Supplementary Information

Ruthenium(II)-catalyzed regioselective direct C4– and C5–diamidation of indoles and mechanistic studies

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1. General information

All experiments were carried out in nitrogen atmosphere. Merck silica gel plates (Art. 5554) pre-coated with a fluorescent indicator was used for analytical TLC. Flash column chromatography was performed using silica gel 9385 (Merck). Melting points were determined using micro-cover glasses on a Fisher-Johns apparatus and are uncorrected. Compound **2a-2n**[1] were prepared according to the reported procedures. Carbonyl-3- indoles and Thianaphthene-3-carboxaldehyde were purchased from Sigma-Aldrich, TCI Chemicals, or Alfa Aesar. All other chemicals were also purchased from Sigma-Aldrich, Alfa Aesar and TCI, and were used as received. ^{1}H NMR and ^{13}C NMR spectra were recorded on a VNS (600 and 150 MHz) or DPX (300 and 75 MHz) spectrometer at the core research center for natural product and medical material of Yeungnam University. $CDCl_3$/DMSO-d_6 were used as a solvent with chemical shift of 7.24 ppm for $CDCl_3$ and 2.50 DMSO-d_6 ppm as reference. The chemical shifts were described in parts per million (δ) relative to TMS (0 ppm) as an internal standard or relative to the resonance of the residual protonated solvent (^{1}H: $CDCl_3$, δ = 7.24 ppm, DMSO-d_6, δ = 2.50 ppm). ^{13}C NMR spectra were referenced to the internal solvent signals (^{13}C: $CDCl_3$, δ = 77.0 ppm, DMSO-d_6, δ = 39.5 ppm) Multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, and m = multiplet or overlap of nonequivalent resonances. All chemical shifts (δ) are expressed in units of ppm and J values are given in Hz. Fourier transform infrared (FTIR) spectra were recorded on a PerkinElmer FT-IR spectrometer Spectrum Two^{TM}. High resolution mass spectra (HRMS) of were obtained with a JEOL JMS-700 spectrometer at the Korea Basic Science Institute. The compound **8** was analyzed for HRMS using Thermo Fisher Q exactive orbitrap mass spectrometer. The crystal structure of the compound was determined by single-crystal diffraction methods at the Korea Basic Science Institute (KBSI, Western Seoul Center, Korea).

2. General procedure for the synthesis of 5, 6, 7 and 8

An oven dried two-necked flask equipped with a magnetic stirrer was charged with a mixture of carbonyl-3-indole **1** (0.5 mmol), dioxazolone **2** (1.1 mmol), [Ru(p-cymene)Cl_2]$_2$ (5 mol%), $AgSbF_6$ (15 mol%), and pivalic acid (10 mol%) in TFE (5 mL). The reaction mixture was vigorously stirred on an oil bath for 20 h at 50 °C, and the progress of the reaction was followed by TLC analysis. After completion, the reaction mixture was cooled to room temperature. The

volatiles were removed *in vacuo* and the residue was purified by silica gel column chromatography and eluded with Hex: EtOAc to obtain the desired products **5**, **6**, **7** and **8**.

3. General procedure for the synthesis of 9

i. General procedure for the synthesis of 9a-9b

In an oven dried two-necked flask, a mixture of **5a** (0.5 mmol) and appropriate wittig reagent (1.1 equivalents) in THF (4 mL) was taken. The reaction mixture was vigorously stirred at 50 ^{o}C, for 6 h and the progress of the reaction was followed by TLC analysis. After completion, the volatiles were removed *in vacuo* and the residue was purified by silica gel column chromatography to obtain the desired products **9a-b**.

ii. General procedure for the synthesis of 9c

In an oven dried two-necked flask, a mixture of **5a** (0.5 mmol), dimethyl malonate (1.1 equivalents), piperidine (2 equivalents) in MeOH (5 mL), was taken. The reaction mixture was stirred at room temperature for 12 h, and the progress of the reaction was followed by TLC analysis. After completion, the volatiles were removed *in vacuo* and the residue was purified by silica gel column chromatography to obtain the desired product **9c**.

iii. General procedure for the synthesis of 9d

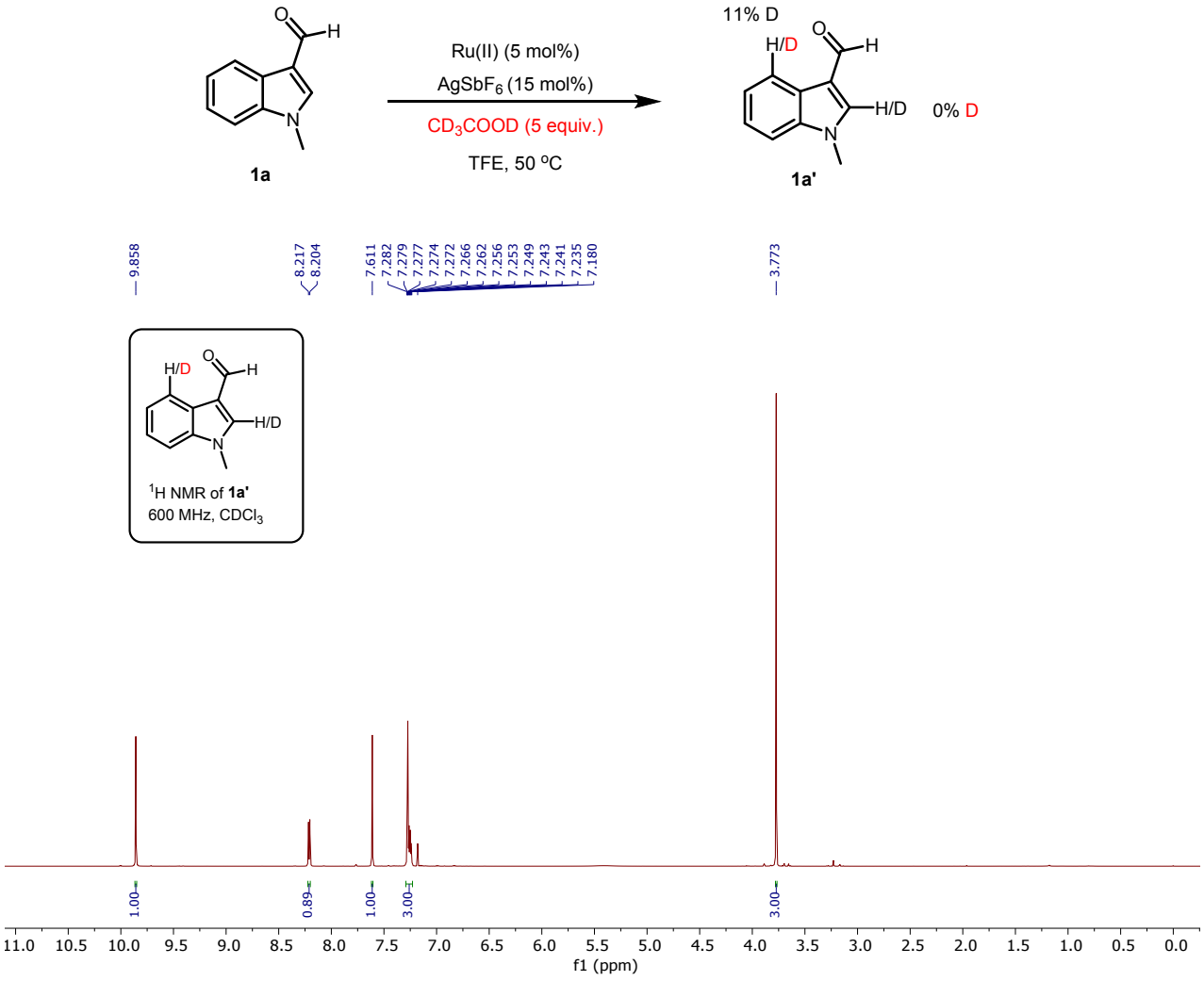
In an oven dried two-necked flask, LAH (2 equivalents) was slowly added to **6g** (0.5 mmol) in THF at 0 °C. The reaction mixture was stirred at room temperature for 2 h, and the progress of the reaction was followed by TLC analysis. After completion, the reaction mixture was quenched by water and the organic phase was extracted with DCM. The organic phase was dried with anhydrous $MgSO_4$. The volatiles were removed *in vacuo* and the residue was purified by silica gel column chromatography to obtain the desired product **9d**.

4. Mechanistic study

a. H/D exchange experiment

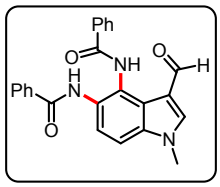
An oven dried 50 mL two necked round bottom flask was charged with indole-3-carboxaldehyde (**1a**) (0.5 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ (5 mol%), $AgSbF_6$ (15 mol%) and CD_3COOD (5

equivalents) in 5 mL of TFE. The reaction mixture was heated at 50 °C for 20 h until the completion of the reaction as indicated by TLC. After completion, the reaction mixture was cooled to room temperature. The volatiles of the filtrate were removed *in vacuo* and the residue was purified by silica gel column chromatography (Hex: EtOAc = 1:1). The analysis of ^{1}H NMR spectra showed the 11% H/D exchange was observed indicating that the C–H activation of indole-3-carboxaldehyde is reversible.



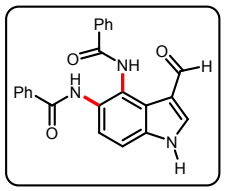
5. Characterization data of synthesized compounds

***N,N′*-(3-Formyl-1-methyl-1*H*-indole-4,5-diyl)dibenzamide (5a):**



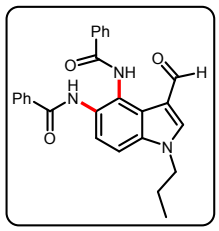
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 87% (173 mg). White solid; mp: 240-242 °C; IR (ATR): 3446, 3018, 1736, 1641, 1442, 1362, 1296, 1222, 1076, 704, 652, 521 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6): δ 11.67 (1H, s), 9.89 (1H, s), 9.64 (1H, s), 8.42 (1H, s), 8.11 (2H, d, J = 7.2 Hz), 7.88 (2H, d, J = 7.2 Hz), 7.72 (1H, d, J = 8.4 Hz), 7.63 (1H, t, J = 7.2 Hz), 7.59-7.54 (4H, m), 7.49 (2H, t, J = 7.8 Hz), 3.94 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 184.9, 165.9, 164.2, 144.0, 136.6, 134.4, 133.5, 132.1, 131.7, 128.7, 128.6, 128.0, 126.9, 125.8, 124.6, 123.5, 119.3, 117.3, 108.9, 33.8. HRMS *m/z* (M^+): calcd for $C_{24}H_{19}N_3O_3$: 397.1426; found: 397.1424.

***N,N′*-(3-Formyl-1*H*-indole-4,5-diyl)dibenzamide (5b):**



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 7:3). Yield: 80% (153 mg). White solid. mp: 230-232 °C. IR (ATR): 3402, 3149, 1731, 1634, 1416, 1123, 1007, 697, 520 cm^{-1}. ^1H NMR (600 MHz, DMSO-d_6): δ 12.61 (1H, s), 11.74 (1H, s), 9.90 (1H, s), 9.70 (1H, s), 8.47 (1H, s), 8.13 (2H, d, J = 7.8 Hz), 7.89 (2H, d, J = 7.8 Hz), 7.68 (1H, d, J = 8.6 Hz), 7.63 (1H, t, J = 7.2 Hz), 7.57 (2H, t, J = 7.2 Hz), 7.54-7.48 (4H, m). ^{13}C NMR (150 MHz, DMSO-d_6): δ 185.7, 166.0, 164.2, 141.4, 136.0, 134.5, 133.5, 132.2, 131.7, 128.6, 128.6, 128.0, 126.9, 125.3, 124.6, 123.7, 118.8, 118.7, 110.4. HRMS *m/z* (M^+): calcd for $C_{23}H_{17}N_3O_3$: 383.1270; found: 383.1273.

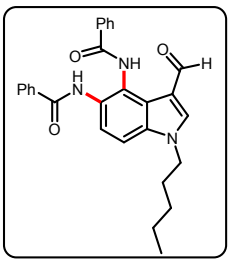
***N,N′*-(3-Formyl-1-propyl-1*H*-indole-4,5-diyl)dibenzamide (5c):**



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 85% (181 mg). White solid. mp: 189-191 °C. IR (ATR): 3042, 2951, 1835, 1504, 1574, 1440, 1383, 1298, 1113, 694, 151, 425 cm^{-1}. ^1H NMR (300 MHz, $CDCl_3$): δ 12.12 (1H, s), 9.96 (1H, s), 9.51 (1H, s), 8.19 (2H, d, J = 7.2 Hz), 8.01 (2H, d, J = 6.9

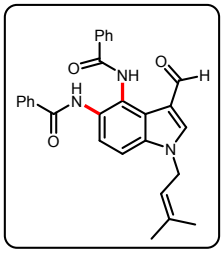
Hz), 7.86 (1H, d, J = 9.0 Hz), 7.73 (1H, s), 7.57-7.53 (3H, m), 7.45-7.42 (3H, m), 7.28 (1H, d, J = 8.4), 4.10 (2H, t, J = 7.1 Hz), 1.93-1.86 (2H, m), 0.95-0.90 (3H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 184.5, 167.5, 165.6, 141.7, 136.3, 134.6, 133.7, 132.2, 131.5, 128.5, 128.56, 128.54, 127.4, 125.8, 125.6, 125.2, 119.4, 118.3, 108.1, 49.4, 22.9, 11.2. HRMS *m/z* (M^+): calcd for $C_{26}H_{23}N_3O_3$: 425.1739; found: 425.1741.

_N,N′_-(3-Formyl-1-pentyl-1_H_-indole-4,5-diyl)dibenzamide (5d):



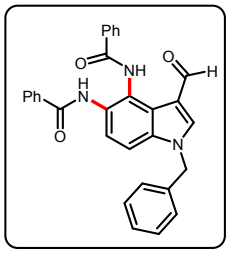
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 80% (181 mg). White solid. mp: 180-182 °C. IR (ATR): 3025, 2939, 1824, 1644, 1440, 1387, 1300, 1185, 700, 405 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 12.10 (1H, s), 9.95 (1H, s), 9.52 (1H, s), 8.19 (2H, d, J = 6.6 Hz), 8.01 (2H, d, J = 7.2 Hz), 7.87 (1H, d, J = 9.0 Hz), 7.73 (1H, s), 7.58-7.55 (3H, m), 7.48-7.46 (1H, m), 7.44-7.40 (2H, m), 7.29 (1H, d, J = 9.0 Hz), 4.14 (2H, t, J = 7.2 Hz), 1.87 (2H, t, J = 7.2 Hz), 1.35-1.27 (4H, m), 0.89-0.86 (3H, m). ^{13}C NMR (150 MHz, $CDCl_3$) δ 184.4, 167.4, 165.6, 141.7, 136.3, 134.6, 133.7, 132.2, 131.5, 128.6, 128.5, 128.4, 127.4, 125.8, 125.6, 125.2, 119.34, 118.3, 108.0, 47.8, 29.2, 28.8, 22.1, 13.8. HRMS m/z (M^+): calcd for $C_{28}H_{27}N_3O_3$: 453.2050; found: 453.2050.

_N,N′_-(3-Formyl-1-(3-methylbut-2-en-1-yl)-1_H_-indole-4,5-diyl)dibenzamide (5e):



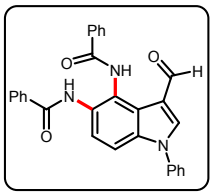
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 76% (171 mg). White solid. mp: 225-227 °C. IR (ATR): 3023, 2820, 1861, 1617, 1439, 1295, 1177, 892, 693, 520 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ 12.12 (1H, s), 9.97 (1H, s), 9.50 (1H, s), 8.20 (2H, d, J = 7.2 Hz), 8.01 (2H, d, J = 7.2 Hz), 7.85 (1H, d, J = 8.4 Hz), 7.74 (1H, s), 7.57 (1H, d, J = 7.2 Hz), 7.53 (2H, t, J = 7.2), 7.47 (1H, t, J = 7.2 Hz), 7.43 (2H, t, J = 7.8 Hz), 7.27 (1H, d, J = 8.4 Hz), 5.37-5.35 (1H, m), 4.68 (2H, d, J = 7.2 Hz), 1.80 (6H, s). ^{13}C NMR (150 MHz, $CDCl_3$): δ 184.4, 167.3, 165.5, 141.2, 139.8, 136.3, 134.5, 133.6, 132.1, 131.4, 128.5, 128.4, 128.4, 127.4, 125.7, 125.6, 125.0, 119.4, 118.2, 117.0, 108.1, 45.2, 25.6, 18.1. HRMS m/z (M^+): calcd for $C_{28}H_{25}N_3O_3$: 451.1896; found: 451.1898.

***N,N′*-(1-Benzyl-3-formyl-1*H*-indole-4,5-diyl)dibenzamide (5f):**



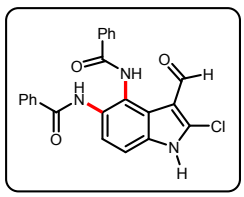
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1).Yield: 89% (211 mg). Brown solid. mp: 210-212 °C. IR (ATR): 3359, 3165, 1837, 1636, 1441, 1383, 1289, 1165, 1017, 691 cm^{-1}. ^1H NMR (600 MHz, DMSO-d_6) δ 12.08 (1H, s), 9.94 (1H, s), 9.50 (1H, s), 8.19 (2H, d, J = 7.2 Hz), 7.99 (2H, d, J = 7.2 Hz), 7.82 (1H, d, J = 9.0 Hz), 7.73 (1H, s), 7.56 (1H, t, J = 7.2 Hz), 7.52 (2H, t, J = 7.8 Hz), 7.46 (1H, t, J = 7.2 Hz), 7.41 (2H, t, J = 7.8 Hz), 7.33-7.31 (3H, m), 7.23 (1H, s), 7.15 (2H, d, J = 6.6 Hz), 5.30 (2H, s).^{13}C NMR (150 MHz, DMSO-d_6): δ 184.7, 167.4, 165.5, 141.9, 136.4, 134.5, 134.4, 133.6, 132.2, 131.5, 129.2, 128.6, 128.5, 128.5, 128.4, 127.4, 127.2, 126.9, 125.7, 125.3, 119.3, 118.7, 108.3, 51.3. HRMS *m/z* (M^+): calcd for $C_{30}H_{23}N_3O_3$: 473.1739; found: 473.1737.

***N,N′*-(3-Formyl-1-phenyl-1*H*-indole-4,5-diyl)dibenzamide (5g):**



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 72% (165 mg). White solid; mp: 252-254 °C. IR (ATR): 3368, 3252, 1743, 1633, 1440, 1290, 1020, 881, 698 cm^{-1}. ^1H NMR (300 MHz, $CDCl_3$): δ 12.05 (1H, s), 9.97 (1H, s), 9.59 (1H, s), 8.20 (2H, d, J = 7.5 Hz), 8.00 (2H, d, J = 7.5 Hz), 7.93 (1H, s), 7.86-7.77 (2H, m), 7.55-7.32 (11H, m). ^{13}C NMR (150 MHz, $CDCl_3$) δ 185.1, 167.3, 165.5, 141.7, 137.2, 136.5, 134.4, 133.5, 132.2, 131.5, 130.0, 128.8, 128.4, 128.4, 127.3, 126.0, 125.6, 124.8, 119.8, 119.2, 109.0. HRMS *m/z* (M^+): calcd for $C_{29}H_{21}N_3O_3$: 459.1583; found:459.1580.

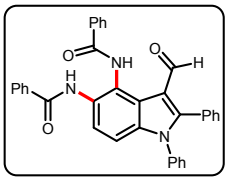
***N,N′*-(2-Chloro-3-formyl-1*H*-indole-4,5-diyl)dibenzamide (5h):**



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 7:3). Yield: 74% (154 mg). White solid; mp: 230-232 °C. IR (ATR): 3520, 3220, 1625, 1443, 1301, 1117, 1014, 762, 617, 407 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 13.65 (1H, s), 11.37 (1H, s), 9.85 (1H, s), 9.80 (1H, s), 8.08 (2H, d, J = 6.0 Hz), 7.87 (2H, d, J = 6.0 Hz), 7.66-7.61 (2H, m), 7.57-7.64 (3H, m), 7.49 (2H, t, J = 6.0 Hz), 7.43 (1H, d, J = 8.6 Hz). ^{13}C NMR (150 MHz,

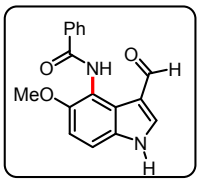
DMSO-d_6): δ 184.0, 165.7, 164.3, 134.3, 133.5, 132.0, 131.6, 128.6, 127.9, 127.0, 126.4, 124.0, 123.6, 119.4, 112.6, 109.8. HRMS *m/z* (M^+): calcd for $C_{23}H_{16}ClN_3O_3$: 417.0880; found: 417.0883.

_N,N'_-(3-Formyl-1,2-diphenyl-1_H_-indole-4,5-diyl)dibenzamide (5i):



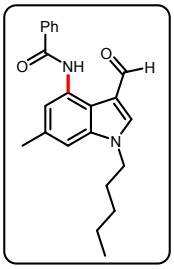
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 73% (195 mg). White solid. mp: 263-265 °C. IR (ATR): 3249, 2835, 1738, 1624, 1426, 1359, 1119, 1014, 916, 803, 694, 594 cm^{-1}. ^1H NMR (300 MHz, $CDCl_3$) δ 12.60 (1H, s), 10.06 (1H, s), 9.61 (1H, s), 8.35 (2H, d, *J* = 5.7 Hz), 8.13 (2H, d, *J* = 6.6 Hz), 7.96 (1H, d, *J* = 9.0 Hz), 7.68-7.64 (2H, m), 7.55-7.51 (8H, m), 7.42-7.39 (4H, m), 7.34-7.27 (3H, m). ^{13}C NMR (75 MHz, $CDCl_3$) δ 187.8, 167.3, 165.5, 153.7, 137.1, 135.5, 134.5, 133.7, 132.1, 131.4, 131.2, 129.8, 129.6, 128.9, 128.4, 128.4, 128.3, 127.8, 127.8, 127.3, 126.2, 125.6, 125.6, 119.1, 116.8, 109.0. HRMS *m/z* (M^+): calcd for $C_{35}H_{25}N_3O_3$: 535.1896; found: 535.1898.

_N,N'_-(3-Formyl-5-methoxy-1_H_-indole-4-yl)dibenzamide (5j):



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 7:3). Yield: 79% (116 mg). White solid. mp:110-112 °C. IR (ATR): 3163, 2929, 1804, 1650, 1415, 1320, 1129, 1005, 932, 880, 754, 698 cm^{-1}. ^1H NMR (600 MHz, DMSO-d_6) δ 12.28 (1H, s), 10.40 (1H, s), 9.74 (1H, s), 8.29 (1H, d, *J* = 3.0 Hz), 8.05 (2H, d, *J* = 7.2 Hz), 7.61 (1H, t, *J* = 7.2 Hz), 7.55 (2H, t, *J* = 7.8 Hz), 7.40 (1H, d, *J* = 8.4 Hz), 7.16 (1H, d, *J* = 9.0 Hz), 3.82 (3H, s).^{13}C NMR (150 MHz, DMSO-d_6): δ 184.6, 164.6, 149.8, 138.8, 134.4, 133.0, 131.4, 128.4, 127.7, 121.8, 119.0, 118.2, 111.0, 110.6, 56.7. HRMS *m/z* (M^+): calcd for $C_{17}H_{14}N_2O_3$: 294.1004; found: 294.1002.

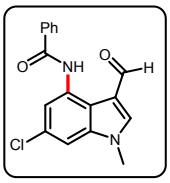
_N_-(3-Formyl-6-methyl-1-pentyl-1_H_-indol-4-yl)benzamide (5k):



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 75% (130 mg). White solid. mp; 90-92 °C. IR (ATR): 3062, 2939, 1630, 1436, 1271, 941, 702, 341 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 12.07 (1H s), 9.56 (1H, s), 8.62 (1H, s), 8.21-8.20 (2H, m), 7.65 (1H, s), 7.53-7.50 (3H, m), 6.87 (1H, s), 4.09 (2H, t, *J* =

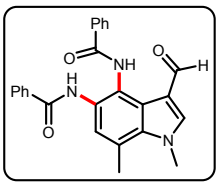
7.2 Hz), 2.51 (3H, s), 1.87-1.85 (2H, m), 1.36-1.29 (4H, m), 0.89 (3H, t, J = 6.6 Hz). ^{13}C NMR (150 MHz, DMSO-d_6): δ 184.4, 166.6, 140.9, 139.1, 136.2, 135.6, 134.0, 131.4, 128.4, 127.7, 118.3, 114.8, 114.0, 105.6, 47.4, 29.1, 28.8, 22.3, 22.2, 13.8. HRMS m/z (M^+): calcd for $C_{22}H_{24}N_2O_2$: 348.1838; found: 348.1840.

_N_-(6-Chloro-3-formyl-1-methyl-1_H_-indol-4-yl)benzamide (5l):



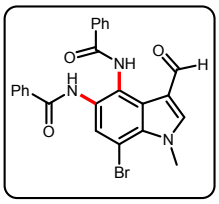
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 80% (125 mg). White solid. mp: 257-259 °C. IR (ATR): 3399, 3025, 1730, 1626, 1522, 1445, 1359, 1277, 1013, 797, 699, 614 cm^{-1}. ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.30 (1H, s), 9.63 (1H, s), 8.63 (1H, d, J = 1.8 Hz), 8.49 (1H, s), 8.10 (2H, d, J = 7.2 Hz), 7.64 (1H, t, J = 7.2 Hz), 7.58 (2H, t, J = 7.8 Hz), 7.50 (1H, d, J = 1.8 Hz), 3.88 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 185.9, 165.5, 145.6, 139.6, 134.5, 133.9, 132.0, 129.5, 128.6, 127.3, 117.2, 113.9, 111.9, 106.7, 33.95. HRMS m/z (M^+): calcd for $C_{17}H_{13}ClN_2O_2$: 312.0666; found: 312.0667.

_N,N′_-(3-Formyl-1,7-dimethyl-1_H_-indole-4,5-diyl)dibenzamide (5m):



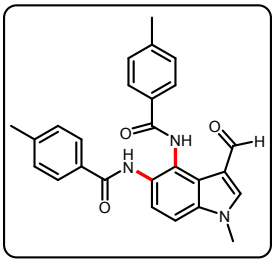
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 78% (160 mg). White solid. mp: 230-232 °C. IR (ATR): 3205, 3022, 1832, 1521, 1443, 1289, 1070, 847, 695, 610, 403cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 12.09 (1H, s), 9.91 (1H, s), 9.34 (1H, s), 8.20 (2H, d, J = 7.2 Hz), 8.00 (2H, d, J = 7.8 Hz), 7.56-7.51 (5H, m), 7.48 (1H, t, J = 7.2 Hz), 7.42 (2H, t, J = 7.2 Hz), 3.95 (3H, s), 2.68 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 184.2, 167.2, 165.5, 144.8, 135.4, 134.5, 133.7, 132.1, 131.5, 128.6, 128.5, 128.4, 127.4, 127.3, 125.4, 123.7, 120.2, 119.8, 117.5, 38.0, 19.1. HRMS m/z (M^+): calcd for $C_{25}H_{21}N_3O_3$: 411.1583; found: 411.1580.

***N,N′*-(7-Bromo-3-formyl-1-methyl-1*H*-indole-4,5-diyl)dibenzamide (5n):**



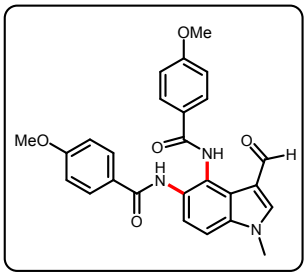
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 71% (169 mg). White solid. mp: 213-215 °C. IR (ATR): 3205, 2944, 1882, 1645, 1430, 1294, 1088, 901, 696, 613, 419 cm^{-1}. ^1H NMR (300 MHz, $CDCl_3$): δ 12.13 (1H, s), 9.88 (1H, s), 9.32 (1H, s), 8.22 (2H, d, J = 7.2 Hz), 7.98 (3H, d, J = 7.2 Hz), 7.63-7.42 (7H, m), 4.10 (3H, s). ^{13}C NMR (75 MHz, $CDCl_3$) δ 184.3, 167.4, 165.5, 146.0, 133.3, 132.4, 131.8, 129.3, 128.6, 128.6, 128.54, 128.51, 127.3, 125.9, 125.2, 121.3, 117.0, 100.7, 99.9, 38.6. HRMS m/z (M^+): calcd for $C_{24}H_{18}BrN_3O_3$: 475.0532; found: 475.0531.

***N,N′*-(3-Formyl-1-methyl-1*H*-indole-4,5-diyl)bis(4-methylbenzamide) (6a):**



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 79% (168 mg). White solid. mp: 286-288 °C. IR (ATR): 3346, 2900, 1760, 1650, 14450, 1360, 1250, 12220, 1057, 698, 640, 510 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 11.86 (1H, s), 9.76 (1H, s), 9.33 (1H, s), 7.93 (2H, d, J = 8.4 Hz), 7.72-7.68 (3H, m), 7.64 (1H, s), 7.18 (2H, d, J = 6.6 Hz), 7.11 (1H, d, J = 9.0 Hz), 7.07 (2H, d, J = 7.8 Hz), 3.67 (3H, s), 2.27 (3H, s), 2.21 (3H, s). ^{13}C NMR (150 MHz, $CDCl_3$) δ 183.9, 166.6, 164.7, 142.5, 142.2, 141.3, 136.2, 131.25, 130.28, 128.6, 127.8, 126.7, 125.0, 124.3, 118.4, 117.5, 107.1, 33.5, 20.9, 20.8. HRMS *m/z* (M^+): calcd for $C_{26}H_{23}N_3O_3$: 425.1739; found: 425.1736.

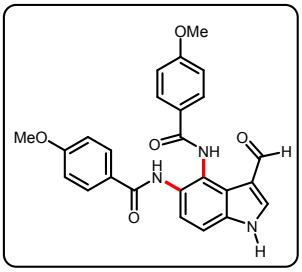
***N,N′*-(3-Formyl-1-methyl-1*H*-indole-4,5-diyl)bis(4-methoxybenzamide) (6b):**



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 81% (185 mg). White solid. mp: 269-271 °C. IR (ATR): 2927, 2850, 1713, 1657, 1514, 1450, 1306, 1263, 1174, 757, 626, 517 cm^{-1}. ^1H NMR (600 MHz, DMSO-d_6) δ 11.63 (1H, s), 9.79 (1H, s), 9.64 (1H, s), 8.42 (1H, s), 8.10 (2H, d, J = 9.0 Hz), 7.84 (2H, d, J = 9.0 Hz), 7.71 (1H, d, J = 9.0 Hz), 7.55 (1H, d, J = 8.4 Hz), 7.11 (2H, d, J = 9.0 Hz), 7.03 (2H, d, J = 8.4 Hz), 3.94 (3H, s), 3.85 (3H, s), 3.80 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 185.0, 165.7, 163.7, 162.4, 161.9, 144.1,

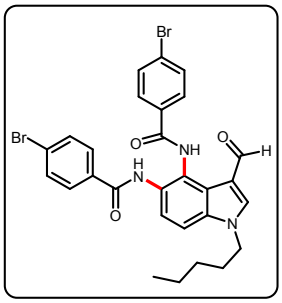
136.5, 130.1, 128.7, 126.5, 125.7, 125.5, 124.6, 123.6, 119.1, 117.3, 113.9, 113.9, 108.6, 55.5, 55.4, 33.85. HRMS *m/z* (M^+): calcd for $C_{26}H_{23}N_3O_5$: 457.1638; found: 457.1636.

***N,N′*-(3-Formyl-1*H*-indole-4,5-diyl)bis(4-methoxybenzamide) (6c):**

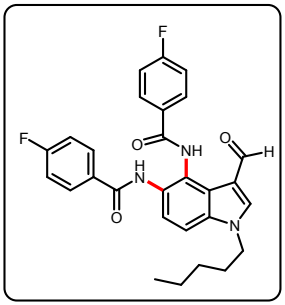


The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 7:3). Yield: 78% (173 mg). White solid. mp: 123-125 °C. IR (ATR): 3400, 3149, 1939, 1727, 1248, 1100, 1009, 754, 556 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 11.67 (^1H NMR (600 MHz, DMSO-d_6) δ 12.59 (1H, s), 11.66 (1H, s), 9.78 (1H, s), 9.69 (1H, s), 8.46 (1H, d, J = 3.0 Hz), 8.11 (2H, d, J = 8.4 Hz), 7.84 (2H, d, J = 8.4 Hz), 7.65 (1H, d, J = 9.0 Hz), 7.48 (1H, d, J = 9.0 Hz), 7.11 (2H, d, J = 8.9 Hz), 7.03 (2H, d, J = 9.0 Hz), 3.85 (3H, s), 3.79 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 185.7, 165.7, 163.6, 162.4, 161.9, 141.5, 135.9, 130.1, 128.7, 126.6, 125.6, 125.3, 124.6, 123.8, 118.7, 118.6, 114.0, 113.9, 110.1, 55.5, 55.4. HRMS *m/z* (M^+): calcd for $C_{25}H_{21}N_3O_5$: 443.1481; found: 443.1479.

***N,N′*-(3-Formyl-1-pentyl-1*H*-indole-4,5-diyl)bis(4-bromobenzamide) (6d):**



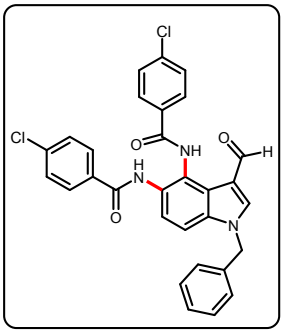
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 77% (234 mg). White solid. mp: 213-233 °C. IR (ATR): 3205, 3022, 1832, 1521, 1443, 1289, 1070, 847, 695, 610 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 12.18 (1H, s), 9.94 (1H, s), 9.54 (1H, s), 8.05 (2H, d, J = 8.4 Hz), 7.85 (3H, d, J = 8.4 Hz), 7.76 (1H, s), 7.66 (2H, d, J = 7.8 Hz), 7.56 (2H, d, J = 7.8 Hz), 7.31 (1H, d, J = 9 Hz), 4.17 (2H t, J = 7.2 Hz,), 1.90-1.88 (2H, m), 1.37-1.28 (4H, m), 0.89 (3H, t, J = 7.2 Hz). ^{13}C NMR (150 MHz, DMSO-d_6): δ 184.5, 166.5, 164.5, 141.6, 136.3, 133.4, 132.4, 131.8, 131.7, 130.0, 129.0, 127.3, 126.3, 125.6, 125.3, 125.0, 119.3, 118.3, 109.9, 108.3, 47.9, 29.2, 28.8, 22.1, 13.8. HRMS *m/z* (M^+): calcd for $C_{28}H_{25}Br_2N_3O_3$: 609.0263; found: 609.0262.



***N,N′*-(3-Formyl-1-pentyl-1*H*-indole-4,5-diyl)bis(4-fluorobenzamide) (6e):**

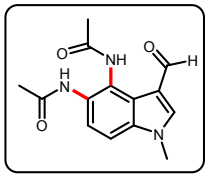
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 75% (183 mg). White solid. mp: 137-139 °C. IR (ATR): 3015, 2744, 1596, 1502, 1446, 1380, 1222, 842, 748, 356 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 12.12 (1H, s), 9.94 (1H, s), 9.51 (1H, s), 8.21 (2H, t, J = 6 Hz), 8.03 (2H, t, J = 5.4 Hz), 7.83-7.79 (2H, m), 7.74 (1H, s), 7.28 (1H, d, J = 9.0 Hz), 7.19 (2H, t, J = 7.8 Hz), 7.09 (2H, t, J = 8.4 Hz), 7.03 (1H, t, J = 8.4 Hz), 4.13 (2H, t, J = 7.2 Hz), 1.88-1.83 (2H, m), 1.35-1.26 (4H, m), 0.87 (3H, t, J = 606). ^{13}C NMR (150 MHz, $CDCl_3$): δ 184.5, 166.35, 166.09 (C-F, $^{1}J_{C\text{-}F}$ = 252 Hz), 165.6 (C-F, $^{1}J_{C\text{-}F}$ = 250.5 Hz), 164.5 (C-F, $^{1}J_{C\text{-}F}$ = 252 Hz), 164.4, 164.0 (C-F, $^{1}J_{C\text{-}F}$ = 250.5 Hz), 141.8, 136.2, 130.97 (C-F, $^{3}J_{C\text{-}F}$ = 9.0 Hz), 130.91 (C-F $^{3}J_{C\text{-}F}$ = 9.0 Hz), 130.69 (C-F, $^{4}J_{C\text{-}F}$ = 3.0 Hz), 130.68, 130.67 (C-F, $^{4}J_{C\text{-}F}$ = 3.0 Hz), 129.99 (C-F, $^{3}J_{C\text{-}F}$ = 10.5 Hz) 129.92 (C-F, $^{3}J_{C\text{-}F}$ = 10.5 Hz), 129.76 (C-F, $^{3}J_{C\text{-}F}$ = 9.0 Hz), 129.74, 129.70 (C-F, $^{3}J_{C\text{-}F}$ = 9.0 Hz), 125.7, 125.3, 125.0, 119.2, 118.2, 115.67 (C-F, $^{2}J_{C\text{-}F}$ = 21.0 Hz), 115.62 (d, $^{2}J_{C\text{-}F}$ = 22.5 Hz), 115.53 (C-F, $^{2}J_{C\text{-}F}$ =, J = 21.0 Hz), 115.4 (C-F, $J_{C\text{-}F}$ =, ^{2}J = 22.5 Hz), 108.1, 47.7, 29.1, 28.7, 22.1, 13.8. ^{19}F NMR (565 Hz, $CDCl_3$) δ -105.8, -106.7, -108.0. HRMS *m/z* (M^+): calcd for $C_{28}H_{25}F_2N_3O_3$: 489.1864; found: 489.1866.

_N,N′_-(3-Formyl-1-(2-methylbenzyl)-1_H_-indole-4,5-diyl)bis(4-chlorobenzamide) (6f):



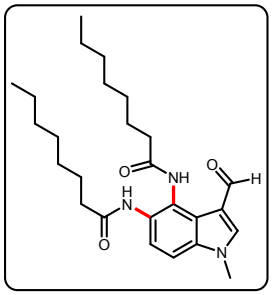
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 77% (208 mg). White solid. mp: 261-263 °C. IR (ATR): 3028, 2930, 1869, 1650, 1540, 1449, 1385, 1298, 1173, 1089, 950, 838, 702, 534 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 12.16 (1H, s), 9.95 (1H s,), 9.57 (1H, s), 8.14 (2H, d, J = 7.2 Hz), 7.93 (2H, d, J = 7.8 Hz), 7.84 (1H, d, J = 9.0 Hz), 7.77 (1H, s), 7.51 (2H, d, J = 7.2 Hz), 7.41-7.37 (5H, m), 7.26-7.27 (1H, m), 7.19 (2H, d, J = 7.8 Hz), 5.37 (2H, s). ^{13}C NMR (150 MHz, $CDCl_3$): δ 184.7, 166.5, 164.5, 141.9, 138.7, 137.9, 136.6, 134.2, 132.9, 131.9, 129.9, 129.3, 128.9, 128.85, 128.82, 128.7, 127.3, 125.6, 125.6, 125.3, 119.4, 118.7, 108.6, 51.4. HRMS m*/z* (M^+): calcd for $C_{31}H_{23}Cl_2N_3O_3$: 541.0960; found: 541.0963.

_N,N′_-(3-Formyl-1-methyl-1_H_-indole-4,5-diyl)diacetamide (6g):



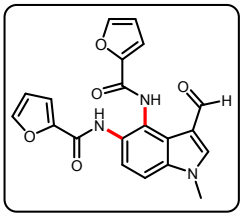
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 74% (101 mg). White solid. mp: 295-297 °C. IR (ATR): 3296, 3100, 2824, 1650, 1455, 1355, 1282, 1122, 645, 587 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 11.35 (1H, s), 9.56 (1H, s), 9.47 (1H, s), 7.69-7.67 (2H, m), 7.14 (1H, d, J = 9.0 Hz), 3.79 (3H, s), 2.34 (3H, s), 2.16 (3H, s). ^{13}C NMR (150 MHz, $CDCl_3$) δ 184.7, 171.0, 169.4, 142.9, 136.7, 125.1, 125.0, 124.5, 119.0, 118.0, 107.6, 34.1, 24.0, 23.9. HRMS m/z (M^+): calcd for $C_{14}H_{15}N_3O_3$: 273.1113; found: 273.1117.

_N,N′_-(3-Formyl-1-methyl-1_H_-indole-4,5-diyl)dioctanamide (6h):



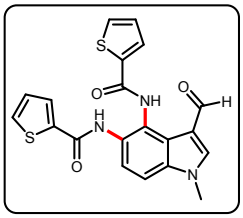
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 77% (170 mg). White solid. mp: 65-67 °C. IR (ATR): 3316, 2922, 2857, 1860, 1639, 1515, 1449, 1364, 1283, 1196, 797, 713, 404 cm^{-1}. ^1H NMR (600 MHz, DMSO-d_6) δ 10.86 (1H, s), 9.68 (1H, s), 9.17 (1H, s), 8.34 (1H, s), 7.53 (1H, d, J = 9.0 Hz), 7.40 (1H, d, J = 9.0 Hz), 3.87 (3H, s), 2.46 (2H, t, J = 7.2 Hz), 2.25 (2H, t, J = 7.2 Hz), 2.09 (1H, d, J = 4.2 Hz), 1.66-1.64 (2H, m), 1.59-1.56(2H, m), 1.29-1.25 (15H, m), 0.87-0.84 (6H, m). ^{13}C NMR (150 MHz, DMSO-d_6): δ 185.0, 176.5, 172.4, 170.4, 143.70, 136.1, 125.7, 123.8, 122.7, 119.2, 117.1, 108.3, 79.17, 78.9, 78.7, 53.5, 36.6, 36.1, 33.7, 31.2, 30.0, 28.6, 28.5, 27.2, 26.7, 25.2, 22.1, 22.0, 13.8. HRMS m/z (M^+): calcd for $C_{26}H_{39}N_3O_3$: 441.2991; found: 441.2995.

_N,N′_-(3-Formyl-1-methyl-1_H_-indole-4,5-diyl)bis(furan-2-carboxamide) (7a):



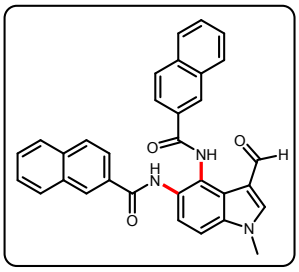
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 75% (141 mg). Brown solid. mp: 259-261 °C. IR (ATR): 2944, 2857, 1859, 1502, 1446, 1380, 1290, 1222, 1164, 944, 842, 748, 582 cm^{-1}. ^1H NMR (600 MHz, DMSO-d_6): δ 11.65 (1H, s), 9.68 (2H, s), 8.44 (1H, s), 8.02 (1H, s), 7.90 (1H, s), 7.66 (1H, d, J = 8.4 Hz), 7.57 (1H, d, J = 8.4 Hz), 7.48 (1H, s), 7.18 (1H, s), 6.76 (1H, s), 6.68 (1H, s), 3.93 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 185.1, 156.8, 155.9, 147.7, 146.8, 146.7, 145.8, 144.3, 136.8, 124.8, 123.8, 123.5, 119.1, 117.3, 116.0, 114.7, 112.4, 112.3, 109.1, 33.91. HRMS m/z (M^+): calcd for $C_{20}H_{15}N_3O_5$: 377.1012; found: 377.1013.

***N,N′*-(3-Formyl-1-methyl-1*H*-indole-4,5-diyl)bis(thiophene-2-carboxamide) (7b):**



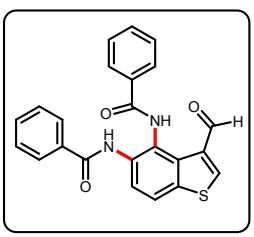
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 73% (149 mg). Brown solid. mp: 173-175 °C. IR (ATR): 3094, 2919, 1844, 1638, 1532, 1436, 1351, 1298, 1071, 930, 846, 734, 647, 516 cm^{-1}. ^1H NMR (600 MHz, DMSO-d_6) δ 11.67 (1H, s), 9.86 (1H, s), 9.70 (1H, s), 8.46 (1H, s), 8.14 (1H, d, J = 4.2 Hz), 7.93 (1H, d, J = 4.8 Hz), 7.83 (1H, d, J = 5.4 Hz), 7.71 (1H, d, J = 3.6 Hz), 7.67 (1H, d, J = 9.0 Hz), 7.58 (1H, d, J = 9.0 Hz), 7.30 (1H, t, J = 4.8 Hz), 7.20 (1H, t, J = 4.2 Hz), 3.94 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 185.6, 161.0, 159.6, 144.7, 140.0, 138.8, 137.1, 133.2, 132.0, 130.8, 129.0, 128.6, 127.0, 125.8, 124.5, 123.9, 119.6, 117.7, 109.5, 34.34. HRMS *m/z* (M^+): calcd for $C_{20}H_{15}N_3O_3S_2$: 409.0555; found: 409.0555.

***N,N′*-(3-Formyl-1-methyl-1*H*-indole-4,5-diyl)bis(2-naphthamide) (7c):**



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 83% (206 mg). White solid. mp: 200-202 °C. IR (ATR): 2924, 2850, 1629, 1446, 1306, 1235, 1195, 1285, 1195, 1033, 756, 624, 624, 470 cm^{-1}. ^1H NMR (600 MHz, DMSO-d_6) δ 11.83 (1H, s), 10.11 (1H, s), 9.67 (1H, s), 8.79 (1H, s), 8.51 (1H, s), 8.43 (1H, s), 8.18 (1H, d, J = 8.4 Hz), 8.08 (2H, t, J = 11.4 Hz), 8.01-7.93 (5H, m), 7.80 (1H, d, J = 8.4 Hz), 7.65-7.53 (5H, m), 3.95 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 185.0, 166.0, 164.4, 143.9, 136.6, 134.4, 134.2, 132.1, 132.0, 131.8, 130.8, 129.1, 128.9, 128.8, 128.7, 128.3, 128.2, 128.1, 127.8, 127.6, 127.5, 126.8, 126.0, 124.7, 124.3, 123.5, 123.4, 119.4, 117.3, 108.9, 33.83. HRMS *m/z* (M^+): calcd for $C_{32}H_{23}N_3O_3$: 497.1739; found: 497.1743.

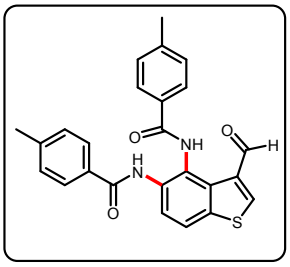
***N,N′*-(3-Formylbenzo[*b*]thiophene-4,5-diyl)dibenzamide (7d):**



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 72% (144 mg). White solid. mp: 152-154 °C. IR (ATR): 3359, 3166, 2925,

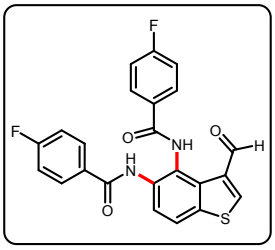
1727, 1656, 1447, 1389, 1281, 1116, 778, 686, 625, 523 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 11.87 (1H, s), 9.78 (1H, s), 9.61 (1H, s), 8.50 (1H, s), 8.15 (2H, d, J = 7.2 Hz), 8.04 (1H, d, J = 9.0 Hz), 7.96 (2H, d, J = 7.2 Hz), 7.81 (1H, d, J = 9 Hz), 7.59 (1H, t, J = 7.8 Hz), 7.53 (2H, t, J = 7.8 Hz), 7.47 (1H, t, J = 7.8 Hz), 7.44-7.40 (2H, m). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.4, 167.3, 165.6, 149.5, 139.1, 137.8, 134.2, 133.4, 132.4, 131.7, 129.8, 128.8, 128.6, 128.6, 128.4, 127.6, 127.4, 127.0, 120.3. HRMS *m/z* (M^+): calcd for $C_{23}H_{16}N_2O_3S$: 400.0882; found: 400.0879.

_N,N′_-(3-Formylbenzo[*b*]thiophene-4,5-diyl)bis(4-methylbenzamide) (7e):



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 75% (161 mg). Brown solid. mp: 155-157 °C. IR (ATR): 3338, 3159, 2924, 1731, 1664, 1615, 1397, 1281, 1114, 732, 628, 527, 450 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 11.79 (1H, s), 9.74 (1H, s), 9.57 (1H, s), 8.47 (1H, s), 8.05-8.01 (3H, m), 7.85 (2H, d, J = 7.8 Hz), 7.78 (1H, d, J = 8.4 Hz), 7.34 (2H, d, J = 7.8 Hz), 7.21 (2H, d, J = 7.8 Hz), 2.43 (3H, s), 2.35 (3H, s). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.4, 167.3, 165.6, 149.5, 139.1, 137.8, 134.2, 133.4, 132.4, 131.7, 129.9, 128.8, 128.5, 128.6, 128.4, 127.6, 127.4, 127.0, 120.3. HRMS *m/z* (M^+): calcd for $C_{25}H_{20}N_2O_3S$: 428.1195; found: 428.1193.

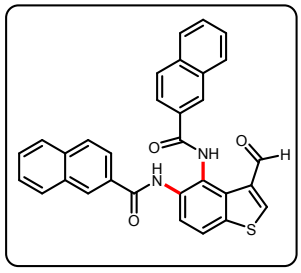
_N,N′_-(3-Formylbenzo[*b*]thiophene-4,5-diyl)bis(4-fluorobenzamide) (7f):



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 75% (164 mg). Brown solid. mp; 220-221 °C. IR (ATR): 3227, 3005, 1735, 1656, 1488, 1288, 1227, 1104, 818, 748, 595 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 111.91 (1H, s), 9.77 (1H, s), 9.57 (1H, s), 8.52 (1H, s), 8.18-8.15 (2H, m), 8.00-7.95 (3H, m), 7.81 (1H, d, J = 6.0 Hz), 7.21 (2H, t, J = 8.4 Hz), 7.10 (2H, t, J = 8.4 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 186.6, 166.3, 166.2 (C-F, $^1J_{C\text{-}F}$ = 255.0 Hz), 165.8 (C-F, ^1J = 252.0 Hz), 164.5 (C-F, $^1J_{C\text{-}F}$ = 255.0 Hz), 164.2 (C-F, $^1J_{C\text{-}F}$ = 252.0 Hz), 150.0, 139.2, 137.7, 130.02 (C-F, ^3J = 9.0 Hz), 130.96 (C-F, ^3J = 9.0 Hz), 130.46 (C-F, ^4J = 3.0 Hz), 130.44 (C-F, ^4J = 3 Hz), 129.8 (C-F, ^3J = 10.5 Hz), 129.7 (C-F, ^3J = 10.5 Hz), 129.6, 129.54 (C-F, ^4J = 3.0 Hz), 129.52 (C-F, ^4J = 3.0 Hz), 128.8, 127.6, 127.0, 120.5, 115.9 (C-F, ^2J = 21.0 Hz), 115.8 (C-F, ^2J =

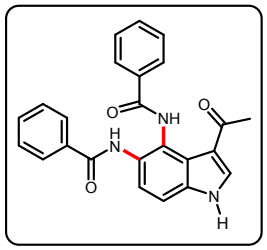
22.0 Hz), 115.7 (C-F, ^2J = 21.0 Hz), 115.6 (C-F, ^2J = 22.0 Hz). ^{19}F NMR (565 Hz, $CDCl_3$) δ -105.8, -106.7, -108.0. HRMS *m/z* (M^+): calcd for $C_{23}H_{14}Cl_2N_2O_3S$: 436.0693; found: 436.0695.

***N,N′*-(3-Formylbenzo[*b*]thiophene-4,5-diyl)bis(2-naphthamide) (7g):**



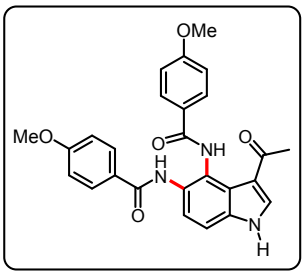
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1).Yield: 65% (163 mg). White solid. mp: 183-185 °C. IR (ATR): 3360, 3190, 2927, 1731, 1650, 1397, 1227, 1109, 956, 774, 627 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 12.06 (1H, s), 9.80 (2H, s), 8.74 (1H, s), 8.50 (2H, d, J = 10.2 Hz), 8.23-8.21 (1H, m), 8.13 (1H, d, J = 9 Hz), 8.04-7.98 (3H, m), 7.89 (1H, d, J = 7.8 Hz), 7.87-7.84 (3H, m), 7.80 (1H, d, J = 7.8 Hz), 7.59-7.54 (2H, m), 7.51-7.44 (2H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 186.3, 167.4, 165.7, 149.4, 139.1, 137.8, 135.1, 134.8, 132.6, 132.6, 131.5, 130.5, 130.0, 129.6, 129.3, 129.1, 128.8, 128.4, 128.2, 128.1, 127.8, 127.7, 127.6, 127.5, 127.0, 126.8, 126.5, 124.4, 123.7, 120.3. HRMS *m/z* (M^+): calcd for $C_{31}H_{20}N_2O_3S$: 500.1195; found: 500.1195.

***N,N′*-(3-Acetyl-1*H*-indole-4,5-diyl)dibenzamide (7h):**



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 7:3). Yield: 73% (144 mg). Brown solid. mp: 151-153 °C. IR (ATR): 3198, 2922, 1721, 1520, 1406, 1163, 696 cm^{-1}. ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.60 (1H s,), 12.50 (1H, s), 9.79 (1H, s), 8.57 (1H, d, J = 3 Hz), 8.11 (2H, d, J = 7.2 Hz), 7.86 (2H, d, J = 7.8 Hz), 7.64-7.61 (2H, m), 7.57 (2H, t, J = 7.8 Hz), 7.54 (1H, t, J = 7.2 Hz), 7.49-7.45 (3H, m), 2.54 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 194.9, 165.9, 164.0, 138.2, 135.8, 134.5, 133.6, 132.1, 131.5, 128.6, 128.6, 128.0, 126.8, 124.8, 124.5, 123.6, 118.6, 117.5, 109.8, 26.93. HRMS *m/z* (M^+): calcd for $C_{24}H_{19}N_3O_3$: 397.1426; found: 397.1424.

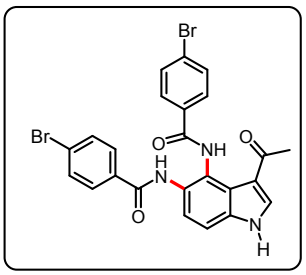
***N,N′*-(3-Acetyl-1*H*-indole-4,5-diyl)bis(4-methoxybenzamide) (7i):**



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 7:3). Yield: 76% (162 mg). Brown solid. mp: 151-153 °C. IR (ATR): 3335, 3158, 2922, 1663, 1613, 1399, 1116, 729, 622, 449, 416 cm^{-1}. ^{1}H NMR (600 MHz,

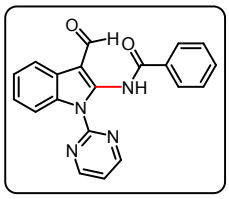
DMSO-d_6) δ 12.57 (1H, s), 12.48 (1H, s), 9.73 (1H, s), 8.57 (1H, d, J = 2.4 Hz), 8.02 (2H, d, J = 8.4 Hz), 7.75 (2H, d, J = 8.4 Hz), 7.61 (1H, d, J = 8.4 Hz), 7.45 (1H, d, J = 9.0 Hz), 7.39 (2H, d, J = 8.4 Hz), 7.29 (2H, d, J = 7.8 Hz), 2.54 (3H, s), 2.40 (3H, s), 2.33 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): 195.0, 165.9, 163.9, 142.4, 141.7, 138.3, 135.8, 131.8, 130.8, 129.2, 129.2, 128.7, 128.1, 127.5, 126.8, 124.8, 124.5, 123.7, 118.6, 117.5, 109.8, 26.9, 21.0, 20.9. HRMS *m/z* (M^+): calcd for $C_{26}H_{23}N_3O_3$: 425.1739; found: 425.1740.

_N,N′_-(3-Acetyl-1_H_-indole-4,5-diyl)bis(4-bromobenzamide) (7j):



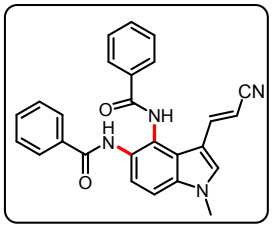
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 7:3). Yield: 84% (232 mg). Brown solid. mp:>300 °C. IR (ATR): 3365, 3167, 2926, 1733, 1651, 1778, 1374, 1224, 1067, 1009, 750, 617, 525, 447 cm^{-1}. ^{1}H NMR (600 MHz, DMSO-d_6) δ 12.59 (1H, s), 12.50 (1H, s), 9.84 (1H, s), 8.56 (1H, d, J = 3.0Hz), 8.03 (2H, d, J = 9.0 Hz), 7.79-7.77 (4H, m), 7.69 (2H, d, J = 8.4 Hz), 7.60 (1H, d, J = 8.4 Hz), 7.47 (1H, d, J = 9.0 Hz), 2.54 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 195.1, 164.9, 163.3, 138.4, 135.9, 133.7, 132.9, 131.7, 131.6, 130.1, 129.0, 126.0, 125.4, 124.8, 124.4, 123.6, 118.7, 117.5, 110.0, 26.95. HRMS *m/z* (M^+): calcd for $C_{24}H_{17}Br_2N_3O_3$: 552.9637; found: 552.9639.

***N*-(3-Formyl-1-(pyrimidin-2-yl)-1*H*-indol-2-yl)benzamide (8):**



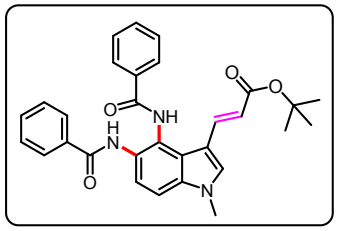
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 69% (117 mg). White solid. mp: 201-203 °C. IR (ATR): 3389, 3161, 1688, 1629, 1557, 1501, 1419, 1375, 1250, 1185, 1108, 750, 651, 522 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ 12.00 (1H, s), 10.26 (1H, s), 8.76 (d, J = 4.8 Hz, 2H), 8.32 (1H, d, J = 8.3 Hz), 8.26 (1H, d, J = 7.5 Hz,), 7.98–7.97 (2H, m), 7.59 (1H, t, J = 7.38 Hz), 7.51 (2H, t, J = 7.86 Hz), 7.32–7.30 (1H, m), 7.25–7.21 (2H, m). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.8, 164.9, 158.1, 157.6, 140.7, 133.8, 133.0, 132.8, 128.XC 9, 127.5, 125.3, 124.4, 124.3, 120.40, 118.1, 114.6, 108.3. HRMS *m/z* (MH^+): calcd for $C_{20}H_{15}N_4O_2$: 343.1190; found: 343.1188.

