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Supporting information

Design, synthesis, and photophysics of bi- and tricyclic fused pyrazolines

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1. Experimental Section

General. ^{1}H NMR and ^{13}C NMR spectra were recorded at 400 MHz for ^{1}H and 100 MHz for ^{13}C spectrometer in DMSO-d_6, $CDCl_3$ or $(CD_3)_2CO$-d_6. Chemical shifts (δ scale) are reported in parts per million (ppm) relative to TMS in ^{1}H NMR and to the residual solvent signals in ^{13}C NMR spectra. The ^{13}C NMR signal patterns for compounds **6h,i** were analyzed by BB (broadband) and for all compounds by APT (attached proton test) and are described as follows: + for secondary or quaternary carbon atom (positive signal), - for primary or tertiary carbon atom (negative signal). The values of the coupling constants (*J*) are given in Hertz (Hz). The 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 mass-spectrometer using the electron ionization (EI) technique (40-200 °C, 70 eV). The abbreviation $[M]^+$ refers to the molecular ion. The IR spectra were obtained with a FT-IR ATR (attenuated total reflection, ZnSe) spectrometer in the 4000-500 cm^{-1} region. Elemental analysis was carried out using a CHNS/O analyser. Melting points were determined using a microscopic melting point meter without correction. The reactions were monitored by analytical thin-layer chromatography (TLC) on aluminium-backed silica-gel plates (Sorbfil UV–254). Visualization of the components was accomplished by short wavelength UV-light (254 nm).

Microwave-heated reactions were carried out in an Anton Paar Monowave 300 microwave synthesis reactor in sealed microwave Pyrex vessels (4-30 mL). The temperature was controlled by external IR sensor. The pressure was monitored by an integrated hydraulic pressure sensor.

3-Chloropentane-2,4-dione and ethyl 2-chloro-3-oxobutanoate, were commercially available. Arylhydrazonoyl chlorides **3a**,**c-i** were synthezised via the Japp–Klingemann reaction as reported previously[2-4]. Commercially available chemicals and solvents were used without further purification. The products were purified by column chromatography on silica gel (0.035–0.070, 60Å) and re-crystallized from ethanol.

General procedure for the synthesis of arylhydrazonoyl chlorides 1b,j,k. An aqueous solution of the corresponding amine (10.0 mmol) in concentrated HCl (30 mmol) was cooled to 0-5 ^{o}C, and a solution of sodium nitrite (11.0 mmol) in 10 mL of water was added dropwise under stirring during 30 min to give aryldiazonium salt. 3-chloropentane-2,4-dione or ethyl 2-chloro-3-oxo-butanoate (10.0 mmol) and sodium acetate in ethanol was added dropwise at 0-5 ^{o}C under stirring. The reaction mixture was left overnight at the temperature of 0-5 ^{o}C, and the next day precipitate was filtered off.

Ethyl 2-(2-(4-acetamidophenyl)hydrazono)-2-chloroacetate (1b). Yellow powder (1.95 g, 69 %). R_f = 0.36 ($CHCl_3$/Hex/Me_2CO, 3:1:1), mp 200-205 ^{o}C. IR (cm^{-1}): 3346, 3214 (N-H), 3065, 2993, 2976, 2934, 2904 (C-H), 1699, 1672 (C=O). ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.30 (t, *J* = 7.1 Hz, 3H), 2.02 (s, 3H), 4.29 (q, *J* = 7.1 Hz, 2H), 7.29 and 7.54 (AA'XX', *J* = 8.9 Hz, 4H), 9.86 (s, 1H), 10.48 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ (-) 14.1, (-) 23.8, (+) 62.0, (+) 112.8, (-) 114.8 (2C), (-) 120.0 (2C), (+) 134.4, (+)

138.1, (+) 159.4, (+) 167.8. Anal. Calcd for $C_{12}H_{14}ClN_3O_3$: C, 50.80; H, 4.97; N, 14.81; O, 16.92. Found: C, 50.7; H, 5.0; N, 14.6; O, 17.1. EIMS (70 eV) *m/z*: M-176 (100), M^+ 283 (9).

Ethyl 2-chloro-2-(2-(4-cyanophenyl)hydrazono)acetate (1g). Yellow powder (2.43 g, 97 %). R_f = 0.58 (Hex/EtOAc, 1:1), mp 175-180 °C. IR (cm^{-1}): 3249 (N-H), 3083, 3047, 2994, 2978, 2931, 2908 (C-H), 2219 (C≡N), 1701 (C=O). ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.38 (t, *J* = 7.1 Hz, 3H), 4.33 (q, *J* = 7.1 Hz, 2H), 7.50 and 7.62 (AA'XX', *J* = 8.8 Hz, 4H), 10.76 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ (-) 14.0, (+) 62.5, (+) 103.7, (-) 114.8 (2C), (+) 116.7, (+) 119.2, (-) 133.7 (2C), (+) 146.4, (+) 158.9. Anal. Calcd for $C_{11}H_{10}ClN_3O_2$: C, 52.50; H, 4.01; N, 16.70; O, 12.71. Found: C, 52.3; H, 4.2; N, 16.5; O, 12.8. EIMS (70 eV) *m/z*: M-135 (100), M^+ 251 (12).

***N*-(4-Cyanophenyl)-2-oxopropanehydrazonoyl chloride (1k).** Yellow powder (2.01 g, 91 %). R_f = 0.51 ($CHCl_3$/Me_2CO, 5:1), mp 195-200 °C. IR (cm^{-1}): 3224 (NH), 3081, 2976 (C-H), 2224 (C≡N), 1688 (C=O). ^{1}H NMR (400 MHz, $(CD_3)_2CO$-d_6): δ 2.58 (s, 3H), 7.63 and 7.77 (AA'XX', *J* = 8.8 Hz, 4H), 10.19 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ (-) 25.4, (+) 104.0, (-) 115.1 (2C), (+) 119.2, (+) 125.4, (-) 133.7 (2C), (+) 146.2, (+) 188.1. Anal. Calcd for $C_{10}H_8ClN_3O$: C, 54.19; H, 3.64; N, 18.96; O, 7.22. Found: C, 54.0; H, 3.7; N, 19.1; O, 7.0. EIMS (70 eV) *m/z*: M-178 (100), M^+ 221 (4).

General procedure for the synthesis of Me-DPPs 2, Ph-DPPs 3 and HMIs 4. A solution of arylhydrazonoyl chloride **1a-k** (1.0 mmol), *N*-methylmaleimide **5**, *N*-phenylmaleimide **6** or norbornene **7** (1.0 mmol) and 0.14 mL (3.0 mmol) TEA in *m*-xylene (4.0 mL) was stirring at 150 °C for 15-180 min under microwave irradiation. The crude product was purified by column chromatography or re-crystallized from ethanol to give pyrazoline derivatives **2a-k, 3a-e, 4a-d**.

Ethyl 1-(4-methoxyphenyl)-5-methyl-4,6-dioxo-1,3a,4,5,6,6*a*-hexahydropyrrolo[3,4-c]pyrazole-3-carboxylate (2a). Green powder (258 mg, 78 %). R_f = 0.63 (Hex/EtOAc, 1:1), mp 160-164 °C. IR (cm^{-1}): 2989, 2958, 2910 (C-H), 1780, 1706 (C=O). ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.30 (t, *J* = 7.0 Hz, 3H), 2.87 (s, 3H), 3.75 (s, 3H), 4.27 (q, *J* = 6.7 Hz, 2H), 4.78 and 5.49 (AB, *J* = 11.2 Hz, 2H), 6.98 and 7.42 (AA'XX', *J* = 8.9 Hz, 4H). ^{13}C NMR (100 MHz, DMSO-d_6): δ (-) 14.1, (-) 25.1, (-) 53.0, (-) 55.3, (+) 60.7, (-) 66.5, (-) 114.4 (2C), (-) 116.3 (2C), (+) 133.6, (+) 136.0, (+) 155.1, (+) 160.5, (+) 171.6, (+) 172.5. Anal. Calcd for $C_{16}H_{17}N_3O_5$: C, 58.00; H, 5.17; N, 12.68. Found: C, 58.2; H, 5.0; N, 12.7. EIMS (70 eV) *m/z*: M^+ 331 (100). HRMS (ESI/Q-TOF): m/z calcd for $C_{16}H_{17}N_3O_5$+H^+: 332.1241 $[M+H]^+$ found 332.1250.

Ethyl 1-(4-acetamidophenyl)-5-methyl-4,6-dioxo-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (2b). Yellow powder (204 mg, 57 %). R_f = 0.21 ($CHCl_3$/Me_2CO/Hex, 3:1:1), mp 250-255 °C. IR (cm^{-1}): 3347 (N-H), 3000, 2973, 2903 (C-H), 1785, 1697, 1682 (C=O). ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.37 (t, *J* = 7.1 Hz, 3H), 2.03 (s, 3H), 2.93 (s, 3H), 4.30 (q, *J* = 7.0 Hz, 2H), 4.76 and 5.45 (AB, *J* = 11.2 Hz, 2H), 7.43 and 7.56 (AA'XX', *J* = 9.0 Hz, 4H), 9.72 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): (-) 14.1, (-) 23.8, (-) 25.2, (-) 53.0, (+) 60.7, (-) 66.1, (-) 115.1 (2C), (-) 119.9 (2C), (+) 134.1, (+) 134.4, (+) 137.6, (+) 160.5, (+) 167.9, (+) 171.5, (+) 172.4. Anal. Calcd for $C_{17}H_{18}N_4O_5$: C, 56.98; H, 5.06; N, 15.63. Found: C, 57.1; H, 5.0; N, 15.5. EIMS (70 eV) *m/z*: M-315 (100), M^+ 358 (36).

Ethyl 5-methyl-4,6-dioxo-1-(*p*-tolyl)-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (2c). Beige powder (249 mg, 79 %). R_f = 0.30 (Hex/Me_2CO, 3:2), 0.32 ($CHCl_3$/Me_2CO, 5:1), mp 259-263 °C. IR (cm^{-1}): 2988, 2954 (C-H), 1787, 1709 (C=O). ^1H NMR (400 MHz, DMSO-d_6): δ 1.30 (t, *J* = 7.1, 3H), 2.28 (s, 3H), 2.87 (s, 3H), 4.28 (qd, *J* = 7.0, 1.1 Hz, 2H), 4.79 and 5.51 (AB, *J* = 11.2 Hz, 2H), 7.19 and 7.38 (AA'XX', *J* = 8.6 Hz, 4H). ^{13}C NMR (100 MHz, DMSO-d_6): δ (-) 14.1, (-) 20.2, (-) 25.1, (-) 53.0, (+) 60.7, (-) 66.1, (-) 114.9 (2C), (-) 129.5 (2C), (+) 131.4, (+) 134.3, (+) 140.0, (+) 160.5, (+) 171.5, (+) 172.4. Anal. Calcd for $C_{16}H_{17}N_3O_4$: C, 60.94; H, 5.43; N, 13.33. Found: C, 60.7; H, 5.5; N, 13.4. EIMS (70 eV) *m/z*: M^+ 315 (100). HRMS (ESI/Q-TOF): m/z calcd for $C_{16}H_{17}N_3O_4+H^+$: 316.1292 $[M+H]^+$ found 316.1301.

Ethyl 5-methyl-4,6-dioxo-1-phenyl-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (2d). Light yellow powder (241 mg, 80 %). R_f = 0.34 ($CHCl_3$/Me_2CO, 5:1), 0.55 (Hex/EtOAc, 1:2), 0.53 (Hex/EtOAc, 2:3), mp 148-149 °C. IR (cm^{-1}): 2984, 2969 (C-H), 1789, 1704 (C=O). ^1H NMR (400 MHz, DMSO-d_6): δ 1.39 (t, *J* = 7.1 Hz, 3H), 2.94 (s, 3H), 4.32 (qd, *J* = 7.0, 1.0 Hz, 2H), 4.78 and 5.47 (AB, *J* = 11.2 Hz, 2H), 7.02 (t, *J* = 7.3 Hz, 1H), 7.33 (dd, *J* = 8.6, 7.5 Hz, 2H), 7.53-7.55 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ (-) 14.1, (-) 25.2, (-) 53.1, (+) 60.8, (-) 65.9, (-) 114.7 (2C), (-) 122.3, (-) 129.1 (2C), (+) 134.9, (+) 142.2, (+) 160.4, (+) 171.4, (+) 172.4. Anal. Calcd for $C_{15}H_{15}N_3O_4$: C, 59.80; H, 5.02; N, 13.95. Found: C, 59.7; H, 5.2; N, 13.7. EIMS (70 eV) *m/z*: M^+ 301 (100). HRMS (ESI/Q-TOF): m/z calcd for $C_{15}H_{15}N_3O_4$+H+: 302.1135 $[M+H]^+$ found 302.1141.

Ethyl 1-(4-chlorophenyl)-5-methyl-4,6-dioxo-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (2e). White powder (258 mg, 77 %). R_f = 0.50 (Hex/EtOAc, 1:1), mp 163-167 °C. IR (cm^{-1}): 2995, 2948, 2909 (C-H), 1789, 1711 (C=O). ^1H NMR (400 MHz, DMSO-d_6): δ 1.37 (t, *J* = 7.1 Hz, 3H), 2.92 (s, 3H), 4.31 (q, *J* = 7.0 Hz, 2H), 4.79 and 5.50 (AB, *J* = 11.1 Hz, 2H), 7.34 and 7.51 (AA'XX', *J* = 9.0 Hz, 4H). ^{13}C NMR (100 MHz, DMSO-d_6): δ (-) 14.1, (-) 25.2, (-) 53.3, (+) 60.9, (-) 65.8, (-) 116.3 (2C), (+) 126.0, (-) 128.9 (2C), (+) 135.7, (+) 141.1, (+) 160.3, (+) 171.3, (+) 172.3. Anal. Calcd for $C_{15}H_{14}ClN_3O_4$: C, 53.66; H, 4.20; N, 12.52. Found: C, 53.9; H, 4.1; N, 12.5. EIMS (70 eV) *m/z*: M-249 (100), M^+ 335 (49).

Ethyl 5-methyl-4,6-dioxo-1-(4-(trifluoromethyl)phenyl)-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (2f). Beige powder (260 mg, 71 %). R_f = 0.50 ($CHCl_3$/EtOAc, 10:1), mp 215-216 °C. IR (cm^{-1}): 2992, 2971, 2945, 2926, 2909 (C-H), 1789, 1715 (C=O). ^1H NMR (400 MHz, DMSO-d_6): δ 1.31 (t, *J* = 7.1 Hz, 3H), 2.87 (s, 3H), 4.31 (qd, *J* = 7.0, 1.2 Hz, 2H), 4.84 and 5.64 (AB, *J* = 11.0 Hz, 2H), 7.62 and 7.74 (AA'XX', *J* = 8.8 Hz, 4H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 14.1, 25.2, 53.4, 61.1, 65.3, 114.7 (2C), 122.0 (q, *J* = 32.0 Hz), 124.5 (q, *J* = 271.0 Hz), 126.4 (q, *J* = 3.7 Hz, 2C), 137.2, 145.1, 160.2, 171.0, 172.2. Anal. Calcd for $C_{16}H_{14}F_3N_3O_4$: C, 52.04; H, 3.82; N, 11.38. Found: C, 51.8; H, 3.9; N, 11.1. EIMS (70 eV) *m/z*: M^+ 369 (100).

Ethyl 1-(4-cyanophenyl)-5-methyl-4,6-dioxo-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (2g). Beige powder (251 mg, 78 %). R_f = 0.53 ($CHCl_3$/Me_2CO, 5:1), 0.56 (Hex/EtOAc, 1:1), mp 215-216 °C. IR (cm^{-1}): 2985, 2949 (C-H), 2217 (C≡N), 1793, 1714 (C=O). ^1H NMR (400 MHz, DMSO-d_6): δ 1.31 (t, *J* = 7.1 Hz, 3H), 2.86 (s, 3H), 4.34 (qd, *J* = 7.1, 2.0 Hz, 2H), 4.83 and 5.65 (AB, *J* = 10.9 Hz,

2H), 7.57 and 7.81 (AA'XX', *J* = 8.9 Hz, 4H). ^{13}C NMR (100 MHz, DMSO-d_6): δ (-) 14.0, (-) 25.2, (-) 53.5, (+) 61.2, (-) 65.0, (+) 103.5, (-) 115.0 (2C), (+) 119.1, (-) 133.4 (2C), (+) 138.1, (+) 145.5, (+) 160.0, (+) 170.8, (+) 172.1. Anal. Calcd for $C_{16}H_{14}N_4O_4$: C, 58.89; H, 4.32; N, 17.17. Found: C, 58.8; H, 4.3; N, 17.1. EIMS (70 eV) *m/z*: M^+ 326 (100).

Ethyl 1-(2-chlorophenyl)-5-methyl-4,6-dioxo-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (2h). White powder (228 mg, 68 %). R_f = 0.59 (Hex/EtOAc, 1:1), mp 165-170 ºC. IR (cm^{-1}): 2991, 2964 (C-H), 1779, 1729, 1702 (C=O). ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.28 (t, *J* = 7.1 Hz, 3H), 2.81 (s, 3H), 4.21-4.29 (m, 2H), 4.78 and 5.69 (AB, *J* = 10.9 Hz, 2H), 7.28-7.33 (m, 1H), 7.37-7.39 (m, 2H), 7.54 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ (-) 14.1, (-) 25.0, (-) 52.9, (+) 60.8, (-) 65.8, (-) 126.3, (+) 127.1, (-) 127.8, (-) 128.0, (-) 130.3, (+) 136.1, (+) 139.1, (+) 160.3, (+) 171.6, (+) 171.7. Anal. Calcd for $C_{15}H_{14}ClN_3O_4$: C, 53.66; H, 4.20; N, 12.52. Found: C, 53.7; H, 4.1; N, 12.4. EIMS (70 eV) *m/z*: M^+ 335 (100).

3-Acetyl-5-methyl-1-(*p*-tolyl)-3*a*,6*a*-dihydropyrrolo[3,4-*c*]pyrazole-4,6(1*H*,5*H*)-dione (2i). Bright yellow crystals (215 mg, 75 %). R_f = 0.38 (Hex/EtOAc, 1:1), mp 167-169 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.28 (s, 3H), 2.41 (s, 3H), 2.84 (s, 3H), 4.76 and 5.53 (AB *J* = 11.1 Hz, 2H), 7.20 and 7.45 (AA'XX', *J* = 8.4 Hz, 4H). ^{13}C NMR (100 MHz, DMSO-d_6: δ 20.2, 25.1, 25.8, 51.7, 66.3, 115.1 (2C), 129.5 (2C), 131.7, 139.6, 141.8, 171.3, 172.2, 190.6. Anal. Calcd for $C_{15}H_{15}N_3O_3$: C, 63.15; H, 5.30; N, 14.73. Found: C, 62.9; H, 5.4; N, 14.6. EIMS (70 eV) *m/z*: M-242 (100), M^+ 285 (80.8).

3-Acetyl-5-methyl-1-phenyl-3*a*,6*a*-dihydropyrrolo[3,4-c]pyrazole-4,6(1*H*,5*H*)-dione (2j). Yellow crystals (245 mg, 91%). R_f = 0.40 (Hex/EtOAc, 1:1), mp 209-211 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.42 (s, 3H), 2.84 (s, 3H), 4.77 and 5.57 (AB, *J* = 11.0 Hz, 2H), 7.07 (t, *J* = 7.3 Hz, 1H), 7.40 (t, *J* = 7.9, 2H), 7.55 (d, *J* = 8.0, 2H). ^{13}C NMR (100 MHz, DMSO-d_6: δ 25.2, 25.8, 51.8, 66.1, 115.0 (2C), 122.6, 129.1 (2C), 141.9, 142.4, 171.2, 172.3, 190.8. Anal. Calcd for $C_{14}H_{13}N_3O_3$: C, 61.99; H, 4.83; N, 15.49. Found: C, 62.1; H, 4.9; N, 15.4. EIMS (70 eV) *m/z*: M-100 (100), M^+ 271 (72.2).

4-(3-Acetyl-5-methyl-4,6-dioxo-4,5,6,6*a*-tetrahydropyrrolo[3,4-*c*]pyrazol-1(3*aH*)-yl)benzonitrile (2k). Beige powder (260 mg, 88 %). R_f = 0.43 ($CHCl_3$/Me_2CO, 5:1), mp 226-227 ºC. IR (cm^{-1}): 2985, 2961, 2926, 2858 (C-H), 2215 (C≡N), 1784, 1698, 1679 (C=O). ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.46 (s, 3H), 2.85 (s, 3H), 4.81 and 5.67 (AB, *J* = 10.8 Hz, 2H), 7.66 and 7.85 (AA'XX', *J* = 8.8 Hz, 4H). ^{13}C NMR (100 MHz, DMSO-d_6): δ (-) 25.2, (-) 26.1, (-) 52.2, (-) 65.3, (+) 103.7, (-) 115.2 (2C), (+) 119.1, (-) 133.5 (2C), (+) 144.8, (+) 145.3, (+) 170.7, (+) 172.1, (+) 191.1. Anal. Calcd for $C_{15}H_{12}N_4O_3$: C, 60.81; H, 4.08; N, 18.91. Found: C, 61.0; H, 4.2; N, 18.4. EIMS (70 eV) *m/z*: M-253 (100), M^+ 296 (30).

Ethyl 4,6-dioxo-5-phenyl-1-(*p*-tolyl)-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (3a). Pale beige powder (253 mg, 66 %). R_f = 0.28 ($CHCl_3$/Me_2CO, 5:1), mp 232-233 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.31 (t, *J* = 7.1 Hz, 3H), 2.29 (s, 3H), 4.30 (q, *J* = 6.8 Hz, 2H), 4.97 and 5.68 (AB, *J* = 11.4 Hz, 2H), 7.21 (d, *J* = 7.8 Hz, 2H), 7.32 (d, *J* = 7.8 Hz, 2H), 7.37-7.57 (m, 5H). ^{13}C NMR (100 MHz, DMSO-d_6: δ 14.1, 20.2, 53.3, 60.8, 66.4, 114.9 (2C), 127.1 (2C), 128.7 (2C), 128.9, 129.5 (2C), 131.4, 131.9, 134.4,

140.1, 160.5, 170.6, 171.6. Anal. Calcd for $C_{21}H_{19}N_3O_4$: C, 66.83; H, 5.07; N, 11.13. Found: C, 66.9; H, 4.9; N, 11.3. (70 eV) *m/z*: M^+ 377 (100). HRMS (ESI/Q-TOF): m/z calcd for $C_{21}H_{19}N_3O_4+H^+$: 378.1448 $[M+H]^+$ found 378.1459.

Ethyl 1-(4-cyanophenyl)-4,6-dioxo-5-phenyl-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (3b). Beige powder (268 mg, 69 %). R_f = 0.26 ($CHCl_3$/Me_2CO, 5:1), mp 209-210 °C. IR (cm^{-1}): 3070, 3054, 2984, 2975, 2956, 2927, 2874, 2861 (C-H), 2216 (C≡N), 1791, 1721 (C=O). ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.39 (t, *J* = 7.1 Hz, 3H), 4.32 (qd, *J* = 7.1, 1.0 Hz, 2H), 4.97 and 5.76 (AB, *J* = 11.2 Hz, 2H), 7.31 (d, *J* = 7.3 Hz, 2H), 7.42-7.50 (m, 3H), 7.67 and 7.73 (AA'XX', *J* = 8.9 Hz, 4H).^{13}C NMR (100 MHz, DMSO-d_6): δ (-) 14.1, (-) 53.7, (+) 61.2, (-) 65.4, (+) 103.5, (-) 115.1 (2C), (+) 119.1, (-) 127.1 (2C), (-) 128.8 (2C), (-) 128.9, (+) 131.9, (-) 133.5 (2C), (+) 138.2, (+) 145.6, (+) 160.1, (+) 169.9, (+) 171.3. Anal. Calcd for $C_{21}H_{16}N_4O_4$: C, 64.94; H, 4.15; N, 14.43. Found: C, 65.0; H, 4.3; N, 14.2. EIMS (70 eV) *m/z*: M^+ 388 (100). HRMS (ESI/Q-TOF): m/z calcd for $C_{21}H_{16}N_4O_4+H^+$: 389.1244 $[M+H]^+$ found 389.1244.

3-Acetyl-5-phenyl-1-(*p*-tolyl)-3*a*,6*a*-dihydropyrrolo[3,4-*c*]pyrazole-4,6(1*H*,5*H*)-dione (3c). Pale yellow powder (245 mg, 70 %). R_f = 0.42 (Hex/EtOAc, 1:1), mp 247-249 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.29 (s, 3H), 2.47 (s, 3H), 4.94 and 5.70 (AB, *J* = 11.3 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.4 Hz, 2H), 7.40-7.55 (m, 5H). ^{13}C NMR (100 MHz, DMSO-d_6: δ 20.2, 25.9, 52.0, 66.7, 115.2 (2C), 127.1 (2C), 128.7, 128.9, 129.5 (2C), 131.8 (2C), 132.0, 139.8, 142.0, 170.4, 171.5, 190.7. Anal. Calcd for $C_{20}H_{17}N_3O_3$: C, 69.15; H, 4.93; N, 12.10. Found: C, 69.0; H, 5.1; N, 12.2. EIMS (70 eV) *m/z*: M-162 (100), M^+ 347 (72.7).

3-Acetyl-1,5-diphenyl-3*a*,6*a*-dihydropyrrolo[3,4-*c*]pyrazole-4,6(1*H*,5*H*)-dione (3d). Light yellow powder (300 mg, 90 %). R_f = 0.43 (Hex/EtOAc, 1:1), mp 221-222 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.60 (s, 3H), 5.06 and 5.51 (AB, *J* = 11.3 Hz, 2H), 7.16 (t, *J* = 7.3 Hz, 1H), 7.31 (d, *J* = 7.7 Hz, 2H), 7.41-7.50 (m, 5H), 7.71 (d, *J* = 8.1 Hz, 2H).^{13}C NMR (100 MHz, DMSO-d_6): δ 26.0, 52.0, 66.5, 115.1 (2C), 122.6, 127.1 (2C), 128.7, 128.9 (2C), 129.1 (2C), 132.0, 142.0, 142.6, 170.3, 171.5, 190.8. Anal. Calcd for $C_{19}H_{15}N_3O_3$: C, 68.46; H, 4.54; N, 12.61. Found: C, 68.6; H, 4.3; N, 12.7. EIMS (70 eV) *m/z*: M-162 (100), M^+ 333 (63.0).

4-(3-Acetyl-4,6-dioxo-5-phenyl-4,5,6,6*a*-tetrahydropyrrolo[3,4-*c*]pyrazol-1(3*aH*)-yl)benzonitrile (3e). Light yellow powder (260 mg, 73 %). R_f = 0.26 (Hex/EtOAc, 1:1), mp 245-247 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.48 (s, 3H), 4.96 (d, *J* = 11.0 Hz, 1H), 5.81 (d, *J* = 11.0 Hz, 1H), 7.24-7.54 (m, 5H), 7.69 and 7.86 (AA'XX', *J* = 8.4 Hz, 4H). ^{13}C NMR (100 MHz, DMSO-d_6: δ 26.2, 52.5, 66.7, 103.8, 115.3 (2C), 119.2, 127.1 (2C), 128.7, 128.9 (2C), 131.9, 133.5 (2C), 145.0, 145.4, 169.8, 171.3, 191.1. Anal. Calcd for $C_{20}H_{14}N_4O_3$: C, 67.03; H, 3.94; N, 15.63. Found: C, 67.2; H, 4.1; N, 15.7. EIMS (70 eV) *m/z*: M-162 (100), M^+ 358 (74.4).

Ethyl 1-(*p*-tolyl)-3a,4,5,6,7,7*a*-hexahydro-1*H*-4,7-methanoindazole-3-carboxylate (4a). Light yellow crystals (200 mg, 66 %). R_f = 0.27 ($CHCl_3$/Me_2CO, 5:1), mp 41-42 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.20 (d, J = 10.5 Hz, 1H), 1.30-1.42 (m, 6H), 1.55-1.64 (m, 2H), 2.29 (s, 3H), 2.68 (br s, 1H), 2.78 (s, 1H), 3.41

and 4.21 (AB, *J* = 10.0 Hz, 2H), 7.08-7.12 (m, 4H), ^{13}C NMR (100 MHz, $DCCl_3$): δ 14.5, 20.7, 24.7, 27.7, 33.2, 40.9, 41.6, 54.2, 60.9, 69.4, 114.0 (2C), 129.7 (2C), 130.5, 140.1, 140.3, 163.2. Anal. Calcd for $C_{18}H_{22}N_2O_2$: C, 72.46; H, 7.43; N, 9.39. Found: C, 72.7; H, 7.3; N, 9.2. EIMS (70 eV) *m/z*: M^+ 298 (100).

Ethyl 1-(4-cyanophenyl)-3*a*,4,5,6,7,7*a*-hexahydro-1*H*-4,7-methanoindazole-3-carboxylate (4b). Yellow powder (229 mg, 74 %). R_f = 0.43 ($CHCl_3$/Me_2CO, 5:1), mp 115-116 °C. IR (cm^{-1}): 2954, 2928, 2874, 2852 (C-H), 2209 (C≡N), 1698 (C=O). ^{1}H NMR (400 MHz, $CDCl_3$): 1.25-1.32 (m, 1H), 1.33-1.49 (m, 6H), 1.60-1.74 (m, 2H), 2.74 (s, 1H), 2.79 (s,1H), 3.49 (d, J = 9.6 Hz, 1H), 4.23 (d, J = 9.6 Hz, 1H), 4.31-4.45 (m, 2H), δ 7.24 and 7.58 (AA'XX', *J* = 8.5, 4H). ^{13}C NMR (100 MHz, $DCCl_3$): δ 14.5, 24.7, 27.7, 33.2, 40.7, 41.3, 54.9, 61.5, 68.7, 103.1, 113.9 (2C), 119.8, 133.6 (2C), 144.7, 145.7, 162.5. Anal. Calcd for $C_{18}H_{19}N_3O_2$: C, 69.88; H, 6.19; N, 13.58. Found: C, 69.9; H, 6.3; N, 13.7. EIMS (70 eV) *m/z*: M^+ 309 (100).

1-(1-*p*-Tolyl-3*a*,4,5,6,7,7*a*-hexahydro-1*H*-4,7-methanoindazol-3-yl)ethan-1-one (4c). Orange powder (238 mg, 89 %). R_f = 0.58 (Hex/EtOAc, 1:1), mp 78-80 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.10-1.15 (m, 2H), 1.30-1.38 (m, 2H), 1.46-1.55 (m, 2H), 2.26 (s, 3H), 2.34 (s, 3H), 2.49 (s, 1H), 2.67 (s, 1H), 3.34 (s, 1H), 4.36 (d, *J* = 9.9, 1H), 7.15 (s, 4H). ^{13}C NMR (100 MHz, DMSO-d_6: δ 20.2, 23.8, 25.3, 26.9, 32.5, 41.0, 51.8, 68.9, 113.9 (2C), 129.7 (2C), 130.1, 139.4, 148.4, 192.3. Anal. Calcd for $C_{17}H_{20}N_2O$: C, 76.09; H, 7.51; N, 10.44. Found: C, 76.2; H, 7.4; N, 10.6. EIMS (70 eV) *m/z*: M-43 (100), M^+ 268 (92.8).

1-(1-Phenyl-3*a*,4,5,6,7,7*a*-hexahydro-1*H*-4,7-methanoindazol-3-yl)ethan-1-one (4d). Dark golden crystals (205 mg, 81 %). R_f = 0.68 (Hex/EtOAc, 1:1), mp 119-121 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.18 (d, *J* = 10.5 Hz, 1H), 1.31 (t, *J* = 9.9 Hz, 2H), 1.41 (t, *J* = 9.0 Hz, 1H), 1.51-1.67 (m, 2H), 2.45 (s, 3H), 2.67 (br s, 1H), 2.79 (s, 1H), 3.40 and 4.22 (AB, *J* = 9.8 Hz, 2H), 6.97 (t, *J* = 7.3 Hz, 1H), 7.56 (d, *J* = 7.9 Hz, 2H), 7.32 (t, *J* = 7.9 Hz, 2H). ^{13}C NMR (100 MHz, $DCCl_3$): δ 24.6, 25.7, 27.7, 33.1, 40.4, 41.6, 52.7, 69.7, 114.1 (2C), 121.5, 129.4 (2C), 142.2, 149.4, 194.0. Anal. Calcd for $C_{16}H_{18}N_2O$: C, 75.56; H, 7.13; N, 11.01. Found: C, 75.7; H, 7.0; N, 11.2. EIMS (70 eV) *m/z*: M-43 (100), M^+ 254 (80).

4-(3-acetyl-3*a*,4,5,6,7,7a-hexahydro-1*H*-4,7-methanoindazol-1-yl)benzonitrile (4e). Golden crystals (210 mg, 75 %). R_f = 0.62 (Hex/EtOAc, 1:1), mp 149-150 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.20-1.26 (m, 2H), 1.32 (t, *J* = 8.9 Hz, 1H), 1.42 (t, *J* = 8.0 Hz, 1H), 2.45 (s, 3H), 2.68 (br s, 1H), 2.75 (br s, 1H), 3.42 and 4.19 (AB, *J* = 9.5 Hz, 2H), 7.22 and 7.56 (AA'XX', *J* = 8.6, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.5, 26.0, 27.6, 33.1, 40.3, 41.3, 53.3, 69.1, 103.4, 114.1 (2C), 119.7, 133.6 (2C), 145.5, 152.0, 194.1. Anal. Calcd for $C_{17}H_{17}N_3O$: C, 73.10; H, 6.13; N, 15.04. Found: C, 73.0; H, 6.3; N, 15.2. EIMS (70 eV) *m/z*: M-43 (100), M^+ 279 (76.2).

