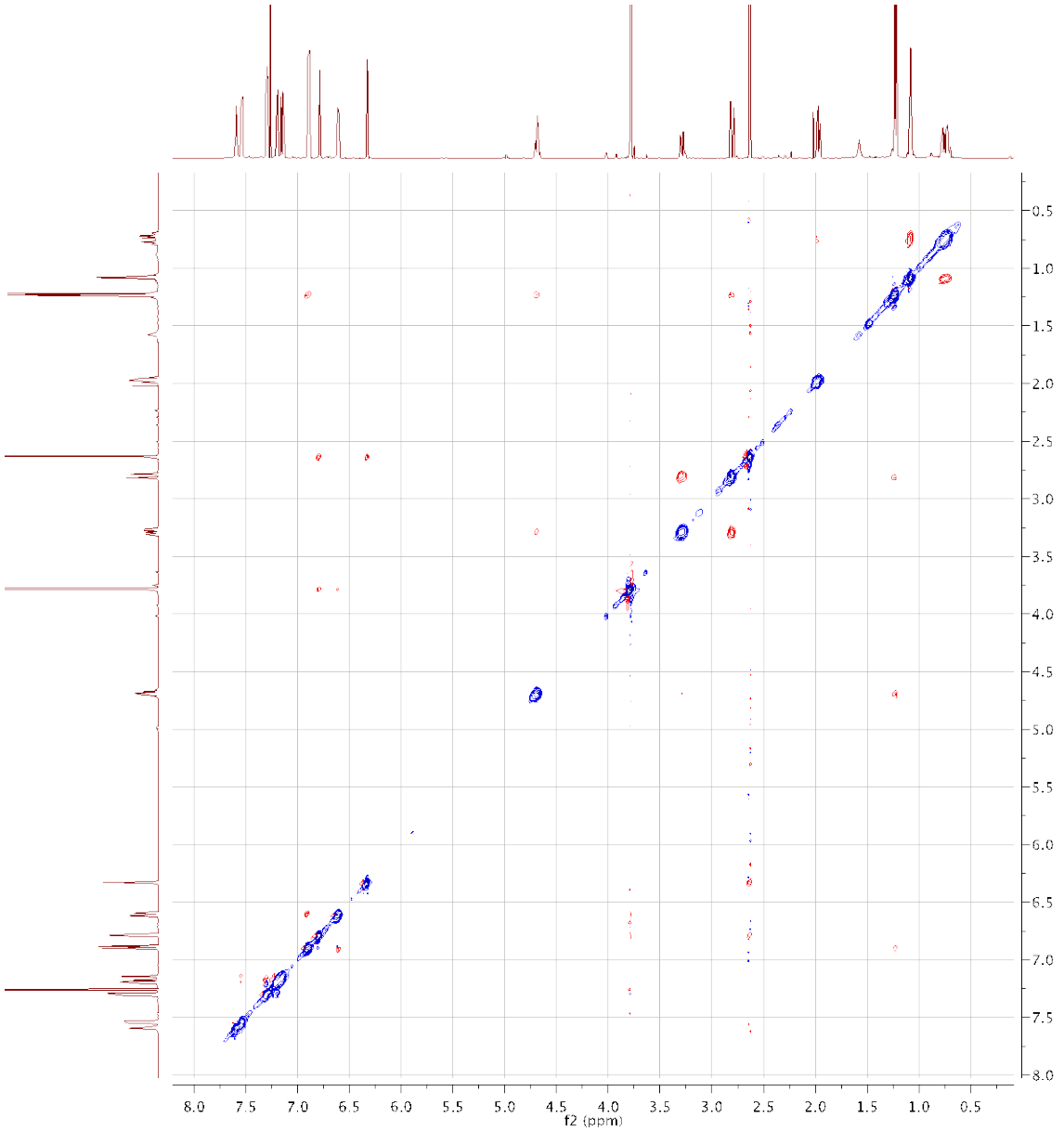
	Parameter	Value
1	Data File Name	81846848/ 14/ pdata/ 1/ 2rr
2	Sample ID	81846848
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	CDCl3
6	Pulse Sequence	hsqcedetgpsisp2.2
7	Acquisition Date	2016-07-18T11:33:56
8	Temperature	300.0
9	Number of Scans	4
10	Spectrometer Frequency	(500.26, 125.79)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(1024, 1024)



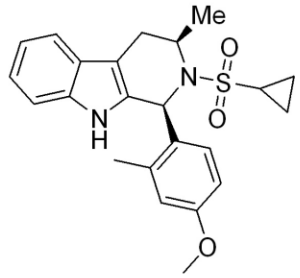


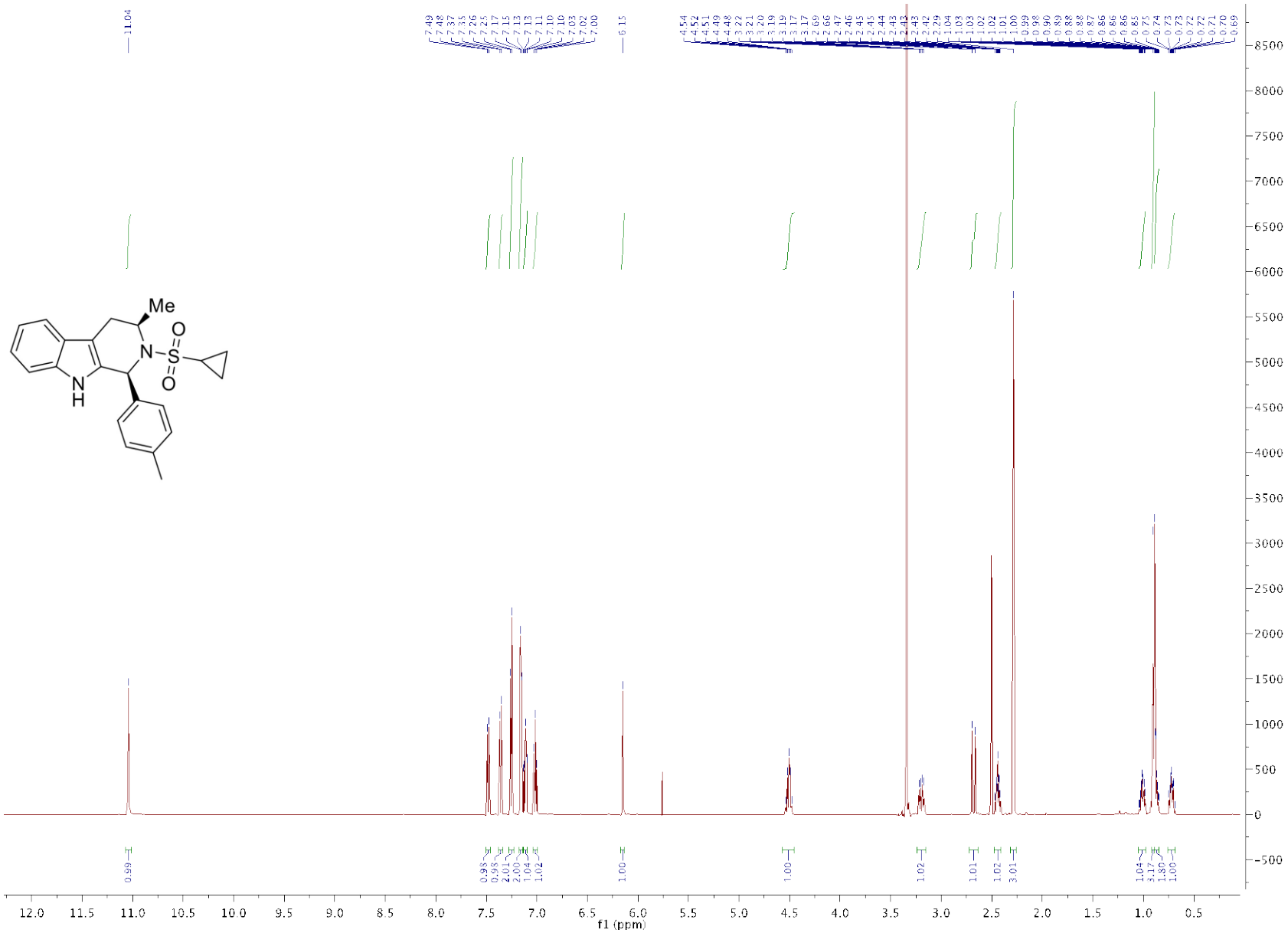
	Parameter	Value
1	Data File Name	81846848/ 15/ pdata/ 1/ 2rr
2	Sample ID	81846848
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	CDCl3
6	Pulse Sequence	hmbcgplpndqf
7	Acquisition Date	2016-07-18T11:54:24
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 125.79)
11	Spectral Width	(4237.3, 30120.5)
12	Lowest Frequency	(-83.7, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(1024, 1024)

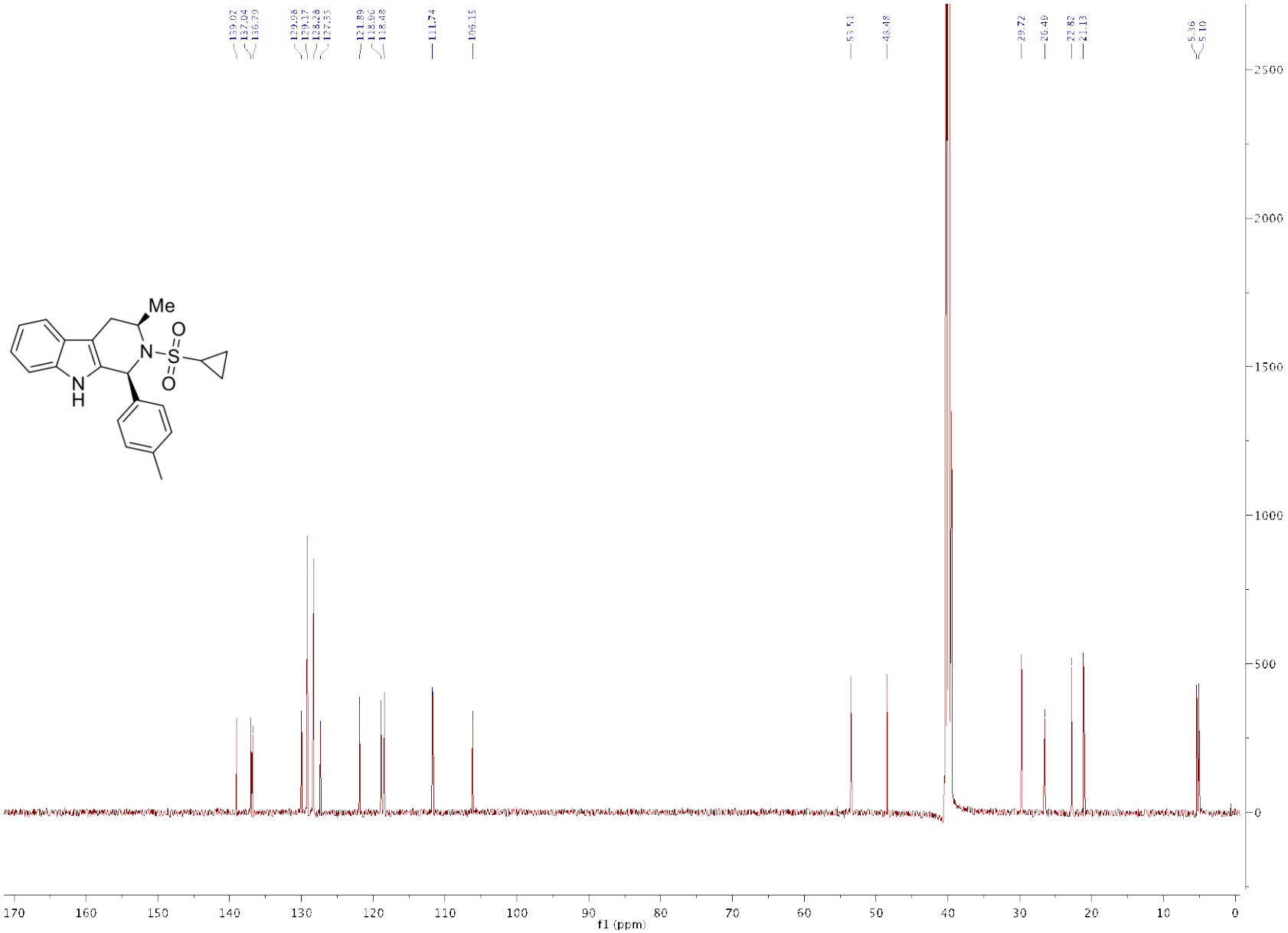




	Parameter	Value
1	Data File Name	81846848/ 16/ pdata/ 1/ 2rr
2	Sample ID	81846848
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	CDCl3
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-07-18T13:17:19
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(4237.3, 4237.3)
12	Lowest Frequency	(-83.7, -83.7)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
O
N
S
O
N
H
f1 (ppm)


139.02
137.04
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127.35
121.89
118.96
118.48
111.74
106.15
53.51
48.48
29.72
26.49
22.82
21.13
5.36
5.10
Me
N
S
O
O
N
H
2500
2000
1500
1000
500
0
170
160
150
140
130
120
110
100
90
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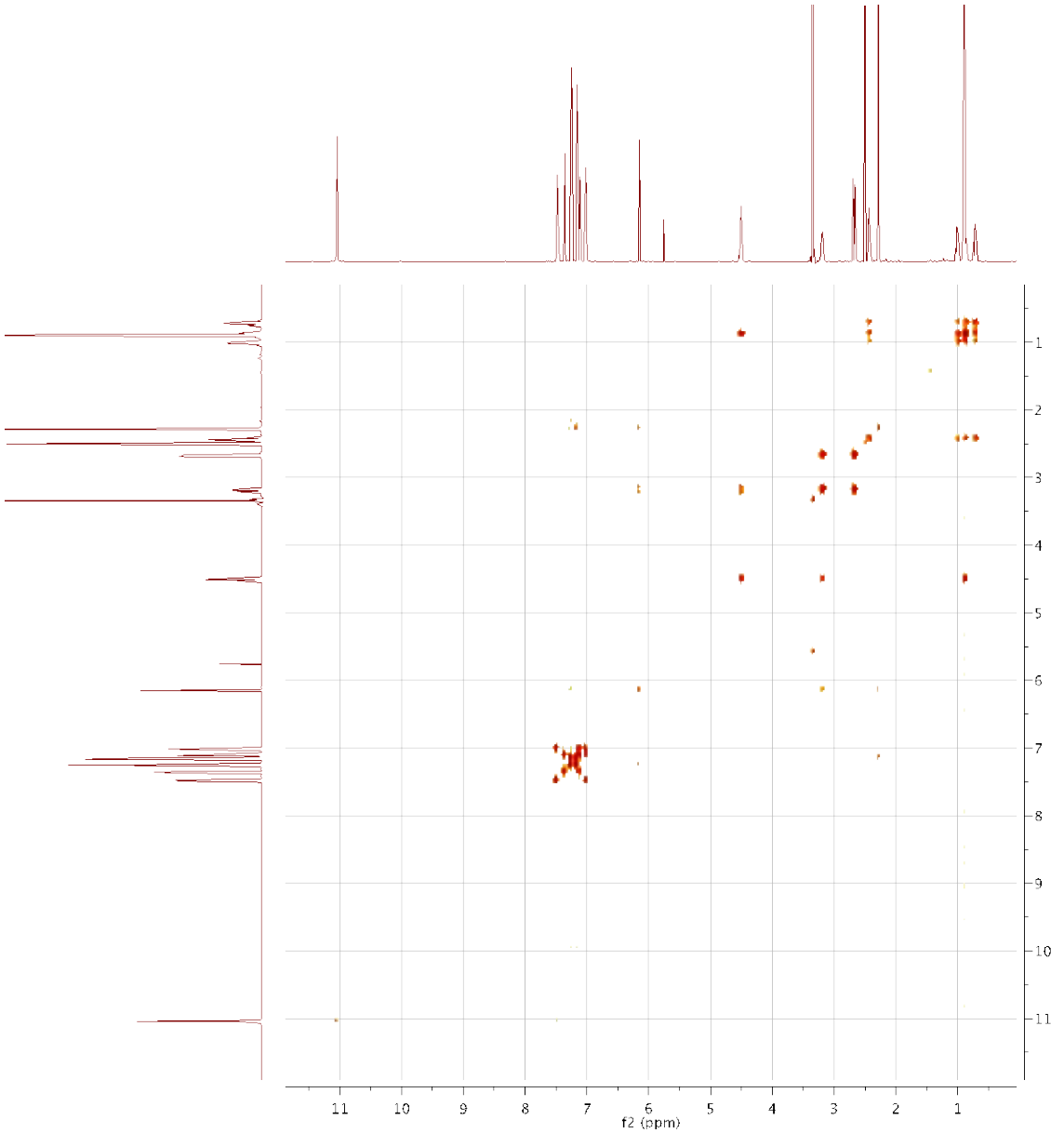
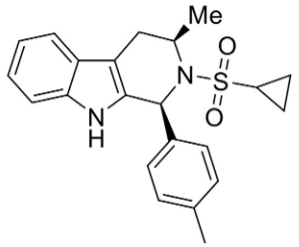
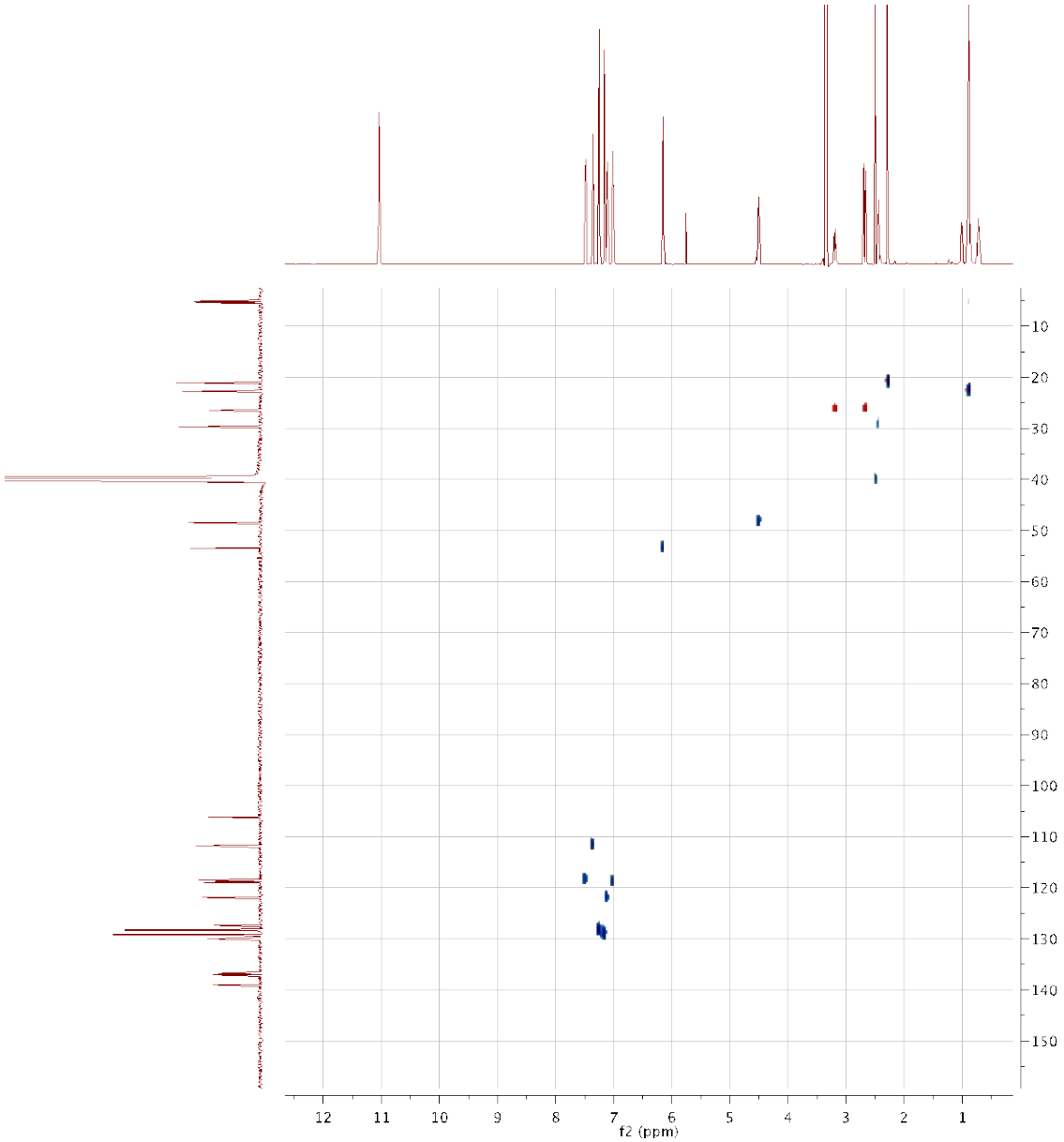
70
60
50
40
30
20
10
0
f1 (ppm)

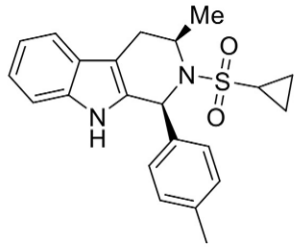


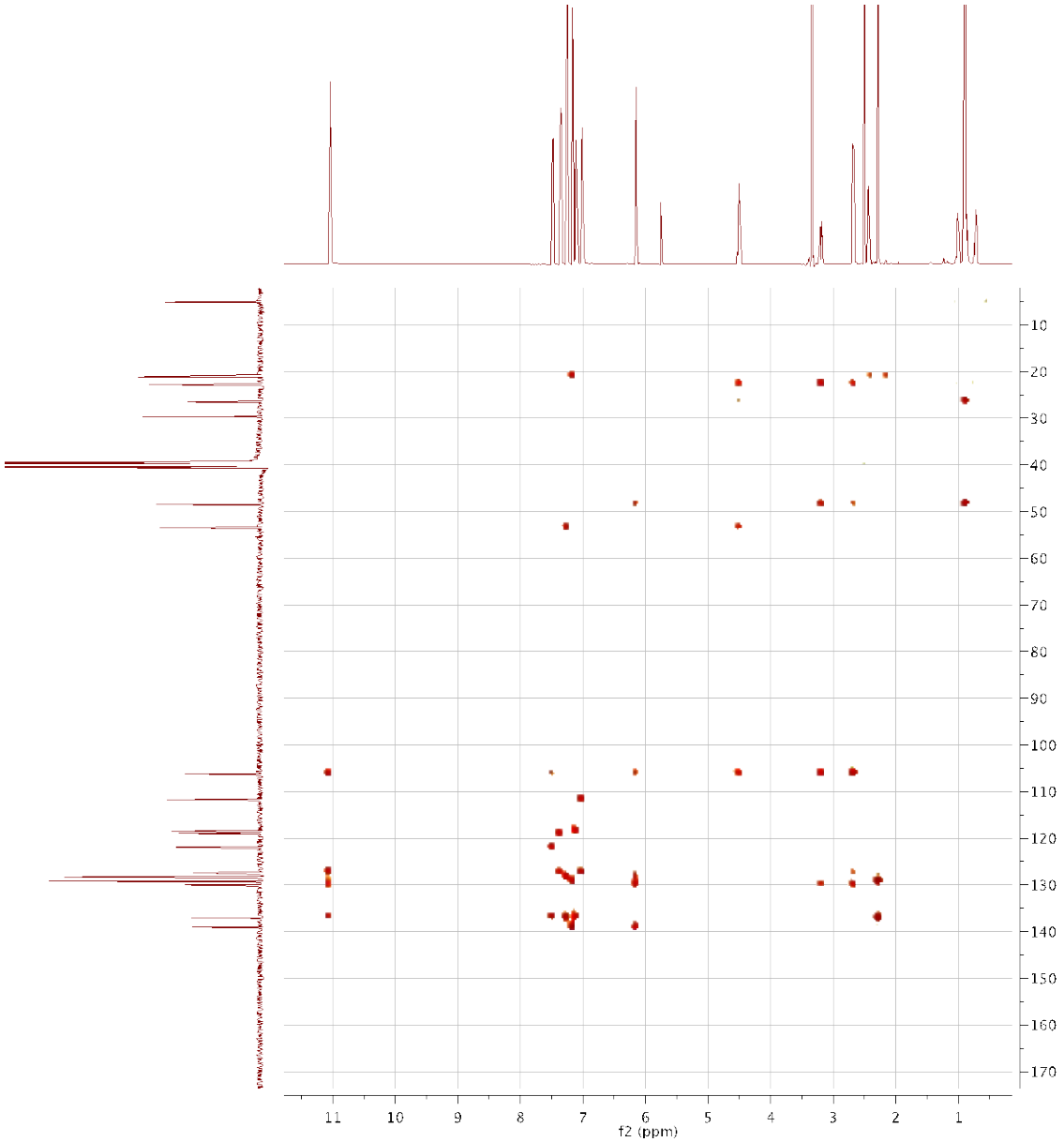
	Parameter	Value
1	Data File Name	81861300/ 13/ pdata/ 1/ 2rr
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T17:24:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-373.1, -373.1)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



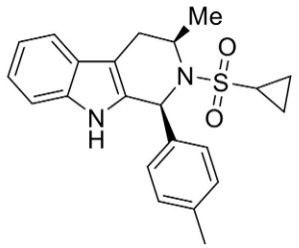


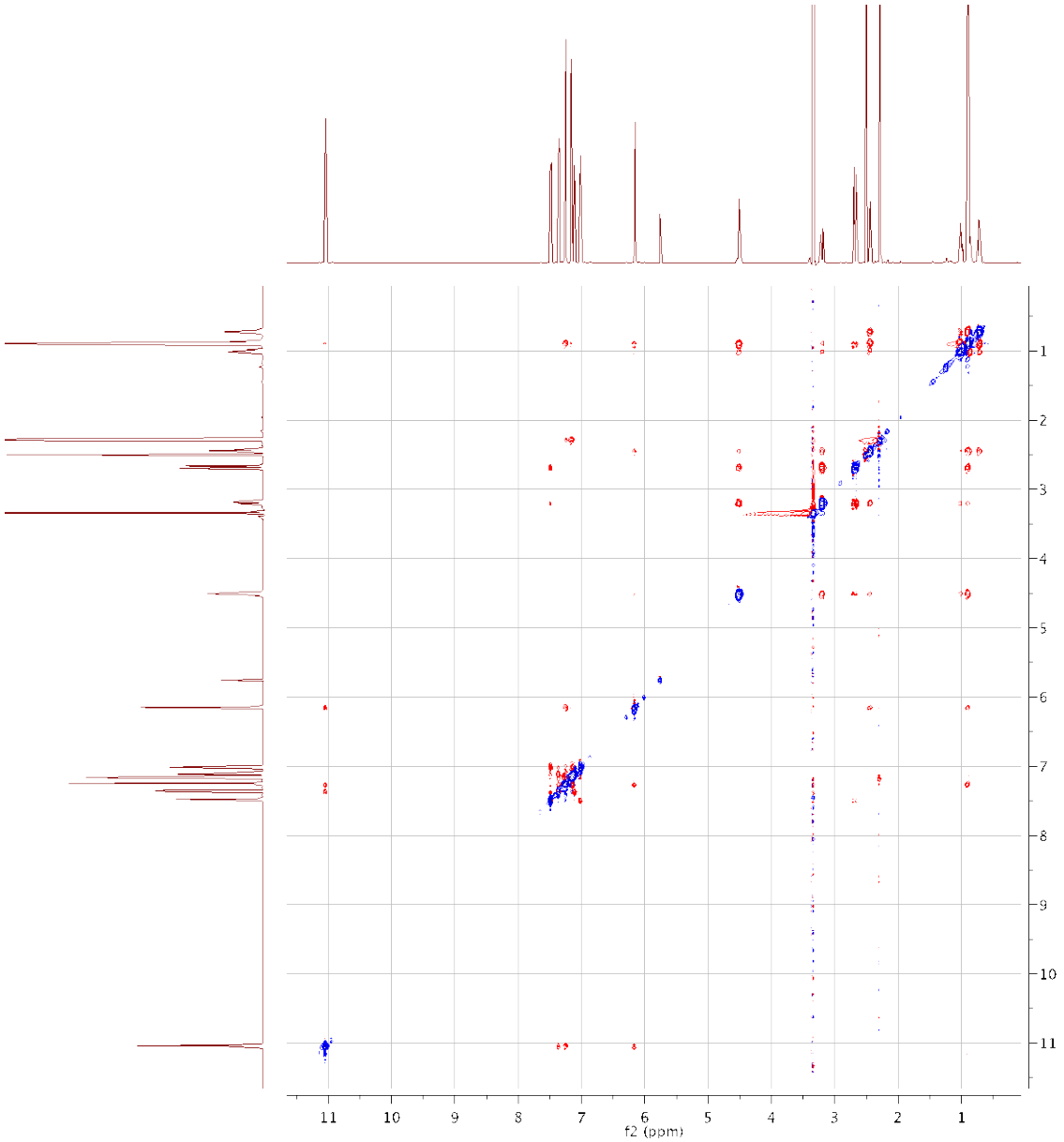
	Parameter	Value
1	Data File Name	81861300/ 14/ pdata/ 1/ 2rr
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T17:45:00
10	Spectrometer Frequency	(500.26, 125.79)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(1024, 1024)



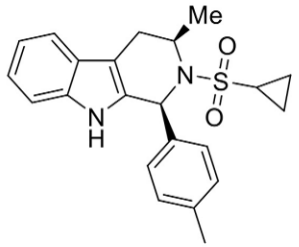


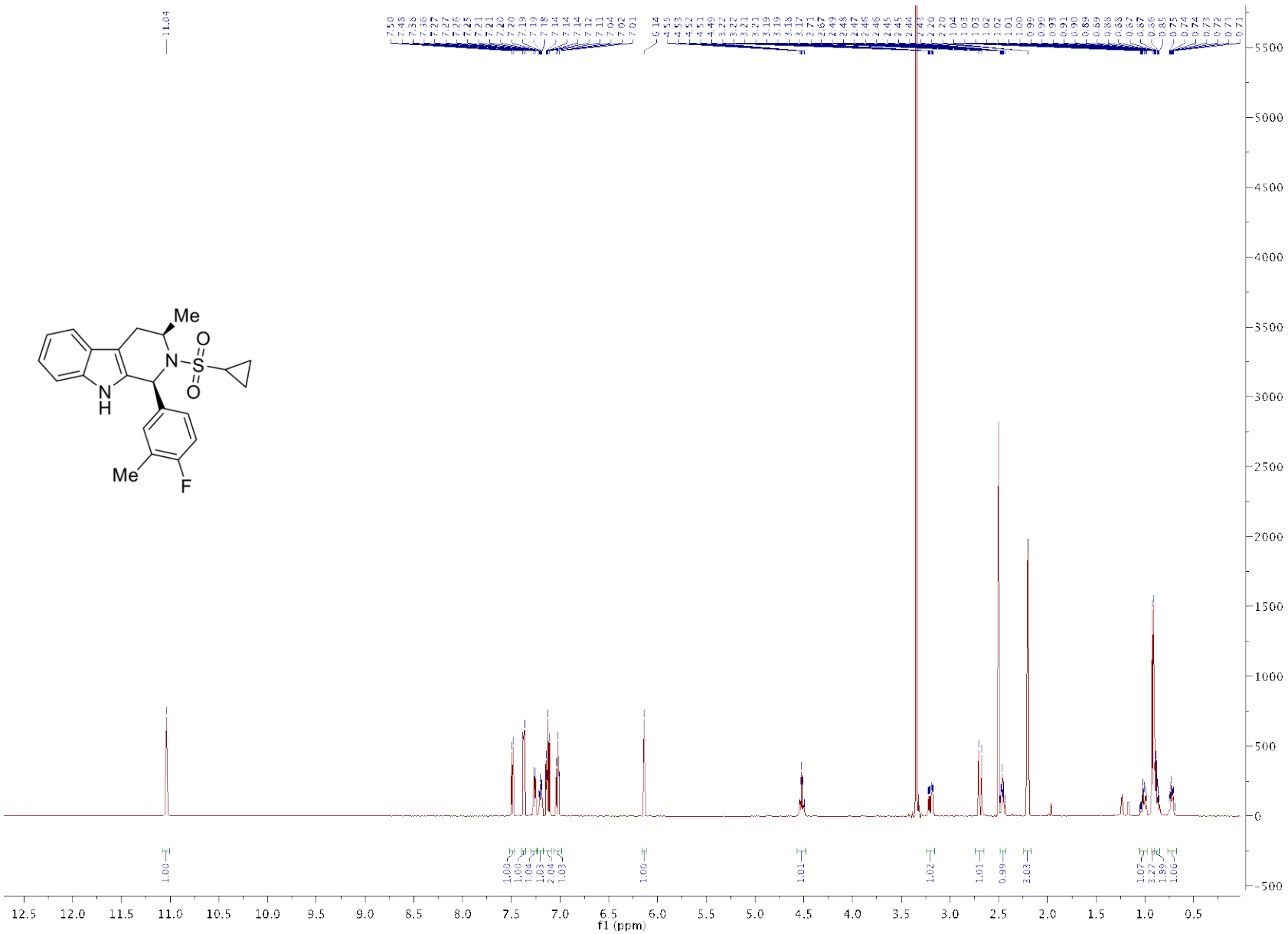
	Parameter	Value
1	Data File Name	81861300/ 15/ pdata/ 1/ 2rr
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T18:06:00
10	Spectrometer Frequency	(500.26, 125.79)
11	Spectral Width	(6329.1, 30120.5)
12	Lowest Frequency	(-373.1, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(1024, 1024)





	Parameter	Value
1	Data File Name	81861300/ 16/ pdata/ 1/ 2rr
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	roesyphpp.2
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T19:29:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-373.1, -373.1)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




11.04
Me
O
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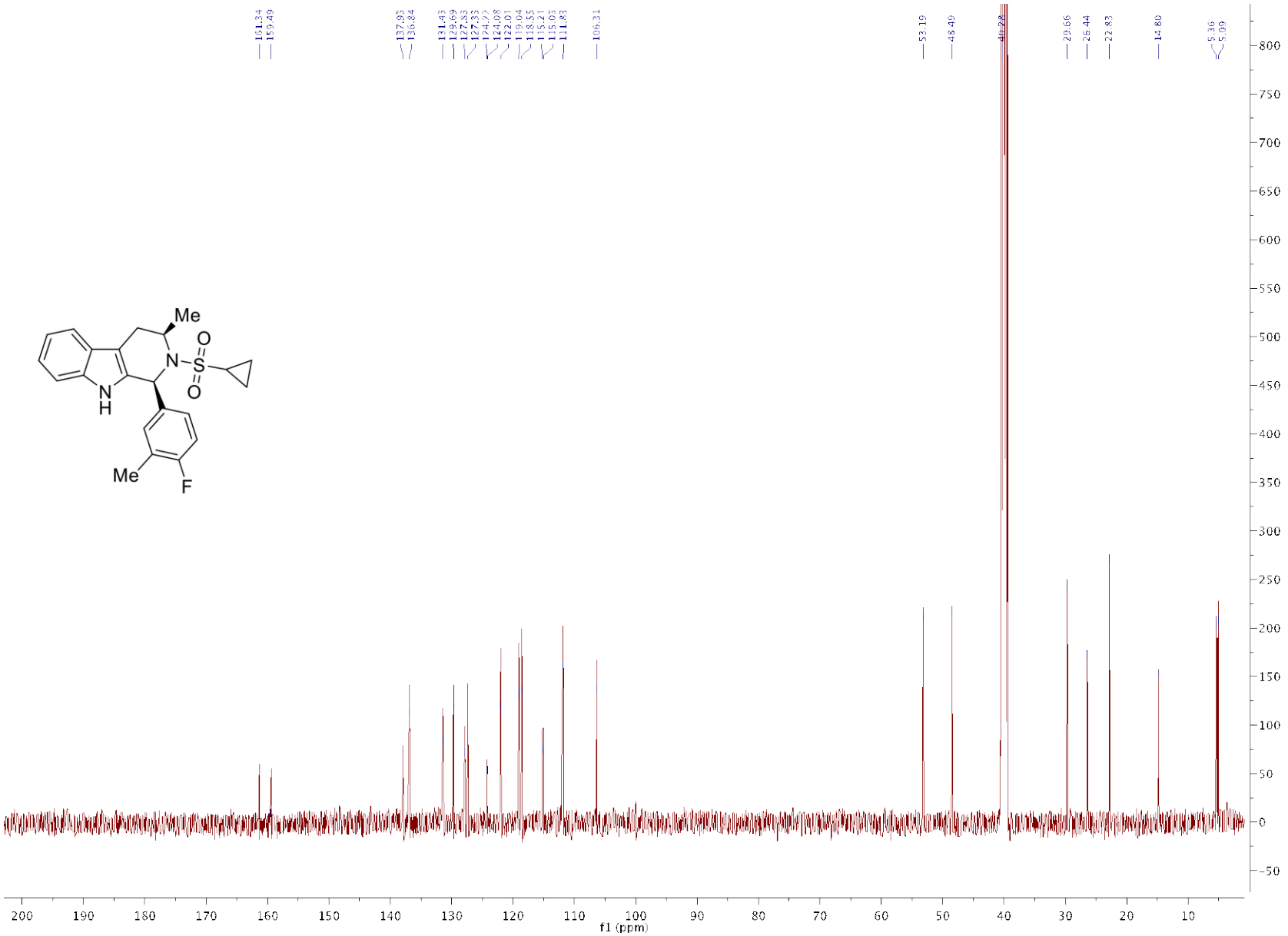
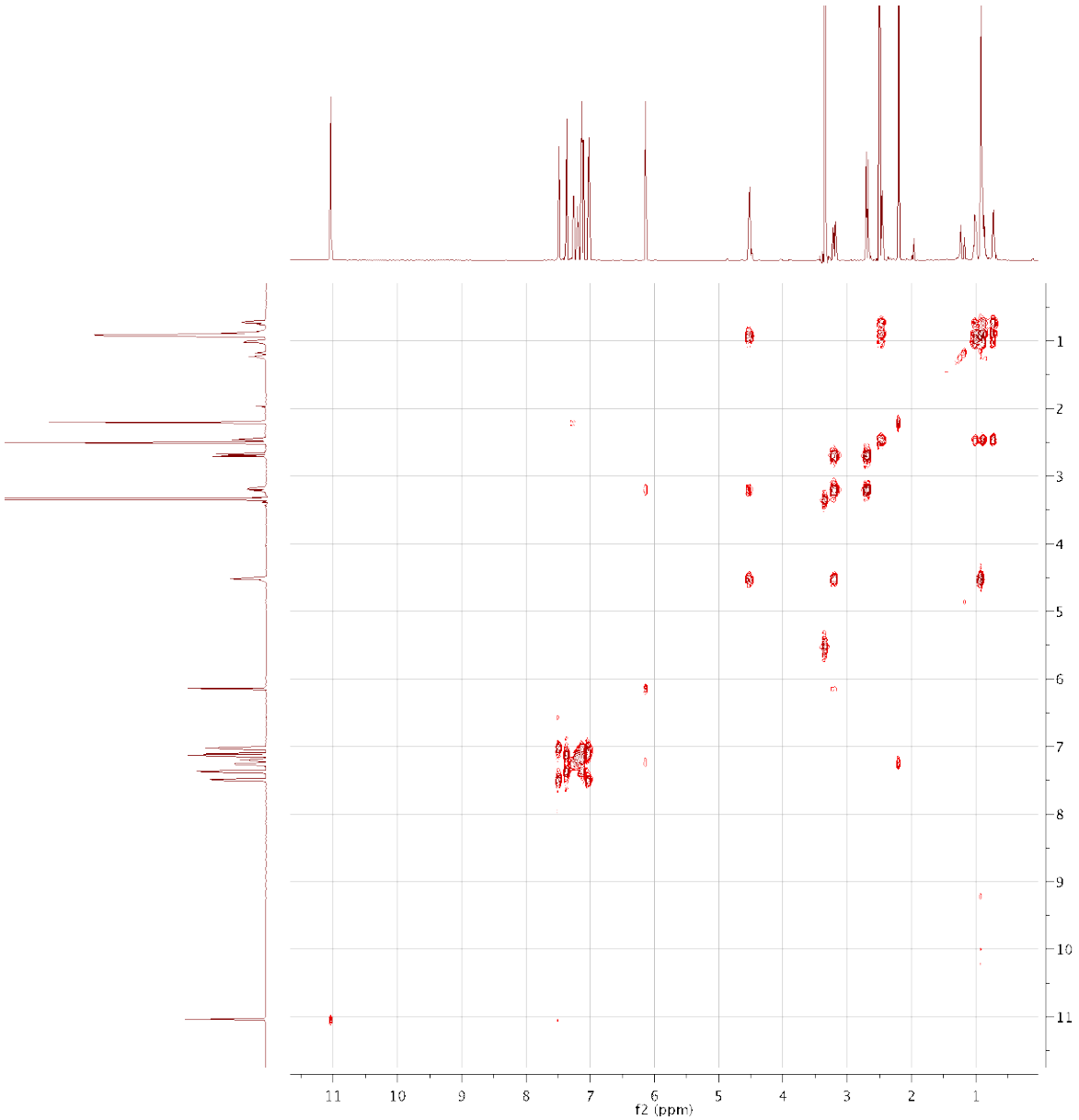
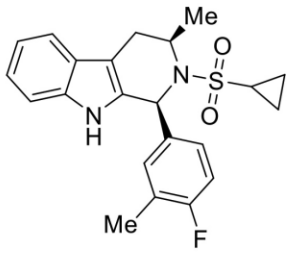
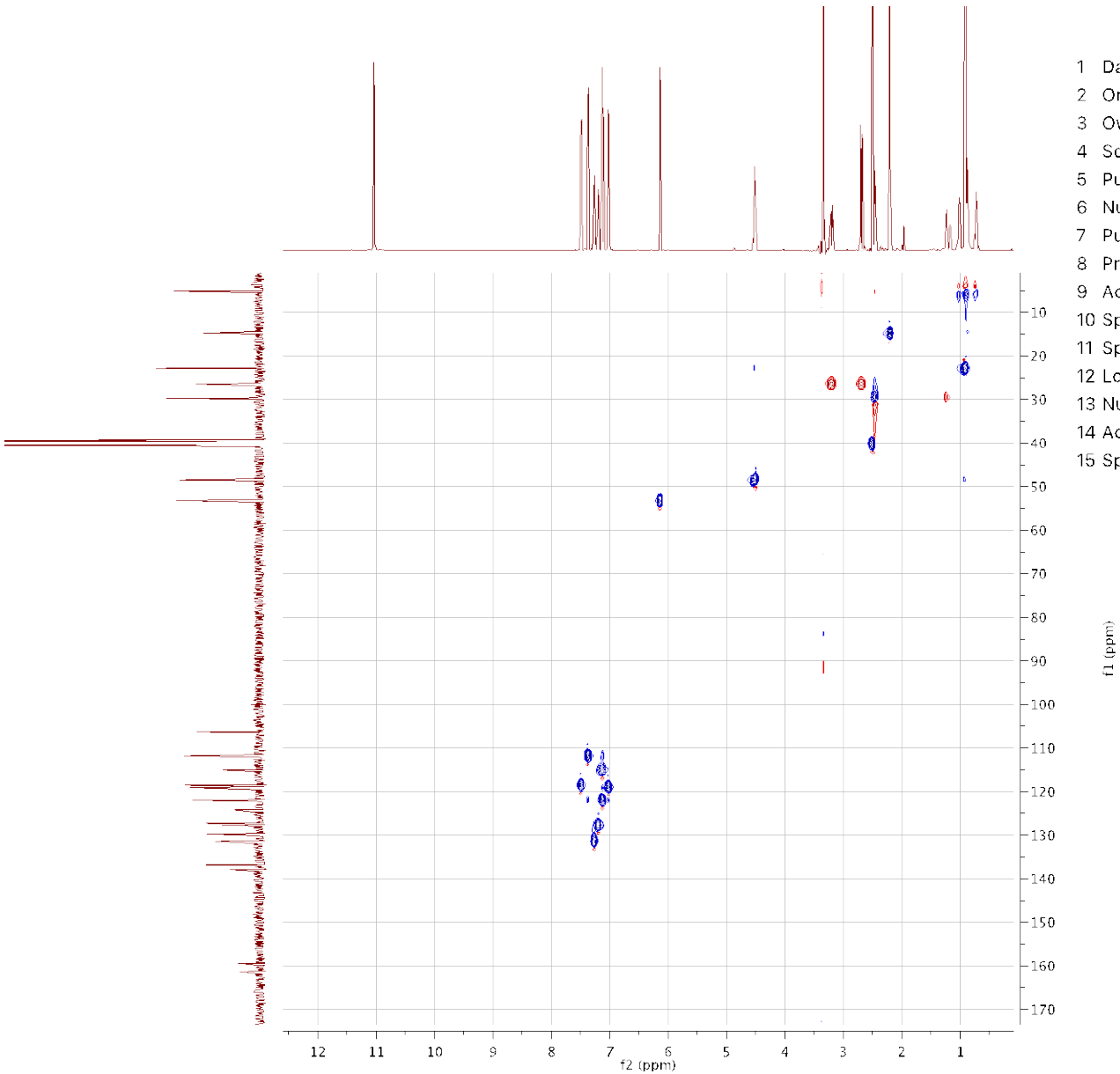
S
O
N
H
Me
F
f1 (ppm)


161.34
159.49
137.95
136.84
131.43
129.69
127.83
127.33
124.08
122.01
119.04
118.55
115.21
115.03
111.83
106.31
53.19
48.49
40.28
29.66
26.44
22.83
14.80
5.36
5.09
Me
O
N
S
O
N
H
Me
F
f1 (ppm)

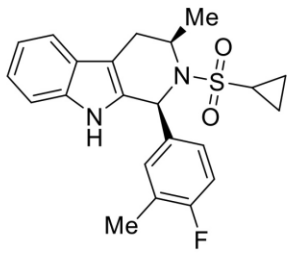


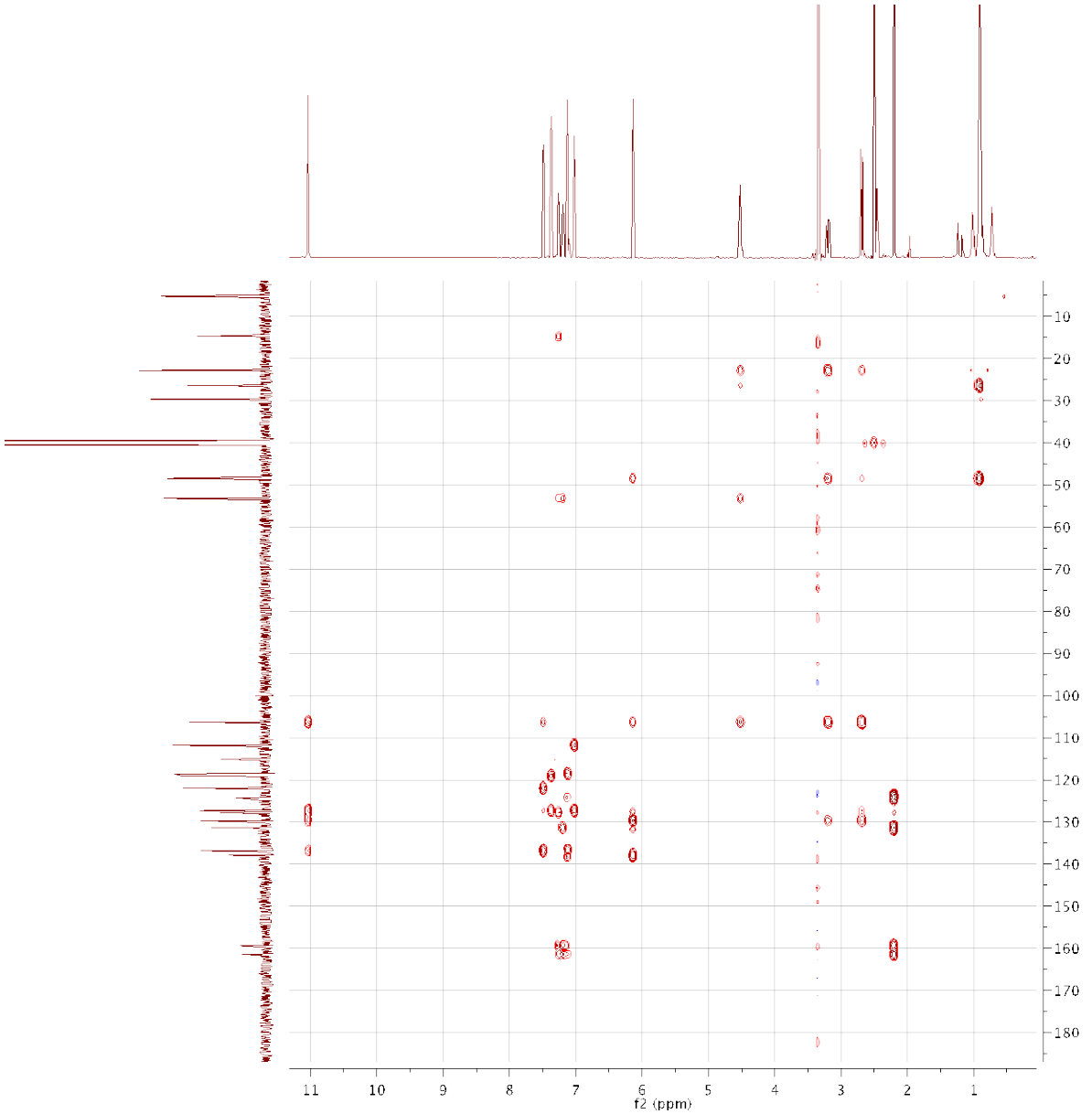
	Parameter	Value
1	Data File Name	81872499/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-19T20:51:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-408.8, -408.8)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



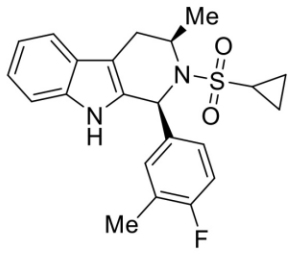


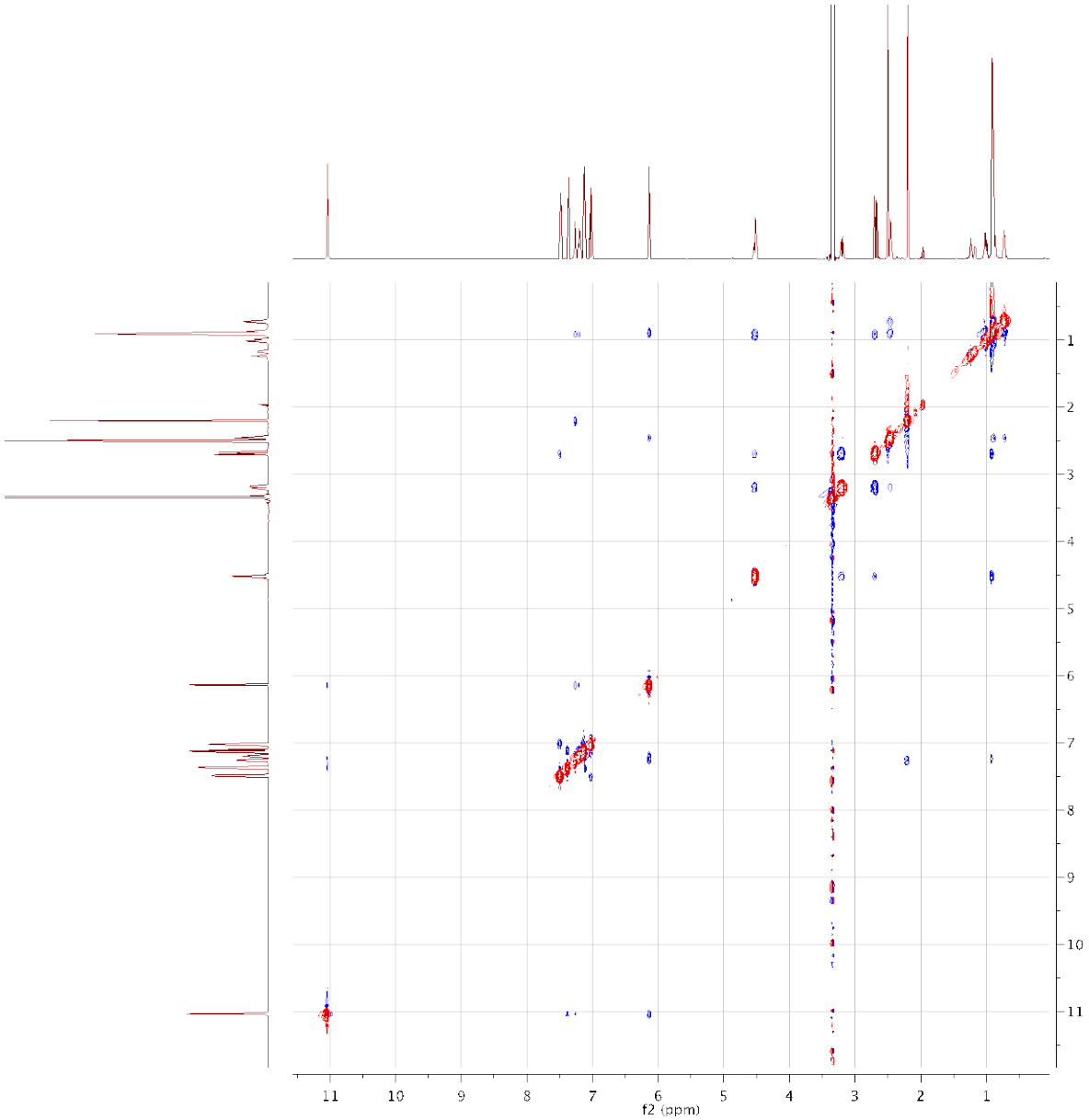
	Parameter	Value
1	Data File Name	81872499/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-19T21:13:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



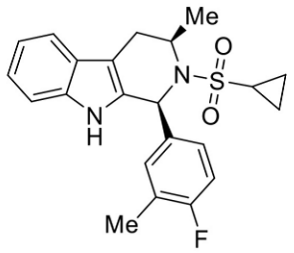


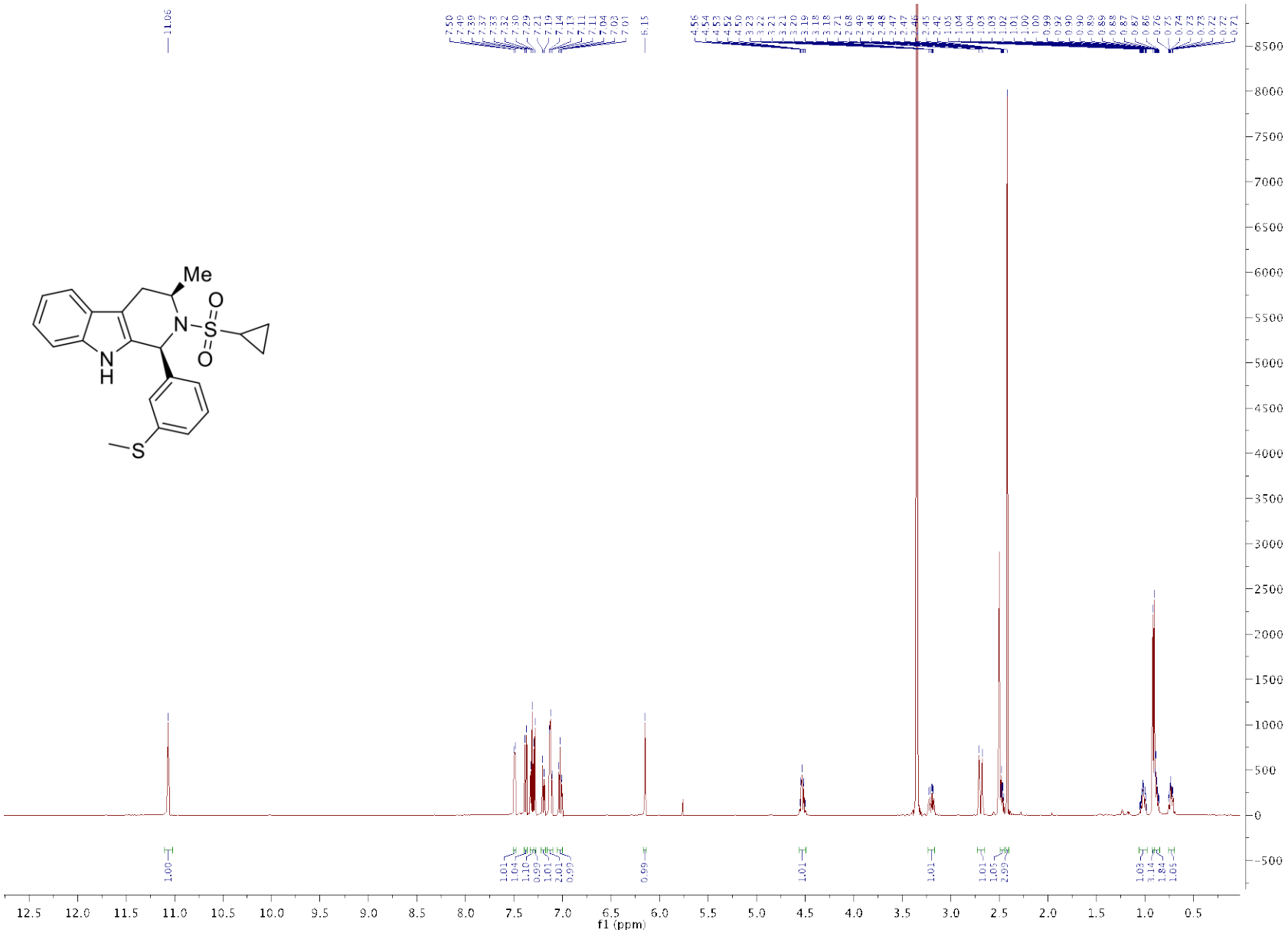
	Parameter	Value
1	Data File Name	81872499/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-19T21:33:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6329.1, 30120.5)
12	Lowest Frequency	(-408.8, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

