

Structural hybrids of sulfonamide and thiazole moieties: Synthesis and evaluation of antimicrobial activity

Samir Y. Abbas,^{a,*} Maha M. Abd El-Aziz,^b Samir M. Awad,^b Mosaad S. Mohamed^b

^aOrganometallic and Organometalloid Chemistry Department, National Research Centre, Cairo, Egypt.

^bPharmaceutical Organic Chemistry Department, Faculty of Pharmacy, Helwan University, Ain Helwan, Cairo, Egypt.

*Corresponding author: sy.abbas@nrc.sci.eg; samiryoussef98@yahoo.com

Experimental Section

NMR spectra were recorded using Bruker spectrometers (^1H NMR 400 MHz; ^{13}C NMR 101 MHz) in DMSO- d_6 with chemical shift in δ from internal TMS.

Synthesis of 4-(arylsulfonamido)-acetophenone thiosemicarbazones 2a-f

A mixture of equimolar amounts (0.01 mole) of *N*-(4-acetylphenyl)methane-(or benzene)-sulfonamide (**1a,b**) and the selected thiosemicarbazides (thiosemicarbazide, *N*-methyl-thiosemicarbazide and *N*-phenyl-thiosemicarbazide) was heated under reflux in a mixture of 1 mL AcOH and 50 mL ethyl alcohol for 0.5 hour. The resultant solid crystals were collected recrystallized from THF.

2-(1-(4-(Methylsulfonamido)phenyl)ethylidene)hydrazinecarbothioamide (2a): Yield 90 %; m.p. 239-241 °C; IR (KBr): ν/cm^{-1} : 3369, 3353, 3318 (NH, NH₂); ^1H NMR: 2.28 (s, 3H, CH₃-C=N), 3.01 (s, 3H, CH₃-SO₂), 7.21 (d, 2H, $J = 8.6$ Hz, Ar-H, AB), 7.91 (m, 3H, 2Ar-H & 1H of NH₂), 8.23 (s, 1H, 1H of NH₂), 10.09 (br, 1H, SO₂-NH); MS, m/z (%): 286 (M⁺; 27.8); Anal. Calcd. for C₁₀H₁₄N₄O₂S₂ (286.37): C, 41.94; H, 4.93; N, 19.56; Found: C, 42.02; H, 4.91; N, 19.53%.

***N*-Methyl-2-(1-(4-(methylsulfonamido)phenyl)ethylidene)hydrazinecarbothioamide (2b):** Yield 85 %; m.p. 246-244 °C; IR (KBr): ν/cm^{-1} : 3355, 3321 (NH); ^1H NMR: 2.28 (s, 3H, CH₃-C=N), 3.02 (s, 3H, CH₃-SO₂), 3.05 (d, 3H, $J = 4.3$ Hz, NHCH₃), 7.24 (d, 2H, $J = 8.5$ Hz, Ar-H, AB), 7.92 (d, 2H, $J = 8.7$ Hz, Ar-H, AB), 8.41 (d, 1H, $J = 4.3$ Hz, NHCH₃), 9.92 (s, 1H, SO₂-NH), 10.17 (s, 1H, N-NH-CS); ^{13}C NMR: 14.27 (CH₃-C=N), 31.53 (NHCH₃), 39.53 (CH₃-SO₂) 119.17 (2CH), 128.18 (2CH), 133.43 (C), 139.77 (C), 147.50 (C), 179.04 (C=S); MS, m/z (%): 300 (M⁺; 38.9); Anal. Calcd. for C₁₁H₁₆N₄O₂S₂ (300.40): C, 43.98; H, 5.37; N, 18.65; Found: C, 43.94; H, 5.34; N, 18.62%

2-(1-(4-(Methylsulfonamido)phenyl)ethylidene)-*N*-phenylhydrazinecarbothioamide (2c): Yield 90 %; m.p. 225-226 °C; IR (KBr): ν/cm^{-1} : 3344, 3332 (NH); ^1H NMR: 2.37 (s, 3H, CH₃-C=N), 3.03 (s, 3H, CH₃-SO₂), 7.22 (m, 3H, Ar-H), 7.37 (t, 2H, $J = 7.6$ Hz, Ar-H), 7.58 (d, 2H, $J = 7.7$ Hz, Ar-H), 7.99 (d, 2H, $J = 8.5$ Hz, Ar-H), 9.95 (s, 1H, NHPh), 9.99 (s, 1H, SO₂-NH), 10.54 (s, 1H, N-NH-CS); MS, m/z (%): 362 (M⁺; 57.1); Anal. Calcd. for C₁₆H₁₈N₄O₂S₂ (362.47): C, 53.02; H, 5.01; N, 15.46; Found: C, 52.98; H, 4.99; N, 15.37%

2-(1-(4-(Phenylsulfonamido)phenyl)ethylidene)hydrazinecarbothioamide (2d): Yield 90 %; m.p. 249-251 °C; IR (KBr): ν/cm^{-1} : 3370, 3348, 3322 (NH, NH₂); ^1H NMR: 2.20 (s, 3H, CH₃-C=N), 7.09 (d, 2H, 8.8 Hz, Ar-H), 7.53-7.59 (m, 3H, Ar-H), 7.77-7.83 (m, 4H, Ar-H), 7.85 (s, 1H, 1H of NH₂), 8.20 (s, 1H, 1H of NH₂), 10.12 (s, 1H, N-NH-CS), 10.45 (br, 1H, SO₂-NH);

MS, m/z (%): 286 (M^+ ; 27.8); MS, m/z (%): 348 (M^+ ; 64.3); Anal. Calcd. for $C_{15}H_{16}N_4O_2S_2$ (348.44): C, 51.70; H, 4.63; N, 16.08; Found: C, 51.74; H, 4.61; N, 16.11%

***N*-Methyl-2-(1-(4-(phenylsulfonamido)phenyl)ethylidene)hydrazinecarbothioamide (2e):** Yield 85 %; m.p. 260-262 °C; IR (KBr): ν/cm^{-1} : 3338, 3298 (NH); 1H NMR: 2.21 (s, 3H, $CH_3-C=N$), 3.02 (d, 3H, $J = 4.5$ Hz, NCH_3), 7.12 (d, 2H, $J = 8.7$ Hz, Ar-H), 7.54-7.64 (m, 3H, Ar-H), 7.78-7.82 (m, 4H, Ar-H), 8.38 (d, 1H, $J = 4.4$ Hz, $NHCH_3$), 10.16 (s, 1H, N-NH-CS), 10.50 (br, 1H, SO_2-NH); MS, m/z (%): 362 (M^+ ; 72.8); Anal. Calcd. for $C_{16}H_{18}N_4O_2S_2$ (362.47): C, 53.02; H, 5.01; N, 15.46; Found: C, 53.99; H, 5.02; N, 15.38%

***N*-Phenyl-2-(1-(4-(phenylsulfonamido)phenyl)ethylidene)hydrazinecarbothioamide (2f):** Yield 90 %; m.p. 203-204 °C; IR (KBr): ν/cm^{-1} : 3363, 3321 (NH); 1H NMR: 2.46 (s, 3H, $CH_3-C=N$), 7.12 (d, 2H, $J = 8.8$ Hz, Ar-H), 7.20 (t, 1H, $J = 7.3$ Hz, Ar-H), 7.36 (t, 2H, $J = 7.8$ Hz, Ar-H), 7.54-7.65 (m, 5H, Ar-H), 7.78 (d, 2H, $J = 8.7$ Hz, Ar-H), 7.88 (d, 2H, $J = 8.8$ Hz, Ar-H), 9.95 (s, 1H, $NHPh$), 10.50 (s, 2H, 2NH); MS, m/z (%): 424 (M^+ ; 74.4); Anal. Calcd. for $C_{21}H_{20}N_4O_2S_2$ (424.54): C, 59.41; H, 4.75; N, 13.20; Found: C, 59.38; H, 4.74; N, 13.17%

Synthesis the derivatives of thiazolidin-4-one 3a-f

A mixture of 0.001 mole of the thiosemicarbazones **2a-f**, 0.001 mole of ethyl chloroacetate and 0.002 mole of fused CH_3COONa was dissolved 40 mL THF (in case of **2d** excess solvent was used). The solution of the reaction mixture was heated under reflux condition for 3 hours. After cooling, the obtained crude products were collected and recrystallized from THF.

***N*-(4-(1-((4-oxothiazolidin-2-ylidene)hydrazono)ethyl)phenyl)methanesulfonamide (3a):** Yield 70 %; m.p. 231-232 °C; IR (KBr): ν/cm^{-1} : 3440, 3370, 3335 (NH); 1H NMR: 2.33 (s, 3H, $CH_3-C=N$), 3.03 (s, 3H, CH_3-SO_2), 3.84 (s, 2H, CH_2 -thiazole), 7.25 (d, 2H, $J = 8.5$ Hz, Ar-H, AB), 7.80 (d, 2H, $J = 8.5$ Hz, Ar-H, AB), 10.08-11.10 (br, 2H, NH); MS, m/z (%): 326 (M^+ ; 32.1); Anal. Calcd. for $C_{12}H_{14}N_4O_3S_2$ (326.39): C, 44.16; H, 4.32; N, 17.17; Found: C, 44.14; H, 4.31; N, 17.15%.

***N*-(4-(1-((3-methyl-4-oxothiazolidin-2-ylidene)hydrazono)ethyl)phenyl)methanesulfonamide (3b):** Yield 70 %; m.p. 250-251 °C; IR (KBr): ν/cm^{-1} : 3429, 3363, 3328 (NH); 1H NMR: 2.40 (s, 3H, $CH_3-C=N$), 3.04 (s, 3H, CH_3-SO_2), 3.20 (s, 3H, NCH_3), 3.93 (s, 2H, CH_2 -thiazole), 7.27 (d, 2H, $J = 8.5$ Hz, Ar-H, AB), 7.84 (d, 2H, $J = 8.5$ Hz, Ar-H, AB), 10.08 (br, 1H, SO_2-NH); ^{13}C NMR: 14.87 (CH_3), 29.88 (CH_3), 32.55 (CH_2), 40.60 (CH_3), 119.18 (2CH), 128.06 (2CH), 133.26, 140.56, 161.34 ($C=N$), 163.50 ($C=N$), 172.67 ($C=O$); MS, m/z (%): 340 (M^+ ; 65.8); Anal. Calcd. for $C_{13}H_{16}N_4O_3S_2$ (340.42): C, 45.87; H, 4.74; N, 16.46; Found: C, 45.85; H, 4.72; N, 16.47%.

***N*-(4-(1-((4-oxo-3-phenylthiazolidin-2-ylidene)hydrazono)ethyl)phenyl)methanesulfonamide (3c):** Yield 80 %; m.p. 258-260 °C; IR (KBr): ν/cm^{-1} : 3388, 3348 (NH); ^1H NMR: 2.13 (s, 3H, $\text{CH}_3\text{-C=N}$), 3.04 (s, 3H, $\text{CH}_3\text{-SO}_2$), 4.09 (s, 2H, $\text{CH}_2\text{-thiazole}$), 7.25 (d, 2H, $J = 8.6$ Hz, Ar-H), 7.37-7.50 (m, 3H, Ar-H), 7.53 (t, 2H, $J = 7.5$ Hz, Ar-H), 7.80 (d, 2H, $J = 8.7$ Hz, Ar-H), 10.12 (br, 1H, $\text{SO}_2\text{-NH}$); MS, m/z (%):402 (M^+ ; 36.2); Anal. Calcd. for $\text{C}_{18}\text{H}_{18}\text{N}_4\text{O}_3\text{S}_2$ (402.49): C, 53.71; H, 4.51; N, 13.92; Found: C, 53.68; H, 4.50; N, 13.89%.

***N*-(4-(1-(4-oxothiazolidin-2-ylidene)hydrazono)ethyl)phenyl)benzenesulfonamide (3d):** Yield 75 %; m.p. 257-258 °C; IR (KBr): ν/cm^{-1} : 3444, 3373, 3332 (NH); ^1H NMR: 2.20 (s, 3H, $\text{CH}_3\text{-C=N}$), 3.85 (s, 2H, $\text{CH}_2\text{-thiazole}$), 7.09-7.82 (m, 9H, Ar-H), 10.12 (s, 1H, NH-thiazole), 10.64 (br, 1H, $\text{SO}_2\text{-NH}$); MS, m/z (%):388 (M^+ ; 65.2); Anal. Calcd. for $\text{C}_{17}\text{H}_{16}\text{N}_4\text{O}_3\text{S}_2$ (388.46): C, 52.56; H, 4.15; N, 14.42; Found: C, 52.54; H, 4.14; N, 14.39%.

***N*-(4-(1-((3-methyl-4-oxothiazolidin-2-ylidene)hydrazono)ethyl)phenyl)benzenesulfonamide (3e):** Yield 75 %; m.p. 236-238 °C; IR (KBr): ν/cm^{-1} : 3444, 3373, 3332 (NH); ^1H NMR: 2.33 (s, 3H, $\text{CH}_3\text{-C=N}$), 3.17 (s, 3H, NCH_3), 3.91 (s, 2H, $\text{CH}_2\text{-thiazole}$), 7.20 (d, 2H, Ph-H), 7.57 (m, 3H, Ph-H), 7.73 (d, 2H, $J = 8.4$ Hz, Ar-H, AB), 7.84 (d, 2H, $J = 8.3$ Hz, Ar-H, AB), 10.76 (br, 1H, $\text{SO}_2\text{-NH}$); MS, m/z (%):402 (M^+ ; 34.4); Anal. Calcd. for $\text{C}_{18}\text{H}_{18}\text{N}_4\text{O}_3\text{S}_2$ (402.49): C, 53.71; H, 4.51; N, 13.92; Found: C, 53.69; H, 4.52; N, 13.89%.