2. ^{1}H and ^{13}C NMR spectra

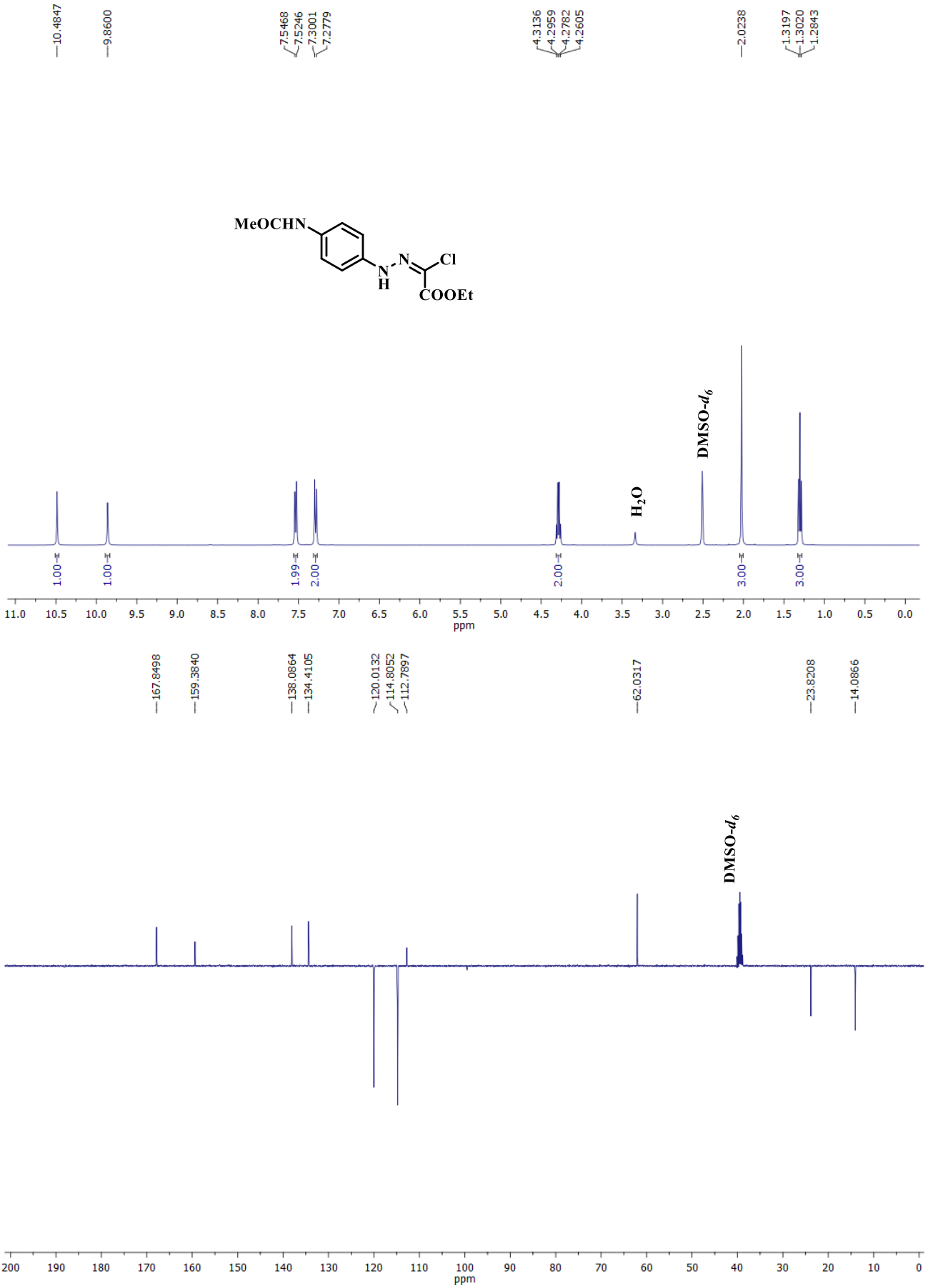


Fig. S1. ^{1}H NMR (400 MHz, DMSO-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6) spectra of ethyl 2-(2-(4-acetamidophenyl)hydrazono)-2-chloroacetate (**1b**).

Fig. S2. ^{1}H NMR (400 MHz, DMSO-*d*$_6$, TMS), ^{13}C NMR APT (100 MHz, DMSO-*d*$_6$) spectra of ethyl 2-chloro-2-(2-(4-cyanophenyl)hydrazono)acetate (**1g**).

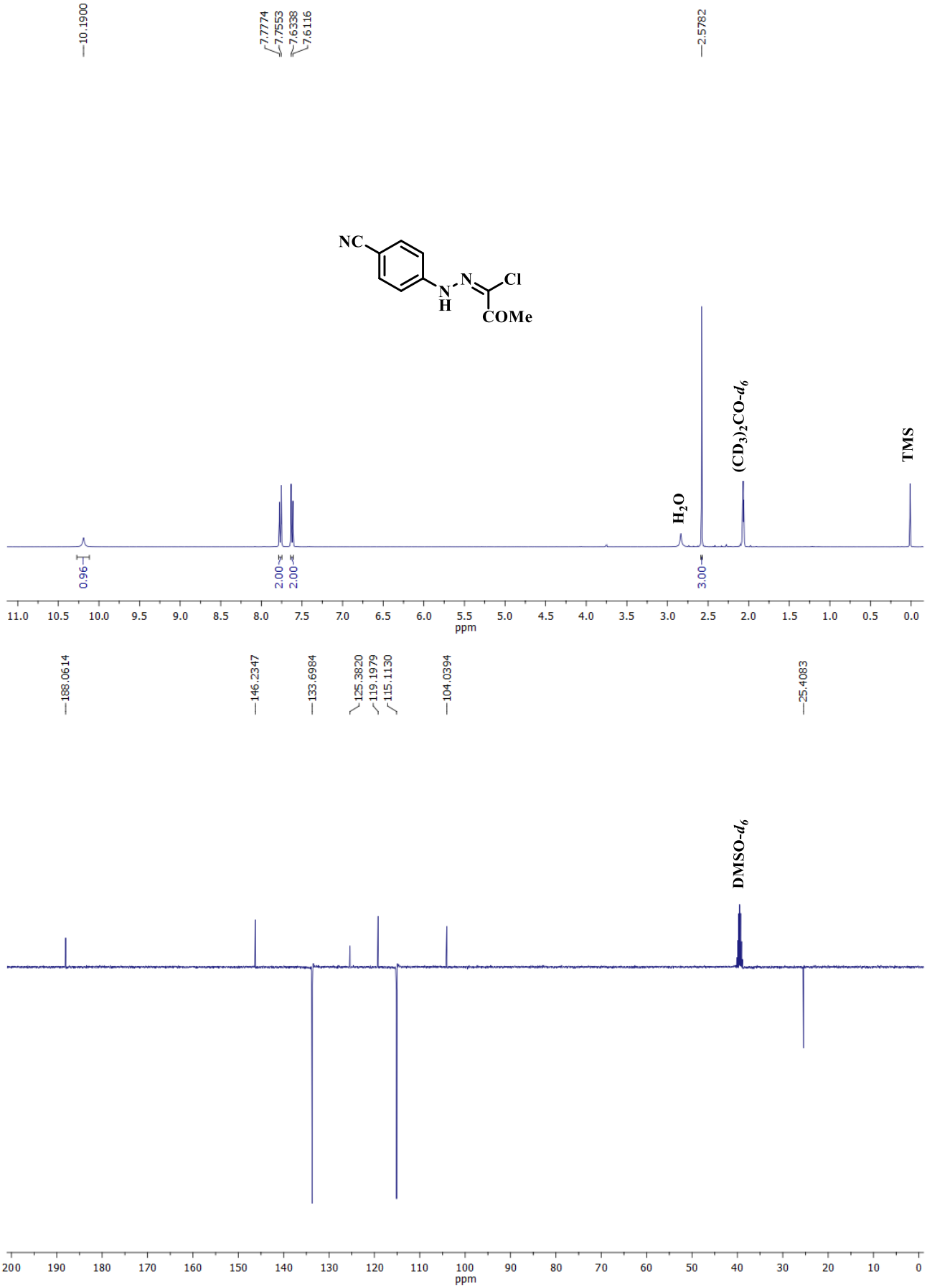


Fig. S3. ^{1}H NMR (400 MHz, $(CD_3)_2CO$-d_6, TMS), ^{13}C NMR APT (100 MHz, DMSO-d_6) spectra of *N*-(4-cyanophenyl)-2-oxopropanehydrazonoyl chloride (**1k**).

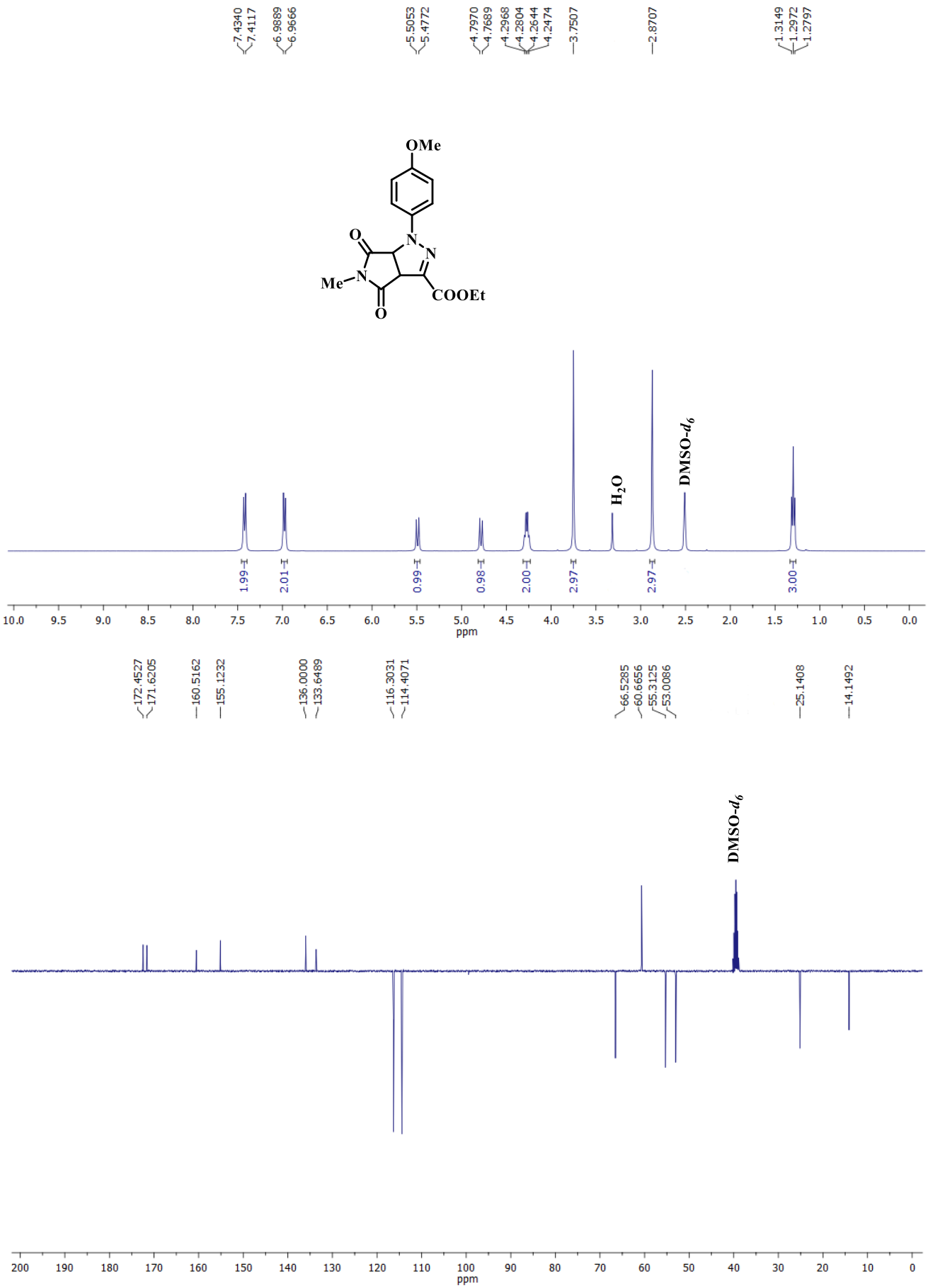


Fig. S4. ^{1}H NMR (400 MHz, DMSO-d_6), ^{13}C NMR APT (100 MHz, DMSO-d_6) spectra of ethyl 1-(4-methoxyphenyl)-5-methyl-4,6-dioxo-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (**2a**).

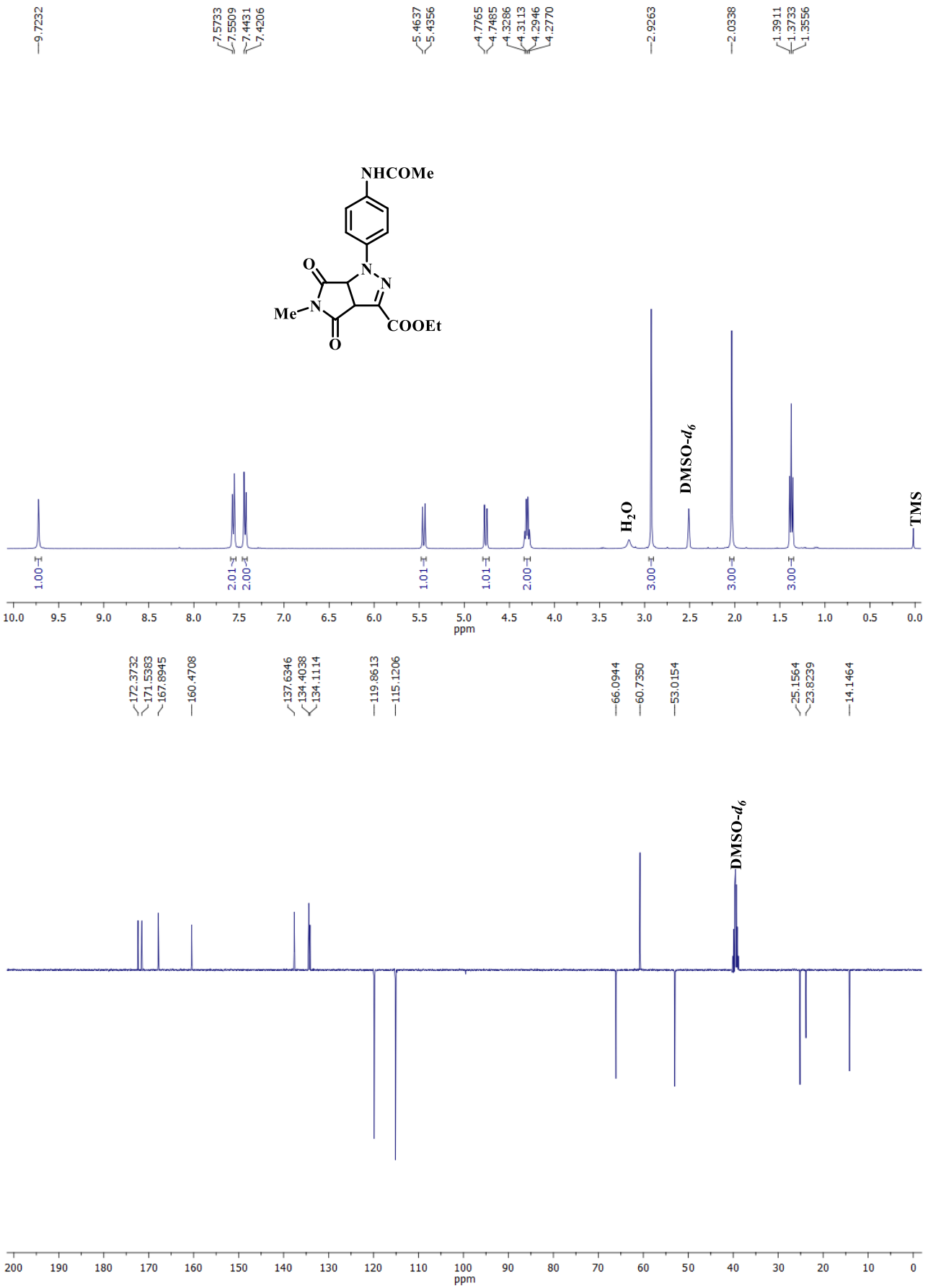


Fig. S5. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR APT (100 MHz, DMSO-d_6) spectra of ethyl 1-(4-acetamidophenyl)-5-methyl-4,6-dioxo-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (**2b**).

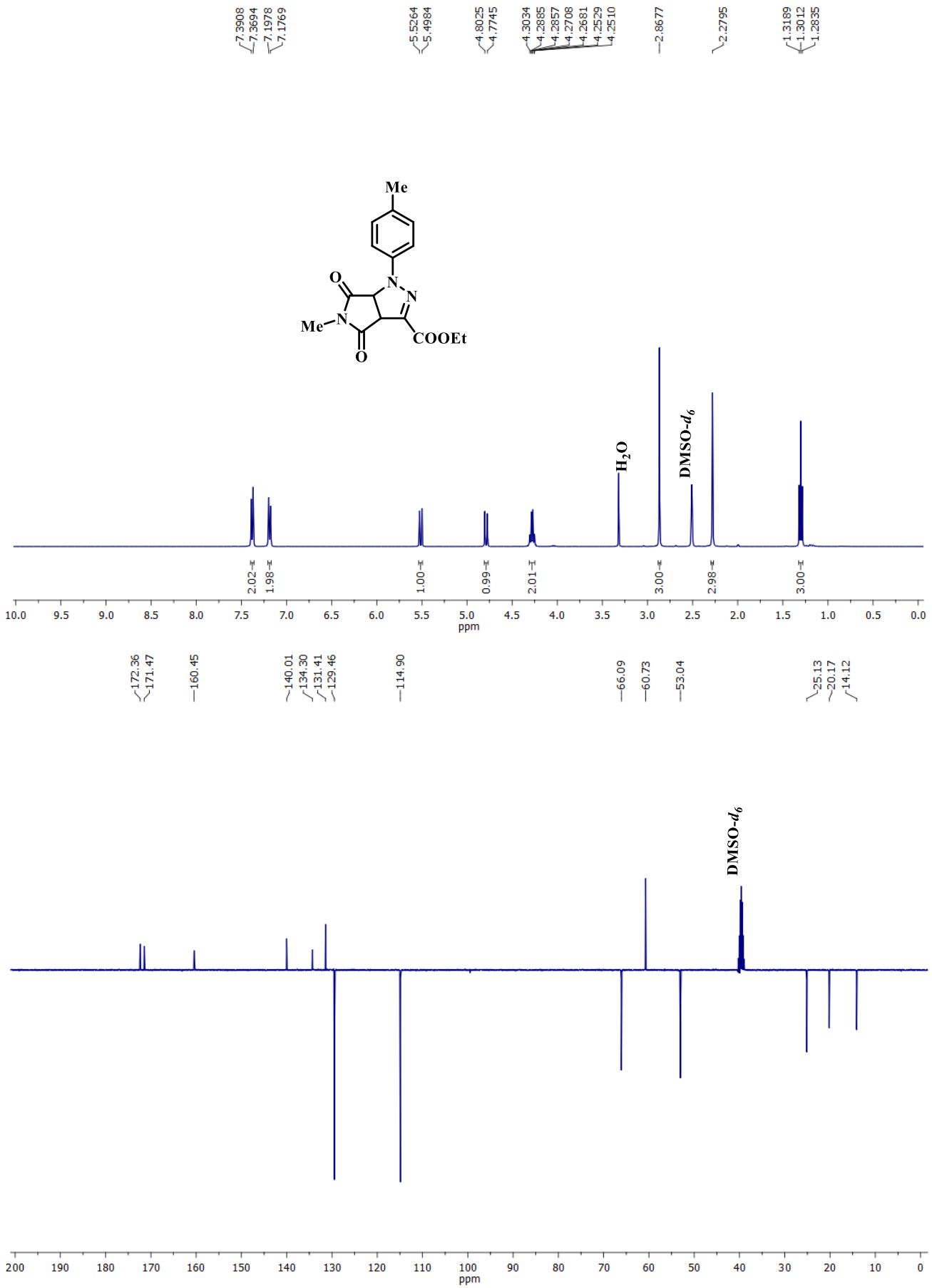


Fig. S6. ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR APT (100 MHz, DMSO-d_6) spectra of ethyl 5-methyl-4,6-dioxo-1-(*p*-tolyl)-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (**2c**).

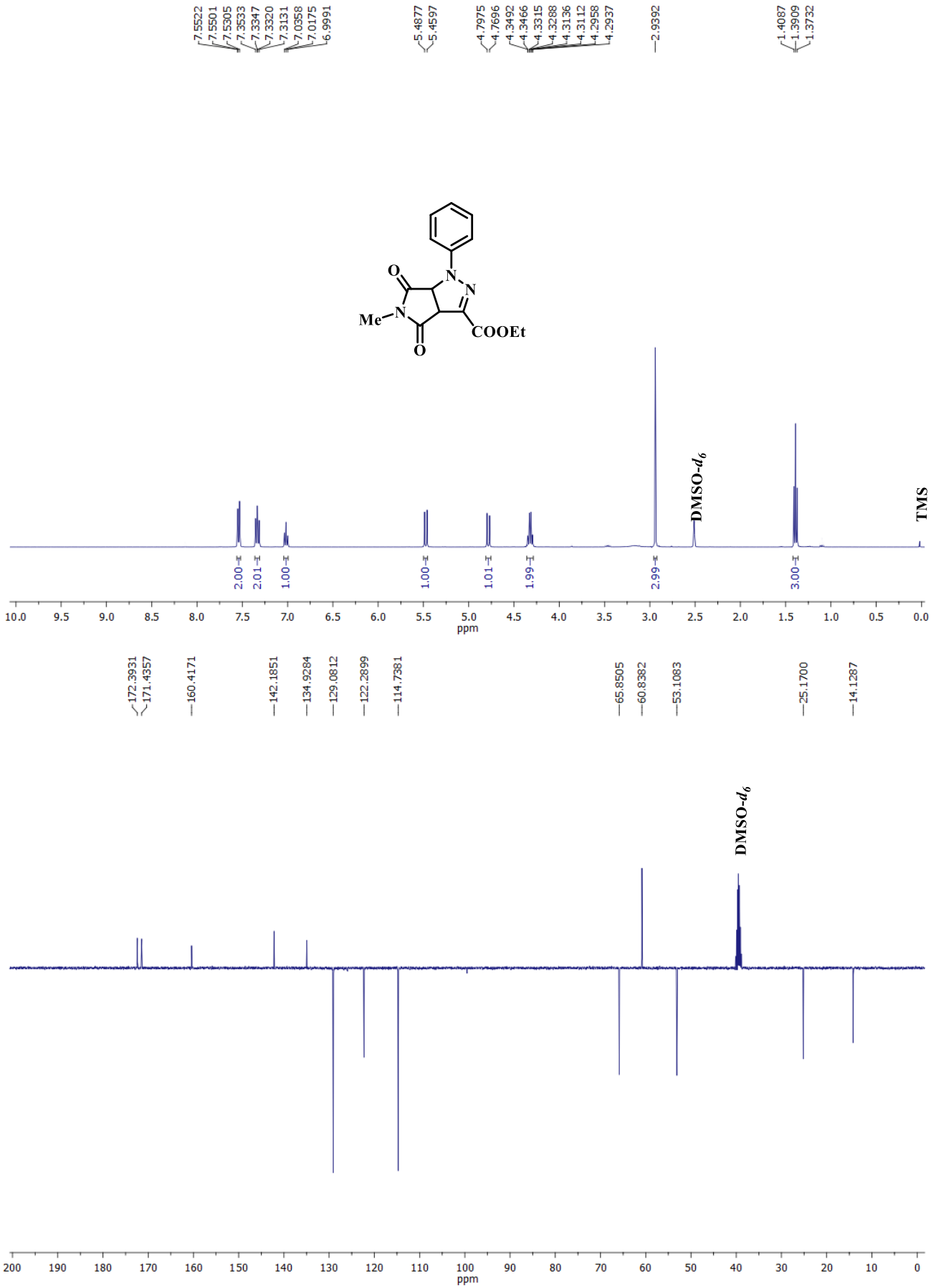


Fig. S7. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR APT (100 MHz, DMSO-d_6) spectra of ethyl 5-methyl-4,6-dioxo-1-phenyl-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (**2d**).

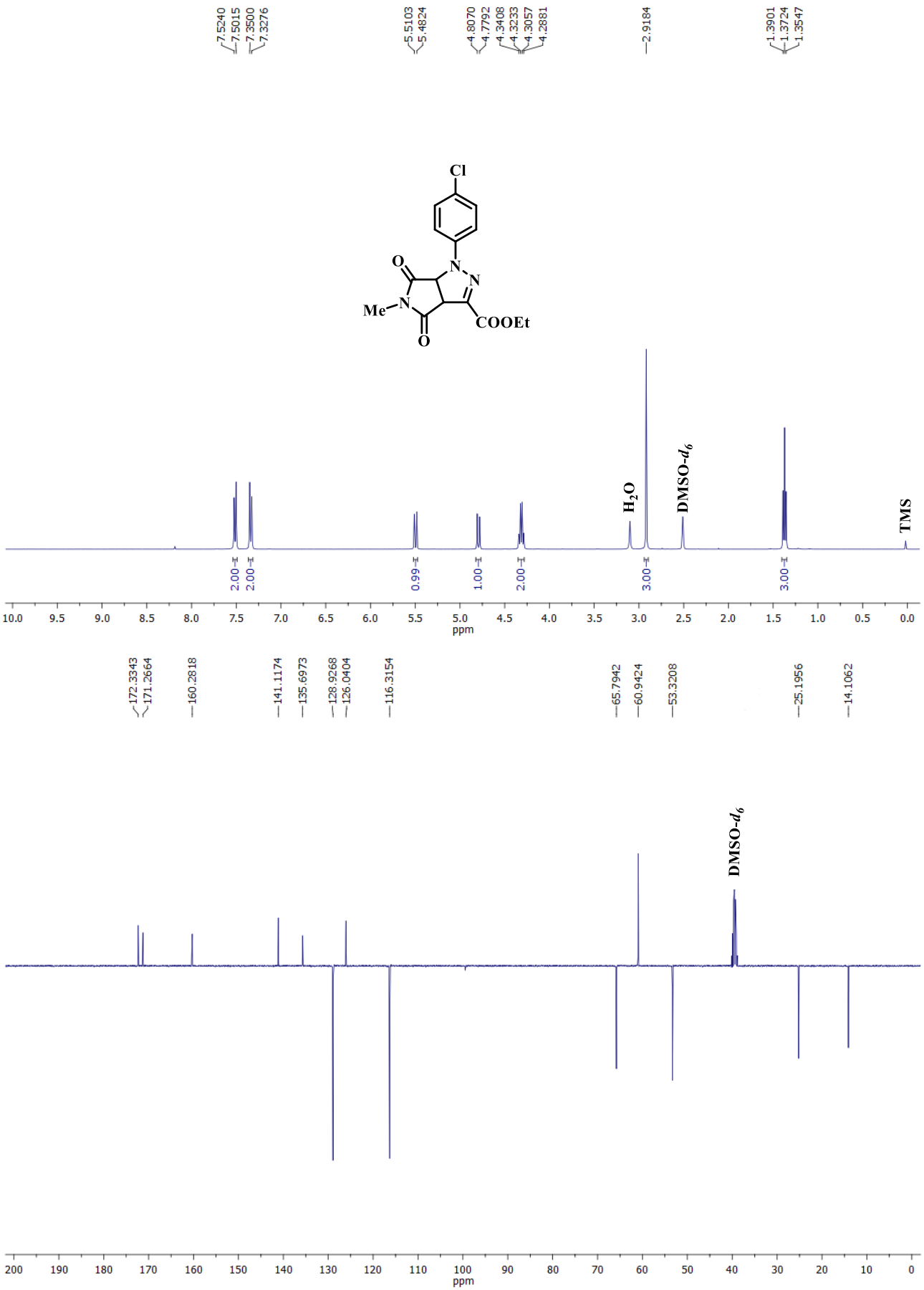


Fig. S8. ^{1}H NMR (400 MHz, DMSO-*d*$_6$, TMS) and ^{13}C NMR APT (100 MHz, DMSO-*d*$_6$) spectra of ethyl 1-(4-chlorophenyl)-5-methyl-4,6-dioxo-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (**2e**).

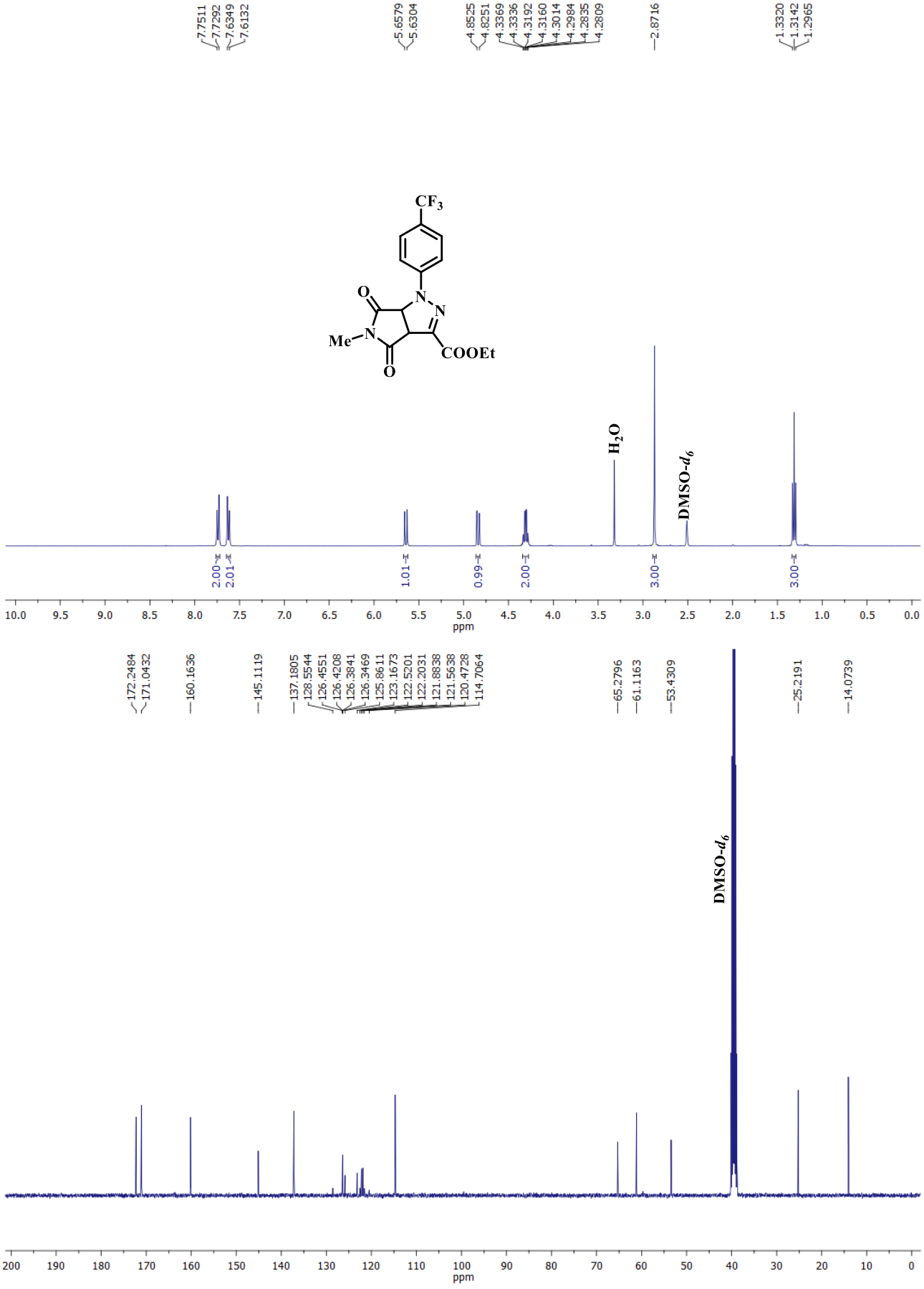


Fig. S9. ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of ethyl 5-methyl-4,6-dioxo-1-(4-(trifluoromethyl)phenyl)-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (**2f**)

