# Supplementary Material

# Design and Evaluation of Dansyl-Derived Chemosensors for Disulfide-Cleavage-Triggered Detection: Photophysical, Metal Sensing, and Thermometric Applications

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**Experimental Section**

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## 1. Experimental Section

### 1.1. Materials

Spectroscopy grade solvents, such as acetonitrile ($CH_3CN$), chloroform ($CHCl_3$), dimethylsulfoxide (DMSO), ethanol (EtOH), and tetrahydrofuran (THF), were used for the spectrophotometric and spectrofluorometric measurements. The starting fine chemicals (dansyl chloride (D0656 >98.0%(T)(HPLC)), 2,2'-thiodianiline (BD64353 98%) and 2,2'-disulfanediyldianiline (BD64662 98%)) used for the synthesis of the target fluorophores were purchased from TCI and BLD Pharm (China). Pyridine employed for the preparation of the target compounds was of analytical grade (p.a.) and dried over molecular sieve (3Å). Solvents for purification of compounds (petroleum ether (PE), dichloromethane (DCM) and methyl-tert-butyl ether (MTBE)) were of p.a. grade and were used without further purification. Silica gel (high-purity grade, pore size 60 Å, 230-400 mesh particle size, 40-63 μm particle size, for flash chromatography) employed for the column chromatography was purchased from Sigma Aldrich. Trifluoromethanesulfonate salts $Co(OTf)_2$, $Cu(OTf)_2$, $Zn(OTf)_2$, $Ag(OTf)$, $Cd(OTf)_2$, were provided from Solchemar, while $Hg(OTf)_2$, $Pb(NO_3)_2$, CuBr and $Hg_2Cl_2$ were purchased from Sigma Aldrich. Poly(methyl methacrylate) (PMMA) (MW ≈ 350.000), IROGRAN® A 92 P 4637 (Polyether-based thermoplastic polyurethane (TPU)) was offered by Huntsman (Germany). The perfluoroalkoxy (PFA) supports for the fabrication of polymer films were purchased from Bohlender GmbH, Germany. Mili-Q ultrapure water was used in all experiments.

### 1.2. Instrumentation

The chemical identities of the compounds under investigation were confirmed through the utilization of various analytical techniques, including $^1$H-NMR, $^{13}$C-NMR, DEPT-135, 2-D COSY, 2D-HSQC, and 2-D HMBC NMR and 2-D NOESY spectroscopic techniques. The $^1$H-NMR and $^{13}$C-NMR spectra were acquired on a Bruker Avance II+600 spectrometer and Avance Neo 400 (Institute of Organic Chemistry with Centre of Phytochemistry - Bulgarian Academy of Sciences / NMR Centre) using 5 mm tubes. The measurements were performed in $CDCl_3$ $CD_3CN$, and DMSO-$d_6$ at 293K, with operating frequencies of 600.13 MHz / 400 MHz and 150.92 MHz / 100 MHz for the $^1$H- and $^{13}$C-nuclei, respectively. The $^1$H- and $^{13}$C- nuclear magnetic resonance (NMR) spectra were standardized using the reference signal of $CDCl_3$, $CD_3CN$, and DMSO-$d_6$ with a chemical shift value (δ) of 7.26 ppm / 1.94 ppm / 2.50 ppm for the $^1$H-NMR and 77.16 ppm / 118.26 ppm, 39.52 ppm for the $^{13}$C-NMR, respectively. The precision of chemical changes is determined at a level of 0.01 ppm for the $^1$H-NMR and 0.1 ppm for the $^{13}$C-NMR. The coupling constants (*J*) are displayed with a precision of 0.1 and denoted in units of hertz (Hz). The spin multiplicity observed in the 1H- nuclear magnetic resonance (NMR) spectroscopy was represented using the following abbreviations: s for singlet, d for doublet, t for triplet, q for quartet, dd for doublet of doublets, dt for doublet of triplets, td for triplet of doublets, and m for multiplet. MestreNova v. 15.0 (Mestrelab Research S.L.) was used for processing the spectra.

High-Resolution Mass Spectrometry analyses have been performed in the Laboratory for Biological Mass Spectrometry–Isabel Moura (PROTEOMASS Scientific Society Facility), using UHR ESI-Qq-TOF IMPACT HD (Bruker-Daltonics, Bremen, Germany). Samples of the corresponding compounds were prepared by dissolution in 50% (v/v) Acetonitrile containing 0.1% (v/v) aqueous formic acid to obtain a working solution of 0.1 µg/mL. Mass spectrometry analysis was carried out by the direct infusion of the compound solutions into the ESI source. MS data were acquired in positive polarity over the mass range of 80 – 1300 m/z. (Capillary voltage: 4500 V, End plate offset: -500 V, Charging voltage: 2000 V, Corona: 4000 nA, Nebulizer gas: 0.4 Bar, Dry Heater: 180 °C, Dry gas: 4.0 L/min).
UV-Vis absorption spectra were recorded on a JASCO V-650 spectrophotometer. Otherwise stated, the fluorescence emission spectra were performed on a HORIBA Scientific FLUOROMAX-4 spectrofluorometer from BIOSCOPE-PROTEOMASS facilities. The second fluorometer equipment constitutes JASCO FP-8350. All photophysical experiments were carried out at 293 K using a quartz cell with 10 mm of optical path.

### 1.3. Synthetic procedures

Synthesis of *N*,*N*'-(thiobis(2,1-phenylene))bis(5-(dimethylamino)naphthalene-1-sulfonamide) (**L1**):
Diamine **2** (1.0 equiv., 216 mg, 1.00 mmol) was dissolved in 3 mL dry pyridine in a 50 mL round bottom flask. Then an excess of dansyl chloride **1** (2.5 equiv., 674 mg, 2.50 mmol) was added as a solid and the formed mixture was stirred at 50°C for 18 h. The reaction outcome was monitored using TLC (mobile phase – DCM, developed 3 times). Workup: The reaction mixture was cooled down to room temperature, then excess of conc. aq. citric acid was added and extracted with DCM (2x40 mL). The organic phase was washed with water, dried over anhydr. $Na_2SO_4$ and evaporated to dryness. The crude product was purified by column chromatography: 65 g silica; DCM:MTBE=100:0.5 v/v. After the column chromatography, the product was boiled with 4 mL PE, cooled down to r.t., decanted and dried *in vacu*o to furnish 375 mg (55%) of **L1** as a yellow powder. m.p. 113-114°C. $^1$H-NMR (600.13 MHz, $CDCl_3$) δ 8.53 (d, *J* = 8.5 Hz, 1H), 8.26–8.20 (m, 2H), 7.47 (dd, *J* = 8.4, 7.5 Hz, 1H), 7.41 (s, 2H), 7.40–7.36 (m, 2H), 7.33 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.11 (d, *J* = 7.5 Hz, 1H), 7.08–7.02 (m, 1H), 6.69 (td, *J* = 7.7, 1.2 Hz, 1H), 6.43 (dd, *J* = 7.9, 1.4 Hz, 1H), 2.86 (s, 12H). $^{13}$C-NMR (150.92 MHz, $CDCl_3$) δ 152.1, 136.8, 134.2, 132.6, 131.3, 130.6, 130.0, 129.6, 129.2, 128.8, 125.7, 125.2, 123.1, 121.5, 118.7, 115.6, 45.6.
$^1$H NMR (400 MHz, $CD_3CN$) δ 8.52 (dt, *J* = 8.6, 1.0 Hz, 2H), 8.26 (dt, *J* = 8.7, 0.8 Hz, 2H), 8.20 (dd, *J* = 7.4, 1.3 Hz, 2H), 8.05 (s, 1H), 7.51 (dd, *J* = 8.5, 7.4 Hz, 2H), 7.44 (dd, *J* = 8.6, 7.6 Hz, 2H), 7.16 (dd, *J* = 7.6, 0.7 Hz, 2H), 7.12 (dd, *J* = 8.1, 1.4 Hz, 2H), 7.09 – 7.01 (m, 2H), 6.77 (ddd, *J* = 7.8, 7.3, 1.5 Hz, 2H), 6.45 (dd, *J* = 7.9, 1.4 Hz, 2H), 2.81 (s, 12H). $^{13}$C NMR (101 MHz, $CD_3CN$) δ 152.95, 137.10, 135.35, 133.15, 131.96, 131.21, 130.58, 130.23, 129.84, 129.49, 128.32, 127.24, 124.12, 123.90, 119.51, 118.26, 116.41, 45.63.

$^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 9.80 (s, 2H), 8.46 (d, *J* = 8.5 Hz, 2H), 8.31 (d, *J* = 8.7 Hz, 2H), 8.14 (dd, *J* = 7.4, 1.2 Hz, 2H), 7.57 (dd, *J* = 8.5, 7.4 Hz, 2H), 7.46 (dd, *J* = 8.6, 7.6 Hz, 2H), 7.19 (d, *J* = 7.1 Hz, 2H), 7.08 (td, *J* = 7.8, 1.5 Hz, 2H), 7.00 (dd, *J* = 8.1, 1.3 Hz, 2H), 6.86 (td, *J* = 7.6, 1.4 Hz, 2H), 6.53 (dd, *J* = 7.9, 1.4 Hz, 2H), 2.80 (s, 12H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 151.27, 136.16, 135.28, 132.50, 130.26, 129.35, 129.27, 129.00, 128.95, 128.45, 128.09, 126.27, 123.85, 123.41, 118.86, 115.27, 45.04.
ESI-HRMS (**L1**): $[M+H]^+$ for $C_{36}H_{34}N_4O_4S_3$ = 683.1772 m/z (-6.3 ppm), $[M+2H]^{2+}$ $C_{36}H_{34}N_4O_4S_3$ = 342.0925 m/z (-5.5 ppm). Calculated $[M+H]^+$ for $C_{36}H_{34}N_4O_4S_3$ = 683.181495 m/z, and $[M+2H]^{2+}$ $C_{36}H_{34}N_4O_4S_3$ = 342.094386 m/z.

Synthesis of *N*,*N*'-(disulfanediylbis(2,1-phenylene))bis(5-(dimethylamino)naphthalene-1-sulfonamide) (**L2**):
Diamine **3** (1.0 equiv., 248 mg, 1.00 mmol) was dissolved in 3 mL dry pyridine in a 50 ml round bottom flask. Then an excess of dansyl chloride **1** (2.5 equiv., 674 mg, 2.50 mmol) was added as a solid and the formed mixture was stirred at r.t. for 48 h. The reaction outcome was monitored using TLC (mobile phase – DCM, developed twice). Workup: excess of conc. aq. citric acid was added to the reaction mixture and extracted with DCM (2x40 mL). The organic phase was washed with water, dried over anhydr. $Na_2SO_4$ and evaporated to dryness. The crude product was purified by column chromatography: 65 g silica; DCM:MTBE=100:0.5 v/v. After the column chromatography, the product was boiled with 4 mL PE, cooled down to room temperature, decanted and dried *in vacuo* to yield 523 mg (73%) of **L2** as a yellow powder. m.p. 180-181 °C. $^{1}$H-NMR (600.13 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.5 Hz, 2H), 8.32 (d, *J* = 8.7 Hz, 2H), 8.25 (dd, *J* = 7.4, 1.3 Hz, 2H), 7.67 (s, 2H), 7.59 (dd, *J* = 8.6, 7.6 Hz, 2H), 7.53 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.45 (dd, *J* = 8.5, 7.4 Hz, 2H), 7.22 (td, *J* = 8.0, 1.6 Hz, 2H), 7.16 (d, *J* = 7.3 Hz, 2H), 6.74 (td, *J* = 7.6, 1.3 Hz, 2H), 6.59 (dd, *J* = 7.7, 1.5 Hz, 2H), 2.80 (s, 12H). $^{13}$C-NMR (150.92 MHz, $CDCl_3$) δ 152.1, 138.8, 136.5, 134.3, 132.0, 131.3, 130.4, 130.0, 129.7, 129.0, 124.2, 123.8, 123.1, 119.8, 118.9, 115.6, 45.5.
$^{1}$H NMR (400 MHz, $CD_3CN$) δ 8.50 (dt, *J* = 8.6, 1.1 Hz, 2H), 8.28 (d, *J* = 8.7 Hz, 2H), 8.11 (dd, *J* = 7.4, 1.3 Hz, 2H), 7.82 (s, 2H), 7.59 (dd, *J* = 8.7, 7.6 Hz, 2H), 7.49 (dd, *J* = 8.5, 7.4 Hz, 2H), 7.24 (dd, *J* = 7.6, 0.7 Hz, 2H), 7.22 – 7.14 (m, 4H), 6.92 (ddd, *J* = 7.9, 7.1, 1.7 Hz, 2H), 6.74 (dd, *J* = 7.9, 1.3 Hz, 2H), 2.78 (s, 12H). $^{13}$C NMR (101 MHz, $CD_3CN$) δ 153.09, 137.23, 135.63, 133.18, 131.91, 131.01, 130.84, 130.64, 130.44, 130.13, 129.54, 127.21, 124.92, 124.16, 119.71, 118.26, 116.37, 45.59.
$^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 10.23 (s, 2H), 8.47 (d, *J* = 8.5 Hz, 2H), 8.35 (d, *J* = 8.7 Hz, 2H), 7.97 (dd, *J* = 7.3, 1.2 Hz, 2H), 7.56 (ddd, *J* = 8.5, 7.5, 5.4 Hz, 4H), 7.25 (d, *J* = 7.0 Hz, 2H), 7.06 (m, 4H), 6.85 (dd, *J* = 7.8, 1.6 Hz, 2H), 6.75 (dd, J = 7.7, 1.5 Hz, 2H), 2.79 (s, 12H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ 151.34, 135.95, 134.71, 133.03, 130.10, 129.24, 129.06, 129.03, 128.53, 128.09, 127.93, 126.99, 125.49, 123.44, 119.20, 115.16, 45.03.
ESI-HRMS (**L2**): $[M+H]^+$ for $C_{36}H_{34}N_4O_4S_4$ = 715.1530 m/z (-0.8 ppm), $[M+2H]^{2+}$ $C_{36}H_{34}N_4O_4S_4$ = 358.0808 m/z (1.06 ppm). Calculated $[M+H]^+$ for $C_{36}H_{34}N_4O_4S_4$ = 715.153566 m/z, and $[M+2H]^{2+}$ $C_{36}H_{34}N_4O_4S_4$ = 358.080421 m/z.

### 1.4. Spectrophotometric and spectrofluorometric measurements

#### 1.4.1. Photophysical characterization and titrations

Stock solutions of each compound were prepared (*ca.* $10^{-3}$ M) in various solvents ($CH_3CN$, DMSO, EtOH, $CHCl_3$, and THF), by dissolving each ligand in a 10 mL volumetric flask and diluting with the corresponding solvent. The working solutions in the range of $10^{-5}$ – $10^{-6}$ M were subsequently prepared by diluting the stock solutions.
Titrations of **L1** were performed by successive additions of microliter aliquots of standard solutions of $Cu^{+}$, $Cu^{2+}$, $Zn^{2+}$, $Ag^{+}$, $Cd^{2+}$, $Hg^{+}$, $Hg^{2+}$ ions prepared in acetonitrile. A correction for the absorbed light was performed when necessary. Temperature-dependent emission spectra were recorded by placing the material between quartz plates and using a temperature-controlled hotplate for variable temperature measurements. Additionally, mixtures with different water fractions ($f_w$ = 0%, 17%, 33%, 55%, 67%, and 83%) were prepared at a final concentration of 10 μM in THF and acetonitrile and characterized using absorption and emission spectroscopy. Luminescence spectra of the compounds in the solid state, as well as in doped polymer thin films, were obtained using a fiber-optic device connected to a spectrofluorometer, with samples excited at the appropriate wavelengths.

**Table S1.** Spectroscopic polarity parameters, physical properties of the different solvents. $\varepsilon_r$: relative permittivity; $\eta$: refractive index; $\alpha$: the solvent's HBD acidity; $\beta$: the solvent´s HBA basicity; $\pi^*$: the solvent´s dipolarity/polarizability.

| Solvent | $\varepsilon_r$ | $\alpha$ | $\beta$ | $\pi^*$ | $\eta$ |
|---|---|---|---|---|---|
| **DMSO** | 47.24 | 0 | 0.76 | 1.00 | 1.47 |
| **EtOH** | 24.3 | 0.86 | 0.75 | 0.54 | 1.36 |
| **$CH_3CN$** | 35.94 | 0.19 | 0.40 | 0.66 | 1.34 |
| **THF** | 7.58 | 0 | 0.55 | 0.58 | 1.40 |
| **$CHCl_3$** | 4.89 | 0.20 | 0.10 | 0.69 | 1.44 |

#### 1.4.2. Fluorescence quantum yield and Lifetime

The relative photoluminescence quantum yields were evaluated using a solution of dansylamide in DMSO ($\phi_F$ = 0.61) as a reference standard to quantify the relative QY of **L1** and **L2** in all tested solvents.[1] Lifetime measurements were conducted using a Tempro Fluorescence Lifetime System equipped with a Horiba Jobin-Yvon NanoLed pulsed diode controller. All experiments were performed at 293 K.

### 1.5. Determination of the limit of detection and quantification (LOD and LOQ)

The determination of the limit of detection (LOD) and limit of quantification (LOQ) started with the collection of ten independent measurements of a solution containing the chosen probe, devoid of any metal ion addition ($y_{blank}$). Final determination of the LOD and LOQ values followed the subsequent formulas: [2,3]
LOD = $y_{dl} = y_{blank} + 3std$, where $y_{dl}$ = signal detection limit and std = standard deviation.
LOQ = $y_{dl} = y_{blank} + 10std$, where $y_{dl}$ = signal detection limit and std = standard deviation.

The final step involved the determination of the minimal detectable and quantified concentration of metal ion by titration with the ligands.

### 1.6. Procedure of polymeric thin films doped with L1

Doped polymer films were fabricated by measuring 100 mg of polymer into one vial and 0.5 mg of compound **L1** in another. To dissolve the polymers, 10 mL of solvent was added to the polymer vial (tetrahydrofuran for TPU and chloroform for PMMA), and 1 mL of solvent was added to the compound vial. For the polyether-based thermoplastic polyurethane (TPU), stirring was required for dissolution, while for the polymethyl methacrylate (PMMA), slight heating along with stirring was necessary. Once both solutions were fully dissolved, the compound solution was combined with the polymer solution and mixed. The resulting mixture was then poured into a perfluoroalkoxyalkane (PFA) mold with a 5 cm diameter and a 15 mL capacity, sourced from Bohlender, GmbH, Germany.


1 M. Montalti, A. Credi, L. Prodi MG, Montalti M, Credi A, Prodi L GM. Handbook of Photochemistry. 3rd ed. BOCA: Taylor & Francis, Boca Raton; 2006.

2 D. Macdougall and W. B. Crummett, Guidelines for data acquisition and data quality evaluation in environmental chemistry, Anal*. Chem.* **52** (1980) 2242–2249, DOI. 10.1021/ac50064a004.

3 G. L. Long and J. D. Winefordner, Limit of Detection A Closer Look at the IUPAC Definition, Anal*. Chem.* **55** (1983) 713A-724A, 10.1021/ac00258a724.

# Display Report

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| Sample Name | MassAccMS | Instrument | impact HD 1819696.00006 |
| Comment | | | |

**Acquisition Parameter**

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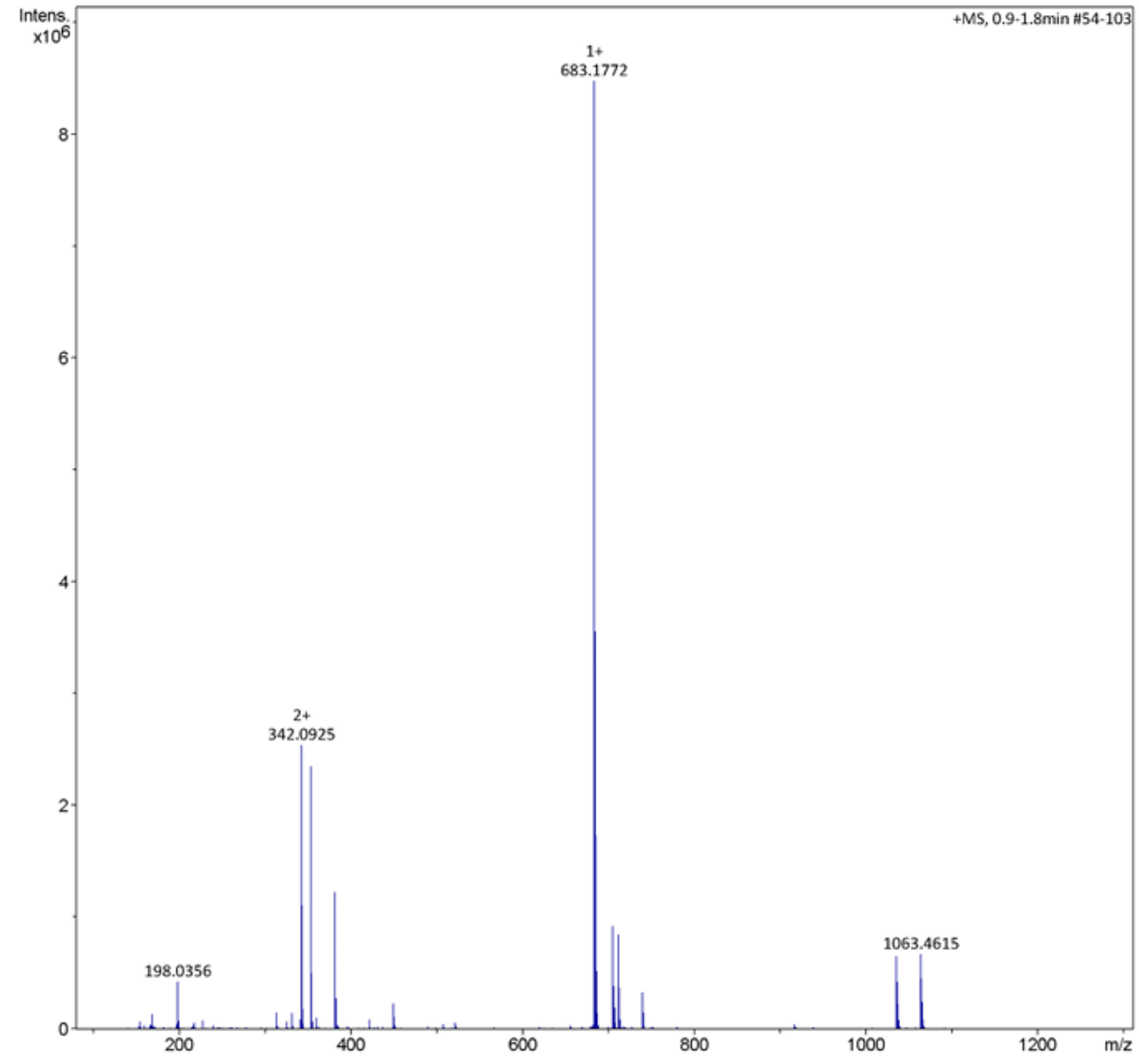


DR-P165.d

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**Figure S1. ESI-HRMS spectrum of compound L1.**

# Display Report

**Analysis Info**

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| Sample Name | ACN | Instrument | impact HD 1819696.00006 |
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| Scan Begin | 80 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 1300 m/z | Set Charging Voltage | 2000 V | Set Divert Valve | Waste |
| | | Set Corona | 4000 nA | Set APCI Heater | 200 °C |

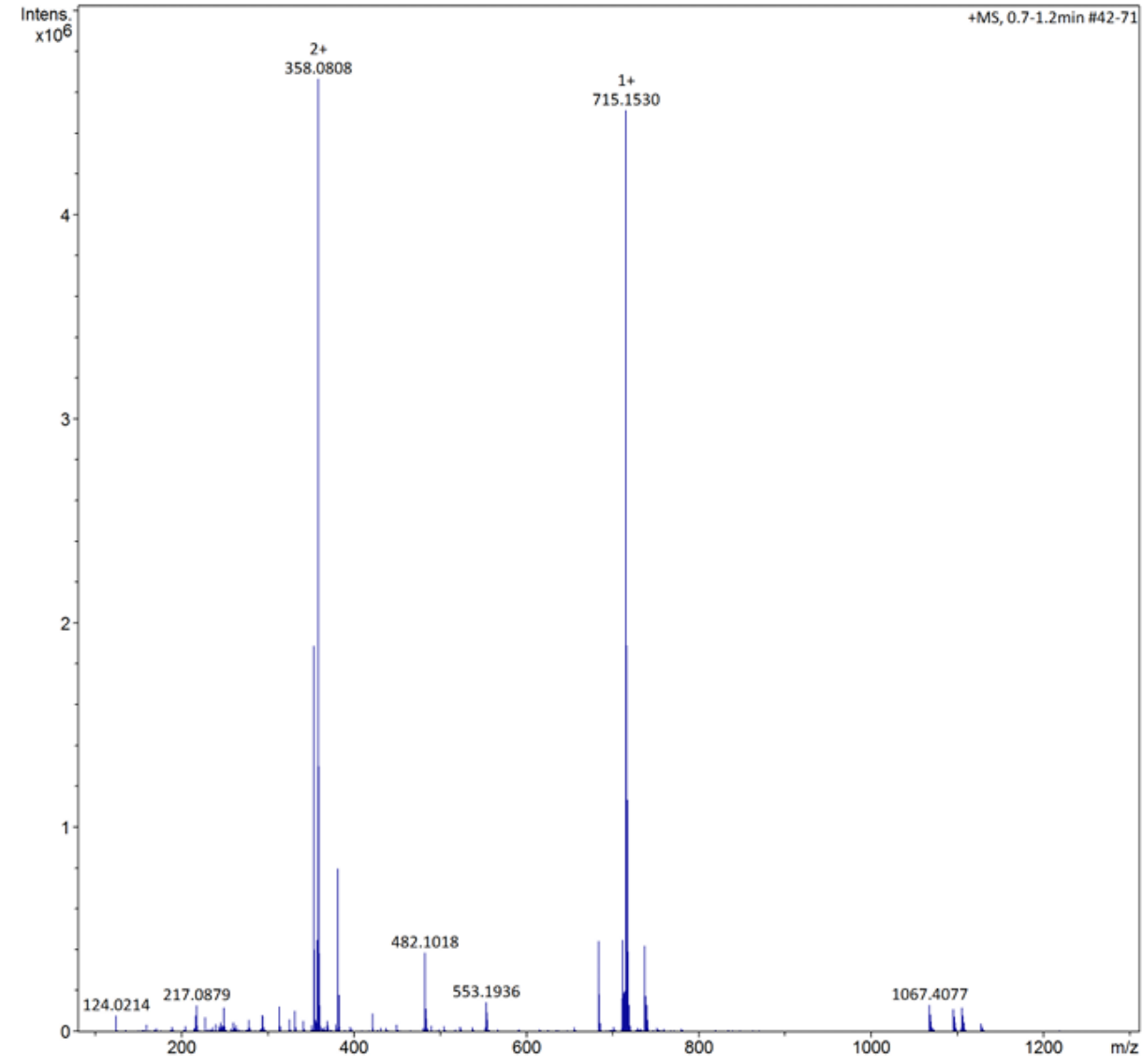


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**Figure S2. ESI-HRMS spectrum of compound L2.**

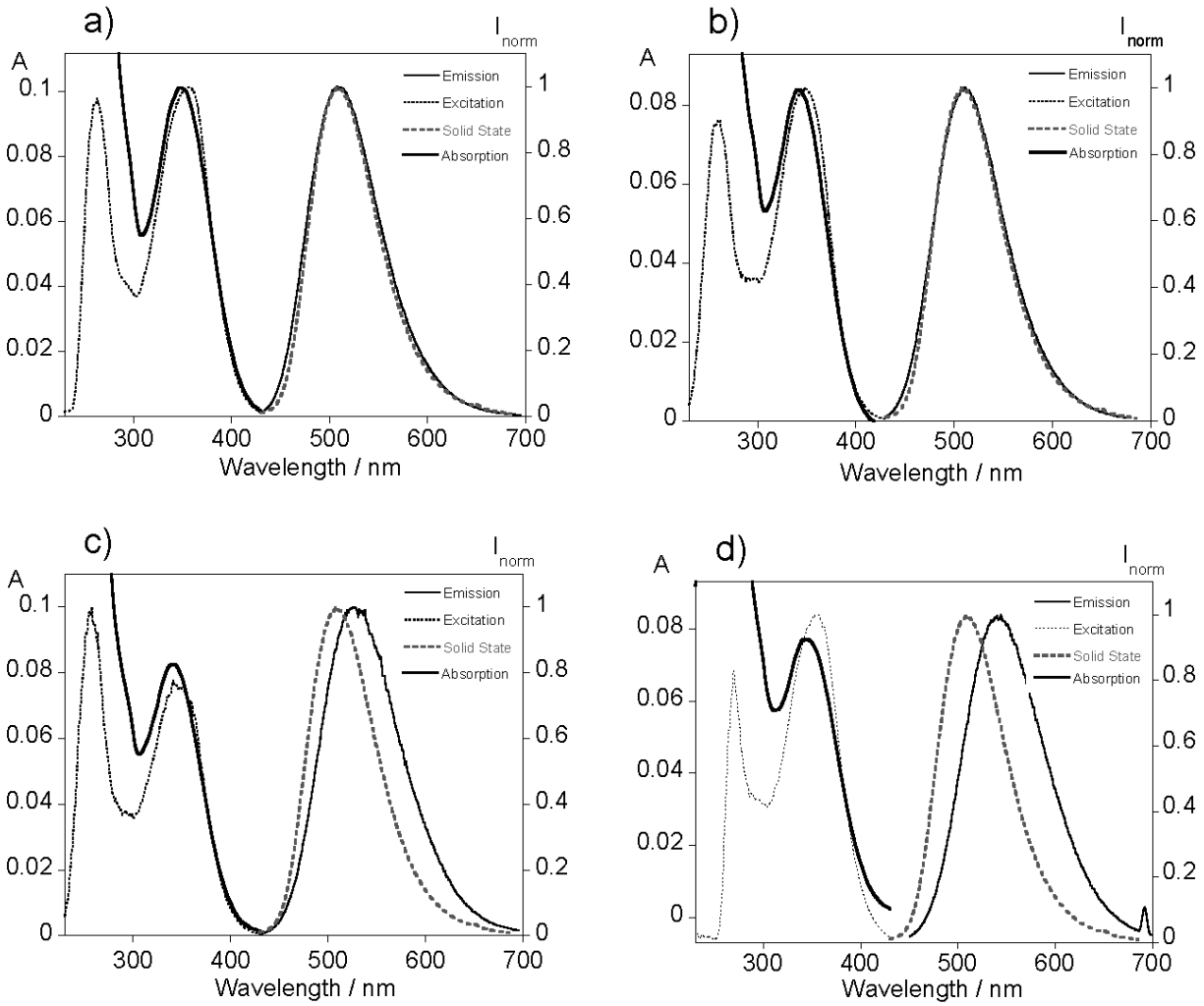



**Figure S3. Photophysical characterization of L1 in a) chloroform, b) THF, c) ethanol and d) DMSO.**

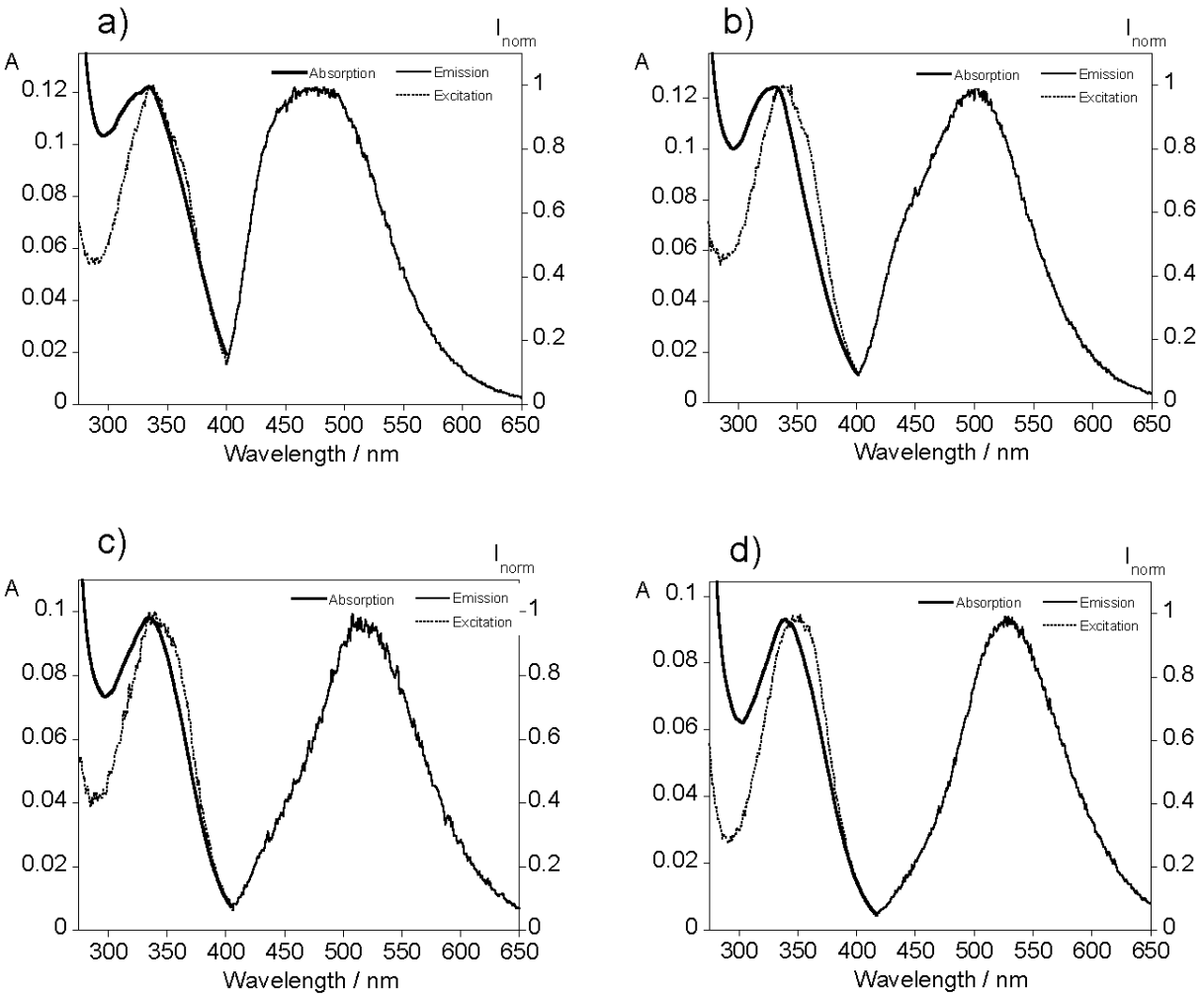



**Figure S4. Photophysical characterization of L2 in a) chloroform, b) THF, c) ethanol and d) DMSO.**

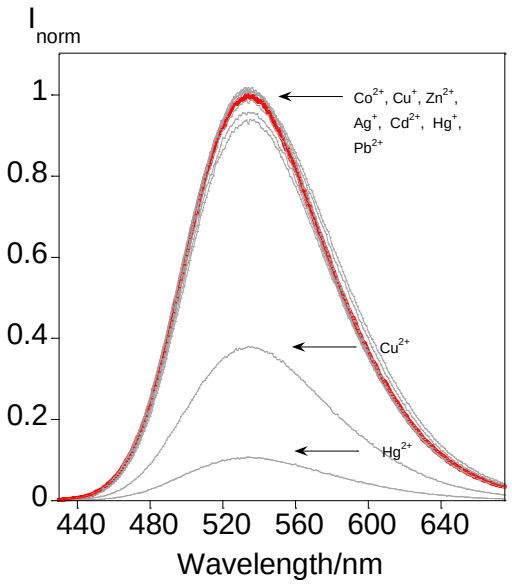



**Figure S5. Emission spectra after the addition of 1 eq. of each metal. For clarity of the reader the red spectrum corresponds L1.**

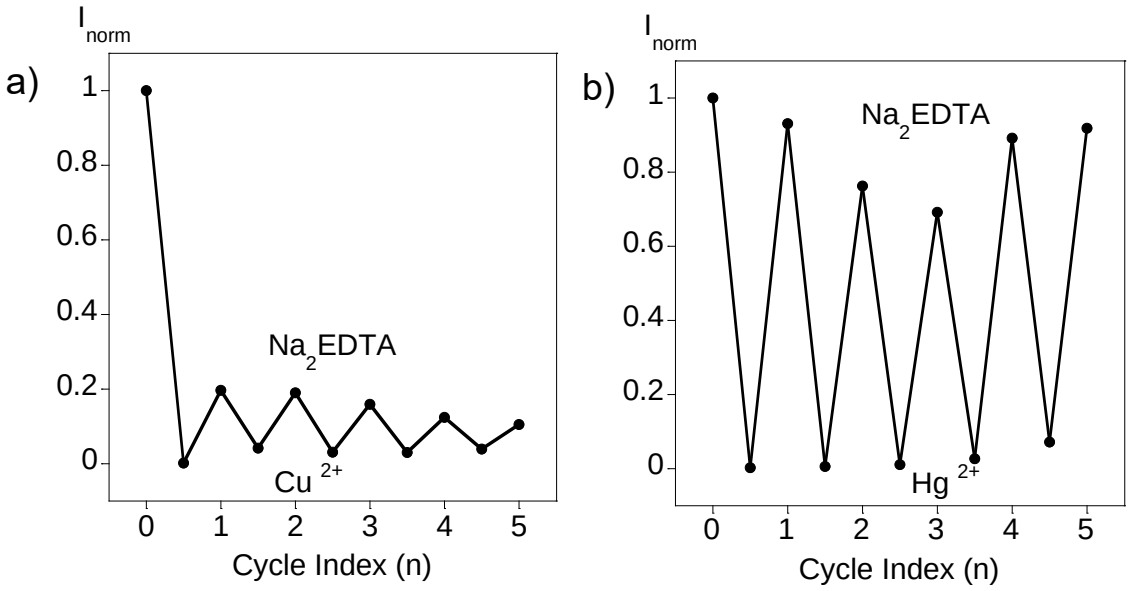



**Figure S6. Reversible changes of fluorescence intensity at 533 nm of L1 upon addition of a) $Cu^{2+}$ and b) $Hg^{2+}$ with $Na_2EDTA$ alternately.**

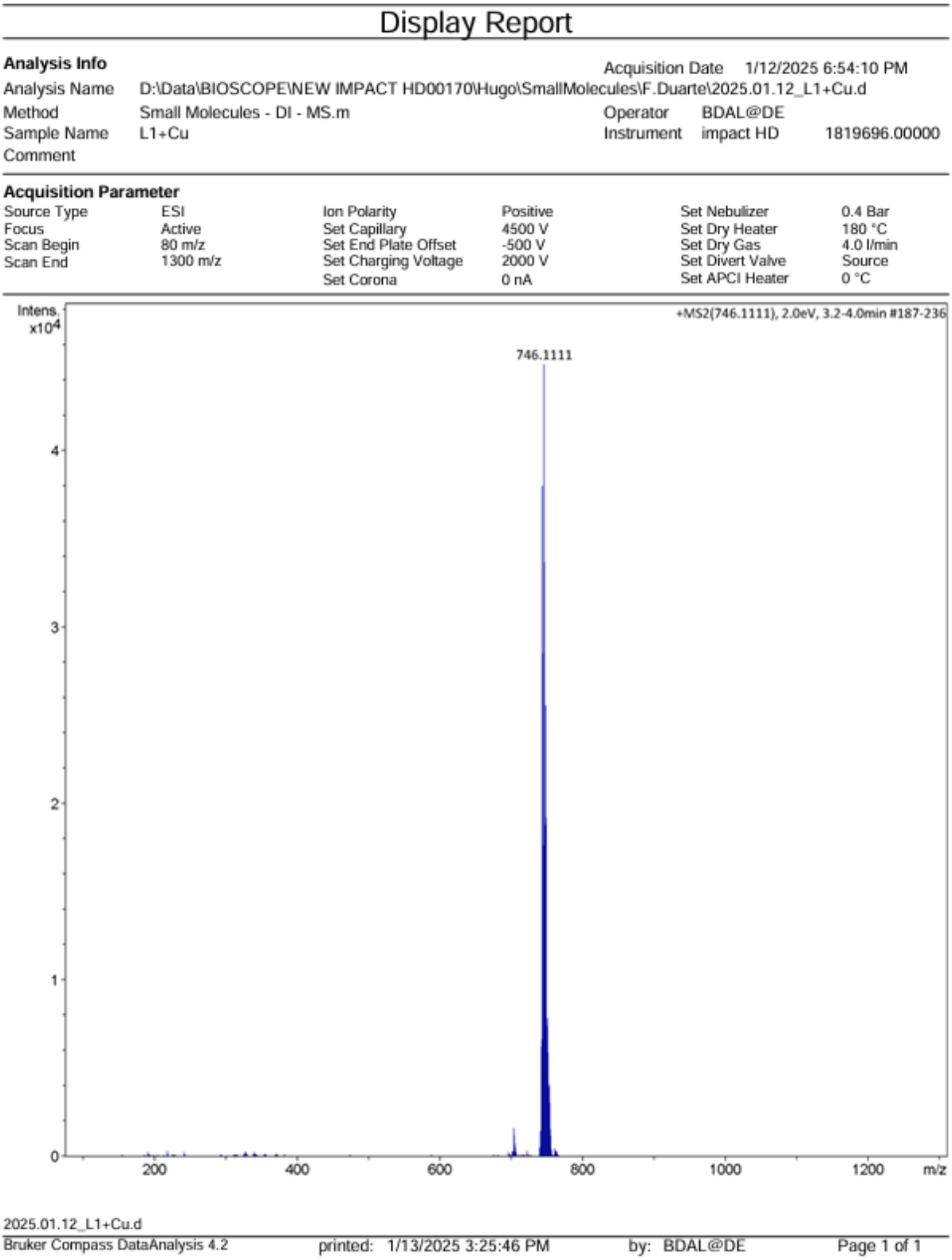



**Figure S7. ESI-HRMS spectrum of compound L1+Cu$^{2+}$ complex.**

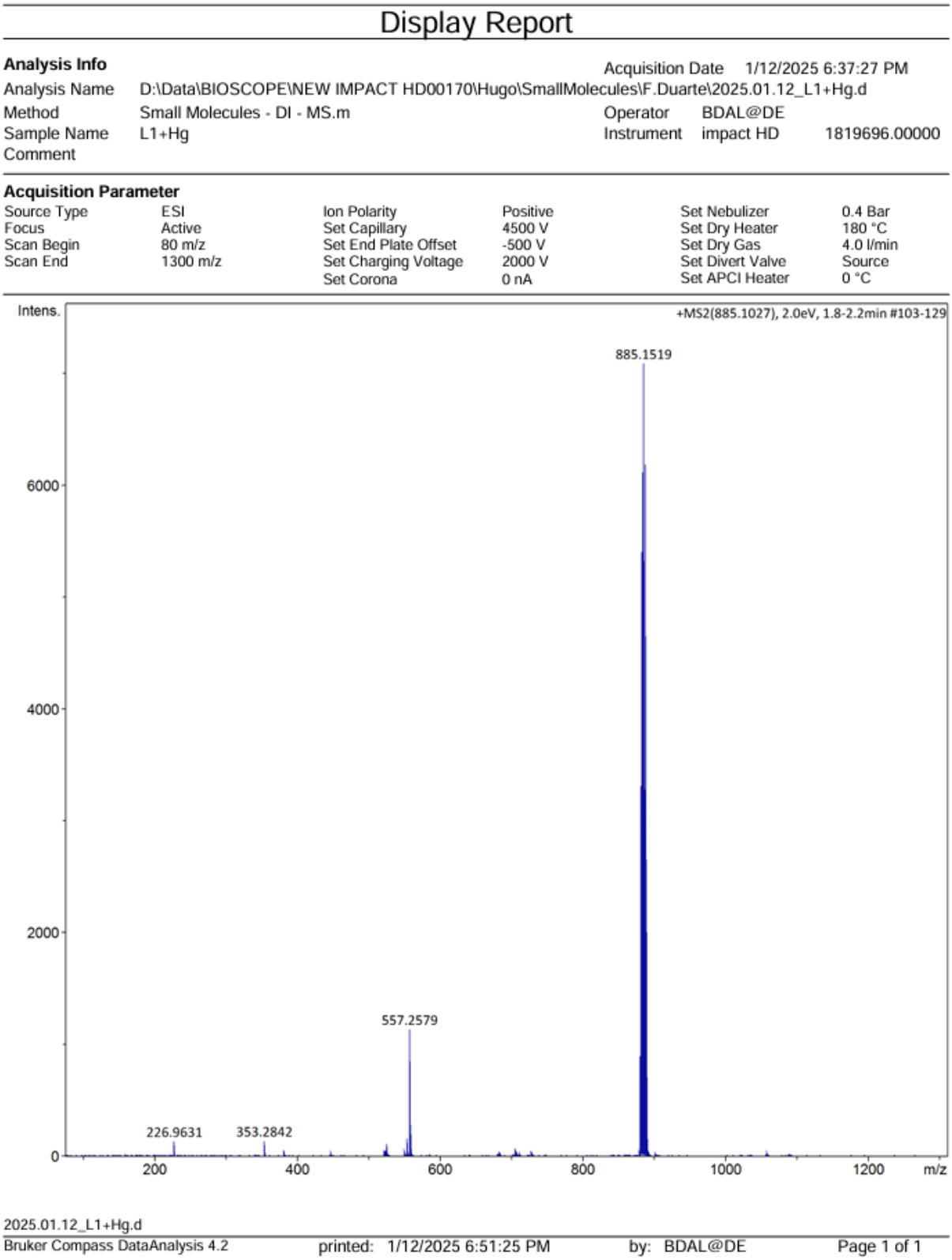



**Figure S8. ESI-HRMS spectrum of compound L1+$Hg^{2+}$ complex.**

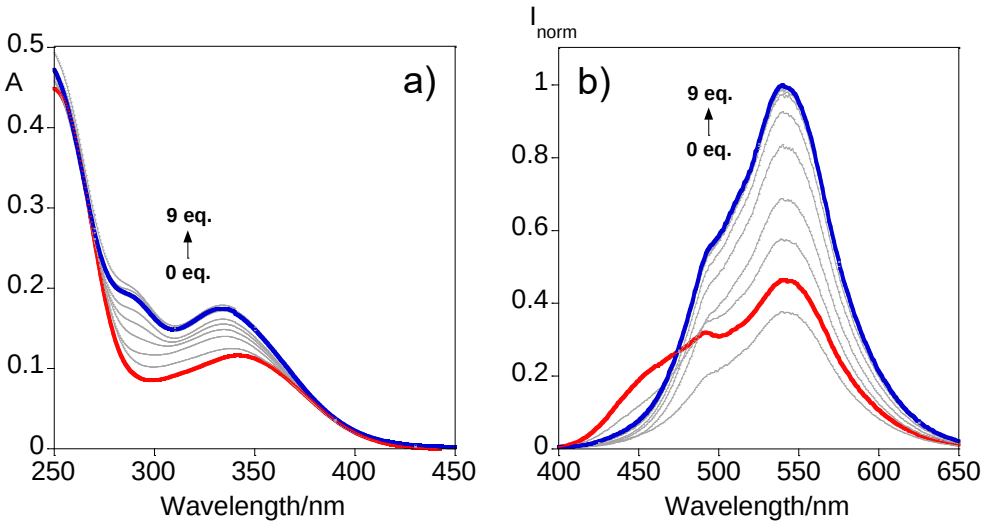



**Figure S9. UV-vis (a) and emission (performed in JASCO FP-8350) (b) spectra response after the addition of up to 9 equivalents of sodium dithionite.**

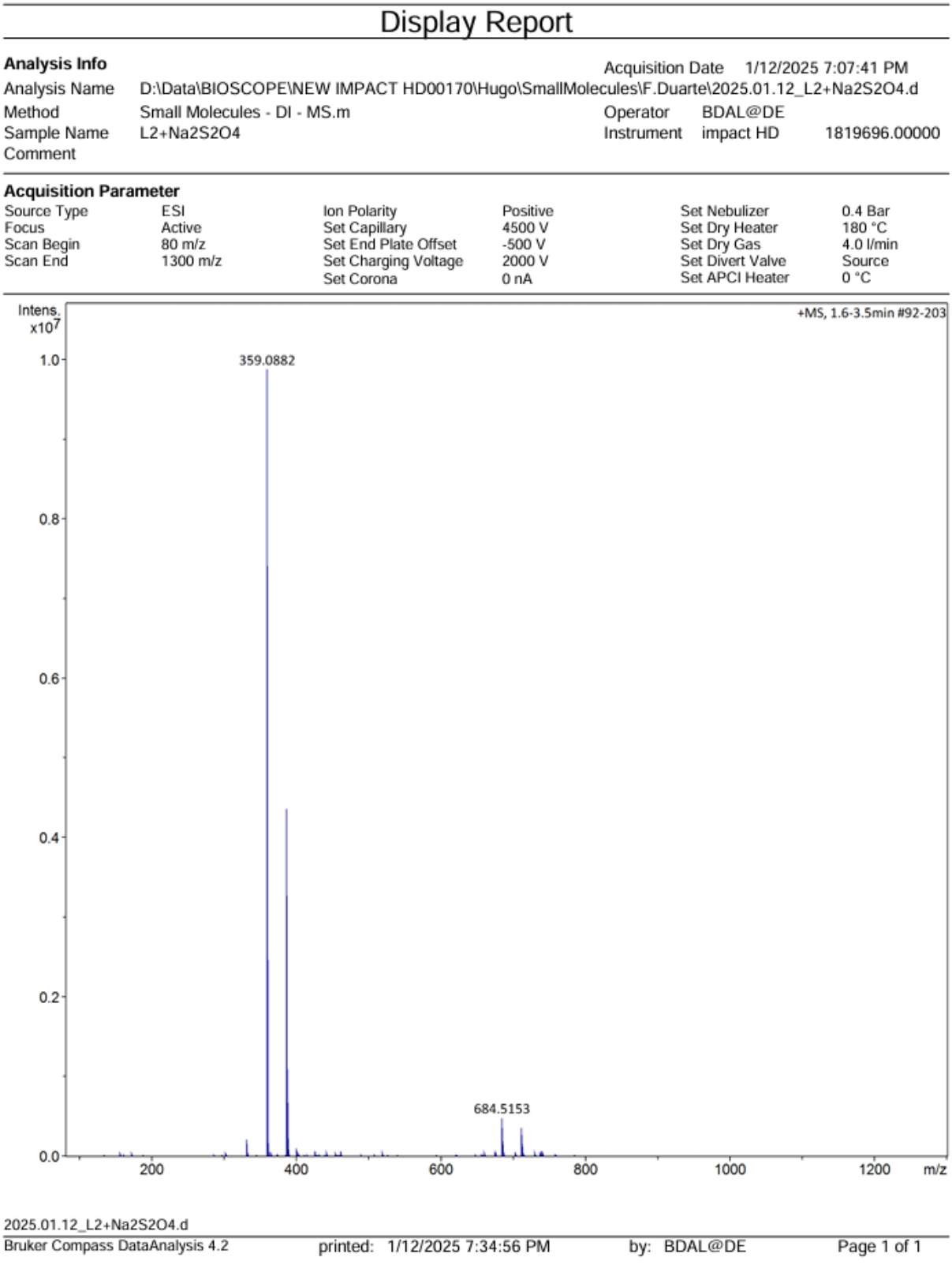


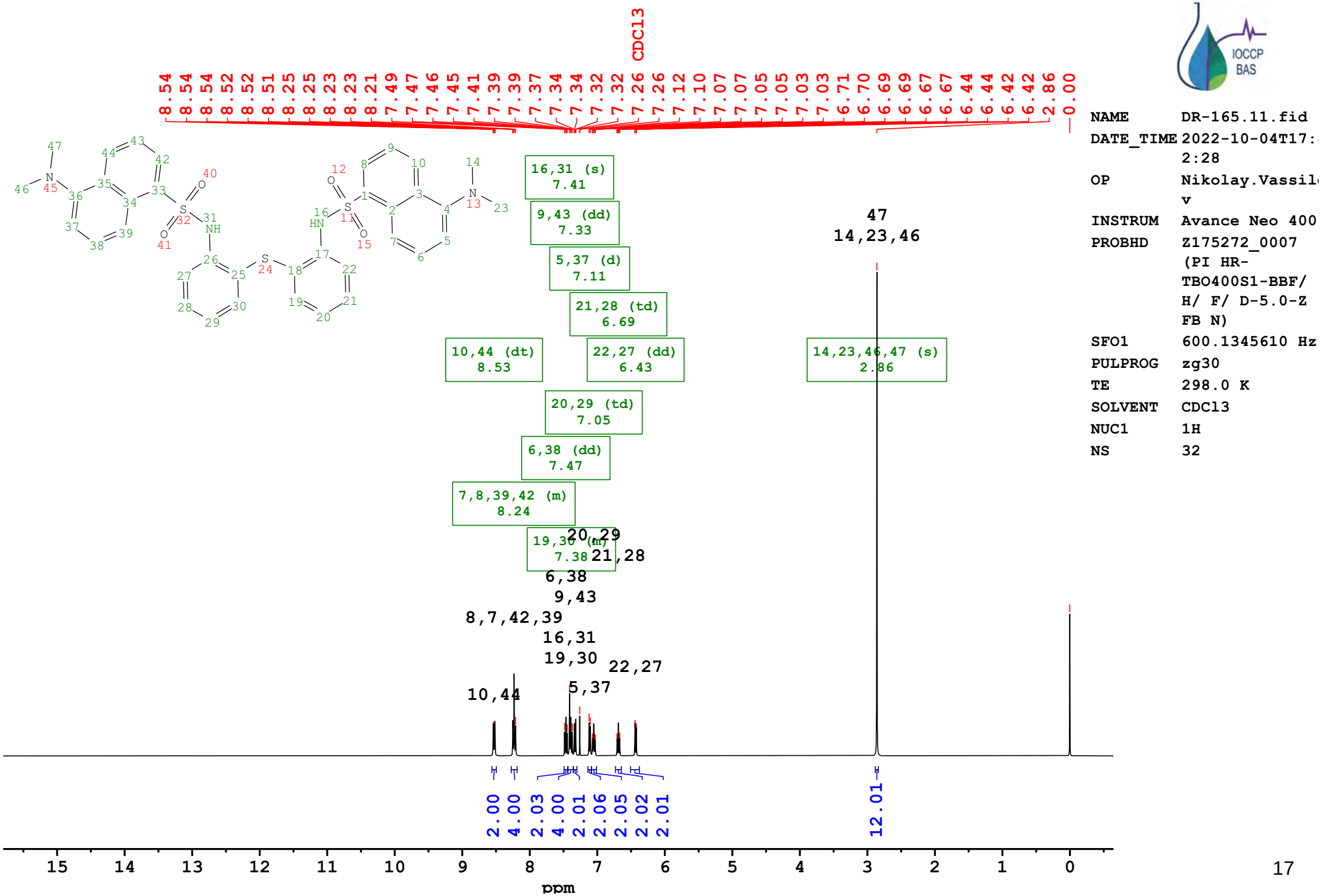

**Figure S10. ESI-HRMS spectrum of compound L2 after the addition of $Na_2S_2O_4$.**

**Determination of the limit of detection and quantification (LOD and LOQ)**

The determination of the Limit of Detection (LOD) and Limit of Quantification (LOQ) began by recording several emission intensities for L1 at the working concentration without the addition of any metal at 534 nm. The measured intensities were as follows: 3325880; 3210490; 3263120; 3208930; 3347470; 3296160; 3326780; 3251750; 3230730. The average emission intensity and its standard deviation were calculated to be 3273478 ± 49572. Using the equations provided in Section 1.5 of the experimental section, the LOD and LOQ were determined to be 3124760 and 2777751, respectively. To express the LOD and LOQ in terms of concentration, extrapolation was performed by comparing these values with the intensities obtained after each addition of metal.

Fig SX1

# L1 chloroform-d ligand only full assignment

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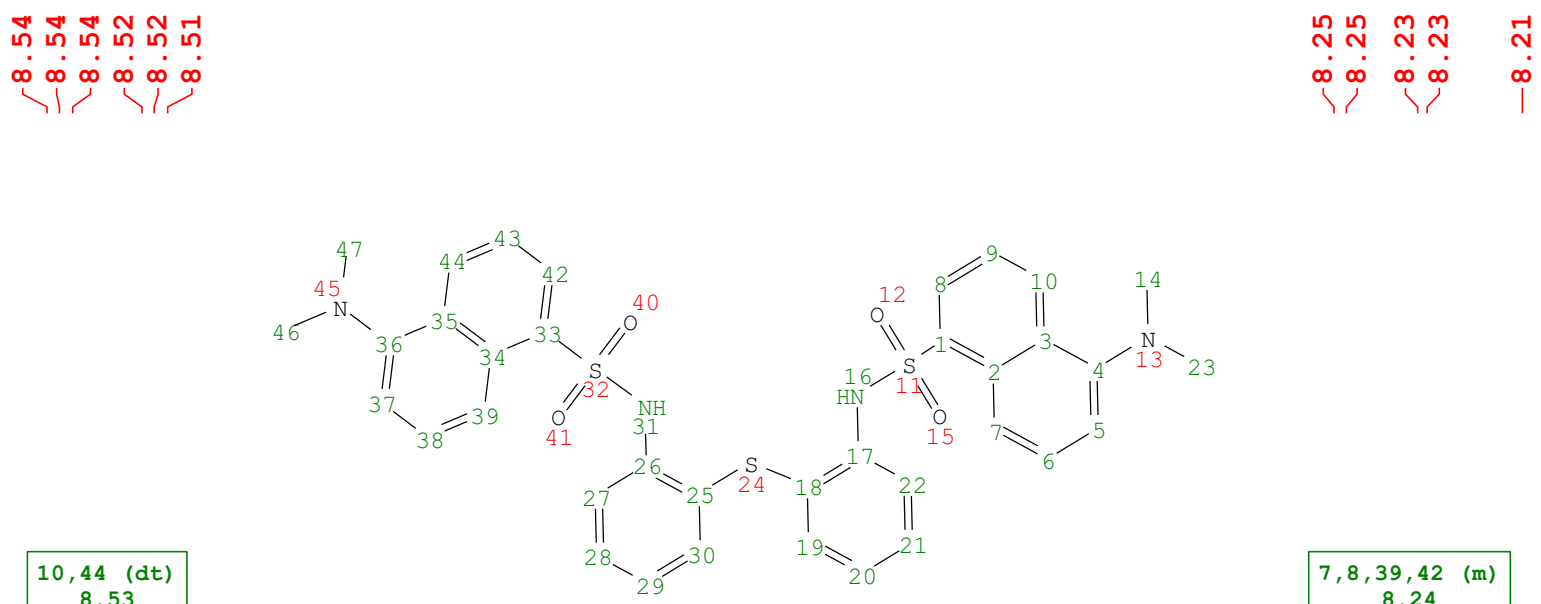
|---|---|
| NAME | DR-165.11.fid |
| DATE_TIME | 2022-10-04T17:2:28 |
| OP | Nikolay.Vassilev |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/F/D-5.0-ZFB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 32 |

Fig SX2

# L1 chloroform-d ligand only full assignment

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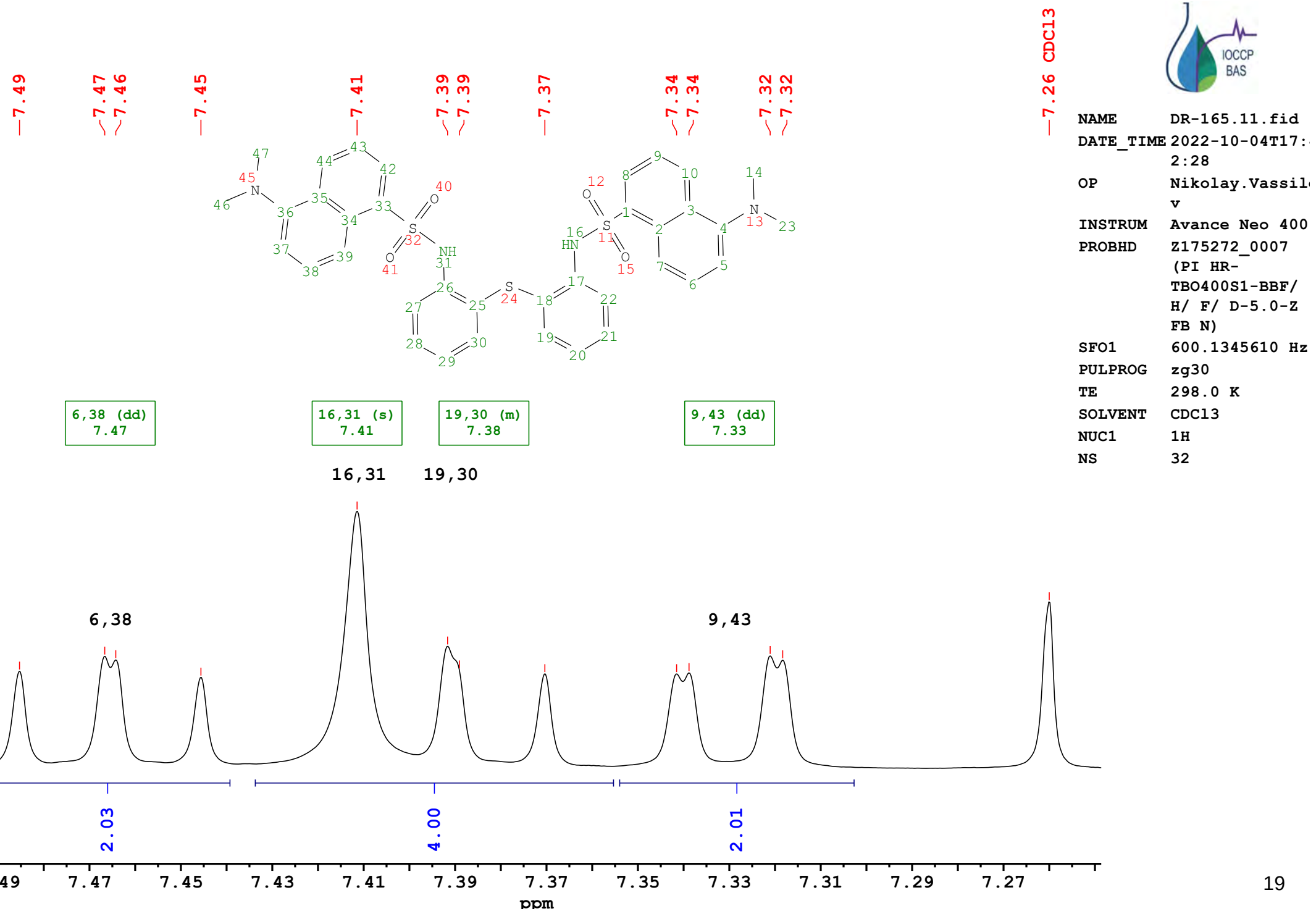
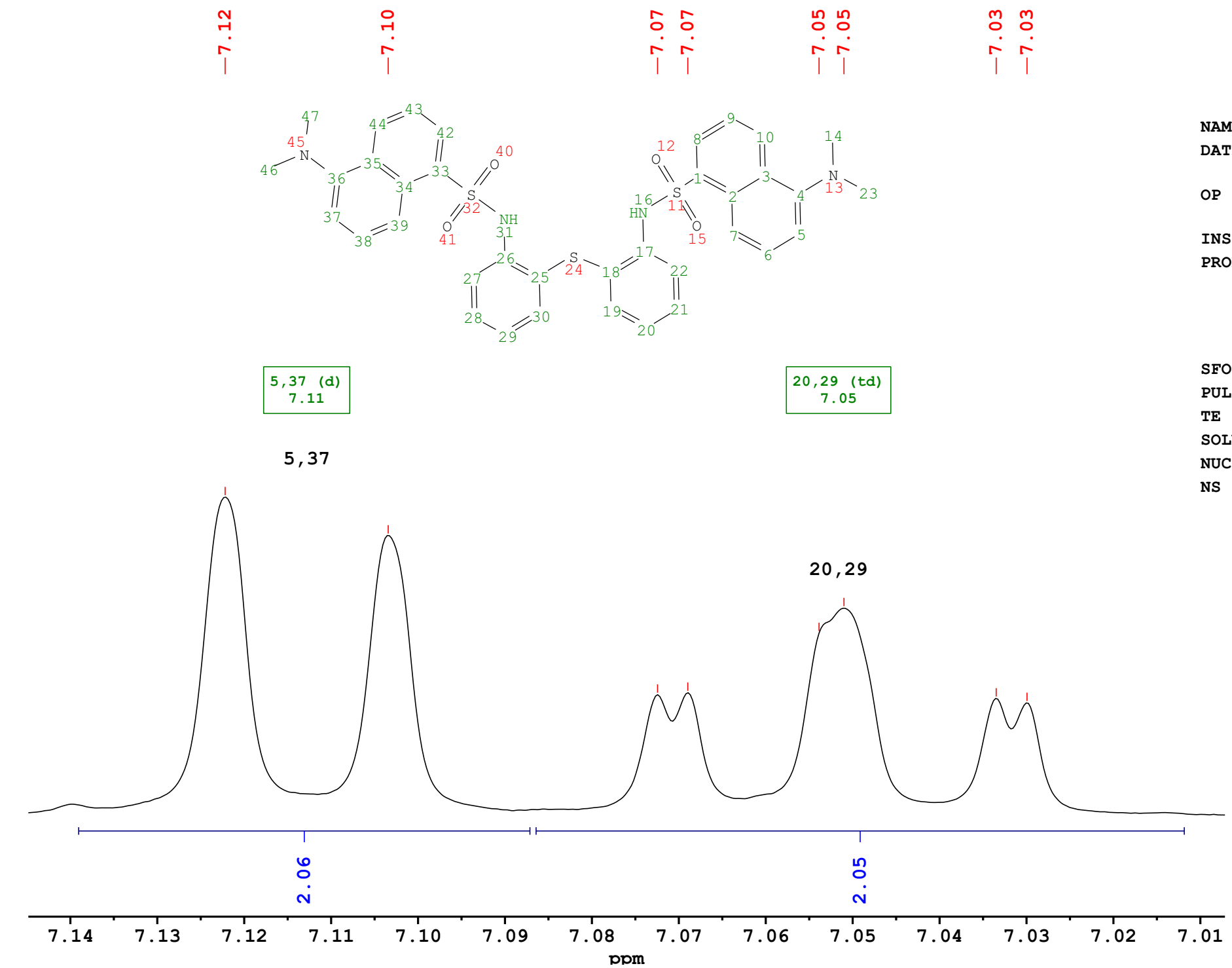
|---|---|
| NAME | DR-165.11.fid |
| DATE_TIME | 2022-10-04T17:2:28 |
| OP | Nikolay.Vassilev |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/F/D-5.0-ZFB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 32 |

**Fig SX3** **L1 chloroform-d ligand only full assignment**



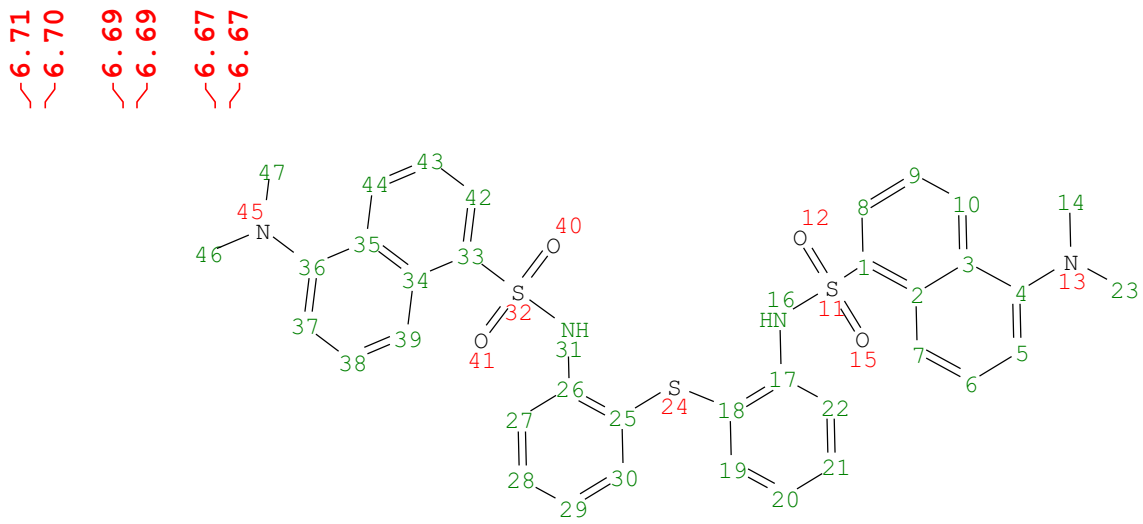

| | |
|---|---|
| NAME | DR-165.11.fid |
| DATE_TIME | 2022-10-04T17:2:28 |
| OP | Nikolay.Vassilev |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 32 |

**Fig SX4** **L1 chloroform-d ligand only full assignment**




| | |
|---|---|
| NAME | DR-165.11.fid |
| DATE_TIME | 2022-10-04T17:2:28 |
| OP | Nikolay.Vassilev |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 32 |

Fig SX5 L1 chloroform-d ligand only full assignment




21,28 (td)
6.69

22,27 (dd)
6.43

21,28

22,27

2.02

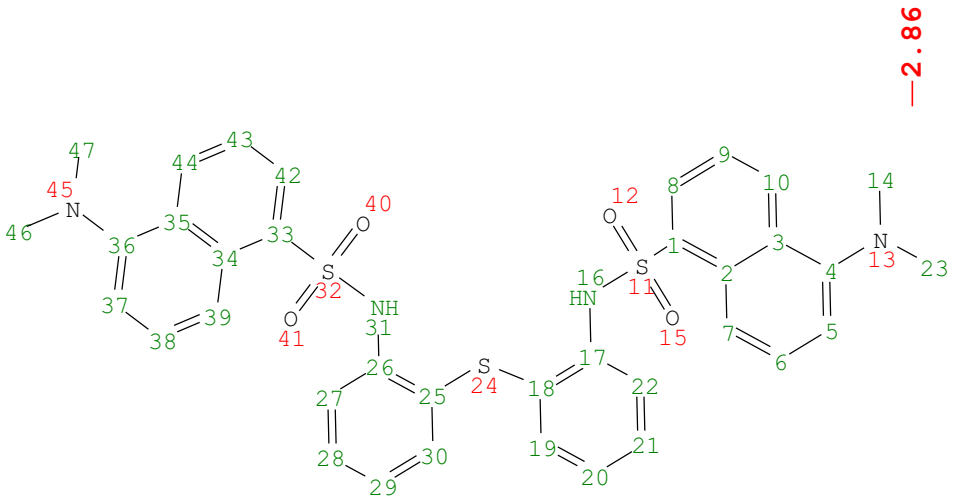
2.01

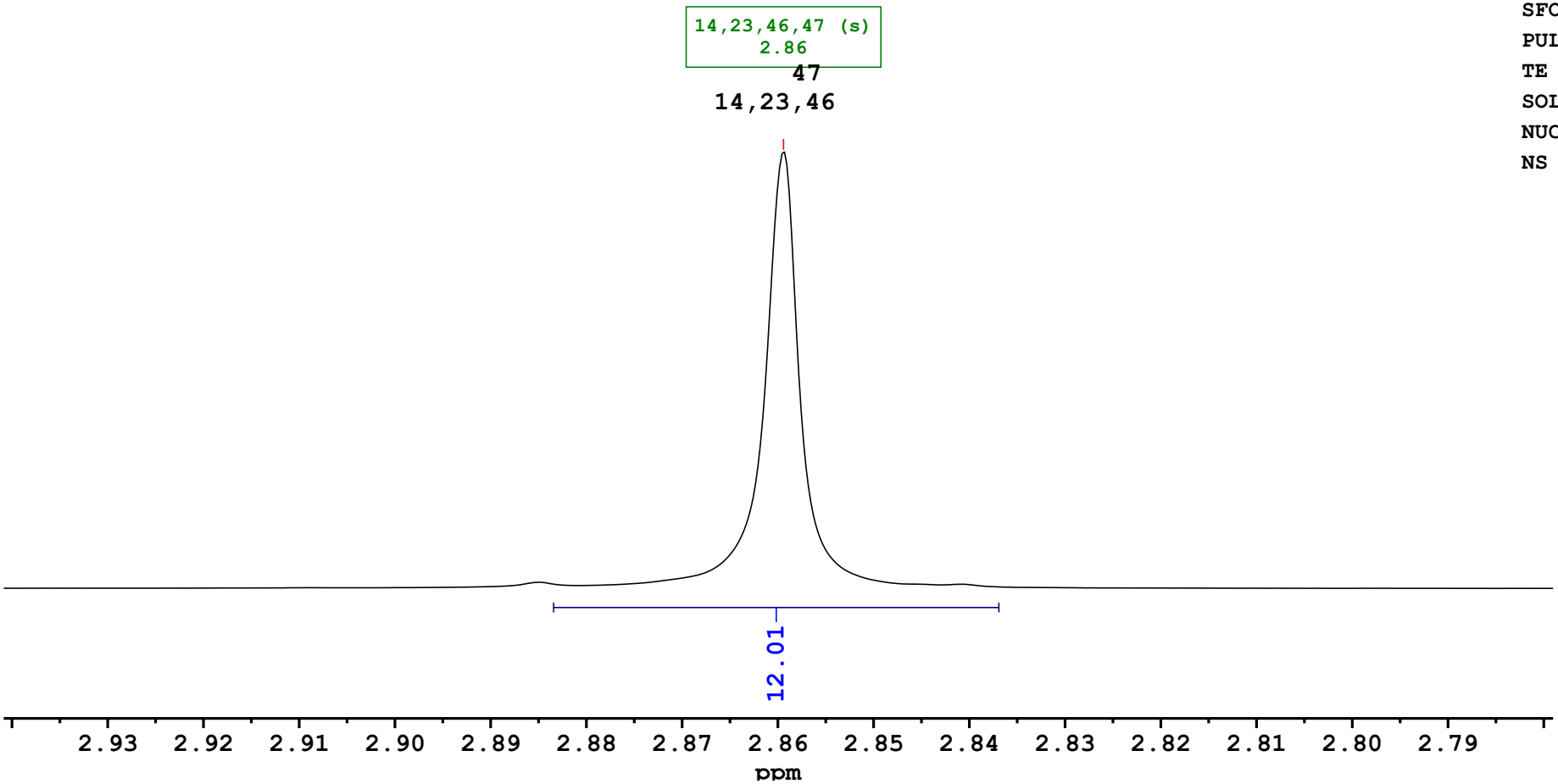
6.74 6.72 6.70 6.68 6.66 6.64 6.62 6.60 6.58 6.56 6.54 6.52 6.50 6.48 6.46 6.44 6.42 6.40 6.38

ppm

| | |
|---|---|
| NAME | DR-165.11.fid |
| DATE_TIME | 2022-10-04T17:2:28 |
| OP | Nikolay.Vassilev |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/F/D-5.0-ZFB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 32 |

**Fig SX6** **L1 chloroform-d ligand only full assignment**

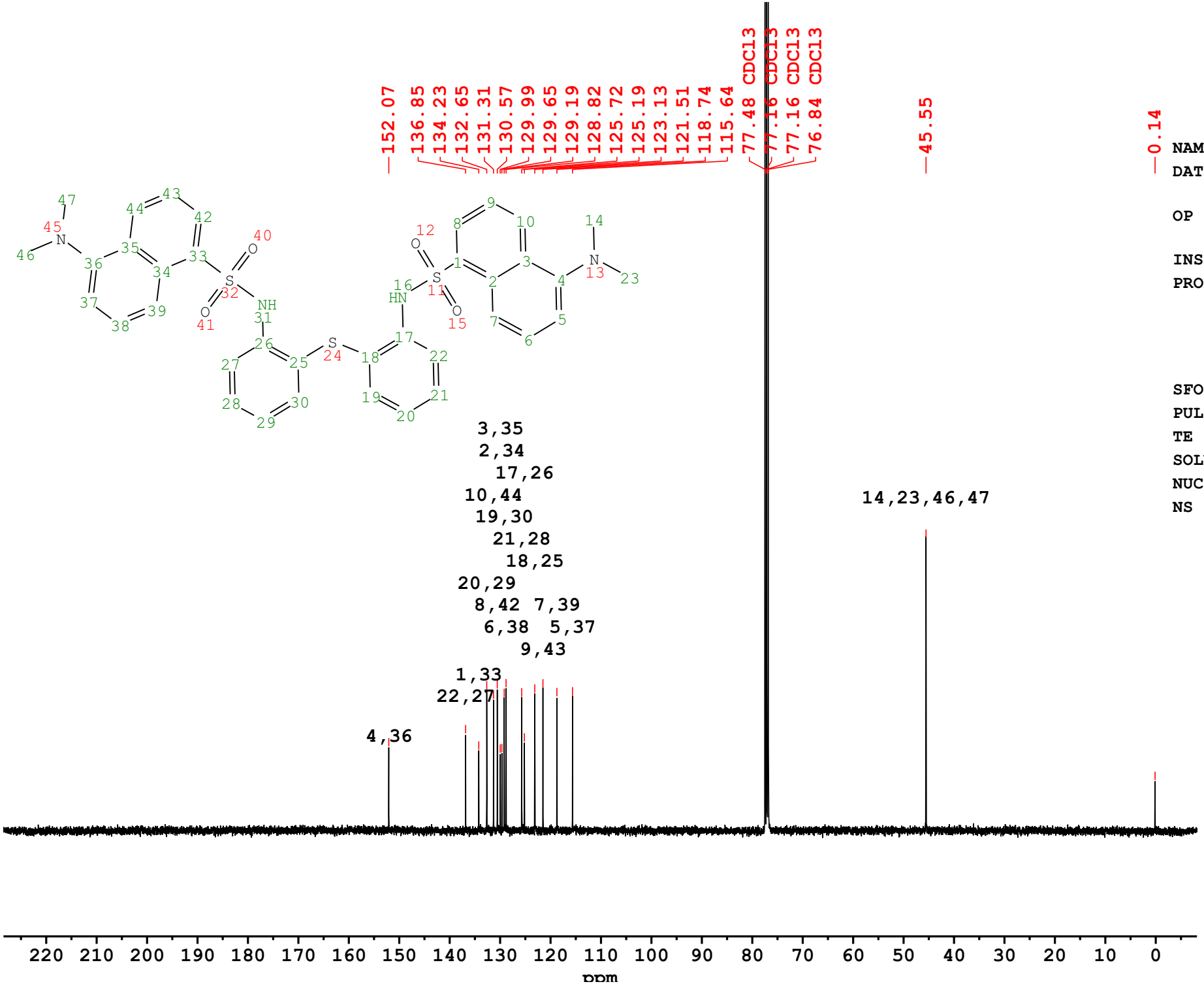



| | |
|---|---|
| NAME | DR-165.11.fid |
| DATE_TIME | 2022-10-04T17:2:28 |
| OP | Nikolay.Vassilv |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 32 |

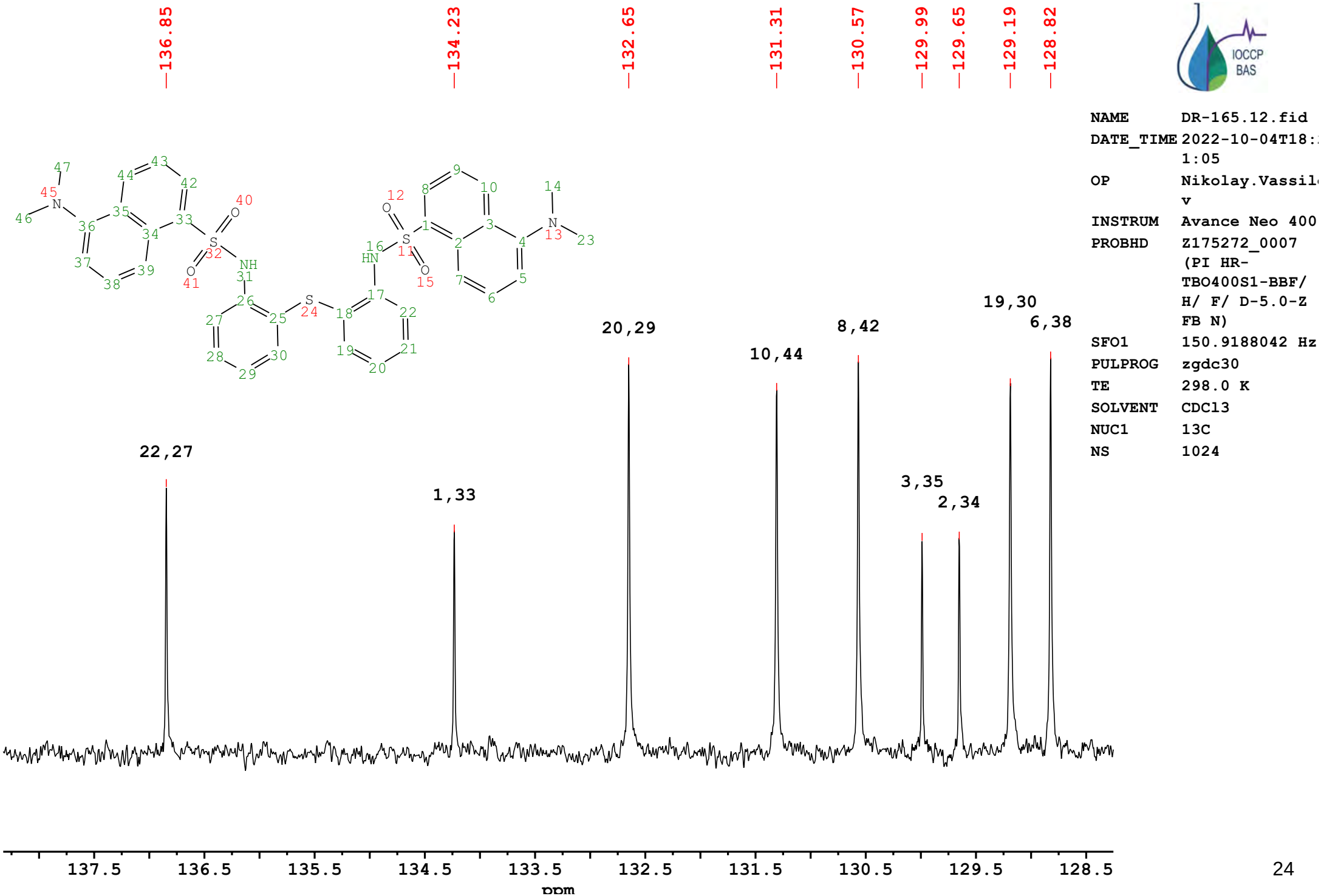
Fig SX7

# L1 chloroform-d ligand only full assignment



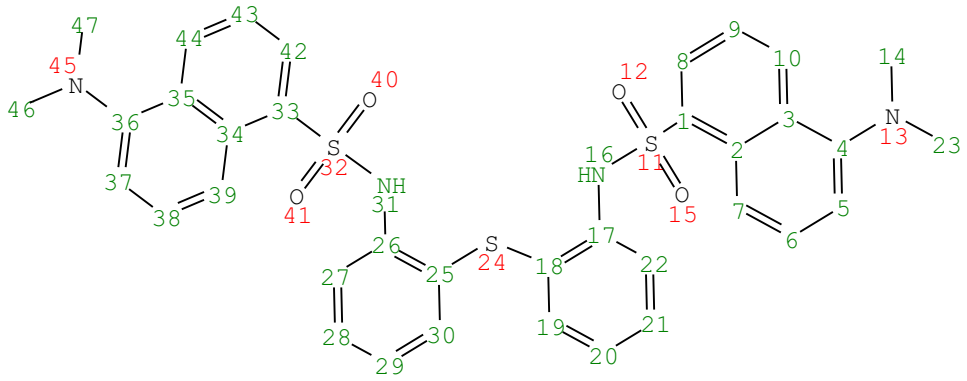

| | |
|---|---|
| NAME | DR-165.12.fid |
| DATE_TIME | 2022-10-04T18:1:05 |
| OP | Nikolay.Vassilv |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 13C |
| NS | 1024 |

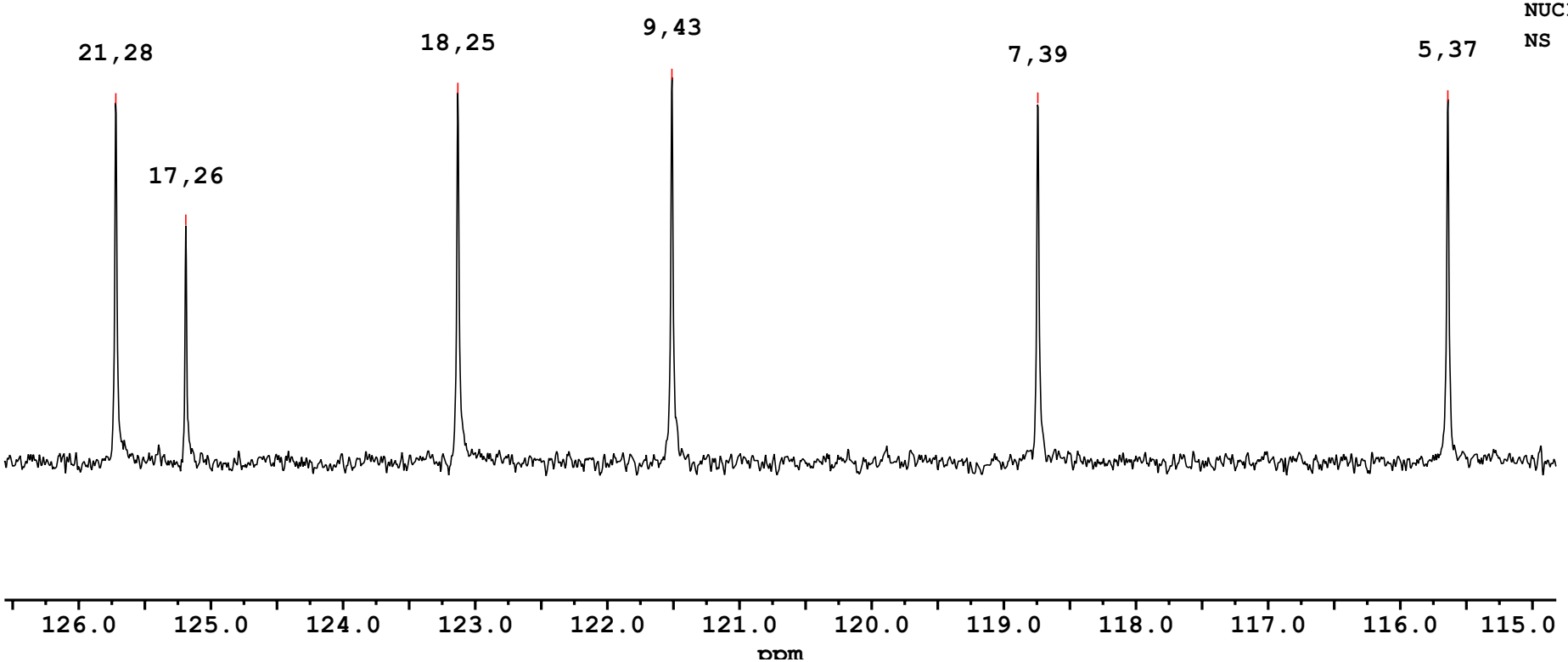
Fig SX8 L1 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-165.12.fid |
| DATE_TIME | 2022-10-04T18:1:05 |
| OP | Nikolay.Vassilev |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 13C |
| NS | 1024 |

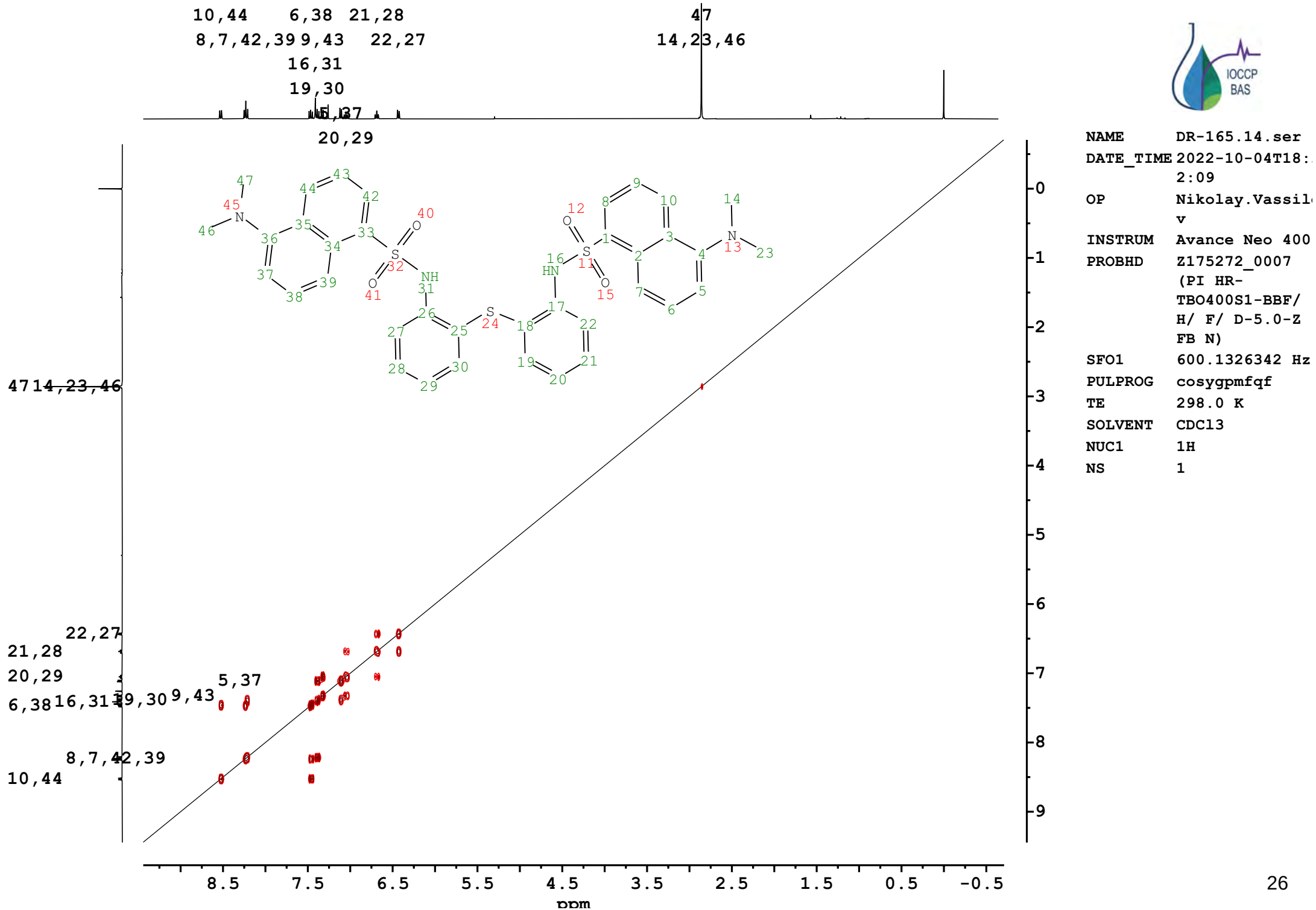
Fig SX9 L1 chloroform-d ligand only full assignment






| | |
|---|---|
| NAME | DR-165.12.fid |
| DATE_TIME | 2022-10-04T18:1:05 |
| OP | Nikolay.Vassilev |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 13C |
| NS | 1024 |

Fig SX10 L1 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-165.14.ser |
| DATE_TIME | 2022-10-04T18:2:09 |
| OP | Nikolay.Vassilev |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 1 |

Fig SX11 L1 chloroform-d ligand only full assignment

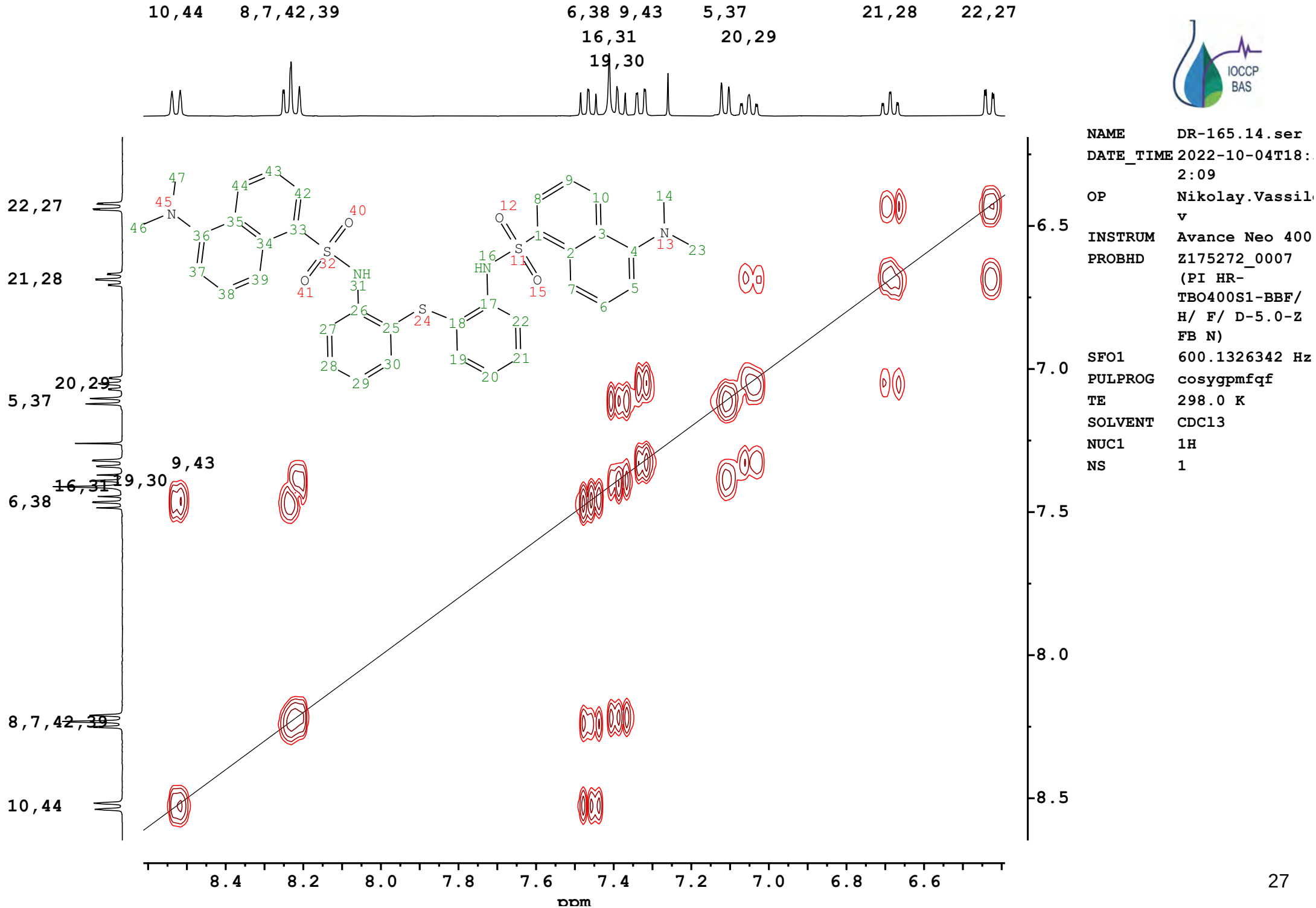
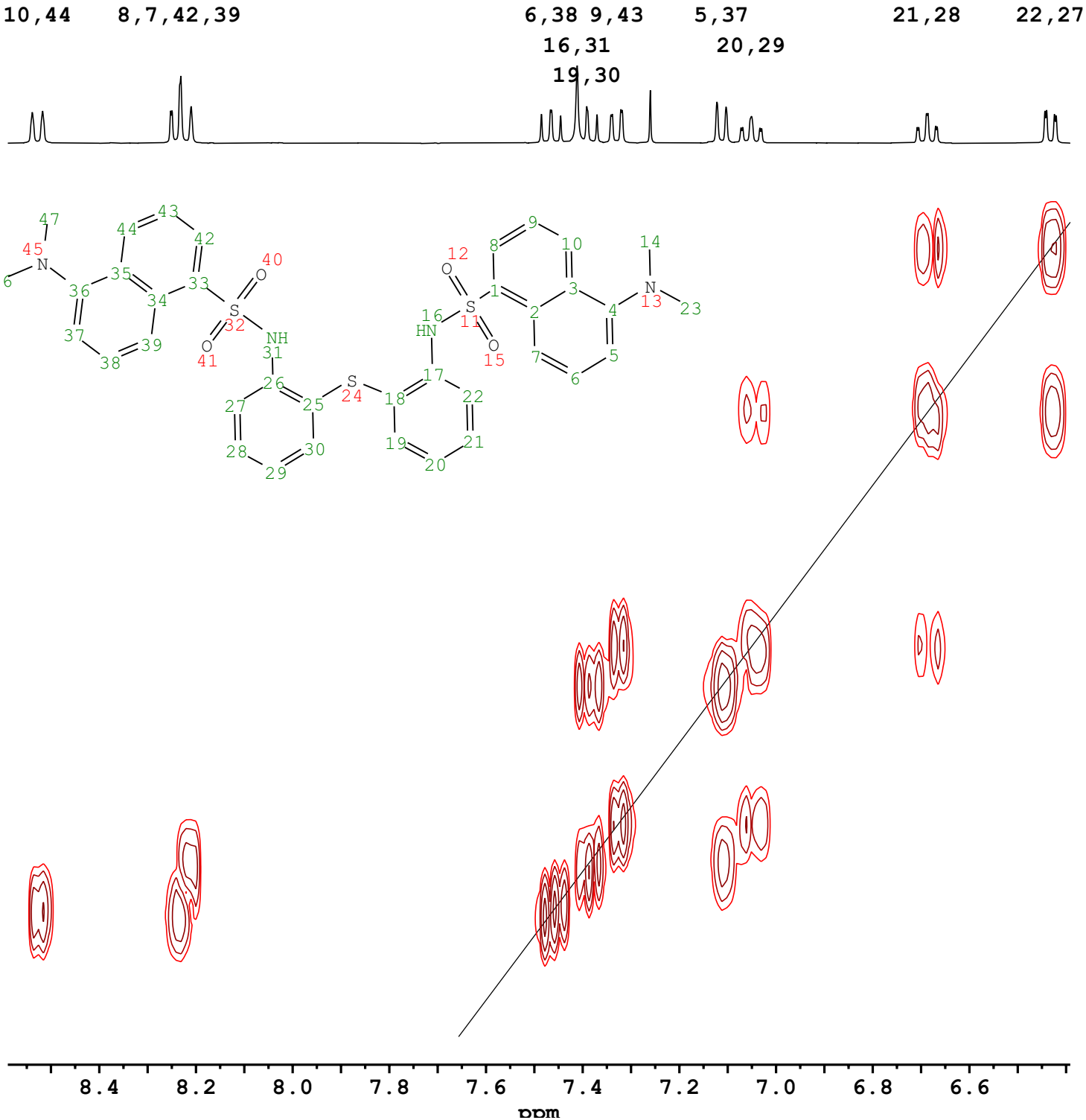


Fig SX12 L1 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-165.14.ser |
| DATE_TIME | 2022-10-04T18:2:09 |
| OP | Nikolay.Vassilev |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 1 |

Fig SX13 L1 chloroform-d ligand only full assignment

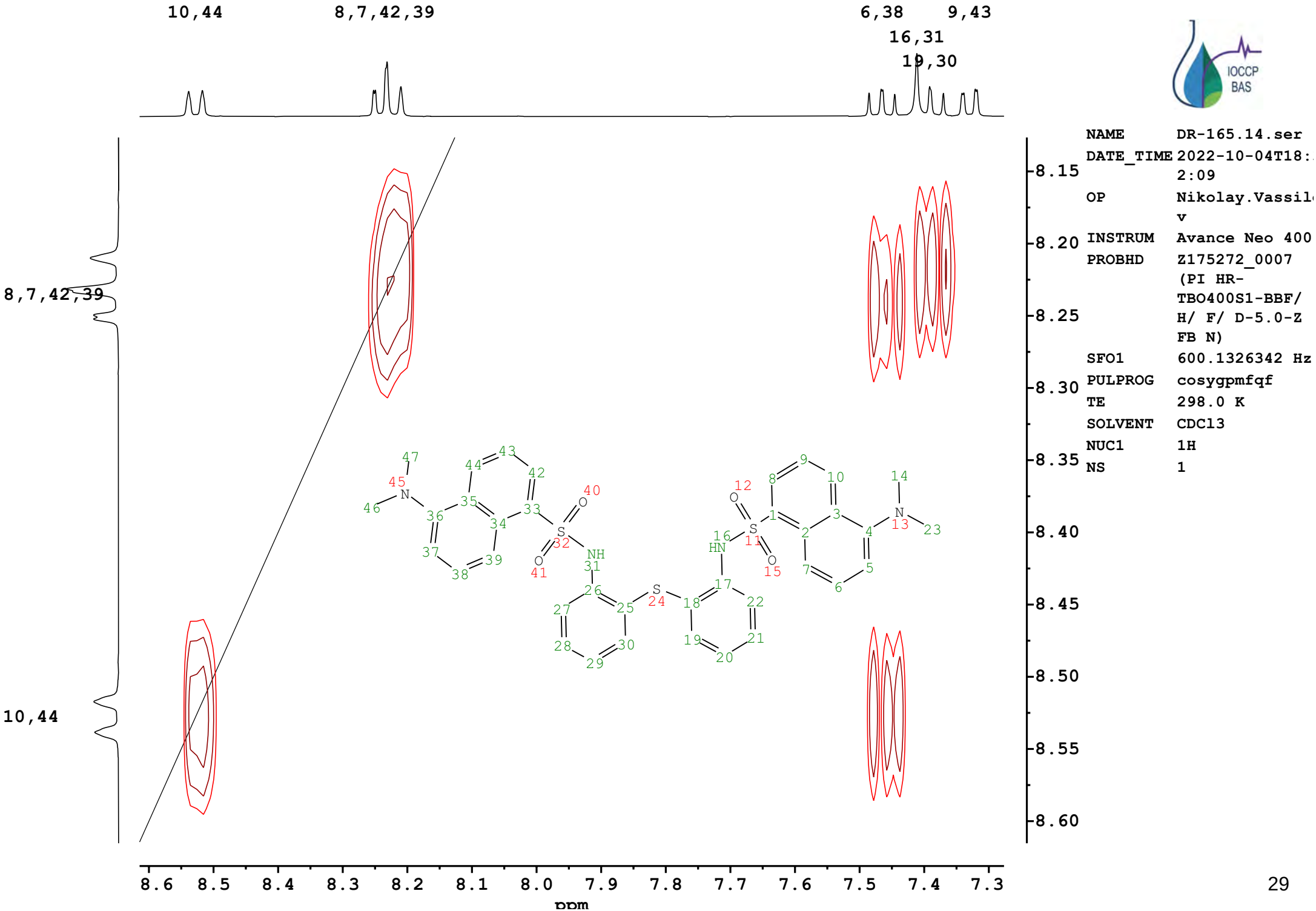
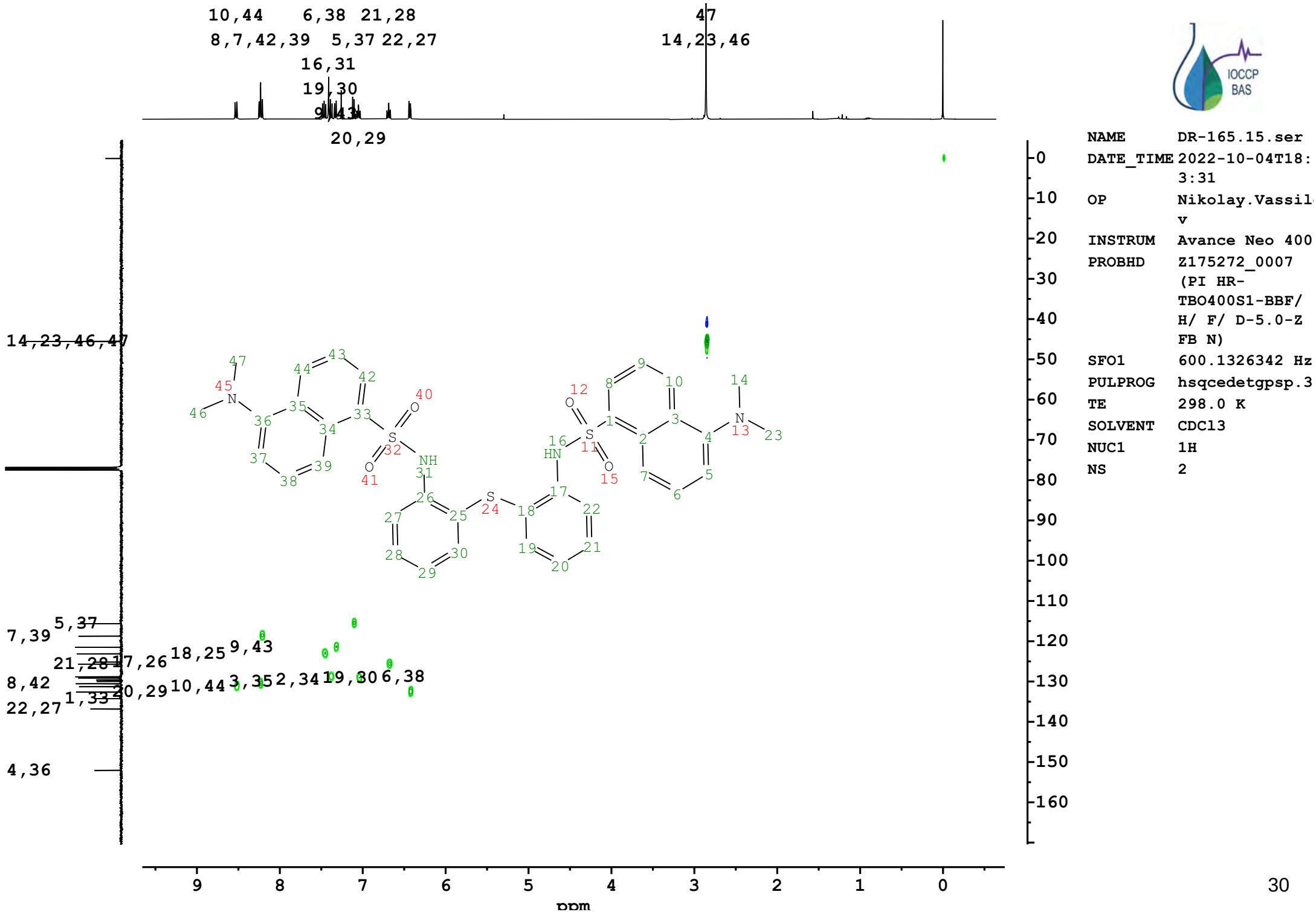
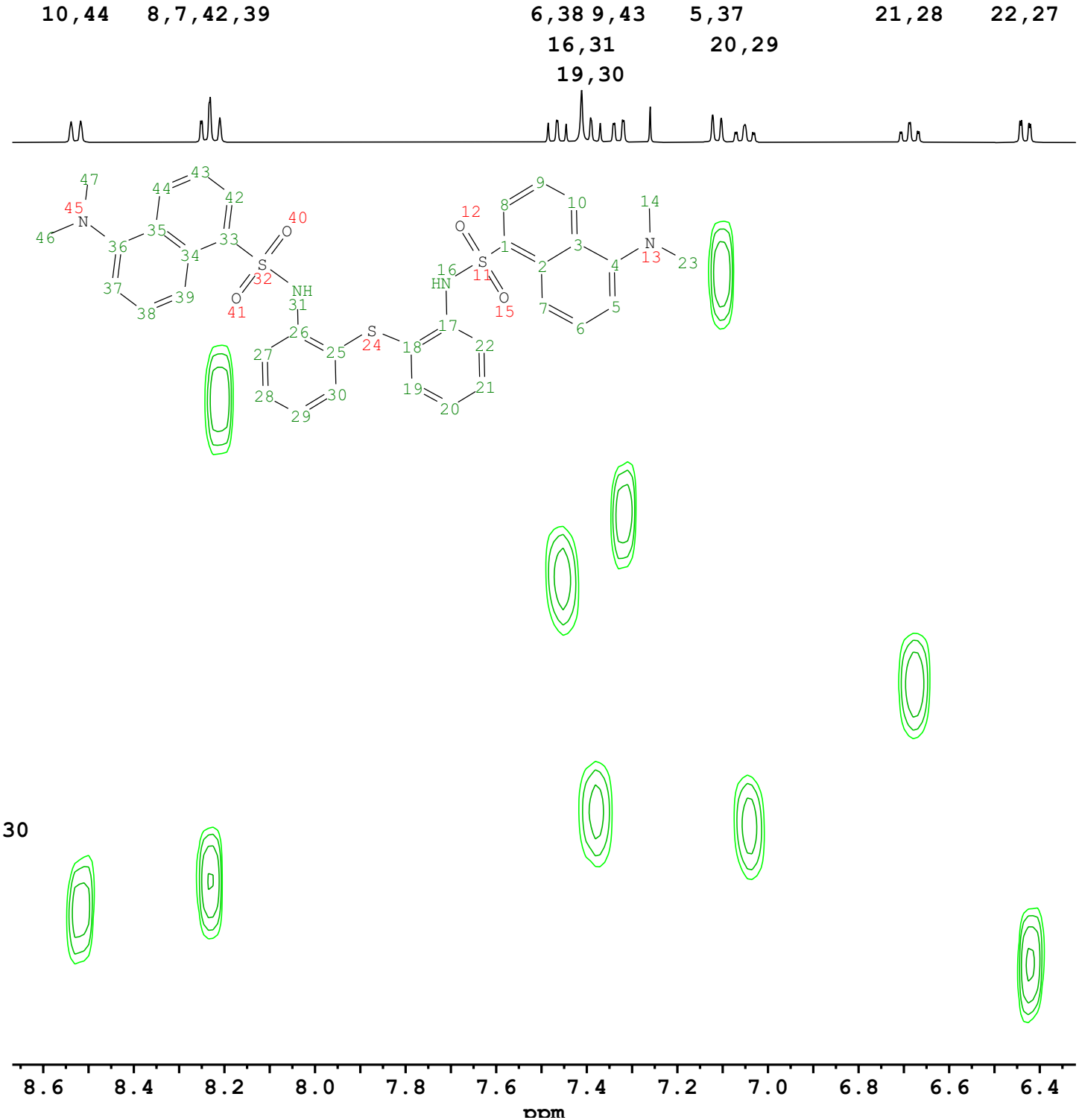


Fig SX14 L1 chloroform-d ligand only full assignment



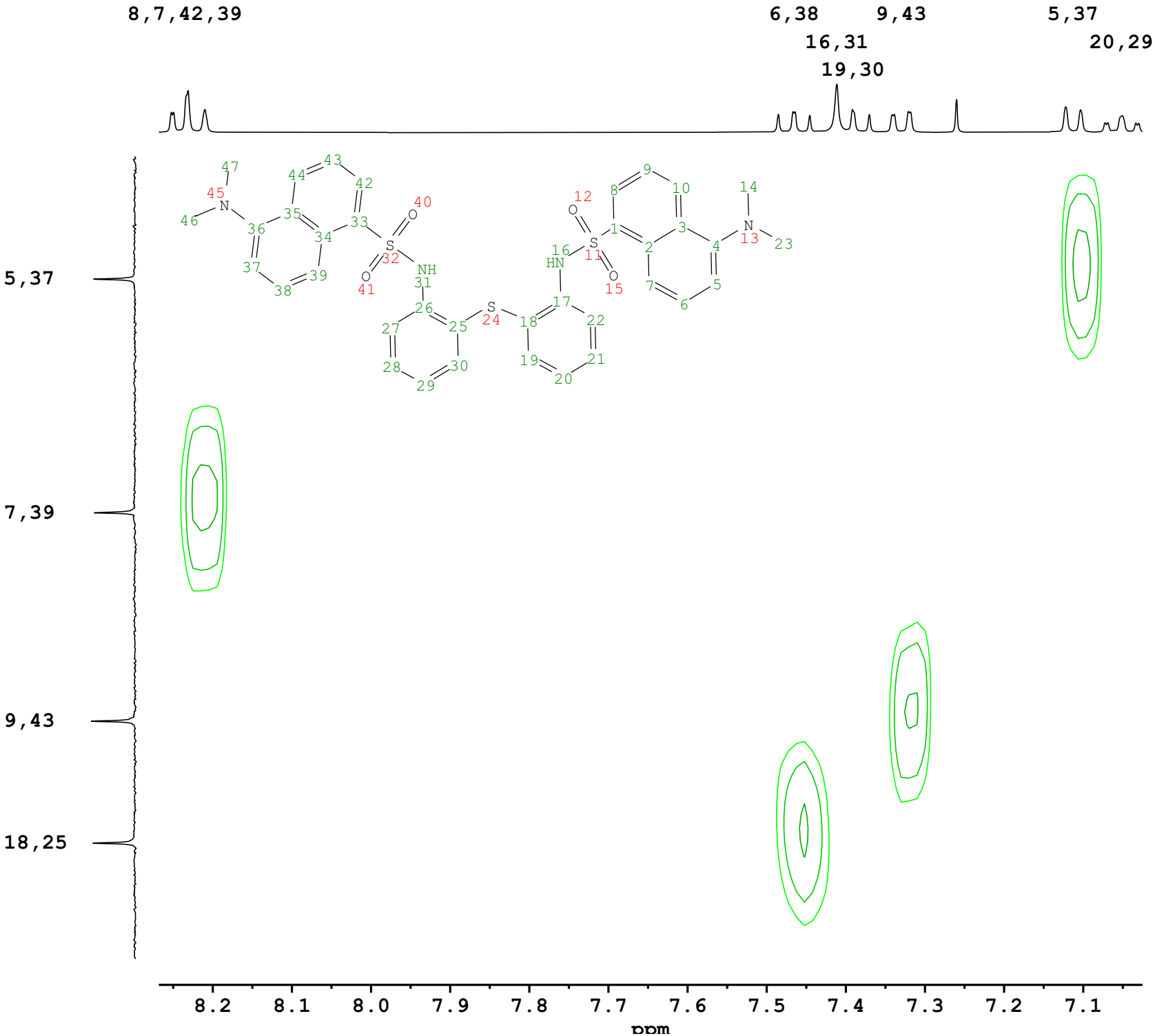

NAME DR-165.15.ser
DATE_TIME 2022-10-04T18:3:31
OP Nikolay.Vassilv
INSTRUM Avance Neo 400
PROBHD Z175272_0007 (PI HR-TBO400S1-BBF/H/ F/ D-5.0-Z FB N)
SFO1 600.1326342 Hz
PULPROG hsqcedetgpsp.3
TE 298.0 K
SOLVENT CDCl3
NUC1 1H
NS 2

Fig SX15 L1 chloroform-d ligand only full assignment



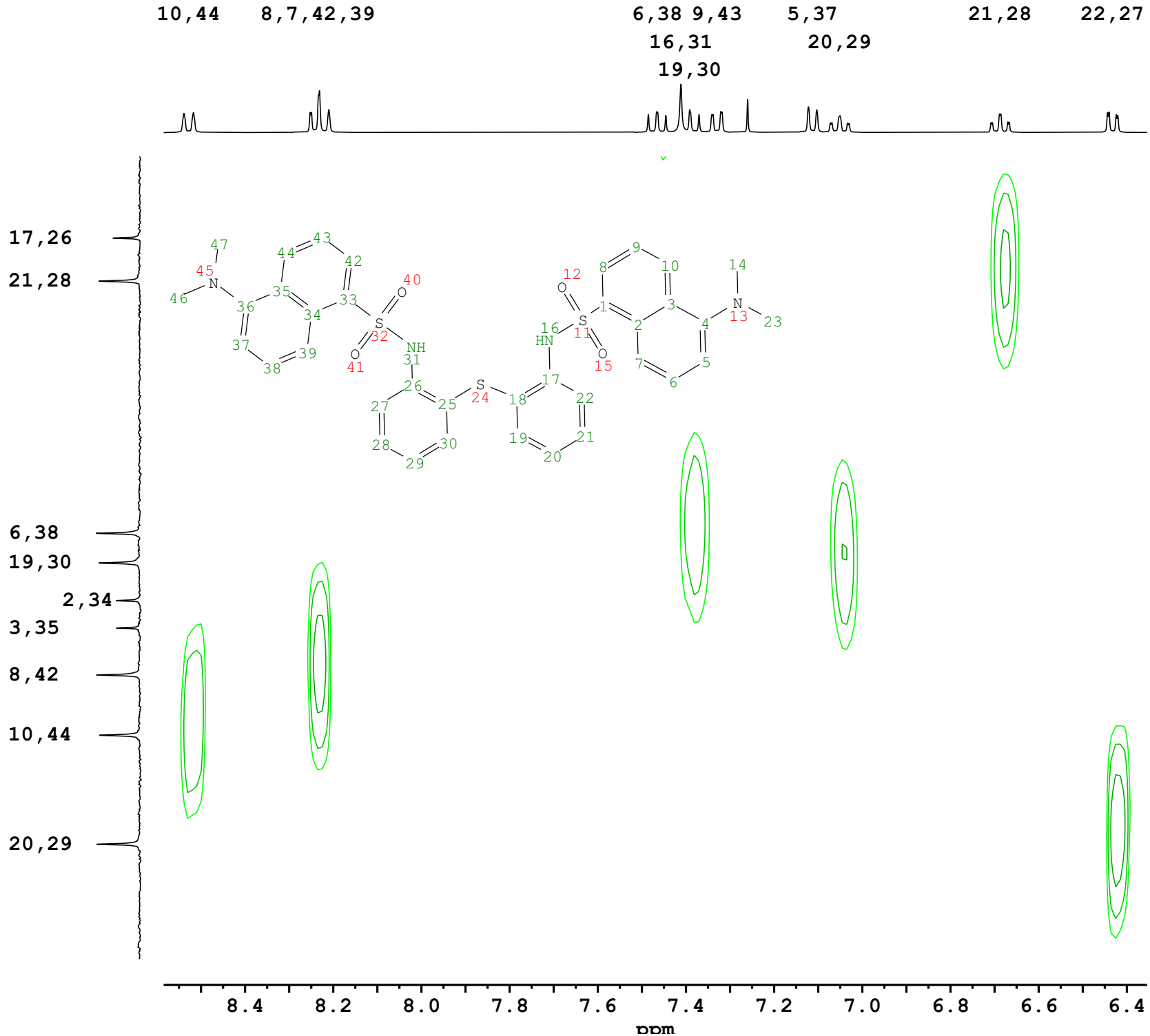

| | |
|---|---|
| NAME | DR-165.15.ser |
| DATE_TIME | 2022-10-04T18:3:31 |
| OP | Nikolay.Vassilv |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 2 |

Fig SX16 L1 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-165.15.ser |
| DATE_TIME | 2022-10-04T18:3:31 |
| OP | Nikolay.Vassilv |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 2 |

Fig SX17 L1 chloroform-d ligand only full assignment

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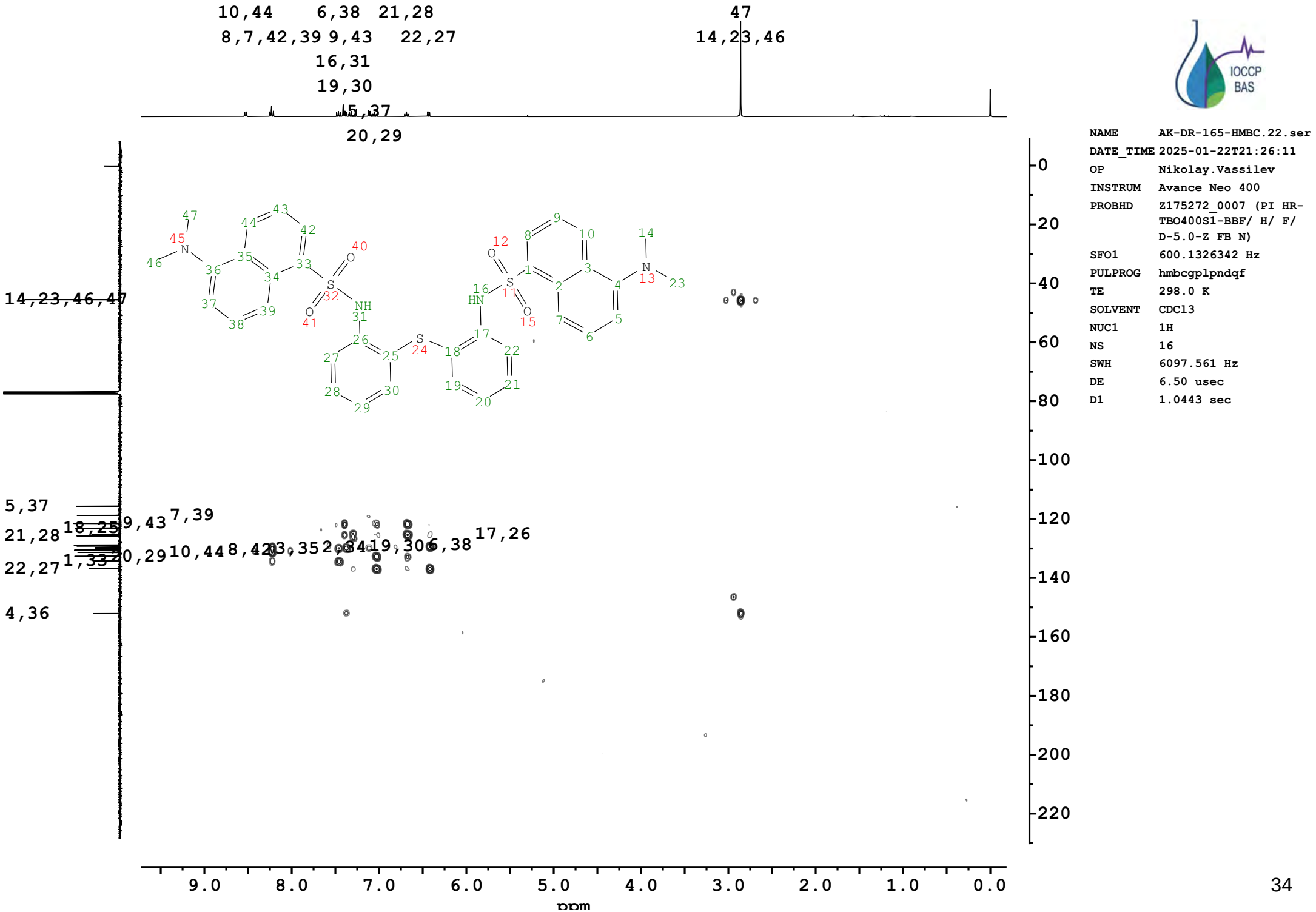
|---|---|
| NAME | DR-165.15.ser |
| DATE_TIME | 2022-10-04T18:3:31 |
| OP | Nikolay.Vassilv |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 2 |

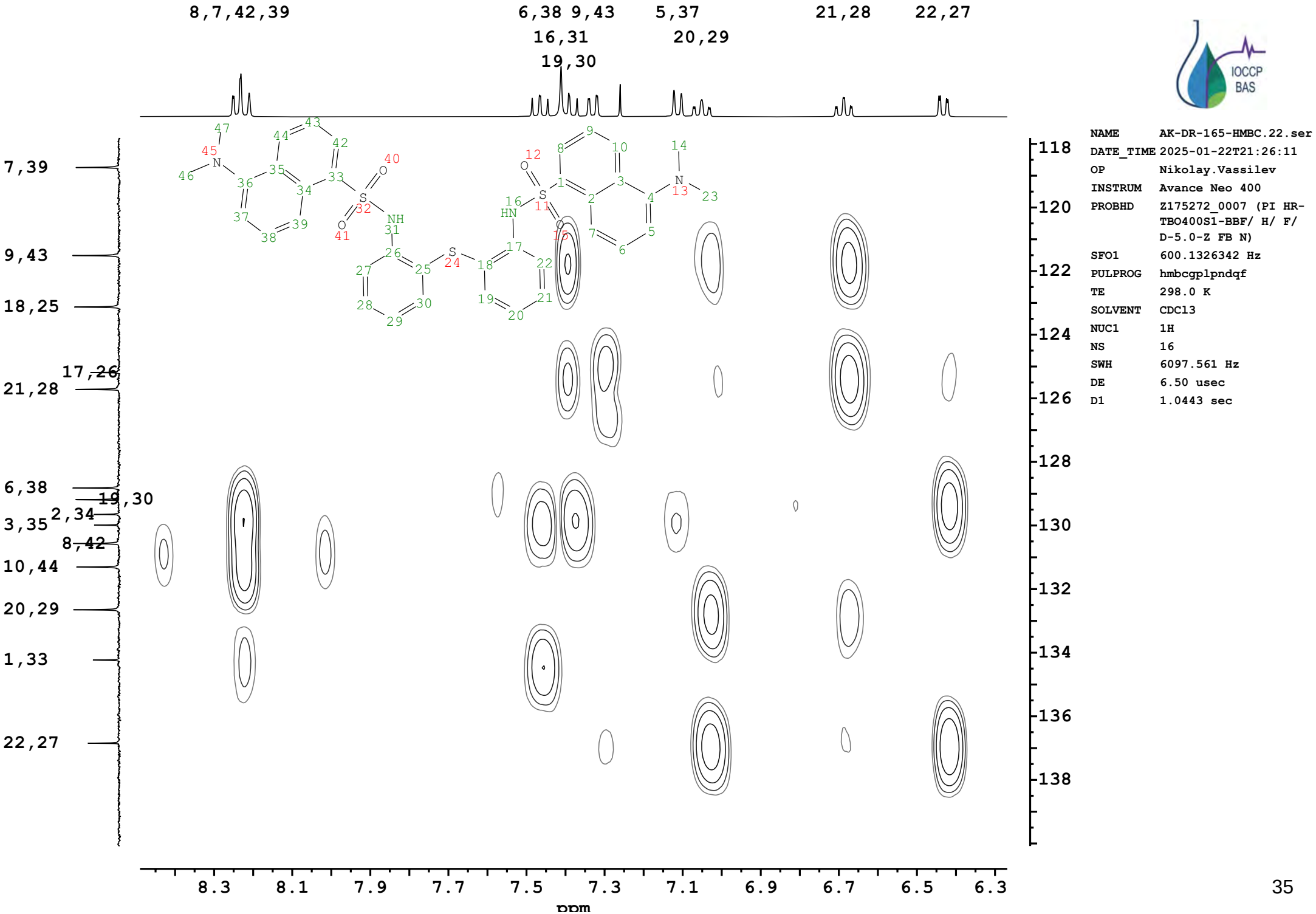
Fig SX18 L1 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-HMBC.22.ser |
| DATE_TIME | 2025-01-22T21:26:11 |
| OP | Nikolay.Vassilev |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX19

# L1 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-HMBC.22.ser |
| DATE_TIME | 2025-01-22T21:26:11 |
| OP | Nikolay.Vassilev |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX20 L1 chloroform-d ligand only full assignment

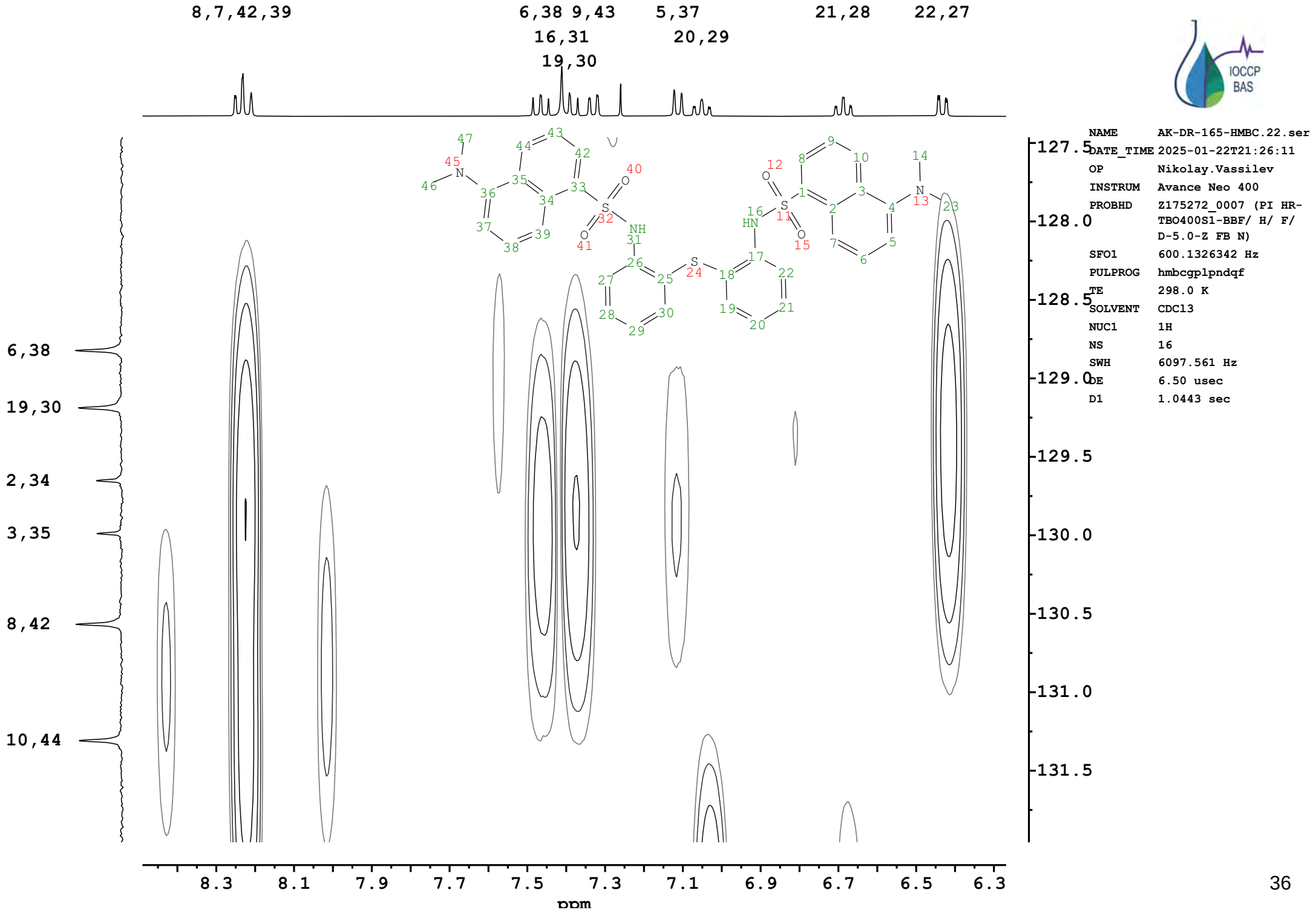
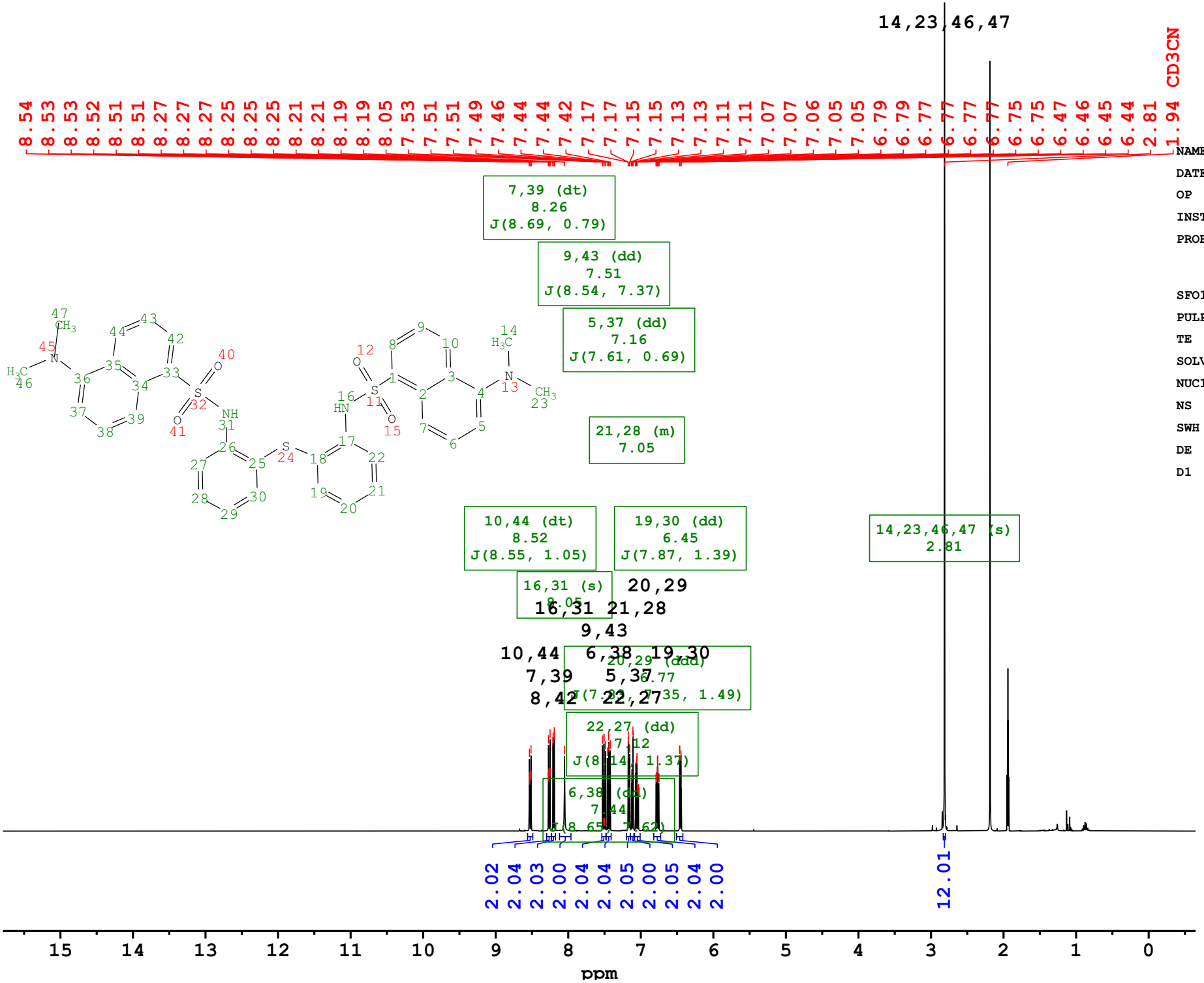
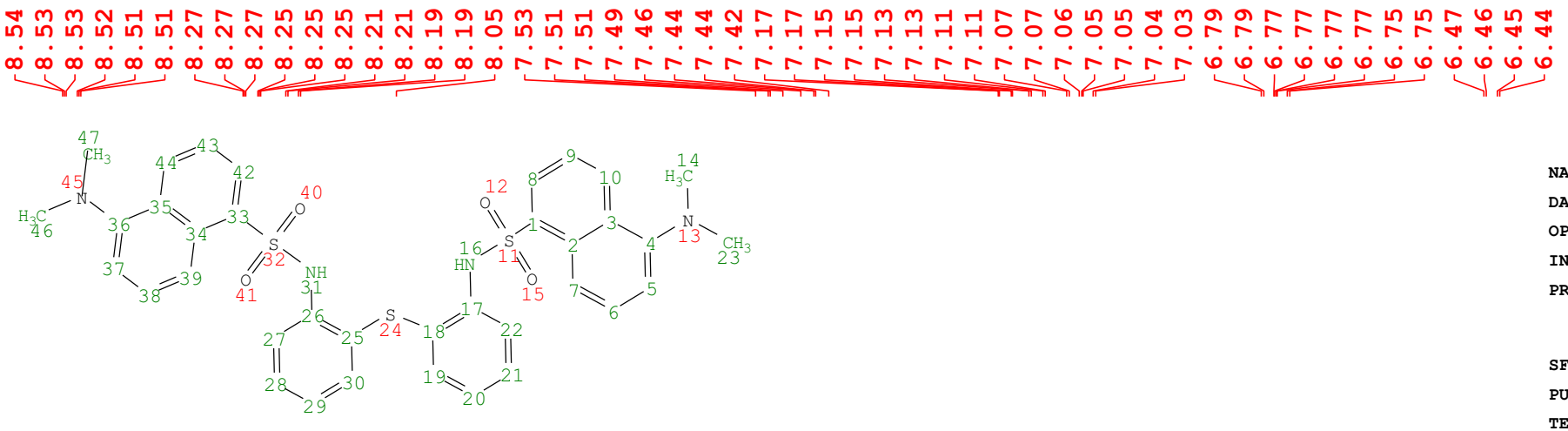