***N*-(4-(1-((4-oxo-3-phenylthiazolidin-2-ylidene)hydrazono)ethyl)phenyl)benzenesulfonamide (3f):** Yield 80 %; m.p. 249-250 °C; IR (KBr): ν/cm^{-1} : 3400, 3384, 3318 (NH); ^1H NMR: 2.10 (s, 3H, $\text{CH}_3\text{-C=N}$), 4.07 (s, 2H, $\text{CH}_2\text{-thiazole}$), 7.15 (d, 2H, 7.8 Hz, Ar-H), 7.39-7.49 (m, 3H, Ar-H), 7.50-7.62 (m, 5H, Ar-H), 7.70 (d, 2H, $J = 7.7$ Hz, Ar-H), 7.82 (d, 2H, $J = 6.8$ Hz, Ar-H), 10.58 (br, 1H, $\text{SO}_2\text{-NH}$); MS, m/z (%):464 (M^+ ; 27.8); Anal. Calcd. for $\text{C}_{23}\text{H}_{20}\text{N}_4\text{O}_3\text{S}_2$ (464.56): C, 59.46; H, 4.34; N, 12.06; Found: C, 59.39; H, 4.32; N, 12.08%.

Synthesis the derivatives of 4-phenyl-2,3-dihydrothiazole 4a-f:

The mixture of 0.001 mole of the thiosemicarbazones **2a-f**, 0.01 mole of chloroacetone and 0.002 mole of fused CH_3COONa was gently heated in 40 mL THF (in case of **2d** excess solvent was used). The solution of the reaction mixture was heated under reflux condition for 6 hours. Then, it was concentrated. After cooling, the obtained crude products were collected and recrystallized from ethyl alcohol to give 4-phenyl-2,3-dihydrothiazole derivatives **4a-f**.

***N*-(4-(1-((4-Methylthiazol-2(3H)-ylidene)hydrazineylidene)ethyl)phenyl)methanesulfonamide (4a):** Yield 60 %; m.p. 209-210 °C; IR (KBr): ν/cm^{-1} : 3267 (NH); ^1H NMR: 2.17 (s, 3H, $\text{CH}_3\text{-thiazole}$), 2.25 (s, 3H, $\text{CH}_3\text{-C=N}$), 3.02 (s, 3H, $\text{CH}_3\text{-SO}_2$), 6.32 (s, 1H, thiazole-H), 7.23 (d, 2H, $J = 8.8$ Hz, Ar-H, AB), 7.72 (d, 2H, $J = 8.8$ Hz, Ar-H, AB), 9.87 (br, 1H, NH-thiazole), 10.97 (br, 1H, $\text{SO}_2\text{-NH}$); MS, m/z (%):

324 (M^+ ; 63.0); Anal. Calcd. for $C_{13}H_{16}N_4O_2S_2$ (324.42): C, 48.13; H, 4.97; N, 17.27; Found: C, 48.09; H, 4.98; N, 17.31%.

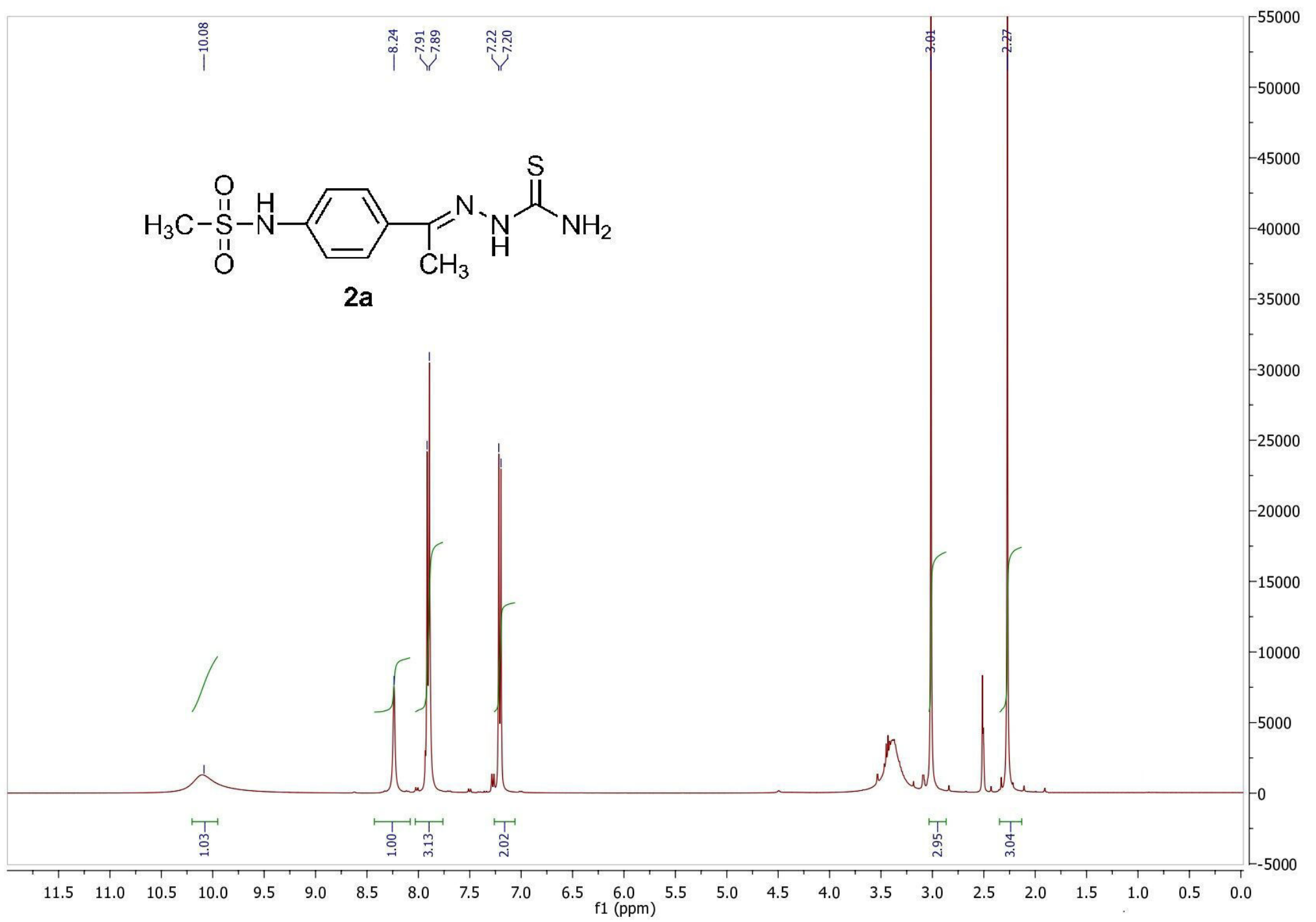
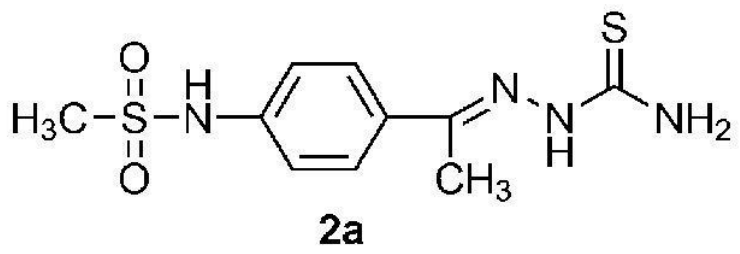
***N*-(4-(1-((3,4-Dimethylthiazol-2(3*H*)-ylidene)hydrazineylidene)ethyl)phenyl)methanesulfonamide (4b):** Yield 65 %; m.p. 258-259 °C; IR (KBr): ν/cm^{-1} : 3254 (NH); 1H NMR: 2.17 (s, 3H, CH_3 -thiazole), 2.25 (s, 3H, CH_3 -C=N), 3.02 (s, 3H, CH_3 -SO₂), 3.20 (s, 3H, NCH₃), 6.30 (s, 1H, thiazole-H), 7.21 (d, 2H, $J = 8.8$ Hz, Ar-H, AB), 7.70 (d, 2H, $J = 8.8$ Hz, Ar-H, AB), 10.97 (br, 1H, SO₂-NH); MS, m/z (%): 338 (M^+ ; 65.2); Anal. Calcd. for $C_{14}H_{18}N_4O_2S_2$ (338.44): C, 49.68; H, 5.36; N, 16.55; Found: C, 49.69; H, 5.37; N, 16.49%.

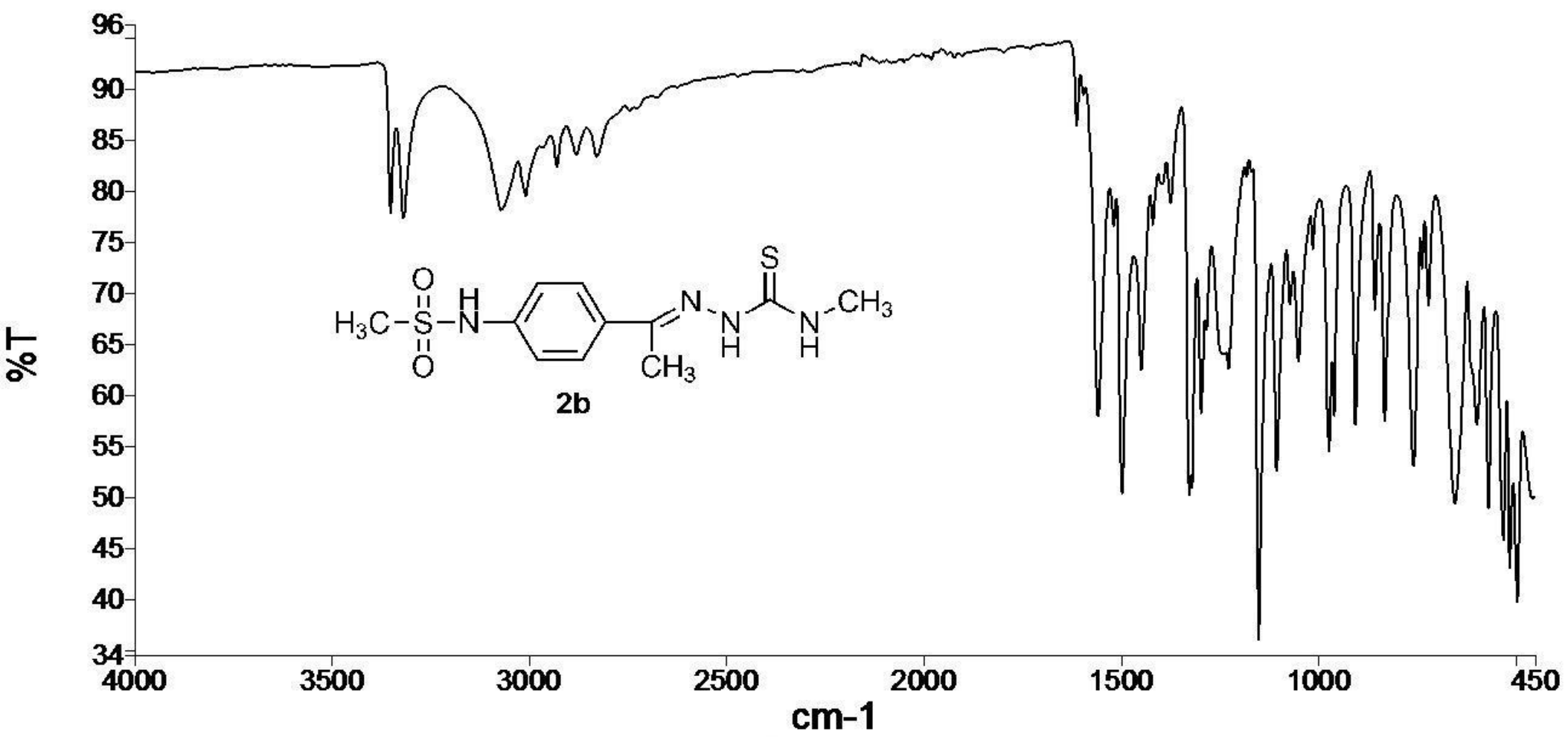
***N*-(4-(1-((4-Methyl-3-phenylthiazol-2(3*H*)-ylidene)hydrazineylidene)ethyl)phenyl)methanesulfonamide (4c):** Yield 60 %; m.p. 245-255 °C; 1H NMR: 2.17 (s, 3H, CH_3 -thiazole), 2.25 (s, 3H, CH_3 -C=N), 3.02 (s, 3H, CH_3 -SO₂), 6.30 (s, 1H, thiazole-H), 7.20-7.70 (m, 9H, Ar-H), 10.97 (br, 1H, SO₂-NH); MS, m/z (%): 400 (M^+ ; 46.2); Anal. Calcd. for $C_{19}H_{20}N_4O_2S_2$ (400.52): C, 56.98; H, 5.03; N, 13.99; Found: C, 57.01; H, 5.01; N, 14.01%.