_N,N′_-(3-(2-Cyanovinyl)-1-methyl-1_H_-indole-4,5-diyl)dibenzamide (9a):



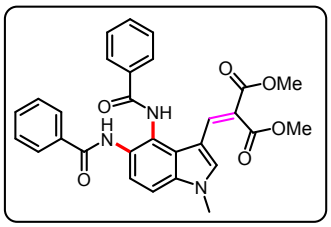
The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 91% (191 mg). White solid. mp: >300 °C. IR (ATR): 3392, 3260, 2203, 1828, 1515, 1443, 1329, 1281, 994, 785, 692, 541 cm^{-1}. ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.10 (1H, s), 9.96 (1H, s), 8.11 (1H, s), 7.99 (2H, d, J = 7.2 Hz), 7.91 (2H, d, J = 7.2 Hz), 7.69 (1H, d, J = 16.8 Hz), 7.60 (1H, t, J = 7.2 Hz), 7.57-7.52 (4H, m), 7.51-7.47 (3H, m), 5.91 (1H, d, J = 16.8 Hz), 3.89 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 165.8, 165.49, 143.9, 136.1, 134.4, 133.9, 131.9, 131.7, 131.6, 128.7, 128.5, 128.3, 127.5, 127.4, 124.1, 122.9, 120.9, 120.1, 110.9, 109.7, 88.9, 33.43. HRMS m/z (M^+): calcd for $C_{26}H_{20}N_4O_2$: 420.1586; found: 420.1588.

tert-Butyl-3-(4,5-bis(benzamido)-1-methyl-1*H*-indol-3-yl)acrylate (9b):



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 88% (218 mg). solid. mp: 260-262 °C. IR (ATR): 3278, 2940, 1844, 1644, 1480, 1276, 1153, 972, 791, 695, 627 cm^{-1}. ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.19 (1H, s), 9.87 (1H, s), 8.11 (1H, s), 8.03 (2H, d, J = 7.2 Hz), 7.92-7.89 (3H, m), 7.60-7.57 (1H, m), 7.56-7.47 (7H, m), 6.12 (1H, d, J = 15.6 Hz), 3.87 (s, 3H), 1.25 (9H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 166.1, 165.7, 165.2, 137.3, 136.1, 134.3, 133.8, 131.8, 131.7, 131.5, 128.5, 127.64, 127.6, 127.3, 123.9, 123.1, 120.5, 114.1, 111.1, 109.4, 78.6, 33.2, 27.7. HRMS m/z (M^+): calcd for $C_{30}H_{29}N_3O_4$: 495.2158; found: 495.2161.

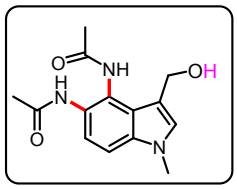
Dimethyl-2-((4,5-bis(benzamido)-1-methyl-1*H*-indol-3-yl)methylene)malonate (9c):



The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 83% (212 mg). White solid. mp: 217-219 °C. IR (ATR): 3240, 3150, 2150, 1760, 1680, 1550, 1460, 1025, 780, 672, 550 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.48 (1H, s), 9.14 (1H, s), 8.20 (1H, s), 8.01 (2H, d, J = 7.8 Hz), 7.65 (2H, d, J = 7.8 Hz), 7.57 (1H, s), 7.51 (1H, t, J = 7.2 Hz), 7.44 (2H, t, J = 7.8 Hz), 7.38 (2H, t, J = 7.8 Hz), 7.23 (2H, t, J = 7.8 Hz), 7.16 (1H, d, J = 9.0 Hz), 3.86 (3H, s), 3.48 (3H, s), 3.30 (3H, s). ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.2, 167.0, 165.9, 165.3, 136.8, 135.8,

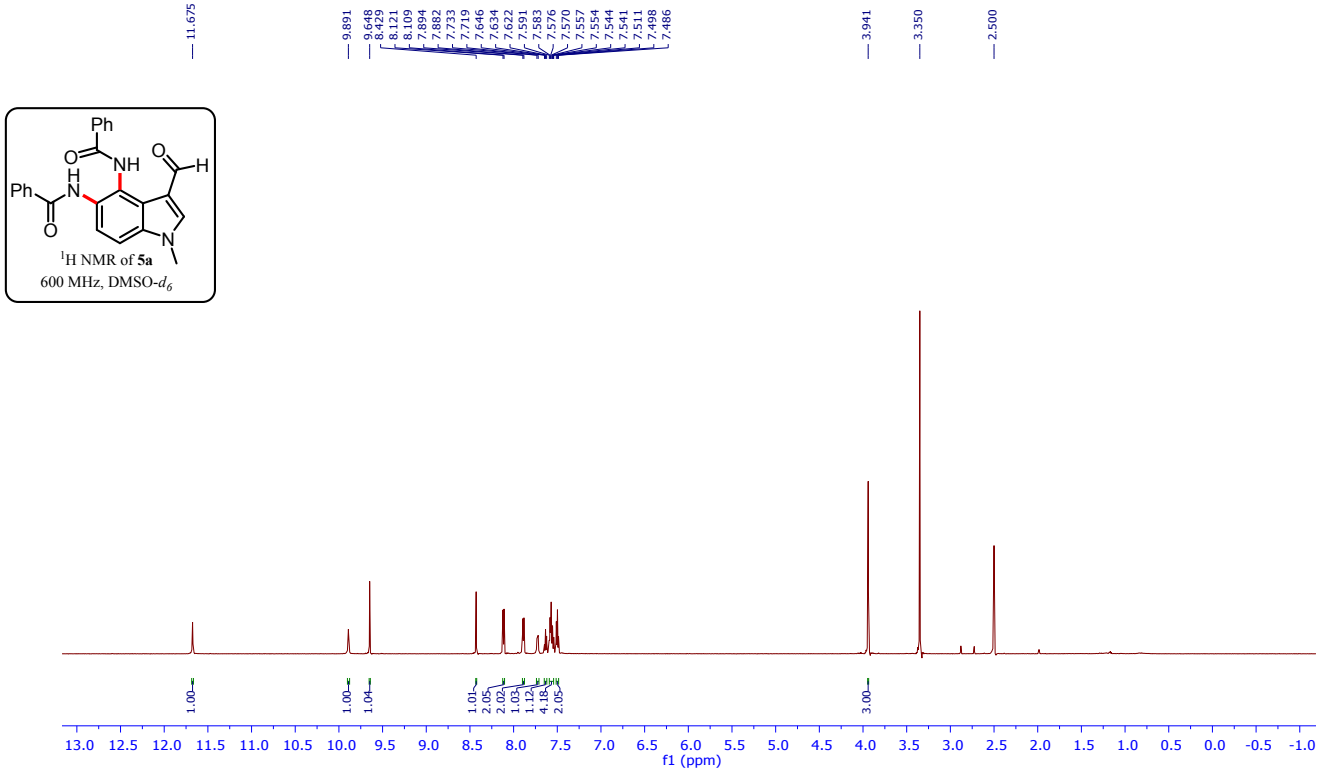
133.4, 133.3, 132.1, 132.04, 131.5, 128.7, 128.6, 128.3, 127.9, 127.8, 127.6, 127.4, 123.9, 123.3, 120.6, 118.4, 109.4, 109.0, 52.5, 52.1, 51.6, 33.5. HRMS *m/z* (M^+): calcd for $C_{29}H_{25}N_3O_6$: 511.1743; found: 511.1742.

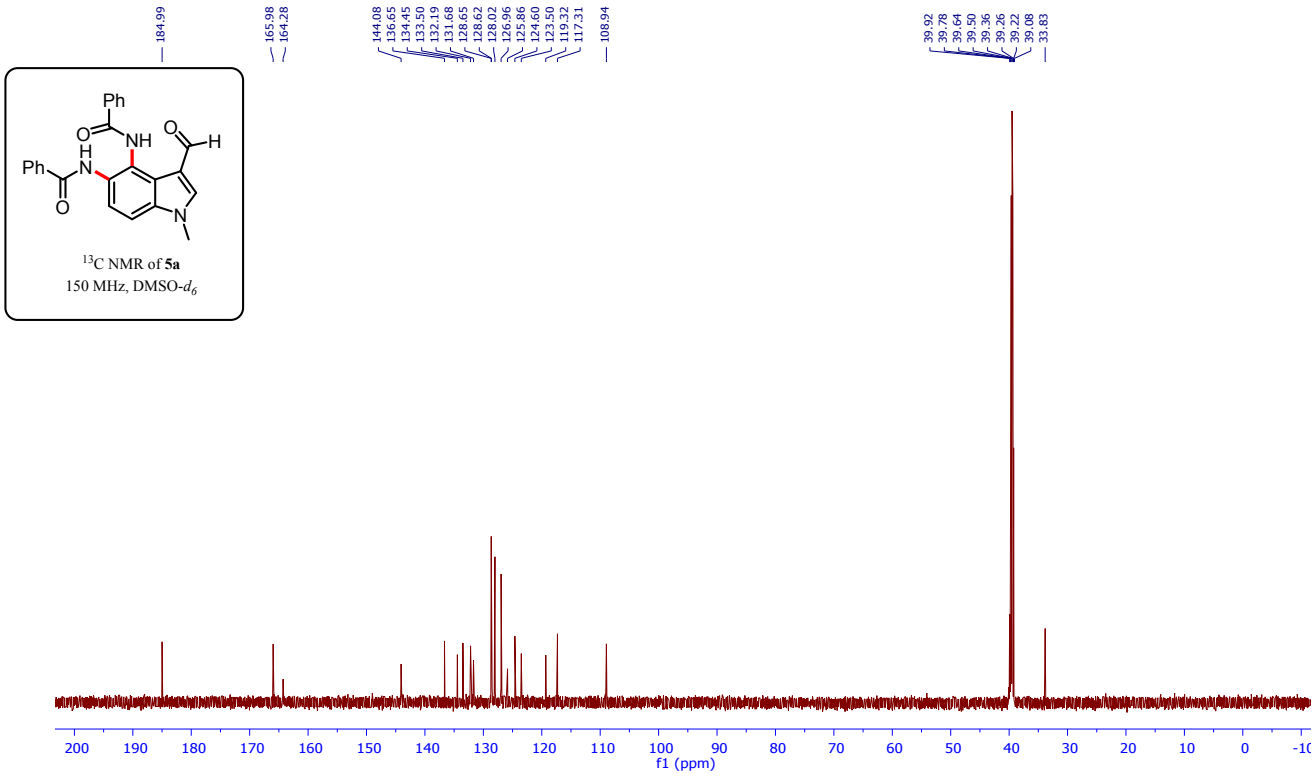
_N_,_N_′-(3-(Hydroxymethyl)-1-methyl-1_H_-indole-4,5-diyl)diacetamide (9d):

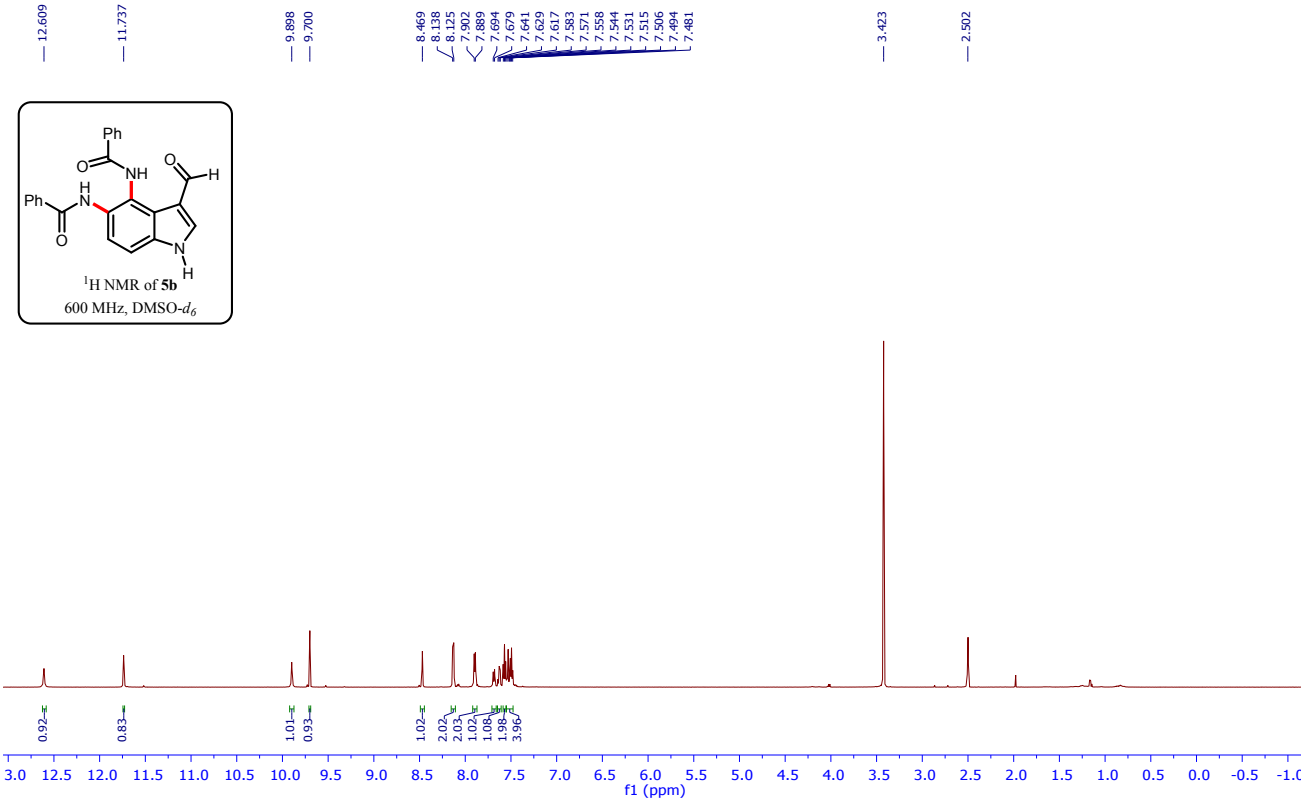


The compound was prepared according to the general procedure and purified by column chromatography (EtOAc/hexane = 1:1). Yield: 91% (125mg). White solid. mp: 277-279 °C. IR (ATR): 3245, 2937, 2203, 1724, 1638, 1448, 1283, 1005, 787, 691, 546 cm^{-1}. ^1H NMR (600 MHz, DMSO-d_6) δ 9.88 (1H, s), 8.96 (1H, s), 7.37 (1H, d, J = 8.7 Hz), 7.27 (1H, d, J = 8.8 Hz), 7.23 (1H, s), 5.58 (1H, t, J = 5.0 Hz), 4.64 (2H, d, J = 4.9 Hz), 3.73 (3H, s), 2.14 (3H, s), 2.01 (3H, s). ^{13}C NMR (150 MHz, DMSO-d_6): δ 169.5, 167.7, 135.3, 128.4, 124.5, 122.4, 121.9, 119.7, 114.2, 107.6, 55.9, 32.4, 23.7, 23.1. HRMS *m/z* (M^+): calcd for $C_{14}H_{17}N_3O_3$: 275.1270; found: 275.1268.

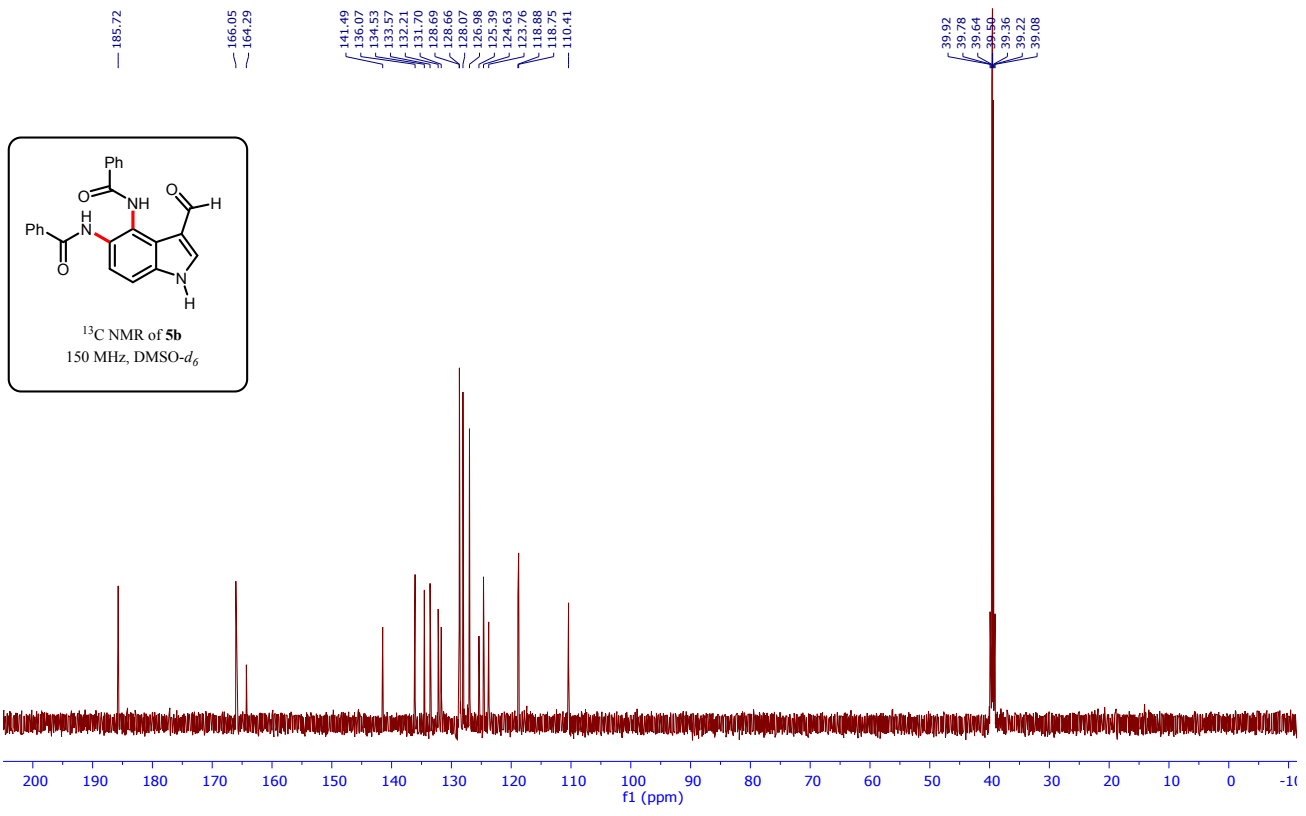
6. ^{1}H NMR and ^{13}C NMR spectra of synthesized compounds



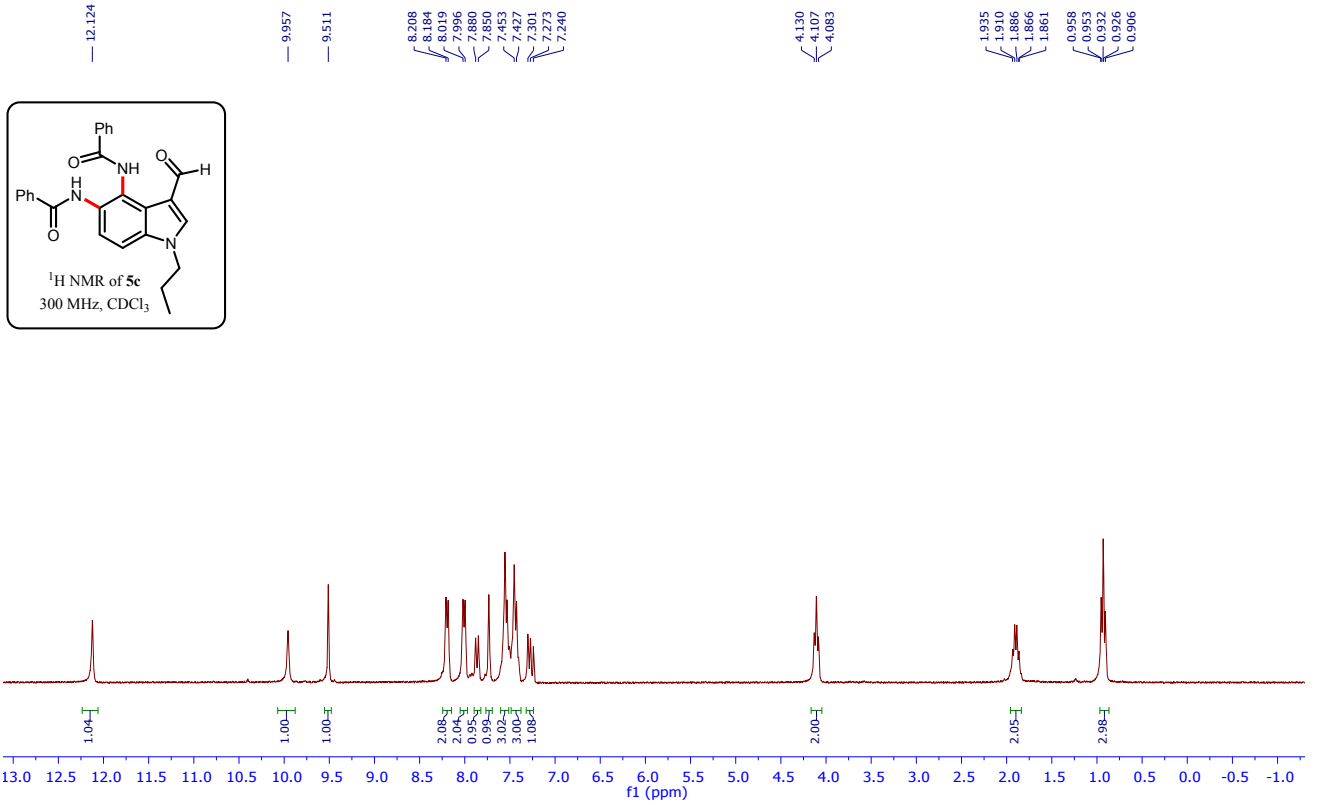


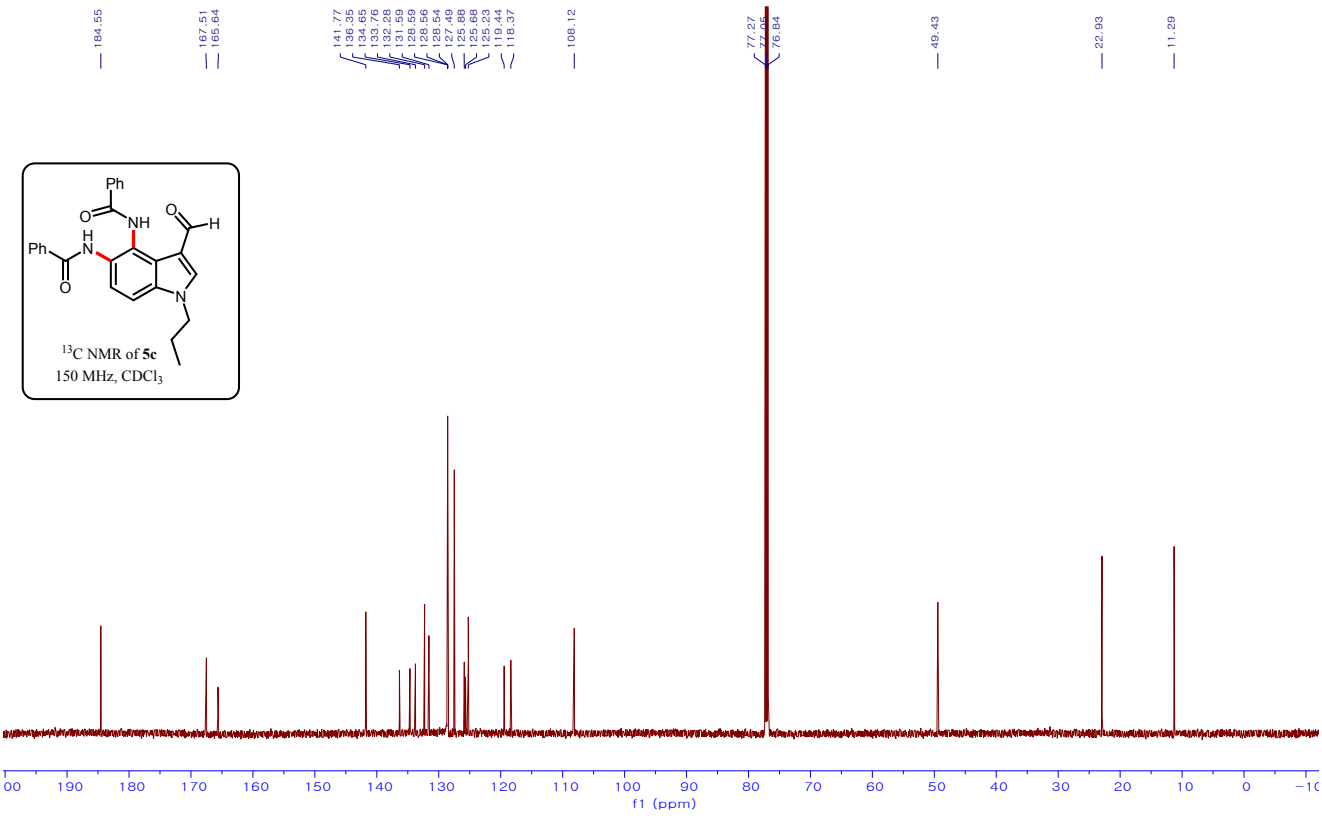


^{1}H NMR of **5b**
600 MHz, DMSO-d_6

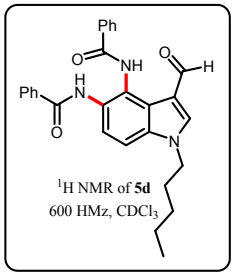


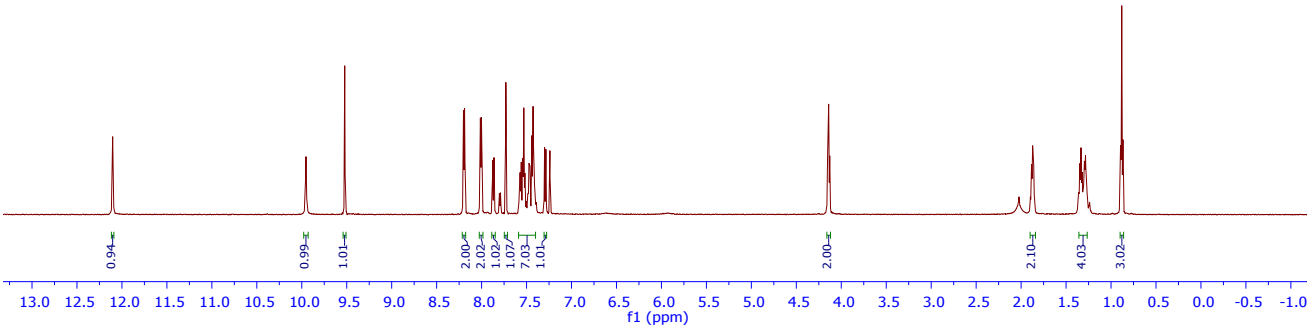
^{13}C NMR of **5b**
150 MHz, DMSO-d_6

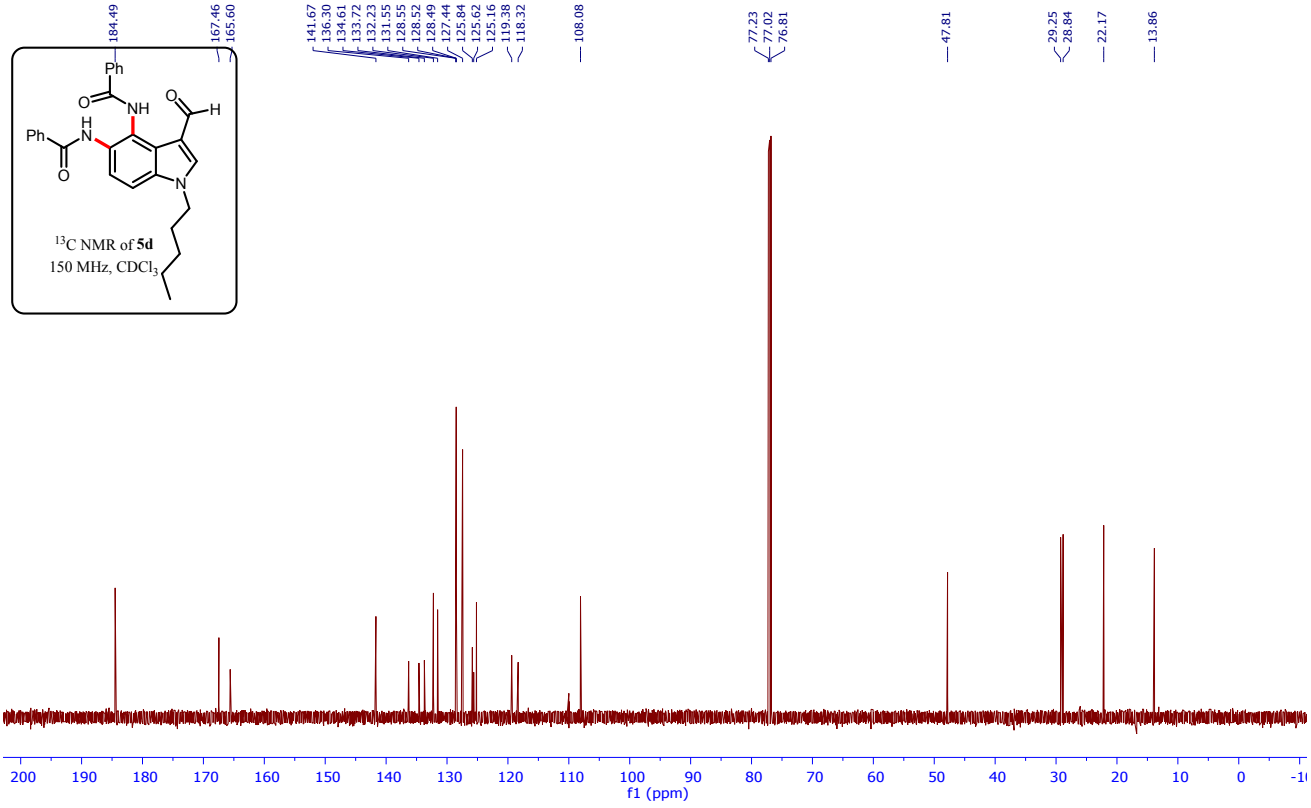

12.124
9.957
9.511
8.208
8.184
8.019
7.996
7.880
7.850
7.453
7.427
7.301
7.273
7.240
4.130
4.107
4.083
1.935
1.910
1.886
1.866
1.861
0.958
0.953
0.932
0.926
0.906
Ph
O
NH
O
H
Ph
N
H
O
N
1H NMR of 5c
300 MHz, CDCl3
1.04
1.00
1.00
2.08
2.04
0.95
0.99
3.02
3.00
1.08
2.00
2.05
2.98
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

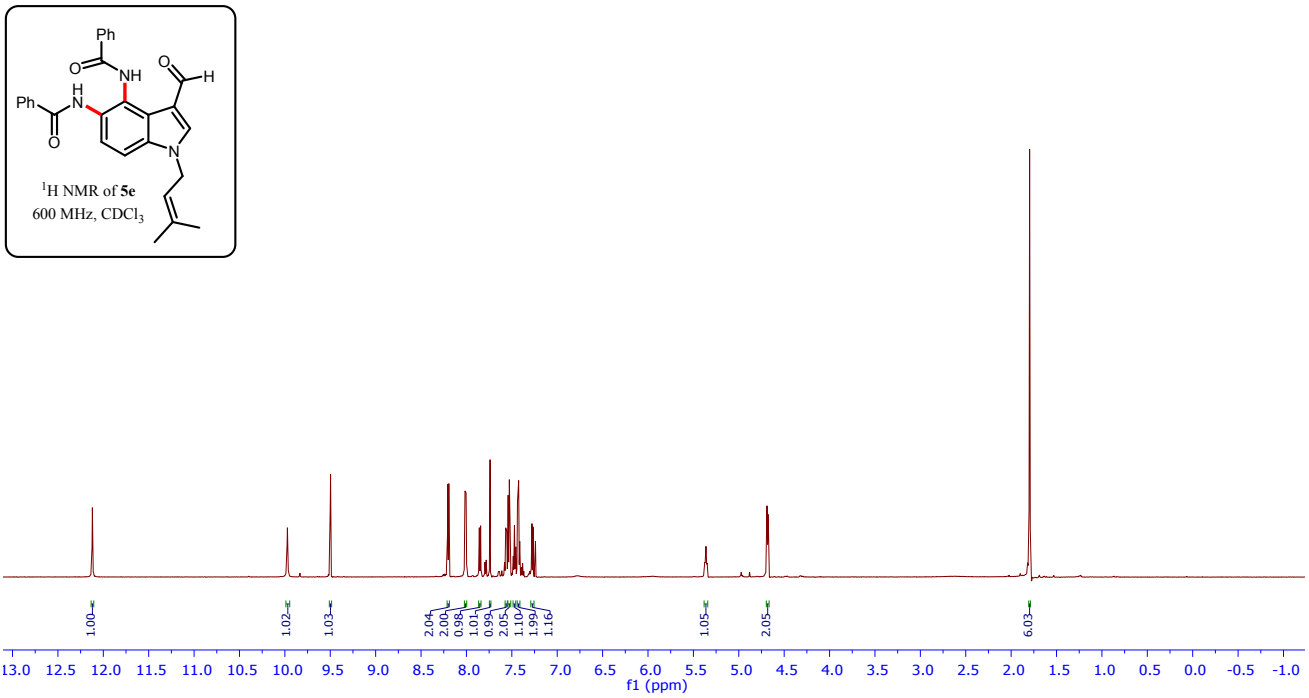

184.55
167.51
165.64
141.77
136.35
134.65
133.76
132.28
131.59
131.56
128.56
128.54
127.49
125.88
125.68
125.23
119.44
118.37
108.12
77.27
77.06
76.84
49.43
22.93
11.29
Ph
O
NH
O
H
Ph
N
H
O
N
13C NMR of 5c
150 MHz, CDCl3
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

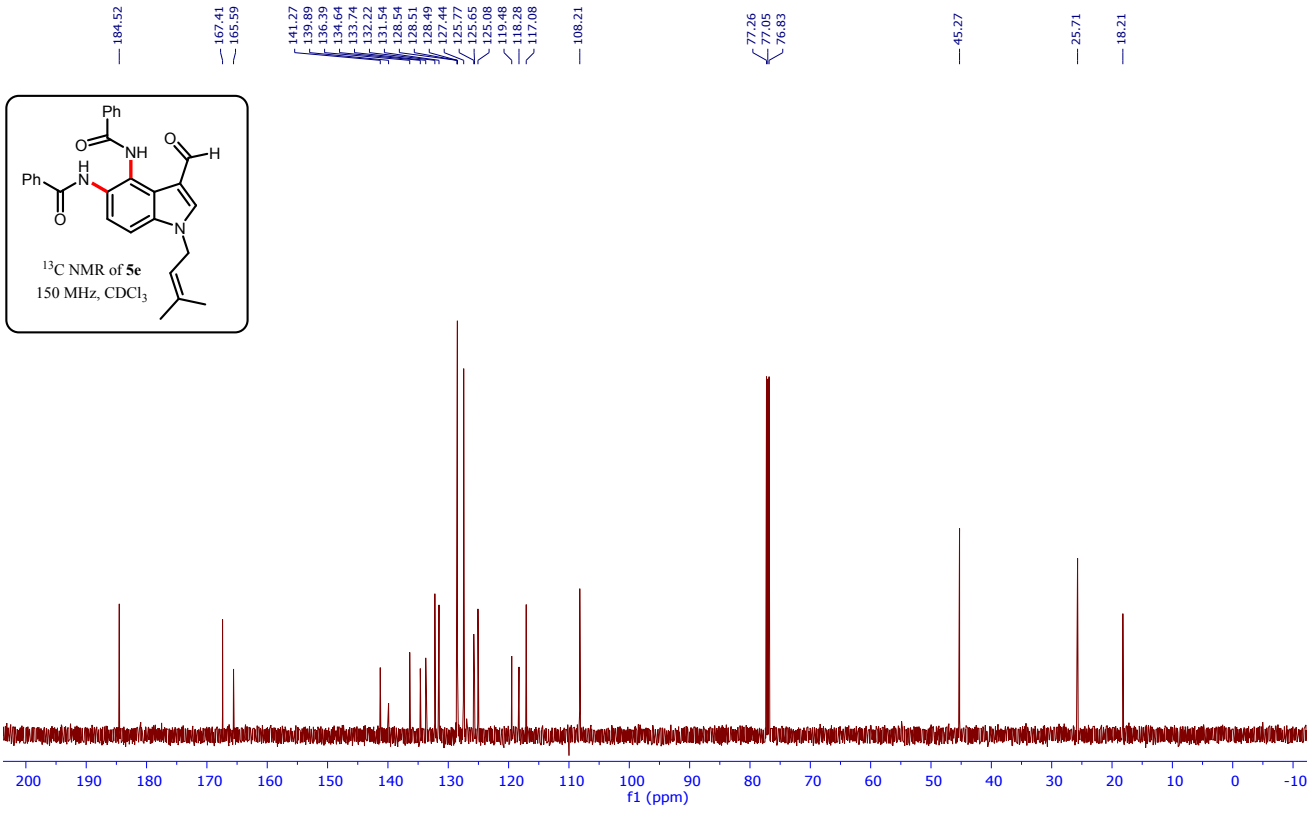

12.103
9.953
9.522
8.201
8.190
8.014
8.002
7.877
7.862
7.730
7.584
7.581
7.576
7.571
7.567
7.562
7.559
7.557
7.544
7.541
7.534
7.530
7.522
7.519
7.517
7.491
7.489
7.486
7.484
7.478
7.474
7.470
7.464
7.462
7.459
7.441
7.438
7.430
7.427
7.416
7.414
7.404
7.300
7.285
7.240
4.152
4.140
4.128
1.884
1.872
1.859
1.358
1.346
1.334
1.323
1.321
1.309
1.300
1.296
1.291
1.284
1.275
1.270
0.892
0.881
0.869
0.866

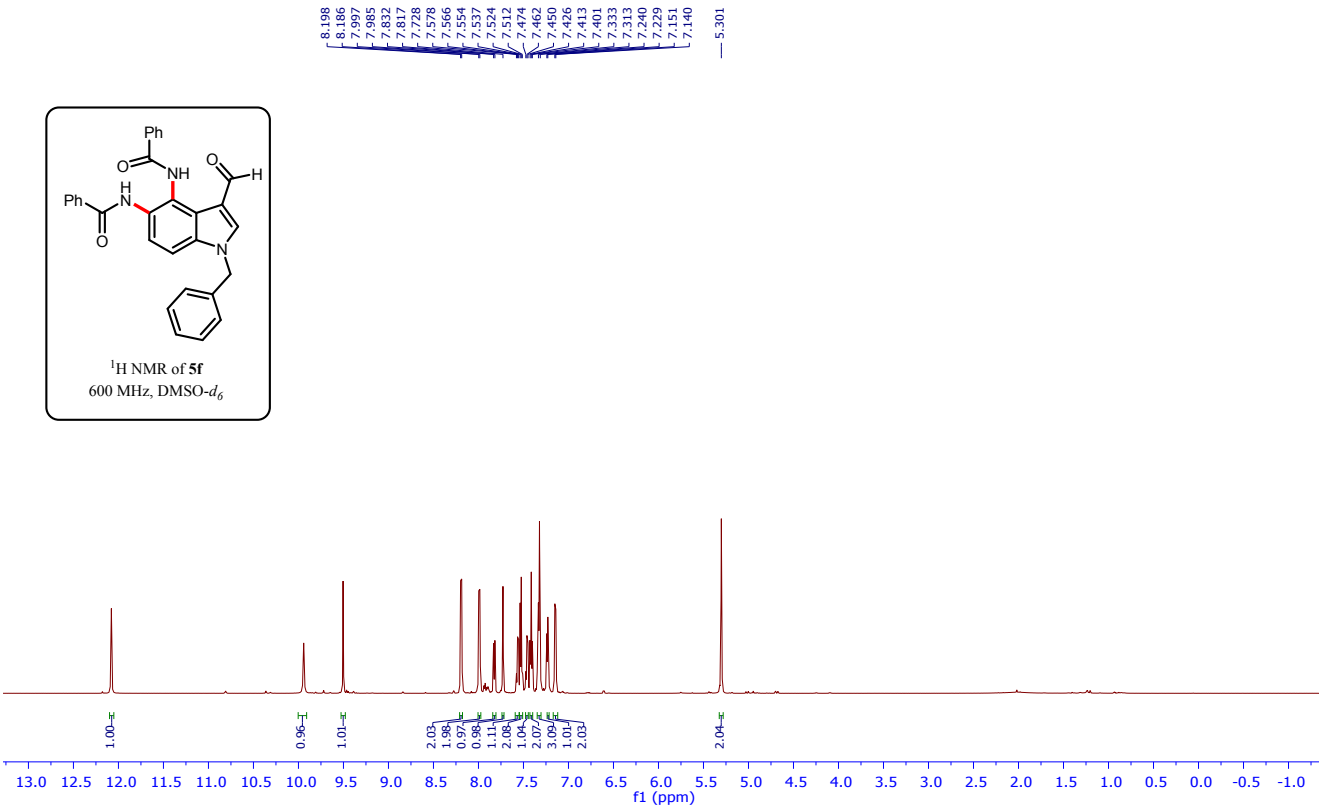

Ph
O
NH
O
H
Ph
H
N
O
N
^{1}H NMR of **5d**
600 HMz, CDCl$_3$


0.94
0.99
1.01
2.00
2.02
1.02
1.07
7.03
1.01
2.00
2.10
4.03
3.02
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

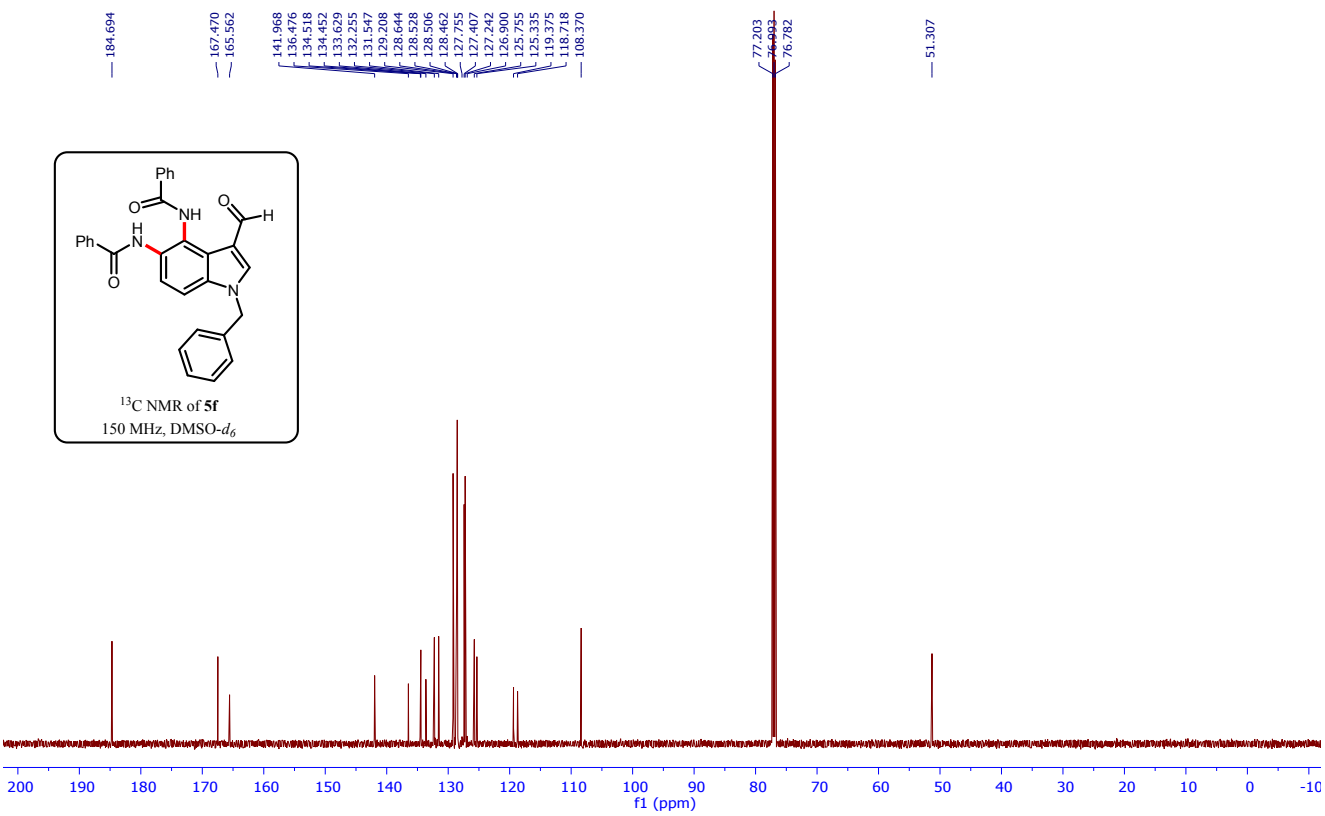

184.49
167.46
165.60
141.67
136.30
134.61
133.72
132.23
131.55
128.55
128.52
128.49
127.44
125.84
125.62
125.16
119.38
118.32
108.08
77.23
77.02
76.81
47.81
29.25
28.84
22.17
13.86
Ph
O
NH
O
H
Ph
H
N
O
N
^{13}C NMR of **5d**
150 MHz, CDCl$_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


12.120
9.972
9.497
8.206
8.194
8.016
8.004
7.858
7.844
7.740
7.579
7.567
7.558
7.555
7.540
7.531
7.528
7.516
7.484
7.471
7.459
7.438
7.425
7.413
7.278
7.264
7.240
5.374
5.362
5.351
4.689
4.677
1.796
Ph
O
NH
O
H
Ph
H
N
O
N
1H NMR of 5e
600 MHz, CDCl3
1.00
1.02
1.03
2.04
2.00
0.98
1.01
0.99
2.05
1.10
1.99
1.16
1.05
2.05
6.03
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

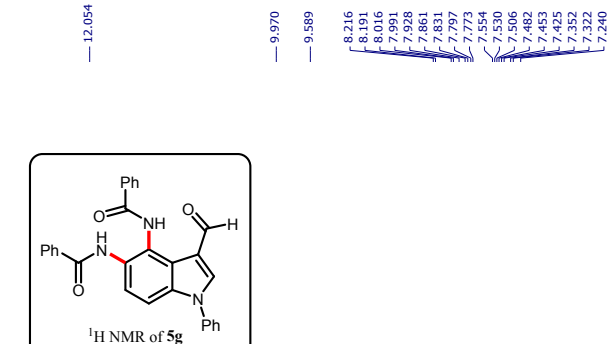

184.52
167.41
165.59
141.27
139.89
136.39
134.64
133.74
132.22
131.54
128.54
128.51
128.49
127.44
125.77
125.65
125.08
119.48
118.28
117.08
108.21
77.26
77.05
76.83
45.27
25.71
18.21
Ph
O
NH
O
H
Ph
H
N
O
N
13C NMR of 5e
150 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



