Electronic Supplementary Information

An Effective and Facile Synthesis of New Blue Fluorophores on the Basis of 8-Azapurine Core

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1. Experimental section

General Information and Materials

All reactants were obtained from Acros Organics and used without further purification. ^{1}H NMR and ^{13}C NMR, spectra were recorded with a Bruker Avance II (Karlsruhe, Germany) (400 MHz for ^{1}H, 100 MHz for ^{13}C) and Bruker Avance NEO (Karlsruhe, Germany) (150 MHz for ^{13}C) spectrometers. Chemical shifts are reported in parts per million (ppm) relative to TMS in ^{1}H NMR, to the residual solvent signals in ^{13}C. Coupling constants (*J*) values are given in Hertz (Hz). Signal splitting patterns are described as a singlet (s), doublet (d), triplet (t), quartet (q), sextet (sext), quintet (quin), multiplet (m), broad (br), doublet of doublets (dd), doublet of triplets (dt) or AA'XX' - spin system of *para*-substituted benzene with two different substituents. Mass spectra were recorded with a Shimadzu GCMS-QP 2010 "Ultra" (Kyoto, Japan) mass spectrometer using the electron impact (EI) ionization technique (40-200 °C, 70 eV). The abbreviation $[M]^+$ refers to the molecular ion. The Fourier-transform infrared (FTIR) spectra were obtained using a Bruker Alpha (NPVO, ZnSe) spectrometer (Ettlingen, Germany).

Elemental analyses were carried out using a CHNS/O analyzer Perkin-Elmer 2400 Series II instrument (Shelton, CT USA). Melting points were determined on a Stuart SMP3 apparatus (Staffordshire, ST15 OSA, UK). The reactions were monitored by analytical thin-layer chromatography (TLC) on aluminium-backed silica-gel plates (Sorbfil UV–254). Visualization of components was accomplished by short wavelength UV-light (254 nm). Solvents were dried and distilled according to the common procedures. All solvents were of spectroscopic grade.

UV-Vis absorption spectra were recorded on a Perkin-Elmer Lambda 35 UV-Vis spectrophotometer (Shelton, CT USA). Fluorescence of the sample solutions was measured using a Hitachi F-7000 spectrophotometer (Tokyo, Japan). The absorption and emission spectra were recorded in CH_2Cl_2 using 10.00 mm quartz cells. The excitation wavelength was at the absorption maxima. Atmospheric oxygen contained in solutions was not removed. Concentration of the compounds in the solution was 5.0×10^{-5} M and 1.0×10^{-6} M for absorption and fluorescence measurements, respectively. The relative fluorescence quantum yields (Φ_F) were determined using quinine sulfate (5×10^{-5} M) in 0.1 M H_2SO_4 as a standard ($\Phi_F = 0.546$).

Diamino-2-arylazoacrylonitriles **1** (DAAs) were obtained according previously described procedure.[1-4]

Preparation and characterization of new compounds.

General procedure for the synthesis of pyrimidine-2(1*H*)-thiones 4a-n. To the solution of 0.52 mmol 2-arylhydrazono-2-cyanoacetamidines **1** in 5 mL $CHCl_3$, were added 0.2 mL (1.4 mmol) of DBU and 0.57 mmol of isothiocyanates **3a-d** at room temperature. The resulting mixture was stirred at reflux for 15-360 min. Then the solvent was evaporated under reduced pressure and residue was purified by column chromatography (eluents – AcOEt/Hexane 4/1).

6-Amino-4-morpholino-1-phenyl-5-(*p*-tolylazo)pyrimidine-2(1*H*)-thione (**4a**). Orange powder (175 mg, 78%). Mp: 129-131 °C. IR ν_{max}/cm^{-1}: 3321, 3030, 2960, 2911, 2854. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si): δ 2.42 (s, 3H, CH_3), 3.82 - 3.94 (m, 4H, CH_2), 4.14 - 4.32 (m, 4H, CH_2), 5.13 (br. s, 1H, NH), 7.26 and 7.46 (AA'XX', J = 8.0 Hz, 4H, CH_{Ar}), 7.35 (d, J = 7.6 Hz, 2H, CH_{Ar}), 7.56 (t, J = 7.2 Hz, 1H, CH_{Ar}), 7.63 (t, J = 7.2 Hz, 2H, CH_{Ar}), 11.84 (br. s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ 20.8, 48.9 (2C), 66.6 (2C), 109.3, 120.8 (2C), 129.1 (2C), 129.2, 129.9 (2C), 130.0 (2C), 137.5, 138.5, 148.5, 149.8, 155.7, 178.1. MS (EI) *m/z* (%): 406 (M^+, 100). Found: C, 61.9; H, 5.7; N, 20.5. $C_{21}H_{22}N_6OS$ requires C, 62.1; H, 5.5; N, 20.7%.

6-Amino-1-(4-methoxyphenyl)-5-(4-methoxyphenylazo)-4-morpholinopyrimidine-2(1*H*)-thione (**4b**). Brown powder (150 mg, 64%). Mp: 223-225 °C. IR ν_{max}/cm^{-1}: 3371, 3001, 2969, 2917, 2852. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.77 - 3.82 (m, 4H, CH_2), 3.84 (s, 3H, CH_3), 3.88 (s, 3H, CH_3), 4.07 - 4.11 (m, 4H, CH_2), 6.74 (br. s, 1H, NH), 6.95 and 7.52 (AA'XX', J = 9.0 Hz, 4H, CH_{Ar}), 7.07 and 7.13 (AA'XX', J = 9.0 Hz, 4H, CH_{Ar}), 11.18 (br. s, 1H, NH). ^{13}C NMR (150 MHz, DMSO-D_6): δ 48.8 (2C), 55.3, 55.5, 66.6 (2C), 109.1, 114.7 (2C), 115.2 (2C), 122.3 (2C), 130.1, 130.2 (2C), 145.9, 148.7, 155.6, 159.4, 159.8, 178.4. MS (EI) *m/z* (%): 452 (M^+, 16). Found: C, 58.1; H, 5.5; N, 18.3. $C_{22}H_{24}N_6O_3S$ requires C, 58.39; H, 5.35; N, 18.57%.

6-Amino-5-(4-methoxyphenylazo)-4-morpholino-1-phenylpyrimidine-2(1*H*)-thione (**4c**). Orange powder (180 mg, 82%). Mp: 218-220 °C. IR ν_{max}/cm^{-1}: 3187, 3030, 2962, 2933, 2897. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.75 - 3.81 (m, 4H, CH_2), 3.82 (br. s,

3H, CH_3), 3.97 - 4.04 (m, 4H, CH_2), 6.79 (s, 1H, NH), 7.06 and 7.30 (AA'XX', J = 9.0 Hz, 4H, CH_{Ar}), 7.47 - 7.53 (m, 1H, CH_{Ar}), 7.54 - 7.60 (m, 4H, CH_{Ar}), 11.14 (br. s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ 48.9 (2C), 55.5, 66.6 (2C), 109.1, 114.7 (2C), 122.4 (2C), 129.1 (2C), 129.2, 130.0 (2C), 137.6, 145.9, 148.4, 155.7, 159.9 177.9. MS (EI) m/z (%): 422 (M^+, 42). Found: C, 59.5; H, 5.0; N, 19.6. $C_{21}H_{22}N_6O_2S$ requires C, 59.70; H, 5.25; N, 19.89%.

6-Amino-1-(4-chlorophenyl)-5-(4-methoxyphenylazo)-4-morpholinopyrimidine-2(1*H*)-thione (**4d**). Orange powder (148 mg, 62%). Mp: 223-225 °C. IR ν_{max}/cm^{-1}: 3237, 3027, 2953, 2905, 2864. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.75 - 3.80 (m, 4H, CH_2), 3.82 (s, 3H, CH_3), 3.98 - 4.04 (m, 4H, CH_2), 7.06 and 7.35 (AA'XX', J = 8.6 Hz, 4H, CH_{Ar}), 7.21 (br. s, 1H, NH), 7.55 - 7.64 (m, 4H, CH_{Ar}), 11.15 (br. s, 1H, NH). ^{13}C NMR (150 MHz, DMSO-d_6): δ 48.9 (2C), 55.5, 66.6 (2C), 109.1, 114.7 (2C), 122.4 (2C), 130.1 (2C), 131.2 (2C), 133.7, 136.6, 145.8, 148.5, 155.8, 159.9, 177.7. MS (EI) *m/z* (%): 456 (M^+, 30). Found: C, 55.0; H, 4.8; N, 18.1. $C_{21}H_{21}ClN_6O_2S$ requires C, 55.20; H, 4.63; N, 18.39%.

6-Amino-5-(4-methoxyphenyl)-4-morpholino-1-(4-(trifluoromethyl)phenylazo)pyrimidine-2(1*H*)-thione (**4e**). Orange powder (189 mg, 74%). Mp: 225-227 °C. IR ν_{max}/cm^{-1}: 3216, 3042, 2958, 2908, 2850. ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ 3.76 - 3.81 (m, 4H, CH_2), 3.82 (s, 3H, CH_3), 3.99 - 4.05 (m, 4H, CH_2), 7.04 - 7.09 (m, 2H, CH_{Ar}), 7.26 (br. s, 1H, NH), 7.54 - 7.60 (m, 4H, CH_{Ar}), 7.92 (d, J = 8.4 Hz, CH_{Ar}), 11.17 (br. s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ 48.9 (2C), 55.5, 66.6 (2C), 109.0, 114.7 (2C), 122.4 (2C), 124.1 (q, $^1J_{C\text{-}F}$ = 264 Hz), 127.1 (m, 2C), 129.4 (q, $^2J_{C\text{-}F}$ = 35 Hz), 130.5 (2C), 141.4, 145.8, 148.4, 155.9, 159.9, 177.3. MS (EI) *m/z* (%): 490 (M^+, 44). Found: C, 53.6; H, 4.5; N, 16.9. $C_{22}H_{21}F_3N_6O_2S$ requires C, 53.87; H, 4.32; N, 17.13%.

6-Amino-1-(4-methoxyphenyl)-4-morpholino-5-(4-(trifluoromethyl)phenylazo)pyrimidine-2(1*H*)-thione (**4f**). Orange powder (183 mg, 81%). Mp: 210-212 °C. IR ν_{max}/cm^{-1}: 3219, 3061, 2962, 2913, 2842. ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ 3.75 - 3.82 (m, 4H, CH_2), 3.87 (s, 3H, CH_3), 4.06 - 4.15 (m, 4H, CH_2), 7.04 -7.17 (m, 5H, CH_{Ar} and NH), 7.62 - 7.72 (m, 4H, CH_{Ar}), 11.35 (br. s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ 48.9 (2C), 55.3, 66.6 (2C), 110.6, 115.2 (2C), 121.3 (2C), 124.2 (q, $^1J_{C\text{-}F}$ = 270 Hz), 126.6 (q, $^3J_{C\text{-}F}$ = 4 Hz, 2C), 127.6 (q, $^2J_{C\text{-}F}$ = 32 Hz), 129.9, 130.2 (2C), 148.9, 154.4, 155.5, 159.5, 179.1. MS (EI) m/z (%): 490 (M^+, 13). Found: C, 53.6; H, 4.5; N, 16.9. $C_{22}H_{21}F_3N_6O_2S$ requires C, 53.87; H, 4.32; N, 17.13%.

6-Amino-4-morpholino-1-(4-(trifluoromethyl)phenyl)-5-(4-(trifluoromethyl)phenylazo)pyrimidine-2(1*H*)-thione (4g) Yellow powder (185 mg, 76%). Mp: 232-238 °C. IR ν_{max}/cm^{-1}: 3371, 3001, 2969, 2917, 2852. ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ 3.79 - 3.87 (m, 4H, CH_2), 4.11 - 4.18 (m, 4H, CH_2), 7.50 and 7.83 (AA'XX', J = 8.2 Hz, 4H, CH_{Ar}), 7.69 - 7.76 (m, 4H, CH_{Ar}), 11.35 (br. s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ 48.9 (2C), 66.6 (2C), 110.5, 121.3 (2C), 124.1 (q, $^1J_{C\text{-}F}$ = 271 Hz), 124.2 (q, $^1J_{C\text{-}F}$ = 270 Hz), 126.6 (q, $^3J_{C\text{-}F}$ = 4 Hz, 2C), 127.2 (q, $^3J_{C\text{-}F}$ = 4 Hz, 2C), 127.7 (q, $^2J_{C\text{-}F}$ = 32 Hz), 129.5 (q, $^2J_{C\text{-}F}$ = 32 Hz), 130.5 (2C), 141.2, 148.6, 154.3, 155.8, 178.0. MS (EI) m/z (%): 528 (M^+, 18). Found: C, 49.7; H, 3.6; N, 15.6. $C_{22}H_{21}F_3N_6O_2S$ requires C, 50.00; H, 3.43; N, 15.90%.

6-Amino-1-(4-methoxyphenyl)-5-(2-methoxyphenylazodiazenyl)-4-morpholinopyrimidine-2(1*H*)-thione (4h). Orange-red powder (171 mg, 72%). Mp: 255-257 °C. IR ν_{max}/cm^{-1}: 3071, 3036, 3004, 2959, 2890. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.75 - 3.81 (m, 4H, CH_2), 3.84 (s, 3H, CH_3), 3.86 (s, 3H, CH_3), 4.01 - 4.07 (m, 4H, CH_2), 7.00 - 7.06 (m, 1H, CH_{Ar}), 7.07 - 7.12 (m, 2H, CH_{Ar}), 7.15 - 7.22 (m, 4H, CH_{Ar} and NH), 7.32 - 7.08 (m, 1H, CH_{Ar}), 7.43 - 7.47 (m, 1H, CH_{Ar}), 11.79 (br. s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ 48.9 (2C), 55.3, 55.8, 66.5 (2C), 110.8, 112.8, 114.7, 115.2 (2C), 121.0, 130.0, 130.2 (2C), 130.3, 140.1, 149.0, 154.7, 155.6, 159.4, 178.6. MS (EI) *m/z* (%): 452 (M^+, 19). Found: C, 58.1; H, 5.5; N, 18.4. $C_{22}H_{24}N_6O_3S$ requires C, 58.39; H, 5.35; N, 18.57%.

6-Amino-5-(2-methoxyphenylazo)-4-morpholino-1-(4-(trifluoromethyl)phenyl)pyrimidine-2(1*H*)-thione (**4i**). The title compound was prepared in accordance with the general procedure **1** (except DMF was used as a solvent). Orange-red powder (192 mg, 75%). Mp: 234-236 °C. IR ν_{max}/cm^{-1}: 3063, 2917, 2908, 2855. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.76 - 3.81 (m, 4H, CH_2), 3.85 (s, 3H, CH_3), 4.02 - 4.08 (m, 4H, CH_2), 7.01 - 7.07 (m, 1H, CH_{Ar}), 7.17 - 7.21 (m, 1H, CH_{Ar}), 7.33 - 7.38 (m, 1H, CH_{Ar}), 7.41 (br. s, 1H, NH), 7.44 - 7.48 (m, 1H, CH_{Ar}), 7.56 and 7.92 (AA'XX', J = 8.4 Hz, 4H, CH_{Ar}), 11.87 (br. s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ 48.9 (2C), 55.9, 66.5 (2C), 110.7, 112.4, 114.7, 121.0, 124.1 (q, $^1J_{C\text{-}F}$ = 271 Hz), 127.2 (q, $^3J_{C\text{-}F}$ = 4 Hz, 2C),

129.4 (q, $^2J_{C\text{-}F}$ = 32 Hz), 130.2, 130.5 (2C), 139.9 (2C), 141.5, 148.6, 154.7, 155.8, 177.4. MS (EI) *m/z* (%): 490 (M^+, 21). Found: C, 53.6; H, 4.5; N, 16.9. $C_{22}H_{21}F_3N_6O_2S$ requires C, 53.87; H, 4.32; N, 17.13%.

6-Amino-1-(4-methoxyphenyl)-4-morpholino-5-(2-(trifluoromethyl)phenyazo)pyrimidine-2(1*H*)-thione (**4j**). The title compound was prepared in accordance with the general procedure **1** (except DMF was used as a solvent). Orange-red powder (181 mg, 80%). Mp: 255-257 °C. IR ν_{max}/cm^{-1}: 3263, 3200, 3014, 2966, 2855. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.76 - 3.82 (m, 4H, CH_2), 3.84 (s, 3H, CH_3), 4.04 - 4.09 (m, 4H, CH_2), 7.06 -7.11 (m, 2H, CH_{Ar}), 7.18 -7.23 (m, 2H, CH_{Ar}), 7.47 - 7.53 (m, 1H, CH_{Ar}), 7.68 - 7.83 (m, 5H, CH_{Ar} and NH), 11.26 (br. s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ 48.9 (2C), 55.3, 66.5 (2C), 111.3, 115.2 (2C), 115.9, 123.5 (q, $^2J_{C\text{-}F}$ = 29 Hz), 124.4 (q, $^1J_{C\text{-}F}$ = 272 Hz), 126.5 (q, $^3J_{C\text{-}F}$ = 5 Hz), 127.8, 130.1, 130.2 (2C), 133.9, 148.7, 149.0, 155.6, 159.5, 179.2. MS (EI) *m/z* (%): 490 (M^+, 15). Found: C, 53.5; H, 4.5; N, 16.8. $C_{22}H_{21}F_3N_6O_2S$ requires C, 53.87; H, 4.32; N, 17.13%.

6-Amino-5-(4-methoxyphenylazo)-1-phenyl-4-(piperidin-1-yl)pyrimidine-2(1*H*)-thione (**4k**). Orange powder (144 mg, 65%). Mp: 130-132 °C. IR ν_{max}/cm^{-1}: 3312, 3038, 2962, 2891, 2858. ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.72 - 1.87 (m, 6H, CH_2), 3.84 (s, 3H, CH_3), 3.93 - 4.18 (m, 4H, CH_2), 6.51 (br. s, 1H, NH), 6.95 (d, J = 8.9 Hz, 2H, CH_{Ar}), 7.23 (d, J = 7.4 Hz, 2H, CH_{Ar}), 7.47 – 7.61 (m, 5H, CH_{Ar}), 11.29 (br. s, 1H, NH). ^{13}C NMR (150 MHz, DMSO-d_6): δ 24.2, 26.5 (2C), 49.3 (2C), 55.5, 108.9, 114.7 (2C), 122.3 (2C), 129.0, 129.1 (2C), 129.9 (2C), 137.6, 141.4, 145.9, 148.2, 155.5, 159.7, 177.4. MS (EI) *m/z* (%): 420 (M^+, 43). Found: C, 63.5; H, 5.9; N, 19.6%; $C_{22}H_{24}N_6OS$ requires C, 62.83; H, 5.75; N, 19.98%.

6-Amino-5-(4-methoxyphenylazo)-4-(piperidin-1-yl)-1-(4-(trifluoromethyl)phenyl)pyrimidine-2(1*H*)-thione (**4l**). Orange powder (167 mg, 65%). Mp**:** 183-185 °C. IR ν_{max}/cm^{-1}: 3289, 3032, 2961, 2923, 2854. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si): δ 1.69 - 1.88 (m, 6H, CH_2), 3.88 (br. s, 3H, CH_3O), 3.95 - 4.20 (m, 4H, CH_2), 4.89 (s, 1H, NH), 6.98 and 7.57 (AA'XX', J = 9.2 Hz, 4H, CH_{Ar}), 7.51 and 7.88 (AA'XX', J = 8.0 Hz, 4H, CH_{Ar}), 11.91 (br. s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ 24.2, 26.5 (2C), 49.4 (2C), 55.5, 108.9, 114.7 (2C), 122.3 (2C), 124.1 (q, $^1J_{C\text{-}F}$ = 271 Hz), 127.1 (m, 2C), 129.3 (q, $^2J_{C\text{-}F}$ = 32 Hz), 130.5 (2C), 141.5, 145.9, 148.2, 155.7, 159.8, 176.8. MS (EI) *m/z* (%): 488 (M^+, 27). Found: C, 56.2; H, 4.9; N, 16.9%; $C_{23}H_{23}F_3N_6OS$ requires C, 56.55; H, 4.75; N, 17.20%.

6-Amino-5-(4-methoxyphenylazo)-1-phenyl-4-(pyrrolidin-1-yl)pyrimidine-2(1*H*)-thione (**4m**). The title compound was prepared in accordance with the general procedure **1** (except DMF was used as a solvent). Orange powder (98 mg, 44%). Mp: 169-171 °C. IR ν_{max}/cm^{-1}: 3161, 3060, 2960, 2942, 2885. ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ 1.82 - 2.06 (m, 4H, CH_2), 3.75 - 4.02 (m, 7H, CH_3 and CH_2), 6.73 (br. s, 1H, NH), 7.05 (d, J = 8.6 Hz, 2H, CH_{Ar}), 7.27 (d, J = 7.4 Hz, 2H, CH_{Ar}), 7.45 - 7.63 (m, 5H, CH_{Ar}), 11.52 (br. s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ 23.2, 26.6, 50.2, 52.4, 55.4, 109.9, 114.6 (2C), 122.3 (2C), 129.0, 129.1 (2C), 130.0 (2C), 137.7, 146.0, 148.0, 153.7, 159.4, 177.3. MS (EI) m/z (%): 406 (M^+, 53). Found: C, 61.8; H, 5.6; N, 20.3. $C_{21}H_{22}N_6OS$ requires C, 62.05; H, 5.46; N, 20.67%.

6-Amino-5-(4-methoxyphenylazo)-4-(pyrrolidin-1-yl)-1-(4-(trifluoromethyl)phenyl)pyrimidine-2(1*H*)-thione (**4n**). The title compound was prepared in accordance with the general procedure **1** (except DMF was used as a solvent). Yellow powder (105 mg, 40%). Mp: 227-229 °C. IR ν_{max}/cm^{-1}: 3207, 3063, 2966, 2918, 2875, 2839. ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.82 - 2.01 (m, 4H, CH_2), 3.77 - 3.98 (m, 7H, CH_2 and CH_3), 7.05 (d, J = 8.9 Hz, 2H, CH_{Ar}), 7.18 (br. s, 1H, NH), 7.50 - 7.57 (m, 4H, CH_{Ar}), 7.91 (d, J = 8.4 Hz, 2H, CH_{Ar}), 11.58 (br. s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ 23.2, 25.3, 50.4, 52.1, 55.5, 110.0, 114.5 (2C), 122.3 (2C), 124.1 (q, $^1J_{C\text{-}F}$ = 271 Hz), 127.0 (q, $^2J_{C\text{-}F}$ = 4 Hz, 2C), 129.4 (q, $^2J_{C\text{-}F}$ = 32 Hz), 130.5 (2C), 141.5, 146.1, 148.0, 153.9, 160.0, 176.8. MS (EI) *m/z* (%): 474 (M^+, 34). Found: C, 55.4; H, 4.6; N, 17.4. $C_{22}H_{21}F_3N_6OS$ requires C, 55.69; H, 4.46; N, 17.71%.

General procedure for the synthesis of 2,3-dihydro-1,2,4-triazine-6-carbonitriles 6a-f. To the solution of 0.35 mmol 2-arylhydrazono-2-cyanoacetamidines **1a-g** in 8 mL toluene were added 0.1 mL (0.70 mmol) of DBU and 1.1 mmol of isothiocyanates **3a-d** at room temperature. The reaction mixture was stirred at reflux for 90-360 min. Then solvent was evaporated under reduced pressure and residue was recrystallized from EtOH.

5-Morpholino-3-(phenylimino)-2-(*p*-tolyl)-2,3-dihydro-1,2,4-triazine-6-carbonitrile (6a). Orange-red powder (141 mg, 70%). Mp: 157-159 °C. IR ν_{max}/cm^{-1}: 3064, 2979, 2954, 2877, 2844, 2225. ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ 2.42 (s, 3H, CH_3),

3.66 - 3.52 (m, 8H, CH_2), 6.88 (t, J = 7.6 Hz, 1H, CH_{Ar}), 6.92 (d, J = 7.6 Hz, 2H, CH_{Ar}), 7.16 (t, J = 7.6 Hz, 2H, CH_{Ar}), 7.28 and 7.50 (AA'XX', J = 8.0 Hz, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, DMSO-d_6): δ 20.7, 45.8 (2C), 65.5 (2C), 109.7, 115.2, 121.9, 122.8 (2C), 125.6 (2C), 128.0 (2C), 129.1 (2C), 137.9, 139.3, 144.6, 147.6, 155.0. MS (EI) *m/z* (%): 372 (M^+, 100). Found: C, 67.4; H, 5.6; N, 22.4; $C_{21}H_{20}N_6O$ requires C, 67.73; H, 5.41; N, 22.57%.

2-(4-Methoxyphenyl)-3-((4-methoxyphenyl)imino)-5-morpholino-2,3-dihydro-1,2,4-triazine-6-carbonitrile (6b). Brown powder (102 mg, 70%). Mp: 172-174 °C. IR ν_{max}/cm^{-1}: 3045, 3004, 2958, 2908, 2843, 2217. ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ 3.69 - 3.76 (m, 7H, CH_2 and CH_3), 3.77 - 3.83 (m, 4H, CH_2), 3.85 (s, 3H, CH_3), 6.71 and 6.93 (AA'XX', J = 8.8 Hz, 4H, CH_{Ar}), 6.98 and 7.51 (AA'XX', J = 8.9 Hz, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, DMSO-d_6): δ 46.4 (2C), 55.5, 55.9, 66.0 (2C), 109.7, 113.8 (2C), 114.2 (2C), 115.8, 124.5 (2C), 127.7 (2C), 128.8, 135.3, 144.8, 150.5, 155.1, 159.3. MS (EI) *m/z* (%): 418 (M^+, 100). Found: C, 63.0; H, 5.5; N, 19.8; $C_{22}H_{22}N_6O_3$ requires C, 63.15; H, 5.30; N, 20.08%.

2-(4-Methoxyphenyl)-5-morpholino-3-((4-(trifluoromethyl)phenyl)imino)-2,3-dihydro-1,2,4-triazine-6-carbonitrile (6c). Orange powder (120 mg, 79%). Mp: 141-143 °C. IR ν_{max}/cm^{-1}: 2968, 2918, 2865, 2843, 2222. ^{1}H NMR (400 MHz, DMSO-d_6, Me_4Si): δ 3.68 - 3.74 (m, 4H, CH_2), 3.78 - 3.83 (m, 4H, CH_2), 3.85 (s, 3H, CH_3), 7.01 and 7.52 (AA'XX', J = 9.0 Hz, 4H, CH_{Ar}), 7.10 and 7.46 (AA'XX', J = 8.3 Hz, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, DMSO-d_6): δ 46.0 (2C), 55.4, 65.5 (2C), 110.2, 113.8 (2C), 115.1, 121.8 (q, $^2J_{C\text{-}F}$ = 32 Hz), 123.3 (2C), 124.8 (q, $^1J_{C\text{-}F}$ = 269 Hz), 125.2 (q, $^3J_{C\text{-}F}$ = 4 Hz, 2C), 127.2 (2C), 134.5, 145.7, 150.2, 151.9, 159.0. MS (EI) *m/z* (%): 455 (M^+, 100). Found: C, 57.6; H, 4.4; N, 18.2; $C_{22}H_{19}F_3N_6O_2$ requires C, 57.89; H, 4.20; N, 18.41%.

3-((4-Methoxyphenyl)imino)-5-morpholino-2-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1,2,4-triazine-6-carbonitrile (6d). Brown powder (56 mg, 40%). Mp: 158-160 °C. IR ν_{max}/cm^{-1}: 2980, 2931, 2888, 2859, 2832, 2246. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.65 - 3.72 (m, 7H, CH_3 and CH_2), 3.76 - 3.86 (m, 4H, CH_2), 6.78 and 7.00 (AA'XX', J = 8.8 Hz, 4H, CH_{Ar}), 7.85 - 7.93 (m, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, DMSO-d_6): δ 46.0 (2C), 55.0, 65.5 (2C), 110.6, 113.4 (2C), 123.9 (q, $^1J_{C\text{-}F}$ = 271 Hz), 124.1 (2C), 125.8 (q, $^3J_{C\text{-}F}$ = 4 Hz, 2C), 126.5 (2C), 128.2 (q, $^2J_{C\text{-}F}$ = 32 Hz), 140.0, 143.6, 144.9, 149.7, 154.7. MS (EI) *m/z* (%): 455 (M^+, 100). Found: C, 57.5; H, 4.4; N, 18.1; $C_{22}H_{19}F_3N_6O_2$ requires C, 57.89; H, 4.20; N, 18.41%.

5-Morpholino-2-(4-(trifluoromethyl)phenyl)-3-((4-(trifluoromethyl)phenyl)imino)-2,3-dihydro-1,2,4-triazine-6-carbonitrile (6e). Yellow powder (119 mg, 78%). Mp: 165-167 °C. IR ν_{max}/cm^{-1}: 3113, 3072, 2974, 2925, 2886, 2225. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.69 - 3.75 (m, 4H, CH_2), 3.78 - 3.87 (m, 4H, CH_2), 7.17 and 7.54 (AA'XX', J = 8.3 Hz, 4H, CH_{Ar}), 7.88 - 7.94 (m, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, DMSO-d_6): δ 46.1 (2C), 55.5 (2C), 111.6, 114.8, 122.1 (q, $^2J_{C\text{-}F}$ = 31 Hz), 123.4 (2C), 123.8 (q, $^1J_{C\text{-}F}$ = 267 Hz), 124.7 (q, $^1J_{C\text{-}F}$ = 269 Hz), 125.2 (q, $^3J_{C\text{-}F}$ = 4 Hz, 2C), 125.9 (q, $^3J_{C\text{-}F}$ = 4 Hz, 2C), 126.7 (2C), 128.5 (q, $^2J_{C\text{-}F}$ = 32 Hz), 144.6, 145.2, 150.0, 151.4. MS (EI) *m/z* (%): 493 (M^+, 100). Found: C, 53.7; H, 3.5; N, 16.7; $C_{22}H_{16}F_6N_6O$ requires C, 53.45; H, 3.26; N, 17.00%.

2-(4-Methoxyphenyl)-5-(piperidin-1-yl)-3-((4-(trifluoromethyl)phenyl)imino)-2,3-dihydro-1,2,4-triazine-6-carbonitrile (6f). Orange powder (125 mg, 79%). Mp: 169-171 °C. IR ν_{max}/cm^{-1}: 3020, 2954, 2928, 2862, 2220. ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.47 - 1.78 (s, 6H, CH_2), 3.64 - 3.78 (m, 4H, CH_2), 3.82 (s, 3H, CH_3), 7.05 (d, J = 8.2 Hz, 2H, CH_{Ar}), 7.14 (d, J = 7.7 Hz, 2H, CH_{Ar}), 7.44 - 7.62 (m, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, DMSO-d_6): δ 23.4, 25.3 (2C), 46.9 (2C), 55.4, 110.2, 113.8 (2C) 115.1, 121.7 (q, $^2J_{C\text{-}F}$ = 31 Hz), 123.4 (2C), 124.8 (q, $^1J_{C\text{-}F}$ = 270 Hz), 125.1 (q, $^3J_{C\text{-}F}$ = 4 Hz, 2C), 127.3, 134.6, 145.9, 149.8, 152.1, 158.9. MS (EI) *m/z* (%): 453 (M^+, 100). Found: C, 60.5; H, 4.8; N, 18.2; $C_{23}H_{21}F_3N_6O$ requires C, 60.79; H, 4.66; N, 18.49%.

General procedure for the synthesis of 2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-ones 7a-n.

To the solution of 0.37 mmol pyrimidine-2(1*H*)-thiones **4a-n** in 10 mL pyridine was added 0.15 g (0.74 mmol) of $Cu(OAc)_2$. The resulting mixture was stirred for 90-240 min at 60 °C. Then mixture was poured onto iced water and solid product was collected by filtration and product was recrystallized from EtOH.

7-Morpholino-4-phenyl-2-(*p*-tolyl)-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-one (7a). White powder (118 mg, 83%). Mp: 289-291 °C. IR ν_{max}/cm^{-1}: 3067, 3041, 2969, 2949, 2905, 2885, 1652. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.42 (s, 3H, CH_3), 3.81 – 4.01 (m, 4H, CH_2), 4.15 - 4.30 (m, 2H, CH_2), 4.52 - 4.68 (m, 2H, CH_2), 7.26 and 7.88 (AA'XX', J = 8.4 Hz, 4H, CH_{Ar}), 7.42 - 7.60 (m, 5H, CH_{Ar}). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.1, 41.6, 48.8, 66.9, 67.1, 119.3 (2C), 123.4, 127.8 (2C), 128.3, 129.3 (2C), 129.9

(2C), 136.3, 136.9, 139.2, 153.7, 153.8, 155.3. MS (EI) m/z (%): 388 (M^+, 100). Found: C, 64.7; H, 5.4; N, 21.3; $C_{21}H_{20}N_6O_2$ requires C, 64.94; H, 5.19; N, 21.64%.

2,4-Bis(4-methoxyphenyl)-7-morpholino-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-one (7b). White powder (112 mg, 78%). Mp: 292-294 °C. IR ν_{max}/cm^{-1}: 2941, 2910, 2852, 2840, 1655. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.59 – 3.90 (m, 10H, CH_3 and CH_2), 3.91 - 4.13 (m, 2H, CH_2), 4.32 - 4.56 (m, 2H, CH_2), 6.93 - 7.20 (m, 4H, CH_{Ar}), 7.36 (d, J = 7.2 Hz, 2H, CH_{Ar}), 7.86 (d, J = 7.6 Hz, 2H, CH_{Ar}). ^{13}C NMR (100 MHz, DMSO-d_6): δ 44.1, 47.7, 55.4, 55.6, 66.1 (2C), 114.3 (2C), 114.9 (2C), 120.8 (2C), 122.9, 129.1 (2C), 129.4, 132.1, 153.2, 153.8, 154.1, 158.7, 159.6. MS (EI) *m/z* (%): 434 (M^+, 100). Found: C, 60.5; H, 5.3; N, 19.1; $C_{22}H_{22}N_6O_4$ requires C, 60.82; H, 5.10; N, 19.34%.

2-(4-Methoxyphenyl)-7-morpholino-4-phenyl-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-one (7c). White powder (169 mg, 80%). Mp: 278-280 °C. IR ν_{max}/cm^{-1}: 3060, 2998, 2970, 2940, 2894, 2881, 1650. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.92 – 4.08 (m, 7H, CH_3 and CH_2), 4.16 - 4.32 (m, 2H, CH_2), 4.46 - 4.70 (m, 2H, CH_2), 6.96 and 7.92 (AA'XX', J = 9.2 Hz, 4H, CH_{Ar}), 7.34 - 7.48 (m, 1H, CH_{Ar}), 7.48 - 7.62 (m, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, $CDCl_3$): δ 44.5, 48.1, 55.6, 66.9, 67.0, 114.5 (2C), 120.9 (2C), 123.2, 127.7 (2C), 128.2, 129.3 (2C), 132.7, 136.4, 153.7, 153.9, 155.3, 160.0. MS (EI) *m/z* (%): 404 (M^+, 100). Found: C, 62.1; H, 5.2; N, 20.6; $C_{21}H_{20}N_6O_3$ requires C, 62.37; H, 4.98; N, 20.78%.

4-(4-Chlorophenyl)-2-(4-methoxyphenyl)-7-morpholino-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-one (7d). White powder (108 mg, 75%). Mp: 288-290 °C. IR ν_{max}/cm^{-1}: 3030, 2985, 2914, 2864, 1658. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.84 – 3.97 (m, 7H, CH_3 and CH_2), 4.16 - 4.27 (m, 2H, CH_2), 4.52 - 4.55 (m, 2H, CH_2), 7.00 and 7.51 (AA'XX', J = 8.8 Hz, 4H, CH_{Ar}), 7.48 and 7.90 (AA'XX', J = 9.2 Hz, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, $CDCl_3$): δ 44.7, 48.2, 55.7, 66.9, 67.0, 114.5 (2C), 120.9 (2C), 123.1, 129.1 (2C), 129.5 (2C), 132.6, 134.0, 134.8, 153.6, 154.9, 160.2. MS (EI) *m/z* (%): 438 (M^+, 100). Found: C, 57.2; H, 4.5; N, 18.9%; $C_{21}H_{19}ClN_6O_3$ requires C, 57.47; H, 4.36; N, 19.15%.

2-(4-Methoxyphenyl)-7-morpholino-4-(4-(trifluoromethyl)phenyl)-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-d]pyrimidin-5-one (7e). White powder (116 mg, 80%). Mp: 289-290 °C. IR ν_{max}/cm^{-1}: 2968, 2954, 2943, 2919, 2889, 2852, 1659. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si): δ 3.83 – 3.99 (m, 7H, CH_3 and CH_2), 4.19 - 4.31 (m, 4H, CH_2), 4.54 - 4.67 (m, 4H, CH_2), 6.99 and 7.94 (AA'XX', J = 9.2 Hz, 4H, CH_{Ar}), 7.69 and 7.80 (AA'XX', J = 8.4 Hz, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, $CDCl_3$): δ 44.7, 48.2, 55.6, 66.9, 114.6 (2C), 121.0 (2C), 123.3, 123.9 (q, $^1J_{C\text{-}F}$ = 271 Hz), 126.2 (q, $^3J_{C\text{-}F}$ = 3 Hz, 2C), 128.1 (q, $^2J_{C\text{-}F}$ = 33 Hz,), 132.6, 139.6, 153.3, 153.7, 154.6, 160.3. MS (EI) *m/z* (%): 472 (M^+, 100). Found: C, 55.6; H, 4.3; N, 17.5; $C_{22}H_{19}F_3N_6O_3$ requires C, 55.93; H, 4.05; N, 17.79%.

4-(4-Methoxyphenyl)-7-morpholino-2-(4-(trifluoromethyl)phenyl)-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-d]pyrimidin-5-one (7f). White powder (122 mg, 85%). Mp: 167-169 °C. IR ν_{max}/cm^{-1}: 3077, 2959, 2919, 2859, 1651. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.76 – 3.88 (m, 7H, CH_3 and CH_2), 3.97 - 4.05 (m, 2H, CH_2), 4.46 - 4.58 (m, 2H, CH_2), 7.08 and 7.37 (AA'XX', J = 8.9 Hz, 4H, CH_{Ar}), 7.92 and 8.19 (AA'XX', J = 8.6 Hz, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, DMSO-d_6): δ 44.2, 47.7, 55.4, 66.0, 66.2, 114.3 (2C), 119.6 (2C), 123.8 (q, $^1J_{C\text{-}F}$ = 271 Hz), 124.5, 127.1 (q, $^3J_{C\text{-}F}$ = 4 Hz, 2C), 128.7 (q, $^2J_{C\text{-}F}$ = 32 Hz), 129.1 (2C), 129.2, 141.2, 153.1, 154.0, 154.1, 158.8. MS (EI) *m/z* (%): 472 (M^+, 100). Found: C, 55.6; H, 4.3; N, 19.5; $C_{22}H_{19}F_3N_6O_3$ requires C, 55.93; H, 4.05; N, 19.79%.