***N*-(4-(1-((4-Methylthiazol-2(3*H*)-ylidene)hydrazineylidene)ethyl)phenyl)benzenesulfonamide (4d):** Yield 65 %; m.p. 254-255 °C; IR (KBr): ν/cm^{-1} : 3284, 3267 (NH); 1H NMR: 1H NMR: 2.12 (s, 3H, CH_3 -thiazole), 2.27 (s, 3H, CH_3 -C=N), 5.98 (s, 1H, thiazole-H), 7.08-7.80 (m, 9H, Ar-H), 9.90 (br, 1H, NH-thiazole), 10.98 (br, 1H, SO₂-NH); MS, m/z (%): 386 (M^+ ; 45.1); Anal. Calcd. for $C_{18}H_{18}N_4O_2S_2$ (386.49): C, 55.94; H, 4.69; N, 14.50; Found: C, 55.91; H, 4.67; N, 14.48%.

***N*-(4-(1-((3,4-Dimethylthiazol-2(3*H*)-ylidene)hydrazineylidene)ethyl)phenyl)benzenesulfonamide (4e):** Yield 70 %; m.p. 207-208 °C; IR (KBr): ν/cm^{-1} : 3367.24 (NH); 1H NMR: 2.12 (s, 3H, CH_3 -thiazole), 2.27 (s, 3H, CH_3 -C=N), 3.38 (s, 3H, NCH₃), 5.98 (s, 1H, thiazole-H), 7.11 (d, 2H, Ph-H), 7.56 (m, 3H, Ph-H), 7.67 (d, 2H, Ar-H, AB), 7.82 (d, 2H, Ar-H, AB), 10.42 (br, 1H, SO₂-NH); MS, m/z (%): 400 (M^+ ; 27.8); Anal. Calcd. for $C_{19}H_{20}N_4O_2S_2$ (400.52): C, 56.98; H, 5.03; N, 13.99; Found: C, 57.01; H, 5.01; N, 13.97%.

***N*-(4-(1-((4-Methyl-3-phenylthiazol-2(3*H*)-ylidene)hydrazineylidene)ethyl)phenyl)benzenesulfonamide (4f):** Yield 65 %; m.p. 213-215 °C; IR (KBr): ν/cm^{-1} : 3277 (NH); 1H NMR: 1.84 (s, 3H, CH_3 -thiazole), 2.00 (s, 3H, CH_3 -C=N), 6.17 (s, 1H, thiazole-H), 7.10 (d, 2H, $J = 8.6$ Hz, Ph-H), 7.39-7.46 (m, 3H, Ar-H), 7.50-7.63 (m, 7H, Ar-H), 7.80 (d, 2H, $J = 7.2$ Hz, Ar-H), 10.43 (br, 1H, SO₂-NH); MS, m/z (%): 462 (M^+ ; 34.1); Anal. Calcd. for $C_{24}H_{22}N_4O_2S_2$ (462.59): C, 62.32; H, 4.79; N, 12.11; Found: C, 62.29; H, 4.80; N, 12.08%.