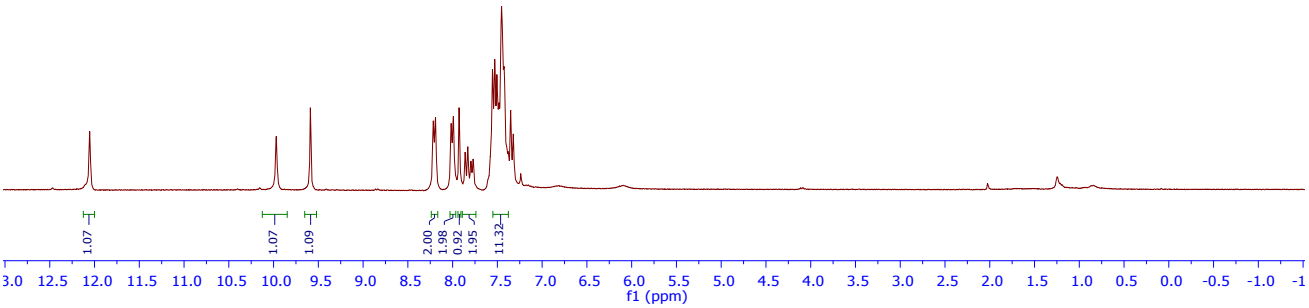
^{1}H NMR of **5f**
600 MHz, DMSO-d_6

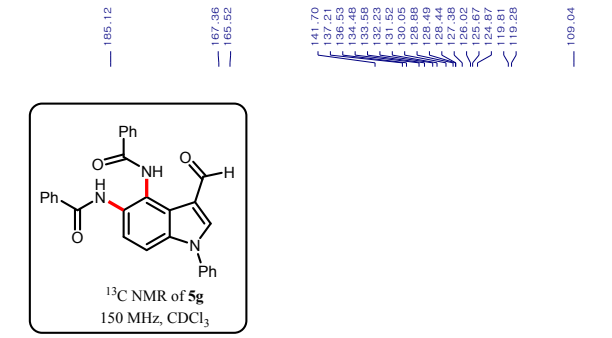


^{13}C NMR of **5f**
150 MHz, DMSO-d_6

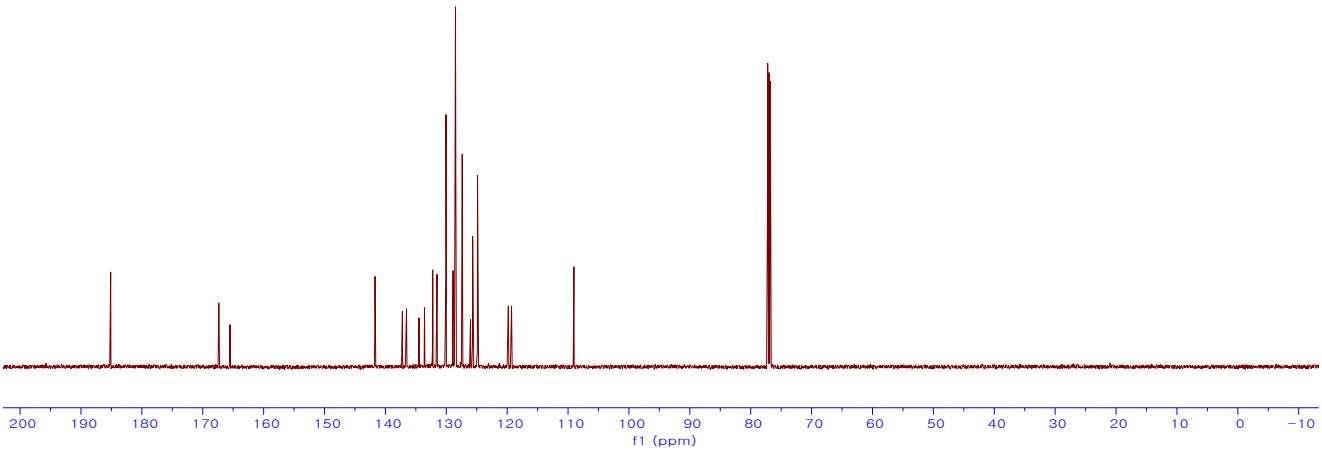


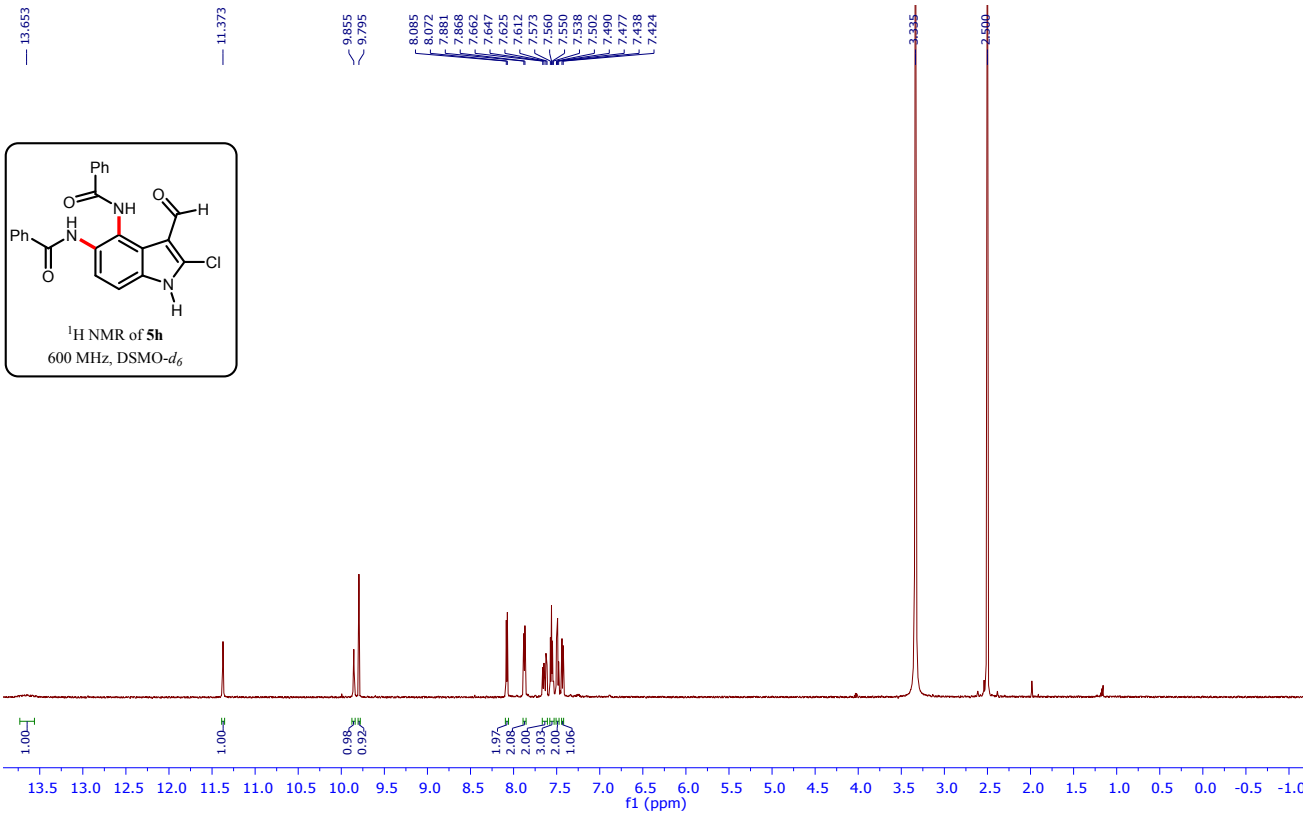
^{1}H NMR of **5g**
300 MHz, $CDCl_3$



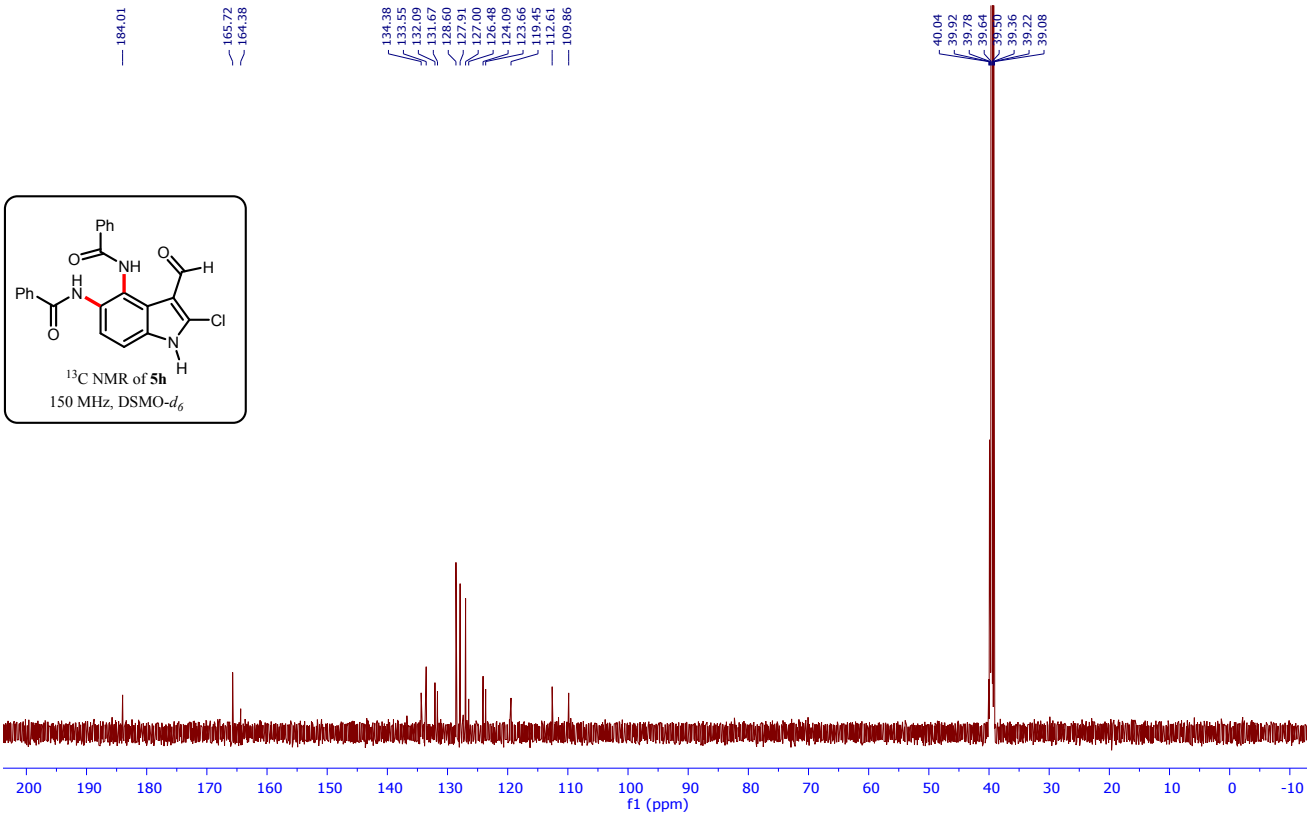


^{13}C NMR of **5g**
150 MHz, $CDCl_3$

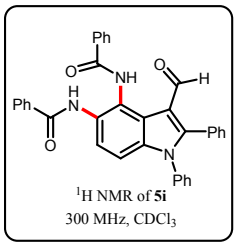




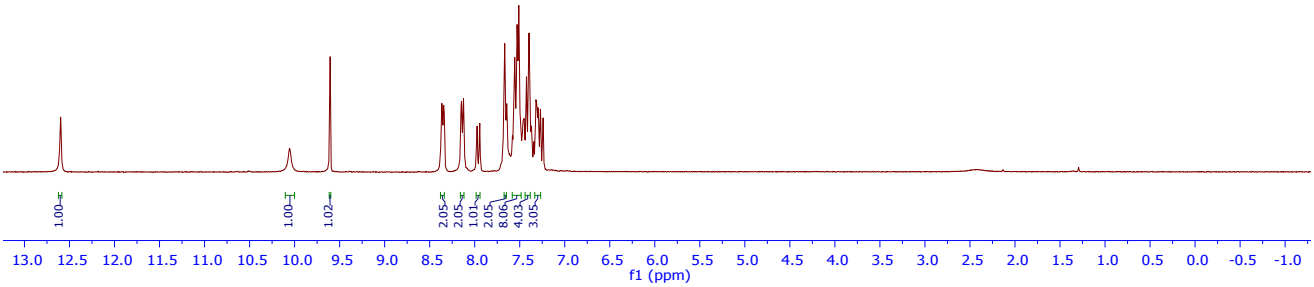
^{1}H NMR of **5h**
600 MHz, DSMO-d_6

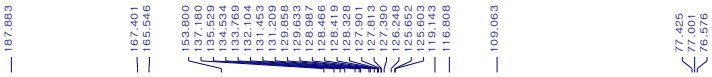


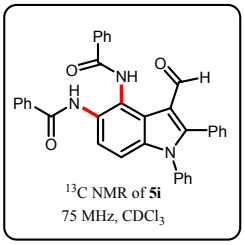
^{13}C NMR of **5h**
150 MHz, DSMO-d_6



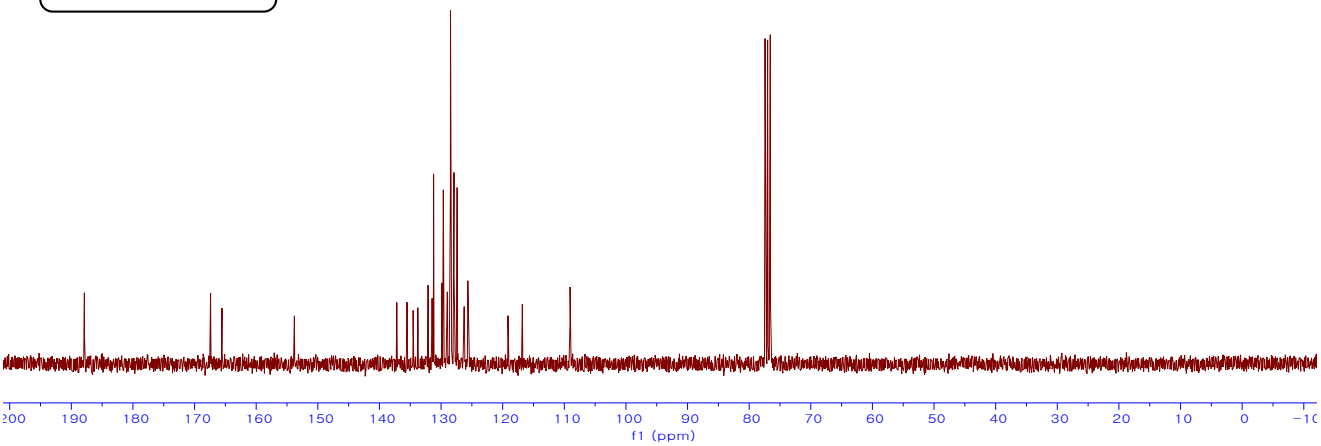
^{1}H NMR of **5i**
300 MHz, $CDCl_3$

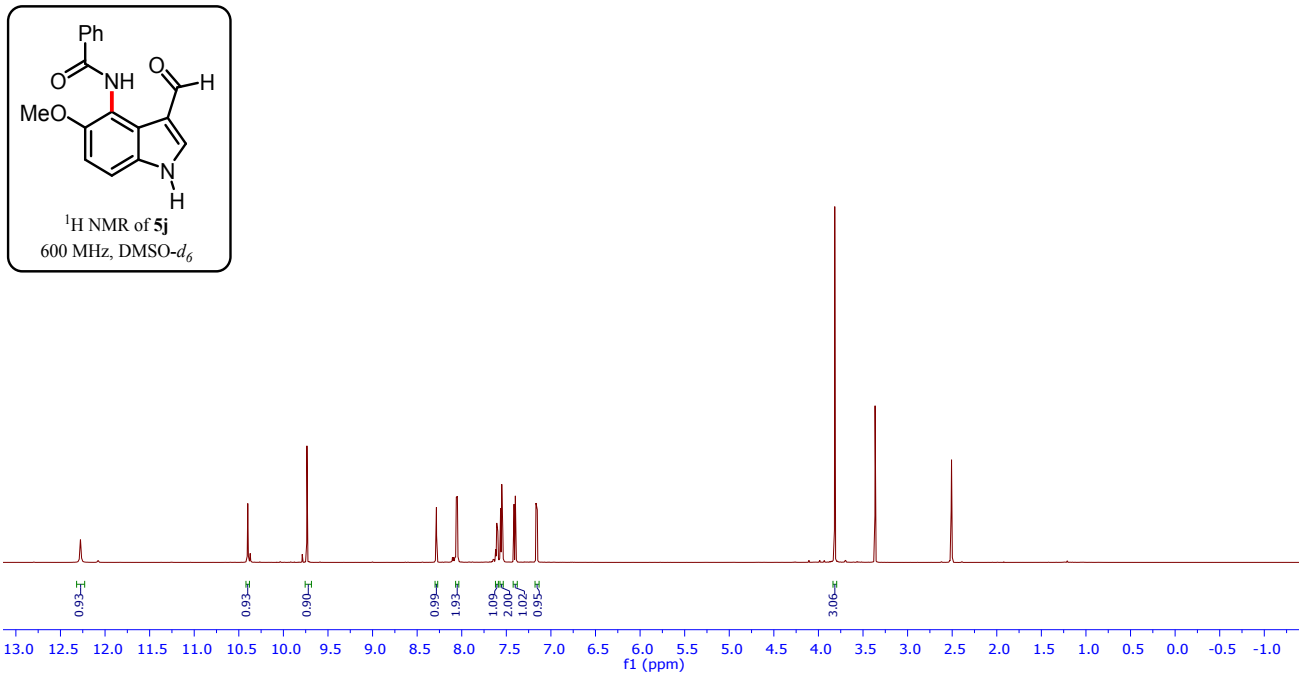




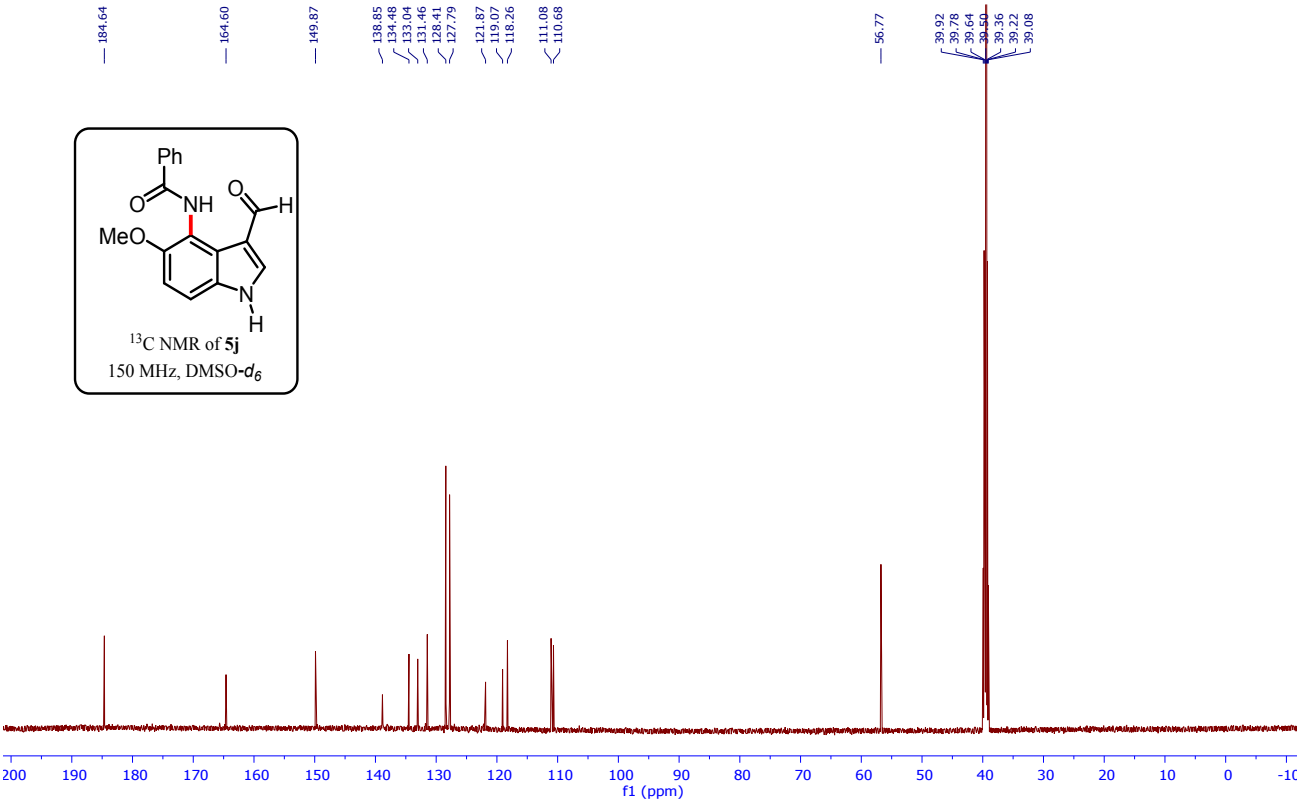


^{13}C NMR of **5i**
75 MHz, $CDCl_3$

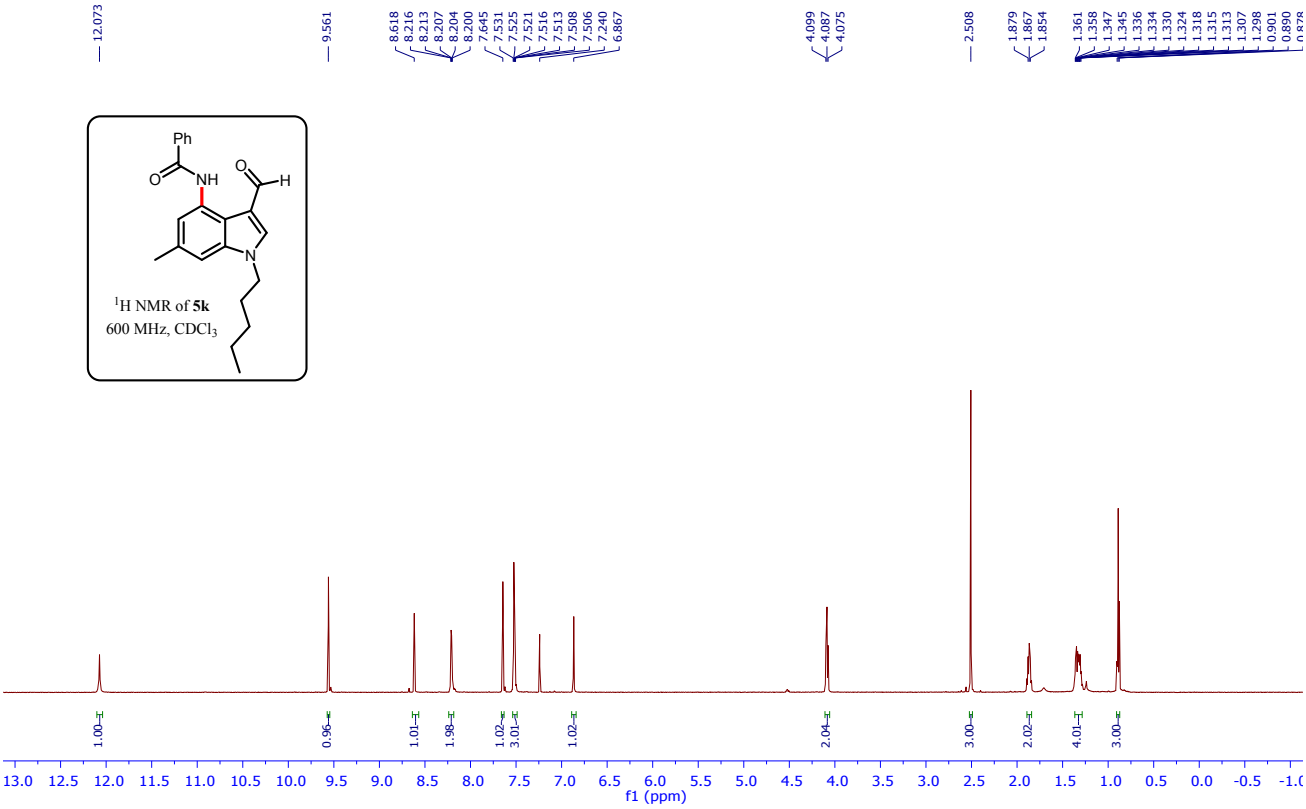


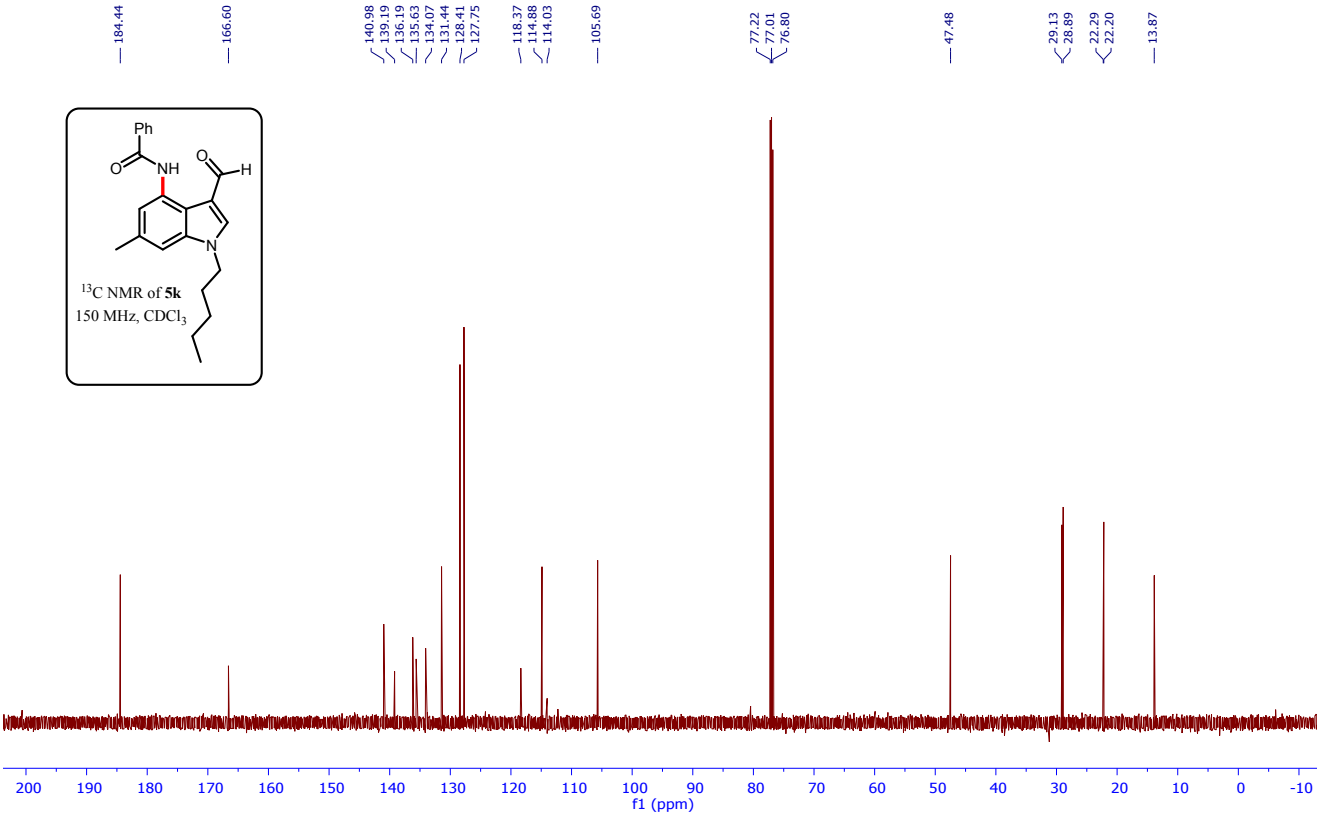


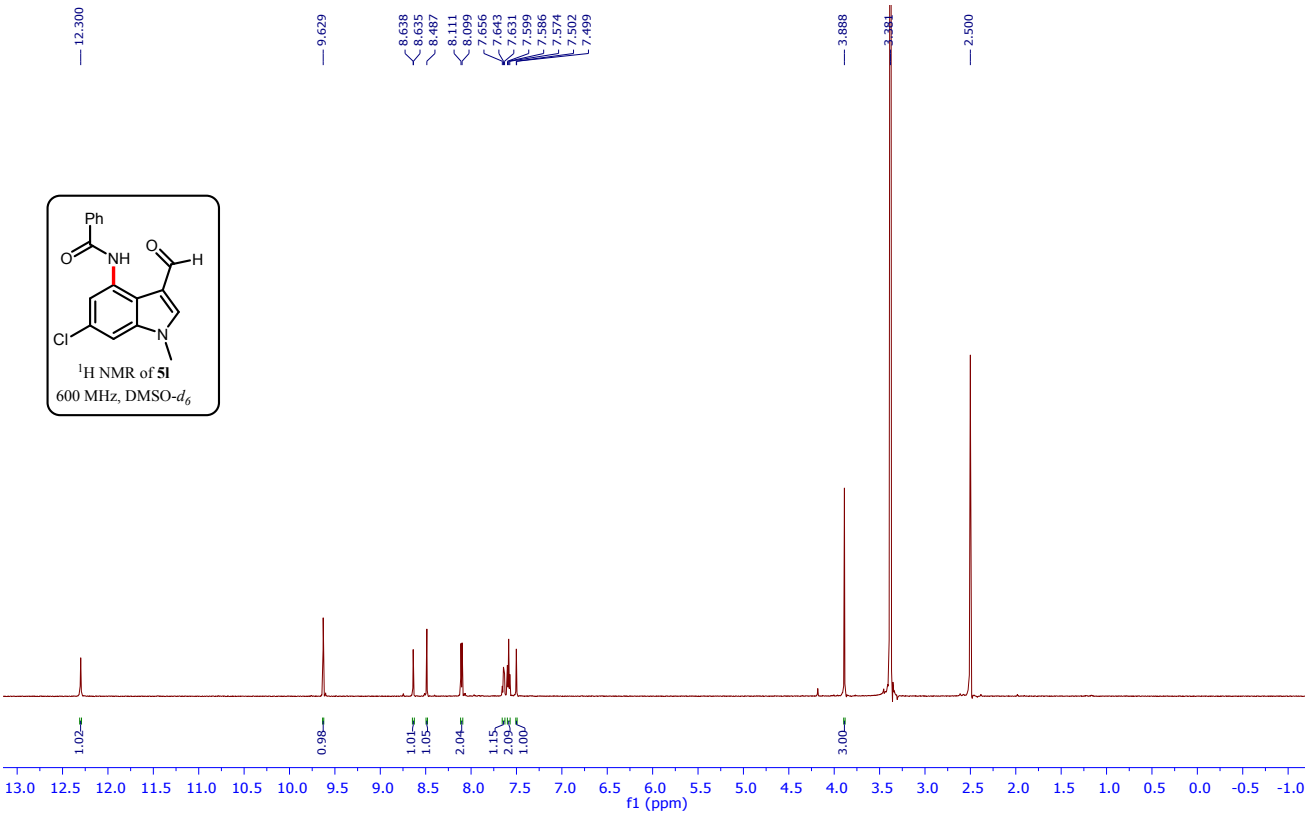
^{1}H NMR of **5j**
600 MHz, DMSO-d_6

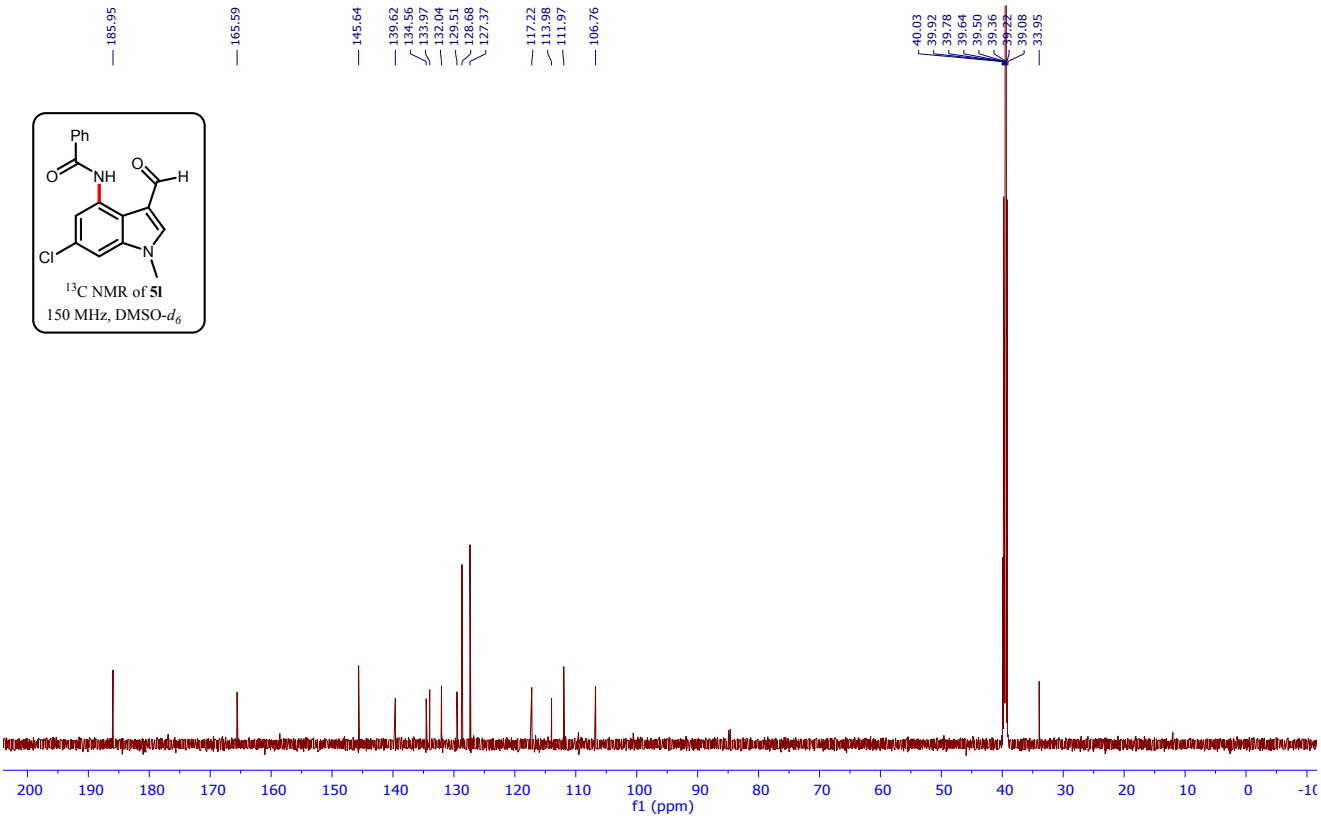


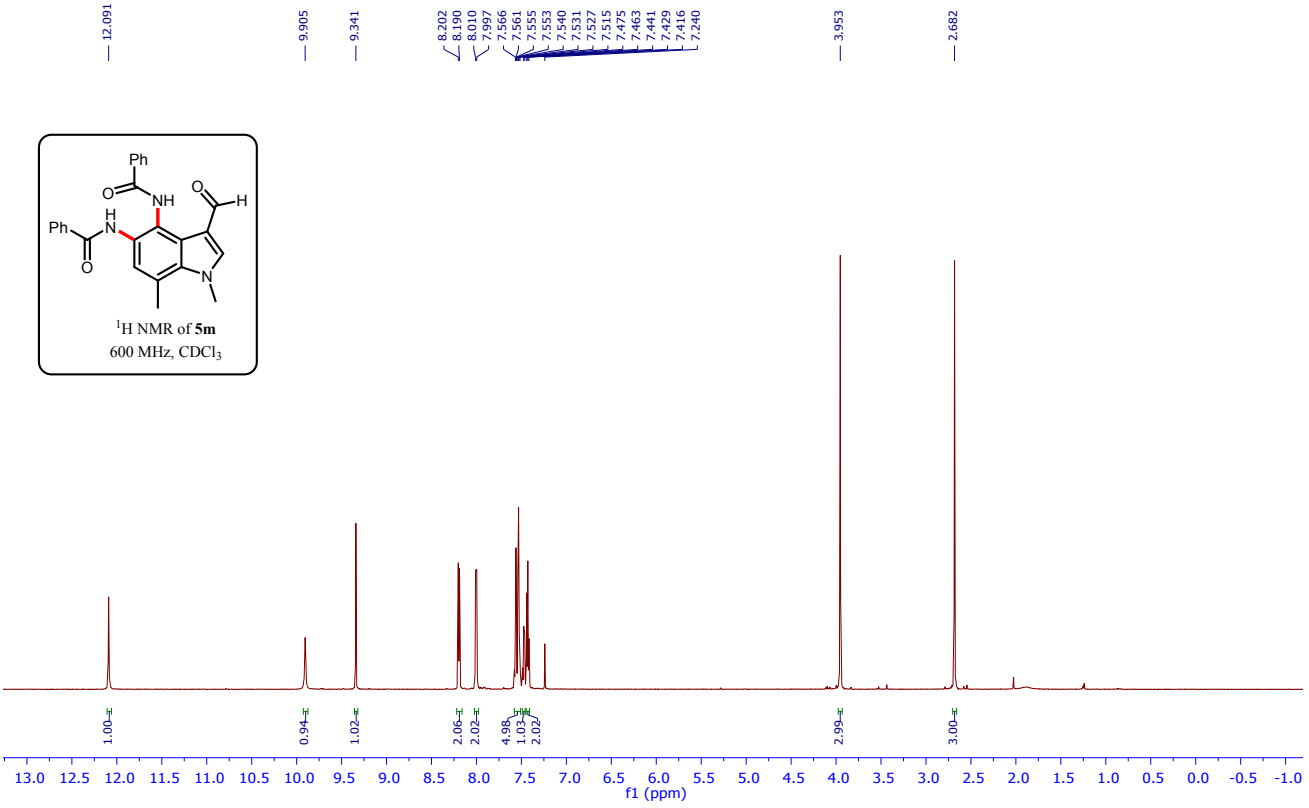
^{13}C NMR of **5j**
150 MHz, DMSO-d_6

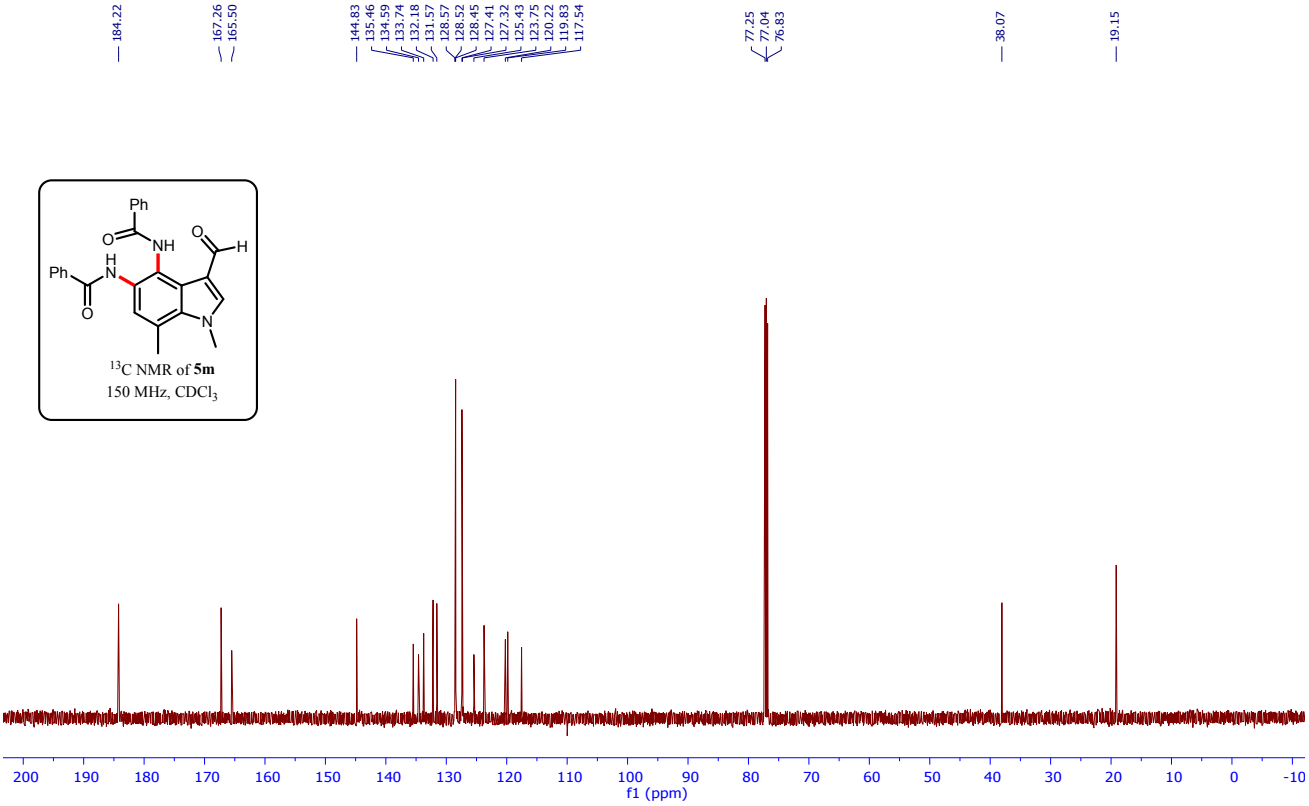

12.073
9.561
8.618
8.216
8.213
8.207
8.204
8.200
7.645
7.531
7.525
7.521
7.516
7.513
7.508
7.506
7.240
6.867
4.099
4.087
4.075
2.508
1.879
1.867
1.854
1.361
1.358
1.347
1.345
1.336
1.334
1.330
1.324
1.318
1.315
1.313
1.307
1.298
0.901
0.890
Ph
NH
O
H
N
^{1}H NMR of **5k**
600 MHz, $CDCl_3$
1.00
0.96
1.01
1.98
1.02
3.01
1.02
2.04
3.00
2.02
4.01
3.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

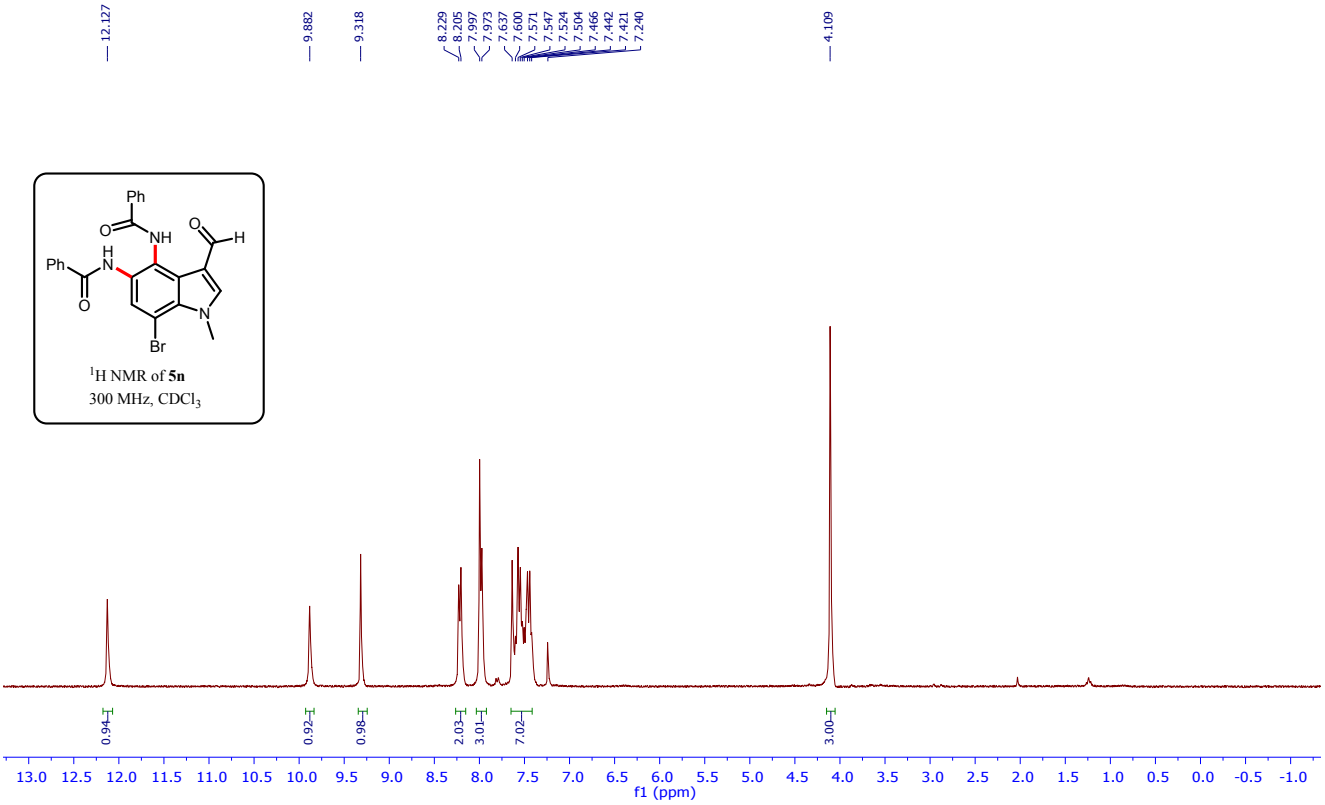

184.44
166.60
140.98
139.19
136.19
135.63
134.07
131.44
128.41
127.75
118.37
114.88
114.03
105.69
77.22
77.01
76.80
47.48
29.13
28.89
22.29
22.20
13.87
Ph
NH
O
H
N
^{13}C NMR of **5k**
150 MHz, $CDCl_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


12.300
9.629
8.638
8.635
8.487
8.111
8.099
7.656
7.643
7.631
7.599
7.586
7.574
7.502
7.499
3.888
3.381
2.500
Ph
O
NH
O
H
Cl
N
1H NMR of 5l
600 MHz, DMSO-d6
1.02
0.98
1.01
1.05
2.04
1.15
2.09
1.00
3.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

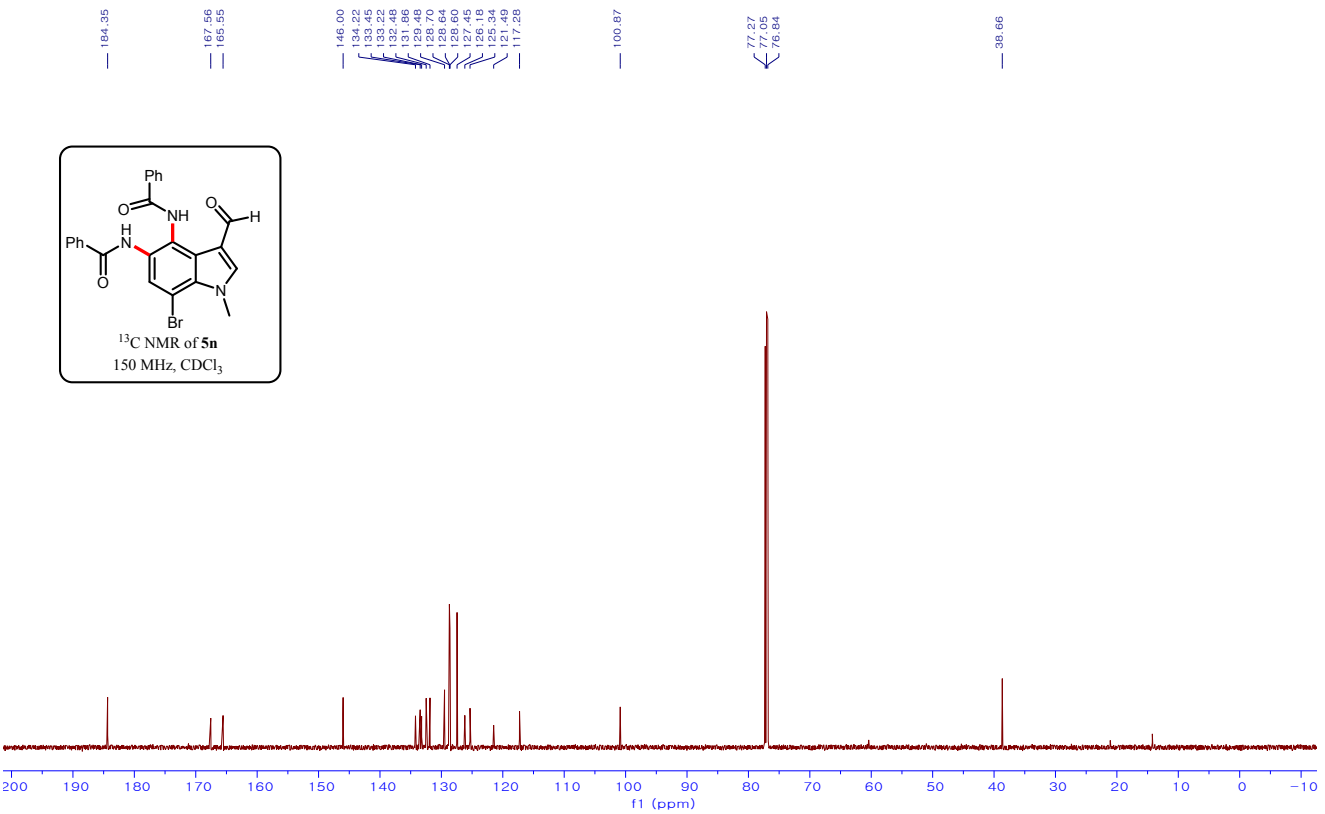

185.95
165.59
145.64
139.62
134.56
133.97
132.04
129.51
128.68
127.37
117.22
113.98
111.97
106.76
40.03
39.92
39.78
39.64
39.50
39.36
39.22
39.08
33.95
Ph
O
NH
O
H
Cl
N
13C NMR of 5l
150 MHz, DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


12.091
9.905
9.341
8.202
8.190
8.010
7.997
7.566
7.561
7.555
7.553
7.540
7.531
7.527
7.515
7.475
7.463
7.441
7.429
7.416
7.240
3.953
2.682
Ph
O
NH
O
H
Ph
H
N
O
N
1H NMR of 5m
600 MHz, CDCl3
1.00
0.94
1.02
2.06
2.02
4.98
1.03
2.02
2.99
3.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

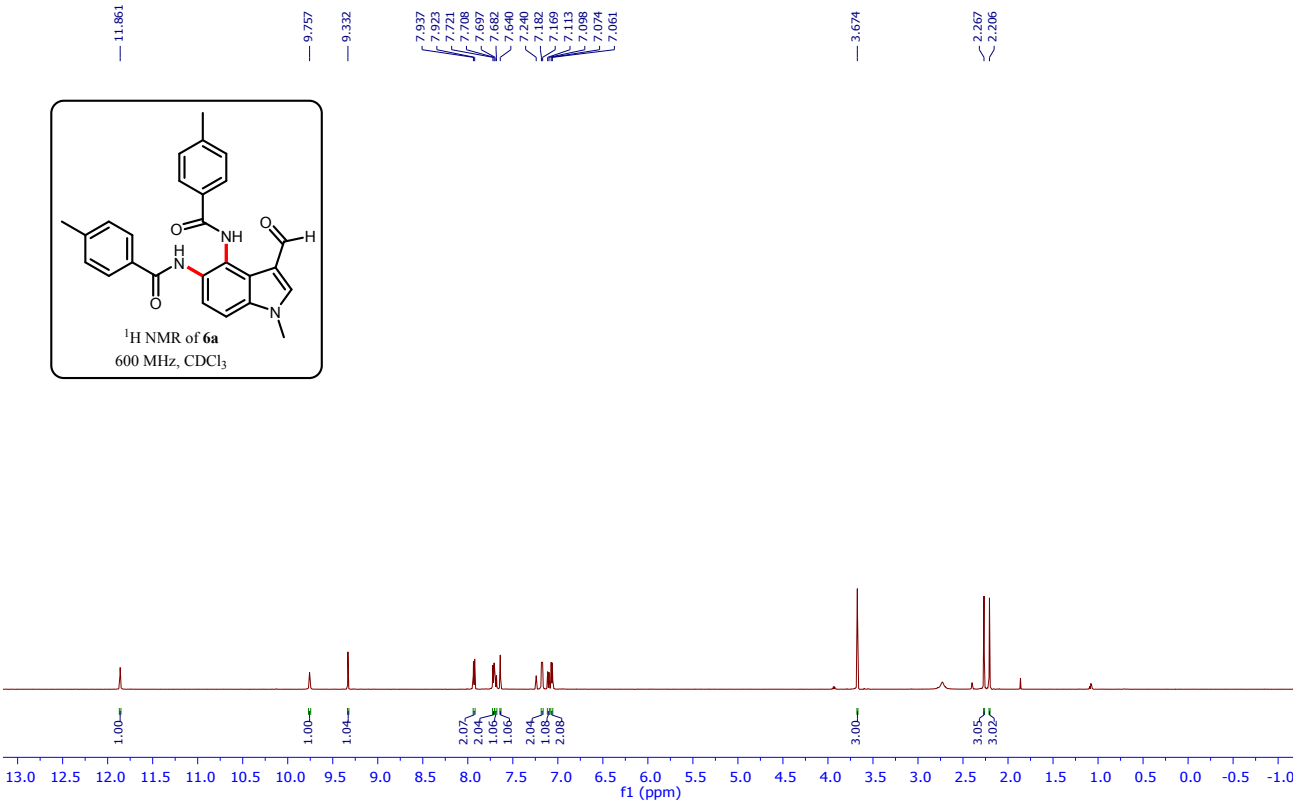

184.22
167.26
165.50
144.83
135.46
134.59
133.74
132.18
131.57
128.57
128.52
128.45
127.41
127.32
125.43
123.75
120.22
119.83
117.54
77.25
77.04
76.83
38.07
19.15
Ph
O
NH
O
H
Ph
H
N
O
N
13C NMR of 5m
150 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



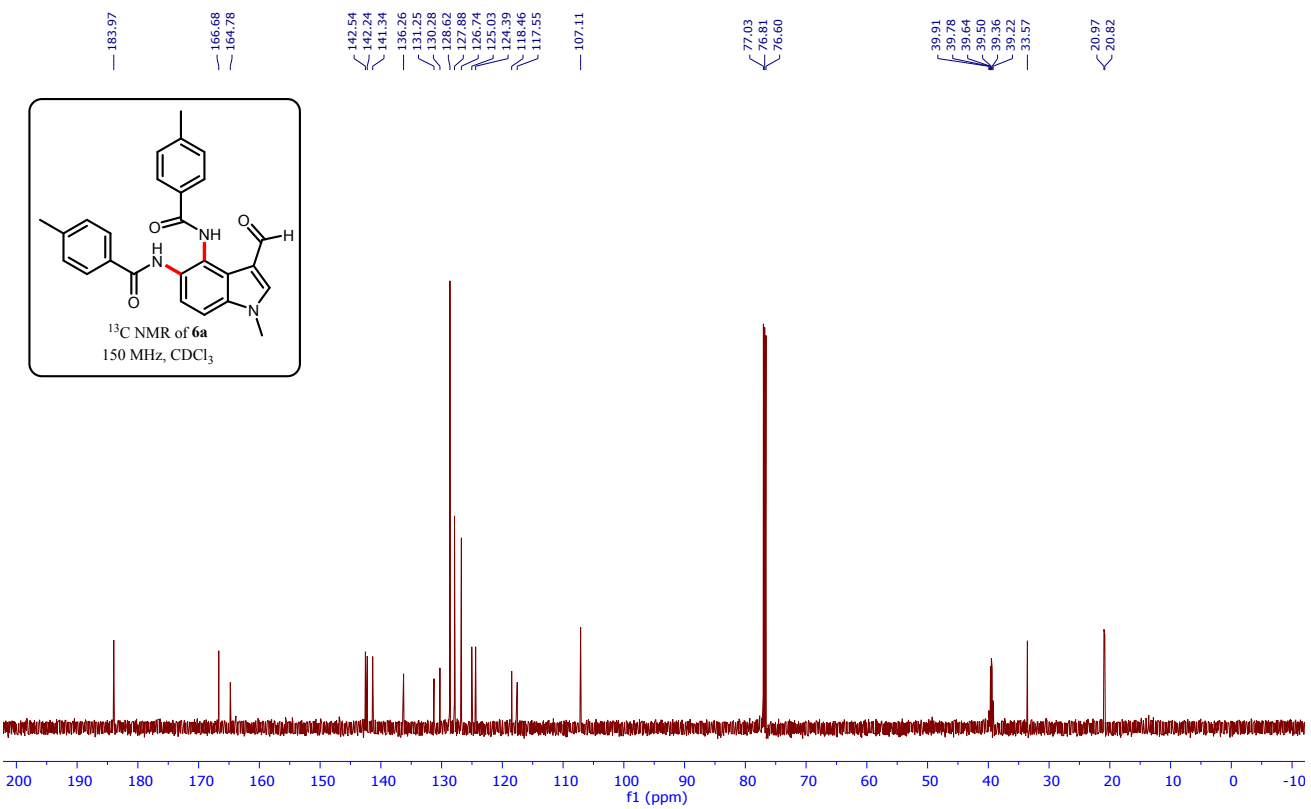
^{1}H NMR of **5n**
300 MHz, $CDCl_3$



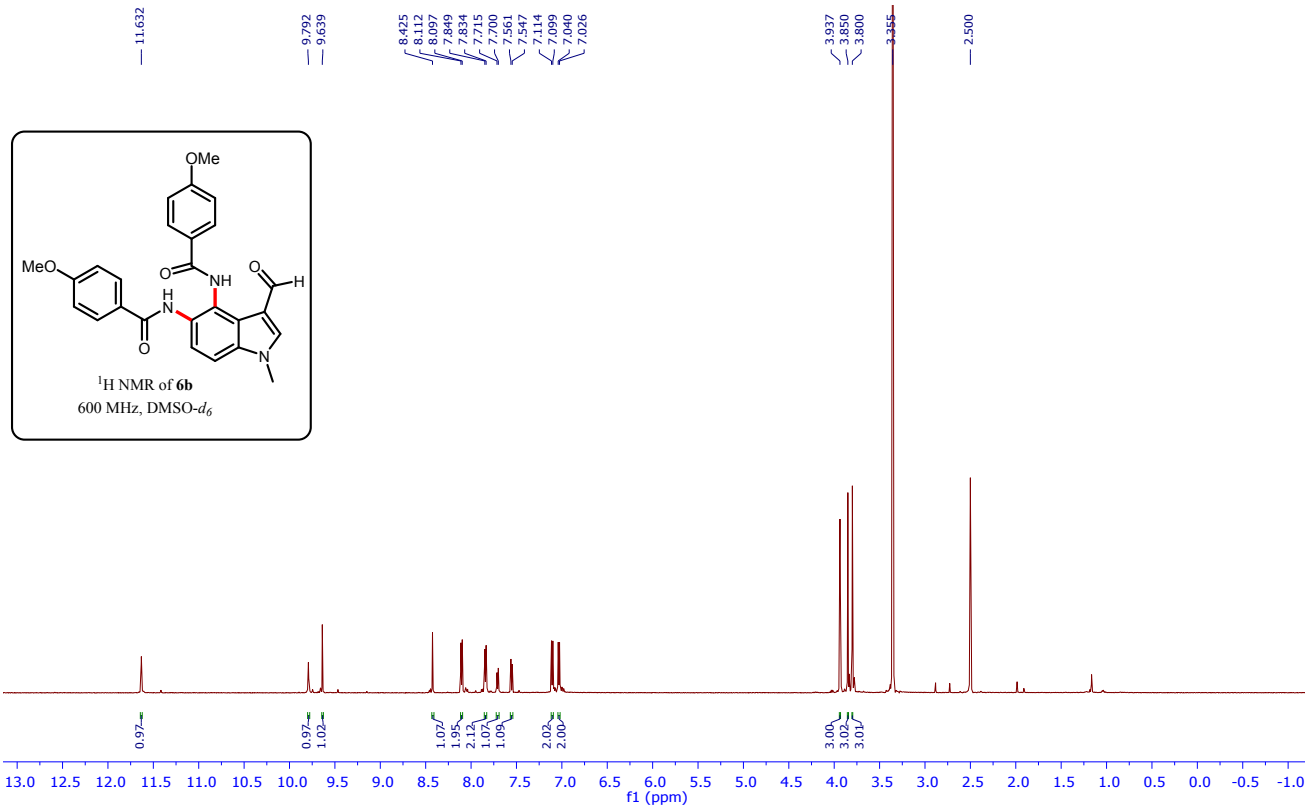
^{13}C NMR of **5n**
150 MHz, $CDCl_3$

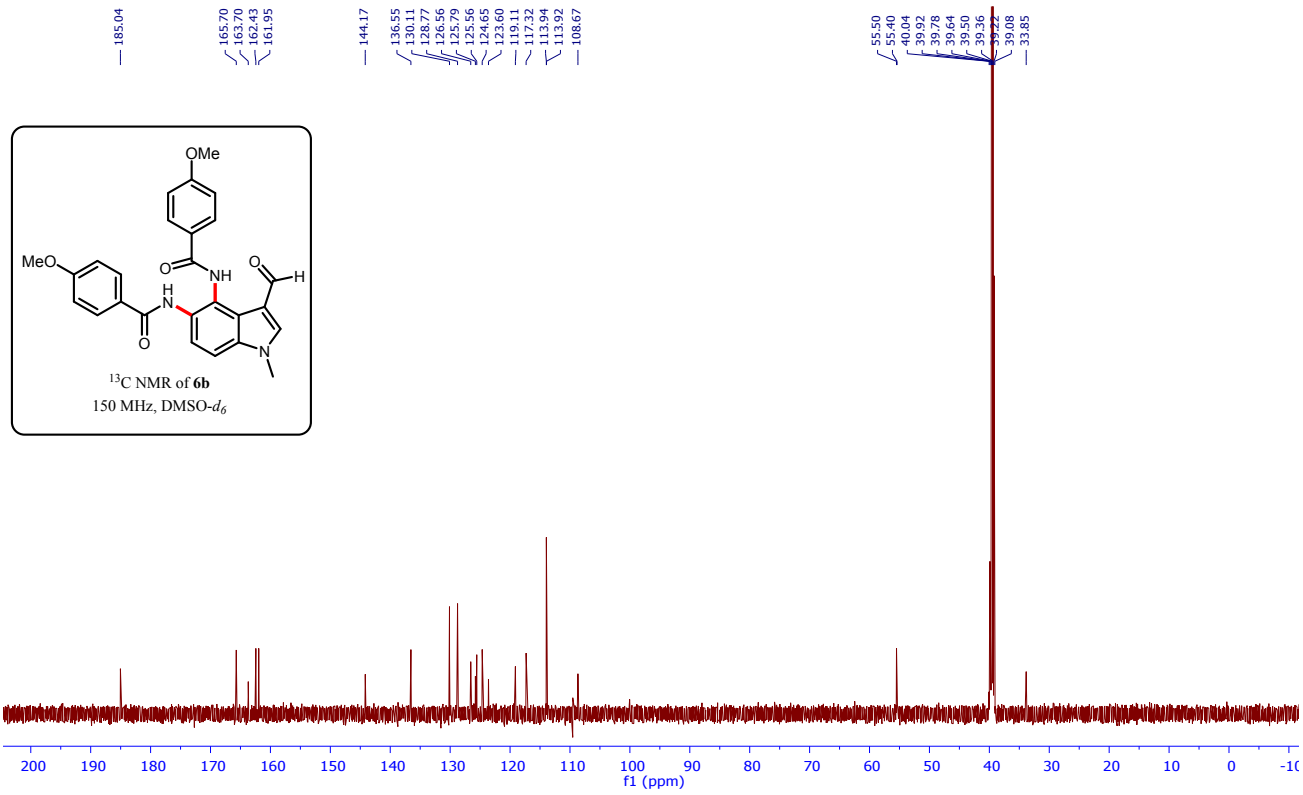


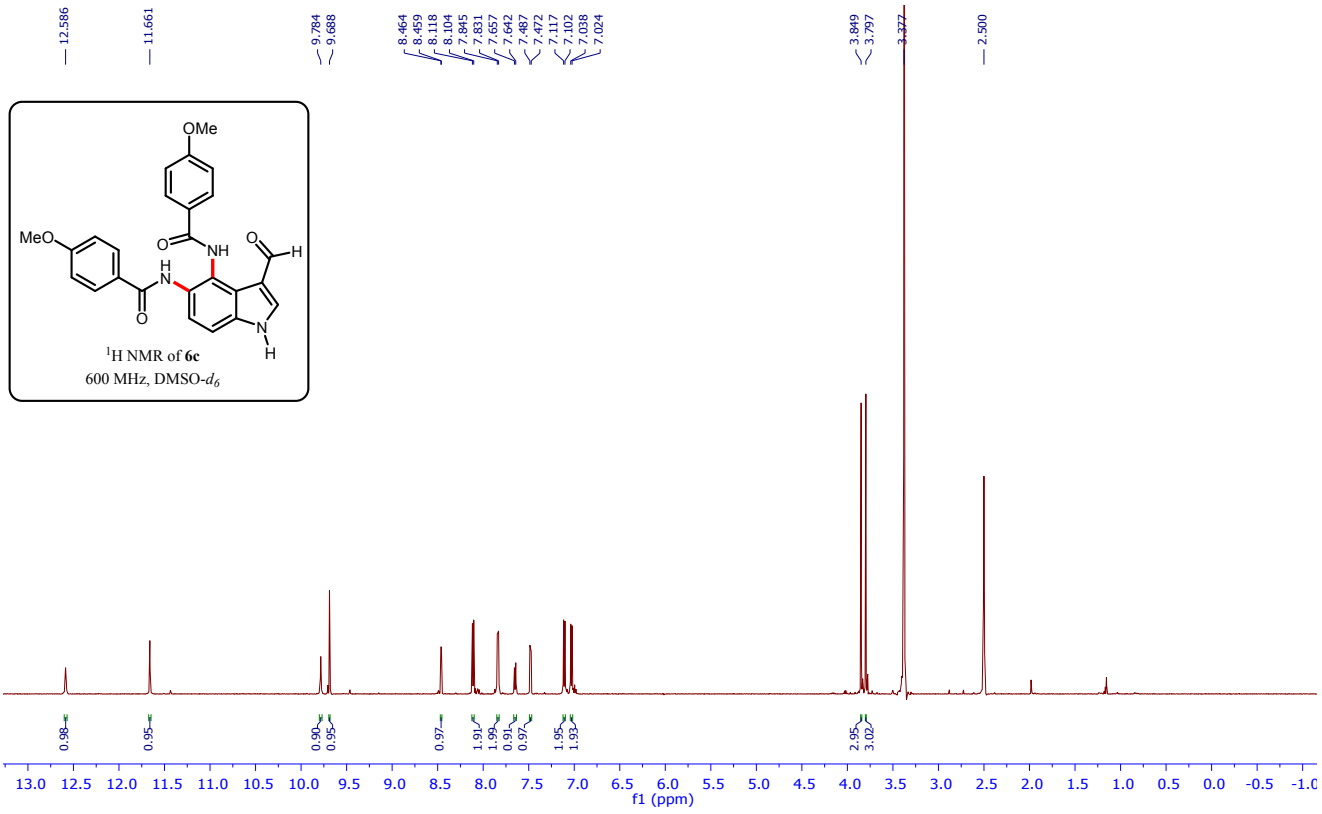
^{1}H NMR of **6a**
600 MHz, $CDCl_3$



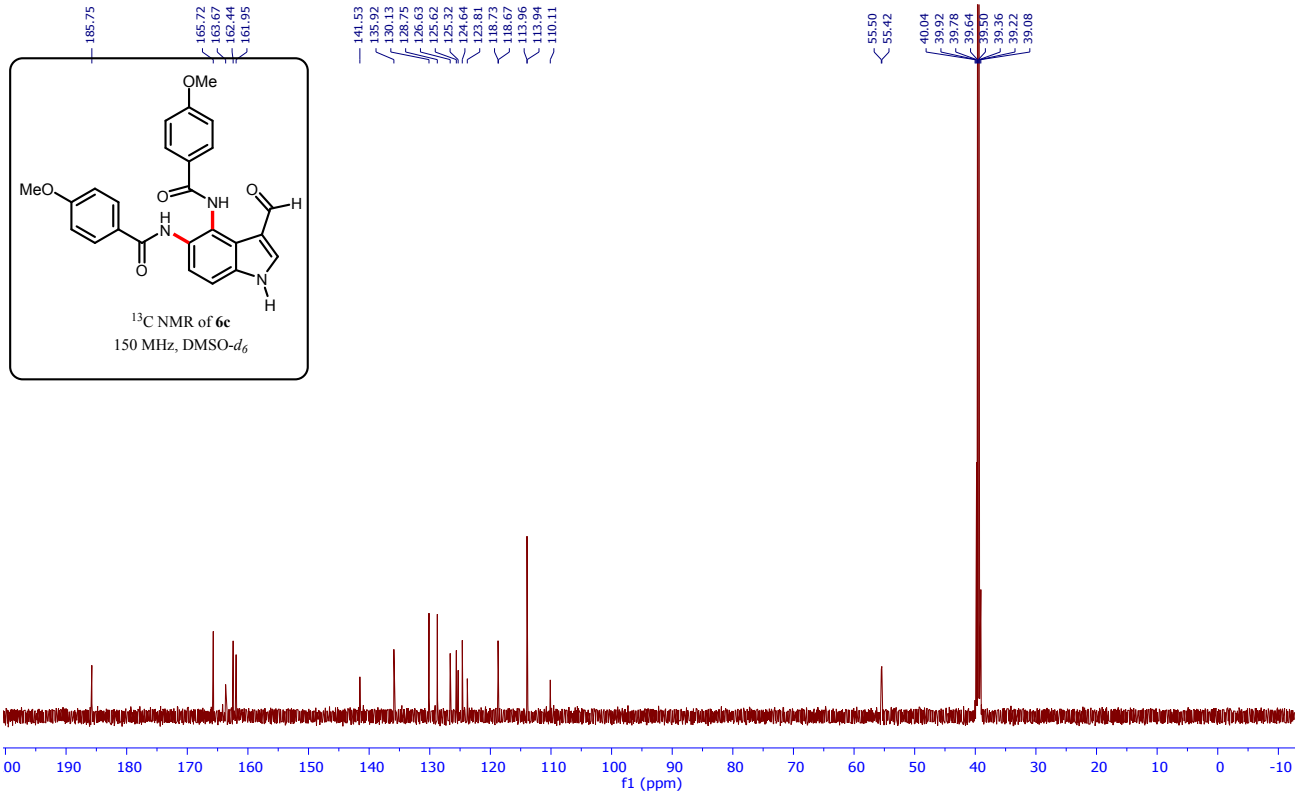
^{13}C NMR of **6a**
150 MHz, $CDCl_3$


11.632
9.792
9.639
8.425
8.112
8.097
7.849
7.834
7.715
7.700
7.561
7.547
7.114
7.099
7.040
7.026
3.937
3.850
3.800
3.355
2.500
OMe
MeO
O
NH
H
N
O
O
H
N
^{1}H NMR of **6b**
600 MHz, DMSO-d_6
0.97
0.97
1.02
1.07
1.95
2.12
1.07
1.09
2.02
2.00
3.00
3.02
3.01
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

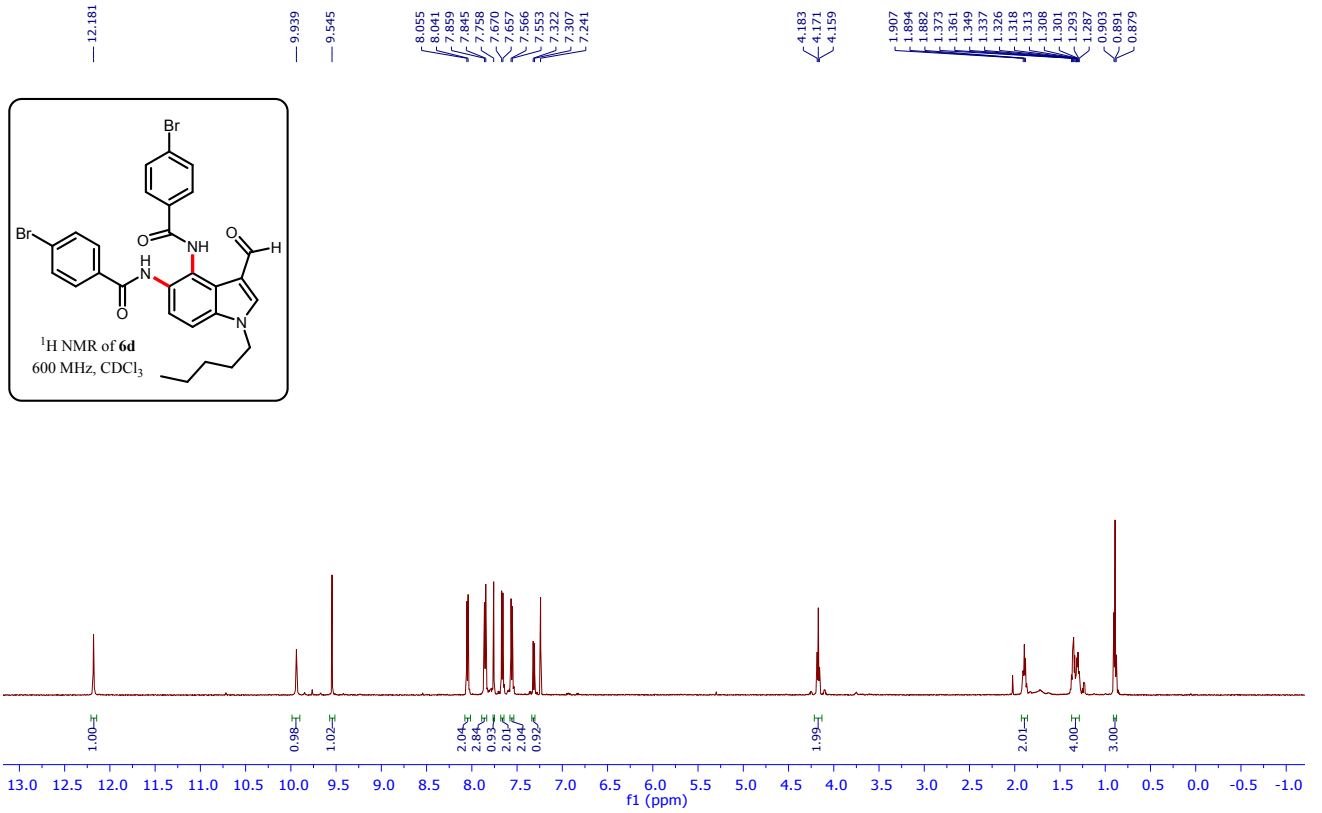

185.04
165.70
163.70
162.43
161.95
144.17
136.55
130.11
128.77
126.56
125.79
125.56
124.65
123.60
119.11
117.32
113.94
113.92
108.67
55.50
55.40
40.04
39.92
39.78
39.64
39.50
39.36
39.22
39.08
33.85
OMe
MeO
O
NH
H
N
O
O
H
N
^{13}C NMR of **6b**
150 MHz, DMSO-d_6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