7-Morpholino-2,4-bis(4-(trifluoromethyl)phenyl)-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-one (7g). White powder (116 mg, 80%). Mp: 292-294 °C. IR ν_{max}/cm^{-1}: 3020, 2930, 2890, 2855, 1665. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.81 –3.99 (m, 4H, CH_2), 4.16 - 4.29 (m, 2H, CH_2), 4.52 - 4.66 (m, 2H, CH_2), 7.66 and 7.80 (AA'XX', J = 8.3 Hz, 4H, CH_{Ar}), 7.75 and 8.13 (AA'XX', $J_{C\text{-}F}$ = 8.6 Hz, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, $CDCl_3$): δ 44.8, 48.2, 66.9, 67.0, 119.5 (2C), 123.5 (q, $^1J_{C\text{-}F}$ = 271 Hz), 123.8 (q, $^1J_{C\text{-}F}$ = 271 Hz), 124.6, 126.5 (q, $^3J_{C\text{-}F}$ = 4 Hz, 2C), 126.8 (q, $^3J_{C\text{-}F}$ = 4 Hz, 2C), 128.1 (2C), 130.4 (q, $^2J_{C\text{-}F}$ = 33 Hz), 130.9 (q, $^2J_{C\text{-}F}$ = 33 Hz) 139.1, 141.2, 153.4, 153.6, 154.5. MS (EI) *m/z* (%): 510 (M^+, 100). Found: C, 51.4; H, 3.4; N, 16.2; $C_{22}H_{16}N_6F_6O_2$ requires C, 51.77; H, 3.16; N, 16.47%.

2-(2-Methoxyphenyl)-4-(4-methoxyphenyl)-7-morpholino-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-one (7h). White powder (112 mg, 78%). Mp: 272-274 °C. IR ν_{max}/cm^{-1}: 2950, 2915, 2855, 2840, 1668. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.76 – 3.84 (m, 10H, CH_3 and CH_2), 3.92 - 4.09 (m, 2H, CH_2), 4.29 - 4.50 (m, 2H, CH_2), 7.04 (d, J = 8.9 Hz, 2H, CH_{Ar}), 7.09 - 7.15 (m,

1H, CH_{Ar}), 7.28 - 7.37 (m, 3H, *CH_{Ar}*), 7.51 - 7.60 (m, 2H, CH_{Ar}). ^{13}C NMR (100 MHz, DMSO-d_6): δ 43.9, 47.6, 55.3, 56.3, 65.9, 66.1, 113.4, 114.2 (2C), 120.6, 123.0, 127.4, 128.4, 129.1 (2C), 129.3, 131.9, 153.1, 153.4 (2C), 154.2, 158.6. MS (EI) *m/z* (%): 434 (M^+, 100). Found: C, 60.5; H, 5.3; N, 19.1; $C_{22}H_{22}N_6O_4$ requires C, 60.82; H, 5.10; N, 19.34%.

2-(2-Methoxyphenyl)-7-morpholino-4-(4-(trifluoromethyl)phenyl)-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-one (7i). White powder (116 mg, 80%). Mp: 228-230 °C. IR ν_{max}/cm^{-1}: 3060, 2990, 2967, 2904, 2884, 1672. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.73 – 3.87 (m, 7H, CH_3 and CH_2), 3.95 - 4.07 (m, 2H, CH_2), 3.37 - 4.48 (m, 2H, CH_2), 7.06 - 7.17 (m, 1H, CH_{Ar}), 7.30 (d, 1H, J = 8.3 Hz, CH_{Ar}), 7.51 - 7.62 (m, 2H, CH_{Ar}), 7.74 and 7.89 (AA'XX', J = 8.3 Hz, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, DMSO-D_6): δ 44.0, 47.7, 56.3, 65.9, 66.1, 113.5, 120.6, 123.1, 124.0 (q, $^1J_{C-F}$ = 271 Hz), 126.1 (q, $^3J_{C-F}$ = 4 Hz, 2C), 128.2 (q, $^2J_{C-F}$ = 32 Hz), 128.3, 128.9 (2C), 132.0, 140.2, 152.6, 153.1, 153.4, 153.5. MS (EI) *m/*z (%): 472 (M^+, 100). Found: C, 55.6; H, 4.3; N, 18.0; $C_{22}H_{19}F_3N_6O_3$ requires C, 55.93; H, 4.05; N, 17.79%.

4-(4-Methoxyphenyl)-7-morpholino-2-(2-(trifluoromethyl)phenyl)-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-one (7j). White powder (105 mg, 73%). Mp: 213-215 °C. IR ν_{max}/cm^{-1}: 3070, 2972, 2925, 2870, 1. ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.74 – 3.84 (m, 7H, CH_3 and CH_2), 3.96 - 4.06 (m, 2H, CH_2), 4.34 - 4.45 (m, 2H, CH_2), 7.04 and 7.34 (AA'XX', J = 8.8 Hz, 4H, CH_{Ar}), 7.79 - 7.95 (m, 3H, CH_{Ar}), 8.02 (d, 1H, J = 7.7 Hz, CH_{Ar}). ^{13}C NMR (100 MHz, $CDCl_3$): δ 44.1, 47.5, 55.4, 65.9, 66.1, 114.2 (2C), 122.6 (q, ^1J = 271 Hz), 123.6 (q, ^2J = 32 Hz), 124.0, 127.9 (q, ^3J = 5 Hz), 128.1, 129.0 (2C), 129.1, 131.1, 134.1, 136.4, 152.9, 153.8, 154.1, 158.7. MS (EI) *m/z* (%): 472 (M^+, 100). Found: C, 55.7; H, 4.3; N, 19.5; $C_{22}H_{19}F_3N_6O_3$ requires C, 55.93; H, 4.05; N, 19.79%.

2-(4-Methoxyphenyl)-4-phenyl-7-(piperidin-1-yl)-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-one (7k). White powder (108 mg, 75%). Mp: 263-265 °C. IR ν_{max}/cm^{-1}: 3032, 3013, 3005, 2970, 2933, 2853, 1656. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si): δ 1.71 – 1.93 (m, 6H, CH_2), 3.87 (s, 3H, CH_3O), 4.11 - 4.23 (m, 2H, CH_2), 4.40 - 4.58 (m, 2H, CH_2), 6.98 and 7.95 (AA'XX', J = 9.2 Hz, 4H, CH_{Ar}), 7.36 - 7.48 (m, 1H, CH_{Ar}), 7.48 - 7.61 (m, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.5, 25.9, 26.9, 45.8, 48.7, 55.6, 114.4 (2C), 120.9 (2C), 123.5, 127.8 (2C), 128.1, 129.2 (2C), 132.8, 136.6, 153.2, 153.8, 155.5, 159.9. MS (EI) *m/z* (%): 402 (M^+, 100). Found: C, 65.5; H, 5.3; N, 20.6%; $C_{22}H_{22}N_6O_2$ requires C, 65.66; H, 5.51; N, 20.88%

2-(4-Methoxyphenyl)-7-(piperidin-1-yl)-4-(4-(trifluoromethyl)phenyl)-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-one (7l). White powder (117 mg, 81%). Mp: 268-270 °C. IR ν_{max}/cm^{-1}: 2982, 2964, 2943, 2920, 2880, 2852, 1659. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si): δ 1.74 – 1.94 (m, 6H, CH_2), 3.87 (s, 3H, CH_3O), 4.09 - 4.24 (m, 2H, CH_2), 4.45 - 4.59 (m, 2H, CH_2), 6.98 and 7.94 (AA'XX', J = 9.2 Hz, 4H, CH_{Ar}), 7.69 and 7.79 (AA'XX', J = 8.4 Hz, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.4, 25.8, 26.9, 45.8, 48.8, 114.6 (2C), 120.9 (2C), 123.5, 123.9 (q, $^1J_{C-F}$ = 271 Hz), 126.2 (q, $^3J_{C-F}$ = 4 Hz, 2C), 128.2, 129.9 (q, $^2J_{C-F}$ = 33 Hz,), 132.7, 139.8, 153.2, 154.8, 160.2. MS (EI) *m/z* (%): 470 (M^+, 100). Found: C, 58.5; H, 4.7; N, 17.5; $C_{23}H_{21}F_3N_6O_2$ requires C, 58.72; H, 4.50; N, 17.86%.

2-(4-Methoxyphenyl)-4-phenyl-7-(pyrrolidin-1-yl)-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-one (7m). White powder (103 mg, 72%). Mp: 246-248 °C. IR ν_{max}/cm^{-1}: 3082, 3050, 2963, 2936, 2922, 2878, 1661. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si): δ 2.00 – 2.09 (m, 2H, CH_2), 2.09 – 2.26 (m, 2H, CH_2), 3.86 (s, 3H, CH_3), 3.95 (t, J = 1.2 Hz, 2H, CH_2), 4.20 (t, J = 1.2 Hz, 2H, CH_2), 6.95 and 7.93 (AA'XX', J = 9.2 Hz, 4H, CH_{Ar}), 7.37 - 7.45 (m, 1H, CH_{Ar}), 7.47 - 7.61 (m, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.1, 26.1, 42.4, 49.6, 55.6, 114.4 (2C), 120.7 (2C), 123.8, 127.8 (2C), 128.0, 129.2 (2C), 133.0, 136.7, 152.9, 153.3, 155.5, 159.8 . MS (EI) *m/z* (%): 388 (M^+, 100). Found: C, 69.6; H, 5.3; N, 21.3; $C_{21}H_{20}N_6O_2$ requires C, 69.94; H, 5.19; N, 21.64%.

2-(4-Methoxyphenyl)-7-(pyrrolidin-1-yl)-4-(4-(trifluoromethyl)phenyl)-2,4-dihydro-5*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-one (7n). White powder (121 mg, 84%). Mp: 266-268 °C. IR ν_{max}/cm^{-1}: 2998, 2982, 2951, 2921, 2889, 2854, 1654. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.02 – 2.14 (m, 2H, CH_2), 2.14 – 2.26 (m, 2H, CH_2), 3.87 (s, 3H, CH_3O), 3.92 – 4.03 (m, 2H, CH_2), 4.17 – 4.29 (m, 2H, CH_2), 6.98 and 7.95 (AA'XX', J = 9.2 Hz, 4H, CH_{Ar}), 7.70 and 7.80 (AA'XX', J = 8.4 Hz, 4H, CH_{Ar}). ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.0, 26.1, 48.5, 49.6, 55.6, 114.6 (2C), 120.8 (2C), 124.0, 124.1 (q, $^1J_{C-F}$ = 271 Hz), 126.1 (q, $^3J_{C-F}$ = 4 Hz, 2C), 128.1

(2C), 129.9 (q, $^{2}J_{C\text{-}F}$ = 51 Hz), 132.9, 139.9, 152.8, 152.9, 154.8, 160.1. MS (EI) *m/*z (%): 456 (M^{+}, 100). Found: C, 57.6; H, 4.4; N, 18.1; $C_{22}H_{19}F_{3}N_{6}O_{2}$ requires C, 57.89; H, 4.20; N, 18.41%.

2. NMR spectra of new compounds

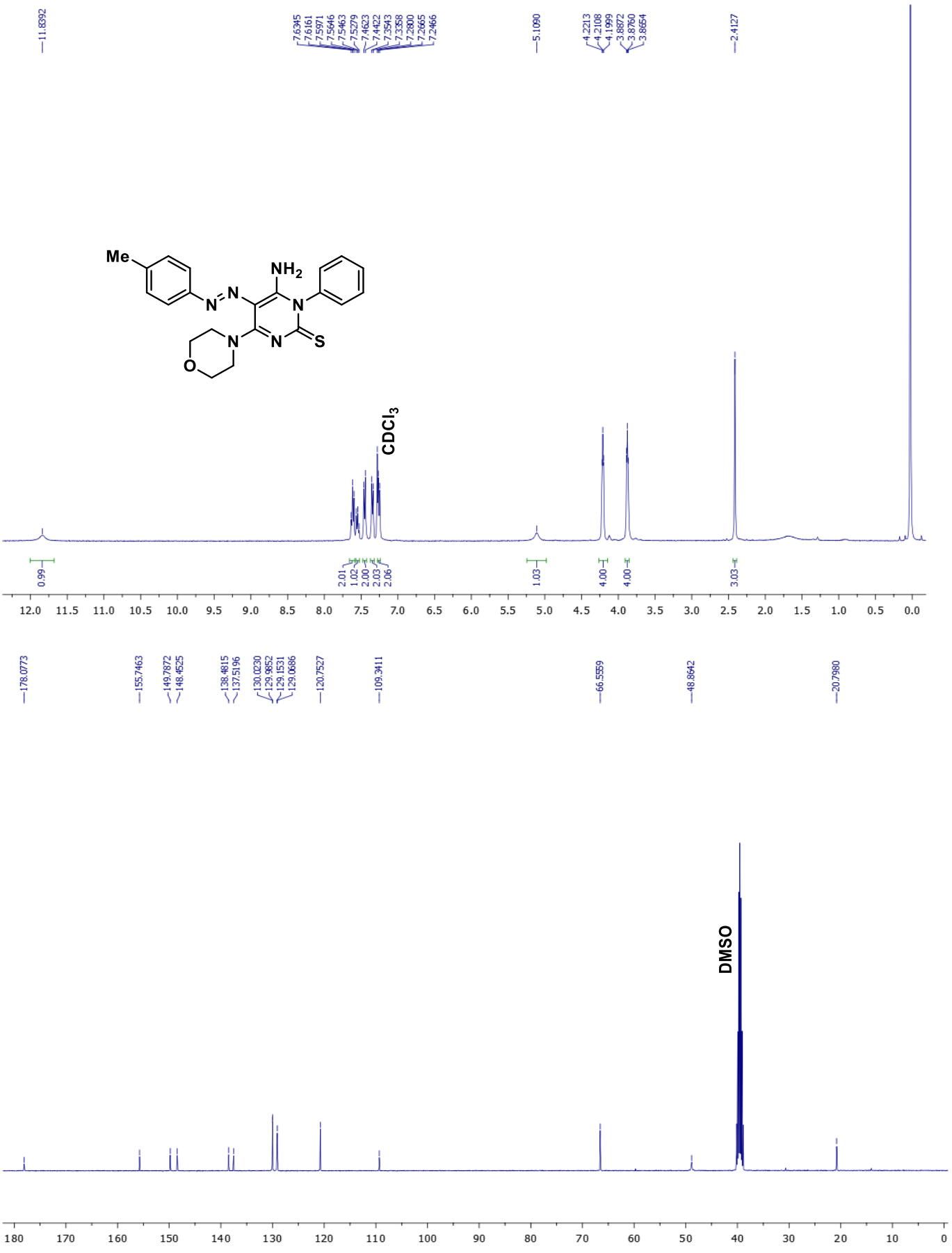


Fig. S1 ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra **4a.**

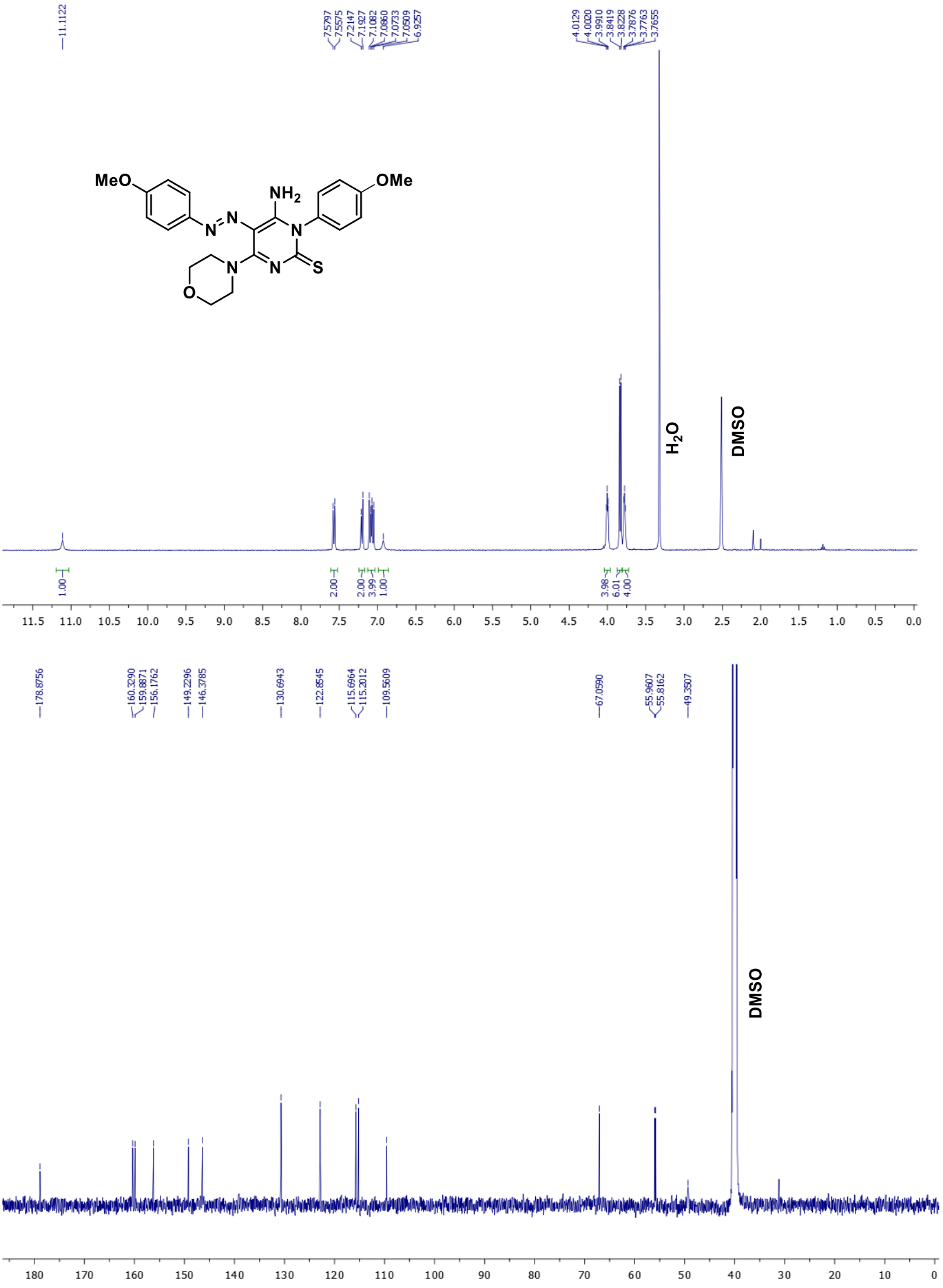


Fig. S2 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (150 MHz, DMSO-d_6) spectra of **4b.**

Fig. S3 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **4c.**

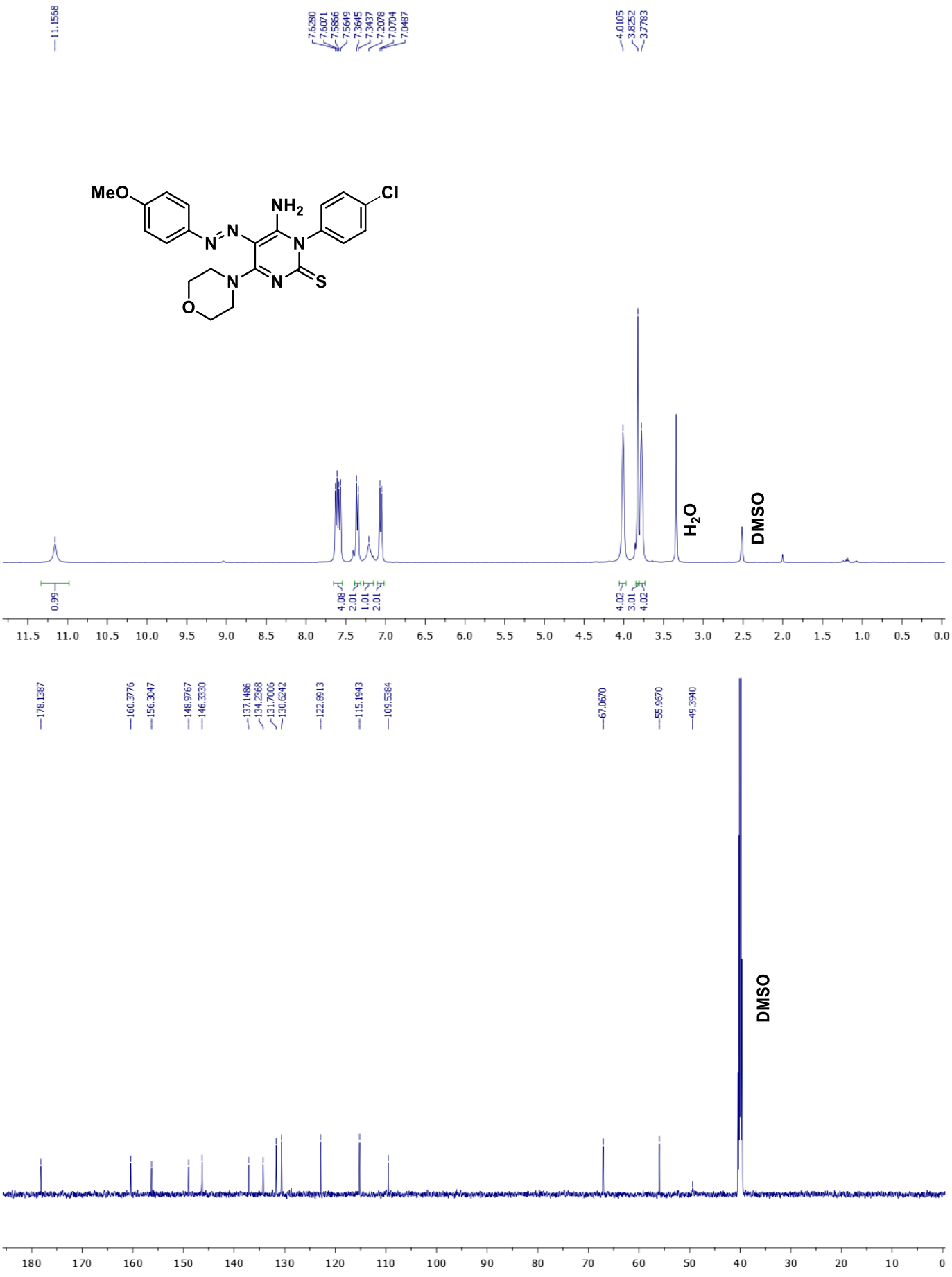


Fig. S4 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (150 MHz, DMSO-d_6) spectra of **4d.**

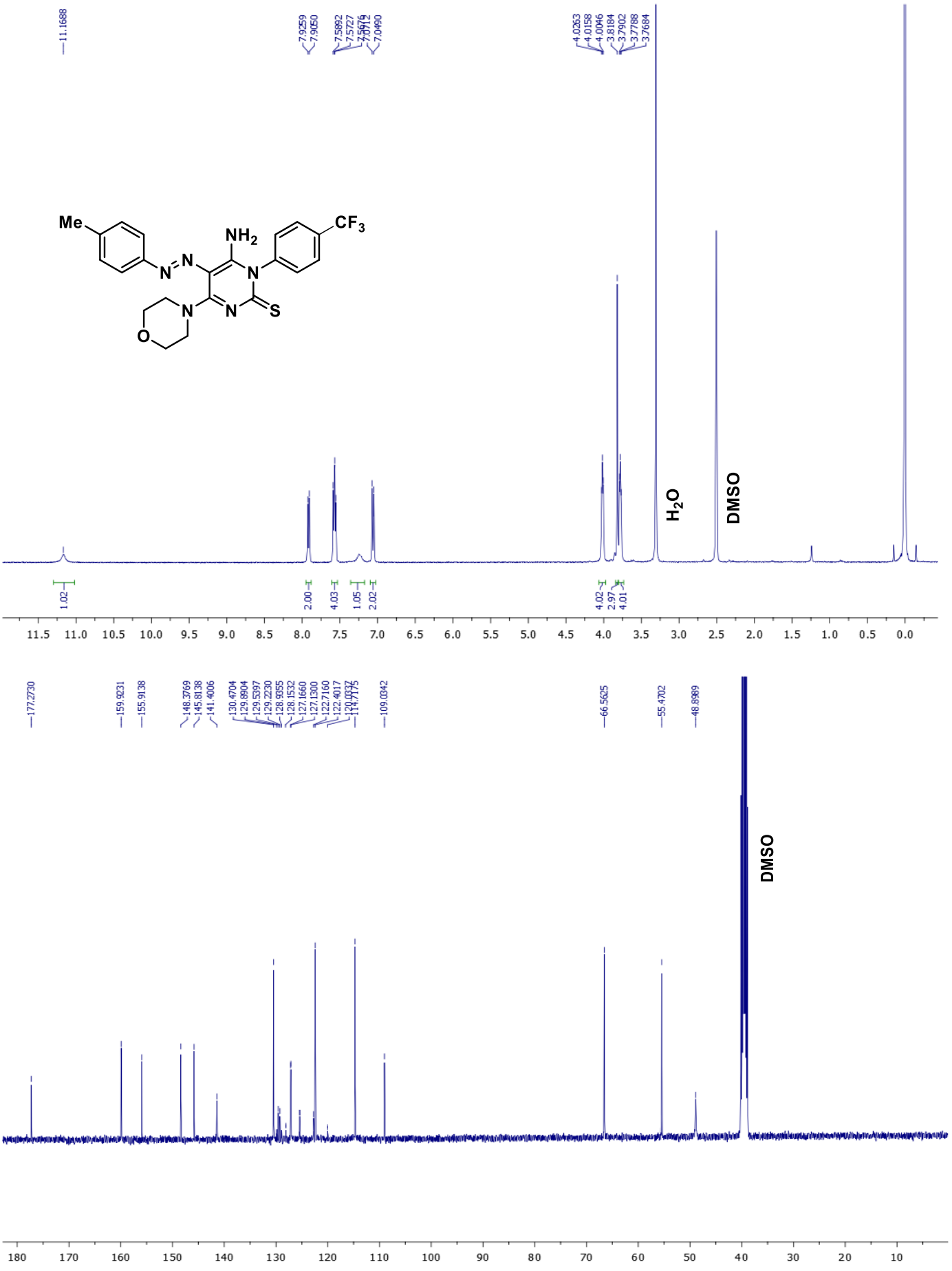


Fig. S5 ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **4e.**

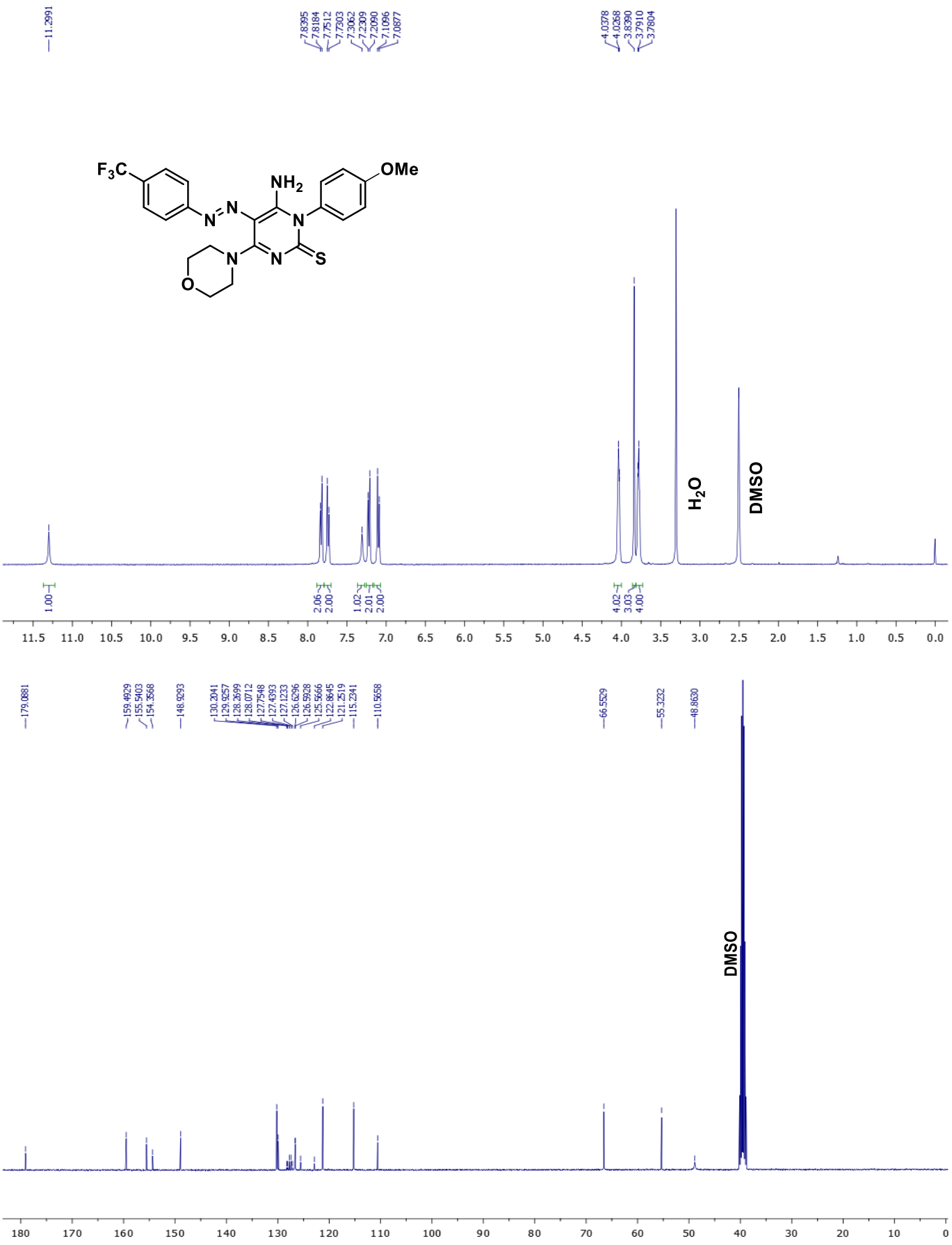


Fig. S6 ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **4f.**

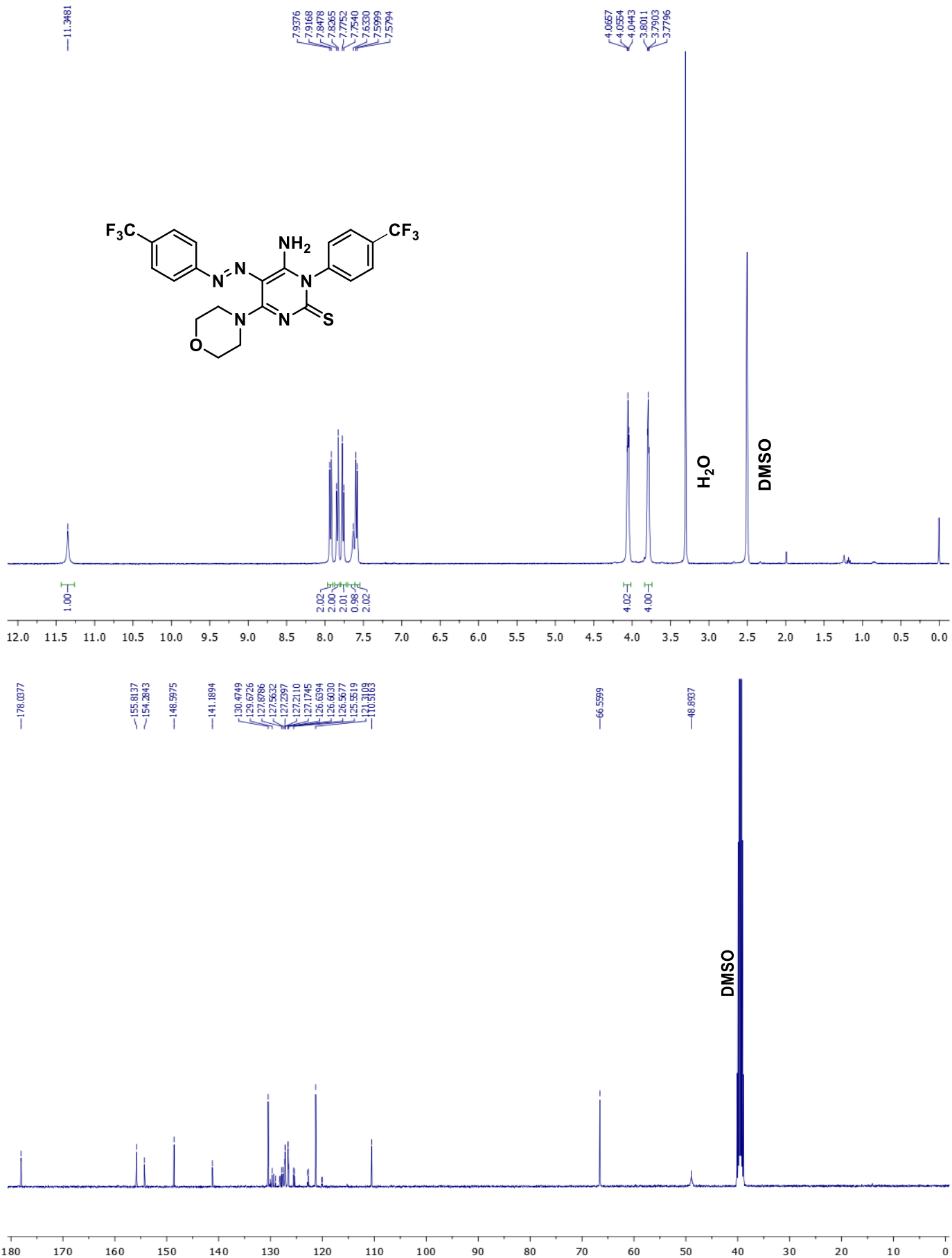


Fig. S7 ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **4g.**

Fig. S8 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **4h.**

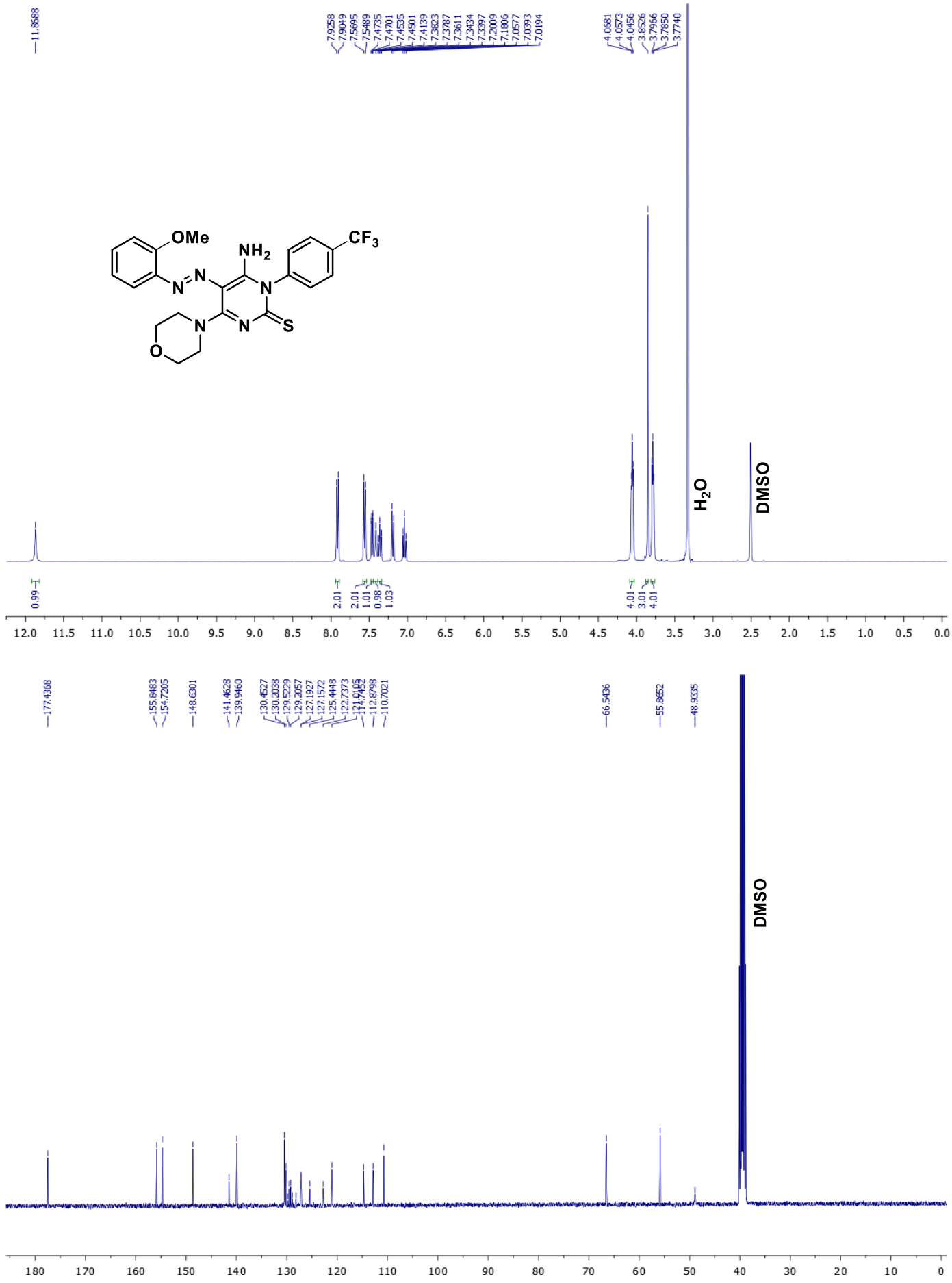


Fig. S9 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **4i.**

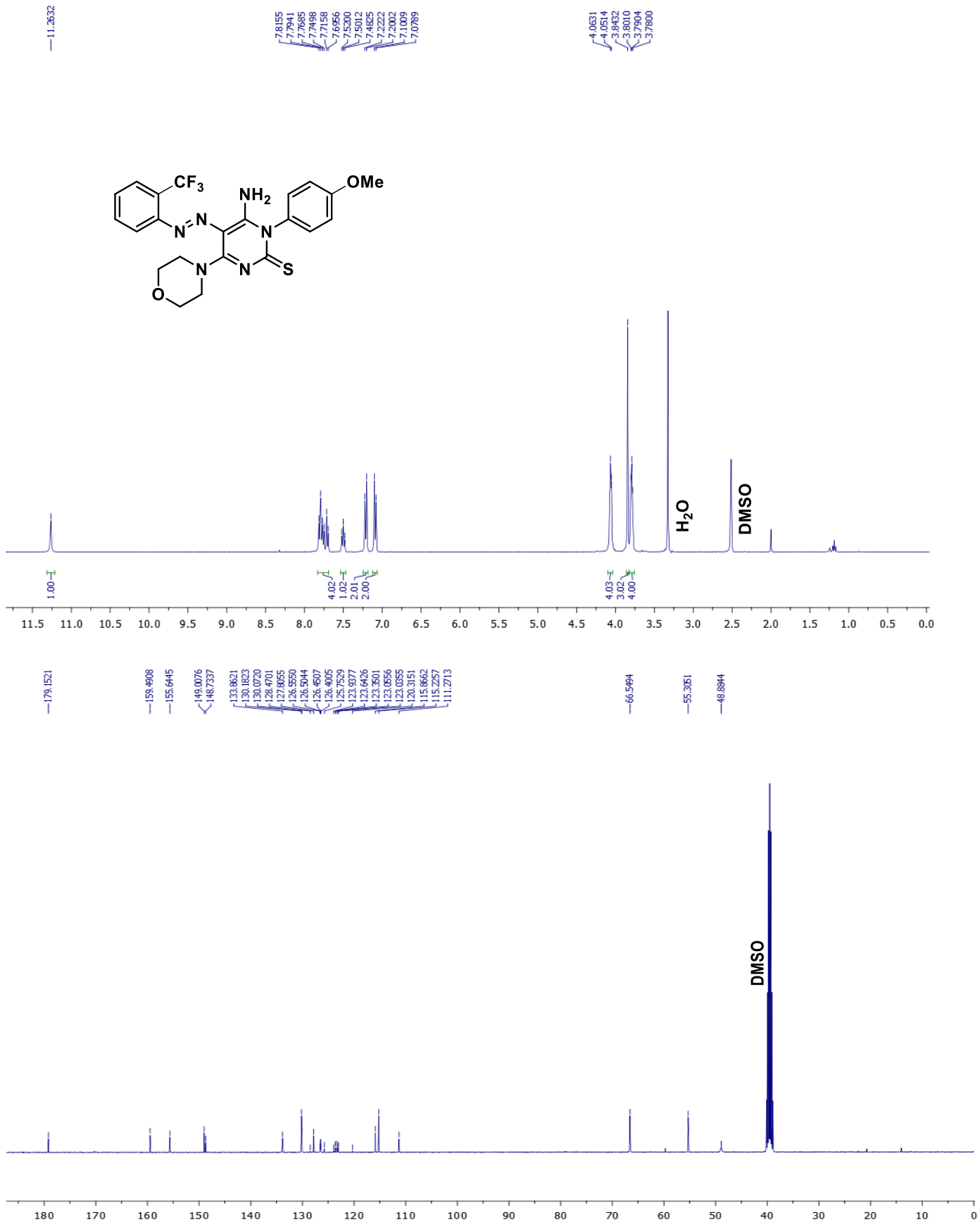


Fig. S10 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **4j.**

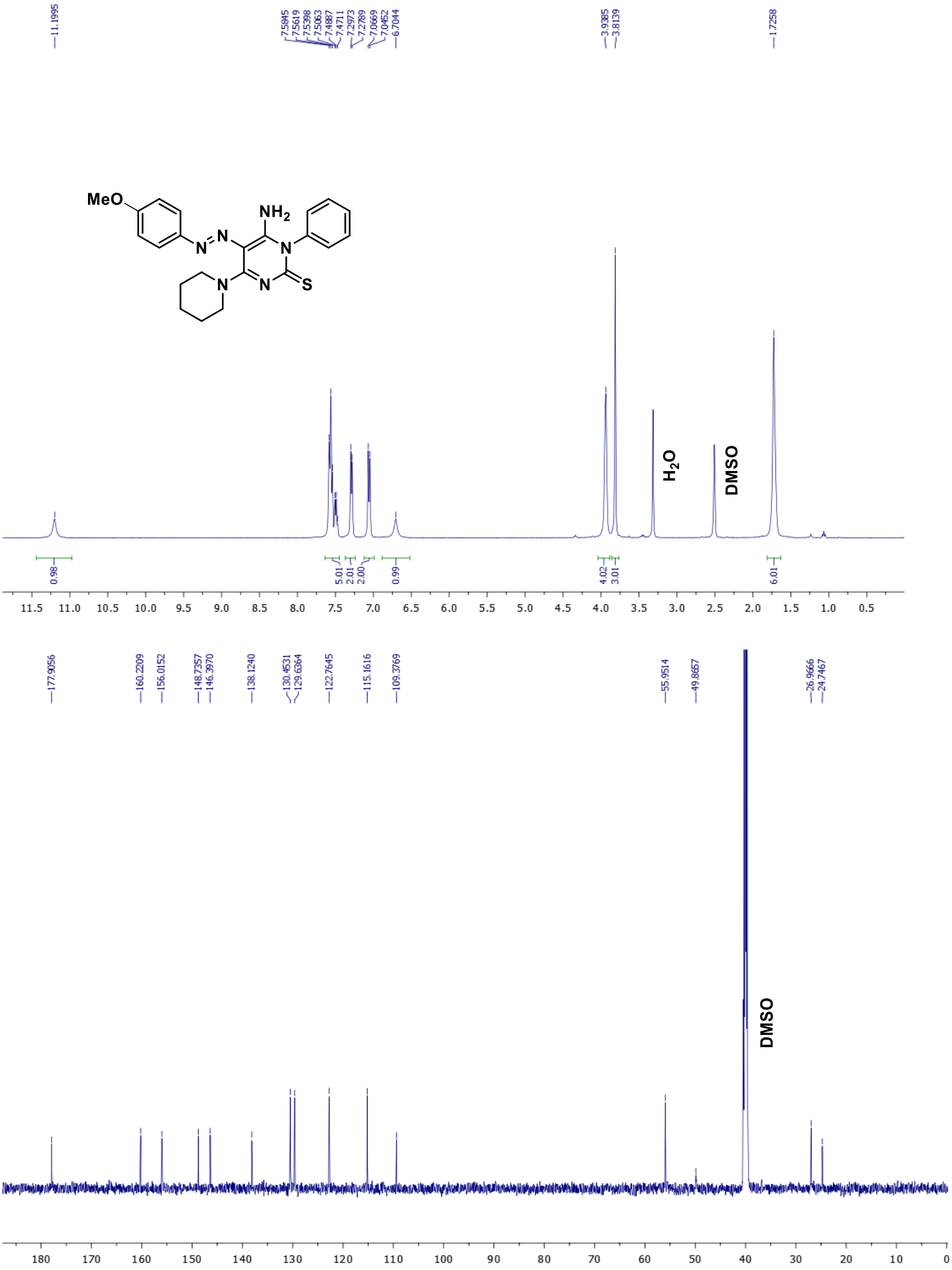


Fig. S11 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (150 MHz, DMSO-d_6) spectra **4k.**