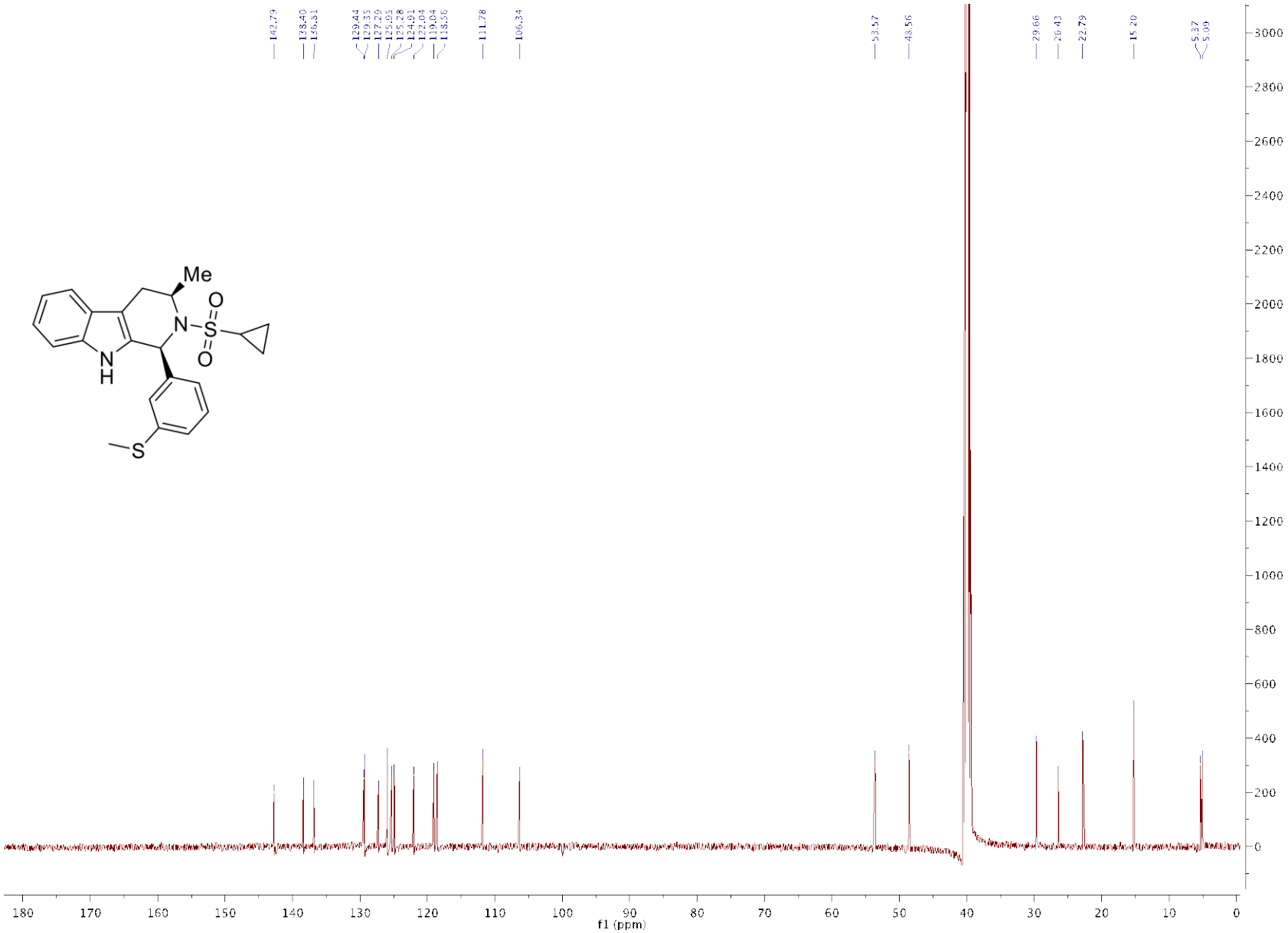




	Parameter	Value
1	Data File Name	81872499/ 16/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	roesyphpp.2
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-19T22:56:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-408.8, -408.8)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
O
N
S
O
N
H
S
f1 (ppm)


142.79
138.40
136.31
129.44
129.35
127.29
125.95
125.28
124.91
122.04
119.04
118.56
111.78
106.34
53.57
48.56
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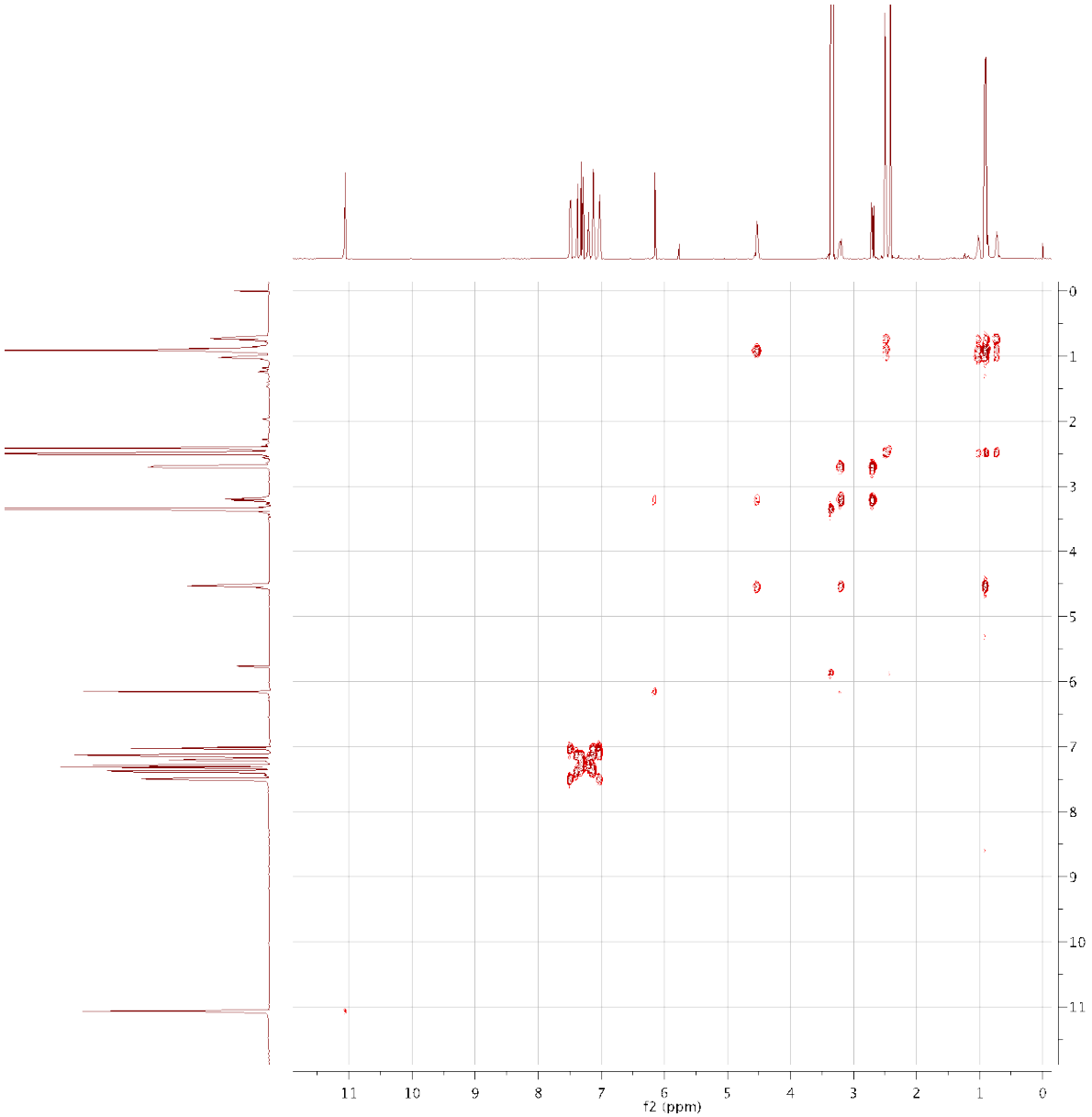
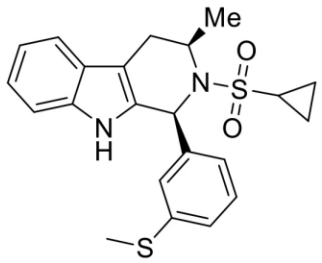
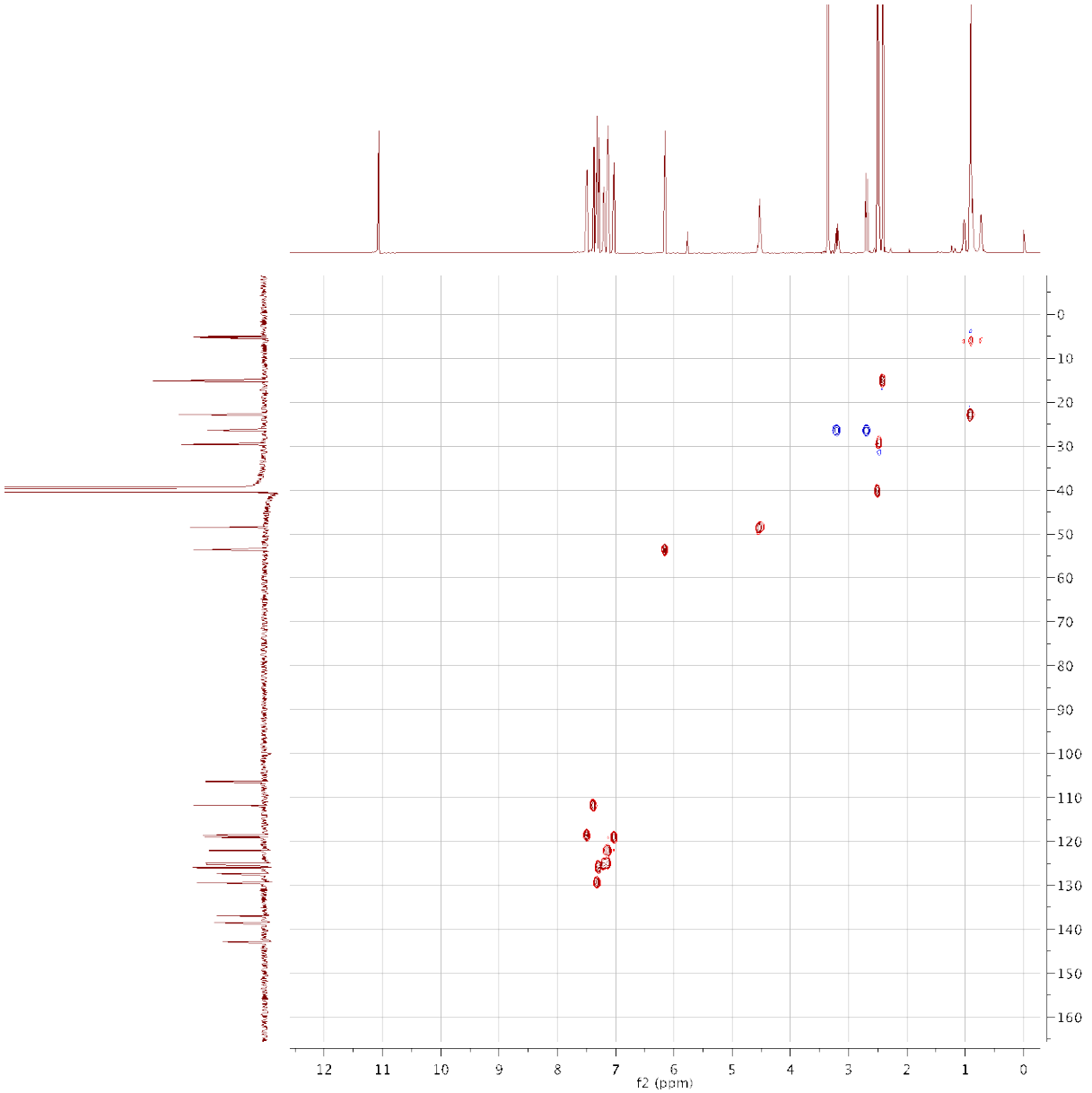
O
N
S
O
N
H
S
f1 (ppm)

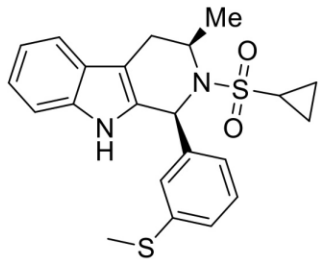


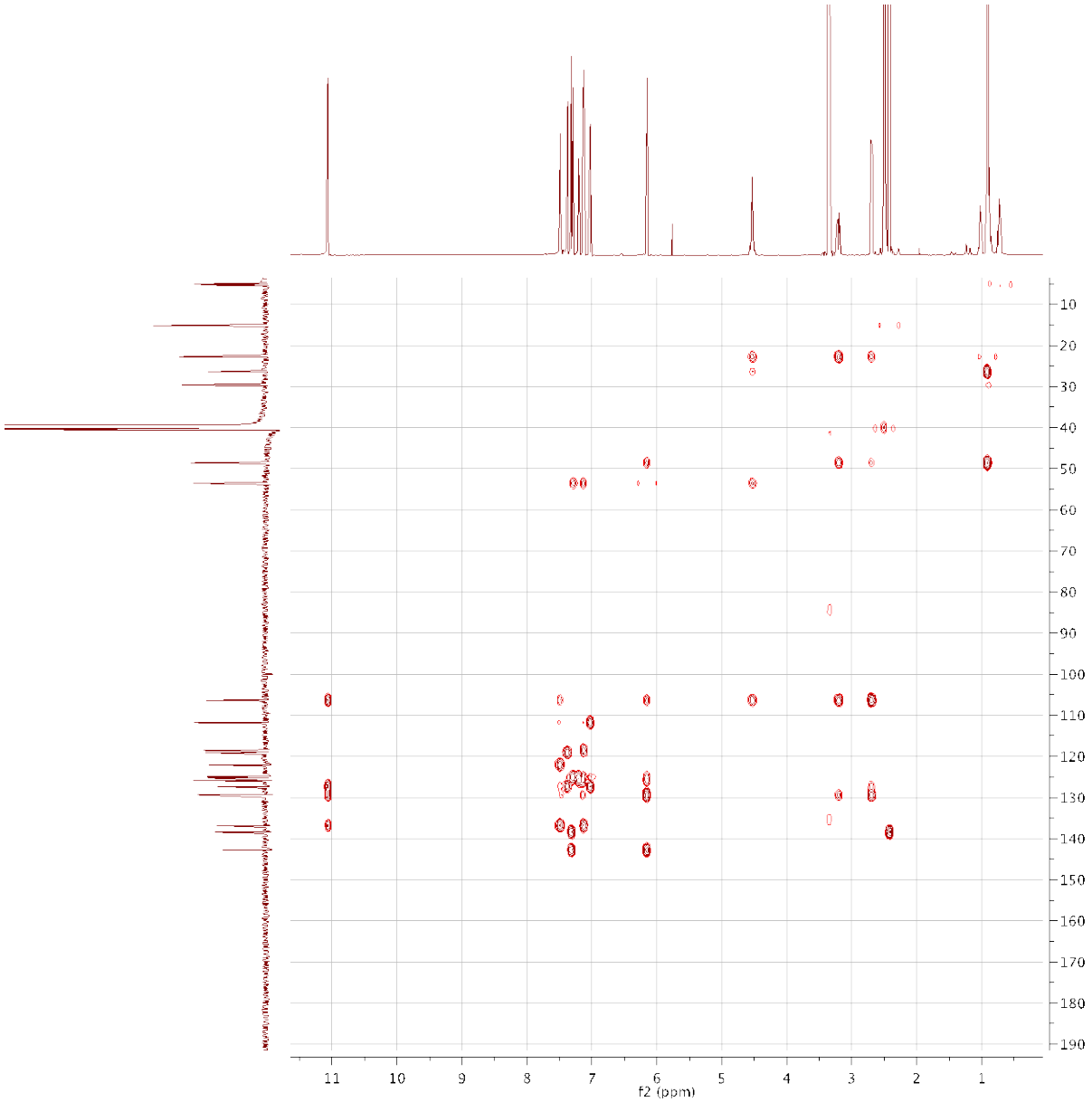
	Parameter	Value
1	Data File Name	81863426/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T12:49:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6024.1, 6024.1)
12	Lowest Frequency	(-77.9, -77.9)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



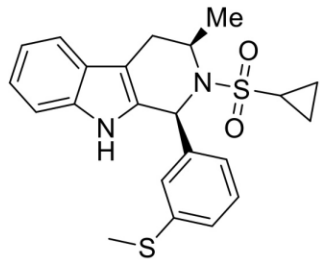


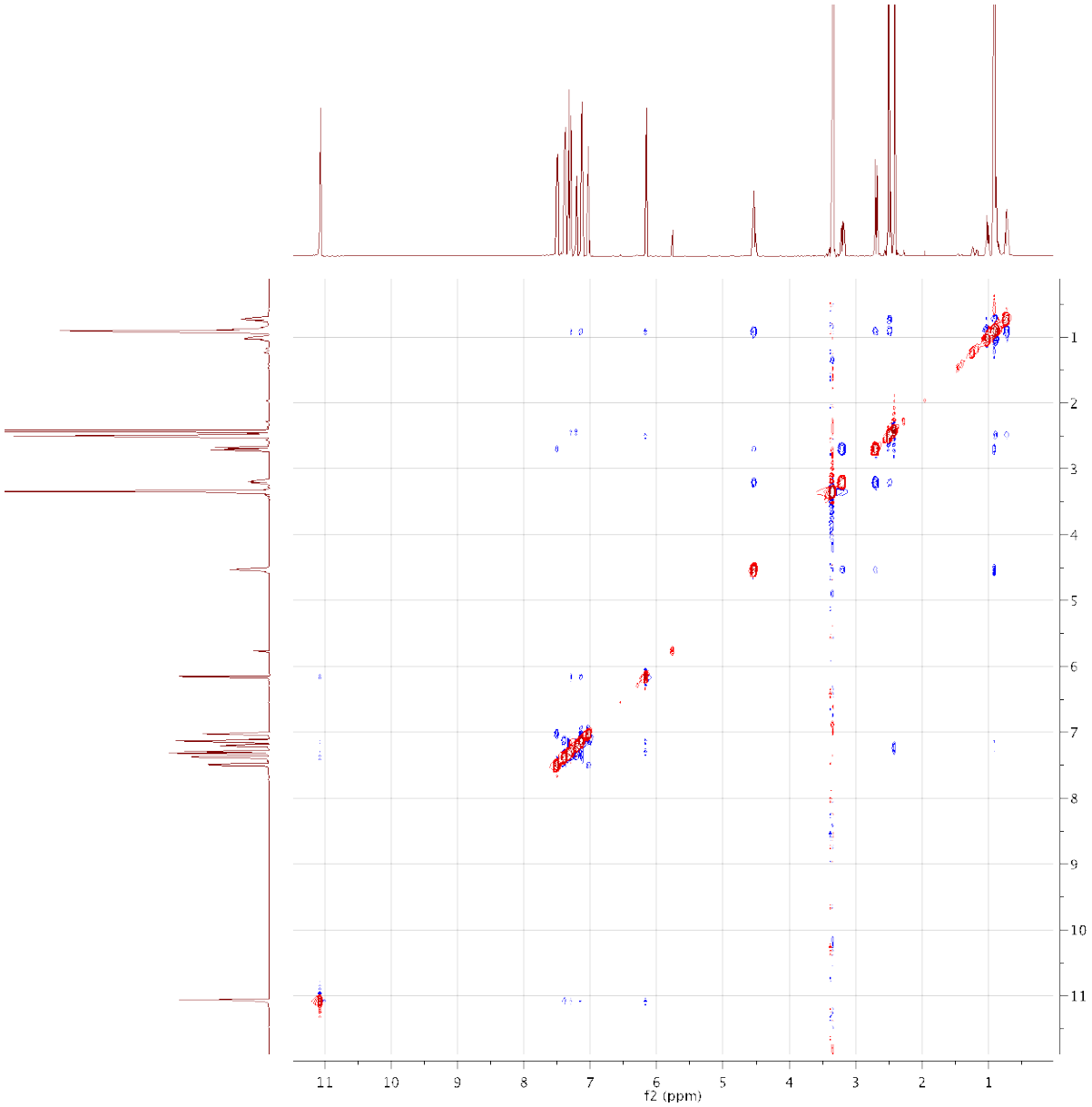
	Parameter	Value
1	Data File Name	81863426/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T13:10:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



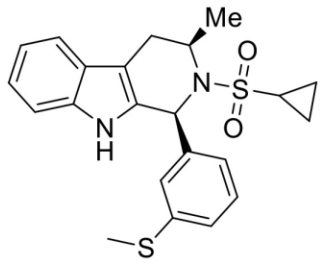


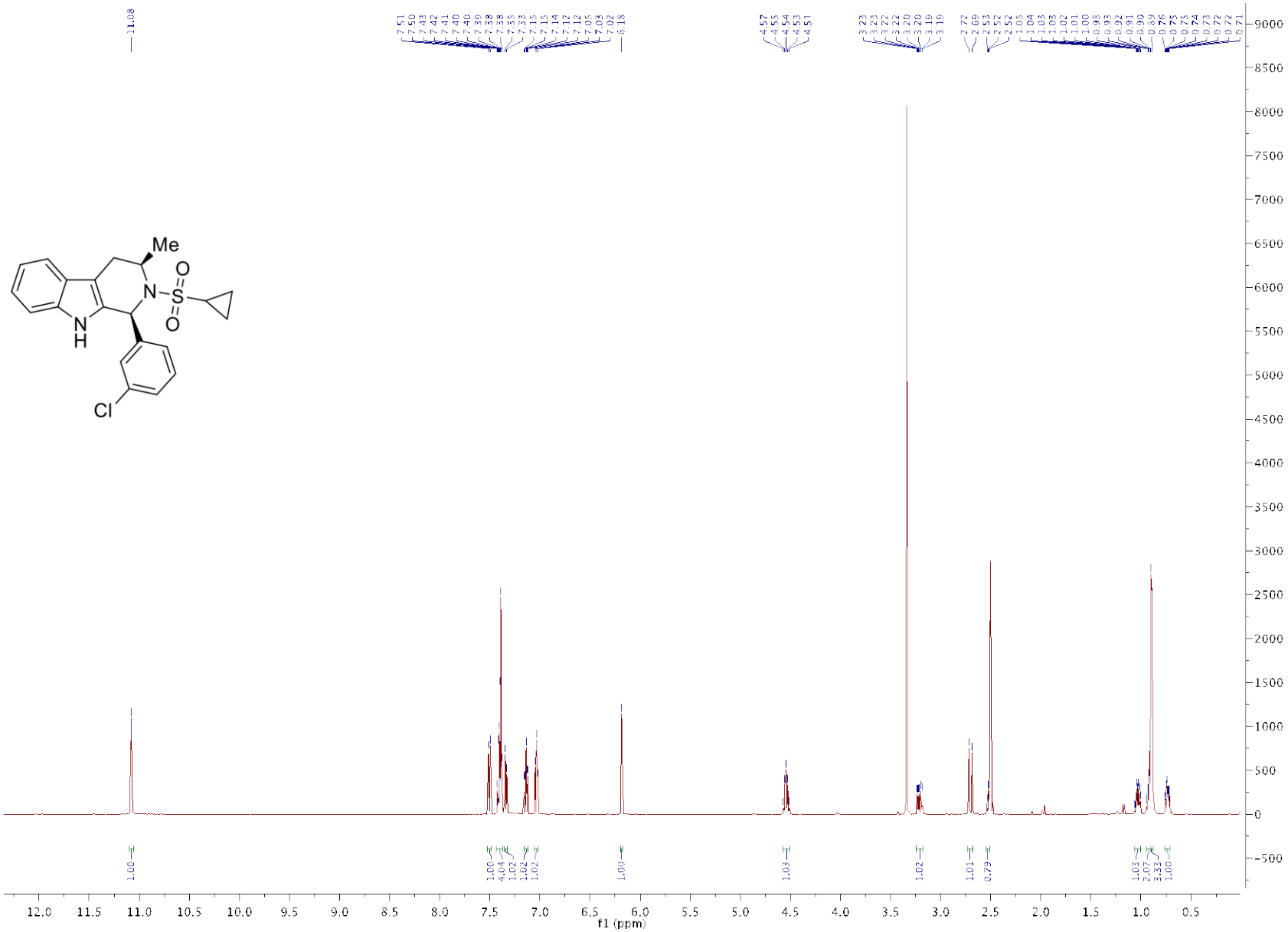
	Parameter	Value
1	Data File Name	81863426/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T13:31:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6024.1, 30120.5)
12	Lowest Frequency	(-77.9, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

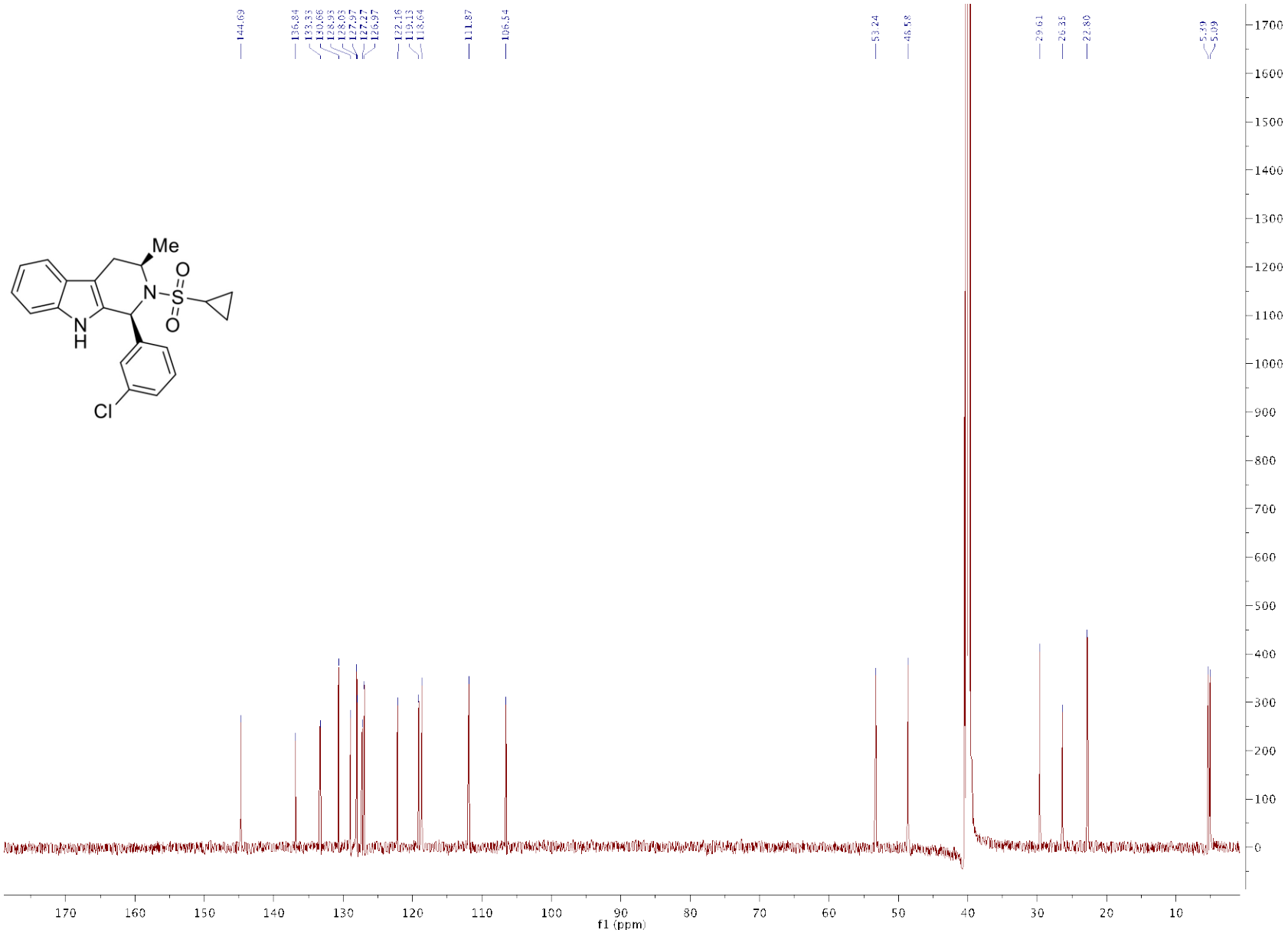




	Parameter	Value
1	Data File Name	81863426/ 16/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	roesyphpp.2
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T14:54:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6024.1, 6024.1)
12	Lowest Frequency	(-77.9, -77.9)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
N
S
O
O
N
H
Cl
f1 (ppm)


144.69
136.84
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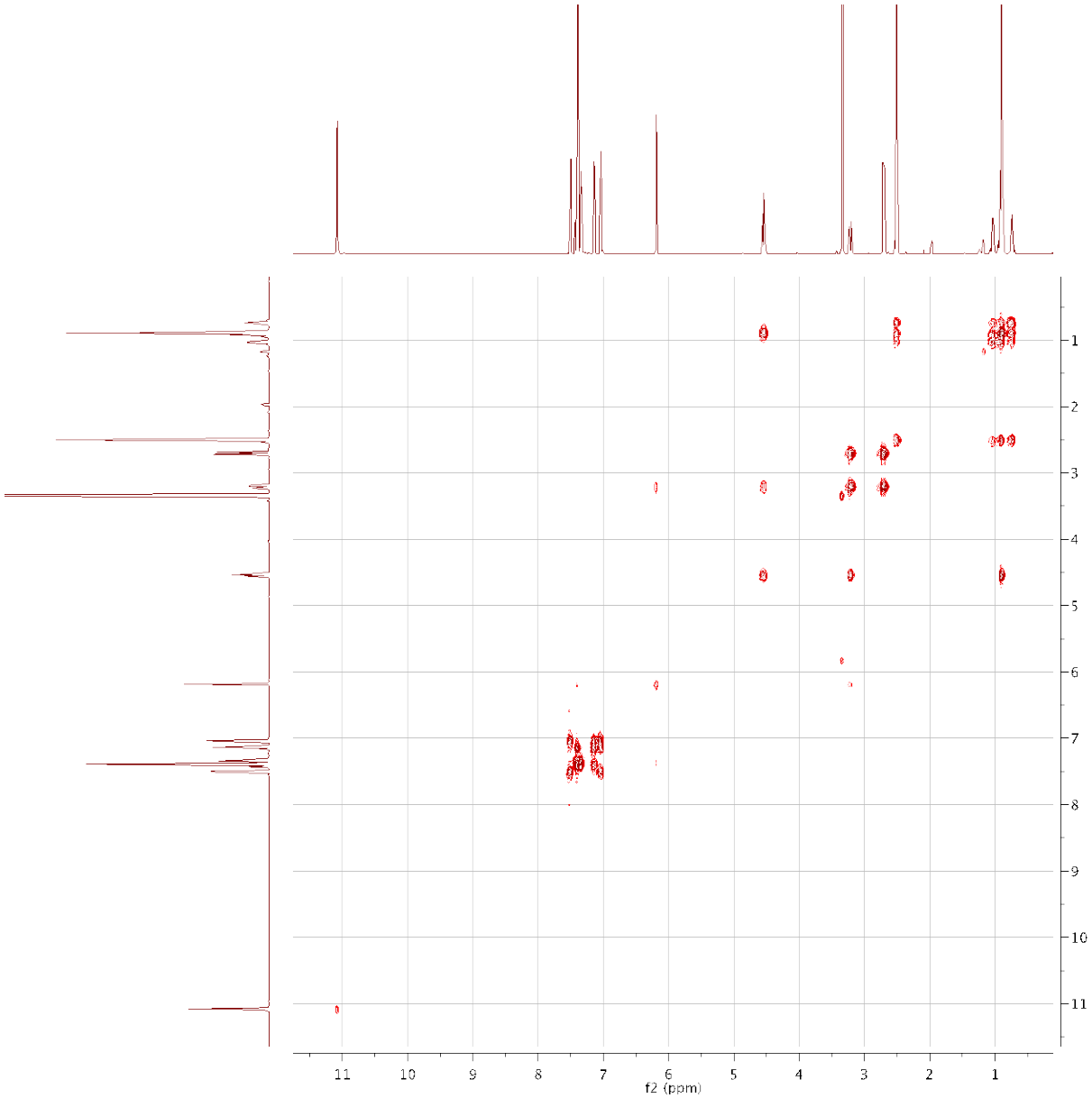
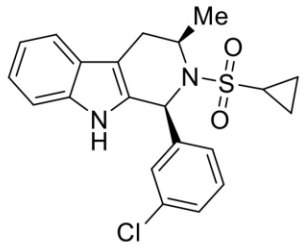
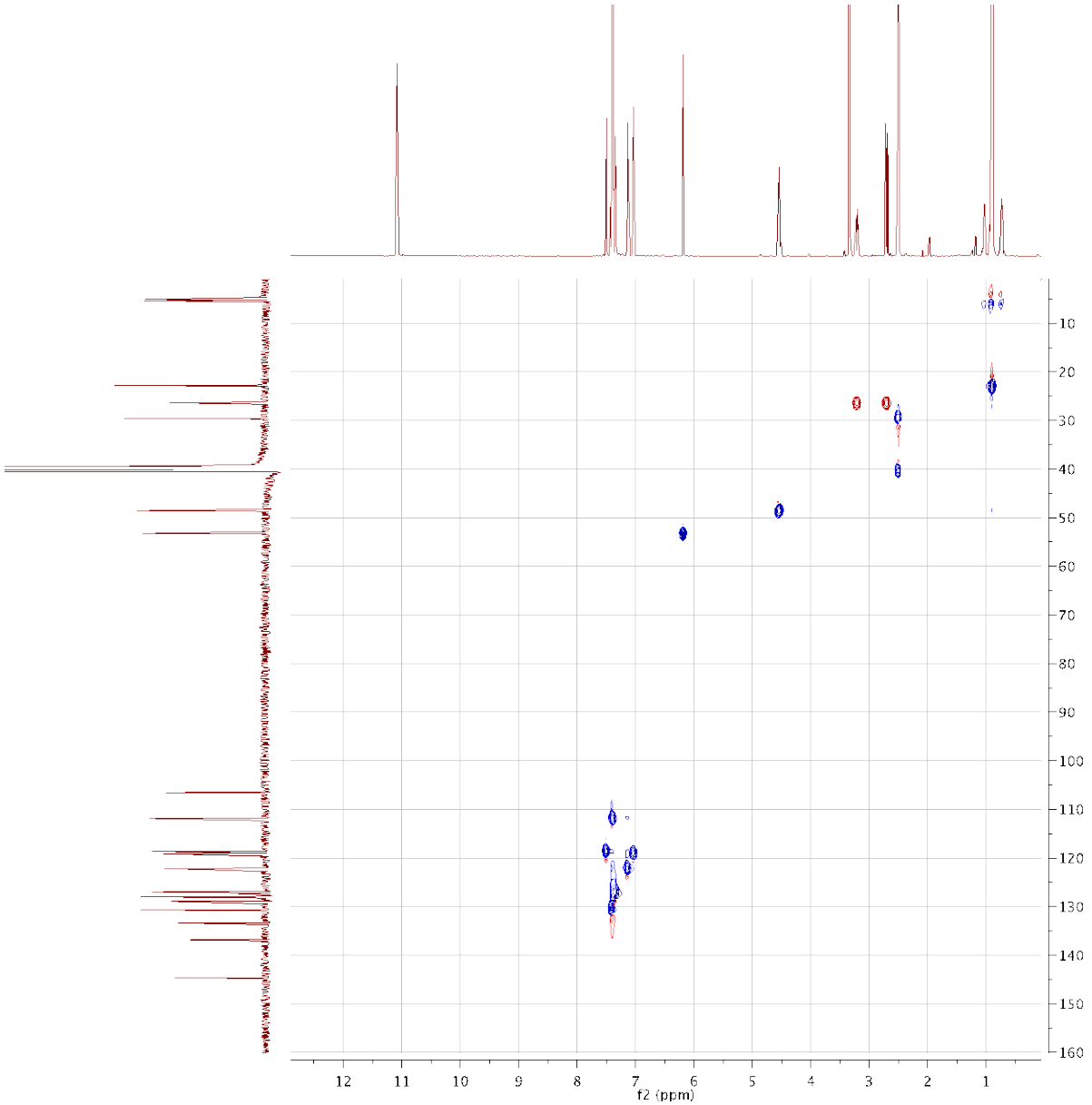
130.66
128.93
128.03
127.97
127.27
126.97
122.16
119.13
118.64
111.87
106.54
53.24
46.58
29.61
26.35
22.80
5.49
5.09
Me
N
S
O
O
N
H
Cl
f1 (ppm)

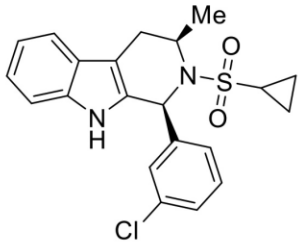


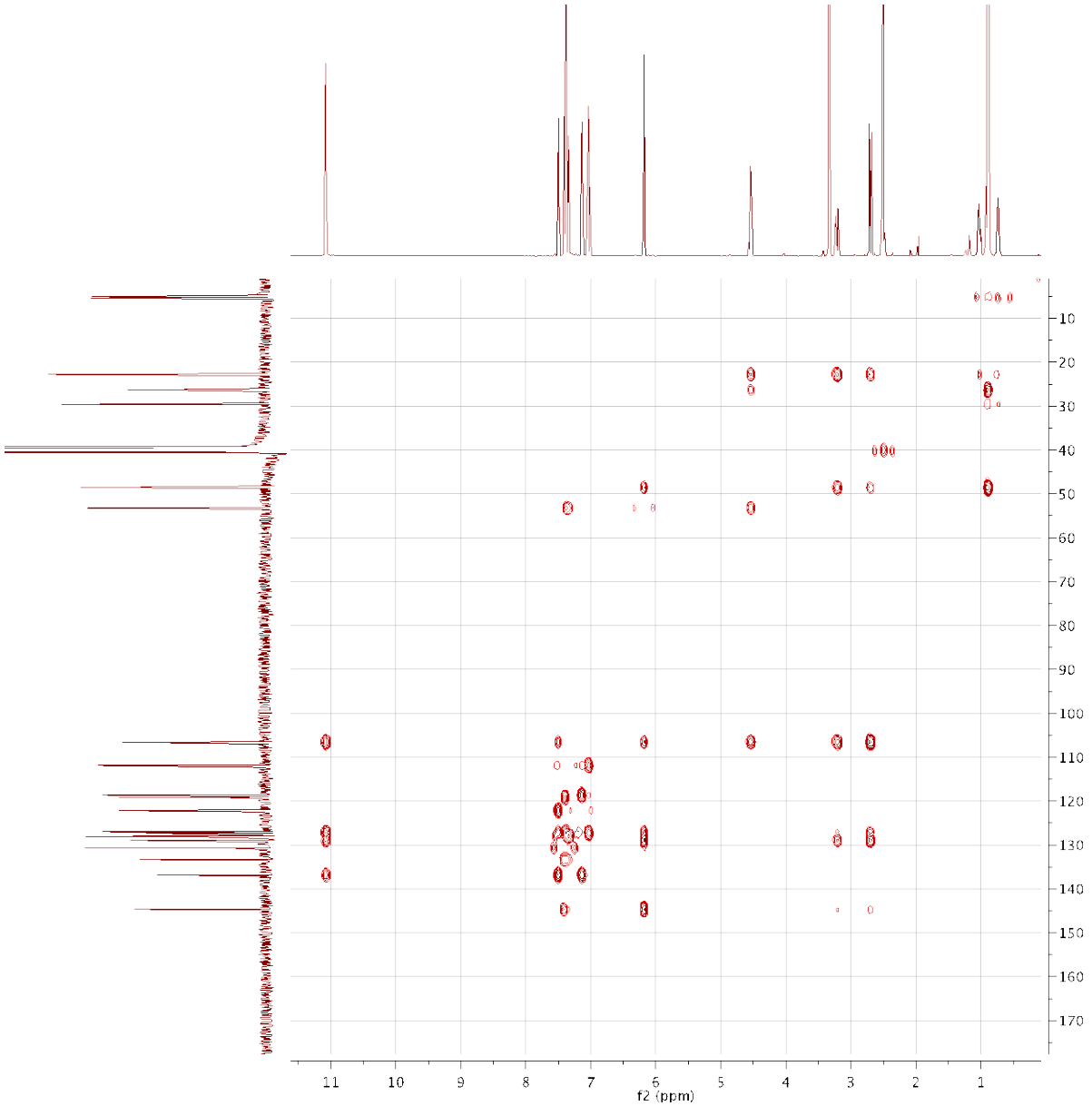
	Parameter	Value
1	Data File Name	81872501/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T06:01:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6097.6, 6097.6)
12	Lowest Frequency	(-140.2, -140.2)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



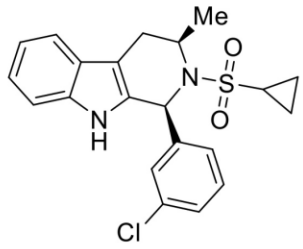


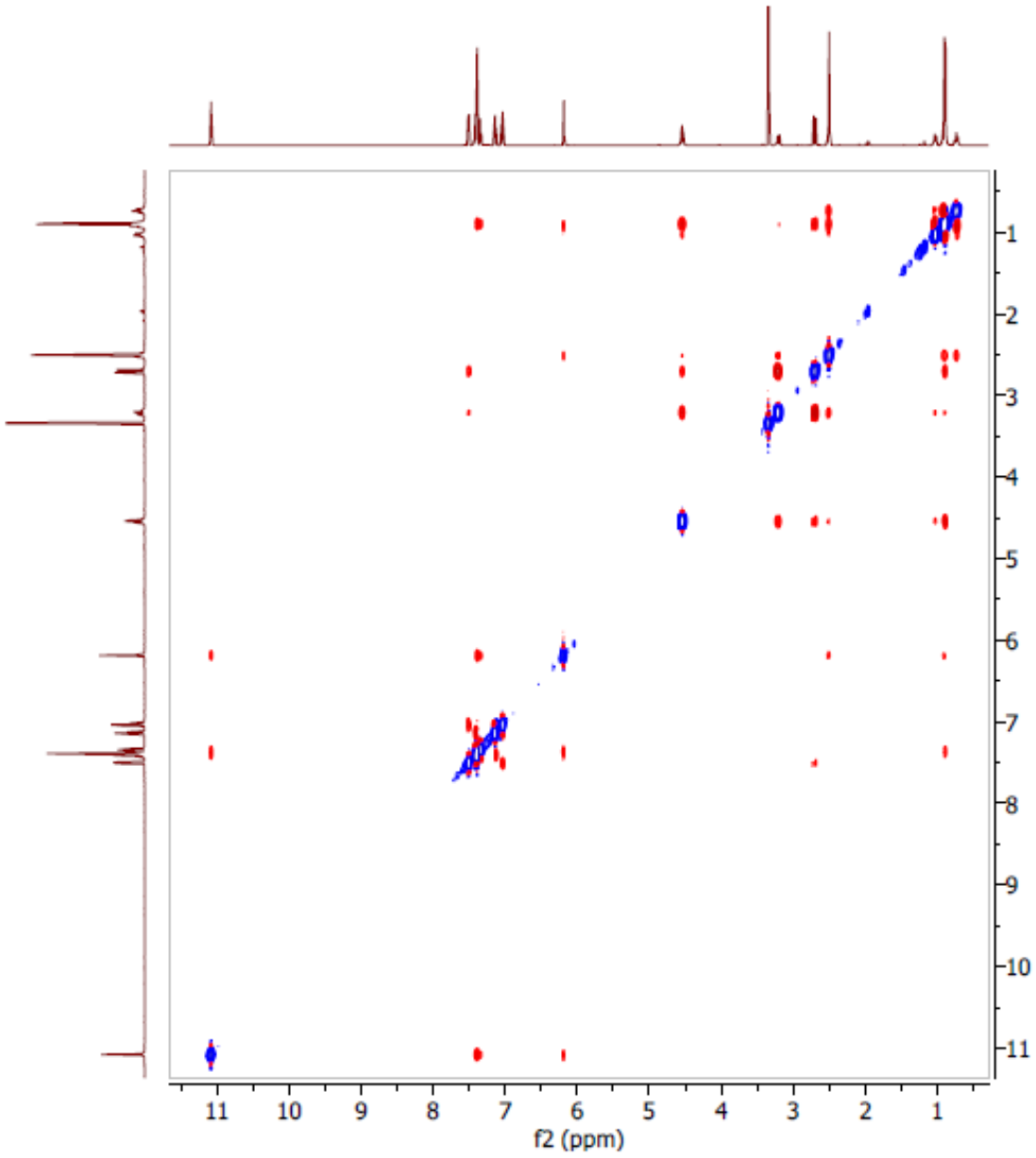
	Parameter	Value
1	Data File Name	81872501/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T06:22:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



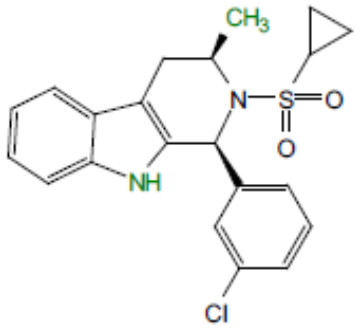


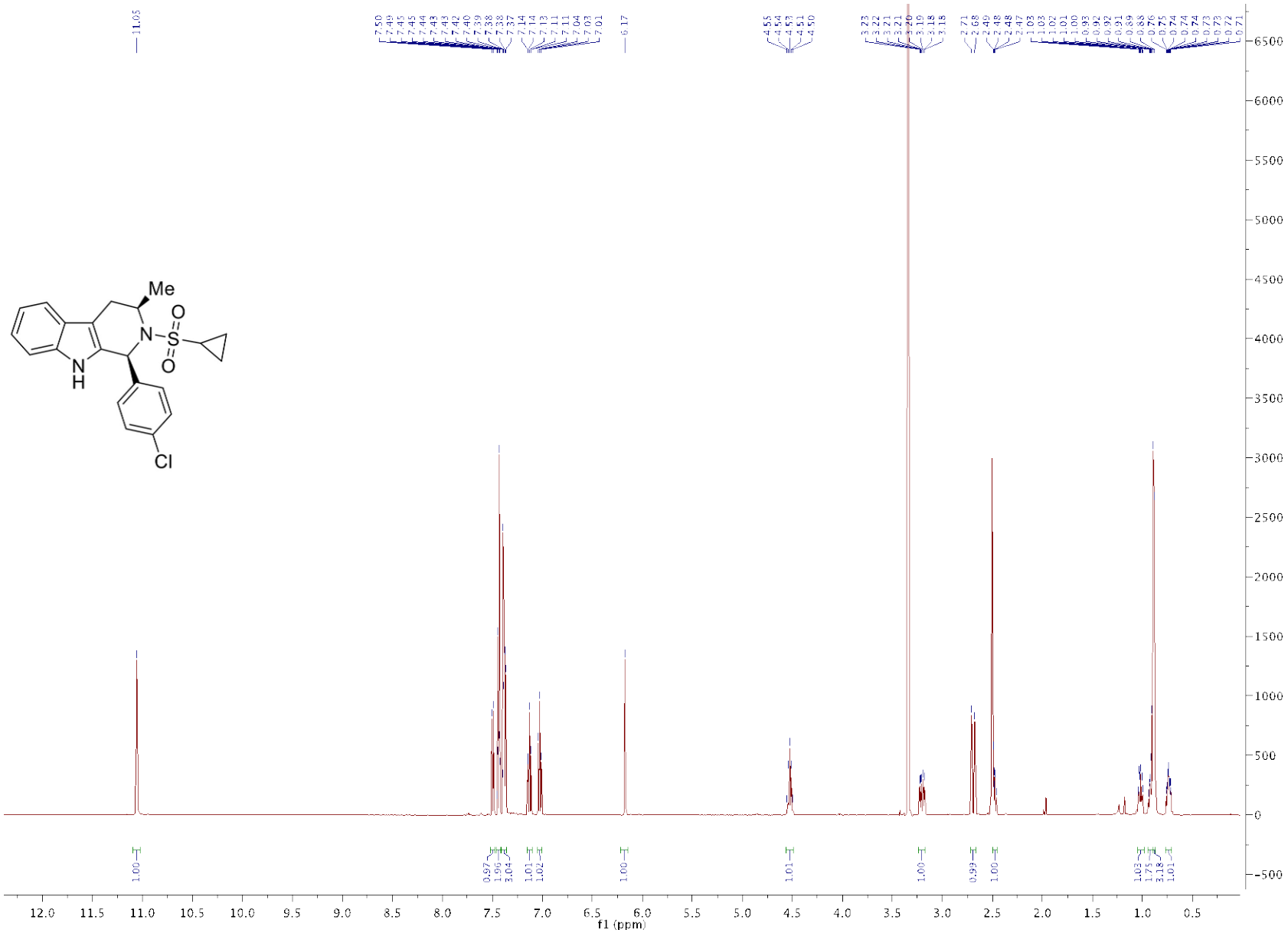
	Parameter	Value
1	Data File Name	81872501/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T06:43:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6097.6, 30120.5)
12	Lowest Frequency	(-140.2, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

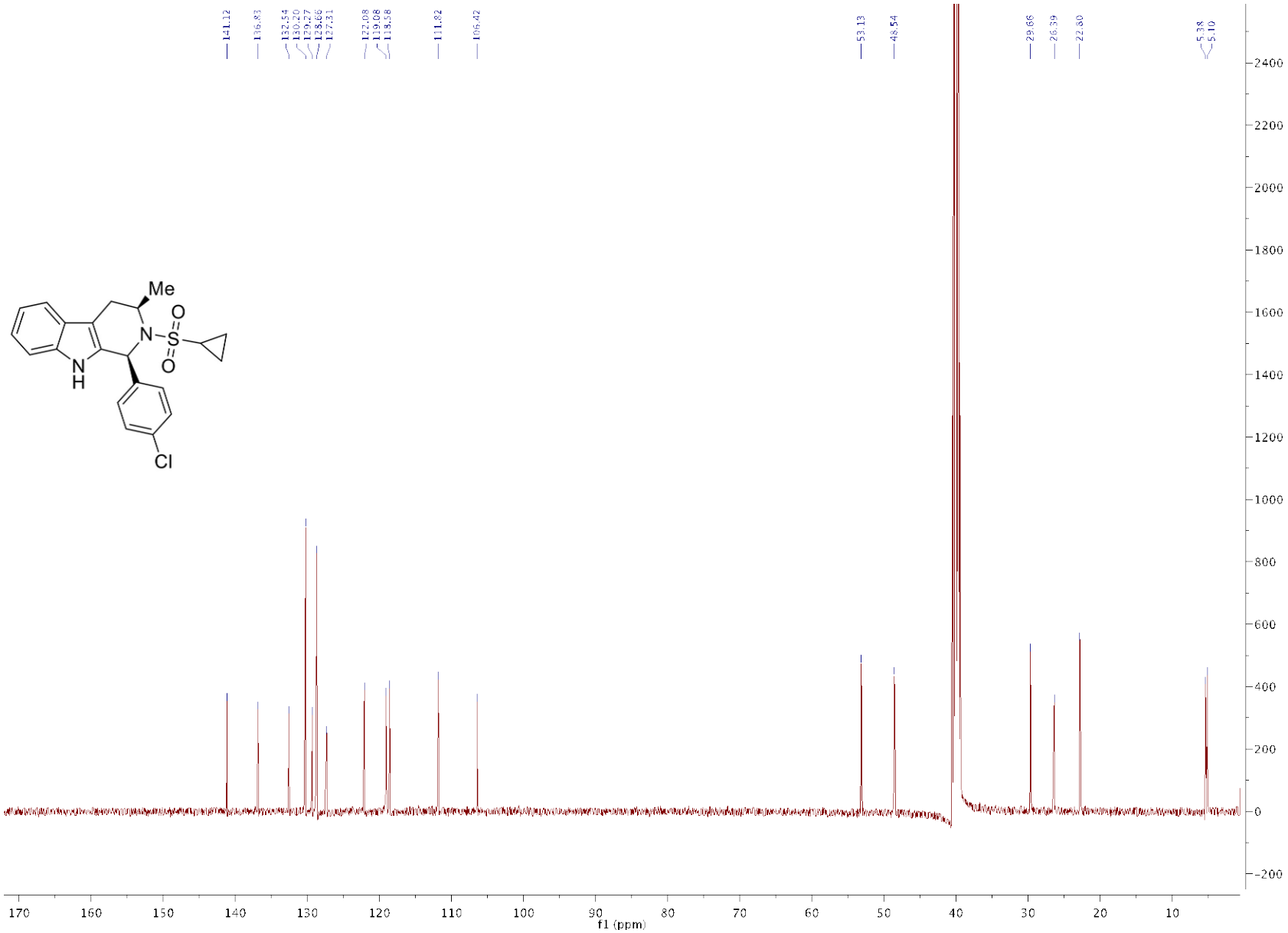




	Parameter	Value
1	Data File Name	W:/ data/ liuy55/ nmr/ 81872501/ 16/ ser
2	Sample ID	81872501
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-08-20T08:06:19
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6097.6, 6097.6)
12	Lowest Frequency	(-140.2, -140.2)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
N
O
S
O
N
H
Cl
f1 (ppm)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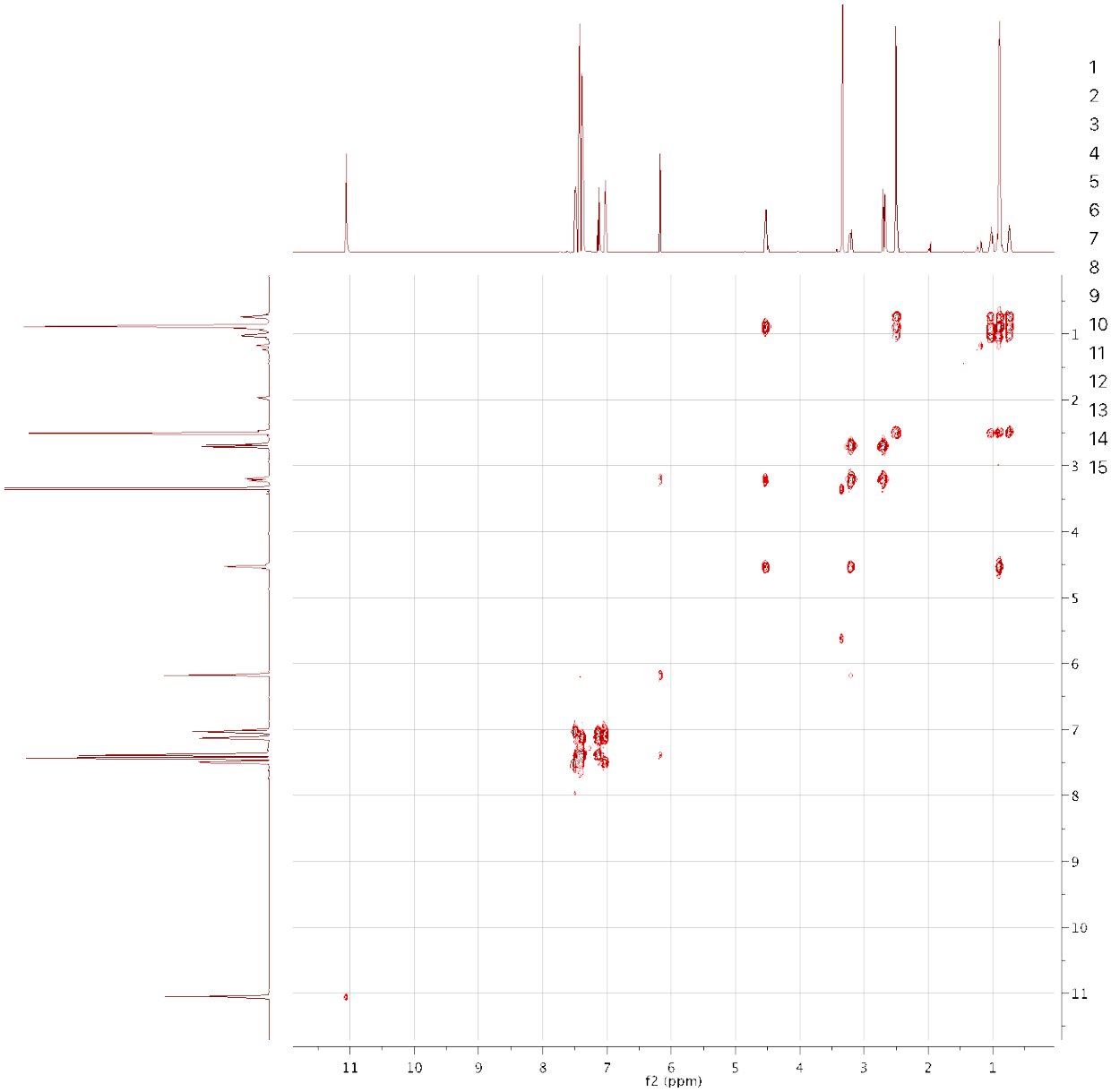
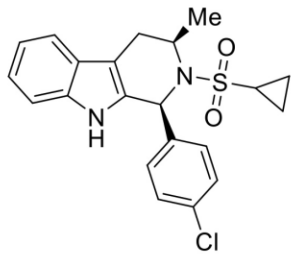
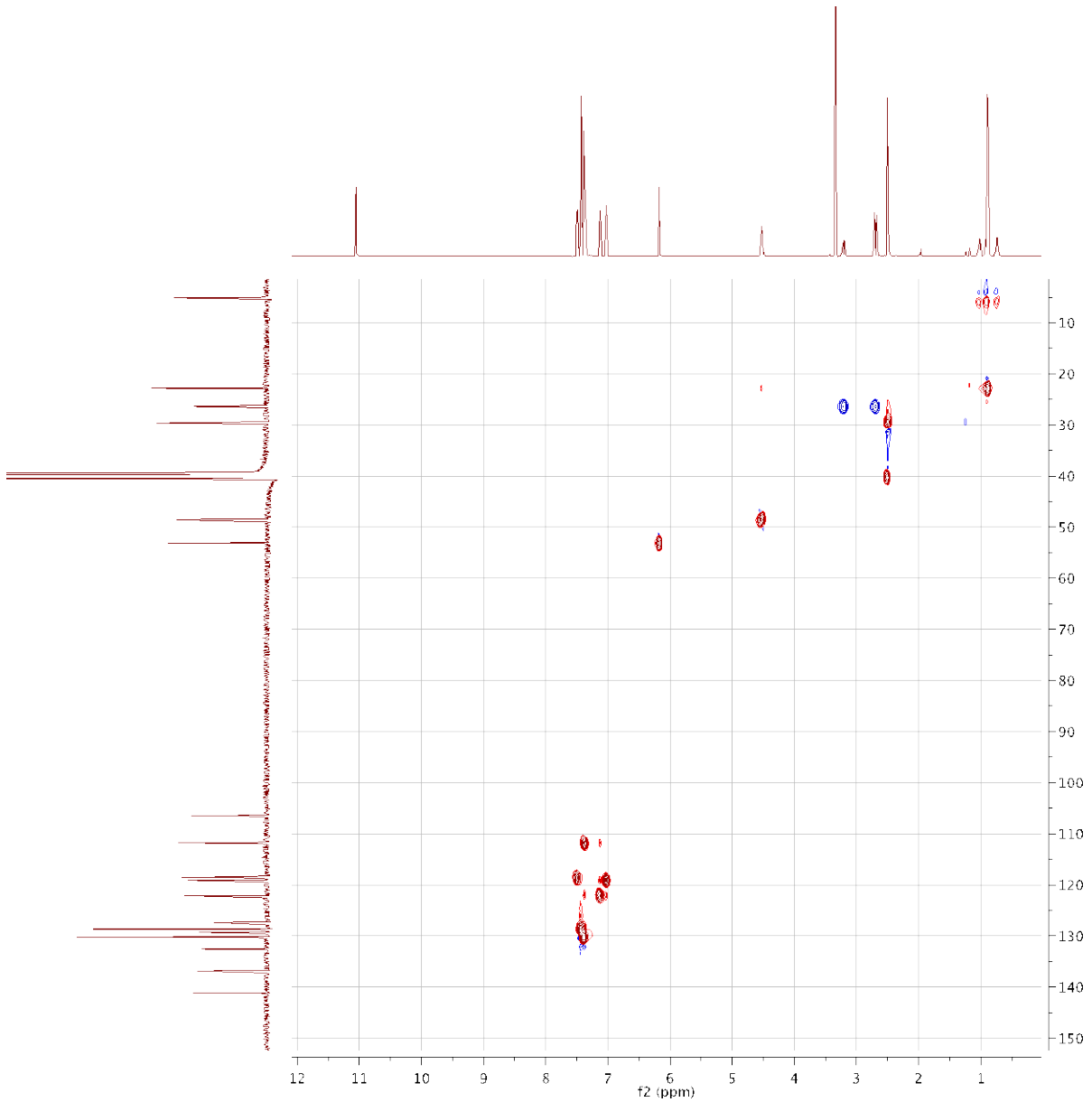
128.66
127.31
122.08
119.08
118.58
111.82
106.42
53.13
48.54
29.66
26.39
23.80
5.38
5.10
Me
N
O
S
O
N
H
Cl
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

