Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Chemoselective *N*-arylation of Aminobenzene Sulfonamides via Copper Catalysed Chan–Evans–Lam Reactions

Weisai Zu,[a] Shuai Liu,[a] Xin Jia*[a] and Liang Xu*[a]

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1. General considerations

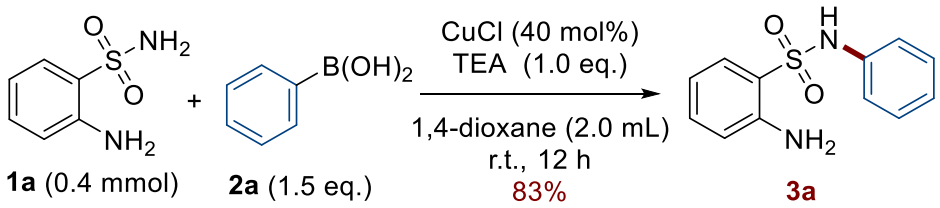
General. Unless otherwise noted, all reactions were carried out under an air atmosphere. Analytical thin-layer chromatography (TLC) was performed on glass plates coated with 0.25 mm 230–400 mesh silica gel containing a fluorescent indicator. Visualization was accomplished by exposure to a UV lamp. All the products in this article are compatible with standard silica gel chromatography. Column chromatography was performed on silica gel (200–300 mesh) using standard methods.

Structural analysis. NMR spectra were measured on a Bruker Ascend 400 spectrometer and chemical shifts (δ) are reported in parts per million (ppm). ^{1}H NMR spectra were recorded at 400 MHz in NMR solvents and referenced internally to corresponding solvent resonance, and ^{13}C NMR spectra were recorded at 100 MHz and referenced to corresponding solvent resonance. Coupling constants are reported in Hz with multiplicities denoted as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and br (broad). Infrared spectra were collected on a Thermo Fisher Nicolet 6700 FT-IR spectrometer using ATR (Attenuated Total Reflectance) method. Absorption maxima (ν max) are reported in wavenumbers (cm^{-1}). High resolution mass spectra (HRMS) were acquired on Thermo Scientific LTQ Orbitrap XL with an ESI source.

Materials. Commercial reagents and solvent were purchased from Adamas, J&K, Energy, Sigma-Aldrich, Alfa Aesar, Acros Organics, TCI and used as received unless otherwise stated.

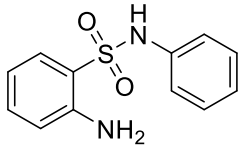
2. Selective N-arylation reaction under Cu catalysis

A. General procedure and experimental data for Cu-catalysed selective arylation of 2-aminobenzenesulfonamides



General procedure A: A flame-dried 100 mL column reaction flask was placed with a stirring bar. Then, 2-aminobenzenesulfonamide **1a** (68.9 mg, 0.4 mmol, 1.0 eq.), CuCl (15.8 mg, 0.16 mmol, 40 mol%), Et_3N (56.0 μL, 0.4 mmol, 1.0 eq.), arylboronic acid (0.6 mmol, 1.5 eq.), and 1,4-dioxane (2.0 mL) were added. The resulting mixture was stirred vigorously at ambient temperature for 12 hours. The reaction mixture was filtered, concentrated and then purified by column chromatography on silica gel to give the target product.

(3a) 2-amino-N-phenylbenzenesulfonamide（CAS: 27332-20-3）



2-amino-*N*-phenylbenzenesulfonamide
Chemical Formula: $C_{12}H_{12}N_2O_2S$
Exact Mass: 248.0619
Molecular Weight: 248.3000

The general procedure A was followed using phenylboronic acid (73.2 mg, 0.6 mmol) as starting material. **3a** was obtained as brown solid (82.8 mg, 83%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

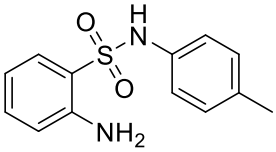
3a (*Molecules* **2013**, *18*, 894-913)

Melting point (°C): 111.2-117.1.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.21 (s, 1H), 7.49 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.20 (t, *J* = 8.0 Hz, 3H), 7.04 (m, 2H), 7.01 – 6.92 (m, 1H), 6.74 (dd, *J* = 8.4, 0.8 Hz, 1H), 6.59 – 6.46 (m, 1H), 5.99 (s, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 146.84, 138.22, 134.37, 130.05, 129.54, 123.95, 119.51, 119.02, 117.36, 115.38.

(3b) 2-amino-N-(p-tolyl)benzenesulfonamide (CAS: 27384-96-9)



2-amino-*N*-(*p*-tolyl)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_2S$
Exact Mass: 262.0776
Molecular Weight: 262.3270

The general procedure A was followed using p-tolylboronic acid (81.6 mg, 0.6 mmol) as starting material. **3b** was obtained as brown solid (88.5 mg, 84%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 124.3-128.2.

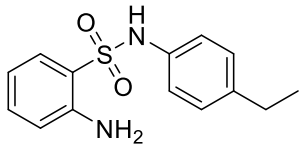
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.03 (s, 1H), 7.44 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.19 (m, 1H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.96 – 6.88 (m, 2H), 6.73 (dd, *J* = 8.4, 0.6 Hz, 1H), 6.52 (m , 1H), 5.97 (s, 2H), 2.16 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 146.82, 135.52, 134.27, 133.28, 130.05, 129.95, 120.20, 119.09, 117.30, 115.34, 20.73.

HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_2S^+$ $(M+H)^+$ 263.0849, found 263.0851.

IR (cm^{-1}): 3458, 3374, 3244, 1618, 1559, 1451, 1132, 846, 760.

(3c) 2-amino-N-(4-ethylphenyl)benzenesulfonamide (CAS: 953730-44-4)



2-amino-*N*-(4-ethylphenyl)benzenesulfonamide
Chemical Formula: $C_{14}H_{16}N_2O_2S$
Exact Mass: 276.0932
Molecular Weight: 276.3540

The general procedure A was followed using (4-ethylphenyl)boronic acid (90.0 mg, 0.6 mmol) as starting material. **3c** was obtained as grey solid (75.1 mg, 68%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 92.3-93.9.

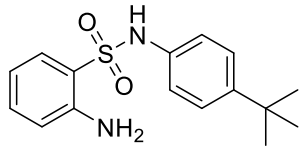
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.06 (s, 1H), 7.46 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.25 – 7.13 (m, 1H), 7.03 (d, *J* = 8.6 Hz, 2H), 6.95 (d, *J* = 8.2 Hz, 2H), 6.73 (dd, *J* = 8.2, 0.8 Hz, 1H), 6.58 – 6.48 (m, 1H), 5.97 (s, 2H), 2.47 (q, *J* = 7.6 Hz, 2H), 1.08 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 146.82, 139.53, 135.75, 134.27, 130.02, 128.77, 120.02, 119.19, 117.33, 115.36, 27.85, 15.94.

HRMS (ESI) m/z calcd for $C_{14}H_{17}N_2O_2S^+$ $(M+H)^+$ 277.1005, found 277.1010.

IR (cm^{-1}): 3468, 3379, 3242, 1617, 1596, 1133, 760, 728.

(3d) 2-amino-N-(4-(tert-butyl)phenyl)benzenesulfonamide (CAS: 1040010-61-4)



2-amino-*N*-(4-(*tert*-butyl)phenyl)benzenesulfonamide
Chemical Formula: $C_{16}H_{20}N_2O_2S$
Exact Mass: 304.1245
Molecular Weight: 304.4080

The general procedure A was followed using (4-(tert-butyl)phenyl)boronic acid (106.8 mg, 0.6 mmol) as starting material. **3d** was obtained as white solid (88.0 mg, 72%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 206.5-211.5.

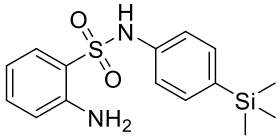
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.12 (s, 1H), 7.50 (dd, J = 8.0, 1.6 Hz, 1H), 7.28 – 7.14 (m, 3H), 7.01 – 6.90 (m, 2H), 6.74 (dd, J = 8.0, 0.8 Hz, 1H), 6.59 – 6.49 (m, 1H), 5.98 (s, 2H), 1.18 (s, 9H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 146.82, 146.21, 135.58, 134.29, 129.99, 126.24, 119.42, 119.21, 117.38, 115.41, 34.38, 31.57.

HRMS (ESI) m/z calcd for $C_{16}H_{21}N_2O_2S^+$ $(M+H)^+$ 305.1318, found 305.1321.

IR (cm^{-1}): 3497, 3393, 3237, 1617, 1451, 1134, 908, 858.

(3e) 2-amino-N-(4-(trimethylsilyl)phenyl)benzenesulfonamide



2-amino-*N*-(4-(trimethylsilyl)phenyl)benzenesulfonamide
Chemical Formula: $C_{15}H_{20}N_2O_2SSi$
Exact Mass: 320.1015
Molecular Weight: 320.4820

The general procedure A was followed using (4-(trimethylsilyl)phenyl)boronic acid (116.5 mg, 0.6 mmol) as starting material. **3e** was obtained as grey solid (86.7 mg, 68%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 162.5-165.4.

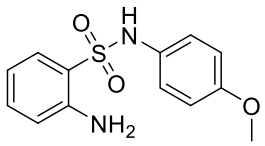
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.30 (s, 1H), 7.53 (dd, J = 8.0, 1.6 Hz, 1H), 7.39 – 7.28 (m, 2H), 7.20 (m, 1H), 7.03 (d, J = 8.4 Hz, 2H), 6.74 (dd, J = 8.4, 0.8 Hz, 1H), 6.60 – 6.50 (m, 1H), 5.99 (s, 2H), 0.15 (s, 9H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 146.97, 139.10, 134.68, 134.54, 134.25, 130.17, 119.27, 118.27, 117.54, 115.56, -0.50.

HRMS (ESI) m/z calcd for $C_{15}H_{21}N_2O_2SSi^+$ $(M+H)^+$ 321.1087, found 321.1090.

IR (cm^{-1}): 3496, 3393, 3245, 1617, 1483, 1136, 835, 757.

(3f) 2-amino-N-(4-methoxyphenyl)benzenesulfonamide（CAS: 33224-44-1）



2-amino-*N*-(4-methoxyphenyl)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_3S$
Exact Mass: 278.0725
Molecular Weight: 278.3260

The general procedure A was followed using (4-methoxyphenyl)boronic acid (91.2 mg, 0.6 mmol) as starting material. **3f** was obtained as grey solid (70.1 mg, 63%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 94.4-97.7.

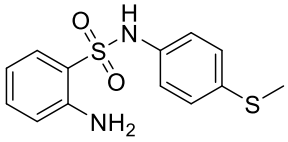
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.29 – 7.23 (m, 1H), 6.96 – 6.91 (m, 2H), 6.79 – 6.68 (m, 4H), 6.68 – 6.61 (m, 1H), 4.85 (s, 2H), 3.72 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.24, 144.95, 134.34, 130.04, 128.68, 126.25, 120.92, 117.89, 117.58, 114.27, 55.38.

HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_3S^+$ $(M+H)^+$ 279.0798, found 279.0801.

IR (cm^{-1}): 3475, 3369, 3271, 1610, 1507, 1479, 1453, 1393, 935.

(3g) 2-amino-N-(4-(methylthio)phenyl)benzenesulfonamide (CAS: 1016512-06-3)



2-amino-*N*-(4-(methylthio)phenyl)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_2S_2$
Exact Mass: 294.0497
Molecular Weight: 294.3870

The general procedure A was followed using (4-(methylthio)phenyl)boronic acid (100.8 mg, 0.6 mmol) as starting material. **3g** was obtained as grey solid (76.7 mg, 65%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 87.6-91.3.

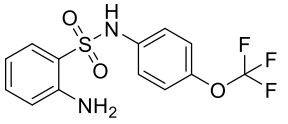
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.17 (s, 1H), 7.46 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.21 (m , 1H), 7.16 – 7.08 (m, 2H), 7.05 – 6.95 (m, 2H), 6.74 (dd, *J* = 8.0, 0.8 Hz, 1H), 6.59 – 6.48 (m, 1H), 5.98 (s, 2H), 2.38 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 146.84, 135.43, 134.41, 133.19, 130.03, 127.68, 120.75, 118.93, 117.37, 115.42, 15.69.

HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_2S_2^+$ $(M+H)^+$ 295.0570, found 295.0571.

IR (cm^{-1}): 3484, 3387, 3290, 1615, 1479, 1134, 838, 747.

(3h) 2-amino-N-(4-(trifluoromethoxy)phenyl)benzenesulfonamide (CAS: 2122297-24-7)



2-amino-*N*-(4-(trifluoromethoxy)phenyl)benzenesulfonamide
Chemical Formula: $C_{13}H_{11}F_3N_2O_3S$
Exact Mass: 332.0442
Molecular Weight: 332.2972

The general procedure A was followed using (4-(trifluoromethoxy)phenyl)boronic acid (125.6 mg, 0.6 mmol) as starting material. **3h** was obtained as grey solid (78.2 mg, 59%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 95.5-98.0.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.47 (s, 1H), 7.51 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.24 (d, *J* = 8.4 Hz, 3H), 7.17 – 7.06 (m, 2H), 6.76 (dd, *J* = 8.4, 0.8 Hz, 1H), 6.60 – 6.52 (m, 1H), 6.01 (s, 2H).

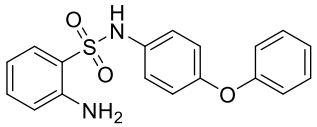
^{13}C NMR (101 MHz, DMSO-d_6) δ 146.90, 144.47, 137.47, 134.60, 129.98, 122.51, 120.72, 120.50 (q, *J* = 254 Hz), 118.66, 117.47, 115.49.

^{19}F NMR (376 MHz, DMSO-d_6) δ -57.12.

HRMS (ESI) m/z calcd for $C_{13}H_{12}F_3N_2O_3S^+$ $(M+H)^+$ 333.0515, found 333.0519.

IR (cm^{-1}): 3467, 3379, 3232, 2360, 1621, 1506, 1453, 819, 735, 696.

(3i) 2-amino-N-(4-phenoxyphenyl)benzenesulfonamide (CAS: 1092226-55-5)



2-amino-*N*-(4-phenoxyphenyl)benzenesulfonamide
Chemical Formula: $C_{18}H_{16}N_2O_3S$
Exact Mass: 340.0882
Molecular Weight: 340.3970

The general procedure A was followed using (4-phenoxyphenyl)boronic acid (128.4 mg, 0.6 mmol) as starting material. **3i** was obtained as grey solid (97.1 mg, 71%) after

purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 83.3-86.0.

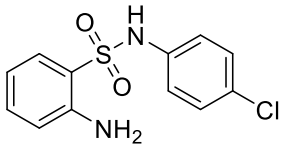
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.11 (s, 1H), 7.44 (dd, J = 8.0, 1.2 Hz, 1H), 7.38 – 7.29 (m, 2H), 7.22 (m, 1H), 7.13 – 7.00 (m, 3H), 6.89 (m, 4H), 6.75 (dd, J = 8.0, 0.8 Hz, 1H), 6.60 – 6.49 (m, 1H), 5.98 (s, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 157.47, 153.18, 146.87, 134.37, 133.74, 130.44, 130.01, 123.62, 122.36, 120.10, 119.01, 118.50, 117.35, 115.41.

HRMS (ESI) m/z calcd for $C_{18}H_{17}N_2O_3S^+$ $(M+H)^+$ 341.0954, found 341.0958.

IR (cm^{-1}): 3496, 3396, 3257, 1615, 1481, 1473, 1137, 892, 752, 728.

(3j) 2-amino-N-(4-chlorophenyl)benzenesulfonamide (CAS: 63132-70-7)



2-amino-*N*-(4-chlorophenyl)benzenesulfonamide
Chemical Formula: $C_{12}H_{11}ClN_2O_2S$
Exact Mass: 282.0230
Molecular Weight: 282.7420

The general procedure A was followed using (4-chlorophenyl)boronic acid (93.6 mg, 0.6 mmol) as starting material. **3j** was obtained as grey solid (88.5 mg, 78%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 104.6-107.5.

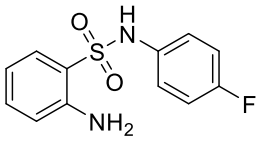
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, J = 8.0, 1.2 Hz, 1H), 7.29 – 7.24 (m, 1H), 7.21 – 7.10 (m, 3H), 7.05 – 6.92 (m, 2H), 6.80 – 6.62 (m, 2H), 4.90 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.00, 134.92, 134.71, 131.42, 129.93, 129.29, 124.02, 120.52, 118.06, 117.84.

HRMS (ESI) m/z calcd for $C_{12}H_{12}ClN_2O_2S^+$ $(M+H)^+$ 283.0302, found 283.0308.

IR (cm^{-1}): 3462, 3377, 3238, 1618, 1478, 1133, 910.6, 758.

(3k) 2-amino-N-(4-fluorophenyl)benzenesulfonamide (CAS: 159048-93-8)



2-amino-*N*-(4-fluorophenyl)benzenesulfonamide
Chemical Formula: $C_{12}H_{11}FN_2O_2S$
Exact Mass: 266.0525
Molecular Weight: 266.2904

The general procedure A was followed using (4-fluorophenyl)boronic acid (84.0 mg, 0.6 mmol) as starting material. **3k** was obtained as gray-green solid (85.9 mg, 81%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

3k (*Molecules* **2013**, *18*, 894-913)

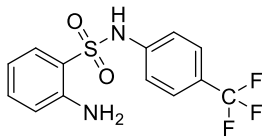
Melting point (°C): 83.3-85.5.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.13 (s, 1H), 7.43 (dd, J = 8.4, 1.6 Hz, 1H), 7.21 (m, 1H), 7.07 (d, J = 1.6 Hz, 2H), 7.05 (s, 2H), 6.75 (dd, J = 8.4, 0.8 Hz, 1H), 6.53 (m, , 1H), 5.98 (s, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 159.26 (d, J = 239 Hz), 146.87, 134.44, 134.38 (d, J = 2 Hz), 129.98, 122.41 (d, J = 8 Hz), 118.71, 117.36, 116.26 (d, J = 23 Hz), 115.43.

^{19}F NMR (376 MHz, DMSO-d_6) δ -118.99.

(3l)2-amino-N-(4-(trifluoromethyl)phenyl)benzenesulfonamide（CAS: 1040000-17-6）



2-amino-*N*-(4-(trifluoromethyl)phenyl)benzenesulfonamide
Chemical Formula: $C_{13}H_{11}F_3N_2O_2S$
Exact Mass: 316.0493
Molecular Weight: 316.2982

The general procedure A was followed using (4-(trifluoromethyl)phenyl)boronic acid (114.0 mg, 0.6 mmol) as starting material. **3l** was obtained as brown solid (82.8 mg, 65%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 70.2-74.4

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.34 – 7.27 (m, 1H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.10 (s, 1H), 6.73 (m, 2H), 4.88 (s, 2H).

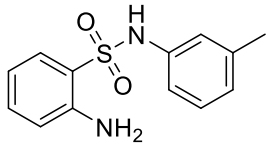
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.03, 139.77, 134.92, 129.87, 127.15 (q, *J* = 32 Hz), 126.49 (q, *J* = 4 Hz), 123.88 (q, *J* = 270 Hz)120.88, 120.63, 118.26, 118.02.

^{19}F NMR (376 MHz, DMSO-d_6) δ -61.28.

HRMS (ESI) m/z calcd for $C_{13}H_{12}F_3N_2O_2S^+$ $(M+H)^+$ 317.0566, found 317.0569.

IR (cm^{-1}): 3486, 3389, 3291, 1616, 1453, 1479, 903, 652.

(3m) 2-amino-N-(m-tolyl)benzenesulfonamide (CAS: 953891-86-6)



2-amino-*N*-(*m*-tolyl)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_2S$
Exact Mass: 262.0776
Molecular Weight: 262.3270

The general procedure A was followed using m-tolylboronic acid (81.6 mg, 0.6 mmol) as starting material. **3m** was obtained as grey solid (74.5 mg, 71%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 73.3-75.6

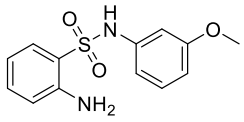
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.14 (s, 1H), 7.49 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.20 (m, 1H), 7.11 – 7.02 (m, 1H), 6.86 (s, 1H), 6.84 (d, *J* = 1.6 Hz, 1H), 6.78 (d, *J* = 7.6 Hz, 1H), 6.74 (dd, *J* = 8.0, 0.8 Hz, 1H), 6.58 – 6.49 (m, 1H), 5.98 (s, 2H), 2.18 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 146.84, 138.80, 138.17, 134.34, 130.06, 129.34, 124.65, 120.01, 119.09, 117.35, 116.47, 115.35, 21.52.

HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_2S^+$ $(M+H)^+$ 263.0849, found 263.0851.

IR (cm^{-1}): 3438, 3359, 3257, 1623, 1478, 1453, 757, 697.

(3n) 2-amino-N-(3-methoxyphenyl)benzenesulfonamide (CAS: 178479-24-8)



2-amino-*N*-(3-methoxyphenyl)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_3S$
Exact Mass: 278.0725
Molecular Weight: 278.3260

The general procedure A was followed using (3-methoxyphenyl)boronic acid (91.2 mg, 0.6 mmol) as starting material. **3n** was obtained as brown solid (76.9 mg, 69%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 81.4-85.7.

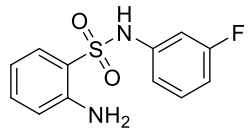
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.24 (s, 1H), 7.52 (dd, J = 8.4, 1.6 Hz, 1H), 7.28 – 7.17 (m, 1H), 7.10 (t, J = 8.0 Hz, 1H), 6.75 (d, J = 7.6 Hz, 1H), 6.58 (m, 4H), 6.00 (s, 2H), 3.65 (s, 3H)

^{13}C NMR (101 MHz, DMSO-d_6) δ 160.13, 146.90, 139.45, 134.44, 130.40, 130.10, 118.94, 117.41, 115.43, 111.52, 109.00, 105.11, 55.41.

HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_3S^+$ $(M+H)^+$ 279.0798, found 279.0799.

IR (cm^{-1}): 3453, 3367, 3281, 1628, 1485, 1049, 880, 699.

(3o) 2-amino-N-(3-fluorophenyl)benzenesulfonamide (CAS: 178479-19-1)



2-amino-*N*-(3-fluorophenyl)benzenesulfonamide
Chemical Formula: $C_{12}H_{11}FN_2O_2S$
Exact Mass: 266.0525
Molecular Weight: 266.2904

The general procedure A was followed using (3-fluorophenyl)boronic acid (84.0 mg, 0.6 mmol) as starting material. **3o** was obtained as white solid (89.3 mg, 84%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 80.1-83.2.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.53 (s, 1H), 7.53 (dd, J = 8.0, 1.2 Hz, 1H), 7.33 – 7.11 (m, 2H), 6.94 – 6.69 (m, 4H), 6.64 – 6.50 (m, 1H), 6.02 (s, 2H).

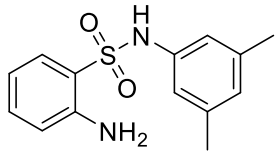
^{13}C NMR (101 MHz, DMSO-d_6) δ 162.71 (d, J = 241 Hz), 146.94, 140.12 (d, J = 10 Hz), 134.67, 131.34 (d, J = 9 Hz), 130.03, 118.51, 117.50, 115.53, 114.96 (d, J = 3 Hz), 110.32 (d, J = 21 Hz), 105.76 (d, J = 25 Hz).

^{19}F NMR (376 MHz, DMSO-d_6) δ -111.72.

HRMS (ESI) m/z calcd for $C_{12}H_{12}FN_2O_2S^+$ $(M+H)^+$ 267.0598, found 267.0600.

IR (cm^{-1}):3494, 3393, 3219, 1610, 1478, 1129, 838, 753.

(3p) 2-amino-N-(3,5-dimethylphenyl)benzenesulfonamide (CAS: 953717-72-1)



2-amino-*N*-(3,5-dimethylphenyl)benzenesulfonamide
Chemical Formula: $C_{14}H_{16}N_2O_2S$
Exact Mass: 276.0932
Molecular Weight: 276.3540

The general procedure A was followed using (3,5-dimethylphenyl)boronic acid (90.0 mg, 0.6 mmol) as starting material. **3p** was obtained as grey solid (72.5 mg, 66%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 137.0-139.8.

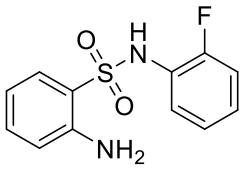
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (dd, J = 8.0, 1.6 Hz, 1H), 7.29 – 7.24 (m, 1H), 6.79 – 6.59 (m, 6H), 4.87 (s, 2H), 2.19 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.02, 138.85, 136.11, 134.35, 130.02, 127.42, 121.11, 120.14, 117.83, 117.69, 21.18.

HRMS (ESI) m/z calcd for $C_{14}H_{17}N_2O_2S^+$ $(M+H)^+$ 277.1005, found 277.1010.

IR (cm^{-1}): 3444, 3412, 3255, 1621, 1597, 1480, 1138, 909, 880.

(3q) 2-amino-N-(2-fluorophenyl)benzenesulfonamide (CAS: 178479-22-6)



2-amino-*N*-(2-fluorophenyl)benzenesulfonamide
Chemical Formula: $C_{12}H_{11}FN_2O_2S$
Exact Mass: 266.0525
Molecular Weight: 266.2904

The general procedure A was followed using (2-fluorophenyl)boronic acid (84.0 mg, 0.6 mmol) as starting material. **3q** was obtained as white solid (49.9 mg, 47%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 135.3-139.1.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.03 (s, 1H), 7.41 (dd, J = 8.0, 1.2 Hz, 1H), 7.29 – 7.19 (m, 2H), 7.19 – 7.01 (m, 3H), 6.77 (dd, J = 8.4, 0.8 Hz, 1H), 6.52 (m,, 1H), 6.04 (s, 2H).

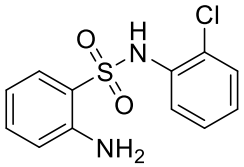
^{13}C NMR (101 MHz, DMSO-d_6) δ 155.12 (d, J = 245 Hz), 146.92, 134.50, 129.76, 126.64 (d, J = 7 Hz), 125.24 (d, J = 13 Hz), 125.02 (d, J = 4 Hz), 124.67, 119.20, 117.35, 116.33 (d, J = 20 Hz), 115.20.

^{19}F NMR (376 MHz, DMSO-d_6) δ -124.60.

HRMS (ESI) m/z calcd for $C_{12}H_{12}FN_2O_2S^+$ $(M+H)^+$ 267.0598, found 267.0594.

IR (cm^{-1}): 3461, 3297, 2358, 1616, 1456, 1252, 918, 760, 747.

(3r) 2-amino-N-(2-chlorophenyl)benzenesulfonamide (CAS: 65493-02-9)



2-amino-*N*-(2-chlorophenyl)benzenesulfonamide
Chemical Formula: $C_{12}H_{11}ClN_2O_2S$
Exact Mass: 282.0230
Molecular Weight: 282.7420

The general procedure A was followed using (2-chlorophenyl)boronic acid (93.8 mg, 0.6 mmol) as starting material. **3r** was obtained as white solid (55.8 mg, 49%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 83.2-85.4.

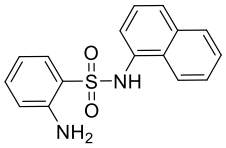
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.70 (s, 1H), 7.38 (m, 2H), 7.30 – 7.17 (m, 3H), 7.13 (m, 1H), 6.82 – 6.73 (d, J= 8.0, 1H), 6.52 (m, 1H), 6.07 (s, 2H)

^{13}C NMR (101 MHz, DMSO-d_6) δ 147.01, 134.52, 134.34, 130.30, 129.60, 128.10, 128.08, 127.19, 125.81, 119.78, 117.43, 115.24.

HRMS (ESI) m/z calcd for $C_{12}H_{12}ClN_2O_2S^+$ $(M+H)^+$ 283.0302, found 283.0307.

IR (cm^{-1}): 3496, 3396, 3257, 1615, 1481, 1473, 1137, 892, 752, 728.

(3s) 2-amino-N-(naphthalen-1-yl)benzenesulfonamide (CAS: 101954-56-7)



2-amino-*N*-(naphthalen-1-yl)benzenesulfonamide
Chemical Formula: $C_{16}H_{14}N_2O_2S$
Exact Mass: 298.0776
Molecular Weight: 298.3600

The general procedure A was followed using naphthalen-1-ylboronic acid (103.2 mg, 0.6 mmol) as starting material. **3s** was obtained as brown solid (73.4 mg, 62%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 125.0-128.8.

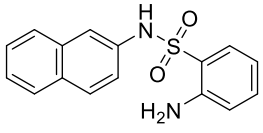
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.11 (s, 1H), 8.20 (dd, J = 8.0, 1.2 Hz, 1H), 7.93 – 7.79 (m, 1H), 7.73 (d, J = 8.4 Hz, 1H), 7.53 – 7.32 (m, 3H), 7.28 (m, 2H), 7.16 , 1H), 6.74 (dd, J = 8.0, 0.8 Hz, 1H), 6.43 (m,, 1H), 6.06 (s, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 146.82, 134.28, 134.26, 132.93, 129.68, 129.45, 128.38, 126.69, 126.64, 126.40, 125.96, 123.43, 122.62, 119.82, 117.24, 115.36.

HRMS (ESI) m/z calcd for $C_{16}H_{15}N_2O_2S^+$ $(M+H)^+$ 299.0849, found 299.0852.

IR (cm^{-1}): 3497, 3396, 3256, 1617, 1456, 1134, 895, 752, 694.

(3t) 2-amino-N-(naphthalen-2-yl)benzenesulfonamide (CAS: 861604-61-7)



2-amino-*N*-(naphthalen-2-yl)benzenesulfonamide
Chemical Formula: $C_{16}H_{14}N_2O_2S$
Exact Mass: 298.0776
Molecular Weight: 298.3600

The general procedure A was followed using naphthalen-2-ylboronic acid (103.2 mg, 0.6 mmol) as starting material. **3t** was obtained as brown solid (56.2 mg, 47%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 105.2-109.8.

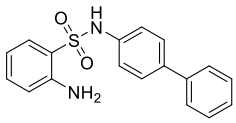
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.46 (s, 1H), 7.77 (d, J = 8.0 Hz, 2H), 7.73 (d, J = 8.0 Hz, 1H), 7.58 (d, J = 7.6 Hz, 1H), 7.50 (s, 1H), 7.42 (d, J = 7.6 Hz, 1H), 7.37 (d, J = 7.2 Hz, 1H), 7.26 (d, J = 8.4 Hz, 1H), 7.16 (t, J = 6.8 Hz, 1H), 6.72 (d, J = 8.0 Hz, 1H), 6.52 (t, J = 7.2 Hz, 1H), 6.05 (s, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 146.92, 135.88, 134.48, 133.72, 130.18, 129.42, 127.97, 127.49, 127.12, 125.28, 120.20, 118.83, 117.38, 115.43, 115.28.

HRMS (ESI) m/z calcd for $C_{16}H_{15}N_2O_2S^+$ $(M+H)^+$ 299.0849, found 299.0851.

IR (cm^{-1}): 3498, 3400, 3222, 2359, 1617, 1559, 1480, 1455, 1132, 751, 696.

(3u) N-([1,1'-biphenyl]-4-yl)-2-aminobenzenesulfonamide (CAS: 1955496-07-7)



***N*-([1,1'-biphenyl]-4-yl)-2-aminobenzenesulfonamide**
Chemical Formula: $C_{18}H_{16}N_2O_2S$
Exact Mass: 324.0932
Molecular Weight: 324.3980

The general procedure A was followed using [1,1'-biphenyl]-4-ylboronic acid (118.8 mg, 0.6 mmol) as starting material. **3u** was obtained as white solid (62.4 mg, 48%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 155.5-158.1.

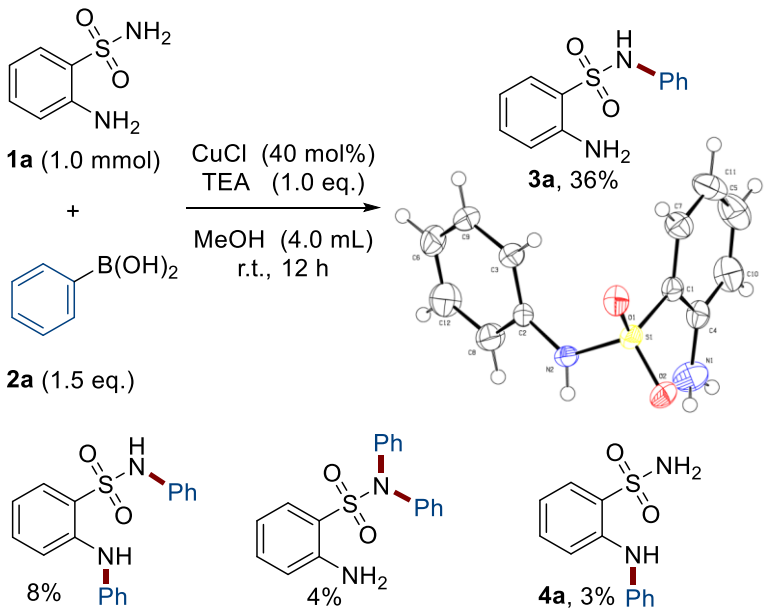
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.36 (s, 1H), 7.63 – 7.47 (m, 5H), 7.40 (t, J = 7.2 Hz, 2H), 7.30 (t, J = 7.6 Hz, 1H), 7.26 – 7.18 (m, 1H), 7.14 (d, J = 8.4 Hz, 2H), 6.81 – 6.71 (m, 1H), 6.62 – 6.53 (m, 1H), 6.03 (s, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 146.89, 139.81, 137.69, 135.60, 134.46, 130.06, 129.33, 127.78, 127.58, 126.70, 119.69, 119.08, 117.44, 115.46.

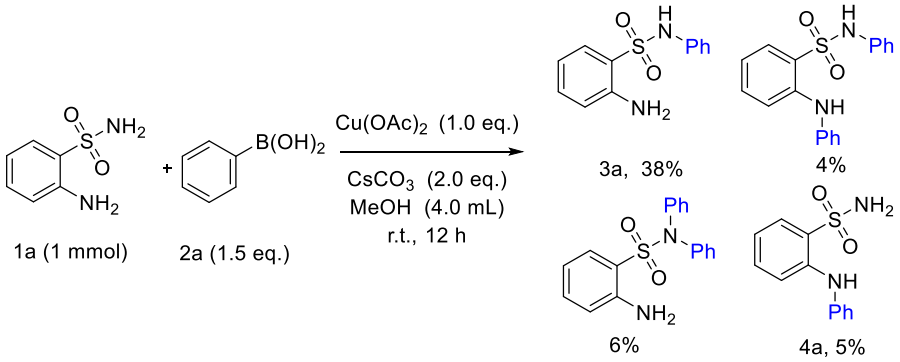
HRMS (ESI) m/z calcd for $C_{18}H_{17}N_2O_2S^+$ $(M+H)^+$ 325.1005, found 325.1009.

IR (cm^{-1}): 3482, 3382, 2362, 1617, 1457, 1135, 917, 843, 759.

B. Separation of different products of Cu-catalyzed reaction of 2-aminobenzenesulfonamide with phenylboronic acid

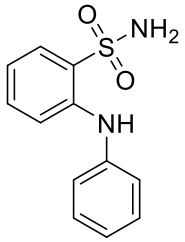


A flame-dried 100 mL column reaction flask was placed with a stirring bar. Then, 2-aminobenzenesulfonamide (172.2 mg, 1 mmol, 1.0 eq.), CuCl (39.5 mg, 0.4 mmol, 40 mol%), Et_3N (140 uL, 1 mmol, 1 eq.), **2a** (182.8 mg, 1.5 mmol, 1.5 eq.) and MeOH (4.0 mL) were added .The resulting mixture was stirred vigorously at ambient temperature for 12 hours. The reaction mixture was filtered, concentrated and then purified by column chromatography on silica gel to give the products. The recovery yield of **1a** was 10%. **4a** was obtained as yellow oil after purification by silica gel flash chromatography (PE:EA = 10:1).



A flame-dried 100 mL column reaction flask was placed with a stirring bar. Then, 2-aminobenzenesulfonamide (172.2 mg, 1 mmol, 1.0 eq.), $Cu(OAc)_2$ (181.6 mg, 1 mmol, 100 mol%), $CsCO_3$ (649.6 mg, 2 mmol, 2 eq.), **2a** (182.8 mg, 1.5 mmol, 1.5 eq.) and MeOH (4.0 mL) were added. The resulting mixture was stirred vigorously at ambient temperature for 12 hours. The reaction mixture was filtered, concentrated and then purified by column chromatography on silica gel to give the products. The recovery yield of **1a** was 22%.

(4a) 2-(phenylamino)benzenesulfonamide (CAS: 23773-76-4)

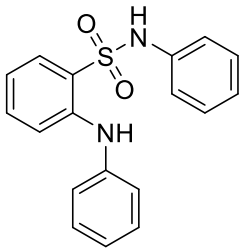


2-(phenylamino)benzenesulfonamide
Chemical Formula: $C_{12}H_{12}N_2O_2S$
Exact Mass: 248.0619
Molecular Weight: 248.3000

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.76 (dd, J = 8.0, 1.6 Hz, 1H), 7.66 (s, 1H), 7.54 (s, 2H), 7.41 – 7.27 (m, 4H), 7.19 (d, J = 7.6 Hz, 2H), 7.05 (t, J = 7.2 Hz, 1H), 6.95 – 6.89 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 141.71, 141.45, 133.57, 129.87, 129.04, 128.98, 123.12, 121.13, 119.07, 116.12.

N-phenyl-2-(phenylamino)benzenesulfonamide



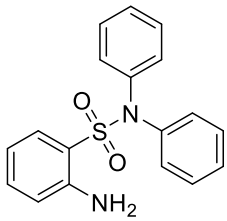
N-phenyl-2-(phenylamino)benzenesulfonamide
Chemical Formula: $C_{18}H_{16}N_2O_2S$
Exact Mass: 324.0932
Molecular Weight: 324.3980

N-phenyl-2-(phenylamino)benzenesulfonamide was obtained as brown solid, after purification by silica gel flash chromatography (PE:EA = 10:1).

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.46 (s, 1H), 7.70 (dd, J = 8.0, 1.5 Hz, 1H), 7.53 (s, 1H), 7.35 (m, 3H), 7.24 – 7.17 (m, 2H), 7.17 – 7.03 (m, 6H), 6.99 (t, J = 7.2 Hz, 1H), 6.85 – 6.79 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 142.71, 141.01, 137.74, 134.68, 130.92, 129.87, 129.64, 124.60, 123.76, 123.29, 122.05, 120.42, 118.84, 116.16.

2-Amino-*N,N*-diphenylbenzenesulfonamide



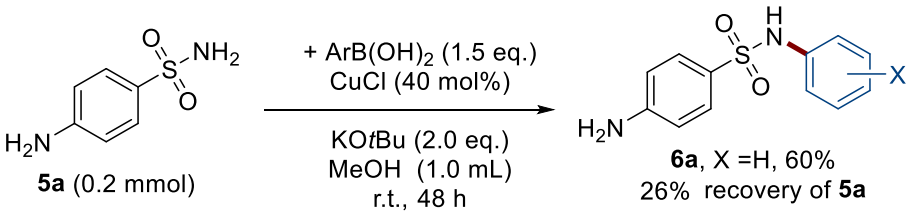
2-amino-*N,N*-diphenylbenzenesulfonamide
Chemical Formula: $C_{18}H_{16}N_2O_2S$
Exact Mass: 324.0932
Molecular Weight: 324.3980

2-Amino-*N,N*-diphenylbenzenesulfonamide was obtained as brown solid, after purification by silica gel flash chromatography (PE:EA= 10:1).

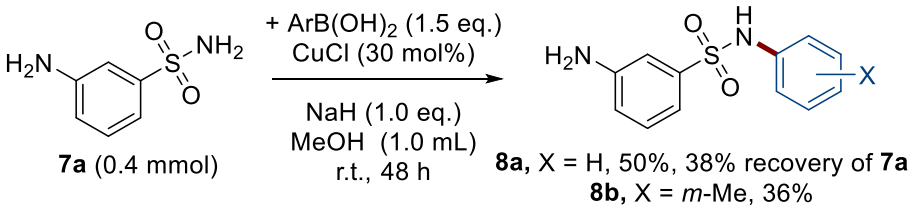
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.39 – 7.23 (m, 12H), 6.85 (dd, J = 8.4, 0. Hz, 1H), 6.53 (m, 1H), 5.94 (s, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 147.44, 141.62, 135.06, 130.52, 129.83, 129.00, 128.13, 118.75, 117.68, 115.73.

C. Reactions between 3- or 4-aminobenzene sulfonamide with arylboronic acids

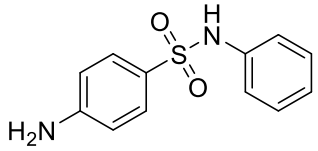


General procedure B: A flame-dried 100 mL column reaction flask was placed with a stirring bar. Then, 4-aminobenzenesulfonamide **5a** (34.5 mg, 0.2 mmol, 1.0 eq.), CuCl (7.9 mg, 0.08 mmol, 40 mol%), KO*t*Bu (44.9 mg, 0.4 mmol, 2.0 eq.), arylboronic acid (0.3 mmol, 1.5 eq.), and MeOH (1.0 mL) were added .The resulting mixture was stirred vigorously at ambient temperature for 48 hours. The reaction mixture was filtered, concentrated and then purified by column chromatography on silica gel to give the target product.



General procedure C: A flame-dried 100 mL column reaction flask was placed with a stirring bar. Then, 3-aminobenzenesulfonamide **7a** (68.9 mg, 0.4 mmol, 1.0 eq.), CuCl (11.9 mg, 0.12 mmol, 30 mol%), NaH (16.0 mg, 60%, 0.4 mmol, 1 eq.), arylboronic acid (0.6 mmol, 1.5 eq.), and MeOH (1.0 mL) were added .The resulting mixture was stirred vigorously at ambient temperature for 48 hours. The reaction mixture was filtered, concentrated and then purified by column chromatography on silica gel to give the target product.

(6a) 4-amino-N-phenylbenzenesulfonamide (CAS: 127-77-5)



4-amino-*N*-phenylbenzenesulfonamide
Chemical Formula: $C_{12}H_{12}N_2O_2S$
Exact Mass: 248.0619
Molecular Weight: 248.3000

The general procedure B was followed using phenylboronic acid **2a** (36.6 mg, 0.3 mmol) as starting material. **6a** was obtained as grey solid (29.9 mg, 60%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 191.3-196.4.

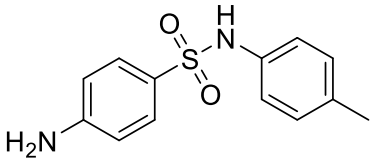
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.84 (s, 1H), 7.39 (d, J = 8.4 Hz, 2H), 7.19 (m, 2H), 7.10 – 7.02 (m, 2H), 6.96 (t, J = 7.6 Hz, 1H), 6.53 (d, J = 8.8 Hz, 2H), 5.95 (s, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 153.28, 138.96, 129.41, 129.17, 124.90, 123.75, 119.88, 113.02.

HRMS (ESI) m/z calcd for $C_{12}H_{13}N_2O_2S^+$ $(M+H)^+$ 249.06922, found 249.06958.

IR (cm-1): 3421, 3475, 3297, 1636, 1592, 1145, 1089, 688, 679.

(6b) 4-amino-N-(p-tolyl)benzenesulfonamide (CAS: 16803-95-5)



4-amino-*N*-(*p*-tolyl)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_2S$
Exact Mass: 262.0776
Molecular Weight: 262.3270

The general procedure B was followed using p-tolylboronic acid (40.8 mg, 0.3 mmol) as starting material. **6b** was obtained as brown solid (33.2 mg, 63%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 187.9-189.9.

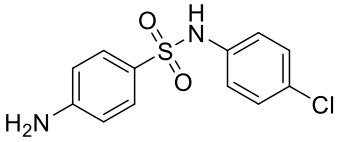
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.65 (s, 1H), 7.34 (d, J = 8.4 Hz, 2H), 7.01 – 6.91 (m, 4H), 6.50 (d, J = 8.8 Hz, 2H), 5.92 (s, 2H), 2.17 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 153.18, 136.31, 132.97, 129.83, 129.14, 124.95, 120.48, 112.98, 20.75.

HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_2S^+$ $(M+H)^+$ 263.0849, found 263.0851.

IR (cm^{-1}): 3413, 3337, 3020, 2341, 1635, 1494, 1142, 807, 674.

(6c) 4-amino-N-(4-chlorophenyl)benzenesulfonamide (CAS: 16803-92-2)



4-amino-*N*-(4-chlorophenyl)benzenesulfonamide
Chemical Formula: $C_{12}H_{11}ClN_2O_2S$
Exact Mass: 282.0230
Molecular Weight: 282.7420

The general procedure B was followed using (4-chlorophenyl)boronic acid (46.8 mg, 0.3 mmol) as starting material. **6c** was obtained as grey solid (25.3 mg, 45%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 189.4-199.0.

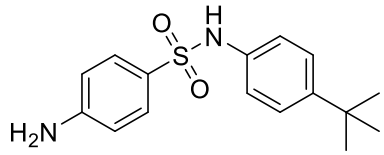
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.00 (s, 1H), 7.41 – 7.35 (m, 2H), 7.29 – 7.23 (m, 2H), 7.09 – 7.03 (m, 2H), 6.53 (m, 2H), 5.99 (s, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 153.46, 137.97, 129.39, 129.20, 127.79, 124.40, 121.41, 113.07.

HRMS (ESI) m/z calcd for $C_{12}H_{12}ClN_2O_2S^+$ $(M+H)^+$ 283.0302, found 283.0306.

IR (cm^{-1}): 3412, 3341, 3096, 2342, 1634, 1457, 1145, 815, 780.

(6d) 4-amino-N-(4-(tert-butyl)phenyl)benzenesulfonamide (CAS: 501356-80-5)



4-amino-*N*-(4-(*tert*-butyl)phenyl)benzenesulfonamide
Chemical Formula: $C_{16}H_{20}N_2O_2S$
Exact Mass: 304.1245
Molecular Weight: 304.4080

The general procedure B was followed using (4-(tert-butyl)phenyl)boronic acid (53.4 mg, 0.3 mmol) as starting material. **6d** was obtained as white solid (36.4 mg, 60%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 131.6-138.1.

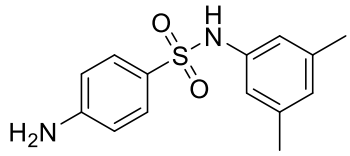
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.74 (s, 1H), 7.39 (d, J = 8.8 Hz, 2H), 7.21 (d, J = 8.8 Hz, 2H), 6.97 (d, J = 8.8 Hz, 2H), 6.53 (d, J = 8.8 Hz, 2H), 5.94 (s, 2H), 1.19 (s, 9H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 153.20, 146.04, 136.26, 129.12, 126.10, 125.27, 119.70, 113.06, 34.36, 31.60.

HRMS (ESI) m/z calcd for $C_{16}H_{21}N_2O_2S^+$ $(M+H)^+$ 305.13183, found 305.13202

IR (cm^{-1}): 3486, 3388.2, 3290, 2343, 1616, 1453, 902, 838.

(6e) 4-amino-N-(3,5-dimethylphenyl)benzenesulfonamide (CAS: 874212-15-4)



4-amino-*N*-(3,5-dimethylphenyl)benzenesulfonamide
Chemical Formula: $C_{14}H_{16}N_2O_2S$
Exact Mass: 276.0932
Molecular Weight: 276.3540

The general procedure B was followed using (3,5-dimethylphenyl)boronic acid (45.0 mg, 0.3 mmol) as starting material. **6e** was obtained as brown solid (37.8 mg, 68%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 145.1-149.7.

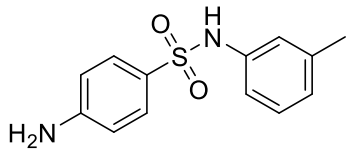
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.70 (s, 1H), 7.38 (d, J = 8.4 Hz, 2H), 6.68 (s, 2H), 6.59 (s, 1H), 6.52 (d, J = 8.8 Hz, 2H), 5.94 (s, 2H), 2.13 (s, 6H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 153.21, 138.86, 138.37, 129.15, 125.28, 125.10, 117.35, 113.01, 21.48.

HRMS (ESI) m/z calcd for $C_{14}H_{17}N_2O_2S^+$ $(M+H)^+$ 277.1005, found 277.1009.

IR (cm^{-1}): 3486, 3388, 3290, 2343, 1615, 1453, 902, 838.

(6f) 4-amino-N-(m-tolyl)benzenesulfonamide (CAS: 16803-94-4)



4-amino-*N*-(*m*-tolyl)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_2S$
Exact Mass: 262.0776
Molecular Weight: 262.3270

The general procedure B was followed using m-tolylboronic acid (40.8 mg, 0.3 mmol) as starting material. **6f** was obtained as brown solid (34.8 mg, 65%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 126.5-131.4.

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.77 (s, 1H), 7.39 (d, J = 8.8 Hz, 2H), 7.06 (t, J = 8.0 Hz, 1H), 6.87 (d, J = 2.0 Hz, 2H), 6.78 (d, J = 7.6 Hz, 1H), 6.53 (d, J = 8.8 Hz, 2H), 5.94 (s, 2H), 2.18 (s, 3H).

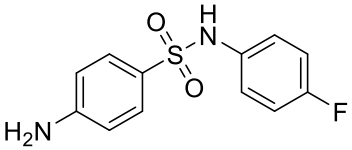
^{13}C NMR (101 MHz, DMSO-d_6) δ 153.24, 138.91, 138.63, 129.22, 129.16, 125.00, 124.45, 120.32, 116.83, 113.02,

21.55.

HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_2S^+$ $(M+H)^+$ 263.0849, found 263.0850.

IR (cm^{-1}): 3414, 3340, 3152, 2361, 1590, 1140, 884, 826.

(6g) 4-amino-N-(4-fluorophenyl)benzenesulfonamide (CAS: 1494-85-5)



4-amino-*N*-(4-fluorophenyl)benzenesulfonamide
Chemical Formula: $C_{12}H_{11}FN_2O_2S$
Exact Mass: 266.0525
Molecular Weight: 266.2904

The general procedure B was followed using (4-fluorophenyl)boronic acid (42.0 mg, 0.3 mmol) as starting material. **6g** was obtained as grey solid (31.9 mg, 60%) after purification by silica gel flash chromatography (PE:EA:MeOH = 3:1:0.2).

Melting point (°C): 161.6-165.0.

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.77 (s, 1H), 7.33 (d, J = 8.8 Hz, 2H), 7.05 (d, J = 6.8 Hz, 4H), 6.52 (d, J = 8.8 Hz, 2H), 5.96 (s, 2H).

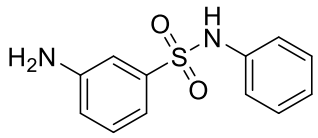
^{13}C NMR (101 MHz, DMSO-d_6) δ 159.14 (d, J = 238 Hz), 153.32, 135.18 (d, J = 3 Hz), 129.16, 124.54, 122.60 (d, J = 8 Hz), 116.10 (d, J = 22 Hz), 113.03.

^{19}F NMR (376 MHz, DMSO-d_6) δ -119.44.

HRMS (ESI) m/z calcd for $C_{12}H_{12}FN_2O_2S^+$ $(M+H)^+$ 267.0598, found 267.0597.

IR (cm^{-1}): 3487, 3394, 2360, 1622, 1446, 1143, 842, 704.

(8a) 3-amino-N-phenylbenzenesulfonamide (CAS: 80-21-7)



3-amino-*N*-phenylbenzenesulfonamide
Chemical Formula: $C_{12}H_{12}N_2O_2S$
Exact Mass: 248.0619
Molecular Weight: 248.3000

The general procedure C was followed using phenylboronic acid **2a** (73.2 mg, 0.6 mmol) as starting material. **8a** was obtained as white solid (49.8 mg, 50%) after purification by silica gel flash chromatography (PE:EA:MeOH = 2:1:0.2).

Melting point (°C): 127.2-131.5.

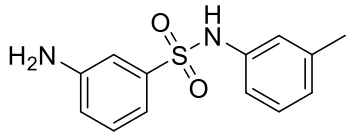
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.12 (s, 1H), 7.22 (t, J = 8.0 Hz, 2H), 7.11 (m, 3H), 7.03 – 6.95 (m, 2H), 6.89 – 6.82 (m, 1H), 6.70 (dd, J = 8.0, 2.0 Hz, 1H), 5.56 (s, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 149.79, 140.69, 138.53, 129.99, 129.50, 124.09, 120.06, 117.99, 113.73, 111.60.

HRMS (ESI) m/z calcd for $C_{12}H_{13}N_2O_2S^+$ $(M+H)^+$ 249.0692, found 249.0693.

IR (cm^{-1}): 3411, 3324, 3079, 2360, 1480, 1456, 1149, 790, 755.

(8b) 3-amino-N-(m-tolyl)benzenesulfonamide (CAS: 953888-95-4)



3-amino-*N*-(*m*-tolyl)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_2S$
Exact Mass: 262.0776
Molecular Weight: 262.3270

The general procedure C was followed using m-tolylboronic acid (81.6 mg, 0.6 mmol) as starting material. **8b** was obtained as brown solid (37.8 mg, 36%) after purification by silica gel flash chromatography (PE:EA:MeOH = 2:1:0.2).

Melting point (°C): 125.3-130.9.

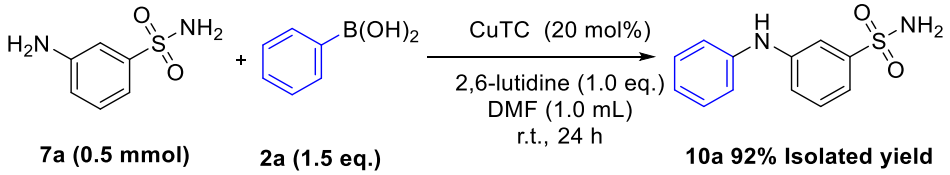
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.05 (s, 1H), 7.17 – 7.05 (m, 2H), 6.96 (t, J = 2.0 Hz, 1H), 6.91 – 6.79 (m, 4H), 6.69 (m, 1H), 5.56 (s, 2H), 2.19 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 149.77, 140.76, 138.75, 138.47, 129.98, 129.30, 124.81, 120.55, 117.97, 117.04, 113.75, 111.62, 21.55.

HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_2S^+$ $(M+H)^+$ 263.0849, found 263.0850.

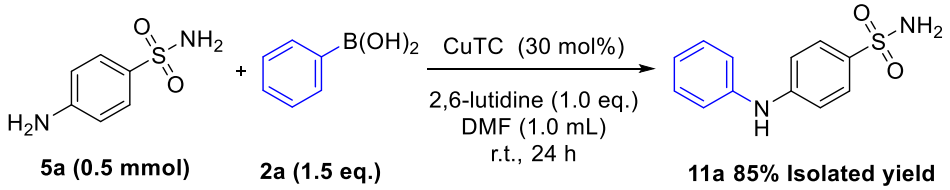
IR (cm^{-1}): 3477, 3385, 3232, 2340, 1626, 1473, 1146, 758, 672.

D. Arylation of phenylamino of 2 or 3- aminobenzenesulfonamide with aryl boronic acid



7a (0.5 mmol) **2a (1.5 eq.)** **10a 92% Isolated yield**

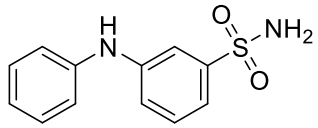
General procedure D: A flame-dried 100 mL pear shaped flask was placed with a stirring bar. Then, 3-aminobenzenesulfonamide (86.1 mg, 0.5 mmol, 1.0 eq.), CuTC (19.1 mg, 0.1 mmol, 20 mol%), 2,6-Lutidine (58.0 μL, 0.5 mmol, 1.0 eq.), arylboronic acid (0.75 mmol, 1.5 eq.) and DMF (1.0 mL) were added. The resulting mixture was stirred vigorously at ambient temperature for 24 hours. The reaction mixture was treated with EtOAc (5.0 mL) and water (5.0 mL). The organic layer was separated, and the aqueous layer was extracted with EtOAc (3 × 5.0 mL). The combined organic phase was washed with brine (2 × 5.0 mL), dried over anhydrous Na_2SO_4, and concentrated to afford residue, which was purified by column chromatography on silica gel to give the target product.



5a (0.5 mmol) **2a (1.5 eq.)** **11a 85% Isolated yield**

General procedure E: A flame-dried 100 mL pear shaped flask was placed with a stirring bar. Then, 4-aminobenzenesulfonamide (86.1 mg, 0.5 mmol, 1.0 eq.), CuTC (28.6 mg, 0.15 mmol, 30 mol%), 2,6-Lutidine (58.0 μL, 0.5 mmol, 1.0 eq.), arylboronic acid (0.75 mmol, 1.5 eq.) and DMF (1.0 mL) were added. The resulting mixture was stirred vigorously at ambient temperature for 24 hours. The reaction mixture was treated with EtOAc (5.0 mL) and water (5.0 mL). The organic layer was separated, and the aqueous layer was extracted with EtOAc (3 × 5.0 mL). The combined organic phase was washed with brine (2 × 5.0 mL), dried over anhydrous Na_2SO_4, and concentrated to afford residue, which was purified by column chromatography on silica gel to give the target product.

(10a) 3-(phenylamino)benzenesulfonamide (CAS: 1294519-72-4)



3-(phenylamino)benzenesulfonamide
Chemical Formula: $C_{12}H_{12}N_2O_2S$
Exact Mass: 248.0619
Molecular Weight: 248.3000

The general procedure D was followed using phenylboronic acid **2a** (91.4 mg, 0.75 mmol) as starting material. **10a** was obtained as white solid (112.6 mg, 92%) after purification by silica gel flash chromatography (PE:EA:Acetone = 4:1:0.3).

Melting point (°C): 114.2-115.9.

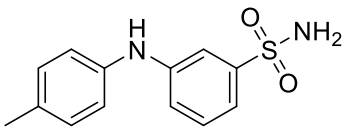
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.52 (s, 1H), 7.52 (t, J = 2.0 Hz, 1H), 7.38 (t, J = 8.0 Hz, 1H), 7.29 (m, 4H), 7.25 – 7.17 (m, 2H), 7.16 – 7.10 (m, 2H), 6.92 (t, J = 7.2 Hz, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 145.48, 144.69, 142.74, 130.27, 129.81, 121.38, 119.30, 118.34, 116.52, 112.72.

HRMS (ESI) m/z calcd for $C_{12}H_{12}N_2O_2S^+$ $(M+H)^+$ 249.0692, found 249.0694.

IR (cm^{-1}): 3337, 3236, 2988, 2344, 1585, 1481, 1149, 864, 680.

(10b) 3-(p-tolylamino)benzenesulfonamide (CAS: 1294519-73-5)



3-(*p*-tolylamino)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_2S$
Exact Mass: 262.0776
Molecular Weight: 262.3270

The general procedure D was followed using p-tolylboronic acid (102.0 mg, 0.75 mmol) as starting material. **10b** was obtained as white solid (113.7 mg, 87%) after purification by silica gel flash chromatography (PE:EA:Acetone = 4:1:0.3).

Melting point (°C): 147.5-152.6.

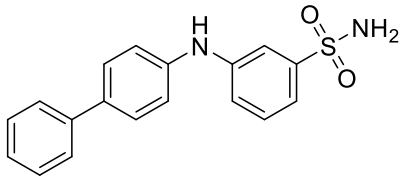
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (s, 1H), 7.47 – 7.41 (m, 1H), 7.34 (t, J = 8.0 Hz, 1H), 7.25 (s, 2H), 7.20 – 7.07 (m, 4H), 7.03 (d, J = 8.4 Hz, 2H), 2.25 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 145.45, 145.37, 139.98, 130.65, 130.23, 130.20, 119.27, 118.60, 115.90, 111.96, 20.82.

HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_2S^+$ $(M+H)^+$ 263.0849, found 263.0848.

IR (cm^{-1}): 3366, 3326, 3236, 1594, 1487, 1150, 783, 731.

(10c) 3-([1,1'-biphenyl]-4-ylamino)benzenesulfonamide



3-([1,1'-biphenyl]-4-ylamino)benzenesulfonamide
Chemical Formula: $C_{18}H_{16}N_2O_2S$
Exact Mass: 324.0932
Molecular Weight: 324.3980

The general procedure D was followed using [1,1'-biphenyl]-4-ylboronic acid (148.5 mg, 0.75 mmol) as starting material. **10c** was obtained as grey solid (105.3 mg, 65%) after purification by silica gel flash chromatography (PE:EA:Acetone = 4:1:0.3).

Melting point (°C): 184.0-186.6.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.68 (s, 1H), 7.69 – 7.59 (m, 4H), 7.57 (t, J = 2.0 Hz, 1H), 7.48 – 7.37 (m, 3H), 7.34 – 7.18 (m, 7H).

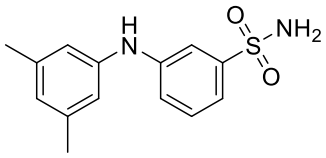
^{13}C NMR (101 MHz, DMSO-d_6) δ 145.54, 144.36, 142.35, 140.35, 132.91, 130.35, 129.36, 128.00, 127.11, 126.40,

119.67, 118.36, 116.82, 113.15.