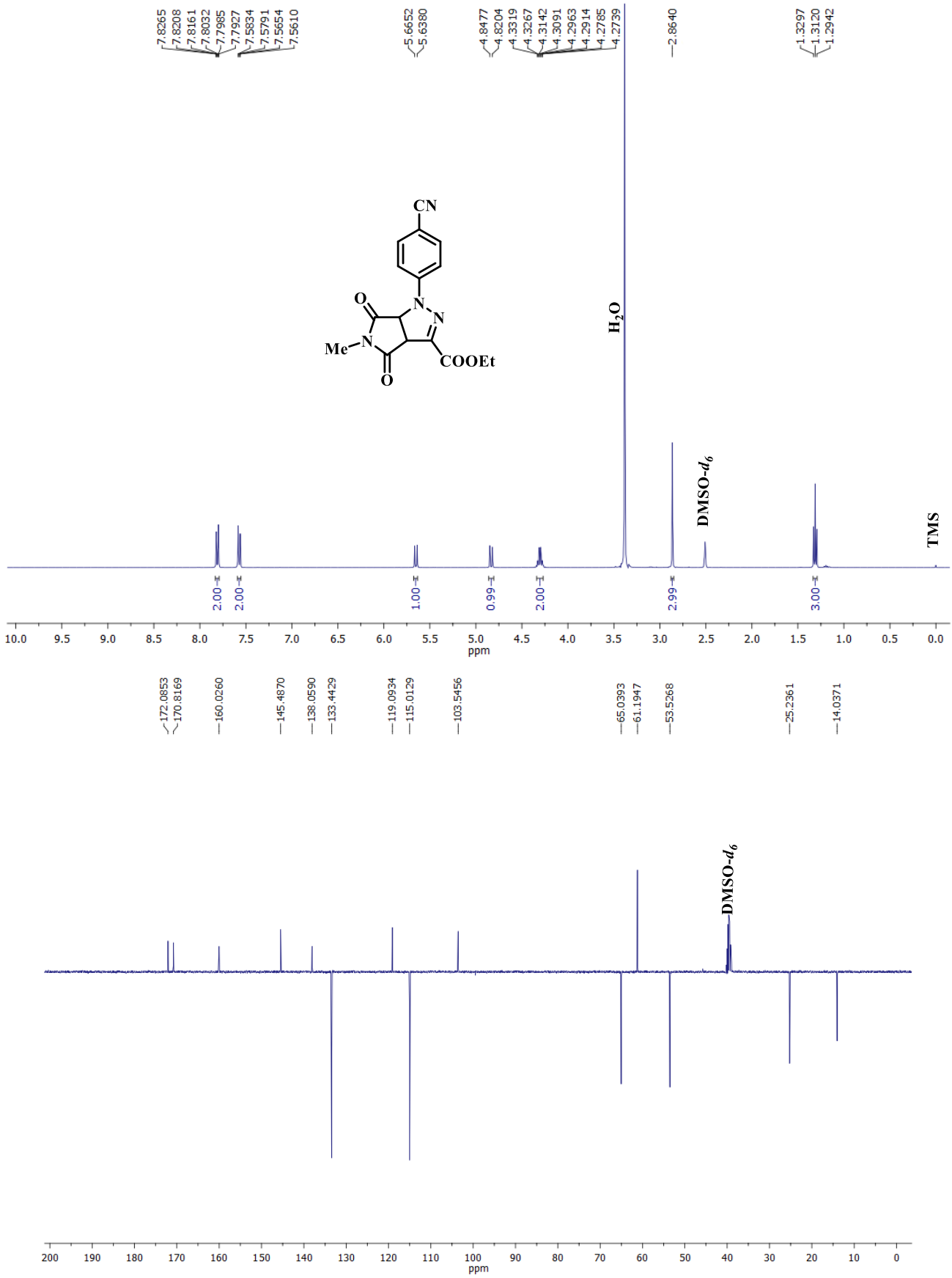
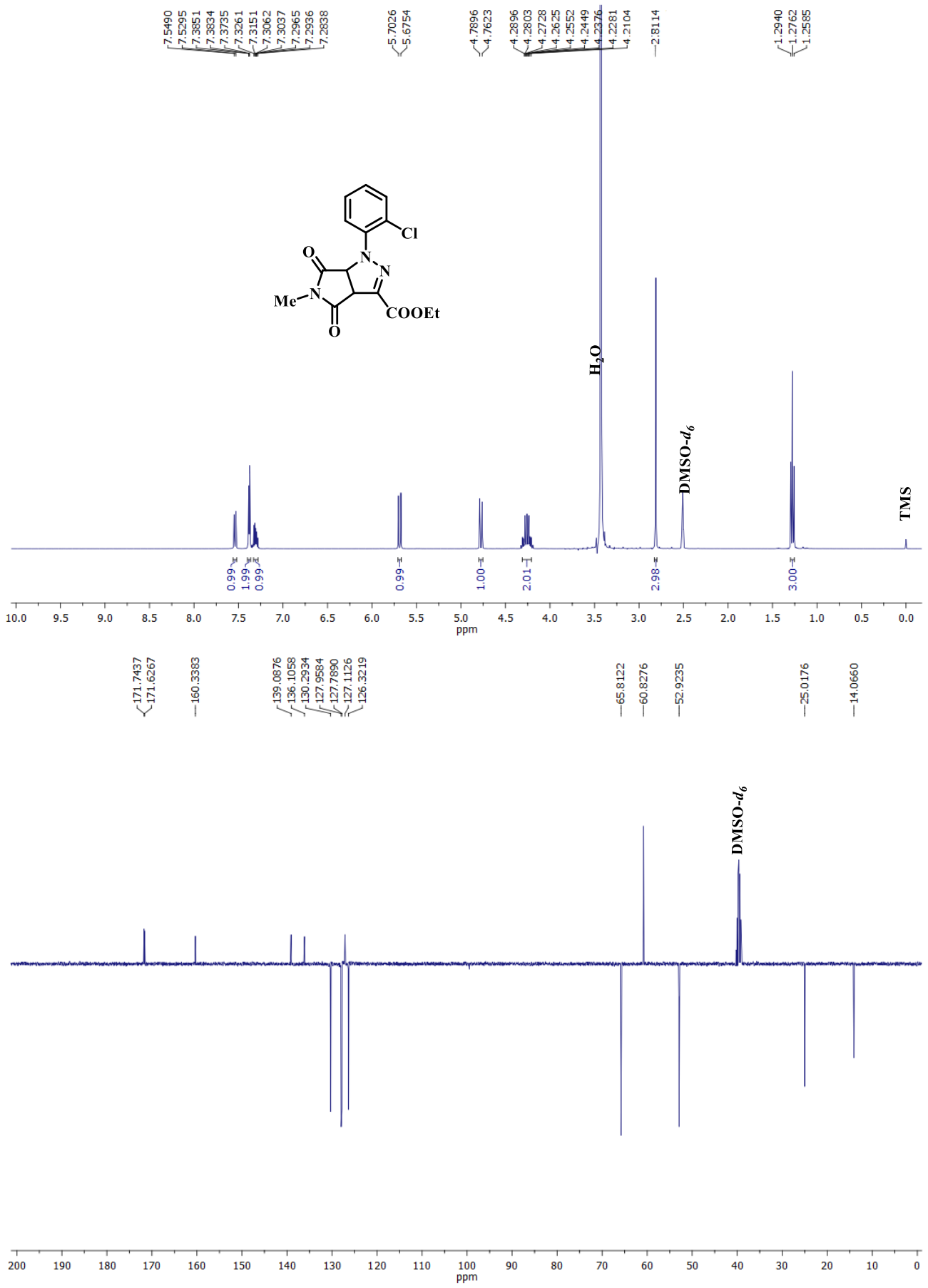


Fig. S10. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR APT (100 MHz, DMSO-d_6) spectra of ethyl 1-(4-cyanophenyl)-5-methyl-4,6-dioxo-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (**2g**).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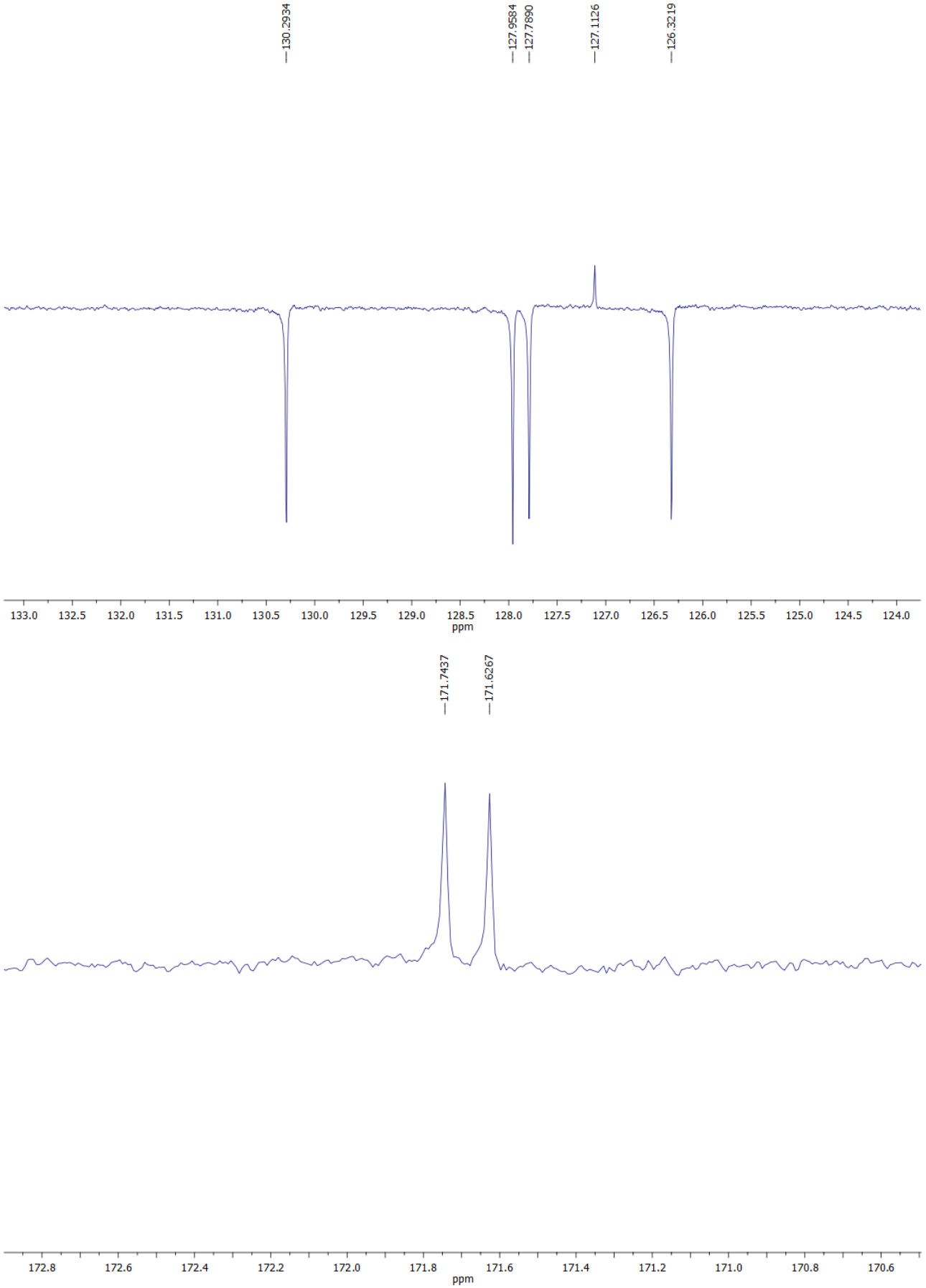


Fig. S11. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR APT (100 MHz, DMSO-d_6) spectra of ethyl 1-(2-chlorophenyl)-5-methyl-4,6-dioxo-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (**2h**).

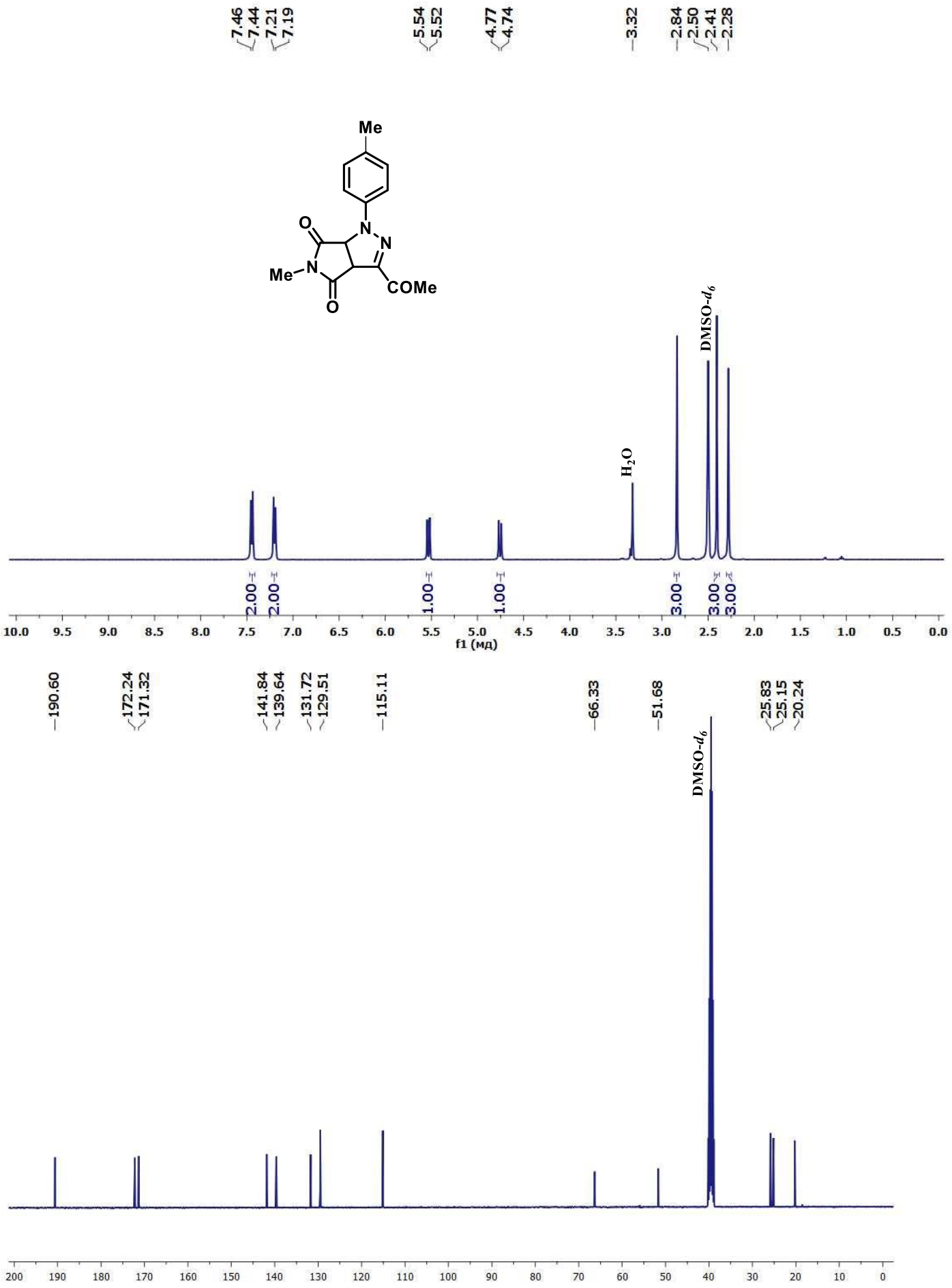


Fig. S12. ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 3-acetyl-5-methyl-1-(*p*-tolyl)-3*a*,6*a*-dihydropyrrolo[3,4-*c*]pyrazole-4,6(1*H*,5*H*)-dione (**2i**).

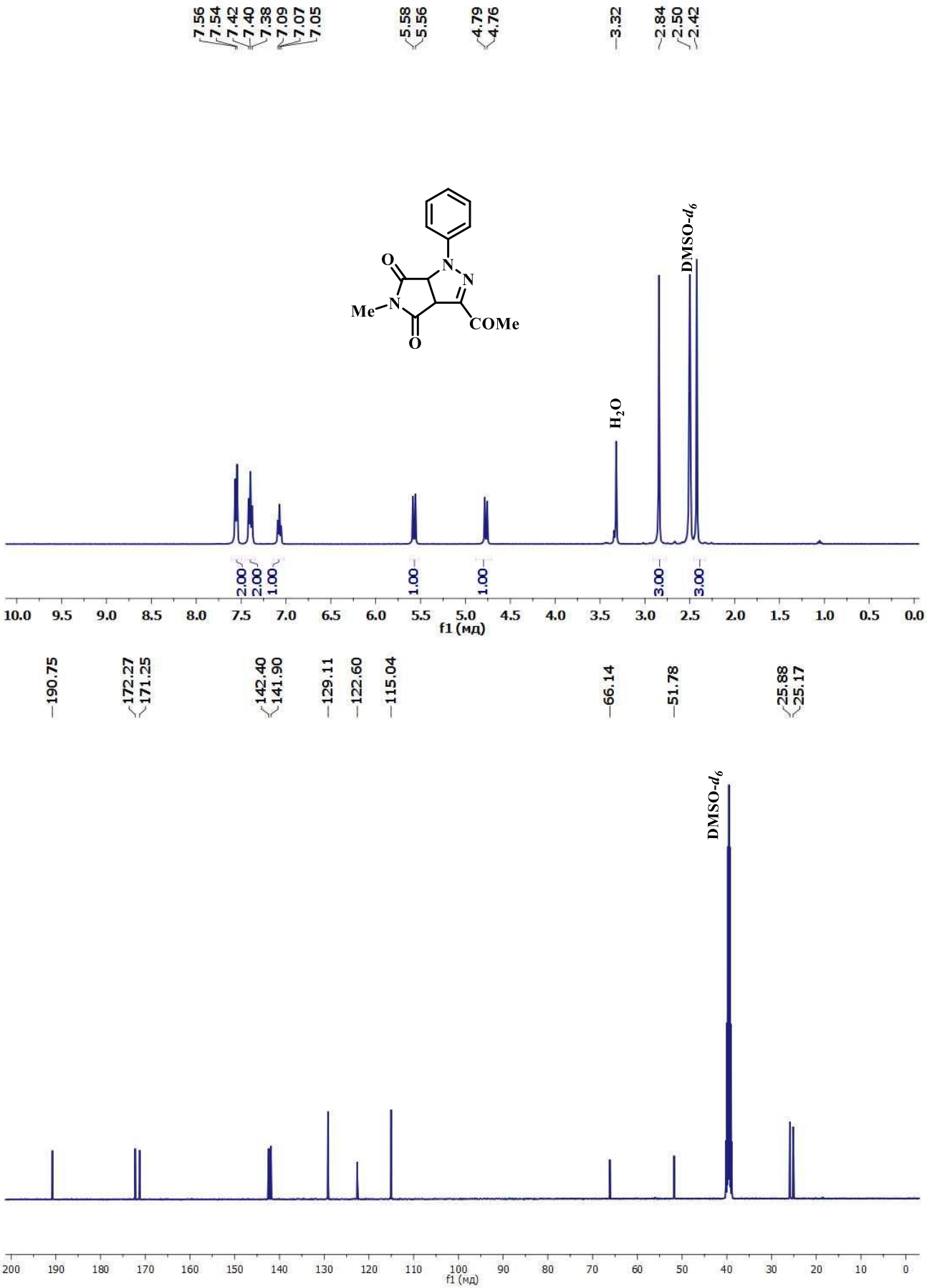


Fig. S13. ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 3-acetyl-5-methyl-1-phenyl-3*a*,6*a*-dihydropyrrolo[3,4-*c*]pyrazole-4,6(1*H*,5*H*)-dione (**2j**).

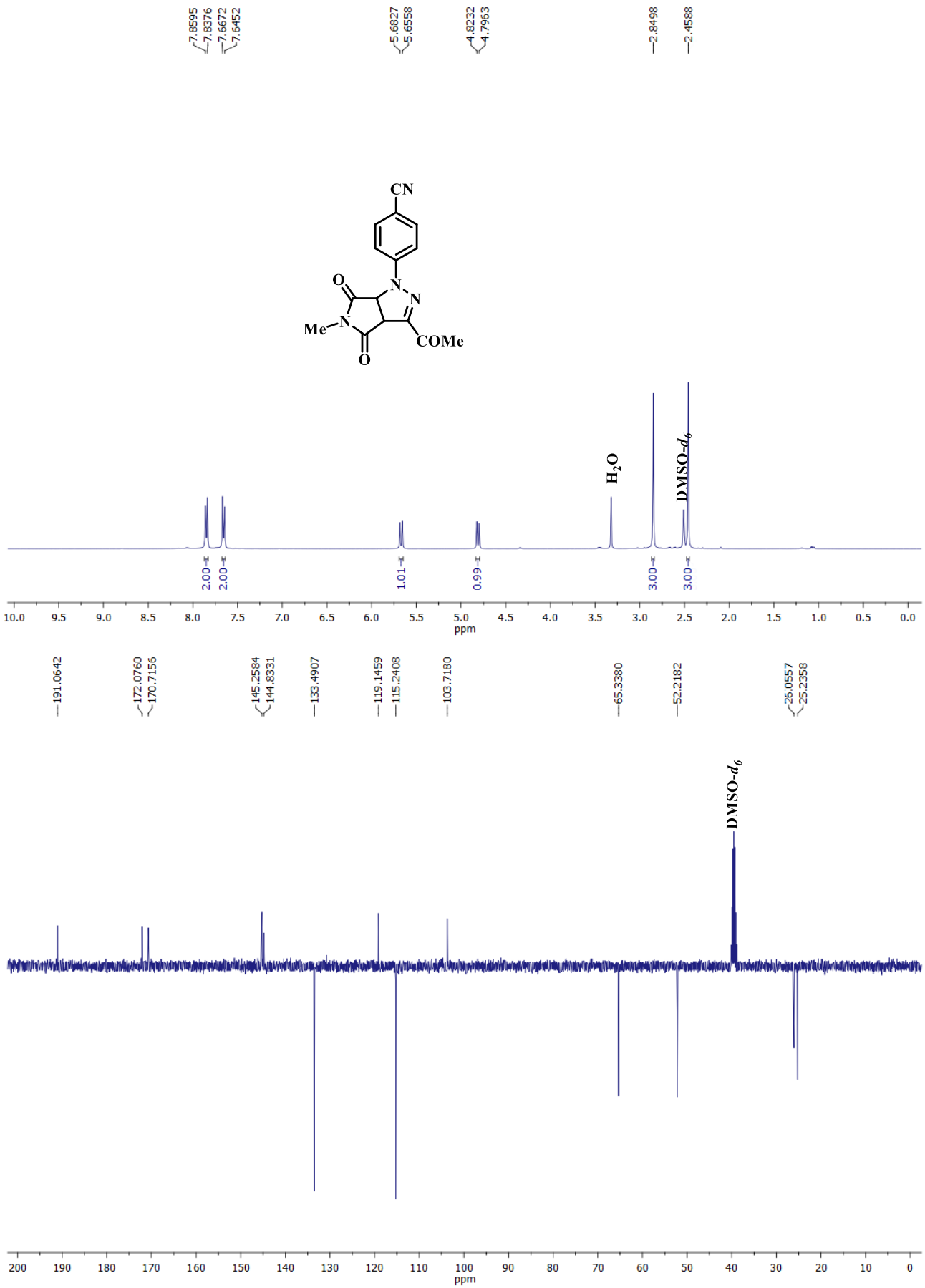


Fig. S14. ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR APT (100 MHz, DMSO-d_6) spectra of 4-(3-acetyl-5-methyl-4,6-dioxo-4,5,6,6*a*-tetrahydropyrrolo[3,4-*c*]pyrazol-1(3*aH*)-yl)benzonitrile (**2k**).

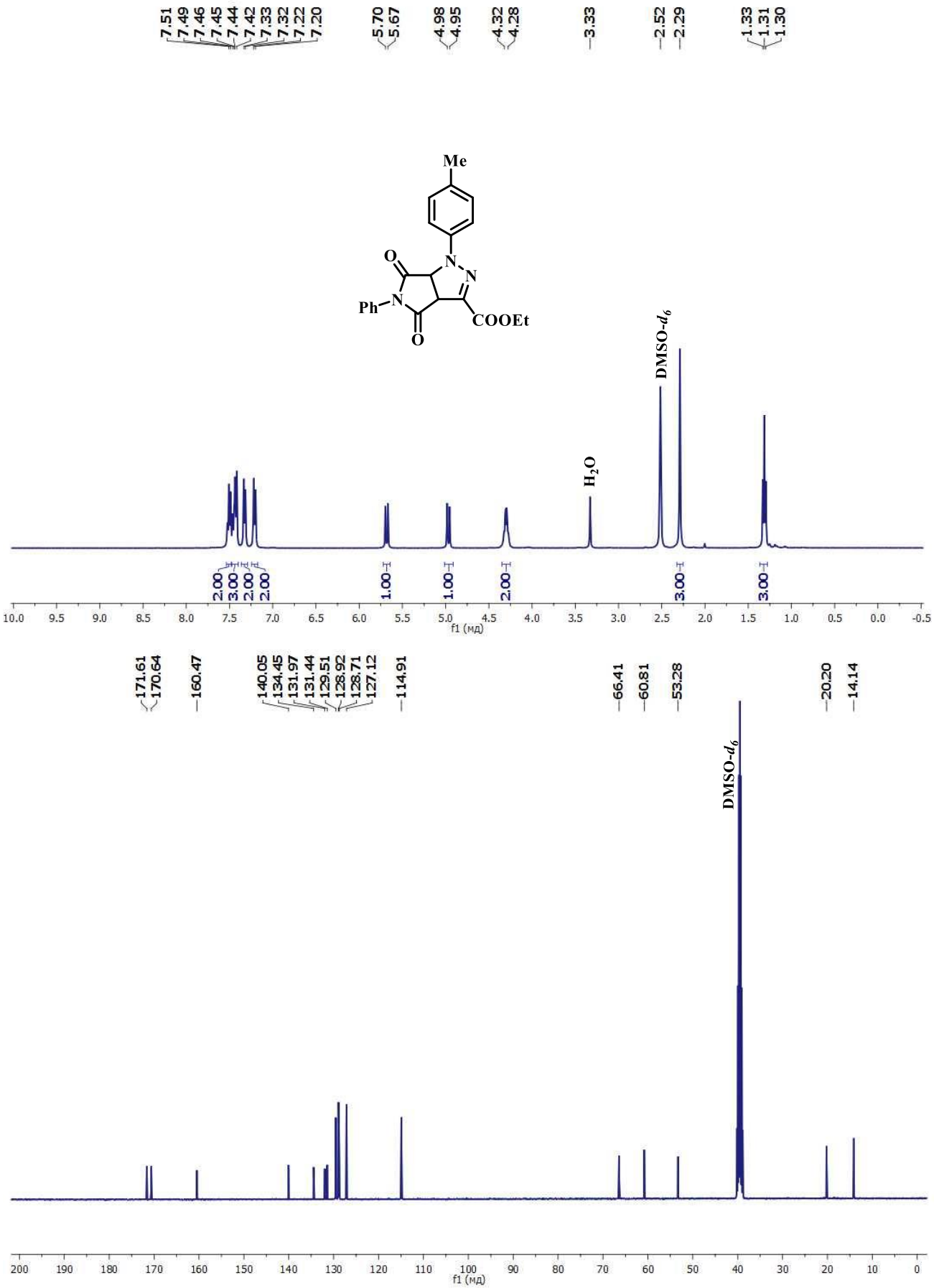
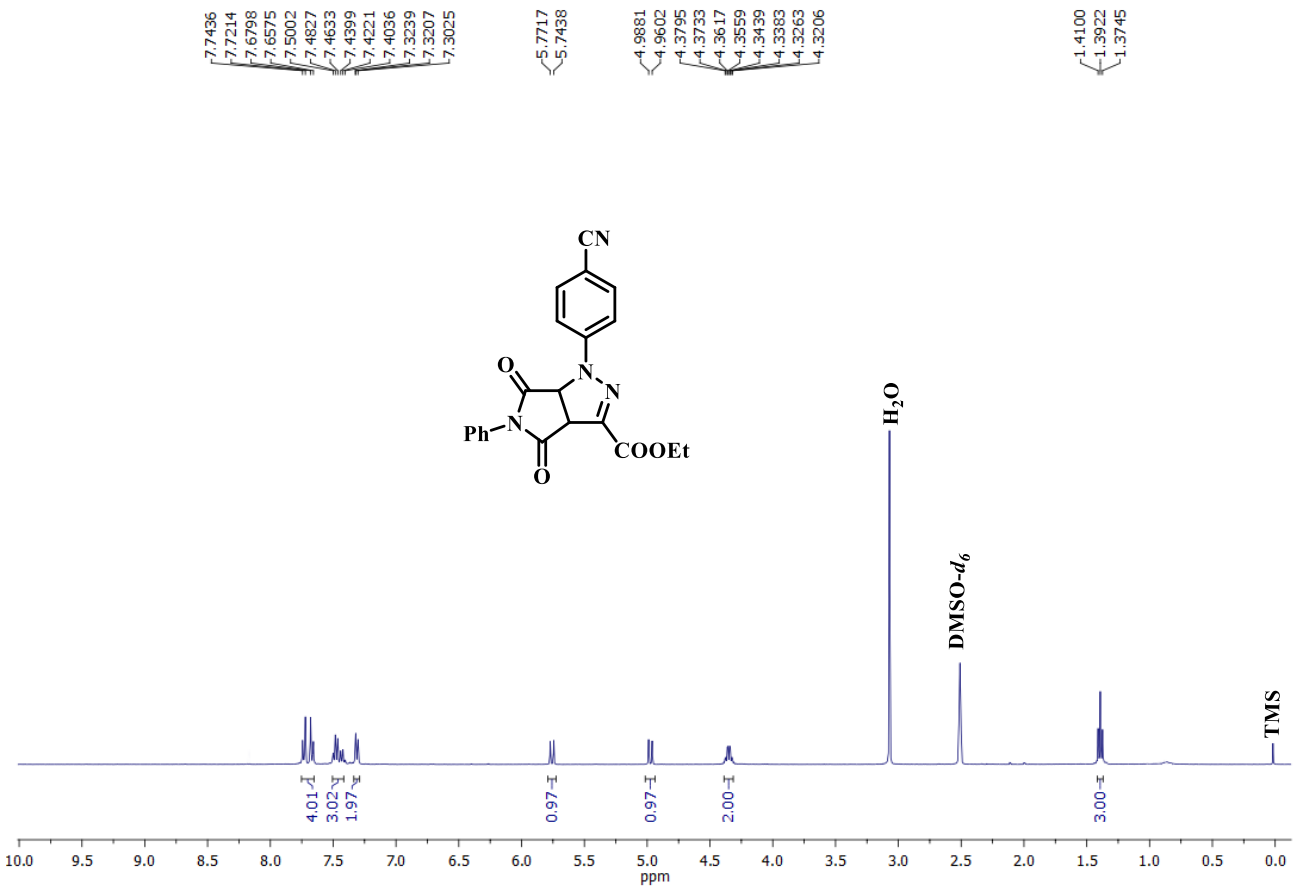


Fig. S15. ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of ethyl 4,6-dioxo-5-phenyl-1-(*p*-tolyl)-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (**3a**).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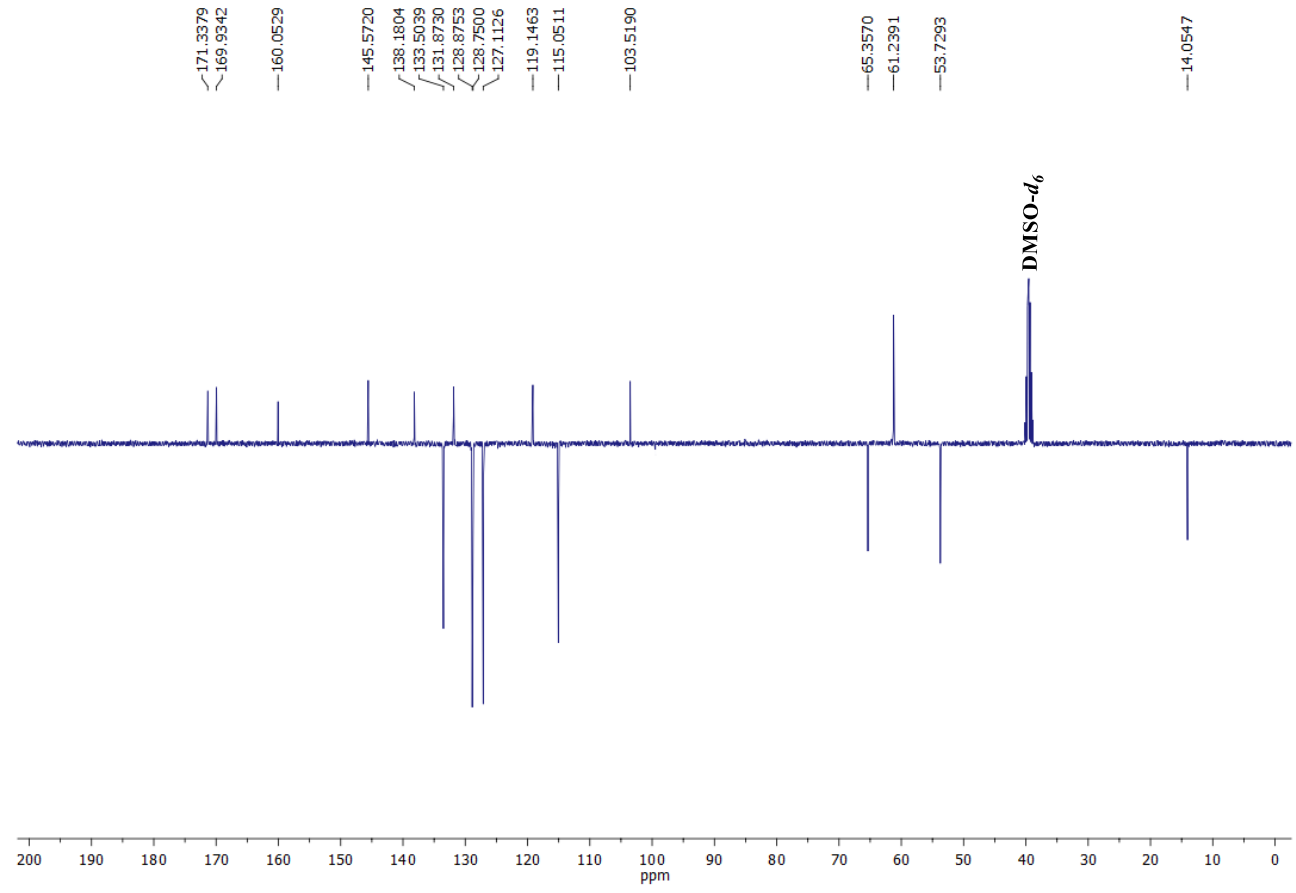
ppm


171.3379
169.9342
160.0529
145.5720
138.1804
133.5039
131.8730
128.8753
128.7500
127.1126
119.1463
115.0511
103.5190
65.3570
61.2391
53.7293
14.0547
DMSO-d6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

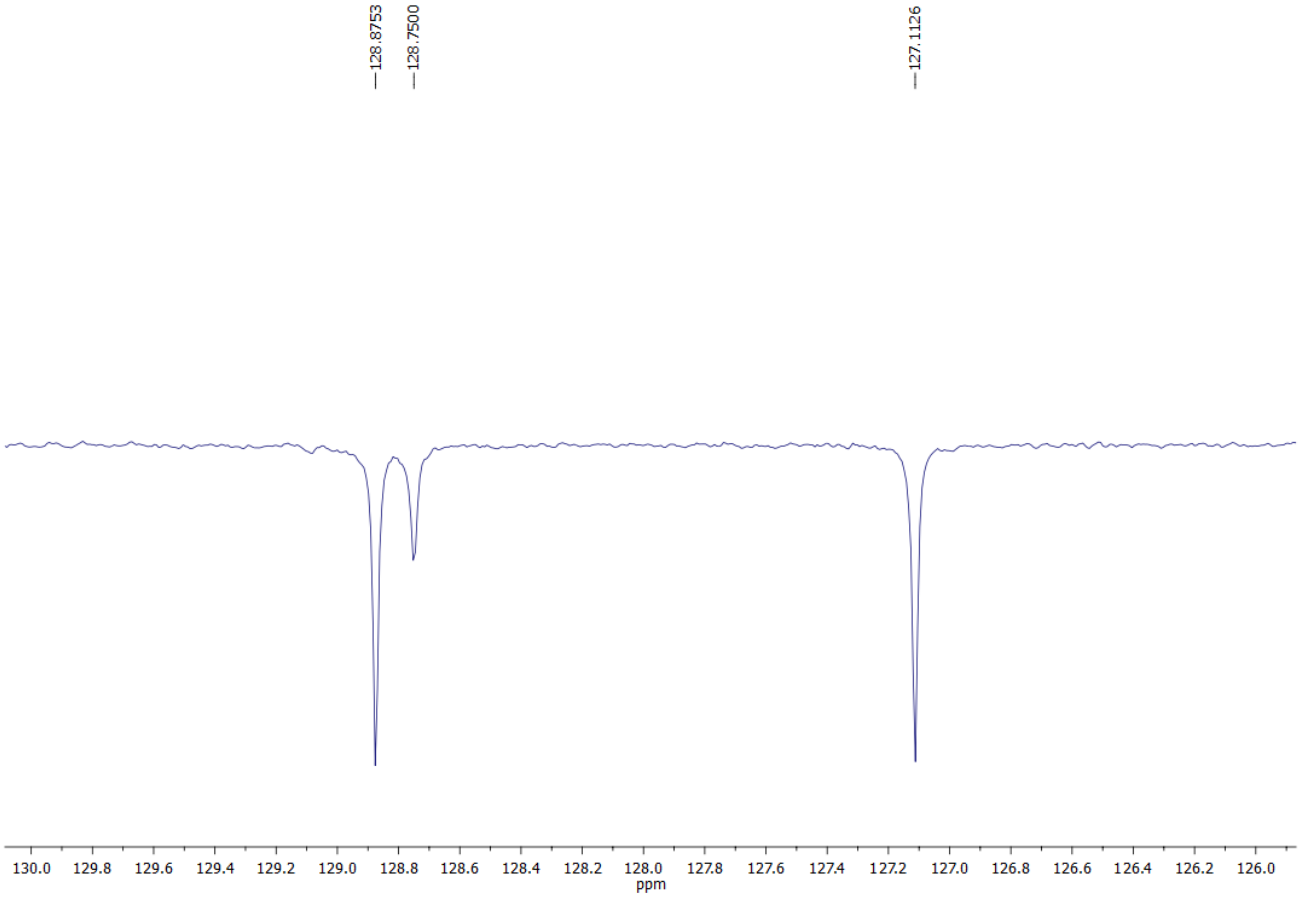


Fig. S16. ^{1}H NMR (400 MHz, DMSO-d_6, TMS) and ^{13}C NMR APT (100 MHz, DMSO-d_6) spectra of ethyl 1-(4-cyanophenyl)-4,6-dioxo-5-phenyl-1,3*a*,4,5,6,6*a*-hexahydropyrrolo[3,4-*c*]pyrazole-3-carboxylate (**3b**).