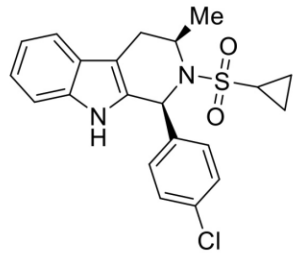


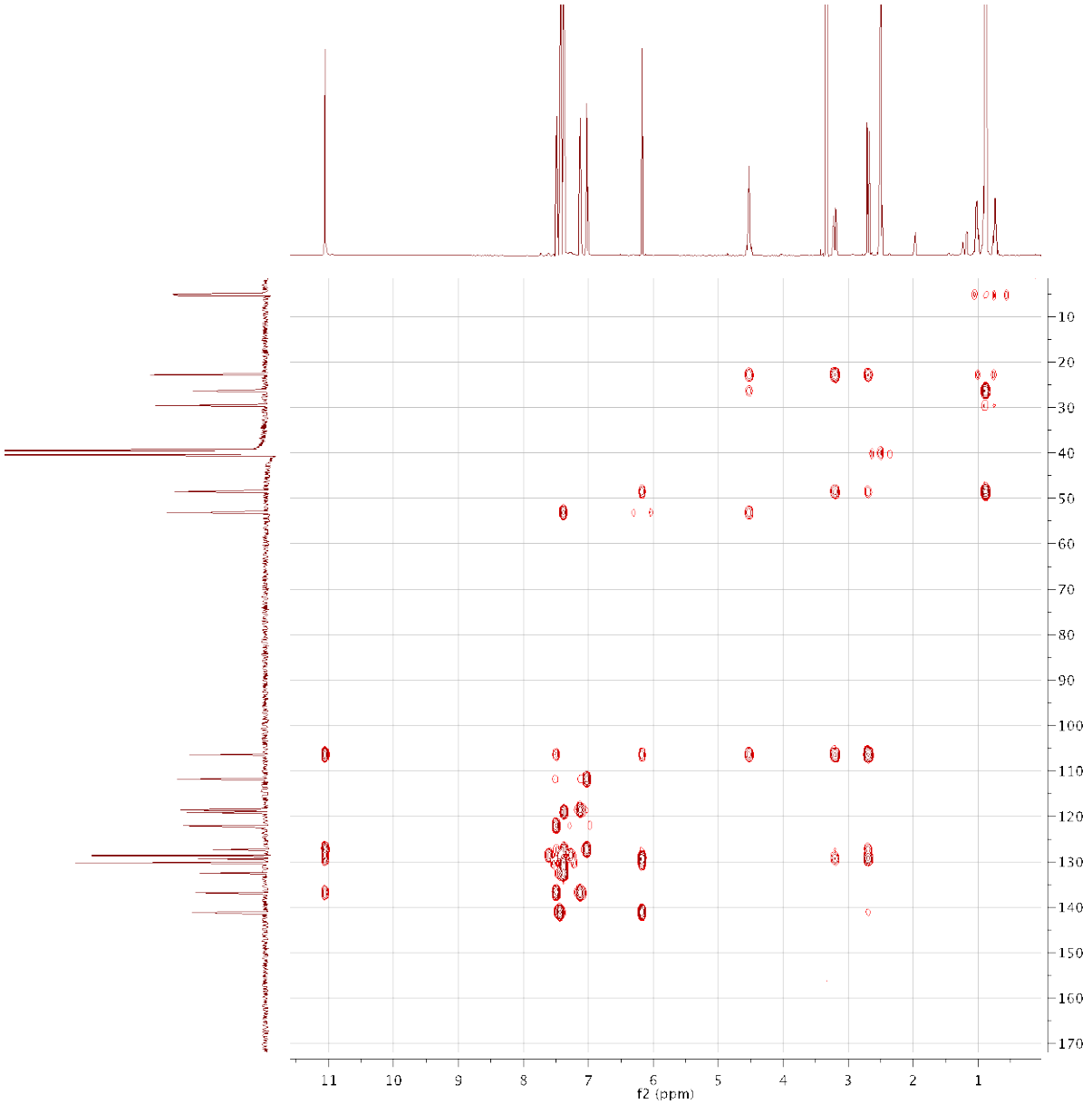
	Parameter	Value
1	Data File Name	81872500/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T01:26:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-362.2, -362.2)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



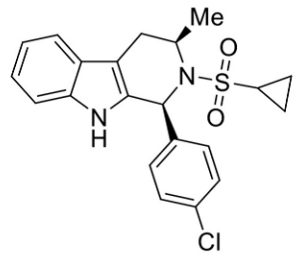


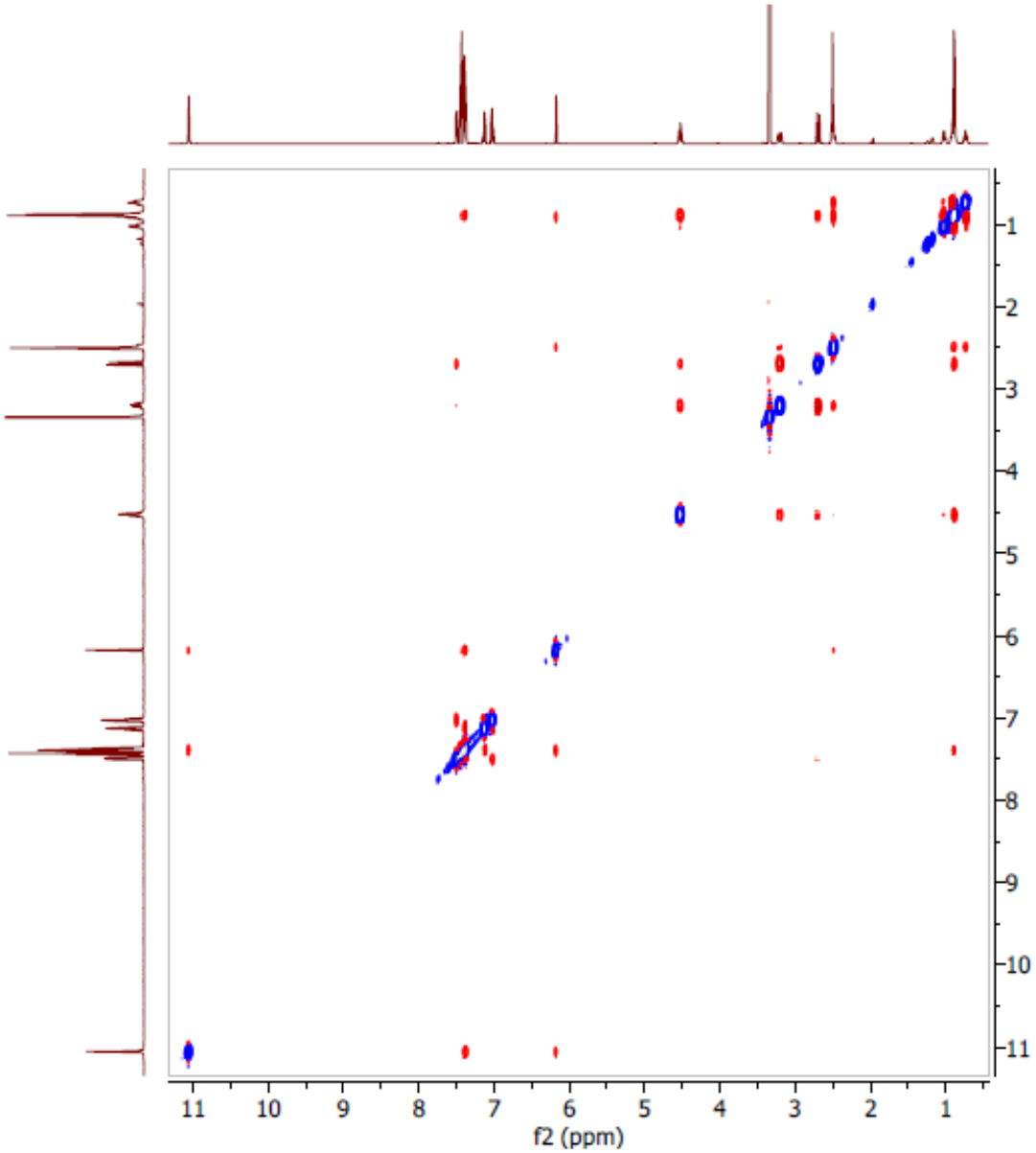
	Parameter	Value
1	Data File Name	81872500/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T01:48:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



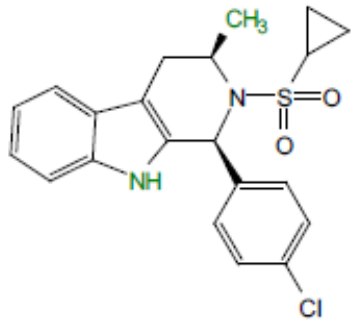


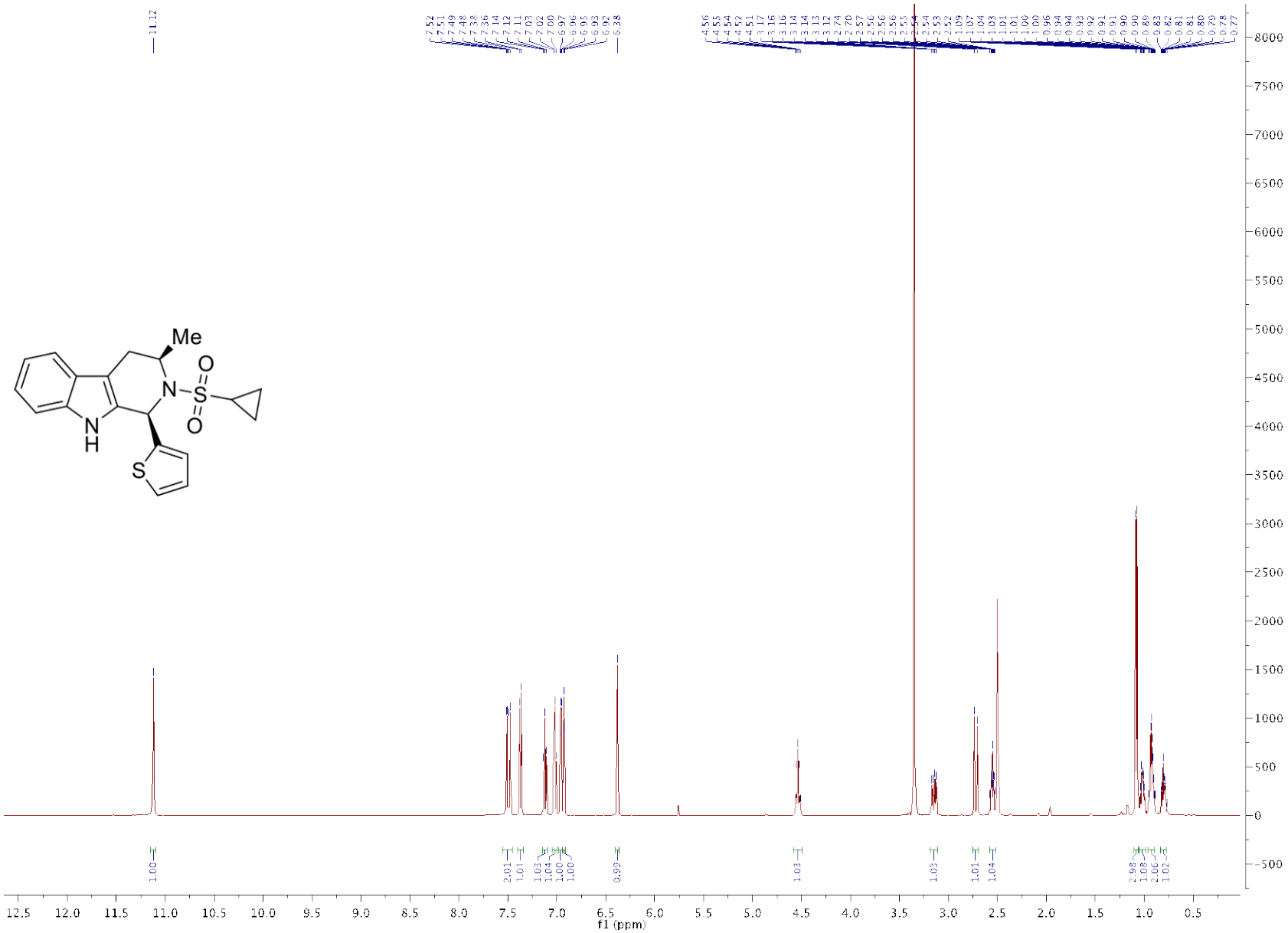
	Parameter	Value
1	Data File Name	81872500/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T02:08:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6329.1, 30120.5)
12	Lowest Frequency	(-362.2, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

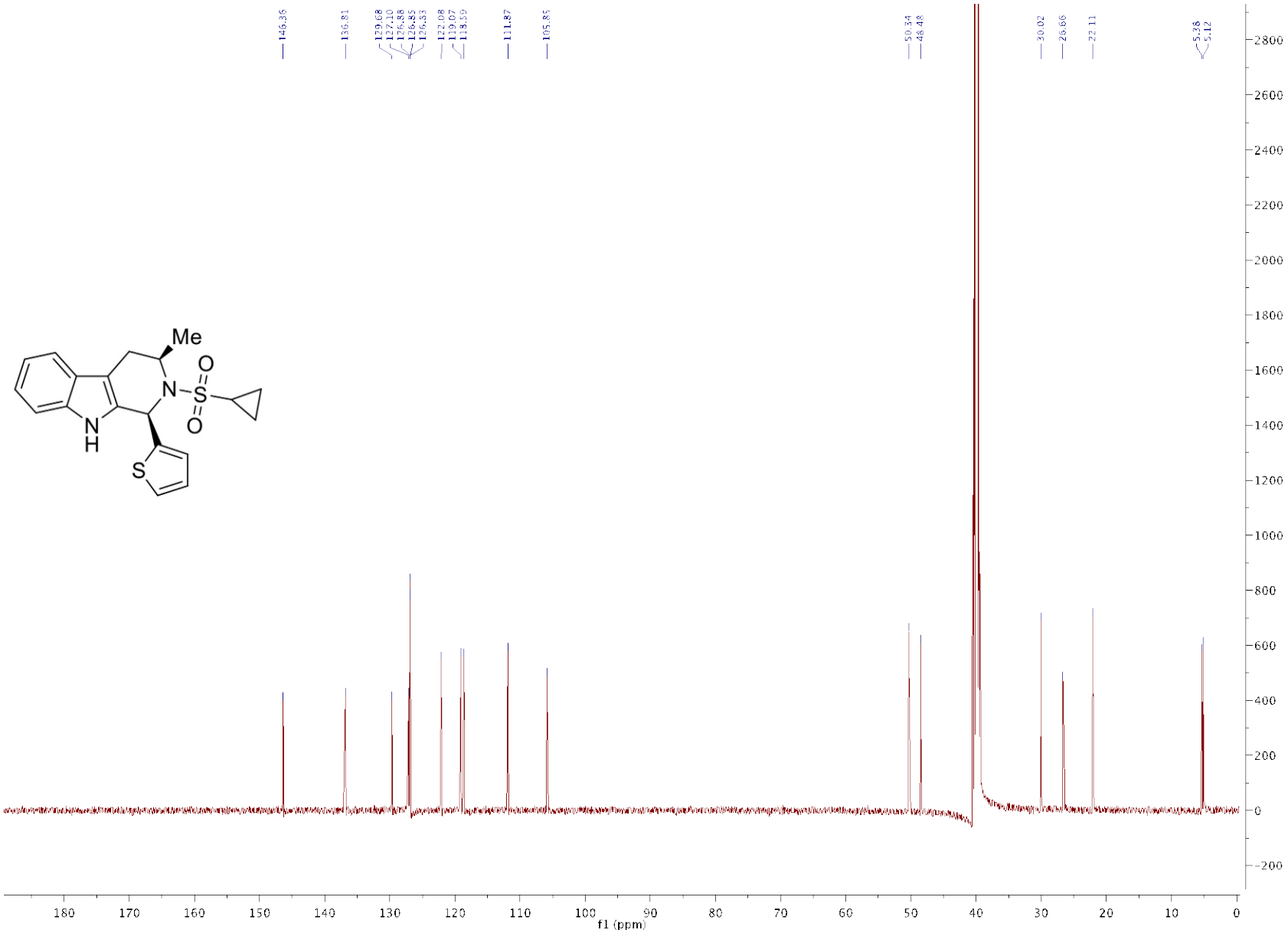




	Parameter	Value
1	Data File Name	W:/ data/ liuy55/ nmr/ 81872500/ 16/ ser
2	Sample ID	81872500
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-08-20T03:31:28
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-362.2, -362.2)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
O
N
S
O
N
H
S
f1 (ppm)


146.36
136.81
129.68
127.10
126.88
126.85
126.53
122.08
119.07
118.59
111.87
105.85
50.34
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22.11
5.38
5.12
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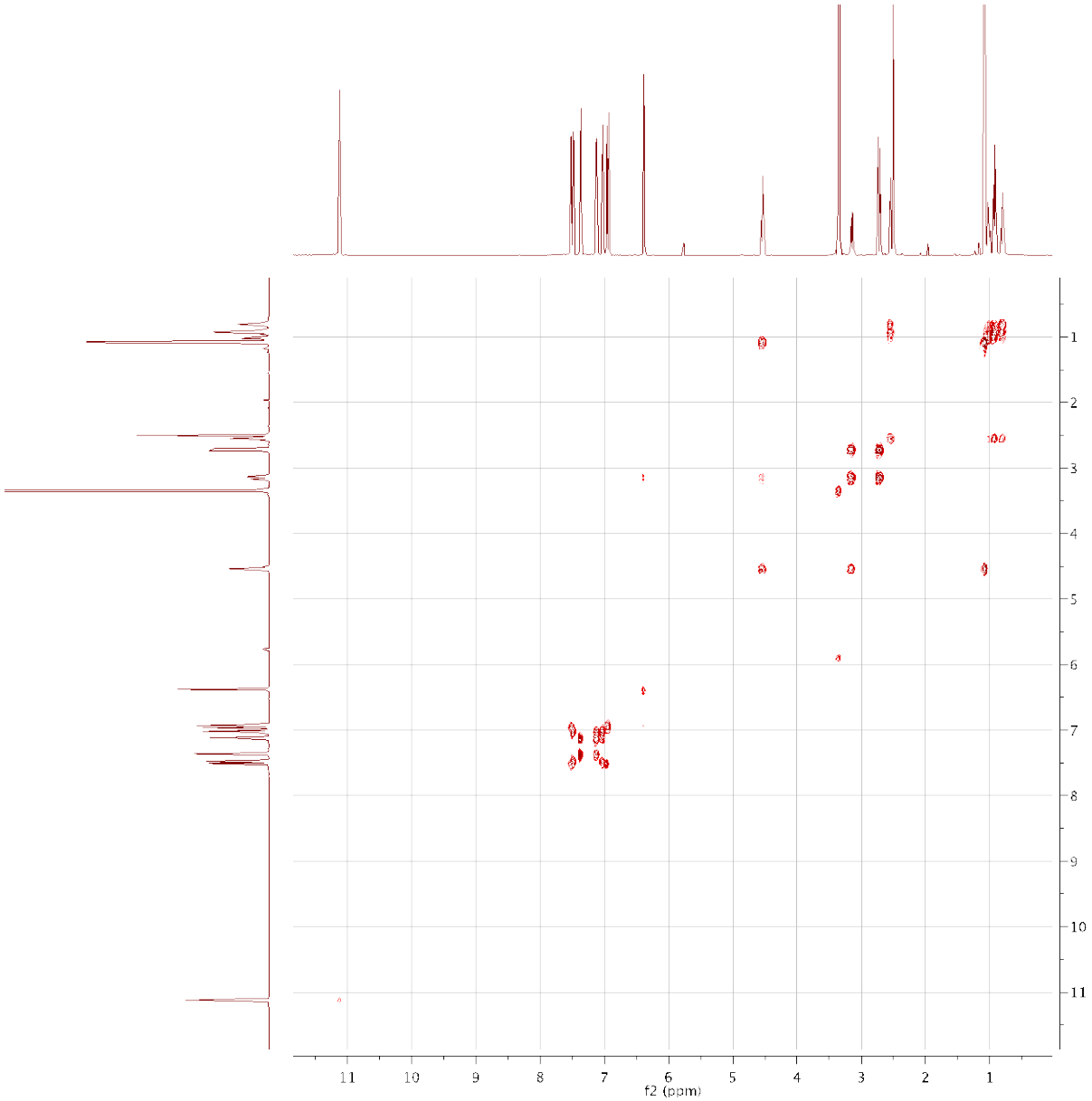
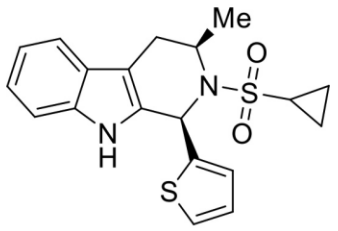
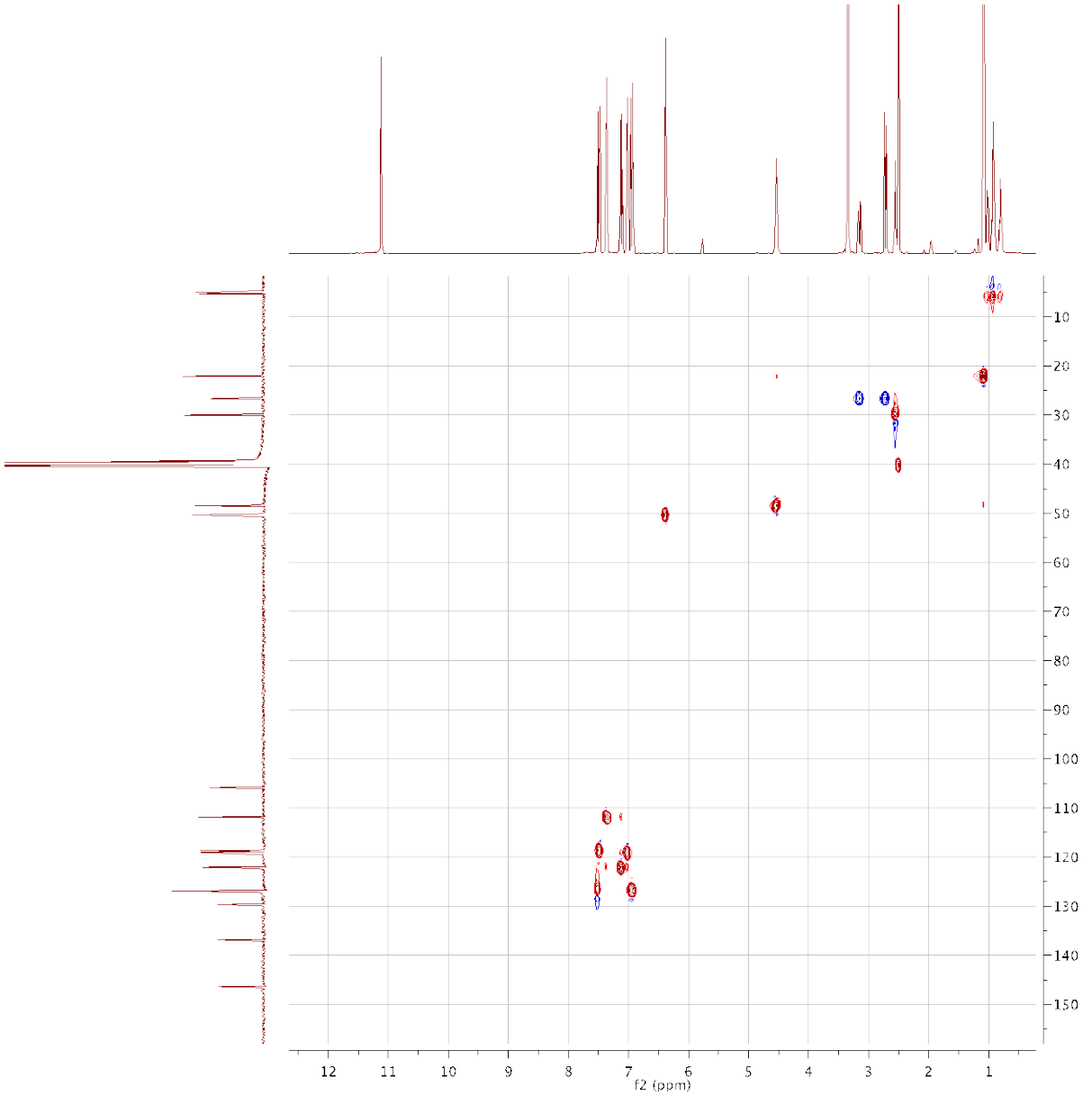
O
N
S
O
N
H
S
f1 (ppm)

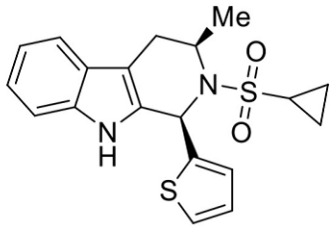


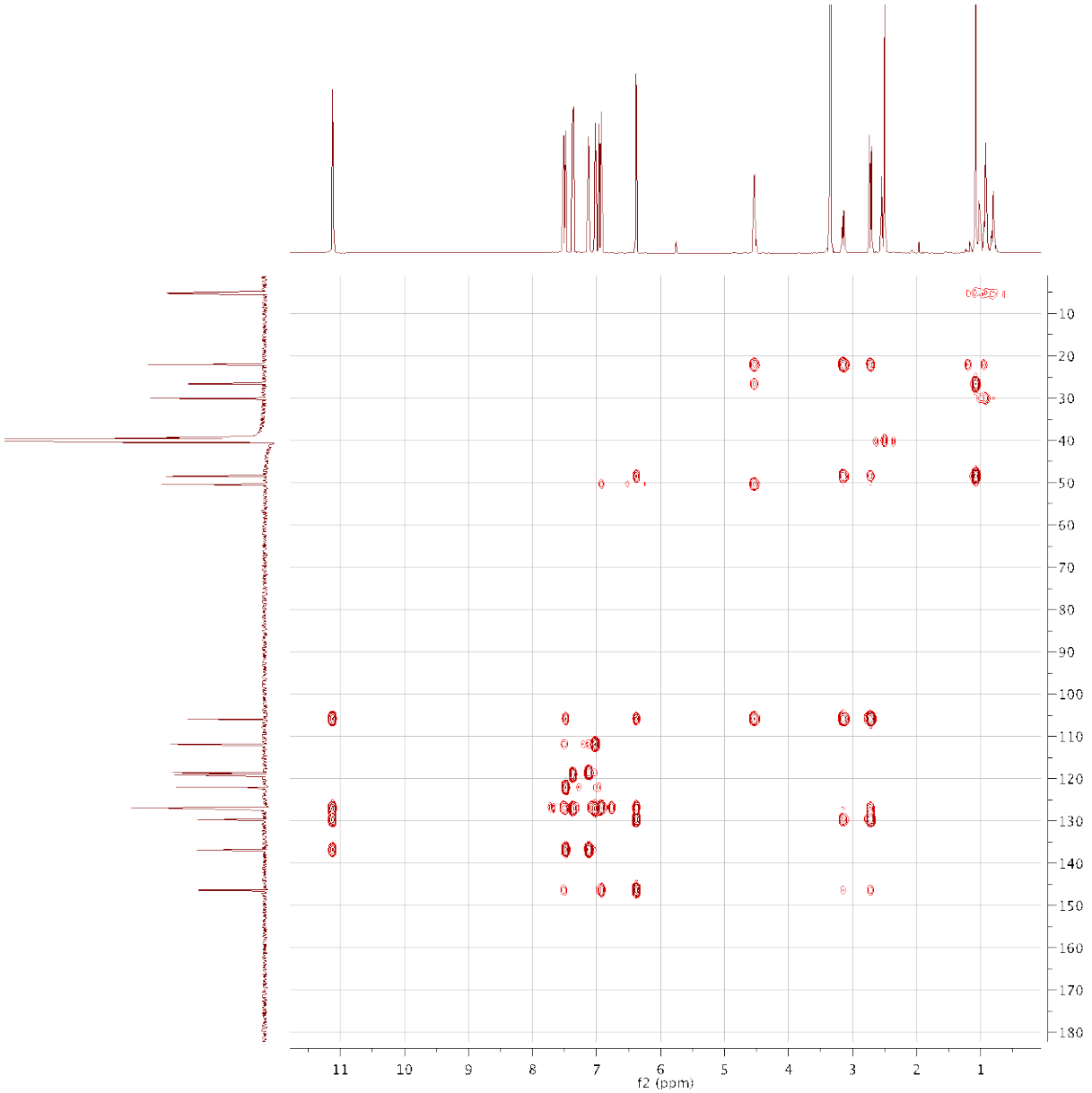
	Parameter	Value
1	Data File Name	81861301/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T21:59:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6172.8, 6172.8)
12	Lowest Frequency	(-140.7, -140.7)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



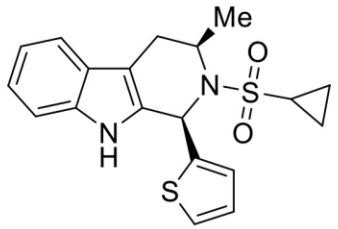


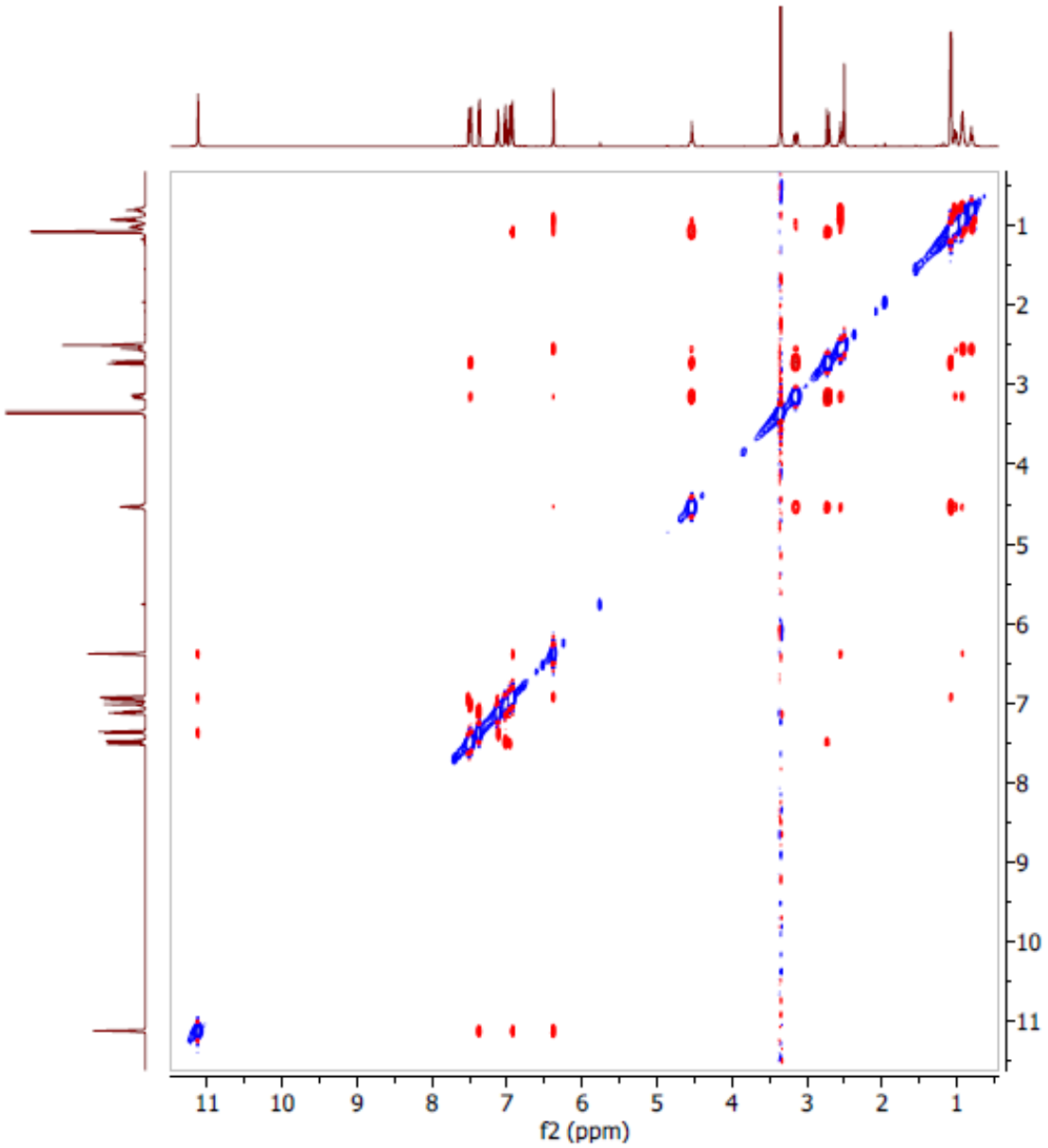
	Parameter	Value
1	Data File Name	81861301/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T22:20:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



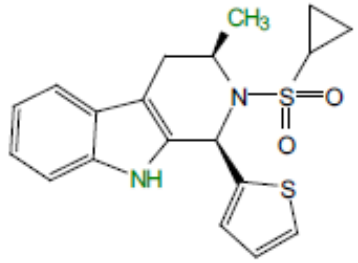


	Parameter	Value
1	Data File Name	81861301/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T22:41:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6172.8, 30120.5)
12	Lowest Frequency	(-140.7, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



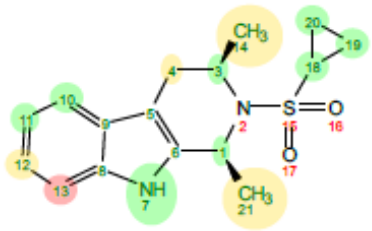


	Parameter	Value
1	Data File Name	W:/ data/ liuy55/ nmr/ 81861301/ 16/ ser
2	Sample ID	81861301
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-08-06T00:04:11
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6172.8, 6172.8)
12	Lowest Frequency	(-140.7, -140.7)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



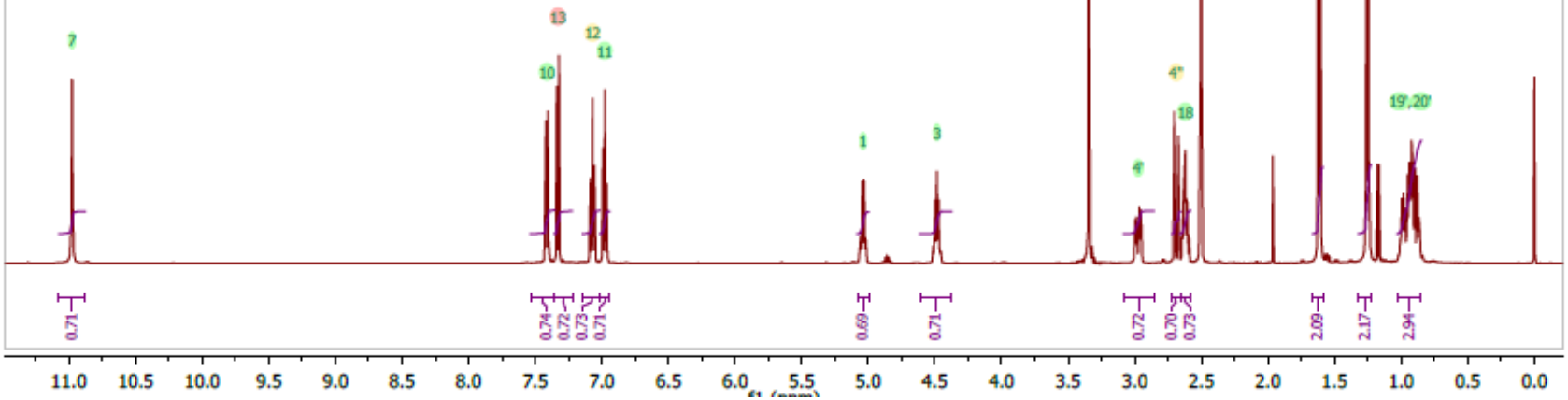
	Parameter	Value
1	Data File Name:	W:/data/liuy55/nmr/81863274/10/fid
2	Sample ID	818613274
3	Origin:	Bruker BioSpin GmbH
4	Owner:	smapchemist
5	Solvent:	DMSO
6	Pulse Sequence:	zg30
7	Acquisition Date:	2016-08-06T01:53:01
8	Temperature:	300.01
9	Number of Scans:	16
10	Spectrometer Frequency	500.2630016
11	Nucleus	1H

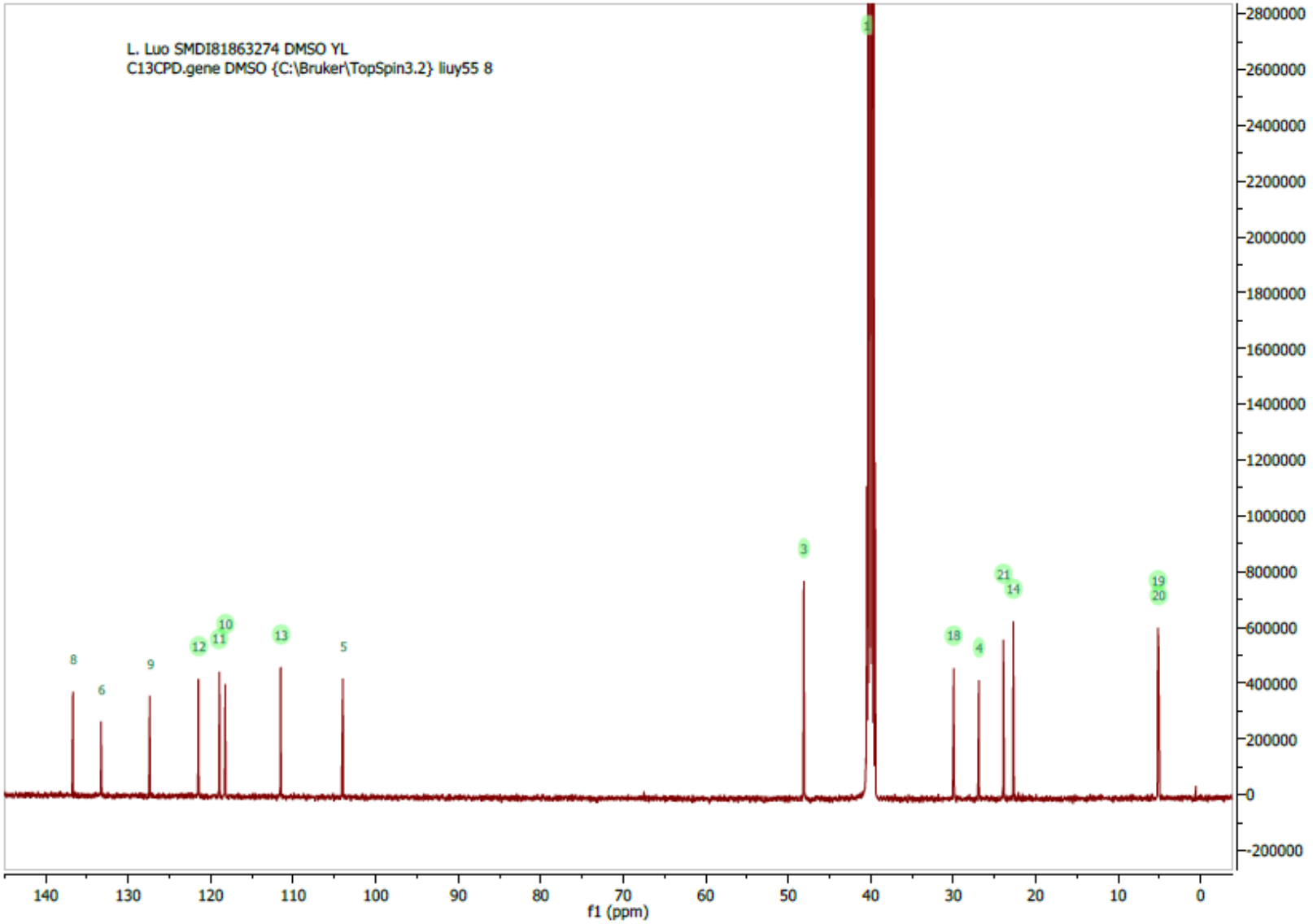
^{1}H NMR (500 MHz, DMSO-d_6) δ 10.98 (s, 1H), 7.41 (d, J = 7.8 Hz, 1H), 7.33 (d, J = 8.1 Hz, 1H), 7.15 – 7.02 (m, 1H), 6.98 (td, J = 0.9, 7.6 Hz, 1H), 5.08 – 5.00 (m, 1H), 4.49 (p, J = 6.9 Hz, 1H), 2.98 (ddd, J = 1.6, 6.0, 15.3 Hz, 1H), 2.69 (d, J = 15.3 Hz, 1H), 2.62 (tt, J = 5.0, 7.8 Hz, 1H), 1.61 (d, J = 6.9 Hz, 3H), 1.25 (d, J = 7.0 Hz, 3H), 1.03 – 0.85 (m, 4H).

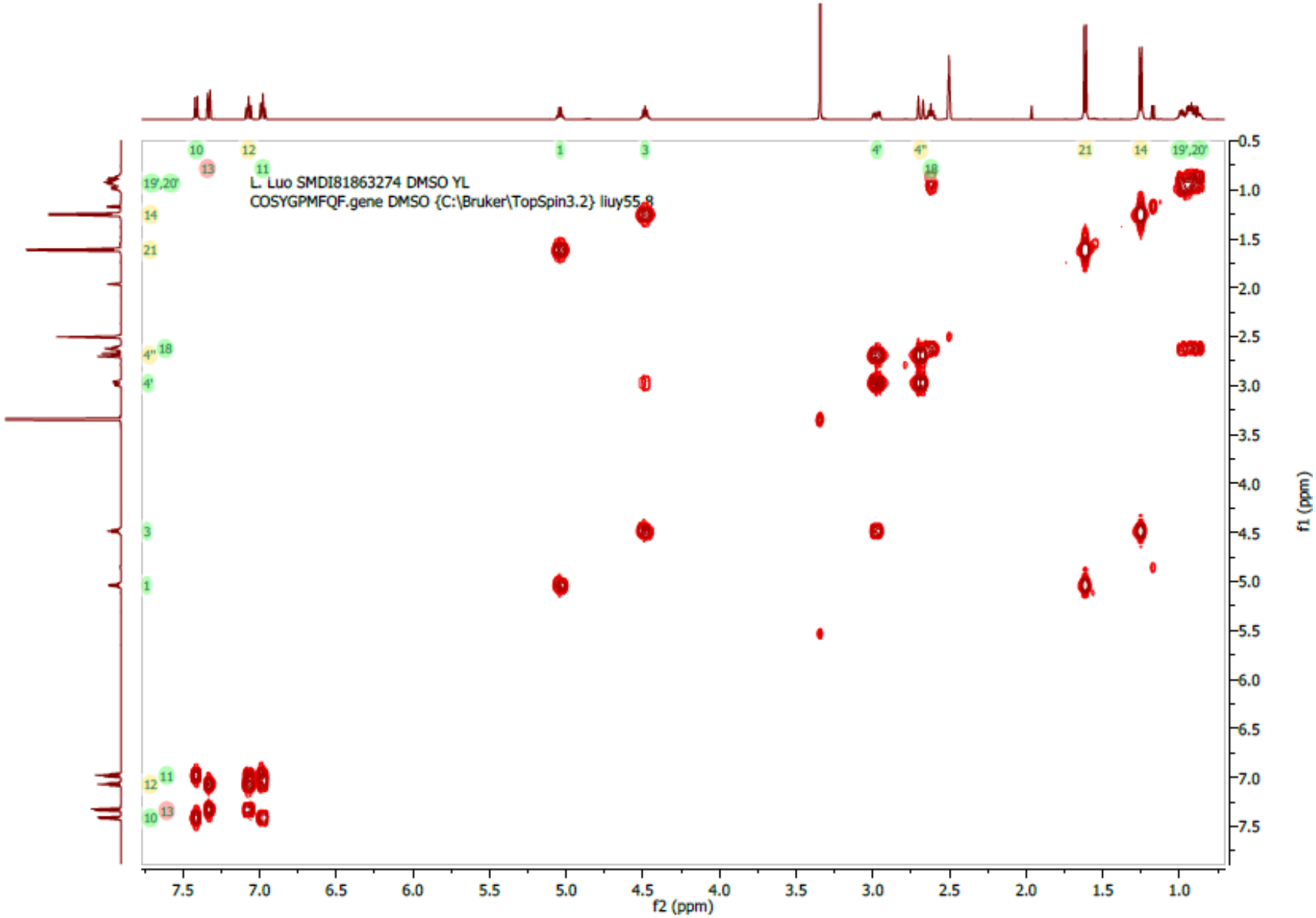


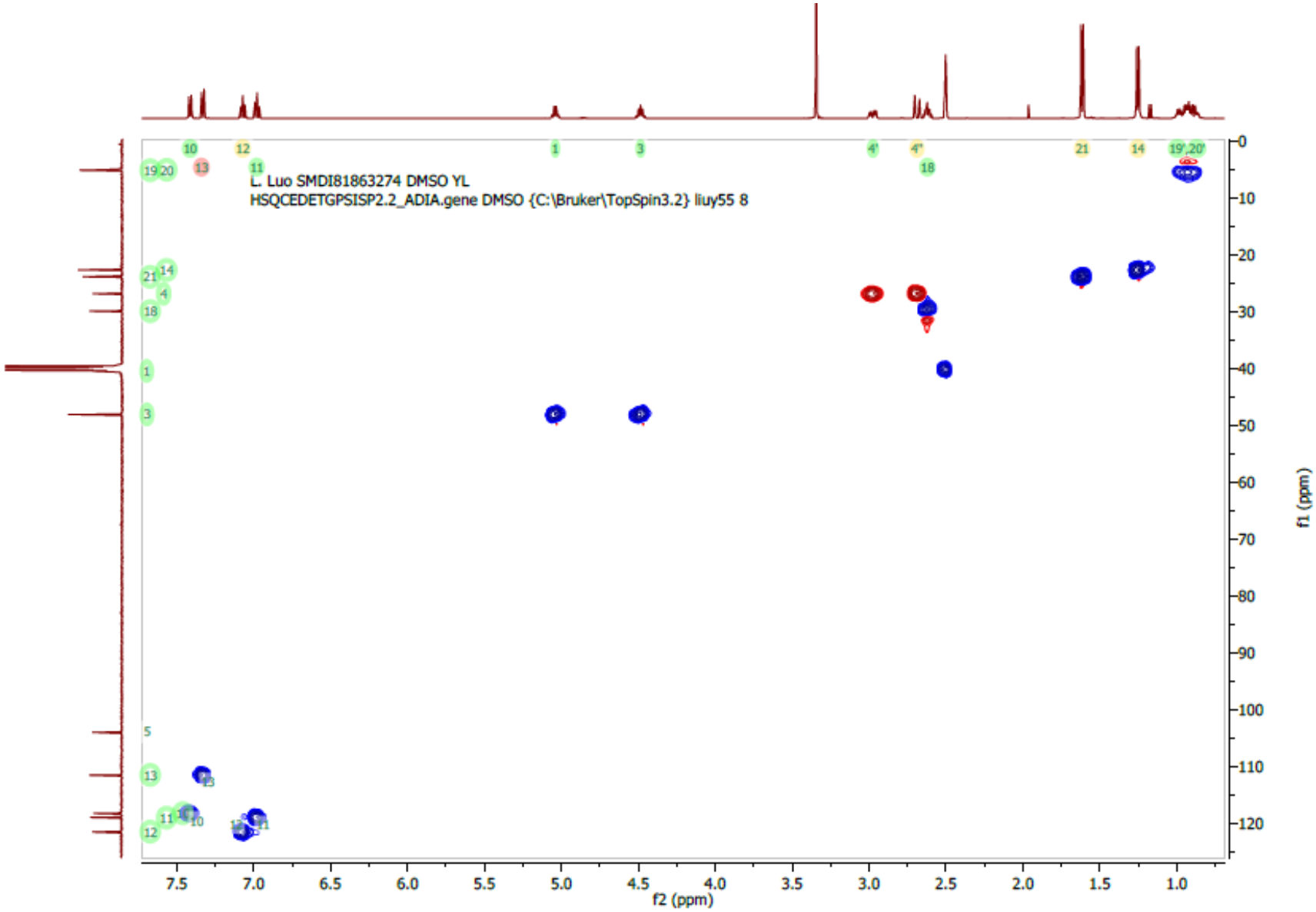
Key evidences:
NOE: H14 and H21;

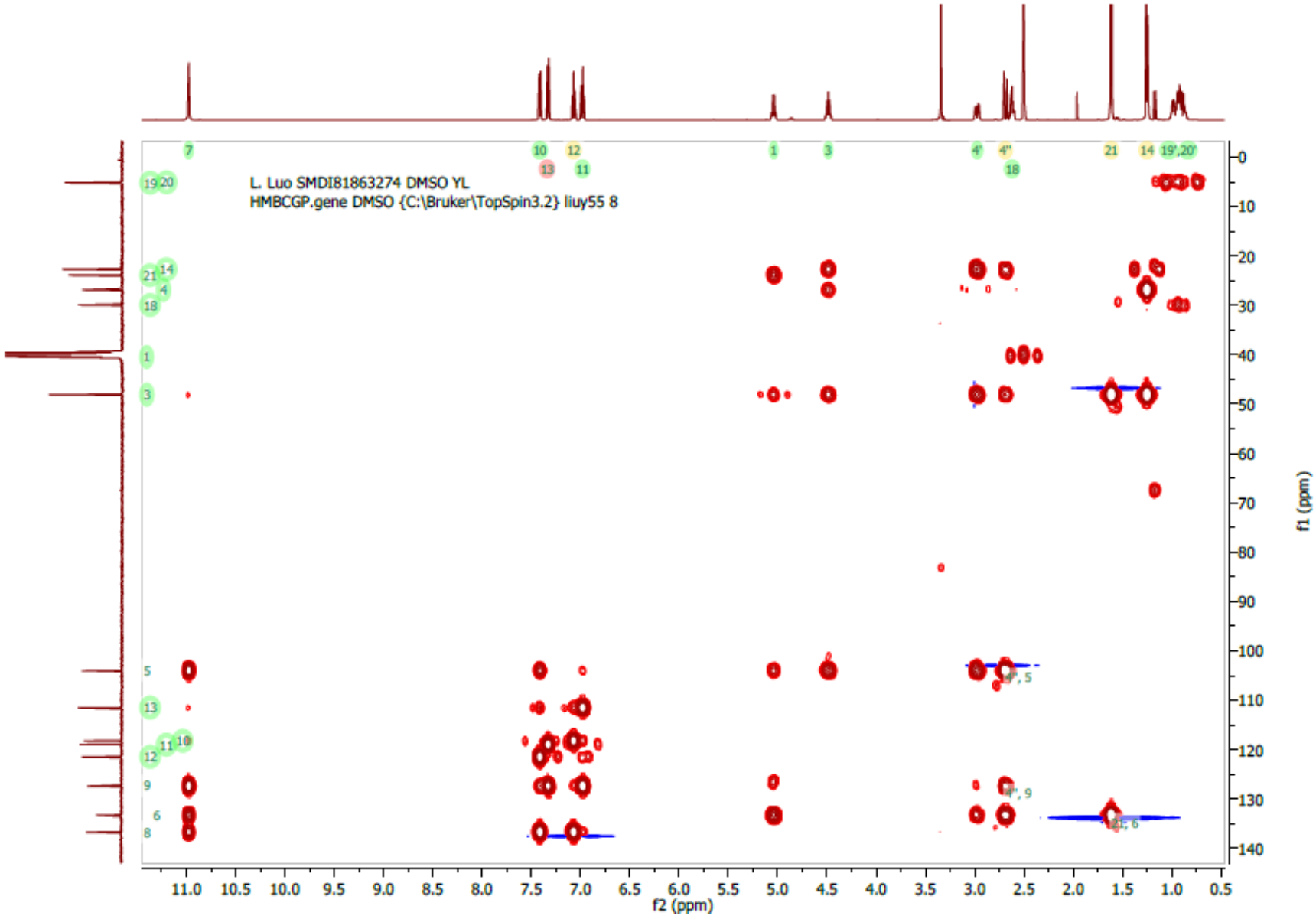
Conclusion: Two methyl are cis.