HRMS (ESI) m/z calcd for $C_{18}H_{17}N_2O_2S^+$ $(M+H)^+$ 325.1005, found 325.1008.

IR (cm^{-1}): 3350, 3270, 1592, 1475, 1291, 1149, 680.

(10d) 3-((3,5-dimethylphenyl)amino)benzenesulfonamide



3-((3,5-dimethylphenyl)amino)benzenesulfonamide
Chemical Formula: $C_{14}H_{16}N_2O_2S$
Exact Mass: 276.0932
Molecular Weight: 276.3540

The general procedure D was followed using (3,5-dimethylphenyl)boronic acid (112.5 mg, 0.75 mmol) as starting material. **10d** was obtained as white solid (126.6 mg, 92%) after purification by silica gel flash chromatography (PE:EA:Acetone = 4:1:0.3).

Melting point (°C): 154.2-159.3.

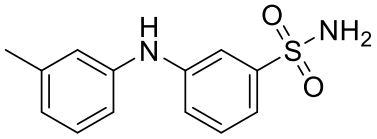
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.35 (s, 1H), 7.47 (t, J = 2.0 Hz, 1H), 7.36 (t, J = 8.0 Hz, 1H), 7.28 (s, 2H), 7.22 – 7.15 (m, 2H), 6.73 (s, 2H), 6.57 (s, 1H), 2.22 (s, 6H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 145.47, 144.94, 142.65, 138.79, 130.19, 123.23, 119.15, 116.29, 113.09, 21.58.

HRMS (ESI) m/z calcd for $C_{14}H_{17}N_2O_2S^+$ $(M+H)^+$ 277.1005, found 277.1008.

IR (cm^{-1}): 3407, 3330, 3244, 1585, 1483, 1153, 748, 682.

(10e) 3-(m-tolylamino)benzenesulfonamide



3-(*m*-tolylamino)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_2S$
Exact Mass: 262.0776
Molecular Weight: 262.3270

The general procedure D was followed using m-tolylboronic acid (102.0 mg, 0.75 mmol) as starting material. **10e** was obtained as white solid (112.8 mg, 86%) after purification by silica gel flash chromatography (PE:EA:Acetone = 4:1:0.3).

Melting point (°C): 159.1-163.4.

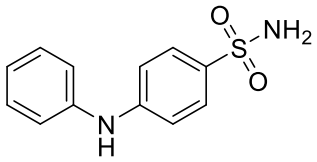
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.43 (s, 1H), 7.49 (t, J = 2.0 Hz, 1H), 7.37 (t, J = 8.0 Hz, 1H), 7.28 (s, 2H), 7.23 – 7.11 (m, 3H), 6.93 (m, 2H), 6.74 (d, J = 7.2 Hz, 1H), 2.27 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 145.47, 144.81, 142.69, 139.05, 130.23, 129.61, 122.23, 119.22, 119.09, 116.39, 115.48, 112.88, 21.67.

HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_2S^+$ $(M+H)^+$ 263.0849, found 263.0850.

IR (cm^{-1}): 3363, 3255, 1600, 1582, 1582, 1147, 1153, 867, 682.

(11a) 4-(phenylamino)benzenesulfonamide (CAS: 6786-93-2)



4-(phenylamino)benzenesulfonamide
Chemical Formula: $C_{12}H_{12}N_2O_2S$
Exact Mass: 248.0619
Molecular Weight: 248.3000

The general procedure E was followed using phenylboronic acid **5a** (91.4 mg, 0.75 mmol) as starting material. **11a** was obtained as white solid (105.0 mg, 85%) after purification by silica gel flash chromatography (PE:EA:Acetone = 3:1:0.3).

Melting point (°C): 145.4-148.1.

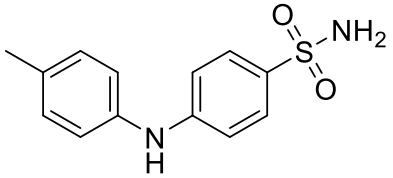
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.67 (s, 1H), 7.67 – 7.59 (m, 2H), 7.35 – 7.27 (m, 2H), 7.16 (m, 2H), 7.12 – 7.08 (m, 2H), 7.07 (s, 2H), 6.97 (t, J = 7.2 Hz, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 147.45, 142.03, 133.99, 129.82, 127.95, 122.09, 119.38, 114.71.

HRMS (ESI) m/z calcd for $C_{12}H_{13}N_2O_2S^+$ $(M+H)^+$ 249.0692, found 249.0690.

IR (cm^{-1}): 3368, 3249, 1585, 1496, 1308, 1141, 730, 693.

(11b) 4-(p-tolylamino)benzenesulfonamide (CAS: 1027579-14-1)



4-(*p*-tolylamino)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_2S$
Exact Mass: 262.0776
Molecular Weight: 262.3270

The general procedure E was followed using p-tolylboronic acid (102.0 mg, 0.75 mmol) as starting material. **11b** was obtained as white solid (113.2 mg, 86%) after purification by silica gel flash chromatography (PE:EA:Acetone = 3:1:0.3).

Melting point (°C): 162.8-166.3.

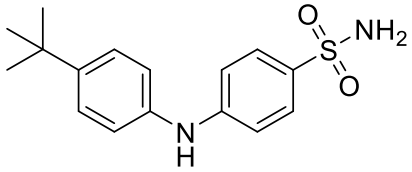
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.54 (s, 1H), 7.66 – 7.55 (m, 2H), 7.13 (d, J = 8.4 Hz, 2H), 7.10 – 6.94 (m, 6H), 2.26 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 148.09, 139.28, 133.38, 131.41, 130.25, 127.95, 120.21, 114.05, 20.86.

HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_2S^+$ $(M+H)^+$ 263.0849, found 263.0846.

IR (cm^{-1}): 3357, 3237, 1588, 1312, 1147, 811, 742.

(11c) 4-((4-(tert-butyl)phenyl)amino)benzenesulfonamide



4-((4-(*tert*-butyl)phenyl)amino)benzenesulfonamide
Chemical Formula: $C_{16}H_{20}N_2O_2S$
Exact Mass: 304.1245
Molecular Weight: 304.4080

The general procedure E was followed using (4-(tert-butyl)phenyl)boronic acid (133.5 mg, 0.75 mmol) as starting material. **11c** was obtained as white solid (123.9 mg, 81%) after purification by silica gel flash chromatography (PE:EA:Acetone = 3:1:0.3).

Melting point (°C): 185.1-188.0.

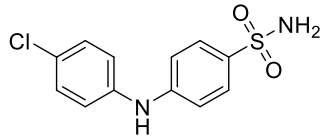
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.58 (s, 1H), 7.61 (d, J = 8.8 Hz, 2H), 7.34 (d, J = 8.8 Hz, 2H), 7.10 (d, J = 8.68Hz, 2H), 7.07 – 7.00 (m, 4H), 1.27 (s, 9H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 147.92, 144.67, 139.28, 133.45, 127.95, 126.44, 119.59, 114.17, 34.42, 31.74.

HRMS (ESI) m/z calcd for $C_{16}H_{21}N_2O_2S^+$ $(M+H)^+$ 305.1318, found 305.1317.

IR (cm^{-1}): 3358, 3259, 2952, 1586, 1497, 1305, 1131, 825.

(11d) 4-((4-chlorophenyl)amino)benzenesulfonamide (CAS: 1348965-14-9)



4-((4-chlorophenyl)amino)benzenesulfonamide
Chemical Formula: $C_{12}H_{11}ClN_2O_2S$
Exact Mass: 282.0230
Molecular Weight: 282.7420

The general procedure E was followed using (4-chlorophenyl)boronic acid (117.0 mg, 0.75 mmol) as starting material. **11d** was obtained as white solid (84.9 mg, 60%) after purification by silica gel flash chromatography (PE:EA:Acetone = 3:1:0.3).

Melting point (°C): 163.2-164.6.

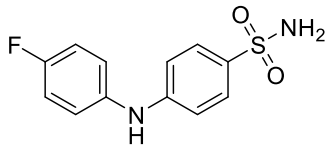
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.78 (s, 1H), 7.68 – 7.61 (m, 2H), 7.36 – 7.29 (m, 2H), 7.19 – 7.14 (m, 2H), 7.11 (m, 4H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 146.84, 141.19, 134.64, 129.64, 127.96, 125.17, 120.50, 115.22.

HRMS (ESI) m/z calcd for $C_{12}H_{12}ClN_2O_2S^+$ $(M+H)^+$ 283.0302, found 283.0307.

IR (cm^{-1}): 3357, 3250, 1519, 1487, 1147, 812, 659.

(11e) 4-((4-fluorophenyl)amino)benzenesulfonamide (CAS: 1294519-59-7)



4-((4-fluorophenyl)amino)benzenesulfonamide
Chemical Formula: $C_{12}H_{11}FN_2O_2S$
Exact Mass: 266.0525
Molecular Weight: 266.2904

The general procedure E was followed using (4-fluorophenyl)boronic acid (105.0 mg, 0.75 mmol) as starting material. **11e** was obtained as grey solid (70.0 mg, 53%) after purification by silica gel flash chromatography (PE:EA:Acetone = 3:1:0.3).

Melting point (°C): 151.6-155.7.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.62 (s, 1H), 7.62 (d, J = 8.8 Hz, 2H), 7.25 – 7.11 (m, 4H), 7.11 – 6.93 (m, 4H).

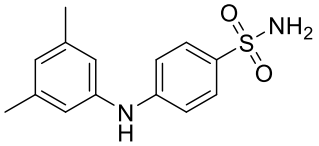
^{13}C NMR (101 MHz, DMSO-d_6) δ 157.92 (d, J = 237 Hz), 147.91, 138.30 (d, J = 2 Hz), 133.81, 127.99, 121.87 (d, J = 8 Hz), 116.42 (d, J = 23 Hz), 114.14.

^{19}F NMR (376 MHz, DMSO-d_6) δ -121.16.

HRMS (ESI) m/z calcd for $C_{12}H_{12}FN_2O_2S^+$ $(M+H)^+$ 267.0598, found 267.0595.

IR (cm^{-1}):,3368, 3249, 1585, 1308, 1141, 693.

(11f) 4-((3,5-dimethylphenyl)amino)benzenesulfonamide (CAS: 1294519-57-5)



4-((3,5-dimethylphenyl)amino)benzenesulfonamide
Chemical Formula: $C_{14}H_{16}N_2O_2S$
Exact Mass: 276.0932
Molecular Weight: 276.3540

The general procedure E was followed using (3,5-dimethylphenyl)boronic acid (112.5 mg, 0.75 mmol) as starting material. **11f** was obtained as brown solid (124.1 mg, 90%) after purification by silica gel flash chromatography (PE:EA:Acetone = 3:1:0.3).

Melting point (°C): 151.1-154.9.

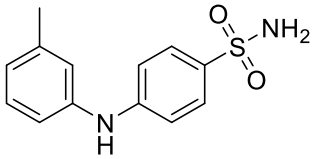
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.52 (s, 1H), 7.61 (d, J = 8.8 Hz, 2H), 7.12 – 7.00 (m, 4H), 6.77 (s, 2H), 6.61 (s, 1H), 2.23 (s, 6H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 147.68, 141.90, 138.83, 133.70, 127.91, 123.88, 117.23, 114.78, 21.54.

HRMS (ESI) m/z calcd for $C_{14}H_{17}N_2O_2S^+$ $(M+H)^+$ 277.1005, found 277.1002.

IR (cm^{-1}): 3381, 3304, 3243, 1582, 1278, 1148, 824.

(11g) 4-(m-tolylamino)benzenesulfonamide (CAS: 1800547-17-4)



4-(*m*-tolylamino)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_2S$
Exact Mass: 262.0776
Molecular Weight: 262.3270

The general procedure E was followed using m-tolylboronic acid (102.0 mg, 0.75 mmol) as starting material. **11g** was obtained as grey solid (116.4 mg, 89%) after purification by silica gel flash chromatography (PE:EA:Acetone = 3:1:0.3).

Melting point (°C): 93.2-96.5.

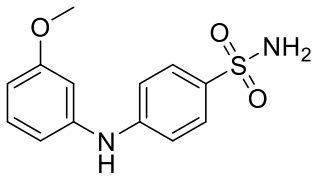
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.60 (s, 1H), 7.67 – 7.57 (m, 2H), 7.19 (t, J = 7.6 Hz, 1H), 7.12 – 7.01 (m, 4H), 6.96 (m, 2H), 6.79 (d, J = 7.6 Hz, 1H), 2.28 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 147.57, 141.97, 139.09, 133.84, 129.64, 127.93, 122.94, 119.99, 116.58, 114.74, 21.63.

HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_2S^+$ $(M+H)^+$ 263.0849, found 263.0845.

IR (cm^{-1}): 3393, 3346, 3250, 1576, 1154, 1091, 720.

(11h) 4-((3-methoxyphenyl)amino)benzenesulfonamide (CAS: 1348122-53-1)



4-((3-methoxyphenyl)amino)benzenesulfonamide
Chemical Formula: $C_{13}H_{14}N_2O_3S$
Exact Mass: 278.0725
Molecular Weight: 278.3260

The general procedure E was followed using (3-methoxyphenyl)boronic acid (114.0 mg, 0.75 mmol) as starting material. **11h** was obtained as grey solid (83.8 mg, 60%) after purification by silica gel flash chromatography (PE:EA:Acetone = 3:1:0.3).

Melting point (°C): 130.9-135.9.

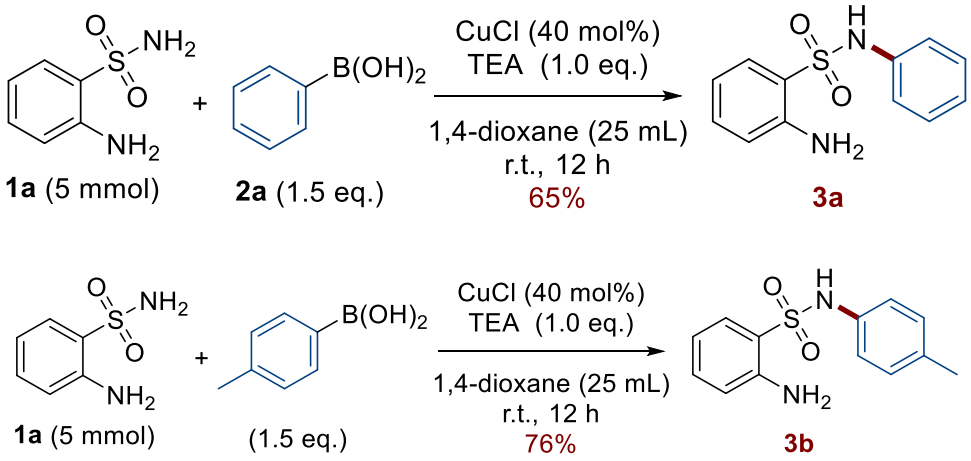
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.68 (s, 1H), 7.64 (d, J = 8.8 Hz, 2H), 7.21 (t, J = 8.0 Hz, 1H), 7.16 – 7.02 (m, 4H), 6.75 (dd, J = 8.0, 1.6 Hz, 1H), 6.69 (t, J = 2.0 Hz, 1H), 6.54 (dd, J = 8.0, 2.0 Hz, 1H), 3.74 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 160.65, 147.21, 143.36, 134.18, 130.59, 127.93, 115.12, 111.47, 107.54, 104.75, 55.42.

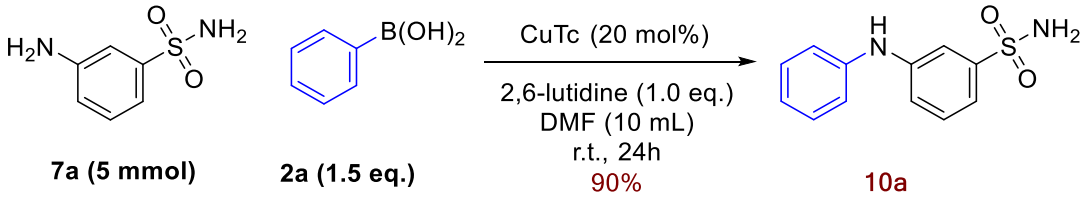
HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2O_3S^+$ $(M+H)^+$ 279.0798, found 279.0799.

IR (cm^{-1}): 3335, 3244, 1585, 1458, 1148, 777, 743.

E. Cu-catalyzed selective arylation of aminobenzenesulfonamide on larger scale



A flame-dried 100 mL column reaction flask was placed with a stirring bar. Then, 2-aminobenzenesulfonamide (861 mg, 5 mmol, 1.0 eq.), CuCl (198 mg, 2 mmol, 40 mol%), Et_3N (700 μL, 5 mmol, 1.0 eq.), arylboronic acid (7.5 mmol, 1.5 eq.) and 1,4-dioxane (25 mL) were added .The resulting mixture was stirred vigorously at ambient temperature for 12 hours. The reaction mixture was filtered, concentrated and then purified by column chromatography on silica gel to give the target products.

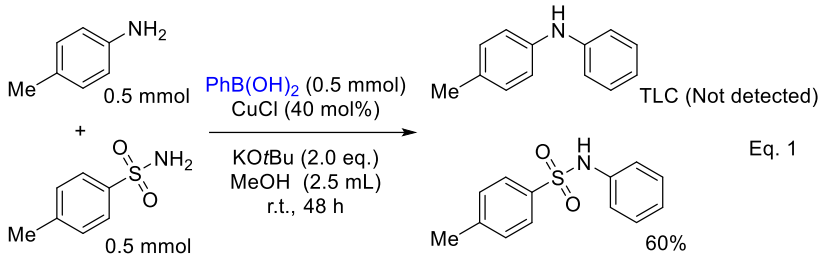


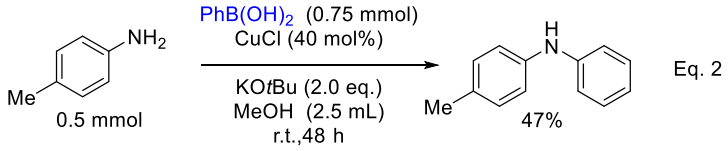
A flame-dried 100 mL pear shaped flask was placed with a stirring bar. Then, 3-aminobenzenesulfonamide (861 mg, 5 mmol, 1.0 eq.), CuTC (191 mg, 1 mmol, 20 mol%), 2,6-Lutidine (576 μL, 5 mmol, 1.0 eq.), arylboronic acid (7.5 mmol, 1.5 eq.) and DMF (10 mL) were added. The resulting mixture was stirred vigorously at ambient temperature (Pear shaped flask open) for 24 hours. The reaction mixture was treated with EtOAc (50 mL) and water (50 mL). The organic layer was separated, and the aqueous layer was extracted with EtOAc (3 × 10.0 mL). The combined organic phase was washed with brine (2 × 10.0 mL), dried over anhydrous Na_2SO_4, and concentrated to afford residue, which was purified by column chromatography on silica gel to give the target product **10a**.

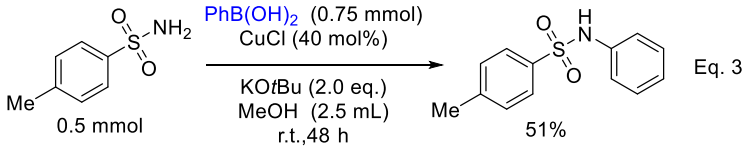
F. Control experiments

The following experiments were performed to give some information of the observed chemoselectivity.

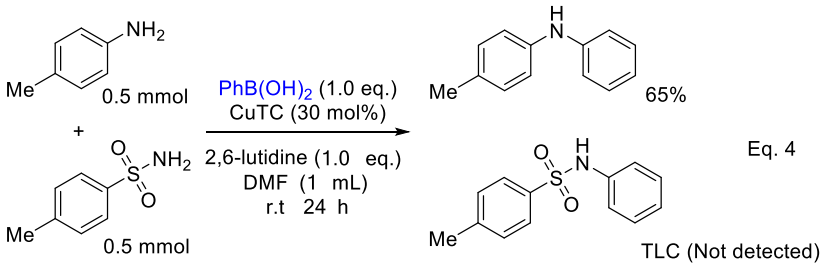
As depicted in Equation 1, when p-toluidine, 4-methylbenzenesulfonamide and phenylboronic acid were mixed in 1:1:1 ratio and exposed to reaction conditions that were depicted in Scheme 4 of the manuscript, selective arylation of the 4-methylbenzenesulfonamide was observed. There was no product deriving from the arylation of the arylamino group. Then p-toluidine and 4-methylbenzenesulfonamide were reacted with $PhB(OH)_2$ under the similar reaction conditions (Eq. 2 and Eq. 3). For p-toluidine, 47% yield of the arylated product was obtained. The yield of the arylated product of 4-methylbenzenesulfonamide was 51%. These data clearly showed the superior reactivity of the sulfonamide group, although both amino and sulfonamide group were competent CEL coupling partners under these conditions.



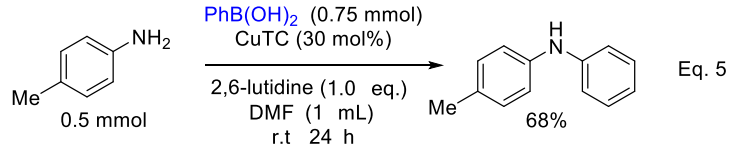




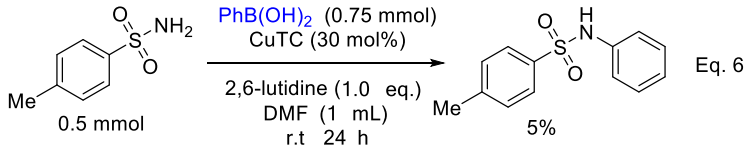
A similar procedure was also performed using the reaction conditions depicted in Scheme 5. In the 1:1:1 mixed case (Eq. 4), selective arylated product of p-toluidine was obtained 65% yield, while 4-methylbenzenesulfonamide was reluctant to be arylated. The separated experiments revealed that the reactivity of arylamino group remained (Eq. 5), while the sulfonamide group was still hard to be arylated (Eq. 6). This implied the observed preference towards arylamino group in Scheme 5 might derive from the instinctive inertness of the sulfonamide group under such conditions.



Eq. 4

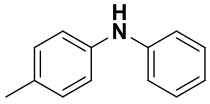


Eq. 5



Eq. 6

4-methyl-N-phenylaniline (CAS: 620-84-8)



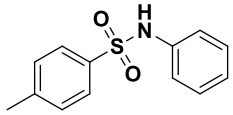
4-methyl-*N*-phenylaniline
Chemical Formula: $C_{13}H_{13}N$
Exact Mass: 183.1048
Molecular Weight: 183.2540

4-methyl-N-phenylaniline (Org. Lett. 2018, 20, 1134-1137)

^{1}H NMR ($CDCl_3$): δ 7.25 (t, *J* = 7.3 Hz, 2H), 7.10 (d, *J* = 8.1 Hz, 2H), 7.02-7.00 (m, 4H), 6.89 (t, *J* = 7.3 Hz, 1H), 5.60 (brs, 1H), 2.32 (s, 3H).

^{13}C NMR ($CDCl_3$): δ 144.1, 140.4, 131.1, 130.0, 129.4, 120.4, 119.0, 117.0, 20.8.

4-methyl-N-phenylbenzenesulfonamide (CAS: 68-34-8)



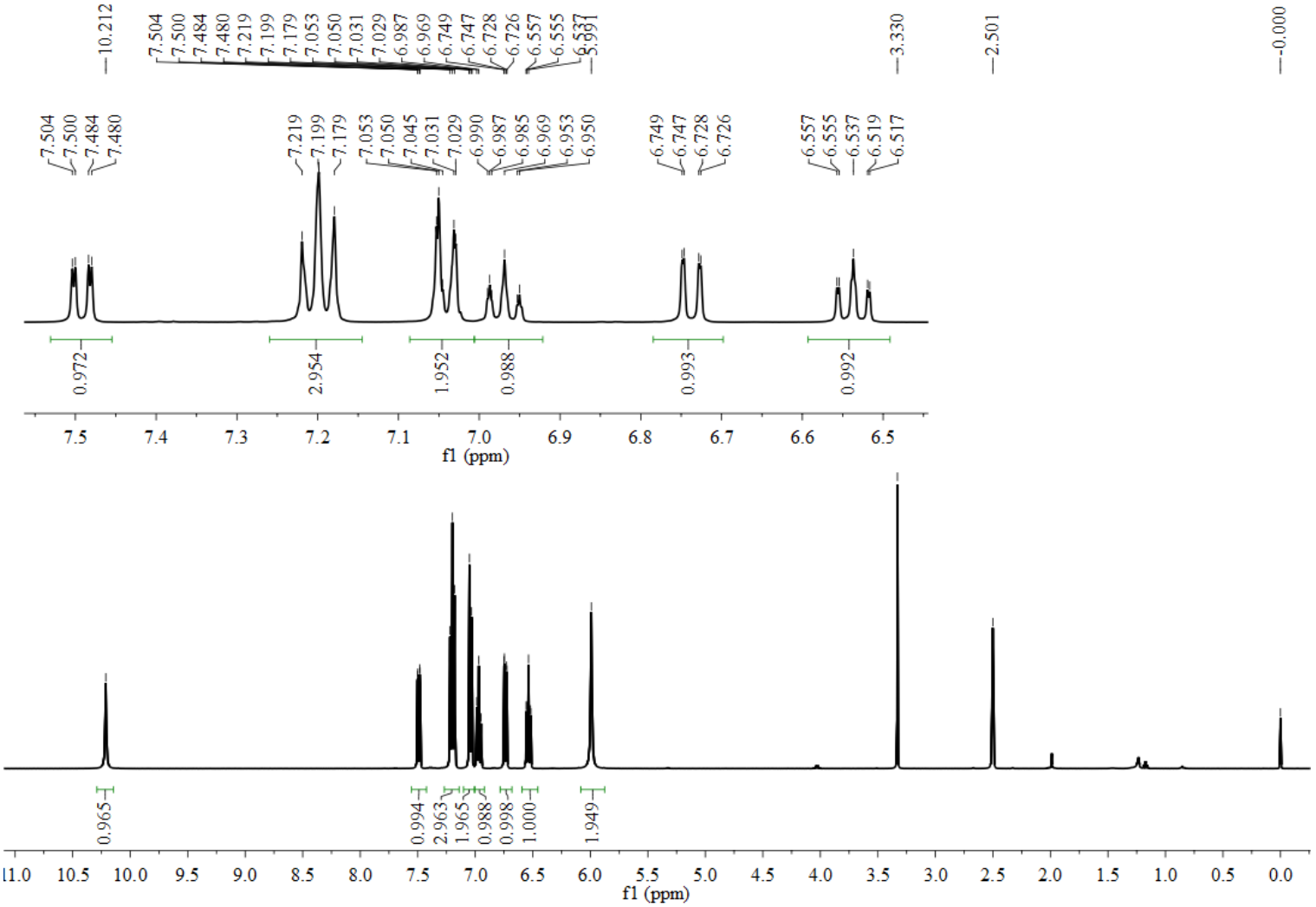
4-methyl-*N*-phenylbenzenesulfonamide
Chemical Formula: $C_{13}H_{13}NO_2S$
Exact Mass: 247.0667
Molecular Weight: 247.3120

4-methyl-N-phenylbenzenesulfonamide (J. Org. Chem. 2018, 83, 14385-14395)

^{1}H NMR ($CDCl_3$): 7.65 (d, *J* = 8.4 Hz, 2H), 7.26-7.22 (m, 4H), 7.12 (t, *J* = 7.6 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 2H), 6.75 (br s, 1H), 2.38 (s, 3H).

^{13}C NMR ($CDCl_3$) δ 143.9, 136.5, 136.1, 129.6, 129.3, 127.3, 125.3, 121.5, 21.5.

3. Copies of NMR spectra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7.500
7.484
7.480
7.219
7.199
7.179
7.053
7.050
7.031
7.029
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6.969
6.749
6.747
6.728
6.726
6.557
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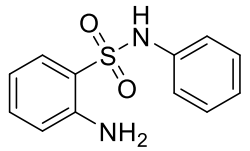
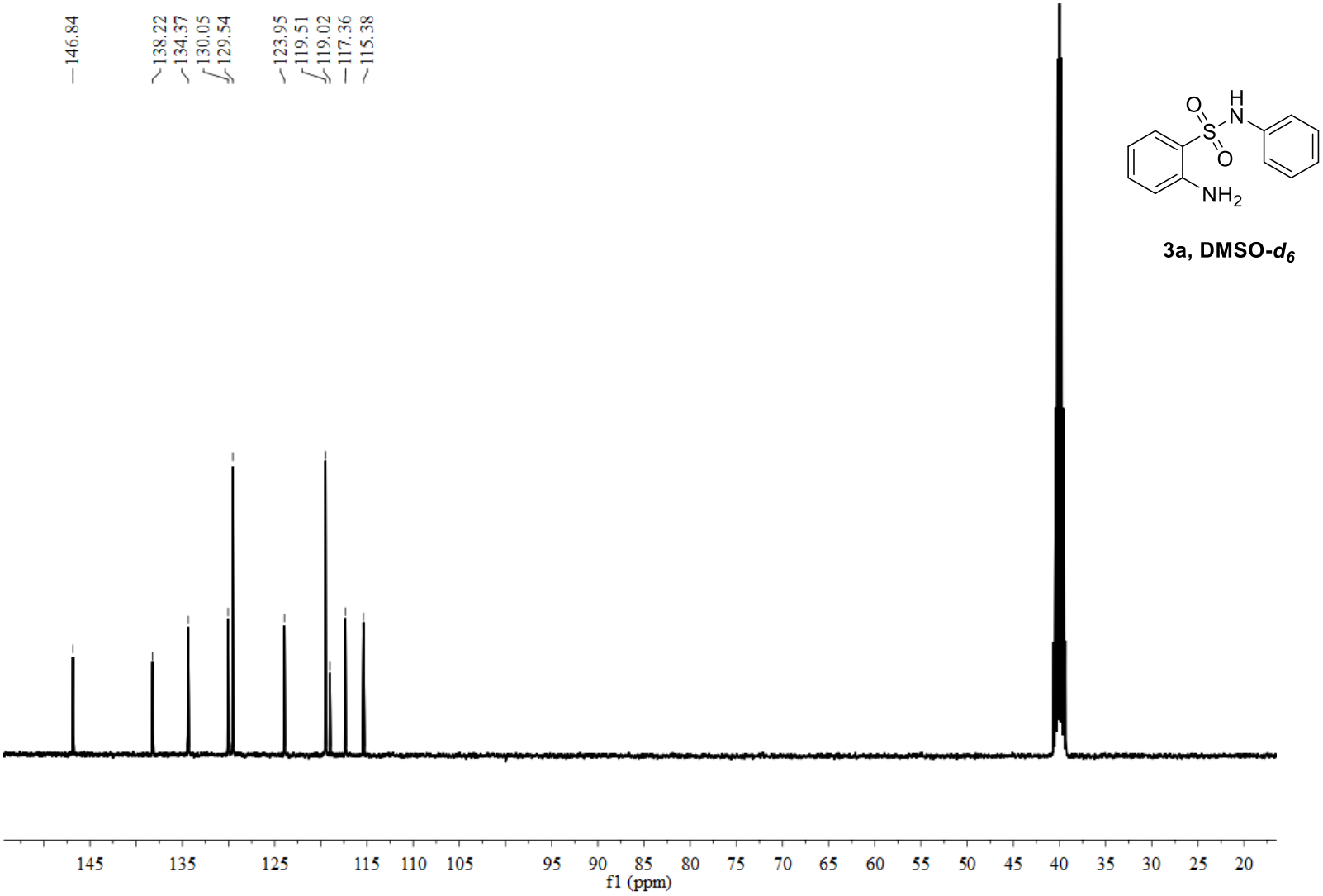
3.330
2.501
0.000
0.972
2.954
1.952
0.988
0.993
0.992
f1 (ppm)
0.965
0.994
2.963
1.965
0.988
0.998
1.000
1.949
f1 (ppm)


O
H
N
S
O
NH2

3a, DMSO-d_6


146.84
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129.54
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119.51
119.02
117.36
115.38
O
H
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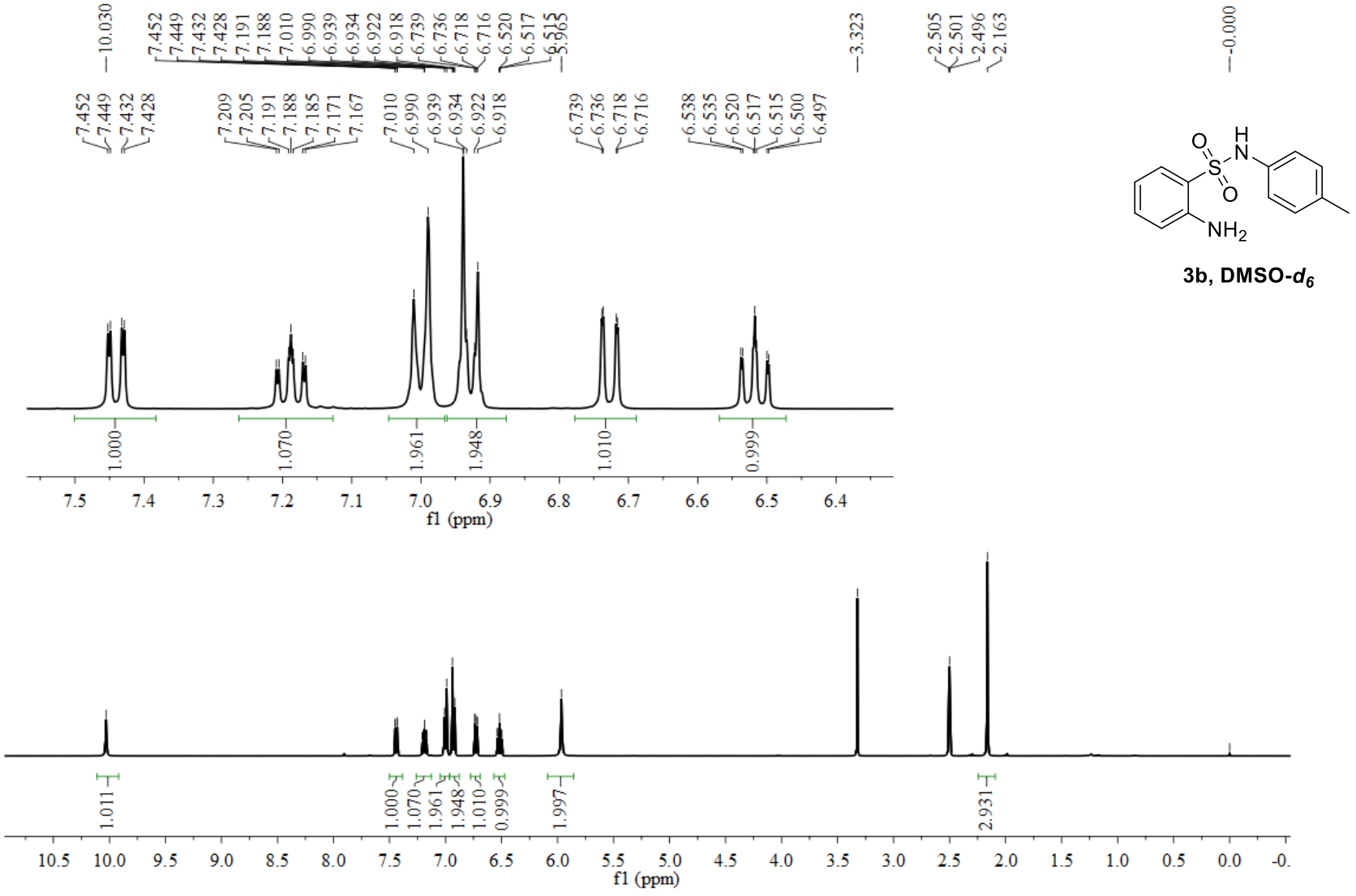
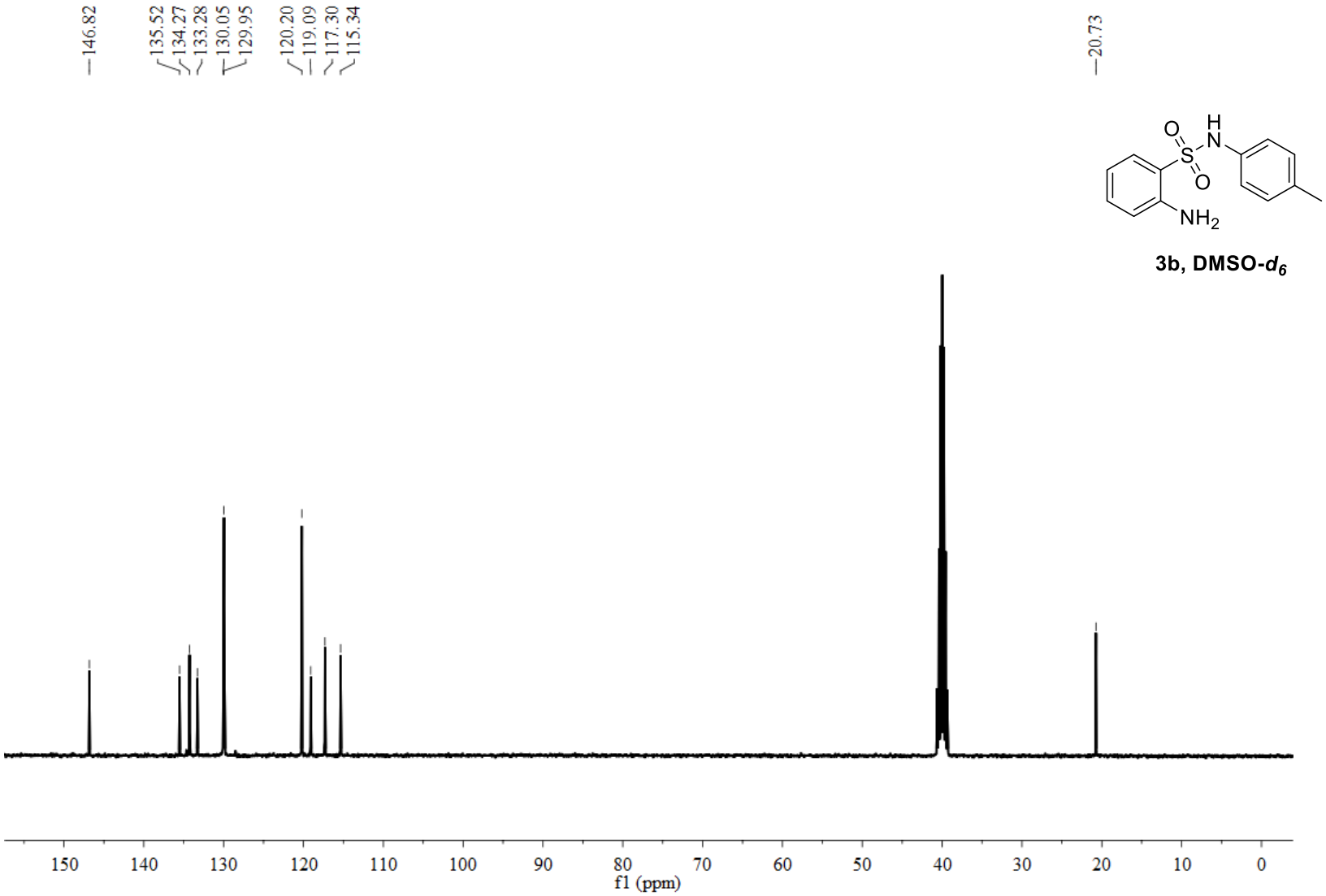
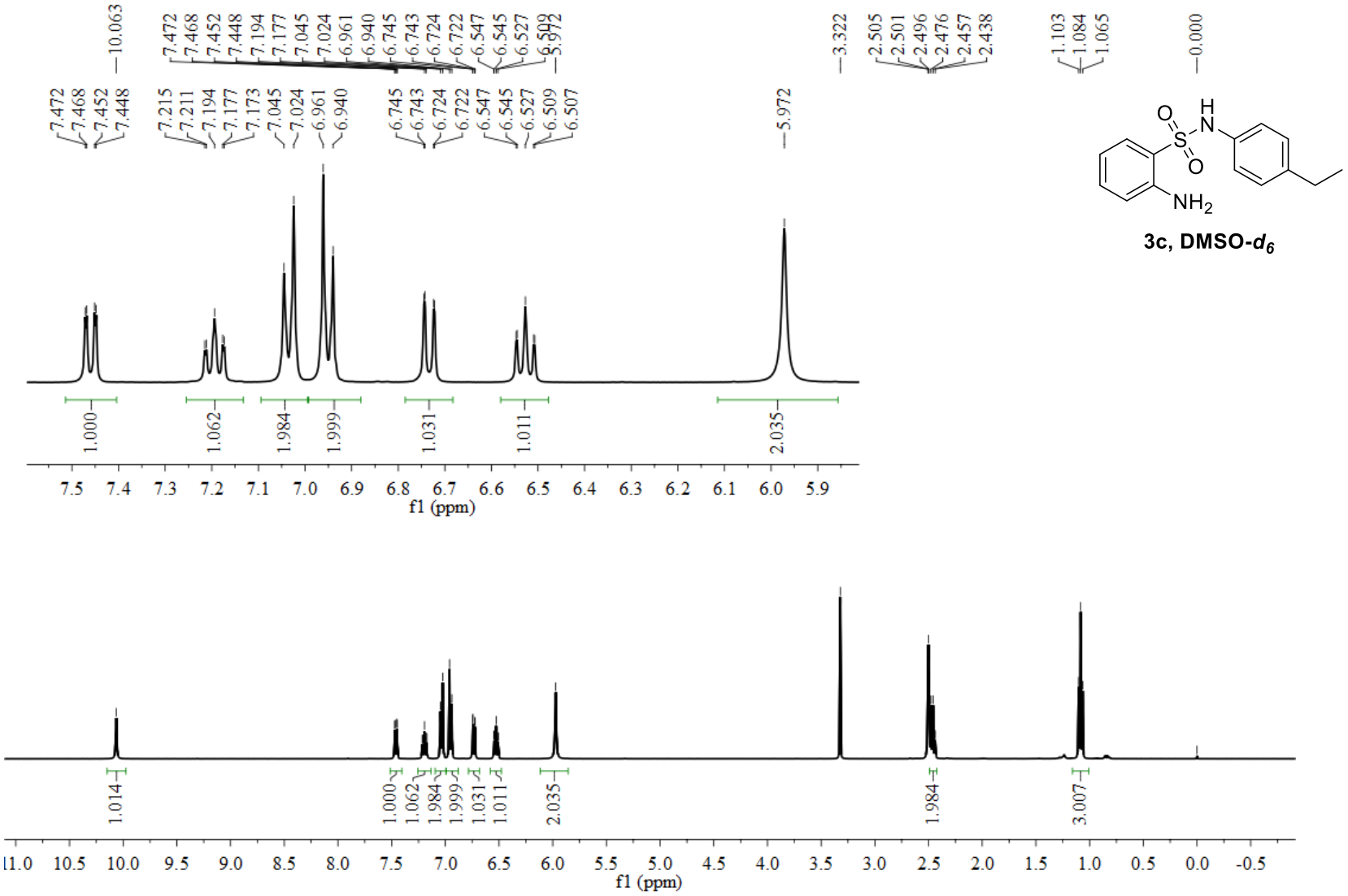
NH2
3a, DMSO-d6
145
135
125
115
110
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
f1 (ppm)

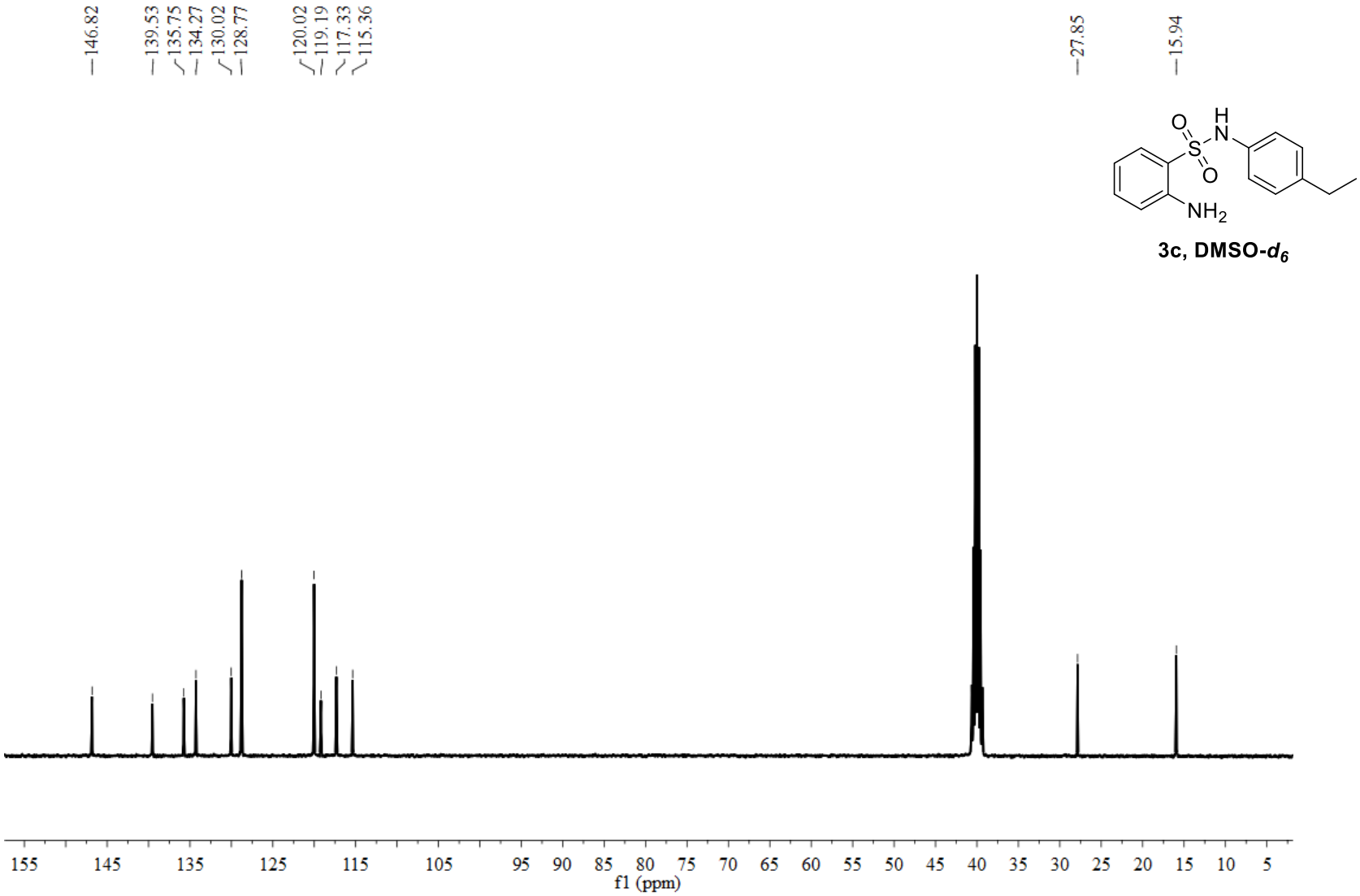

10.030
7.452
7.449
7.432
7.428
7.191
7.188
7.010
6.990
6.939
6.934
6.922
6.918
6.739
6.736
6.718
6.716
6.520
6.517
5.965
3.323
2.505
2.501
2.496
2.163
0.000
7.209
7.205
7.185
7.171
7.167
6.538
6.535
6.515
6.500
6.497
1.000
1.070
1.961
1.948
1.010
0.999
f1 (ppm)
1.011
1.997
2.931

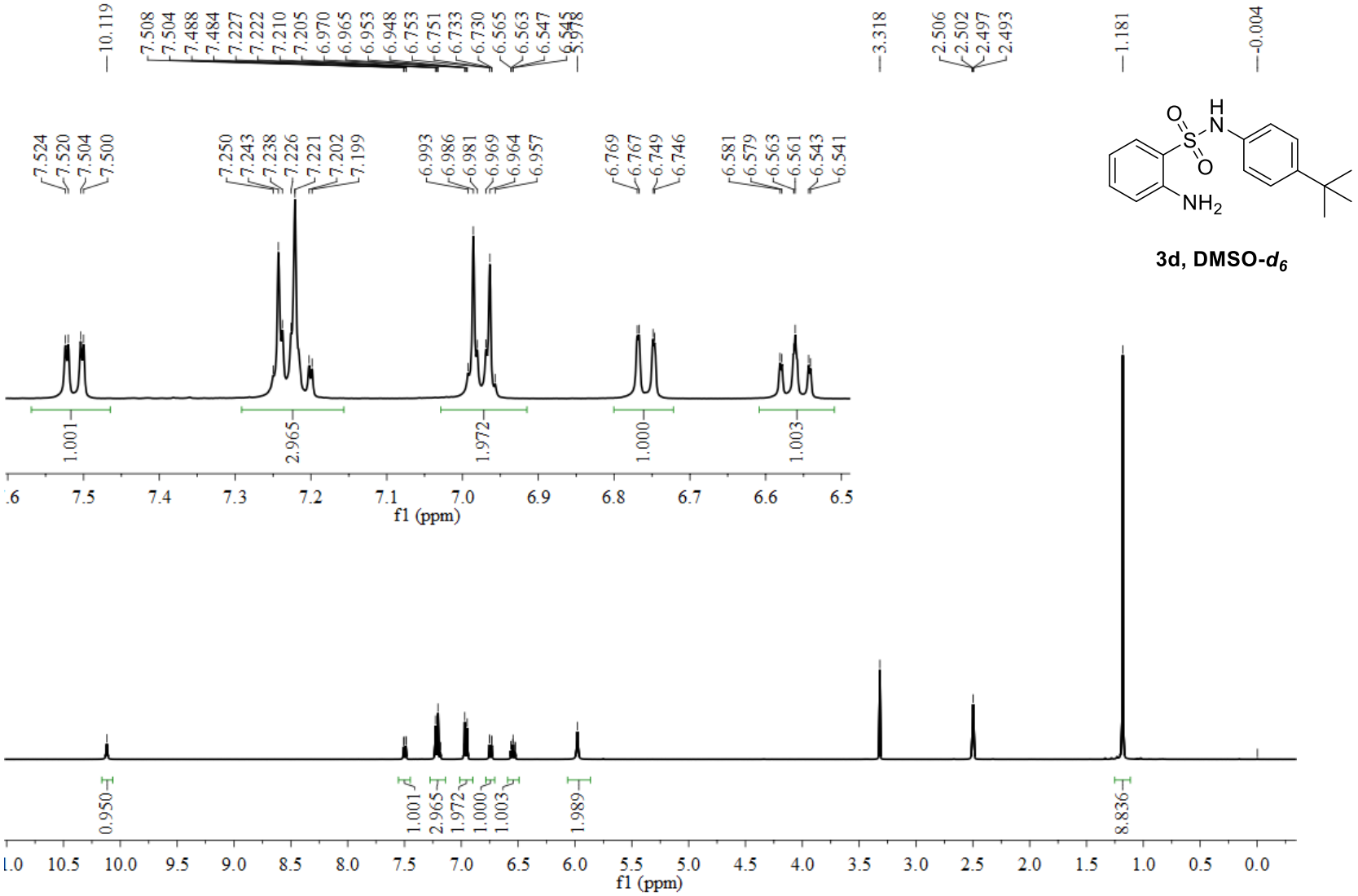
3b, DMSO-*d*$_6$


146.82
135.52
134.27
133.28
130.05
129.95
120.20
119.09
117.30
115.34
20.73
O
H
N
S
O
NH2
3b, DMSO-d6
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

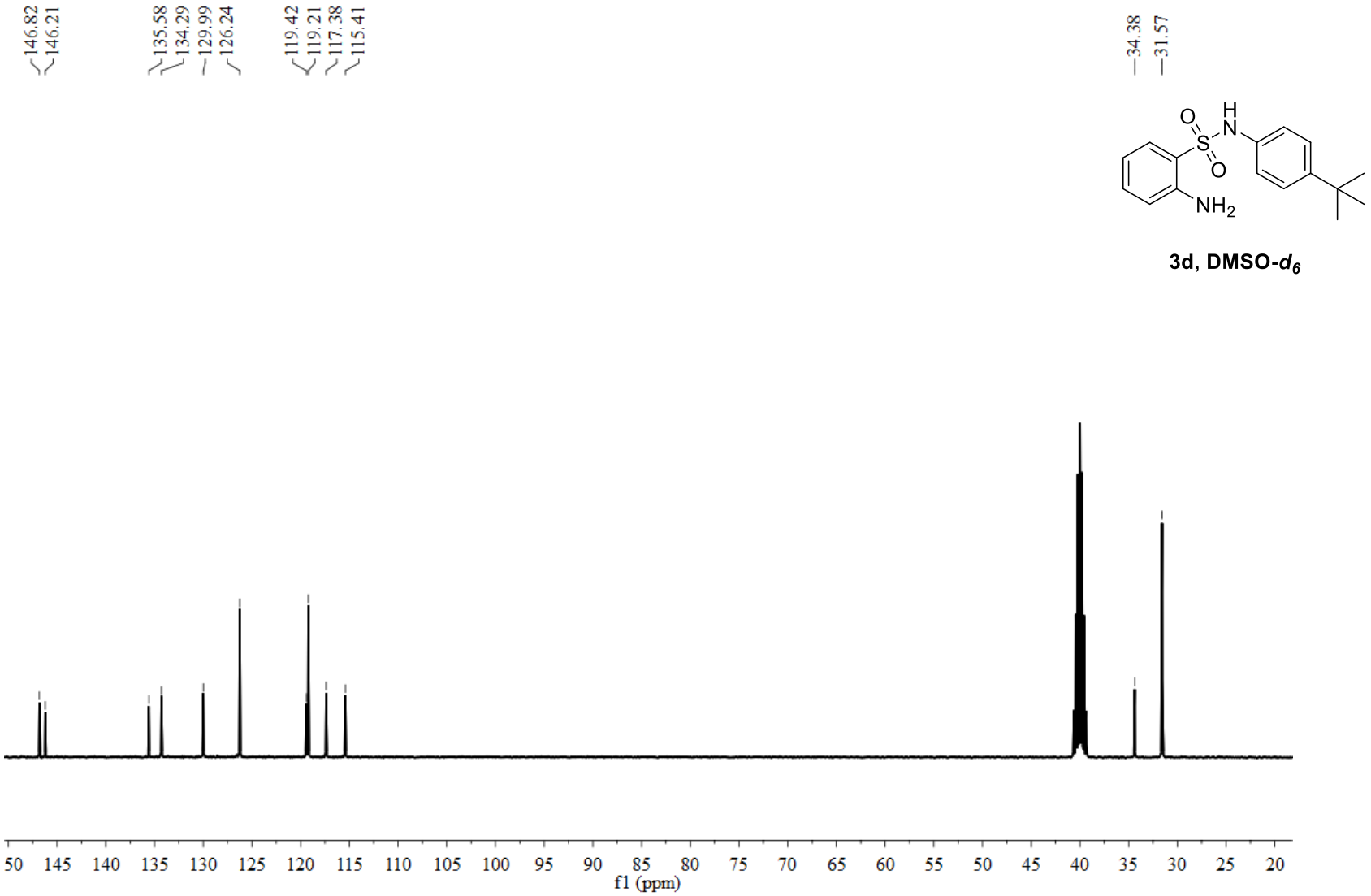

10.063
7.472
7.468
7.452
7.448
7.215
7.211
7.194
7.177
7.173
7.045
7.024
6.961
6.940
6.745
6.743
6.724
6.722
6.547
6.545
6.527
6.509
6.507
5.972
3.322
2.505
2.501
2.496
2.476
2.457
2.438
1.103
1.084
1.065
0.000
1.000
1.062
1.984
1.999
1.031
1.011
2.035
f1 (ppm)
1.014
3.007

3c, DMSO-*d*$_6$

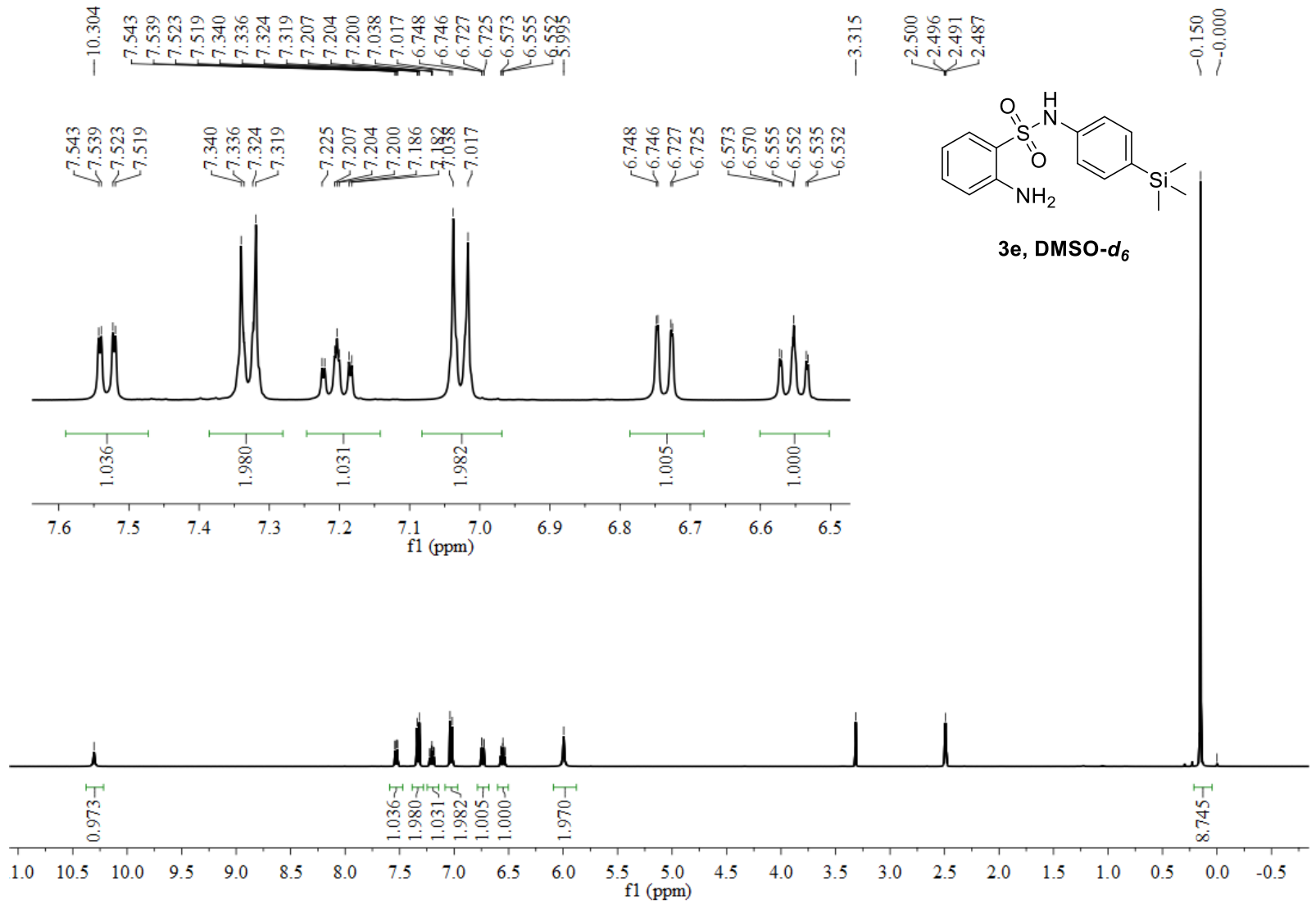

146.82
139.53
135.75
134.27
130.02
128.77
120.02
119.19
117.33
115.36
27.85
15.94
O
H
N
S
O
NH2
3c, DMSO-d6
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
f1 (ppm)


10.119
7.508
7.504
7.488
7.484
7.227
7.222
7.210
7.205
6.970
6.965
6.953
6.948
6.753
6.751
6.733
6.730
6.565
6.563
6.547
6.545
5.978
3.318
2.506
2.502
2.497
2.493
1.181
-0.004
7.524
7.520
7.504
7.500
7.250
7.243
7.238
7.226
7.221
7.202
7.199
6.993
6.986
6.981
6.969
6.964
6.957
6.769
6.767
6.749
6.746
6.581
6.579
6.563
6.561
6.543
6.541
1.001
2.965
1.972
1.000
1.003
f1 (ppm)
0.950
1.001
2.965
1.972
1.000
1.003
1.989
8.836
f1 (ppm)
O
S
O
H
N
NH2