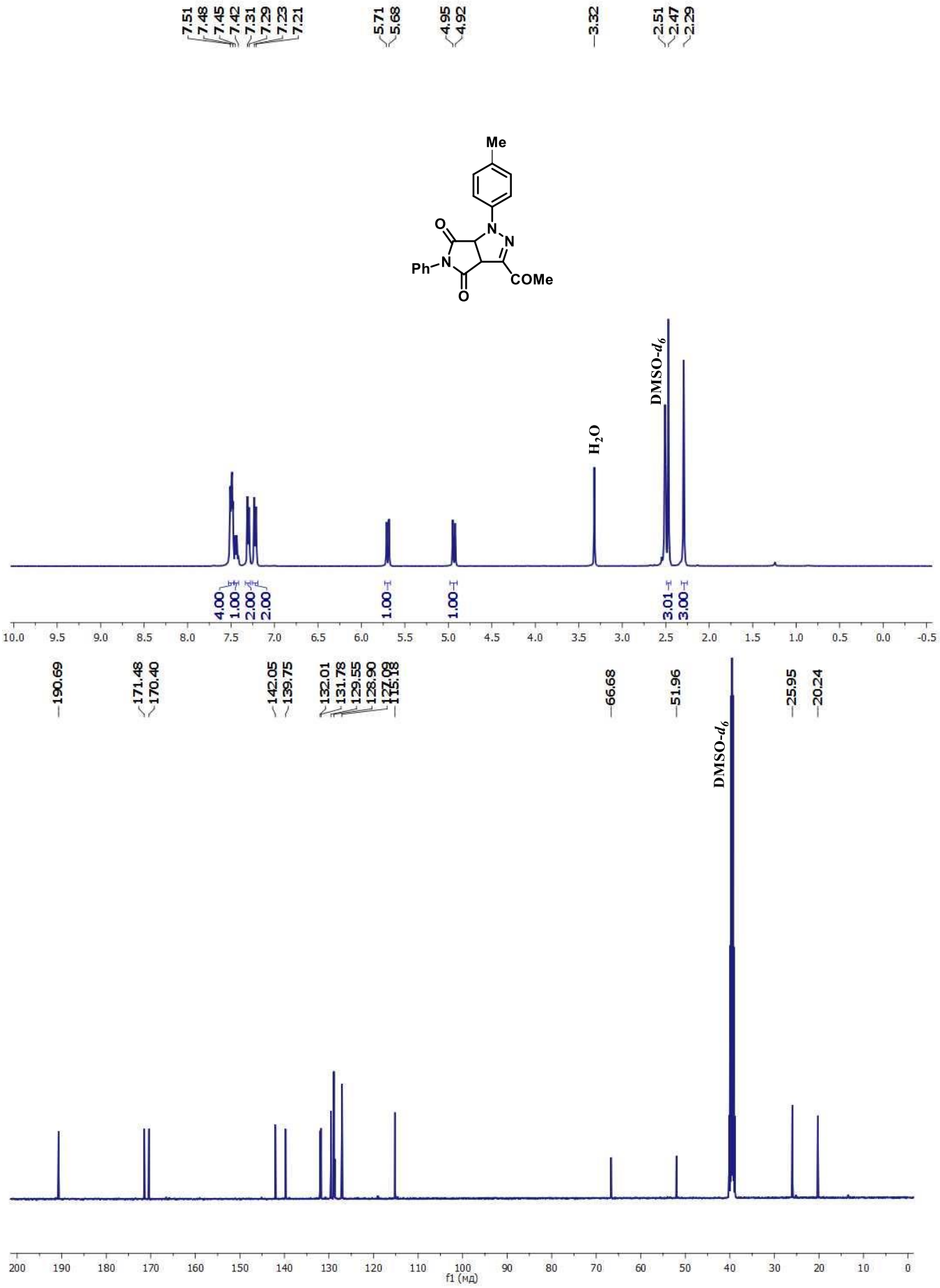


Fig. S17. ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 3-acetyl-5-phenyl-1-(*p*-tolyl)-3*a*,6*a*-dihydropyrrolo[3,4-*c*]pyrazole-4,6(1*H*,5*H*)-dione **(3c).**

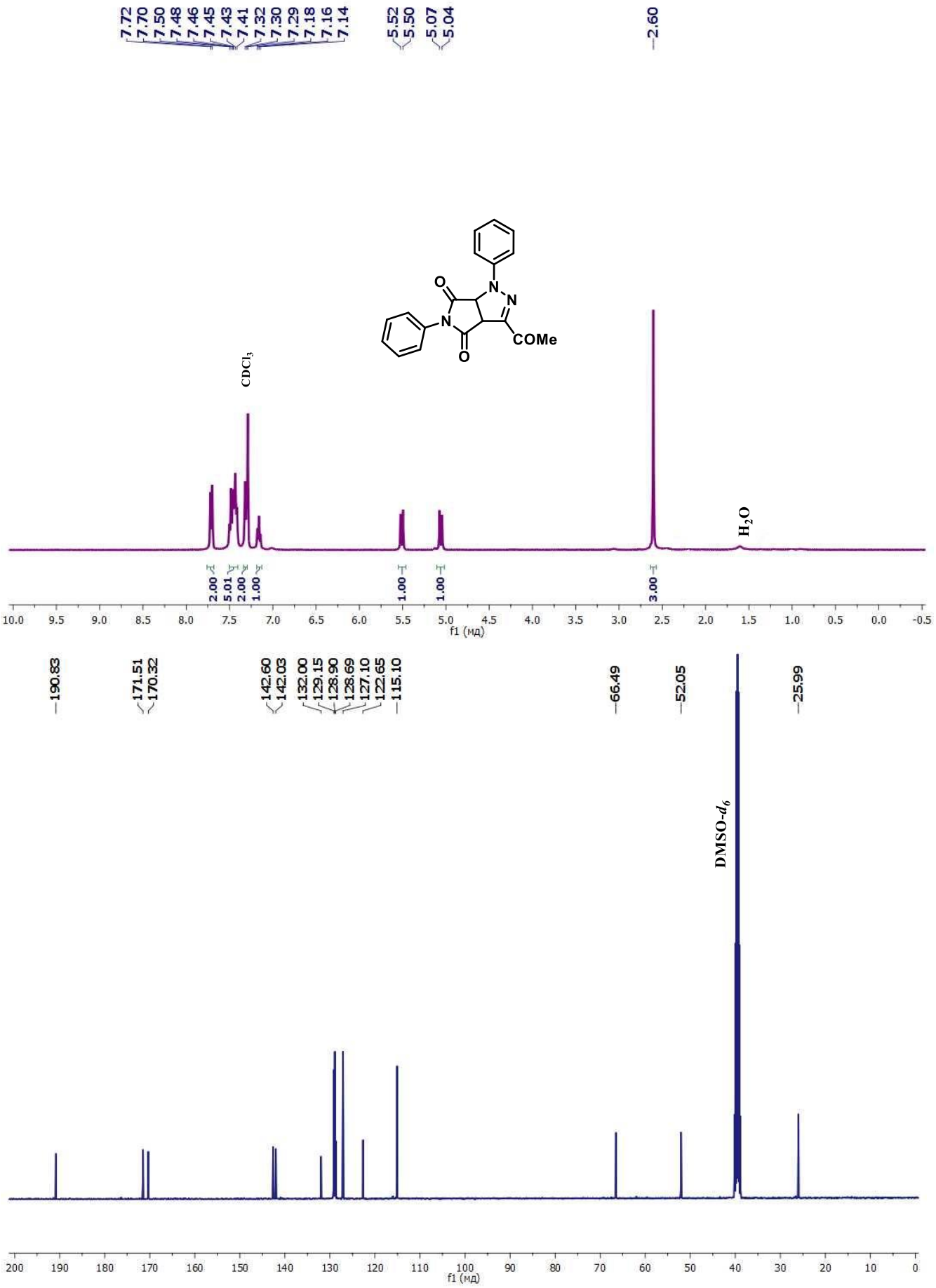


Fig. S18. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 3-acetyl-1,5-diphenyl-3*a*,6*a*-dihydropyrrolo[3,4-*c*]pyrazole-4,6(1*H*,5*H*)-dione (**3d**).

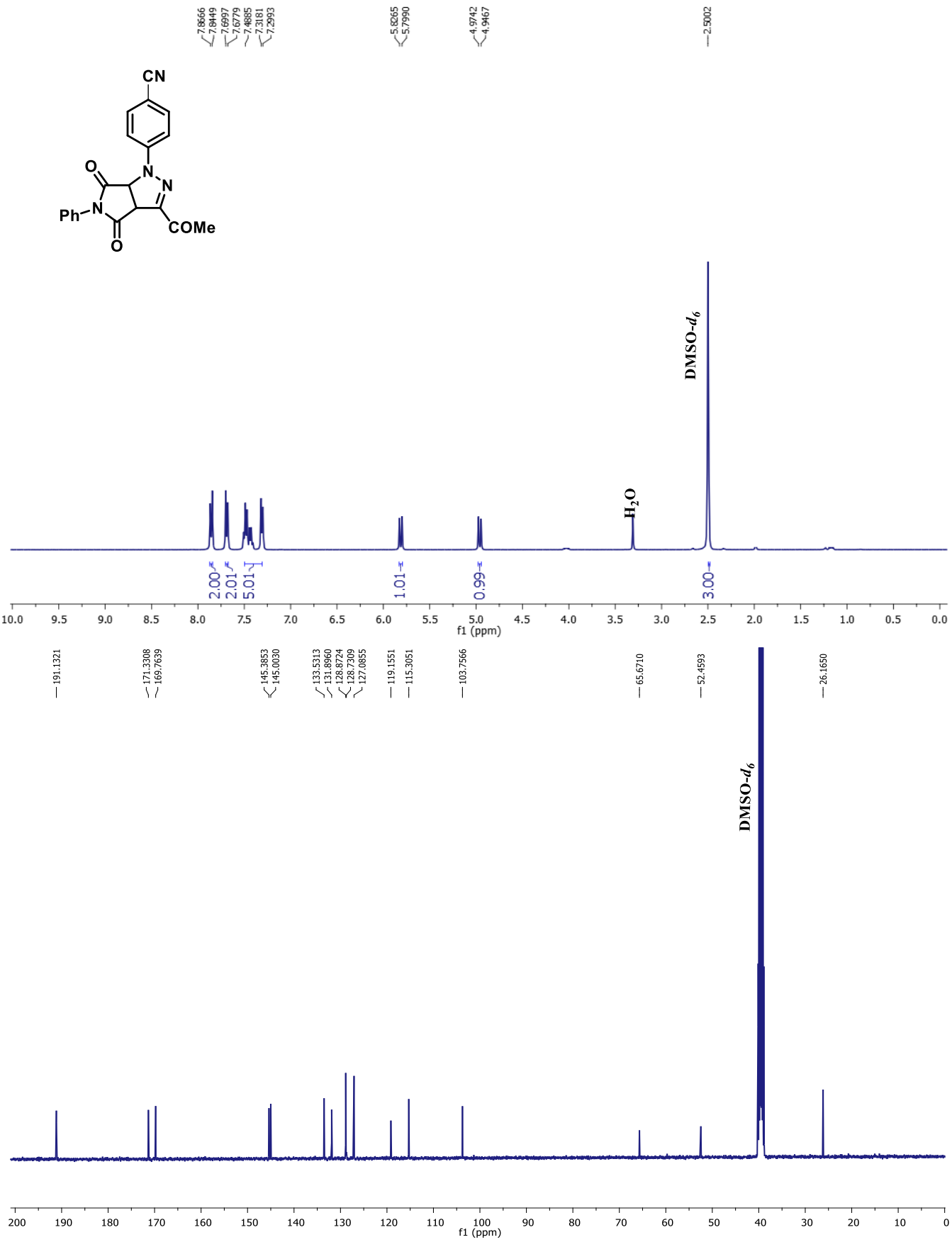


Fig. S19. ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of (3-acetyl-4,6-dioxo-5-phenyl-4,5,6,6*a*-tetrahydropyrrolo[3,4-*c*]pyrazol-1(3*aH*)-yl)benzonitrile (**3e**).

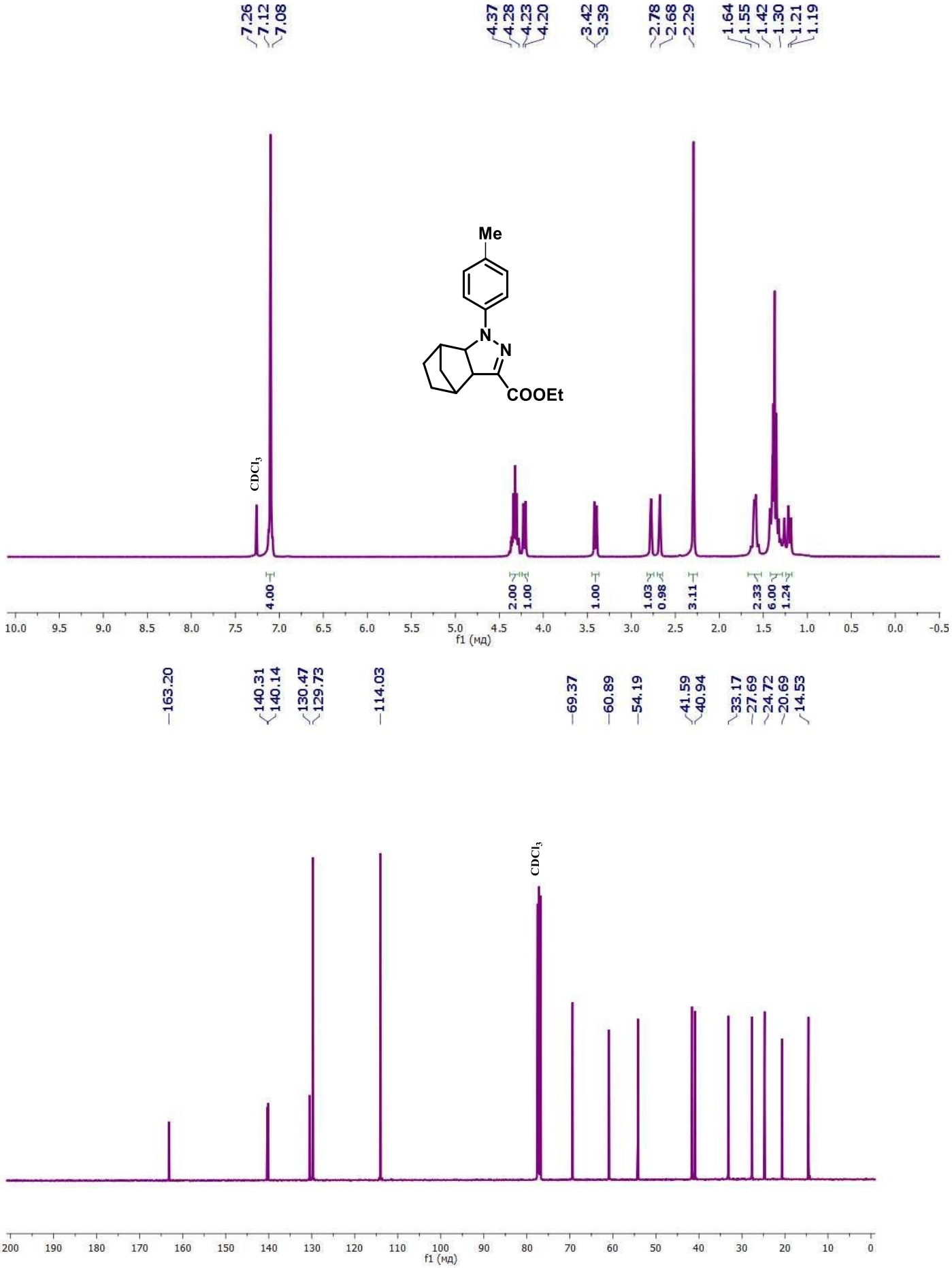


Fig. S20. ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of ethyl 1-(*p*-tolyl)-3*a*,4,5,6,7,7*a*-hexahydro-1*H*-4,7-methanoindazole-3-carboxylate (**4a**).

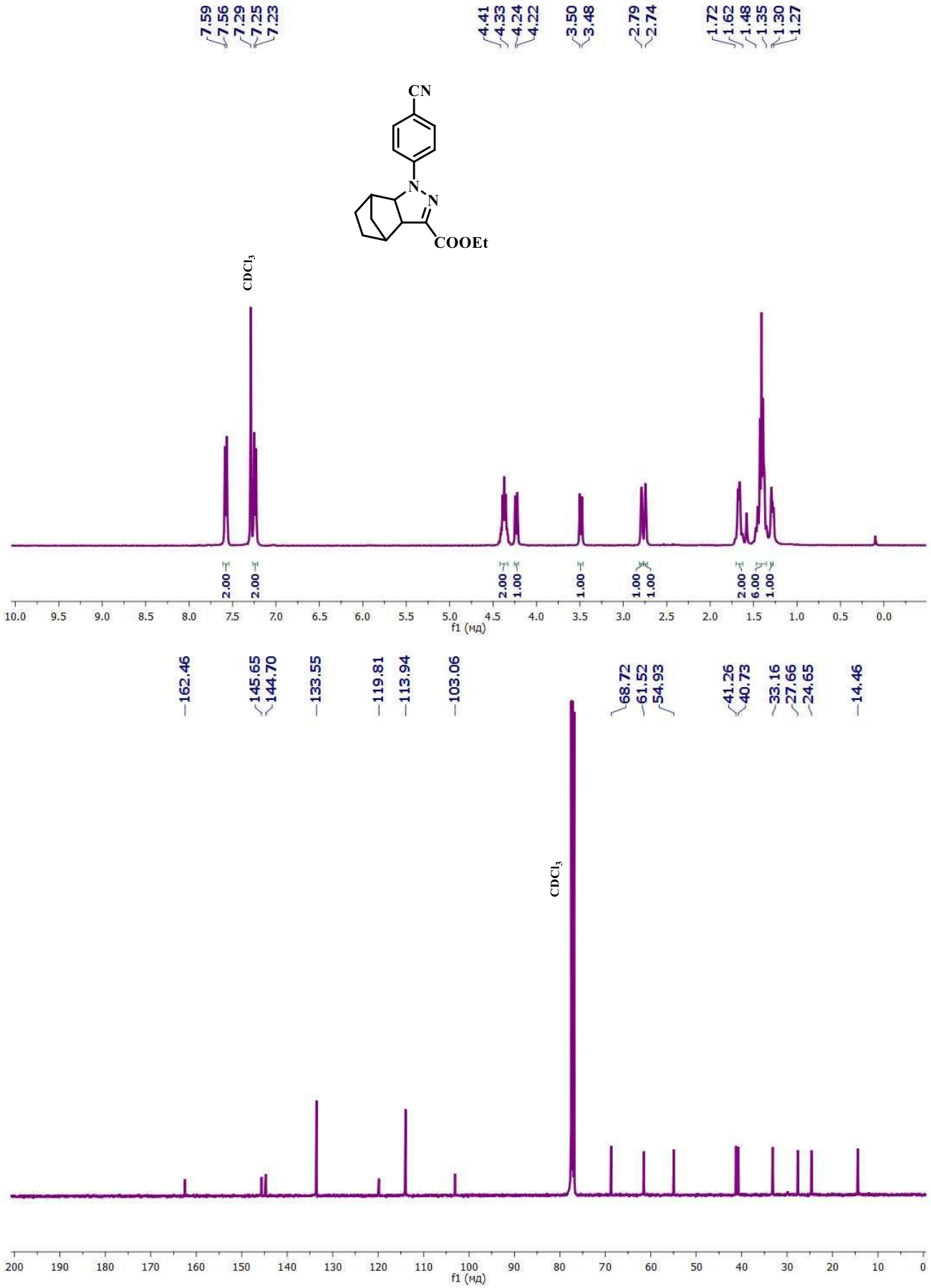


Fig. S21. ^{1}H NMR (400 MHz, $CDCl_3$, TMS) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of ethyl 1-(4-cyanophenyl)-3*a*,4,5,6,7,7*a*-hexahydro-1*H*-4,7-methanoindazole-3-carboxylate (**4b**).

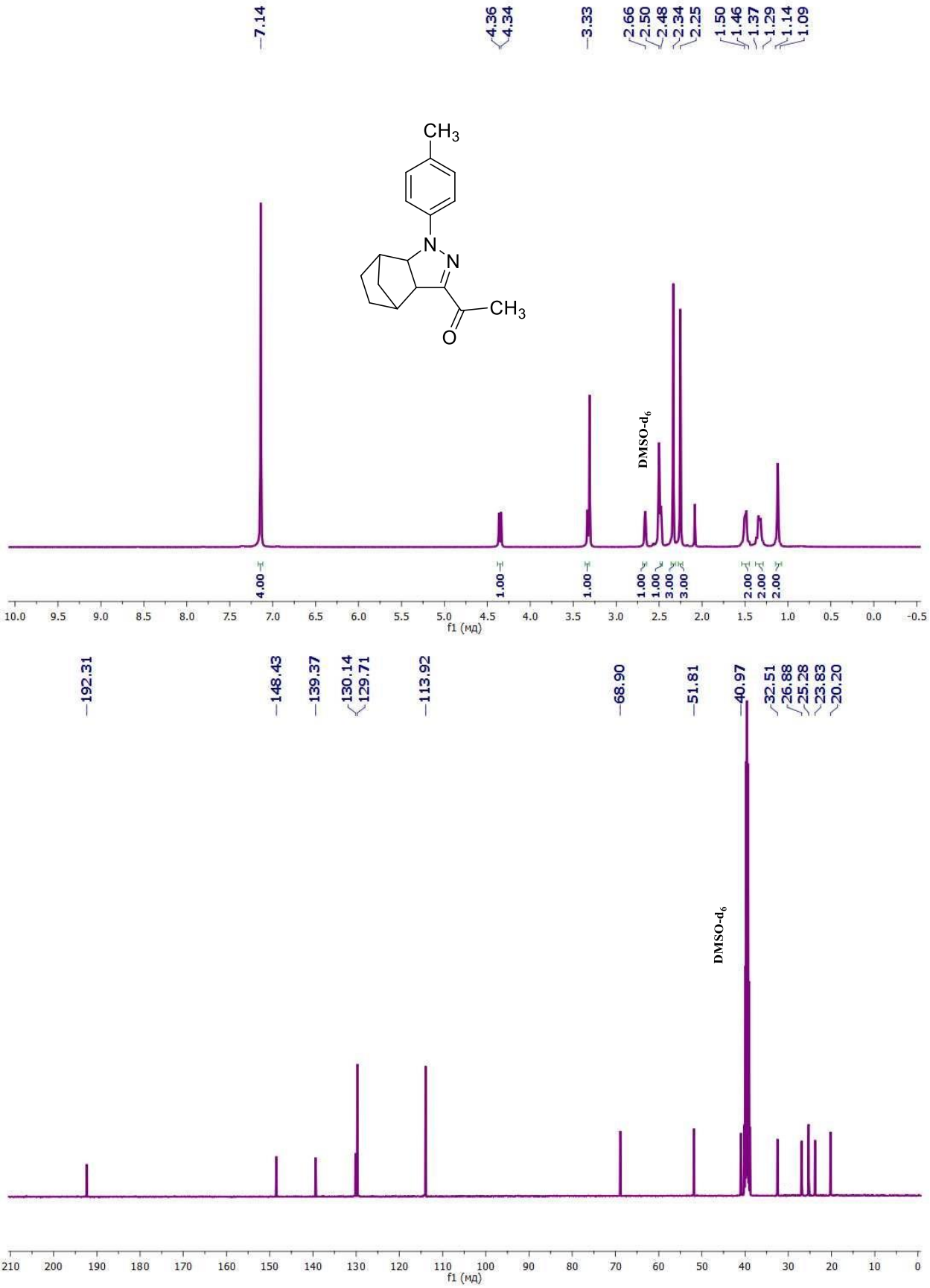


Fig. S22. ^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) spectra of 1-(1-tolyl-3*a*,4,5,6,7,7*a*-hexahydro-1*H*-4,7-methanoindazol-3-yl)ethan-1-one (**4c**)

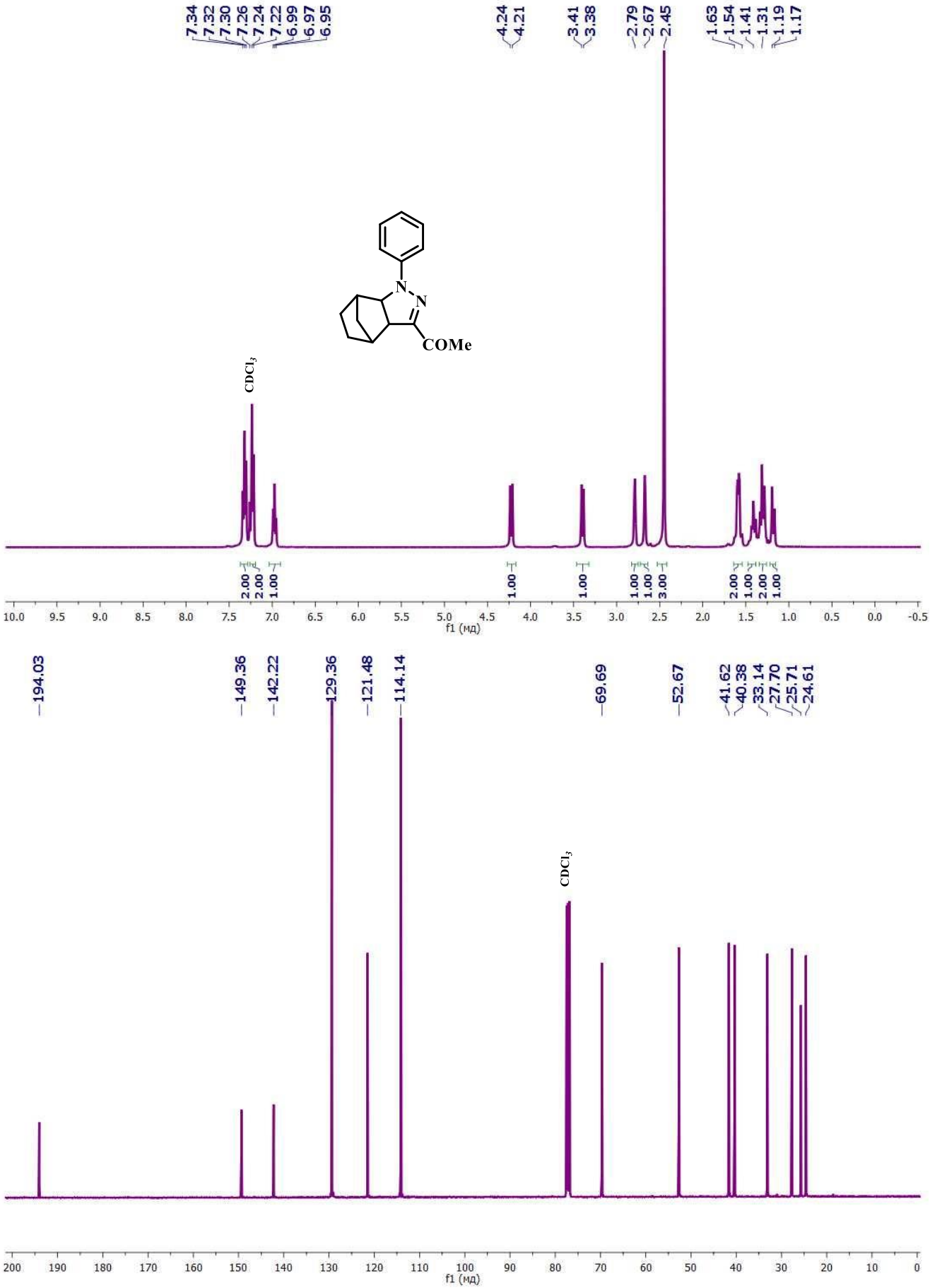


Fig. S23. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of 1-(1-phenyl-3*a*,4,5,6,7,7*a*-hexahydro-1*H*-4,7-methanoindazol-3-yl)ethan-1-one (**4d**)

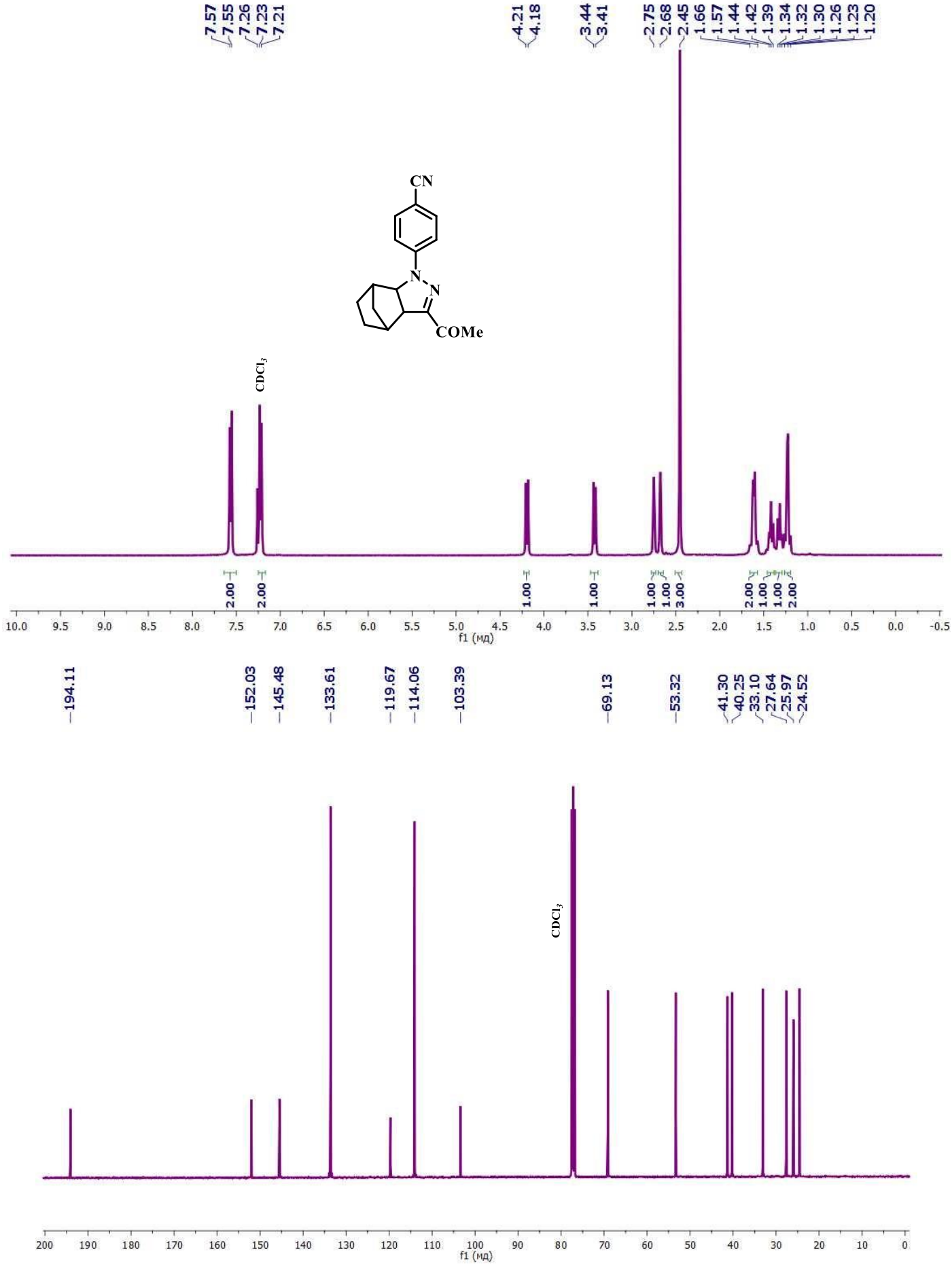


Fig. S24. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of 4-(3-acetyl-3*a*,4,5,6,7,7*a*-hexahydro-1*H*-4,7-methanoindazol-1-yl)benzonitrile (**4e**)

3. XRD crystal data Me-DPP 2h and HMIs 4b,d

The XRD experiments were accomplished on an «Xcalibur 3» diffractometer on standard procedure (MoK-irradiation, graphite monochromator, ω-scans with 1° step at 295(2) K). Empirical absorption correction was applied. Using Olex2[5], the structures were solved with the Superflip[6] structure solution program using Charge Flipping or SHELXS[7] by Direct Method (compounds **2h**, **4d)** and refined with the SHELXL[7] refinement package using Least Squares minimization in anisotropic approximation for non-hydrogen atoms. H-atoms were placed in the calculated positions and refined isotropically in the "rider" model.

Crystal structures were obtained by slow evaporation of the diluted solutions of compounds **2h** in a mixture of AcOEt/hexane **4d** in a mixture of $CHCl_3$/EtOH.

The results of XRD experiments were registered in the Cambridge Structural Database with numbers CCDC 2044826 (for compound **2h**), and CCDC 2044827 (for compound **4d**). These data may be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif

Crystal Data **2h**. $C_{15}H_{14}ClN_3O_4$, M = 335.74, monoclinic, a = 15.872(2) Å, b = 6.0495(4) Å, c = 16.2381(19) Å, β = 106.271(11)°, V = 1658.0(6) $Å^3$, space group $P2_1/n$, Z = 4, μ(MoK_α) = 0.280 mm^{-1}, 15847 reflections measured, 4123 unique (R_{int} = 0.0527) which were used in all calculations. The final R_1 = 0.1098, wR_2 = 0.0606 (all data) and R_1 = 0.0380, wR_2 = 0.0568 (I>2σ(I)). $\Delta\rho_{\bar{e}}$= 0.372/-0.279 $\bar{e}Å^{-3}$.