Fig SX21 L1 acetonitrile-d3 ligand only full assignment




NAME AK-DR-165-0.21.fid
DATE_TIME 2024-12-20T17:05:58
OP Dessislava.Gerginova
INSTRUM Avance Neo 400
PROBHD Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N)
SFO1 600.1345610 Hz
PULPROG zg30
TE 298.0 K
SOLVENT CD3CN
NUC1 1H
NS 256
SWH 9615.385 Hz
DE 6.50 usec
D1 2.0000 sec

**Fig SX22** **L1 acetonitrile-d3 ligand only full assignment**






| | |
|---|---|
| NAME | AK-DR-165-0.21.fid |
| DATE_TIME | 2024-12-20T17:05:58 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

10,44 (dt)
8.52
J(8.55, 1.05)

7,39 (dt)
8.26
J(8.69, 0.79)

8,42 (dd)
8.20
J(7.35, 1.26)

16,31 (s)
8.05

9,43 (dd)
7.51
J(8.54, 7.37)

6,38 (dd)
7.44
J(8.65, 7.62)

22,27 (dd)
7.12
J(8.14, 1.37)

5,37 (dd)
7.16
J(7.61, 0.69)

21,28 (m)
7.05

20,29 (ddd)
6.77
J(7.83, 7.35, 1.49)

19,30 (dd)
6.45
J(7.87, 1.39)

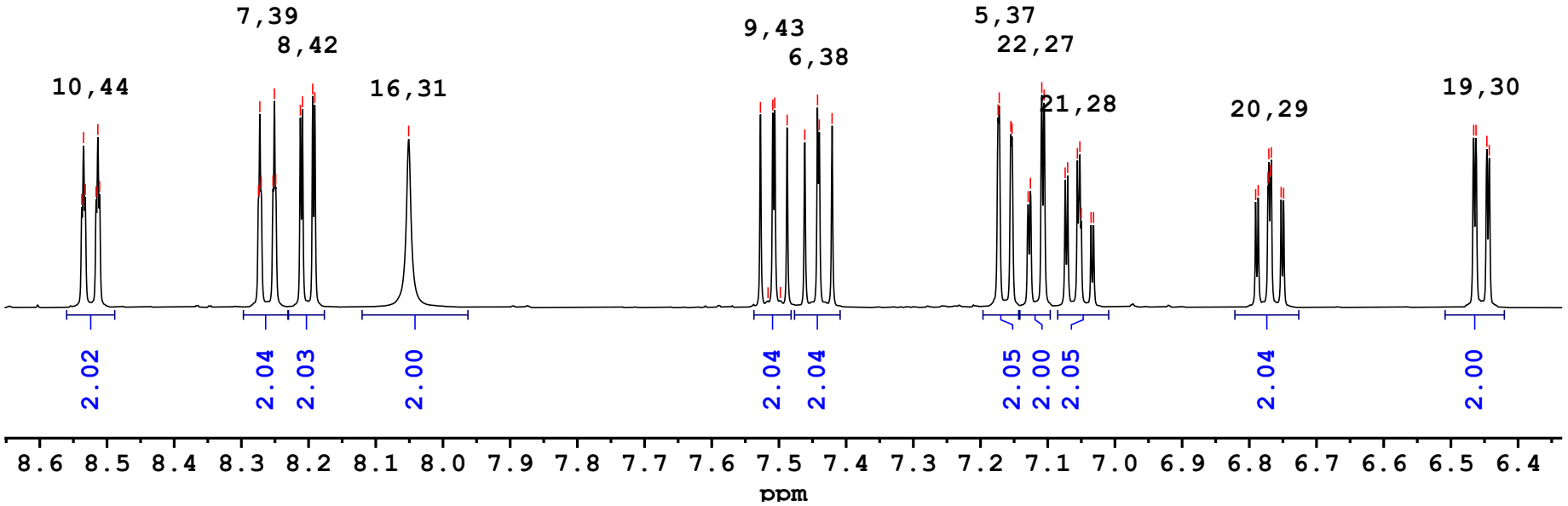
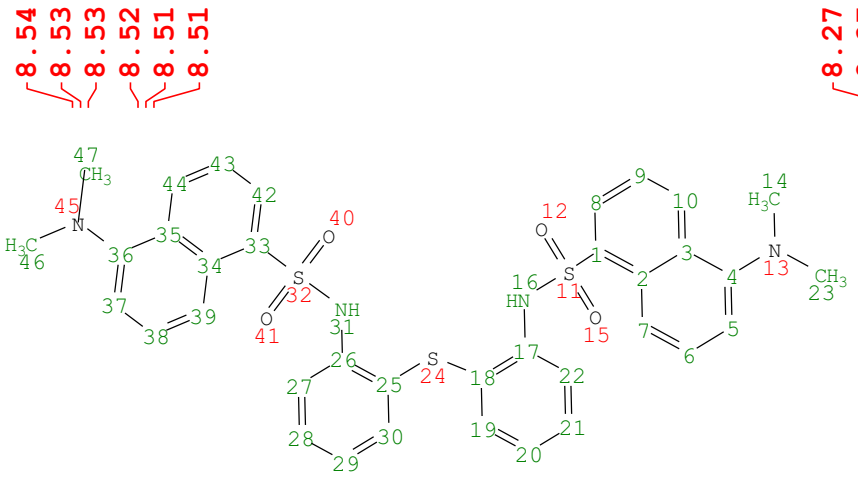


**Fig SX23** **L1 acetonitrile-d3 ligand only full assignment**




| | |
|---|---|
| NAME | AK-DR-165-0.21.fid |
| DATE_TIME | 2024-12-20T17:05:58 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

10,44 (dt)
8.52
J(8.55, 1.05)

8,42 (dd)
8.20
J(7.35, 1.26)

7,39 (dt)
8.26
J(8.69, 0.79)

16,31 (s)
8.05

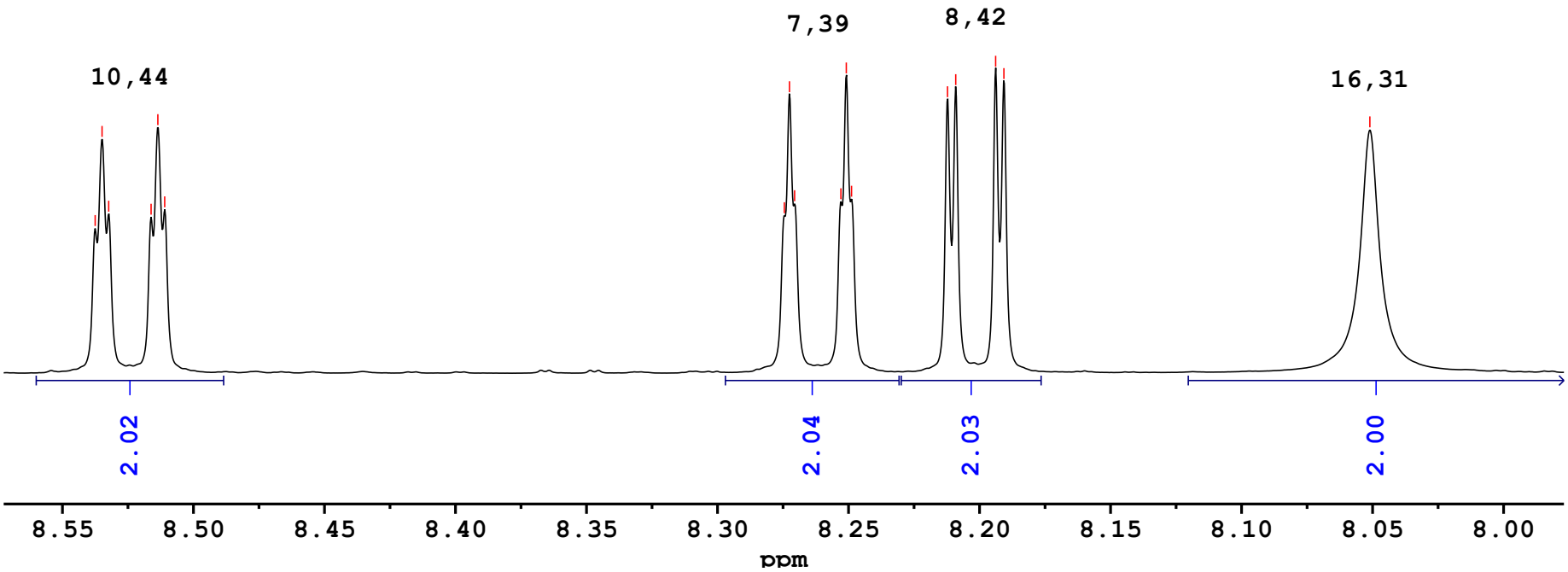
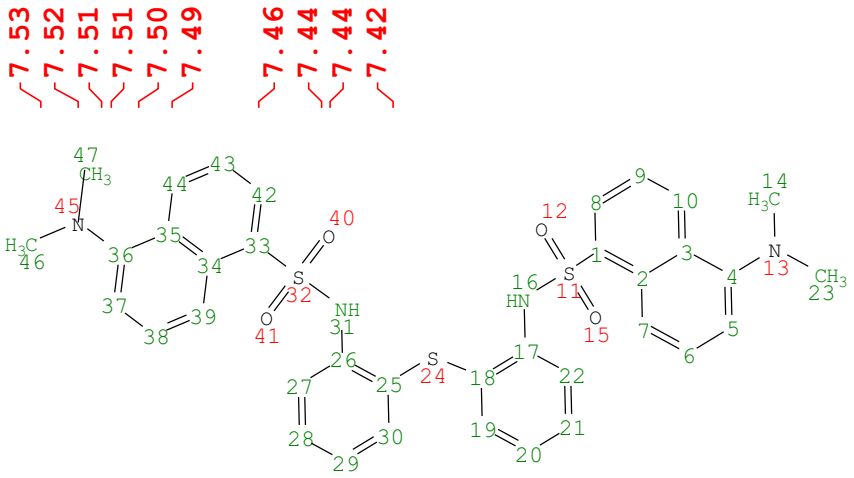


**Fig SX24** **L1 acetonitrile-d3 ligand only full assignment**








| | |
|---|---|
| NAME | AK-DR-165-0.21.fid |
| DATE_TIME | 2024-12-20T17:05:58 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

9,43 (dd)
7.51
J(8.54, 7.37)

6,38 (dd)
7.44
J(8.65, 7.62)

22,27 (dd)
7.12
J(8.14, 1.37)

5,37 (dd)
7.16
J(7.61, 0.69)

21,28 (m)
7.05

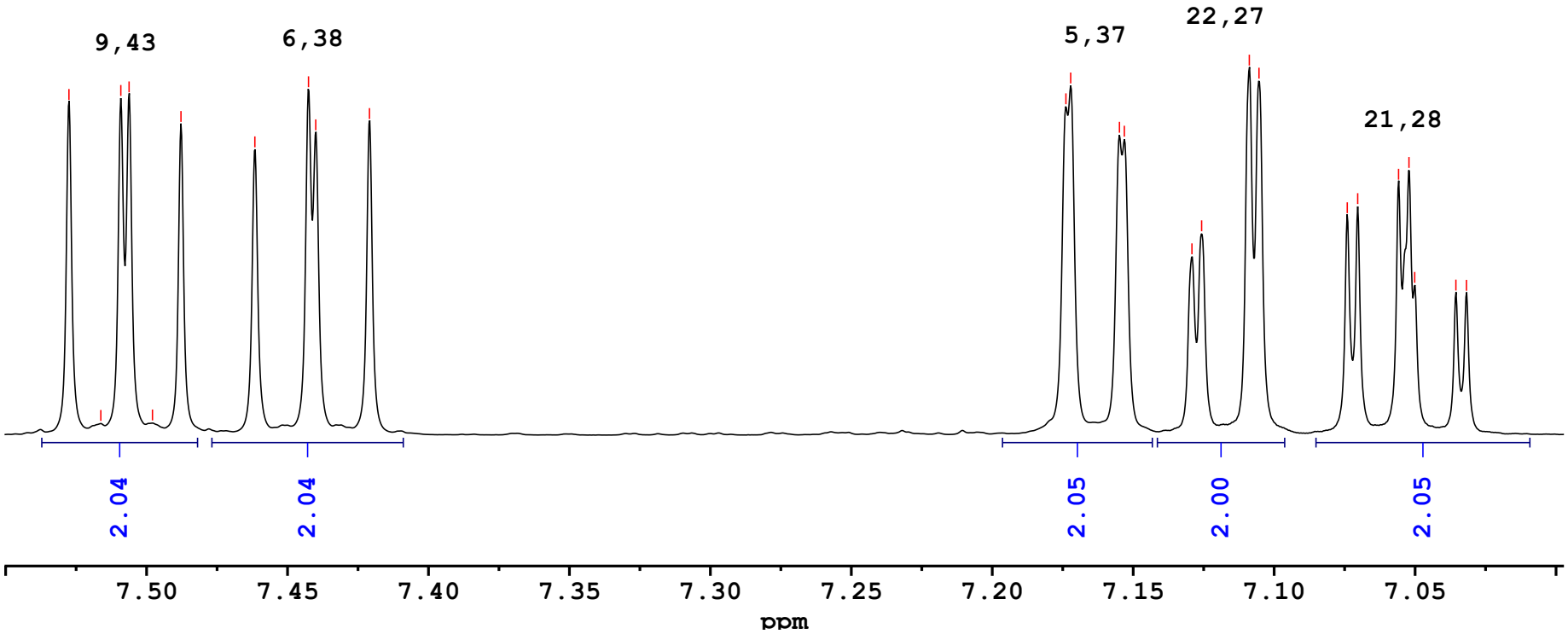
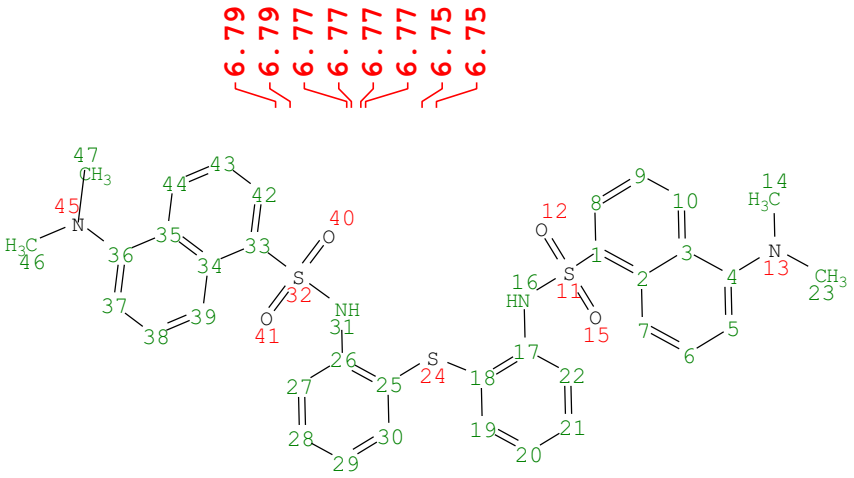


**Fig SX25** **L1 acetonitrile-d3 ligand only full assignment**




| | |
|---|---|
| NAME | AK-DR-165-0.21.fid |
| DATE_TIME | 2024-12-20T17:05:58 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

20,29 (ddd)
6.77
J(7.83, 7.35, 1.49)

19,30 (dd)
6.45
J(7.87, 1.39)

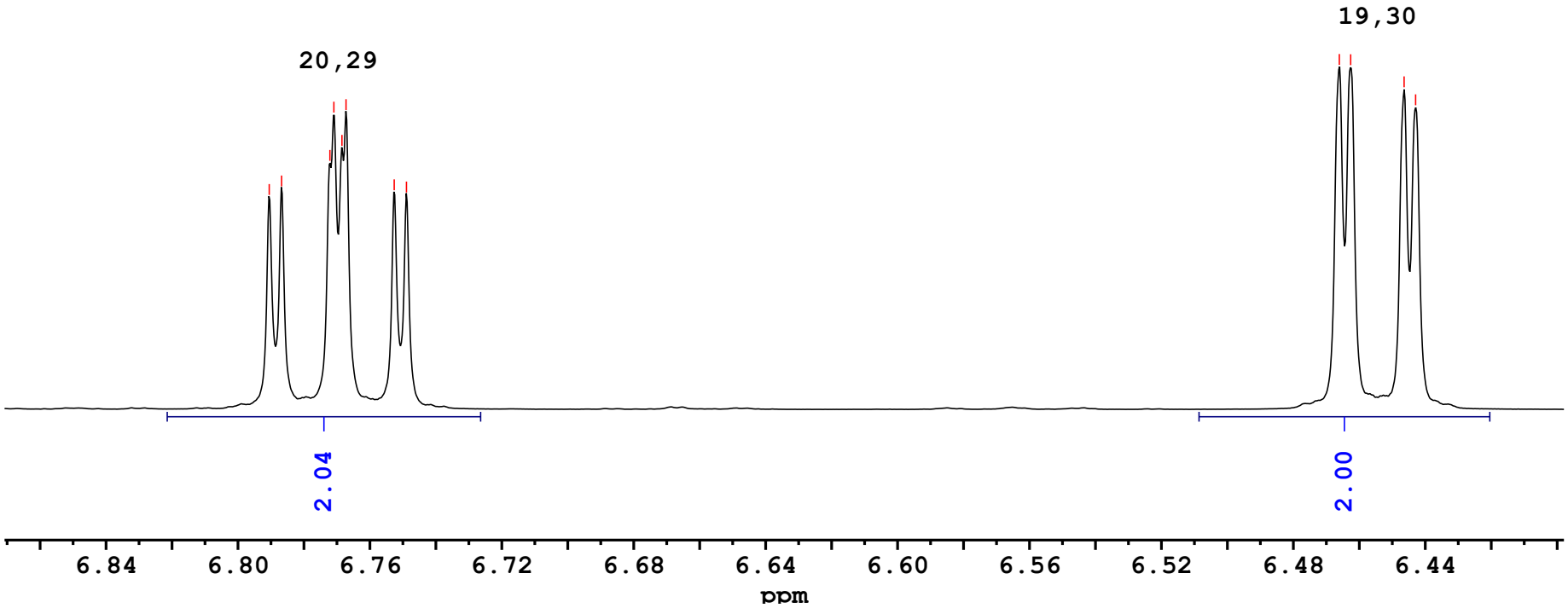
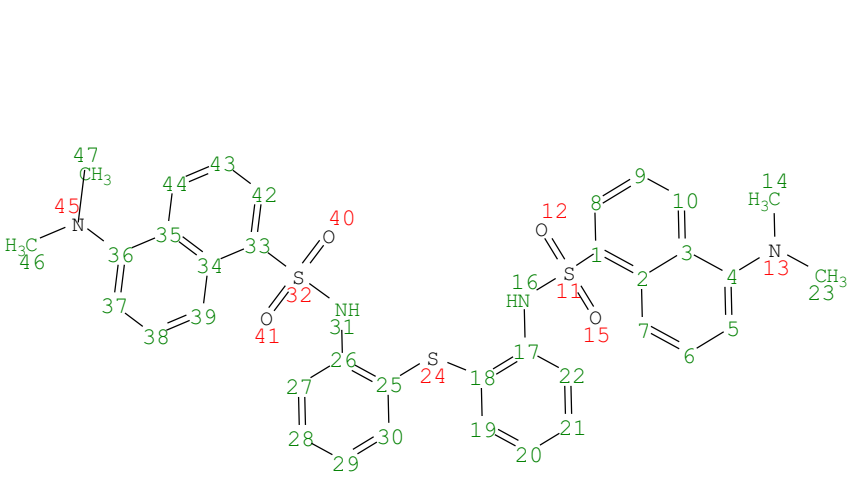


**Fig SX26** **L1 acetonitrile-d3 ligand only full assignment**




| | |
|---|---|
| NAME | AK-DR-165-0.21.fid |
| DATE_TIME | 2024-12-20T17:05:58 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

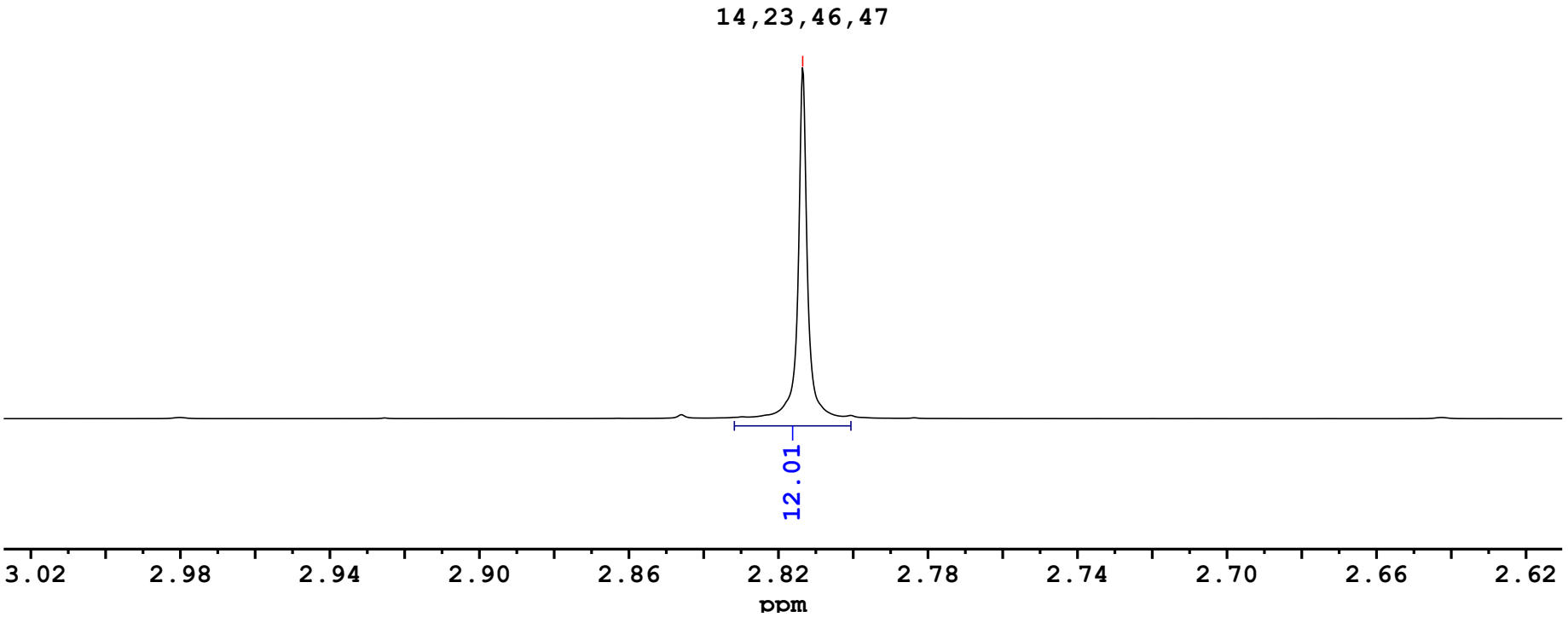
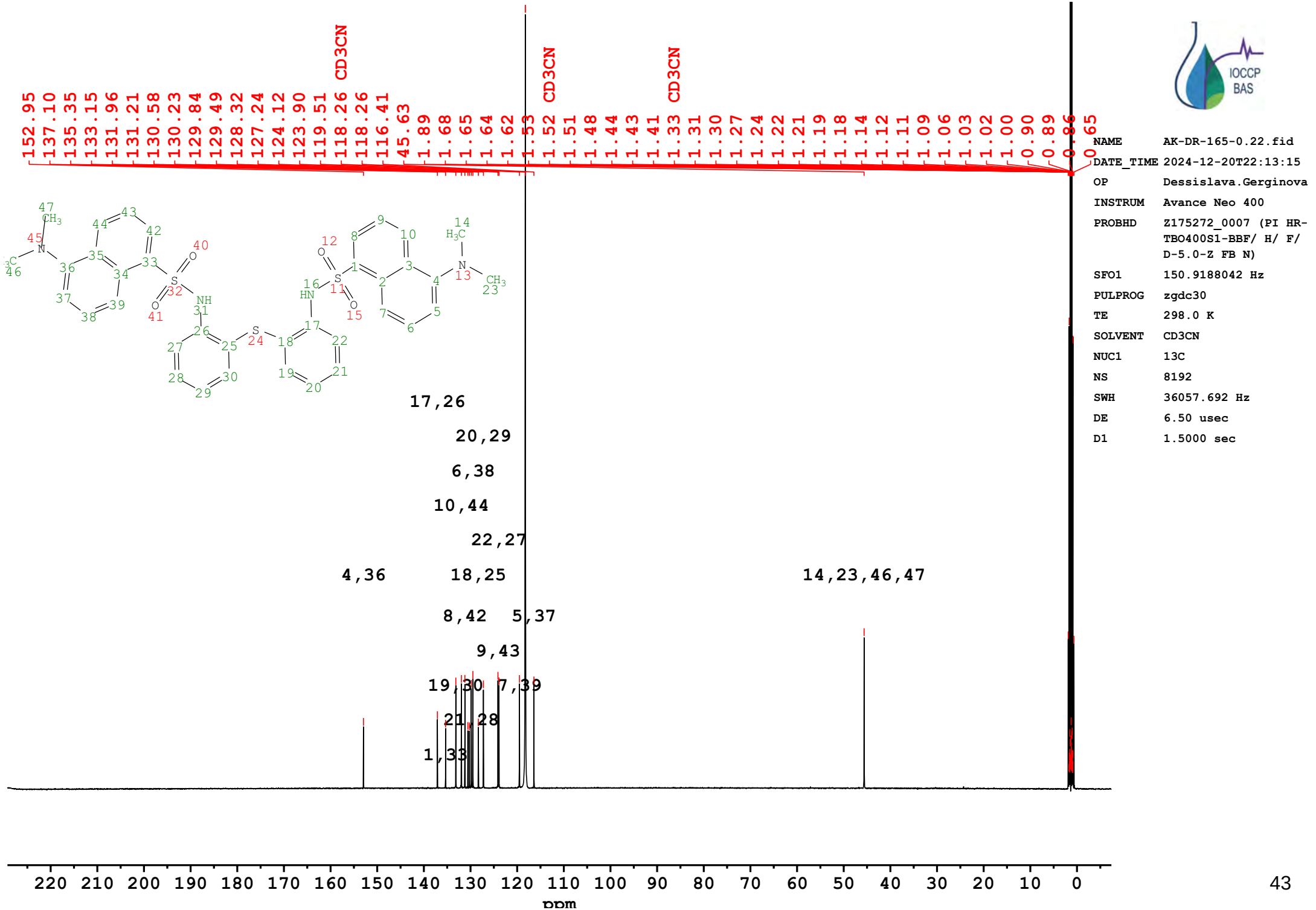
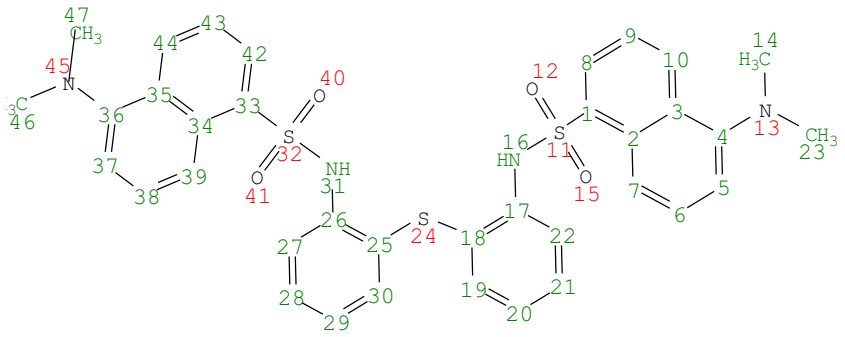


Fig SX27 L1 acetonitrile-d3 ligand only full assignment




NAME AK-DR-165-0.22.fid
DATE_TIME 2024-12-20T22:13:15
OP Dessislava.Gerginova
INSTRUM Avance Neo 400
PROBHD Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N)
SFO1 150.9188042 Hz
PULPROG zgdc30
TE 298.0 K
SOLVENT CD3CN
NUC1 13C
NS 8192
SWH 36057.692 Hz
DE 6.50 usec
D1 1.5000 sec

Fig SX28 L1 acetonitrile-d3 ligand only full assignment



137.10 135.35 133.15 131.96 131.21 130.58 130.23 129.84 129.49 128.32 127.24 124.12 123.90 119.51 118.26 CD3CN 118.26 116.41

| | |
|---|---|
| NAME | AK-DR-165-0.22.fid |
| DATE_TIME | 2024-12-20T22:13:15 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

2,34 10,44 6,38 20,29 9,43 7,26 1,33 19,30 8,42 21,28 18,25 22,27 7,39 5,37 3,35

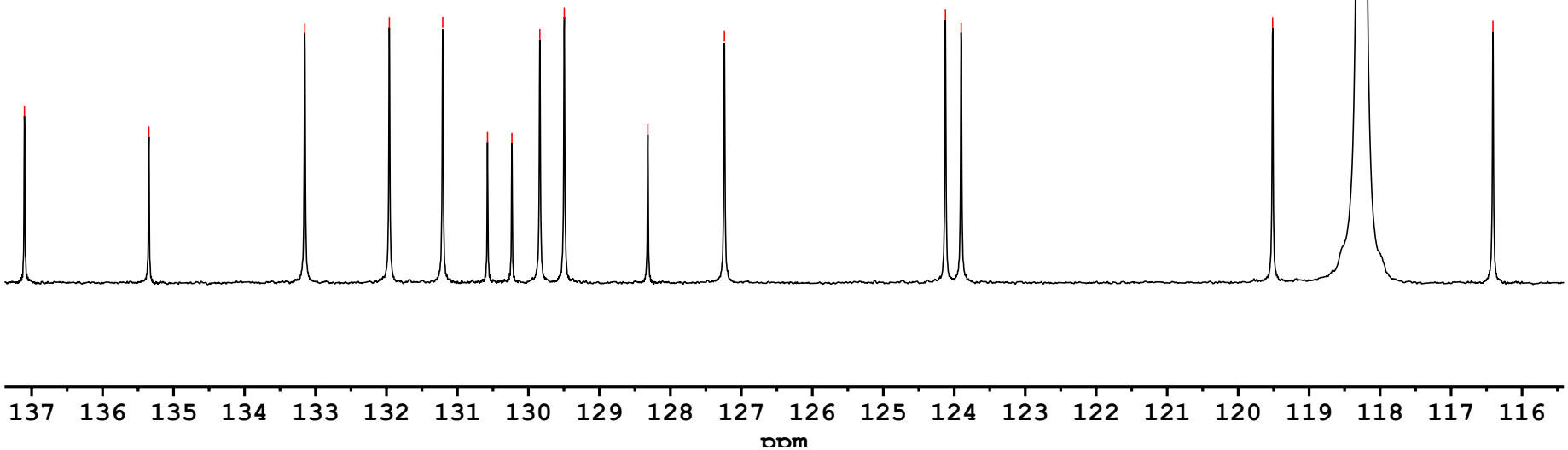
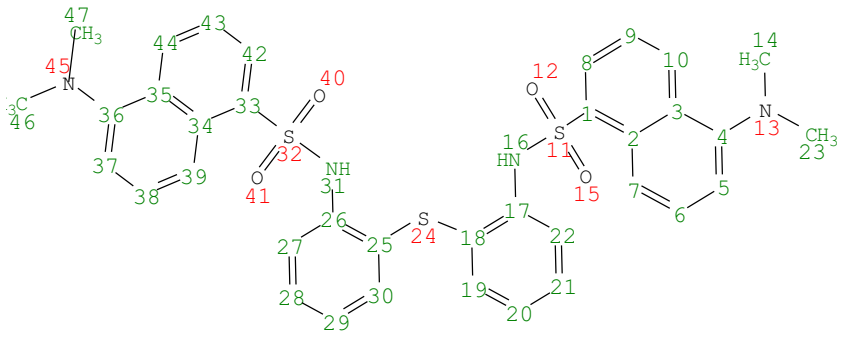


**Fig SX29** **L1 acetonitrile-d3 ligand only full assignment**

131.96 131.21 130.58 130.23 129.84 129.49



| | |
|---|---|
| NAME | AK-DR-165-0.22.fid |
| DATE_TIME | 2024-12-20T22:13:15 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

10,44 8,42 3,35 2,34 21,28 6,38

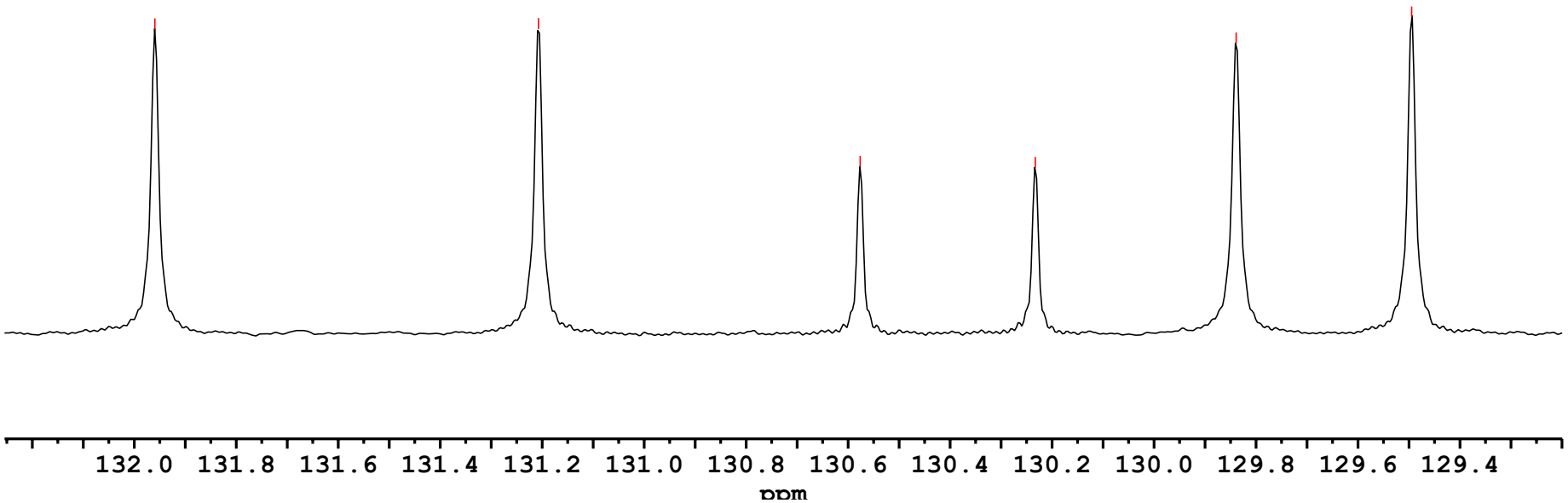
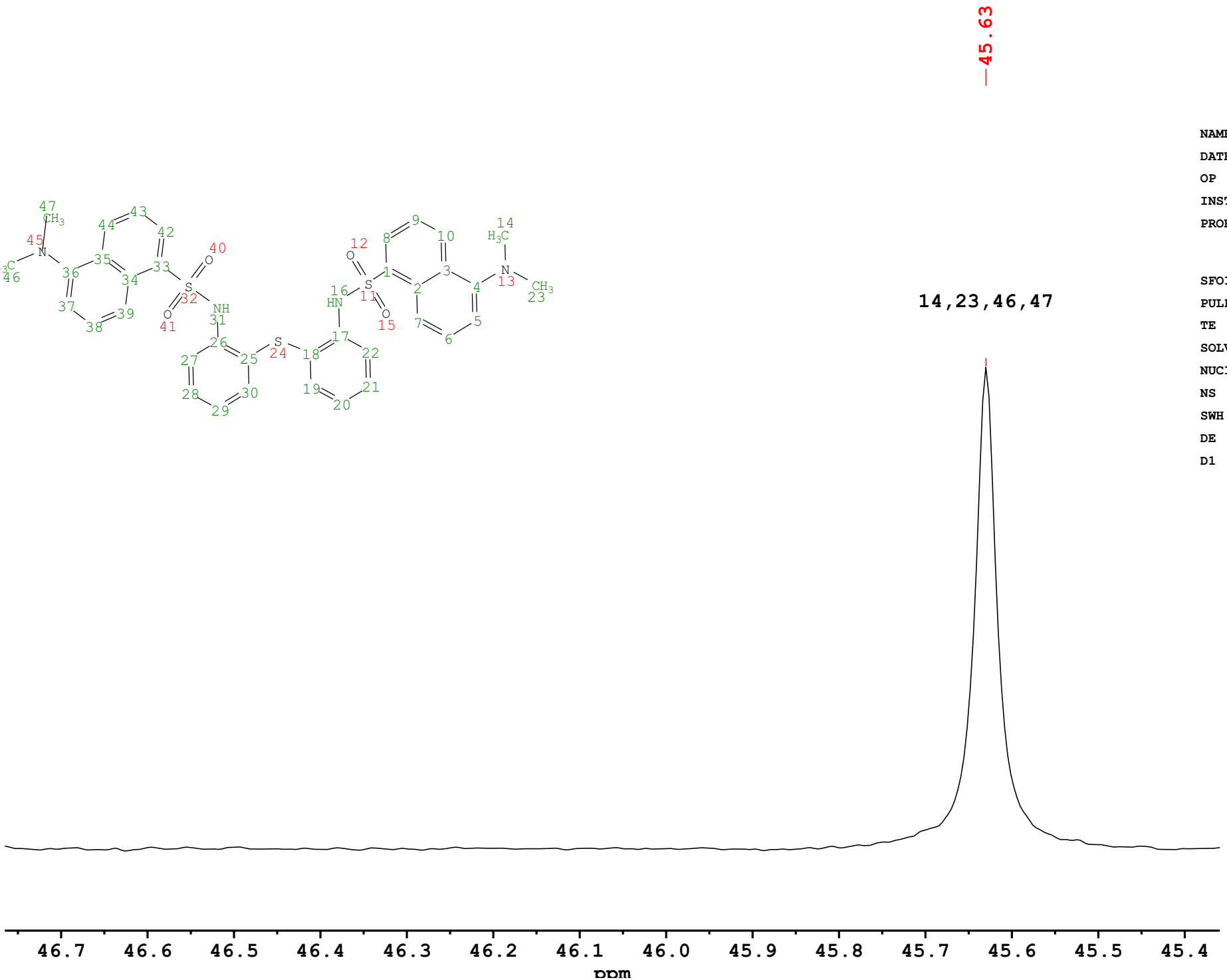


**Fig SX30** **L1 acetonitrile-d3 ligand only full assignment**

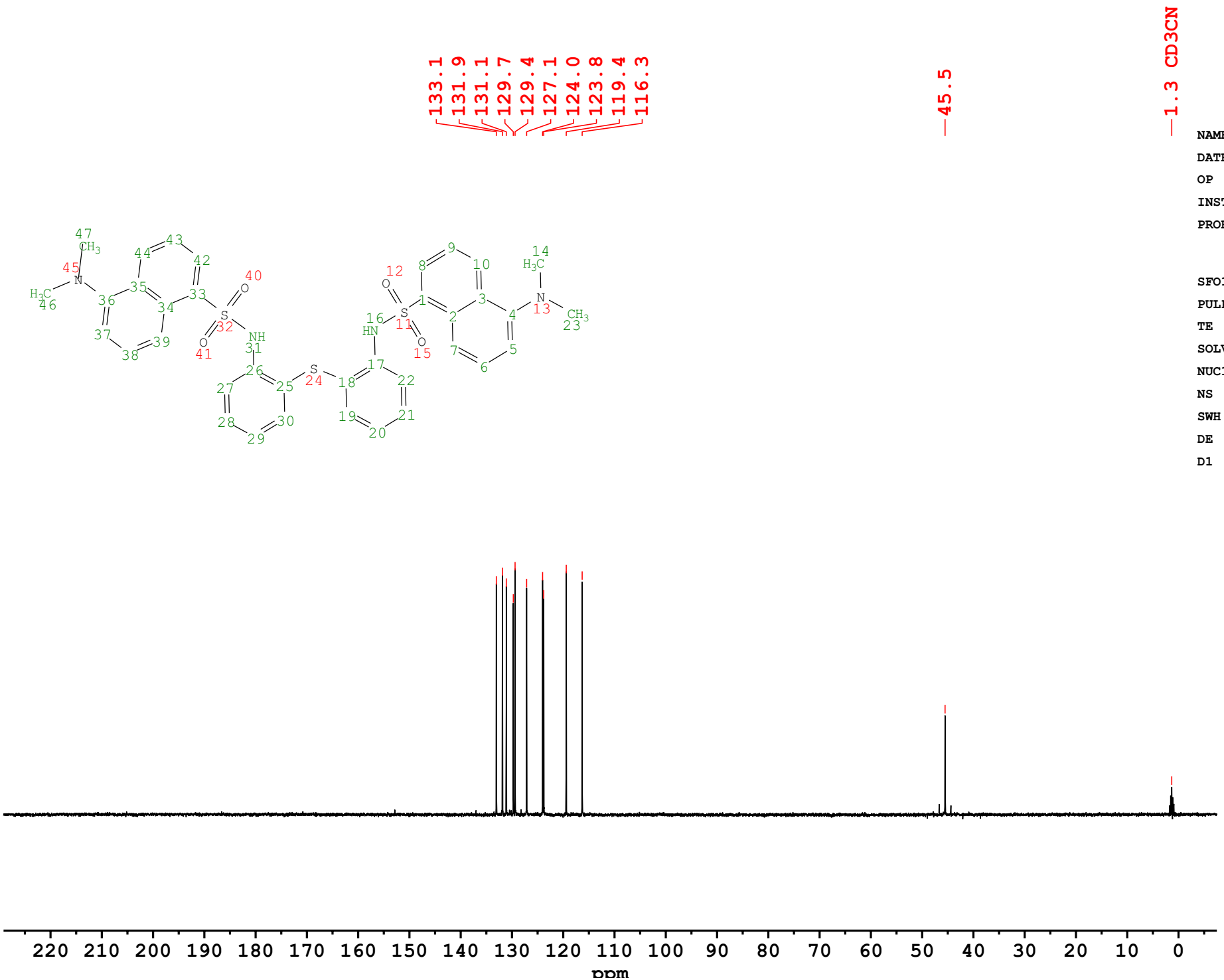





| | |
|---|---|
| NAME | AK-DR-165-0.22.fid |
| DATE_TIME | 2024-12-20T22:13:15 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

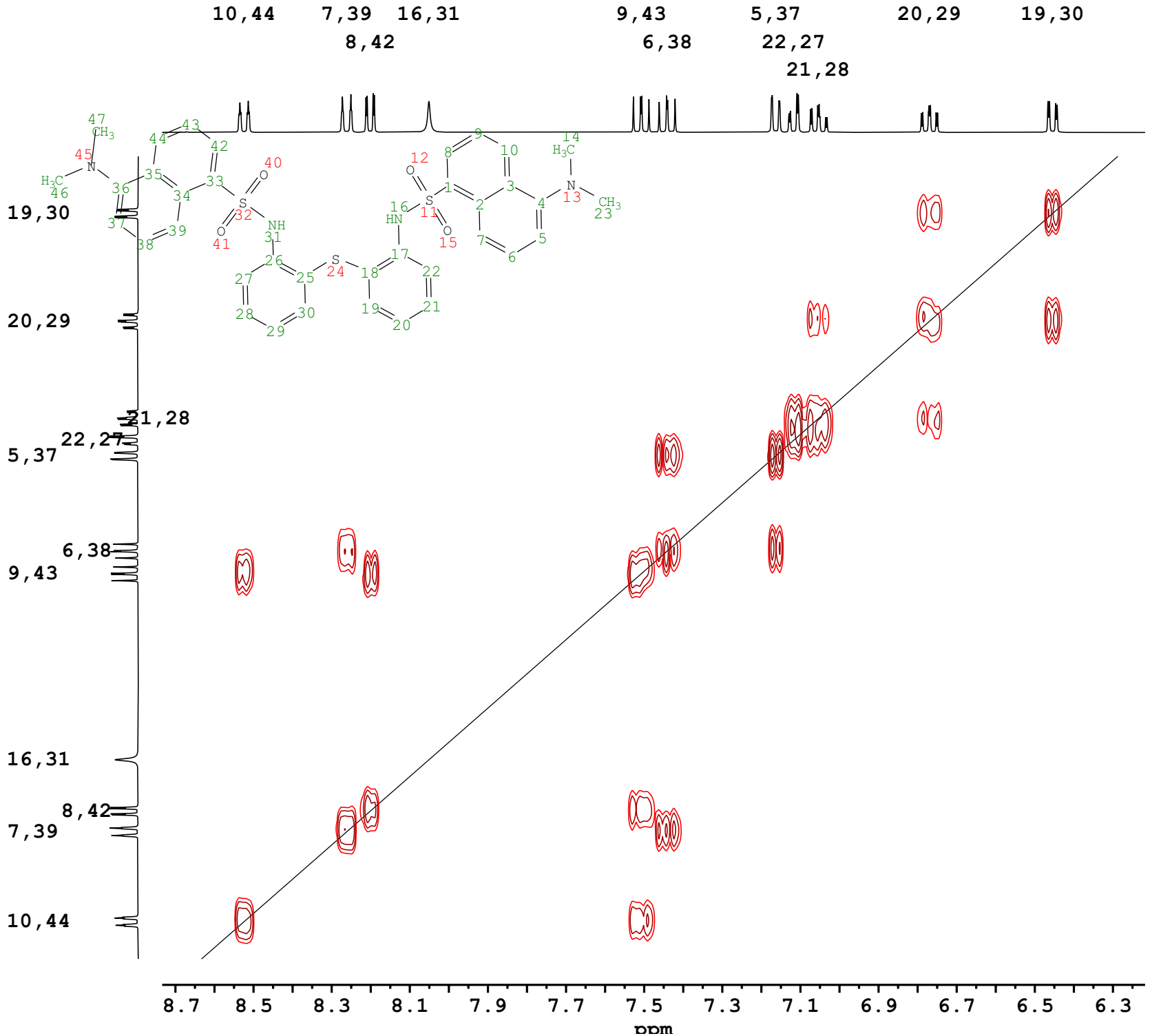
Fig SX31 L1 acetonitrile-d3 ligand only full assignment





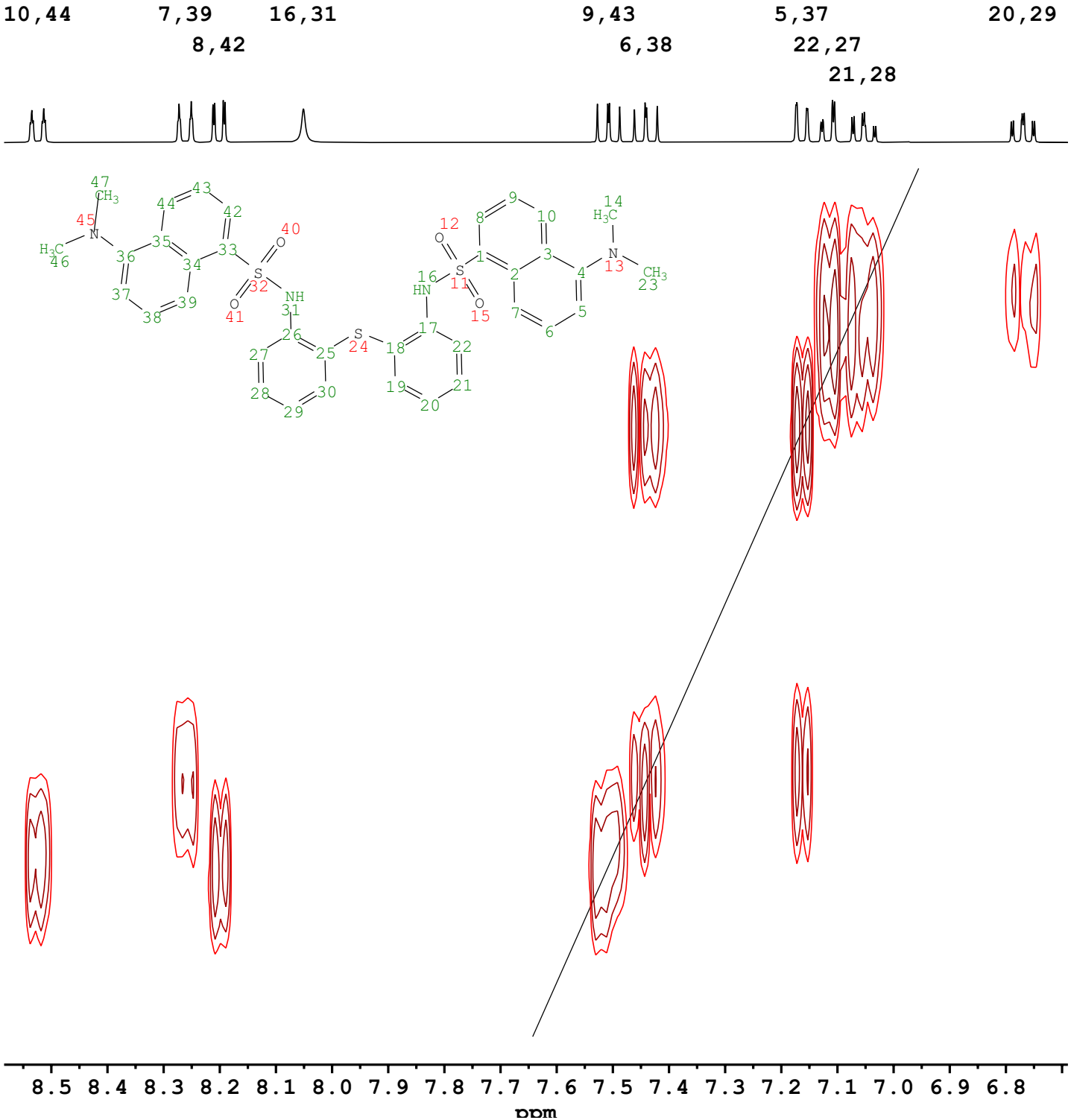

| | |
|---|---|
| NAME | AK-DR-165-0.22.fid |
| DATE_TIME | 2024-12-20T22:13:15 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9319844 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 35714.286 Hz |
| DE | 18.00 usec |
| D1 | 1.5000 sec |

Fig SX32 L1 acetonitrile-d3 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-0.24.ser |
| DATE_TIME | 2024-12-20T23:22:47 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 4 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 0.9750 sec |

Fig SX33 L1 acetonitrile-d3 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-0.24.ser |
| DATE_TIME | 2024-12-20T23:22:47 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 4 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 0.9750 sec |

Fig SX34 L1 acetonitrile-d3 ligand only full assignment

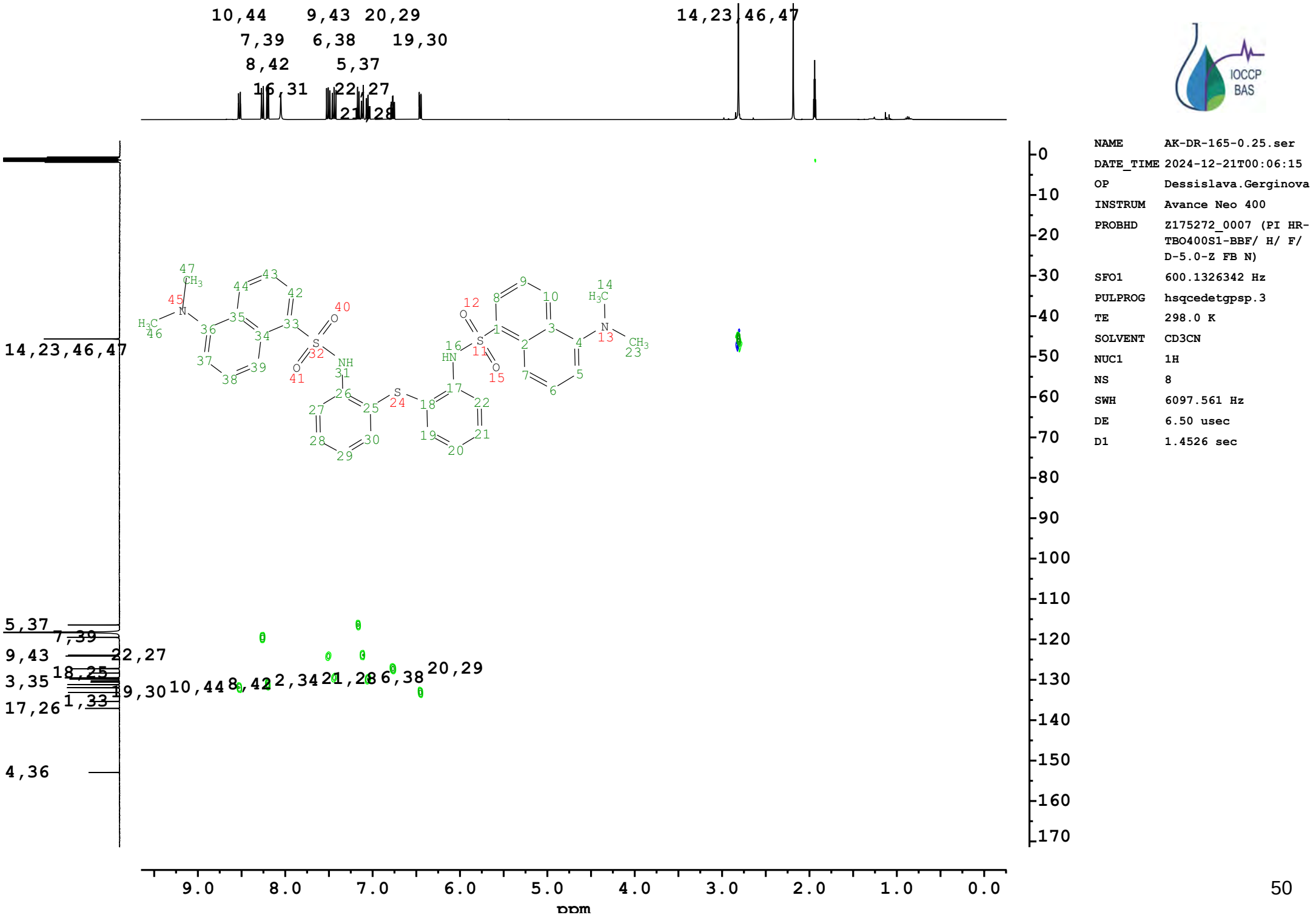
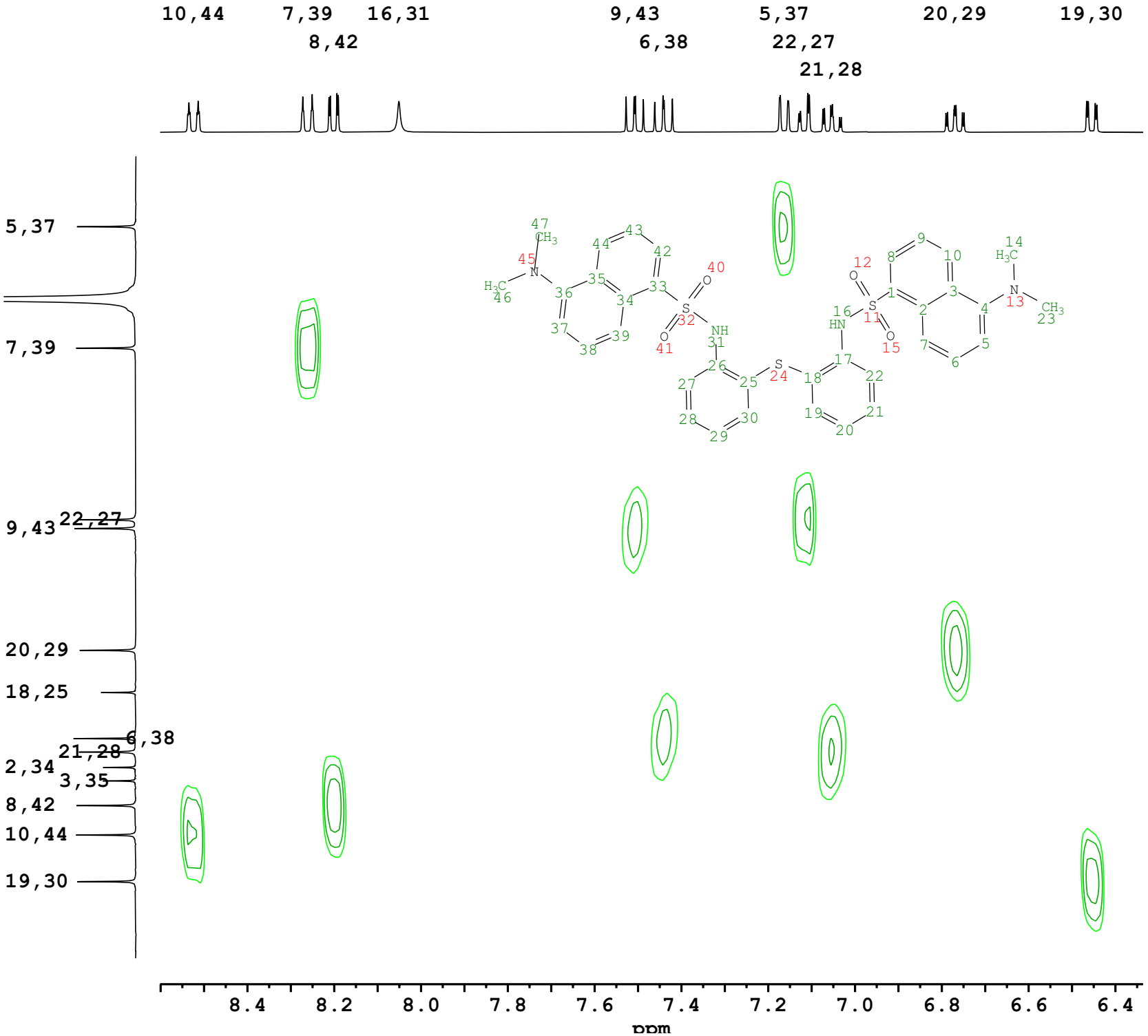


Fig SX35 L1 acetonitrile-d3 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-0.25.ser |
| DATE_TIME | 2024-12-21T00:06:15 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

**Fig SX36** **L1 acetonitrile-d3 ligand only full assignment**

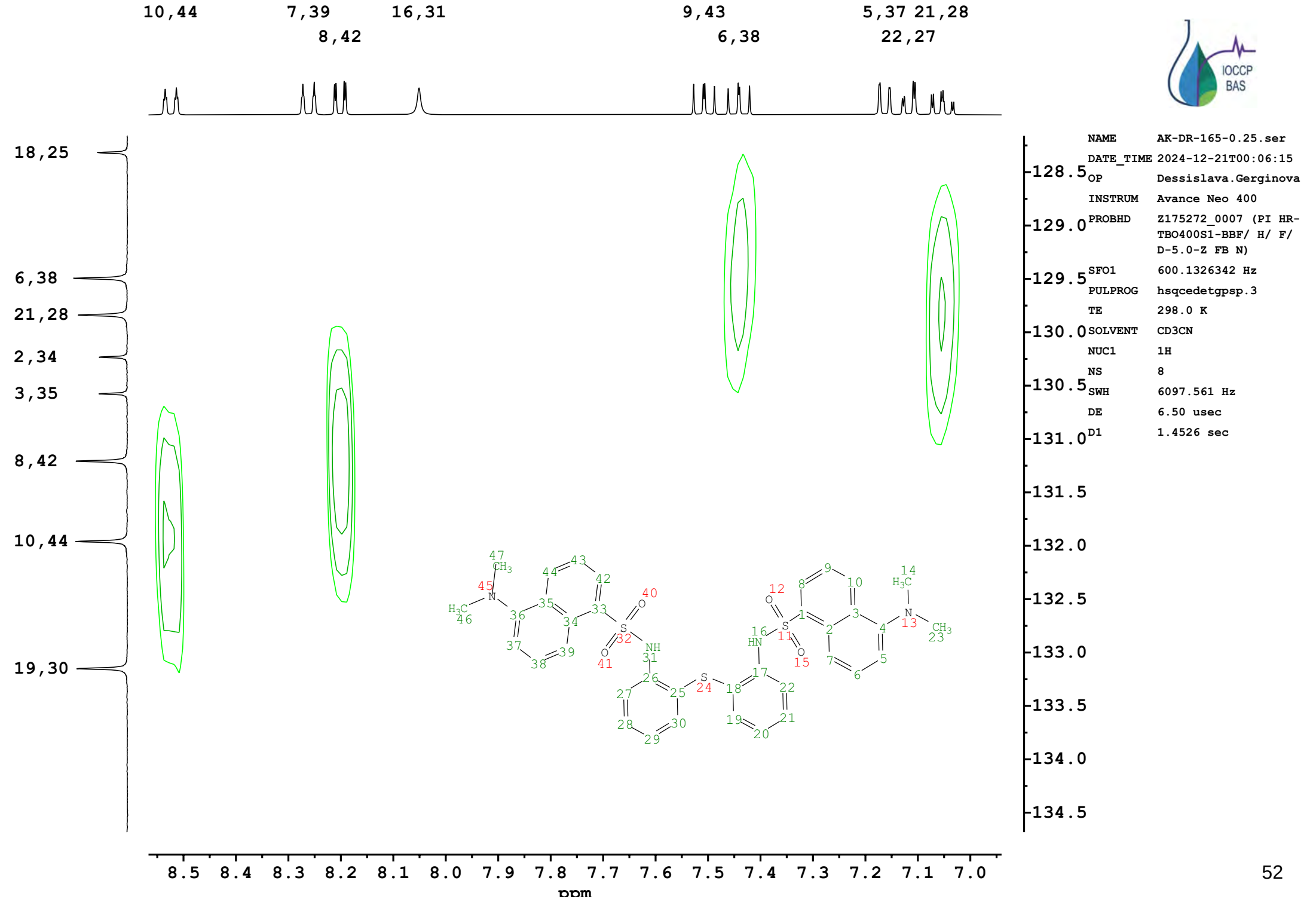


Fig SX37 L1 acetonitrile-d3 ligand only full assignment

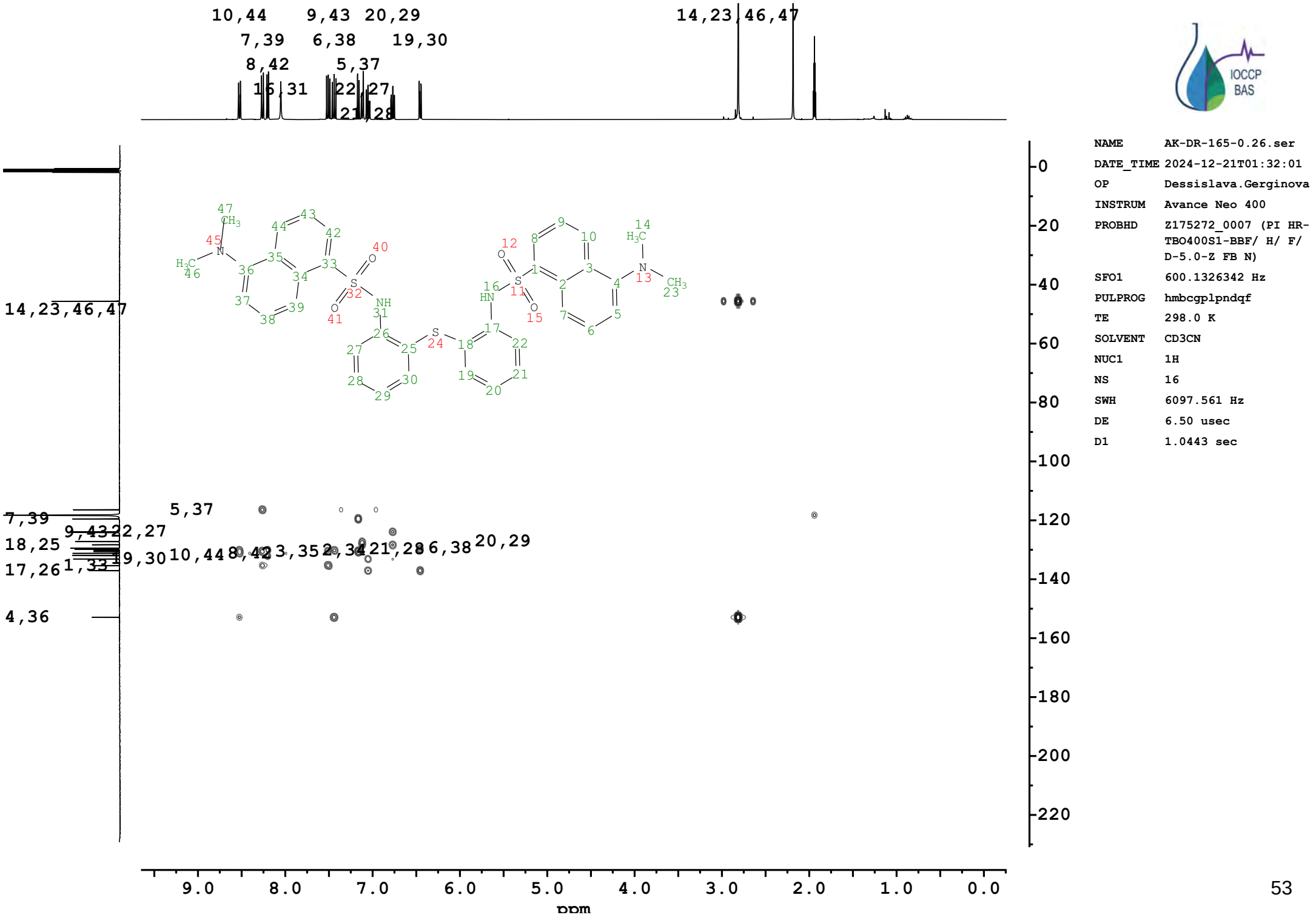
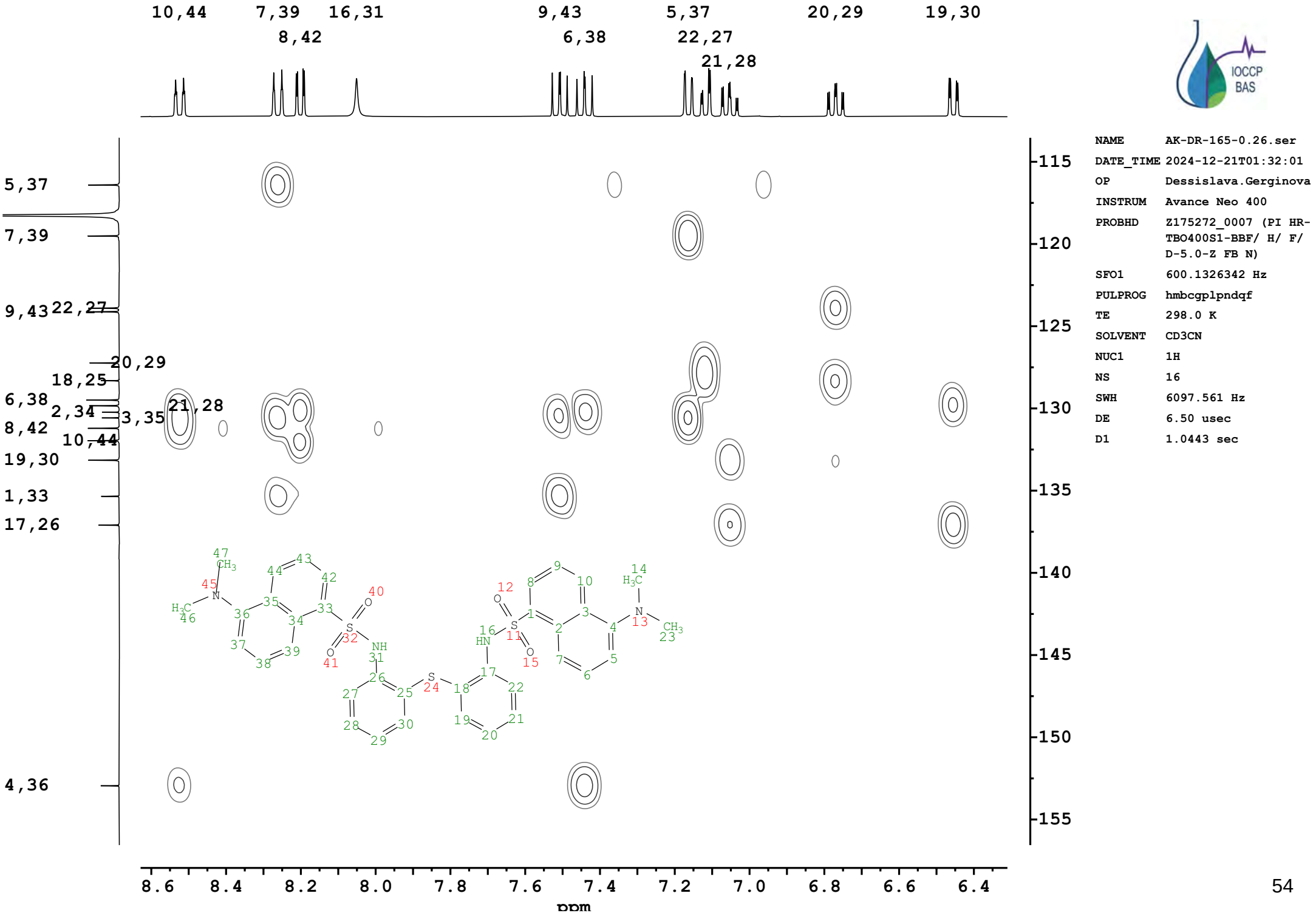
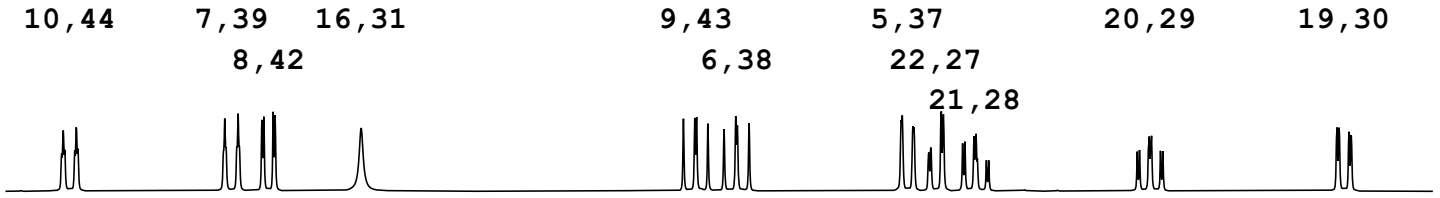


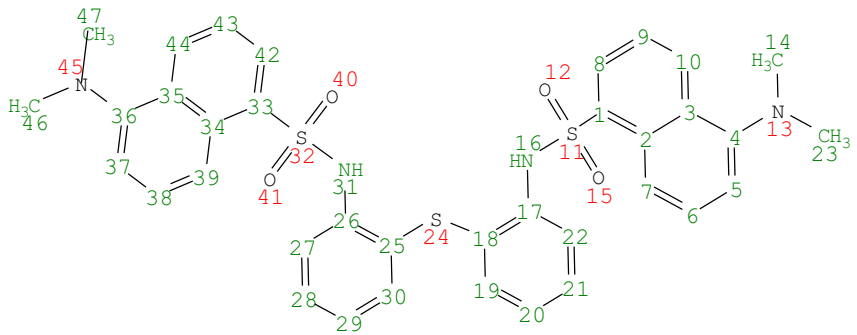
Fig SX38 L1 acetonitrile-d3 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-0.26.ser |
| DATE_TIME | 2024-12-21T01:32:01 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

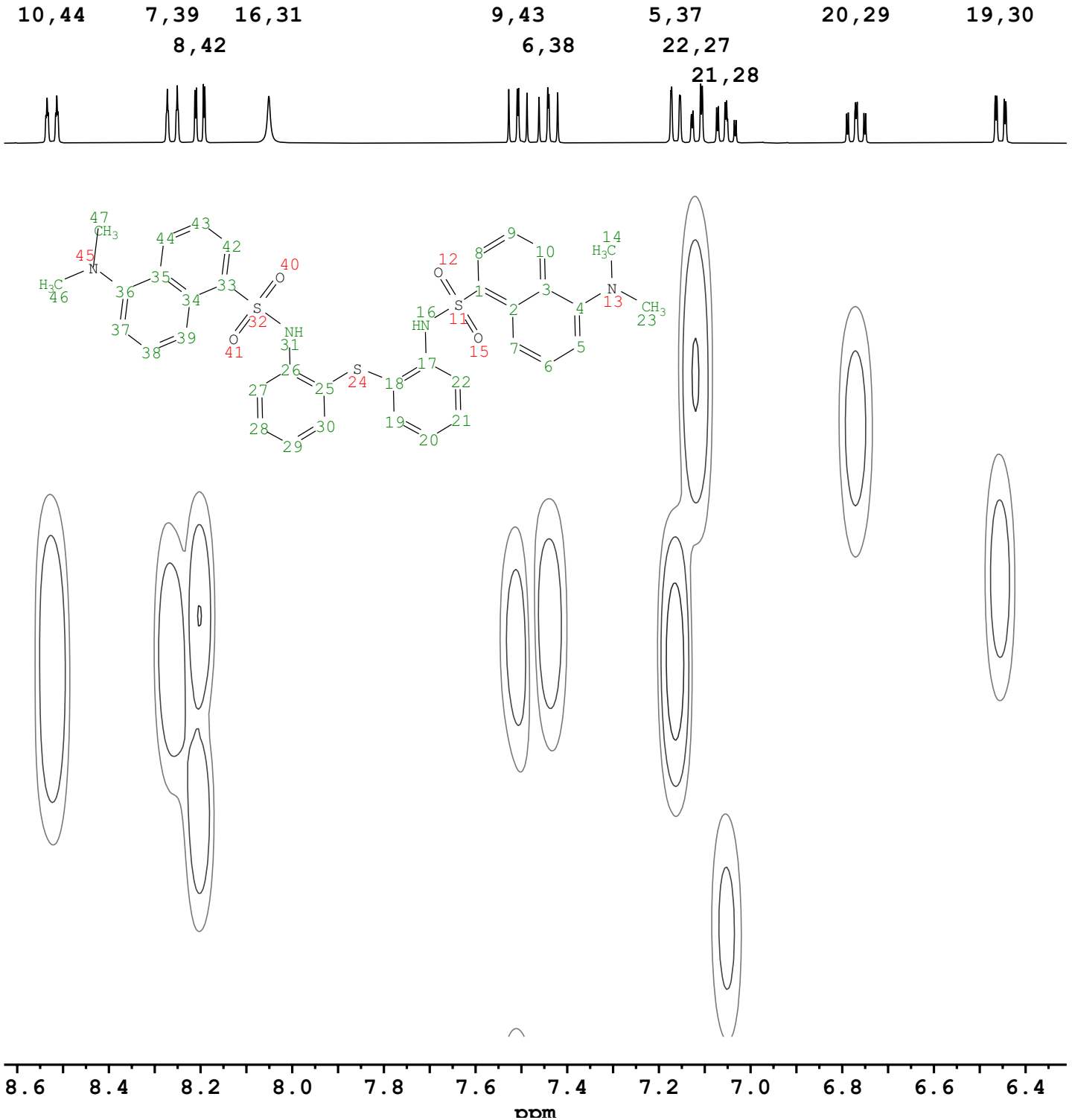
Fig SX39 L1 acetonitrile-d3 ligand only full assignment



| | |
|---|---|
| NAME | AK-DR-165-0.26.ser |
| DATE_TIME | 2024-12-21T01:32:01 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

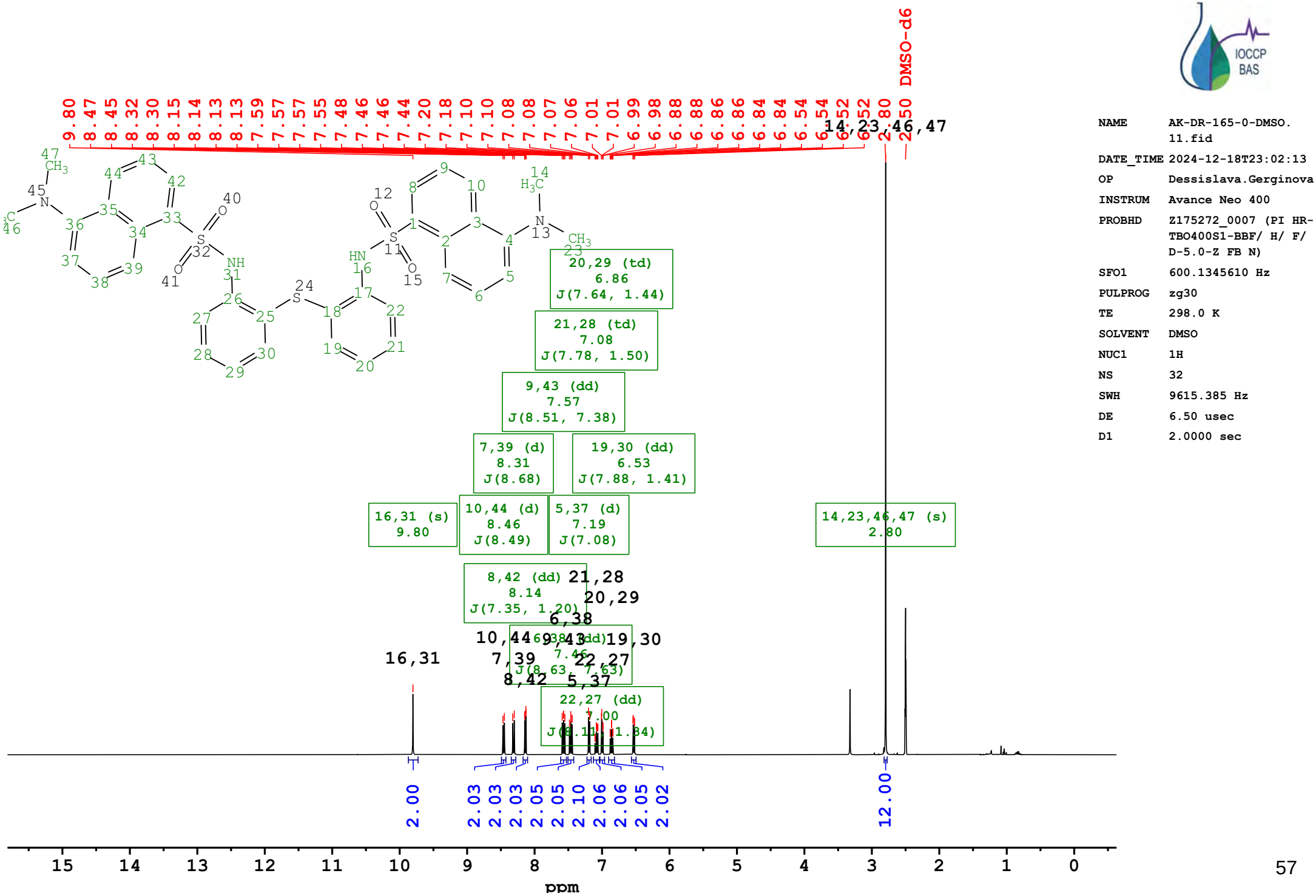
Fig SX40 L1 acetonitrile-d3 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-0.26.ser |
| DATE_TIME | 2024-12-21T01:32:01 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX41

# L1 dmso-d6 ligand only full assignment



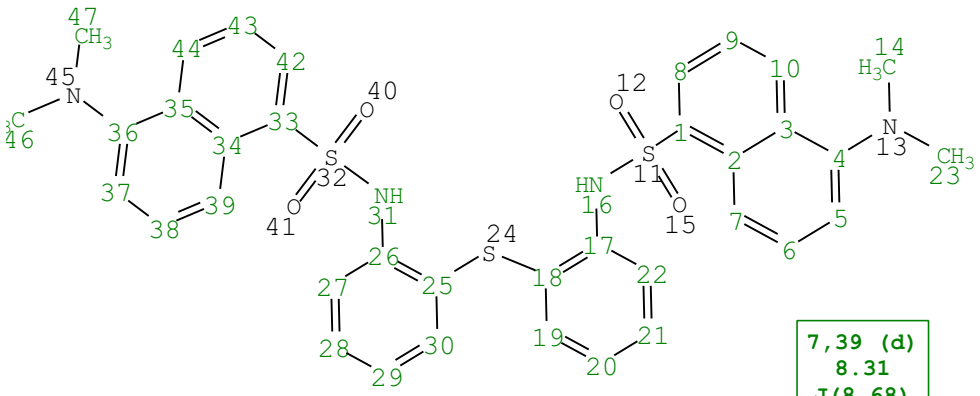

| | |
|---|---|
| NAME | AK-DR-165-0-DMSO.11.fid |
| DATE_TIME | 2024-12-18T23:02:13 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

Fig SX42

# L1 dmso-d6 ligand only full assignment

9.80

8.47 8.45 8.32 8.30 8.15 8.14 8.13 8.13 7.59 7.57 7.57 7.55 7.48 7.46 7.46 7.44 7.20 7.18 7.10 7.10 7.08 7.08 7.07 7.06 7.01 7.01 6.99 6.98 6.88 6.88 6.86 6.86 6.84 6.84 6.54 6.54 6.52 6.52




16,31 (s)
9.80

7,39 (d)
8.31
J(8.68)

10,44 (d)
8.46
J(8.49)

8,42 (dd)
8.14
J(7.35, 1.20)

20,29 (td)
6.86
J(7.64, 1.44)

6,38 (dd)
7.46
J(8.63, 7.63)

22,27 (dd)
7.00
J(8.11, 1.34)

9,43 (dd)
7.57
J(8.51, 7.38)

5,37 (d)
7.19
J(7.08)

19,30 (dd)
6.53
J(7.88, 1.41)

21,28 (td)
7.08
J(7.78, 1.50)

| | |
|---|---|
| NAME | AK-DR-165-0-DMSO.11.fid |
| DATE_TIME | 2024-12-18T23:02:13 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

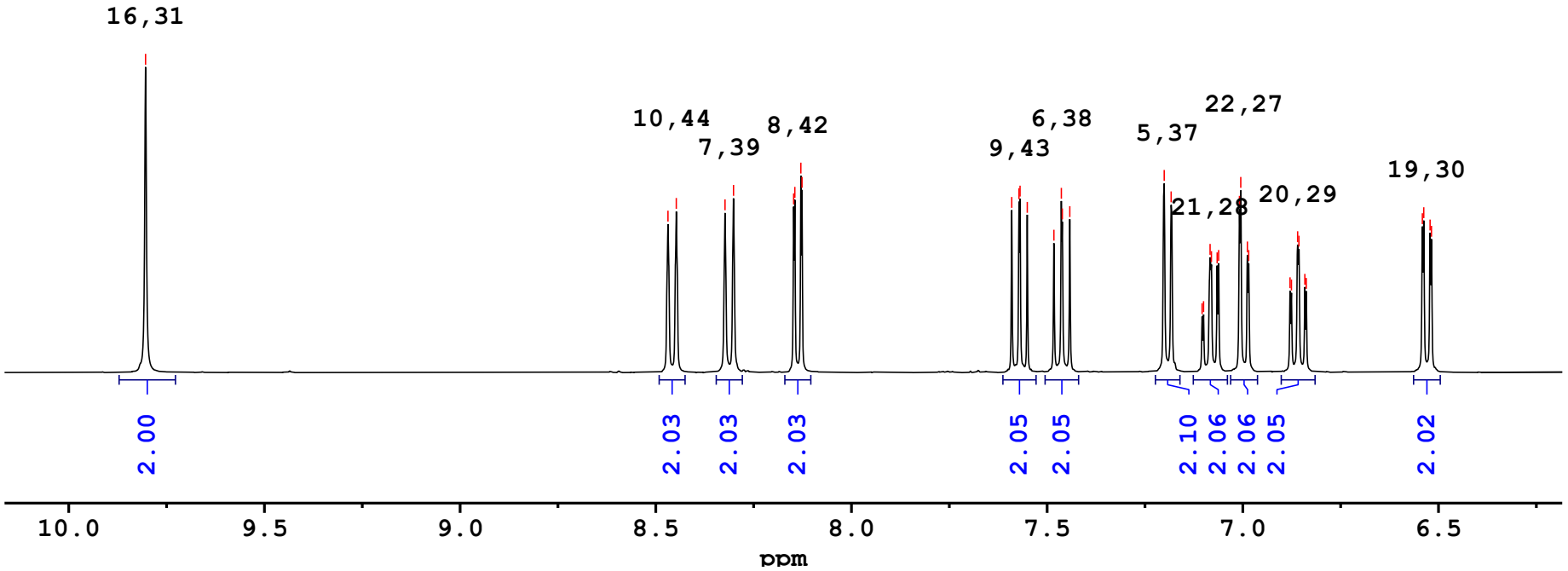
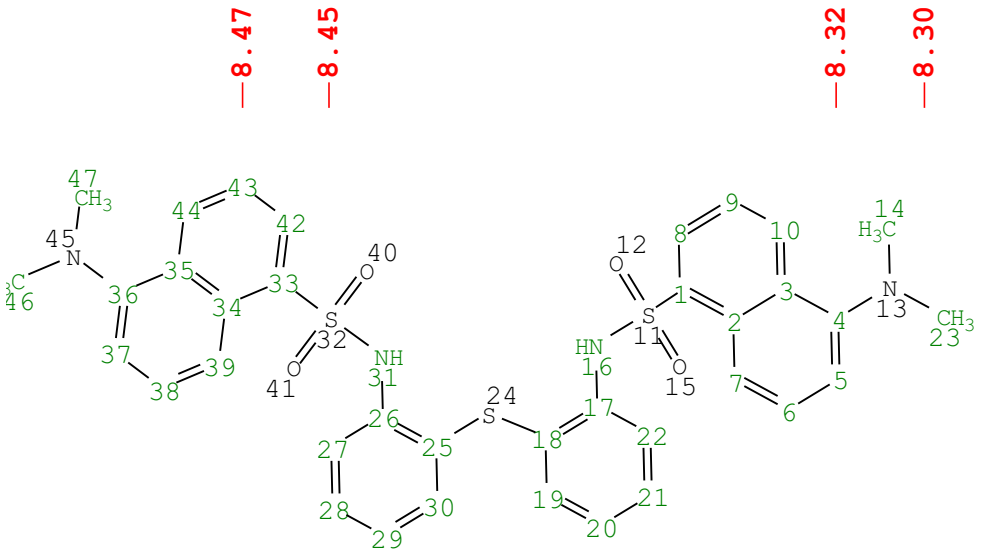


**Fig SX43** **L1 dmso-d6 ligand only full assignment**




10,44 (d)
8.46
J(8.49)

7,39 (d)
8.31
J(8.68)

8,42 (dd)
8.14
J(7.35, 1.20)

| | |
|---|---|
| NAME | AK-DR-165-0-DMSO.11.fid |
| DATE_TIME | 2024-12-18T23:02:13 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

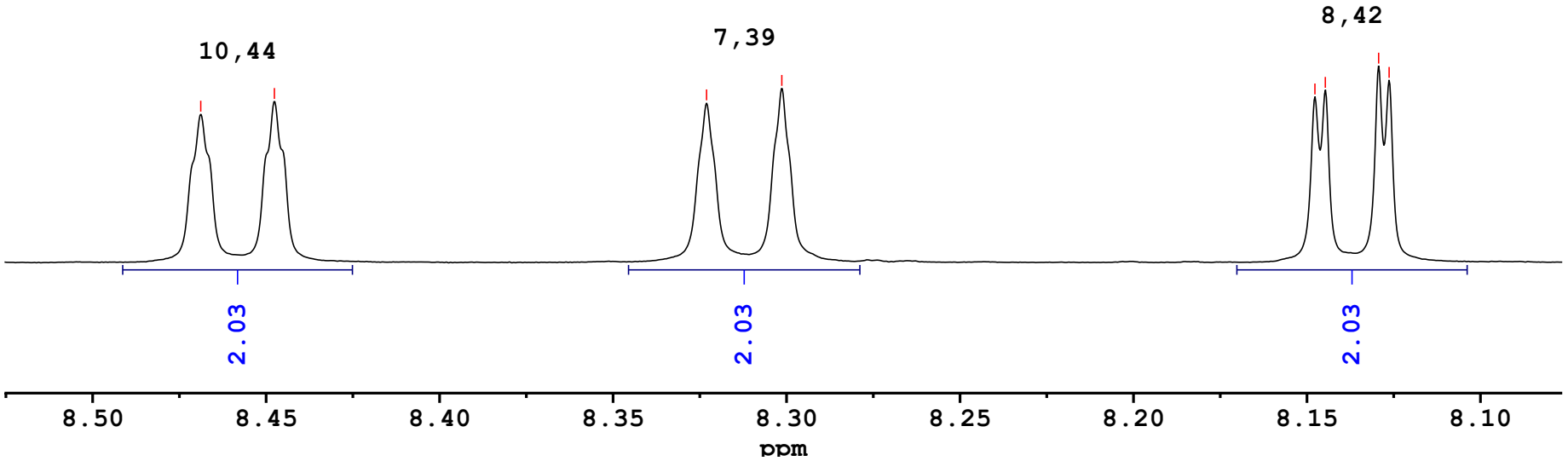
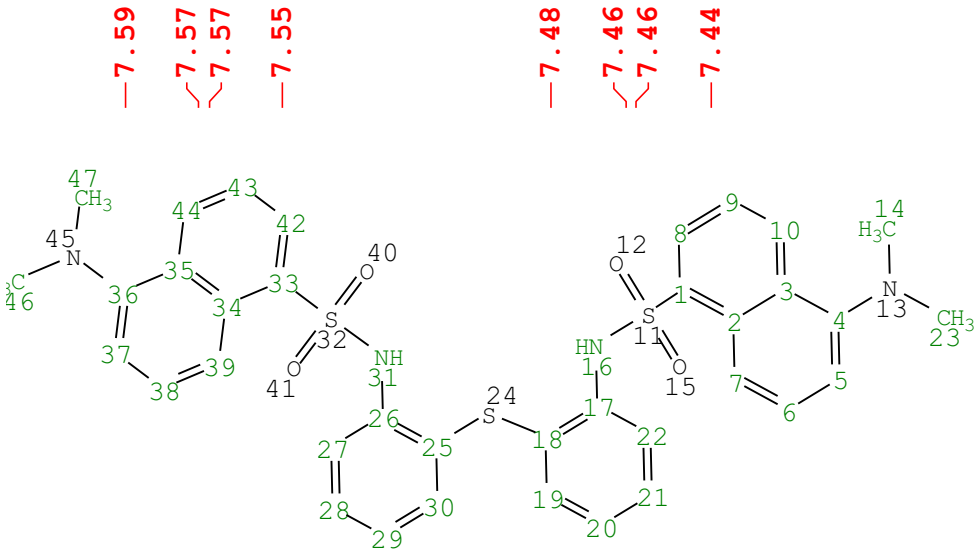


**Fig SX44** **L1 dmso-d6 ligand only full assignment**




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO.11.fid |
| DATE_TIME | 2024-12-18T23:02:13 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

9,43 (dd)
7.57
J(8.51, 7.38)

6,38 (dd)
7.46
J(8.63, 7.63)

5,37 (d)
7.19
J(7.08)

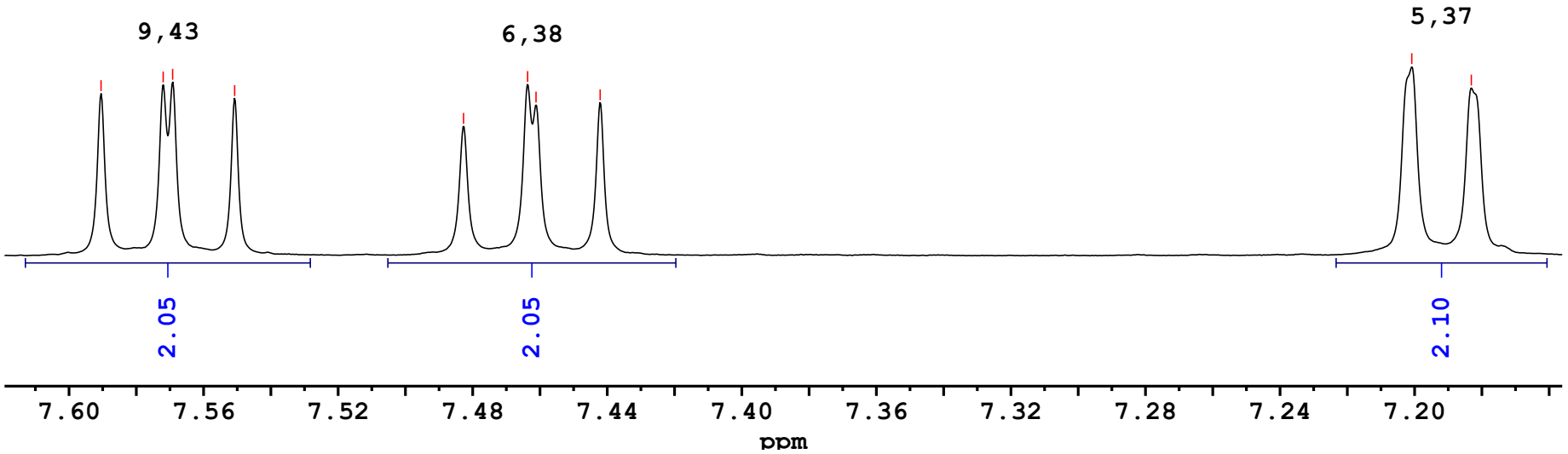
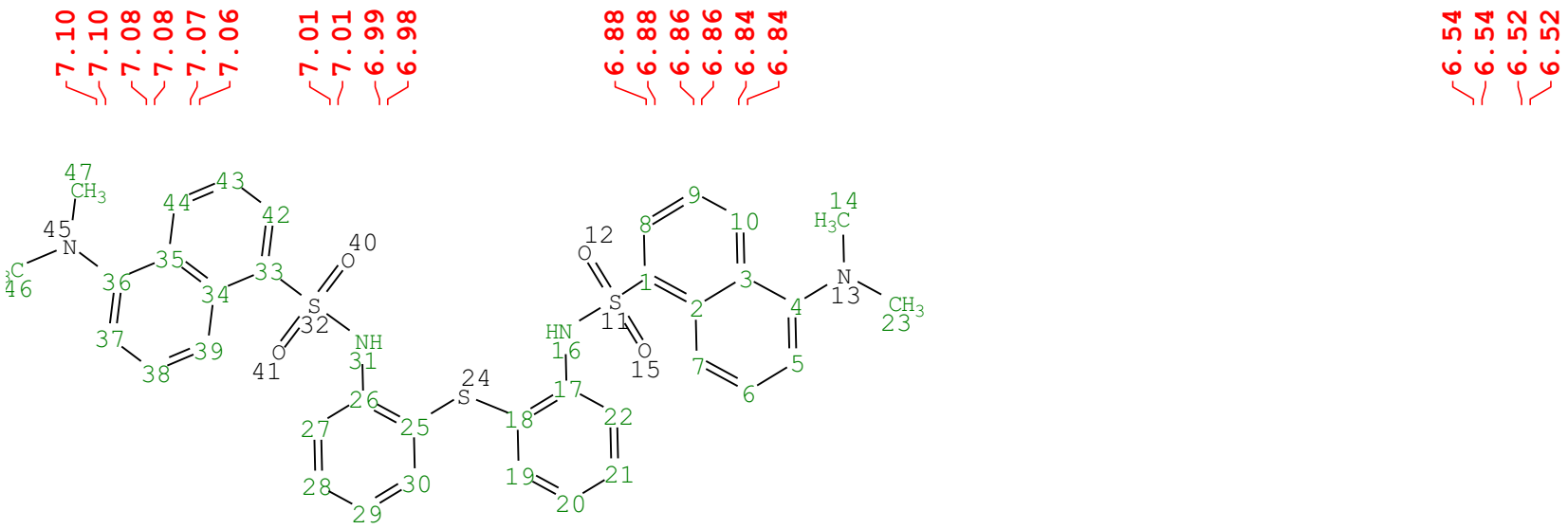


**Fig SX45** **L1 dmso-d6 ligand only full assignment**




| 21,28 (td) | 22,27 (dd) | 20,29 (td) | 19,30 (dd) |
|---|---|---|---|
| 7.08 | 7.00 | 6.86 | 6.53 |
| J(7.78, 1.50) | J(8.11, 1.34) | J(7.64, 1.44) | J(7.88, 1.41) |

| | |
|---|---|
| NAME | AK-DR-165-0-DMSO.11.fid |
| DATE_TIME | 2024-12-18T23:02:13 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

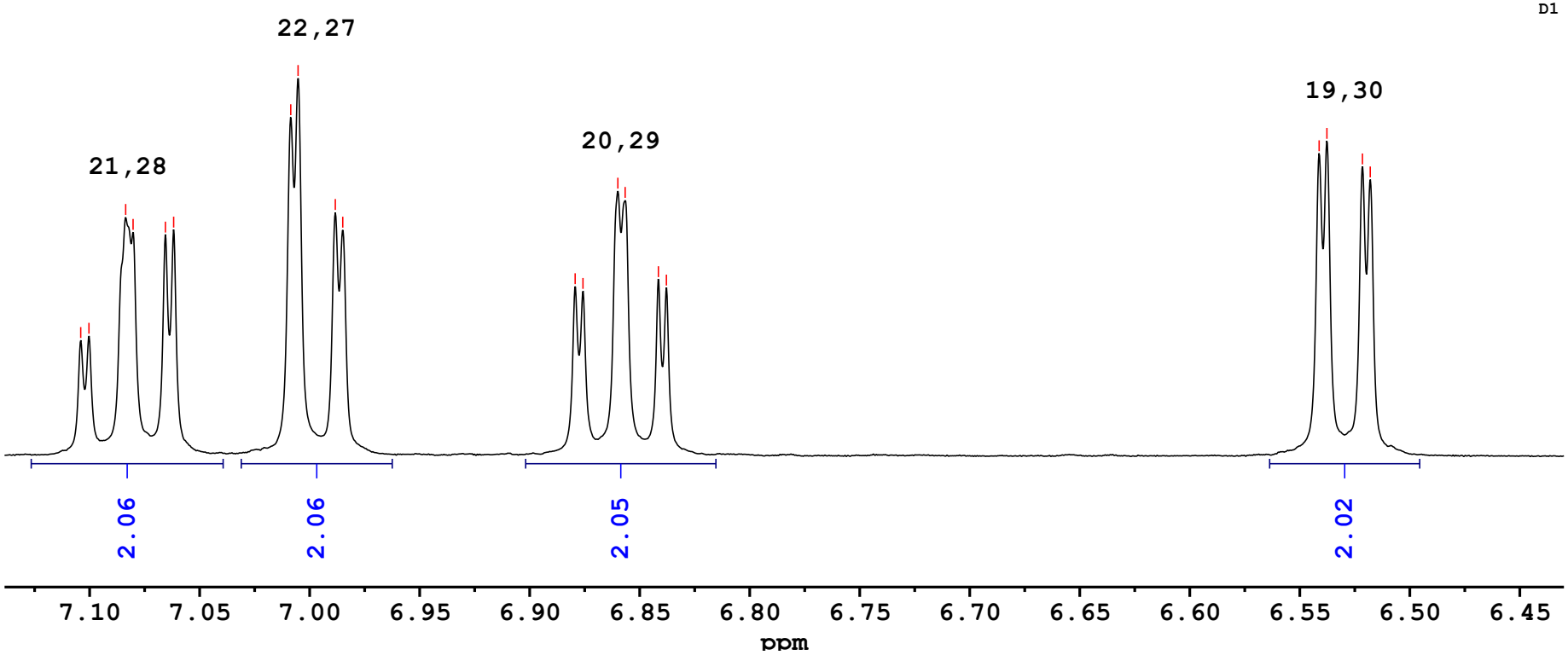
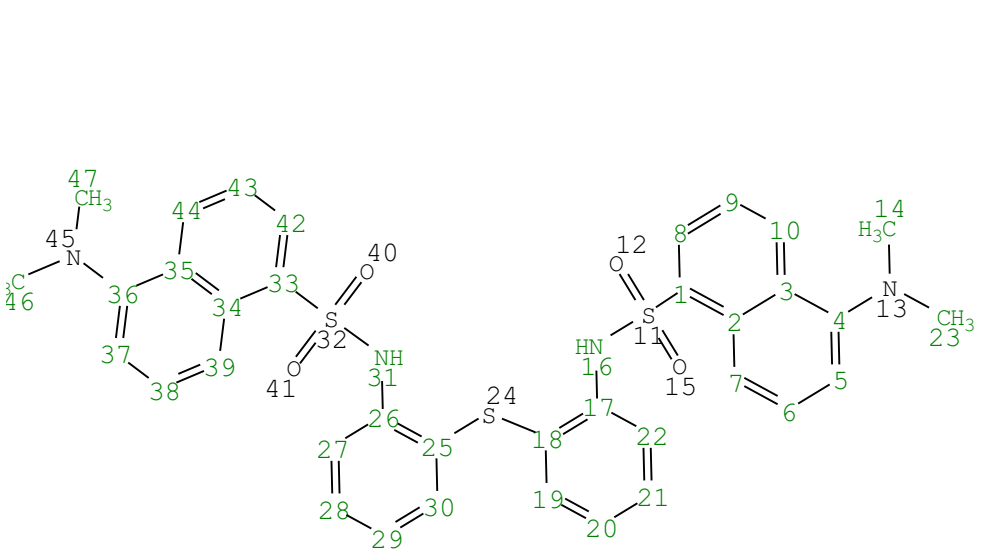


**Fig SX46** **L1 dmso-d6 ligand only full assignment**




14,23,46,47 (s)
2.80

| | |
|---|---|
| NAME | AK-DR-165-0-DMSO.11.fid |
| DATE_TIME | 2024-12-18T23:02:13 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

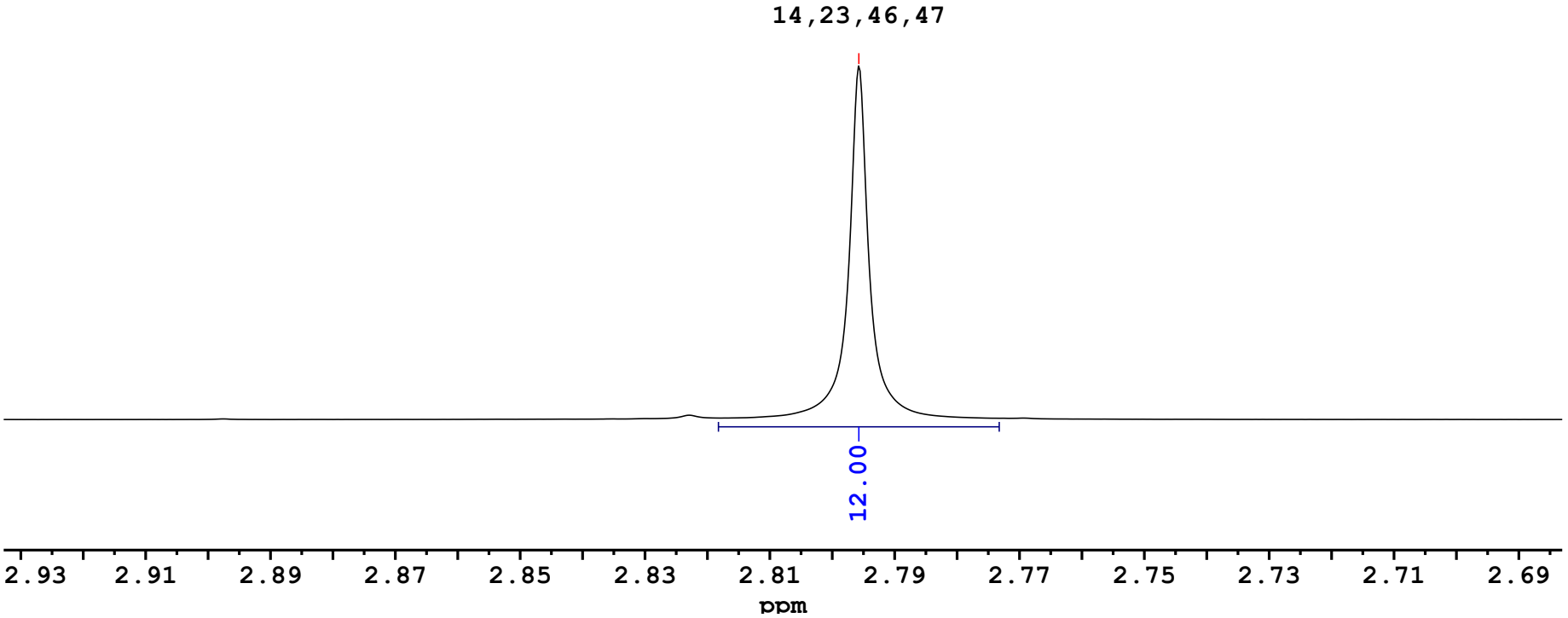
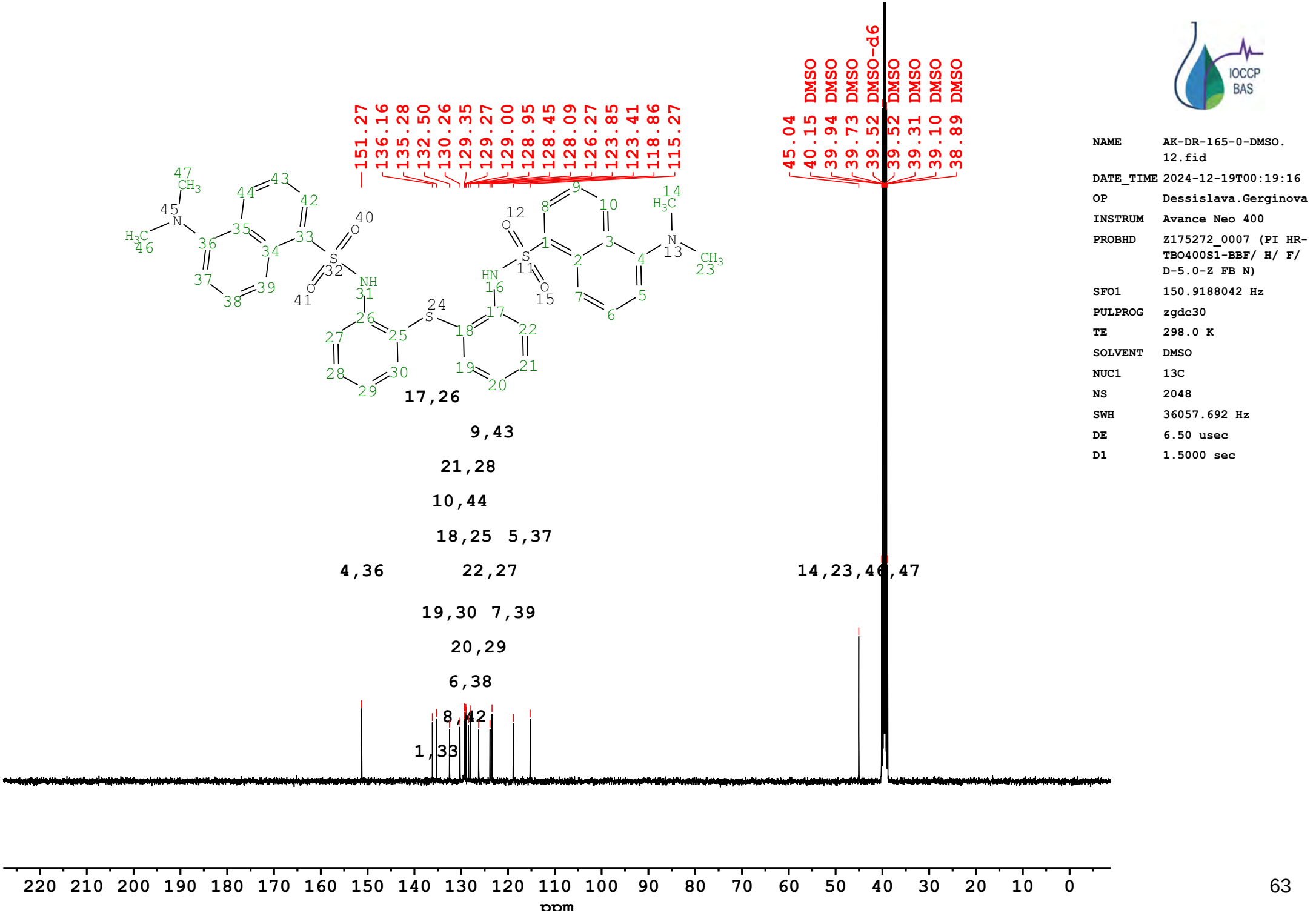


Fig SX47

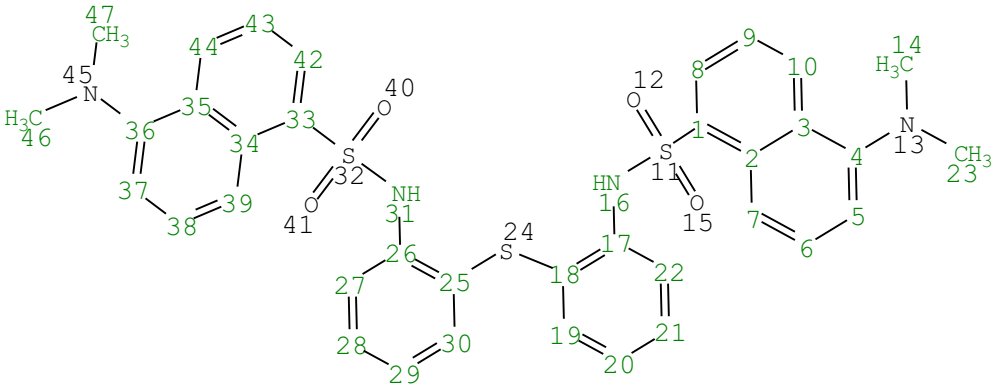
# L1 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO. 12.fid |
| DATE_TIME | 2024-12-19T00:19:16 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 2048 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

**Fig SX48** **L1 dmso-d6 ligand only full assignment**

136.16 135.28 132.50 130.26 129.35 129.27 129.00 128.95 128.45 128.09



| | |
|---|---|
| NAME | AK-DR-165-0-DMSO.12.fid |
| DATE_TIME | 2024-12-19T00:19:16 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 2048 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

2,34 8,42 6,38 17,26 1,33 19,30 10,44 18,25 21,28 3,35

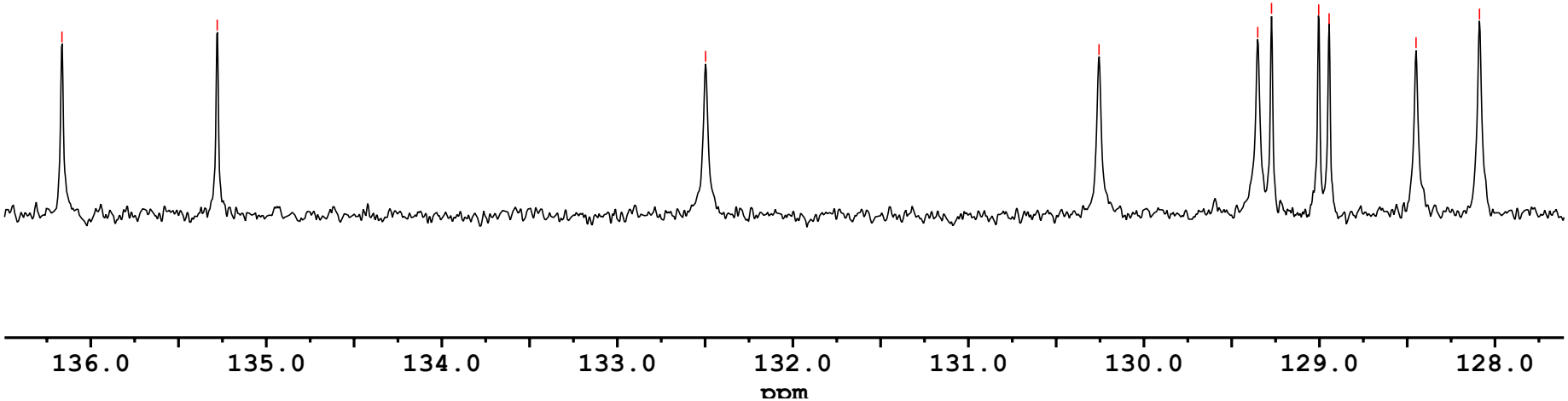
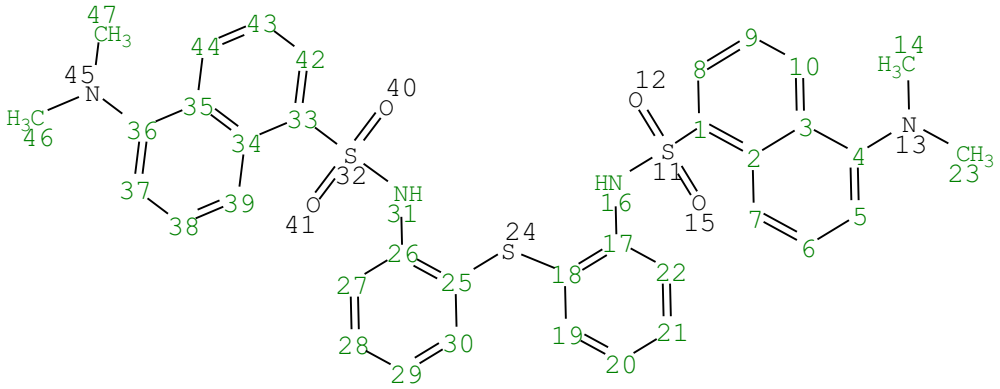


**Fig SX49** **L1 dmso-d6 ligand only full assignment**



| | |
|---|---|
| NAME | AK-DR-165-0-DMSO. 12.fid |
| DATE_TIME | 2024-12-19T00:19:16 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 2048 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

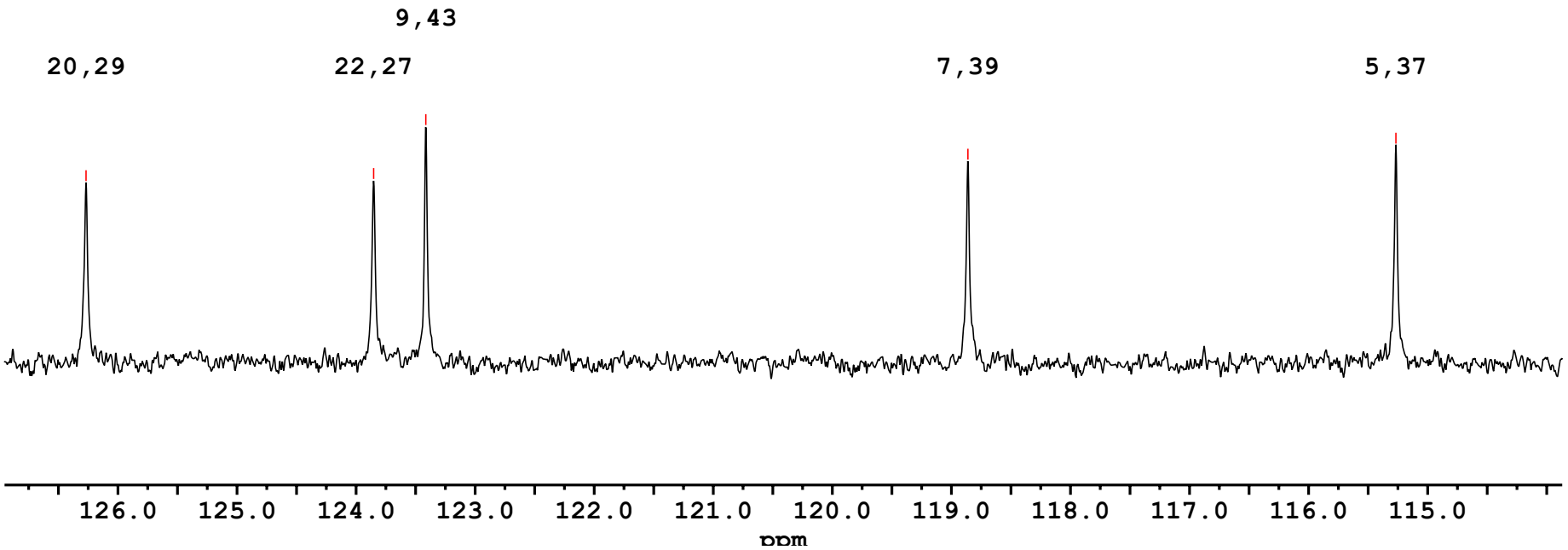
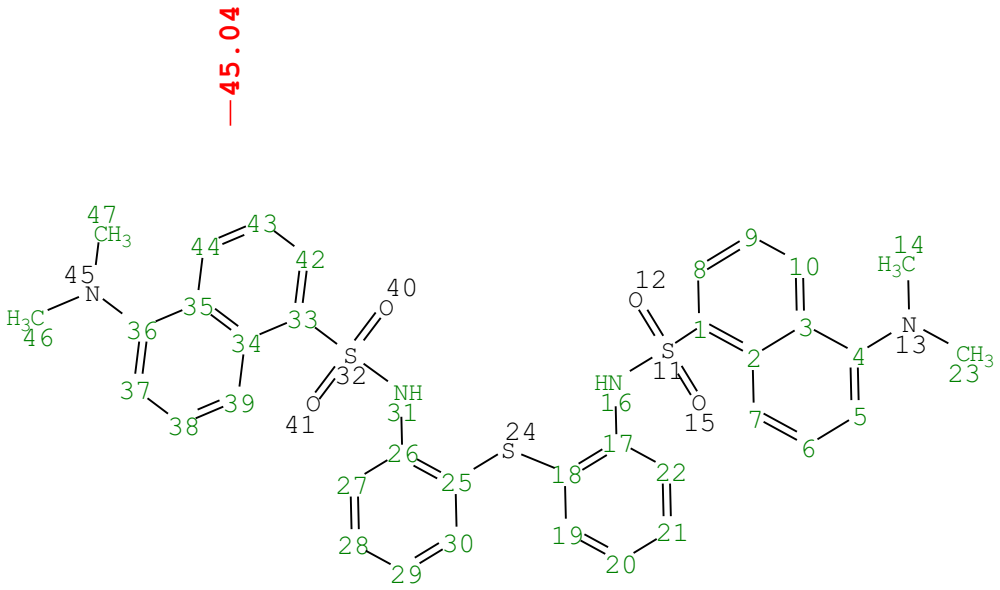


Fig SX50

# L1 dmso-d6 ligand only full assignment




—45.04

—40.15 DMSO
—39.94 DMSO
—39.73 DMSO
—39.52 DMSO-d6
—39.52 DMSO
—39.31 DMSO
—39.10 DMSO
—38.89 DMSO

14,23,46,47

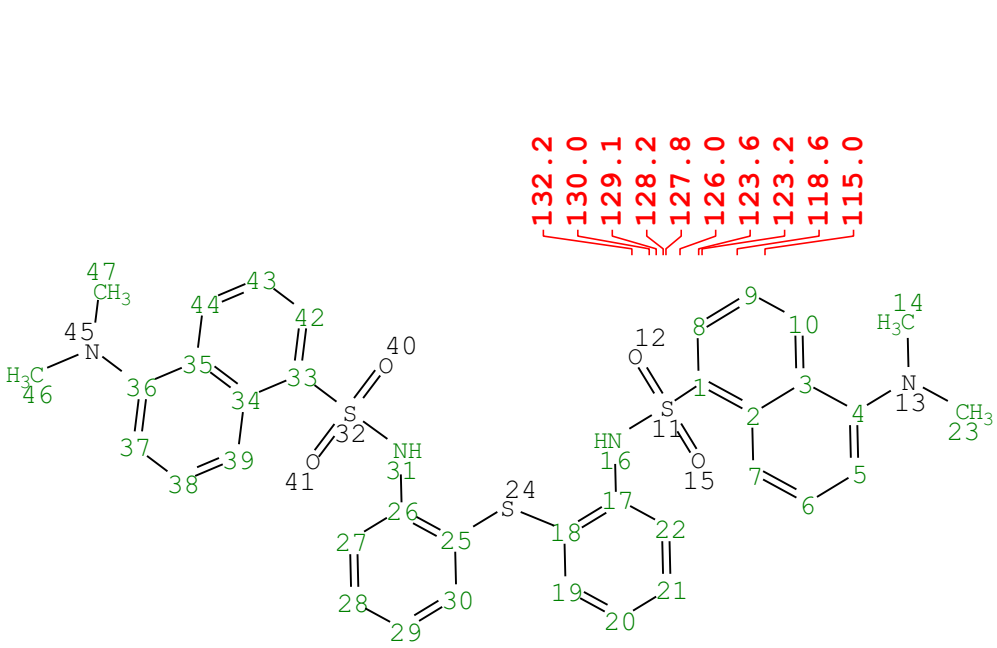
| | |
|---|---|
| NAME | AK-DR-165-0-DMSO. 12.fid |
| DATE_TIME | 2024-12-19T00:19:16 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 2048 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

47.0 46.5 46.0 45.5 45.0 44.5 44.0 43.5 43.0 42.5 42.0 41.5 41.0 40.5 40.0 39.5 39.0 38.5

ppm

Fig SX51

# L1 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO.12.fid |
| DATE_TIME | 2024-12-19T00:19:16 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9319844 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 2048 |
| SWH | 35714.286 Hz |
| DE | 18.00 usec |
| D1 | 1.5000 sec |

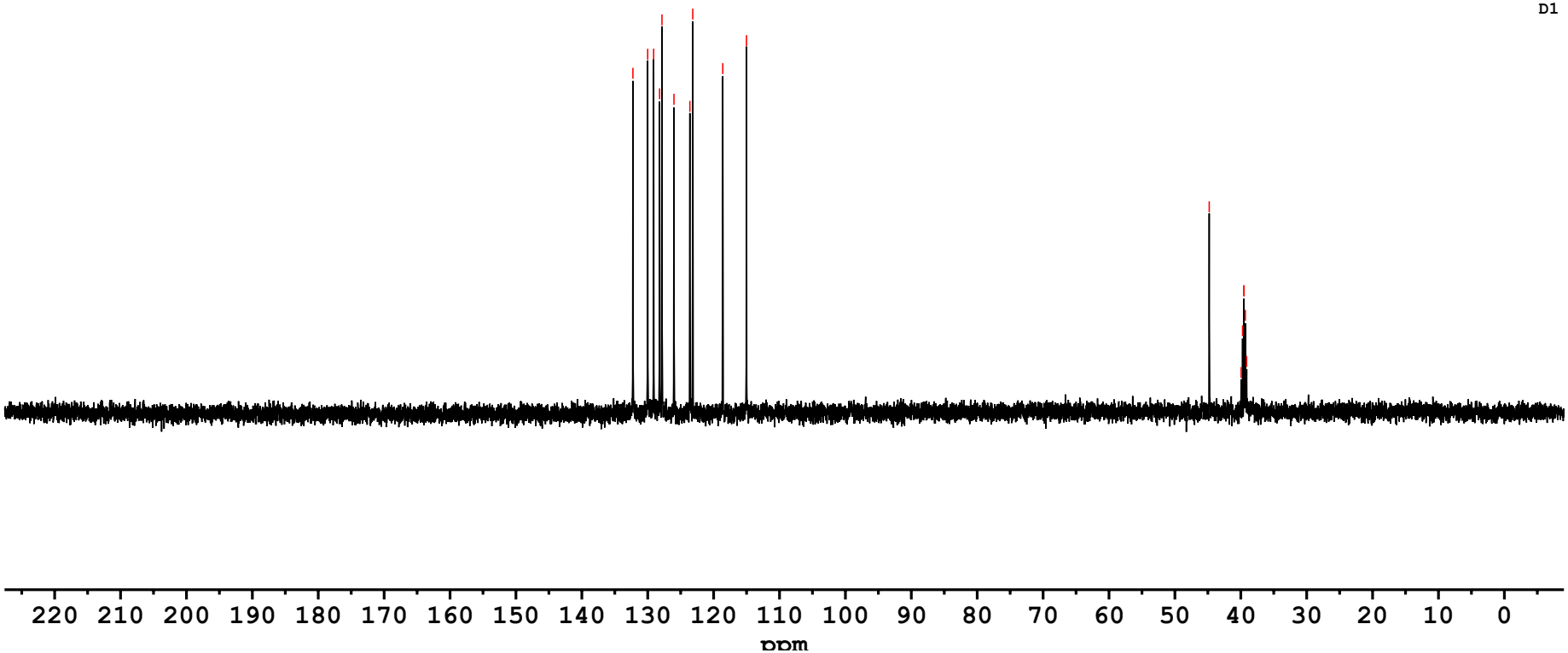
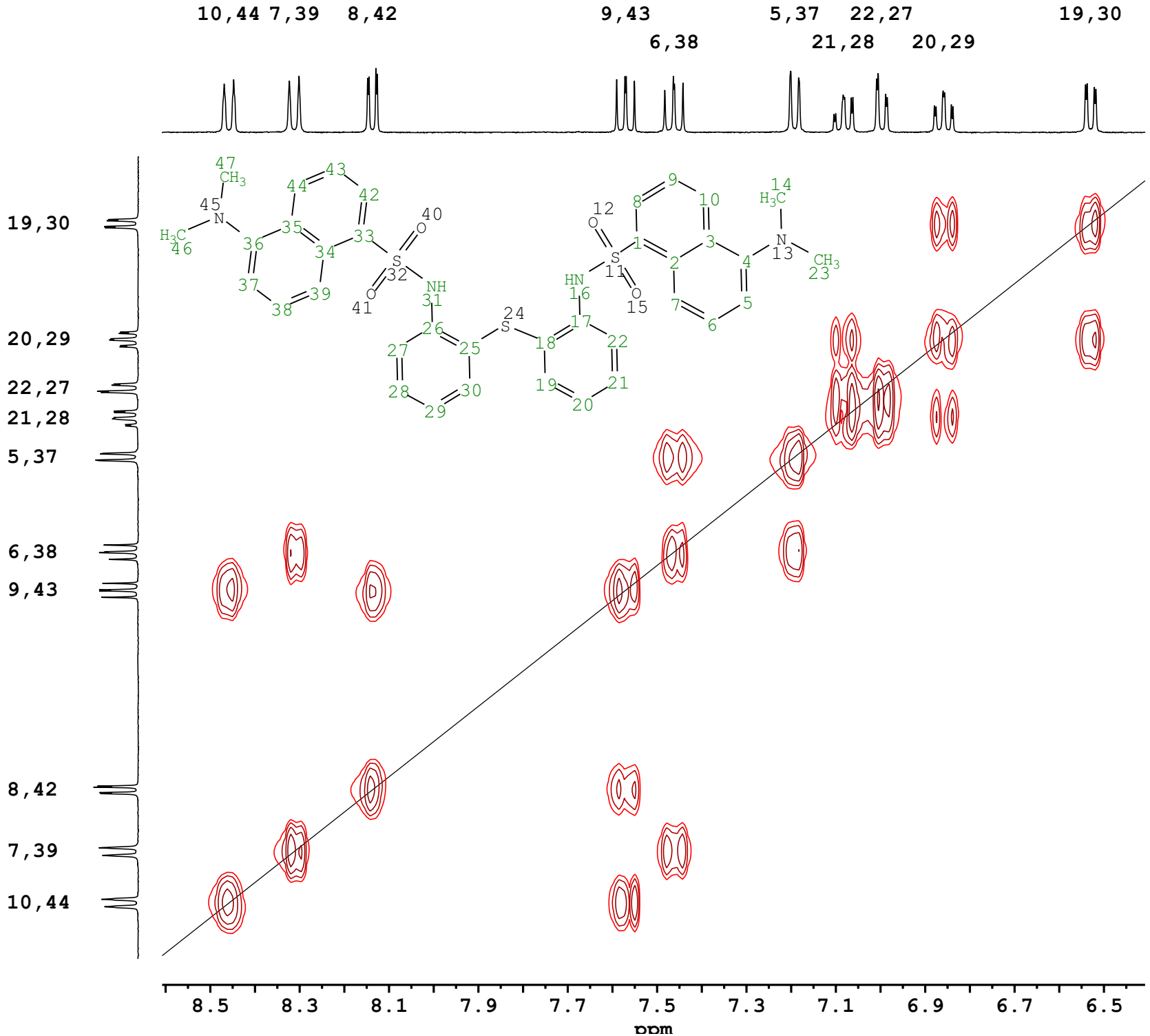


Fig SX52

# L1 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO.14.ser |
| DATE_TIME | 2024-12-19T01:02:21 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 1 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0221 sec |