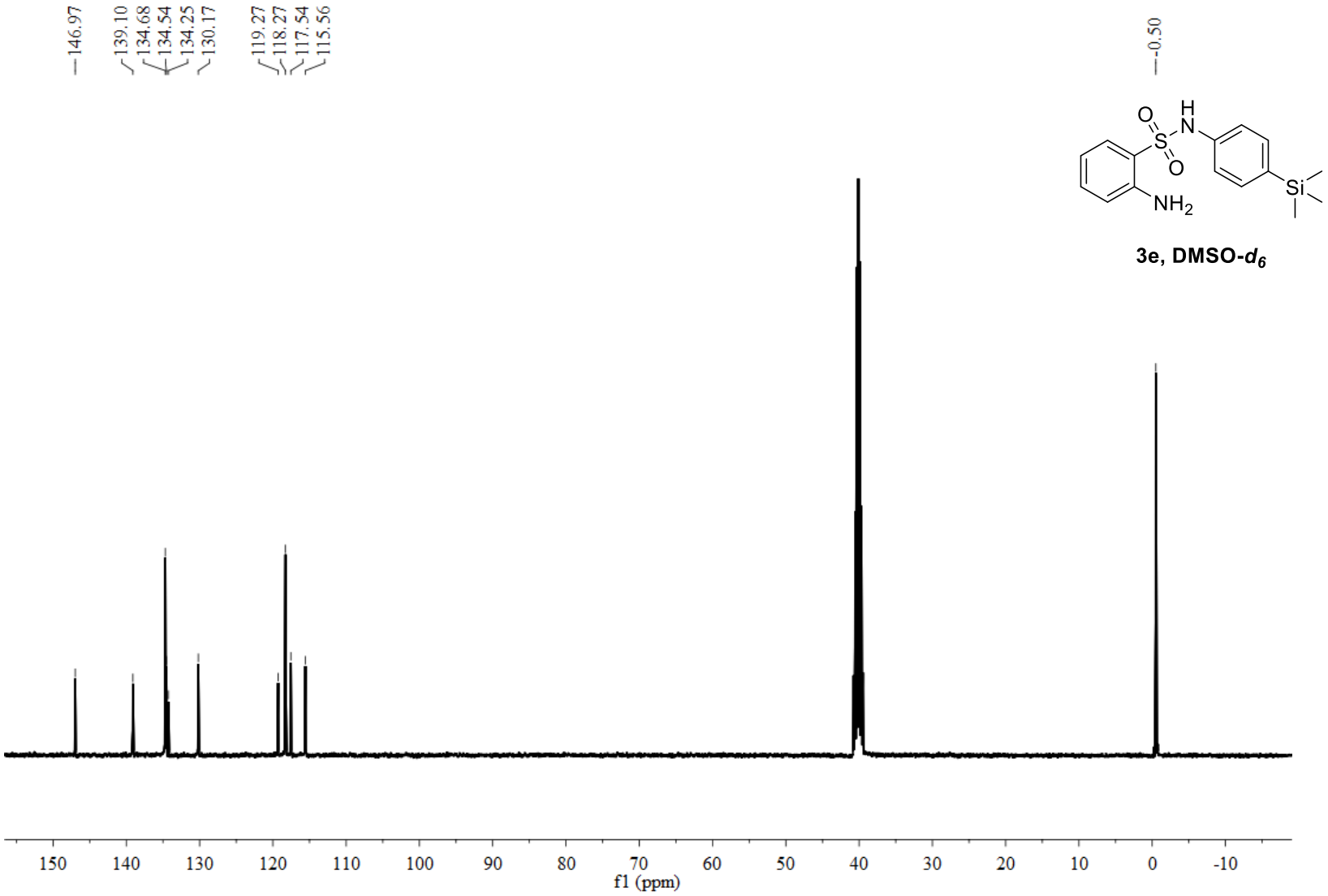
3d, DMSO-*d*$_6$

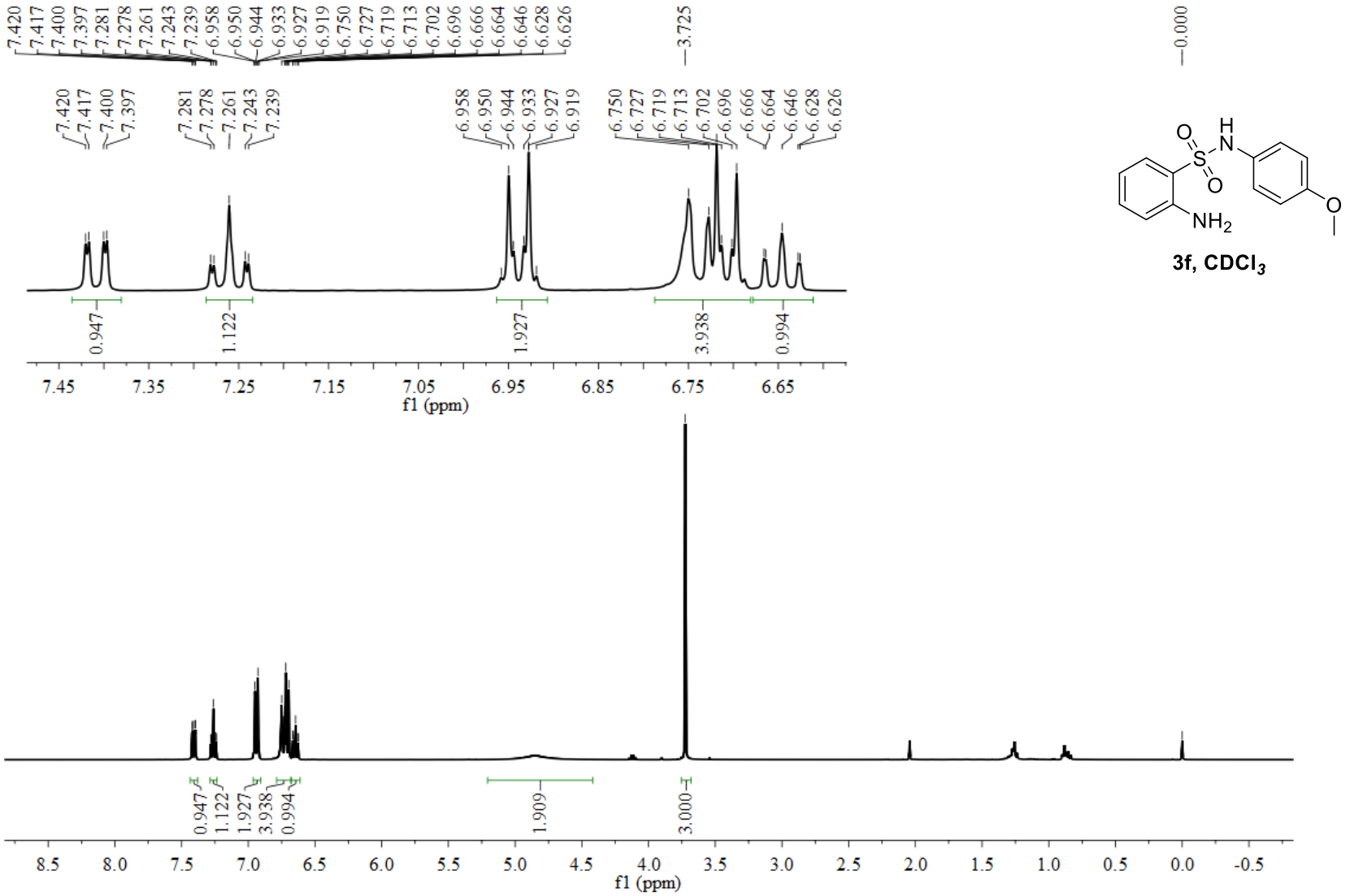

146.82
146.21
135.58
134.29
129.99
126.24
119.42
119.21
117.38
115.41
34.38
31.57
O
S
O
H
N
NH2
50 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)

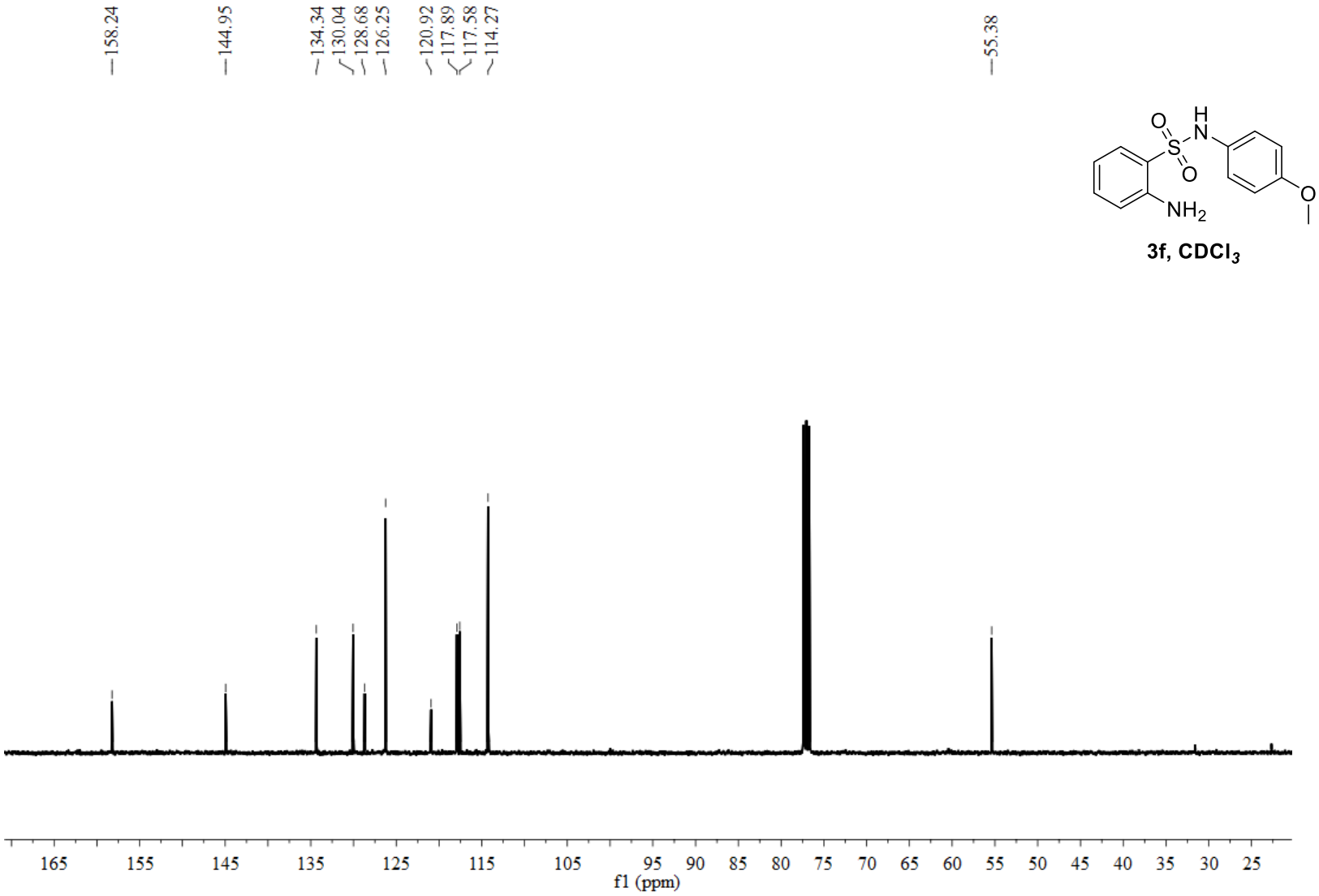
3d, DMSO-d_6

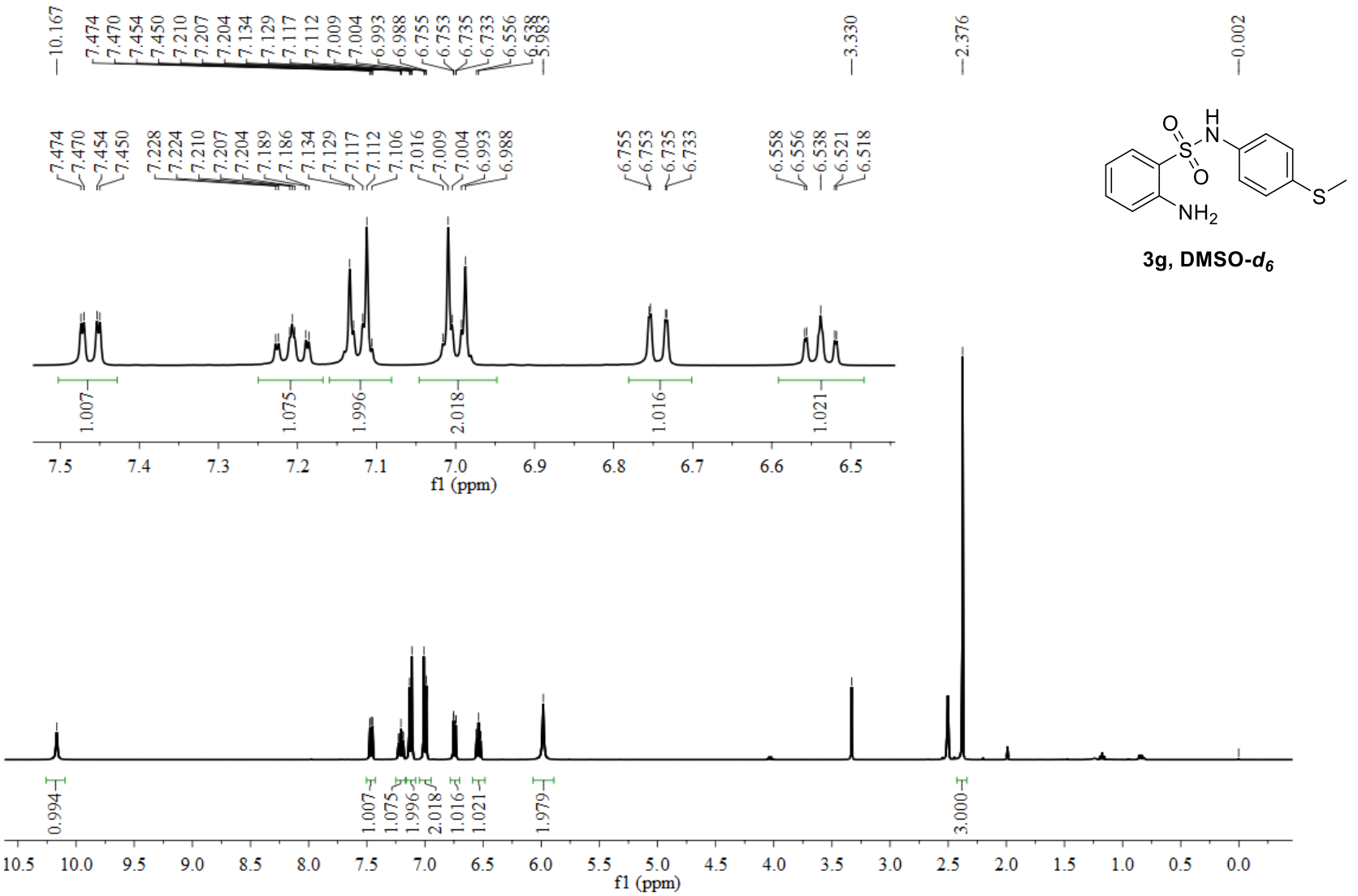

10.304
7.543
7.539
7.523
7.519
7.340
7.336
7.324
7.319
7.207
7.204
7.200
7.038
7.017
6.748
6.746
6.727
6.725
6.573
6.555
6.552
3.995
3.315
2.500
2.496
2.491
2.487
0.150
-0.000
1.036
1.980
1.031
1.982
1.005
1.000
f1 (ppm)
0.973
1.036
1.980
1.031
1.982
1.005
1.000
1.970
8.745
f1 (ppm)

3e, DMSO-d_6

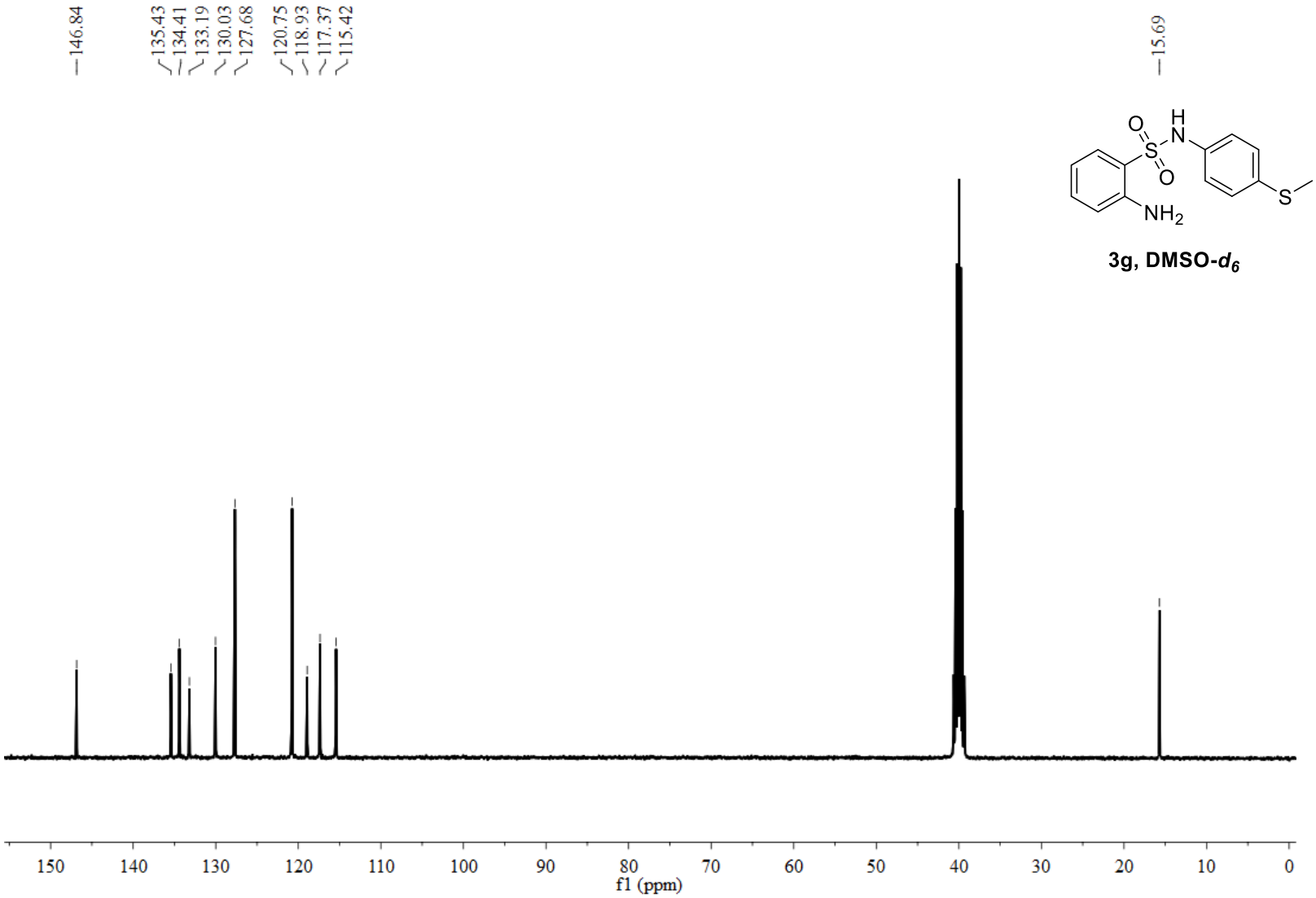

146.97
139.10
134.68
134.54
134.25
130.17
119.27
118.27
117.54
115.56
-0.50
O
H
N
S
O
NH2
Si
3e, DMSO-d6
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

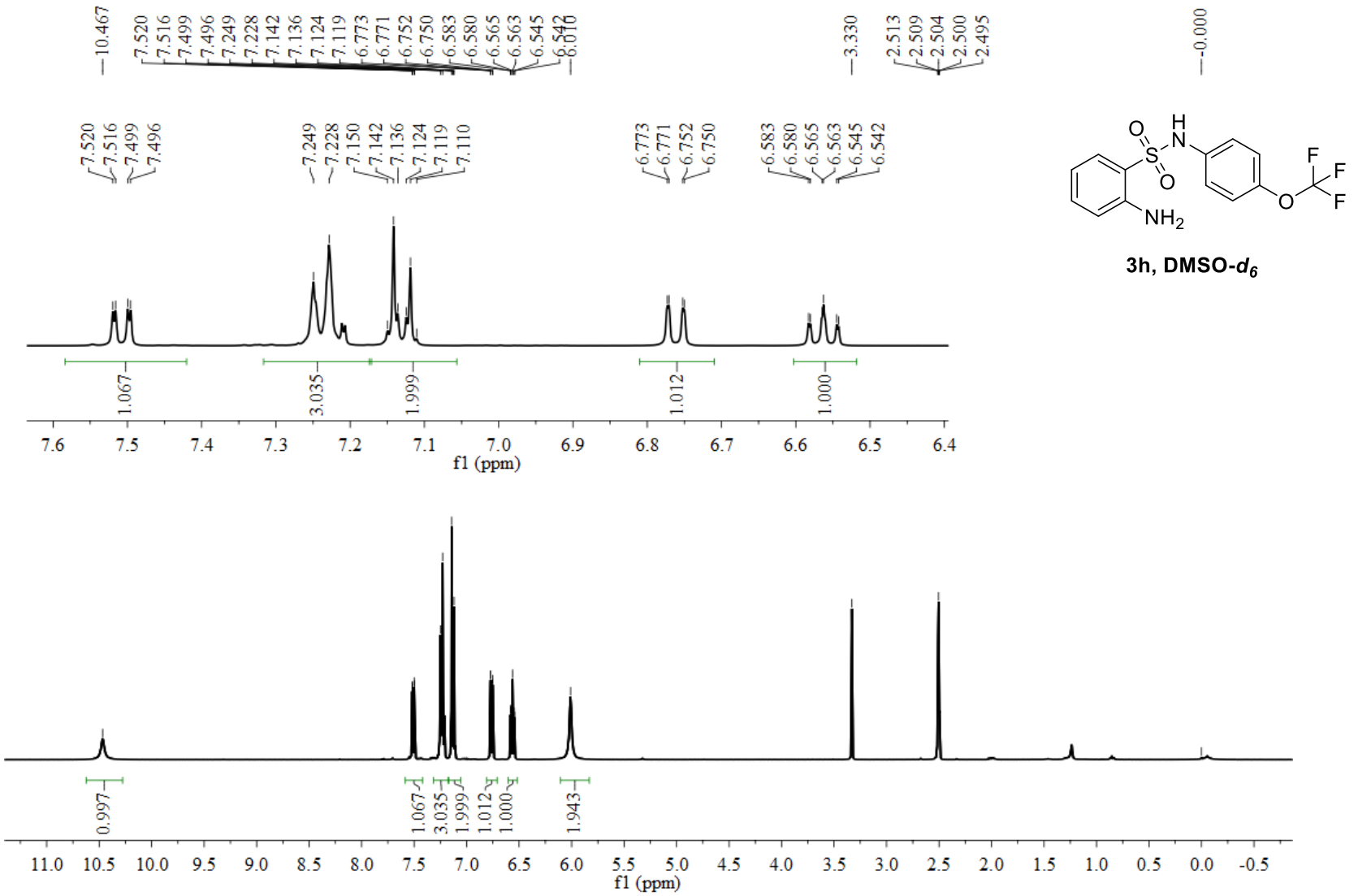

7.420
7.417
7.400
7.397
7.281
7.278
7.261
7.243
7.239
6.958
6.950
6.944
6.933
6.927
6.919
6.750
6.727
6.719
6.713
6.702
6.696
6.666
6.664
6.646
6.628
6.626
3.725
0.000
0.947
1.122
1.927
3.938
0.994
1.909
3.000
f1 (ppm)
3f, CDCl3


158.24
144.95
134.34
130.04
128.68
126.25
120.92
117.89
117.58
114.27
55.38
O
H
N
S
O
O
NH2
O
3f, CDCl3
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
f1 (ppm)

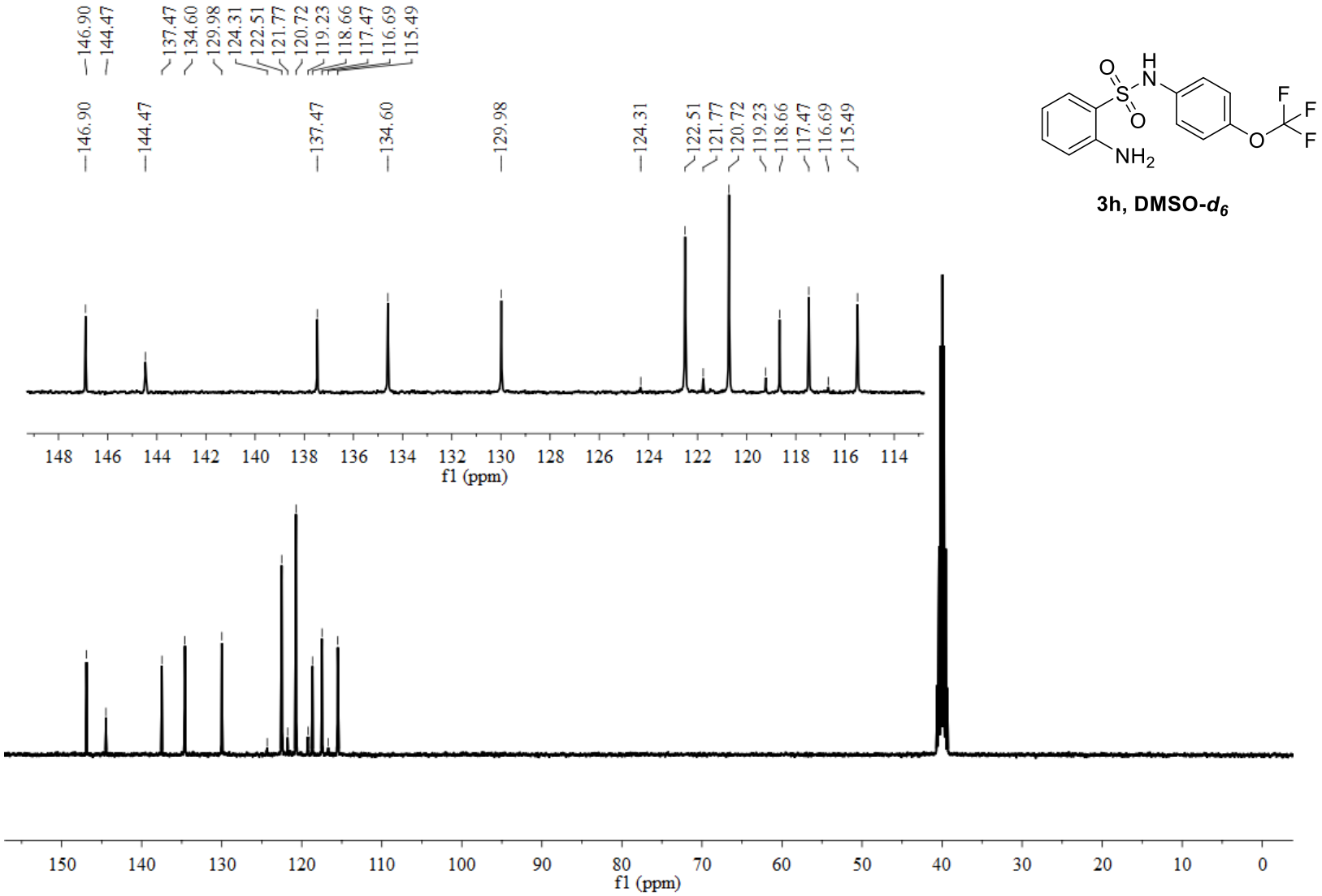

10.167
7.474
7.470
7.454
7.450
7.210
7.207
7.204
7.134
7.129
7.117
7.112
7.009
7.004
6.993
6.988
6.755
6.753
6.735
6.733
6.556
6.538
3.983
3.330
2.376
0.002
7.228
7.224
7.189
7.186
7.106
7.016
6.558
6.521
6.518
1.007
1.075
1.996
2.018
1.016
1.021
0.994
1.979
3.000
f1 (ppm)
NH2

3g, DMSO-d_6

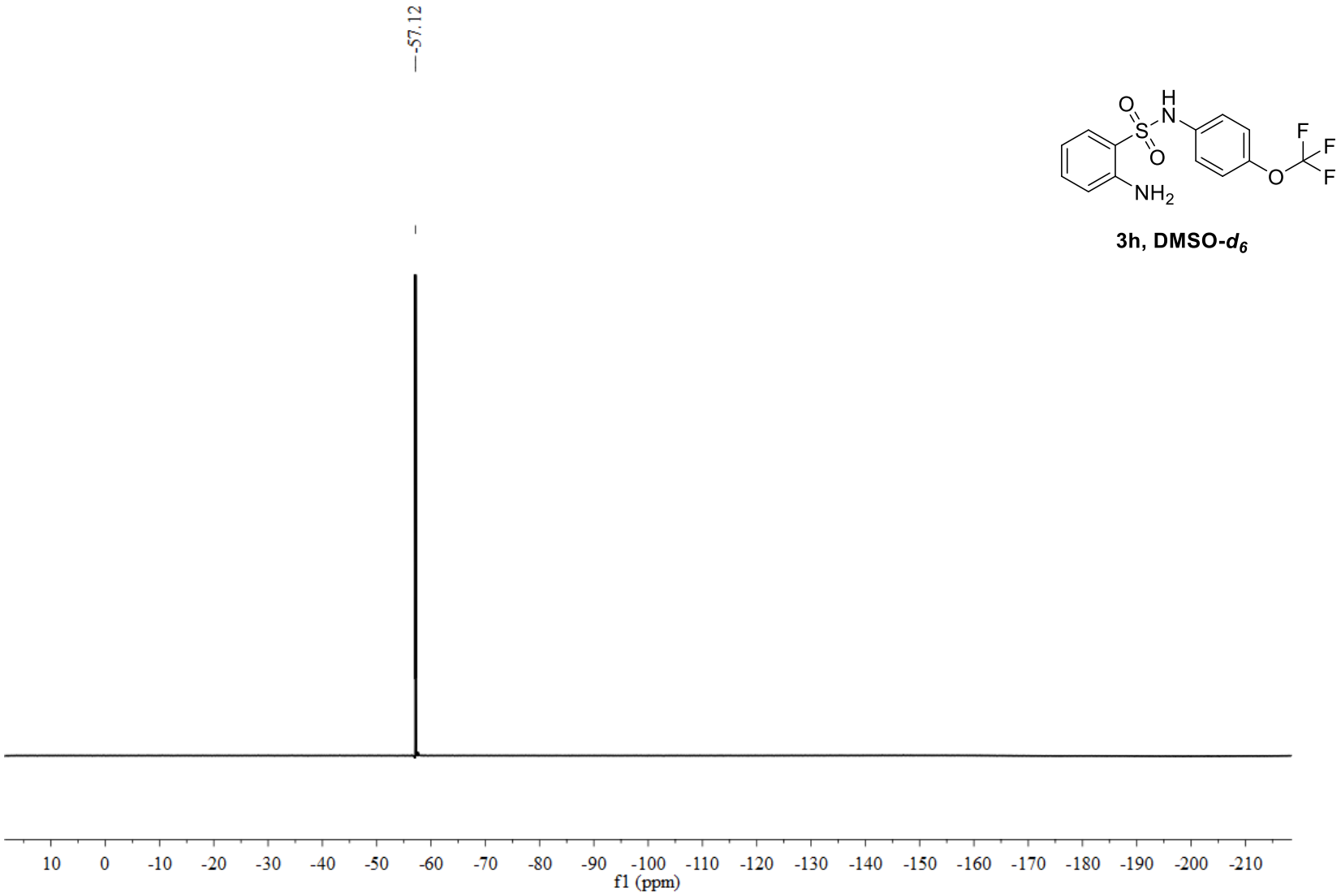

146.84
135.43
134.41
133.19
130.03
127.68
120.75
118.93
117.37
115.42
15.69
O
H
N
S
O
NH2
S
3g, DMSO-d6
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.467
7.520
7.516
7.499
7.496
7.249
7.228
7.142
7.136
7.124
7.119
6.773
6.771
6.752
6.750
6.583
6.580
6.565
6.563
6.545
6.542
6.010
3.330
2.513
2.509
2.504
2.500
2.495
-0.000
1.067
3.035
1.999
1.012
1.000
f1 (ppm)
0.997
1.067
3.035
1.999
1.012
1.000
1.943
f1 (ppm)

3h, DMSO-*d*$_6$

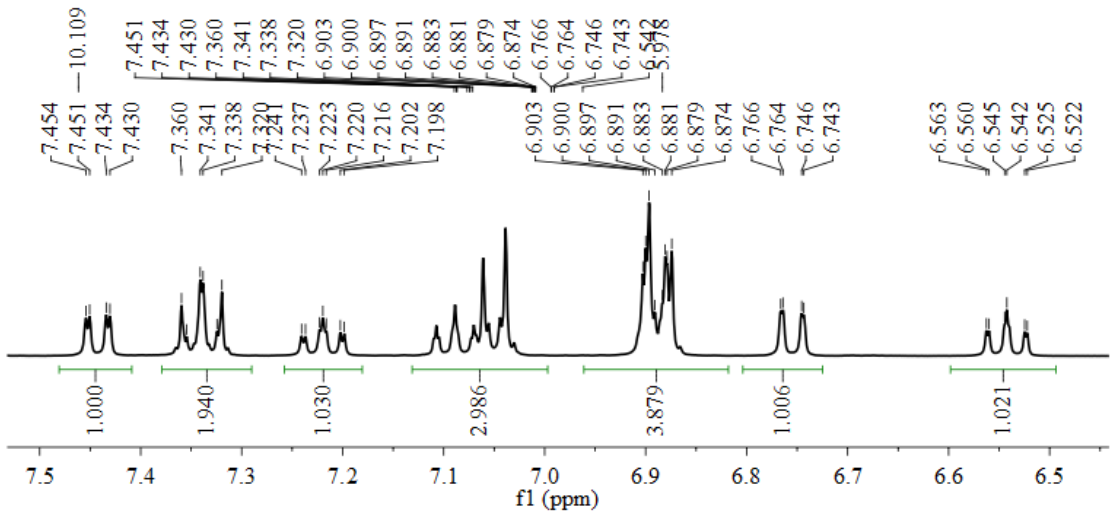

146.90
144.47
137.47
134.60
129.98
124.31
122.51
121.77
120.72
119.23
118.66
117.47
116.69
115.49
148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114
f1 (ppm)
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
O
S
O
H
N
NH2
F
F
F
O

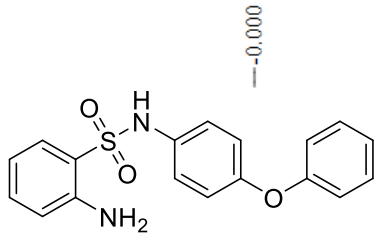
3h, DMSO-d_6


-57.12
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

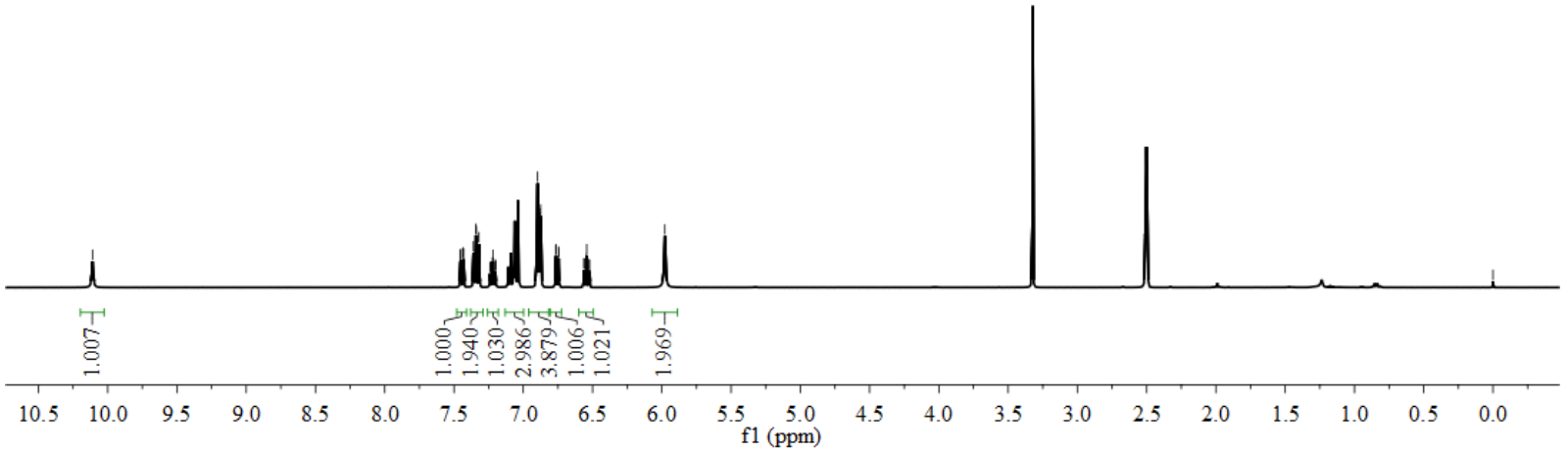
O
H
N
S
O
F
F
F
O
NH2

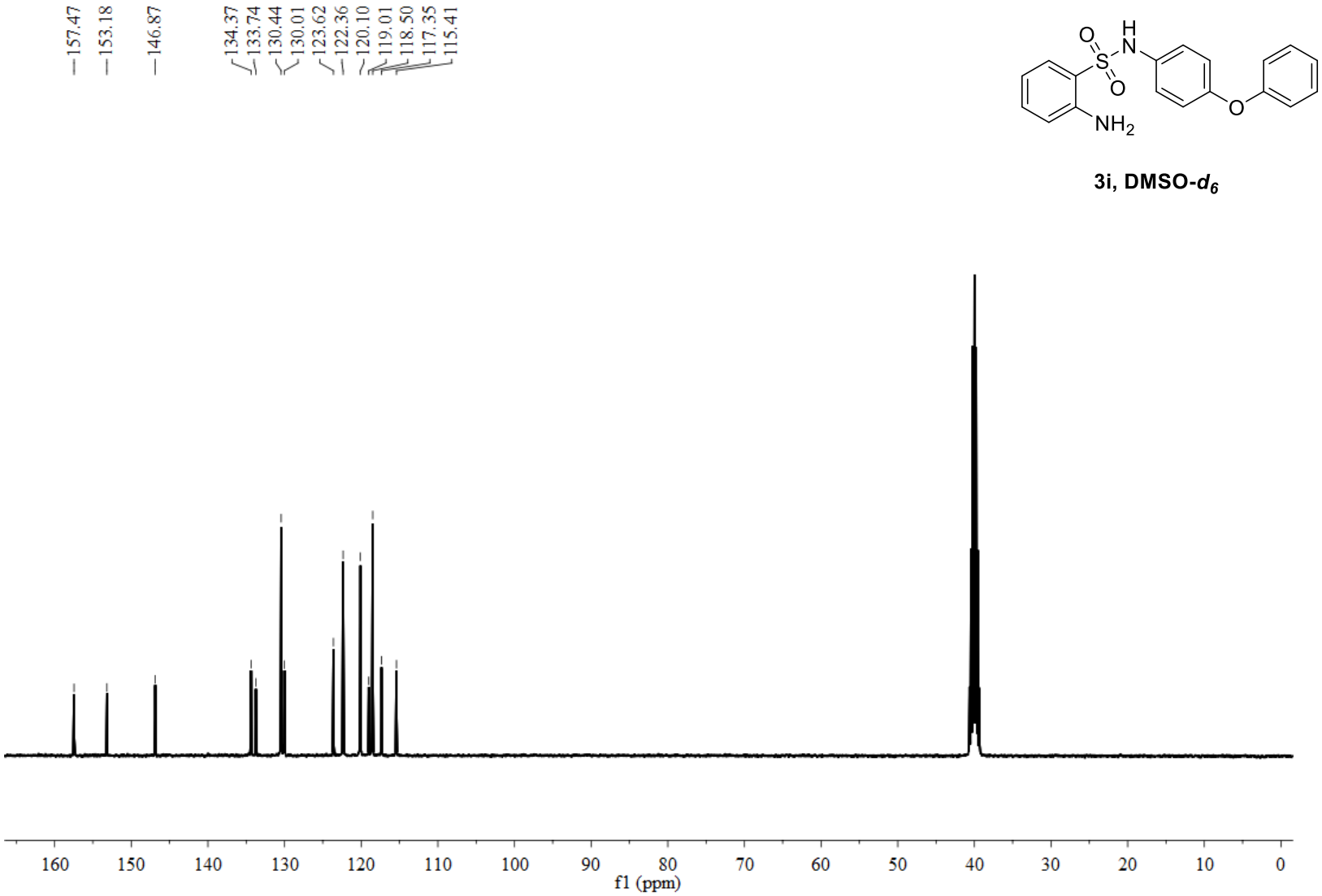
3h, DMSO-d_6


10.109
7.451
7.434
7.430
7.360
7.341
7.338
7.320
6.903
6.900
6.897
6.891
6.883
6.881
6.879
6.874
6.766
6.764
6.746
6.743
5.978
7.454
7.451
7.434
7.430
7.360
7.341
7.338
7.320
7.241
7.237
7.223
7.220
7.216
7.202
7.198
6.903
6.900
6.897
6.891
6.883
6.881
6.879
6.874
6.766
6.764
6.746
6.743
6.563
6.560
6.545
6.542
6.525
6.522
1.000
1.940
1.030
2.986
3.879
1.006
1.021
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
f1 (ppm)

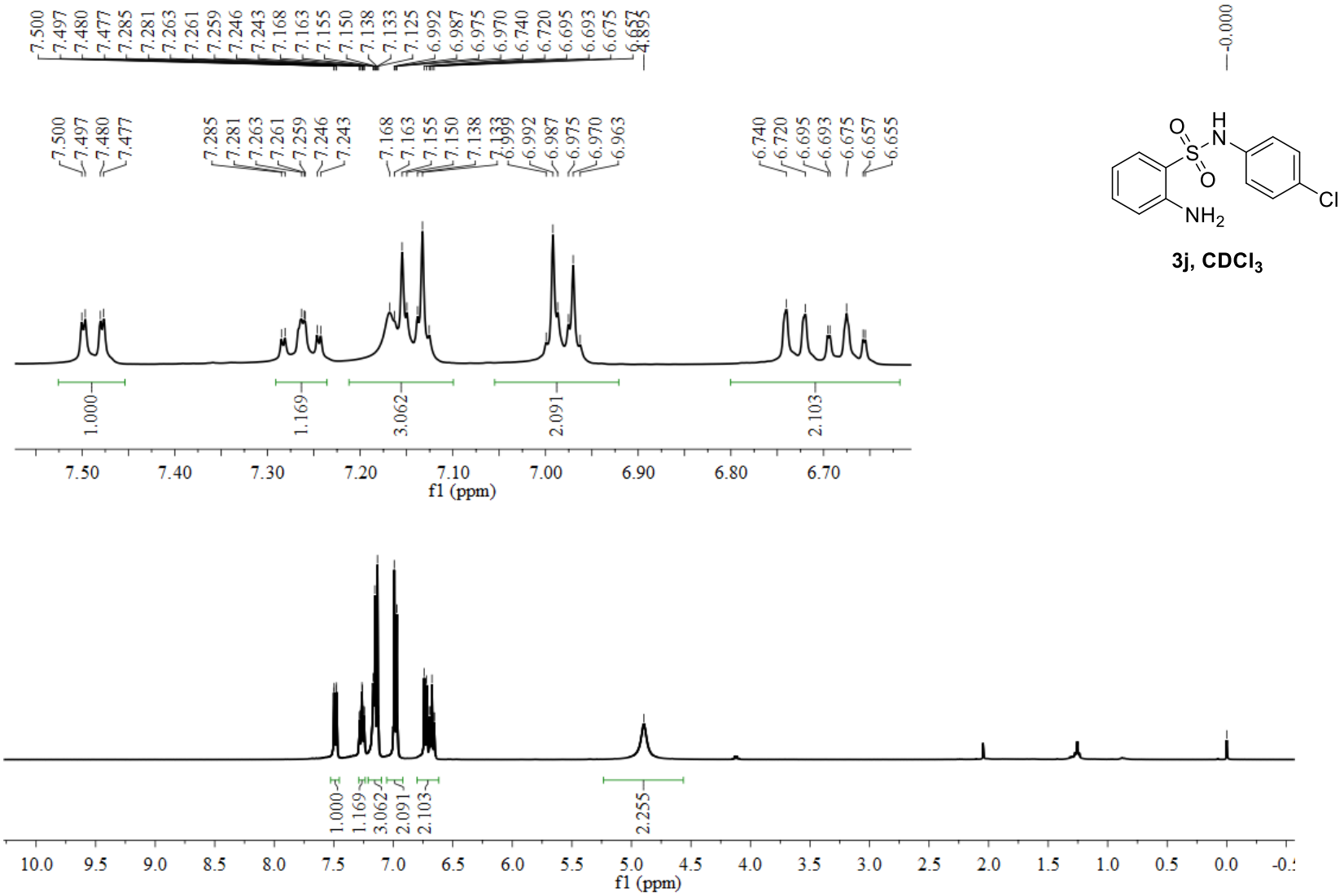

0.000
O
H
N
S
O
NH2
O

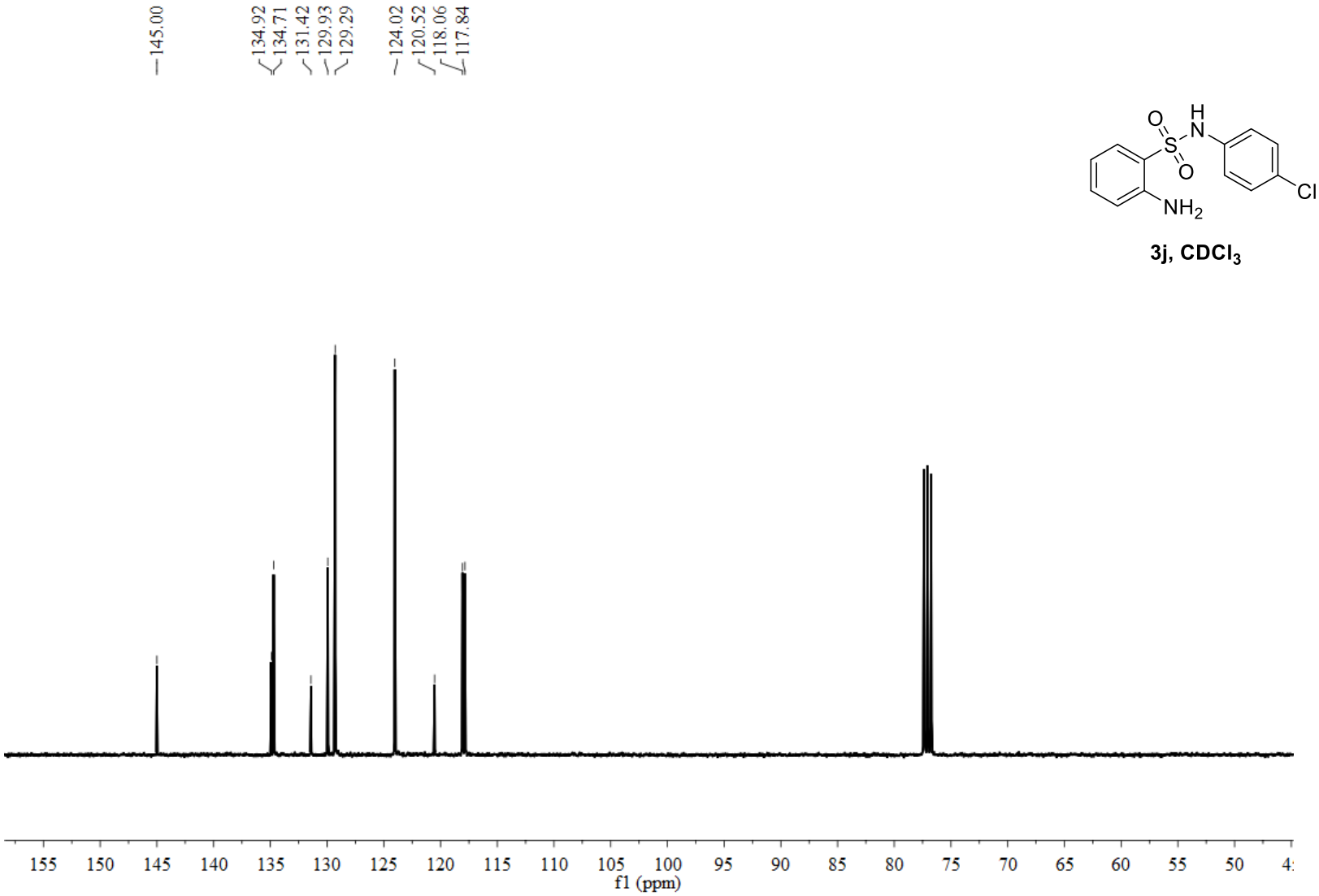
3i, DMSO-*d*$_6$


1.007
1.000
1.940
1.030
2.986
3.879
1.006
1.021
1.969
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

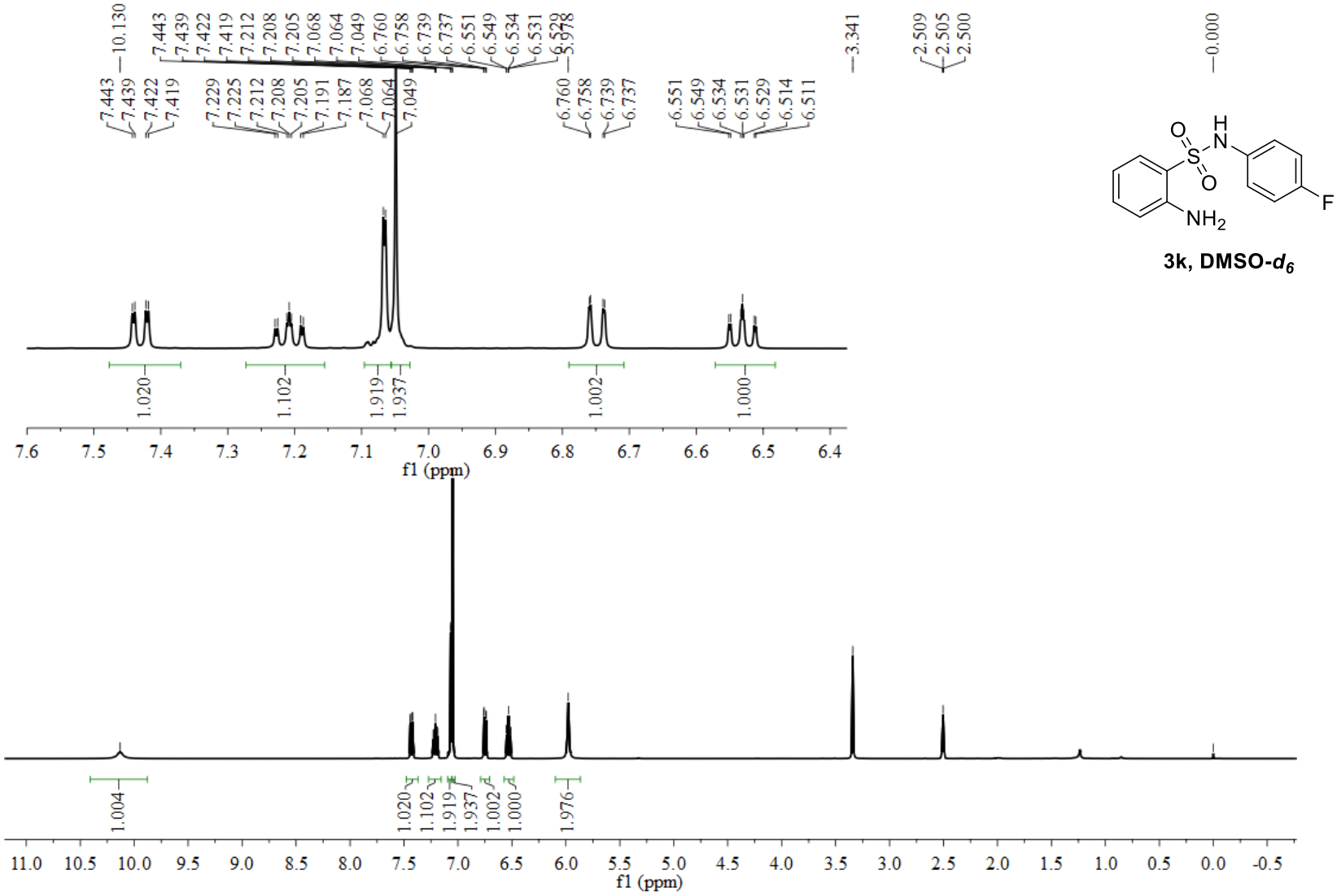

157.47
153.18
146.87
134.37
133.74
130.44
130.01
123.62
122.36
120.10
119.01
118.50
117.35
115.41
O
S
O
H
N
NH2
O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3i, DMSO-d_6

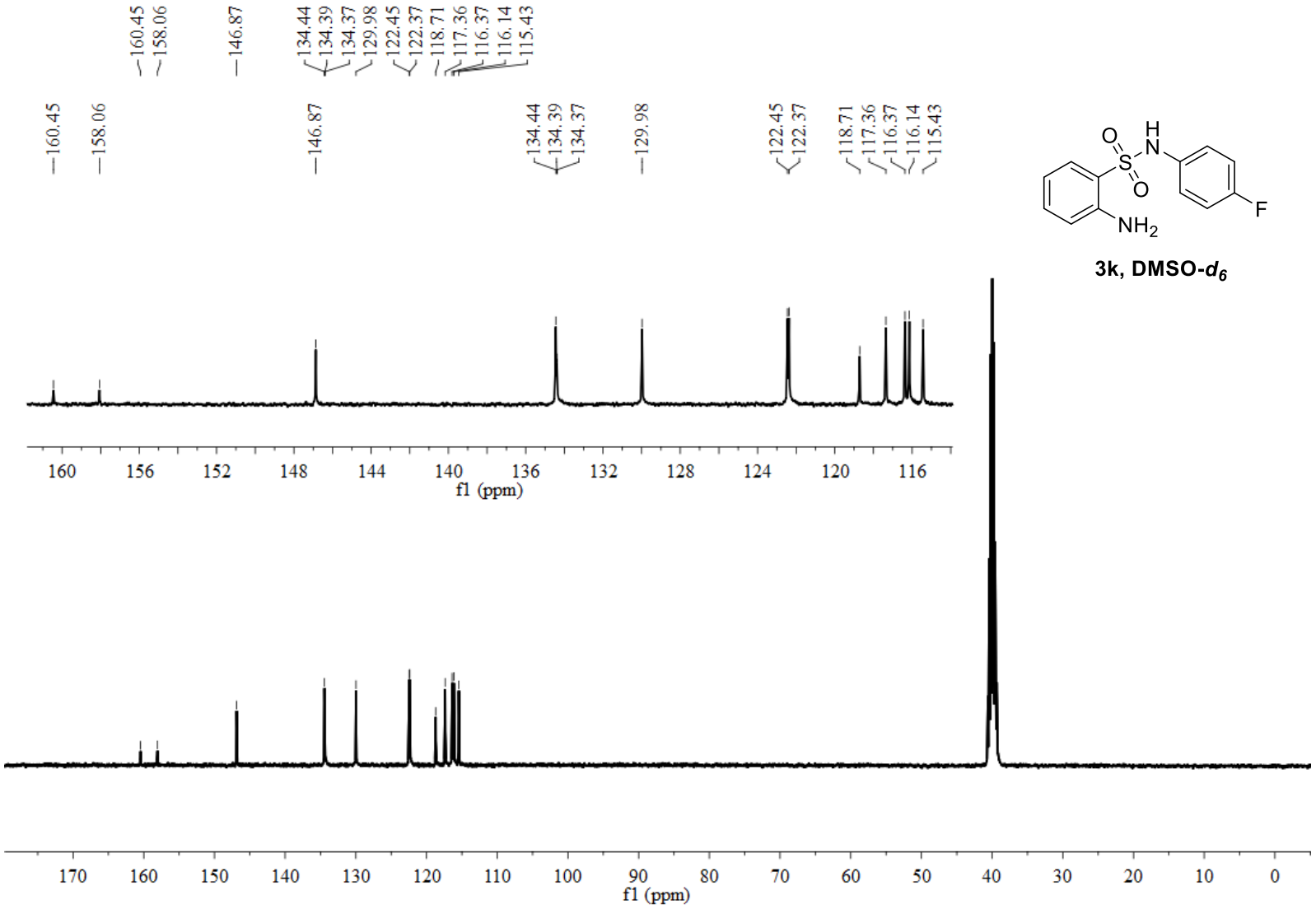

7.500
7.497
7.480
7.477
7.285
7.281
7.263
7.261
7.259
7.246
7.243
7.168
7.163
7.155
7.150
7.138
7.133
7.125
6.992
6.987
6.975
6.970
6.740
6.720
6.695
6.693
6.675
6.657
6.655
4.893
-0.000
1.000
1.169
3.062
2.091
2.103
2.255
f1 (ppm)
3j, CDCl3


145.00
134.92
134.71
131.42
129.93
129.29
124.02
120.52
118.06
117.84
O
H
N
S
O
Cl
NH2
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50
f1 (ppm)

3j, $CDCl_3$

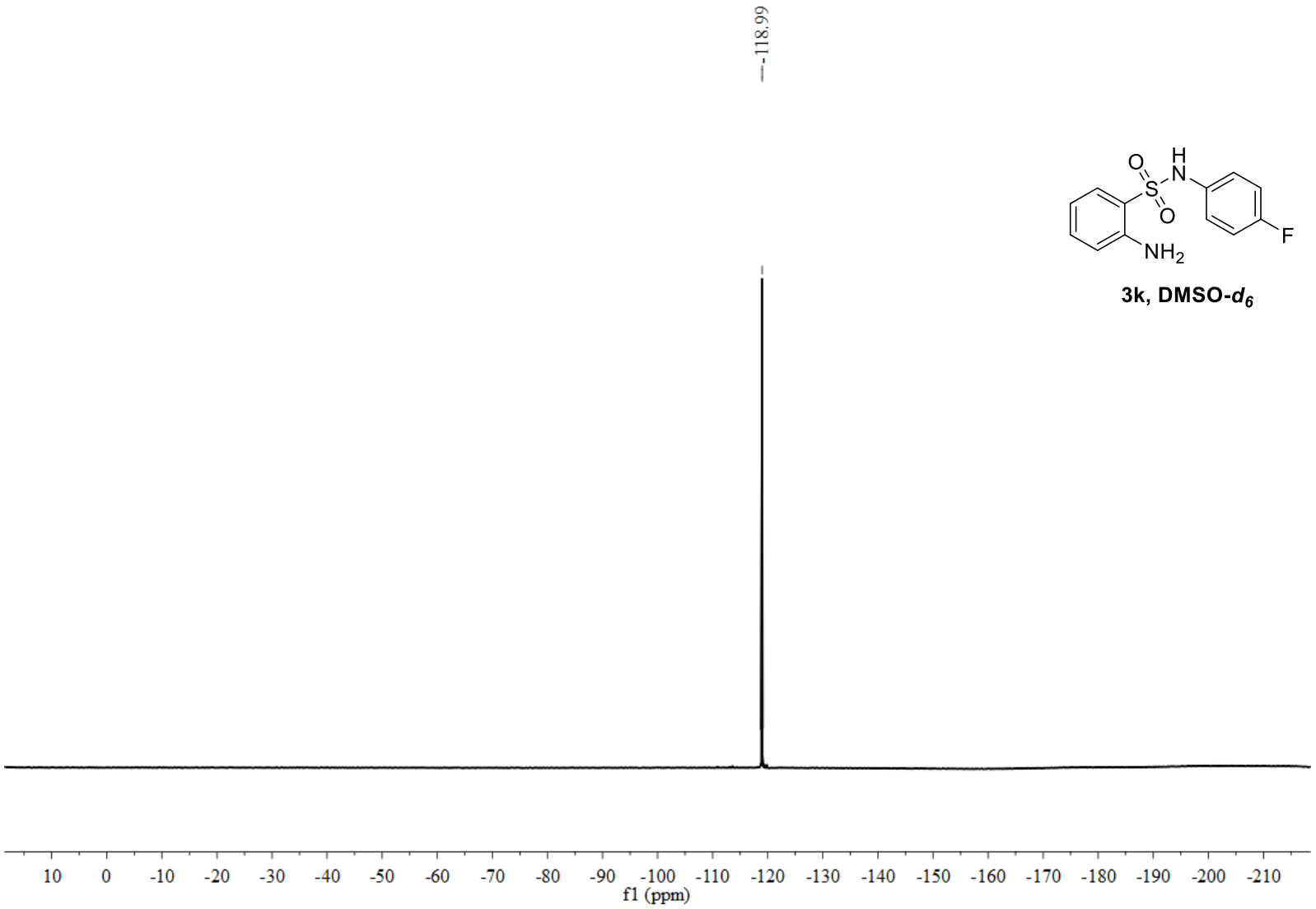

10.130
7.443
7.439
7.422
7.419
7.212
7.208
7.205
7.068
7.064
7.049
6.760
6.758
6.739
6.737
6.551
6.549
6.534
6.531
6.529
5.978
3.341
2.509
2.505
2.500
0.000
7.443
7.439
7.422
7.419
7.229
7.225
7.212
7.208
7.205
7.191
7.187
7.068
7.064
7.049
6.760
6.758
6.739
6.737
6.551
6.549
6.534
6.531
6.529
6.514
6.511
1.020
1.102
1.919
1.937
1.002
1.000
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4
f1 (ppm)
1.004
1.020
1.102
1.919
1.937
1.002
1.000
1.976
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
O
S
O
H
N
NH2
F