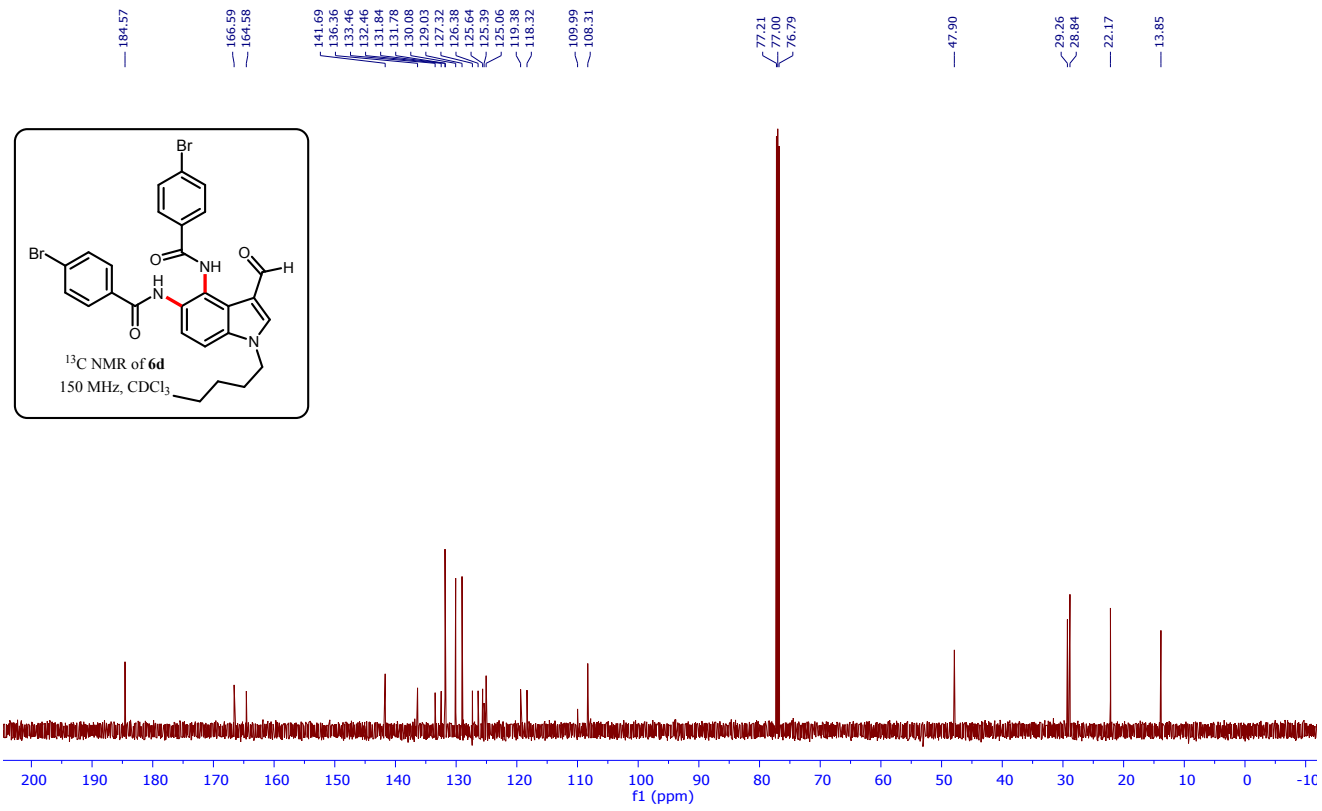


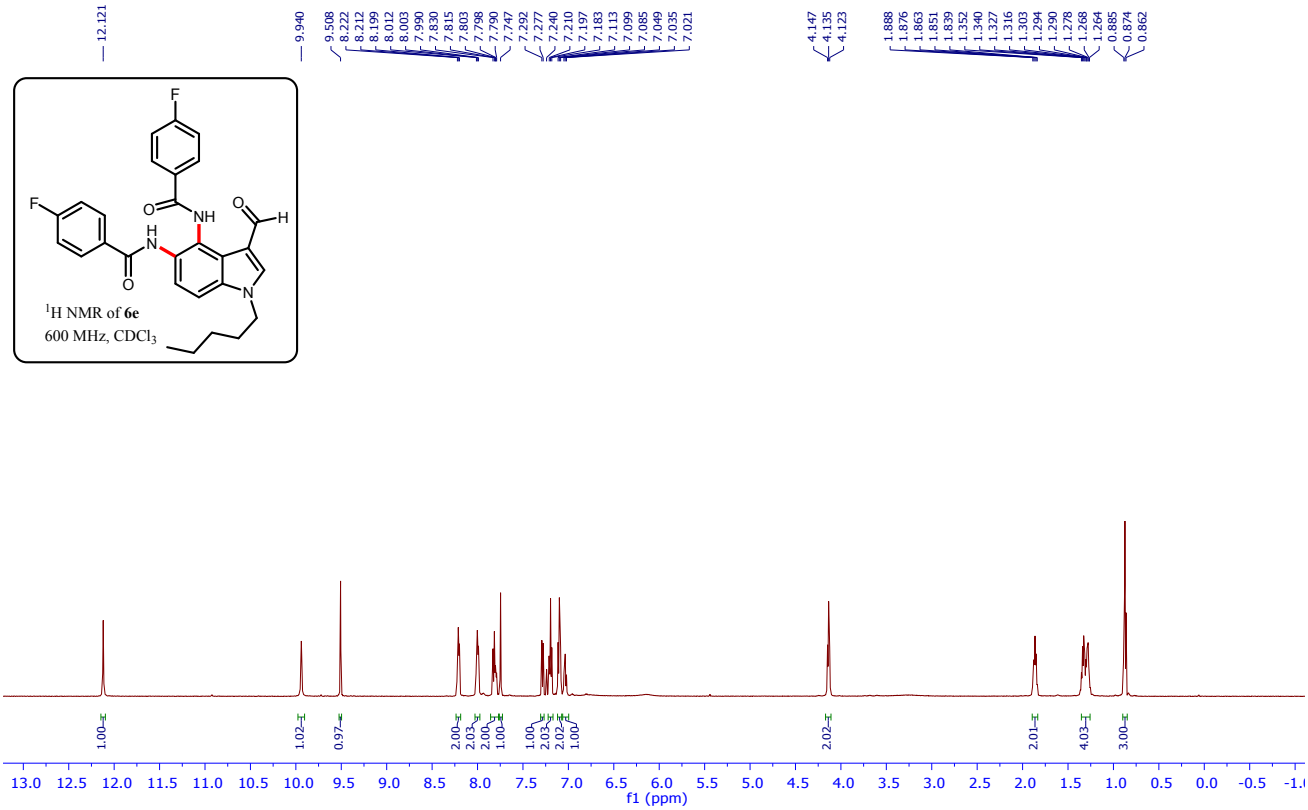
^{1}H NMR of **6c**
600 MHz, DMSO-d_6

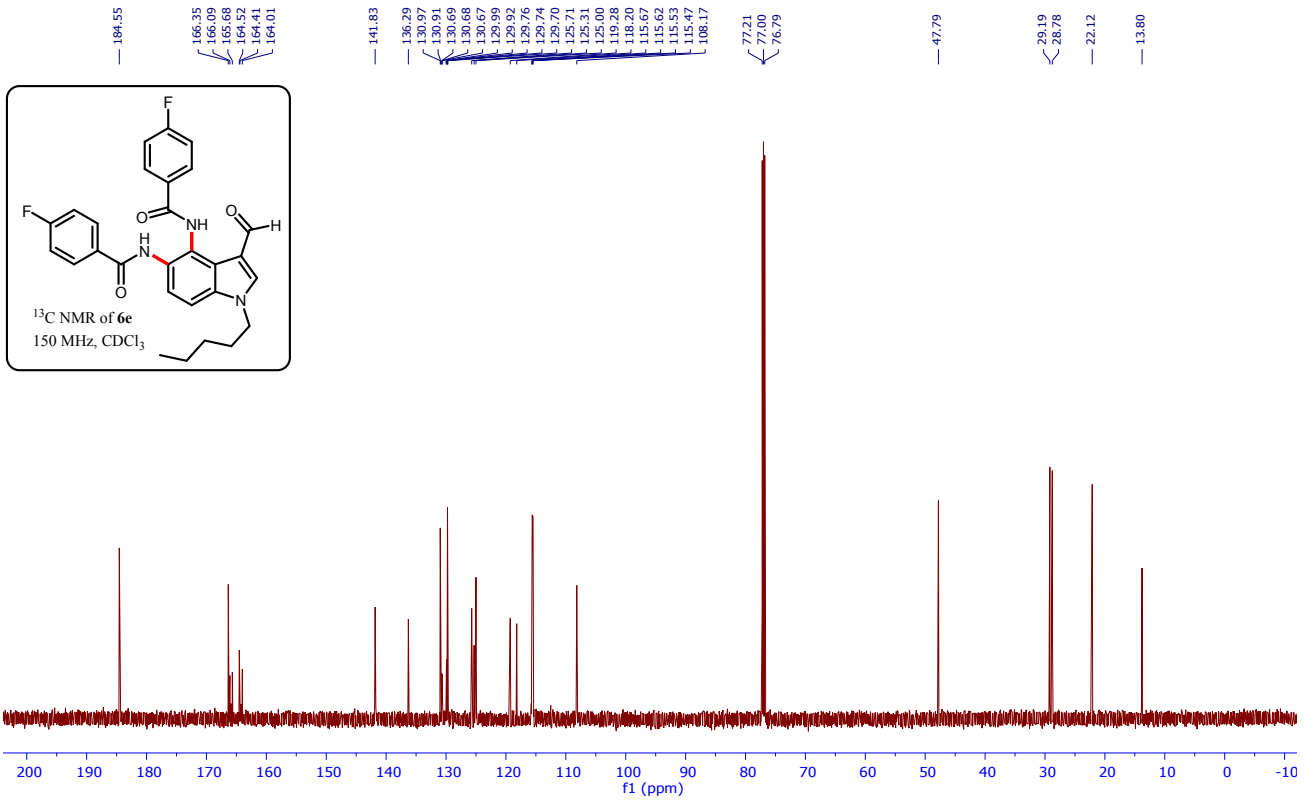


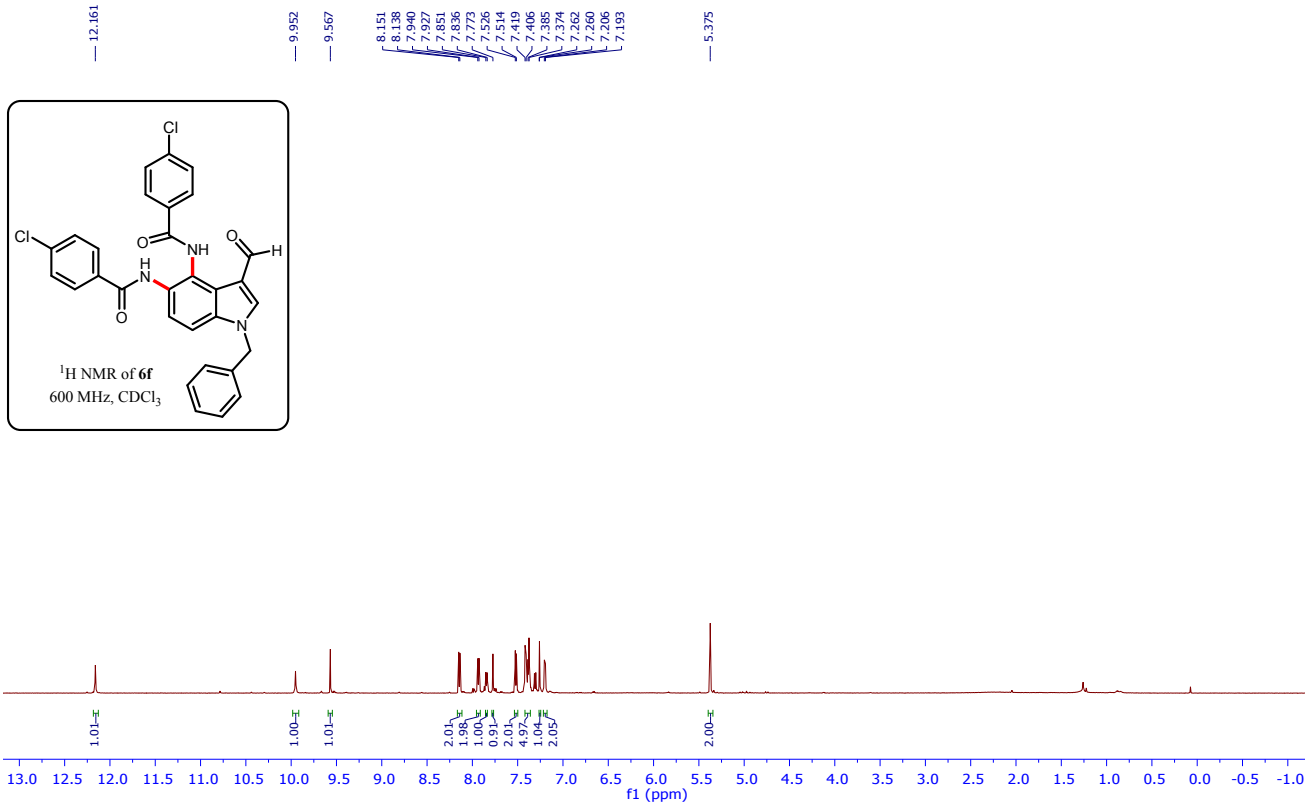
^{13}C NMR of **6c**
150 MHz, DMSO-d_6

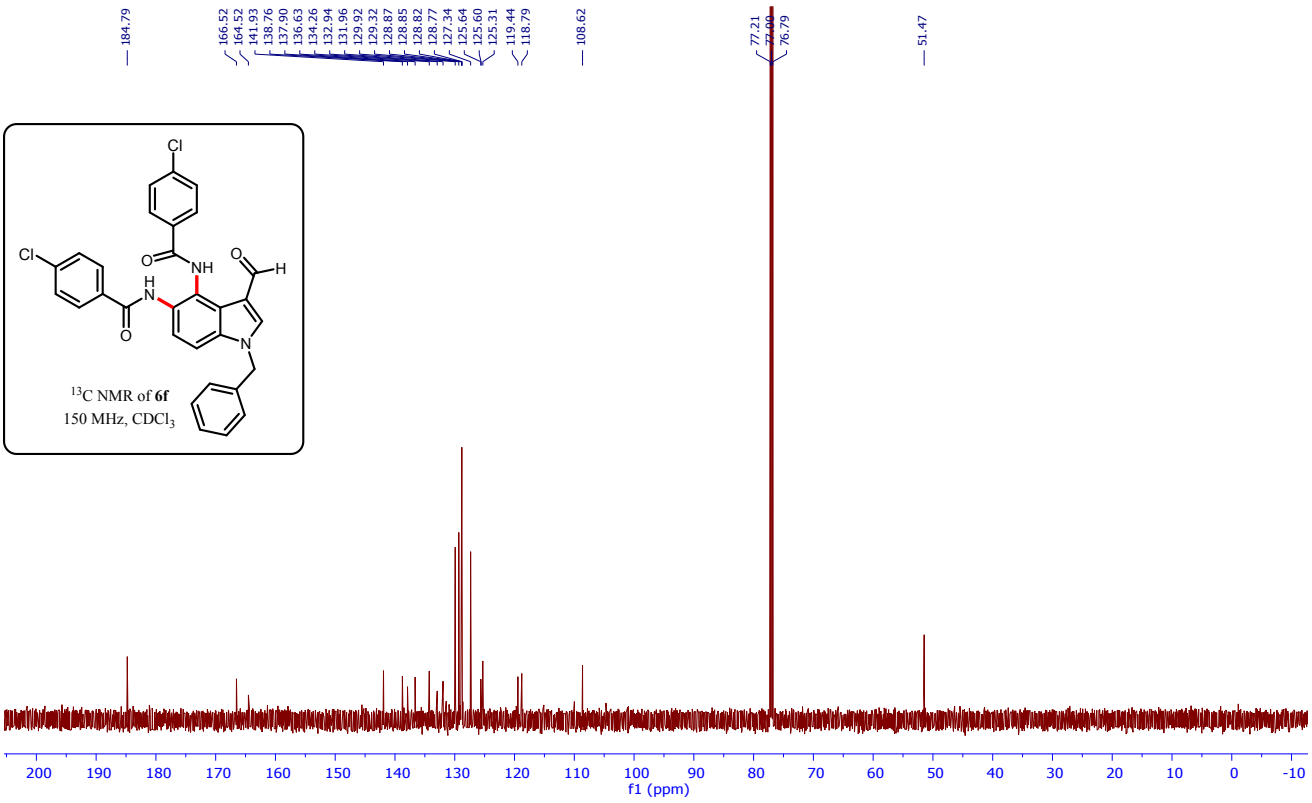

12.181
9.939
9.545
8.055
8.041
7.859
7.845
7.758
7.670
7.657
7.566
7.553
7.322
7.307
7.241
4.183
4.171
4.159
1.907
1.894
1.882
1.373
1.361
1.349
1.337
1.326
1.318
1.313
1.308
1.301
1.293
1.287
0.903
0.891
0.879
Br
Br
O
NH
O
H
H
N
O
N
1H NMR of 6d
600 MHz, CDCl3
1.00
0.98
1.02
2.04
2.84
0.93
2.01
2.04
0.92
1.99
2.01
4.00
3.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

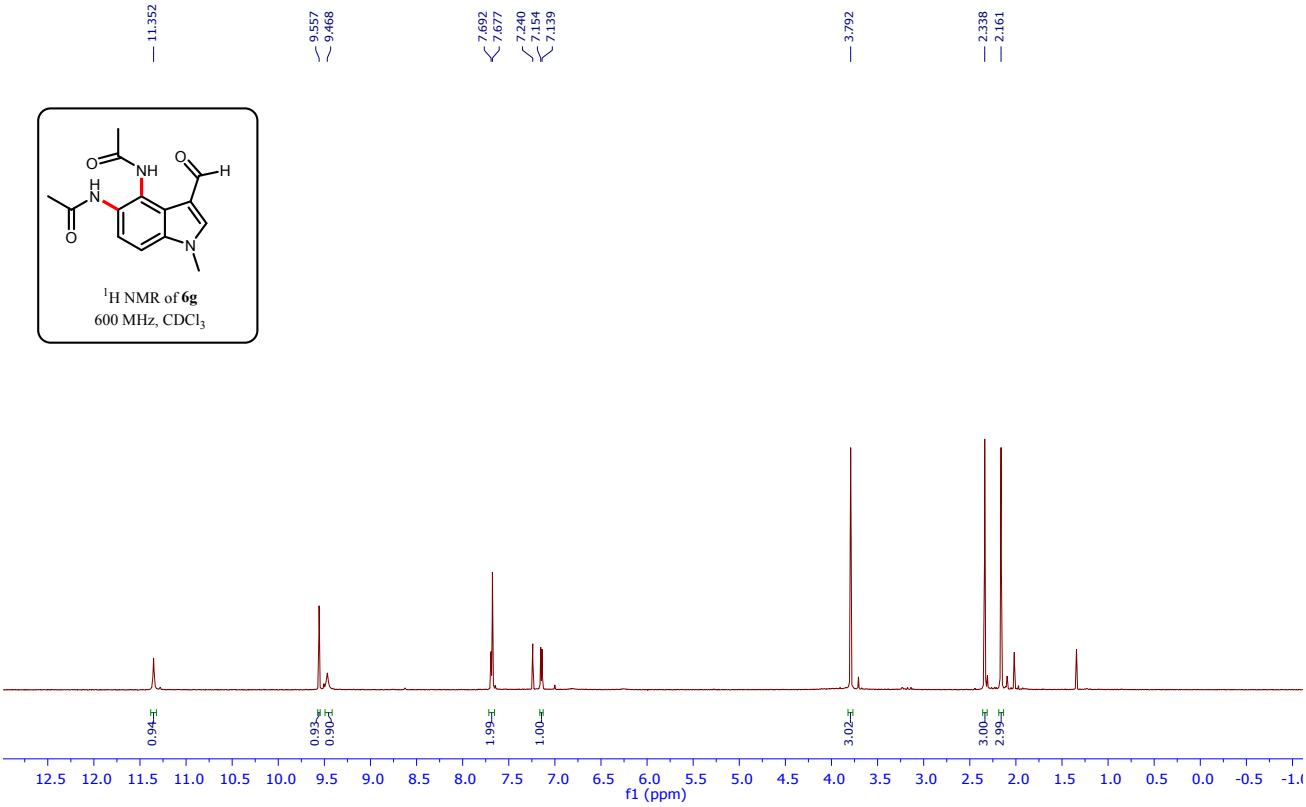

184.57
166.59
164.58
141.69
136.36
133.46
132.46
131.84
131.78
130.08
129.03
127.32
126.38
125.64
125.39
125.06
119.38
118.32
109.99
108.31
77.21
77.00
76.79
47.90
29.26
28.84
22.17
13.85
Br
Br
O
NH
O
H
H
N
O
N
13C NMR of 6d
150 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


12.121
9.940
9.508
8.222
8.212
8.199
8.012
8.003
7.990
7.830
7.815
7.803
7.798
7.790
7.747
7.292
7.277
7.240
7.210
7.197
7.183
7.113
7.099
7.085
7.049
7.035
7.021
4.147
4.135
4.123
1.888
1.876
1.863
1.851
1.839
1.352
1.340
1.327
1.316
1.303
1.294
1.290
1.278
1.268
1.264
0.885
0.874
0.862
F
F
O
NH
O
H
H
N
O
N
1H NMR of 6e
600 MHz, CDCl3
1.00
1.02
0.97
2.00
2.03
2.00
1.00
1.00
2.03
2.02
1.00
2.02
2.01
4.03
3.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

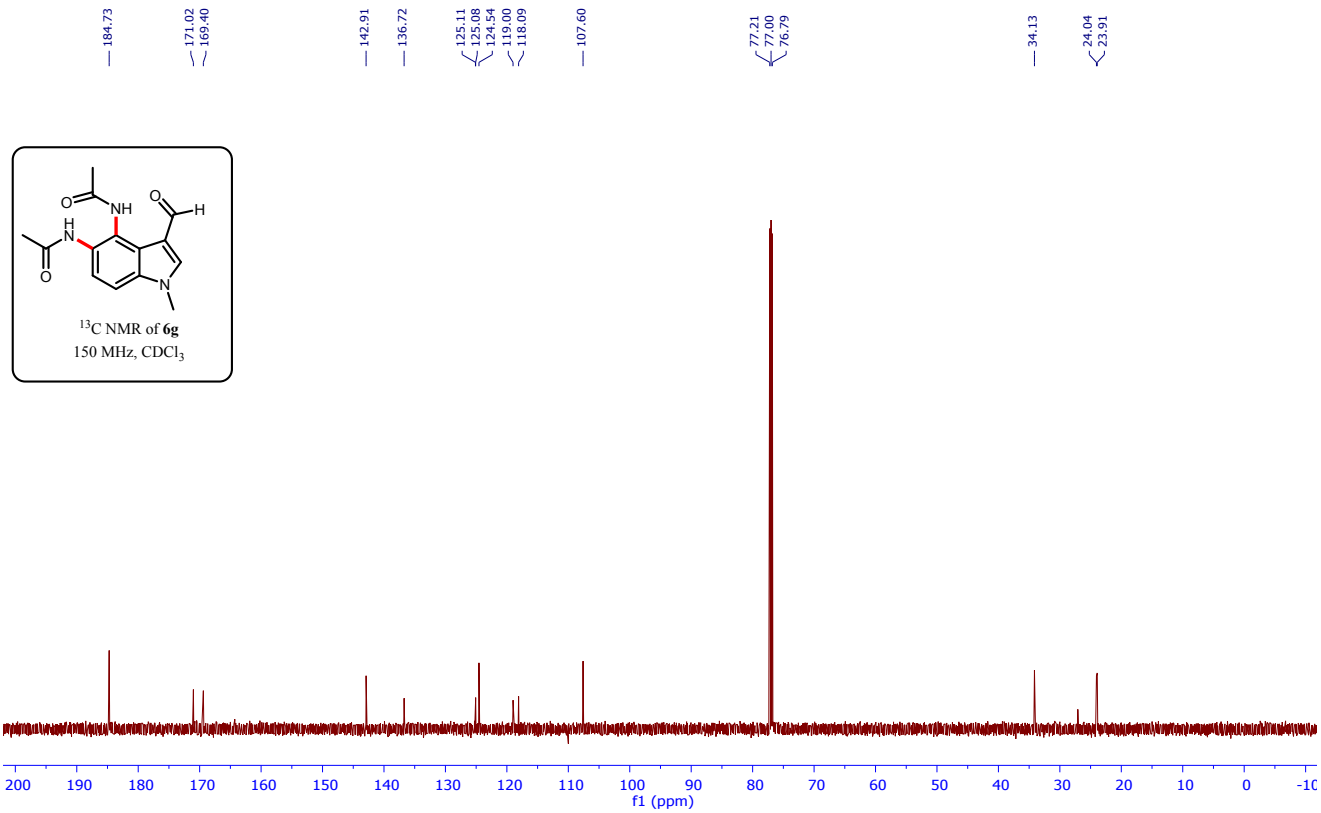

184.55
166.35
166.09
165.68
164.52
164.41
164.01
141.83
136.29
130.97
130.91
130.69
130.68
130.67
129.99
129.92
129.76
129.74
129.70
125.71
125.31
125.00
119.28
118.20
115.67
115.62
115.53
115.47
108.17
77.21
77.00
76.79
47.79
29.19
28.78
22.12
13.80
F
F
O
NH
O
H
H
N
O
N
13C NMR of 6e
150 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


12.161
9.952
9.567
8.151
8.138
7.940
7.927
7.851
7.836
7.773
7.526
7.514
7.419
7.406
7.385
7.374
7.262
7.260
7.206
7.193
5.375
Cl
Cl
O
NH
O
H
H
N
O
N
^{1}H NMR of **6f**
600 MHz, $CDCl_3$
1.01
1.00
1.01
2.01
1.98
1.00
0.91
2.01
4.97
1.04
2.05
2.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

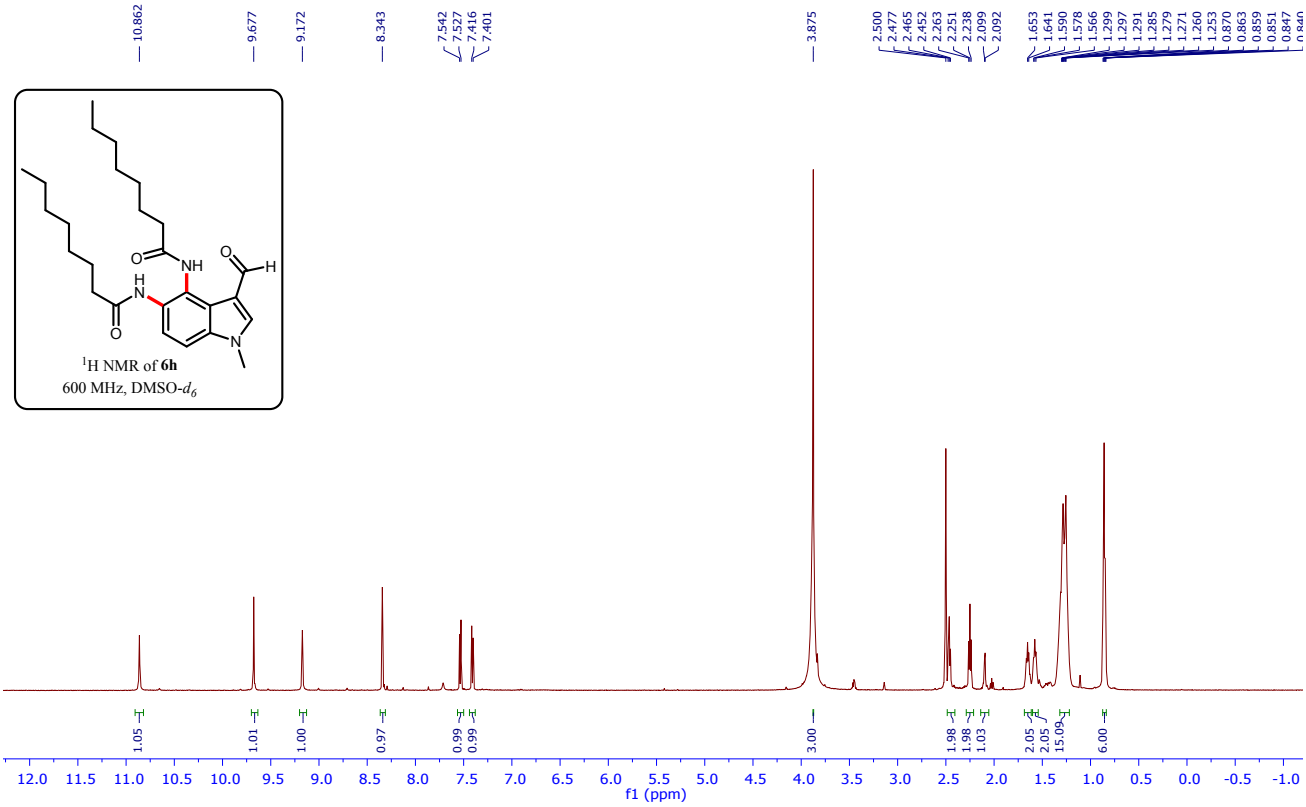

184.79
166.52
164.52
141.93
138.76
137.90
136.63
134.26
132.94
131.96
129.92
129.32
128.87
128.85
128.82
128.77
127.34
125.64
125.60
125.31
119.44
118.79
108.62
77.21
77.00
76.79
51.47
Cl
Cl
O
NH
O
H
H
N
O
N
^{13}C NMR of **6f**
150 MHz, $CDCl_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

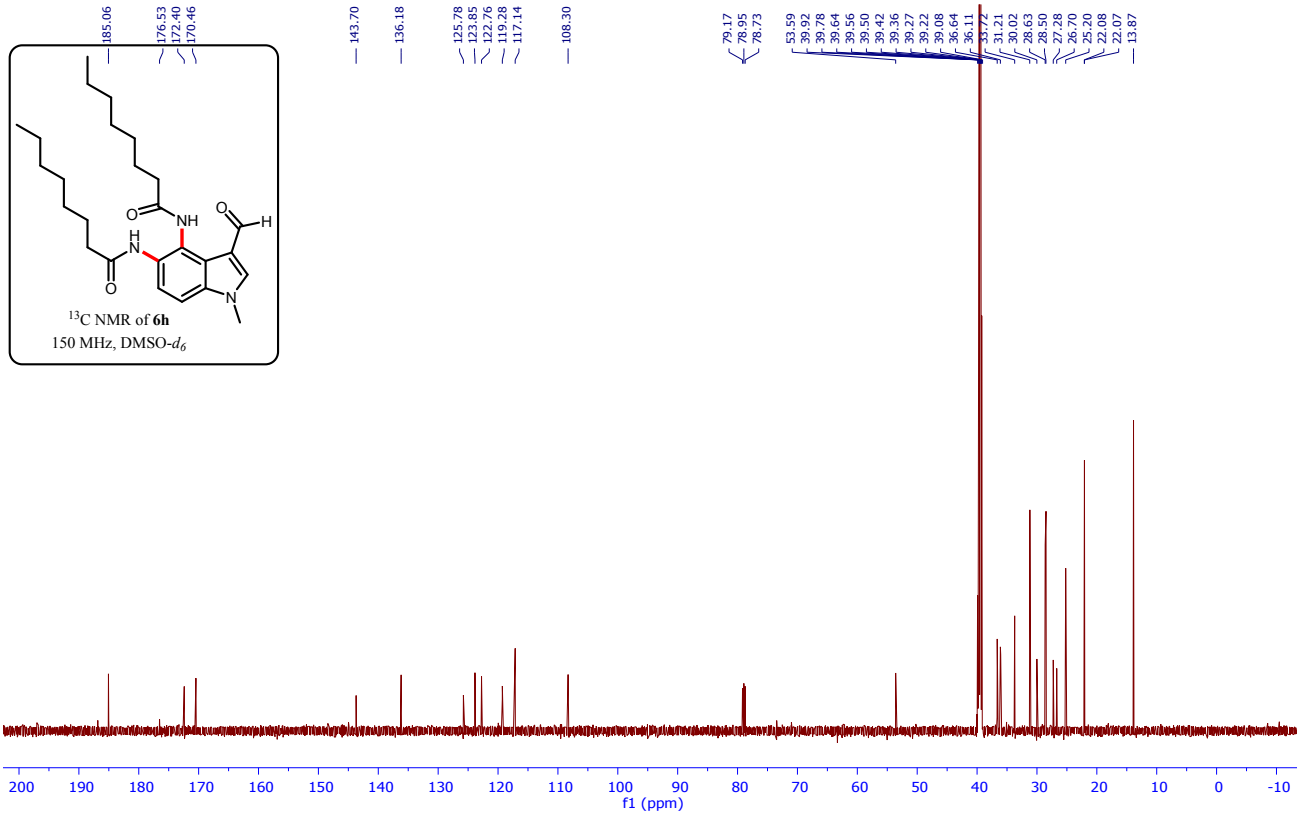


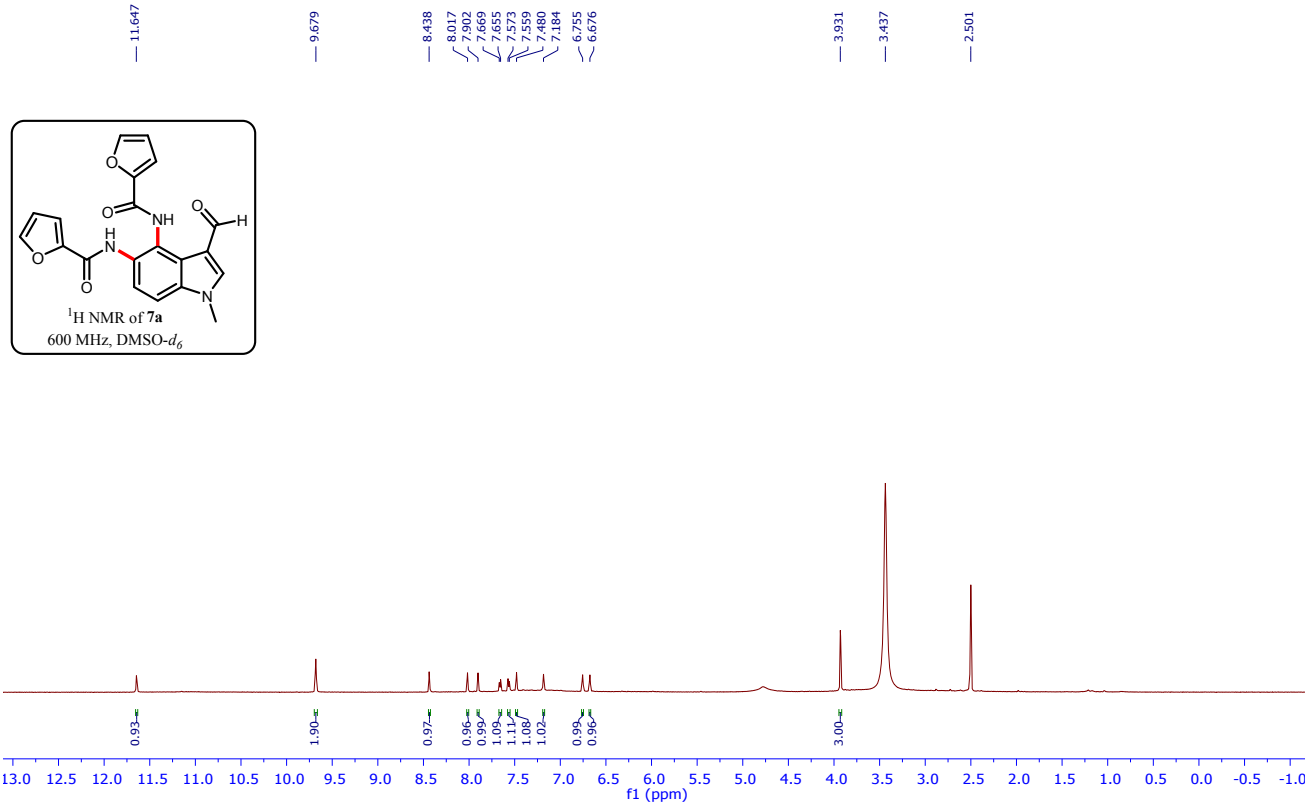
^{1}H NMR of **6g**
600 MHz, $CDCl_3$



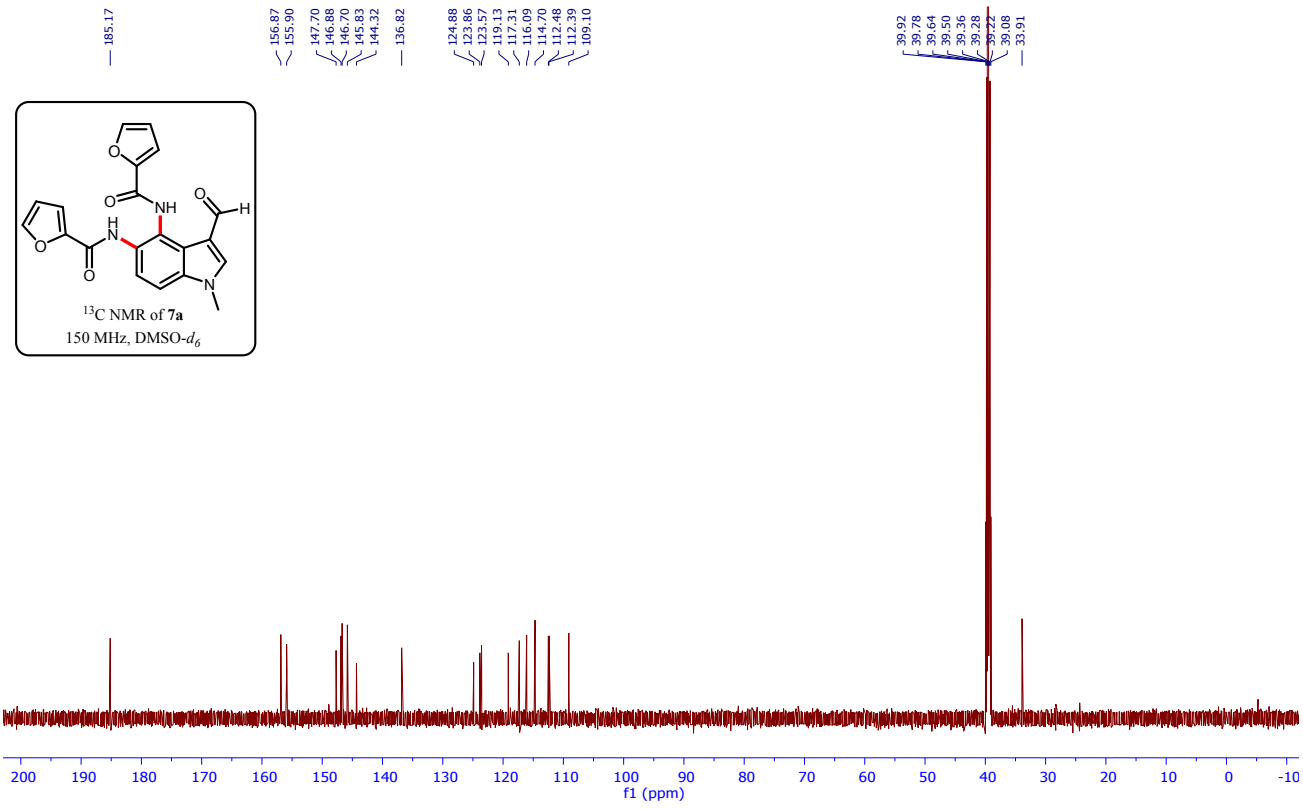
^{13}C NMR of **6g**
150 MHz, $CDCl_3$


10.862
9.677
9.172
8.343
7.542
7.527
7.416
7.401
3.875
2.500
2.477
2.465
2.452
2.263
2.251
2.238
2.099
2.092
1.653
1.641
1.590
1.578
1.566
1.299
1.297
1.291
1.285
1.279
1.271
1.260
1.253
0.870
0.863
0.859
0.851
0.847
1.05
1.01
1.00
0.97
0.99
0.99
3.00
1.98
1.98
1.03
2.05
2.05
15.09
6.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
NH
H
N
O
O
H
N
O
^{1}H NMR of **6h**
600 MHz, DMSO-d_6

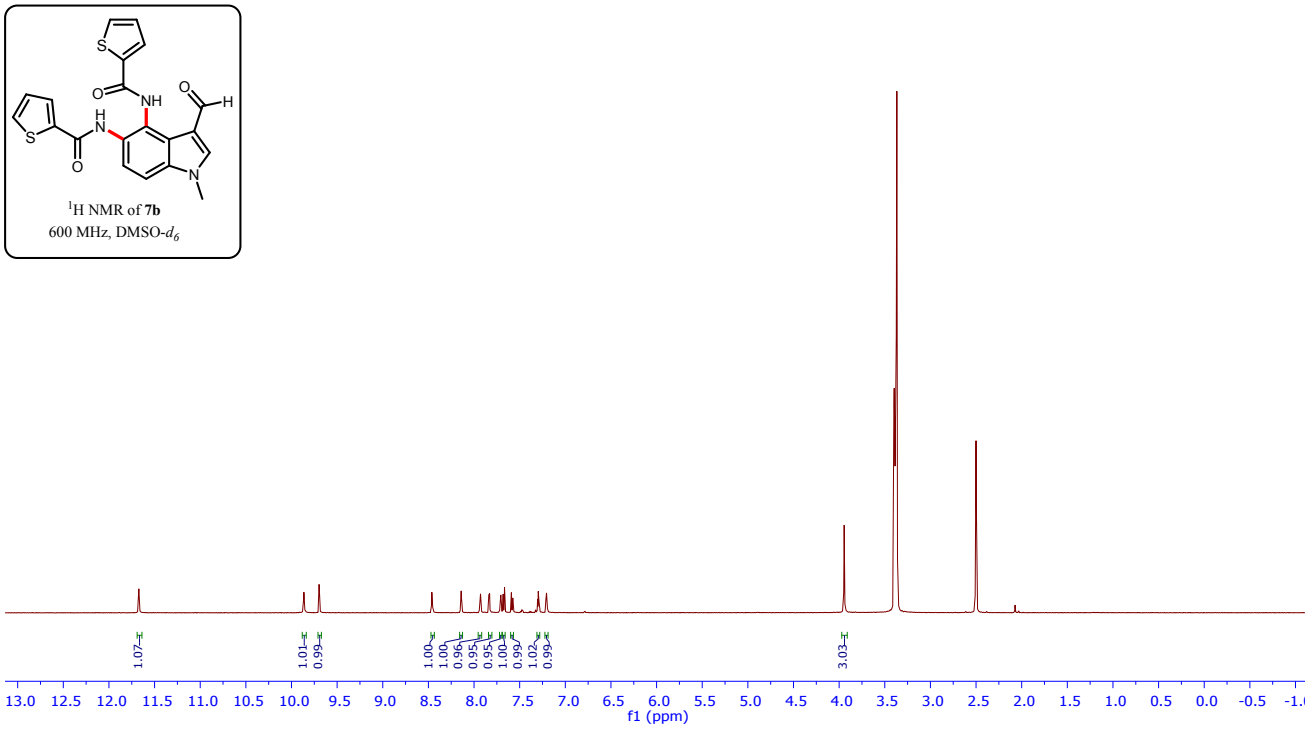

185.06
176.53
172.40
170.46
143.70
136.18
125.78
123.85
122.76
119.28
117.14
108.30
79.17
78.95
78.73
53.59
39.92
39.78
39.64
39.56
39.50
39.42
39.36
39.27
39.22
39.08
36.64
36.11
33.72
31.21
30.02
28.63
28.50
27.28
26.70
25.20
22.08
22.07
13.87
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
NH
H
N
O
O
H
N
O
^{13}C NMR of **6h**
150 MHz, DMSO-d_6