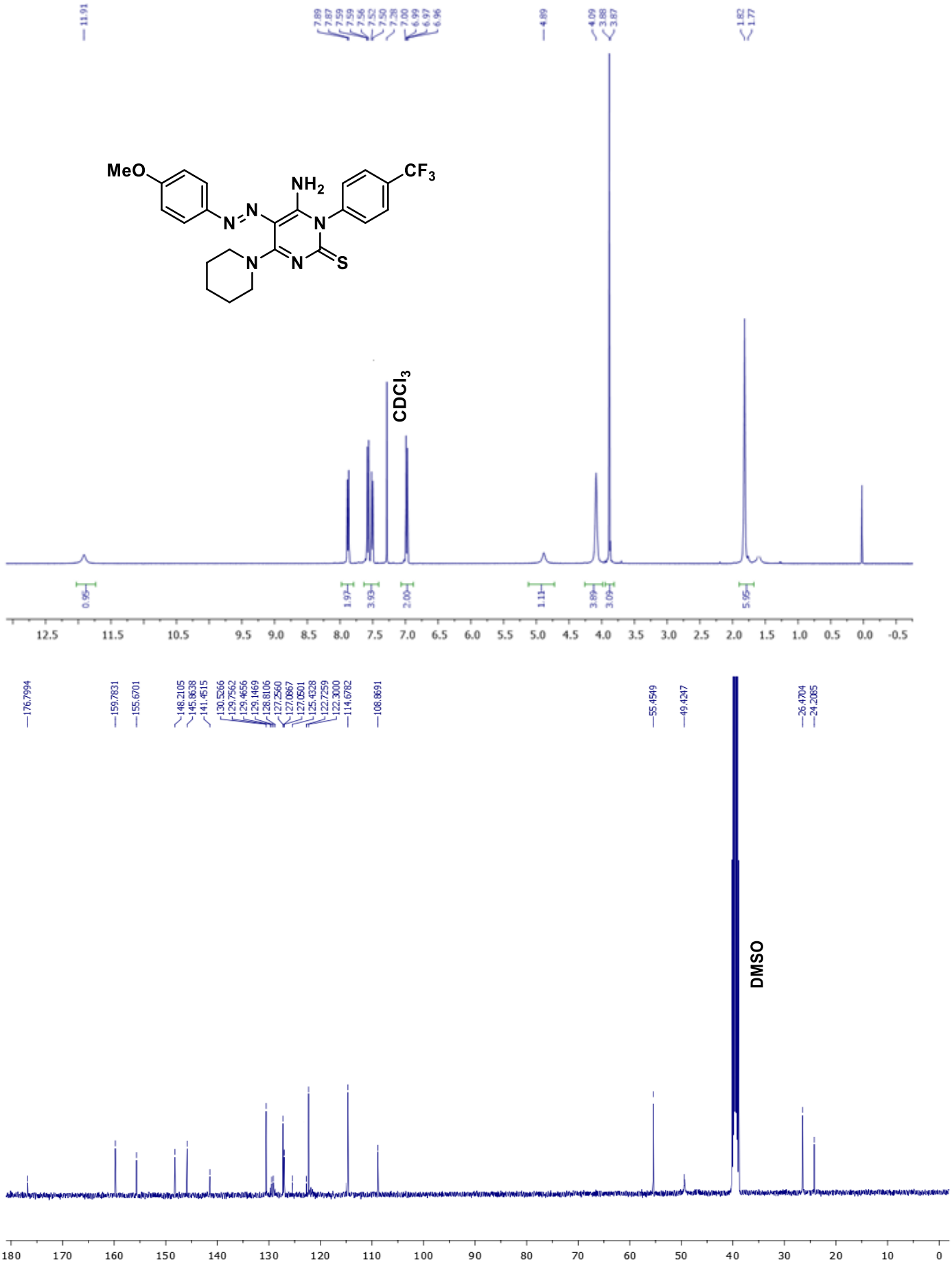


Fig. S12 ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **4l.**

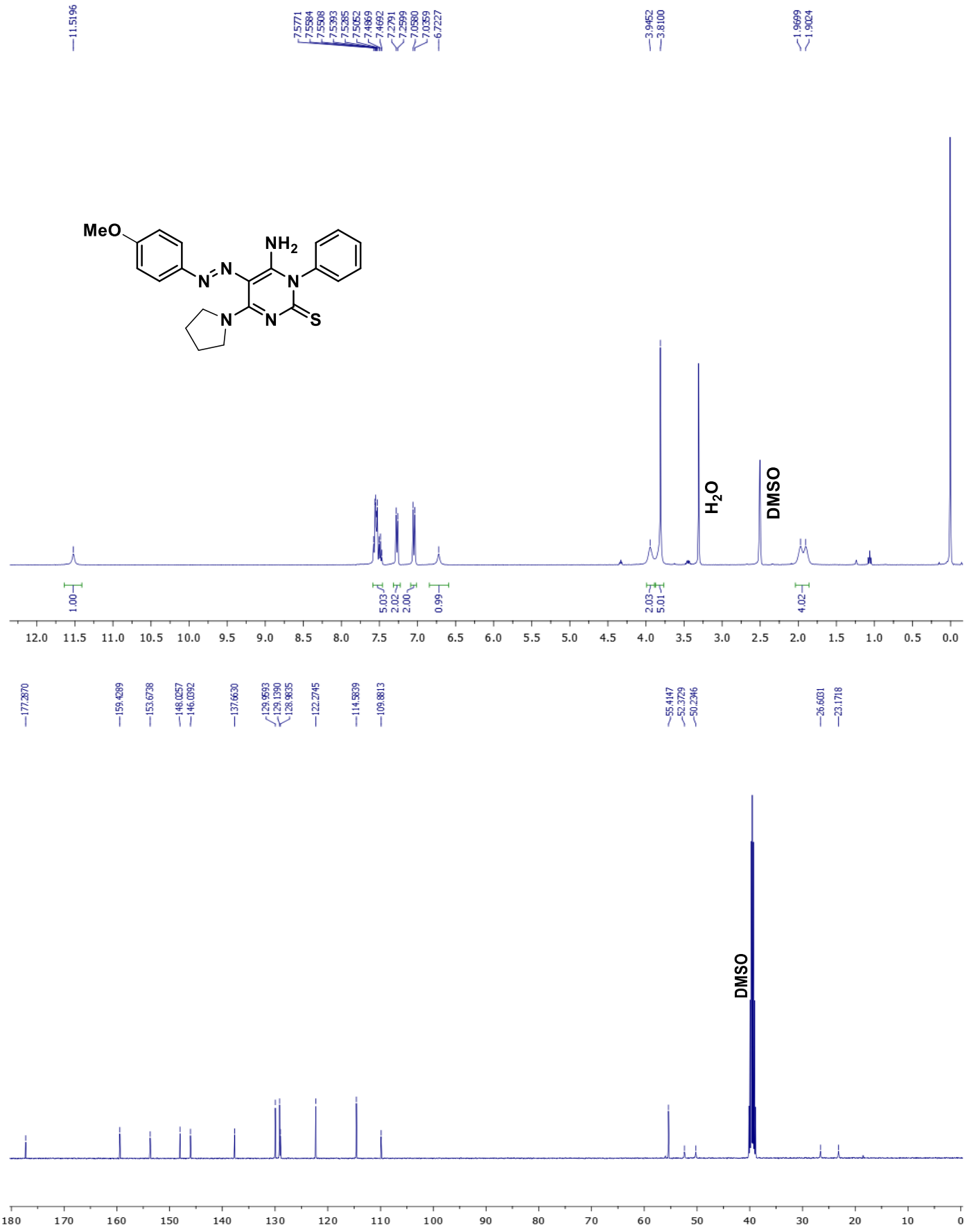


Fig. S13 ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **4m.**

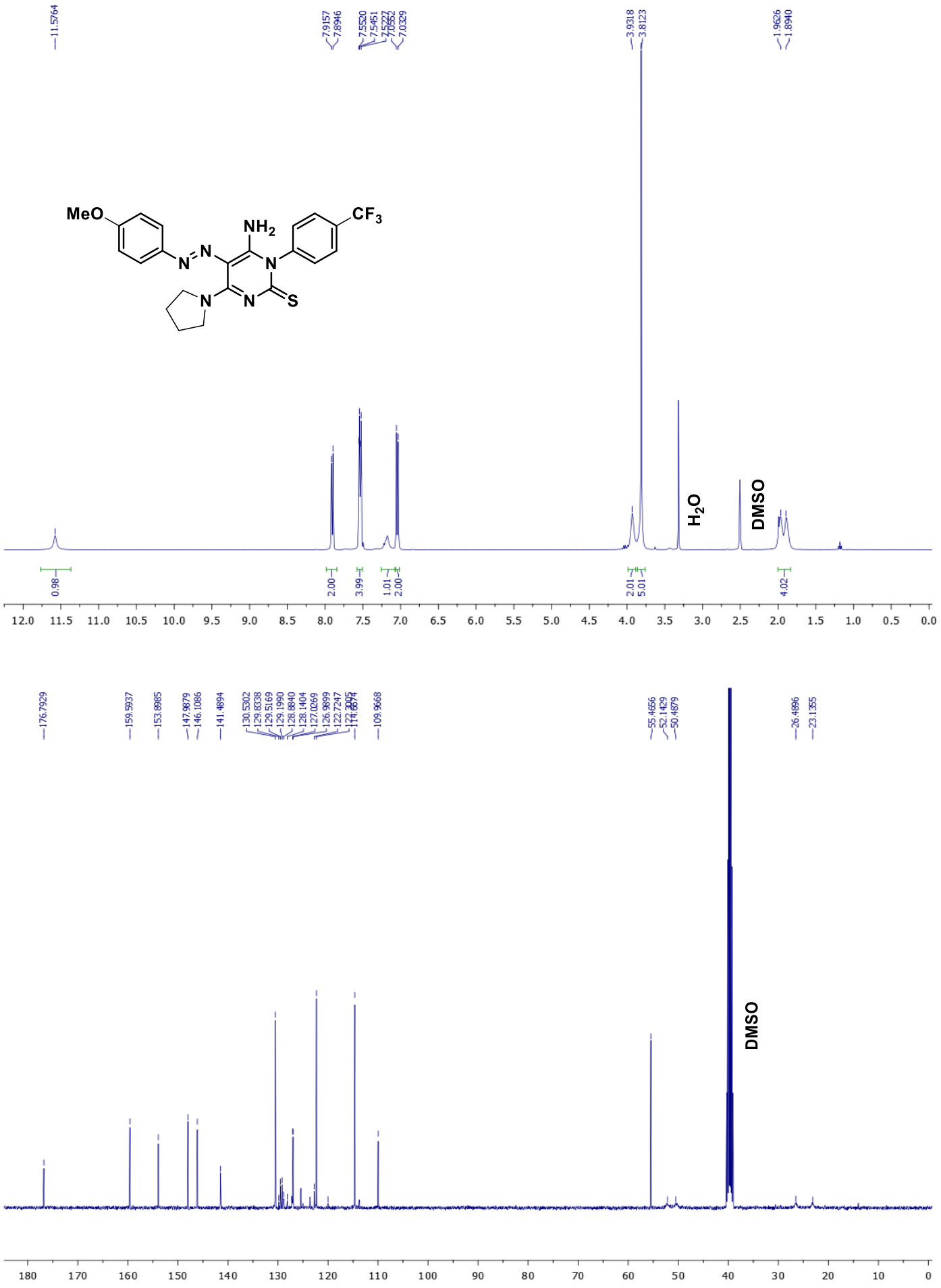


Fig. S14 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **4n.**

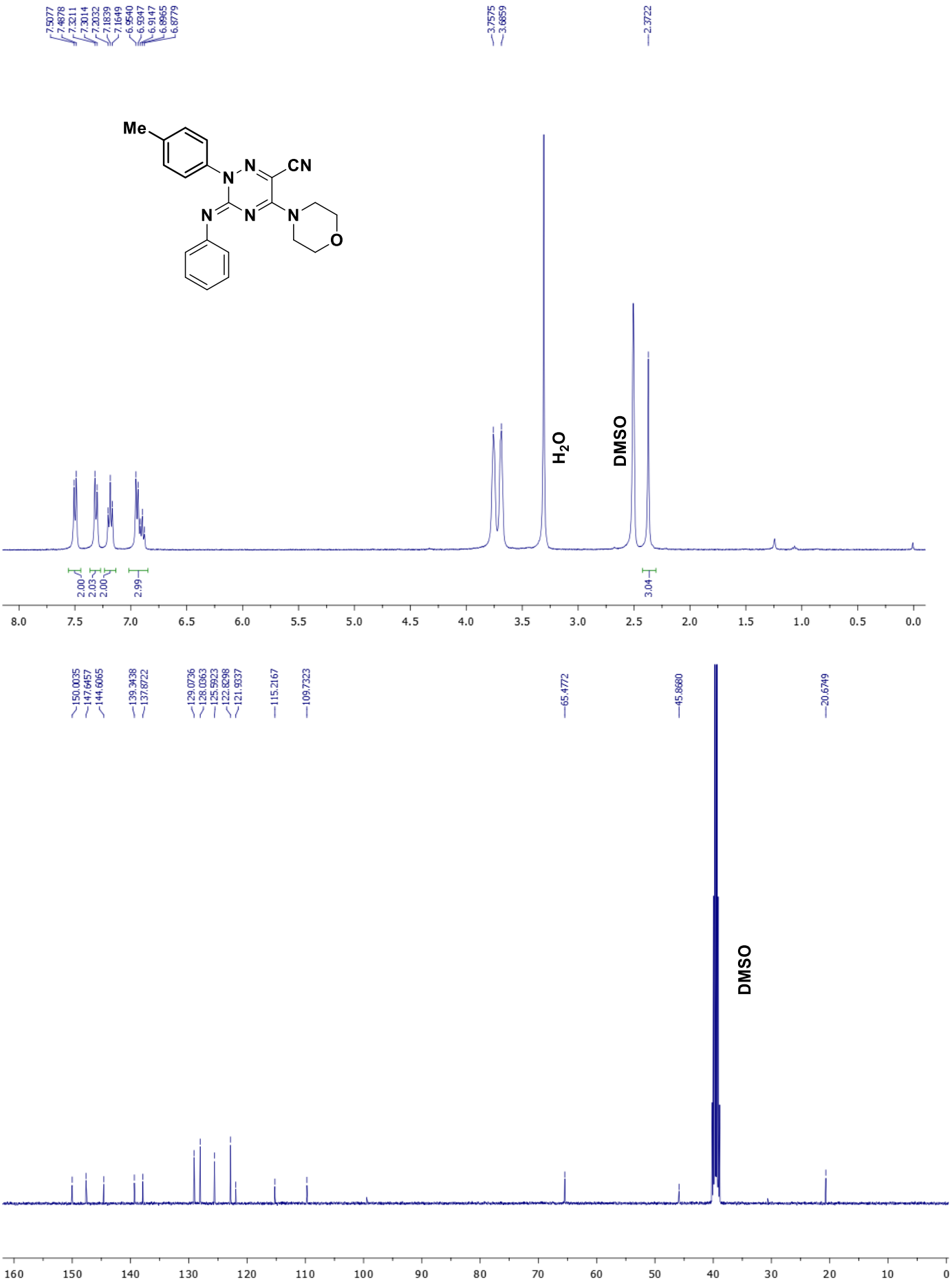


Fig. S15 ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra **6a.**

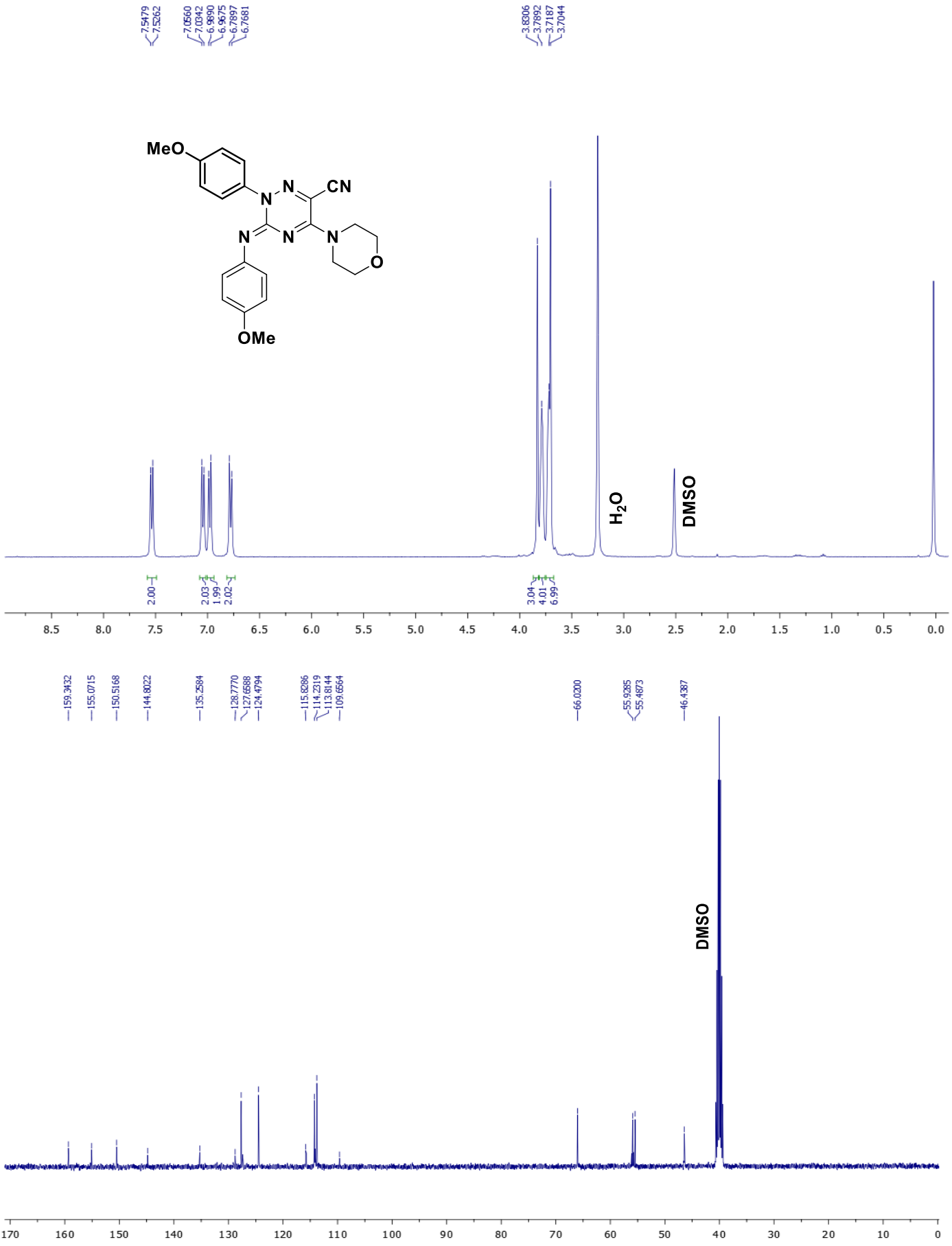


Fig. S16 ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **6b.**

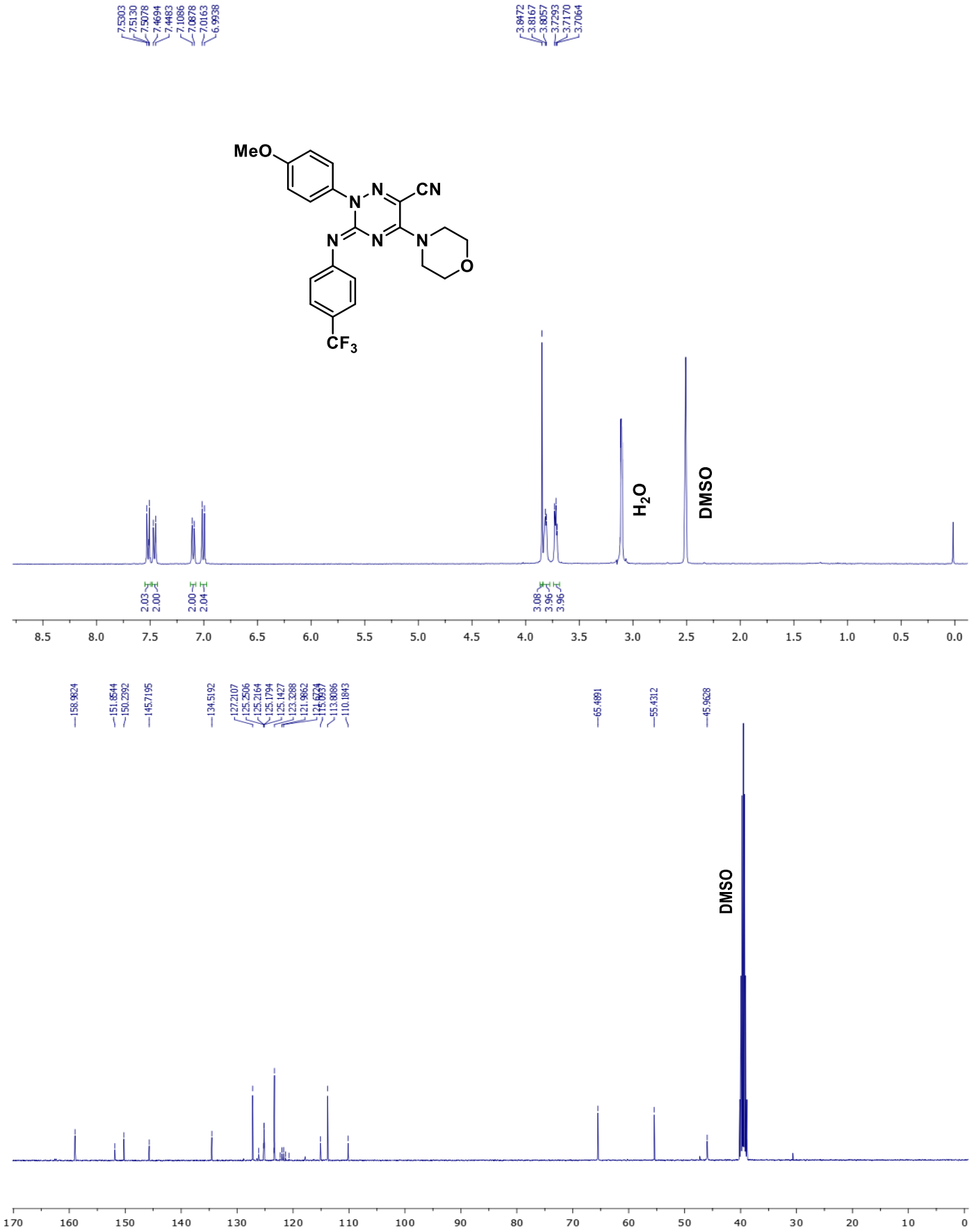


Fig. S17 ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **6c.**

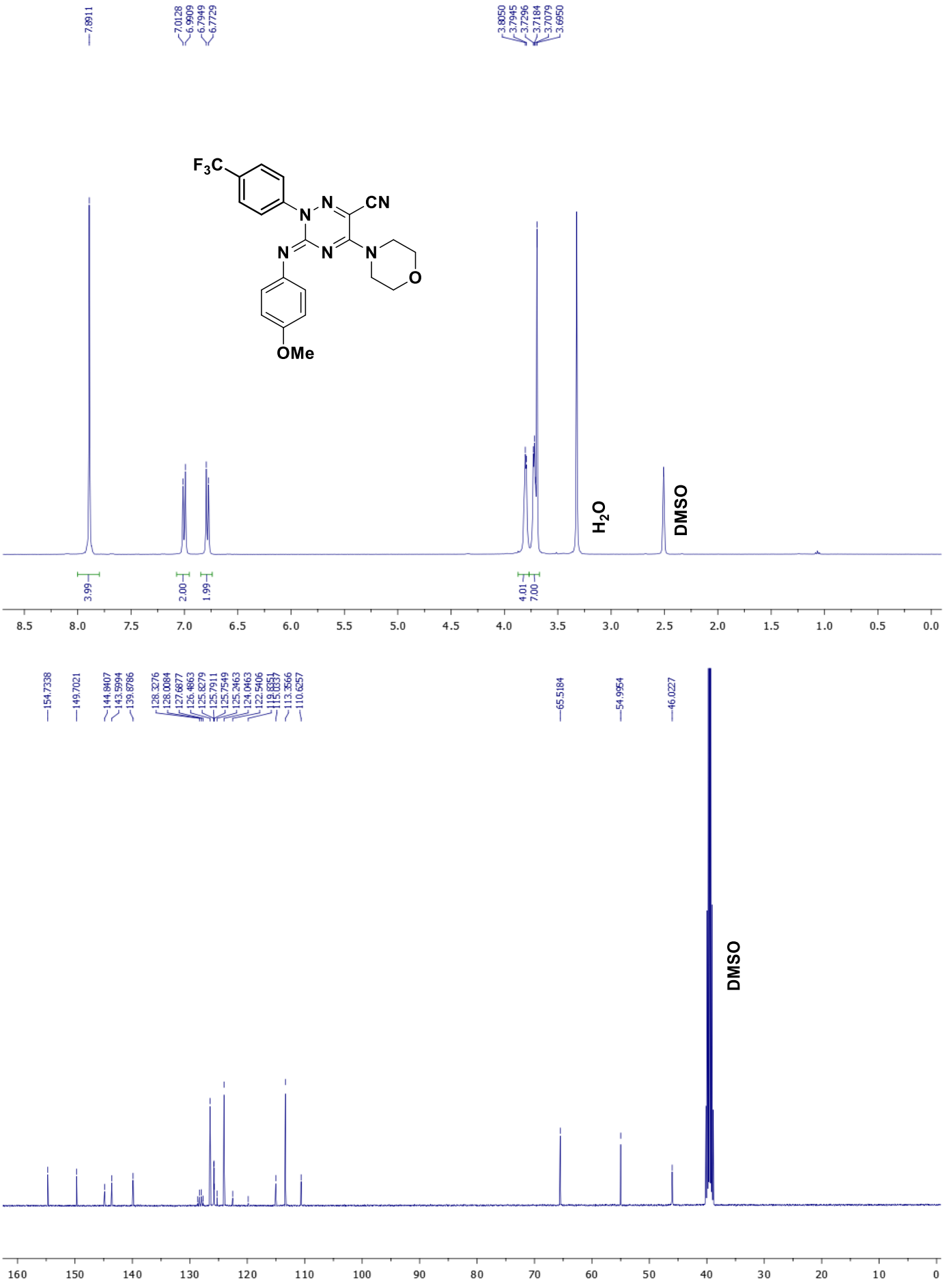


Fig. S18 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **6d.**

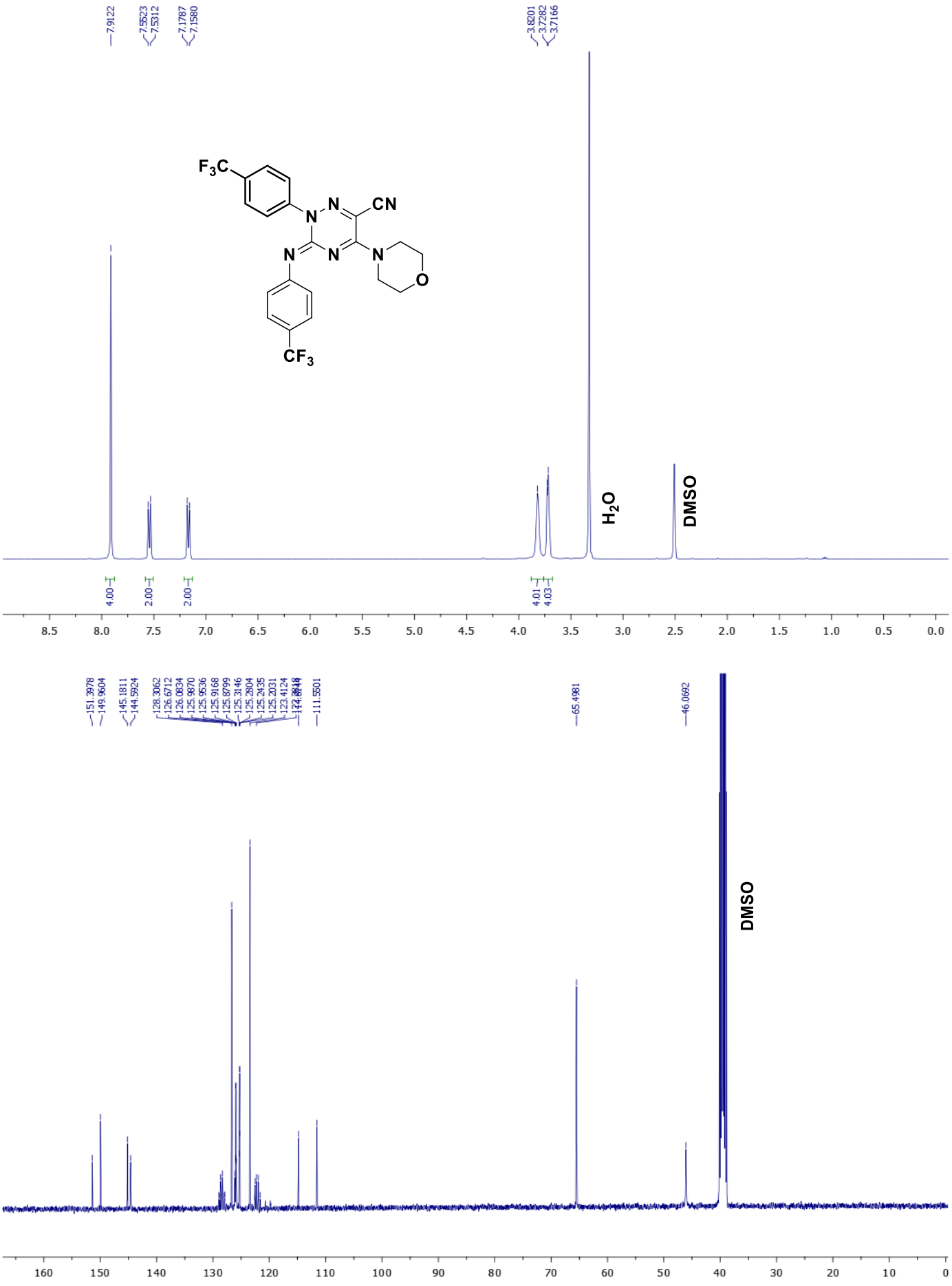


Fig. S19 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **6e.**

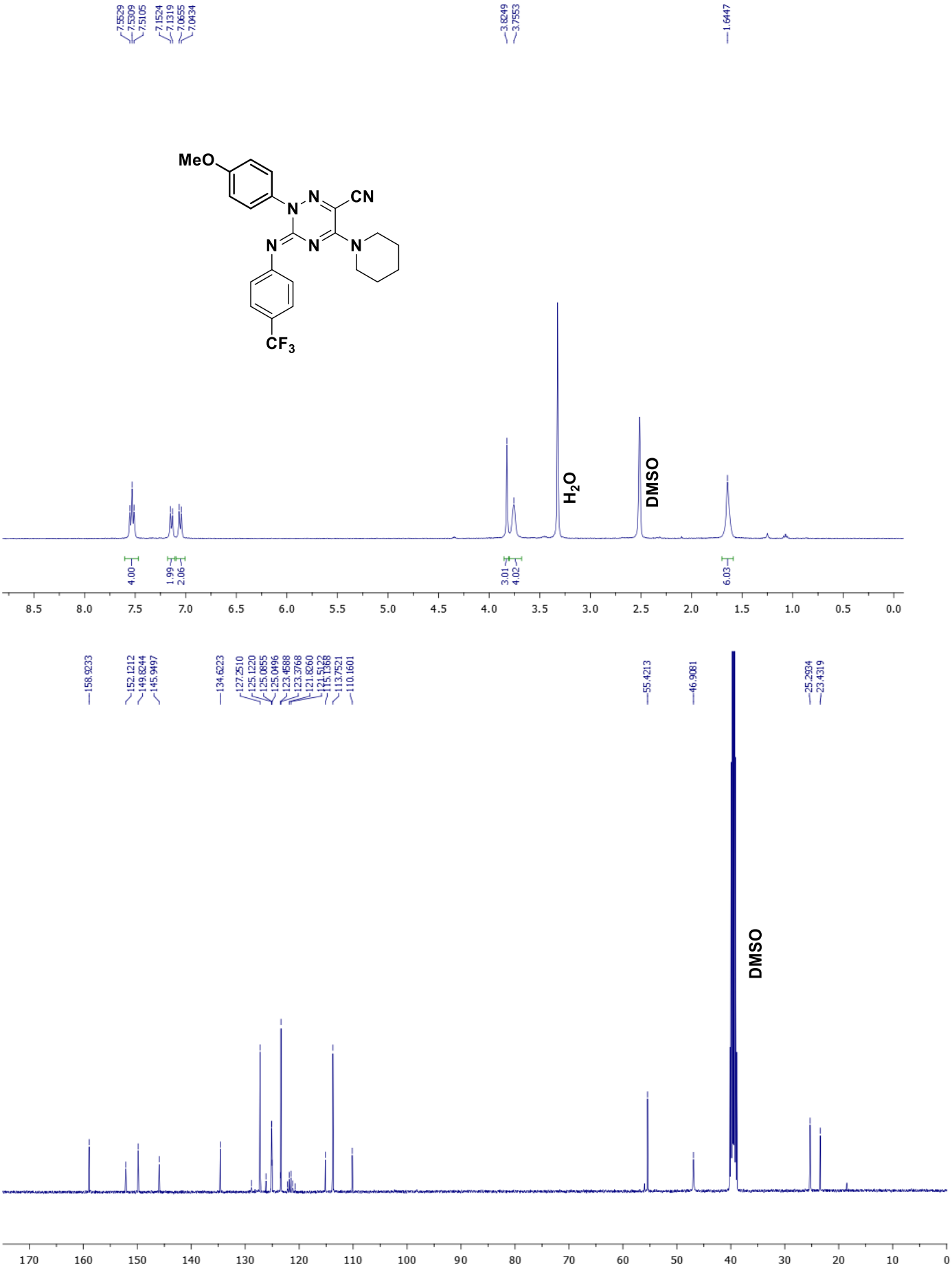


Fig. S20 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **6f.**

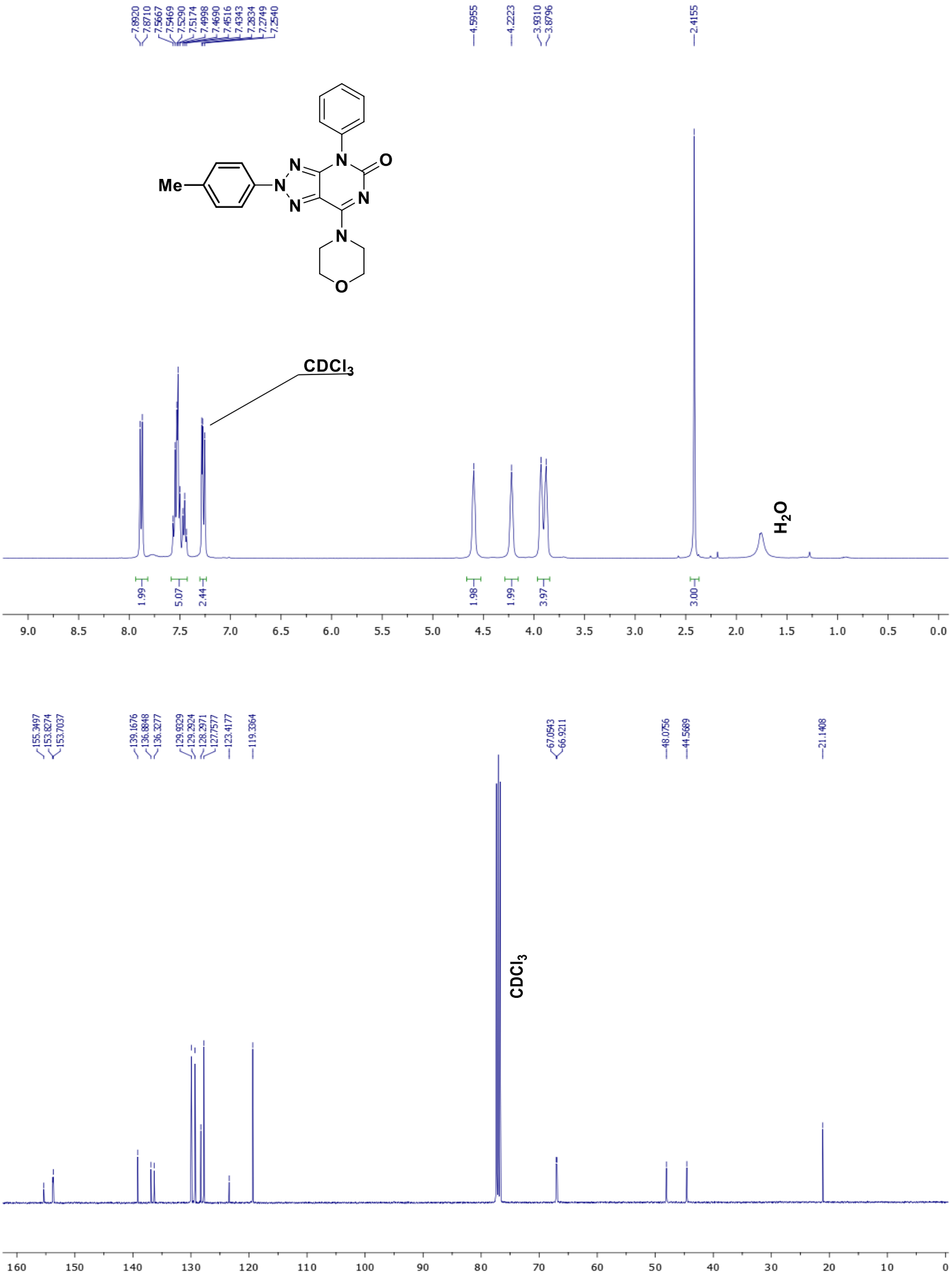


Fig. S21 ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **7a.**

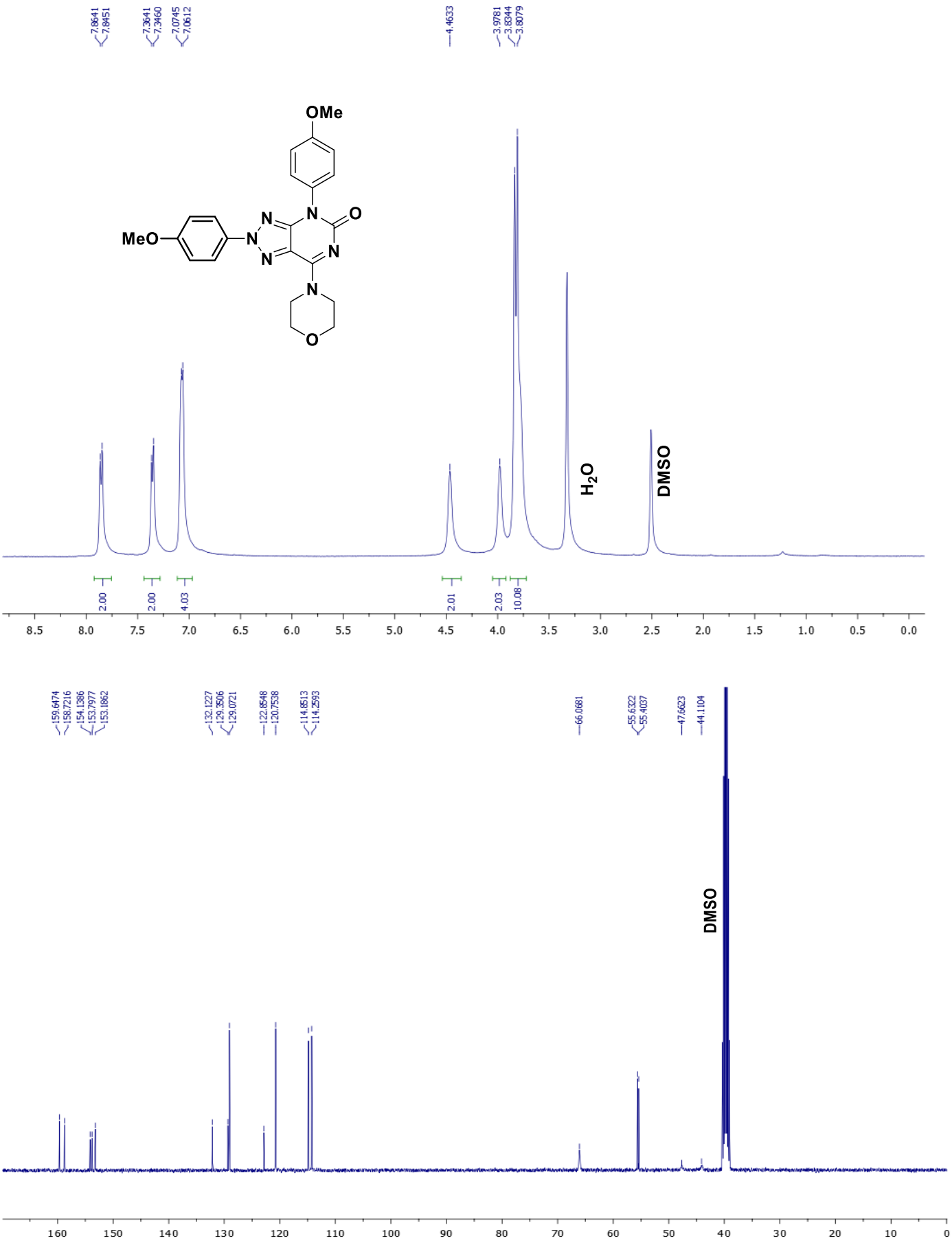


Fig. S22 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **7b.**

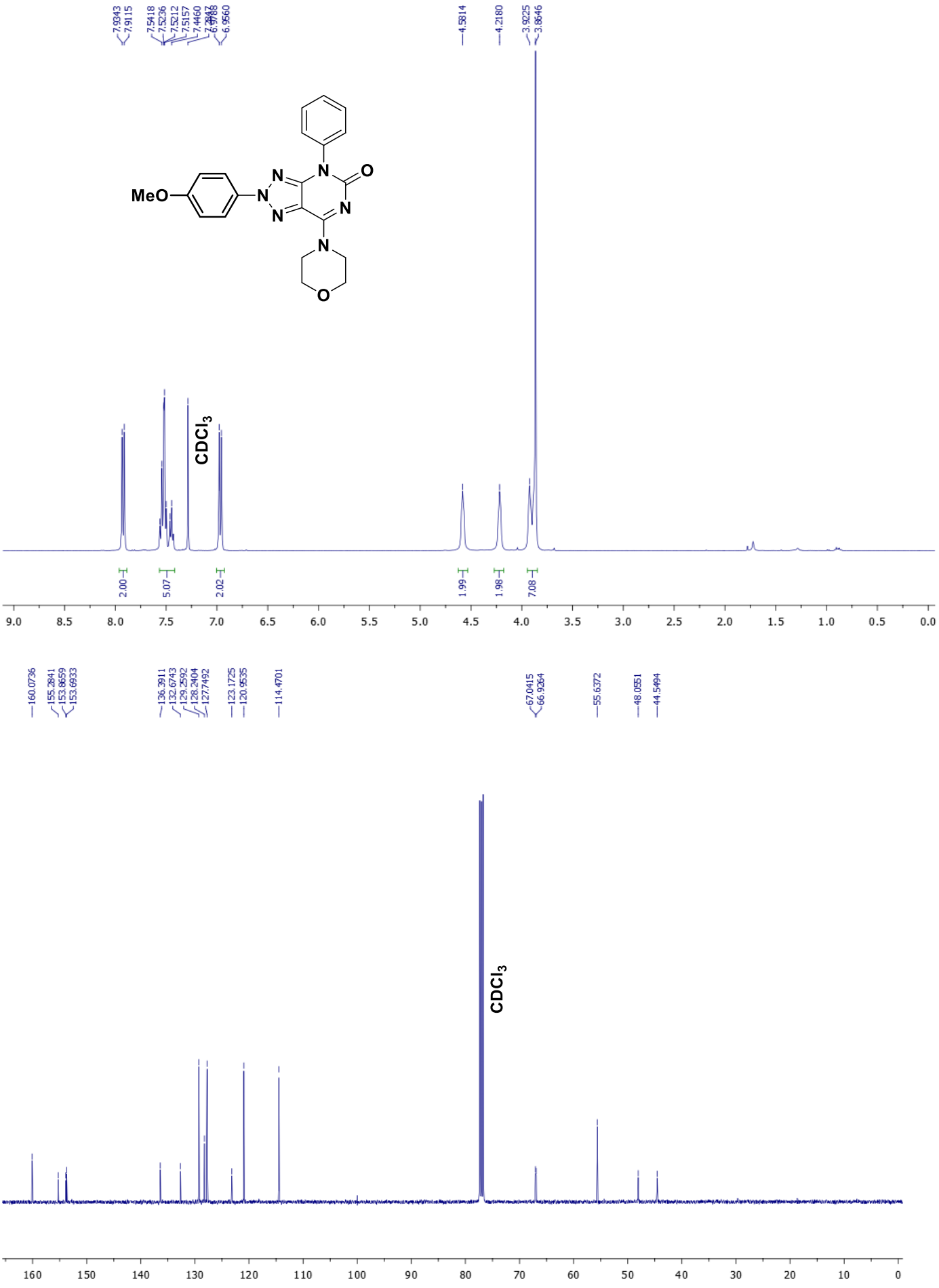


Fig. S23 ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **7c.**

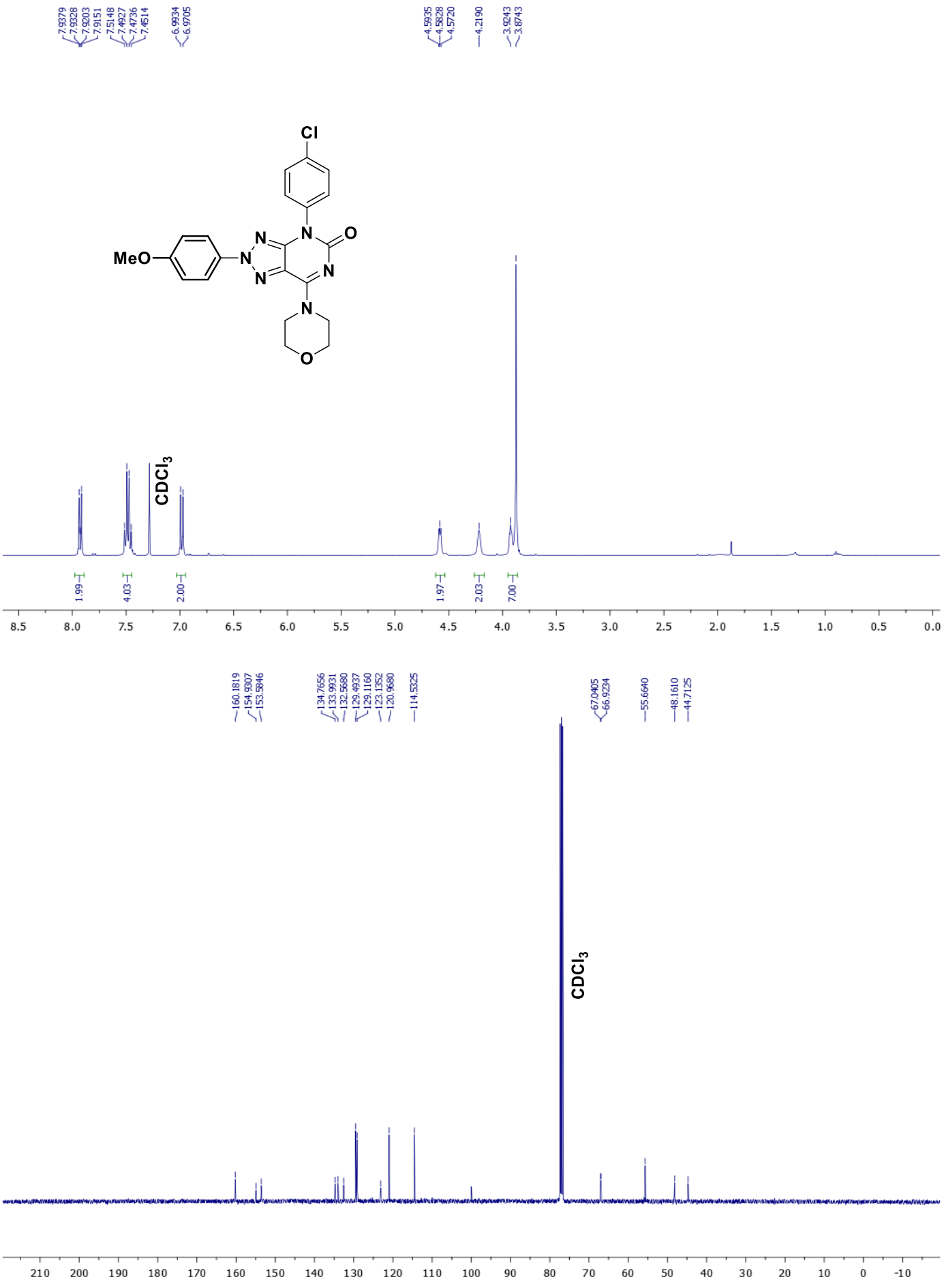


Fig. S24 ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **7d.**

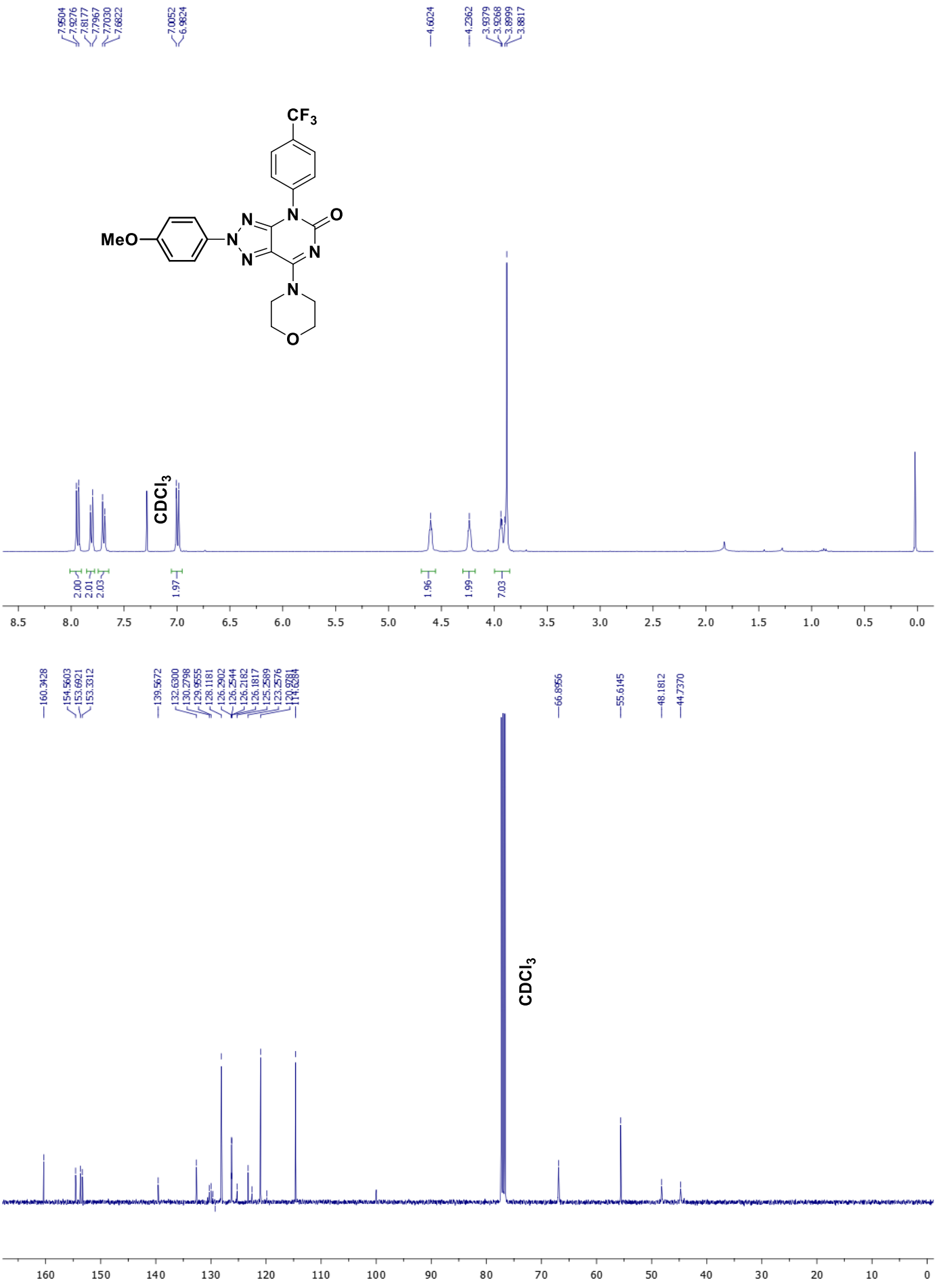


Fig. S25 ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **7e.**

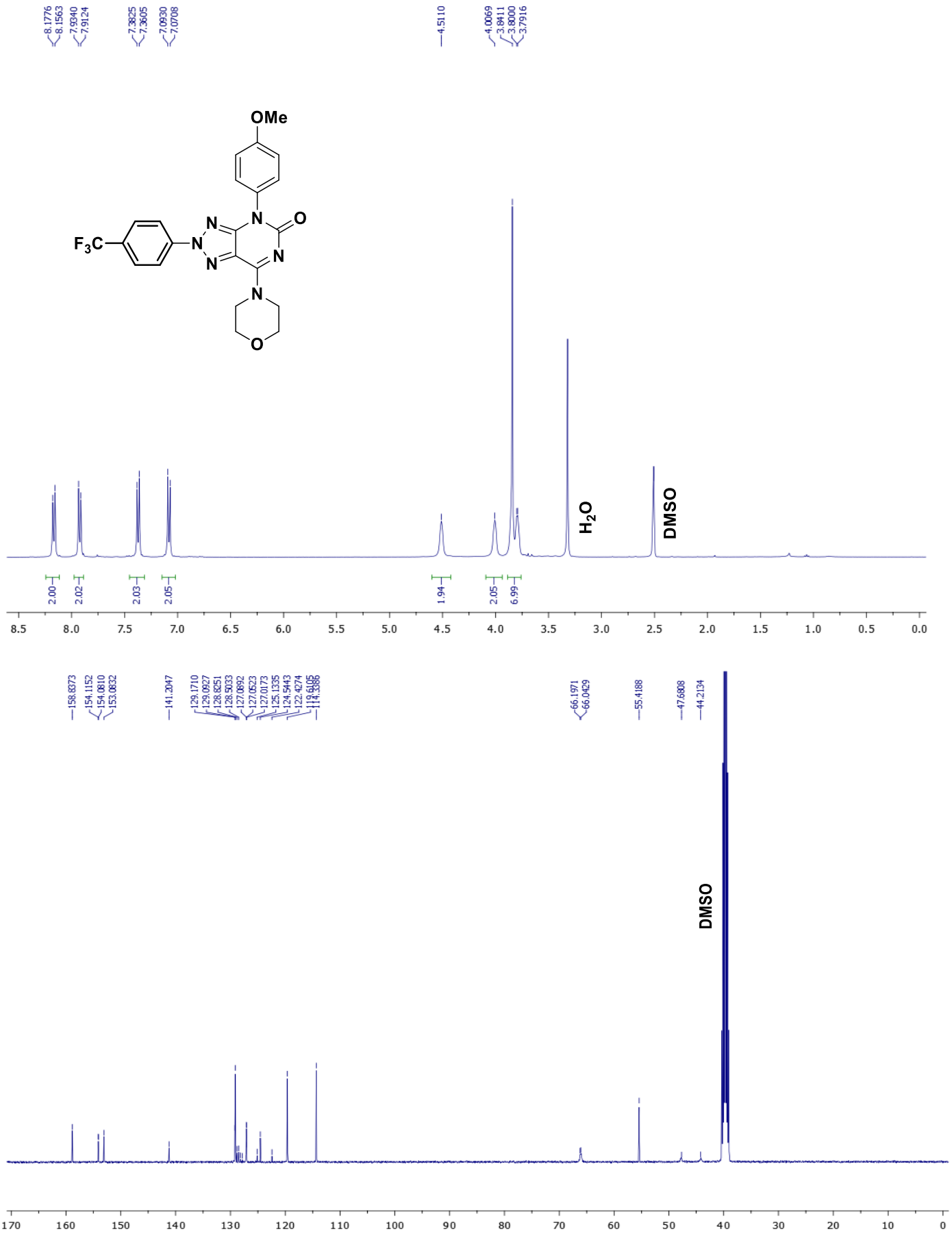


Fig. S26 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **7f.**

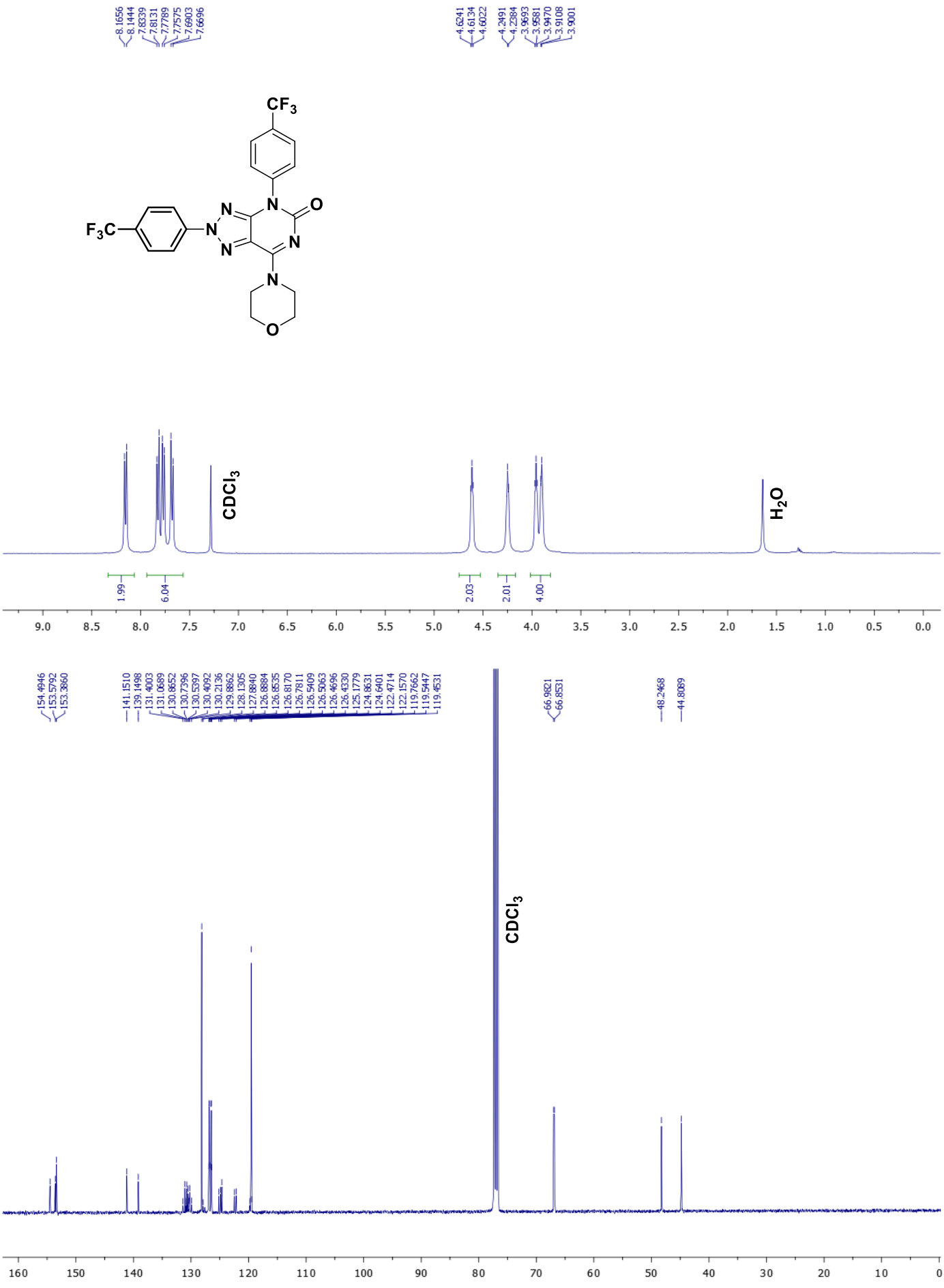


Fig. S27 ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **7g.**

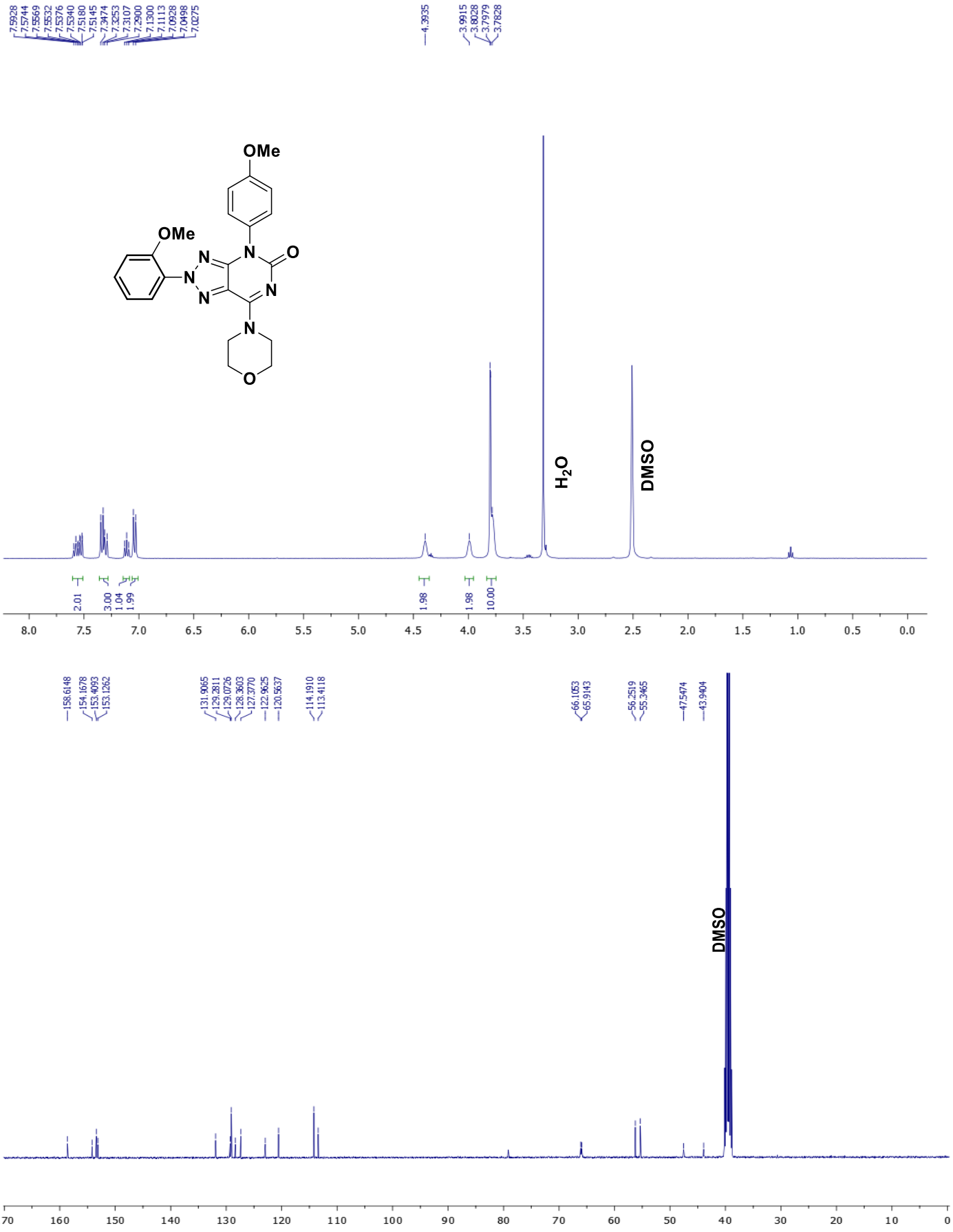


Fig. S28 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **7h.**

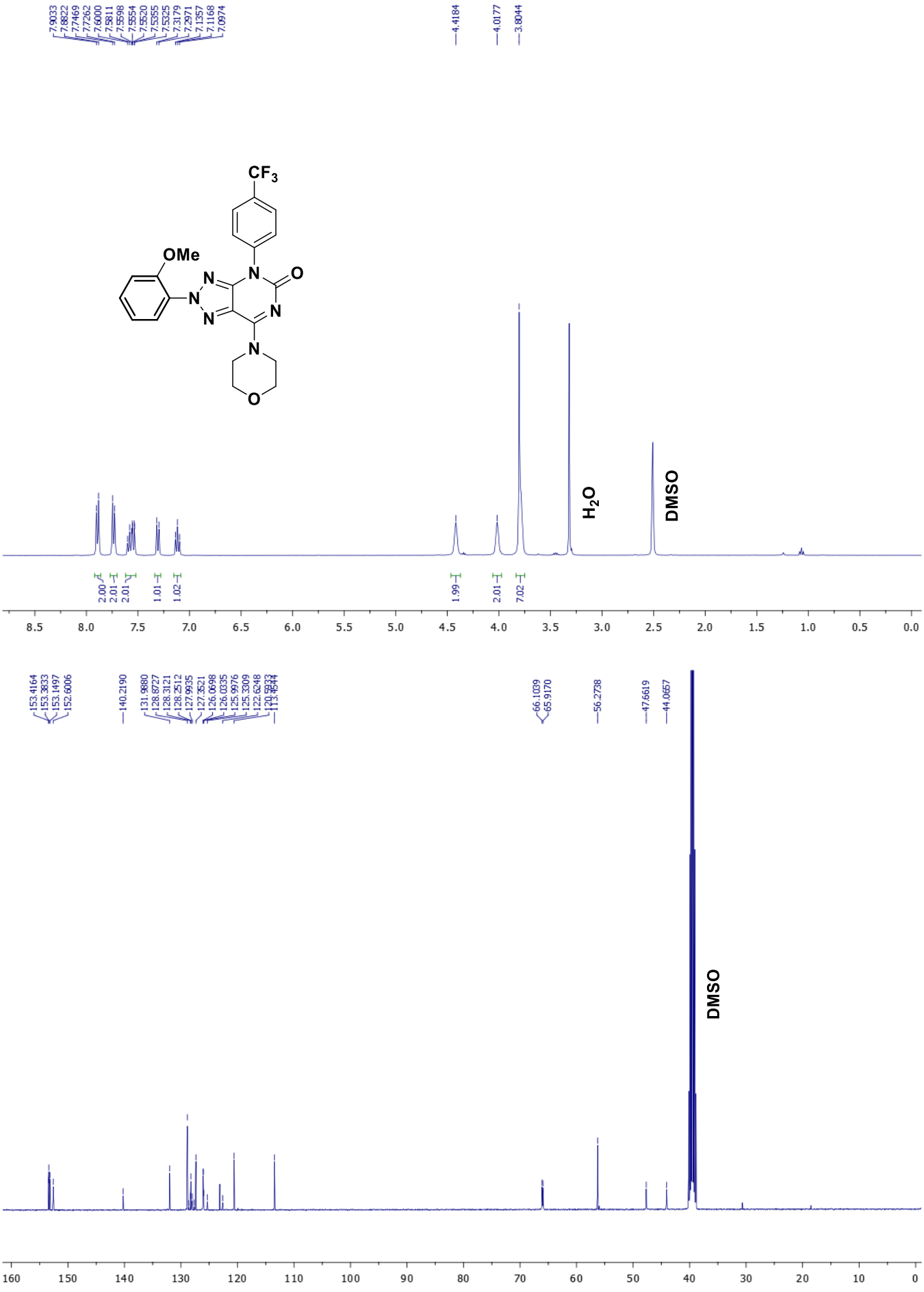


Fig. S29 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **7i.**

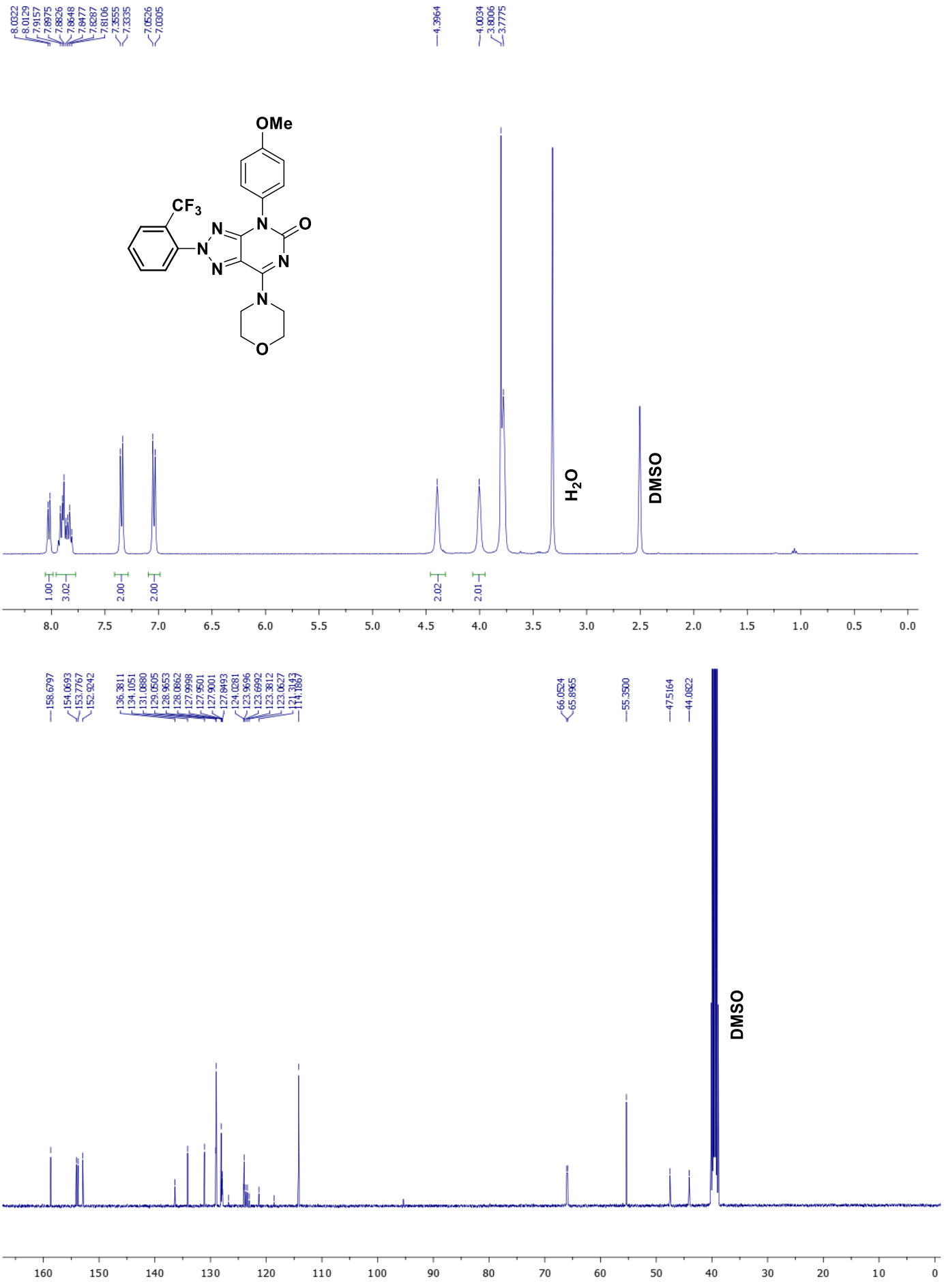


Fig. S30 ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of **7j.**

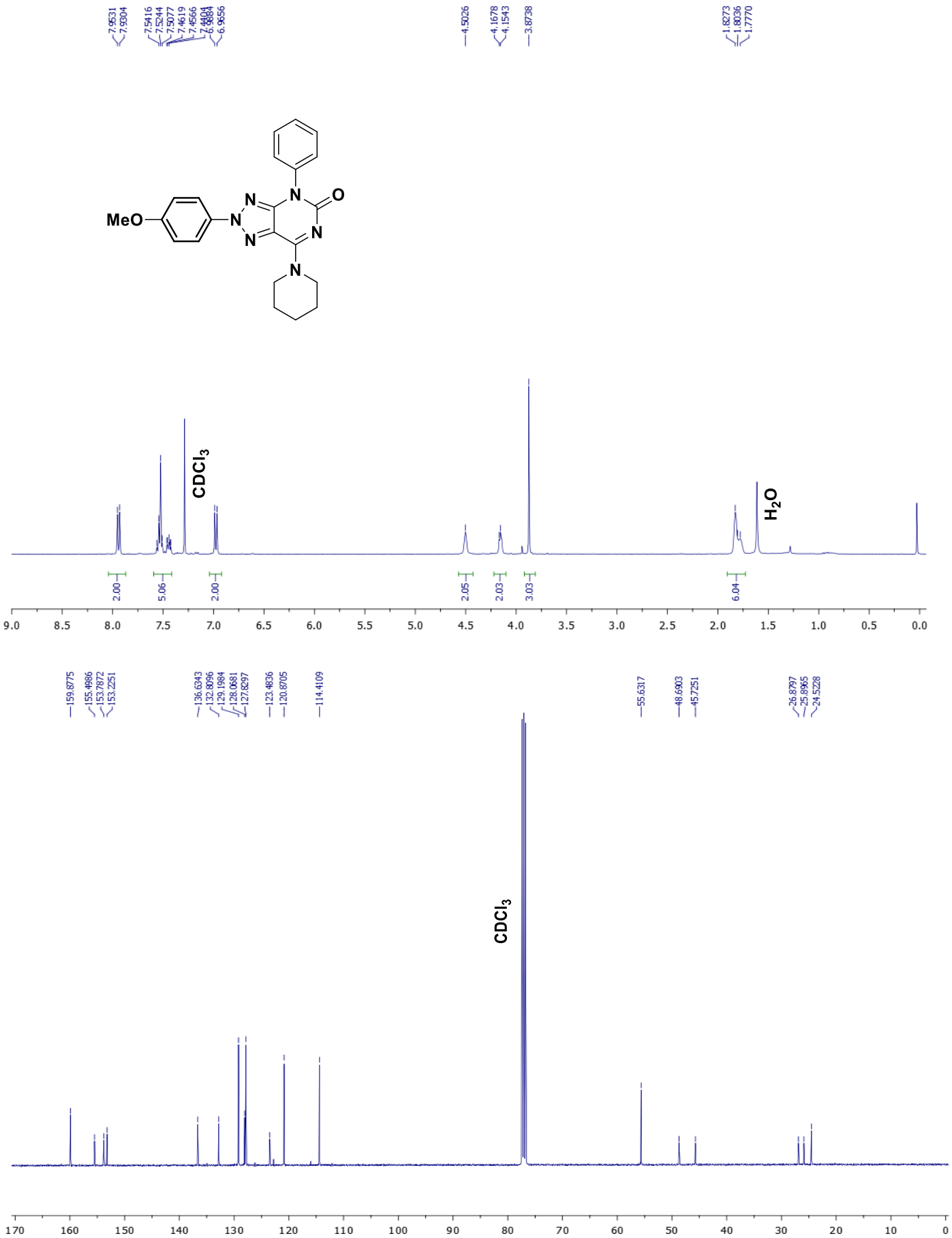


Fig. S31 ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **7k.**

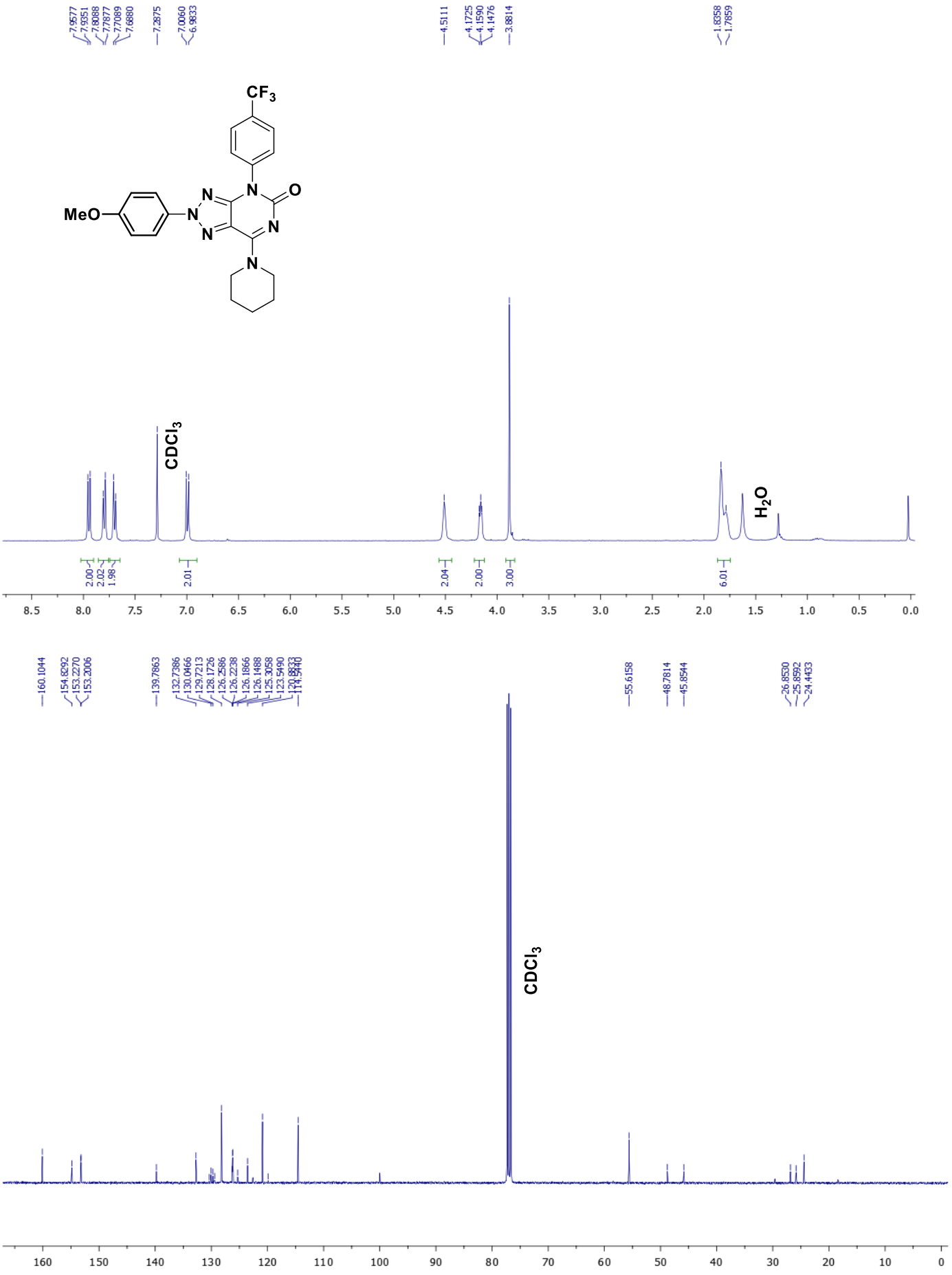


Fig. S32 ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **7l.**

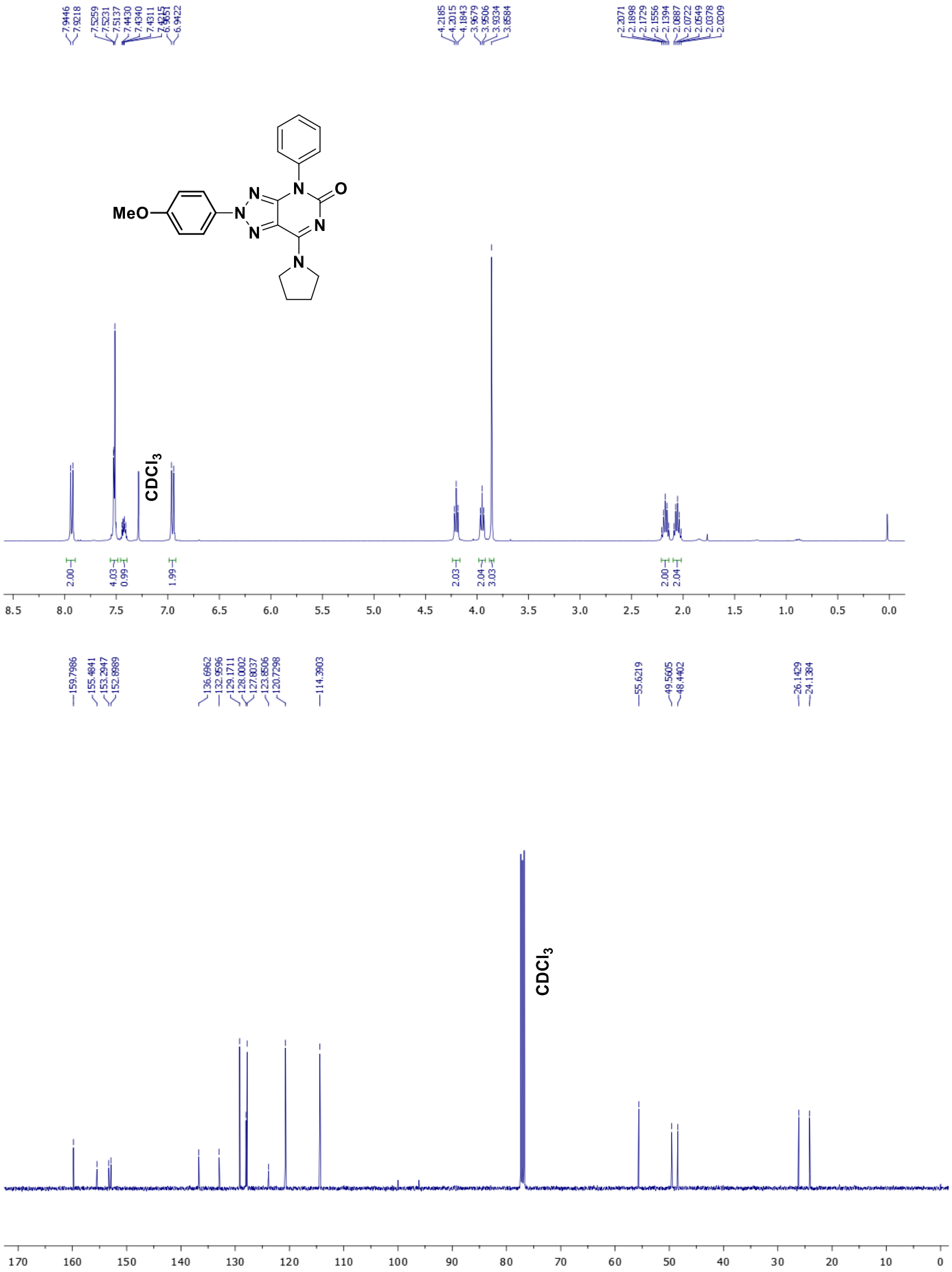


Fig. S33 ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **7m.**

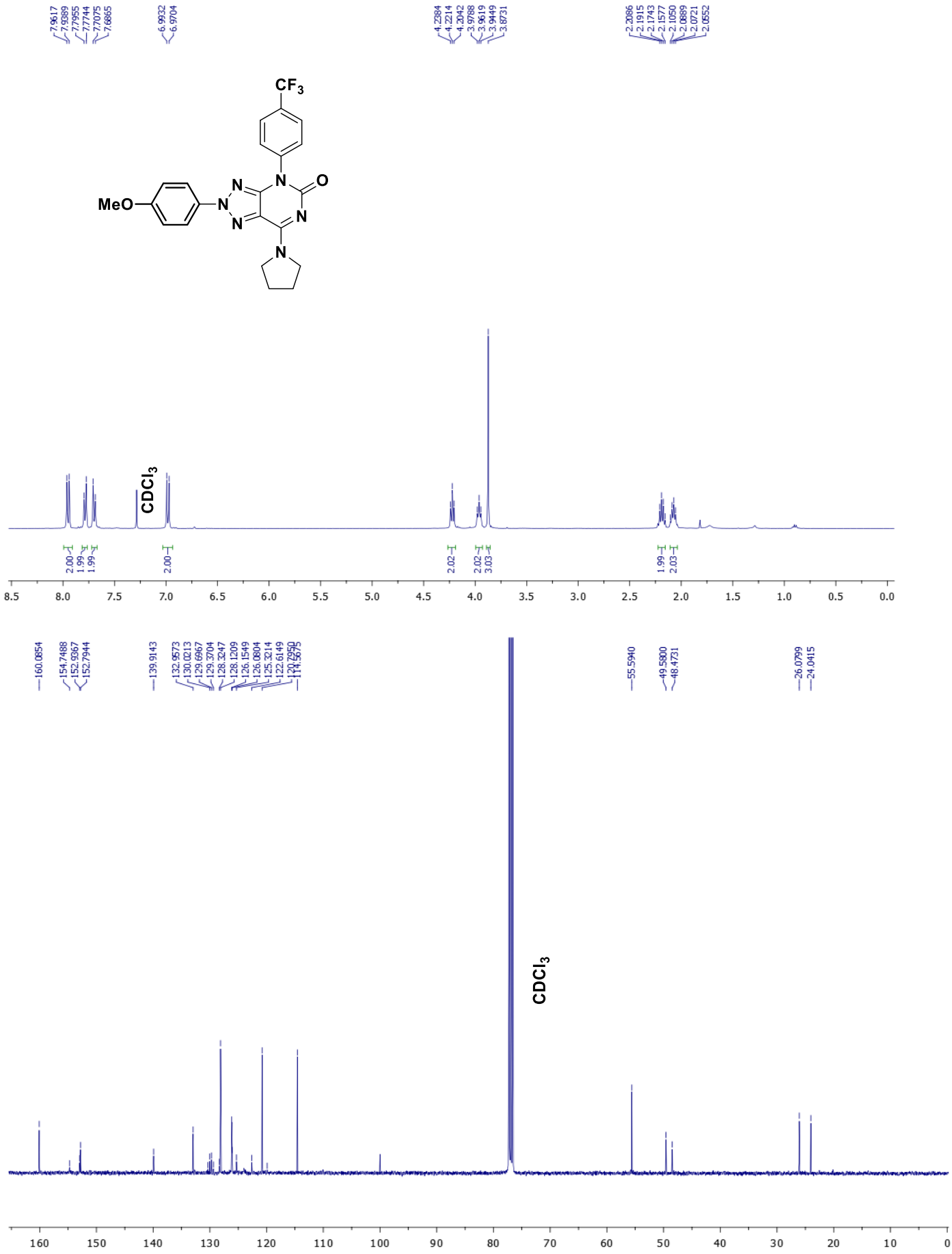


Fig. S34 ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **7n.**

3. XRD crystal data

The XRD analysis was of the single crystal $C_{21}H_{22}N_6OS$ was performed on an automated diffractometer "Xcalibur 3" on standard procedure (MoK-irradiation, graphite monochromator, ω-scans with 1o step, T= 150.01(10) K). Empirical absorption correction was applied. Using Olex2[5] the structure was solved with the Superflip[6] structure solution program using Charge Flipping and refined with the ShelXL[7] refinement package using Least Squares minimization. All non-hydrogen atoms were refined in the anisotropic approximation; H-atoms were added in the calculated positions and refined in the "rider" model.
CCDC 1859079 and CCDC 1859080 for **4a** and **7k** can be obtained free of charge from the Cambridge Crystallographic Data Centre via link www.ccdc.cam.ac.uk/data_request/cif.

Crystal Data for 4a. $C_{21}H_{22}N_6OS$, M =406.51, monoclinic, a = 6.4066(5) Å, b = 18.5404(16) Å, c = 16.5770(16) Å, β = 91.794(7)°, V = 1968.1(3) Å^3, T = 295(2), space group $P2_1/c$, Z = 4, μ(Mo Kα) = 0.191 mm^{-1}. On the angles 4.4 < 2Θ < 56.56° 7951 reflections measured, 4680 unique (R_{int} = 0.0622) which were used in all calculations. The final R^1 = 0.1936, wR^2 = 0.0948 (all data) and R^1 = 0.0696, wR^2 = 0.0681 (I>2σ(I)). Largest diff. peak/hole 0.24/-0.27 ēÅ^{-3}.
In according XRD data, the compound is crystallized in the centrosymmetric space group of the monoclinic system. The general stereometry of the molecule was shown on the Fig. 2. The azagroup and 4-MePh-substituent in the molecule are placed approximately in the plane of the heterocycle, and N=N bond distance 1.281 Å well distinguished from single N-C bonds distances. The Ph-substituent is turned toward the plane of the heterocycles on the angle 84°. The morpholino-group has a "chair" conformation with (pseudo)axial placed pyrimidine moiety. The measured C=S bond distance 1.667 Å is typical for thiones. The conformation of the molecule is ordered by intramolecular H-bond between amino- and azagroup. The protons of the NH-group of the molecule were localized by direct method and refined independently. The localization of the protons confirms the amino- rather than iminoform of the molecule. Any significantly shortened contacts in the crystal do not observed.