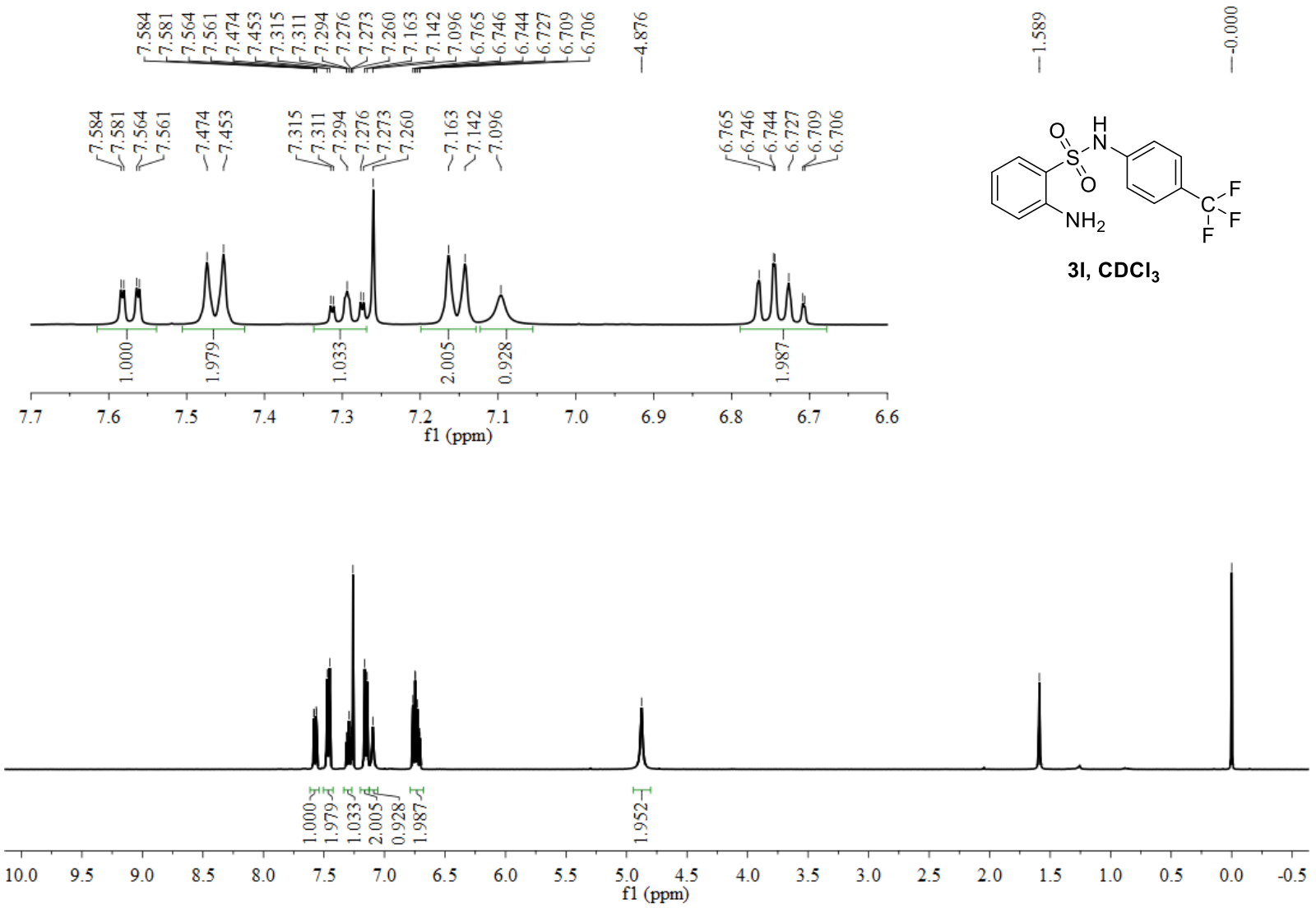
3k, DMSO-d_6

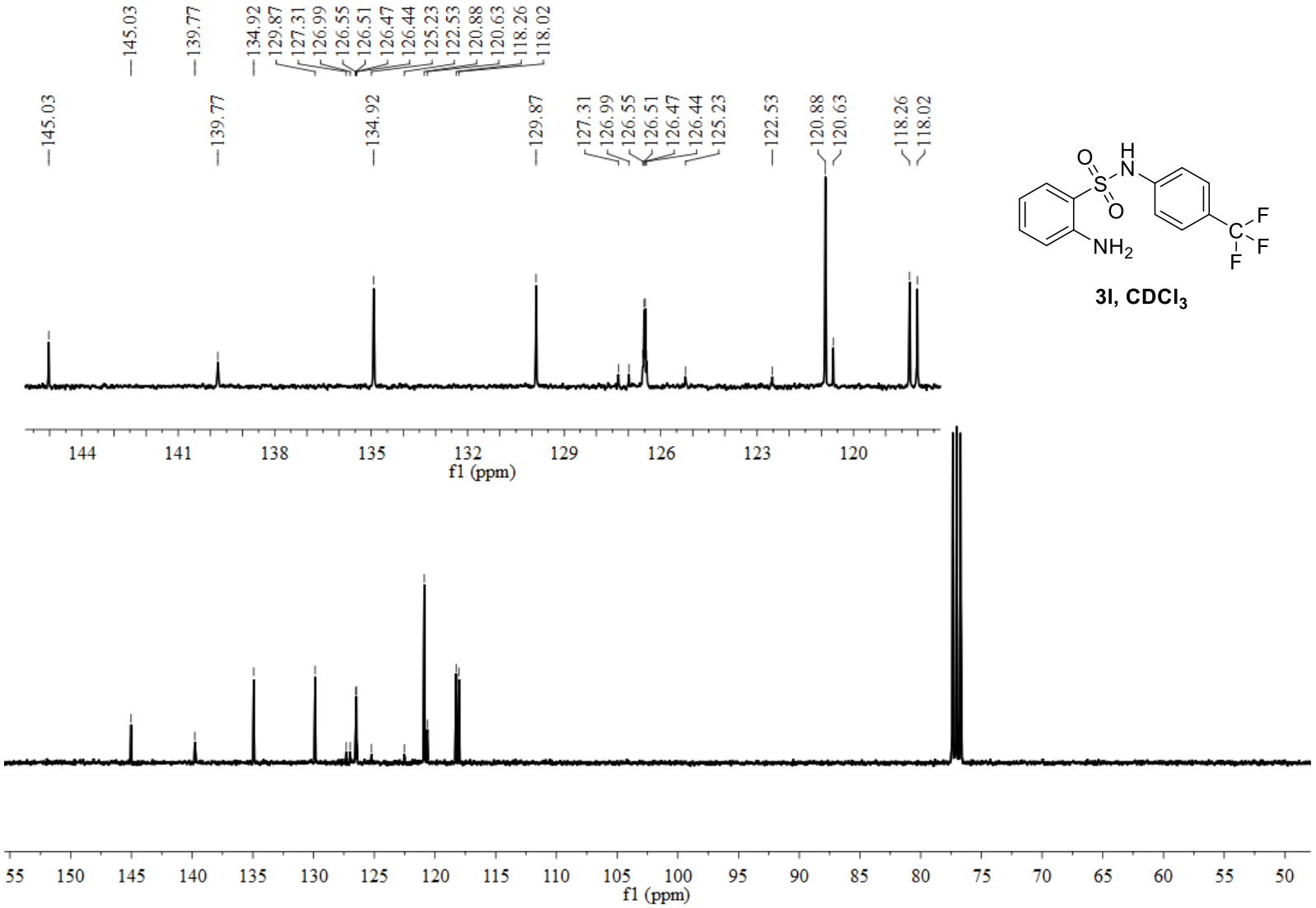

160.45
158.06
146.87
134.44
134.39
134.37
129.98
122.45
122.37
118.71
117.36
116.37
116.14
115.43
f1 (ppm)
f1 (ppm)

O
S
O
H
N
NH2
F

3k, DMSO-*d*$_6$

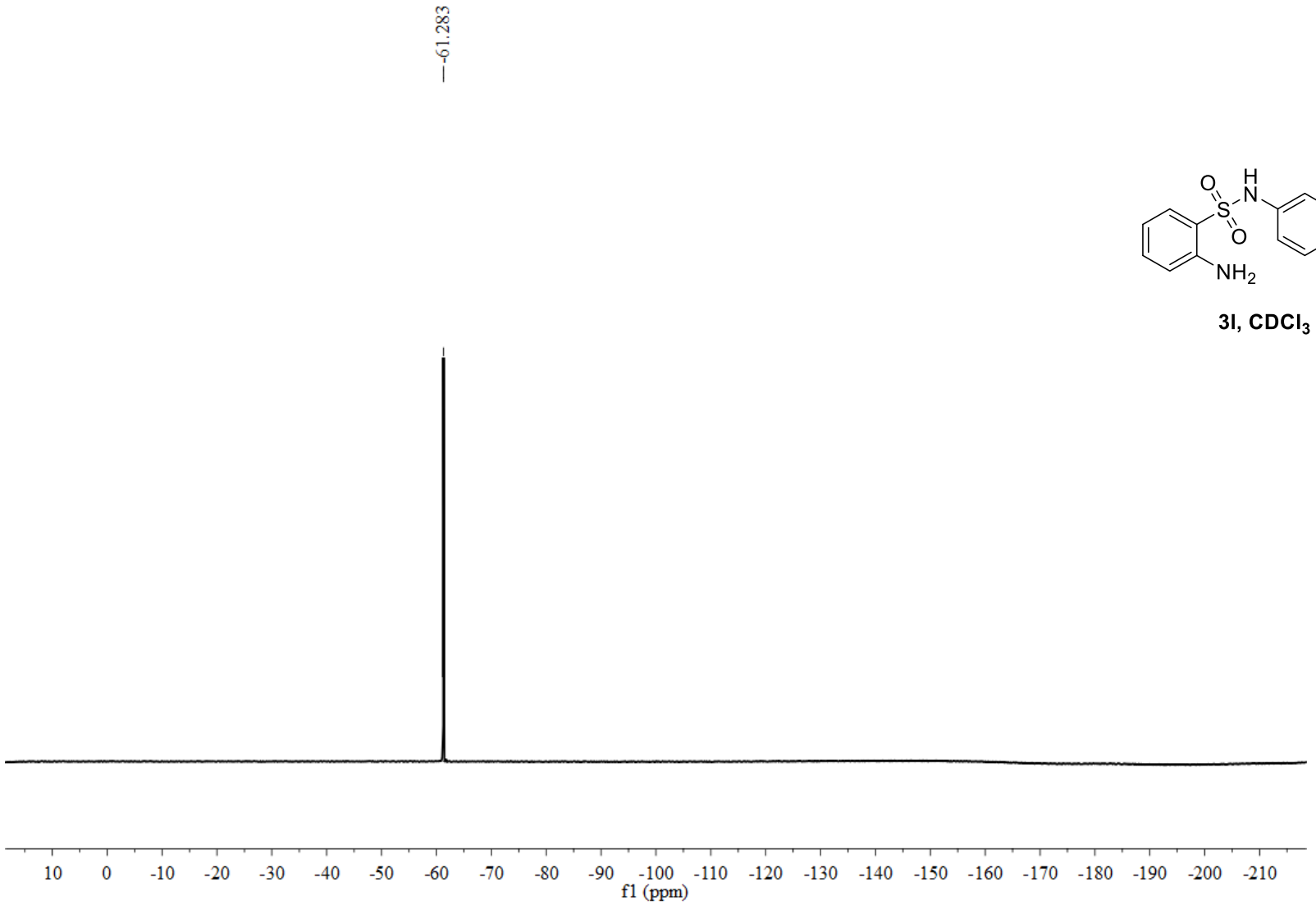

-118.99
O
H
N
S
O
NH2
F
3k, DMSO-d6
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


7.584
7.581
7.564
7.561
7.474
7.453
7.315
7.311
7.294
7.276
7.273
7.260
7.163
7.142
7.096
6.765
6.746
6.744
6.727
6.709
6.706
4.876
1.589
0.000
1.000
1.979
1.033
2.005
0.928
1.987
1.952
f1 (ppm)
3l, CDCl3


145.03
139.77
134.92
129.87
127.31
126.99
126.55
126.51
126.47
126.44
125.23
122.53
120.88
120.63
118.26
118.02
144
141
138
135
132
129
126
123
120
f1 (ppm)
55
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
f1 (ppm)

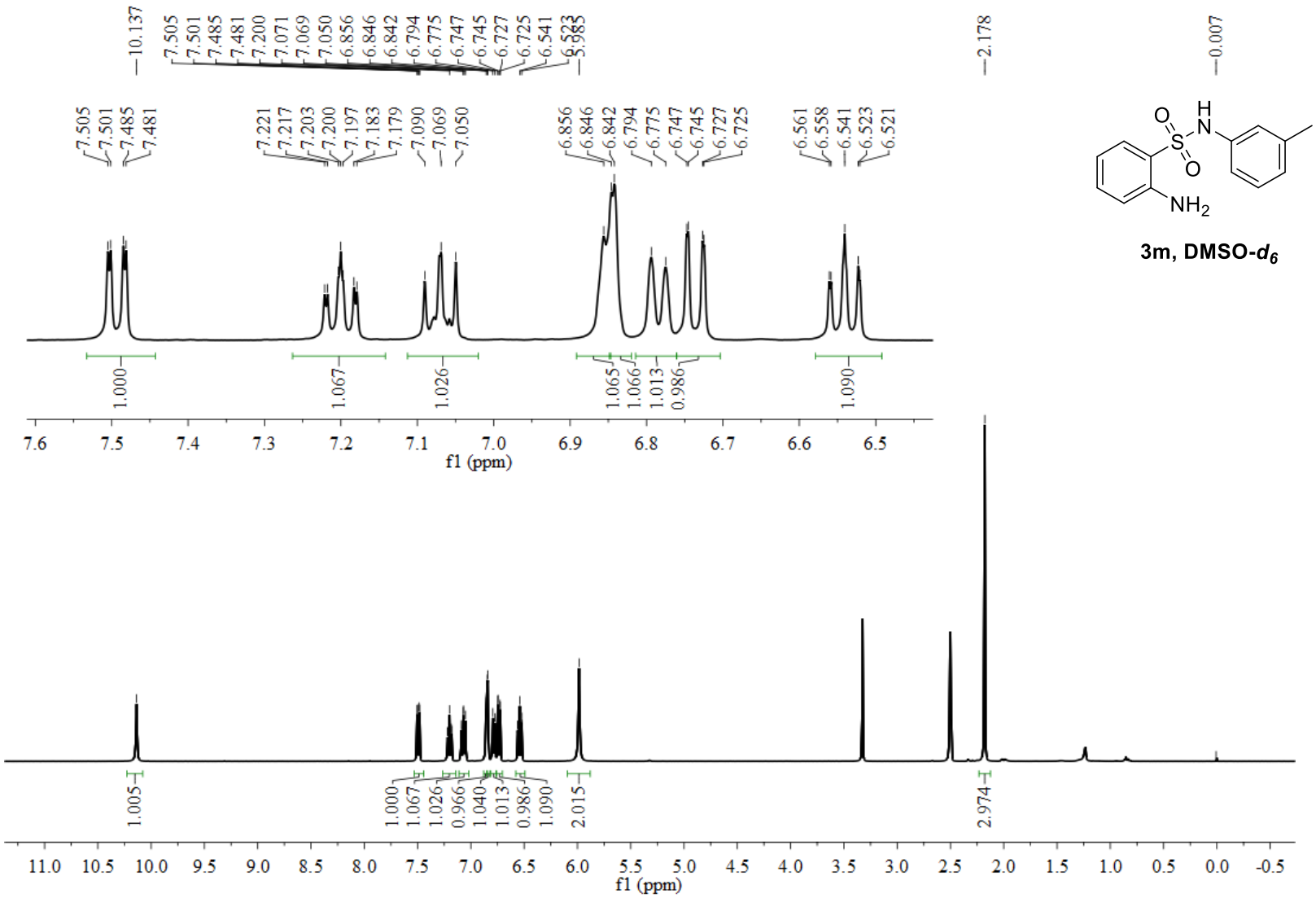
O
H
N
S
O
NH2
C
F
F
F

3l, $CDCl_3$

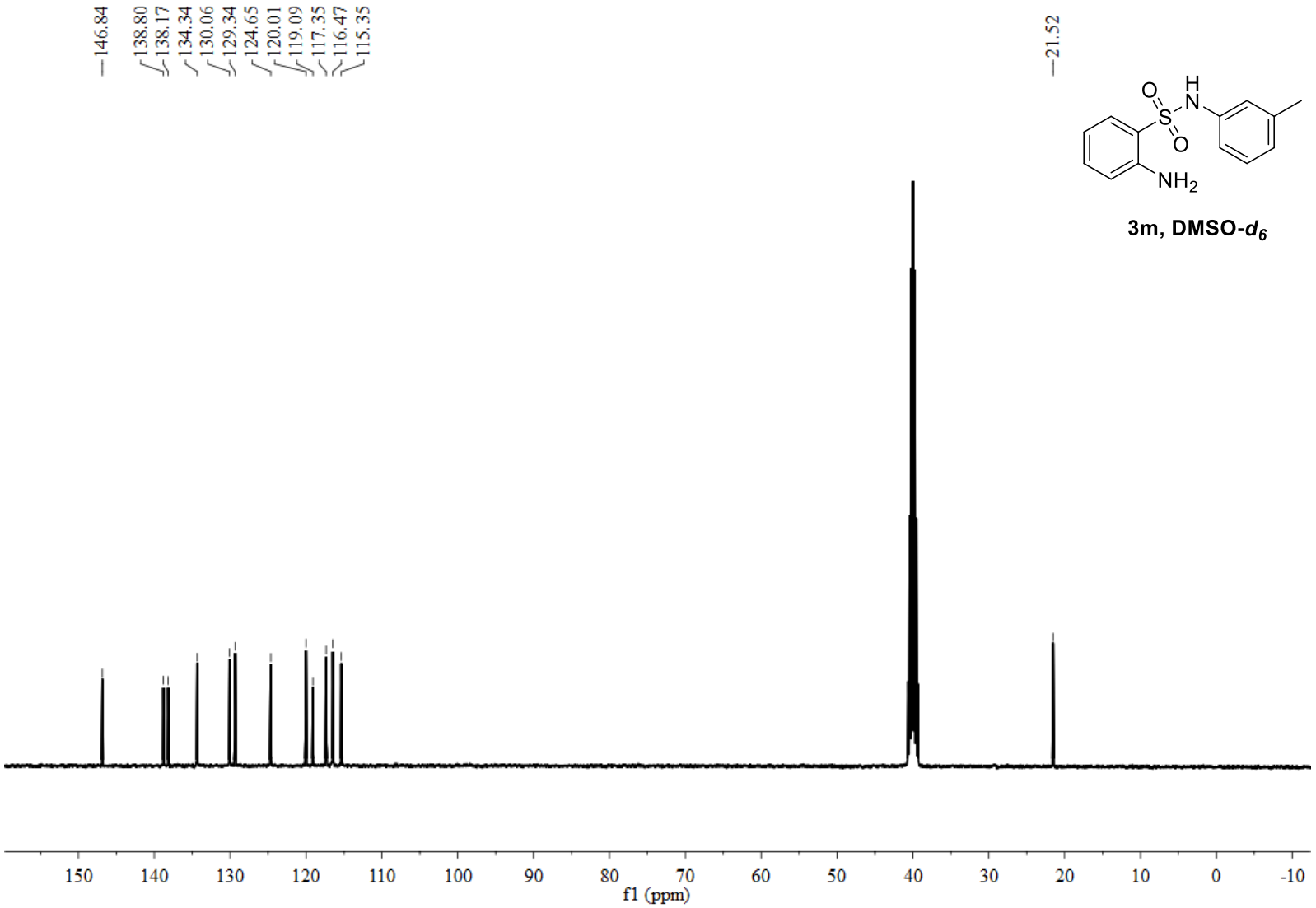

-61.283
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

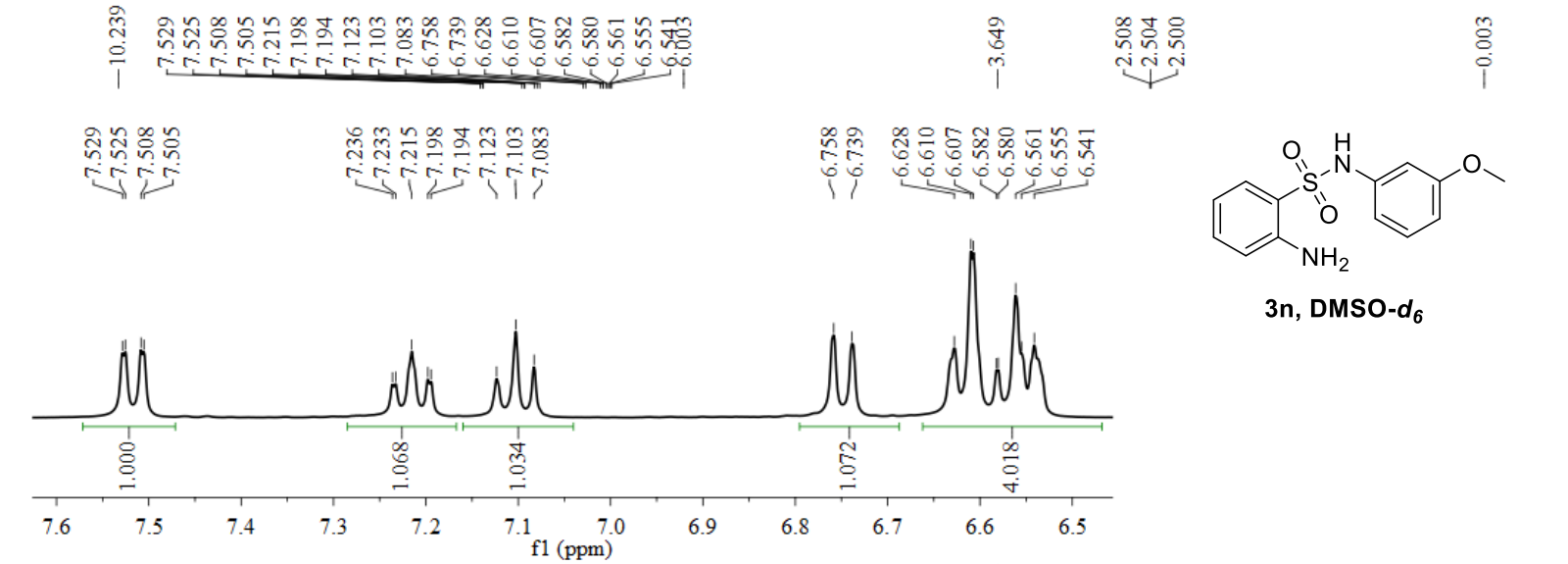
O
H
N
S
O
NH2
C
F
F
F

3l, $CDCl_3$

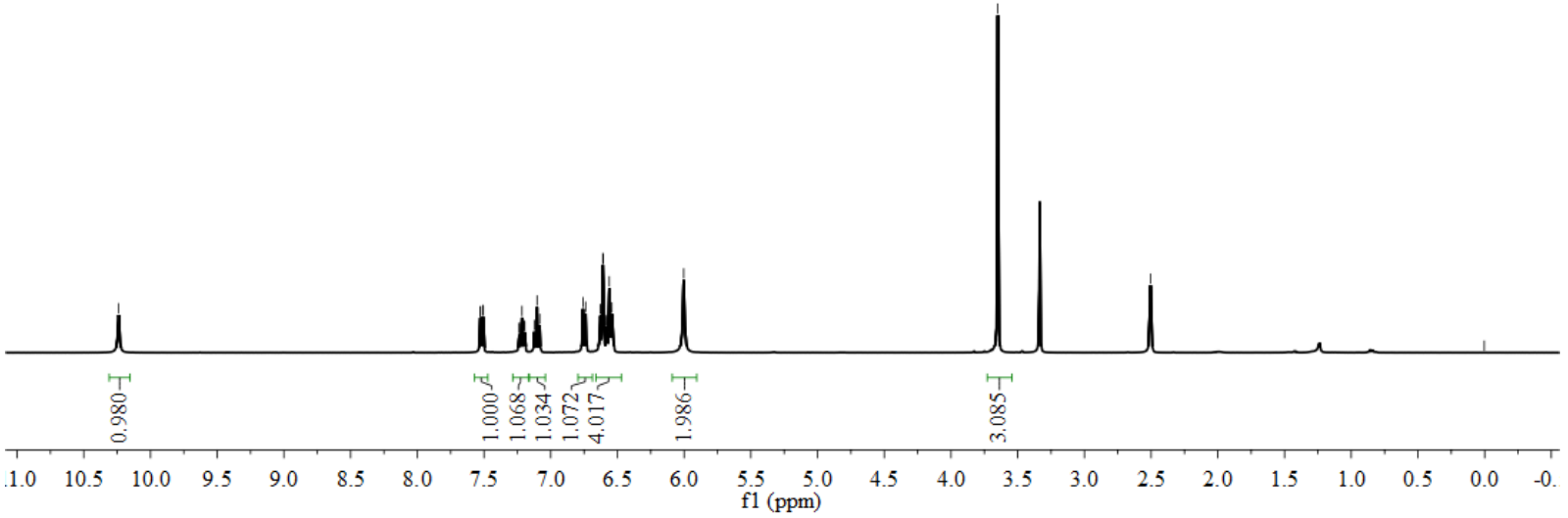

10.137
7.505
7.501
7.485
7.481
7.200
7.071
7.069
7.050
6.856
6.846
6.842
6.794
6.775
6.747
6.745
6.727
6.725
6.541
6.523
5.983
2.178
0.007
7.221
7.217
7.203
7.200
7.197
7.183
7.179
7.090
7.069
7.050
6.856
6.846
6.842
6.794
6.775
6.747
6.745
6.727
6.725
6.561
6.558
6.541
6.523
6.521
1.000
1.067
1.026
1.065
1.066
1.013
0.986
1.090
f1 (ppm)
1.005
1.000
1.067
1.026
0.966
1.040
1.013
0.986
1.090
2.015
2.974
f1 (ppm)

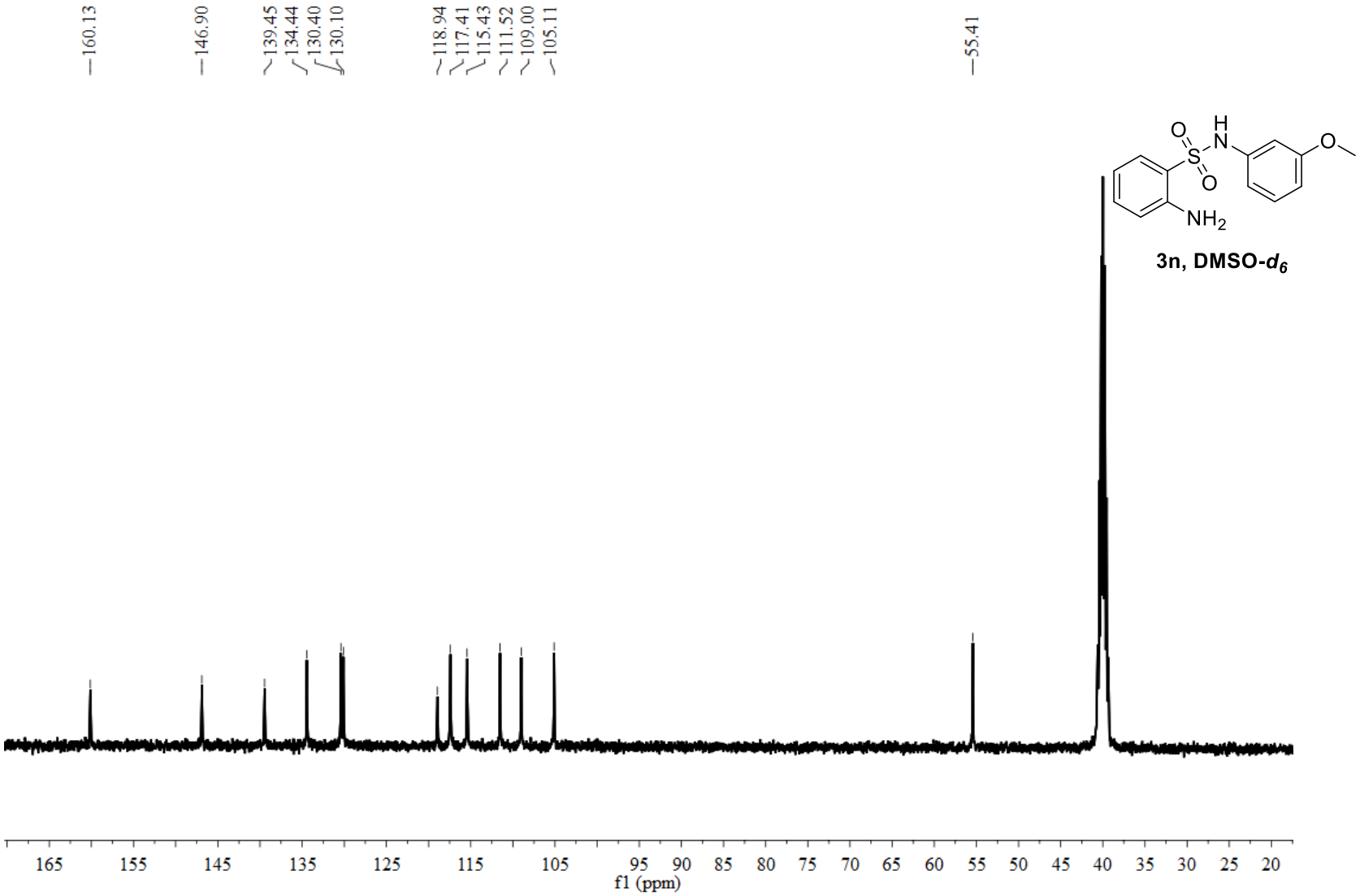
3m, DMSO-d_6

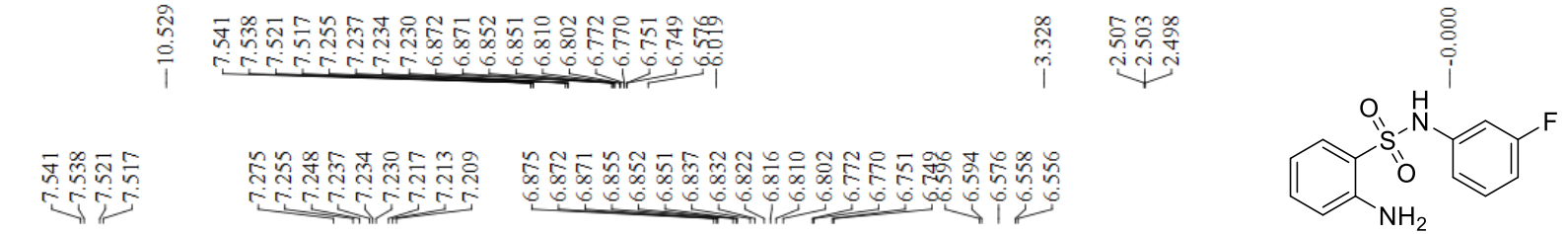

146.84
138.80
138.17
134.34
130.06
129.34
124.65
120.01
119.09
117.35
116.47
115.35
21.52
O
H
N
S
O
NH2
3m, DMSO-d6
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


10.239
7.529
7.525
7.508
7.505
7.215
7.198
7.194
7.123
7.103
7.083
6.758
6.739
6.628
6.610
6.607
6.582
6.580
6.561
6.555
6.541
6.003
3.649
2.508
2.504
2.500
0.003
1.000
1.068
1.034
1.072
4.018
f1 (ppm)

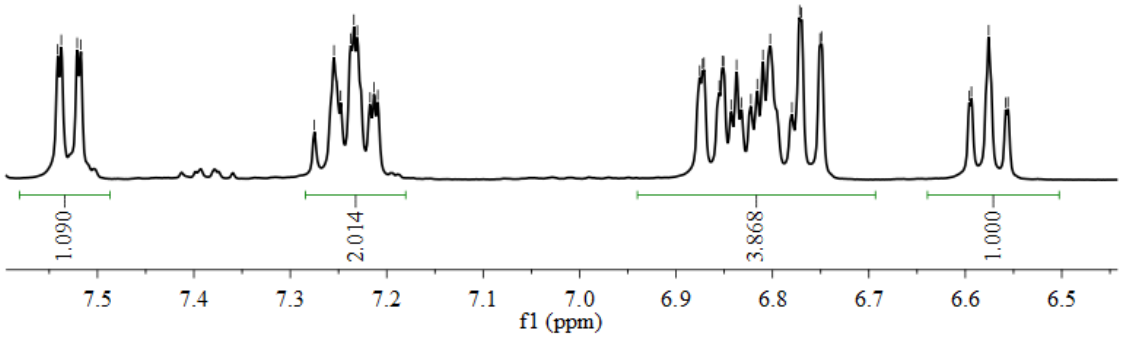
3n, DMSO-*d*$_6$

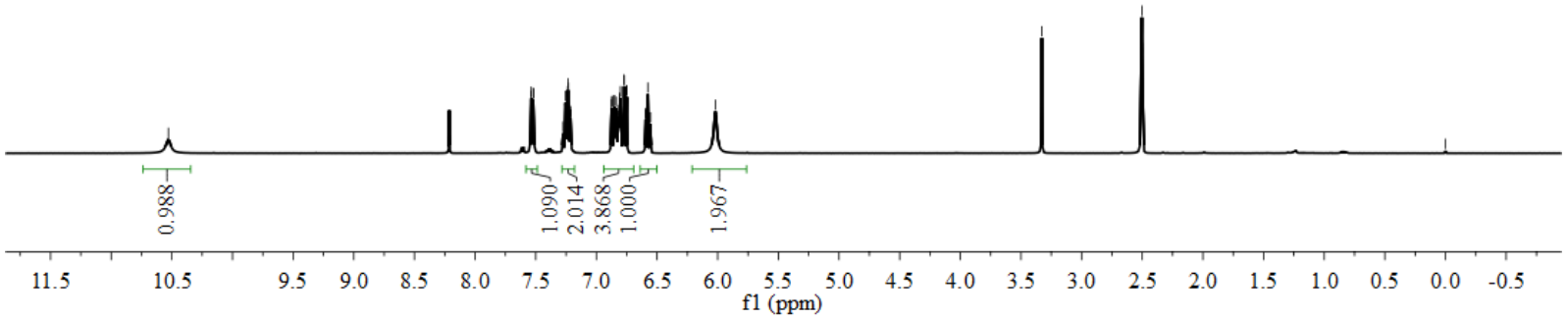

0.980
1.000
1.068
1.034
1.072
4.017
1.986
3.085
f1 (ppm)

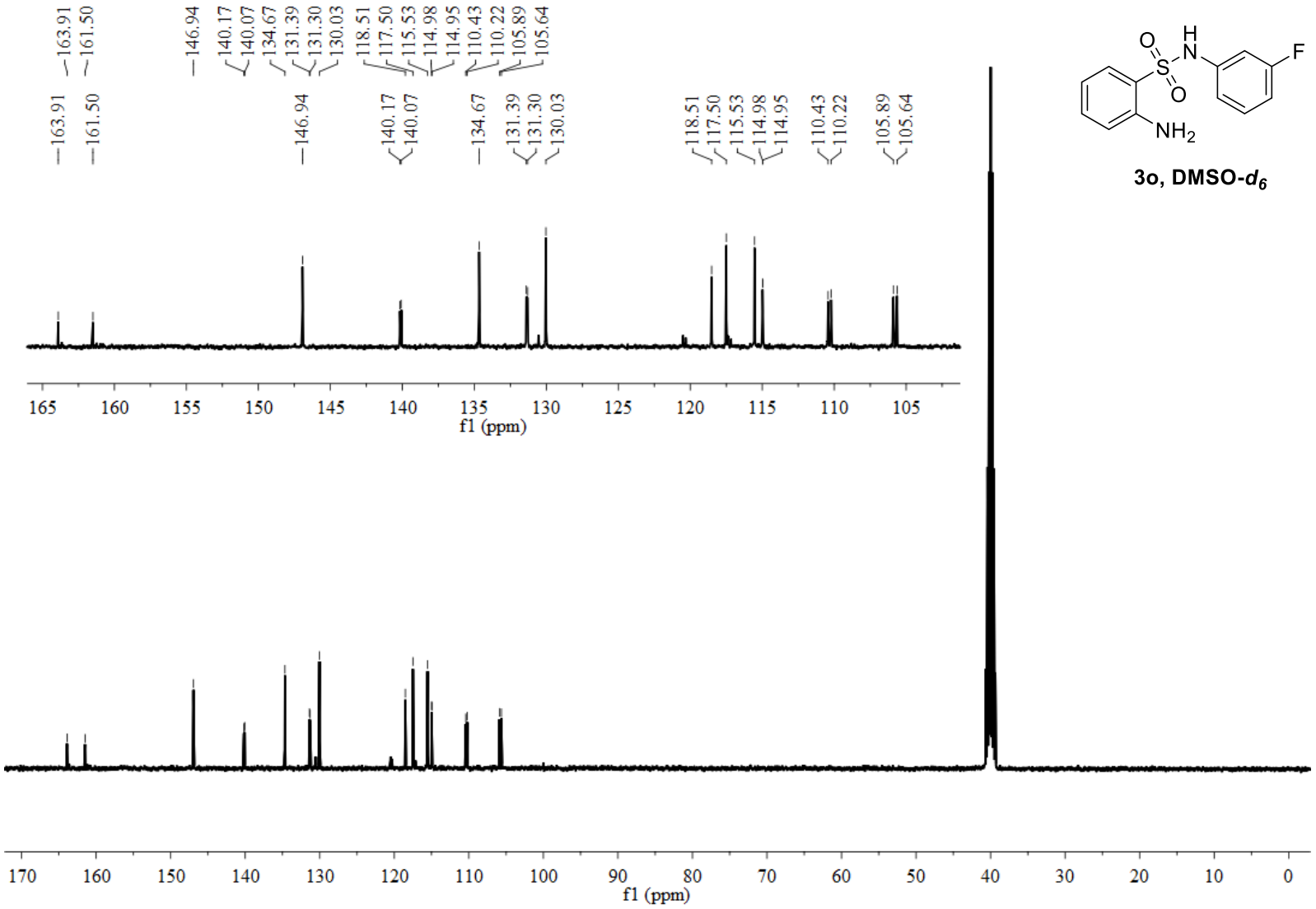

160.13
146.90
139.45
134.44
130.40
130.10
118.94
117.41
115.43
111.52
109.00
105.11
55.41
O
H
N
S
O
O
O
NH2
3n, DMSO-d6
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
f1 (ppm)


10.529
7.541
7.538
7.521
7.517
7.255
7.237
7.234
7.230
6.872
6.871
6.852
6.851
6.810
6.802
6.772
6.770
6.751
6.749
6.576
6.019
3.328
2.507
2.503
2.498
0.000
7.541
7.538
7.521
7.517
7.275
7.255
7.248
7.237
7.234
7.230
7.217
7.213
7.209
6.875
6.872
6.871
6.855
6.852
6.851
6.837
6.832
6.822
6.816
6.810
6.802
6.772
6.770
6.751
6.594
6.576
6.558
6.556
O
S
O
H
N
F
NH2

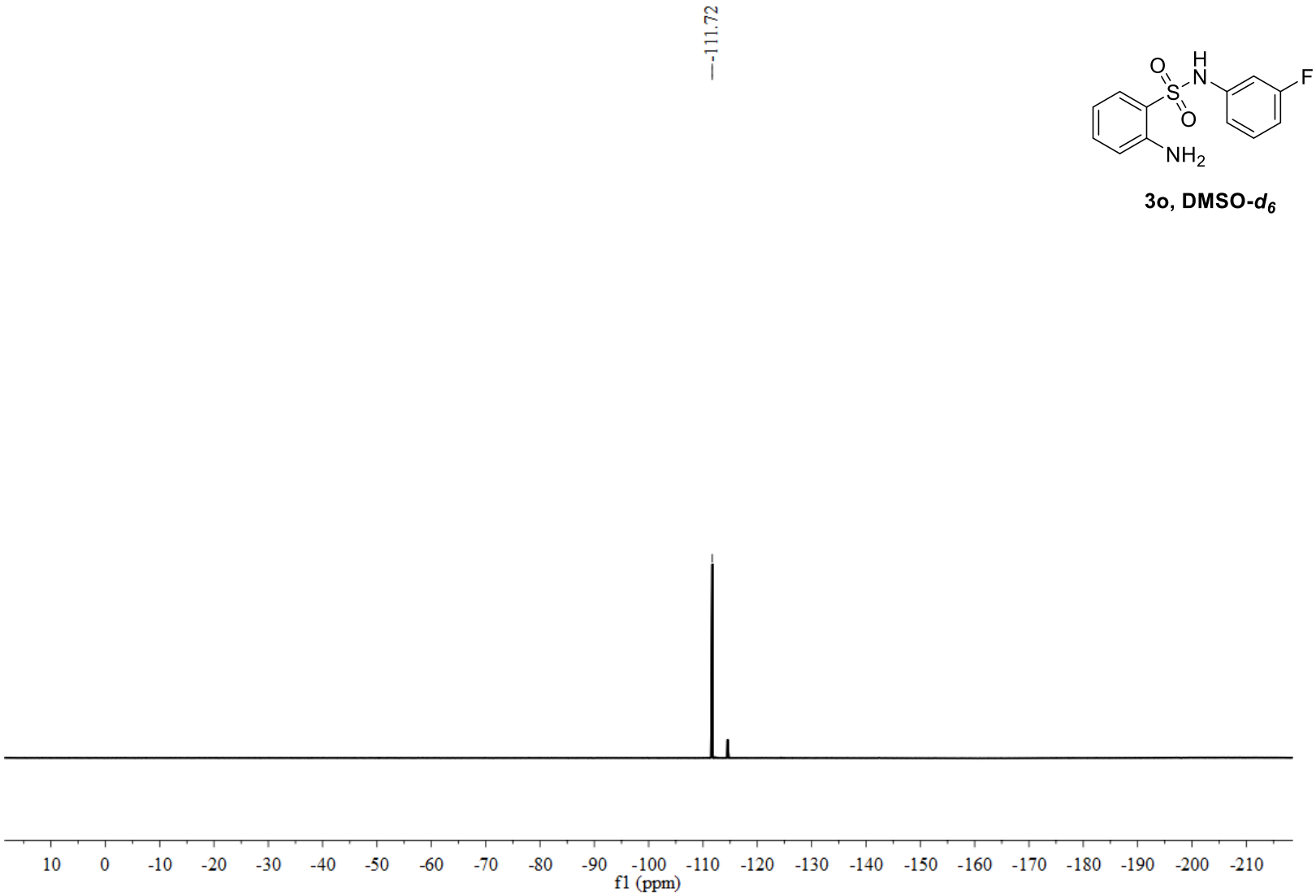
3o, DMSO-*d*$_6$


1.090
2.014
3.868
1.000
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
f1 (ppm)

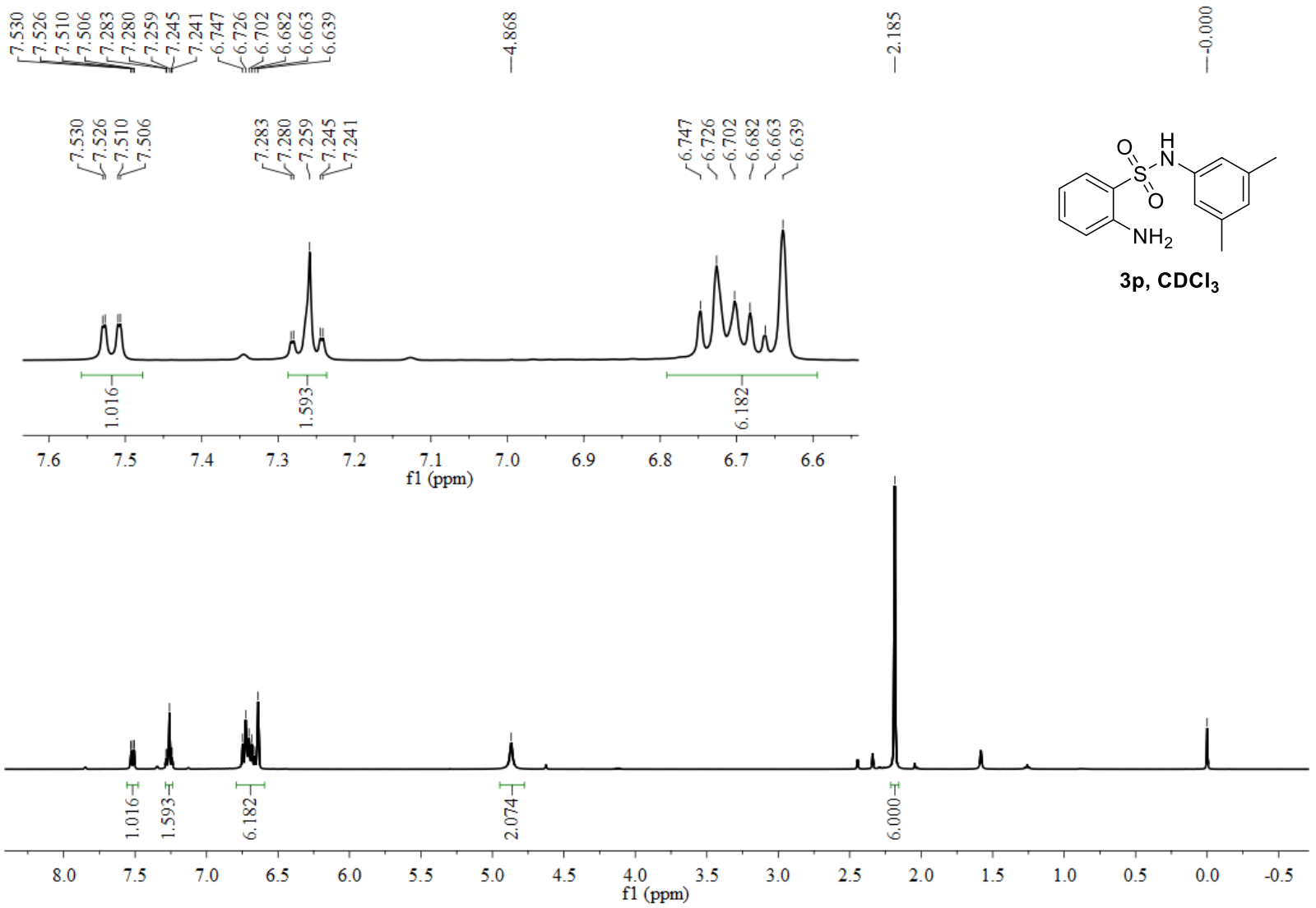

0.988
1.090
2.014
3.868
1.000
1.967
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

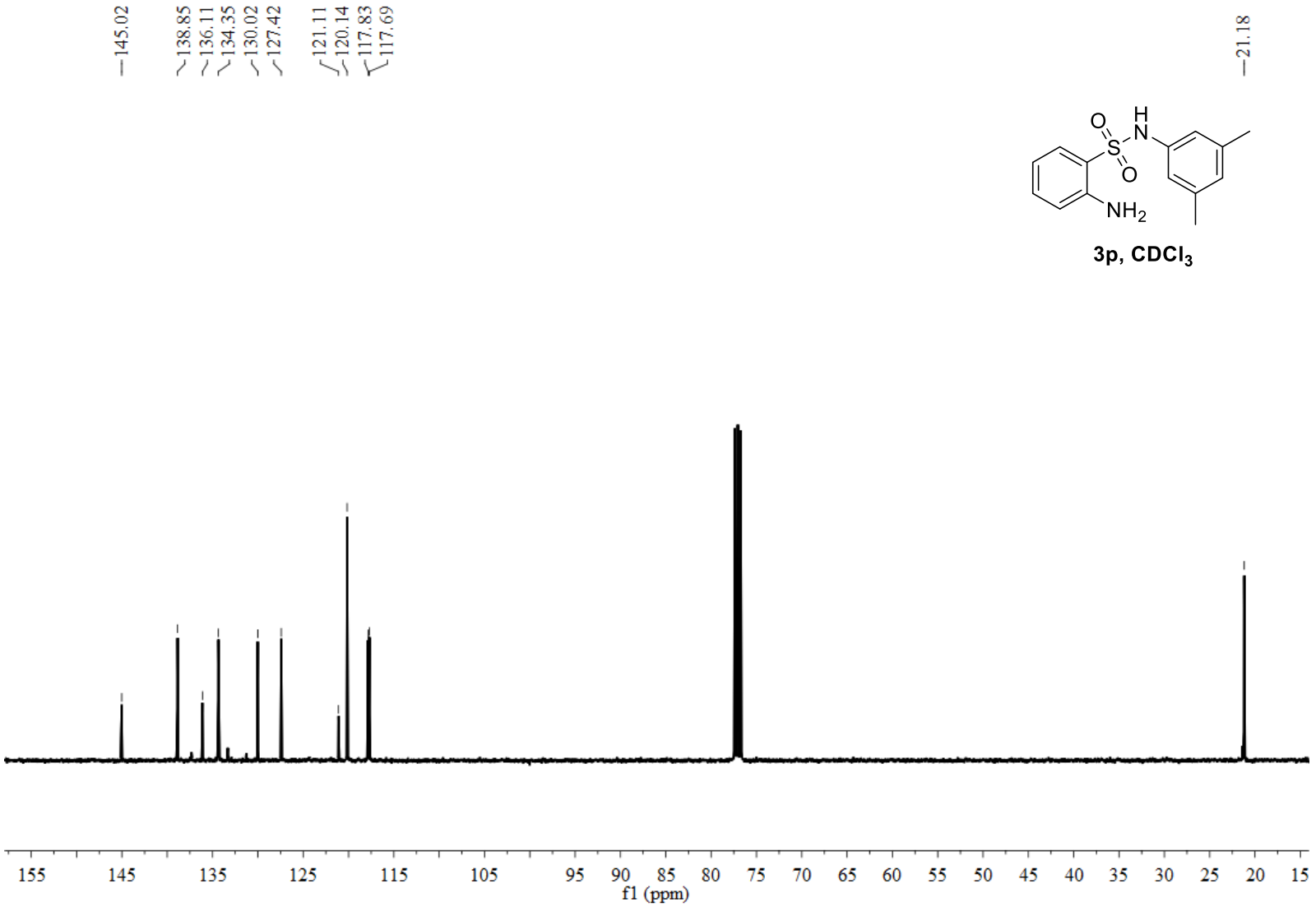

163.91
161.50
146.94
140.17
140.07
134.67
131.39
131.30
130.03
118.51
117.50
115.53
114.98
114.95
110.43
110.22
105.89
105.64
f1 (ppm)
f1 (ppm)
O
H
N
S
O
F
NH2

3o, DMSO-d_6

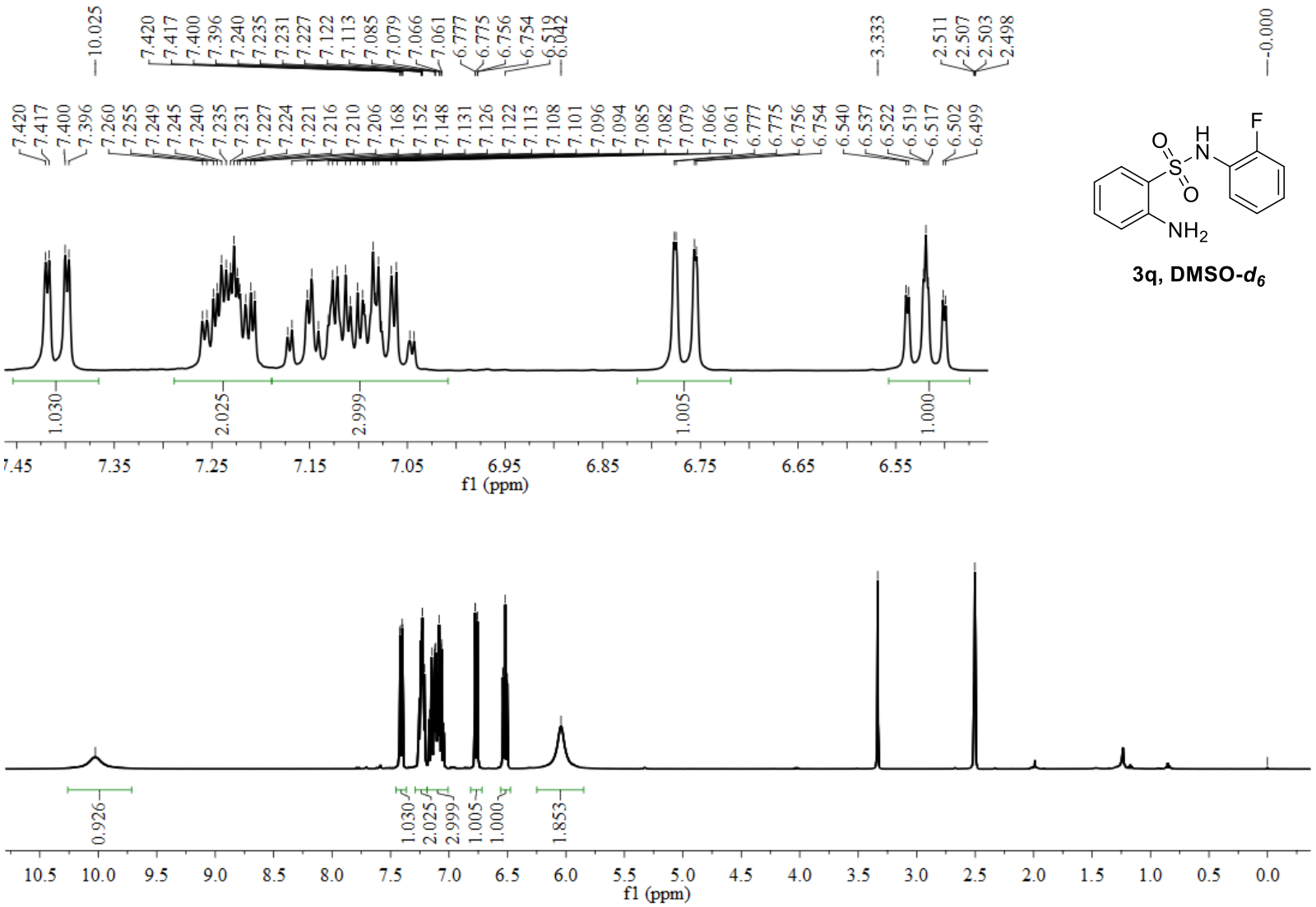

-111.72
O
H
N
S
O
F
NH2
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

3o, DMSO-d_6


7.530
7.526
7.510
7.506
7.283
7.280
7.259
7.245
7.241
6.747
6.726
6.702
6.682
6.663
6.639
4.868
2.185
0.000
1.016
1.593
6.182
f1 (ppm)
2.074
6.000
NH2
3p, CDCl3

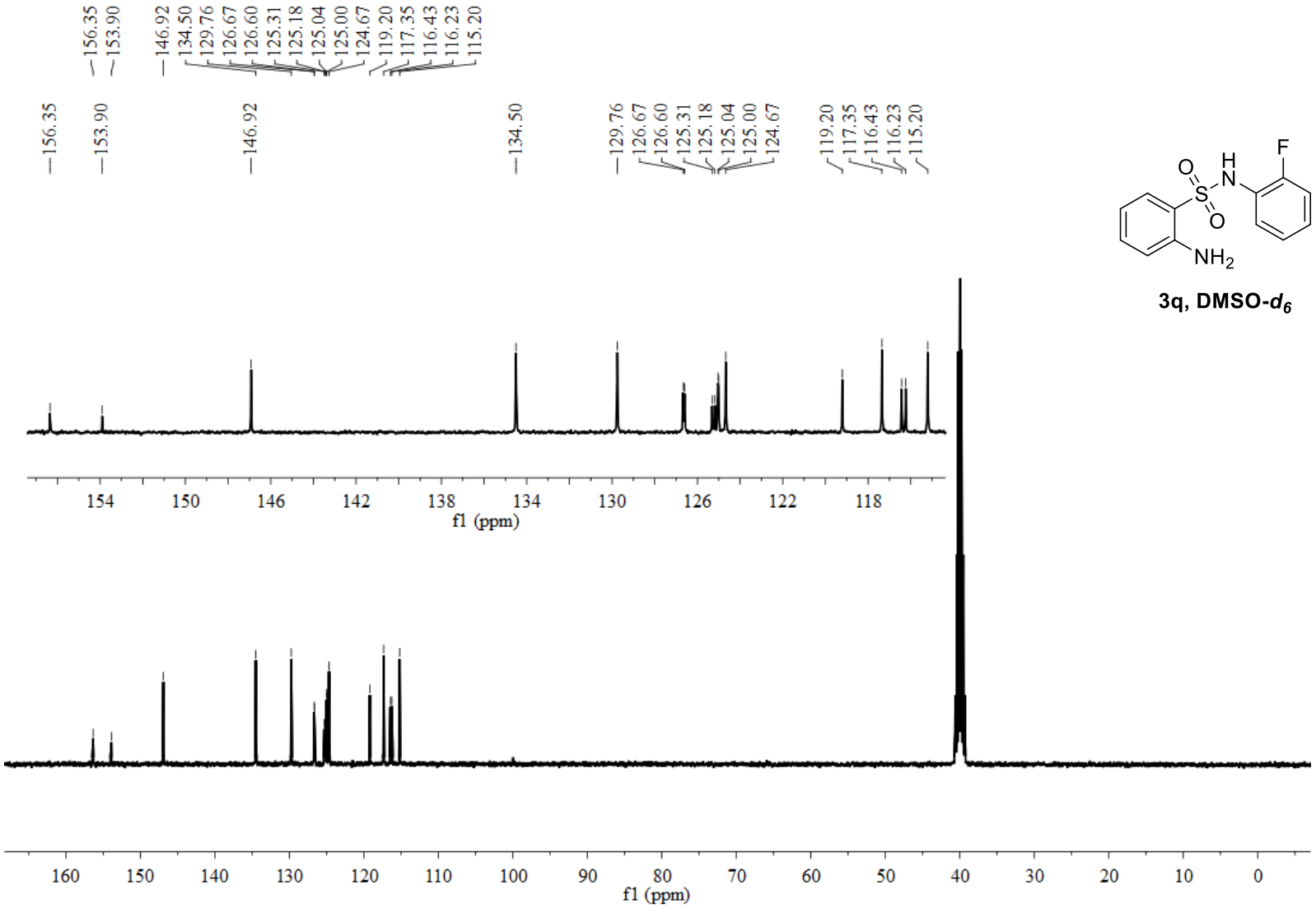

145.02
138.85
136.11
134.35
130.02
127.42
121.11
120.14
117.83
117.69
21.18
O
S
O
H
N
NH2
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
f1 (ppm)

3p, $CDCl_3$

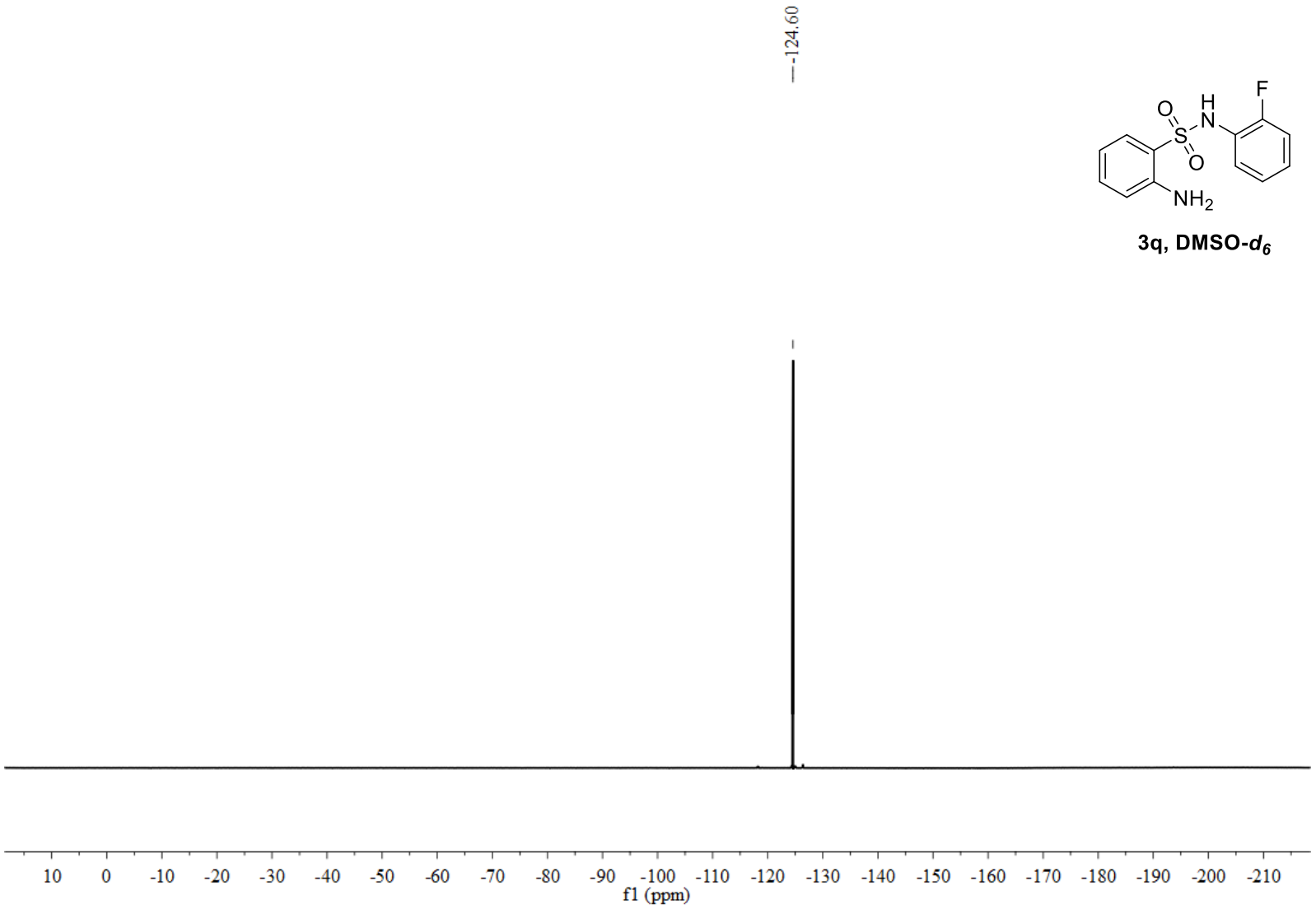

10.025
7.420
7.417
7.400
7.396
7.240
7.235
7.231
7.227
7.122
7.113
7.085
7.079
7.066
7.061
6.777
6.775
6.756
6.754
6.519
6.042
3.333
2.511
2.507
2.503
2.498
0.000
7.420
7.417
7.400
7.396
7.260
7.255
7.249
7.245
7.240
7.235
7.231
7.227
7.224
7.221
7.216
7.210
7.206
7.168
7.152
7.148
7.131
7.126
7.122
7.113
7.108
7.101
7.096
7.094
7.085
7.082
7.079
7.066
7.061
6.777
6.775
6.756
6.754
6.540
6.537
6.522
6.519
6.517
6.502
6.499
1.030
2.025
2.999
1.005
1.000
7.45
7.35
7.25
7.15
7.05
6.95
6.85
6.75
6.65
6.55
f1 (ppm)
0.926
1.030
2.025
2.999
1.005
1.000
1.853
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