Crystal Data **4d**. $C_{16}H_{18}N_2O$, M = 254.32, monoclinic, a = 11.5162(17) Å, b = 7.2314(9) Å, c = 16.393(3) Å, β = 95.819(14)°, V = 1358.2(4) $Å^3$, space group $P2_1/n$, Z = 4, μ(MoK_α) = 0.079 mm^{-1}, 8074 reflections measured, 3358 unique (R_{int} = 0.0315) which were used in all calculations. The final wR_2 = 0.0834 (all data) and R_1 = 0.0401 (I>2σ(I)). $\Delta\rho_{\bar{e}}$ = 0.189/-0.127 $\bar{e}Å^{-3}$.

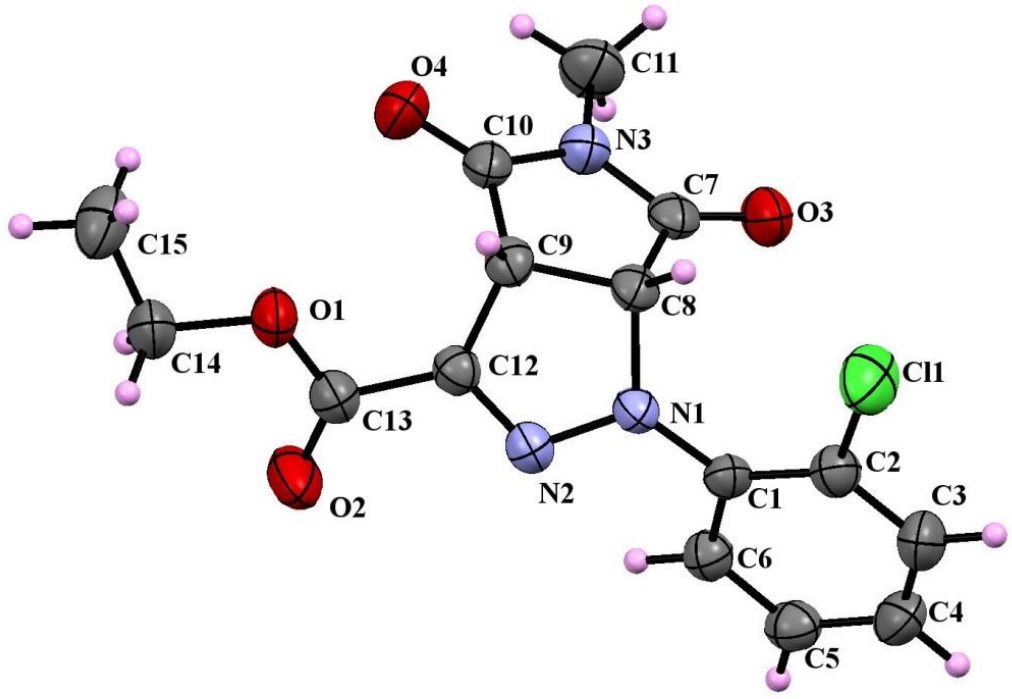


Fig. S25. The compound **2h** in the thermal ellipsoids of the 50% probability (disordering of the Et-group was omitted for clarity).

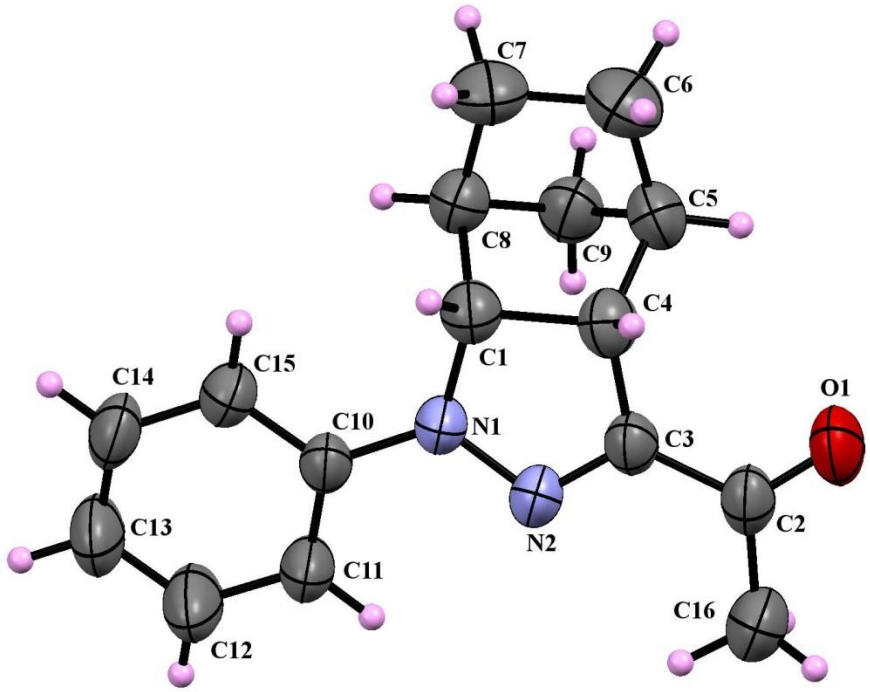
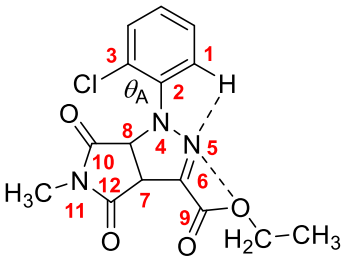
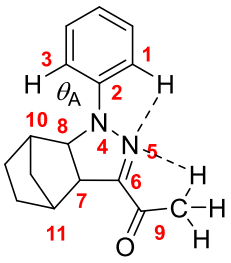


Fig. S26. The compound **4d** in the thermal ellipsoids of the 50% probability**.**

Table S1. Selected bonds lengths (in Å) for the compounds **2h**, **4b**, **4d** according to X-ray data





Entry	Compd	C2-N4	N4-N5	N5-C6	C6-C7	C7-C8	C8-N4	C6-C9	θ_A	C10C8C7-C6	C_1H-N	N_5-H_{CH3}	N5-O
1	**2h**	1.415	1.355	1.285	1.500	1.522	1.476	1.471	45.29	108.99	2.412		2.812
2	**4d**	1.394	1.347	1.406	1.500	1.551	1.464	1.453	178.8	120.94	2.503	2.467	

4. Photophysical nvestigation

The absorption and emission spectra were recorded in chloroform using 10.00 mm quartz cells at room temperature. The excitation wavelength was at the absorption maxima. Atmospheric oxygen contained in the solutions was not removed. The concentrations of the compounds in solution were 5.0×10^{-5} M and 1.0×10^{-6} M for absorption and fluorescence measurements, respectively. The relative fluorescence quantum yields (QY) were determined using quinine sulphate (1×10^{-6} M) in 0.1 M H_2SO_4 as a standard (Φ_F = 54.0 %).[5]

Suitable single crystals of pyrazolines **6g** and **8** for XRD structural analysis were obtained by slow evaporation of a solution of the compounds in ethyl acetate at room temperature. XRD data were obtained on a CCD area detector diffractometer using the standard procedure (MoK-irradiation, graphite monochromator, ω-scanning with 1° step, T = 295(2) K). Empirical absorption correction was applied. Using Olex2,[6] the structure was solved with the Superflip[7] structure solution program using Charge Flipping and refined with the ShelXL[8] refinement package using Least Squares minimization in anisotropic approximation for nonhydrogen atoms. The H-atoms were added at the calculated position and refined in the "rider" model. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via link www.ccdc.cam.ac.uk/data_request/cif.

Table S2. Photophysical properties of Me-DTPs **2a-l**, Ph-DTPs **3a-e** and HMIs **4a-d**

Entry	Compd	UV-Vis[a]		Fluorescence[b]		Stokes shift, (nm/cm^{-1})
		λ_{abs}max, (nm)	ε_{max}, ($M^{-1}\cdot cm^{-1}$)	λ_{em}max, (nm)	Φ_F[c], (%)	
1	**2a**	364	20700	512	1.7	148/7949
2	**2b**	361	16900	494	4.0	133/7458
3	**2c**	356	12600	491	7.6	135/7723
4	**2d**	349	13726	469	10.8	120/7331
5	**2e**	350	15200	474	10.8	124/7474
6	**2f**	341	18100	449	42.3	108/7054
7	**2g**	346	18700	448	77.7	102/6580
8	**2h**	320	18900	471	5.1	151/10010
9	**2i**	371	13000	500	18.6	129/6954
10	**2j**	361	13200	486	16.0	125/7125
11	**2k**	356	18000	459	13.9	102/6256
12	**3a**	356	10300	492	9.2	136/7765
13	**3b**	344	15600	448	71.9	104/6748
14	**3c**	370	12300	501	16.4	131/7067
15	**3d**	362	13400	485	12.8	123/7006
16	**3e**	356	15200	458	14.0	102/6256
17	**4a**	370	16300	487	26.3	117/6493
18	**4b**	363	16800	443	93.1	80/4975
19	**4c**	385	16900	499	13.6	114/5934
20	**4d**	378	17400	488	38.9	110/5963
21	**4e**	375	24600	457	32.7	82/4785

[a]UV-vis absorption wavelengths at room temperature at a concentration of 5×10^{-5} M.

[b]Fluorescence wavelengths at room temperature at a concentration of 1×10^{-6} M.

[c]The relative quantum yield, were definite with the standard - quinine sulfate (solution c = 0.1M H_2SO_4, Φ_F = 54.0 %).

Table S3. Photophysical properties of Ph-DPPs **3a**, **b**, **e** and HMI **4d** in dependent of concentration

Entry	Compd	*c*, M	UV-Vis[b]		Fluorescence[c]		*SS*, nm/cm^{-1}
			λ_{abs}max, nm	ε_{max}, M^{-1} cm^{-1}	λ_{em}max, nm	*QY*,[d] %	
1	**3a**	1.0×10^{-6}	353	13000	481	9.2	128/7539
2		2.5×10^{-6}	353	8400	490	6.4	137/7920
3		5.0×10^{-6}	353	9000	492	5.9	139/8003
4	**3b**	1.0×10^{-6}	349	17000	447	71.9	107/7040
5		2.5×10^{-6}	344	19600	448	68.3	104/6748
6		5.0×10^{-6}	344	19000	448	60.7	104/6748
7	**3e**	1.0×10^{-6}	371	12000	460	17.7	89/5215
8		2.5×10^{-6}	371	13600	473	8.4	102/5813
9		5.0×10^{-6}	371	13600	496	4.1	125/6793
10	**4d**	1.0×10^{-6}	373	32000	458	32.7	85/4976
11		2.5×10^{-6}	376	19600	457	31.7	81/4714
12		5.0×10^{-6}	376	17000	458	31.0	82/4762

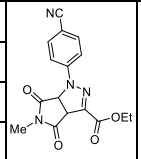
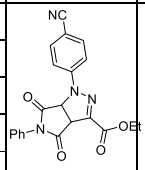
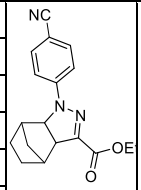
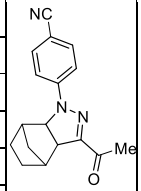
[a]The experiment was repeated several times. [b]UV-vis absorption wavelengths at room temperature at a concentration of 5×10^{-5} M. [c] Fluorescence wavelengths at room temperature at a concentration of 1×10^{-6} M. [d]The relative quantum yield, were definite with the standard - quinine sulfate (solution c = 0.1M H_2SO_4, Φ_F = 54.0 %).

Table S4. Lifetime values of Me-DPPs **2i-k**, Ph-DPPs **3a-e**, and HMIs **4b-c** obtained in $CHCl_3$

Entry	Compd	τ_1[a] (ns)	A_1[b]	τ_2[a] (ns)	A_2[b]	τ_3[a] (ns)	A_3[b]	$\langle\tau\rangle_f$[c] (ns)	χ^2
1	**2i**	0.0830085	-0.1266	0.6796846	1.0744	3.640079	0.0522	0.9098	1.140
2	**2j**	1.20049	0.7467	1.916438	0.2533	-	-	1.3818	1.112
3	**2k**	1.580955	0.0619	0.2382781	0.9113	4.411467	0.0269	0.4337	1.106
4	**3a**	0.1440308	-0.2094	0.9638026	1.1377	2.808342	0.0716	1.2674	1.012
5	**3b**	2.1449	0.2329	0.234713	-0.0739	5.047551	0.8410	4.7272	1.048
6	**3c**	0.6716223	0.931	3.508906	0.069	-	-	0.8674	1.098
7	**3d**	1.199454	0.8333	2.183725	0.1667	-	-	1.3635	1.028
8	**3e**	1.305331	0.0496	0.2403628	0.8996	3.512939	0.0508	0.4594	1.186
9	**4b**	1.506172	0.2404	0.3154246	-0.1705	4.330757	0.5878	3.3694	
10	**4b**	1.547604	0.2404	0.2504187	-0.0649	3.807704	0.8245	3.4952	1.093
11	**4d**	1.080918	0.5294	2.2946150	0.4706	-	-	1.65208	1.141

[a]Fluorescence lifetime. [b]Fractional contribution. [c]Weighted mean lifetime. [d]χ^2-Chi-squared.

Table S5. Absorption ($c = 5\times10^{-5}$ M) and emission ($c = 1\times10^{-6}$ M) properties of pyrazolines **2g**, **3b**, **4b** and **4d** in different solvents

Entry	Structure	Compd	Solvent	$E_T(30)^a$	UV-Vis		Fluorescence		Stokes Shift, nm/cm^{-1}
					λ_{abs}max, nm	ε_{max}, M^{-1} cm^{-1}	λ_{em}max, nm	*QY*,b %	
1		**2g**	Toluene	33.9	346	19500	441	50.5	95/6226
2			1,4-Dioxane	36.0	344	24200	442	80.8	98/6445
3			$CHCl_3$	39.1	345	17100	448	59.7	103/6664
4			EtOAc	38.1	342	23300	442	92.4	100/6615
5			DMF	43.2	348	24674	450	53.3	102/6513
6			DMSO	45.1	350	23100	455	41.0	105/6593
7			MeCN		345	22500	450	69.6	105/6763
8			EtOH	51.9	346	32050	460	18.6	114/7163
9			1-BuOH	50.2	345	23900	457	47.7	112/7104
10			Ethylene glycole		350	13800	466	30.1	116/7112
11		**3b**	Toluene	33.9	345	16300	442	67.7	97/6361
12			1,4-Dioxane	36.0	344	15600	443	61.7	99/6496
13			$CHCl_3$	39.1	344	15900	448	71.9	104/6748
14			EtOAc	38.1	341	20400	443	65.9	102/6752
15			DMF	43.2	349	22000	451	47.6	102/6480
16			DMSO	45.1	352	24995	457	49.8	105/6527
17			MeCN		344	24800	460	16.6	113/7079
18			EtOH	51.9	347	18379	460	16.6	120/7673
19			BuOH	50.2	350	24500	457	25.6	107/7020
20			$CH_2(OH)CH_2OH$		351	19100	465	5.7	114/6985
21		**4b**	Toluene	33.9	361	23200	432	60.6	71/4553
22			1,4-Dioxane	36.0	360	20600	437	57.2	77/4894
23			$CHCl_3$	39.1	363	17300	443	93.1	80/4975
24			EtOAc	38.1	358	12000	436	57.6	78/4997
25			MeCN	43.2	359	11300	446	54.6	87/5434
26			DMF	45.1	363	31300	446	82.0	83/5127
27			DMSO		364	32300	449	82.3	85/5201
28			EtOH	51.9	361	12100	457	58.6	96/5819
29			BuOH	50.2	361	12100	453	70.0	92/5626
30			$CH_2(OH)CH_2OH$		364	20500	464	54.0	100/5921
31		**4d**	Toluene	33.9	374	25900	444	3.2	70/4215
32			1,4-Dioxane	36.0	371	30100	447	5.6	76/4583
33			$CHCl_3$	39.1	375	24600	456	33.2	81/4737
34			EtOAc	38.1	369	28000	449	5.5	80/4829
35			DMF	43.2	374	31200	460	23.4	86/4999
36			DMSO	45.1	378	29600	463	35.2	85//4857
37			MeCN		372	30000	461	25.6	89/5190
38			EtOH	51.9	376	32400	484	35.9	108/5935
39			BuOH	50.2	376	34800	476	35.1	100/5587
40			Ethylene glycole		379	19100	490	18.9	111/5977

[a] Reichardt empirical polarity parameter.

[b]Значение относительного квантового выхода, стандарт – хинин сульфат (раствор c = 0.1M H_2SO_4, Φ_F = 54.0 %).

Table S6. The UV-Vis and fluorescence data of DTP **1c** in DMSO-water mixture with different water volume fractions.

№	Water content, %	UV-Vis		Fluorescence		
		λ_{abs}max, nm	ε_{max}, M^{-1} cm^{-1}	λ_{em}max, nm	Φ_F, %	SS, nm/cm^{-1}
1	0	351	28400	455	51.5	104/6512
2	10	350	31800	458	40.6	108/6737
3	20	350	39400	461	32.3	111/6879
4	30	351	30200	463	27.7	112/6892
5	40	350	29800	465	20.4	115/7066
6	50	351	29400	470	15.0	119/7213
7	60	352	29200	472	11.4	120/7223
8	70	351	29800	474	8.6	123/7393
9	80	352	27800	474	7.6	122/7312
10	90	352	26600	478	5.9	126/7489

[a]UV-vis absorption wavelengths at room temperature at a concentration of 5×10^{-5} M.
[b]Fluorescence quantum yields measured using a 0.1 M H_2SO_4 solution of quinine sulphate (Φ_F = 54.0)

5. 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 (DMSO, EtOH, DMF, $CHCl_3$, Toluene, MeCN). We compared the results obtained by employing different functionals with the experimental data. 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.

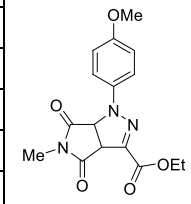
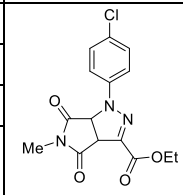
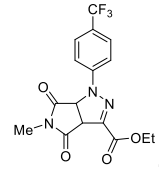
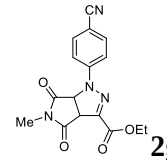
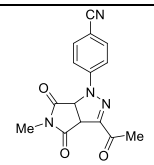
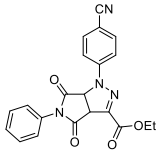
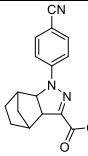
The atomic charge population analysis, electric multiple moments, electronic density, and electrostatic potential were also computed using Mulliken's and the CHelpG procedure[16] for both the ground and the S_1 excited (vertical and relaxed) states.

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.

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 were 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 S7. Stability of the different isomers of Me-DPPs **2a**,**e-g**,**k**, Ph-DPP **3b** and HMI **4b** in $CHCl_3$ in kJ/mol

Entry	Compd	Rotamer	Δ*E*	Δ(*E*+ZPE)	Δ*H*	Δ*G*	*f*
1	 **2a**	A	2.5	3.5	3.0	5.1	0.064
2		B		2.3	3.3	2.7	5.1
3		C		0.1	0.7	0.5	0.7
4		D		0.0	0.0	0.0	0.0
5		E		32.7	32.2	32.0	33.5
6		F		32.2	32.4	32.2	33.2
7		G		32.8	32.8	32.6	33.3
8		H		32.0	31.5	31.4	32.1
9	 **2e**	A	2.4	2.8	2.4	5.3	0.105
10		B		0.0	0.0	0.0	0.0
11		C		32.8	32.6	32.5	33.5
12		D		32.9	32.3	32.3	33.1
13	 **2f**	A		2.4	2.6	2.3	4.6
14		B		0.0	0.0	0.0	0.0
15		C		33.2	33.0	32.9	32.9
16		D		33.2	32.9	32.8	34.4
17	 **2g**	A		2.3	2.8	2.3	5.8
18		B		0.0	0.0	0.0	0.0
19		C		33.3	33.4	33.1	34.9
20		D		33.4	33.2	33.0	34.7
21	 **2k**	A		0.0	0.0	0.0	0.0
22		B		1.5	1.7	1.5	2.6
23	 **3b**	A		1.7	2.3	1.9	5.2
24		B		0.0	0.0	0.0	0.0
25	 **4b**	A		0.0	0.0	0.0	0.0
26		B		2.13	2.42	2.33	2.29

Rotamers spectroscopical and other properties will be computed for those rotamers having $f > 0.1$ (10%)

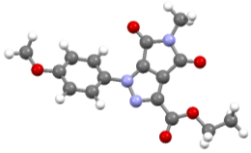
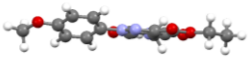
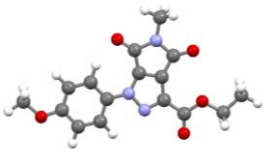
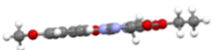
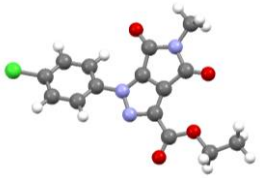
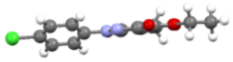
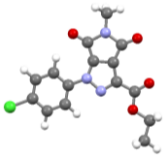
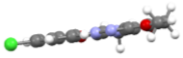
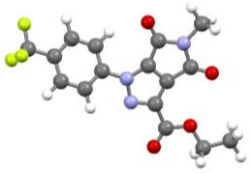
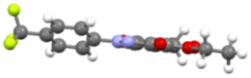
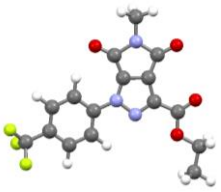
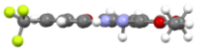
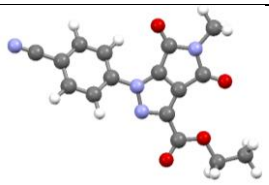
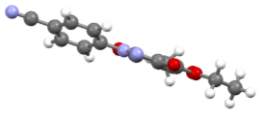
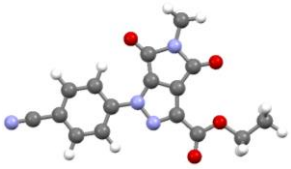
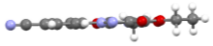
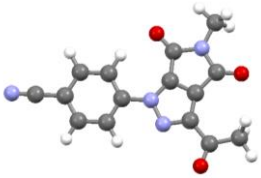
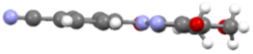
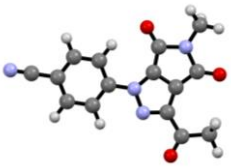
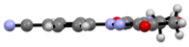
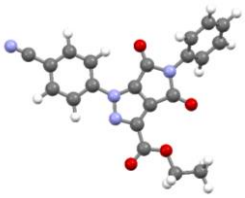
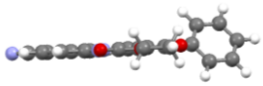
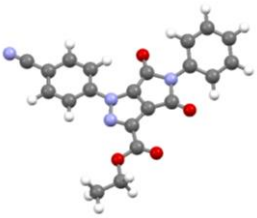
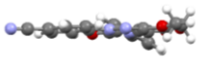
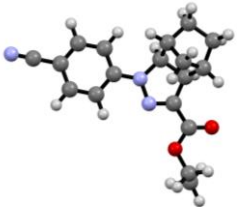
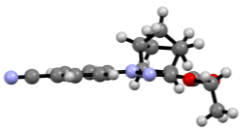
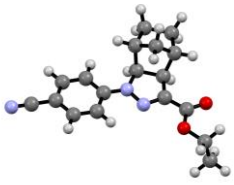
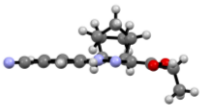
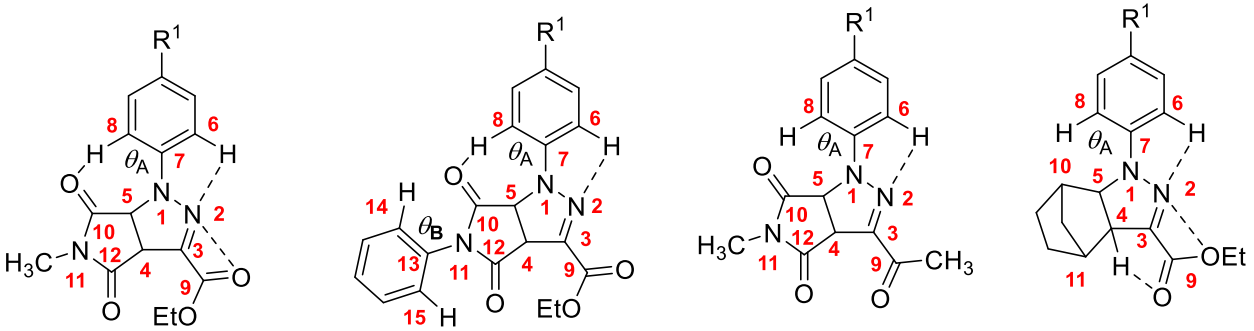
Entry	Compd	S_0		S_1	
1	**2a**				
2	**2e**				
3	**2f**				
4	**2g**				
5	**2k**				
6	**3b**				
7	**4b**				

Fig. S27. Optimized geometries of the investigated molecules **2a**, **e-g**,k, **3b** and **4b** in their ground (*GS*) and exciting (*ES*) state, in $CHCl_3$ and depicted from two orthogonal viewpoints. Level of theory: DFT /IEF-PCM(UFF). Legend of colours: white (H), grey (C), lilac (N), and red (O).

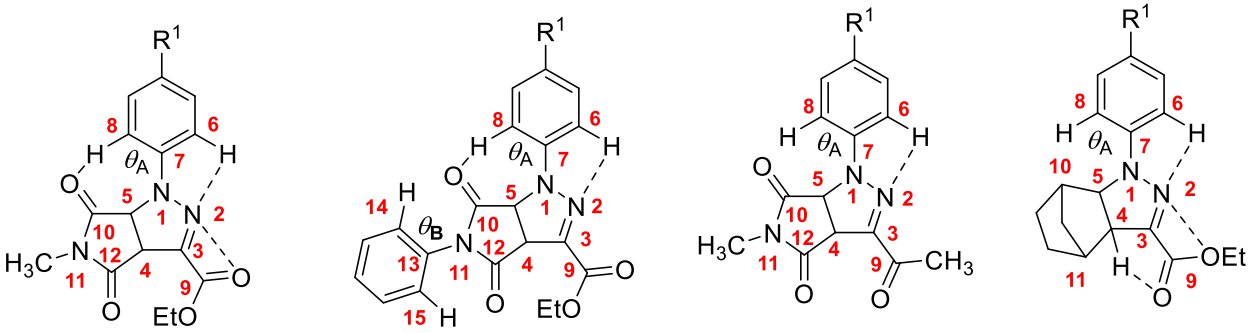
Table S8. Selected bonds lengths (in Å) and angles (in grad) for the GS (S_0) optimized geometries of compounds **2a**, **e-g**,k, **3b** and **4b** in $CHCl_3$

The selected bond lengths (Å) and bond angles (°) B3LYP/6-311G+(d,p) calculation.



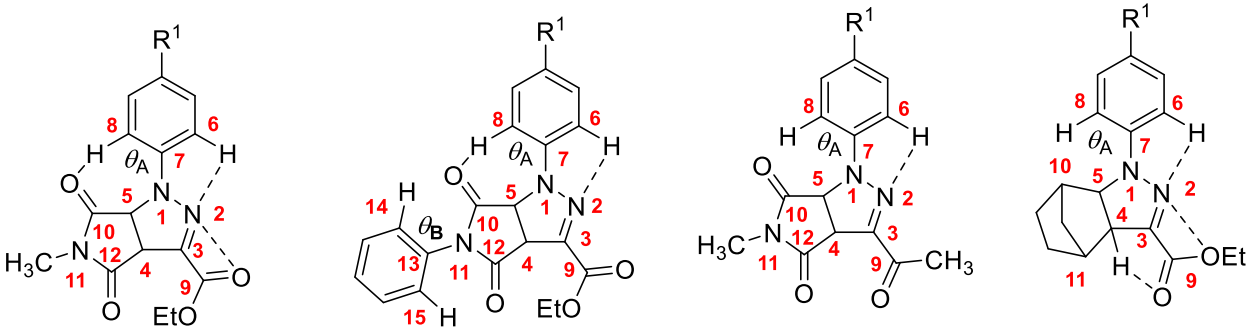
Entry	Compd	C7-N1	N1-N2	N2-C3	C3-C4	C4-C5	C5-N1	C3-C9	*C9=O*	C9-OEt	C10-O	C12-O	N11-C13	θ_A	Θ_B	C10C8C7-C6
1	**2a**	1.428	1.339	1.334	1.407	1.372	1.351	1.485	1.210	1.329	1.210	1.207	1.451	27.8	-	177.0
2	**2e**	1.427	1.341	1.332	1.408	1.371	1.352	1.486	1.209	1.328	1.209	1.206	1.452	26.5		177.1
3	**2f**	1.426	1.341	1.331	1.409	1.370	1.353	1.487	1.209	1.328	1.209	1.206	1.452	26.6	-	177.2
4	**2g**	1.425	1.342	1.332	1.409	1.369	1.353	1.487	1.209	1.328	1.209	1.206	1.452	25.6		177.2
5	**2k**	1.427	1.341	1.331	1.411	1.371	1.356	1.498	1.214	-	1.210	1.208	1.453	-2.81	-	179.9
6	**3b**	1.427	1.342	1.327	1.408	1.370	1.359	1.488	1.209	1.326	1.207	1.203	1.428	1.1	57.5.	179.2
7	**4b**	1.382	1.350	1.287	1.505	1.580	1.477	1.478	1.216	1.332				-1.30		109.1

Table S9. Selected bonds lengths (in Å) and angles (in grad) for the ES (S_{1r}) optimized geometries of compounds **2a**, **e-g**,**k**, **3b** and **4b** in $CHCl_3$



Entry	Compd	C7-N1	N1-N2	N2-C3	C3-C4	C4-C5	C5-N1	C3-C9	*C9=O*	*C9-OEt*	*C10-O*	*C12-O*	*N11-C13*	θ_A	Θ_B	C10C5C4-C3
1	**2a**	1.355	1.391	1.313	1.425	1.387	1.392	1.493	1.205	1.322	1.235	1.222	1.445	0.14	-	179.9
2	**2d**	1.416	1.367	1.309	1.425	1.440	1.357	1.488	1.205	1.323	1.225	1.222	1.420	1.50		179.8
3	**2e**	1.415	1.365	1.309	1.425	1.440	1.361	1.488	1.204	1.322	1.224	1.221	1.419	-0.64	-	179.4
4	**2f**	1.412	1.366	1.308	1.425	1.439	1.361	1.489	1.204	1.322	1.224	1.220	1.419	-3.20	-	179.9
5	**2k**	1.413	1.366	1,311	1.426	1.439	1.359	1.503	1.208	-	1.224	1.224	1.420	-1.02	-	179.1
6	**3e**	1.412	1.354	1.311	1.425	1.415	1.375	1.488	1.205	1.324	1.227	1.220	1.380	3.90	27.5	179.7
7	**4b**	1.365	1.366	1.356	1.488	1.542	1.468	1.437	1.236	1.334	-	-	-	4.14	-	117.6

Table S10. Selected non-covalent bonding lengths (in Å) and angles (*grad*) for the optimized geometries of compound **2a**, **e-g**,**k**, **3b** and **4b** in *GS* and *ES* in the mixture of $CHCl_3$



Entry	Compd	S_0						S_{1r}					
		C6H-N2	C8H-O=C10	N2-O=C9	N1N2O=C9	C14H-O=C10	C15H-O=C12	C6H-N2	C8H-O=C10	N2-C9=O	C14H-C10=O	C14H-O=C10	C15H-O=C12
1	**2a**	2.553	2.405	2.839	163.8	-	-	2.396	2.036	2.787	170.5	-	-
2	**2d**	2.533	2.373	2.838	163.8	-	-	2.404	2.141	2.080	169.2	-	-
3	**2e**	2.551	2.363	2.836	163.8	-	-	2.401	2.137	2.680	169.2	-	-
4	**2f**	2.506	2.342	2.834	163.9			2.401	2.137	2.680	169.2	-	-
5	**2k**	2/403	2.090	-	-	-	-	2.402	2.132	-	-	-	-
6	**3e**	2.395	2.095	2.794	166.6	2.205	2.213	2.396	2.093	2.829	164.4	2.833	2.852
7	**4b**	2.463		2.700	165.2			2.376		2.701	165.0		

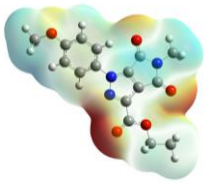
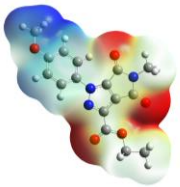
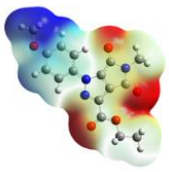
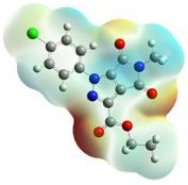
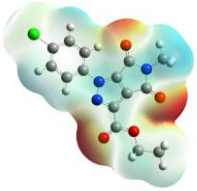
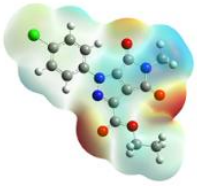
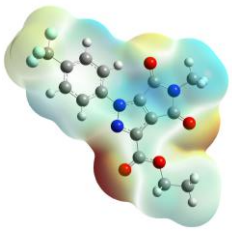
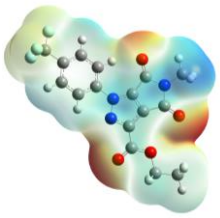
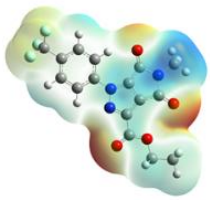
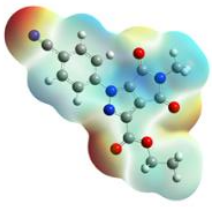
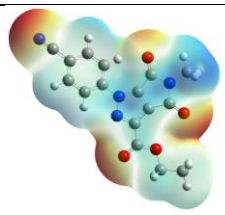
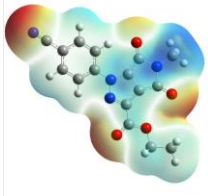
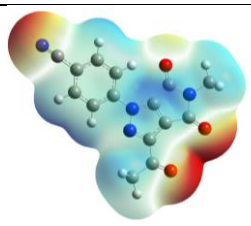
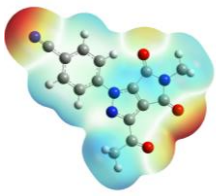
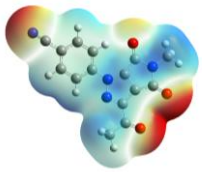
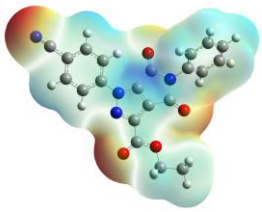
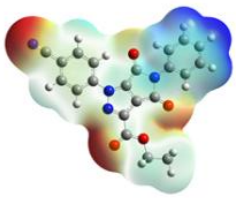
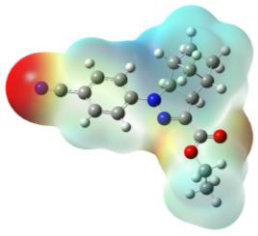
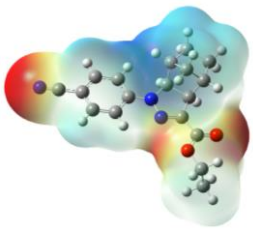
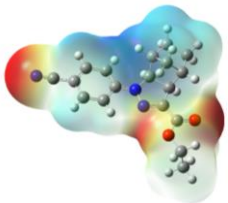
Entry	Compd	S_0	S_{1v}	S_{1r}
1	**2a**			
2	**2e**			
3	**2f**			
4	**2g**			
5	**2k**			
6	**3b**			
7	**4b**			

Fig. S28. Plot of MEPs of complexes **2a**, **e-g**,**k**, **3b** and **4b** calculated at (TD-)DFT ω-B97X-D / 6−311++G** // IEF-PCM(UFF) level of theory, for GS and ESs in $CHCl_3$. The red and blue colors correspond to negative and positive potential regions, respectively. Green color corresponds to the neutral region.