Crystal data for triazolopyrimidine 7k. $C_{22}H_{22}N_6O_2$, *M* =402.45, orthorhombic, *a* = 21.5416(13) Å, *b* = 5.9720(4) Å, *c* = 15.4401(15) Å, *V* = 1986.3(3) Å^3, space group $Pna2_1$, *Z* = 2, μ(Mo Kα) = 0.090 mm^{-1}. On the angles 4.62 < 2Θ < 61.42° 6843 reflections measured, 2840 unique (R_{int} = 0.0381) which were used in all calculations. The final R^1 = 0.1100, wR^2 = 0.0984 (all data) and R^1 = 0.0482, wR^2 = 0.0780 (I>2σ(I)). Largest diff. peak/hole 0.15/-0.19 ēÅ^{-3}. In according XRD data, the compound is crystallized in the non-centrosymmetric space group. The mean configuration of the molecule is shown on the Figure 2. The 4-MeOPh-group is placed approximately in the plane of the heterocycle. The Ph-group is turned toward the triazole ring on the angle 53°. The piperidine moiety has a "chair" conformation with the heterocycle in the (pseudo)axial position. In the crystal the strong intermolecular T-like interaction C_{Ar}-H…O=C [-1-x, -1-y, z-0.5] is observed with H…O distance 2.256 Å (0.46 Å less when sum of the V-d-W radii).

4. Quantum mechanical calculations

The ground state molecular geometry of the compounds under investigation was fully optimized at density functional theory (DFT) level, both in vacuo and in solvents (EtOH, DMF, $CHCl_3$, Toluene, MeCN). We compared the results obtained by employing different functionals with the experimental data. In particular, we chose hybrid (viz. B3LYP[8], and M06−2X[9]), long-range corrected (viz. CAM−B3LYP[10] and ωB97X[11]), coupled with the 6−311++G** and aug-cc-pVTZ basis sets. The D3 version of Grimme's semi-empirical dispersion with Becke-Johnson damping GD3BJ[12] was also included in the case of the B3LYP, CAM-B3LYP, and ωB97X functionals. Solvent effects were taken into account via the implicit polarizable continuum model in its integral equation formalism (IEF−PCM).[13] For geometry optimizations and frequency calculations, the PCM molecular cavity was built according to the universal force field (UFF)[14] radii within the value used in the last implementation of the PCM (based on a continuum surface charge formalism). For topological analysis and the evaluation of energetics, SMD parameterization was employed.[15] The standard values for dielectric constants and refractive indexes were always assumed. The vibrational frequencies and thermochemicals were computed in harmonic approximation at T = 298.15 K and p = 1 atm, and no imaginary frequencies were found.

The atomic charge population analysis, electric multiple moments, electronic density, and electrostatic potential were also computed using Mulliken's and the CHelpG procedure[16] for both the ground and the S_1 excited (vertical and relaxed) states.

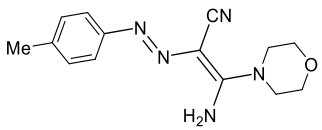
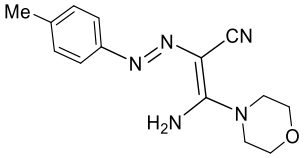
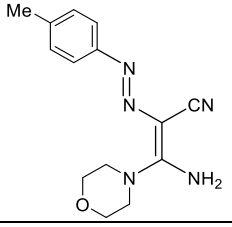
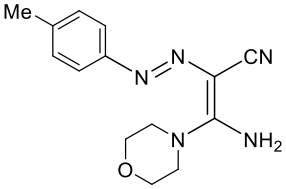
To investigate the presence and nature of possible intramolecular H-bonding interactions the non-covalent interaction (NCI) index combined with the second derivative of the reduced density gradient along the second main axis of variation were employed.[17] this procedure was applied both to the ground and first singlet excited states.

NMR chemical shift were computed according to the protocol suggested in.[18]

The integration grid for the electronic density for topological and RDG analysis was set to 150 radial shells and 974 angular points. For the rest of the calculations, the integration grid was set as 99 radial shells and 590 angular points. The convergence criteria of the self-consistent field was set to 10^{-12} for the RMS change in the density matrix and 10^{-10} for the maximum change in the density matrix. The Convergence criteria for optimizations were set to 2 x 10^{-6} a.u. for maximum force, 1 x 10^{-6} a.u. for RMS force, 6 x 10^{-6} a.u. for maximum displacement and 4 x 10^{-6} a.u. for RMS displacement.

All calculations were performed using the GAUSSIAN G09.D01 software package.[19] The location of BCPs and subsequent calculation of SF values were performed using a modified version of the PROAIMV program.[20]

Table S1. Stability of the different isomers of DAA **1a** in different solvents

			
1a/t	**1a/t´**	**1a/c**	**1a/c´**

	Δ / (kJ/mol)								
	Toluene			DMF			MeCN		
Compd	*E*+ZPE	*H*	*G*	*E*+ZPE	*H*	*G*	*E*+ZPE	*H*	*G*
1a/c´	17.6	17.4	18.1	16.6	16.6	17.2	16.3	16.5	16.4
1a/c	4.5	4.8	3.4	3.0	3.6	0.8	3.3	3.7	2.7
1a/t´	6.2	6.0	6.5	13.3	12.9	13.9	13.6	13.0	15.0
1a/t	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

	Δ / (kJ/mol)					
	Chloroform			Ethanol		
Compd	*E*+ZPE	*H*	*G*	*E*+ZPE	*H*	*G*
1a/c´	18.1	17.3	23.6	17.4	17.3	18.6
1a/c	4.2	4.2	7.2	3.9	4.1	3.8
1a/t´	10.8	9.7	16.7	13.3	12.8	14.1
1a/t	0.0	0.0	0.0	0.0	0.0	0.0