Fig SX53

# L1 dmso-d6 ligand only full assignment

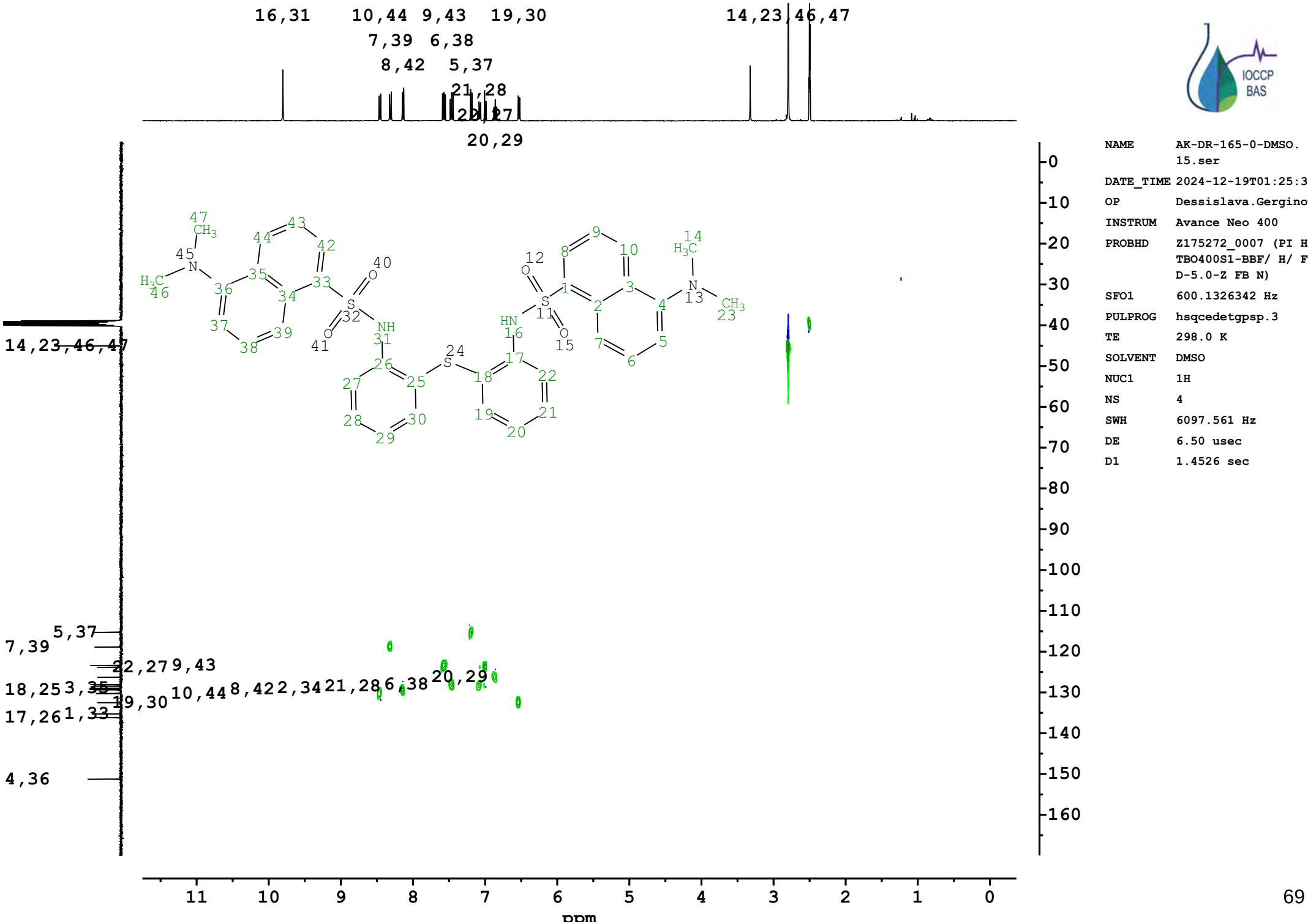
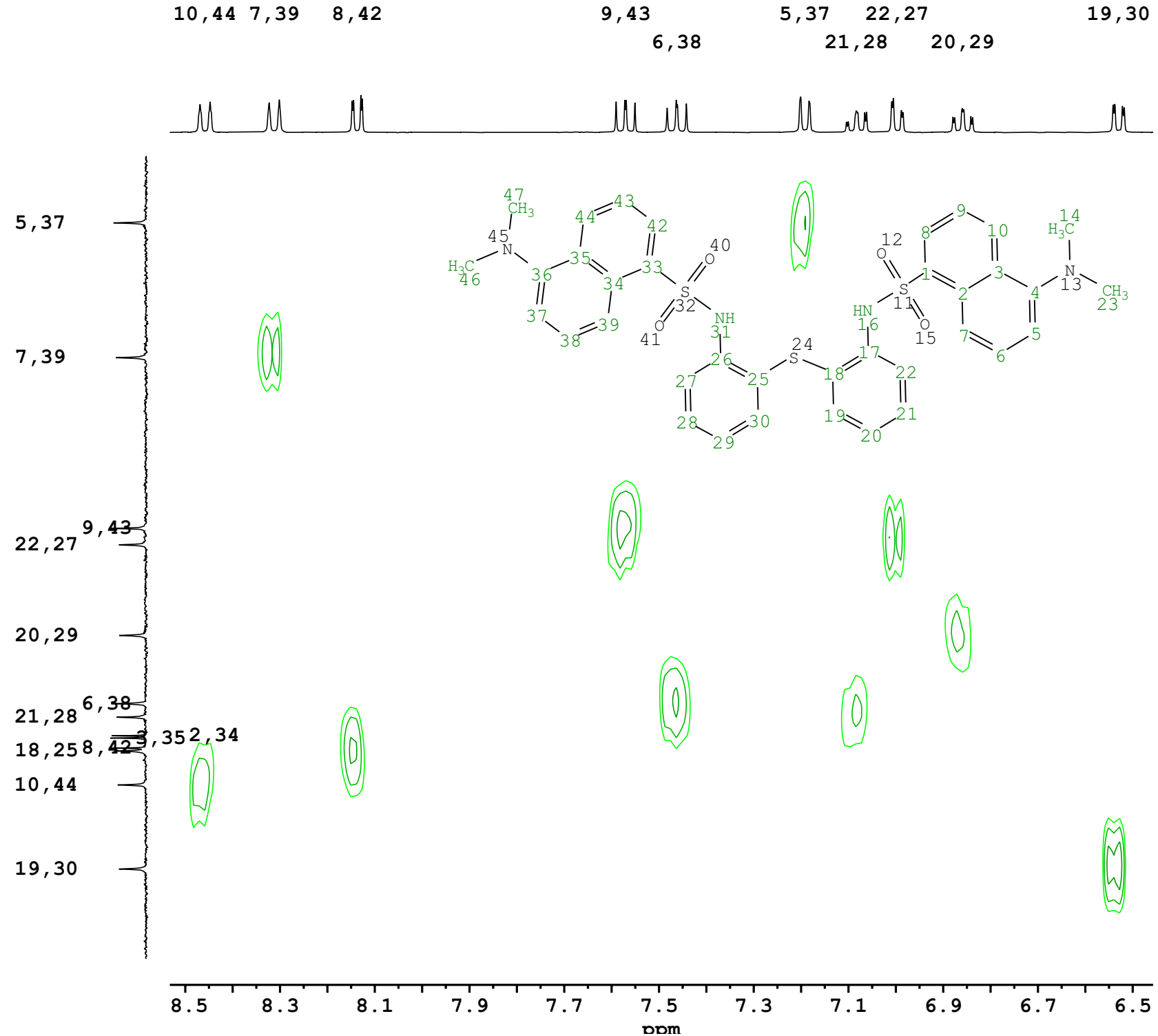


Fig SX54

# L1 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO. 15.ser |
| DATE_TIME | 2024-12-19T01:25:34 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 4 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX55

# L1 dmso-d6 ligand only full assignment

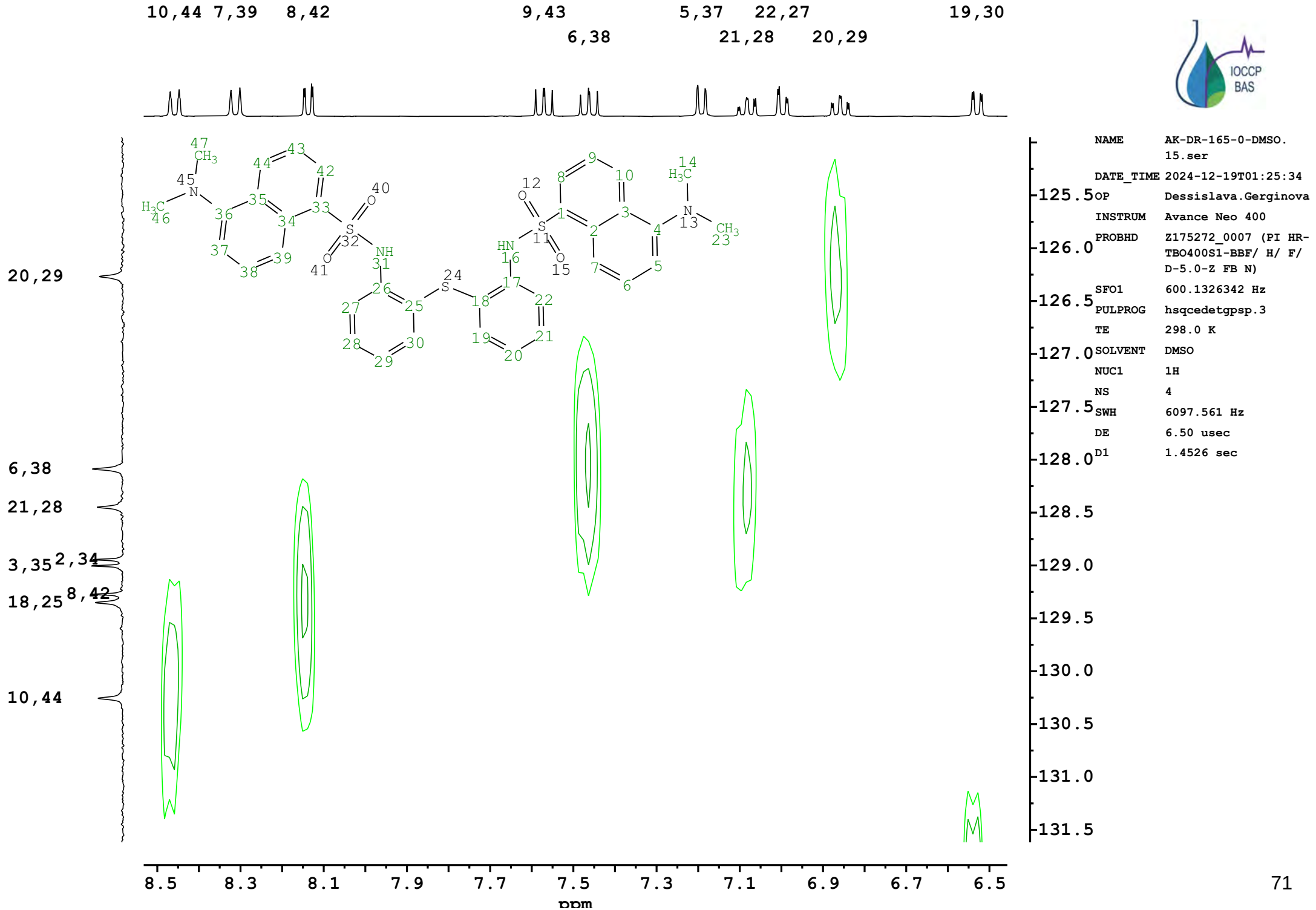
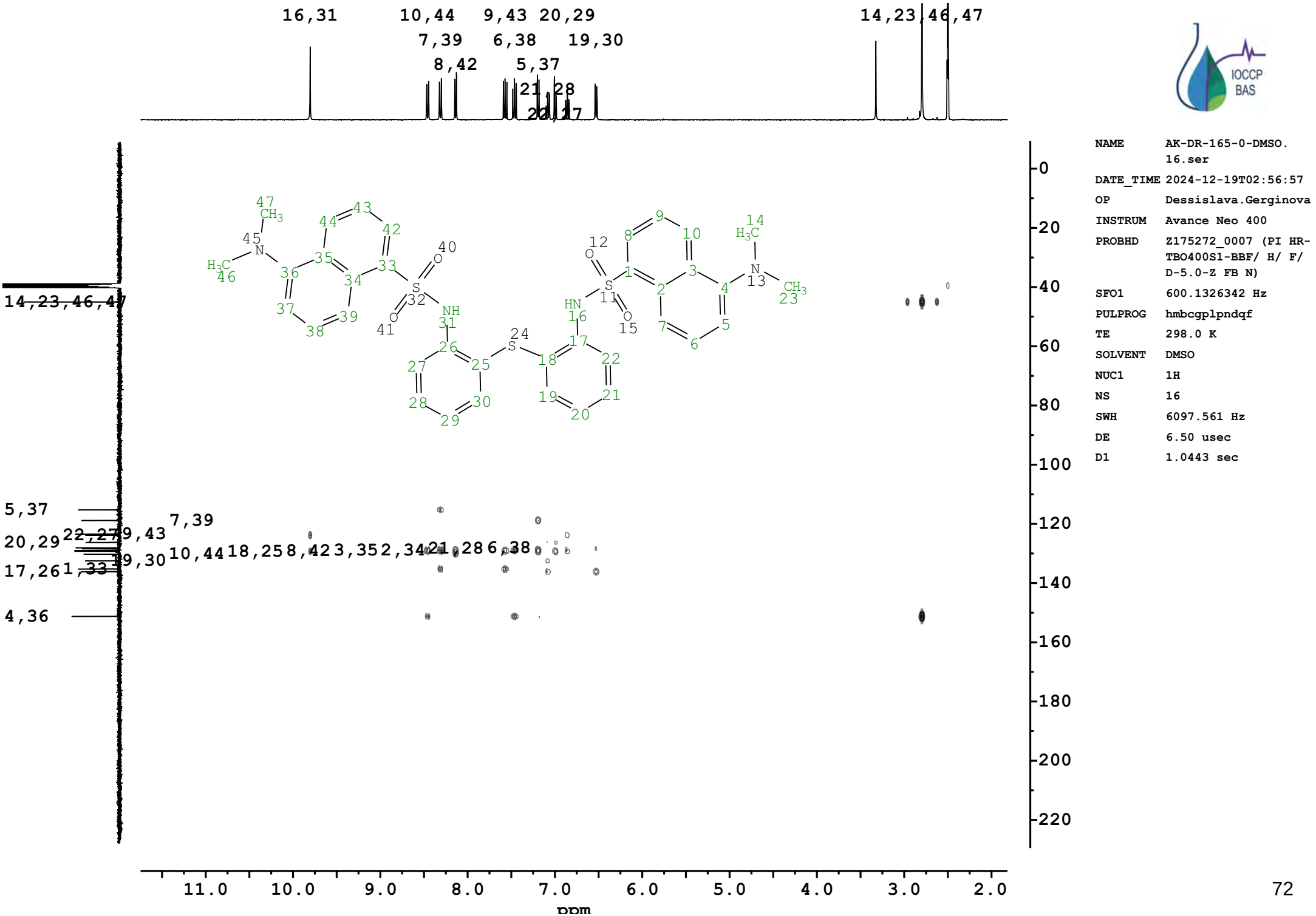


Fig SX56

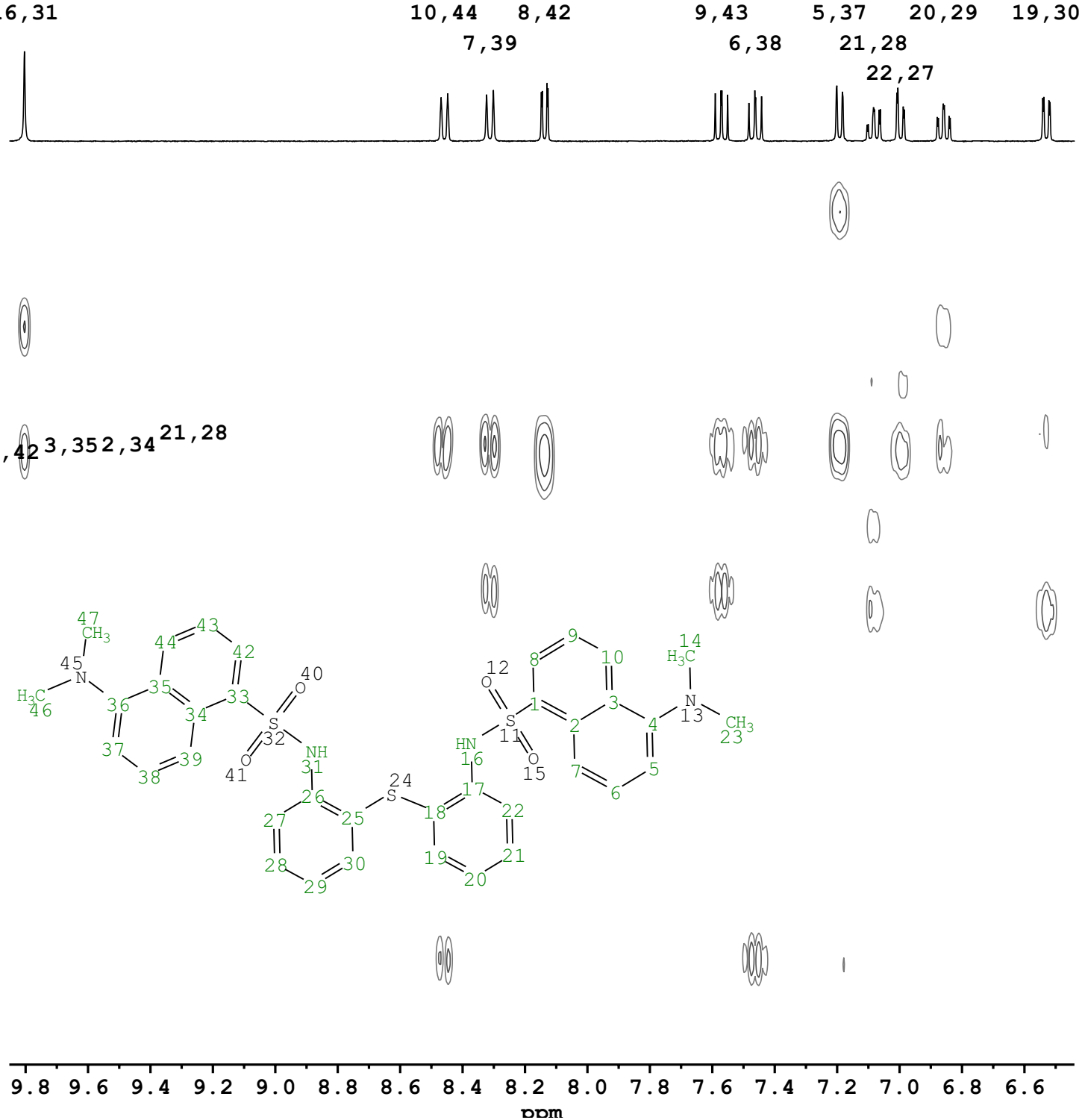
# L1 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO.16.ser |
| DATE_TIME | 2024-12-19T02:56:57 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX57

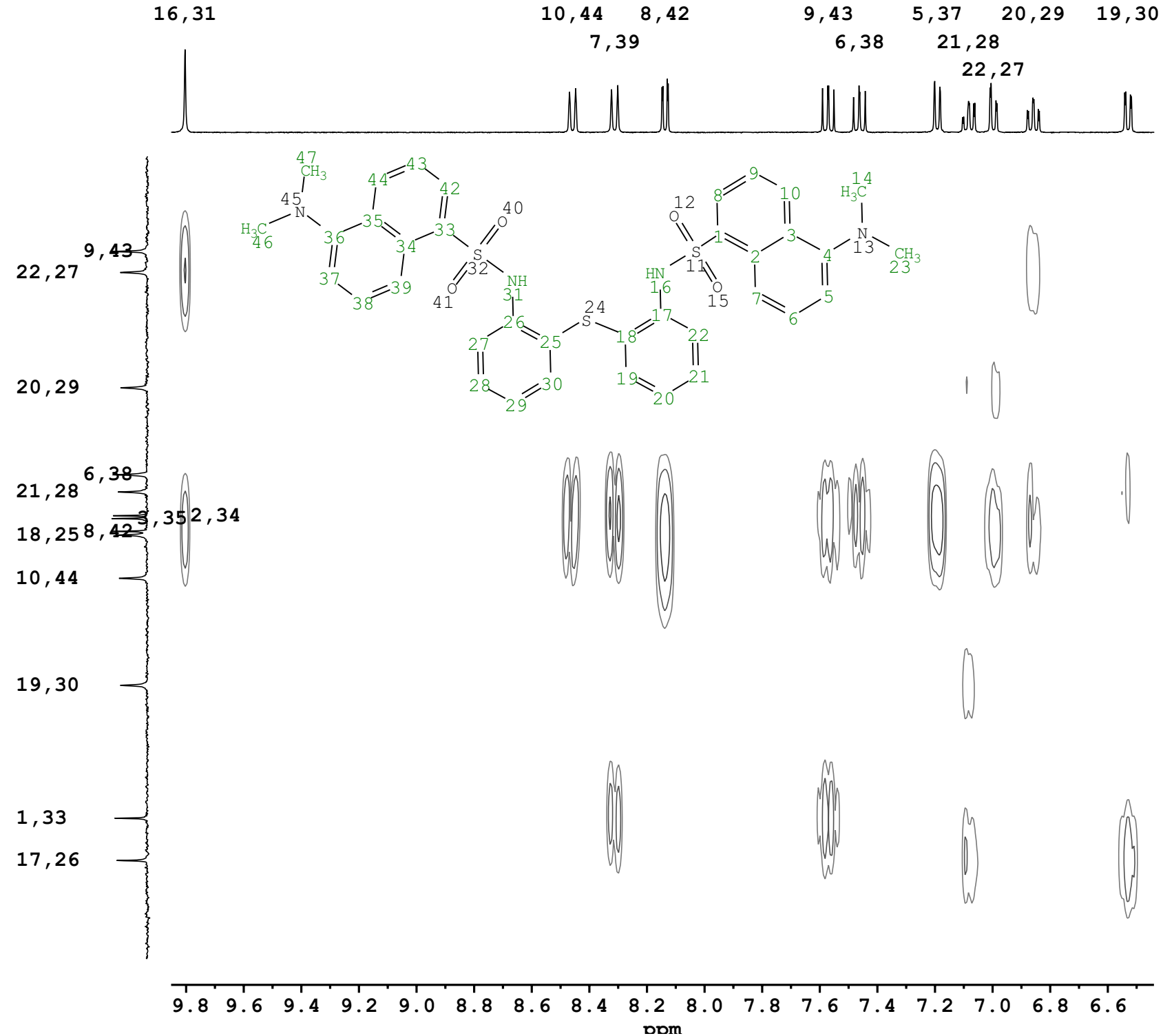
# L1 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO. 16.ser |
| DATE_TIME | 2024-12-19T02:56:57 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

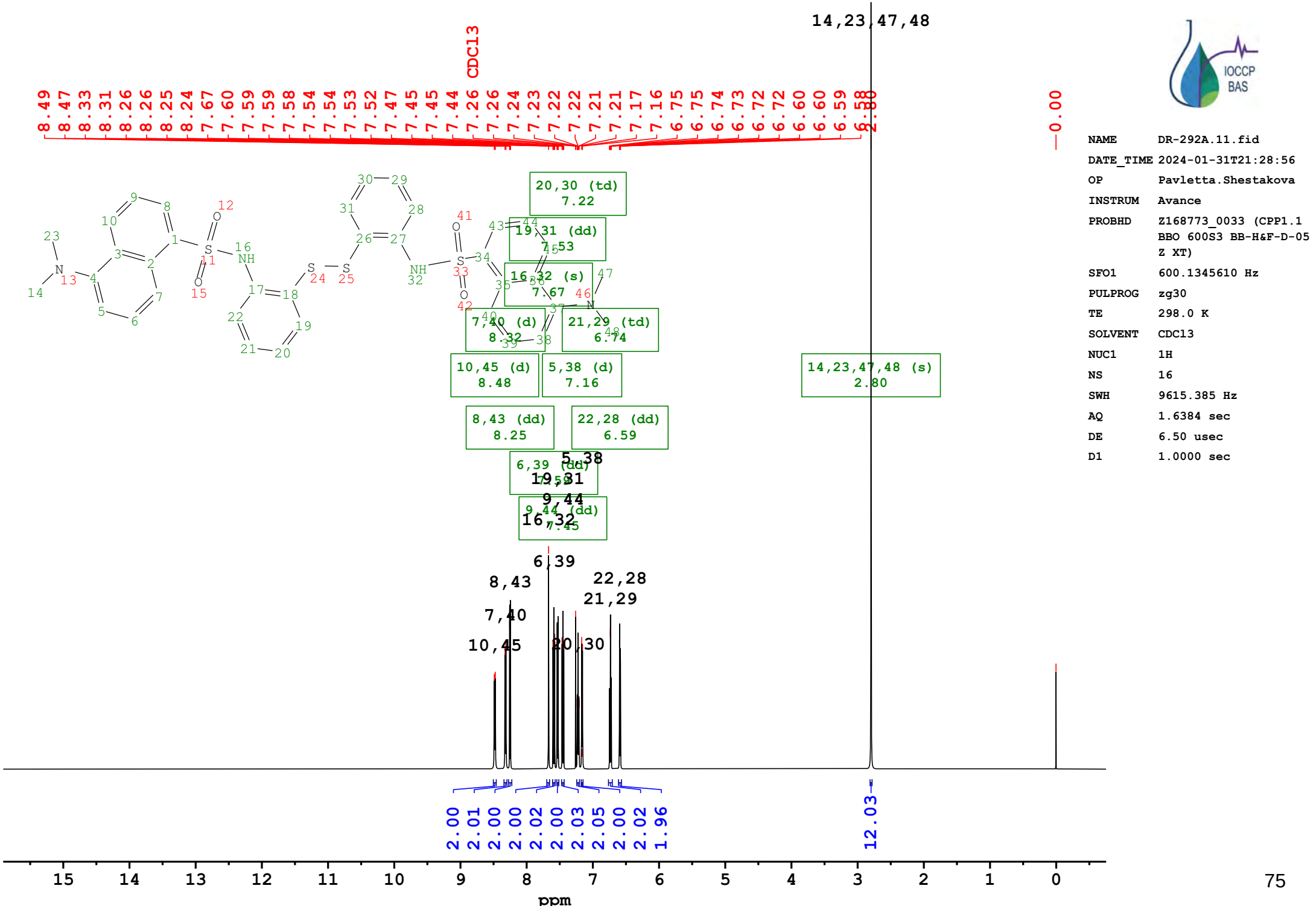
Fig SX58

# L1 dmso-d6 ligand only full assignment



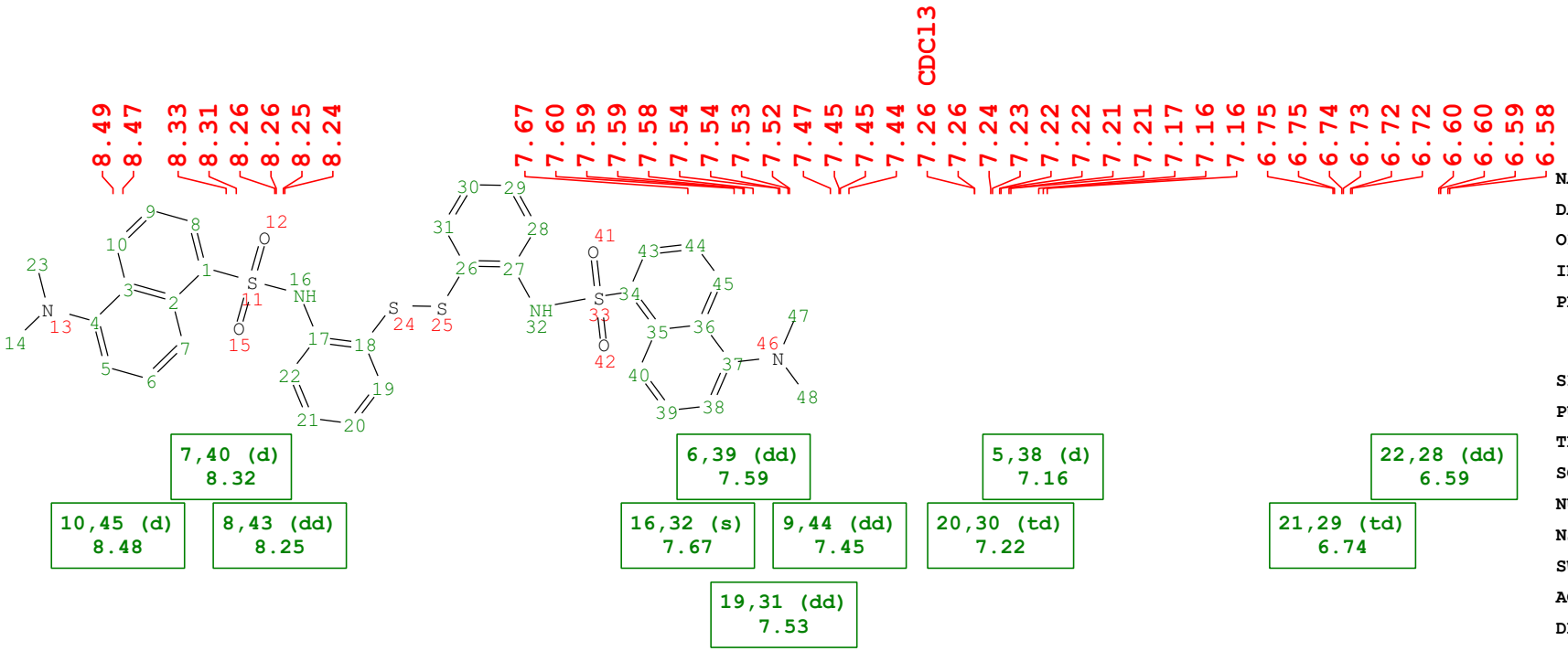

| | |
|---|---|
| NAME | AK-DR-165-0-DMSO. 16.ser |
| DATE_TIME | 2024-12-19T02:56:57 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX59 L2 chloroform-d ligand only full assignment




NAME DR-292A.11.fid
DATE_TIME 2024-01-31T21:28:56
OP Pavletta.Shestakova
INSTRUM Avance
PROBHD Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT)
SFO1 600.1345610 Hz
PULPROG zg30
TE 298.0 K
SOLVENT CDC13
NUC1 1H
NS 16
SWH 9615.385 Hz
AQ 1.6384 sec
DE 6.50 usec
D1 1.0000 sec

**Fig SX60** **L2 chloroform-d ligand only full assignment**




| | |
|---|---|
| NAME | DR-292A.11.fid |
| DATE_TIME | 2024-01-31T21:28:56 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 16 |
| SWH | 9615.385 Hz |
| AQ | 1.6384 sec |
| DE | 6.50 usec |
| D1 | 1.0000 sec |

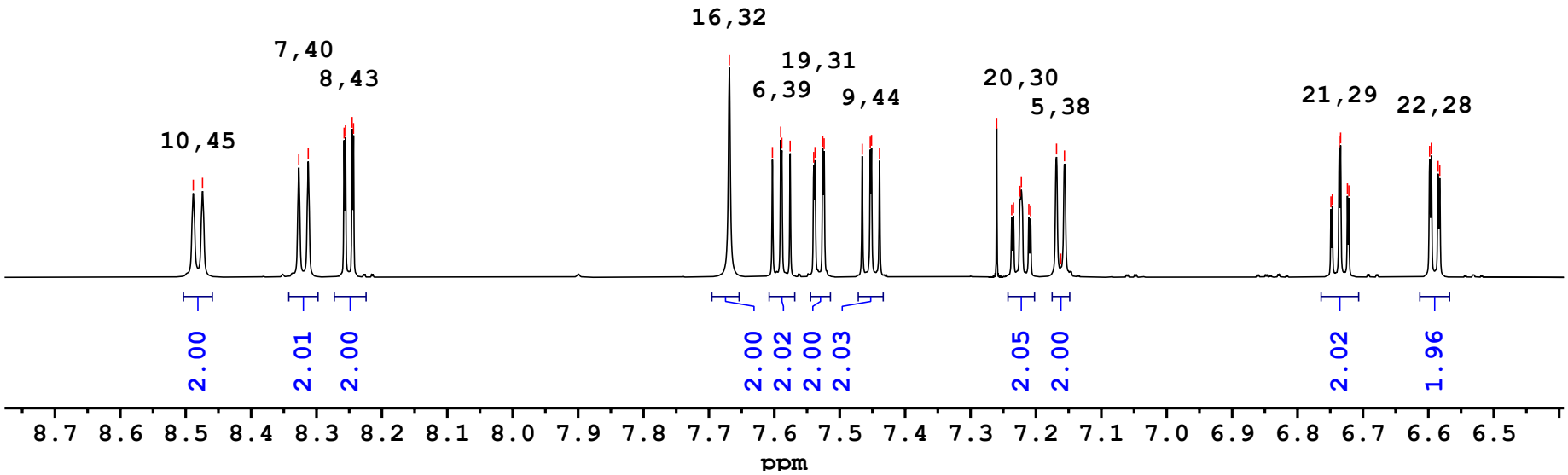
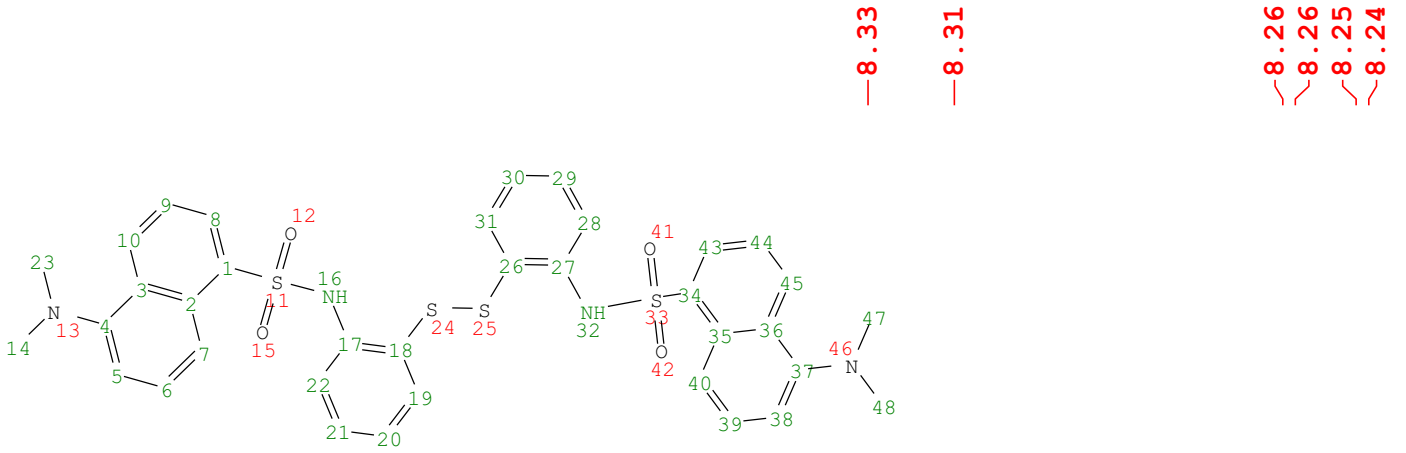


Fig SX61 L2 chloroform-d ligand only full assignment




10,45 (d)
8.48

7,40 (d)
8.32

8,43 (dd)
8.25

| | |
|---|---|
| NAME | DR-292A.11.fid |
| DATE_TIME | 2024-01-31T21:28:56 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 16 |
| SWH | 9615.385 Hz |
| AQ | 1.6384 sec |
| DE | 6.50 usec |
| D1 | 1.0000 sec |

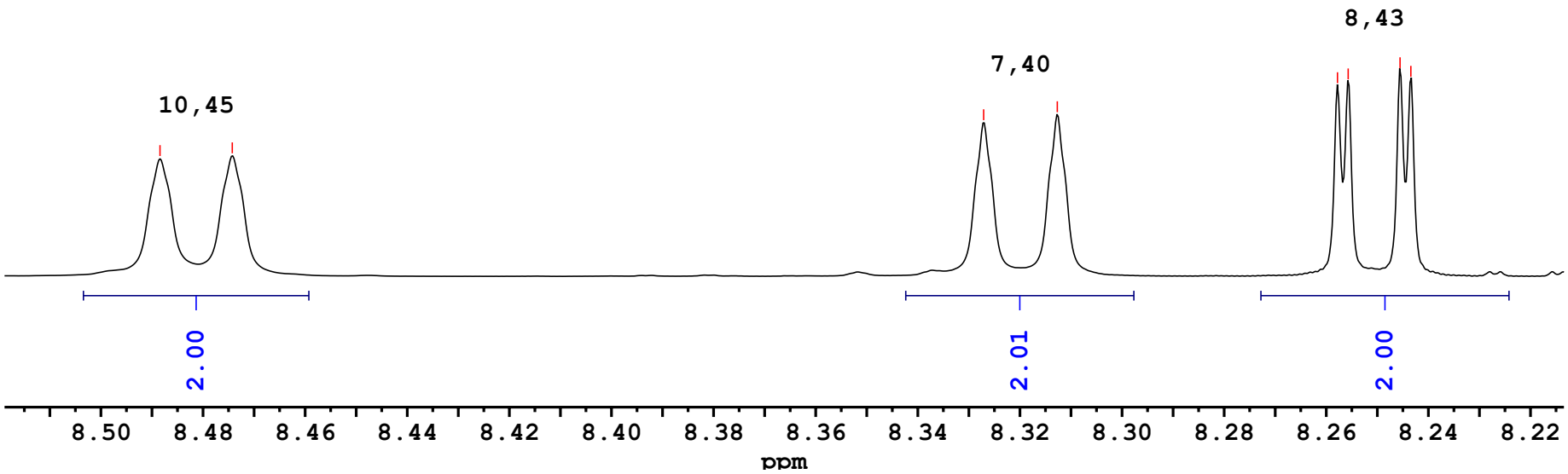
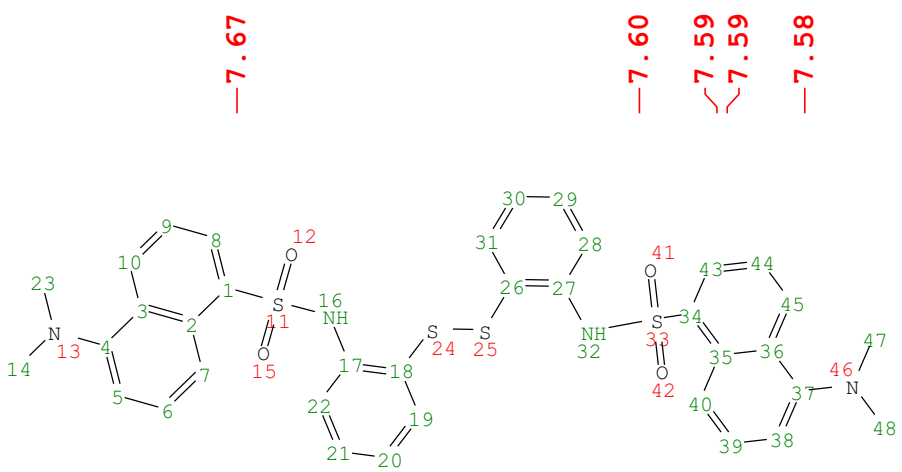


**Fig SX62** **L2 chloroform-d ligand only full assignment**






16,32 (s) 7.67

6,39 (dd) 7.59

19,31 (dd) 7.53

9,44 (dd) 7.45

| | |
|---|---|
| NAME | DR-292A.11.fid |
| DATE_TIME | 2024-01-31T21:28:56 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 16 |
| SWH | 9615.385 Hz |
| AQ | 1.6384 sec |
| DE | 6.50 usec |
| D1 | 1.0000 sec |

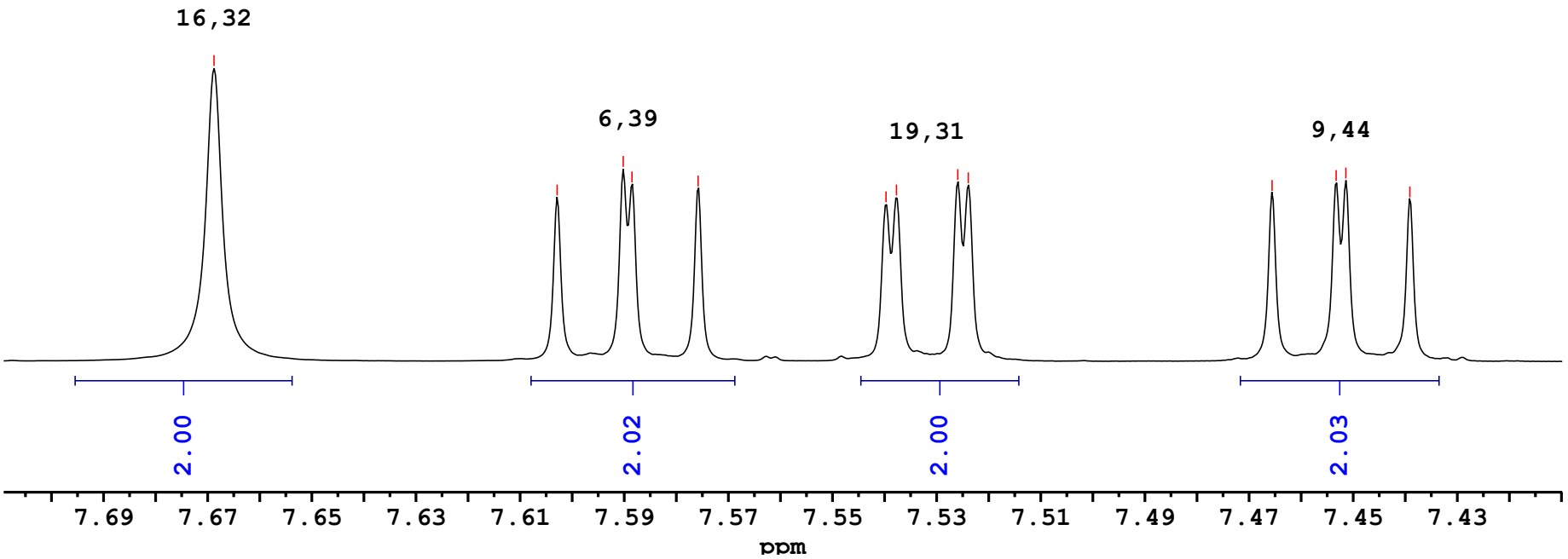
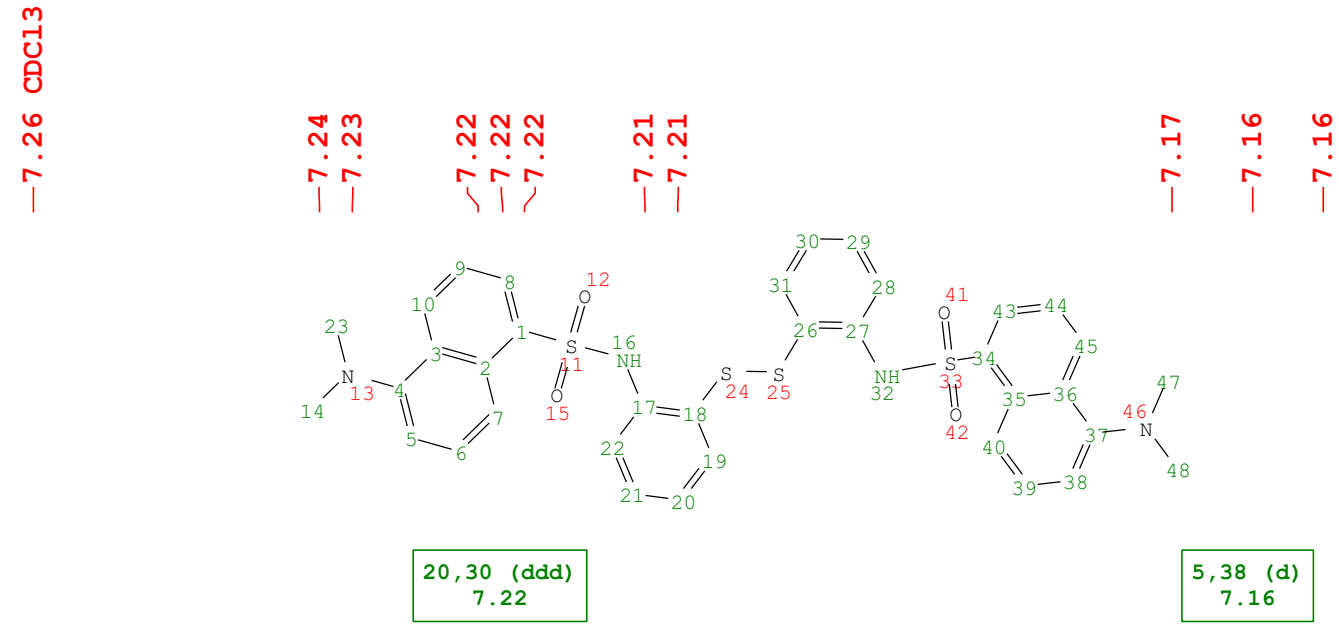


**Fig SX63** **L2 chloroform-d ligand only full assignment**




| | |
|---|---|
| NAME | DR-292A.11.fid |
| DATE_TIME | 2024-01-31T21:28:56 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 16 |
| SWH | 9615.385 Hz |
| AQ | 1.6384 sec |
| DE | 6.50 usec |
| D1 | 1.0000 sec |

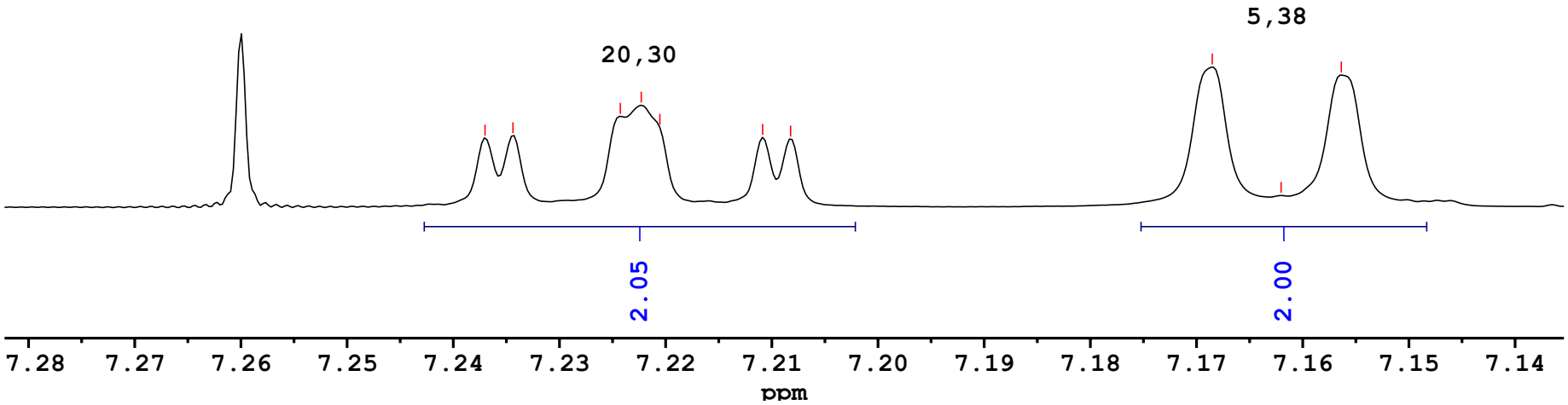


**Fig SX64** **L2 chloroform-d ligand only full assignment**

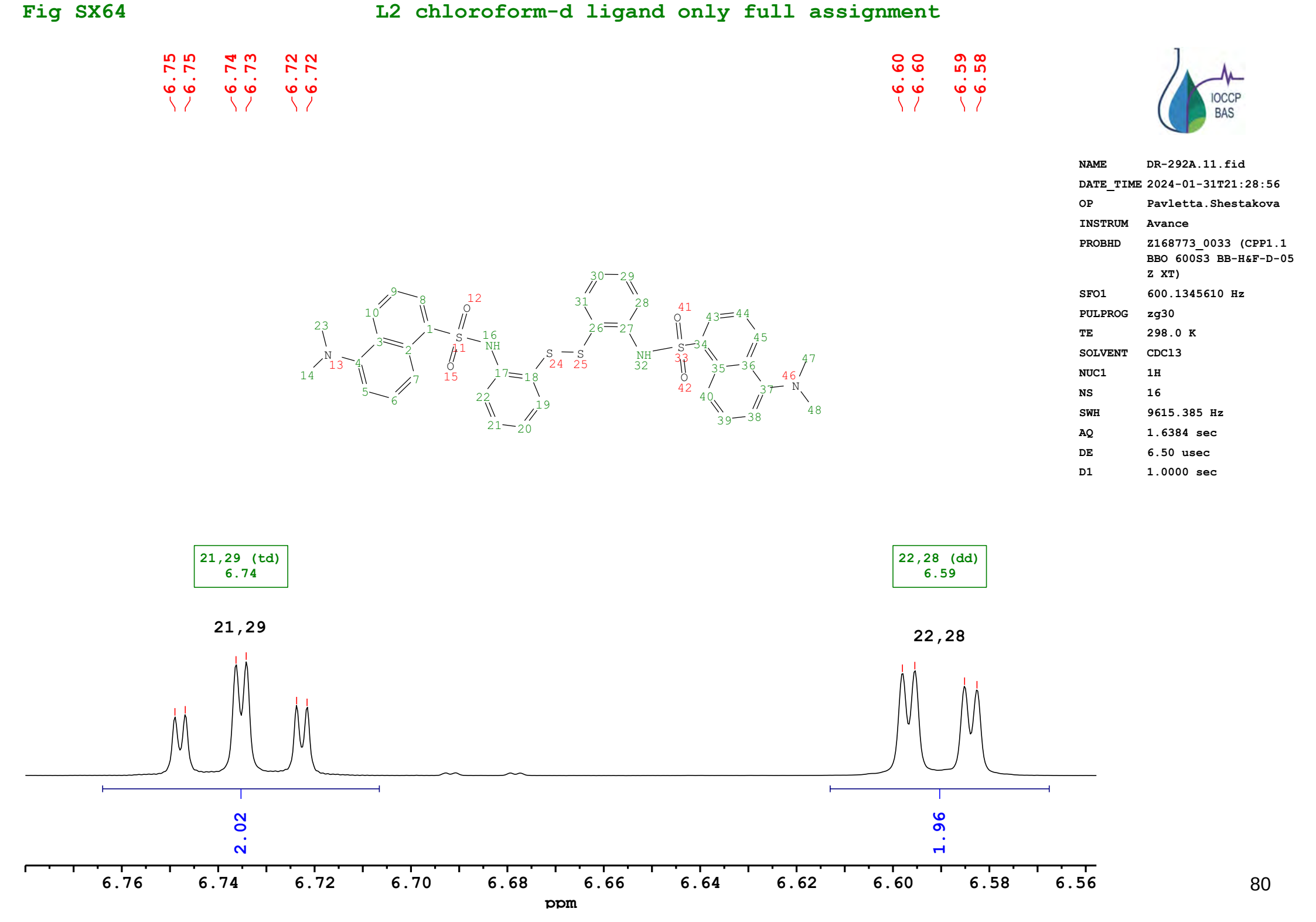
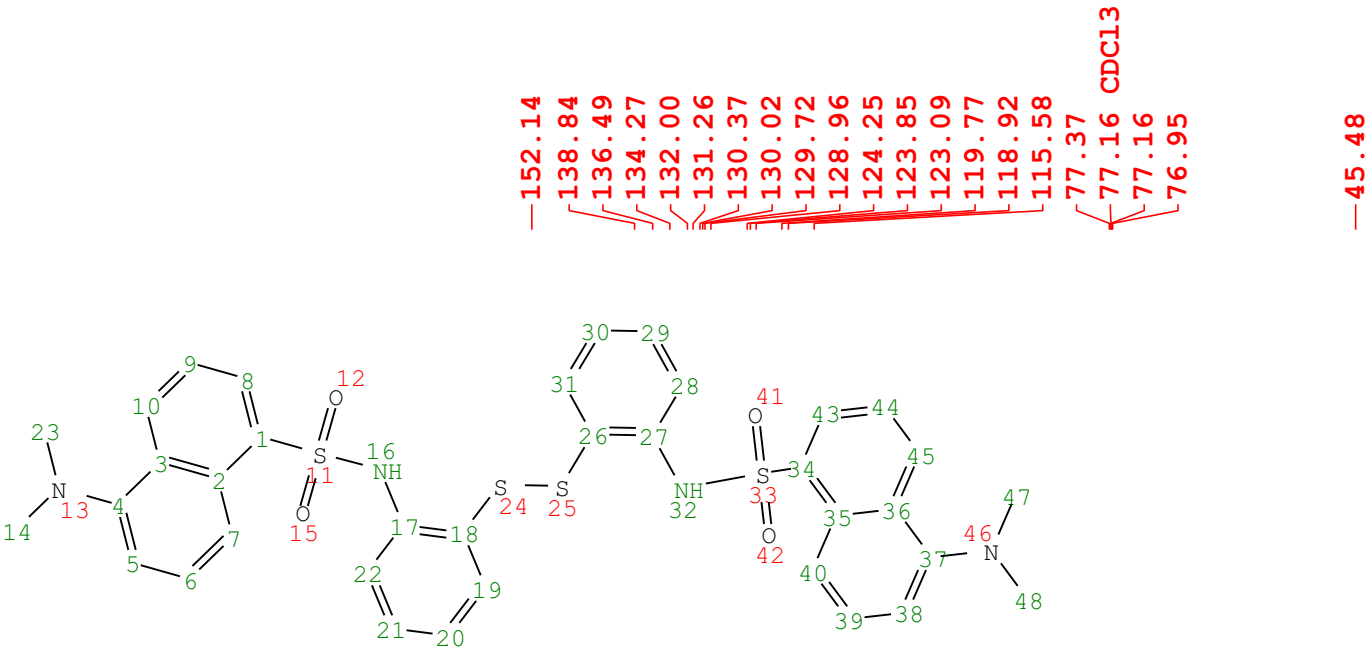


Fig SX65 L2 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-292A.12.fid |
| DATE_TIME | 2024-01-31T21:33:25 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 13C |
| NS | 128 |
| SWH | 36057.692 Hz |
| AQ | 0.4588 sec |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

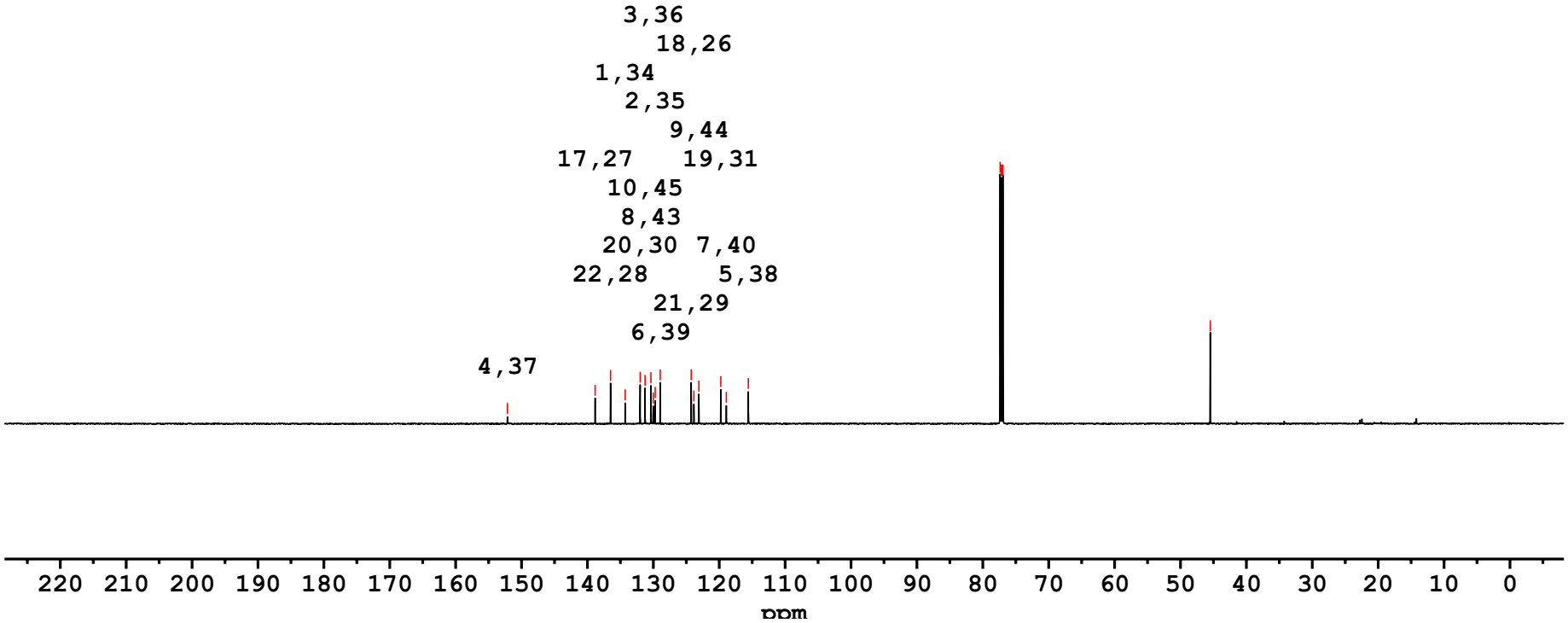
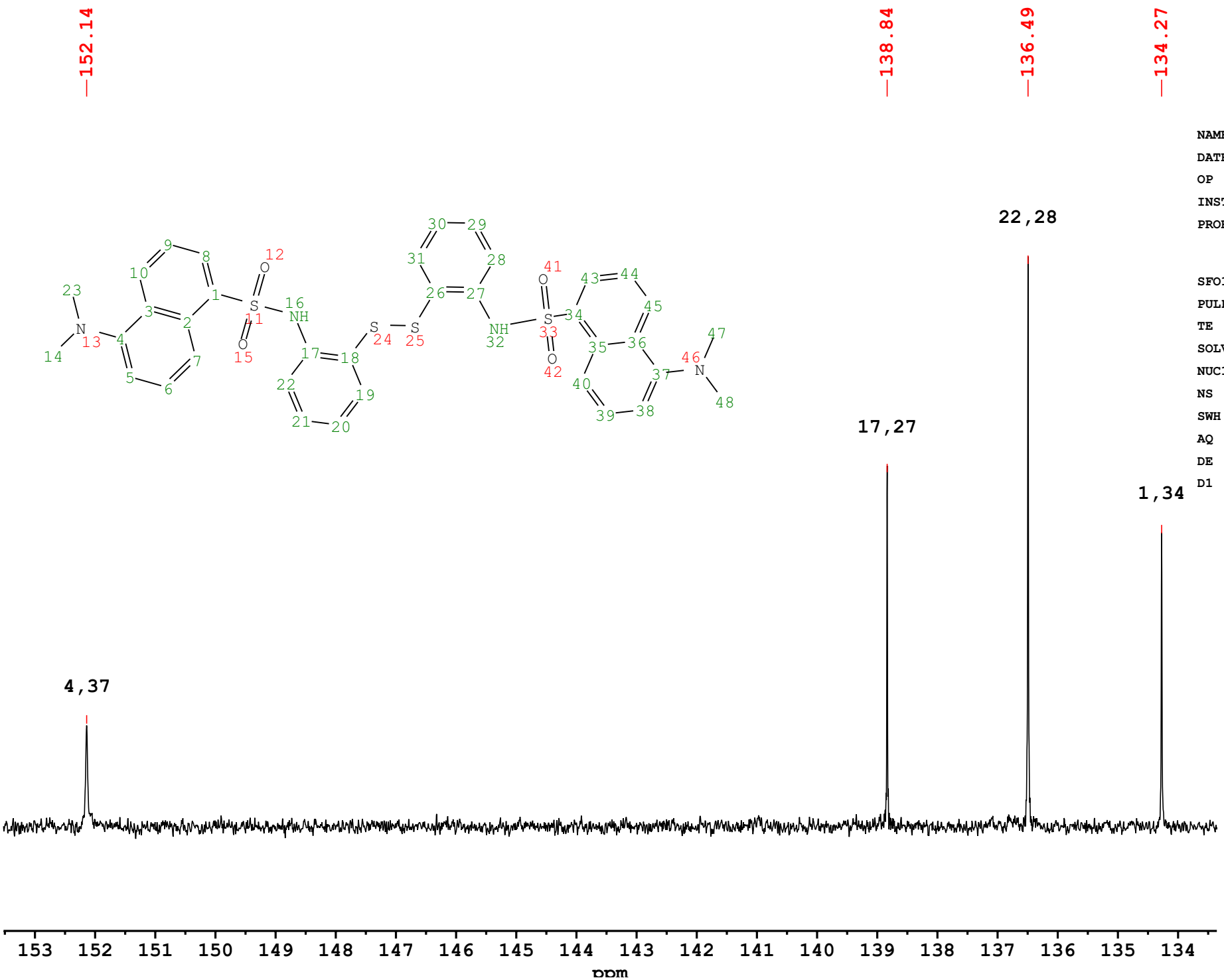
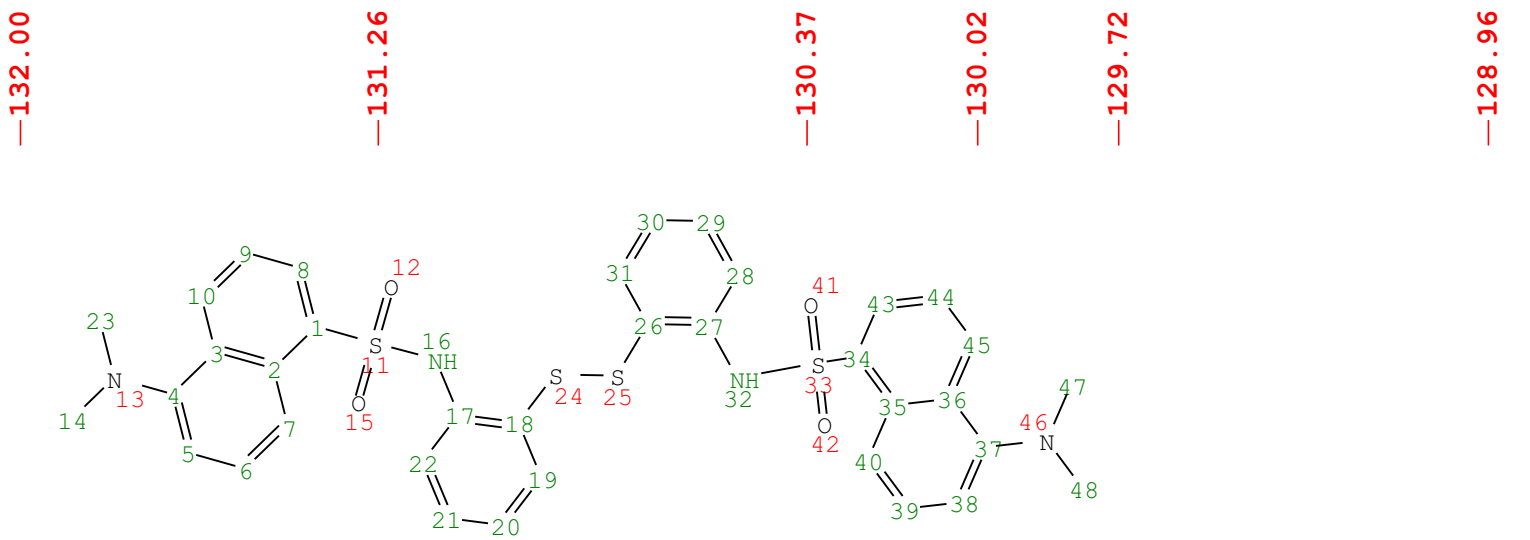


Fig SX66 L2 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-292A.12.fid |
| DATE_TIME | 2024-01-31T21:33:25 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 13C |
| NS | 128 |
| SWH | 36057.692 Hz |
| AQ | 0.4588 sec |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

**Fig SX67** **L2 chloroform-d ligand only full assignment**






| | |
|---|---|
| NAME | DR-292A.12.fid |
| DATE_TIME | 2024-01-31T21:33:25 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 13C |
| NS | 128 |
| SWH | 36057.692 Hz |
| AQ | 0.4588 sec |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

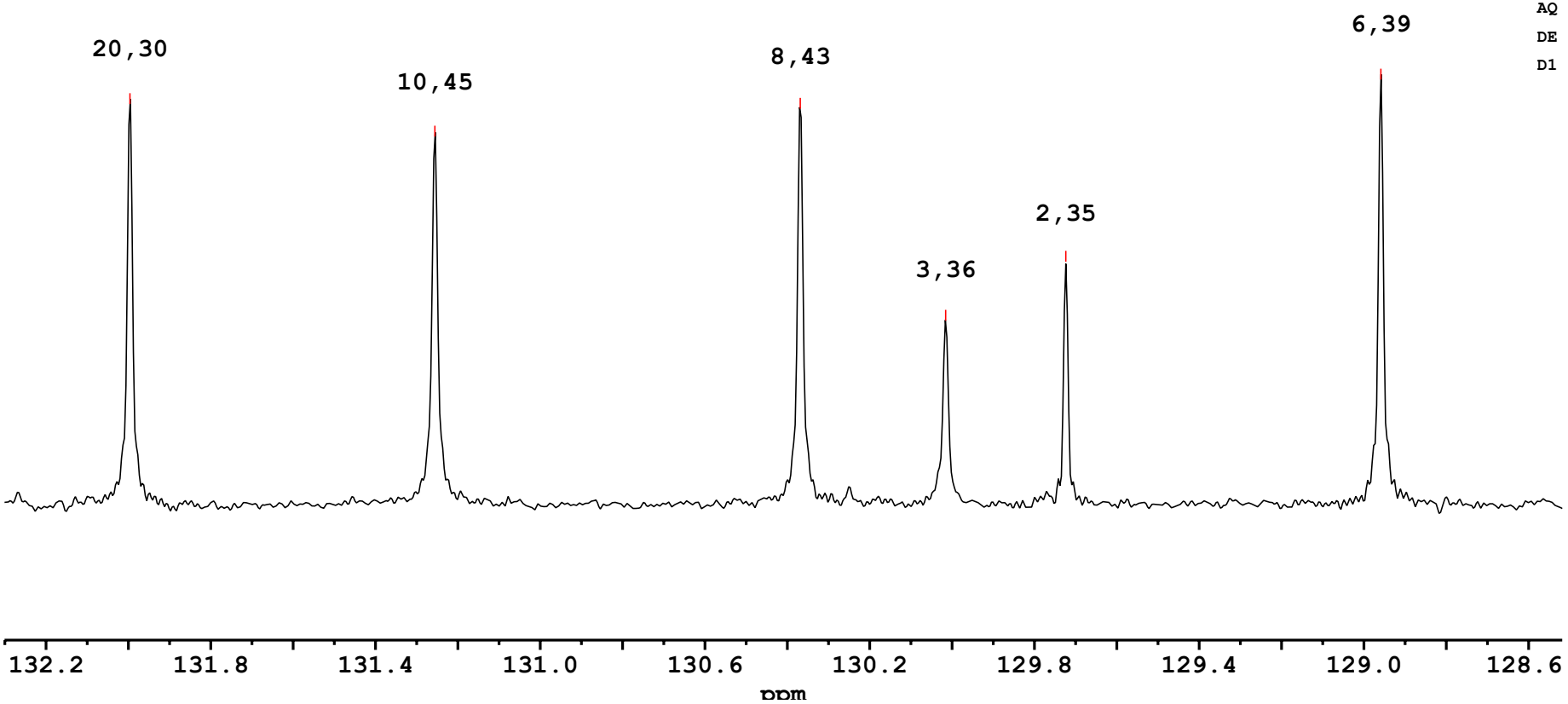
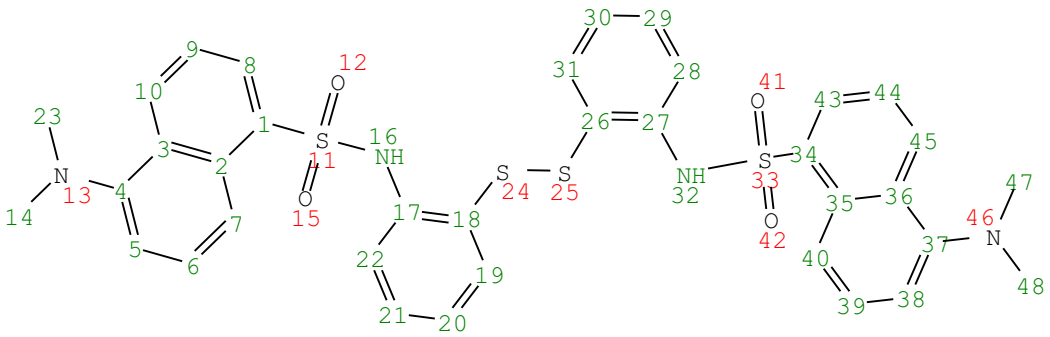
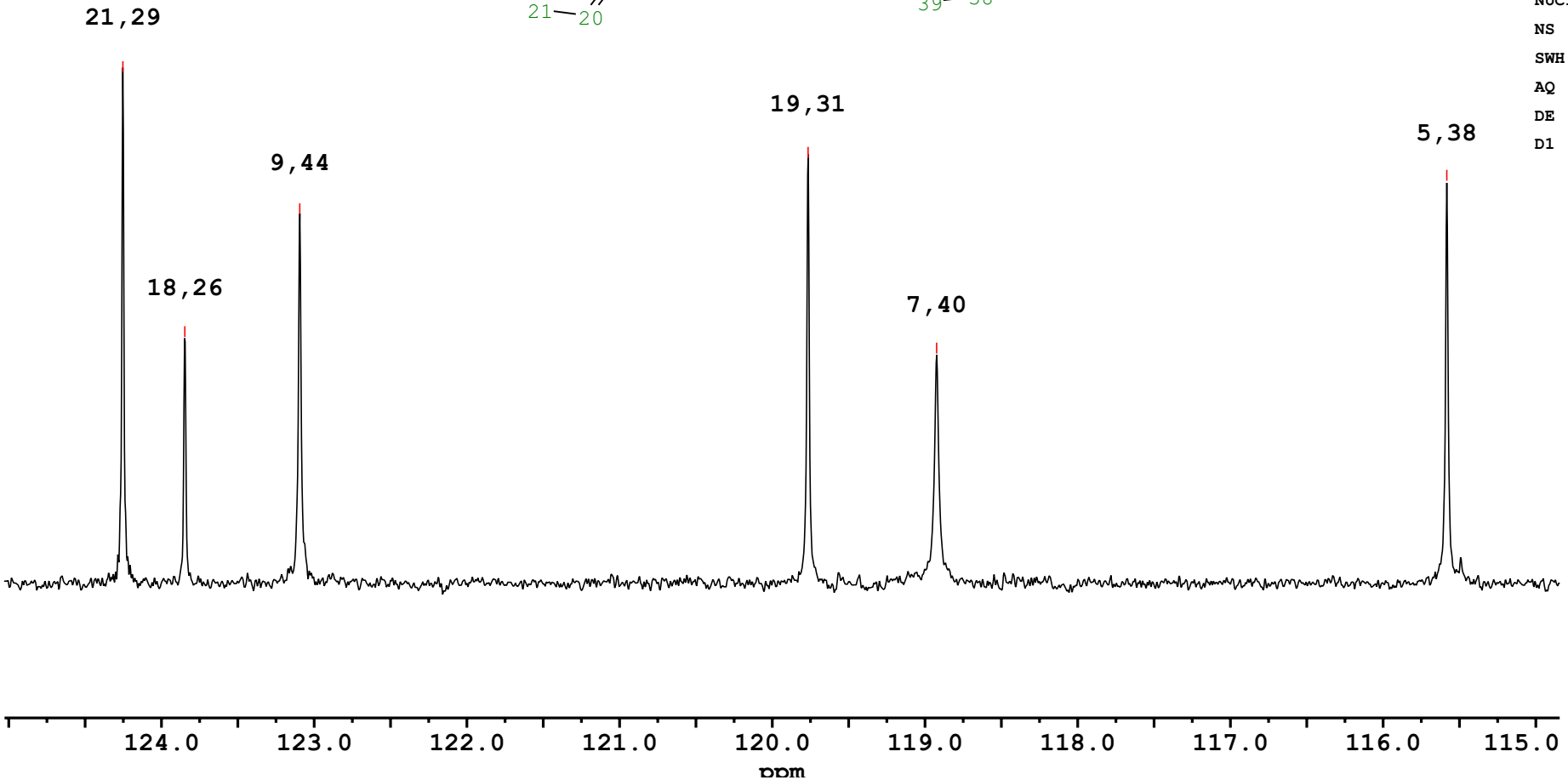


Fig SX68 L2 chloroform-d ligand only full assignment

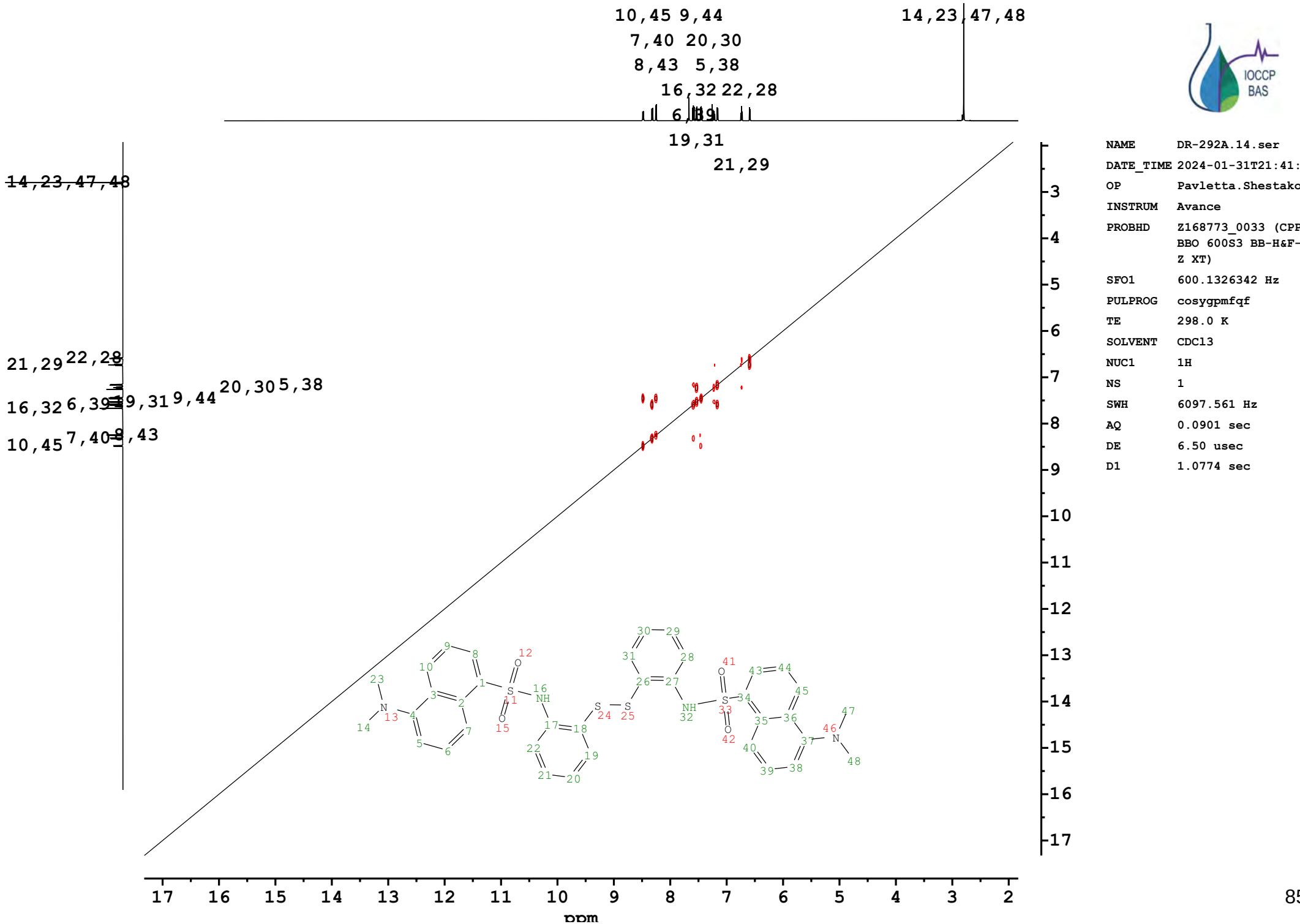





| | |
|---|---|
| NAME | DR-292A.12.fid |
| DATE_TIME | 2024-01-31T21:33:25 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 13C |
| NS | 128 |
| SWH | 36057.692 Hz |
| AQ | 0.4588 sec |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

Fig SX69

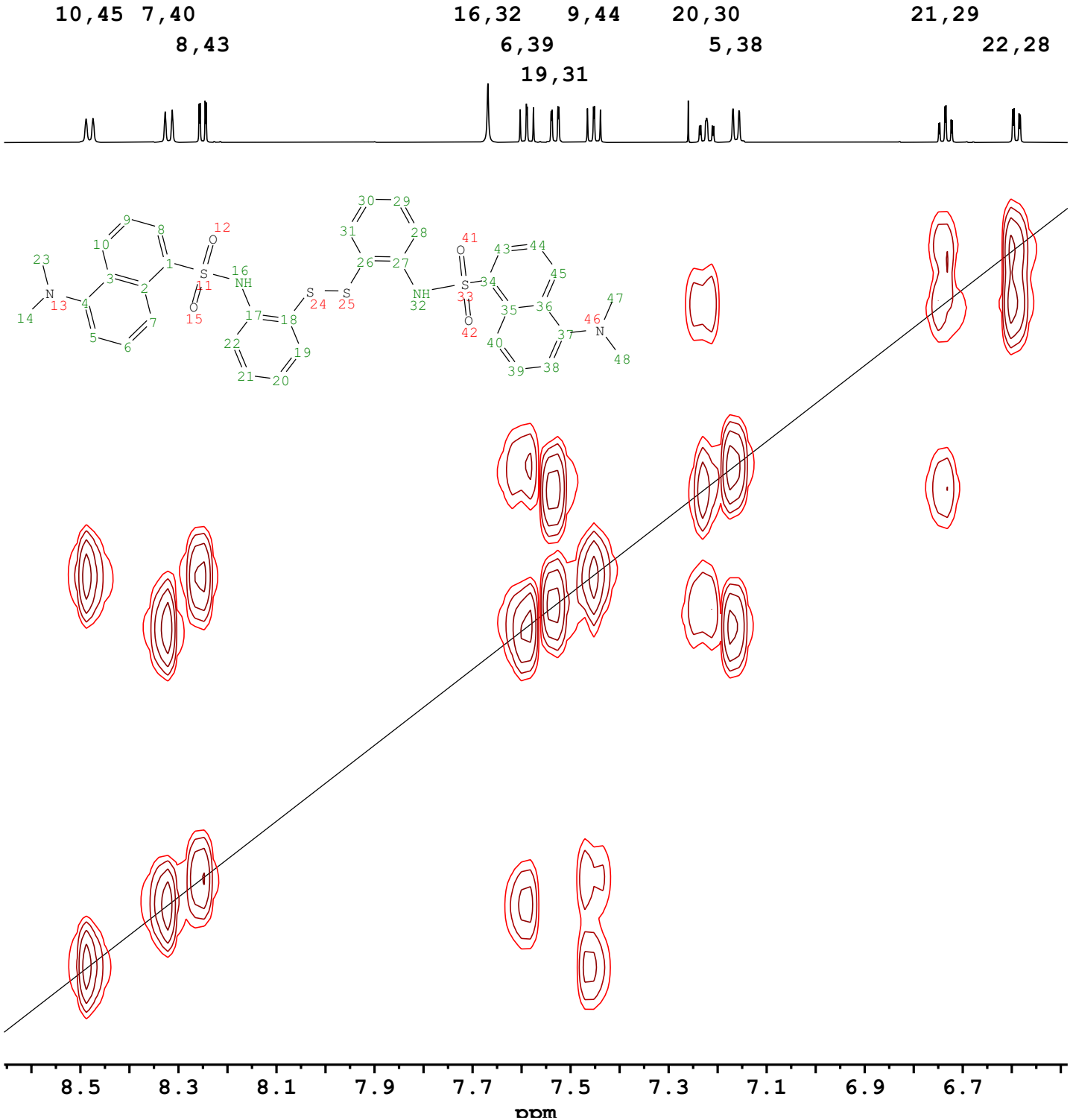
# L2 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-292A.14.ser |
| DATE_TIME | 2024-01-31T21:41:32 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 1 |
| SWH | 6097.561 Hz |
| AQ | 0.0901 sec |
| DE | 6.50 usec |
| D1 | 1.0774 sec |

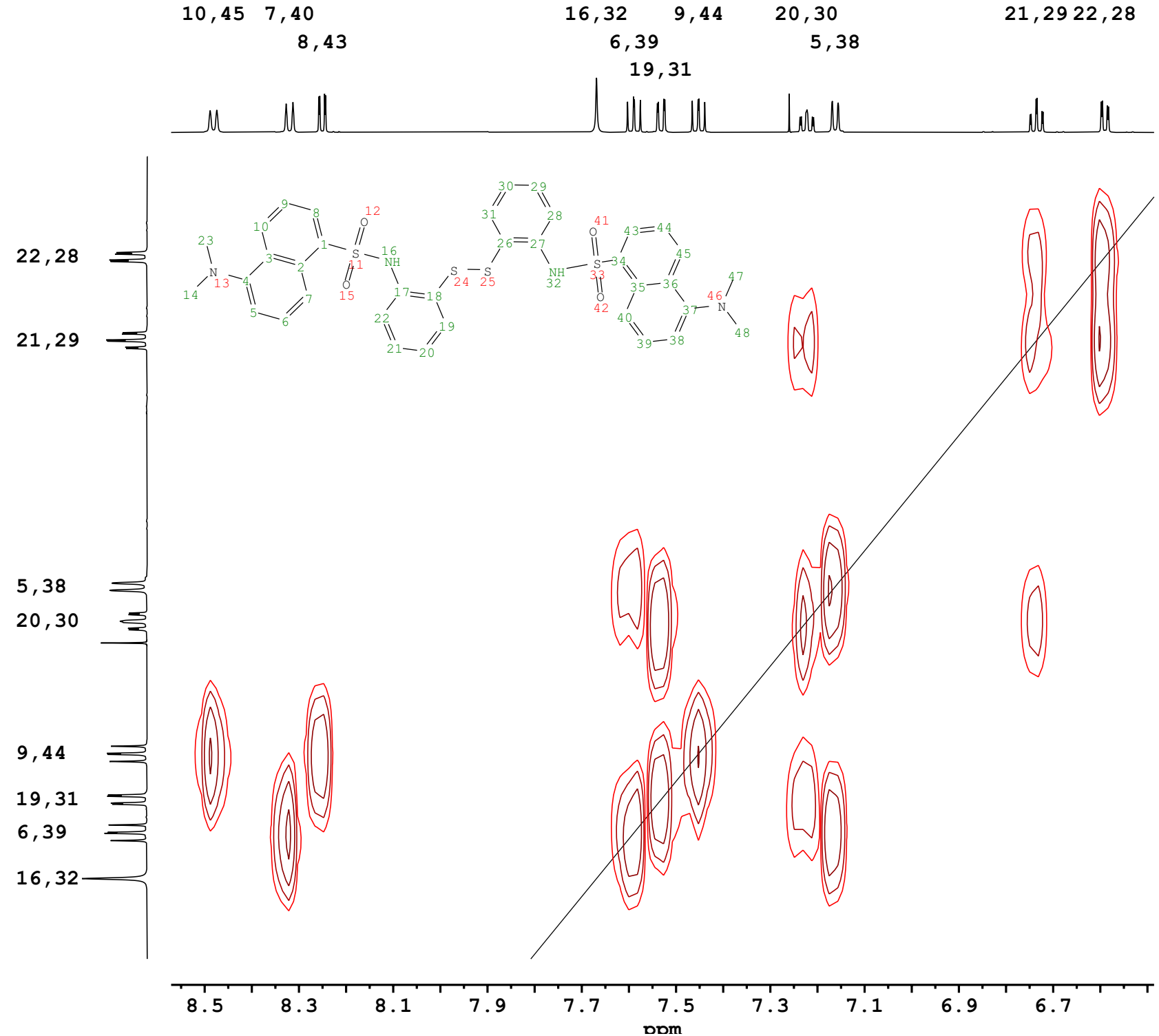
Fig SX70

# L2 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-292A.14.ser |
| DATE_TIME | 2024-01-31T21:41:32 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 1 |
| SWH | 6097.561 Hz |
| AQ | 0.0901 sec |
| DE | 6.50 usec |
| D1 | 1.0774 sec |

Fig SX71 L2 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-292A.14.ser |
| DATE_TIME | 2024-01-31T21:41:32 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 1 |
| SWH | 6097.561 Hz |
| AQ | 0.0901 sec |
| DE | 6.50 usec |
| D1 | 1.0774 sec |

Fig SX72 L2 chloroform-d ligand only full assignment

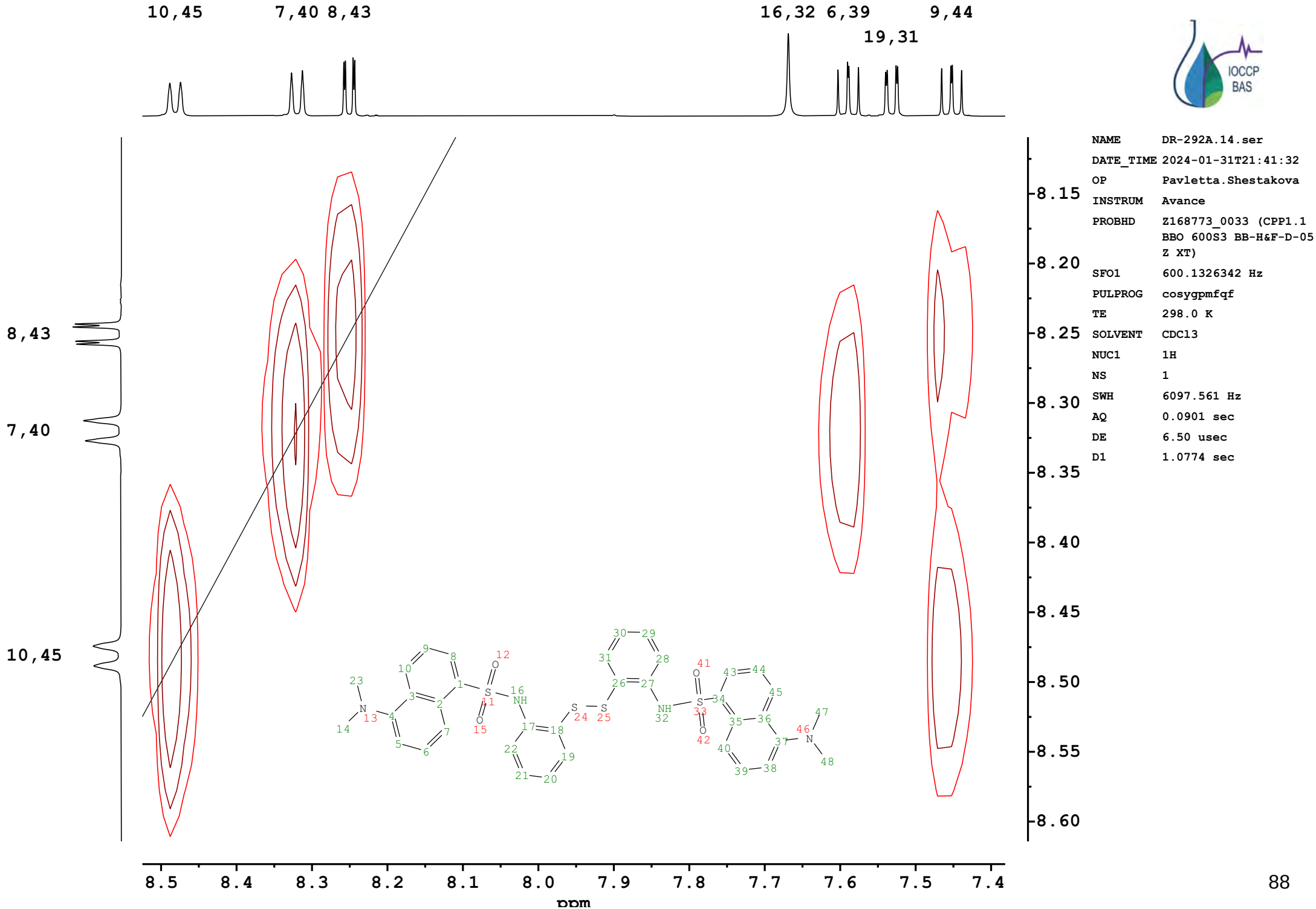


Fig SX73 L2 chloroform-d ligand only full assignment

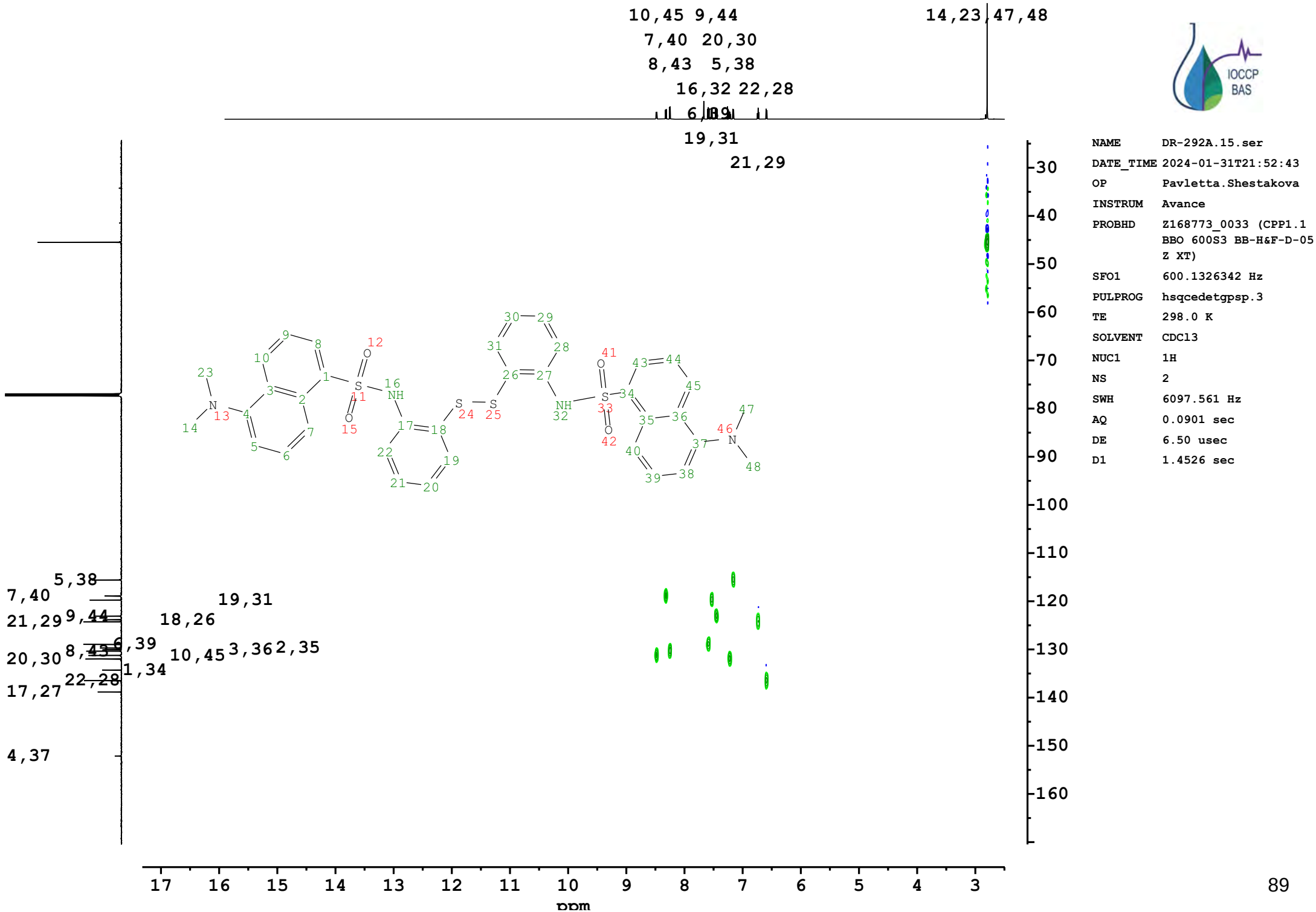
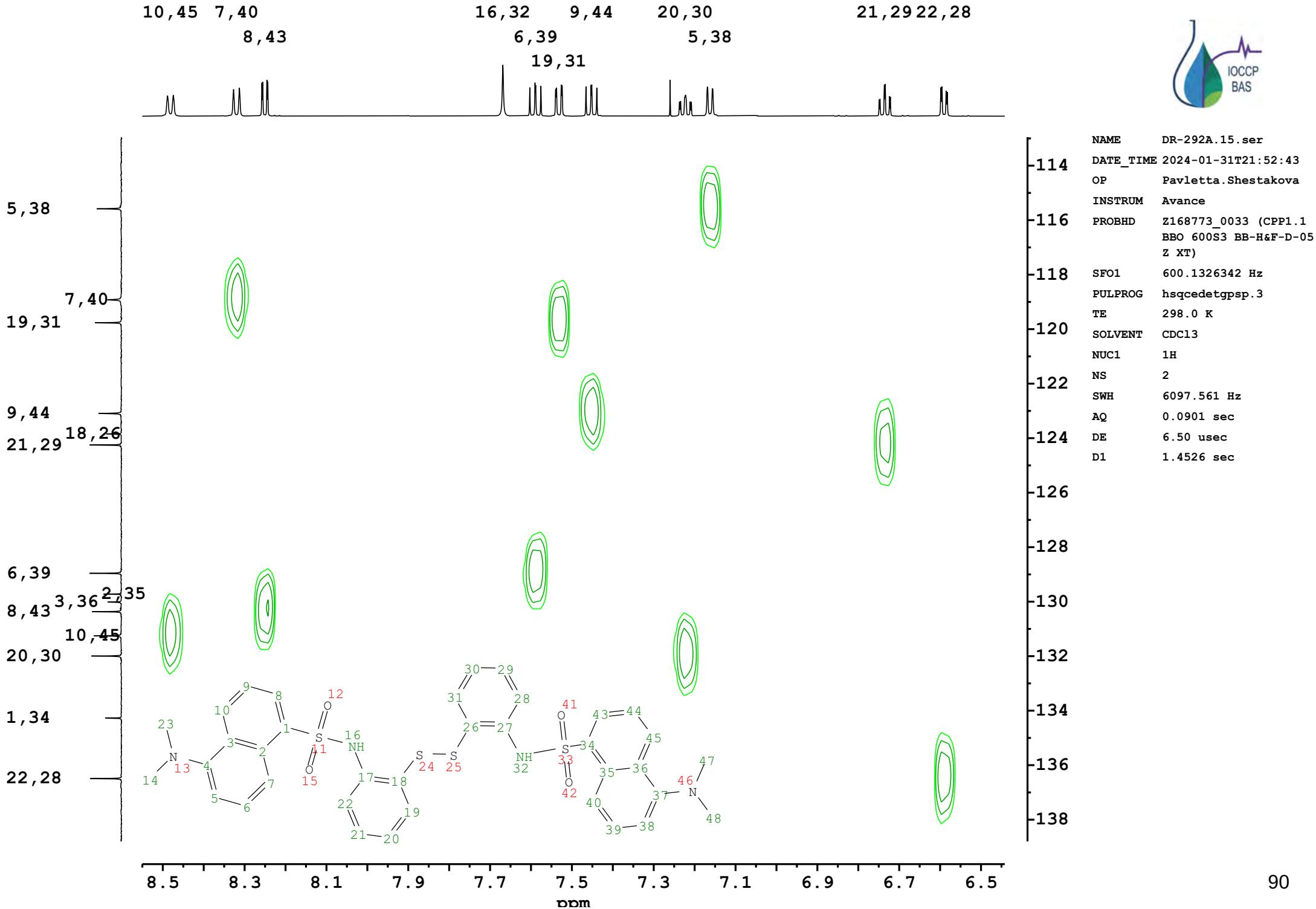


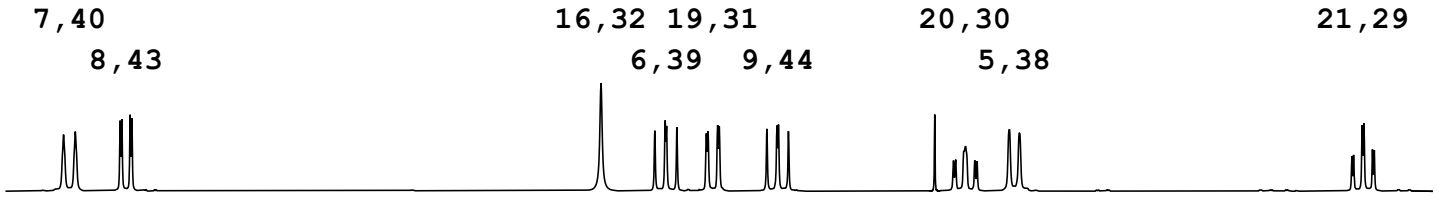
**Fig SX74** **L2 chloroform-d ligand only full assignment**

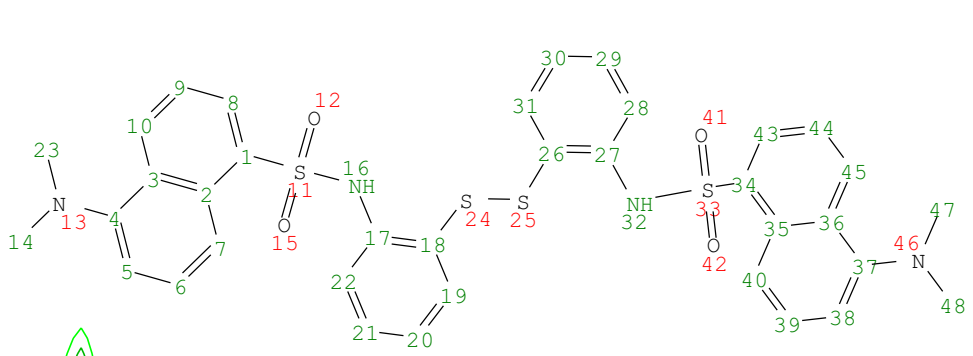



| | |
|---|---|
| NAME | DR-292A.15.ser |
| DATE_TIME | 2024-01-31T21:52:43 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 2 |
| SWH | 6097.561 Hz |
| AQ | 0.0901 sec |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX75

# L2 chloroform-d ligand only full assignment

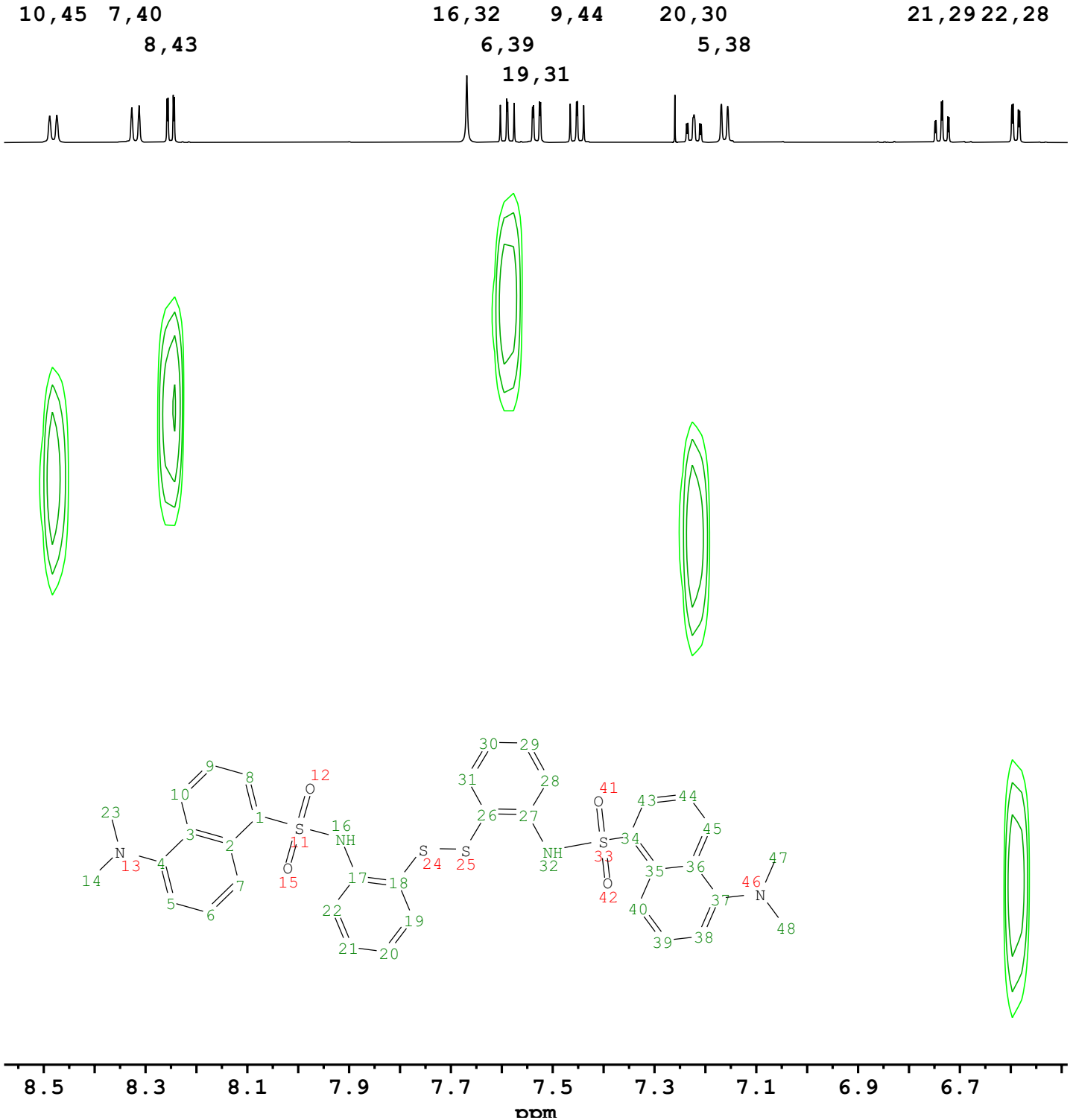


| | |
|---|---|
| NAME | DR-292A.15.ser |
| DATE_TIME | 2024-01-31T21:52:43 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 2 |
| SWH | 6097.561 Hz |
| AQ | 0.0901 sec |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX76

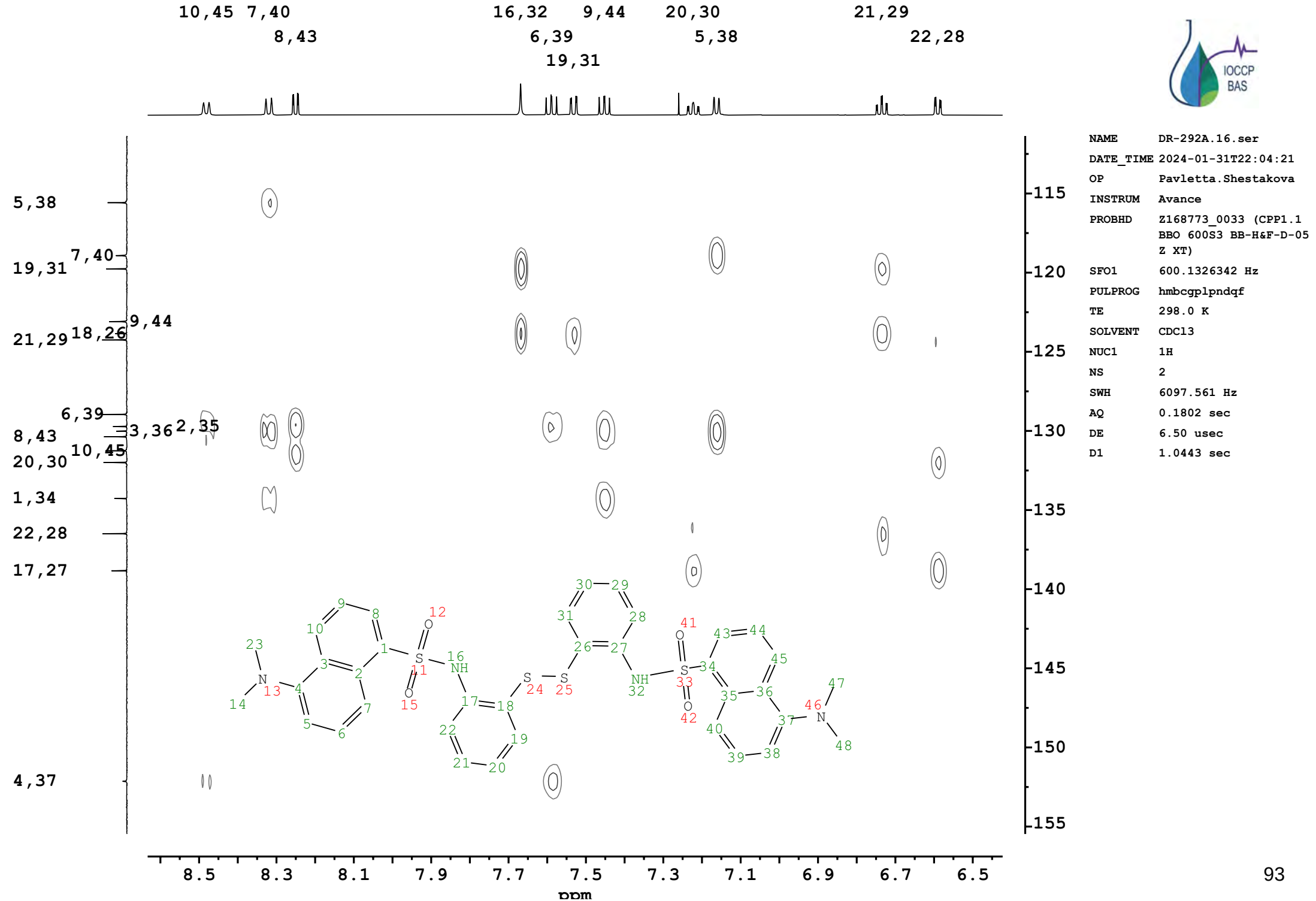
# L2 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-292A.15.ser |
| DATE_TIME | 2024-01-31T21:52:43 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 2 |
| SWH | 6097.561 Hz |
| AQ | 0.0901 sec |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

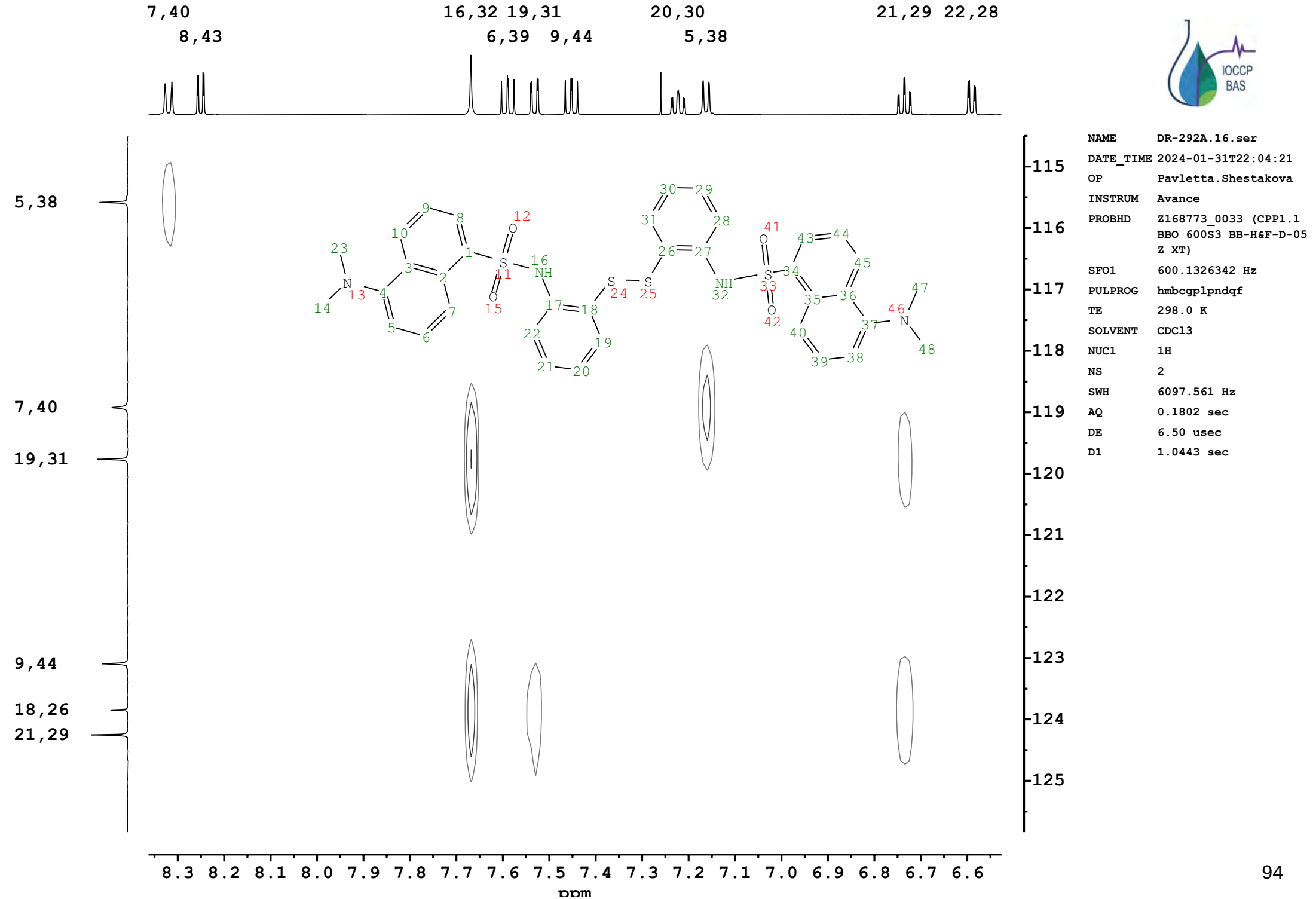
Fig SX77

# L2 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-292A.16.ser |
| DATE_TIME | 2024-01-31T22:04:21 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 2 |
| SWH | 6097.561 Hz |
| AQ | 0.1802 sec |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

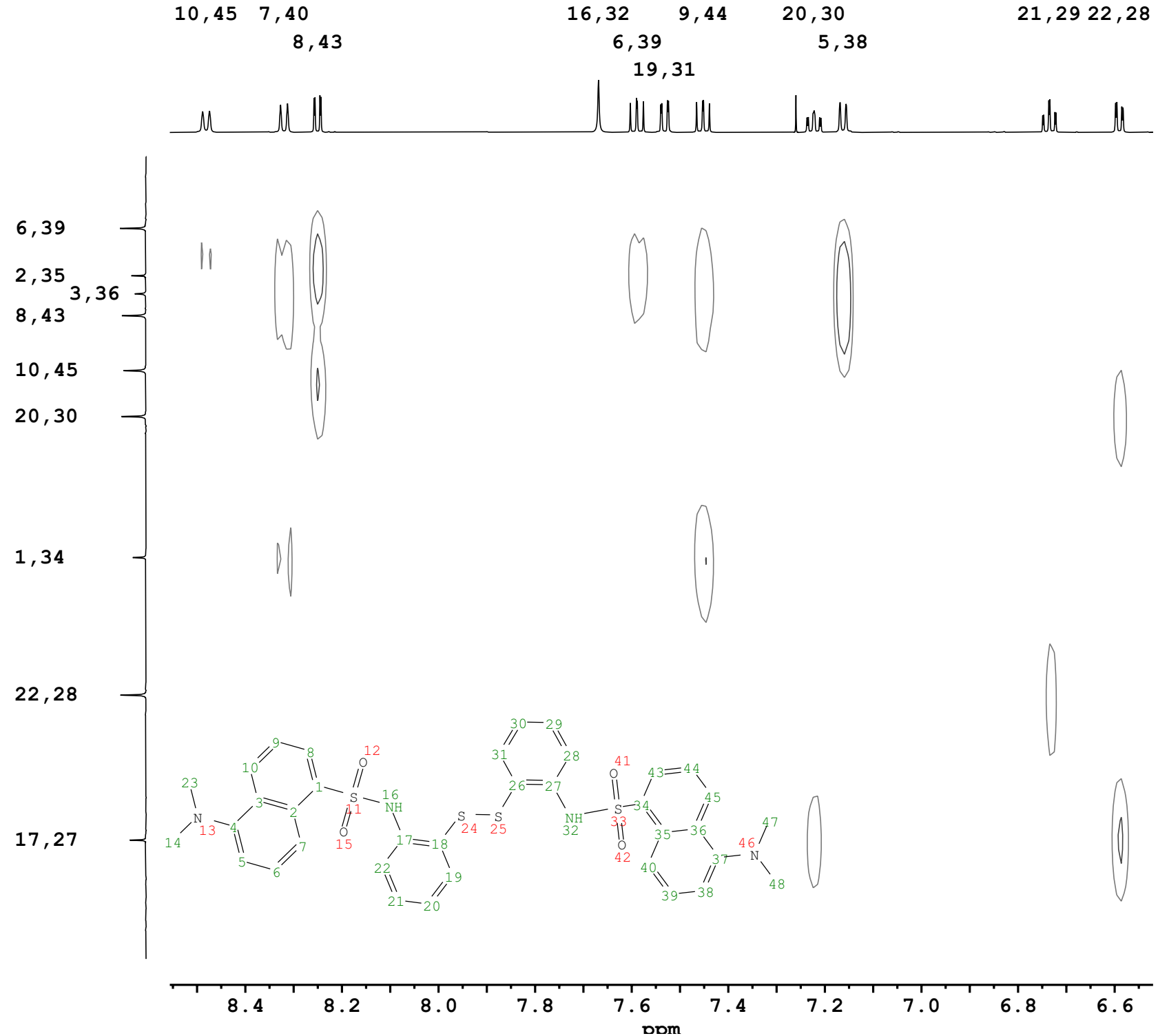
Fig SX78 L2 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-292A.16.ser |
| DATE_TIME | 2024-01-31T22:04:21 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 2 |
| SWH | 6097.561 Hz |
| AQ | 0.1802 sec |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

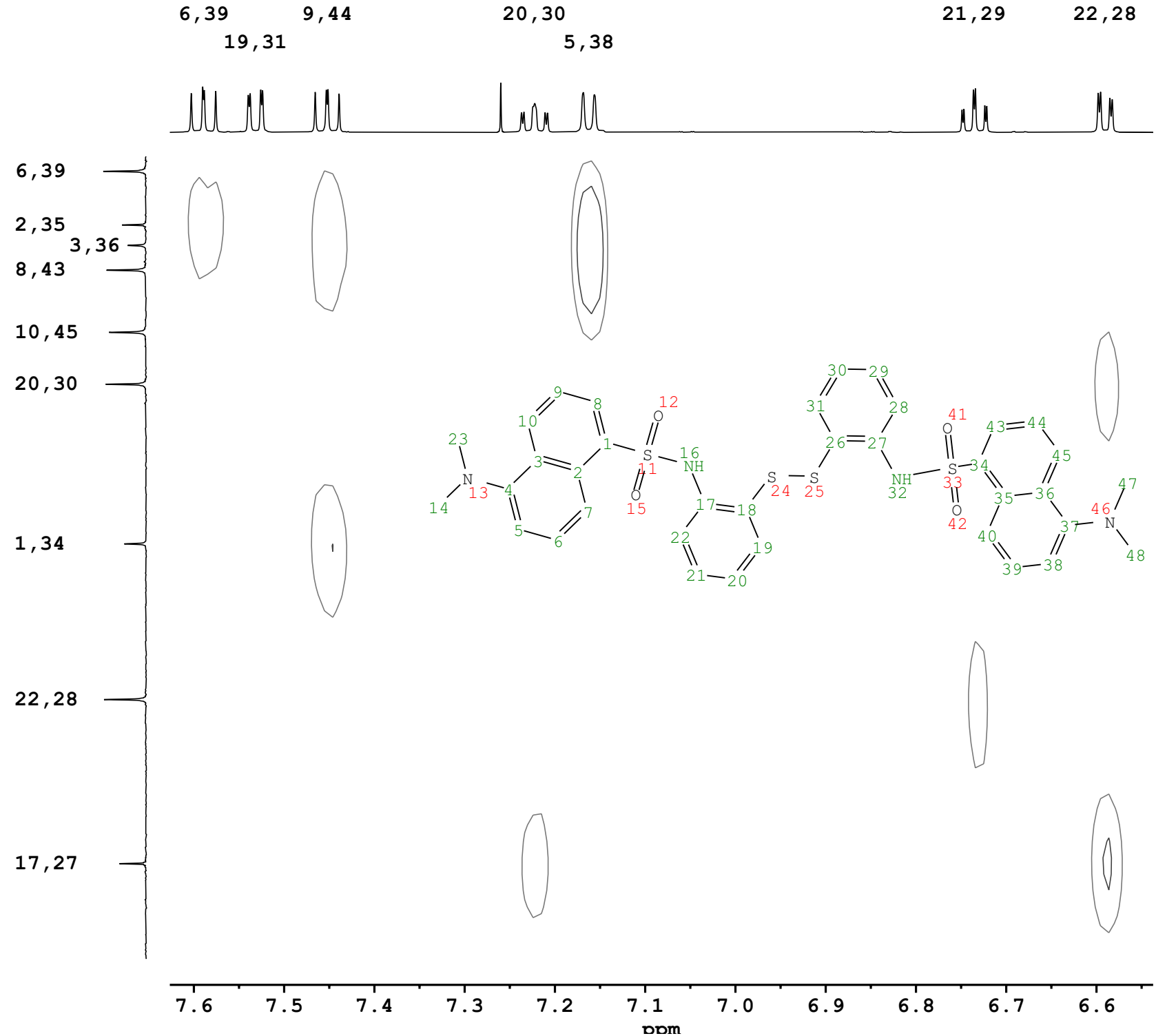
Fig SX79

# L2 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-292A.16.ser |
| DATE_TIME | 2024-01-31T22:04:21 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 2 |
| SWH | 6097.561 Hz |
| AQ | 0.1802 sec |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX80 L2 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-292A.16.ser |
| DATE_TIME | 2024-01-31T22:04:21 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 2 |
| SWH | 6097.561 Hz |
| AQ | 0.1802 sec |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX81 L2 chloroform-d ligand only full assignment

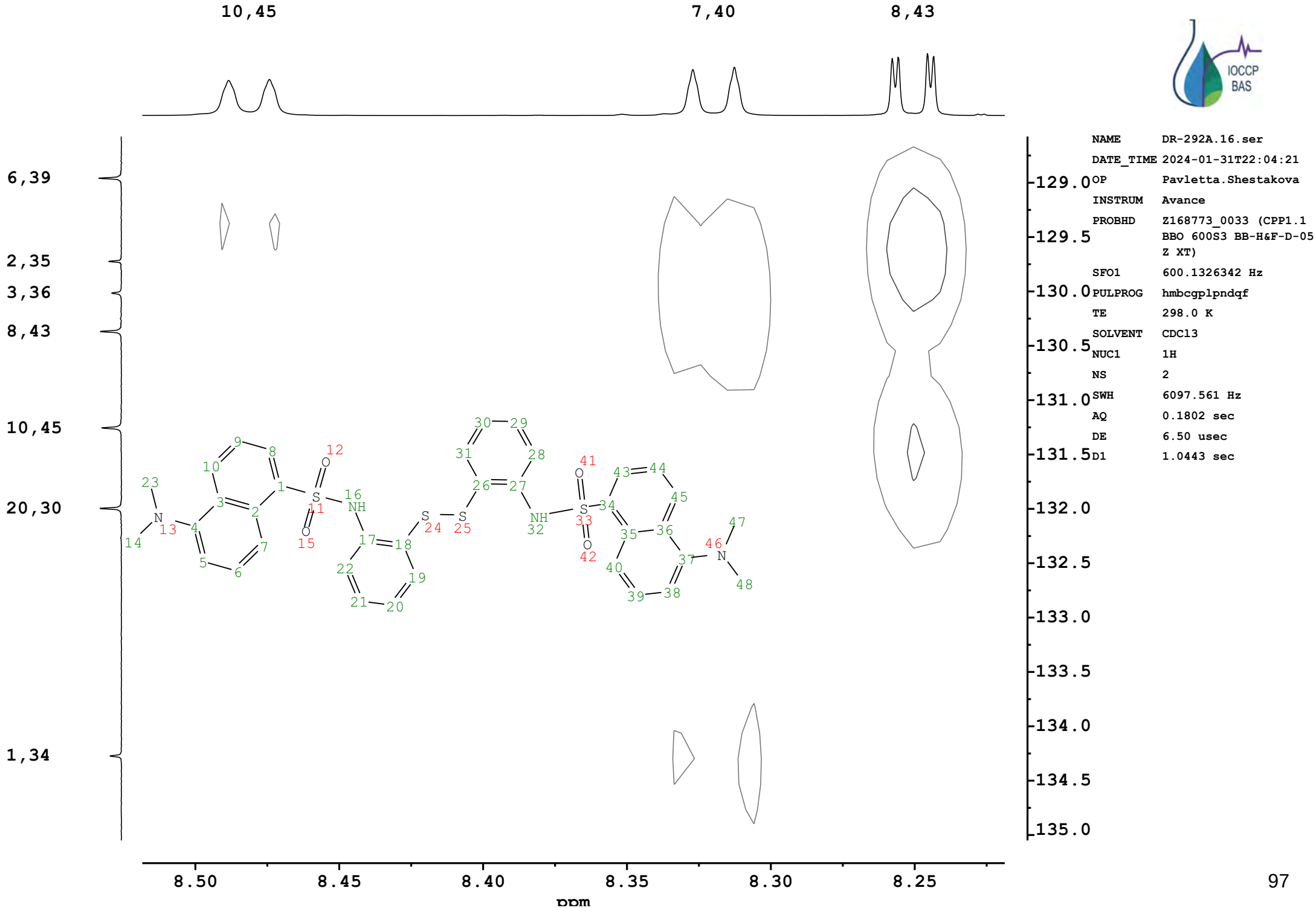
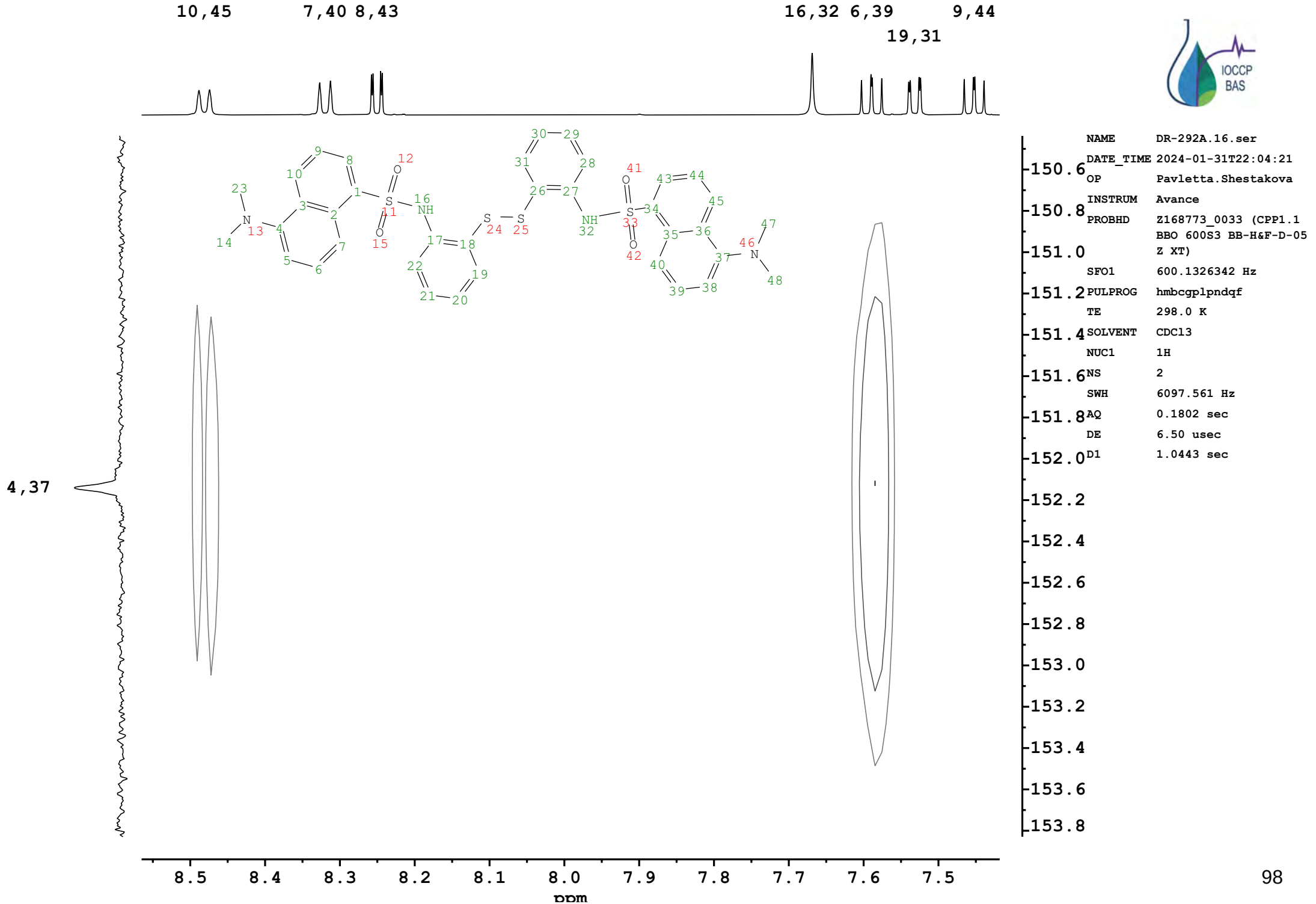


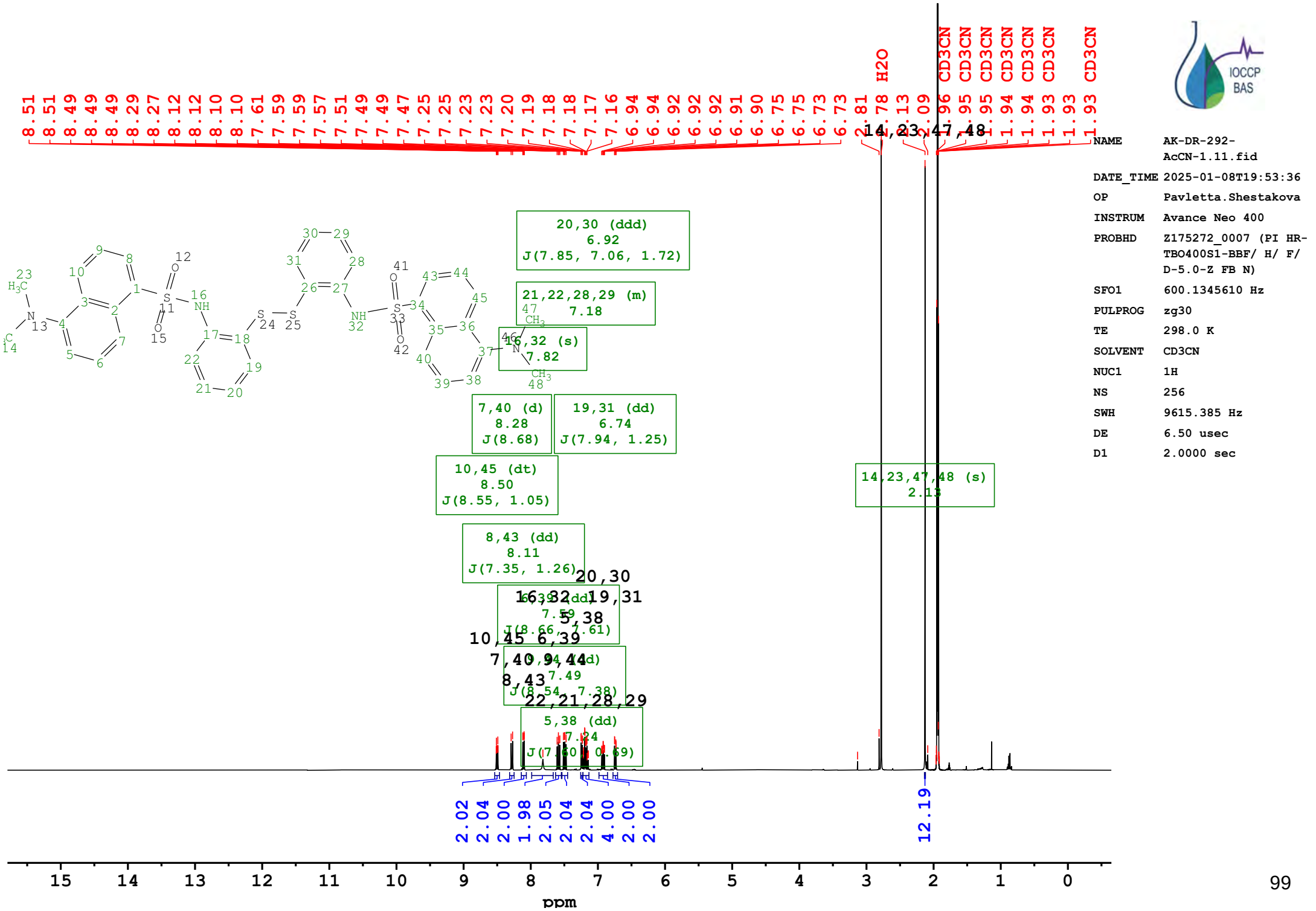
Fig SX82

# L2 chloroform-d ligand only full assignment




| | |
|---|---|
| NAME | DR-292A.16.ser |
| DATE_TIME | 2024-01-31T22:04:21 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance |
| PROBHD | Z168773_0033 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CDCl3 |
| NUC1 | 1H |
| NS | 2 |
| SWH | 6097.561 Hz |
| AQ | 0.1802 sec |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

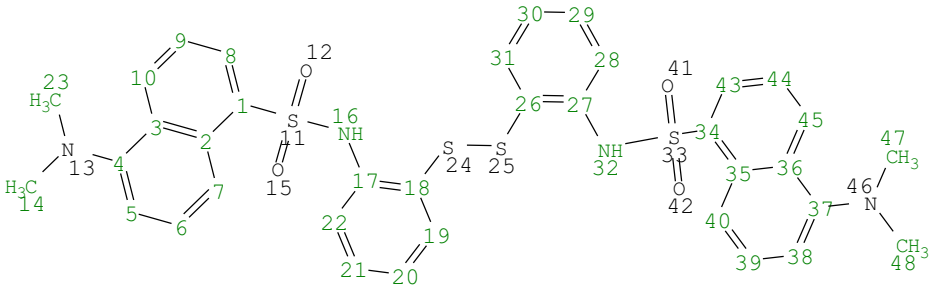
Fig SX83 L2 acetonitrile-d3 ligand only full assignment




NAME AK-DR-292-AcCN-1.11.fid
DATE_TIME 2025-01-08T19:53:36
OP Pavletta.Shestakova
INSTRUM Avance Neo 400
PROBHD Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N)
SFO1 600.1345610 Hz
PULPROG zg30
TE 298.0 K
SOLVENT CD3CN
NUC1 1H
NS 256
SWH 9615.385 Hz
DE 6.50 usec
D1 2.0000 sec

**Fig SX84** **L2 acetonitrile-d3 ligand only full assignment**

8.51 8.51 8.51 8.49 8.49 8.49 8.29 8.27 8.12 8.12 8.10 8.10 7.82 7.61 7.59 7.59 7.57 7.51 7.49 7.49 7.47 7.25 7.25 7.23 7.23 7.22 7.21 7.20 7.19 7.18 7.18 7.17 7.16 7.16 7.15 7.14 6.94 6.94 6.93 6.92 6.92 6.92 6.91 6.90 6.75 6.75 6.73 6.73



| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.11.fid |
| DATE_TIME | 2025-01-08T19:53:36 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

10,45 (dt) 8.50 J(8.55, 1.05)

7,40 (d) 8.28 J(8.68)

8,43 (dd) 8.11 J(7.35, 1.26)

16,32 (s) 7.82

6,39 (dd) 7.59 J(8.66, 7.61)

9,44 (dd) 7.49 J(8.54, 7.38)

5,38 (dd) 7.24 J(7.60, 0.69)

21,22,28,29 (m) 7.18

20,30 (ddd) 6.92 J(7.85, 7.06, 1.72)