F
H
N
O
S
O
NH2

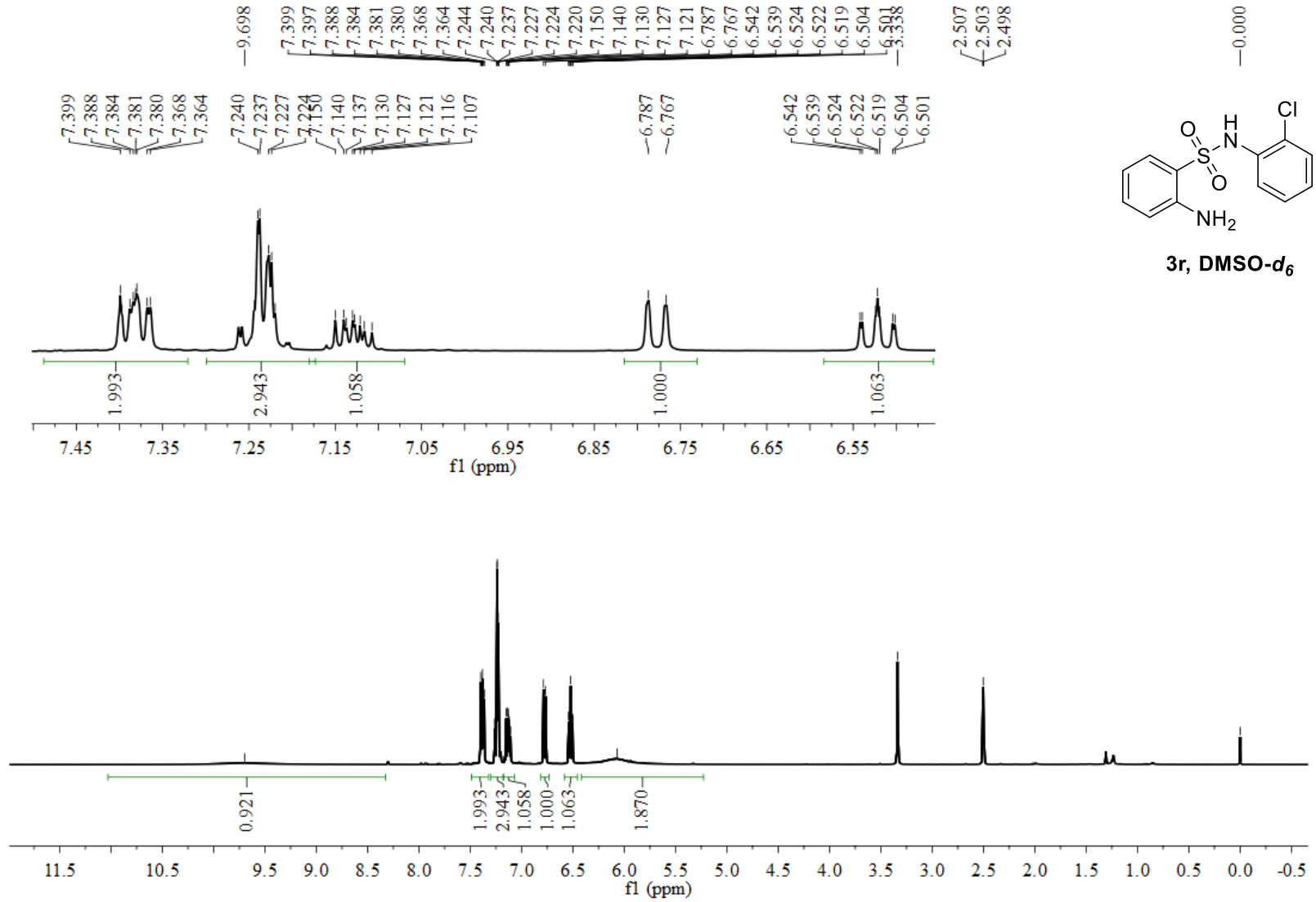
3q, DMSO-*d*$_6$


156.35
153.90
146.92
134.50
129.76
126.67
126.60
125.31
125.18
125.04
125.00
124.67
119.20
117.35
116.43
116.23
115.20
154
150
146
142
138
134
130
126
122
118
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
H
N
F
S
O
NH2

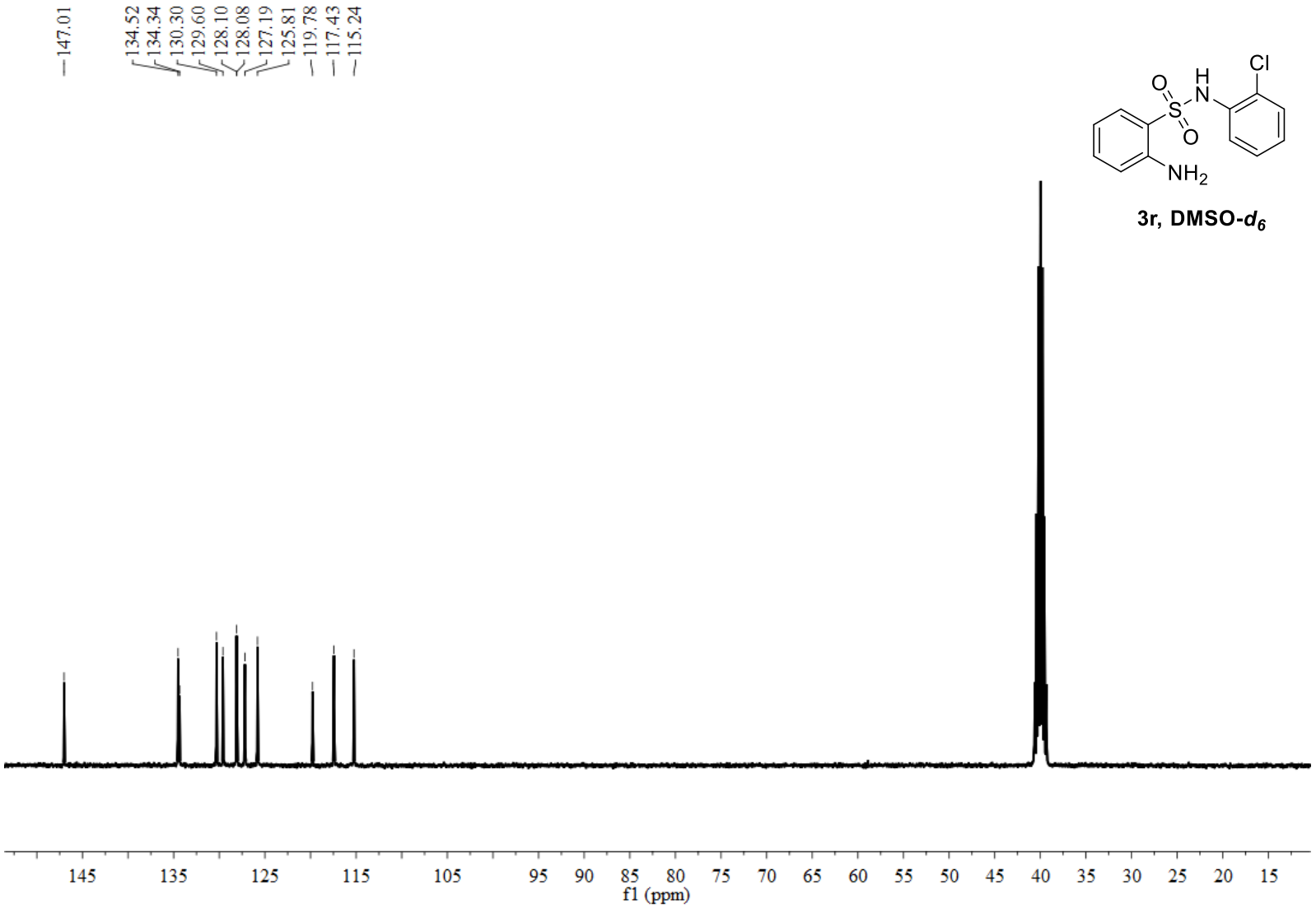
3q, DMSO-d_6

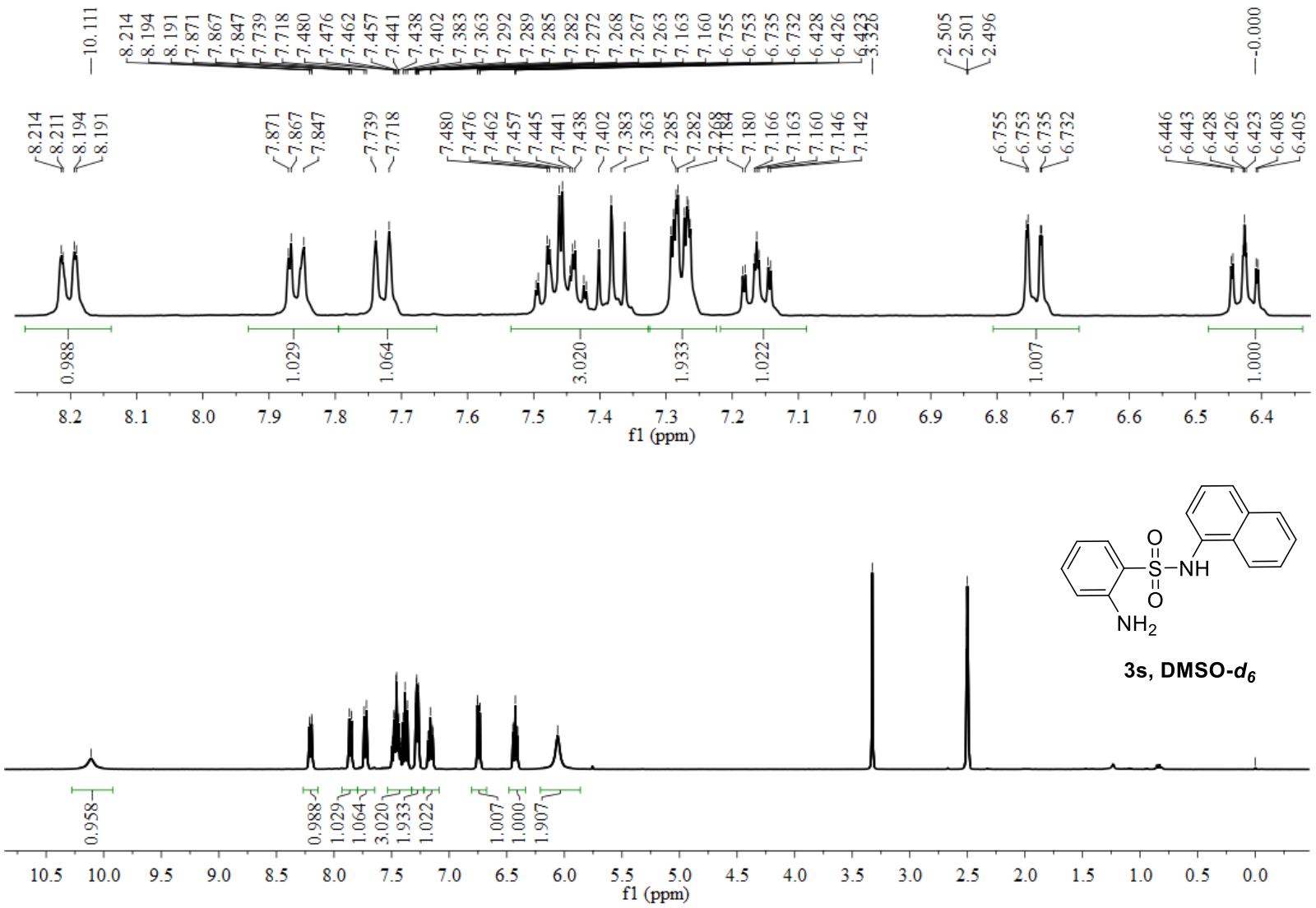

-124.60
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

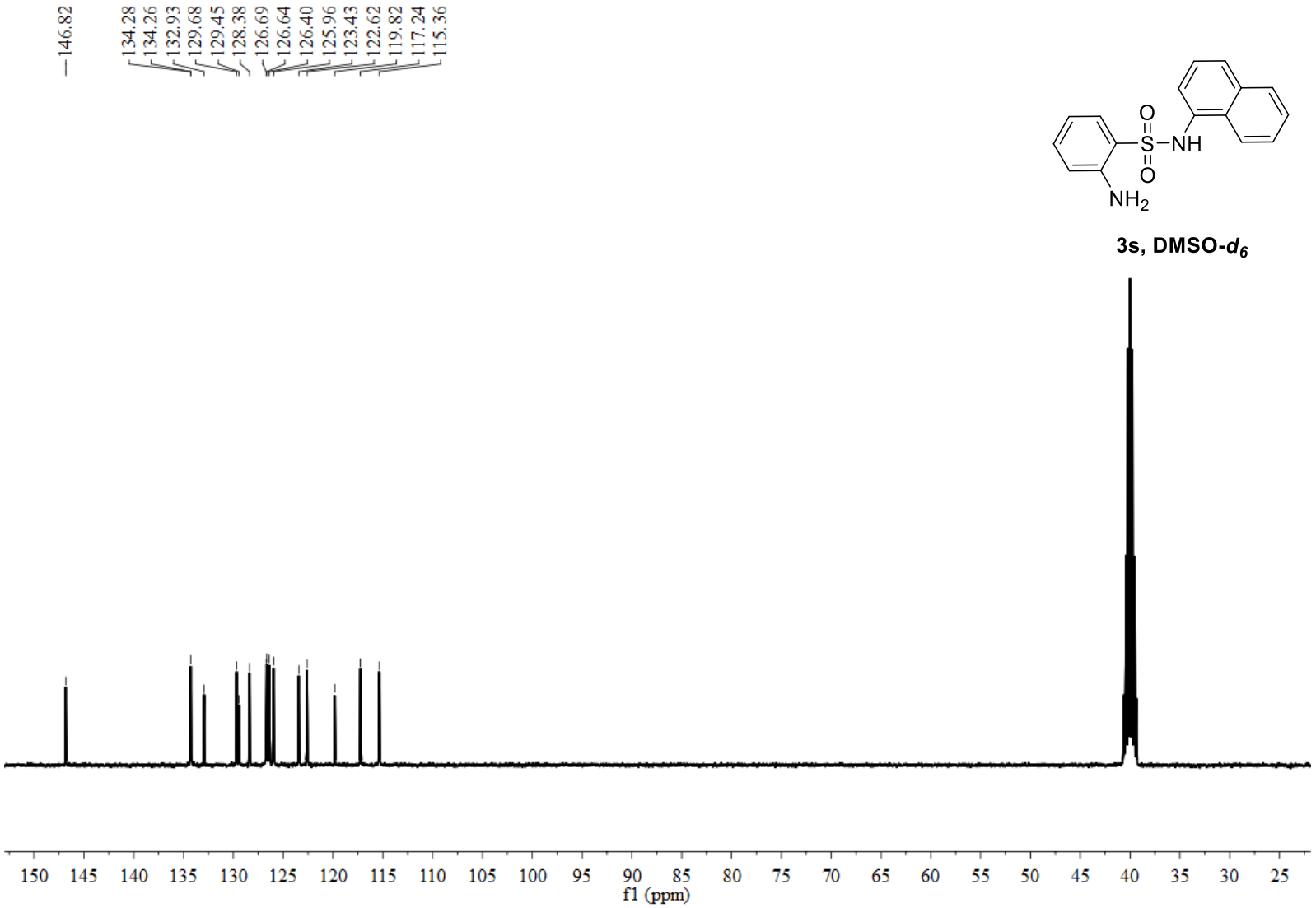
3q, DMSO-d_6

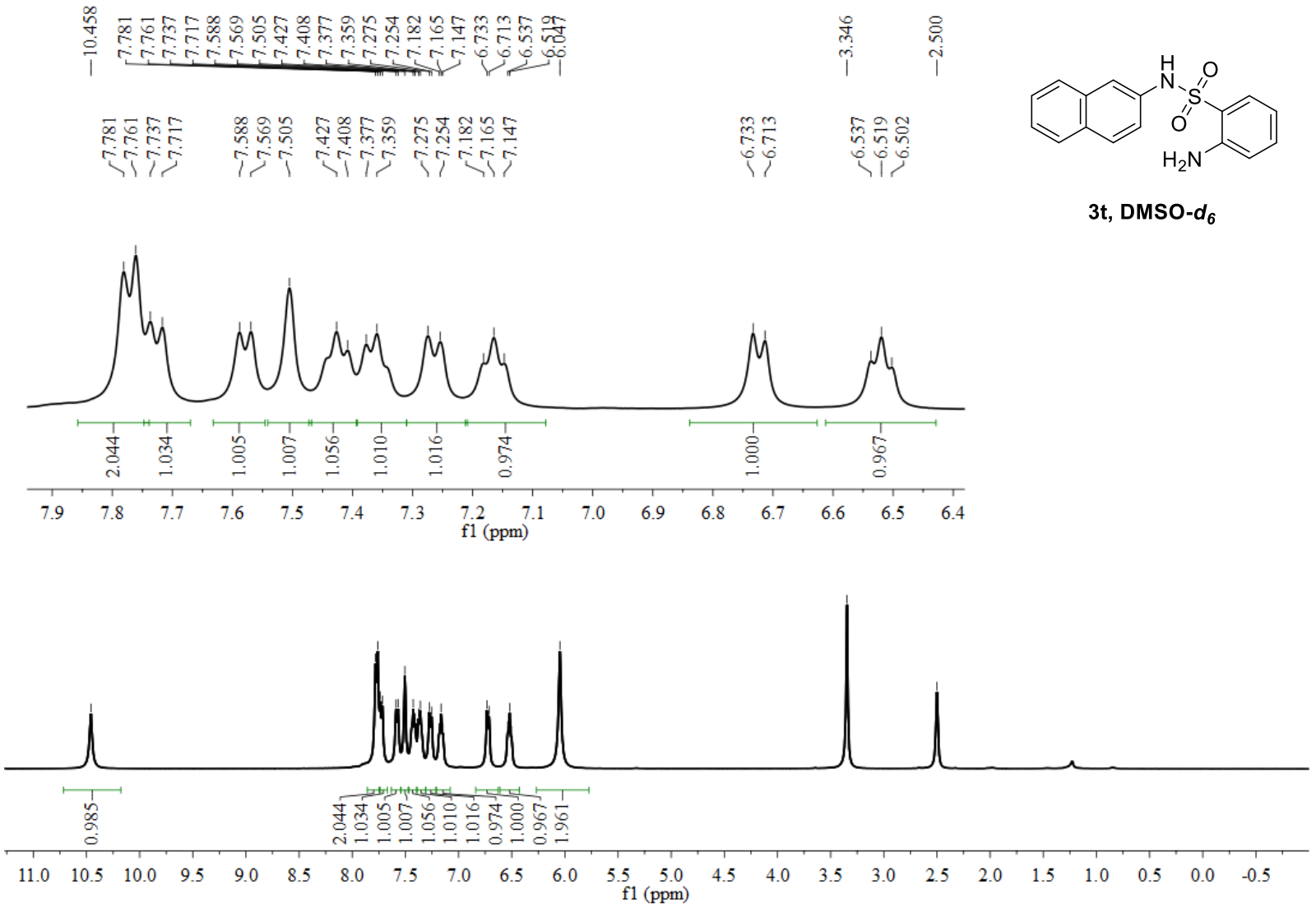

9.698
7.399
7.397
7.388
7.384
7.381
7.380
7.368
7.364
7.244
7.240
7.237
7.227
7.224
7.220
7.150
7.140
7.130
7.127
7.121
6.787
6.767
6.542
6.539
6.524
6.522
6.519
6.504
6.501
3.338
2.507
2.503
2.498
0.000
1.993
2.943
1.058
1.000
1.063
f1 (ppm)
0.921
1.870
Cl
H
N
O
S
O
NH2

3r, DMSO-d_6

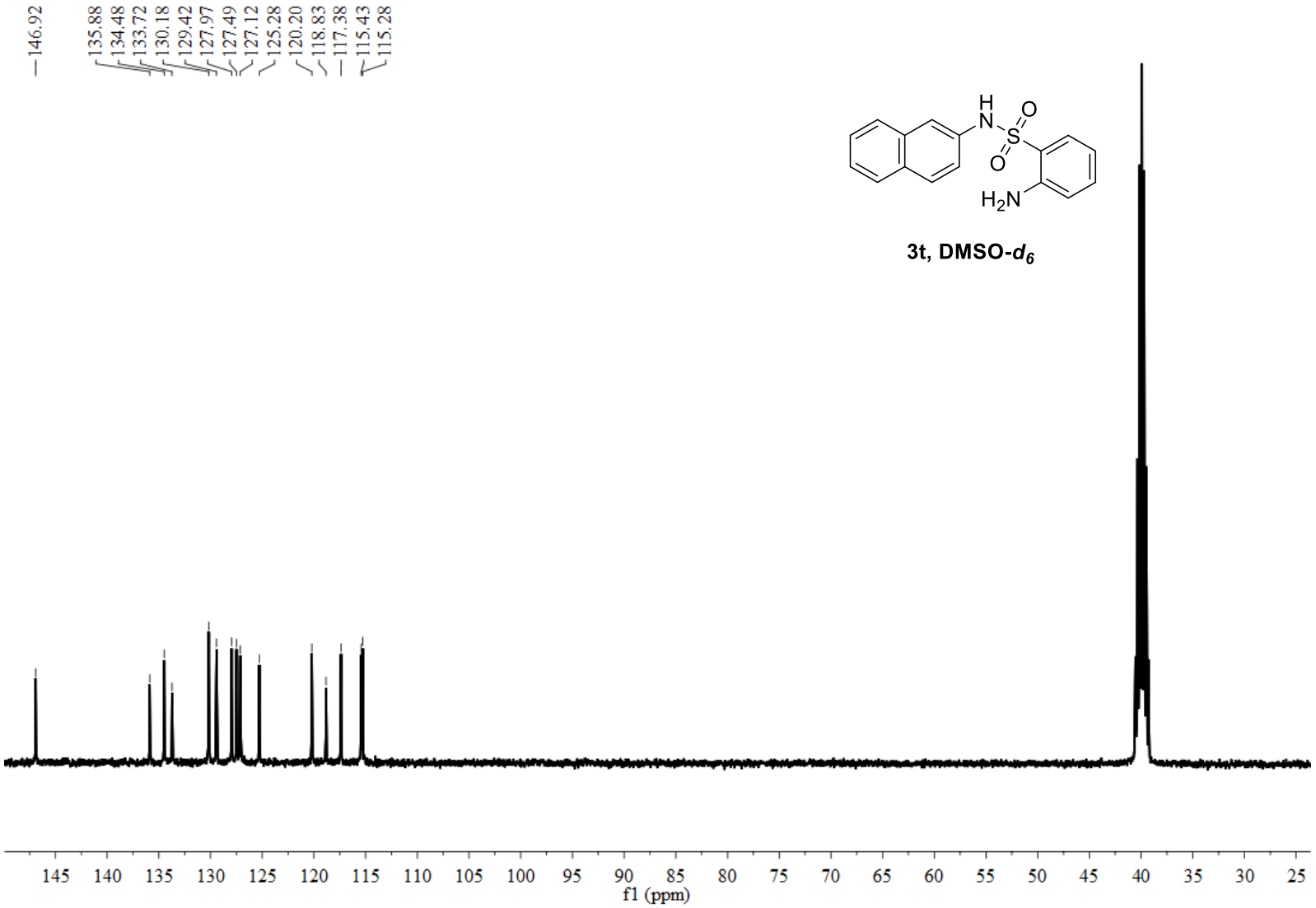

147.01
134.52
134.34
130.30
129.60
128.10
128.08
127.19
125.81
119.78
117.43
115.24
Cl
H
N
O
S
O
NH2
3r, DMSO-d6
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
f1 (ppm)


10.111
8.214
8.194
8.191
7.871
7.867
7.847
7.739
7.718
7.480
7.476
7.462
7.457
7.441
7.438
7.402
7.383
7.363
7.292
7.289
7.285
7.282
7.272
7.268
7.267
7.263
7.163
7.160
6.755
6.753
6.735
6.732
6.428
6.426
6.423
2.505
2.501
2.496
0.000
0.988
1.029
1.064
3.020
1.933
1.022
1.007
1.000
f1 (ppm)
NH2
S
O
NH
3s, DMSO-d6
0.958
0.907
f1 (ppm)

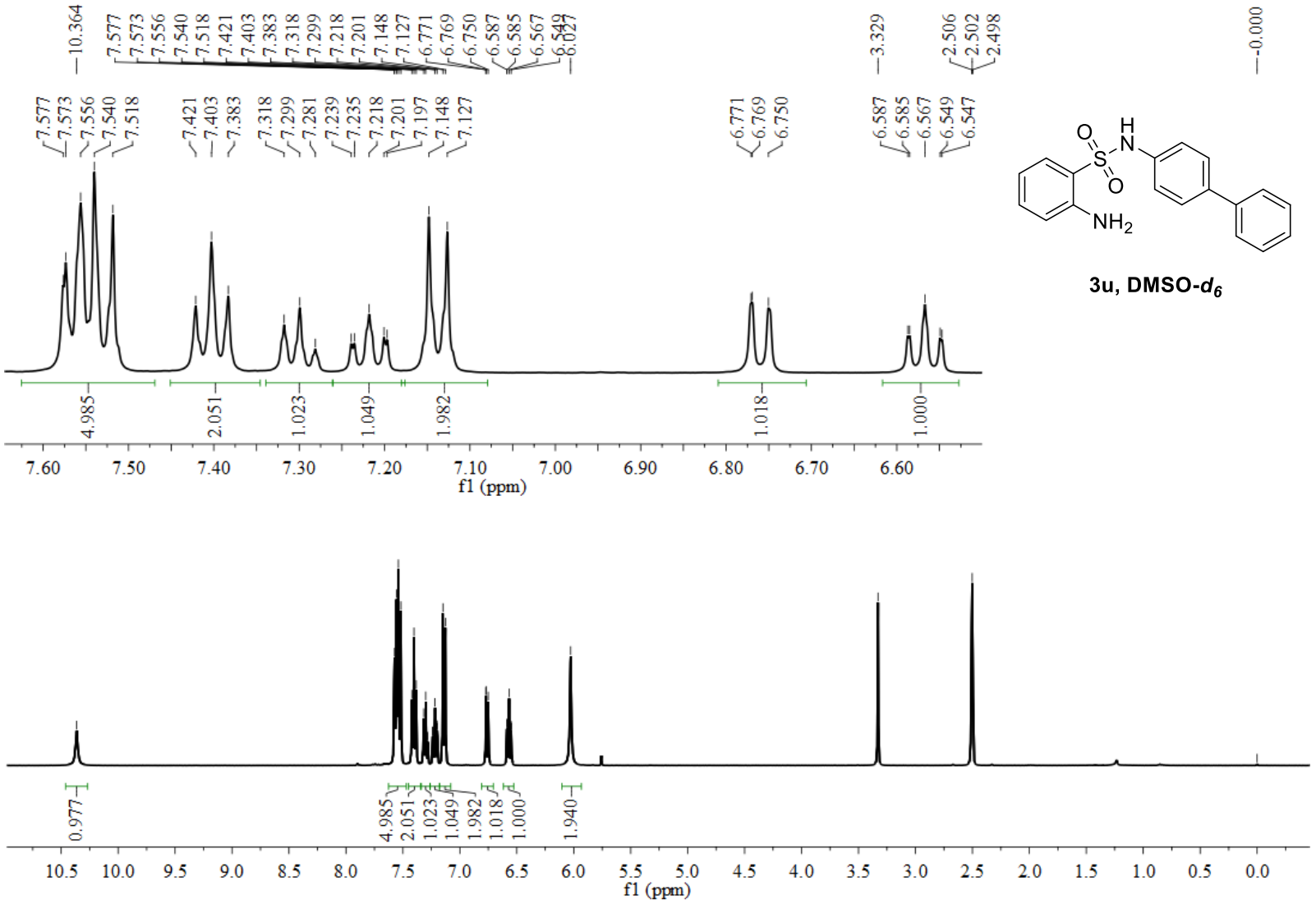

146.82
134.28
134.26
132.93
129.68
129.45
128.38
126.69
126.64
126.40
125.96
123.43
122.62
119.82
117.24
115.36
O
S
NH
O
NH2
3s, DMSO-d6
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)


10.458
7.781
7.761
7.737
7.717
7.588
7.569
7.505
7.427
7.408
7.377
7.359
7.275
7.254
7.182
7.165
7.147
6.733
6.713
6.537
6.519
6.502
3.346
2.500
2.044
1.034
1.005
1.007
1.056
1.010
1.016
0.974
1.000
0.967
f1 (ppm)
0.985
1.961

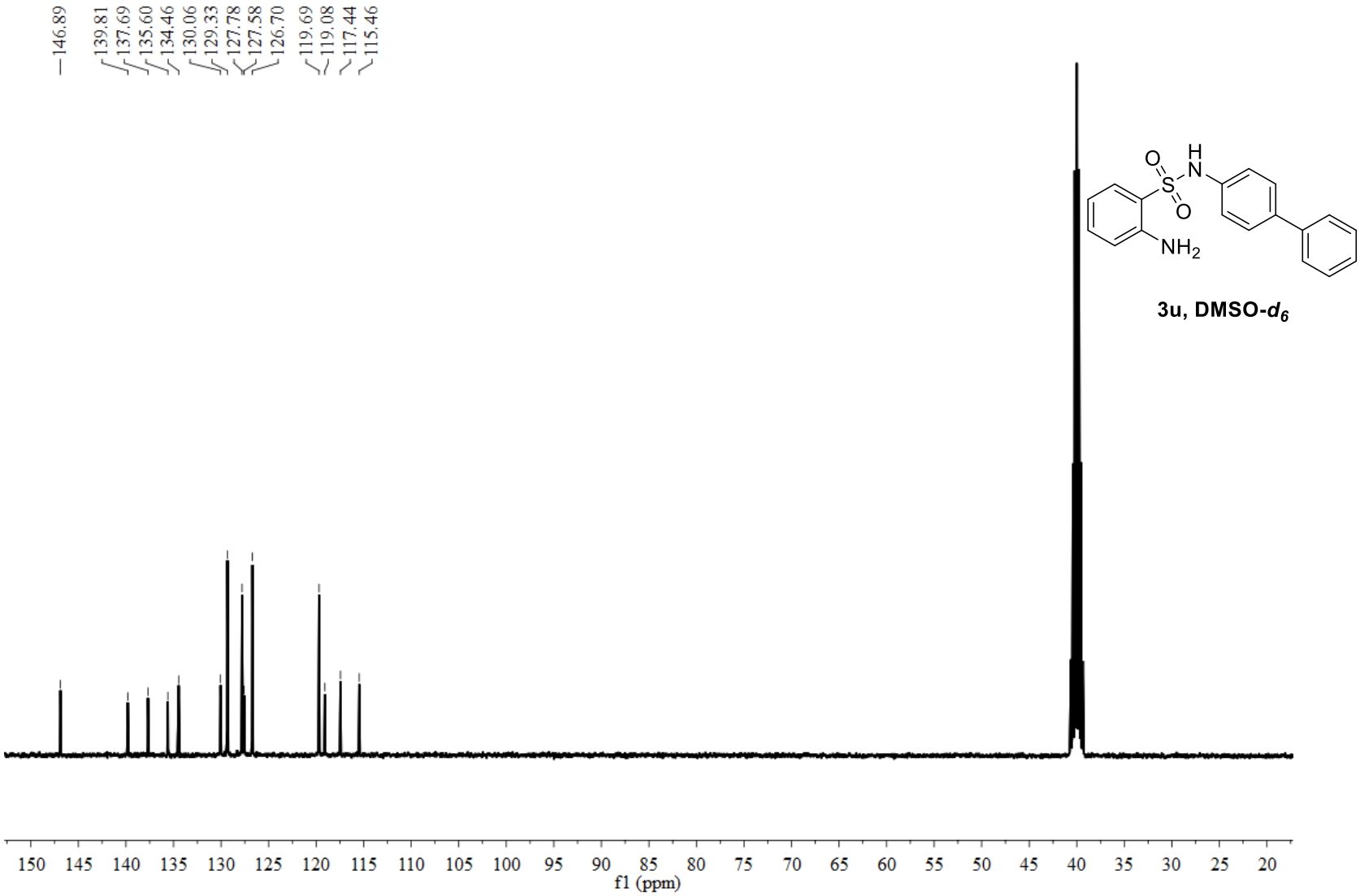
3t, DMSO-*d*$_6$


146.92
135.88
134.48
133.72
130.18
129.42
127.97
127.49
127.12
125.28
120.20
118.83
117.38
115.43
115.28
H
N
S
O
O
H_2N
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)

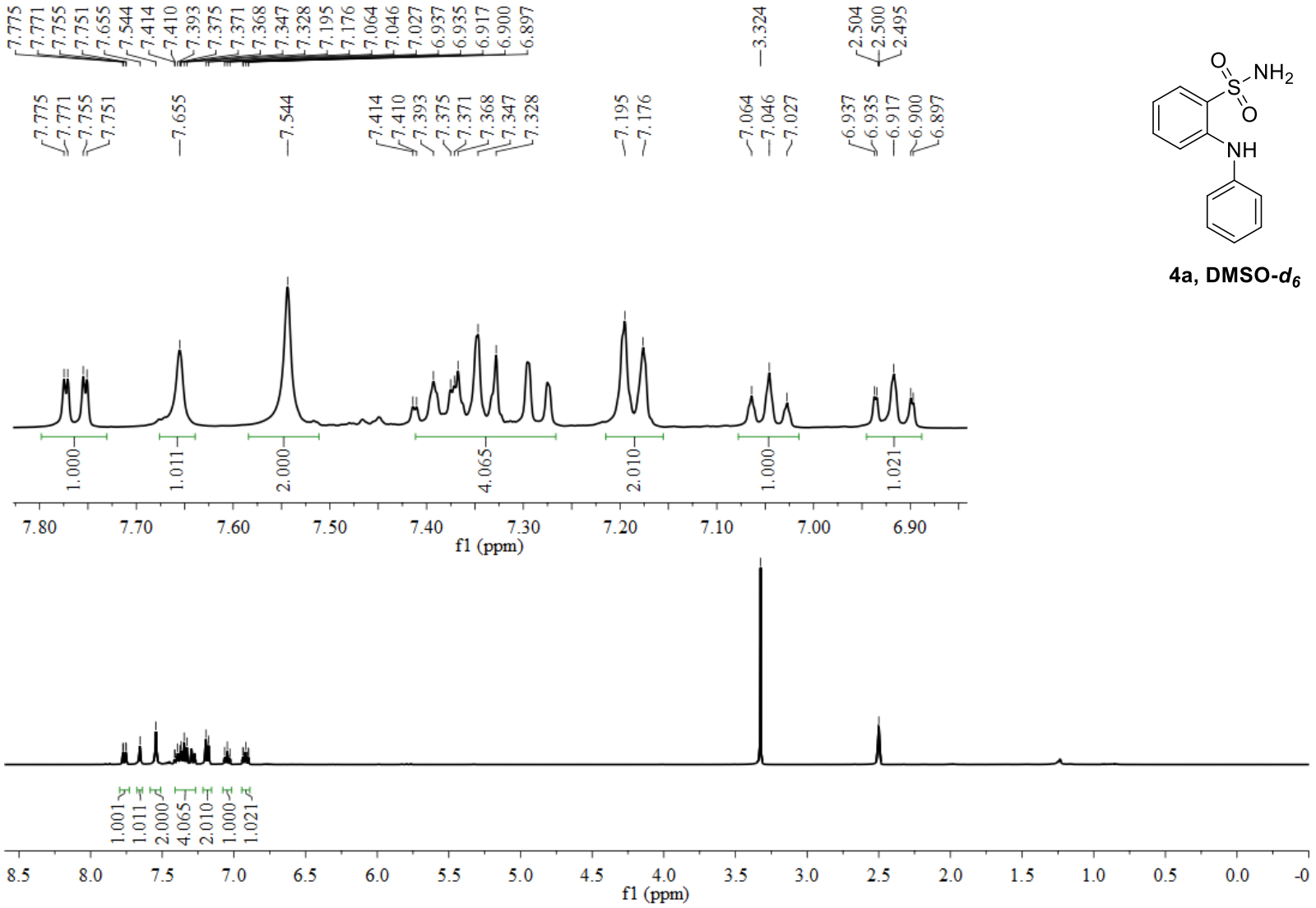
3t, DMSO-d_6


10.364
7.577
7.573
7.556
7.540
7.518
7.421
7.403
7.383
7.318
7.299
7.218
7.201
7.148
7.127
6.771
6.769
6.750
6.587
6.585
6.567
6.549
6.027
3.329
2.506
2.502
2.498
0.000
4.985
2.051
1.023
1.049
1.982
1.018
1.000
0.977
1.940
f1 (ppm)
O
S
O
H
N
NH2

3u, DMSO-d_6

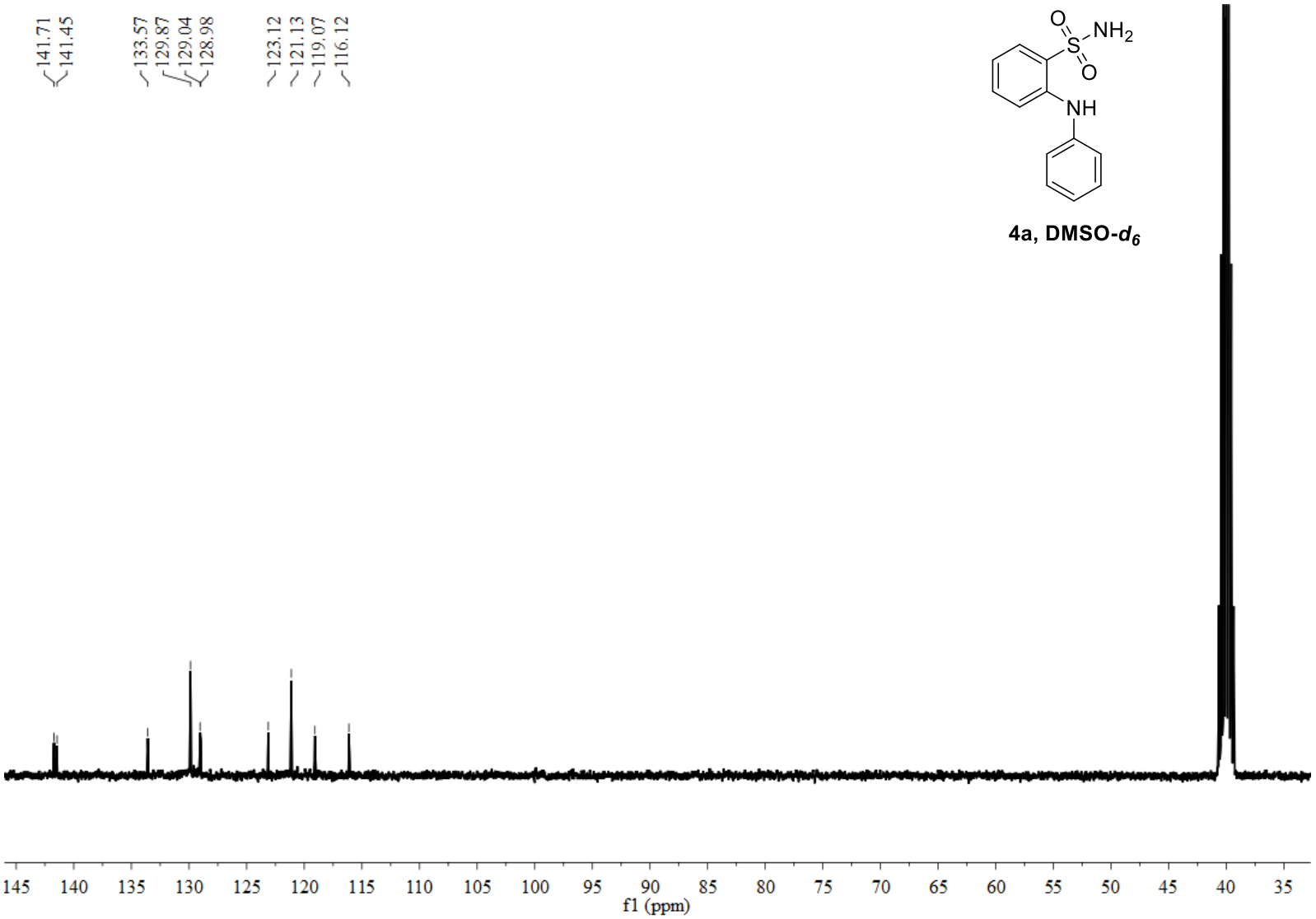

146.89
139.81
137.69
135.60
134.46
130.06
129.33
127.78
127.58
126.70
119.69
119.08
117.44
115.46
O
H
N
S
O
NH2
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)

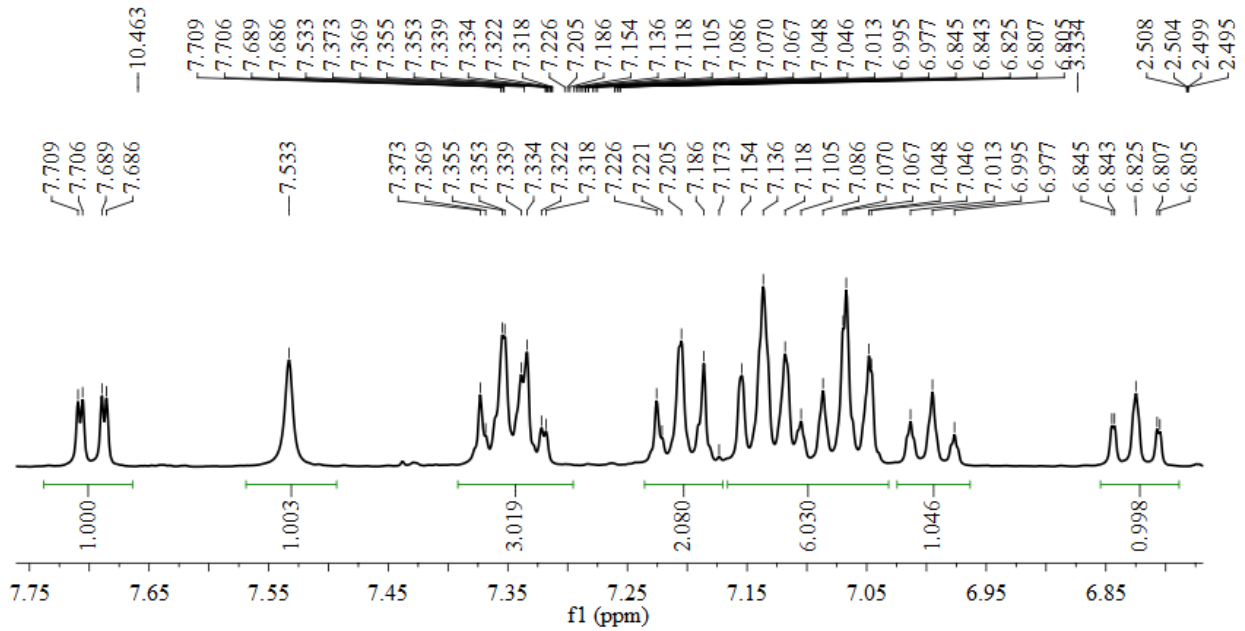
3u, DMSO-d_6

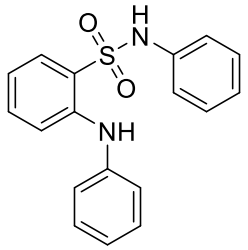

7.775
7.771
7.755
7.751
7.655
7.544
7.414
7.410
7.393
7.375
7.371
7.368
7.347
7.328
7.195
7.176
7.064
7.046
7.027
6.937
6.935
6.917
6.900
6.897
3.324
2.504
2.500
2.495
1.000
1.011
2.000
4.065
2.010
1.000
1.021
7.80
7.70
7.60
7.50
7.40
7.30
7.20
7.10
7.00
6.90
f1 (ppm)
1.001
1.011
2.000
4.065
2.010
1.000
1.021
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

O
NH2
S
O
NH

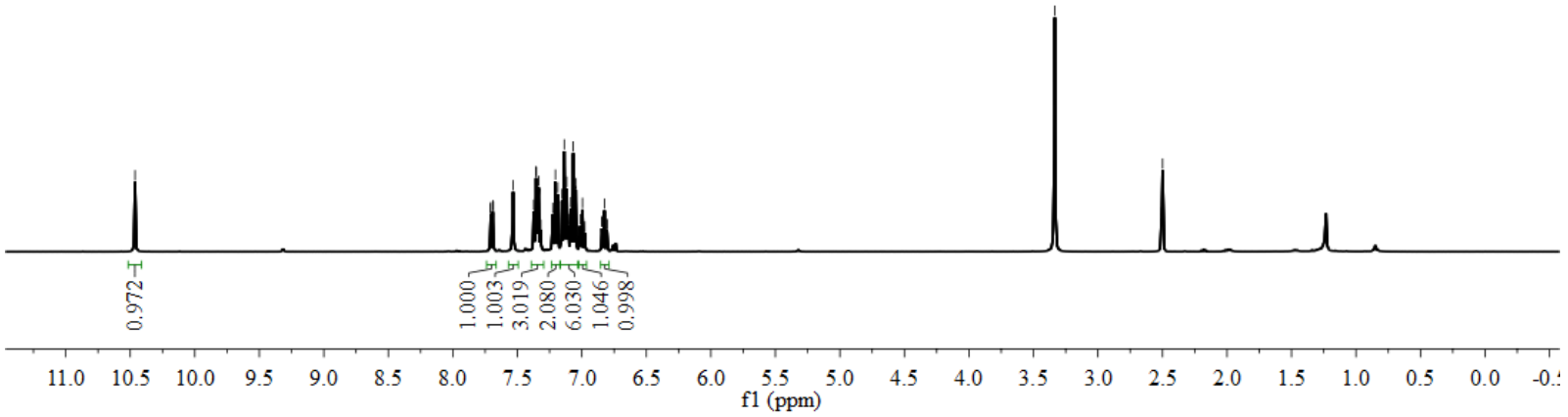
4a, DMSO-d_6

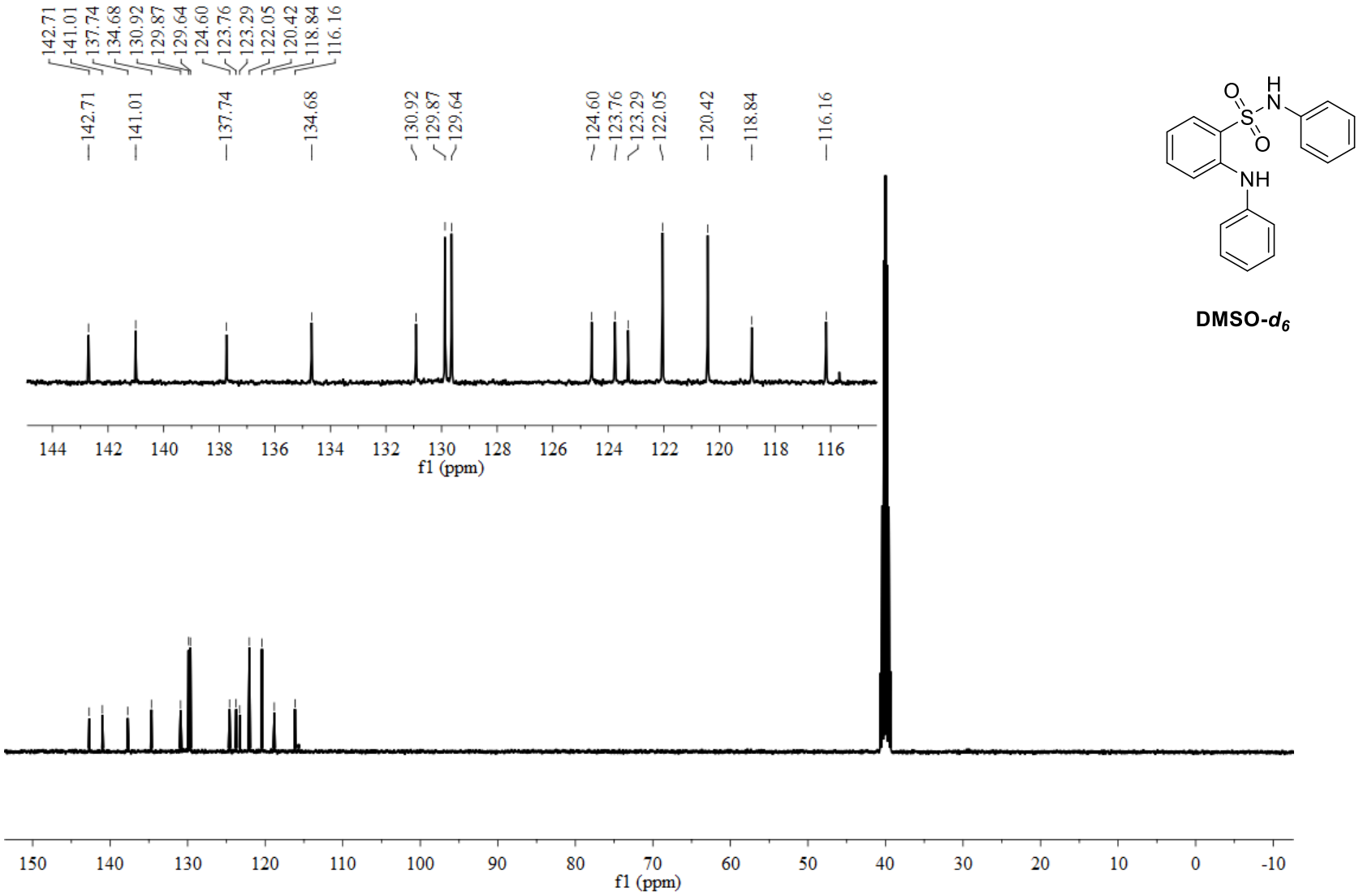

141.71
141.45
133.57
129.87
129.04
128.98
123.12
121.13
119.07
116.12
O
NH2
S
O
NH
4a, DMSO-d6
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

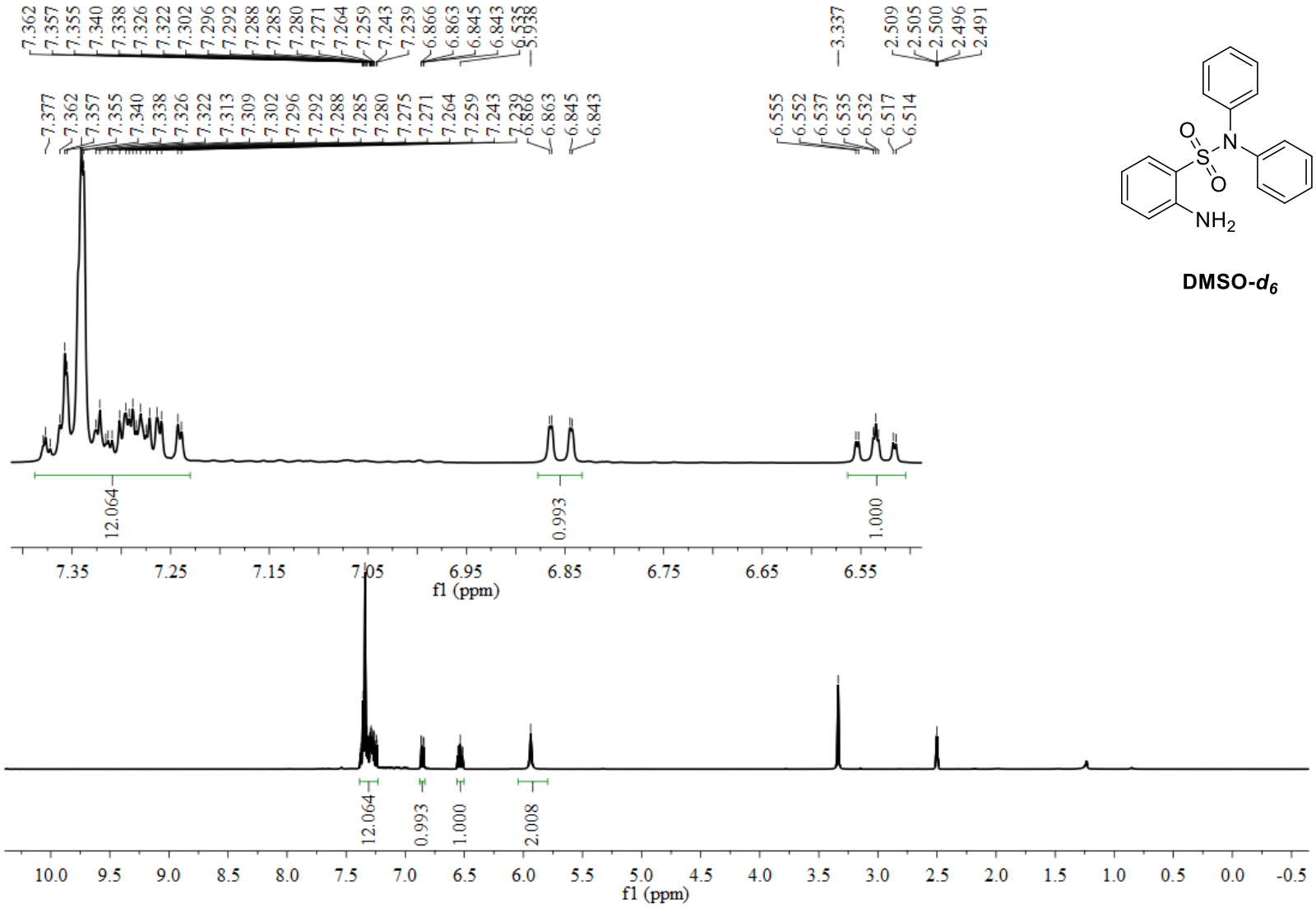

10.463
7.709
7.706
7.689
7.686
7.533
7.373
7.369
7.355
7.353
7.339
7.334
7.322
7.318
7.226
7.205
7.186
7.154
7.136
7.118
7.105
7.086
7.070
7.067
7.048
7.046
7.013
6.995
6.977
6.845
6.843
6.825
6.807
6.805
3.334
2.508
2.504
2.499
2.495
1.000
1.003
3.019
2.080
6.030
1.046
0.998
7.75
7.65
7.55
7.45
7.35
7.25
7.15
7.05
6.95
6.85
f1 (ppm)



DMSO-d_6

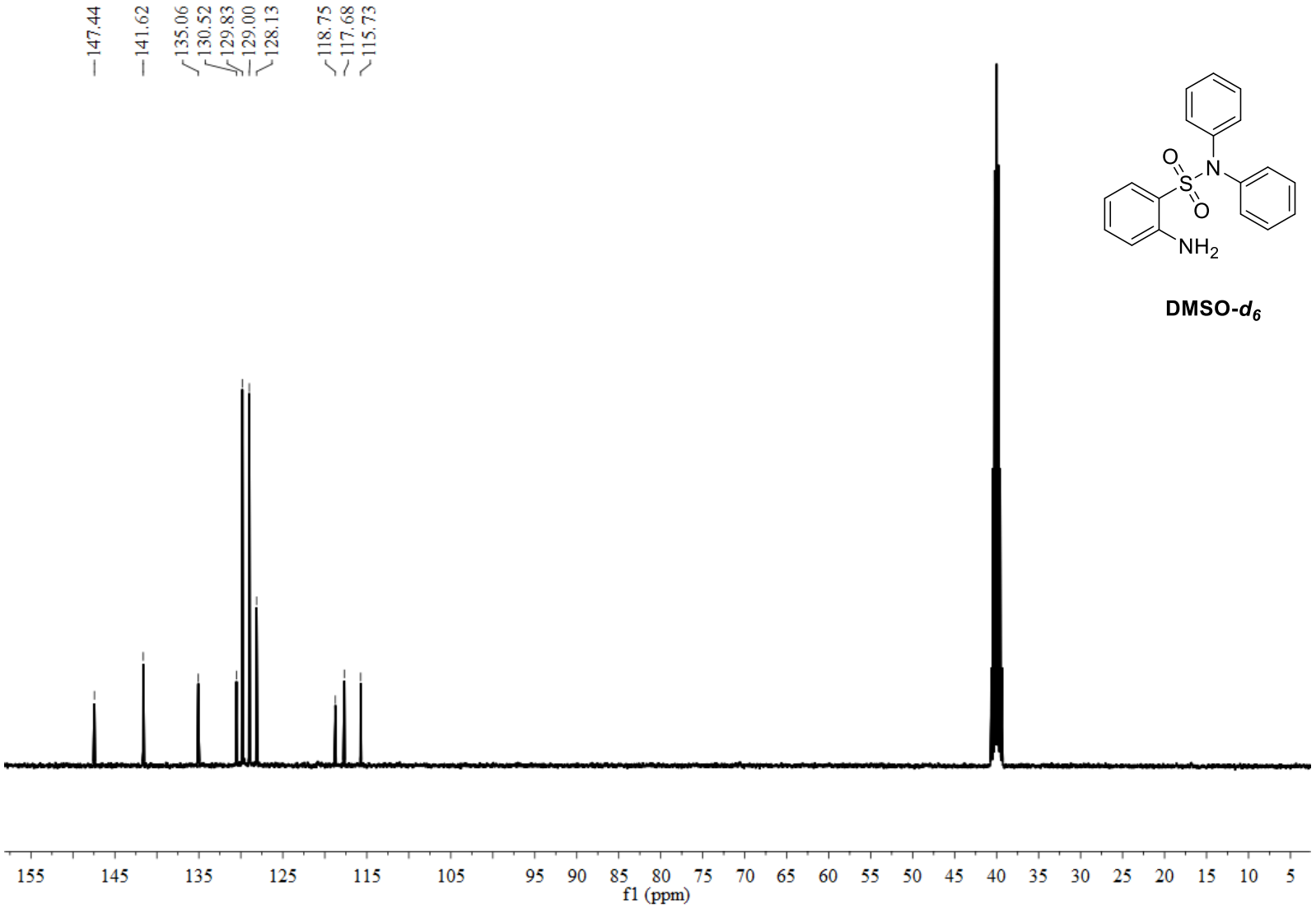

0.972
1.000
1.003
3.019
2.080
6.030
1.046
0.998
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

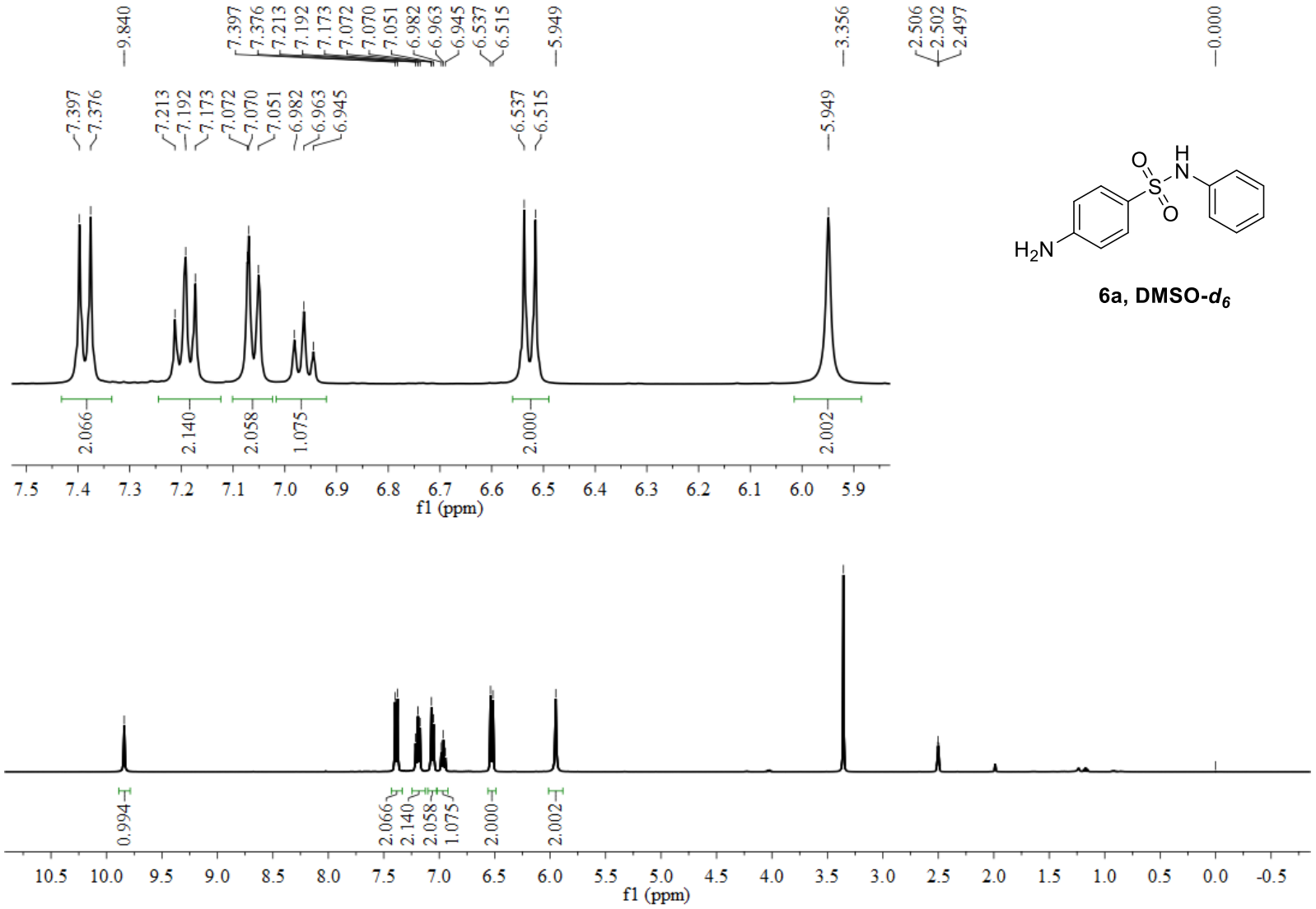

142.71
141.01
137.74
134.68
130.92
129.87
129.64
124.60
123.76
123.29
122.05
120.42
118.84
116.16
f1 (ppm)
f1 (ppm)
DMSO-d_6