Legend of map colours: red (negative potential), blue (positive potential). Legend of elements: hydrogen (white), carbon (grey), nitrogen (blue), oxygen (red), sulphur (yellow), chlorine (

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

Optimised Geometries (S_0) in chloroform

Mol-2a/A_s0_chl.out

```
    * SCF ENERGY / A.U. =   -1158.72296531

       6         1.476105    1.665831    0.625846
       6         0.408921    2.581518    0.571799
       6        -0.718210    1.800112    0.606930
       6        -0.027218    3.995675    0.437118
       6        -1.943242    2.647603    0.490640
       6        -1.131770   -0.674082    0.730844
       6        -2.395839   -0.629485    1.321212
       6        -0.631652   -1.856871    0.199860
       6        -3.163292   -1.781417    1.366501
       1        -2.777811    0.295362    1.739442
       6        -1.398835   -3.018697    0.255089
       1         0.351814   -1.872792   -0.256603
       6        -2.669747   -2.982293    0.838361
       1        -4.148640   -1.774261    1.820330
       1        -0.998323   -3.934435   -0.162408
       7        -1.434611    3.938239    0.396020
       7        -0.332934    0.508399    0.679659
       7         1.003863    0.419013    0.695451
       8         0.599194    5.024466    0.366322
       8        -3.113700    2.341920    0.476962
       8        -3.491140   -4.053562    0.939287
       6         2.932646    1.952266    0.626393
       8         3.372421    3.080465    0.616549
       8         3.671082    0.848162    0.638029
       6         5.102305    1.045344    0.644869
       1         5.365702    1.628259    1.531916
       1         5.375163    1.622083   -0.243297
       6         5.743049   -0.322552    0.653032
       1         5.458190   -0.891570   -0.236079
       1         6.830899   -0.211907    0.658729
       1         5.447980   -0.885834    1.542386
       6        -3.027776   -5.298242    0.434935
       1        -3.832094   -6.010608    0.615843
       1        -2.829152   -5.237926   -0.640684
       1        -2.125238   -5.624980    0.962986
       6        -2.258931    5.127046    0.277587
       1        -2.066507    5.800395    1.115354
       1        -2.043670    5.642777   -0.660625
       1        -3.302233    4.811967    0.291275
```

Mol-2a/B_s0_chl.out

```
    * SCF ENERGY / A.U. =   -1158.72305162

       6         1.449555    1.693767    0.656341
       6         0.406094    2.637346    0.657233
       6        -0.740351    1.886128    0.596344
```

6	0.010214	4.068728	0.644308
6	-1.939686	2.775062	0.522753
6	-1.211999	-0.580617	0.493695
6	-2.503501	-0.545037	1.001208
6	-0.699660	-1.743914	-0.087042
6	-3.312108	-1.678261	0.919661
1	-2.892321	0.358550	1.457805
6	-1.498474	-2.871577	-0.158906
1	0.311352	-1.755318	-0.478195
6	-2.810328	-2.845659	0.337956
1	-4.318003	-1.634071	1.318169
1	-1.127292	-3.787107	-0.607513
7	-1.396475	4.054252	0.560467
7	-0.387357	0.582992	0.565358
7	0.945956	0.458561	0.604842
8	0.664453	5.081346	0.690352
8	-3.117020	2.506068	0.446982
8	-3.512812	-3.995694	0.209475
6	2.912039	1.943171	0.707028
8	3.378348	3.060137	0.745761
8	3.622878	0.821158	0.702869
6	5.058023	0.981825	0.746706
1	5.315243	1.544458	1.648469
1	5.365741	1.564685	-0.125983
6	5.664044	-0.401784	0.748652
1	5.381896	-0.952361	-0.152804
1	6.754070	-0.318749	0.776013
1	5.338067	-0.968534	1.624843
6	-4.850199	-4.017695	0.689421
1	-5.223121	-5.021248	0.486983
1	-4.883288	-3.826830	1.767580
1	-5.469372	-3.284228	0.161400
6	-2.186360	5.271466	0.528118
1	-1.977974	5.874387	1.414276
1	-1.953086	5.849735	-0.368562
1	-3.238346	4.986682	0.516667

Mol-2a/C_s0_chl.out

* SCF ENERGY / A.U. = -1158.72385828

6	1.426432	1.584180	0.664740
6	0.380536	2.521926	0.591937
6	-0.764218	1.765894	0.616589
6	-0.019092	3.945413	0.447841
6	-1.966855	2.642222	0.482049
6	-1.229373	-0.699572	0.743704
6	-2.506067	-0.624866	1.302702
6	-0.740195	-1.896133	0.233652
6	-3.297411	-1.760963	1.338223
1	-2.879312	0.311030	1.704009
6	-1.531924	-3.041699	0.278891
1	0.253785	-1.935273	-0.197860
6	-2.815466	-2.975446	0.830877
1	-4.293066	-1.730791	1.767907
1	-1.139909	-3.968751	-0.121306
7	-1.425963	3.920819	0.385606
7	-0.406324	0.466574	0.701249

7	0.927494	0.349196	0.734982
8	0.634289	4.958526	0.385722
8	-3.144460	2.366849	0.457655
8	-3.659819	-4.029837	0.919841
6	2.897828	1.785062	0.676509
8	3.711303	0.890543	0.719184
8	3.185147	3.081598	0.632123
6	4.584642	3.435230	0.635464
1	5.055766	2.986868	-0.244075
1	5.046316	3.010596	1.531430
6	4.660526	4.943676	0.615671
1	4.172738	5.368201	1.497080
1	5.708813	5.254398	0.614178
1	4.176359	5.345224	-0.278345
6	-3.209520	-5.285920	0.431919
1	-4.028822	-5.983313	0.603622
1	-2.991252	-5.236119	-0.640433
1	-2.321805	-5.624371	0.977227
6	-2.220923	5.127754	0.251549
1	-2.047841	5.788342	1.103751
1	-1.959062	5.648602	-0.671763
1	-3.270183	4.834412	0.221514

Mol-2a/D_s0_chl.out

* SCF ENERGY / A.U. = -1158.72391329

6	1.381041	1.608729	0.490469
6	0.360265	2.568036	0.617815
6	-0.799642	1.835930	0.656324
6	0.000035	3.998776	0.789632
6	-1.973525	2.736668	0.864941
6	-1.321264	-0.619665	0.566617
6	-2.627405	-0.518800	0.108031
6	-0.818795	-1.832037	1.046944
6	-3.460556	-1.636846	0.137037
1	-3.008233	0.424025	-0.269334
6	-1.642294	-2.943905	1.066352
1	0.203937	-1.893950	1.401413
6	-2.968683	-2.853249	0.618242
1	-4.477709	-1.542596	-0.222427
1	-1.279827	-3.897002	1.437038
7	-1.401368	4.003327	0.931508
7	-0.473437	0.529308	0.555280
7	0.853763	0.384078	0.450108
8	0.677141	4.997618	0.819600
8	-3.153248	2.486164	0.960447
8	-3.693541	-3.994203	0.689608
6	2.853206	1.781997	0.402851
8	3.646523	0.873486	0.309187
8	3.167345	3.072520	0.444133
6	4.571715	3.397902	0.369605
1	4.978467	2.965483	-0.548849
1	5.077365	2.938029	1.223709
6	4.680243	4.904215	0.386968
1	4.248926	5.314385	1.303797
1	5.733863	5.192639	0.338370
1	4.159550	5.340793	-0.469346

6	-5.053835	-3.949191	0.281805
1	-5.444193	-4.954763	0.435888
1	-5.623508	-3.238696	0.890740
1	-5.139226	-3.684756	-0.777718
6	-2.160208	5.225529	1.123525
1	-1.834412	5.729176	2.035994
1	-2.020857	5.892505	0.270204
1	-3.212436	4.954850	1.209974

Mol-2a/E_s0_chl.out

* SCF ENERGY / A.U. = -1158.71147446

6	1.293925	1.377510	-0.238828
6	0.352823	2.341191	0.165829
6	-0.795227	1.629701	0.401421
6	0.090977	3.757722	0.523816
6	-1.868539	2.534661	0.916217
6	-1.420303	-0.795883	0.220539
6	-2.791067	-0.623205	0.020244
6	-0.890136	-2.051487	0.491120
6	-3.631397	-1.720444	0.105143
1	-3.198603	0.357728	-0.199310
6	-1.733590	-3.158152	0.564086
1	0.176752	-2.168157	0.647199
6	-3.109871	-2.993418	0.374803
1	-4.700236	-1.613567	-0.046872
1	-1.306913	-4.130965	0.775375
7	-1.252790	3.781291	0.946479
7	-0.546795	0.330251	0.137100
7	0.726492	0.169301	-0.254434
8	0.804399	4.730615	0.506166
8	-3.008606	2.295995	1.242097
8	-4.011912	-4.000539	0.431340
6	2.684878	1.628108	-0.719824
8	2.949227	2.675781	-1.263429
8	3.626284	0.698172	-0.573850
6	3.486490	-0.470826	0.268399
1	2.941163	-1.235719	-0.288516
1	2.919343	-0.207734	1.164692
6	4.886034	-0.922916	0.616878
1	5.418099	-0.145506	1.171420
1	4.832043	-1.821190	1.238550
1	5.452569	-1.161501	-0.286973
6	-3.530937	-5.314392	0.677884
1	-3.034303	-5.375705	1.652145
1	-4.409326	-5.959008	0.677679
1	-2.842935	-5.634819	-0.111874
6	-1.909589	4.999284	1.385260
1	-1.419536	5.391492	2.279063
1	-1.873840	5.748141	0.591464
1	-2.946945	4.754856	1.613528

Mol-2a/F_s0_chl.out

* SCF ENERGY / A.U. = -1158.71163960

6	1.315572	1.416439	-0.033084

6	0.360554	2.406277	0.262431
6	-0.825129	1.726171	0.371495
6	0.079457	3.847550	0.480932
6	-1.945877	2.679495	0.637524
6	-1.480601	-0.691639	0.139073
6	-2.628295	-0.657502	0.919155
6	-1.179968	-1.805613	-0.649390
6	-3.502878	-1.743640	0.913372
1	-2.853232	0.208581	1.532085
6	-2.042535	-2.887766	-0.647648
1	-0.281111	-1.815168	-1.255703
6	-3.209210	-2.864125	0.131329
1	-4.395447	-1.702452	1.525359
1	-1.834250	-3.764858	-1.251530
7	-1.313870	3.917071	0.681396
7	-0.581437	0.417835	0.146975
7	0.722866	0.222154	-0.094560
8	0.808103	4.808486	0.510346
8	-3.129449	2.479380	0.788162
8	-3.987904	-3.968803	0.061524
6	2.756438	1.635723	-0.354785
8	3.108223	2.703535	-0.801842
8	3.648268	0.663690	-0.177010
6	3.392467	-0.549698	0.571516
1	2.831063	-1.239606	-0.061030
1	2.795090	-0.310538	1.454849
6	4.742012	-1.112775	0.953104
1	5.293736	-0.409319	1.582121
1	4.600291	-2.043148	1.510425
1	5.336926	-1.330082	0.062162
6	-5.170705	-3.999901	0.848473
1	-5.859263	-3.199711	0.556296
1	-5.633779	-4.966689	0.653817
1	-4.934331	-3.917138	1.914966
6	-2.001664	5.169332	0.937545
1	-1.625591	5.624710	1.856152
1	-1.850288	5.856354	0.102679
1	-3.064080	4.950485	1.044216

Mol-2a/G_s0_chl.out

* SCF ENERGY / A.U. = -1158.71143733

6	1.349930	1.387202	1.170208
6	0.358458	2.360788	0.942678
6	-0.789373	1.644305	0.723258
6	0.012836	3.803460	0.862163
6	-1.946279	2.566252	0.509425
6	-1.346457	-0.805087	0.699138
6	-2.447577	-0.751992	-0.156914
6	-1.061010	-1.952486	1.428775
6	-3.272601	-1.858889	-0.267540
1	-2.659038	0.145110	-0.729163
6	-1.884451	-3.069950	1.309768
1	-0.203296	-1.972860	2.092395
6	-2.995789	-3.024266	0.461074
1	-4.135119	-1.844420	-0.925576
1	-1.653547	-3.956949	1.886835

7	-1.375661	3.829033	0.617735
7	-0.492424	0.332218	0.824785
7	0.810710	0.167978	1.091230
8	0.690882	4.795656	0.962425
8	-3.111739	2.326731	0.290967
8	-3.856279	-4.053015	0.279278
6	2.771909	1.654127	1.536926
8	3.068351	2.735713	1.991762
8	3.710210	0.721520	1.387596
6	3.531020	-0.522221	0.668493
1	2.964289	-0.332909	-0.246142
1	2.968155	-1.213508	1.298433
6	4.915810	-1.045857	0.364769
1	5.478397	-1.210751	1.287436
1	4.832607	-1.998650	-0.165768
1	5.468702	-0.343183	-0.264043
6	-3.603291	-5.264894	0.976631
1	-3.628954	-5.107812	2.060393
1	-4.403388	-5.946832	0.690688
1	-2.637419	-5.691121	0.684144
6	-2.114600	5.068325	0.459317
1	-1.932434	5.716484	1.318277
1	-1.807848	5.581089	-0.455301
1	-3.174726	4.821295	0.404272

Mol-2a/H_s0_chl.out

* SCF ENERGY / A.U. = -1158.71173590

6	1.257988	1.401712	1.394669
6	0.332573	2.379247	0.987222
6	-0.823720	1.684412	0.742596
6	0.093609	3.799614	0.629176
6	-1.881061	2.605471	0.223969
6	-1.480370	-0.734660	0.910317
6	-2.844264	-0.551722	1.093835
6	-0.955088	-2.000493	0.637336
6	-3.709446	-1.640534	0.992267
1	-3.244563	0.432128	1.314208
6	-1.811641	-3.083437	0.548908
1	0.112280	-2.126994	0.493369
6	-3.193291	-2.910905	0.721535
1	-4.771342	-1.482593	1.135336
1	-1.431680	-4.077206	0.336078
7	-1.247213	3.843018	0.198106
7	-0.594672	0.380937	1.004797
7	0.673955	0.201461	1.403276
8	0.820932	4.761985	0.652278
8	-3.023427	2.384102	-0.106719
8	-3.945359	-4.030077	0.608280
6	2.650171	1.633291	1.881608
8	2.925320	2.677257	2.427169
8	3.580472	0.692339	1.737095
6	3.426466	-0.477334	0.897943
1	2.864453	-0.209394	-0.000139
1	2.869859	-1.233016	1.456247
6	4.820280	-0.949339	0.553117
1	5.382445	-1.192349	1.458510

1	4.754587	-1.849102	-0.065270
1	5.363387	-0.181268	-0.003730
6	-5.353063	-3.904329	0.755257
1	-5.768460	-3.233477	-0.004390
1	-5.758450	-4.906055	0.616174
1	-5.613257	-3.542153	1.755722
6	-1.882879	5.070454	-0.245487
1	-1.844560	5.818298	0.549169
1	-1.378723	5.456384	-1.134164
1	-2.921211	4.840393	-0.483969

Mol-2e/A_s0_chl.out

* SCF ENERGY / A.U. = -1503.80737453

6	1.446630	1.689501	0.643044
6	0.401960	2.633725	0.649084
6	-0.743966	1.884879	0.586719
6	0.007754	4.066498	0.648928
6	-1.943580	2.777036	0.521445
6	-1.210556	-0.584128	0.476997
6	-2.511832	-0.538583	0.969025
6	-0.683255	-1.747851	-0.079804
6	-3.307652	-1.677341	0.892719
1	-2.909338	0.370041	1.407065
6	-1.476070	-2.887894	-0.145189
1	0.332277	-1.759457	-0.458055
6	-2.780538	-2.839660	0.339506
1	-4.323981	-1.658299	1.270123
1	-1.083466	-3.802367	-0.576198
7	-1.399090	4.054183	0.568302
7	-0.389983	0.580839	0.548075
7	0.944743	0.456136	0.584491
8	0.664415	5.076491	0.702345
8	-3.120457	2.507799	0.444146
6	2.909688	1.940358	0.698115
8	3.372551	3.058236	0.739546
8	3.620601	0.819230	0.695232
6	5.056054	0.980317	0.746579
1	5.307845	1.542014	1.650414
1	5.367553	1.564312	-0.123928
6	5.662274	-0.403096	0.750177
1	5.385151	-0.952813	-0.153360
1	6.752073	-0.319578	0.783226
1	5.332161	-0.970765	1.624212
6	-2.187824	5.272859	0.545668
1	-1.974430	5.870250	1.434275
1	-1.957341	5.855212	-0.349002
1	-3.240187	4.989533	0.537418
17	-3.776190	-4.270938	0.253446

Mol-2e/B_s0_chl.out

* SCF ENERGY / A.U. = -1503.80829451

6	1.381317	1.602300	0.511772
6	0.359055	2.562869	0.632260
6	-0.800568	1.833247	0.668137

6	-0.000112	3.995959	0.794424
6	-1.975482	2.738037	0.865946
6	-1.318053	-0.624746	0.582314
6	-2.631390	-0.513537	0.135087
6	-0.804331	-1.836876	1.039357
6	-3.453537	-1.635876	0.155028
1	-3.017808	0.433779	-0.223827
6	-1.624243	-2.959583	1.049584
1	0.221656	-1.899853	1.383018
6	-2.940779	-2.846043	0.610731
1	-4.479615	-1.566707	-0.188878
1	-1.243244	-3.911287	1.403437
7	-1.402108	4.003047	0.929153
7	-0.473175	0.525029	0.574400
7	0.855765	0.378861	0.476344
8	0.679008	4.992795	0.821890
8	-3.155318	2.487611	0.956283
6	2.854373	1.776873	0.422781
8	3.647546	0.867782	0.338087
8	3.164863	3.067766	0.450231
6	4.568414	3.397248	0.368077
1	4.972308	2.959273	-0.548989
1	5.078351	2.945013	1.223638
6	4.671487	4.903960	0.374044
1	4.243386	5.319184	1.290074
1	5.723803	5.195653	0.318008
1	4.145012	5.332404	-0.482840
6	-2.160374	5.227829	1.109899
1	-1.839396	5.735253	2.021898
1	-2.013669	5.889459	0.253757
1	-3.213595	4.959473	1.190718
17	-3.971215	-4.254812	0.631348

Mol-2e/C_s0_chl.out

* SCF ENERGY / A.U. = -1503.79579992

6	1.306371	1.409538	-0.035227
6	0.353473	2.398803	0.273614
6	-0.831018	1.721209	0.394419
6	0.080209	3.842052	0.492869
6	-1.946351	2.682196	0.673294
6	-1.482962	-0.700295	0.142444
6	-2.686748	-0.627734	0.837407
6	-1.124161	-1.842763	-0.571263
6	-3.551526	-1.717695	0.816156
1	-2.957769	0.264742	1.390044
6	-1.985119	-2.934015	-0.583578
1	-0.185417	-1.876484	-1.111344
6	-3.190887	-2.859476	0.108573
1	-4.493202	-1.676726	1.352273
1	-1.722382	-3.830622	-1.134235
7	-1.309731	3.915903	0.710320
7	-0.588719	0.411623	0.160120
7	0.714385	0.217645	-0.096153
8	0.812911	4.799514	0.509552
8	-3.129078	2.488213	0.836888
6	2.743954	1.631475	-0.374540

8	3.084632	2.698424	-0.830993
8	3.639884	0.663246	-0.203003
6	3.395426	-0.548230	0.552673
1	2.832022	-1.242788	-0.073192
1	2.804608	-0.307917	1.440076
6	4.750468	-1.104090	0.924805
1	5.304036	-0.395941	1.546836
1	4.617465	-2.033170	1.486333
1	5.338823	-1.321508	0.029576
6	-1.991872	5.171106	0.969877
1	-1.578605	5.643969	1.863049
1	-1.878851	5.842781	0.116609
1	-3.047765	4.950758	1.125988
17	-4.272235	-4.229140	0.088103

Mol-2e/D_s0_chl.out

* SCF ENERGY / A.U. = -1503.79578023

6	1.255632	1.390646	1.382043
6	0.329057	2.370309	0.978440
6	-0.828045	1.679580	0.734782
6	0.092151	3.794693	0.632123
6	-1.886970	2.609421	0.228853
6	-1.480006	-0.743717	0.899266
6	-2.851452	-0.547783	1.035332
6	-0.944524	-2.012098	0.682617
6	-3.706719	-1.641115	0.941994
1	-3.258030	0.442154	1.209545
6	-1.799527	-3.105071	0.601217
1	0.126399	-2.142318	0.577290
6	-3.171824	-2.907398	0.729262
1	-4.777740	-1.505911	1.044114
1	-1.401585	-4.099945	0.433644
7	-1.250236	3.844148	0.207680
7	-0.597494	0.373228	0.990935
7	0.673609	0.191713	1.385176
8	0.822770	4.753729	0.659669
8	-3.031943	2.392998	-0.094913
6	2.645931	1.623975	1.877036
8	2.910892	2.664804	2.432722
8	3.580298	0.688752	1.729688
6	3.433967	-0.476393	0.882600
1	2.875537	-0.204378	-0.016486
1	2.877249	-1.237094	1.434081
6	4.831038	-0.941478	0.541983
1	5.388958	-1.189116	1.448716
1	4.771927	-1.836804	-0.083387
1	5.374439	-0.167402	-0.006152
6	-1.886415	5.076761	-0.221983
1	-1.844868	5.816453	0.580024
1	-1.384163	5.470306	-1.108280
1	-2.925597	4.849914	-0.459615
17	-4.244582	-4.279995	0.624868

Mol-2f/A_s0_chl.out

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    * SCF ENERGY / A.U. =   -1381.19234981

       6         1.443341    1.688712    0.636372
       6         0.398264    2.633592    0.649978
       6        -0.747827    1.886705    0.585351
       6         0.006170    4.067286    0.659424
       6        -1.946982    2.781670    0.528450
       6        -1.211296   -0.583848    0.460518
       6        -2.516450   -0.537436    0.939437
       6        -0.670671   -1.747244   -0.089744
       6        -3.305949   -1.681506    0.858586
       1        -2.918295    0.372198    1.370691
       6        -1.462029   -2.884695   -0.157032
       1         0.348631   -1.753001   -0.456809
       6        -2.775672   -2.846505    0.314343
       1        -4.324930   -1.659033    1.228291
       1        -1.058964   -3.798811   -0.582485
       7        -1.400712    4.057316    0.582067
       7        -0.393765    0.581966    0.536581
       7         0.941893    0.456955    0.569355
       8         0.665016    5.075325    0.717179
       8        -3.124152    2.514118    0.452130
       6         2.906972    1.938937    0.693120
       8         3.369314    3.056701    0.738154
       8         3.616713    0.817518    0.688106
       6         5.052516    0.976824    0.742490
       1         5.302902    1.537810    1.647130
       1         5.366284    1.560799   -0.127187
       6         5.656806   -0.407392    0.746821
       1         5.380758   -0.956513   -0.157399
       1         6.746634   -0.325293    0.782013
       1         5.324287   -0.974810    1.620098
       6        -2.187724    5.277424    0.566222
       1        -1.969407    5.871658    1.455687
       1        -1.959896    5.861829   -0.327773
       1        -3.240552    4.995869    0.561662
       6        -3.594972   -4.101834    0.236867
       9        -4.857209   -3.924084    0.657209
       9        -3.662511   -4.583218   -1.020772
       9        -3.067354   -5.091109    0.987797
```

Mol-2f/B_s0_chl.out

```
    * SCF ENERGY / A.U. =   -1381.19325217

       6         1.379271    1.600887    0.528686
       6         0.355891    2.562431    0.641155
       6        -0.803419    1.833998    0.678900
       6        -0.002865    3.997203    0.792803
       6        -1.978972    2.741328    0.867565
       6        -1.317439   -0.626267    0.605093
       6        -2.630867   -0.515232    0.161062
       6        -0.794291   -1.837504    1.060352
       6        -3.447037   -1.643184    0.179756
       1        -3.018414    0.432497   -0.194682
       6        -1.613149   -2.957504    1.067932
```

1	0.232820	-1.893996	1.400647
6	-2.935402	-2.855205	0.631297
1	-4.472602	-1.570998	-0.164311
1	-1.225072	-3.908594	1.419726
7	-1.405065	4.005967	0.924008
7	-0.475133	0.524436	0.595541
7	0.854945	0.377891	0.502106
8	0.677233	4.993196	0.814966
8	-3.158882	2.491416	0.956209
6	2.852866	1.774891	0.438049
8	3.645184	0.864374	0.363554
8	3.162952	3.065718	0.450205
6	4.566730	3.394070	0.362066
1	4.966973	2.950891	-0.554113
1	5.078883	2.945777	1.218319
6	4.670749	4.900663	0.359845
1	4.247172	5.320823	1.275709
1	5.723038	5.191175	0.297611
1	4.140830	5.325134	-0.496892
6	-2.162860	5.232763	1.094294
1	-1.843861	5.745869	2.003772
1	-2.012783	5.888138	0.233973
1	-3.216553	4.966003	1.173890
6	-3.785742	-4.092376	0.645686
9	-3.852352	-4.642790	1.874873
9	-3.291967	-5.049721	-0.166458
9	-5.047626	-3.859154	0.251881

Mol-2f/C_s0_chl.out

* SCF ENERGY / A.U. = -1381.18061856

6	1.303028	1.410810	-0.045842
6	0.350962	2.398855	0.273152
6	-0.833727	1.722624	0.389979
6	0.081258	3.841101	0.505760
6	-1.947280	2.684425	0.678347
6	-1.484781	-0.698445	0.123514
6	-2.692208	-0.621177	0.809578
6	-1.114098	-1.845047	-0.581706
6	-3.550754	-1.717197	0.791591
1	-2.967749	0.275991	1.351684
6	-1.972792	-2.934726	-0.586791
1	-0.171711	-1.876309	-1.114780
6	-3.187518	-2.866777	0.098205
1	-4.494159	-1.668342	1.323651
1	-1.699091	-3.833942	-1.130435
7	-1.308096	3.915948	0.725365
7	-0.592954	0.414135	0.142377
7	0.710476	0.221229	-0.117883
8	0.816602	4.796061	0.530168
8	-3.130108	2.491295	0.841061
6	2.741705	1.633694	-0.382108
8	3.082324	2.702007	-0.834877
8	3.636626	0.664976	-0.211037
6	3.389751	-0.548761	0.540648
1	2.828304	-1.241395	-0.089092
1	2.796405	-0.310677	1.426990

6	4.743548	-1.105825	0.915269
1	5.295258	-0.399621	1.541123
1	4.608657	-2.036533	1.473627
1	5.334534	-1.320708	0.021189
6	-1.986953	5.170033	0.999566
1	-1.574380	5.629859	1.899847
1	-1.869489	5.852142	0.155304
1	-3.043902	4.951049	1.150150
6	-4.082157	-4.072424	0.084556
9	-5.252122	-3.856767	0.705726
9	-3.505756	-5.130547	0.692203
9	-4.369469	-4.472253	-1.170304

Mol-2f/D_s0_chl.out

* SCF ENERGY / A.U. = -1381.18061748

6	1.254711	1.387549	1.378345
6	0.325592	2.368607	0.981280
6	-0.831382	1.679348	0.737422
6	0.088684	3.795188	0.642494
6	-1.891182	2.612884	0.236801
6	-1.476588	-0.748013	0.891706
6	-2.848736	-0.551902	1.007478
6	-0.930325	-2.016855	0.691019
6	-3.698300	-1.650736	0.910042
1	-3.257613	0.438916	1.168578
6	-1.784185	-3.106711	0.605180
1	0.142380	-2.141360	0.602583
6	-3.163687	-2.919216	0.711393
1	-4.769739	-1.510345	0.997795
1	-1.377474	-4.101381	0.448758
7	-1.254271	3.847074	0.220946
7	-0.598093	0.370795	0.985850
7	0.675184	0.188764	1.375504
8	0.820188	4.753116	0.673607
8	-3.036268	2.398263	-0.087138
6	2.645709	1.621079	1.872837
8	2.908264	2.660605	2.431788
8	3.581041	0.687986	1.721696
6	3.435333	-0.476412	0.873104
1	2.877573	-0.203270	-0.026048
1	2.878359	-1.237734	1.423494
6	4.832674	-0.940875	0.533032
1	5.389933	-1.189474	1.439888
1	4.774057	-1.835495	-0.093373
1	5.376308	-0.166144	-0.013919
6	-1.890936	5.082117	-0.201554
1	-1.847252	5.817750	0.604015
1	-1.390184	5.479500	-1.086954
1	-2.930682	4.856882	-0.438127
6	-4.053451	-4.124870	0.618260
9	-3.804869	-5.007352	1.607647
9	-3.871245	-4.796636	-0.536764
9	-5.357095	-3.814584	0.689561

Mol-2g/A_s0_chl.out

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    * SCF ENERGY / A.U. =   -1136.45579535

       6         1.438877    1.681695    0.629067
       6         0.393236    2.626057    0.646337
       6        -0.753497    1.879857    0.593109
       6         0.004565    4.060629    0.651841
       6        -1.951996    2.778601    0.551407
       6        -1.211532   -0.593695    0.469104
       6        -2.534931   -0.536322    0.901202
       6        -0.653062   -1.768911   -0.035095
       6        -3.320366   -1.678750    0.821172
       1        -2.952805    0.384056    1.292091
       6        -1.438576   -2.910207   -0.106075
       1         0.378472   -1.783570   -0.365406
       6        -2.772154   -2.863759    0.319241
       1        -4.352288   -1.653633    1.153311
       1        -1.024253   -3.833649   -0.495597
       7        -1.402762    4.052812    0.589123
       7        -0.398501    0.573692    0.544966
       7         0.938179    0.450267    0.569174
       8         0.666451    5.067120    0.696275
       8        -3.131397    2.514756    0.499229
       6         2.902519    1.934925    0.678685
       8         3.361736    3.054193    0.714016
       8         3.614303    0.815103    0.680295
       6         5.050067    0.978181    0.731750
       1         5.299787    1.546390    1.632046
       1         5.361229    1.556594   -0.142526
       6         5.657756   -0.404419    0.745540
       1         5.383032   -0.960527   -0.154798
       1         6.747351   -0.319140    0.779932
       1         5.327044   -0.966485    1.622954
       6        -2.188100    5.274242    0.574319
       1        -1.966010    5.869973    1.461808
       1        -1.961991    5.856073   -0.321739
       1        -3.241311    4.994219    0.573535
       6        -3.585203   -4.048765    0.244452
       7        -4.237143   -5.003431    0.182625
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Mol-2g/B_s0_chl.out

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    * SCF ENERGY / A.U. =   -1136.45665810

       6         1.374723    1.597079    0.519941
       6         0.350739    2.558404    0.633635
       6        -0.808579    1.830568    0.667645
       6        -0.007116    3.993084    0.789812
       6        -1.983985    2.738659    0.857813
       6        -1.318681   -0.631046    0.592000
       6        -2.642100   -0.517999    0.171025
       6        -0.784375   -1.845120    1.023900
       6        -3.454726   -1.644120    0.193124
       1        -3.037667    0.432341   -0.168484
       6        -1.597030   -2.969465    1.037723
       1         0.249104   -1.902613    1.343809
       6        -2.931768   -2.867363    0.626319
```

1	-4.487423	-1.576690	-0.130878
1	-1.203231	-3.922819	1.372481
7	-1.409427	4.002272	0.919464
7	-0.479850	0.520457	0.581148
7	0.851062	0.374654	0.489524
8	0.673921	4.988110	0.816380
8	-3.164175	2.489006	0.944019
6	2.848901	1.771006	0.432528
8	3.640202	0.860084	0.353742
8	3.159530	3.061303	0.453500
6	4.563903	3.389462	0.370559
1	4.966529	2.949308	-0.545993
1	5.073169	2.937787	1.226742
6	4.668626	4.895938	0.374071
1	4.242254	5.313110	1.290000
1	5.721306	5.185962	0.316473
1	4.141962	5.323774	-0.482979
6	-2.166493	5.229047	1.094302
1	-1.847295	5.738063	2.005981
1	-2.015420	5.887674	0.236686
1	-3.220405	4.962795	1.172388
6	-3.771142	-4.036322	0.645557
7	-4.443423	-4.978627	0.662230