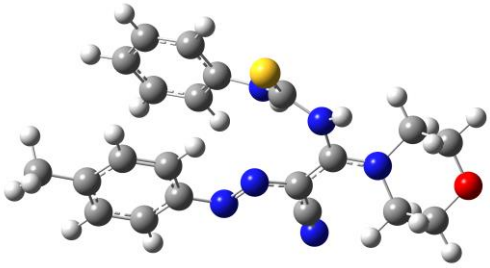
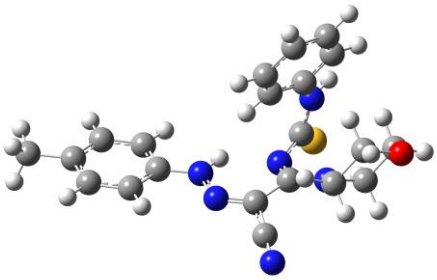
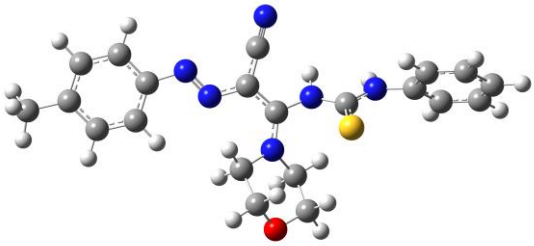
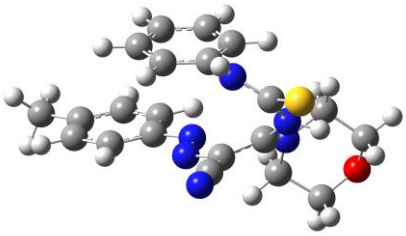
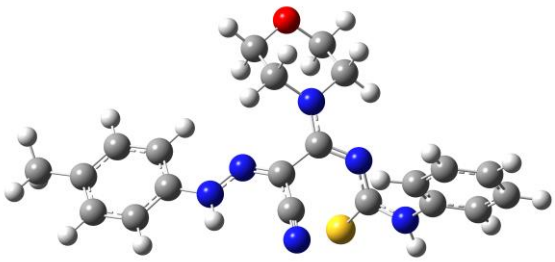
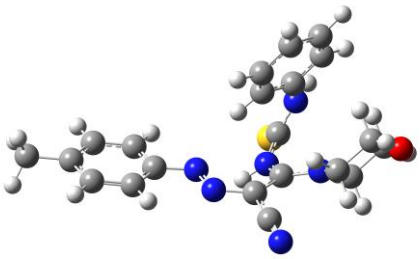
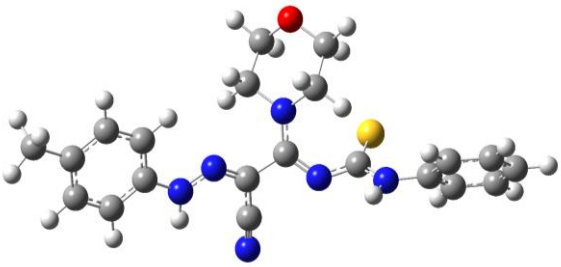
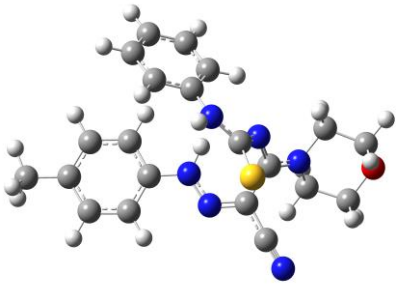
	
A(*tt*)	A(*tc*)
	
A(*ct*)	A(*cc*)
	
B(*tt*)	B(*tc*)
	
B(*ct*)	B(*cc*)

Fig. S35 Optimized geometry for the reaction intermediates **A** and **B** isomers obtained at the DFT M06-2X (SMD) / aug-cc-pVTZ level.

Both **A** and **B** tautomers may assume different conformations due to possible rotations about angles α, β, and γ. These rotations generate two possible rotamers each (namely, *trans* and *cis*). On the whole, eight possible combinations, but some of them coincide, so we eventually have just four possible distinct rotamers for **A** and for **B**, named *tt*, *tc*, *ct*, and *cc*.

Table S2 Differences of Thermochemicals (T = 298.15 K and p = 1.00 atm) for the reaction intermediates A and B tautomers formation in different solvents (kJ/mol).

Compd	Δ / (kJ/mol)									
	E	ZPE	*E+ZPE*	*H*	*G*	*E*	ZPE	*E+ZPE*	*H*	*G*
Toluene						DMF				
A2(cc)	30.6	0.2	28.7	28.3	34.6	A2(cc)	18.1	2.6	17.8	16.9
A2(ct)	33.2	0.0	31.2	32.0	30.9	A2(ct)	25.1	0.0	22.2	23.1
A2(tc)	28.7	2.2	28.9	28.4	35.4	A2(tc)	34.0	2.8	34.0	33.4
A2(tt)	20.4	0.8	19.1	19.6	19.6	A2(tt)	11.0	3.6	11.7	10.8
B2(cc)	0.0	2.0	0.0	0.0	3.2	B2(cc)	0.0	2.9	0.0	0.0
B2(ct)	21.5	0.9	20.4	21.0	19.2	B2(ct)	21.8	1.5	20.4	21.0
B2(tc)	19.0	1.4	18.4	18.1	21.3	B2(tc)	23.0	3.4	23.5	22.7
B2(tt)	4.3	0.3	2.7	3.7	0.0	B2(tt)	1.7	1.6	0.5	1.3
MeCN						$CHCl_3$				
A2(cc)	18.6	2.3	18.8	17.5	28.2	A2(cc)	25.7	0.8	24.9	24.1
A2(ct)	24.2	0.0	22.2	22.5	24.2	A2(ct)	29.6	0.0	28.0	28.5
A2(tc)	34.0	2.5	34.4	33.4	43.3	A2(tc)	30.8	2.1	31.3	30.6
A2(tt)	11.3	3.3	12.5	11.4	20.4	A2(tt)	16.8	1.5	16.6	16.3
B2(cc)	0.0	2.4	0.3	0.0	5.1	B2(cc)	0.0	1.6	0.0	0.0
B2(ct)	20.8	1.2	19.9	20.1	22.0	B2(ct)	21.0	0.9	20.3	20.6
B2(tc)	22.7	3.1	23.8	22.5	32.3	B2(tc)	20.5	1.8	20.7	20.0
B2(tt)	1.0	1.0	0.0	0.4	0.0	B2(tt)	2.2	1.0	1.6	2.1
EtOH										
A2(cc)	18.5	2.2	17.7	17.1	25.0					
A2(ct)	26.8	0.0	23.7	25.0	21.7					
A2(tc)	34.5	2.9	34.4	33.9	42.1					
A2(tt)	11.5	3.1	11.5	11.0	18.9					
B2(cc)	0.0	3.0	0.0	0.0	4.9					
B2(ct)	22.3	1.5	20.8	21.6	20.8					
B2(tc)	22.7	4.0	23.7	22.7	30.9					
B2(tt)	1.7	1.5	0.2	1.0	0.0					
A2(cc)	18.5	2.2	17.7	17.1	25.0					

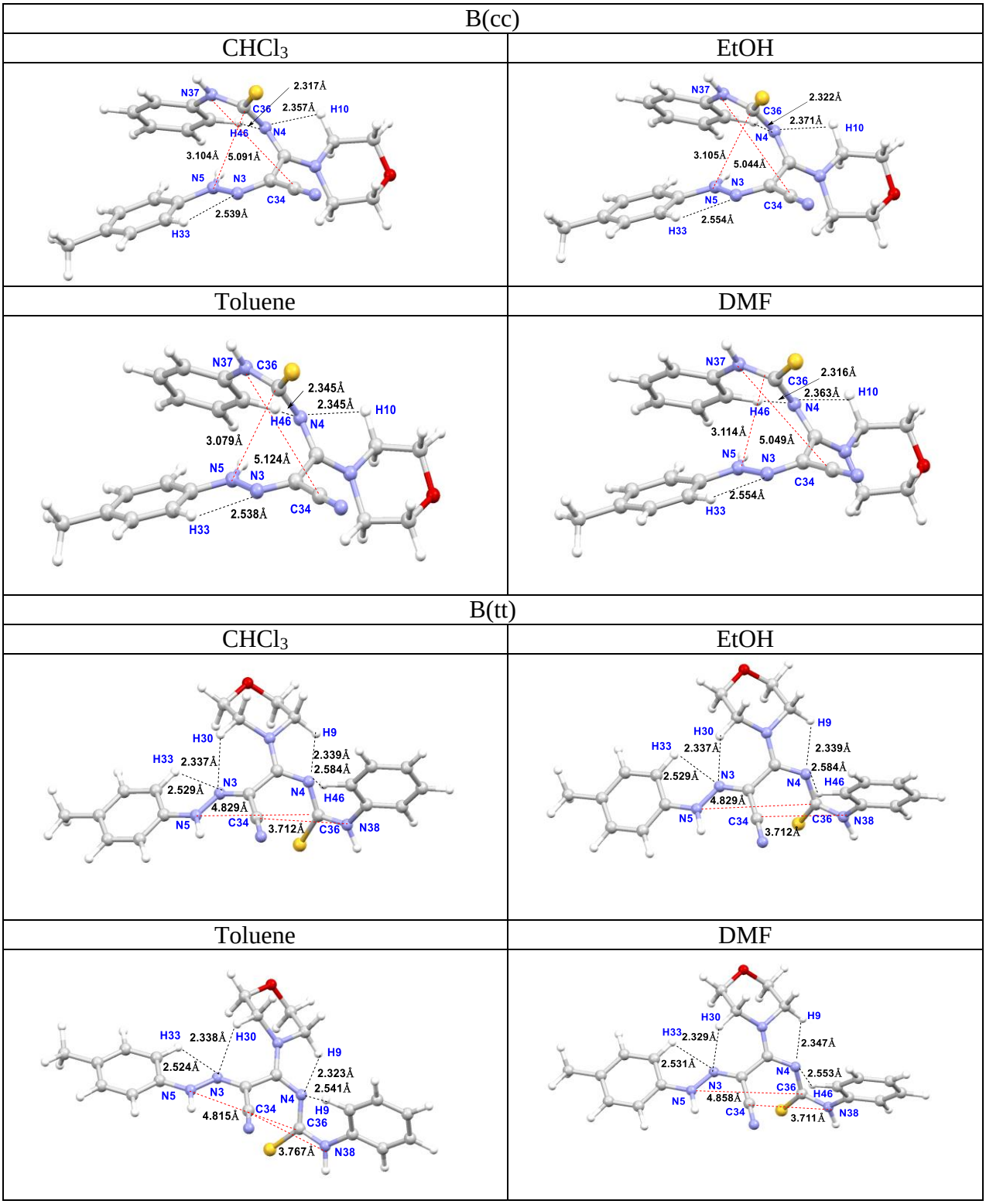


Fig. S36 Distances between the nucleophilic and electrophilic centers in the optimized structures of stable isomers of intermediate B, B(*cc*) and B(*tt*), in different solvents, and intramolecular hydrogen bonds.

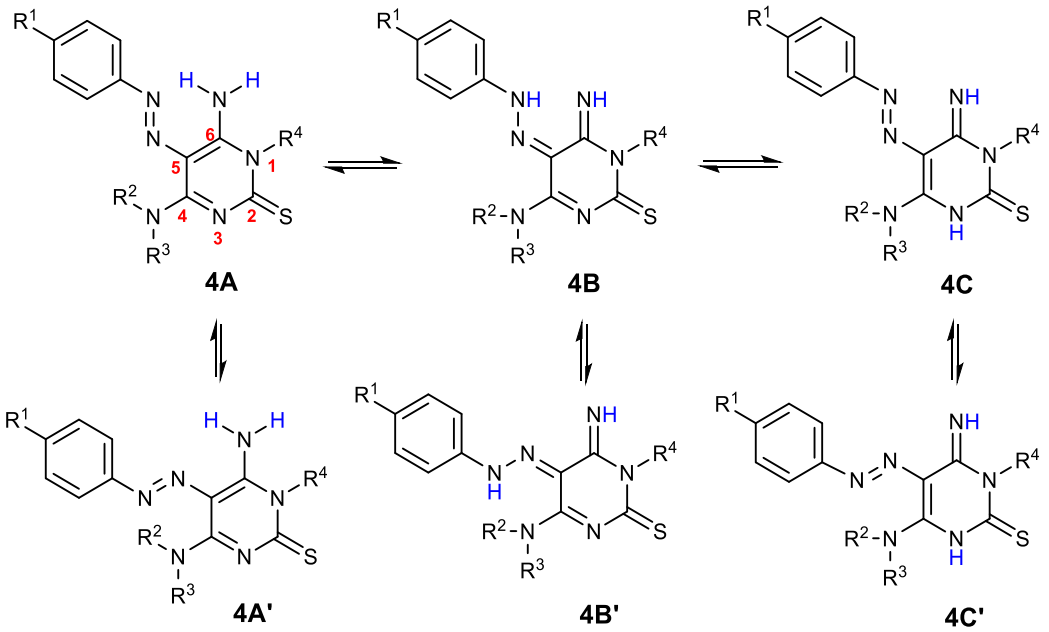
Table S3 Charges (*q*) and electrostatic potential (*EP*) of the intermediate B active centers for stable isomers B(*cc*) and B(*tt*) optimized structures in different solvents.

Entry	Isomer	Solvent	N37/N38		C34		N5		C36	
			q, e	*EP*, a.u.	*q*, e	*EP*, a.u.	*q*, e	*EP*, a.u.	*q*, e	*EP*, a.u.
1	B(*cc*)	$CHCl_3$	-0.502	-18.330	0.291	-14.744	-0.043	-18.285	0.414	-14.646
2		EtOH	-0.537	-18.329	0.289	-14.746	-0.022	-18.281	0.432	-14.647
3		Toluene	-0.429	-18.340	0.391	-14.728	-0.238	-18.271	0.617	-14.652
4		DMF	-0.499	-18.341	0.404	-14.730	-0.186	-18.256	0.658	-14.659
5	B(*tt*)	$CHCl_3$	-0.636	-18.356	0.438	-14.726	-0.152	-18.272	0.664	-14.666
6		EtOH	-0.646	-18.359	0.460	-14.723	-0.114	-18.265	0.460	-14.723
7		Toluene	-0.588	-18.352	0.428	-14.727	-0.155	-18.277	0.614	-14.661
8		DMF	-0.683	-18.361	0.448	-14.723	-0.147	-18.265	0.711	-14.673

Table S4 Thermochemical analysis (T = 298.15 K and p = 1.00 atm) of the cyclization of stable isomers of intermediate B, B(*cc*) and B(*tt*)[a].

Entry	Interme-diate	Solvent	T, K	Reaction I				Reaction II			
				ΔE	$\Delta(ZPE+E)$	ΔH	ΔG	ΔE	$\Delta(ZPE+E)$	ΔH	ΔG
1		Toluene	298	65.2	39.2	43.0	-4.9	-63.4	-61.1	-66.1	-53.1
2		DMF	298	71.7	45.6	49.3	1.3	-58.4	-56.0	-58.8	-53.0
3		MeCN	298	72.2	45.6	49.4	-0.1	-57.7	-55.3	-58.1	-51.2
4	B(*cc*)	EtOH	298	-55.3	-53.1	-55.7	-50.2	76.7	50.4	54.2	5.5
5		EtOH	351	-55.3	-53.1	-56.1	-49.2	76.7	50.4	54.0	-3.1
6		$CHCl_3$	298	-60.5	-57.7	-60.6	-54.5	69.8	42.8	46.9	-4.5
7		$CHCl_3$	334	-60.5	-57.7	-60.9	-53.7	69.8	42.8	46.8	-10.6
8		Toluene	298	60.9	36.6	39.3	-1.7	-67.8	-63.7	-69.8	-49.9
9		DMF	298	69.9	45.1	48.0	5.5	-60.1	-56.5	-60.1	-48.8
10		MeCN	298	71.2	45.9	49.0	5.0	-58.7	-54.9	-58.6	-46.2
11	B (*tt*)	EtOH	298	-57.0	-53.2	-56.7	-45.3	74.9	50.2	53.2	10.4
12		EtOH	351	-57.0	-53.2	-57.2	-43.3	74.9	50.2	52.9	2.9
13		$CHCl_3$	298	-62.7	-59.3	-62.7	-53.7	67.5	41.2	44.8	-3.7
14		$CHCl_3$	334	-62.7	-59.3	-63.0	-52.5	67.5	41.2	44.7	-9.5

[a]Values are reported in units of (kJ/mol).



Scheme S1 Putative tautomeric/rotameric forms of compounds **4**.

Table S5 Intermediate B stable isomers Charge in different solvents.