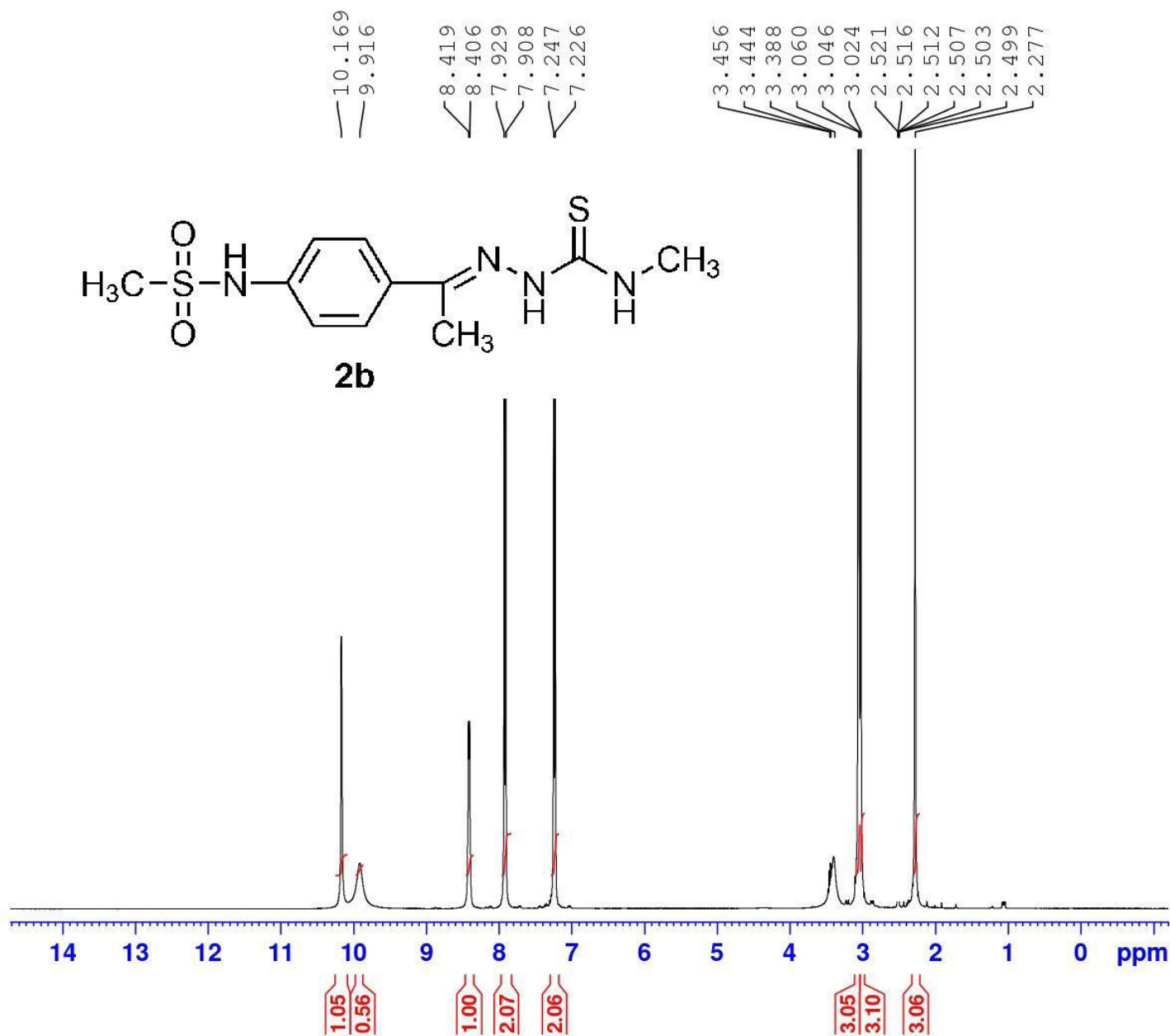


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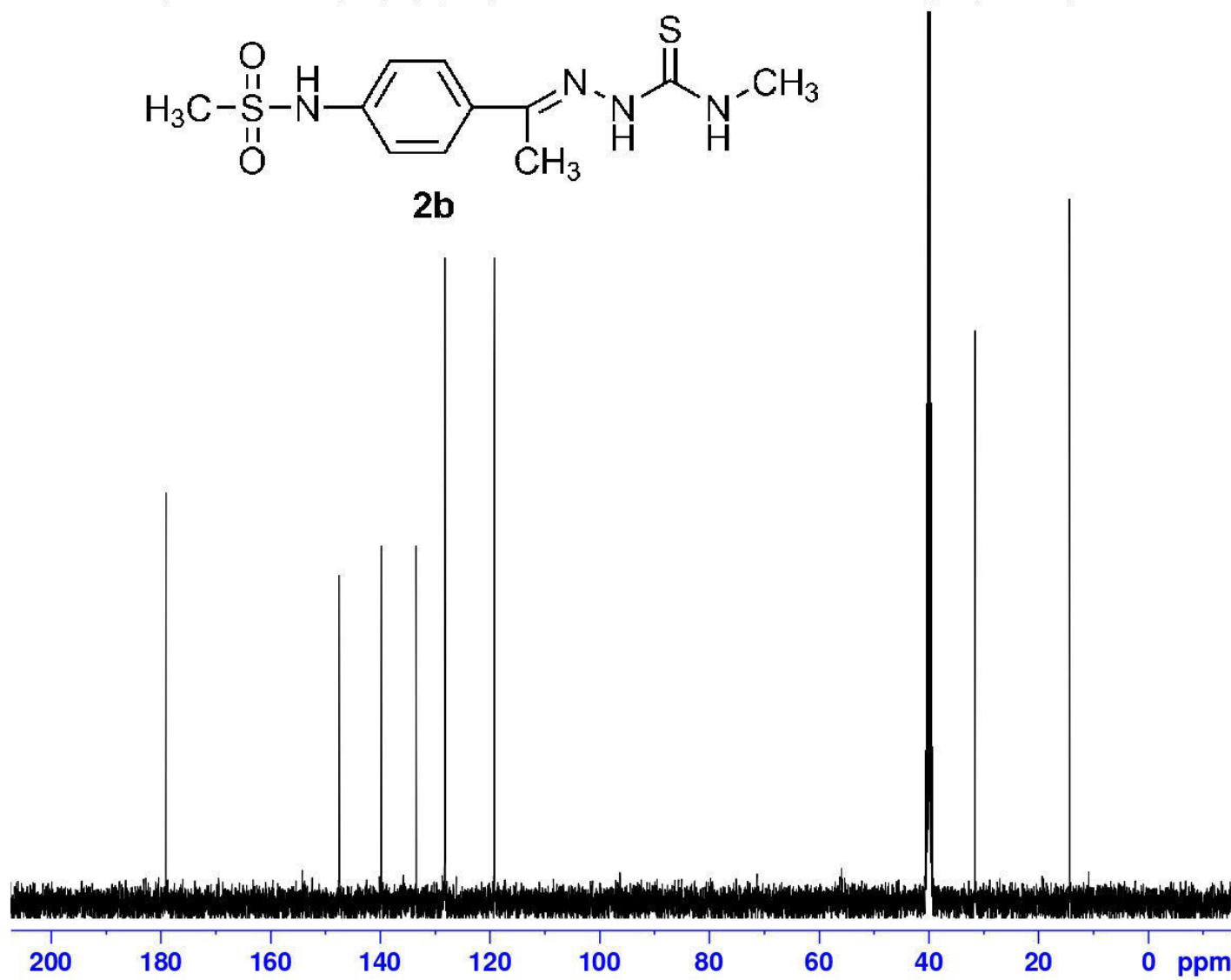
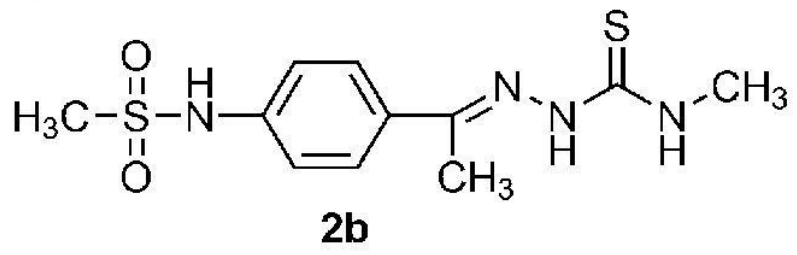
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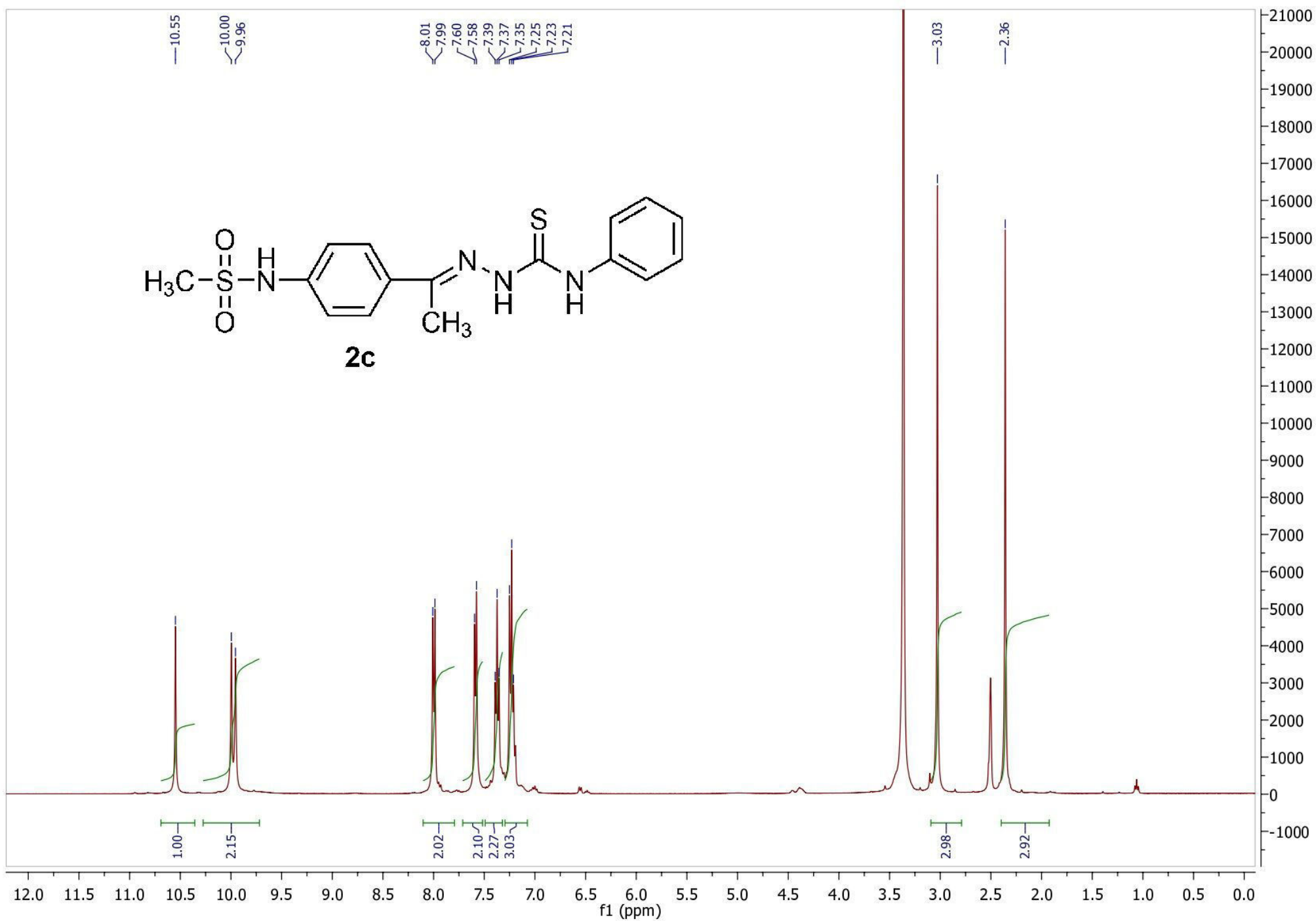
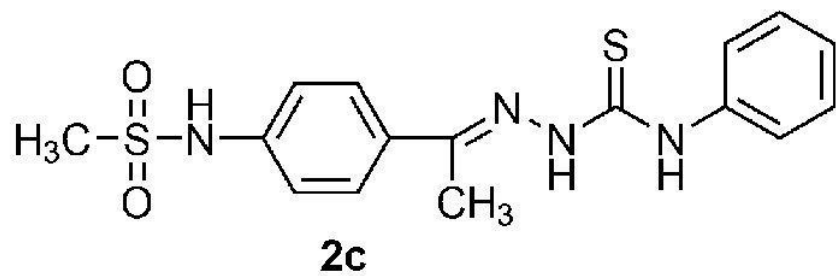
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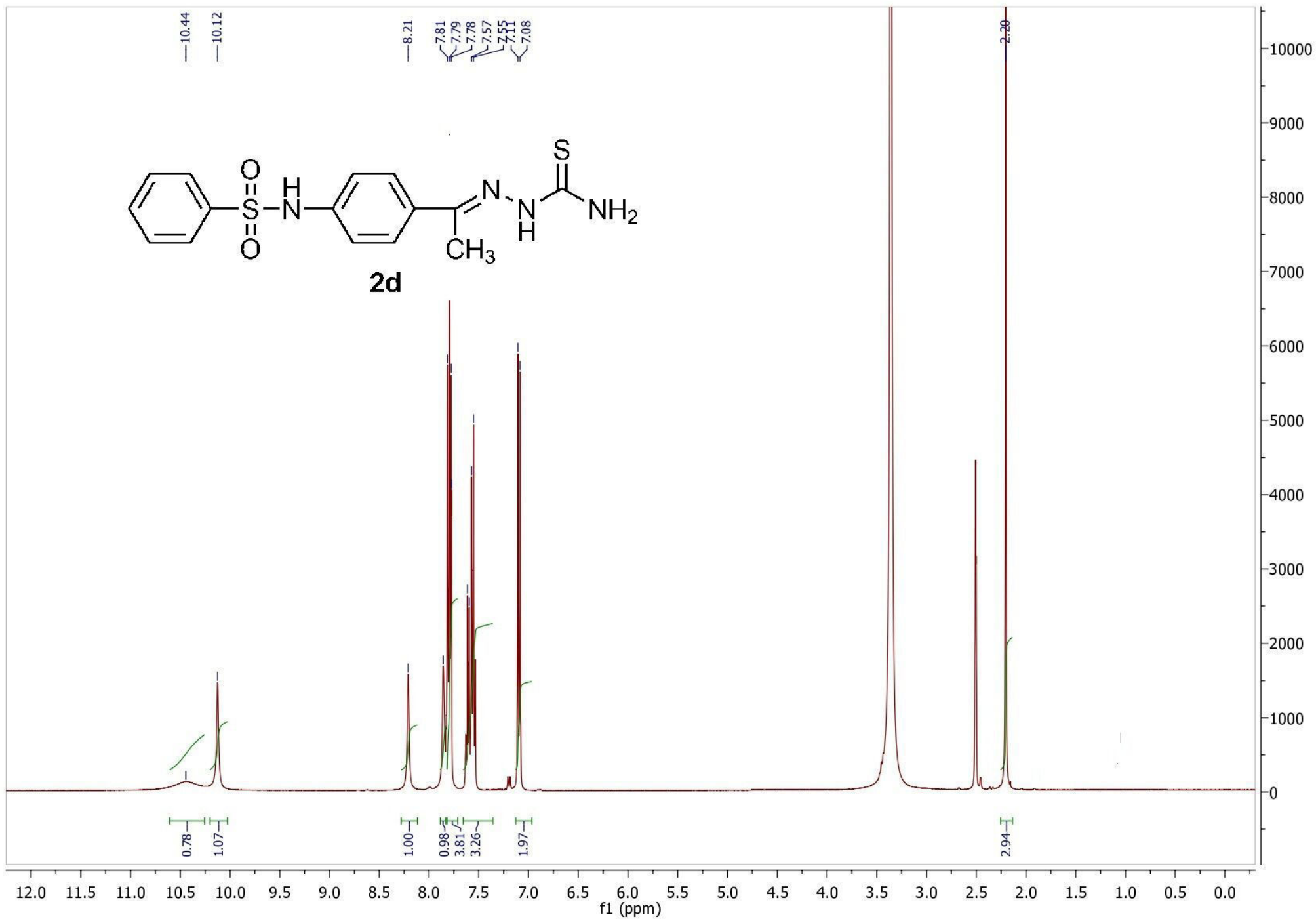
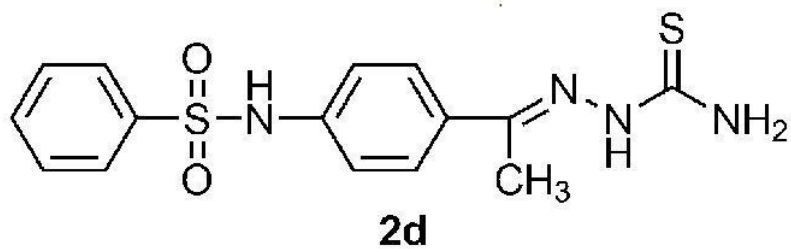
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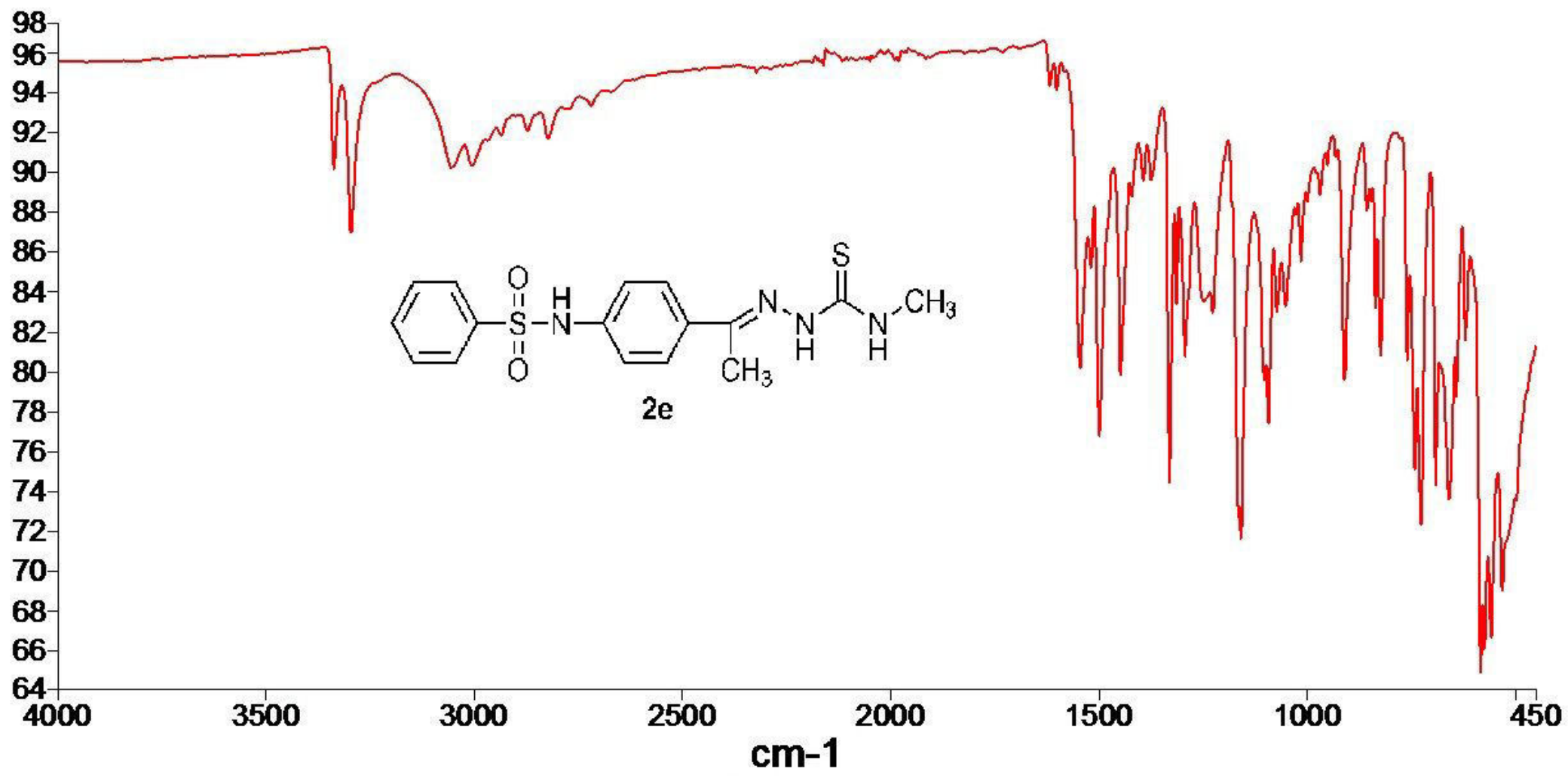
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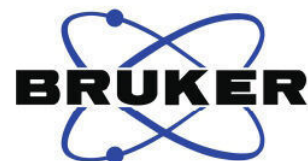
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 PC 1.40