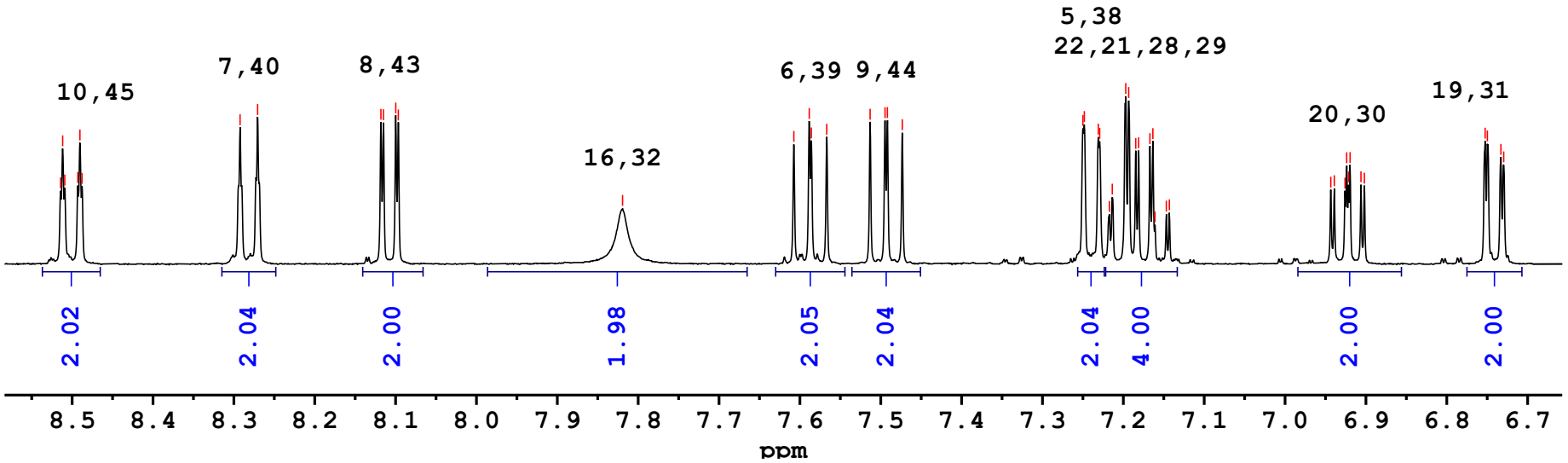
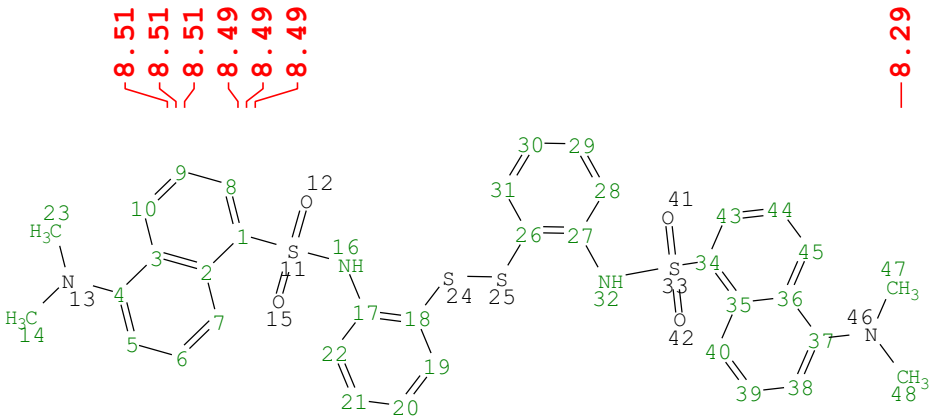


**Fig SX85** **L2 acetonitrile-d3 ligand only full assignment**




| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.11.fid |
| DATE_TIME | 2025-01-08T19:53:36 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

10,45 (dt)
8.50
J(8.55, 1.05)

7,40 (d)
8.28
J(8.68)

8,43 (dd)
8.11
J(7.35, 1.26)

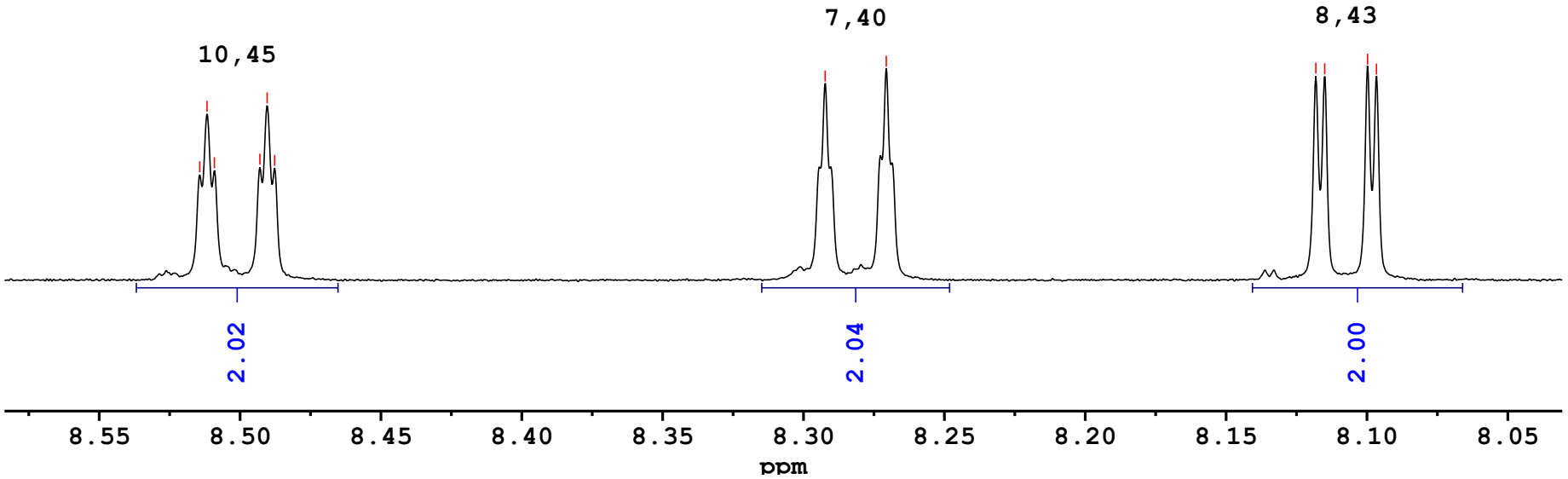
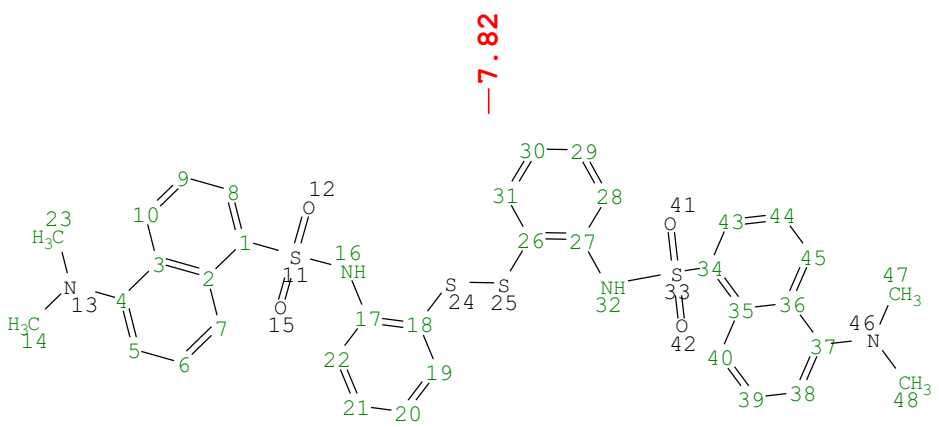


**Fig SX86** **L2 acetonitrile-d3 ligand only full assignment**




| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.11.fid |
| DATE_TIME | 2025-01-08T19:53:36 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

16,32 (s)
7.82

6,39 (dd)
7.59
J(8.66, 7.61)

9,44 (dd)
7.49
J(8.54, 7.38)

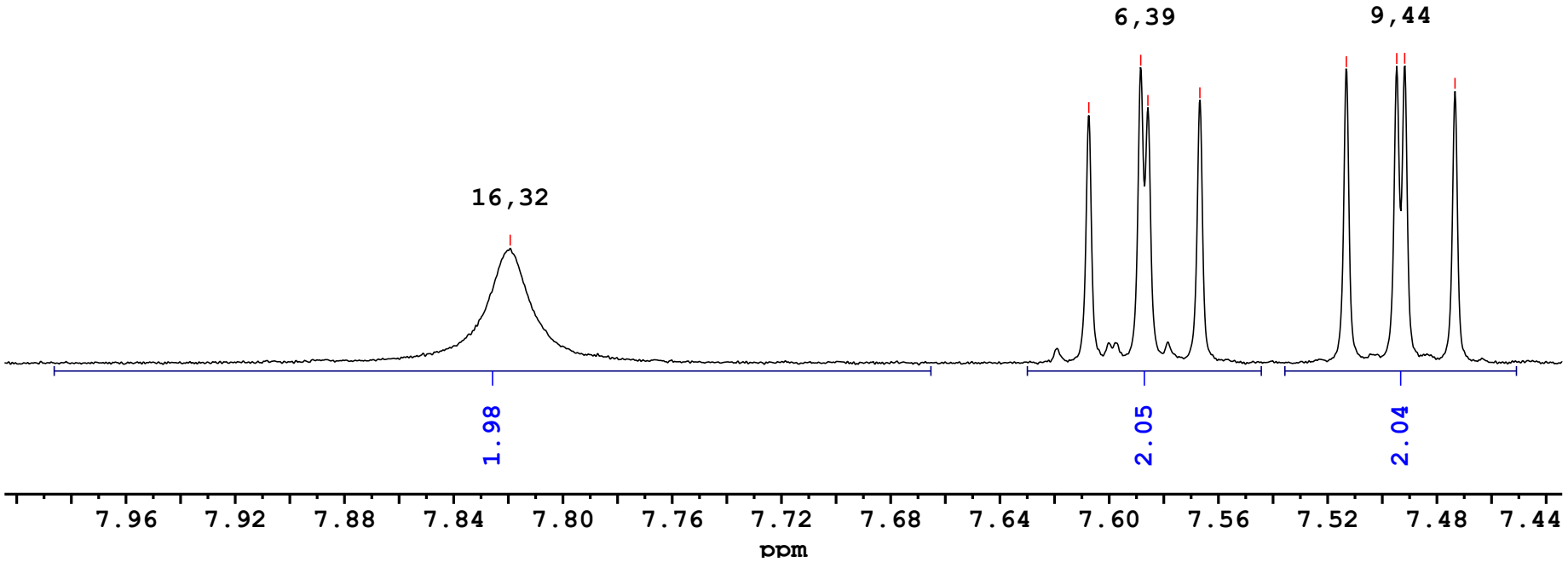
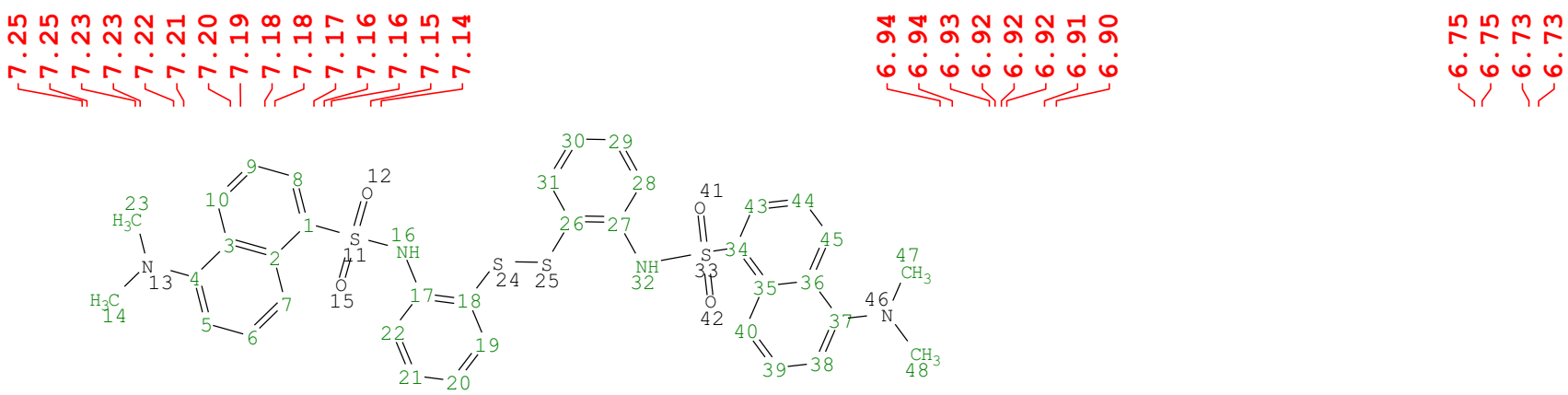


**Fig SX87** **L2 acetonitrile-d3 ligand only full assignment**




IOCCP BAS

| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.11.fid |
| DATE_TIME | 2025-01-08T19:53:36 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

5,38 (dd)
7.24
J(7.60, 0.69)

21,22,28,29 (m)
7.18

20,30 (ddd)
6.92
J(7.85, 7.06, 1.72)

19,31 (dd)
6.74
J(7.94, 1.25)

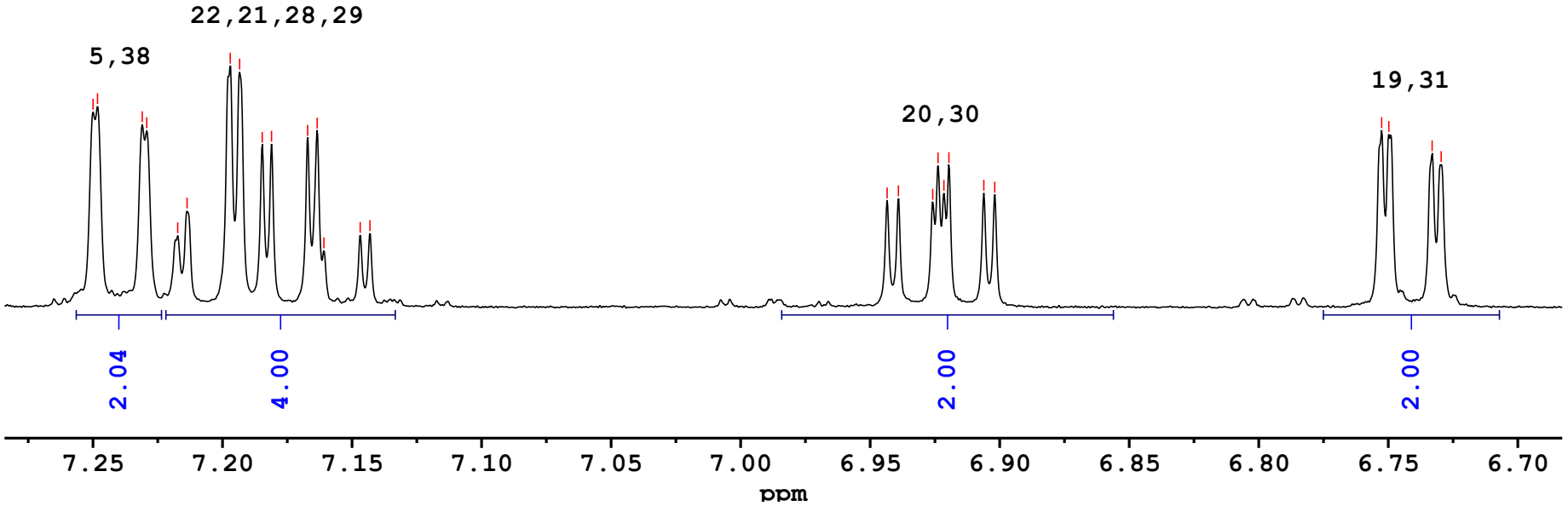
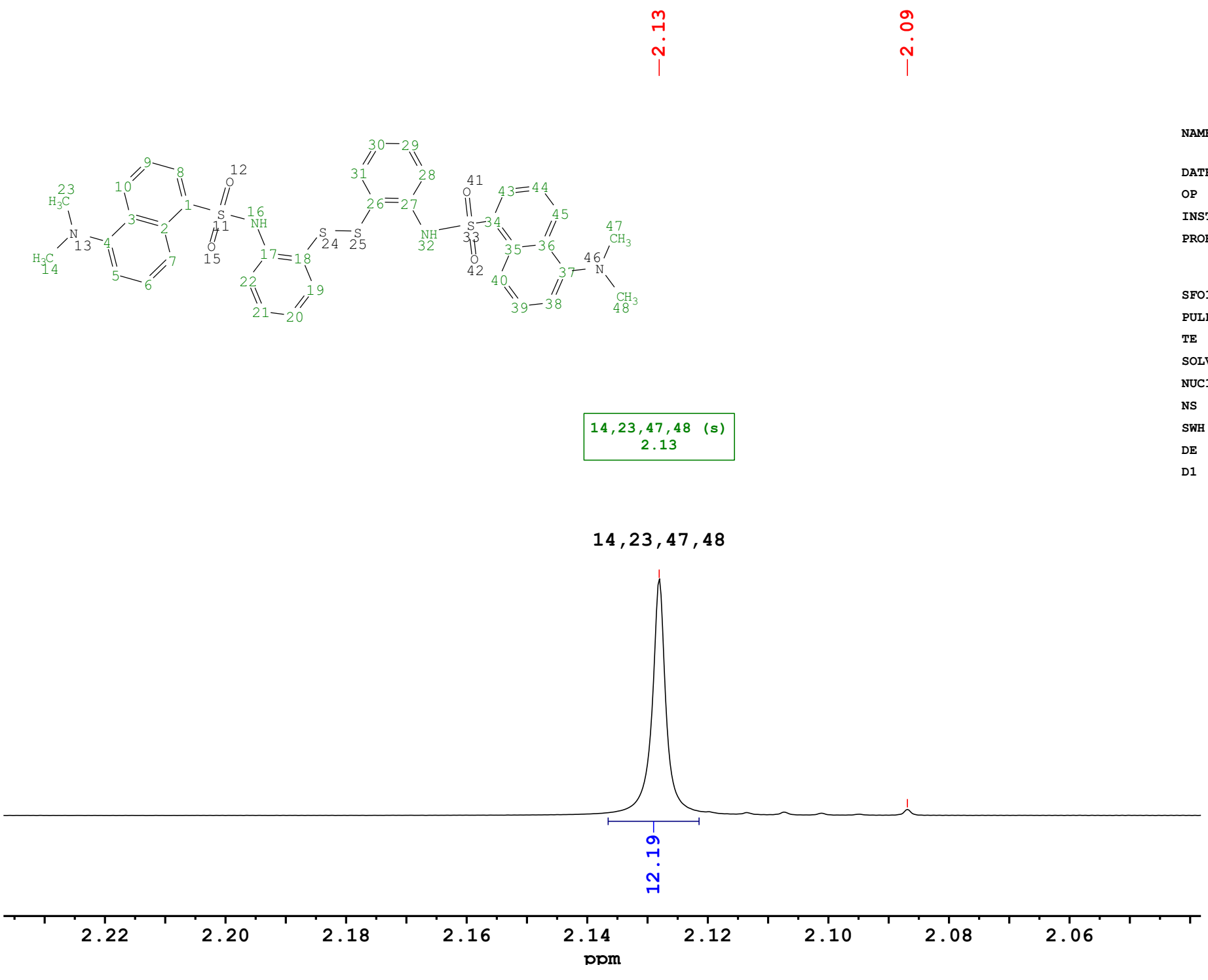


**Fig SX88** **L2 acetonitrile-d3 ligand only full assignment**

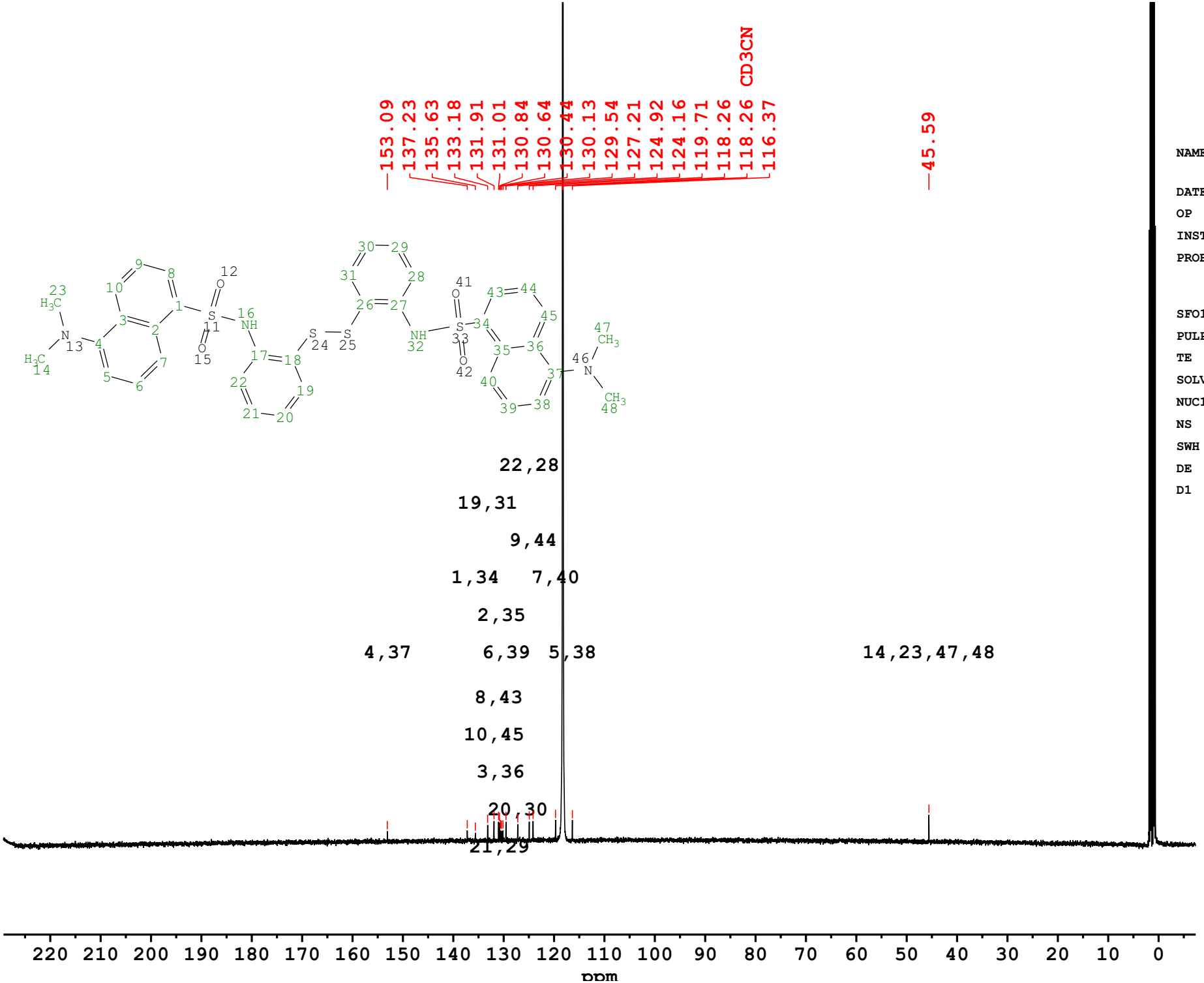





| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.11.fid |
| DATE_TIME | 2025-01-08T19:53:36 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

Fig SX89

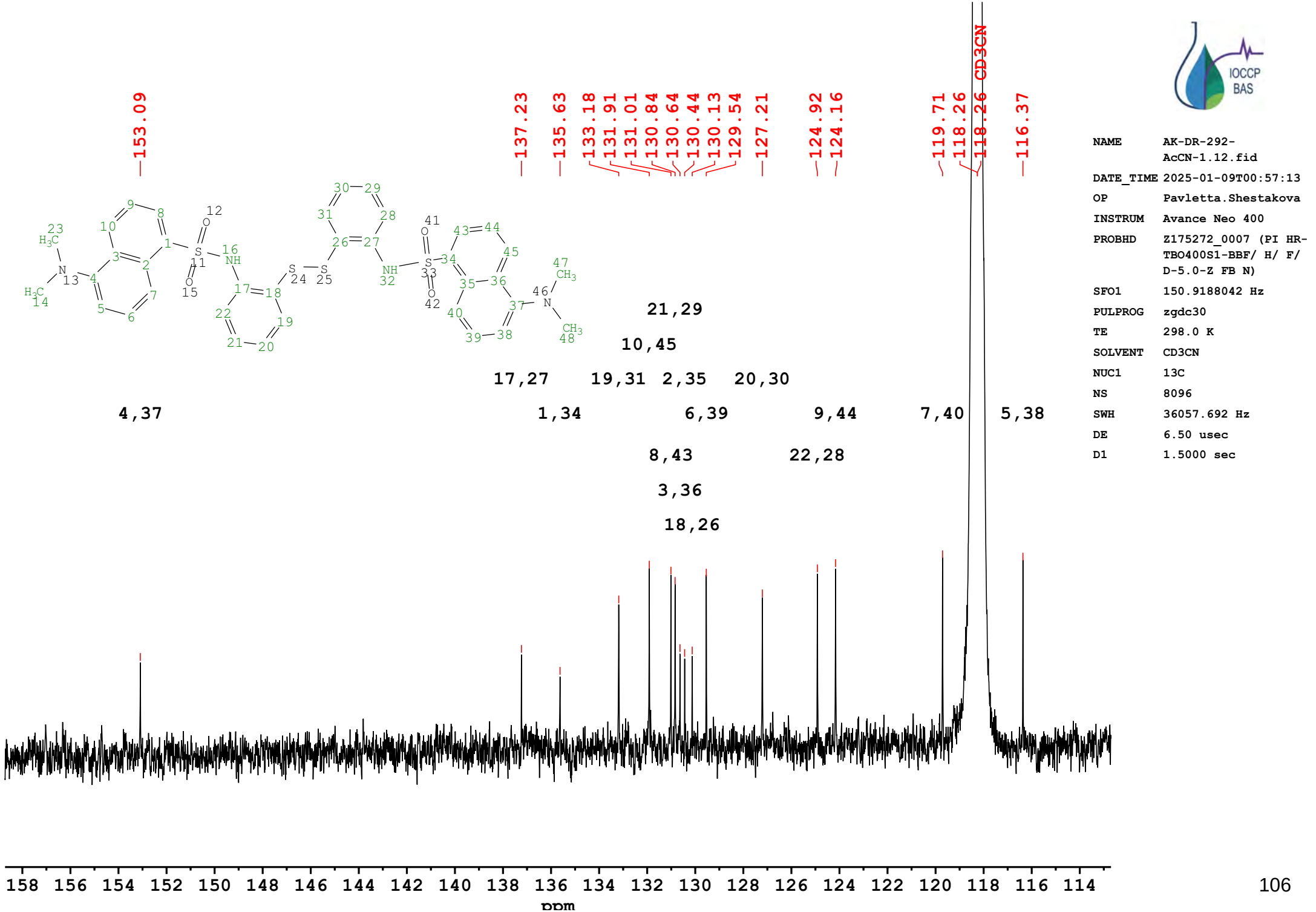
# L2 acetonitrile-d3 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.12.fid |
| DATE_TIME | 2025-01-09T00:57:13 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8096 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

Fig SX90 L2 acetonitrile-d3 ligand only full assignment

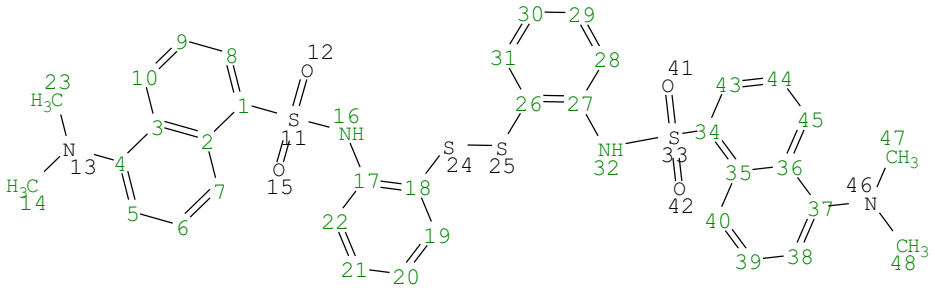





| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.12.fid |
| DATE_TIME | 2025-01-09T00:57:13 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8096 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

**Fig SX91** **L2 acetonitrile-d3 ligand only full assignment**

133.18 131.91 131.01 130.84 130.64 130.44 130.13 129.54



| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.12.fid |
| DATE_TIME | 2025-01-09T00:57:13 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8096 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

3,36

19,31 10,45 8,43 2,35 18,26 6,39

21,29

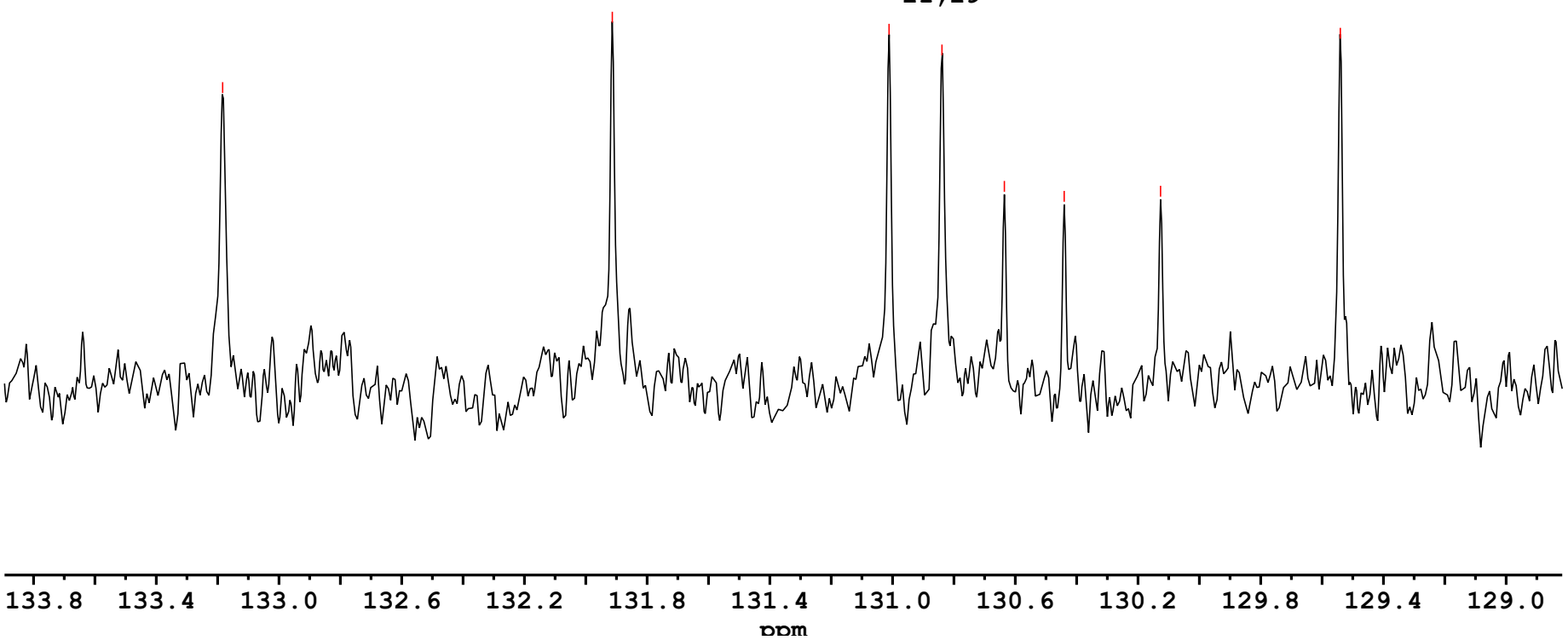
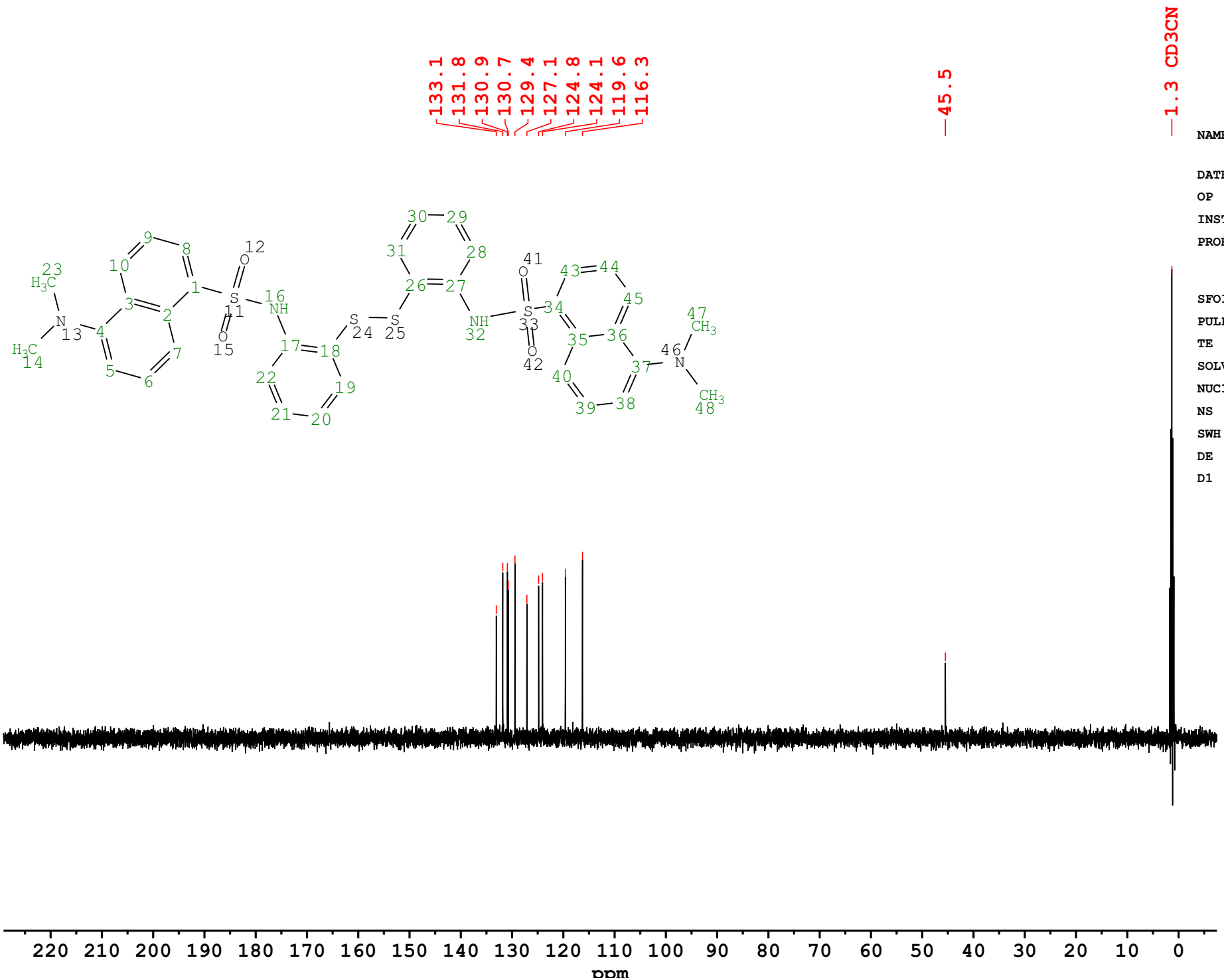


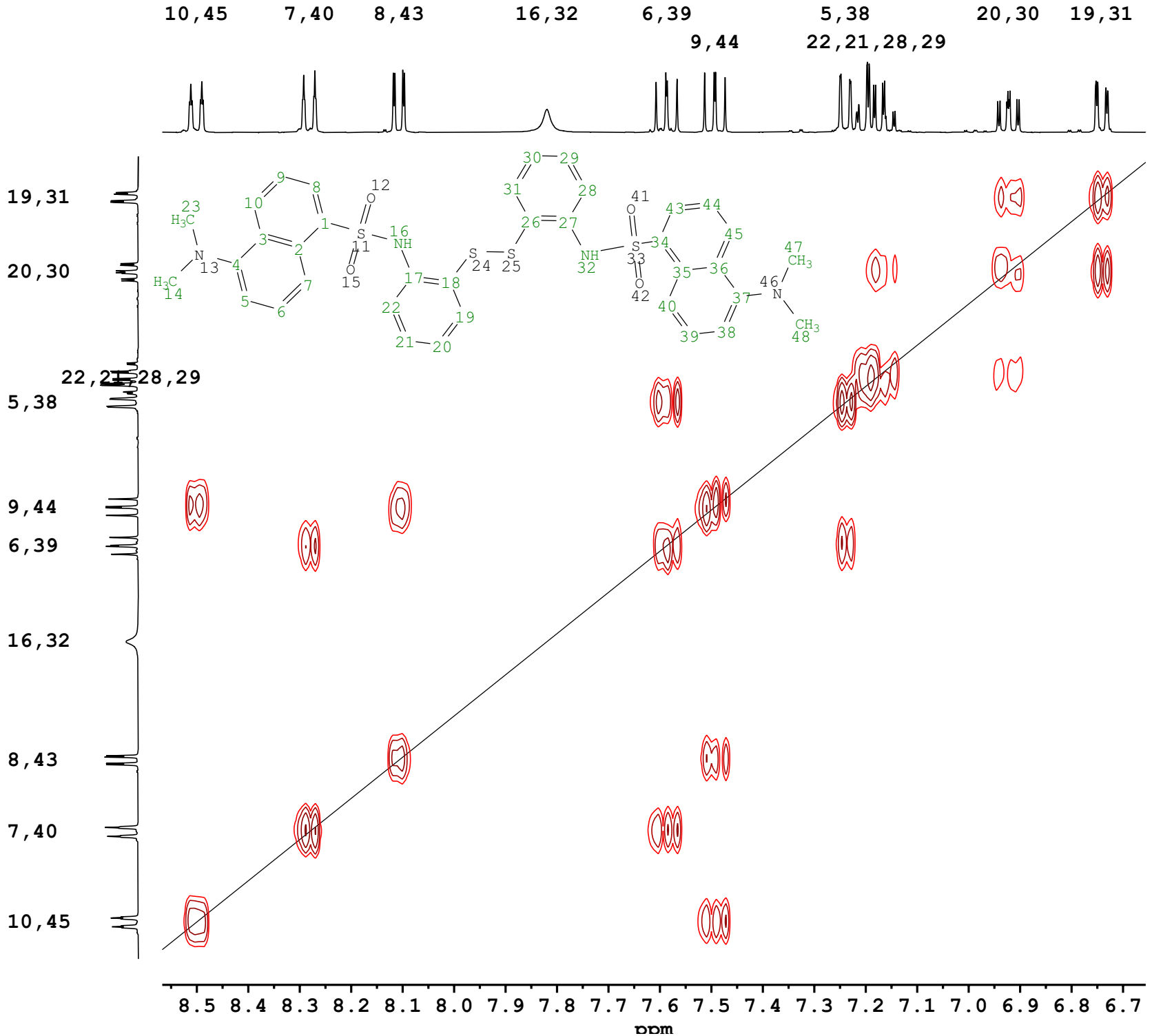
Fig SX92 L2 acetonitrile-d3 ligand only full assignment





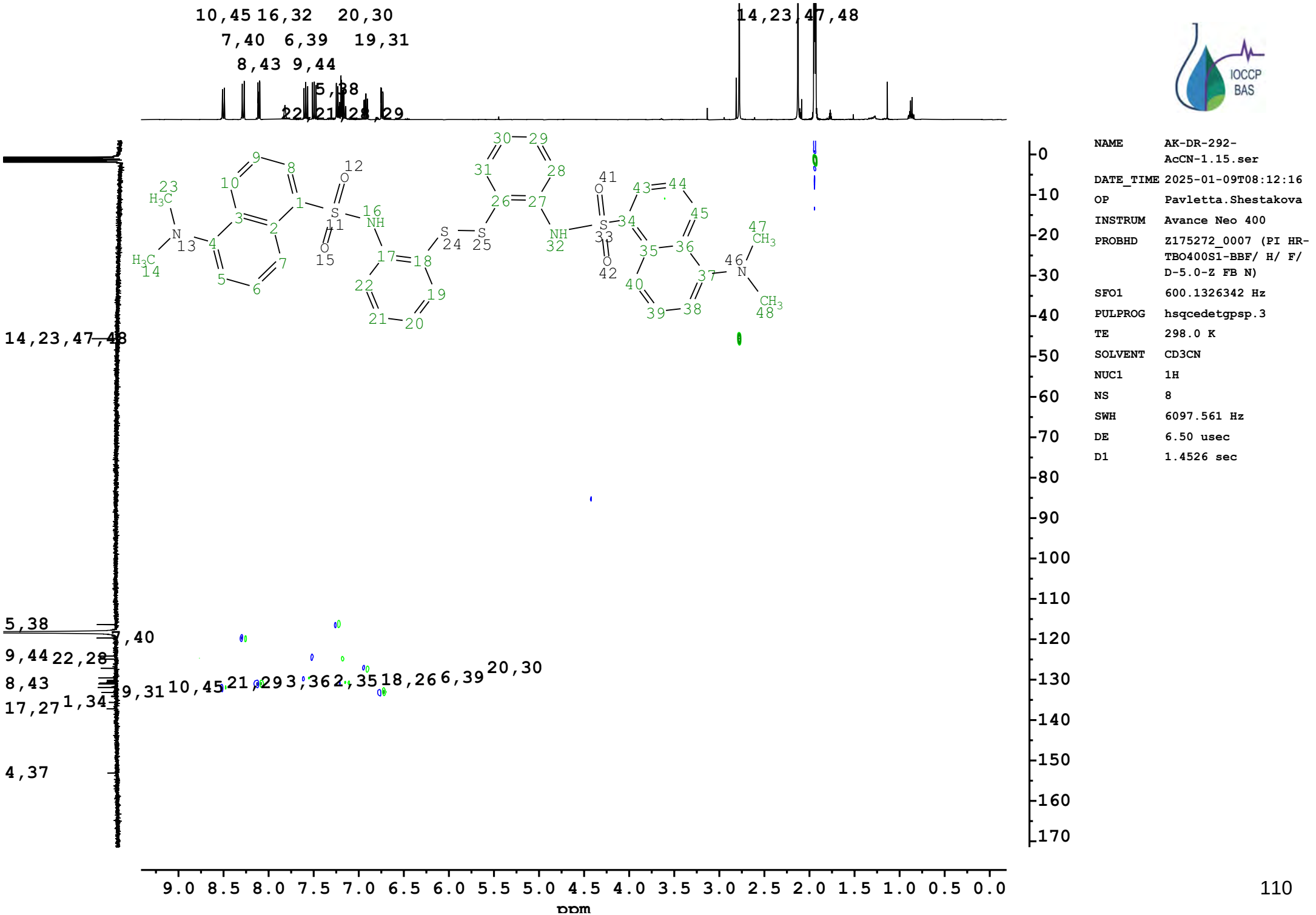

| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.12.fid |
| DATE_TIME | 2025-01-09T00:57:13 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9319844 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8096 |
| SWH | 35714.286 Hz |
| DE | 18.00 usec |
| D1 | 1.5000 sec |

**Fig SX93** **L2 acetonitrile-d3 ligand only full assignment**



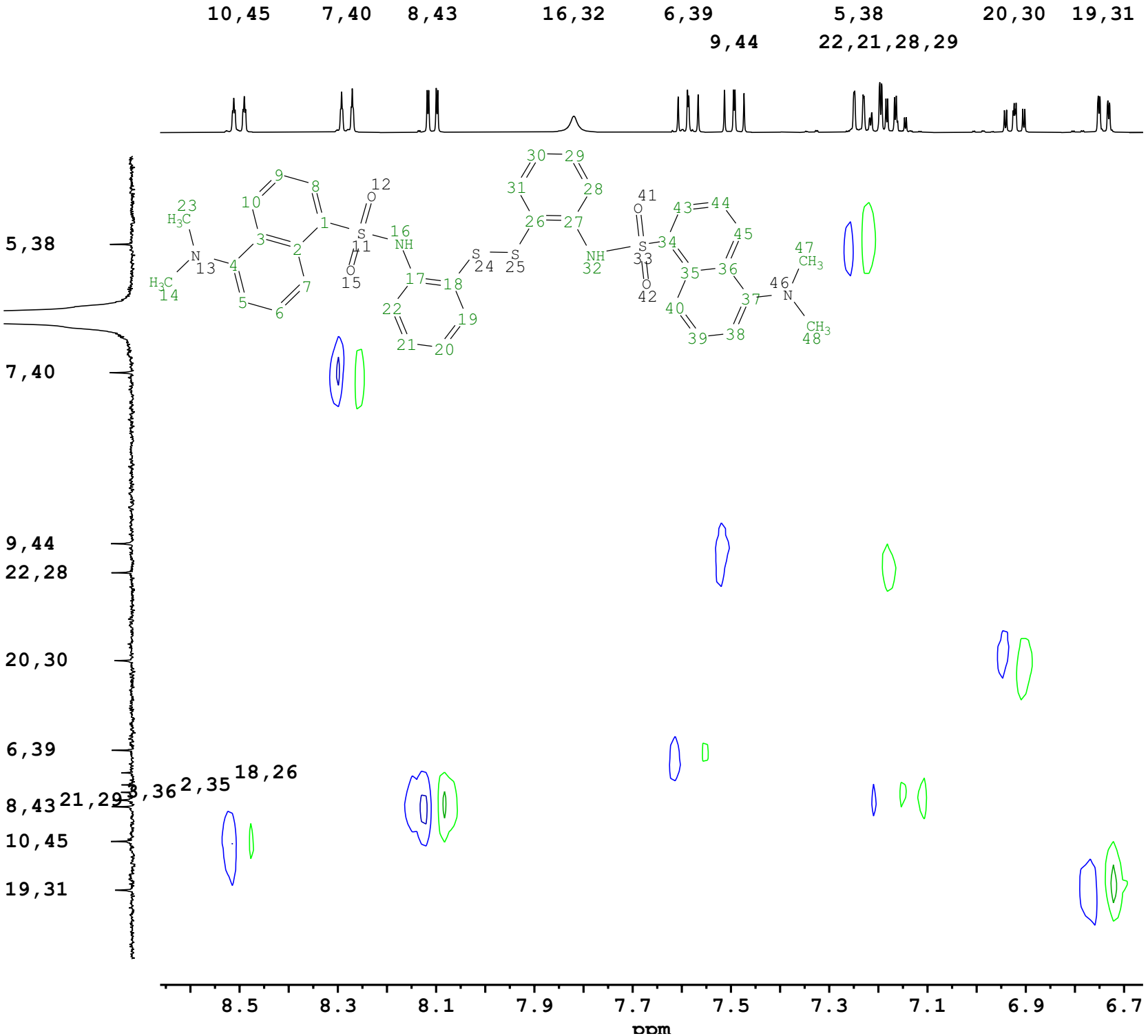

| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.14.ser |
| DATE_TIME | 2025-01-09T07:28:41 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 4 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 0.9689 sec |

Fig SX94 L2 acetonitrile-d3 ligand only full assignment



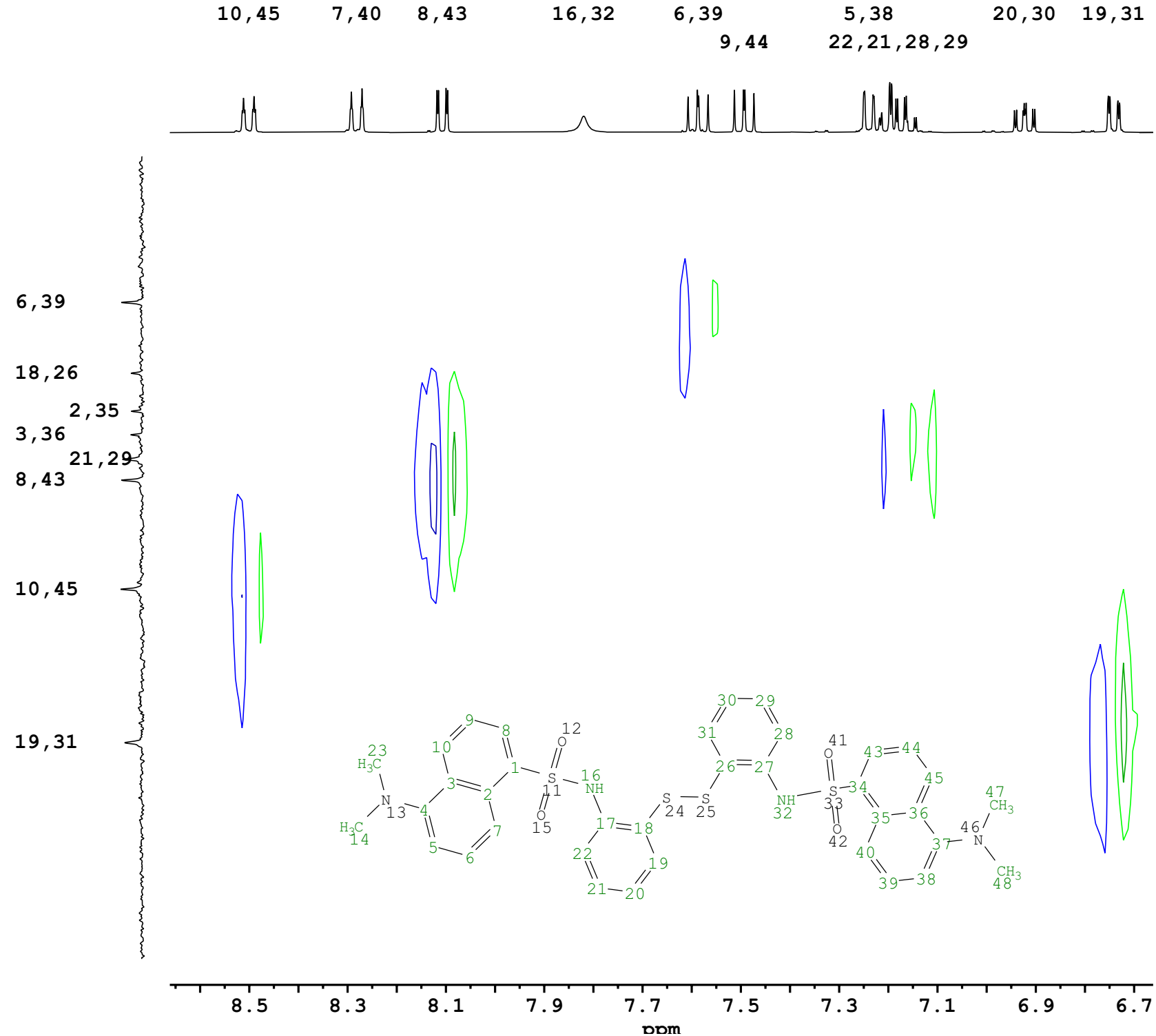

| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.15.ser |
| DATE_TIME | 2025-01-09T08:12:16 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

**Fig SX95** **L2 acetonitrile-d3 ligand only full assignment**



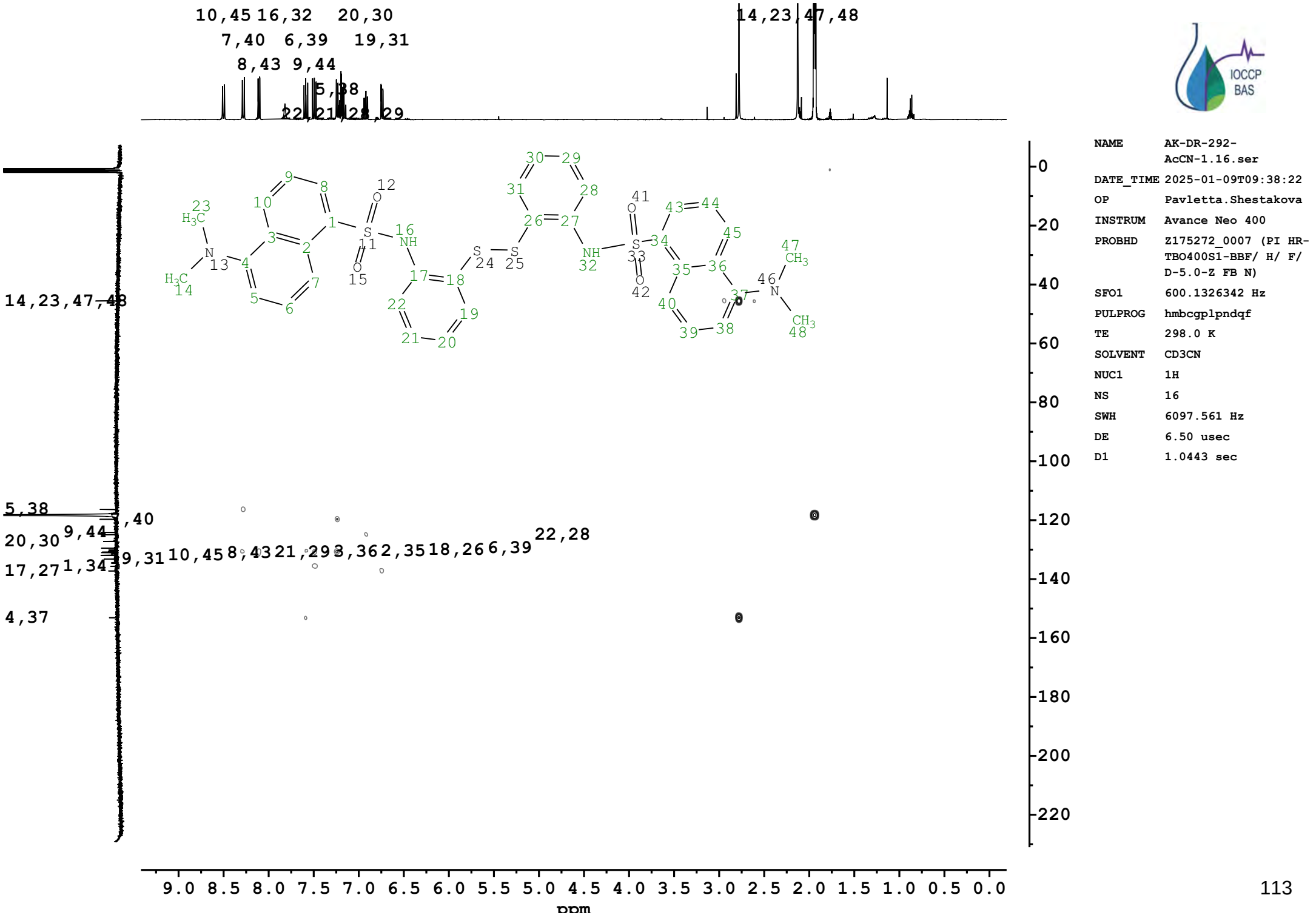

| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.15.ser |
| DATE_TIME | 2025-01-09T08:12:16 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX96 L2 acetonitrile-d3 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.15.ser |
| DATE_TIME | 2025-01-09T08:12:16 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

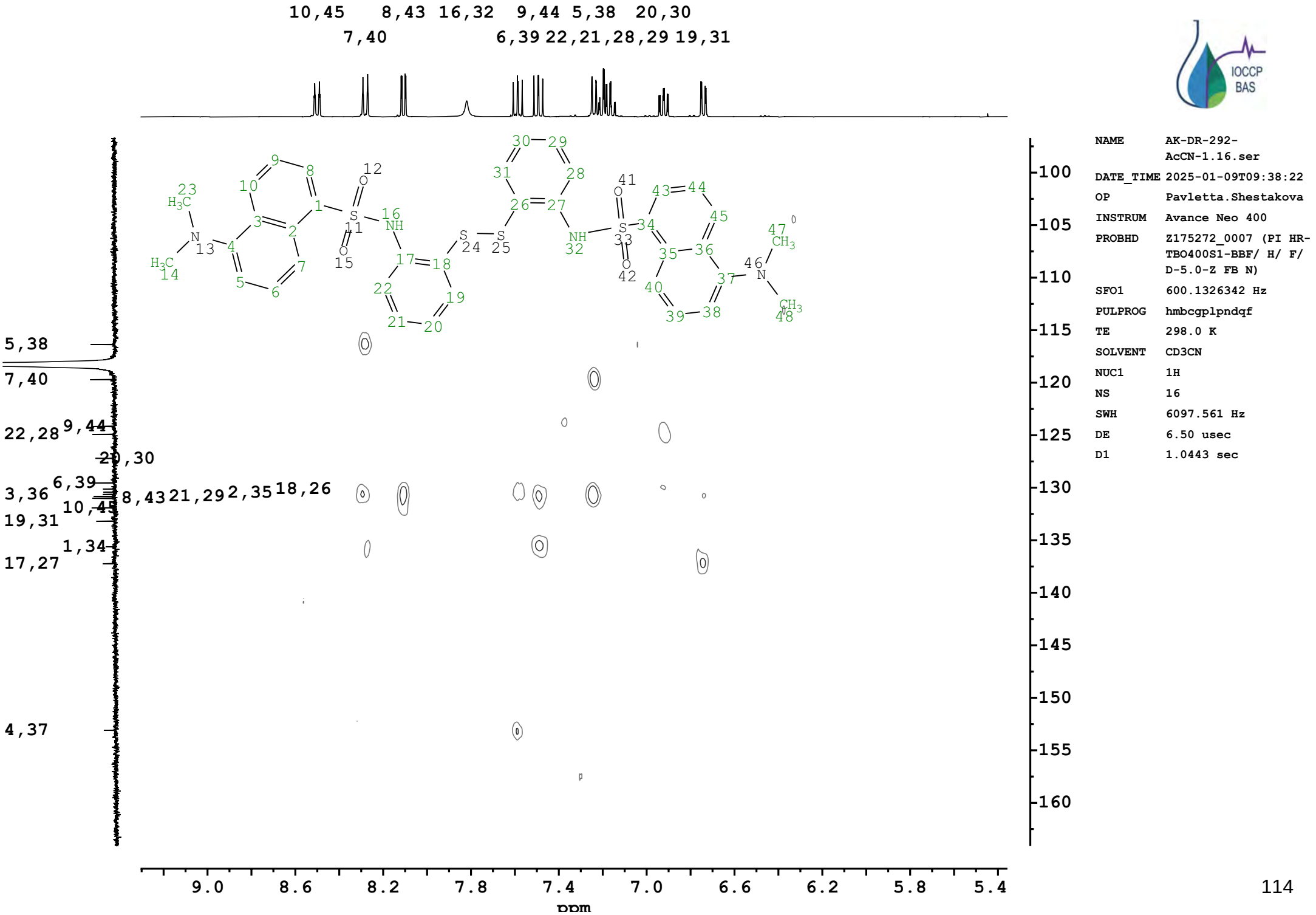
Fig SX97 L2 acetonitrile-d3 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.16.ser |
| DATE_TIME | 2025-01-09T09:38:22 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX98

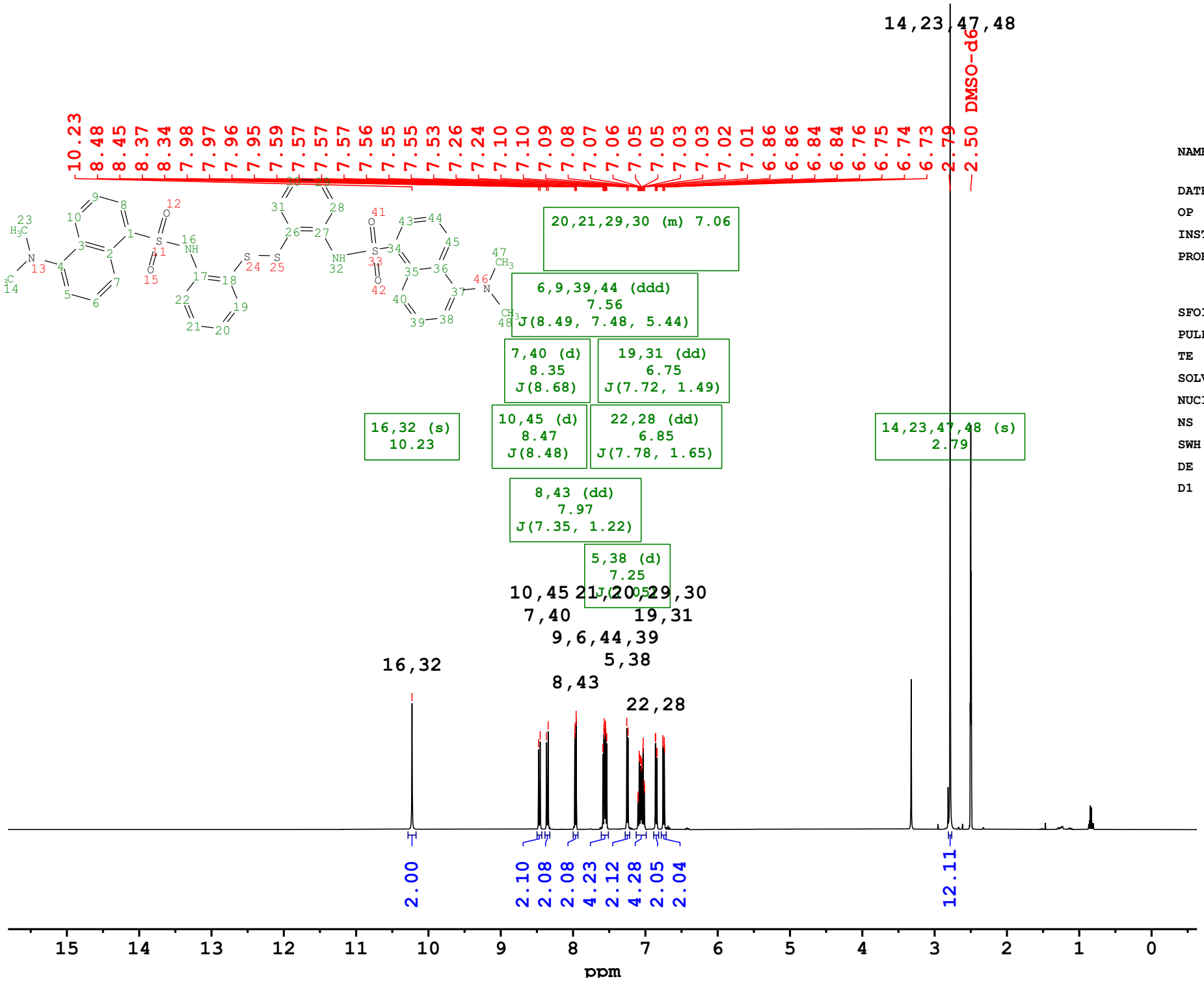
# L2 acetonitrile-d3 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-AcCN-1.16.ser |
| DATE_TIME | 2025-01-09T09:38:22 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX99

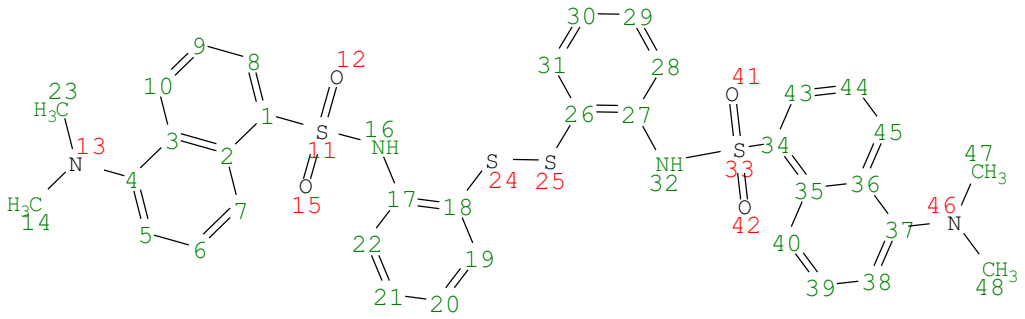
# L2 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.11.fid |
| DATE_TIME | 2024-12-19T03:08:04 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

**Fig SX100** **L2 dmso-d6 ligand only full assignment**

8.48 8.45 8.37 8.34 7.98 7.97 7.96 7.95 7.59 7.57 7.57 7.57 7.56 7.55 7.55 7.53 7.26 7.24 7.10 7.09 7.08 7.07 7.06 7.05 7.05 7.03 7.03 7.02 7.01 6.86 6.86 6.84 6.84 6.76 6.75 6.74 6.73



| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.11.fid |
| DATE_TIME | 2024-12-19T03:08:04 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

7,40 (d) 8.35 J(8.68)

20,21,29,30 (m) 7.06

19,31 (dd) 6.75 J(7.72, 1.49)

10,45 (d) 8.47 J(8.48)

8,43 (dd) 7.97 J(7.35, 1.22)

6,9,39,44 (ddd) 7.56 J(8.49, 7.48, 5.44)

5,38 (d) 7.25 J(7.05)

22,28 (dd) 6.85 J(7.78, 1.65)

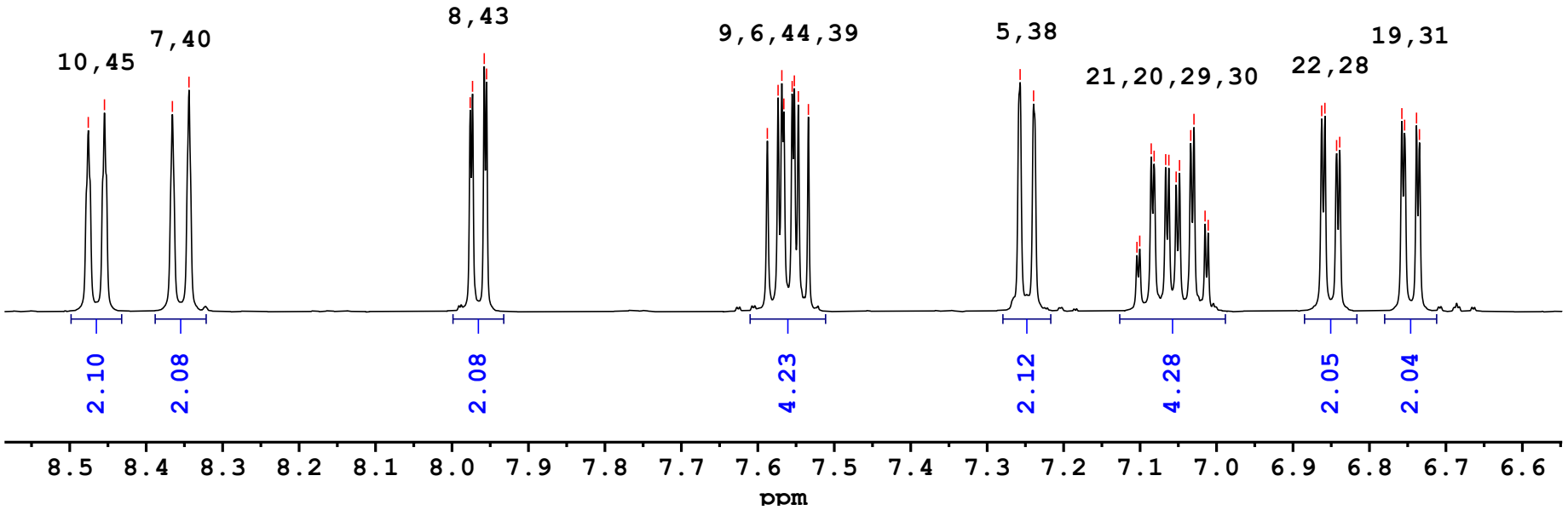
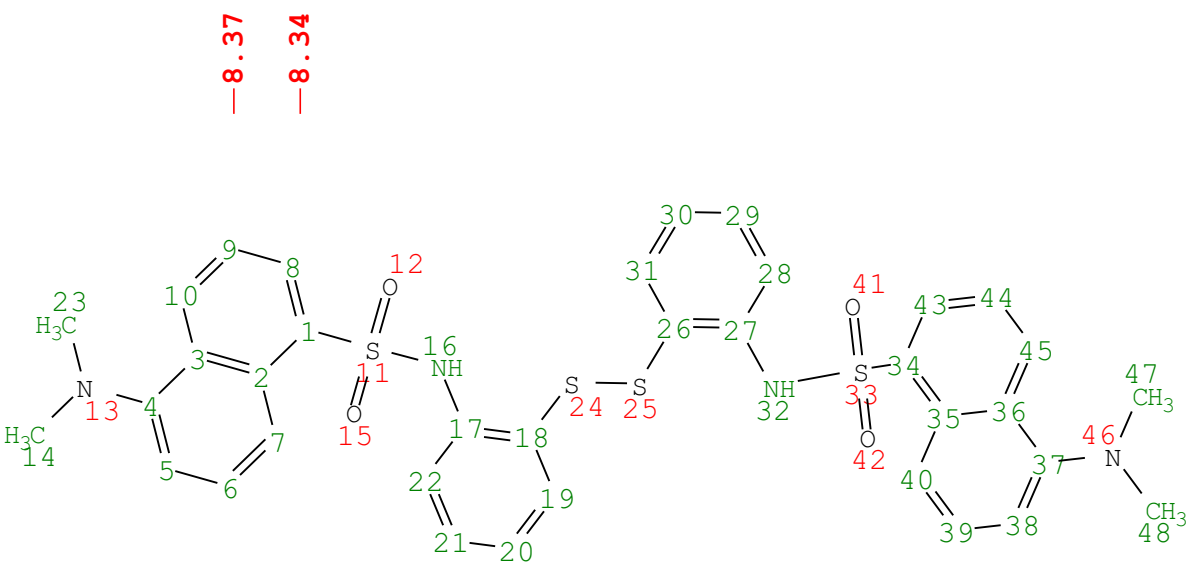


**Fig SX101** **L2 dmso-d6 ligand only full assignment**




| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.11.fid |
| DATE_TIME | 2024-12-19T03:08:04 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

10,45 (d)
8.47
J(8.48)

7,40 (d)
8.35
J(8.68)

8,43 (dd)
7.97
J(7.35, 1.22)

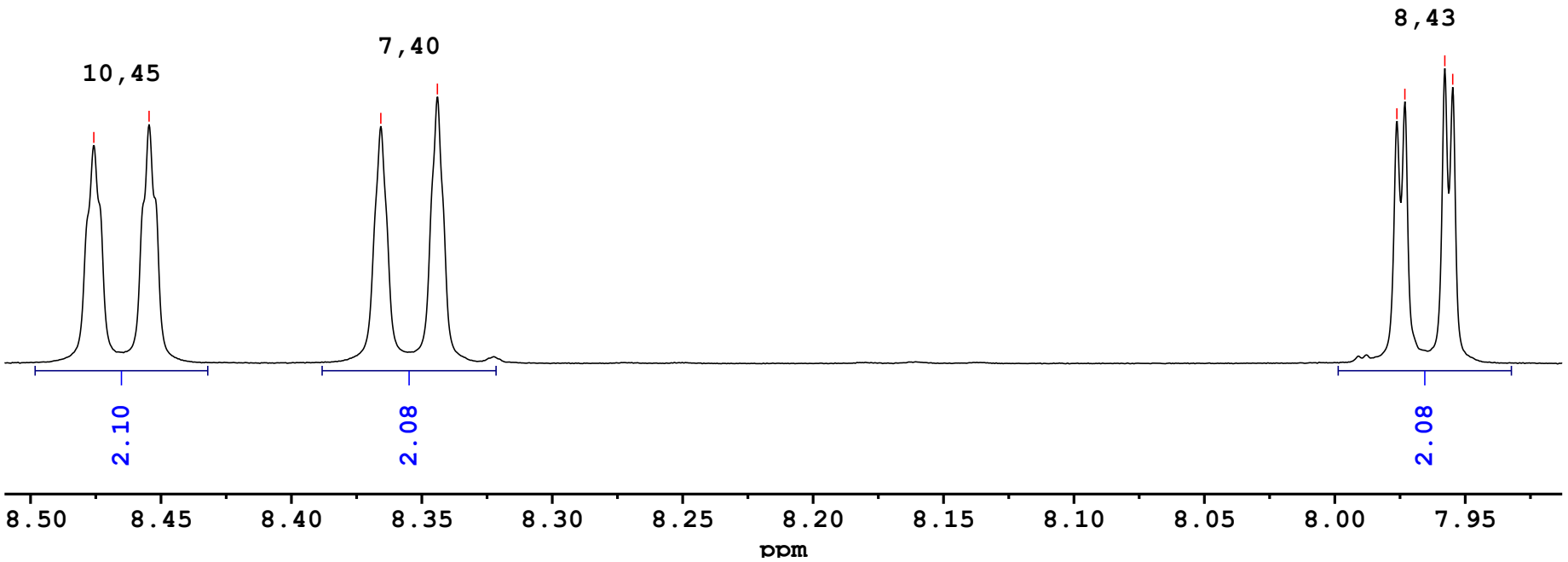
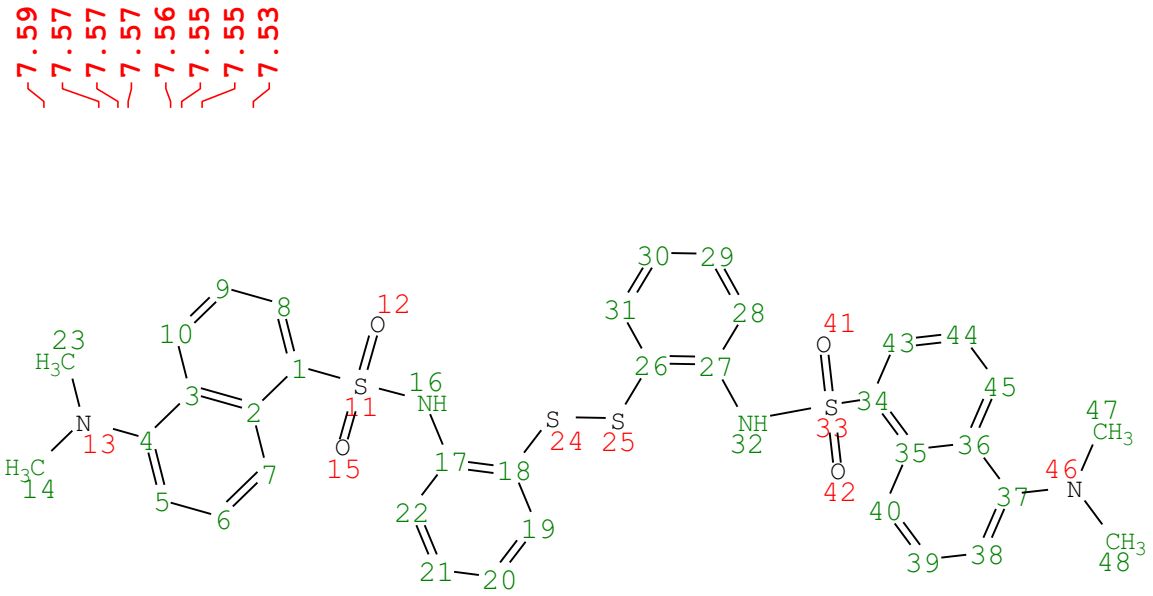


Fig SX102

# L2 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.11.fid |
| DATE_TIME | 2024-12-19T03:08:04 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

6,9,39,44 (ddd)
7.56
J(8.49, 7.48, 5.44)

5,38 (d)
7.25
J(7.05)

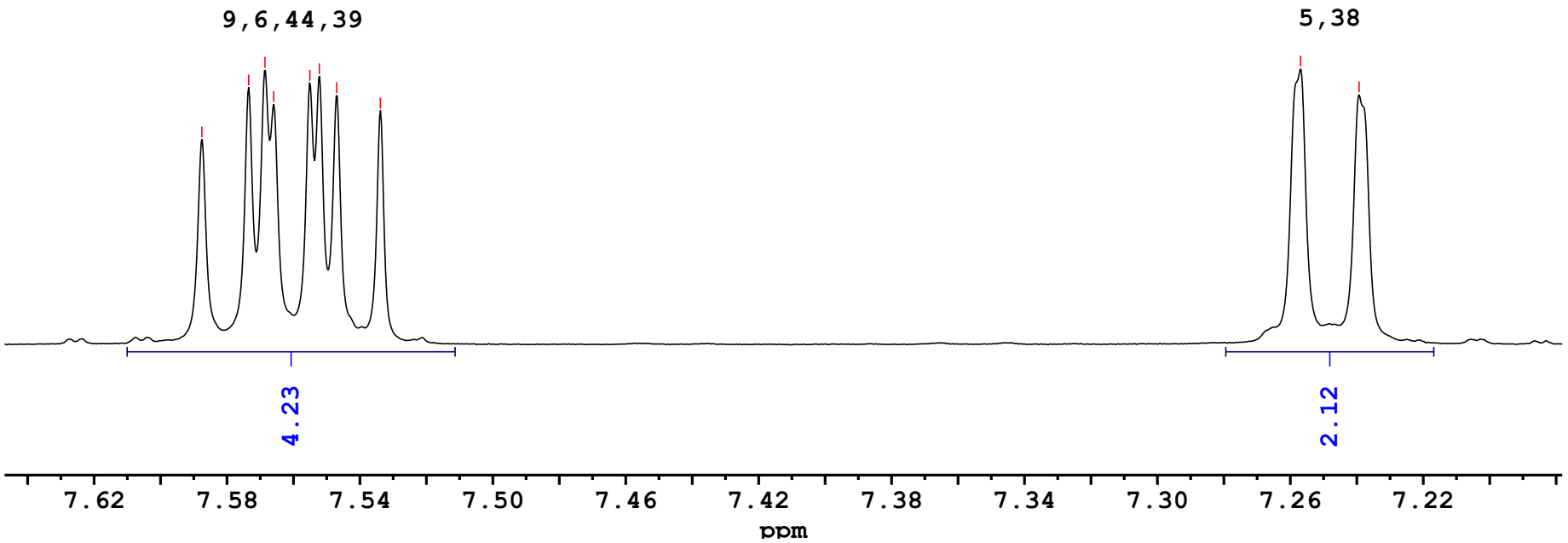
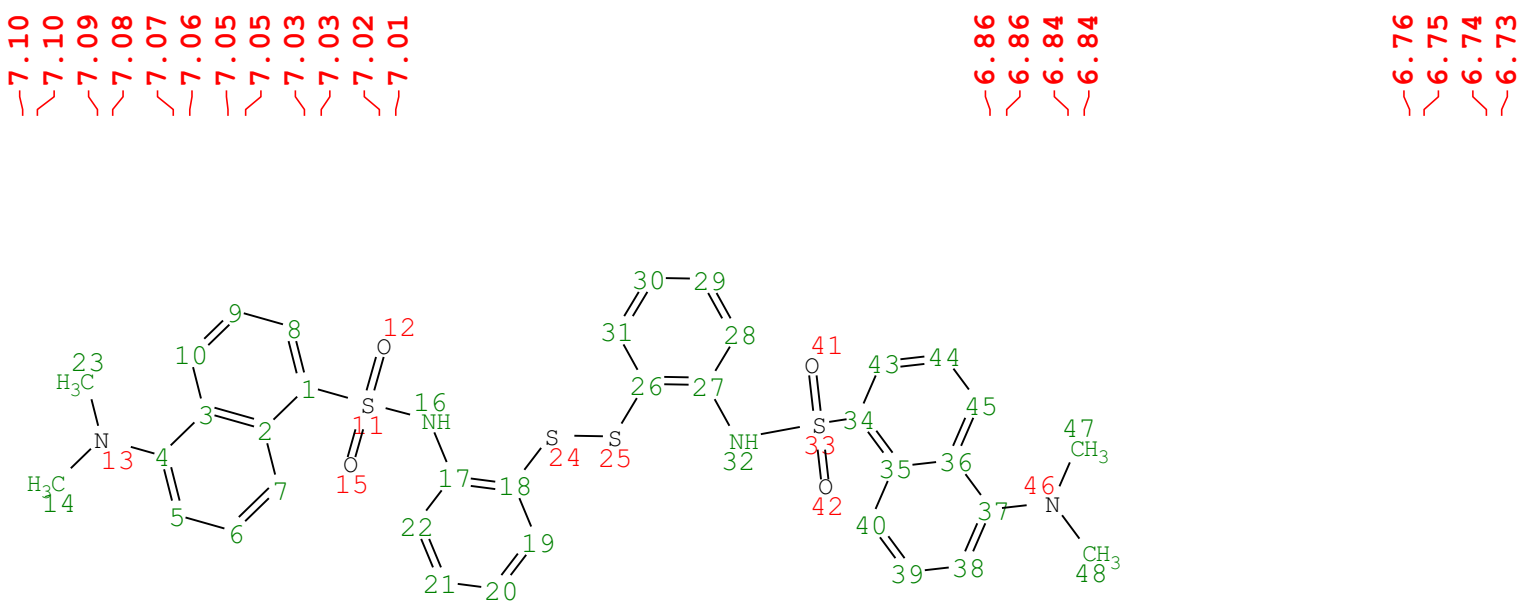


Fig SX103 L2 dmso-d6 ligand only full assignment






| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.11.fid |
| DATE_TIME | 2024-12-19T03:08:04 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

20,21,29,30 (m) 7.06

22,28 (dd) 6.85 J(7.78, 1.65)

19,31 (dd) 6.75 J(7.72, 1.49)

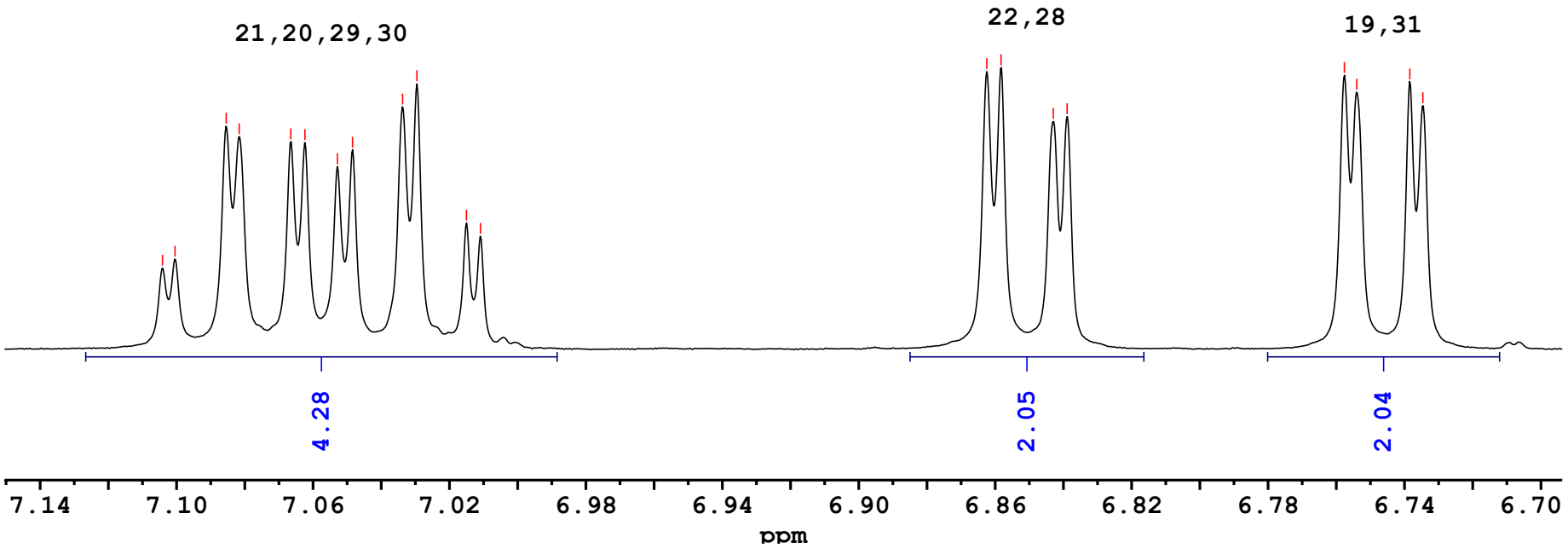
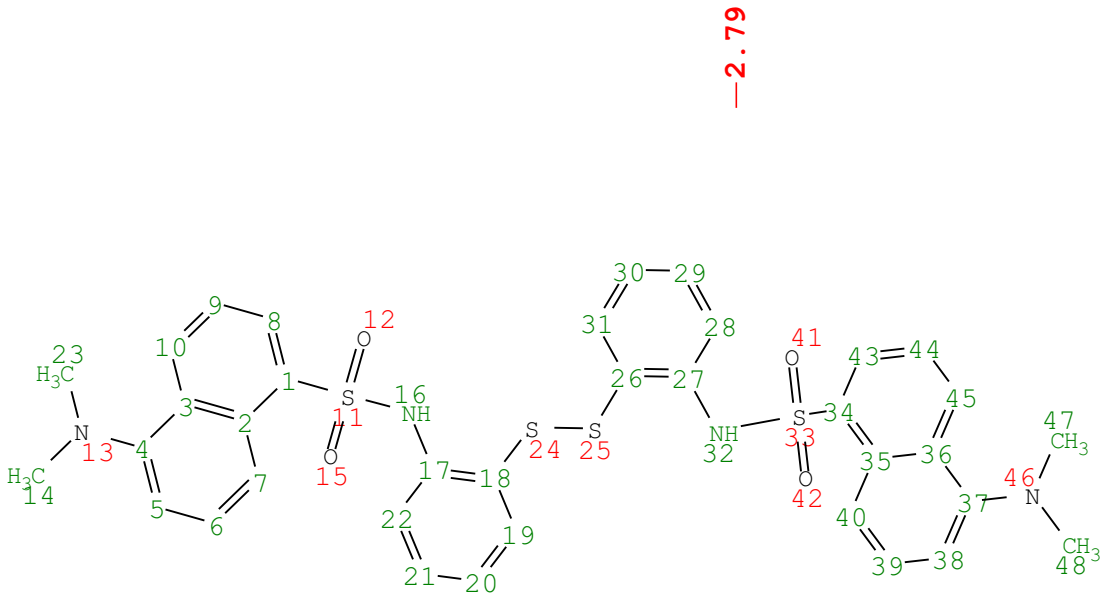


**Fig SX104** **L2 dmso-d6 ligand only full assignment**




| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.11.fid |
| DATE_TIME | 2024-12-19T03:08:04 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

14,23,47,48 (s)
2.79

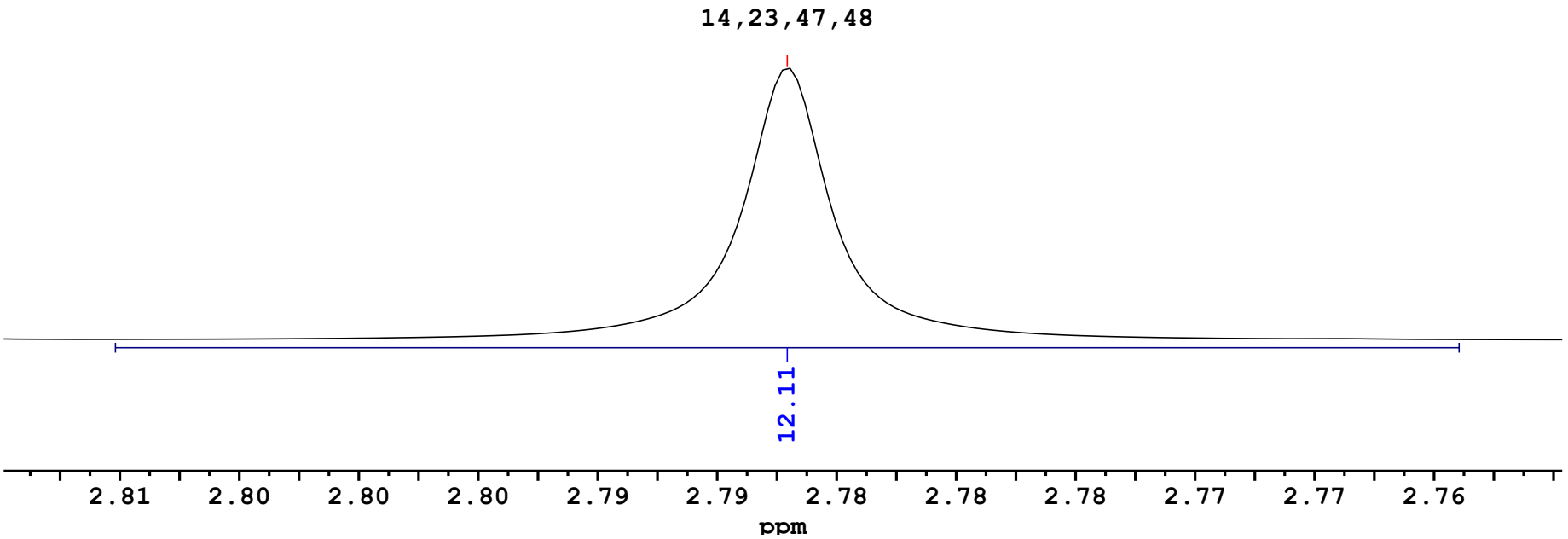
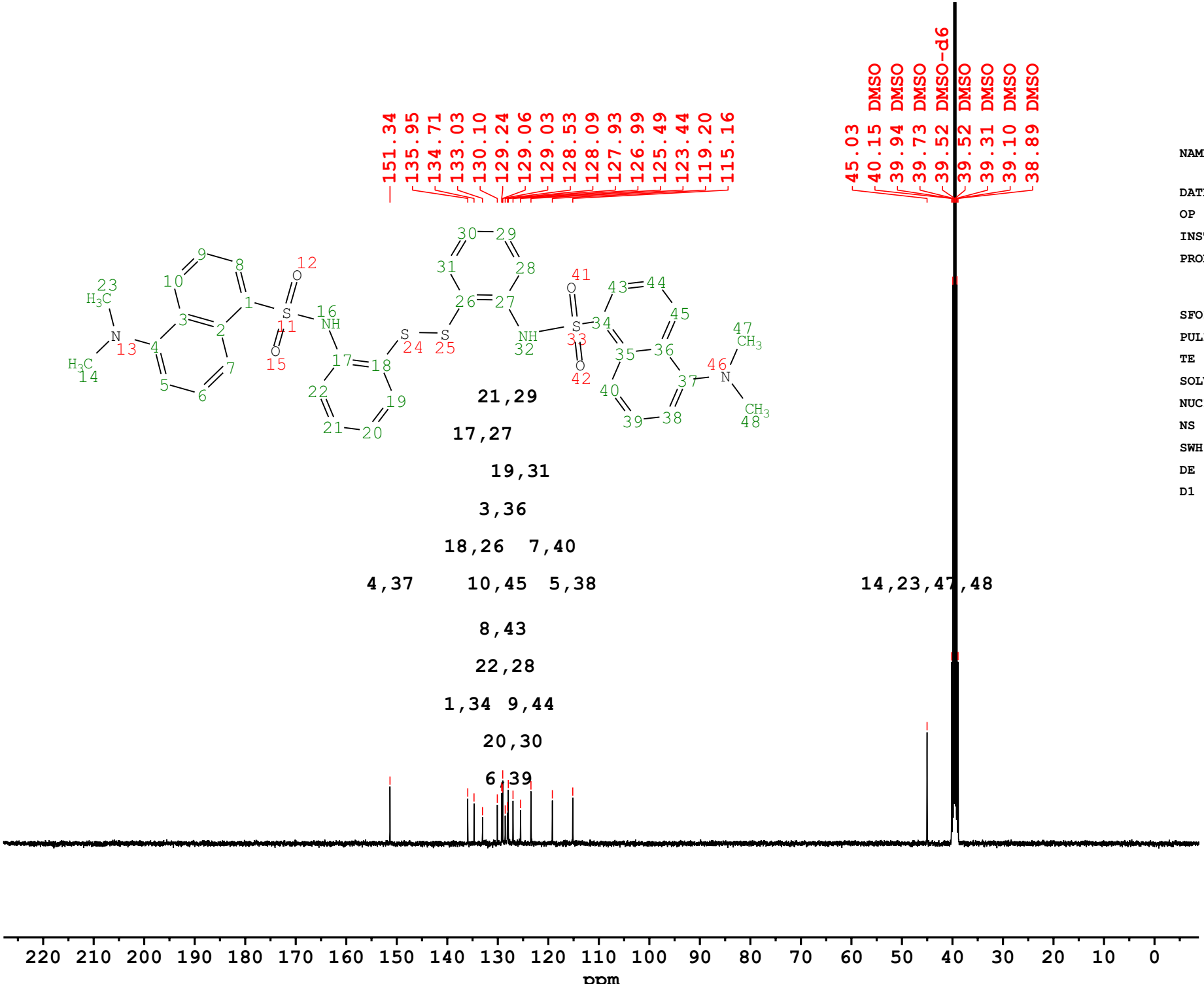


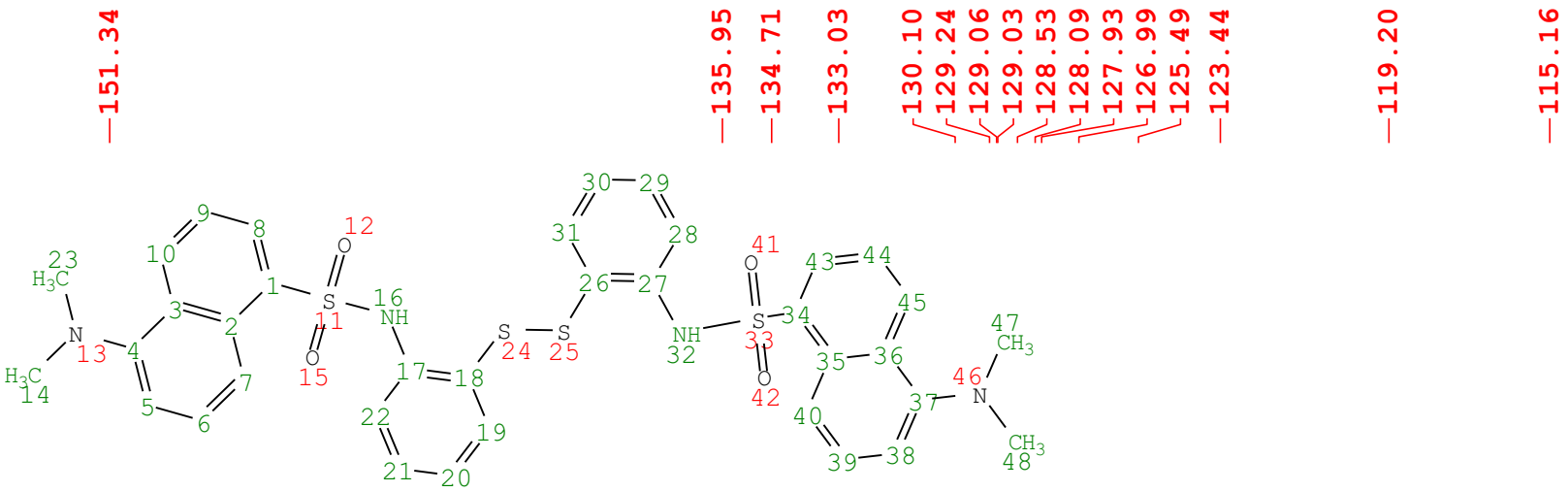
Fig SX105

# L2 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-0-DMSO. 12.fid |
| DATE_TIME | 2024-12-19T04:25:04 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 2048 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

**Fig SX106** **L2 dmso-d6 ligand only full assignment**






| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.12.fid |
| DATE_TIME | 2024-12-19T04:25:04 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 2048 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

2,35
21,29
22,28
1,34 17,27 8,43 9,44
4,37 18,26 10,45 19,31 7,40 5,38
3,36
20,30
6,39

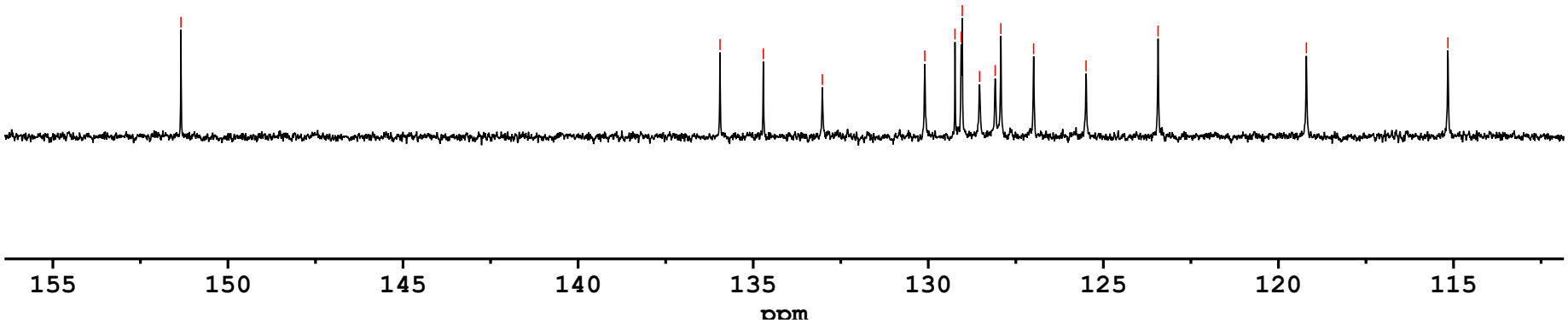
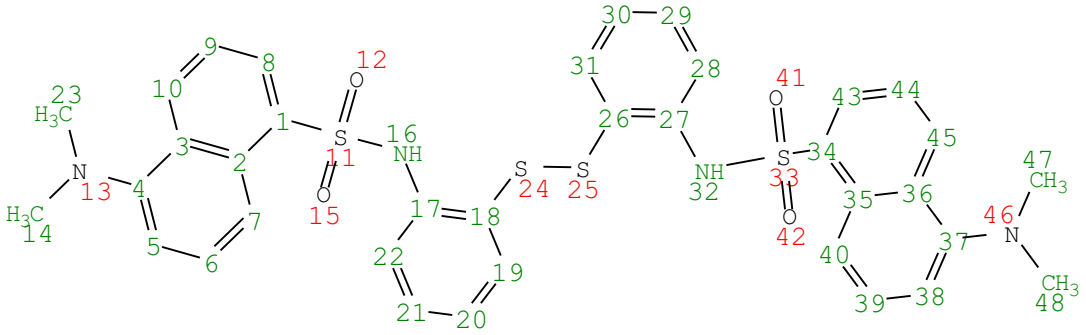


**Fig SX107** **L2 dmso-d6 ligand only full assignment**

130.10 129.24 129.06 129.03 128.53 128.09 127.93 126.99 125.49



| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.12.fid |
| DATE_TIME | 2024-12-19T04:25:04 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 2048 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

3,36 6,39

10,45 8,43 22,28 21,29 20,30 19,31

2,35

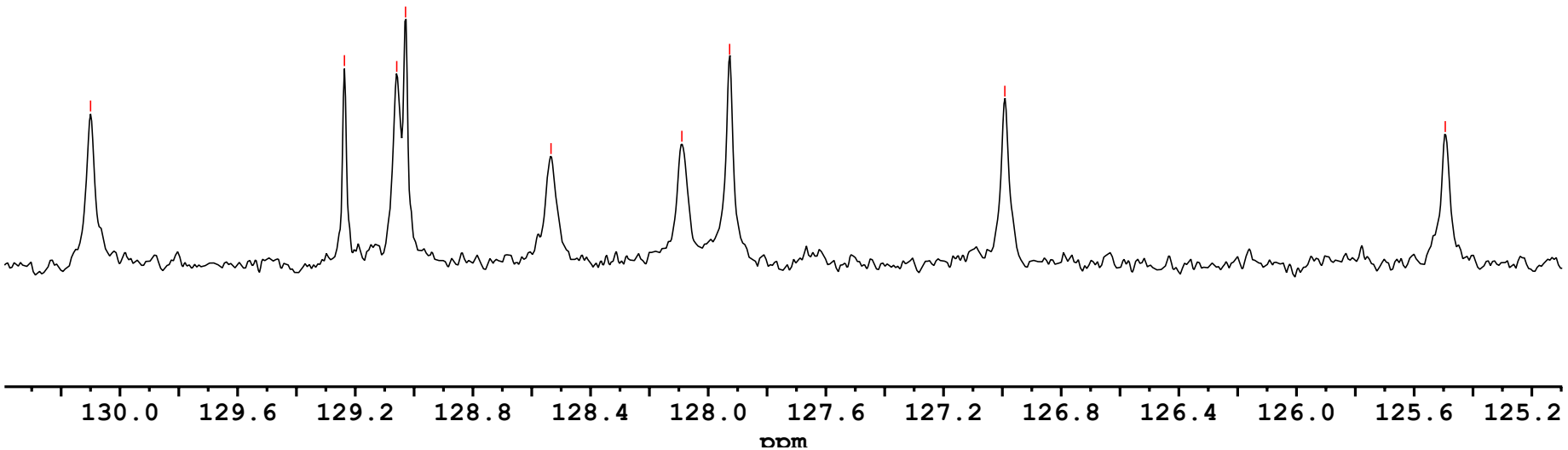
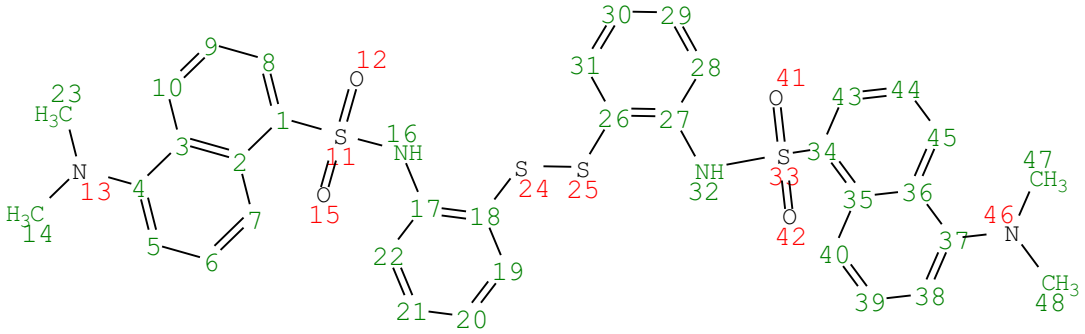
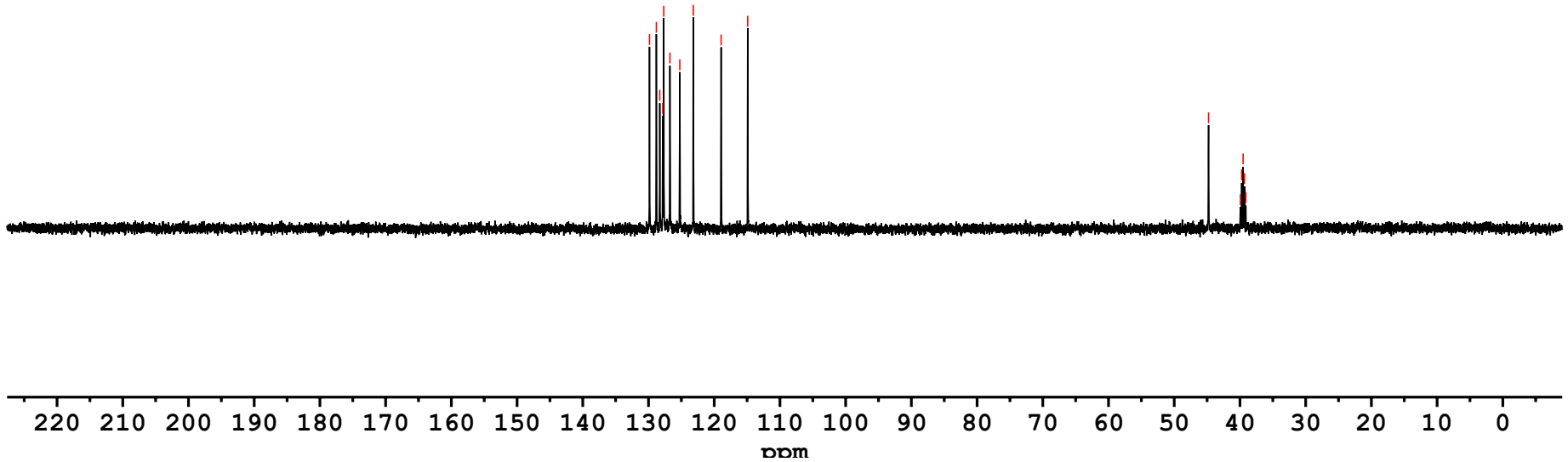


Fig SX108

# L2 dmso-d6 ligand only full assignment

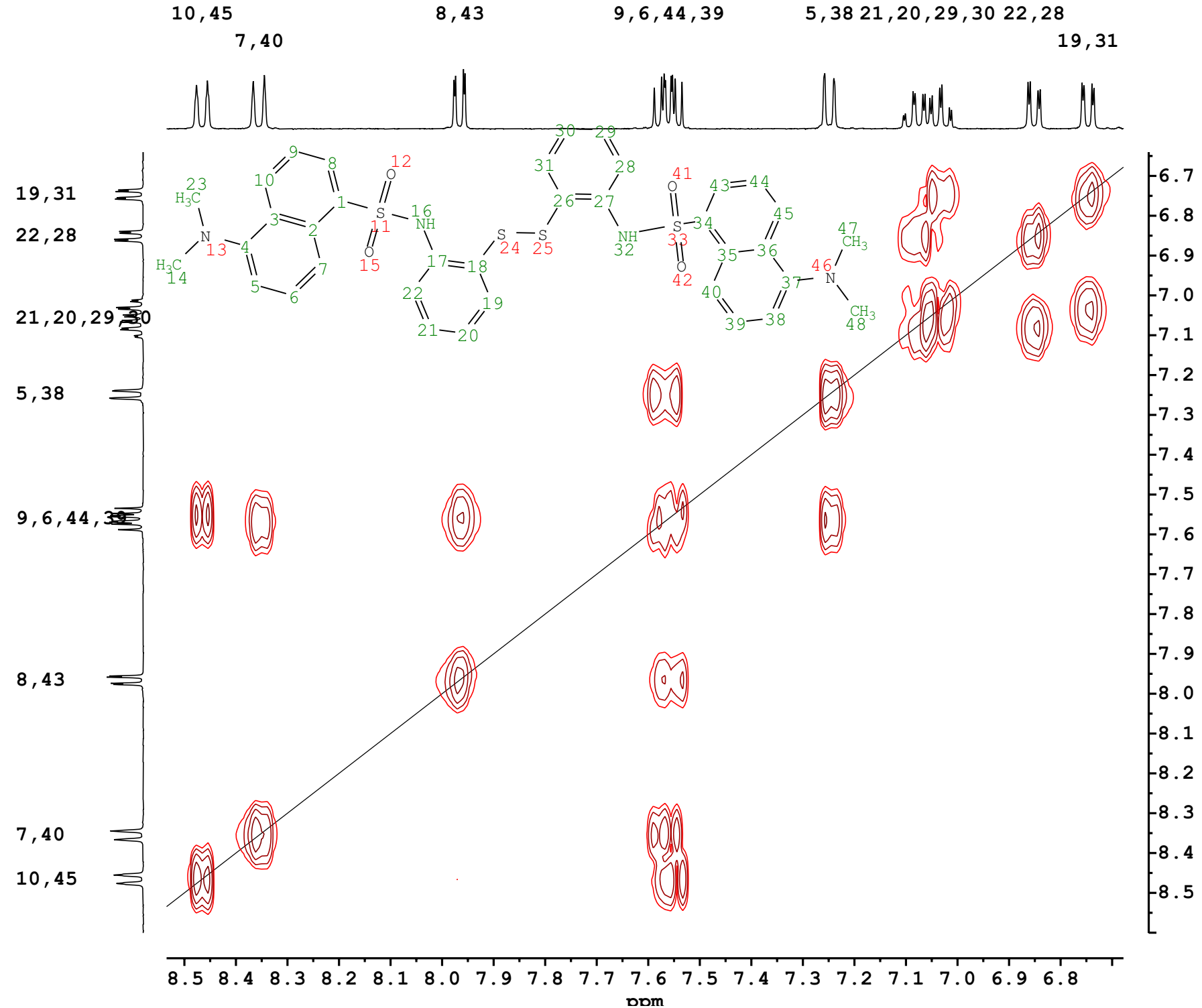





| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.13.fid |
| DATE_TIME | 2024-12-19T05:02:12 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9319844 Hz |
| PULPROG | deptsp135 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 800 |
| SWH | 35714.286 Hz |
| DE | 18.00 usec |
| D1 | 2.0000 sec |

Fig SX109

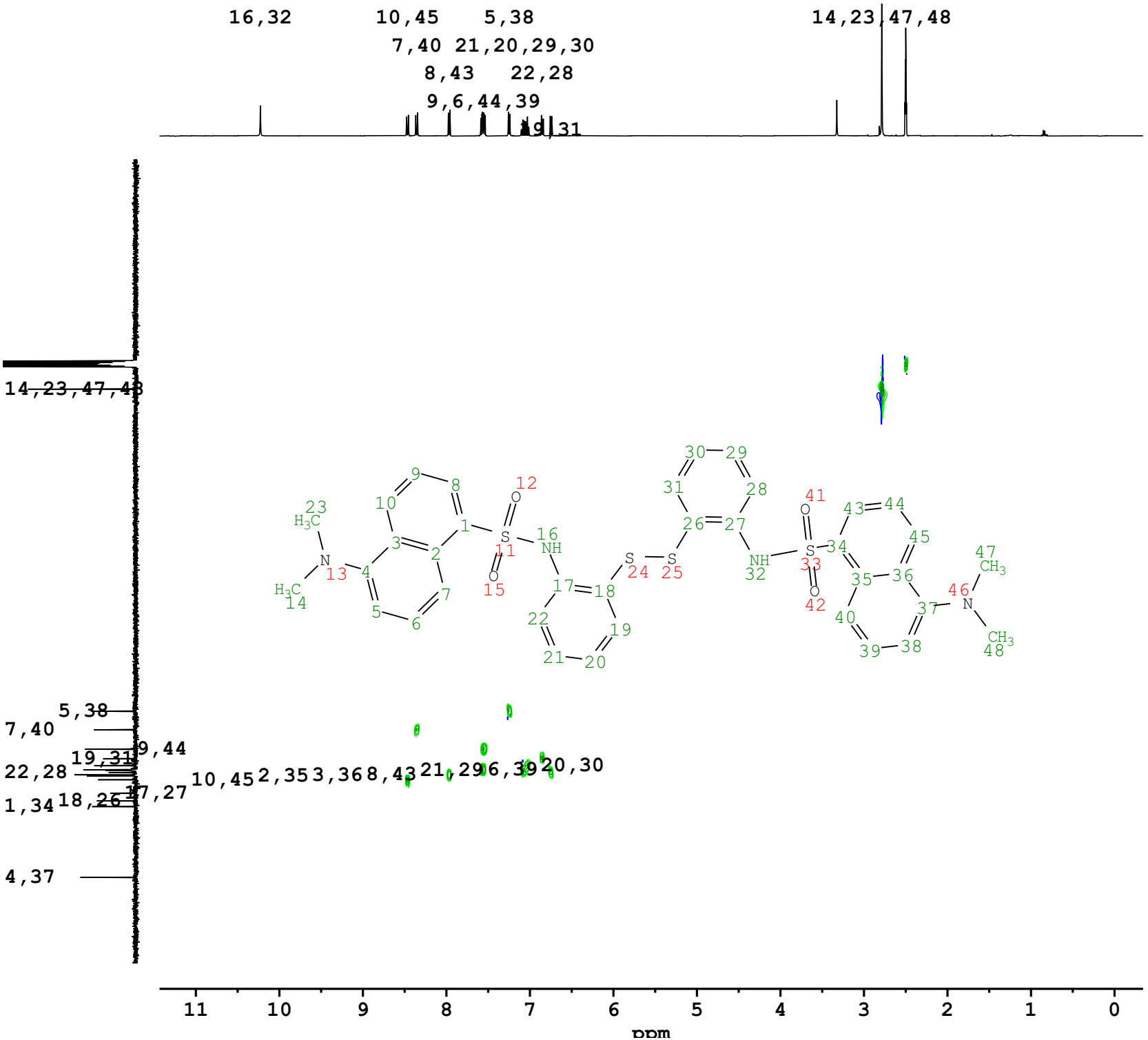
# L2 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.14.ser |
| DATE_TIME | 2024-12-19T05:08:08 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 1 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0139 sec |

Fig SX110

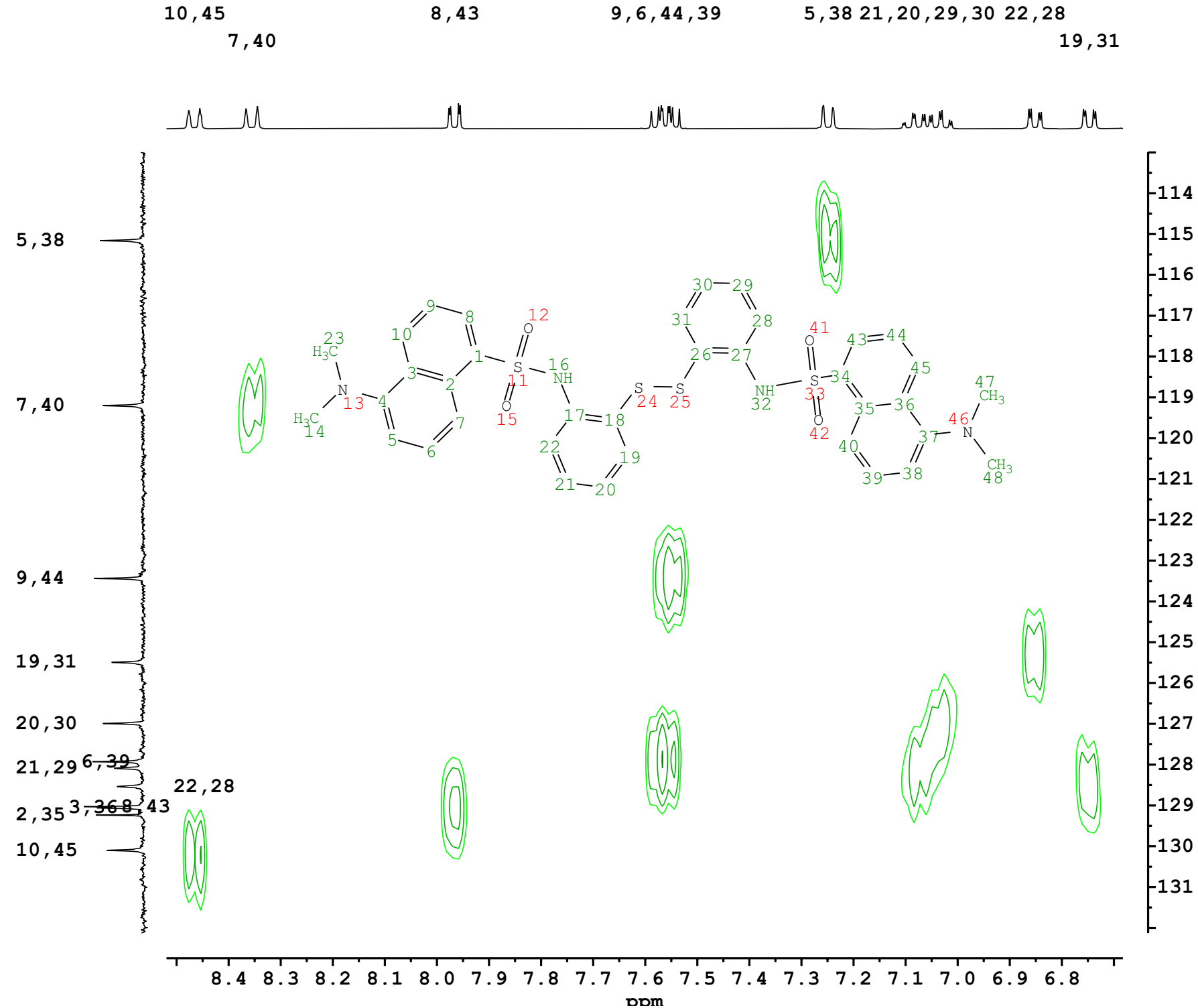
L2 dmso-d6 ligand only full assignment




NAME AK-DR-292-0-DMSO.15.ser
DATE_TIME 2024-12-19T05:31:26
OP Dessislava.Gerginova
INSTRUM Avance Neo 400
PROBHD Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N)
SFO1 600.1326342 Hz
PULPROG hsqcedetgpsp.3
TE 298.0 K
SOLVENT DMSO
NUC1 1H
NS 4
SWH 6097.561 Hz
DE 6.50 usec
D1 1.4526 sec

Fig SX111

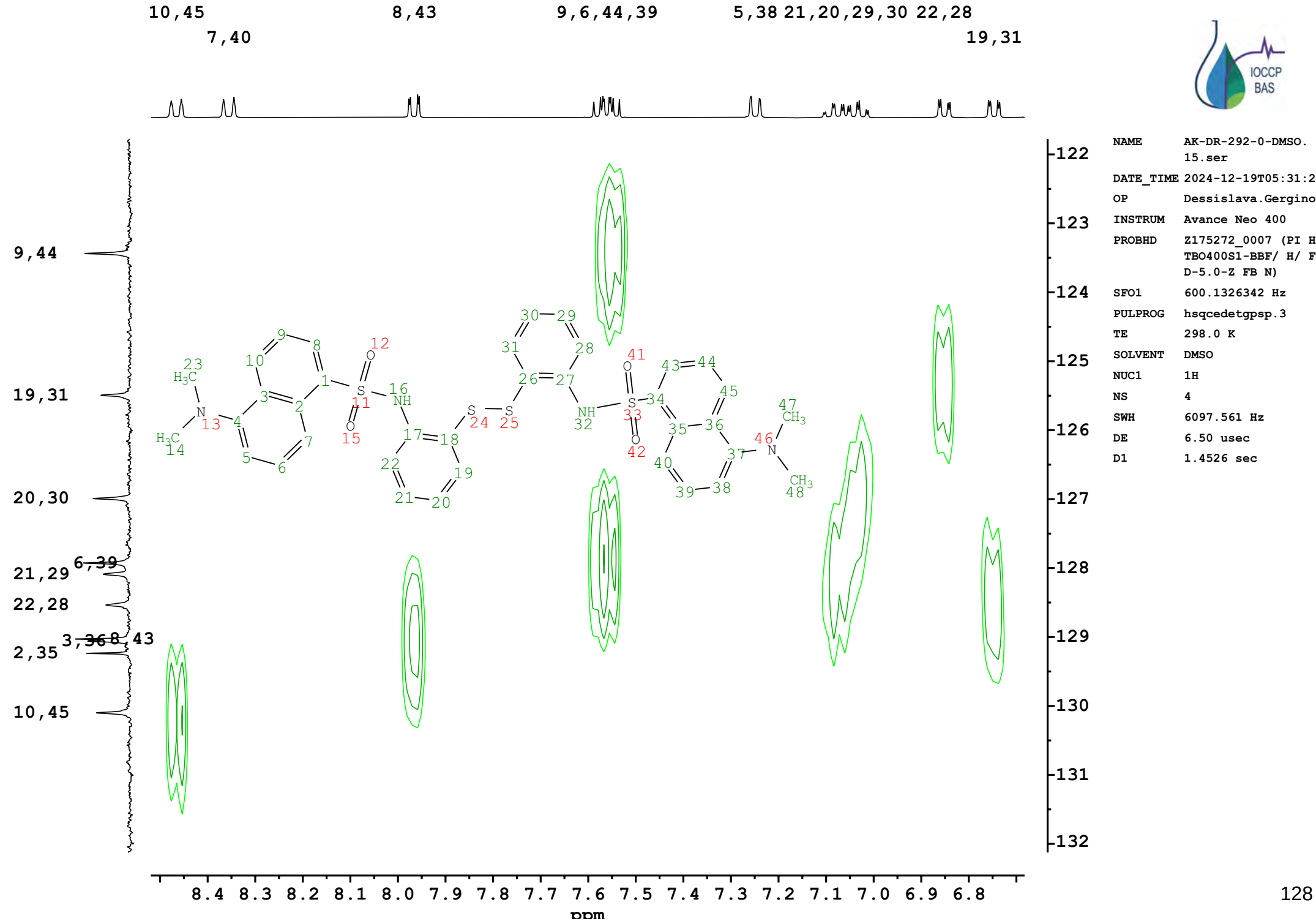
# L2 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.15.ser |
| DATE_TIME | 2024-12-19T05:31:26 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 4 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX112

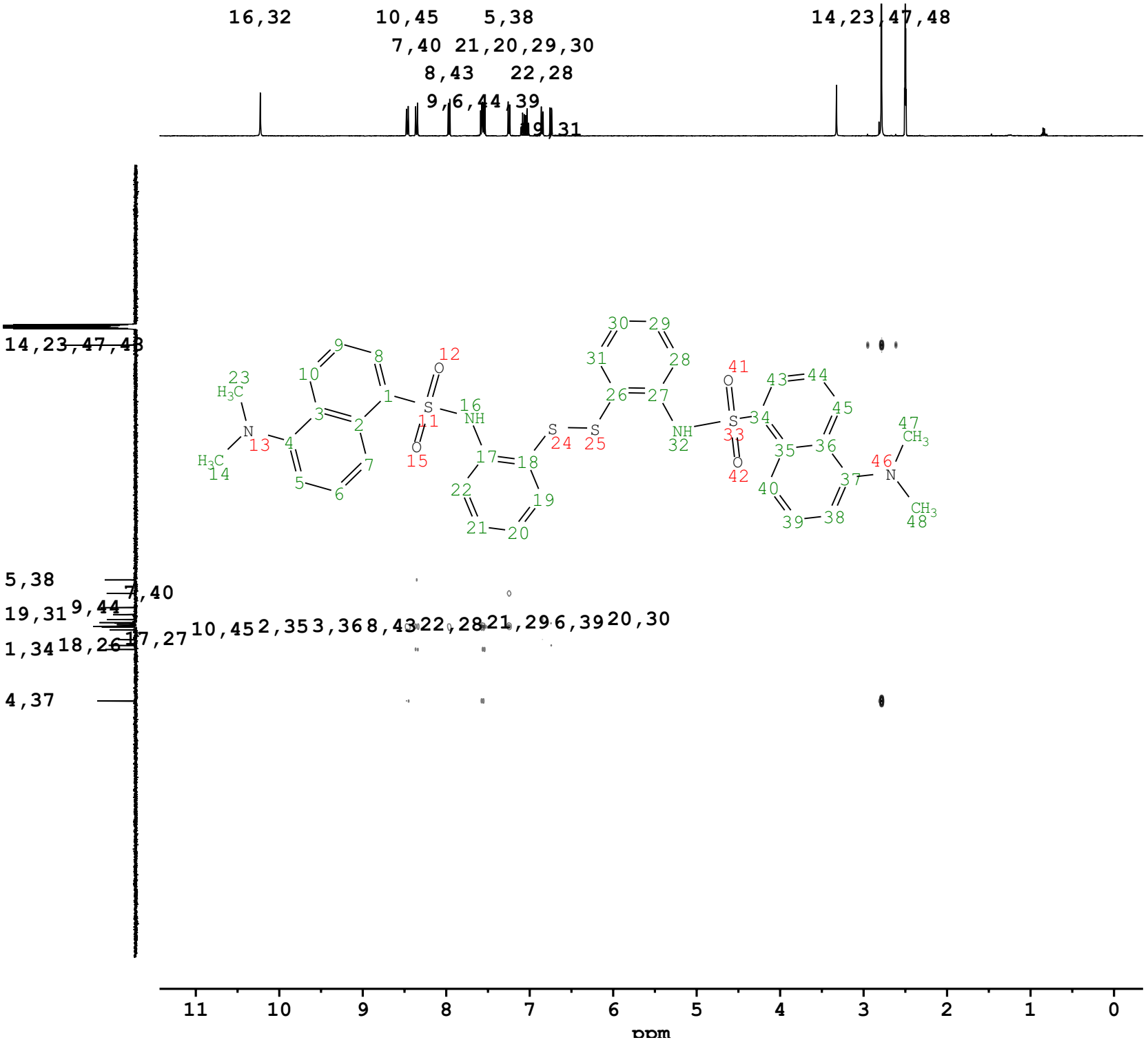
# L2 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.15.ser |
| DATE_TIME | 2024-12-19T05:31:26 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 4 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX113

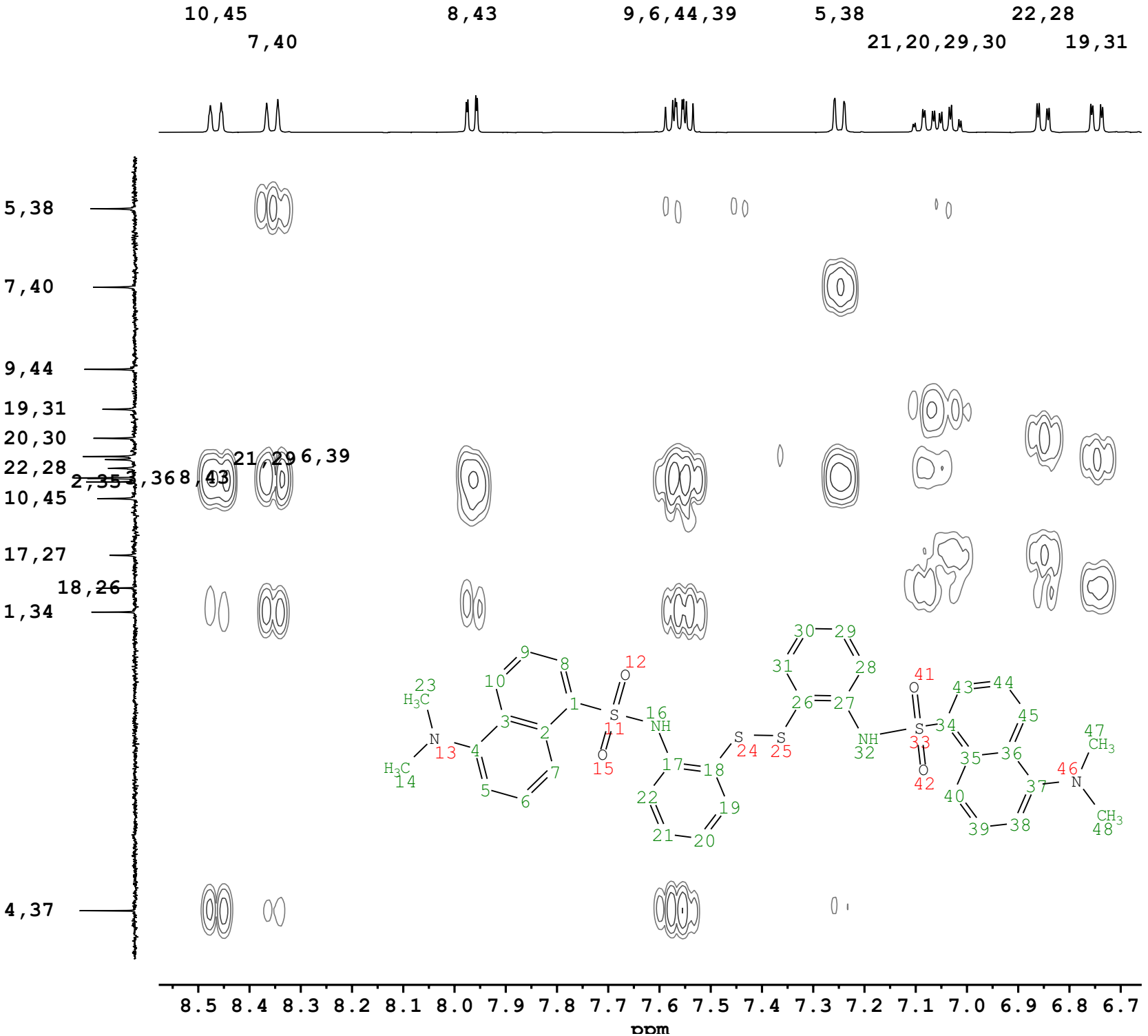
L2 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.16.ser |
| DATE_TIME | 2024-12-19T07:03:15 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX114

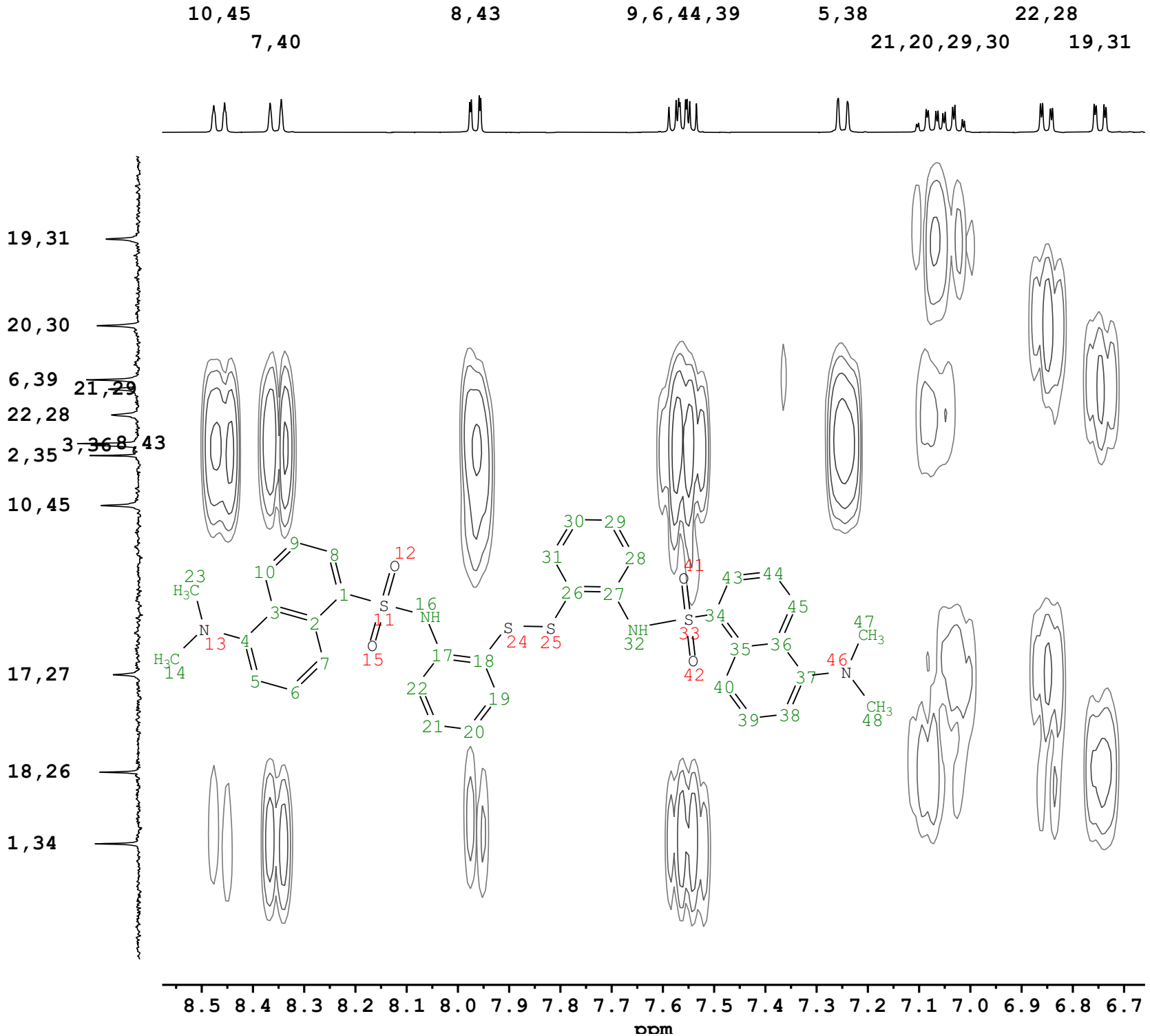
# L2 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.16.ser |
| DATE_TIME | 2024-12-19T07:03:15 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX115