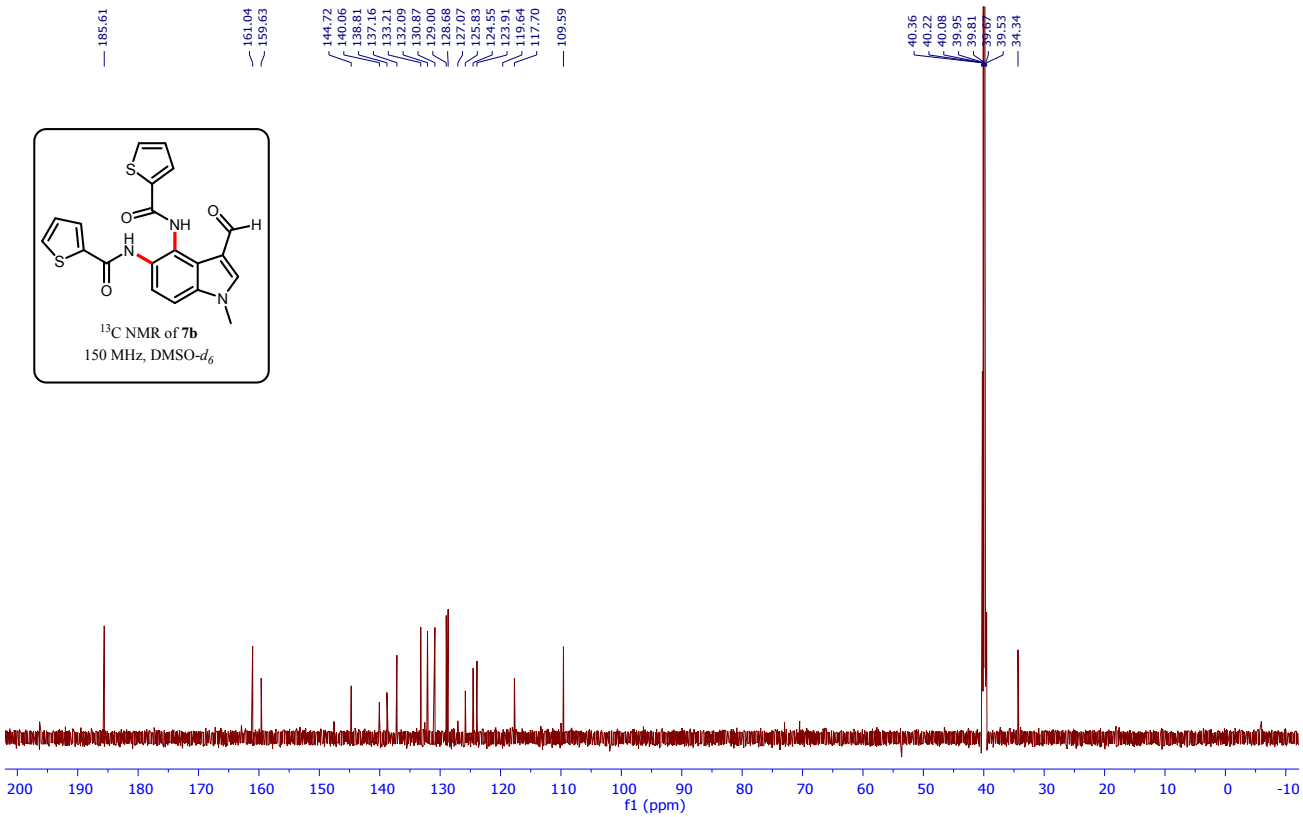
^{1}H NMR of **7a**
600 MHz, DMSO-d_6



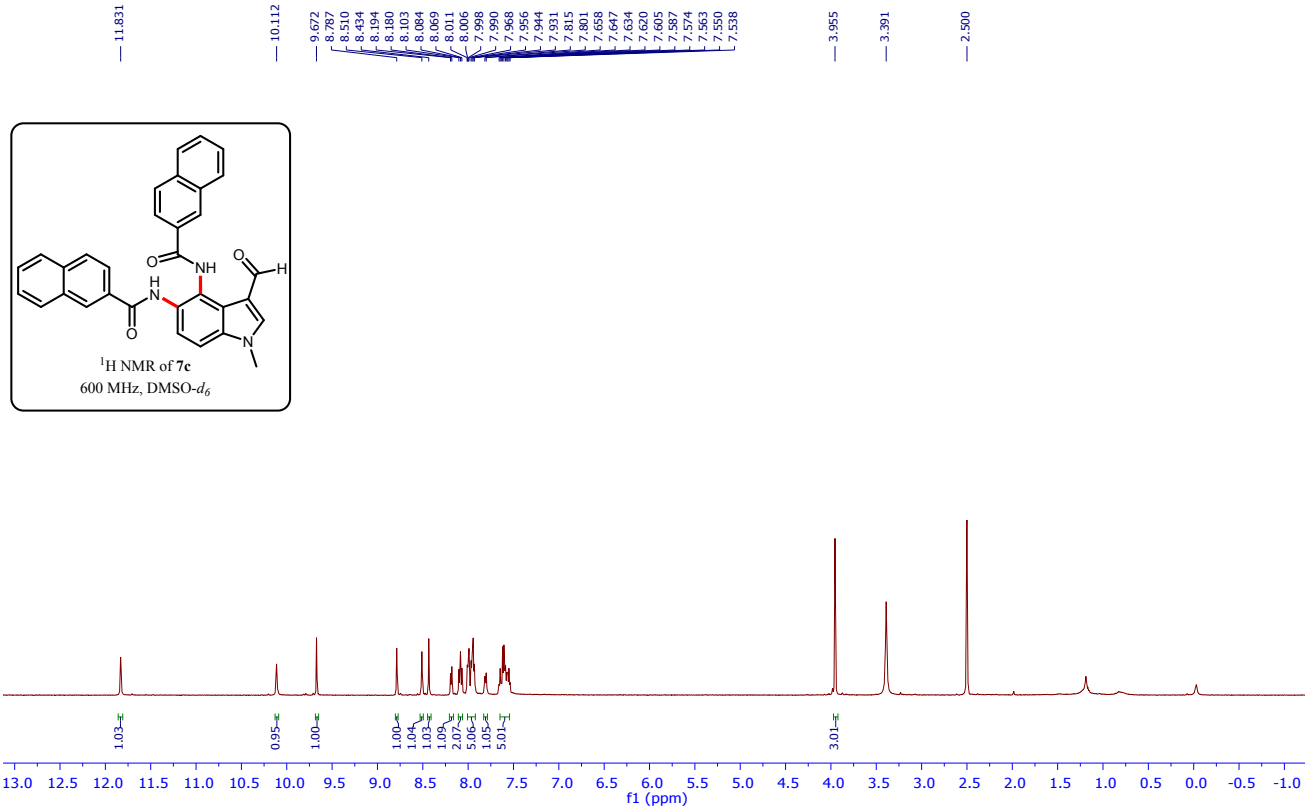
^{13}C NMR of **7a**
150 MHz, DMSO-d_6

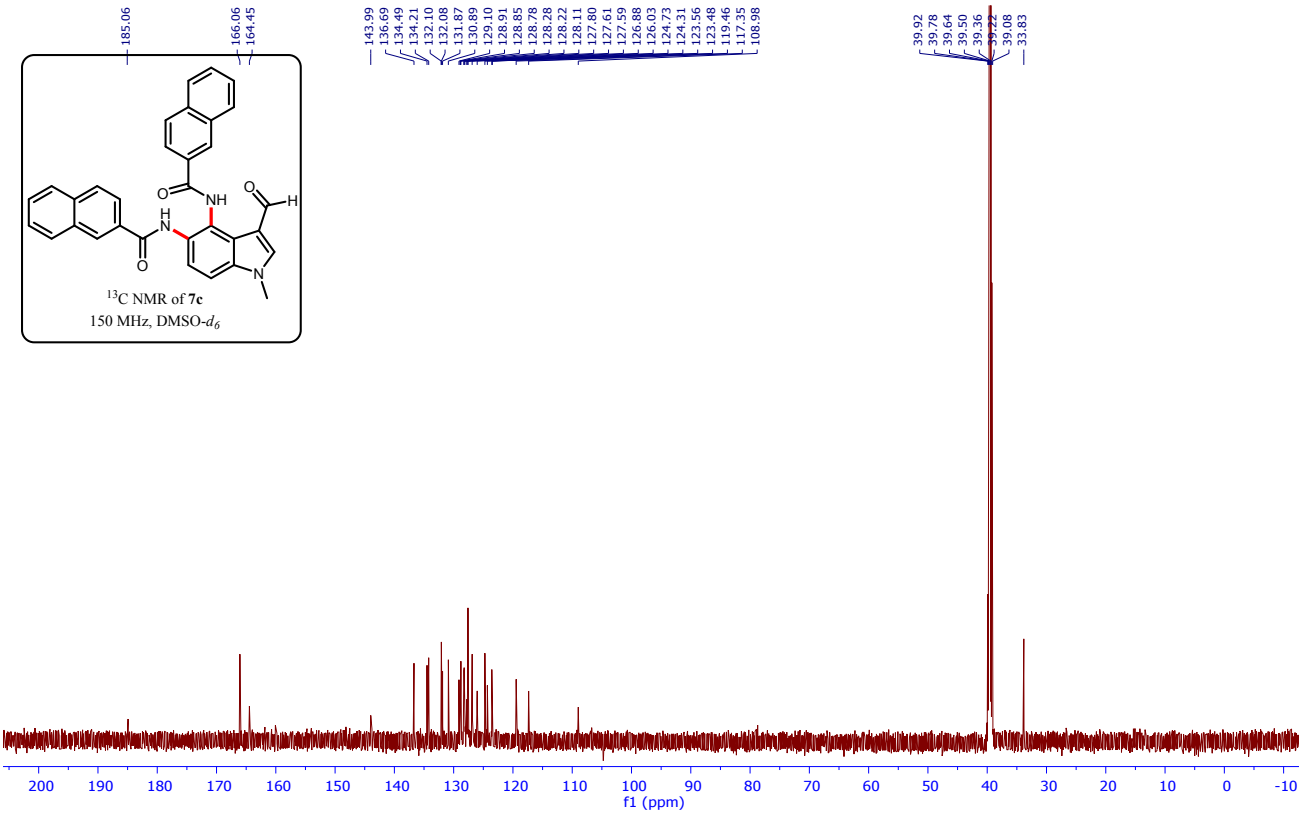


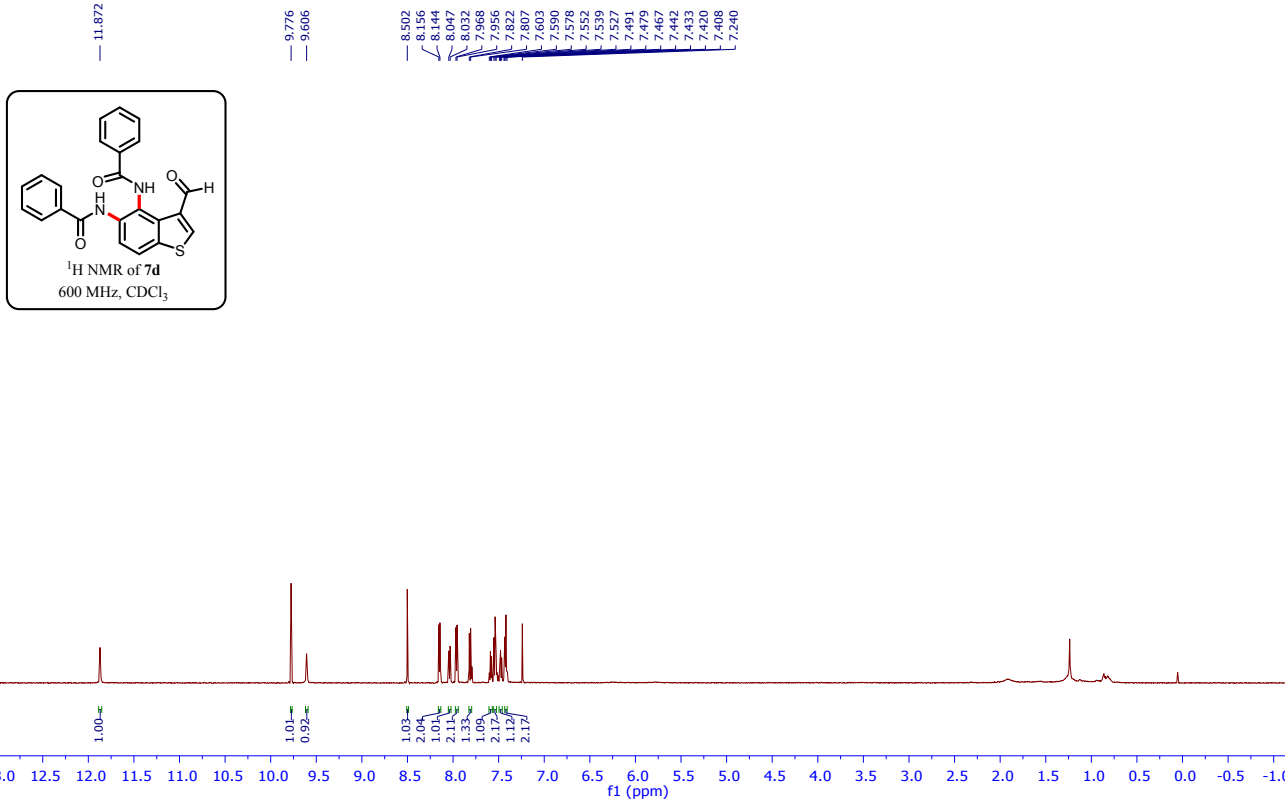
^{1}H NMR of **7b**
600 MHz, DMSO-d_6

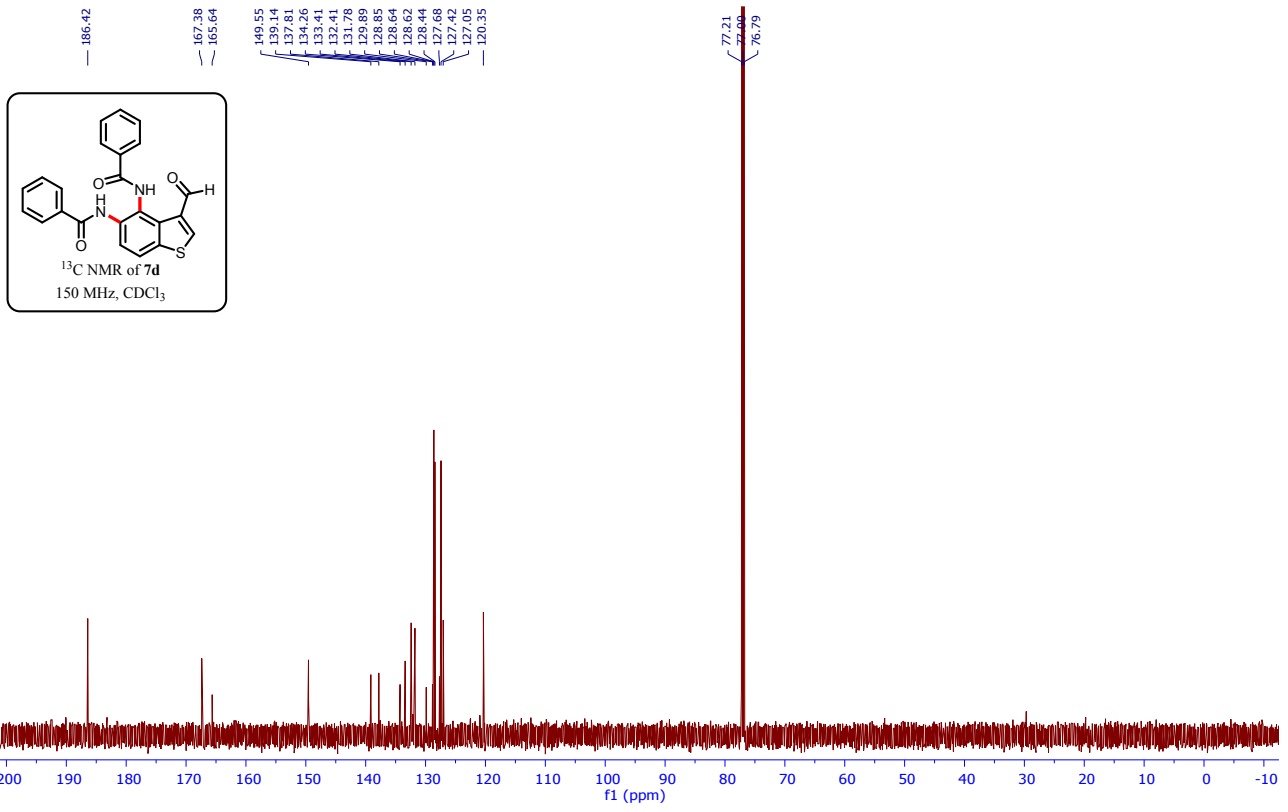


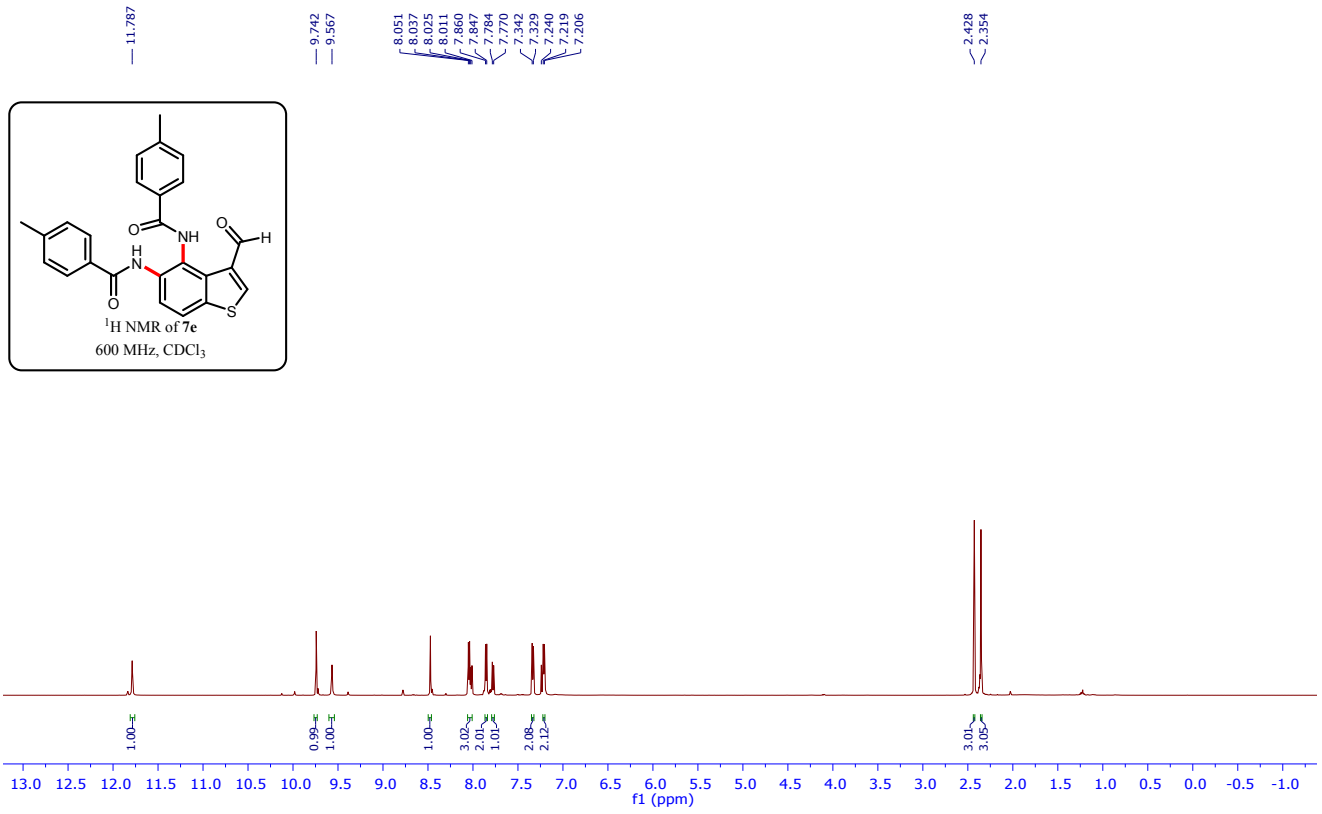
^{13}C NMR of **7b**
150 MHz, DMSO-d_6

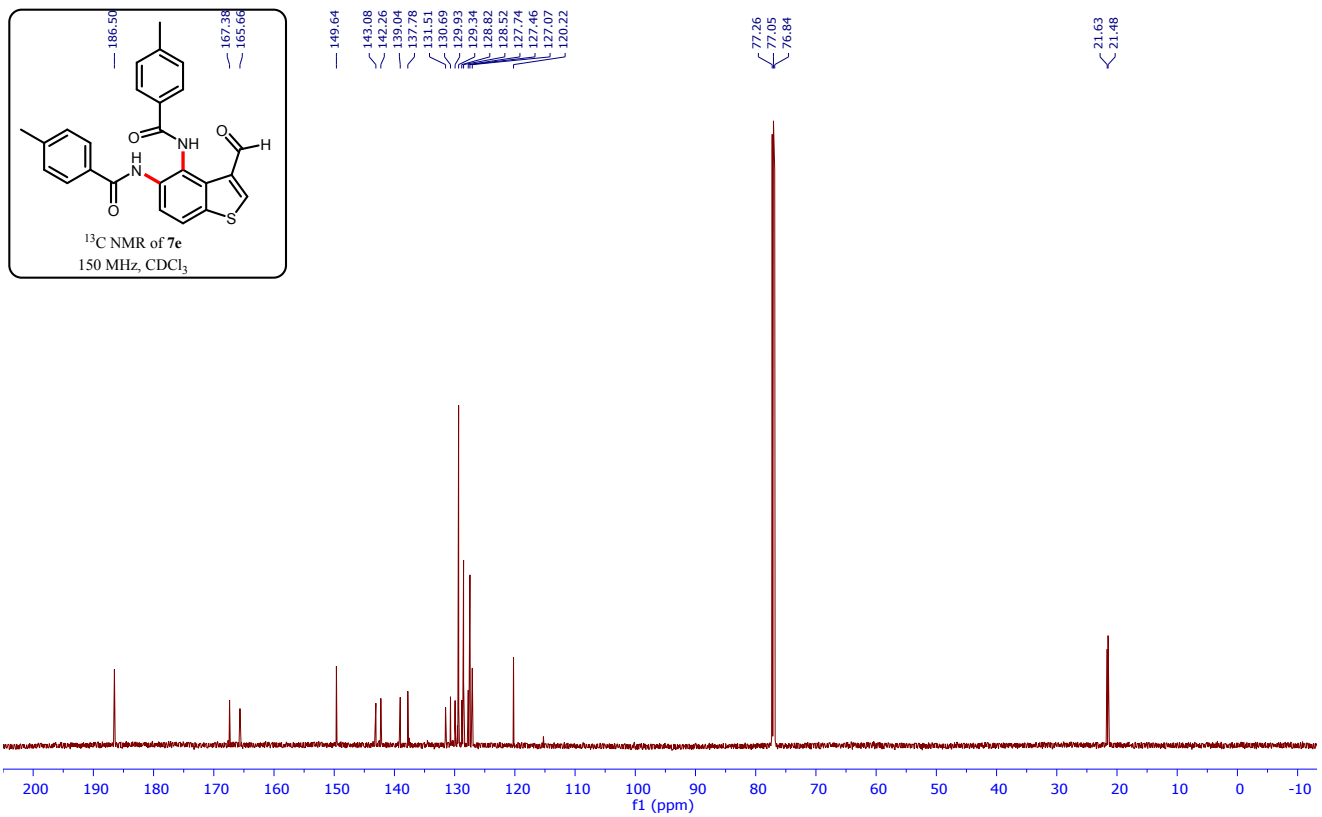

11.831
10.112
9.672
8.787
8.510
8.434
8.194
8.180
8.103
8.084
8.069
8.011
8.006
7.998
7.990
7.968
7.956
7.944
7.931
7.815
7.801
7.658
7.647
7.634
7.620
7.605
7.587
7.574
7.563
7.550
7.538
3.955
3.391
2.500
NH
H
N
O
O
O
H
N
^{1}H NMR of **7c**
600 MHz, DMSO-d_6
1.03
0.95
1.00
1.00
1.04
1.03
1.09
2.07
5.06
1.05
5.01
3.01
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

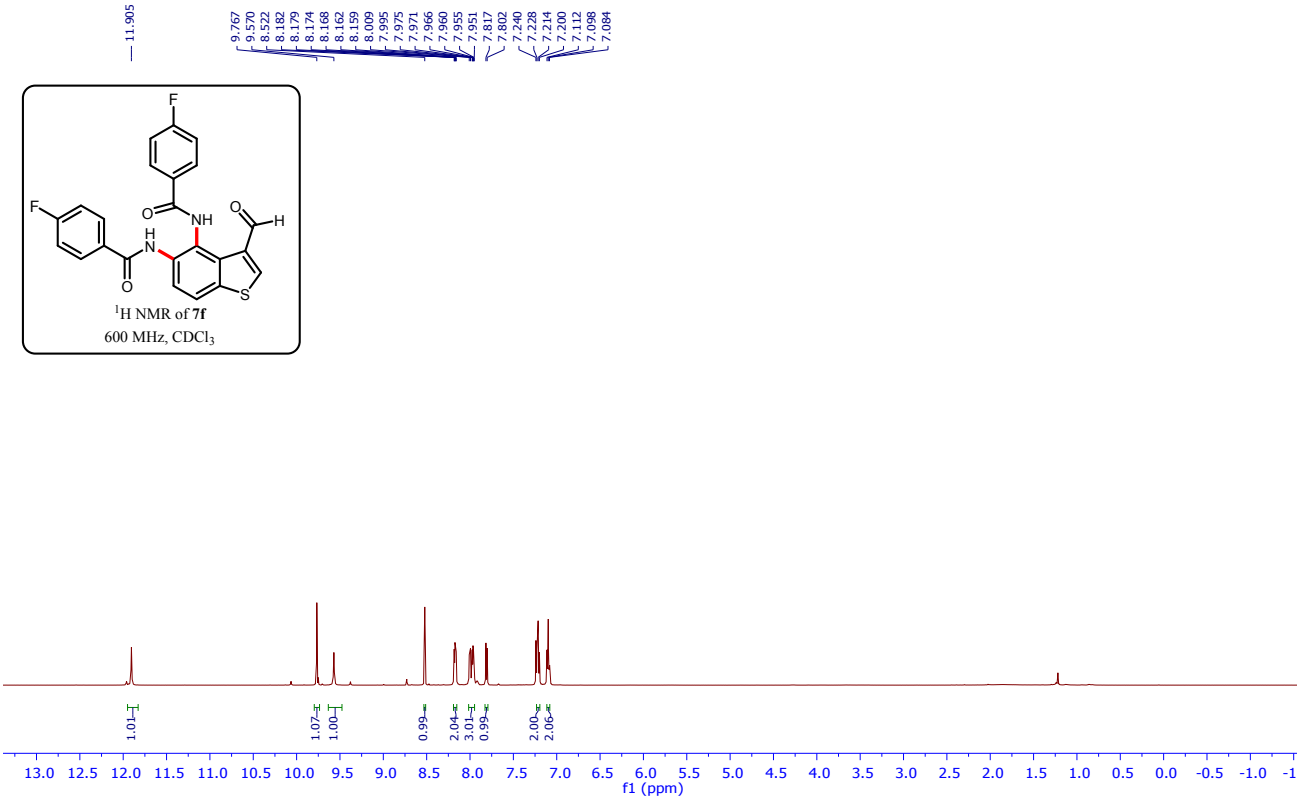

185.06
166.06
164.45
143.99
136.69
134.49
134.21
132.10
132.08
131.87
130.89
129.10
128.91
128.85
128.78
128.28
128.22
128.11
127.80
127.61
127.59
126.88
126.03
124.73
124.31
123.56
123.48
119.46
117.35
108.98
39.92
39.78
39.64
39.50
39.36
39.22
39.08
33.83
NH
H
N
O
O
O
H
N
^{13}C NMR of **7c**
150 MHz, DMSO-d_6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


11.872
9.776
9.606
8.502
8.156
8.144
8.047
8.032
7.968
7.956
7.822
7.807
7.603
7.590
7.578
7.552
7.539
7.527
7.491
7.479
7.467
7.442
7.433
7.420
7.408
7.240
NH
O
H
N
O
S
1H NMR of 7d
600 MHz, CDCl3
1.00
1.01
0.92
1.03
2.04
1.01
2.11
1.33
1.09
2.17
1.12
2.17
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

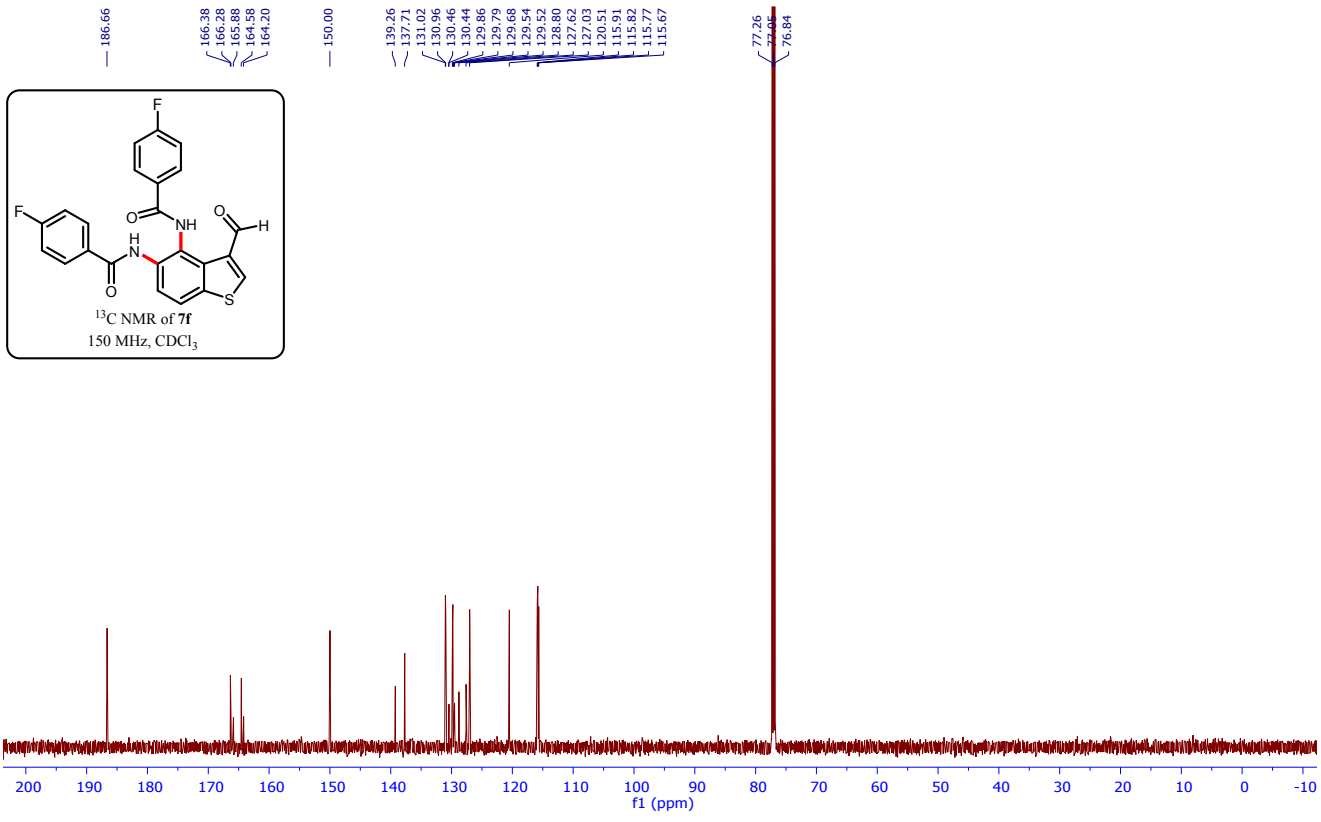

186.42
167.38
165.64
149.55
139.14
137.81
134.26
133.41
132.41
131.78
129.89
128.85
128.64
128.62
128.44
127.68
127.42
127.05
120.35
77.21
77.00
76.79
NH
O
H
N
O
S
13C NMR of 7d
150 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


11.787
9.742
9.567
8.051
8.037
8.025
8.011
7.860
7.847
7.784
7.770
7.342
7.329
7.240
7.219
7.206
2.428
2.354
1H NMR of 7e
600 MHz, CDCl3
1.00
0.99
1.00
1.00
3.02
2.01
1.01
2.08
2.12
3.01
3.05
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

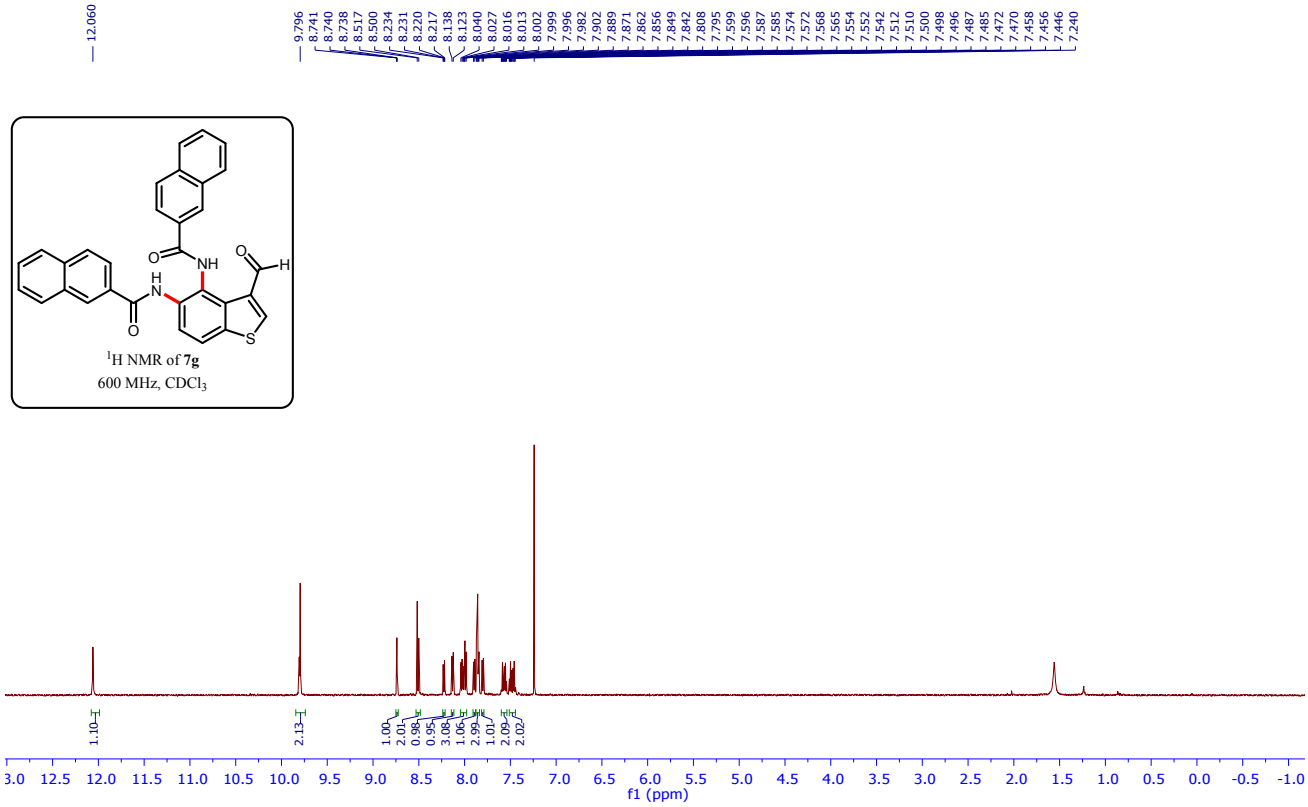

186.50
167.38
165.66
149.64
143.08
142.26
139.04
137.78
131.51
130.69
129.93
129.34
128.82
128.52
127.74
127.46
127.07
120.22
77.26
77.05
76.84
21.63
21.48
13C NMR of 7e
150 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



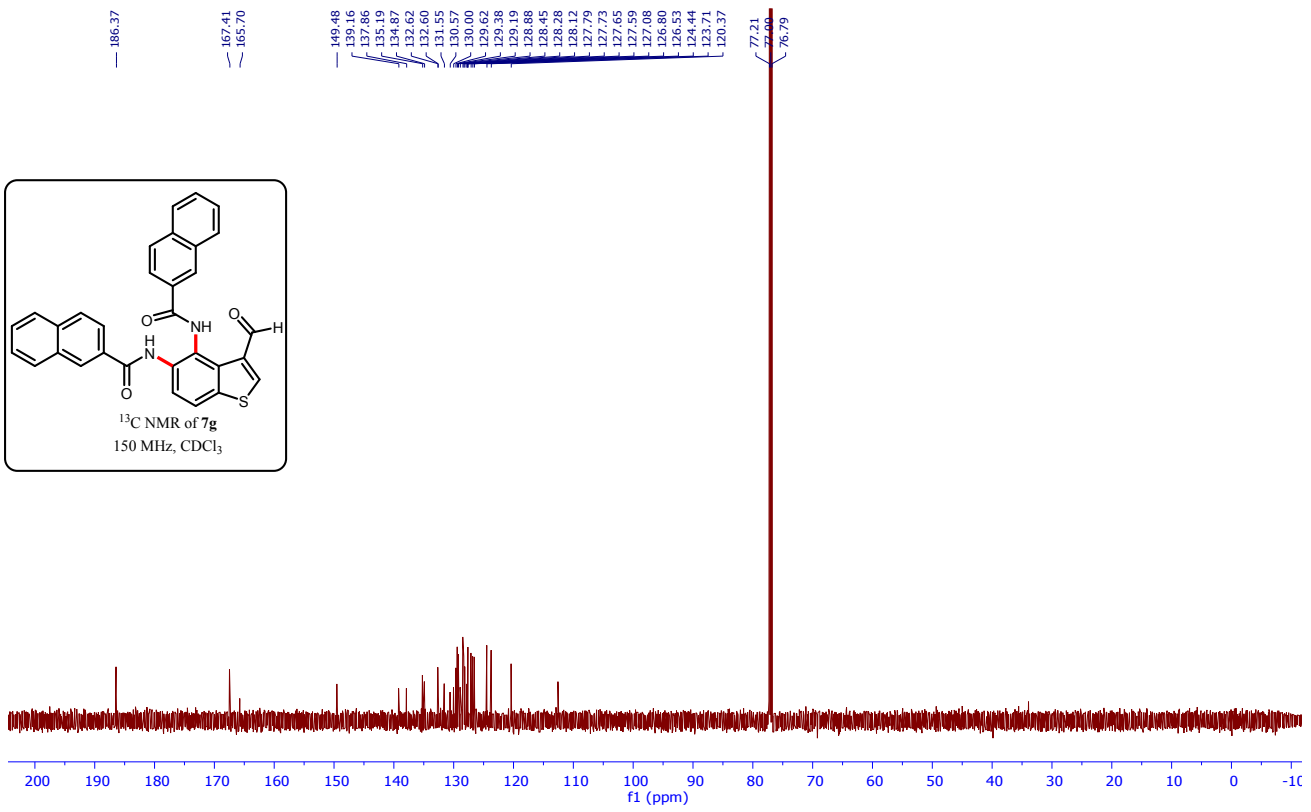
^{1}H NMR of **7f**
600 MHz, $CDCl_3$



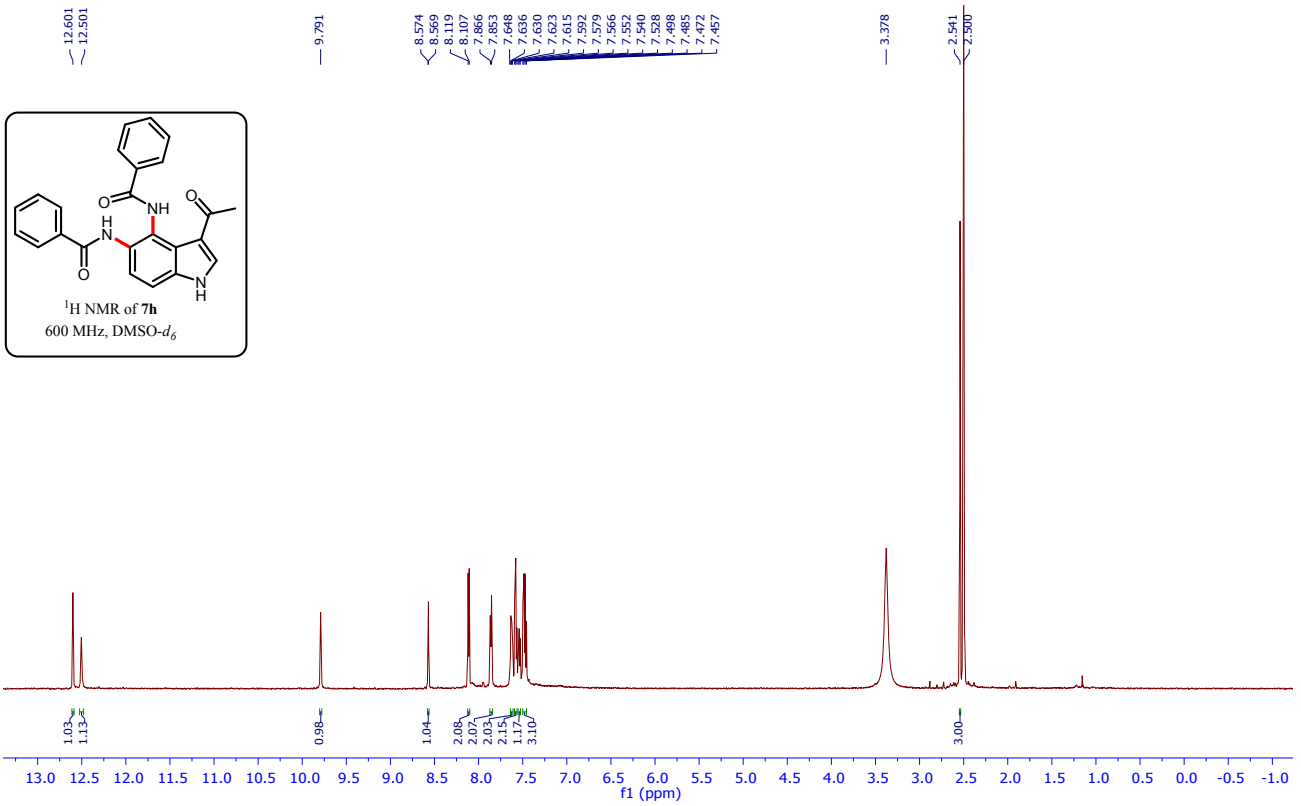
^{13}C NMR of **7f**
150 MHz, $CDCl_3$



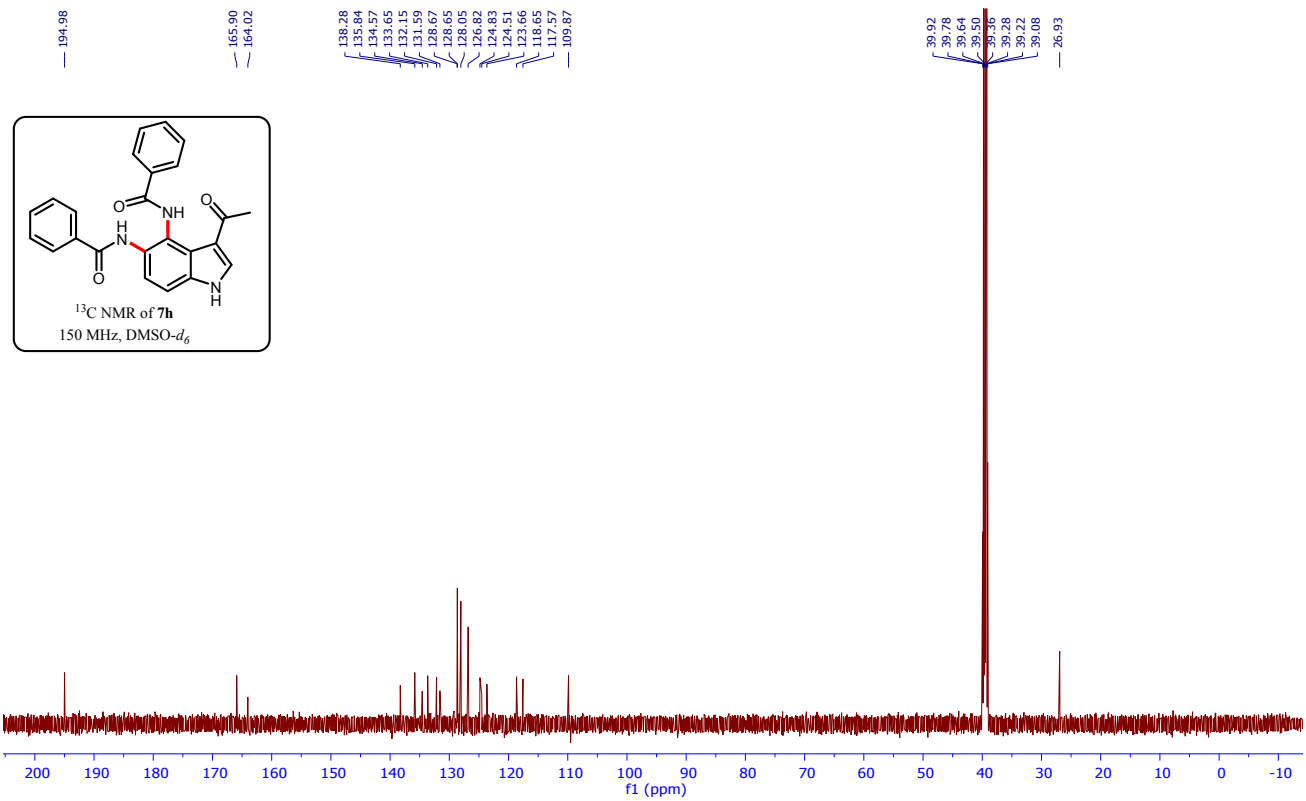
^{1}H NMR of **7g**
600 MHz, $CDCl_3$



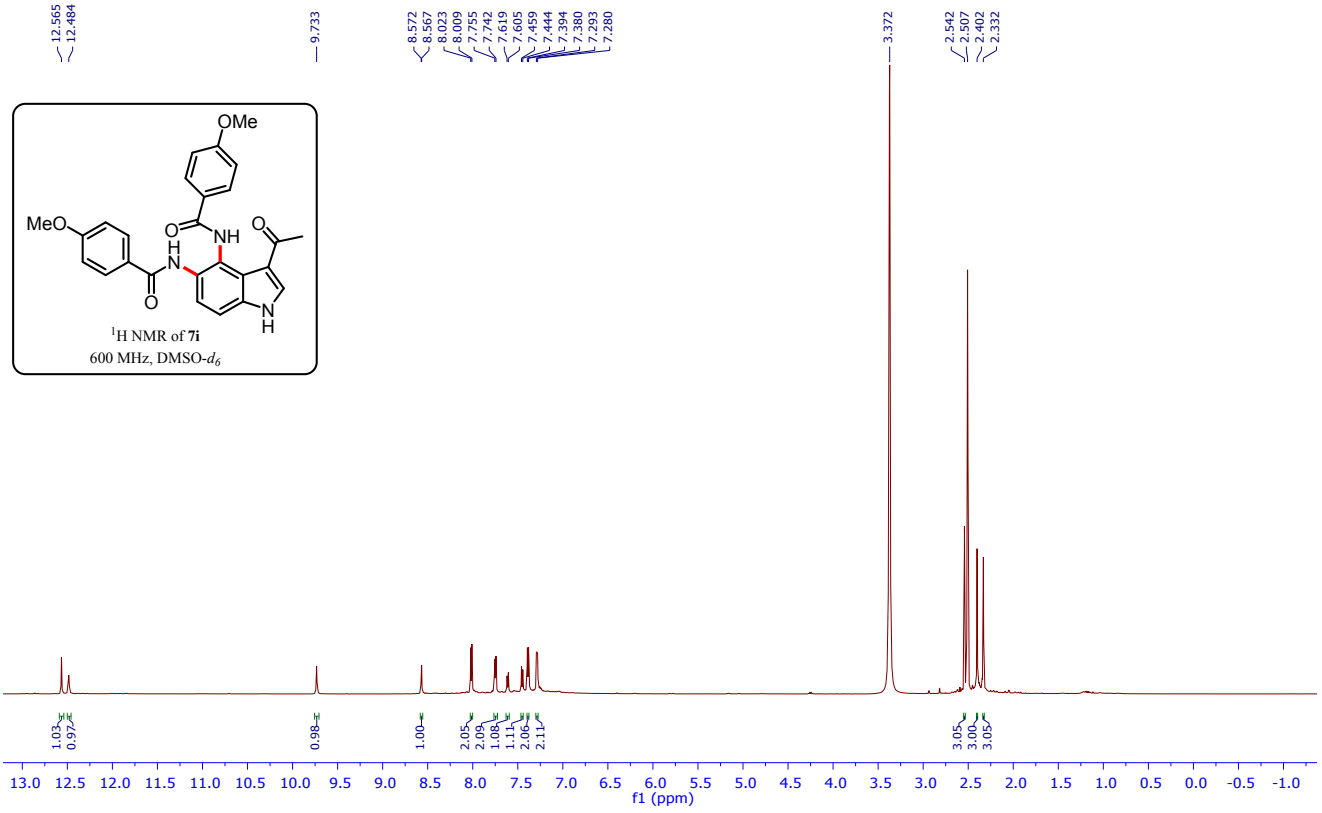
^{13}C NMR of **7g**
150 MHz, $CDCl_3$



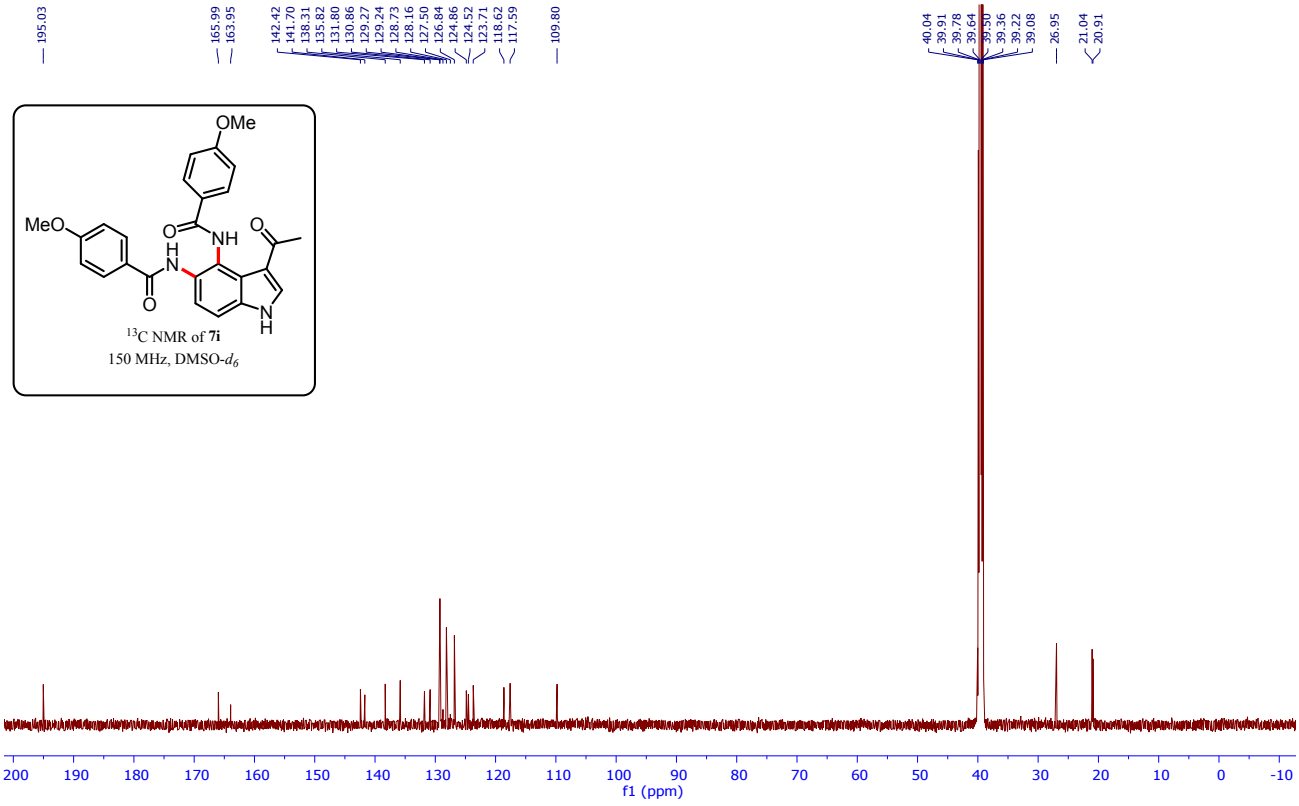
^{1}H NMR of **7h**
600 MHz, DMSO-d_6



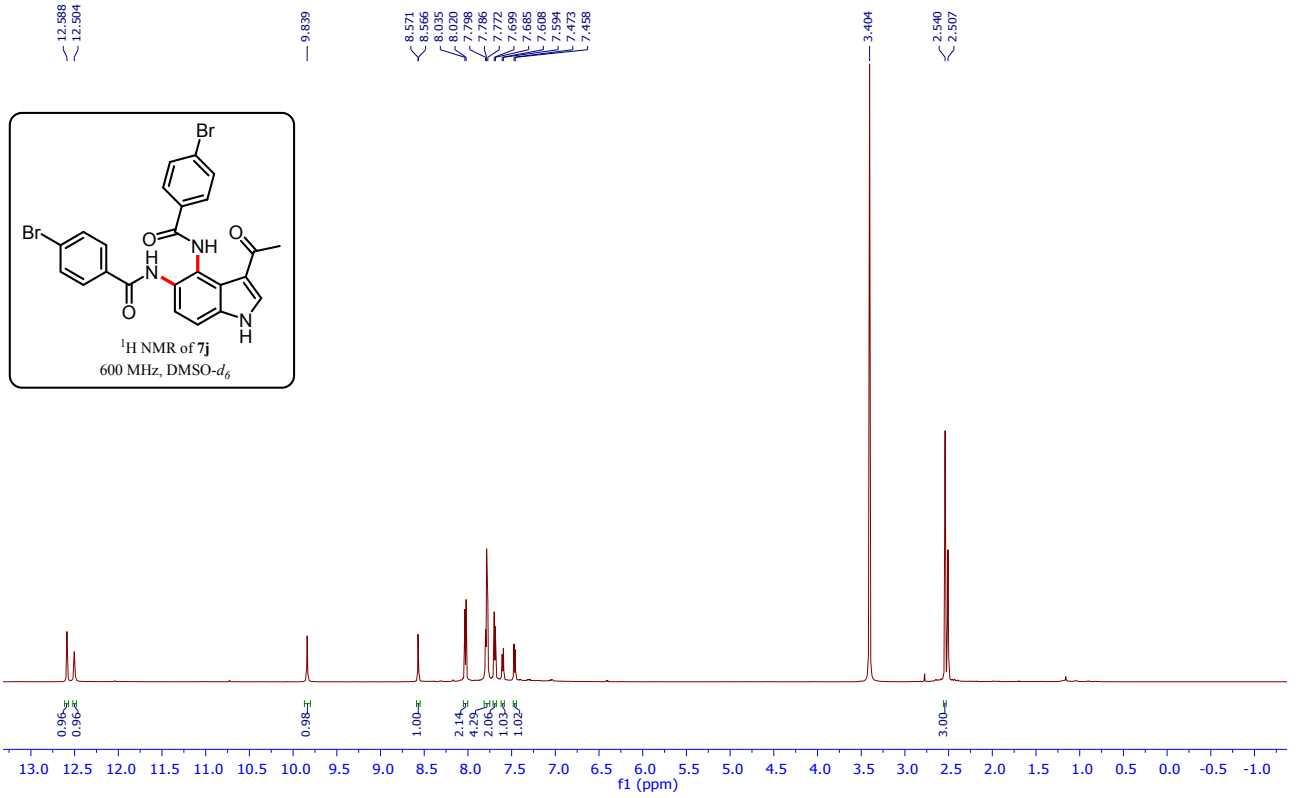
^{13}C NMR of **7h**
150 MHz, DMSO-d_6



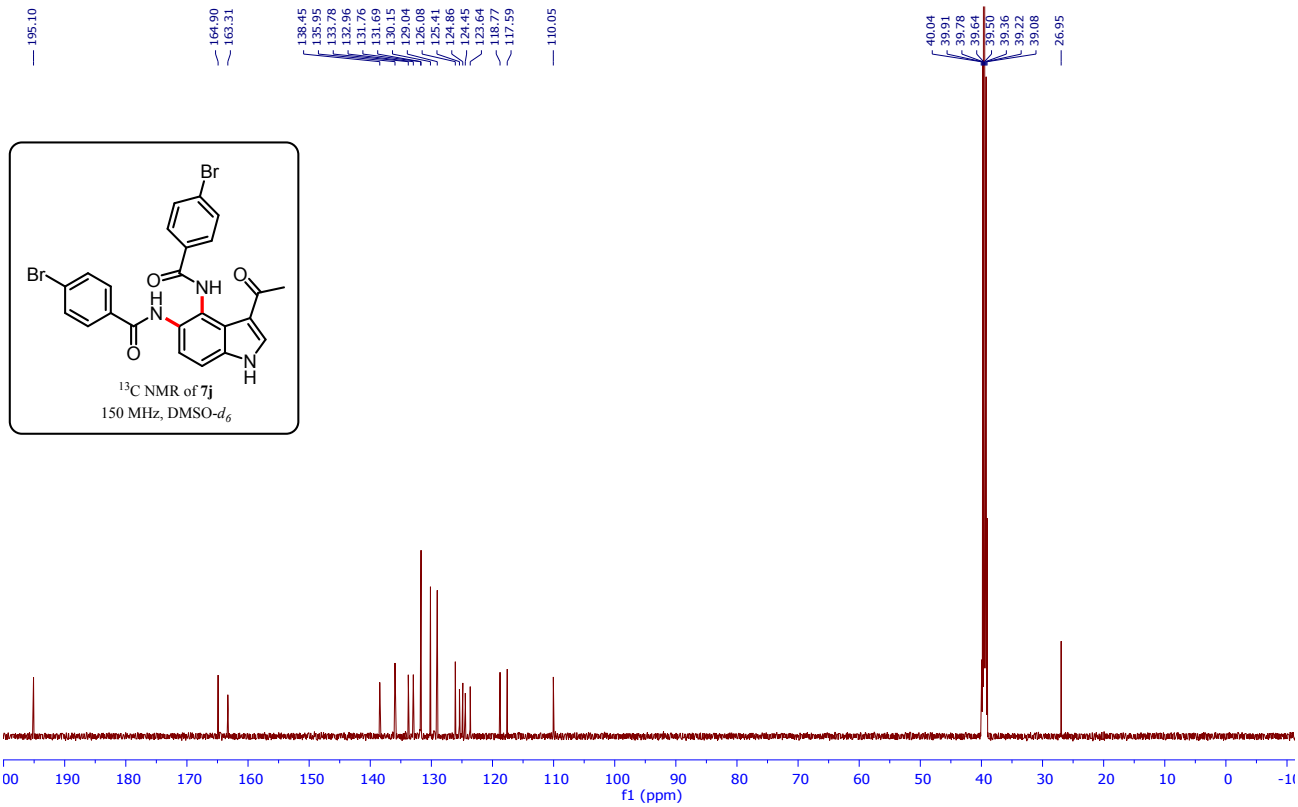
^{1}H NMR of **7i**
600 MHz, DMSO-d_6



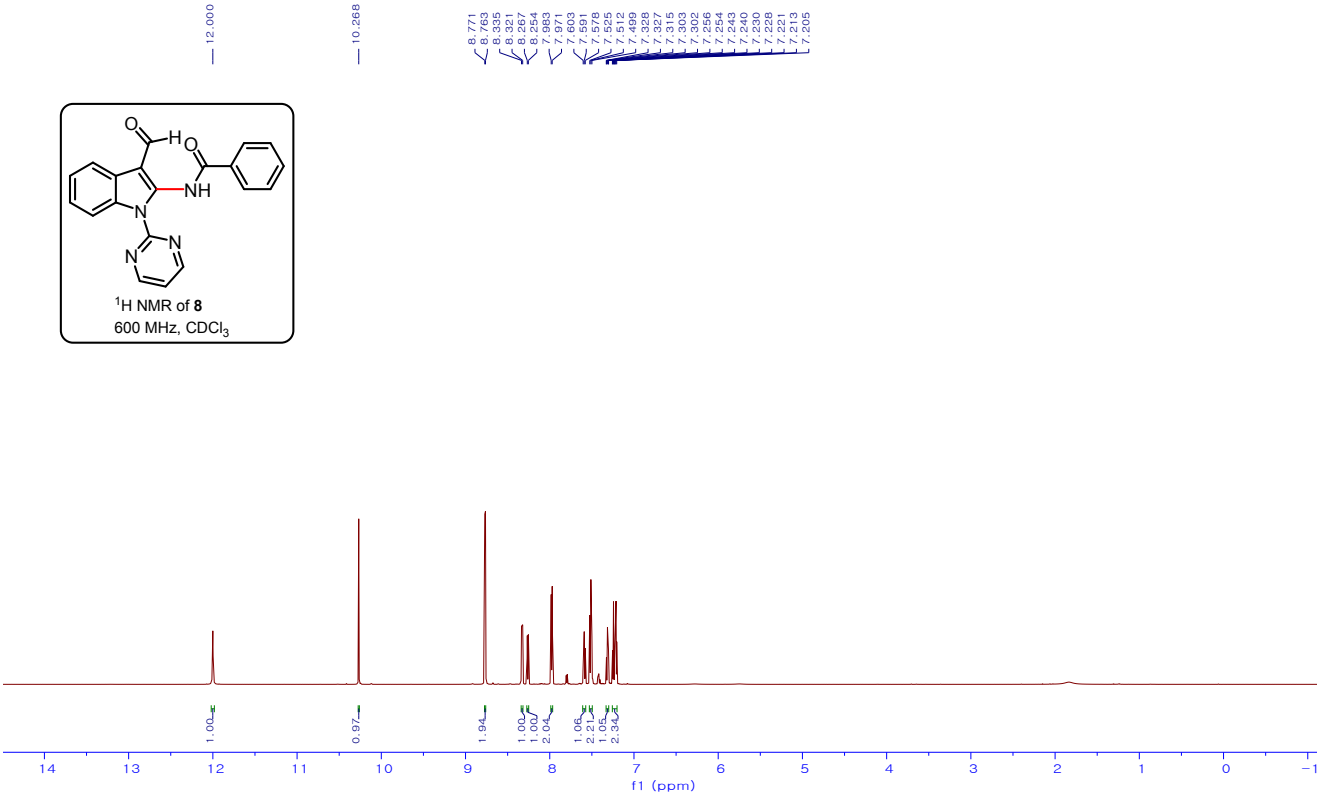
^{13}C NMR of **7i**
150 MHz, DMSO-d_6

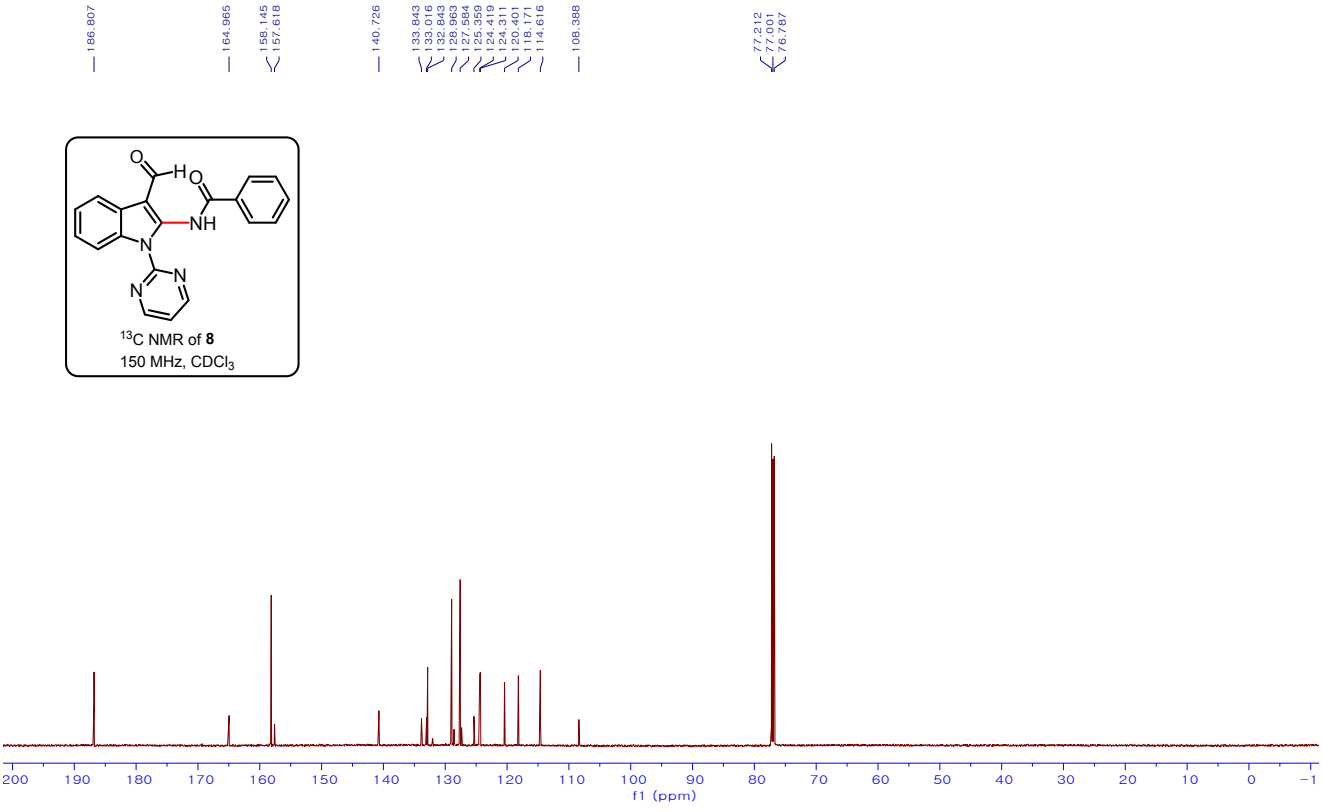


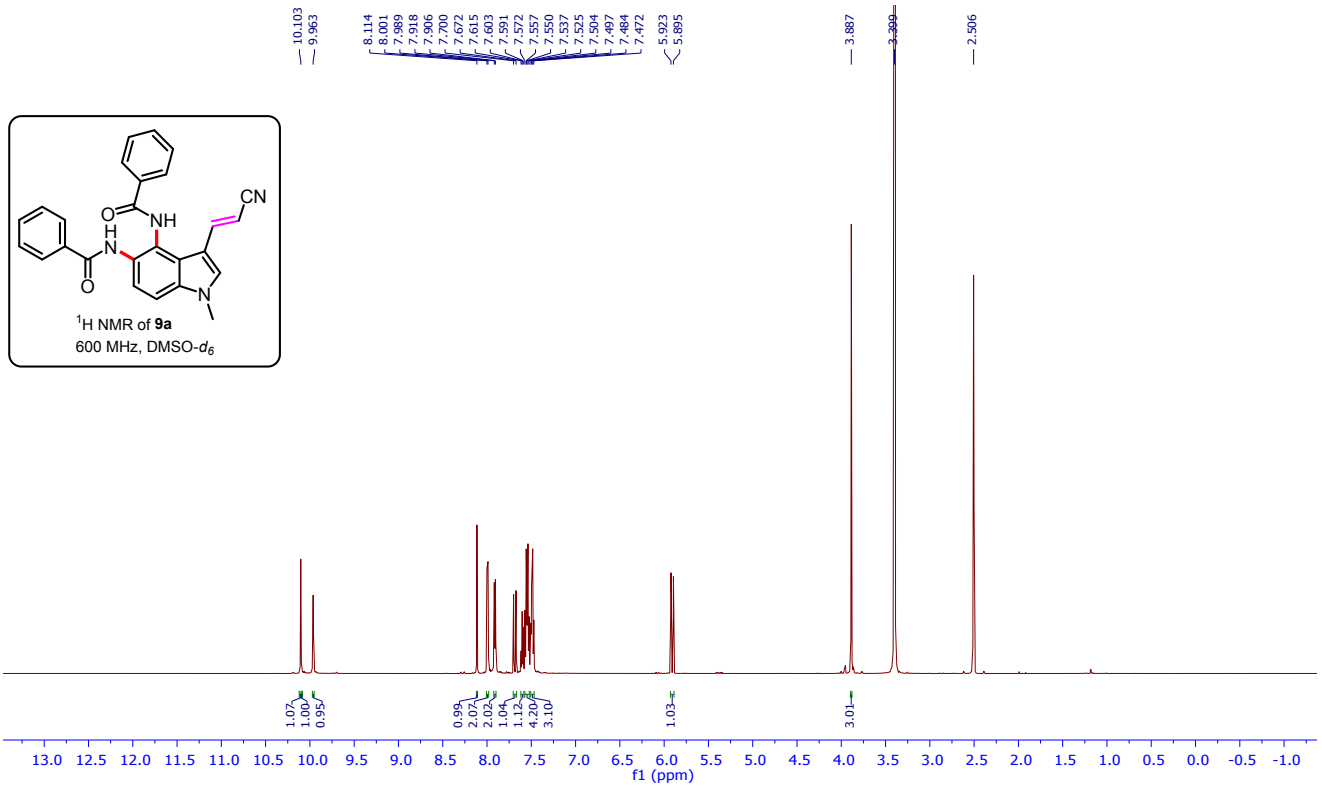
^{1}H NMR of **7j**
600 MHz, DMSO-d_6

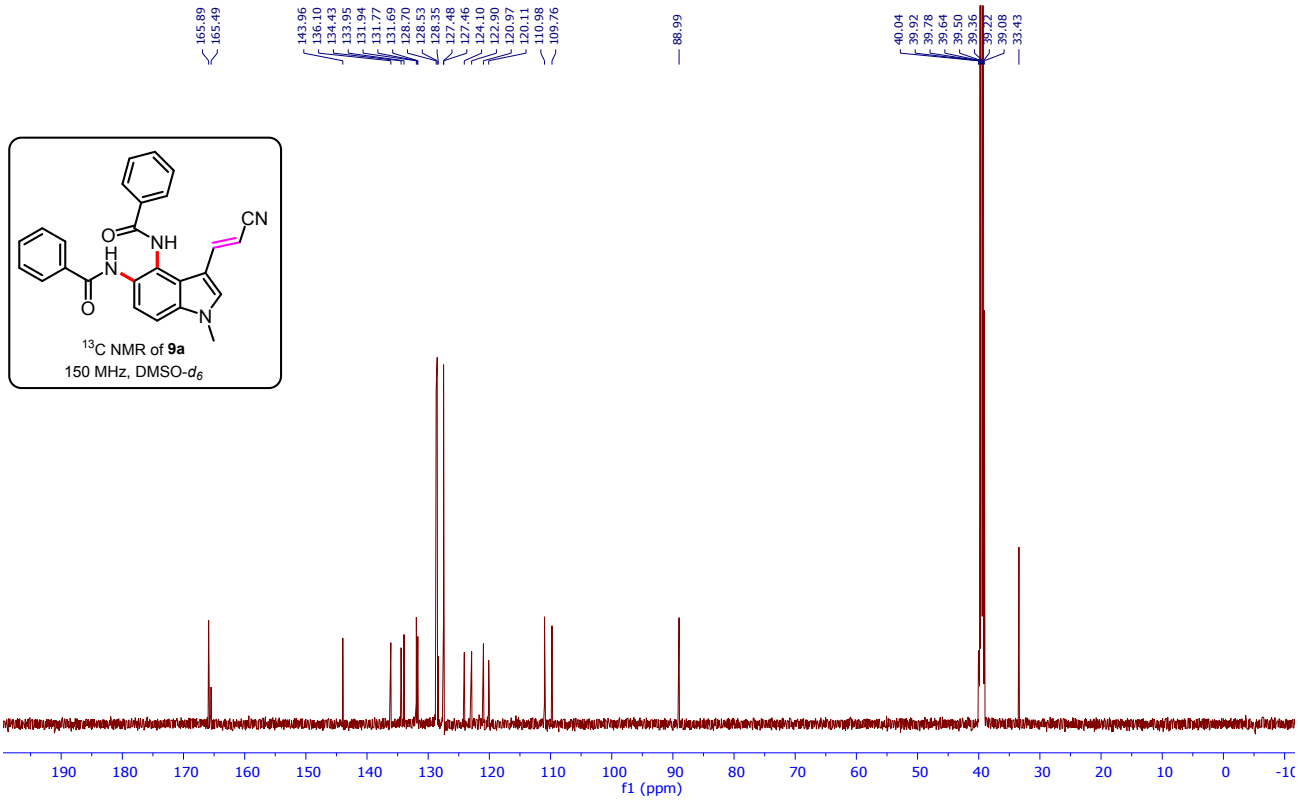


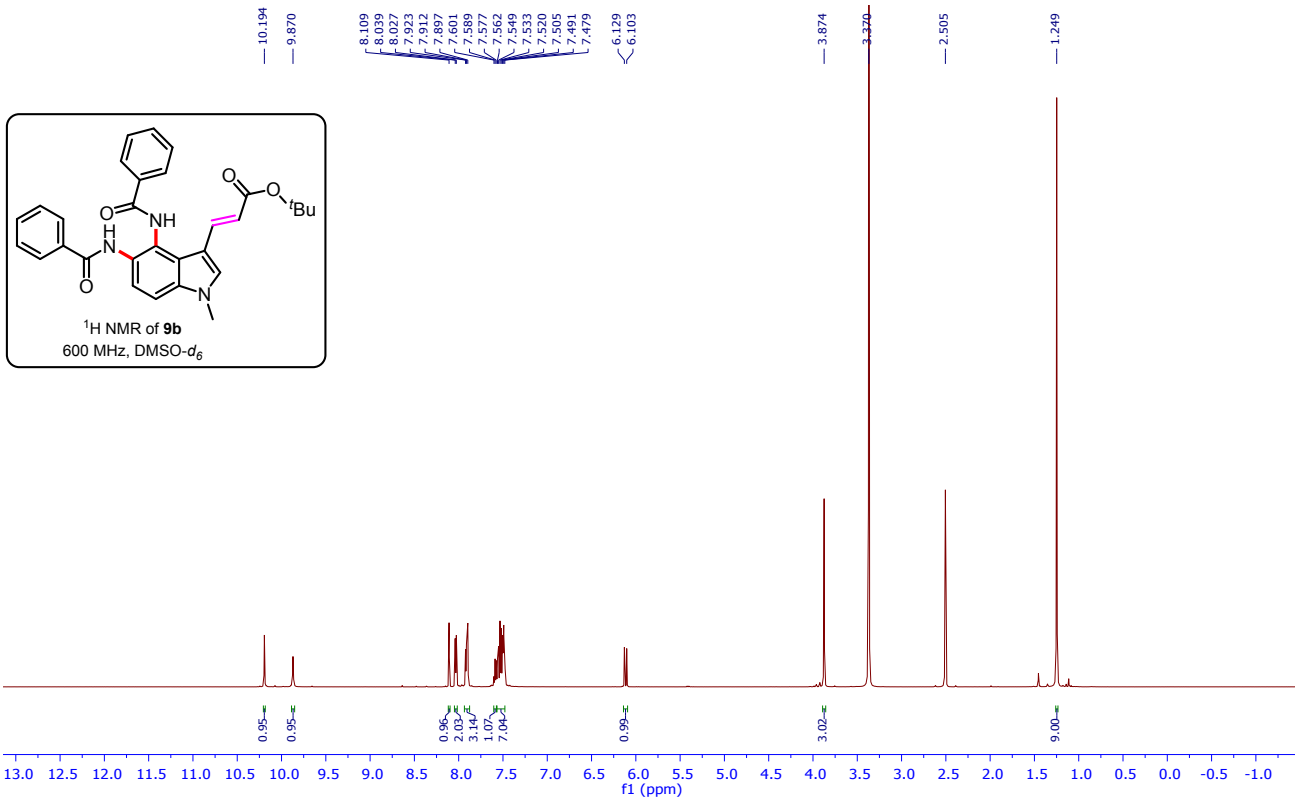
^{13}C NMR of **7j**
150 MHz, DMSO-d_6


12.000
10.268
8.771
8.763
8.345
8.321
8.267
8.254
7.983
7.971
7.603
7.591
7.578
7.565
7.512
7.499
7.328
7.327
7.315
7.303
7.302
7.256
7.254
7.243
7.240
7.230
7.228
7.221
7.213
7.205
O
H
O
NH
N
N
N
1H NMR of 8
600 MHz, CDCl3
1.00
0.97
1.94
1.00
1.00
2.04
1.06
2.21
1.05
2.34
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)