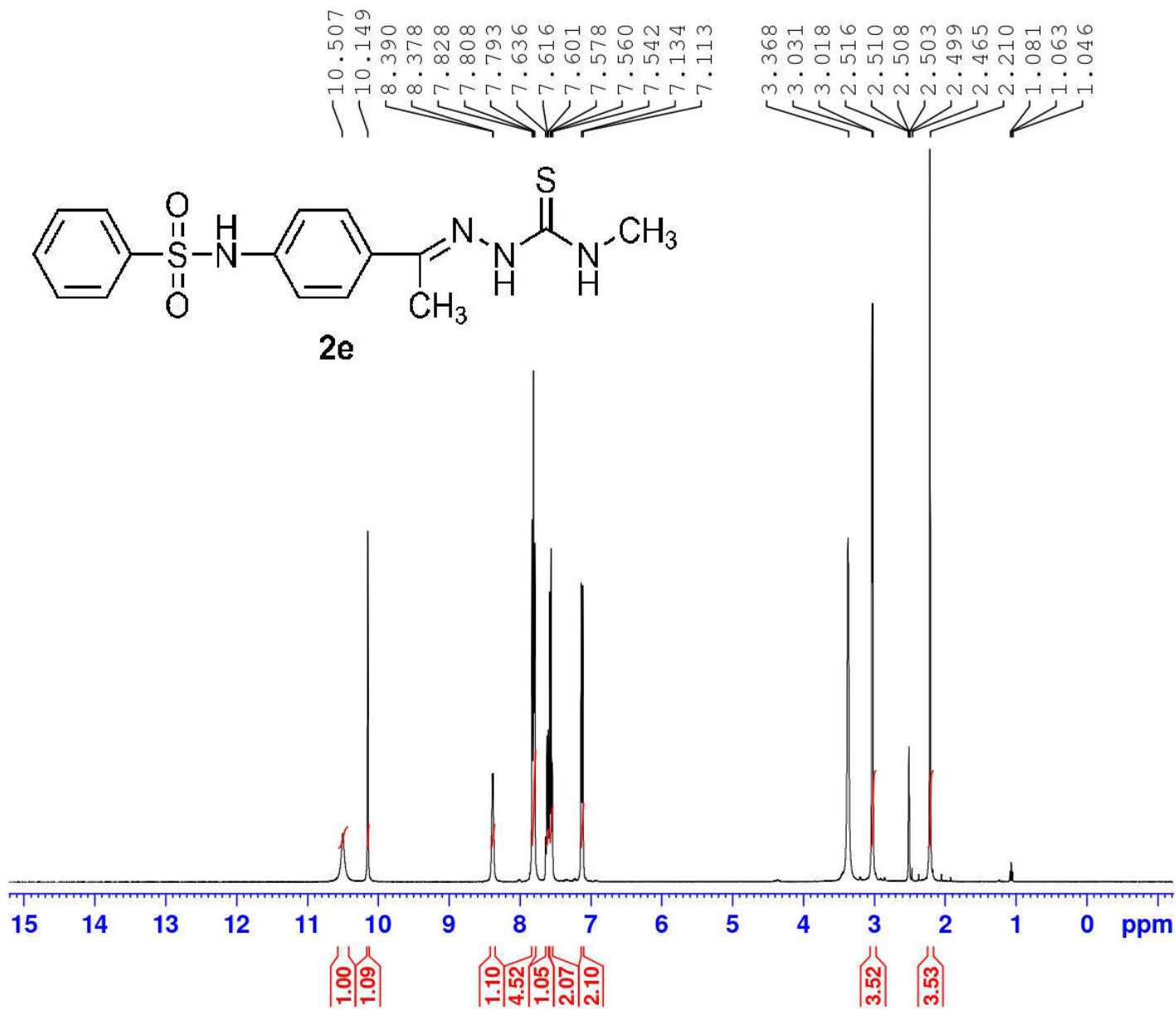


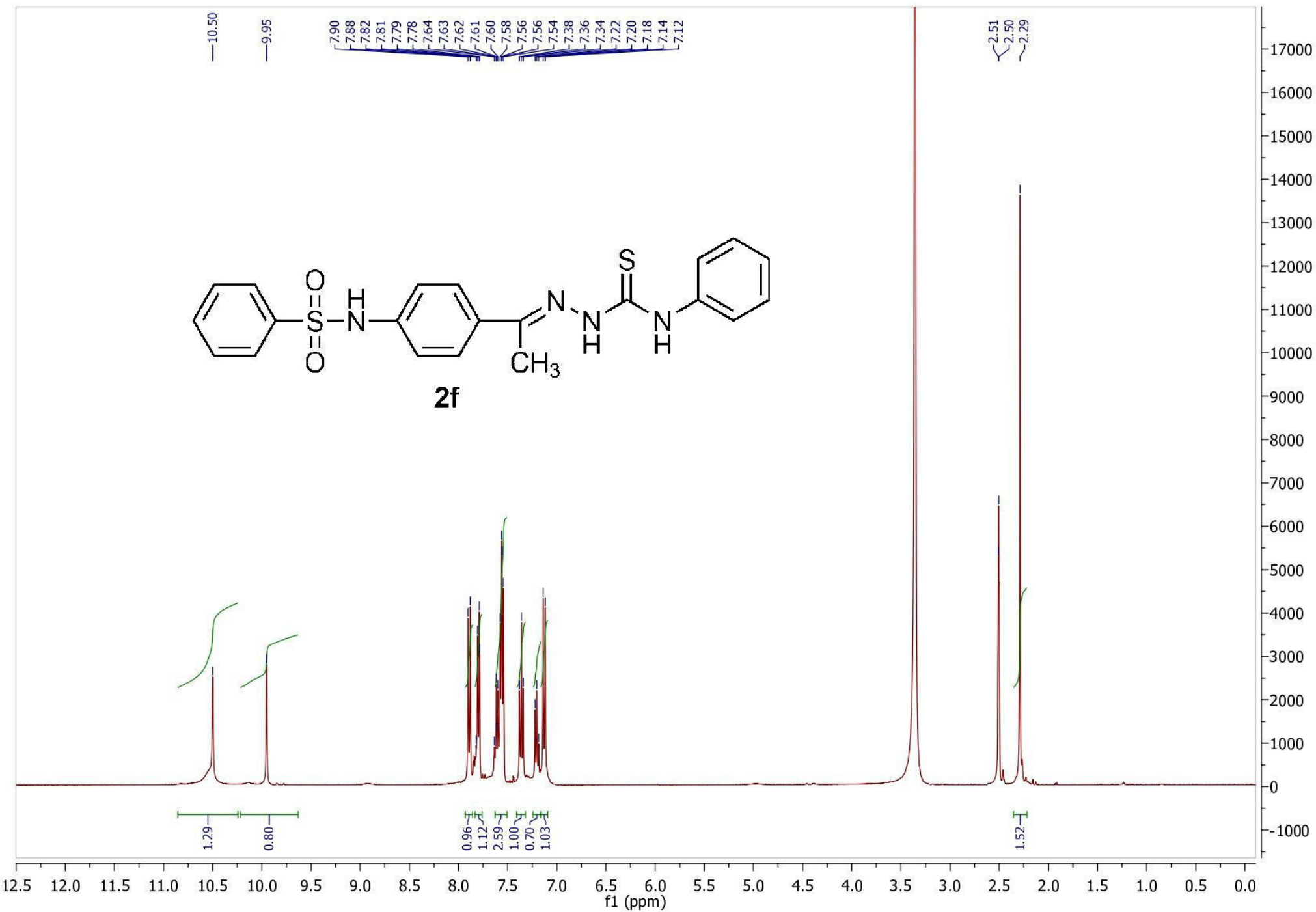
Current Data Parameters
NAME maha-mohamed-S5
EXPNO 1
PROCNO 1

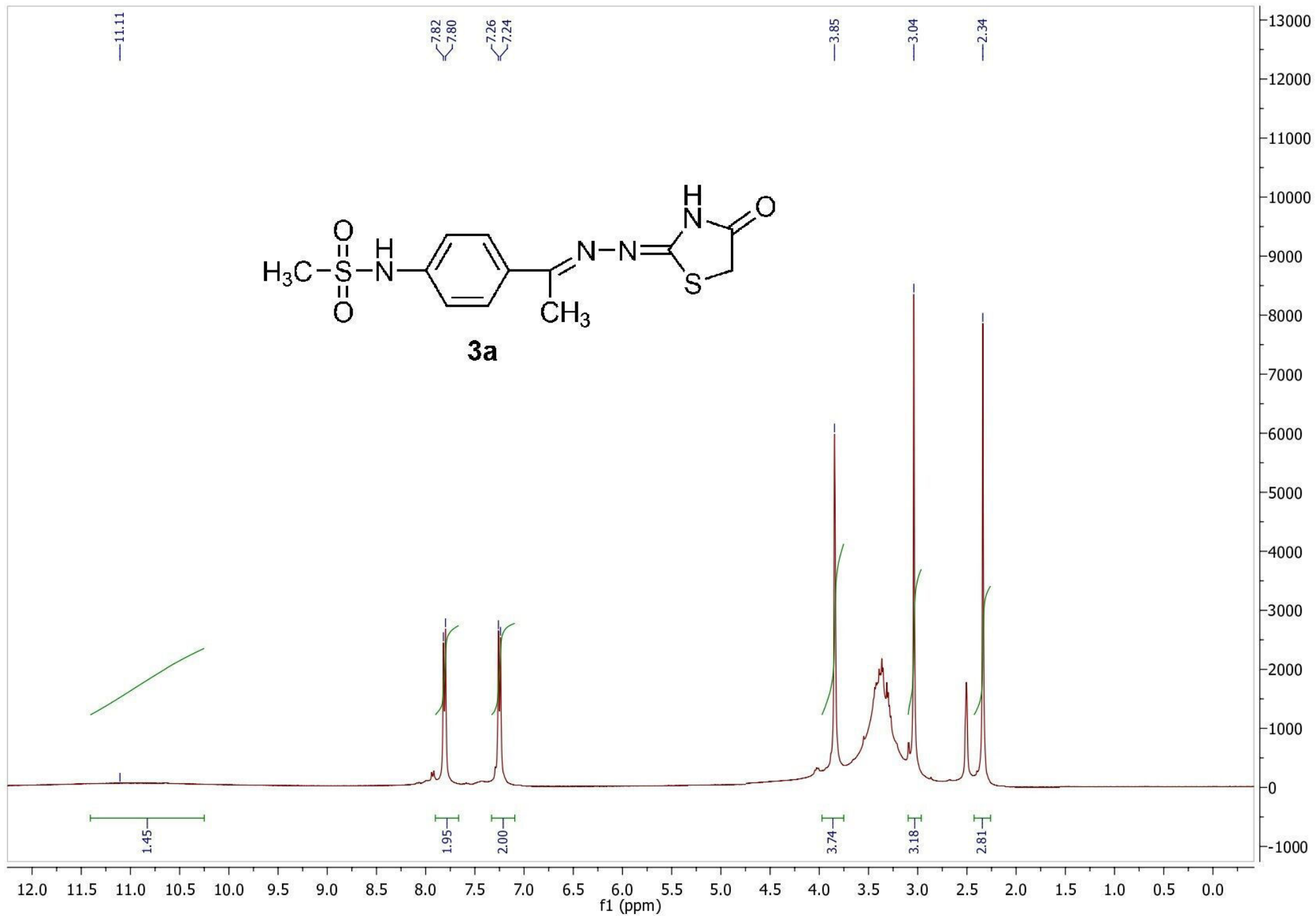
F2 - Acquisition Parameters
Date_ 20220901
Time 14.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 17
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