7.362
7.357
7.355
7.340
7.338
7.326
7.322
7.302
7.296
7.292
7.288
7.285
7.280
7.271
7.264
7.259
7.243
7.239
6.866
6.863
6.845
6.843
6.535
5.938
3.337
2.509
2.505
2.500
2.496
2.491
7.377
7.362
7.357
7.355
7.340
7.338
7.326
7.322
7.313
7.309
7.302
7.296
7.292
7.288
7.285
7.280
7.275
7.271
7.264
7.259
7.243
7.239
6.866
6.863
6.845
6.843
6.555
6.552
6.537
6.535
6.532
6.517
6.514
12.064
0.993
1.000
7.35
7.25
7.15
7.05
6.95
6.85
6.75
6.65
6.55
f1 (ppm)
12.064
0.993
1.000
2.008
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

O
S
O
N
NH2

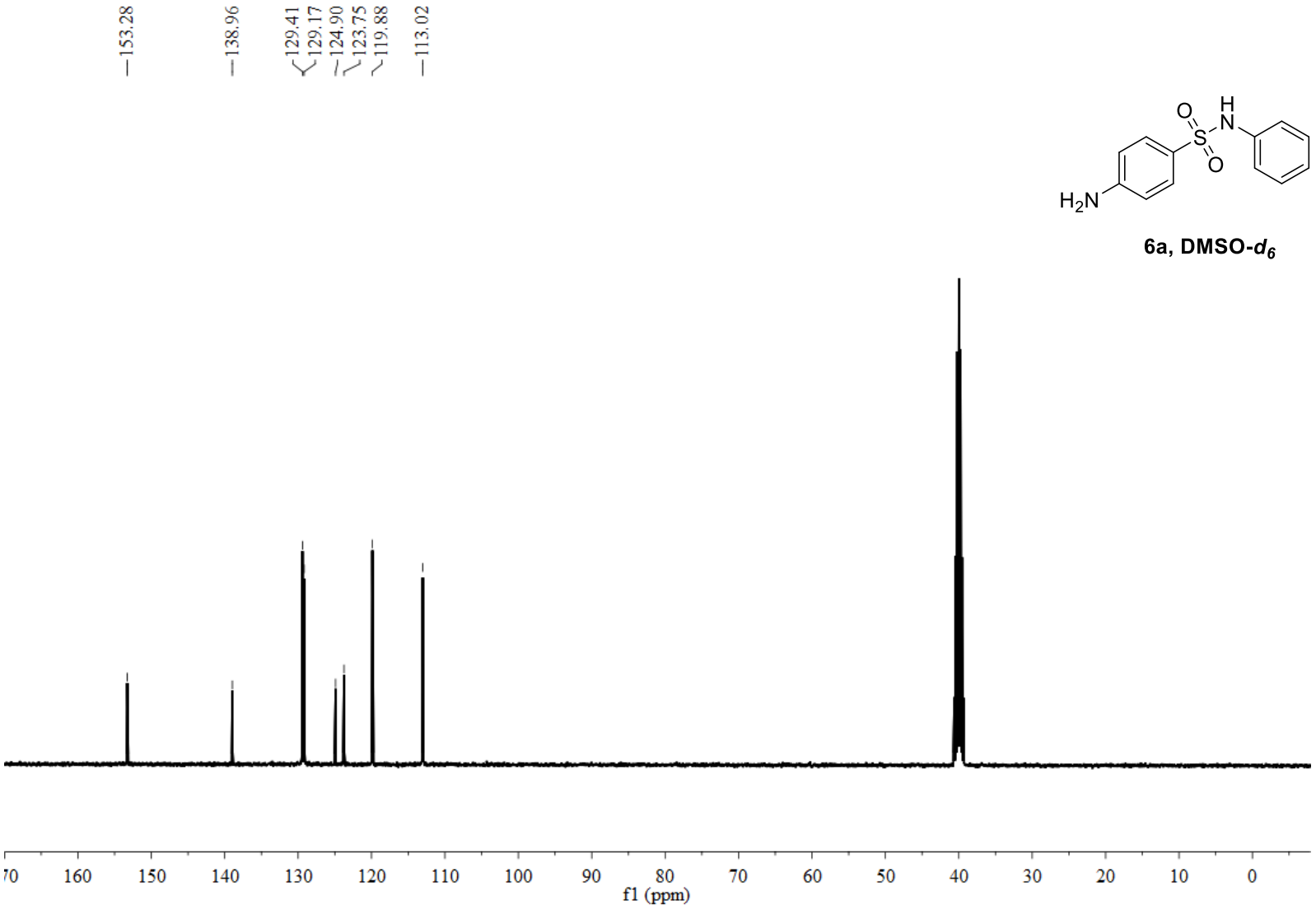
DMSO-d_6

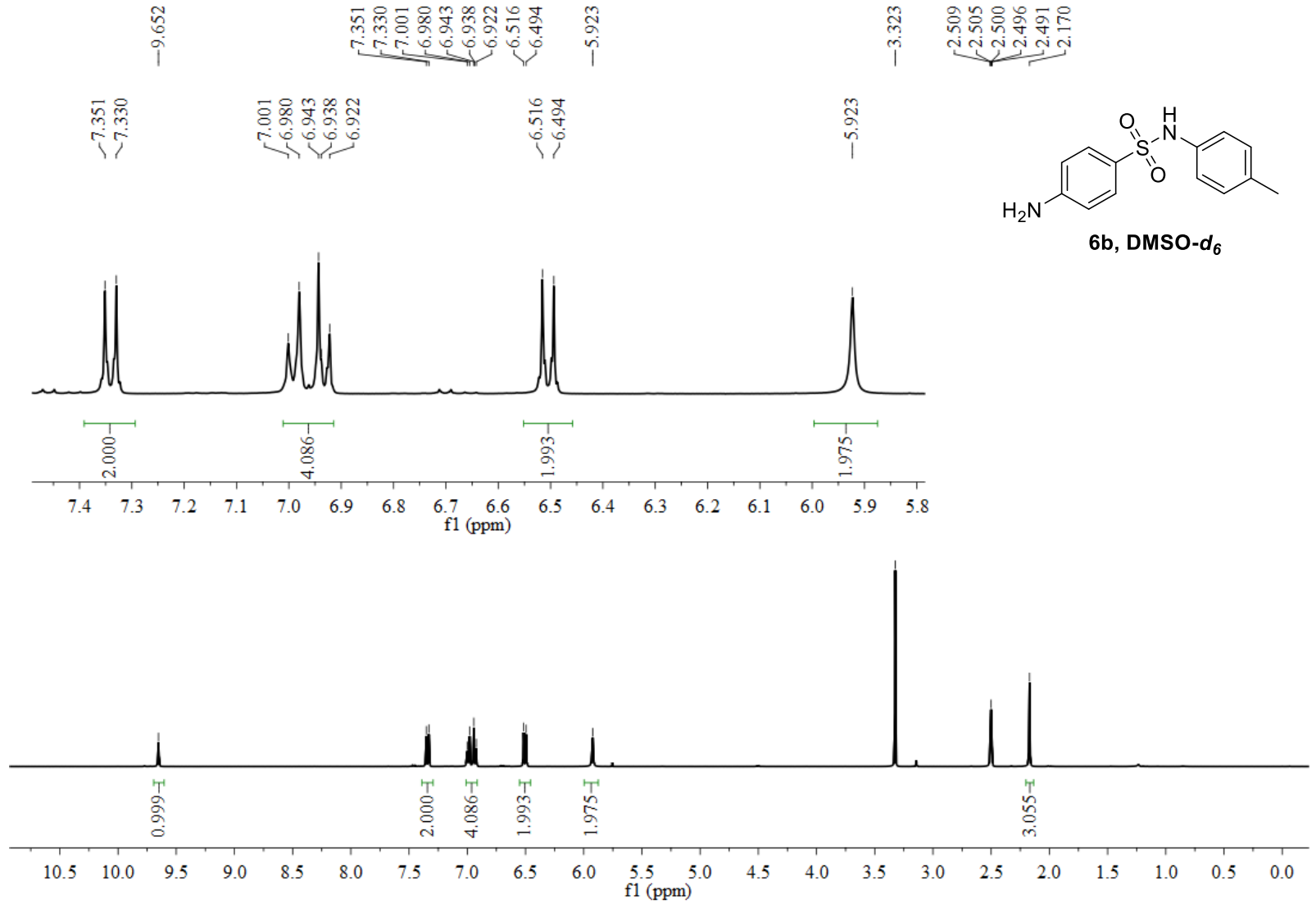

147.44
141.62
135.06
130.52
129.83
129.00
128.13
118.75
117.68
115.73
O
S
N
O
NH2
DMSO-d6
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
f1 (ppm)


9.840
7.397
7.376
7.213
7.192
7.173
7.072
7.070
7.051
6.982
6.963
6.945
6.537
6.515
5.949
3.356
2.506
2.502
2.497
0.000
2.066
2.140
2.058
1.075
2.000
2.002
f1 (ppm)
0.994
f1 (ppm)

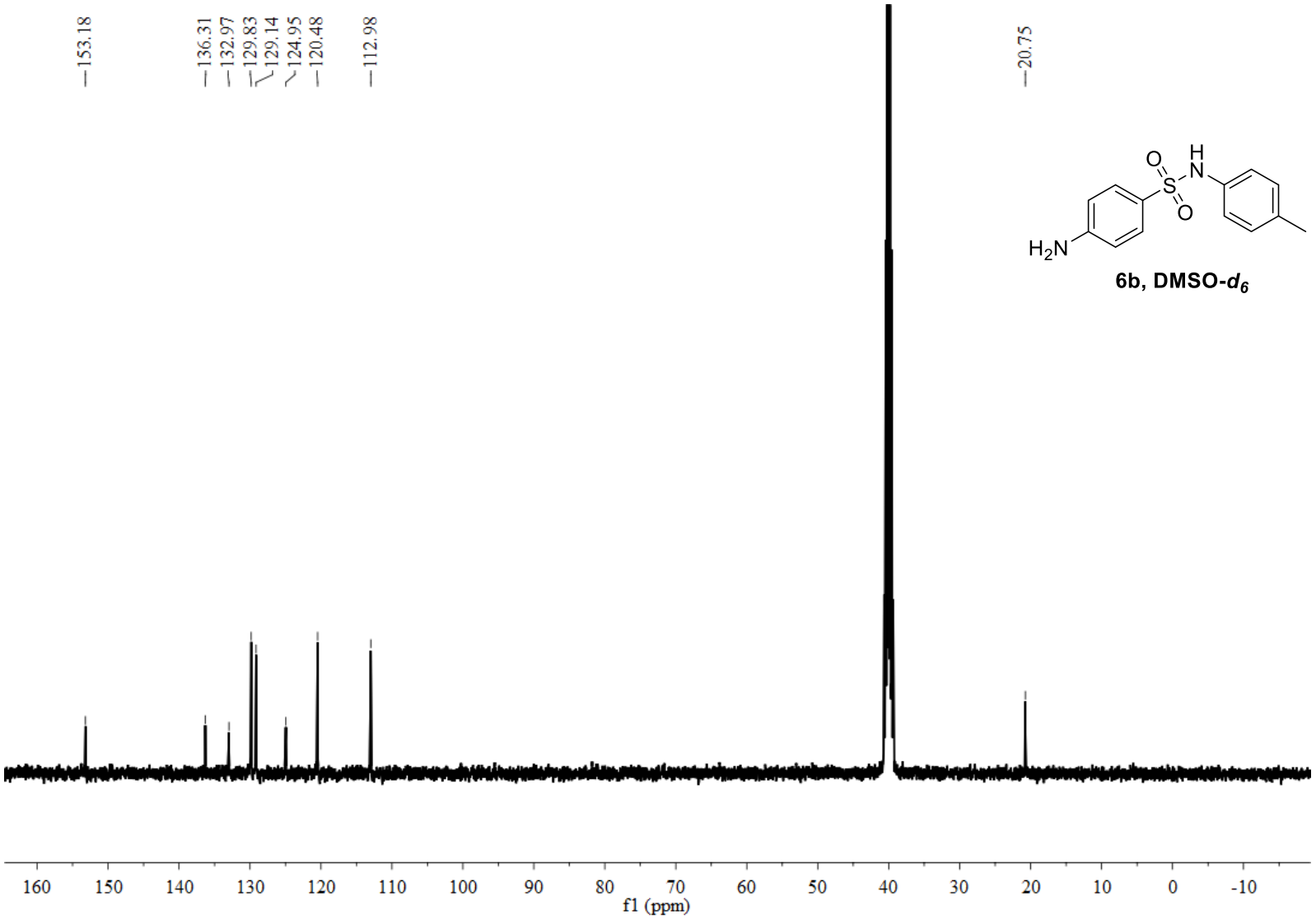
O
H
N
S
O
H_2N

6a, DMSO-*d*$_6$


153.28
138.96
129.41
129.17
124.90
123.75
119.88
113.02
O
H
N
S
O
H2N
6a, DMSO-d6
70
160
150
140
130
120
110
100
90
80
f1 (ppm)
70
60
50
40
30
20
10
0

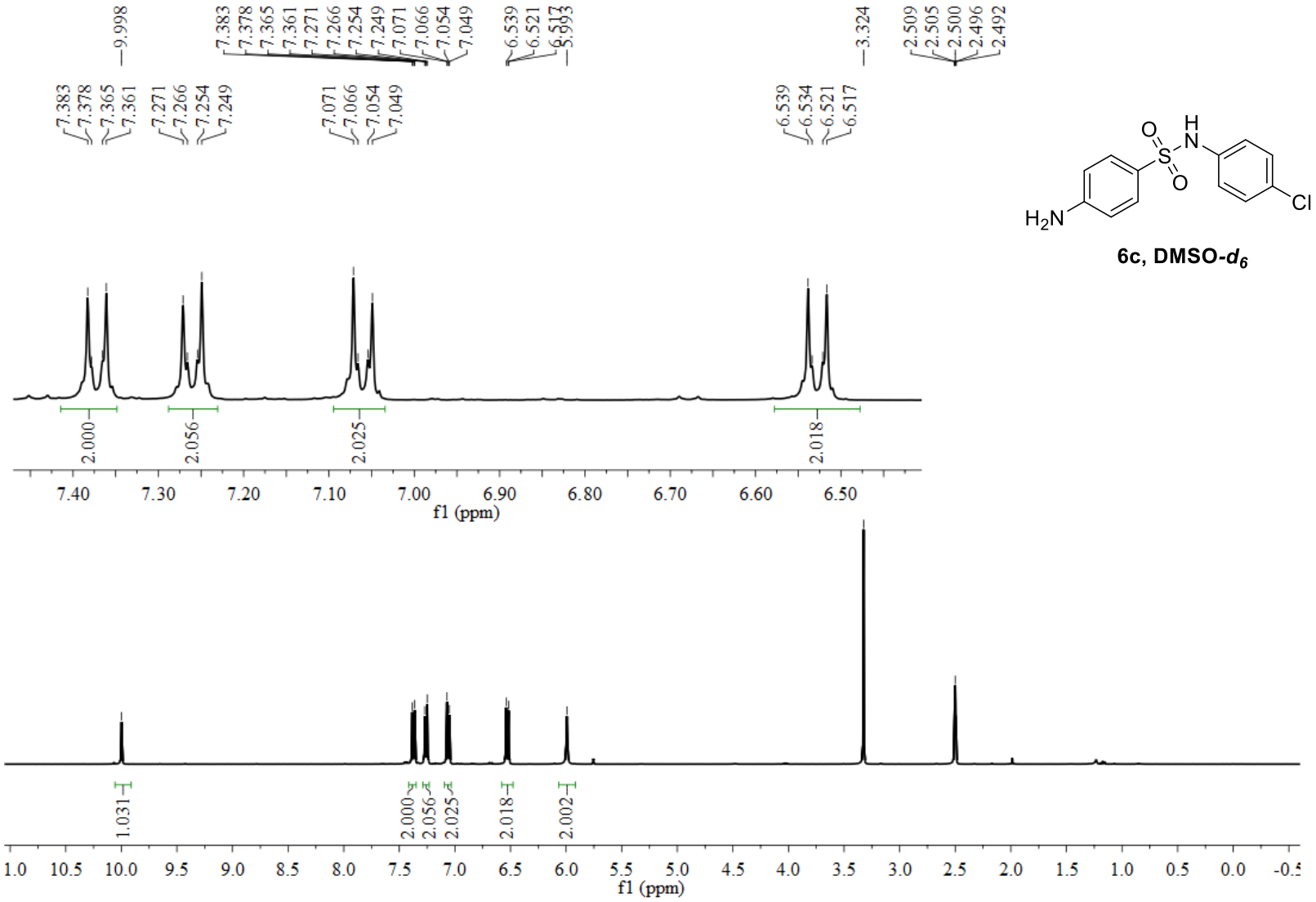

9.652
7.351
7.330
7.001
6.980
6.943
6.938
6.922
6.516
6.494
5.923
3.323
2.509
2.505
2.500
2.496
2.491
2.170
2.000
4.086
1.993
1.975
f1 (ppm)
0.999
2.000
4.086
1.993
1.975
3.055
f1 (ppm)

6b, DMSO-d_6

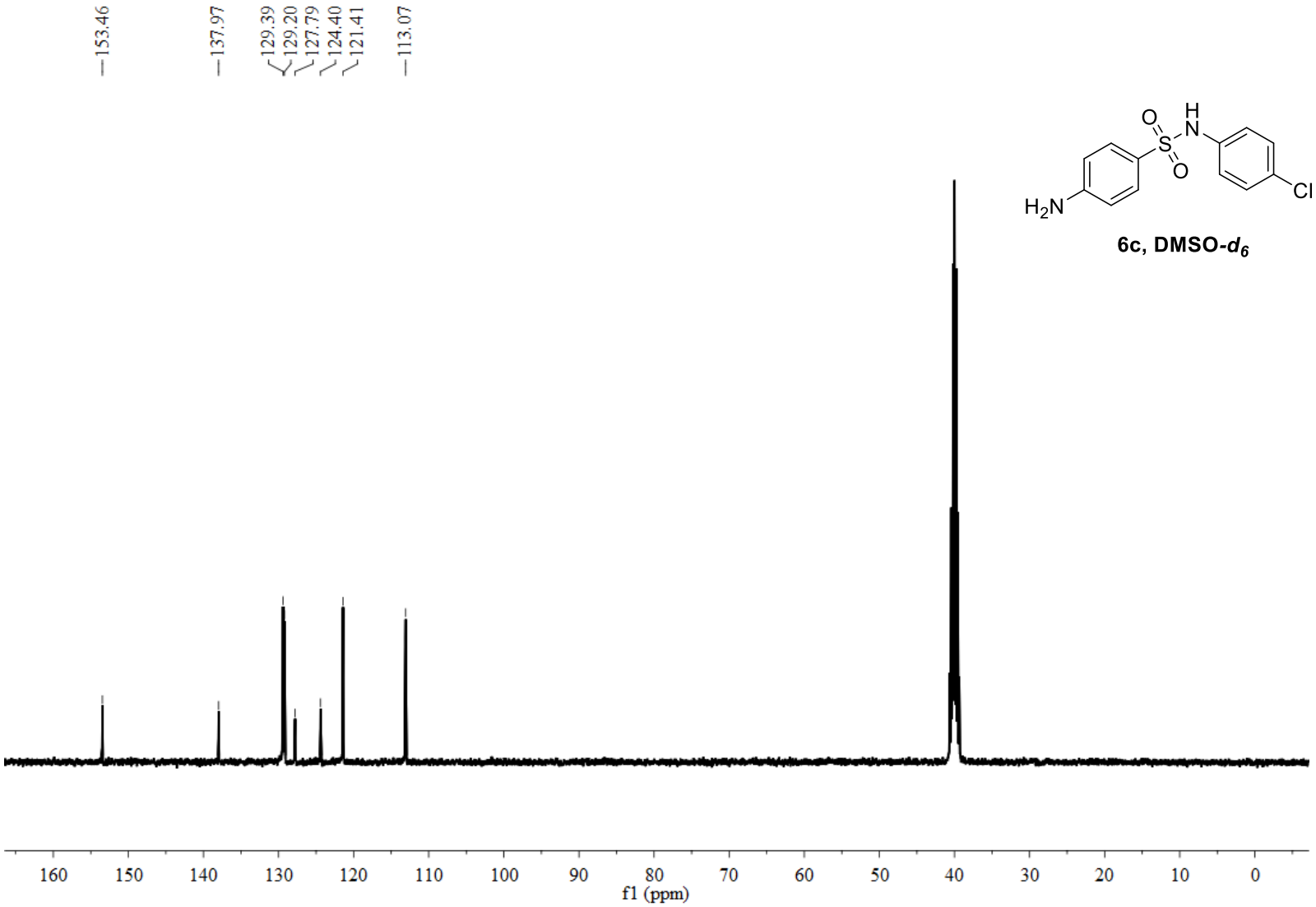

153.18
136.31
132.97
129.83
129.14
124.95
120.48
112.98
20.75
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

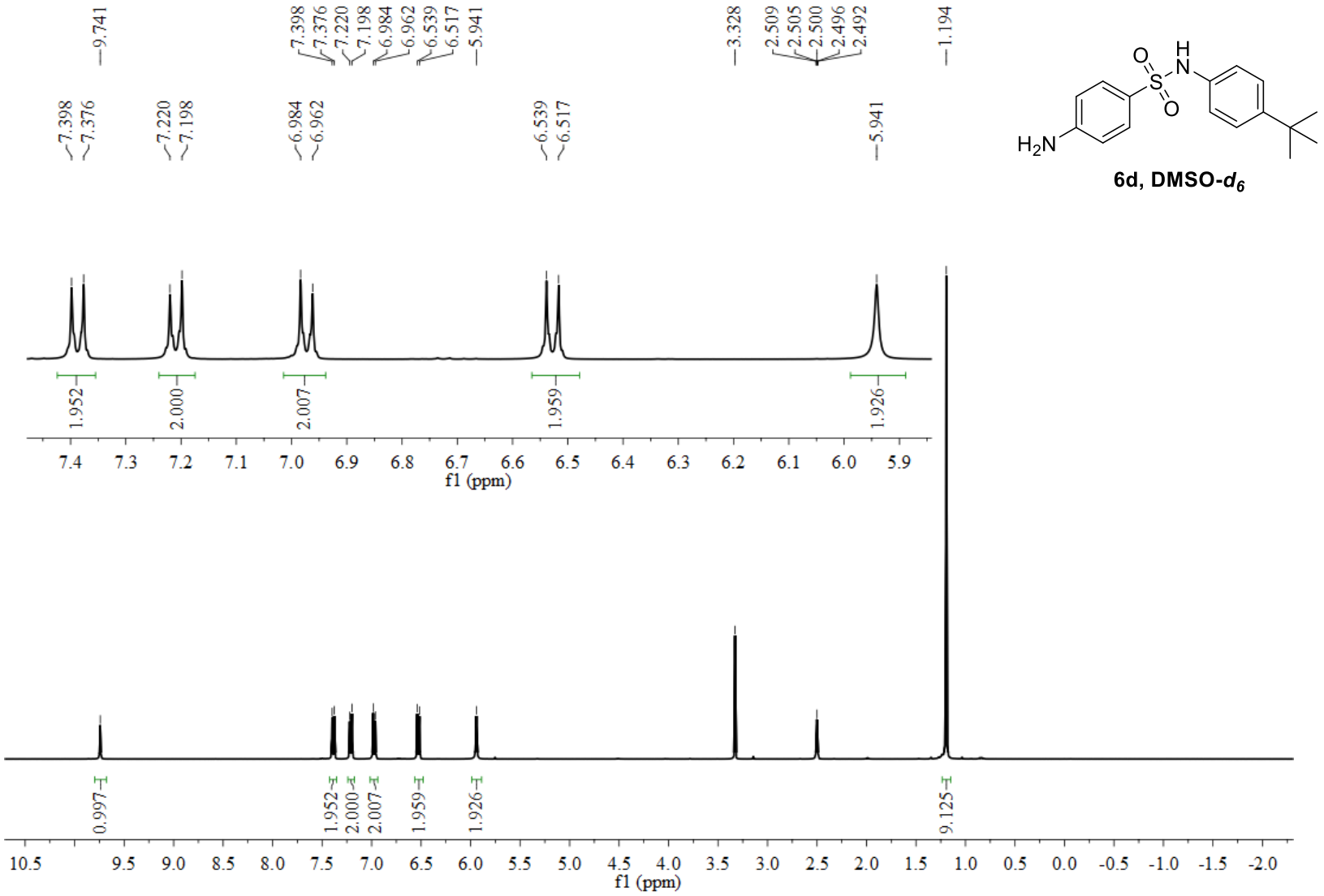
O
H
N
S
O
H2N

6b, DMSO-d_6

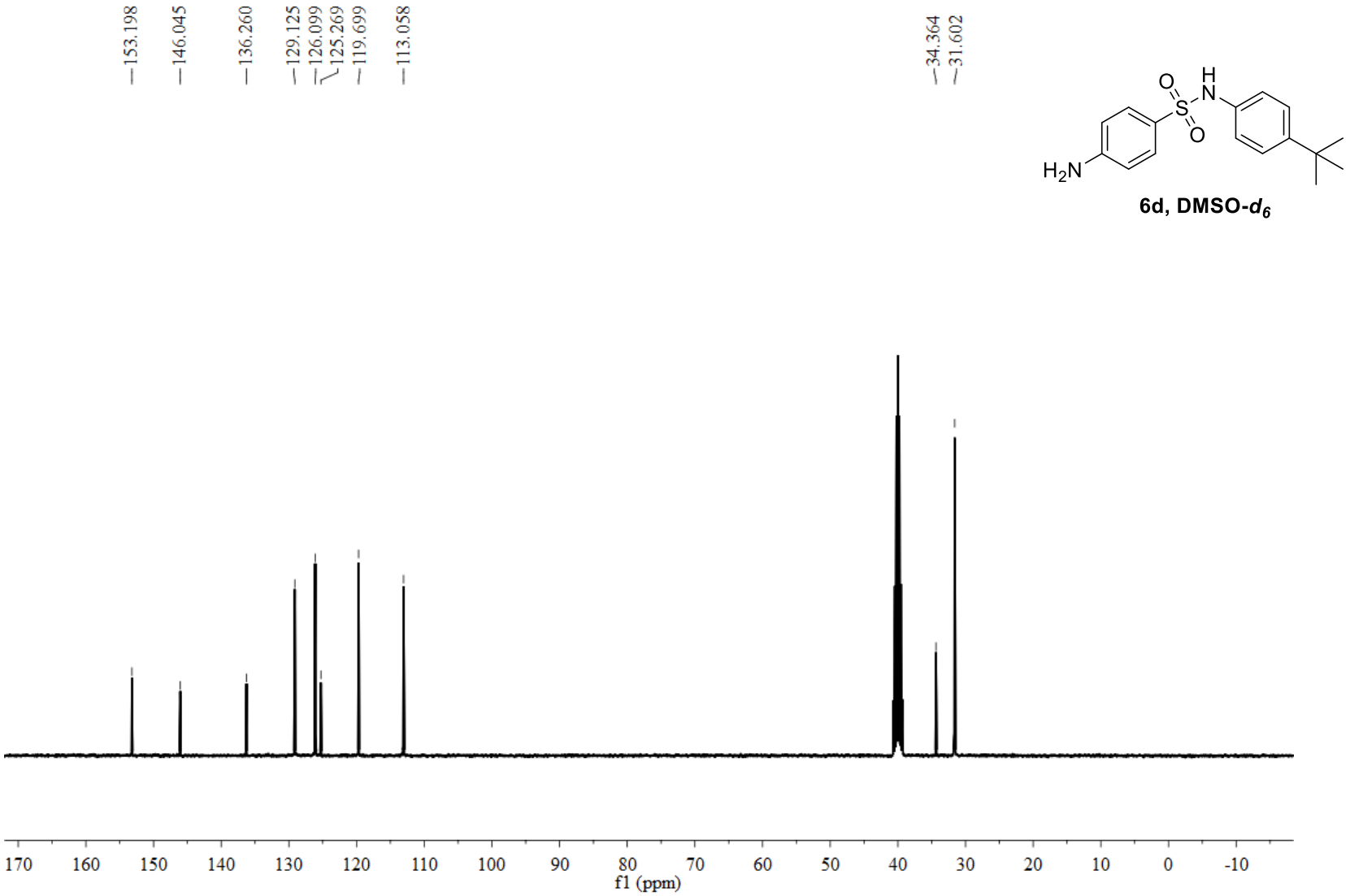

9.998
7.383
7.378
7.365
7.361
7.271
7.266
7.254
7.249
7.071
7.066
7.054
7.049
6.539
6.521
6.517
5.993
3.324
2.509
2.505
2.500
2.496
2.492
2.000
2.056
2.025
2.018
f1 (ppm)
1.031
2.000
2.056
2.025
2.018
2.002
f1 (ppm)

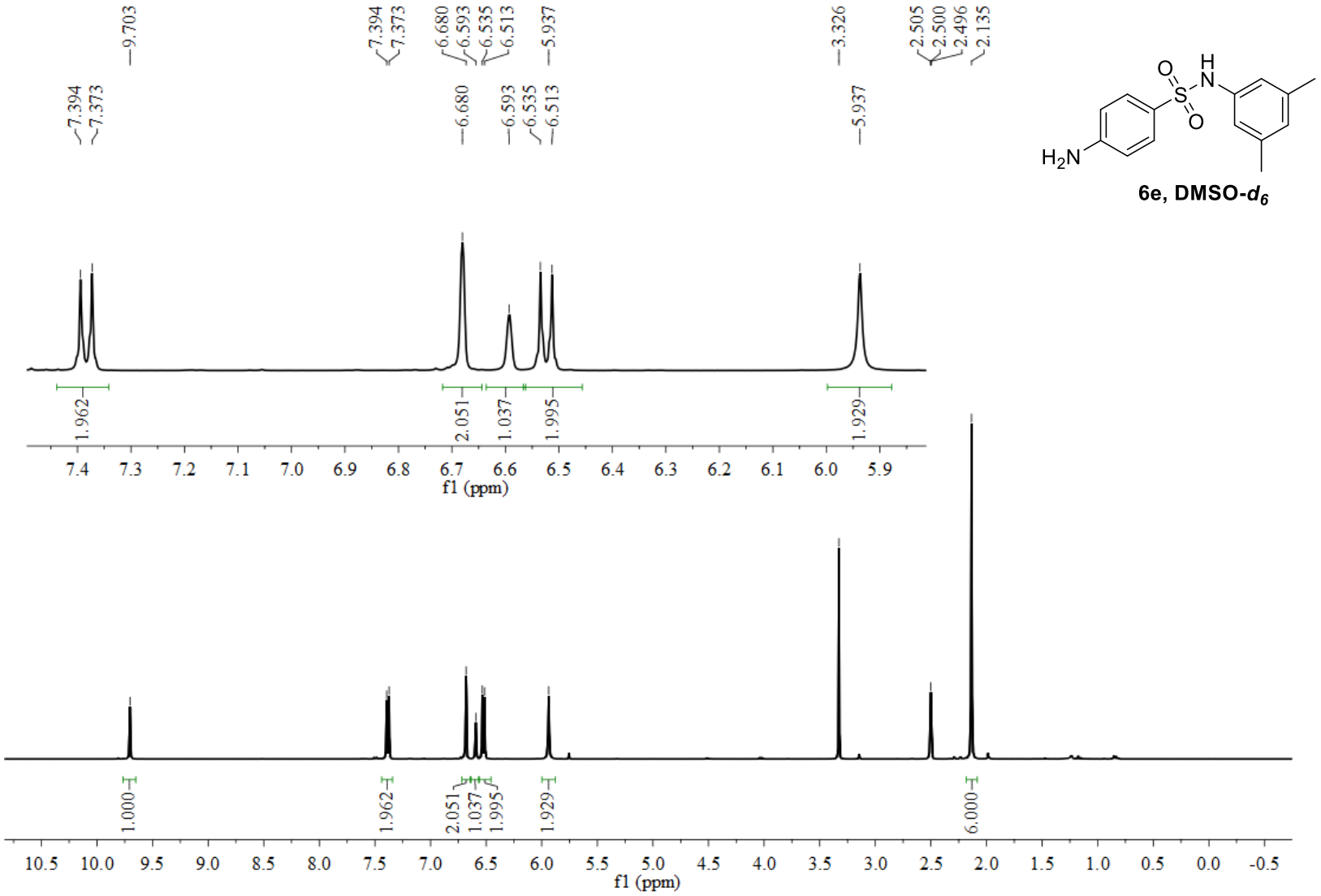
6c, DMSO-d_6

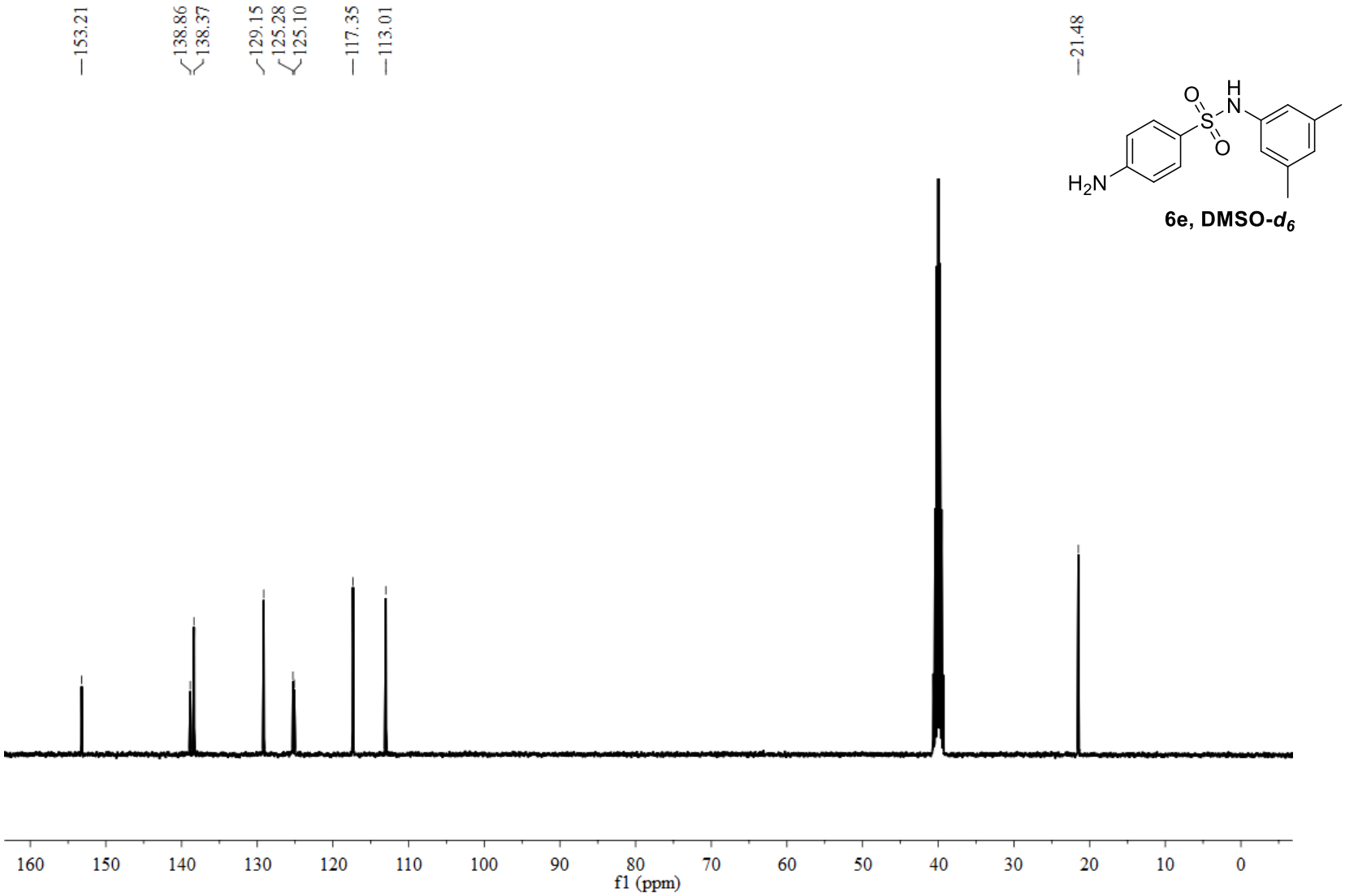

153.46
137.97
129.39
129.20
127.79
124.40
121.41
113.07
O
H
N
S
O
H2N
Cl
6c, DMSO-d6
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

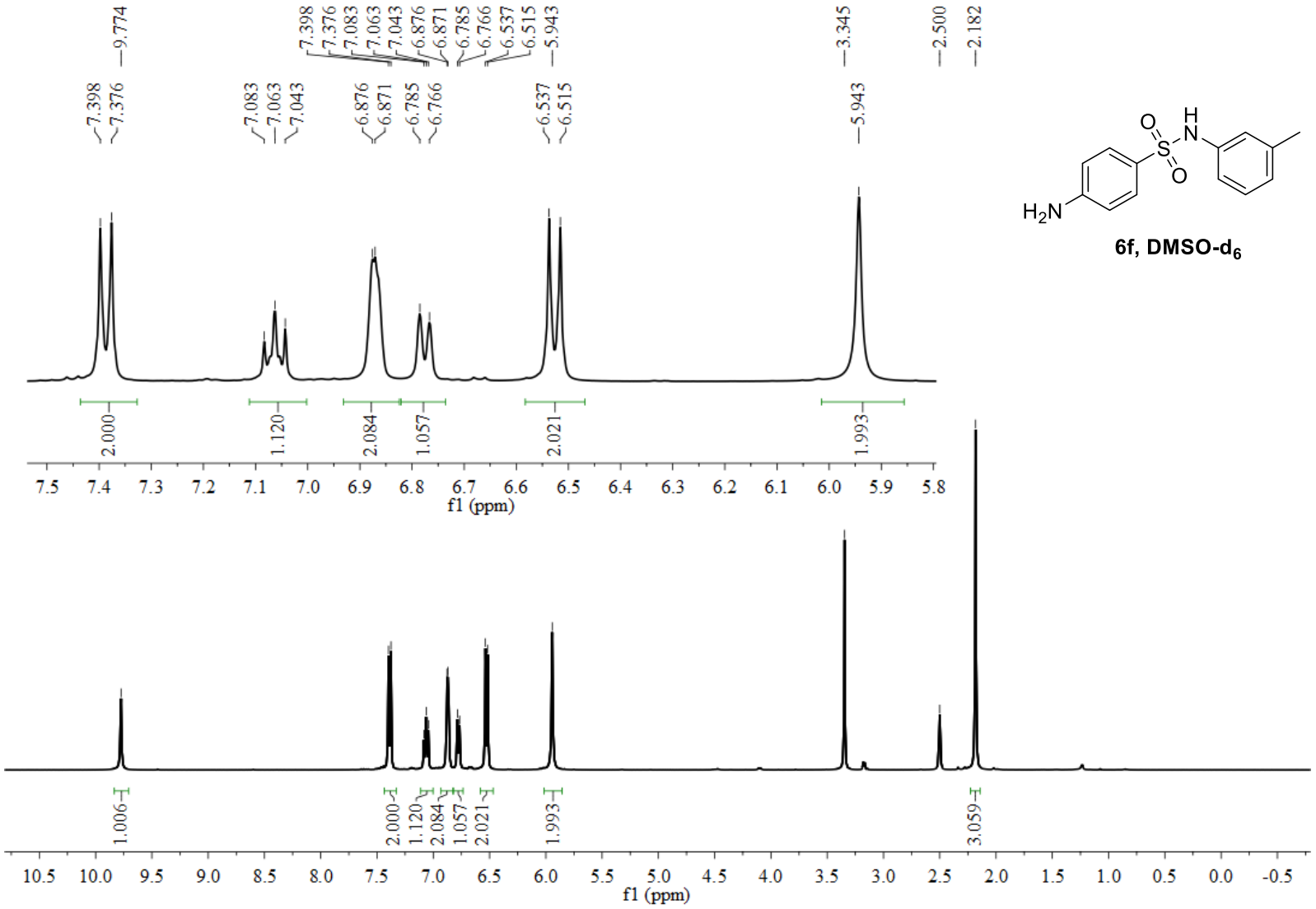

9.741
7.398
7.376
7.220
7.198
6.984
6.962
6.539
6.517
5.941
3.328
2.509
2.505
2.500
2.496
2.492
1.194
1.952
2.000
2.007
1.959
1.926
f1 (ppm)
0.997
1.952
2.000
2.007
1.959
1.926
9.125
f1 (ppm)

6d, DMSO-d_6

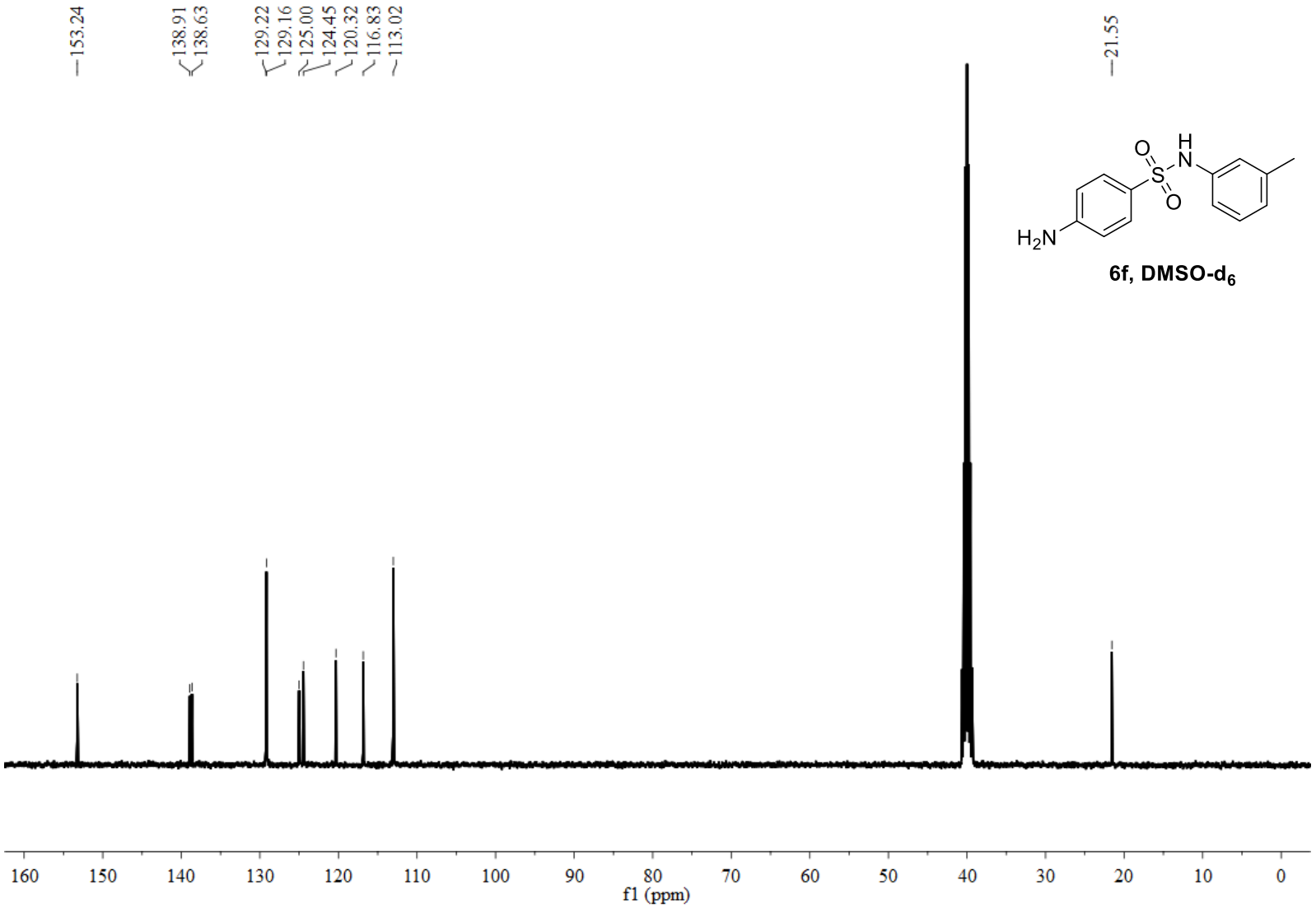

153.198
146.045
136.260
129.125
126.099
125.269
119.699
113.058
34.364
31.602
O
H
N
S
O
H_2N
6d, DMSO-d_6
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

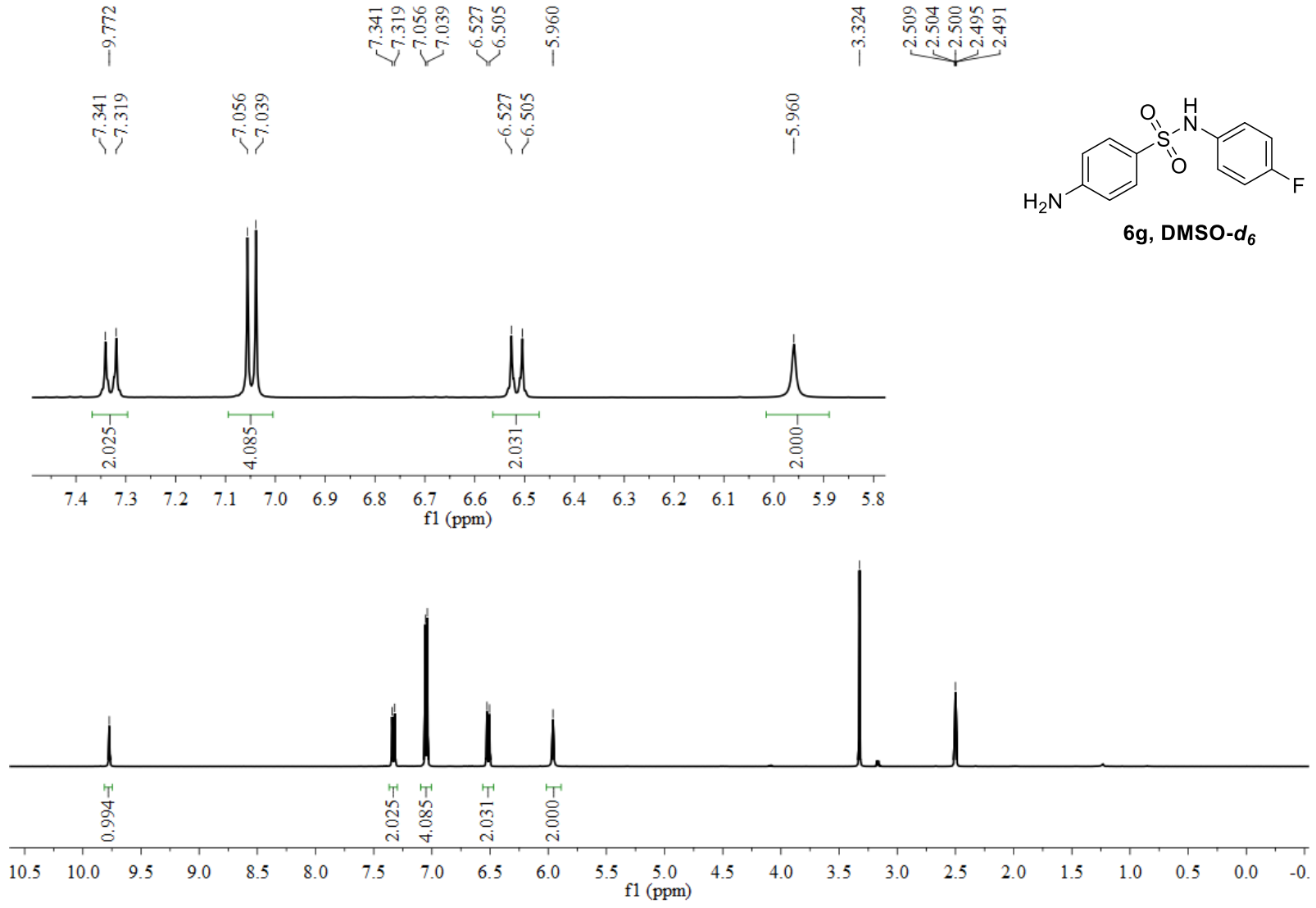

9.703
7.394
7.373
6.680
6.593
6.535
6.513
5.937
3.326
2.505
2.500
2.496
2.135
1.962
2.051
1.037
1.995
1.929
1.000
6.000
f1 (ppm)
6e, DMSO-d6


153.21
138.86
138.37
129.15
125.28
125.10
117.35
113.01
21.48
H2N
O
S
O
H
N
6e, DMSO-d6
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.774
7.398
7.376
7.083
7.063
7.043
6.876
6.871
6.785
6.766
6.537
6.515
5.943
3.345
2.500
2.182
2.000
1.120
2.084
1.057
2.021
1.993
f1 (ppm)
1.006
2.000
1.120
2.084
1.057
2.021
1.993
3.059
f1 (ppm)

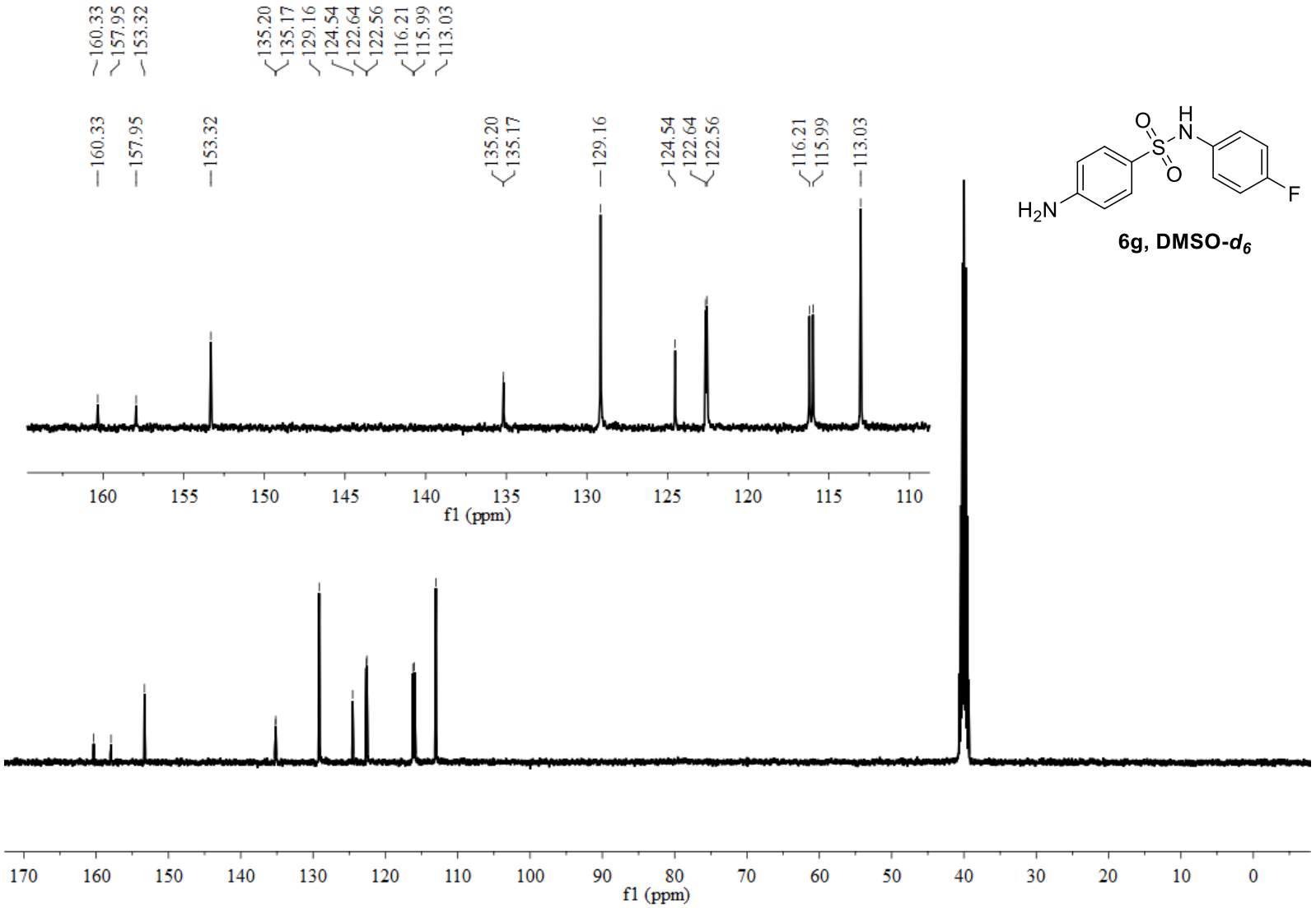
6f, DMSO-d_6

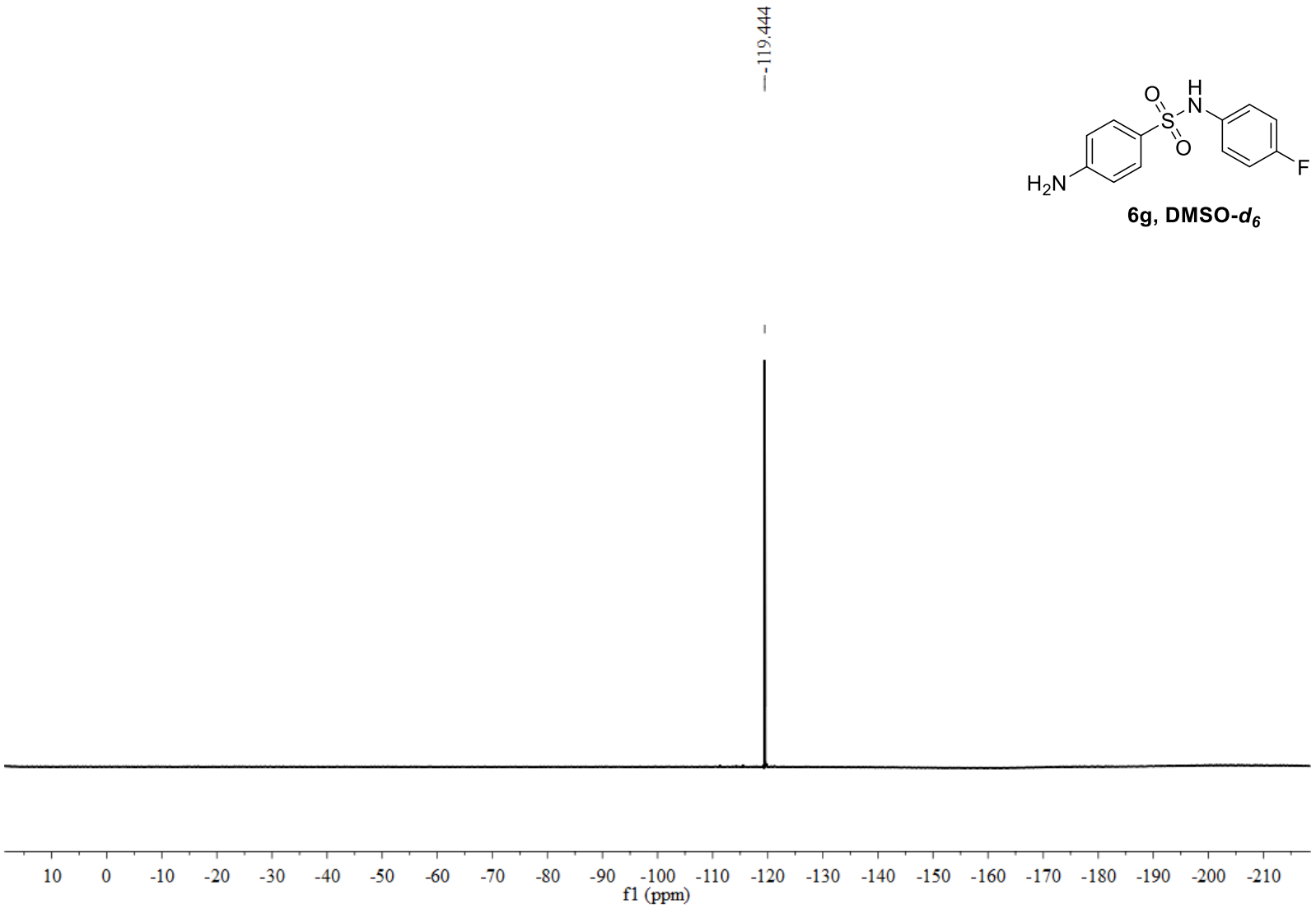

153.24
138.91
138.63
129.22
129.16
125.00
124.45
120.32
116.83
113.02
21.55
H2N
O
S
O
H
N
6f, DMSO-d6
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.772
7.341
7.319
7.056
7.039
6.527
6.505
5.960
3.324
2.509
2.504
2.500
2.495
2.491
2.025
4.085
2.031
2.000
f1 (ppm)
0.994
2.025
4.085
2.031
2.000
f1 (ppm)

O
H
N
S
O
H2N
F

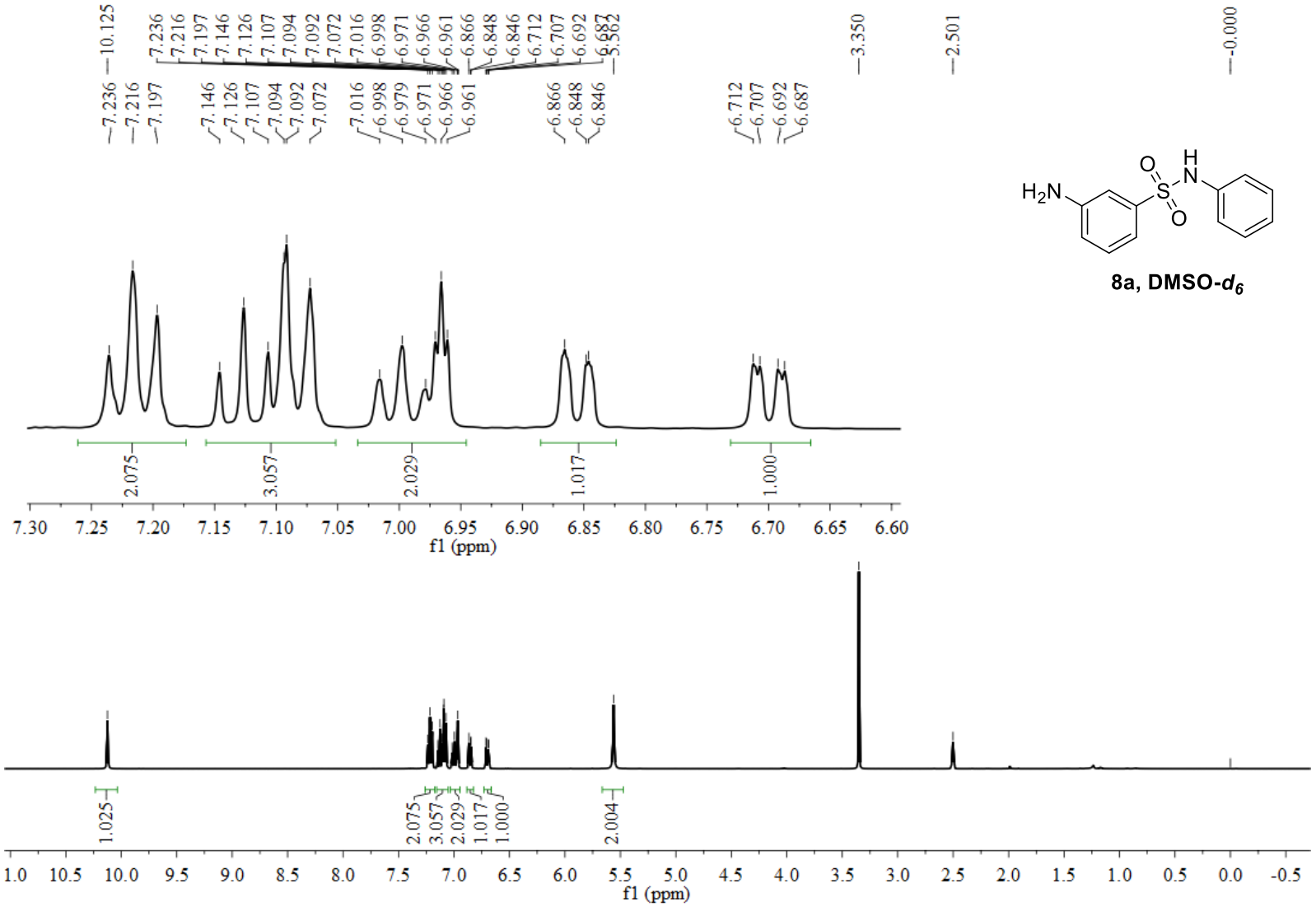
6g, DMSO-d_6


160.33
157.95
153.32
135.20
135.17
129.16
124.54
122.64
122.56
116.21
115.99
113.03
160
155
150
145
140
135
130
125
120
115
110
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
H2N
O
S
O
H
N
F
6g, DMSO-d6