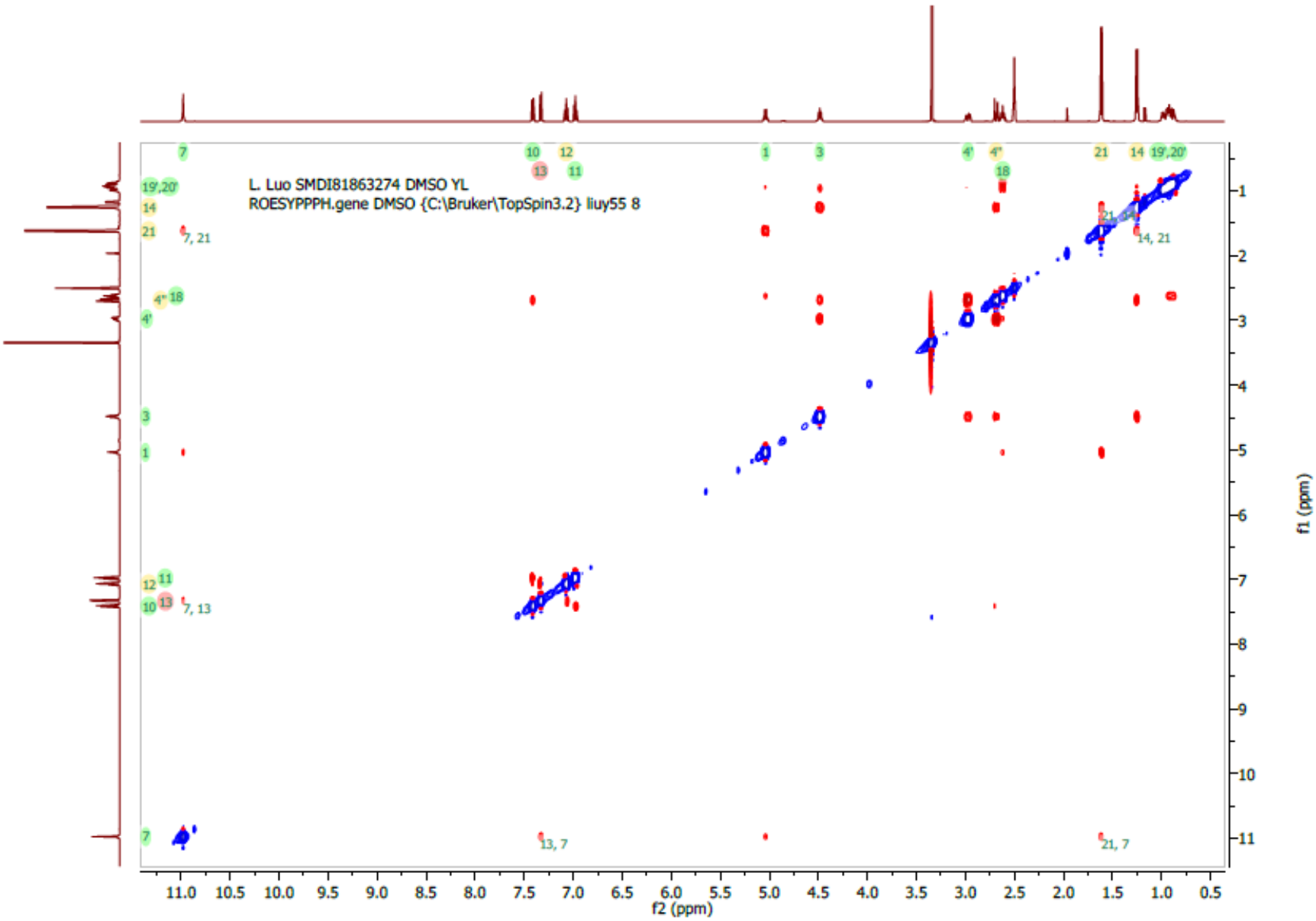


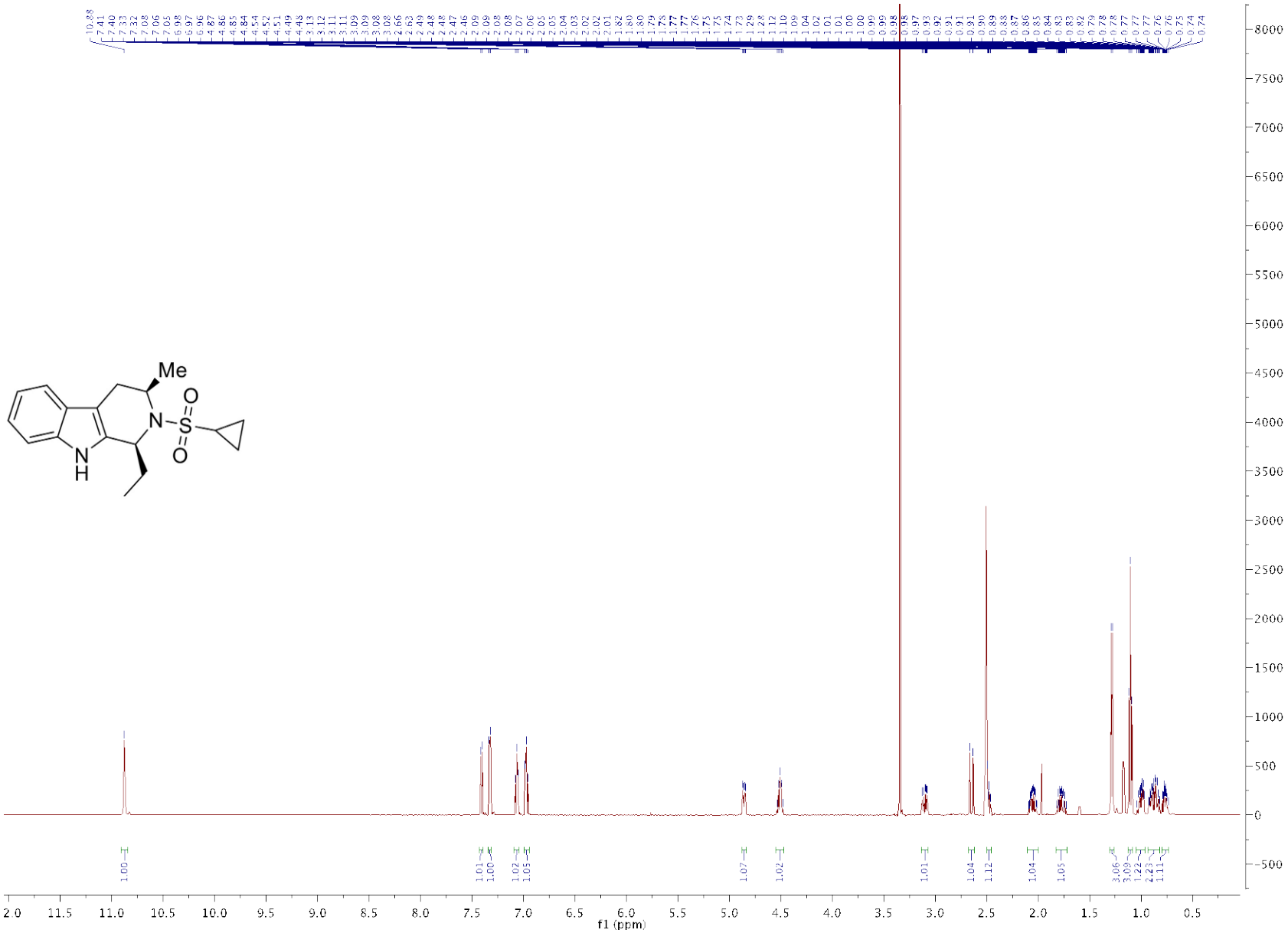

L. Luo SMDI81863274 DMSO YL
C13CPD.gene DMSO {C:\Bruker\TopSpin3.2} liuy55 8
1
3
21
14
19
20
18
4
8
6
9
12
11
10
13
5
2800000
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
-200000
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

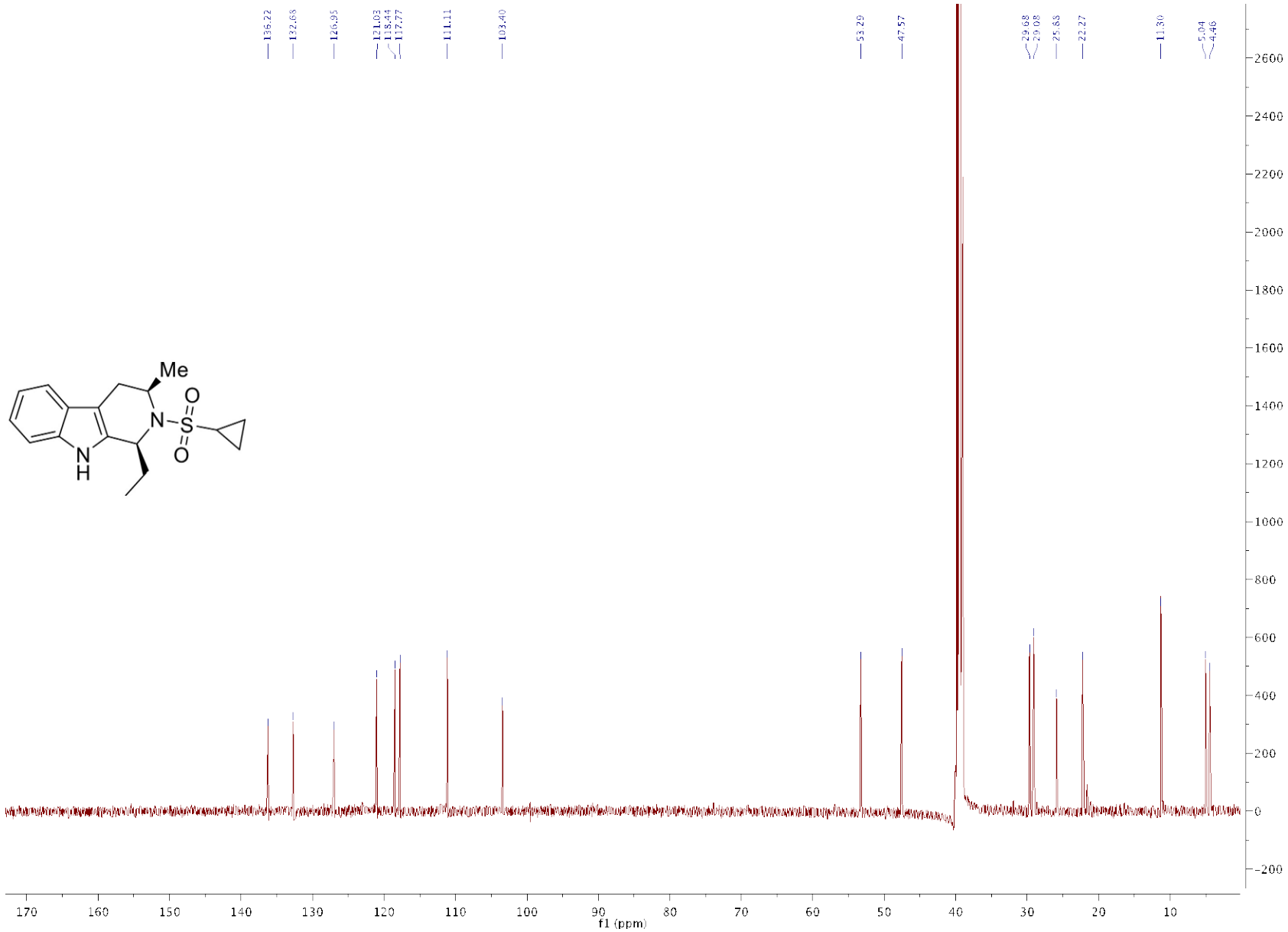

L. Luo SMDI81863274 DMSO YL
COSYGPMFQF.gene DMSO {C:\Bruker\TopSpin3.2} liuy55-8
10
12
1
3
4'
4"
21
14
19',20'
13
11
18
19',20'
14
21
4"
18
4'
3
1
12
11
10
13
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f2 (ppm)
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
f1 (ppm)

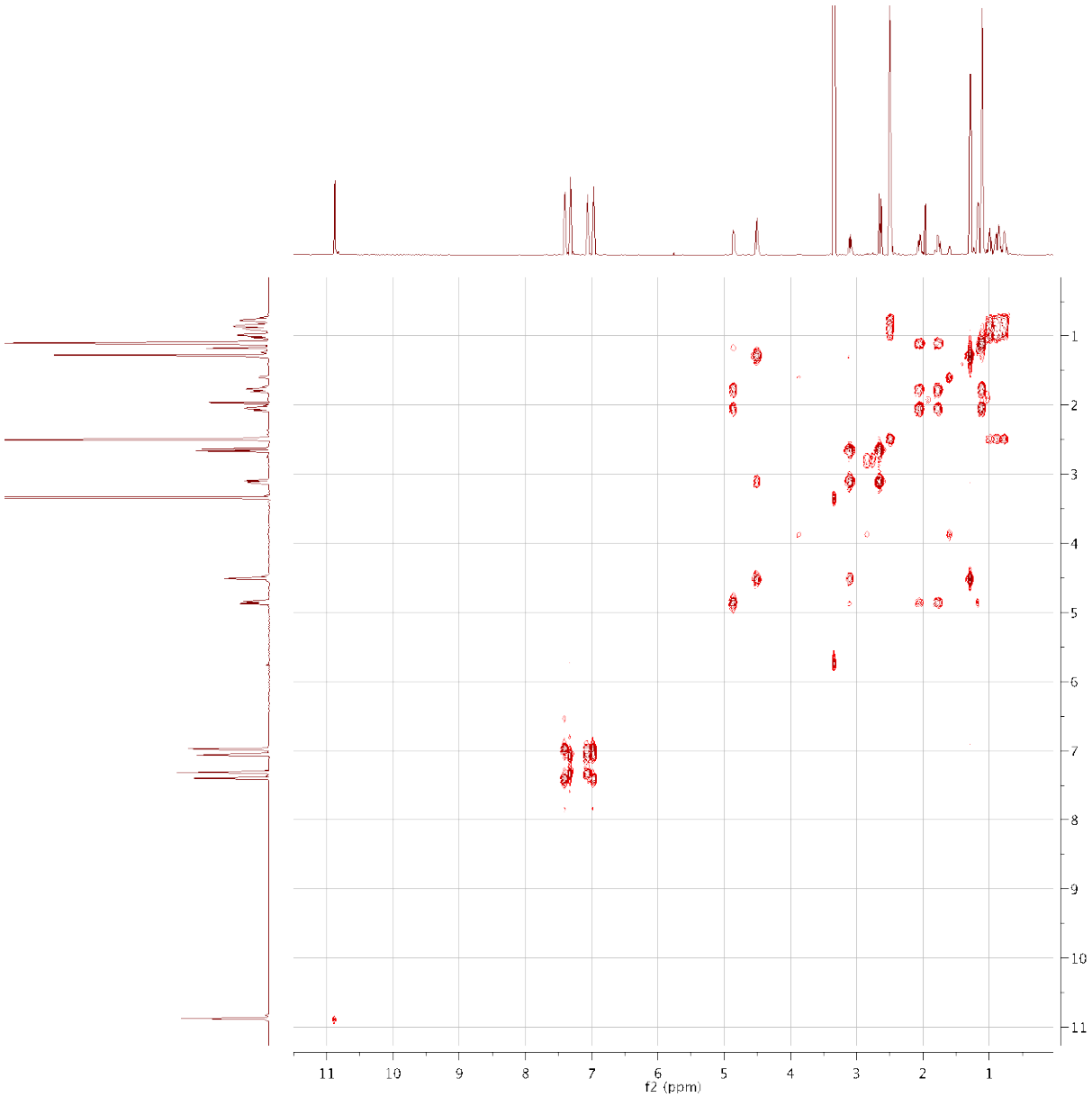

L. Luo SMDI81863274 DMSO YL
HSQCEDETGPSISP2.2_ADIA.gene DMSO {C:\Bruker\TopSpin3.2} liuy55 8
f2 (ppm)
f1 (ppm)


L. Luo SMDI81863274 DMSO YL
HMBCGP.gene DMSO {C:\Bruker\TopSpin3.2} liuy55 8
f2 (ppm)
f1 (ppm)

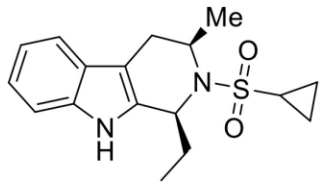

L. Luo SMDI81863274 DMSO YL
ROESYPPPH.gene DMSO {C:\Bruker\TopSpin3.2} liuy55 8
7, 21
14, 21
7, 13
13, 7
21, 7
f2 (ppm)
f1 (ppm)

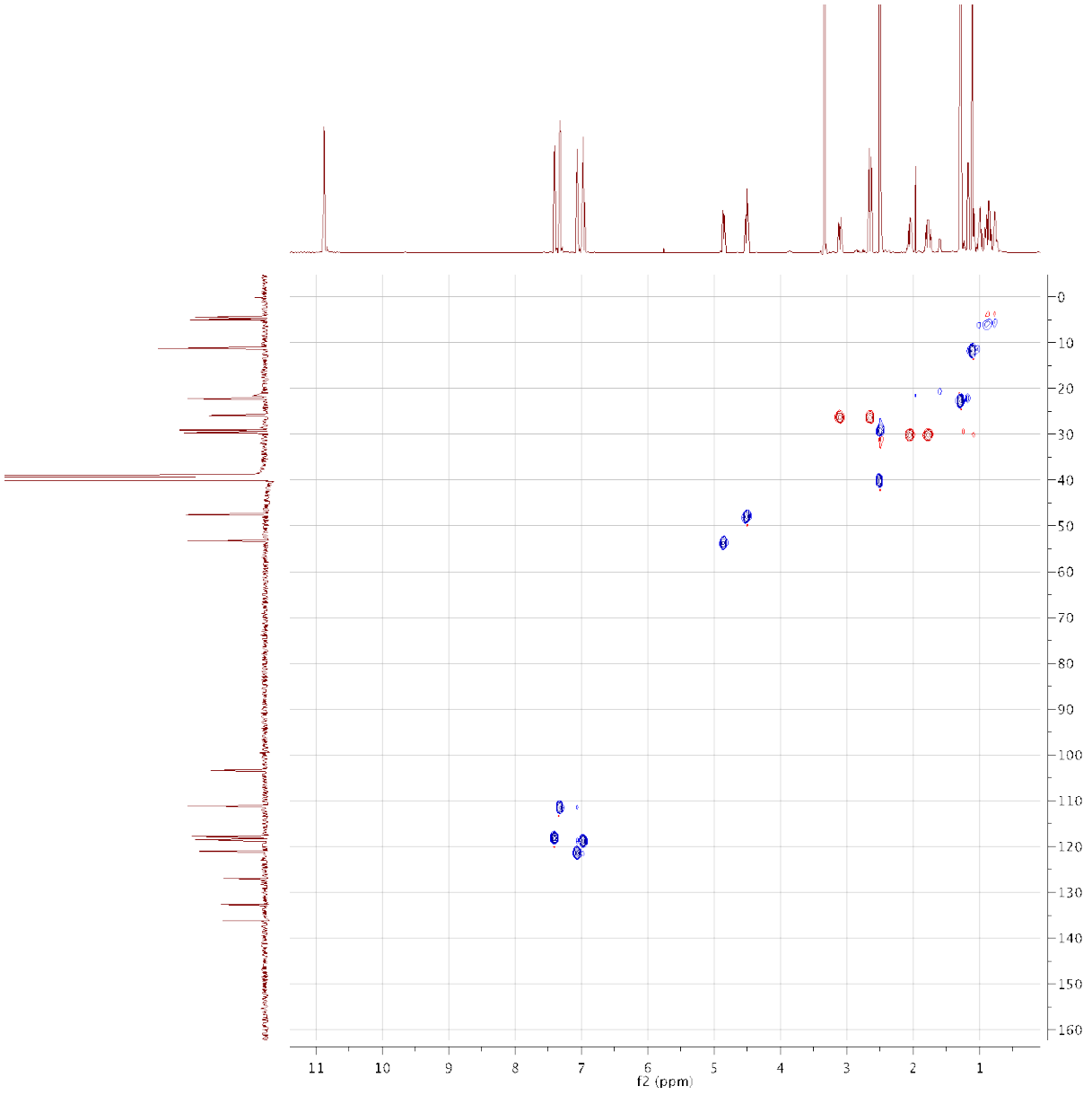

Me
O
N
S
O
N
H
f1 (ppm)


136.22
132.68
126.95
121.03
118.44
117.77
111.11
103.40
53.29
47.57
29.68
29.08
25.88
22.27
11.30
5.04
4.46
Me
O
O
N
S
N
H
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

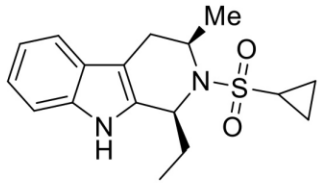


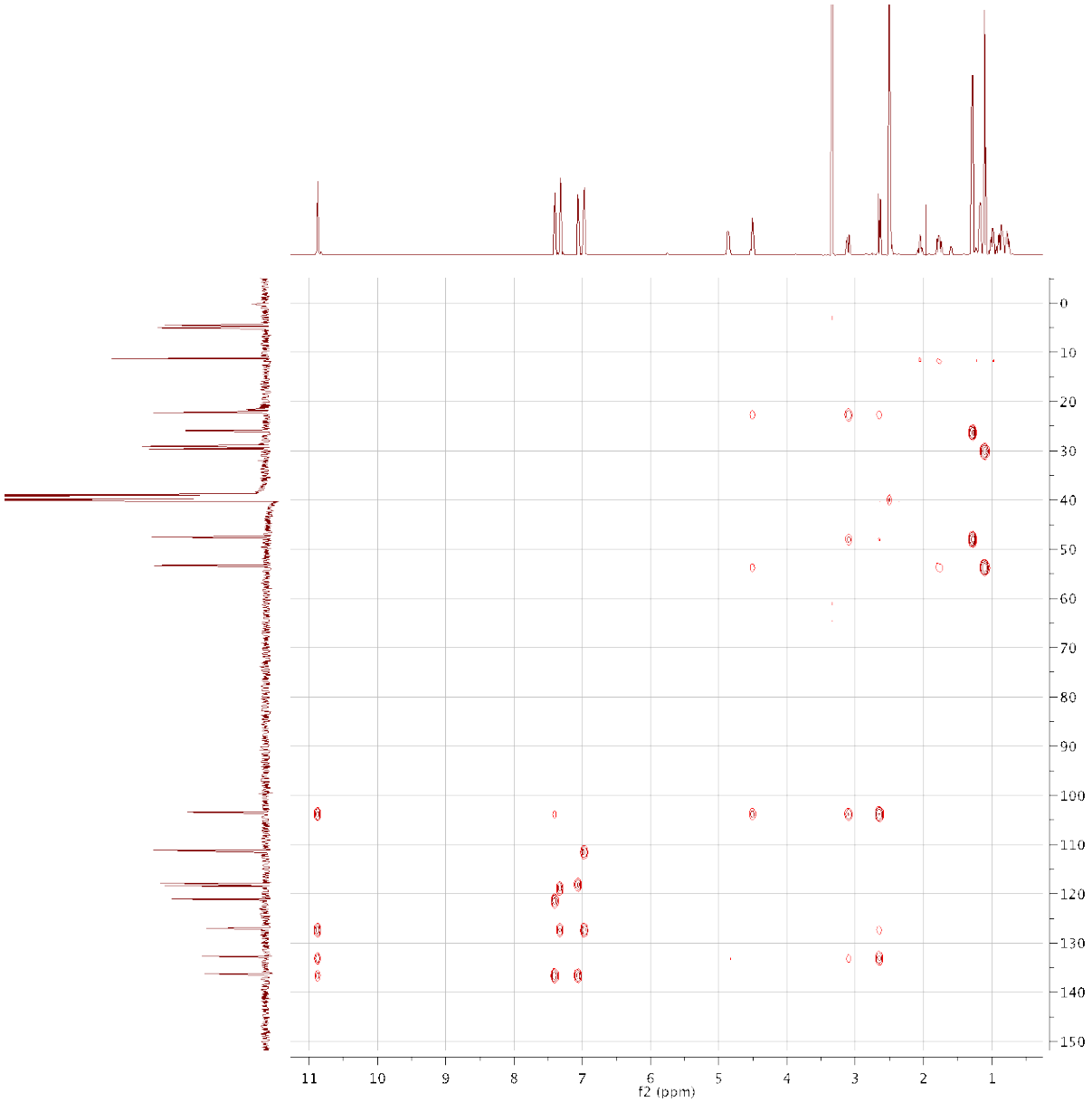
	Parameter	Value
1	Data File Name	81837693/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-07-06T21:13:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(5952.4, 5952.4)
12	Lowest Frequency	(-109.5, -109.5)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



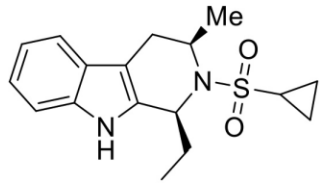


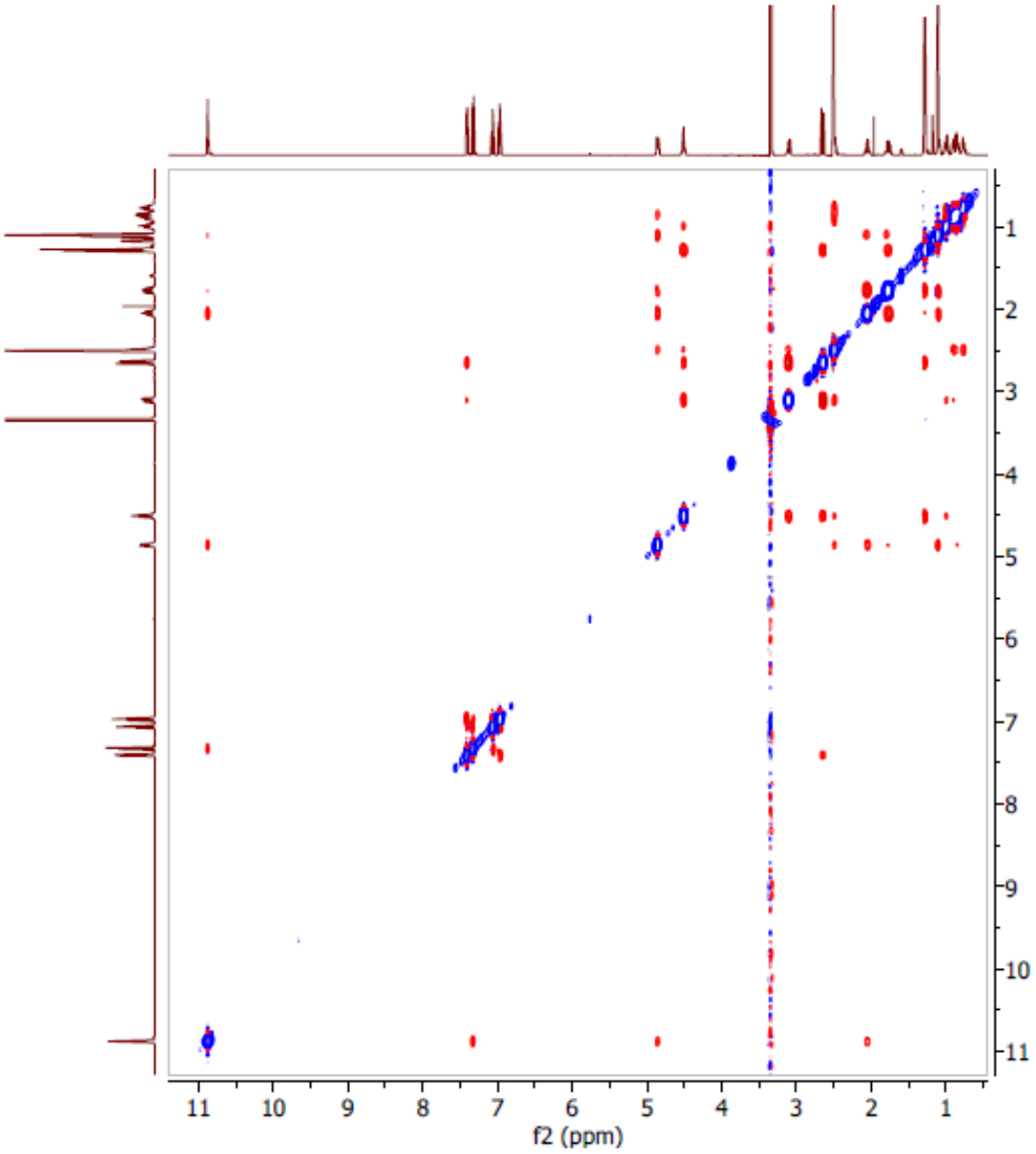
	Parameter	Value
1	Data File Name	81837693/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-07-06T21:35:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



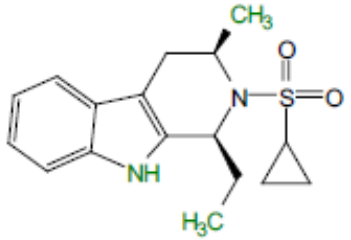


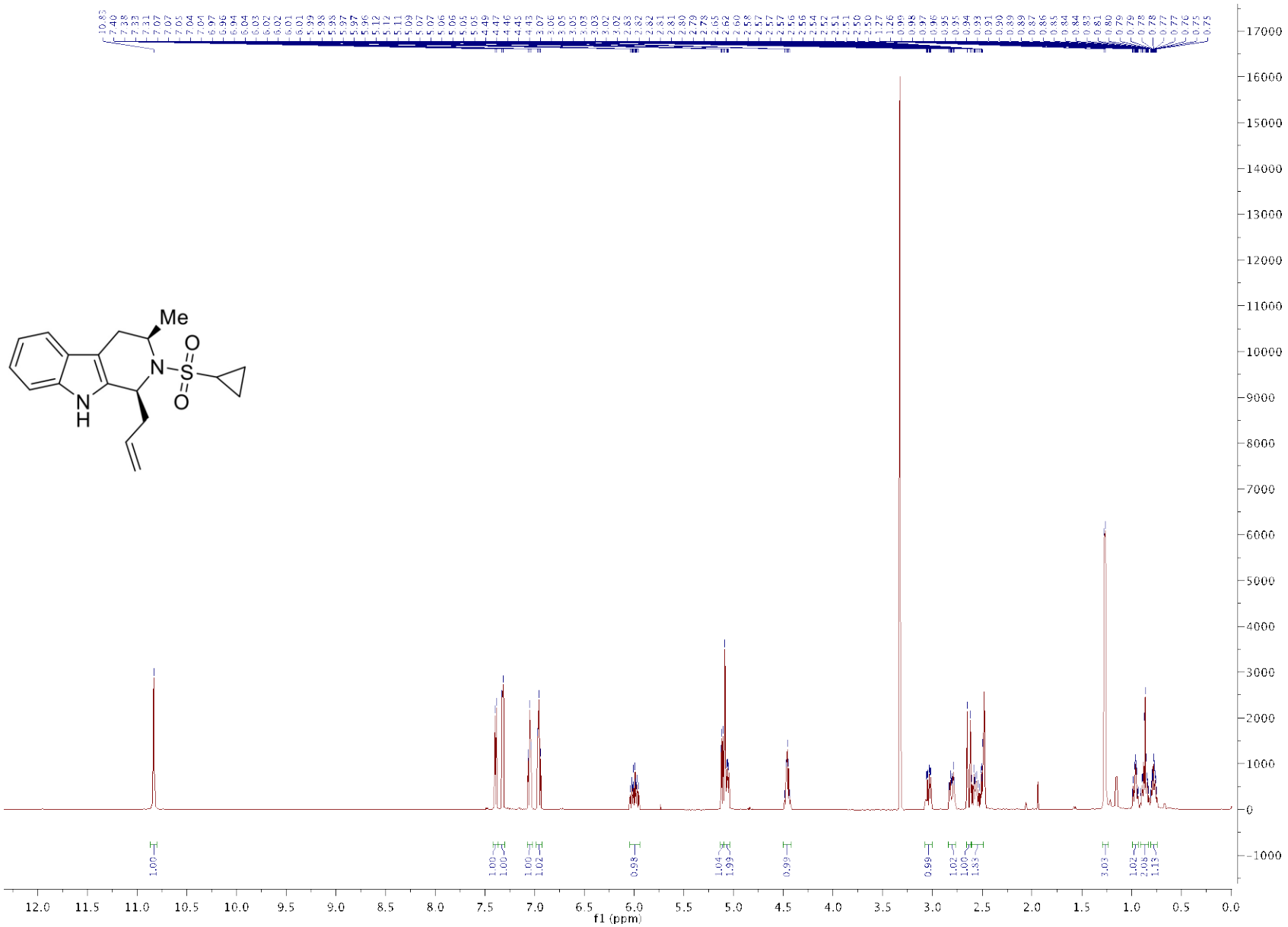
	Parameter	Value
1	Data File Name	81837693/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-07-06T21:55:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(5952.4, 30120.5)
12	Lowest Frequency	(-109.5, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

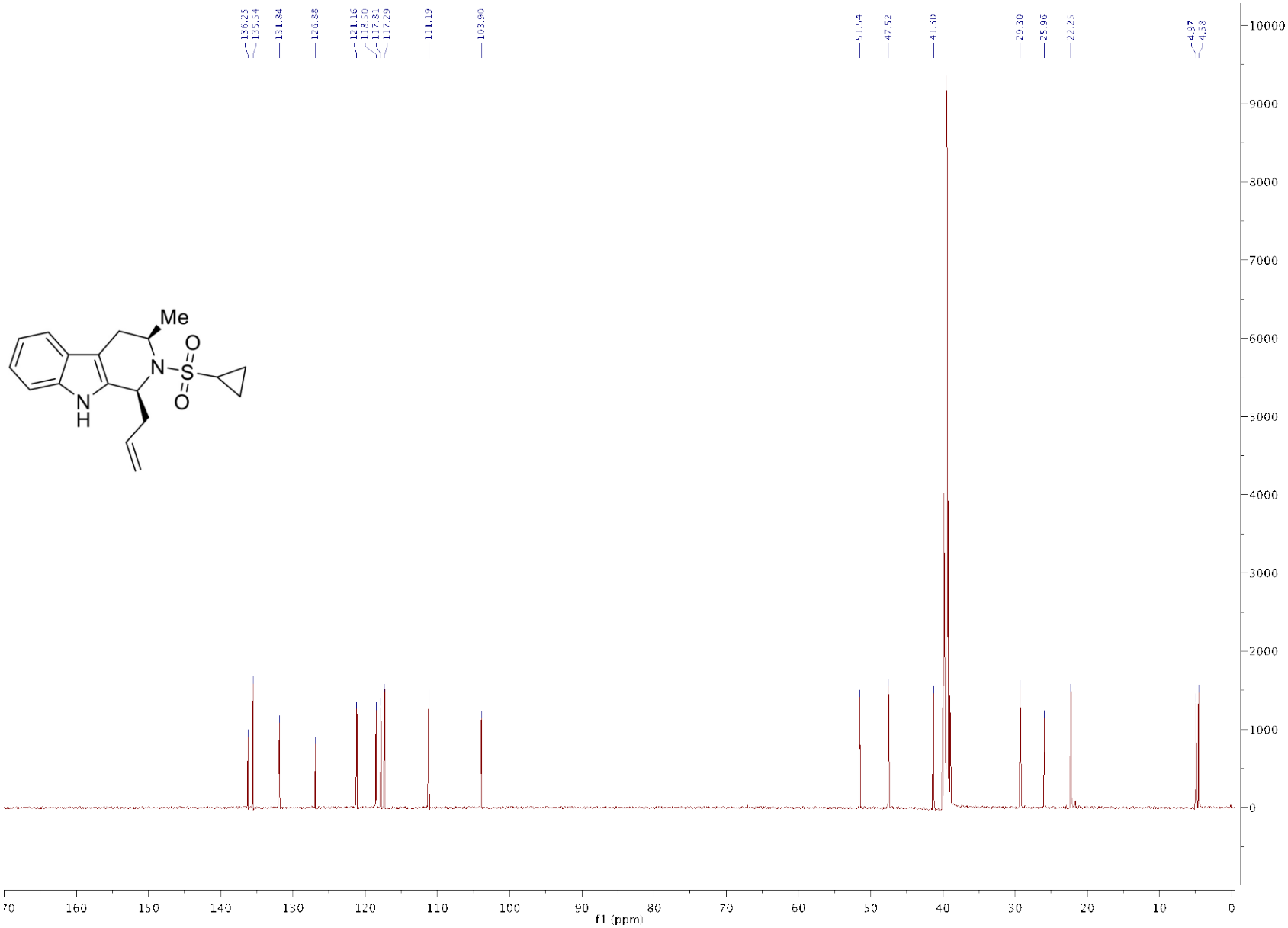




	Parameter	Value
1	Data File Name	W:/ data/ liuy55/ nmr/ 81837693/ 16/ ser
2	Sample ID	81837693
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-07-06T23:18:43
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(5952.4, 5952.4)
12	Lowest Frequency	(-109.5, -109.5)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
O
N
S
O
N
H
f1 (ppm)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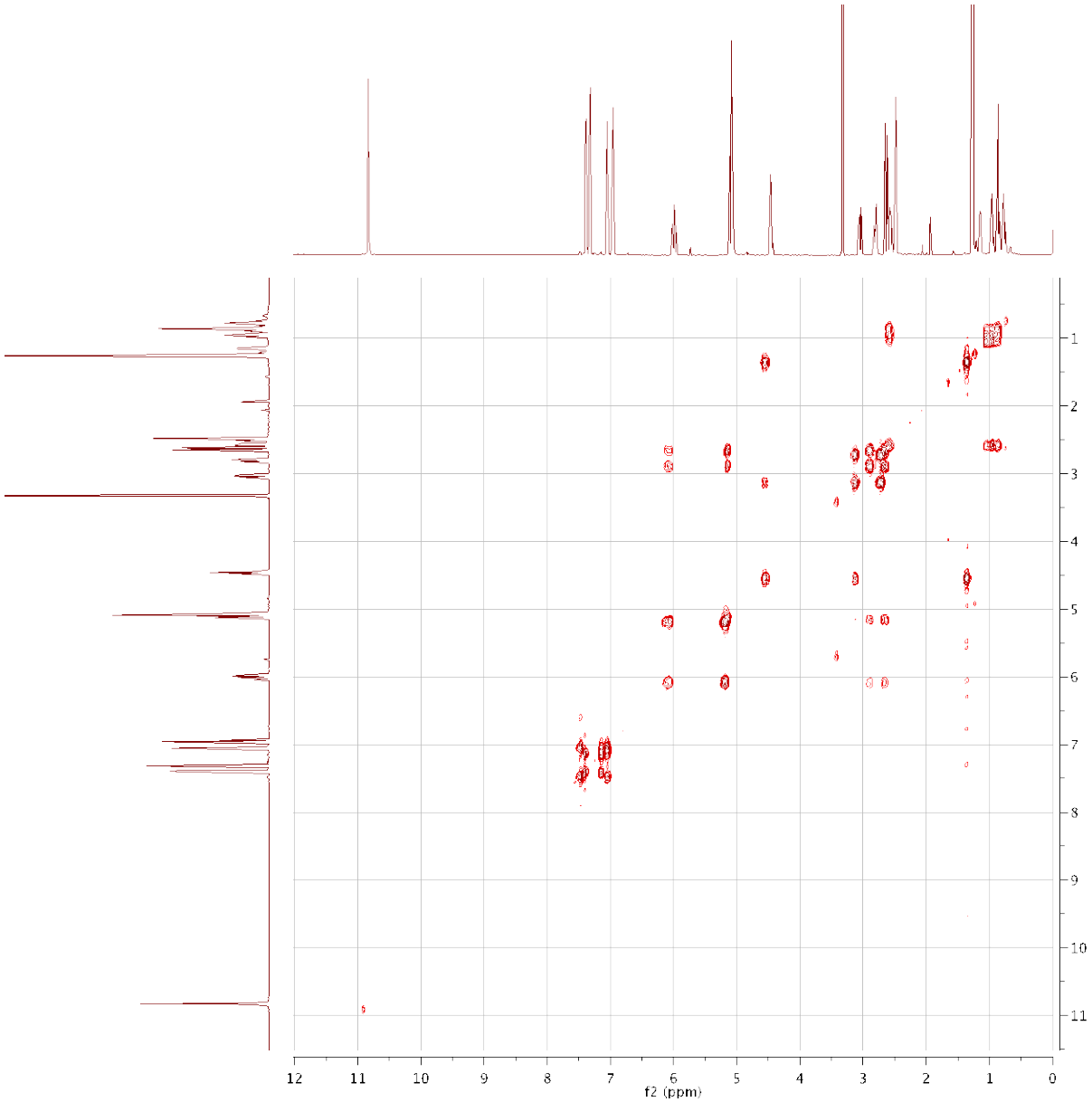
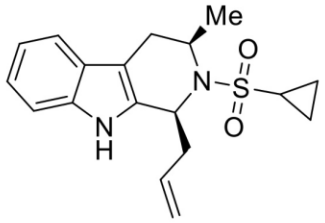
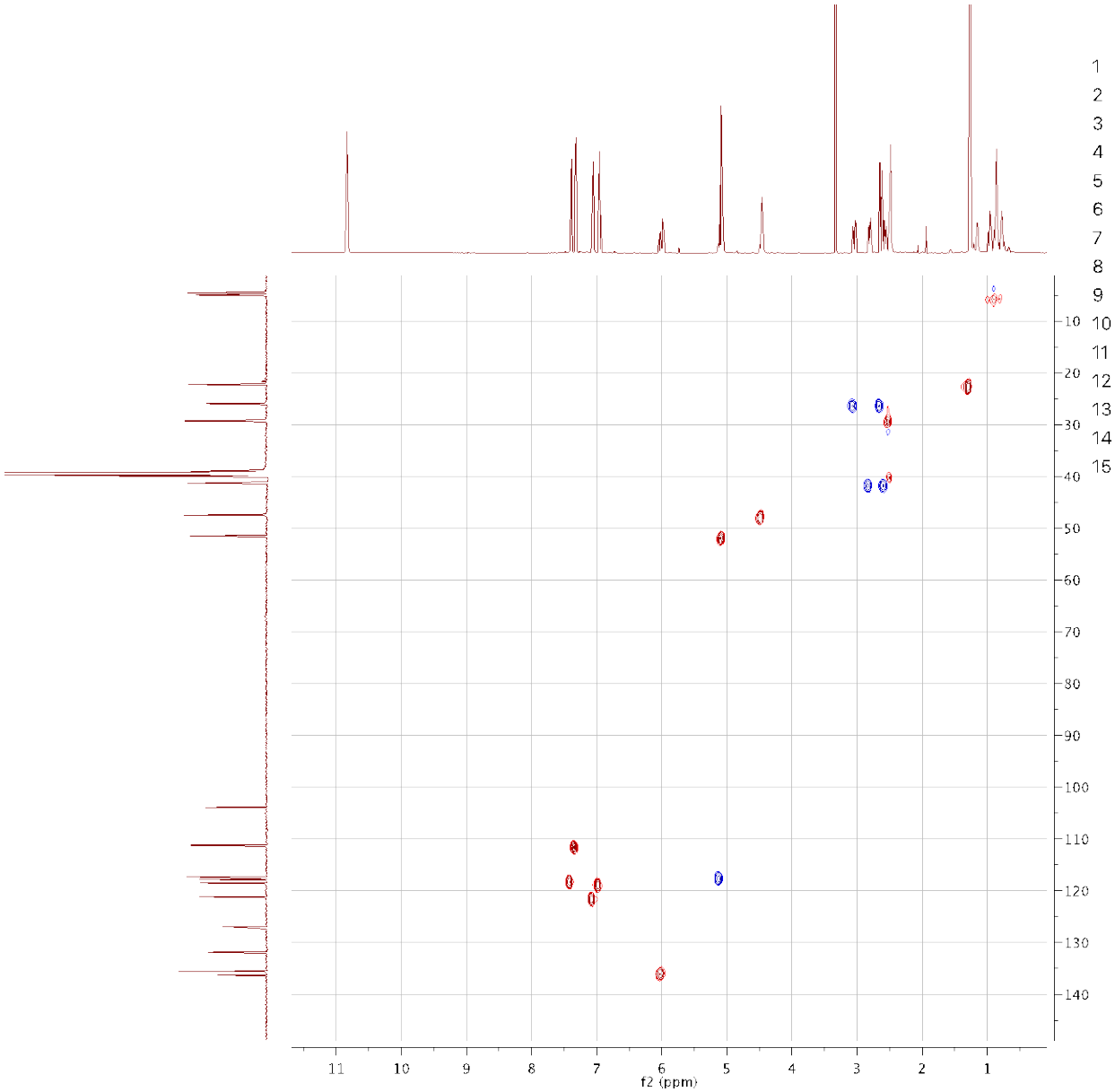
126.88
121.16
118.50
117.81
117.29
111.19
103.90
51.54
47.52
41.30
29.30
25.96
22.25
4.97
4.38
Me
N
O
S
O
N
H
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
f1 (ppm)

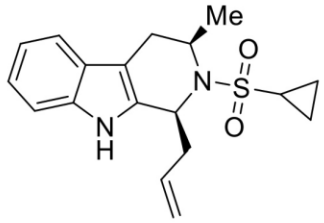


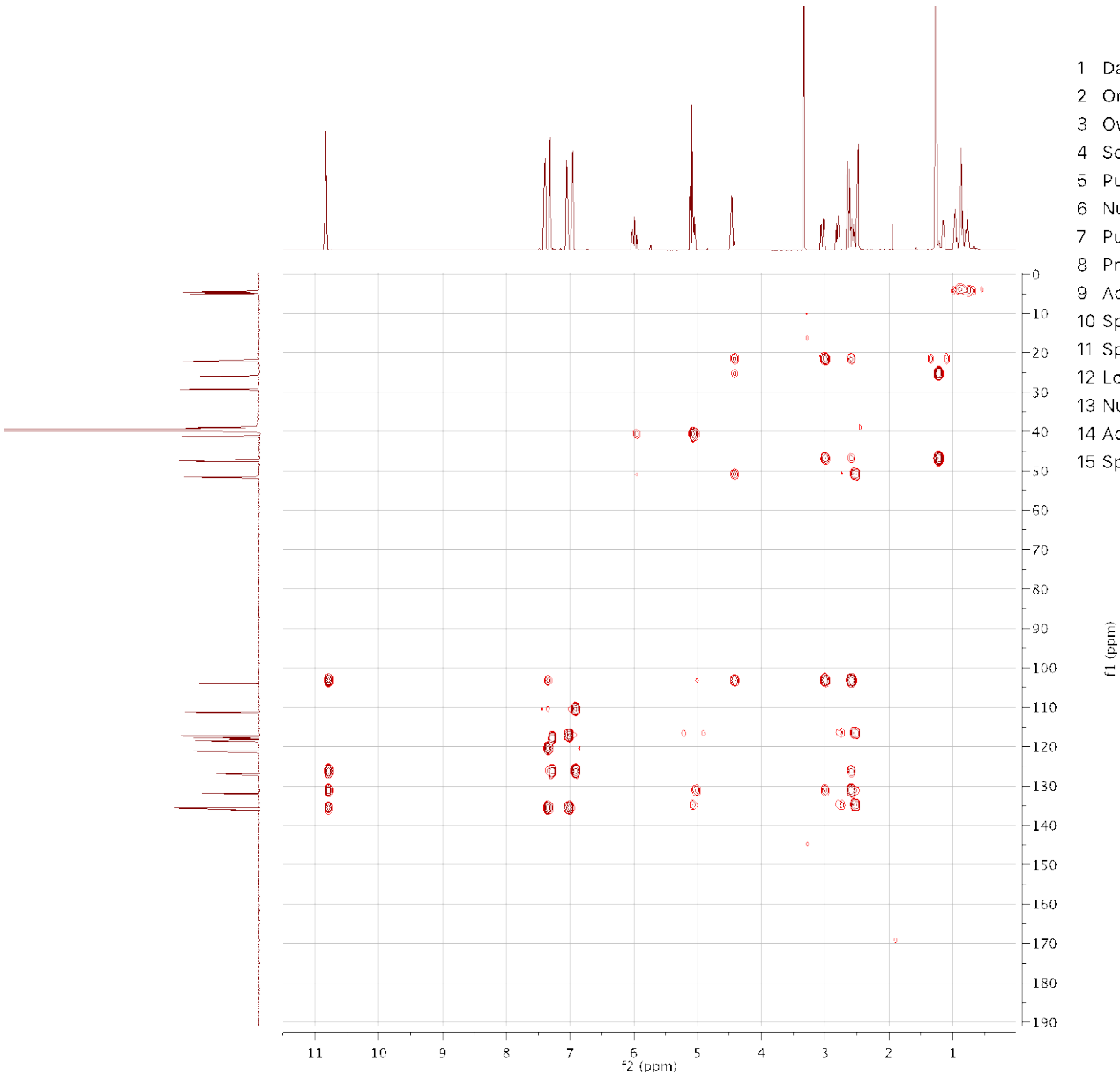
	Parameter	Value
1	Data File Name	81837683/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-07-06T16:39:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6578.9, 6578.9)
12	Lowest Frequency	(-432.2, -432.2)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



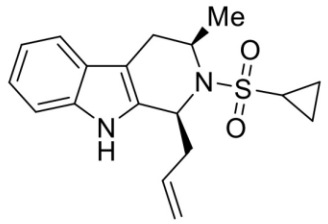


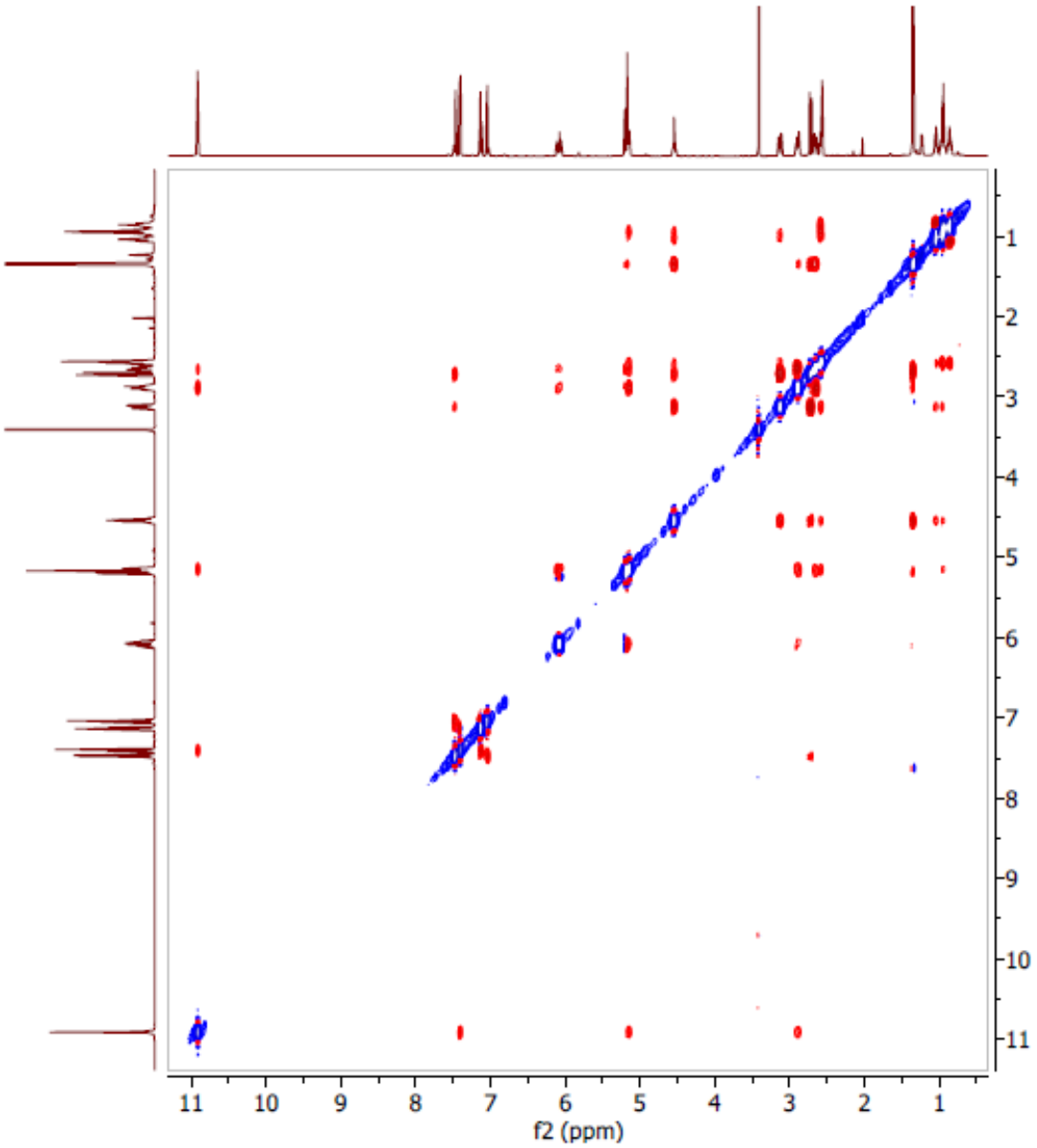
	Parameter	Value
1	Data File Name	81837683/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-07-06T17:00:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



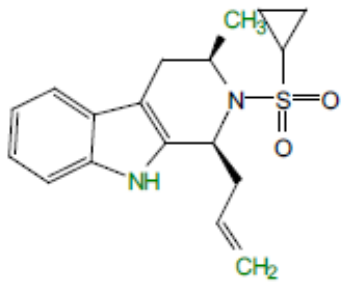


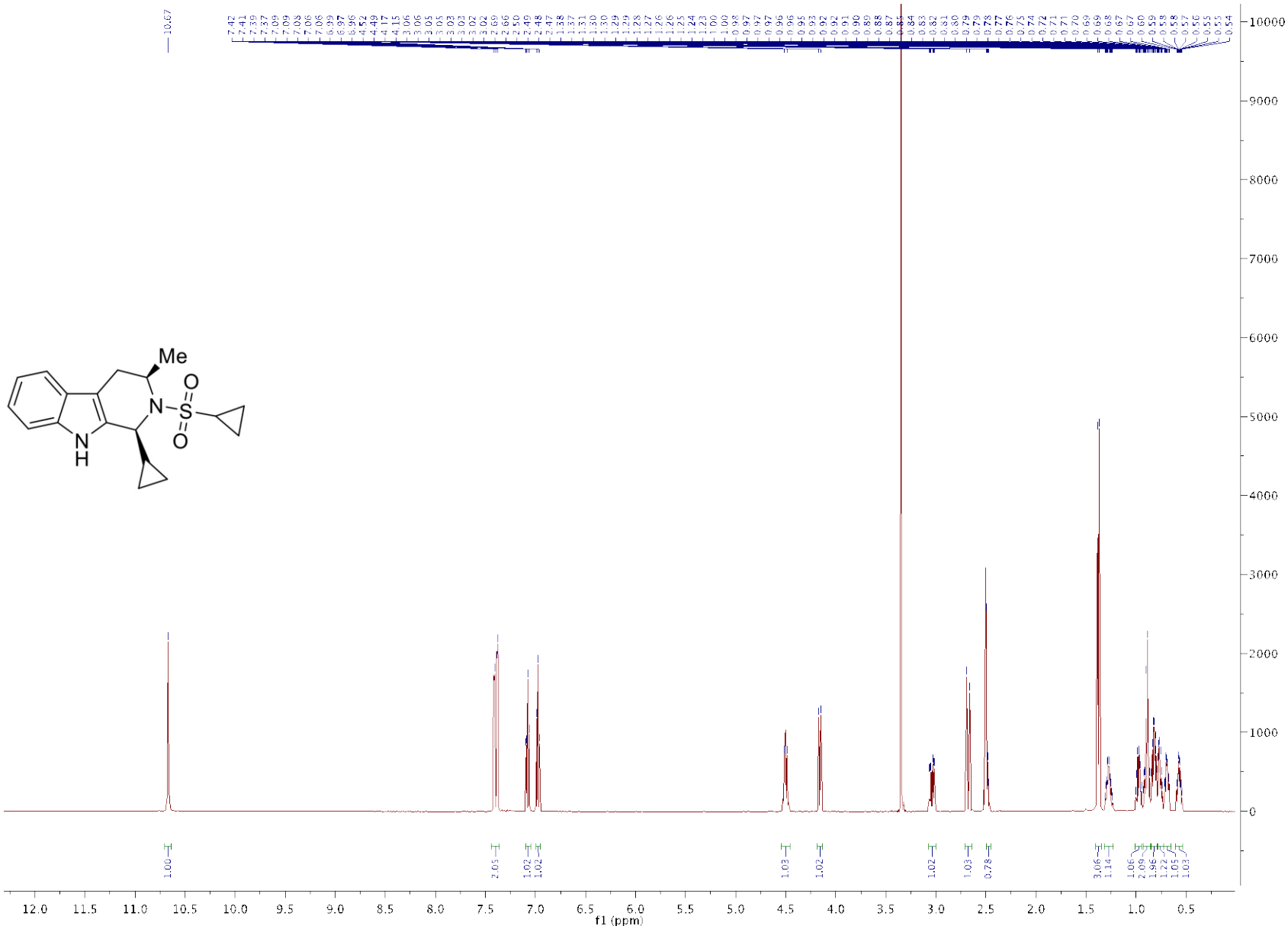
	Parameter	Value
1	Data File Name	81837683/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-07-06T17:21:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6578.9, 30120.5)
12	Lowest Frequency	(-494.4, -1370.4)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

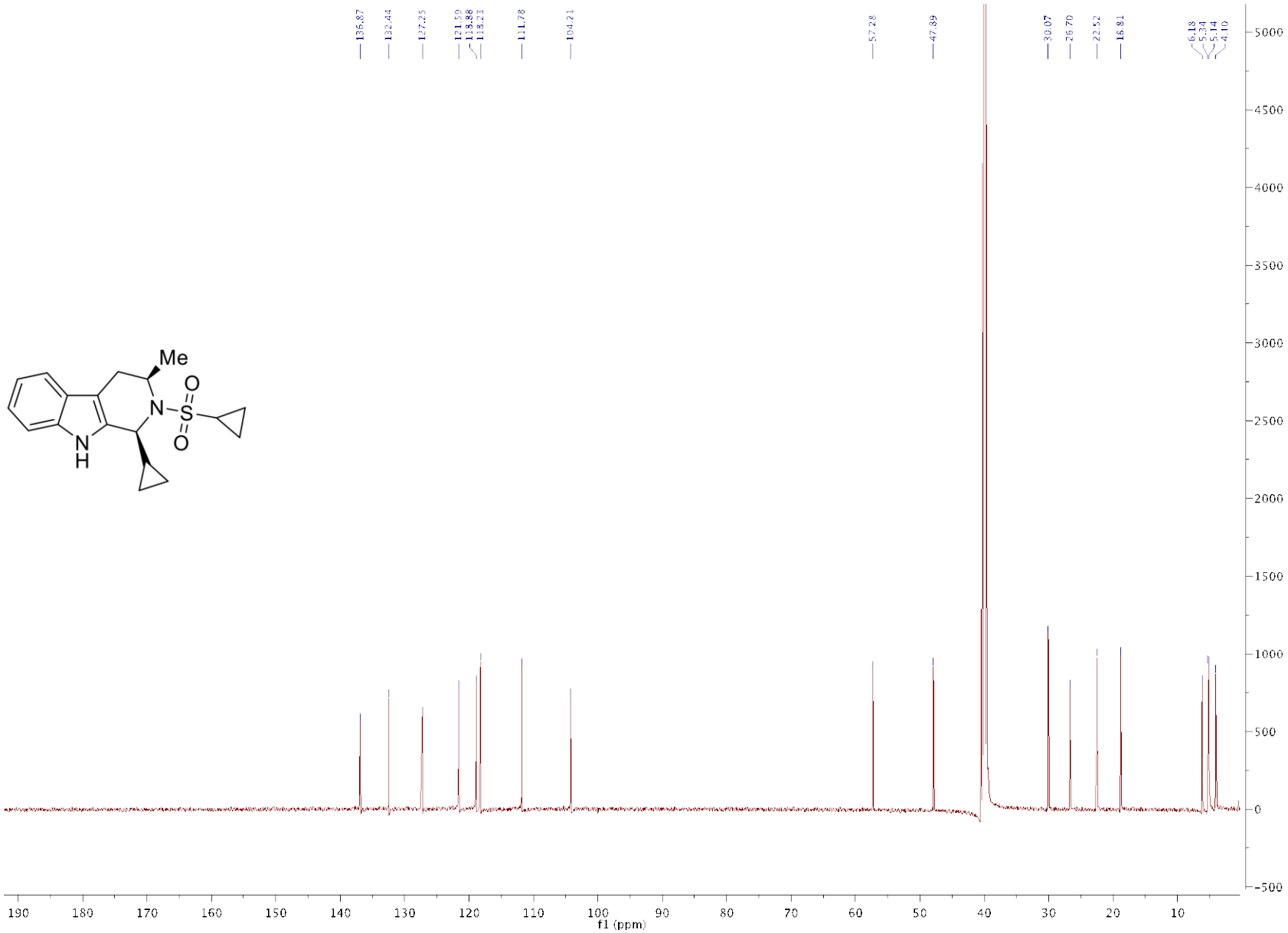




	Parameter	Value
1	Data File Name	W:/ data/ liuy55/ nmr/ 81837683/ 16/ ser
2	Sample ID	81837683
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-07-06T18:44:08
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6578.9, 6578.9)
12	Lowest Frequency	(-433.1, -433.1)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
O
N
S
O
N
H
f1 (ppm)


136.87
132.44
127.25
121.59
118.88
118.23
111.78
104.21
57.28
47.89
30.07
26.70
22.52
16.81
6.18
5.34
5.14
4.10
Me
O
N
S
O
N
H
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190
180
170
160
150
140
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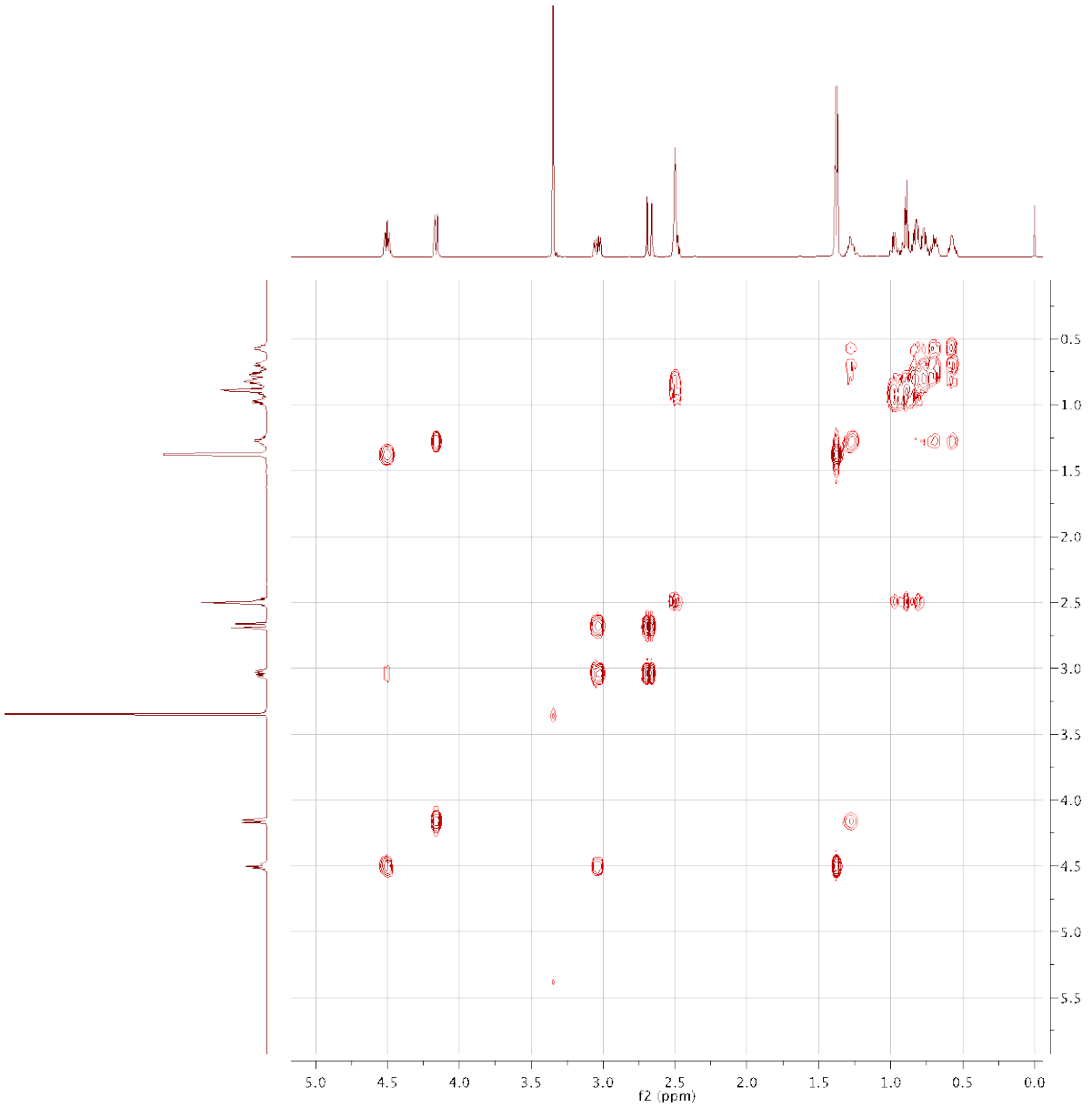
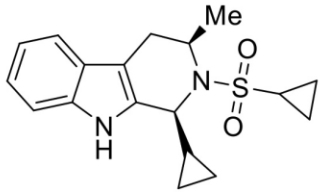
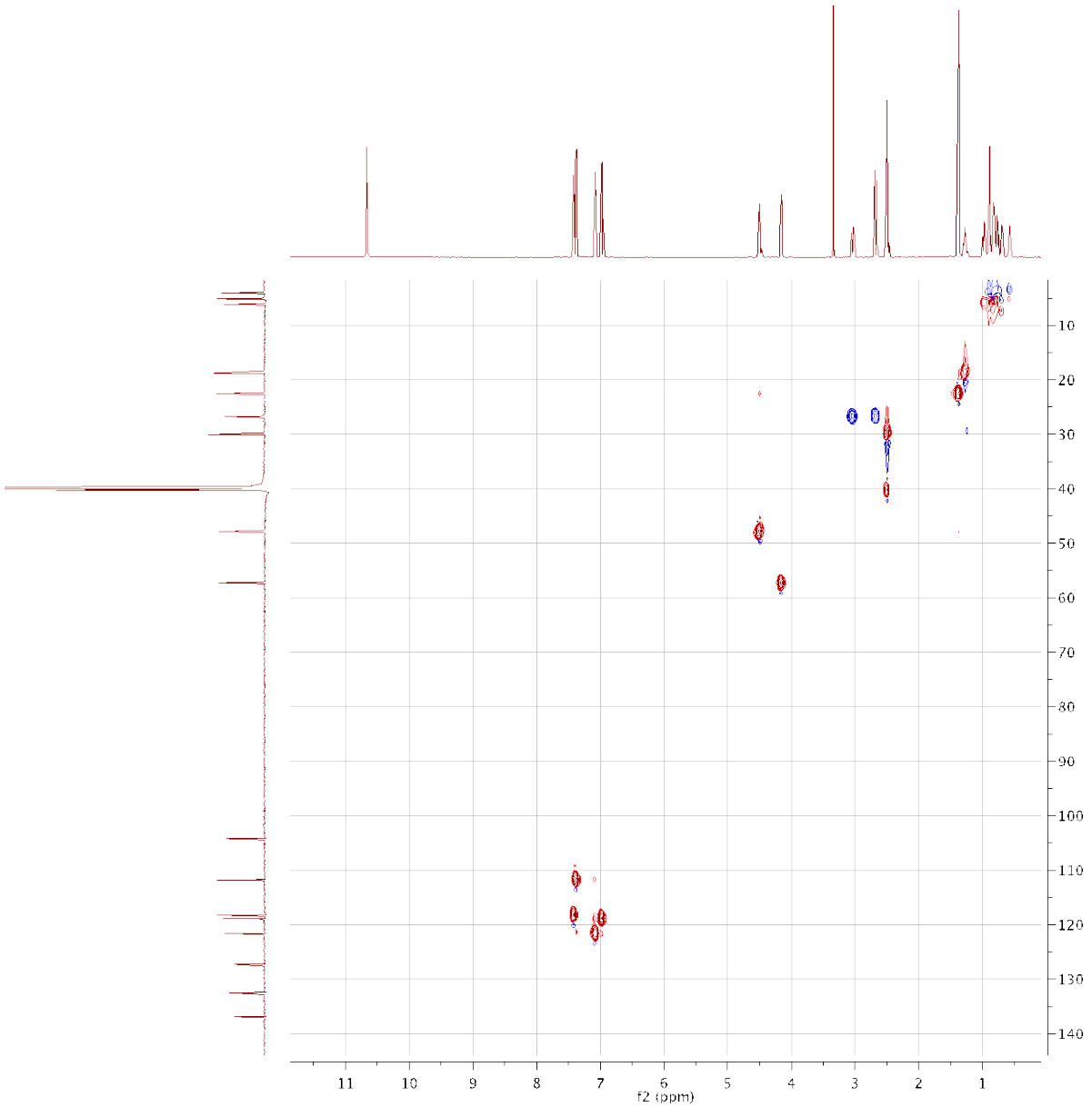
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

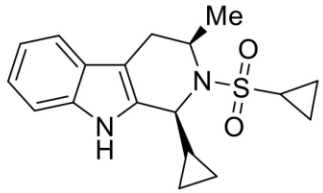


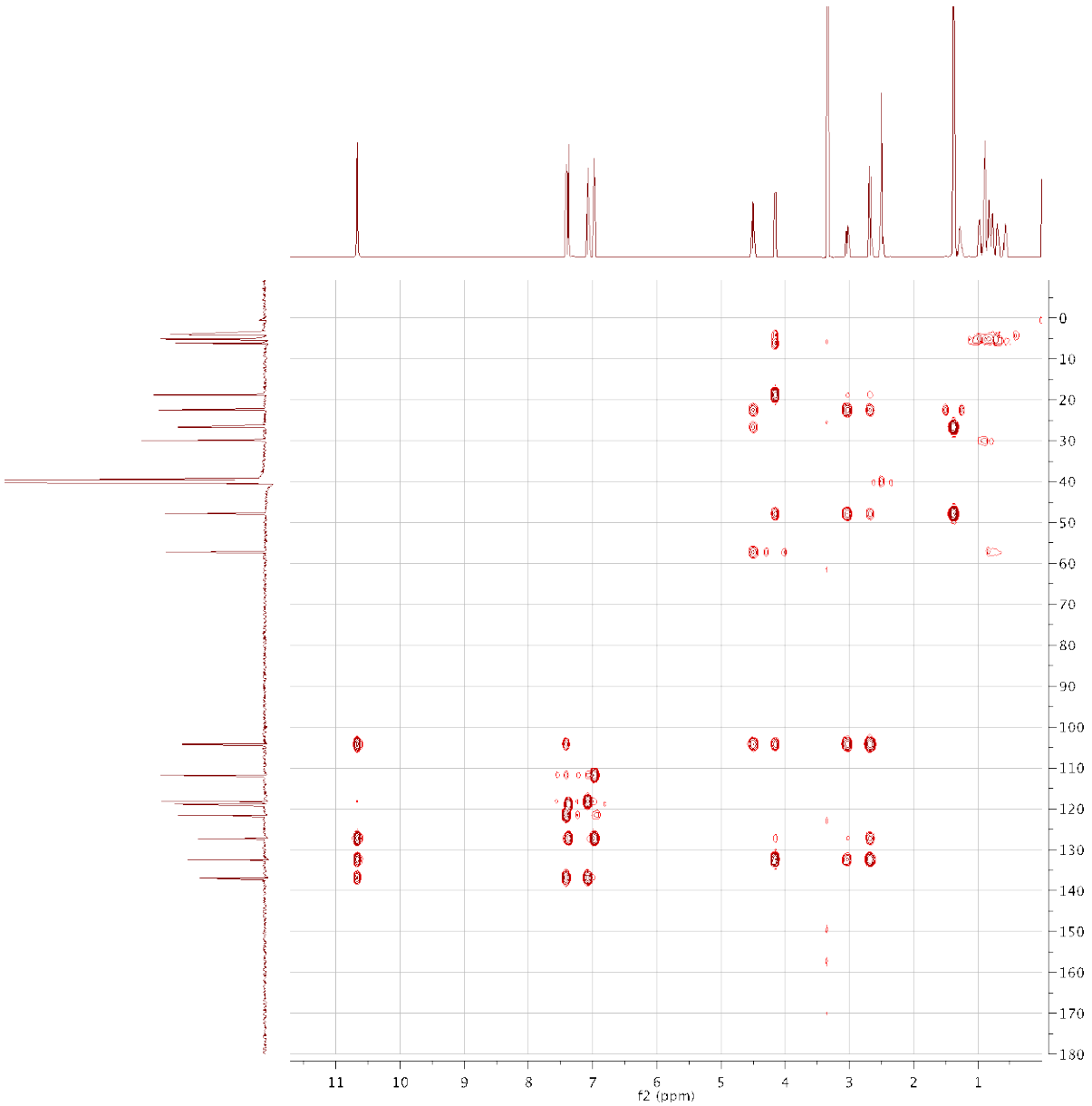
	Parameter	Value
1	Data File Name	81868898/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T19:46:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-471.0, -471.0)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



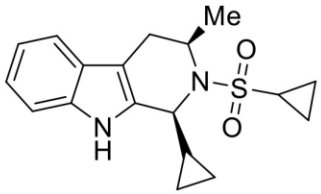


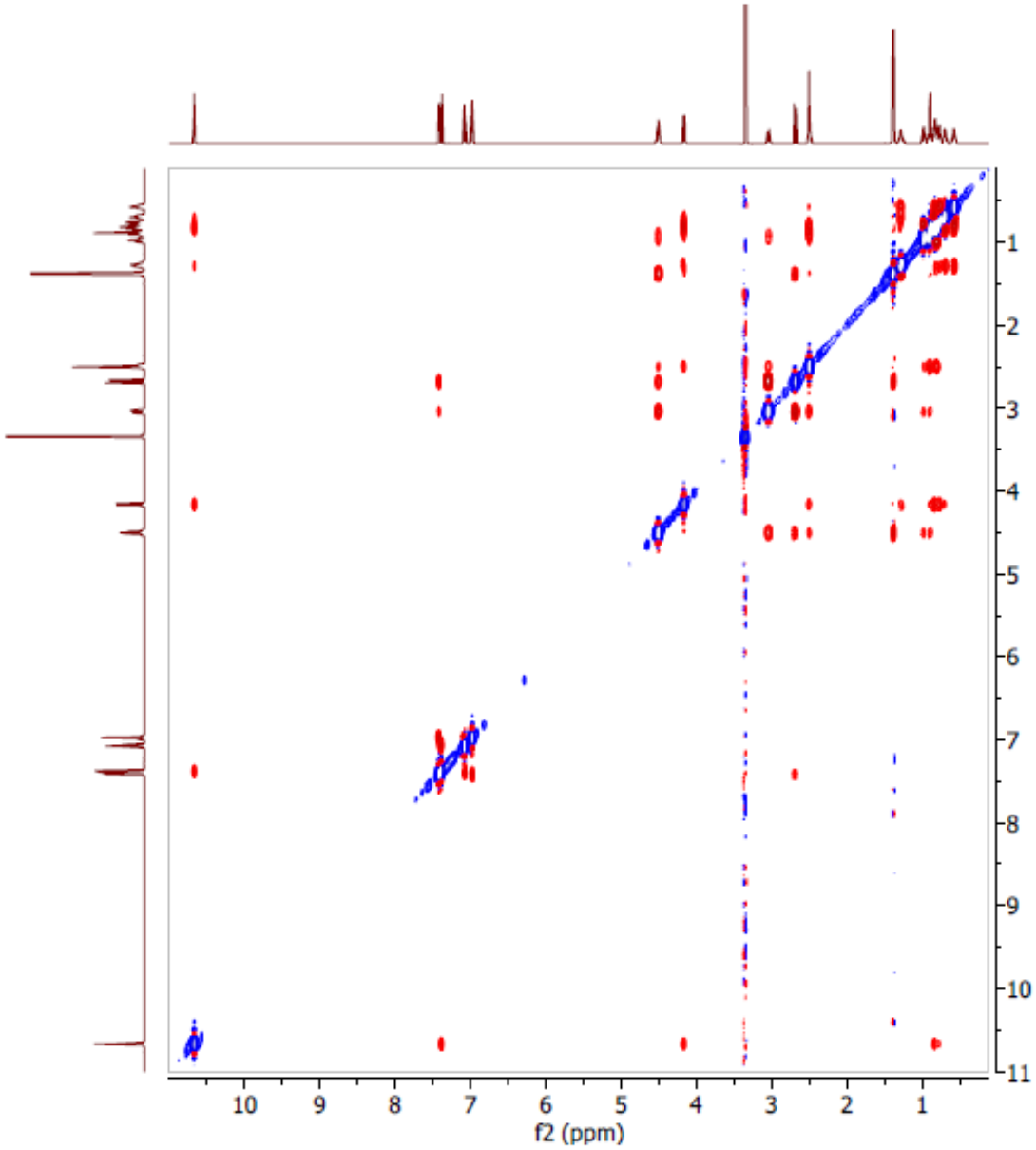
	Parameter	Value
1	Data File Name	81868898/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T20:08:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



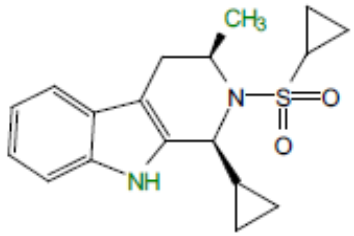


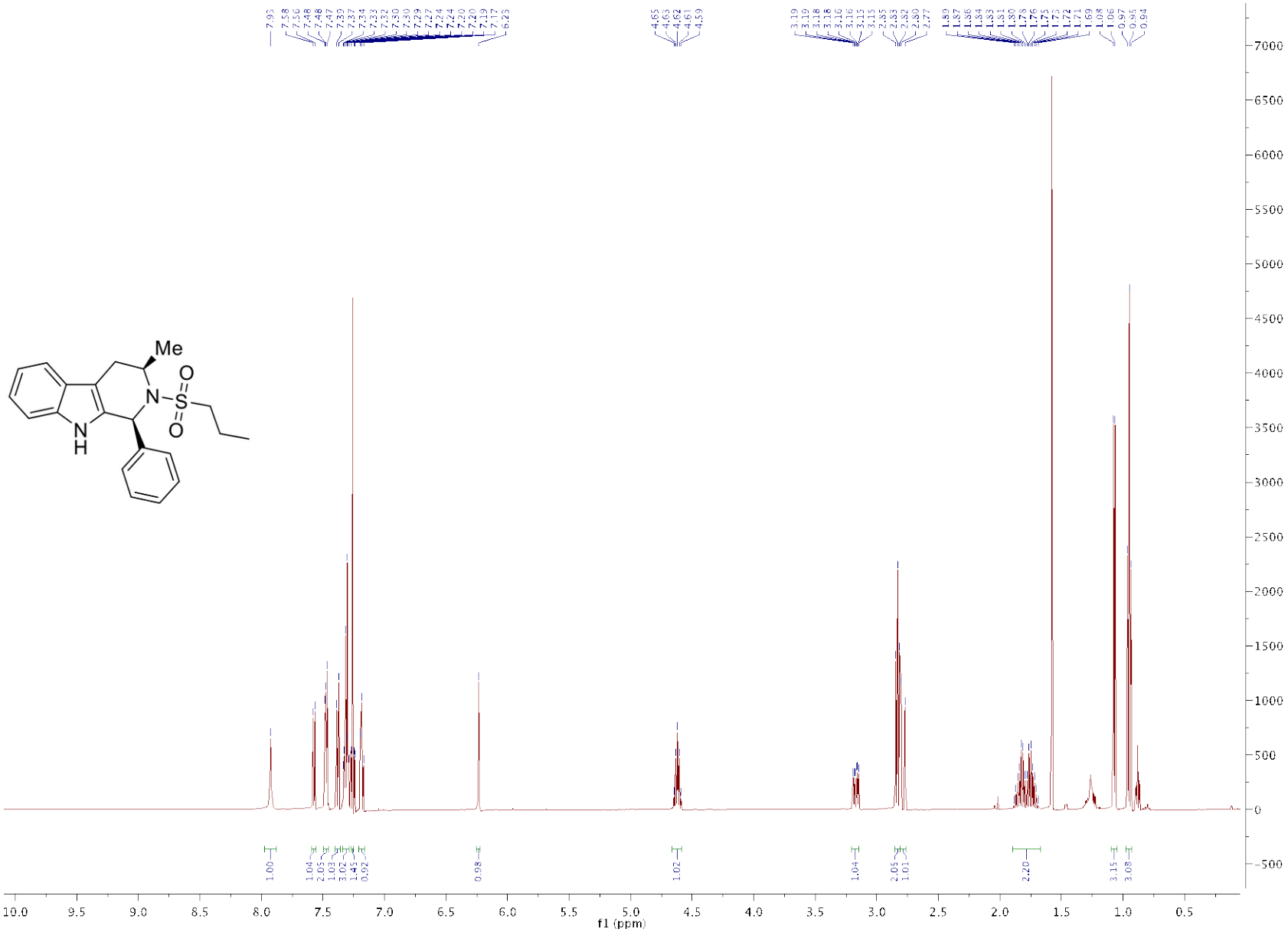
	Parameter	Value
1	Data File Name	81868898/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T20:28:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6329.1, 30120.5)
12	Lowest Frequency	(-471.0, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

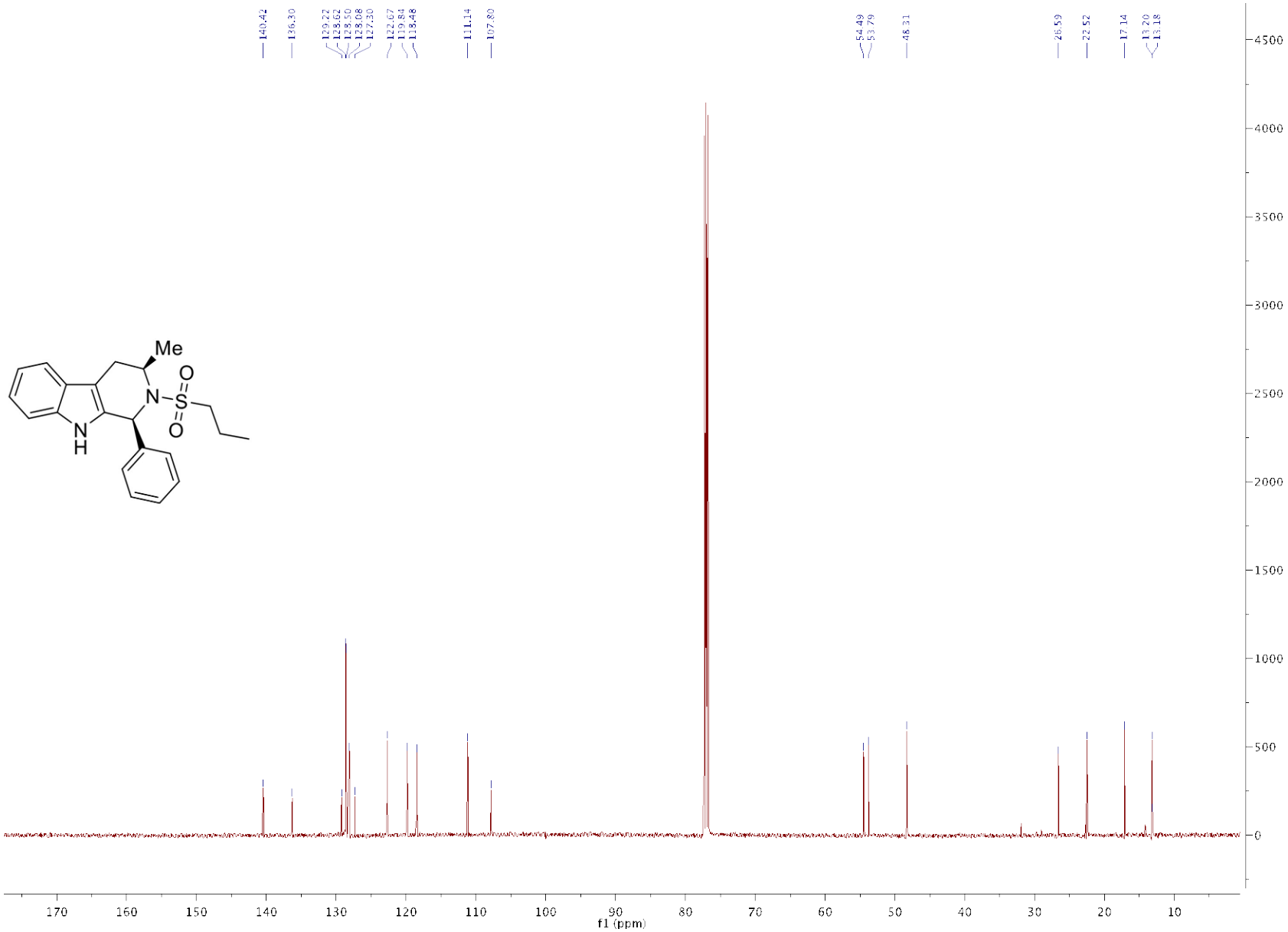




	Parameter	Value
1	Data File Name	W:/ data/ liuy55/ nmr/ 81868898/ 16/ ser
2	Sample ID	81868898
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-08-20T21:51:41
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-473.8, -473.8)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
O
N
S
O
N
H
f1 (ppm)


140.42
136.30
129.22
128.62
128.50
128.08
127.30
122.67
119.84
118.48
111.14
107.80
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53.79
48.31
26.59
22.52
17.14
13.20
13.18
Me
O
N
S
O
N
H
4500
4000
3500
3000
2500
2000
1500
1000
500
0
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140
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120
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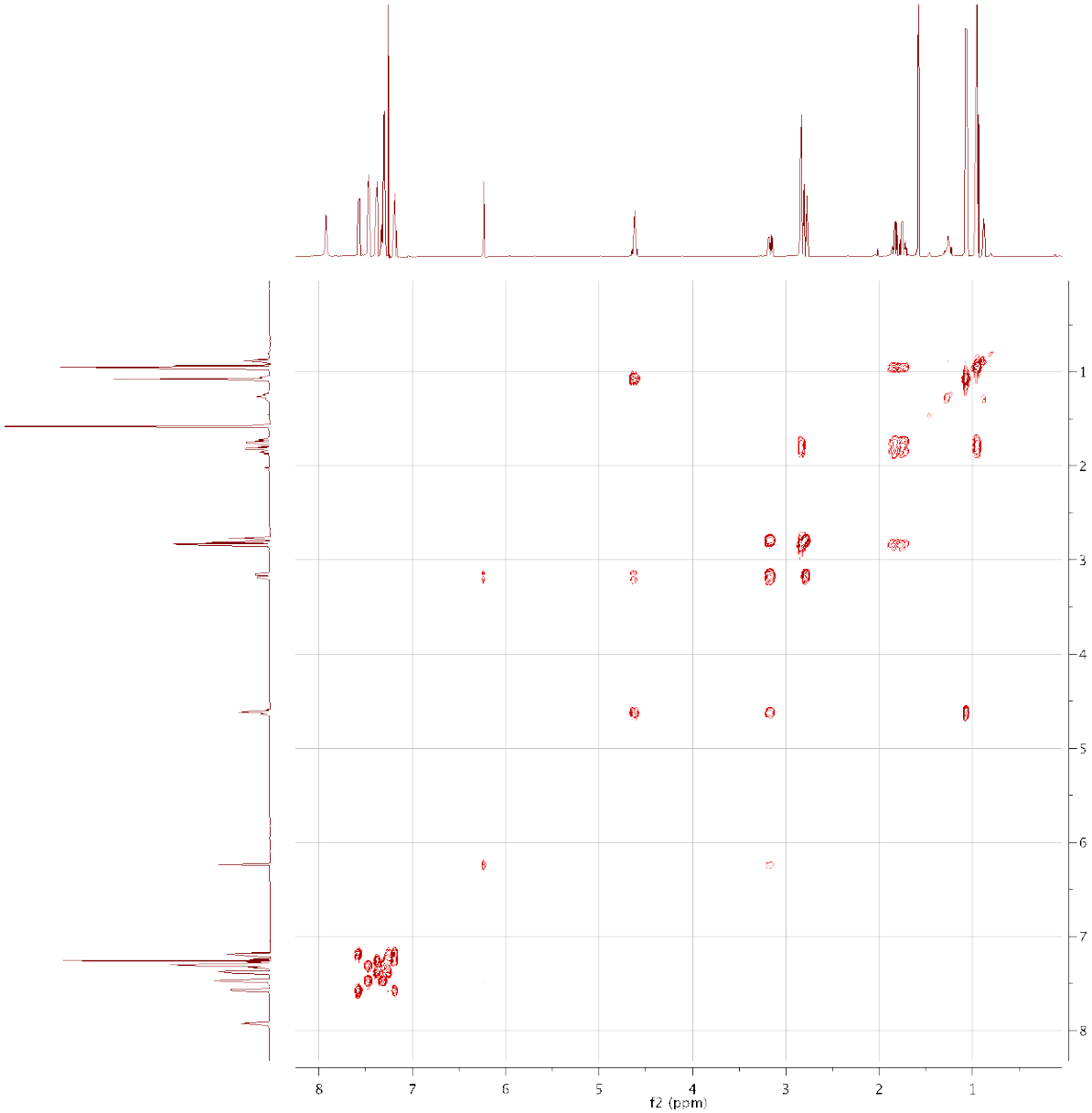
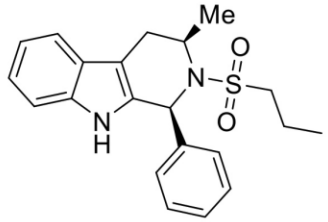
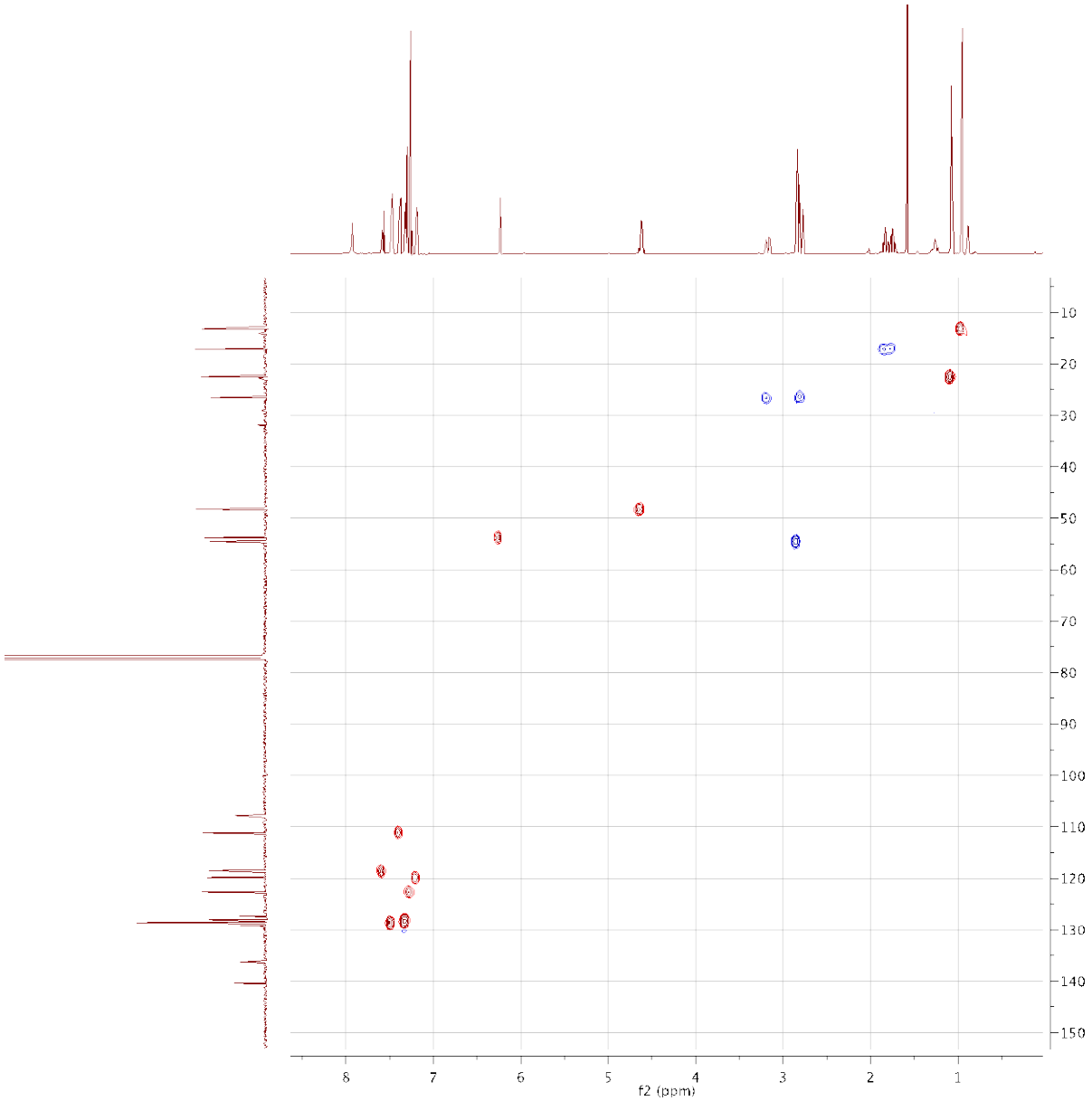
80
70
60
50
40
30
20
10
f1 (ppm)

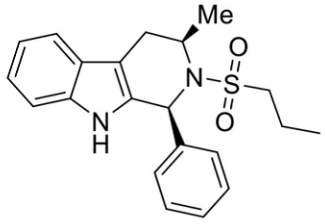


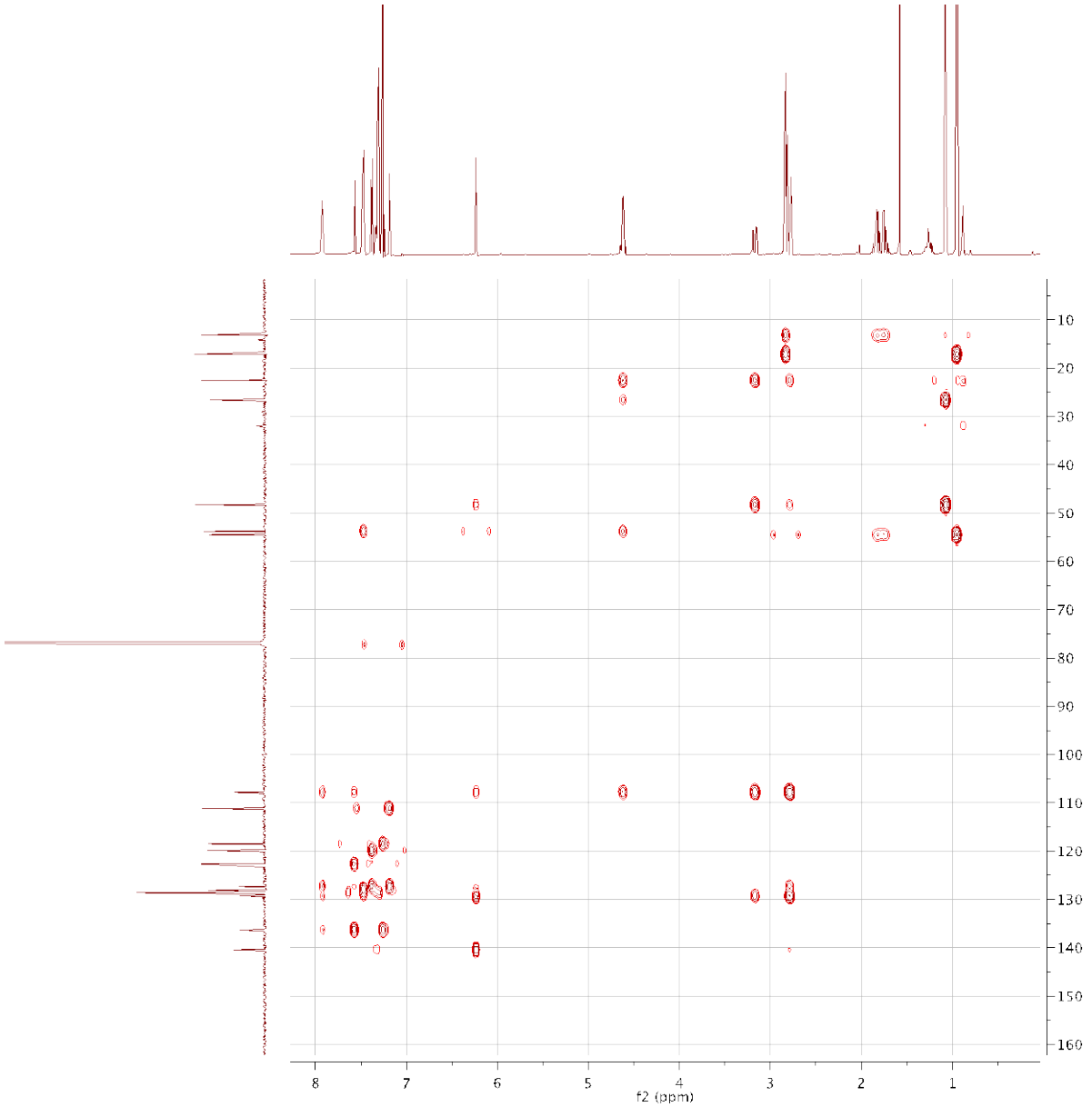
	Parameter	Value
1	Data File Name	81491872/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	CDCl3
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	9.0000
8	Presaturation Frequency	
9	Acquisition Date	2015-07-09T09:17:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(4629.6, 4629.6)
12	Lowest Frequency	(-335.6, -335.6)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



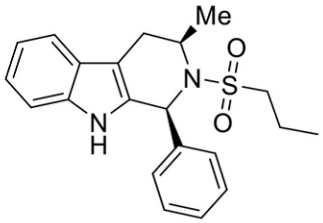


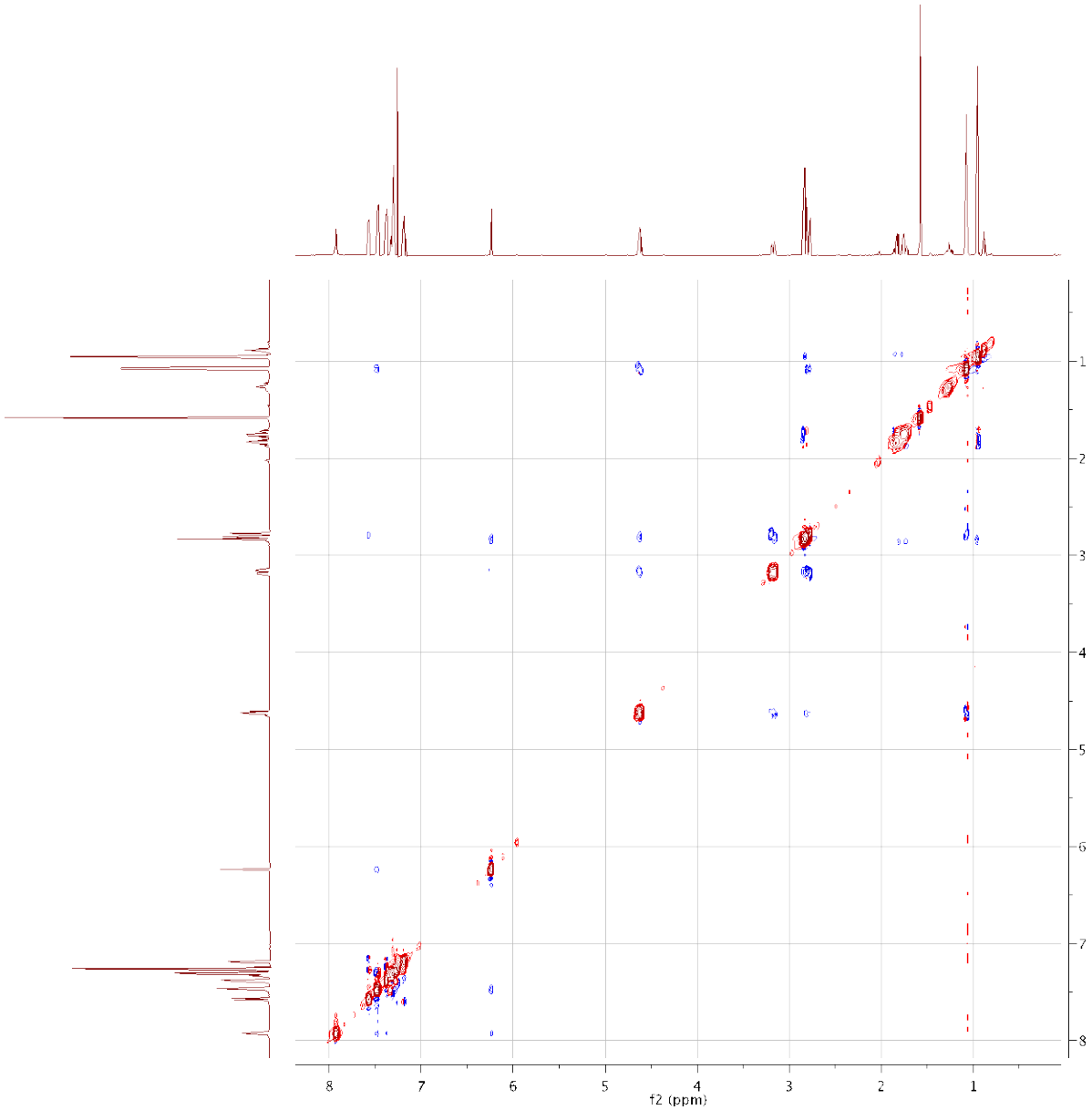
	Parameter	Value
1	Data File Name	81491872/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	CDCl3
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	9.0000
8	Presaturation Frequency	
9	Acquisition Date	2015-07-09T09:39:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



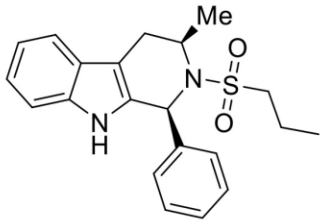


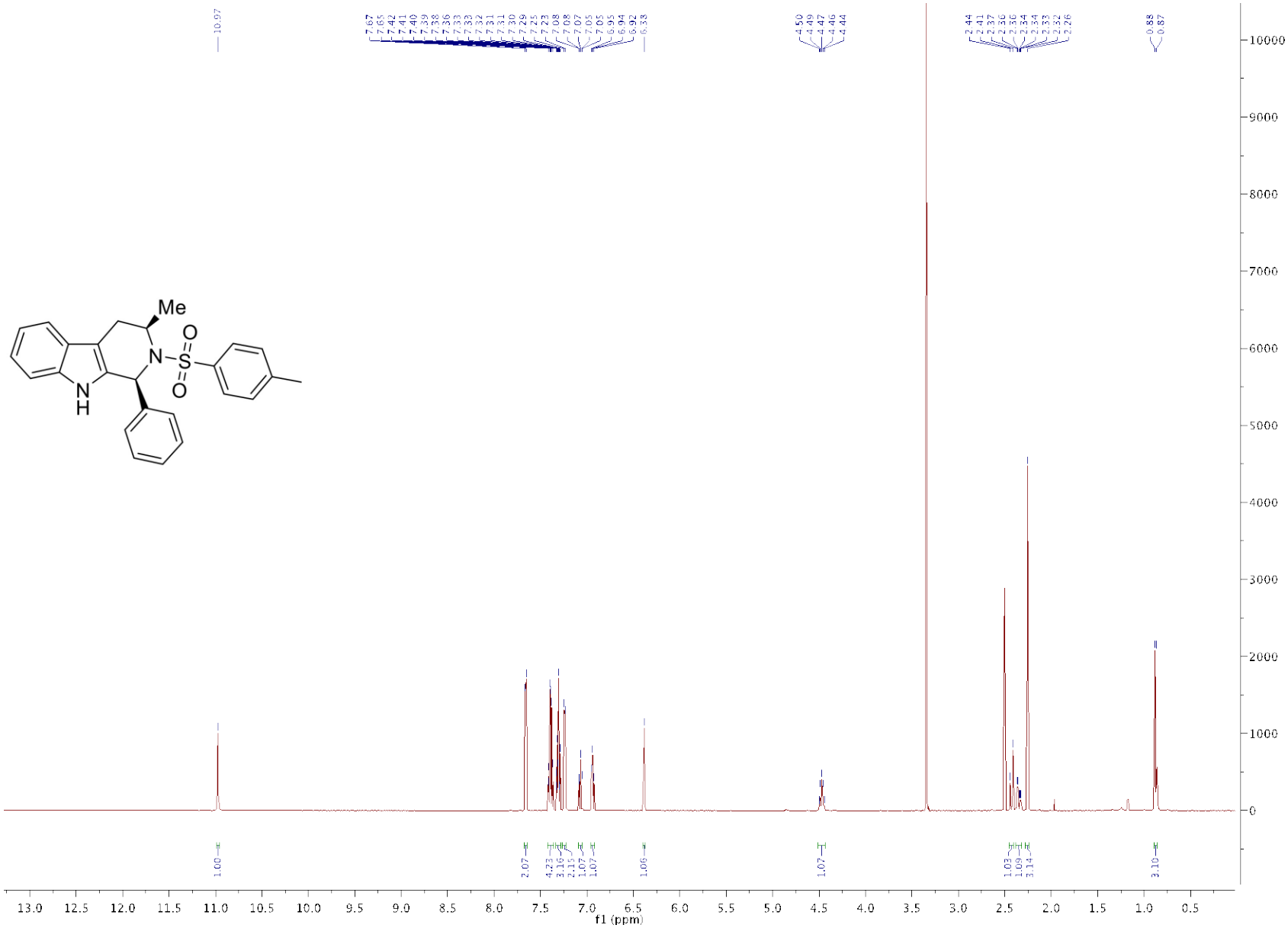
	Parameter	Value
1	Data File Name	81491872/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	CDCl3
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	9.0000
8	Presaturation Frequency	
9	Acquisition Date	2015-07-09T09:59:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(4629.6, 30120.5)
12	Lowest Frequency	(-335.6, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

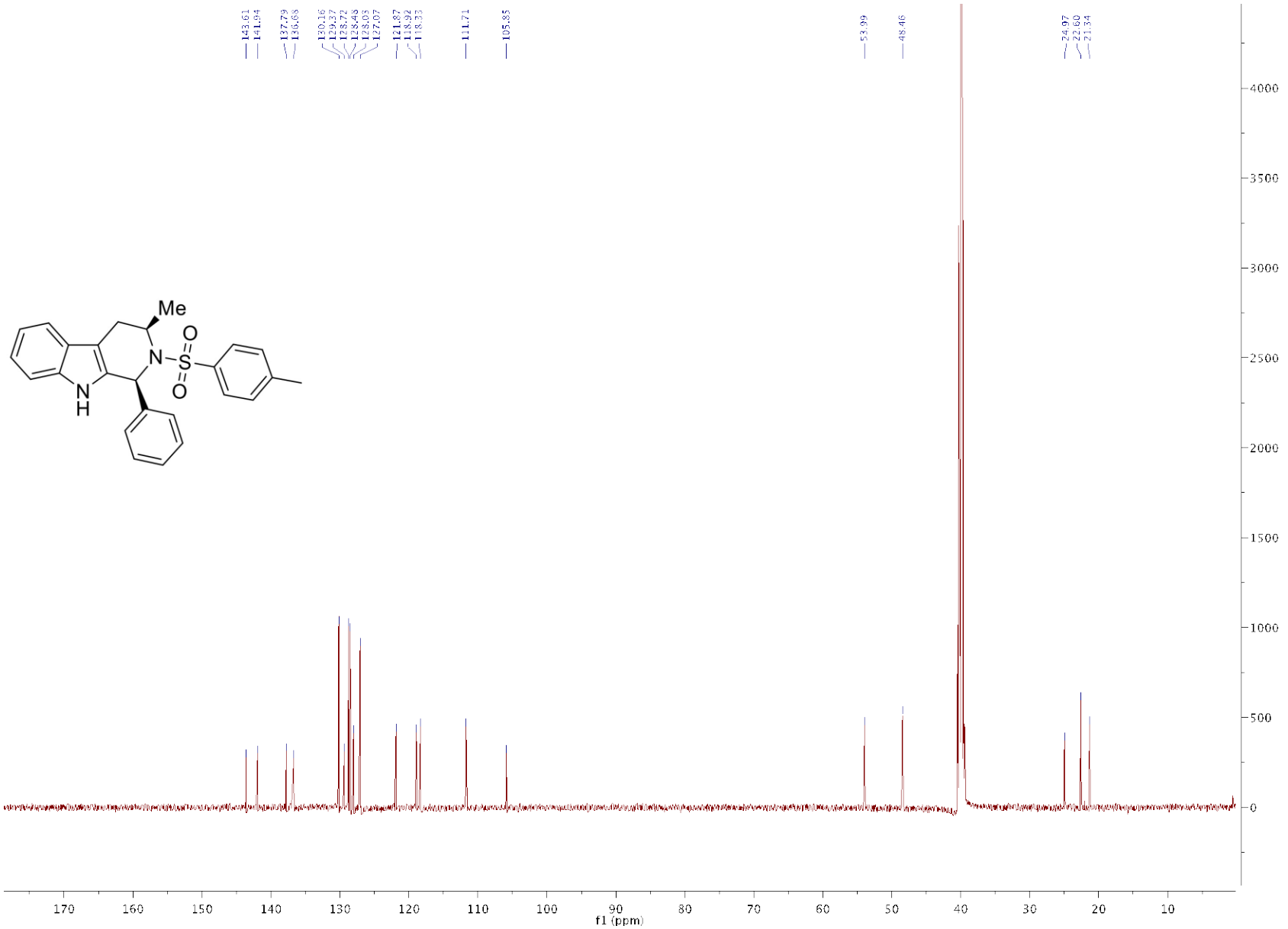




	Parameter	Value
1	Data File Name	81491872/ 16/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	CDCl3
5	Pulse Sequence	roesyphpp.2
6	Number of Scans	16
7	Pulse Width	9.0000
8	Presaturation Frequency	
9	Acquisition Date	2015-07-09T11:22:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(4672.9, 4672.9)
12	Lowest Frequency	(-368.6, -368.6)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
N
H
N
S
O
O
f1 (ppm)


143.61
141.94
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130.16
129.37
128.72
128.48
128.03
127.07
121.87
118.92
118.33
111.71
105.85
53.99
48.46
24.97
22.60
21.34
Me
N
H
O
S
O
4000
3500
3000
2500
2000
1500
1000
500
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100
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80
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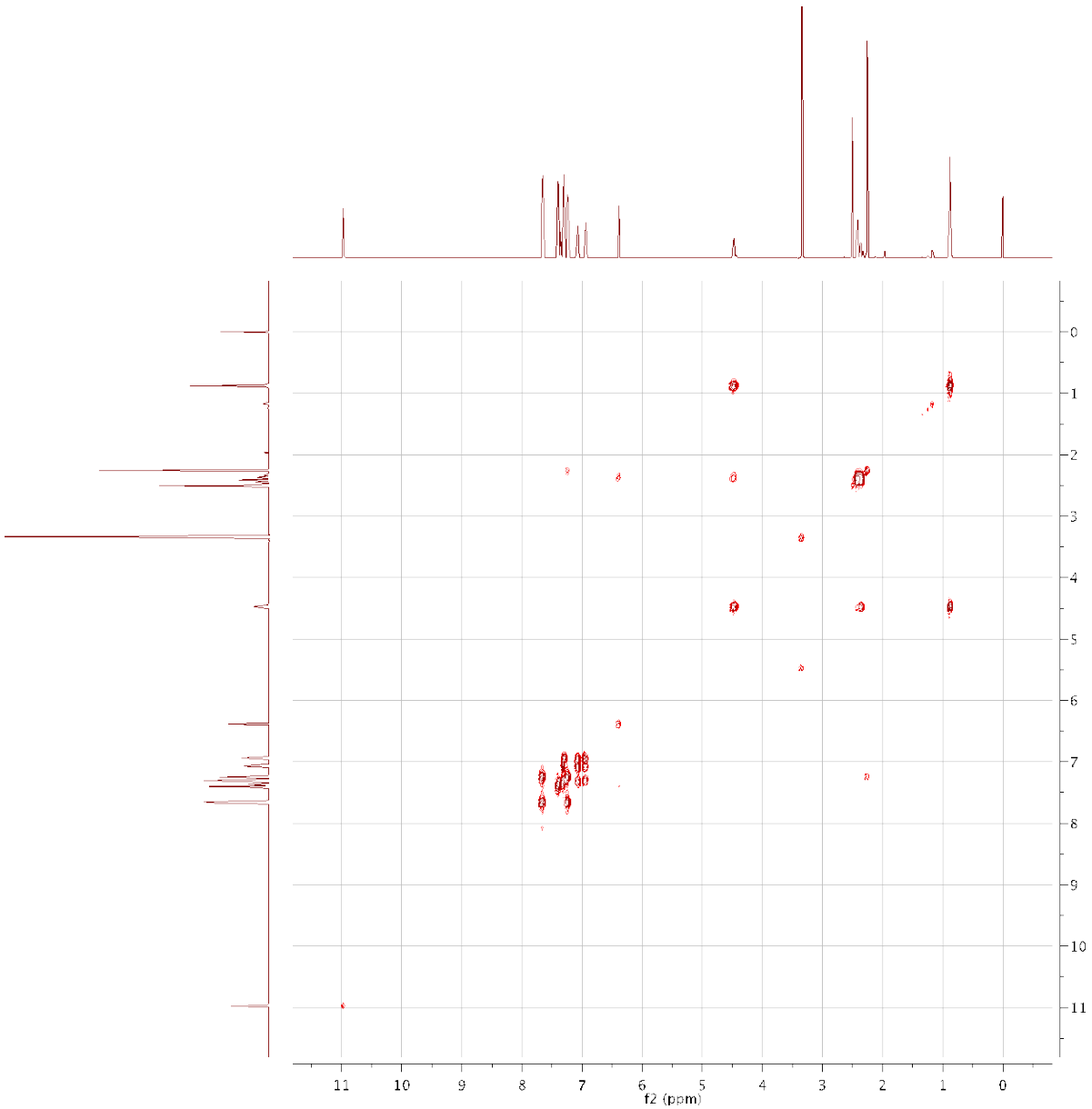
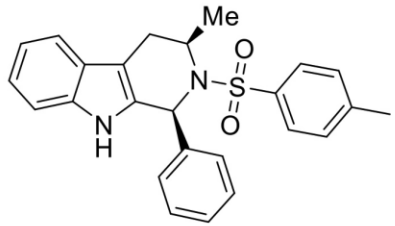
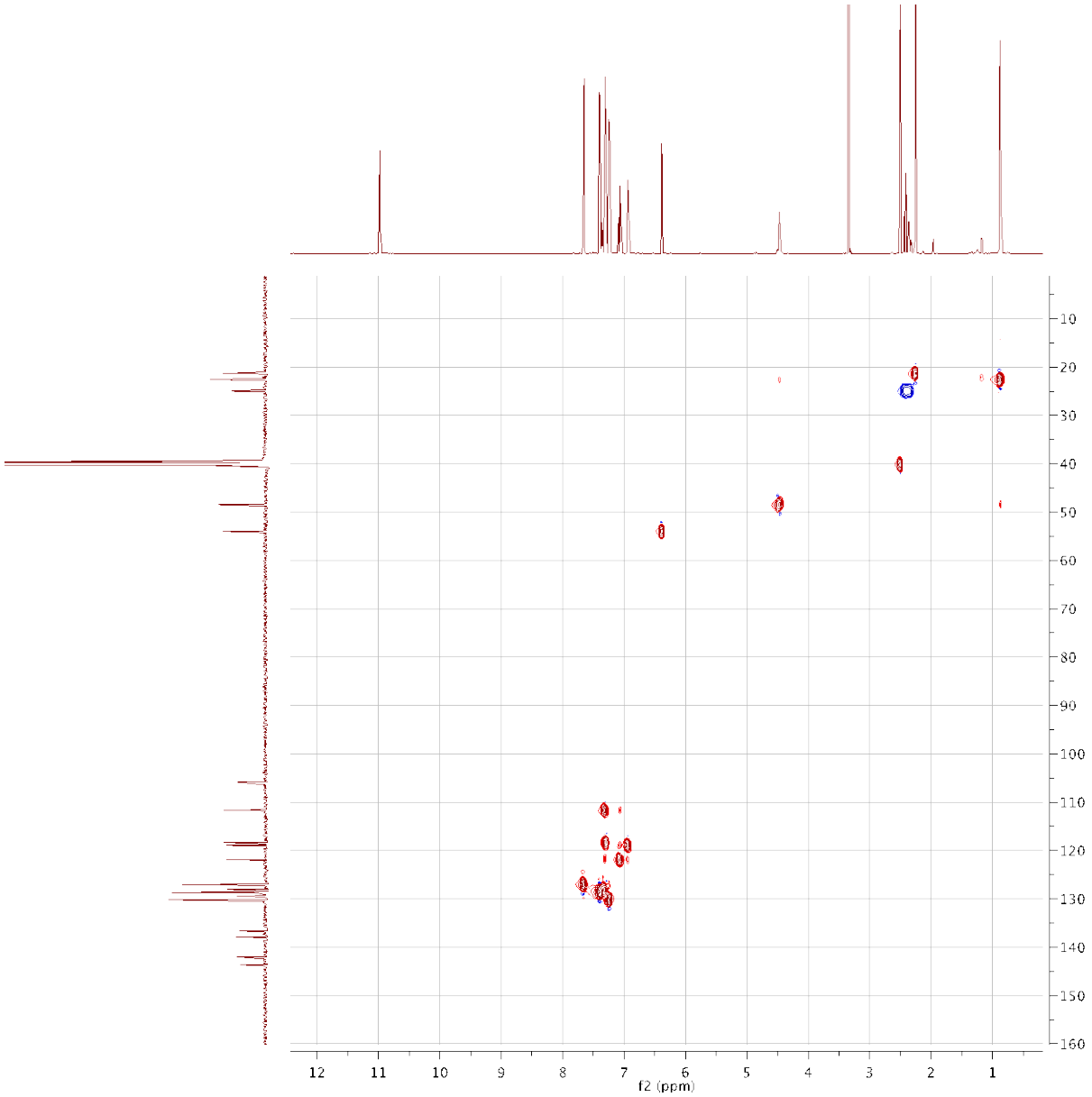
60
50
40
30
20
10
f1 (ppm)

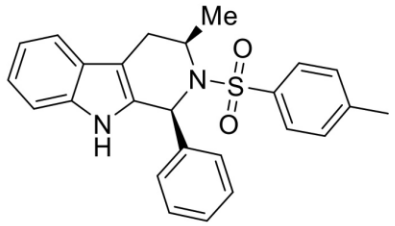


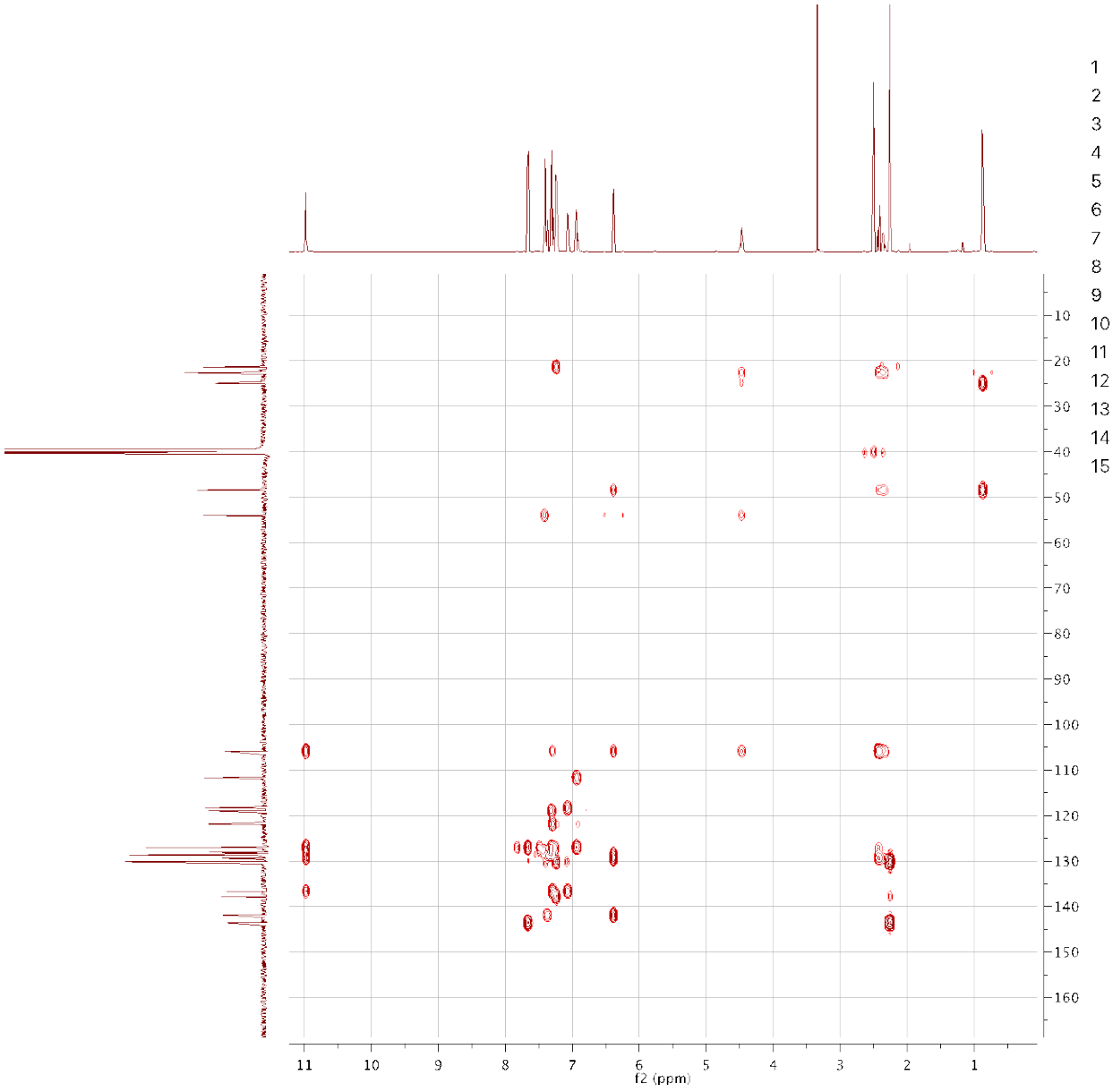
	Parameter	Value
1	Data File Name	81837747/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-07-07T01:33:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-423.0, -423.0)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