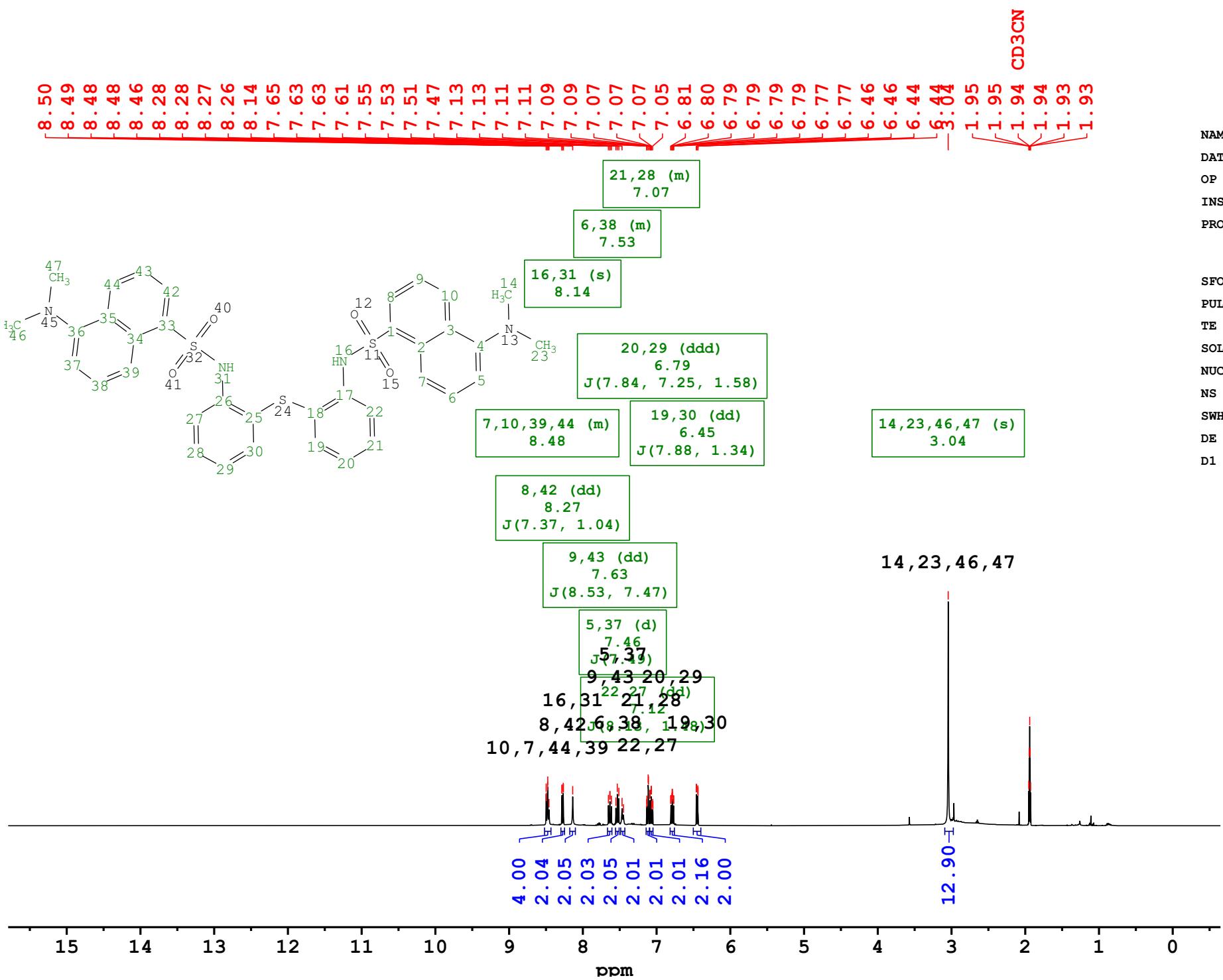
# L2 dmso-d6 ligand only full assignment




| | |
|---|---|
| NAME | AK-DR-292-0-DMSO.16.ser |
| DATE_TIME | 2024-12-19T07:03:15 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX116

# L1 acetonitrile-d3 ligand + 1equiv. Cu(II)

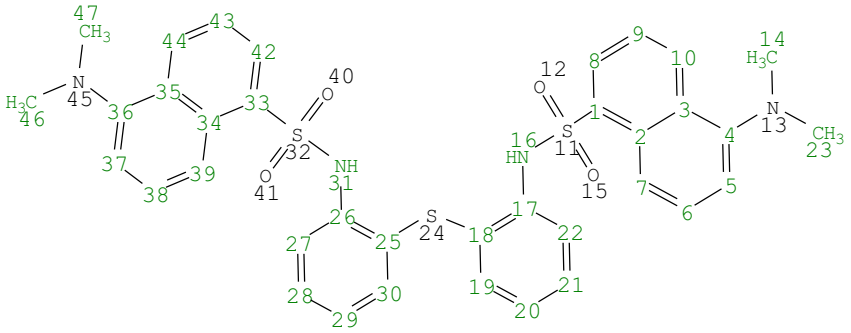



| | |
|---|---|
| NAME | AK-DR-165-Cu1.21.fid |
| DATE_TIME | 2024-12-21T02:05:29 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

**Fig SX117** **L1 acetonitrile-d3 ligand + 1equiv. Cu(II)**

8.50 8.49 8.48 8.48 8.46 8.28 8.28 8.27 8.26 8.14

7.65 7.63 7.63 7.61 7.55 7.53 7.51 7.47 7.45 7.13 7.13 7.11 7.11 7.09 7.09 7.07 7.07 7.07 7.05 7.05 6.81 6.80 6.79 6.79 6.79 6.79 6.77 6.77 6.46 6.46 6.44 6.44



| | |
|---|---|
| NAME | AK-DR-165-Cu1.21.fid |
| DATE_TIME | 2024-12-21T02:05:29 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

8,42 (dd)
8.27
J(7.37, 1.04)

5,37 (d)
7.46
J(7.49)

22,27 (dd)
7.12
J(8.13, 1.48)

7,10,39,44 (m)
8.48

16,31 (s)
8.14

9,43 (dd)
7.63
J(8.53, 7.47)

6,38 (m)
7.53

21,28 (m)
7.07

20,29 (ddd)
6.79
J(7.84, 7.25, 1.58)

19,30 (dd)
6.45
J(7.88, 1.34)

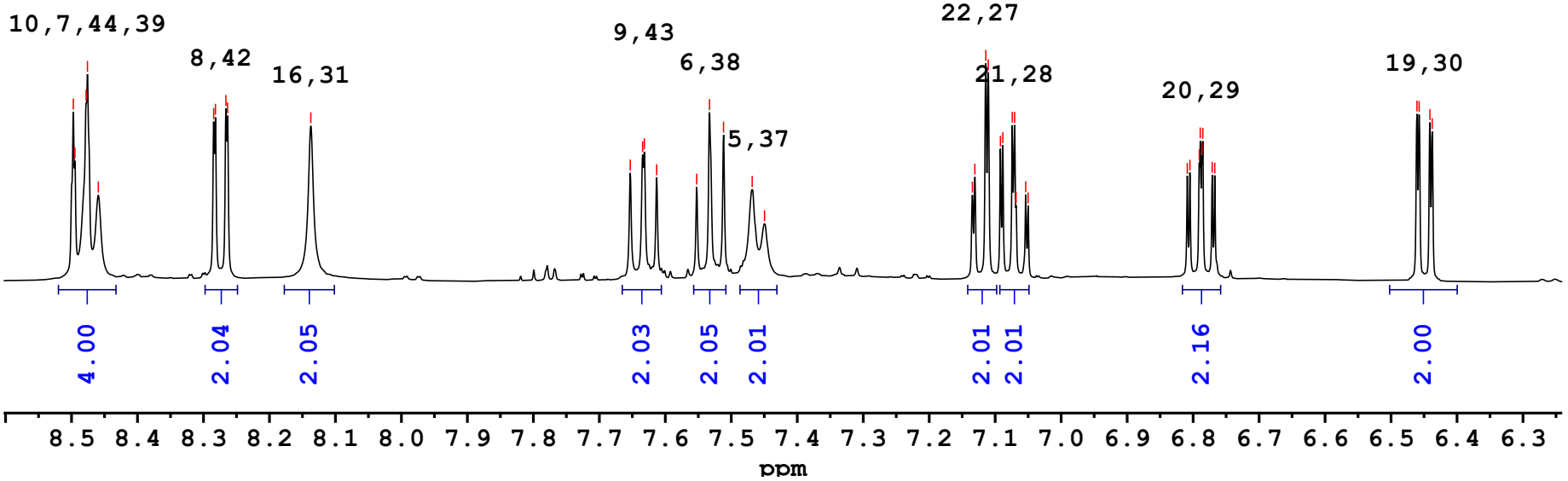
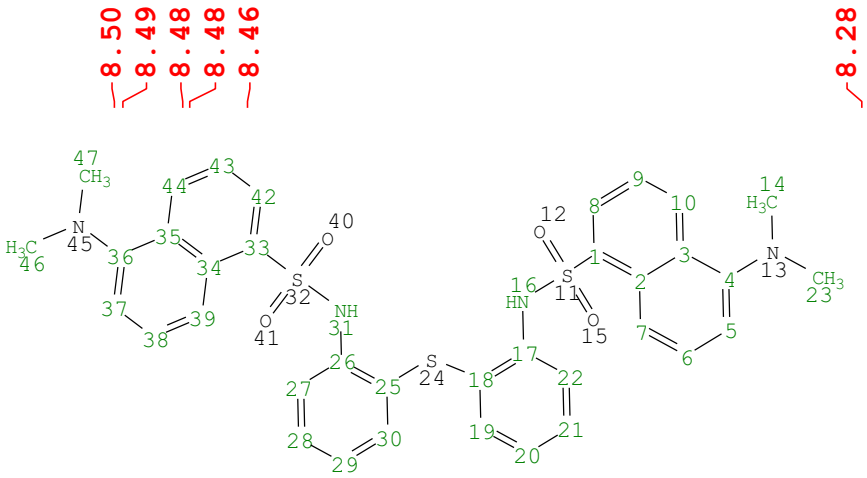


**Fig SX118** **L1 acetonitrile-d3 ligand + 1equiv. Cu(II)**




| | |
|---|---|
| NAME | AK-DR-165-Cu1.21.fid |
| DATE_TIME | 2024-12-21T02:05:29 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

7,10,39,44 (m)
8.48

8,42 (dd)
8.27
J(7.37, 1.04)

16,31 (s)
8.14

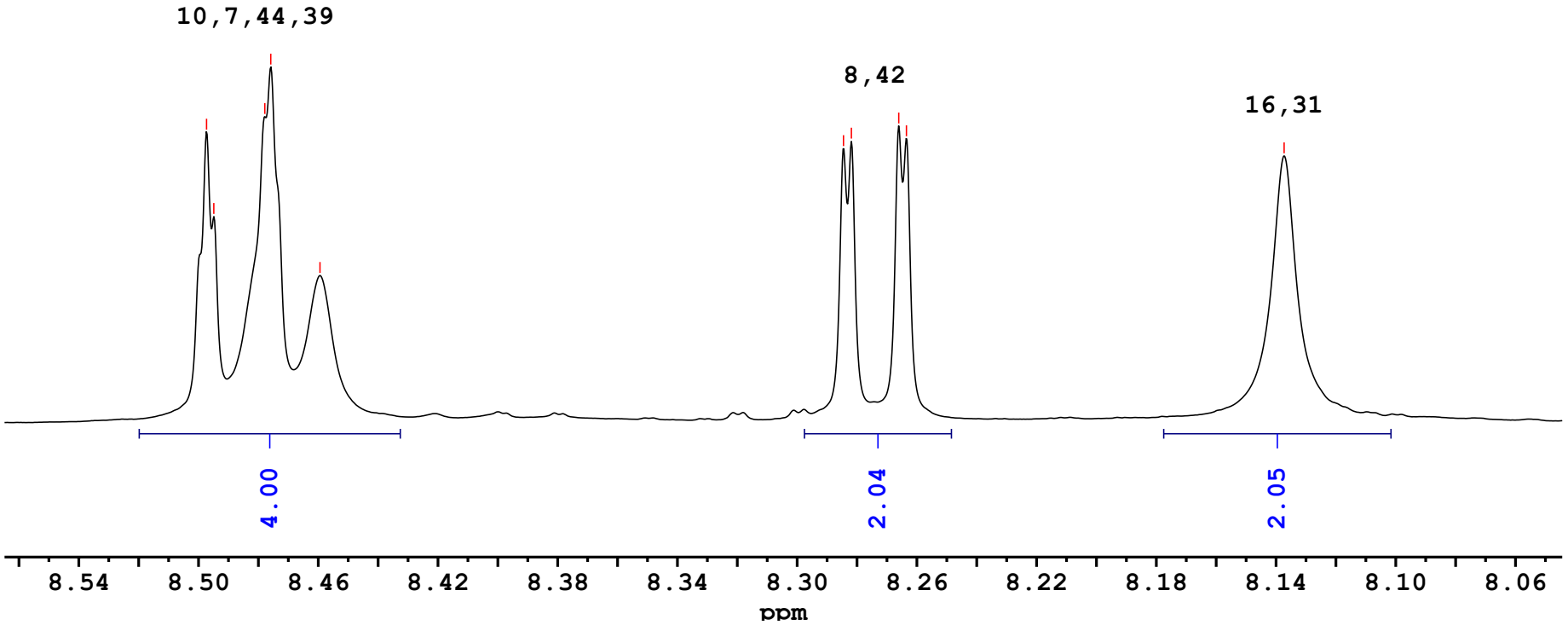
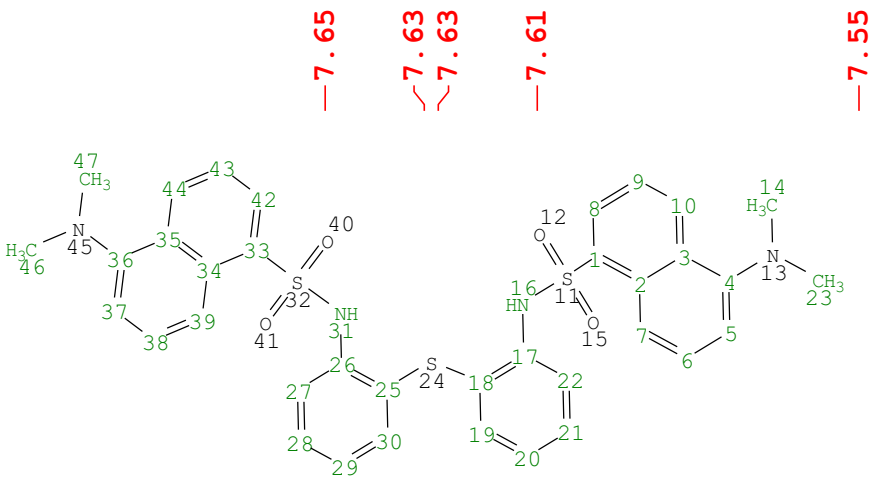


**Fig SX119** **L1 acetonitrile-d3 ligand + 1equiv. Cu(II)**




| | |
|---|---|
| NAME | AK-DR-165-Cu1.21.fid |
| DATE_TIME | 2024-12-21T02:05:29 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

9,43 (dd)
7.63
J(8.53, 7.47)

6,38 (m)
7.53

5,37 (d)
7.46
J(7.49)

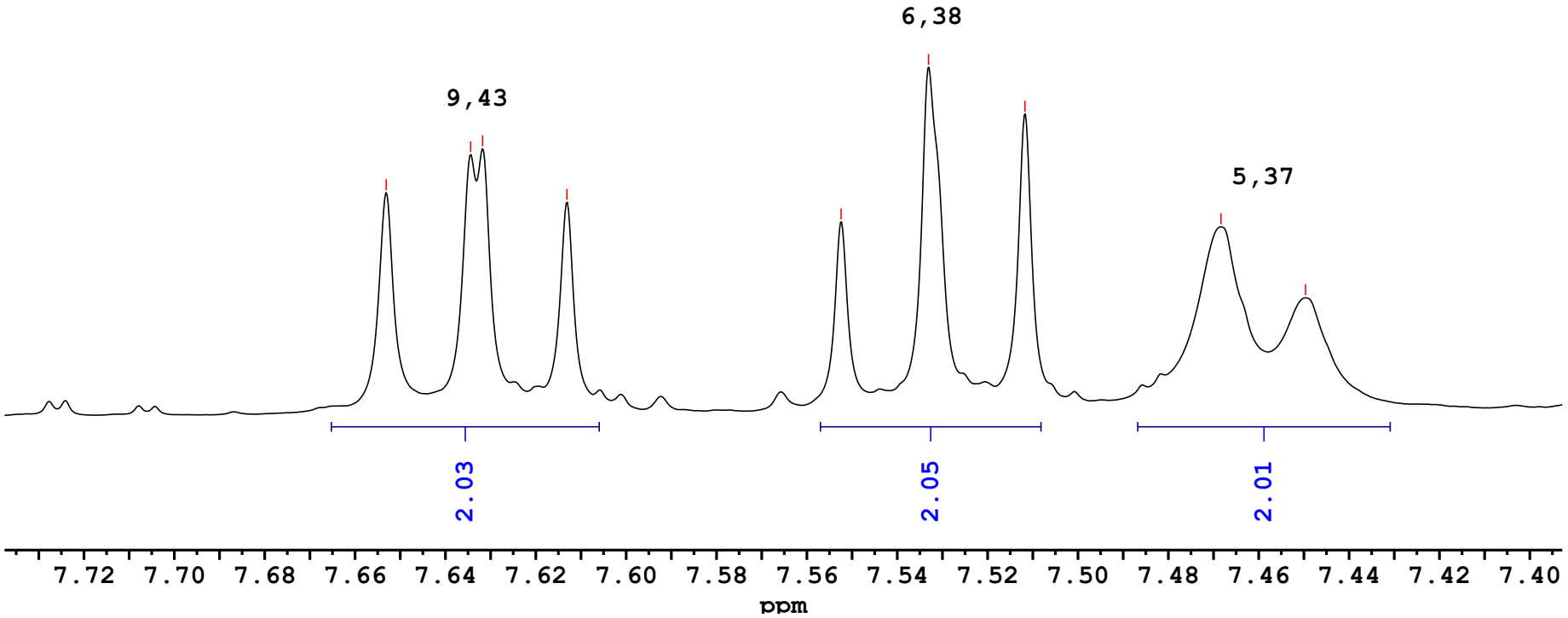
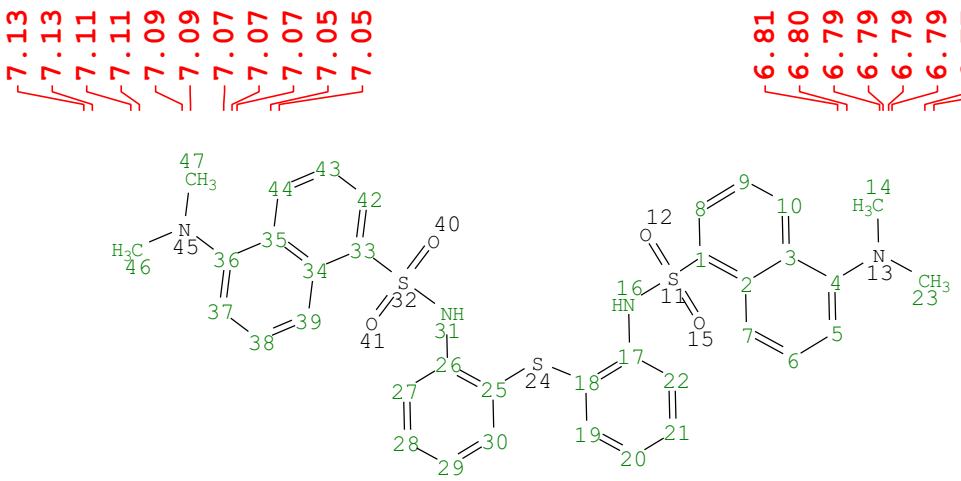


**Fig SX120** **L1 acetonitrile-d3 ligand + 1equiv. Cu(II)**







22,27 (dd)
7.12
J(8.13, 1.48)

21,28 (m)
7.07

20,29 (ddd)
6.79
J(7.84, 7.25, 1.58)

19,30 (dd)
6.45
J(7.88, 1.34)

| | |
|---|---|
| NAME | AK-DR-165-Cu1.21.fid |
| DATE_TIME | 2024-12-21T02:05:29 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

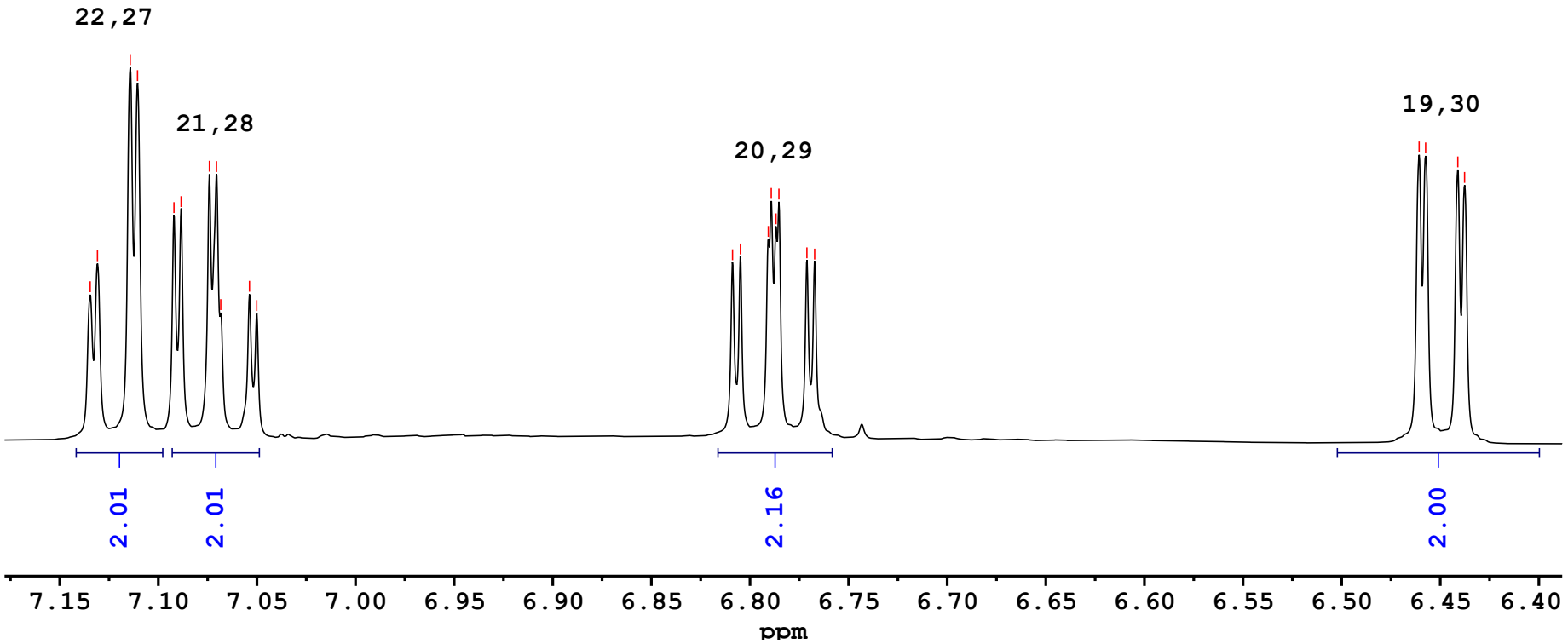
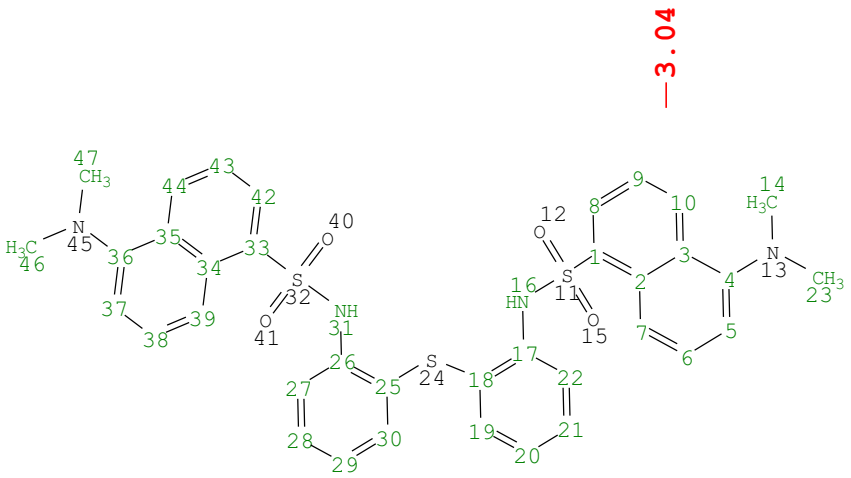


**Fig SX121** **L1 acetonitrile-d3 ligand + 1equiv. Cu(II)**




| | |
|---|---|
| NAME | AK-DR-165-Cu1.21.fid |
| DATE_TIME | 2024-12-21T02:05:29 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

14,23,46,47 (s)
3.04

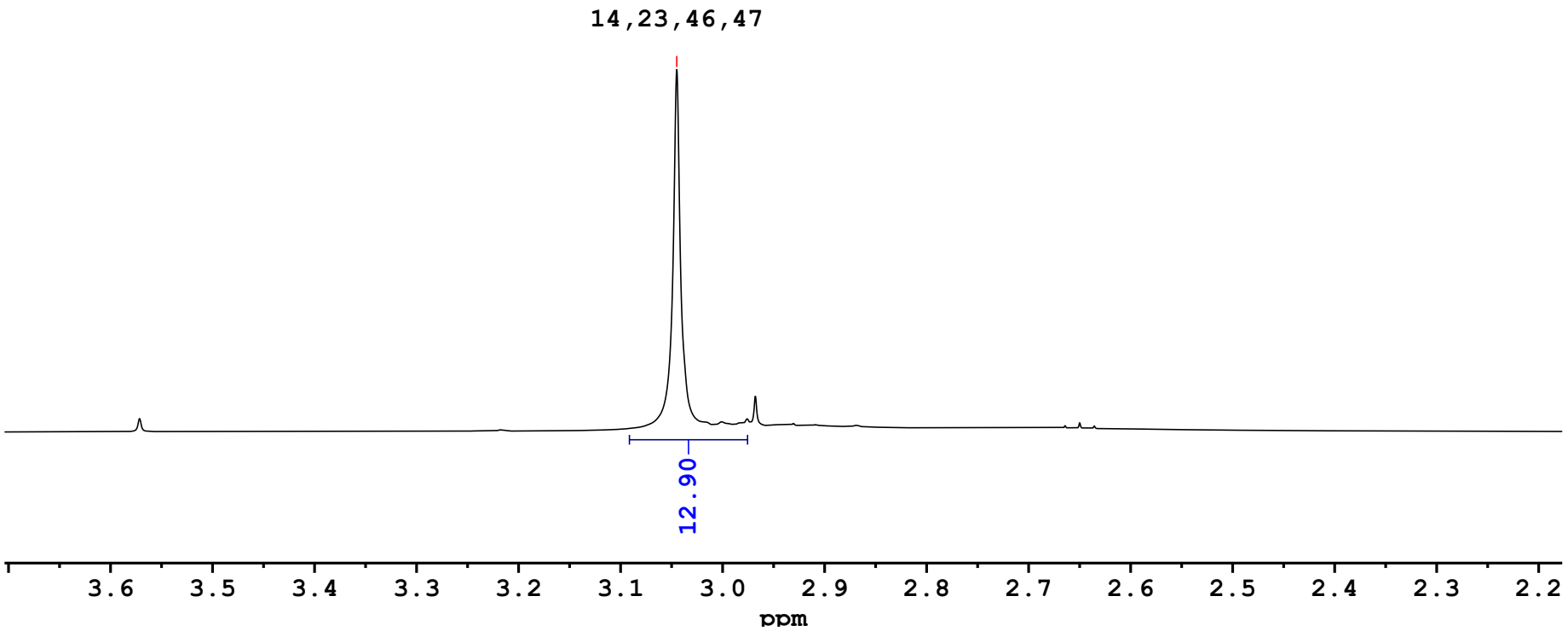
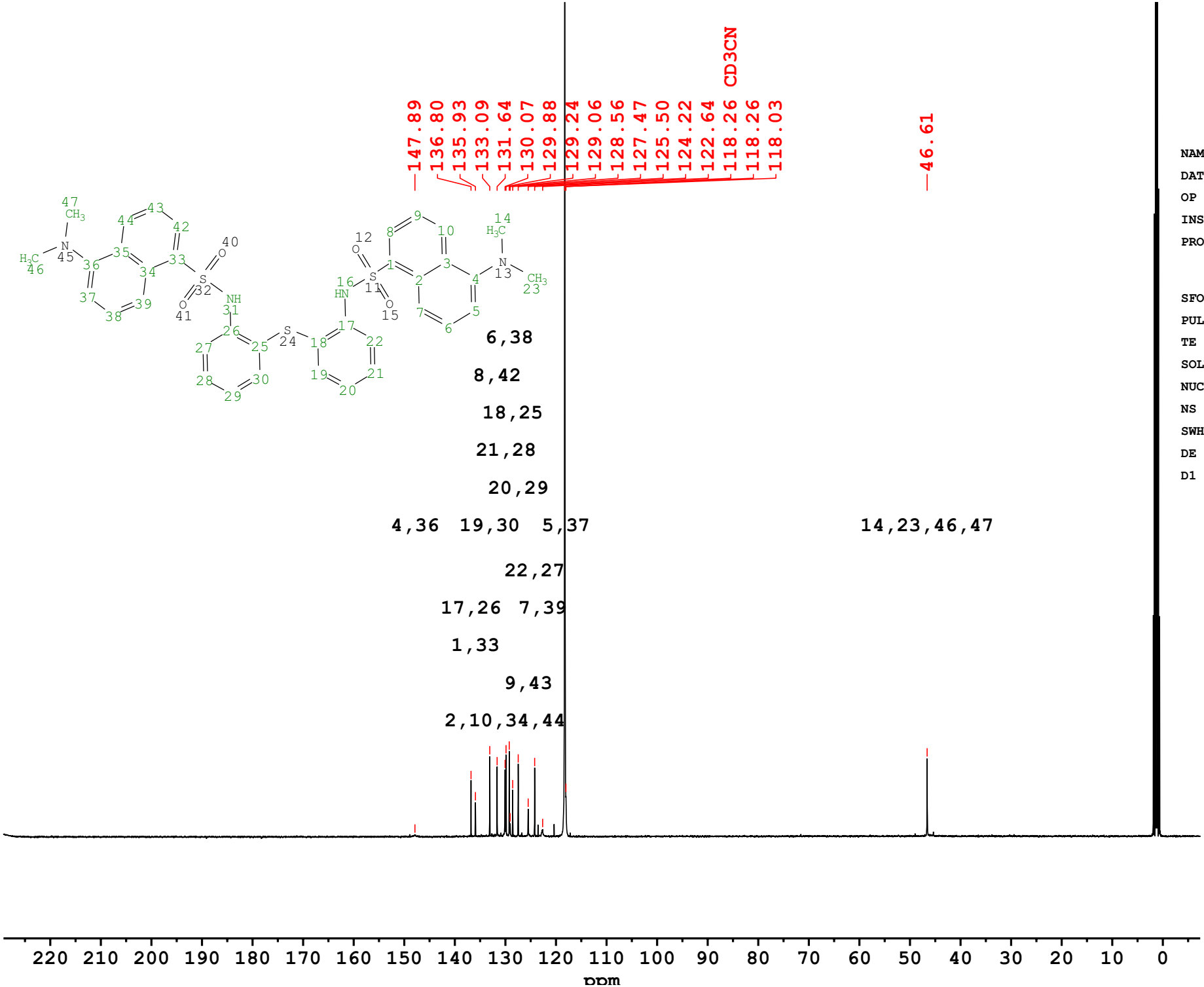


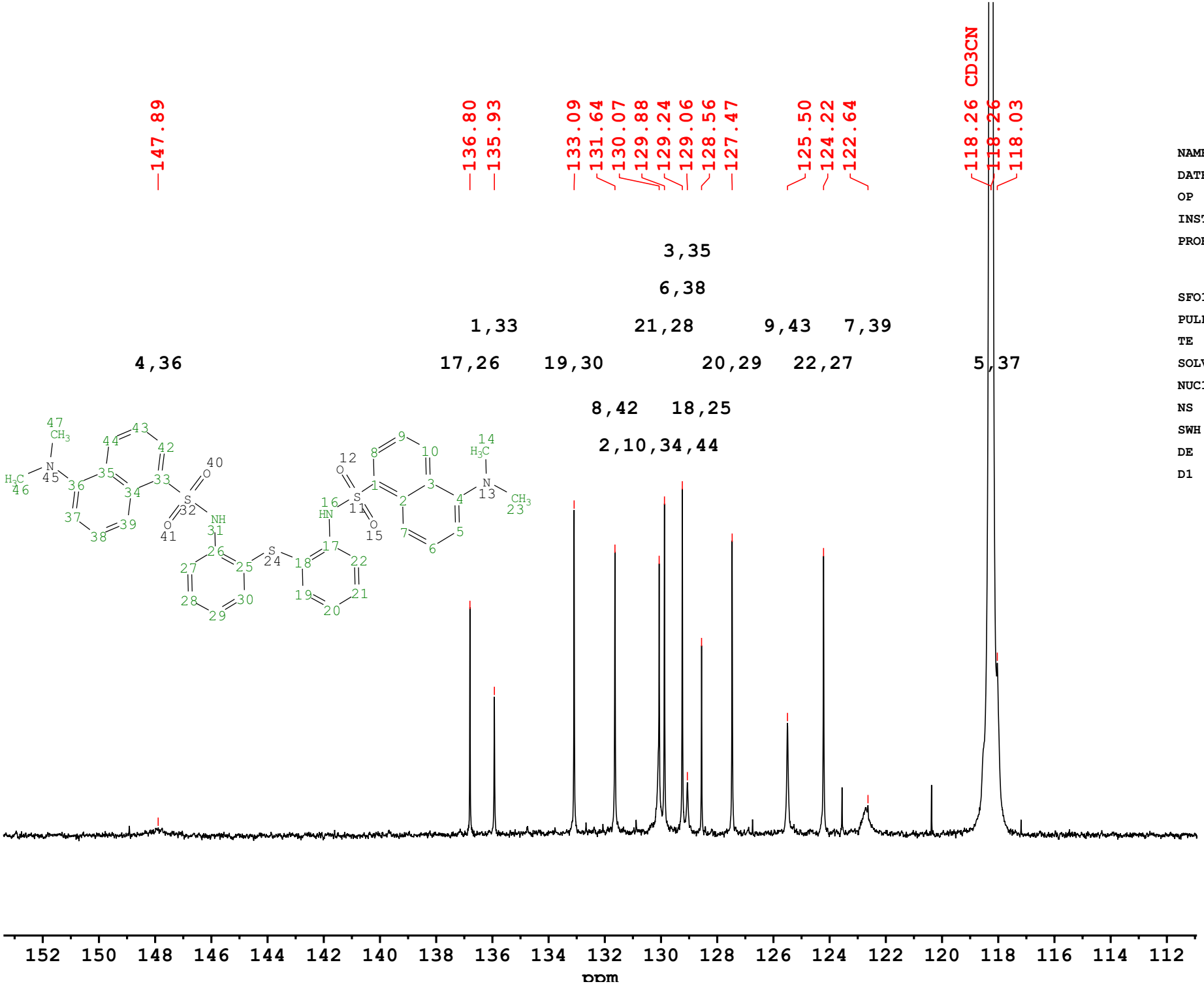
Fig SX122

# L1 acetonitrile-d3 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-Cu1.22.fid |
| DATE_TIME | 2024-12-21T07:12:43 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

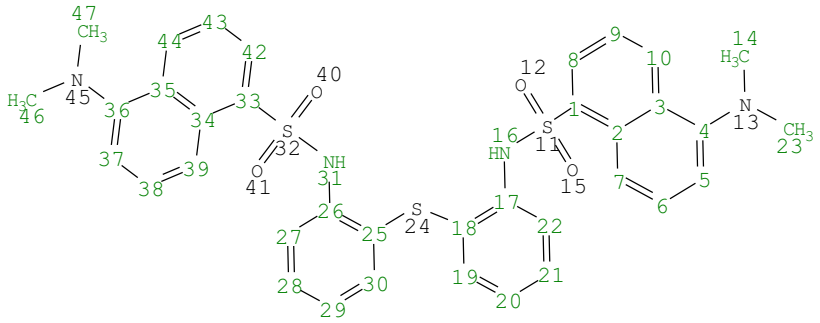
Fig SX123 L1 acetonitrile-d3 ligand + 1equiv. Cu(II)




NAME AK-DR-165-Cu1.22.fid
DATE_TIME 2024-12-21T07:12:43
OP Dessislava.Gerginova
INSTRUM Avance Neo 400
PROBHD Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N)
SFO1 150.9188042 Hz
PULPROG zgdc30
TE 298.0 K
SOLVENT CD3CN
NUC1 13C
NS 8192
SWH 36057.692 Hz
DE 6.50 usec
D1 1.5000 sec

**Fig SX124** **L1 acetonitrile-d3 ligand + 1equiv. Cu(II)**

136.80 135.93 133.09 131.64 130.07 129.88 129.24 129.06 128.56 127.47 125.50 124.22 122.64



| | |
|---|---|
| NAME | AK-DR-165-Cu1.22.fid |
| DATE_TIME | 2024-12-21T07:12:43 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

2,10,34,44

1,33 18,25

17,26 19,30 8,42 21,28 20,29 9,43 22,27 7,39

6,38

3,35

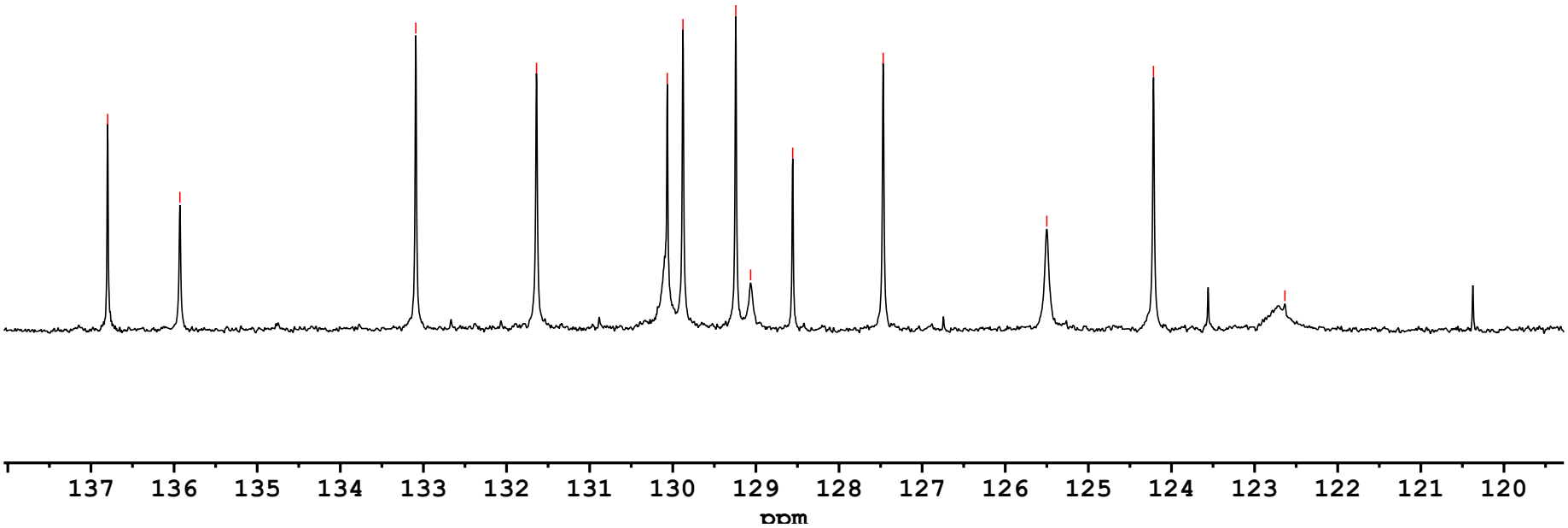
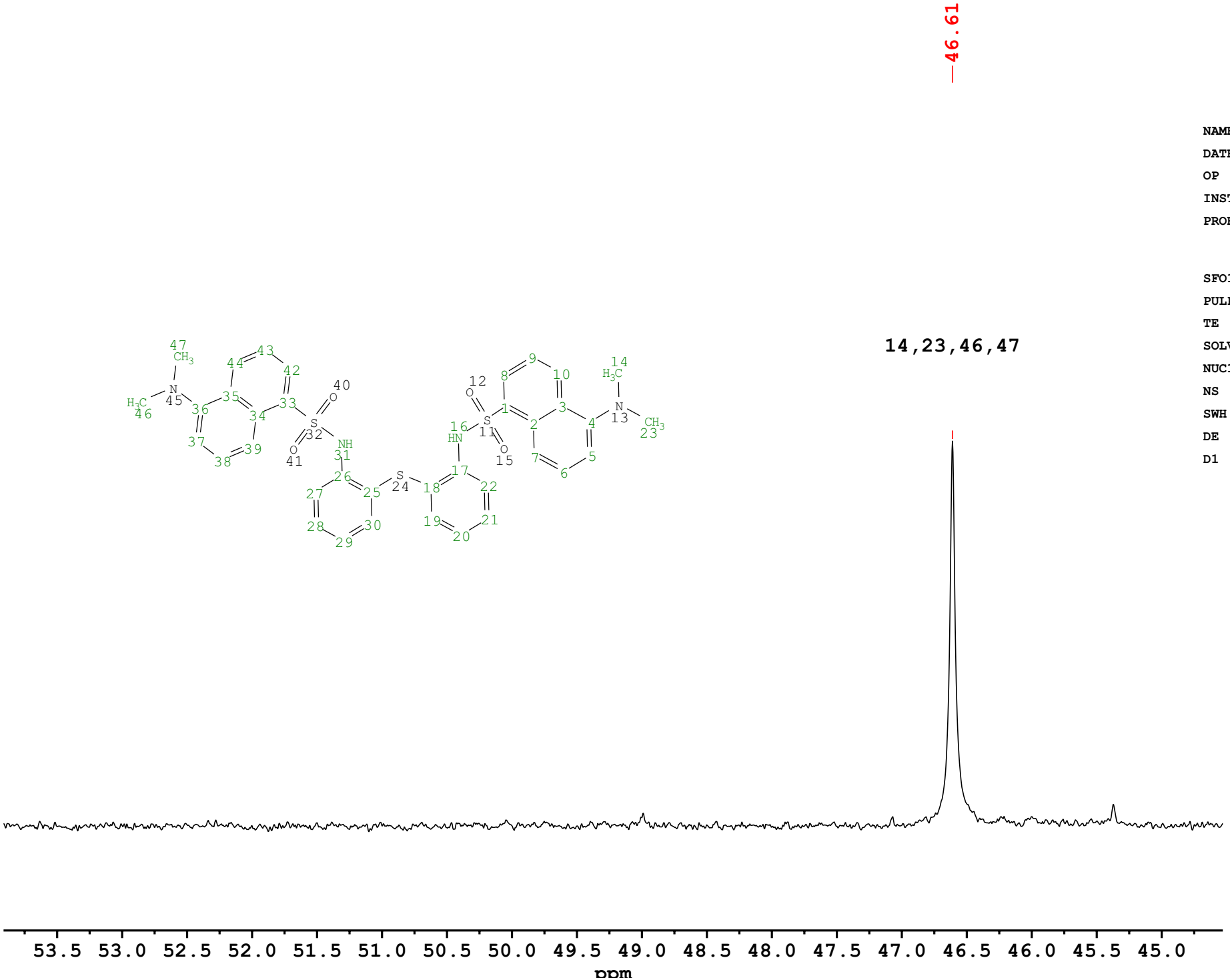


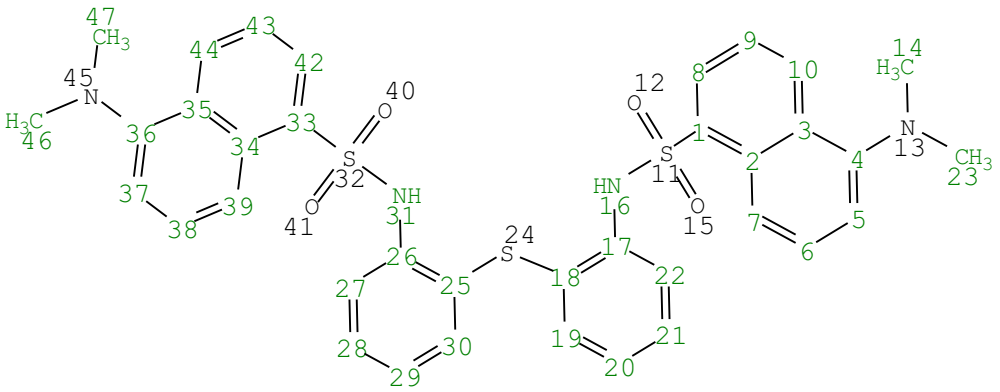
**Fig SX125** **L1 acetonitrile-d3 ligand + 1equiv. Cu(II)**




| | |
|---|---|
| NAME | AK-DR-165-Cu1.22.fid |
| DATE_TIME | 2024-12-21T07:12:43 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

**Fig SX126** **L1 acetonitrile-d3 ligand + 1equiv. Cu(II)**



131.8 130.4 128.8 128.6 128.0 126.2 124.3 123.0 116.8

45.4 39.5 DMSO-d6

0.4 0.2 -0.0

| | |
|---|---|
| NAME | AK-DR-165-Cu1.22.fid |
| DATE_TIME | 2024-12-21T07:12:43 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9319844 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 35714.286 Hz |
| DE | 18.00 usec |
| D1 | 1.5000 sec |

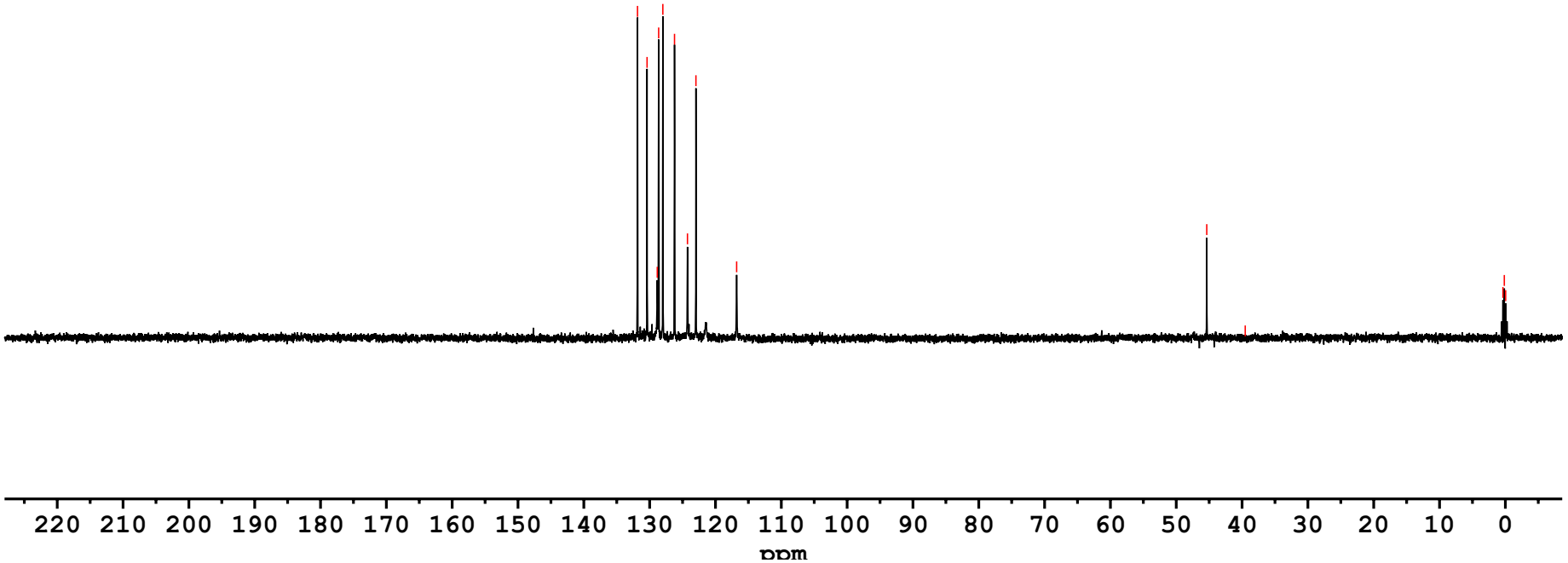


Fig SX127 L1 acetonitrile-d3 ligand + 1equiv. Cu(II)

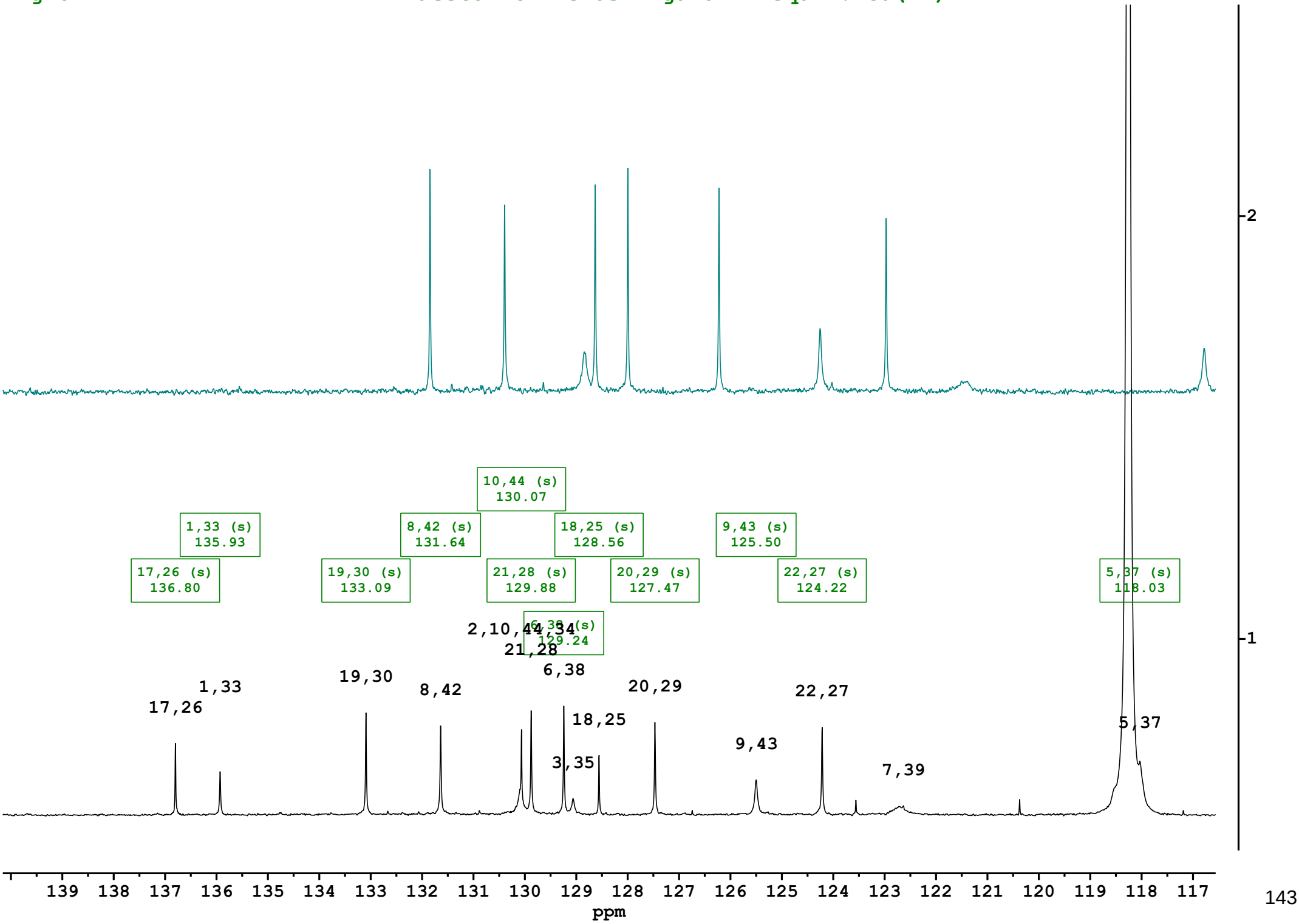
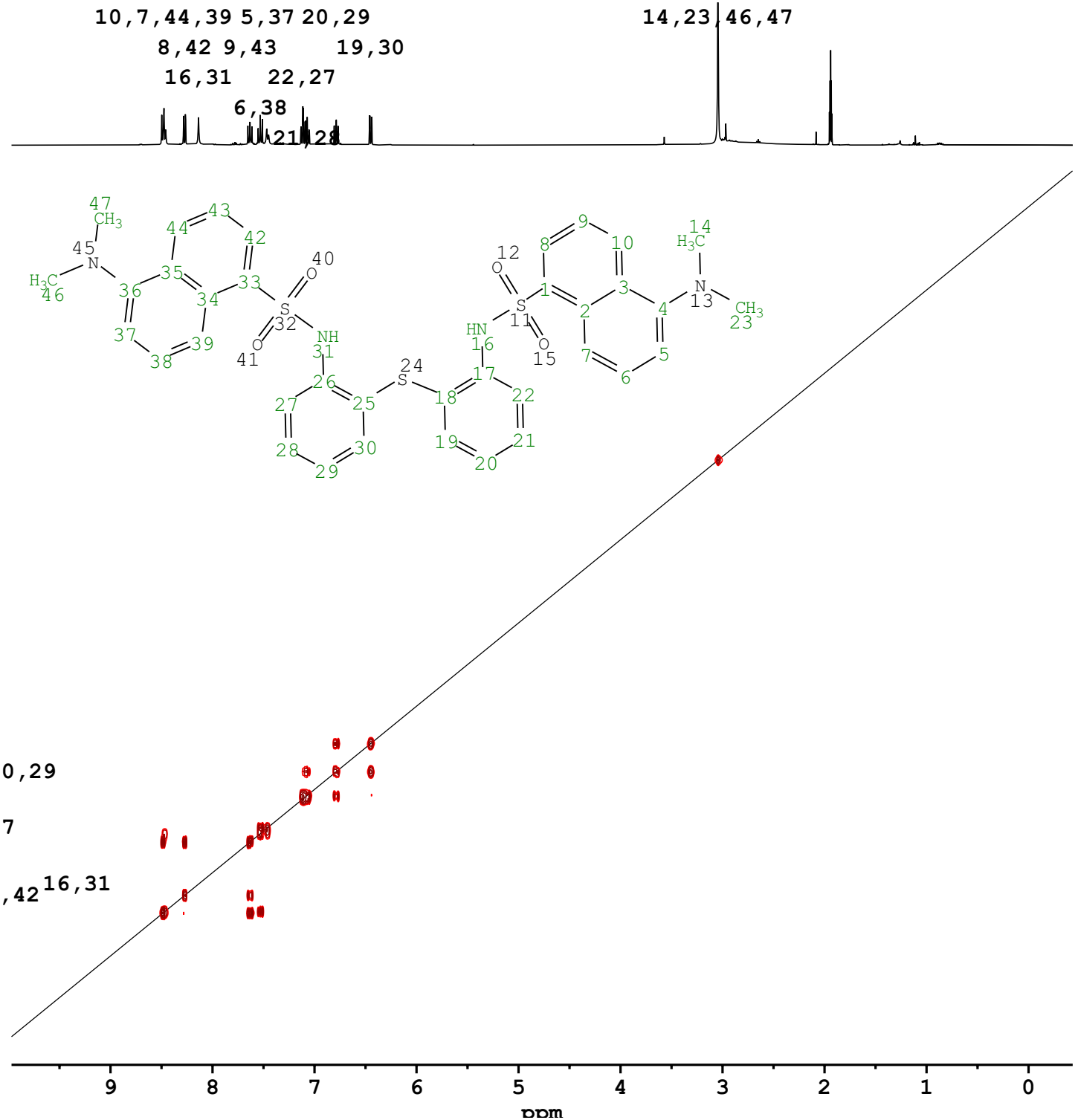


Fig SX128

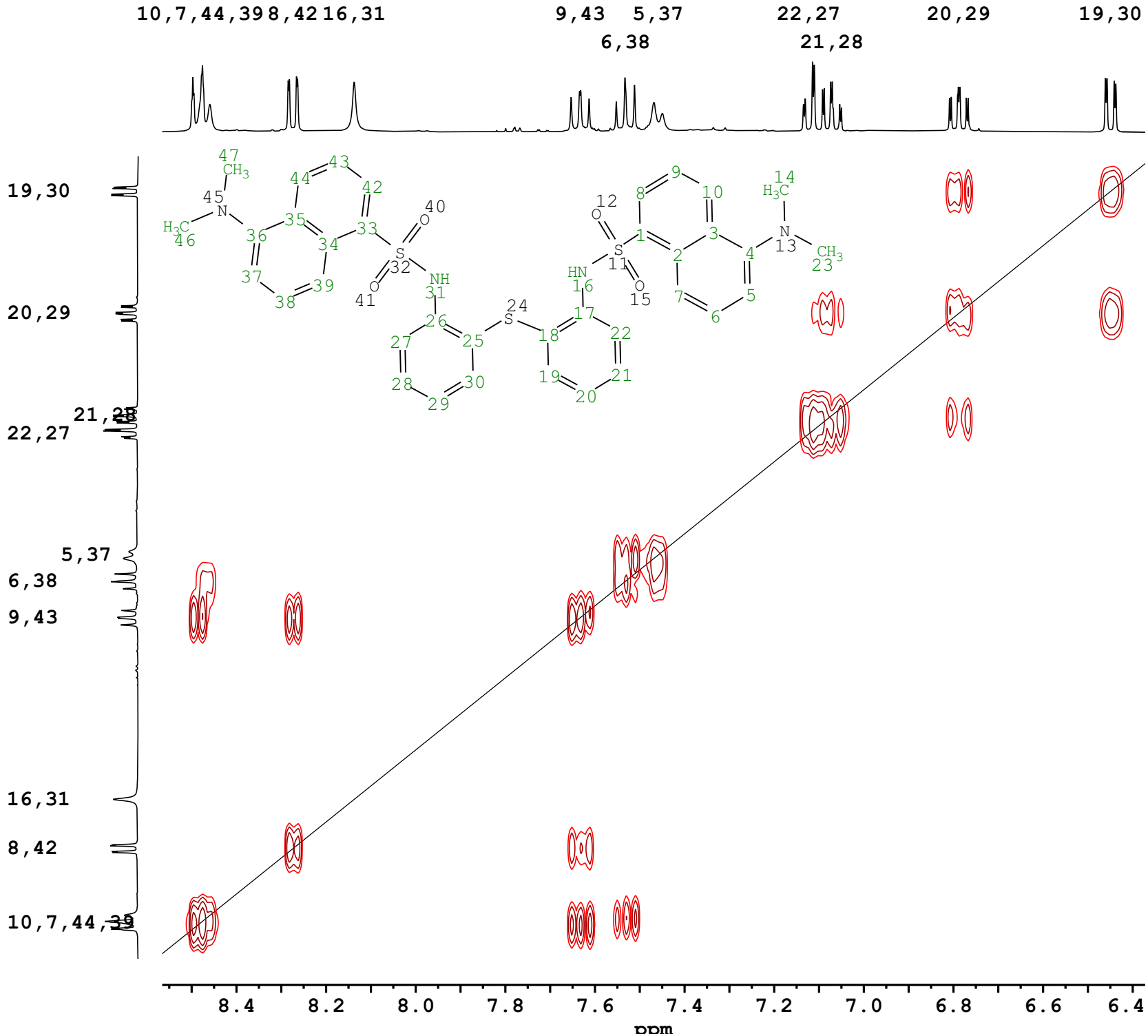
# L1 acetonitrile-d3 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-Cu1.24.ser |
| DATE_TIME | 2024-12-21T08:22:39 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 4 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 0.9914 sec |

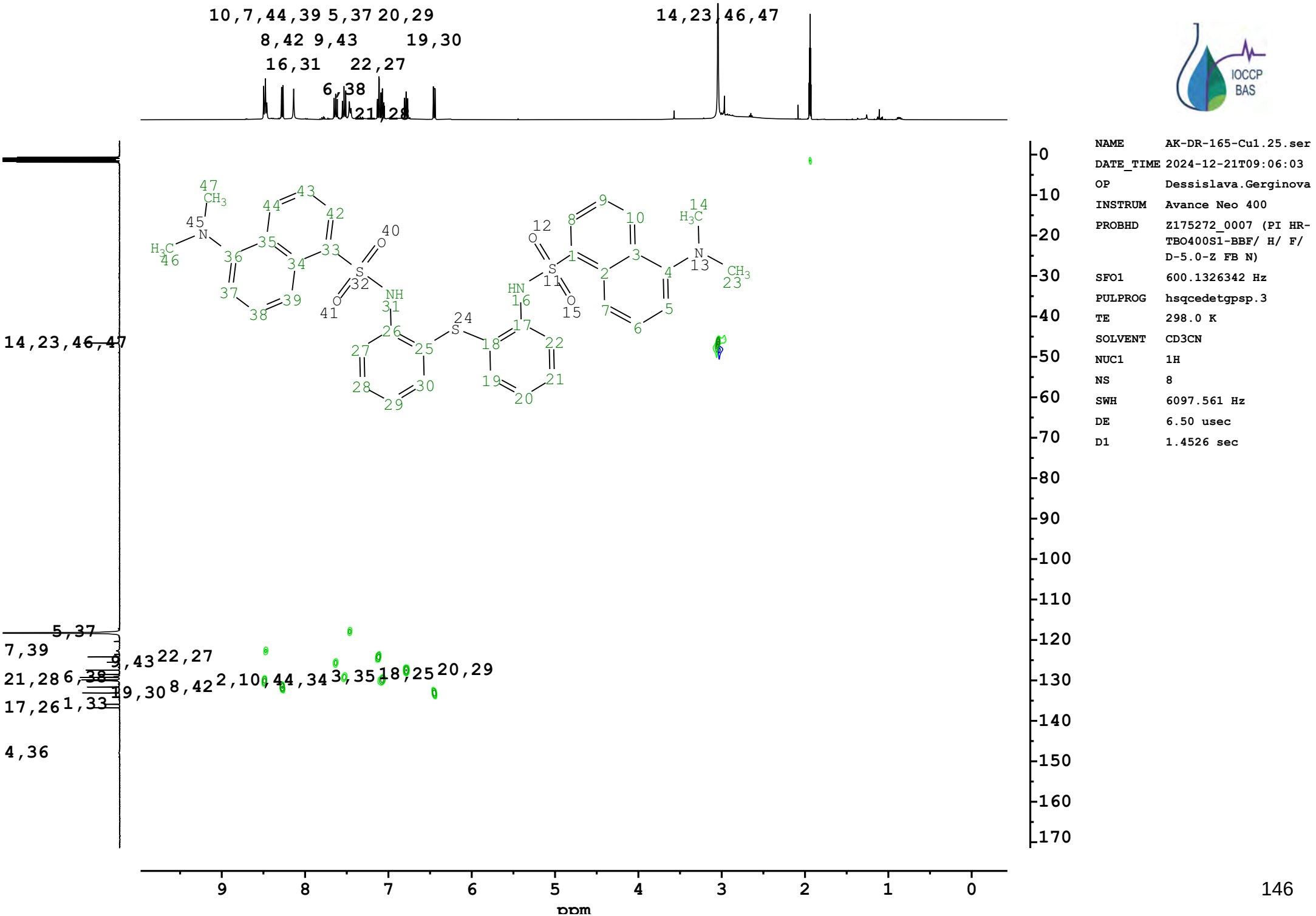
Fig SX129

L1 acetonitrile-d3 ligand + 1equiv. Cu(II)



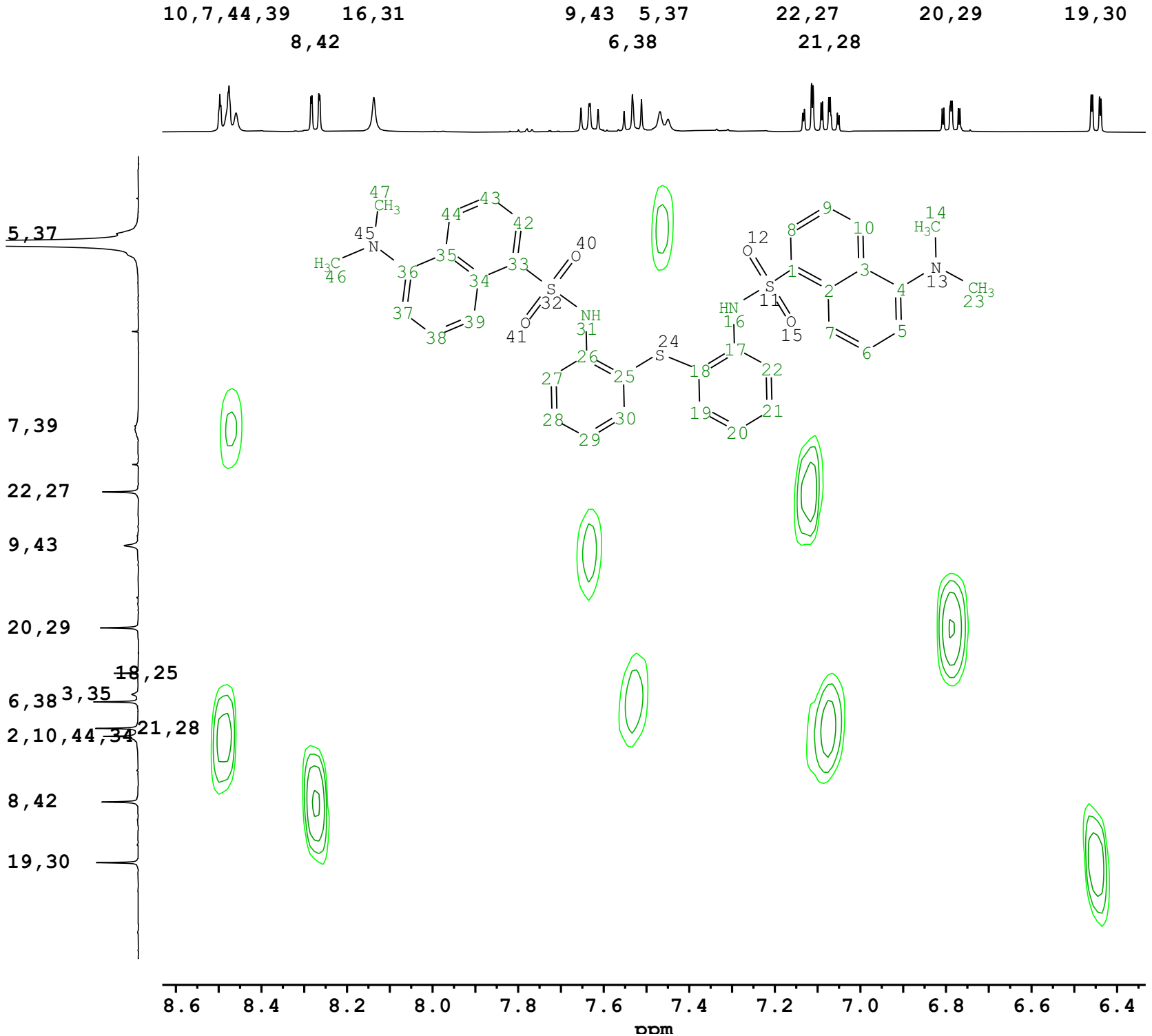

| | |
|---|---|
| NAME | AK-DR-165-Cu1.24.ser |
| DATE_TIME | 2024-12-21T08:22:39 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 4 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 0.9914 sec |

Fig SX130 L1 acetonitrile-d3 ligand + 1equiv. Cu(II)



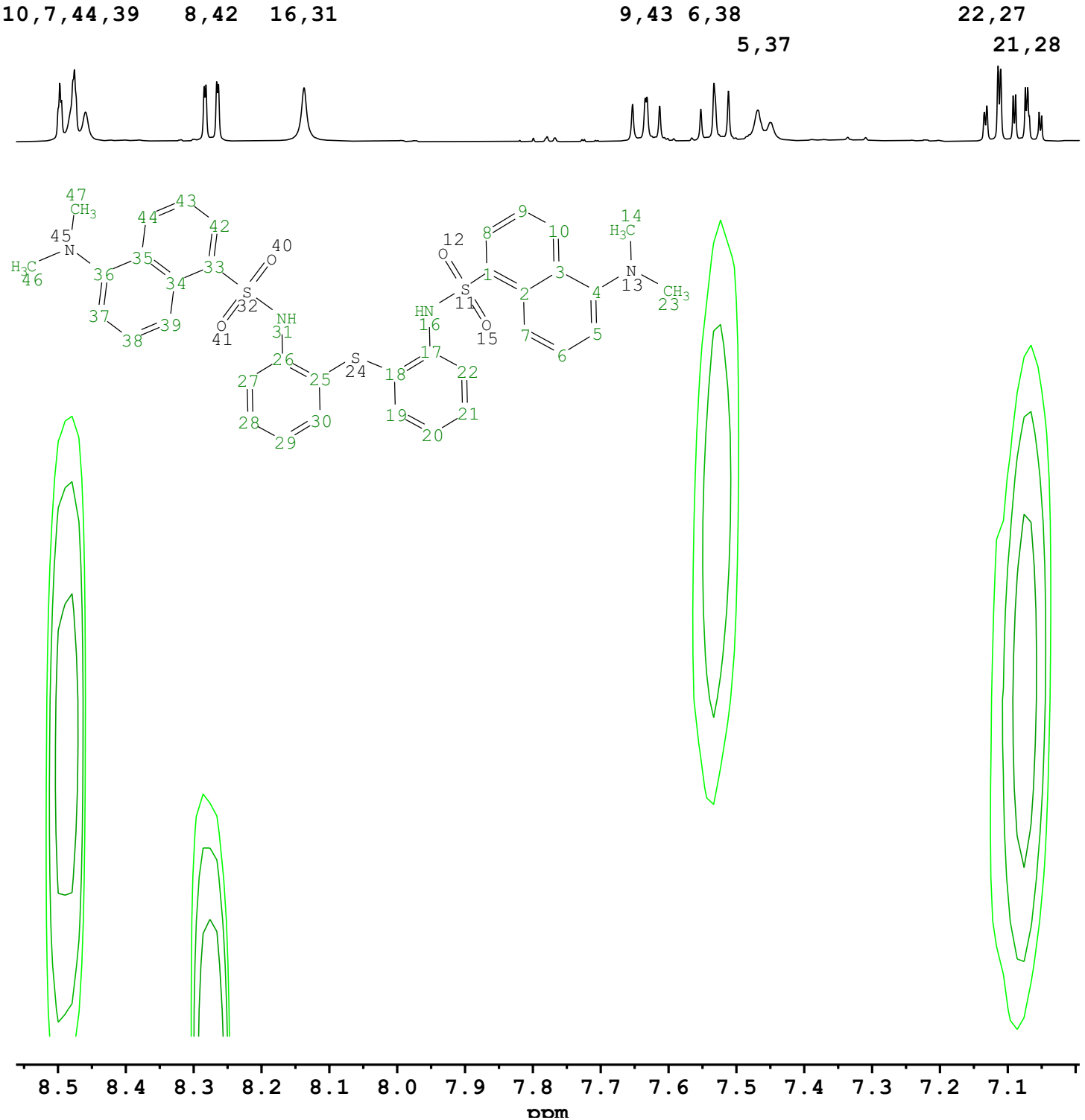

| | |
|---|---|
| NAME | AK-DR-165-Cu1.25.ser |
| DATE_TIME | 2024-12-21T09:06:03 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX131 L1 acetonitrile-d3 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-Cu1.25.ser |
| DATE_TIME | 2024-12-21T09:06:03 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

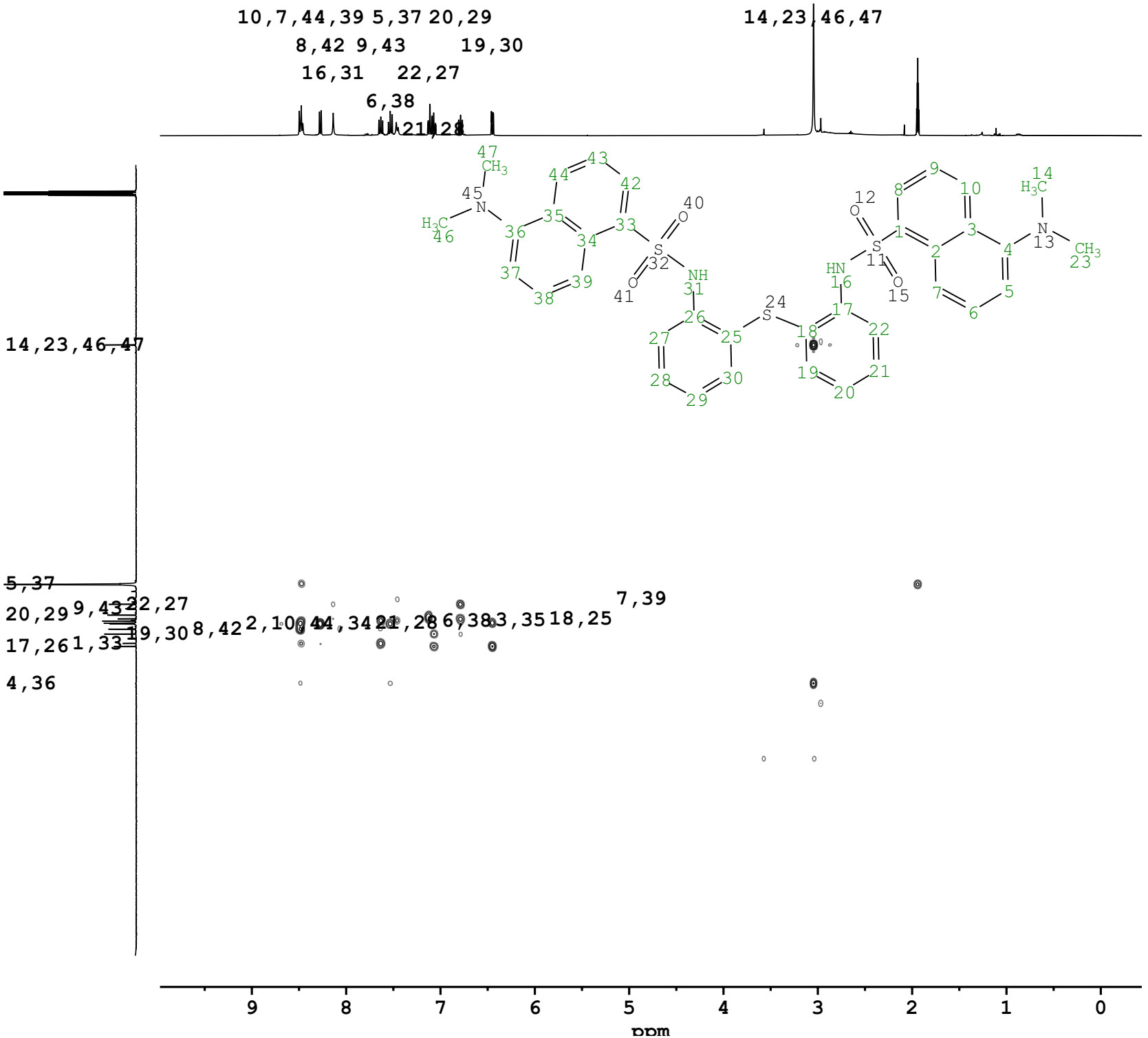
Fig SX132 L1 acetonitrile-d3 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-Cu1.25.ser |
| DATE_TIME | 2024-12-21T09:06:03 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

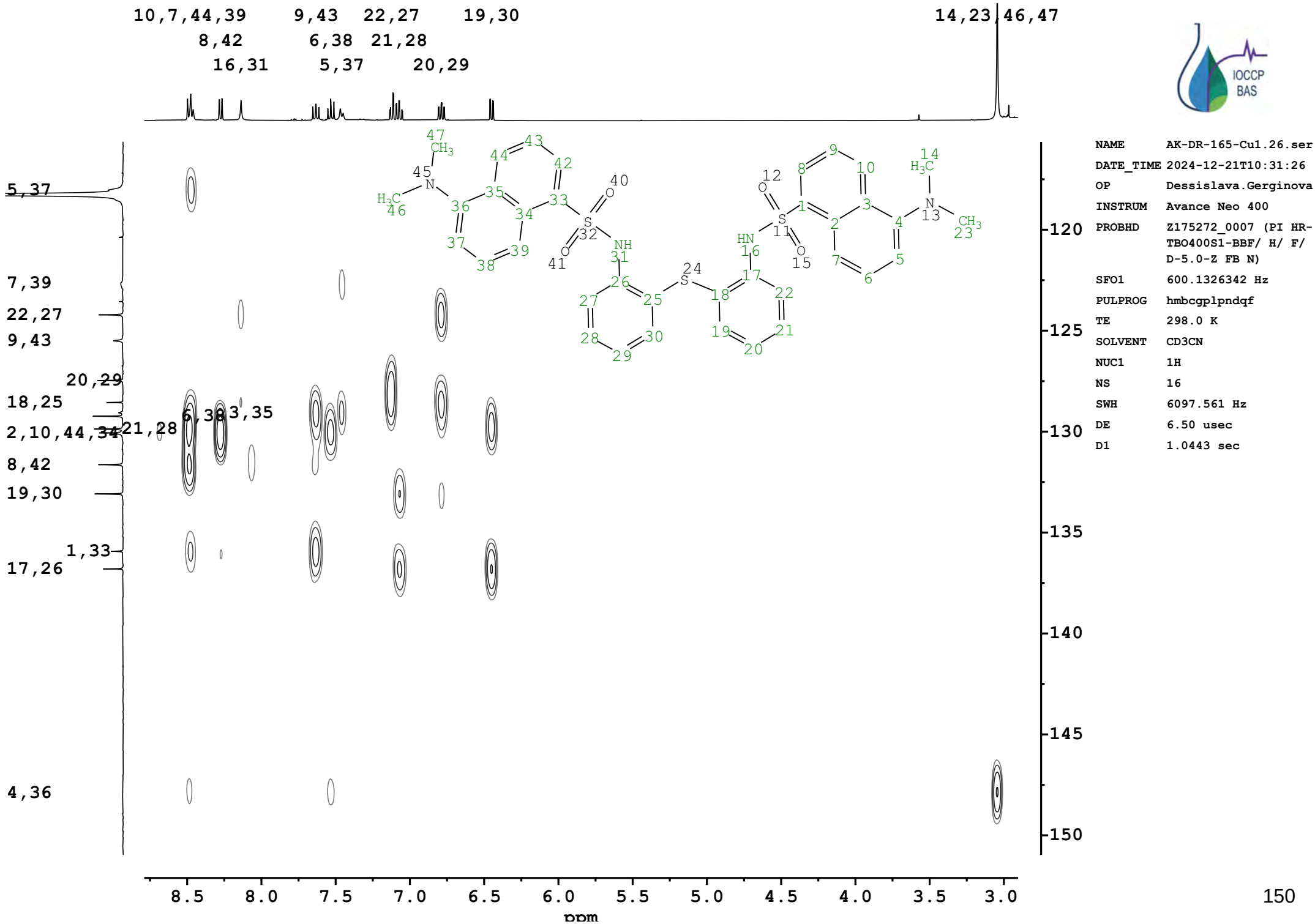
Fig SX133

# L1 acetonitrile-d3 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-Cu1.26.ser |
| DATE_TIME | 2024-12-21T10:31:26 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

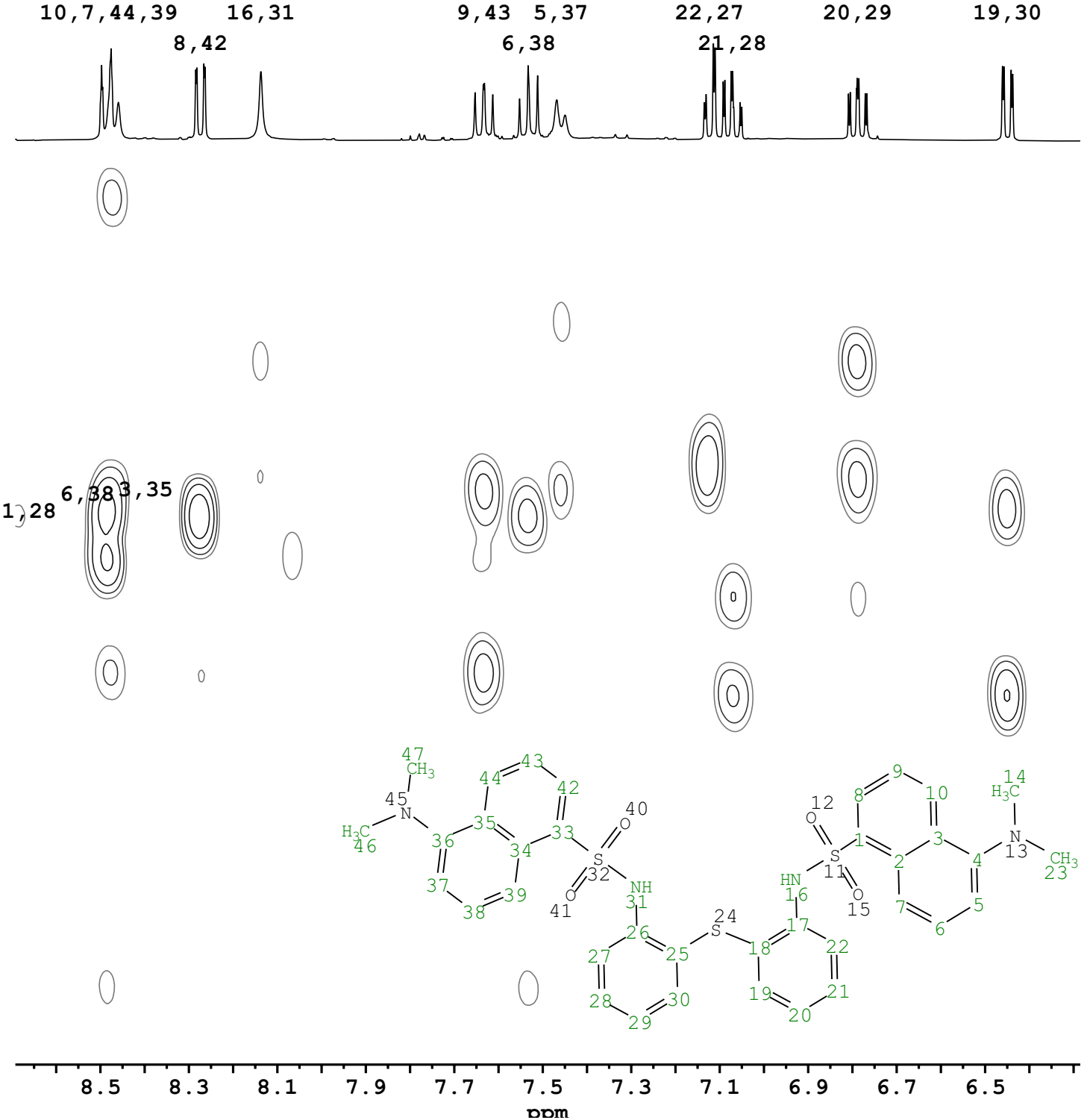
**Fig SX134** **L1 acetonitrile-d3 ligand + 1equiv. Cu(II)**




| | |
|---|---|
| NAME | AK-DR-165-Cu1.26.ser |
| DATE_TIME | 2024-12-21T10:31:26 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

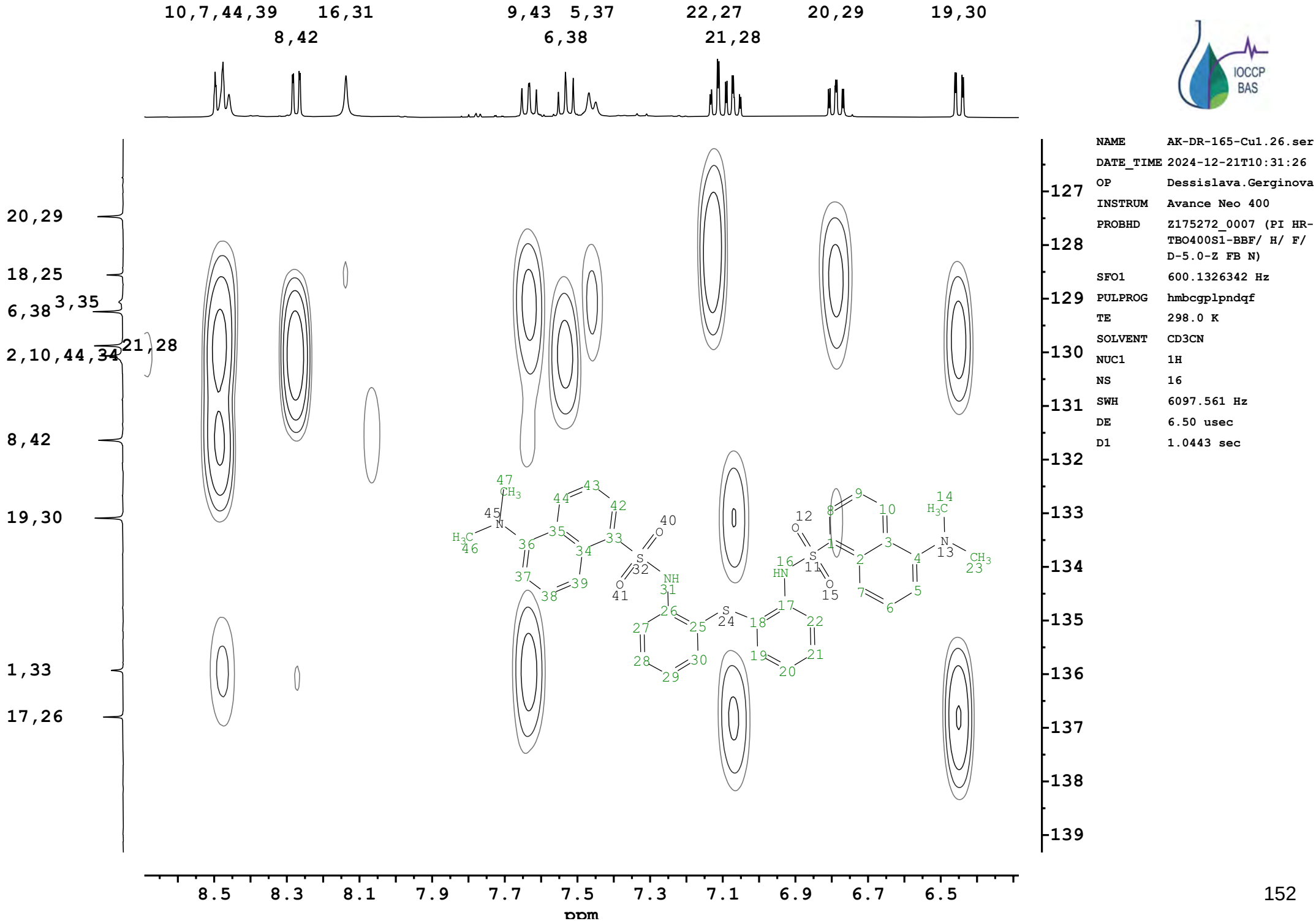
Fig SX135

L1 acetonitrile-d3 ligand + 1equiv. Cu(II)



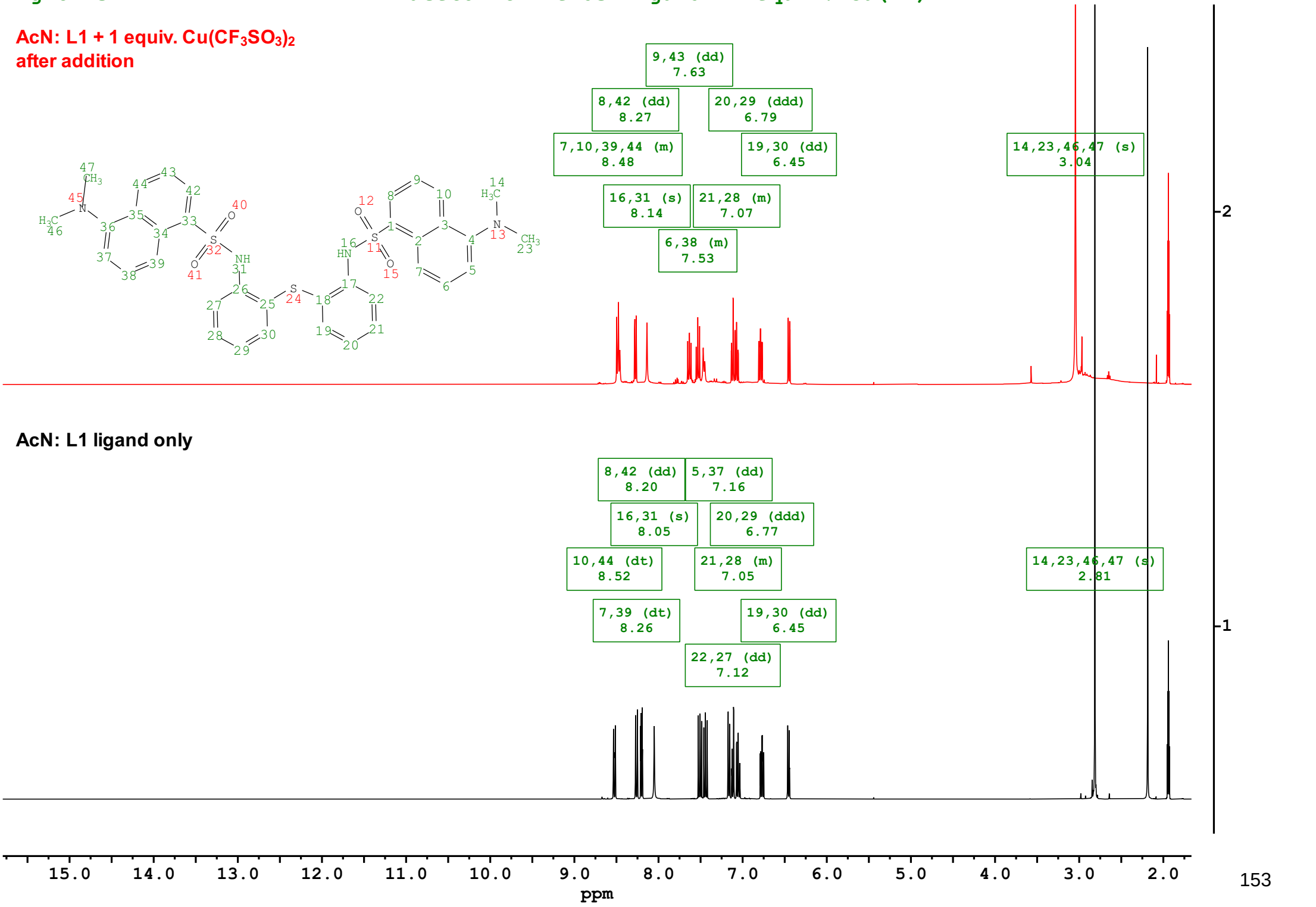

| | |
|---|---|
| NAME | AK-DR-165-Cu1.26.ser |
| DATE_TIME | 2024-12-21T10:31:26 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX136 L1 acetonitrile-d3 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-Cu1.26.ser |
| DATE_TIME | 2024-12-21T10:31:26 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX137 L1 acetonitrile-d3 ligand + 1equiv. Cu(II)



**AcN: L1 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition**




**AcN: L1 ligand only**



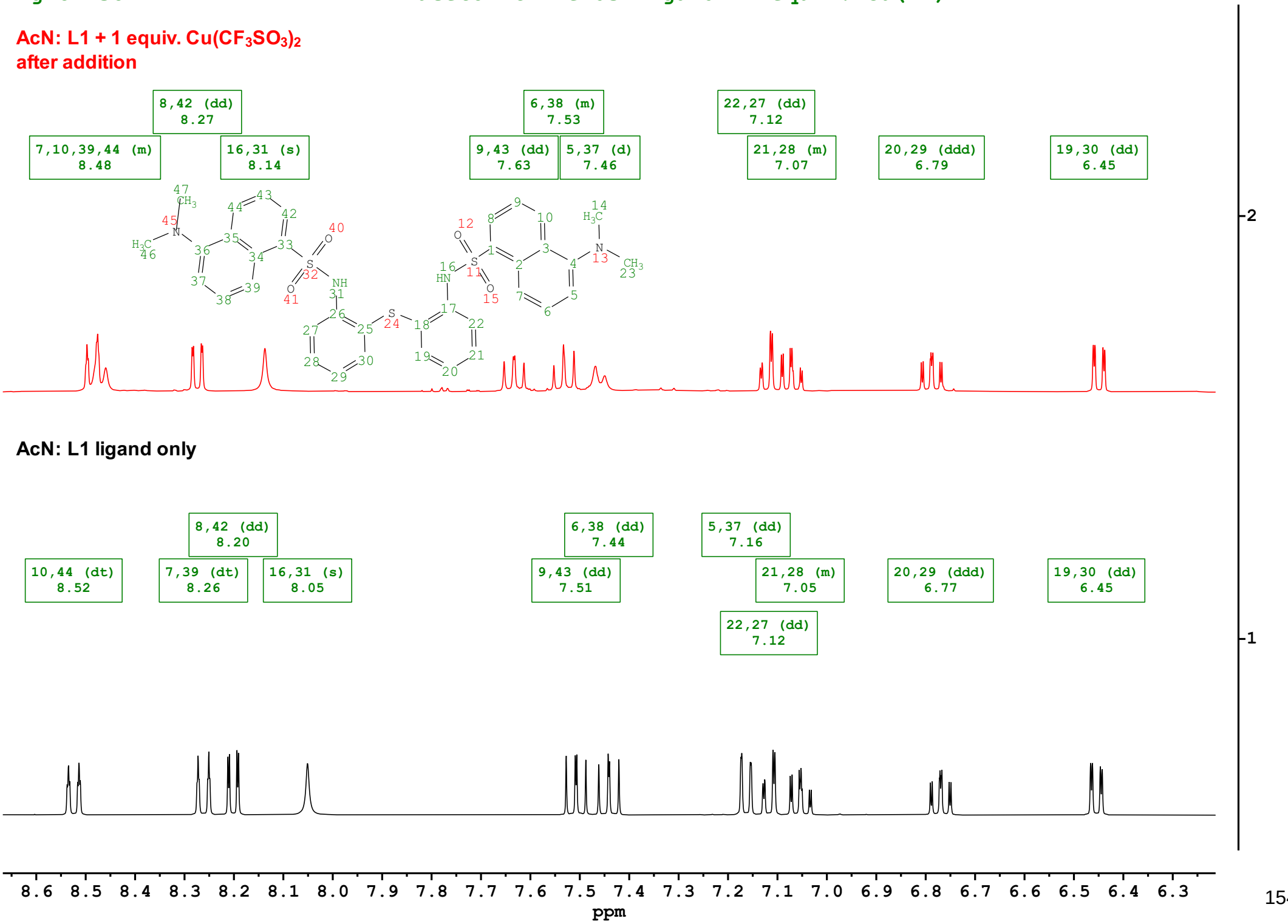
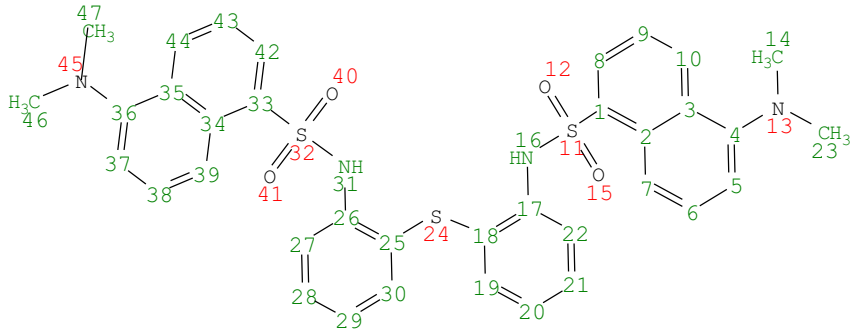



Fig SX139 L1 acetonitrile-d3 ligand + 1equiv. Cu(II)

**AcN: L1 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition**



14,23,46,47 (s)
3.04

**AcN: L1 ligand only**

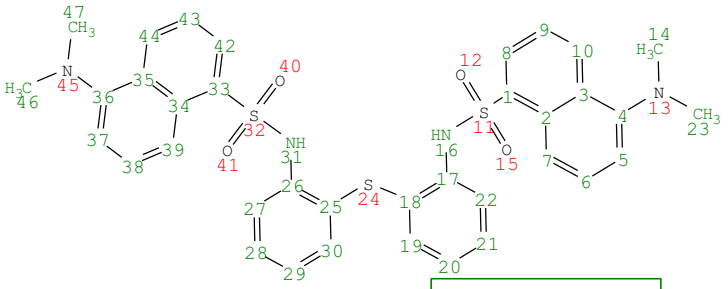
14,23,46,47 (s)
2.81

3.50 3.45 3.40 3.35 3.30 3.25 3.20 3.15 3.10 3.05 3.00 2.95 2.90 2.85 2.80
ppm

Fig SX140

L1 acetonitrile-d3 ligand + 1equiv. Cu(II)

AcN: L1 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition



18,25 (s) 128.56

21,28 (s) 129.88

19,30 (s) 133.09

4,36 (s) 147.89

20,29 (s) 127.47

22,27 (s) 124.22

17,26 (s) 136.80

5,37 (s) 118.03

1,33 (s) 135.93

14,23,46,47 (s) 46.61

AcN: L1 ligand only

6,38 (s) 129.49

10,44 (s) 131.96

22,27 (s) 123.90

4,36 (s) 152.95

18,25 (s) 128.32

14,23,46,47 (s) 45.63

8,42 (s) 131.21

9,43 (s) 124.12

19,30 (s) 133.15

5,37 (s) 116.41

2

1

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

ppm

Fig SX141 L1 acetonitrile-d3 ligand + 1equiv. Cu(II)

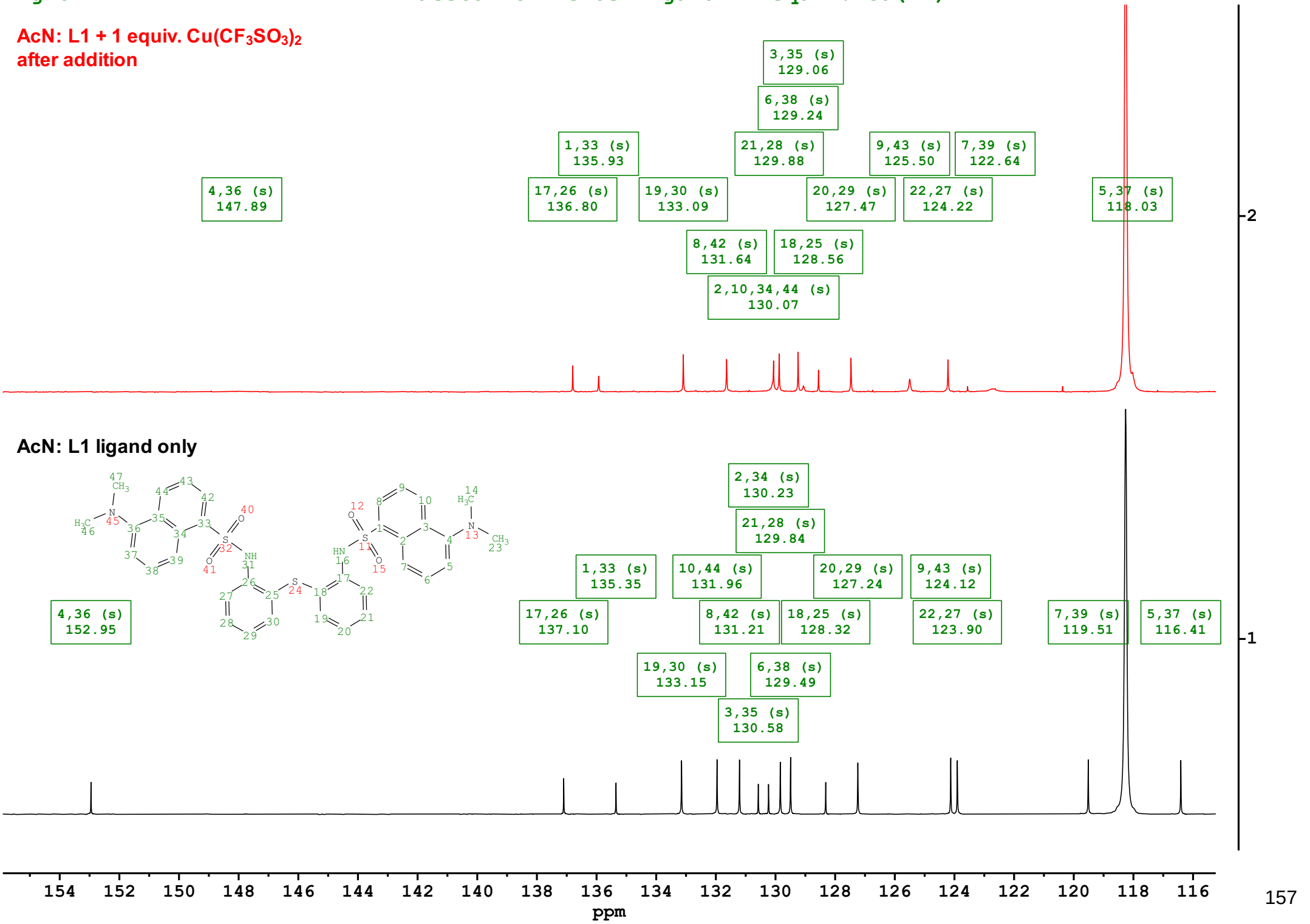
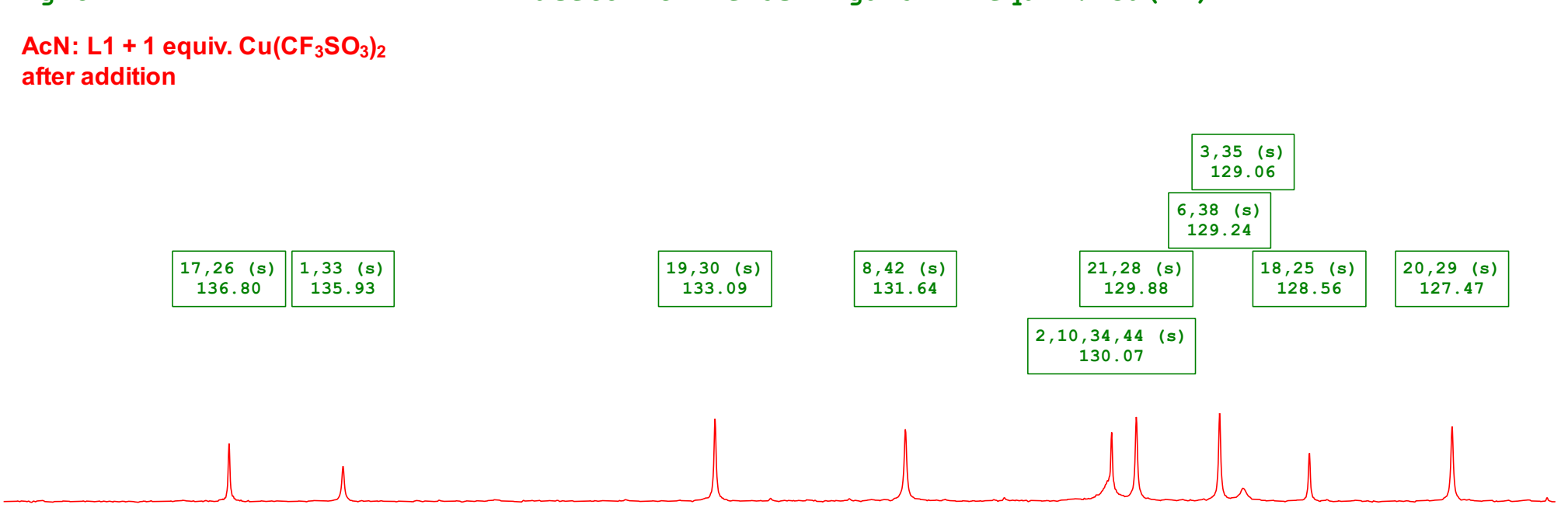


Fig SX142 L1 acetonitrile-d3 ligand + 1equiv. Cu(II)

AcN: L1 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition




AcN: L1 ligand only

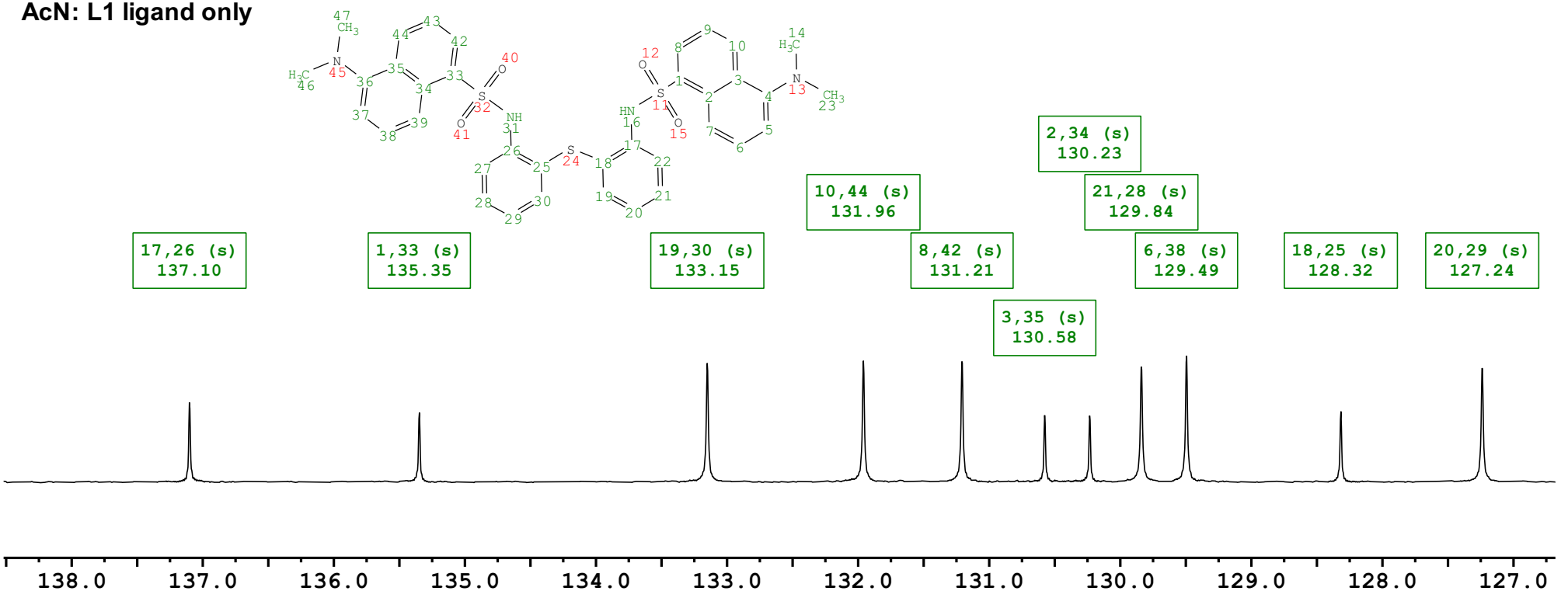


Fig SX143 L1 acetonitrile-d3 ligand + 1equiv. Cu(II)

AcN: L1 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition

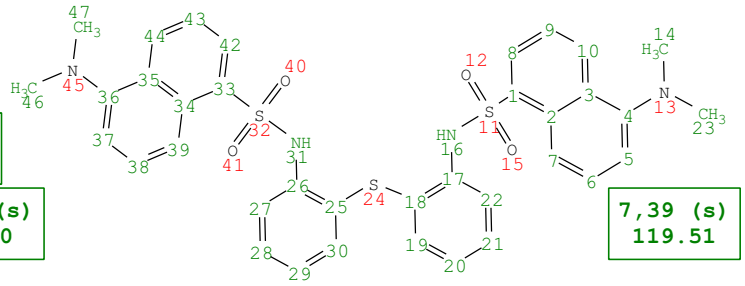
9,43 (s) 125.50

22,27 (s) 124.22

7,39 (s) 122.64

5,37 (s) 118.03

AcN: L1 ligand only



9,43 (s) 124.12

22,27 (s) 123.90

7,39 (s) 119.51

5,37 (s) 116.41

126.0 125.0 124.0 123.0 122.0 121.0 120.0 119.0 118.0 117.0 116.0 115.0

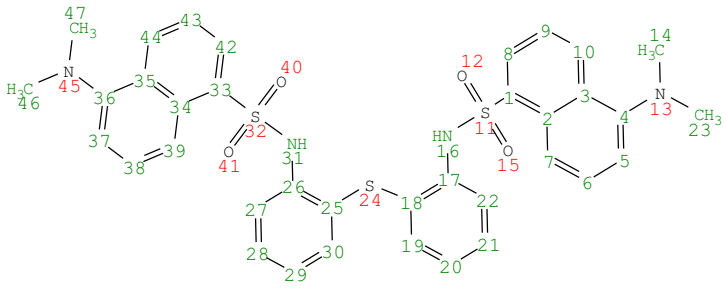
ppm

Fig SX144 L1 acetonitrile-d3 ligand + 1equiv. Cu(II)

AcN: L1 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition

14,23,46,47 (s)
46.61

AcN: L1 ligand only

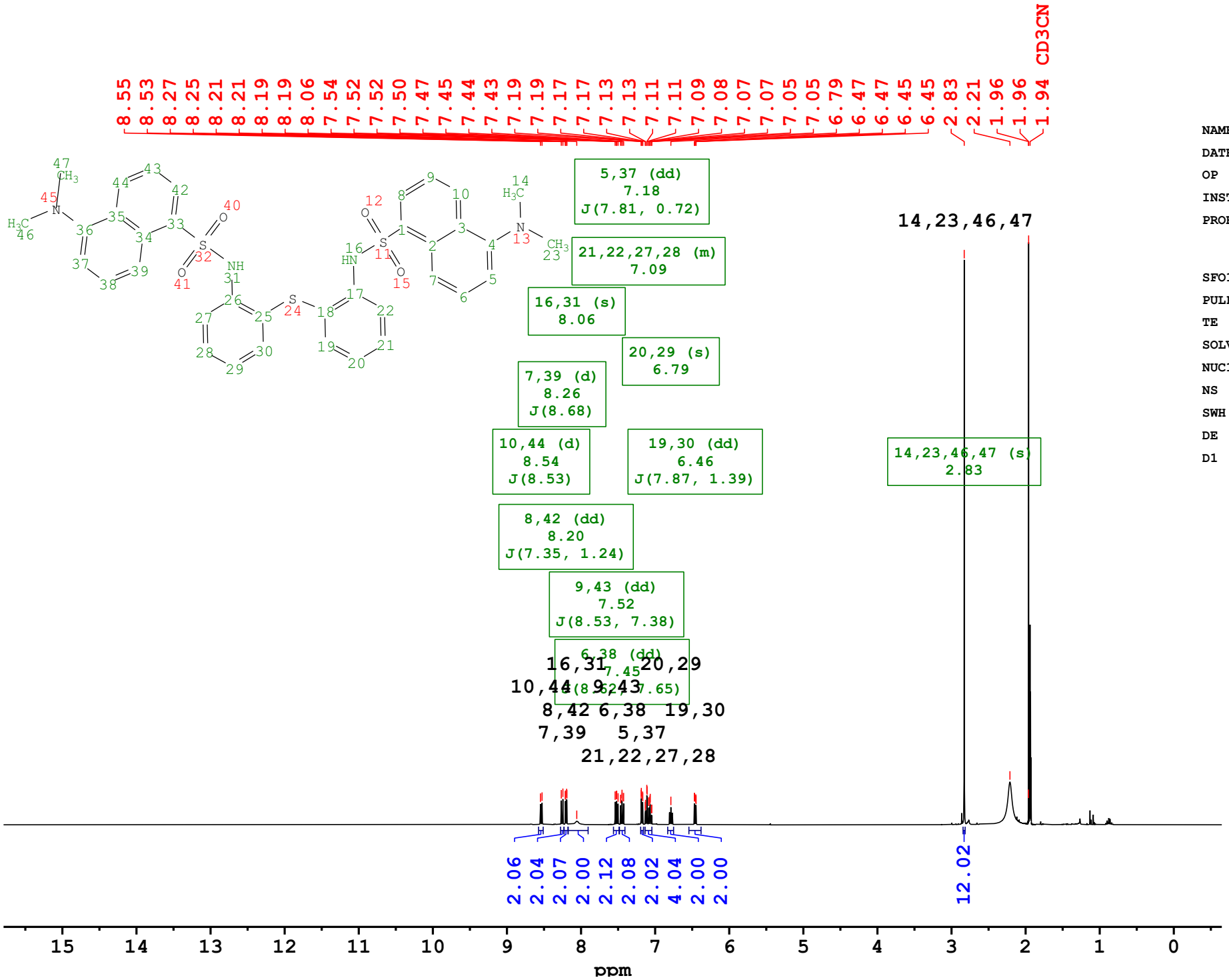


14,23,46,47 (s)
45.63

53.0 52.5 52.0 51.5 51.0 50.5 50.0 49.5 49.0 48.5 48.0 47.5 47.0 46.5 46.0 45.5 45.0
ppm

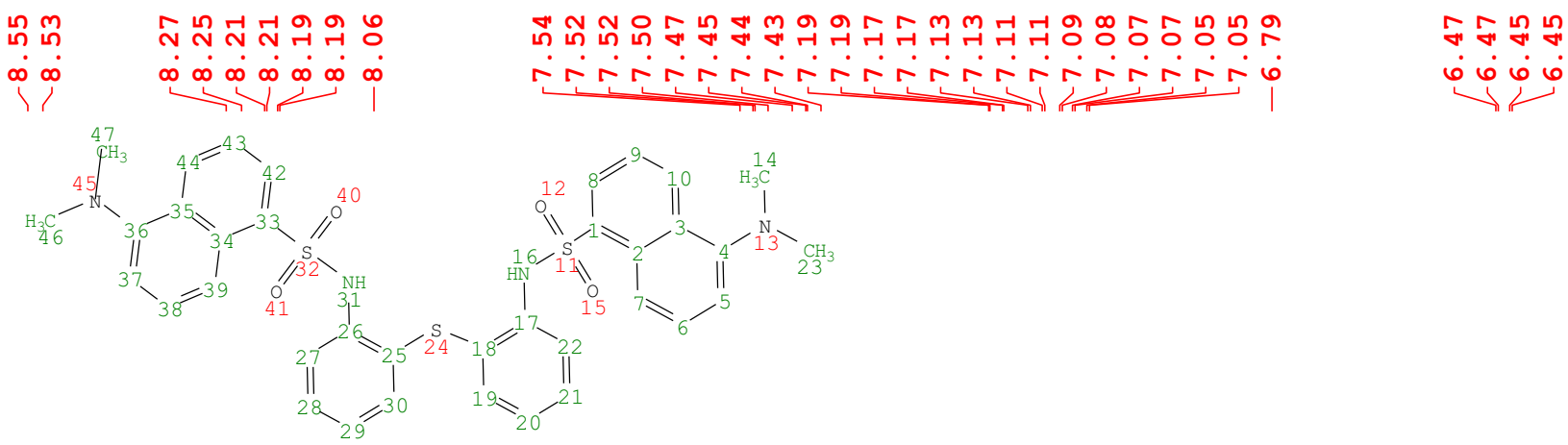
Fig SX145

# L1 acetonitrile-d3 ligand + 1equiv. Hg(II)




| | |
|---|---|
| NAME | AK-DR-165-Hg2.11.fid |
| DATE_TIME | 2025-01-09T11:01:29 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

**Fig SX146** **L1 acetonitrile-d3 ligand + 1equiv. Hg(II)**




| NAME | AK-DR-165-Hg2.11.fid |
|---|---|
| DATE_TIME | 2025-01-09T11:01:29 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

10,44 (d) 8.54 J(8.53)

8,42 (dd) 8.20 J(7.35, 1.24)

7,39 (d) 8.26 J(8.68)

16,31 (s) 8.06

6,38 (dd) 7.45 J(8.62, 7.65)

9,43 (dd) 7.52 J(8.53, 7.38)

5,37 (dd) 7.18 J(7.81, 0.72)

21,22,27,28 (m) 7.09

20,29 (s) 6.79

19,30 (dd) 6.46 J(7.87, 1.39)

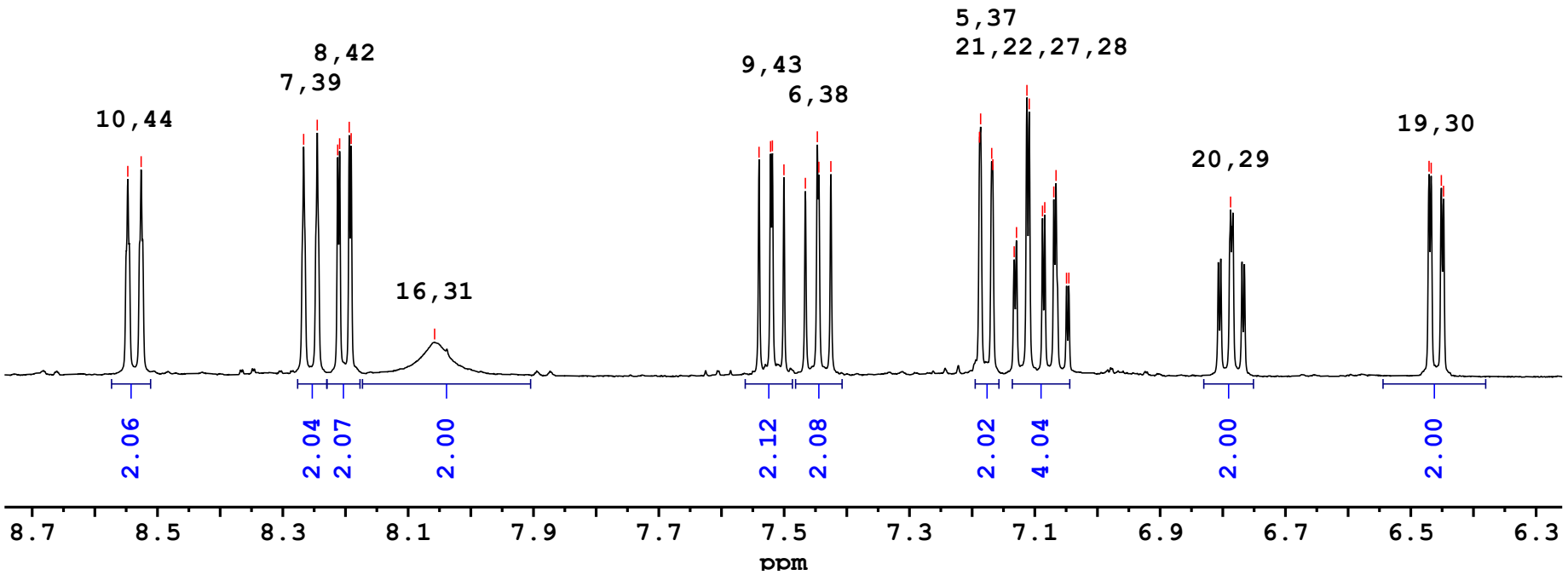
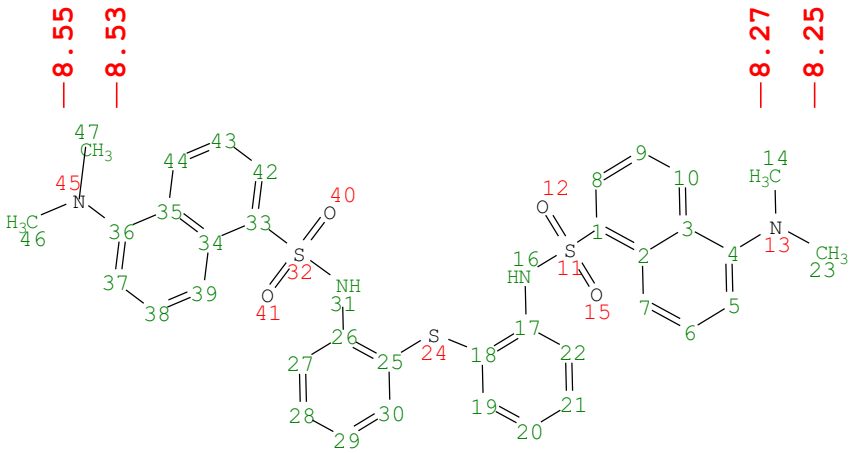


**Fig SX147** **L1 acetonitrile-d3 ligand + 1equiv. Hg(II)**




| | |
|---|---|
| NAME | AK-DR-165-Hg2.11.fid |
| DATE_TIME | 2025-01-09T11:01:29 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

10,44 (d)
8.54
J(8.53)

7,39 (d)
8.26
J(8.68)

8,42 (dd)
8.20
J(7.35, 1.24)

16,31 (s)
8.06

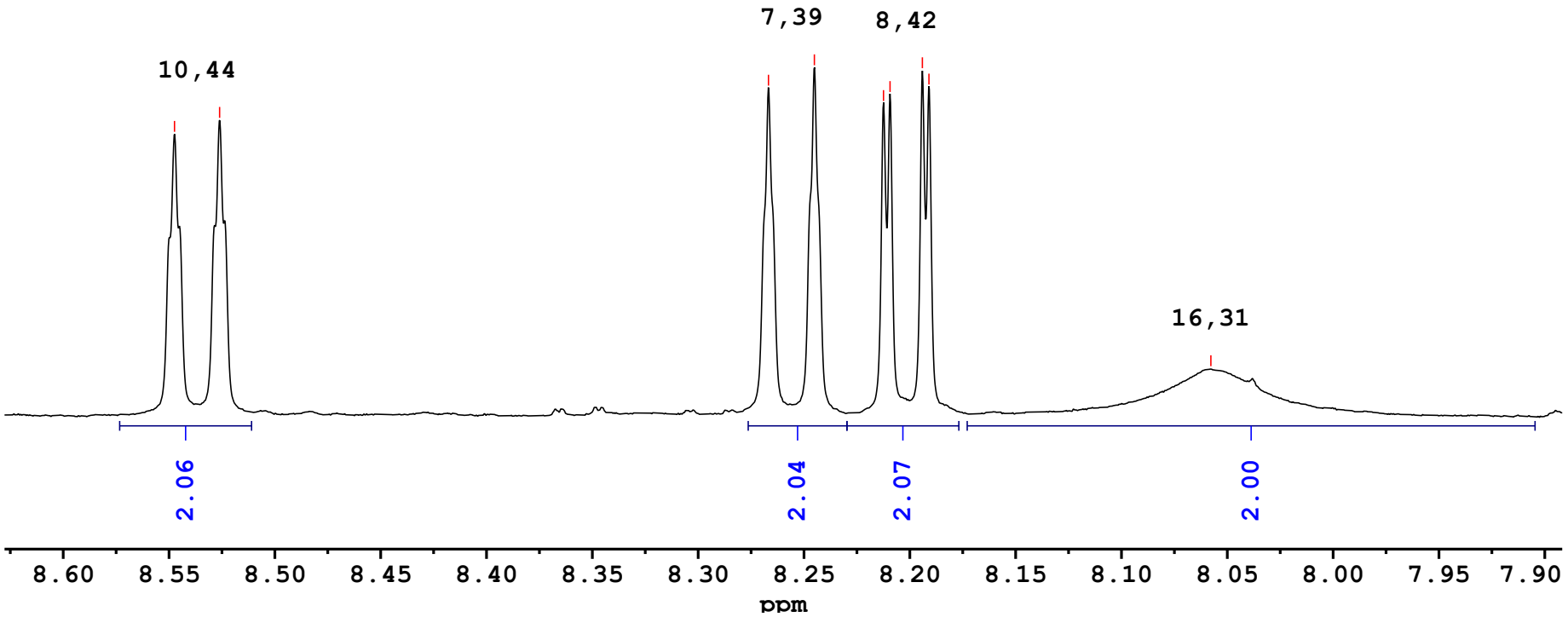
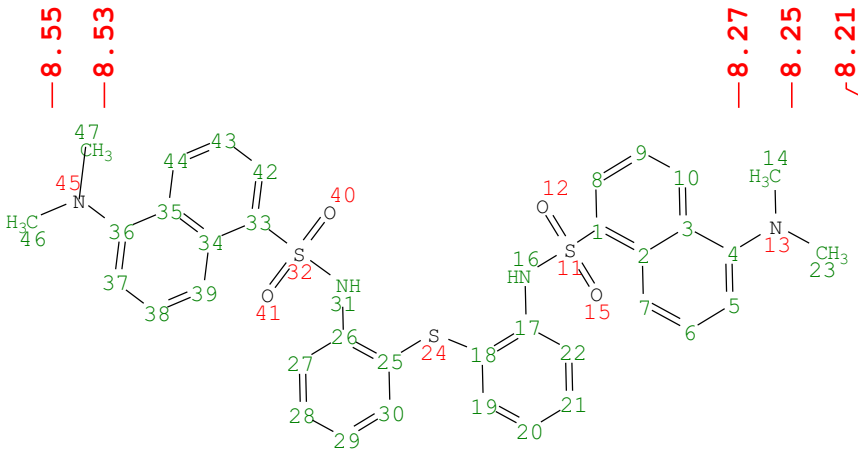


**Fig SX148** **L1 acetonitrile-d3 ligand + 1equiv. Hg(II)**




| | |
|---|---|
| NAME | AK-DR-165-Hg2.11.fid |
| DATE_TIME | 2025-01-09T11:01:29 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

10,44 (d)
8.54
J(8.53)

8,42 (dd)
8.20
J(7.35, 1.24)

7,39 (d)
8.26
J(8.68)

16,31 (s)
8.06

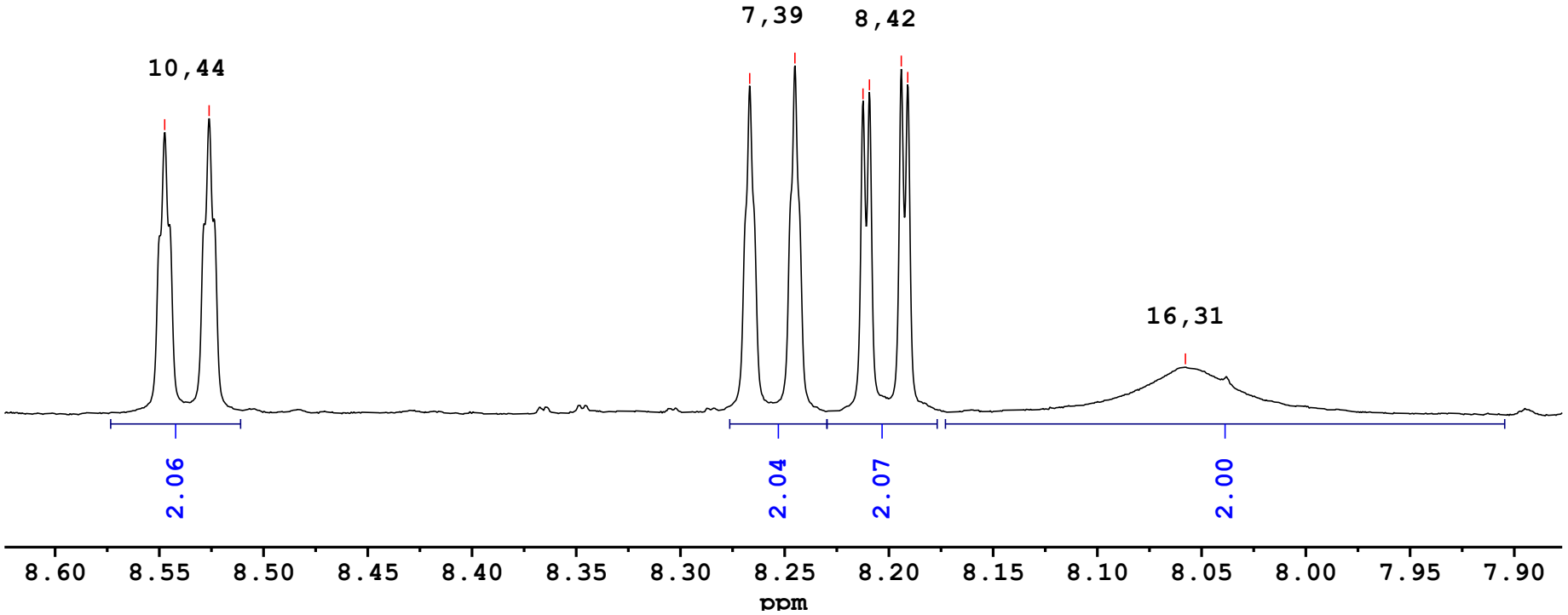
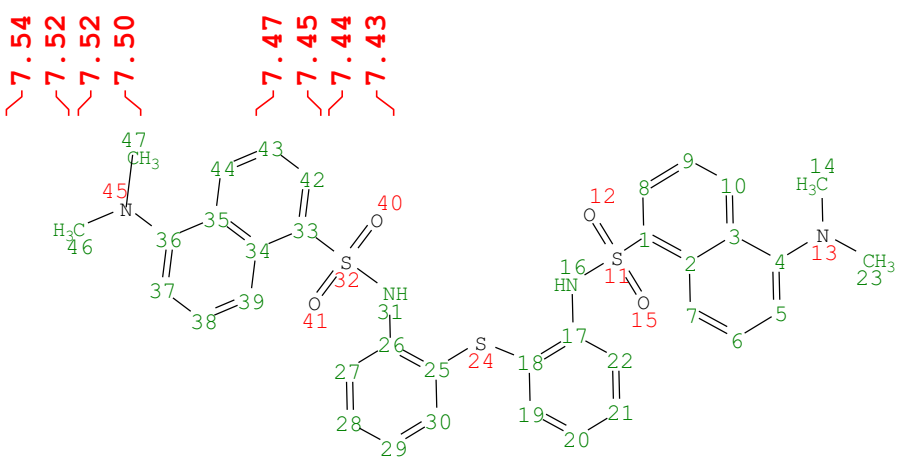


**Fig SX149** **L1 acetonitrile-d3 ligand + 1equiv. Hg(II)**




| | |
|---|---|
| NAME | AK-DR-165-Hg2.11.fid |
| DATE_TIME | 2025-01-09T11:01:29 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

9,43 (dd)
7.52
J(8.53, 7.38)

6,38 (dd)
7.45
J(8.62, 7.65)

5,37 (dd)
7.18
J(7.81, 0.72)

21,22,27,28 (m)
7.09

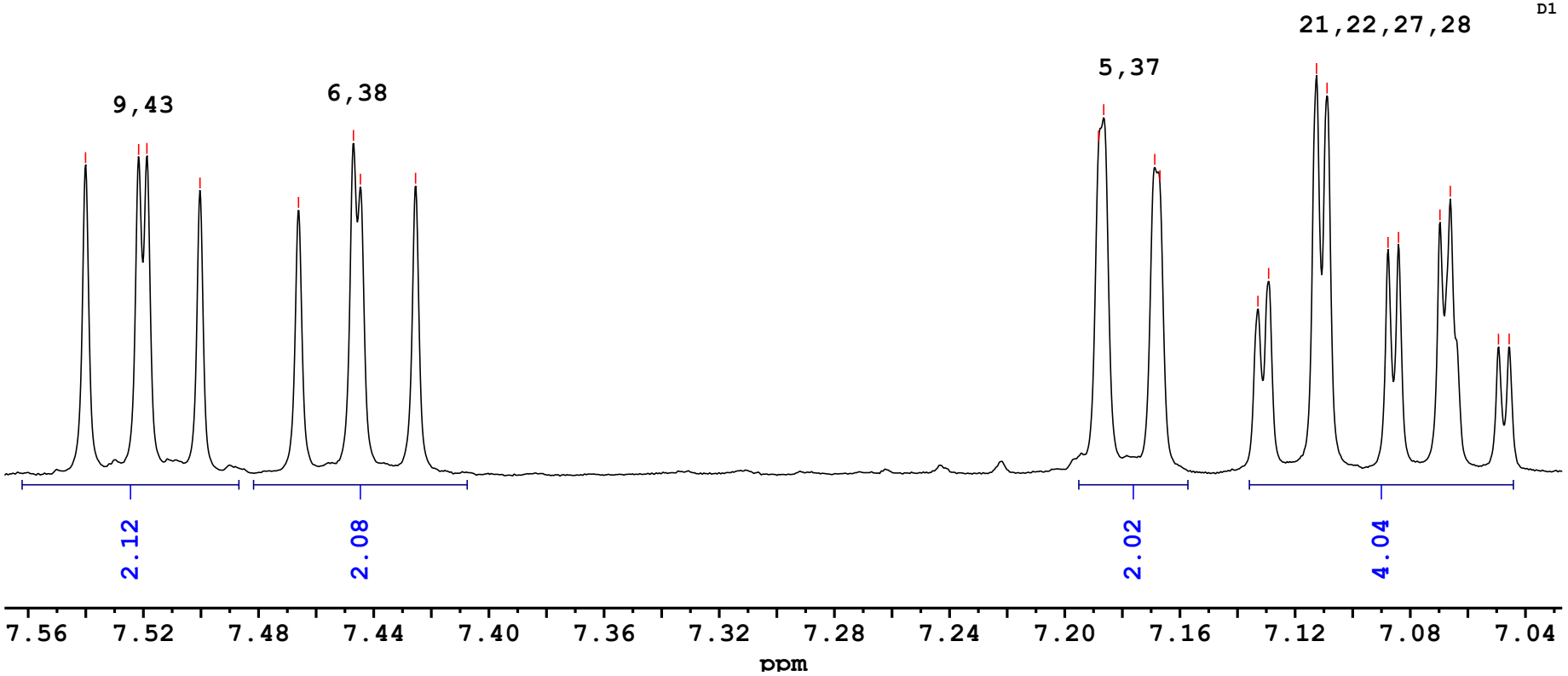
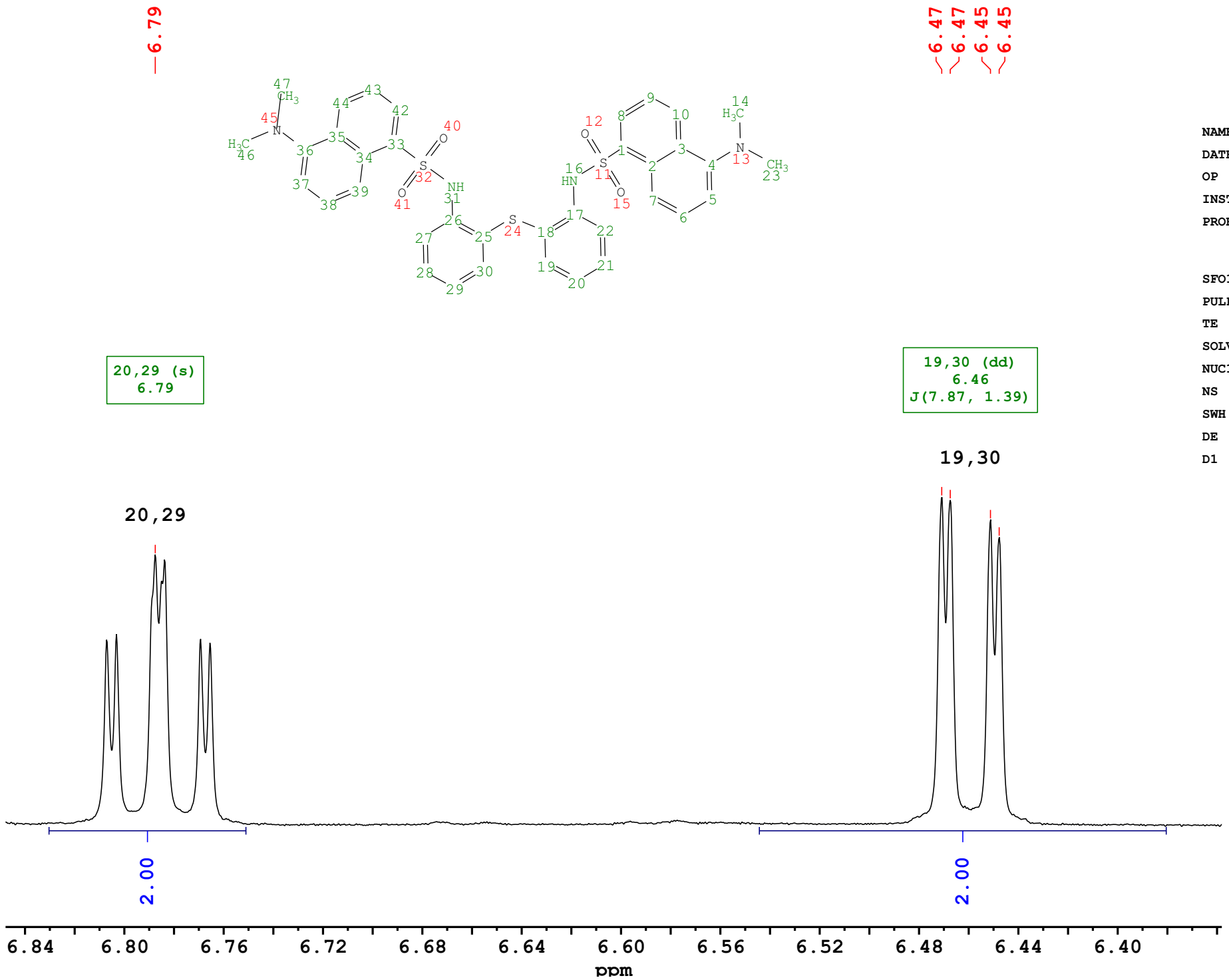