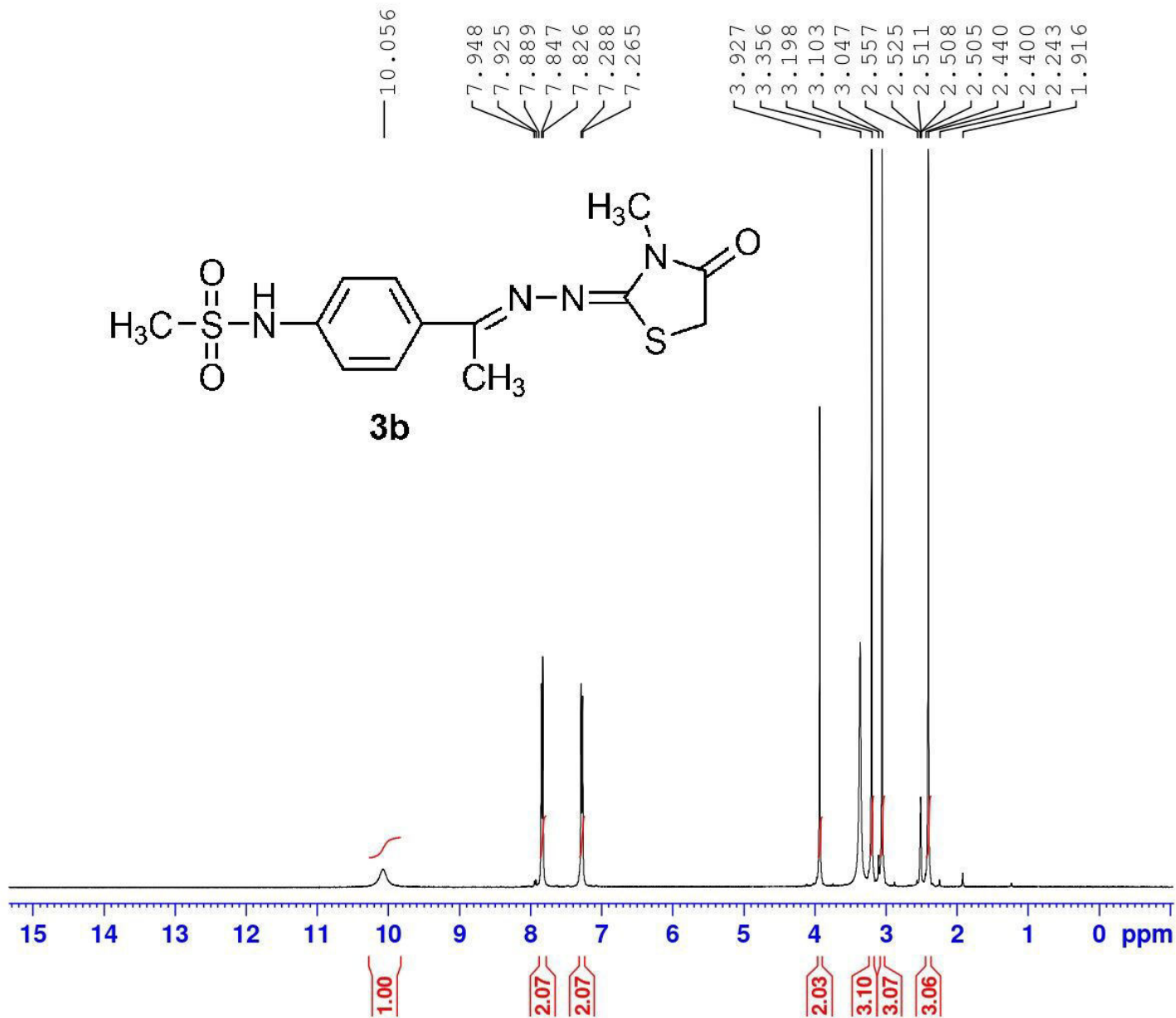


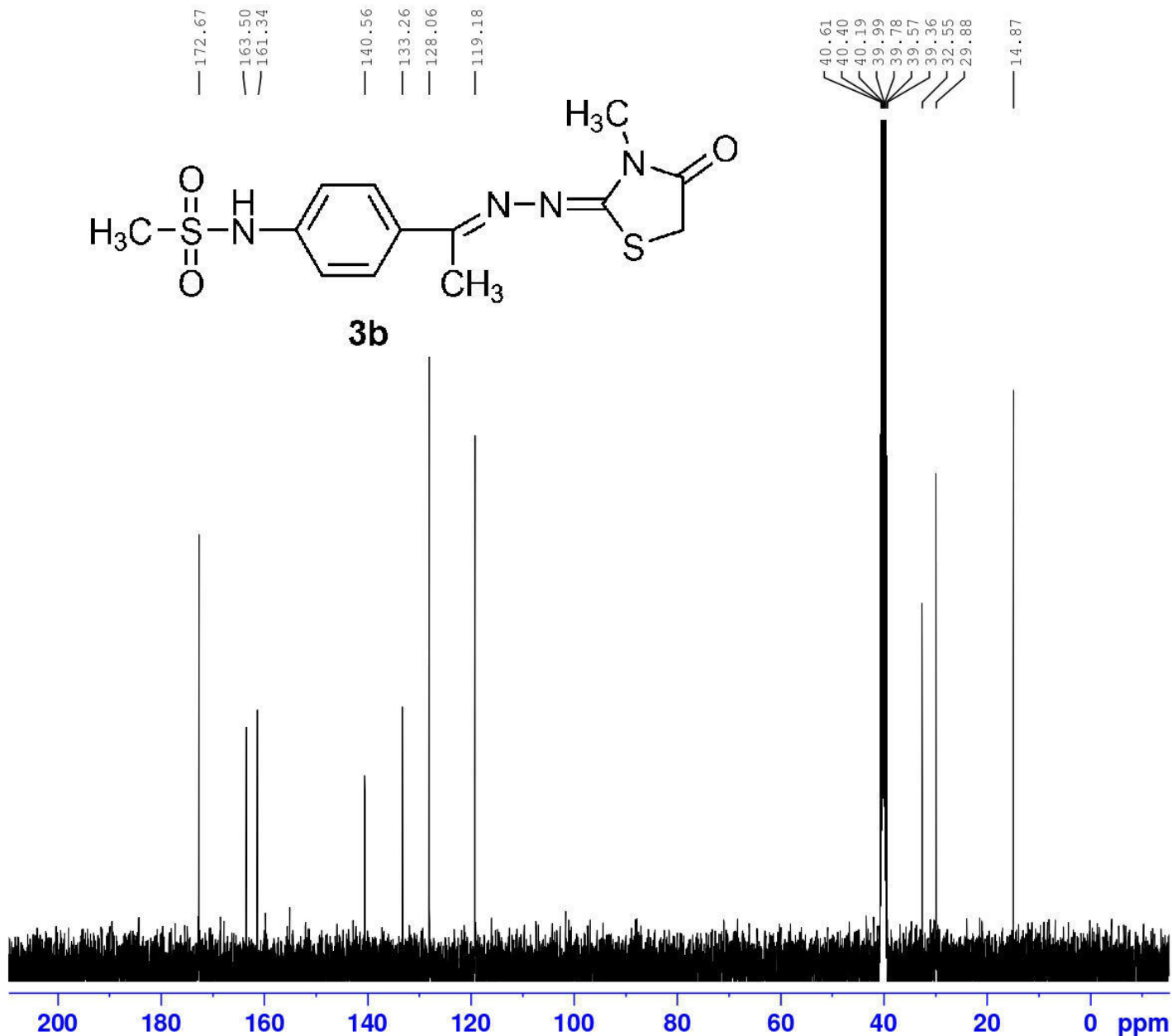
Current Data Parameters
NAME maha-mohamed-S2A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220901
Time 13.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 14
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





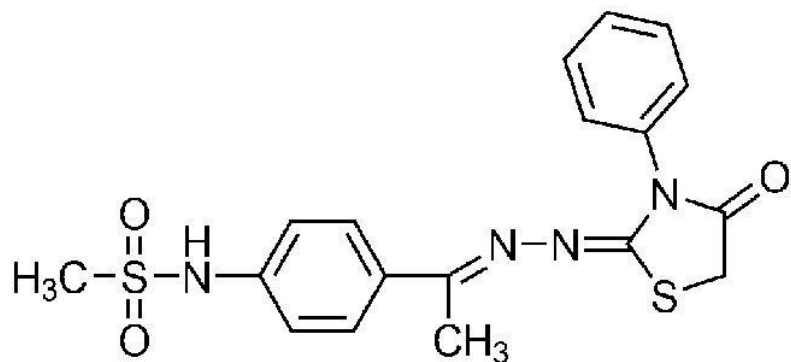
Current Data Parameters
 NAME maha-mohamed-S2A
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220901
 Time 13.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 604
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 205.37
 DW 20.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6278588 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 47.00000000 W

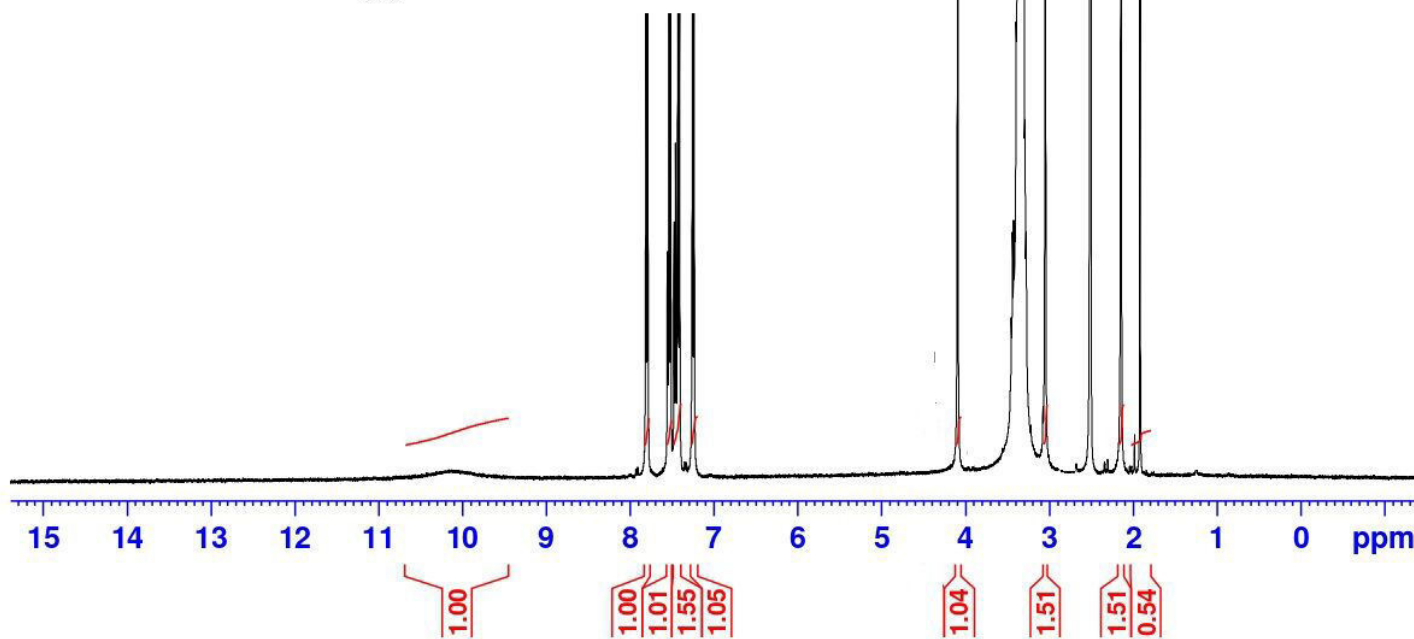
==== CHANNEL f2 =====
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 18.00000000 W
 PLW12 0.34722000 W
 PLW13 0.28125000 W

F2 - Processing parameters
 SI 32768
 SF 100.6177975 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



10.120
7.811
7.788
7.554
7.537
7.516
7.473
7.456
7.431
7.426
7.409
7.257
7.235

4.095
3.453
3.439
3.423
3.411
3.393
3.345
3.301
3.289
3.277
3.043
2.516
2.512
2.507
2.504
2.500
2.143