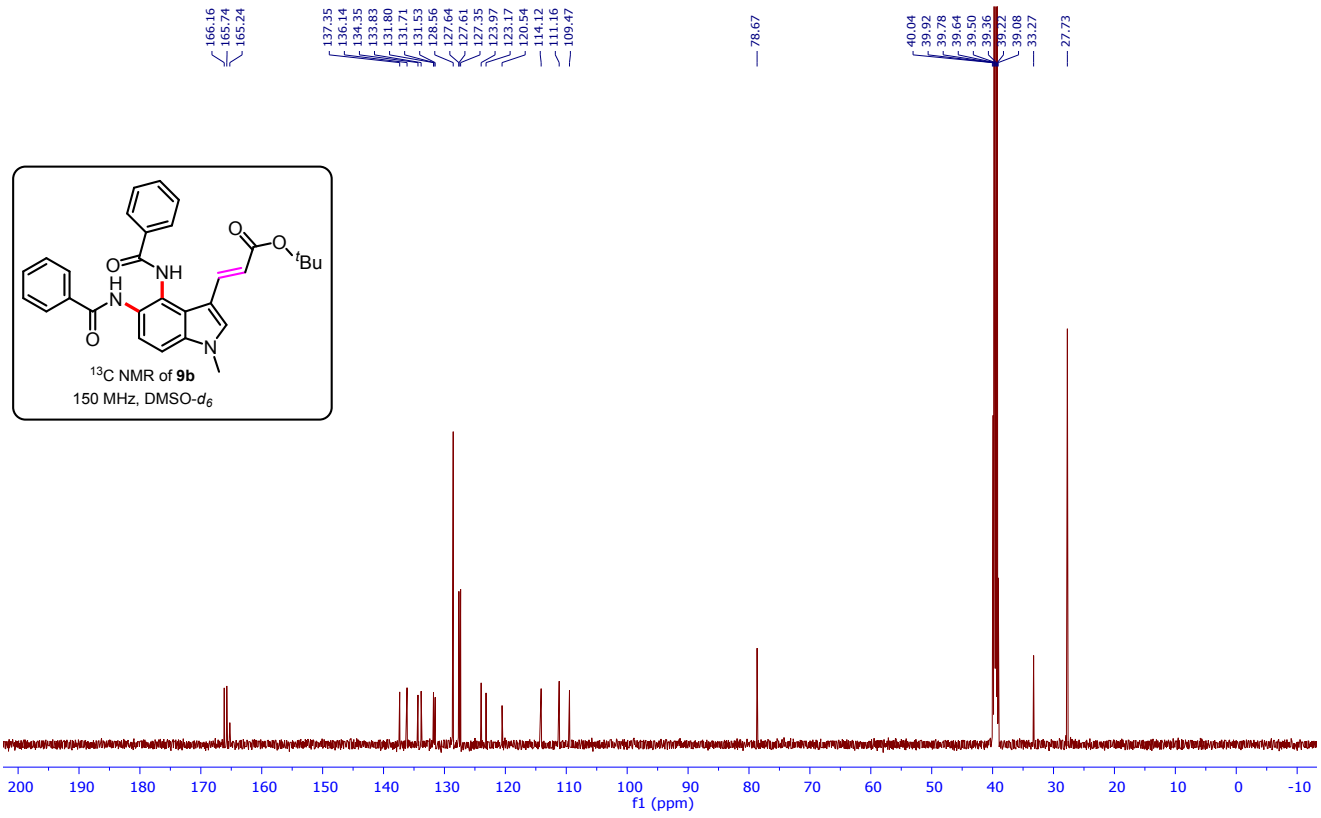

186.807
164.965
158.145
157.618
140.726
133.843
133.016
132.643
128.963
127.584
125.359
124.419
124.311
120.401
118.171
114.616
108.388
77.212
77.001
76.787
O
H
O
NH
N
N
N
13C NMR of 8
150 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)


10.103
9.963
8.114
8.001
7.989
7.918
7.906
7.700
7.672
7.615
7.603
7.591
7.572
7.557
7.550
7.537
7.525
7.504
7.497
7.484
7.472
5.923
5.895
3.887
3.399
2.506
1.07
1.00
0.95
0.99
2.07
2.02
1.04
1.12
4.20
3.10
1.03
3.01
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
CN
NH
O
H
N
O
N
^{1}H NMR of **9a**
600 MHz, DMSO-d_6

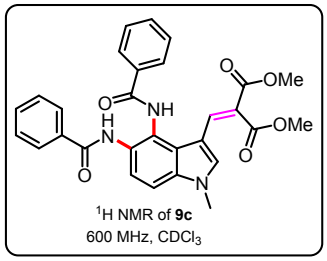

165.89
165.49
143.96
136.10
134.43
133.95
131.94
131.77
131.69
128.70
128.53
128.35
127.48
127.46
124.10
122.90
120.97
120.11
110.98
109.76
88.99
40.04
39.92
39.78
39.64
39.50
39.36
39.22
39.08
33.43
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
CN
NH
O
H
N
O
N
^{13}C NMR of **9a**
150 MHz, DMSO-d_6



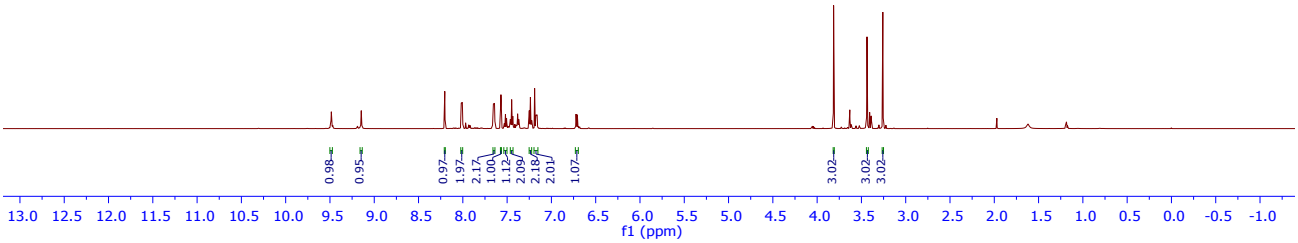
^{1}H NMR of **9b**
600 MHz, DMSO-d_6

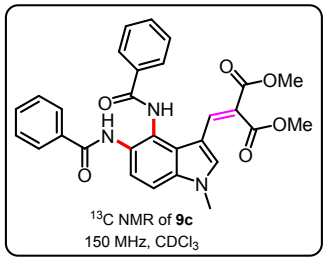


^{13}C NMR of **9b**
150 MHz, DMSO-d_6

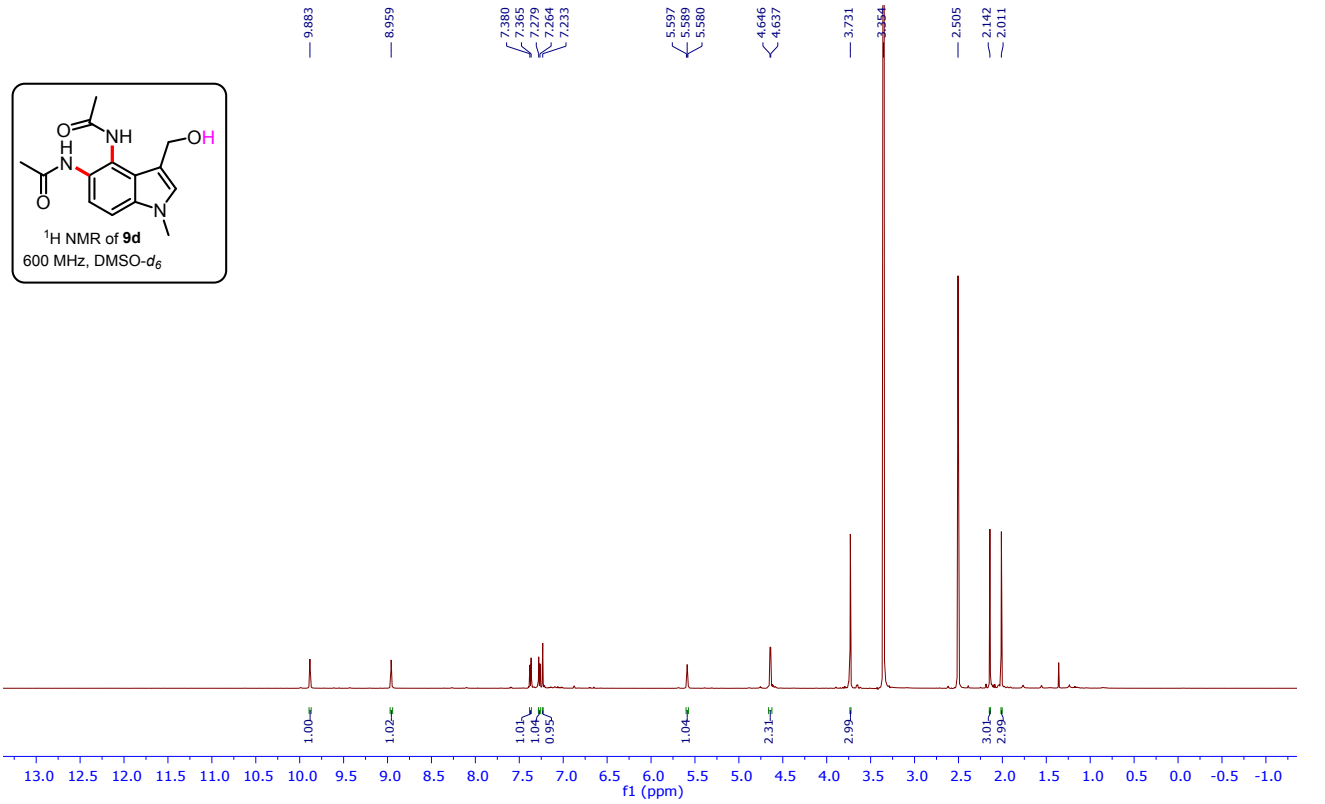


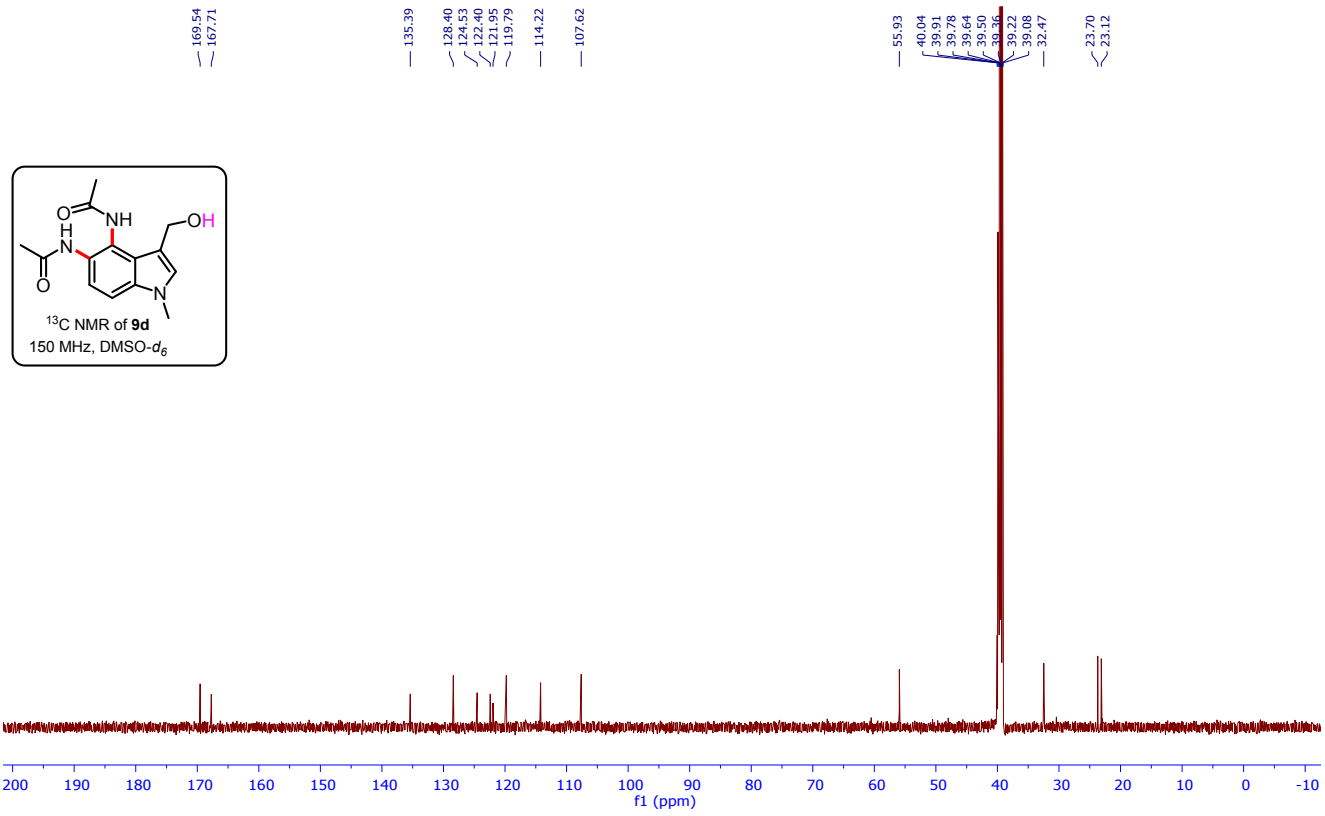
^{1}H NMR of **9c**
600 MHz, $CDCl_3$





^{13}C NMR of **9c**
150 MHz, $CDCl_3$


9.883
8.959
7.380
7.365
7.279
7.264
7.233
5.597
5.589
5.580
4.646
4.637
3.731
3.354
2.505
2.142
2.011
1.00
1.02
1.01
1.04
0.95
1.04
2.31
2.99
3.01
2.99
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
NH
OH
O
H
N
O
N
^{1}H NMR of **9d**
600 MHz, DMSO-d_6


169.54
167.71
135.39
128.40
124.53
122.40
121.95
119.79
114.22
107.62
55.93
40.04
39.91
39.78
39.64
39.50
39.36
39.22
39.08
32.47
23.70
23.12
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
NH
OH
O
H
N
O
N
^{13}C NMR of **9d**
150 MHz, DMSO-d_6

7. Computational details

All calculations were performed using DFT implemented in the Jaguar 9.1 suite of ab initio quantum chemistry programs.[2,3] Geometry optimizations were carried out with Becke's three-parameter exchange functional B3LYP including Grimme's D3 dispersion correction (B3LYP-D3)[4-9] using the 6-31G** basis set[10] for the main group elements. Ruthenium was represented using the Los Alamos double-ζ basis[11-13] which includes relativistic effective core potentials. The electronic energies of the optimized structures were re-evaluated by single-point calculations using the same functional and triple-ζ basis set, cc-pVTZ(-f),[14] that contains a double set of polarization functions. Single-point calculations for the transition metal employed LACV3P basis involving decontracted exponents to match the effective core potential in triple-ζ quality. Analytical vibrational frequencies with the harmonic approximation were obtained using the same level of theory as geometry optimization in order to confirm the proper convergence of local minima for the intermediates or first-order saddle points for the transition states on the potential energy surface. Solvation energies were calculated using a self-consistent reaction field (SCRF)[15-17] approach based on accurate numerical solutions of the Poisson-Boltzmann equation utilizing 6-31G** basis at the optimized gas-phase geometry with the dielectric constant of ε = 8.55 for trifluoroethanol (TFE). The solvation energies are subject to the empirical parametrization of the atomic radii that are used to generate the solute surface.[18] The solution-phase Gibbs free energies G(sol) were obtained with the following protocols:

$$G(sol) = G(gas) + G^{solv}$$

$$G(gas) = H(gas) - TS(gas)$$

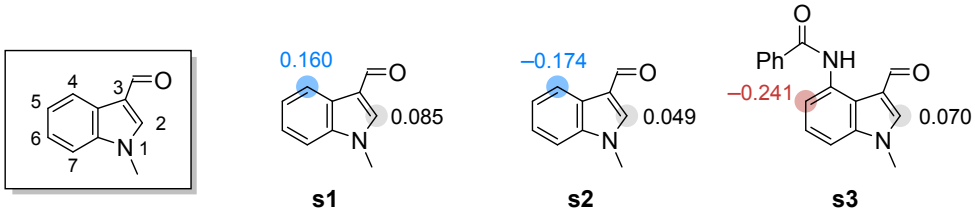
$$H(gas) = E(SCF) + ZPE$$

$$\Delta E(SCF) = \Sigma E(SCF) \text{ for products} - \Sigma E(SCF) \text{ for reactants}$$

$$\Delta G(sol) = \Sigma G(sol) \text{ for products} - \Sigma G(sol) \text{ for reactants}$$

where G(gas) is the free energy in gas phase; G^{solv} is the free energy of solvation; H(gas) is the enthalpy in gas phase; T is the temperature (298.15K); S(gas) is the entropy in gas phase; E(SCF) is the electronic energy computed from the self-consistent field procedure; ZPE is the zero-point energy. Note that the entropy here refers to the vibrational, rotational, and translational entropy of the solute(s), and the entropy of the solvent is included implicitly in the continuum solvation model.

7.1 Electronic features of indole substrates



Site	Fukui index (HOMO)	Natural Population Analysis (charge)	
C2	0.085	0.049	0.070
C4	0.160	–0.174	–
C5	0.040	–0.211	–0.241
C6	0.091	–0.196	–0.168
C7	0.138	–0.244	–0.268

Figure S1. NPA charge analysis and Fukui index of **1a** and **4a**.

Electronic features of each carbon of **1a** and **4a** were evaluated using Fukui index and natural population analysis (NPA) as summarized in Figure S5. Both Fukui index and NPA indicate C4-site is more nucleophilic than C2-site for **1a** as shown in **s1** and **s2**. Thus, it can be assumed that C4-ruthenation would be more efficient, if the *electrophilic* nature of the metal center overrides the C–H acidity of substrate during C–H metalation. In mono amidation product **4a**, an implemented amide group increases the electron density of C5 site through resonance, increasing the NPA charge difference between C2- and C4- position as shown in **s3**.

7.2 Distortion-interaction analysis of the second C–H ruthenation step.

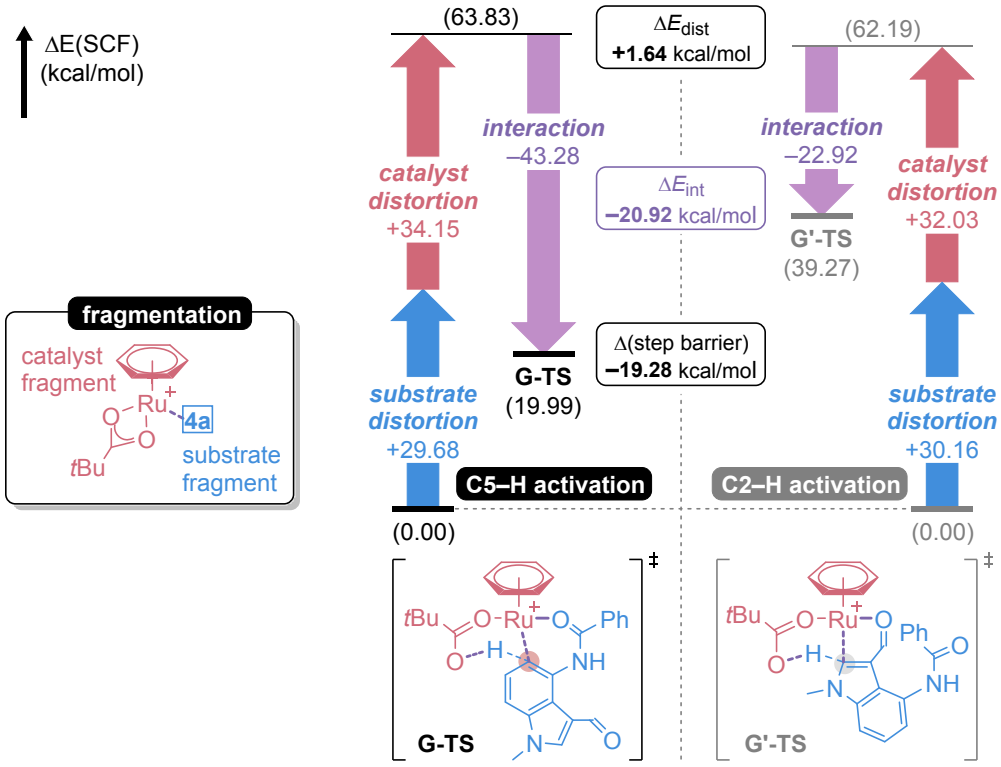


Figure S2. Distortion-interaction analysis diagram for **G-TS** and **G'-TS**.

The energy difference in C–H ruthenation step between **G-TS** for C4-site and **G'-TS** for C2-site is investigated using an activation-strain model. As summarized in Figure S6, the interaction energy (E_{int}) engenders a notable preference to **G-TS**, while the distortion energy (E_{dist}) of each fragment has marginal impact. Therefore, the second C–H ruthenation process can be described as *electrophilic* CMD (*e*CMD) process, favoring the more nucleophilic site and featuring a sensitive change in E_{int}.

7.3 Possibility of C6-amidation reaction

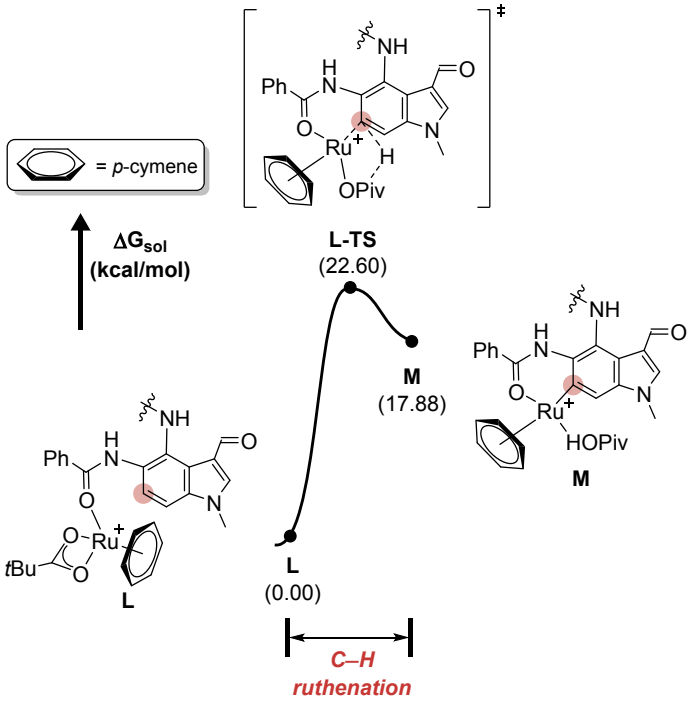


Figure S3. DFT-calculated energy profile for C6–H activation.

The possibility of C6–H activation was examined as depicted in Figure S3. While the C–H ruthenation transition state **L-TS** is accessible owing to the presence of an adjacent C5-amide group, the destabilization of resulting ruthenacycle **M** is of notable difference. Steric congestion between two neighboring amide groups enforces the complex **M** to be unstable compared to what found in first and second C–H activation product, **C** and **H**, showing differences of 5.3 and 7.8 kcal/mol respectively.

7.4 Energy components for DFT-optimized structures

Table S1. Computed Energy Components for Optimized Structures

Components	**E(SCF)/(eV)**	**ZPE/(kcal/mol)**	**S(gas)/(cal/mol·K)**	**G^{solv}/(kcal/mol)**
	B3LYP-D3 /cc-pVTZ(-f)	B3LYP-D3 /LACVP/6-31G**	B3LYP-D3 /LACVP/6-31G**	B3LYP-D3 /LACVP/6-31G**

PivOH	–9446.946	92.54	86.59	–6.78
1a	–14058.439	105.28	97.12	–9.33
2a	–16012.652	75.29	94.07	–6.75
4a	–24940.441	173.96	134.11	–12.70
5a	–35822.219	241.85	171.23	–16.42
CO_2	–5133.566	7.29	51.16	–2.29
A	–32031.576	314.70	196.71	–40.63
B	–36643.594	327.90	203.39	–39.06
B-sub[a]	–14058.327			
B-cat[b]	–22583.139			
B-TS	–36642.582	325.25	195.74	–40.63
B-TS-sub[a]	–14057.252			
B-TS-cat[b]	–22581.785			
B'-TS	–36642.445	325.47	195.83	–39.27
B'-TS-sub[a]	–14057.299			
B'-TS-cat[b]	–22581.773			
C	–36643.293	328.24	198.40	–36.66
C'	–36643.242	328.43	192.99	–37.01
D	–43208.992	311.12	205.15	–39.44
D-TS	–43208.207	308.74	207.56	–45.58
E	–38075.523	300.57	195.52	–44.09
E-TS	–38075.035	299.93	191.00	–43.38

F	–38076.895	301.90	193.09	–43.23
F-TS	–47524.510	393.00	230.14	–40.30
G	–47525.781	396.40	238.03	–38.33
G-sub[a]	–24940.277			
G-cat[b]	–22583.178			
G-TS	–47524.914	392.95	235.06	–39.00
G-TS-sub[a]	–24938.990			
G-TS-cat[b]	–22581.697			
G'-TS	–47524.078	393.51	235.22	–44.04
G'-TS-sub[a]	–24938.969			
G'-TS-cat[b]	–22581.789			
H	–47525.547	396.36	235.46	–36.16
I	–54091.199	379.16	240.66	–40.39
I-TS	–54090.461	378.00	238.29	–44.51
J	-48957.930	368.69	239.82	–38.66
J-TS	–48957.445	368.73	226.78	–40.62
K	–48959.438	370.11	227.48	–42.34
K-TS	–58407.270	461.49	264.89	–38.84
L	–58407.918	464.70	262.71	–39.88
L-TS	–58406.684	460.98	268.21	–40.25
M	–58407.254	464.39	260.60	–37.69

[a] Electronic energies of the substrate fragment for distortion-interaction analysis.

[b] Electronic energies of the catalyst fragment for distortion-interaction analysis.

7.5 Cartesian coordinates for DFT-optimized structures

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PivOH

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H	-1.654826641	2.281059265	-3.559230566
O	-1.659597754	1.657928944	-2.813710928
O	-1.664160371	3.632249355	-1.738672376
C	-1.665239573	2.420909882	-1.688892603
C	-1.672607899	1.570924640	-0.418055385
C	-1.679743528	2.501371384	0.802846849
H	-1.685678482	1.907136917	1.722615719
H	-0.797830105	3.147343397	0.810263813
H	-2.561450720	3.147745609	0.799773753
C	-2.935413837	0.681452274	-0.424368173
H	-2.947987318	0.019050913	-1.293396354
H	-2.956537724	0.067026064	0.481922150
H	-3.845842600	1.289754748	-0.440865487
C	-0.409483701	0.682072699	-0.409882337
H	-0.402765423	0.062069982	0.492776483
H	-0.382894754	0.024828702	-1.282650590
H	0.500843287	1.290730357	-0.408181667

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1a

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C	0.524967790	0.637573659	-2.129291534
C	0.548275948	-0.015405540	-0.888962805
C	0.558002293	0.749171376	0.301905423
C	0.535112679	2.146059275	0.298438251
C	0.508555830	2.772841930	-0.944209278
C	0.504664183	2.028269529	-2.141177416
C	0.568036735	-1.403731227	-0.490489393
C	0.587800205	-1.414422035	0.893718302
N	0.591433167	-0.136814386	1.377844691
H	0.519990623	0.048925467	-3.039297581
H	0.532591760	2.719737530	1.220052242
H	0.487572998	3.857756138	-0.991276324
H	0.483219236	2.556551218	-3.089919806
H	0.607143402	-2.260268927	1.568313956
C	0.536205649	0.257684797	2.771665573
H	-0.425785482	0.726085722	3.006968975
H	0.665738761	-0.623390853	3.402439594
H	1.337209105	0.969011366	2.995053053
C	0.576572537	-2.575883865	-1.342234015
O	0.563318968	-2.548194885	-2.565455914
H	0.594777584	-3.548002481	-0.797606826

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2a

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N	-2.099320412	-0.102104813	-3.830556154
O	-2.235720873	1.021766424	-2.972558737
C	-2.442506075	-1.109673262	-3.098371029
O	-2.798698187	-0.771263123	-1.827199817
C	-2.664314985	0.607228160	-1.750301361
O	-2.886109591	1.279242754	-0.791355968
C	-2.478272676	-2.509218931	-3.506713152
C	-2.100422382	-2.862605095	-4.812402725
C	-2.891088963	-3.494969130	-2.599247217
C	-2.137715101	-4.196979523	-5.200687408
C	-2.924555063	-4.829186440	-2.999523878
C	-2.549227715	-5.181765079	-4.296816349
H	-1.781830907	-2.090853214	-5.505198479
H	-3.181427002	-3.213361979	-1.592894912
H	-1.844856501	-4.471688747	-6.209261417
H	-3.244180202	-5.592799187	-2.297296524
H	-2.576347589	-6.222636223	-4.605216980

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4a

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C	2.252142906	-0.559548199	-3.200581551
C	2.209328175	-1.140697002	-1.905212402
C	2.344299793	-2.534888506	-1.815418720
C	2.423731327	-1.407150626	-4.321178913
C	2.153021097	0.792869925	-3.733657837
C	2.556417227	-2.794497252	-4.237837791

N	2.433278322	-0.614816010	-5.470617294
C	2.509974957	-3.331799030	-2.957860708
H	2.685773134	-3.414000273	-5.118370056
H	2.606529951	-4.405460835	-2.825991869
H	2.308202028	-2.990473747	-0.837930083
C	2.275434732	0.683037162	-5.114192009
C	1.979927778	2.074918747	-3.104939461
H	2.255636454	1.467303514	-5.858929634
C	2.599484921	-1.127872586	-6.817044258
H	1.799354196	-1.835453510	-7.056574821
H	2.564130306	-0.299080849	-7.525921345
H	3.562424183	-1.639557004	-6.914410591
O	1.848339081	2.294678926	-1.898806572
H	1.964239359	2.930378675	-3.811828852
N	2.061360359	-0.302047253	-0.794022560
C	1.948650718	-0.676115572	0.529405713
O	1.945690036	-1.843929291	0.915785372
C	1.811854839	0.452430815	1.515281439
C	2.226143837	1.769422412	1.271441579
C	1.269950747	0.125228435	2.767226219
C	2.081535339	2.742002964	2.261252403
H	2.666814089	2.047966480	0.321901232
C	1.118347526	1.099807262	3.748595953
H	0.978024006	-0.903676212	2.947284222
C	1.523702621	2.413427830	3.497120142
H	2.408316851	3.758792162	2.063357115
H	0.687179565	0.836270392	4.710317612
H	1.408905506	3.175618172	4.262904167
H	1.926807642	0.687836885	-1.020595789

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5a

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C	1.980175138	-4.022118568	-0.417817622
C	0.950666726	-3.528314114	-1.252502680
C	1.325511217	-2.839859009	-2.426542997
C	3.326846361	-3.749176979	-0.743370354
C	2.014426708	-4.805227280	0.810745299
C	3.705690145	-3.039896727	-1.884102106
N	4.138834953	-4.306082249	0.245933801
C	2.689969063	-2.600485802	-2.715276241
H	4.745839596	-2.842049122	-2.118091822
H	2.923003674	-2.073606968	-3.629943609
C	3.356033802	-4.927935600	1.159510136
C	0.990454793	-5.507099152	1.539177895
H	3.788955212	-5.449301243	2.002725363
C	5.588101387	-4.236238003	0.254215449
H	5.918445110	-3.193029881	0.272276968
H	5.967872620	-4.743883133	1.142305493
H	5.998297215	-4.721074104	-0.637267768
O	-0.192350239	-5.634626389	1.211742282
H	1.343782544	-5.992027760	2.472451925
N	-0.385989338	-3.815961361	-0.885262609
H	-0.460354775	-4.596445560	-0.221206129
C	-1.461267114	-2.970207691	-0.907372594
O	-1.413623333	-1.810990453	-1.351575851
C	-2.742155552	-3.515901089	-0.353663921
C	-2.982658863	-4.880881310	-0.133718804
C	-3.752461195	-2.586142778	-0.064867333
C	-4.208086014	-5.300241947	0.382019281
C	-4.972945213	-3.008604765	0.453347087
C	-5.203015327	-4.367781162	0.679396212
H	-2.227526903	-5.622757912	-0.364277542
H	-3.556045771	-1.536503792	-0.253855646
H	-4.385668755	-6.358560562	0.548159897
H	-5.745502472	-2.279622316	0.680521131
H	-6.155930042	-4.699055672	1.082717180
C	0.398039669	-2.331554890	-4.665712357
N	0.325817347	-2.372090101	-3.296242476
O	1.378120184	-2.715210676	-5.303545475
C	-0.826864302	-1.792113900	-5.360967159
C	-0.765920460	-1.725817323	-6.759972095
C	-1.996813893	-1.369720697	-4.708023071
C	-1.845791459	-1.246585131	-7.495707035
H	0.144174278	-2.060474634	-7.245690346
C	-3.076543331	-0.888420403	-5.448739052
H	-2.091457844	-1.407736659	-3.627565145
C	-3.004260063	-0.824014664	-6.840976715
H	-1.784298897	-1.201354027	-8.579358101
H	-3.975574970	-0.562294185	-4.933567047
H	-3.847811460	-0.446659774	-7.412489891
H	-0.480237842	-1.984247684	-2.805096388

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CO_2

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C	-2.814436436	0.000000000	-3.463116884
O	-2.262597084	-0.126832008	-2.440206766
O	-3.366275787	0.126832008	-4.486027241

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A

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C	0.152070373	0.694550872	-3.075703382
C	-1.005001187	0.319390029	-2.356092930
C	1.458598137	0.671165228	-2.472401381
H	-1.962594390	0.278428435	-2.864662409
C	-0.911831379	-0.126278475	-0.990773618
C	1.533616900	0.237858459	-1.129012108
H	2.510255337	0.115231343	-0.671074510
C	0.369765550	-0.155786902	-0.391910791
H	0.481950849	-0.563944578	0.605908394
H	0.058674831	0.927935123	-4.130017757
C	2.700927973	1.044837117	-3.259332418
H	3.560509920	0.688497901	-2.677943945
C	2.791963339	2.580398321	-3.364519835
H	3.711461782	2.865656137	-3.883868217
H	1.947035670	2.982421637	-3.934727669
H	2.795002699	3.055119753	-2.378489494
C	2.761817217	0.380139470	-4.645132542
H	2.646043301	-0.704738557	-4.578760147
H	1.983641148	0.762873888	-5.314155579
H	3.725116730	0.601339221	-5.113570690
C	-2.132898331	-0.632806122	-0.277788609
H	-2.756191015	-1.222699285	-0.955167711
H	-1.860768437	-1.257303953	0.575327992
H	-2.728980541	0.211808488	0.086074367
Ru	0.434918761	-1.344989657	-2.291743279
O	0.627268136	-2.299934387	-4.186338425
C	-0.296268523	-3.132585526	-3.895229340
O	-0.887722194	-2.941280127	-2.770473957
C	-0.695293546	-4.259298801	-4.826192856
C	0.467657685	-4.586944103	-5.778028011
C	-1.088764548	-5.496117592	-3.996495008
C	-1.920043349	-3.752969980	-5.628679276
H	0.167018548	-5.384937763	-6.463488579
H	0.757830262	-3.713600636	-6.366726398
H	1.349100351	-4.926161766	-5.223933220
H	-1.881258607	-5.261372566	-3.281777382
H	-1.443275332	-6.288354397	-4.662505150
H	-0.227452129	-5.886892319	-3.443488121
H	-2.248404503	-4.534757137	-6.320384026
H	-2.753708363	-3.509913445	-4.963128567
H	-1.666370153	-2.864336014	-6.215128899
O	0.482670724	-3.508307457	0.079887480
C	1.415097237	-3.819223404	-0.817900658
O	1.667759299	-3.010997295	-1.713952541
C	2.167590618	-5.137402534	-0.678653955
C	2.953999519	-5.413190842	-1.969605803
C	3.136504412	-4.986908913	0.522028744
C	1.162185192	-6.282192707	-0.411492884
H	3.508628845	-6.349184036	-1.863150001
H	2.283697605	-5.504941463	-2.828903675
H	3.663058281	-4.610103607	-2.181023359
H	2.606284380	-4.776089668	1.457110643
H	3.689228296	-5.921046257	0.655627787
H	3.860304117	-4.185209274	0.347578824
H	1.702874780	-7.231844425	-0.384856790
H	0.652948916	-6.190834045	0.556863666
H	0.401938289	-6.345424652	-1.195194364
H	0.341075510	-4.241132259	0.699167788

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B

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C	-0.774099886	0.532889068	-2.609713078
C	-1.775982380	-0.272475302	-1.995347142
C	0.419029295	0.916716576	-1.930068851
H	-2.635856390	-0.595920563	-2.571943283
C	-1.590740681	-0.758064568	-0.667213798
C	0.570905864	0.442743868	-0.591034412
H	1.501543283	0.631417632	-0.066304706
C	-0.410365224	-0.362042546	0.041907366
H	-0.228319243	-0.752736807	1.037590027
H	-0.883905351	0.790796757	-3.659251451
C	1.477508903	1.751407504	-2.629430294
H	1.313982606	1.617616653	-3.706851244
C	2.911609411	1.297313333	-2.315681458
H	3.617182255	1.847835779	-2.945358992

H	3.184709787	1.502713799	-1.273890376
H	3.040390968	0.227167502	-2.502042770
C	1.266350150	3.241221905	-2.292606354
H	0.258501530	3.576259613	-2.558858156
H	1.413537383	3.422826052	-1.221486211
H	1.986014724	3.857659101	-2.840620041
C	-2.577454567	-1.715284705	-0.060471199
H	-2.948013544	-2.416484594	-0.813347995
H	-2.124543428	-2.290234089	0.751109183
H	-3.431466818	-1.159060121	0.343434542
Ru	0.167744577	-1.339166403	-1.896377087
O	0.244559169	-2.376989126	-3.761173248
C	-0.013401768	-3.486528635	-3.183485985
O	-0.290052861	-3.415490627	-1.928988934
C	0.011300791	-4.819303989	-3.905201674
C	0.563855767	-4.644217968	-5.328577995
C	0.899909616	-5.790197372	-3.096457958
C	-1.443142176	-5.346578598	-3.940419197
H	0.549350798	-5.608417988	-5.846370220
H	-0.034482535	-3.933543444	-5.904531956
H	1.595780492	-4.281173229	-5.307881355
H	0.535578668	-5.897590637	-2.071399689
H	0.890689969	-6.774624348	-3.574658394
H	1.935120821	-5.437444210	-3.065120459
H	-1.463251948	-6.326982975	-4.426546097
H	-1.846304655	-5.453392982	-2.929245949
H	-2.095002651	-4.674372673	-4.508378506
C	4.319298267	-3.905315876	-2.702001572
C	4.119720459	-3.298924685	-3.948083878
C	4.927406788	-3.702292204	-5.008557320
H	3.345275402	-2.551176786	-4.073054790
C	5.312971115	-4.897403717	-2.559448719
C	3.678187132	-3.782514095	-1.406919718
C	6.131484509	-5.303298950	-3.613036871
N	5.280114174	-5.354581356	-1.231768012
C	5.921110153	-4.685622692	-4.843423843
H	6.894234657	-6.064568043	-3.486249685
H	6.536424160	-4.969406128	-5.691371441
H	4.790037155	-3.249838114	-5.985876083
C	4.310336590	-4.704712391	-0.559931517
C	2.589663267	-2.962523460	-1.054943800
H	4.114972115	-4.919320583	0.482353300
C	6.155461311	-6.389933109	-0.699518979
H	7.199516296	-6.080174446	-0.797290683
H	5.926806450	-6.551621914	0.354596198
H	6.005222321	-7.323468208	-1.248676538
O	2.139332771	-2.087324142	-1.843525529
H	2.120450497	-3.100907803	-0.069726080

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B-TS

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C	-0.748140216	0.642014265	-2.913578749
C	-1.279367208	0.324509591	-1.637929797
C	0.622672737	0.999402463	-3.096934557
H	-2.307721138	-0.009306731	-1.551578641
C	-0.438680798	0.333124161	-0.480794609
C	1.432935476	1.020792365	-1.923416734
H	2.494708061	1.216264486	-2.027464390
C	0.923729360	0.709632158	-0.633293629
H	1.590661645	0.692255795	0.221043274
H	-1.381843805	0.511911750	-3.784068823
C	1.186246634	1.350070715	-4.464090824
H	2.263568163	1.511264563	-4.329783440
C	0.567545712	2.672941685	-4.955326080
H	1.029284358	2.977881193	-5.898758888
H	-0.507917881	2.559758186	-5.131420612
H	0.710171223	3.479576349	-4.229554653
C	1.004709125	0.222556040	-5.494956017
H	1.511237621	-0.693658412	-5.180365086
H	-0.052053537	-0.018199677	-5.649714947
H	1.418715119	0.531166255	-6.459549904
C	-0.987377584	-0.114694335	0.843794703
H	-1.588123679	-1.019499421	0.719308615
H	-0.187928811	-0.320936054	1.558581471
H	-1.631257057	0.667313695	1.261443138
Ru	0.486977905	-1.006584406	-2.070832491
O	-0.384739041	-2.173934221	-3.558868885
C	0.272113472	-3.016901016	-4.273551464
O	1.502478004	-3.224931717	-4.138306618
C	-0.503862083	-3.787994146	-5.351214409
C	-0.377580881	-5.291163921	-5.020212650
C	-1.979883790	-3.369423151	-5.387560368
C	0.175178245	-3.494428635	-6.706439495

H	-0.878901362	-5.881790638	-5.793769360
H	0.671986163	-5.592492580	-4.975378036
H	-0.849033535	-5.525186539	-4.059263706
H	-2.085376501	-2.304584265	-5.615197659
H	-2.504254580	-3.938320637	-6.161794186
H	-2.470344782	-3.557603598	-4.428665638
H	-0.323896497	-4.061223030	-7.498837948
H	0.108874954	-2.430800438	-6.960951805
H	1.229829669	-3.778640270	-6.682708263
C	2.893584251	-2.627781153	-1.029885530
C	2.606636047	-1.838849187	-2.161624670
C	3.705047131	-1.168042660	-2.736780643
H	1.917220950	-2.357895613	-3.034846067
C	4.210839272	-2.764854431	-0.547000587
C	2.060086012	-3.450559378	-0.193505764
C	5.287364483	-2.090751648	-1.123482585
N	4.182053089	-3.664786577	0.527165234
C	5.006619930	-1.278349876	-2.225018501
H	6.300771713	-2.204130173	-0.752664745
H	5.819715977	-0.751193047	-2.714159012
H	3.545660734	-0.592397034	-3.644307852
C	2.910455227	-4.076574802	0.726660907
C	0.644411862	-3.475367069	-0.199108914
H	2.669156551	-4.768767834	1.522608638
C	5.355138302	-4.082583904	1.285479784
H	5.827235222	-3.214213133	1.753265738
H	5.051428318	-4.785968304	2.061534882
H	6.074678421	-4.570336342	0.622049510
O	-0.083674558	-2.693053961	-0.855716527
H	0.128239676	-4.205756187	0.440268874

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B'-TS

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C	-1.120968819	-0.729129314	-8.334472656
C	-0.802105546	-0.229859248	-9.611492157
C	-0.580759466	-1.970697641	-7.842157364
H	-1.179362655	0.737640381	-9.924161911
C	0.101286314	-0.948914409	-10.464110374
C	0.281025290	-2.683656693	-8.714312553
H	0.794221342	-3.564721107	-8.348532677
C	0.628865600	-2.183566332	-10.006495476
H	1.341688275	-2.725406408	-10.618214607
H	-1.723147750	-0.122733466	-7.664281845
C	-0.901978850	-2.416965723	-6.426662445
H	-0.956744611	-1.497659564	-5.828270912
C	0.183226049	-3.309370995	-5.809536934
H	-0.031076431	-3.463924885	-4.748248577
H	0.208089173	-4.299672127	-6.279043198
H	1.173850894	-2.853934526	-5.901048183
C	-2.288235903	-3.092418194	-6.400985241
H	-3.068622112	-2.437509775	-6.803212166
H	-2.282334805	-4.016376495	-6.989544868
H	-2.559764862	-3.348059177	-5.372377872
C	0.452212393	-0.398172826	-11.816893578
H	0.491364658	0.693461120	-11.798206329
H	1.408487558	-0.785615444	-12.173826218
H	-0.322272509	-0.693505168	-12.534912109
Ru	1.108171344	-0.637038469	-8.434240341
C	1.847285986	3.535335541	-8.666650772
C	1.555557251	4.841025352	-8.239970207
C	1.784673095	5.889431953	-9.119715691
C	2.337021589	3.327338457	-9.983517647
C	1.775913119	2.230065107	-8.071737289
C	2.572176933	4.381481171	-10.872509003
N	2.548307180	1.962621093	-10.165495872
C	2.287330866	5.662931442	-10.419552803
H	2.958963394	4.208773613	-11.871231079
H	2.454906225	6.509553909	-11.077527046
H	1.579251528	6.907207012	-8.803555489
C	2.219987154	1.278120875	-9.028409958
C	1.342142701	1.751574755	-6.816111565
H	3.048851728	0.403101742	-8.795989037
C	3.298577309	1.404010057	-11.283437729
H	4.278694153	1.885182142	-11.348362923
H	3.439082384	0.337328166	-11.111712456
H	2.760272026	1.561560035	-12.221813202
O	1.121161461	0.518855035	-6.635106087
H	1.194543242	2.421033382	-5.960970402
C	3.953577995	-1.249312520	-7.783580780
O	2.733545303	-1.579333186	-7.546276093
O	4.279859066	-0.294368654	-8.535481453
C	5.052603722	-2.080447197	-7.106915474
C	5.924799442	-1.108714581	-6.282710075

C	4.454512596	-3.165309429	-6.199536800
C	5.898444653	-2.720048428	-8.230141640
H	5.342641354	-0.634606361	-5.485022068
H	6.746811390	-1.661077619	-5.816655159
H	6.345071316	-0.325688541	-6.918252468
H	5.261631012	-3.739659309	-5.734173775
H	3.843867302	-2.727057219	-5.405011654
H	3.824650526	-3.857072592	-6.766149044
H	6.317519665	-1.954288840	-8.887759209
H	6.722111702	-3.290059090	-7.789150238
H	5.298600674	-3.409595013	-8.834763527
H	1.175744772	5.029820919	-7.240949154

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C

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C	-0.757540762	0.723296523	-3.131927729
C	-1.572080970	0.487010807	-1.994219184
C	0.579174340	1.227079988	-3.039131641
H	-2.579907656	0.107674964	-2.118154764
C	-1.010896087	0.594181418	-0.702349424
C	1.107904434	1.379029274	-1.725801349
H	2.139373064	1.692725062	-1.600589871
C	0.351345688	1.031577349	-0.574696243
H	0.802679181	1.099902749	0.409213424
H	-1.167761326	0.510685623	-4.113687992
C	1.361506581	1.648831248	-4.270915985
H	2.400749207	1.804424047	-3.954171181
C	0.820912182	3.001925945	-4.776420593
H	1.418711066	3.359146595	-5.620495319
H	-0.216439128	2.903743982	-5.115773201
H	0.849671304	3.763900280	-3.991237402
C	1.361865520	0.594210327	-5.387888432
H	1.767575979	-0.358626962	-5.039534092
H	0.354154289	0.411071062	-5.776593208
H	1.974088550	0.938754082	-6.226747990
C	-1.782943606	0.193963870	0.522750080
H	-2.671452522	-0.391605467	0.263205379
H	-1.154792786	-0.408308834	1.191021919
H	-2.100947857	1.092938423	1.070390940
Ru	0.446672827	-0.741830289	-1.911772370
O	0.042118073	-2.338092566	-3.348567247
C	0.711200953	-3.067560434	-4.093244076
O	1.999502420	-2.890472174	-4.322183132
C	0.109322414	-4.284408569	-4.778662682
C	0.651636899	-5.516118050	-4.007339478
C	-1.422922373	-4.230714798	-4.687642097
C	0.569163978	-4.342546940	-6.250448227
H	0.234198496	-6.427146912	-4.446406364
H	1.742318153	-5.569754601	-4.067290783
H	0.361458749	-5.482082844	-2.951475859
H	-1.819715858	-3.351952553	-5.205110073
H	-1.846721172	-5.122986794	-5.157593250
H	-1.759090185	-4.191120625	-3.648486137
H	0.150532961	-5.236279964	-6.722782612
H	0.217606932	-3.469722033	-6.810238838
H	1.657772422	-4.387555599	-6.330227375
C	2.702728748	-2.596092463	-1.170976162
C	2.414555788	-1.388982773	-1.835719466
C	3.520991087	-0.782965899	-2.459698677
H	2.351732016	-2.188632488	-3.726301908
C	3.999856710	-3.151998520	-1.149189115
C	1.857420325	-3.511354208	-0.441839844
C	5.084506989	-2.543896675	-1.782298446
N	3.939494133	-4.357273579	-0.437521368
C	4.816825867	-1.345183492	-2.436190844
H	6.078347206	-2.978765011	-1.775374889
H	5.622670650	-0.831774712	-2.952378511
H	3.388933659	0.143026695	-3.009993553
C	2.671190500	-4.566061497	-0.016067248
C	0.489686131	-3.298737049	-0.165586516
H	2.415206909	-5.444635391	0.560739517
C	5.080078125	-5.235984802	-0.210825175
H	5.859880924	-4.702753544	0.339946032
H	4.760340691	-6.101864815	0.370250136
H	5.486481667	-5.576605320	-1.167500854
O	-0.164448053	-2.309818745	-0.578307688
H	-0.048193362	-4.021327972	0.464310735

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C'

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C	-1.164083719	-0.422913313	-8.674798965
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C	-0.948268056	-1.586268306	-7.845489025
H	-0.828487873	0.549754143	-10.579134941
C	0.145115405	-1.407051086	-10.535245895
C	-0.145839319	-2.608825445	-8.370336533
H	0.133514822	-3.453386784	-7.753907204
C	0.433133274	-2.489612341	-9.676243782
H	1.112989545	-3.264062643	-10.018209457
H	-1.717466831	0.417594463	-8.268573761
C	-1.497677922	-1.592139006	-6.433086395
H	-1.441027164	-0.552177906	-6.087143421
C	-0.675560296	-2.445519209	-5.459999084
H	-1.047935367	-2.302121162	-4.441999912
H	-0.755828083	-3.514895916	-5.684691429
H	0.380071968	-2.157607555	-5.480384827
C	-2.980156183	-2.018583298	-6.456688881
H	-3.576362848	-1.382619977	-7.118963242
H	-3.081376314	-3.054542065	-6.797469139
H	-3.403865814	-1.949823976	-5.450518608
C	0.580877364	-1.402746320	-11.974367142
H	0.679779887	-0.388220161	-12.365262032
H	1.527756929	-1.931905866	-12.111545563
H	-0.175750121	-1.916518688	-12.579200745
Ru	1.042303920	-0.596386731	-8.535349846
C	2.795944214	3.255982161	-8.387284279
C	3.157331705	4.479220867	-7.816728115
C	3.865193844	5.392774582	-8.596693039
C	3.157404661	2.981128216	-9.725272179
C	2.094227552	2.069520473	-7.933280468
C	3.864989281	3.884902716	-10.514232635
N	2.690772772	1.686594248	-10.058264732
C	4.214296341	5.100880623	-9.925145149
H	4.133162022	3.662107944	-11.541615486
H	4.765045643	5.834202766	-10.505571365
H	4.152033806	6.349014759	-8.170490265
C	2.031464577	1.129826784	-9.018736839
C	1.542803884	1.614835382	-6.735940456
C	2.977277040	1.056389689	-11.335287094
H	4.038952351	1.170850158	-11.571078300
H	2.742426395	-0.002998289	-11.258347511
H	2.389286518	1.513922572	-12.137815475
O	1.040913582	0.437032998	-6.681294441
H	1.541718006	2.198799372	-5.811351776
C	3.870310307	-1.234421134	-7.285404682
O	2.821499109	-1.576179624	-7.855428696
O	4.274535179	0.015451179	-7.185693741
C	4.794752598	-2.248797417	-6.630435944
C	4.877558231	-1.894947410	-5.124638081
C	4.229865551	-3.664730549	-6.816133022
C	6.193440914	-2.128564596	-7.277744770
H	3.892116785	-1.946201921	-4.649437904
H	5.531917572	-2.614887714	-4.624457359
H	5.286161423	-0.892955899	-4.972857475
H	4.895587444	-4.387497425	-6.336232662
H	3.238458157	-3.757957458	-6.363622665
H	4.146653175	-3.924702168	-7.875379086
H	6.604811668	-1.123911500	-7.154411316
H	6.871030807	-2.841030598	-6.798521519
H	6.157838345	-2.363666296	-8.346828461
H	2.891804218	4.716613293	-6.791113377
H	3.623565912	0.637933612	-7.578835964

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D

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C	-0.644406199	0.699306607	-3.091603994
C	-1.462617993	0.394820780	-1.973901749
C	0.652254999	1.293055892	-2.967283726
H	-2.444119930	-0.038223919	-2.124006033
C	-0.928796113	0.511646211	-0.672370732
C	1.141468048	1.463341355	-1.643593311
H	2.144751787	1.848966479	-1.494661927
C	0.393010348	1.045272350	-0.513070881
H	0.822235465	1.130264997	0.479051411
H	-1.029548168	0.489273041	-4.084370613
C	1.416438699	1.783755898	-4.184574127
H	2.416074514	2.077429533	-3.841165543
C	0.729176104	3.041999340	-4.750216007
H	1.308739185	3.446883678	-5.585127831
H	-0.274520993	2.805542469	-5.121196270
H	0.634041965	3.823550224	-3.990068436
C	1.589105964	0.701672673	-5.263229847
H	2.114629984	-0.169600397	-4.865891933
H	0.622299790	0.372457922	-5.661642551
H	2.165250063	1.099231482	-6.103838921

C	-1.700913906	0.047273222	0.529530883
H	-2.468262911	-0.678112566	0.251461715
H	-1.035942197	-0.416861594	1.261533976
H	-2.191286325	0.902130961	1.009300828
Ru	0.642255306	-0.722016454	-1.883462071
C	3.063241243	-2.267161608	-0.982915342
C	2.663905382	-1.154259562	-1.734406948
C	3.705470324	-0.452396542	-2.356287241
C	4.417563438	-2.645410061	-0.864314795
C	2.306546926	-3.230078220	-0.215102345
C	5.447096825	-1.945254803	-1.490249991
N	4.473360062	-3.794230700	-0.056859989
C	5.056213856	-0.837826490	-2.240317822
H	6.487289429	-2.240644932	-1.406129241
H	5.814100266	-0.256731629	-2.757679939
H	3.486707449	0.409214884	-2.976765156
C	3.227975130	-4.137226582	0.328013062
C	0.918442190	-3.198884726	-0.031472839
H	3.056448460	-4.997397900	0.961268902
C	5.702663422	-4.498294353	0.282537133
H	6.383217335	-3.825435877	0.811535358
H	5.468134403	-5.348907948	0.923888266
H	6.190101147	-4.857496262	-0.628192306
O	0.153617308	-2.340438366	-0.558369040
H	0.440573126	-3.946978331	0.615250468
O	1.829555154	-2.551438570	-4.073246002
N	0.612533867	-2.198654413	-3.426422119
C	-0.326307088	-2.808161259	-4.089592934
C	1.537475467	-3.328752756	-5.154920101
O	0.157269329	-3.494792461	-5.152169704
C	-1.766495347	-2.812496662	-3.859817266
O	2.300147295	-3.781680822	-5.941410065
C	-2.619460344	-2.834502459	-4.977818012
C	-2.297317505	-2.821753025	-2.559598446
C	-3.998921394	-2.825647354	-4.790814877
H	-2.200315237	-2.854980469	-5.978388786
C	-3.678663492	-2.822671175	-2.389073849
H	-1.634377718	-2.828090191	-1.703117728
C	-4.529191494	-2.814941883	-3.498242378
H	-4.659093857	-2.834023952	-5.652196407
H	-4.095401287	-2.839716196	-1.386476994
H	-5.605666161	-2.814640045	-3.355849981

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D-TS

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C	-0.819349885	0.477462679	-3.154044390
C	-1.567222238	0.273472697	-1.962071300
C	0.424131662	1.173123002	-3.166759491
H	-2.513645887	-0.253847957	-2.011360884
C	-1.025916934	0.627713442	-0.709828079
C	0.937908709	1.551376820	-1.894185305
H	1.908871889	2.032791138	-1.839445949
C	0.260937184	1.248795986	-0.690254748
H	0.714386046	1.507750154	0.260322899
H	-1.227718234	0.106738098	-4.087853432
C	1.126826882	1.513365030	-4.467955112
H	2.119710684	1.898772955	-4.206068993
C	0.364036977	2.645339966	-5.186070442
H	0.899690747	2.937096834	-6.093842506
H	-0.638649642	2.315757513	-5.479402065
H	0.261178046	3.531050920	-4.551375866
C	1.314851165	0.285182953	-5.376323223
H	1.848264098	-0.518875539	-4.863492012
H	0.353264272	-0.110845134	-5.720985889
H	1.882904172	0.569804907	-6.266566277
C	-1.715734005	0.256662697	0.572278976
H	-2.794116735	0.158153206	0.429376036
H	-1.326327443	-0.709652364	0.915467858
H	-1.526927352	0.996839583	1.353952408
Ru	0.621506035	-0.785664618	-1.865281224
C	3.146737814	-2.156234980	-1.131090164
C	2.667380571	-1.015874147	-1.779920936
C	3.602814436	-0.275825888	-2.508847475
C	4.489902020	-2.560932636	-1.255533934
C	2.491814137	-3.155570269	-0.324650556
C	5.420528412	-1.838186860	-1.999725461
N	4.637931347	-3.770660639	-0.555825830
C	4.948586941	-0.679520607	-2.612171650
H	6.451400280	-2.157854319	-2.106461048
H	5.630239487	-0.081309199	-3.208942652
H	3.305089712	0.606249988	-3.060991764
C	3.461001158	-4.117837906	-0.001139131
C	1.154972672	-3.090041399	0.082764879
H	3.364018917	-5.022513866	0.583763003