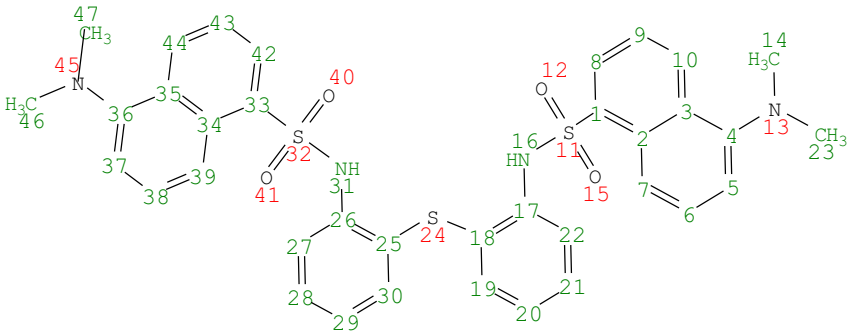
Fig SX150 L1 acetonitrile-d3 ligand + 1equiv. Hg(II)

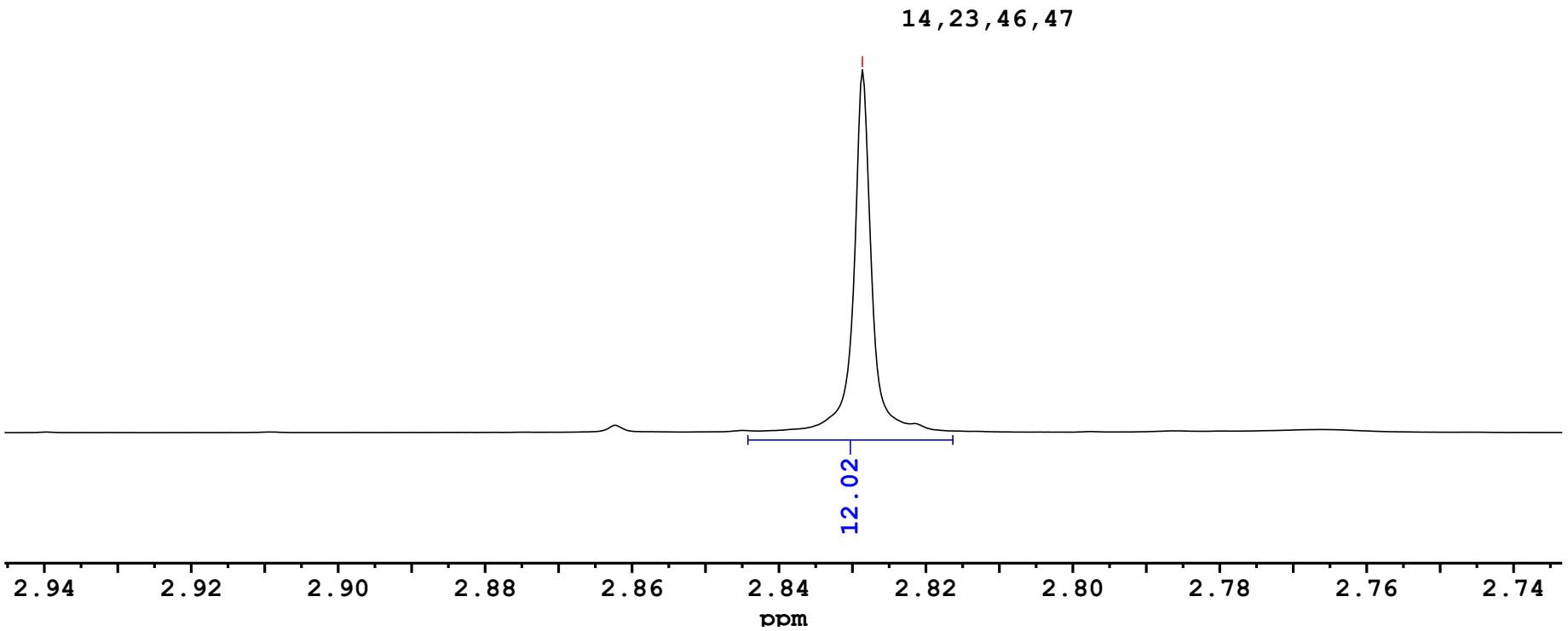





| | |
|---|---|
| NAME | AK-DR-165-Hg2.11.fid |
| DATE_TIME | 2025-01-09T11:01:29 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

**Fig SX151** **L1 acetonitrile-d3 ligand + 1equiv. Hg(II)**

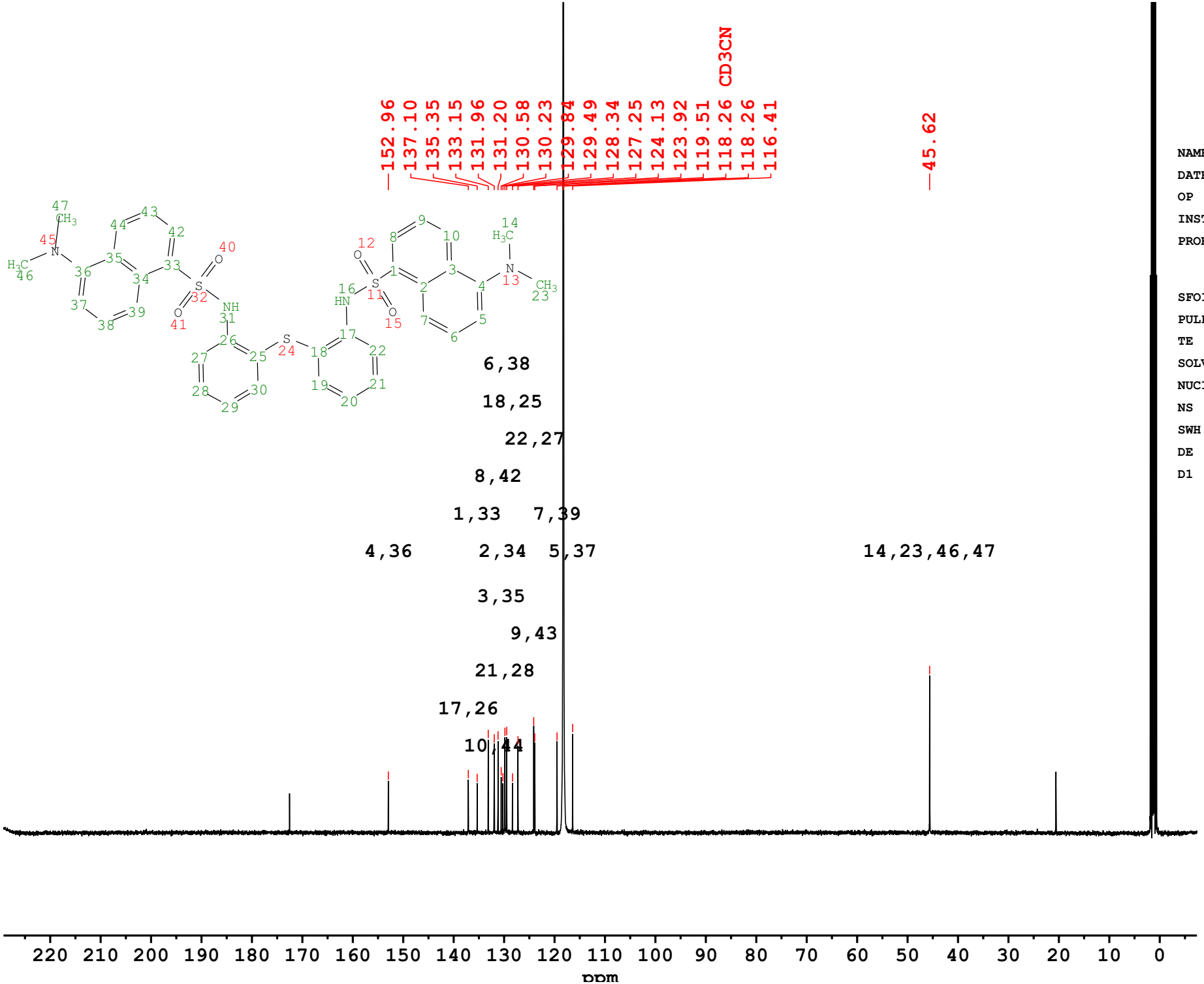





| | |
|---|---|
| NAME | AK-DR-165-Hg2.11.fid |
| DATE_TIME | 2025-01-09T11:01:29 |
| OP | Pavletta.Shestakova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

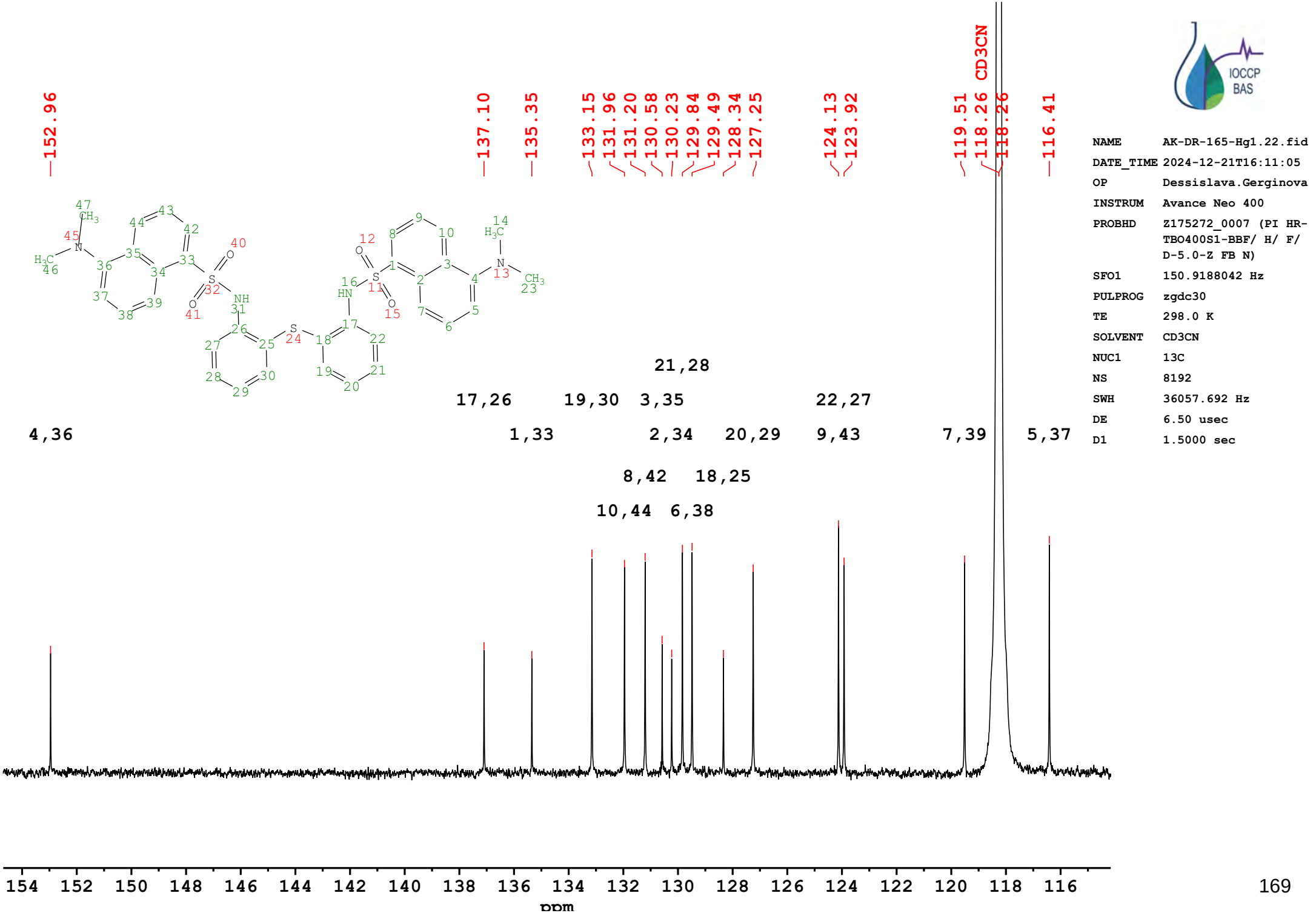
Fig SX152

# L1 acetonitrile-d3 ligand + 1equiv. Hg(II)




| | |
|---|---|
| NAME | AK-DR-165-Hg1.22.fid |
| DATE_TIME | 2024-12-21T16:11:05 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

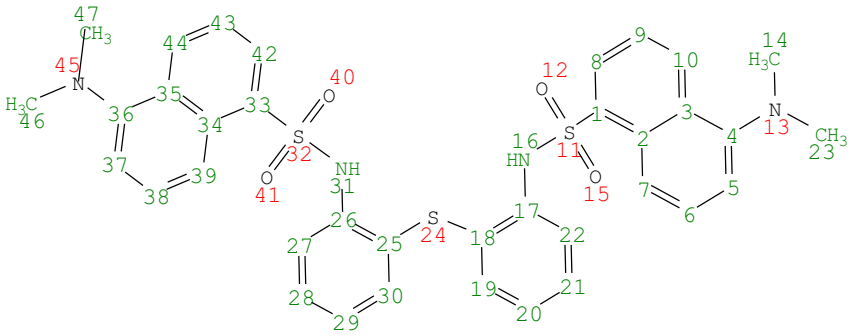
Fig SX153 L1 acetonitrile-d3 ligand + 1equiv. Hg(II)




NAME AK-DR-165-Hg1.22.fid
DATE_TIME 2024-12-21T16:11:05
OP Dessislava.Gerginova
INSTRUM Avance Neo 400
PROBHD Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N)
SFO1 150.9188042 Hz
PULPROG zgdc30
TE 298.0 K
SOLVENT CD3CN
NUC1 13C
NS 8192
SWH 36057.692 Hz
DE 6.50 usec
D1 1.5000 sec

**Fig SX154** **L1 acetonitrile-d3 ligand + 1equiv. Hg(II)**

137.10 135.35 133.15 131.96 131.20 130.58 130.23 129.84 129.49 128.34 127.25 124.13 123.92



| | |
|---|---|
| NAME | AK-DR-165-Hg1.22.fid |
| DATE_TIME | 2024-12-21T16:11:05 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

10,44 3,35 22,27

17,26 1,33 19,30 8,42 2,34 6,38 18,25 20,29 9,43

21,28

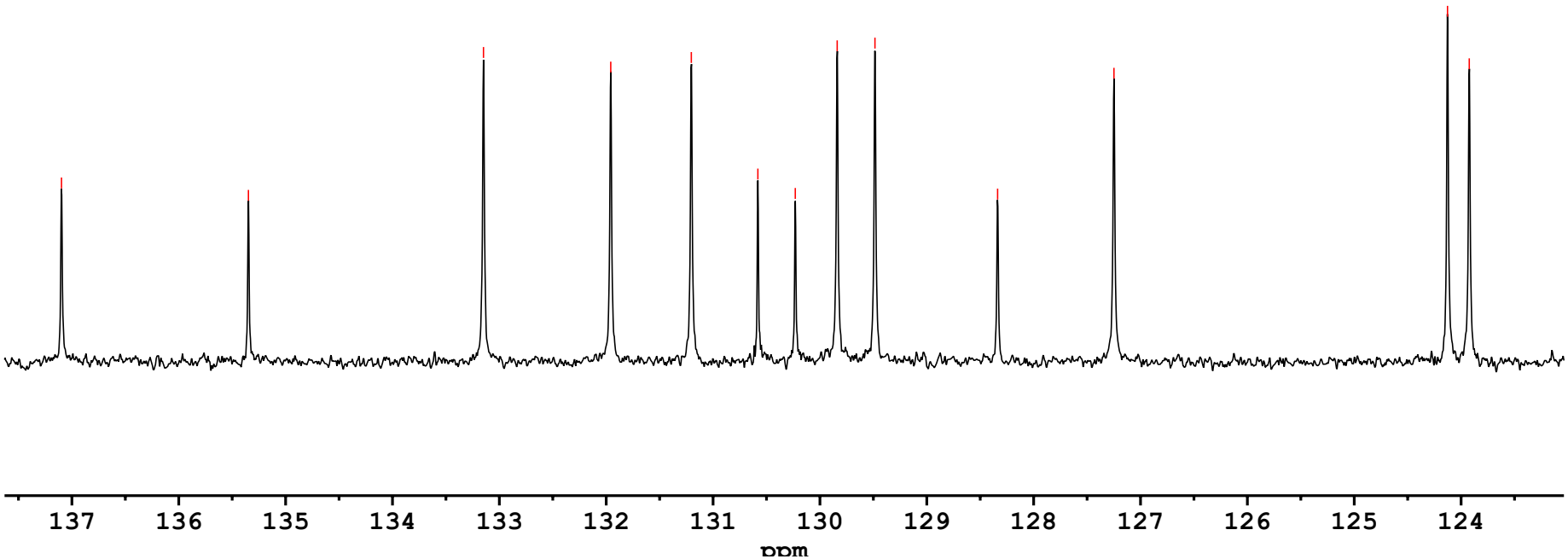
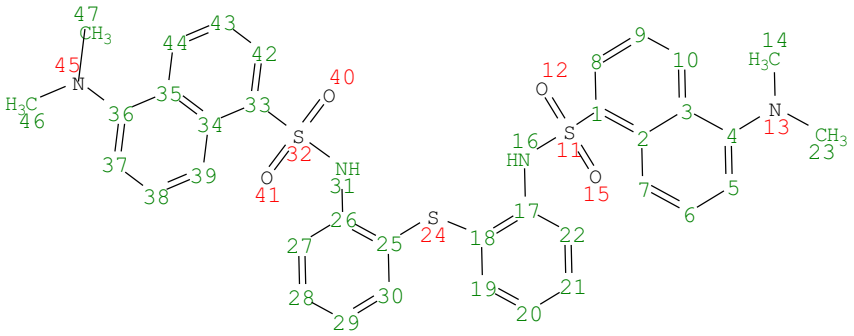


Fig SX155 L1 acetonitrile-d3 ligand + 1equiv. Hg(II)



45.62

| | |
|---|---|
| NAME | AK-DR-165-Hg1.22.fid |
| DATE_TIME | 2024-12-21T16:11:05 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

14,23,46,47

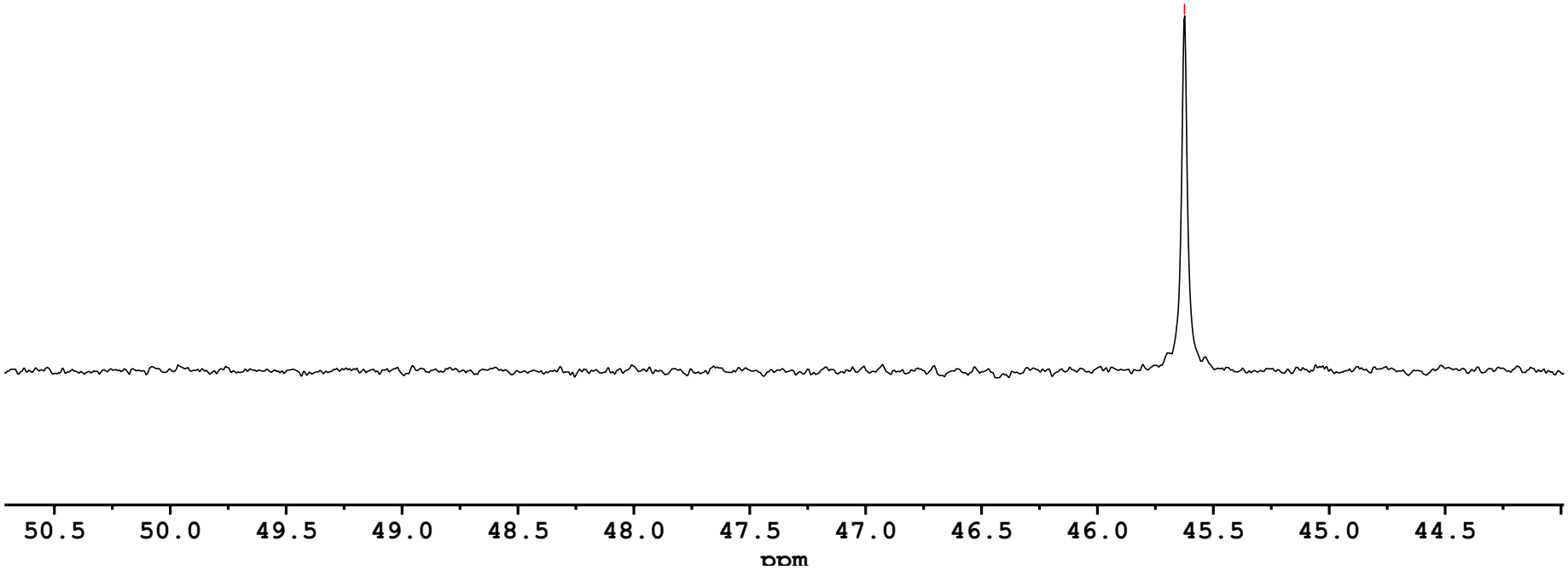
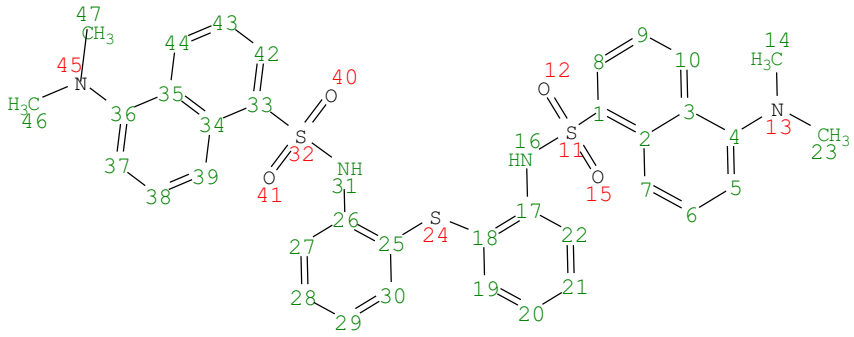


Fig SX156

# L1 acetonitrile-d3 ligand + 1equiv. Hg(II)



133.1
131.9
131.1
129.8
129.4
127.2
124.0
123.8
119.4
116.3

45.5

1.3 CD3CN

| | |
|---|---|
| NAME | AK-DR-165-Hg1.22.fid |
| DATE_TIME | 2024-12-21T16:11:05 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9319844 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 35714.286 Hz |
| DE | 18.00 usec |
| D1 | 1.5000 sec |

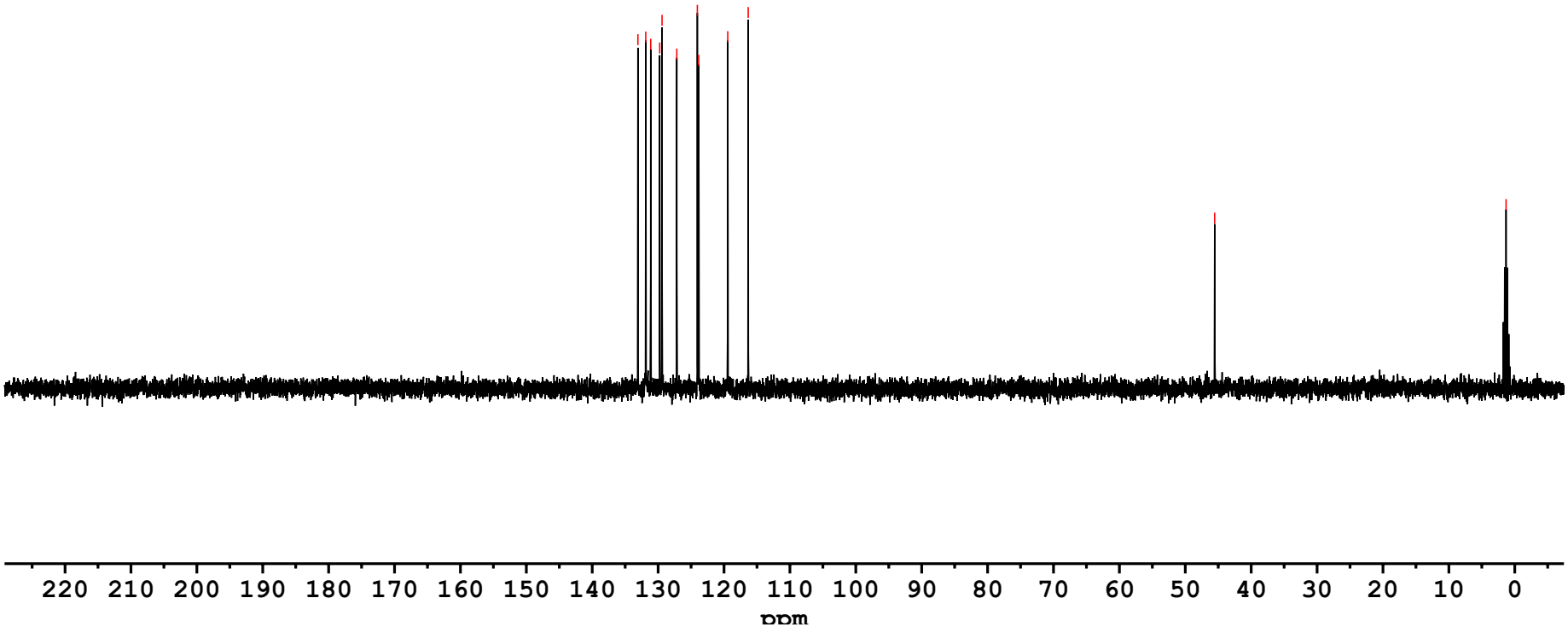
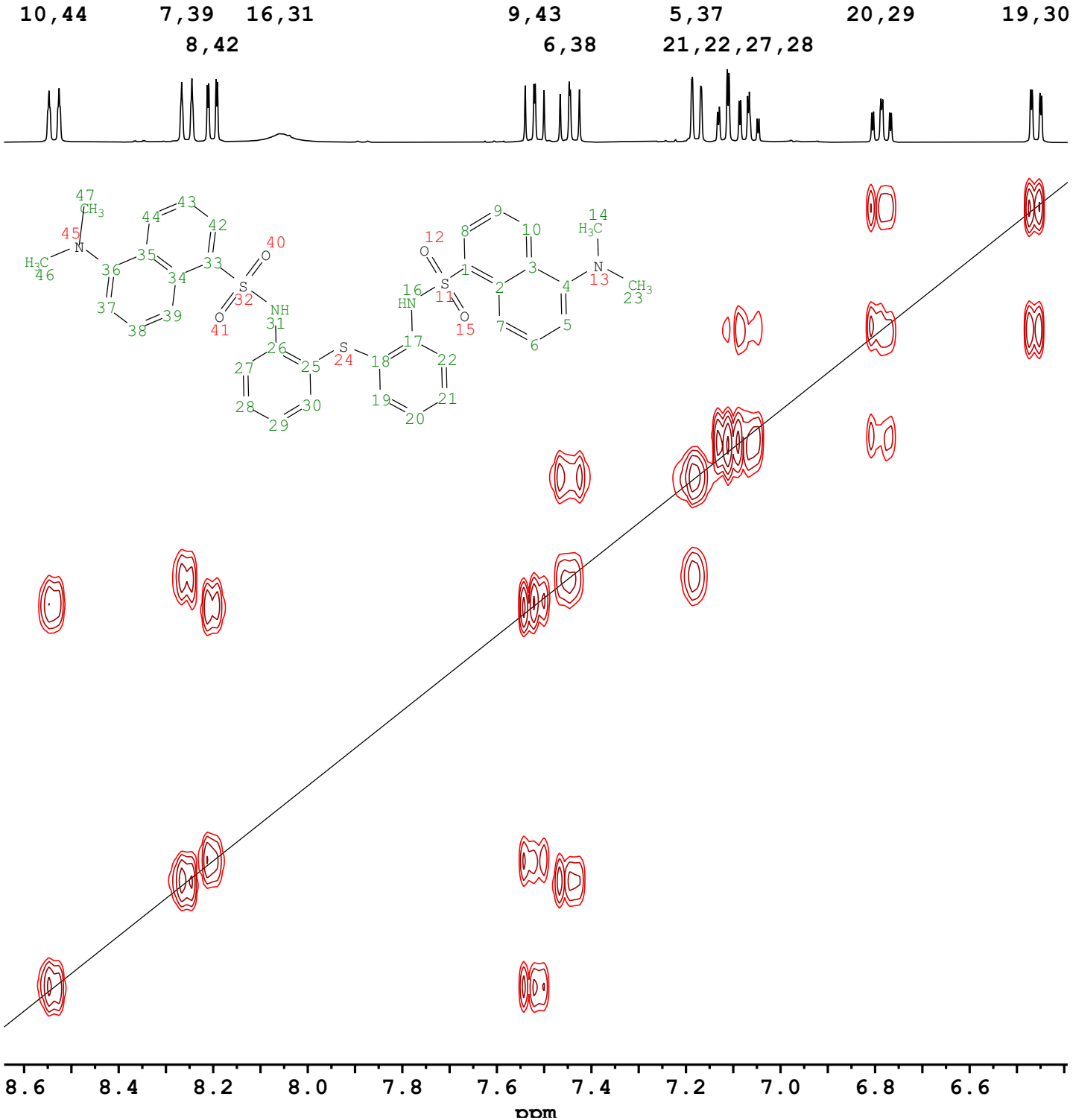


Fig SX157

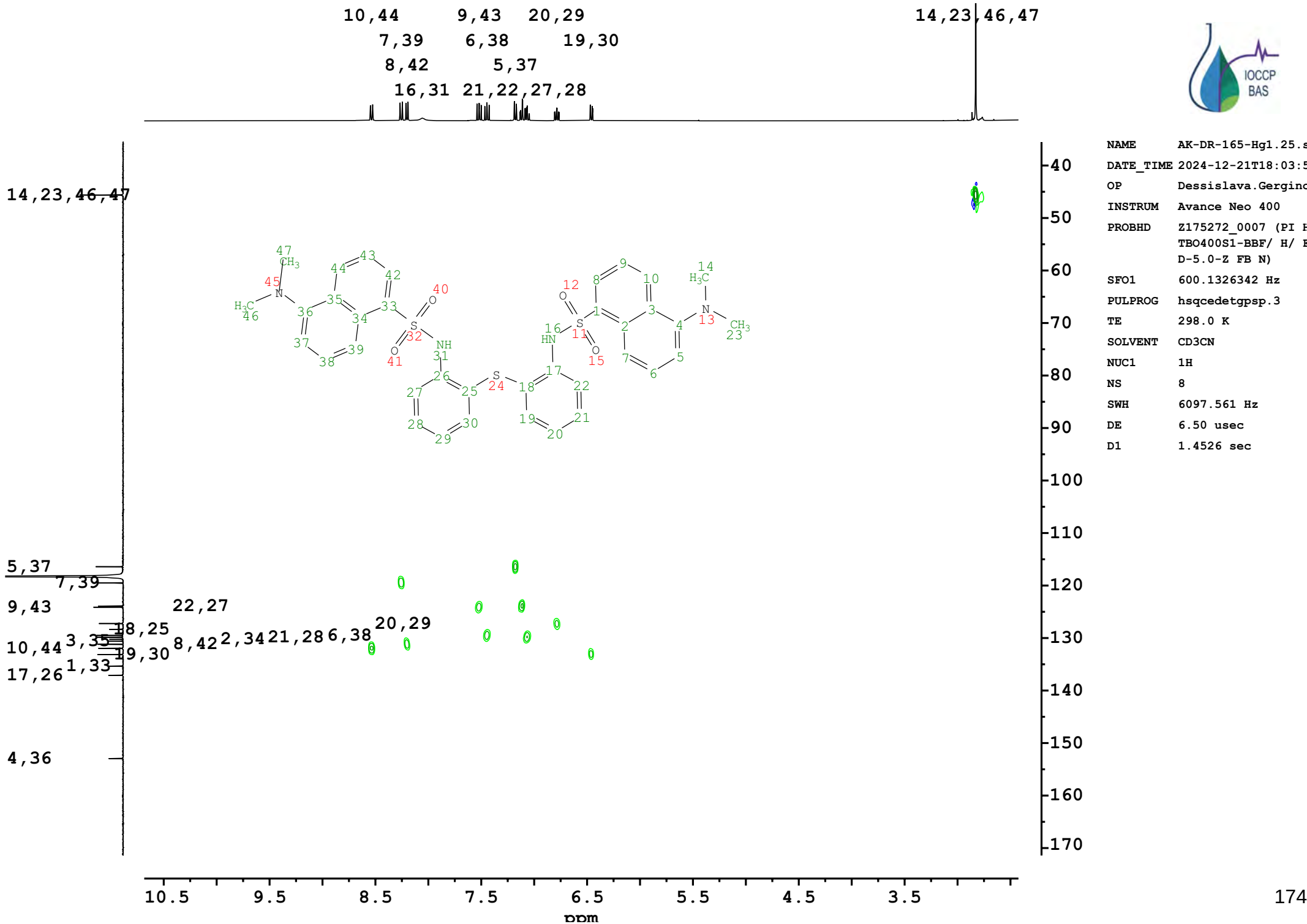
# L1 acetonitrile-d3 ligand + 1equiv. Hg(II)




| | |
|---|---|
| NAME | AK-DR-165-Hg1.24.ser |
| DATE_TIME | 2024-12-21T17:20:42 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 4 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0017 sec |

Fig SX158

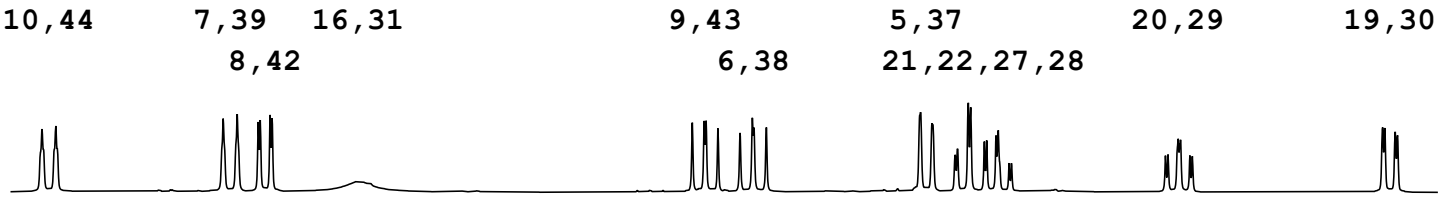
L1 acetonitrile-d3 ligand + 1equiv. Hg(II)



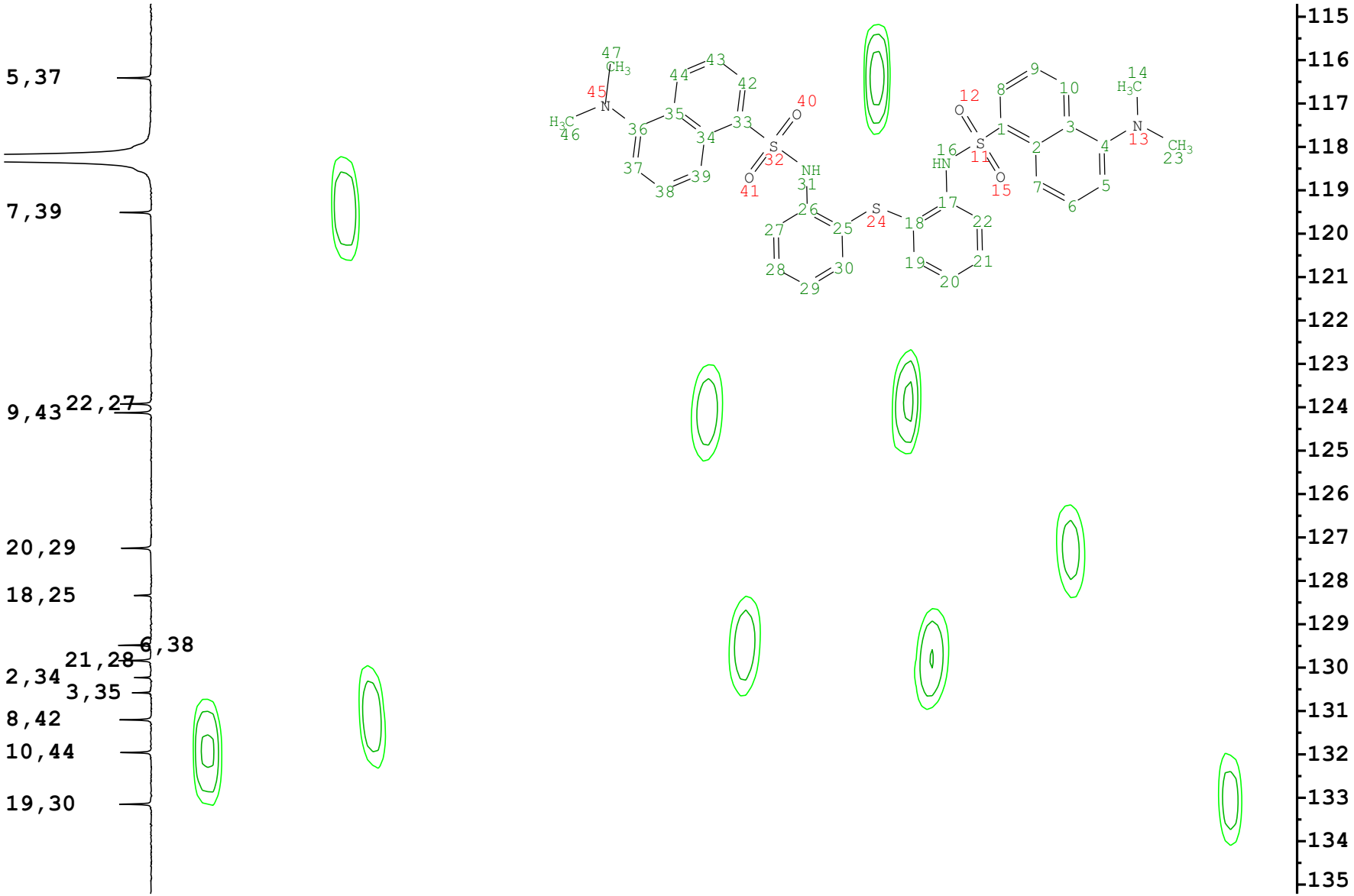

| | |
|---|---|
| NAME | AK-DR-165-Hg1.25.ser |
| DATE_TIME | 2024-12-21T18:03:53 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

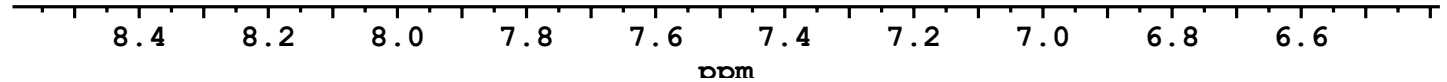
Fig SX159

# L1 acetonitrile-d3 ligand + 1equiv. Hg(II)



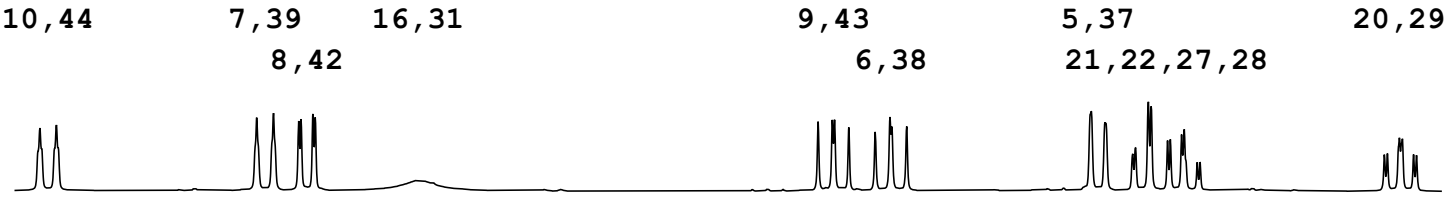


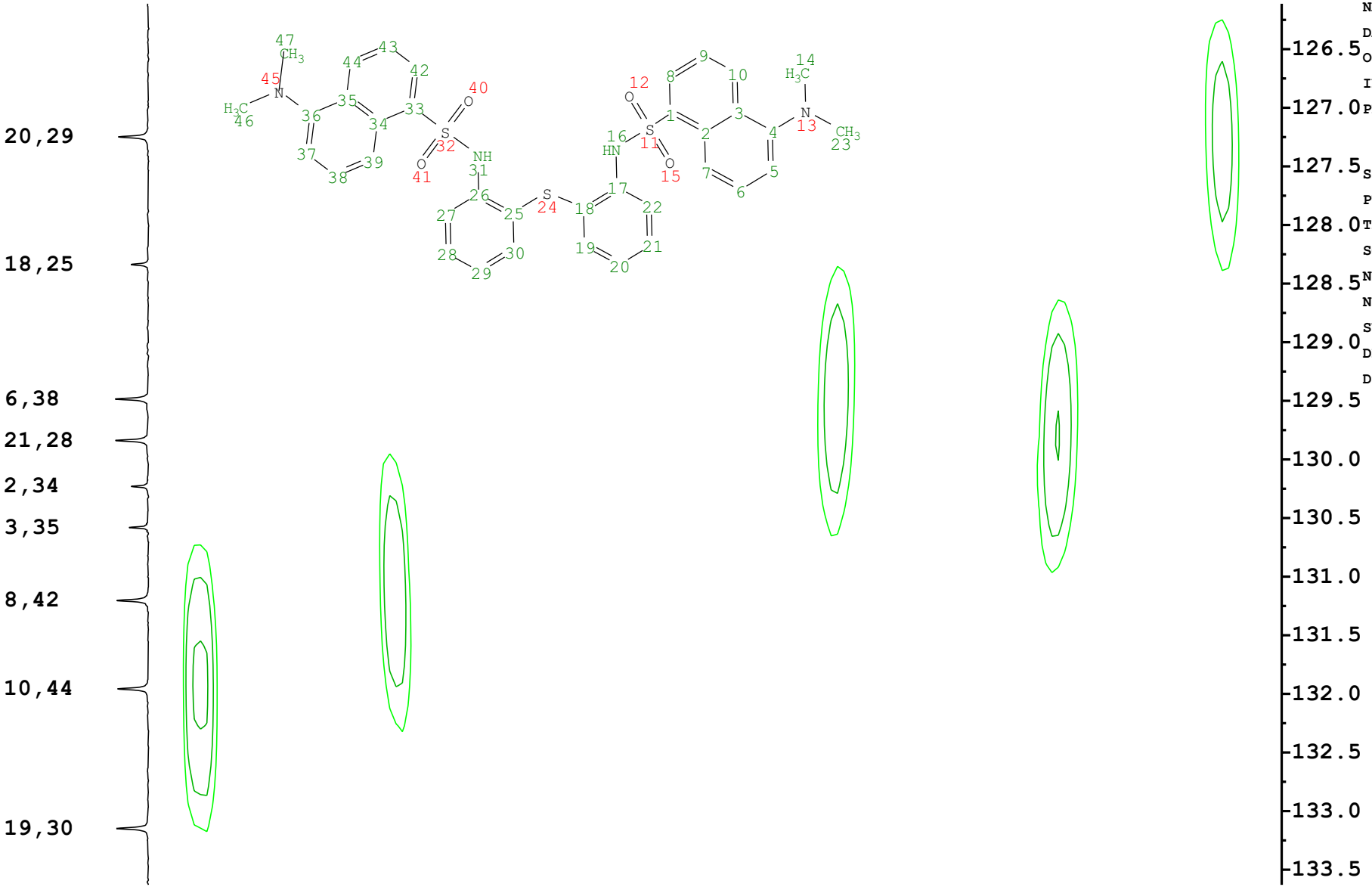

| | |
|---|---|
| NAME | AK-DR-165-Hg1.25.ser |
| DATE_TIME | 2024-12-21T18:03:53 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

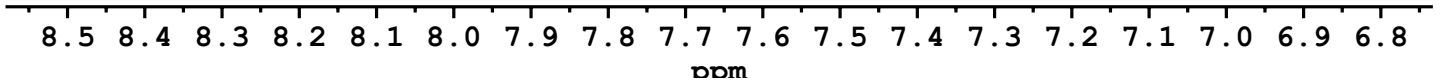
Fig SX160 L1 acetonitrile-d3 ligand + 1equiv. Hg(II)







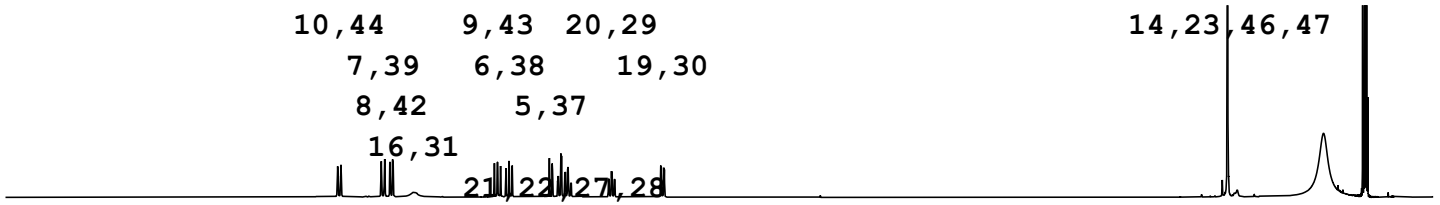


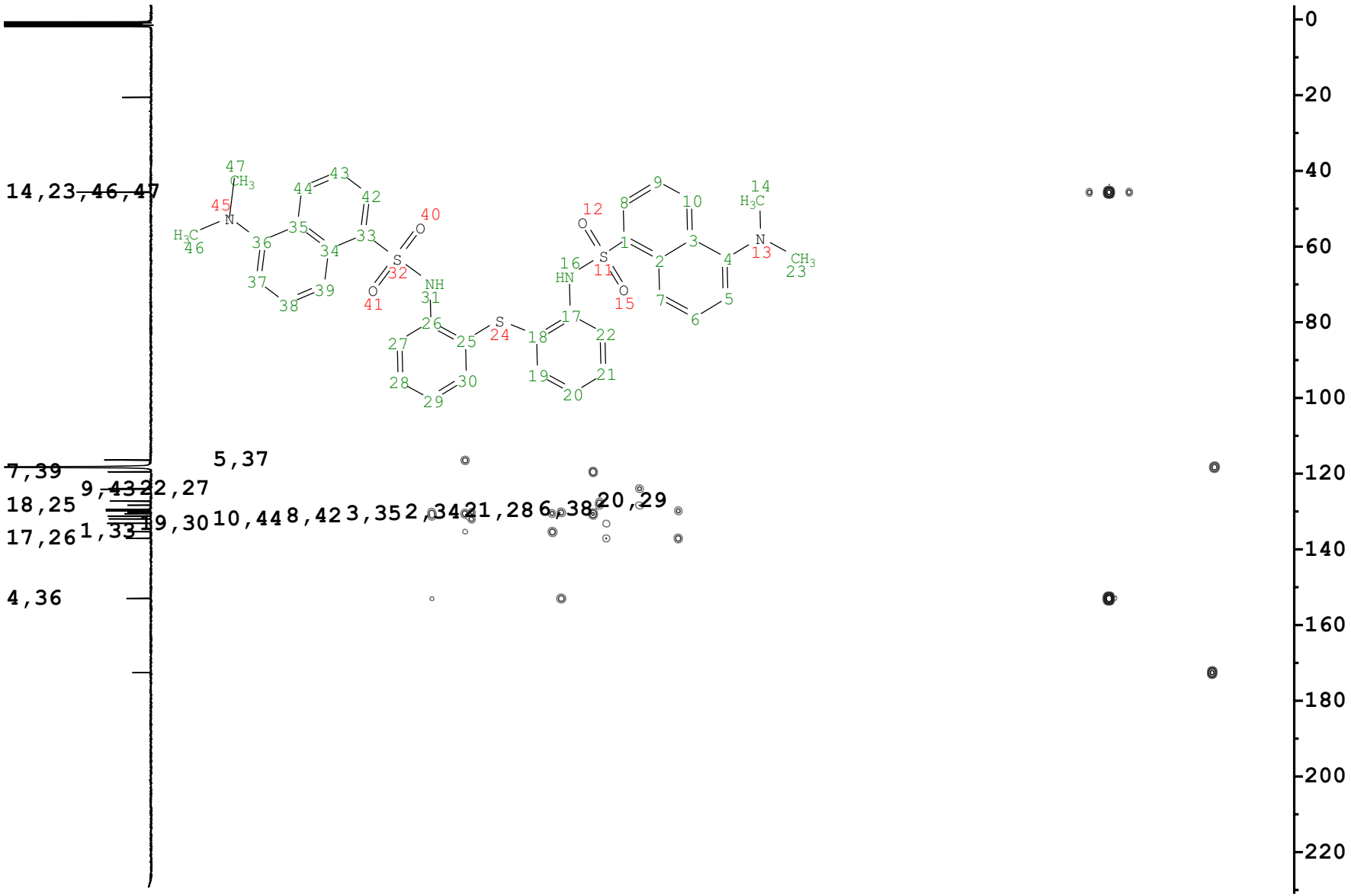




| | |
|---|---|
| NAME | AK-DR-165-Hg1.25.ser |
| DATE_TIME | 2024-12-21T18:03:53 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX161

# L1 acetonitrile-d3 ligand + 1equiv. Hg(II)

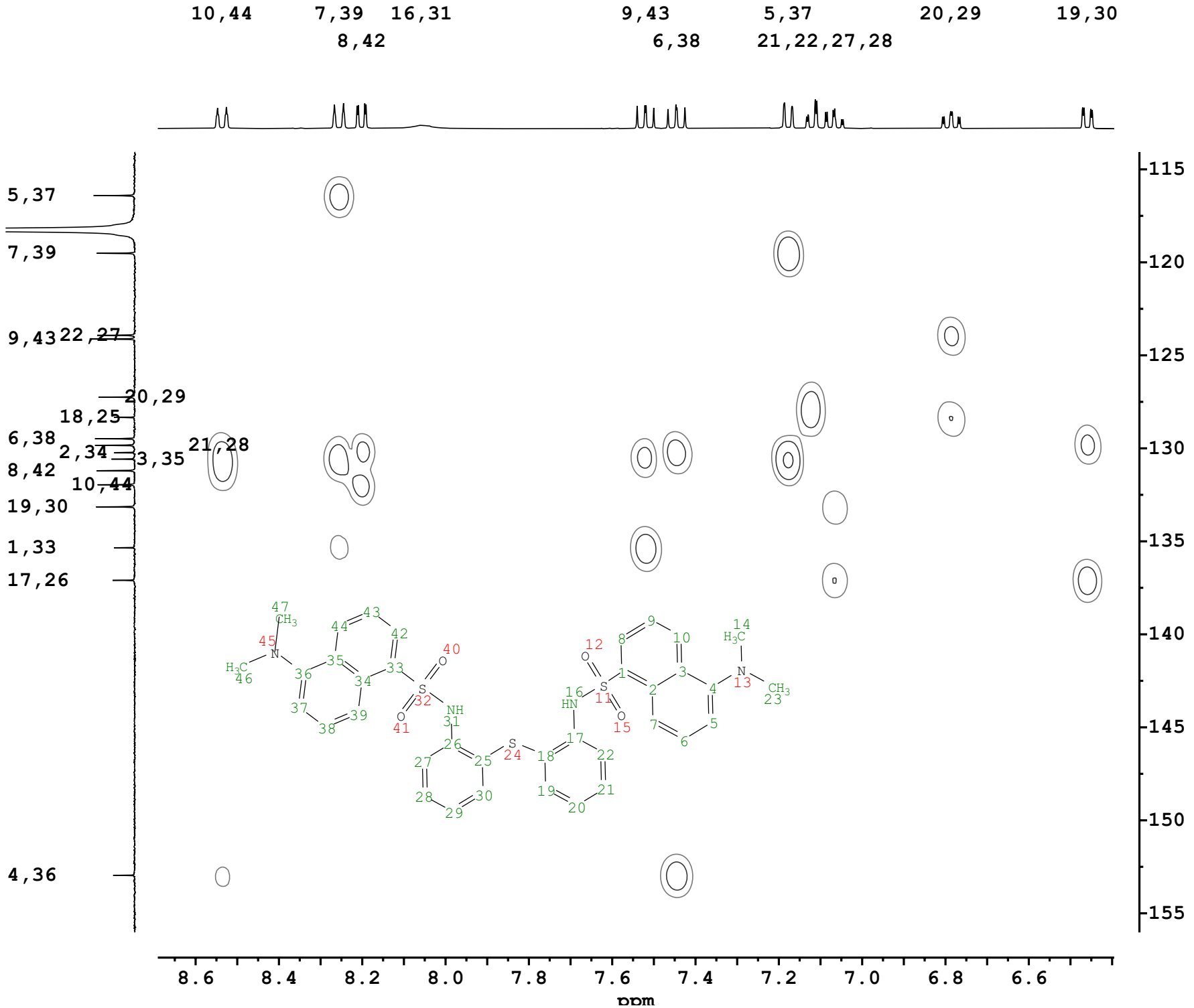



| | |
|---|---|
| NAME | AK-DR-165-Hg1.26.ser |
| DATE_TIME | 2024-12-21T19:28:50 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX162

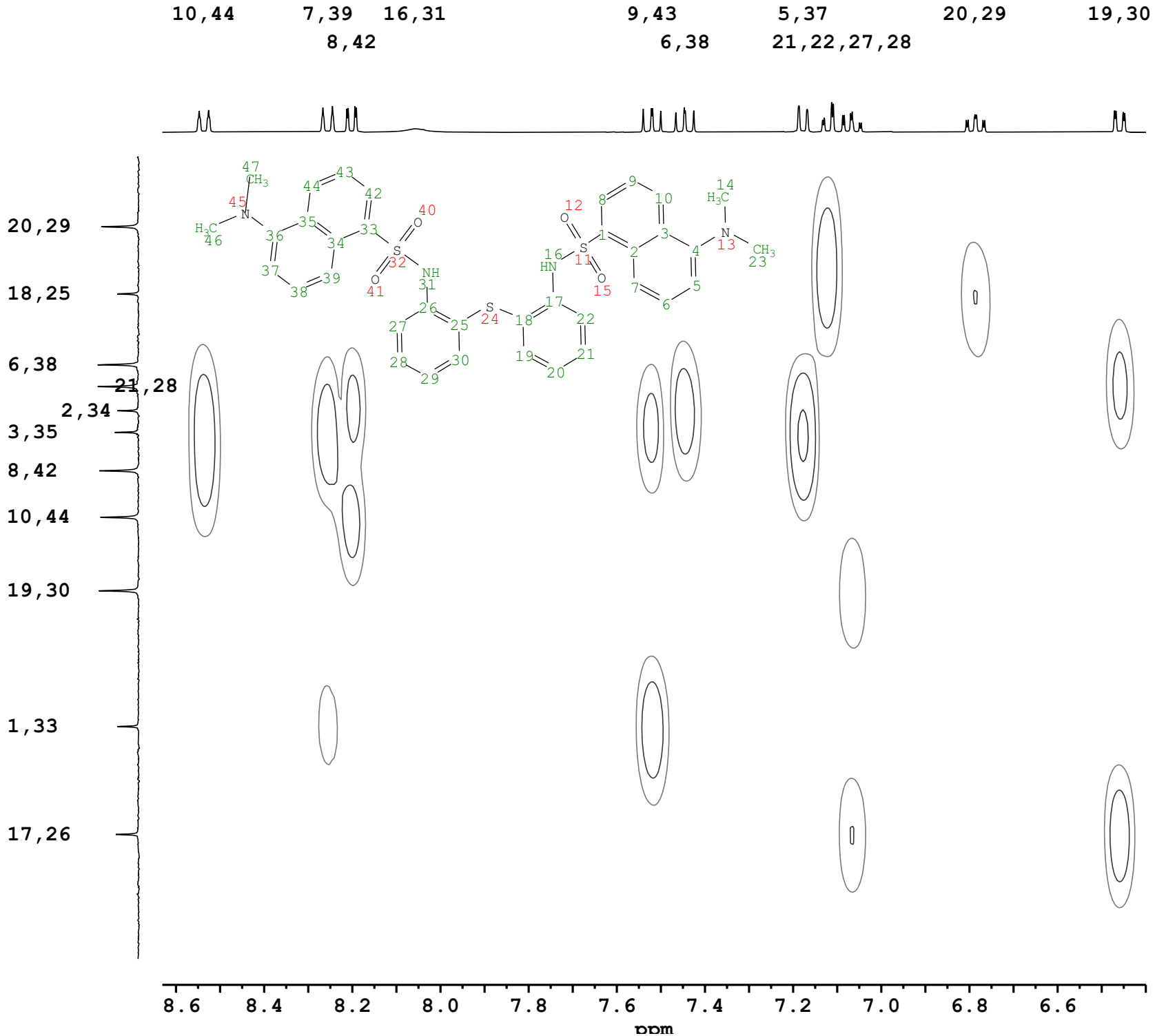
# L1 acetonitrile-d3 ligand + 1equiv. Hg(II)




| | |
|---|---|
| NAME | AK-DR-165-Hg1.26.ser |
| DATE_TIME | 2024-12-21T19:28:50 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX163

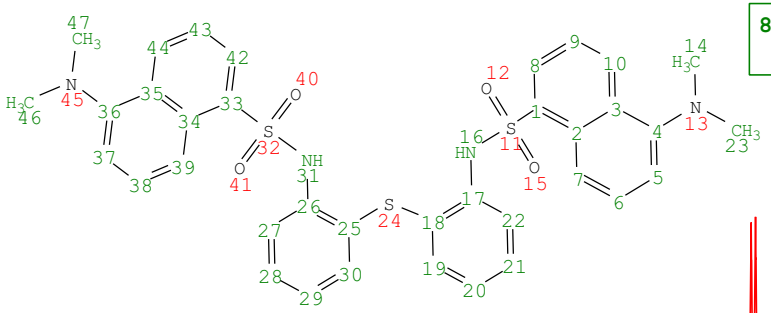
# L1 acetonitrile-d3 ligand + 1equiv. Hg(II)




| | |
|---|---|
| NAME | AK-DR-165-Hg1.26.ser |
| DATE_TIME | 2024-12-21T19:28:50 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | CD3CN |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX164 L1 acetonitrile-d3 ligand + 1equiv. Hg(II)

AcN: L1 + 1 equiv. $Hg(CH_3COO)_2$ after addition



16,31 (s) 8.06
21,22,27,28 (m) 7.09
7,39 (d) 8.26
6,38 (dd) 7.45
10,44 (d) 8.54
9,43 (dd) 7.52
19,30 (dd) 6.46
14,23,46,47 (s) 2.83
8,42 (dd) 8.20
20,29 (s) 6.79
5,37 (dd) 7.18

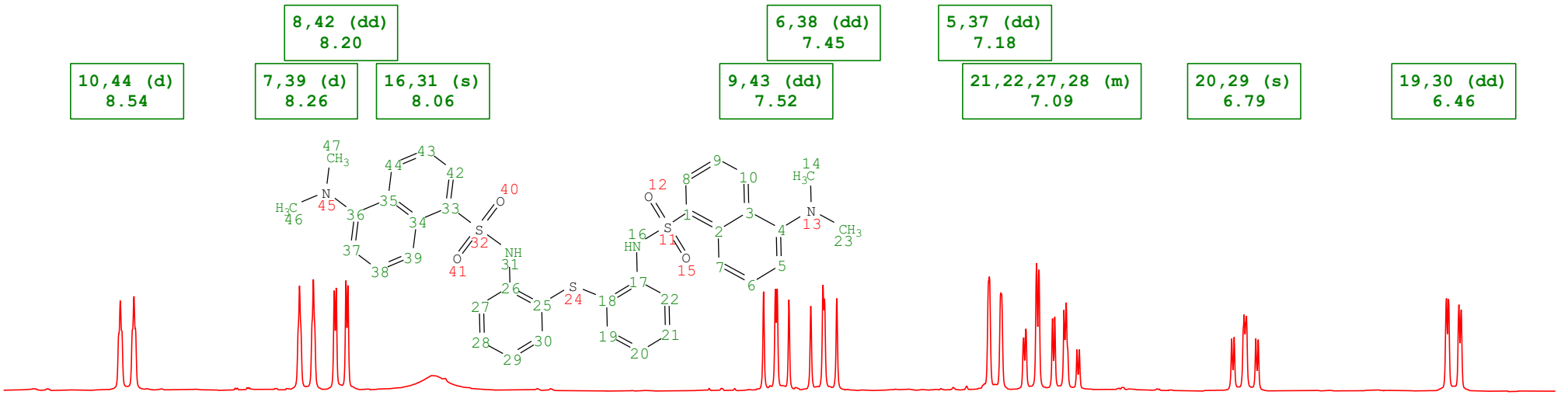
AcN: L1 (DR-292) ligand only

8,42 (dd) 8.20
5,37 (dd) 7.16
16,31 (s) 8.05
20,29 (ddd) 6.77
10,44 (dt) 8.52
21,28 (m) 7.05
14,23,46,47 (s) 2.81
7,39 (dt) 8.26
9,43 (dd) 7.51
19,30 (dd) 6.45
22,27 (dd) 7.12

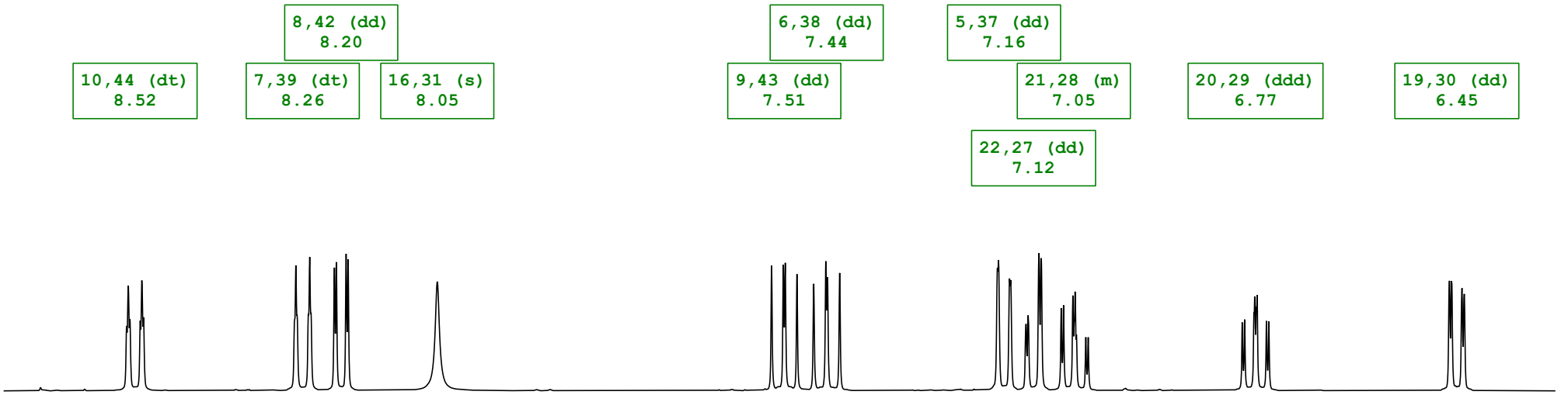
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0
ppm

Fig SX165 L1 acetonitrile-d3 ligand + 1equiv. Hg(II)

**AcN: L1 + 1 equiv. $Hg(CH_3COO)_2$ after addition**




**AcN: L1 (DR-292) ligand only**



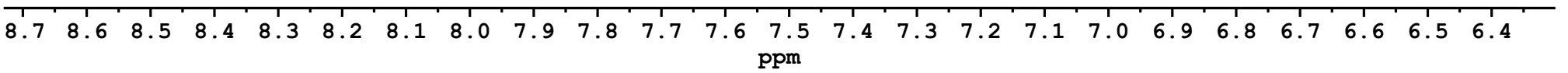
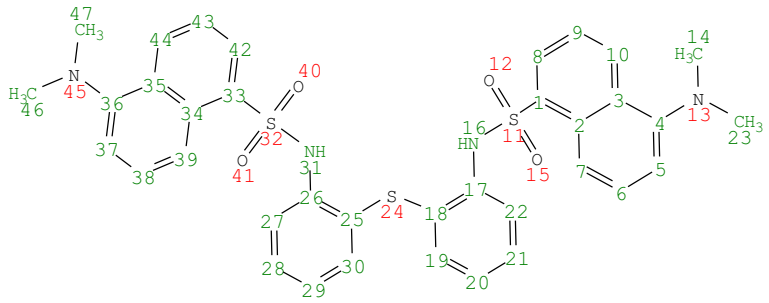



Fig SX166 L1 acetonitrile-d3 ligand + 1equiv. Hg(II)

AcN: L1 + 1 equiv. $Hg(CH_3COO)_2$ after addition



14,23,46,47 (s)
2.83

AcN: L1 (DR-292) ligand only

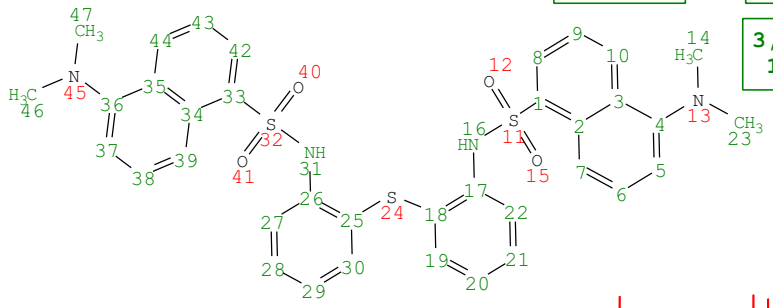
14,23,46,47 (s)
2.81

2.86 2.86 2.85 2.85 2.84 2.84 2.83 2.83 2.82 2.82 2.81 2.81 2.80 2.80
ppm

Fig SX167

L1 acetonitrile-d3 ligand + 1equiv. Hg(II)

AcN: L1 + 1 equiv. $Hg(CH_3COO)_2$ after addition



8,42 (s) 131.20

1,33 (s) 135.35

7,39 (s) 119.51

4,36 (s) 152.96

2,34 (s) 130.23

14,23,46,47 (s) 45.62

3,35 (s) 130.58

9,43 (s) 124.13

AcN: L1 (DR-292) ligand only

10,44 (s) 131.96

22,27 (s) 123.90

4,36 (s) 152.95

18,25 (s) 128.32

14,23,46,47 (s) 45.63

8,42 (s) 131.21

9,43 (s) 124.12

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

ppm

Fig SX168 L1 acetonitrile-d3 ligand + 1equiv. Hg(II)

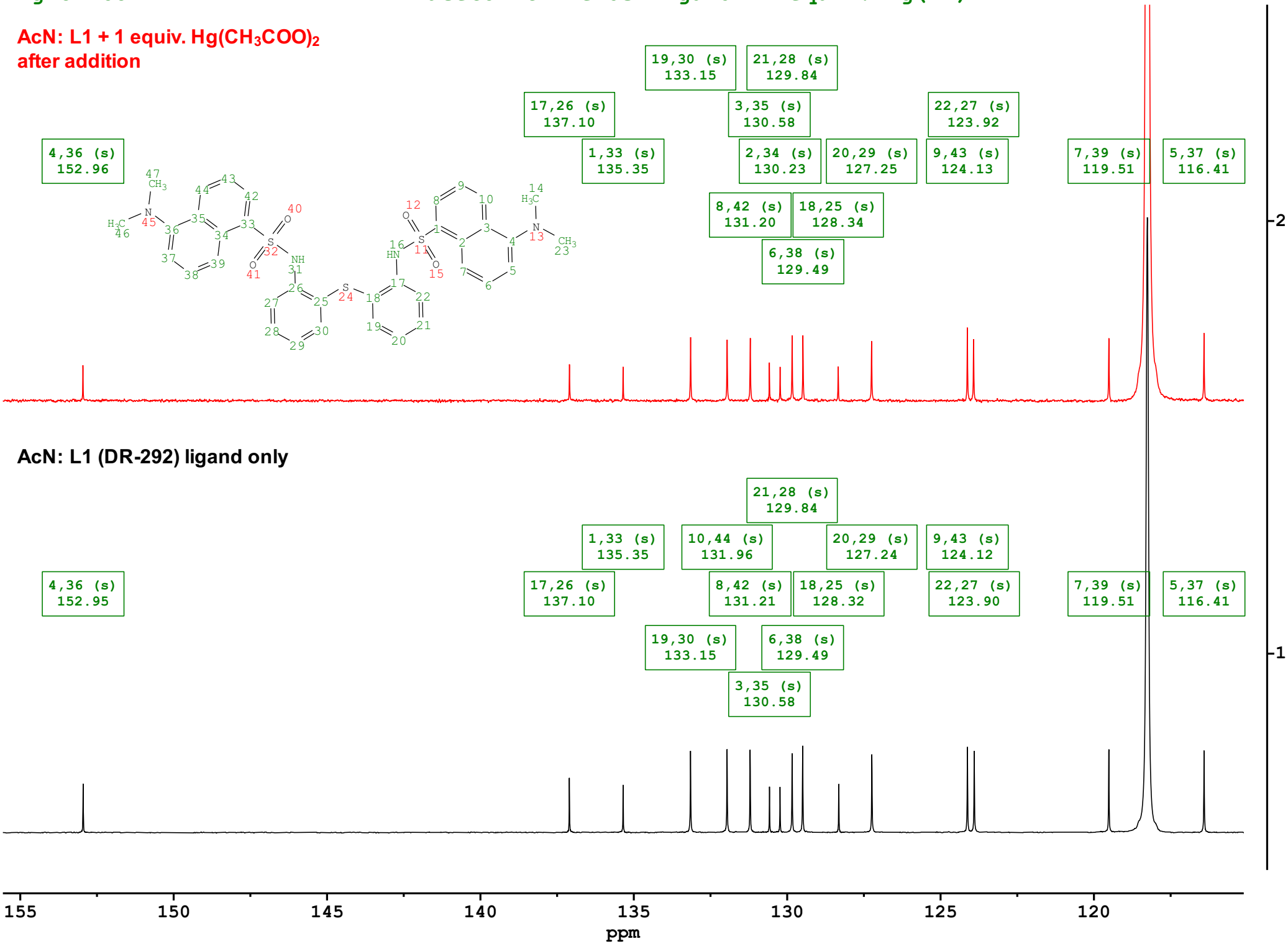


Fig SX169 L1 acetonitrile-d3 ligand + 1equiv. Hg(II)

**AcN: L1 + 1 equiv. $Hg(CH_3COO)_2$ after addition**




**AcN: L1 (DR-292) ligand only**



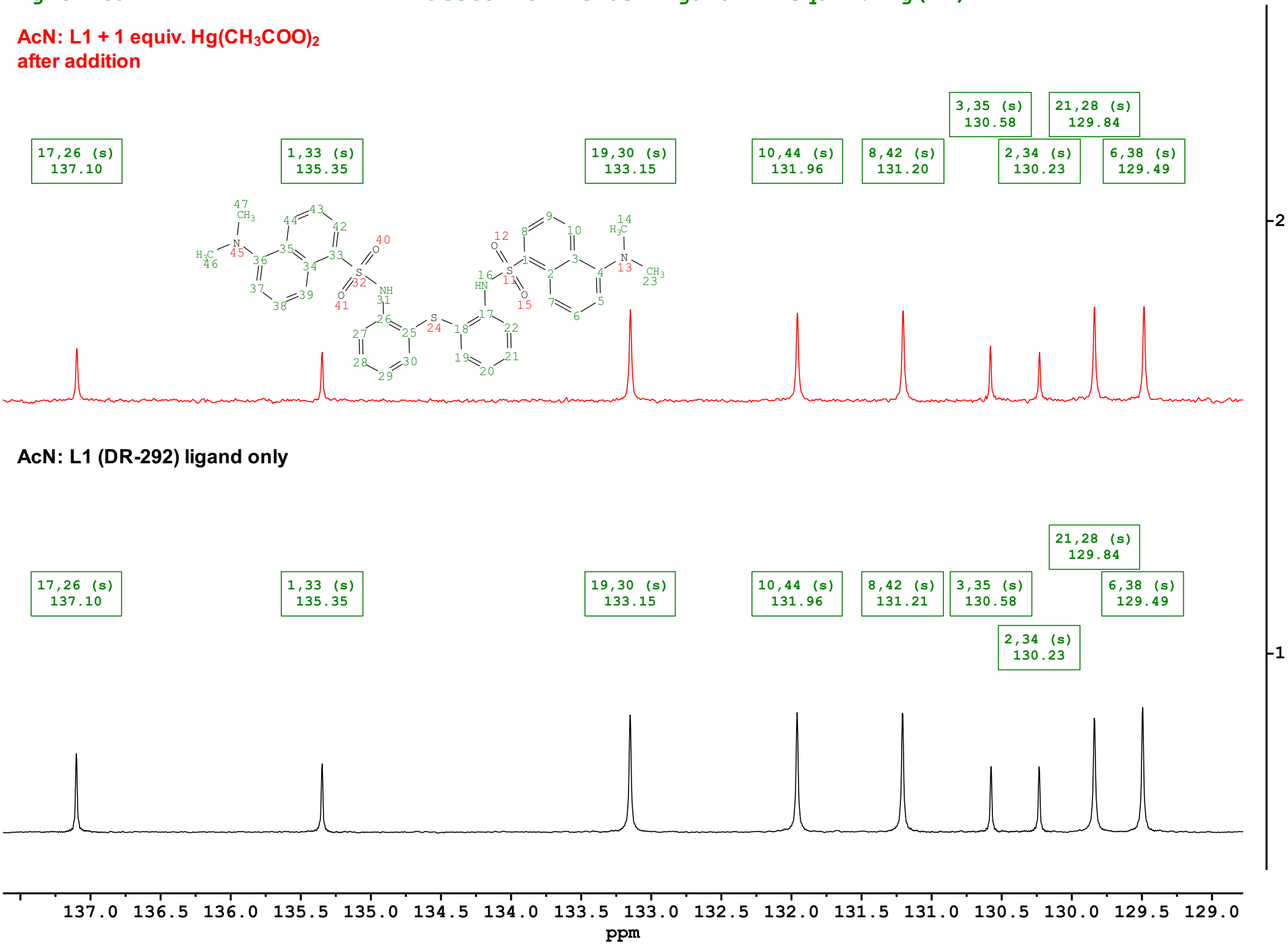
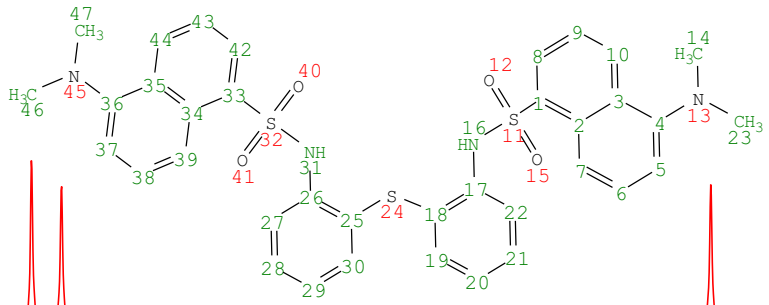



Fig SX170 L1 acetonitrile-d3 ligand + 1equiv. Hg(II)

AcN: L1 + 1 equiv. $Hg(CH_3COO)_2$ after addition



18,25 (s) 128.34

20,29 (s) 127.25

22,27 (s) 123.92

9,43 (s) 124.13

7,39 (s) 119.51

5,37 (s) 116.41

AcN: L1 (DR-292) ligand only

18,25 (s) 128.32

20,29 (s) 127.24

9,43 (s) 124.12

22,27 (s) 123.90

7,39 (s) 119.51

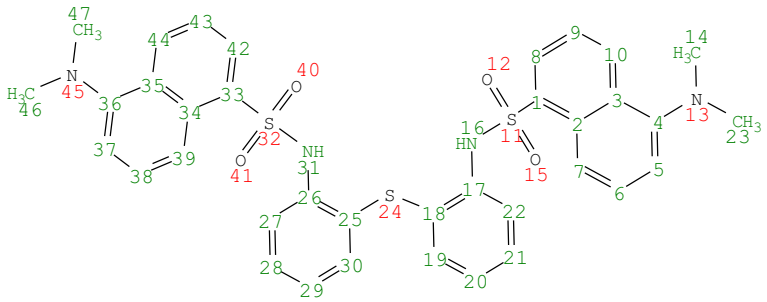
5,37 (s) 116.41

128.5 127.5 126.5 125.5 124.5 123.5 122.5 121.5 120.5 119.5 118.5 117.5 116.5

ppm

Fig SX171 L1 acetonitrile-d3 ligand + 1equiv. Hg(II)

**AcN: L1 + 1 equiv. $Hg(CH_3COO)_2$ after addition**



14,23,46,47 (s)
45.62

-2

**AcN: L1 ligand only**

14,23,46,47 (s)
45.63

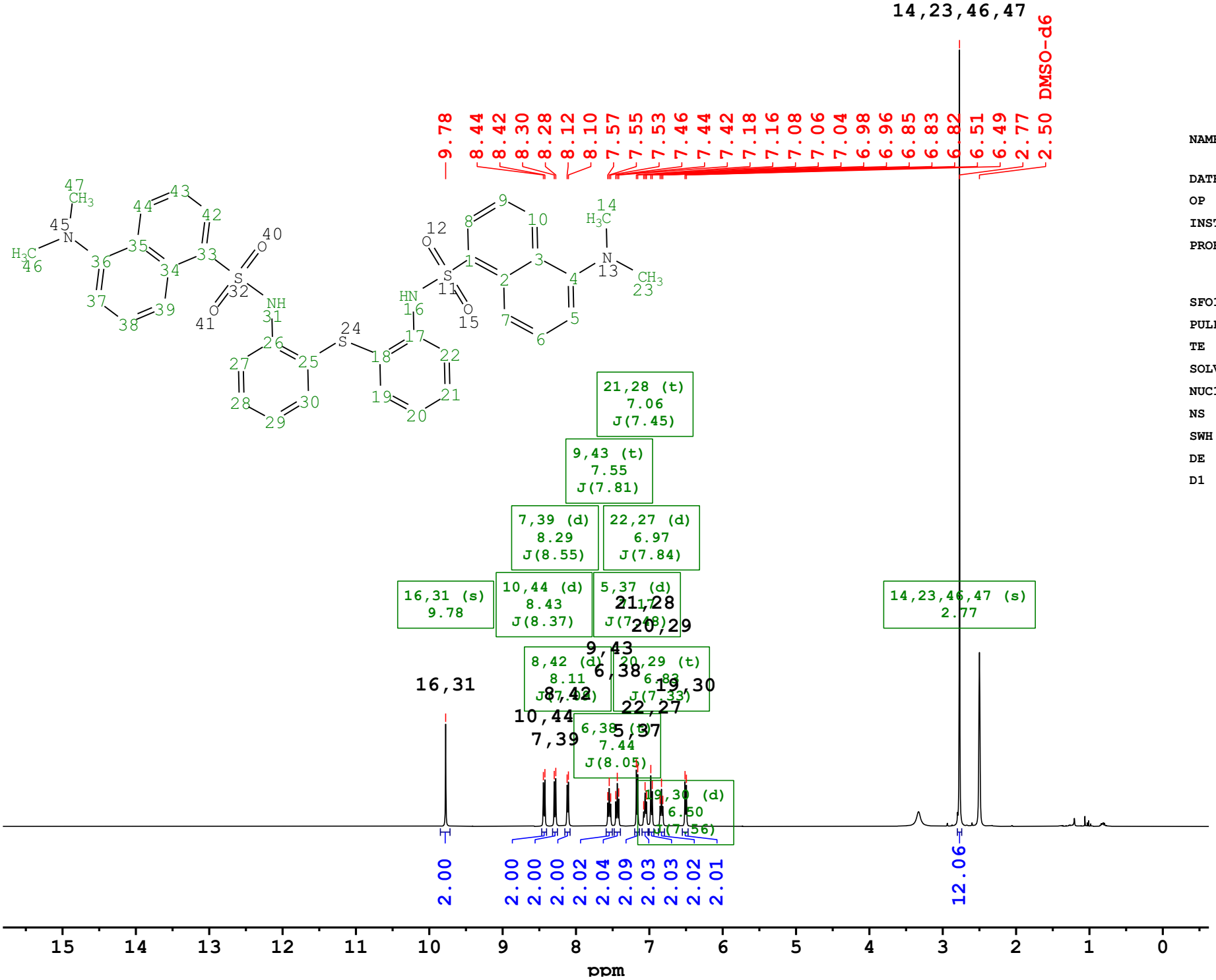
-1

46.30 46.20 46.10 46.00 45.90 45.80 45.70 45.60 45.50 45.40

ppm

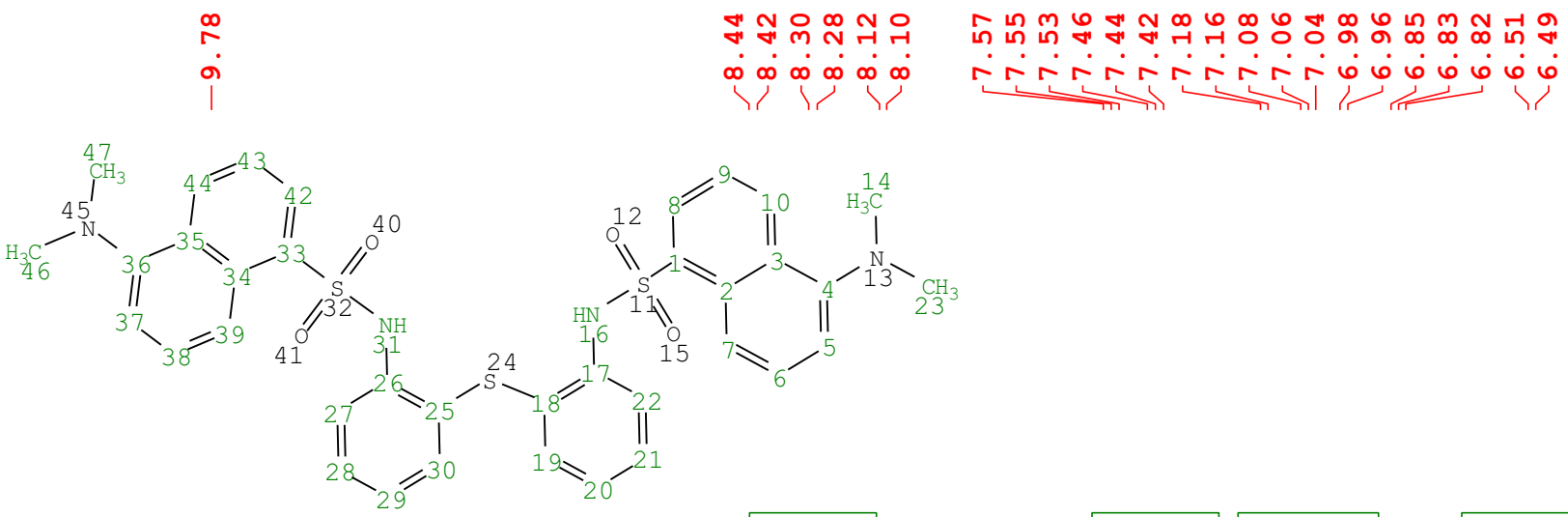
Fig SX172

L1 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.11.fid |
| DATE_TIME | 2024-12-19T21:40:20 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

**Fig SX173** **L1 dmso-d6 ligand + 1equiv. Cu(II)**






| NAME | AK-DR-165-0-DMSO-Cu.11.fid |
|---|---|
| DATE_TIME | 2024-12-19T21:40:20 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

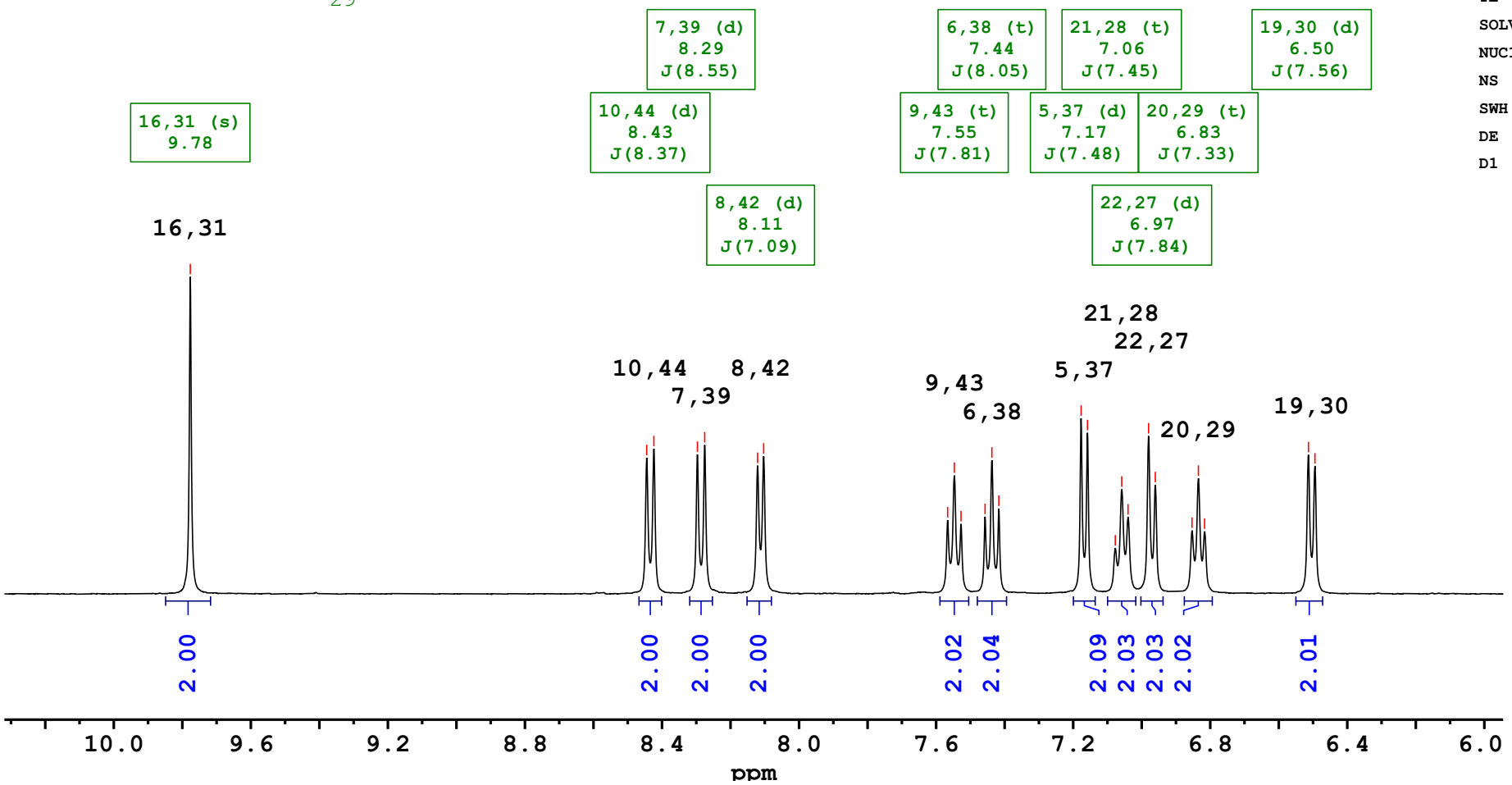
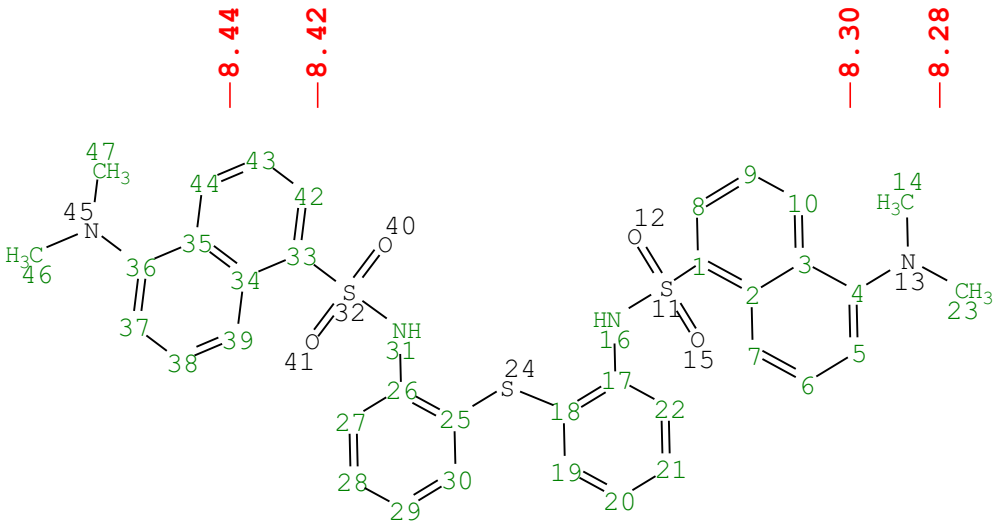


**Fig SX174** **L1 dmso-d6 ligand + 1equiv. Cu(II)**




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.11.fid |
| DATE_TIME | 2024-12-19T21:40:20 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

10,44 (d)
8.43
J(8.37)

7,39 (d)
8.29
J(8.55)

8,42 (d)
8.11
J(7.09)

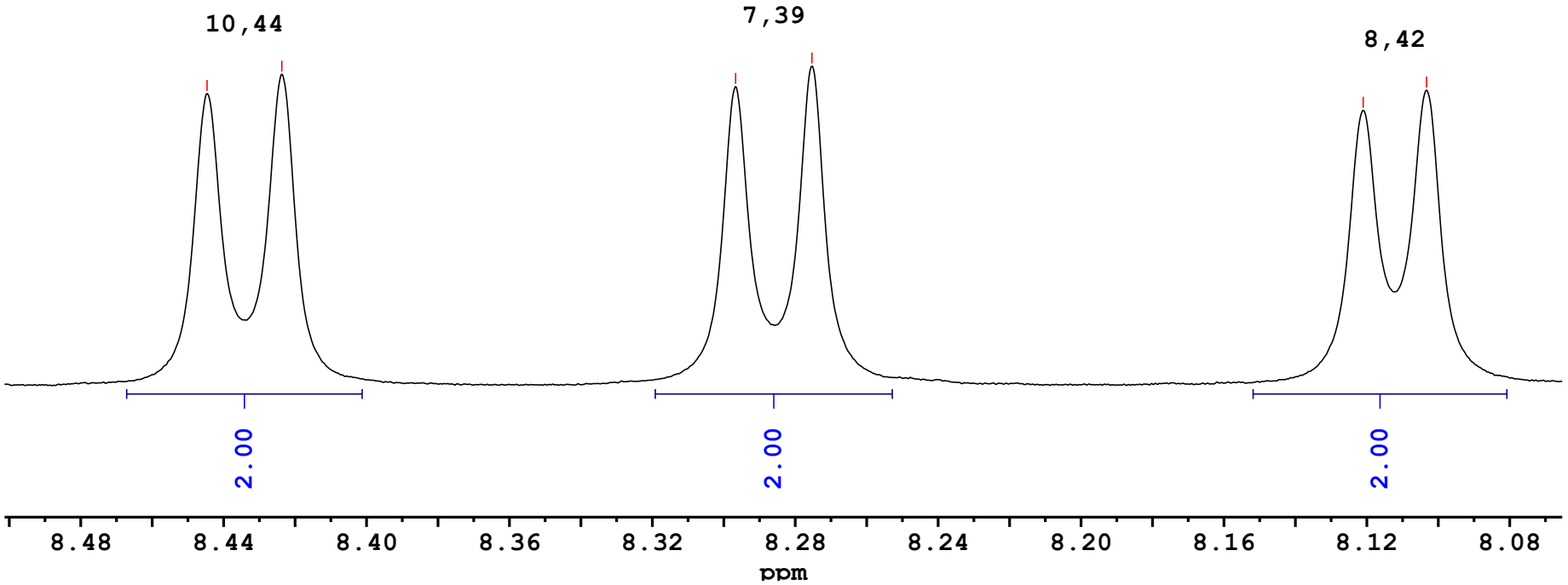
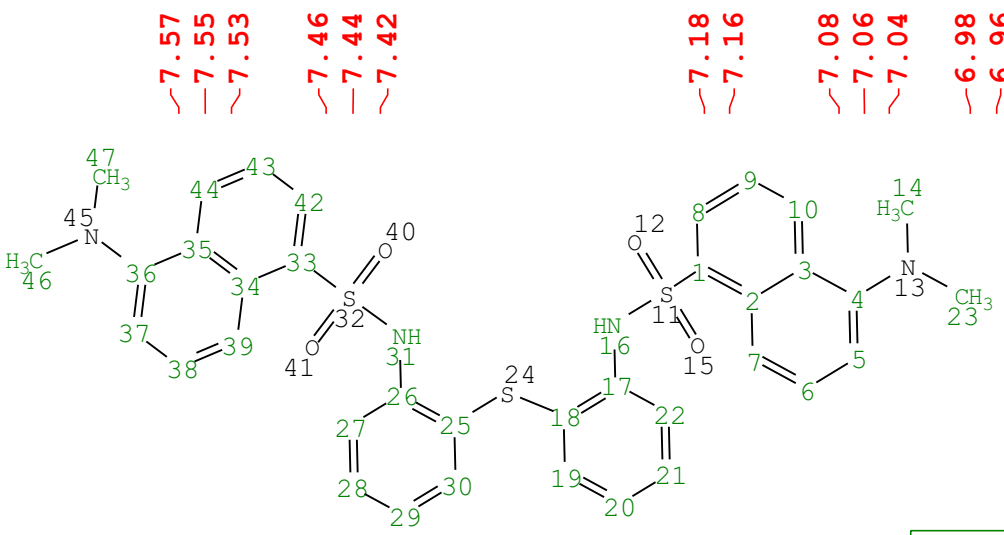


**Fig SX175** **L1 dmso-d6 ligand + 1equiv. Cu(II)**




| NAME | AK-DR-165-0-DMSO-Cu.11.fid |
|---|---|
| DATE_TIME | 2024-12-19T21:40:20 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

9,43 (t) 7.55 J(7.81)

6,38 (t) 7.44 J(8.05)

5,37 (d) 7.17 J(7.48)

21,28 (t) 7.06 J(7.45)

22,27 (d) 6.97 J(7.84)

20,29 (t) 6.83 J(7.33)

19,30 (d) 6.50 J(7.56)

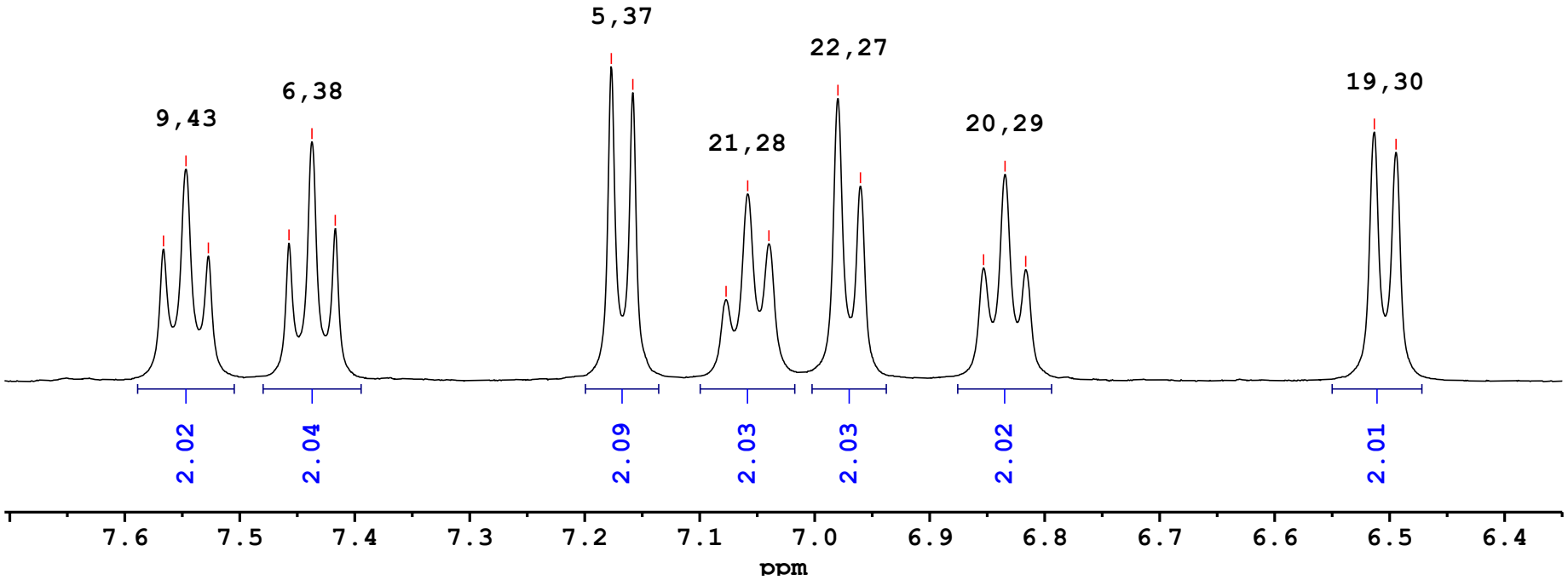
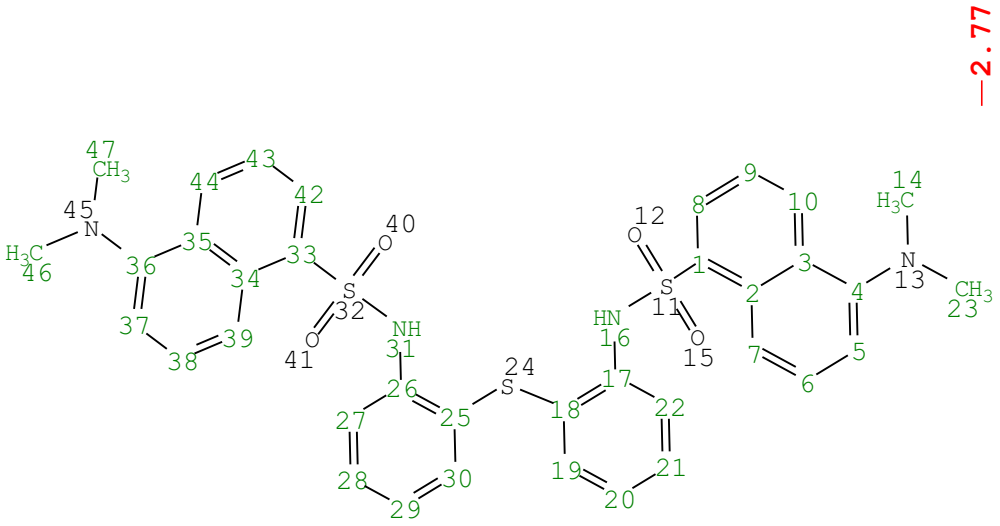


**Fig SX176** **L1 dmso-d6 ligand + 1equiv. Cu(II)**




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.11.fid |
| DATE_TIME | 2024-12-19T21:40:20 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 32 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

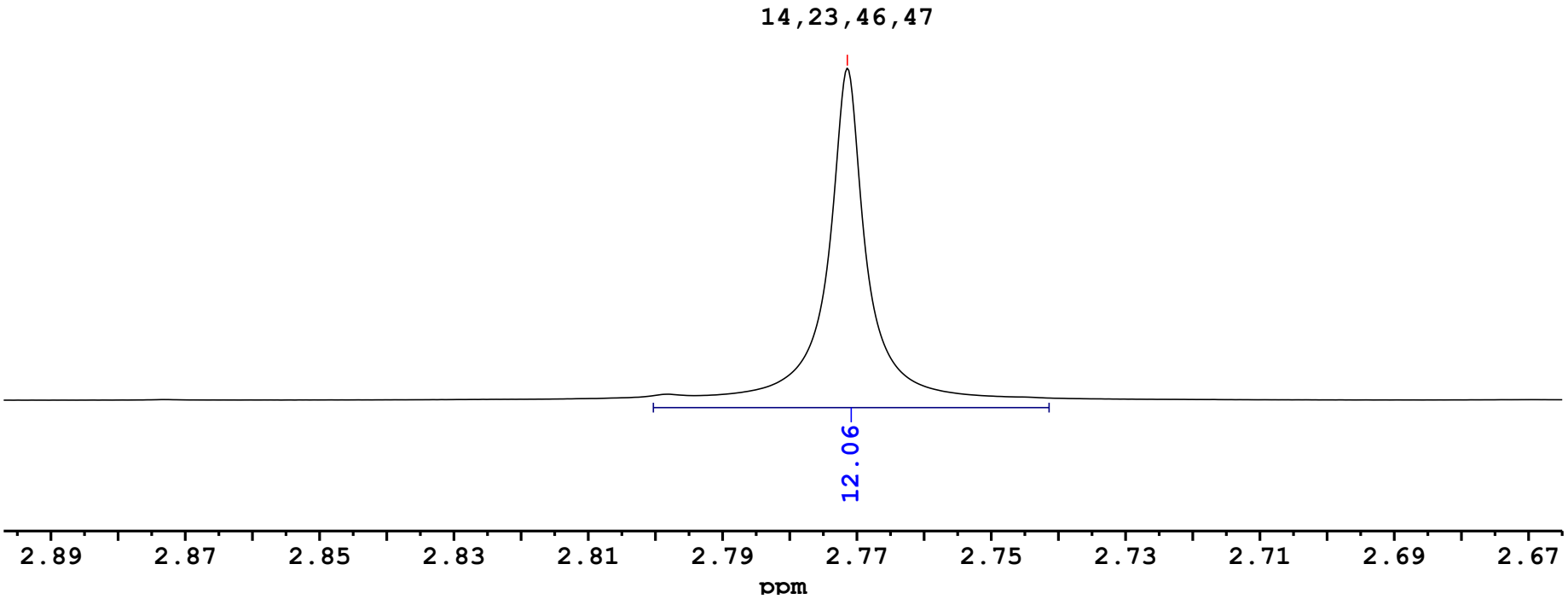
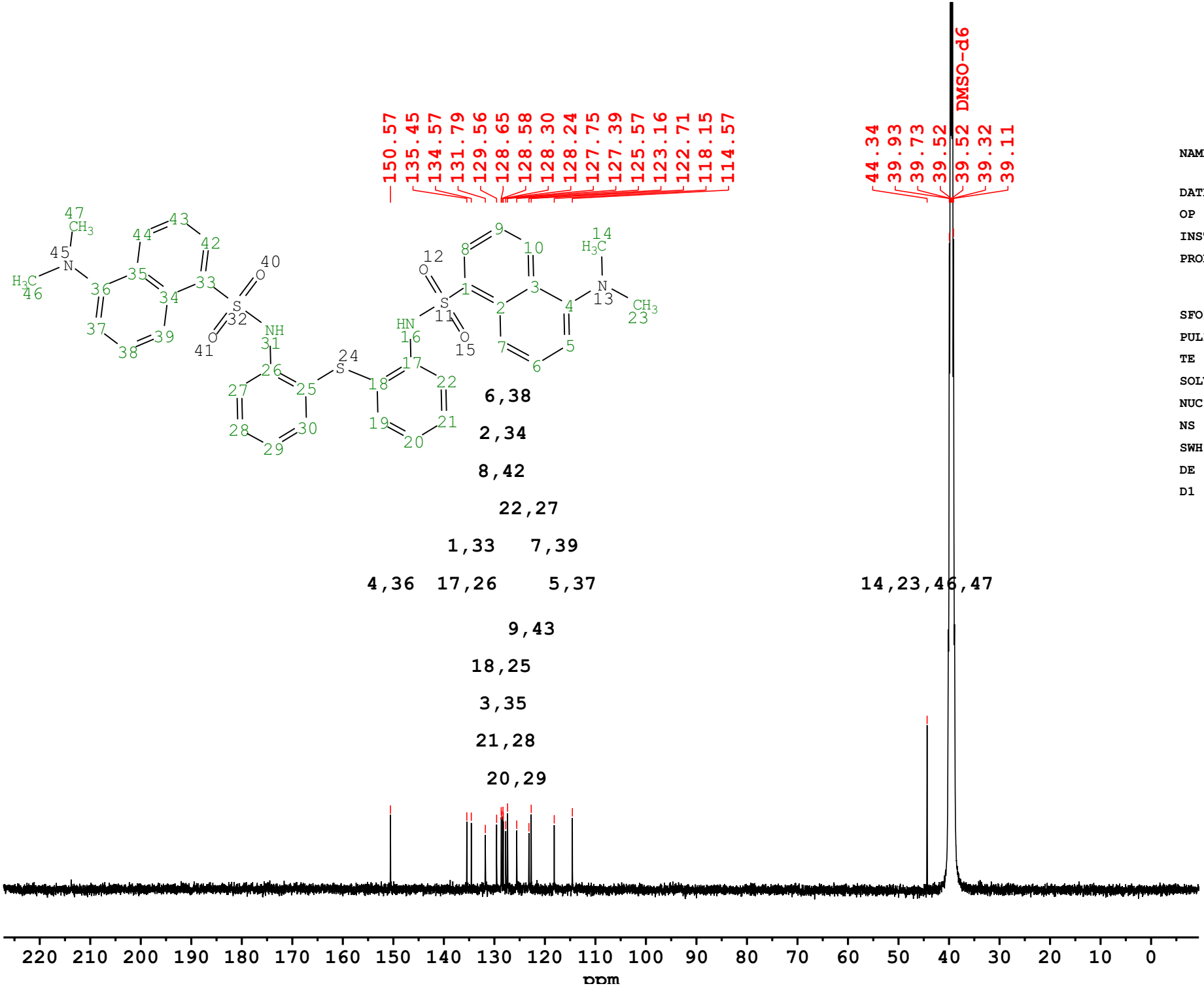


Fig SX177

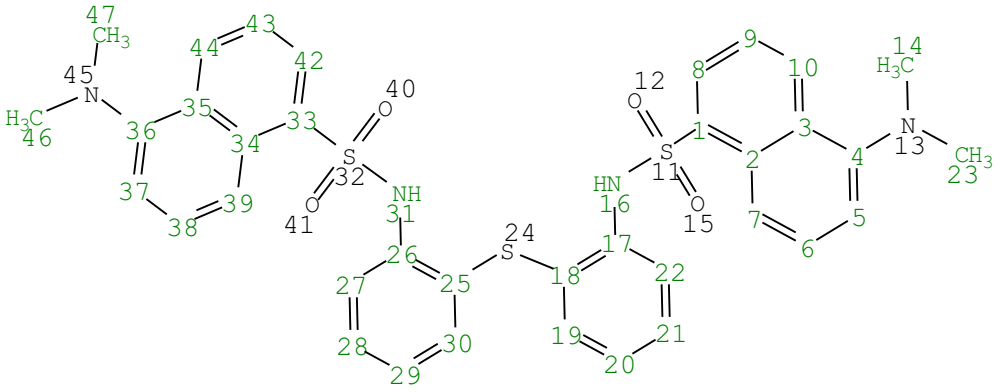
L1 dmso-d6 ligand + 1equiv. Cu(II)




NAME AK-DR-165-0-DMSO-Cu.12.fid
DATE_TIME 2024-12-19T22:18:57
OP Dessislava.Gerginova
INSTRUM Avance Neo 400
PROBHD Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N)
SFO1 150.9188042 Hz
PULPROG zgdc30
TE 298.0 K
SOLVENT DMSO
NUC1 13C
NS 1024
SWH 36057.692 Hz
DE 6.50 usec
D1 1.5000 sec

**Fig SX178** **L1 dmso-d6 ligand + 1equiv. Cu(II)**

150.57 135.45 134.57 131.79 129.56 128.65 128.58 128.30 128.24 127.75 127.39 125.57 123.16 122.71 118.15 114.57




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.12.fid |
| DATE_TIME | 2024-12-19T22:18:57 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 1024 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

6,38 2,34 1,33 8,42 22,27 4,36 17,26 19,30 18,25 20,29 9,43 7,39 5,37 3,35 21,28 10,44

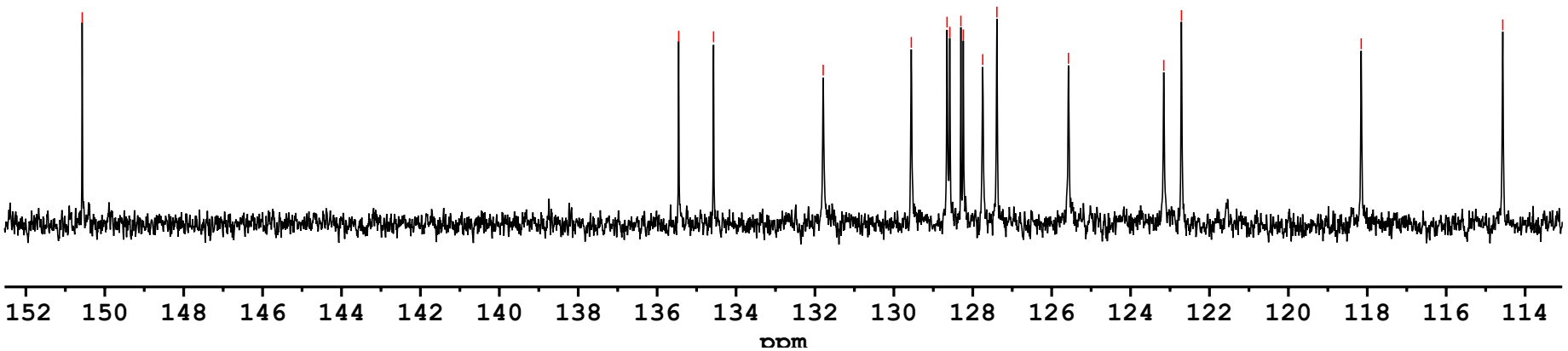
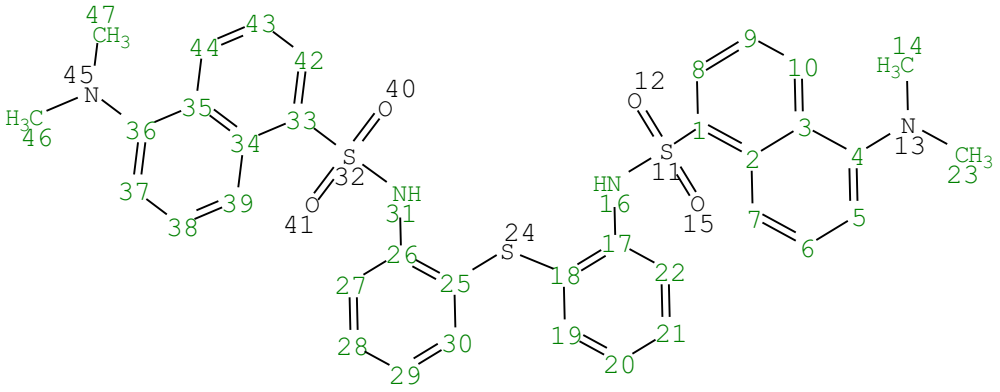


**Fig SX179** **L1 dmso-d6 ligand + 1equiv. Cu(II)**

131.79 129.56 128.65 128.58 128.30 128.24 127.75 127.39 125.57



| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.12.fid |
| DATE_TIME | 2024-12-19T22:18:57 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 1024 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

8,42 6,38

19,30 10,44 18,25 2,34 21,28 20,29

3,35

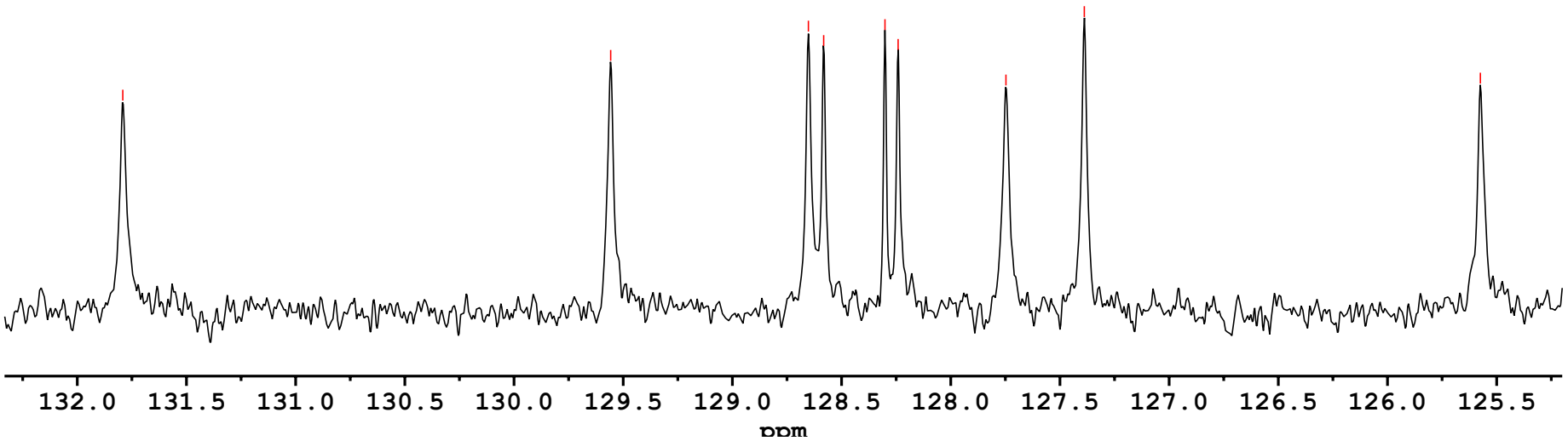
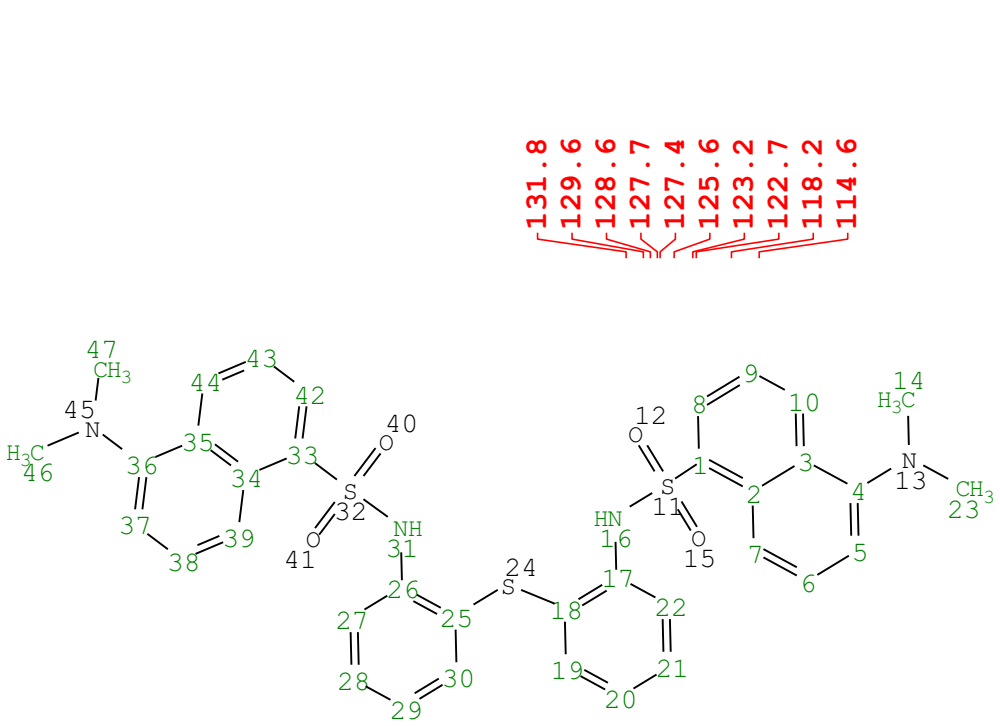


Fig SX180

L1 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.12.fid |
| DATE_TIME | 2024-12-19T22:18:57 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9319844 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 1024 |
| SWH | 35714.286 Hz |
| DE | 18.00 usec |
| D1 | 1.5000 sec |

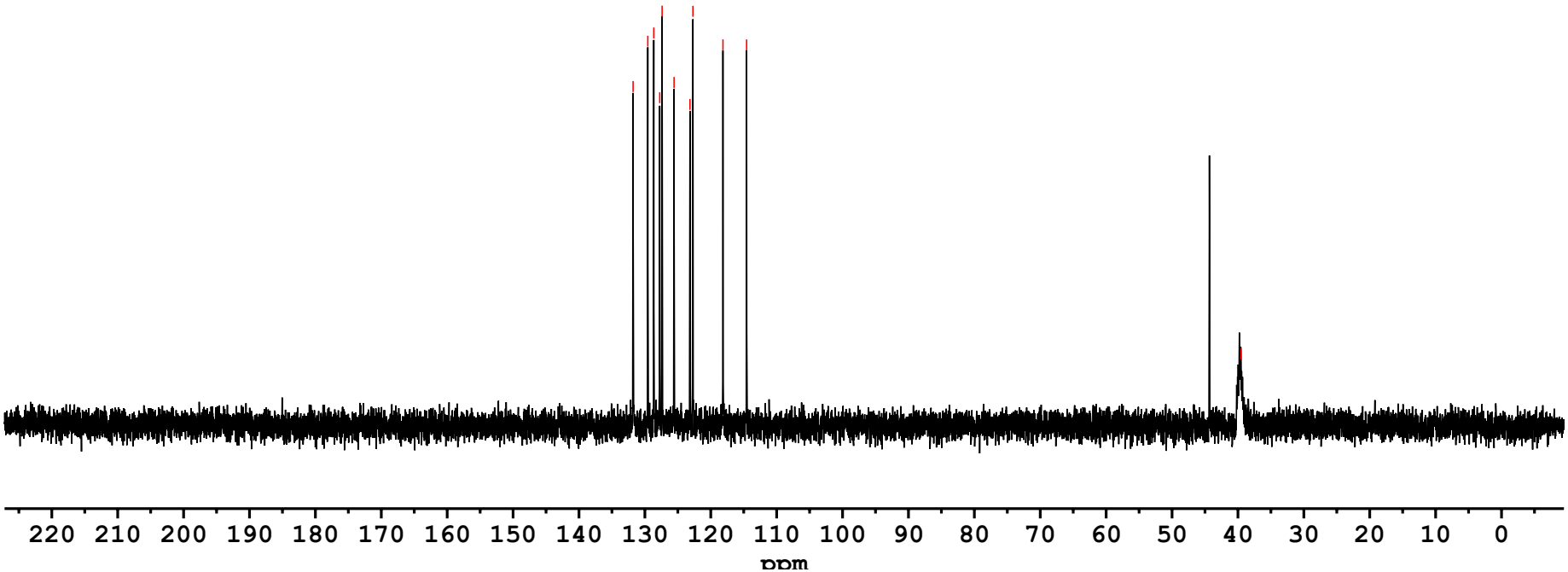
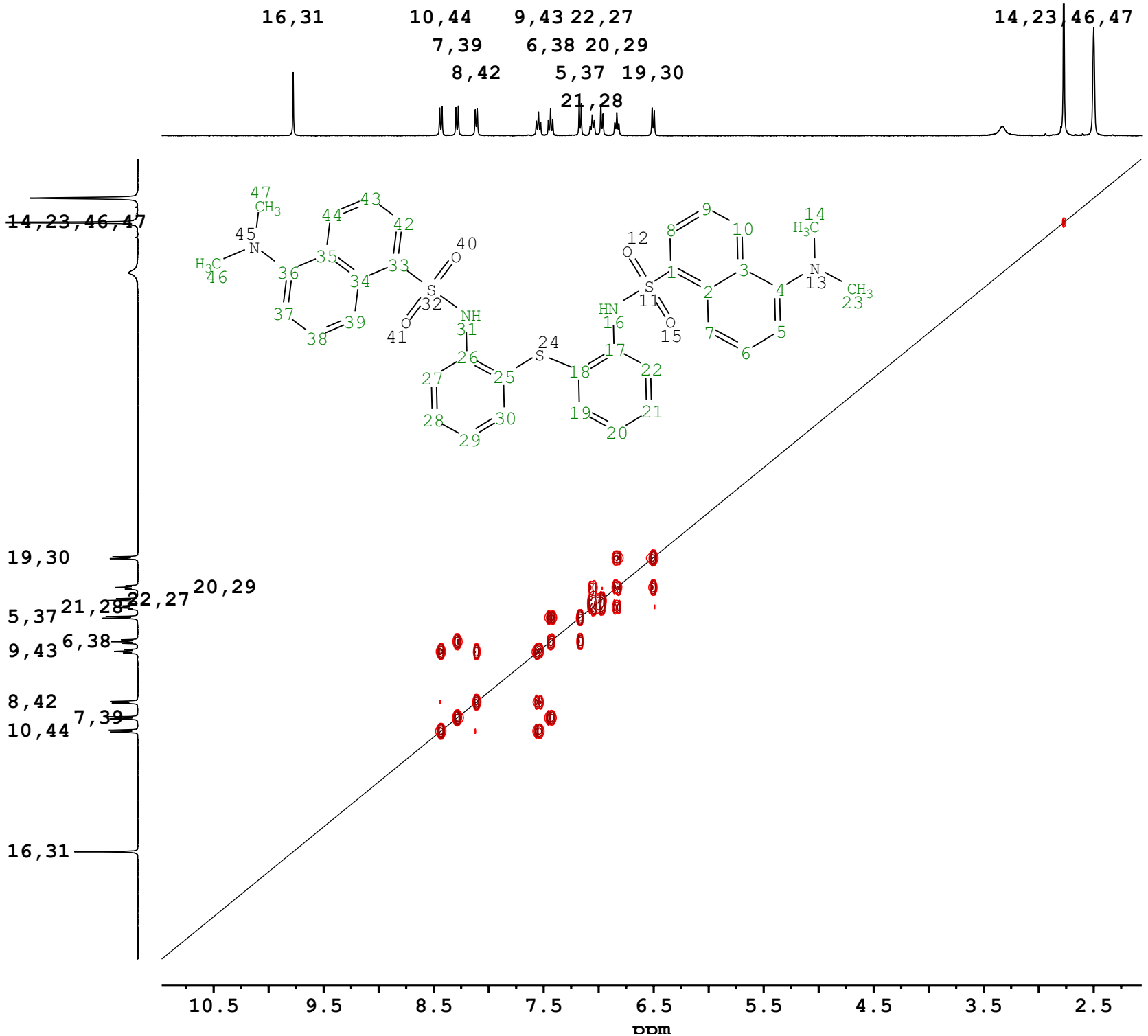


Fig SX181

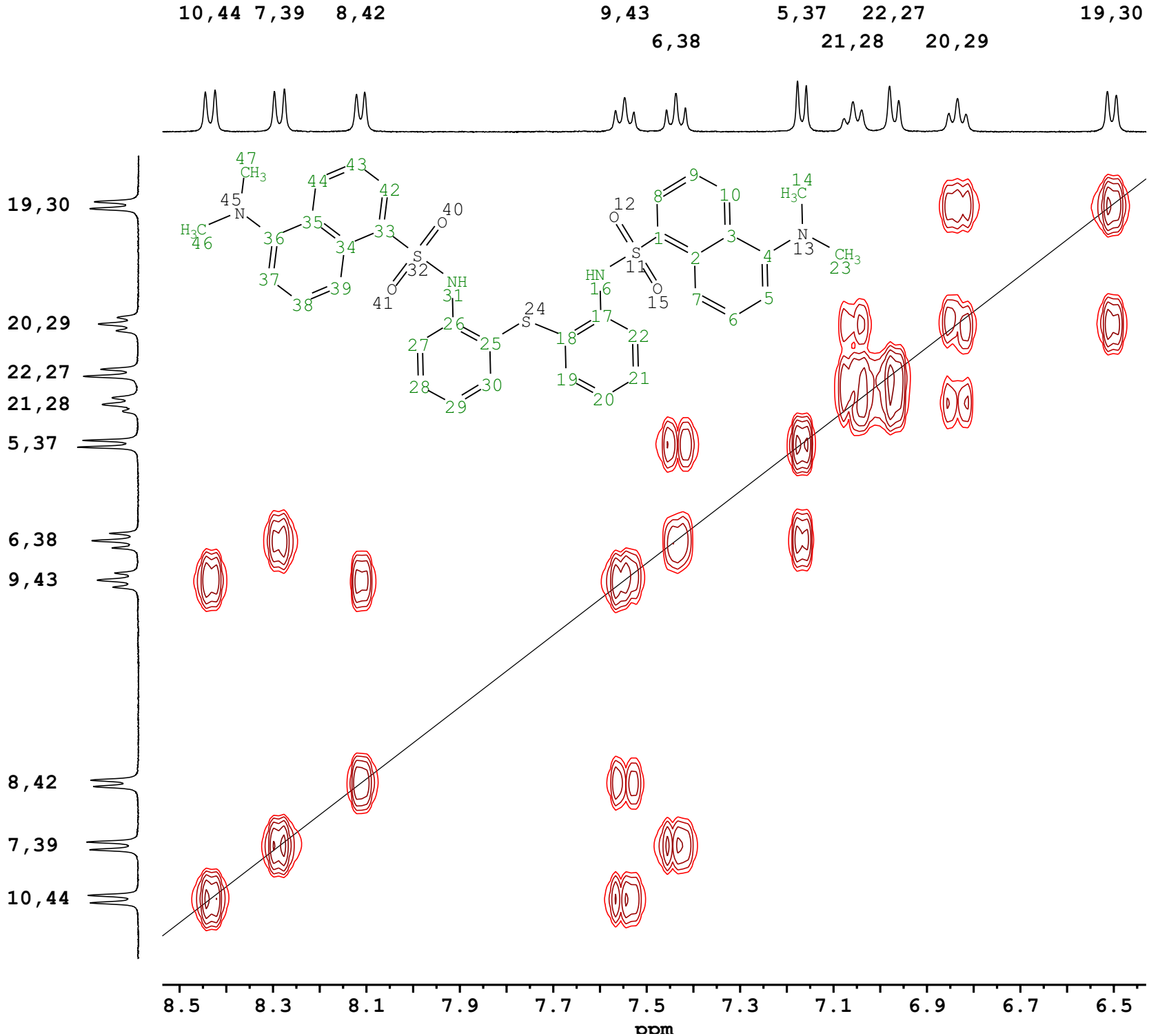
L1 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.14.ser |
| DATE_TIME | 2024-12-19T22:43:51 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 1 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0057 sec |

Fig SX182

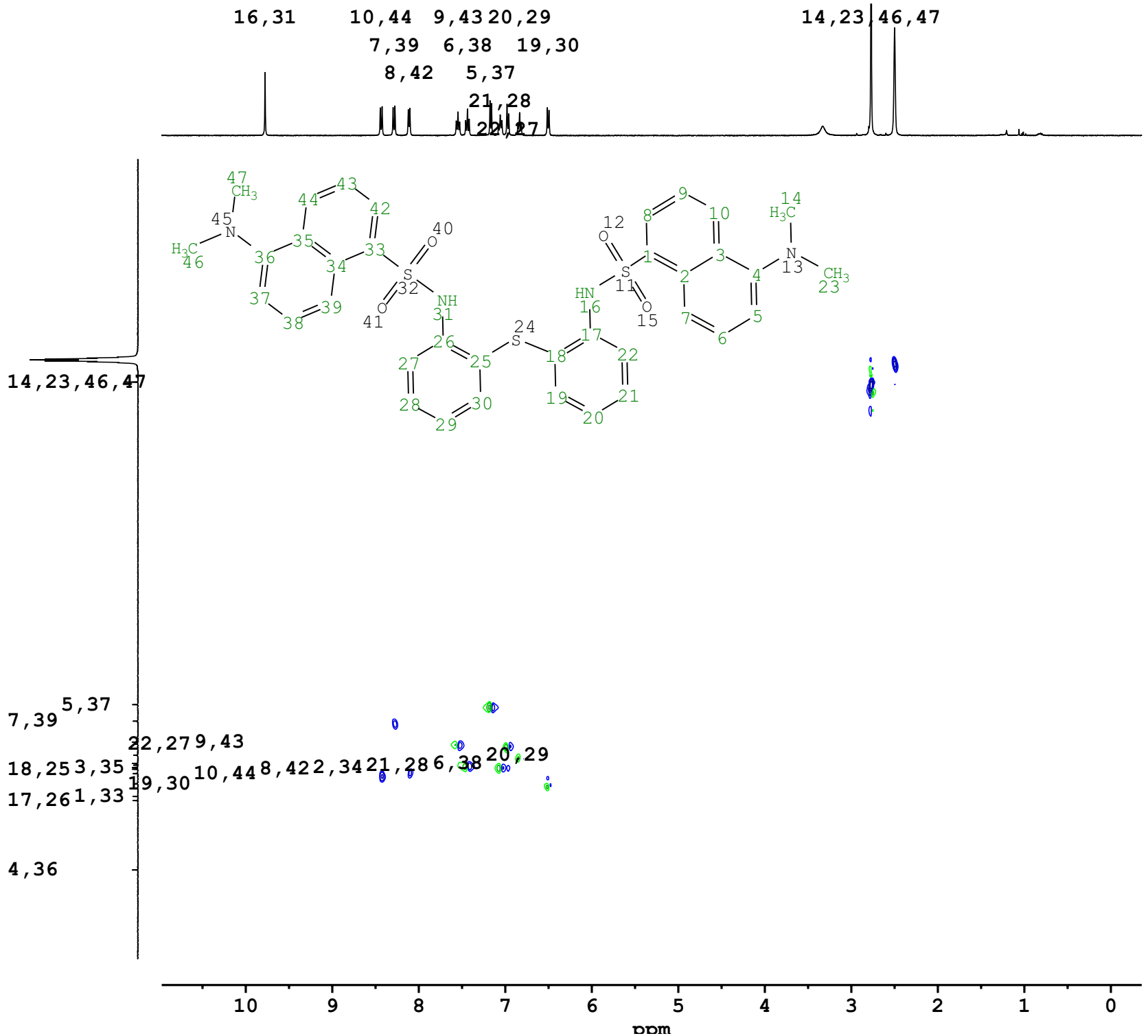
L1 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.14.ser |
| DATE_TIME | 2024-12-19T22:43:51 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 1 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0057 sec |