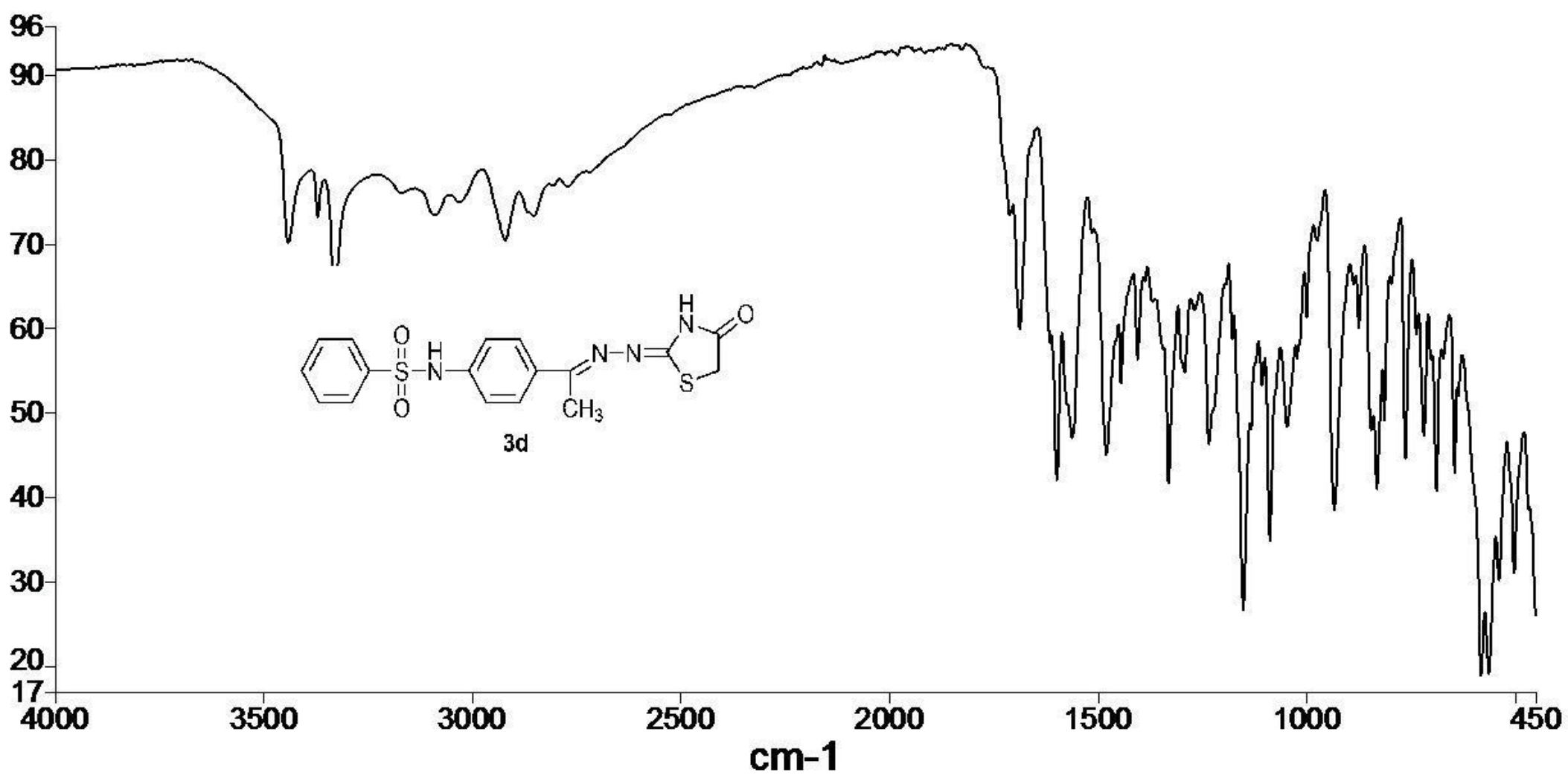


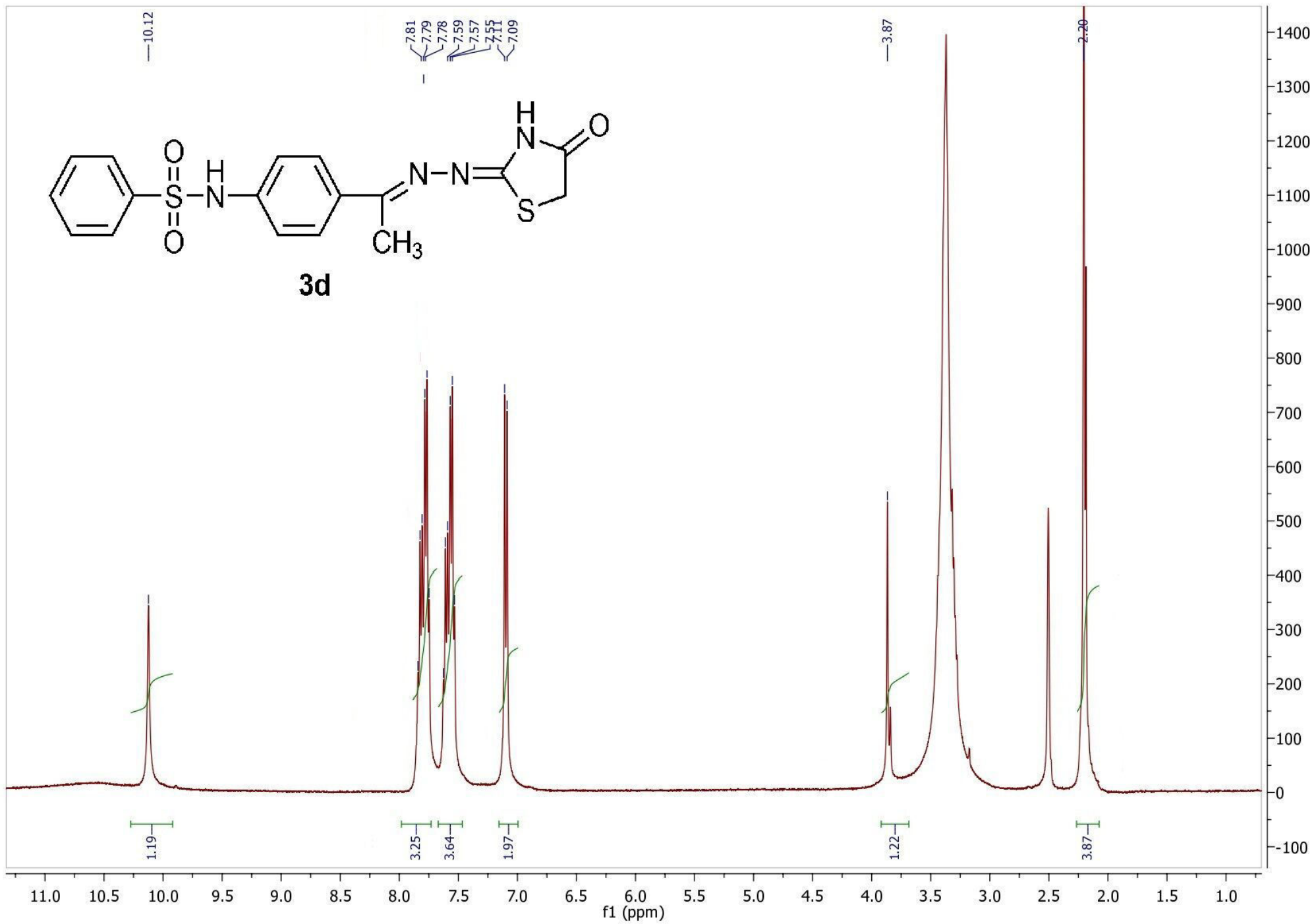
Current Data Parameters
NAME maha-mohamed-S3A
EXPNO 1
PROCNO 1

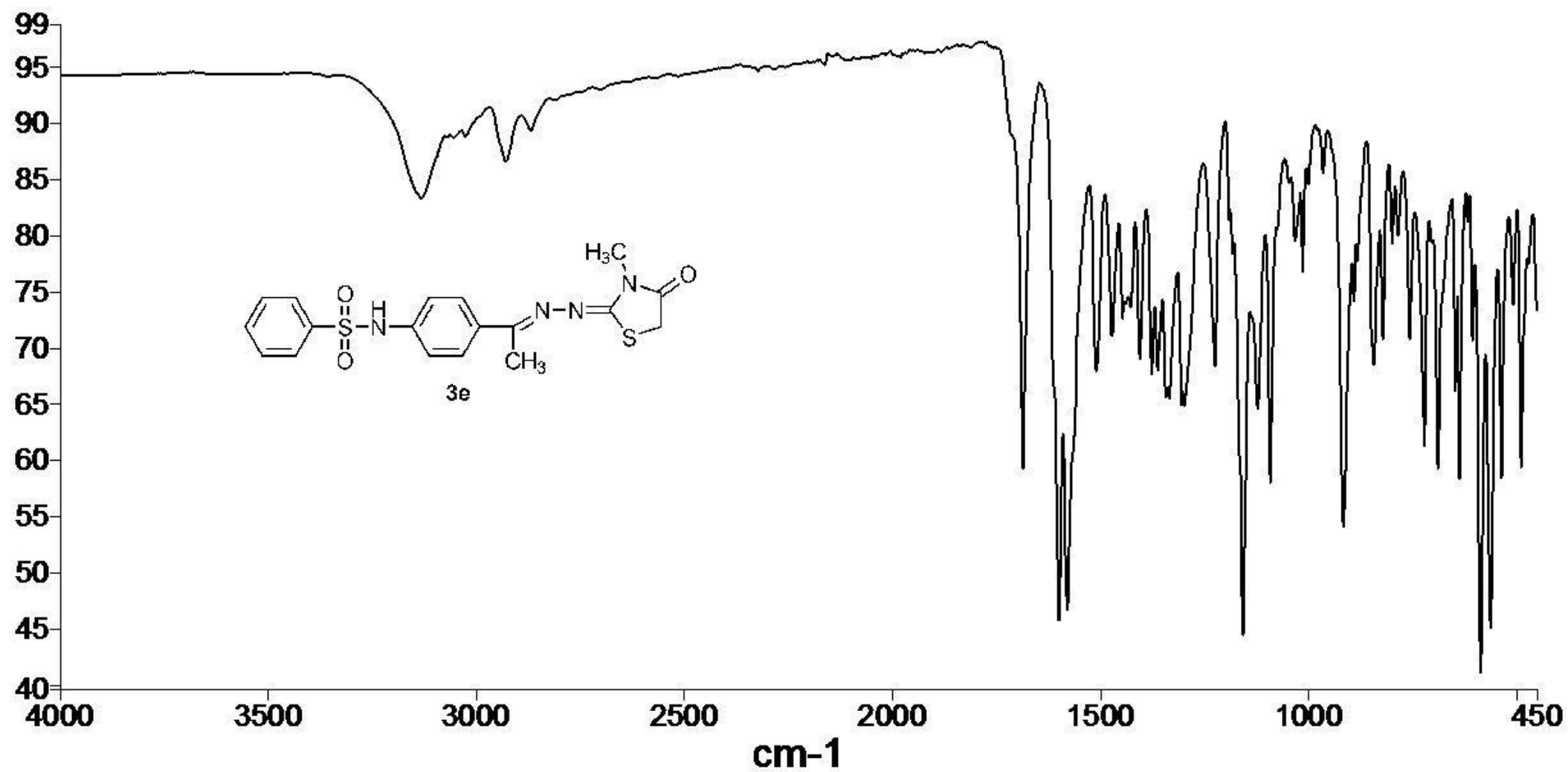
F2 - Acquisition Parameters
Date_ 20220901
Time 14.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 88
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







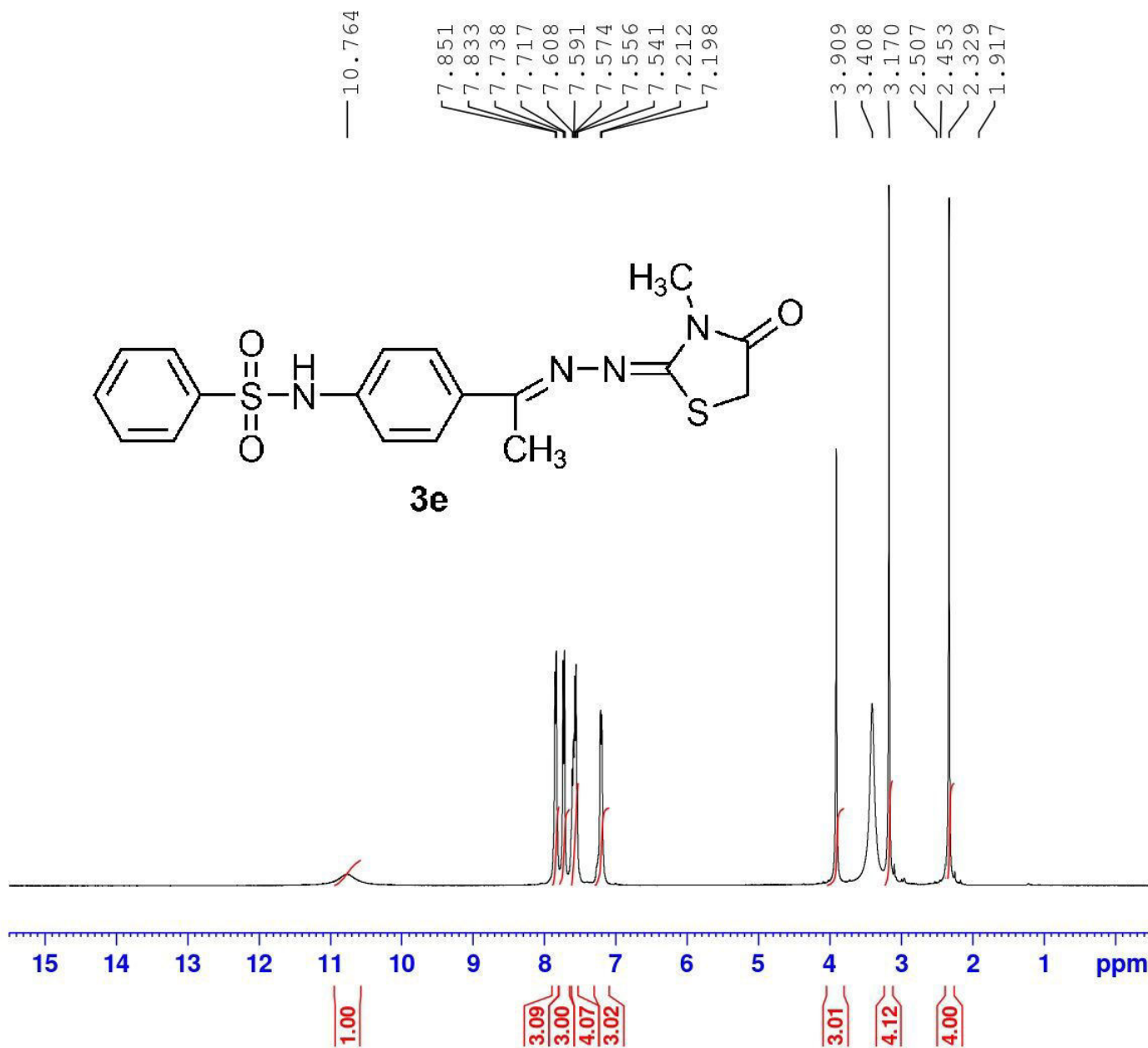


Current Data Parameters
NAME maha-aziz-S5A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220822
Time 8.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 79
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