Mol-2g/C_s0_chl.out

* SCF ENERGY / A.U. = -1136.44399210

6	1.300277	1.401813	-0.049512
6	0.348006	2.389881	0.270605
6	-0.835779	1.713624	0.390597
6	0.077588	3.832898	0.499143
6	-1.949874	2.675645	0.677421
6	-1.485487	-0.706818	0.123747
6	-2.694368	-0.628541	0.811928
6	-1.114655	-1.852336	-0.581691
6	-3.551485	-1.721142	0.795840
1	-2.968629	0.268759	1.354525
6	-1.970822	-2.943953	-0.590248
1	-0.172080	-1.883011	-1.114401
6	-3.188576	-2.877691	0.097668
1	-4.494915	-1.679980	1.328930
1	-1.701840	-3.843597	-1.133121
7	-1.311605	3.907454	0.720122
7	-0.594824	0.404653	0.143038
7	0.708820	0.212177	-0.120006
8	0.812518	4.788070	0.519216
8	-3.132240	2.481208	0.841759
6	2.738561	1.624802	-0.388791
8	3.076395	2.690319	-0.849815
8	3.634558	0.658549	-0.211428
6	3.389811	-0.548854	0.551299
1	2.833268	-1.249527	-0.074005
1	2.792494	-0.304642	1.433276
6	4.744258	-1.097128	0.936272
1	5.290644	-0.382839	1.557593
1	4.610668	-2.023011	1.502896
1	5.339591	-1.318235	0.046633

6	-1.991359	5.162394	0.988839
1	-1.578163	5.626962	1.886340
1	-1.875210	5.840182	0.140930
1	-3.047964	4.943261	1.141560
6	-4.070819	-4.014576	0.093413
7	-4.778657	-4.930605	0.091210

Mol-2g/D_s0_chl.out

* SCF ENERGY / A.U. = -1136.44392749

6	1.250771	1.382330	1.378778
6	0.320894	2.362715	0.980433
6	-0.836414	1.673764	0.739971
6	0.085078	3.788643	0.637313
6	-1.895806	2.606971	0.236457
6	-1.479161	-0.753573	0.899397
6	-2.854429	-0.555256	1.002067
6	-0.931225	-2.023279	0.714555
6	-3.702258	-1.650943	0.906291
1	-3.264182	0.436999	1.151548
6	-1.780739	-3.116513	0.627802
1	0.142214	-2.148231	0.637493
6	-3.165361	-2.929248	0.720328
1	-4.775496	-1.516461	0.983826
1	-1.376001	-4.112122	0.482557
7	-1.258053	3.840246	0.216348
7	-0.602688	0.365069	0.991157
7	0.671893	0.183896	1.379252
8	0.817736	4.745583	0.664936
8	-3.040974	2.391702	-0.086749
6	2.641919	1.617897	1.872956
8	2.902009	2.657759	2.432199
8	3.578463	0.686460	1.721392
6	3.433852	-0.478253	0.872902
1	2.876151	-0.205479	-0.026409
1	2.877412	-1.239893	1.423432
6	4.831634	-0.941714	0.533415
1	5.388645	-1.189772	1.440558
1	4.773953	-1.836453	-0.092886
1	5.374910	-0.166637	-0.013372
6	-1.893526	5.074354	-0.211204
1	-1.849609	5.812839	0.591706
1	-1.391722	5.467745	-1.097761
1	-2.933298	4.849105	-0.447568
6	-4.043475	-4.065384	0.623382
7	-4.746650	-4.981400	0.542343

Mol-2k/A_s0_chl.out

* SCF ENERGY / A.U. = -1021.94900327

6	1.422955	1.490257	0.588364
6	0.399350	2.461004	0.588635
6	-0.770229	1.748036	0.588827
6	0.061852	3.907009	0.588636
6	-1.938350	2.693556	0.589008
6	-1.282288	-0.732231	0.588817

6	-2.668919	-0.590962	0.588987
6	-0.677858	-1.991629	0.588747
6	-3.465244	-1.729032	0.589087
1	-3.129909	0.390222	0.589043
6	-1.477288	-3.124920	0.588845
6	-2.871391	-2.994890	0.589016
1	-4.545567	-1.633667	0.589219
1	-1.023124	-4.109774	0.588791
7	-1.345665	3.946513	0.588892
7	-0.451722	0.426579	0.588701
7	0.882801	0.274524	0.588424
8	0.758295	4.891035	0.588441
8	-3.129840	2.480442	0.589202
6	2.903892	1.665703	0.588069
8	3.361206	2.791114	0.588288
6	-2.090494	5.193300	0.588961
1	-1.847040	5.774259	1.480809
1	-1.847025	5.774339	-0.302829
1	-3.152190	4.947903	0.588941
1	0.400792	-2.079372	0.588618
6	-3.696837	-4.173042	0.589117
7	-4.358061	-5.123400	0.589200
6	3.748354	0.424531	0.587486
1	3.521367	-0.183372	1.468731
1	3.521083	-0.182710	-0.294146
1	4.801313	0.706199	0.587419

Mol-2k/B_s0_chl.out

* SCF ENERGY / A.U. = -1021.94843369

6	1.353769	1.524437	0.656445
6	0.321603	2.485389	0.606025
6	-0.844361	1.765321	0.580619
6	-0.026863	3.927966	0.570349
6	-2.015816	2.703119	0.526722
6	-1.334459	-0.717236	0.598272
6	-2.721908	-0.586093	0.611373
6	-0.719038	-1.970738	0.572636
6	-3.509421	-1.730161	0.596129
1	-3.190802	0.391163	0.630693
6	-1.509939	-3.110051	0.558867
6	-2.905009	-2.990842	0.570690
1	-4.590462	-1.643769	0.605365
1	-1.047894	-4.090974	0.538586
7	-1.428350	3.962237	0.515588
7	-0.512454	0.448763	0.612310
7	0.820257	0.305434	0.658074
8	0.671497	4.913716	0.583765
8	-3.205663	2.487541	0.499120
6	2.841244	1.693730	0.698372
8	3.563126	0.718531	0.739277
6	-2.179023	5.205488	0.484208
1	-2.068008	5.739453	1.430658
1	-1.816659	5.831575	-0.332976
1	-3.228073	4.959491	0.321775
1	0.360473	-2.048593	0.563268
6	-3.722170	-4.174854	0.556373

7	-4.378241	-5.128695	0.544214
6	3.350481	3.104114	0.686647
1	4.440335	3.099822	0.703857
1	2.988745	3.627579	-0.204416
1	2.962526	3.648588	1.554010

Mol-3b/A_s0_chl.out

* SCF ENERGY / A.U. = -1328.12946553

6	1.489336	1.661731	0.603651
6	0.439105	2.600354	0.574690
6	-0.703672	1.849589	0.503779
6	0.059877	4.031724	0.642106
6	-1.906809	2.739430	0.524366
6	-1.140875	-0.635671	0.425856
6	-2.467981	-0.547099	0.010324
6	-0.563142	-1.856390	0.779022
6	-3.238758	-1.701528	-0.037922
1	-2.903515	0.406368	-0.264468
6	-1.334262	-3.007946	0.721734
6	-2.672335	-2.930224	0.316186
1	-4.274454	-1.649855	-0.355298
1	-0.904102	-3.965068	0.995752
7	-1.361851	4.024532	0.601926
7	-0.341196	0.542922	0.487527
7	0.995379	0.428861	0.546163
8	0.731815	5.025394	0.722072
8	-3.083764	2.473838	0.483514
6	2.950544	1.924270	0.677551
8	3.401725	3.046773	0.708069
8	3.667330	0.808400	0.705932
6	5.101558	0.978642	0.779194
1	5.334349	1.550003	1.682087
1	5.423244	1.556524	-0.091533
6	5.715267	-0.401125	0.805005
1	5.455573	-0.960344	-0.097846
1	6.803837	-0.310799	0.854518
1	5.374942	-0.962760	1.679012
1	0.471352	-1.898733	1.095948
6	-3.473404	-4.124763	0.268652
7	-4.116620	-5.086549	0.230039
6	-2.155944	5.209910	0.649391
6	-1.957508	6.204472	-0.306541
6	-3.112114	5.354806	1.653223
6	-2.728031	7.363701	-0.250530
1	-1.207735	6.068993	-1.079500
6	-3.888877	6.510485	1.689999
1	-3.243721	4.569993	2.391339
6	-3.695648	7.516045	0.742643
1	-2.574906	8.144789	-0.988355
1	-4.640048	6.626934	2.464712
1	-4.297803	8.418519	0.778480

Mol-3b/B_s0_chl.out

* SCF ENERGY / A.U. = -1328.13009743

6	1.386306	1.580347	0.645939
6	0.356751	2.540218	0.598537
6	-0.803358	1.814217	0.531900
6	0.017109	3.982846	0.617440
6	-1.980667	2.741081	0.495876
6	-1.279968	-0.673369	0.483310
6	-2.665101	-0.551615	0.389907
6	-0.657566	-1.922850	0.528952
6	-3.443313	-1.701341	0.344269
1	-3.139788	0.422220	0.354982
6	-1.439237	-3.067509	0.482571
6	-2.832032	-2.958036	0.390188
1	-4.522542	-1.621842	0.272348
1	-0.972255	-4.045671	0.518034
7	-1.401522	4.012297	0.545836
7	-0.466465	0.497810	0.535357
7	0.866638	0.359812	0.603707
8	0.714512	4.960560	0.684500
8	-3.165290	2.515286	0.435282
6	2.861915	1.749864	0.730596
8	3.649304	0.834004	0.785759
8	3.175751	3.038563	0.740376
6	4.580789	3.360858	0.839653
1	5.095463	2.920234	-0.018978
1	4.973388	2.905044	1.752939
6	4.689922	4.866811	0.860419
1	4.154670	5.283204	1.717704
1	5.742834	5.152307	0.934310
1	4.275780	5.299217	-0.054053
1	0.419986	-1.994200	0.601029
6	-3.639179	-4.148136	0.345558
7	-4.287116	-5.106884	0.308898
6	-2.164077	5.219472	0.556067
6	-1.925506	6.187364	-0.417795
6	-3.127701	5.412483	1.544544
6	-2.661901	7.369796	-0.394452
1	-1.171047	6.013754	-1.178518
6	-3.870072	6.590951	1.548601
1	-3.290875	4.647410	2.296941
6	-3.636045	7.570669	0.583598
1	-2.477921	8.130881	-1.145939
1	-4.626361	6.744852	2.311642
1	-4.211713	8.490859	0.594307

Mol-4b/A_s0_chl.out

* SCF ENERGY / A.U. = -1087.83166139

6	1.691066	-0.619295	-0.179297
6	1.508363	0.754837	-0.465763
6	0.167889	0.907497	-0.593649
6	-1.802506	-0.634242	-0.408786
6	-2.741375	0.391931	-0.545745
6	-2.201836	-1.967224	-0.286854

6	-4.093382	0.082598	-0.566621
1	-2.419517	1.425096	-0.629932
6	-3.554708	-2.273372	-0.305165
6	-4.502143	-1.251328	-0.446161
1	-4.831970	0.870168	-0.670701
1	-3.879739	-3.304198	-0.212914
7	-0.431597	-0.300347	-0.391764
7	0.506982	-1.238005	-0.142653
6	2.957291	-1.346567	0.065661
8	4.033285	-0.783737	0.076564
8	2.783959	-2.650623	0.272706
6	3.974760	-3.436073	0.497528
1	3.613248	-4.326898	1.013059
1	4.643073	-2.881246	1.159938
6	4.646431	-3.787894	-0.814286
1	4.993687	-2.889395	-1.330317
1	5.511585	-4.428518	-0.619299
1	3.955972	-4.329966	-1.466258
1	-1.457176	-2.746366	-0.180831
6	-5.903256	-1.572716	-0.466359
7	-7.032335	-1.830297	-0.482886
6	0.194337	2.403095	-0.863956
6	-0.166401	3.415490	0.243331
6	1.775430	2.242389	-0.706606
1	-0.157929	2.705437	-1.853390
6	1.081887	4.326505	0.176493
6	-0.003059	2.771137	1.633013
1	-1.128452	3.910025	0.089566
6	2.092139	3.193054	0.468506
1	2.358021	2.475576	-1.600745
1	1.080670	5.111015	0.940698
1	1.224317	4.785178	-0.808395
1	-0.416640	3.431239	2.401021
1	-0.525401	1.811403	1.709543
6	1.540087	2.627190	1.789107
1	3.142374	3.487901	0.517789
1	1.905128	3.224567	2.629698
1	1.852703	1.592847	1.957700

Mol-4b/B_s0_chl.out

* SCF ENERGY / A.U. = -1087.83145305

6	1.362408	-0.972770	0.377345
6	1.373825	0.373018	-0.061371
6	0.085118	0.645721	-0.380447
6	-2.056324	-0.656492	-0.306854
6	-2.834309	0.426129	-0.725686
6	-2.630976	-1.902039	-0.044403
6	-4.202605	0.263320	-0.883257
1	-2.373863	1.388838	-0.924055
6	-4.000030	-2.061763	-0.202465
6	-4.787557	-0.981434	-0.620419
1	-4.818311	1.095843	-1.206150
1	-4.462164	-3.022469	-0.001973
7	-0.667453	-0.466367	-0.145101
7	0.119776	-1.459855	0.316293
6	2.458734	-1.842434	0.864678

8	2.335156	-2.998879	1.202111
8	3.614497	-1.168623	0.876447
6	4.777130	-1.881201	1.349721
1	5.619263	-1.336131	0.920967
1	4.757602	-2.894578	0.942288
6	4.830382	-1.885409	2.863813
1	3.977628	-2.423918	3.284396
1	5.747553	-2.382084	3.193994
1	4.833486	-0.862737	3.251152
1	-2.007976	-2.726488	0.279959
6	-6.206351	-1.149520	-0.779735
7	-7.349671	-1.283256	-0.907730
6	0.318422	2.088921	-0.796979
6	-0.048052	3.257492	0.141437
6	1.840508	1.785890	-0.419190
1	0.124628	2.308824	-1.849873
6	1.296610	4.021689	0.137793
6	-0.122281	2.772269	1.601290
1	-0.921815	3.825848	-0.185447
6	2.127696	2.834730	0.677111
1	2.546182	1.848125	-1.250882
1	1.298475	4.888316	0.807262
1	1.604289	4.341569	-0.864027
1	-0.543756	3.558971	2.233916
1	-0.756079	1.886350	1.712590
6	1.365292	2.492769	1.969681
1	3.192369	3.025853	0.827274
1	1.696841	3.148203	2.780577
1	1.533682	1.459907	2.287777

Excited states (S_1)

Optimised Geometries (S_1)

Mol-2a/C_s1r_chl.out

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    * SCF ENERGY / A.U. =   -1159.03281272

       6         1.411677    1.676564    0.563903
       6         0.339464    2.613725    0.574422
       6        -0.819276    1.850522    0.585698
       6        -0.041832    4.030370    0.577608
       6        -1.984115    2.686243    0.598236
       6        -1.145840   -0.618335    0.601231
       6        -2.569482   -0.555555    0.619288
       6        -0.488828   -1.885566    0.602288
       6        -3.290344   -1.711987    0.639820
       1        -3.064749    0.411402    0.617645
       6        -1.225070   -3.037056    0.623188
       1         0.591089   -1.912018    0.586756
       6        -2.638519   -2.969492    0.643514
       1        -4.372546   -1.695293    0.654848
       1        -0.716028   -3.990941    0.624171
       7        -1.432399    3.994218    0.599278
       7        -0.412501    0.520642    0.583897
       7         0.977611    0.436942    0.569192
       8         0.622424    5.056029    0.565187
       8        -3.197012    2.456181    0.608552
       8        -3.432928   -4.024073    0.666970
       6         2.887469    1.903114    0.549340
       8         3.704801    1.017644    0.534554
       8         3.159657    3.196662    0.555522
       6         4.552551    3.574338    0.543043
       1         5.016346    3.149111   -0.349757
       1         5.034905    3.138852    1.420958
       6         4.615355    5.082640    0.551072
       1         4.137073    5.487836    1.444570
       1         5.661035    5.398594    0.542924
       1         4.120236    5.497938   -0.328481
       6        -2.877647   -5.341696    0.679162
       1        -3.730322   -6.014264    0.701435
       1        -2.289664   -5.516507   -0.224216
       1        -2.264342   -5.488780    1.570650
       6        -2.243869    5.190262    0.599172
       1        -1.848175    5.901908    1.324551
       1        -2.252879    5.659760   -0.387770
       1        -3.259825    4.909878    0.872503
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Mol-2a/D_s1r_chl.out

```
    * SCF ENERGY / A.U. =   -1159.03286243

       6         1.403853    1.695963    0.568801
       6         0.340862    2.644601    0.578014
       6        -0.824805    1.893540    0.592729
```

6	-0.026088	4.064555	0.577451
6	-1.981899	2.741328	0.604623
6	-1.177764	-0.571107	0.609345
6	-2.599160	-0.484968	0.626656
6	-0.540742	-1.849908	0.609028
6	-3.354424	-1.627784	0.643200
1	-3.076364	0.491384	0.626937
6	-1.303640	-2.975613	0.625610
1	0.538319	-1.898014	0.595550
6	-2.721482	-2.888829	0.643082
1	-4.432564	-1.547783	0.656252
1	-0.851386	-3.959149	0.625954
7	-1.417194	4.042849	0.600763
7	-0.430099	0.558441	0.593182
7	0.956923	0.461196	0.577480
8	0.648264	5.083736	0.561214
8	-3.197913	2.523904	0.617811
8	-3.357923	-4.045398	0.658616
6	2.882167	1.905454	0.552653
8	3.689012	1.010499	0.540567
8	3.169925	3.195732	0.554203
6	4.567719	3.555172	0.540031
1	5.025762	3.120237	-0.351055
1	5.044461	3.116751	1.419547
6	4.650567	5.062505	0.542074
1	4.177910	5.477624	1.434023
1	5.700374	5.364419	0.532521
1	4.160879	5.480914	-0.339064
6	-4.787378	-4.075746	0.677292
1	-5.054102	-5.128675	0.688172
1	-5.167001	-3.585801	1.576141
1	-5.190270	-3.598391	-0.218205
6	-2.215866	5.247590	0.598677
1	-1.820938	5.951847	1.331736
1	-2.209797	5.721917	-0.385913
1	-3.237344	4.976168	0.860159

Mol-2e/A_s1r_chl.out

* SCF ENERGY / A.U. = -1504.11126605

6	1.431101	1.698815	0.592066
6	0.375942	2.657016	0.607748
6	-0.819637	1.853749	0.613075
6	0.059133	4.038329	0.604407
6	-1.981213	2.656329	0.612912
6	-1.168353	-0.644235	0.609464
6	-2.558672	-0.596179	0.660631
6	-0.498448	-1.866128	0.563139
6	-3.282063	-1.779452	0.664317
1	-3.082937	0.352107	0.694115
6	-1.226187	-3.045172	0.567930
1	0.581217	-1.892513	0.524000
6	-2.612528	-2.993980	0.618473
1	-4.363370	-1.750816	0.703606
1	-0.713606	-3.997891	0.532026
7	-1.389516	3.990238	0.617374
7	-0.417988	0.557151	0.603901

7	0.946790	0.482689	0.592951
8	0.674857	5.093830	0.586484
8	-3.194863	2.488414	0.609155
6	2.895908	1.958640	0.583733
8	3.348454	3.074851	0.594693
8	3.602836	0.841075	0.563897
6	5.041395	0.985812	0.556515
1	5.335789	1.544981	1.446886
1	5.324588	1.566049	-0.323960
6	5.635566	-0.401672	0.536374
1	5.323967	-0.947348	-0.356376
1	6.725095	-0.325754	0.530773
1	5.334506	-0.968447	1.419547
6	-2.191302	5.162001	0.576172
1	-1.622384	5.994453	0.988749
1	-2.434651	5.394844	-0.471608
1	-3.128784	4.975636	1.101115
17	-3.528093	-4.482216	0.624823

Mol-2e/B_s1r_chl.out

* SCF ENERGY / A.U. = -1504.11223076

6	1.405325	1.727454	0.574612
6	0.343628	2.679576	0.593631
6	-0.847063	1.867692	0.606477
6	0.014427	4.058756	0.589113
6	-2.014440	2.662273	0.610784
6	-1.178982	-0.632192	0.609498
6	-2.569366	-0.593074	0.666154
6	-0.500804	-1.849496	0.563482
6	-3.284760	-1.781081	0.675789
1	-3.099817	0.351750	0.699522
6	-1.220687	-3.033328	0.574227
1	0.578851	-1.868706	0.520094
6	-2.607130	-2.991194	0.630214
1	-4.366069	-1.759636	0.719412
1	-0.701751	-3.982585	0.538650
7	-1.432598	3.999226	0.609786
7	-0.436701	0.574460	0.597716
7	0.927914	0.509030	0.580269
8	0.620928	5.120349	0.565837
8	-3.227044	2.485382	0.613168
6	2.882791	1.922149	0.557008
8	3.680495	1.021031	0.531638
8	3.172322	3.211622	0.573603
6	4.571838	3.572003	0.559269
1	5.025685	3.147214	-0.338517
1	5.049873	3.123268	1.432532
6	4.652485	5.079057	0.578404
1	4.182092	5.483419	1.476475
1	5.701893	5.381977	0.569850
1	4.160749	5.507036	-0.296958
6	-2.243756	5.165160	0.571786
1	-1.678420	6.002619	0.978949
1	-2.496781	5.393819	-0.474476
1	-3.175749	4.972669	1.104205
17	-3.512862	-4.485320	0.643811

Mol-2f/A_s1r_chl.out

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    * SCF ENERGY / A.U. =   -1381.56239266

       6         1.426465    1.699327    0.592051
       6         0.375049    2.660128    0.617611
       6        -0.822784    1.861643    0.632770
       6         0.065671    4.041910    0.618875
       6        -1.982807    2.664729    0.645758
       6        -1.177470   -0.636605    0.630111
       6        -2.567649   -0.581773    0.669469
       6        -0.508587   -1.860384    0.603721
       6        -3.290592   -1.764494    0.681665
       1        -3.087812    0.368710    0.690919
       6        -1.242881   -3.033133    0.617213
       1         0.571114   -1.887879    0.575382
       6        -2.633122   -2.988539    0.659697
       1        -4.371861   -1.723824    0.715301
       1        -0.725191   -3.984201    0.600304
       7        -1.386774    3.999723    0.645645
       7        -0.423542    0.561040    0.619059
       7         0.939221    0.484203    0.596235
       8         0.681594    5.095735    0.596013
       8        -3.196158    2.502792    0.654289
       6         2.892176    1.955601    0.572619
       8         3.347102    3.070688    0.590059
       8         3.595549    0.836592    0.535816
       6         5.034623    0.977071    0.517105
       1         5.338458    1.525975    1.410671
       1         5.311564    1.565693   -0.359764
       6         5.624191   -0.411918    0.477146
       1         5.303128   -0.947212   -0.418521
       1         6.713848   -0.339211    0.462732
       1         5.329166   -0.987048    1.356942
       6        -2.184621    5.172455    0.611201
       1        -1.605763    6.006743    1.005654
       1        -2.447029    5.396405   -0.434479
       1        -3.114273    4.992509    1.152514
       6        -3.418233   -4.267095    0.621949
       9        -2.798567   -5.263153    1.279185
       9        -4.639393   -4.134974    1.164898
       9        -3.604554   -4.703026   -0.642627
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Mol-2f/B_s1r_chl.out

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    * SCF ENERGY / A.U. =   -1381.56334002

       6         1.396917    1.728064    0.555545
       6         0.339628    2.682972    0.597155
       6        -0.853434    1.876069    0.624178
       6         0.018335    4.062691    0.607135
       6        -2.018815    2.671300    0.654580
       6        -1.192285   -0.624086    0.617571
       6        -2.582131   -0.577770    0.674439
       6        -0.515925   -1.843281    0.579089
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6	-3.297496	-1.764934	0.692235
1	-3.107875	0.369360	0.705205
6	-1.242824	-3.020670	0.598337
1	0.563495	-1.863902	0.537098
6	-2.632635	-2.984756	0.658371
1	-4.378489	-1.731143	0.739568
1	-0.719384	-3.968345	0.572012
7	-1.432309	4.009217	0.651858
7	-0.445971	0.578755	0.600776
7	0.916102	0.510712	0.561434
8	0.624983	5.122649	0.580385
8	-3.231030	2.500733	0.677334
6	2.874912	1.918158	0.516853
8	3.668415	1.014525	0.467764
8	3.169213	3.206226	0.545319
6	4.569925	3.561726	0.513561
1	5.007455	3.148040	-0.397392
1	5.060021	3.098703	1.372532
6	4.656861	5.068002	0.552770
1	4.201928	5.461394	1.463600
1	5.707245	5.366919	0.532465
1	4.153739	5.510308	-0.308880
6	-2.239418	5.176421	0.632604
1	-1.660593	6.014012	1.019809
1	-2.520912	5.400201	-0.407993
1	-3.158637	4.988361	1.188798
6	-3.410903	-4.267703	0.626231
9	-2.775471	-5.263680	1.267938
9	-4.624089	-4.145287	1.189405
9	-3.615315	-4.697584	-0.637593

Mol-2g/A_s1r_chl.out

* SCF ENERGY / A.U. = -1136.73527164

6	1.424170	1.691651	0.592701
6	0.370692	2.651100	0.609163
6	-0.825411	1.851677	0.616831
6	0.059984	4.032818	0.605652
6	-1.986718	2.652871	0.618693
6	-1.174568	-0.645830	0.613621
6	-2.566491	-0.592750	0.656926
6	-0.502171	-1.868529	0.575256
6	-3.288397	-1.773318	0.661013
1	-3.087295	0.357334	0.684624
6	-1.230588	-3.043213	0.580200
1	0.577432	-1.892222	0.542174
6	-2.626494	-3.002158	0.623106
1	-4.370078	-1.740222	0.694338
1	-0.715744	-3.995275	0.550315
7	-1.392996	3.989260	0.620629
7	-0.424438	0.550878	0.607721
7	0.940183	0.476036	0.595046
8	0.674659	5.086781	0.586068
8	-3.199264	2.488342	0.617937
6	2.890055	1.951488	0.582451
8	3.341222	3.067997	0.591869
8	3.595885	0.834039	0.562966

6	5.035072	0.977486	0.553968
1	5.330354	1.537550	1.443431
1	5.317399	1.556450	-0.327572
6	5.627833	-0.410530	0.534957
1	5.314996	-0.957036	-0.356833
1	6.717388	-0.335457	0.528154
1	5.327334	-0.975914	1.419194
6	-2.191788	5.160780	0.575629
1	-1.620284	5.995525	0.979925
1	-2.437408	5.386387	-0.473889
1	-3.129560	4.978825	1.101899
6	-3.378357	-4.220939	0.628695
7	-3.982476	-5.202050	0.633192

Mol-2g/B_s1r_chl.out

* SCF ENERGY / A.U. = -1136.73624420

6	1.397328	1.720494	0.572414
6	0.337682	2.674179	0.593679
6	-0.853858	1.866466	0.608816
6	0.015017	4.053820	0.590162
6	-2.020735	2.659895	0.616310
6	-1.187118	-0.632969	0.611083
6	-2.579091	-0.588241	0.659696
6	-0.506898	-1.851220	0.573517
6	-3.293543	-1.773250	0.670311
1	-3.105737	0.358618	0.686870
6	-1.228002	-3.030462	0.584946
1	0.572704	-1.868192	0.536205
6	-2.623933	-2.997958	0.633386
1	-4.375269	-1.746888	0.707931
1	-0.707139	-3.979241	0.555843
7	-1.436487	3.999183	0.613500
7	-0.444492	0.568901	0.598837
7	0.919681	0.502716	0.578776
8	0.620694	5.113737	0.565685
8	-3.232314	2.486822	0.622077
6	2.876021	1.913753	0.552428
8	3.671293	1.011061	0.523010
8	3.166613	3.202445	0.572207
6	4.567022	3.561406	0.556479
1	5.018219	3.138984	-0.343699
1	5.045740	3.108757	1.427282
6	4.649628	5.068178	0.580776
1	4.181537	5.470078	1.481141
1	5.699483	5.369451	0.571538
1	4.157260	5.499992	-0.292324
6	-2.244410	5.165060	0.572782
1	-1.675786	6.004715	0.970710
1	-2.501284	5.386291	-0.474830
1	-3.176014	4.977219	1.107870
6	-3.368490	-4.221216	0.645762
7	-3.967217	-5.205579	0.655777

Mol-2k/A_s1r_chl.out

```
    * SCF ENERGY / A.U. =   -1097.41789337

       6         1.421860    1.683097    0.593280
       6         0.370749    2.644748    0.610295
       6        -0.826939    1.847943    0.617712
       6         0.063461    4.027053    0.606828
       6        -1.986599    2.651461    0.619491
       6        -1.181794   -0.649039    0.613838
       6        -2.573494   -0.592311    0.657283
       6        -0.512551   -1.873363    0.575228
       6        -3.298480   -1.771023    0.661367
       1        -3.091961    0.359027    0.685119
       6        -1.243986   -3.046187    0.580166
       1         0.566968   -1.899985    0.541964
       6        -2.639757   -3.001517    0.623275
       1        -4.380065   -1.735112    0.694816
       1        -0.731591   -3.999558    0.550117
       7        -1.389910    3.986863    0.621586
       7        -0.428554    0.546041    0.608065
       7         0.935273    0.468306    0.595092
       8         0.680549    5.079492    0.587219
       8        -3.199401    2.489818    0.618529
       6         2.887086    1.940390    0.583379
       8         3.343567    3.054013    0.597017
       8         3.592422    0.820647    0.558863
       6         5.019772    0.973362    0.549778
       1         5.348251    1.494491    1.449287
       1         5.333261    1.529449   -0.333982
       6        -2.185992    5.160006    0.575764
       1        -1.612972    5.993693    0.980126
       1        -2.430225    5.385805   -0.474102
       1        -3.124696    4.980201    1.101127
       6        -3.394839   -4.218335    0.628859
       7        -4.001642   -5.197775    0.633359
       1         5.417084   -0.037689    0.526711
```

Mol-2k/B_s1r_chl.out

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    * SCF ENERGY / A.U. =   -1097.41879232

       6         1.407359    1.709474    0.579763
       6         0.351139    2.666631    0.600315
       6        -0.843018    1.863063    0.612544
       6         0.033660    4.047207    0.597143
       6        -2.007237    2.660399    0.618352
       6        -1.185030   -0.635438    0.611418
       6        -2.576802   -0.585341    0.658033
       6        -0.509359   -1.856112    0.573353
       6        -3.295852   -1.767609    0.666126
       1        -3.099966    0.363420    0.685542
       6        -1.235014   -3.032602    0.582267
       1         0.570230   -1.877263    0.537577
       6        -2.630868   -2.994770    0.628686
       1        -4.377520   -1.737121    0.702154
       1        -0.717788   -3.983352    0.552762
       7        -1.418241    3.997970    0.617542
```

7	-0.437809	0.563916	0.601735
7	0.925527	0.493127	0.583809
8	0.643453	5.104829	0.574458
8	-3.219304	2.491790	0.621718
6	2.885814	1.896858	0.562286
8	3.680584	0.994797	0.528365
8	3.181392	3.186119	0.589905
6	4.574847	3.527654	0.576535
1	5.043464	3.153858	-0.334201
1	5.072883	3.104414	1.449208
6	-2.221898	5.166557	0.575305
1	-1.651470	6.004182	0.974932
1	-2.475150	5.389014	-0.473002
1	-3.155668	4.981670	1.107642
6	-3.380243	-4.215141	0.638402
7	-3.983006	-5.197041	0.646267
1	4.604771	4.613177	0.605963

Mol-3b/A_s1r_chl.out

* SCF ENERGY / A.U. = -1328.43995055

6	1.413190	1.709702	0.601148
6	0.357549	2.664939	0.584518
6	-0.821630	1.883235	0.563508
6	0.062740	4.046278	0.584648
6	-1.987899	2.670158	0.552326
6	-1.174585	-0.627526	0.535753
6	-2.563079	-0.580590	0.428555
6	-0.507410	-1.851336	0.624676
6	-3.284516	-1.762062	0.413669
1	-3.080556	0.368752	0.360151
6	-1.233526	-3.026811	0.606966
1	0.569669	-1.872788	0.706289
6	-2.626765	-2.989899	0.501949
1	-4.363757	-1.729666	0.330982
1	-0.719580	-3.977455	0.676304
7	-1.417735	4.041396	0.573556
7	-0.422068	0.566811	0.554270
7	0.930148	0.490612	0.581582
8	0.720581	5.071072	0.639824
8	-3.193563	2.457095	0.471130
6	2.876862	1.961295	0.622097
8	3.344761	3.072381	0.621984
8	3.580869	0.838360	0.638760
6	5.017747	0.977098	0.655385
1	5.300627	1.547756	1.542429
1	5.321585	1.542924	-0.227804
6	5.606793	-0.413130	0.665910
1	5.307657	-0.970603	-0.223898
1	6.696709	-0.342625	0.678071
1	5.287640	-0.965919	1.551673
6	-3.377034	-4.208971	0.484141
7	-3.980464	-5.190763	0.469938
6	-2.183448	5.164950	0.601277
6	-3.487349	5.135416	1.176310
6	-1.687130	6.385077	0.056824
6	-4.245818	6.282417	1.201098

1	-3.853418	4.221775	1.614997
6	-2.478708	7.508553	0.077410
1	-0.708116	6.405250	-0.393527
6	-3.753108	7.466659	0.649683
1	-5.227073	6.264208	1.657718
1	-2.110655	8.428766	-0.357743
1	-4.362967	8.361902	0.667865

Mol-3b/B_s1r_chl.out

* SCF ENERGY / A.U. = -1328.44084701

6	1.389230	1.737966	0.634187
6	0.329238	2.689707	0.601875
6	-0.846593	1.901789	0.575430
6	0.025019	4.069602	0.594692
6	-2.017132	2.682258	0.553112
6	-1.188494	-0.610478	0.558252
6	-2.575630	-0.569996	0.433740
6	-0.517106	-1.830491	0.663867
6	-3.291933	-1.754572	0.417903
1	-3.096352	0.376529	0.352960
6	-1.238098	-3.009183	0.645048
1	0.558970	-1.846806	0.758726
6	-2.630072	-2.978860	0.522735
1	-4.370206	-1.727366	0.321783
1	-0.720931	-3.957031	0.727149
7	-1.454550	4.055804	0.571402
7	-0.441061	0.587632	0.577826
7	0.910161	0.517650	0.618073
8	0.674333	5.100490	0.652525
8	-3.221213	2.462658	0.465513
6	2.865237	1.920289	0.669891
8	3.658093	1.014143	0.719801
8	3.176271	3.206966	0.637163
6	4.579927	3.541292	0.666784
1	5.064828	3.069720	-0.190722
1	5.014413	3.124886	1.578156
6	4.690496	5.046368	0.623286
1	4.194601	5.498794	1.483989
1	5.745233	5.329942	0.641800
1	4.240732	5.444148	-0.288378
6	-3.375341	-4.201035	0.504101
7	-3.975250	-5.184963	0.489212
6	-2.226838	5.175463	0.585788
6	-1.734321	6.393958	0.034811
6	-3.533979	5.142633	1.152651
6	-2.532729	7.512799	0.041028
1	-0.752751	6.416174	-0.409760
6	-4.299504	6.285314	1.163479
1	-3.897436	4.230239	1.596126
6	-3.810482	7.467926	0.605620
1	-2.167628	8.431589	-0.399625
1	-5.283577	6.264734	1.613882
1	-4.425859	8.359545	0.612460

Mol-4b/A_s1r_chl.out