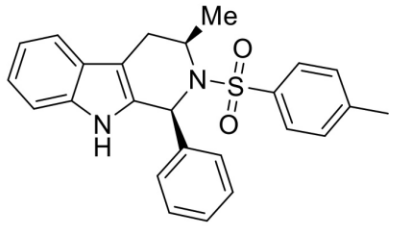


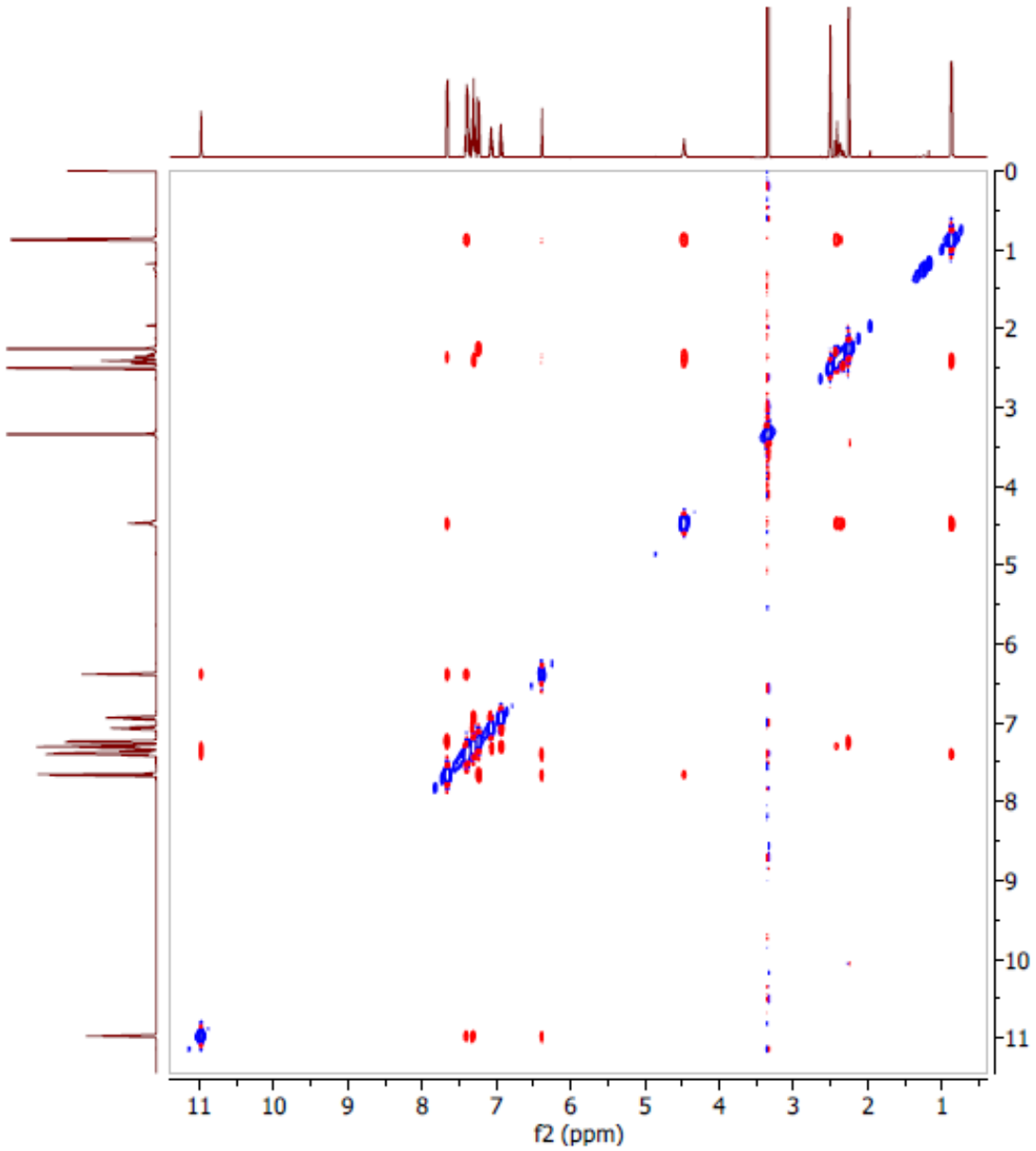
	Parameter	Value
1	Data File Name	81837747/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-07-07T01:55:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



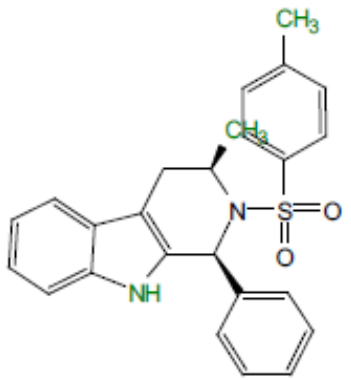


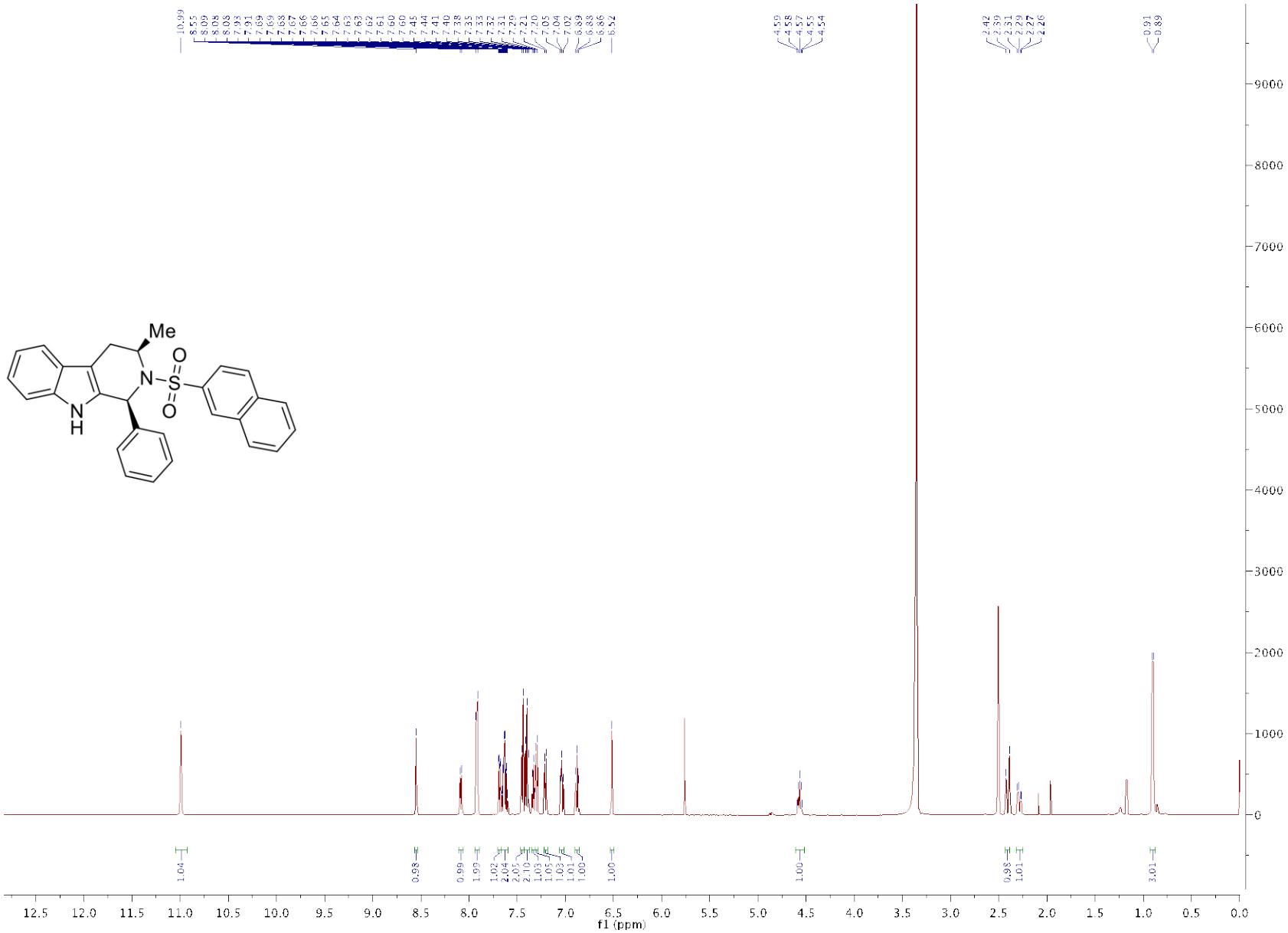
	Parameter	Value
1	Data File Name	81837747/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-07-07T02:15:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6329.1, 30120.5)
12	Lowest Frequency	(-423.0, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

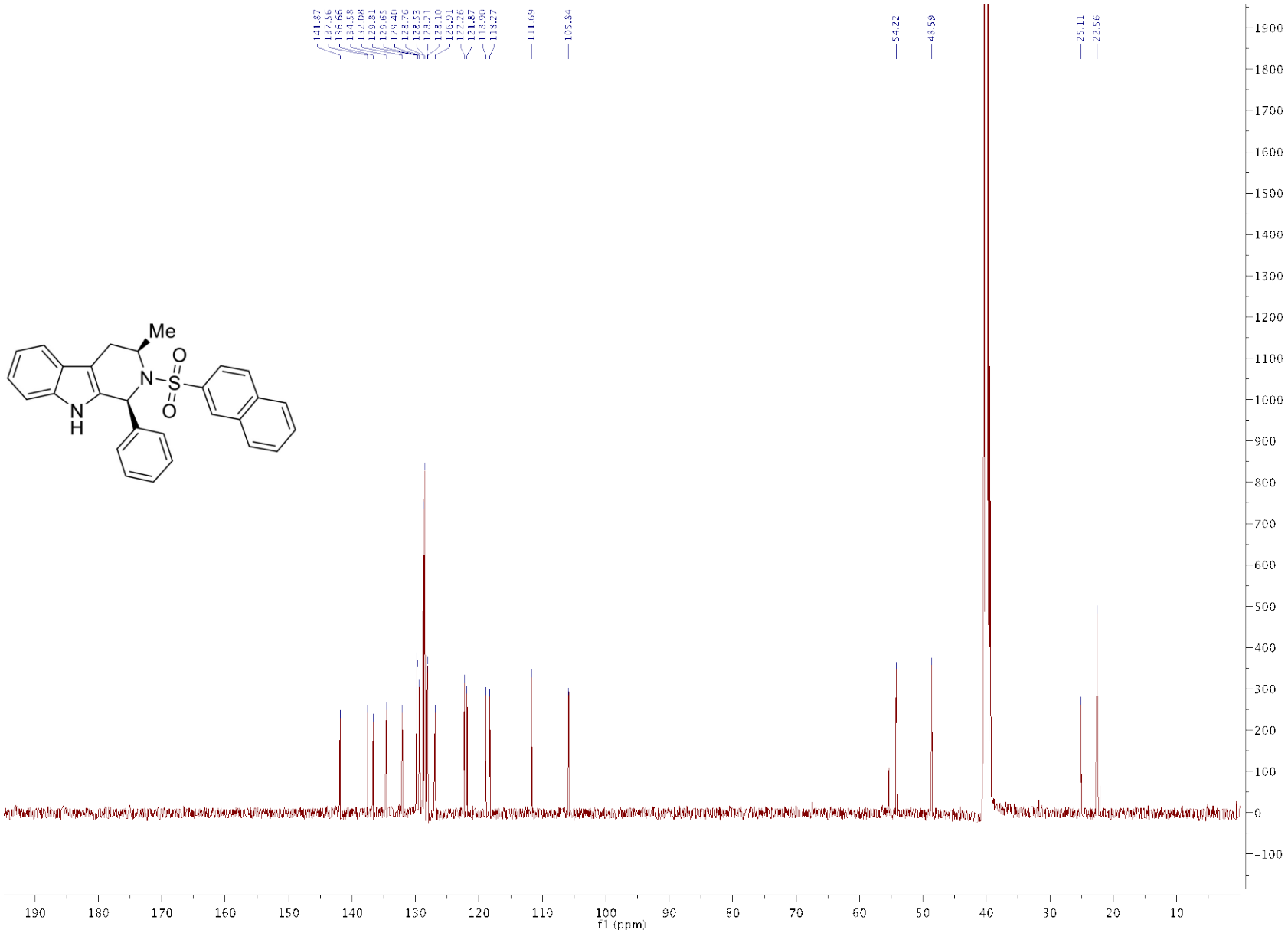




	Parameter	Value
1	Data File Name	W:/ data/ liuy55/ nmr/ 81837747/ 16/ ser
2	Sample ID	81837747
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-07-07T03:38:32
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-423.0, -423.0)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
N
S
O
O
N
H
f1 (ppm)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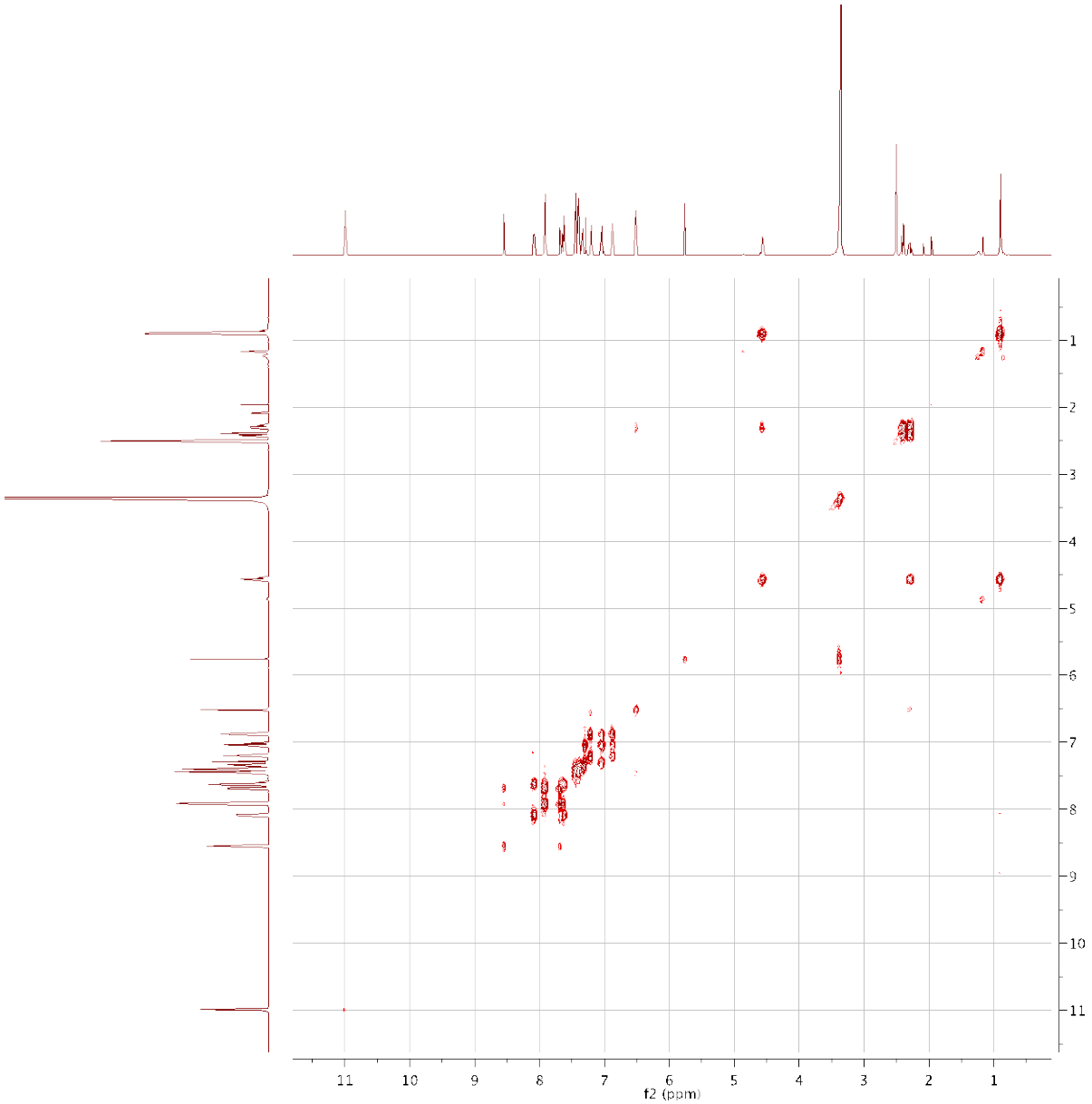
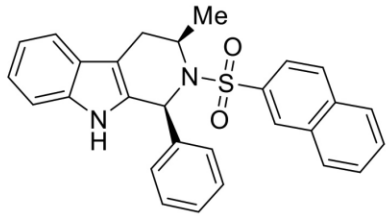
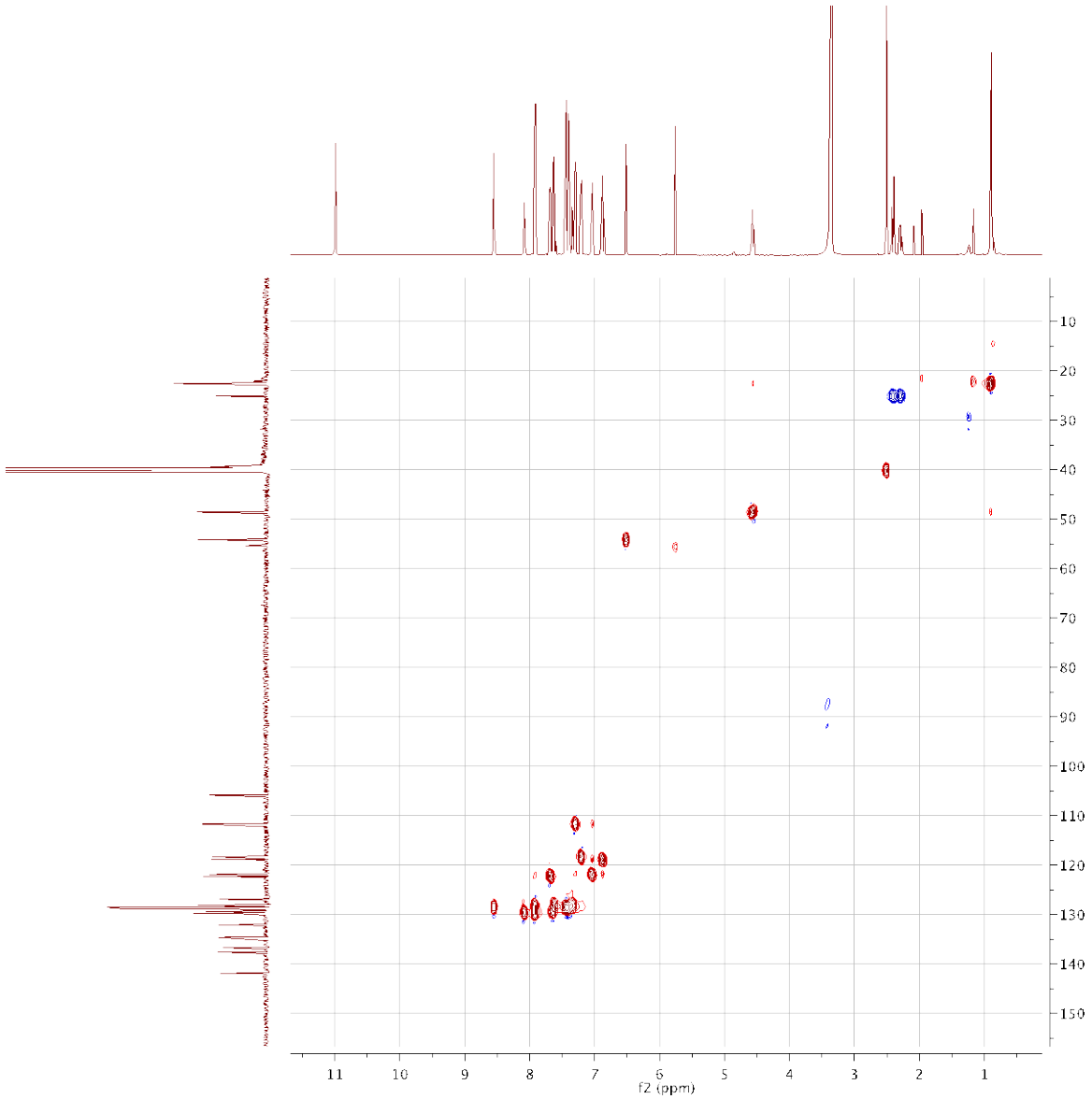
137.56
136.66
134.58
132.08
129.81
129.65
129.40
128.76
128.53
128.21
128.10
126.91
122.26
121.87
118.90
118.27
111.69
105.84
54.22
48.59
25.11
22.56
Me
N
S
O
O
N
H
f1 (ppm)

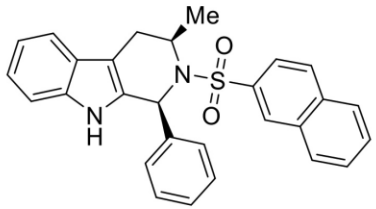


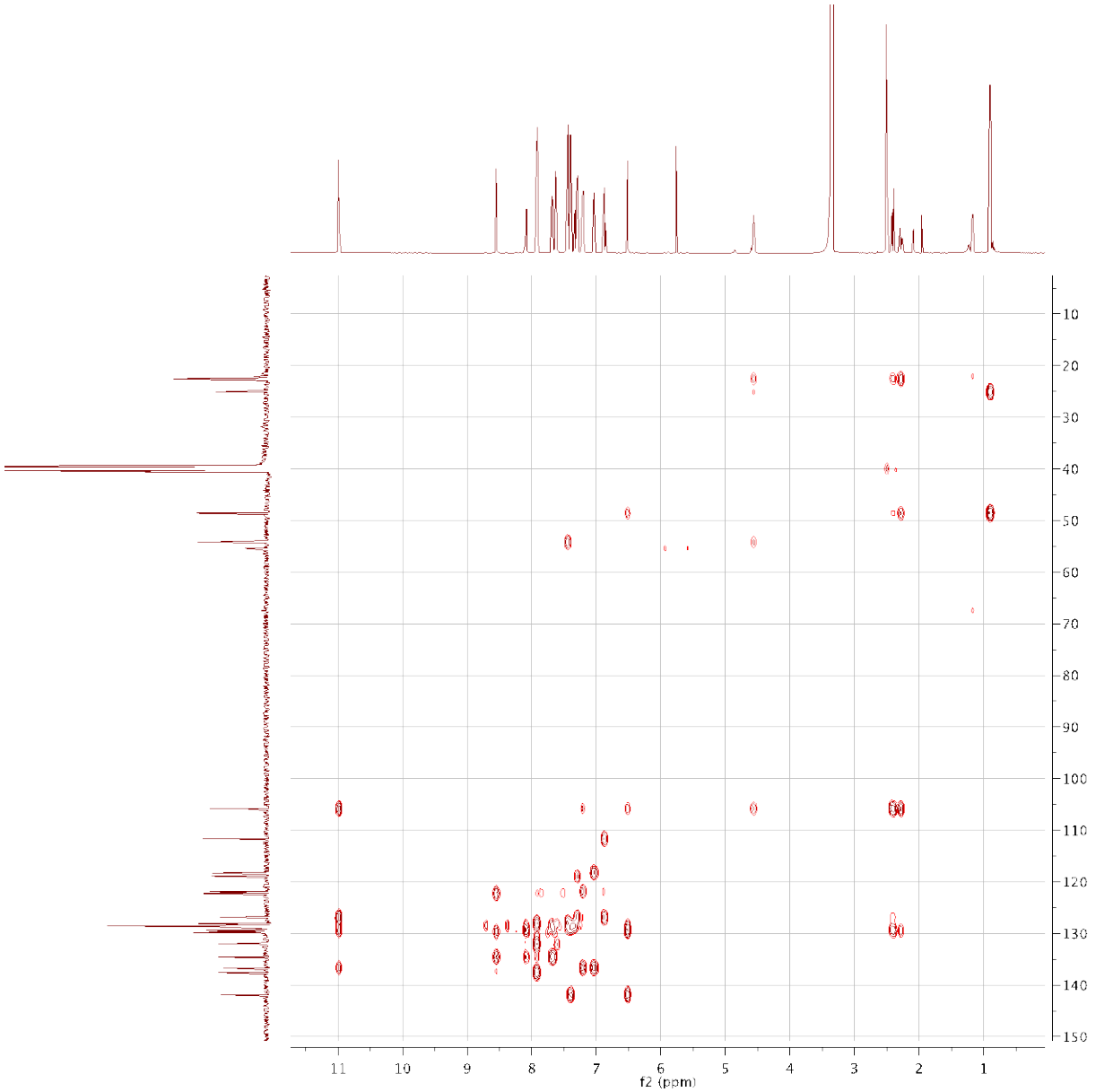
	Parameter	Value
1	Data File Name	81850332/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-07-20T20:35:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(5952.4, 5952.4)
12	Lowest Frequency	(-18.2, -18.2)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



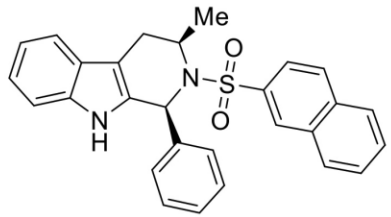


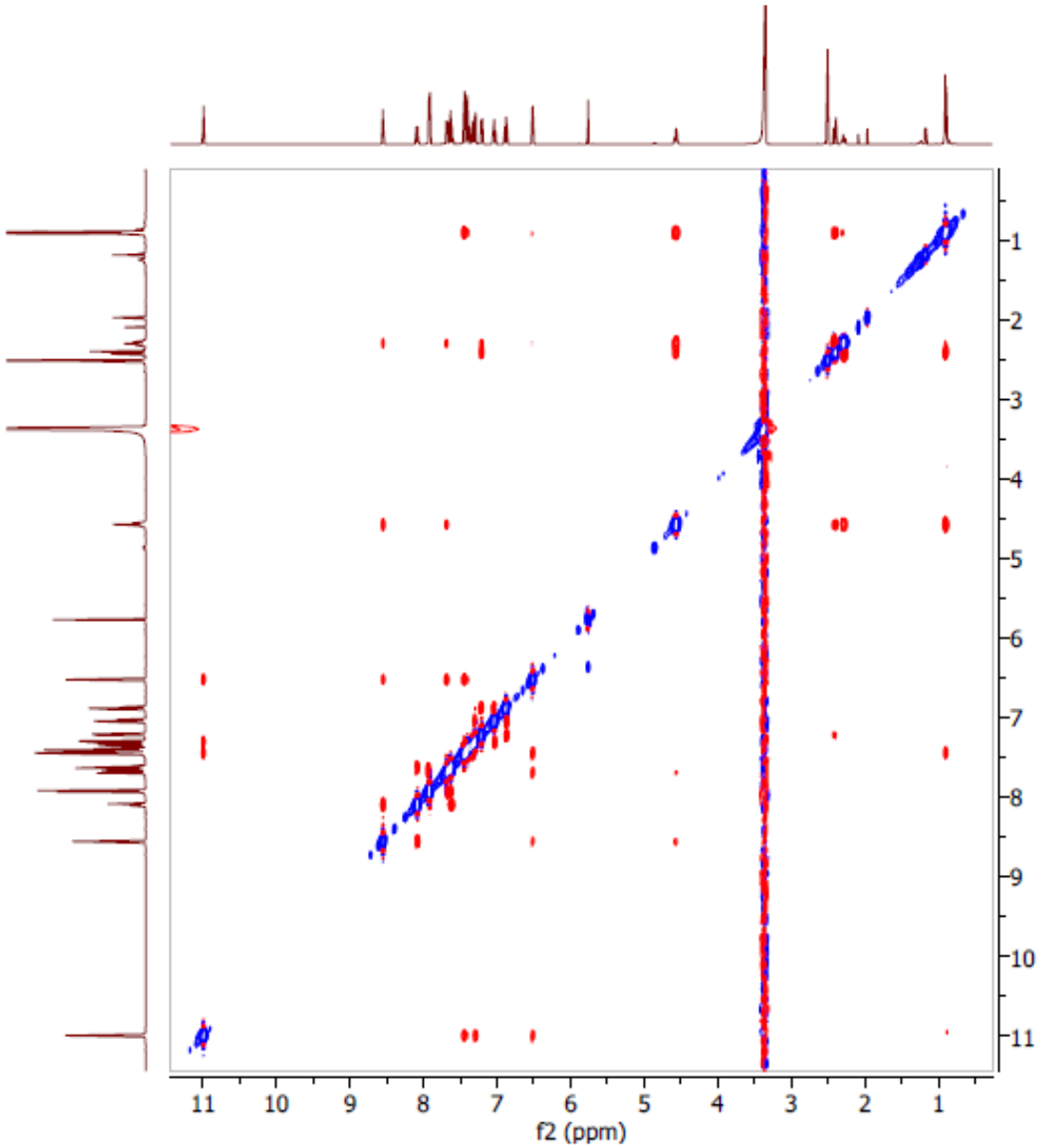
	Parameter	Value
1	Data File Name	81850332/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-07-20T20:57:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



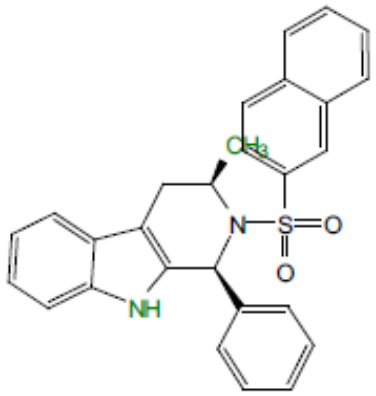


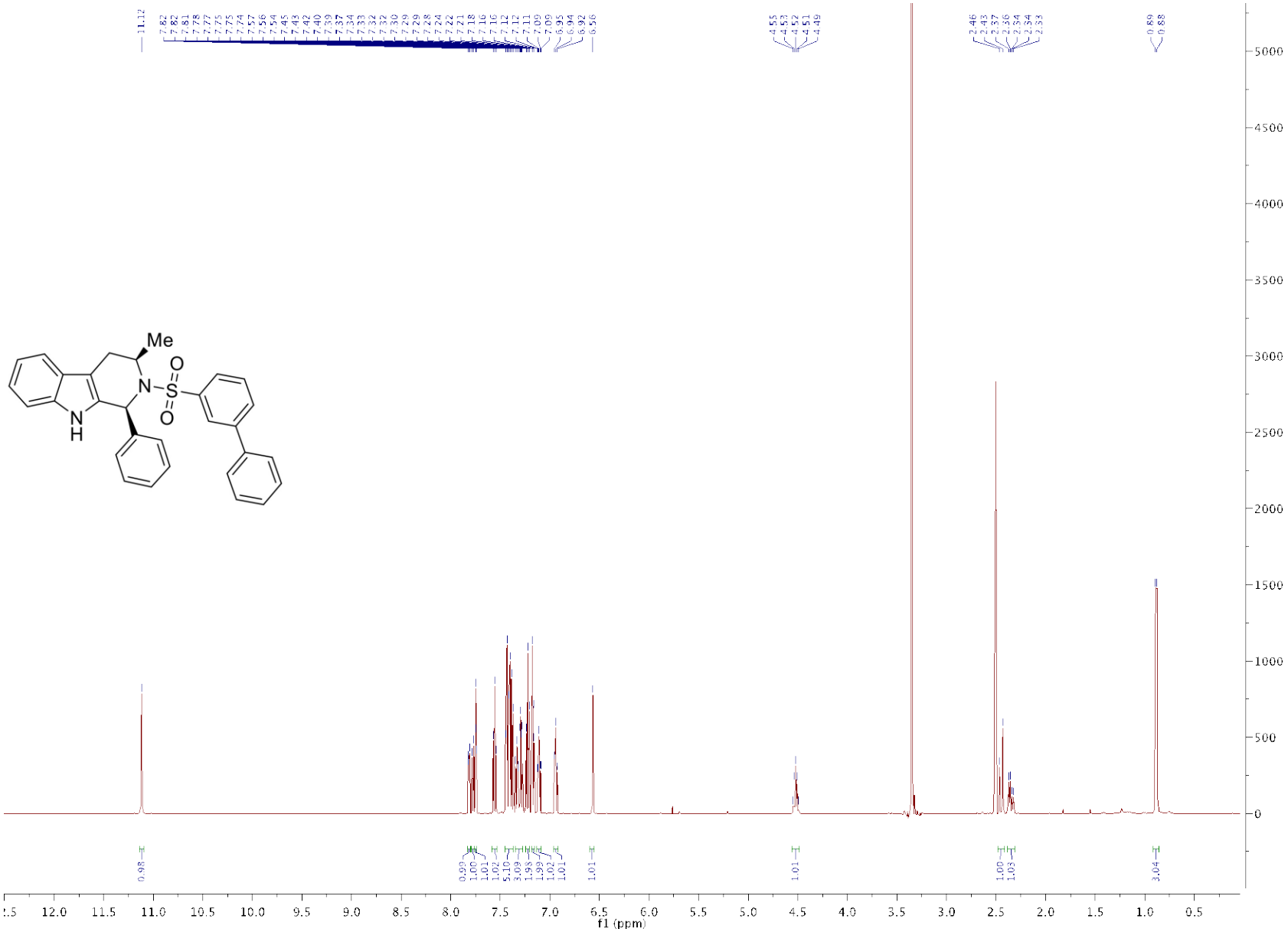
	Parameter	Value
1	Data File Name	81850332/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-07-20T21:17:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(5952.4, 30120.5)
12	Lowest Frequency	(-18.2, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)





	Parameter	Value
1	Data File Name	W:/ data/ liuy55/ nmr/ 81850332/ 16/ ser
2	Sample ID	81850332
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-07-20T22:40:34
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(5952.4, 5952.4)
12	Lowest Frequency	(-18.2, -18.2)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)

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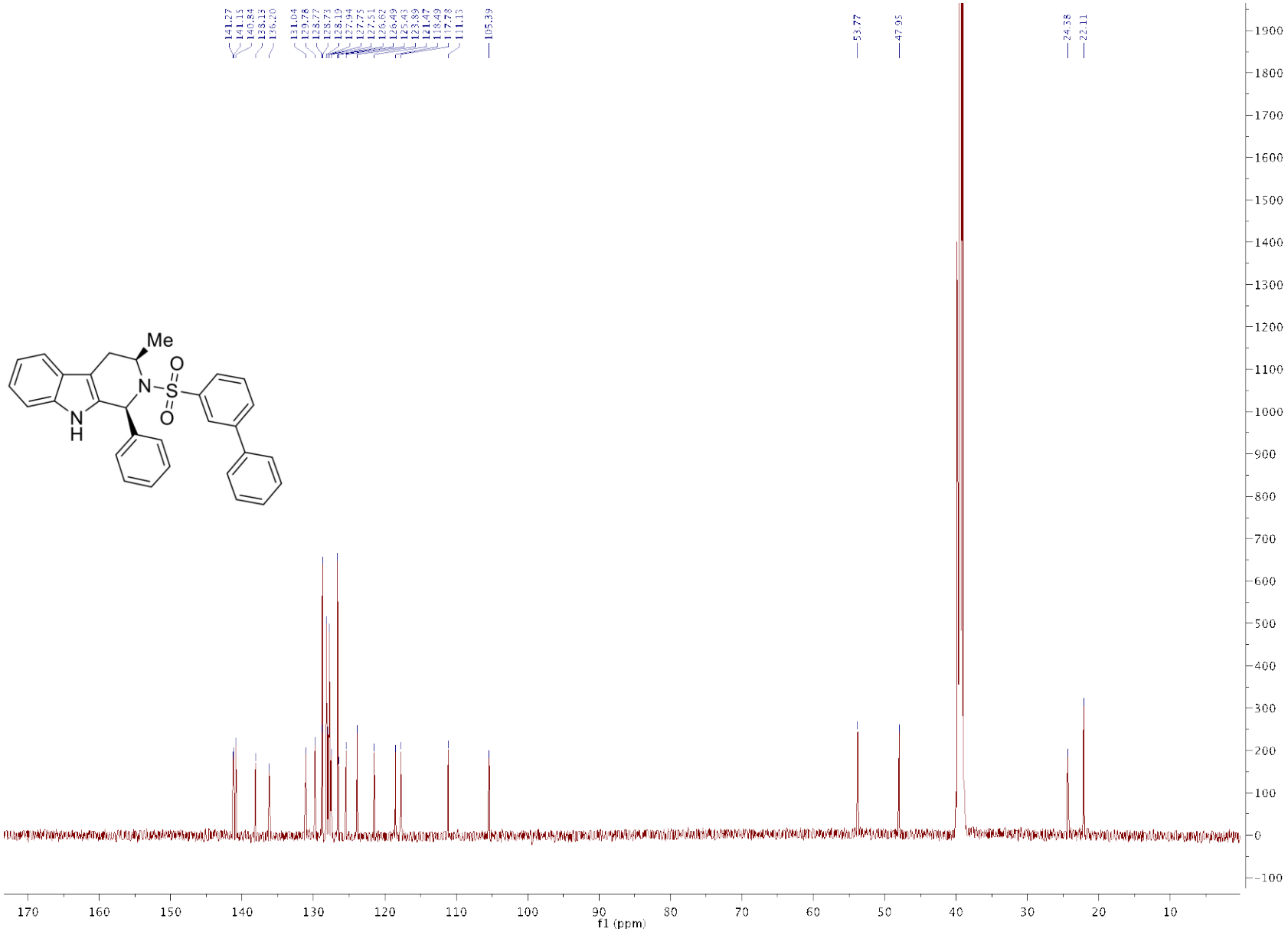
7.82
7.81
7.78
7.77
7.75
7.75
7.74
7.57
7.56
7.54
7.45
7.43
7.42
7.40
7.39
7.37
7.34
7.33
7.32
7.32
7.30
7.29
7.29
7.28
7.24
7.22
7.21
7.18
7.16
7.16
7.12
7.12
7.11
7.09
7.09
6.95
6.94
6.92
6.56
4.55
4.53
4.52
4.51
4.49
2.46
2.43
2.37
2.36
2.34
2.34
2.33
0.89
0.88
Me
N
S
O
O
N
H
0.98
0.99
1.00
1.01
1.02
5.10
3.09
1.98
1.99
1.02
1.01
1.01
1.01
1.00
1.03
3.04
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
f1 (ppm)


141.27
141.15
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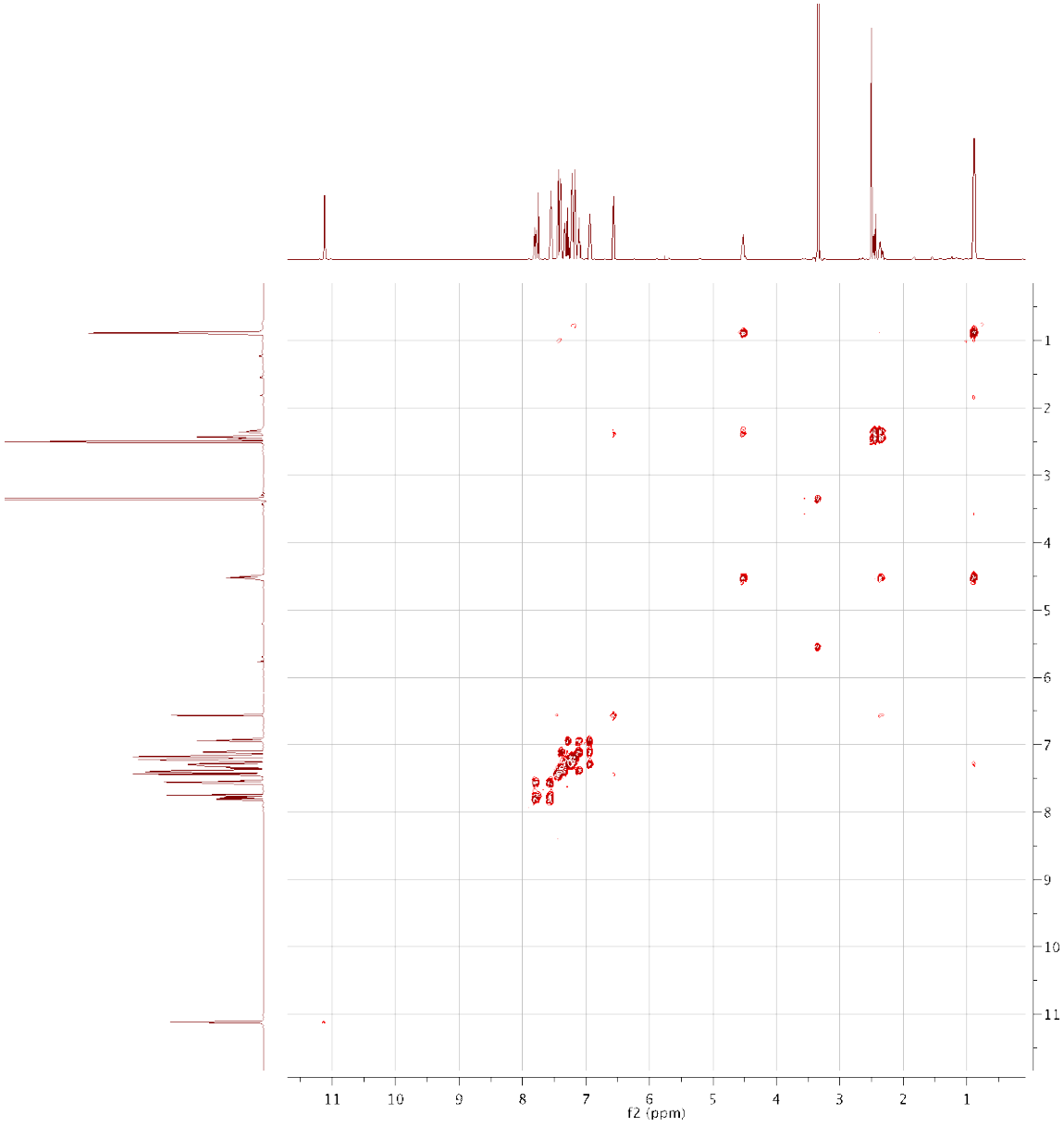
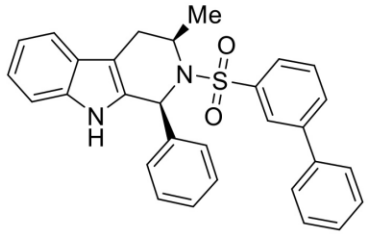
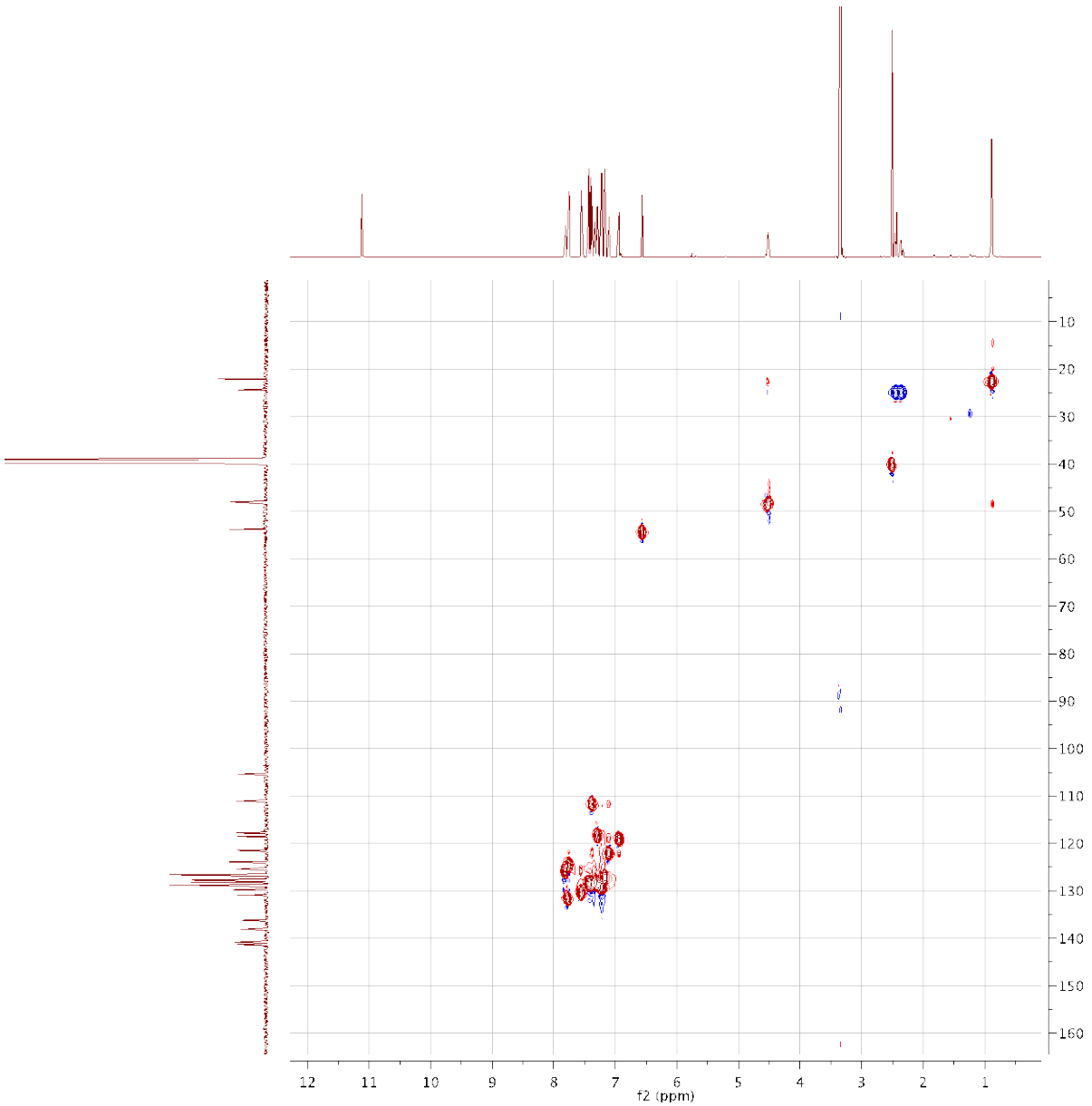
138.13
136.20
131.04
129.78
128.77
128.73
128.19
127.94
127.75
127.51
126.62
126.49
125.43
123.89
121.47
118.49
117.78
111.15
105.39
53.77
47.95
24.38
22.11
Me
O
N
S
O
N
H
f1 (ppm)

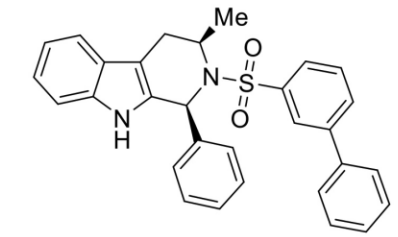


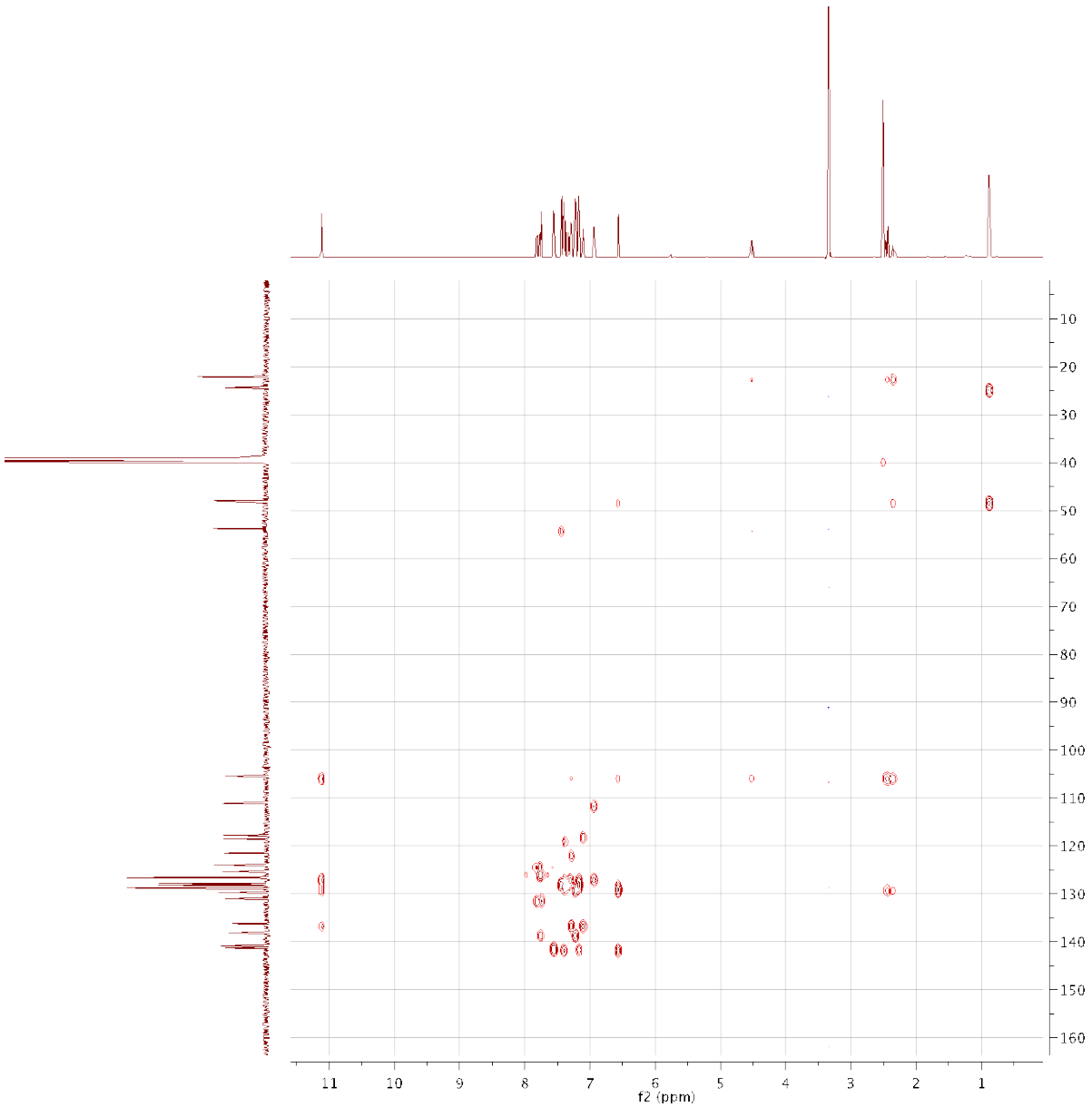
	Parameter	Value
1	Data File Name	81863425/ 13/ pdata/ 1/ 2rr
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T08:14:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6410.3, 6410.3)
12	Lowest Frequency	(-431.3, -431.3)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



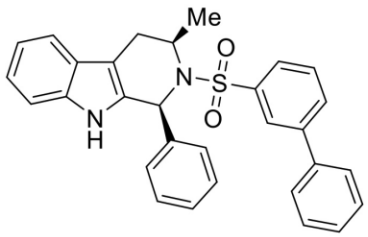


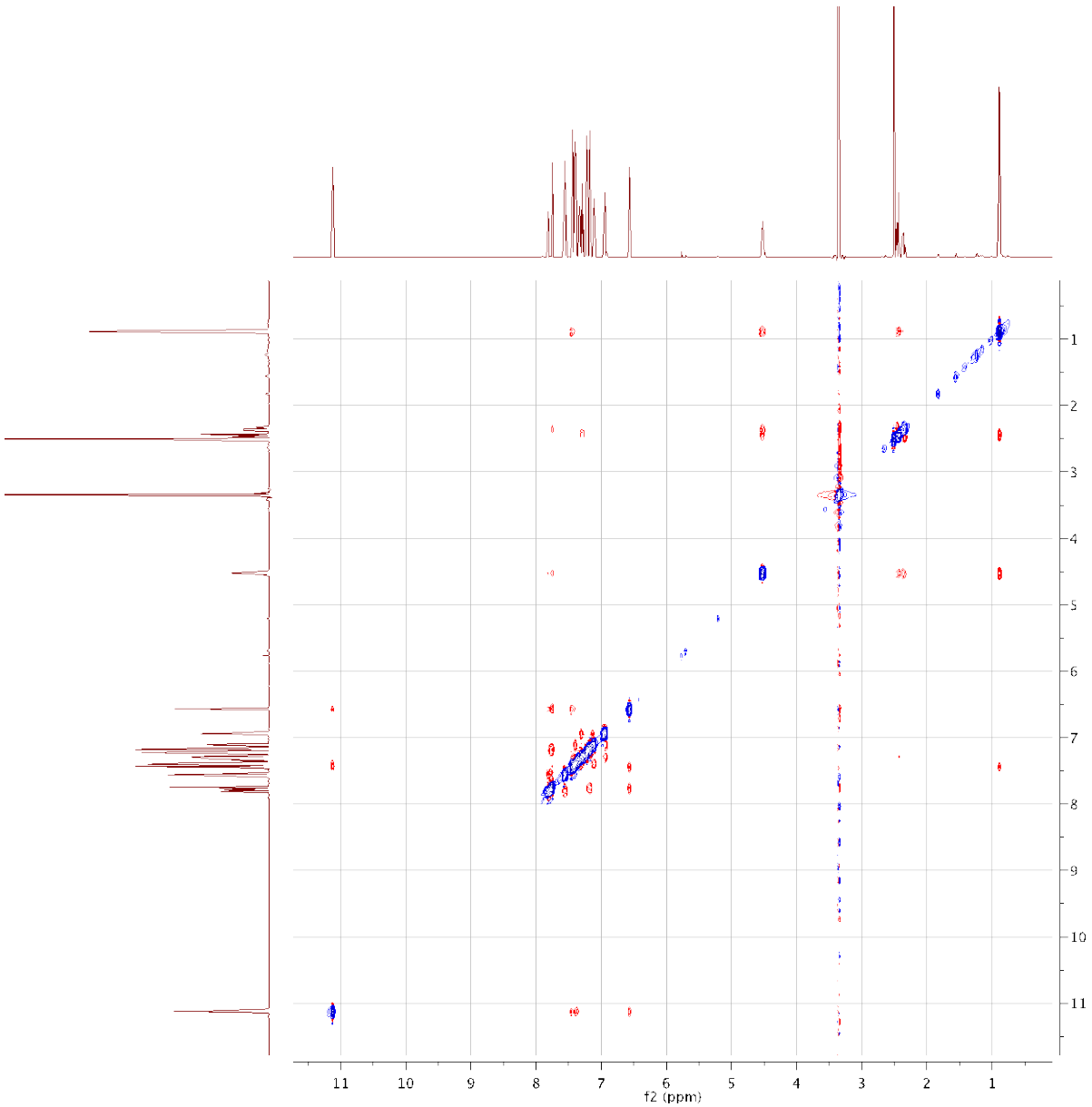
	Parameter	Value
1	Data File Name	81863425/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T08:36:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



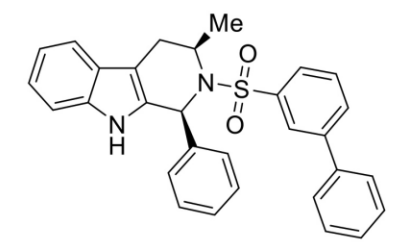


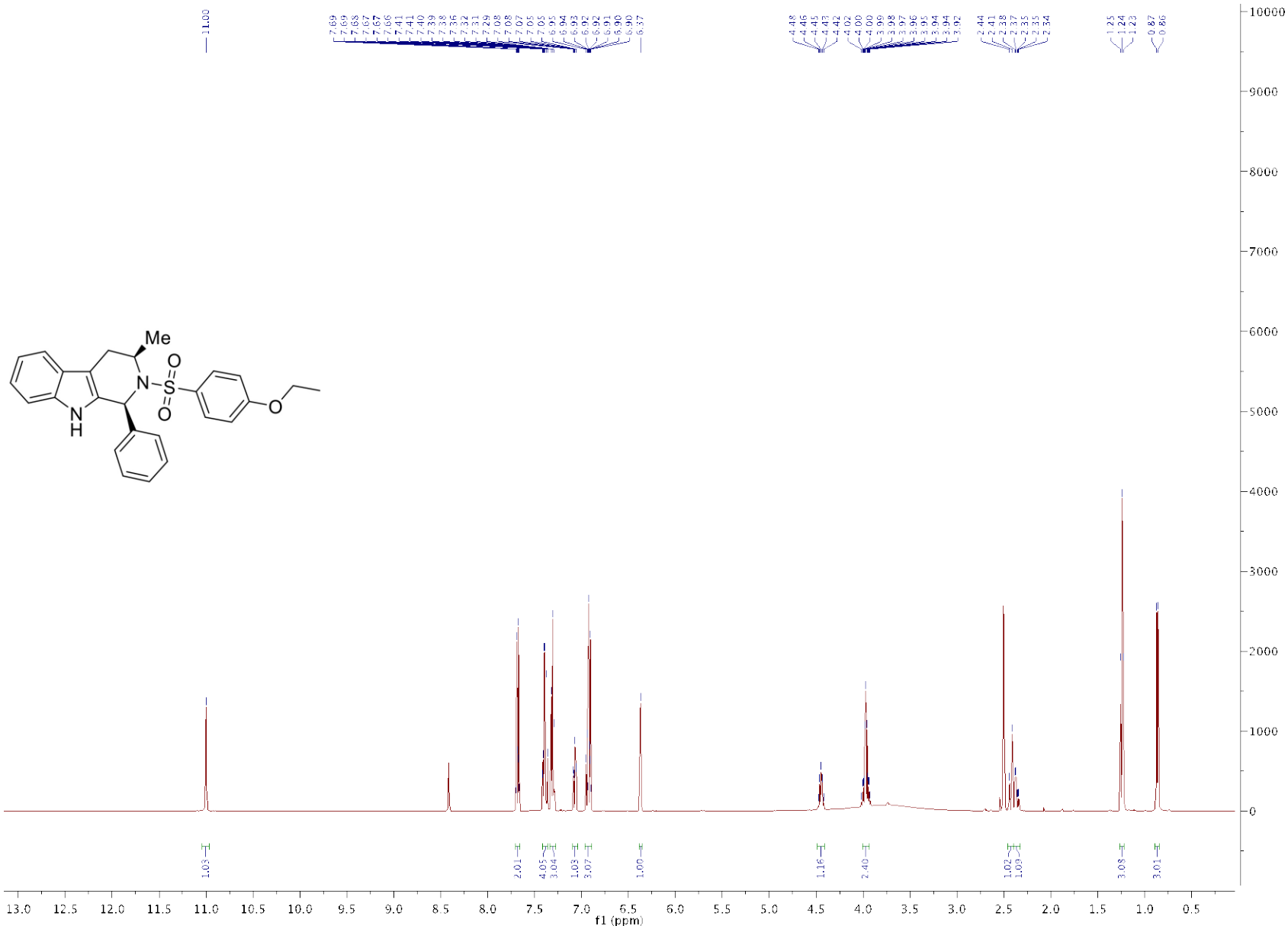
	Parameter	Value
1	Data File Name	81863425/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T08:56:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6410.3, 30120.5)
12	Lowest Frequency	(-431.3, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