ESP Charges, *e*												
B(tt)												
TOLUENE			DMF			$CHCl_3$			EtOH			
1	O	-0.512211	1	O	-0.559697	1	O	-0.550960	1	O	-0.583049
2	N	-0.219675	2	N	-0.127867	2	N	-0.166609	2	N	-0.168101
3	N	-0.203560	3	N	-0.260828	3	N	-0.208837	3	N	-0.265759
4	N	-0.565714	4	N	-0.645830	4	N	-0.623335	4	N	-0.659111
5	N	-0.155579	5	N	-0.146928	5	N	-0.152199	5	N	-0.114295
6	C	0.447114	6	C	0.415629	6	C	0.443874	6	C	0.458041
7	C	0.015086	7	C	0.079649	7	C	0.030862	7	C	0.045693
8	C	0.006050	8	C	-0.043140	8	C	-0.048162	8	C	-0.055115
9	H	0.031114	9	H	0.049922	9	H	0.054644	9	H	0.059475
10	H	0.071040	10	H	0.088961	10	H	0.087130	10	H	0.094497
11	C	-0.176196	11	C	-0.175452	11	C	-0.151928	11	C	-0.132197
12	H	0.143468	12	H	0.150780	12	H	0.137876	12	H	0.142167
13	C	0.179104	13	C	0.181406	13	C	0.183493	13	C	0.146533
14	C	-0.263776	14	C	-0.276202	14	C	-0.283636	14	C	-0.313136
15	H	0.161404	15	H	0.176971	15	H	0.173211	15	H	0.185867
16	C	-0.245067	16	C	-0.270376	16	C	-0.255493	16	C	-0.228184
17	H	0.159100	17	H	0.177305	17	H	0.169546	17	H	0.167102
18	C	0.187018	18	C	0.276046	18	C	0.260147	18	C	0.249748
19	H	0.062239	19	H	0.051216	19	H	0.052360	19	H	0.065431
20	H	0.063256	20	H	0.056488	20	H	0.055345	20	H	0.062804
21	C	-0.133184	21	C	-0.275147	21	C	-0.230774	21	C	-0.227436
22	H	0.133837	22	H	0.168510	22	H	0.158110	22	H	0.160749
23	H	0.072047	23	H	0.145338	23	H	0.109340	23	H	0.134471
24	C	-0.260321	24	C	-0.301004	24	C	-0.324175	24	C	-0.303948
25	H	0.077705	25	H	0.092900	25	H	0.099123	25	H	0.092836
26	H	0.089454	26	H	0.096592	26	H	0.103746	26	H	0.100126
27	H	0.073251	27	H	0.090810	27	H	0.091472	27	H	0.093386
28	C	0.311774	28	C	0.350627	28	C	0.342140	28	C	0.336364
29	H	0.029649	29	H	0.032105	29	H	0.031150	29	H	0.040648
30	H	-0.003439	30	H	-0.017856	30	H	-0.012163	30	H	-0.005329
31	C	0.213079	31	C	0.205627	31	C	0.205404	31	C	0.214190
32	C	-0.087522	32	C	-0.085022	32	C	-0.083886	32	C	-0.114413
33	H	0.080651	33	H	0.086976	33	H	0.076998	33	H	0.092034
34	C	0.427962	34	C	0.448053	34	C	0.437751	34	C	0.460092
35	N	-0.515101	35	N	-0.567343	35	N	-0.538458	35	N	-0.568882
36	C	0.613783	36	C	0.711168	36	C	0.664582	36	C	0.703434
37	S	-0.569967	37	S	-0.671898	37	S	-0.614107	37	S	-0.659039
38	N	-0.588033	38	N	-0.682733	38	N	-0.635788	38	N	-0.646598
39	H	0.287145	39	H	0.330349	39	H	0.306557	39	H	0.321709
40	C	0.473372	40	C	0.530911	40	C	0.512000	40	C	0.486339
41	C	-0.283308	41	C	-0.330469	41	C	-0.312393	41	C	-0.311657
42	C	-0.313982	42	C	-0.371140	42	C	-0.335936	42	C	-0.341977
43	C	-0.072187	43	C	-0.066422	43	C	-0.065297	43	C	-0.054955
44	H	0.165240	44	H	0.194602	44	H	0.179201	44	H	0.188701
45	C	-0.033904	45	C	-0.034969	45	C	-0.038325	45	C	-0.037003
46	H	0.172106	46	H	0.210494	46	H	0.189030	46	H	0.201567
47	C	-0.171924	47	C	-0.190568	47	C	-0.168460	47	C	-0.187444
48	H	0.111575	48	H	0.122226	48	H	0.113219	48	H	0.113837
49	H	0.100647	49	H	0.112723	49	H	0.104089	49	H	0.109847
50	H	0.119334	50	H	0.132853	50	H	0.119700	50	H	0.130377
51	H	0.296045	51	H	0.333656	51	H	0.308821	51	H	0.319567
B(cc)												
1	O	-0.531300	1	O	-0.418467	1	O	-0.531300	1	O	-0.567022
2	N	-0.142908	2	N	-0.363419	2	N	-0.142908	2	N	-0.118372
3	N	-0.337428	3	N	-0.173326	3	N	-0.337428	3	N	-0.354634
4	N	-0.312667	4	N	-0.793549	4	N	-0.312667	4	N	-0.314756
5	N	-0.043170	5	N	-0.185806	5	N	-0.043170	5	N	-0.022047
6	C	0.214987	6	C	0.593160	6	C	0.214987	6	C	0.193078
7	C	0.281820	7	C	0.027079	7	C	0.281820	7	C	0.300793
8	C	-0.096643	8	C	0.227830	8	C	-0.096643	8	C	-0.079874
9	H	0.055437	9	H	0.012695	9	H	0.055437	9	H	0.050908

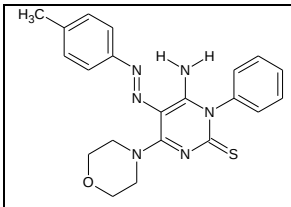
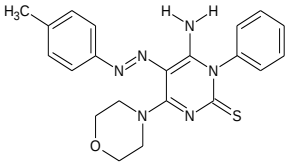
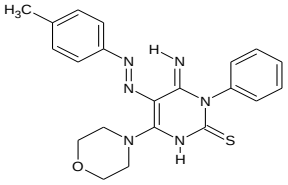
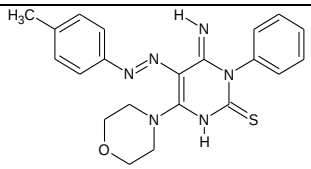
10	H	0.126817	10	H	0.070074	10	H	0.126817	10	H	0.133490
11	C	-0.217081	11	C	-0.188299	11	C	-0.217081	11	C	-0.208280
12	H	0.141130	12	H	0.151295	12	H	0.141130	12	H	0.148966
13	C	0.223116	13	C	0.193998	13	C	0.223116	13	C	0.197945
14	C	-0.200798	14	C	-0.238548	14	C	-0.200798	14	C	-0.219931
15	H	0.130223	15	H	0.164610	15	H	0.130223	15	H	0.150442
16	C	-0.269425	16	C	-0.278401	16	C	-0.269425	16	C	-0.257426
17	H	0.168822	17	H	0.182913	17	H	0.168822	17	H	0.172465
18	C	0.226210	18	C	0.179588	18	C	0.226210	18	C	0.228017
19	H	0.040993	19	H	0.055989	19	H	0.040993	19	H	0.047385
20	H	0.058775	20	H	0.065283	20	H	0.058775	20	H	0.063083
21	C	0.011996	21	C	-0.263362	21	C	0.011996	21	C	-0.016070
22	H	0.080988	22	H	0.201038	22	H	0.080988	22	H	0.096854
23	H	0.031421	23	H	0.161305	23	H	0.031421	23	H	0.051114
24	C	-0.346514	24	C	-0.318708	24	C	-0.346514	24	C	-0.323765
25	H	0.108043	25	H	0.098295	25	H	0.108043	25	H	0.104818
26	H	0.102815	26	H	0.097823	26	H	0.102815	26	H	0.097829
27	H	0.097032	27	H	0.095028	27	H	0.097032	27	H	0.094136
28	C	0.252943	28	C	-0.105921	28	C	0.252943	28	C	0.244111
29	H	0.059696	29	H	0.108454	29	H	0.059696	29	H	0.068278
30	H	0.021574	30	H	0.132424	30	H	0.021574	30	H	0.026303
31	C	0.138217	31	C	0.159934	31	C	0.138217	31	C	0.117921
32	C	-0.082145	32	C	-0.066094	32	C	-0.082145	32	C	-0.093810
33	H	0.103050	33	H	0.071904	33	H	0.103050	33	H	0.102307
34	C	0.291330	34	C	0.404563	34	C	0.291330	34	C	0.289142
35	N	-0.497460	35	N	-0.544411	35	N	-0.497460	35	N	-0.519070
36	C	0.413633	36	C	0.658321	36	C	0.413633	36	C	0.431911
37	N	-0.501927	37	N	-0.499518	37	N	-0.501927	37	N	-0.537512
38	H	0.297211	38	H	0.373564	38	H	0.297211	38	H	0.322100
39	S	-0.536964	39	S	-0.582472	39	S	-0.536964	39	S	-0.583542
40	C	0.370608	40	C	0.234936	40	C	0.370608	40	C	0.387632
41	C	-0.275309	41	C	-0.180470	41	C	-0.275309	41	C	-0.285117
42	C	-0.182205	42	C	-0.191576	42	C	-0.182205	42	C	-0.216188
43	C	-0.038388	43	C	-0.127597	43	C	-0.038388	43	C	-0.038644
44	H	0.158972	44	H	0.142521	44	H	0.158972	44	H	0.163887
45	C	-0.118068	45	C	-0.123087	45	C	-0.118068	45	C	-0.106427
46	H	0.095783	46	H	0.157269	46	H	0.095783	46	H	0.113389
47	C	-0.133072	47	C	-0.109908	47	C	-0.133072	47	C	-0.147943
48	H	0.107298	48	H	0.130393	48	H	0.107298	48	H	0.108811
49	H	0.124944	49	H	0.126458	49	H	0.124944	49	H	0.129984
50	H	0.113762	50	H	0.115636	50	H	0.113762	50	H	0.122236
51	H	0.213825	51	H	0.358561	51	H	0.213825	51	H	0.251097

Table S6 Intermediate B stable isomers Electrostatic Potential in different solvents

EP (a.u.)							
B(tt)							
TOLUENE		DMF		$CHCl_3$		EtOH	
1 Atom	-22.338908	1 Atom	-22.337406	1 Atom	-22.339839	1 Atom	-22.345717
2 Atom	-18.317770	2 Atom	-18.310068	2 Atom	-18.315004	2 Atom	-18.313696
3 Atom	-18.298710	3 Atom	-18.291507	3 Atom	-18.295331	3 Atom	-18.292135
4 Atom	-18.401119	4 Atom	-18.409874	4 Atom	-18.405389	4 Atom	-18.408365
5 Atom	-18.277241	5 Atom	-18.265386	5 Atom	-18.271898	5 Atom	-18.265949
6 Atom	-14.643157	6 Atom	-14.642354	6 Atom	-14.643297	6 Atom	-14.643489
7 Atom	-14.673553	7 Atom	-14.671486	7 Atom	-14.672967	7 Atom	-14.671723
8 Atom	-14.713975	8 Atom	-14.710869	8 Atom	-14.712573	8 Atom	-14.712457
9 Atom	-1.086700	9 Atom	-1.088136	9 Atom	-1.086878	9 Atom	-1.088238
10 Atom	-1.086186	10 Atom	-1.078286	10 Atom	-1.082786	10 Atom	-1.081423
11 Atom	-14.752165	11 Atom	-14.751738	11 Atom	-14.751622	11 Atom	-14.751597
12 Atom	-1.083781	12 Atom	-1.076822	12 Atom	-1.080473	12 Atom	-1.077077
13 Atom	-14.746419	13 Atom	-14.746107	13 Atom	-14.745737	13 Atom	-14.745881
14 Atom	-14.745256	14 Atom	-14.741256	14 Atom	-14.743348	14 Atom	-14.741447
15 Atom	-1.067533	15 Atom	-1.053997	15 Atom	-1.061557	15 Atom	-1.054833
16 Atom	-14.752807	16 Atom	-14.752389	16 Atom	-14.752038	16 Atom	-14.752196
17 Atom	-1.084450	17 Atom	-1.077351	17 Atom	-1.080671	17 Atom	-1.077403
18 Atom	-14.696040	18 Atom	-14.689586	18 Atom	-14.693830	18 Atom	-14.692501
19 Atom	-1.091698	19 Atom	-1.082890	19 Atom	-1.087247	19 Atom	-1.082159
20 Atom	-1.085905	20 Atom	-1.075844	20 Atom	-1.081649	20 Atom	-1.077326
21 Atom	-14.702235	21 Atom	-14.692342	21 Atom	-14.698439	21 Atom	-14.694226
22 Atom	-1.078281	22 Atom	-1.064840	22 Atom	-1.072854	22 Atom	-1.067648
23 Atom	-1.068604	23 Atom	-1.053051	23 Atom	-1.062355	23 Atom	-1.054007
24 Atom	-14.759483	24 Atom	-14.758012	24 Atom	-14.758436	24 Atom	-14.757919
25 Atom	-1.099900	25 Atom	-1.095450	25 Atom	-1.097804	25 Atom	-1.095432
26 Atom	-1.098663	26 Atom	-1.095581	26 Atom	-1.096866	26 Atom	-1.095481
27 Atom	-1.098846	27 Atom	-1.094157	27 Atom	-1.096144	27 Atom	-1.094376
28 Atom	-14.700596	28 Atom	-14.698370	28 Atom	-14.699993	28 Atom	-14.701138
29 Atom	-1.091327	29 Atom	-1.087286	29 Atom	-1.089430	29 Atom	-1.088479
30 Atom	-1.097745	30 Atom	-1.095997	30 Atom	-1.096532	30 Atom	-1.095068
31 Atom	-14.698973	31 Atom	-14.695644	31 Atom	-14.697177	31 Atom	-14.695747
32 Atom	-14.750416	32 Atom	-14.748378	32 Atom	-14.748869	32 Atom	-14.748087
33 Atom	-1.079577	33 Atom	-1.069700	33 Atom	-1.074169	33 Atom	-1.069302
34 Atom	-14.726964	34 Atom	-14.723406	34 Atom	-14.725736	34 Atom	-14.722778
35 Atom	-18.396647	35 Atom	-18.407051	35 Atom	-18.401578	35 Atom	-18.405685
36 Atom	-14.661277	36 Atom	-14.672730	36 Atom	-14.666443	36 Atom	-14.670851
37 Atom	-59.330744	37 Atom	-59.349164	37 Atom	-59.339061	37 Atom	-59.346413
38 Atom	-18.352403	38 Atom	-18.361497	38 Atom	-18.356463	38 Atom	-18.358766
39 Atom	-1.010818	39 Atom	-1.010913	39 Atom	-1.010606	39 Atom	-1.008589
40 Atom	-14.721290	40 Atom	-14.731529	40 Atom	-14.725936	40 Atom	-14.729744
41 Atom	-14.765136	41 Atom	-14.770252	41 Atom	-14.767190	41 Atom	-14.768867
42 Atom	-14.770579	42 Atom	-14.780294	42 Atom	-14.774450	42 Atom	-14.778245
43 Atom	-14.765393	43 Atom	-14.769885	43 Atom	-14.767123	43 Atom	-14.768683
44 Atom	-1.089262	44 Atom	-1.084981	44 Atom	-1.087507	44 Atom	-1.084178
45 Atom	-14.767526	45 Atom	-14.773520	45 Atom	-14.769963	45 Atom	-14.772059
46 Atom	-1.103251	46 Atom	-1.105580	46 Atom	-1.104368	46 Atom	-1.103416
47 Atom	-14.769910	47 Atom	-14.774522	47 Atom	-14.771488	47 Atom	-14.773164
48 Atom	-1.096710	48 Atom	-1.093103	48 Atom	-1.094881	48 Atom	-1.092402
49 Atom	-1.099296	49 Atom	-1.096436	49 Atom	-1.097979	49 Atom	-1.095414
50 Atom	-1.099645	50 Atom	-1.096232	50 Atom	-1.097869	50 Atom	-1.095420
51 Atom	-0.959168	51 Atom	-0.938356	51 Atom	-0.950339	51 Atom	-0.939302
B(cc)							
1 Atom	-22.350757	1 Atom	-22.351802	1 Atom	-22.337811	1 Atom	-22.342451
2 Atom	-18.326319	2 Atom	-18.321694	2 Atom	-18.299545	2 Atom	-18.292887
3 Atom	-18.292459	3 Atom	-18.282445	3 Atom	-18.308757	3 Atom	-18.308488
4 Atom	-18.399840	4 Atom	-18.409024	4 Atom	-18.381493	4 Atom	-18.378832
5 Atom	-18.271176	5 Atom	-18.256668	5 Atom	-18.285337	5 Atom	-18.280899
6 Atom	-14.645190	6 Atom	-14.645801	6 Atom	-14.628719	6 Atom	-14.624168
7 Atom	-14.673453	7 Atom	-14.672709	7 Atom	-14.677580	7 Atom	-14.676887
8 Atom	-14.714829	8 Atom	-14.709617	8 Atom	-14.698323	8 Atom	-14.692834
9 Atom	-1.083254	9 Atom	-1.074989	9 Atom	-1.069694	9 Atom	-1.064852
10 Atom	-1.089515	10 Atom	-1.076717	10 Atom	-1.066288	10 Atom	-1.056844
11 Atom	-14.747684	11 Atom	-14.746299	11 Atom	-14.758362	11 Atom	-14.757401
12 Atom	-1.079613	12 Atom	-1.072095	12 Atom	-1.085136	12 Atom	-1.079977
13 Atom	-14.742154	13 Atom	-14.741010	13 Atom	-14.752499	13 Atom	-14.752565
14 Atom	-14.740258	14 Atom	-14.734719	14 Atom	-14.753721	14 Atom	-14.750915
15 Atom	-1.062620	15 Atom	-1.047824	15 Atom	-1.075555	15 Atom	-1.066513
16 Atom	-14.748549	16 Atom	-14.746967	16 Atom	-14.762320	16 Atom	-14.763764
17 Atom	-1.080497	17 Atom	-1.072478	17 Atom	-1.091121	17 Atom	-1.089454
18 Atom	-14.708109	18 Atom	-14.705938	18 Atom	-14.696551	18 Atom	-14.695519
19 Atom	-1.106564	19 Atom	-1.108105	19 Atom	-1.097918	19 Atom	-1.096700

20 Atom -1.095843	20 Atom -1.089105	20 Atom -1.085483	20 Atom -1.082445
21 Atom -14.710438	21 Atom -14.703632	21 Atom -14.691965	21 Atom -14.685917
22 Atom -1.089220	22 Atom -1.074906	22 Atom -1.062966	22 Atom -1.053403
23 Atom -1.076574	23 Atom -1.065277	23 Atom -1.058890	23 Atom -1.051348
24 Atom -14.755913	24 Atom -14.753806	24 Atom -14.762374	24 Atom -14.761412
25 Atom -1.096607	25 Atom -1.091786	25 Atom -1.100430	25 Atom -1.097319
26 Atom -1.095090	26 Atom -1.090584	26 Atom -1.100520	26 Atom -1.098682
27 Atom -1.095348	27 Atom -1.090909	27 Atom -1.100501	27 Atom -1.098353
28 Atom -14.716496	28 Atom -14.716859	28 Atom -14.694162	28 Atom -14.693215
29 Atom -1.103849	29 Atom -1.100700	29 Atom -1.082929	29 Atom -1.079792
30 Atom -1.119731	30 Atom -1.127074	30 Atom -1.093009	30 Atom -1.091513
31 Atom -14.693472	31 Atom -14.687934	31 Atom -14.709578	31 Atom -14.708789
32 Atom -14.745521	32 Atom -14.741654	32 Atom -14.762881	32 Atom -14.765102
33 Atom -1.075274	33 Atom -1.063781	33 Atom -1.095270	33 Atom -1.097097
34 Atom -14.727925	34 Atom -14.729705	34 Atom -14.743793	34 Atom -14.745845
35 Atom -18.398503	35 Atom -18.413507	35 Atom -18.423078	35 Atom -18.431769
36 Atom -14.651811	36 Atom -14.659511	36 Atom -14.646441	36 Atom -14.647901
37 Atom -18.340548	37 Atom -18.341171	37 Atom -18.330243	37 Atom -18.328852
38 Atom -0.994106	38 Atom -0.979078	38 Atom -0.990654	38 Atom -0.987217
39 Atom -59.321187	39 Atom -59.340084	39 Atom -59.327079	39 Atom -59.336598
40 Atom -14.718913	40 Atom -14.725344	40 Atom -14.693186	40 Atom -14.691488
41 Atom -14.774668	41 Atom -14.784516	41 Atom -14.742913	41 Atom -14.742280
42 Atom -14.761452	42 Atom -14.760352	42 Atom -14.745120	42 Atom -14.740043
43 Atom -14.770840	43 Atom -14.778685	43 Atom -14.743294	43 Atom -14.742675
44 Atom -1.112351	44 Atom -1.119449	44 Atom -1.066734	44 Atom -1.063526
45 Atom -14.764443	45 Atom -14.765813	45 Atom -14.741559	45 Atom -14.737081
46 Atom -1.083182	46 Atom -1.070240	46 Atom -1.078663	46 Atom -1.071453
47 Atom -14.770401	47 Atom -14.774056	47 Atom -14.747448	47 Atom -14.744596
48 Atom -1.104166	48 Atom -1.104648	48 Atom -1.075437	48 Atom -1.072578
49 Atom -1.095068	49 Atom -1.088228	49 Atom -1.074191	49 Atom -1.066802
50 Atom -1.100641	50 Atom -1.096991	50 Atom -1.076973	50 Atom -1.071858
51 Atom -0.953407	51 Atom -0.931028	51 Atom -0.962193	51 Atom -0.949069

Tautomeric/rotameric forms of 5-(arylazo)pyrimidine-2(1*H*)-thione **4a**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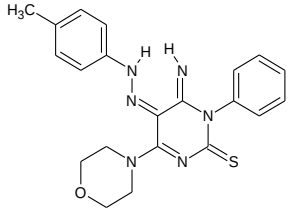	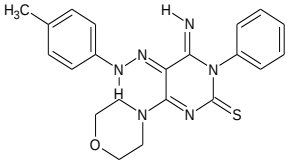		
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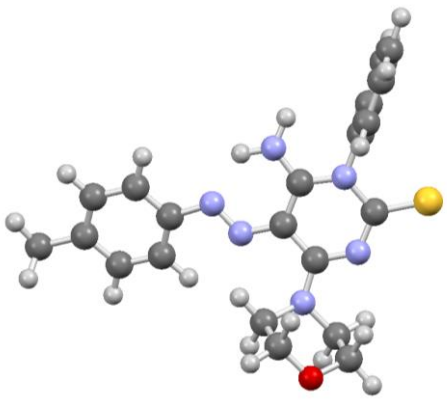
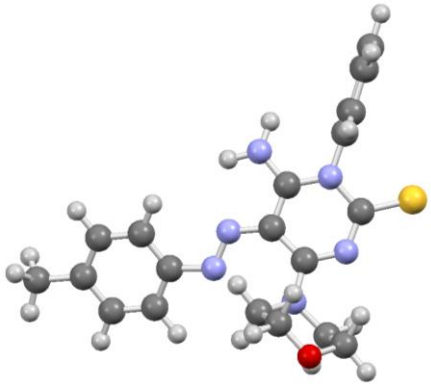


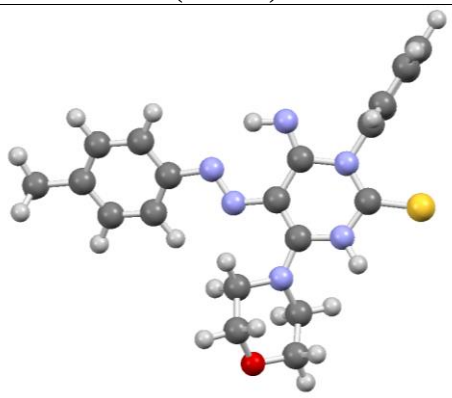
4A

Δ*E* / (kJ / mol) = 0.0
Δ(*E* + ZPE) / (kJ / mol) = 0.0
Δ*H* / (kJ / mol) = 0.0
Δ*G* / (kJ / mol) = 0.0



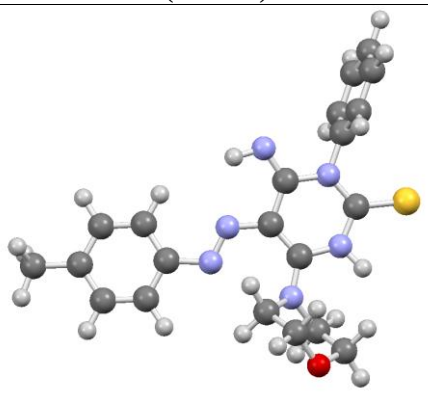
4A'

Δ*E* / (kJ / mol) = 17.0
Δ(*E* + ZPE) / (kJ / mol) = 16.9
Δ*H* / (kJ / mol) = 19.9
Δ*G* / (kJ / mol) = 7.7



4B

Δ*E* / (kJ / mol) = 47.2
Δ(*E* + ZPE) / (kJ / mol) = 48.2
Δ*H* / (kJ / mol) = 51.1
Δ*G* / (kJ / mol) = 39.0



4B',

Δ*E* / (kJ / mol) = 61.0
Δ(*E* + ZPE) / (kJ / mol) = 61.6
Δ*H* / (kJ / mol) = 62.12
Δ*G* / (kJ / mol) = 58.2

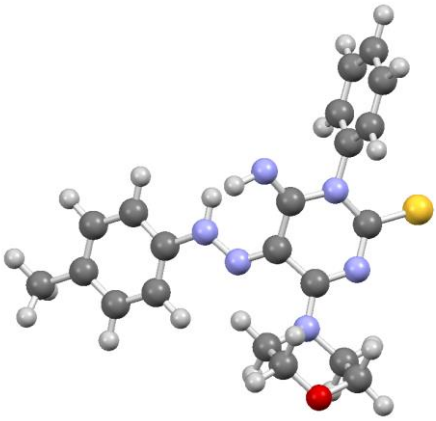
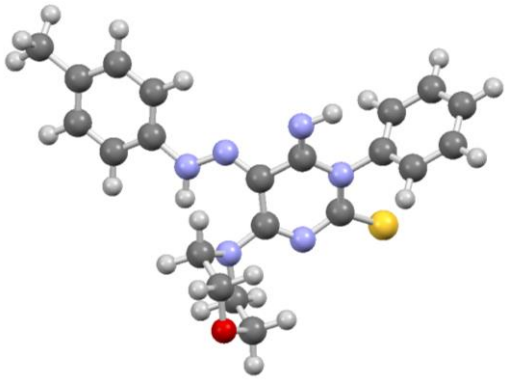
	
4C	**4C'**
ΔE / (kJ / mol) = 60.3 $\Delta(E$ + ZPE) / (kJ / mol) = 61.9 ΔH / (kJ / mol) = 64.6 ΔG / (kJ / mol) = 53.9	ΔE / (kJ / mol) = 55.5 $\Delta(E$ + ZPE) / (kJ / mol) = 57.6 ΔH / (kJ / mol) = 57.3 ΔG / (kJ / mol) = 57.9

Fig. S37 Tautomer study. Relative electronic energy (ΔE) also with zero point energy ($\Delta(E+ZPE)$), Gibbs free energy (ΔG), enthalpy (ΔH), computed at 298.15 K and 1.00 atm, for ground state of possible 5-(arylazo)pyrimidine-2(1*H*)-thione **4a** tautomer/rotamers in $CDCl_3$. Level of theory: DFT M06-2X (SMD) / aug-cc-pVTZ.

Stability of the different 5-(arylazo)pyrimidine-2(1*H*)-thione **4a** isomers of **A, B** and **C** in different solvents. These data refer to T = 298.15 K and p = 1.00 atm. All differences are in units of kJ/mol.

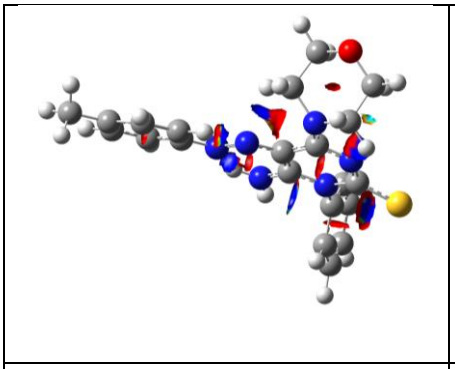
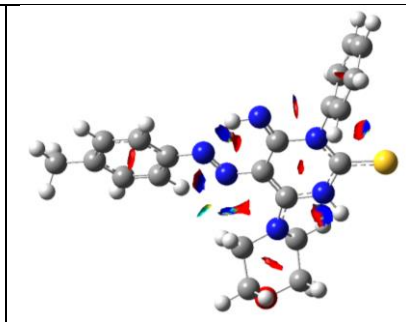
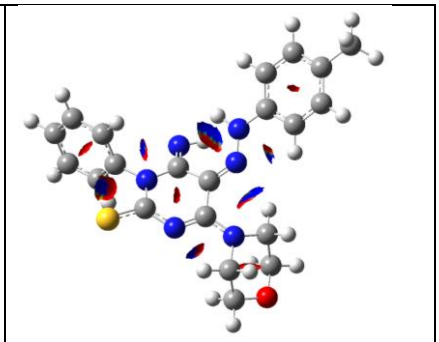
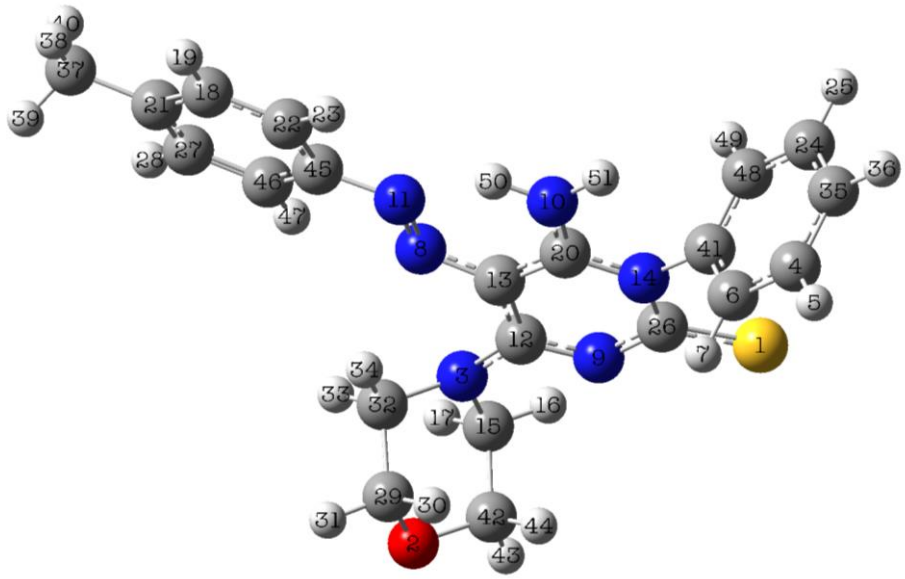
		
4a-A	**4a-B**	**4a-C**

Fig. S38 Color scaling of weak interactions in molecule of 5-(arylazo)pyrimidine-2(1*H*)-thione **4a**. The surfaces are colored on a blue-green-red scale. Blue indicates strong attractive interactions and red indicates strong non-bonded overlap putative tautomer forms of compound **4a**.

Table S7 Illustrates the calculated vs. experimental chemical shifts in of the protons of compound **4a** in ^{1}H NMR spectrum the most stable tautomers/rotamers A and A'.



		mPW1LYP/6-311+G(2d,p)				WP04/DGTZVP			
	Exp	A	A'	B	C	A	A'	B	C
5	7.63	7.358	7.3671	7.272	7.232	7.470	7.4596	7.349	7.344
7	7.35	7.020	7.0345	7.040	6.951	7.127	7.1525	7.166	7.065
16	3.82-3.94	4.892	4.6691	3.344	4.834	5.036	4.8066	3.543	4.959
17	3.82-3.94	3.115	3.0196	3.468	3.085	3.112	3.0250	3.461	3.056
19	7.26	7.011	7.0931	7.055	6.947	7.130	7.1891	7.158	7.063
23	7.46	7.271	7.5156	7.483	6.543	7.333	7.5470	7.536	6.647
25	7.63	7.325	7.3482	7.247	7.243	7.417	7.4544	7.339	7.353
28	7.26	7.059	7.0116	7.035	7.055	7.161	7.1333	7.158	7.176
30	4.14-4.32	3.355	3.2250	3.384	3.393	3.393	3.2779	3.420	3.418
31	4.14-4.32	3.387	3.4205	3.494	3.554	3.531	3.5645	3.662	3.697
33	3.82-3.94	3.686	3.3544	3.745	3.686	3.765	3.4298	3.837	3.724
34	3.82-3.94	4.029	2.6401	3.255	3.824	4.227	2.6877	3.454	3.989
36	7.56	7.323	7.3388	7.221	7.212	7.421	7.4493	7.299	7.312
38	2.42	2.029	2.0775	2.042	2.091	2.064	2.1070	2.075	2.144
39	2.42	2.381	2.3345	2.360	2.187	2.511	2.4465	2.480	2.275
40	2.42	2.384	2.3983	2.391	2.333	2.525	2.5303	2.521	2.466
43	4.14-4.32	3.627	3.5996	3.660	3.684	3.763	3.7329	3.833	3.822
44	4.14-4.32	3.588	3.5125	3.614	3.525	3.609	3.5550	3.678	3.542
47	7.46	7.417	7.1473	7.369	7.296	7.590	7.2942	7.541	7.466
49	7.35	7.047	7.1204	6.918	6.942	7.177	7.2518	7.020	7.044
50	11.84	10.991	6.5208	9.959	7.190	11.311	6.6496	9.940	6.934
51	5.13	4.370	3.9050	7.593	8.659	4.419	3.8712	7.842	8.756

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6. The Coordinates of compounds optimized at B3LYP/6-31G**level

Ground state
3,3-diamino-2-(phenylazo)acrylonitrile
1a/c (MeCN)
37

8	3.84464762	-2.53373996	0.71322235
7	2.42157417	-0.34945738	-0.38515858
7	-0.16621057	0.81226244	-0.13458268
7	3.20236059	1.76912974	-0.87566320
7	-1.24746185	1.36861034	0.18824495
6	2.21847368	0.97302339	-0.43194168
6	0.97174391	1.56104955	-0.05880019
6	3.48499164	-1.02790348	-1.13504616
1	3.96342566	-0.34492778	-1.83366022
1	3.00821360	-1.82851061	-1.70923316
6	-4.76758956	0.32617163	0.46326785
1	-5.68700669	0.74123540	0.86354868
6	-4.78655379	-0.93490676	-0.13364806
6	-3.58838635	1.05994510	0.55112098
1	-3.57939421	2.04093253	1.01418860
6	-3.58139641	-1.44229862	-0.63743117
1	-3.57553720	-2.42093737	-1.10803271
6	2.84146233	-1.87033416	1.46336002
1	3.29990383	-1.08314573	2.07739187
1	2.38664902	-2.61326904	2.11904731
6	1.76990770	-1.25272787	0.57146502
1	1.23669705	-2.02928531	0.01590683
1	1.06190771	-0.70702739	1.18716796
6	-6.06368705	-1.72120166	-0.26283610
1	-6.83036144	-1.33951553	0.41332336
1	-5.89897256	-2.77788956	-0.04128806
1	-6.45462455	-1.65866541	-1.28295375
6	4.49268184	-1.63669236	-0.17369750
1	5.23870105	-2.21005031	-0.72425677
1	4.99592197	-0.84423996	0.39682817
6	-2.39349942	0.54218408	0.05080662
6	-2.39875571	-0.72258352	-0.55297165
1	-1.47973527	-1.13133609	-0.95481406
1	4.16883064	1.47608536	-0.86026692
1	3.01530774	2.74040068	-1.08116380
6	0.92641140	2.93162244	0.30121963
7	0.87803299	4.04916618	0.59477127

1a/c (DMF)
37

8	3.84265036	-2.53911786	0.70660815
7	2.42445393	-0.34578562	-0.38279177
7	-0.16586490	0.81286163	-0.13380926
7	3.20281668	1.77405957	-0.86956833
7	-1.24778874	1.36886553	0.18750981

6	2.21919246	0.97612986	-0.42865389
6	0.97120584	1.56249863	-0.05683462
6	3.48817481	-1.02176916	-1.13418071
1	3.97015627	-0.33566945	-1.82730046
1	3.01131449	-1.81775184	-1.71485456
6	-4.76928370	0.32994368	0.45270704
1	-5.69051514	0.74876310	0.84489742
6	-4.78571220	-0.93603155	-0.13363612
6	-3.59030487	1.06381030	0.54079166
1	-3.58324726	2.04859360	0.99583261
6	-3.57828626	-1.44788550	-0.62708245
1	-3.57018709	-2.43057077	-1.08915832
6	2.83822111	-1.87874436	1.45704971
1	3.29558371	-1.09621583	2.07795590
1	2.37999377	-2.62464410	2.10713763
6	1.76952102	-1.25365765	0.56689876
1	1.23567195	-2.02572703	0.00562589
1	1.06147157	-0.71063945	1.18501773
6	-6.06222457	-1.72276909	-0.26281684
1	-6.83054411	-1.33947814	0.41064934
1	-5.89811064	-2.77886930	-0.03795004
1	-6.45152193	-1.66338501	-1.28382001
6	4.49227984	-1.63745946	-0.17371425
1	5.23955869	-2.20730974	-0.72614613
1	4.99544987	-0.84841641	0.40189394
6	-2.39314289	0.54178382	0.05053582
6	-2.39589266	-0.72797463	-0.54257208
1	-1.47513267	-1.14080090	-0.93624346
1	4.16968132	1.48240290	-0.85279831
1	3.01503028	2.74527974	-1.07453347
6	0.92409098	2.93293951	0.30347558
7	0.87454170	4.05035537	0.59710574

1a/c (Toluene)

37

8	3.72007230	-2.69857377	0.53160947
7	2.50044803	-0.28253548	-0.27579504
7	-0.15404976	0.80576461	-0.11014978
7	3.25725408	1.86422884	-0.66177279
7	-1.23835910	1.37244763	0.15515185
6	2.23751540	1.03882915	-0.30597303
6	0.97377420	1.59026138	-0.02387629
6	3.56464490	-0.90421090	-1.06947282
1	4.12600424	-0.14891052	-1.61541968
1	3.08932006	-1.57099749	-1.79819045
6	-4.74888417	0.33081961	0.46234437
1	-5.66531911	0.74580206	0.86867632
6	-4.77019986	-0.93249311	-0.12773281
6	-3.57188027	1.06726348	0.53326452
1	-3.55193324	2.05186053	0.98666789
6	-3.57161520	-1.44044923	-0.64439610
1	-3.57172565	-2.41915026	-1.11459787

6	2.72074985	-2.09203591	1.32960458
1	3.19155812	-1.44894833	2.08637628
1	2.18716396	-2.89706445	1.83553332
6	1.74267308	-1.26543691	0.50206038
1	1.17432841	-1.90805772	-0.17728718
1	1.04472606	-0.76066175	1.16334371
6	-6.04747540	-1.72154201	-0.23829779
1	-6.80374887	-1.34721892	0.45347114
1	-5.87880901	-2.77866481	-0.02214836
1	-6.45856740	-1.65501383	-1.25003829
6	4.47050437	-1.72690545	-0.16718457
1	5.21303933	-2.26108677	-0.76069790
1	4.98994953	-1.06999526	0.54603305
6	-2.38375049	0.54482848	0.02662131
6	-2.39025296	-0.71932995	-0.57399870
1	-1.47188519	-1.11958736	-0.98509292
1	4.19893878	1.62387114	-0.38910173
1	3.06210705	2.85377610	-0.71867118
6	0.88887102	2.98507023	0.25022149
7	0.87416785	4.12161221	0.45244589

1a/**c′** (MeCN)