```
    * SCF ENERGY / A.U. =   -1088.11830346

       6         1.671513   -0.631093   -0.273004
       6         1.472294    0.754482   -0.591554
       6         0.144966    0.925751   -0.736204
       6        -1.787602   -0.580075   -0.461139
       6        -2.758124    0.444914   -0.730658
       6        -2.213884   -1.921650   -0.158435
       6        -4.082685    0.138906   -0.702167
       1        -2.429635    1.452211   -0.954195
       6        -3.547304   -2.207166   -0.134044
       6        -4.508495   -1.193935   -0.402905
       1        -4.825109    0.900512   -0.903706
       1        -3.884191   -3.210851    0.092929
       7        -0.479760   -0.280296   -0.496089
       7         0.491375   -1.263393   -0.232024
       6         2.950135   -1.289309   -0.011921
       8         4.009476   -0.690098   -0.039261
       8         2.821757   -2.589022    0.264358
       6         4.030715   -3.329966    0.519654
       1         3.700433   -4.181739    1.113433
       1         4.704071   -2.714165    1.117743
       6         4.687897   -3.777950   -0.770577
       1         5.022786   -2.920482   -1.356719
       1         5.558705   -4.395921   -0.537680
       1         3.994965   -4.371819   -1.370562
       1        -1.464353   -2.673076    0.043923
       6        -5.884913   -1.500035   -0.373550
       7        -7.017794   -1.749480   -0.349904
       6         0.181647    2.434491   -0.901835
       6        -0.171606    3.371250    0.271498
       6         1.760210    2.242768   -0.741518
       1        -0.159848    2.814344   -1.866034
       6         1.086893    4.267195    0.278288
       6        -0.032875    2.634376    1.614853
       1        -1.123907    3.886612    0.144228
       6         2.076260    3.102905    0.500144
       1         2.364246    2.516221   -1.607417
       1         1.090156    4.995543    1.093382
       1         1.245639    4.792608   -0.667566
       1        -0.441863    3.249324    2.419468
       1        -0.572806    1.684387    1.626572
       6         1.504581    2.452636    1.772160
       1         3.128554    3.374209    0.576739
       1         1.873915    2.978517    2.655208
       1         1.798828    1.405228    1.868676
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Mol-4b/B_s1r_chl.out

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    * SCF ENERGY / A.U. =   -1088.11845650

       6         1.340642   -1.034626    0.300509
       6         1.362290    0.310486   -0.198999
       6         0.095912    0.612373   -0.538046
       6        -2.034016   -0.615926   -0.351354
       6        -2.822600    0.467706   -0.871397
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6	-2.665782	-1.847295	0.047508
6	-4.168939	0.320387	-0.990023
1	-2.340922	1.391595	-1.166201
6	-4.017615	-1.973758	-0.078663
6	-4.798100	-0.903431	-0.597137
1	-4.775631	1.127165	-1.380921
1	-4.507595	-2.892704	0.217465
7	-0.703902	-0.476191	-0.245808
7	0.092043	-1.518191	0.253784
6	2.437478	-1.841086	0.833059
8	2.336886	-2.970804	1.261125
8	3.587782	-1.145864	0.784637
6	4.758455	-1.773849	1.337622
1	5.590799	-1.279276	0.837596
1	4.755222	-2.831248	1.068522
6	4.825157	-1.584953	2.840457
1	3.990537	-2.086174	3.333725
1	5.755773	-2.014382	3.219766
1	4.806024	-0.523420	3.097398
1	-2.050895	-2.644130	0.440116
6	-6.195562	-1.044627	-0.723870
7	-7.345591	-1.157207	-0.828615
6	0.341617	2.080523	-0.835975
6	-0.023366	3.171232	0.191775
6	1.853788	1.729304	-0.456244
1	0.164881	2.394051	-1.866104
6	1.326910	3.917723	0.270075
6	-0.128700	2.574866	1.606367
1	-0.884655	3.772108	-0.101012
6	2.133234	2.682102	0.724953
1	2.582268	1.832117	-1.261461
1	1.328042	4.727014	1.004860
1	1.655054	4.314227	-0.694863
1	-0.549058	3.315351	2.290280
1	-0.777215	1.696172	1.642017
6	1.347271	2.245577	1.973375
1	3.195966	2.842255	0.904575
1	1.675024	2.824970	2.839287
1	1.499067	1.189985	2.209666

Optimised geometries (GS)

Mol-2g/A_s0_ac.out
    * SCF ENERGY / A.U. =   -1136.46213679

6	1.442399	1.687565	0.656333
6	0.394019	2.630123	0.661044
6	-0.749134	1.879677	0.594773
6	-0.004504	4.062877	0.650969
6	-1.950987	2.770284	0.516832
6	-1.206513	-0.589327	0.474741
6	-2.507871	-0.546175	0.970757
6	-0.670557	-1.746538	-0.090825
6	-3.297905	-1.685375	0.888574
1	-2.901982	0.358401	1.419211
6	-1.458135	-2.886587	-0.161833
1	0.343185	-1.749158	-0.473218
6	-2.770858	-2.852817	0.325414
1	-4.313173	-1.673306	1.269533
1	-1.061886	-3.796409	-0.599423
7	-1.409076	4.048054	0.564181
7	-0.391675	0.576156	0.552316
7	0.944484	0.454230	0.591268
8	0.651880	5.074055	0.698775
8	-3.125994	2.497930	0.427123
6	2.906746	1.936672	0.721533
8	3.370213	3.053391	0.788835
8	3.615806	0.815773	0.696735
6	5.053545	0.971463	0.747471
1	5.309289	1.523445	1.655854
1	5.365098	1.560099	-0.119839
6	5.657629	-0.412584	0.738135
1	5.377673	-0.955877	-0.168472
1	6.747459	-0.327349	0.766254
1	5.333814	-0.986502	1.610558
6	-2.200677	5.265273	0.535246
1	-2.003930	5.858607	1.430351
1	-1.959351	5.850758	-0.354403
1	-3.252125	4.979985	0.510241
6	-3.587440	-4.035095	0.248380
7	-4.242737	-4.987546	0.183946

Mol-2g/A_s0_dcm.out
    * SCF ENERGY / A.U. =   -1136.46039615

6	1.442225	1.688357	0.639421
6	0.393939	2.630598	0.650521
6	-0.749957	1.880706	0.589672
6	-0.002962	4.063372	0.653120
6	-1.951648	2.773124	0.530103
6	-1.205961	-0.590217	0.469953
6	-2.516731	-0.540102	0.939880
6	-0.660329	-1.756060	-0.068408
6	-3.305095	-1.680620	0.860161
1	-2.920711	0.372069	1.363446
6	-1.447159	-2.896783	-0.137199
1	0.361092	-1.764458	-0.429379

6	-2.769074	-2.856537	0.323982
1	-4.327573	-1.662249	1.220789
1	-1.043133	-3.813173	-0.553279
7	-1.408419	4.050009	0.576560
7	-0.392321	0.576520	0.544503
7	0.944143	0.455389	0.576420
8	0.653950	5.073626	0.705393
8	-3.128272	2.502730	0.456177
6	2.906581	1.938403	0.695910
8	3.370380	3.055933	0.742064
8	3.614816	0.816788	0.689408
6	5.052110	0.972409	0.741078
1	5.305486	1.532573	1.645238
1	5.365549	1.553952	-0.130278
6	5.653183	-0.413077	0.745154
1	5.374538	-0.962190	-0.158311
1	6.743136	-0.331782	0.777554
1	5.322569	-0.978935	1.620216
6	-2.198619	5.268327	0.555960
1	-1.999372	5.856618	1.453825
1	-1.956469	5.858443	-0.330324
1	-3.250259	4.983865	0.530005
6	-3.584456	-4.040015	0.249865
7	-4.238452	-4.993437	0.188170

Mol-2g/A_s0_diox.out

* SCF ENERGY / A.U. = -1136.44598514

6	1.427152	1.695169	0.614838
6	0.383086	2.641747	0.649651
6	-0.768370	1.899870	0.602485
6	0.006673	4.079699	0.692293
6	-1.962985	2.810606	0.609257
6	-1.214295	-0.587457	0.463847
6	-2.595913	-0.498814	0.621265
6	-0.583252	-1.811736	0.233630
6	-3.360522	-1.655527	0.541829
1	-3.077222	0.457214	0.794069
6	-1.351982	-2.963130	0.158729
1	0.492010	-1.854209	0.116588
6	-2.741469	-2.887693	0.311829
1	-4.436968	-1.601859	0.661782
1	-0.877745	-3.921944	-0.019969
7	-1.404742	4.077883	0.664784
7	-0.414470	0.589934	0.541351
7	0.922192	0.468048	0.551423
8	0.670936	5.081423	0.738903
8	-3.146991	2.562832	0.577166
6	2.894920	1.937311	0.642169
8	3.367000	3.049142	0.661306
8	3.594067	0.806671	0.642130
6	5.029223	0.958338	0.667919
1	5.301443	1.528981	1.560287
1	5.332253	1.532673	-0.212105
6	5.629470	-0.427812	0.675665
1	5.337920	-0.985340	-0.218134
1	6.720077	-0.350541	0.692960
1	5.309647	-0.987193	1.558502

6	-2.182987	5.302495	0.678099
1	-1.853521	5.936409	1.502972
1	-2.060816	5.842522	-0.263703
1	-3.230376	5.033631	0.813453
6	-3.535042	-4.085394	0.232764
7	-4.171673	-5.049775	0.167336

Mol-2g/A_s0_dmso.out

* SCF ENERGY / A.U. = -1136.45801784

6	1.444891	1.692195	0.655115
6	0.395352	2.634014	0.660010
6	-0.746489	1.881409	0.596834
6	-0.008247	4.065725	0.644412
6	-1.950650	2.766718	0.512999
6	-1.203174	-0.585921	0.477933
6	-2.494085	-0.551799	1.000965
6	-0.677246	-1.733062	-0.116246
6	-3.284658	-1.690330	0.916154
1	-2.878870	0.344455	1.473542
6	-1.465017	-2.872570	-0.190617
1	0.328487	-1.727952	-0.519361
6	-2.767615	-2.847482	0.323361
1	-4.292033	-1.685921	1.317666
1	-1.077399	-3.774596	-0.651374
7	-1.412965	4.046234	0.558748
7	-0.388091	0.579024	0.555686
7	0.947932	0.458045	0.592811
8	0.644653	5.079427	0.686085
8	-3.123858	2.488445	0.418627
6	2.909856	1.938881	0.718499
8	3.377052	3.054472	0.777517
8	3.615181	0.815449	0.702854
6	5.053313	0.965948	0.755324
1	5.310187	1.520407	1.661811
1	5.369315	1.549409	-0.113741
6	5.653061	-0.419732	0.752726
1	5.373235	-0.966467	-0.151793
1	6.743030	-0.337032	0.781654
1	5.327404	-0.989220	1.627275
6	-2.208171	5.260497	0.526571
1	-1.980682	5.875432	1.399295
1	-2.002109	5.825434	-0.385089
1	-3.259280	4.973715	0.547055
6	-3.584803	-4.028735	0.241608
7	-4.240780	-4.980343	0.172452

Mol-2g/A_s0_etoh.out

* SCF ENERGY / A.U. = -1136.45846995

6	1.441294	1.662947	0.663445
6	0.395598	2.603200	0.670464
6	-0.747580	1.856037	0.598998
6	0.004637	4.032425	0.661615
6	-1.940685	2.753369	0.503613
6	-1.214873	-0.606526	0.476504
6	-2.500492	-0.561936	1.011310
6	-0.703734	-1.754356	-0.127920

6	-3.303269	-1.691757	0.925596
1	-2.869445	0.334960	1.496237
6	-1.503460	-2.885786	-0.202016
1	0.299071	-1.756781	-0.538602
6	-2.801806	-2.850120	0.321770
1	-4.307565	-1.680435	1.334896
1	-1.128762	-3.789553	-0.670326
7	-1.394284	4.030498	0.563257
7	-0.391130	0.553098	0.554356
7	0.944855	0.428727	0.595852
8	0.677088	5.037274	0.719716
8	-3.115894	2.487216	0.391603
6	2.898360	1.931423	0.717737
8	3.339036	3.063057	0.756091
8	3.628019	0.828737	0.715376
6	5.066625	1.007141	0.754461
1	5.314769	1.573673	1.655732
1	5.358975	1.588344	-0.124079
6	5.685646	-0.369555	0.759077
1	5.407027	-0.925814	-0.140209
1	6.774494	-0.271798	0.781217
1	5.371488	-0.935473	1.640362
6	-2.175576	5.255202	0.520461
1	-1.967390	5.856837	1.407298
1	-1.932108	5.825421	-0.378493
1	-3.230124	4.981211	0.505336
6	-3.632097	-4.021730	0.238448
7	-4.299979	-4.965002	0.168185

Mol-2g/A_s0_mecn.out

* SCF ENERGY / A.U. = -1136.46121233

6	1.444468	1.692463	0.647974
6	0.394829	2.633771	0.654347
6	-0.747118	1.881324	0.589881
6	-0.008030	4.065389	0.647344
6	-1.950956	2.768686	0.515410
6	-1.203053	-0.587099	0.472095
6	-2.499312	-0.546627	0.981618
6	-0.671726	-1.741169	-0.103941
6	-3.289562	-1.685930	0.902119
1	-2.888258	0.355667	1.439262
6	-1.459224	-2.881509	-0.172152
1	0.337924	-1.741217	-0.497026
6	-2.767020	-2.850407	0.328439
1	-4.300844	-1.676597	1.293544
1	-1.066989	-3.789107	-0.617806
7	-1.411932	4.047776	0.562364
7	-0.388341	0.578671	0.547044
7	0.947860	0.458345	0.583856
8	0.645756	5.078806	0.696636
8	-3.125486	2.493347	0.427968
6	2.909092	1.939441	0.711995
8	3.376132	3.055432	0.772866
8	3.615294	0.817070	0.694930
6	5.053632	0.967784	0.750703
1	5.307167	1.520421	1.659282
1	5.370652	1.553053	-0.116773

6	5.651096	-0.419078	0.746666
1	5.371917	-0.962244	-0.160242
1	6.741120	-0.339119	0.779279
1	5.320301	-0.989259	1.618879
6	-2.206221	5.263411	0.536532
1	-2.042327	5.836923	1.451102
1	-1.936710	5.868673	-0.331272
1	-3.255040	4.975466	0.469186
6	-3.583543	-4.032877	0.253934
7	-4.238823	-4.985505	0.191324

Mol-2g/B_s0_ac.out

* SCF ENERGY / A.U. = -1136.46272244

6	1.372285	1.613531	0.515872
6	0.342676	2.568654	0.639327
6	-0.810273	1.831592	0.679924
6	-0.031689	3.999232	0.803665
6	-1.992791	2.723188	0.893659
6	-1.313833	-0.625656	0.593303
6	-2.610036	-0.526470	0.092231
6	-0.806609	-1.822155	1.099355
6	-3.426229	-1.650076	0.110098
1	-2.977745	0.409495	-0.312463
6	-1.620247	-2.946151	1.106777
1	0.204420	-1.867036	1.486842
6	-2.928962	-2.856316	0.616340
1	-4.438242	-1.595876	-0.275869
1	-1.248129	-3.886547	1.498420
7	-1.432503	3.993657	0.943067
7	-0.475499	0.525728	0.587524
7	0.854980	0.386991	0.485835
8	0.639194	5.001744	0.829627
8	-3.166431	2.454942	1.008745
6	2.846383	1.784672	0.414601
8	3.631611	0.868521	0.322873
8	3.168644	3.071388	0.438229
6	4.577493	3.382825	0.342541
1	4.965342	2.941386	-0.579572
1	5.089114	2.923276	1.192910
6	4.706975	4.886931	0.349066
1	4.299859	5.309481	1.271509
1	5.764713	5.156248	0.282717
1	4.182853	5.327777	-0.503113
6	-2.200499	5.211122	1.135163
1	-1.909409	5.696665	2.068987
1	-2.032786	5.892690	0.299015
1	-3.254797	4.938648	1.178237
6	-3.771346	-4.023011	0.629459
7	-4.446867	-4.963324	0.641285

Mol-2g/B_s0_dcm.out

* SCF ENERGY / A.U. = -1136.46105211

6	1.374509	1.603990	0.509600
6	0.347588	2.561902	0.628191
6	-0.808694	1.829594	0.663383
6	-0.017900	3.994251	0.791133

6	-1.987450	2.730375	0.864569
6	-1.315407	-0.629977	0.585631
6	-2.629294	-0.521965	0.134645
6	-0.792312	-1.836117	1.051830
6	-3.445151	-1.645685	0.160919
1	-3.013378	0.422203	-0.233853
6	-1.607053	-2.959161	1.068953
1	0.232831	-1.889353	1.398495
6	-2.932791	-2.861168	0.628180
1	-4.470543	-1.583057	-0.186397
1	-1.222319	-3.906626	1.429979
7	-1.419055	3.996691	0.925833
7	-0.476748	0.521517	0.573164
7	0.854114	0.379466	0.477455
8	0.658976	4.992535	0.819323
8	-3.165259	2.472859	0.959904
6	2.848716	1.778202	0.418776
8	3.638119	0.865782	0.329705
8	3.164277	3.066601	0.449515
6	4.570809	3.388468	0.362053
1	4.966369	2.952869	-0.559651
1	5.081367	2.928988	1.213153
6	4.685896	4.894015	0.374304
1	4.271566	5.308963	1.296837
1	5.740600	5.175260	0.310324
1	4.157180	5.331239	-0.476816
6	-2.181094	5.218749	1.113287
1	-1.860677	5.722230	2.027594
1	-2.038134	5.883853	0.259355
1	-3.233349	4.947023	1.194343
6	-3.775010	-4.028035	0.651247
7	-4.449681	-4.968721	0.671219

Mol-2g/B_s0_diox.out
* SCF ENERGY / A.U. = -1136.44715756

6	1.351215	1.607244	0.575998
6	0.328218	2.574044	0.647361
6	-0.838094	1.854202	0.679405
6	-0.015483	4.020080	0.679886
6	-2.011237	2.791068	0.731548
6	-1.331864	-0.628834	0.643091
6	-2.713302	-0.501462	0.773275
6	-0.721915	-1.879371	0.524146
6	-3.499301	-1.646448	0.783368
1	-3.178211	0.473976	0.862182
6	-1.512500	-3.018397	0.536441
1	0.353513	-1.951810	0.424738
6	-2.901777	-2.904802	0.666140
1	-4.575802	-1.562323	0.883937
1	-1.055116	-3.997396	0.444906
7	-1.424179	4.048238	0.738074
7	-0.509902	0.536401	0.632425
7	0.822109	0.389829	0.570948
8	0.672209	5.008237	0.662063
8	-3.200711	2.571910	0.760189
6	2.830440	1.764567	0.514750
8	3.610263	0.848044	0.422446

8	3.155679	3.052087	0.574601
6	4.563821	3.358804	0.515756
1	4.974560	2.924679	-0.400254
1	5.056010	2.884882	1.370174
6	4.695849	4.862758	0.543135
1	4.262017	5.275445	1.457264
1	5.754144	5.135551	0.506625
1	4.190097	5.313827	-0.314129
6	-2.177623	5.288092	0.768929
1	-1.826883	5.912578	1.592426
1	-2.058363	5.829526	-0.172253
1	-3.227805	5.037964	0.917715
6	-3.717174	-4.090317	0.679049
7	-4.371286	-5.045110	0.689830

Mol-2g/B_s0_dmso.out

* SCF ENERGY / A.U. = -1136.45855212

6	1.370147	1.615007	0.512502
6	0.340511	2.570107	0.636044
6	-0.812056	1.832824	0.680684
6	-0.034396	4.001088	0.795854
6	-1.994738	2.724476	0.895054
6	-1.314814	-0.624700	0.596322
6	-2.610302	-0.527251	0.093103
6	-0.806838	-1.820357	1.103317
6	-3.424830	-1.651867	0.110012
1	-2.978553	0.407541	-0.313632
6	-1.618575	-2.945484	1.109690
1	0.203282	-1.863987	1.493234
6	-2.926350	-2.857234	0.616799
1	-4.436242	-1.599302	-0.277701
1	-1.245650	-3.885140	1.502256
7	-1.434760	3.995104	0.938691
7	-0.477264	0.526994	0.590086
7	0.852954	0.388298	0.486014
8	0.635949	5.004062	0.815292
8	-3.168033	2.456396	1.014746
6	2.844101	1.785653	0.408417
8	3.628865	0.869819	0.310083
8	3.167549	3.071947	0.438157
6	4.576748	3.380986	0.340600
1	4.961453	2.944511	-0.585112
1	5.090095	2.915451	1.186589
6	4.711178	4.884172	0.355565
1	4.308255	5.303441	1.281323
1	5.769820	5.149668	0.288757
1	4.187857	5.332544	-0.493136
6	-2.201938	5.211941	1.135579
1	-1.918475	5.688798	2.076264
1	-2.026438	5.900171	0.306667
1	-3.257140	4.941723	1.167497
6	-3.767345	-4.024512	0.629444
7	-4.442409	-4.965128	0.641124

Mol-2g/B_s0_etoh.out
* SCF ENERGY / A.U. = -1136.45909613

6	1.383554	1.594009	0.526591
6	0.357535	2.549223	0.647860
6	-0.796944	1.816459	0.684127
6	-0.009200	3.976206	0.819884
6	-1.971636	2.715248	0.898857
6	-1.311385	-0.636270	0.590514
6	-2.597764	-0.531479	0.066151
6	-0.820307	-1.830554	1.115967
6	-3.422233	-1.648944	0.082461
1	-2.951286	0.400934	-0.359730
6	-1.642116	-2.948601	1.121250
1	0.183706	-1.878510	1.521333
6	-2.941768	-2.853092	0.609073
1	-4.427385	-1.592094	-0.320884
1	-1.283802	-3.887960	1.528178
7	-1.405068	3.983537	0.956425
7	-0.465542	0.510404	0.589274
7	0.864950	0.368027	0.491030
8	0.676149	4.973571	0.853414
8	-3.148230	2.454443	1.009294
6	2.852704	1.778766	0.430303
8	3.650104	0.867475	0.353919
8	3.161270	3.066140	0.436718
6	4.566196	3.404578	0.335875
1	4.956638	2.963958	-0.585231
1	5.084575	2.962372	1.190901
6	4.656179	4.911229	0.330106
1	4.245932	5.329998	1.253076
1	5.705579	5.208138	0.252194
1	4.112645	5.329353	-0.521634
6	-2.162627	5.209294	1.145420
1	-1.856837	5.697763	2.072839
1	-1.995843	5.881193	0.301249
1	-3.218762	4.946805	1.200709
6	-3.794866	-4.011161	0.623058
7	-4.482497	-4.942695	0.635613

Mol-2g/B_s0_mecn.out
* SCF ENERGY / A.U. = -1136.46176523

6	1.373151	1.612552	0.510437
6	0.343639	2.567468	0.633795
6	-0.809070	1.830219	0.675433
6	-0.031061	3.997850	0.797084
6	-1.991080	2.721909	0.890593
6	-1.313299	-0.626435	0.591182
6	-2.610599	-0.526038	0.093050
6	-0.805921	-1.823013	1.096905
6	-3.427872	-1.648866	0.113553
1	-2.977988	0.410081	-0.311570
6	-1.620578	-2.946299	1.106898
1	0.205629	-1.868644	1.482848
6	-2.930359	-2.855219	0.619465
1	-4.440709	-1.594059	-0.270069
1	-1.248605	-3.886762	1.498419

7	-1.430912	3.992484	0.938852
7	-0.474350	0.524489	0.583308
7	0.856106	0.385812	0.480780
8	0.640053	5.000818	0.820279
8	-3.164631	2.454010	1.007811
6	2.846958	1.784560	0.410740
8	3.632761	0.868750	0.315633
8	3.169157	3.070745	0.440507
6	4.577792	3.384315	0.343925
1	4.963741	2.949219	-0.581948
1	5.091127	2.920395	1.190741
6	4.704382	4.888615	0.358602
1	4.301570	5.305229	1.285633
1	5.761144	5.160318	0.288042
1	4.174934	5.332395	-0.488766
6	-2.198621	5.209837	1.133784
1	-1.900047	5.697442	2.064089
1	-2.038728	5.889312	0.294464
1	-3.252096	4.936060	1.186246
6	-3.773790	-4.021052	0.635509
7	-4.450209	-4.960733	0.649932

Optimised geometries (ES) – B rotamers

Mol-2g/B_s1r_ac.out
* SCF ENERGY / A.U. = -1136.50322484

6	1.391696	1.734676	0.570739
6	0.327177	2.684356	0.590999
6	-0.862469	1.871350	0.606671
6	-0.006343	4.062769	0.585652
6	-2.031646	2.665752	0.612836
6	-1.188310	-0.630830	0.610207
6	-2.583224	-0.588852	0.657957
6	-0.501869	-1.848648	0.574754
6	-3.295984	-1.778139	0.669683
1	-3.111938	0.358492	0.683838
6	-1.220515	-3.033001	0.587201
1	0.578935	-1.865105	0.537936
6	-2.619641	-3.003120	0.634832
1	-4.378992	-1.754443	0.706760
1	-0.695202	-3.980722	0.559607
7	-1.454124	4.004072	0.609232
7	-0.450043	0.574525	0.597371
7	0.916290	0.511391	0.577147
8	0.603132	5.131473	0.560212
8	-3.250271	2.483639	0.616980
6	2.869833	1.926730	0.550231
8	3.665233	1.012723	0.519530
8	3.173560	3.213853	0.570884
6	4.581583	3.553737	0.554994
1	5.023509	3.130124	-0.350296
1	5.053520	3.089543	1.424507
6	4.686895	5.060700	0.587661
1	4.228972	5.465800	1.493461
1	5.742646	5.344190	0.577819
1	4.201430	5.506426	-0.284028
6	-2.269076	5.168693	0.572179
1	-1.696331	6.013944	0.953458
1	-2.548541	5.375017	-0.472898
1	-3.188141	4.982425	1.130928
6	-3.362042	-4.231650	0.648401
7	-3.961601	-5.224886	0.659511

Mol-2g/B_s1r_dcm.out
* SCF ENERGY / A.U. = -1136.50110550

6	1.394969	1.730134	0.572340
6	0.331666	2.681190	0.592199
6	-0.859085	1.869621	0.607014
6	0.001085	4.060475	0.587707
6	-2.027777	2.664444	0.613446
6	-1.187998	-0.632312	0.609923
6	-2.582890	-0.588419	0.655753
6	-0.503089	-1.851001	0.575834
6	-3.297075	-1.776953	0.666888
1	-3.110663	0.359574	0.680564
6	-1.223499	-3.034325	0.587669
1	0.577829	-1.868174	0.540613

6	-2.622637	-3.002904	0.633364
1	-4.380131	-1.751936	0.702441
1	-0.699682	-3.982947	0.561167
7	-1.448198	4.003038	0.610610
7	-0.447904	0.572024	0.597677
7	0.918308	0.507254	0.578371
8	0.610453	5.128263	0.563279
8	-3.246328	2.484444	0.617656
6	2.873173	1.923135	0.552889
8	3.670360	1.011235	0.524790
8	3.172802	3.211653	0.571223
6	4.578549	3.557369	0.555852
1	5.024077	3.132193	-0.347061
1	5.051920	3.098282	1.427436
6	4.675618	5.065107	0.583065
1	4.213170	5.470696	1.486265
1	5.729639	5.355220	0.573416
1	4.187515	5.504473	-0.290295
6	-2.261433	5.168424	0.574320
1	-1.685167	6.013587	0.950689
1	-2.545717	5.372905	-0.469941
1	-3.178981	4.984458	1.136657
6	-3.366851	-4.230489	0.646286
7	-3.967920	-5.222734	0.656849

Mol-2g/B_s1r_diox.out

* SCF ENERGY / A.U. = -1136.49210729

6	1.405668	1.714354	0.572057
6	0.346785	2.670166	0.593437
6	-0.847872	1.863650	0.608332
6	0.027773	4.052357	0.590877
6	-2.015088	2.659311	0.617267
6	-1.187254	-0.637495	0.609975
6	-2.582075	-0.587400	0.648995
6	-0.507472	-1.859129	0.582185
6	-3.300616	-1.773706	0.659521
1	-3.107002	0.362677	0.669122
6	-1.233764	-3.038971	0.593345
1	0.573885	-1.878222	0.552491
6	-2.632903	-3.003020	0.632120
1	-4.383848	-1.744664	0.689656
1	-0.715231	-3.990766	0.571871
7	-1.427596	3.999572	0.614442
7	-0.440896	0.563266	0.598118
7	0.924734	0.492909	0.578285
8	0.635789	5.117097	0.566440
8	-3.233091	2.487641	0.624347
6	2.883753	1.911857	0.551781
8	3.688012	1.009074	0.522304
8	3.167899	3.206104	0.571050
6	4.565672	3.570373	0.554006
1	5.018171	3.150387	-0.348397
1	5.048608	3.117094	1.423935
6	4.637416	5.079989	0.580939
1	4.165736	5.476518	1.483125
1	5.685669	5.391138	0.569200
1	4.135810	5.509497	-0.289380

6	-2.233844	5.167728	0.577320
1	-1.649472	6.010412	0.948370
1	-2.520301	5.373167	-0.466808
1	-3.153466	4.988406	1.138812
6	-3.382866	-4.227654	0.644068
7	-3.988617	-5.216714	0.653748

Mol-2g/B_s1r_dmso.out

* SCF ENERGY / A.U. = -1136.50420646

6	1.390086	1.736867	0.569404
6	0.324982	2.685863	0.590084
6	-0.864125	1.872167	0.606414
6	-0.009904	4.063844	0.584298
6	-2.033536	2.666361	0.612640
6	-1.188466	-0.630127	0.610344
6	-2.583392	-0.589075	0.658975
6	-0.501285	-1.847529	0.574424
6	-3.295452	-1.778730	0.671135
1	-3.112568	0.357956	0.685244
6	-1.219078	-3.032377	0.587313
1	0.579467	-1.863637	0.536869
6	-2.618197	-3.003251	0.635831
1	-4.378438	-1.755679	0.708912
1	-0.693050	-3.979670	0.559344
7	-1.456979	4.004566	0.608478
7	-0.451086	0.575716	0.597066
7	0.915302	0.513383	0.576100
8	0.599630	5.132973	0.558144
8	-3.252189	2.483267	0.616999
6	2.868167	1.928552	0.548083
8	3.662745	1.013614	0.515415
8	3.173818	3.215030	0.570494
6	4.582948	3.552034	0.554263
1	5.022863	3.129951	-0.352661
1	5.054395	3.084570	1.422219
6	4.692422	5.058560	0.590884
1	4.236866	5.462648	1.498366
1	5.749026	5.338725	0.581043
1	4.208193	5.508207	-0.279519
6	-2.272735	5.168820	0.571004
1	-1.701710	6.014104	0.954688
1	-2.549789	5.376053	-0.474483
1	-3.192572	4.981443	1.127943
6	-3.359715	-4.232239	0.649854
7	-3.958539	-5.225954	0.661340

Mol-2g/B_s1r_etoh.out

* SCF ENERGY / A.U. = -1136.50352676

6	1.391209	1.735342	0.570375
6	0.326512	2.684815	0.590746
6	-0.862971	1.871599	0.606600
6	-0.007426	4.063097	0.585264
6	-2.032219	2.665939	0.612770
6	-1.188357	-0.630616	0.610249
6	-2.583275	-0.588919	0.658276
6	-0.501692	-1.848307	0.574635

6	-3.295823	-1.778318	0.670122
1	-3.112129	0.358330	0.684288
6	-1.220079	-3.032811	0.587206
1	0.579096	-1.864658	0.537587
6	-2.619202	-3.003159	0.635115
1	-4.378824	-1.754817	0.707418
1	-0.694548	-3.980401	0.559482
7	-1.454992	4.004223	0.609007
7	-0.450360	0.574888	0.597291
7	0.915990	0.511996	0.576864
8	0.602068	5.131931	0.559622
8	-3.250852	2.483526	0.616961
6	2.869330	1.927279	0.549643
8	3.664478	1.012983	0.518395
8	3.173644	3.214204	0.570785
6	4.582004	3.553216	0.554799
1	5.023338	3.130010	-0.350952
1	5.053776	3.088088	1.423881
6	4.688569	5.060051	0.588570
1	4.231353	5.464903	1.494850
1	5.744579	5.342538	0.578721
1	4.203483	5.506907	-0.282764
6	-2.270189	5.168732	0.571826
1	-1.697966	6.013994	0.953833
1	-2.548925	5.375329	-0.473376
1	-3.189487	4.982128	1.130029
6	-3.361335	-4.231827	0.648811
7	-3.960670	-5.225210	0.660026

Mol-2g/B_s1r_mecn.out

* SCF ENERGY / A.U. = -1136.50396437

6	1.390490	1.736319	0.569799
6	0.325533	2.685487	0.590353
6	-0.863710	1.871963	0.606495
6	-0.009015	4.063576	0.584673
6	-2.033062	2.666210	0.612684
6	-1.188427	-0.630303	0.610316
6	-2.583350	-0.589019	0.658733
6	-0.501431	-1.847808	0.574489
6	-3.295585	-1.778582	0.670765
1	-3.112410	0.358090	0.684921
6	-1.219438	-3.032532	0.587250
1	0.579333	-1.864003	0.537114
6	-2.618559	-3.003217	0.635551
1	-4.378577	-1.755369	0.708372
1	-0.693588	-3.979932	0.559355
7	-1.456265	4.004443	0.608677
7	-0.450825	0.575419	0.597166
7	0.915549	0.512884	0.576414
8	0.600506	5.132599	0.558715
8	-3.251708	2.483359	0.616963
6	2.868586	1.928092	0.548708
8	3.663369	1.013381	0.516599
8	3.173758	3.214730	0.570614
6	4.582612	3.552457	0.554473
1	5.023051	3.129915	-0.351996
1	5.054162	3.085887	1.422872

6	4.691035	5.059098	0.589978
1	4.234873	5.463516	1.497000
1	5.747425	5.340100	0.580127
1	4.206503	5.507685	-0.280793
6	-2.271821	5.168789	0.571305
1	-1.700372	6.014062	0.954404
1	-2.549461	5.375803	-0.474083
1	-3.191473	4.981684	1.128682
6	-3.360297	-4.232090	0.649442
7	-3.959305	-5.225686	0.660819