Fig SX183

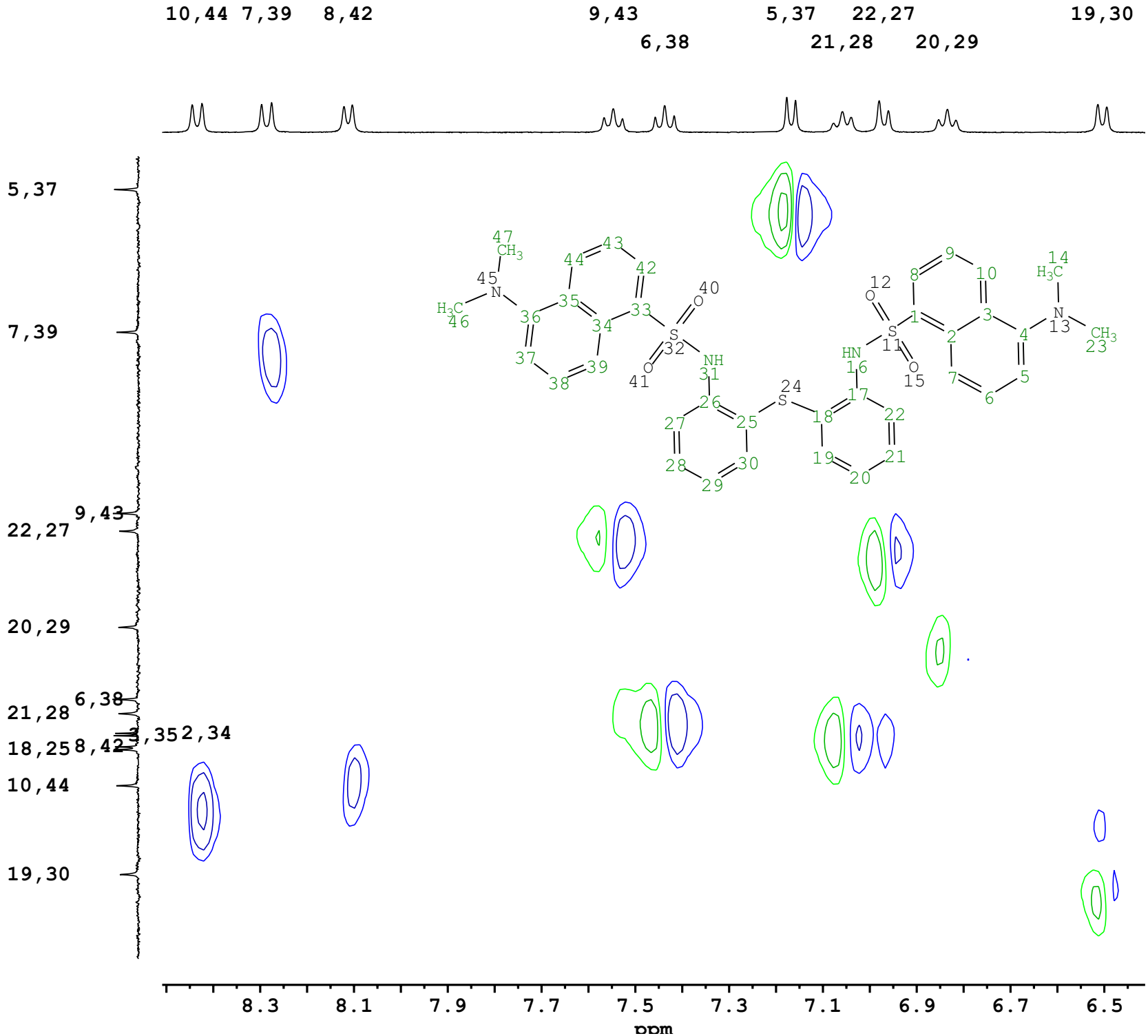
# L1 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.15.ser |
| DATE_TIME | 2024-12-19T22:55:09 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 2 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX184

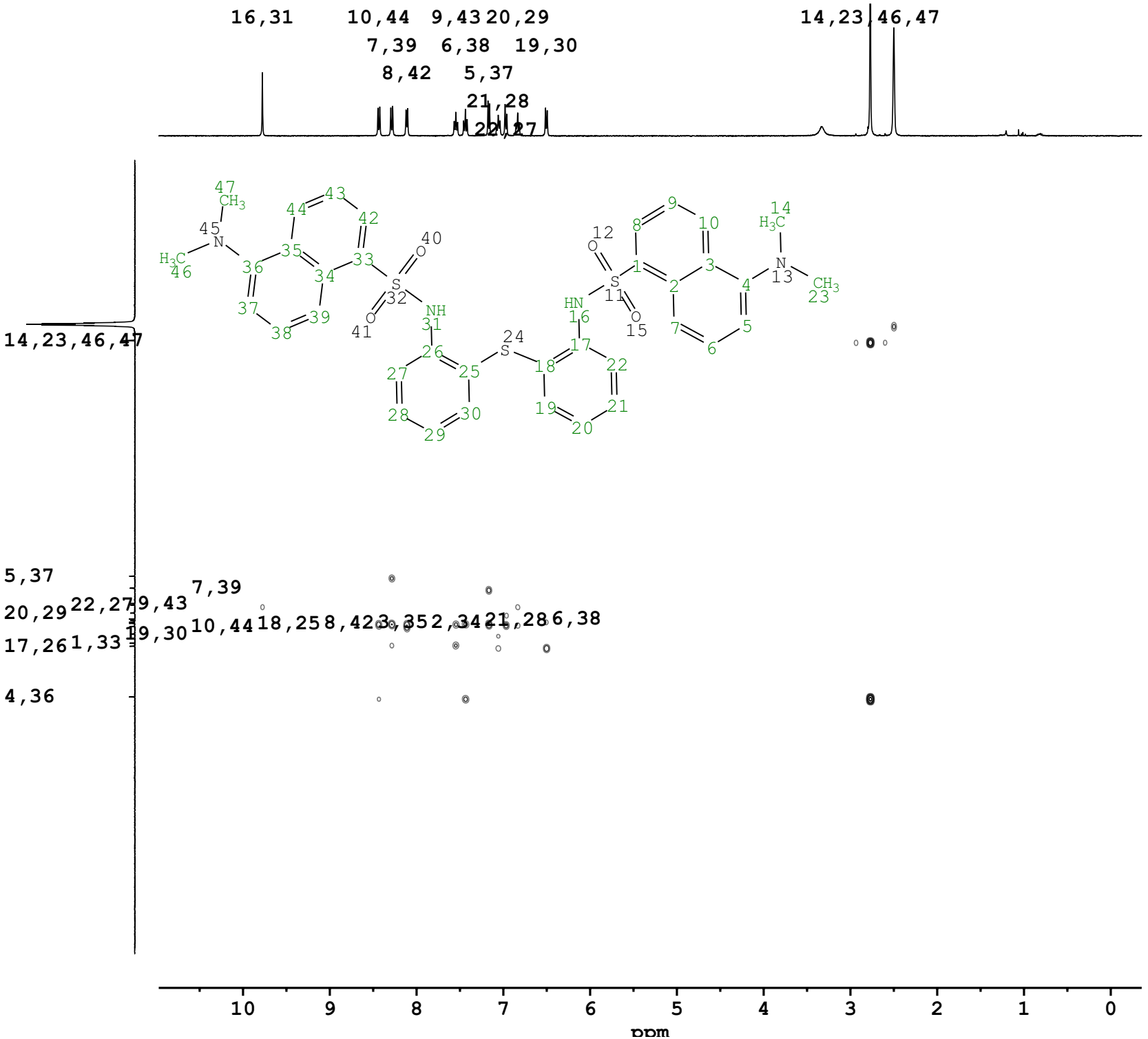
L1 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.15.ser |
| DATE_TIME | 2024-12-19T22:55:09 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 2 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX185

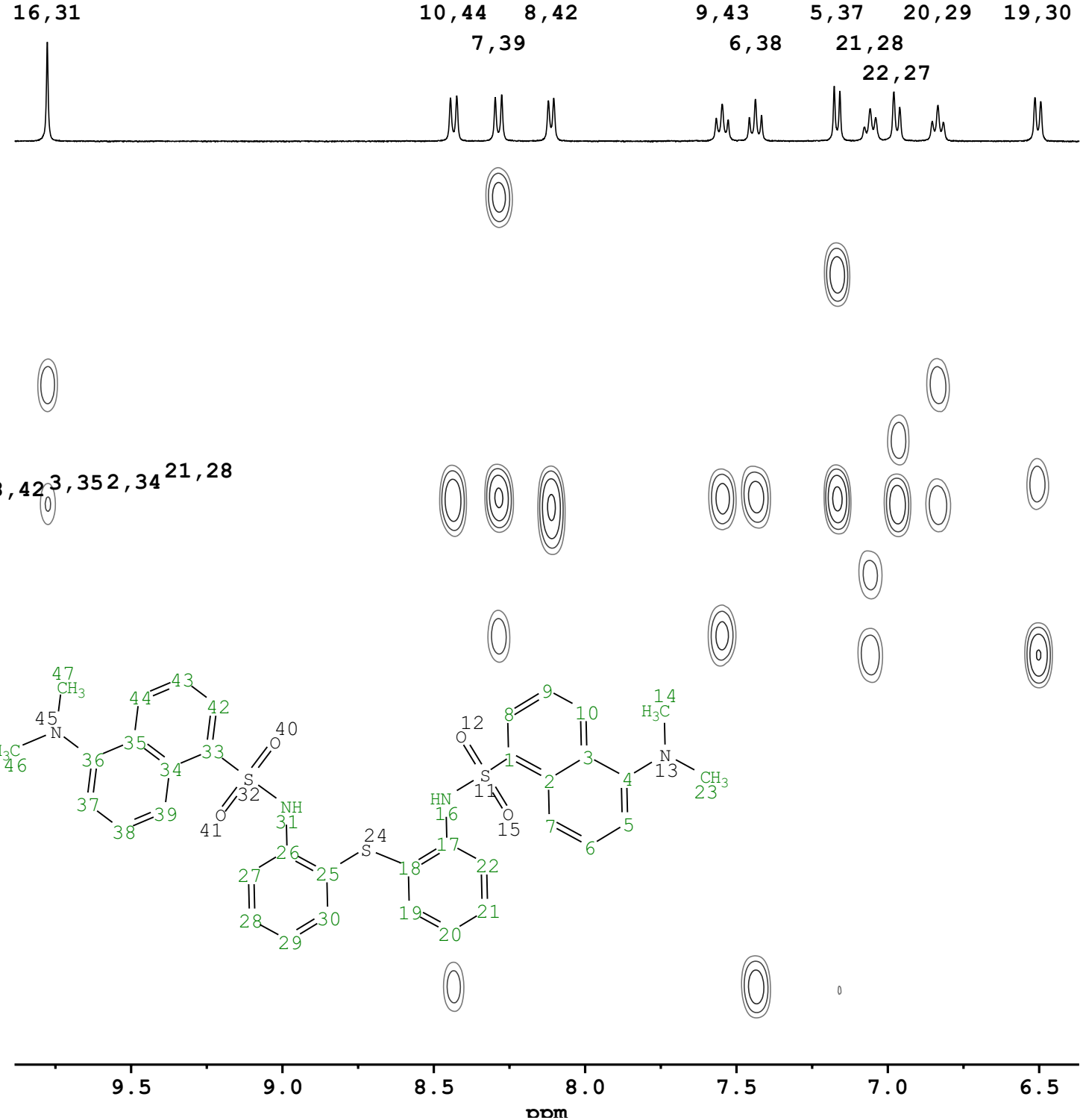
# L1 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.16.ser |
| DATE_TIME | 2024-12-19T23:37:44 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX186

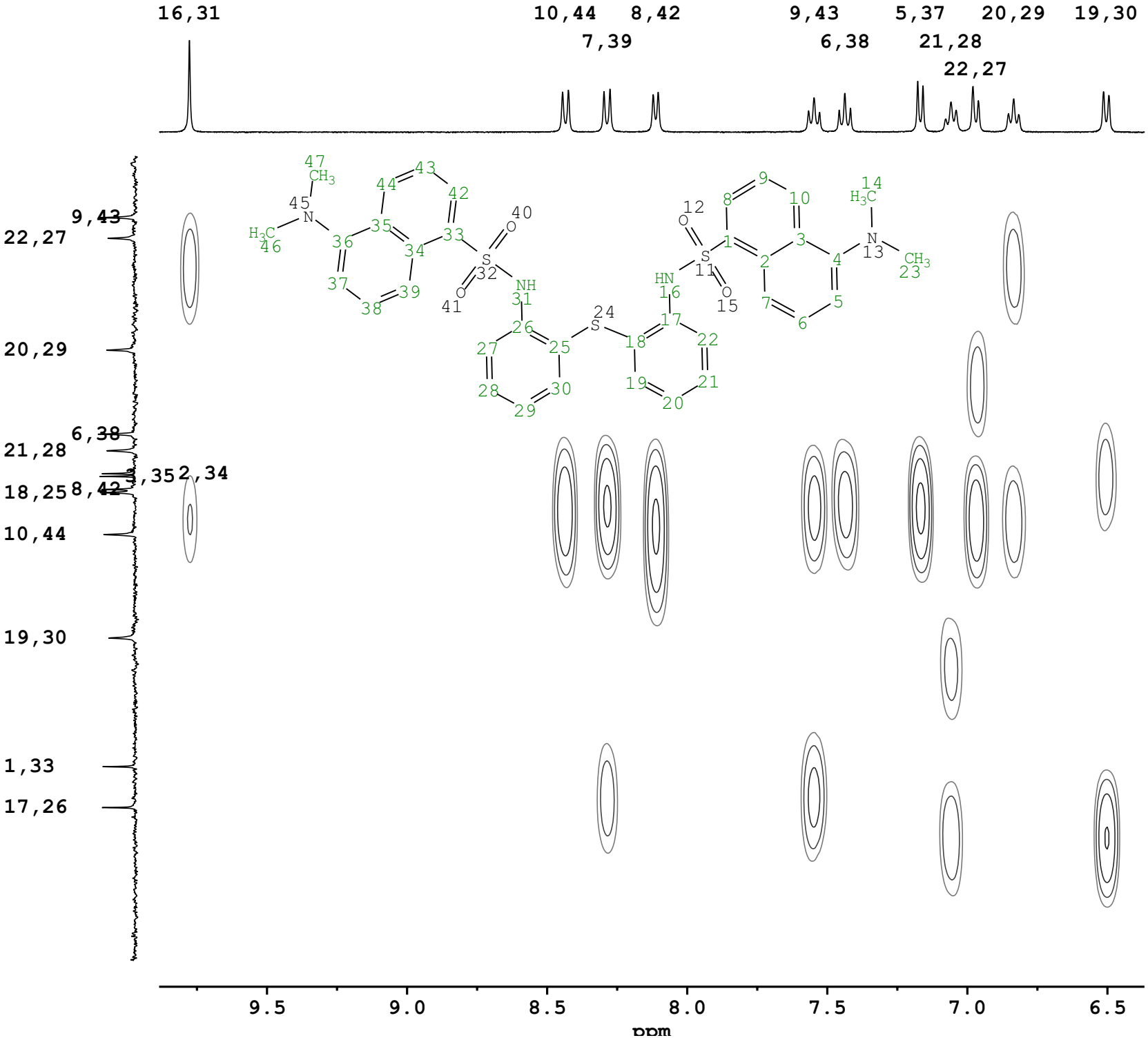
L1 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.16.ser |
| DATE_TIME | 2024-12-19T23:37:44 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX187

L1 dmso-d6 ligand + 1equiv. Cu(II)

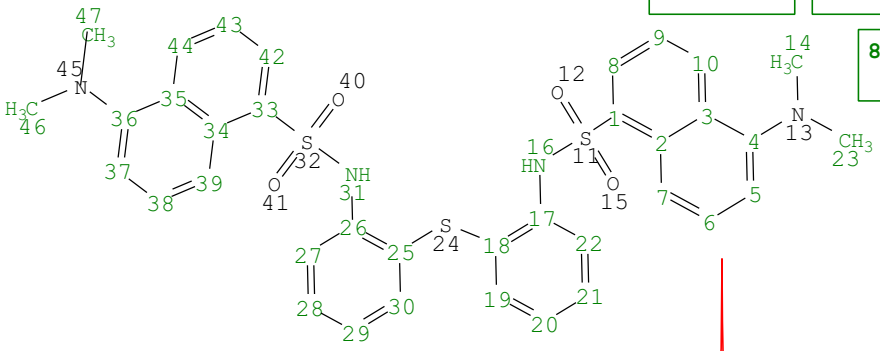



| | |
|---|---|
| NAME | AK-DR-165-0-DMSO-Cu.16.ser |
| DATE_TIME | 2024-12-19T23:37:44 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX188

L1 dmso-d6 ligand + 1equiv. Cu(II)

**DMSO: L1 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition**



9,43 (t) 7.55

7,39 (d) 8.29 | 21,28 (t) 7.06

16,31 (s) 9.78 | 10,44 (d) 8.43 | 5,37 (d) 7.17

14,23,46,47 (s) 2.77

8,42 (d) 8.11 | 22,27 (d) 6.97

6,38 (t) 7.44

**DMSO: L1 ligand only**

9,43 (dd) 7.57

7,39 (d) 8.31 | 21,28 (td) 7.08

16,31 (s) 9.80 | 10,44 (d) 8.46 | 5,37 (d) 7.19

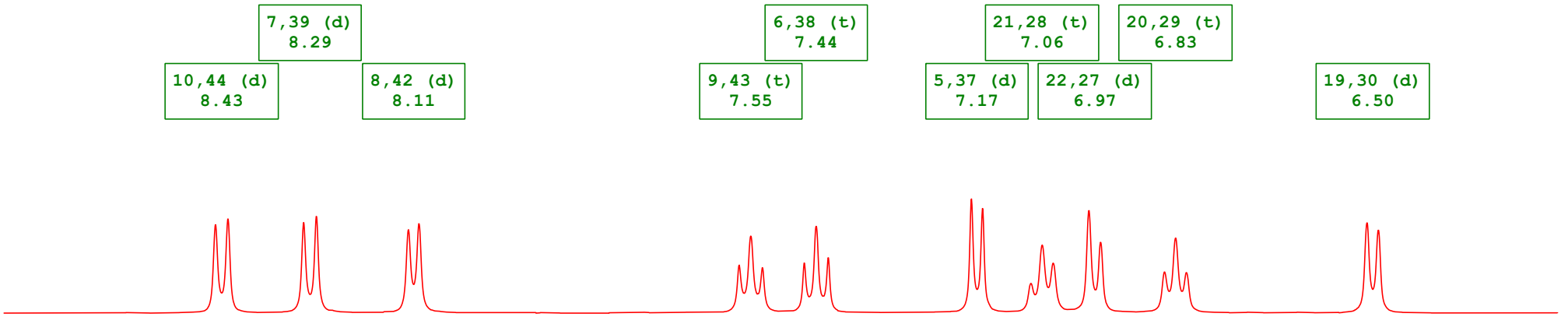
14,23,46,47 (s) 2.80

8,42 (dd) 8.14 | 20,29 (td) 6.86

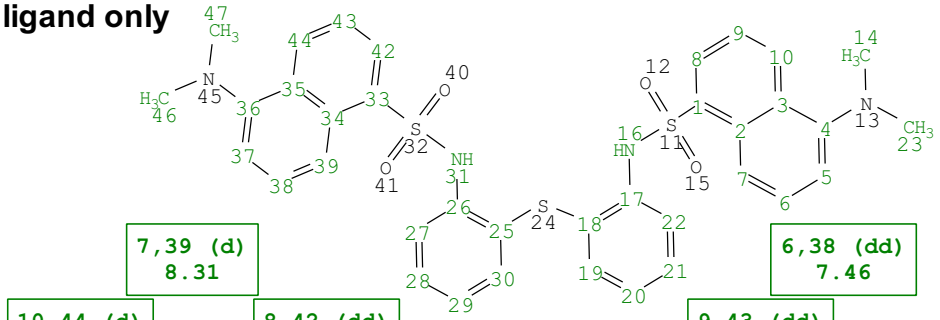
6,38 (dd) 7.46

Fig SX189 L1 dmso-d6 ligand + 1equiv. Cu(II)

**DMSO: L1 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition**




**DMSO: L1 ligand only**



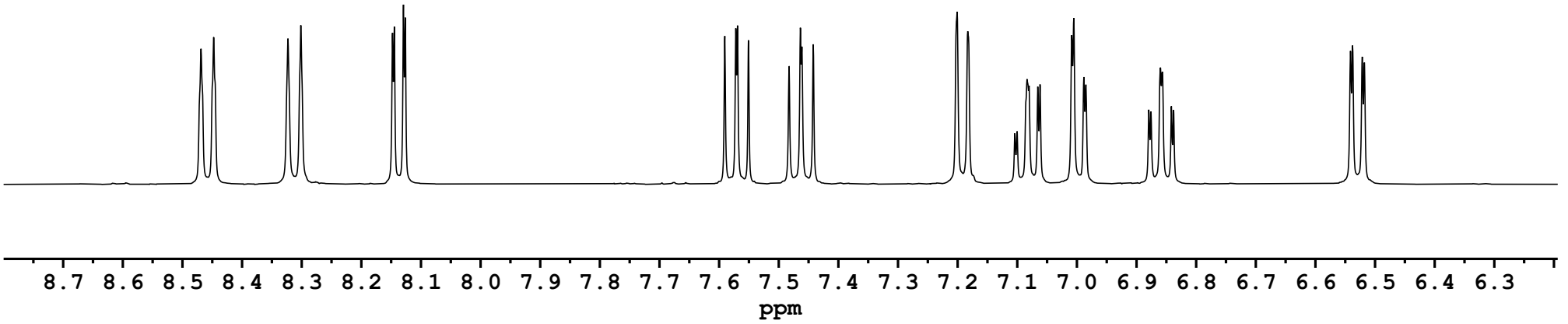
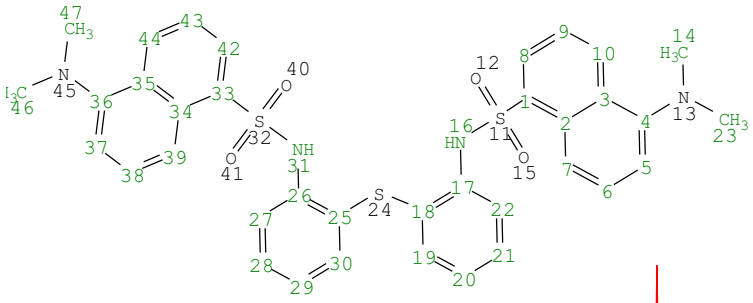


Fig SX190

L1 dmso-d6 ligand + 1equiv. Cu(II)

DMSO: L1 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition



22,27 (s) 123.16

17,26 (s) 135.45

7,39 (s) 118.15

4,36 (s) 150.57

1,33 (s) 134.57

5,37 (s) 114.57

14,23,46,47 (s) 44.34

9,43 (s) 122.71

18,25 (s) 128.65

DMSO: L1 ligand only

10,44 (s) 130.26

18,25 (s) 129.35

4,36 (s) 151.27

22,27 (s) 123.85

14,23,46,47 (s) 45.04

19,30 (s) 132.50

5,37 (s) 115.27

20,29 (s) 126.27

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

ppm

Fig SX191 L1 dmso-d6 ligand + 1equiv. Cu(II)

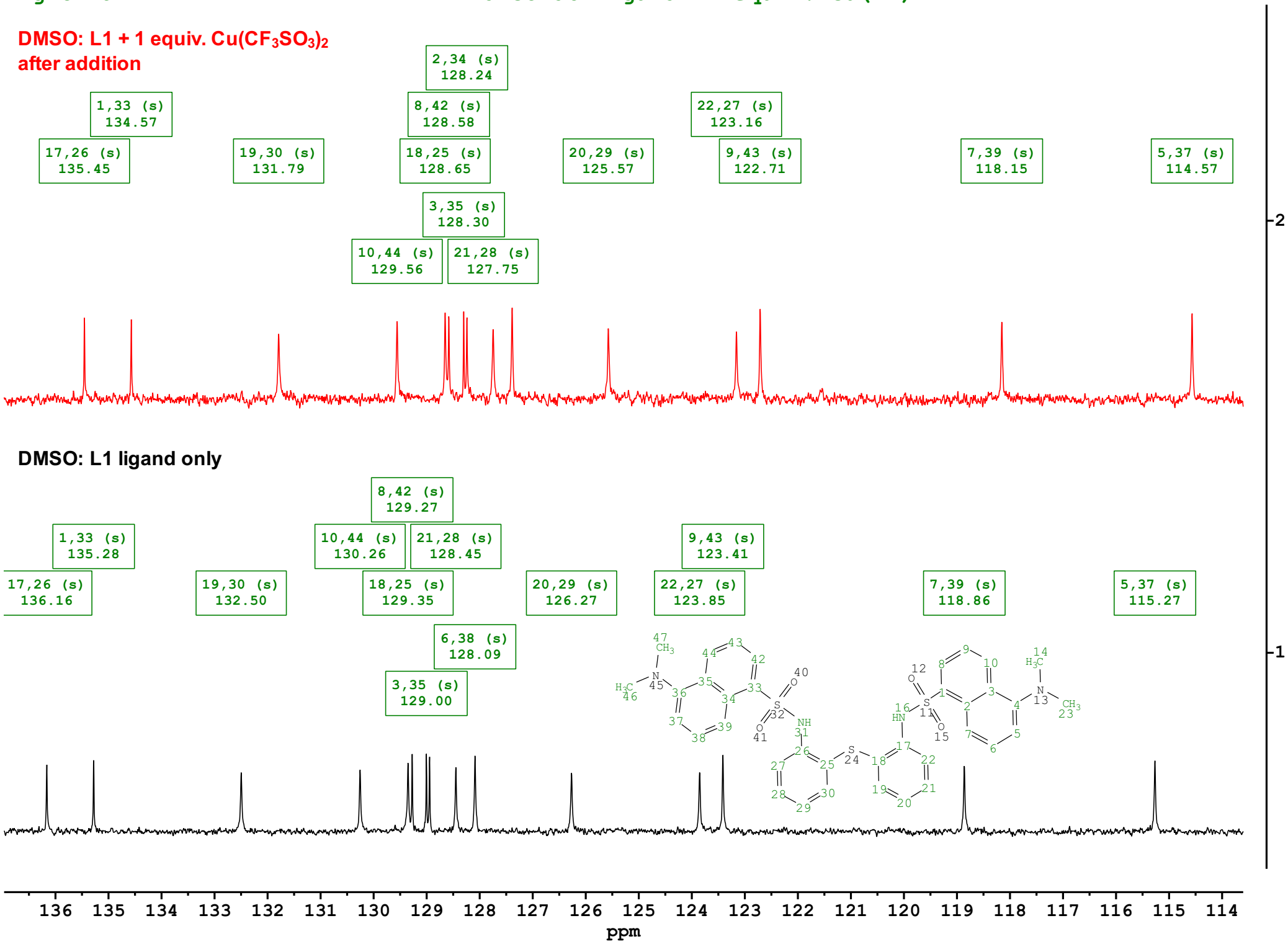


Fig SX192 L1 dmso-d6 ligand + 1equiv. Hg(II)

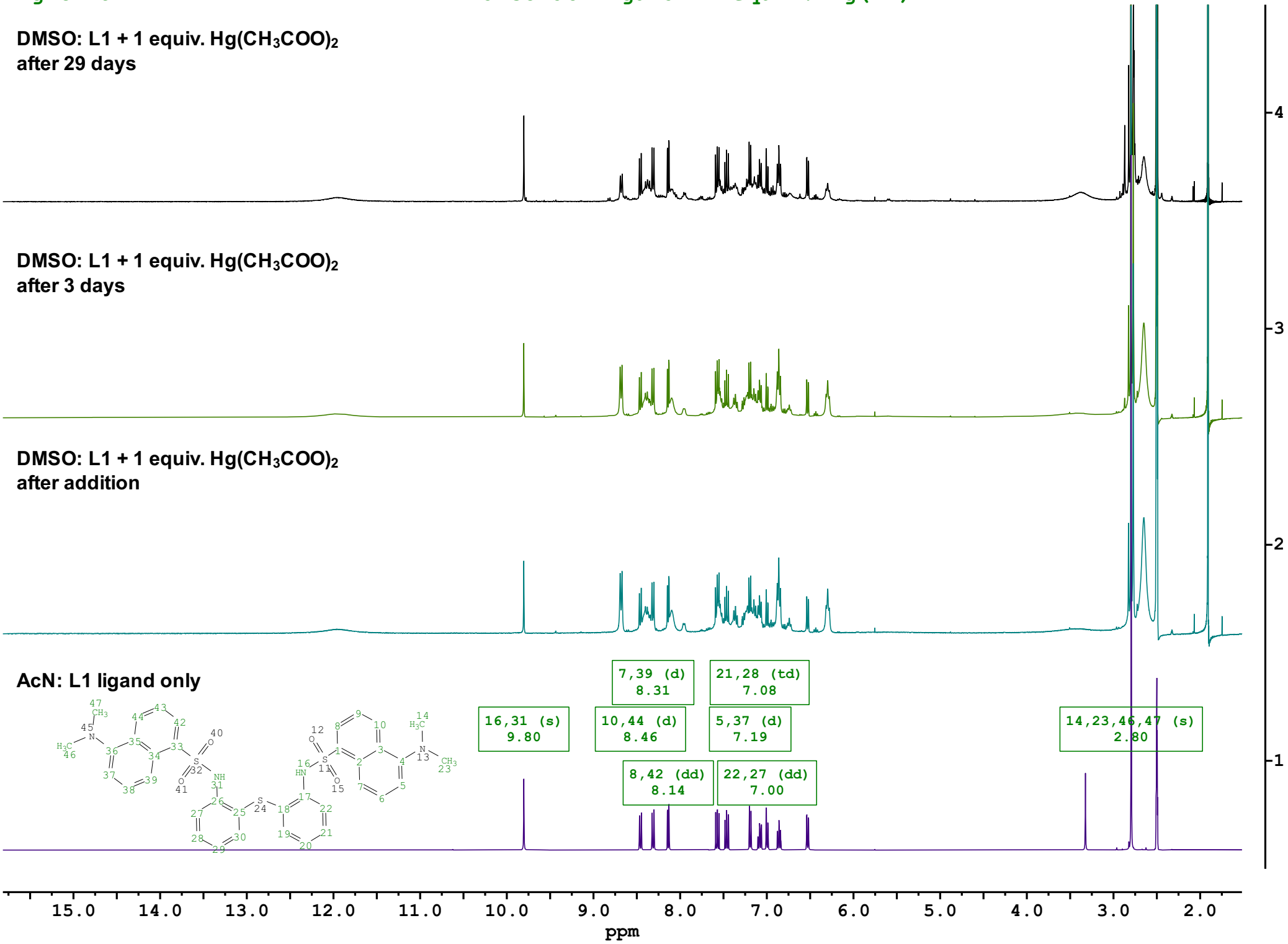


Fig SX193 L1 dmso-d6 ligand + 1equiv. Hg(II)

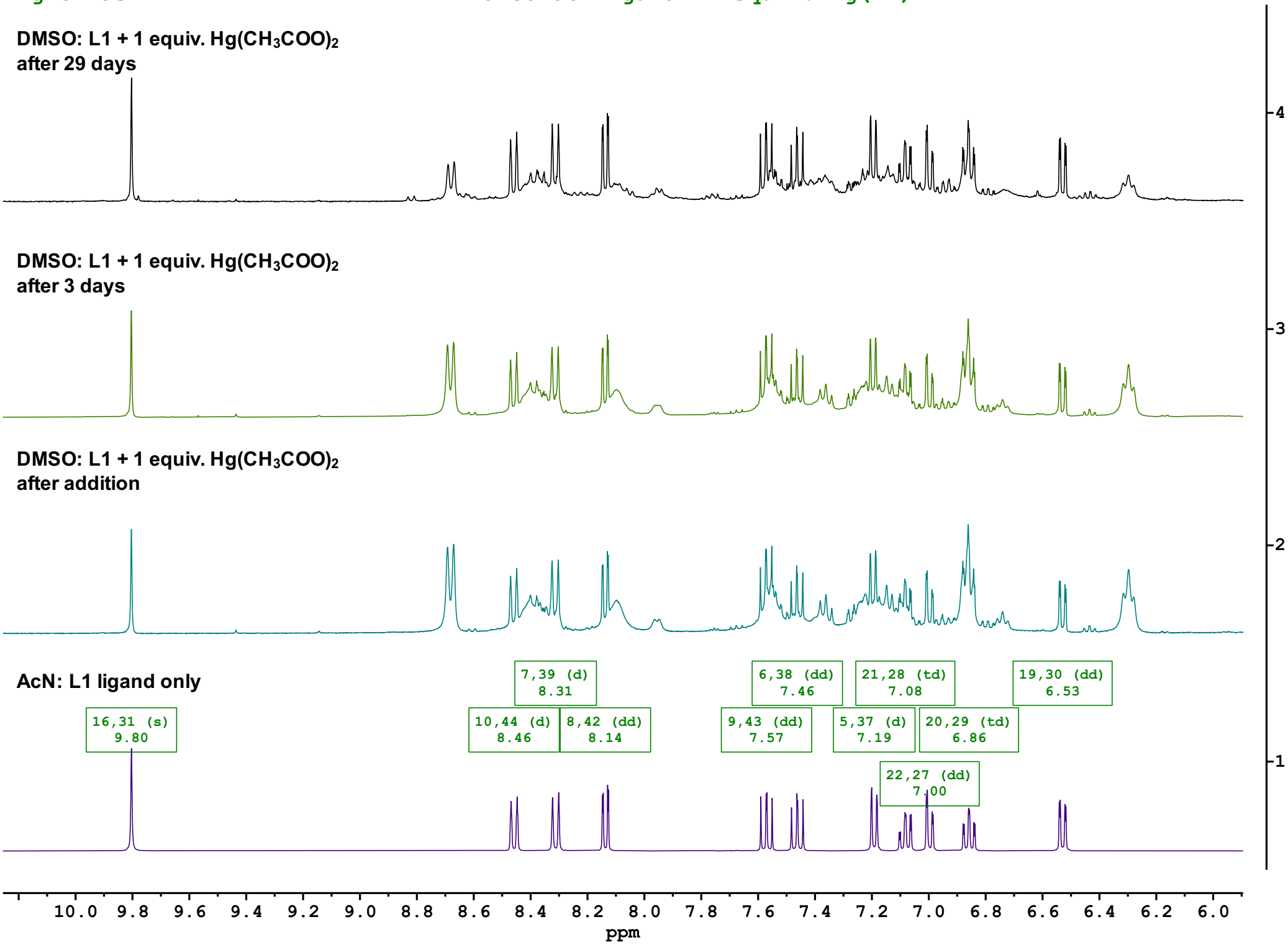
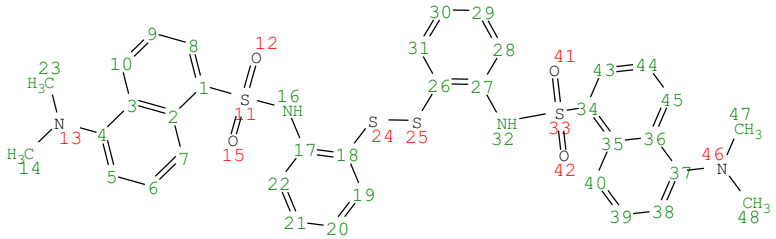


Fig SX194

L2 acetonitrile-d3 ligand + 1equiv. Cu(II)

AcN: L2 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition



5,38 (dd) 8.03

6,39 (m) 7.86

9,44 (m) 7.83

10,45 (dt) 8.38

8,43 (dd) 8.27

7,40 (d) 8.88

19,20,22,28,30,31 (m) 7.05

16,32 (s) 8.10

14,23,47,48 (s) 3.41

AcN: L2 ligand only

9,44 (dd) 7.49

16,32 (s) 7.82

7,40 (d) 8.28

19,31 (dd) 6.74

10,45 (dt) 8.50

20,30 (ddd) 6.92

8,43 (dd) 8.11

6,39 (dd) 7.59

5,38 (dd) 7.24

14,23,47,48 (s) 2.78

2

1

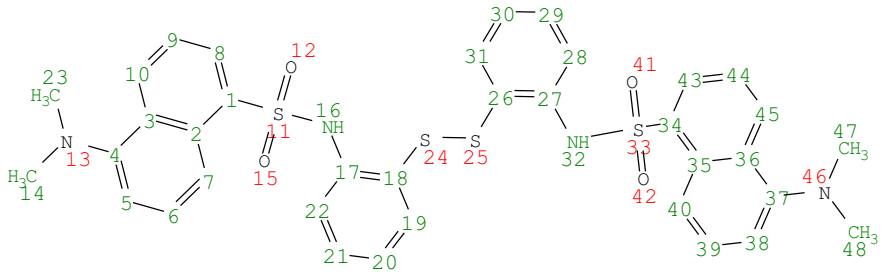
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0

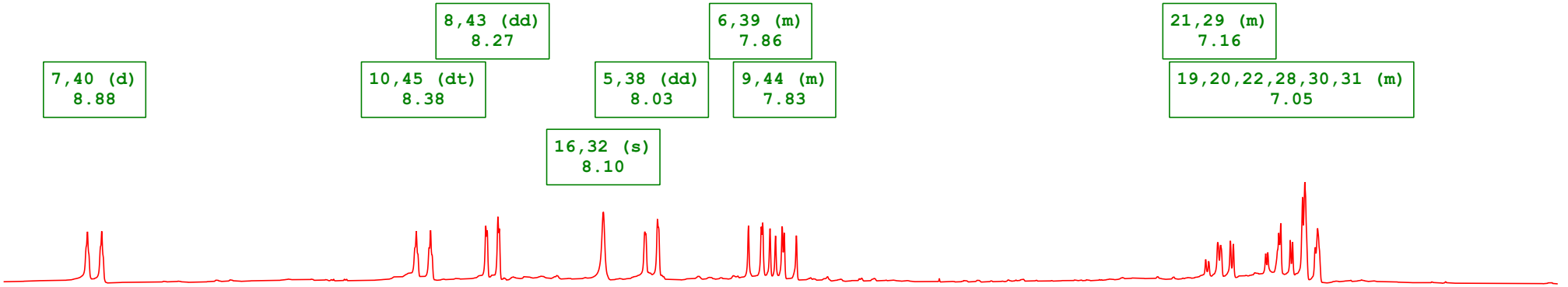
ppm

Fig SX195

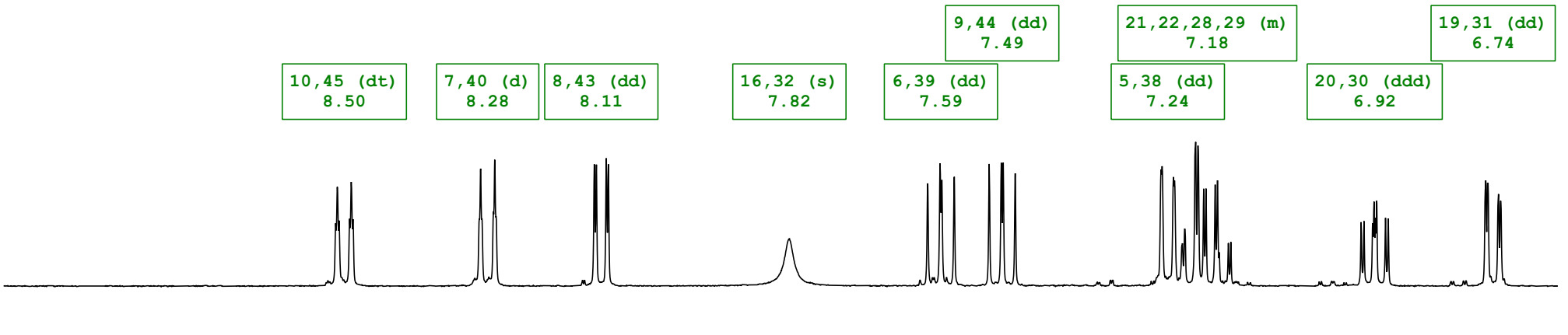
L2 acetonitrile-d3 ligand + 1equiv. Cu(II)

AcN: L2 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition






AcN: L2 ligand only



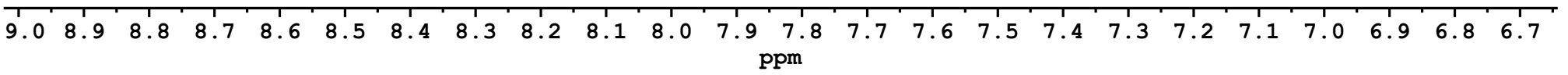
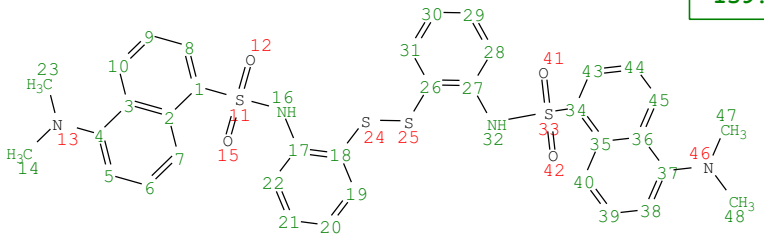



Fig SX196

L2 acetonitrile-d3 ligand + 1equiv. Cu(II)

AcN: L2 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition



8,43 (s) 132.12

10,45 (s) 126.84

4,37 (s) 139.51

5,38 (s) 120.69

14,23,47,48 (s) 48.22

9,44 (s) 128.34

6,39 (s) 128.85

AcN: L2 ligand only

8,43 (s) 131.01

2,35 (s) 130.44

4,37 (s) 153.09

6,39 (s) 129.54

14,23,47,48 (s) 45.59

1,34 (s) 135.63

5,38 (s) 116.37

17,27 (s) 137.23

7,40 (s) 119.71

2

1

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

ppm

Fig SX197 L2 acetonitrile-d3 ligand + 1equiv. Cu(II)

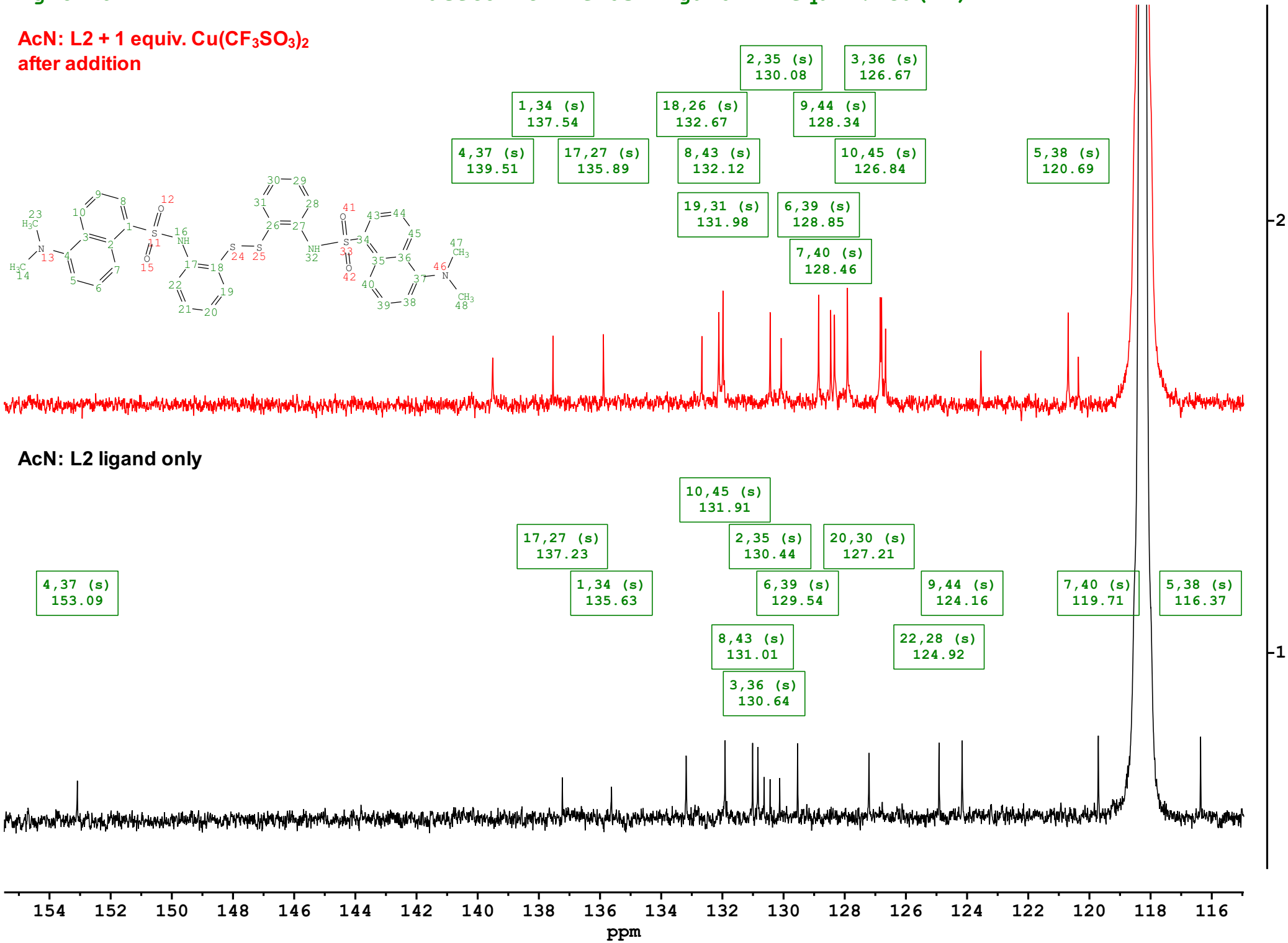
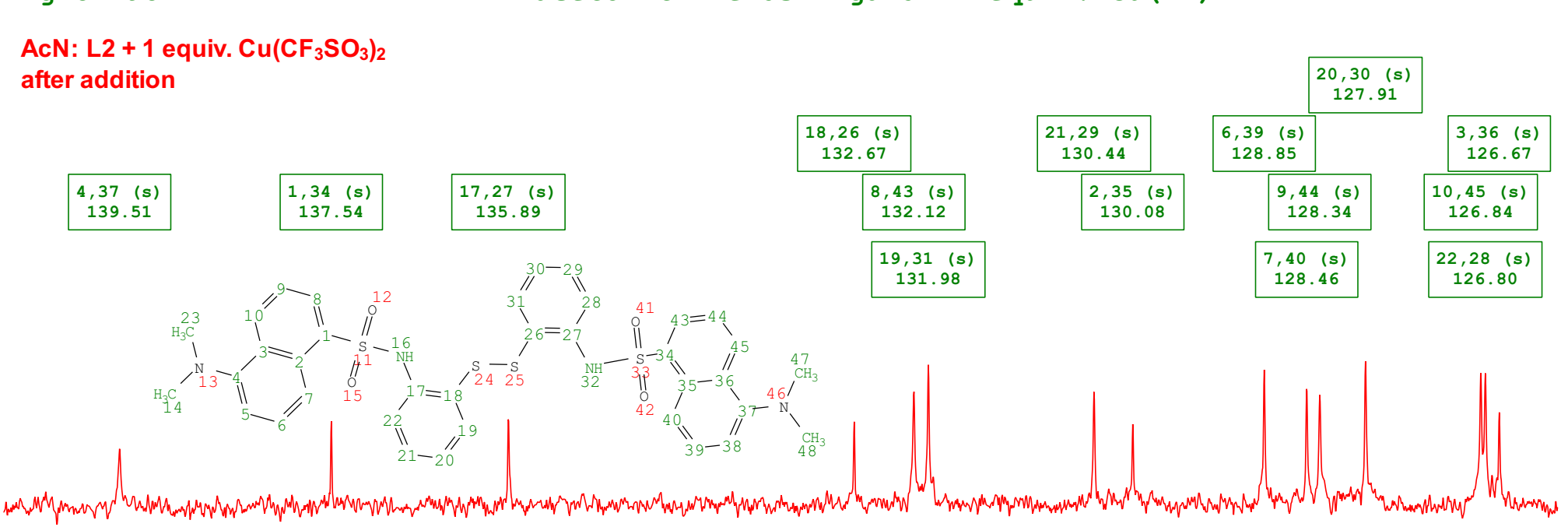


Fig SX198 L2 acetonitrile-d3 ligand + 1equiv. Cu(II)

AcN: L2 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition




AcN: L2 ligand only

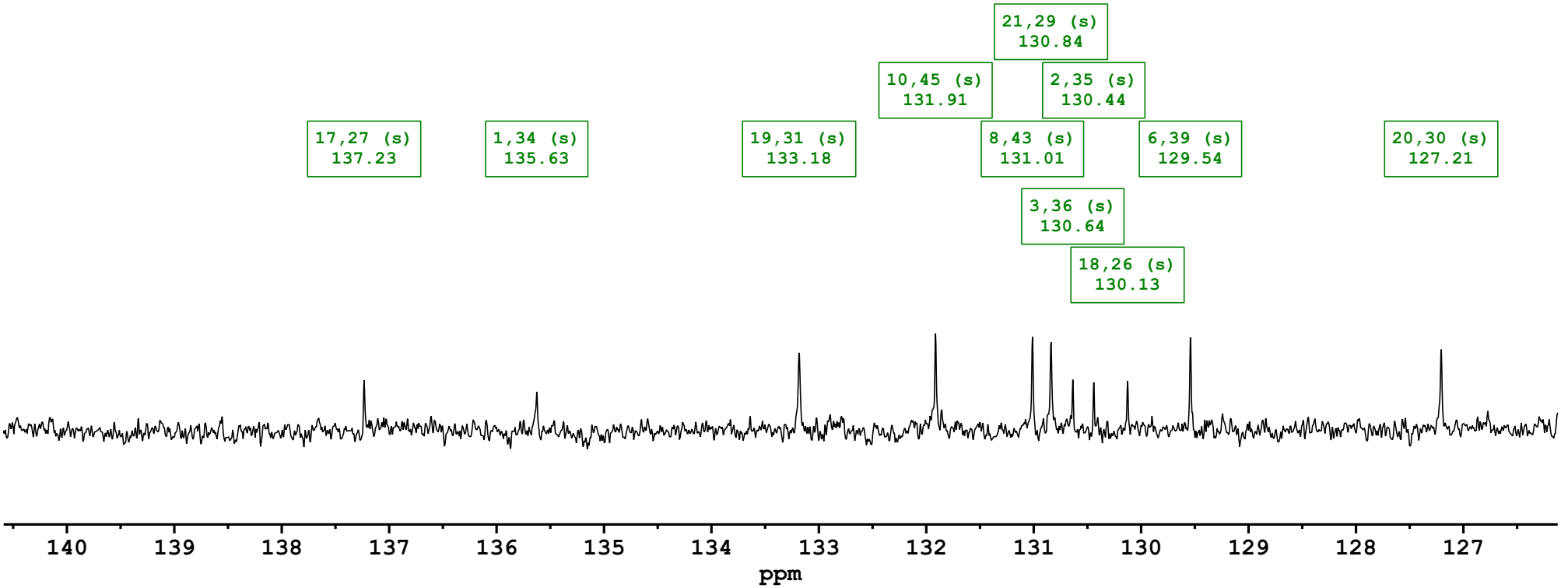
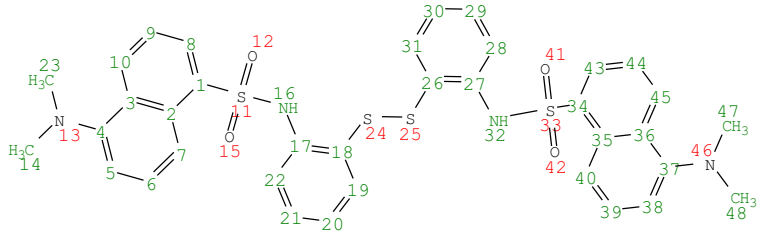


Fig SX199

L2 acetonitrile-d3 ligand + 1equiv. Cu(II)

AcN: L2 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition

5,38 (s)
120.69



AcN: L2 ligand only

7,40 (s)
119.71

5,38 (s)
116.37

-2

-1

121.0 120.5 120.0 119.5 119.0 118.5 118.0 117.5 117.0 116.5 116.0 115.5

ppm

Fig SX200 L2 acetonitrile-d3 ligand + 1equiv. Hg(II)

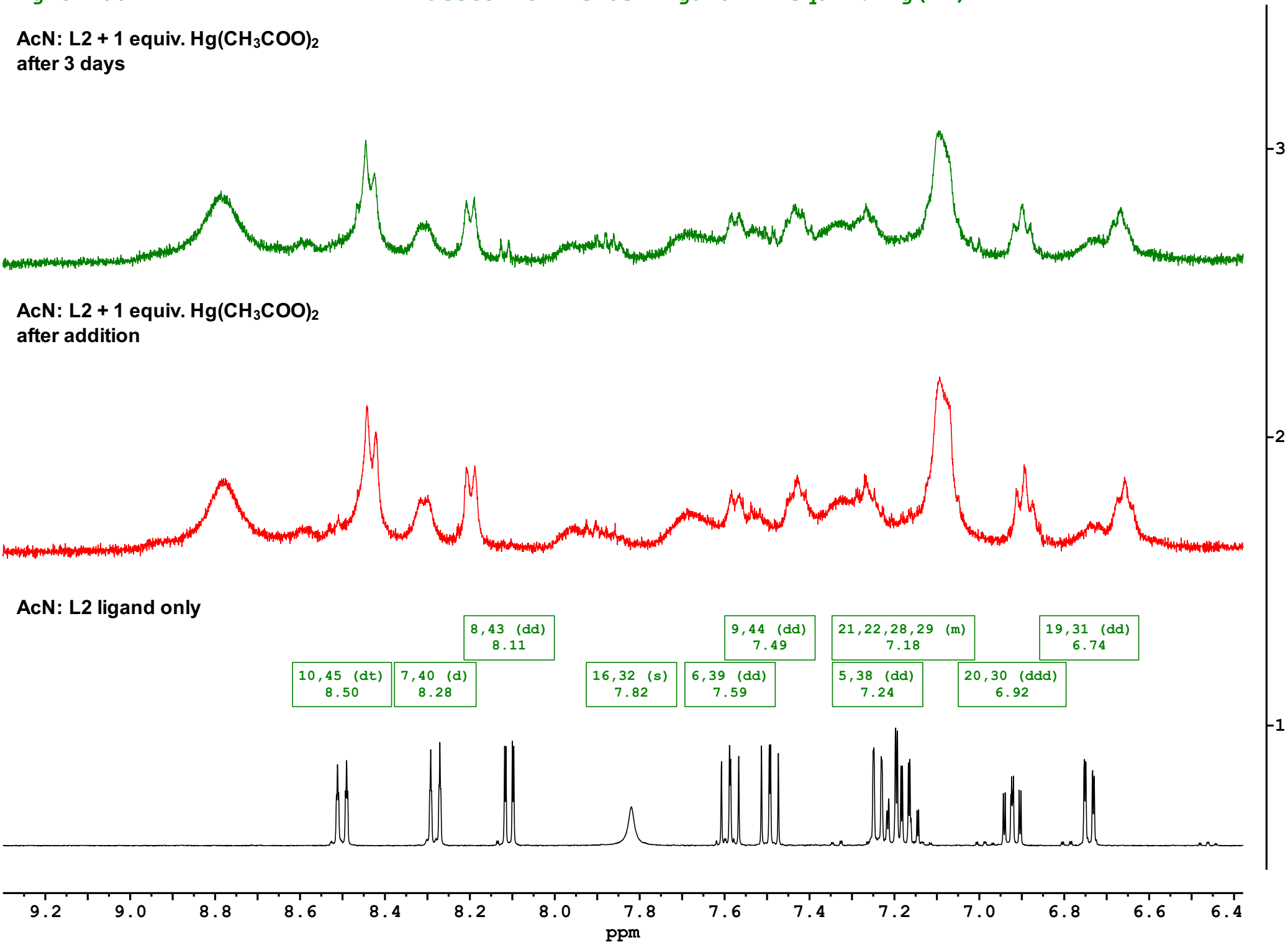


Fig SX201 L2 acetonitrile-d3 ligand + 1equiv. sodium dithionite

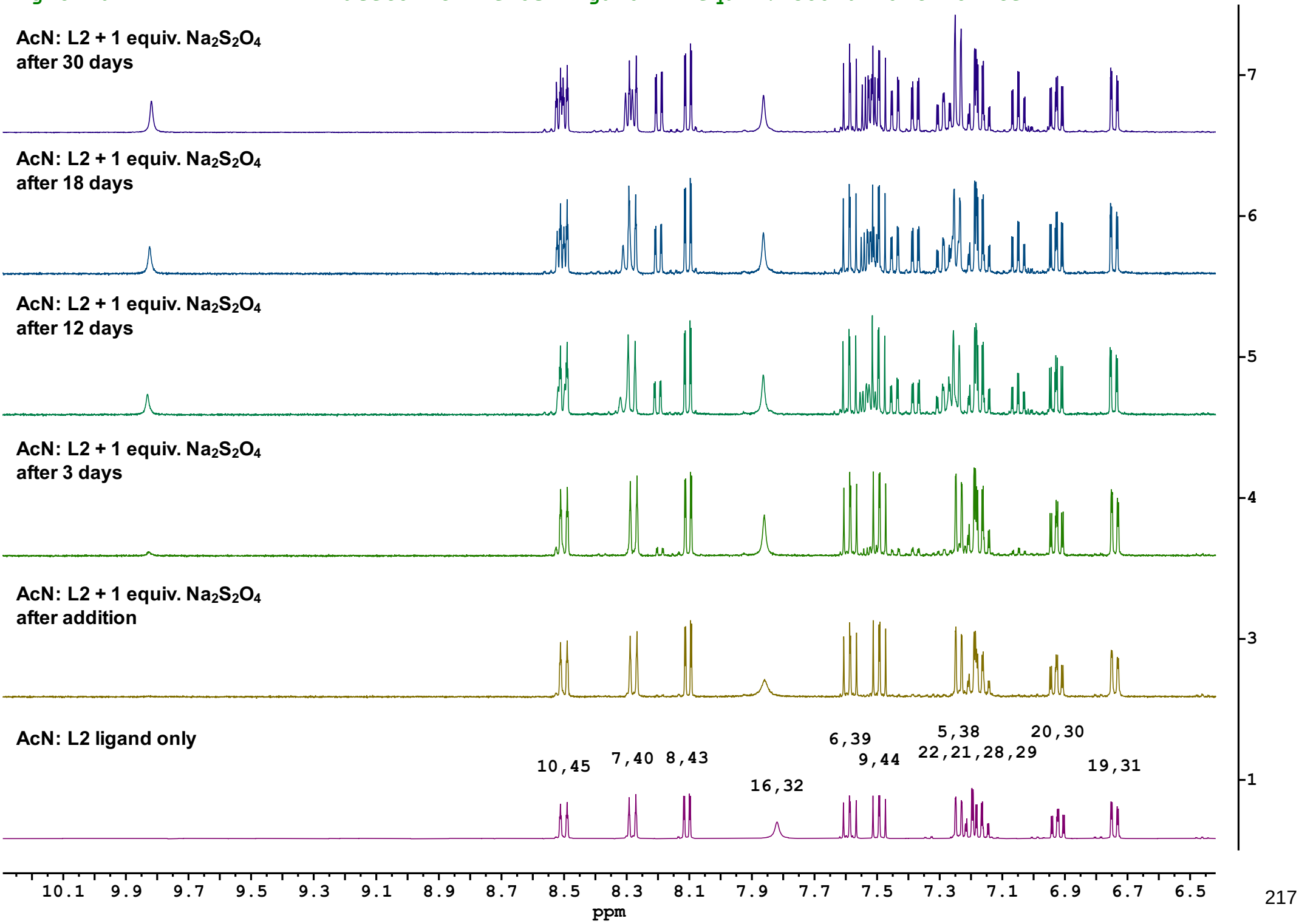


Fig SX202 L2 acetonitrile-d3 ligand + 1equiv. sodium dithionite

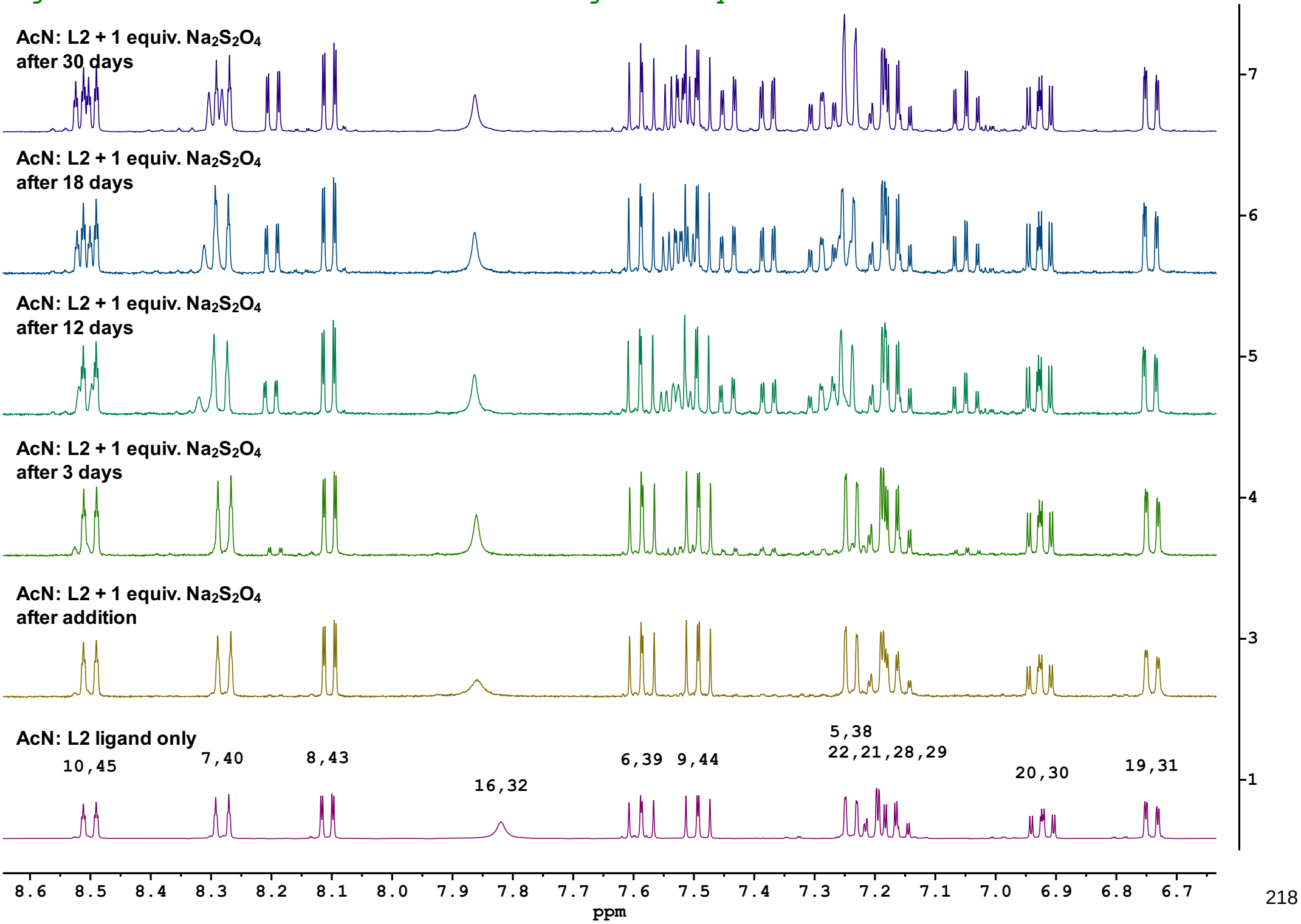


Fig SX203 L2 acetonitrile-d3 ligand + 1equiv. sodium dithionite

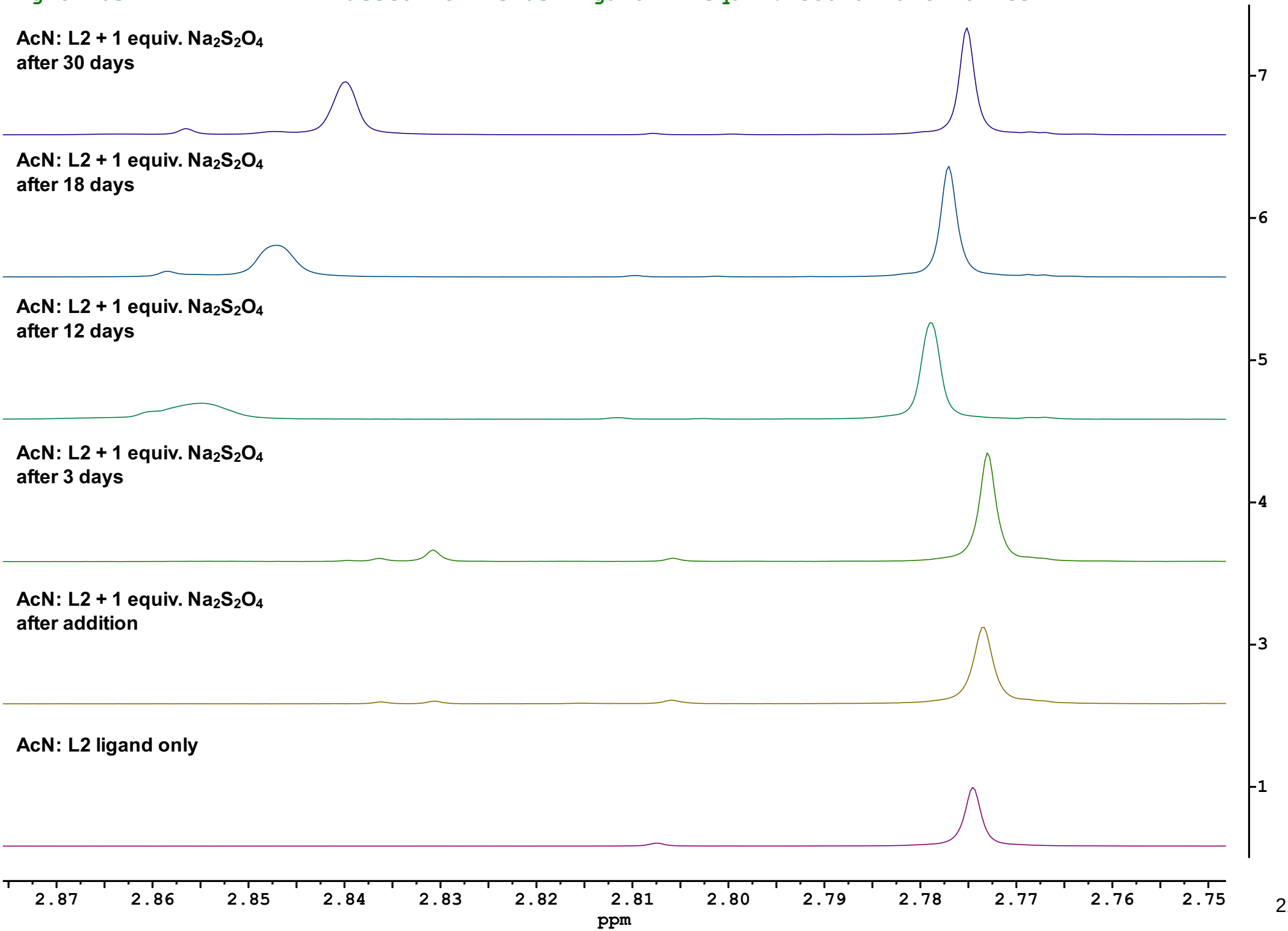


Fig SX204 L2 acetonitrile-d3 ligand + 1equiv. sodium dithionite

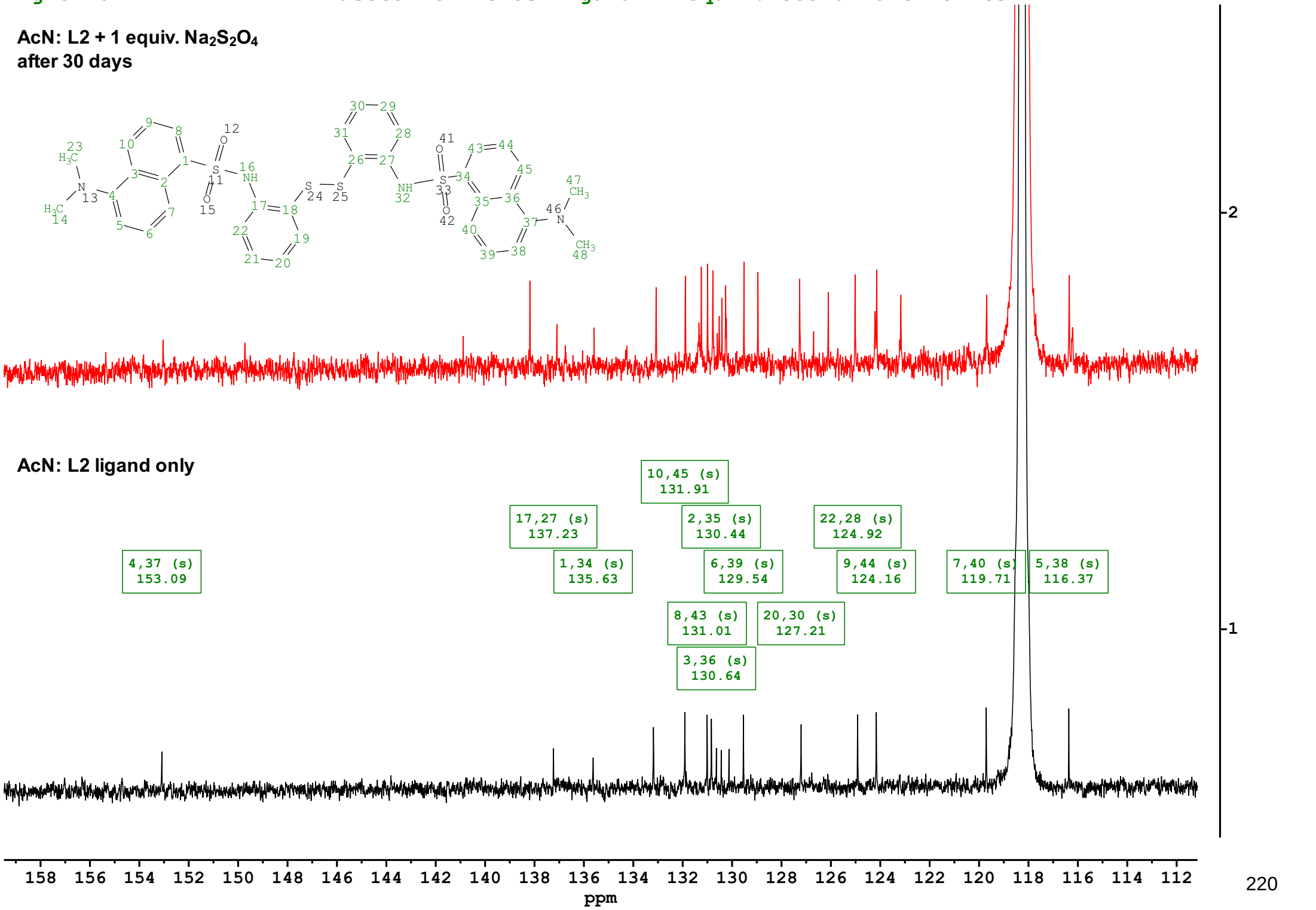
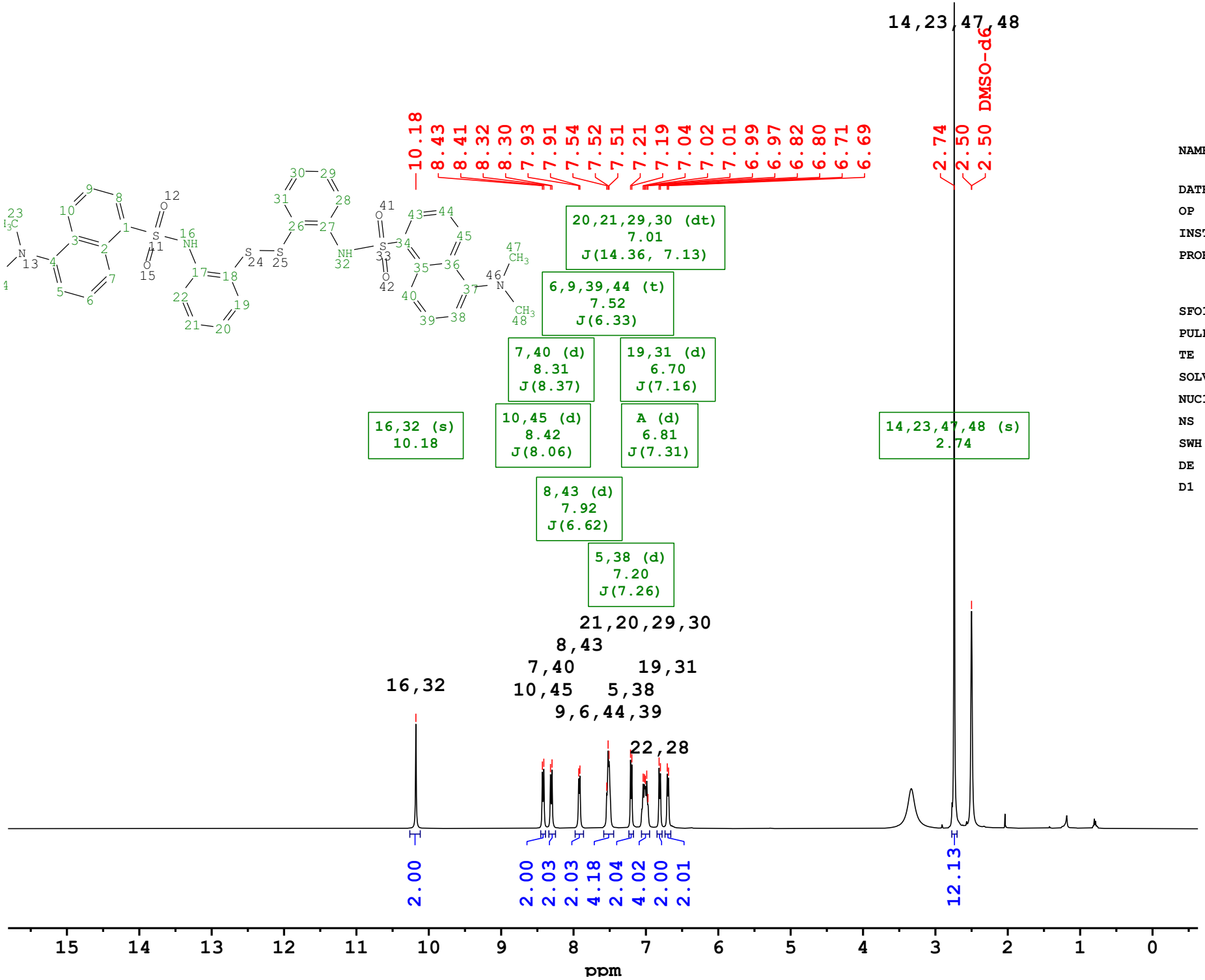


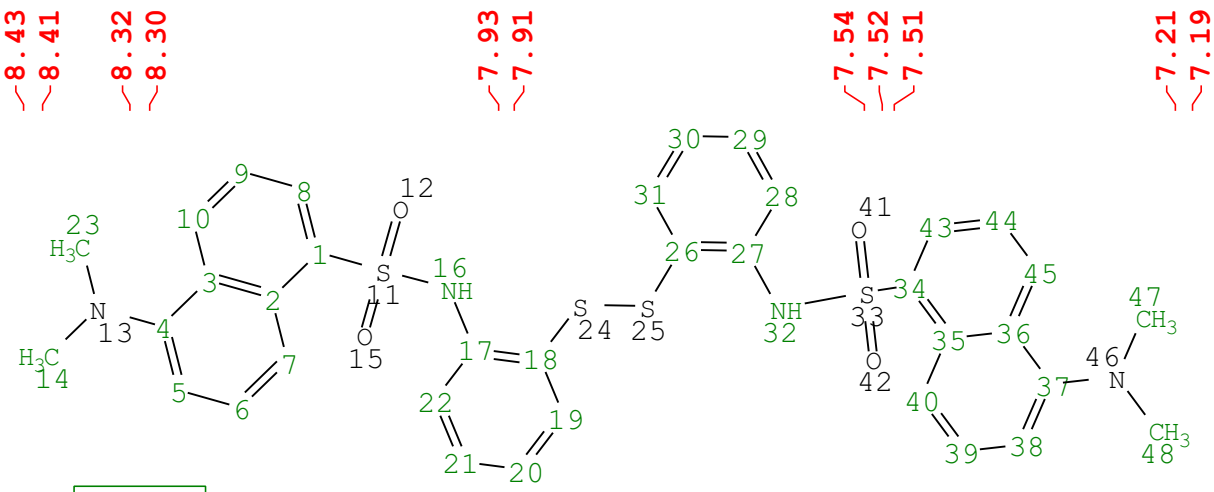
Fig SX205

L2 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu.11.fid |
| DATE_TIME | 2024-12-23T00:07:19 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

**Fig SX206** **L2 dmso-d6 ligand + 1equiv. Cu(II)**




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu. 11.fid |
| DATE_TIME | 2024-12-23T00:07:19 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

7,40 (d)
8.31
J(8.37)

20,21,29,30 (dt)
7.01
J(14.36, 7.13)

19,31 (d)
6.70
J(7.16)

10,45 (d)
8.42
J(8.06)

8,43 (d)
7.92
J(6.62)

6,9,39,44 (t)
7.52
J(6.33)

5,38 (d)
7.20
J(7.26)

A (d)
6.81
J(7.31)

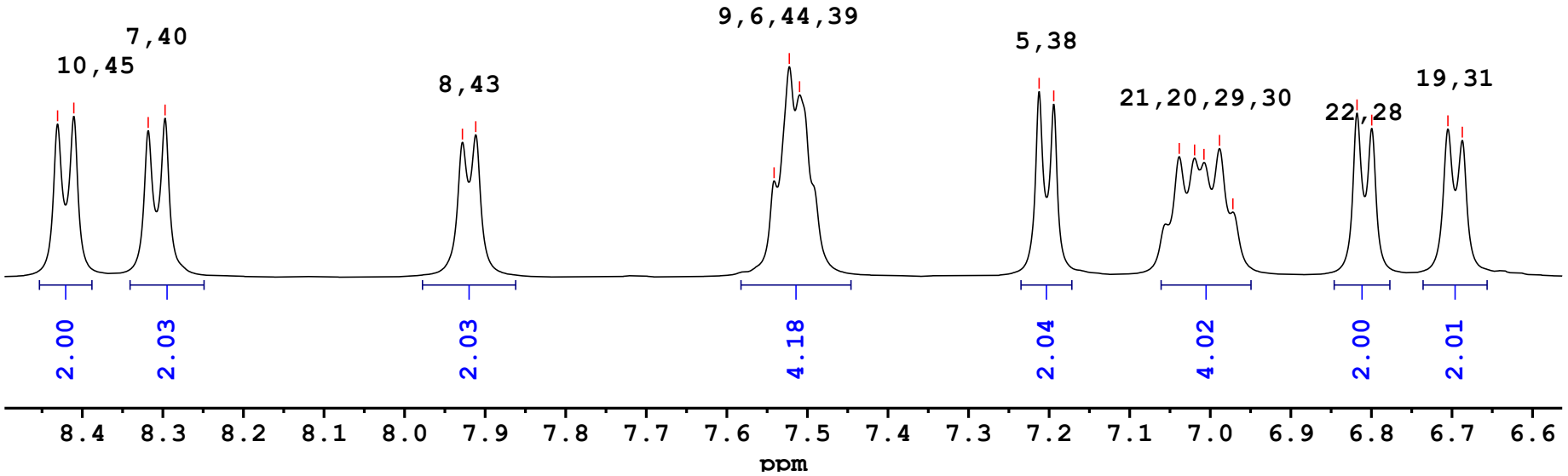
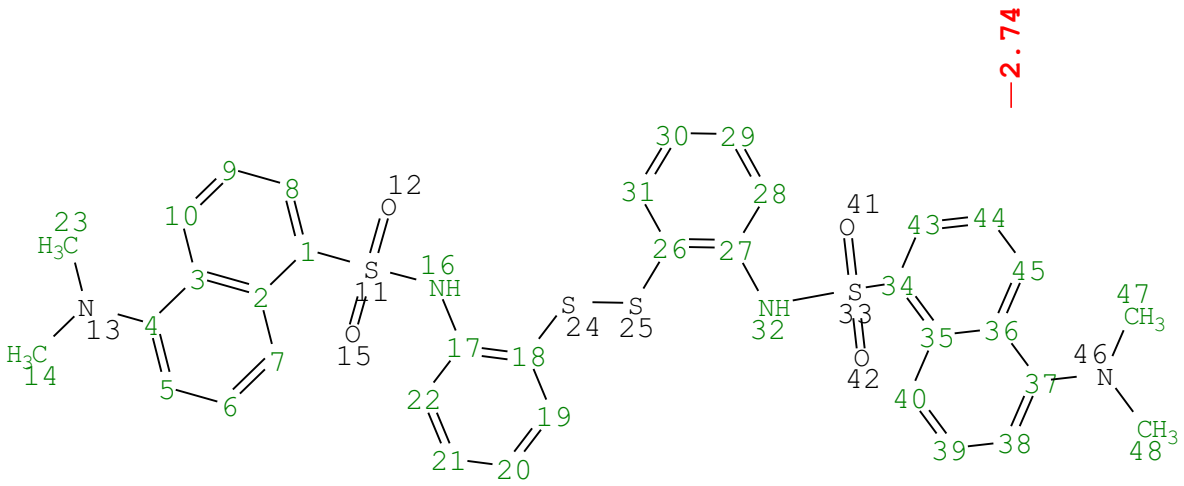


**Fig SX207** **L2 dmso-d6 ligand + 1equiv. Cu(II)**




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu. 11.fid |
| DATE_TIME | 2024-12-23T00:07:19 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

14,23,47,48 (s)
2.74

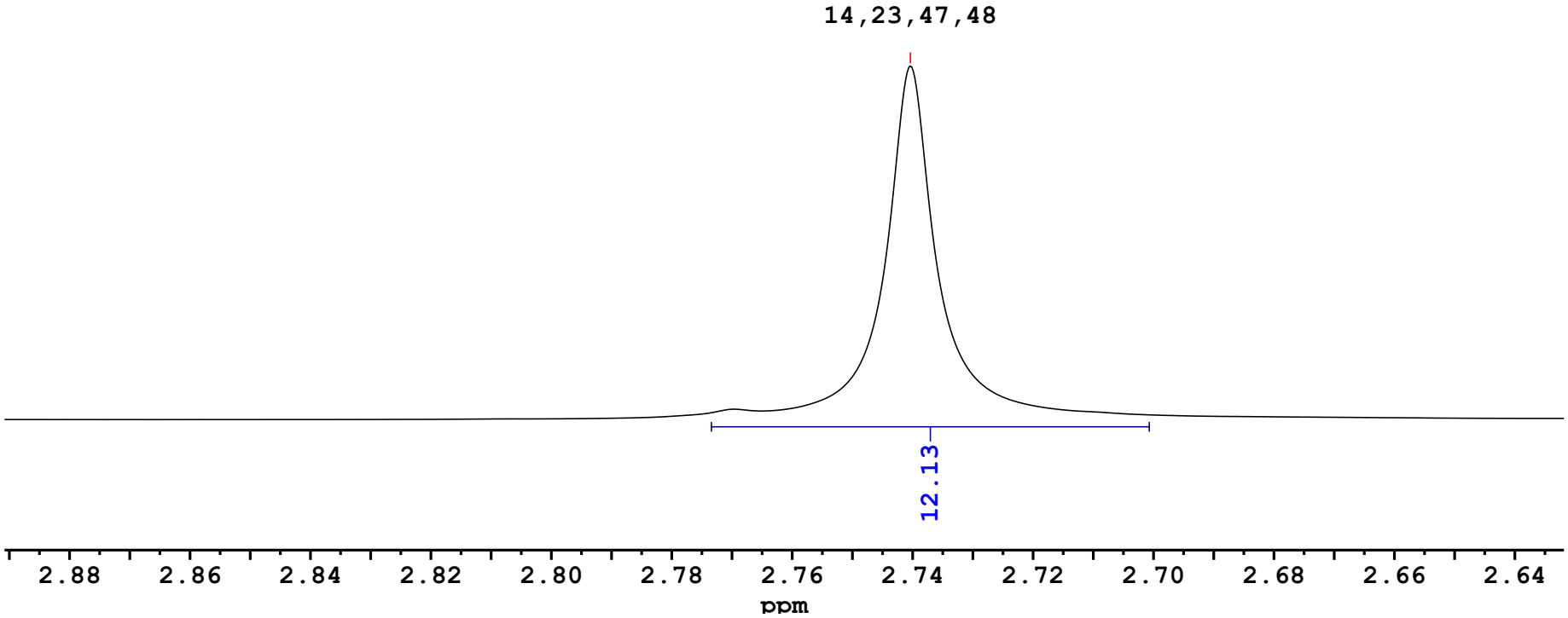
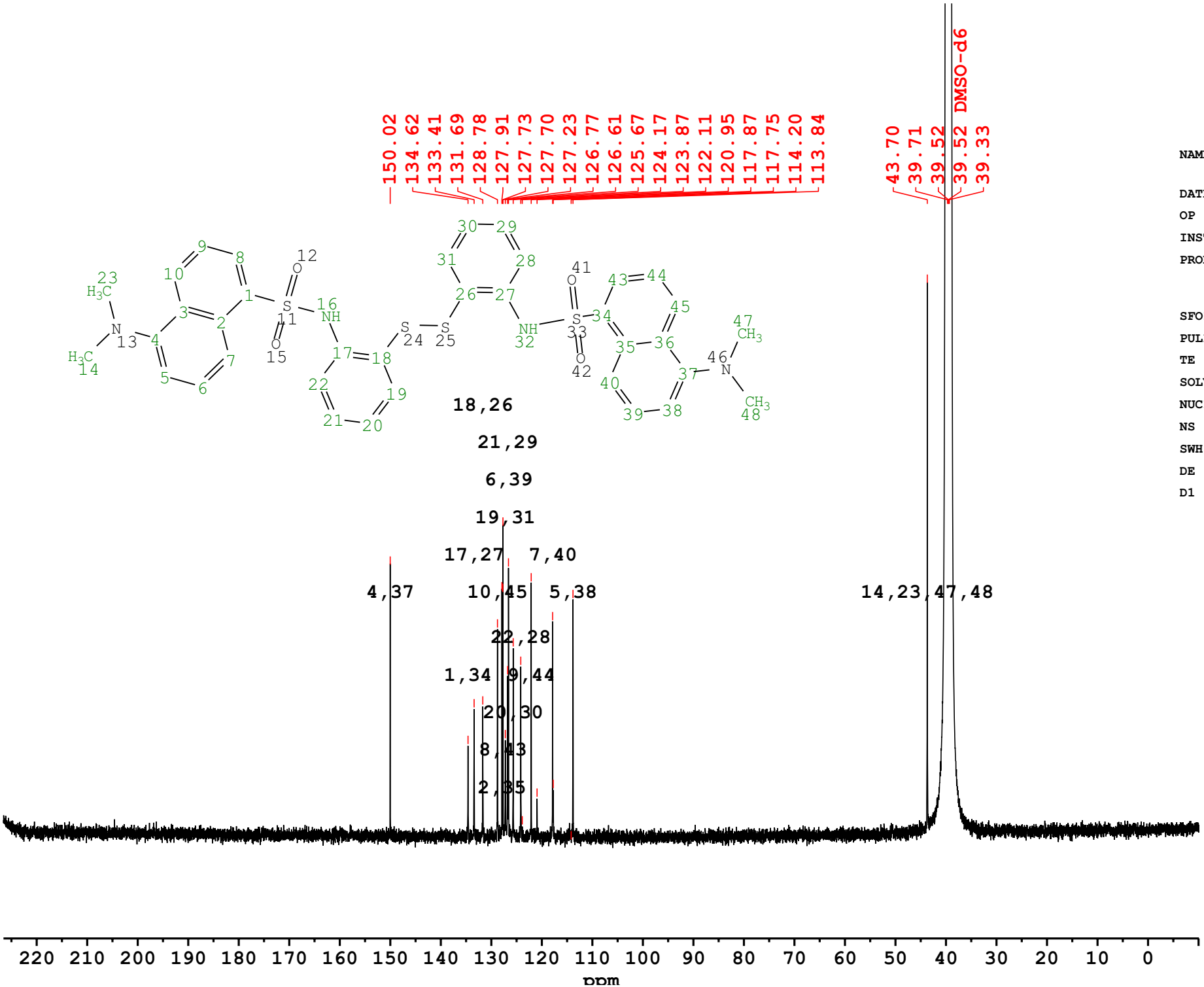


Fig SX208

# L2 dmso-d6 ligand + 1equiv. Cu(II)

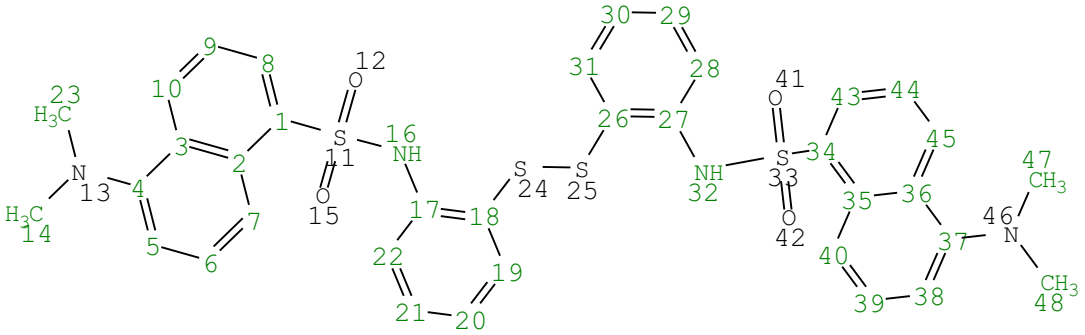



IOCCP BAS

| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu. 12.fid |
| DATE_TIME | 2024-12-23T05:14:43 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

**Fig SX209** **L2 dmso-d6 ligand + 1equiv. Cu(II)**

150.02 134.62 133.41 131.69 128.78 127.91 127.73 127.70 127.23 126.77 126.61 125.67 124.17 123.87 122.11 120.95 117.87 117.75 114.20 113.84



| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu.12.fid |
| DATE_TIME | 2024-12-23T05:14:43 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

3,36 8,43 20,30 1,34 18,26 19,31 9,44 4,37 17,27 10,45 22,28 7,40 5,38 6,39 21,29 2,35

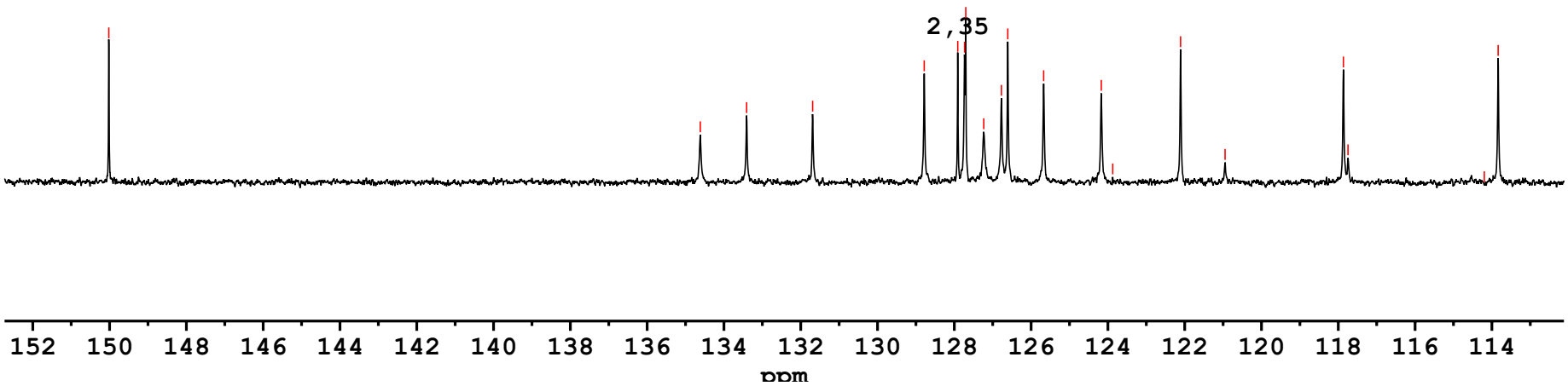
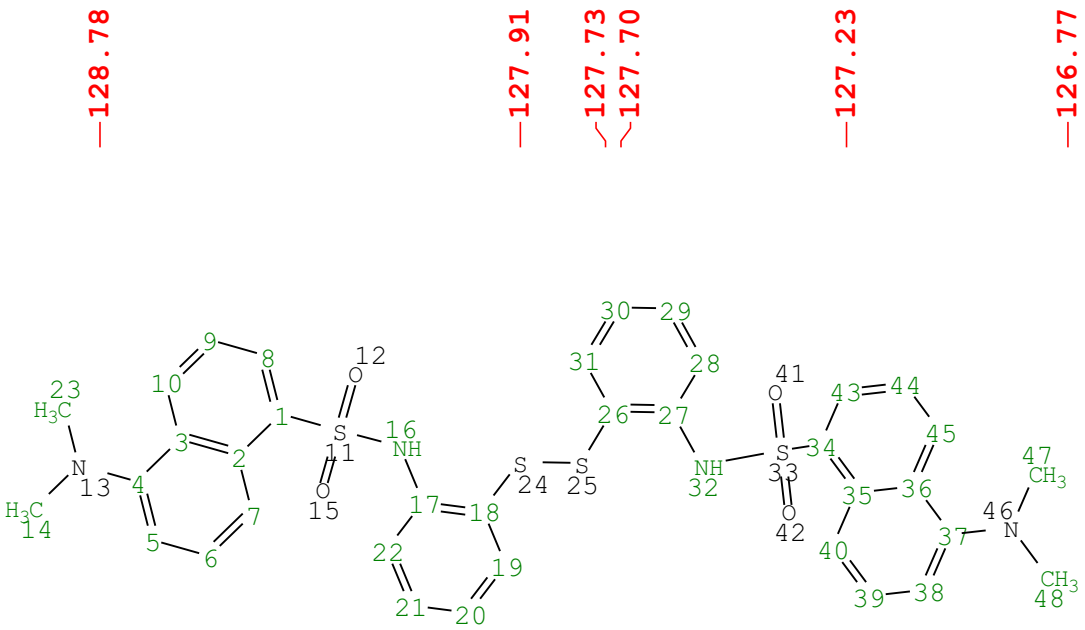


Fig SX210 L2 dmso-d6 ligand + 1equiv. Cu(II)






| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu.12.fid |
| DATE_TIME | 2024-12-23T05:14:43 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9188042 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 36057.692 Hz |
| DE | 6.50 usec |
| D1 | 1.5000 sec |

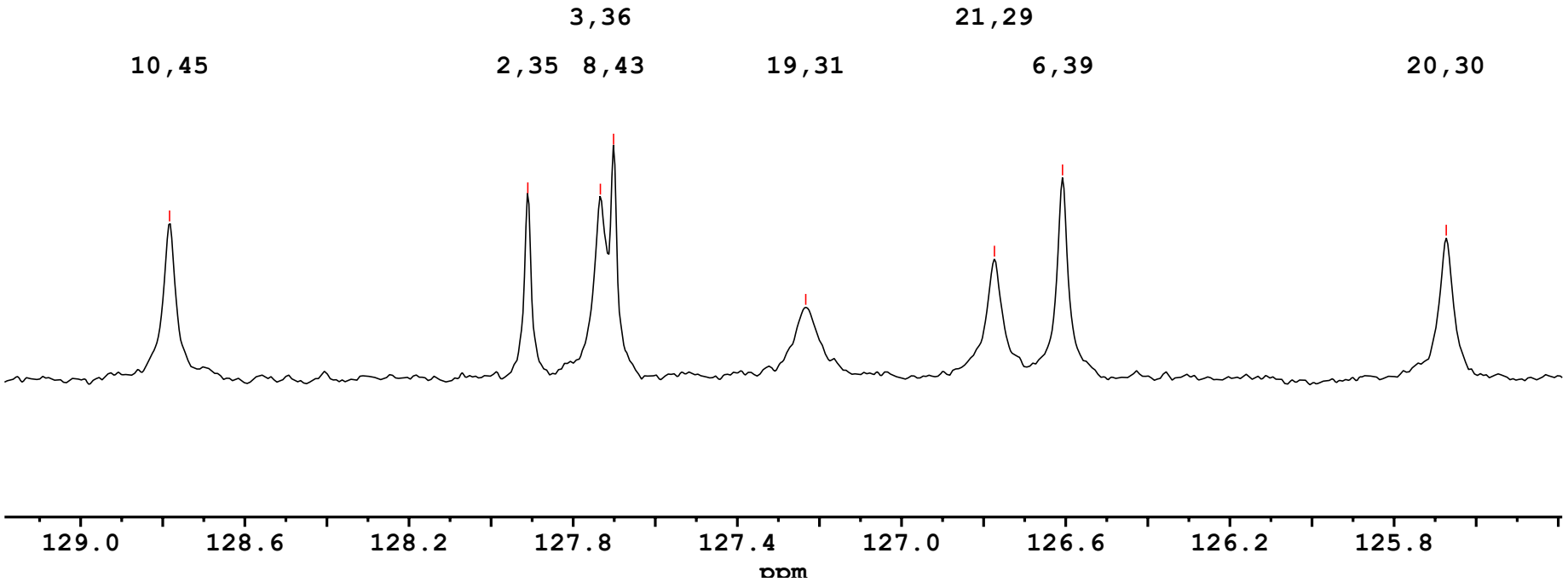
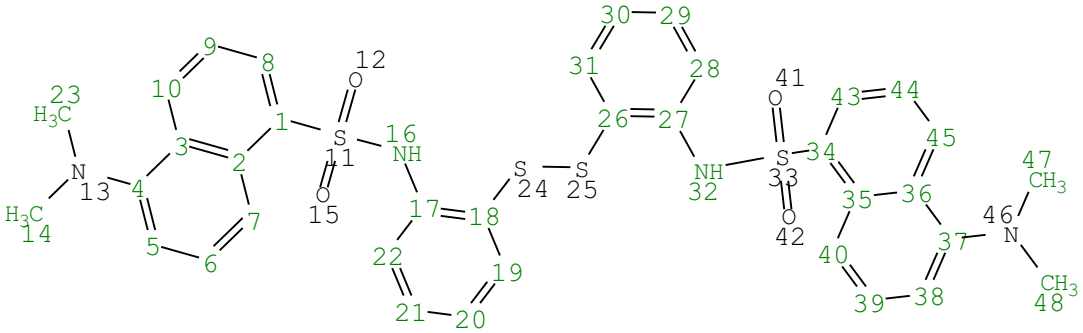


Fig SX211

# L2 dmso-d6 ligand + 1equiv. Cu(II)



128.6
127.5
127.0
126.5
126.4
125.4
123.9
121.9
117.6
113.6

43.5
39.5 DMSO-d6
39.5

| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu.12.fid |
| DATE_TIME | 2024-12-23T05:14:43 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9319844 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 8192 |
| SWH | 35714.286 Hz |
| DE | 18.00 usec |
| D1 | 1.5000 sec |

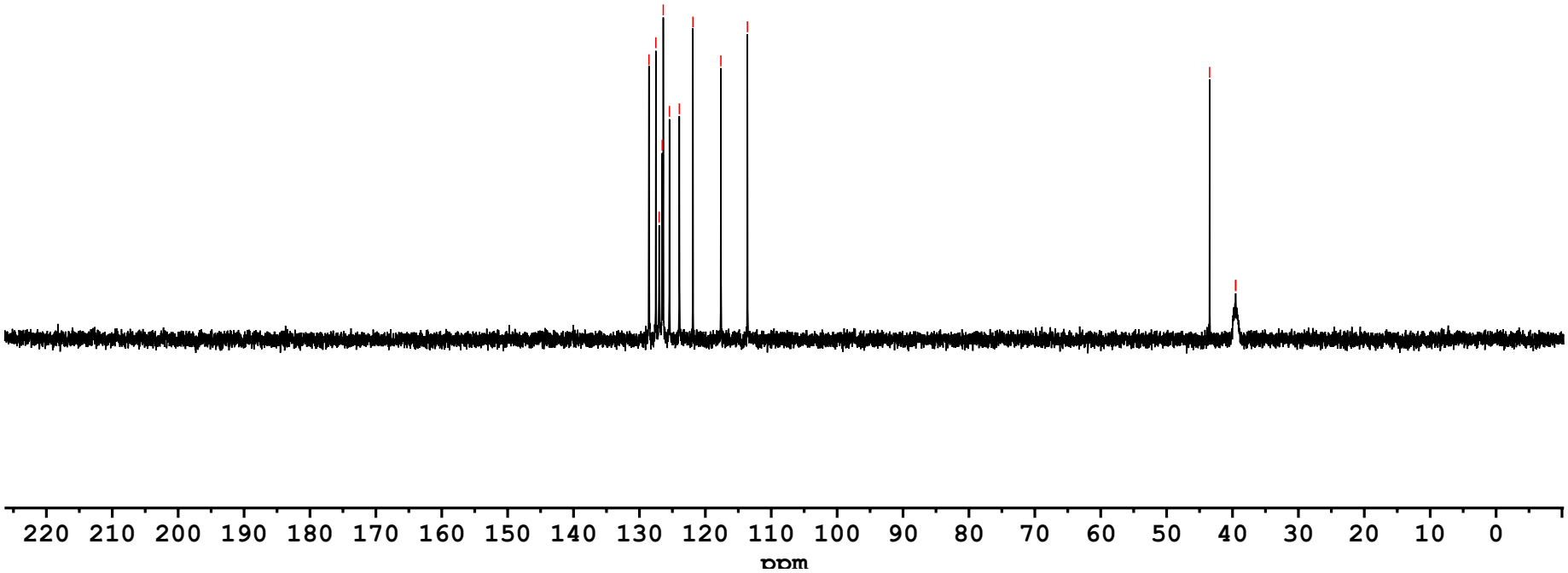
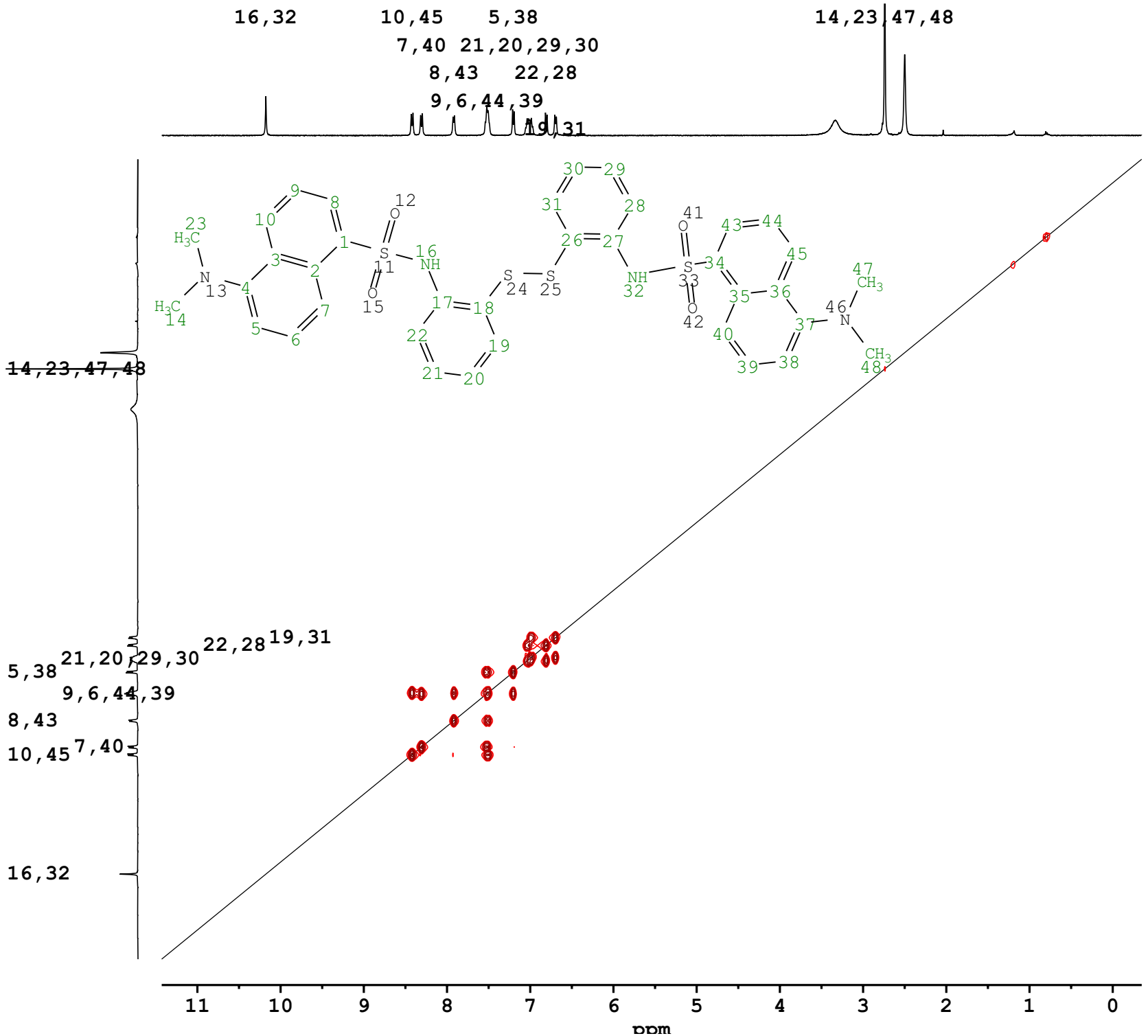


Fig SX212

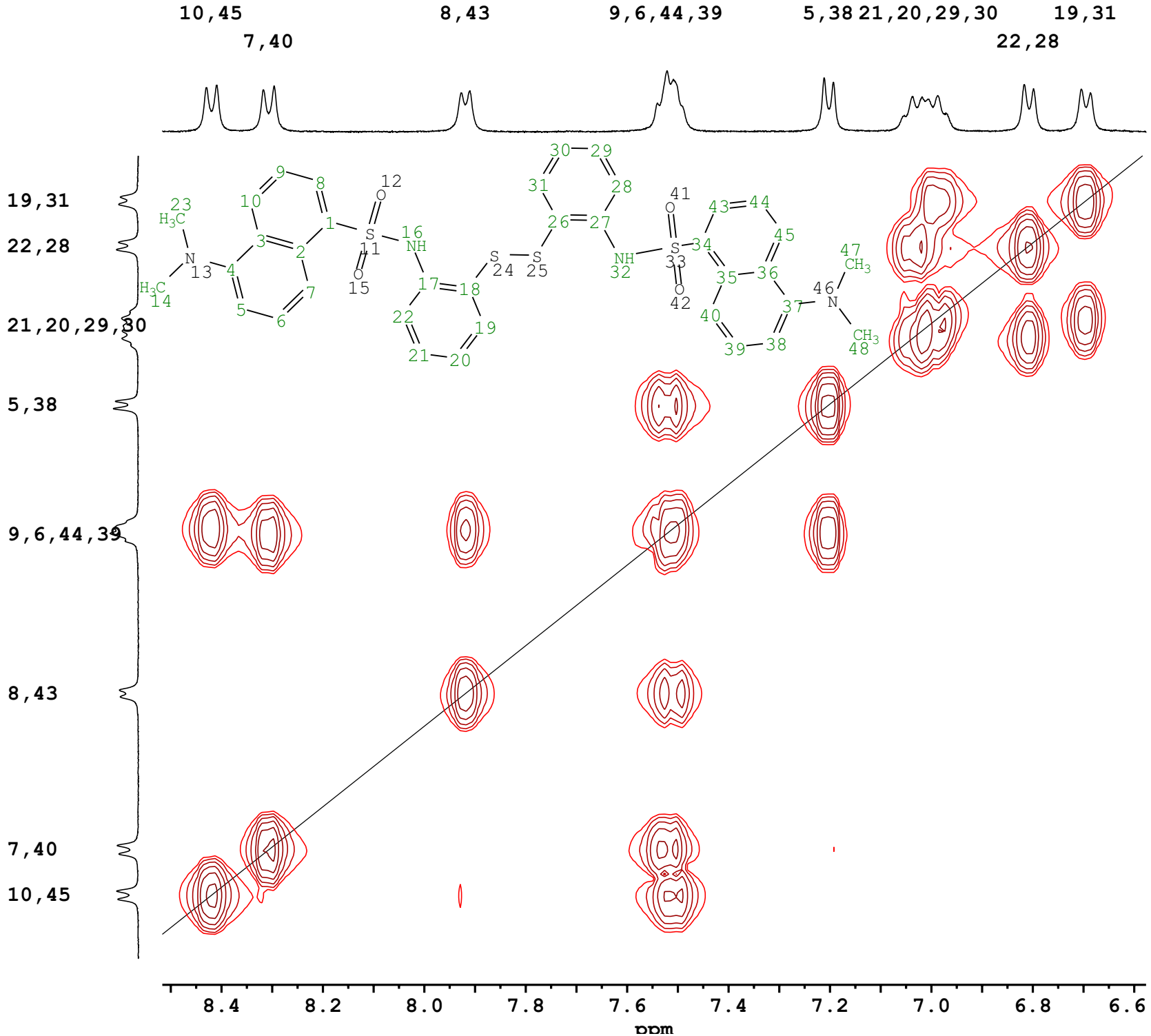
L2 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu.14.ser |
| DATE_TIME | 2024-12-23T06:24:27 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 4 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0160 sec |

Fig SX213

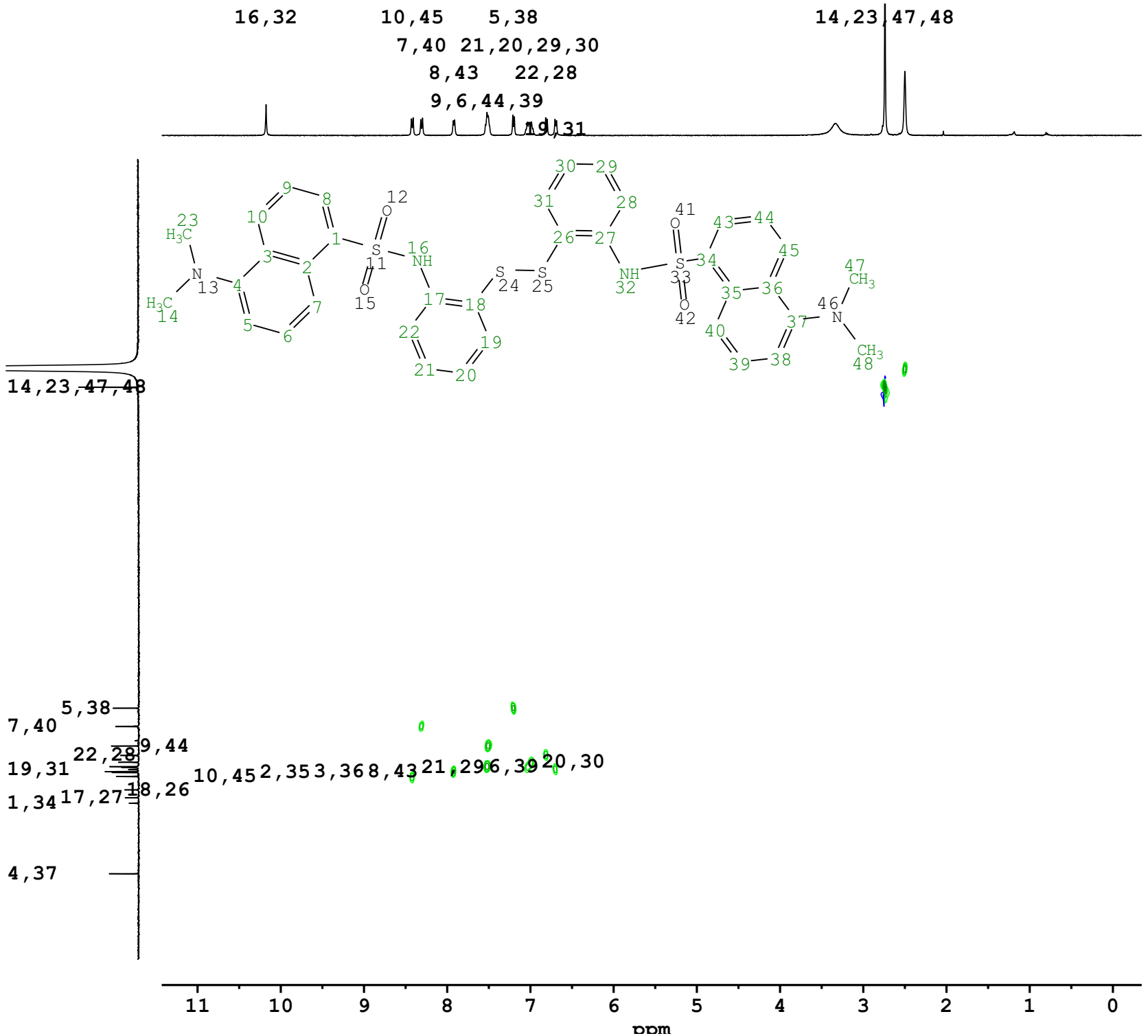
L2 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu.14.ser |
| DATE_TIME | 2024-12-23T06:24:27 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 4 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0160 sec |

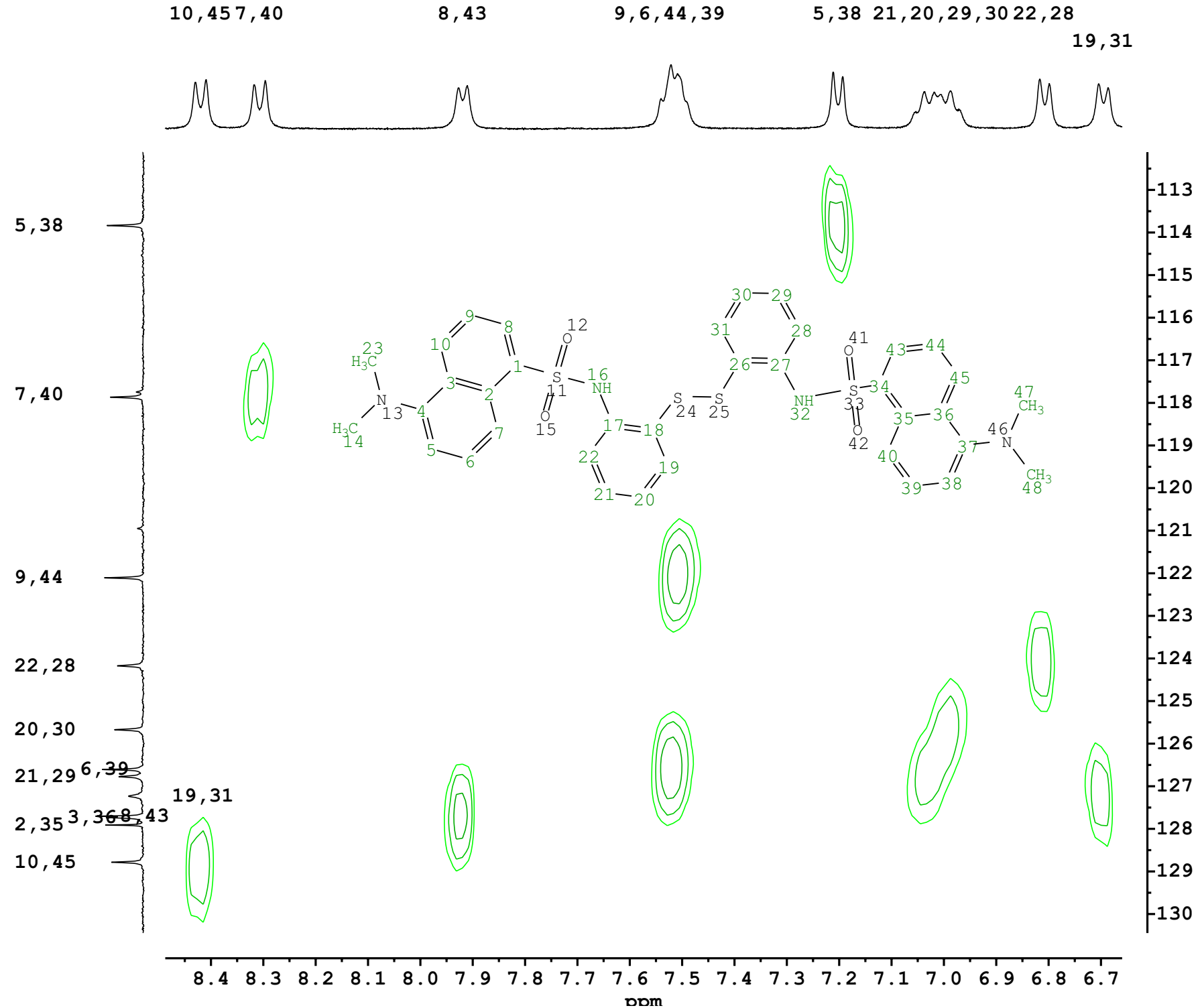
Fig SX214

L2 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu.15.ser |
| DATE_TIME | 2024-12-23T07:10:18 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

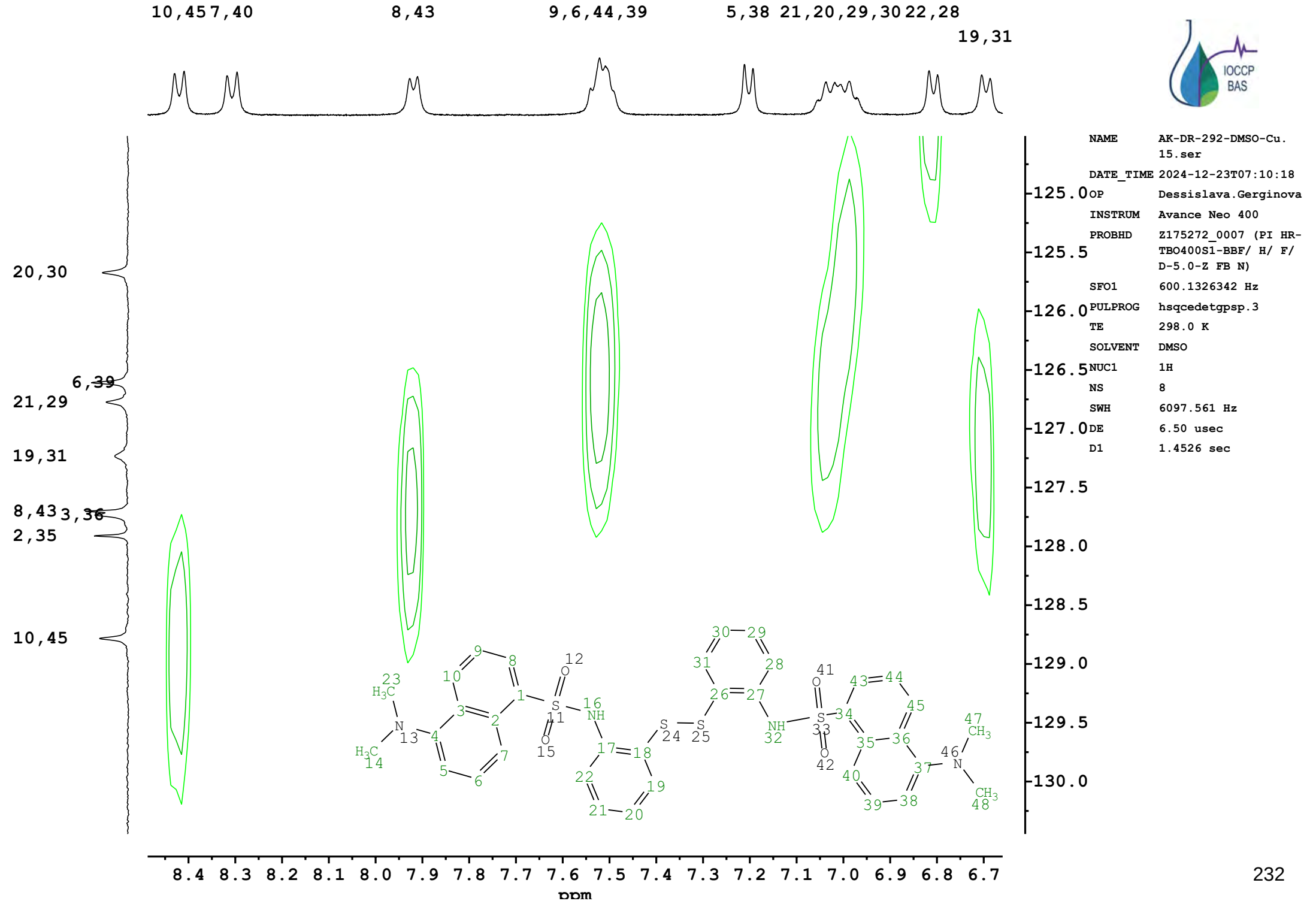
Fig SX215 L2 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu.15.ser |
| DATE_TIME | 2024-12-23T07:10:18 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX216

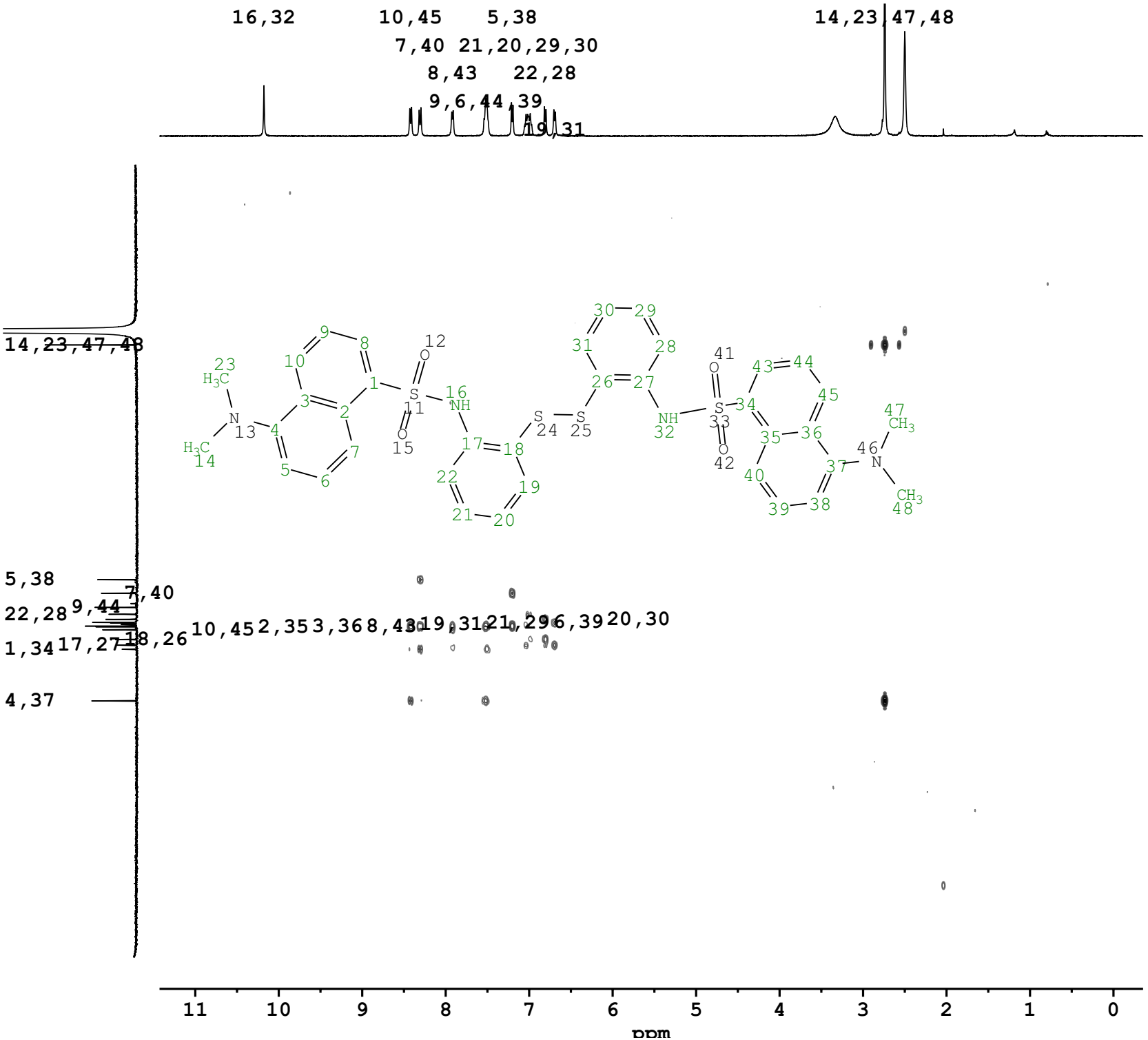
L2 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu.15.ser |
| DATE_TIME | 2024-12-23T07:10:18 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX217

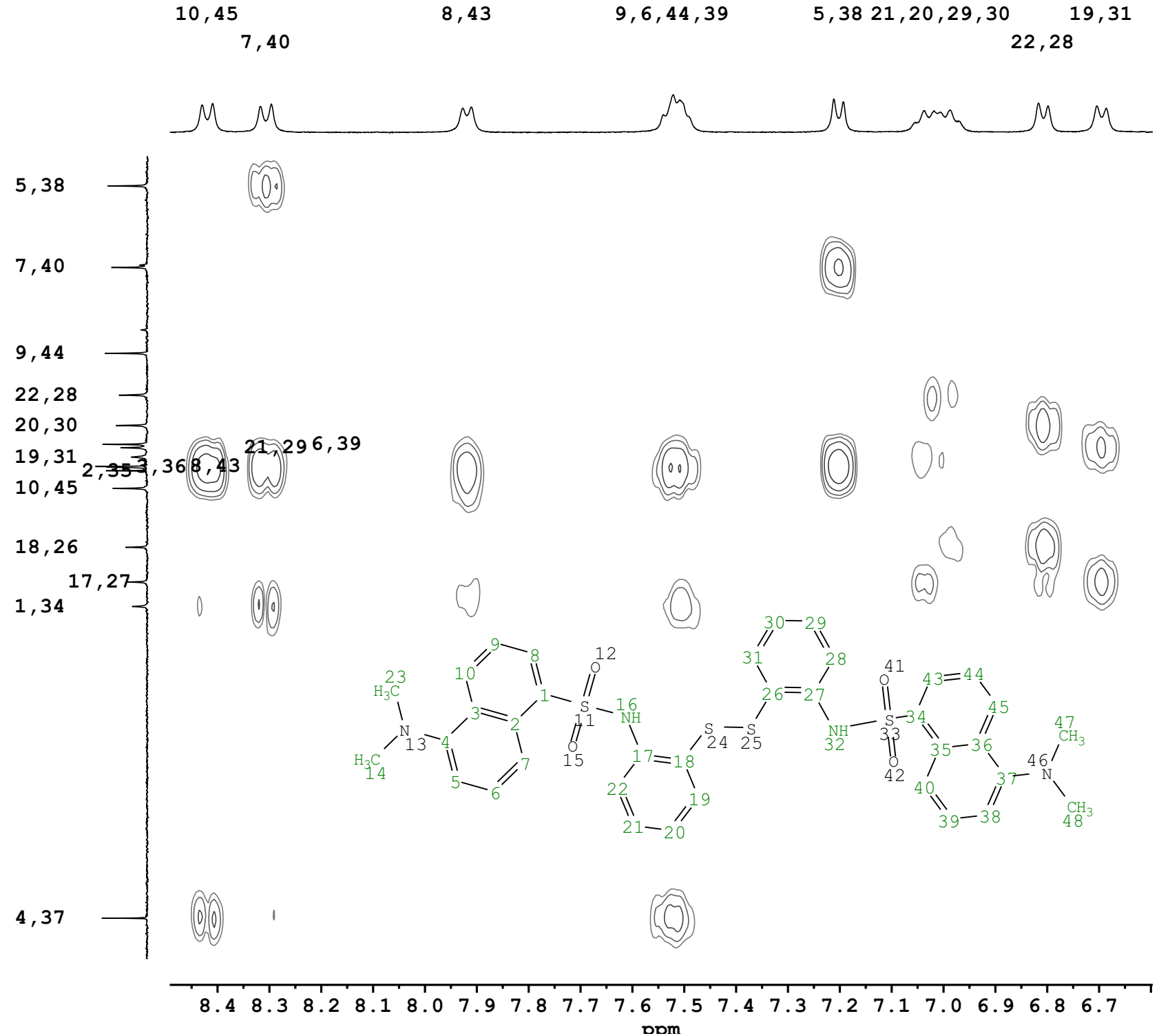
L2 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu.16.ser |
| DATE_TIME | 2024-12-23T08:42:07 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX218

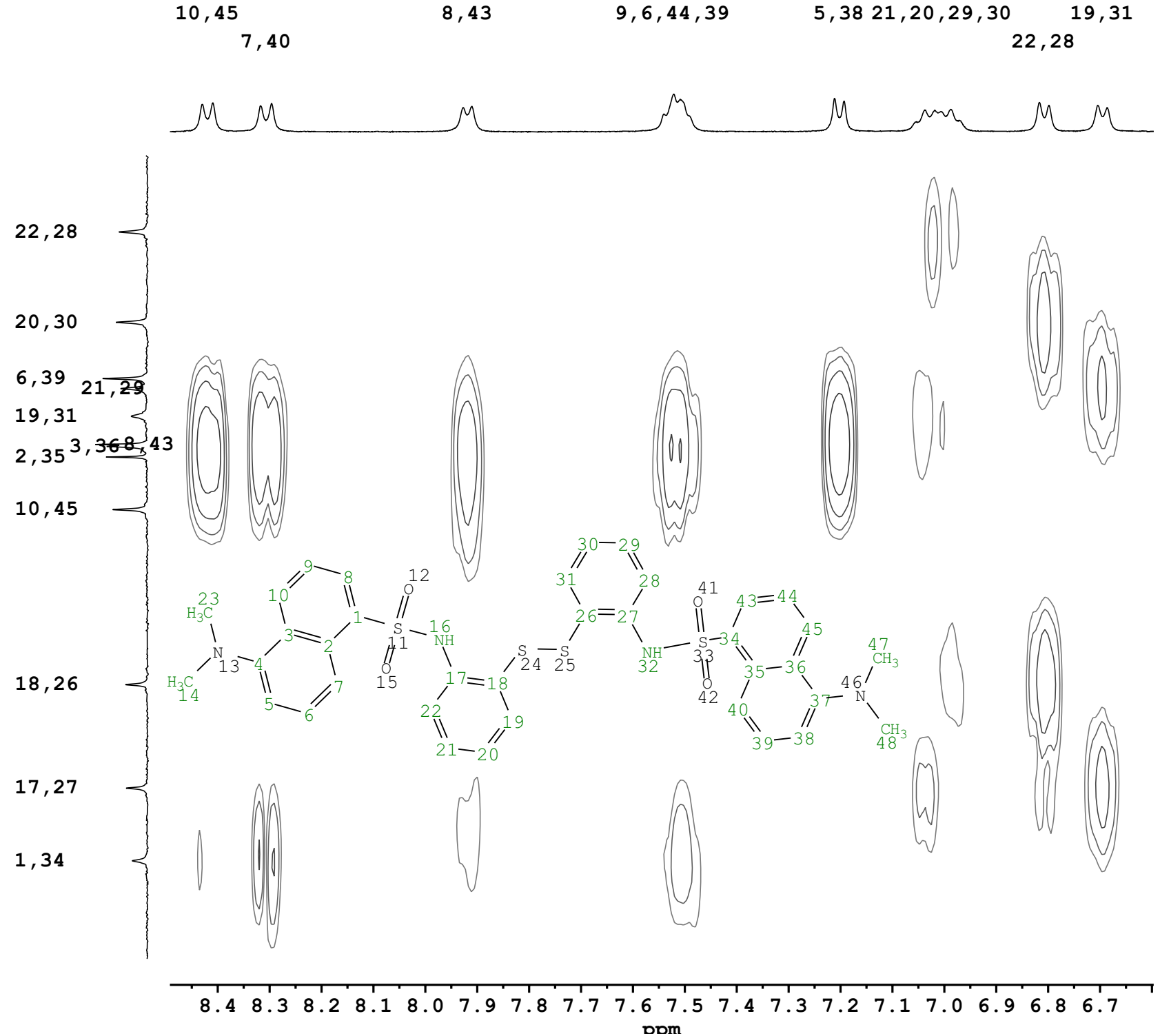
L2 dmso-d6 ligand + 1equiv. Cu(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu.16.ser |
| DATE_TIME | 2024-12-23T08:42:07 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX219