37

8	3.53377604	-2.55799329	0.85018219
7	2.17292141	-0.40594842	-0.36318664
7	-0.27886853	1.39055416	0.11491339
7	3.06772545	1.53603633	-1.23322186
7	-0.66996860	0.27156232	-0.31395223
6	2.11533203	0.91292672	-0.52771447
6	1.04482907	1.71109512	0.02450938
6	3.04935519	-1.28820464	-1.14140789
1	3.48140123	-0.76083372	-1.98912449
1	2.42382511	-2.10038874	-1.52306690
6	-3.91986328	-1.42408713	-0.66543685
1	-4.28624633	-2.34671946	-1.10410444
6	-4.81573543	-0.56033520	-0.03565657
6	-2.56277142	-1.12132851	-0.73826375
1	-1.87069789	-1.79783581	-1.22895942
6	-4.30693735	0.61991091	0.52355736
1	-4.98745027	1.30343055	1.02300984
6	2.71028073	-1.69760950	1.61837744
1	3.31767475	-0.89050678	2.04961483
1	2.28791723	-2.29479835	2.42669545
6	1.58158904	-1.09490767	0.78688582
1	0.90818319	-1.87276689	0.42007888
1	1.02092441	-0.39333551	1.39874678
6	-6.28565966	-0.87465383	0.05152009
1	-6.51277788	-1.82840185	-0.42703158
1	-6.88050006	-0.09739512	-0.43569066
1	-6.61324589	-0.92790639	1.09322057
6	4.12657451	-1.86569040	-0.23556681
1	4.73310907	-2.58540047	-0.78506965
1	4.77283555	-1.06072008	0.13999049

6	-2.06810215	0.05967048	-0.18466557
6	-2.95773338	0.93291912	0.45772336
1	-2.58707912	1.84835067	0.90168358
1	2.94579198	2.50096027	-1.50599159
1	3.97626852	1.12192970	-1.38715196
6	1.34547289	3.04812943	0.38462636
7	1.60248646	4.13626345	0.68412810

1a/c′ (DMF)

37

8	3.52640280	-2.56636613	0.84440815
7	2.17474646	-0.40308199	-0.36133146
7	-0.27822552	1.39163687	0.11584081
7	3.07008032	1.53991504	-1.22821398
7	-0.66846811	0.27272950	-0.31399241
6	2.11676949	0.91580727	-0.52492870
6	1.04518286	1.71308541	0.02645801
6	3.05024779	-1.28438423	-1.14143850
1	3.48608291	-0.75459021	-1.98566295
1	2.42337681	-2.09272348	-1.52909831
6	-3.91662838	-1.42679411	-0.66111502
1	-4.28172006	-2.35166101	-1.09619022
6	-4.81376214	-0.56095379	-0.03625270
6	-2.55977944	-1.12345020	-0.73398819
1	-1.86702755	-1.80191602	-1.22104942
6	-4.30635204	0.62200869	0.51827699
1	-4.98774676	1.30757252	1.01376379
6	2.70535716	-1.70629681	1.61500640
1	3.31510599	-0.90408671	2.05219403
1	2.27906839	-2.30521961	2.42006720
6	1.58011980	-1.09432860	0.78559154
1	0.90226407	-1.86694347	0.41585134
1	1.02294697	-0.39255657	1.40056500
6	-6.28344638	-0.87537863	0.04989959
1	-6.50903088	-1.83362989	-0.42040346
1	-6.87768569	-0.10307977	-0.44600584
1	-6.61418951	-0.91938644	1.09105931
6	4.12320002	-1.86931271	-0.23572811
1	4.73019754	-2.58651283	-0.78811183
1	4.77055387	-1.06768390	0.14539068
6	-2.06642968	0.06017711	-0.18504208
6	-2.95739897	0.93558139	0.45248825
1	-2.58805565	1.85334467	0.89276894
1	2.94859166	2.50520361	-1.49987191
1	3.97943267	1.12675815	-1.37990472
6	1.34435126	3.05044674	0.38647954
7	1.60015608	4.13891412	0.68557290

1a/c′ (Toluene)

37

8	3.37537055	-2.69513267	0.75411254
7	2.17292180	-0.38237766	-0.31084130
7	-0.26354749	1.42810430	0.15167969
7	3.13931885	1.55017495	-1.12371837
7	-0.63860448	0.30673990	-0.26971079
6	2.13316080	0.94725509	-0.44935003
6	1.07149417	1.74920382	0.06172152
6	2.98295296	-1.26893183	-1.14827671
1	3.44868945	-0.71094820	-1.95843304
1	2.30438757	-2.00713308	-1.58760566
6	-3.86813500	-1.41084380	-0.66860325
1	-4.22225120	-2.33716064	-1.10903315
6	-4.77699134	-0.54952031	-0.05717291
6	-2.51306478	-1.09952194	-0.72068407
1	-1.80605492	-1.76803742	-1.19992188
6	-4.28621402	0.63764239	0.50224035
1	-4.98036053	1.31947371	0.98445630
6	2.62702531	-1.82422670	1.58250600
1	3.29816450	-1.09446108	2.05700872
1	2.17172413	-2.43946734	2.35873346
6	1.54096905	-1.08913000	0.80301345
1	0.79860742	-1.78649632	0.40896731
1	1.04134111	-0.37750035	1.45622751
6	-6.24604182	-0.87274665	0.01081038
1	-6.46382345	-1.82715798	-0.47064738
1	-6.84022493	-0.10039461	-0.48459246
1	-6.58745110	-0.93091545	1.04772408
6	4.01312409	-1.99097824	-0.29087557
1	4.55526481	-2.72497391	-0.88772068
1	4.73289797	-1.27127146	0.12639916
6	-2.03817555	0.08592704	-0.16412732
6	-2.93983154	0.95948387	0.45692283
1	-2.57454607	1.88006420	0.89424535
1	3.06951707	2.54088984	-1.30602498
1	4.07087235	1.16206223	-1.10907652
6	1.37381660	3.10777391	0.35146208
7	1.66644674	4.20395412	0.57100121

1a/t (MeCN)

37

8	-5.48478292	-0.46329933	0.96950840
7	-3.03511963	-0.09961455	-0.39376176
7	0.57235754	0.10419372	-0.23425601
7	-1.38883441	-1.63871793	-0.91310267
7	1.50329377	0.94766790	-0.17862519
6	-1.73707166	-0.39878151	-0.53661656
6	-0.70331838	0.57164191	-0.37066798
6	-4.11397335	-0.91727782	-0.95996127
1	-3.71037971	-1.69721065	-1.60207286
1	-4.73072156	-0.25177200	-1.57230894
6	5.15623754	0.84549853	0.25891395
1	5.96008383	1.56681041	0.36498709

6	5.45042229	-0.51752990	0.27600547
6	3.84723412	1.29464505	0.10694905
1	3.62453122	2.35623749	0.09285435
6	4.38811070	-1.42169391	0.13625337
1	4.59714962	-2.48744222	0.14390778
6	-4.43944035	0.29358081	1.55253846
1	-3.82746880	-0.35400575	2.19474685
1	-4.90406957	1.06636161	2.16532668
6	-3.54593608	0.94559746	0.50113856
1	-4.10908328	1.67649691	-0.08614858
1	-2.72781528	1.44694211	1.01140490
6	6.86082780	-1.01740627	0.44072846
1	7.56830268	-0.18849125	0.49151219
1	7.14683315	-1.66180686	-0.39467921
1	6.96026360	-1.60838723	1.35535601
6	-4.96601462	-1.50135494	0.15405438
1	-5.81696113	-2.03726617	-0.26643762
1	-4.36859966	-2.19295935	0.76366858
6	2.79807156	0.38593903	-0.02801230
6	3.07994558	-0.98754302	-0.01229028
1	2.27556018	-1.70515285	-0.11785661
1	-1.98390203	-2.42510856	-0.69237755
1	-0.40193697	-1.82625238	-1.03031538
6	-0.95602437	1.95715120	-0.51728355
7	-1.13568978	3.09141395	-0.64998772

1a/t (DMF)

37

8	-5.48677426	-0.47040462	0.96265953
7	-3.03407229	-0.09847090	-0.39476495
7	0.57272338	0.10855765	-0.23145754
7	-1.38506723	-1.63350449	-0.91619347
7	1.50405966	0.95147848	-0.17365360
6	-1.73561045	-0.39539422	-0.53642735
6	-0.70294543	0.57576513	-0.36589205
6	-4.11068282	-0.91592725	-0.96510654
1	-3.70531466	-1.69326497	-1.60929963
1	-4.72783127	-0.24951512	-1.57614449
6	5.15922099	0.84300916	0.24439235
1	5.96560648	1.56313298	0.33889802
6	5.44956852	-0.52055122	0.27304732
6	3.85071575	1.29462140	0.09596853
1	3.63136470	2.35679881	0.07316773
6	4.38373666	-1.42271784	0.14889916
1	4.58929401	-2.48905180	0.16675322
6	-4.44373691	0.28672323	1.54883488
1	-3.83130867	-0.36094349	2.19085187
1	-4.91011181	1.05706340	2.16342869
6	-3.54862521	0.94344269	0.50168161
1	-4.11082328	1.67559180	-0.08503673
1	-2.73267763	1.44436451	1.01593238
6	6.85921217	-1.02322902	0.43321330

1	7.56885541	-0.19603564	0.48263292
1	7.14175760	-1.66728630	-0.40376064
1	6.96042235	-1.61559049	1.34675165
6	-4.96327031	-1.50450713	0.14581868
1	-5.81145124	-2.04208689	-0.27813406
1	-4.36560765	-2.19689325	0.75445280
6	2.79819134	0.38793395	-0.02479945
6	3.07618358	-0.98614768	0.00362331
1	2.26918184	-1.70264503	-0.08907401
1	-1.97965637	-2.42146073	-0.69983824
1	-0.39776237	-1.81945169	-1.03258517
6	-0.95654162	1.96170650	-0.50602828
7	-1.13653509	3.09653136	-0.63301978

1a/t (Toluene)

37

8	-5.66800596	-0.26841456	0.67399489
7	-3.00484019	-0.22193177	-0.25723886
7	0.61270410	0.03373847	-0.16282264
7	-1.32804638	-1.73240055	-0.76985166
7	1.52258778	0.89206267	-0.14520077
6	-1.68916040	-0.47351324	-0.41280984
6	-0.68071753	0.49881776	-0.26806163
6	-4.04815326	-0.96643348	-0.96979836
1	-3.62185179	-1.82552122	-1.48323134
1	-4.48107419	-0.29695572	-1.72240331
6	5.19438437	0.87580123	-0.02790818
1	5.99142709	1.60459803	-0.13149871
6	5.51215735	-0.45876846	0.21859651
6	3.87075828	1.28735609	-0.13929362
1	3.61951066	2.32485317	-0.32838946
6	4.46016016	-1.37442970	0.34973286
1	4.68968858	-2.41695588	0.54861334
6	-4.66174691	0.40346154	1.40603512
1	-4.24584960	-0.27041675	2.16793251
1	-5.13928162	1.24731258	1.90425400
6	-3.53797805	0.90768774	0.50757422
1	-3.90907842	1.68034906	-0.17351636
1	-2.75656121	1.33513762	1.13199382
6	6.93989981	-0.91193665	0.36957523
1	7.63698462	-0.13905323	0.04267483
1	7.13073411	-1.81391547	-0.21655068
1	7.16447734	-1.14659002	1.41414056
6	-5.13801027	-1.39121357	0.00021036
1	-5.96140698	-1.85851839	-0.54058880
1	-4.73644134	-2.11021888	0.72911246
6	2.83362189	0.36566722	-0.01359796
6	3.13749749	-0.97759576	0.23817280
1	2.33652608	-1.69702884	0.35239622
1	-1.87363076	-2.50597166	-0.41808760
1	-0.32998552	-1.88712213	-0.82822541
6	-0.95051731	1.88767149	-0.39919413

7	-1.17716434	3.01251705	-0.52145543

1a/t′ (MeCN)

37

8	-5.27698301	-0.79328302	1.00210009
7	-2.96471043	0.00291018	-0.42853116
7	0.64108613	0.84719845	-0.22712657
7	-1.15746311	-1.38836968	-0.84561591
7	1.22826419	-0.26865018	-0.26659436
6	-1.63333488	-0.18446289	-0.52889447
6	-0.71669458	0.90893397	-0.36601612
6	-3.93707676	-0.94007469	-0.99207834
1	-3.45910286	-1.61233312	-1.70217068
1	-4.67521693	-0.34290581	-1.53602942
6	4.70857720	-1.44060359	-0.00308734
1	5.23453168	-2.38588852	-0.09019439
6	5.42647523	-0.27887213	0.28019094
6	3.32749727	-1.40574727	-0.17485620
1	2.77425912	-2.31297268	-0.39409441
6	4.71586998	0.92483592	0.38547124
1	5.25697317	1.83994365	0.60773602
6	-4.33773885	0.09354578	1.58329165
1	-3.61232460	-0.47544726	2.18029642
1	-4.89236407	0.76251379	2.24205005
6	-3.59319620	0.91680815	0.53576926
1	-4.28203879	1.57655424	0.00103504
1	-2.84556431	1.51847128	1.04555547
6	6.91834643	-0.30416557	0.47806438
1	7.32425937	-1.29619925	0.27534992
1	7.17956413	-0.03260654	1.50480523
1	7.41217171	0.41211965	-0.18337055
6	-4.64026236	-1.70287419	0.11910847
1	-5.41651538	-2.34551841	-0.29628825
1	-3.91869358	-2.31917840	0.67271131
6	2.63271839	-0.20117305	-0.07105023
6	3.34061783	0.97346082	0.21725874
1	2.81072812	1.91341032	0.30727181
1	-1.73297682	-2.21375842	-0.74646639
1	-0.14549938	-1.49252431	-0.86866497
6	-1.19833640	2.23666004	-0.50161929
7	-1.58676257	3.31761925	-0.63293901

1a/t′ (DMF)

37

8	-5.29126275	-0.77788212	0.99366722
7	-2.96164818	-0.00436887	-0.42242478
7	0.64326666	0.84294145	-0.22663628
7	-1.15475198	-1.39547448	-0.83806754
7	1.23113043	-0.27263322	-0.26238581
6	-1.63079145	-0.19090713	-0.52400585

6	-0.71448513	0.90347821	-0.36463178
6	-3.93496337	-0.94432988	-0.98887798
1	-3.45536354	-1.62473138	-1.68998657
1	-4.66348465	-0.34609166	-1.54464175
6	4.71316917	-1.43913854	0.00002611
1	5.24026226	-2.38396966	-0.08529385
6	5.42968818	-0.27571844	0.27930123
6	3.33191550	-1.40674703	-0.17011152
1	2.77978824	-2.31542007	-0.38626839
6	4.71748265	0.92705990	0.38285984
1	5.25742332	1.84349466	0.60260831
6	-4.34983611	0.10442248	1.57709059
1	-3.63277557	-0.46656268	2.18247090
1	-4.90378899	0.78036363	2.22928741
6	-3.59119051	0.91824918	0.53228258
1	-4.27067312	1.58149038	-0.01025508
1	-2.84308554	1.51595947	1.04618326
6	6.92159600	-0.29776537	0.47523668
1	7.32916082	-1.29022629	0.27773435
1	7.18418268	-0.01994156	1.49998190
1	7.41366483	0.41530693	-0.19104866
6	-4.65355282	-1.69549231	0.12015485
1	-5.43066282	-2.33441099	-0.29947722
1	-3.94132431	-2.31555042	0.68196068
6	2.63556265	-0.20297108	-0.06853984
6	3.34208965	0.97331442	0.21609970
1	2.81096438	1.91275134	0.30467291
1	-1.72998750	-2.22057713	-0.73481175
1	-0.14281390	-1.49975167	-0.86029359
6	-1.19664178	2.23041848	-0.50572271
7	-1.58537410	3.31063323	-0.64179016

2a/t′ (Toluene)

37

8	-5.42829073	-0.63786947	0.86522023
7	-2.92618203	-0.09644299	-0.32654290
7	0.66959169	0.81934268	-0.23414353
7	-1.09520761	-1.46110291	-0.72099651
7	1.26537675	-0.28837427	-0.26525823
6	-1.58743661	-0.24119569	-0.45818793
6	-0.69607854	0.86316015	-0.36413564
6	-3.88950368	-1.00698336	-0.94916026
1	-3.37818552	-1.76089960	-1.54531013
1	-4.51371509	-0.41074449	-1.62398484
6	4.75577072	-1.42104413	0.02421262
1	5.29180244	-2.36224268	-0.03998661
6	5.45916181	-0.24568667	0.27953327
6	3.37532858	-1.40483160	-0.14834224
1	2.83046755	-2.32154600	-0.34620068
6	4.73613926	0.95222159	0.35519121
1	5.26769906	1.87818795	0.55324633
6	-4.49077722	0.20498699	1.50721195

1	-3.88077423	-0.38487810	2.20583192
1	-5.06131445	0.94213403	2.07257475
6	-3.57515434	0.91396660	0.51430264
1	-4.14410760	1.60676176	-0.11308888
1	-2.83042821	1.47753826	1.07108529
6	6.95179417	-0.24763323	0.47392287
1	7.36854334	-1.24495744	0.32684381
1	7.21541888	0.08390810	1.48202898
1	7.43873544	0.43121392	-0.23077682
6	-4.77937541	-1.63984269	0.10960328
1	-5.55849489	-2.24163372	-0.35929110
1	-4.18317725	-2.28286265	0.77404928
6	2.66988001	-0.20651406	-0.07263517
6	3.36203062	0.98246159	0.18673450
1	2.81543715	1.91464615	0.25040469
1	-1.64159745	-2.27954318	-0.49869049
1	-0.07723086	-1.53254626	-0.72034730
6	-1.20419312	2.18078008	-0.53639623
7	-1.63618879	3.23905554	-0.69752732

Intermediate B stable isomers (B(tt) and B(cc)
B(cc) (DMF)

8	-5.664987	-0.020172	-1.632372
7	-2.986519	-0.023708	-0.766885
7	-0.129860	1.767875	0.213287
7	-1.354560	-0.990488	0.532632
7	0.753825	0.934479	-0.252253
6	-1.939776	0.074237	0.045321
6	-1.378327	1.438007	0.325780
6	-3.706924	-1.288140	-0.942508
1	-3.351610	-2.010342	-0.211297
1	-3.509316	-1.661745	-1.951812
6	4.308396	0.697735	-1.144508
1	4.961412	-0.008699	-1.646999
6	4.836401	1.884813	-0.635470
6	2.956292	0.398177	-1.020404
1	2.555477	-0.529630	-1.418336
6	3.962681	2.767414	0.009576
1	4.350881	3.695665	0.417184
6	-4.983808	1.203444	-1.416048
1	-5.163630	1.559278	-0.392735
1	-5.387687	1.927822	-2.123113
6	-3.489515	1.036757	-1.646472
1	-3.307641	0.720081	-2.678267
1	-2.963411	1.973326	-1.477365
6	6.299236	2.215947	-0.766573
1	6.836680	1.420322	-1.284575
1	6.758498	2.354839	0.215749
1	6.440590	3.144171	-1.326534
6	-5.195258	-1.025599	-0.751514
1	-5.758630	-1.933294	-0.967481
1	-5.381437	-0.726970	0.288606
6	2.109605	1.293909	-0.372593
6	2.610702	2.485662	0.151115
1	1.952705	3.175663	0.663945
6	-2.252753	2.438597	0.851784

7	-2.999868	3.213877	1.261605
6	-0.691473	-1.004750	1.709124
7	0.456293	-1.724393	1.761419
1	0.897728	-1.720270	2.673760
16	-1.263578	-0.263957	3.127520
6	1.247836	-2.277997	0.728329
6	2.611314	-2.426729	1.011784
6	0.752239	-2.694342	-0.511347
6	3.470026	-2.970713	0.068043
1	2.989468	-2.103867	1.976275
6	1.629307	-3.230864	-1.452432
1	-0.300799	-2.616249	-0.736598
6	2.985154	-3.369681	-1.176094
1	4.523077	-3.073829	0.304111
1	1.235836	-3.551282	-2.410576
1	3.655483	-3.789544	-1.916720
1	0.480144	0.020425	-0.616549

B(cc) (MeCN)

8	-5.631701	-0.000466	-1.697773
7	-2.975642	-0.009107	-0.763466
7	-0.129125	1.766110	0.248699
7	-1.363472	-0.995831	0.546259
7	0.751127	0.936482	-0.231176
6	-1.939533	0.075937	0.064721
6	-1.376703	1.435464	0.364677
6	-3.688503	-1.272580	-0.974972
1	-3.350337	-2.003809	-0.244702
1	-3.463346	-1.631899	-1.983804
6	4.298561	0.704884	-1.153194
1	4.948761	-0.001487	-1.659382
6	4.828536	1.894643	-0.652342
6	2.948274	0.402427	-1.015747
1	2.546089	-0.527994	-1.406136
6	3.958496	2.777401	-0.002490
1	4.348183	3.708018	0.398212
6	-4.961501	1.221994	-1.442773
1	-5.169330	1.558341	-0.418342
1	-5.349570	1.956807	-2.147758
6	-3.461160	1.064398	-1.637276
1	-3.251160	0.767322	-2.669641
1	-2.944957	2.000396	-1.437504
6	6.289833	2.227955	-0.797141
1	6.823395	1.432166	-1.318786
1	6.757451	2.368850	0.180905
1	6.424582	3.155590	-1.359619
6	-5.182554	-1.018733	-0.820318
1	-5.735779	-1.924766	-1.067216
1	-5.398913	-0.736595	0.218384
6	2.105223	1.298363	-0.363322
6	2.608269	2.493169	0.151723
1	1.953099	3.183872	0.667104
6	-2.248599	2.429292	0.907337
7	-2.992506	3.200732	1.330124
6	-0.697386	-1.019207	1.722048
7	0.449490	-1.740629	1.765963
1	0.893485	-1.742634	2.677123

16	-1.265484	-0.289393	3.146902
6	1.237798	-2.289645	0.727658
6	2.601106	-2.444970	1.008642
6	0.738980	-2.697715	-0.513488
6	3.456734	-2.986715	0.060672
1	2.981360	-2.129086	1.974585
6	1.612944	-3.232085	-1.458834
1	-0.314026	-2.614198	-0.736700
6	2.968767	-3.377284	-1.185036
1	4.509605	-3.095177	0.294986
1	1.217017	-3.546032	-2.418074
1	3.636558	-3.795578	-1.928786
1	0.474598	0.025670	-0.601210

B(cc) (Toluene)

8	-5.689175	0.042567	-1.555565
7	-2.994314	-0.005836	-0.759719
7	-0.113810	1.761692	0.239456
7	-1.340015	-1.005495	0.479194
7	0.789651	0.920470	-0.172492
6	-1.923620	0.075097	0.033477
6	-1.363909	1.434105	0.329260
6	-3.744342	-1.256600	-0.896449
1	-3.378617	-1.971435	-0.162566
1	-3.585781	-1.655675	-1.903719
6	4.352911	0.738769	-1.049931
1	5.024343	0.032099	-1.526566
6	4.847525	1.956708	-0.585908
6	3.009685	0.407257	-0.915872
1	2.640316	-0.546081	-1.282516
6	3.949526	2.838233	0.024914
1	4.311935	3.791190	0.397398
6	-4.985260	1.256210	-1.369063
1	-5.132637	1.630129	-0.347441
1	-5.397133	1.977291	-2.075003
6	-3.499821	1.055807	-1.635283
1	-3.357601	0.725970	-2.670046
1	-2.948106	1.981259	-1.490708
6	6.301885	2.321395	-0.725387
1	6.857205	1.537220	-1.241868
1	6.763736	2.473171	0.253769
1	6.421348	3.248932	-1.291065
6	-5.222621	-0.958790	-0.672445
1	-5.814764	-1.854082	-0.862589
1	-5.375904	-0.643132	0.368041
6	2.138990	1.302961	-0.302473
6	2.606463	2.526395	0.175629
1	1.924668	3.213231	0.660115
6	-2.259530	2.448957	0.794601
7	-3.038304	3.228300	1.128817
6	-0.688935	-1.055387	1.669361
7	0.449741	-1.803131	1.708732
1	0.879853	-1.812980	2.624786
16	-1.253492	-0.337319	3.083818
6	1.239748	-2.344286	0.673234
6	2.601463	-2.514514	0.953576
6	0.744276	-2.730590	-0.576997

6	3.455399	-3.050044	0.002123
1	2.985126	-2.207446	1.920697
6	1.617631	-3.255072	-1.527630
1	-0.309458	-2.640837	-0.794273
6	2.970533	-3.416524	-1.251328
1	4.506058	-3.170282	0.239187
1	1.223111	-3.554084	-2.492059
1	3.637075	-3.830770	-1.997920
1	0.535882	-0.019626	-0.474600

B(cc) $CHCl_3$

8	5.243320	-1.773194	0.552781
7	2.883210	-0.339288	0.012851
7	-0.239536	0.872805	1.089810
7	1.843244	1.404724	-1.061619
7	-0.872679	0.799044	-0.044398
6	1.974027	0.635185	-0.013182
6	1.050202	0.774097	1.161255
6	3.948866	-0.413584	-0.990982
1	3.966108	0.511115	-1.563296
1	3.740343	-1.253443	-1.661857
6	-4.272723	0.737050	-1.436075
1	-4.741177	0.550240	-2.396898
6	-5.063355	1.065340	-0.334993
6	-2.889586	0.644650	-1.329242
1	-2.285624	0.392857	-2.195646
6	-4.421271	1.306323	0.884315
1	-5.015304	1.569583	1.753877
6	4.243198	-1.652913	1.548861
1	4.454500	-0.790562	2.194572
1	4.273842	-2.563704	2.146541
6	2.870344	-1.498551	0.911369
1	2.647271	-2.383380	0.305651
1	2.098727	-1.399667	1.671028
6	-6.562496	1.159071	-0.441810
1	-6.892301	1.028258	-1.473435
1	-6.920884	2.129543	-0.089784
1	-7.046729	0.391446	0.167991
6	5.277106	-0.624770	-0.275257
1	6.069806	-0.779631	-1.007099
1	5.513162	0.262303	0.326810
6	-2.277279	0.887726	-0.103143
6	-3.042128	1.224957	1.013202
1	-2.559506	1.425531	1.961002
6	1.621196	0.877738	2.468815
7	2.131616	0.931908	3.499753
6	1.403842	2.685066	-0.991464
7	0.581351	3.105093	-1.989463
1	0.299358	4.072592	-1.891820
16	1.896122	3.788307	0.190012
6	-0.125699	2.379758	-2.973582
6	-1.311707	2.960370	-3.440350
6	0.300493	1.160692	-3.510536
6	-2.066954	2.328232	-4.416688
1	-1.639726	3.906512	-3.021751
6	-0.476109	0.531173	-4.481435
1	1.232207	0.720383	-3.189531

6	-1.658768	1.102152	-4.938223
1	-2.983154	2.792108	-4.763488
1	-0.135758	-0.412911	-4.891698
1	-2.250259	0.604299	-5.697225
1	-0.376461	0.616068	-0.917045

B(cc) EtOH

8	5.206613	-1.825007	0.517141
7	2.877572	-0.325236	0.006862
7	-0.224015	0.899421	1.100955
7	1.869289	1.454239	-1.044167
7	-0.852951	0.794493	-0.033293
6	1.987989	0.664379	-0.008929
6	1.066697	0.806770	1.167842
6	3.926970	-0.429964	-1.011316
1	3.968226	0.493250	-1.584623
1	3.683381	-1.262332	-1.679220
6	-4.240493	0.673278	-1.448548
1	-4.700832	0.442926	-2.404074
6	-5.040834	1.051697	-0.369957
6	-2.858617	0.583133	-1.324653
1	-2.245500	0.285599	-2.170498
6	-4.409476	1.346096	0.843398
1	-5.010873	1.648143	1.695317
6	4.218687	-1.675422	1.526464
1	4.466123	-0.818372	2.165807
1	4.230062	-2.586054	2.124880
6	2.844781	-1.484242	0.905455
1	2.588136	-2.361937	0.303295
1	2.086565	-1.365739	1.676156
6	-6.538729	1.137221	-0.493509
1	-6.857387	0.979375	-1.524946
1	-6.904125	2.113995	-0.166812
1	-7.024787	0.382325	0.131020
6	5.259256	-0.677606	-0.317990
1	6.033024	-0.858426	-1.063801
1	5.533599	0.200468	0.280015
6	-2.256554	0.881088	-0.104986
6	-3.030893	1.270283	0.987670
1	-2.559433	1.513756	1.931385
6	1.644676	0.948745	2.466615
7	2.155548	1.047685	3.494466
6	1.398530	2.720601	-0.961845
7	0.566086	3.132721	-1.949723
1	0.261733	4.093991	-1.848386
16	1.873207	3.829878	0.230977
6	-0.136460	2.396245	-2.932430
6	-1.337290	2.958502	-3.382295
6	0.308442	1.189655	-3.481118
6	-2.091098	2.318090	-4.354943
1	-1.676711	3.897123	-2.955857
6	-0.465006	0.553220	-4.450192
1	1.248548	0.759065	-3.171055
6	-1.663412	1.104691	-4.890297
1	-3.020318	2.766277	-4.688293
1	-0.111878	-0.382217	-4.869711
1	-2.253959	0.600525	-5.646257

1	-0.355823	0.562306	-0.894513

B(tt) $CHCl_3$

8	-2.466064	-2.277870	1.156551
7	-1.356413	-0.834697	-0.992036
7	1.294038	0.190394	-0.449169
7	-0.685314	-0.815483	-3.183526
7	2.361915	0.865268	-0.146020
6	-0.485602	-0.469934	-1.938845
6	0.670567	0.385696	-1.567070
6	-2.345889	-1.885259	-1.242865
1	-2.130361	-2.365547	-2.194024
1	-3.340234	-1.429166	-1.286703
6	4.880990	1.236671	2.506717
1	5.775814	1.823067	2.686438
6	4.448001	0.328428	3.472228
6	4.188356	1.408225	1.313342
1	4.538614	2.117958	0.571188
6	3.290791	-0.409935	3.203144
1	2.934167	-1.125757	3.937241
6	-1.487268	-1.280884	1.391696
1	-0.486931	-1.733793	1.402591
1	-1.699138	-0.849149	2.370116
6	-1.548567	-0.206118	0.317276
1	-2.545700	0.247863	0.318761
1	-0.809169	0.566759	0.497587
6	5.197759	0.133524	4.763193
1	6.046577	0.815137	4.831761
1	5.576596	-0.888873	4.843384
1	4.548402	0.310349	5.624359
6	-2.275572	-2.896375	-0.104837
1	-3.065162	-3.639481	-0.217542
1	-1.301084	-3.401904	-0.127311
6	3.039791	0.660544	1.071379
6	2.584175	-0.255346	2.019446
1	1.693703	-0.839297	1.825679
6	1.099979	1.374420	-2.514775
7	1.457577	2.213299	-3.218389
6	0.295874	-0.993172	-4.095801
16	1.820548	-1.673077	-3.778423
7	-0.036849	-0.699900	-5.375832
1	0.624207	-1.019875	-6.071701
6	-1.235209	-0.121229	-5.858124
6	-1.778964	-0.630200	-7.038193
6	-1.839690	0.964965	-5.224336
6	-2.930691	-0.066054	-7.573680
1	-1.297361	-1.470881	-7.525915
6	-2.999234	1.513602	-5.760359
1	-1.391833	1.387105	-4.334461
6	-3.550710	1.002294	-6.932346
1	-3.346236	-0.468637	-8.490211
1	-3.464736	2.358362	-5.265627
1	-4.451413	1.439163	-7.347181
1	2.751311	1.547303	-0.798141

B(tt) EtOH

8	-2.545998	-2.242324	1.183361
7	-1.314446	-0.923180	-0.986177
7	1.303330	0.159781	-0.476186
7	-0.677547	-0.897772	-3.190286
7	2.356473	0.852066	-0.173316
6	-0.468702	-0.542140	-1.947709
6	0.673100	0.337331	-1.594918
6	-2.294125	-1.985392	-1.226624
1	-2.025961	-2.529948	-2.128970
1	-3.283413	-1.534426	-1.358834
6	4.890751	1.233580	2.462439
1	5.800016	1.803333	2.623637
6	4.437758	0.362469	3.454340
6	4.199580	1.387876	1.266278
1	4.562069	2.067815	0.502200
6	3.258909	-0.349893	3.211567
1	2.881871	-1.029123	3.969828
6	-1.561263	-1.243994	1.414527
1	-0.573497	-1.713826	1.505262
1	-1.816255	-0.754540	2.354450
6	-1.555850	-0.229720	0.284367
1	-2.543550	0.239834	0.216525
1	-0.813822	0.541488	0.461450
6	5.199749	0.172067	4.738289
1	5.902866	0.989702	4.904527
1	5.770106	-0.761475	4.714547
1	4.521820	0.119007	5.592922
6	-2.294228	-2.930759	-0.033508
1	-3.083928	-3.672925	-0.150998
1	-1.325907	-3.443150	0.030031
6	3.030921	0.662806	1.049328
6	2.551438	-0.210109	2.025151
1	1.637579	-0.766770	1.859214
6	1.084026	1.315795	-2.558798
7	1.428163	2.135282	-3.291663
6	0.296179	-1.054020	-4.112093
16	1.815668	-1.763052	-3.813214
7	-0.031049	-0.720377	-5.381956
1	0.613606	-1.042543	-6.093412
6	-1.219316	-0.105095	-5.845837
6	-1.755305	-0.553006	-7.054470
6	-1.818678	0.957903	-5.168395
6	-2.896783	0.046780	-7.573439
1	-1.274735	-1.372268	-7.578522
6	-2.968403	1.541925	-5.689574
1	-1.379234	1.336319	-4.254876
6	-3.513822	1.090318	-6.888731
1	-3.306507	-0.308198	-8.512238
1	-3.430946	2.366540	-5.159035
1	-4.407194	1.554186	-7.290443
1	2.732847	1.548325	-0.819383

5-(Tolylazo)pyrimidine-2(1*H*)-thione **4a**

Isomer A

S	-4.24088300	1.10173900	-0.98252600
O	0.66651800	4.92888900	1.09702600
N	0.42659400	2.55989000	-0.44398300
C	-4.82650600	-2.62424400	1.53330600
H	-5.30491300	-2.73447000	2.49871000
C	-3.88085000	-1.62287100	1.34225200
H	-3.61496600	-0.93865300	2.13928400
N	1.37959700	-0.08115300	-0.13634200
N	-1.70450700	1.75957500	-0.63397100
N	-0.67100300	-2.05810900	0.45607500
N	1.81575000	-1.22352200	0.15991800
C	-0.43235500	1.50546000	-0.37119500
C	0.03211600	0.17299100	-0.07718800
N	-2.27829400	-0.46892200	-0.09286600
C	-0.07286900	3.84909400	-0.93319500
H	-0.92566600	3.68257200	-1.58507900
H	0.74252200	4.31469200	-1.49522100
C	5.14542300	-2.77041700	0.40149100
H	5.56810900	-3.68895200	0.79394300
C	-0.97123800	-0.80487800	0.10957000
C	5.98158000	-1.83135400	-0.19805200
C	3.77677800	-2.54705300	0.50191000
H	3.12685500	-3.27808800	0.96924800
C	-4.55378200	-3.32815900	-0.75840200
H	-4.82168500	-3.98481700	-1.57696500
C	-2.65489500	0.81888400	-0.57242700
C	5.40567500	-0.65594900	-0.69651400
H	6.04234600	0.08203000	-1.17447800
C	1.14468900	3.69721200	1.59077400
H	0.36588200	3.21030500	2.19713700
H	1.99979700	3.92284800	2.22972500
C	1.56145500	2.75259300	0.46479900
H	2.38351800	3.19452600	-0.10640100
H	1.89905000	1.80562600	0.87124100
C	-5.16208900	-3.47538900	0.48514500
H	-5.90234700	-4.25187500	0.63553700
C	7.46337200	-2.06644800	-0.32689200
H	7.76333600	-2.98389600	0.18025800
H	8.02921100	-1.23757000	0.10455300
H	7.75314300	-2.15018300	-1.37745400
C	-3.28521900	-1.48237200	0.09634800
C	-0.44835100	4.74257600	0.23979000
H	-0.74666200	5.73279700	-0.10460200
H	-1.28057600	4.28648800	0.79201500
C	3.21974300	-1.37014500	0.01004400
C	4.04523000	-0.41919900	-0.60055800
H	3.60573000	0.48634300	-0.99914900
C	-3.60973000	-2.32797600	-0.95729300
H	-3.14129900	-2.17808600	-1.92307200
H	0.32334300	-2.27367500	0.52536400
H	-1.38876400	-2.76534900	0.48551800

Isomer B

S	-4.26763800	-1.64191700	0.35086200
O	2.10047300	-4.83246600	-0.22774800
N	0.53079700	-2.50553200	-0.02632000
C	-5.27234300	2.48763800	-1.14478700
H	-5.80684000	2.72618600	-2.05620500
C	-4.22681600	1.57390400	-1.17702100
H	-3.93078800	1.08888600	-2.09933500
N	1.28575600	0.21216100	-0.04438900
N	-1.66479000	-1.83209900	0.09530200
N	-1.08239000	2.09391100	-0.54431800
N	1.62267000	1.39924700	-0.25175900
C	-0.35002300	-1.46069100	-0.02349400
C	-0.05498300	-0.11757600	-0.15815300
N	-2.46757800	0.32568300	-0.02923400
C	0.44941100	-3.56287200	0.98821600
H	-0.54783500	-3.60491700	1.42566500
H	1.16030600	-3.33011400	1.79200700
C	4.81960000	3.20818600	-0.40562900
H	5.17887800	4.15251200	-0.79987900
C	-1.15394700	0.85592900	-0.29102500
C	5.70796300	2.35282200	0.24247400
C	3.47807900	2.87133800	-0.54745500
H	2.78222400	3.53790400	-1.04356200
C	-4.94243400	2.79025800	1.22483000
H	-5.21999700	3.26331600	2.15888500
C	-2.75615700	-0.98827000	0.13737400
C	5.21350400	1.14493600	0.75096000
H	5.88974900	0.47586200	1.27395700
C	2.14522800	-3.84035400	-1.23468500
H	1.42366000	-4.08313100	-2.02710100
H	3.15228400	-3.86168400	-1.65124900
C	1.84262000	-2.45685000	-0.67237800
H	2.61590900	-2.16408000	0.04407600
H	1.82347400	-1.72153600	-1.47446700
C	-5.63117900	3.09433000	0.05519400
H	-6.44786000	3.80593700	0.07810700
C	7.16118500	2.70967500	0.41130000
H	7.38412200	3.67909000	-0.03505300
H	7.80307600	1.96208300	-0.06110500
H	7.43092500	2.75267600	1.46932600
C	-3.55401500	1.27675800	-0.00286000
C	0.82174900	-4.89917400	0.36391400
H	0.86483100	-5.67633000	1.12713700
H	0.07289400	-5.17823000	-0.39141600
C	3.00530500	1.65848000	-0.05533700
C	3.88200200	0.79422700	0.60896700
H	3.50323600	-0.13255700	1.02003000
C	-3.89515700	1.87709900	1.19789100
H	-3.34482600	1.62507100	2.09645000
H	-0.10838200	2.35139000	-0.68021700
H	-1.90942300	-2.81026200	0.03738200