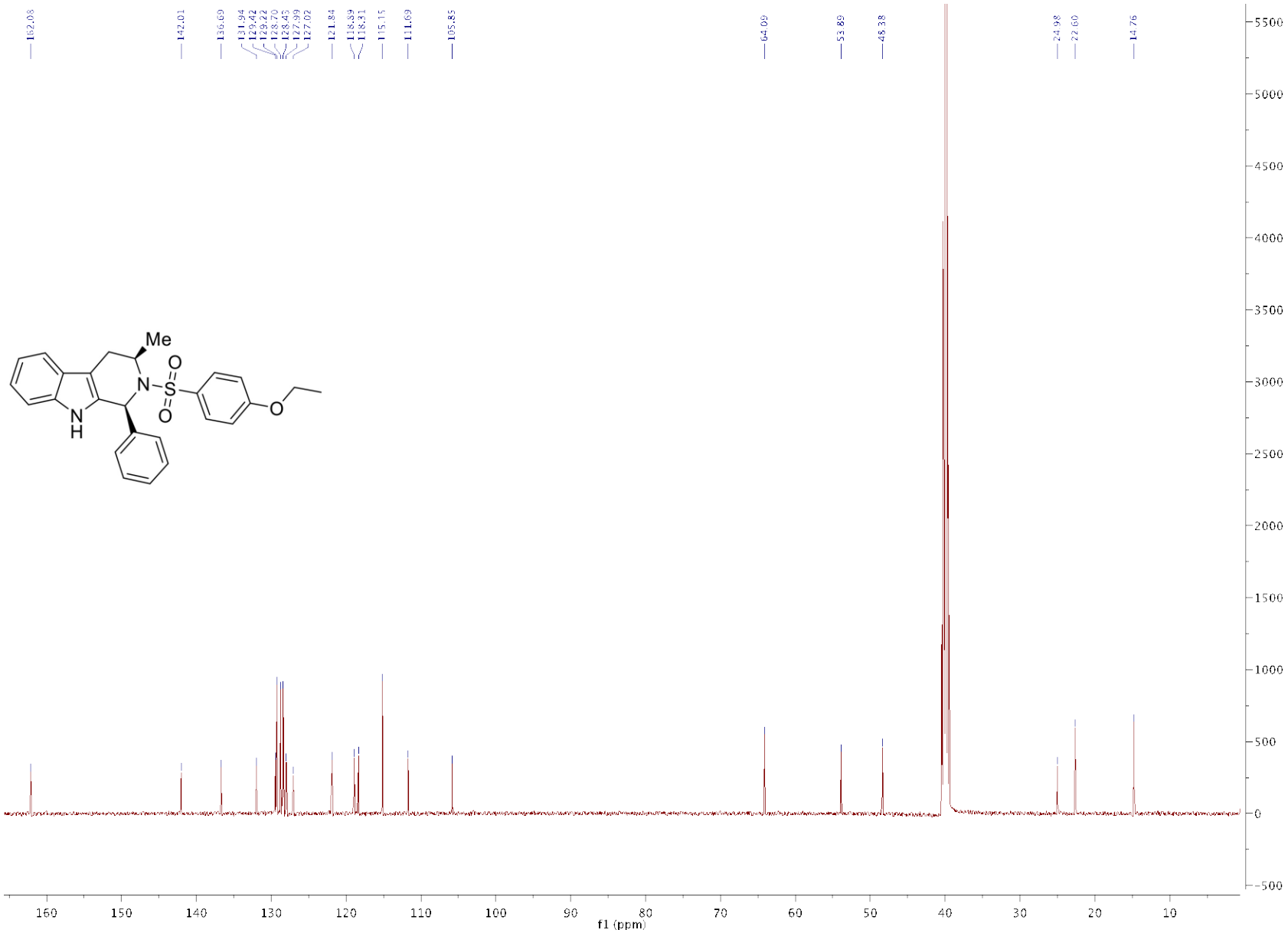




	Parameter	Value
1	Data File Name	81863425/ 16/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	roesyphpp.2
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T10:19:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6410.3, 6410.3)
12	Lowest Frequency	(-431.3, -431.3)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
O
N
S
O
N
H
O
f1 (ppm)


162.08
142.01
136.69
131.94
129.42
128.72
128.70
128.43
127.99
127.02
121.84
118.39
118.31
115.15
111.69
105.85
64.09
53.89
45.38
24.98
22.60
14.76
Me
O
N
S
O
O
N
H
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
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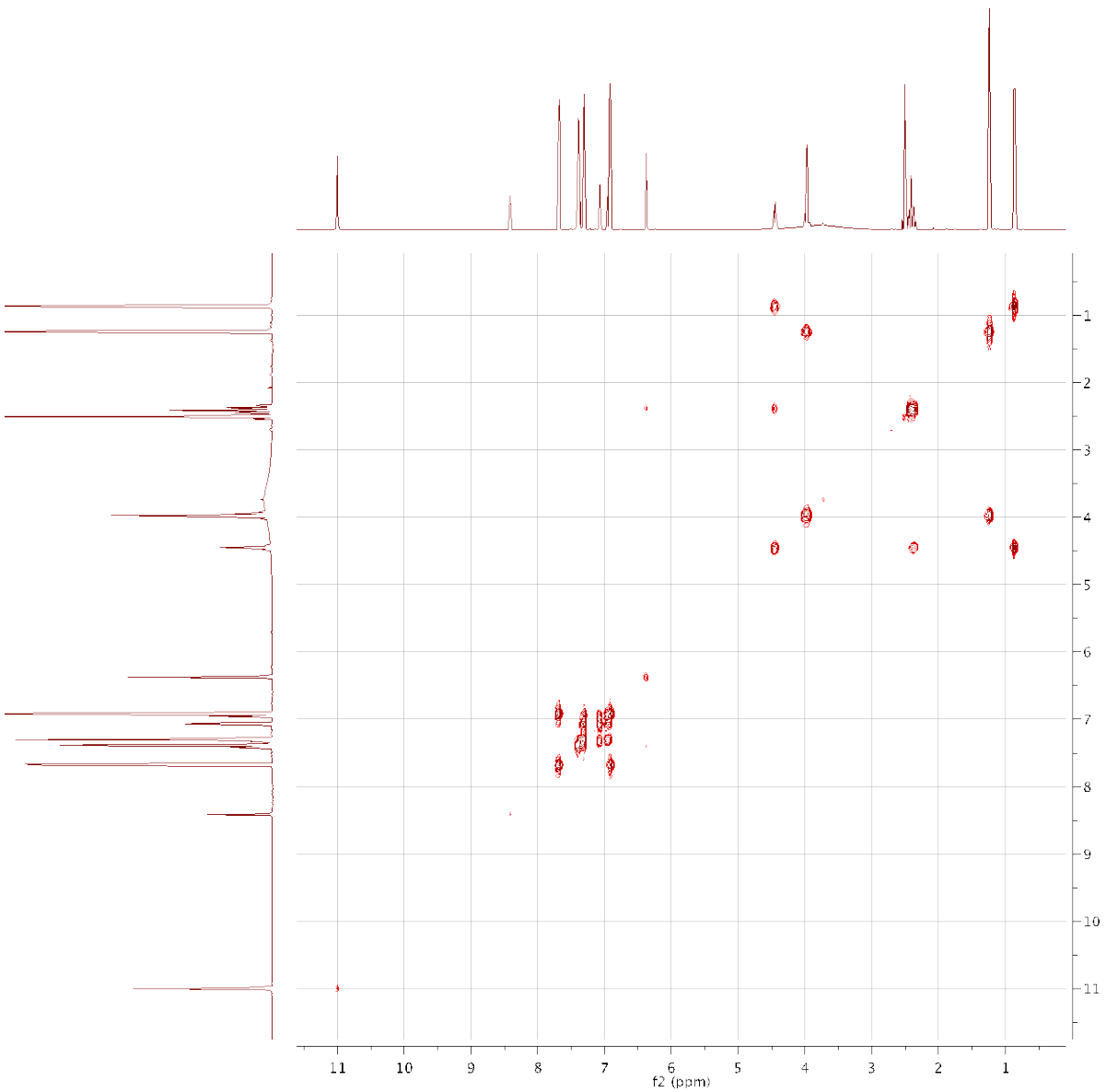
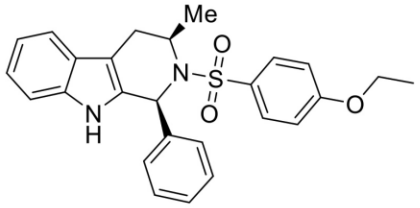
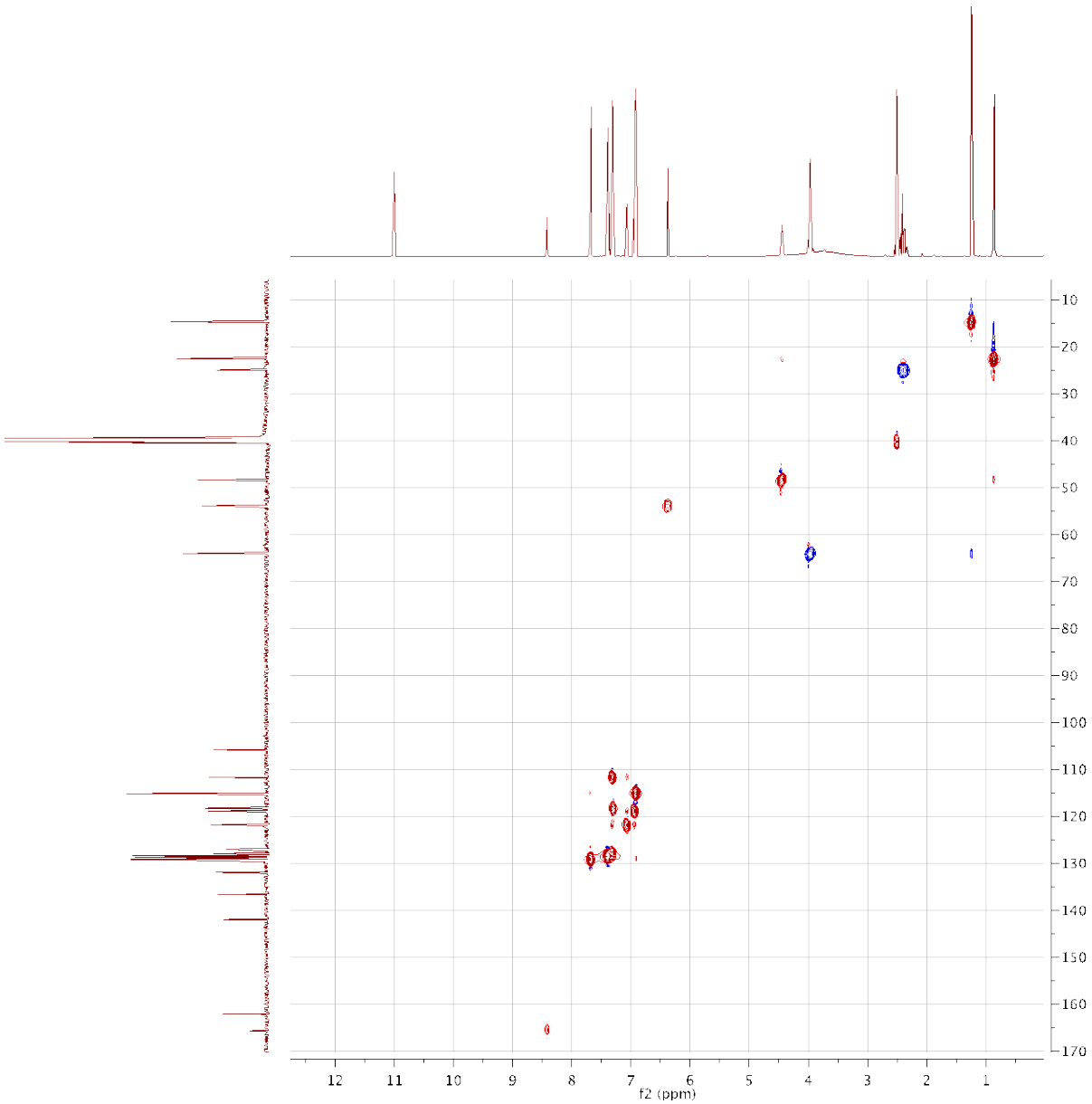
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

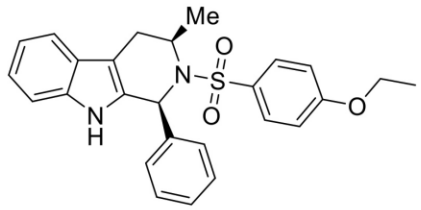


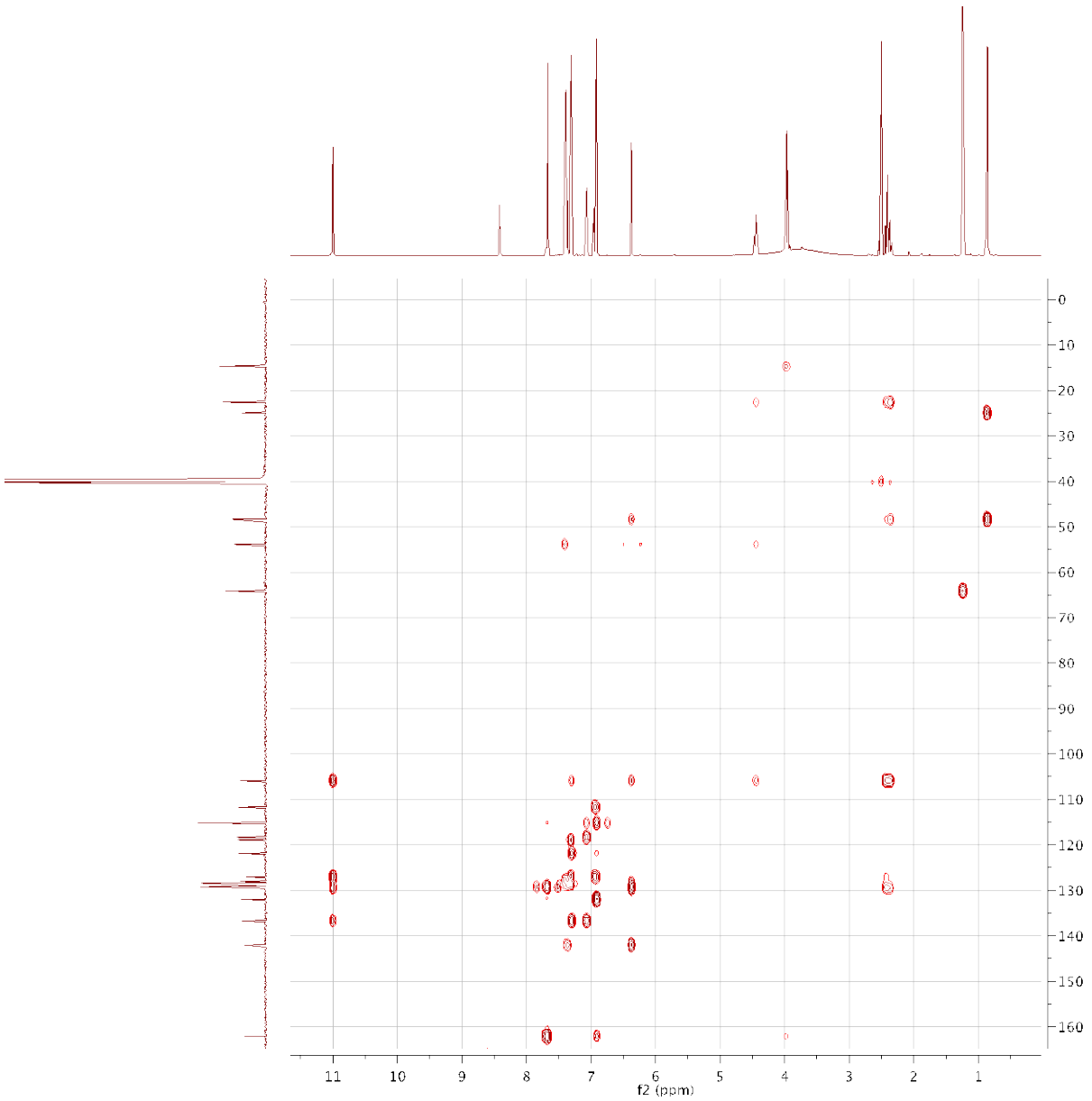
	Parameter	Value
1	Data File Name	81863285/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T15:12:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6493.5, 6493.5)
12	Lowest Frequency	(-413.8, -413.8)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)





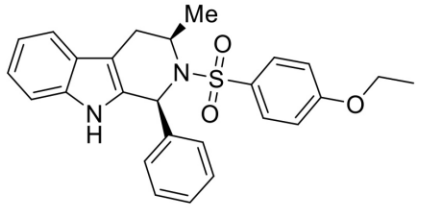
	Parameter	Value
1	Data File Name	81863285/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T15:33:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

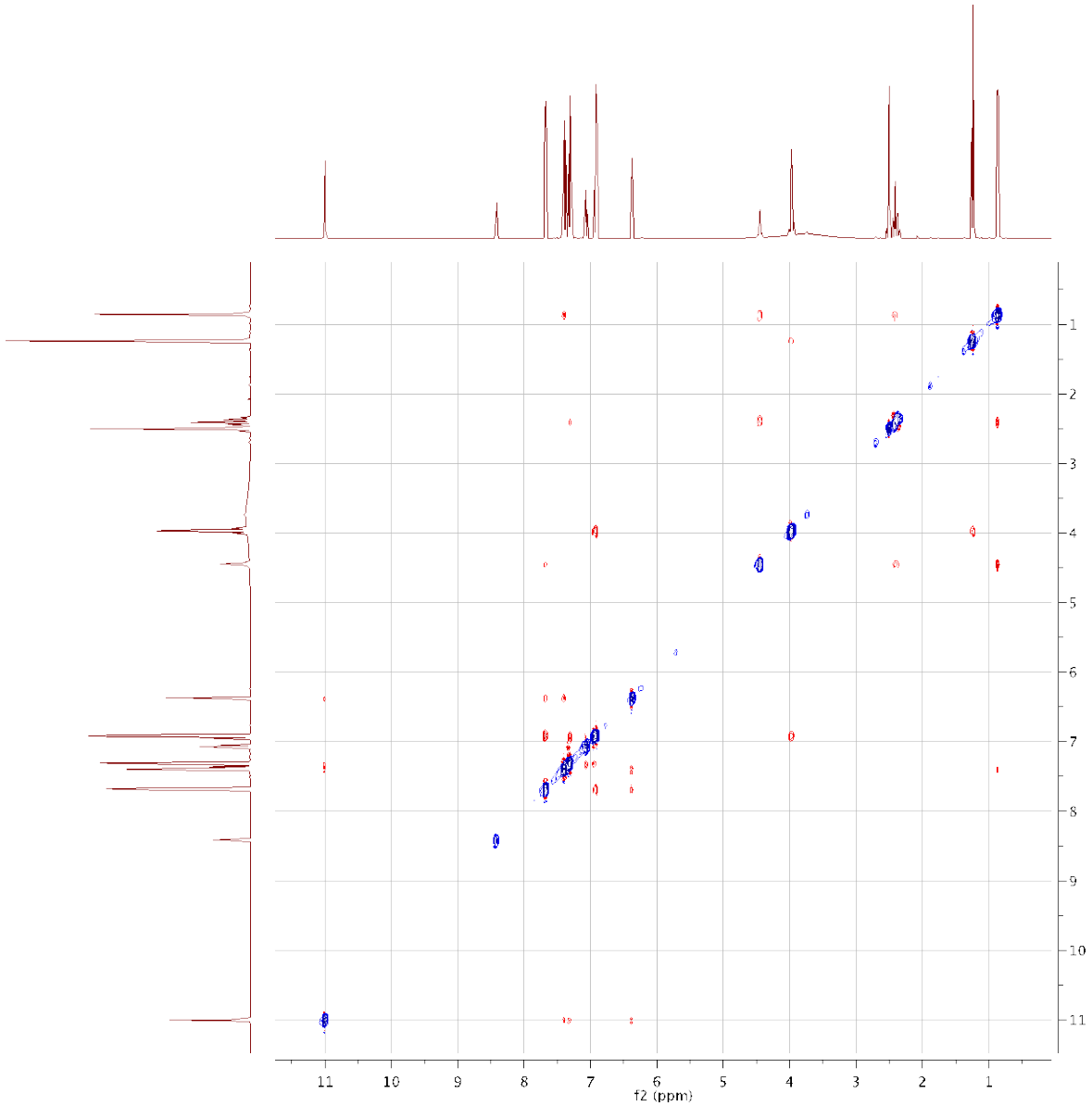




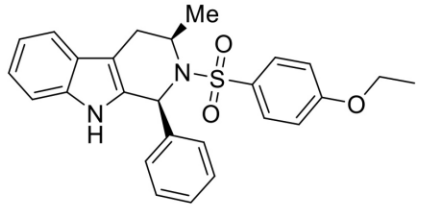
	Parameter	Value
1	Data File Name	81863285/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T15:54:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6493.5, 30120.5)
12	Lowest Frequency	(-413.8, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

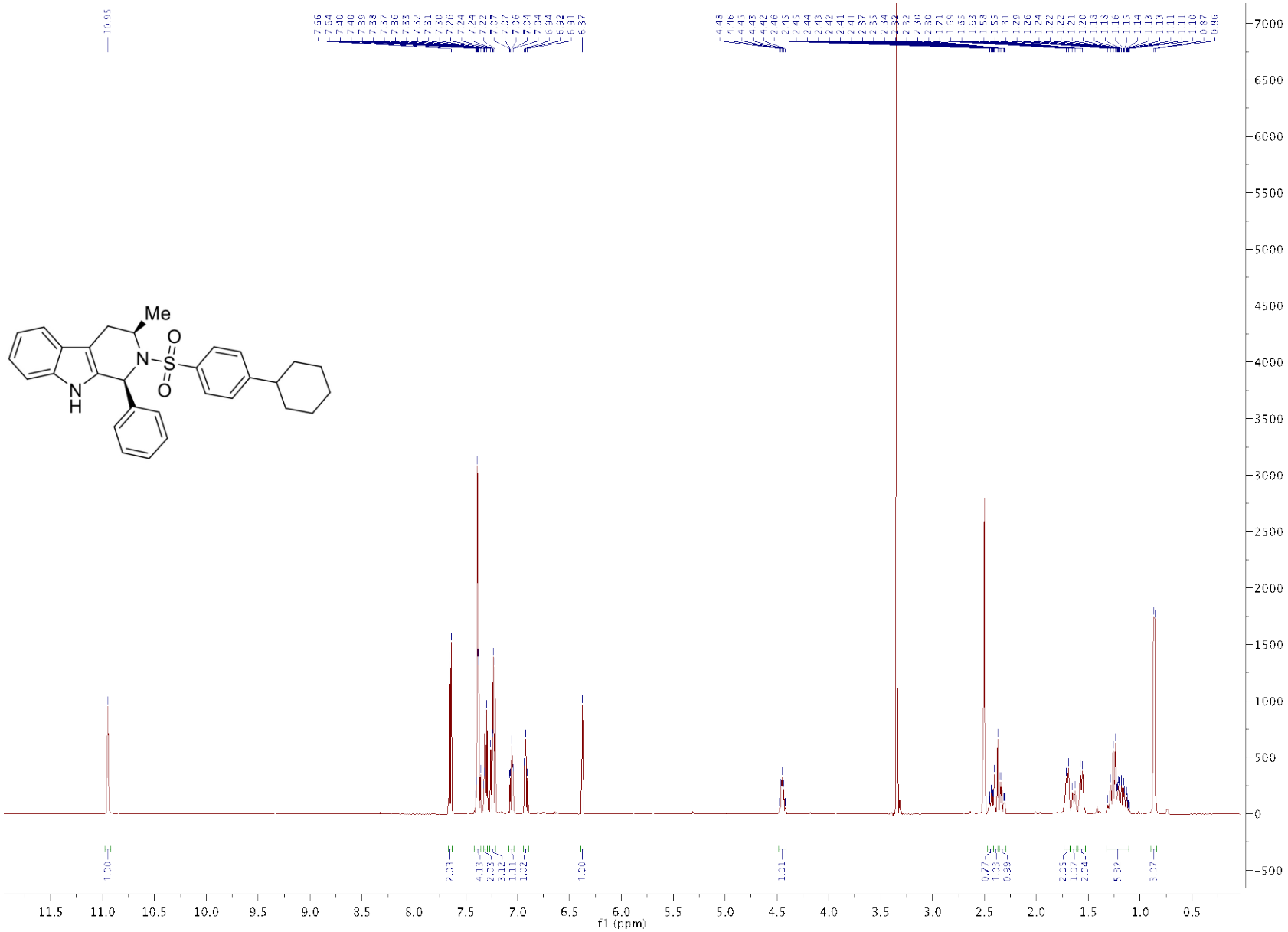
f1 (ppm)

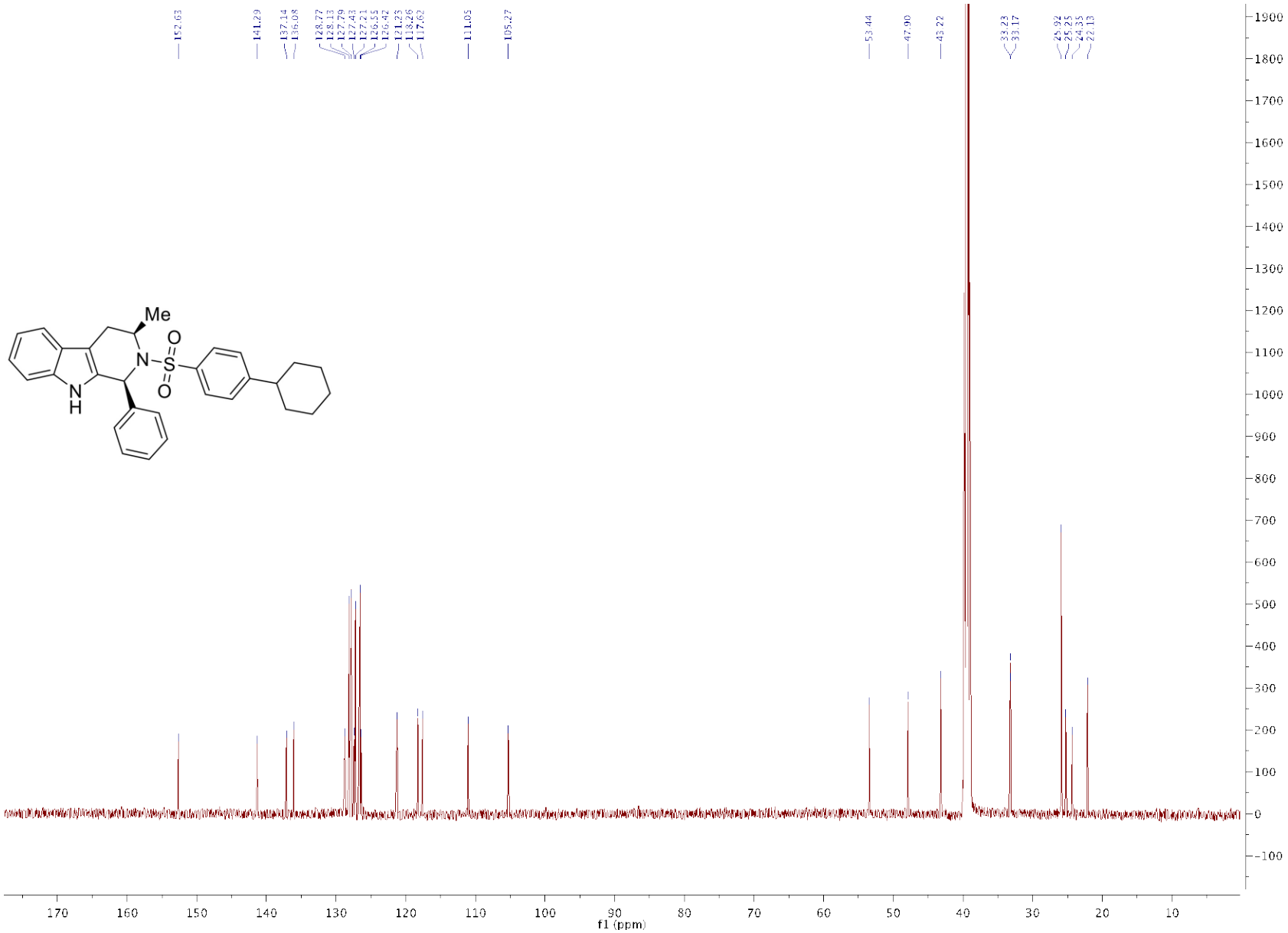




	Parameter	Value
1	Data File Name	81863285/ 16/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	roesyphpp.2
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T17:17:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6493.5, 6493.5)
12	Lowest Frequency	(-413.8, -413.8)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
N
O
S
O
N
H
f1 (ppm)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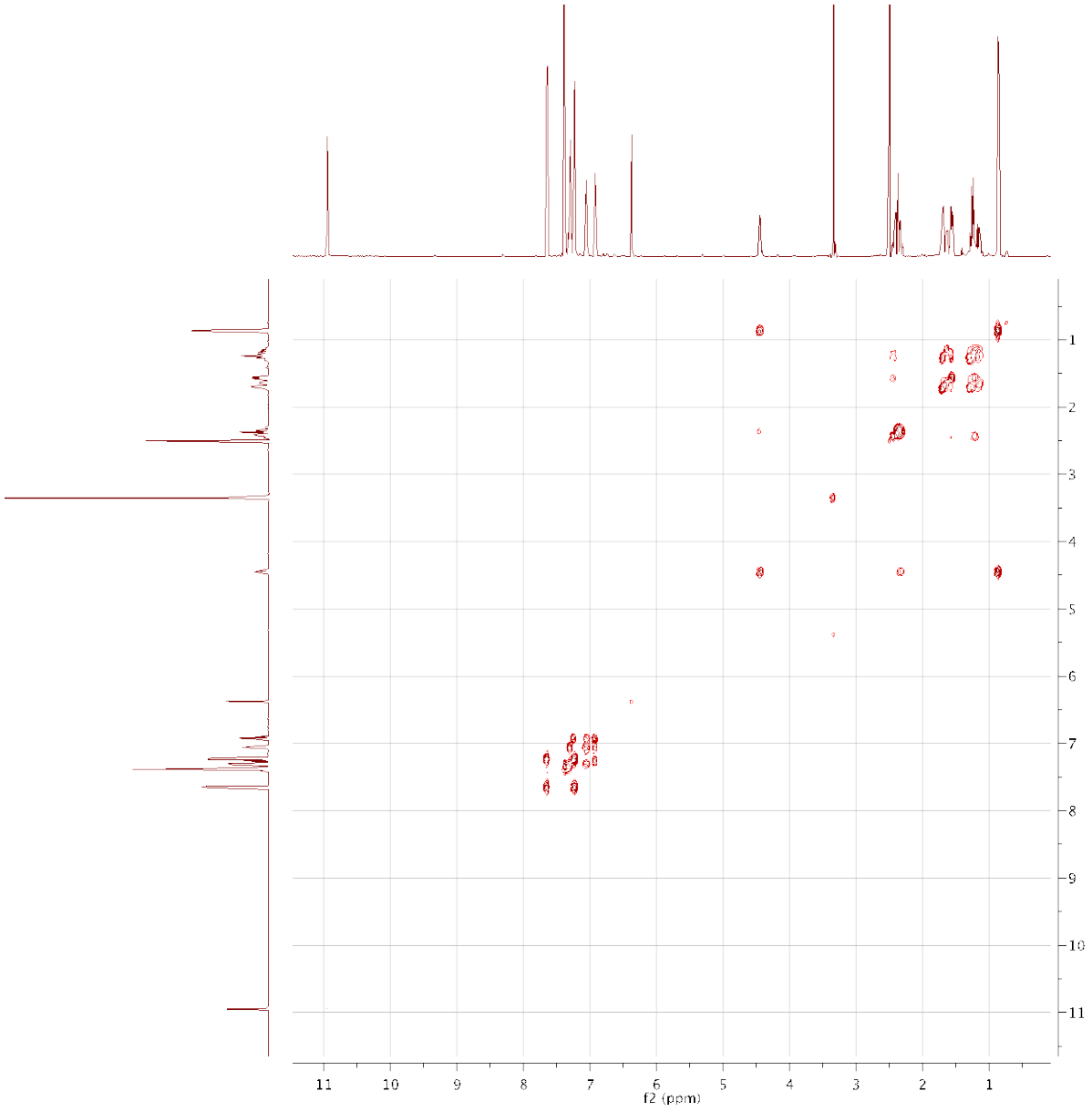
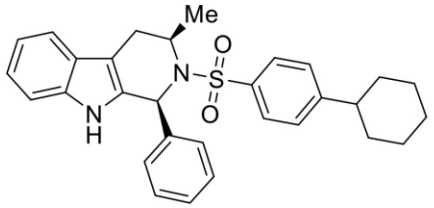
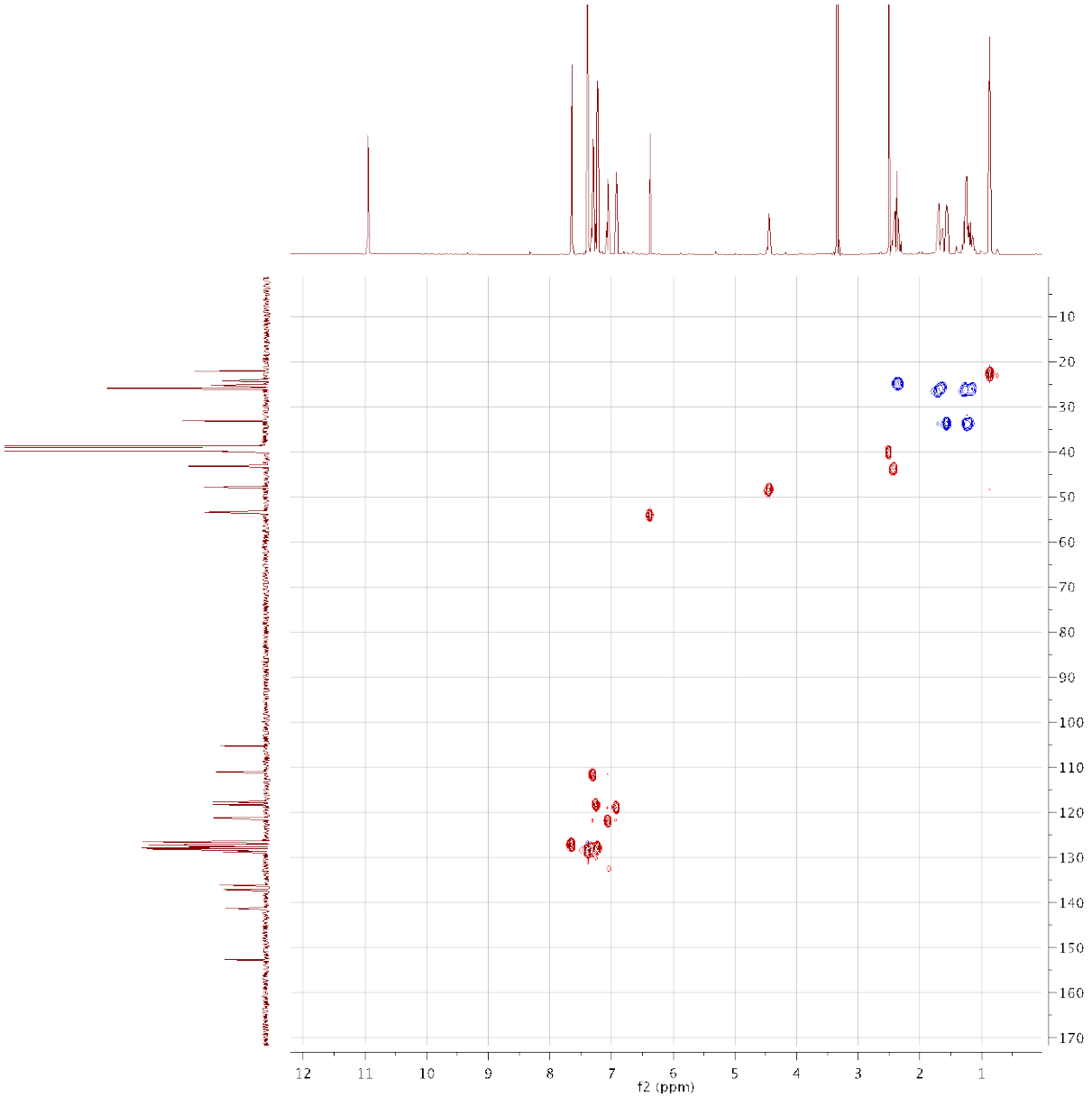
128.13
127.79
127.43
127.21
126.55
126.42
121.25
118.26
117.62
111.05
105.27
53.44
47.90
43.22
33.23
33.17
21.92
21.25
20.35
20.13
Me
N
O
S
O
N
H
f1 (ppm)

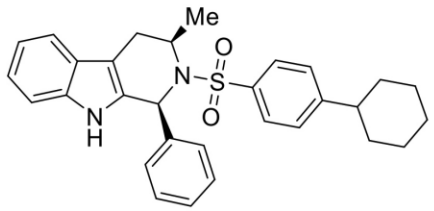


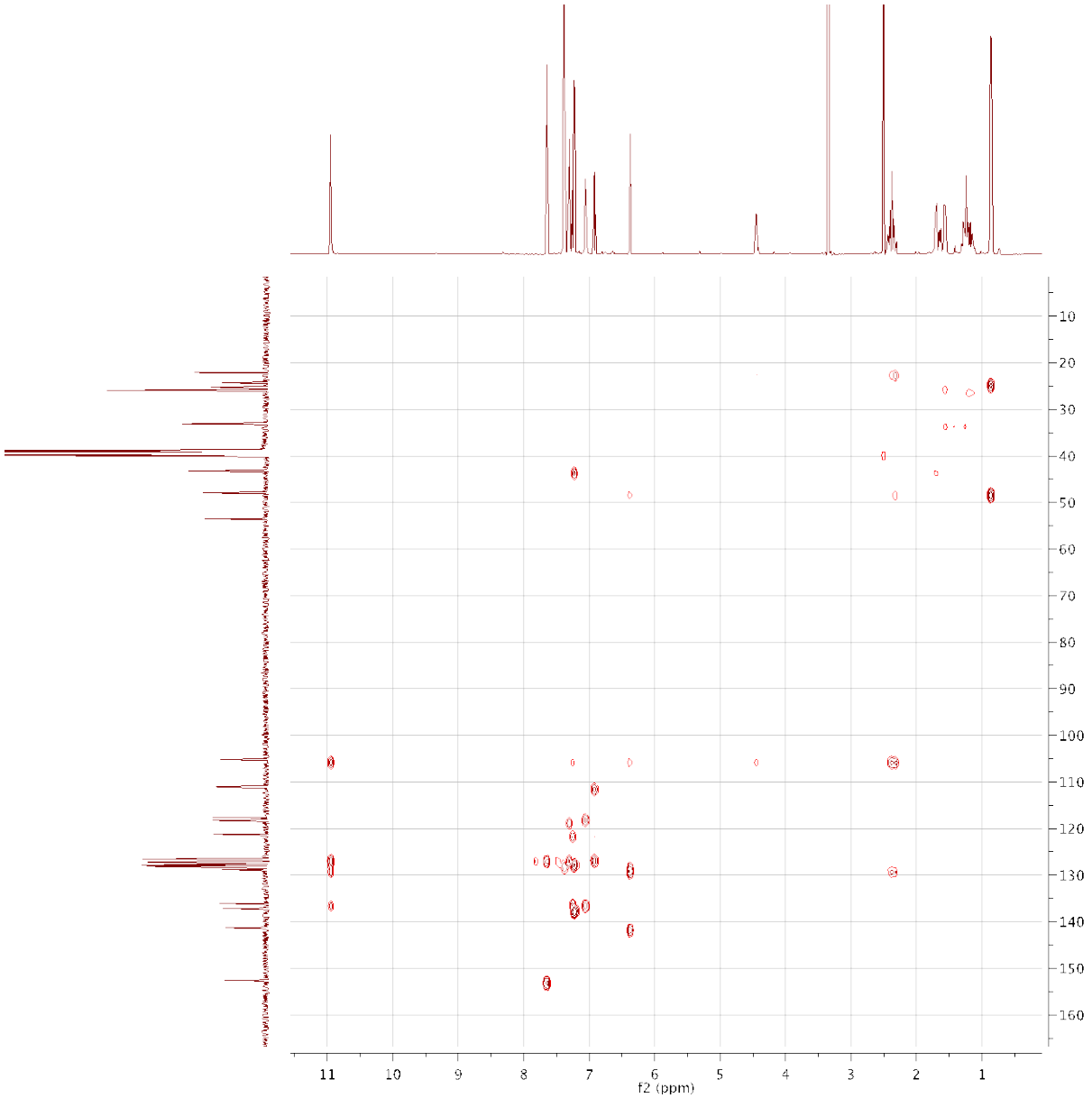
	Parameter	Value
1	Data File Name	81856448/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T03:39:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-472.8, -472.8)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)





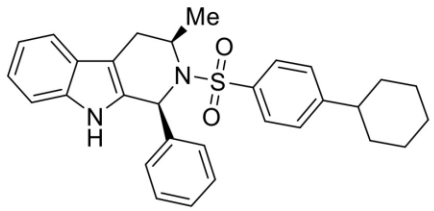
	Parameter	Value
1	Data File Name	81856448/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T04:01:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

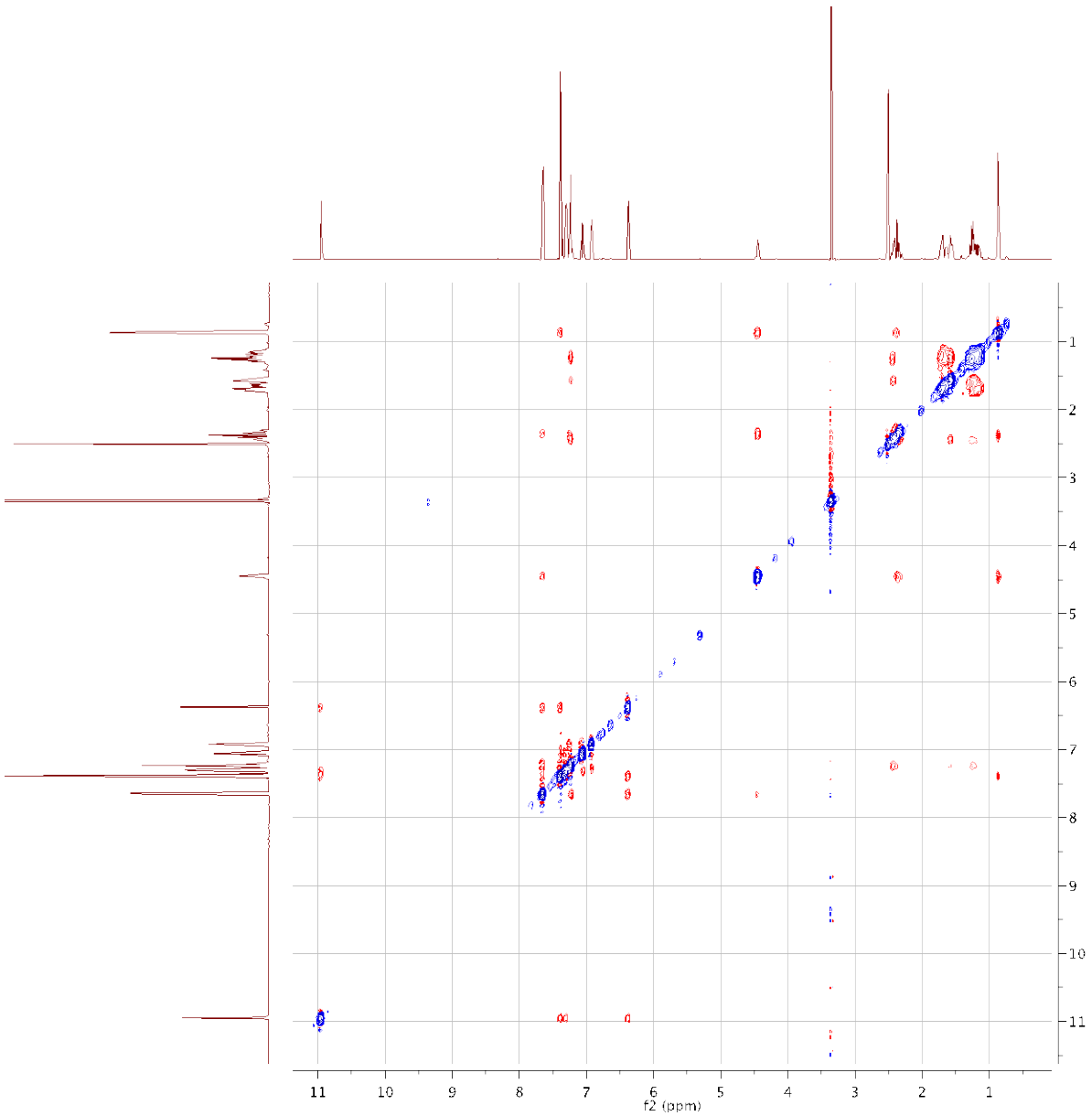




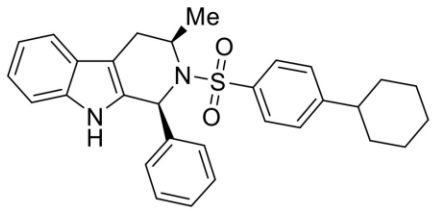
	Parameter	Value
1	Data File Name	81856448/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T04:21:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6329.1, 30120.5)
12	Lowest Frequency	(-472.8, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

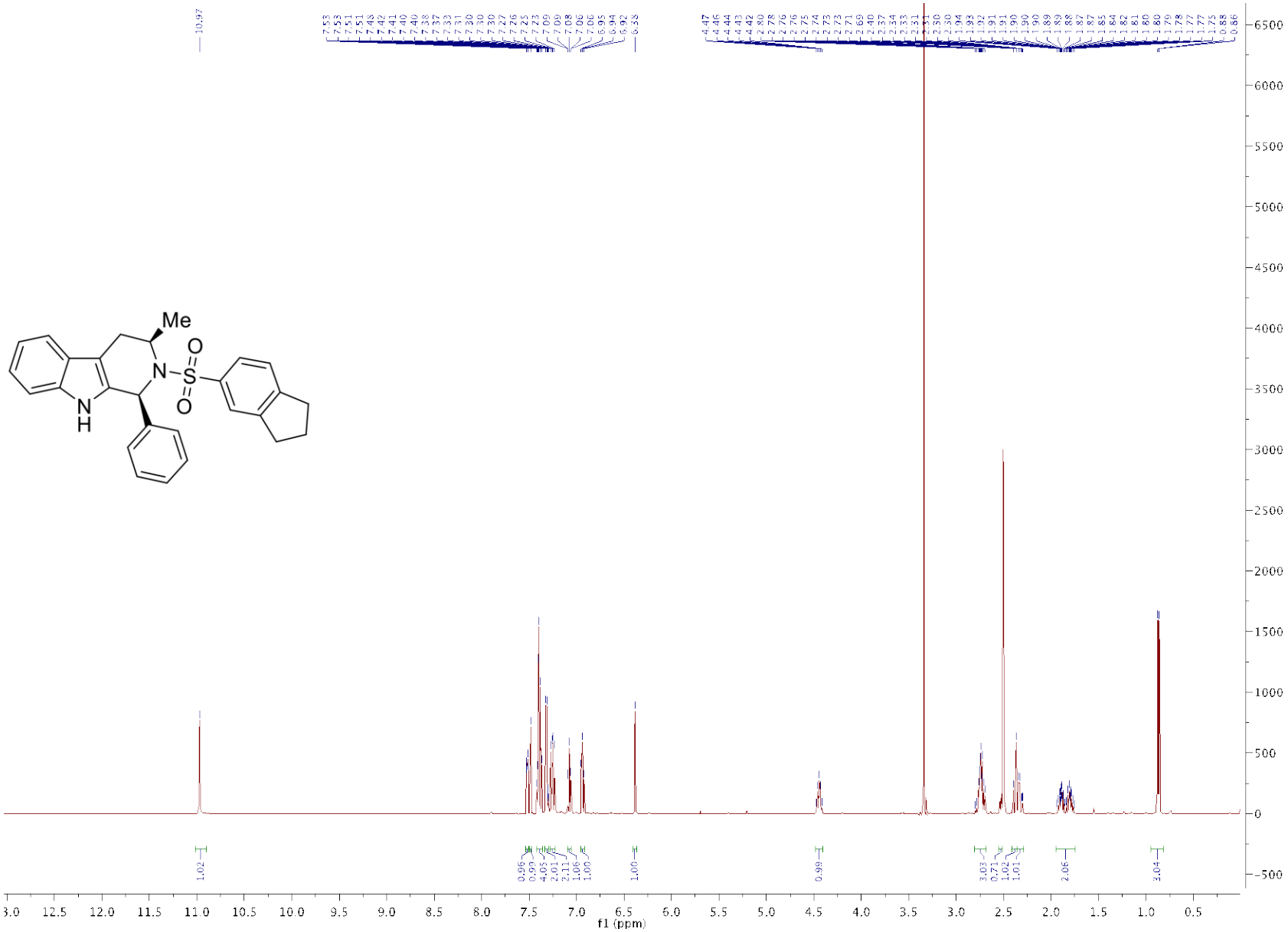
f1 (ppm)

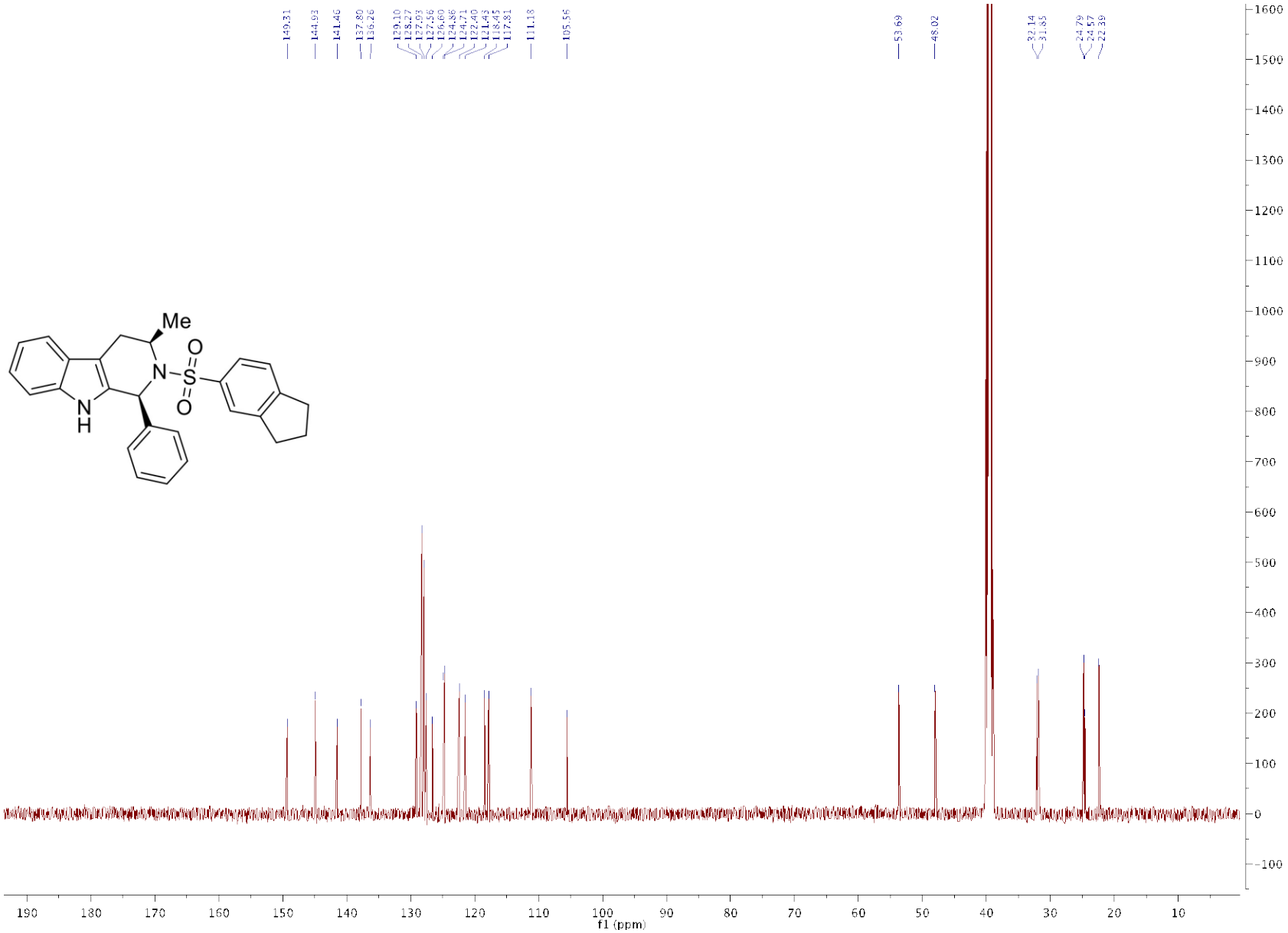


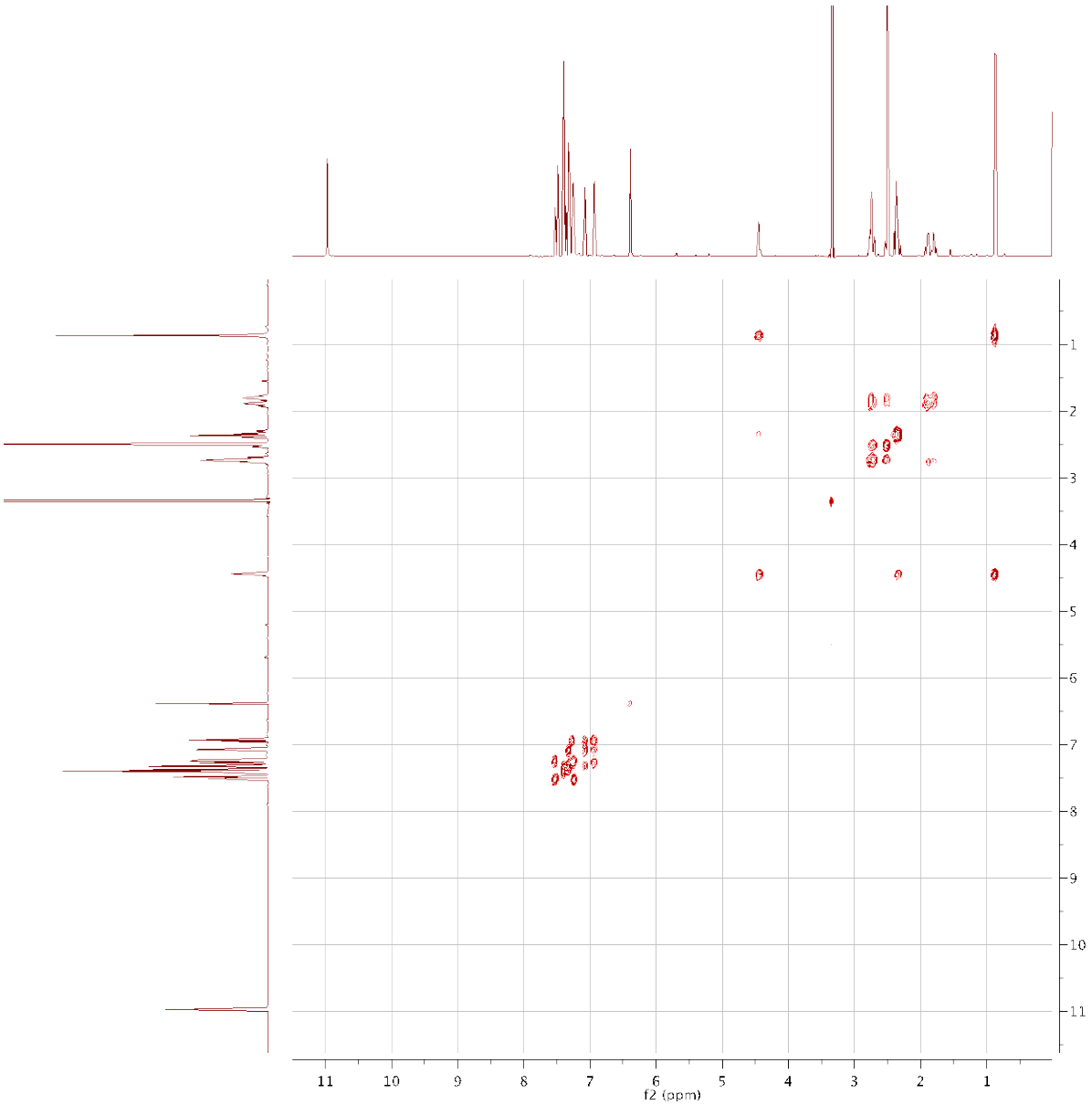


	Parameter	Value
1	Data File Name	81856448/ 16/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	roesyphpp.2
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-05T05:44:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-472.8, -472.8)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)