-119.444
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

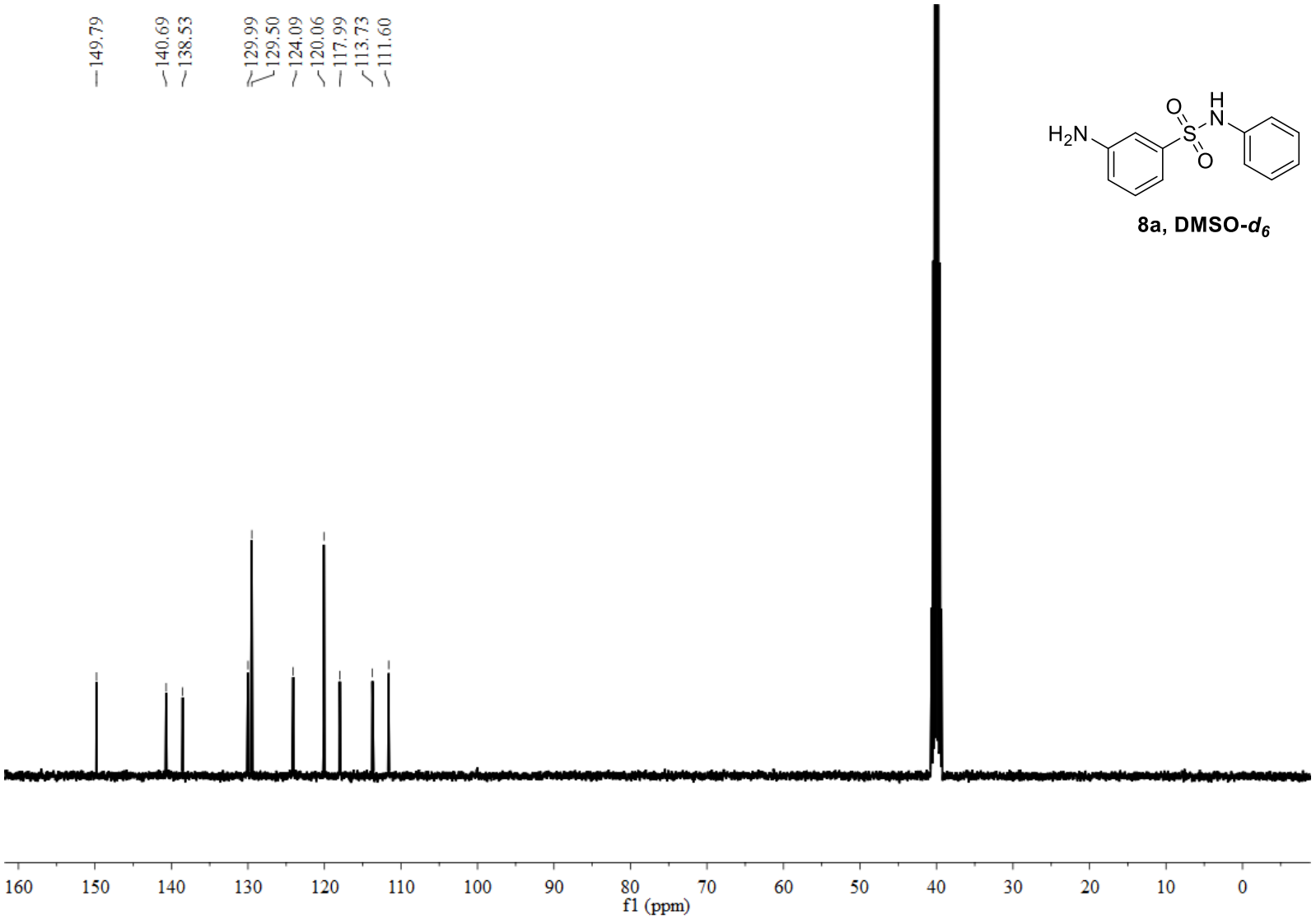
O
H
N
S
O
H2N
F

6g, DMSO-d_6


10.125
7.236
7.216
7.197
7.146
7.126
7.107
7.094
7.092
7.072
7.016
6.998
6.979
6.971
6.966
6.961
6.866
6.848
6.846
6.712
6.707
6.692
6.687
5.582
3.350
2.501
-0.000
2.075
3.057
2.029
1.017
1.000
f1 (ppm)
1.025
2.004

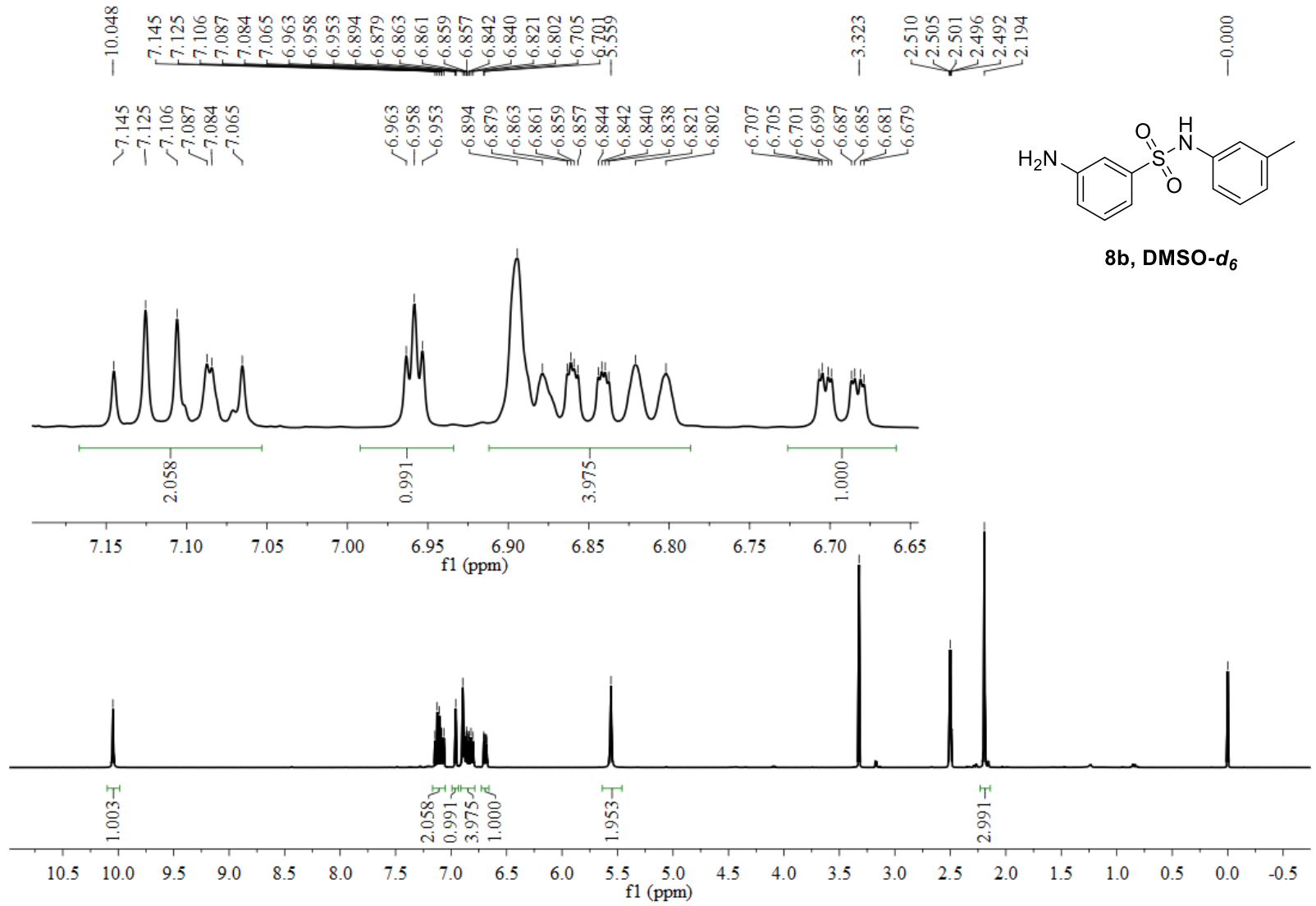
H2N
O
S
O
H
N

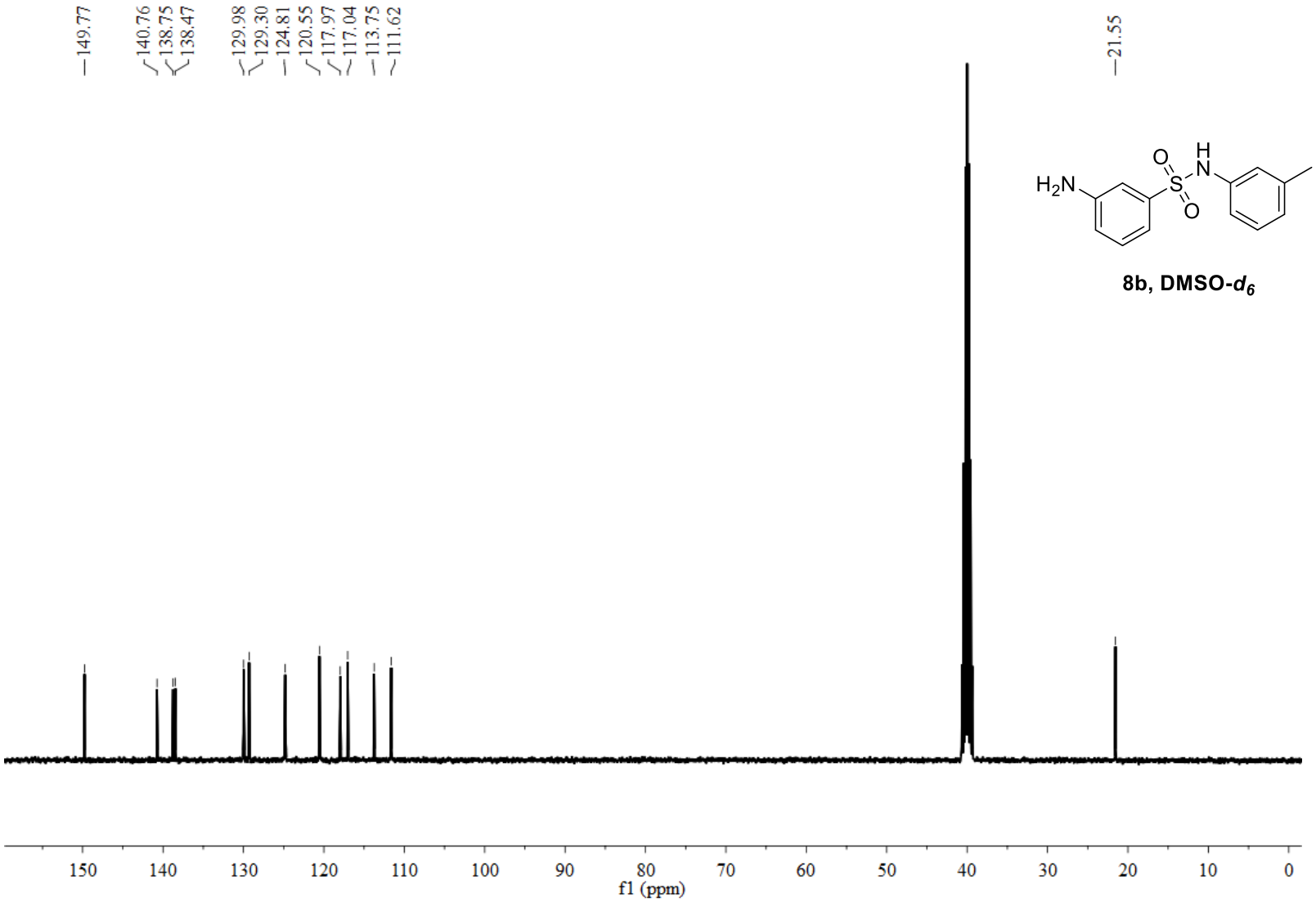
8a, DMSO-*d*$_6$


149.79
140.69
138.53
129.99
129.50
124.09
120.06
117.99
113.73
111.60
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

H2N
O
S
O
H
N

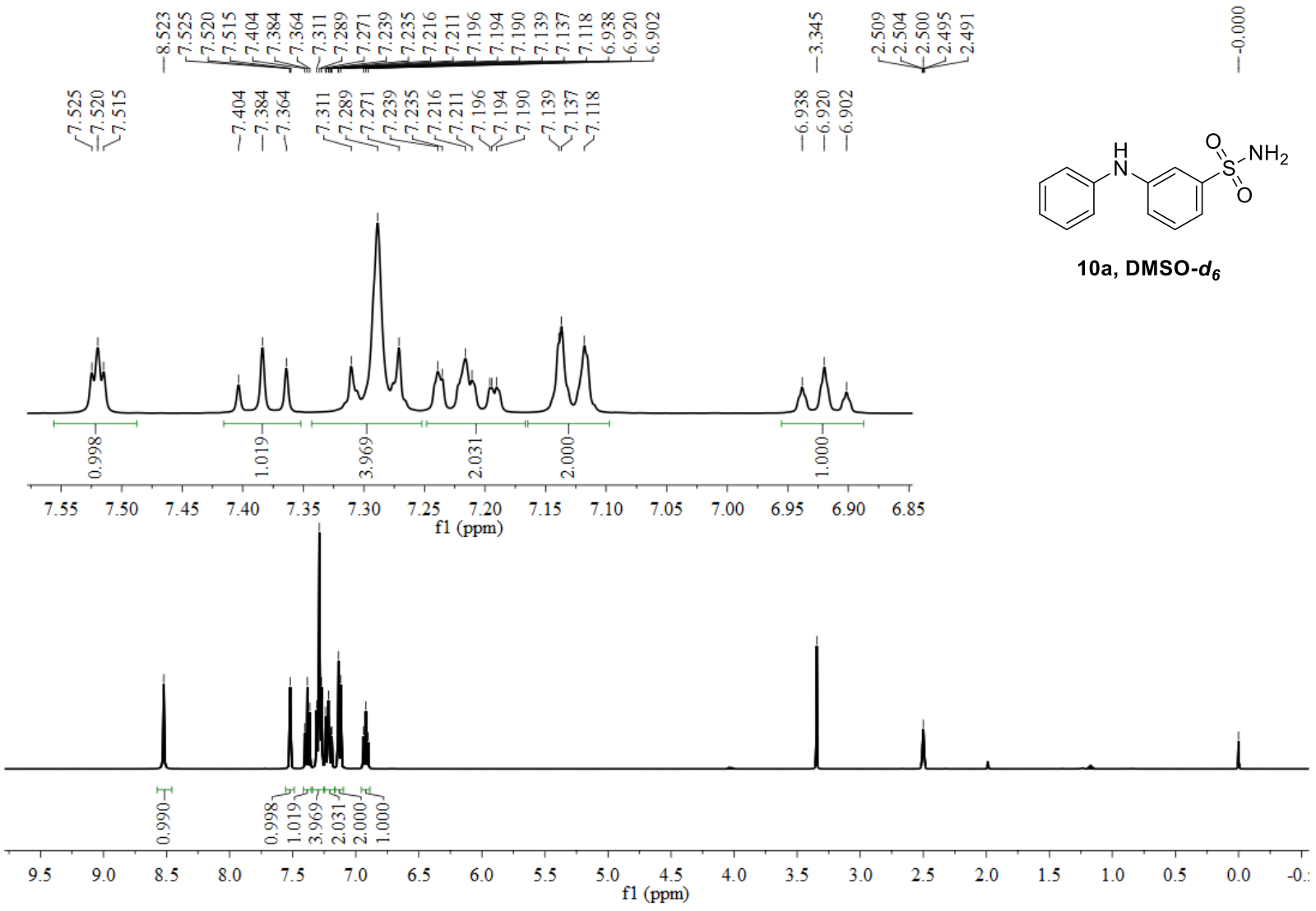
8a, DMSO-d_6


10.048
7.145
7.125
7.106
7.087
7.084
7.065
6.963
6.958
6.953
6.894
6.879
6.863
6.861
6.859
6.857
6.842
6.840
6.821
6.802
6.705
6.701
5.559
3.323
2.510
2.505
2.501
2.496
2.492
2.194
0.000
H2N
O
S
O
H
N
8b, DMSO-d6
2.058
0.991
3.975
1.000
f1 (ppm)
1.003
2.058
0.991
3.975
1.000
1.953
2.991
f1 (ppm)

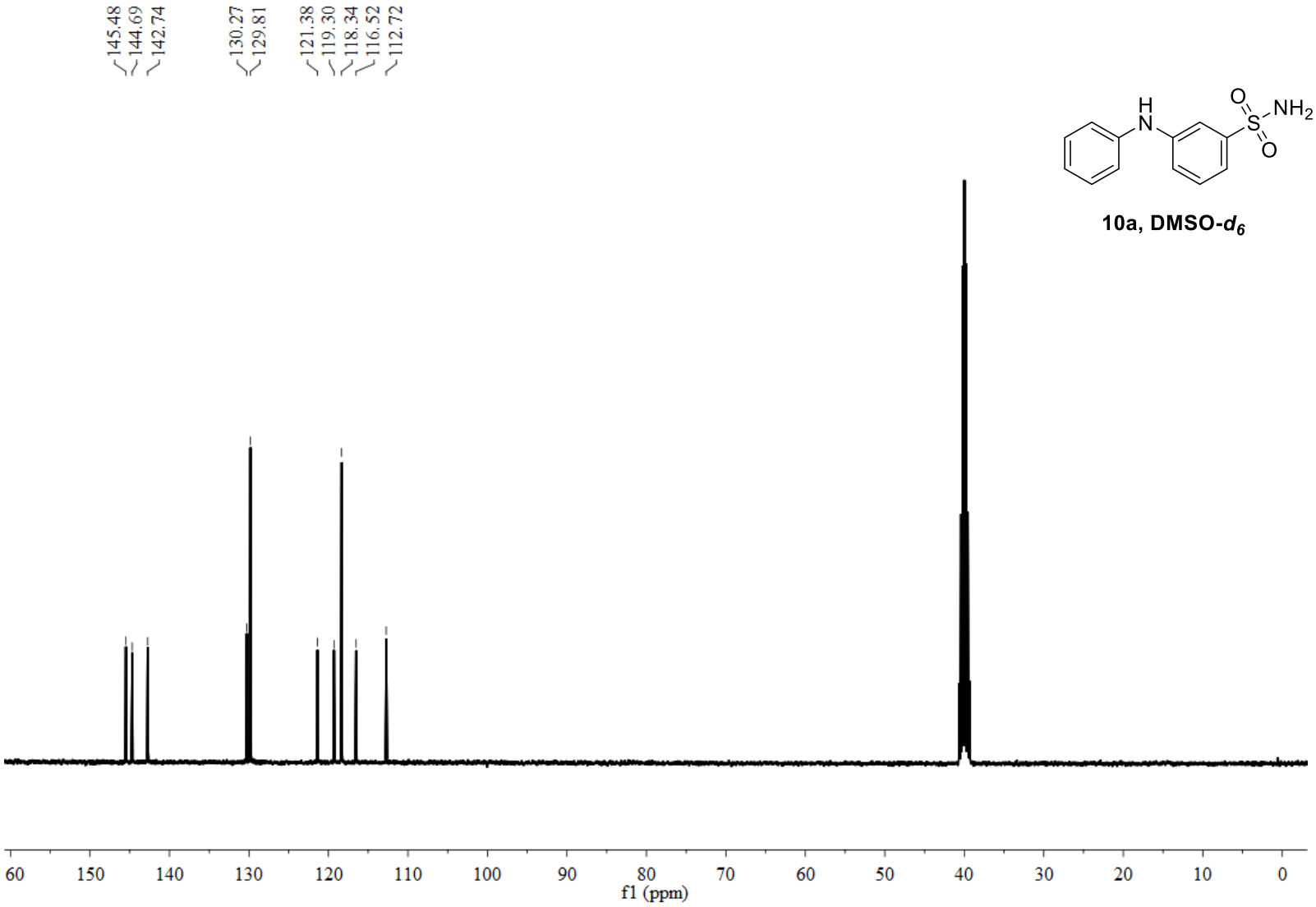

149.77
140.76
138.75
138.47
129.98
129.30
124.81
120.55
117.97
117.04
113.75
111.62
21.55
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

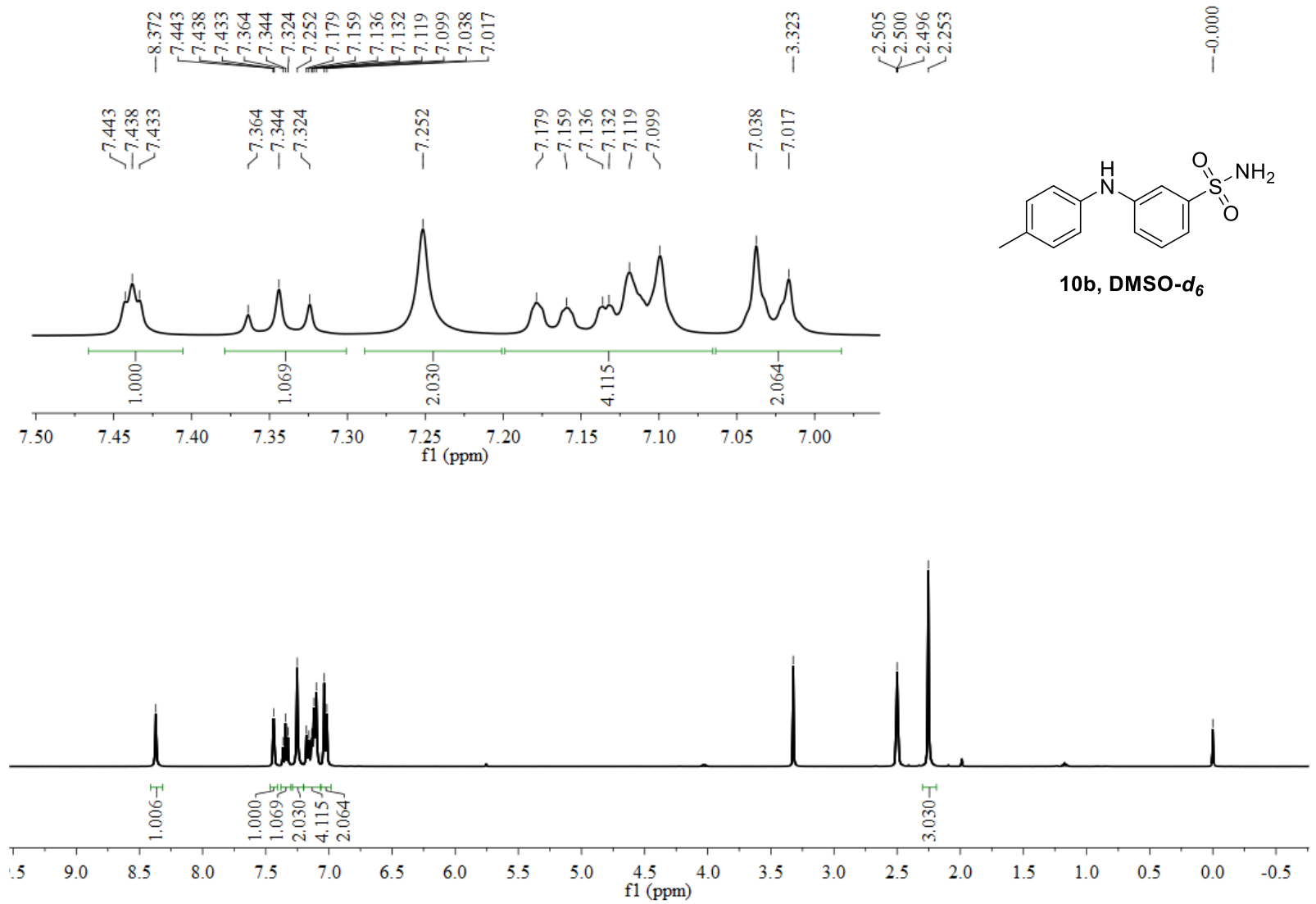
H2N
O
S
O
H
N

8b, DMSO-d_6

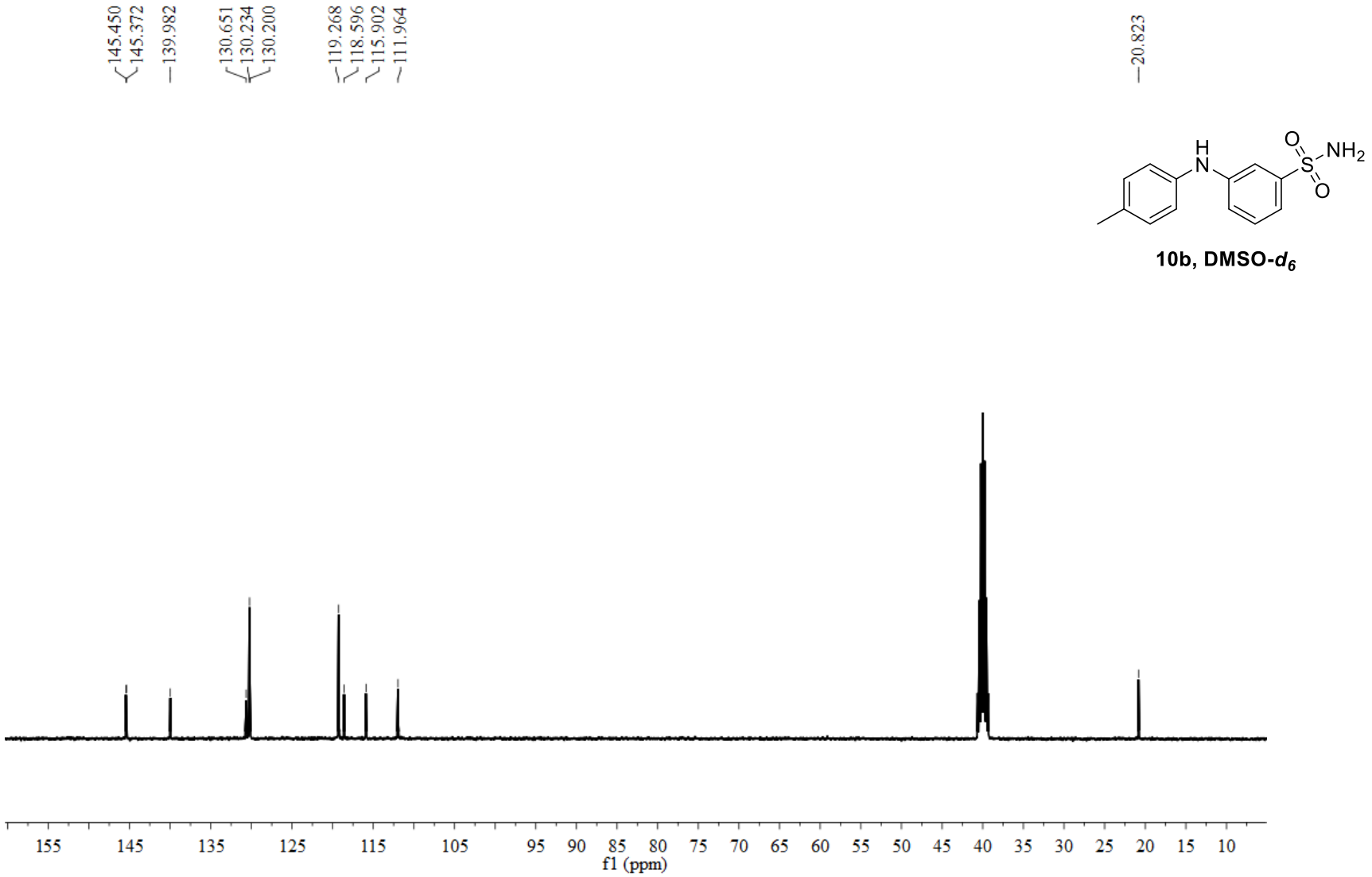

8.523
7.525
7.520
7.515
7.404
7.384
7.364
7.311
7.289
7.271
7.239
7.235
7.216
7.211
7.196
7.194
7.190
7.139
7.137
7.118
6.938
6.920
6.902
3.345
2.509
2.504
2.500
2.495
2.491
0.000
0.998
1.019
3.969
2.031
2.000
1.000
f1 (ppm)
0.990
f1 (ppm)

10a, DMSO-d_6

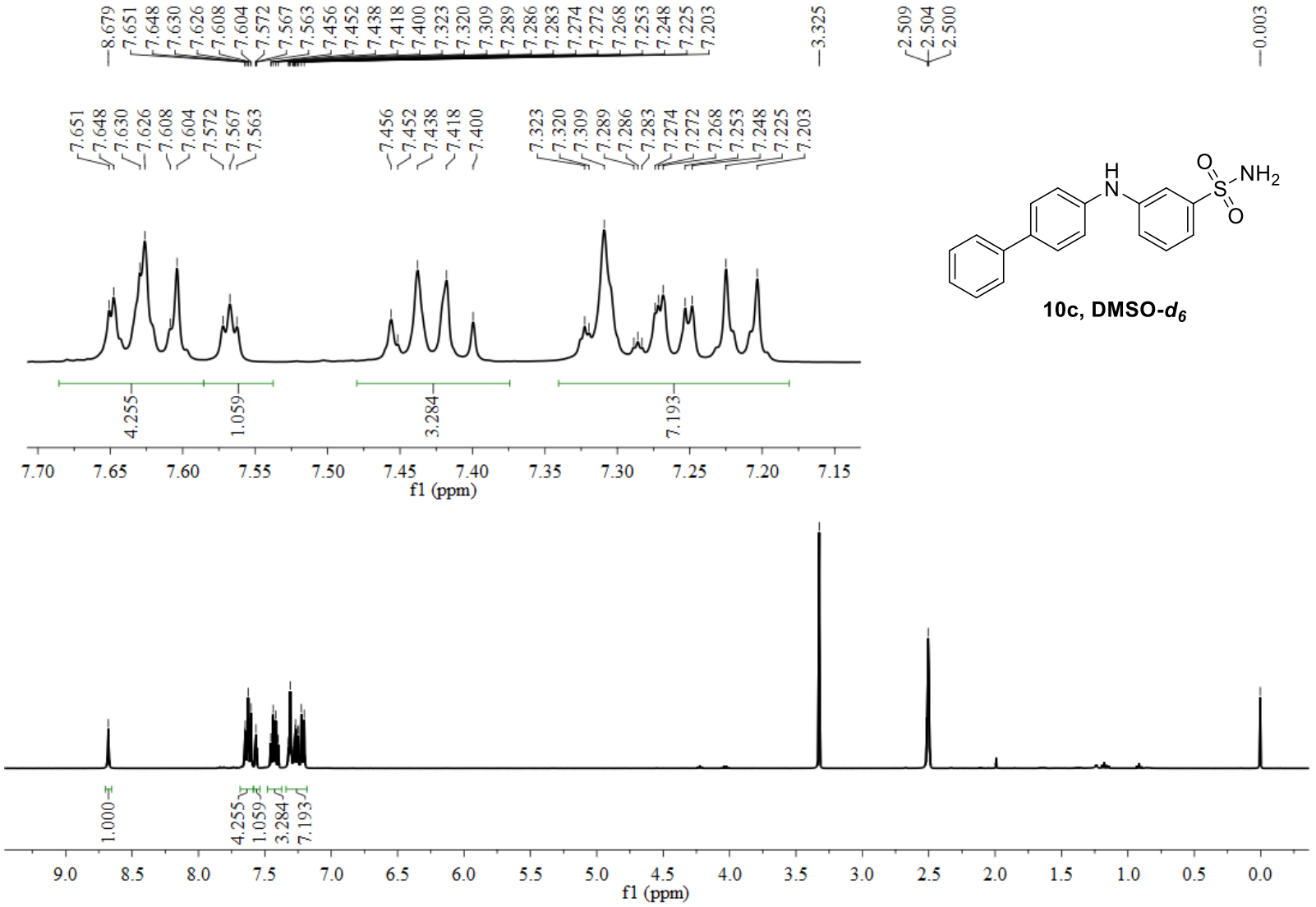

145.48
144.69
142.74
130.27
129.81
121.38
119.30
118.34
116.52
112.72
H
N
O
S
NH2
O
10a, DMSO-d6
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

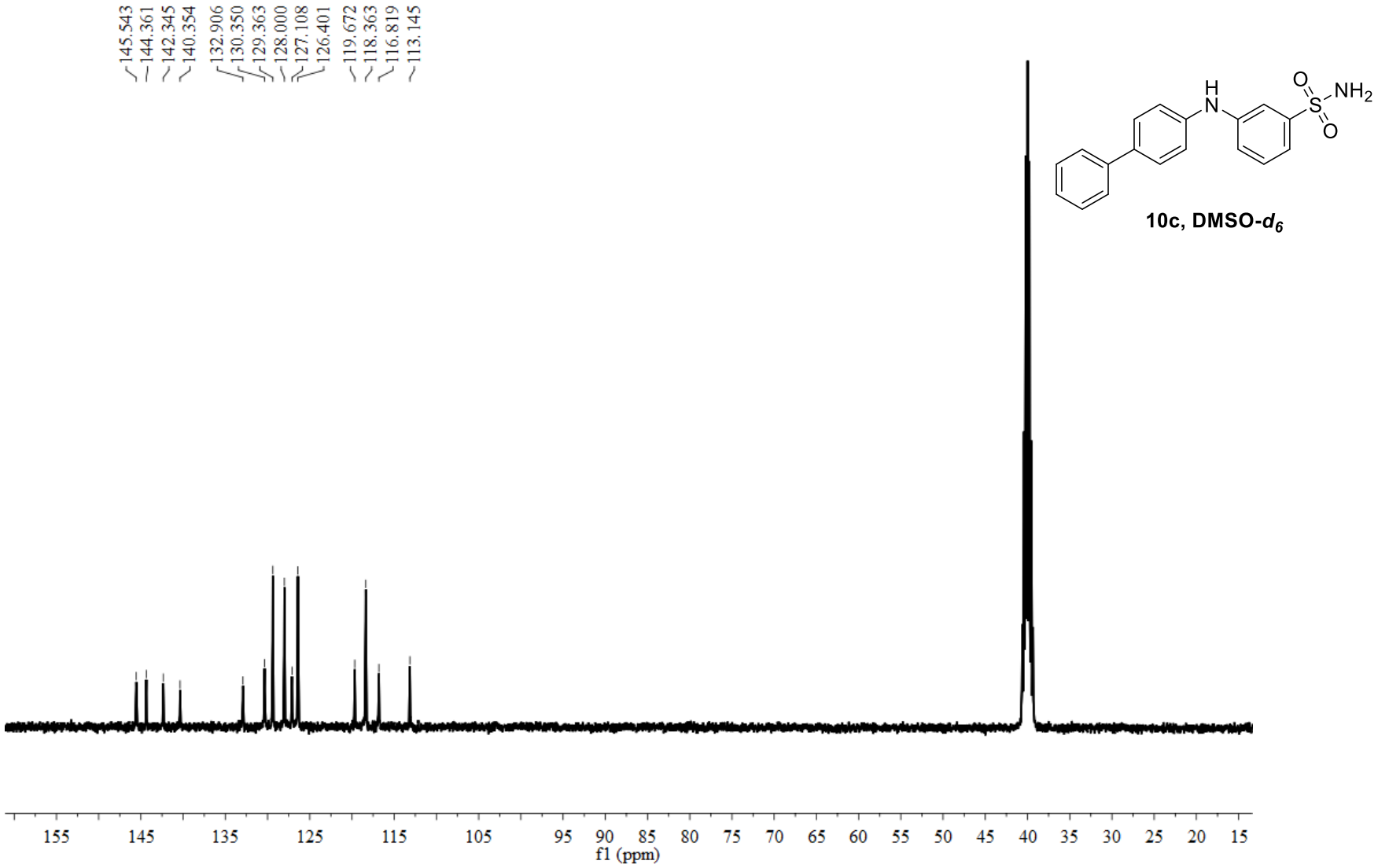

8.372
7.443
7.438
7.433
7.364
7.344
7.324
7.252
7.179
7.159
7.136
7.132
7.119
7.099
7.038
7.017
3.323
2.505
2.500
2.496
2.253
0.000
1.000
1.069
2.030
4.115
2.064
f1 (ppm)
1.006
3.030
f1 (ppm)

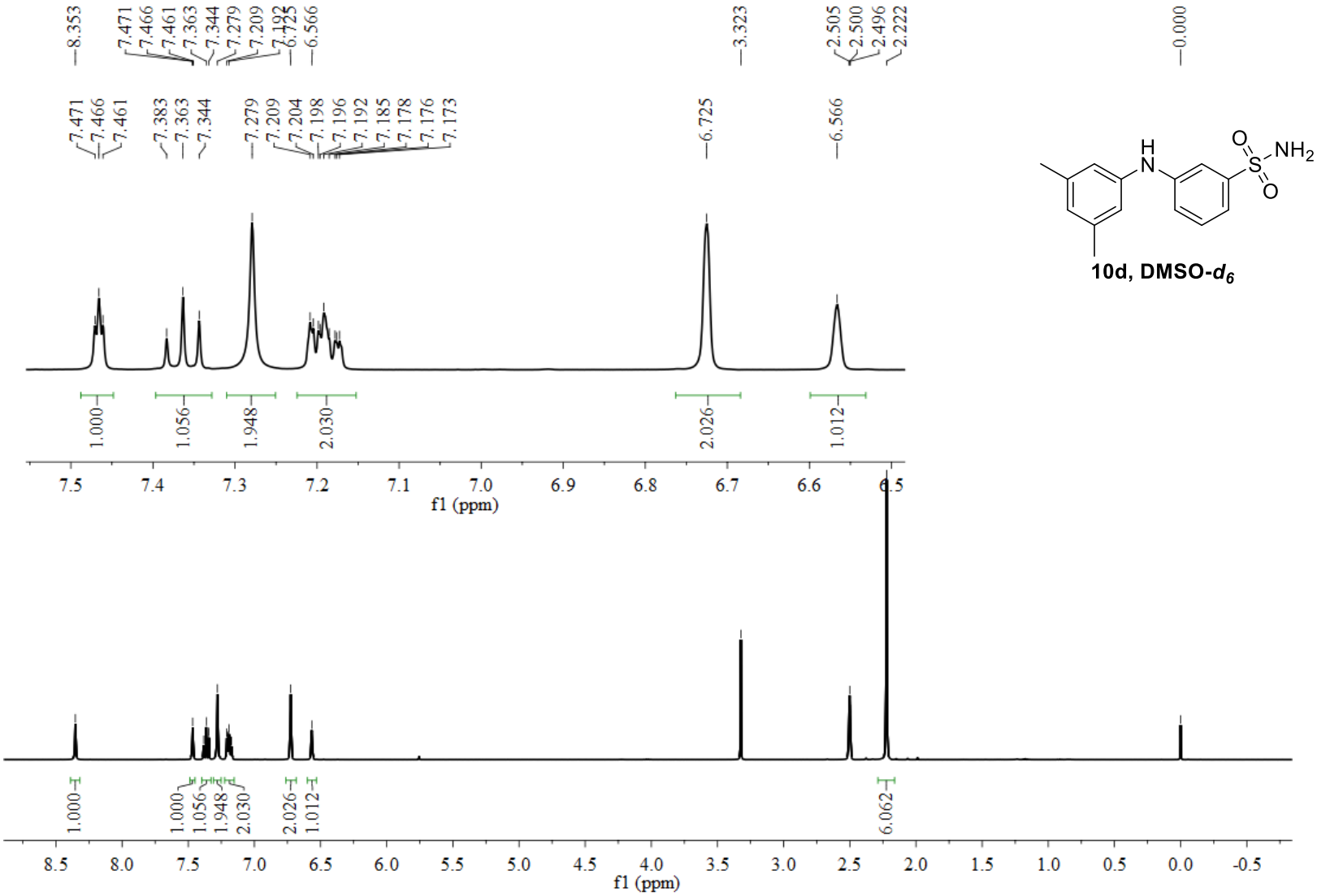
10b, DMSO-d_6

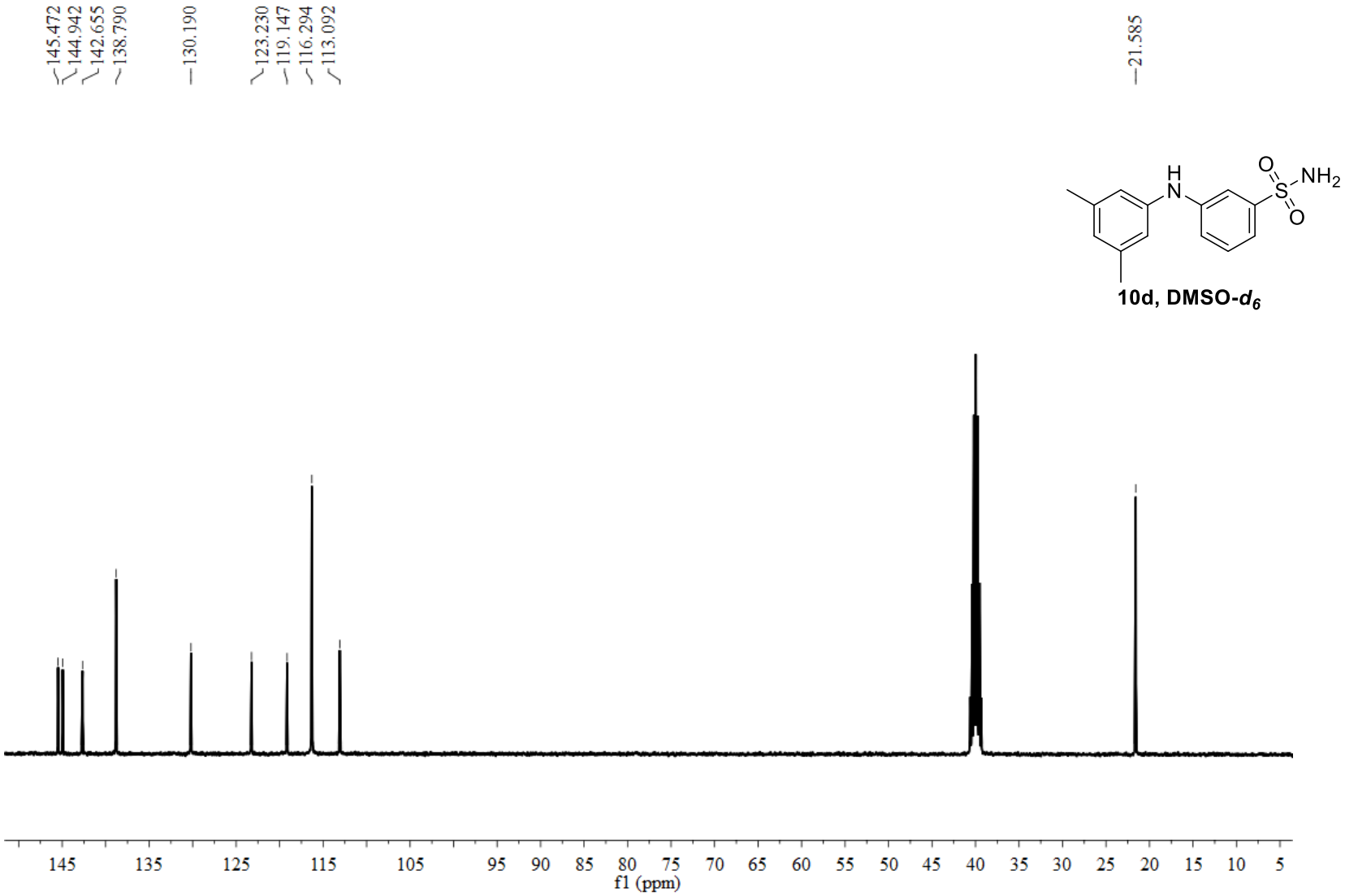

145.450
145.372
139.982
130.651
130.234
130.200
119.268
118.596
115.902
111.964
20.823
H
N
O
S
NH2
O
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)

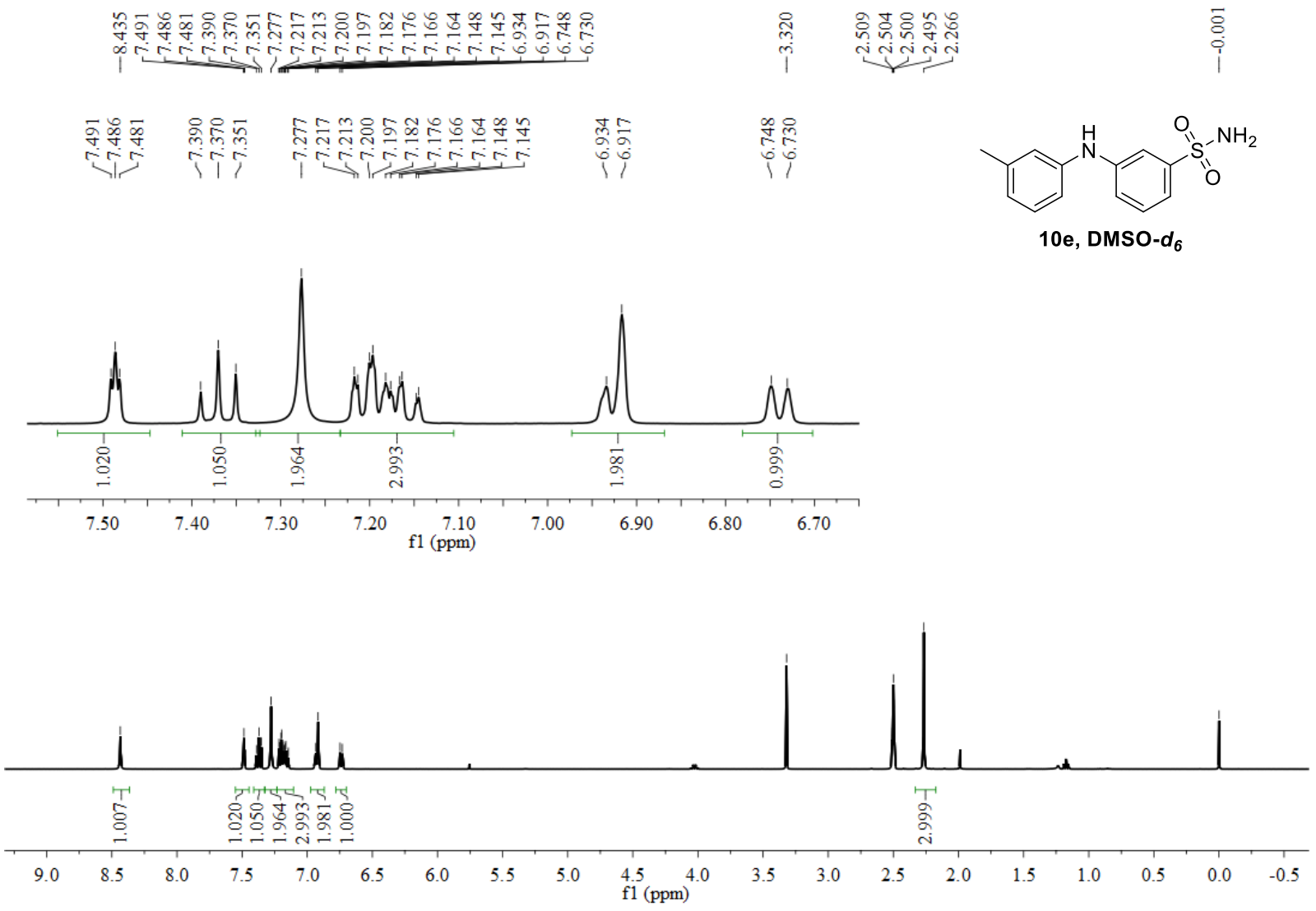
10b, DMSO-d_6

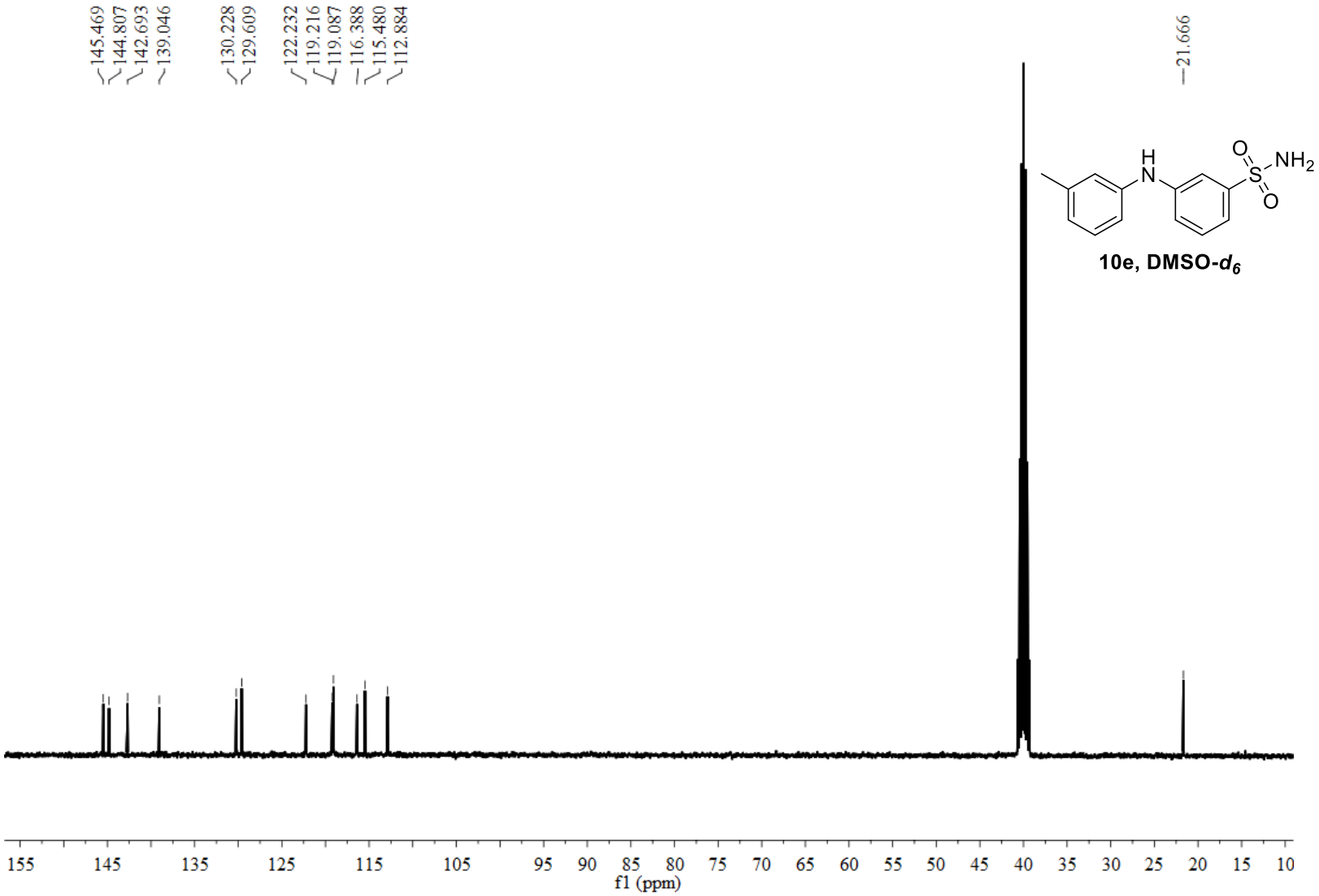

8.679
7.651
7.648
7.630
7.626
7.608
7.604
7.572
7.567
7.563
7.456
7.452
7.438
7.418
7.400
7.323
7.320
7.309
7.289
7.286
7.283
7.274
7.272
7.268
7.253
7.248
7.225
7.203
3.325
2.509
2.504
2.500
0.003
4.255
1.059
3.284
7.193
f1 (ppm)
1.000
10c, DMSO-d6

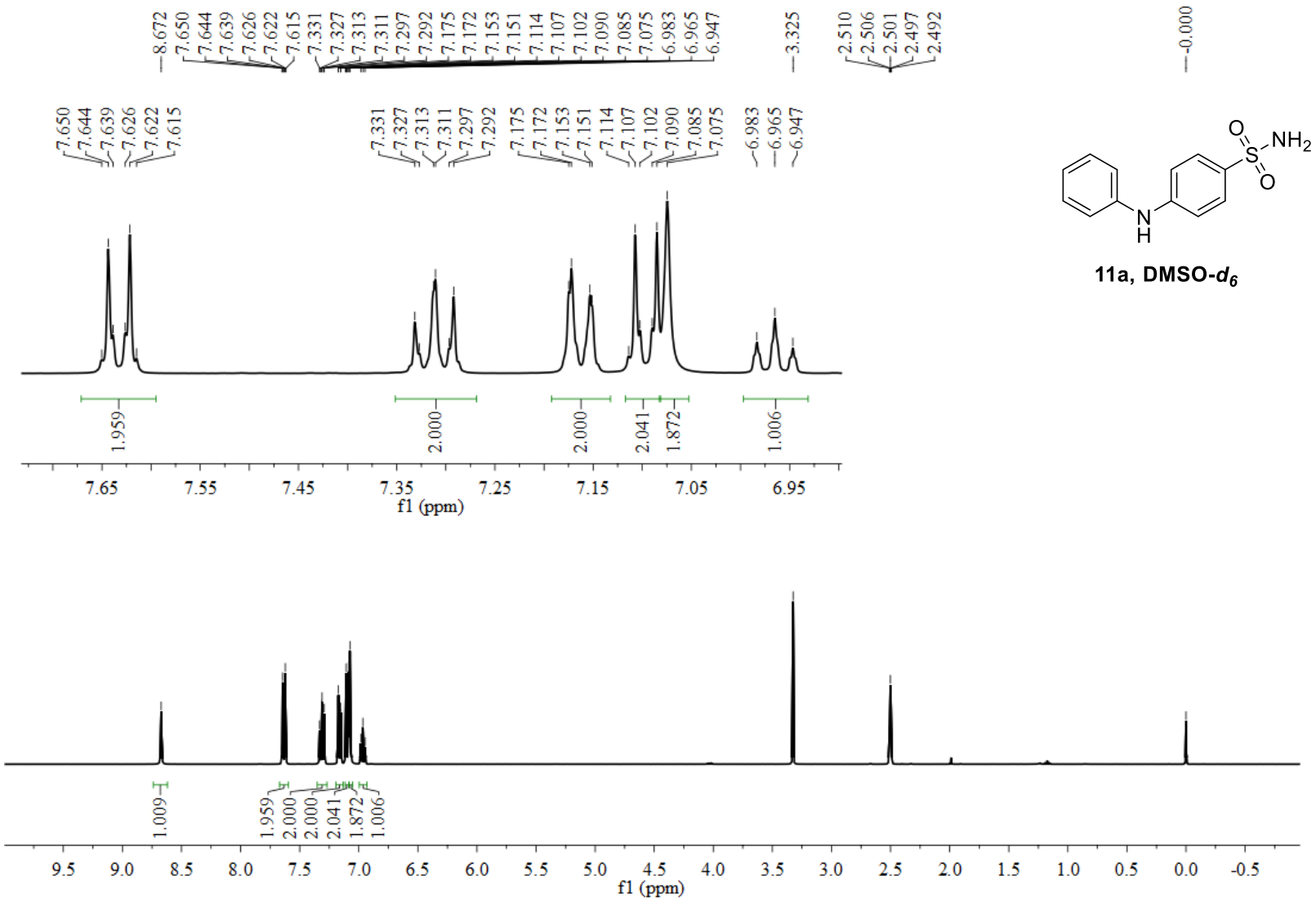

145.543
144.361
142.345
140.354
132.906
130.350
129.363
128.000
127.108
126.401
119.672
118.363
116.819
113.145
H
N
O
S
NH2
O
10c, DMSO-d6
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
f1 (ppm)


8.353
7.471
7.466
7.461
7.383
7.363
7.344
7.279
7.209
7.204
7.198
7.196
7.192
7.185
7.178
7.176
7.173
6.725
6.566
3.323
2.505
2.500
2.496
2.222
0.000
1.000
1.056
1.948
2.030
2.026
1.012
6.062
f1 (ppm)
NH2
10d, DMSO-d6

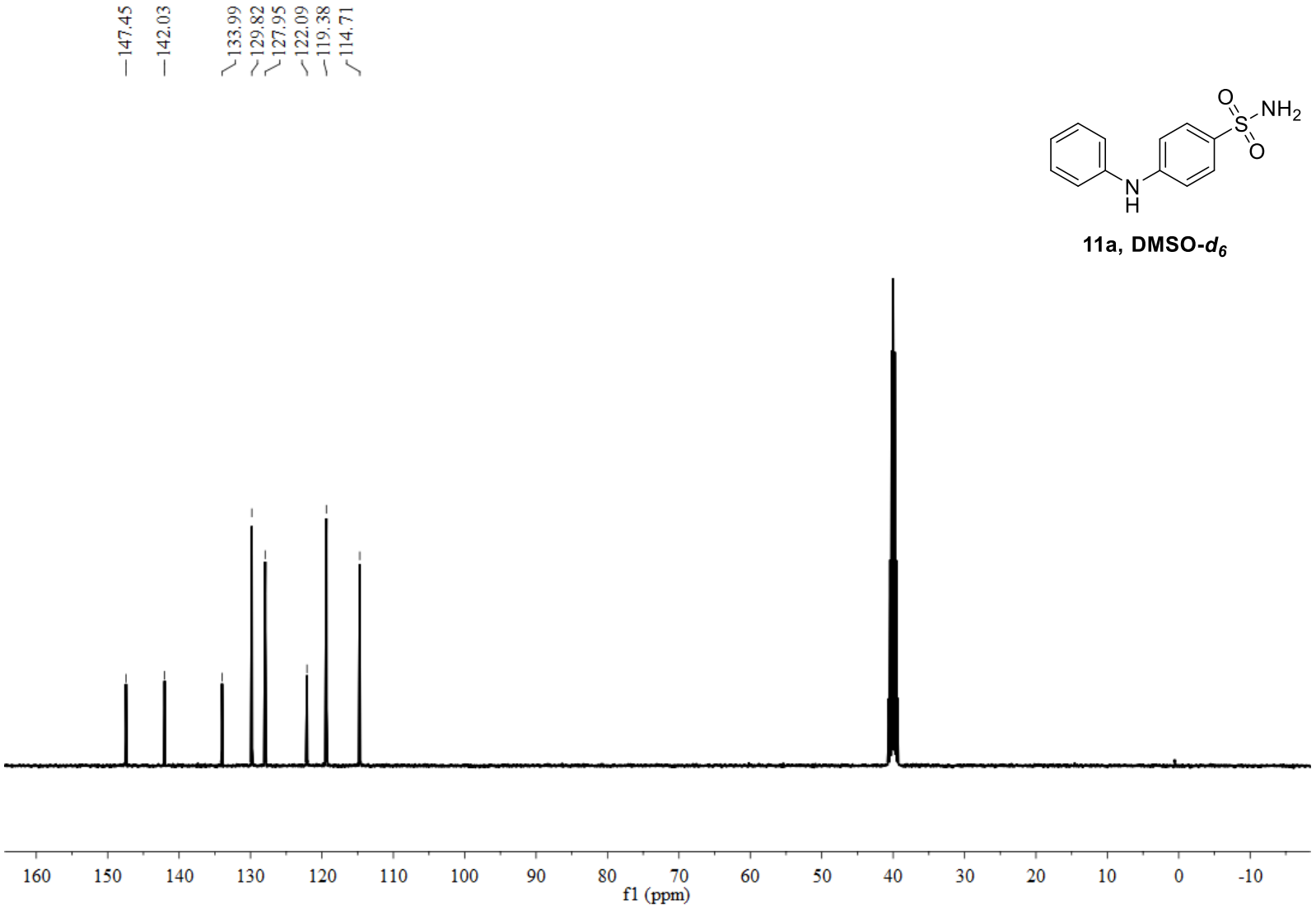

145.472
144.942
142.655
138.790
130.190
123.230
119.147
116.294
113.092
21.585
H
N
O
S
NH2
O
10d, DMSO-d6
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
f1 (ppm)


8.435
7.491
7.486
7.481
7.390
7.370
7.351
7.277
7.217
7.213
7.200
7.197
7.182
7.176
7.166
7.164
7.148
7.145
6.934
6.917
6.748
6.730
3.320
2.509
2.504
2.500
2.495
2.266
-0.001
NH2
10e, DMSO-d6
1.020
1.050
1.964
2.993
1.981
0.999
f1 (ppm)
1.007
1.020
1.050
1.964
2.993
1.981
1.000
2.999
f1 (ppm)