C	5.873721123	-4.543311119	-0.505573571
H	6.675818920	-3.935536861	-0.078864664
H	5.722703457	-5.426669121	0.115938038
H	6.155524254	-4.856782436	-1.514706492
O	0.347122818	-2.187342644	-0.287696183
H	0.758997142	-3.834575176	0.784477353
N	0.450932175	-2.256271839	-3.009004354
C	-0.257955641	-3.072640896	-3.741501570
O	2.279621363	-2.856362820	-3.994786024
C	1.940378547	-3.618003368	-4.896391869
O	2.293964624	-4.265112400	-5.821871281
O	0.188642189	-3.806643486	-4.686697483
C	-1.732856512	-3.100700617	-3.460898638
C	-2.596748590	-3.148101807	-4.563127041
C	-2.245203972	-3.075105667	-2.157478809
C	-3.975574493	-3.138736010	-4.356435299
H	-2.181887388	-3.202214003	-5.564057350
C	-3.625870466	-3.080555916	-1.961659431
H	-1.569670200	-3.054141045	-1.309772372
C	-4.491581917	-3.101000786	-3.058706284
H	-4.646933079	-3.169887304	-5.209143639
H	-4.026782036	-3.079222441	-0.951995492
H	-5.566274643	-3.100519180	-2.902246237

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E

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C	-0.810211122	1.212411523	-2.994403362
C	-1.308472157	1.225724339	-1.669331789
C	0.574363708	1.357614636	-3.263450623
H	-2.370105982	1.074720860	-1.499491096
C	-0.453028768	1.440543532	-0.552457869
C	1.424355149	1.489824176	-2.130046129
H	2.496087313	1.560310006	-2.284365416
C	0.928122044	1.566624761	-0.804402828
H	1.621629834	1.688633323	0.020489268
H	-1.502305031	1.044229984	-3.811302900
C	1.142577529	1.406759977	-4.668259144
H	2.187139034	1.077200413	-4.595965385
C	1.146217227	2.868872881	-5.164996147
H	1.605888486	2.924853802	-6.156012535
H	0.123439364	3.252365351	-5.244369507
H	1.706327081	3.525205851	-4.491434097
C	0.419862032	0.475168228	-5.651738644
H	0.338947684	-0.541179419	-5.255045414
H	-0.590710461	0.832371652	-5.878752708
H	0.968322456	0.443888694	-6.597110271
C	-1.007119060	1.400447607	0.842494011
H	-1.247600079	0.361612558	1.099195957
H	-0.289066732	1.779977202	1.572471023
H	-1.928960323	1.984258294	0.915995300
Ru	0.295778185	-0.611714602	-1.863062382
C	2.221004009	-2.665407419	-0.893024445
C	2.136894703	-1.529608130	-1.703201652
C	3.256466150	-1.242148519	-2.489942074
C	3.357544184	-3.497934103	-0.909815371
C	1.271992803	-3.284126997	0.001120009
C	4.479176044	-3.209384441	-1.687178612
N	3.094852686	-4.591687202	-0.070975237
C	4.408238411	-2.056184530	-2.464983225
H	5.354515553	-3.849299431	-1.699703217
H	5.253051281	-1.788612485	-3.092489719
H	3.247821569	-0.401279598	-3.175240517
C	1.865359664	-4.463363171	0.469983310
C	0.013803170	-2.743871450	0.305237412
H	1.470570445	-5.212004185	1.143304348
C	3.985000372	-5.734801292	0.079234548
H	4.972030640	-5.398444653	0.406620979
H	3.575186491	-6.417995930	0.823830009
H	4.075691223	-6.253677845	-0.879525423
O	-0.448798925	-1.698020577	-0.231601715
H	-0.626046121	-3.222205400	1.055502892
N	-0.321636528	-1.835016727	-3.076279640
C	-0.516978979	-3.191356421	-2.820812464
O	-1.542011142	-3.549967766	-2.246603251
C	0.541300237	-4.131521225	-3.289254189
C	1.570171118	-3.740862846	-4.155981064
C	0.514652014	-5.435095787	-2.774299860
C	2.573652744	-4.645990849	-4.492837429
H	1.586641192	-2.732060432	-4.554612637
C	1.521742344	-6.336204052	-3.110030174
H	-0.301045418	-5.717090607	-2.116306543
C	2.553839445	-5.941123009	-3.967334032
H	3.371335268	-4.344027042	-5.164540291

H	1.497288465	-7.348405361	-2.715989828
H	3.335405350	-6.646744251	-4.235706806

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E-TS

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C	-0.872864604	1.276490569	-2.855266333
C	-1.319665670	1.235442638	-1.510482669
C	0.509134352	1.427536488	-3.170400381
H	-2.369508266	1.056149960	-1.302746892
C	-0.411578566	1.397224903	-0.417335898
C	1.405846357	1.491161108	-2.065929174
H	2.472815990	1.532686234	-2.261554003
C	0.958223939	1.529291749	-0.709130168
H	1.682176471	1.596975446	0.095050916
H	-1.595268130	1.138640046	-3.651694536
C	1.023629069	1.522293687	-4.594417572
H	2.086184978	1.246092677	-4.562162399
C	0.932245553	2.988944292	-5.063450336
H	1.360642195	3.089335680	-6.065063000
H	-0.112511463	3.315227509	-5.109778404
H	1.470919013	3.664593220	-4.391410351
C	0.317590743	0.569849014	-5.570793152
H	0.345069140	-0.460799456	-5.209464073
H	-0.728702128	0.853403211	-5.727632046
H	0.810513198	0.616778910	-6.546199322
C	-0.924483538	1.299192071	0.992687225
H	-1.466107130	0.356752694	1.123228550
H	-0.111682363	1.338387728	1.720817447
H	-1.620408297	2.118316650	1.202162981
Ru	0.253336132	-0.431140304	-1.809590101
C	2.097354889	-2.713151932	-0.997895837
C	2.027992487	-1.626442552	-1.877194762
C	3.152078629	-1.363955140	-2.671767235
C	3.256088734	-3.510629416	-0.928272009
C	1.129051447	-3.298034668	-0.113293596
C	4.389491081	-3.233902693	-1.691263676
N	2.990615368	-4.561866760	-0.041311931
C	4.321208000	-2.133825541	-2.549977541
H	5.275650501	-3.858207703	-1.649908185
H	5.179453850	-1.894059658	-3.169850349
H	3.112579823	-0.577624977	-3.418067217
C	1.733670473	-4.437731743	0.436104059
C	-0.159622252	-2.774968624	0.142849028
H	1.331697106	-5.158597469	1.135440826
C	3.904112101	-5.668486118	0.218487874
H	4.870727062	-5.283277035	0.552055061
H	3.486768007	-6.306255341	0.998359144
H	4.038349152	-6.253814220	-0.695813298
O	-0.621997595	-1.737128019	-0.393145204
H	-0.807784438	-3.283013105	0.868407011
N	0.313067257	-1.798328161	-3.124815941
C	-0.098719463	-3.121644020	-3.099036217
O	-1.305551291	-3.306063890	-2.937063456
C	0.857109547	-4.220915794	-3.400849819
C	1.974691391	-4.045091152	-4.225785732
C	0.596624970	-5.476418495	-2.832679033
C	2.840385437	-5.112558365	-4.457376003
H	2.156185150	-3.079354525	-4.682959557
C	1.473310709	-6.535873890	-3.052642107
H	-0.293154001	-5.601910591	-2.224181652
C	2.598667860	-6.353817463	-3.863005877
H	3.701736927	-4.978660107	-5.105001926
H	1.272976041	-7.506987572	-2.608831167
H	3.275675774	-7.183828831	-4.045723438

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C	-0.848507106	0.583131313	-3.036702633
C	-1.546464443	0.401629984	-1.805016518
C	0.365917563	1.320354819	-3.073610067
H	-2.376899719	-0.295409560	-1.781494737
C	-1.148773670	1.086946368	-0.598671556
C	0.810674429	1.891074061	-1.837790012
H	1.784456134	2.372722626	-1.811948895
C	0.035458256	1.848023415	-0.640974402
H	0.423811316	2.297929764	0.266430110
H	-1.173008680	0.004903470	-3.890968323
C	1.223166585	1.470809460	-4.318430424
H	2.266742468	1.387897372	-3.983436584
C	1.025345206	2.882219791	-4.908852577
H	1.683677673	3.025098085	-5.770994186
H	-0.007661756	3.019549370	-5.245891571
H	1.251282573	3.664127111	-4.176757813

C	0.975940943	0.382892787	-5.370428562
H	1.055674434	-0.617229998	-4.935808182
H	-0.015441165	0.481346875	-5.825541019
H	1.710500121	0.474679947	-6.175711632
C	-1.915539265	0.862223864	0.671633184
H	-2.069772959	-0.209658310	0.827232718
H	-1.386464596	1.266709089	1.537184000
H	-2.898439884	1.341743588	0.606513679
Ru	0.466334164	-0.274583250	-1.495976686
C	2.549754143	-2.963639736	-1.116085529
C	2.253594875	-2.261044979	-2.302358866
C	3.335600615	-1.973259330	-3.155468941
C	3.830826759	-3.526716471	-0.935681224
C	1.767306209	-3.317629576	0.039689567
C	4.877897263	-3.320535183	-1.829480410
N	3.804292202	-4.265455723	0.256410748
C	4.613183498	-2.497585058	-2.927749157
H	5.856224060	-3.765402555	-1.681651235
H	5.406638622	-2.290626049	-3.638596058
H	3.138061285	-1.391211152	-4.049773216
C	2.589419127	-4.142484665	0.826680779
C	0.591764092	-2.699446917	0.531395137
H	2.374840736	-4.601903439	1.782896399
C	4.935252190	-5.022368908	0.781162560
H	5.773114681	-4.350178242	0.985469997
H	4.639044285	-5.518838406	1.705608487
H	5.246502876	-5.776738644	0.053717304
O	0.055240799	-1.652336597	0.086063802
H	0.133701265	-3.132172823	1.432377577
N	0.939260781	-1.882195950	-2.627204180
C	-0.040945575	-2.717595339	-3.121387243
O	-1.229947209	-2.390754223	-3.095373392
C	0.365184158	-4.051603794	-3.679049492
C	1.416724324	-4.223001957	-4.588760853
C	-0.405854404	-5.160474777	-3.302477598
C	1.706453204	-5.489733696	-5.095578194
H	1.991433382	-3.367729664	-4.923637867
C	-0.101768047	-6.427712440	-3.793853045
H	-1.245505095	-5.010589600	-2.631225586
C	0.956949055	-6.595019817	-4.690307140
H	2.512950420	-5.611877441	-5.812891006
H	-0.697442710	-7.283231735	-3.489060402
H	1.187356114	-7.581395626	-5.082486153

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C	-2.599670410	-1.763305306	-1.106403828
C	-2.779315948	-0.925557911	0.019544369
C	-2.094673157	-1.217014313	-2.327187538
H	-3.013551712	-1.381954789	0.976297379
C	-2.503019094	0.480350107	-0.017402561
C	-1.881254077	0.193931013	-2.399118900
H	-1.457503676	0.625765979	-3.296484232
C	-2.066492319	1.023963928	-1.266951323
H	-1.751083851	2.059107542	-1.320438027
H	-2.743526459	-2.830566883	-1.000408173
C	-1.790709019	-2.071166277	-3.543654680
H	-0.945399106	-1.588930488	-4.052327633
C	-3.009083748	-2.035123825	-4.490674973
H	-2.790259361	-2.593354464	-5.406088352
H	-3.882645845	-2.494912863	-4.016319275
H	-3.274065733	-1.010667562	-4.770092010
C	-1.381805182	-3.510369539	-3.207656622
H	-0.557876170	-3.533099413	-2.489067078
H	-2.219182014	-4.086257458	-2.799517632
H	-1.054669619	-4.021413326	-4.117690563
C	-2.616792917	1.342259169	1.207706928
H	-2.476491690	0.748705745	2.114694357
H	-1.861205697	2.129710436	1.180339456
H	-3.610160112	1.804078460	1.251306176
Ru	-0.692429721	-0.611455917	-0.668085515
C	1.569709301	-0.000137674	-3.094992161
C	1.474484921	-0.305677652	-1.695005655
C	1.731124520	-1.645768881	-1.291496873
C	2.052360296	-1.031656265	-3.941967964
C	1.364386320	1.149395943	-3.954598427
C	2.312090635	-2.350722313	-3.535799026
N	2.179720640	-0.525500238	-5.226901531
C	2.119307995	-2.649348974	-2.204096079
H	2.658417225	-3.097847700	-4.241555214
H	2.320008516	-3.647705793	-1.830465317
H	1.805172682	-1.868124485	-0.237484053
C	1.777971387	0.769709408	-5.225930691

C	0.659731746	2.406390429	-3.776445866
H	1.772600293	1.353069425	-6.137073040
C	2.666454077	-1.278097630	-6.376262665
H	2.017301083	-2.136486292	-6.571521759
H	2.667109966	-0.628690839	-7.252285957
H	3.685647249	-1.630719066	-6.195599079
O	-0.061152425	2.688103914	-2.828929424
H	0.774278283	3.115990877	-4.622201920
N	1.085581064	0.551104784	-0.636556447
C	1.171921015	1.991050959	-0.554855943
O	0.305071026	2.580456495	0.058563951
C	2.408863783	2.638248682	-1.058423877
C	3.610717297	1.943900228	-1.258316636
C	2.355339766	4.021852493	-1.290086031
C	4.741566181	2.626623631	-1.703013539
H	3.676466465	0.881965339	-1.046290636
C	3.482051611	4.695534706	-1.747408867
H	1.417352557	4.539349556	-1.122592807
C	4.676323414	3.998158216	-1.955949426
H	5.674731731	2.090286732	-1.846038342
H	3.434322596	5.763547421	-1.937451959
H	5.557504177	4.526355267	-2.308623552
C	0.842968881	-1.147985935	1.937713265
O	1.724124908	-0.291716427	1.615089774
O	-0.144578189	-1.456930518	1.188702345
C	1.019892216	-1.897332788	3.258421659
C	2.277393818	-2.783787251	3.086255312
C	1.262157679	-0.862533212	4.376527309
C	-0.206638053	-2.764283657	3.573697567
H	3.154450893	-2.174351215	2.852300167
H	2.471944094	-3.331168413	4.013716698
H	2.137661219	-3.519864559	2.285687685
H	1.455001593	-1.380586147	5.321044922
H	2.120505810	-0.228821740	4.143112659
H	0.386953622	-0.219041467	4.516143799
H	-0.382603675	-3.505904436	2.789789438
H	-0.051331915	-3.291560888	4.519850731
H	-1.109401345	-2.152744293	3.668566227
H	1.455890536	0.171138436	0.447105259

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C	-0.026685309	1.173160195	-2.678124666
C	-0.770370901	0.654663682	-1.569154143
C	1.389911056	1.048413157	-2.726526022
H	-1.855693221	0.666128874	-1.612741709
C	-0.127949476	0.019013971	-0.477738470
C	2.049383640	0.431491166	-1.605035186
H	3.118575335	0.249836117	-1.647155643
C	1.305023074	-0.077600375	-0.523234546
H	1.817944884	-0.636107028	0.252496898
H	-0.565537512	1.574619293	-3.527445555
C	2.227416754	1.498437643	-3.909403563
H	3.061043262	0.786751151	-3.974877596
C	-0.906019688	-0.586676657	0.659803987
H	-1.886963010	-0.936254561	0.327161223
Ru	0.492752492	-0.949952602	-2.427739143
O	-0.872505307	-1.794626117	-3.815958023
C	0.087776616	-2.238045931	-4.536805153
O	1.258589506	-1.815466523	-4.232486725
C	-0.141151264	-3.275916815	-5.613612175
C	1.099546671	-3.388388395	-6.513553619
C	-0.390819550	-4.612800598	-4.870090008
C	-1.386955857	-2.889830112	-6.434683323
H	0.929215968	-4.150131702	-7.280283928
H	1.313707471	-2.439960003	-7.015992641
H	1.984051347	-3.671010017	-5.936472893
H	-1.273623228	-4.543925285	-4.229013920
H	-0.549446166	-5.410371304	-5.602464199
H	0.465537041	-4.883648396	-4.244340420
H	-1.596756816	-3.671247244	-7.171498299
H	-2.261971474	-2.775331020	-5.790270805
H	-1.230165243	-1.949764848	-6.974197865
C	4.260862350	-2.244365215	-0.082515903
C	3.231558084	-2.814596653	-0.865664184
C	3.385921478	-2.843366623	-2.253904819
C	5.380296707	-1.686773062	-0.746402502
C	4.498182774	-2.063099623	1.339930773
C	5.526231289	-1.677588224	-2.135791540
N	6.252833366	-1.189166903	0.221715495
C	4.510028362	-2.275675058	-2.872773886
H	6.396412849	-1.242172599	-2.615181446
H	4.575199604	-2.308805943	-3.955368996

H	2.616087198	-3.283007622	-2.869495392
C	5.726731300	-1.415277004	1.449017882
C	3.739181519	-2.491570473	2.485067606
H	6.256082058	-1.117943645	2.344622850
C	7.541042805	-0.575416744	-0.068852350
H	7.405992508	0.303441137	-0.706015229
H	8.011921883	-0.267616600	0.865535796
H	8.193268776	-1.290324926	-0.579028726
O	2.692134380	-3.148964405	2.454458952
H	4.159646034	-2.197271109	3.465369463
N	2.103671551	-3.351235151	-0.209413782
H	2.233271599	-3.493909836	0.806152344
C	0.858150005	-3.485104322	-0.707414150
O	0.518464804	-3.024069548	-1.837951779
C	-0.152869806	-4.191312313	0.109920919
C	0.159124568	-4.903896332	1.281709194
C	-1.487894297	-4.121532917	-0.327587813
C	-0.856495321	-5.515777588	2.010672331
C	-2.495514154	-4.740390778	0.404035896
C	-2.181949615	-5.434840202	1.576051235
H	1.181129098	-4.989312649	1.633281469
H	-1.708846211	-3.581663847	-1.242339015
H	-0.612278402	-6.062665462	2.915939331
H	-3.524591923	-4.684545994	0.062197324
C	1.482566237	1.468711138	-5.249795914
H	2.179653645	1.703008056	-6.059862137
H	1.059560180	0.478798836	-5.438349247
H	0.680651069	2.214241266	-5.290547371
C	2.805575848	2.896997690	-3.607104301
H	3.477055311	3.207355499	-4.413872242
H	2.004768848	3.640703201	-3.528696537
H	3.372391462	2.908636332	-2.669621706
H	-1.057705402	0.158665776	1.449086785
H	-0.374223769	-1.436360598	1.096539974
H	-2.969337702	-5.917481899	2.147665024

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C	-1.096912384	0.922131002	-2.851754189
C	-1.549598813	0.470660627	-1.594729066
C	0.244934767	1.384822607	-3.054052353
H	-2.550153017	0.063600190	-1.495630383
C	-0.652256012	0.424774945	-0.475502580
C	1.101732016	1.375064015	-1.920541286
H	2.141544580	1.657738328	-2.047885895
C	0.668091357	0.917641699	-0.641193151
H	1.370912313	0.870262265	0.183037311
H	-1.757823586	0.827555776	-3.705753088
C	0.733841240	1.888720393	-4.400211334
H	1.829177380	1.812373877	-4.381699562
C	-1.104514837	-0.185211390	0.821925998
H	-1.681086183	-1.095380545	0.637020826
Ru	0.315151781	-0.700919151	-2.170210123
O	-0.249683887	-1.809982181	-3.863686085
C	0.264572442	-2.940847874	-4.162214279
O	1.336187243	-3.378221750	-3.646014214
C	-0.483001709	-3.835317850	-5.156899929
C	-1.120490789	-4.960268497	-4.304720402
C	-1.572369099	-3.046857119	-5.898964882
C	0.524597228	-4.439927578	-6.152598381
H	-1.680950046	-5.640151501	-4.954523563
H	-0.352043182	-5.534710407	-3.780043125
H	-1.812551379	-4.548908710	-3.561913729
H	-1.141917586	-2.220725298	-6.473898411
H	-2.095614433	-3.709712029	-6.595500469
H	-2.304096937	-2.627645016	-5.203826904
H	0.008389305	-5.133857250	-6.823510647
H	0.989516854	-3.660821915	-6.766299248
H	1.315466762	-4.981683731	-5.629439831
C	4.071866512	-1.813796520	-0.435123563
C	2.771560431	-2.054666758	-0.927881420
C	2.376692533	-1.492437005	-2.168181658
C	4.939612389	-0.996663511	-1.200796843
C	4.829360962	-2.223408222	0.737332821
C	4.594707012	-0.442397296	-2.441676378
N	6.149396420	-0.903047383	-0.528526068
C	3.321681499	-0.717742264	-2.901615858
H	5.300489902	0.144590616	-3.019387960
H	3.016312599	-0.346808255	-3.876044750
H	1.809062004	-2.388260365	-2.901175261
C	6.078871727	-1.630691290	0.617569566
C	4.487722874	-3.104263067	1.825510383
H	6.926183224	-1.696837544	1.286437869

C	7.310572624	-0.170624077	-1.016899586
H	7.058609486	0.883910120	-1.159803152
H	8.116032600	-0.247161910	-0.285785973
H	7.650187016	-0.591553569	-1.967687845
O	3.424452782	-3.720616817	1.945020080
H	5.269928455	-3.225523949	2.598050833
N	1.935928822	-2.914456367	-0.204699203
H	2.380795956	-3.359666348	0.617725670
C	0.633474708	-3.203198671	-0.445162117
O	-0.111534551	-2.513440132	-1.192523718
C	0.044166923	-4.384687901	0.222585395
C	0.827643514	-5.384796143	0.824360669
C	-1.355432272	-4.519867897	0.201806024
C	0.213335648	-6.488516808	1.409933209
C	-1.961036563	-5.625881672	0.786655962
C	-1.177570224	-6.611173153	1.394260287
H	1.909323931	-5.320021629	0.833635926
H	-1.951413989	-3.755126476	-0.283661306
H	0.823200643	-7.258486271	1.871761680
H	-3.042179585	-5.723659039	0.768134594
H	-1.650817394	-7.476483345	1.849003673
C	0.223148882	1.055603743	-5.586379528
H	0.724618196	1.375388503	-6.504586697
H	0.403179973	-0.011484688	-5.434490204
H	-0.852026343	1.194702148	-5.743926525
C	0.361210138	3.376388311	-4.557468414
H	0.756215870	3.768558264	-5.499661922
H	-0.727262676	3.502380133	-4.571514606
H	0.762139559	3.982955933	-3.739172459
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H	-0.255148739	-0.439448684	1.459913611

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C	-0.570451558	-1.945367575	-7.786795139
H	-1.228794098	0.890548289	-9.674992561
C	-0.030867394	-0.789586365	-10.386608124
C	0.218810827	-2.624733448	-8.750888824
H	0.729445338	-3.537396669	-8.468499184
C	0.498271465	-2.059258461	-10.030337334
H	1.154729486	-2.581911564	-10.716804504
H	-1.634558201	-0.080021806	-7.427420139
C	-0.831978738	-2.476648569	-6.388758183
H	-0.848899424	-1.597844124	-5.730553150
C	0.266560405	-3.419445753	-5.880589485
H	0.102058962	-3.634882450	-4.821159363
H	0.251352787	-4.379596233	-6.409077644
H	1.258449435	-2.973710537	-5.995637417
C	-2.225214005	-3.137142897	-6.343682766
H	-3.015619278	-2.443866730	-6.650492668
H	-2.263755322	-4.012042522	-7.001606464
H	-2.446739435	-3.470232248	-5.325355530
C	0.243312195	-0.176132768	-11.729957581
H	0.354196280	0.907945931	-11.652822495
H	1.140851617	-0.595964074	-12.187754631
H	-0.603698373	-0.381841868	-12.395234108
Ru	1.116083384	-0.611404002	-8.414374352
C	1.979594111	3.542606354	-8.733364105
C	1.763125539	4.883405209	-8.329734802
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C	2.423258781	3.280442715	-10.056973457
C	1.875912786	2.256554365	-8.097178459
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N	2.578985214	1.904424429	-10.204029083
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C	2.261440039	1.263459682	-9.042307854
C	1.535032153	1.777517676	-6.810585976
H	3.083938599	0.416943640	-8.753109932
C	3.282137632	1.289240360	-11.321870804
H	4.287889481	1.711017489	-11.404223442
H	3.357825279	0.217738345	-11.138344765
H	2.742139101	1.466651440	-12.255511284
O	1.295290470	0.548239112	-6.621296406
H	1.499560833	2.425273657	-5.926520348
N	1.298406243	5.121427536	-7.033025265
C	1.354139328	6.312726498	-6.311382771
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C	0.779852748	6.231693268	-4.930733681

C	-0.195142314	5.299538612	-4.542156219
C	1.256601691	7.159467220	-3.994602442
C	-0.668363690	5.284783363	-3.230888844
H	-0.632567465	4.614863396	-5.265995979
C	0.788871765	7.136952400	-2.683649302
H	1.995169640	7.886230469	-4.316049099
C	-0.171632782	6.198426247	-2.298866034
H	-1.433618546	4.571562767	-2.939320087
H	1.170890093	7.852454662	-1.961764216
H	-0.539169014	6.184552193	-1.277006626
C	3.948308229	-1.253116012	-7.706380367
O	2.724478006	-1.636453152	-7.598727226
O	4.304523945	-0.246798545	-8.369132042
C	5.014422417	-2.090101242	-6.982796669
C	5.787671089	-1.138952494	-6.043368340
C	4.382291794	-3.235429287	-6.179417610
C	5.966301918	-2.648085833	-8.063723564
H	5.133009911	-0.736463785	-5.262534618
H	6.596048832	-1.689362526	-5.551530361
H	6.220603943	-0.304545373	-6.600039005
H	5.169734478	-3.817065477	-5.689775467
H	3.709791660	-2.854221106	-5.405405998
H	3.809644461	-3.908073664	-6.823912144
H	6.410112858	-1.838337302	-8.648316383
H	6.770948887	-3.216125011	-7.586429119
H	5.437854767	-3.322478056	-8.746883392
H	0.925219655	4.327450752	-6.539364815

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H

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C	-0.567348301	0.726609886	-1.730771780
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H	-1.366068721	-0.251387209	0.004621356
C	0.816572905	-0.377033174	-0.003333796
C	1.881628156	0.728018641	-1.946882725
H	2.783755541	0.964938939	-2.499432325
C	1.981226444	0.030532965	-0.701093078
H	2.959790707	-0.258484781	-0.339121610
H	-1.542224765	0.944604456	-2.153724909
C	0.472131342	1.604916215	-3.883798838
H	1.422949195	1.598722100	-4.421632767
C	0.853813291	-1.164612532	1.296569586
H	0.056289654	-1.916876435	1.221452832
Ru	0.764932394	-1.203228354	-2.080056190
O	-0.250012279	-1.633219004	-3.963259935
C	-0.327767998	-2.715827465	-4.567177296
O	0.598223209	-3.650498390	-4.479257584
C	-1.534757614	-3.097393751	-5.404193401
C	-2.392528057	-1.856074810	-5.685088634
C	-1.092097044	-3.768563509	-6.720630169
C	-2.323933363	-4.110367298	-4.531150341
H	-3.276199341	-2.147596121	-6.259657383
H	-2.722943783	-1.382206082	-4.757646561
H	-1.836512327	-1.115451217	-6.268237591
H	-0.483097821	-4.655656338	-6.533844948
H	-1.977972507	-4.071734905	-7.286731720
H	-0.514654994	-3.077179670	-7.343025208
H	-3.241146088	-4.393942356	-5.055412292
H	-1.735492468	-5.013213634	-4.348042488
H	-2.598067045	-3.674033880	-3.564971924
C	3.935842514	-4.226691246	-2.153646469
C	2.686682701	-3.589532375	-1.943352342
C	2.414349556	-2.350457191	-2.564082384
C	4.853907585	-3.632658958	-3.049886703
C	4.580221653	-5.437238693	-1.665994287
C	4.592385769	-2.444952726	-3.732244015
N	5.990963936	-4.436292171	-3.112688065
C	3.379357338	-1.825516105	-3.464607239
H	5.302773476	-2.020872355	-4.434270859
H	3.152070761	-0.898438513	-3.981205463
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C	5.822305202	-5.498755455	-2.292334080
C	4.169525146	-6.412871838	-0.694882035
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C	7.163417339	-4.147712708	-3.925553322
H	7.603459358	-3.190923214	-3.629718065
H	7.901700497	-4.937765121	-3.783085823
H	6.888738632	-4.104293823	-4.983462811
O	3.117375374	-6.390944958	-0.045140341
H	4.884755611	-7.240338802	-0.527881861
N	1.754883647	-4.265701294	-1.117001057
H	2.144388199	-5.071933270	-0.594598055

C	0.438981056	-4.021639824	-1.013331413
O	-0.127209768	-3.014042139	-1.532256365
C	-0.410163283	-4.965493202	-0.249839842
C	-0.053224344	-6.305315018	-0.022139309
C	-1.633870721	-4.479526520	0.239970222
C	-0.906875372	-7.133692265	0.703289688
C	-2.478437185	-5.311858177	0.966726124
C	-2.114715576	-6.640463829	1.201885343
H	0.874193013	-6.709745884	-0.407281011
H	-1.907259464	-3.449195862	0.039330430
H	-0.628740609	-8.168604851	0.876233697
H	-3.419232845	-4.927800655	1.349322677
H	-2.773994207	-7.290874481	1.769315362
C	2.177141905	-1.900905967	1.539042354
H	2.992600679	-1.200567961	1.751880050
H	2.079764843	-2.557986021	2.407775402
H	2.462999105	-2.515085936	0.681173503
C	0.518972874	-0.227446750	2.476304293
H	-0.444576532	0.274326384	2.341313839
H	0.474315822	-0.796236336	3.410073996
H	1.288769126	0.544334054	2.585921288
H	-0.258067042	1.035650849	-4.466485977
H	0.122126460	2.640761614	-3.813981533

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C	-1.560796618	1.260151386	-2.437630892
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C	-0.683761477	0.741698980	-0.193487152
C	0.763551831	1.793169022	-1.890121102
H	1.742500424	2.165657759	-2.170719385
C	0.556628823	1.309447169	-0.559039235
H	1.378946304	1.308792472	0.147988960
H	-2.370884895	1.218898058	-3.156337976
C	0.000094821	2.217262030	-4.276032448
H	1.039080858	1.954382420	-4.512515068
C	-0.907227993	0.114749320	1.155904889
H	-1.410306573	-0.850276172	1.046901703
Ru	0.147142678	-0.363655061	-1.992716193
C	3.915242672	-2.364752293	-0.969784141
C	2.533726931	-2.049907446	-1.053698421
C	2.105863571	-1.008253217	-1.892003298
C	4.826038361	-1.642834902	-1.774573684
C	4.718362808	-3.319050789	-0.218060434
C	4.429441452	-0.630445123	-2.647240639
N	6.110308170	-2.131303072	-1.535623193
C	3.071729183	-0.336905003	-2.681138992
H	5.139481068	-0.101336643	-3.273919106
H	2.737335920	0.426748723	-3.374286652
C	6.039093971	-3.118464947	-0.614736915
C	4.367152214	-4.297682285	0.771790564
H	6.928486824	-3.633610010	-0.277620435
C	7.313133717	-1.638877034	-2.188426495
H	7.449253082	-0.574220538	-1.976399899
H	8.176791191	-2.189490318	-1.813180447
H	7.241612911	-1.781722069	-3.270744562
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H	5.215299129	-4.885184288	1.172236085
N	1.656080723	-2.829415321	-0.260702103
H	2.128620386	-3.525529623	0.346596092
C	0.322762936	-2.884318590	-0.326624393
O	-0.379198253	-2.169503212	-1.106225491
C	-0.397946626	-3.842541695	0.547578216
C	-1.660165429	-4.285901070	0.119221389
C	0.120729446	-4.296641827	1.770707250
C	-2.383527040	-5.185845375	0.893296301
C	-0.616742730	-5.190033436	2.545572281
C	-1.864321470	-5.639900208	2.109436274
H	-2.054143667	-3.928324461	-0.824278295
H	1.085928917	-3.958370924	2.128513098
H	-3.352458239	-5.535282612	0.548323393
H	-0.214221448	-5.532843113	3.493845224
H	-2.432114363	-6.338799477	2.716610670
C	-0.901620388	1.574850559	-5.339490891
H	-0.559119701	1.862966537	-6.337093830
H	-0.886102319	0.484054685	-5.278923988
H	-1.940312505	1.911029935	-5.246952534
C	-0.126471892	3.754390478	-4.306183338
H	0.109222516	4.134609699	-5.304829121
H	-1.148115635	4.064946651	-4.059504032
H	0.553188264	4.228033066	-3.591119051

H	-1.540055752	0.761061192	1.774303913
H	0.036951929	-0.045787226	1.681016326
N	0.069485255	-1.467205882	-3.813191652
O	1.094084859	-1.212696552	-4.763098717
C	-0.579443038	-2.502327919	-4.261699677
O	-0.033625372	-2.990174055	-5.404257298
C	1.042220473	-2.178441048	-5.727209091
O	1.763755441	-2.294097900	-6.660597801
C	-1.779194713	-3.147285223	-3.748985291
C	-2.761211872	-2.409415007	-3.069788456
C	-1.970730543	-4.515436649	-4.003570080
C	-3.924299240	-3.042158842	-2.643844366
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H	-4.689757824	-2.472376108	-2.126382113
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H	-5.018741608	-4.897336006	-2.550542593

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C	-0.585755587	0.251597017	-0.645261526
C	0.605106890	0.664358556	-2.765911579
H	1.547501326	0.739383876	-3.296511173
C	0.612459064	0.444817275	-1.355250359
H	1.564797282	0.318943858	-0.855273426
H	-2.783467054	0.791857719	-3.254891634
C	-0.642510295	0.971468210	-4.968851566
H	0.278060377	0.619930685	-5.439992428
C	-0.649951458	-0.088750772	0.833648801
H	-1.434831023	-0.850967586	0.934089720
Ru	-0.522436082	-1.311584353	-2.399848223
C	2.678311348	-4.071668625	-1.356129169
C	1.421667814	-3.416707277	-1.378526092
C	1.189846754	-2.421716690	-2.337426186
C	3.627132654	-3.752076149	-2.354397774
C	3.303141117	-5.088959694	-0.524195492
C	3.394342899	-2.805863619	-3.351799011
N	4.760365963	-4.536963940	-2.153213739
C	2.173531532	-2.149676323	-3.313410759
H	4.124071598	-2.597221136	-4.126896381
H	1.950969696	-1.434040546	-4.096431732
C	4.562847614	-5.323692322	-1.071374297
C	2.854320526	-5.745557308	0.669554651
H	5.327536583	-6.009859085	-0.733142436
C	5.939130306	-4.512673855	-3.006323338
H	6.368640900	-3.506908178	-3.027858019
H	6.681808949	-5.208243370	-2.613737583
H	5.673004627	-4.811226845	-4.024343967
O	1.779029846	-5.540444851	1.247769475
H	3.556295395	-6.488338947	1.092628360
N	0.459732622	-3.828828096	-0.423679560
H	0.832571447	-4.453558445	0.318293333
C	-0.852502346	-3.572548866	-0.425836504
O	-1.416702271	-2.770021677	-1.233517170
C	-1.721962929	-4.225150108	0.582680225
C	-1.385762811	-5.435961246	1.208403349
C	-2.939660311	-3.597682714	0.897692204
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C	-3.448266983	-5.355852127	2.471473932
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H	-3.200687647	-2.671317577	0.397461176
H	-1.983669043	-6.931018353	2.626729250
H	-4.729471684	-3.663182974	2.086135626
H	-4.115300179	-5.794313431	3.207787991
C	0.652331531	-0.675372303	1.391316891
H	1.445683002	0.078951448	1.434300780
H	0.488540381	-1.030480385	2.412347078
H	1.007201195	-1.518842578	0.792810798
C	-1.087000251	1.156534314	1.633520007
H	-2.041597605	1.558008552	1.278271317
H	-1.201455593	0.901733577	2.691277027
H	-0.335476637	1.949649811	1.555263519
H	-1.488102436	0.444156587	-5.418472290
H	-0.758195519	2.037634134	-5.194930553
C	-2.201994896	-2.336470127	-4.744292259
N	-1.202531576	-2.345510244	-3.903005600

C	-0.901316166	-3.804573536	-5.906246662
O	-0.074027047	-3.321925163	-5.047452450
O	-2.127185106	-3.047848225	-5.865727425
O	-0.782964826	-4.683365822	-6.710441589
C	-3.504100800	-1.711099386	-4.450051785
C	-4.201937199	-1.082244158	-5.490198135
C	-4.046825409	-1.775701642	-3.157424450
C	-5.428909779	-0.476910889	-5.222681522
H	-3.786378145	-1.074842930	-6.492915154
C	-5.280699730	-1.180422902	-2.907578468
H	-3.510695934	-2.302274227	-2.374550343
C	-5.966219425	-0.522140741	-3.933791876
H	-5.970109463	0.018661985	-6.022565842
H	-5.717167854	-1.242310524	-1.915017843
H	-6.927596569	-0.058991279	-3.732763052

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C	-0.989158630	-5.729656696	-0.316787839
C	1.363537073	-5.062170982	0.005037060
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C	2.059078693	-3.328426838	1.728177190
H	3.043109179	-3.672266960	1.383518577
C	1.991289735	-3.549080133	3.250623465
H	2.805793524	-3.012567282	3.747281790
H	1.050500751	-3.174712896	3.668187618
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H	2.128162861	-1.651187181	0.323201925
H	0.941559494	-1.446084619	1.621774435
H	2.666821003	-1.248247504	1.959492087
C	-2.034732342	-6.612364292	-0.943030417
H	-2.766648531	-6.011996746	-1.492066503
H	-1.592179894	-7.328757286	-1.640324831
H	-2.569539547	-7.172492027	-0.168295503
Ru	0.121133745	-4.237504482	-2.416833878
C	3.520719051	-1.677617669	-2.781970263
C	2.209827185	-2.140998125	-2.497901201
C	1.939381957	-3.515640974	-2.643453360
C	4.498402596	-2.618453264	-3.175288200
C	4.186701775	-0.385841906	-2.768693209
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N	5.695762157	-1.942872286	-3.383291245
C	2.964703798	-4.418694019	-3.017106771
H	5.025090218	-4.686816692	-3.599379778
H	2.728737354	-5.476309776	-3.097565651
C	5.505405903	-0.623583913	-3.142739296
C	3.693062782	0.934088647	-2.482724190
H	6.313407421	0.086606801	-3.254772663
C	6.940419674	-2.573327780	-3.801786661
H	6.808182240	-3.060275555	-4.771652699
H	7.715334892	-1.811211944	-3.889003038
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H	4.443541527	1.744003415	-2.541729927
N	1.262872815	-1.194087744	-2.069831371
C	0.044726107	-1.418652058	-1.555500031
O	-0.463666618	-2.584538698	-1.456384778
C	-0.766767204	-0.292416275	-1.056400657
C	-0.198185638	0.907597184	-0.596522748
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C	-2.978270292	0.563653588	-0.567600727
H	-2.588588953	-1.396781445	-1.382454515
C	-2.411297798	1.759622574	-0.118661813
H	-0.583523095	2.851430655	0.227660984
H	-4.056216717	0.434714347	-0.560981870
H	-3.050040483	2.560690403	0.241719842
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N	-0.514990568	-4.642940044	-4.013038158
C	-1.923641443	-4.636945724	-4.157837868
O	-2.625268936	-4.429695129	-3.158586740
C	-2.446514606	-4.872865200	-5.513247013
C	-1.582584739	-5.104309082	-6.597501755
C	-3.837615013	-4.859784126	-5.709569454

C	-2.111053228	-5.320788860	-7.866916180
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H	-4.484540939	-4.678152561	-4.857563496
C	-3.495334625	-5.307049274	-8.057970047
H	-1.447357655	-5.500057220	-8.707160950
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H	-5.432209015	-5.067238808	-7.135936737

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C	2.635607243	-4.858707905	-0.484191924
H	-0.183192223	-5.661855698	1.321715474
C	0.172713369	-6.371230602	-0.710399508
C	2.300832272	-5.590970993	-1.655790567
H	2.958569288	-5.520762920	-2.515794039
C	1.114366174	-6.359746456	-1.769805670
H	0.879249334	-6.871400356	-2.695716858
H	1.909841299	-4.375182629	1.503475666
C	3.917197704	-4.046198368	-0.390730590
H	4.442860126	-4.172880173	-1.345232606
C	4.822331429	-4.598897457	0.726781368
H	5.778404236	-4.067318439	0.733312190
H	4.362704277	-4.464270115	1.712108970
H	5.026683807	-5.665302753	0.589426339
C	3.641087770	-2.543211699	-0.204882607
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H	3.054671288	-2.349090576	0.699415088
H	4.584942341	-1.996544361	-0.116965383
C	-1.110576630	-7.146239281	-0.816196620
H	-1.912681699	-6.661000729	-0.254601508
H	-1.418631434	-7.235655785	-1.859811544
H	-0.969778955	-8.153248787	-0.407898694
Ru	0.500314236	-4.157137394	-1.333674669
C	1.455648184	-1.158883810	-4.438795090
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C	1.811323404	-1.995775342	-5.519857883
C	1.587469339	0.204837382	-4.932048321
C	1.762883663	-3.389300108	-5.456286907
N	2.151152611	-1.194836617	-6.606665134
C	1.346496463	-3.946435928	-4.259291172
H	2.001371384	-4.011216164	-6.312267780
H	1.196793914	-5.015796185	-4.207216740
C	2.013663530	0.104156651	-6.253257275
C	1.317384005	1.474439025	-4.316627502
H	2.216917276	0.899395287	-6.957704544
C	2.544297218	-1.699570894	-7.915009975
H	1.732016683	-2.286649704	-8.353685379
H	2.769373417	-0.857879937	-8.571032524
H	3.434240580	-2.328887463	-7.825025558
O	0.883720338	1.644231915	-3.171537876
H	1.517486334	2.358121872	-4.951318264
N	0.690066159	-0.889309764	-2.168221235
C	0.381502718	-1.172281861	-0.895017862
O	0.292922527	-2.341374874	-0.415588617
C	0.132897556	-0.047224466	0.038229920
C	0.766438663	1.198254108	-0.095831849
C	-0.754811227	-0.267449170	1.104503989
C	0.496592581	2.213226080	0.819004714
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C	-1.025315166	0.754549086	2.008517027
H	-1.234063387	-1.235672712	1.202293754
C	-0.400740743	1.996706128	1.866480827
H	0.990115643	3.174252272	0.712965131
H	-1.724621058	0.585712135	2.821790457
H	-0.612394333	2.794130564	2.572777510
H	0.674598217	0.115547270	-2.434582949
N	-1.004093766	-3.741599798	-2.373357296
C	-1.721176744	-4.718350887	-3.043013334
O	-1.201238155	-5.591144085	-3.748361111
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C	-3.988274097	-5.716558933	-3.155766010
C	-5.160350800	-3.421324730	-2.065787792
H	-3.166522503	-2.597408533	-2.042608738
C	-5.362815380	-5.670714378	-2.947571039
H	-3.513005495	-6.589846611	-3.590784073
C	-5.949456692	-4.524672031	-2.399567366
H	-5.620916843	-2.528181553	-1.654042959
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H	-5.980753422	-6.522623539	-3.215222359

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C	0.078934349	-6.000097275	0.004592536
C	1.771743774	-6.161243439	-1.788536668
H	2.018919945	-6.420325279	-2.812660694
C	0.481385142	-6.450710773	-1.295151234
H	-0.262593418	-6.891081810	-1.948585629
H	3.064453125	-4.497683048	0.932081997
C	4.074540615	-5.064539433	-1.619770765
H	3.958715439	-5.172656059	-2.705734015
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H	4.853665352	-7.101154327	-1.375481606
C	4.501499176	-3.613855362	-1.346118808
H	3.740885258	-2.906565666	-1.689748287
H	4.682975769	-3.433026075	-0.281552404
H	5.435667515	-3.397722483	-1.874129176
C	-1.325062513	-6.213651657	0.491657883
H	-1.591517687	-5.477575779	1.253876209
H	-2.020161152	-6.127368927	-0.345961273
H	-1.420072794	-7.212840557	0.932887673
Ru	0.813258767	-4.247797489	-1.134192228
C	2.182431221	-1.289477110	-3.511079073
C	1.085043430	-1.811653018	-2.780319452
C	0.553918958	-3.080523968	-3.172336817
C	2.753805161	-2.058674335	-4.546966076
C	2.934280157	-0.048386898	-3.464132786
C	2.259830952	-3.316719532	-4.938612938
N	3.816336155	-1.346966863	-5.083367348
C	1.175744891	-3.803719282	-4.252148628
H	2.706455231	-3.871842384	-5.756531715
H	0.731861532	-4.755330086	-4.523386002
C	3.918925285	-0.154268950	-4.439764500
C	2.703075171	1.170490623	-2.723432064
H	4.670430660	0.569118679	-4.726042271
C	4.649837971	-1.804022551	-6.189666748
H	4.042057037	-1.947868109	-7.087495327
H	5.414248466	-1.054018378	-6.395141125
H	5.138559341	-2.747205496	-5.930006504
O	1.725096464	1.400287390	-2.008092642
H	3.473897219	1.953299046	-2.851775408
N	0.478333801	-1.004432440	-1.818215728
C	-0.000788796	-1.388276219	-0.604754448
O	0.165722266	-2.545653820	-0.131639212
C	-0.665832281	-0.357025027	0.215509117
C	-1.144909263	0.841937780	-0.340030521
C	-0.826196134	-0.599092841	1.590193748
C	-1.759029746	1.787915826	0.474799991
H	-1.058080077	1.034015656	-1.403962970
C	-1.440738559	0.350758135	2.398317575
H	-0.460445106	-1.530592680	2.007188320
C	-1.905362964	1.546015620	1.842546225
H	-2.130196810	2.711145878	0.041227940
H	-1.557539225	0.162884846	3.461158037
H	-2.385837555	2.286847830	2.474709034
H	0.748695314	-0.003692664	-1.881684899
N	-0.551807821	-3.600433826	-2.504933119
C	-1.562572122	-4.314621449	-3.130917072
O	-2.009925365	-5.362938881	-2.668275595
C	-2.131420374	-3.689399242	-4.368656635
C	-2.048498631	-2.310640812	-4.619064331
C	-2.783826828	-4.521356106	-5.288288116
C	-2.594946146	-1.777981639	-5.784530163
H	-1.585584879	-1.655054569	-3.888339043
C	-3.316523552	-3.987341642	-6.459492683
H	-2.864013195	-5.580769062	-5.067022324
C	-3.220487118	-2.616271019	-6.710547924
H	-2.541038752	-0.708624184	-5.967885971
H	-3.641712189	-2.199912548	-7.621119022
H	-3.811724901	-4.637383461	-7.174655437

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C	0.242987692	-7.063230038	-1.025092602
C	2.397531509	-5.995166302	-1.644954443
H	3.107560873	-5.728360653	-2.419280052
C	1.251038074	-6.783833981	-1.981901646
H	1.095361114	-7.094856262	-3.007534742
H	1.596177816	-5.306225777	1.619947672
C	3.733407021	-4.545295238	-0.044076186
H	3.944787264	-3.987369061	-0.966114700
C	4.954233170	-5.431842327	0.278746516
H	5.836303234	-4.808513165	0.455754876
H	4.774879932	-6.023722649	1.183239222
H	5.180980682	-6.122924805	-0.539106846
C	3.479607821	-3.527606249	1.077042699
H	2.574532032	-2.946168900	0.890070319
H	3.387269735	-4.017007351	2.053240061
H	4.326895714	-2.838842869	1.145116091
C	-1.007665873	-7.816436291	-1.378619552
H	-1.869892836	-7.371004581	-0.874772191
H	-1.185026884	-7.782986164	-2.453530312
H	-0.922135115	-8.861480713	-1.058457494
Ru	0.526495039	-4.858080387	-1.179891467
C	3.023207188	-1.540814161	-3.699780226
C	1.839039564	-2.074769974	-3.148197889
C	1.424934268	-3.348074913	-3.563331842
C	3.807741880	-2.340501785	-4.564015865
C	3.708630562	-0.264710277	-3.594655037
C	3.437561989	-3.632370949	-4.941251278
N	4.929940701	-1.606315017	-4.938929081
C	2.237009048	-4.107575417	-4.438261509
H	4.044468880	-4.232502937	-5.610471725
H	1.895183682	-5.097197056	-4.722715378
C	4.863282681	-0.380466789	-4.364128113
C	3.296342850	0.983064950	-2.999198198
H	5.628184795	0.362449646	-4.548958302
C	5.972079277	-2.088769436	-5.833501339
H	5.549305916	-2.325708866	-6.814281940
H	6.731123447	-1.314489365	-5.951030731
H	6.441111565	-2.985701561	-5.418262482
O	2.197806120	1.209982038	-2.484267950
H	4.045507431	1.796321273	-3.049874783
N	1.102961540	-1.275189161	-2.243613005
C	0.641884506	-1.641665220	-1.025928617
O	0.697599530	-2.806474447	-0.555808485
C	0.054177929	-0.571189404	-0.184273675
C	-0.451255560	0.619034708	-0.730228066
C	-0.033541206	-0.793914318	1.198568463
C	-1.029165745	1.573948383	0.102148533
H	-0.420691103	0.795223892	-1.799385548
C	-0.600997806	0.169171453	2.026850224
H	0.344289005	-1.724817157	1.607047081
C	-1.101964235	1.353617072	1.479365468
H	-1.428619504	2.488052845	-0.326011389
H	-0.658929050	-0.003587134	3.097386599
H	-1.553227544	2.101625681	2.124853134
H	1.293912530	-0.263030052	-2.350725889
N	0.200056762	-3.921691179	-3.092845917
C	-0.528419971	-4.659451008	-4.106878281
O	-0.855068684	-5.819226742	-3.930294752
C	-0.902070045	-3.900390387	-5.331822872
C	-0.947408915	-2.497053385	-5.372766018
C	-1.256464958	-4.639646530	-6.470806599
C	-1.331421256	-1.848589778	-6.543002129
H	-0.711246073	-1.911080360	-4.492400169
C	-1.625189543	-3.986537933	-7.642637730
H	-1.234245777	-5.723248482	-6.417606831
C	-1.661700130	-2.589747667	-7.680438519
H	-1.377043009	-0.763824821	-6.567992687
H	-1.953461647	-2.079172611	-8.593916893
H	-1.887896538	-4.562708378	-8.524814606
O	-1.739058256	-2.692178488	-2.160224915
H	-0.706769586	-3.164585829	-2.640321255
C	-2.177787542	-3.483446836	-1.255781531
O	-1.524714708	-4.479557514	-0.815493047
C	-3.560095072	-3.186649084	-0.677997887
C	-4.014595985	-4.313370228	0.259886384
C	-3.445878983	-1.852541804	0.097499490
C	-4.548567295	-3.026316404	-1.852176309
H	-5.005943775	-4.081027508	0.661049545
H	-4.075021744	-5.268602371	-0.270603150
H	-3.322788477	-4.435791492	1.097782373
H	-3.107439995	-1.044359922	-0.555814505
H	-4.425980568	-1.584885240	0.505535960

H	-2.740318537	-1.933907390	0.930473208
H	-5.541046143	-2.773821115	-1.465702653
H	-4.224422455	-2.233504772	-2.529913425
H	-4.635343075	-3.955643892	-2.425630093

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L

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C	0.599095643	-1.728005171	-3.095662355
C	0.781305254	-0.576225400	-2.263372183
C	1.611228824	-2.717281580	-3.208197832
H	-0.052380104	0.101764299	-2.113065243
C	1.980625391	-0.371208936	-1.540589571
C	2.840920687	-2.504556417	-2.488863468
H	3.603848457	-3.272542715	-2.475980759
C	3.008535624	-1.366470337	-1.674401999
H	3.891310930	-1.299982071	-1.049143195
H	-0.361489266	-1.891189933	-3.572202682
C	1.368891478	-3.955695868	-4.051116943
H	0.286293000	-4.135411739	-4.034925938
C	2.061147213	-5.210933208	-3.508552790
H	1.768140912	-6.082201958	-4.101379871
H	3.151431561	-5.136145115	-3.572206259
H	1.781357527	-5.386034012	-2.468617439
C	1.788834810	-3.657424927	-5.505173206
H	1.261188865	-2.788351774	-5.910625458
H	2.865293503	-3.461169958	-5.566051483
H	1.567111969	-4.518509388	-6.143000603
C	2.154277325	0.773455620	-0.581200242
H	1.195795417	1.240864992	-0.344553947
H	2.602769852	0.422208905	0.352344900
H	2.811435223	1.536730409	-1.013214588
Ru	1.132313848	-2.399902582	-1.059195995
O	0.498975217	-4.421954155	-0.680170417
C	-0.677386999	-4.024315357	-0.352149248
O	-0.866398096	-2.760159492	-0.377971798
C	-1.774892807	-5.014527798	-0.007283821
C	-1.362324238	-5.822946072	1.243336201
C	-3.093610048	-4.271220684	0.255180269
C	-1.911336064	-5.966527462	-1.220312715
H	-2.085134745	-6.629642963	1.402523637
H	-0.375261575	-6.271911621	1.130318880
H	-1.356386185	-5.192718029	2.135494232
H	-3.413991213	-3.700082302	-0.620855570
H	-3.876874924	-4.995259285	0.500951886
H	-2.991189480	-3.576830626	1.093555808
H	-2.705802202	-6.693842411	-1.026251435
H	-2.174351931	-5.414835453	-2.130430460
H	-0.982994378	-6.514494419	-1.394990921
C	3.804214001	-5.380713940	-0.170904130
C	4.940631390	-5.277310371	-1.016982555
C	5.830908775	-4.189101219	-0.863156021
C	5.497565269	-6.098797321	-2.083013773
C	3.587265968	-4.320004940	0.733395815
N	2.967825174	-6.491614342	-0.339970917
C	4.504688740	-3.253540277	0.851910532
N	2.482647419	-4.318449020	1.612567902
C	5.638029099	-3.163749456	0.066822045
N	6.880906105	-4.346944809	-1.761598945
C	6.677988052	-5.478937626	-2.478826523
C	4.995439529	-7.267316341	-2.765024424
H	6.347622871	-2.352387428	0.186211511
C	8.009866714	-3.436252832	-1.878040791
H	4.291547775	-2.490518570	1.591611266
H	7.374559879	-5.784087181	-3.248023748
O	3.892167330	-7.789411068	-2.592396975
H	5.681362152	-7.692391872	-3.523250103
H	8.550079346	-3.379569769	-0.928485692
H	8.687886238	-3.801202297	-2.650510550
H	7.662601471	-2.435953617	-2.153092146
H	3.144103050	-7.008346558	-1.214218736
C	2.174269676	-7.139182091	0.571566641
O	2.142093420	-6.858284950	1.783253193
C	1.323024631	-8.235106468	0.026831644
C	1.027726412	-8.378111839	-1.338518381
C	0.751381695	-9.122982979	0.951748550
C	0.179418847	-9.396769524	-1.766330123
H	1.439690351	-7.696788311	-2.071913481
C	-0.090672784	-10.142475128	0.518615663
H	0.975723505	-8.992771149	2.004859447
C	-0.380022496	-10.280214310	-0.841519475
H	-0.047767337	-9.497207642	-2.823388338
H	-0.523175240	-10.829274178	1.240095377
H	-1.040031552	-11.074159622	-1.179137588

C	1.626003742	-3.304490328	1.782112956
O	1.611690044	-2.279592752	1.025323391
C	0.667257786	-3.407305002	2.900494576
H	2.264759541	-5.257862568	1.999372482
C	-0.476372957	-2.592367172	2.864407539
C	0.848583579	-4.311208248	3.962329626
C	-1.436852574	-2.698592901	3.865806818
H	-0.610170603	-1.916083574	2.028917789
C	-0.116454251	-4.411714554	4.959712029
H	1.741248012	-4.925459385	4.020767212
C	-1.260444641	-3.609718800	4.911053658
H	-2.325690031	-2.076059580	3.830125332
H	0.025325701	-5.111184597	5.777758598
H	-2.011962891	-3.692639351	5.690845490

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L-TS

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C	2.707295418	-3.787744284	-1.282584071
C	1.478077769	-3.502521992	-1.931227326
C	1.550185919	-2.956145763	-3.229918957
C	3.929662466	-3.428183556	-1.907174230
C	3.068241358	-4.347445965	0.006903492
C	3.994607687	-2.919786215	-3.196267843
N	4.972970486	-3.709348917	-1.025022507
C	2.793569565	-2.724592209	-3.892102242
H	4.941625118	-2.689016819	-3.673635006
H	2.780798912	-1.598361611	-4.606179714
C	4.454935074	-4.251461506	0.101491667
C	2.285444736	-5.028114319	1.014536023
H	5.096049309	-4.563960552	0.915448308
C	6.374870300	-3.425640106	-1.289253354
H	6.526039600	-2.350124359	-1.420925617
H	6.975904465	-3.768897057	-0.446451366
H	6.703516960	-3.946298122	-2.193909883
O	1.095065117	-5.329282761	0.923285127
H	2.848703384	-5.315467358	1.923611999
N	0.285693586	-3.834592581	-1.247028947
H	0.431914419	-4.525990009	-0.496761441
C	-0.843152821	-3.066093445	-1.118249655
O	-0.982818723	-1.976680160	-1.706584215
C	-1.915835857	-3.593770742	-0.231236219
C	-1.987460494	-4.929961681	0.195130691
C	-2.909631729	-2.686257362	0.169726521
C	-3.032348633	-5.342458248	1.018780947
C	-3.947294235	-3.102368593	0.997438669
C	-4.010360718	-4.431523800	1.423583388
H	-1.243714571	-5.655437946	-0.114029594
H	-2.846064329	-1.659285307	-0.173335105
H	-3.084172726	-6.377374172	1.342776060
H	-4.706454754	-2.392320871	1.311579227
H	-4.821470261	-4.757313251	2.068522930
C	0.137225449	-2.306698799	-5.163549900
N	0.350727439	-2.557402611	-3.860807657
O	0.939850748	-2.622543097	-6.091414928
C	-1.127955317	-1.631460547	-5.549569130
C	-1.213538289	-1.110194206	-6.851329327
C	-2.217982292	-1.486911416	-4.673260212
C	-2.363141298	-0.445949256	-7.266621590
H	-0.366990089	-1.221742988	-7.519428253
C	-3.366587877	-0.825760126	-5.099242210
H	-2.188217640	-1.876215458	-3.661876202
C	-3.442400694	-0.302373707	-6.391648293
H	-2.416609049	-0.035467058	-8.270381927
H	-4.204237938	-0.717782855	-4.417031765
H	-4.338938236	0.218662888	-6.714698792
H	-0.323383242	-2.176959276	-3.165887594
C	2.183959007	-5.733748913	-5.382675171
C	3.546557903	-5.522738457	-5.041871548
C	4.512258530	-5.071087360	-5.990865231
H	3.844636440	-5.637983322	-4.004898071
Ru	2.771182537	-3.623684645	-5.920664310
H	1.473990321	-6.016105175	-4.613799095
C	1.730499387	-5.469167709	-6.707276344
C	4.037548065	-4.834083080	-7.316102028
C	5.961145401	-4.866212368	-5.587759495
C	2.684440374	-5.049963951	-7.684723854
C	0.271217406	-5.545351982	-7.058813572
H	4.707212448	-4.395878315	-8.048089981
H	2.353190660	-4.800054073	-8.686734200
H	5.959862709	-4.741820335	-4.496698856
C	6.587807178	-3.606178284	-6.204976559
C	6.781186581	-6.127734661	-5.919370174
H	7.569424152	-3.420229673	-5.758449554