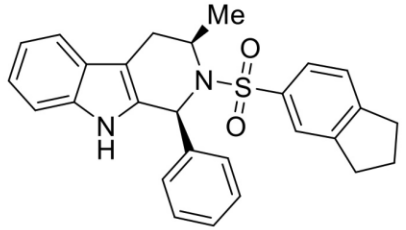


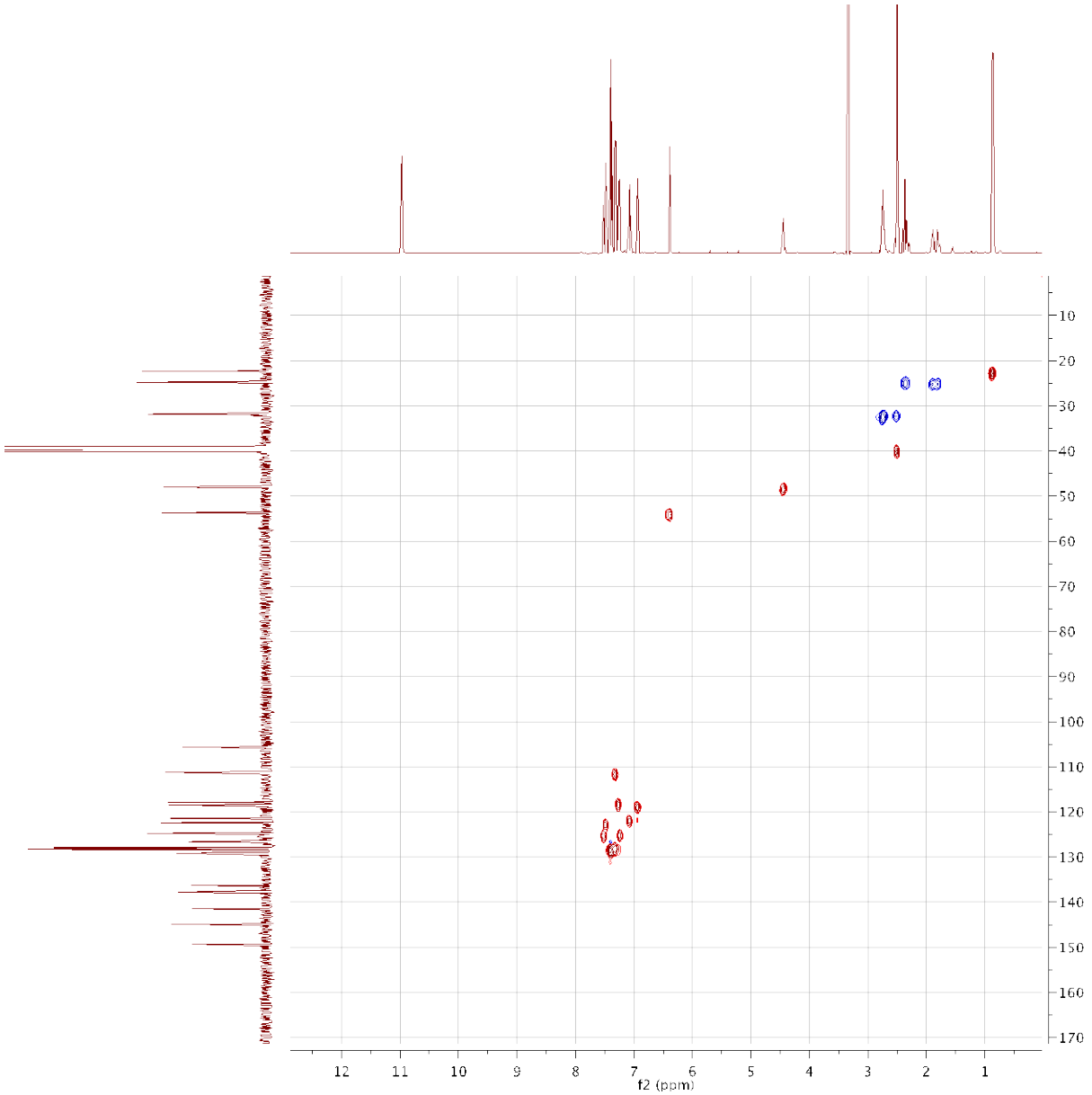

Me
O
N
S
O
N
H
f1 (ppm)


149.31
144.93
141.46
137.80
136.26
129.10
128.27
127.93
127.56
126.60
124.86
124.71
122.40
121.43
118.45
117.81
111.18
105.56
53.69
48.02
32.14
31.85
24.79
24.57
22.39
Me
O
N
S
O
N
H
f1 (ppm)

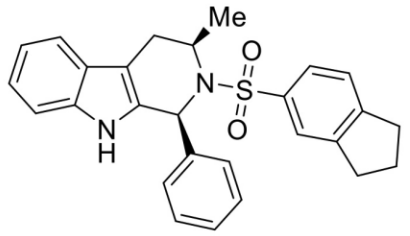


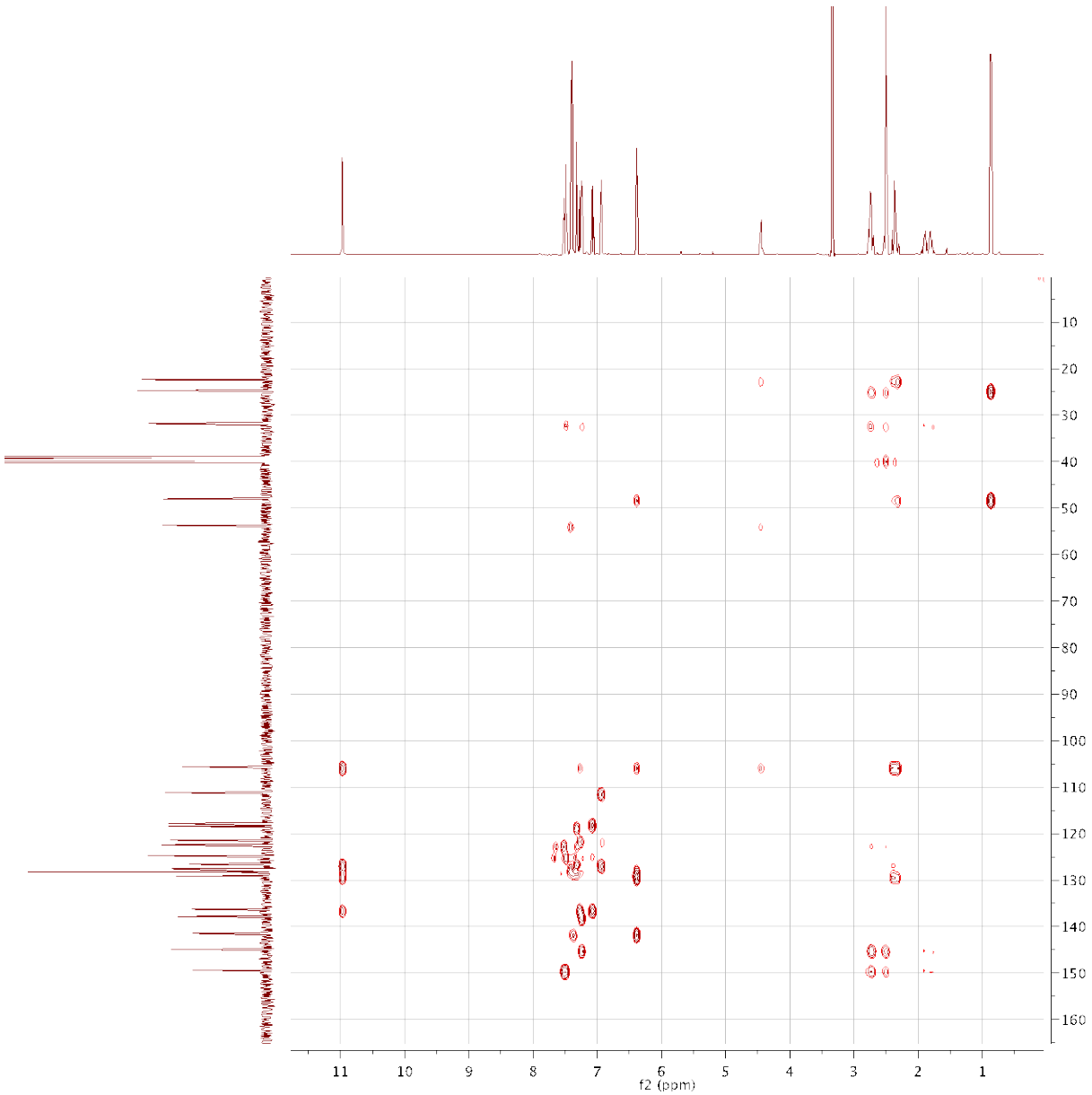
	Parameter	Value
1	Data File Name	81872502/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	cosygpmfqf
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T10:37:00
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-416.7, -416.7)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)



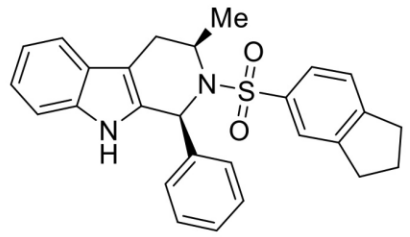


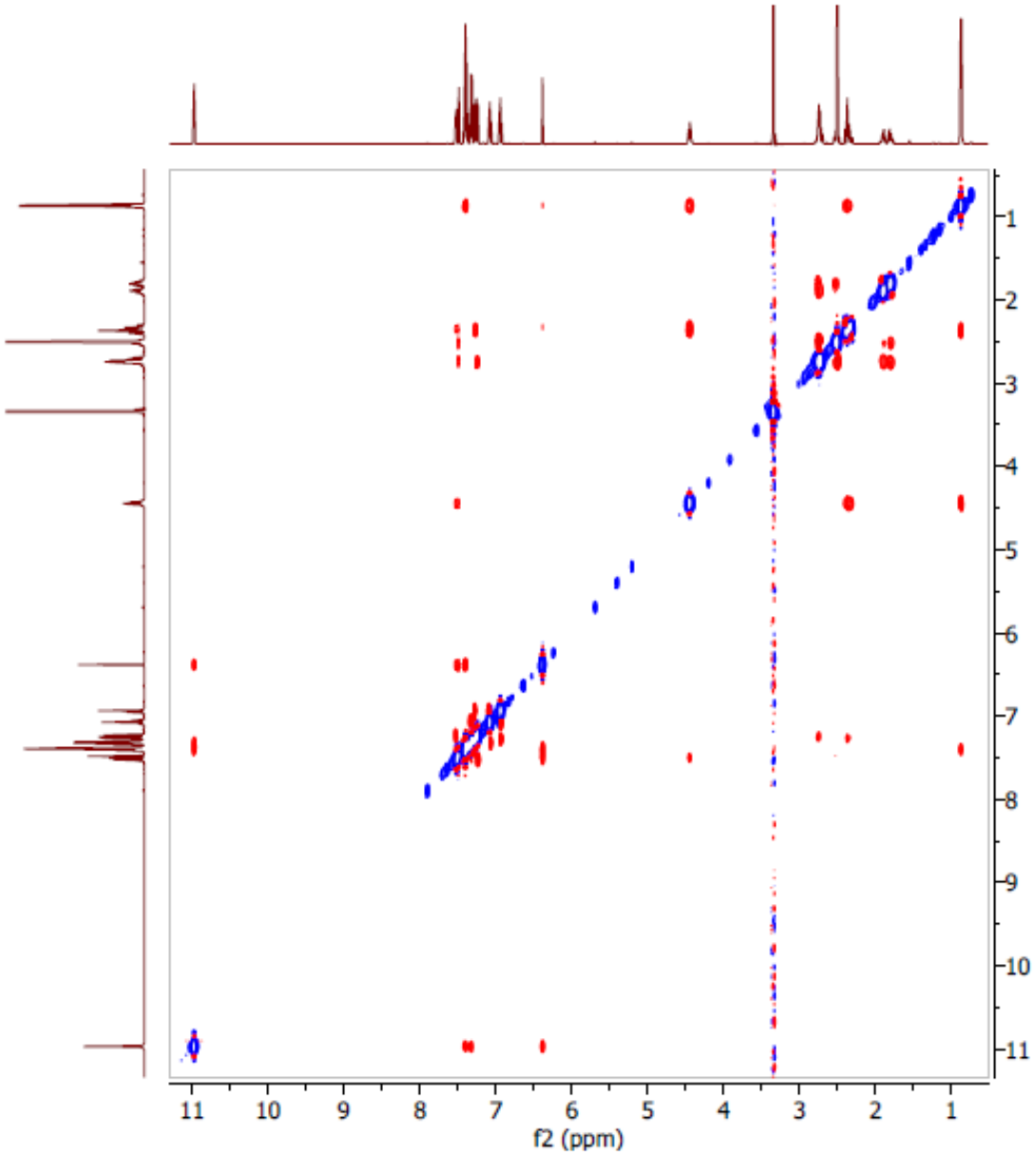
	Parameter	Value
1	Data File Name	81872502/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T10:58:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



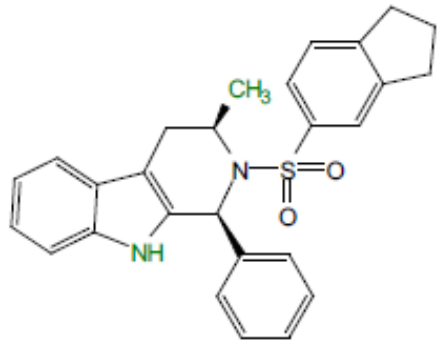


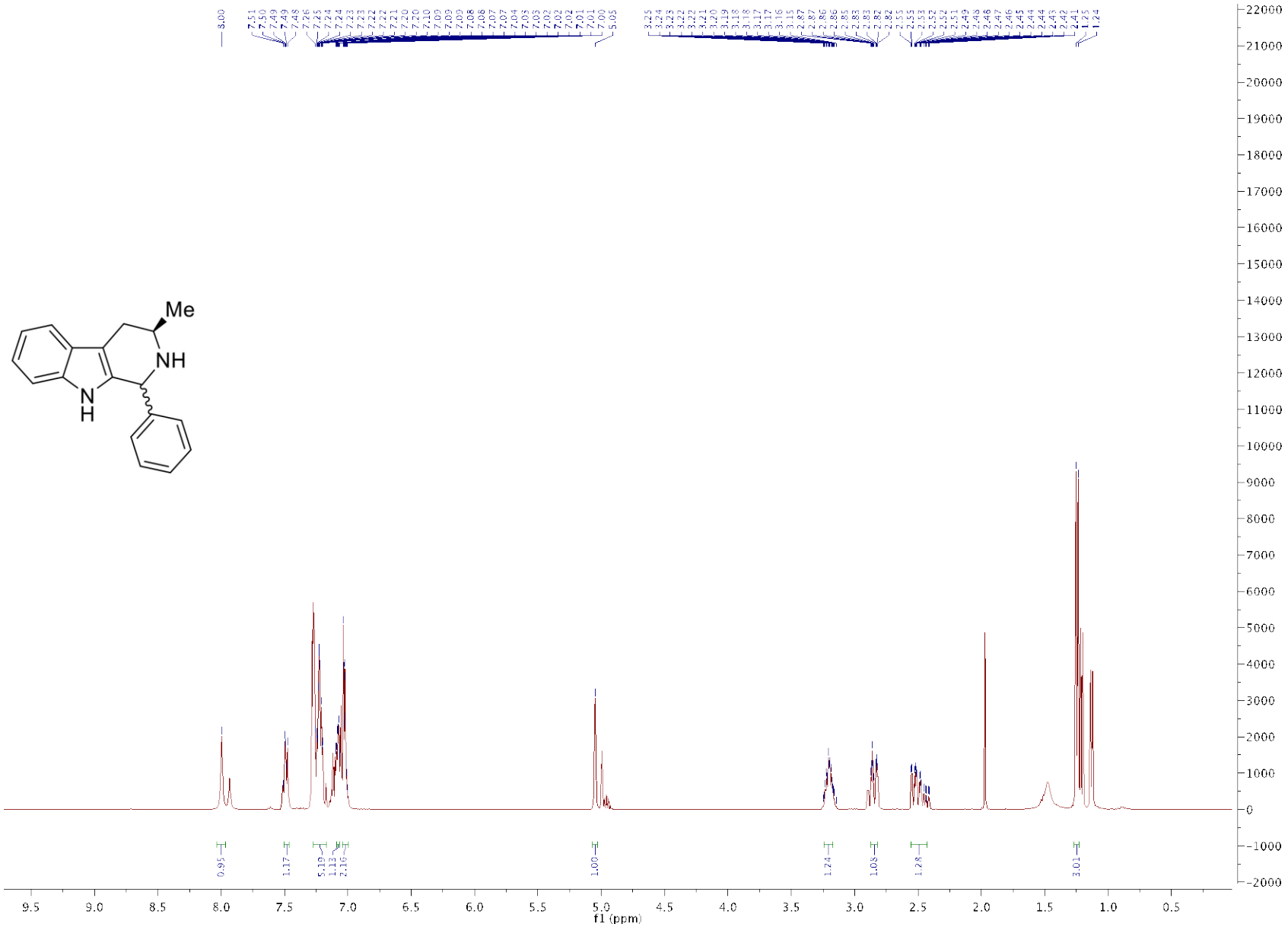
	Parameter	Value
1	Data File Name	81872502/ 15/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-20T11:19:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6329.1, 30120.5)
12	Lowest Frequency	(-416.7, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)

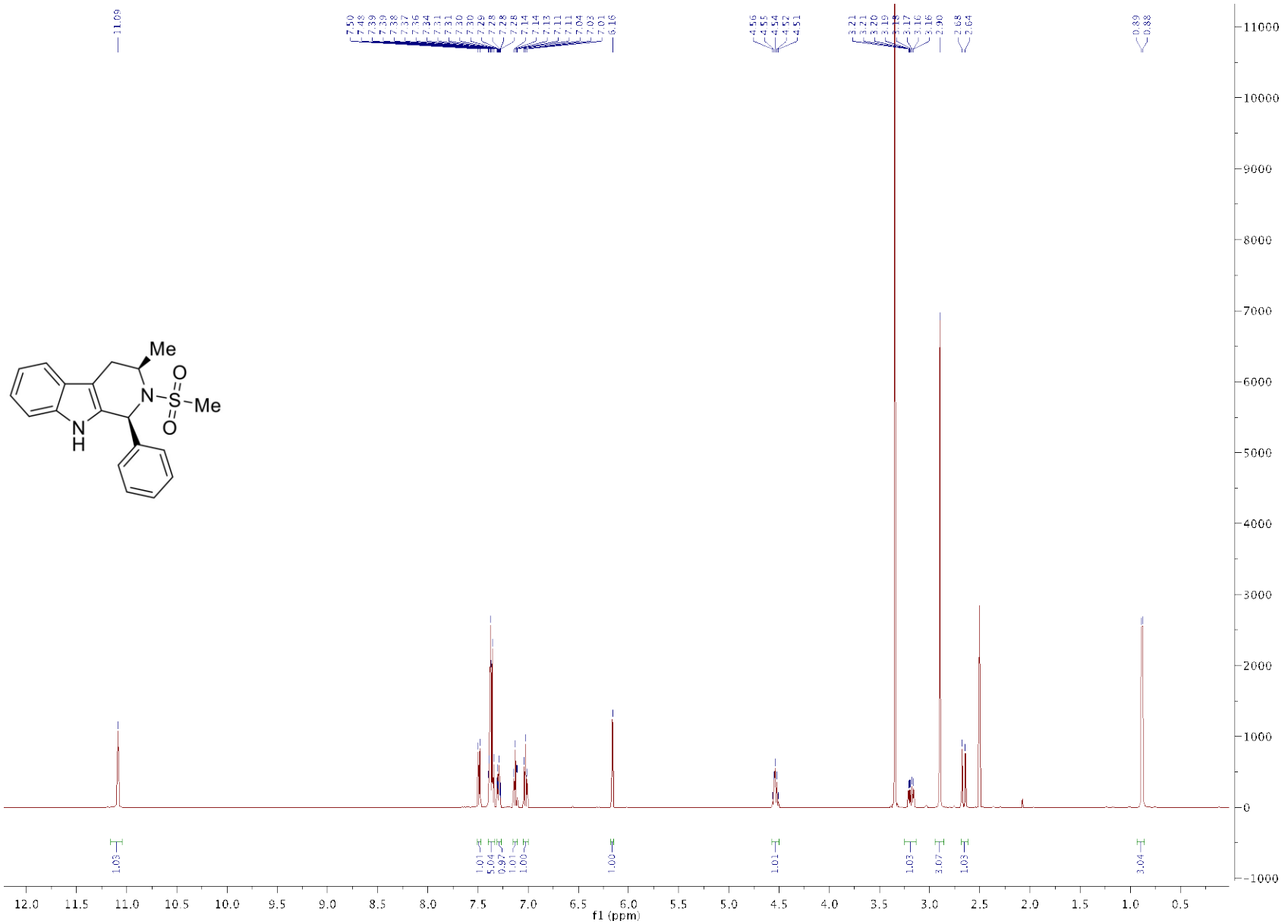




	Parameter	Value
1	Data File Name	W:/ data/ liuy55/ nmr/ 81872502/ 16/ ser
2	Sample ID	81872502
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-08-20T12:42:08
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6329.1, 6329.1)
12	Lowest Frequency	(-416.7, -416.7)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)




Me
NH
N
H
f1 (ppm)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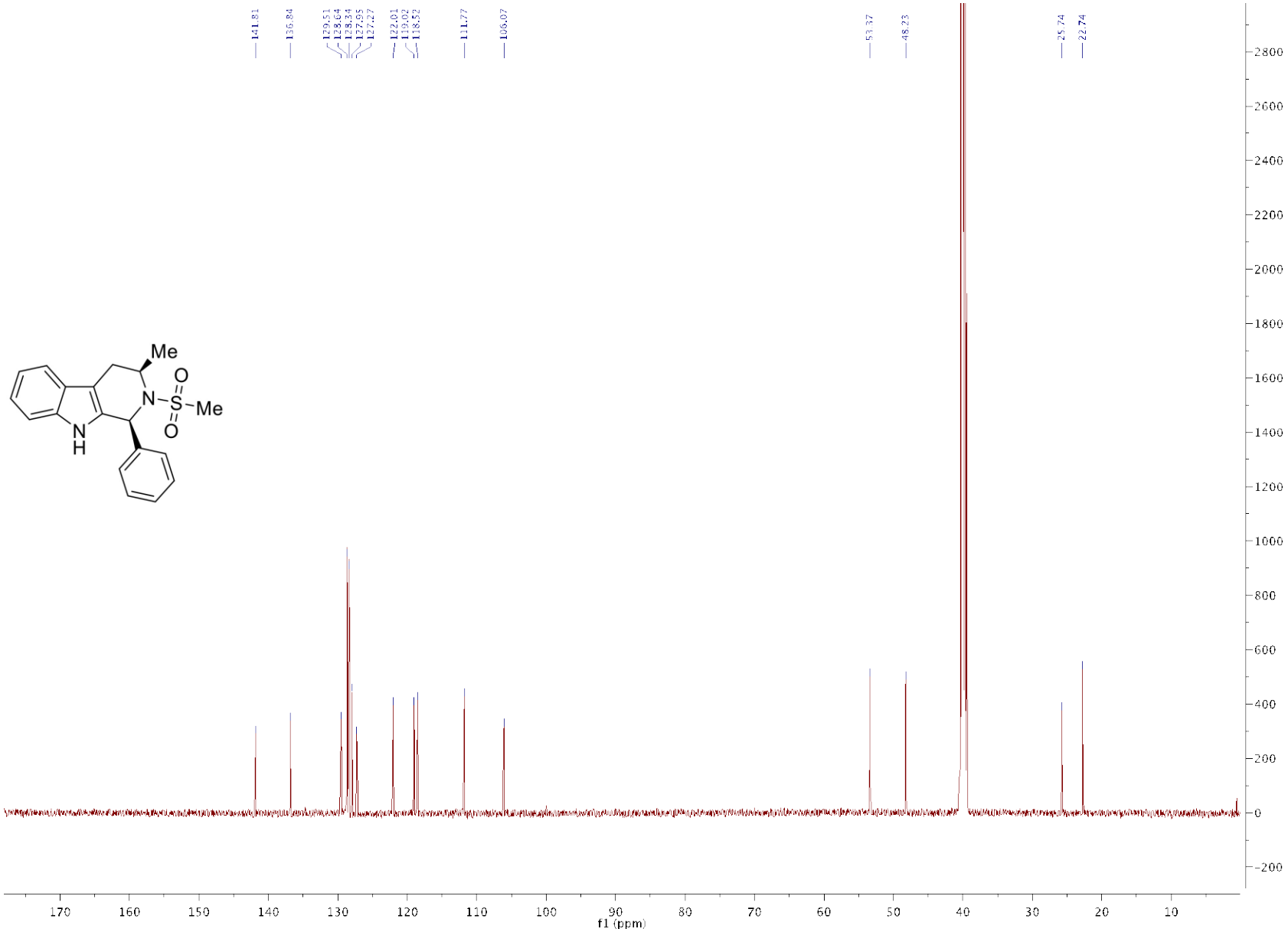
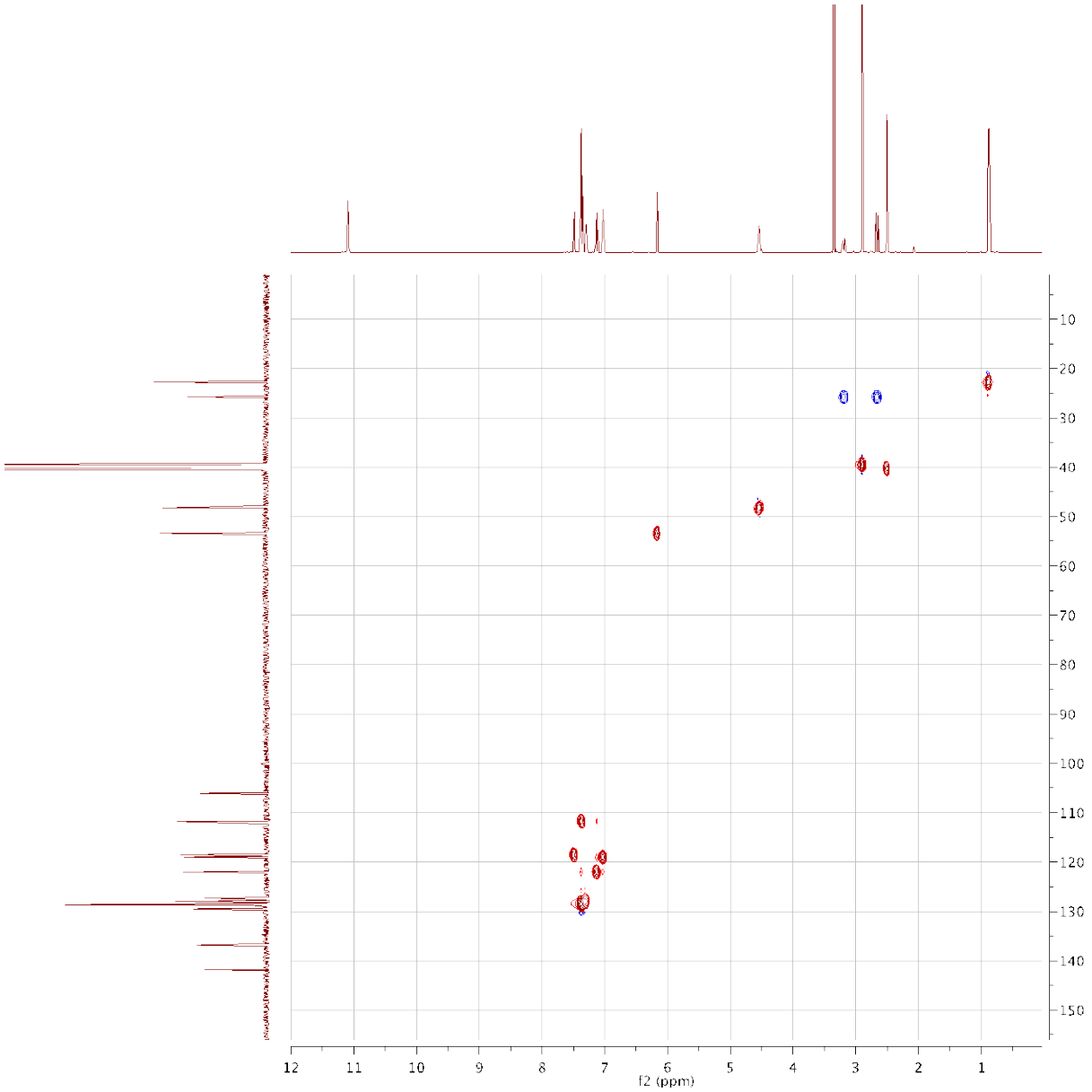
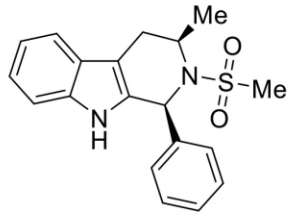
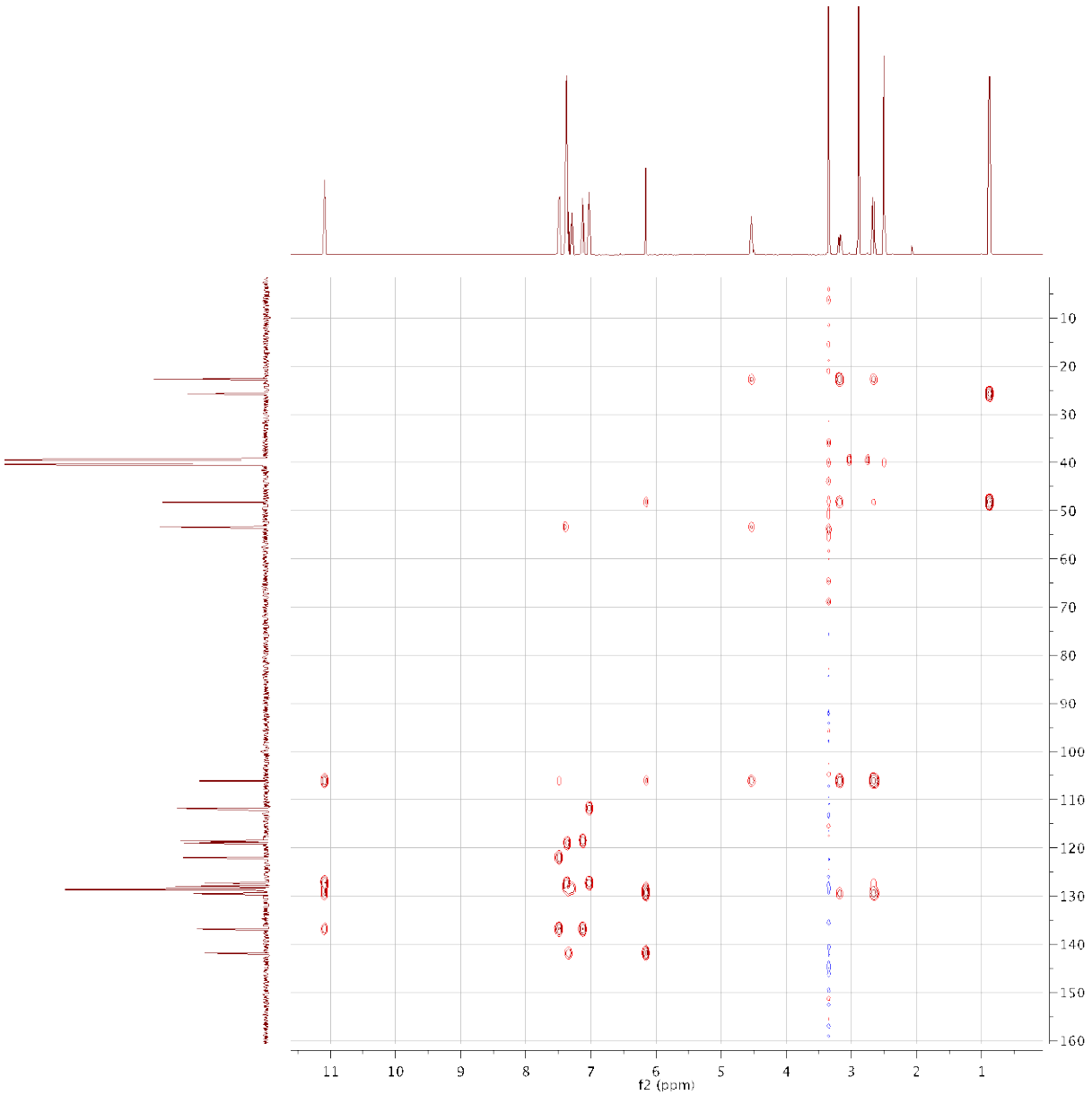
7.39
7.38
7.37
7.36
7.34
7.31
7.31
7.30
7.30
7.29
7.28
7.28
7.28
7.14
7.14
7.13
7.11
7.11
7.04
7.03
7.01
6.16
4.56
4.55
4.54
4.52
4.51
3.21
3.21
3.20
3.19
3.18
3.17
3.16
3.16
2.90
2.68
2.64
0.89
0.88
Me
O
N
S
Me
O
N
H
1.03
1.01
5.04
0.97
1.01
1.00
1.00
1.01
1.03
3.07
1.03
3.04
f1 (ppm)


141.81
136.84
129.51
128.64
128.34
127.95
127.27
122.01
119.02
118.52
111.77
106.07
53.37
48.23
25.74
22.74
Me
O
N
S
Me
O
N
H
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

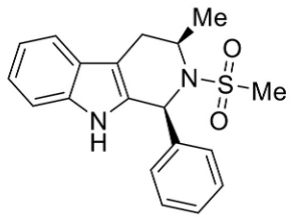


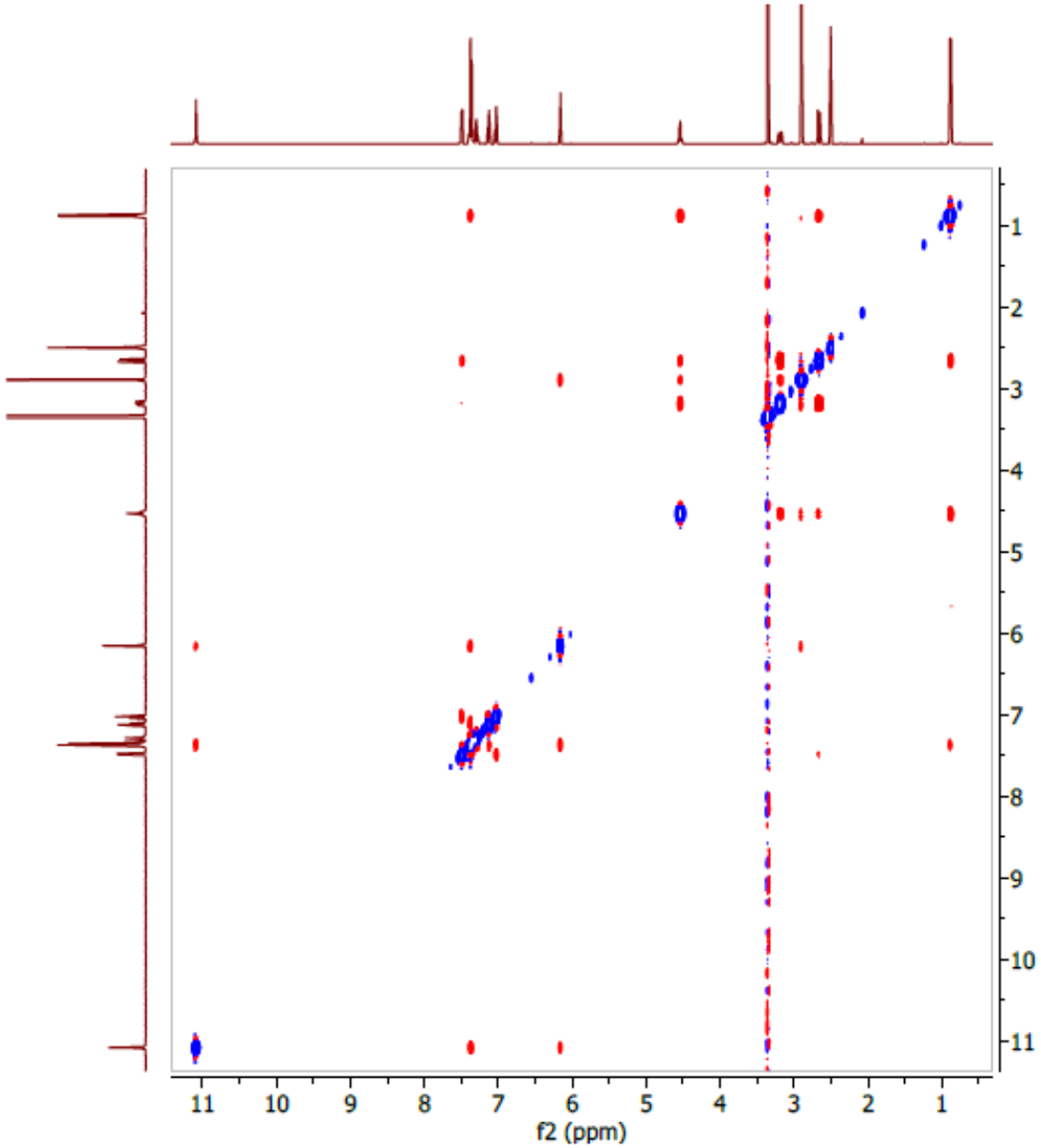
	Parameter	Value
1	Data File Name	81875262/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-31T17:03:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)



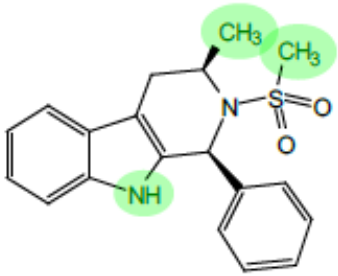


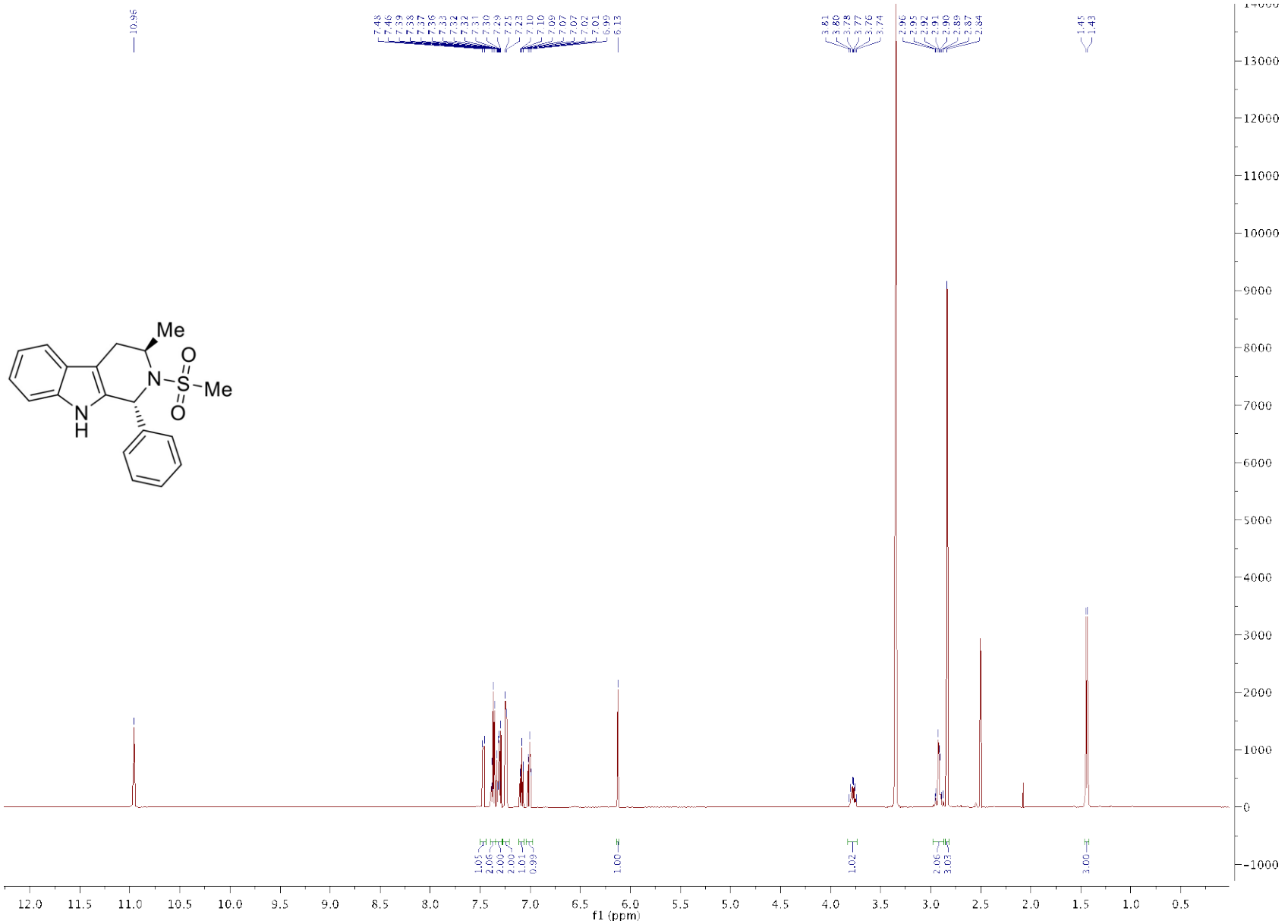
	Parameter	Value
1	Data File Name	81875262/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-31T17:23:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(6410.3, 30120.5)
12	Lowest Frequency	(-429.0, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)





	Parameter	Value
1	Data File Name	W:/ data/ liuy55/ nmr/ 81875262/ 15/ ser
2	Sample ID	81875262
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-08-31T18:45:31
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(6410.3, 6410.3)
12	Lowest Frequency	(-429.0, -429.0)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)

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7.33
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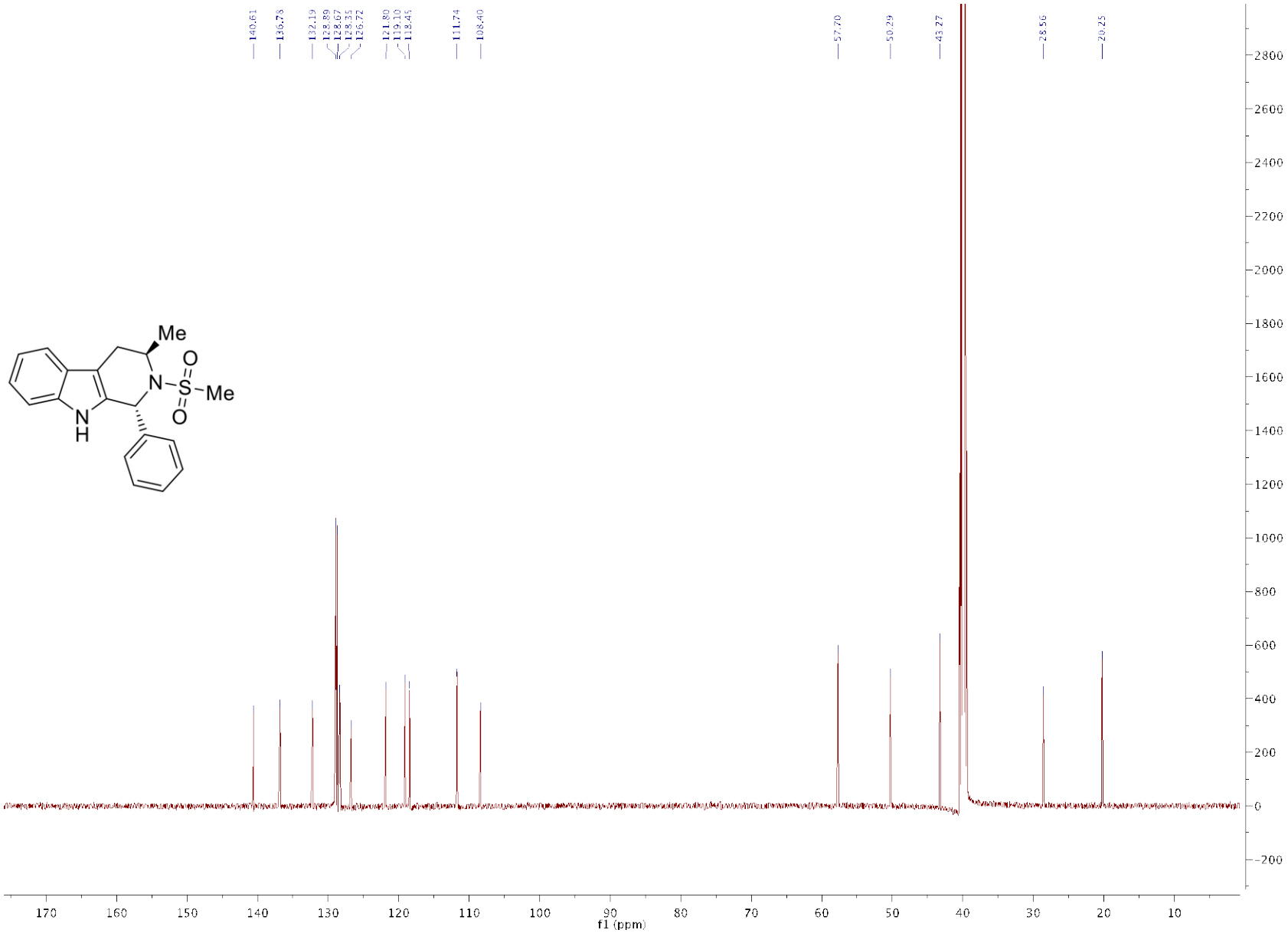
7.32
7.31
7.30
7.29
7.25
7.23
7.10
7.10
7.09
7.07
7.07
7.02
7.01
6.99
6.13
3.81
3.80
3.78
3.77
3.76
3.74
2.96
2.95
2.92
2.91
2.90
2.89
2.87
2.84
1.45
1.43
Me
O
N
S
Me
O
N
H
1.05
2.06
2.00
2.00
1.01
0.99
1.00
1.02
2.06
3.03
3.00
f1 (ppm)


140.61
136.78
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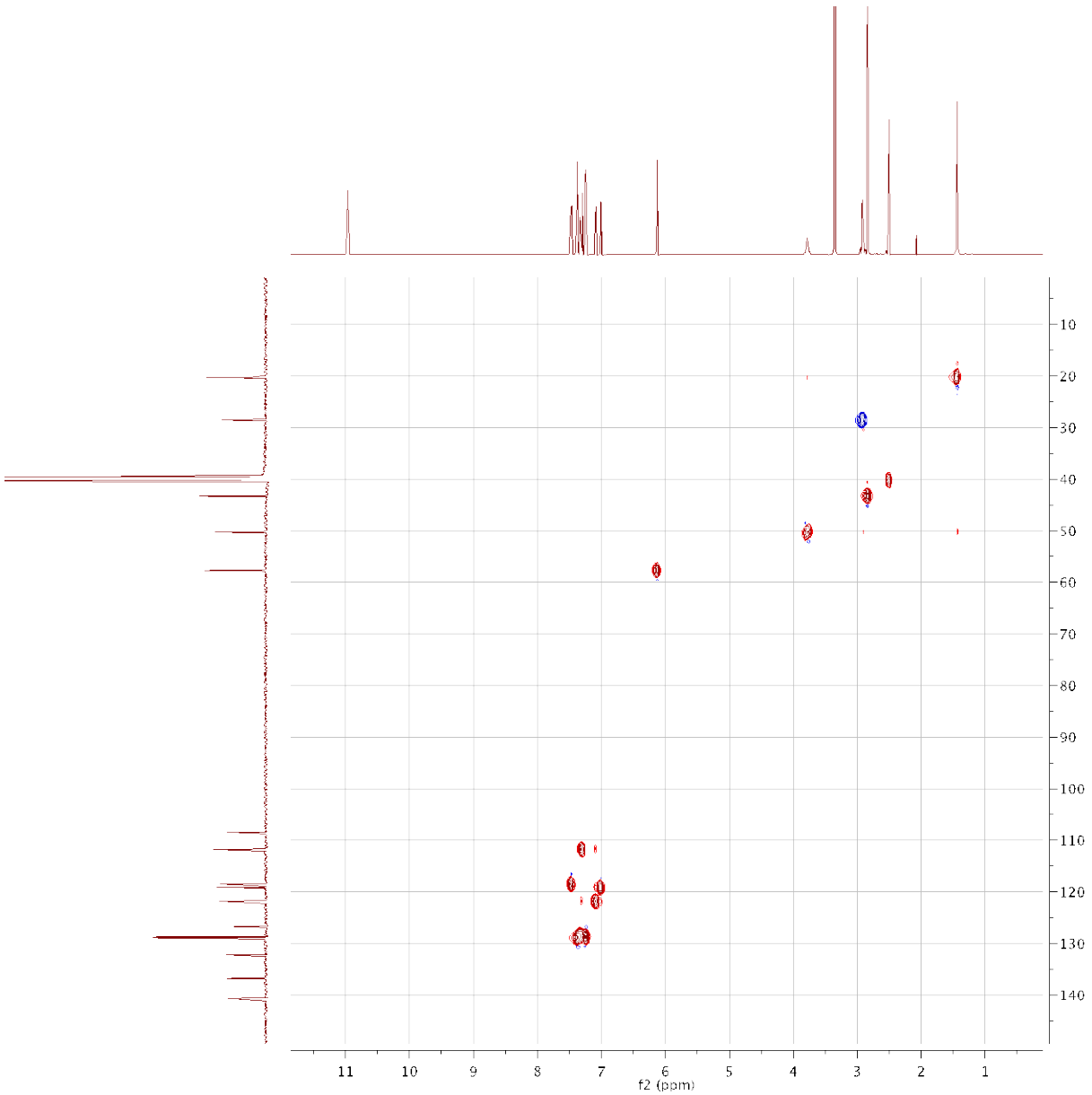
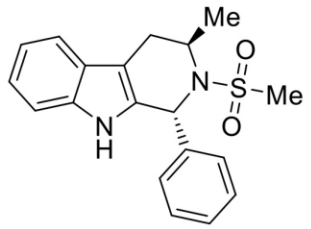
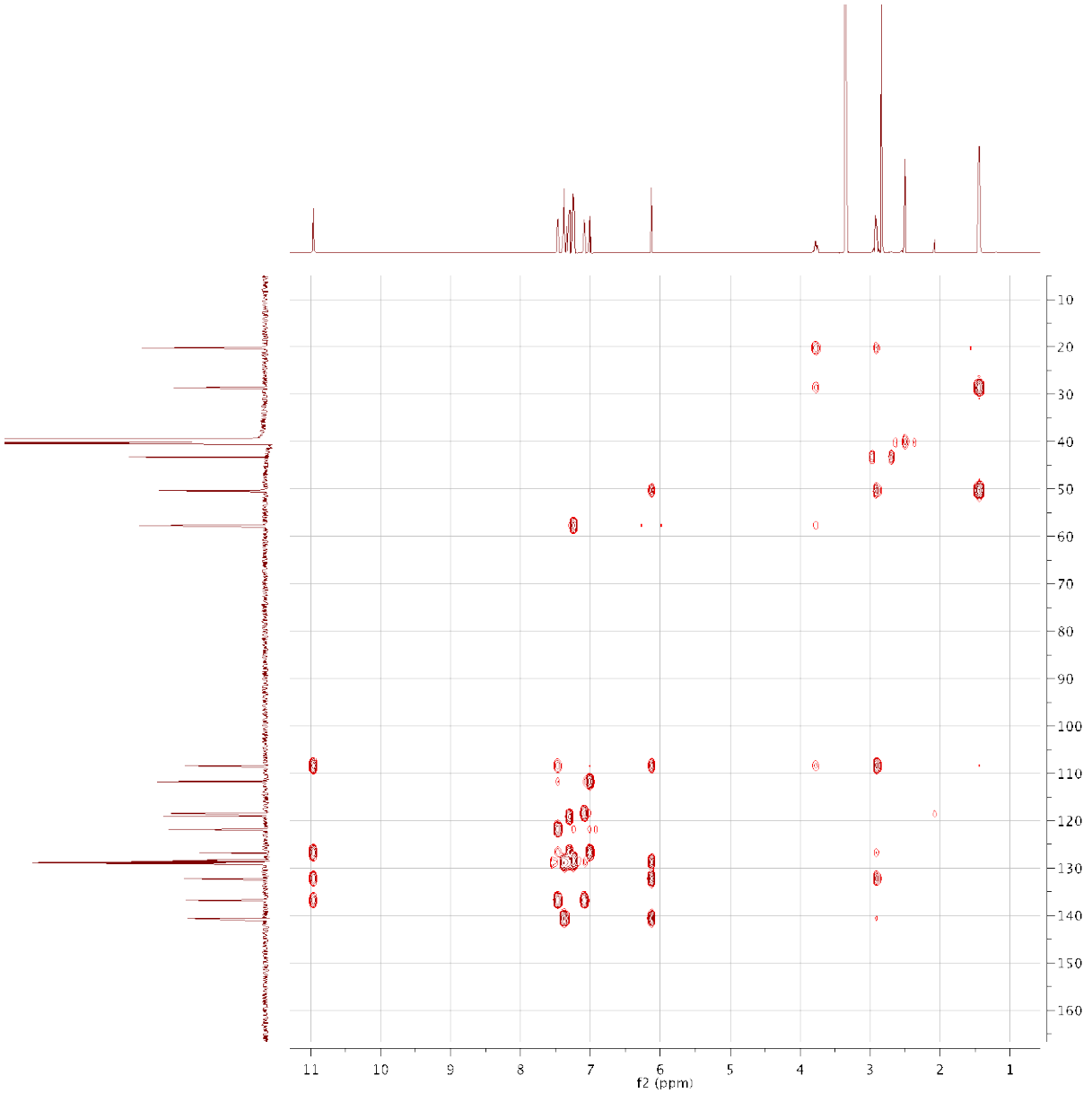
128.35
126.72
121.80
119.10
118.45
111.74
108.40
57.70
50.29
43.27
28.56
20.25
Me
N
S
Me
O
O
N
H
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

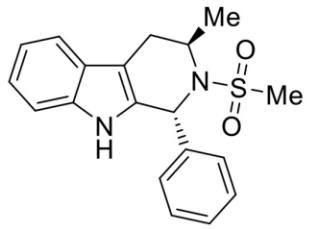


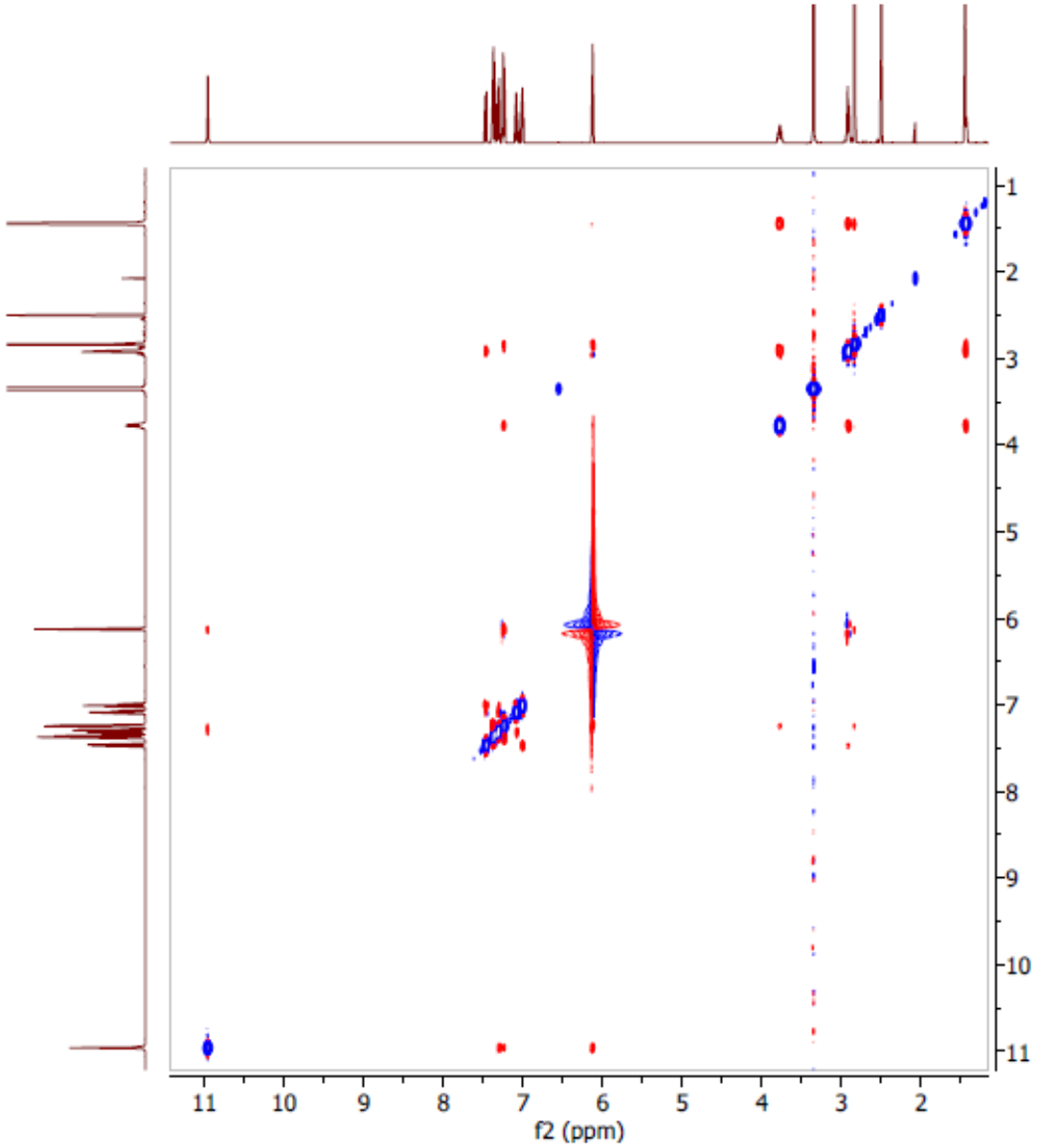
	Parameter	Value
1	Data File Name	81875265/ 13/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hsqcedetgpsisp2.2
6	Number of Scans	4
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-31T21:15:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(8012.8, 25125.6)
12	Lowest Frequency	(-1505.1, -1241.7)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)





	Parameter	Value
1	Data File Name	81875265/ 14/ ser
2	Origin	Bruker BioSpin GmbH
3	Owner	smapchemist
4	Solvent	DMSO
5	Pulse Sequence	hmbcgplpndqf
6	Number of Scans	16
7	Pulse Width	7.7500
8	Presaturation Frequency	
9	Acquisition Date	2016-08-31T21:36:00
10	Spectrometer Frequency	(500.26, 125.80)
11	Spectral Width	(5555.6, 30120.5)
12	Lowest Frequency	(272.4, -1226.6)
13	Nucleus	(1H, 13C)
14	Acquired Size	(512, 256)
15	Spectral Size	(512, 512)





	Parameter	Value
1	Data File Name	W:/ data/ liuy55/ nmr/ 81875265/ 15/ ser
2	Sample ID	81875265
3	Origin	Bruker BioSpin GmbH
4	Owner	smapchemist
5	Solvent	DMSO
6	Pulse Sequence	roesyphpp.2
7	Acquisition Date	2016-08-31T22:59:14
8	Temperature	300.0
9	Number of Scans	16
10	Spectrometer Frequency	(500.26, 500.26)
11	Spectral Width	(5555.6, 5555.6)
12	Lowest Frequency	(272.4, 272.4)
13	Nucleus	(1H, 1H)
14	Acquired Size	(1024, 256)
15	Spectral Size	(1024, 1024)