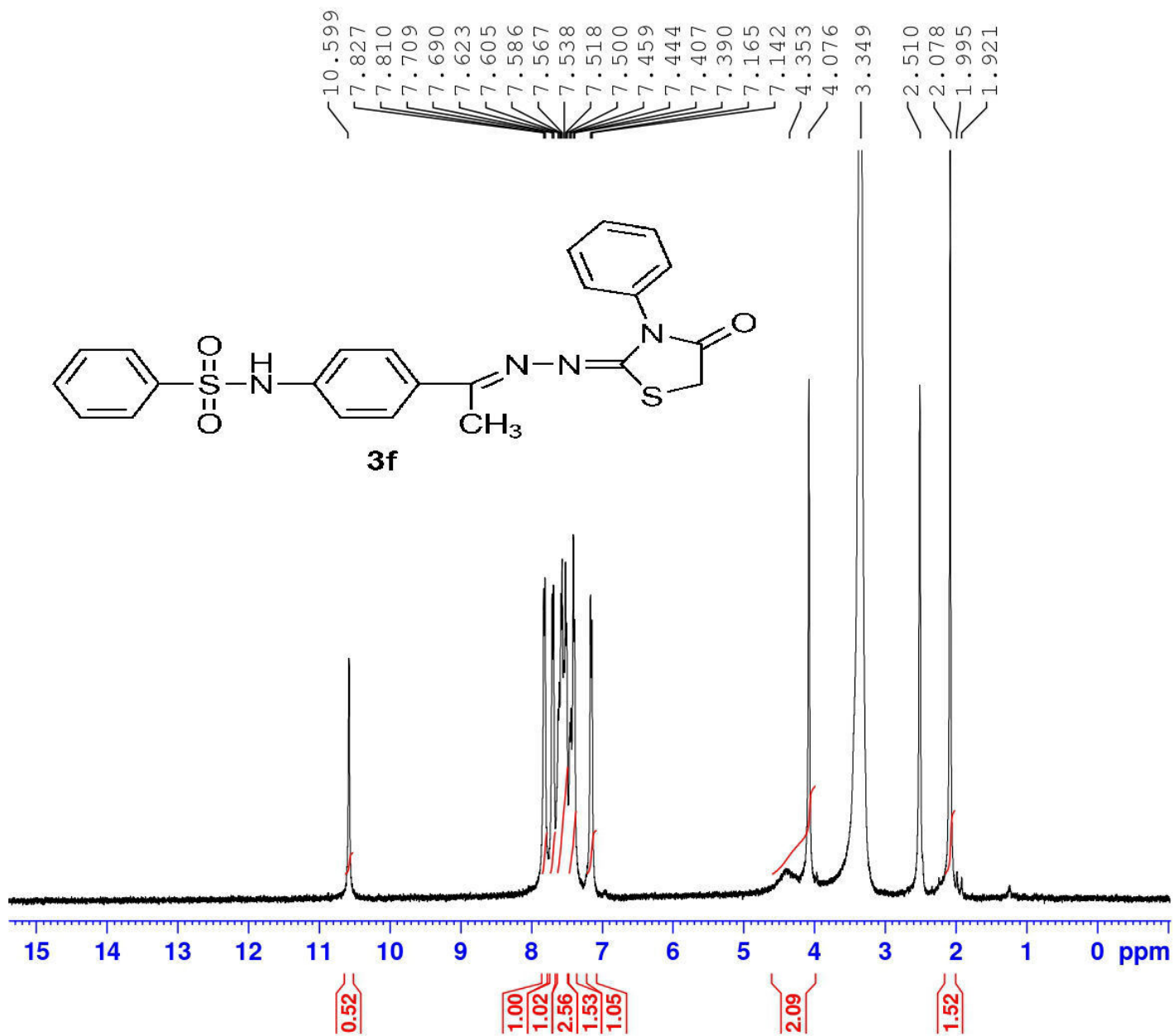


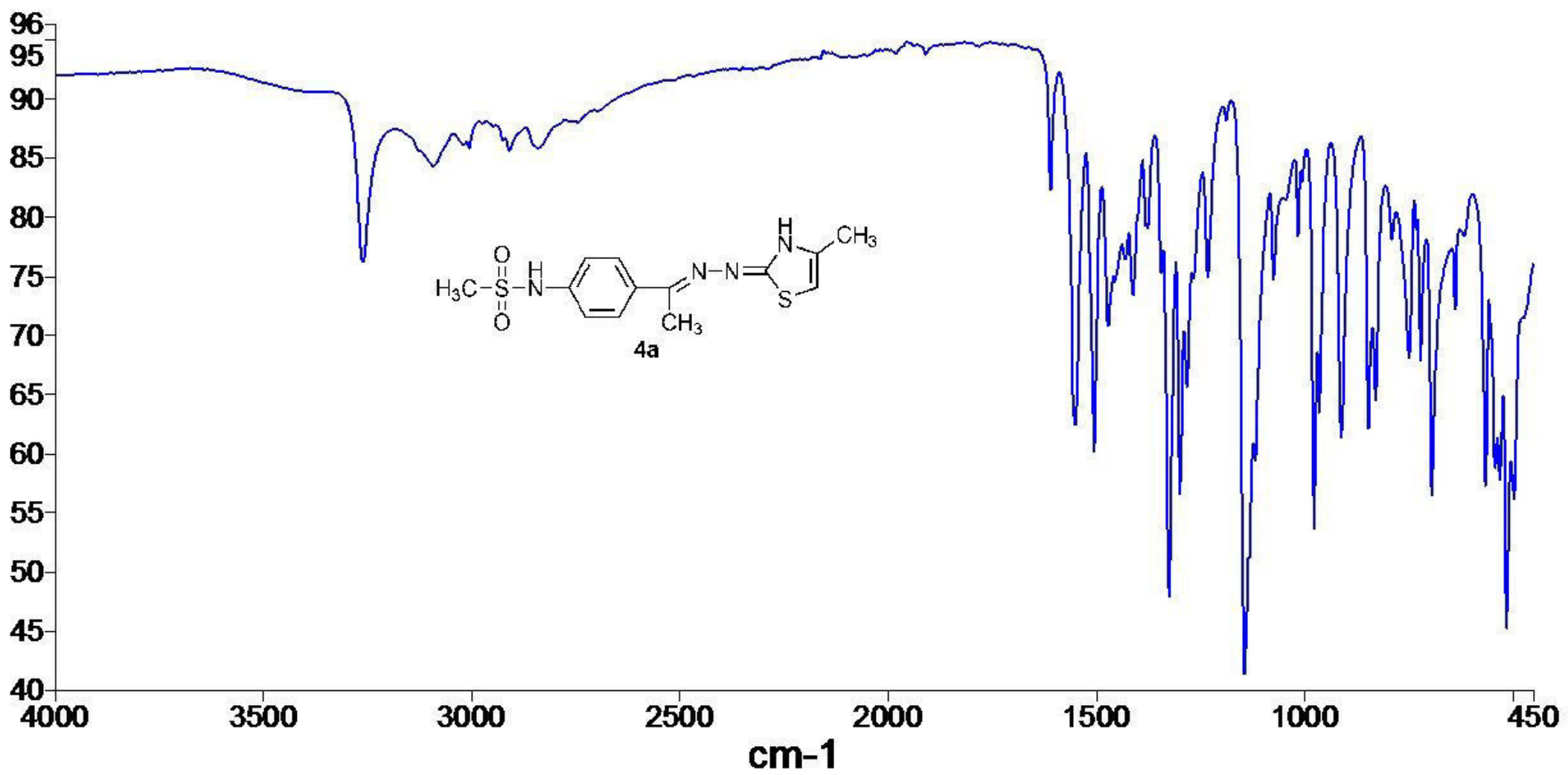
Current Data Parameters
NAME maha-mohamed-S6A
EXPNO 1
PROCNO 1

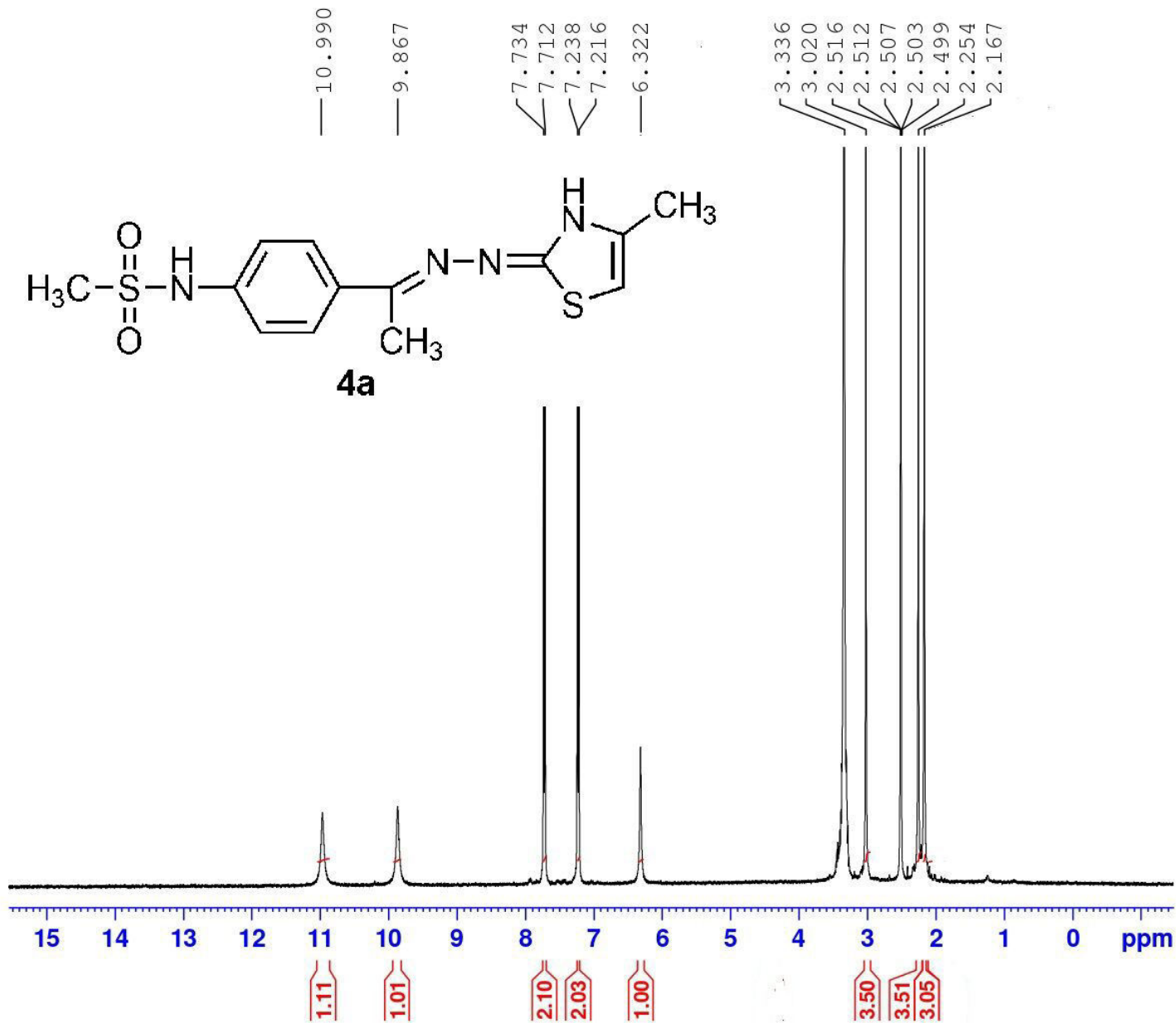
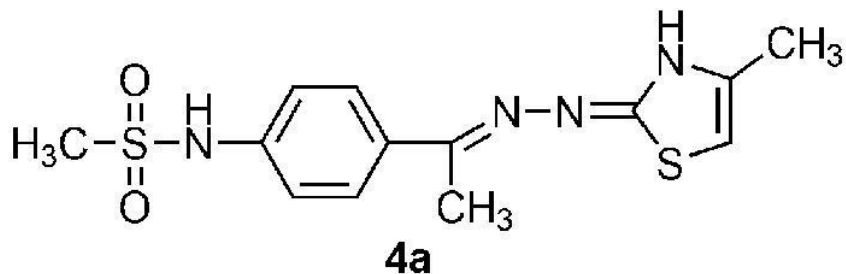
F2 - Acquisition Parameters
Date_ 20220901
Time 14.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





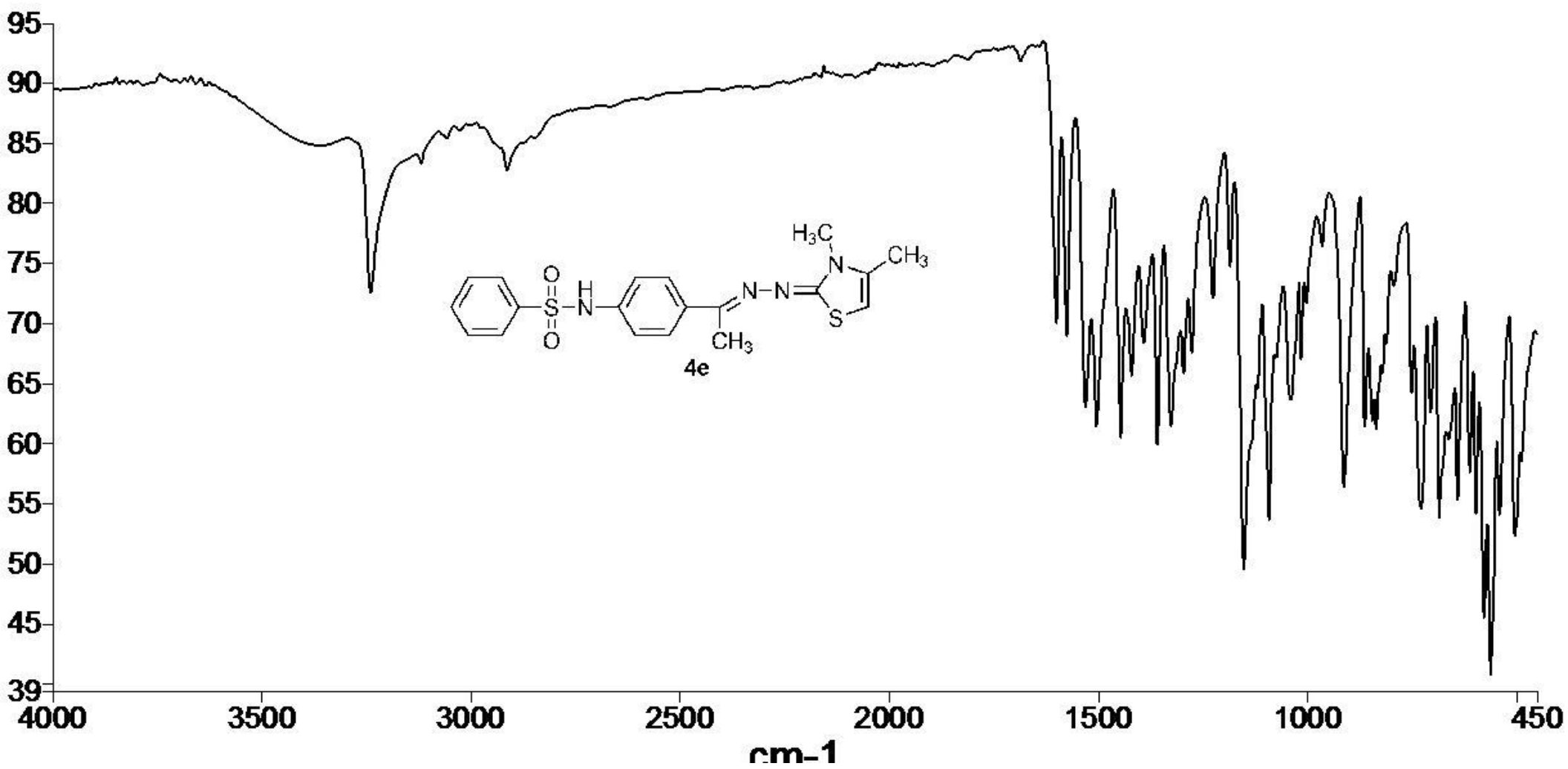


Current Data Parameters
NAME maha-mohamed-S1B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220901
Time 14.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 37
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME maha-aziz-S5B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220822
Time 8.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 67
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 205.37
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10.425
7.817
7.797
7.679
7.657
7.625
7.607
7.589
7.572
7.553
7.535
7.138
7.133
7.116
5.979
5.977
3.382
3.347
2.507
2.274
2.119