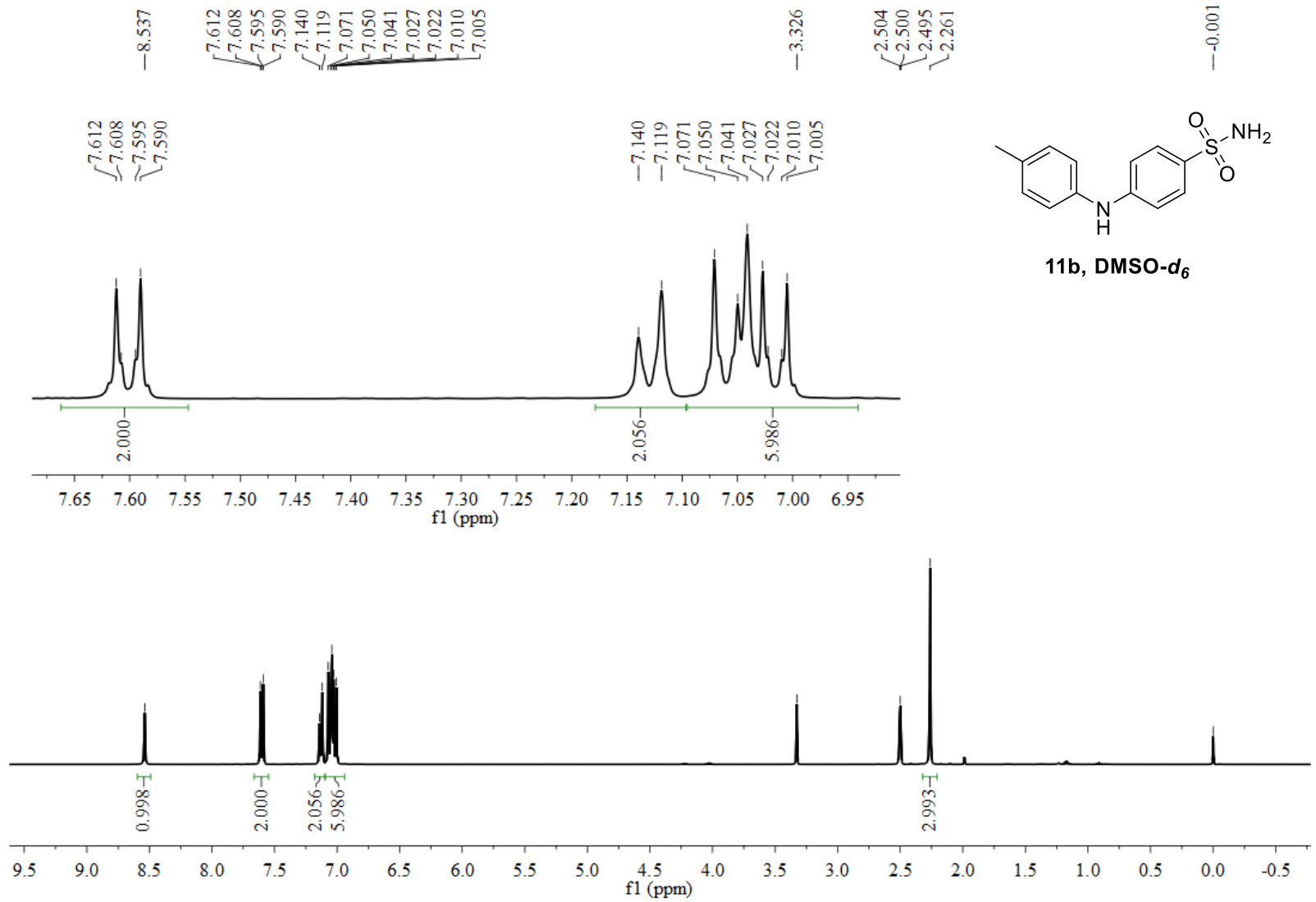

145.469
144.807
142.693
139.046
130.228
129.609
122.232
119.216
119.087
116.388
115.480
112.884
21.666
H
N
O
S
O
NH2
10e, DMSO-d6
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)


8.672
7.650
7.644
7.639
7.626
7.622
7.615
7.331
7.327
7.313
7.311
7.297
7.292
7.175
7.172
7.153
7.151
7.114
7.107
7.102
7.090
7.085
7.075
6.983
6.965
6.947
3.325
2.510
2.506
2.501
2.497
2.492
0.000
1.959
2.000
2.000
2.041
1.872
1.006
f1 (ppm)
1.009
1.959
2.000
2.000
2.041
1.872
1.006
f1 (ppm)

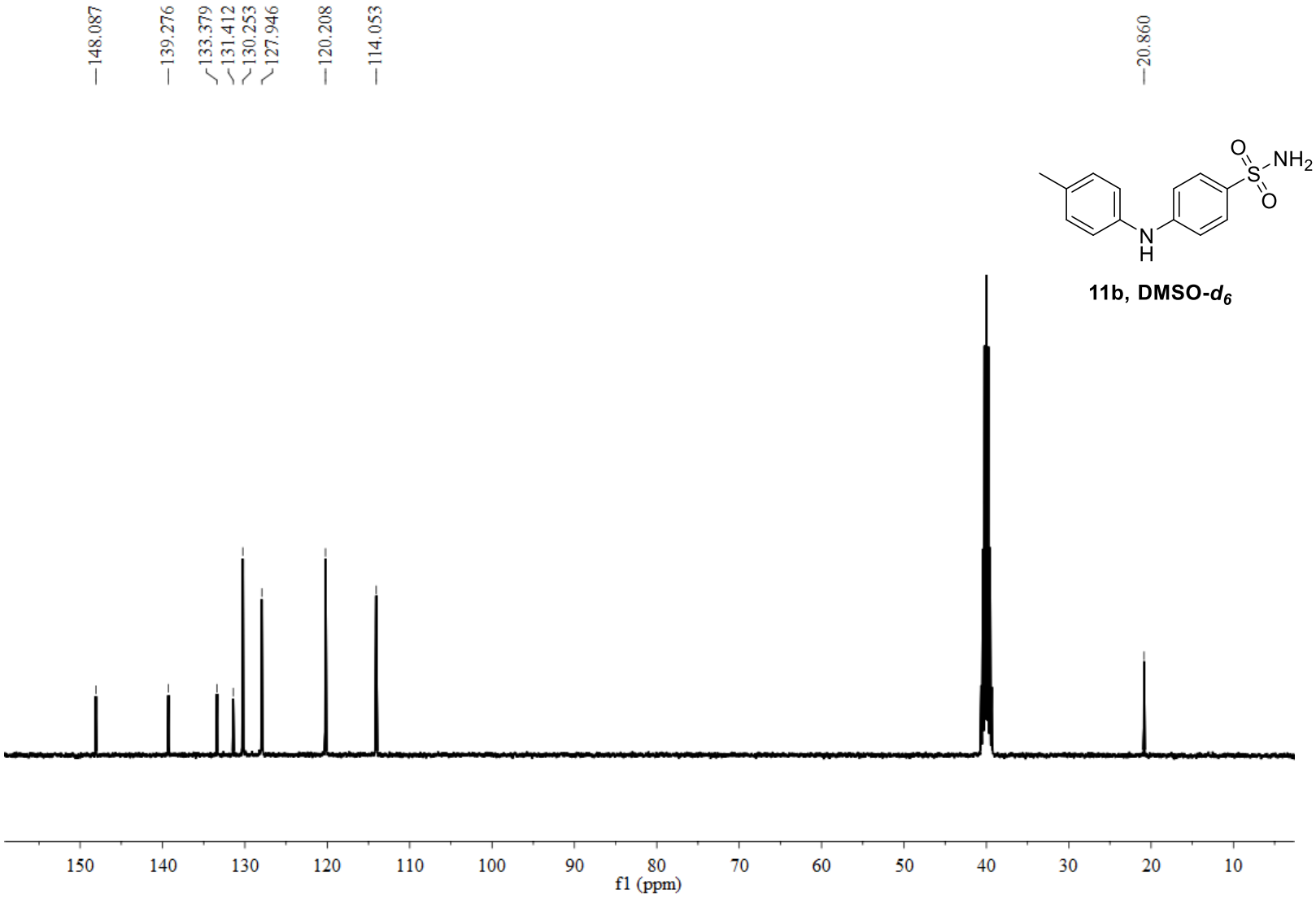
11a, DMSO-d_6

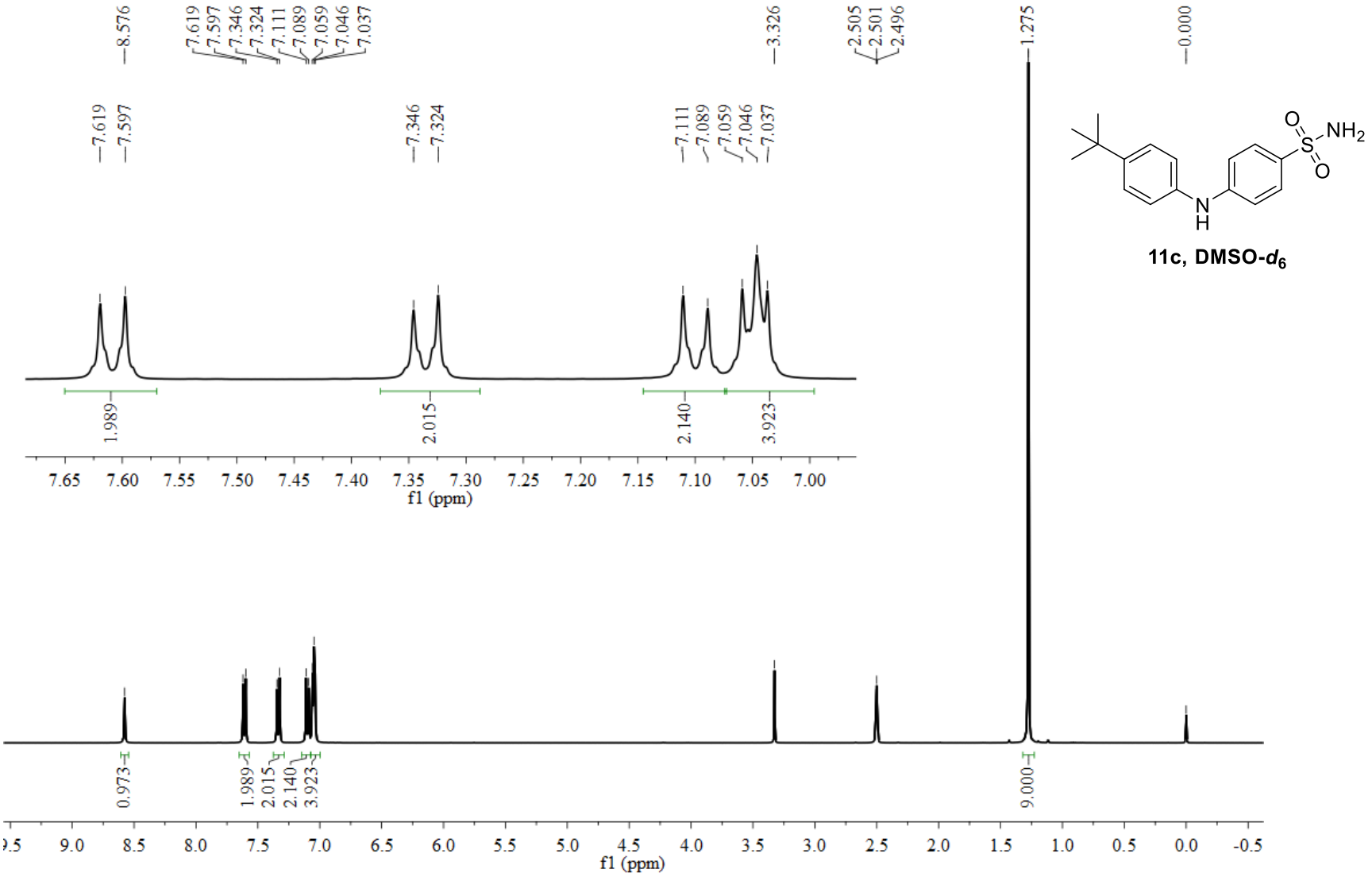

147.45
142.03
133.99
129.82
127.95
122.09
119.38
114.71
O
NH2
S
O
N
H
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

11a, DMSO-d_6

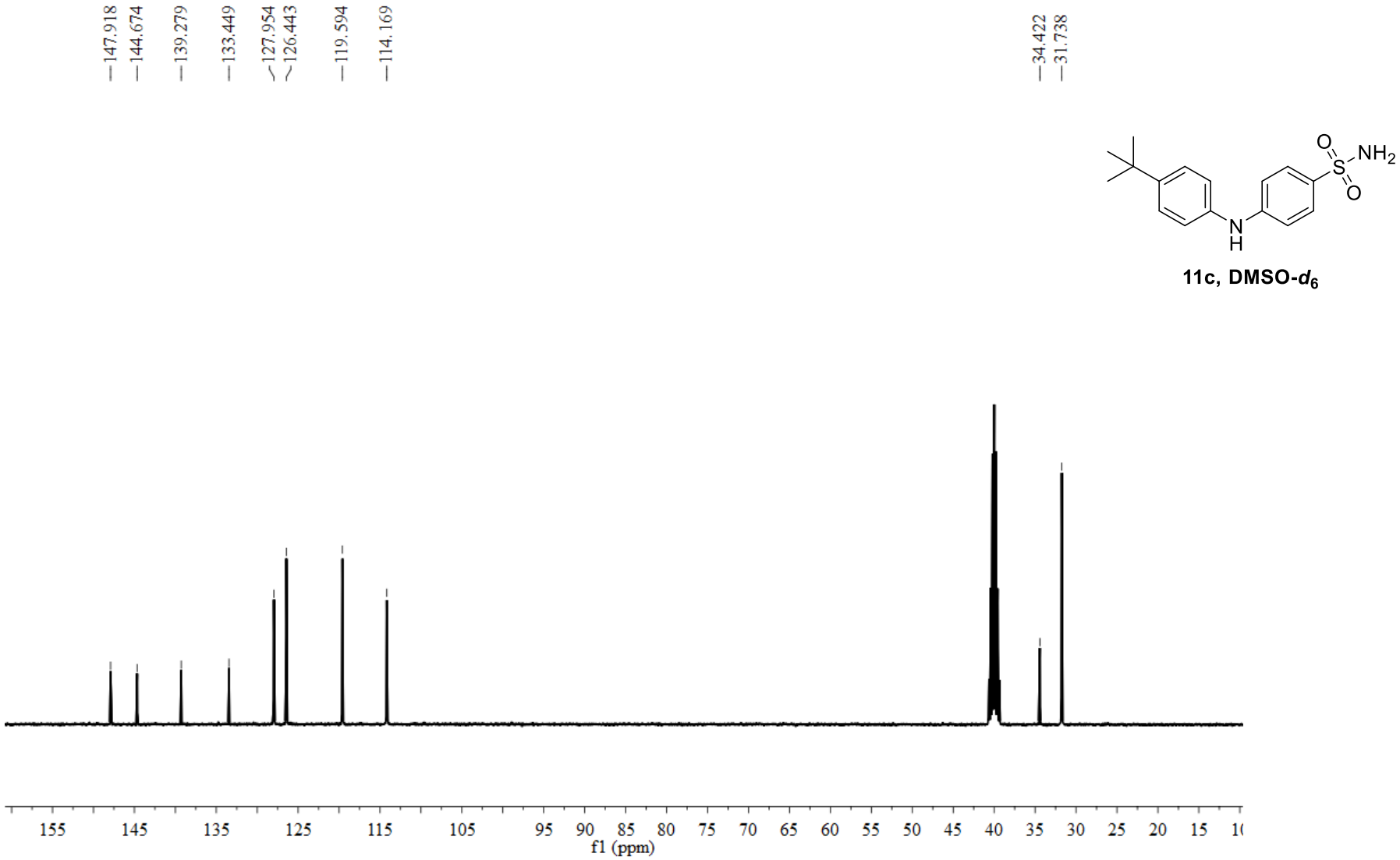

8.537
7.612
7.608
7.595
7.590
7.140
7.119
7.071
7.050
7.041
7.027
7.022
7.010
7.005
3.326
2.504
2.500
2.495
2.261
0.001
2.000
2.056
5.986
f1 (ppm)
0.998
2.000
2.056
5.986
2.993
f1 (ppm)

11b, DMSO-d_6

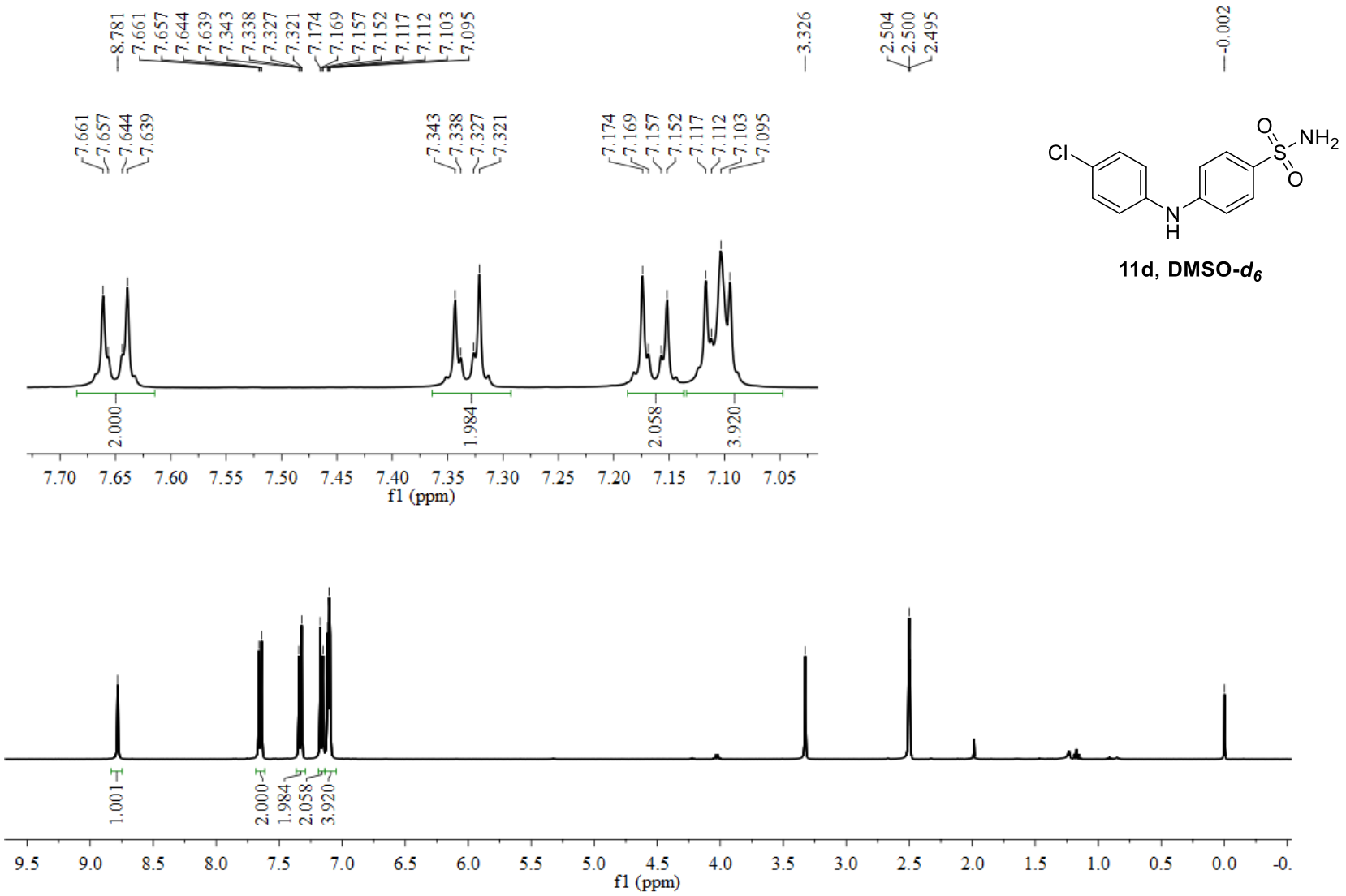

148.087
139.276
133.379
131.412
130.253
127.946
120.208
114.053
20.860
O
NH2
S
O
N
H
11b, DMSO-d6
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

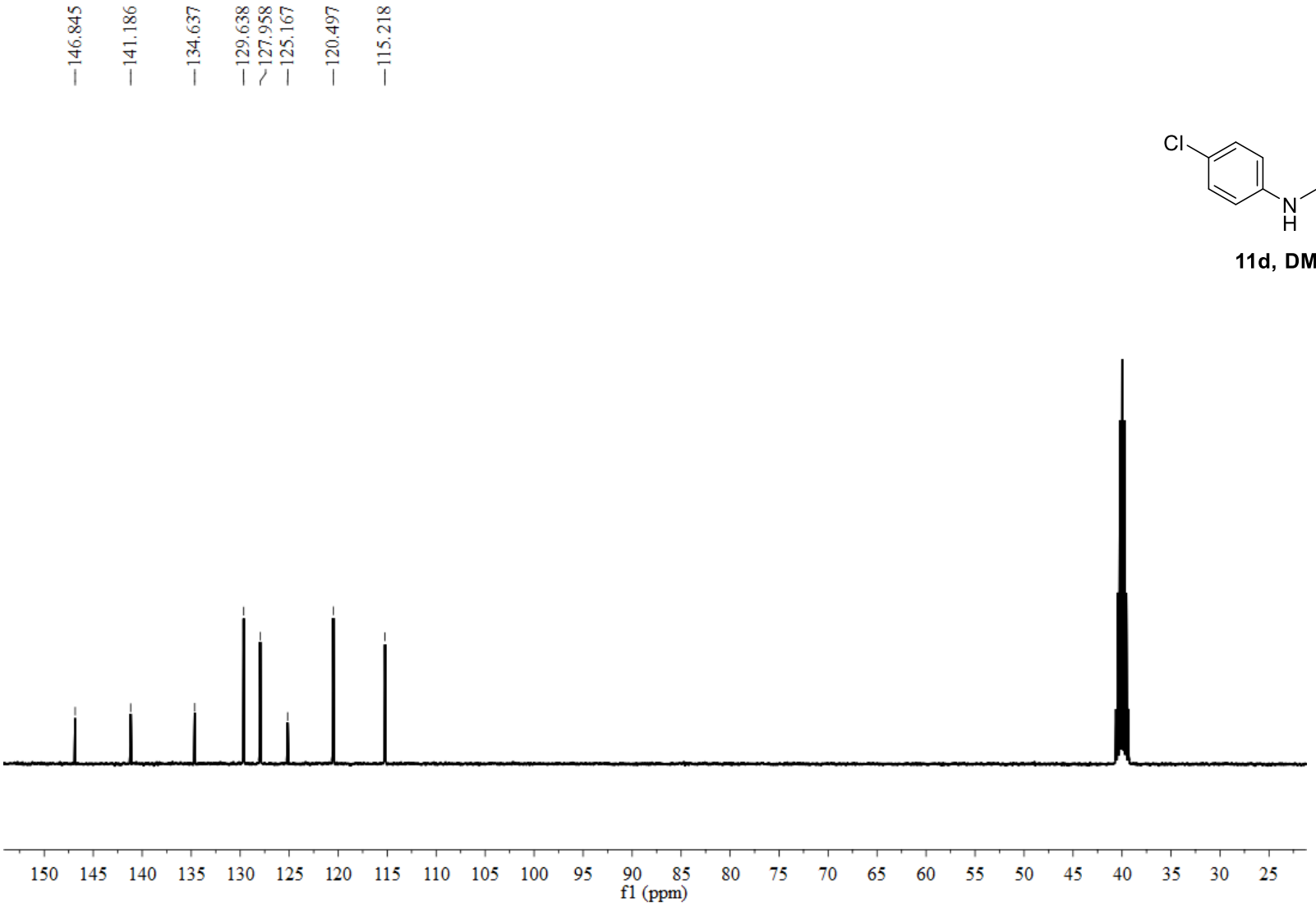

8.576
7.619
7.597
7.346
7.324
7.111
7.089
7.059
7.046
7.037
3.326
2.505
2.501
2.496
1.275
0.000
1.989
2.015
2.140
3.923
0.973
9.000
f1 (ppm)
O
NH2
S
O
N
H

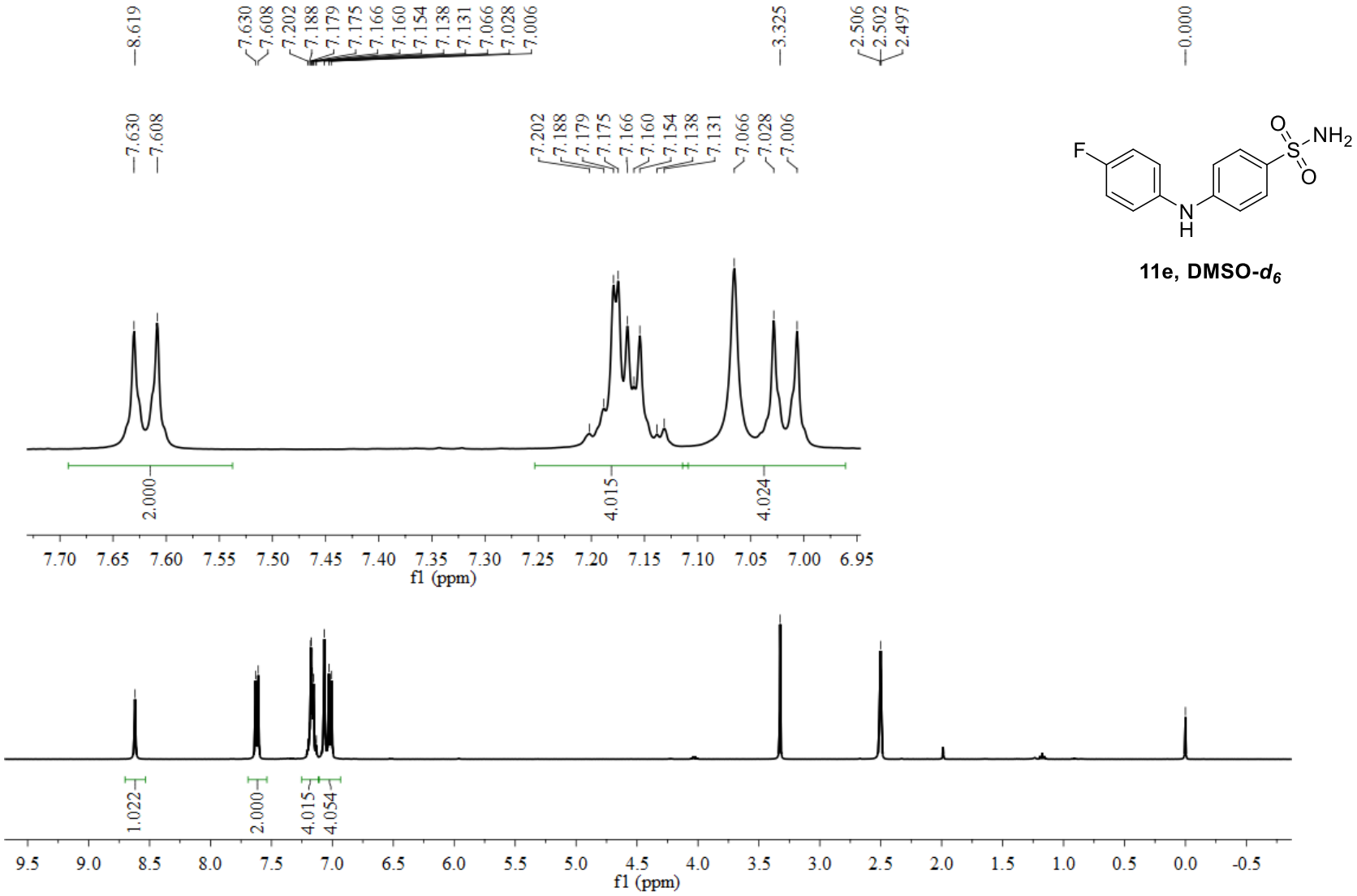
11c, DMSO-d_6


147.918
144.674
139.279
133.449
127.954
126.443
119.594
114.169
34.422
31.738
O
NH2
S
O
N
H
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
f1 (ppm)

11c, DMSO-d_6

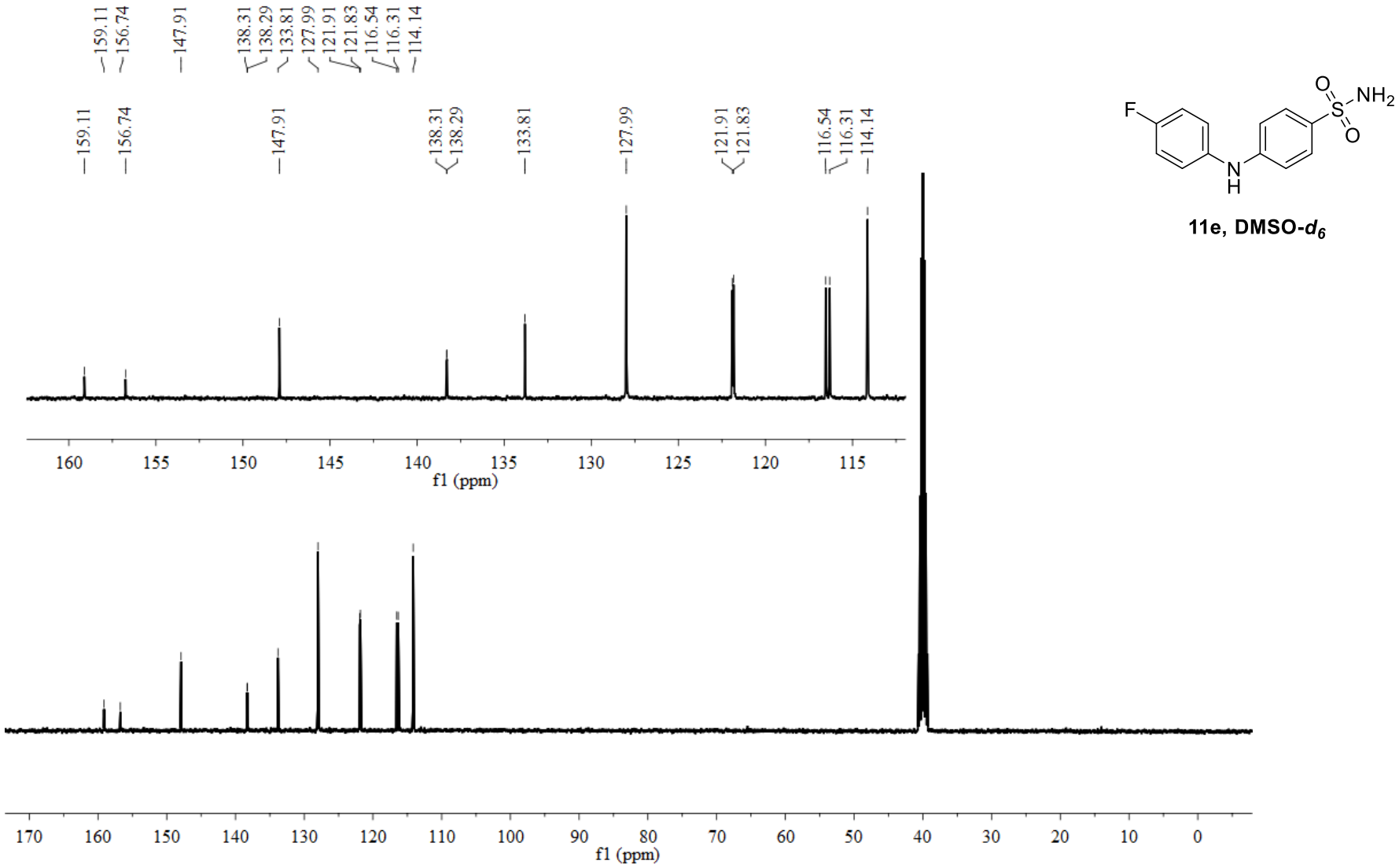

8.781
7.661
7.657
7.644
7.639
7.343
7.338
7.327
7.321
7.174
7.169
7.157
7.152
7.117
7.112
7.103
7.095
3.326
2.504
2.500
2.495
-0.002
Cl
N
H
O
S
O
NH2
11d, DMSO-d6
2.000
1.984
2.058
3.920
f1 (ppm)
1.001
2.000
1.984
2.058
3.920
f1 (ppm)


146.845
141.186
134.637
129.638
127.958
125.167
120.497
115.218
Cl
N
H
S
O
O
NH2
11d, DMSO-d6
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)


8.619
7.630
7.608
7.202
7.188
7.179
7.175
7.166
7.160
7.154
7.138
7.131
7.066
7.028
7.006
3.325
2.506
2.502
2.497
0.000
2.000
4.015
4.024
7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95
f1 (ppm)
1.022
2.000
4.015
4.054
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

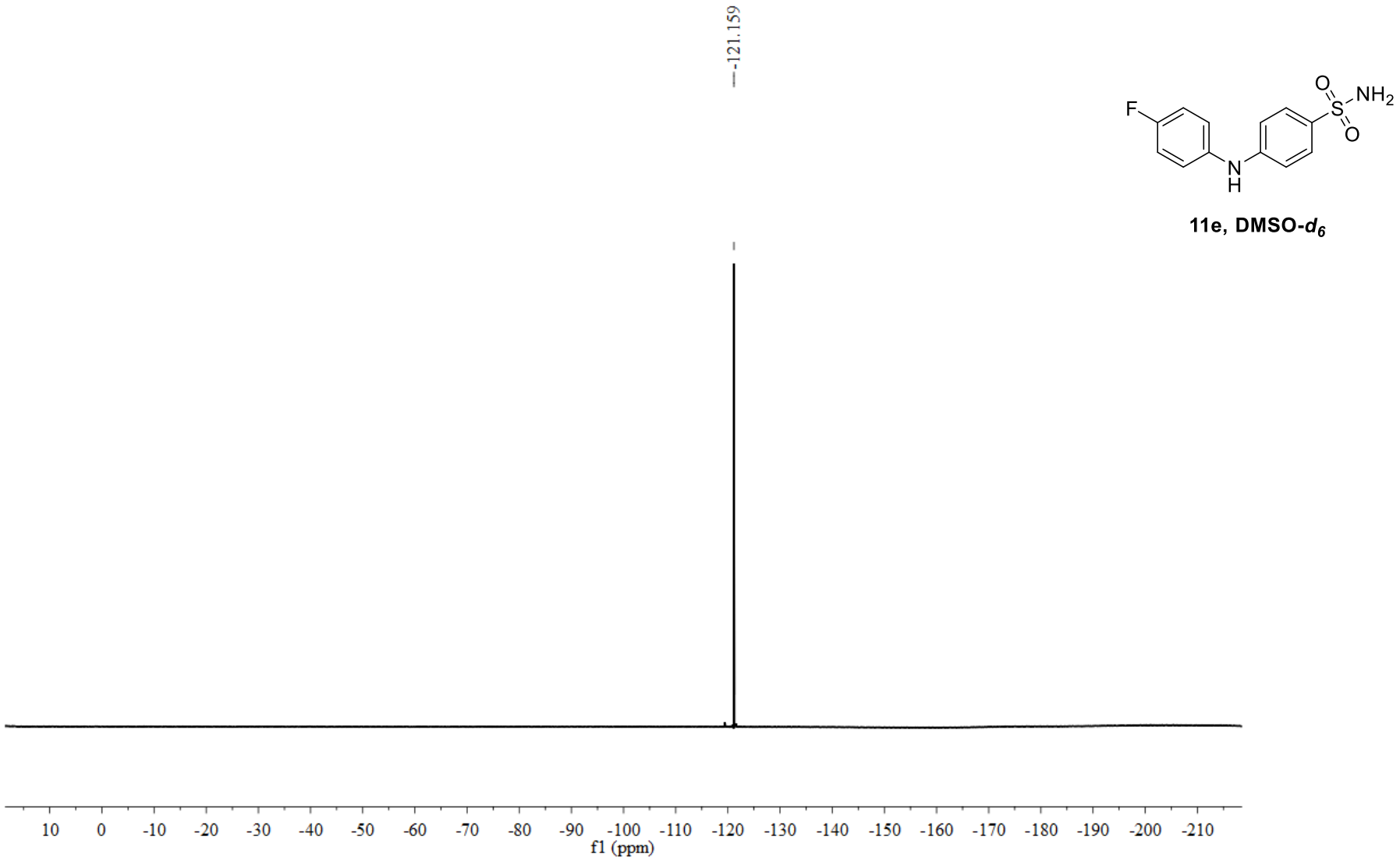
F
N
H
O
S
O
NH2

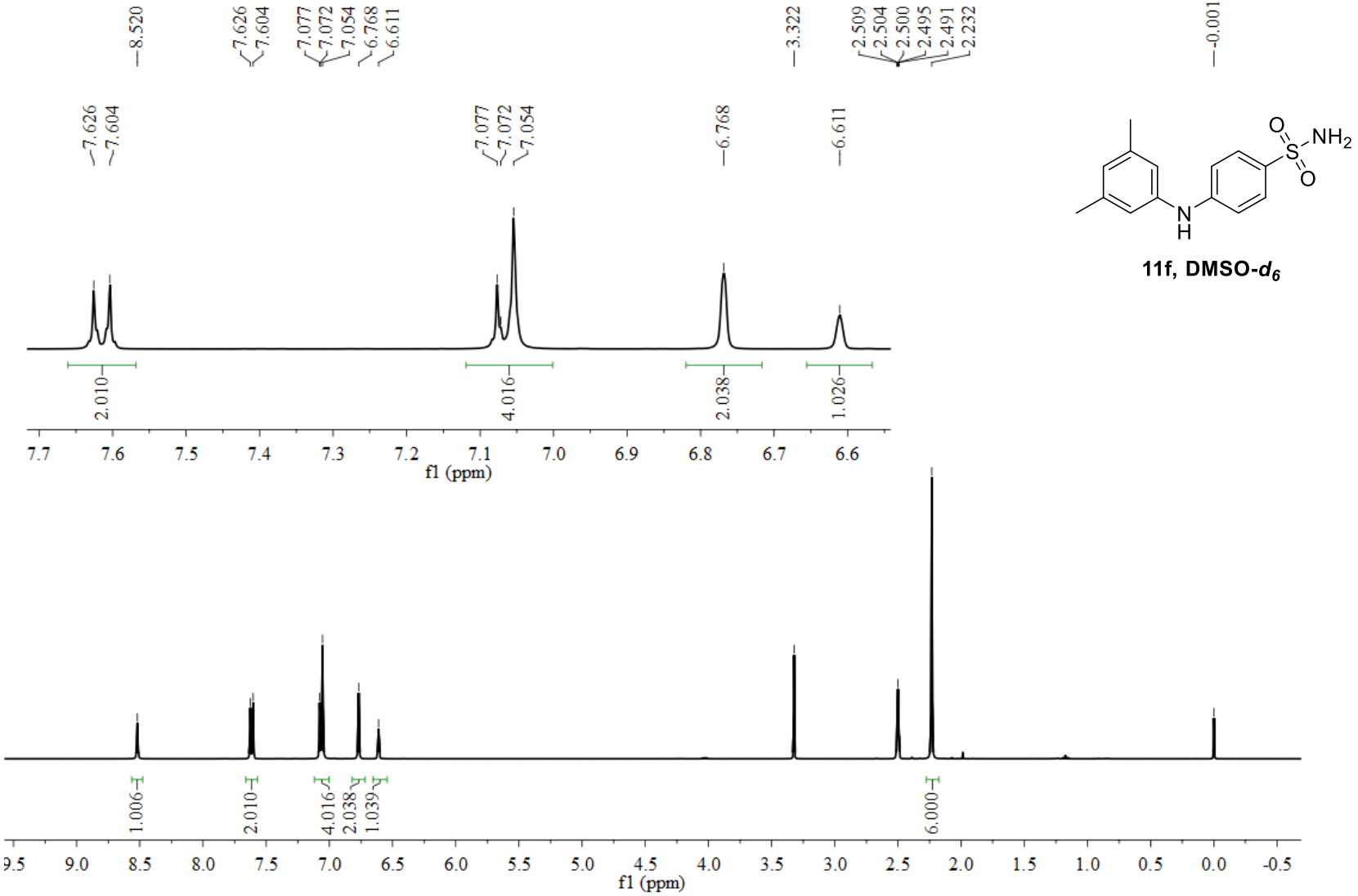
11e, DMSO-d_6


159.11
156.74
147.91
138.31
138.29
133.81
127.99
121.91
121.83
116.54
116.31
114.14
f1 (ppm)
f1 (ppm)

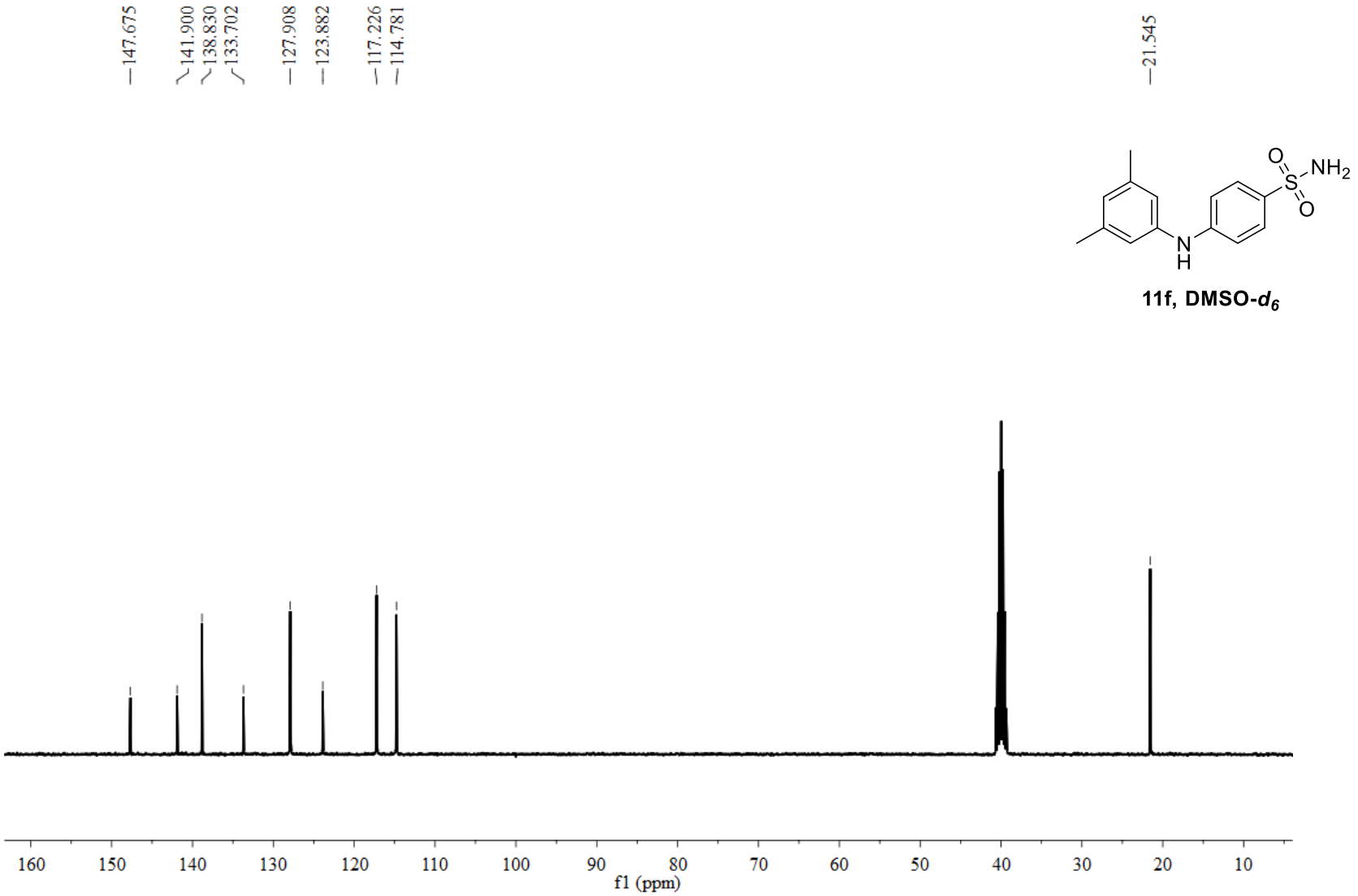
F
N
H
O
S
O
NH2

11e, DMSO-d_6

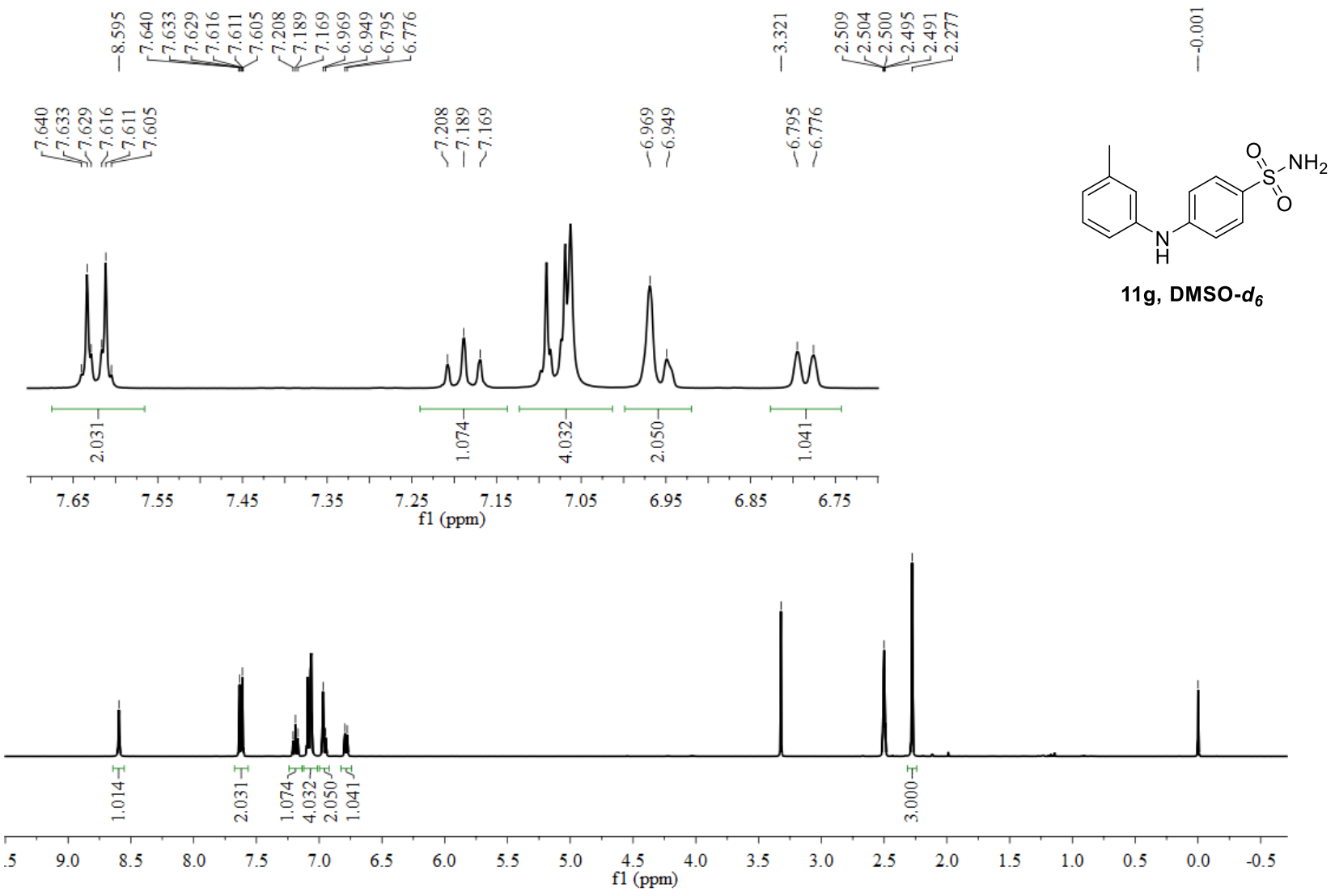

-121.159
F
O
NH2
S
O
N
H
11e, DMSO-d6
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


8.520
7.626
7.604
7.077
7.072
7.054
6.768
6.611
3.322
2.509
2.504
2.500
2.495
2.491
2.232
-0.001
2.010
4.016
2.038
1.026
f1 (ppm)
1.006
2.010
4.016
2.038
1.039
6.000
f1 (ppm)
NH2
O
S
O
N
H

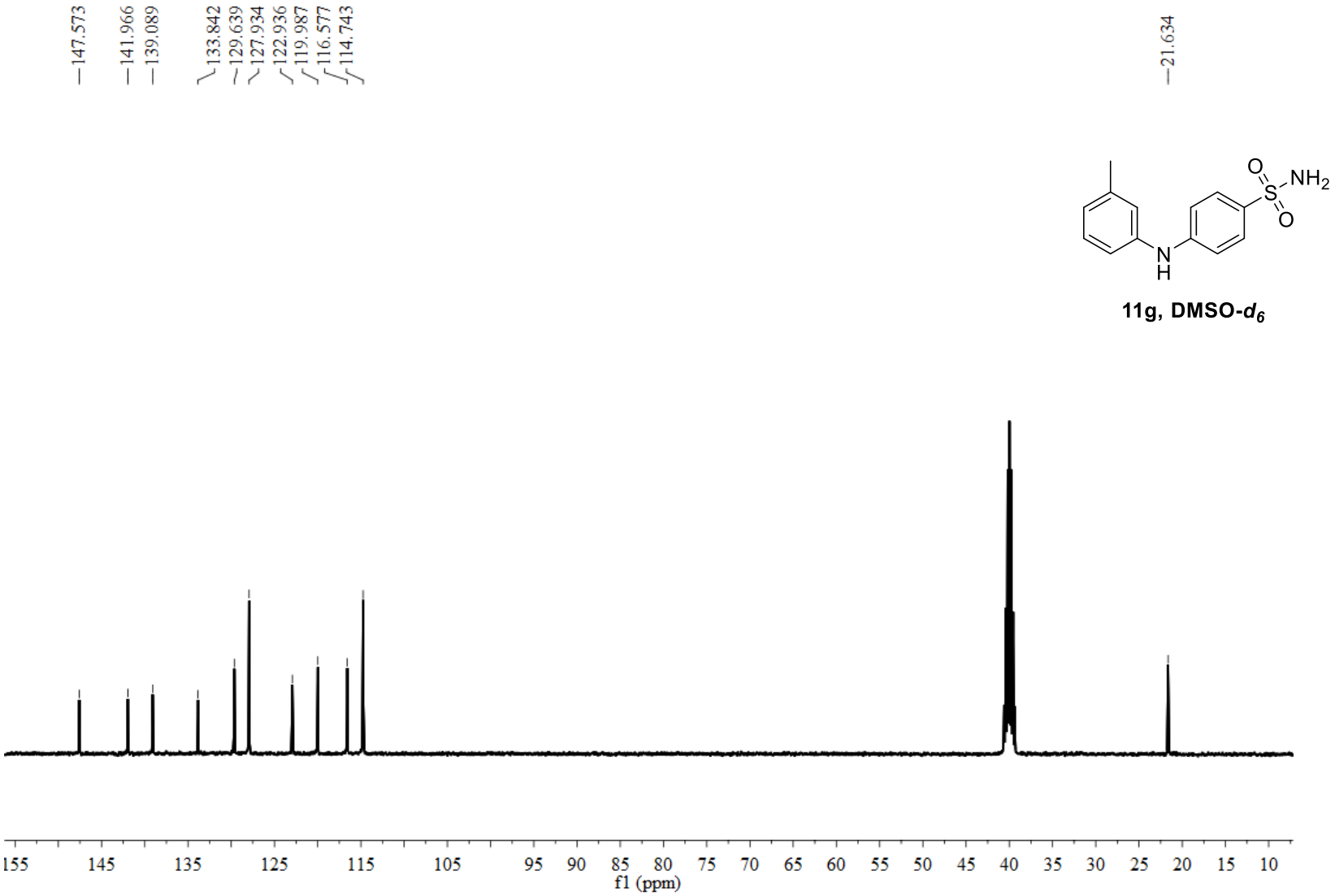
11f, DMSO-d_6


147.675
141.900
138.830
133.702
127.908
123.882
117.226
114.781
21.545
O
S
NH2
O
N
H
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

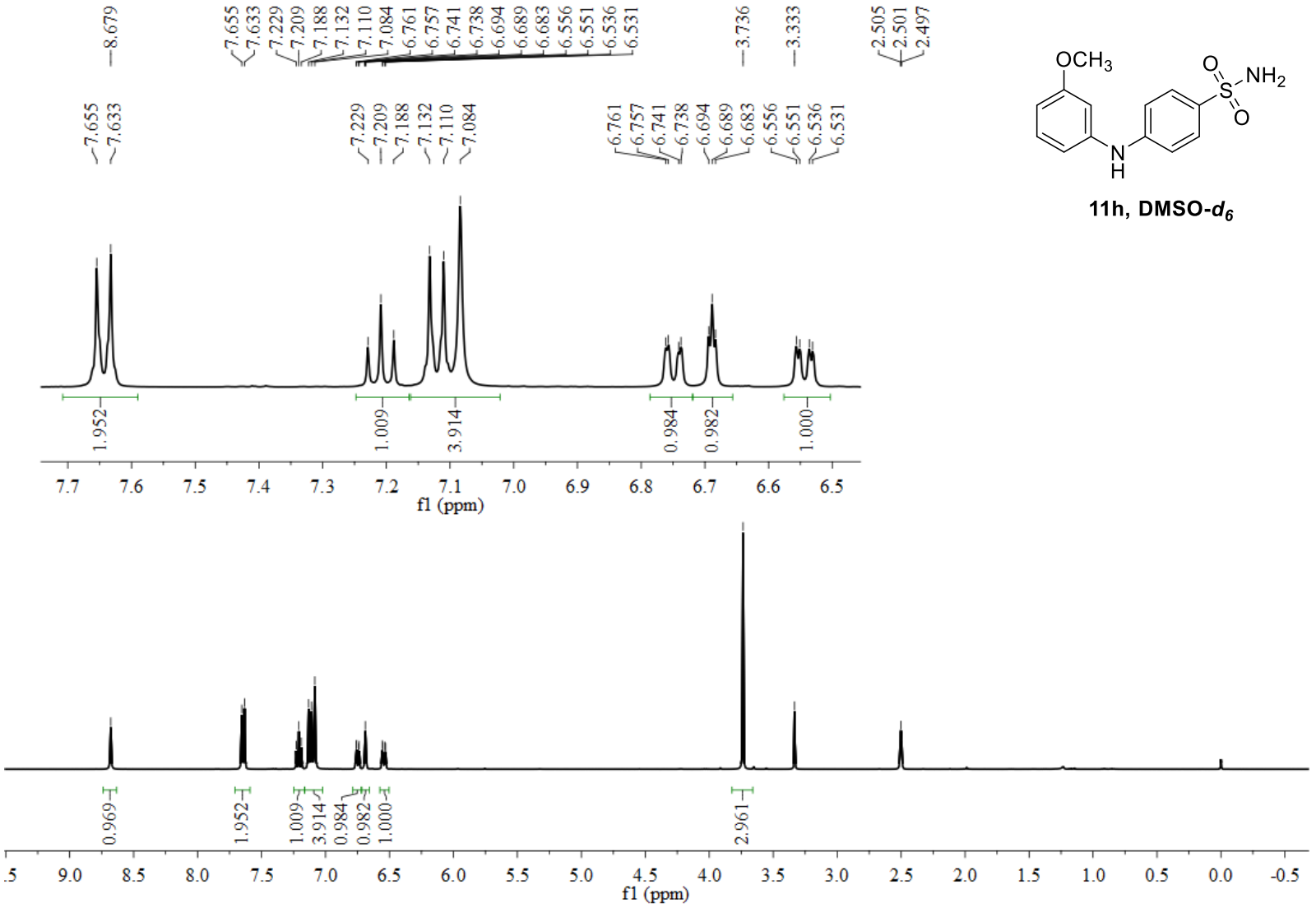
11f, DMSO-d_6


8.595
7.640
7.633
7.629
7.616
7.611
7.605
7.208
7.189
7.169
6.969
6.949
6.795
6.776
3.321
2.509
2.504
2.500
2.495
2.491
2.277
-0.001
2.031
1.074
4.032
2.050
1.041
7.65
7.55
7.45
7.35
7.25
7.15
7.05
6.95
6.85
6.75
f1 (ppm)
1.014
2.031
1.074
4.032
2.050
1.041
3.000
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

11g, DMSO-d_6

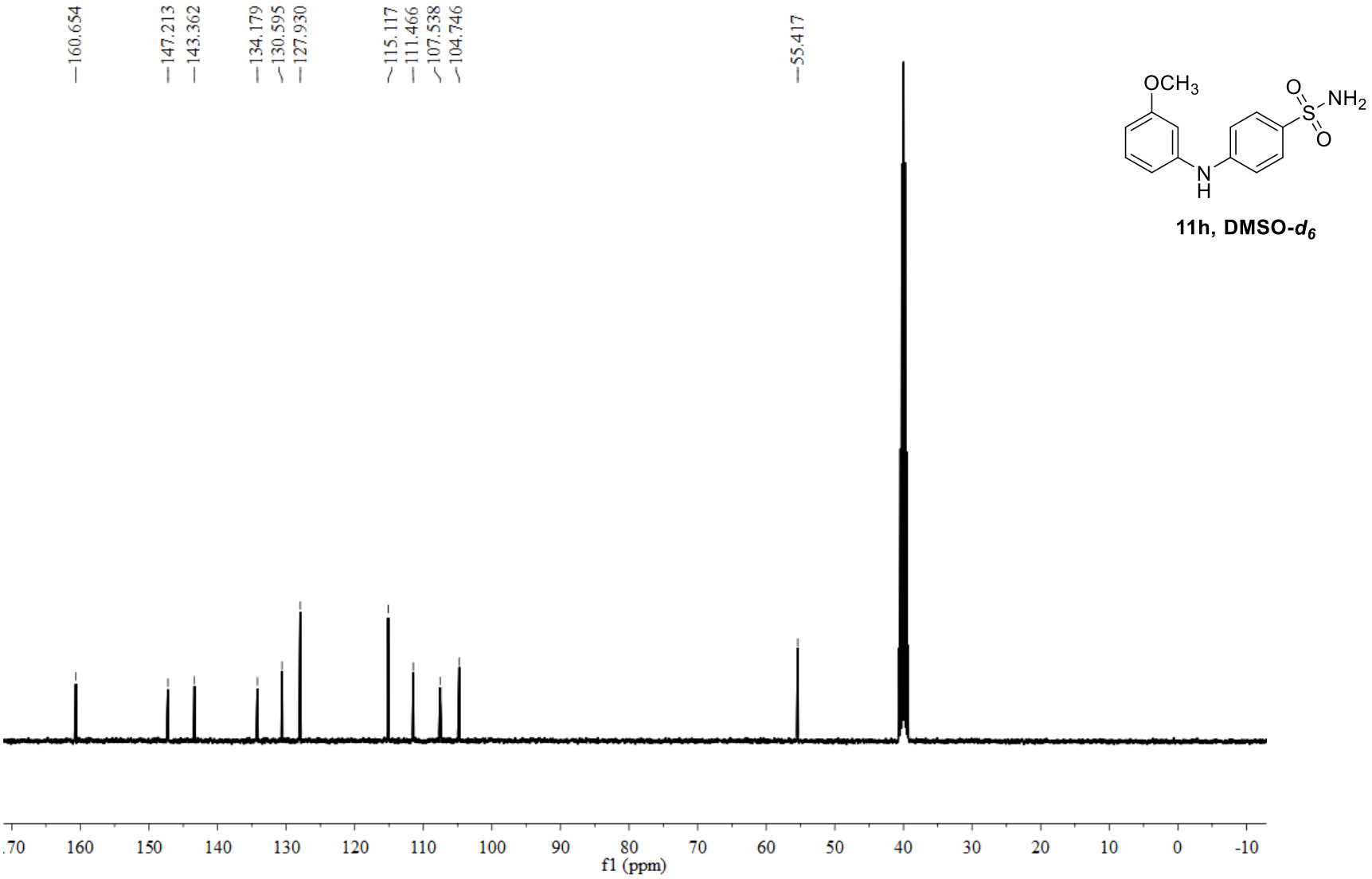

147.573
141.966
139.089
133.842
129.639
127.934
122.936
119.987
116.577
114.743
21.634
O
NH2
S
O
N
H
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)

11g, DMSO-d_6


8.679
7.655
7.633
7.229
7.209
7.188
7.132
7.110
7.084
6.761
6.757
6.741
6.738
6.694
6.689
6.683
6.556
6.551
6.536
6.531
3.736
3.333
2.505
2.501
2.497
1.952
1.009
3.914
0.984
0.982
1.000
f1 (ppm)
0.969
1.952
1.009
3.914
0.984
0.982
1.000
2.961
f1 (ppm)

OCH3
O
S
NH2
O
N
H

11h, DMSO-d_6


160.654
147.213
143.362
134.179
130.595
127.930
115.117
111.466
107.538
104.746
55.417
OCH3
O
S
NH2
O
N
H
11h, DMSO-d6
70
160
150
140
130
120
110
100
90
80
f1 (ppm)
70
60
50
40
30
20
10
0
-10