Isomer C

S	-3.75473000	-0.39770800	1.94359500
O	0.28610600	-5.28315500	-0.92892800
N	0.22243200	-2.75183100	0.30931400
C	-5.04513000	2.48635200	-1.29084800
H	-5.84886300	2.35290600	-2.00471300
C	-4.13292300	1.46022400	-1.07896200
H	-4.21057000	0.52007400	-1.61191300
N	1.29994000	-0.12717900	-0.13470300
N	-1.68112300	-1.60582600	0.87479700
N	-0.83582500	1.46948600	-1.63354300
N	1.82355700	1.04523600	-0.43112900
C	-0.50897800	-1.61606800	0.30574300
C	0.03568900	-0.36194700	-0.24354400
N	-2.15603100	0.58270600	0.05613300
C	-0.27910700	-3.94173400	0.99966600
H	-1.08058300	-3.64889600	1.67303900
H	0.55348100	-4.36676000	1.56892800
C	4.98393800	2.89463600	-0.06846700
H	5.33824700	3.91052100	-0.20581800
C	-0.98463100	0.61978600	-0.68988600
C	5.87320600	1.90710200	0.35286000
C	3.64867300	2.60561100	-0.31689600
H	2.97290600	3.38885000	-0.64472500
C	-3.89372400	3.85146600	0.32920500
H	-3.80355100	4.77915200	0.88121800
C	-2.45479500	-0.47942700	0.92968700
C	5.37806200	0.61139600	0.51290700
H	6.05026000	-0.17655000	0.83668500
C	0.74773400	-4.14277800	-1.61761700
H	-0.06617800	-3.71564200	-2.22223400
H	1.54538000	-4.47572700	-2.28283600
C	1.27008000	-3.07470000	-0.65739800
H	2.13677400	-3.45897200	-0.11044100
H	1.57289500	-2.18878500	-1.20678400
C	-4.92651600	3.68111300	-0.58731600
H	-5.64050600	4.47913400	-0.75229200
C	7.31421200	2.22761800	0.65284400
H	7.62825600	3.14094300	0.14597000
H	7.97203500	1.41719100	0.33413300
H	7.46427000	2.37320300	1.72615000
C	-3.11228200	1.63970300	-0.15778100
C	-0.75816300	-4.95714700	-0.02752600
H	-1.05643500	-5.88696700	0.45621100
H	-1.61590100	-4.54570400	-0.57686300
C	3.17791100	1.30598000	-0.14614100
C	4.04764600	0.29995700	0.27014300
H	3.67732200	-0.70774800	0.40256500
C	-2.97983800	2.82730600	0.54500300
H	-2.17746000	2.93286100	1.26558700
H	0.04365900	1.30723900	-2.11908700
H	1.21436000	1.84339800	-0.59902000

Isomer A’

S	-4.05439500	1.09224500	-1.42039300
O	0.76141500	4.77513400	1.15626000
N	0.56992100	2.35002400	-0.28300800
C	-5.17060500	-2.21860300	1.54819000
H	-5.71999500	-2.18258300	2.48087000
C	-4.12996300	-1.32343500	1.32543600
H	-3.85749300	-0.57997700	2.06499000
N	1.22873800	-0.64391000	0.12521700
N	-1.54131500	1.64115000	-0.79638600
N	-0.90938800	-2.11221400	0.72604500
N	2.24978000	-0.02693700	-0.25217300
C	-0.33321600	1.34216600	-0.33752200
C	0.00402600	-0.00151000	0.06050900
N	-2.34046900	-0.46670700	-0.09275200
C	0.26866300	3.63671800	-0.91198900
H	-0.48136800	3.48977600	-1.68449900
H	1.19979100	4.00087700	-1.35729900
C	5.76898000	-0.89023500	-0.85234400
H	6.61077100	-0.45688600	-1.38151900
C	-1.08732800	-0.87206800	0.23706200
C	5.93217200	-2.09708600	-0.17557500
C	4.54445700	-0.23211600	-0.85394600
H	4.41181700	0.70850100	-1.37591000
C	-4.80688200	-3.19288300	-0.62904100
H	-5.07680000	-3.91206700	-1.39255200
C	-2.55735900	0.77511800	-0.77013800
C	4.82942800	-2.62839700	0.50490000
H	4.94424600	-3.56029100	1.04984100
C	1.01247100	3.54178000	1.79120900
H	0.09053800	3.17434500	2.26688700
H	1.75867900	3.72913600	2.56465000
C	1.52402100	2.48080500	0.81589500
H	2.49930600	2.76096200	0.40930800
H	1.63094800	1.53792000	1.34399100
C	-5.50769400	-3.15203400	0.57335900
H	-6.32135700	-3.84563000	0.74779900
C	7.25429800	-2.81793800	-0.16059800
H	8.01622000	-2.25601200	-0.70142700
H	7.16557600	-3.80296300	-0.62560000
H	7.60520000	-2.96845700	0.86313000
C	-3.44183300	-1.37082200	0.12139100
C	-0.20954400	4.63378400	0.13326200
H	-0.34878100	5.62126300	-0.30666000
H	-1.16170800	4.28927500	0.55809600
C	3.45074100	-0.78030800	-0.18909600
C	3.60277500	-1.98662200	0.50361900
H	2.76262500	-2.40092100	1.04575100
C	-3.76847700	-2.29880100	-0.86022000
H	-3.22880100	-2.29095000	-1.80012600
H	0.05067600	-2.41174700	0.81101800
H	-1.64674500	-2.79548600	0.66069400

Isomer B’

S	-4.12432800	1.38896600	-0.93234000
O	1.12269200	4.88192600	0.69408500
N	0.66776000	2.26837800	-0.26367000
C	-5.33509200	-2.33060200	1.33864400
H	-5.93082300	-2.37322200	2.24225800
C	-4.27285300	-1.43929800	1.25375100
H	-4.02409400	-0.77963500	2.07627100
N	1.21784800	-0.68971900	0.23175400
N	-1.54610700	1.60885800	-0.51273400
N	-1.08144900	-2.12379600	0.89159800
N	2.26627500	-0.06435900	-0.04221600
C	-0.25213800	1.27447200	-0.17759300
C	-0.00115900	-0.03441400	0.19830400
N	-2.41534500	-0.47079100	-0.00272400
C	0.49720300	3.43640200	-1.12562600
H	-0.24019300	3.23446500	-1.90306800
H	1.45758900	3.60952300	-1.62139500
C	5.83377100	-0.91118300	-0.31802600
H	6.76656500	-0.37528800	-0.45654600
C	-1.13634100	-0.95007200	0.41734700
C	5.85059400	-2.29865000	-0.19803300
C	4.63625000	-0.20619300	-0.26488200
H	4.61870300	0.87317700	-0.36351600
C	-4.86437900	-3.11266500	-0.89358200
H	-5.09345500	-3.76371300	-1.72838600
C	-2.65070600	0.78224900	-0.46805400
C	4.62952200	-2.96377700	-0.02498600
H	4.62576400	-4.04584800	0.06176500
C	1.22627300	3.76940100	1.56249900
H	0.26437500	3.60467100	2.06997700
H	1.97982800	4.02426800	2.30803200
C	1.63183400	2.50350200	0.81270400
H	2.62871900	2.60884700	0.37920700
H	1.64209600	1.65407200	1.49086000
C	-5.63161700	-3.16555000	0.26578800
H	-6.46090800	-3.85942600	0.33400700
C	7.13754200	-3.07803100	-0.25942300
H	7.99619400	-2.41528900	-0.37069400
H	7.13197100	-3.77150200	-1.10401700
H	7.27845400	-3.66875500	0.64889900
C	-3.52176200	-1.39452700	0.09066700
C	0.14607200	4.67217600	-0.30176700
H	0.13399700	5.56325800	-0.92973300
H	-0.84363300	4.55764700	0.16725500
C	3.43105900	-0.87839600	-0.08301200
C	3.43159300	-2.27358400	0.03117600
H	2.49273800	-2.79736400	0.15520500
C	-3.80077400	-2.22328900	-0.98370300
H	-3.18900400	-2.16545900	-1.87596400
H	-0.11255400	-2.33506400	1.12276100
H	-1.78682200	2.57395200	-0.68561900

Isomer C’

S	-3.58048200	0.57052800	-2.10764700
O	0.20467400	4.75104800	1.16429500
N	0.62865200	2.34137100	-0.26767800
C	-5.54139200	-1.85805600	1.13561500
H	-6.37441900	-1.54655800	1.75391600
C	-4.46834800	-0.99676900	0.93784500
H	-4.44970400	-0.00961400	1.38465200
N	1.18787200	-0.56194500	0.33519800
N	-1.41088700	1.49565900	-0.94665200
N	-1.03923600	-1.60231500	1.68319400
N	2.28152900	0.00713100	-0.11148100
C	-0.29584900	1.32186000	-0.31674600
C	0.03733900	0.02573200	0.29285000
N	-2.28755400	-0.52065800	-0.04854900
C	0.29358000	3.59575600	-0.95654100
H	-0.26506000	3.36296300	-1.86043800
H	1.23783000	4.08251300	-1.21492400
C	5.80960800	-0.79225700	-0.78671500
H	6.65939000	-0.32703700	-1.27440700
C	-1.13403700	-0.77016900	0.73271200
C	5.95338000	-2.05081500	-0.20732300
C	4.59399000	-0.11925300	-0.75663600
H	4.50004700	0.85805700	-1.21931500
C	-4.47527500	-3.51338500	-0.25739200
H	-4.47934800	-4.49025400	-0.72528500
C	-2.35923000	0.49555900	-1.00084900
C	4.83266600	-2.61887500	0.40530000
H	4.91894100	-3.59970800	0.86177000
C	0.47287900	3.55355200	1.85781400
H	-0.46938900	3.05634500	2.13327100
H	1.00792300	3.82449700	2.76857900
C	1.31379500	2.60073200	1.01220100
H	2.28216400	3.05901800	0.79070200
H	1.48042800	1.66833300	1.55134100
C	-5.54520500	-3.11482000	0.53847000
H	-6.38301300	-3.78411600	0.69270100
C	7.27313300	-2.77721100	-0.22069700
H	7.98264300	-2.29244400	-0.89228500
H	7.14832900	-3.81168900	-0.54733800
H	7.71673600	-2.79811900	0.77824400
C	-3.40896800	-1.40116500	0.13628200
C	-0.51063900	4.50483600	-0.03543200
H	-0.68131200	5.47399400	-0.50350900
H	-1.47781600	4.03800700	0.18848000
C	3.49346800	-0.70637300	-0.13875400
C	3.61049200	-1.96581600	0.44895200
H	2.74871500	-2.41278800	0.92678800
C	-3.40135300	-2.65516800	-0.46107400
H	-2.56262300	-2.94081300	-1.08515400
H	-1.91016800	-2.11260000	1.82464300
H	2.23319000	0.90310000	-0.59197300

Isothiocyanate

3a (MeCN)

14

6	-2.53566081	1.20689006	-0.00000000
6	-1.14662319	1.21693554	-0.00000000
6	-0.46282809	0.00000047	-0.00000001
6	-1.14662222	-1.21693514	0.00000000
6	-2.53565981	-1.20689080	-0.00000000
6	-3.23167663	-0.00000066	0.00000000
1	-3.07464219	2.14686870	-0.00000000
1	-0.58739179	2.14456209	-0.00000000
1	-0.58739005	-2.14456124	0.00000000
1	-3.07464042	-2.14686988	0.00000001
1	-4.31530066	-0.00000111	0.00000001
7	0.91953856	0.00000095	0.00000000
6	2.09014457	0.00000050	0.00000000
16	3.68850952	-0.00000031	-0.00000000

3a (DMF)

14

6	-2.53546802	1.20678425	-0.00000000
6	-1.14653911	1.21688462	-0.00000000
6	-0.46279595	0.00000013	-0.00000001
6	-1.14653884	-1.21688452	0.00000000
6	-2.53546774	-1.20678447	0.00000000
6	-3.23143733	-0.00000019	0.00000000
1	-3.07452299	2.14675109	0.00000002
1	-0.58732552	2.14455842	-0.00000000
1	-0.58732504	-2.14455819	0.00000000
1	-3.07452249	-2.14675142	0.00000002
1	-4.31508820	-0.00000032	0.00000000
7	0.91943040	0.00000030	-0.00000000
6	2.08992772	0.00000017	0.00000000
16	3.68829294	-0.00000010	0.00000000

3a (Toluene)

14

6	-2.53523470	1.20555302	-0.00000006
6	-1.14709690	1.21504591	0.00000007
6	-0.45982117	0.00000098	0.00000013
6	-1.14709489	-1.21504513	0.00000007
6	-2.53523273	-1.20555455	-0.00000006
6	-3.23158925	-0.00000133	-0.00000013
1	-3.07384349	2.14552828	-0.00000011
1	-0.58788963	2.14236523	0.00000013
1	-0.58788608	-2.14236353	0.00000014
1	-3.07383993	-2.14553073	-0.00000011
1	-4.31490909	-0.00000223	-0.00000026
7	0.91999106	0.00000211	0.00000024
6	2.09338876	0.00000079	0.00000005
16	3.68590725	-0.00000062	-0.00000012

5-(Tolylazo)pyrimidine (**4a**)

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4a/A′ (MeCN)
   51

  16     -4.07780781      1.16619979     -1.39305421
   8      1.02104706      4.79912393      1.09503961
   7      0.56133932      2.34442078     -0.24028305
   6     -5.23959630     -2.12892415      1.54349105
   1     -5.79465738     -2.06914452      2.47218245
   6     -4.17831571     -1.25767148      1.31715639
   1     -3.89497624     -0.51293298      2.05248100
   7      1.20353313     -0.65411189      0.13642887
   7     -1.54233073      1.64137918     -0.81125080
   7     -0.95748253     -2.09797953      0.73468036
   7      2.22544752     -0.06769452     -0.28485608
   6     -0.32750544      1.33905006     -0.32532162
   6     -0.01488815     -0.00378050      0.06460496
   7     -2.36696340     -0.44917379     -0.10383507
   6      0.33075471      3.63172861     -0.90079178
   1     -0.46131258      3.52922342     -1.63671018
   1      1.26395068      3.90404399     -1.40385627
   6      5.76386849     -0.93273297     -0.78351198
   1      6.63235198     -0.47668935     -1.24709118
   6     -1.11663364     -0.87088055      0.24652781
   6      5.88595401     -2.18091003     -0.17357060
   6      4.54384226     -0.26309750     -0.80074008
   1      4.44989961      0.70895103     -1.27319799
   6     -4.86760977     -3.15326632     -0.61241909
   1     -5.13481043     -3.88961235     -1.36108986
   6     -2.55359487      0.78917053     -0.75517953
   6      4.74666294     -2.74306602      0.42153592
   1      4.82825203     -3.71106059      0.90670569
   6      1.20205480      3.56526879      1.76514978
   1      0.28127912      3.29862009      2.30198215
   1      2.00490149      3.70754434      2.48949774
   6      1.57771793      2.43384852      0.80978646
   1      2.55195921      2.62167695      0.35156940
   1      1.62611781      1.51054583      1.37965674
   6     -5.58495226     -3.07278047      0.57948436
   1     -6.41251566     -3.74951766      0.75820234
   6      7.19733754     -2.91769202     -0.14734494
   1      7.99222341     -2.32326841     -0.59950983
   1      7.12192294     -3.86150568     -0.69432665
   1      7.48733241     -3.15980464      0.87828637
   6     -3.48290765     -1.34002464      0.11819396
   6     -0.01113247      4.69898940      0.12642615
   1     -0.09610192      5.67343939     -0.35500941
   1     -0.96237710      4.45601258      0.61863140
   6      3.41785335     -0.83703080     -0.21311164
   6      3.52593025     -2.08840259      0.40850784
   1      2.65878585     -2.53538253      0.87926781
   6     -3.80725516     -2.28446059     -0.84810876
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1	-3.24194465	-2.32464160	-1.77254257
1	-0.01588241	-2.40646225	0.93675877
1	-1.71816213	-2.76011650	0.78588485

4a/A′ (DMF)

51

16	-4.07835812	1.17201483	-1.38771771
8	1.03657259	4.80001223	1.08897478
7	0.56299251	2.34227142	-0.23708138
6	-5.24522179	-2.12337001	1.54022083
1	-5.80152557	-2.06237804	2.46811964
6	-4.18201494	-1.25431233	1.31536573
1	-3.89836352	-0.50996280	2.05100891
7	1.20168489	-0.65621657	0.13944640
7	-1.54138840	1.64222678	-0.80825197
7	-0.96122538	-2.09944288	0.73353420
7	2.22384591	-0.06997896	-0.28146551
6	-0.32697210	1.33823219	-0.32230983
6	-0.01614349	-0.00490450	0.06792536
7	-2.36831086	-0.44821541	-0.10358844
6	0.33773429	3.62786642	-0.90232344
1	-0.45711014	3.52643154	-1.63552682
1	1.27070514	3.89279860	-1.40977190
6	5.76018462	-0.93827686	-0.78650031
1	6.62794748	-0.48320456	-1.25242527
6	-1.11874138	-0.87148047	0.24744255
6	5.88258051	-2.18573476	-0.17538469
6	4.54075267	-0.26774537	-0.80192264
1	4.44676411	0.70385985	-1.27534890
6	-4.87196110	-3.14866039	-0.61483457
1	-5.13938380	-3.88477165	-1.36368528
6	-2.55364118	0.79145413	-0.75248490
6	4.74413549	-2.74636880	0.42251278
1	4.82601087	-3.71385699	0.90872240
6	1.21114343	3.56763320	1.76248383
1	0.28983160	3.30737886	2.30180066
1	2.01490573	3.70778389	2.48631402
6	1.58046685	2.43038308	0.81178392
1	2.55585976	2.61042868	0.35278911
1	1.62374509	1.50922336	1.38575785
6	-5.59096244	-3.06654708	0.57579118
1	-6.42012210	-3.74165483	0.75343789
6	7.19343666	-2.92288519	-0.14948721
1	7.98815817	-2.33035896	-0.60452402
1	7.11710277	-3.86828654	-0.69366665
1	7.48531344	-3.16231226	0.87629034
6	-3.48533230	-1.33780196	0.11729604
6	0.00435054	4.70172665	0.12079190
1	-0.07456349	5.67443990	-0.36527091
1	-0.94931958	4.46818186	0.61327589
6	3.41559435	-0.84007880	-0.21132636
6	3.52394494	-2.09087160	0.41126511

1	2.65754212	-2.53673641	0.88453969
6	-3.80980749	-2.28180977	-0.84923061
1	-3.24351416	-2.32310972	-1.77305025
1	-0.02032439	-2.40891267	0.93741228
1	-1.72285818	-2.76051361	0.78488531

4a/A′ (TOL)

51

16	-4.07488814	1.20101665	-1.35972337
8	1.06597987	4.79297859	1.07584878
7	0.57802947	2.33459878	-0.23582524
6	-5.22402320	-2.16273719	1.54652311
1	-5.76243225	-2.13100257	2.48604009
6	-4.16925859	-1.28332406	1.32644316
1	-3.87645761	-0.55703617	2.07586049
7	1.19024888	-0.67461908	0.14502433
7	-1.53685062	1.65878268	-0.77486433
7	-0.98026518	-2.10900058	0.72201678
7	2.21525080	-0.08561462	-0.26409192
6	-0.32900805	1.33930139	-0.30868650
6	-0.02335995	-0.01102474	0.08108110
7	-2.37677131	-0.43804956	-0.09704085
6	0.34631438	3.61636214	-0.90442911
1	-0.46093680	3.50673146	-1.62325383
1	1.27335622	3.87907008	-1.42458896
6	5.74116896	-0.95351723	-0.81452356
1	6.59822557	-0.50382363	-1.30434347
6	-1.13141153	-0.86792834	0.24350244
6	5.88011375	-2.18809308	-0.18292674
6	4.51992917	-0.28864619	-0.82096480
1	4.40815811	0.67189518	-1.31158115
6	-4.90088329	-3.11095475	-0.64924979
1	-5.19049948	-3.81469169	-1.42023553
6	-2.56458173	0.81726518	-0.73936755
6	4.75570830	-2.74101395	0.44507979
1	4.85074146	-3.69780834	0.94951835
6	1.24178261	3.56814281	1.75503367
1	0.32453579	3.31510491	2.30630958
1	2.05145623	3.71408592	2.47164616
6	1.59751879	2.42249591	0.80763689
1	2.57309216	2.59193022	0.34464575
1	1.64081088	1.50033760	1.38066312
6	-5.58921764	-3.07432671	0.56067768
1	-6.41445044	-3.75510555	0.73306580
6	7.19386058	-2.92171991	-0.17084359
1	7.98399900	-2.32674389	-0.63049375
1	7.11752744	-3.86430013	-0.71980071
1	7.49863420	-3.16304439	0.85049103
6	-3.49595250	-1.32546163	0.11314033
6	0.02502408	4.69482548	0.11761786
1	-0.05426137	5.66858440	-0.36622940
1	-0.92611134	4.46466257	0.61612695

6	3.40708345	-0.85388846	-0.20221589
6	3.53340175	-2.09052286	0.44226015
1	2.67809631	-2.52662087	0.94254378
6	-3.84656042	-2.23430890	-0.87801559
1	-3.31102486	-2.23203160	-1.82053703
1	-0.03209532	-2.43015760	0.85357580
1	-1.73338065	-2.77836377	0.68619093

4a/A (MeCN)

51

16	-4.24627242	1.16666319	-1.02851812
8	1.00922633	5.01539768	0.96906122
7	0.42507287	2.55120688	-0.31339488
6	-4.90591158	-2.53203295	1.54188814
1	-5.38190699	-2.62721222	2.51067072
6	-3.93350787	-1.55636793	1.34389240
1	-3.64091919	-0.88373865	2.14247459
7	1.35418637	-0.09385279	-0.11887660
7	-1.70525531	1.77261524	-0.63125030
7	-0.73828225	-2.05155698	0.47646608
7	1.77577066	-1.23279812	0.19995316
6	-0.43039976	1.50916677	-0.31557559
6	0.00513243	0.17236779	-0.03941934
7	-2.31322442	-0.44245697	-0.10203935
6	0.05842217	3.83790891	-0.91312224
1	-0.83359412	3.72057556	-1.52092573
1	0.89546284	4.14343301	-1.54930082
6	5.05703090	-2.88202993	0.39996046
1	5.45650217	-3.80810439	0.79988293
6	-1.00930502	-0.79969323	0.13201256
6	5.91362701	-1.97879689	-0.22994754
6	3.69753136	-2.61149764	0.52081505
1	3.03258850	-3.31552893	1.00965192
6	-4.64885294	-3.26246819	-0.74614194
1	-4.92561610	-3.92561444	-1.55716242
6	-2.64593011	0.83859377	-0.57742981
6	5.36821618	-0.79035785	-0.73642156
1	6.02090928	-0.07933024	-1.23364568
6	1.33309369	3.78083222	1.58238014
1	0.51235033	3.47093313	2.24417713
1	2.22977093	3.94464753	2.18137330
6	1.59719615	2.67800373	0.56163542
1	2.47098576	2.92342446	-0.04915542
1	1.78902435	1.75104434	1.09152787
6	-5.26528121	-3.38068259	0.49782065
1	-6.02411620	-4.13861424	0.65410306
6	7.38113151	-2.27023500	-0.38863517
1	7.68132674	-3.12476509	0.21929902
1	7.98461919	-1.40700858	-0.09879492
1	7.61757869	-2.49730642	-1.43232845
6	-3.33987048	-1.44046212	0.09395179
6	-0.15377174	4.88701700	0.16505848

1	-0.33905364	5.86113762	-0.28840697
1	-1.01239912	4.61258492	0.79282805
6	3.17180671	-1.42207762	0.01975634
6	4.01691261	-0.50672986	-0.61985727
1	3.61034612	0.41219820	-1.02385098
6	-3.67698934	-2.28923301	-0.95309256
1	-3.19028964	-2.17698423	-1.91546087
1	0.24186635	-2.29471114	0.60285420
1	-1.45844795	-2.76030557	0.51081233

4a/A (DMF)

51

16	-4.24723645	1.16679216	-1.03175077
8	1.01728672	5.01553877	0.96944266
7	0.42290821	2.55238818	-0.31167922
6	-4.90312968	-2.52753580	1.54826879
1	-5.37651299	-2.62075334	2.51855018
6	-3.93128232	-1.55249706	1.34574638
1	-3.63654413	-0.87838543	2.14232356
7	1.35345197	-0.09351089	-0.12293238
7	-1.70627400	1.77315802	-0.63294357
7	-0.73901305	-2.05194332	0.46995775
7	1.77435985	-1.23294286	0.19503521
6	-0.43127820	1.50978992	-0.31743383
6	0.00450481	0.17255401	-0.04372380
7	-2.31398687	-0.44200337	-0.10530688
6	0.05687920	3.83982885	-0.90993391
1	-0.83850938	3.72489942	-1.51330331
1	0.89141447	4.14303522	-1.55060136
6	5.05148889	-2.88991547	0.38944202
1	5.44754373	-3.82095118	0.78123288
6	-1.01000465	-0.79968179	0.12739082
6	5.91211578	-1.98173972	-0.22755369
6	3.69223514	-2.61801132	0.50807424
1	3.02425601	-3.32596444	0.98705374
6	-4.65161824	-3.26283911	-0.73854738
1	-4.93026707	-3.92790954	-1.54737844
6	-2.64663625	0.83917705	-0.57999224
6	5.37090043	-0.78692861	-0.72318056
1	6.02682601	-0.07159303	-1.20988382
6	1.34026320	3.77994499	1.58015020
1	0.52166822	3.47086462	2.24527254
1	2.23928677	3.94053048	2.17657949
6	1.59850050	2.67637948	0.55881772
1	2.47105141	2.91909199	-0.05490773
1	1.78969510	1.74927937	1.08877334
6	-5.26467577	-3.37866833	0.50714123
1	-6.02287523	-4.13652377	0.66704073
6	7.37922981	-2.27467370	-0.38430909
1	7.67795827	-3.13007397	0.22321558
1	7.98370208	-1.41253558	-0.09322575
1	7.61695760	-2.50164583	-1.42781646

6	-3.34079322	-1.43905360	0.09414239
6	-0.14822447	4.88890536	0.16945704
1	-0.33404245	5.86334641	-0.28321953
1	-1.00591235	4.61634238	0.79962573
6	3.17047445	-1.42251811	0.01744427
6	4.01977557	-0.50190866	-0.60880789
1	3.61696887	0.42251266	-1.00404441
6	-3.68048249	-2.29002356	-0.95018586
1	-3.19644078	-2.18029865	-1.91418636
1	0.24108908	-2.29534601	0.59643502
1	-1.45940135	-2.76043561	0.50557774

4a/A (Toluene)

51

16	-4.24049991	1.16699675	-1.00413618
8	0.98071121	5.00939725	0.97709056
7	0.42923046	2.55528064	-0.33364267
6	-4.89424107	-2.55746874	1.53263932
1	-5.37190243	-2.66095996	2.49945352
6	-3.92824319	-1.57503935	1.34231059
1	-3.64431170	-0.90280339	2.14384055
7	1.35464032	-0.10165069	-0.10633347
7	-1.70088126	1.77827842	-0.60629888
7	-0.73167758	-2.05705424	0.46282659
7	1.77394909	-1.24811208	0.19460750
6	-0.43111464	1.51088415	-0.31274298
6	0.00921253	0.17021747	-0.03528613
7	-2.31036257	-0.44313516	-0.09269312
6	0.02471607	3.84120542	-0.90931065
1	-0.87843405	3.70779326	-1.49775450
1	0.84288201	4.17477872	-1.55640084
6	5.07423027	-2.85541988	0.43222812
1	5.48569787	-3.76525467	0.85610100
6	-1.00900942	-0.79885084	0.12961581
6	5.91734347	-1.96142069	-0.22609074
6	3.71296964	-2.59803289	0.55082004
1	3.05862337	-3.29468250	1.06315920
6	-4.64185162	-3.25976892	-0.76251280
1	-4.92427416	-3.90903715	-1.58241440
6	-2.65385261	0.84867889	-0.56421082
6	5.35542703	-0.79634162	-0.76460219
1	5.99665525	-0.09438155	-1.28875772
6	1.34491070	3.77790209	1.56416846
1	0.54747835	3.43877248	2.24138410
1	2.24883132	3.95757610	2.14833907
6	1.61147704	2.69520714	0.52115110
1	2.46674179	2.97470791	-0.10201832
1	1.84165218	1.76139335	1.02267582
6	-5.25166664	-3.39666629	0.48171364
1	-6.00886331	-4.15729666	0.63072358
6	7.38798514	-2.23949020	-0.38357406
1	7.69952096	-3.08596069	0.22992061

1	7.98489770	-1.37074283	-0.09660044
1	7.62870443	-2.47206262	-1.42485133
6	-3.33536945	-1.44257135	0.09387240
6	-0.19081611	4.86884415	0.18910269
1	-0.40204525	5.84826947	-0.24102278
1	-1.03657661	4.56663040	0.82130076
6	3.17078243	-1.43015668	0.02002523
6	4.00205090	-0.52585819	-0.65066325
1	3.57592285	0.37084802	-1.08278763
6	-3.67663985	-2.27943698	-0.96152724
1	-3.20462654	-2.14379836	-1.92785252
1	0.25483441	-2.29208134	0.56019973
1	-1.45319267	-2.76258229	0.48079587

4a (MeCN)

48

8	5.36239629	-0.74898696	0.94621113
7	2.86800521	-1.09880080	-0.35246163
7	-0.63845383	-2.03915570	-0.28728394
7	0.97094911	0.18204815	-0.22740188
7	-1.16450306	-0.85233829	-0.15058761
6	1.53188744	-1.00252999	-0.29697494
6	0.65339483	-2.17590005	-0.36743834
6	3.69597456	0.09153107	-0.58407649
1	3.05955889	0.94002546	-0.81860882
1	4.34051594	-0.13077827	-1.44028818
6	-4.76397705	-0.20255098	-0.81356139
1	-5.38463141	0.29230703	-1.55360138
6	-5.37086323	-0.85302750	0.26869091
6	-3.38497798	-0.18328178	-0.96027806
1	-2.92116888	0.31876772	-1.80031493
6	-4.55567021	-1.49238503	1.20173993
1	-5.00560891	-2.00430413	2.04545763
6	4.55505598	-1.87530979	1.22816346
1	3.92113831	-1.66857395	2.10084514
1	5.22407892	-2.70396827	1.46151557
6	3.66984975	-2.26122988	0.04540981
1	4.27962182	-2.57725369	-0.80554533
1	3.04223388	-3.08710573	0.36504999
6	-6.86923822	-0.85431706	0.40919157
1	-7.34035117	-1.30940923	-0.46575668
1	-7.25034515	0.16687520	0.49037681
1	-7.18072879	-1.40865765	1.29527914
6	4.55862931	0.37747335	0.63321240
1	5.23311209	1.20790833	0.42468862
1	3.92514458	0.63433252	1.49257396
6	-2.59778790	-0.82313836	-0.00829734
6	-3.16881269	-1.47939870	1.07041156
1	-2.53481121	-1.97303956	1.79858623
6	1.06276078	-3.50791205	-0.70238885
7	1.36485504	-4.57600035	-1.00467376
6	-0.37676022	0.33374269	-0.15232595

7	-1.01019017	1.44084533	-0.02985131
6	-0.31665733	2.66208673	-0.06415184
6	-0.56015796	3.59039783	0.95513133
6	0.53663537	3.02336880	-1.11607123
6	0.05647061	4.83751052	0.93948432
1	-1.23511551	3.31781294	1.75922805
6	1.14023184	4.27608300	-1.13232542
1	0.71538892	2.32075126	-1.92171172
6	0.91006880	5.18831840	-0.10351019
1	-0.13699257	5.53908876	1.74347667
1	1.79383196	4.54137356	-1.95621611
1	1.38498310	6.16236756	-0.11911425

2-Tolyl-1,2,3-triazolopyrimidine

7a (MeCN)

49

6	5.00129390	-1.05071987	-0.07203591
6	3.74947706	-0.44395929	-0.09152224
6	2.61459065	-1.24501128	-0.07296588
6	2.71429586	-2.63401052	-0.03360715
6	3.97337137	-3.21500751	-0.01784855
6	5.13730586	-2.43845806	-0.03591754
1	5.88808840	-0.42645084	-0.08665350
1	3.65705837	0.63360966	-0.12146387
1	1.82219845	-3.24616617	-0.01463550
1	4.05416975	-4.29665932	0.01254804
6	-0.74949325	-0.41693211	-0.14753195
6	-0.13532518	0.84145833	-0.05641580
6	-2.20329113	-0.45713442	-0.23322868
6	-2.25622803	1.92384186	-0.06919298
7	1.32522286	-0.63402737	-0.09154025
7	1.17712833	0.69330493	-0.02032238
7	0.22205482	-1.33211606	-0.17277934
7	-0.84591244	2.00521284	-0.02150980
7	-2.85004297	0.69618150	-0.19007826
8	-2.90327758	2.95592696	0.00137831
6	-0.17287535	3.26935391	0.06861490
6	-0.20521473	4.14165250	-1.01396578
6	0.52440427	3.59072879	1.22783770
6	0.46332298	5.35828189	-0.92784965
1	-0.75201878	3.86647256	-1.90832635
6	1.19886588	4.80607968	1.30316314
1	0.53640975	2.89516288	2.05933518
6	1.16713986	5.69011333	0.22807912
1	0.43865777	6.04467097	-1.76620611
1	1.74512671	5.06136165	2.20366968
1	1.69027959	6.63734540	0.29029955
6	-4.35087626	-1.59646432	-0.53262213
6	-2.32617986	-2.94172608	-0.38747497
6	-4.98175220	-2.51932554	0.49834289
1	-4.56842128	-1.96324898	-1.54138012
1	-4.73219509	-0.58562695	-0.42589985

6	-3.04319282	-3.80718982	0.64012770
1	-2.47545219	-3.35600826	-1.39007149
1	-1.26457039	-2.91954763	-0.16704145
1	-6.05302085	-2.60056282	0.31377969
1	-4.82075223	-2.11459189	1.50639149
1	-2.68885345	-4.83538403	0.56507979
1	-2.83430849	-3.42780779	1.64947179
7	-2.89522358	-1.59296569	-0.36063847
8	-4.44160974	-3.82798887	0.41605722
6	6.49160598	-3.09405479	-0.01945661
1	6.60530363	-3.72768168	0.86371180
1	6.62328734	-3.73154140	-0.89757283
1	7.28805345	-2.34908134	-0.01361848

7a (DMF)
49

6	4.95960336	-1.22250516	-0.03320548
6	3.73108907	-0.56989762	-0.04079438
6	2.56800169	-1.32921935	-0.06107615
6	2.61677867	-2.72140178	-0.07325927
6	3.85369996	-3.34826979	-0.06619365
6	5.04492451	-2.61453609	-0.04616166
1	5.86858373	-0.63090560	-0.01790047
1	3.67874262	0.51083740	-0.03195589
1	1.70256558	-3.30035194	-0.08867482
1	3.89497737	-4.43265207	-0.07581017
6	-0.76364312	-0.37981670	-0.11468491
6	-0.10282126	0.85683342	-0.05128822
6	-2.21910809	-0.36758257	-0.18264039
6	-2.18258774	2.01861866	-0.08164434
7	1.30203026	-0.67185041	-0.07084713
7	1.20344712	0.66092314	-0.02246119
7	0.17358770	-1.33029983	-0.12953323
7	-0.76923635	2.04673966	-0.03151059
7	-2.82063627	0.80940789	-0.18162505
8	-2.78986844	3.07407315	-0.03476553
6	-0.05034894	3.28503003	0.05554692
6	-0.08142035	4.17390401	-1.01333179
6	0.68626276	3.56755303	1.20065202
6	0.62846919	5.36676565	-0.92768388
1	-0.66038378	3.93084397	-1.89645304
6	1.40193710	4.75894434	1.27507872
1	0.69703458	2.86106484	2.02289415
6	1.37159853	5.65944297	0.21393663
1	0.60441666	6.06591367	-1.75552067
1	1.97815852	4.98336014	2.16512584
1	1.92609157	6.58871890	0.27598442
6	-4.41216969	-1.42149912	-0.41481734
6	-2.42231405	-2.83938236	-0.37637146
6	-5.07889555	-2.43212556	0.50370051
1	-4.64492377	-1.65411381	-1.46013307
1	-4.76090895	-0.41898526	-0.18603778

6	-3.18696002	-3.78052914	0.54235282
1	-2.54237406	-3.15834624	-1.41786448
1	-1.36916666	-2.86435596	-0.11770985
1	-6.14994174	-2.45795225	0.30230754
1	-4.91905422	-2.14279061	1.55104198
1	-2.85476899	-4.80454976	0.37054046
1	-2.99230290	-3.51297222	1.58973003
7	-2.95704440	-1.48167034	-0.24540609
8	-4.57896304	-3.74048791	0.28856481
6	6.37467797	-3.31816253	-0.03836292
1	6.47031729	-3.95787478	0.84277452
1	6.48076812	-3.95732331	-0.91860939
1	7.19714048	-2.60198363	-0.03295115

7a (Toluene)

49

6	4.98851711	-1.10441903	-0.05927602
6	3.74428639	-0.48412195	-0.06904223
6	2.60160550	-1.27349093	-0.07237098
6	2.68733803	-2.66318158	-0.06508911
6	3.93961936	-3.25722771	-0.05673055
6	5.11076140	-2.49299301	-0.05348821
1	5.88162529	-0.48929825	-0.05764242
1	3.65636843	0.59413004	-0.07558076
1	1.78631474	-3.26182478	-0.06695161
1	4.00995203	-4.33996391	-0.05162529
6	-0.74965019	-0.40179294	-0.12243884
6	-0.11678483	0.85180064	-0.06064321
6	-2.20524296	-0.42203057	-0.18502797
6	-2.23258763	1.96242986	-0.07346148
7	1.32070124	-0.64809526	-0.08316440
7	1.19359030	0.68114306	-0.03370792
7	0.20659402	-1.33266779	-0.13970267
7	-0.81103501	2.02668838	-0.03756893
7	-2.83444426	0.73060921	-0.17183387
8	-2.86686825	2.99334616	-0.01926393
6	-0.12787475	3.28386713	0.05667477
6	-0.33896671	4.25784449	-0.91322342
6	0.74908035	3.51126936	1.11187014
6	0.33419038	5.46976900	-0.82171665
1	-1.03419404	4.06684372	-1.72057081
6	1.42628249	4.72316437	1.19091816
1	0.89965844	2.74601732	1.86359887
6	1.22006407	5.70370392	0.22636879
1	0.16671551	6.23210382	-1.57320697
1	2.10983637	4.90132021	2.01254927
1	1.74438120	6.64969507	0.29300492
6	-4.37670638	-1.52009536	-0.40345424
6	-2.36175668	-2.90239233	-0.39214098
6	-5.01280604	-2.53987526	0.52673570
1	-4.62218479	-1.76092911	-1.44438216
1	-4.73004792	-0.51760798	-0.17817576

6	-3.09651279	-3.85688979	0.53962743
1	-2.49438036	-3.22912635	-1.43043931
1	-1.30249559	-2.90323978	-0.15574367
1	-6.08578326	-2.59320868	0.34175237
1	-4.84632161	-2.24300072	1.57129617
1	-2.75680095	-4.87831020	0.36484324
1	-2.88643411	-3.58595444	1.58390006
7	-2.92026295	-1.55851038	-0.25062916
8	-4.48975214	-3.83777951	0.30950404
6	6.45867889	-3.16259823	-0.04576759
1	6.57273172	-3.80084010	0.83399668
1	6.58482564	-3.79470844	-0.92835983
1	7.26398267	-2.42724174	-0.03787622