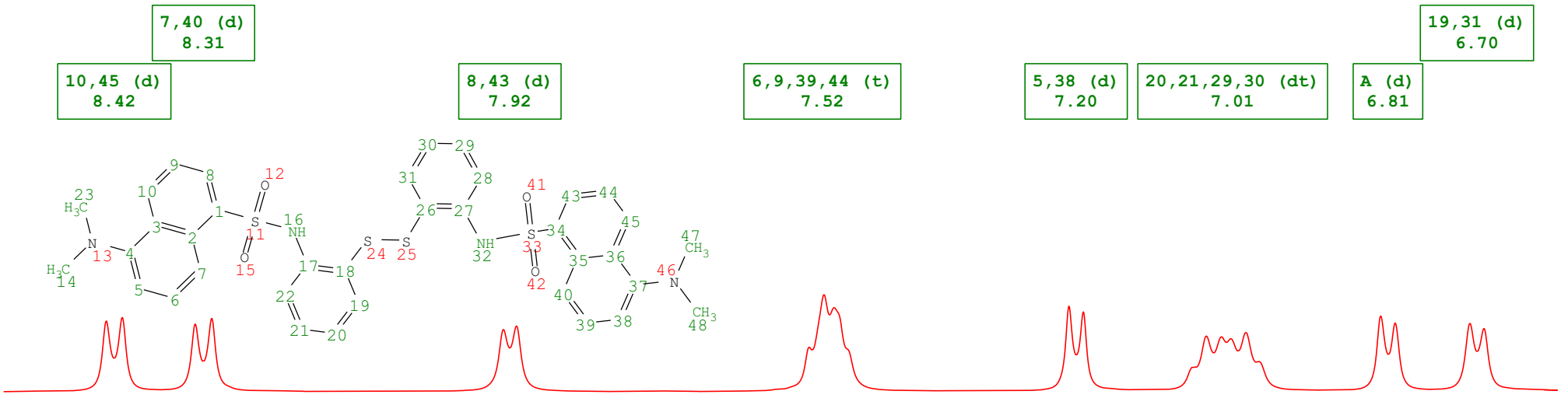
L2 dmso-d6 ligand + 1equiv. Cu(II)



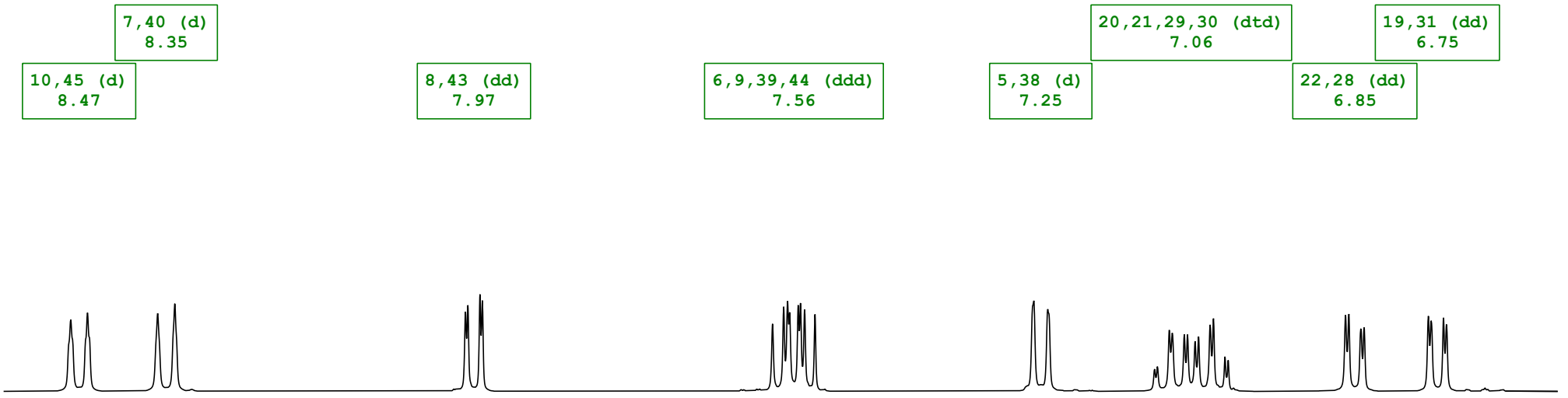

| | |
|---|---|
| NAME | AK-DR-292-DMSO-Cu.16.ser |
| DATE_TIME | 2024-12-23T08:42:07 |
| OP | Dessislava.Gerginova |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX220 L2 dmso-d6 ligand + 1equiv. Cu(II)

**DMSO: L2 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition**




**DMSO: L2 ligand only**



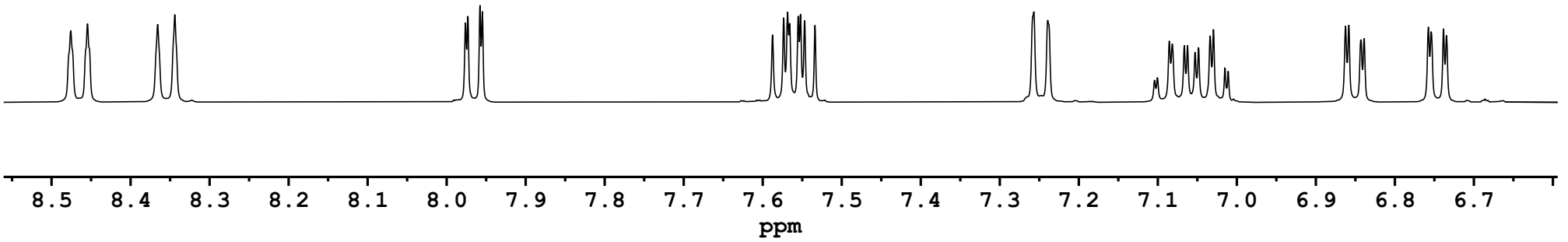



Fig SX221 L2 dmso-d6 ligand + 1equiv. Cu(II)

**DMSO: L2 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition**



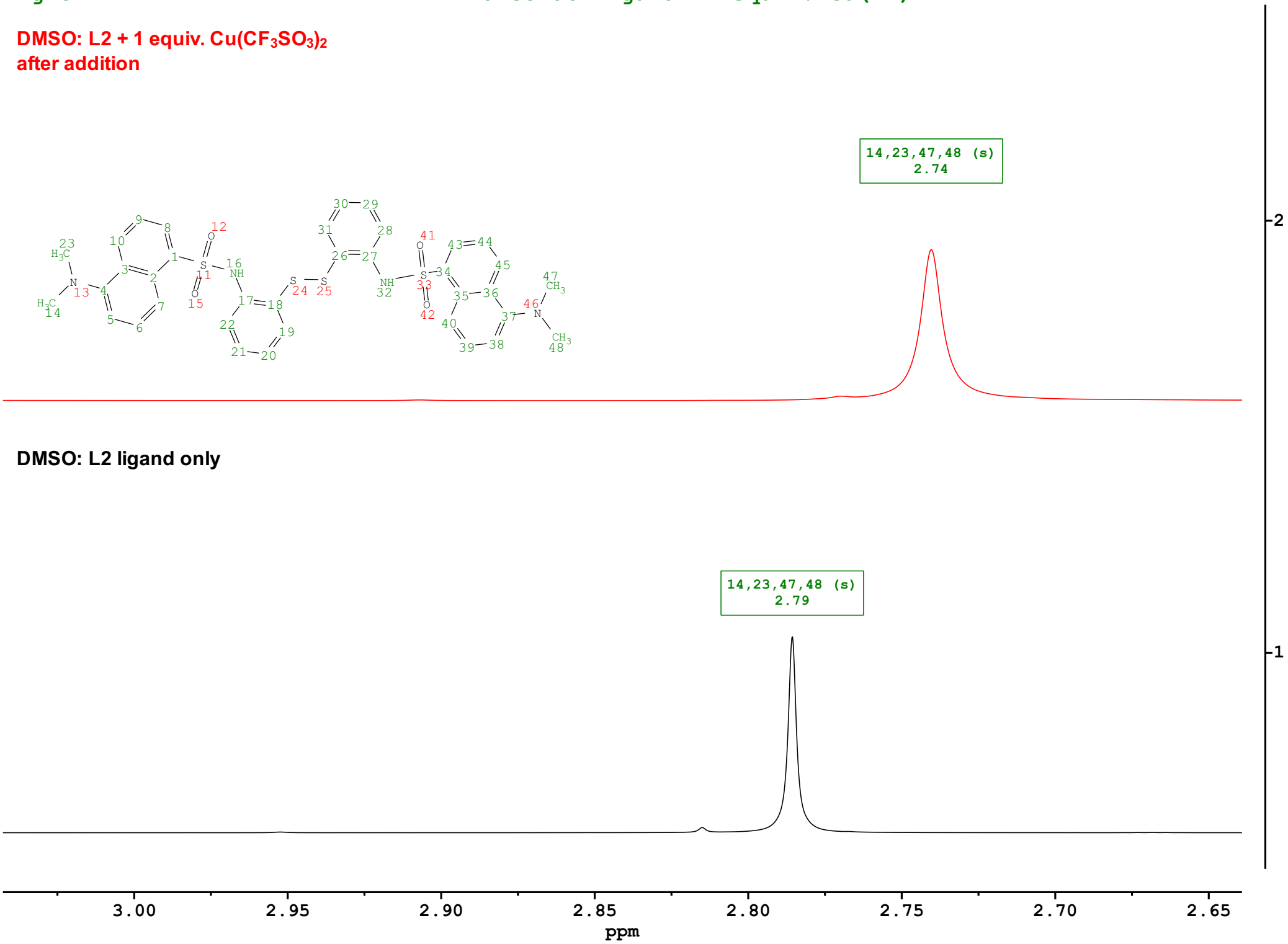
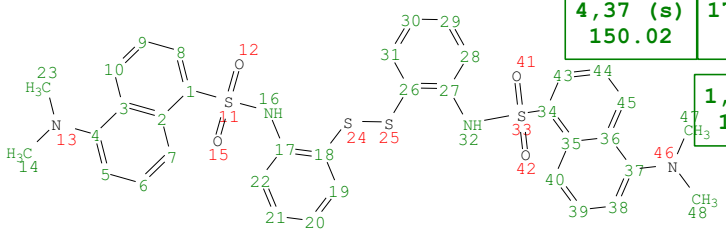


Fig SX222

L2 dmso-d6 ligand + 1equiv. Cu(II)

DMSO: L2 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition



22,28 (s) 124.17

10,45 (s) 128.78

4,37 (s) 150.02

17,27 (s) 133.41

5,38 (s) 113.84

1,34 (s) 134.62

7,40 (s) 117.87

19,31 (s) 127.23

14,23,47,48 (s) 43.70

-2

DMSO: L2 ligand only

8,43 (s) 129.03

18,26 (s) 134.71

5,38 (s) 115.16

4,37 (s) 151.34

10,45 (s) 130.10

14,23,47,48 (s) 45.03

1,34 (s) 135.95

7,40 (s) 119.20

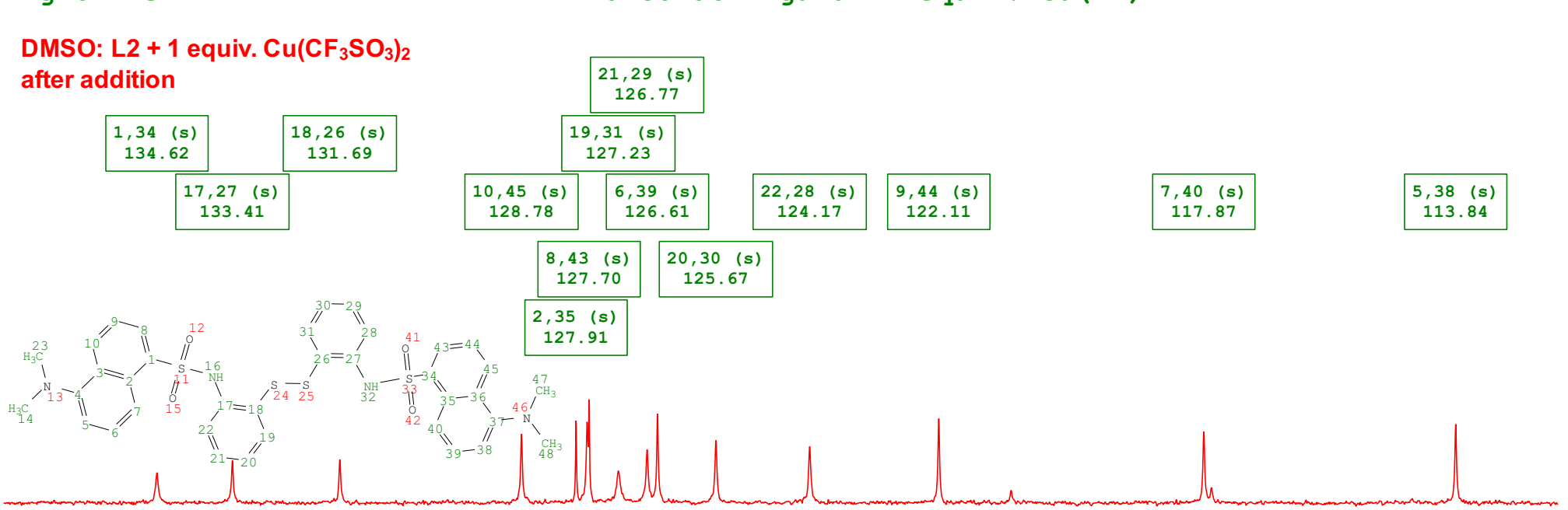
3,36 (s) 129.06

-1

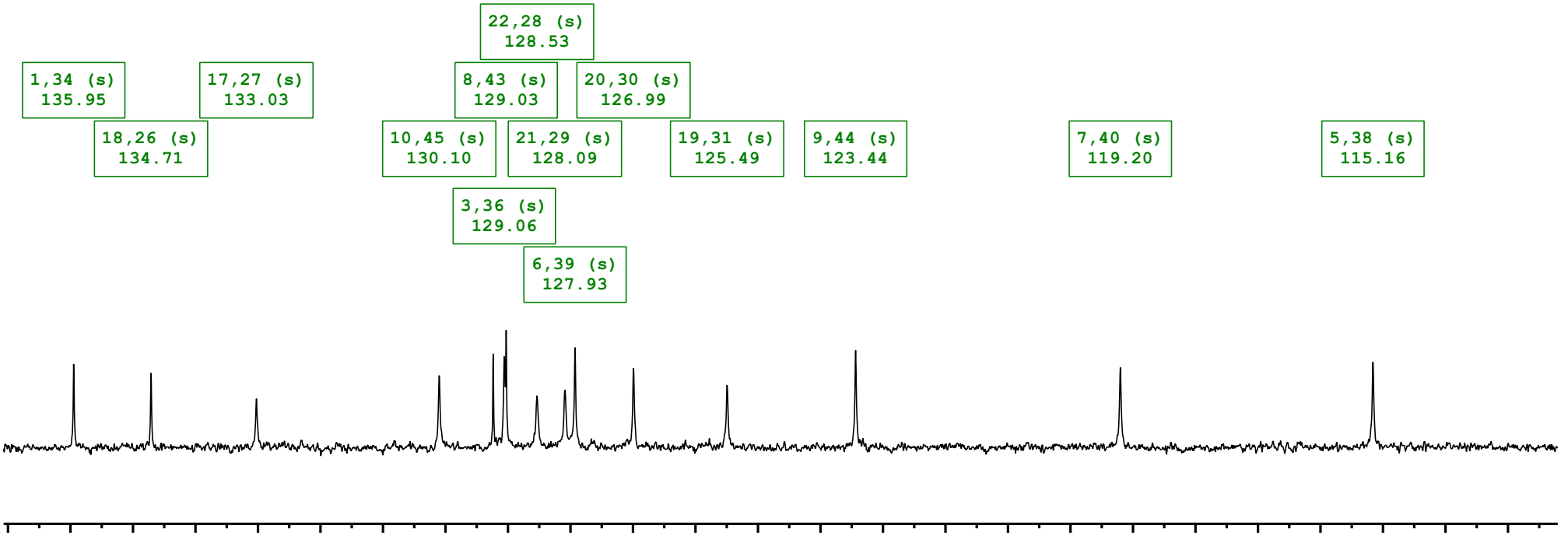
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

ppm

**DMSO: L2 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition**




**DMSO: L2 ligand only**



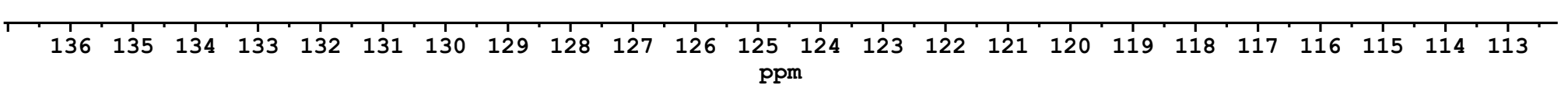



Fig SX224 L2 dmso-d6 ligand + 1equiv. Cu(II)

**DMSO: L2 + 1 equiv. $Cu(CF_3SO_3)_2$ after addition**




**DMSO: L2 ligand only**



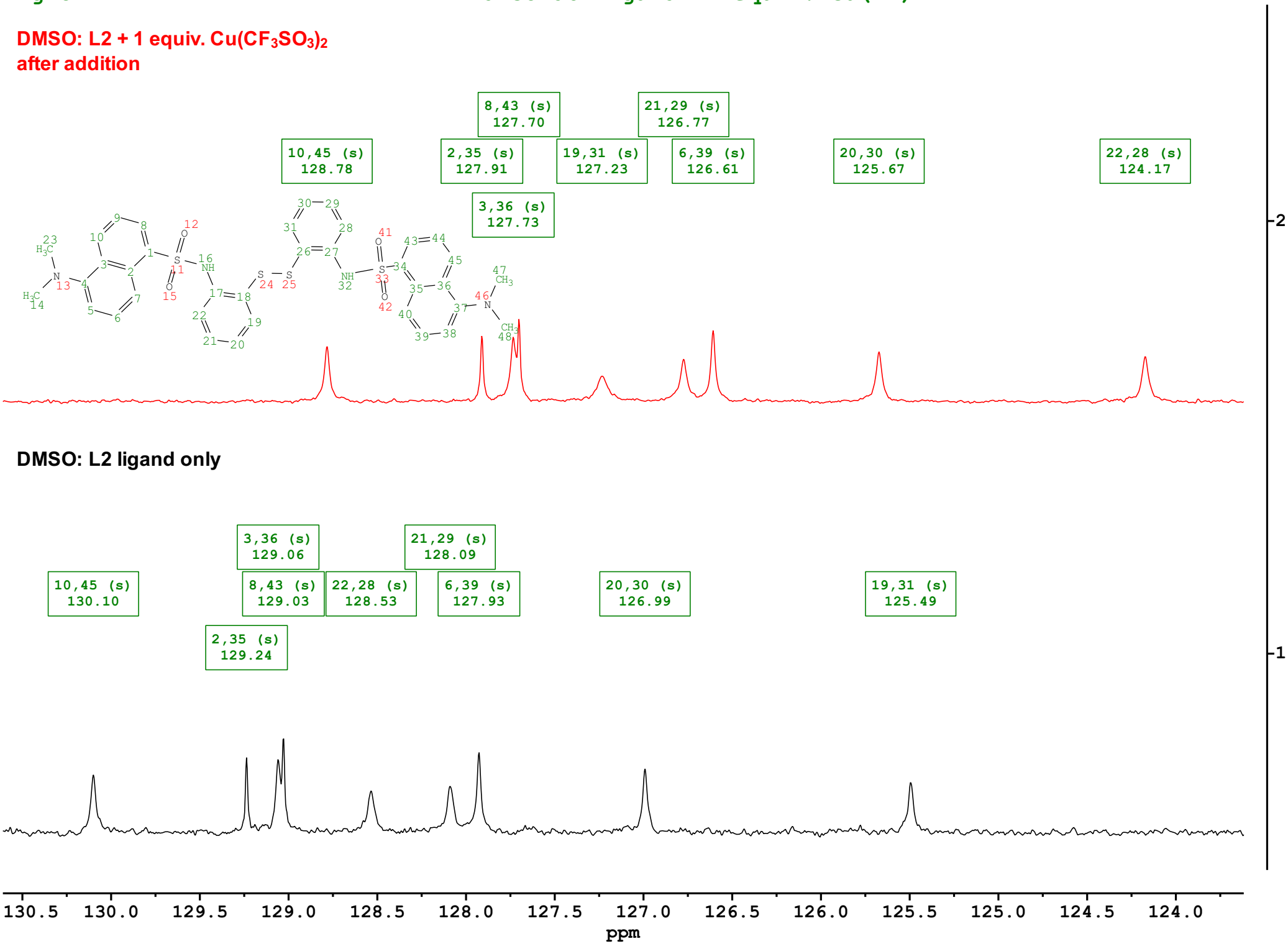
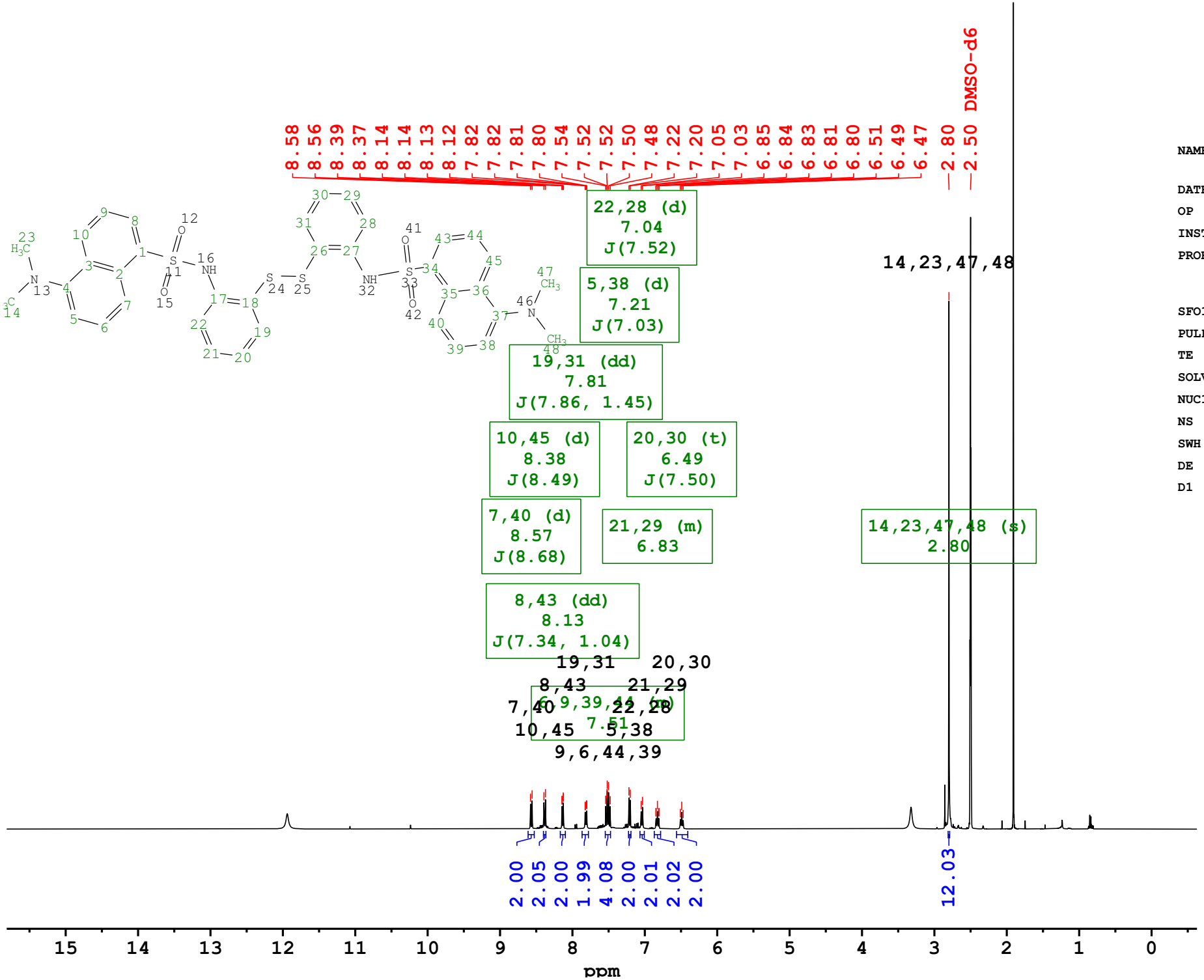



Fig SX225

L2 dmso-d6 ligand + 1equiv. Hg(II)

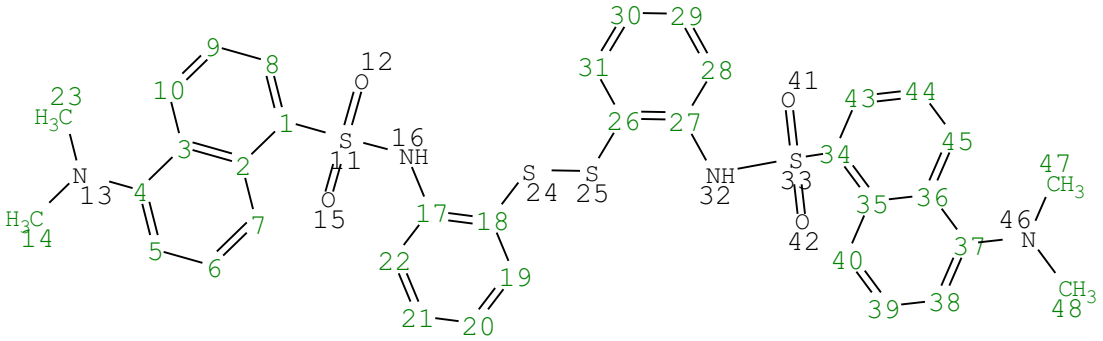



NAME AK-DR-292-DMSO-Hg4.11.fid
DATE_TIME 2025-01-16T20:26:14
OP Miroslav.Dangalov
INSTRUM Avance Neo 400
PROBHD Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N)
SFO1 600.1345610 Hz
PULPROG zg30
TE 298.0 K
SOLVENT DMSO
NUC1 1H
NS 256
SWH 9615.385 Hz
DE 6.50 usec
D1 2.0000 sec

Fig SX226

L2 dmso-d6 ligand + 1equiv. Hg(II)

8.58 8.56 8.39 8.37 8.14 8.14 8.13 8.12 7.82 7.82 7.81 7.80 7.54 7.52 7.52 7.50 7.48 7.22 7.20 7.05 7.03 6.85 6.84 6.83 6.81 6.80 6.51 6.49 6.47



| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.11.fid |
| DATE_TIME | 2025-01-16T20:26:14 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

10,45 (d) 8.38 J(8.49)

19,31 (dd) 7.81 J(7.86, 1.45)

22,28 (d) 7.04 J(7.52)

7,40 (d) 8.57 J(8.68)

8,43 (dd) 8.13 J(7.34, 1.04)

6,9,39,44 (m) 7.51

5,38 (d) 7.21 J(7.03)

21,29 (m) 6.83

20,30 (t) 6.49 J(7.50)

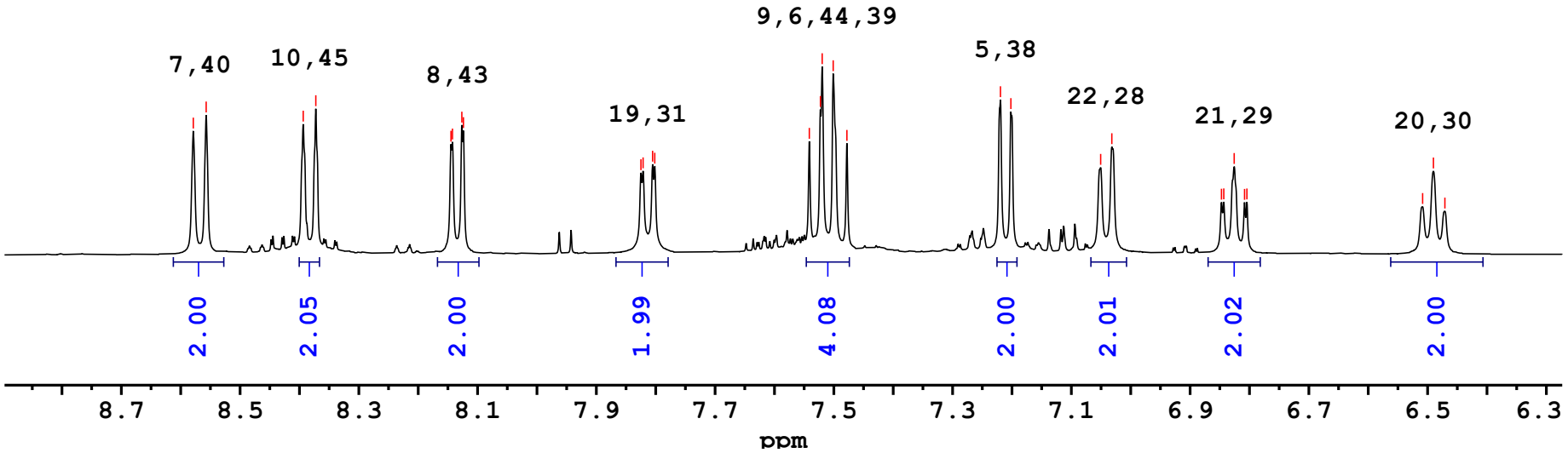
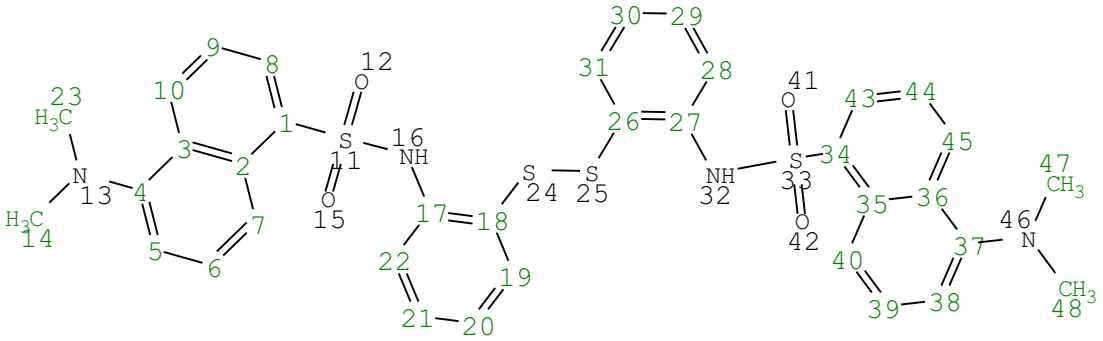


**Fig SX227** **L2 dmso-d6 ligand + 1equiv. Hg(II)**

8.58 8.56 8.39 8.37 8.14 8.14 8.13 8.12 7.82 7.82 7.81 7.80



| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.11.fid |
| DATE_TIME | 2025-01-16T20:26:14 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

| 7,40 (d) | 10,45 (d) | 8,43 (dd) | 19,31 (dd) |
|---|---|---|---|
| 8.57 | 8.38 | 8.13 | 7.81 |
| J(8.68) | J(8.49) | J(7.34, 1.04) | J(7.86, 1.45) |

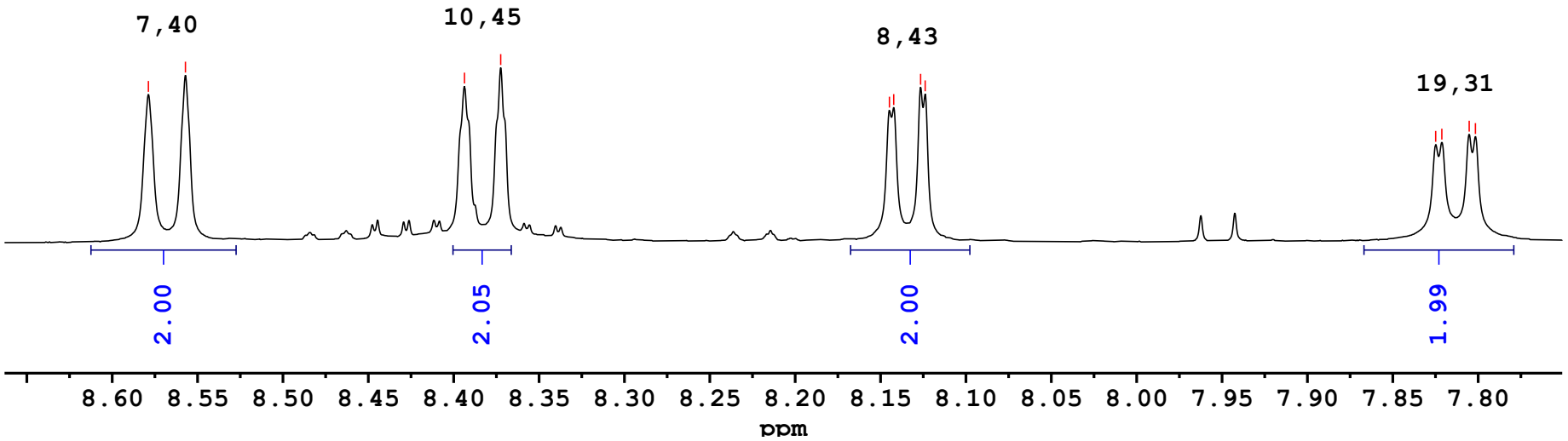
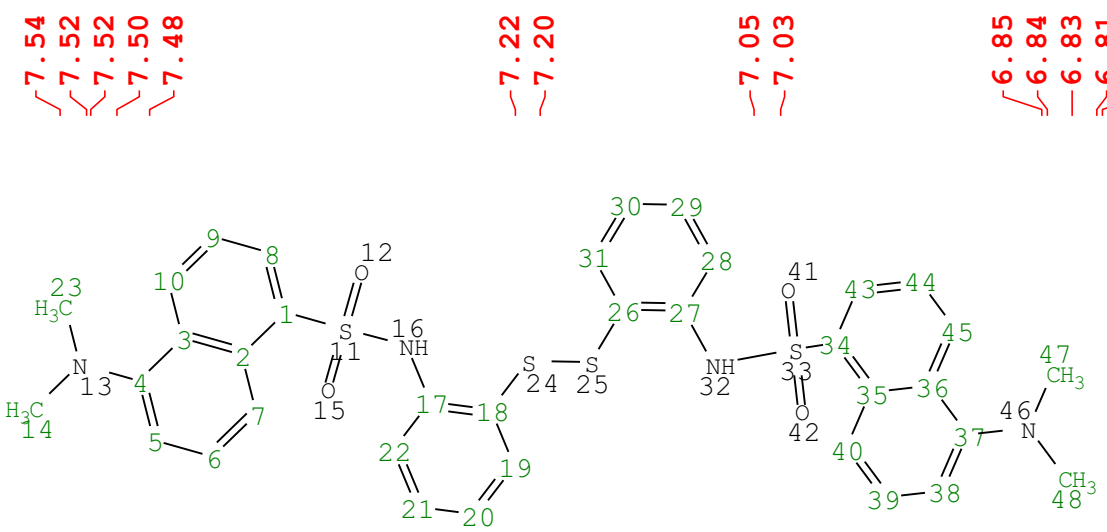


Fig SX228 L2 dmso-d6 ligand + 1equiv. Hg(II)






| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.11.fid |
| DATE_TIME | 2025-01-16T20:26:14 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

6,9,39,44 (m)
7.51

5,38 (d)
7.21
J(7.03)

22,28 (d)
7.04
J(7.52)

21,29 (m)
6.83

20,30 (t)
6.49
J(7.50)

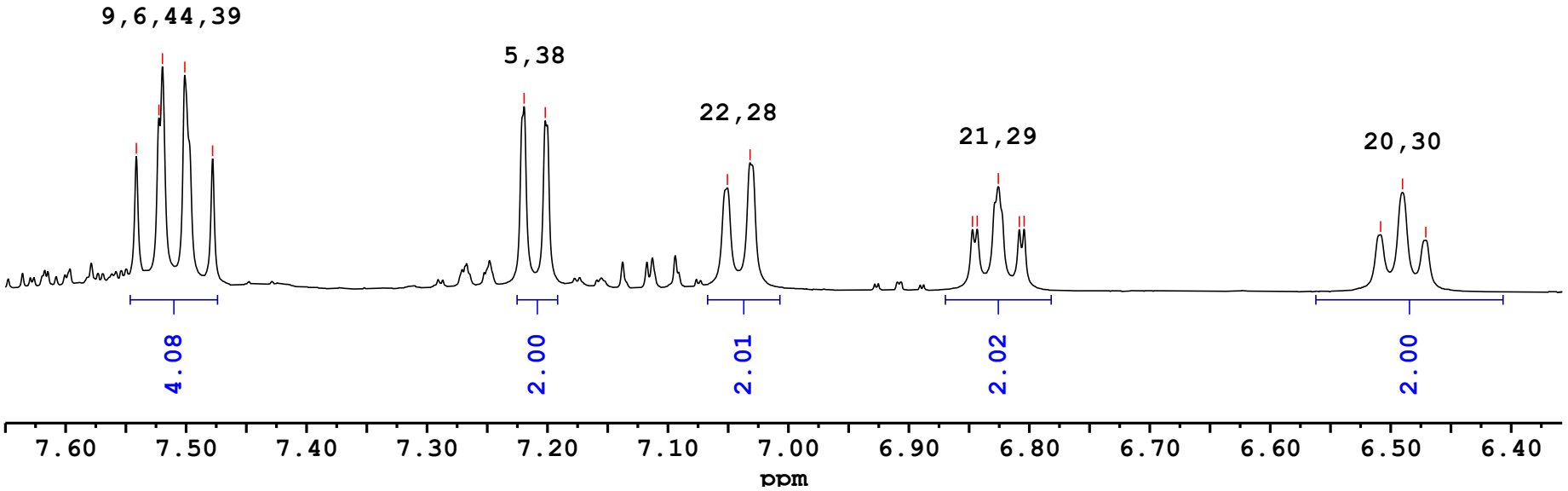
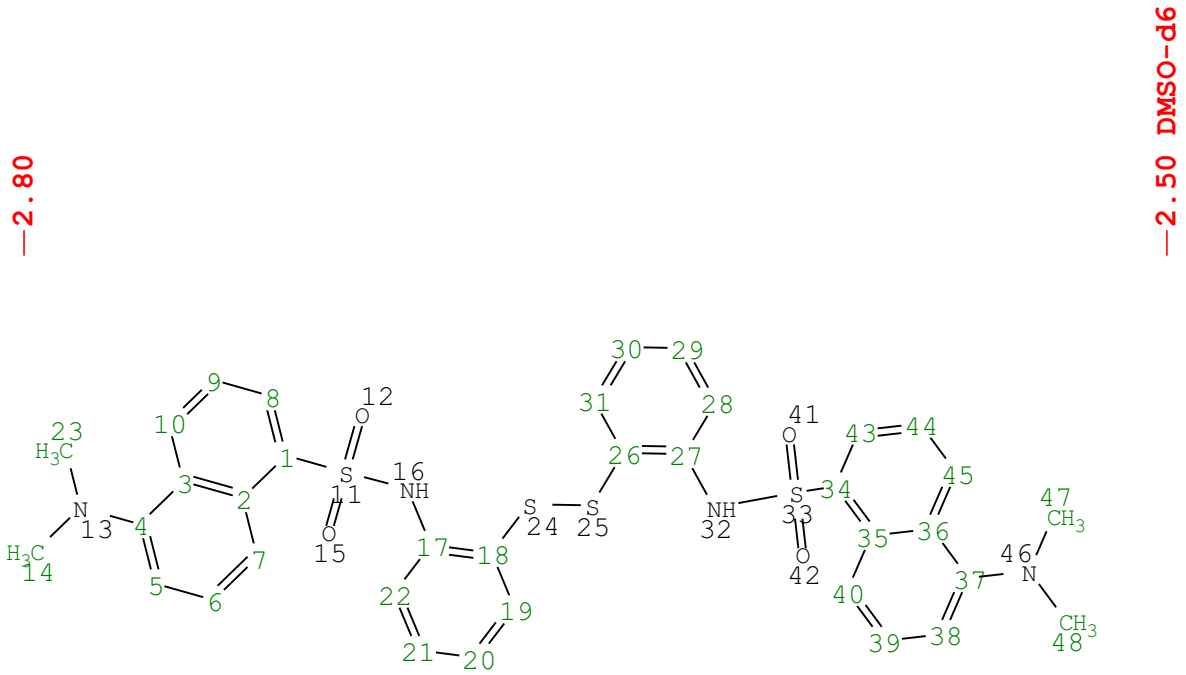


**Fig SX229** **L2 dmso-d6 ligand + 1equiv. Hg(II)**




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.11.fid |
| DATE_TIME | 2025-01-16T20:26:14 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1345610 Hz |
| PULPROG | zg30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 256 |
| SWH | 9615.385 Hz |
| DE | 6.50 usec |
| D1 | 2.0000 sec |

**14,23,47,48 (s)**
**2.80**

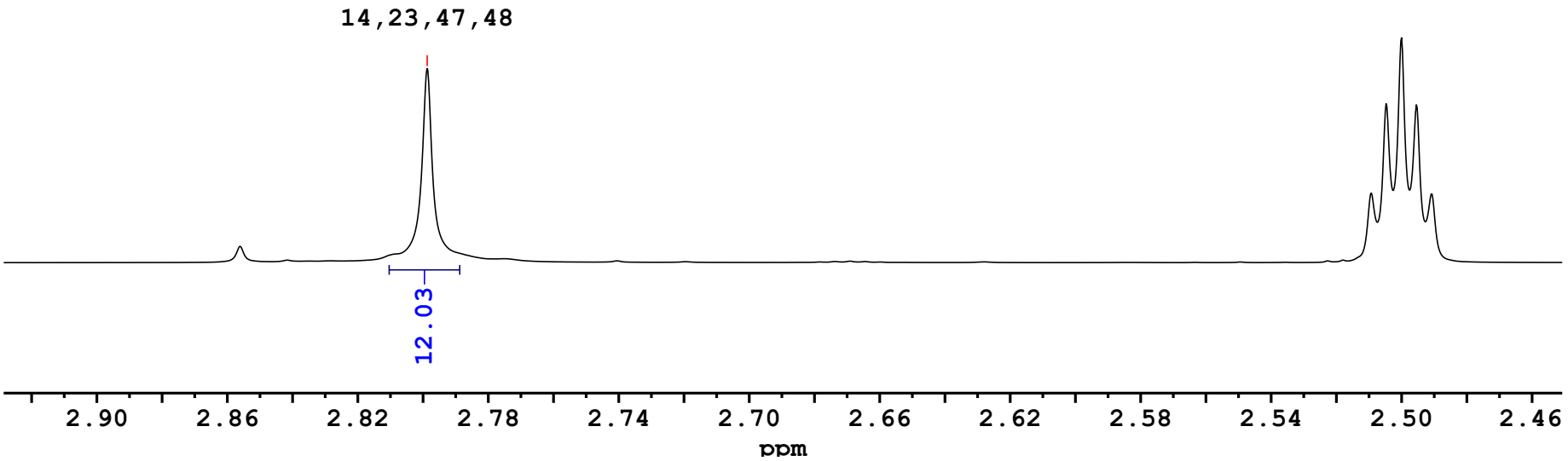
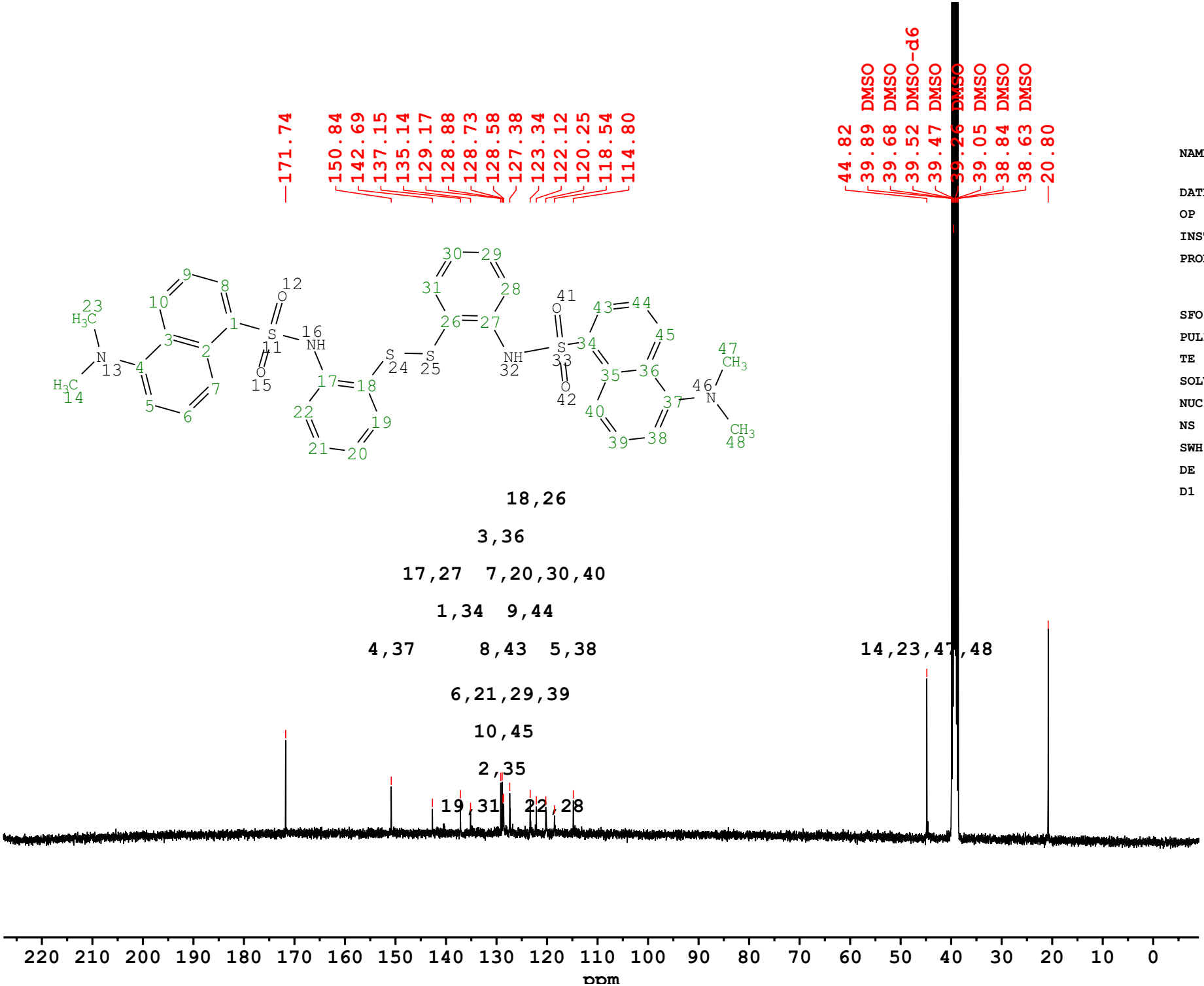


Fig SX230

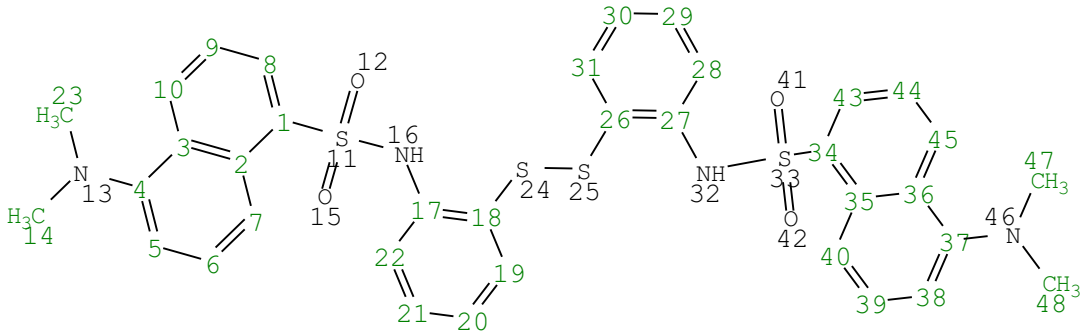
L2 dmso-d6 ligand + 1equiv. Hg(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.18.fid |
| DATE_TIME | 2025-01-17T12:24:17 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9319844 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 16384 |
| SWH | 35714.286 Hz |
| DE | 18.00 usec |
| D1 | 1.5000 sec |

Fig SX231 L2 dmso-d6 ligand + 1equiv. Hg(II)

150.84 142.69 137.15 135.14 129.17 128.88 128.73 128.58 127.38 123.34 122.12 120.25 118.54 114.80



| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.18.fid |
| DATE_TIME | 2025-01-17T12:24:17 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9319844 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 16384 |
| SWH | 35714.286 Hz |
| DE | 18.00 usec |
| D1 | 1.5000 sec |

3,36 19,31 8,43 7,20,30,40 4,37 17,27 1,34 6,21,29,39 9,44 22,28 5,38 10,45 18,26 2,35

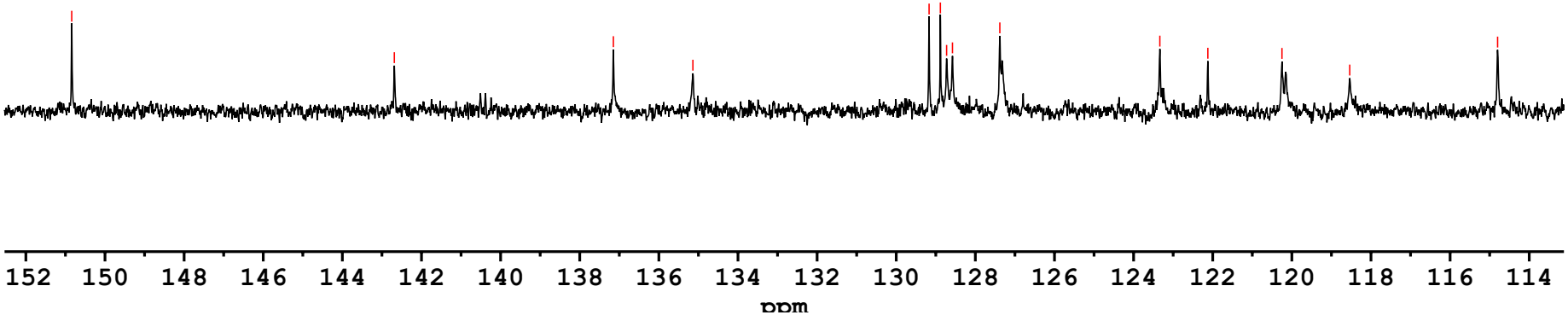
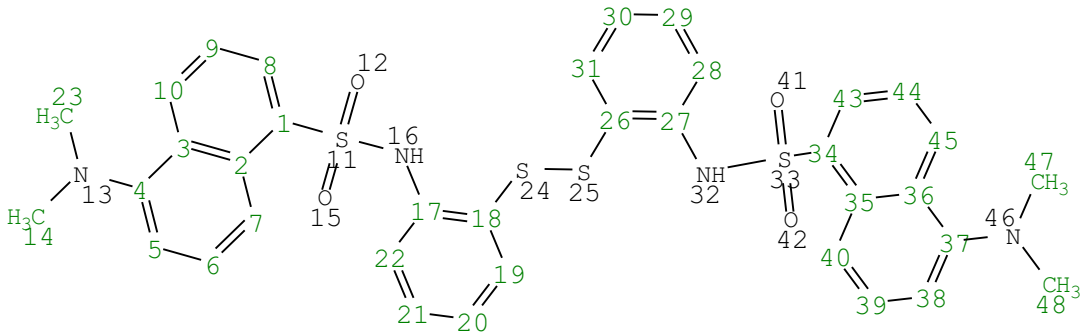


**Fig SX232** **L2 dmso-d6 ligand + 1equiv. Hg(II)**

129.17
128.88
128.73
128.58
127.38
123.34
122.12
120.25
118.54



| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.18.fid |
| DATE_TIME | 2025-01-17T12:24:17 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9319844 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 16384 |
| SWH | 35714.286 Hz |
| DE | 18.00 usec |
| D1 | 1.5000 sec |

2,35
10,45
8,43
6,21,29,39
9,44
18,26
7,20,30,40
22,28
3,36

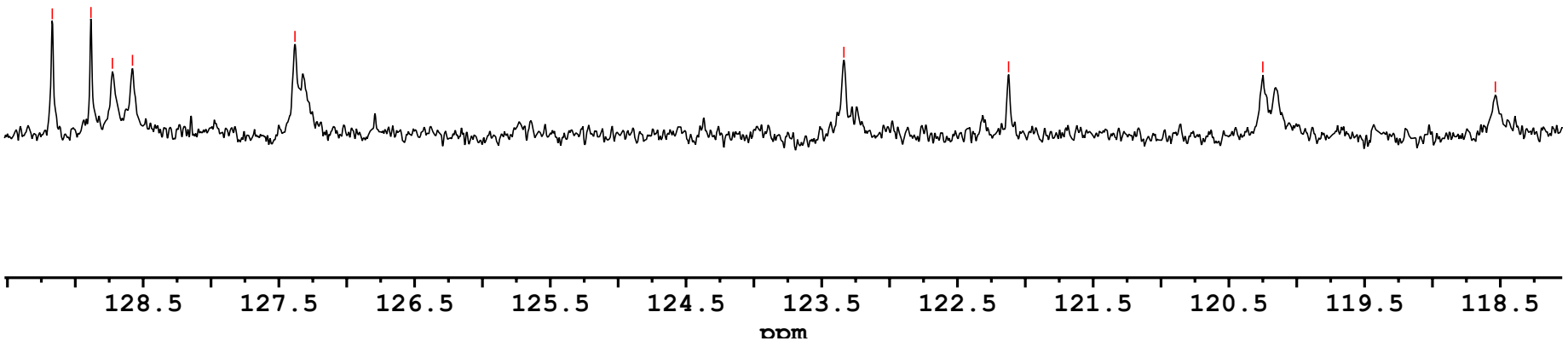
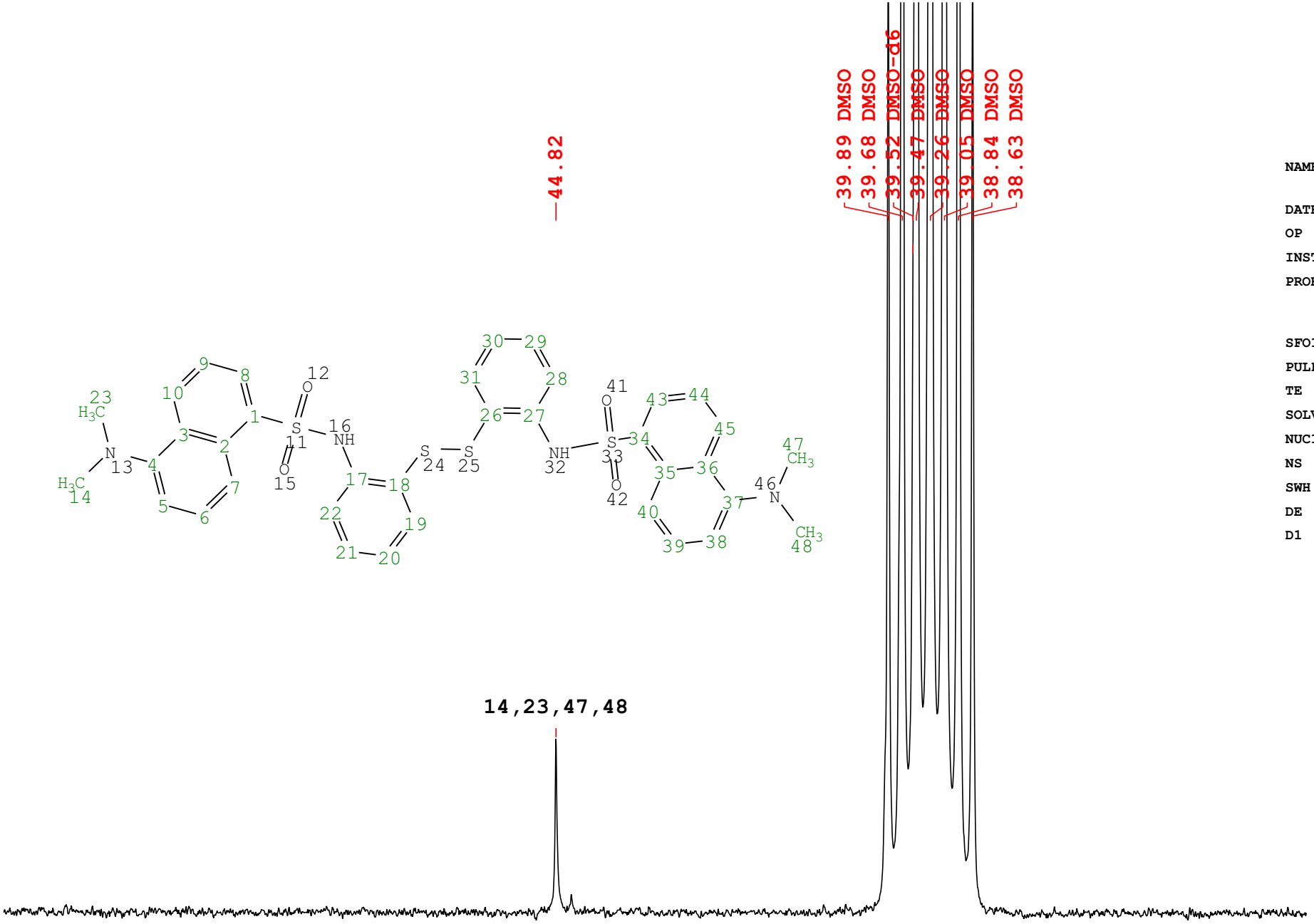


Fig SX233

L2 dmso-d6 ligand + 1equiv. Hg(II)

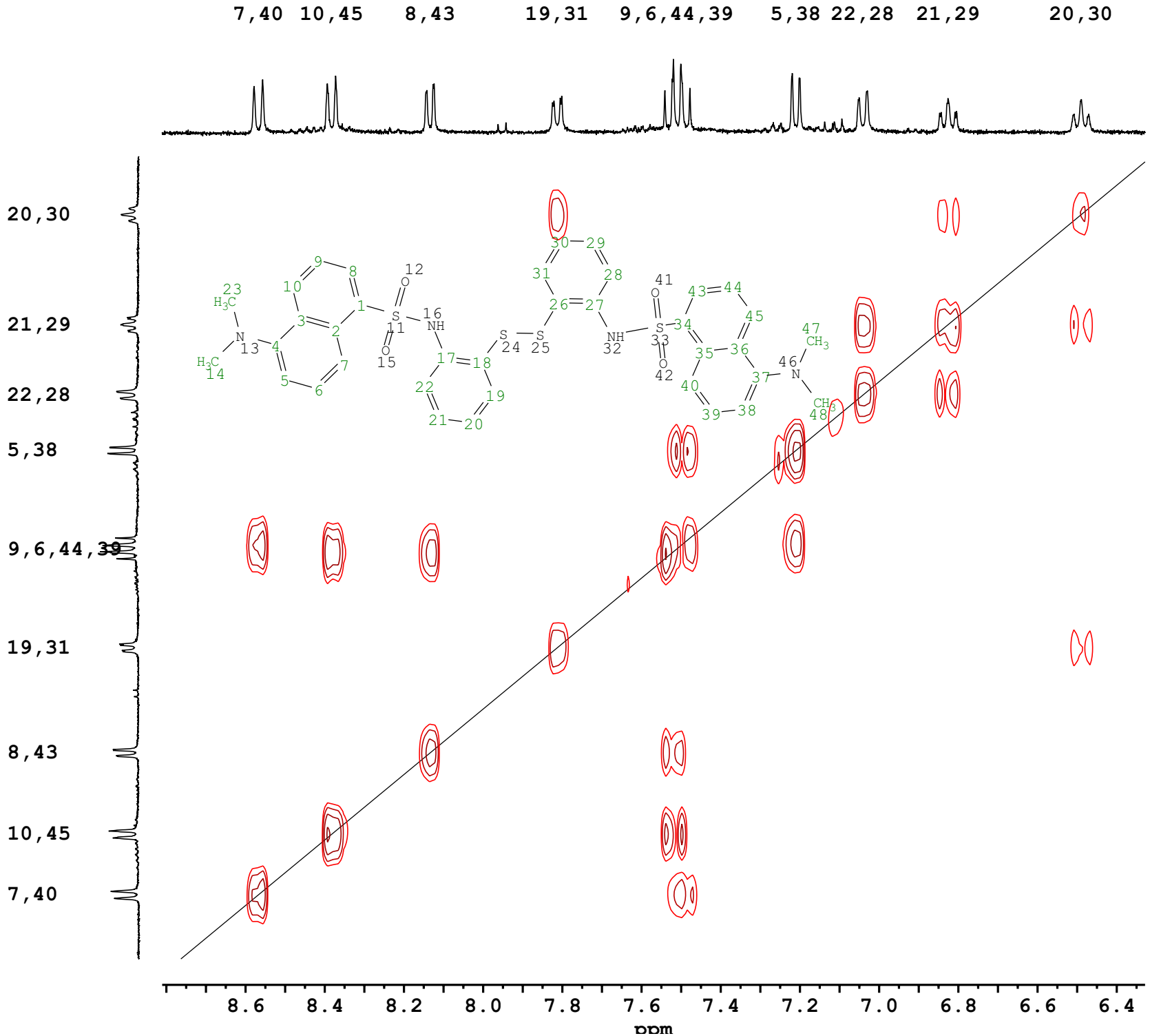





| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.18.fid |
| DATE_TIME | 2025-01-17T12:24:17 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 150.9319844 Hz |
| PULPROG | zgdc30 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 13C |
| NS | 16384 |
| SWH | 35714.286 Hz |
| DE | 18.00 usec |
| D1 | 1.5000 sec |

Fig SX234

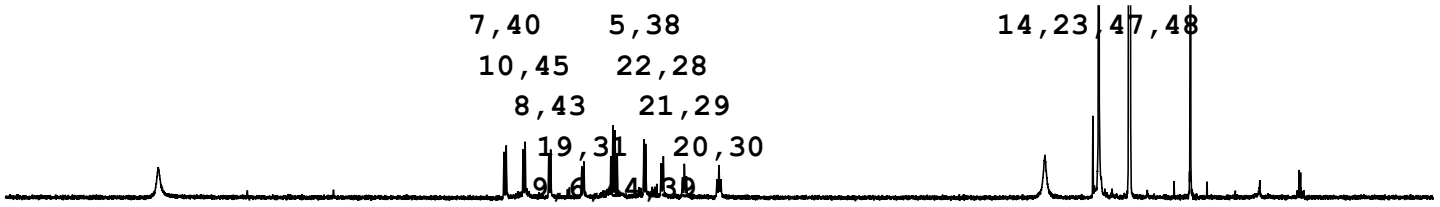
L2 dmso-d6 ligand + 1equiv. Hg(II)

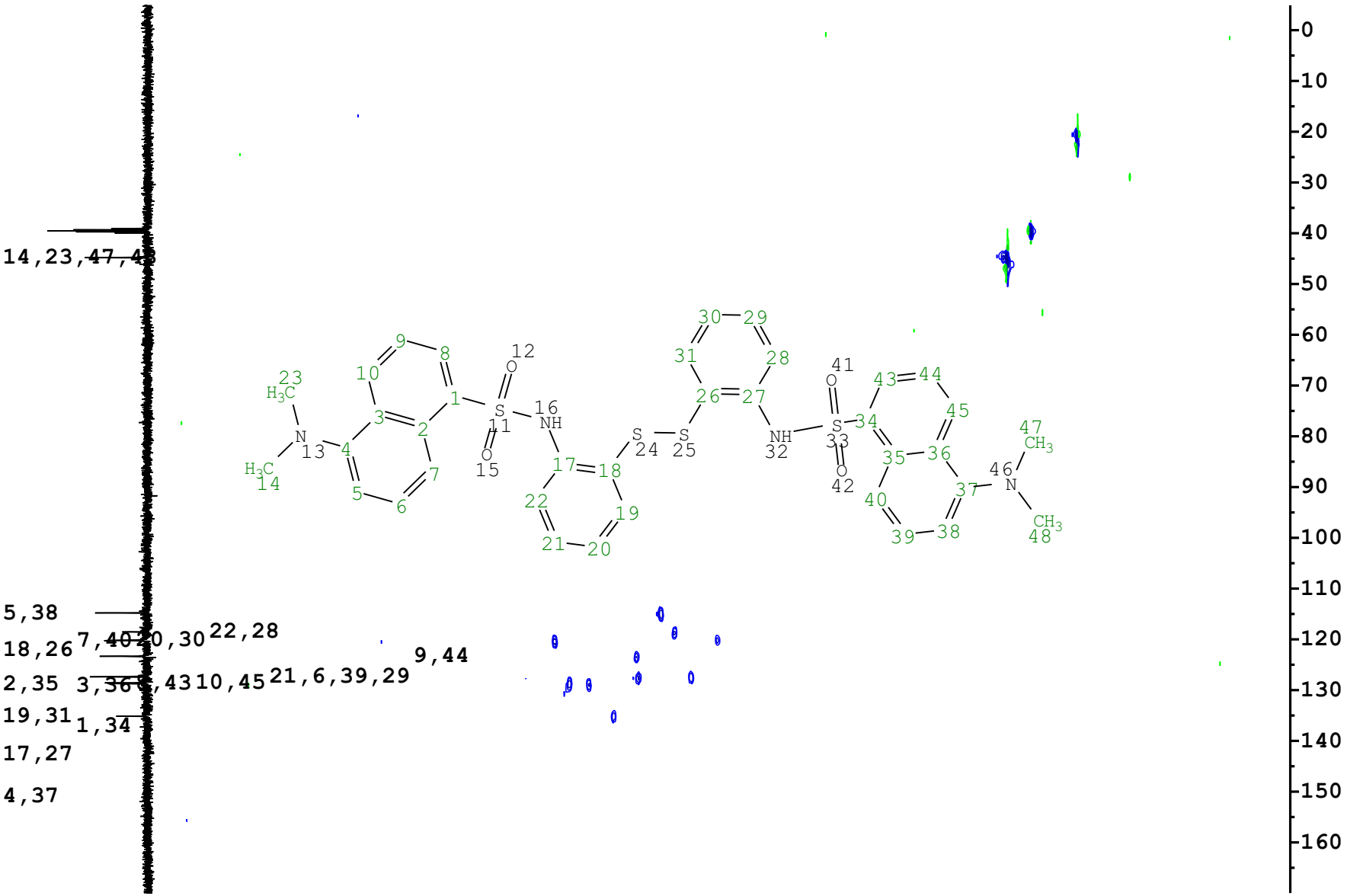



| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.14.ser |
| DATE_TIME | 2025-01-16T22:25:58 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | cosygpmfqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 4 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0795 sec |

Fig SX235

L2 dmso-d6 ligand + 1equiv. Hg(II)

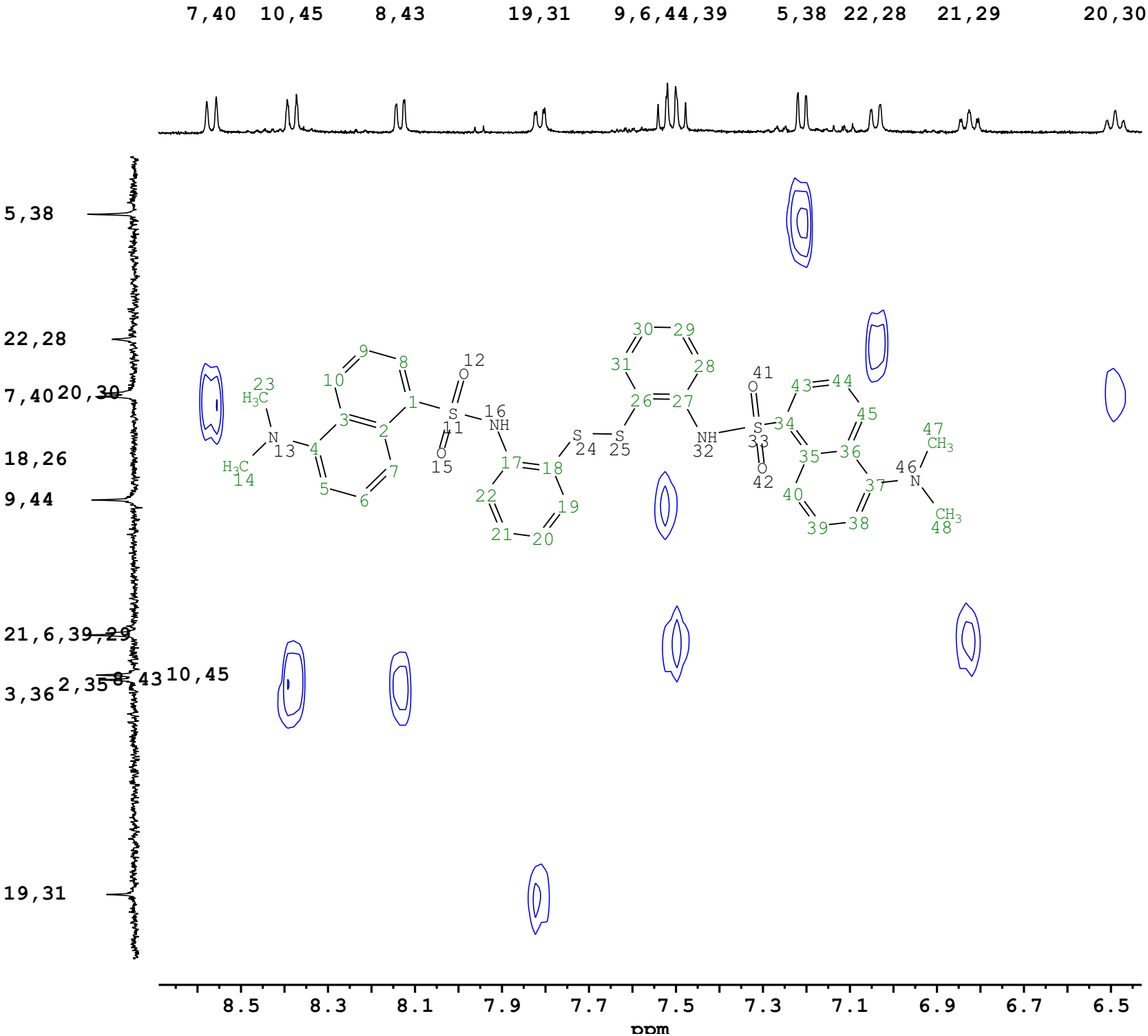



| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.15.ser |
| DATE_TIME | 2025-01-16T23:10:55 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX236

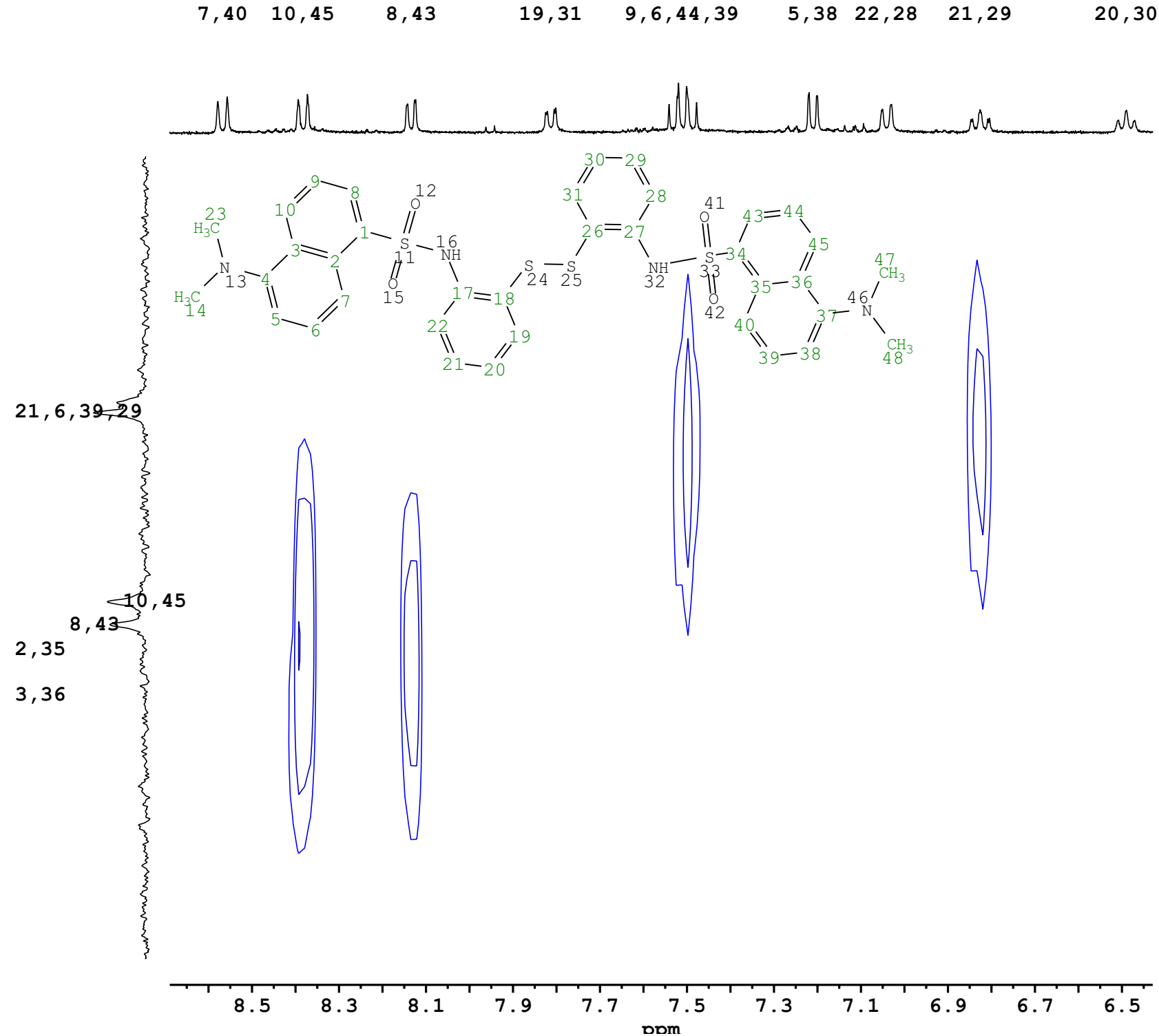
L2 dmso-d6 ligand + 1equiv. Hg(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.15.ser |
| DATE_TIME | 2025-01-16T23:10:55 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX237

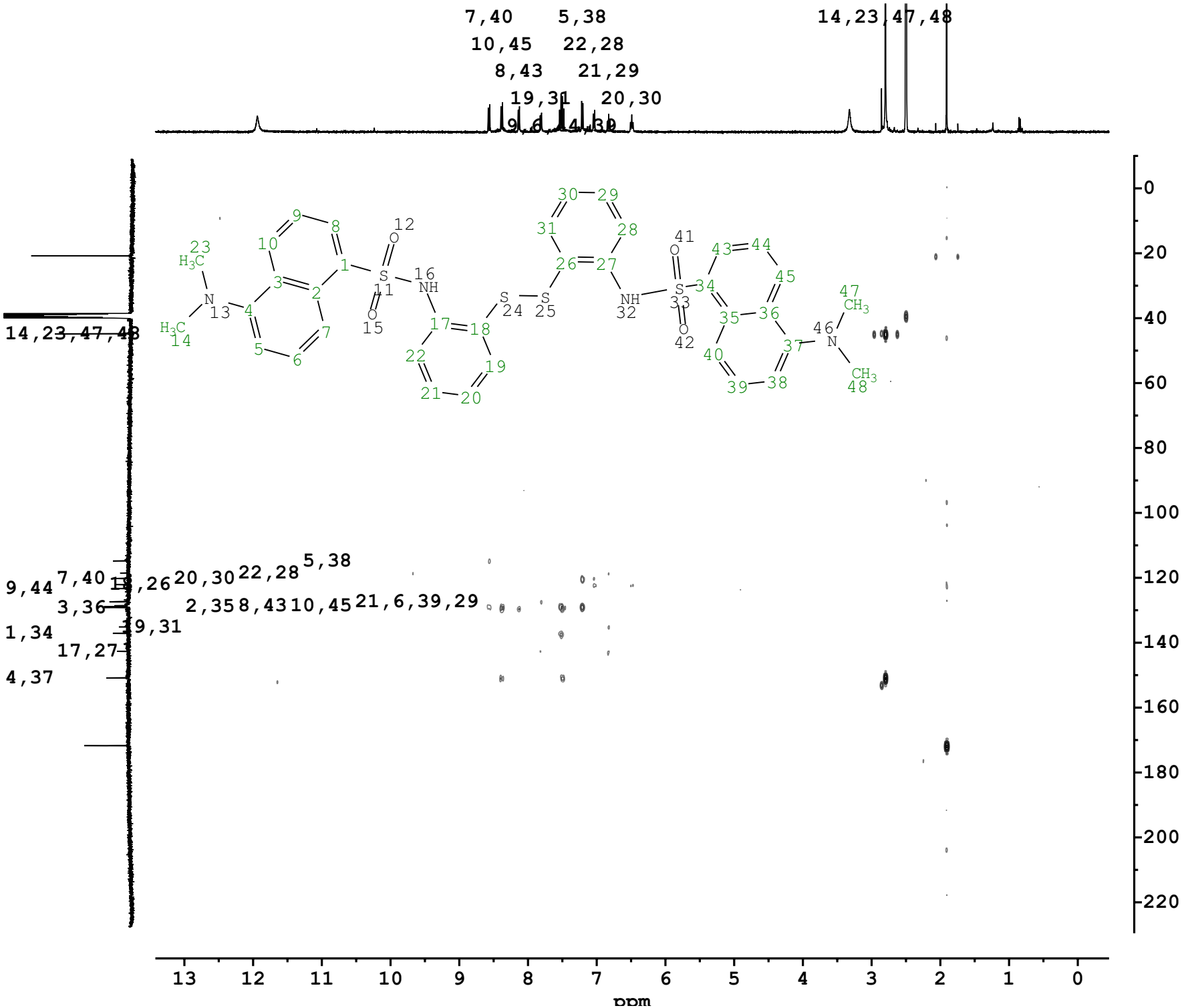
L2 dmso-d6 ligand + 1equiv. Hg(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.15.ser |
| DATE_TIME | 2025-01-16T23:10:55 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hsqcedetgpsp.3 |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 8 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.4526 sec |

Fig SX238

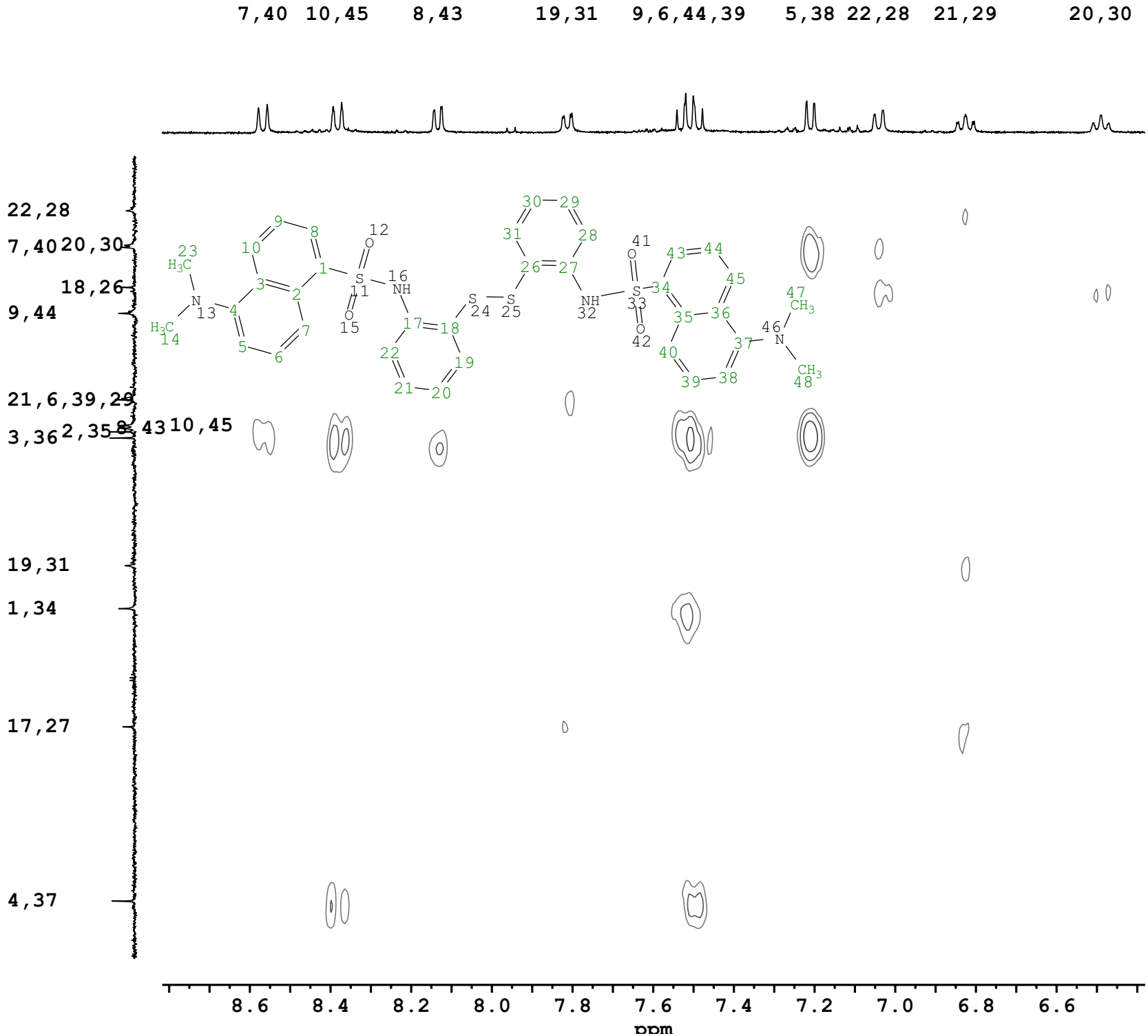
L2 dmso-d6 ligand + 1equiv. Hg(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.16.ser |
| DATE_TIME | 2025-01-17T00:40:29 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX239

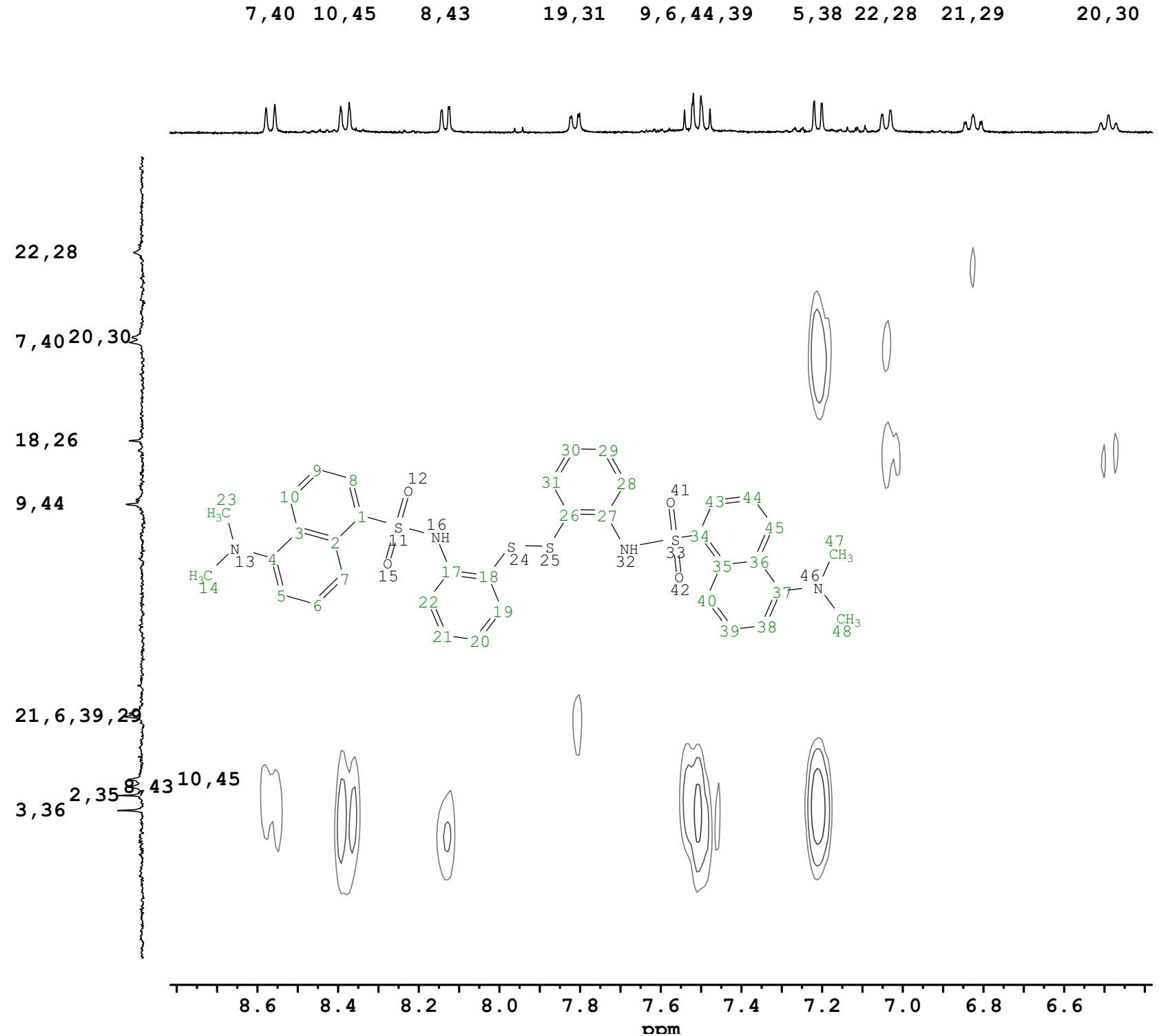
L2 dmso-d6 ligand + 1equiv. Hg(II)




| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.16.ser |
| DATE_TIME | 2025-01-17T00:40:29 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX240

L2 dmso-d6 ligand + 1equiv. Hg(II)

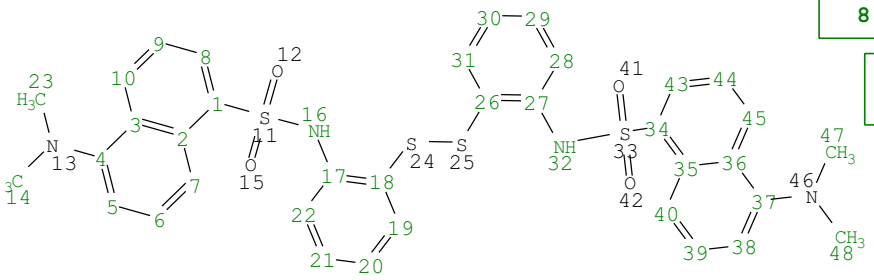



| | |
|---|---|
| NAME | AK-DR-292-DMSO-Hg4.16.ser |
| DATE_TIME | 2025-01-17T00:40:29 |
| OP | Miroslav.Dangalov |
| INSTRUM | Avance Neo 400 |
| PROBHD | Z175272_0007 (PI HR-TBO400S1-BBF/ H/ F/ D-5.0-Z FB N) |
| SFO1 | 600.1326342 Hz |
| PULPROG | hmbcgplpndqf |
| TE | 298.0 K |
| SOLVENT | DMSO |
| NUC1 | 1H |
| NS | 16 |
| SWH | 6097.561 Hz |
| DE | 6.50 usec |
| D1 | 1.0443 sec |

Fig SX241

L2 dmso-d6 ligand + 1equiv. Hg(II)

DMSO: L2 + 1 equiv. $Hg(CH_3COO)_2$ after addition



19,31 (dd) 7.81

10,45 (d) 8.38

21,29 (m) 6.83

7,40 (d) 8.57

5,38 (d) 7.21

8,43 (dd) 8.13

20,30 (t) 6.49

6,9,39,44 (m) 7.51

14,23,47,48 (s) 2.80

DMSO: L2 ligand only

6,9,39,44 (ddd) 7.56

7,40 (d) 8.35

22,28 (dd) 6.85

16,32 (s) 10.23

10,45 (d) 8.47

5,38 (d) 7.25

8,43 (dd) 7.97

20,21,29,30 (dtd) 7.06

14,23,47,48 (s) 2.79

2

1

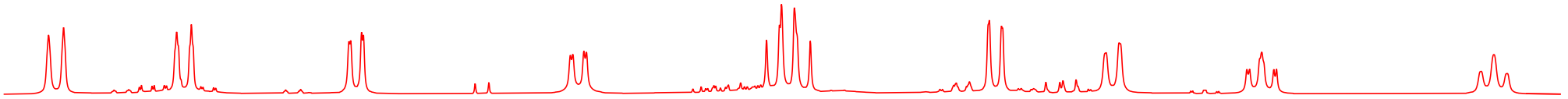
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0

ppm

Fig SX242 L2 dmso-d6 ligand + 1equiv. Hg(II)

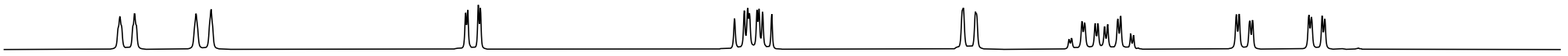
**DMSO: L2 + 1 equiv. $Hg(CH_3COO)_2$ after addition**

7,40 (d) 8.57 | 10,45 (d) 8.38 | 8,43 (dd) 8.13 | 19,31 (dd) 7.81 | 6,9,39,44 (m) 7.51 | 5,38 (d) 7.21 | 22,28 (d) 7.04 | 21,29 (m) 6.83 | 20,30 (t) 6.49



**DMSO: L2 ligand only**

7,40 (d) 8.35 | 10,45 (d) 8.47 | 8,43 (dd) 7.97 | 6,9,39,44 (ddd) 7.56 | 5,38 (d) 7.25 | 20,21,29,30 (dtd) 7.06 | 22,28 (dd) 6.85 | 19,31 (dd) 6.75



8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5

ppm

Fig SX243 L2 dmso-d6 ligand + 1equiv. Hg(II)

DMSO: L2 + 1 equiv. $Hg(CH_3COO)_2$
after addition

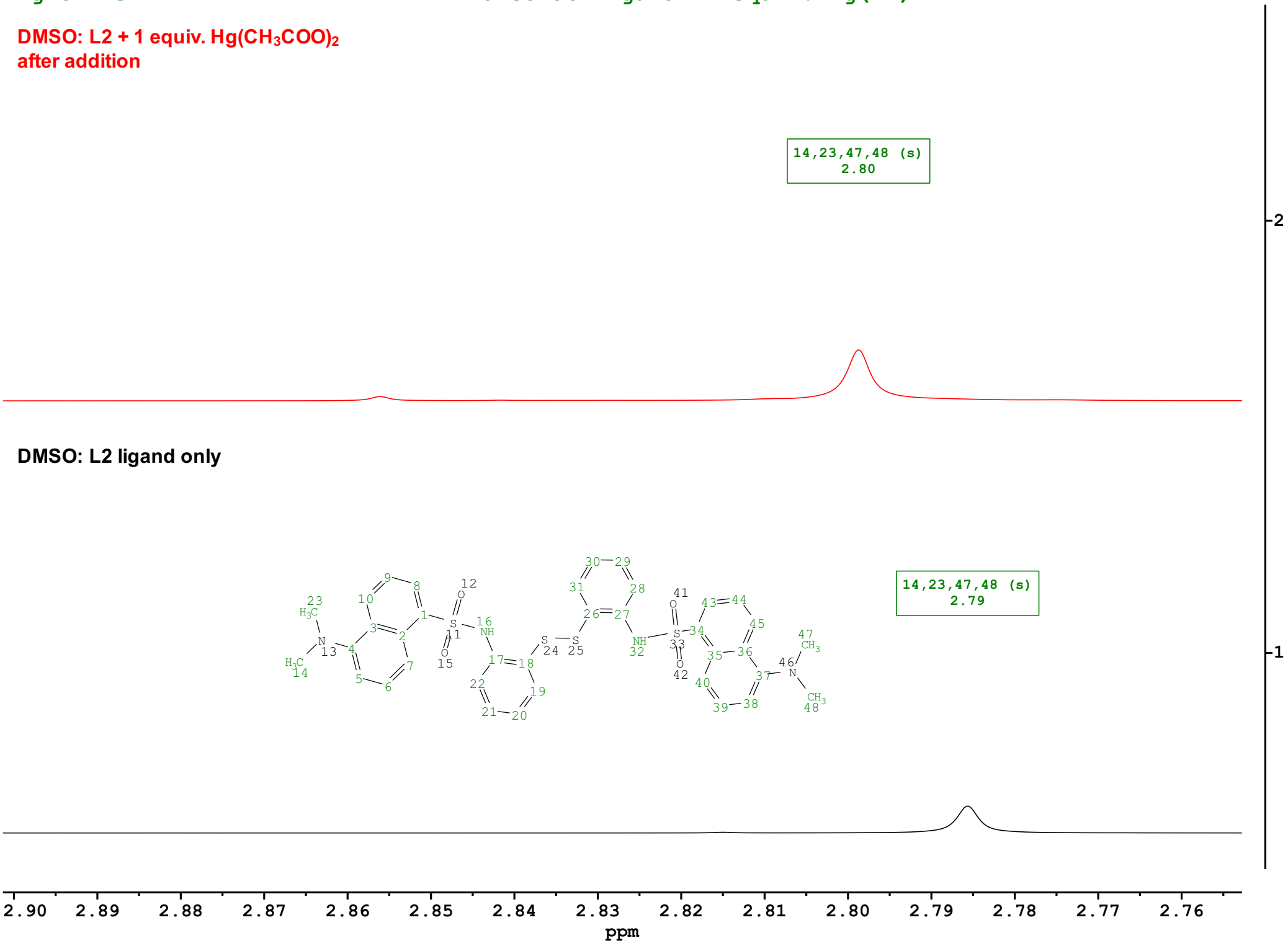
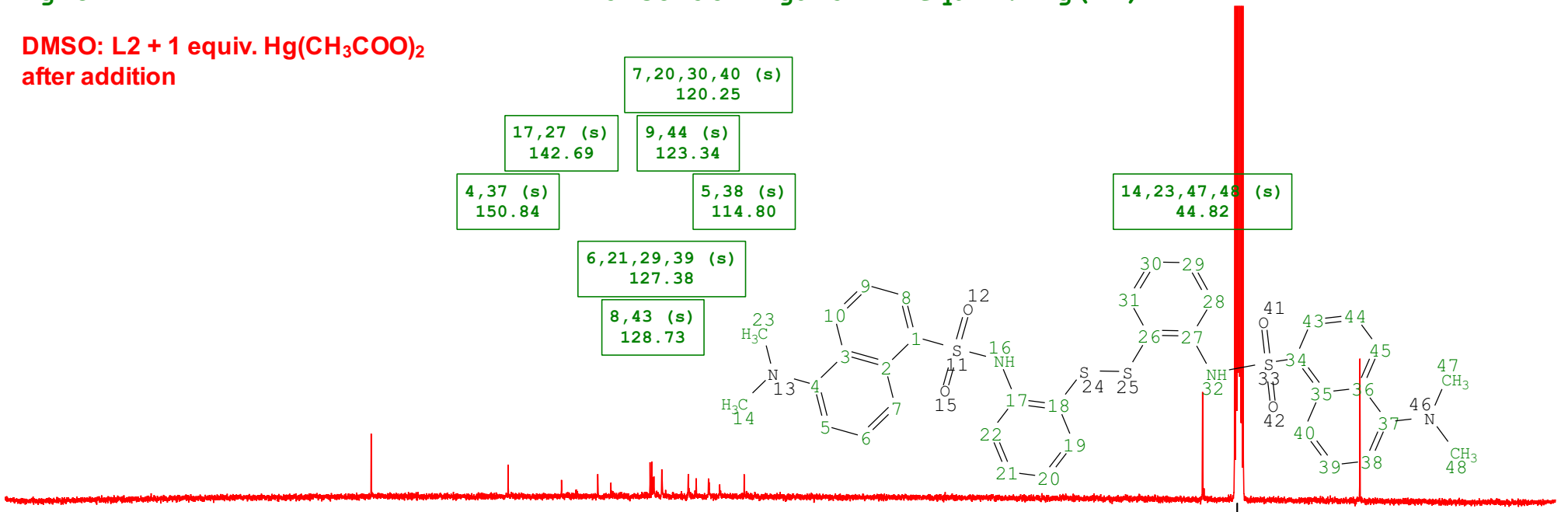


Fig SX244

L2 dmso-d6 ligand + 1equiv. Hg(II)

DMSO: L2 + 1 equiv. $Hg(CH_3COO)_2$ after addition




DMSO: L2 ligand only

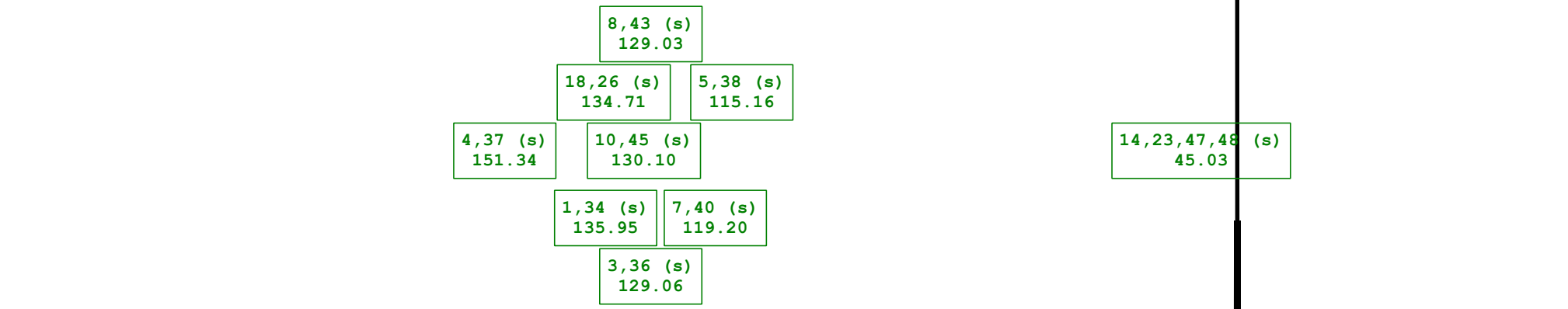


Fig SX245 L2 dmso-d6 ligand + 1equiv. Hg(II)

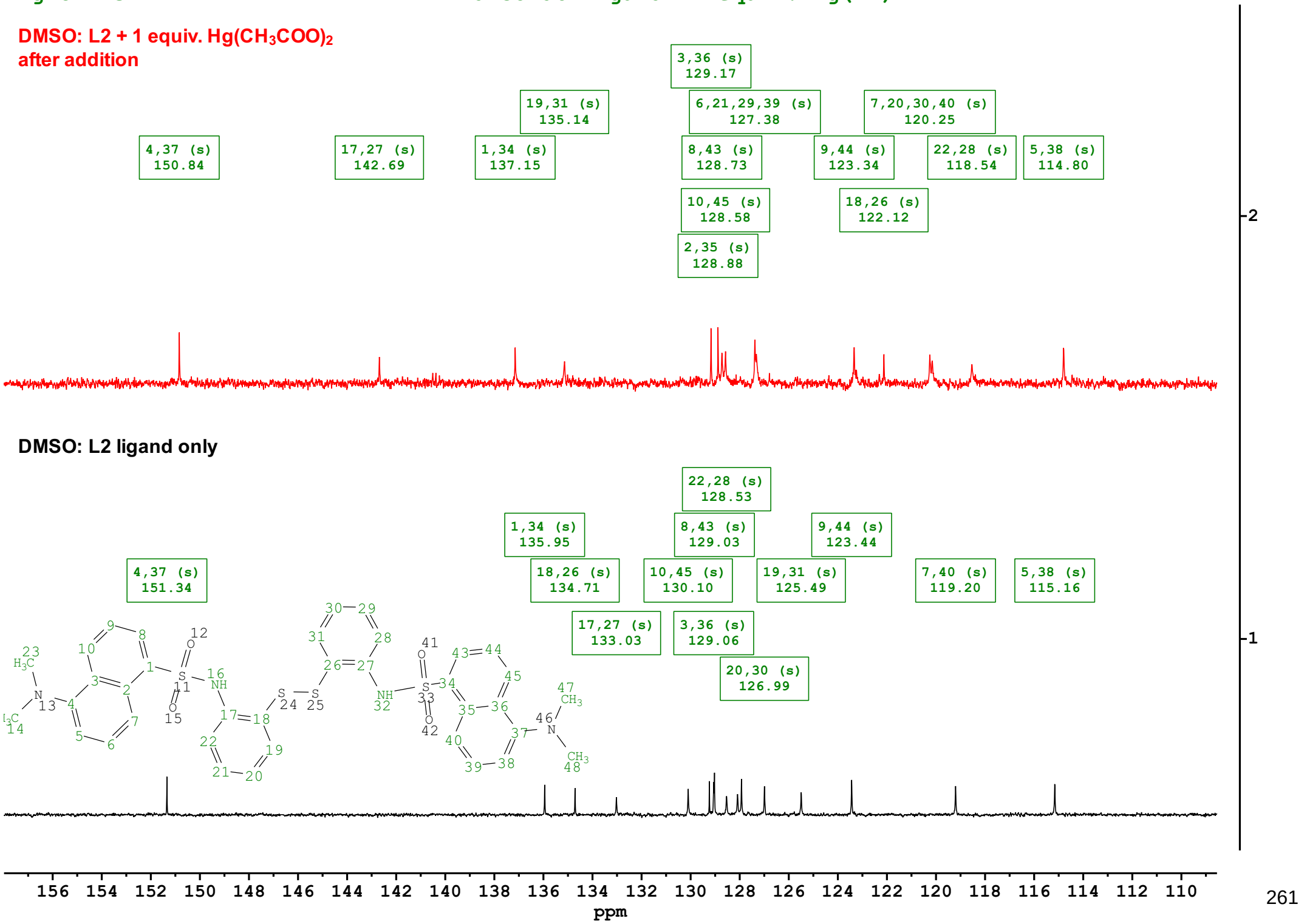


Fig SX246 L2 dmso-d6 ligand + 1equiv. Hg(II)

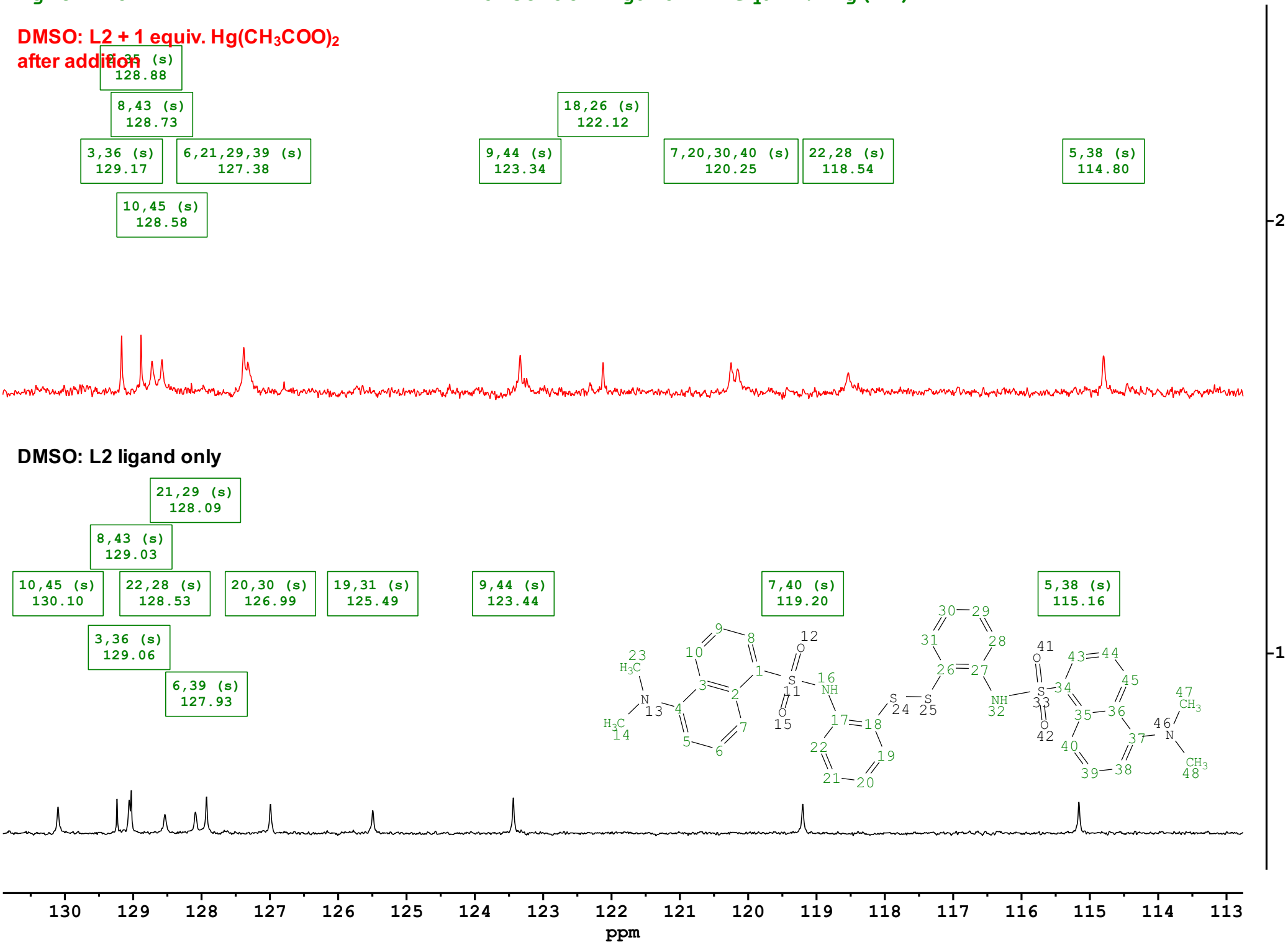


Fig SX247 L2 dmso-d6 ligand + 1equiv. sodium dithionite

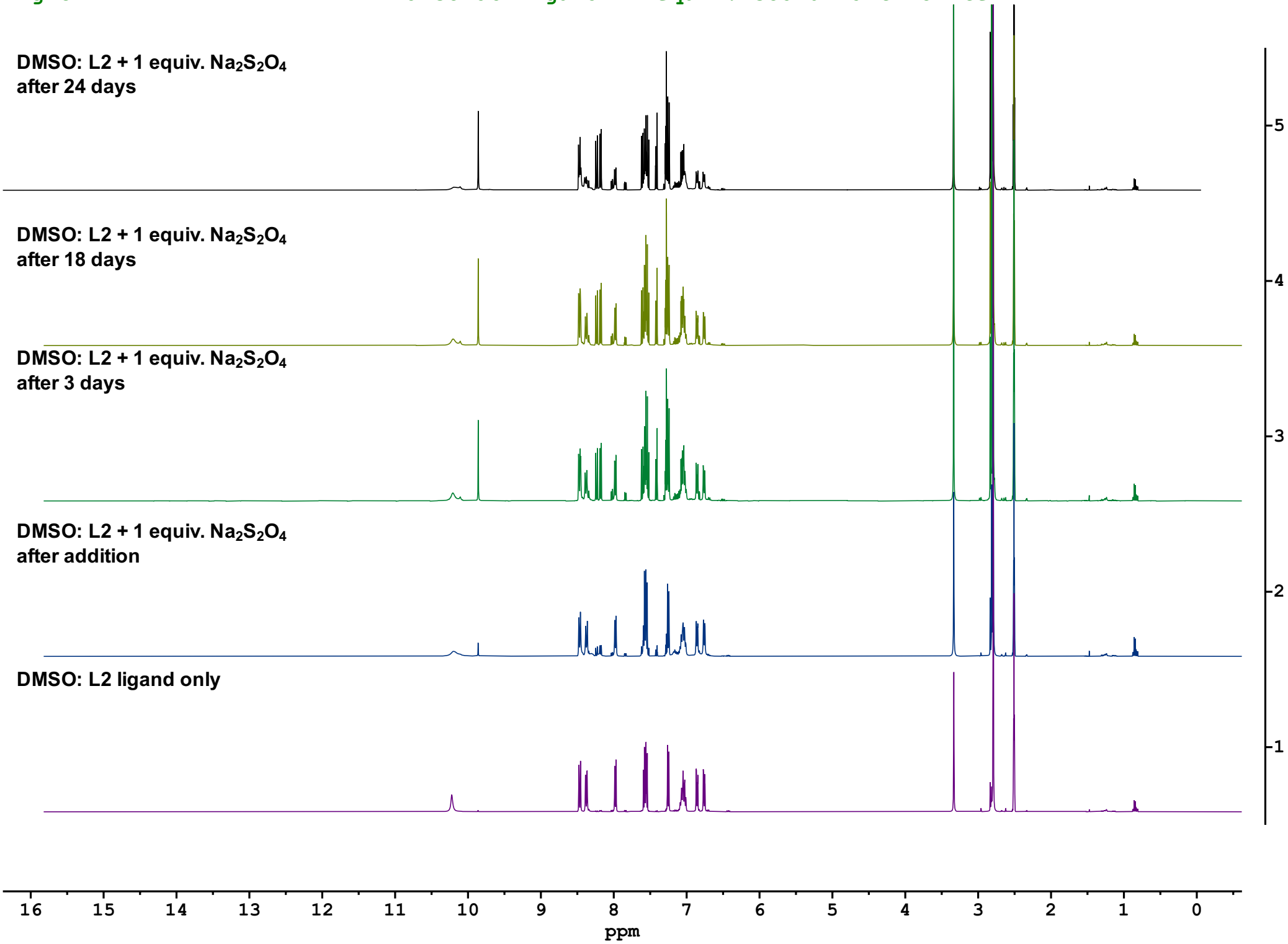


Fig SX248 L2 dmso-d6 ligand + 1equiv. sodium dithionite

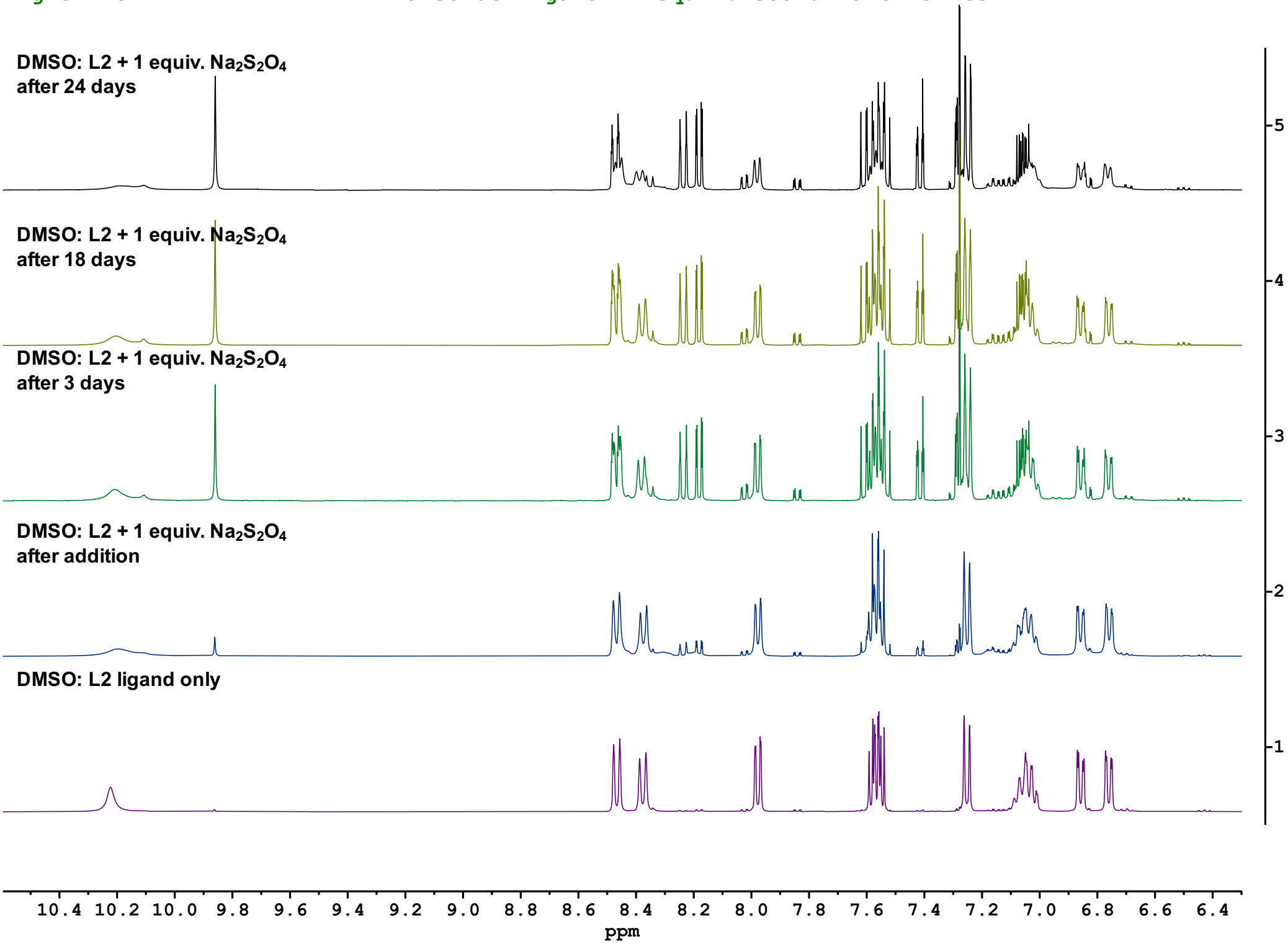


Fig SX249 L2 dmso-d6 ligand + 1equiv. sodium dithionite

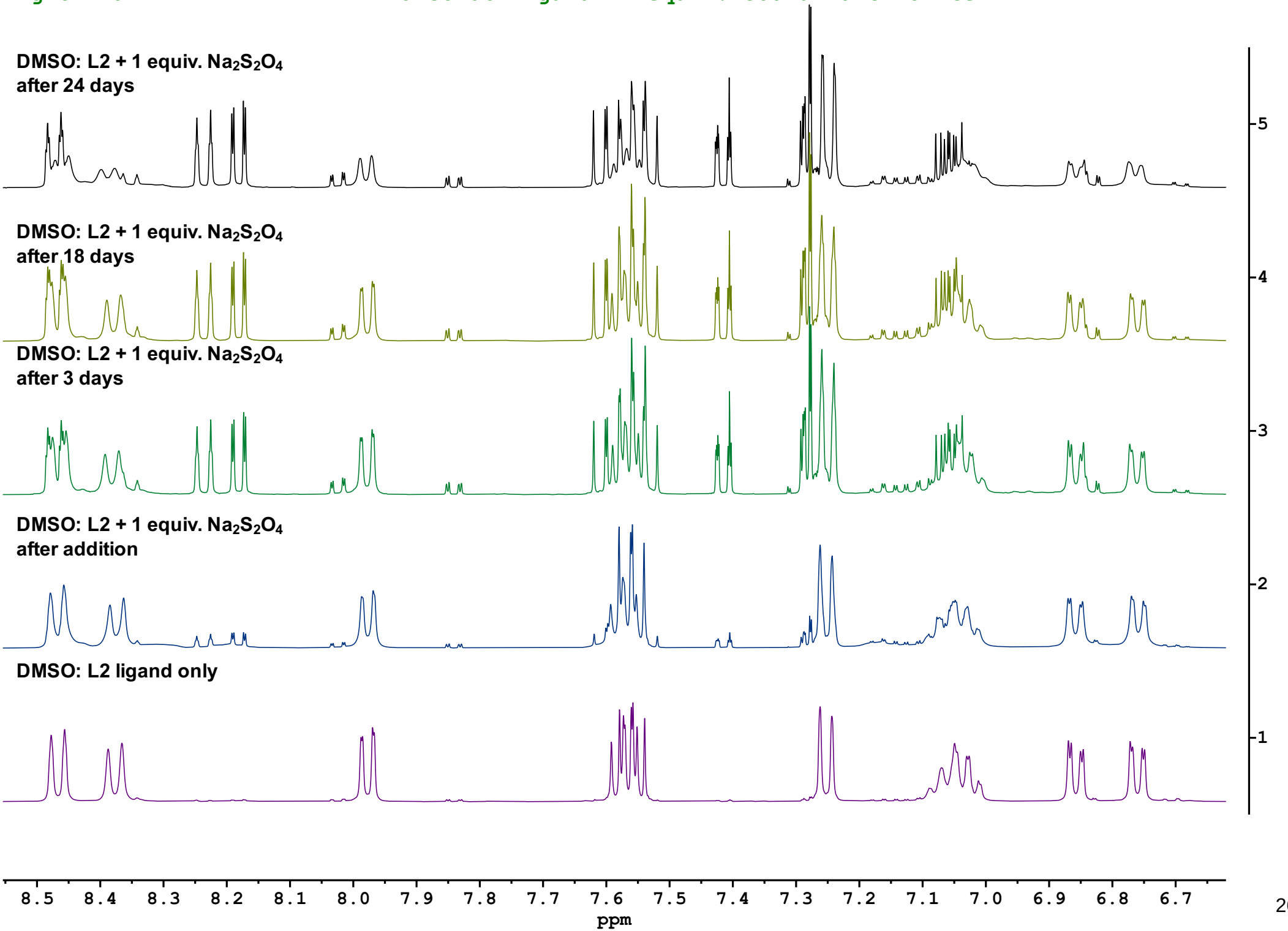


Fig SX250 L2 dmso-d6 ligand + 1equiv. sodium dithionite

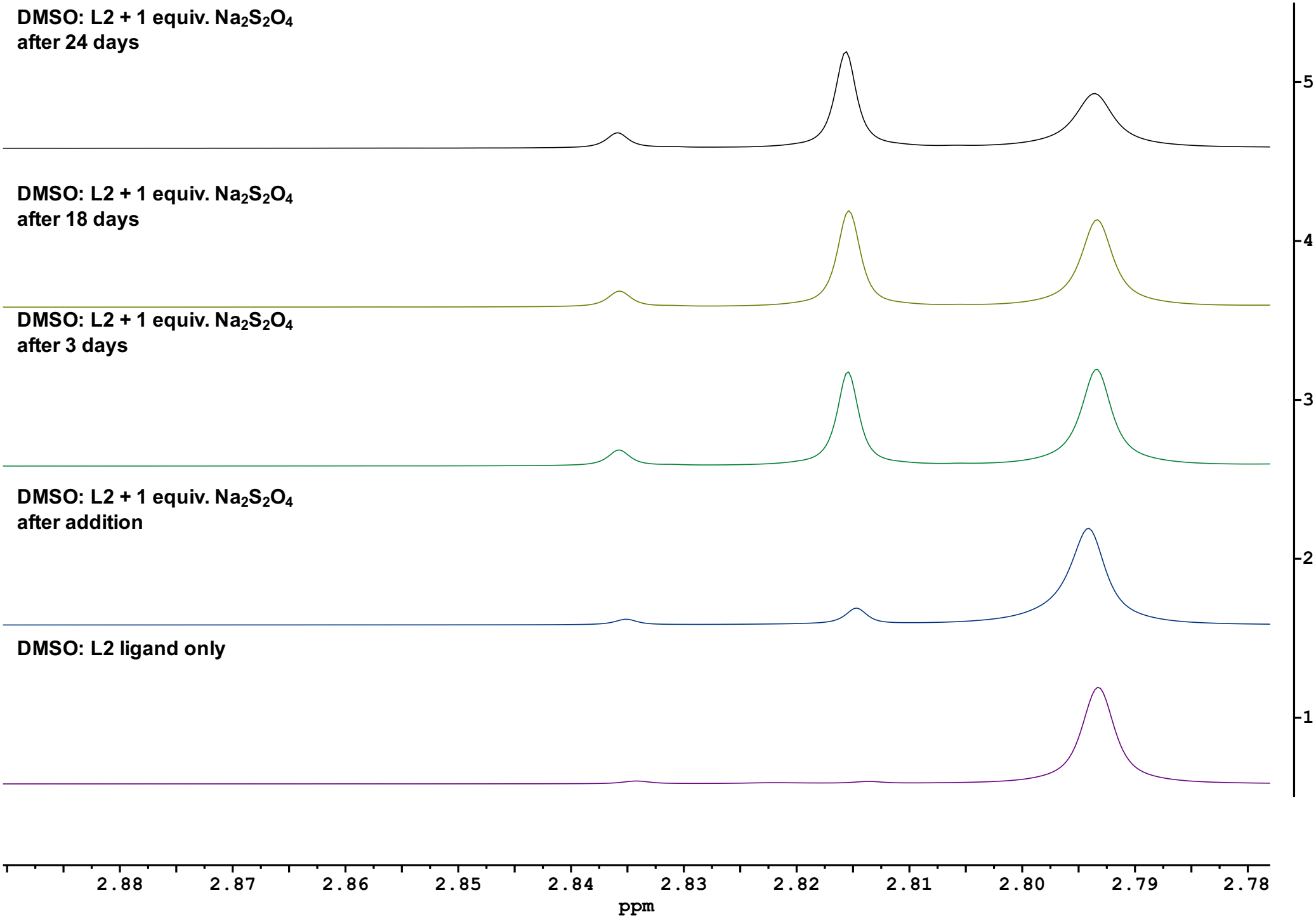


Fig SX251 L2 dmso-d6 ligand + 1equiv. sodium dithionite

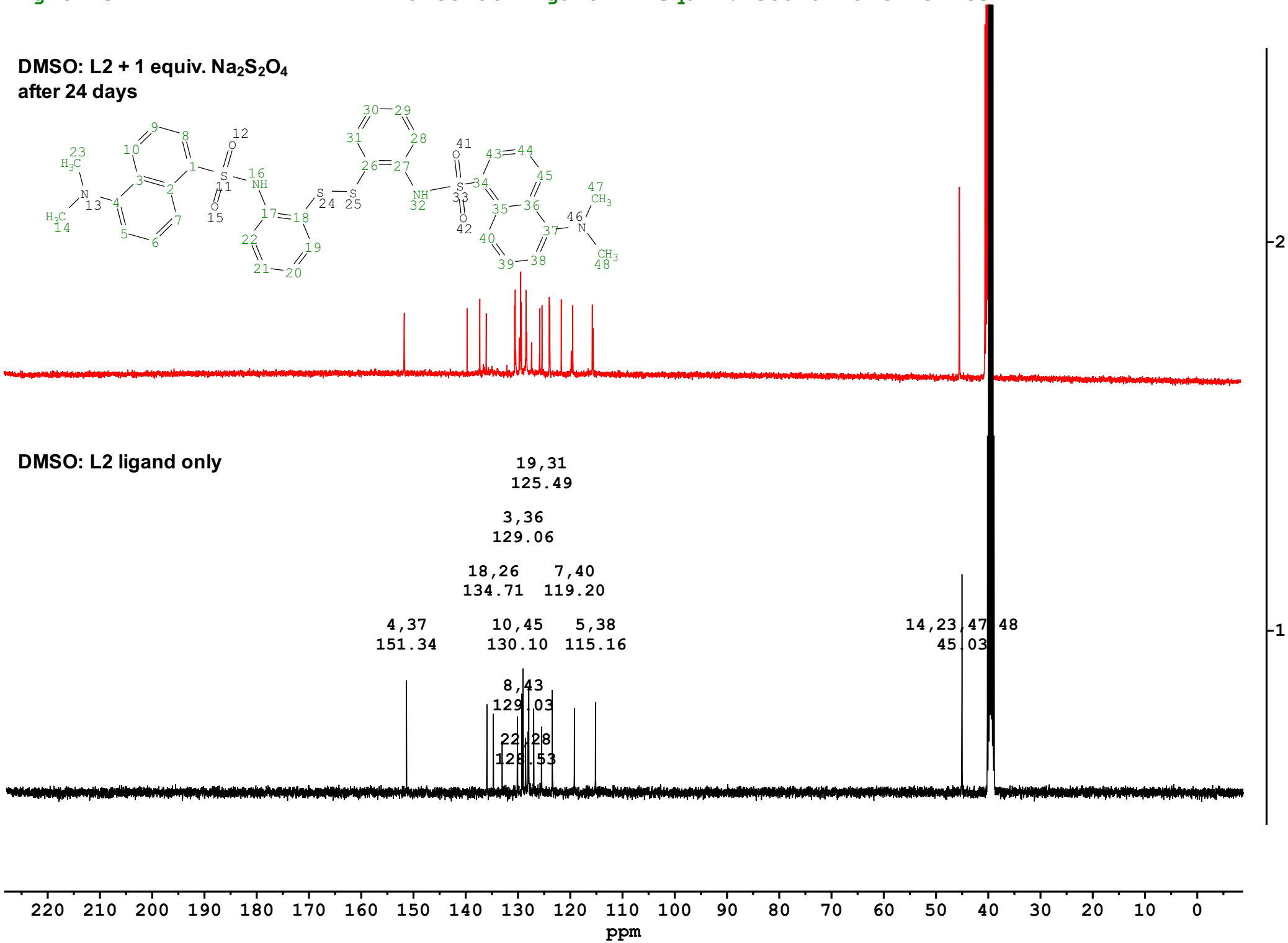


Fig SX252 L2 dmso-d6 ligand + 1equiv. sodium dithionite

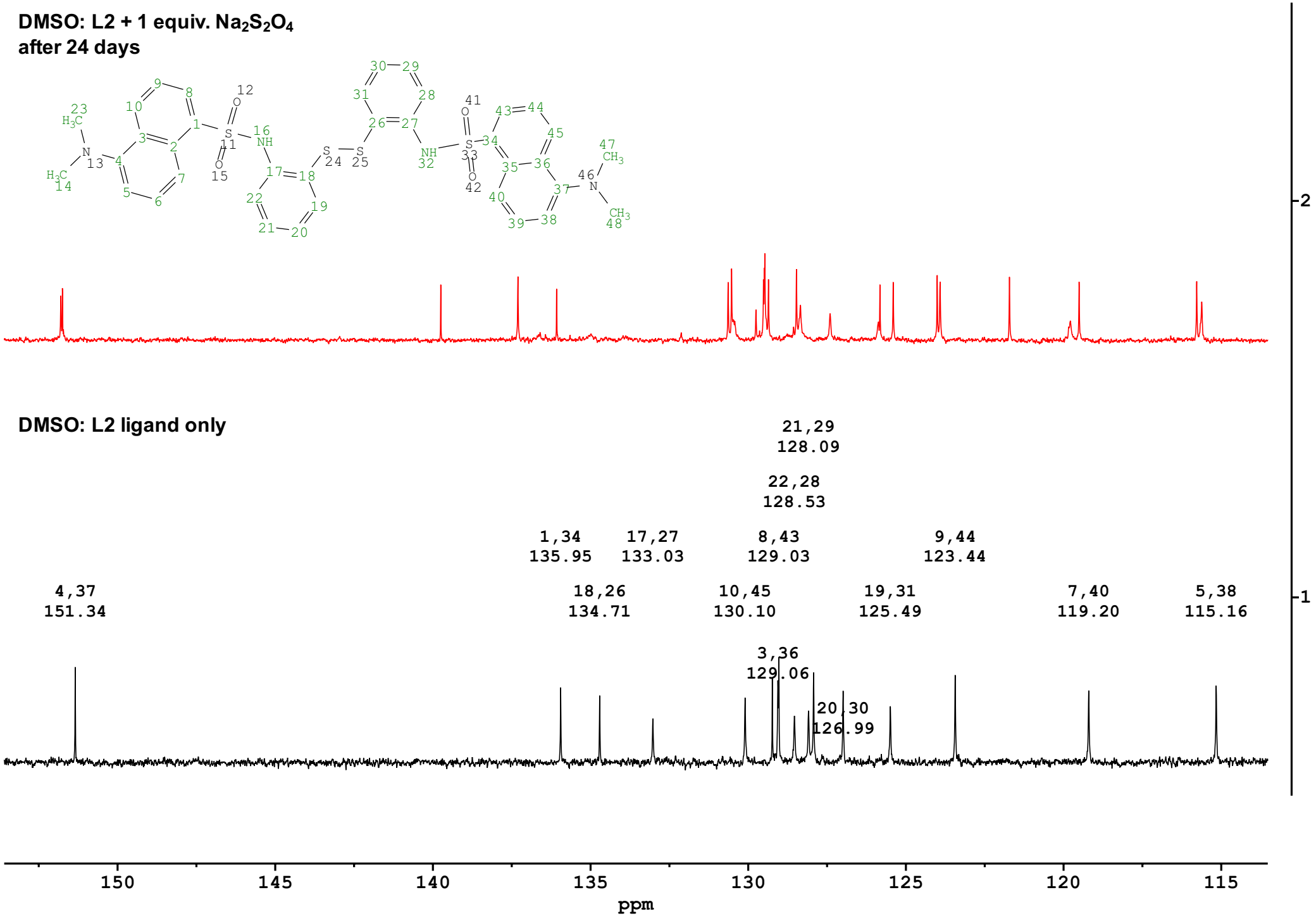
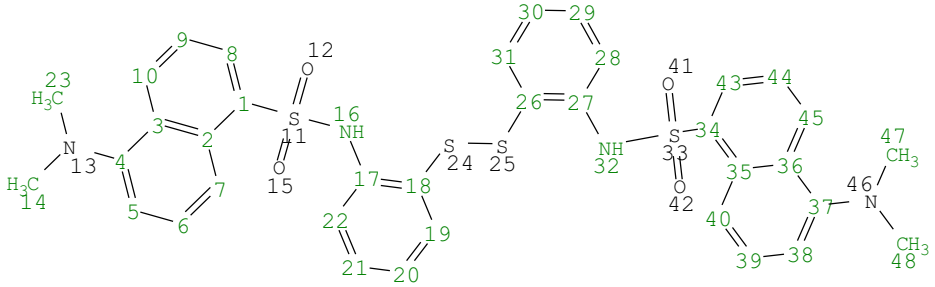
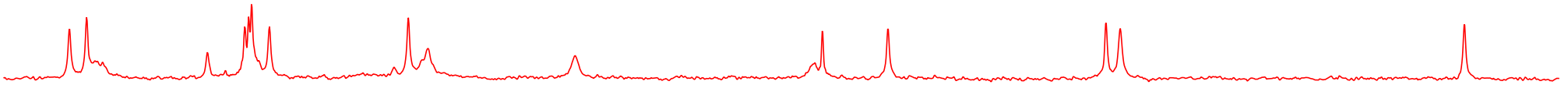


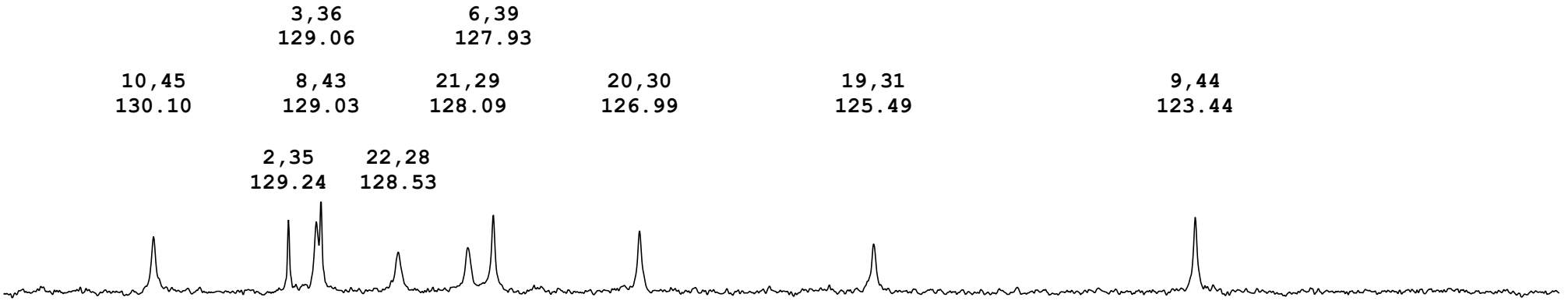
Fig SX253 L2 dmso-d6 ligand + 1equiv. sodium dithionite

**DMSO: L2 + 1 equiv. $Na_2S_2O_4$**
**after 24 days**





**DMSO: L2 ligand only**



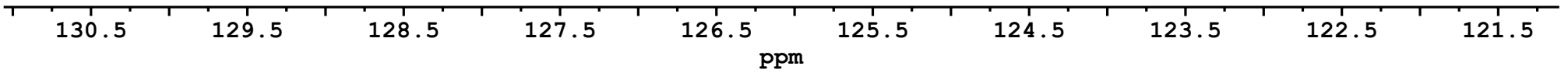



**Fig SX254** **L2 dmso-d6 ligand + 1equiv. sodium dithionite**