H	6.743865967	-3.720602751	-7.283013344
H	5.954207420	-2.727342129	-6.053482056
H	6.361259937	-7.017994404	-5.440297604
H	6.801777363	-6.302884579	-7.000576496
H	7.814771175	-6.011456966	-5.578357220
H	-0.349719137	-5.624595165	-6.163830757
H	-0.033056222	-4.650895596	-7.608807564
H	0.082670406	-6.420535564	-7.690067291
O	3.596130848	-1.891204357	-6.777230263
C	3.413821459	-0.718443632	-6.313577652
O	2.846749783	-0.486386150	-5.198827267
C	3.983765125	0.472302496	-7.088734627
C	5.297907352	0.854695797	-6.364868641
C	4.273378372	0.086818852	-8.546832085
C	2.985752583	1.643983960	-7.021703720
H	6.020693779	0.031450823	-6.396588326
H	5.750932693	1.720564008	-6.857950211
H	5.106476307	1.113996863	-5.319470882
H	4.689515591	0.947984457	-9.078894615
H	4.989475727	-0.736675978	-8.605417252
H	3.359094143	-0.223638296	-9.062661171
H	2.770128727	1.919180512	-5.987154007
H	3.405562401	2.514022112	-7.536267281
H	2.040300131	1.384970784	-7.510070324

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M

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C	1.246245265	-6.949226379	-2.646195650
C	0.608993471	-5.725527287	-2.948948622
C	1.044020653	-5.020698071	-4.096601486
C	2.349761248	-7.345299721	-3.428770304
C	1.089803934	-7.965435505	-1.619124770
C	2.786062956	-6.638999939	-4.549042702
N	2.871079922	-8.518998146	-2.889654875
C	2.108521700	-5.477261066	-4.938455105
H	3.649687290	-6.993998528	-5.096745968
H	3.466952085	-4.346363068	-3.997823000
C	2.116161108	-8.881254196	-1.821113944
C	0.050160151	-8.185764313	-0.642023325
H	2.330744982	-9.786211014	-1.268839478
C	4.022934914	-9.230695724	-3.418681145
H	4.909829617	-8.589629173	-3.394699812
H	4.210941315	-10.115779877	-2.809667110
H	3.835396528	-9.543978691	-4.450717926
O	-0.986082554	-7.528267384	-0.529229224
H	0.220191136	-9.047428131	0.032522108
N	-0.449417412	-5.318117619	-2.097386599
H	-0.859080493	-6.103743076	-1.569926620
C	-0.645176351	-4.079335690	-1.547460198
O	0.043627229	-3.087984800	-1.866252661
C	-1.741667032	-3.938568354	-0.548502743
C	-2.752484560	-4.893167019	-0.352994561
C	-1.755596161	-2.754748344	0.208141893
C	-3.749201298	-4.667815208	0.593926132
C	-2.750255346	-2.537514925	1.155848861
C	-3.749103546	-3.494825363	1.351219177
H	-2.778192043	-5.807119370	-0.933511078
H	-0.976023436	-2.020139694	0.038356923
H	-4.529138088	-5.409107685	0.737985194
H	-2.748320580	-1.623498082	1.742496490
H	-4.527345181	-3.325250149	2.089885712
C	0.227934524	-3.133651733	-5.479626656
N	0.413578689	-3.775311708	-4.326107025
O	0.702807903	-3.524451494	-6.587063789
C	-0.536193907	-1.864859223	-5.432702065
C	-0.249848902	-0.890196681	-6.400946140
C	-1.480425119	-1.595266938	-4.428199291
C	-0.887101471	0.346820474	-6.354017258
H	0.486105859	-1.112307787	-7.166336060
C	-2.117100239	-0.357834667	-4.390325069
H	-1.720855832	-2.343193769	-3.680967331
C	-1.818898439	0.614845514	-5.347993374
H	-0.654216945	1.104559302	-7.096041679
H	-2.847870588	-0.153456390	-3.613868713
H	-2.313530922	1.581099153	-5.310466290
H	0.197543755	-3.275289774	-3.438828707
C	2.319682598	-6.117318153	-8.217658043
C	3.613156796	-6.258792877	-7.634379864
C	4.549062252	-5.197299480	-7.614972115
H	3.859888077	-7.189265251	-7.136029243
Ru	2.564300776	-4.479016781	-6.728564739
H	1.600571156	-6.925724983	-8.148165703
C	1.961073160	-4.901400566	-8.869254112

C	4.161598206	-3.983870983	-8.282063484
C	5.929024220	-5.360019684	-6.998239994
C	2.929354906	-3.853279114	-8.948589325
C	0.581402957	-4.694018364	-9.428280830
H	4.825032711	-3.126515865	-8.238220215
H	2.660828829	-2.908719301	-9.408207893
H	5.924988270	-6.316262722	-6.457372665
C	6.280292034	-4.257154465	-5.986727238
C	6.987741947	-5.449526310	-8.114686012
H	7.288577080	-4.418873310	-5.592317104
H	6.264888763	-3.262445927	-6.445947647
H	5.583635807	-4.251359940	-5.145632267
H	6.756815434	-6.249742031	-8.824581146
H	7.045079708	-4.507927418	-8.672612190
H	7.976362705	-5.645370007	-7.688013554
H	-0.105516367	-5.474542141	-9.094417572
H	0.184295714	-3.728263378	-9.105487823
H	0.619549751	-4.707361698	-10.523468018
O	3.118504763	-2.697131634	-5.581934452
C	3.470137596	-2.507744789	-4.406455040
O	3.739326000	-3.496942759	-3.575317144
C	3.576241493	-1.118731022	-3.801883459
C	4.860575676	-1.019034505	-2.952333450
C	3.570188046	-0.061168842	-4.914916039
C	2.327037334	-0.947216392	-2.896370888
H	5.756257534	-1.176575422	-3.562726021
H	4.922831059	-0.018761436	-2.513637781
H	4.861556530	-1.750992775	-2.141566992
H	3.617594242	0.935520113	-4.466583252
H	4.431097507	-0.177350864	-5.580705643
H	2.659768581	-0.126107171	-5.516158104
H	2.253429890	-1.738081694	-2.146845341
H	2.395007849	0.016812861	-2.382678270
H	1.405956626	-0.949779034	-3.486309528

8.6 Vibrational frequencies for DFT-optimized structures

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PivOH

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48.63 218.96 243.31 262.86 289.36 296.47
357.68 367.49 385.38 515.99 575.58 609.10
728.55 787.03 870.69 950.96 960.62 984.06
1056.72 1062.74 1157.44 1239.69 1252.92 1281.29
1366.80 1414.42 1422.86 1451.47 1492.39 1500.01
1505.80 1515.17 1520.07 1539.96 1835.02 3043.61
3045.27 3053.18 3113.72 3115.18 3126.62 3135.46
3137.43 3139.62 3756.48

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94.69 118.36 143.05 151.84 187.99 255.43
278.04 338.82 418.94 440.26 517.06 547.70
583.30 585.98 616.45 743.70 763.99 782.41
783.48 803.38 823.84 874.67 949.52 996.98
1017.01 1040.38 1049.57 1092.83 1151.65 1155.40
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1407.36 1413.35 1444.05 1467.95 1492.16 1510.97
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2875.47 3044.30 3108.40 3152.47 3181.00 3194.00
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2a

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47.11 96.43 134.13 207.35 319.65 326.25
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893.93 943.83 951.02 988.78 988.90 1013.20
1016.68 1051.74 1088.24 1118.83 1183.55 1201.39
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1629.25 1664.00 1671.35 1950.89 3188.26 3199.59
3208.42 3218.60 3222.01

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4a

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32.25 35.90 54.95 91.56 111.16 128.26
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591.85 610.08 631.97 639.06 669.86 700.58
721.84 737.99 756.01 769.41 783.30 798.73
808.09 819.15 842.11 866.54 897.16 902.30
950.12 971.53 985.44 989.28 1007.48 1014.17
1017.34 1057.83 1084.17 1094.27 1117.08 1128.79
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1386.24 1405.02 1410.64 1438.65 1466.08 1488.45
1490.26 1494.32 1528.31 1536.32 1543.74 1587.50
1613.24 1637.22 1642.75 1661.18 1676.94 1734.27
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3189.31 3190.17 3201.41 3213.77 3220.82 3232.79
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5a

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28.10 31.24 33.22 43.71 47.74 53.51
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374.51 406.67 413.93 417.16 435.37 452.93
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1201.60 1223.77 1226.38 1229.21 1241.72 1282.83
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CO_2

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641.84 641.85 1372.93 2440.54

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B

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1413.35 1416.47 1416.83 1425.48 1428.41 1439.68
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B-TS

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931.36 949.69 953.32 958.99 959.67 976.95
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3138.98 3143.77 3150.93 3169.48 3189.47 3204.55
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B'-TS

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3207.16 3213.72 3222.06 3223.74 3226.06 3243.49

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C

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14.28 24.10 25.59 38.35 45.45 67.14
80.35 88.80 101.35 112.81 120.42 134.86
138.12 151.82 167.55 175.34 181.31 193.10
196.36 212.10 225.15 234.48 246.32 248.62
263.34 267.37 271.09 283.92 284.57 296.29
302.93 308.47 316.84 318.13 331.38 350.42
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547.26 554.73 566.93 602.37 609.01 611.31
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1188.49 1195.56 1219.47 1222.35 1230.95 1231.46
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1492.48 1495.64 1498.13 1500.10 1501.14 1502.52
1504.73 1508.24 1510.58 1515.90 1518.17 1519.16
1522.54 1531.39 1534.95 1539.76 1575.73 1578.71
1611.75 1637.30 1643.01 1708.01 3021.84 3038.67
3043.58 3045.10 3052.04 3054.33 3057.19 3059.07
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C'

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D

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10.80 21.47 29.56 35.20 53.11 59.16
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119.10 133.15 142.18 148.33 162.79 168.69
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D-TS

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E

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E-TS

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624.36 627.21 628.88 630.60 657.71 667.89
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F-TS

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G

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G-TS

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G'-TS

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H

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I-TS

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J

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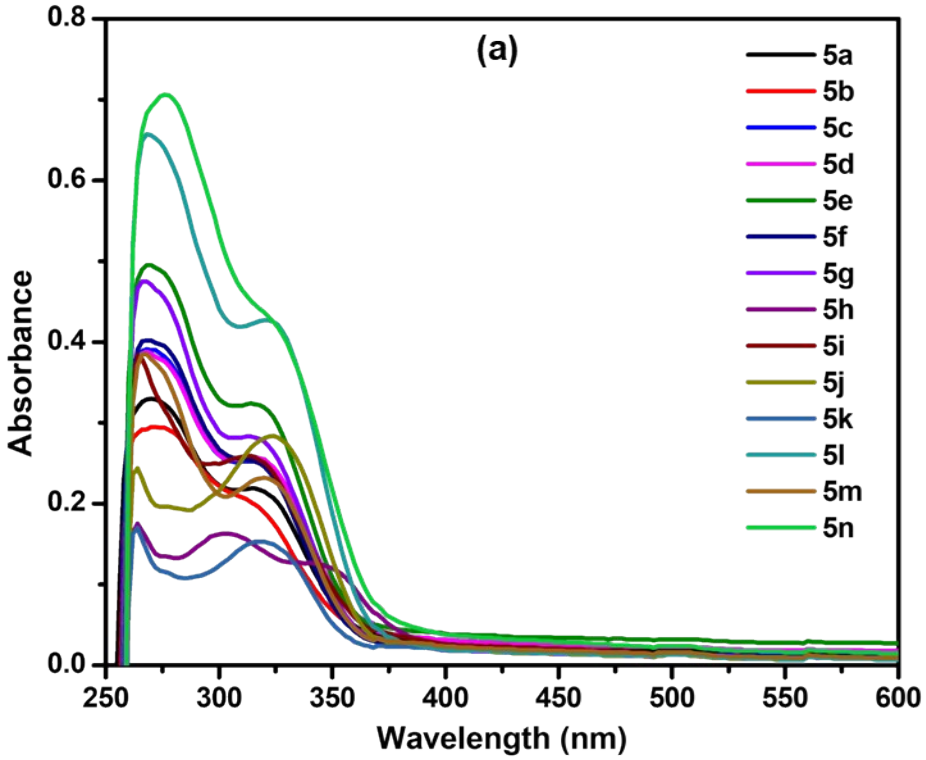
3422.50

8. Chemosensors application

Instrumentation and procedure for metal sensing measurements

UV–Vis and fluorescence spectra were recorded using a UV 3220 spectrometer (Optizen) and spectrofluorometer (HITACHI) F-2700 equipped with a Xe arc lamp, respectively. The stock solutions of chloride and nitrate metal salts (Ag^{+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Ce^{3+}, Cu^{2+}, Co^{2+}, Fe^{3+}, Hg^{2+}, Mn^{2+}, Na^{+}, Ni^{2+}, Pb^{2+}, Sn^{2+}, Sr^{2+}, Ti^{3+} and Zn^{2+}) were first prepared with 10 mM in pH 7.4 phosphate buffer solution (PBS). A stock solution of compounds **5a–5o**, **6a–6h**, and **7a–7j** (1.0×10^{-5} mol/L) was prepared in DMSO. Before the spectroscopic measurements, test solutions were prepared in 1.0 mL of PBS solution and 0.97 mL of DMSO mixed with 5 μL stock solution of **7i** (1.0×10^{-5} mol/L) and 25 μL of each metal ions stock into cuvettes with the final volume of 2.0 mL respectively. Fe^{3+} metal ions were detected by adding a different aliquot of stock solution of 0 – 10 mM with **7i** (1.0×10^{-5} mol/L). All UV–Vis spectra were recorded at room temperature after the addition of samples for a few seconds. All the fluorescence measurements were carried out after 2 min of incubation at 324 nm (λ_{exc}) emission wavelength range from 300–700 nm with 5 nm of slit width, 250 V of photomultiplier tube voltage, and a scan speed of 240 nm/min.


(a)
Absorbance
Wavelength (nm)
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0.6
0.8
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300
350
400
450
500
550
600
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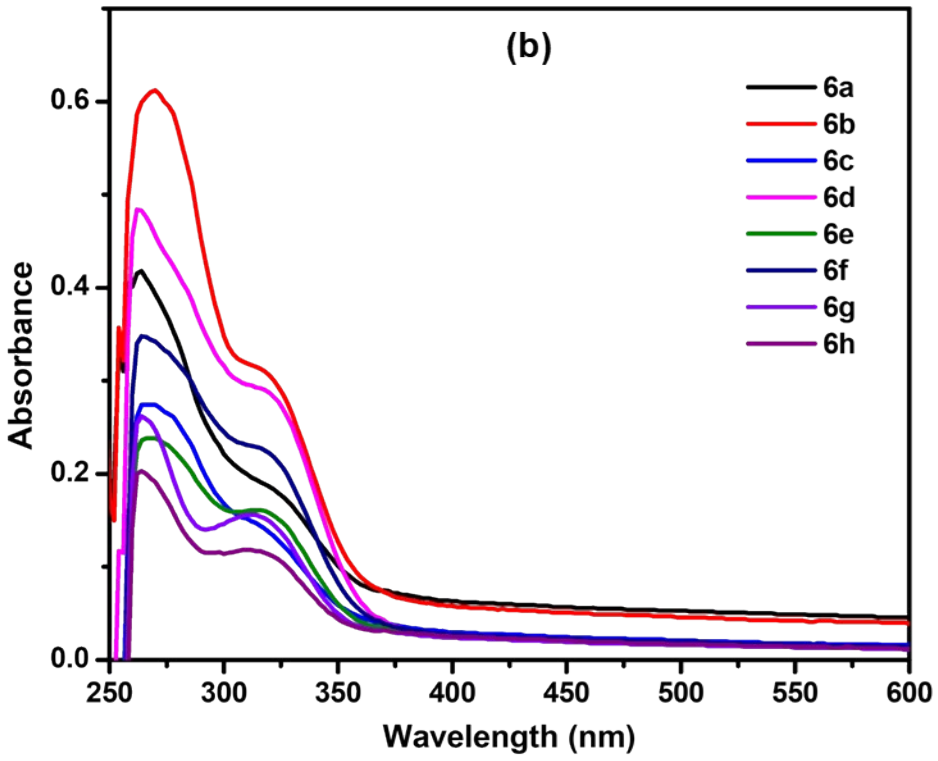
5b
5c
5d
5e
5f
5g
5h
5i
5j
5k
5l
5m
5n


(b)
Absorbance
Wavelength (nm)
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0.2
0.4
0.6
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300
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400
450
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600
6a
6b
6c
6d
6e
6f
6g
6h

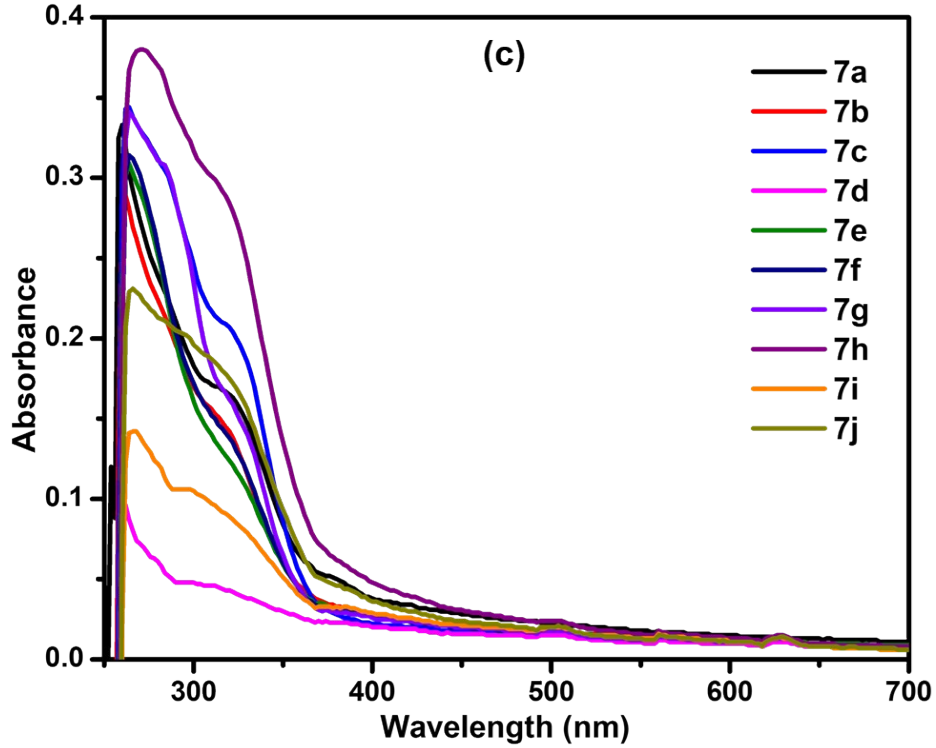
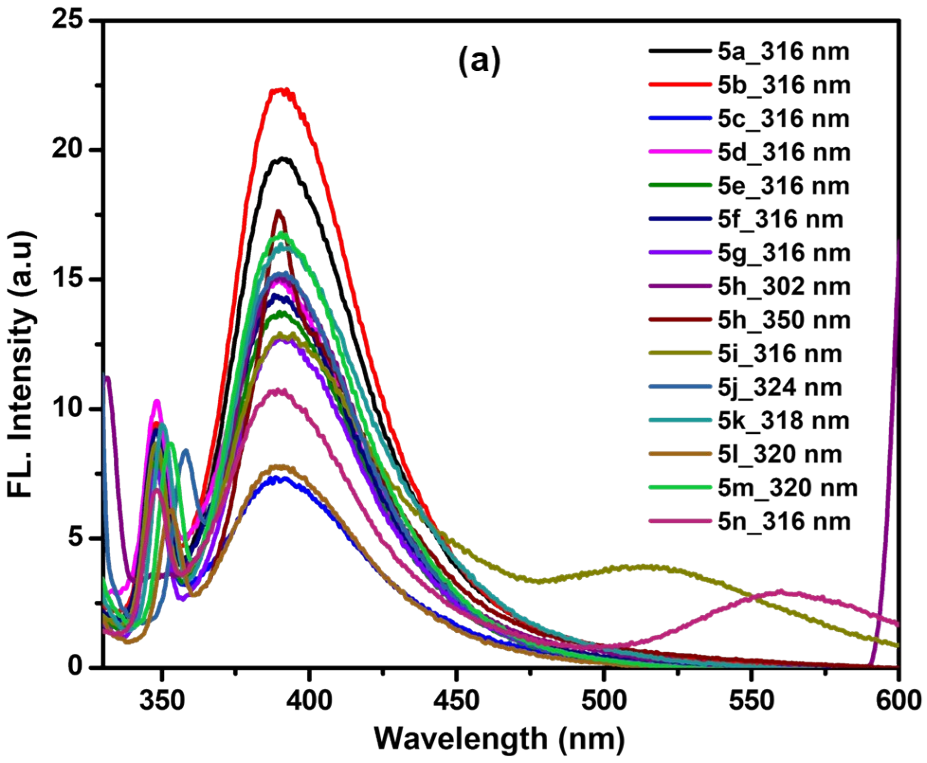


Fig. S4. Absorption spectral properties of (a) **5a-5n**, (b) **6a-6h**, and (c) **7a-7j**.



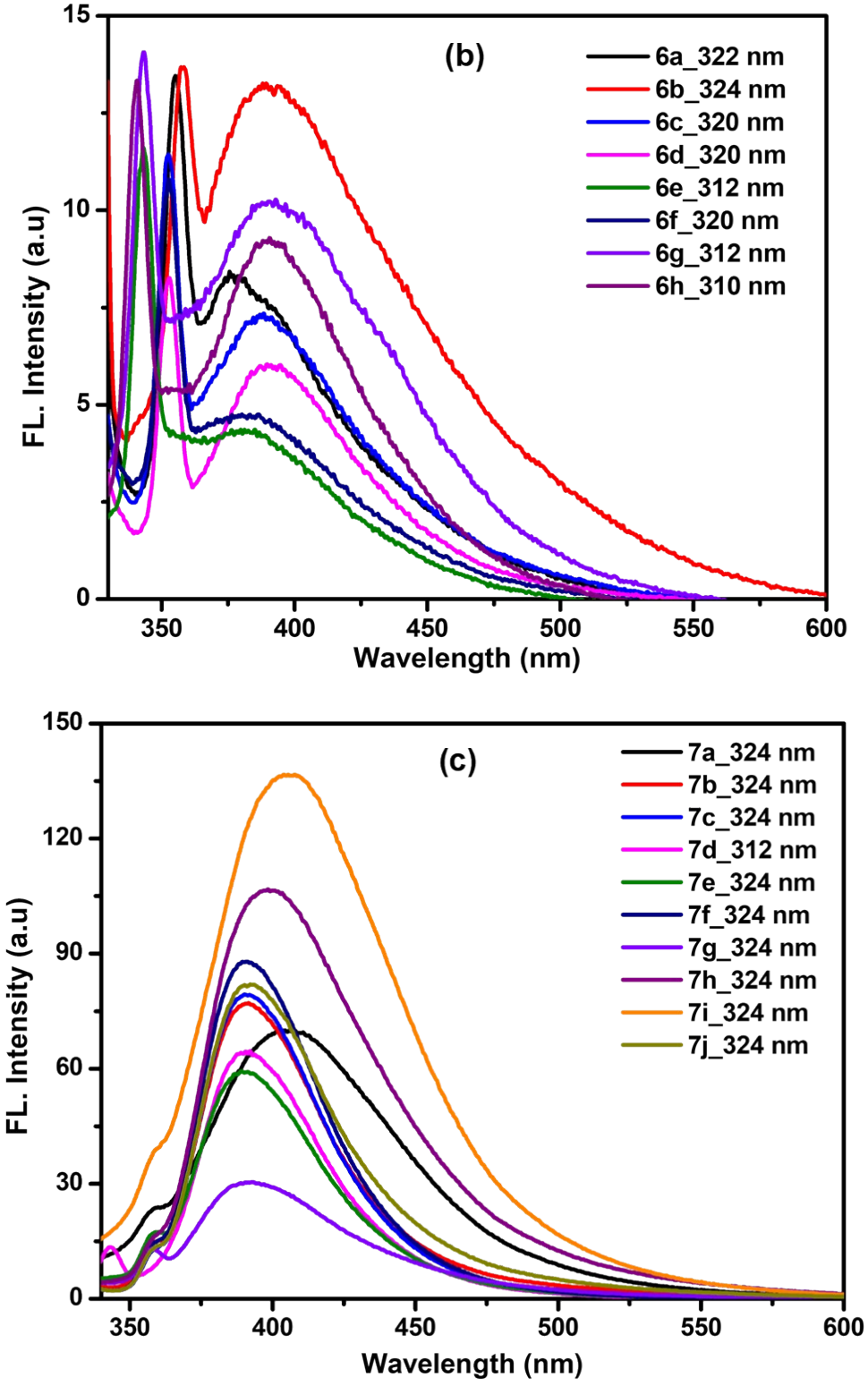


Fig. S5. Fluorescence spectral properties of (a) **5a-5n**, (b) **6a-6h**, and (c) **7a-7j**.

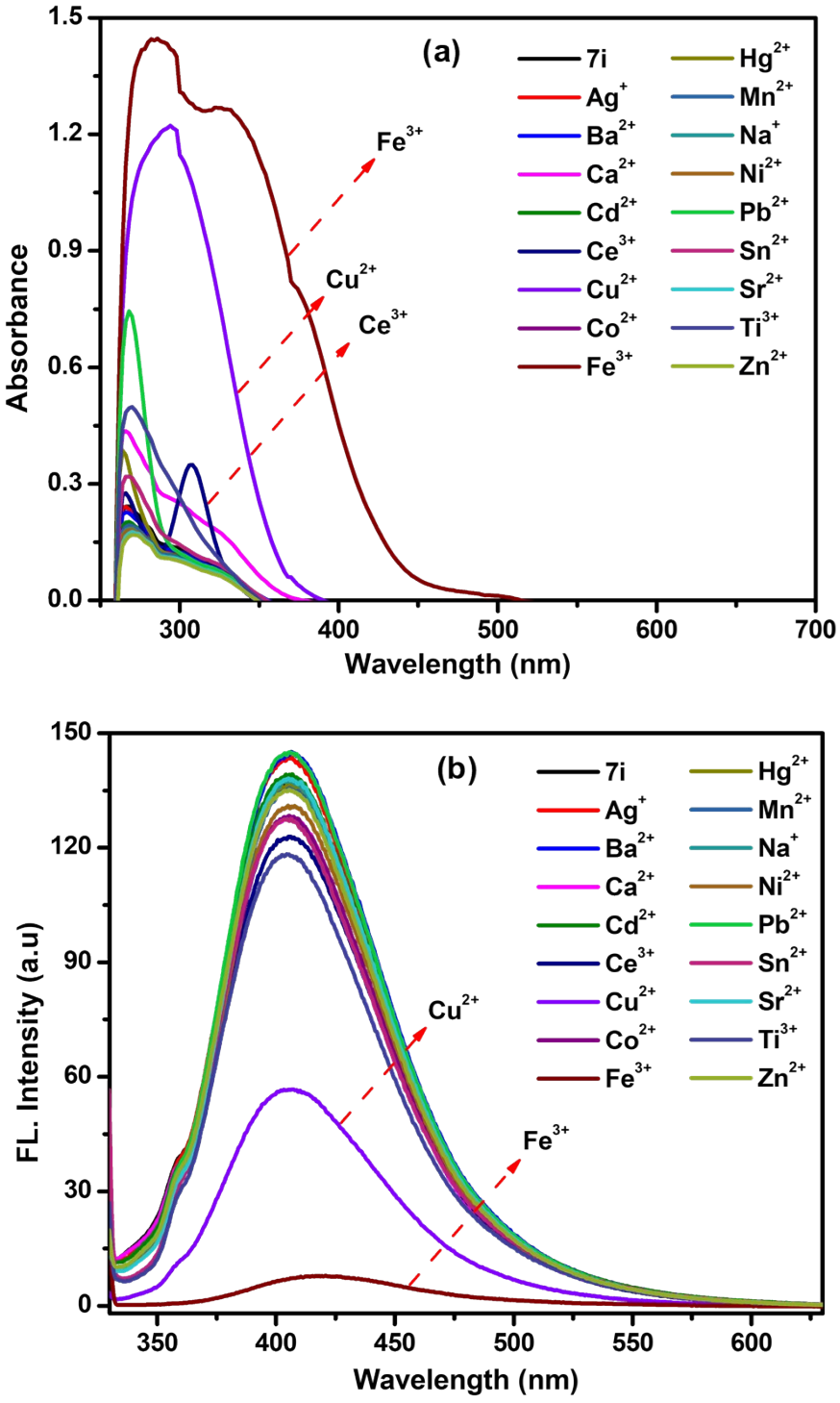


Fig. S6. (a) Absorption and (b) Fluorescence spectral properties of **7i** (1.0×10^{-5} mol/L) system in the presence of various metal ions (Ag^{+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Ce^{3+}, Cu^{2+}, Co^{2+}, Fe^{3+}, Hg^{2+}, Mn^{2+}, Na^{+}, Ni^{2+}, Pb^{2+}, Sn^{2+}, Sr^{2+}, Ti^{3+}, and Zn^{2+}) at 10 mM pH 7.4.

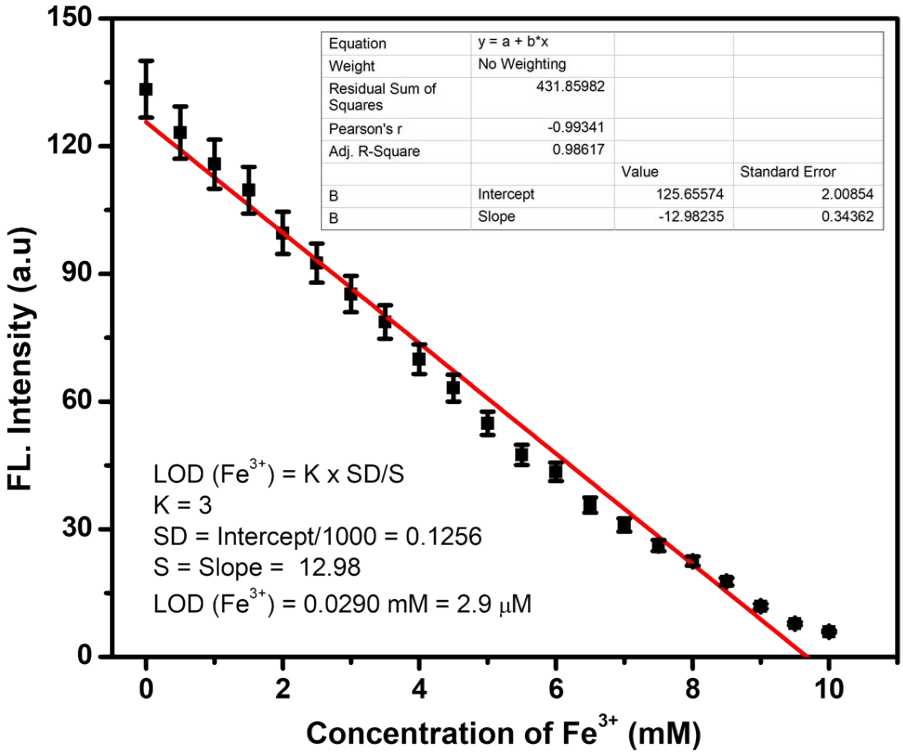


Fig. S7. Calibration curve of **7i** in the presence of Fe^{3+} ions using the monitored emission wavelength at 405 nm in **7i**-Fe^{3+} systems. The detection limit (LOD) was determined from the following equation: LOD = K × SD/S, where K = 3; SD is the standard deviation of the blank solution; S is the slope of the calibration curve.

9. References

1. V. Bizet and L. Buglioni, C. Bolm, *Angew. Chem., Int. Ed.*, 2014, **53**, 5639–5642.
2. R. G. Parr and Yang, W. Theory of Atoms and Molecules. Oxford University Press: New York, **1989**.
3. A. D. Bochevarov, E. Harder, T. F. Hughes, J. R. Greenwood, D. A. Braden, D. M. Philipp, D. Rinaldo, M. D. Halls, J. Zhang and R. J. Friesner, *Int. J. Quantum Chem.*, **2013**, *113*, 2110.
4. J. C. Slater, Quantum Theory of Molecules and Solids, Vol. 4: McGraw-Hill: New York, **1974**.
5. S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.*, **1980**, *58*, 1200–1211.
6. A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098–3100.
7. C. Lee, W. Yang and R. G. Parr, Density. *Phys. Rev. B*, 1988, **37**, 785–789.
8. A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648–5652.
9. S. Grimme, J. Antony, S. Ehrlich, S. A. Krieg, *J. Chem. Phys.* 2010, **132**, 154104
10. W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.* 1972, **56**, 2257–2261.
11. P. J. Hay and W. R. Wadt, *J. Chem. Phys.* 1985, **82**, 270–283.
12. W. R. Wadt and P. J. Hay, *J. Chem. Phys*. 1985, **82**, 284-298.
13. P. J. Hay and W. R. Wadt, *J. Chem. Phys.* 1985, **82**, 299–310.
14. T. H. Dunning, *J. Chem. Phys.* 1989, **90**, 1007–1023.
15. B. Marten, K. Kim, C. Cortis, R. A. Friesner, R. B. Murphy, M. N. Ringnalda, D. Sitkoff and B. Honig, *J. Phys. Chem.* 1996, **100**, 11775–11788.
16. M. Friedrichs, R. H. Zhou, S. R. Edinger, R. A. Friesner, *J. Phys. Chem.*, *B* 1999, **103**, 3057–3061.
17. S. R. Edinger, C. Cortis, P. S. Shenkin and R. A. Friesner, *J. Phys. Chem.*, *B* 1997, **101**, 1190–1197.
18. A. A. Rashin and B. Honig, *J. Phys. Chem.* 1985, **89**, 5588–5593.

10. X-Ray crystallographic structure and data of compound 5i

Empirical Formula $C_{35}H_{25}N_3O_3$, M = 535.58, Orthorhombic, Space group P_{bca}, a = 12.0479(5) Å, b = 18.5786(9) Å, c = 24.7785(12) Å, V = 5546.2(4) Å^3, Z = 8, T = 223(2) K, ρ_{calcd} = 1.283 Mg/m^3, $2\Theta_{max.}$ = 25.242°, Refinement of 378 parameters on 6880 independent reflections out of 223588 collected reflections (R_{int} = 0.0601) led to R1 = 0.0497 [I >2σ(I)], wR_2 = 0.1322 (all data) and S = 1.040 with the largest difference peak and hole of 0.223 and -0.205 e.Å^{-3} respectively. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 2070102). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif.

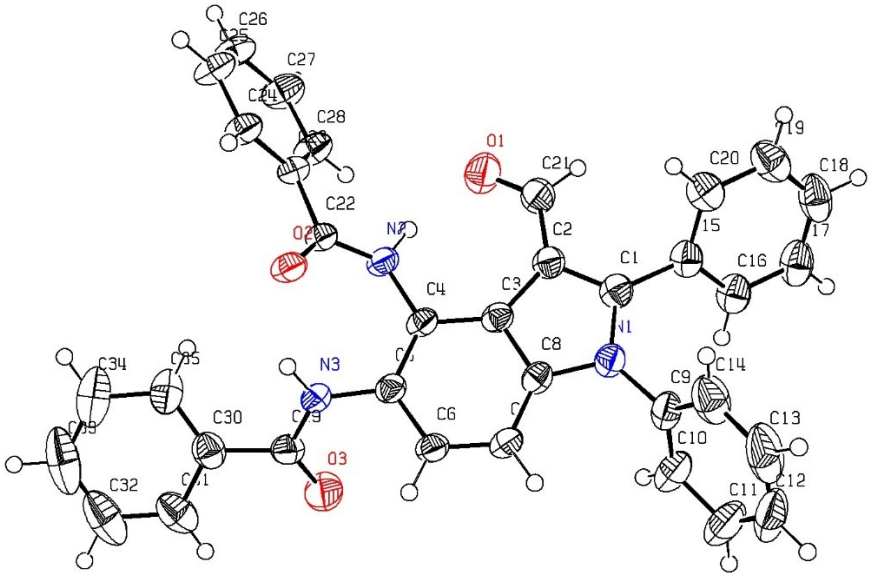


Fig. S8. X-ray crystal structure of compound **5i**.

Table S2. Crystal data and structure refinement for **5i**.

Identification code	**5i**	
Empirical formula	C35 H25 N3 O3	
Formula weight	535.58	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 12.0479(5) Å	α= 90°.
	b = 18.5786(9) Å	β= 90°.
	c = 24.7785(12) Å	γ = 90°.
Volume	5546.2(4) $Å^3$	
Z	8	
Density (calculated)	1.283 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	2240	
Crystal size	0.243 x 0.217 x 0.074 mm^3	
Theta range for data collection	2.192 to 28.307°.	
Index ranges	-16<=h<=16, -24<=k<=24, -33<=l<=33	
Reflections collected	223588	
Independent reflections	6880 [R(int) = 0.0601]	
Completeness to theta = 25.242°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.7144	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6880 / 0 / 378	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0497, wR2 = 0.1250	
R indices (all data)	R1 = 0.0597, wR2 = 0.1322	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.223 and -0.205 $e.Å^{-3}$	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5i**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	4888(1)	4736(1)	4009(1)	38(1)
C(1)	3979(1)	4447(1)	4257(1)	40(1)
C(2)	3077(1)	4907(1)	4185(1)	39(1)
C(3)	3467(1)	5511(1)	3866(1)	34(1)
C(4)	2979(1)	6138(1)	3649(1)	33(1)
C(5)	3663(1)	6625(1)	3380(1)	34(1)
C(6)	4783(1)	6462(1)	3279(1)	37(1)
C(7)	5256(1)	5836(1)	3460(1)	37(1)
C(8)	4593(1)	5383(1)	3766(1)	35(1)
C(9)	5983(1)	4437(1)	3961(1)	44(1)
C(10)	6861(1)	4802(1)	4189(1)	58(1)
C(11)	7931(2)	4544(2)	4122(1)	79(1)
C(12)	8107(2)	3930(2)	3831(1)	91(1)
C(13)	7225(3)	3568(1)	3604(1)	93(1)
C(14)	6148(2)	3818(1)	3665(1)	66(1)
C(15)	4048(1)	3772(1)	4571(1)	41(1)
C(16)	4860(2)	3690(1)	4969(1)	48(1)
C(17)	4904(2)	3070(1)	5274(1)	56(1)
C(18)	4152(2)	2528(1)	5189(1)	60(1)
C(19)	3350(2)	2596(1)	4795(1)	58(1)
C(20)	3297(2)	3216(1)	4484(1)	50(1)
C(21)	2035(1)	4809(1)	4462(1)	51(1)
O(1)	1269(1)	5236(1)	4477(1)	69(1)
N(2)	1830(1)	6255(1)	3728(1)	36(1)
C(22)	1096(1)	6488(1)	3352(1)	33(1)
O(2)	1355(1)	6660(1)	2888(1)	39(1)
C(23)	-83(1)	6529(1)	3535(1)	34(1)
C(24)	-907(1)	6551(1)	3144(1)	43(1)

C(25)	-2006(1)	6615(1)	3292(1)	51(1)
C(26)	-2294(1)	6672(1)	3828(1)	52(1)
C(27)	-1485(1)	6644(1)	4219(1)	53(1)
C(28)	-381(1)	6566(1)	4075(1)	46(1)
N(3)	3238(1)	7293(1)	3199(1)	37(1)
C(29)	3701(1)	7937(1)	3311(1)	42(1)
O(3)	4534(1)	8000(1)	3590(1)	68(1)
C(30)	3129(1)	8576(1)	3073(1)	45(1)
C(31)	3741(2)	9203(1)	3012(1)	60(1)
C(32)	3276(3)	9803(1)	2781(1)	81(1)
C(33)	2189(3)	9799(1)	2633(1)	92(1)
C(34)	1553(2)	9195(1)	2712(1)	84(1)
C(35)	2022(2)	8576(1)	2924(1)	60(1)

Table S4. Bond lengths [Å] and angles [°] for **5i**.

N(1)-C(1)	1.3653(19)
N(1)-C(8)	1.3907(18)
N(1)-C(9)	1.4369(19)
C(1)-C(2)	1.394(2)
C(1)-C(15)	1.478(2)
C(2)-C(21)	1.443(2)
C(2)-C(3)	1.451(2)
C(3)-C(8)	1.4001(19)
C(3)-C(4)	1.4113(19)
C(4)-C(5)	1.3924(19)
C(4)-N(2)	1.4143(17)
C(5)-C(6)	1.4057(19)
C(5)-N(3)	1.4162(18)
C(6)-C(7)	1.371(2)
C(6)-H(6)	0.9400
C(7)-C(8)	1.386(2)

C(7)-H(7)	0.9400
C(9)-C(10)	1.376(3)
C(9)-C(14)	1.379(3)
C(10)-C(11)	1.385(2)
C(10)-H(10)	0.9400
C(11)-C(12)	1.366(4)
C(11)-H(11)	0.9400
C(12)-C(13)	1.379(4)
C(12)-H(12)	0.9400
C(13)-C(14)	1.387(3)
C(13)-H(13)	0.9400
C(14)-H(14)	0.9400
C(15)-C(20)	1.390(2)
C(15)-C(16)	1.397(2)
C(16)-C(17)	1.379(2)
C(16)-H(16)	0.9400
C(17)-C(18)	1.371(3)
C(17)-H(17)	0.9400
C(18)-C(19)	1.380(3)
C(18)-H(18)	0.9400
C(19)-C(20)	1.387(2)
C(19)-H(19)	0.9400
C(20)-H(20)	0.9400
C(21)-O(1)	1.218(2)
C(21)-H(21)	0.9400
N(2)-C(22)	1.3553(17)
N(2)-H(2)	0.90(2)
C(22)-O(2)	1.2334(17)
C(22)-C(23)	1.4941(18)
C(23)-C(24)	1.386(2)
C(23)-C(28)	1.387(2)
C(24)-C(25)	1.378(2)
C(24)-H(24)	0.9400

C(25)-C(26)	1.378(2)
C(25)-H(25)	0.9400
C(26)-C(27)	1.376(2)
C(26)-H(26)	0.9400
C(27)-C(28)	1.385(2)
C(27)-H(27)	0.9400
C(28)-H(28)	0.9400
N(3)-C(29)	1.3489(19)
N(3)-H(3)	0.871(19)
C(29)-O(3)	1.2242(19)
C(29)-C(30)	1.493(2)
C(30)-C(35)	1.384(3)
C(30)-C(31)	1.386(2)
C(31)-C(32)	1.373(3)
C(31)-H(31)	0.9400
C(32)-C(33)	1.361(4)
C(32)-H(32)	0.9400
C(33)-C(34)	1.373(4)
C(33)-H(33)	0.9400
C(34)-C(35)	1.385(3)
C(34)-H(34)	0.9400
C(35)-H(35)	0.9400
C(1)-N(1)-C(8)	109.25(12)
C(1)-N(1)-C(9)	128.44(13)
C(8)-N(1)-C(9)	122.23(12)
N(1)-C(1)-C(2)	109.07(13)
N(1)-C(1)-C(15)	121.65(13)
C(2)-C(1)-C(15)	129.17(14)
C(1)-C(2)-C(21)	122.72(14)
C(1)-C(2)-C(3)	106.98(13)
C(21)-C(2)-C(3)	129.65(14)
C(8)-C(3)-C(4)	118.47(13)
C(8)-C(3)-C(2)	106.15(12)

C(4)-C(3)-C(2)	135.37(13)
C(5)-C(4)-C(3)	118.14(12)
C(5)-C(4)-N(2)	123.06(13)
C(3)-C(4)-N(2)	118.76(12)
C(4)-C(5)-C(6)	120.94(13)
C(4)-C(5)-N(3)	120.49(12)
C(6)-C(5)-N(3)	118.57(12)
C(7)-C(6)-C(5)	121.50(13)
C(7)-C(6)-H(6)	119.3
C(5)-C(6)-H(6)	119.3
C(6)-C(7)-C(8)	117.10(13)
C(6)-C(7)-H(7)	121.5
C(8)-C(7)-H(7)	121.5
C(7)-C(8)-N(1)	127.96(13)
C(7)-C(8)-C(3)	123.47(13)
N(1)-C(8)-C(3)	108.55(12)
C(10)-C(9)-C(14)	121.25(17)
C(10)-C(9)-N(1)	118.76(15)
C(14)-C(9)-N(1)	119.88(17)
C(9)-C(10)-C(11)	119.8(2)
C(9)-C(10)-H(10)	120.1
C(11)-C(10)-H(10)	120.1
C(12)-C(11)-C(10)	119.7(3)
C(12)-C(11)-H(11)	120.1
C(10)-C(11)-H(11)	120.1
C(11)-C(12)-C(13)	120.3(2)
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	120.9(2)
C(12)-C(13)-H(13)	119.6
C(14)-C(13)-H(13)	119.6
C(9)-C(14)-C(13)	118.2(2)
C(9)-C(14)-H(14)	120.9

C(13)-C(14)-H(14)	120.9
C(20)-C(15)-C(16)	118.95(15)
C(20)-C(15)-C(1)	120.78(14)
C(16)-C(15)-C(1)	120.26(15)
C(17)-C(16)-C(15)	120.27(17)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(18)-C(17)-C(16)	120.37(17)
C(18)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
C(17)-C(18)-C(19)	120.19(16)
C(17)-C(18)-H(18)	119.9
C(19)-C(18)-H(18)	119.9
C(18)-C(19)-C(20)	120.12(18)
C(18)-C(19)-H(19)	119.9
C(20)-C(19)-H(19)	119.9
C(19)-C(20)-C(15)	120.10(17)
C(19)-C(20)-H(20)	120.0
C(15)-C(20)-H(20)	120.0
O(1)-C(21)-C(2)	126.29(15)
O(1)-C(21)-H(21)	116.9
C(2)-C(21)-H(21)	116.9
C(22)-N(2)-C(4)	126.30(12)
C(22)-N(2)-H(2)	115.8(12)
C(4)-N(2)-H(2)	113.5(12)
O(2)-C(22)-N(2)	123.96(12)
O(2)-C(22)-C(23)	120.65(12)
N(2)-C(22)-C(23)	115.39(12)
C(24)-C(23)-C(28)	119.09(13)
C(24)-C(23)-C(22)	118.10(13)
C(28)-C(23)-C(22)	122.78(12)
C(25)-C(24)-C(23)	120.38(15)
C(25)-C(24)-H(24)	119.8

C(23)-C(24)-H(24)	119.8
C(26)-C(25)-C(24)	120.28(15)
C(26)-C(25)-H(25)	119.9
C(24)-C(25)-H(25)	119.9
C(27)-C(26)-C(25)	119.87(15)
C(27)-C(26)-H(26)	120.1
C(25)-C(26)-H(26)	120.1
C(26)-C(27)-C(28)	120.14(16)
C(26)-C(27)-H(27)	119.9
C(28)-C(27)-H(27)	119.9
C(27)-C(28)-C(23)	120.20(14)
C(27)-C(28)-H(28)	119.9
C(23)-C(28)-H(28)	119.9
C(29)-N(3)-C(5)	124.28(12)
C(29)-N(3)-H(3)	119.1(12)
C(5)-N(3)-H(3)	116.6(12)
O(3)-C(29)-N(3)	122.62(15)
O(3)-C(29)-C(30)	121.68(15)
N(3)-C(29)-C(30)	115.70(13)
C(35)-C(30)-C(31)	118.89(17)
C(35)-C(30)-C(29)	123.35(15)
C(31)-C(30)-C(29)	117.74(16)
C(32)-C(31)-C(30)	120.7(2)
C(32)-C(31)-H(31)	119.7
C(30)-C(31)-H(31)	119.7
C(33)-C(32)-C(31)	120.1(2)
C(33)-C(32)-H(32)	120.0
C(31)-C(32)-H(32)	120.0
C(32)-C(33)-C(34)	120.2(2)
C(32)-C(33)-H(33)	119.9
C(34)-C(33)-H(33)	119.9
C(33)-C(34)-C(35)	120.3(3)
C(33)-C(34)-H(34)	119.8

C(35)-C(34)-H(34)	119.8
C(30)-C(35)-C(34)	119.7(2)
C(30)-C(35)-H(35)	120.2
C(34)-C(35)-H(35)	120.2

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5i**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	36(1)	41(1)	37(1)	3(1)	-2(1)	5(1)
C(1)	41(1)	45(1)	33(1)	2(1)	-2(1)	1(1)
C(2)	36(1)	46(1)	34(1)	6(1)	-2(1)	-1(1)
C(3)	30(1)	43(1)	30(1)	1(1)	-2(1)	-1(1)
C(4)	26(1)	44(1)	30(1)	1(1)	-2(1)	1(1)
C(5)	29(1)	41(1)	32(1)	2(1)	-5(1)	-1(1)
C(6)	28(1)	46(1)	36(1)	4(1)	-2(1)	-4(1)
C(7)	26(1)	48(1)	38(1)	0(1)	-1(1)	2(1)
C(8)	32(1)	41(1)	33(1)	-1(1)	-4(1)	3(1)
C(9)	44(1)	48(1)	38(1)	9(1)	7(1)	16(1)
C(10)	40(1)	76(1)	57(1)	3(1)	-2(1)	17(1)
C(11)	43(1)	117(2)	78(1)	28(1)	6(1)	28(1)
C(12)	76(2)	104(2)	94(2)	53(2)	43(1)	57(2)
C(13)	123(2)	58(1)	98(2)	20(1)	58(2)	45(2)
C(14)	88(2)	47(1)	64(1)	4(1)	22(1)	15(1)
C(15)	48(1)	44(1)	31(1)	2(1)	3(1)	6(1)
C(16)	54(1)	54(1)	35(1)	2(1)	-2(1)	8(1)
C(17)	69(1)	63(1)	35(1)	9(1)	4(1)	22(1)
C(18)	86(1)	50(1)	45(1)	13(1)	20(1)	19(1)
C(19)	75(1)	43(1)	56(1)	-1(1)	18(1)	-1(1)
C(20)	58(1)	51(1)	40(1)	1(1)	4(1)	-1(1)

C(21)	45(1)	59(1)	48(1)	20(1)	6(1)	2(1)
O(1)	48(1)	86(1)	73(1)	37(1)	22(1)	16(1)
N(2)	26(1)	48(1)	33(1)	6(1)	1(1)	0(1)
C(22)	27(1)	39(1)	34(1)	-1(1)	-2(1)	-2(1)
O(2)	28(1)	58(1)	32(1)	5(1)	-2(1)	-5(1)
C(23)	26(1)	38(1)	37(1)	-3(1)	-1(1)	-2(1)
C(24)	31(1)	61(1)	36(1)	-1(1)	-2(1)	-3(1)
C(25)	28(1)	74(1)	52(1)	-5(1)	-6(1)	-2(1)
C(26)	27(1)	69(1)	60(1)	-9(1)	6(1)	-2(1)
C(27)	40(1)	77(1)	43(1)	-9(1)	10(1)	0(1)
C(28)	34(1)	68(1)	37(1)	-7(1)	-2(1)	1(1)
N(3)	28(1)	41(1)	41(1)	6(1)	-7(1)	-2(1)
C(29)	36(1)	45(1)	44(1)	5(1)	-2(1)	-6(1)
O(3)	56(1)	54(1)	92(1)	5(1)	-34(1)	-14(1)
C(30)	52(1)	42(1)	40(1)	2(1)	5(1)	3(1)
C(31)	81(1)	42(1)	58(1)	-1(1)	19(1)	-4(1)
C(32)	140(2)	40(1)	62(1)	4(1)	28(2)	7(1)
C(33)	165(3)	54(1)	57(1)	9(1)	6(2)	45(2)
C(34)	105(2)	77(2)	70(1)	2(1)	-20(1)	42(1)
C(35)	64(1)	56(1)	61(1)	7(1)	-12(1)	13(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **5i**.

	x	y	z	U(eq)
H(6)	5218	6790	3082	44
H(7)	5996	5719	3379	45
H(10)	6734	5224	4388	69
H(11)	8533	4791	4278	95
H(12)	8833	3755	3785	109
H(13)	7355	3146	3404	111

H(14)	5546	3571	3510	80
H(16)	5379	4059	5029	57
H(17)	5452	3018	5541	67
H(18)	4183	2108	5401	72
H(19)	2839	2222	4736	70
H(20)	2752	3261	4215	59
H(21)	1937	4374	4649	61
H(2)	1542(16)	5993(10)	4000(8)	52(5)
H(24)	-715	6522	2777	51
H(25)	-2560	6620	3025	61
H(26)	-3043	6729	3926	62
H(27)	-1682	6678	4585	64
H(28)	168	6538	4343	55
H(3)	2627(15)	7278(9)	3011(7)	45(5)
H(31)	4482	9217	3131	72
H(32)	3709	10218	2726	97
H(33)	1872	10211	2476	111
H(34)	795	9202	2622	101
H(35)	1591	8158	2966	72

Table S7. Torsion angles [°] for **5i**.

C(8)-N(1)-C(1)-C(2)	-0.74(17)
C(9)-N(1)-C(1)-C(2)	-177.38(14)
C(8)-N(1)-C(1)-C(15)	-177.23(13)
C(9)-N(1)-C(1)-C(15)	6.1(2)
N(1)-C(1)-C(2)-C(21)	-170.85(15)
C(15)-C(1)-C(2)-C(21)	5.3(3)
N(1)-C(1)-C(2)-C(3)	0.73(17)
C(15)-C(1)-C(2)-C(3)	176.87(14)
C(1)-C(2)-C(3)-C(8)	-0.45(16)

C(21)-C(2)-C(3)-C(8)	170.34(16)
C(1)-C(2)-C(3)-C(4)	178.35(15)
C(21)-C(2)-C(3)-C(4)	-10.9(3)
C(8)-C(3)-C(4)-C(5)	-4.8(2)
C(2)-C(3)-C(4)-C(5)	176.51(15)
C(8)-C(3)-C(4)-N(2)	177.27(13)
C(2)-C(3)-C(4)-N(2)	-1.4(2)
C(3)-C(4)-C(5)-C(6)	6.7(2)
N(2)-C(4)-C(5)-C(6)	-175.52(13)
C(3)-C(4)-C(5)-N(3)	-174.09(12)
N(2)-C(4)-C(5)-N(3)	3.7(2)
C(4)-C(5)-C(6)-C(7)	-3.0(2)
N(3)-C(5)-C(6)-C(7)	177.74(13)
C(5)-C(6)-C(7)-C(8)	-2.5(2)
C(6)-C(7)-C(8)-N(1)	-177.63(14)
C(6)-C(7)-C(8)-C(3)	4.4(2)
C(1)-N(1)-C(8)-C(7)	-177.77(14)
C(9)-N(1)-C(8)-C(7)	-0.9(2)
C(1)-N(1)-C(8)-C(3)	0.44(16)
C(9)-N(1)-C(8)-C(3)	177.34(13)
C(4)-C(3)-C(8)-C(7)	-0.7(2)
C(2)-C(3)-C(8)-C(7)	178.32(13)
C(4)-C(3)-C(8)-N(1)	-179.02(12)
C(2)-C(3)-C(8)-N(1)	0.01(15)
C(1)-N(1)-C(9)-C(10)	-118.42(18)
C(8)-N(1)-C(9)-C(10)	65.3(2)
C(1)-N(1)-C(9)-C(14)	65.3(2)
C(8)-N(1)-C(9)-C(14)	-110.94(18)
C(14)-C(9)-C(10)-C(11)	-0.3(3)
N(1)-C(9)-C(10)-C(11)	-176.49(17)
C(9)-C(10)-C(11)-C(12)	0.2(3)
C(10)-C(11)-C(12)-C(13)	-0.1(3)
C(11)-C(12)-C(13)-C(14)	0.1(4)

C(10)-C(9)-C(14)-C(13)	0.3(3)
N(1)-C(9)-C(14)-C(13)	176.46(17)
C(12)-C(13)-C(14)-C(9)	-0.2(3)
N(1)-C(1)-C(15)-C(20)	-130.67(16)
C(2)-C(1)-C(15)-C(20)	53.6(2)
N(1)-C(1)-C(15)-C(16)	50.7(2)
C(2)-C(1)-C(15)-C(16)	-125.03(18)
C(20)-C(15)-C(16)-C(17)	-0.7(2)
C(1)-C(15)-C(16)-C(17)	177.97(15)
C(15)-C(16)-C(17)-C(18)	0.0(3)
C(16)-C(17)-C(18)-C(19)	0.5(3)
C(17)-C(18)-C(19)-C(20)	-0.4(3)
C(18)-C(19)-C(20)-C(15)	-0.2(3)
C(16)-C(15)-C(20)-C(19)	0.8(2)
C(1)-C(15)-C(20)-C(19)	-177.87(15)
C(1)-C(2)-C(21)-O(1)	169.43(19)
C(3)-C(2)-C(21)-O(1)	-0.1(3)
C(5)-C(4)-N(2)-C(22)	45.7(2)
C(3)-C(4)-N(2)-C(22)	-136.50(15)
C(4)-N(2)-C(22)-O(2)	-3.3(2)
C(4)-N(2)-C(22)-C(23)	176.92(13)
O(2)-C(22)-C(23)-C(24)	19.1(2)
N(2)-C(22)-C(23)-C(24)	-161.14(14)
O(2)-C(22)-C(23)-C(28)	-159.07(15)
N(2)-C(22)-C(23)-C(28)	20.7(2)
C(28)-C(23)-C(24)-C(25)	0.5(2)
C(22)-C(23)-C(24)-C(25)	-177.68(15)
C(23)-C(24)-C(25)-C(26)	1.3(3)
C(24)-C(25)-C(26)-C(27)	-1.8(3)
C(25)-C(26)-C(27)-C(28)	0.6(3)
C(26)-C(27)-C(28)-C(23)	1.2(3)
C(24)-C(23)-C(28)-C(27)	-1.7(3)
C(22)-C(23)-C(28)-C(27)	176.38(16)

C(4)-C(5)-N(3)-C(29)	127.85(16)
C(6)-C(5)-N(3)-C(29)	-52.9(2)
C(5)-N(3)-C(29)-O(3)	-1.0(3)
C(5)-N(3)-C(29)-C(30)	179.14(13)
O(3)-C(29)-C(30)-C(35)	-156.52(18)
N(3)-C(29)-C(30)-C(35)	23.4(2)
O(3)-C(29)-C(30)-C(31)	21.9(2)
N(3)-C(29)-C(30)-C(31)	-158.24(15)
C(35)-C(30)-C(31)-C(32)	-3.5(3)
C(29)-C(30)-C(31)-C(32)	178.03(17)
C(30)-C(31)-C(32)-C(33)	3.2(3)
C(31)-C(32)-C(33)-C(34)	-0.1(4)
C(32)-C(33)-C(34)-C(35)	-2.6(4)
C(31)-C(30)-C(35)-C(34)	0.8(3)
C(29)-C(30)-C(35)-C(34)	179.18(18)
C(33)-C(34)-C(35)-C(30)	2.2(3)

Symmetry transformations used to generate equivalent atoms:

Table S8. Hydrogen bonds for **5i** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3)...O(2)	0.871(19)	1.940(18)	2.6694(15)	140.4(16)
N(2)-H(2)...O(1)	0.90(2)	1.86(2)	2.7351(18)	161.5(18)

Symmetry transformations used to generate equivalent atoms: