Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Effective Modulation of 2,1,3-Benzothiadiazoles and 2,1,3-Benzoselenadiazoles Photoluminescence Properties by Pd-Catalyzed C–H Bond Arylations

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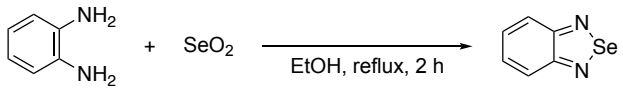
1. General Methods

All reactions were carried out under argon atmosphere with standard Schlenk techniques. DMA, 2,1,3-benzothiadiazole, aryl bromides were purchased from chemical suppliers and were not purified before use. 2,1,3-benzoselenadiazole was prepared according the literature.[1] ^{1}H NMR spectra were recorded on Bruker GPX (400 MHz) spectrometer. Chemical shifts (δ) were reported in parts per million relative to residual chloroform (7.28 ppm for ^{1}H; 77.23 ppm for ^{13}C), constants were reported in Hertz. ^{1}H NMR assignment abbreviations were the following: singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublets (dd), doublet of triplets (dt), and multiplet (m). ^{13}C NMR spectra were recorded at 100 MHz on the same spectrometer and reported in ppm. All reagents were weighed and handled in air. UV-Vis absorption spectra were recorded at room temperature using a Specord 205 UV/Vis/NIR spectrophotometer in quartz cuvettes of 1 cm pathlength. Molar absorptivity determination was verified by linear least-squares fit of values obtained from independent solutions at varying concentrations ranging from 10^{-4} to 10^{-5} M. The sample solutions for the emission spectra were prepared in dichloromethane HPLC grade solvent. Steady-state luminescence spectra were measured using an Edinburgh FS920 Steady State Fluorimeter combined with a FL920 Fluorescence Lifetime Spectrometer. All samples for steady-state measurements were excited at 350 nm. The spectra were corrected for the wavelength dependence of the detector, and the quoted emission maxima refer to the values after correction. Luminescence quantum yields were determined using $[Ru(bpy)_3]Cl_2$ (Φ= 0.028 in air-equilibrated aqueous solution)[2] as standard.

Procedure A (Palladium-catalyzed direct C4 arylation): To a 20 mL oven dried Schlenk tube, 2,1,3-benzothiadiazole (1.5 mmol) or 2,1,3- benzoselenadiazole (1.5 mmol), aryl bromide (1 mmol), PivOK (280 mg, 2 mmol), DMA (4 mL) and $Pd(OAc)_2$ (2.2 mg, 0.01 mmol, 1 mol%) were successively added. The reaction mixture was evacuated by vacuum-argon cycles (5 times) and stirred at 150 °C (oil bath temperature) for 16 hours (see tables and schemes). After cooling the reaction at room temperature and concentration, the crude mixture was purified by silica column chromatography to afford the desired arylated products.

Procedure B (Palladium-catalyzed one-pot direct C4,C7-diarylation): To a 20 mL oven dried Schlenk tube, 2,1,3-benzothiadiazole (136 mg, 1 mmol), aryl bromide (3 mmol), PivOK (420 mg, 3 mmol), DMA (4 mL) and $Pd(OAc)_2$ (2.2 mg, 0.01 mmol, 1 mol%) were successively added. The reaction mixture was evacuated by vacuum-argon cycles (5 times) and stirred at 150 °C (oil bath temperature) for 16 hours. After cooling the reaction at room temperature and concentration, the crude mixture was purified by silica column chromatography to afford the desired diarylated products.

Preparation of benzo[c][1,2,5]selenadiazole



Benzo[c][1,2,5]selenadiazole is prepare following the procedure described by Smith.[3] A solution of *o*-phenylenediamine (1.08 g, 10 mmol) in ethanol (55 mL) was heated to reflux in a round-bottomed single- necked flask and then SeO_2 (1.17 g, 10.5 mmol) in hot water (30 mL) was added. The reaction mixture was stirred and refluxed for 2 h. The solvent was removed using a rotary evaporator and then the residue was dissolved in ethyl acetate (15 mL). The organic layer was washed with water (2 x 10 mL), dried over Na_2SO_4, filtrated and concentrated under vacuo. The crude product was purified by purified by flash chromatography on silica gel (CH_2Cl_2, 100) to afford the desired product (1.8 g, 99%) ^{1}H NMR (d, CDCl3): 7.46–7.50 (m, 2H), 7.84– 7.87 (m, 2H). This product should be stored under argon at 0 ºC to prevent its degradation.

2. Product characterizations

4-(Benzo[*c*][1,2,5]thiadiazol-4-yl)benzonitrile (1): Following the general procedure **A** using 4-bromobenzonitrile (182 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 90-10) to afford the desired compound **1** (199 mg, 84%) as a white solid (Mp = 196-198 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.16 – 8.04 (m, 3H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.80 – 7.72 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.5, 152.9, 141.7, 132.4, 132.4, 129.9, 129.5, 128.4, 122.0, 118.8, 112.0. Elemental analysis: calcd (%) for $C_{13}H_7N_3S$ (237.28): C 65.81, H 2.97; found: C 65.59, H 3.21.

4-(4-Nitrophenyl)benzo[*c*][1,2,5]thiadiazole (2): Following the general procedure **A** using 4-bromonitrobenzene (202 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-EtOAc, 98-2) to afford the desired compound **2** (190 mg, 74%) as a white solid (Mp = 180-183 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.38 (d, *J* = 8.8 Hz, 2H), 8.13 (d, *J* = 8.8 Hz, 2H), 8.09 (dd, *J* = 1.4 and 8.5 Hz, 1H), 7.77 (dd, *J* = 1.4 and 7.0 Hz, 1H), 7.73 (dd, *J* = 7.0 and 8.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.5, 152.9, 147.6, 143.6, 132.0, 130.1, 129.4, 128.7, 123.8, 122.3. Elemental analysis: calcd (%) for $C_{12}H_7N_3O_2S$ (257.27): C 56.02, H 2.74; found: C 56.22, H 2.58.

4-(Benzo[*c*][1,2,5]thiadiazol-4-yl)benzaldehyde (3): Following the general procedure **A** using 4-bromobenzaldehyde (185 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 90-10) to afford the desired compound **3** (173 mg, 72%) as a white solid (Mp = 136-138 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm)

10.14 (s, 1H), 8.15 (d, J = 8.4 Hz, 2H), 8.10 (dd, J = 1.4 and 8.6 Hz, 1H), 8.07 (d, J = 8.4 Hz, 2H), 7.80 (dd, J = 1.4 and 7.0 Hz, 1H), 7.75 (dd, J = 7.0 and 8.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 191.9, 155.5, 153.1, 143.3, 135.9, 133.1, 129.9, 129.9, 129.5, 128.5, 121.8. Elemental analysis: calcd (%) for $C_{13}H_8N_2OS$ (240.28): C 64.98, H 3.36; found: C 65.19, H 3.47.

Ethyl 4-(benzo[c][1,2,5]thiadiazol-4-yl)benzoate (4): Following the general procedure **A** using ethyl 4-bromobenzoate (229 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-EtOAc,95-5) to afford the desired compound **4** (193 mg, 68%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.21 – 8.17 (m, 2H), 8.04 – 8.00 (m, 3H), 7.74 – 7.66 (m, 2H), 4.42 (q, J = 7.1 Hz, 2H), 1.42 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 166.6, 155.8, 153.5, 141.9, 133.7, 130.5, 130.0, 129.7, 129.4, 128.4, 121.6, 61.3, 14.6. This is a known compound and the spectral data are identical to those reported in literature.[4]

1-(4-(Benzo[*c*][1,2,5]thiadiazol-4-yl)phenyl)propan-1-one (5): Following the general procedure **A** using 4-bromopropiophenone (213 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 90-10) to afford the desired compound **5** (174 mg, 65%) as a white solid (Mp = 108-110 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.16 (d, J = 8.4 Hz, 2H), 8.11 – 8.03 (m, 3H), 7.78 (dd, J = 1.5 and 7.0 Hz, 1H), 7.74 (dd, J = 7.0 and 8.4 Hz, 1H), 3.10 (q, J = 7.2 Hz, 2H), 1.29 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 200.4, 155.6, 153.2, 141.7, 136.5, 133.4, 129.5, 129.4, 128.3, 128.2, 121.4, 31.9, 8.3. Elemental analysis: calcd (%) for $C_{15}H_{12}N_2OS$ (268.33): C 67.14, H 4.51; found: C 67.28, H 4.79.

(4-(Benzo[*c*][1,2,5]thiadiazol-4-yl)phenyl)(phenyl)methanone (6): Following the general procedure **A** using 4-bromobenzophenone (261 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-EtOAc,95-5) to afford the desired compound **6** (209 mg, 66%) as an orange solid (Mp = 134-137 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.12 – 8.06 (m, 3H), 8.03 – 7.98 (m, 2H), 7.93 – 7.88 (m, 2H), 7.81 (dd, J = 1.3, 7.0 Hz, 1H), 7.75 (dd, J = 7.0, 8.6 Hz, 1H), 7.68 – 7.61 (m, 1H), 7.57 – 7.52 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 196.3, 155.6, 153.2, 141.3, 137.6, 137.2, 133.4, 132.5, 130.4, 130.1, 129.6, 129.2, 128.4, 128.3, 121.5. Elemental analysis: calcd (%) for $C_{19}H_{12}N_2OS$ (316.38): C 72.13, H 3.82; found: C 72.41, H 3.63.

4-(4-Chlorophenyl)benzo[*c*][1,2,5]thiadiazole (7): Following the general procedure **A** using 1-bromo-4-chlorobenzene (191 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 95-5) to afford the desired compound **7** (135 mg, 55%) as a yellow solid (Mp = 110-113 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02 (dd, J = 3.2, 6.7 Hz, 1H), 7.88 (d, J = 8.5 Hz, 2H), 7.71 – 7.66 (m, 2H), 7.51 (d, J = 8.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.6, 153.3, 135.7, 134.5, 133.3, 130.5, 129.6, 128.8, 127.7,

120.9. Elemental analysis: calcd (%) for $C_{12}H_7ClN_2S$ (246.71): C 58.42, H 2.86; found: C 58.59, H 2.61.

4-Phenylbenzo[*c*][1,2,5]thiadiazole (8): Following the general procedure **A** using bromobenzene (157 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 95-5) to afford the desired compound **8** (127 mg, 60%) as a yellow solid (Mp = 70-71 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02 – 7.96 (m, 1H), 7.93 – 7.89 (m, 2H), 7.69 – 7.64 (m, 2H), 7.56 – 7.50 (m, 2H), 7.47 – 7.42 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.9, 153.8, 137.6, 134.9, 129.9, 129.5, 128.9, 128.7, 128.0, 120.8. This is a known compound and the spectral data are identical to those reported in literature.[4]

4-(4-(*Tert*-butyl)phenyl)benzo[*c*][1,2,5]thiadiazole (9): Following the general procedure **A** using 1-bromo-4-(tert-butyl)benzene (213 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 95-5) to afford the desired compound **9** (164 mg, 61%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.00 (dd, J = 3.8 and 6.0 Hz, 1H), 7.89 (d, J = 8.4 Hz, 2H), 7.71 (s, 2H), 7.59 (d, J = 8.5 Hz, 2H), 1.42 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.6, 153.6, 151.5, 134.5, 134.5, 129.7, 128.9, 127.4, 125.6, 120.2, 34.7, 31.3. Elemental analysis: calcd (%) for $C_{16}H_{16}N_2S$ (268.37): C 71.61, H 6.01; found: C 71.85, H 6.22.

4-(4-Methoxyphenyl)benzo[*c*][1,2,5]thiadiazole (10): Following the general procedure **A** using 4-bromoanisole (187 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 95-5) to afford the desired compound **10** (157 mg, 65%) as a yellow solid (Mp = 125-127 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.97 – 7.86 (m, 3H), 7.67 – 7.61 (m, 2H), 7.09 – 7.04 (m, 2H), 3.88 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.1, 155.9, 154.9, 134.4, 130.7, 130.1, 130.0, 127.1, 120.1, 114.3, 55.6. This is a known compound and the spectral data are identical to those reported in literature.[4]

3-(Benzo[c][1,2,5]thiadiazol-4-yl)benzonitrile (11): Following the general procedure **A** using 3-bromobenzonitrile (182 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 90-10) to afford the desired compound **11** (178 mg, 75%) as a white solid (Mp = 178-180 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.32 – 8.27 (m, 1H), 8.21 (ddd, J = 1.3, 1.9 and 7.9 Hz, 1H), 8.13 – 8.07 (m, 1H), 7.79 – 7.71 (m, 3H), 7.67 (t, J = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.5, 153.0, 138.5, 133.5, 132.8, 132.0, 131.7, 129.5, 129.4, 128.1, 121.8, 118.7, 112.9. Elemental analysis: calcd (%) for $C_{13}H_7N_3S$ (237.28): C 65.81, H 2.97; found: C 65.97, H 2.82.

4-(3-(Trifluoromethyl)phenyl)benzo[*c*][1,2,5]thiadiazole (12): Following the general procedure **A** using 1-bromo-3-(trifluoromethyl)benzene (225 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5

mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-toluene, 80-20) to afford the desired compound **12** (222 mg, 79%) as a yellow solid (Mp = 50-52 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.22 (s, 1H), 8.18 (dd, *J* = 1.6 and 7.5 Hz, 1H), 8.08 (dd, *J* = 2.1 and 7.8 Hz, 1H), 7.78 – 7.72 (m, 3H), 7.69 (dd, *J* = 5.3 and 13.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.5, 153.2, 138.0, 133.0, 132.6, 131.1 (q, *J* = 32.3 Hz), 129.5, 129.0, 128.1, 126.0 (q, *J* = 3.8 Hz), 125.0 (q, *J* = 3.8 Hz), 124.2 (q, *J* = 272.3 Hz), 121.4. This is a known compound and the spectral data are identical to those reported in literature.[4]

4-(3-Nitrophenyl)benzo[*c*][1,2,5]thiadiazole (13): Following the general procedure **A** using 3-bromonitrobenzene (202 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 90-10) to afford the desired compound **13** (178 mg, 69%) as a white solid (Mp = 158-160 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.86 (t, *J* = 2.0 Hz, 1H), 8.40 – 8.28 (m, 2H), 8.12 (dd, *J* = 1.3 and 8.6 Hz, 1H), 7.83 – 7.80 (m, 1H), 7.79 – 7.72 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.5, 153.0, 148.6, 138.8, 135.2, 131.8, 129.5, 129.5, 128.3, 124.1, 123.1, 122.0. Elemental analysis: calcd (%) for $C_{12}H_7N_3O_2S$ (257.27): C 56.02, H 2.74; found: C 56.18, H 2.98.

4-(3-Chlorophenyl)benzo[*c*][1,2,5]thiadiazole (14): Following the general procedure **A** using 1-bromo-3-chlorobenzene (191 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 95-5) to afford the desired compound **14** (178 mg, 72%) as a white solid (Mp = 175-178 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.08 – 8.03 (m, 1H), 7.96 (t, *J* = 1.9 Hz, 1H), 7.85 (dt, *J* = 1.6 and 7.4 Hz, 1H), 7.72 (dd, *J* = 1.1 and 4.9 Hz, 2H), 7.52 – 7.43 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.5, 153.2, 139.0, 134.5, 133.0, 129.8, 129.5, 129.3, 128.4, 128.0, 127.4, 121.2. Elemental analysis: calcd (%) for $C_{12}H_7ClN_2S$ (246.71): C 58.42, H 2.86; found: C 58.57, H 3.06.

2-(Benzo[c][1,2,5]thiadiazol-4-yl)benzonitrile (15): Following the general procedure **A** using 2-bromobenzonitrile (182 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 90-10) to afford the desired compound **15** (166 mg, 70%) as a white solid (Mp =177-179 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.14 (dd, *J* = 2.1 and 7.9 Hz, 1H), 7.89 (dd, *J* = 1.4 and 7.8 Hz, 1H), 7.85 – 7.81 (m, 1H), 7.80 – 7.74 (m, 3H), 7.59 (td, *J* = 1.5 and 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.1, 153.3, 140.9, 133.7, 132.6, 131.4, 131.1, 129.9, 129.2, 128.6, 122.3, 118.2, 112.6. Elemental analysis: calcd (%) for $C_{13}H_7N_3S$ (237.28): C 65.81, H 2.97; found: C 65.67, H 3.22.

2-(Benzo[c][1,2,5]thiadiazol-4-yl)benzaldehyde (16): Following the general procedure **A** using 2-bromobenzaldehyde (185 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 90-10) to afford the desired

compound **3** (103 mg, 43%) as a yellow solid (Mp = 169-171 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.81 (s, 1H), 8.23 – 8.06 (m, 2H), 7.79 – 7.73 (m, 2H), 7.68 – 7.65 (m, 1H), 7.62 (dd, *J* = 1.2, 6.9 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 191.3, 154.7, 154.4, 140.4, 134.5, 133.8, 131.7, 131.4, 130.2, 129.2, 129.0, 128.3, 121.8. Elemental analysis: calcd (%) for $C_{13}H_8N_2OS$ (240.28): C 64.98, H 3.36; found: C 65.19, H 3.47.

4-(Benzo[*d*][1,3]dioxol-5-yl)benzo[*c*][1,2,5]thiadiazole (17): Following the general procedure **A** using 5-bromo-1,3-benzodioxole (201 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 98-2) to afford the desired compound **17** (115 mg, 45%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.99 (dd, *J* = 1.6, 8.2 Hz, 1H), 7.71 – 7.62 (m, 2H), 7.48 (d, *J* = 1.8 Hz, 1H), 7.44 (dd, *J* = 1.8, 8.1 Hz, 1H), 7.00 (d, *J* = 8.1 Hz, 1H), 6.07 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.6, 153.5, 147.9, 134.2, 131.4, 129.6, 127.2, 123.1, 120.2, 109.7, 108.5, 101.3. Elemental analysis: calcd (%) for $C_{13}H_8N_2O_2S$ (256.28): C 60.93, H 3.15; found: C 60.76, H 3.20.

4-(Naphthalen-2-yl)benzo[*c*][1,2,5]thiadiazole (18): Following the general procedure **A** using 2-bromonaphthalene (207 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-toluene, 85-15) to afford the desired compound **18** (157 mg, 60%) as a yellow solid (Mp = 94-96 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.46 (s, 1H), 8.11 – 8.02 (m, 3H), 8.02 – 7.97 (m, 1H), 7.97 – 7.91 (m, 1H), 7.84 (dd, *J* = 1.1, 7.0 Hz, 1H), 7.75 (dd, *J* = 7.0, 8.7 Hz, 1H), 7.59 – 7.53 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.7, 153.7, 134.8, 134.5, 133.4, 133.2, 129.7, 128.6, 128.5, 128.1, 128.0, 127.7, 126.9, 126.5, 126.4, 120.6. Elemental analysis: calcd (%) for $C_{16}H_{10}N_2S$ (262.33): C 73.26, H 3.84; found: C 73.49, H 4.07.

4-(Fluoren-3-yl)benzo[*c*][1,2,5]thiadiazole (19): Following the general procedure **A** using 3-bromofluorene (245 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 98-2) to afford the desired compound **19** (168 mg, 56%) as a yellow solid (Mp = 200-203 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.16 (t, *J* = 1.1 Hz, 1H), 8.03 (dd, *J* = 1.3 and 8.6 Hz, 1H), 7.99 – 7.95 (m, 2H), 7.88 (d, *J* = 7.5 Hz, 1H), 7.78 (dd, *J* = 1.3 and 7.0 Hz, 1H), 7.73 (dd, *J* = 7.0 and 8.6 Hz, 1H), 7.61 (dt, *J* = 1.1 and 7.4 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.37 (td, *J* = 1.2 and 7.4 Hz, 1H), 4.05 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.7, 153.7, 143.7, 143.6, 142.0, 141.3, 135.9, 134.9, 129.7, 128.1, 127.6, 127.0, 126.9, 125.9, 125.1, 120.3, 120.2, 120.0, 37.1. Elemental analysis: calcd (%) for $C_{19}H_{12}N_2S$ (300.38): C 75.97, H 4.03; found: C 76.29, H 4.19.

4-(Pyren-1-yl)benzo[*c*][1,2,5]thiadiazole (20): Following the general procedure **A** using 1-bromopyrene (281 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 98-2) to afford the desired

compound **20** (145 mg, 43%) as a yellow solid (Mp = 216-218 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.34 (d, *J* = 7.9 Hz, 1H), 8.26 (dd, *J* = 1.2, 7.6 Hz, 1H), 8.22 – 8.14 (m, 5H), 8.05 (t, *J* = 7.6 Hz, 1H), 8.00 (d, *J* = 9.3 Hz, 1H), 7.87 (d, *J* = 9.2 Hz, 1H), 7.85 – 7.80 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.2, 154.9, 134.5, 132.6, 131.5, 131.4, 130.9, 130.7, 129.4, 129.2, 128.1, 127.9, 127.7, 127.4, 126.1, 125.4, 125.2, 125.1, 125.0, 124.8, 124.6, 121.0. Elemental analysis: calcd (%) for $C_{22}H_{12}N_2S$ (336.41): C 78.55, H 3.60; found: C 78.91, H 3.34.

4-(6-Methoxypyridin-2-yl)benzo[*c*][1,2,5]thiadiazole (21): Following the general procedure **A** using 2-bromo-6-methoxypyridine (188 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 95-5) to afford the desired compound **21** (127 mg, 52%) as a yellow solid (Mp = 130-133 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.62 (dd, *J* = 1.2 and 7.1 Hz, 1H), 8.49 (dd, *J* = 0.8 and 7.4 Hz, 1H), 8.08 (dd, *J* = 1.2 and 8.7 Hz, 1H), 7.82 – 7.75 (m, 2H), 6.83 (dd, *J* = 0.8 and 8.3 Hz, 1H), 4.10 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 163.5, 155.9, 152.9, 150.8, 139.2, 131.8, 129.6, 128.9, 121.9, 118.0, 110.7, 53.3. Elemental analysis: calcd (%) for $C_{12}H_9N_3OS$ (243.29): C 59.24, H 3.73; found: C 59.44, H 4.07.

4-(6-(Trifluoromethyl)pyridin-2-yl)benzo[*c*][1,2,5]thiadiazole (22): Following the general procedure **A** using 2-bromo-6-(trifluoromethyl)pyridine (225 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 95-5) to afford the desired compound **22** (194 mg, 69%) as a white solid (Mp = 102-104 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (d, *J* = 8.0 Hz, 1H), 8.68 (dd, *J* = 1.1 and 7.1 Hz, 1H), 8.14 (dd, *J* = 1.1 and 8.8 Hz, 1H), 8.08 (t, *J* = 7.9 Hz, 1H), 7.81 (dd, *J* = 7.1 and 8.8 Hz, 1H), 7.73 (dd, *J* = 0.9 and 7.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.8, 154.2, 152.7, 148.1 (q, *J* = 34.7 Hz), 138.0, 130.3, 130.1, 129.8, 127.4, 123.0, 121.5 (q, *J* = 274.4 Hz), 119.3 (q, *J* = 2.8 Hz). Elemental analysis: calcd (%) for $C_{12}H_6F_3N_3S$ (281.26): C 51.25, H 2.15; found: C 51.40, H 1.98.

4-(Quinolin-3-yl)benzo[*c*][1,2,5]thiadiazole (23): Following the general procedure **A** using 3-bromoquinoline (208 mg, 1 mmol) and 2,1,3-benzothiadiazole (204 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-EtOAc, 80-20) to afford the desired compound **23** (203 mg, 77%) as a yellow solid (Mp = 166-168 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.46 (s, 1H), 8.87 (s, 1H), 8.22 (d, *J* = 8.5 Hz, 1H), 8.11 (dd, *J* = 1.1, 8.8 Hz, 1H), 7.99 (dd, *J* = 1.4, 8.2 Hz, 1H), 7.89 (dd, *J* = 1.1, 6.9 Hz, 1H), 7.85 – 7.74 (m, 2H), 7.65 (ddd, *J* = 1.1, 6.9, 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 155.6, 153.4, 150.6, 147.6, 136.3, 131.1, 130.1, 130.0, 129.6, 129.2, 128.4, 128.1, 127.8, 127.1, 121.5. Elemental analysis: calcd (%) for $C_{15}H_9N_3S$ (263.31): C 68.42, H 3.45; found: C 68.79, H 3.62.

4,7-Bis(4-chlorophenyl)benzo[*c*][1,2,5]thiadiazole (24): Following the general procedure **B** using 1-bromo-4-chlorobenzene (574 mg, 3 mmol) and 2,1,3-benzothiadiazole (136 mg, 1 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 95-5) to afford the desired compound **24** (228 mg, 64%) as a yellow solid (Mp = 130-131 ºC). ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 8.20 – 7.70 (m, 6H), 7.69 – 7.47 (m, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 153.1, 152.3, 133.5, 132.6, 130.9, 128.7, 112.8. This is a known compound and the spectral data are identical to those reported in literature.[5]

4,7-Bis(3-(trifluoromethyl)phenyl)benzo[*c*][1,2,5]thiadiazole (25): Following the general procedure **B** using 1-bromo-3-(trifluoromethyl)benzene (675 mg, 3 mmol) and 2,1,3-benzothiadiazole (136 mg, 1 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-toluene, 85-15) to afford the desired compound **25** (297 mg, 70%) as a yellow solid (Mp = 138-141 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.27 (s, 2H), 8.22 (d, J = 7.8 Hz, 2H), 7.88 (s, 2H), 7.79 – 7.75 (m, 2H), 7.75 – 7.66 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 153.8, 137.8, 132.6, 131.2 (q, J = 32.4 Hz), 129.1, 128.3, 126.1 (q, J = 3.9 Hz), 125.2 (q, J = 3.8 Hz), 124.1 (q, J = 271.5 Hz). Elemental analysis: calcd (%) for $C_{20}H_{10}F_6N_2S$ (424.36): C 56.61, H 2.38; found: C 56.45, H 2.17.

4,7-Bis(3,5-bis(trifluoromethyl)phenyl)benzo[*c*][1,2,5]thiadiazole (26): Following the general procedure **B** using 1-bromo-3,5-bis(trifluoromethyl)benzene (879 mg, 3 mmol) and 2,1,3-benzothiadiazole (136 mg, 1 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-toluene, 90-10) to afford the desired compound **26** (420mg, 75%) as a white solid (Mp = 176-178 ºC).). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.51 (s, 4H), 8.02 (s, 2H), 7.96 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 153.4, 138.7, 132.1 (q, J = 33.5 Hz), 131.7, 129.4 (m), 128.5, 123.3 (q, J = 272.2 Hz), 122.3 (m). Elemental analysis: calcd (%) for $C_{22}H_8F_{12}N_2S$ (560.36): C 47.16, H 1.44; found: C 47.39, H 1.21.

4-(Benzo[*d*][1,3]dioxol-5-yl)-7-(3,5-bis(trifluoromethyl)phenyl)benzo[*c*][1,2,5]thiadiazole (27): Following the general procedure **A** using 1-bromo-3,5-bis(trifluoromethyl)benzene (146 mg, 0.5 mmol) and 4-(benzo[*d*][1,3]dioxol-5-yl)2,1,3-benzothiadiazole (**17**) (192 mg, 0.75 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 99-1) to afford the desired compound **27** (89 mg, 38%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.49 (s, 2H), 7.98 (s, 1H), 7.88 (dd, J = 1.8, 7.4 Hz, 1H), 7.80 (dd, J = 1.7, 7.4 Hz, 1H), 7.56 – 7.46 (m, 2H), 7.03 (dd, J = 1.7, 8.2 Hz, 1H), 6.10 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 154.0, 153.5, 148.3, 148.1, 139.2, 134.8, 131.9 (q, J = 33.3 Hz), 130.9, 129.5, 128.9, 128.8, 127.2, 123.4, 123.4 (q, J = 274.2 Hz), 121.8 (m), 109.7, 108.7, 101.5. Elemental analysis: calcd (%) for $C_{21}H_{10}F_6N_2O_2S$ (468.37): C 53.85, H 2.15; found: C 54.01, H 2.46.

4-(Benzo[*c*][1,2,5]selenadiazol-4-yl)benzonitrile (28): Following the general procedure **A** using 4-bromobenzonitrile (182 mg, 1 mmol) and 2,1,3-benzoselenadiazole (274 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 90-10) to afford the desired compound **28** (148 mg, 52%) as a yellow solid (Mp =198-202 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.01 (d, *J* = 8.4 Hz, 2H), 7.98 – 7.95 (m, 1H), 7.83 (d, *J* = 8.4 Hz, 2H), 7.63 (dd, *J* = 6.8, 8.5 Hz, 1H), 7.58 (d, *J* = 6.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 161.0, 158.6, 142.3, 134.1, 132.2, 130.2, 129.5, 128.8, 124.0, 118.8, 111.8. Elemental analysis: calcd (%) for $C_{13}H_7N_3Se$ (284.18): C 54.95, H 2.48; found: C 55.10, H 2.57.

4-(4-(*Tert*-butyl)phenyl)benzo[*c*][1,2,5]selenadiazole (29): Following the general procedure **A** using 1-bromo-4-(tert-butyl)benzene (213 mg, 1 mmol) and 2,1,3-benzoselenadiazole (274 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 95-5) to afford the desired compound **29** (173 mg, 55%) as a yellow solid (Mp = 84-88 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.84 (dd, *J* = 1.3, 8.9 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 2H), 7.59 – 7.55 (m, 3H), 7.52 (dd, *J* = 1.3, 6.7 Hz, 1H), 1.42 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 151.3, 136.1, 135.0, 129.9, 129.1, 128.8, 127.7, 125.5, 122.3, 34.7, 31.4. Elemental analysis: calcd (%) for $C_{16}H_{16}N_2Se$ (315.28): C 60.95, H 5.12; found: C 60.86, H 5.29.

4-(3,5-Bis(trifluoromethyl)phenyl)benzo[*c*][1,2,5]selenadiazole (30): Following the general procedure **A** using 1-bromo-3,5-bis(trifluoromethyl)benzene (293 mg, 1 mmol) and 4 2,1,3-benzoselenadiazole (274 mg, 1.5 mmol), the residue was purified by flash chromatography on silica gel (petroleum ether-Et_2O, 95-5) to afford the desired compound **30** (225 mg, 57%) as a white solid (Mp = 66-69 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.38 (s, 2H), 8.00 (s, 2H), 7.65 – 7.62 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.9, 158.4, 139.6, 131.7 (q, *J* = 33.3 Hz), 132.9, 129.6 (m), 129.4, 128.9, 124.3, 123.4 (q, *J* = 273.2 Hz), 121.9 (m). Elemental analysis: calcd (%) for $C_{14}H_6F_6N_2Se$ (395.17): C 42.55, H 1.53; found: C 42.34, H 1.29.

3. Crystal structure report of compound 18

X-ray crystallographic study

(C_{16} H_{10} N_2 S); *M* = 262.32. APEXII, Bruker-AXS diffractometer, Mo-Kα radiation (λ = 0.71073 Å), *T* = 150(2) K; monoclinic *C* 2/*c* (I.T.#15), a = 48.765(5), b = 7.4625(8), c = 7.0053(7) Å, β = 96.573(4) °, *V* = 2532.5(5) Å^3. *Z* = 8, *d* = 1.376 g.cm^{-3}, μ = 0.241 mm^{-1}. The structure was solved by dual-space algorithm using the *SHELXT* program [1], and then refined with full-matrix least-square methods based on F^2(*SHELXL*) [2]. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their

calculated positions. A final refinement on F^2 with 2908 unique intensities and 172 parameters converged at $\omega R(F^2) = 0.1899$ ($R(F) = 0.0763$) for 2425 observed reflections with $I > 2\sigma(I)$.

[1] G. M. Sheldrick, Acta Cryst. A71 (2015) 3-8
[2] Sheldrick G.M., Acta Cryst. C71 (2015) 3-8

Structural data

Empirical formula	$C_{16}\,H_{10}\,N_2\,S$
Formula weight	262.32 g/mol
Temperature	150(2) *K*
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, *C* 2/*c*
Unit cell dimensions	a = 48.765(5) Å, α = 90 °
	b = 7.4625(8) Å, β = 96.573(4) °
	c = 7.0053(7) Å, γ = 90 °
Volume	2532.5(5) $Å^3$
Z, Calculated density	8, 1.376 $g.cm^{-3}$
Absorption coefficient	0.241 mm^{-1}
F(000)	1088
Crystal size	0.600 x 0.510 x 0.140 mm
Crystal color	yellow
Theta range for data collection	3.007 to 27.480 °
h_min, h_max	-62, 62
k_min, k_max	-9, 9
l_min, l_max	-9, 8
Reflections collected / unique	15916 / 2908 [R(int)[a] = 0.0719]
Reflections [I>2σ]	2425
Completeness to theta_max	0.998
Absorption correction type	multi-scan
Max. and min. transmission	0.967 , 0.436
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2908 / 0 / 172
[b]S (Goodness-of-fit)	1.109
Final *R* indices [I>2σ]	$R1^c$ = 0.0763, $wR2^d$ = 0.1899
R indices (all data)	$R1^c$ = 0.0870, $wR2^d$ = 0.2022
Largest diff. peak and hole	1.596 and -1.090 $e^-.Å^{-3}$

$^{a}R_{int} = \sum |F_o^2 - < F_o^2 >| / \sum [F_o^2]$

$^{b}S = \{\sum [w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$

$^{c}R1 = \sum | |F_o| - |F_c| | / \sum |F_o|$

$^{d}wR2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$

$w = 1 / [\sigma(F_o^2) + aP^2 + bP]$ where $P = [2F_c^2 + MAX(F_o^2, 0)] /3$

Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters ($Å^2$). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
C1	0.68129(4)	0.3464(3)	0.7360(3)	1	0.0152(4)
C2	0.70564(4)	0.4518(3)	0.7884(3)	1	0.0186(5)
C3	0.70488(5)	0.6409(3)	0.7791(3)	1	0.0216(5)
H3	0.720920	0.711062	0.814302	1	0.026
C4	0.67993(5)	0.7188(3)	0.7169(3)	1	0.0205(5)
H4	0.678731	0.845752	0.709501	1	0.025
C5	0.65586(4)	0.6149(3)	0.6632(3)	1	0.0182(4)
H5	0.639246	0.675460	0.617890	1	0.022
C6	0.65543(4)	0.4305(3)	0.6736(3)	1	0.0156(4)
C7	0.62950(4)	0.3300(3)	0.6211(3)	1	0.0164(4)
C8	0.62908(5)	0.1635(3)	0.5205(3)	1	0.0194(5)
H8	0.645990	0.109103	0.497127	1	0.023
C9	0.60460(5)	0.0812(3)	0.4573(3)	1	0.0259(5)
H9	0.604718	-0.028784	0.389160	1	0.031
C10	0.57903(5)	0.1585(3)	0.4925(3)	1	0.0274(6)
C11	0.55331(6)	0.0797(4)	0.4234(4)	1	0.0396(7)
H11	0.552880	-0.028280	0.351314	1	0.048
C12	0.52916(6)	0.1584(5)	0.4599(4)	1	0.0475(9)
H12	0.512074	0.105263	0.411201	1	0.057
C13	0.52922(6)	0.3157(5)	0.5677(4)	1	0.0461(8)
H13	0.512202	0.367053	0.593482	1	0.055
C14	0.55368(5)	0.3971(4)	0.6370(4)	1	0.0356(6)
H14	0.553523	0.504192	0.710299	1	0.043
C15	0.57922(5)	0.3205(3)	0.5986(3)	1	0.0253(5)

C16	0.60478(4)	0.4030(3)	0.6618(3)	1	0.0204(5)
H16	0.604951	0.511005	0.733757	1	0.024
N1	0.68595(4)	0.1688(2)	0.7582(3)	1	0.0198(4)
N2	0.72813(4)	0.3519(2)	0.8467(3)	1	0.0251(5)
S1	0.71813(2)	0.14556(7)	0.83514(9)	1	0.0271(3)

Anisotropic displacement parameters ($Å^2$)

The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a^{*2} U_{11} + ... + 2 h k a* b* U_{12}].

Atom	U11	U22	U33	U23	U13	U12
C1	0.0100(10)	0.0173(10)	0.0183(9)	-0.0032(7)	0.0022(8)	-0.0027(7)
C2	0.0093(10)	0.0239(11)	0.0227(10)	-0.0023(8)	0.0022(8)	-0.0019(8)
C3	0.0149(11)	0.0227(11)	0.0276(11)	-0.0037(8)	0.0043(9)	-0.0089(8)
C4	0.0225(11)	0.0148(9)	0.0245(10)	0.0001(8)	0.0041(8)	-0.0030(8)
C5	0.0145(10)	0.0206(10)	0.0193(10)	0.0002(8)	0.0012(8)	0.0021(8)
C6	0.0110(10)	0.0213(10)	0.0146(9)	-0.0013(7)	0.0019(7)	-0.0025(7)
C7	0.0106(10)	0.0226(10)	0.0155(9)	0.0012(7)	-0.0006(7)	-0.0021(7)
C8	0.0152(11)	0.0259(11)	0.0173(10)	-0.0007(8)	0.0020(8)	-0.0056(8)
C9	0.0242(12)	0.0343(12)	0.0191(10)	-0.0060(9)	0.0025(9)	-0.0128(10)
C10	0.0142(12)	0.0505(15)	0.0168(10)	0.0033(9)	-0.0016(8)	-0.0134(9)
C11	0.0237(14)	0.0700(19)	0.0239(12)	0.0016(12)	-0.0035(10)	-0.0257(13)
C12	0.0167(13)	0.091(3)	0.0318(14)	0.0142(14)	-0.0082(11)	-0.0232(14)
C13	0.0101(12)	0.090(2)	0.0371(15)	0.0206(15)	-0.0007(10)	-0.0017(13)
C14	0.0136(12)	0.0625(17)	0.0306(13)	0.0073(12)	0.0019(9)	0.0044(11)
C15	0.0096(11)	0.0469(14)	0.0188(10)	0.0057(9)	-0.0007(8)	-0.0025(9)
C16	0.0130(11)	0.0294(11)	0.0184(10)	-0.0009(8)	-0.0001(8)	-0.0010(8)
N1	0.0122(9)	0.0161(8)	0.0306(10)	-0.0030(7)	-0.0002(7)	0.0000(6)
N2	0.0085(9)	0.0257(10)	0.0405(12)	-0.0031(8)	0.0002(8)	-0.0011(7)
S1	0.0124(3)	0.0203(4)	0.0474(4)	-0.0036(2)	-0.0018(3)	0.00404(19)

Bond lengths [Å]

C1	- N1	= 1.350(3)
C1	- C6	= 1.431(3)
C1	- C2	= 1.437(3)
C2	- N2	= 1.350(3)
C2	- C3	= 1.413(3)
C3	- C4	= 1.374(3)
C3	- H3	= 0.9500
C4	- C5	= 1.421(3)
C4	- H4	= 0.9500
C5	- C6	= 1.378(3)
C5	- H5	= 0.9500
C6	- C7	= 1.480(3)
C7	- C16	= 1.382(3)
C7	- C8	= 1.427(3)
C8	- C9	= 1.371(3)
C8	- H8	= 0.9500
C9	- C10	= 1.420(4)
C9	- H9	= 0.9500
C10	- C15	= 1.419(4)
C10	- C11	= 1.420(3)
C11	- C12	= 1.366(5)
C11	- H11	= 0.9500
C12	- C13	= 1.395(5)
C12	- H12	= 0.9500
C13	- C14	= 1.377(4)
C13	- H13	= 0.9500
C14	- C15	= 1.424(3)
C14	- H14	= 0.9500
C15	- C16	= 1.415(3)
C16	- H16	= 0.9500
N1	- S1	= 1.609(2)
N2	- S1	= 1.6141(19)

Angles [°]

N1	- C1	- C6	= 126.58(18)
N1	- C1	- C2	= 112.63(19)
C6	- C1	- C2	= 120.77(18)

N2	- C2	- C3	=	125.60(2)
N2	- C2	- C1	=	113.20(2)
C3	- C2	- C1	=	121.23(19)
C4	- C3	- C2	=	117.07(19)
C4	- C3	- H3	=	121.50
C2	- C3	- H3	=	121.50
C3	- C4	- C5	=	121.80(2)
C3	- C4	- H4	=	119.10
C5	- C4	- H4	=	119.10
C6	- C5	- C4	=	123.20(2)
C6	- C5	- H5	=	118.40
C4	- C5	- H5	=	118.40
C5	- C6	- C1	=	115.83(18)
C5	- C6	- C7	=	120.67(19)
C1	- C6	- C7	=	123.50(18)
C16	- C7	- C8	=	118.80(2)
C16	- C7	- C6	=	119.33(19)
C8	- C7	- C6	=	121.81(19)
C9	- C8	- C7	=	120.80(2)
C9	- C8	- H8	=	119.60
C7	- C8	- H8	=	119.60
C8	- C9	- C10	=	120.80(2)
C8	- C9	- H9	=	119.60
C10	- C9	- H9	=	119.60
C15	- C10	- C11	=	118.90(3)
C15	- C10	- C9	=	118.90(2)
C11	- C10	- C9	=	122.10(3)
C12	- C11	- C10	=	120.40(3)
C12	- C11	- H11	=	119.80
C10	- C11	- H11	=	119.80
C11	- C12	- C13	=	121.00(3)
C11	- C12	- H12	=	119.50
C13	- C12	- H12	=	119.50
C14	- C13	- C12	=	120.70(3)
C14	- C13	- H13	=	119.70
C12	- C13	- H13	=	119.70
C13	- C14	- C15	=	119.80(3)
C13	- C14	- H14	=	120.10
C15	- C14	- H14	=	120.10
C16	- C15	- C10	=	119.20(2)

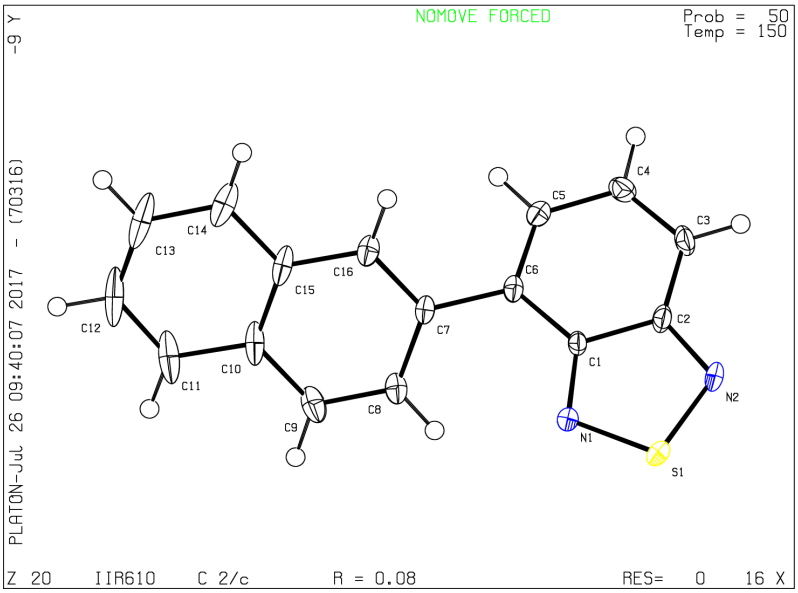
C16	- C15	- C14	=	121.60(2)
C10	- C15	- C14	=	119.20(2)
C7	- C16	- C15	=	121.50(2)
C7	- C16	- H16	=	119.30
C15	- C16	- H16	=	119.30
C1	- N1	- S1	=	106.80(14)
C2	- N2	- S1	=	106.35(16)
N1	- S1	- N2	=	101.03(10)

Torsion angles [°]

N1	- C1	- C2	- N2	=	0.70(3)
C6	- C1	- C2	- N2	=	179.03(19)
N1	- C1	- C2	- C3	=	-178.70(2)
C6	- C1	- C2	- C3	=	-0.40(3)
N2	- C2	- C3	- C4	=	-179.60(2)
C1	- C2	- C3	- C4	=	-0.30(3)
C2	- C3	- C4	- C5	=	-0.30(3)
C3	- C4	- C5	- C6	=	1.70(3)
C4	- C5	- C6	- C1	=	-2.20(3)
C4	- C5	- C6	- C7	=	178.15(18)
N1	- C1	- C6	- C5	=	179.60(2)
C2	- C1	- C6	- C5	=	1.60(3)
N1	- C1	- C6	- C7	=	-0.80(3)
C2	- C1	- C6	- C7	=	-178.81(18)
C5	- C6	- C7	- C16	=	-35.10(3)
C1	- C6	- C7	- C16	=	145.40(2)
C5	- C6	- C7	- C8	=	141.70(2)
C1	- C6	- C7	- C8	=	-37.90(3)
C16	- C7	- C8	- C9	=	3.00(3)
C6	- C7	- C8	- C9	=	-173.76(19)
C7	- C8	- C9	- C10	=	-0.80(3)
C8	- C9	- C10	- C15	=	-1.60(3)
C8	- C9	- C10	- C11	=	177.80(2)
C15	- C10	- C11	- C12	=	-0.40(4)
C9	- C10	- C11	- C12	=	-179.90(2)
C10	- C11	- C12	- C13	=	-0.90(4)
C11	- C12	- C13	- C14	=	1.20(4)
C12	- C13	- C14	- C15	=	0.00(4)

C11	- C10	- C15	- C16	= -177.70(2)
C9	- C10	- C15	- C16	= 1.70(3)
C11	- C10	- C15	- C14	= 1.60(3)
C9	- C10	- C15	- C14	= -179.00(2)
C13	- C14	- C15	- C16	= 177.90(2)
C13	- C14	- C15	- C10	= -1.40(4)
C8	- C7	- C16	- C15	= -2.80(3)
C6	- C7	- C16	- C15	= 174.01(19)
C10	- C15	- C16	- C7	= 0.50(3)
C14	- C15	- C16	- C7	= -178.80(2)
C6	- C1	- N1	- S1	= -178.80(17)
C2	- C1	- N1	- S1	= -0.60(2)
C3	- C2	- N2	- S1	= 178.89(19)
C1	- C2	- N2	- S1	= -0.50(2)
C1	- N1	- S1	- N2	= 0.31(18)
C2	- N2	- S1	- N1	= 0.09(18)

Structure visualisation



4. Crystal structure report of compound 20

X-ray crystallographic study

(C_{22} H_{12} N_2 S); *M* = 336.40. D8 VENTURE Bruker AXS diffractometer [*], Mo-Kα radiation (λ = 0.71073 Å), *T* = 150(2) K; triclinic *P* -1 (I.T.#2), a = 8.4312(8), b = 9.1773(9), c = 10.6084(11) Å, α = 83.752(4), β = 69.103(3), γ = 87.077(3) °, *V* = 762.22(13) $Å^3$. *Z* = 2, *d* = 1.466 $g.cm^{-3}$, μ = 0.218 mm^{-1}. The structure was solved by dual-space algorithm using the *SHELXT* program [1], and then refined with full-matrix least-square methods based on F^2(*SHELXL*) [2]. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 3480 unique intensities and 226 parameters converged at ω$R(F^2)$ = 0.0950 ($R(F)$ = 0.0361) for 3037 observed reflections with $I > 2\sigma(I)$.

[1] G. M. Sheldrick, Acta Cryst. A71 (2015) 3-8

[2] Sheldrick G.M., Acta Cryst. C71 (2015) 3-8

[*] Thanks to FEDER founds

Structural data

Empirical formula	C_{22} H_{12} N_2 S
Formula weight	336.40 g/mol
Temperature	150(2) *K*
Wavelength	0.71073 Å
Crystal system, space group	triclinic, *P* -1
Unit cell dimensions	a = 8.4312(8) Å, α = 83.752(4) °
	b = 9.1773(9) Å, β = 69.103(3) °
	c = 10.6084(11) Å, γ = 87.077(3) °
Volume	762.22(13) $Å^3$
Z, Calculated density	2, 1.466 $g.cm^{-3}$
Absorption coefficient	0.218 mm^{-1}
F(000)	348
Crystal size	0.310 x 0.290 x 0.140 mm
Crystal color	yellow
Theta range for data collection	3.186 to 27.478 °
h_min, h_max	-10, 10
k_min, k_max	-11, 11
l_min, l_max	-13, 13
Reflections collected / unique	17768 / 3480 [R(int)[a] = 0.0376]
Reflections [I>2σ]	3037
Completeness to theta_max	0.998

Absorption correction type	multi-scan
Max. and min. transmission	0.970 , 0.892
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3480 / 0 / 226
[b]S (Goodness-of-fit)	1.065
Final *R* indices [I>2σ]	$R1^c$ = 0.0361, $wR2^d$ = 0.0950
R indices (all data)	$R1^c$ = 0.0433, $wR2^d$ = 0.0992
Largest diff. peak and hole	0.371 and -0.357 $e^-.Å^{-3}$

[a] $R_{int} = \sum |F_o^2 - < F_o^2 >| / \sum [F_o^2]$

[b] $S = \{\sum [w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$

[c] $R1 = \sum | |F_o| - |F_c| | / \sum |F_o|$

[d] $wR2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$

$w = 1 / [\sigma(F_o^2) + aP^2 + bP]$ where $P = [2F_c^2 + MAX(F_o^2, 0)] /3$

Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters (Å^2). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
C1	0.49040(17)	0.63630(14)	0.13768(13)	1	0.0160(3)
C2	0.34692(17)	0.54255(14)	0.18135(13)	1	0.0146(3)
C3	0.32247(17)	0.43371(14)	0.29280(13)	1	0.0150(3)
C4	0.44838(18)	0.41890(15)	0.35576(14)	1	0.0183(3)
H4	0.435552	0.345124	0.428700	1	0.022
C5	0.58501(18)	0.50746(15)	0.31381(14)	1	0.0197(3)
H5	0.666091	0.494098	0.357511	1	0.024
C6	0.60952(17)	0.62100(15)	0.20466(14)	1	0.0178(3)
C7	0.74453(18)	0.71942(16)	0.16485(16)	1	0.0228(3)
H7	0.824198	0.710853	0.209990	1	0.027
C8	0.76252(19)	0.82911(17)	0.06008(17)	1	0.0268(3)
H8	0.853395	0.896037	0.035233	1	0.032
C9	0.64956(19)	0.84234(16)	-0.00885(16)	1	0.0248(3)
H9	0.665636	0.916519	-0.081930	1	0.030
C10	0.51210(18)	0.74750(14)	0.02815(14)	1	0.0184(3)

C11	0.39123(19)	0.75931(15)	-0.03979(14)	1	0.0206(3)
H11	0.407133	0.830495	-0.115137	1	0.025
C12	0.25536(18)	0.67073(15)	0.00189(14)	1	0.0193(3)
H12	0.177123	0.681220	-0.044571	1	0.023
C13	0.22645(17)	0.56103(14)	0.11484(13)	1	0.0158(3)
C14	0.08130(18)	0.47448(15)	0.16460(14)	1	0.0186(3)
H14	0.000041	0.485466	0.120988	1	0.022
C15	0.05425(18)	0.37294(14)	0.27657(15)	1	0.0186(3)
H15	-0.047510	0.318178	0.310532	1	0.022
C16	0.17333(17)	0.34940(14)	0.34052(13)	1	0.0160(3)
C17	0.13400(17)	0.23880(14)	0.46062(14)	1	0.0160(3)
C18	-0.00384(18)	0.25543(15)	0.57611(14)	1	0.0192(3)
H18	-0.070151	0.342884	0.580632	1	0.023
C19	-0.05196(18)	0.14733(16)	0.68961(14)	1	0.0210(3)
H19	-0.148701	0.165027	0.766919	1	0.025
C20	0.03696(19)	0.01943(15)	0.69021(14)	1	0.0211(3)
H20	0.004398	-0.051688	0.766599	1	0.025
C21	0.17982(17)	-0.00398(14)	0.57289(14)	1	0.0181(3)
C22	0.22839(17)	0.10465(14)	0.45845(14)	1	0.0162(3)
N1	0.27906(16)	-0.12547(13)	0.55337(13)	1	0.0236(3)
N2	0.36331(15)	0.06366(13)	0.35396(13)	1	0.0211(3)
S1	0.41735(5)	-0.09834(4)	0.40224(4)	1	0.02562(12)

Anisotropic displacement parameters ($Å^2$)

The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a^{*2} U_{11} + ... + 2 h k a* b* U_{12}].

Atom	U11	U22	U33	U23	U13	U12
C1	0.0166(6)	0.0141(6)	0.0154(6)	-0.0056(5)	-0.0026(5)	0.0026(5)
C2	0.0161(6)	0.0123(6)	0.0145(6)	-0.0057(5)	-0.0034(5)	0.0033(5)
C3	0.0166(6)	0.0127(6)	0.0148(6)	-0.0046(5)	-0.0040(5)	0.0028(5)
C4	0.0205(7)	0.0180(6)	0.0168(6)	-0.0024(5)	-0.0071(5)	0.0019(5)
C5	0.0194(7)	0.0228(7)	0.0192(7)	-0.0057(5)	-0.0090(5)	0.0026(5)
C6	0.0161(6)	0.0173(6)	0.0183(7)	-0.0075(5)	-0.0028(5)	0.0023(5)

C7	0.0169(7)	0.0239(7)	0.0271(8)	-0.0089(6)	-0.0056(6)	0.0002(5)
C8	0.0199(7)	0.0226(7)	0.0328(8)	-0.0047(6)	-0.0018(6)	-0.0062(6)
C9	0.0227(7)	0.0196(7)	0.0257(8)	0.0006(6)	-0.0013(6)	-0.0019(6)
C10	0.0186(7)	0.0149(6)	0.0175(6)	-0.0033(5)	-0.0012(5)	0.0019(5)
C11	0.0258(7)	0.0170(6)	0.0155(6)	-0.0007(5)	-0.0036(6)	0.0034(5)
C12	0.0237(7)	0.0183(6)	0.0170(7)	-0.0039(5)	-0.0088(5)	0.0050(5)
C13	0.0187(6)	0.0132(6)	0.0152(6)	-0.0053(5)	-0.0052(5)	0.0034(5)
C14	0.0207(7)	0.0160(6)	0.0222(7)	-0.0042(5)	-0.0113(6)	0.0025(5)
C15	0.0180(7)	0.0145(6)	0.0237(7)	-0.0030(5)	-0.0075(5)	-0.0011(5)
C16	0.0183(6)	0.0120(6)	0.0167(6)	-0.0031(5)	-0.0049(5)	0.0025(5)
C17	0.0170(6)	0.0138(6)	0.0178(6)	-0.0023(5)	-0.0063(5)	-0.0011(5)
C18	0.0203(7)	0.0145(6)	0.0223(7)	-0.0052(5)	-0.0062(6)	0.0017(5)
C19	0.0213(7)	0.0209(7)	0.0182(7)	-0.0066(5)	-0.0020(5)	-0.0031(5)
C20	0.0252(7)	0.0195(7)	0.0178(7)	0.0004(5)	-0.0066(6)	-0.0061(5)
C21	0.0188(7)	0.0142(6)	0.0228(7)	-0.0011(5)	-0.0090(6)	-0.0022(5)
C22	0.0152(6)	0.0153(6)	0.0179(6)	-0.0028(5)	-0.0052(5)	-0.0010(5)
N1	0.0215(6)	0.0167(6)	0.0315(7)	0.0008(5)	-0.0091(5)	0.0002(5)
N2	0.0180(6)	0.0179(6)	0.0244(6)	-0.0030(5)	-0.0039(5)	0.0016(4)
S1	0.01971(19)	0.01770(18)	0.0350(2)	-0.00389(14)	-0.00451(16)	0.00434(13)

Bond lengths [Å]

C1	- C6	= 1.4164(19)	
C1	- C10	= 1.4263(19)	
C1	- C2	= 1.4275(18)	
C2	- C13	= 1.4233(19)	
C2	- C3	= 1.4241(18)	
C3	- C16	= 1.4128(18)	
C3	- C4	= 1.4363(19)	
C4	- C5	= 1.355(2)	
C4	- H4	= 0.9500	
C5	- C6	= 1.435(2)	
C5	- H5	= 0.9500	
C6	- C7	= 1.4031(19)	
C7	- C8	= 1.387(2)	
C7	- H7	= 0.9500	
C8	- C9	= 1.386(2)	
C8	- H8	= 0.9500	
C9	- C10	= 1.400(2)	

C9 - H9 = 0.9500
C10 - C11 = 1.437(2)
C11 - C12 = 1.351(2)
C11 - H11 = 0.9500
C12 - C13 = 1.4362(19)
C12 - H12 = 0.9500
C13 - C14 = 1.3979(19)
C14 - C15 = 1.3853(19)
C14 - H14 = 0.9500
C15 - C16 = 1.3953(19)
C15 - H15 = 0.9500
C16 - C17 = 1.4882(18)
C17 - C18 = 1.3717(19)
C17 - C22 = 1.4293(18)
C18 - C19 = 1.425(2)
C18 - H18 = 0.9500
C19 - C20 = 1.361(2)
C19 - H19 = 0.9500
C20 - C21 = 1.417(2)
C20 - H20 = 0.9500
C21 - N1 = 1.3482(18)
C21 - C22 = 1.4349(19)
C22 - N2 = 1.3460(18)
N1 - S1 = 1.6127(14)
N2 - S1 = 1.6162(13)

Angles [°]

C6 - C1 - C10 = 119.91(12)
C6 - C1 - C2 = 120.12(12)
C10 - C1 - C2 = 119.96(12)
C13 - C2 - C3 = 120.28(12)
C13 - C2 - C1 = 119.52(12)
C3 - C2 - C1 = 120.18(12)
C16 - C3 - C2 = 119.18(12)
C16 - C3 - C4 = 122.70(12)
C2 - C3 - C4 = 118.07(12)
C5 - C4 - C3 = 121.70(13)
C5 - C4 - H4 = 119.20

C3 - C4 - H4 = 119.20
C4 - C5 - C6 = 121.25(13)
C4 - C5 - H5 = 119.40
C6 - C5 - H5 = 119.40
C7 - C6 - C1 = 119.15(13)
C7 - C6 - C5 = 122.19(13)
C1 - C6 - C5 = 118.64(12)
C8 - C7 - C6 = 120.48(14)
C8 - C7 - H7 = 119.80
C6 - C7 - H7 = 119.80
C9 - C8 - C7 = 120.84(14)
C9 - C8 - H8 = 119.60
C7 - C8 - H8 = 119.60
C8 - C9 - C10 = 120.67(14)
C8 - C9 - H9 = 119.70
C10 - C9 - H9 = 119.70
C9 - C10 - C1 = 118.91(13)
C9 - C10 - C11 = 122.17(13)
C1 - C10 - C11 = 118.92(12)
C12 - C11 - C10 = 120.99(13)
C12 - C11 - H11 = 119.50
C10 - C11 - H11 = 119.50
C11 - C12 - C13 = 121.51(13)
C11 - C12 - H12 = 119.20
C13 - C12 - H12 = 119.20
C14 - C13 - C2 = 118.65(12)
C14 - C13 - C12 = 122.30(13)
C2 - C13 - C12 = 119.03(12)
C15 - C14 - C13 = 120.95(13)
C15 - C14 - H14 = 119.50
C13 - C14 - H14 = 119.50
C14 - C15 - C16 = 121.38(13)
C14 - C15 - H15 = 119.30
C16 - C15 - H15 = 119.30
C15 - C16 - C3 = 119.46(12)
C15 - C16 - C17 = 117.96(12)
C3 - C16 - C17 = 122.54(12)
C18 - C17 - C22 = 116.31(12)
C18 - C17 - C16 = 121.34(12)
C22 - C17 - C16 = 122.16(12)

C17	- C18	- C19	=	122.91(13)
C17	- C18	- H18	=	118.50
C19	- C18	- H18	=	118.50
C20	- C19	- C18	=	121.76(13)
C20	- C19	- H19	=	119.10
C18	- C19	- H19	=	119.10
C19	- C20	- C21	=	117.68(13)
C19	- C20	- H20	=	121.20
C21	- C20	- H20	=	121.20
N1	- C21	- C20	=	125.99(13)
N1	- C21	- C22	=	113.33(13)
C20	- C21	- C22	=	120.65(13)
N2	- C22	- C17	=	126.07(13)
N2	- C22	- C21	=	113.22(12)
C17	- C22	- C21	=	120.68(12)
C21	- N1	- S1	=	105.98(10)
C22	- N2	- S1	=	106.03(10)
N1	- S1	- N2	=	101.44(6)

Torsion angles [°]

C6	- C1	- C2	- C13	= 178.77(11)
C10	- C1	- C2	- C13	= 0.02(18)
C6	- C1	- C2	- C3	= 0.29(18)
C10	- C1	- C2	- C3	= -178.46(11)
C13	- C2	- C3	- C16	= -3.05(18)
C1	- C2	- C3	- C16	= 175.42(11)
C13	- C2	- C3	- C4	= 179.59(11)
C1	- C2	- C3	- C4	= -1.94(18)
C16	- C3	- C4	- C5	= -175.63(13)
C2	- C3	- C4	- C5	= 1.64(19)
C3	- C4	- C5	- C6	= 0.40(2)
C10	- C1	- C6	- C7	= 2.18(19)
C2	- C1	- C6	- C7	= -176.57(12)
C10	- C1	- C6	- C5	= -179.55(12)
C2	- C1	- C6	- C5	= 1.70(18)
C4	- C5	- C6	- C7	= 176.16(13)
C4	- C5	- C6	- C1	= -2.05(19)
C1	- C6	- C7	- C8	= -0.80(2)

C5 - C6 - C7 - C8 = -179.05(13)

C6 - C7 - C8 - C9 = -1.10(2)

C7 - C8 - C9 - C10 = 1.70(2)

C8 - C9 - C10 - C1 = -0.30(2)

C8 - C9 - C10 - C11 = 179.12(13)

C6 - C1 - C10 - C9 = -1.61(19)

C2 - C1 - C10 - C9 = 177.14(12)

C6 - C1 - C10 - C11 = 178.94(12)

C2 - C1 - C10 - C11 = -2.31(18)

C9 - C10 - C11 - C12 = -176.94(13)

C1 - C10 - C11 - C12 = 2.50(2)

C10 - C11 - C12 - C13 = -0.30(2)

C3 - C2 - C13 - C14 = 2.52(18)

C1 - C2 - C13 - C14 = -175.96(11)

C3 - C2 - C13 - C12 = -179.39(11)

C1 - C2 - C13 - C12 = 2.13(18)

C11 - C12 - C13 - C14 = 176.00(13)

C11 - C12 - C13 - C2 = -2.00(2)

C2 - C13 - C14 - C15 = 0.20(2)

C12 - C13 - C14 - C15 = -177.82(12)

C13 - C14 - C15 - C16 = -2.40(2)

C14 - C15 - C16 - C3 = 1.90(2)

C14 - C15 - C16 - C17 = 179.71(12)

C2 - C3 - C16 - C15 = 0.86(19)

C4 - C3 - C16 - C15 = 178.10(12)

C2 - C3 - C16 - C17 = -176.87(11)

C4 - C3 - C16 - C17 = 0.37(19)

C15 - C16 - C17 - C18 = -62.15(17)

C3 - C16 - C17 - C18 = 115.61(15)

C15 - C16 - C17 - C22 = 112.64(15)

C3 - C16 - C17 - C22 = -69.60(17)

C22 - C17 - C18 - C19 = 0.60(2)

C16 - C17 - C18 - C19 = 175.71(13)

C17 - C18 - C19 - C20 = -0.10(2)

C18 - C19 - C20 - C21 = -0.50(2)

C19 - C20 - C21 - N1 = -177.58(13)

C19 - C20 - C21 - C22 = 0.40(2)

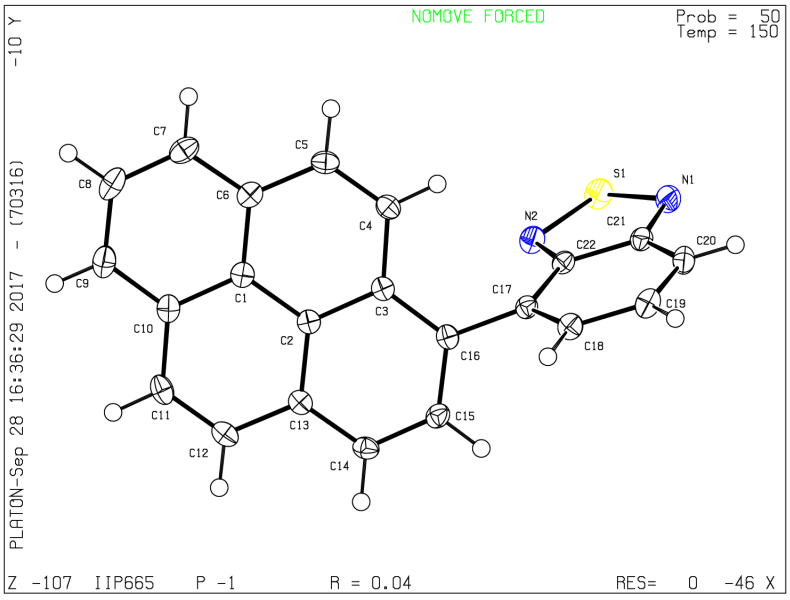
C18 - C17 - C22 - N2 = 177.32(13)

C16 - C17 - C22 - N2 = 2.30(2)

C18 - C17 - C22 - C21 = -0.68(19)

C16	- C17	- C22	- C21	= -175.71(12)
N1	- C21	- C22	- N2	= 0.16(17)
C20	- C21	- C22	- N2	= -178.06(12)
N1	- C21	- C22	- C17	= 178.40(12)
C20	- C21	- C22	- C17	= 0.20(2)
C20	- C21	- N1	- S1	= 177.74(12)
C22	- C21	- N1	- S1	= -0.37(14)
C17	- C22	- N2	- S1	= -178.00(11)
C21	- C22	- N2	- S1	= 0.13(14)
C21	- N1	- S1	- N2	= 0.41(11)
C22	- N2	- S1	- N1	= -0.32(11)

Structure visualisation



5. Crystal structure report of compound 26

X-ray crystallographic study

(C_{22} H_8 F_{12} N_2 S); M = 560.36. APEXII, Bruker-AXS diffractometer, Mo-Kα radiation (λ = 0.71073 Å), T = 150(2) K; monoclinic P $2_1/c$ (I.T.#14), a = 8.3373(17), b = 23.536(5), c = 11.577(2) Å, β = 111.527(7) °, V = 2113.4(7) $Å^3$. Z = 4, d = 1.761 $g.cm^{-3}$, μ = 0.274 mm^{-1}. The structure was solved by dual-space algorithm using the *SHELXT* program [1], and then refined with full-matrix least-square methods based on F^2(*SHELXL*) [2]. All non-hydrogen atoms were

refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 4745 unique intensities and 344 parameters converged at $\omega R(F^2) = 0.1760$ ($R(F) = 0.0733$) for 3865 observed reflections with $I > 2\sigma(I)$.

[1] G. M. Sheldrick, Acta Cryst. A71 (2015) 3-8
[2] Sheldrick G.M., Acta Cryst. C71 (2015) 3-8

Structural data

Empirical formula	$C_{22}\ H_8\ F_{12}\ N_2\ S$
Formula weight	560.36 g/mol
Temperature	150(2) *K*
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, *P* $2_1/c$
Unit cell dimensions	a = 8.3373(17) Å, α = 90 °
	b = 23.536(5) Å, β = 111.527(7) °
	c = 11.577(2) Å, γ = 90 °
Volume	2113.4(7) $Å^3$
Z, Calculated density	4, 1.761 $g.cm^{-3}$
Absorption coefficient	0.274 mm^{-1}
F(000)	1112
Crystal size	0.520 x 0.510 x 0.350 mm
Crystal color	colourless
Theta range for data collection	3.135 to 27.478 °
h_min, h_max	-10, 10
k_min, k_max	-26, 30
l_min, l_max	-12, 15
Reflections collected / unique	15301 / 4745 [R(int)[a] = 0.0525]
Reflections [I>2σ]	3865
Completeness to theta_max	0.981
Absorption correction type	multi-scan
Max. and min. transmission	0.909 , 0.727
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4745 / 0 / 344
[b]S (Goodness-of-fit)	1.144
Final *R* indices [I>2σ]	$R1^c$ = 0.0733, $wR2^d$ = 0.1760
R indices (all data)	$R1^c$ = 0.0899, $wR2^d$ = 0.1858
Largest diff. peak and hole	0.638 and -0.747 $e^-.Å^{-3}$

$^{a}R_{int} = \sum |F_o^2 - < F_o^2 >| / \sum [F_o^2]$

$^{b}S = \{\sum [w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$

$^{c}R1 = \sum | |F_o| - |F_c| | / \sum |F_o|$

$^{d}wR2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$

$w = 1 / [\sigma(F_o^2) + aP^2 + bP]$ where $P = [2F_c^2 + MAX(F_o^2, 0)] /3$

Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters ($Å^2$). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
C1	0.1688(4)	0.48045(12)	0.6663(3)	1	0.0166(6)
C2	0.1854(4)	0.44105(13)	0.5765(3)	1	0.0163(6)
C3	0.2498(4)	0.45895(13)	0.4837(3)	1	0.0169(6)
C4	0.2890(4)	0.51562(13)	0.4830(3)	1	0.0188(6)
H4	0.328597	0.529308	0.420924	1	0.023
C5	0.2722(4)	0.55449(13)	0.5720(3)	1	0.0191(6)
H5	0.300305	0.593255	0.566412	1	0.023
C6	0.2174(4)	0.53865(13)	0.6656(3)	1	0.0171(6)
C7	0.2106(4)	0.57957(12)	0.7610(3)	1	0.0170(6)
C8	0.1517(4)	0.63520(13)	0.7264(3)	1	0.0212(6)
H8	0.112985	0.646383	0.641764	1	0.025
C9	0.1506(4)	0.67385(13)	0.8172(3)	1	0.0235(7)
C10	0.2083(4)	0.65892(14)	0.9410(3)	1	0.0236(7)
H10	0.206322	0.685671	1.001944	1	0.028
C11	0.2695(4)	0.60396(13)	0.9753(3)	1	0.0200(6)
C12	0.2680(4)	0.56419(13)	0.8857(3)	1	0.0187(6)
H12	0.306232	0.526474	0.909847	1	0.022
C13	0.0908(5)	0.73375(15)	0.7791(4)	1	0.0328(8)
C14	0.3425(5)	0.58880(15)	1.1110(3)	1	0.0267(7)
C15	0.2747(4)	0.41799(12)	0.3937(3)	1	0.0168(6)
C16	0.2282(4)	0.43267(13)	0.2693(3)	1	0.0170(6)
H16	0.177489	0.468650	0.240717	1	0.020
C17	0.2560(4)	0.39468(13)	0.1871(3)	1	0.0188(6)

C18	0.3288(5)	0.34169(14)	0.2264(3)	1	0.0245(7)
H18	0.347537	0.315897	0.169519	1	0.029
C19	0.3734(5)	0.32726(14)	0.3496(3)	1	0.0253(7)
C20	0.3464(4)	0.36455(14)	0.4342(3)	1	0.0220(7)
H20	0.376588	0.353759	0.518652	1	0.026
C21	0.2065(4)	0.40934(14)	0.0522(3)	1	0.0224(7)
C22	0.4593(6)	0.27123(17)	0.3941(4)	1	0.0402(10)
F1	-0.0225(4)	0.73688(10)	0.6630(3)	1	0.0572(8)
F2	0.2219(4)	0.76801(10)	0.7852(3)	1	0.0516(7)
F3	0.0163(4)	0.75680(10)	0.8521(3)	1	0.0567(8)
F4	0.4730(7)	0.62092(16)	1.1757(4)	0.805(6)	0.0623(14)
F5	0.2310(5)	0.5882(3)	1.1656(3)	0.805(6)	0.0764(19)
F6	0.4148(7)	0.53571(13)	1.1333(3)	0.805(6)	0.0534(11)
F4B	0.301(3)	0.5431(8)	1.1269(13)	0.195(6)	0.0623(14)
F5B	0.497(3)	0.6002(13)	1.1511(18)	0.195(6)	0.0764(19)
F6B	0.280(3)	0.6295(6)	1.1697(12)	0.195(6)	0.0534(11)
F7	0.1017(3)	0.45387(10)	0.01880(19)	1	0.0371(6)
F8	0.3429(3)	0.42090(11)	0.0231(2)	1	0.0388(6)
F9	0.1231(3)	0.36615(10)	-0.0215(2)	1	0.0398(6)
F10	0.6294(4)	0.27555(13)	0.4253(3)	1	0.0693(10)
F11	0.4062(6)	0.23144(12)	0.3076(3)	1	0.0908(14)
F12	0.4341(4)	0.25153(11)	0.4937(3)	1	0.0545(8)
N1	0.1013(4)	0.45684(11)	0.7445(2)	1	0.0209(6)
N2	0.1300(4)	0.38830(11)	0.5886(2)	1	0.0216(6)
S1	0.06530(12)	0.39100(3)	0.70383(8)	1	0.0239(2)

Anisotropic displacement parameters ($Å^2$)

The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a^{*2} U_{11} + ... + 2 h k a* b* U_{12}].

Atom	U11	U22	U33	U23	U13	U12
C1	0.0217(15)	0.0153(14)	0.0112(14)	0.0008(11)	0.0039(11)	0.0020(11)
C2	0.0189(14)	0.0155(14)	0.0119(14)	-0.0001(11)	0.0025(11)	0.0013(11)
C3	0.0195(15)	0.0186(14)	0.0118(14)	0.0008(11)	0.0046(11)	0.0023(11)

C4	0.0218(15)	0.0196(15)	0.0174(16)	0.0005(11)	0.0102(12)	-0.0005(12)
C5	0.0239(16)	0.0156(14)	0.0178(16)	-0.0025(11)	0.0077(12)	-0.0022(12)
C6	0.0194(15)	0.0167(14)	0.0131(15)	-0.0017(11)	0.0035(11)	0.0005(11)
C7	0.0183(14)	0.0144(14)	0.0183(16)	-0.0038(11)	0.0065(12)	-0.0026(11)
C8	0.0259(16)	0.0178(15)	0.0205(17)	-0.0016(12)	0.0094(13)	-0.0021(12)
C9	0.0274(17)	0.0117(14)	0.0295(19)	-0.0036(12)	0.0083(14)	-0.0017(12)
C10	0.0276(17)	0.0197(15)	0.0249(18)	-0.0097(13)	0.0113(14)	-0.0072(13)
C11	0.0206(15)	0.0216(15)	0.0178(16)	-0.0062(12)	0.0072(12)	-0.0066(12)
C12	0.0205(15)	0.0171(14)	0.0180(16)	-0.0040(11)	0.0066(12)	-0.0027(11)
C13	0.042(2)	0.0181(16)	0.036(2)	-0.0039(14)	0.0128(17)	0.0021(15)
C14	0.0299(18)	0.0260(17)	0.0238(18)	-0.0075(13)	0.0093(14)	-0.0072(14)
C15	0.0213(15)	0.0152(14)	0.0139(15)	0.0002(11)	0.0063(12)	0.0012(11)
C16	0.0208(15)	0.0152(14)	0.0164(15)	0.0018(11)	0.0085(12)	0.0016(11)
C17	0.0247(16)	0.0183(14)	0.0137(15)	0.0012(11)	0.0073(12)	0.0018(12)
C18	0.0326(18)	0.0195(15)	0.0235(17)	-0.0029(12)	0.0130(14)	0.0056(13)
C19	0.0337(19)	0.0171(15)	0.0250(18)	0.0017(13)	0.0105(14)	0.0072(13)
C20	0.0266(17)	0.0202(15)	0.0176(16)	0.0029(12)	0.0063(13)	0.0067(13)
C21	0.0258(17)	0.0222(15)	0.0217(17)	-0.0023(12)	0.0114(13)	0.0012(13)
C22	0.063(3)	0.0258(19)	0.032(2)	0.0069(16)	0.018(2)	0.0212(18)
F1	0.0760(19)	0.0240(12)	0.0487(16)	0.0016(11)	-0.0042(14)	0.0135(12)
F2	0.0652(17)	0.0199(11)	0.0703(19)	0.0031(11)	0.0255(14)	-0.0106(11)
F3	0.086(2)	0.0263(12)	0.071(2)	0.0008(12)	0.0450(17)	0.0201(13)
F4	0.082(3)	0.045(2)	0.0277(19)	0.0053(14)	-0.0173(17)	-0.041(2)
F5	0.044(2)	0.169(6)	0.0258(18)	0.031(2)	0.0233(15)	0.033(3)
F6	0.098(3)	0.0316(16)	0.0192(15)	0.0045(11)	0.0075(16)	0.0189(17)
F4B	0.082(3)	0.045(2)	0.0277(19)	0.0053(14)	-0.0173(17)	-0.041(2)
F5B	0.044(2)	0.169(6)	0.0258(18)	0.031(2)	0.0233(15)	0.033(3)
F6B	0.098(3)	0.0316(16)	0.0192(15)	0.0045(11)	0.0075(16)	0.0189(17)
F7	0.0500(14)	0.0423(13)	0.0189(11)	0.0092(9)	0.0124(9)	0.0214(10)
F8	0.0337(12)	0.0606(16)	0.0272(12)	0.0093(10)	0.0170(10)	0.0019(11)
F9	0.0622(15)	0.0369(12)	0.0169(11)	-0.0066(9)	0.0105(10)	-0.0119(11)
F10	0.066(2)	0.0588(19)	0.092(2)	0.0435(17)	0.0394(18)	0.0433(15)
F11	0.167(4)	0.0256(13)	0.056(2)	-0.0063(13)	0.013(2)	0.0413(18)
F12	0.085(2)	0.0304(12)	0.0551(18)	0.0235(12)	0.0340(15)	0.0208(13)
N1	0.0310(15)	0.0168(12)	0.0152(13)	-0.0019(10)	0.0087(11)	-0.0035(11)
N2	0.0345(15)	0.0156(12)	0.0148(13)	-0.0006(10)	0.0093(11)	-0.0038(11)
S1	0.0417(5)	0.0164(4)	0.0160(4)	-0.0011(3)	0.0136(3)	-0.0058(3)

Bond lengths [Å]

C1 - N1 = 1.349(4)
C1 - C6 = 1.429(4)
C1 - C2 = 1.437(4)
C2 - N2 = 1.350(4)
C2 - C3 = 1.430(4)
C3 - C4 = 1.374(4)
C3 - C15 = 1.489(4)
C4 - C5 = 1.423(4)
C4 - H4 = 0.9500
C5 - C6 = 1.373(4)
C5 - H5 = 0.9500
C6 - C7 = 1.483(4)
C7 - C12 = 1.392(4)
C7 - C8 = 1.404(4)
C8 - C9 = 1.392(5)
C8 - H8 = 0.9500
C9 - C10 = 1.380(5)
C9 - C13 = 1.506(5)
C10 - C11 = 1.394(5)
C10 - H10 = 0.9500
C11 - C12 = 1.394(4)
C11 - C14 = 1.505(5)
C12 - H12 = 0.9500
C13 - F1 = 1.331(5)
C13 - F3 = 1.334(5)
C13 - F2 = 1.340(5)
C14 - F4B = 1.165(14)
C14 - F5B = 1.22(2)
C14 - F5 = 1.301(5)
C14 - F4 = 1.311(5)
C14 - F6 = 1.370(5)
C14 - F6B = 1.381(14)
C15 - C16 = 1.391(4)
C15 - C20 = 1.398(4)
C16 - C17 = 1.386(4)
C16 - H16 = 0.9500
C17 - C18 = 1.389(4)
C17 - C21 = 1.502(4)
C18 - C19 = 1.378(5)

C18	- H18	= 0.9500
C19	- C20	= 1.393(5)
C19	- C22	= 1.499(5)
C20	- H20	= 0.9500
C21	- F7	= 1.328(4)
C21	- F8	= 1.328(4)
C21	- F9	= 1.345(4)
C22	- F11	= 1.323(5)
C22	- F12	= 1.329(5)
C22	- F10	= 1.333(6)
N1	- S1	= 1.615(3)
N2	- S1	= 1.613(3)

Angles [°]

N1	- C1	- C6	= 126.00(3)
N1	- C1	- C2	= 113.20(3)
C6	- C1	- C2	= 120.80(3)
N2	- C2	- C3	= 125.90(3)
N2	- C2	- C1	= 113.00(3)
C3	- C2	- C1	= 121.00(3)
C4	- C3	- C2	= 116.50(3)
C4	- C3	- C15	= 122.00(3)
C2	- C3	- C15	= 121.50(3)
C3	- C4	- C5	= 122.20(3)
C3	- C4	- H4	= 118.90
C5	- C4	- H4	= 118.90
C6	- C5	- C4	= 123.10(3)
C6	- C5	- H5	= 118.40
C4	- C5	- H5	= 118.40
C5	- C6	- C1	= 116.20(3)
C5	- C6	- C7	= 121.80(3)
C1	- C6	- C7	= 122.00(3)
C12	- C7	- C8	= 119.30(3)
C12	- C7	- C6	= 120.80(3)
C8	- C7	- C6	= 119.90(3)
C9	- C8	- C7	= 119.50(3)
C9	- C8	- H8	= 120.20
C7	- C8	- H8	= 120.20

C10 - C9 - C8 = 121.40(3)
C10 - C9 - C13 = 119.60(3)
C8 - C9 - C13 = 118.90(3)
C9 - C10 - C11 = 118.90(3)
C9 - C10 - H10 = 120.50
C11 - C10 - H10 = 120.50
C10 - C11 - C12 = 120.60(3)
C10 - C11 - C14 = 118.90(3)
C12 - C11 - C14 = 120.50(3)
C7 - C12 - C11 = 120.20(3)
C7 - C12 - H12 = 119.90
C11 - C12 - H12 = 119.90
F1 - C13 - F3 = 107.10(3)
F1 - C13 - F2 = 106.40(3)
F3 - C13 - F2 = 106.40(3)
F1 - C13 - C9 = 112.50(3)
F3 - C13 - C9 = 112.10(3)
F2 - C13 - C9 = 111.80(3)
F4B - C14 - F5B = 118.30(16)
F5 - C14 - F4 = 108.70(4)
F5 - C14 - F6 = 104.00(4)
F4 - C14 - F6 = 101.70(4)
F4B - C14 - F6B = 112.00(14)
F5B - C14 - F6B = 101.10(14)
F4B - C14 - C11 = 110.70(7)
F5B - C14 - C11 = 108.10(9)
F5 - C14 - C11 = 114.90(3)
F4 - C14 - C11 = 113.10(3)
F6 - C14 - C11 = 113.20(3)
F6B - C14 - C11 = 105.50(6)
C16 - C15 - C20 = 119.60(3)
C16 - C15 - C3 = 120.40(3)
C20 - C15 - C3 = 120.00(3)
C17 - C16 - C15 = 119.80(3)
C17 - C16 - H16 = 120.10
C15 - C16 - H16 = 120.10
C16 - C17 - C18 = 121.20(3)
C16 - C17 - C21 = 120.90(3)
C18 - C17 - C21 = 117.90(3)
C19 - C18 - C17 = 118.70(3)

C19	- C18	- H18	= 120.70				
C17	- C18	- H18	= 120.70				
C18	- C19	- C20	= 121.40(3)				
C18	- C19	- C22	= 119.00(3)				
C20	- C19	- C22	= 119.50(3)				
C19	- C20	- C15	= 119.40(3)				
C19	- C20	- H20	= 120.30				
C15	- C20	- H20	= 120.30				
F7	- C21	- F8	= 107.30(3)				
F7	- C21	- F9	= 106.30(3)				
F8	- C21	- F9	= 106.60(3)				
F7	- C21	- C17	= 112.60(3)				
F8	- C21	- C17	= 112.10(3)				
F9	- C21	- C17	= 111.50(3)				
F11	- C22	- F12	= 107.10(4)				
F11	- C22	- F10	= 106.70(4)				
F12	- C22	- F10	= 106.40(3)				
F11	- C22	- C19	= 112.20(3)				
F12	- C22	- C19	= 113.40(3)				
F10	- C22	- C19	= 110.70(4)				
C1	- N1	- S1	= 106.10(2)				
C2	- N2	- S1	= 106.30(2)				
N2	- S1	- N1	= 101.32(14)				

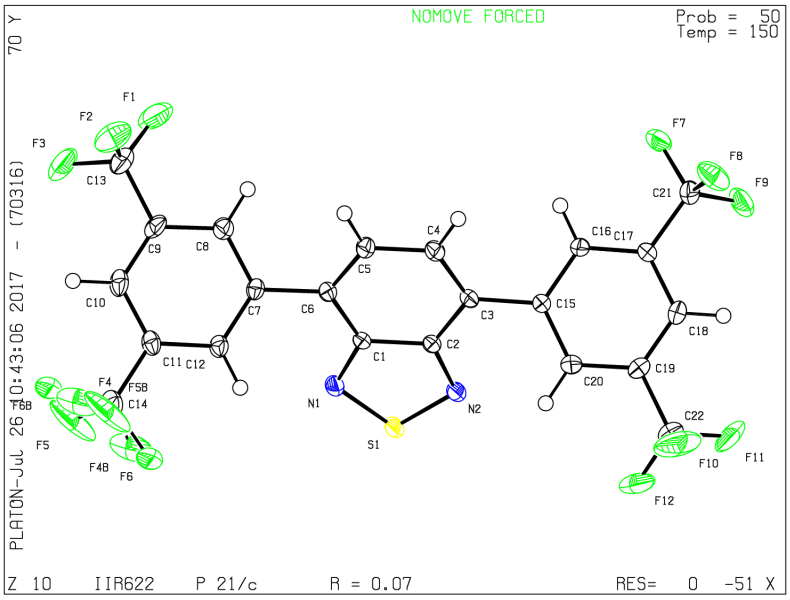
Torsion angles [°]

N1	- C1	- C2	- N2	= 0.00(4)			
C6	- C1	- C2	- N2	= -178.50(3)			
N1	- C1	- C2	- C3	= 178.20(3)			
C6	- C1	- C2	- C3	= -0.40(4)			
N2	- C2	- C3	- C4	= 175.80(3)			
C1	- C2	- C3	- C4	= -2.10(4)			
N2	- C2	- C3	- C15	= -4.80(5)			
C1	- C2	- C3	- C15	= 177.30(3)			
C2	- C3	- C4	- C5	= 2.00(5)			
C15	- C3	- C4	- C5	= -177.30(3)			
C3	- C4	- C5	- C6	= 0.50(5)			
C4	- C5	- C6	- C1	= -2.90(5)			
C4	- C5	- C6	- C7	= 176.50(3)			

N1 - C1 - C6 - C5 = -175.50(3)
C2 - C1 - C6 - C5 = 2.80(4)
N1 - C1 - C6 - C7 = 5.00(5)
C2 - C1 - C6 - C7 = -176.70(3)
C5 - C6 - C7 - C12 = -136.80(3)
C1 - C6 - C7 - C12 = 42.70(4)
C5 - C6 - C7 - C8 = 40.80(4)
C1 - C6 - C7 - C8 = -139.70(3)
C12 - C7 - C8 - C9 = -0.50(5)
C6 - C7 - C8 - C9 = -178.10(3)
C7 - C8 - C9 - C10 = 0.90(5)
C7 - C8 - C9 - C13 = 178.70(3)
C8 - C9 - C10 - C11 = 0.30(5)
C13 - C9 - C10 - C11 = -177.50(3)
C9 - C10 - C11 - C12 = -1.80(5)
C9 - C10 - C11 - C14 = 176.30(3)
C8 - C7 - C12 - C11 = -1.00(5)
C6 - C7 - C12 - C11 = 176.60(3)
C10 - C11 - C12 - C7 = 2.20(5)
C14 - C11 - C12 - C7 = -175.80(3)
C10 - C9 - C13 - F1 = -153.90(4)
C8 - C9 - C13 - F1 = 28.20(5)
C10 - C9 - C13 - F3 = -33.10(5)
C8 - C9 - C13 - F3 = 149.10(3)
C10 - C9 - C13 - F2 = 86.40(4)
C8 - C9 - C13 - F2 = -91.50(4)
C10 - C11 - C14 - F4B = 140.50(15)
C12 - C11 - C14 - F4B = -41.50(16)
C10 - C11 - C14 - F5B = -88.50(15)
C12 - C11 - C14 - F5B = 89.50(14)
C10 - C11 - C14 - F5 = 67.20(5)
C12 - C11 - C14 - F5 = -114.70(5)
C10 - C11 - C14 - F4 = -58.40(5)
C12 - C11 - C14 - F4 = 119.70(4)
C10 - C11 - C14 - F6 = -173.40(4)
C12 - C11 - C14 - F6 = 4.60(5)
C10 - C11 - C14 - F6B = 19.00(10)
C12 - C11 - C14 - F6B = -162.90(10)
C4 - C3 - C15 - C16 = -42.50(4)
C2 - C3 - C15 - C16 = 138.20(3)

C4	- C3	- C15	- C20	=	137.00(3)
C2	- C3	- C15	- C20	=	-42.30(4)
C20	- C15	- C16	- C17	=	-1.10(5)
C3	- C15	- C16	- C17	=	178.40(3)
C15	- C16	- C17	- C18	=	0.40(5)
C15	- C16	- C17	- C21	=	179.80(3)
C16	- C17	- C18	- C19	=	0.10(5)
C21	- C17	- C18	- C19	=	-179.30(3)
C17	- C18	- C19	- C20	=	0.10(5)
C17	- C18	- C19	- C22	=	-177.30(4)
C18	- C19	- C20	- C15	=	-0.80(5)
C22	- C19	- C20	- C15	=	176.60(3)
C16	- C15	- C20	- C19	=	1.20(5)
C3	- C15	- C20	- C19	=	-178.20(3)
C16	- C17	- C21	- F7	=	-14.90(4)
C18	- C17	- C21	- F7	=	164.50(3)
C16	- C17	- C21	- F8	=	106.30(4)
C18	- C17	- C21	- F8	=	-74.30(4)
C16	- C17	- C21	- F9	=	-134.30(3)
C18	- C17	- C21	- F9	=	45.10(4)
C18	- C19	- C22	- F11	=	-32.80(6)
C20	- C19	- C22	- F11	=	149.80(4)
C18	- C19	- C22	- F12	=	-154.30(4)
C20	- C19	- C22	- F12	=	28.30(6)
C18	- C19	- C22	- F10	=	86.20(4)
C20	- C19	- C22	- F10	=	-91.20(4)
C6	- C1	- N1	- S1	=	178.50(3)
C2	- C1	- N1	- S1	=	0.10(3)
C3	- C2	- N2	- S1	=	-178.20(3)
C1	- C2	- N2	- S1	=	-0.10(3)
C2	- N2	- S1	- N1	=	0.20(2)
C1	- N1	- S1	- N2	=	-0.10(2)

Structure visualisation



6. Crystal structure report of compound 30

X-ray crystallographic study

(C_{14} H_6 F_6 N_2 Se); M = 395.17. D8 VENTURE Bruker AXS diffractometer [*], Mo-Kα radiation (λ = 0.71073 Å), T = 150(2) K; tetragonal $P\,4_2/n$ (I.T.#86), a = 35.191(2), c = 4.3928(3) Å, V = 5440.1(8) Å^3. Z = 16, d = 1.930 g.cm^{-3}, μ = 2.830 mm^{-1}. The structure was solved by dual-space algorithm using the *SHELXT* program [1], and then refined with full-matrix least-square methods based on F^2(*SHELXL*) [2]. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 6225 unique intensities and 409 parameters converged at ω$R(F^2)$ = 0.1337 ($R(F)$ = 0.0614) for 5193 observed reflections with $I > 2\sigma(I)$.

[1] G. M. Sheldrick, Acta Cryst. A71 (2015) 3-8
[2] Sheldrick G.M., Acta Cryst. C71 (2015) 3-8

[*] Thanks to FEDER founds

Structural data

Empirical formula	C_{14} H_6 F_6 N_2 Se
Formula weight	395.17 g/mol

Temperature	150(2) *K*
Wavelength	0.71073 Å
Crystal system, space group	tetragonal, $P\,4_2/n$
Unit cell dimensions	a = 35.191(2) Å, α = 90 °
	b = 35.191 Å, β = 90 °
	c = 4.3928(3) Å, γ = 90 °
Volume	5440.1(8) $Å^3$
Z, Calculated density	16, 1.930 $g.cm^{-3}$
Absorption coefficient	2.830 mm^{-1}
F(000)	3072
Crystal size	0.600 x 0.220 x 0.210 mm
Crystal color	yellow
Theta range for data collection	2.952 to 27.471 °
h_min, h_max	-44, 45
k_min, k_max	-42, 45
l_min, l_max	-5, 5
Reflections collected / unique	34119 / 6225 [R(int)[a] = 0.0515]
Reflections [I>2σ]	5193
Completeness to theta_max	0.997
Absorption correction type	multi-scan
Max. and min. transmission	0.552 , 0.361
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6225 / 15 / 409
[b]S (Goodness-of-fit)	1.090
Final *R* indices [I>2σ]	$R1^c$ = 0.0614, $wR2^d$ = 0.1337
R indices (all data)	$R1^c$ = 0.0757, $wR2^d$ = 0.1410
Largest diff. peak and hole	1.198 and -1.027 $e^-.Å^{-3}$

[a] $R_{int} = \sum |F_o^2 - \langle F_o^2 \rangle| / \sum [F_o^2]$

[b] $S = \{\sum [w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$

[c] $R1 = \sum | |F_o| - |F_c| | / \sum |F_o|$

[d] $wR2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$

$w = 1 / [\sigma(F_o^2) + aP^2 + bP]$ where $P = [2F_c^2 + MAX(F_o^2, 0)] /3$

Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters ($Å^2$). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
Se1	0.50686(2)	0.85557(2)	0.95099(12)	1	0.02567(14)
N1	0.48074(12)	0.89789(11)	0.8658(11)	1	0.0275(9)
N2	0.47440(11)	0.82488(11)	0.7572(10)	1	0.0245(9)
C1	0.44745(13)	0.84696(12)	0.6414(12)	1	0.0220(10)
C2	0.45104(13)	0.88729(13)	0.7011(12)	1	0.0252(10)
C3	0.42328(15)	0.91299(13)	0.5819(14)	1	0.0314(12)
H3	0.425380	0.939505	0.618726	1	0.038
C4	0.39413(15)	0.89917(15)	0.4171(15)	1	0.0362(13)
H4	0.375829	0.916240	0.336052	1	0.043
C5	0.39016(15)	0.85925(14)	0.3614(15)	1	0.0331(12)
H5	0.369022	0.850690	0.245681	1	0.040
C6	0.41561(13)	0.83284(13)	0.4683(12)	1	0.0241(10)
C7	0.40990(13)	0.79166(13)	0.4139(12)	1	0.0245(10)
C8	0.37404(14)	0.77569(14)	0.4589(13)	1	0.0271(10)
H8	0.353592	0.791415	0.522620	1	0.032
C9	0.36782(15)	0.73730(15)	0.4123(13)	1	0.0321(12)
C10	0.39680(17)	0.71392(15)	0.3170(13)	1	0.0350(13)
H10	0.392418	0.687654	0.281639	1	0.042
C11	0.43256(16)	0.72957(14)	0.2736(13)	1	0.0318(12)
C12	0.43961(14)	0.76789(14)	0.3226(12)	1	0.0265(10)
H12	0.464436	0.777888	0.294301	1	0.032
C13	0.3295(2)	0.72128(17)	0.4847(15)	1	0.0491(17)
C14	0.46426(19)	0.70441(16)	0.1652(14)	1	0.0466(16)
F1	0.3015(3)	0.7413(3)	0.322(2)	0.481(7)	0.0528(11)
F2	0.3165(2)	0.7309(2)	0.776(2)	0.481(7)	0.0528(11)
F3	0.3210(3)	0.6868(3)	0.442(3)	0.481(7)	0.0528(11)
F1B	0.3309(2)	0.7085(2)	0.7806(17)	0.519(7)	0.0528(11)
F2B	0.3272(3)	0.6865(2)	0.341(2)	0.519(7)	0.0528(11)
F3B	0.3020(3)	0.7418(3)	0.435(2)	0.519(7)	0.0528(11)
F4	0.45529(17)	0.69126(17)	-0.1165(15)	0.601(5)	0.0488(9)
F5	0.45932(19)	0.66895(18)	0.3232(18)	0.601(5)	0.0488(9)
F6	0.4969(2)	0.7142(2)	0.2158(18)	0.601(5)	0.0488(9)
F4B	0.4983(3)	0.7134(4)	0.342(3)	0.399(5)	0.0488(9)
F5B	0.4817(3)	0.7181(2)	-0.113(2)	0.399(5)	0.0488(9)
F6B	0.4639(3)	0.6696(3)	0.170(3)	0.399(5)	0.0488(9)
Se2	0.51380(2)	0.95470(2)	0.27361(12)	1	0.02435(13)
N21	0.54986(11)	0.91860(10)	0.2577(10)	1	0.0218(8)

N22	0.54107(12)	0.98533(10)	0.5119(10)	1	0.0256(9)
C21	0.57886(13)	0.93094(12)	0.4272(11)	1	0.0196(9)
C22	0.57414(13)	0.96815(12)	0.5645(12)	1	0.0229(10)
C23	0.60411(16)	0.98452(14)	0.7422(13)	1	0.0335(12)
H23	0.600874	1.008396	0.839652	1	0.040
C24	0.63717(15)	0.96508(14)	0.7676(13)	1	0.0308(11)
H24	0.657472	0.975948	0.880536	1	0.037
C25	0.64235(14)	0.92889(13)	0.6302(12)	1	0.0238(10)
H25	0.666244	0.916614	0.651813	1	0.029
C26	0.61421(12)	0.91086(12)	0.4670(11)	1	0.0199(9)
C27	0.62090(12)	0.87234(12)	0.3404(11)	1	0.0180(9)
C28	0.65535(12)	0.86391(12)	0.1979(11)	1	0.0187(9)
H28	0.673910	0.883294	0.174812	1	0.022
C29	0.66288(12)	0.82772(12)	0.0897(10)	1	0.0176(9)
C30	0.63621(12)	0.79879(12)	0.1202(11)	1	0.0190(9)
H30	0.641162	0.774088	0.042493	1	0.023
C31	0.60222(13)	0.80683(13)	0.2668(11)	1	0.0212(9)
C32	0.59428(12)	0.84310(12)	0.3731(11)	1	0.0193(9)
H32	0.570597	0.848108	0.468803	1	0.023
C33	0.70046(13)	0.81943(14)	-0.0549(12)	1	0.0233(10)
C34	0.57390(14)	0.77573(13)	0.3166(13)	1	0.0268(11)
F21	0.71315(9)	0.84912(9)	-0.2182(8)	1	0.0409(8)
F22	0.72701(9)	0.81237(12)	0.1503(8)	1	0.0481(10)
F23	0.69939(9)	0.79028(9)	-0.2418(8)	1	0.0414(8)
F24	0.55672(19)	0.77906(18)	0.5994(19)	0.511(5)	0.0449(9)
F25	0.5844(3)	0.7426(2)	0.272(2)	0.511(5)	0.0449(9)
F26	0.5421(2)	0.7823(2)	0.133(2)	0.511(5)	0.0449(9)
F24B	0.5827(3)	0.7440(3)	0.137(2)	0.489(5)	0.0449(9)
F25B	0.5399(2)	0.7838(2)	0.281(2)	0.489(5)	0.0449(9)
F26B	0.5786(2)	0.76094(19)	0.601(2)	0.489(5)	0.0449(9)

Anisotropic displacement parameters ($Å^2$)

The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a^{*2} U_{11} + ... + 2 h k a* b* U_{12}].

Atom	U11	U22	U33	U23	U13	U12
Se1	0.0242(2)	0.0212(2)	0.0316(3)	-0.0026(2)	0.0000(2)	0.00199(18)
N1	0.026(2)	0.0215(19)	0.035(3)	-0.0016(18)	0.0015(18)	0.0014(16)
N2	0.0211(19)	0.0180(18)	0.034(2)	-0.0016(17)	-0.0005(18)	0.0014(15)
C1	0.019(2)	0.018(2)	0.029(3)	-0.0006(19)	0.0069(19)	0.0015(16)
C2	0.020(2)	0.021(2)	0.035(3)	-0.003(2)	0.004(2)	0.0016(17)
C3	0.033(3)	0.015(2)	0.046(3)	0.000(2)	0.004(2)	0.0048(19)
C4	0.028(3)	0.024(2)	0.056(4)	0.004(3)	-0.003(3)	0.008(2)
C5	0.024(2)	0.025(2)	0.050(4)	0.000(2)	-0.004(2)	0.0004(19)
C6	0.020(2)	0.020(2)	0.032(3)	0.000(2)	0.003(2)	0.0024(17)
C7	0.024(2)	0.021(2)	0.029(3)	-0.001(2)	-0.001(2)	-0.0001(17)
C8	0.024(2)	0.024(2)	0.033(3)	-0.001(2)	0.001(2)	-0.0024(18)
C9	0.033(3)	0.028(3)	0.034(3)	0.005(2)	-0.010(2)	-0.006(2)
C10	0.050(3)	0.021(2)	0.034(3)	-0.003(2)	-0.013(3)	-0.005(2)
C11	0.040(3)	0.025(2)	0.030(3)	-0.004(2)	-0.008(2)	0.009(2)
C12	0.027(2)	0.026(2)	0.027(3)	0.001(2)	-0.001(2)	0.0023(19)
C13	0.060(4)	0.045(4)	0.042(4)	0.004(3)	-0.007(3)	-0.027(3)
C14	0.063(4)	0.035(3)	0.042(4)	-0.013(3)	-0.012(3)	0.027(3)
F1	0.0410(16)	0.0455(15)	0.072(3)	0.004(2)	0.005(2)	-0.0144(12)
F2	0.0410(16)	0.0455(15)	0.072(3)	0.004(2)	0.005(2)	-0.0144(12)
F3	0.0410(16)	0.0455(15)	0.072(3)	0.004(2)	0.005(2)	-0.0144(12)
F1B	0.0410(16)	0.0455(15)	0.072(3)	0.004(2)	0.005(2)	-0.0144(12)
F2B	0.0410(16)	0.0455(15)	0.072(3)	0.004(2)	0.005(2)	-0.0144(12)
F3B	0.0410(16)	0.0455(15)	0.072(3)	0.004(2)	0.005(2)	-0.0144(12)
F4	0.0437(15)	0.0415(14)	0.061(3)	-0.010(2)	0.0120(19)	0.0131(11)
F5	0.0437(15)	0.0415(14)	0.061(3)	-0.010(2)	0.0120(19)	0.0131(11)
F6	0.0437(15)	0.0415(14)	0.061(3)	-0.010(2)	0.0120(19)	0.0131(11)
F4B	0.0437(15)	0.0415(14)	0.061(3)	-0.010(2)	0.0120(19)	0.0131(11)
F5B	0.0437(15)	0.0415(14)	0.061(3)	-0.010(2)	0.0120(19)	0.0131(11)
F6B	0.0437(15)	0.0415(14)	0.061(3)	-0.010(2)	0.0120(19)	0.0131(11)
Se2	0.0218(2)	0.0158(2)	0.0354(3)	-0.0039(2)	0.0033(2)	0.00413(17)
N21	0.0186(18)	0.0168(17)	0.030(2)	-0.0035(16)	0.0041(16)	0.0035(14)
N22	0.030(2)	0.0134(17)	0.033(2)	-0.0063(17)	0.0048(18)	0.0038(15)
C21	0.024(2)	0.0134(19)	0.022(2)	0.0007(17)	0.0045(18)	-0.0020(16)
C22	0.028(2)	0.013(2)	0.028(3)	-0.0007(19)	0.007(2)	-0.0002(17)
C23	0.043(3)	0.022(2)	0.036(3)	-0.010(2)	0.004(3)	-0.004(2)
C24	0.036(3)	0.025(2)	0.031(3)	-0.006(2)	-0.004(2)	-0.010(2)
C25	0.025(2)	0.022(2)	0.025(3)	0.0005(19)	0.000(2)	-0.0008(18)
C26	0.019(2)	0.016(2)	0.025(2)	0.0006(18)	0.0046(18)	-0.0026(16)

C27	0.019(2)	0.017(2)	0.018(2)	-0.0004(17)	0.0002(17)	0.0032(16)
C28	0.0144(19)	0.019(2)	0.023(2)	0.0004(18)	0.0003(17)	-0.0028(15)
C29	0.016(2)	0.023(2)	0.013(2)	-0.0023(17)	-0.0003(17)	0.0028(16)
C30	0.020(2)	0.017(2)	0.021(2)	-0.0021(17)	-0.0021(18)	0.0025(16)
C31	0.019(2)	0.020(2)	0.025(2)	0.0029(19)	-0.0030(19)	-0.0027(16)
C32	0.0145(19)	0.022(2)	0.022(2)	0.0049(18)	0.0018(17)	0.0000(16)
C33	0.017(2)	0.030(2)	0.023(2)	-0.003(2)	0.0015(19)	0.0023(18)
C34	0.025(2)	0.019(2)	0.037(3)	0.002(2)	0.001(2)	-0.0051(18)
F21	0.0351(17)	0.0370(17)	0.051(2)	0.0019(16)	0.0227(16)	-0.0017(13)
F22	0.0210(15)	0.096(3)	0.0268(17)	-0.0045(18)	-0.0008(13)	0.0200(17)
F23	0.0402(18)	0.0402(18)	0.044(2)	-0.0242(16)	0.0159(16)	-0.0046(14)
F24	0.0369(13)	0.0274(12)	0.070(3)	0.007(2)	0.008(2)	-0.0099(10)
F25	0.0369(13)	0.0274(12)	0.070(3)	0.007(2)	0.008(2)	-0.0099(10)
F26	0.0369(13)	0.0274(12)	0.070(3)	0.007(2)	0.008(2)	-0.0099(10)
F24B	0.0369(13)	0.0274(12)	0.070(3)	0.007(2)	0.008(2)	-0.0099(10)
F25B	0.0369(13)	0.0274(12)	0.070(3)	0.007(2)	0.008(2)	-0.0099(10)
F26B	0.0369(13)	0.0274(12)	0.070(3)	0.007(2)	0.008(2)	-0.0099(10)

Bond lengths [Å]

Se1	- N2	= 1.788(4)	
Se1	- N1	= 1.790(4)	
N1	- C2	= 1.325(7)	
N2	- C1	= 1.327(6)	
C1	- C6	= 1.443(7)	
C1	- C2	= 1.449(6)	
C2	- C3	= 1.431(7)	
C3	- C4	= 1.346(8)	
C3	- H3	= 0.9500	
C4	- C5	= 1.433(7)	
C4	- H4	= 0.9500	
C5	- C6	= 1.373(7)	
C5	- H5	= 0.9500	
C6	- C7	= 1.482(6)	
C7	- C8	= 1.396(7)	
C7	- C12	= 1.398(7)	
C8	- C9	= 1.384(7)	
C8	- H8	= 0.9500	
C9	- C10	= 1.376(8)	

C9 - C13 = 1.495(8)
C10 - C11 = 1.387(8)
C10 - H10 = 0.9500
C11 - C12 = 1.388(7)
C11 - C14 = 1.502(8)
C12 - H12 = 0.9500
C13 - F3B = 1.227(10)
C13 - F3 = 1.263(11)
C13 - F1B = 1.376(9)
C13 - F2B = 1.380(10)
C13 - F2 = 1.399(10)
C13 - F1 = 1.408(11)
C14 - F6 = 1.219(9)
C14 - F6B = 1.227(10)
C14 - F4 = 1.358(8)
C14 - F5 = 1.438(9)
C14 - F5B = 1.450(10)
C14 - F4B = 1.462(12)
Se2 - N22 = 1.783(4)
Se2 - N21 = 1.797(4)
N21 - C21 = 1.336(6)
N22 - C22 = 1.332(6)
C21 - C26 = 1.441(6)
C21 - C22 = 1.451(6)
C22 - C23 = 1.433(7)
C23 - C24 = 1.354(8)
C23 - H23 = 0.9500
C24 - C25 = 1.421(7)
C24 - H24 = 0.9500
C25 - C26 = 1.377(7)
C25 - H25 = 0.9500
C26 - C27 = 1.484(6)
C27 - C28 = 1.396(6)
C27 - C32 = 1.399(6)
C28 - C29 = 1.385(6)
C28 - H28 = 0.9500
C29 - C30 = 1.391(6)
C29 - C33 = 1.496(6)
C30 - C31 = 1.388(6)
C30 - H30 = 0.9500

C31 - C32 = 1.388(6)
C31 - C34 = 1.496(6)
C32 - H32 = 0.9500
C33 - F23 = 1.314(6)
C33 - F22 = 1.322(6)
C33 - F21 = 1.344(6)
C34 - F25 = 1.237(10)
C34 - F25B = 1.240(10)
C34 - F26B = 1.362(10)
C34 - F24 = 1.386(9)
C34 - F26 = 1.399(11)
C34 - F24B = 1.402(11)

Angles [°]

N2 - Se1 - N1 = 94.30(19)
C2 - N1 - Se1 = 106.60(3)
C1 - N2 - Se1 = 106.60(3)
N2 - C1 - C6 = 123.70(4)
N2 - C1 - C2 = 116.20(4)
C6 - C1 - C2 = 120.00(4)
N1 - C2 - C3 = 124.10(4)
N1 - C2 - C1 = 116.30(4)
C3 - C2 - C1 = 119.60(5)
C4 - C3 - C2 = 119.30(5)
C4 - C3 - H3 = 120.40
C2 - C3 - H3 = 120.40
C3 - C4 - C5 = 121.40(5)
C3 - C4 - H4 = 119.30
C5 - C4 - H4 = 119.30
C6 - C5 - C4 = 122.80(5)
C6 - C5 - H5 = 118.60
C4 - C5 - H5 = 118.60
C5 - C6 - C1 = 117.00(4)
C5 - C6 - C7 = 121.20(5)
C1 - C6 - C7 = 121.80(4)
C8 - C7 - C12 = 118.40(4)
C8 - C7 - C6 = 119.60(4)
C12 - C7 - C6 = 122.00(4)

C9 - C8 - C7 = 121.00(5)
C9 - C8 - H8 = 119.50
C7 - C8 - H8 = 119.50
C10 - C9 - C8 = 120.80(5)
C10 - C9 - C13 = 120.50(5)
C8 - C9 - C13 = 118.60(5)
C9 - C10 - C11 = 118.50(5)
C9 - C10 - H10 = 120.80
C11 - C10 - H10 = 120.80
C10 - C11 - C12 = 121.80(5)
C10 - C11 - C14 = 118.90(5)
C12 - C11 - C14 = 119.30(5)
C11 - C12 - C7 = 119.50(5)
C11 - C12 - H12 = 120.30
C7 - C12 - H12 = 120.30
F3B - C13 - F1B = 112.90(8)
F3B - C13 - F2B = 113.10(8)
F1B - C13 - F2B = 98.40(6)
F3 - C13 - F2 = 106.90(7)
F3 - C13 - F1 = 103.80(8)
F2 - C13 - F1 = 96.50(8)
F3B - C13 - C9 = 116.80(7)
F3 - C13 - C9 = 122.90(7)
F1B - C13 - C9 = 107.00(6)
F2B - C13 - C9 = 106.90(6)
F2 - C13 - C9 = 113.50(6)
F1 - C13 - C9 = 109.60(6)
F6 - C14 - F4 = 118.80(7)
F6 - C14 - F5 = 105.80(6)
F4 - C14 - F5 = 96.70(6)
F6B - C14 - F5B = 110.60(8)
F6B - C14 - F4B = 102.40(8)
F5B - C14 - F4B = 91.60(8)
F6 - C14 - C11 = 118.30(6)
F6B - C14 - C11 = 125.20(7)
F4 - C14 - C11 = 108.50(5)
F5 - C14 - C11 = 105.60(6)
F5B - C14 - C11 = 112.70(5)
F4B - C14 - C11 = 108.20(6)
N22 - Se2 - N21 = 94.02(18)

C21 - N21 - Se2 = 106.80(3)
C22 - N22 - Se2 = 107.30(3)
N21 - C21 - C26 = 124.60(4)
N21 - C21 - C22 = 115.90(4)
C26 - C21 - C22 = 119.40(4)
N22 - C22 - C23 = 123.70(4)
N22 - C22 - C21 = 116.00(4)
C23 - C22 - C21 = 120.30(4)
C24 - C23 - C22 = 118.30(5)
C24 - C23 - H23 = 120.80
C22 - C23 - H23 = 120.80
C23 - C24 - C25 = 121.90(5)
C23 - C24 - H24 = 119.10
C25 - C24 - H24 = 119.10
C26 - C25 - C24 = 122.80(5)
C26 - C25 - H25 = 118.60
C24 - C25 - H25 = 118.60
C25 - C26 - C21 = 117.30(4)
C25 - C26 - C27 = 120.10(4)
C21 - C26 - C27 = 122.60(4)
C28 - C27 - C32 = 118.10(4)
C28 - C27 - C26 = 120.00(4)
C32 - C27 - C26 = 121.80(4)
C29 - C28 - C27 = 121.00(4)
C29 - C28 - H28 = 119.50
C27 - C28 - H28 = 119.50
C28 - C29 - C30 = 120.70(4)
C28 - C29 - C33 = 119.60(4)
C30 - C29 - C33 = 119.60(4)
C31 - C30 - C29 = 118.50(4)
C31 - C30 - H30 = 120.80
C29 - C30 - H30 = 120.80
C30 - C31 - C32 = 121.20(4)
C30 - C31 - C34 = 119.50(4)
C32 - C31 - C34 = 119.30(4)
C31 - C32 - C27 = 120.50(4)
C31 - C32 - H32 = 119.80
C27 - C32 - H32 = 119.80
F23 - C33 - F22 = 107.40(4)
F23 - C33 - F21 = 106.40(4)

F22 - C33 - F21 = 106.00(4)
F23 - C33 - C29 = 113.10(4)
F22 - C33 - C29 = 111.80(4)
F21 - C33 - C29 = 111.60(4)
F25B - C34 - F26B = 108.70(6)
F25 - C34 - F24 = 110.60(6)
F25 - C34 - F26 = 107.60(6)
F24 - C34 - F26 = 98.90(6)
F25B - C34 - F24B = 108.90(7)
F26B - C34 - F24B = 100.70(6)
F25 - C34 - C31 = 117.80(6)
F25B - C34 - C31 = 117.20(5)
F26B - C34 - C31 = 109.40(5)
F24 - C34 - C31 = 111.10(5)
F26 - C34 - C31 = 109.10(5)
F24B - C34 - C31 = 110.70(5)

Torsion angles [°]

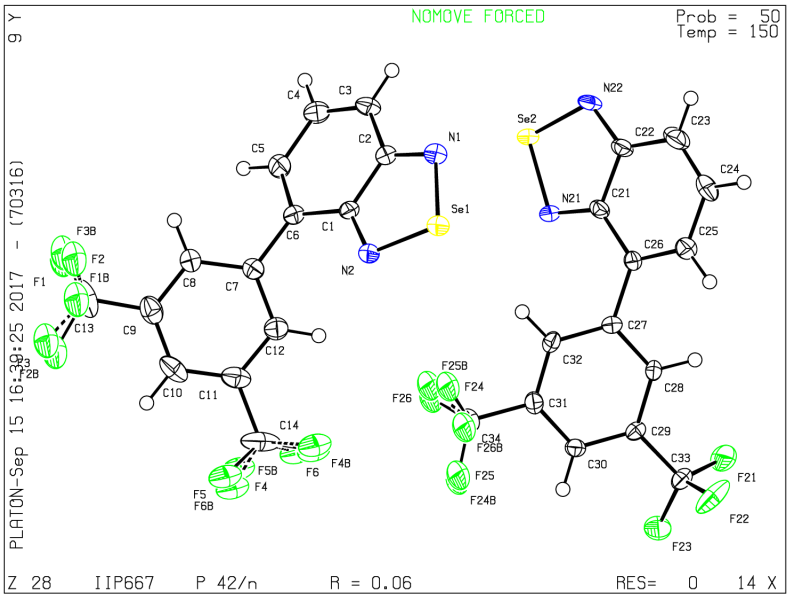
N2 - Se1 - N1 - C2 = -1.00(4)
N1 - Se1 - N2 - C1 = 0.90(4)
Se1 - N2 - C1 - C6 = -179.70(4)
Se1 - N2 - C1 - C2 = -0.50(5)
Se1 - N1 - C2 - C3 = -178.90(4)
Se1 - N1 - C2 - C1 = 0.90(6)
N2 - C1 - C2 - N1 = -0.20(7)
C6 - C1 - C2 - N1 = 178.90(5)
N2 - C1 - C2 - C3 = 179.50(5)
C6 - C1 - C2 - C3 = -1.30(7)
N1 - C2 - C3 - C4 = -180.00(6)
C1 - C2 - C3 - C4 = 0.30(8)
C2 - C3 - C4 - C5 = 0.70(9)
C3 - C4 - C5 - C6 = -0.60(10)
C4 - C5 - C6 - C1 = -0.40(8)
C4 - C5 - C6 - C7 = 178.10(5)
N2 - C1 - C6 - C5 = -179.60(5)
C2 - C1 - C6 - C5 = 1.30(7)
N2 - C1 - C6 - C7 = 1.90(8)
C2 - C1 - C6 - C7 = -177.20(5)

C5 - C6 - C7 - C8 = -45.20(8)
C1 - C6 - C7 - C8 = 133.20(5)
C5 - C6 - C7 - C12 = 135.80(6)
C1 - C6 - C7 - C12 = -45.70(8)
C12 - C7 - C8 - C9 = -0.50(8)
C6 - C7 - C8 - C9 = -179.50(5)
C7 - C8 - C9 - C10 = -0.70(9)
C7 - C8 - C9 - C13 = 175.80(5)
C8 - C9 - C10 - C11 = 1.10(9)
C13 - C9 - C10 - C11 = -175.40(5)
C9 - C10 - C11 - C12 = -0.30(9)
C9 - C10 - C11 - C14 = -179.10(5)
C10 - C11 - C12 - C7 = -1.00(8)
C14 - C11 - C12 - C7 = 177.90(5)
C8 - C7 - C12 - C11 = 1.30(8)
C6 - C7 - C12 - C11 = -179.70(5)
C10 - C9 - C13 - F3B = -148.10(8)
C8 - C9 - C13 - F3B = 35.30(9)
C10 - C9 - C13 - F3 = -5.30(11)
C8 - C9 - C13 - F3 = 178.10(8)
C10 - C9 - C13 - F1B = 84.30(7)
C8 - C9 - C13 - F1B = -92.30(7)
C10 - C9 - C13 - F2B = -20.30(9)
C8 - C9 - C13 - F2B = 163.10(7)
C10 - C9 - C13 - F2 = 125.90(7)
C8 - C9 - C13 - F2 = -50.70(8)
C10 - C9 - C13 - F1 = -127.50(8)
C8 - C9 - C13 - F1 = 55.90(9)
C10 - C11 - C14 - F6 = -157.60(7)
C12 - C11 - C14 - F6 = 23.50(9)
C10 - C11 - C14 - F6B = -16.20(11)
C12 - C11 - C14 - F6B = 164.90(9)
C10 - C11 - C14 - F4 = 63.20(7)
C12 - C11 - C14 - F4 = -115.70(6)
C10 - C11 - C14 - F5 = -39.50(7)
C12 - C11 - C14 - F5 = 141.60(6)
C10 - C11 - C14 - F5B = 123.50(7)
C12 - C11 - C14 - F5B = -55.40(8)
C10 - C11 - C14 - F4B = -136.80(8)
C12 - C11 - C14 - F4B = 44.30(9)

N22	- Se2	- N21	- C21	=	0.60(3)
N21	- Se2	- N22	- C22	=	0.30(4)
Se2	- N21	- C21	- C26	=	-178.00(4)
Se2	- N21	- C21	- C22	=	-1.20(5)
Se2	- N22	- C22	- C23	=	178.50(4)
Se2	- N22	- C22	- C21	=	-1.00(5)
N21	- C21	- C22	- N22	=	1.60(7)
C26	- C21	- C22	- N22	=	178.50(4)
N21	- C21	- C22	- C23	=	-177.90(5)
C26	- C21	- C22	- C23	=	-1.00(7)
N22	- C22	- C23	- C24	=	-176.90(5)
C21	- C22	- C23	- C24	=	2.60(8)
C22	- C23	- C24	- C25	=	-1.60(8)
C23	- C24	- C25	- C26	=	-1.10(8)
C24	- C25	- C26	- C21	=	2.60(7)
C24	- C25	- C26	- C27	=	-177.40(5)
N21	- C21	- C26	- C25	=	175.10(5)
C22	- C21	- C26	- C25	=	-1.50(7)
N21	- C21	- C26	- C27	=	-4.90(7)
C22	- C21	- C26	- C27	=	178.40(4)
C25	- C26	- C27	- C28	=	-43.50(7)
C21	- C26	- C27	- C28	=	136.60(5)
C25	- C26	- C27	- C32	=	133.10(5)
C21	- C26	- C27	- C32	=	-46.90(7)
C32	- C27	- C28	- C29	=	0.50(7)
C26	- C27	- C28	- C29	=	177.20(4)
C27	- C28	- C29	- C30	=	0.00(7)
C27	- C28	- C29	- C33	=	-178.50(4)
C28	- C29	- C30	- C31	=	-1.20(7)
C33	- C29	- C30	- C31	=	177.30(4)
C29	- C30	- C31	- C32	=	1.90(7)
C29	- C30	- C31	- C34	=	-176.90(4)
C30	- C31	- C32	- C27	=	-1.40(7)
C34	- C31	- C32	- C27	=	177.40(4)
C28	- C27	- C32	- C31	=	0.20(7)
C26	- C27	- C32	- C31	=	-176.50(4)
C28	- C29	- C33	- F23	=	-156.40(4)
C30	- C29	- C33	- F23	=	25.10(6)
C28	- C29	- C33	- F22	=	82.20(6)
C30	- C29	- C33	- F22	=	-96.40(5)

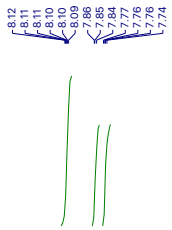
C28	- C29	- C33	- F21	= -36.40(6)
C30	- C29	- C33	- F21	= 145.10(4)
C30	- C31	- C34	- F25	= 12.10(9)
C32	- C31	- C34	- F25	= -166.80(7)
C30	- C31	- C34	- F25B	= -140.10(7)
C32	- C31	- C34	- F25B	= 41.00(9)
C30	- C31	- C34	- F26B	= 95.50(6)
C32	- C31	- C34	- F26B	= -83.30(6)
C30	- C31	- C34	- F24	= 141.10(5)
C32	- C31	- C34	- F24	= -37.80(7)
C30	- C31	- C34	- F26	= -111.00(6)
C32	- C31	- C34	- F26	= 70.20(7)
C30	- C31	- C34	- F24B	= -14.50(8)
C32	- C31	- C34	- F24B	= 166.60(6)

Structure visualisation



7. Copy of ^{1}H and ^{13}NMR charts of new compounds

1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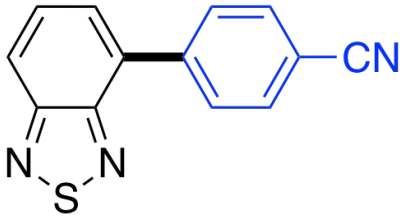
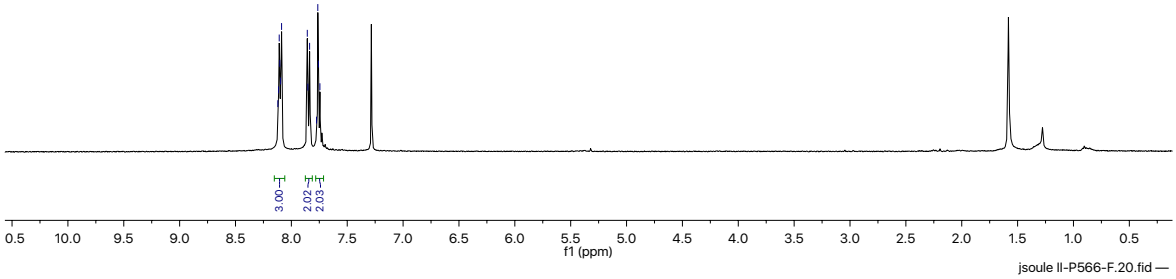
7.76
7.74


CN
N
S
N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6.0
5.5
5.0
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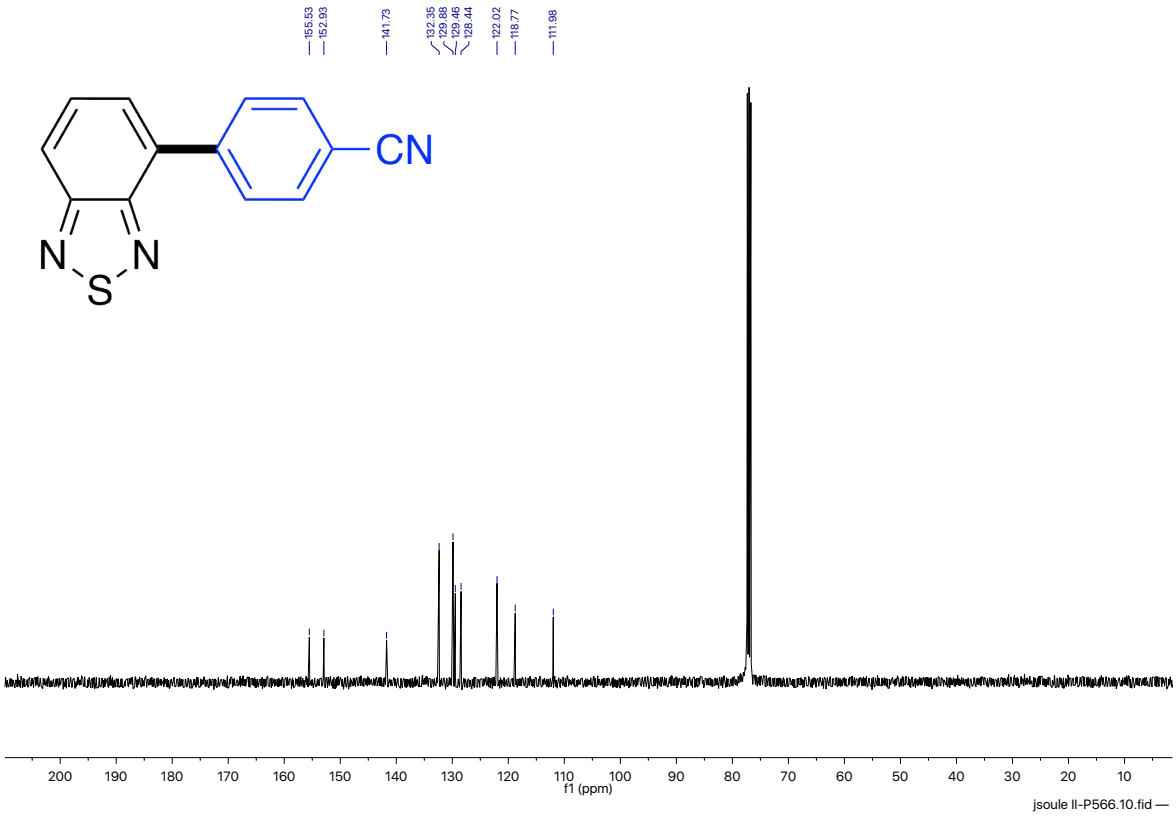
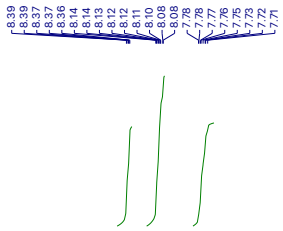
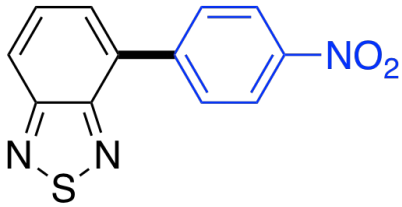
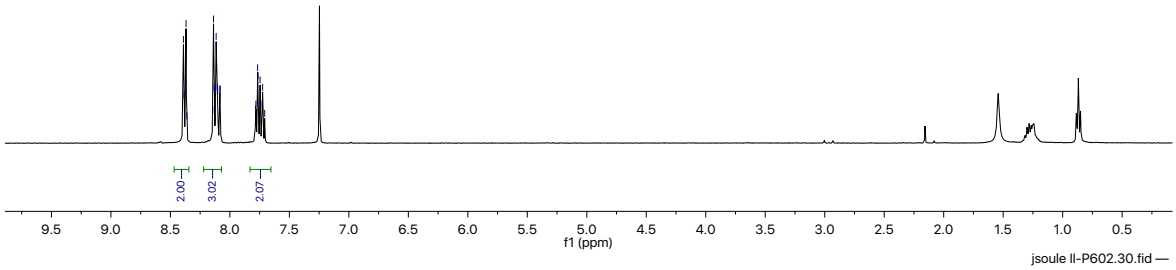
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
jsoule II-P566-F.20.fid


155.53
152.93
141.73
132.35
129.88
129.46
128.44
122.02
118.77
111.98
CN
N
S
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
jsoule II-P566.10.fid

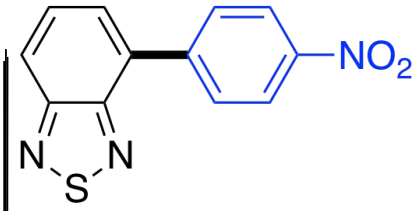
2

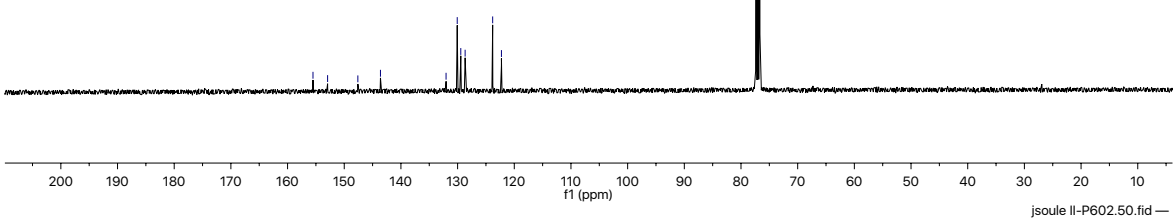

8.39
8.39
8.37
8.37
8.37
8.36
8.14
8.14
8.13
8.12
8.12
8.11
8.10
8.08
8.08
7.78
7.78
7.77
7.76
7.75
7.73
7.72
7.71


NO2
N
S
N

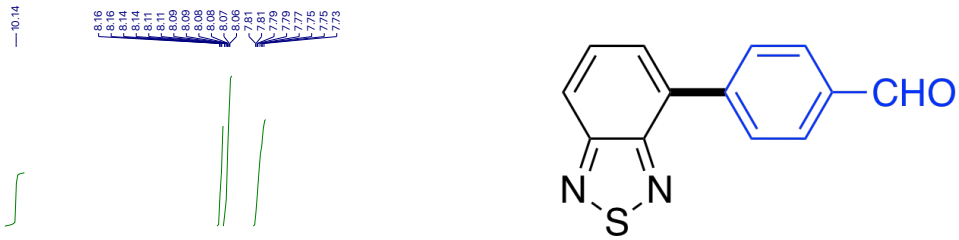

2.00
3.02
2.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
jsoule II-P602.30.fid

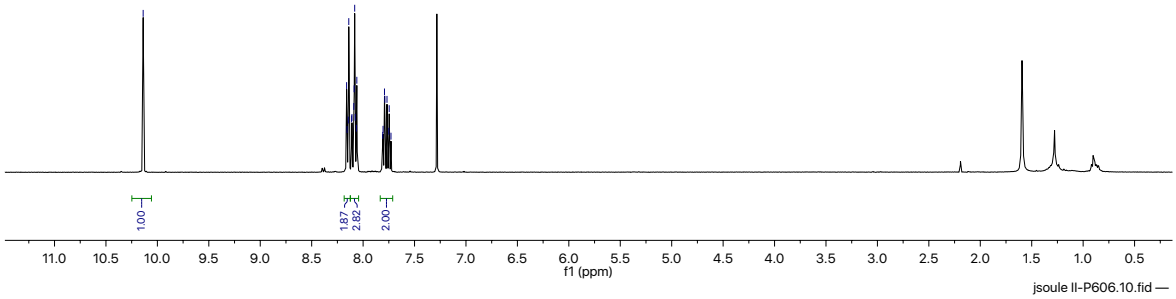

155.51
152.94
147.60
143.61
132.04
130.07
129.44
128.67
123.81
122.27

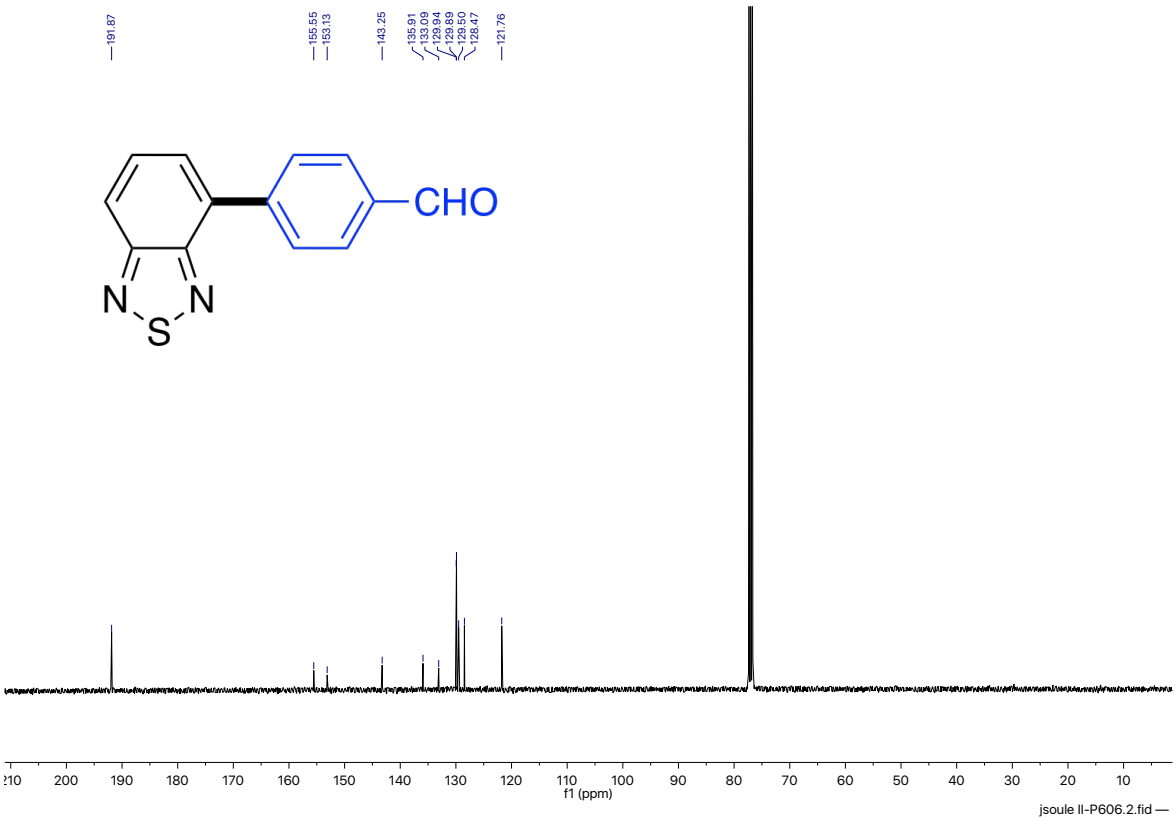

NO2
N
S
N


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
jsoule II-P602.50.fid

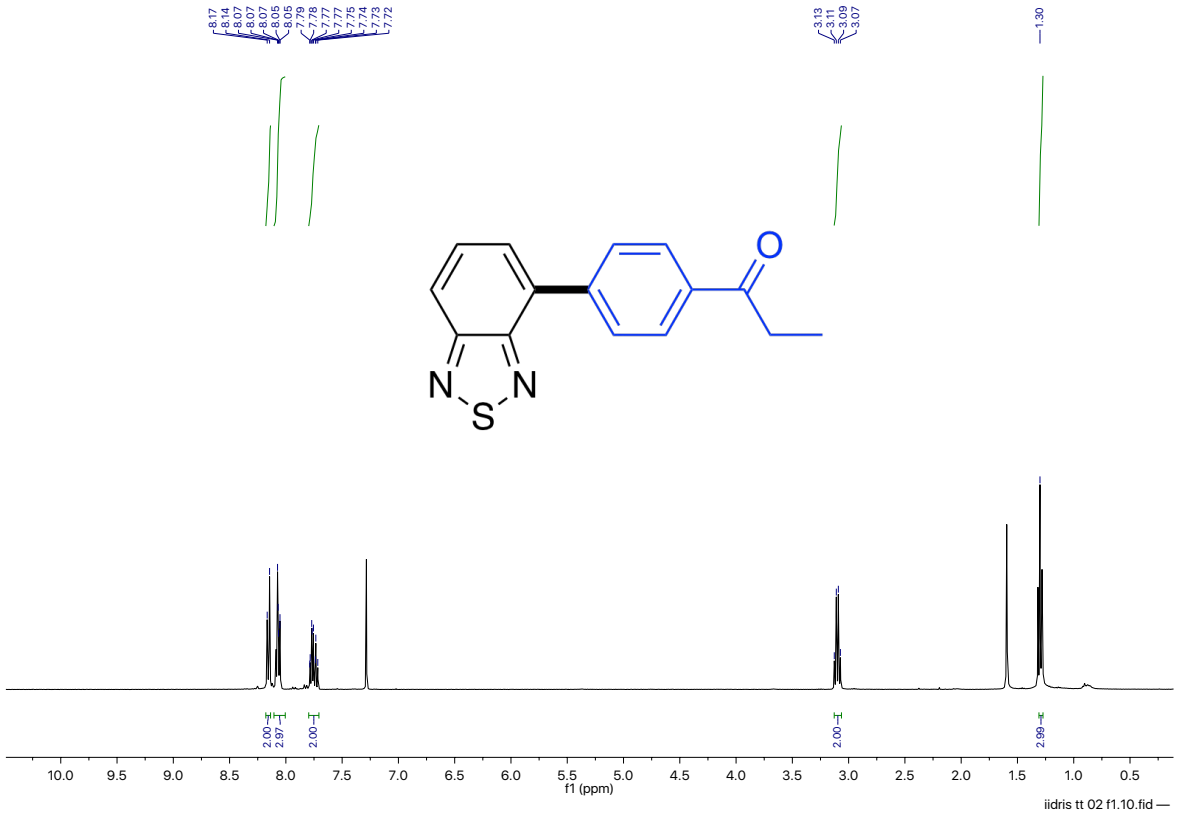
3

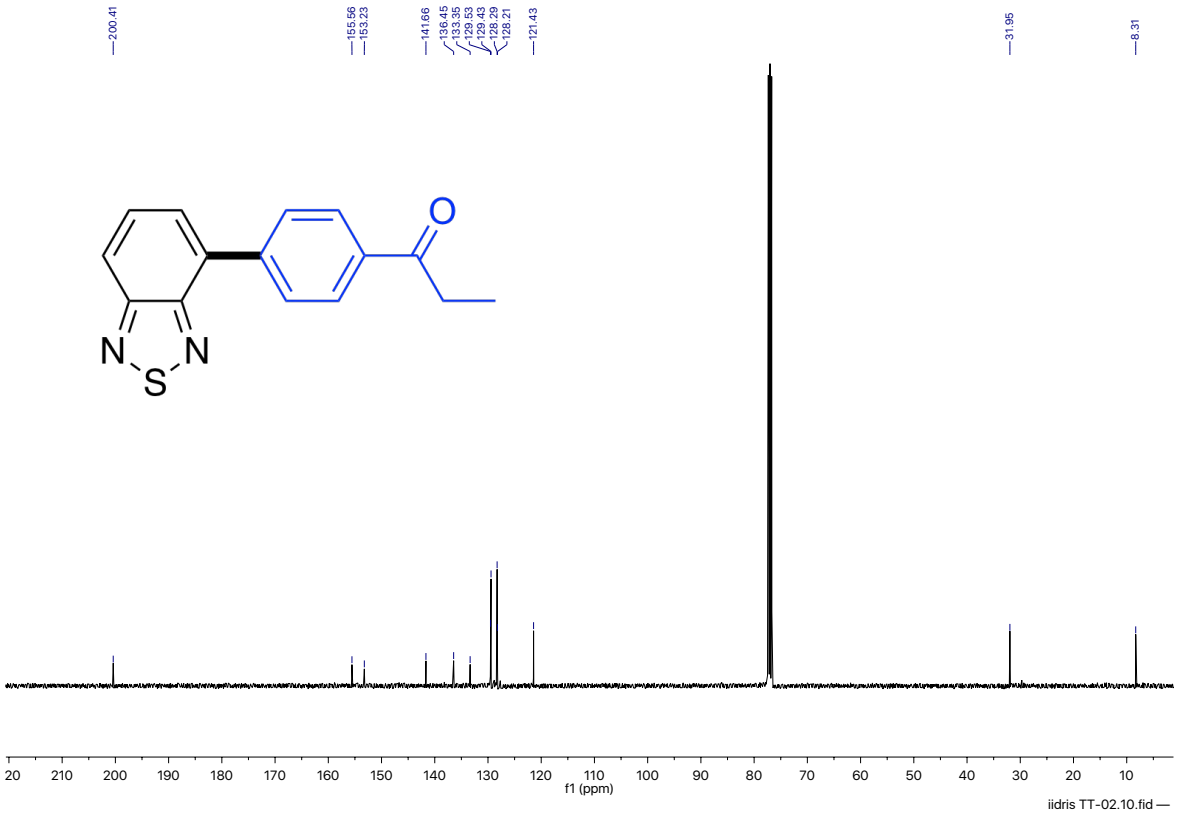

10.14
8.16
8.16
8.14
8.14
8.11
8.11
8.09
8.09
8.08
8.08
8.07
8.06
7.81
7.81
7.79
7.79
7.77
7.75
7.75
7.73
CHO
N
S
N


1.00
1.87
2.82
2.00
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
f1 (ppm)
jsoule II-P606.10.fid

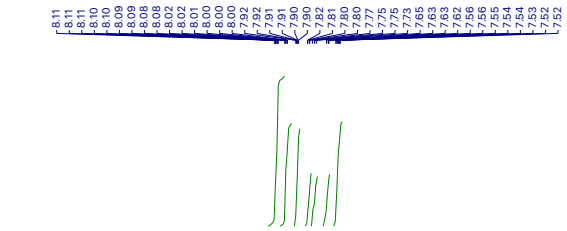

191.87
155.55
153.13
143.25
135.91
133.09
129.94
129.89
129.50
128.47
121.76
CHO
N
S
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
jsoule II-P606.2.fid

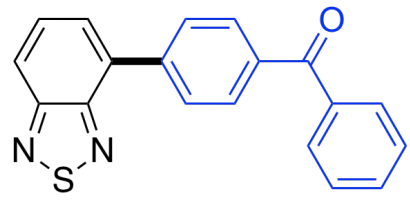
5

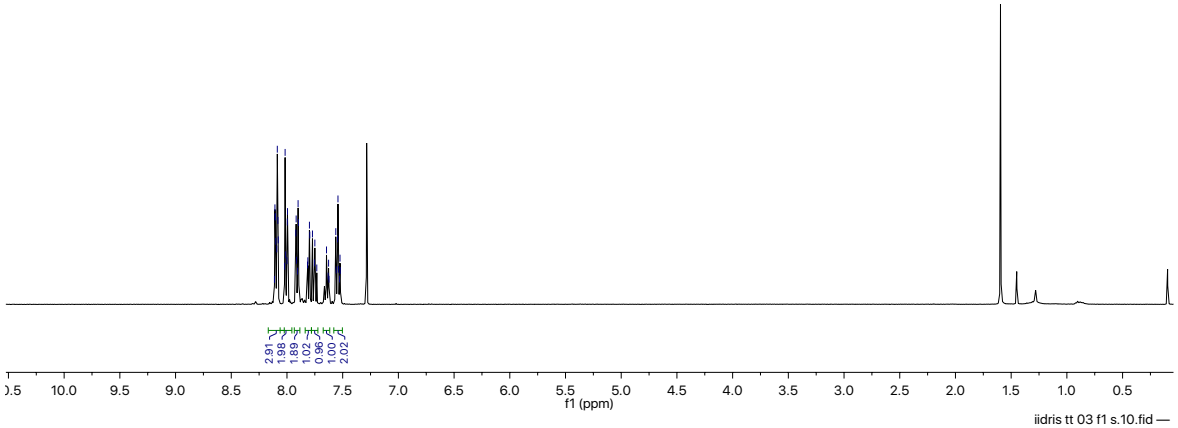

8.17
8.14
8.07
8.07
8.07
8.05
8.05
7.78
7.78
7.77
7.77
7.75
7.74
7.73
7.72
3.13
3.11
3.09
3.07
1.30
O
N
S
N
2.00
2.97
2.00
2.00
2.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
iidris tt 02 f1.10.fid

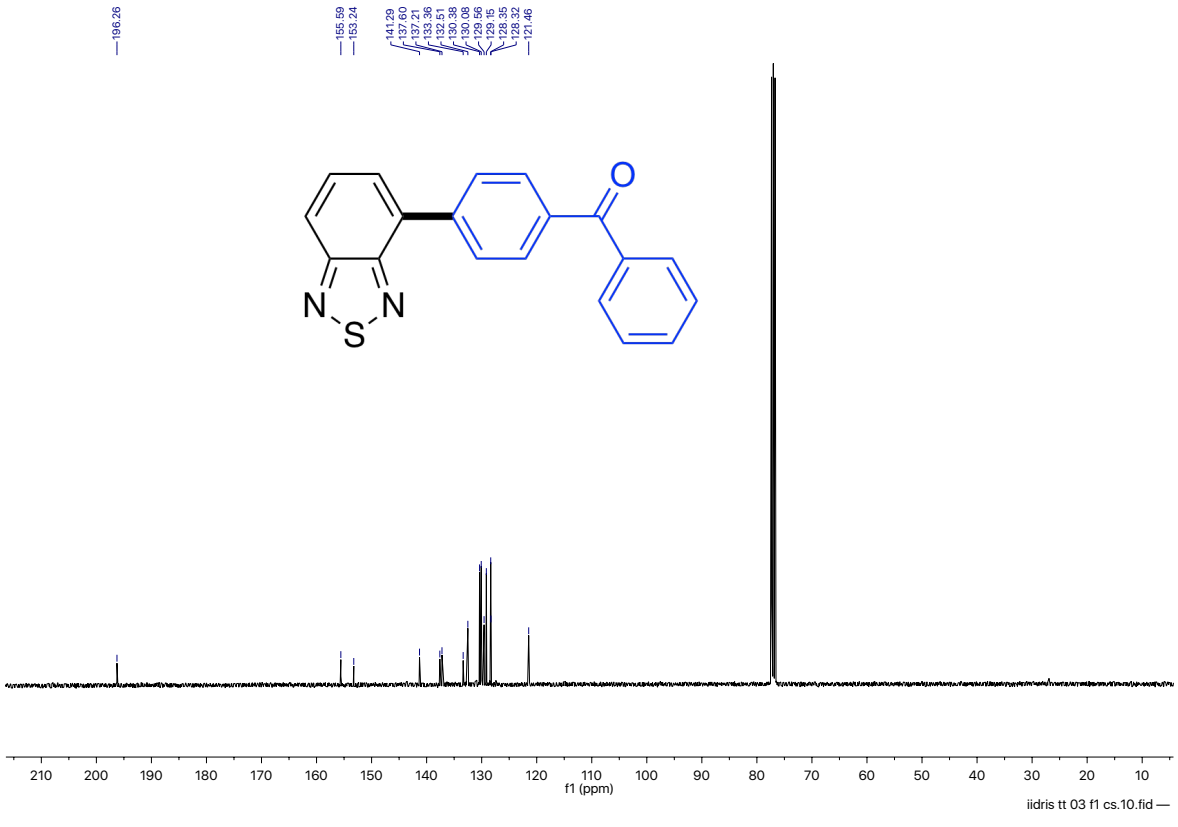

200.41
155.56
153.23
141.66
136.45
133.35
129.53
129.43
128.29
128.21
121.43
31.95
8.31
O
N
S
N
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
iidris TT-02.10.fid

6

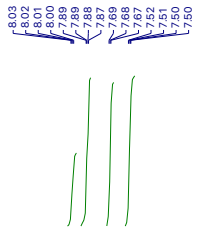

8.11
8.11
8.11
8.10
8.10
8.09
8.09
8.08
8.08
8.02
8.02
8.01
8.00
8.00
8.00
7.92
7.92
7.91
7.91
7.90
7.90
7.82
7.81
7.80
7.80
7.77
7.75
7.75
7.73
7.65
7.63
7.63
7.62
7.56
7.56
7.55
7.54
7.54
7.53
7.52
7.52

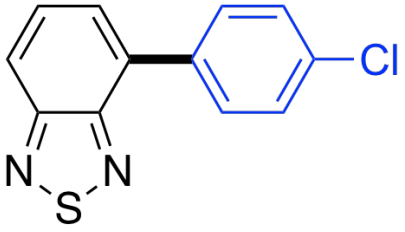

O
N
S
N

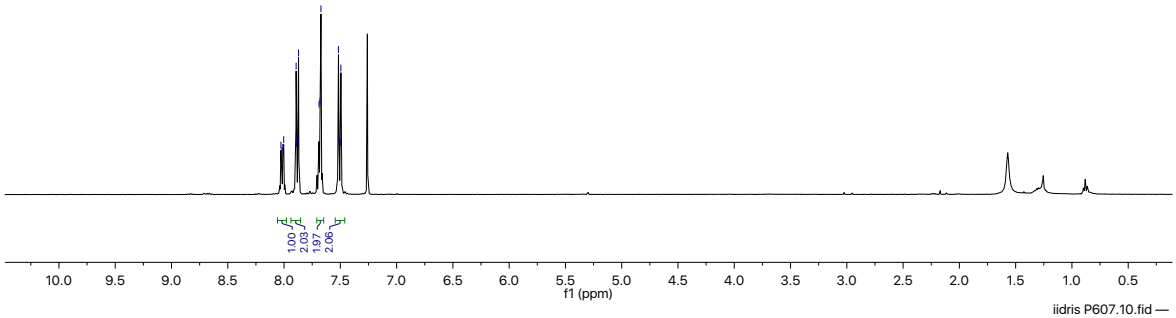

2.91
1.98
1.89
1.02
0.96
1.00
2.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
iidris tt 03 f1 s.10.fid


196.26
155.59
153.24
141.29
137.60
137.21
133.38
133.11
130.38
130.08
129.56
129.15
128.35
128.32
121.46
O
N
S
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
iidris tt 03 f1 cs.10.fid

7

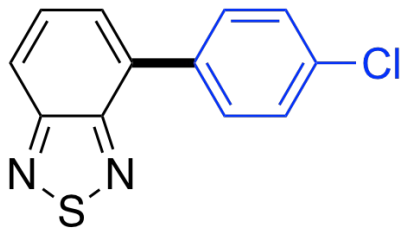

8.03
8.02
8.01
8.00
7.89
7.89
7.88
7.87
7.69
7.68
7.67
7.52
7.51
7.50
7.50


Cl
N
S
N


1.00
2.03
1.97
2.06
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
f1 (ppm)
iidris P607.10.fid

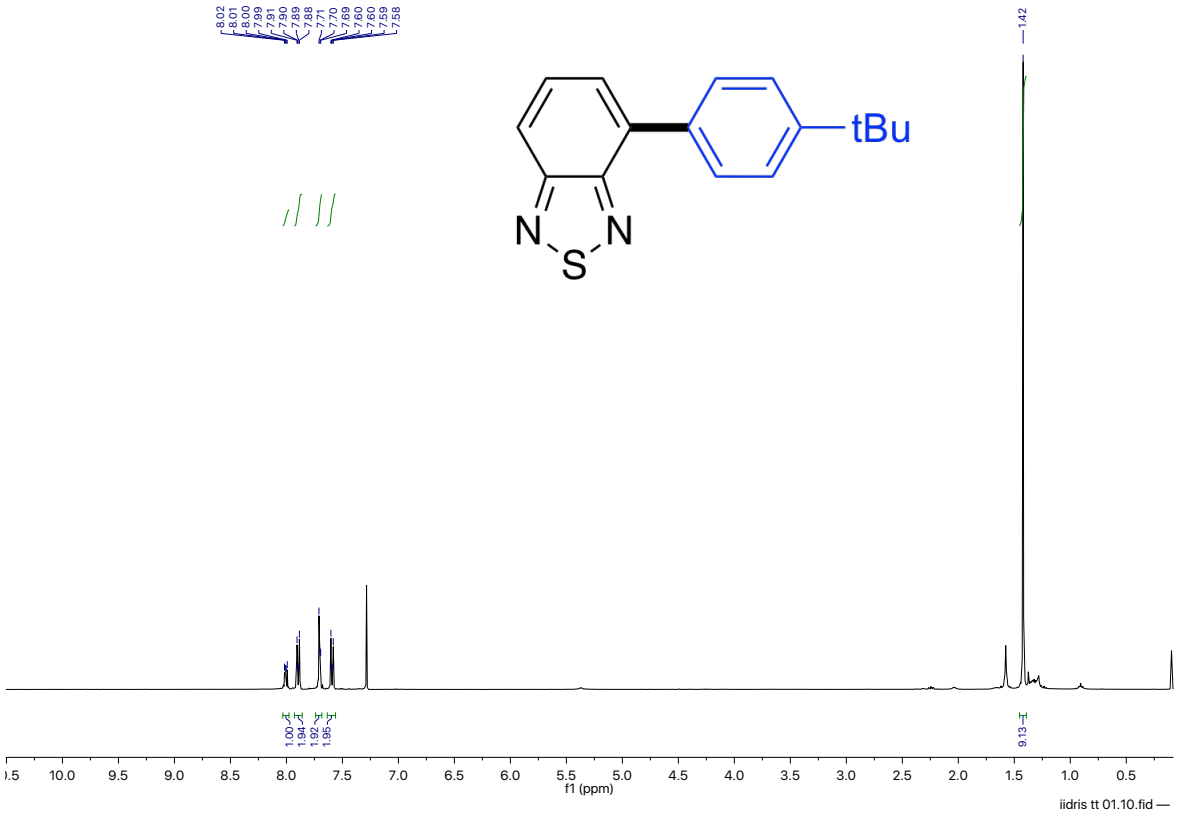

155.56
153.28

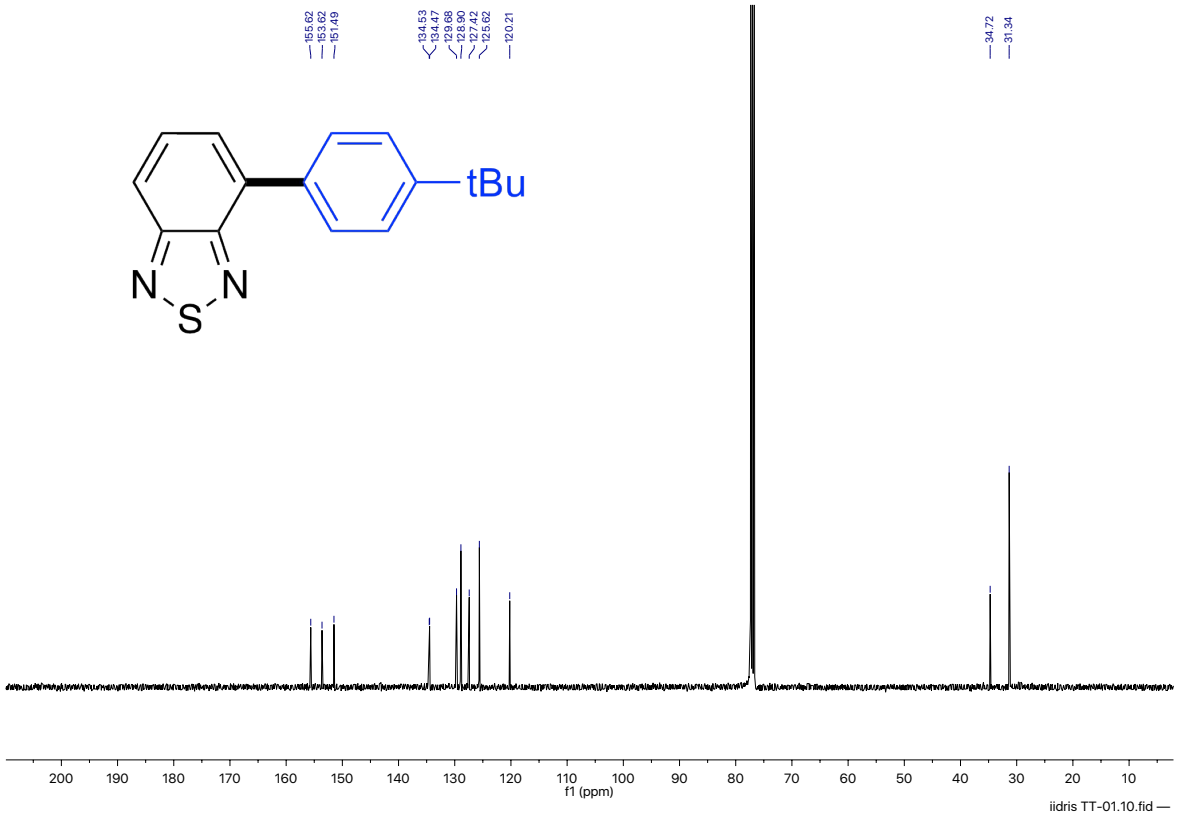
135.71
134.52
133.30
130.50
129.57
128.81
127.65
120.91


Cl
N
S
N

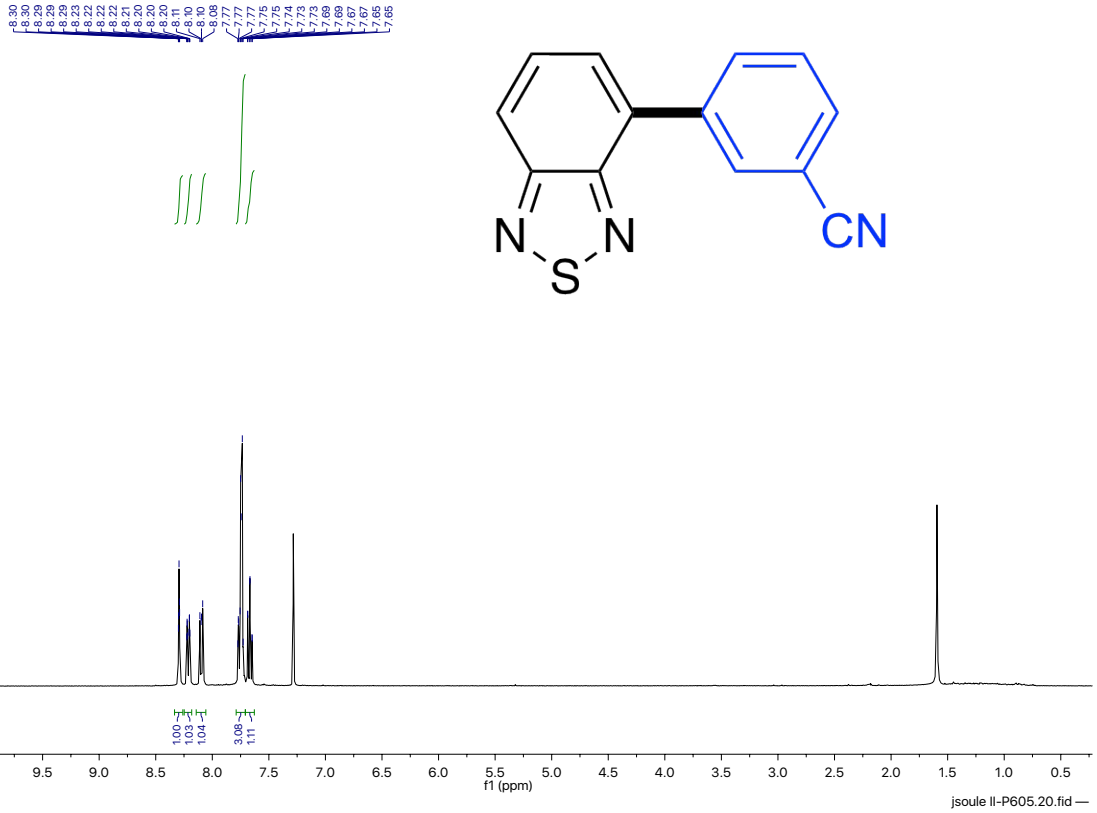
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
iidris P-607.11.fid

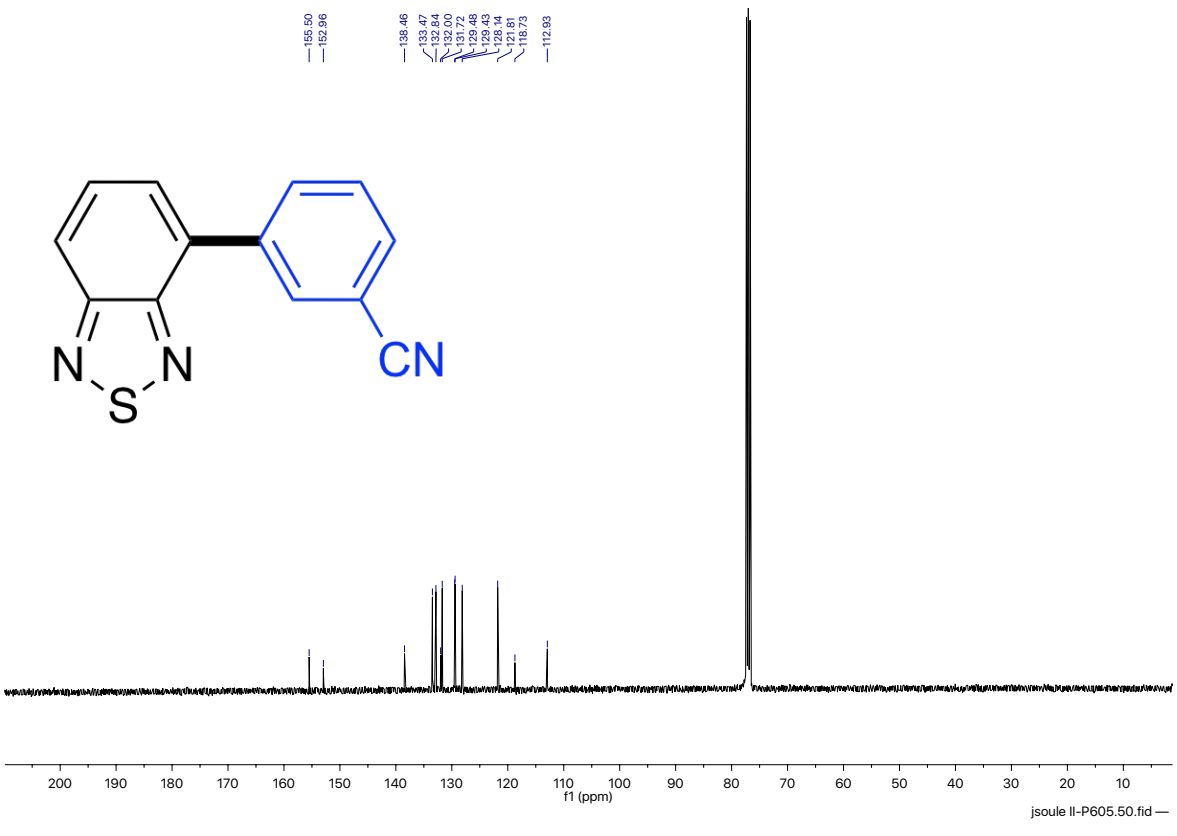
9


8.02
8.01
8.00
7.99
7.91
7.90
7.89
7.88
7.71
7.70
7.69
7.60
7.60
7.59
7.58
1.42
tBu
N
S
N
1.00
1.94
1.92
1.95
9.13
f1 (ppm)
iidris tt 01.10.fid

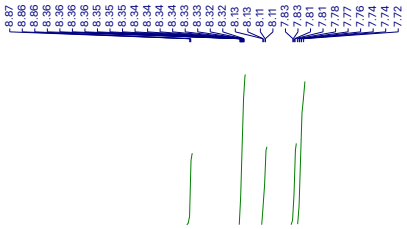

155.62
153.62
151.49
134.53
134.47
129.68
128.90
127.42
125.62
120.21
34.72
31.34
tBu
N
S
N
f1 (ppm)
iidris TT-01.10.fid

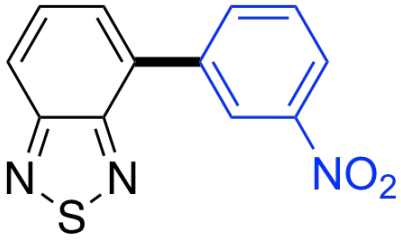
11

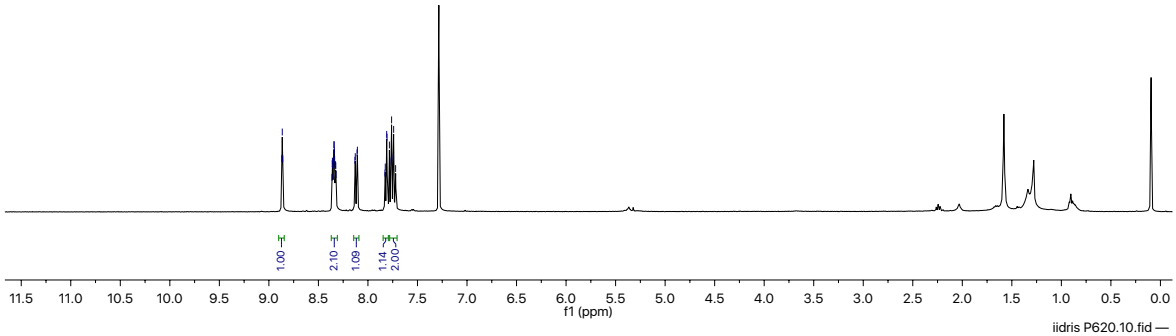

8.30
8.30
8.29
8.29
8.29
8.23
8.22
8.22
8.22
8.21
8.20
8.20
8.20
8.11
8.10
8.10
8.08
7.77
7.77
7.75
7.75
7.74
7.73
7.73
7.69
7.69
7.67
7.67
7.65
7.65
N
S
N
CN
1.00
1.03
1.04
3.08
1.11
f1 (ppm)
jsoule II-P605.20.fid


155.50
152.96
138.46
133.47
132.84
132.00
131.72
129.48
129.43
128.14
121.61
118.73
112.93
N
S
N
CN
f1 (ppm)
jsoule II-P605.50.fid

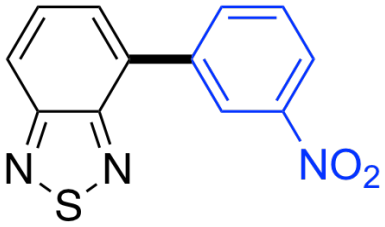
13


8.87
8.86
8.86
8.36
8.36
8.36
8.35
8.35
8.35
8.34
8.34
8.34
8.34
8.33
8.32
8.32
8.13
8.11
7.83
7.83
7.81
7.81
7.78
7.77
7.77
7.76
7.74
7.74
7.72


N
S
N
NO2

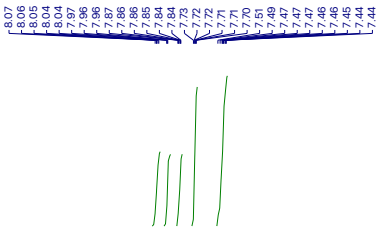

1.00
2.10
1.09
1.14
2.00
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
iidris P620.10.fid —

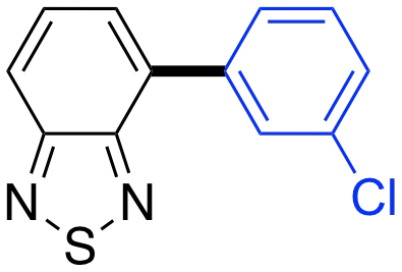

155.52
152.97
148.55
138.83
135.15
131.83
129.53
129.46
128.30
124.13
123.08
121.96

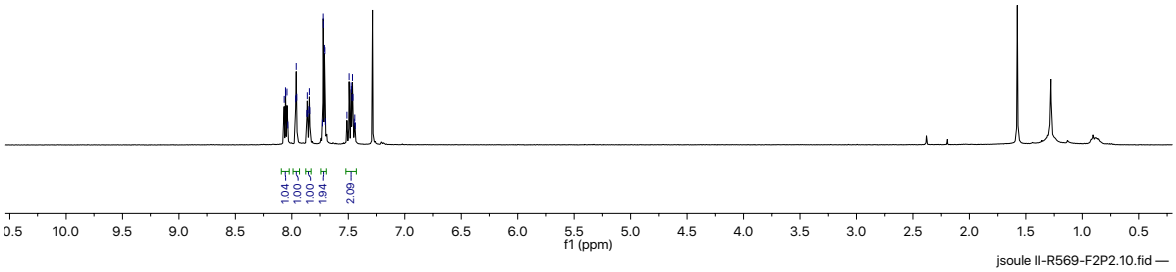

N
S
N
NO2

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
iidris P620.11.fid —

14

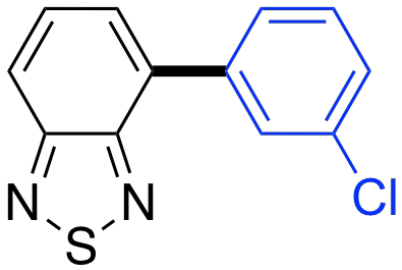

8.07
8.06
8.05
8.04
8.04
7.97
7.96
7.87
7.86
7.86
7.85
7.84
7.84
7.73
7.72
7.72
7.71
7.71
7.70
7.51
7.49
7.47
7.47
7.47
7.47
7.46
7.46
7.45
7.44
7.44


N
S
N
Cl


1.04
1.00
1.00
1.94
2.09
0.5
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
f1 (ppm)
jsoule II-R569-F2P2.10.fid

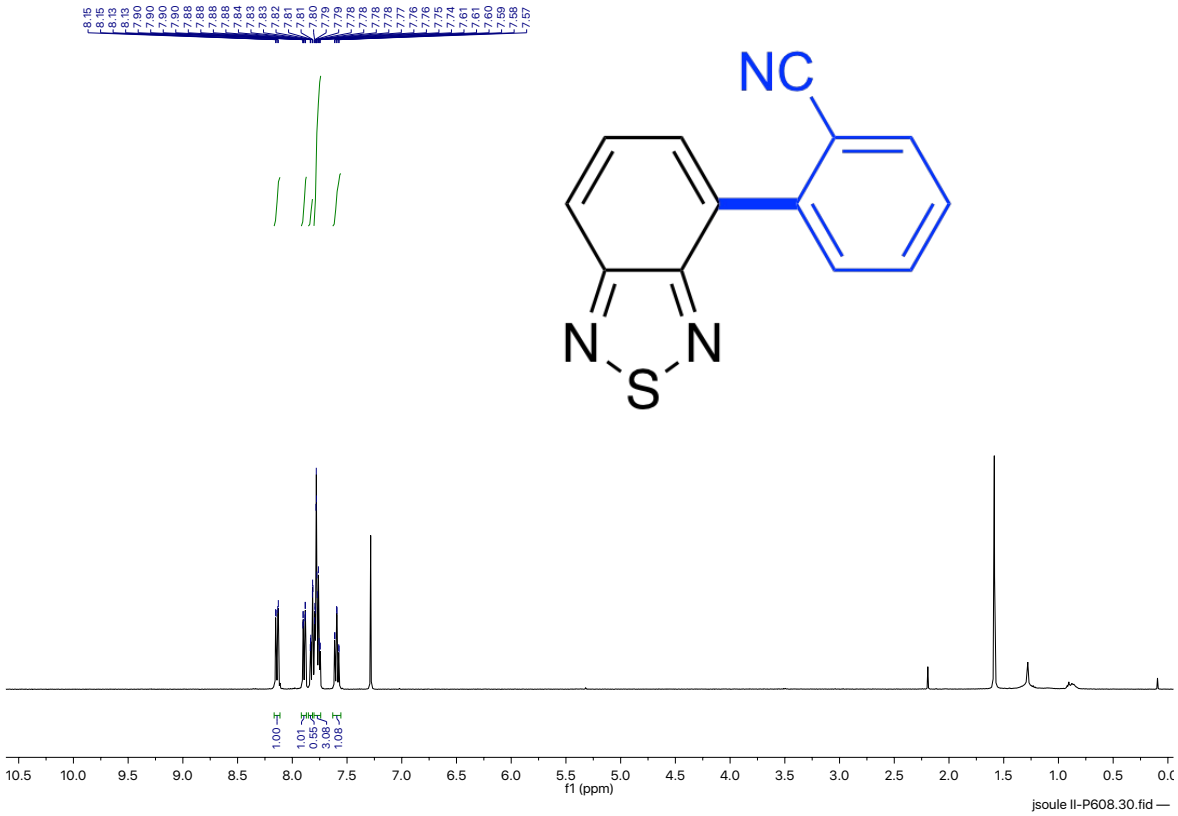

155.53
153.19

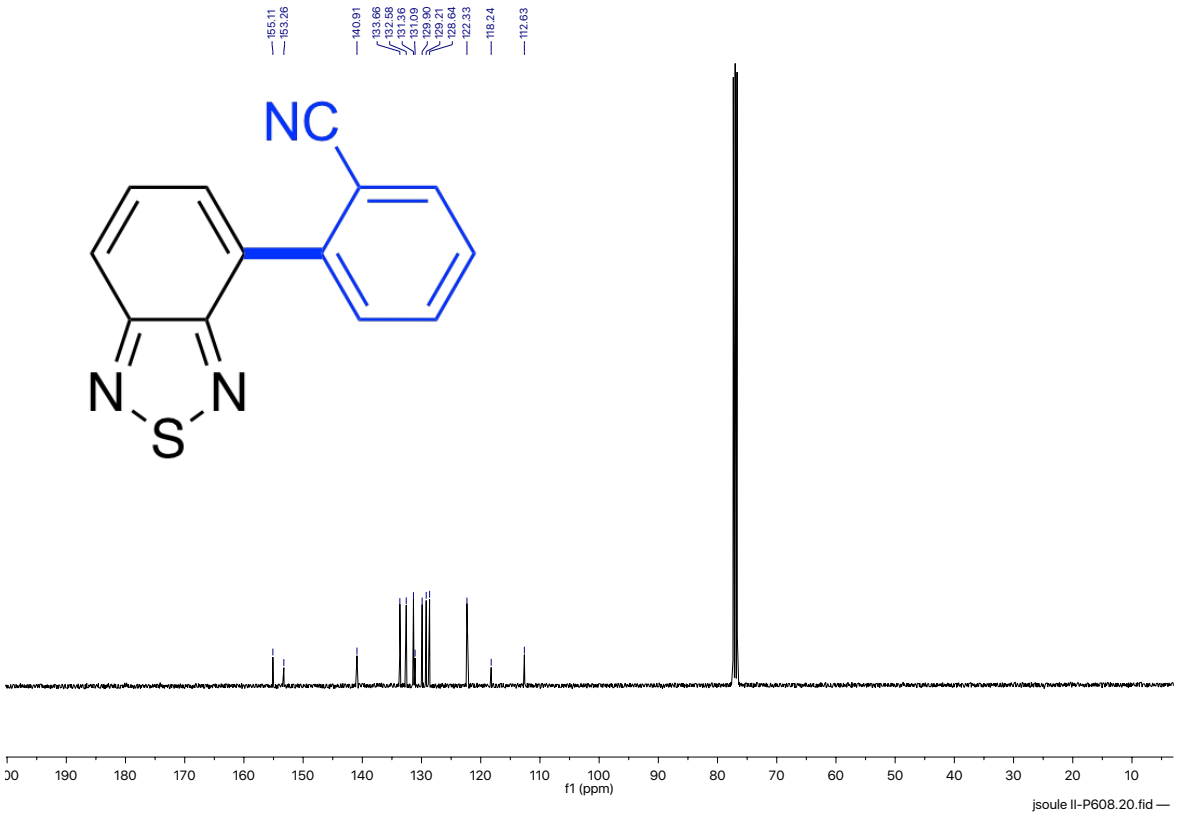
139.02
134.52
133.05
129.80
129.51
129.30
128.42
127.95
127.40
121.19

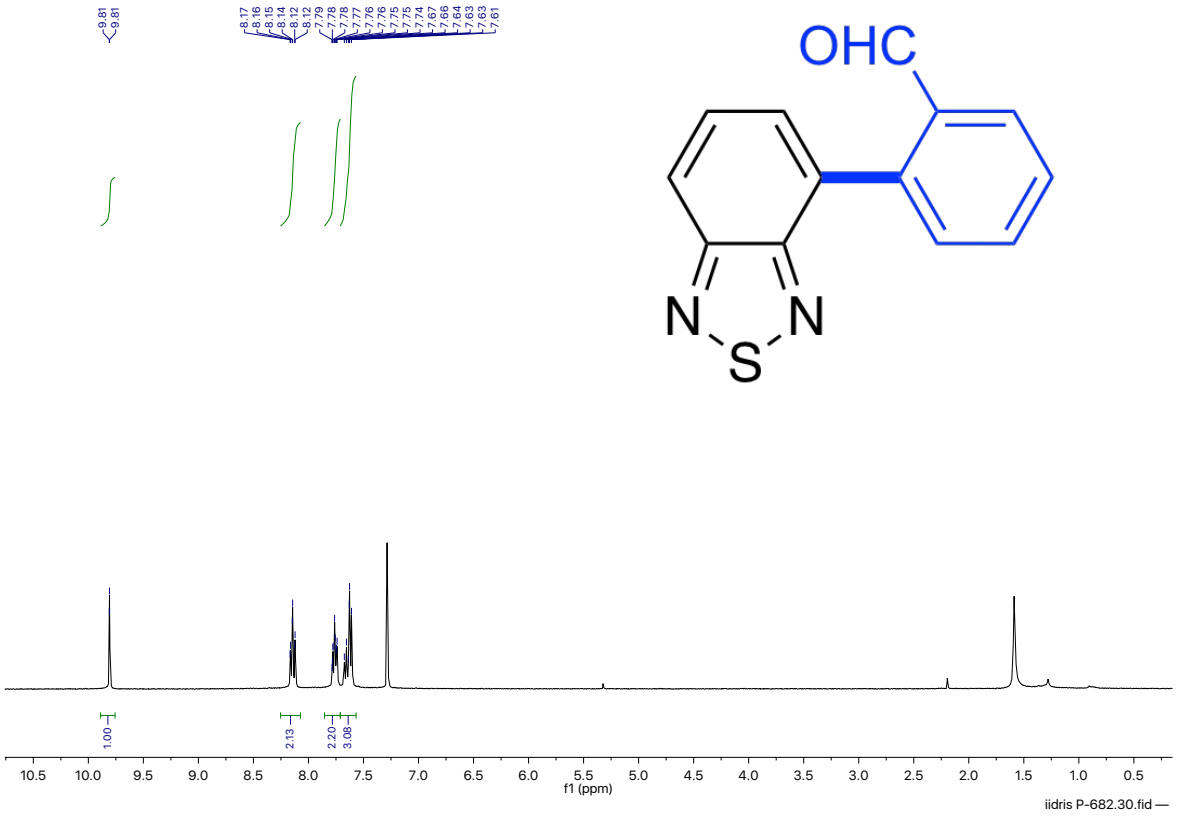

N
S
N
Cl

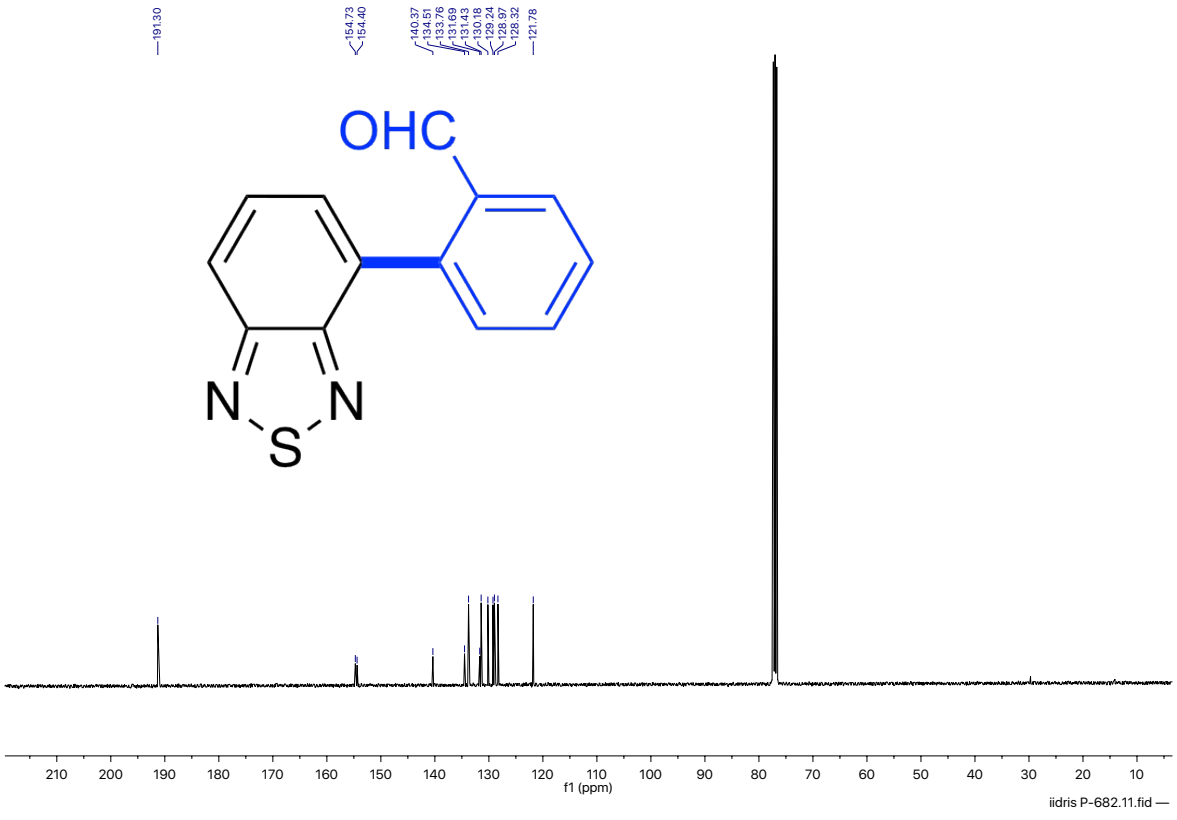
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
jsoule II-P604.10.fid

15

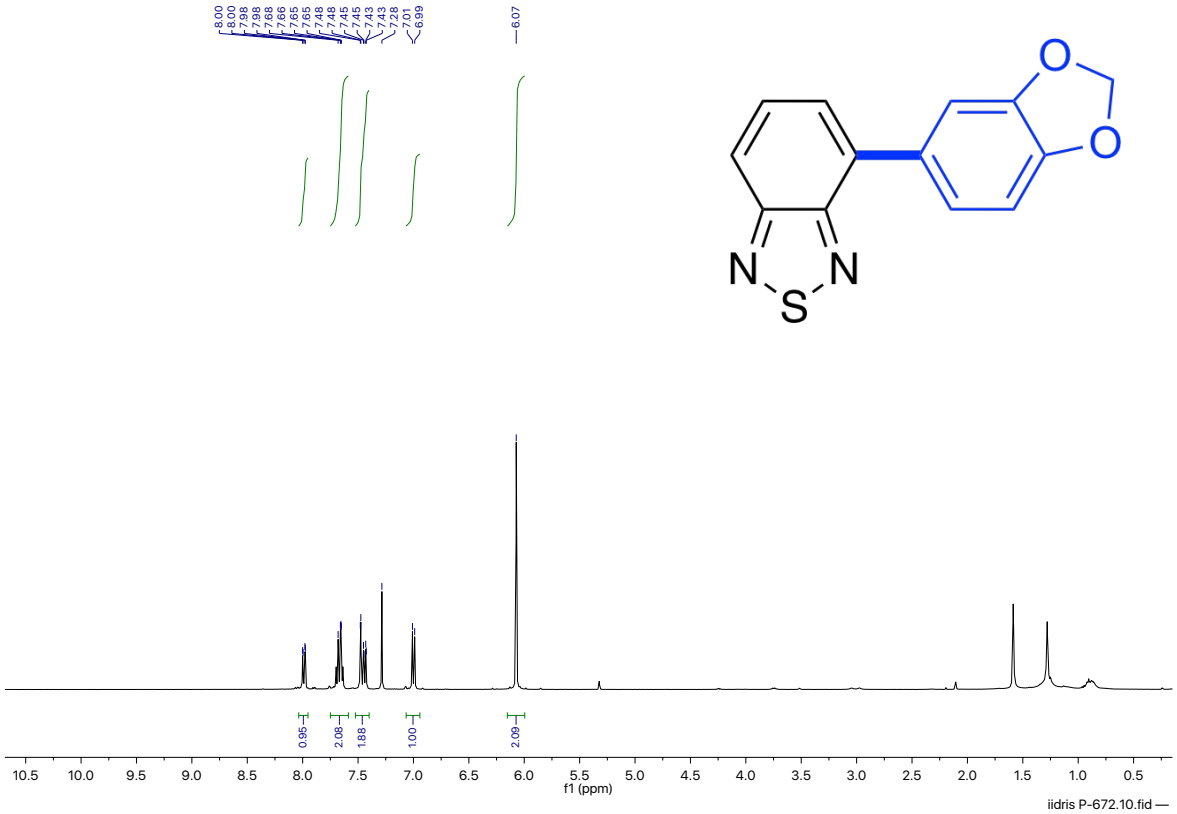

8.15
8.15
8.13
8.13
7.90
7.90
7.90
7.90
7.88
7.88
7.88
7.88
7.84
7.83
7.83
7.82
7.81
7.81
7.80
7.79
7.78
7.78
7.78
7.78
7.77
7.76
7.76
7.75
7.74
7.61
7.61
7.60
7.59
7.58
7.57
NC
N
S
N
1.00
1.01
0.55
3.08
1.08
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
jsoule II-P608.30.fid

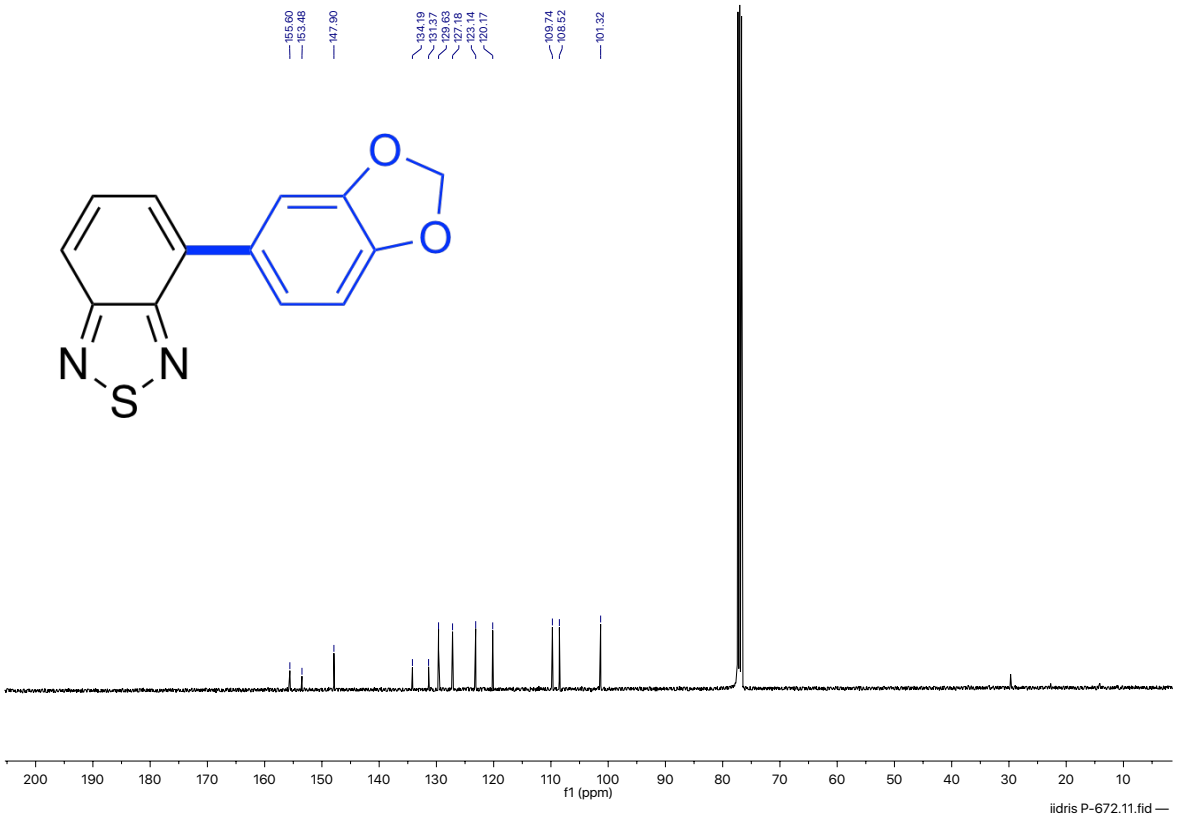

155.11
153.26
140.91
133.66
132.58
131.36
131.09
130.90
129.21
128.64
122.33
118.24
112.63
NC
N
S
N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
jsoule II-P608.20.fid


9.81
9.81
8.17
8.16
8.15
8.14
8.12
8.12
7.79
7.78
7.78
7.77
7.76
7.75
7.75
7.74
7.67
7.66
7.64
7.63
7.63
7.61
OHC
N
S
N
1.00
2.13
2.20
3.08
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
f1 (ppm)
iidris P-682.30.fid

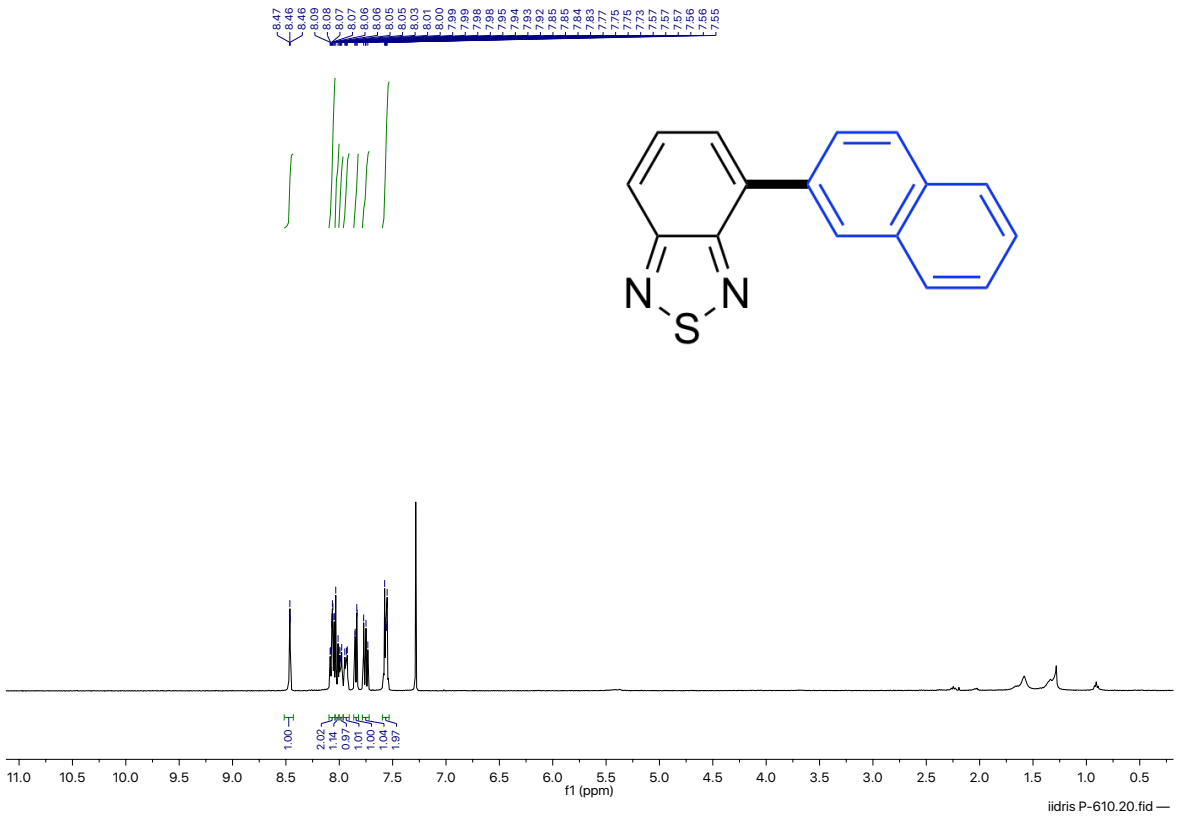

191.30
154.73
154.40
140.37
134.51
133.76
131.69
131.43
130.18
129.24
128.97
128.32
121.78
OHC
N
S
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
iidris P-682.11.fid

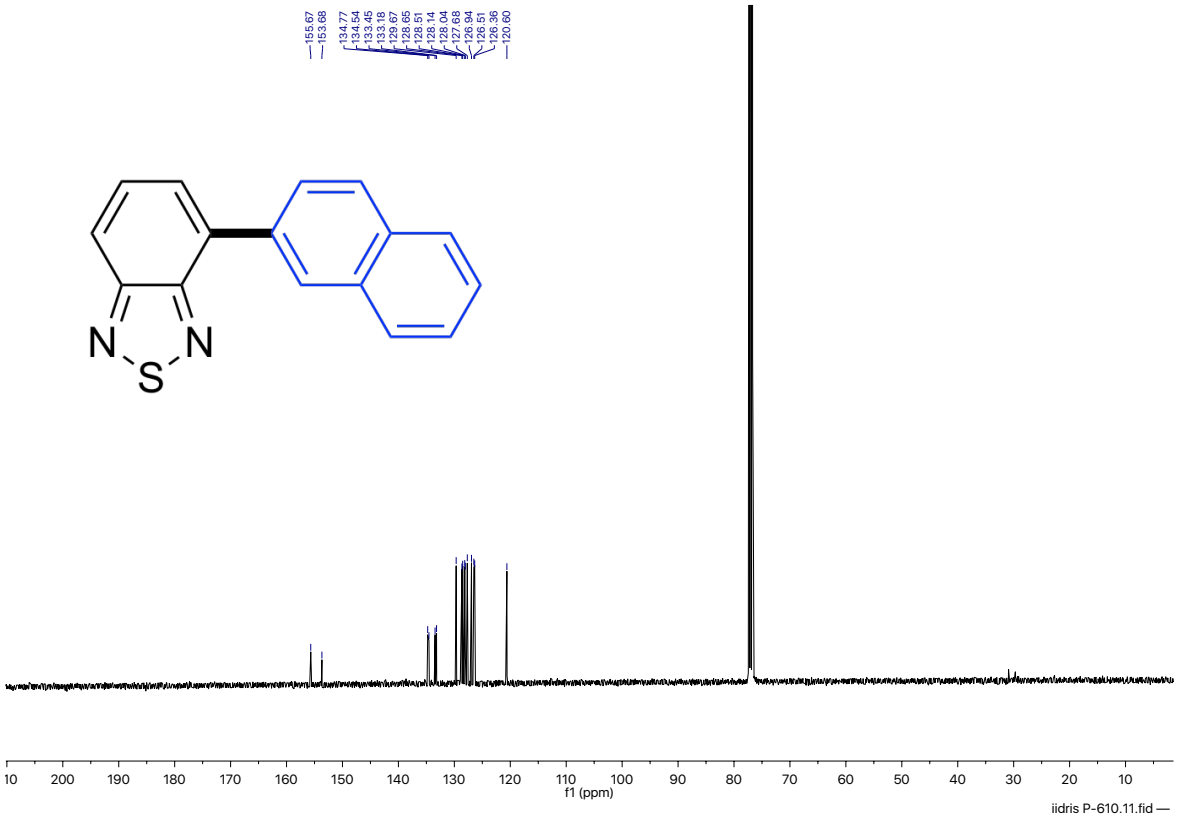
17


8.00
8.00
7.98
7.98
7.68
7.66
7.65
7.65
7.48
7.48
7.45
7.45
7.43
7.43
7.28
7.01
6.99
6.07
O
O
N
S
N
0.95
2.08
1.88
1.00
2.09
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
f1 (ppm)
iidris P-672.10.fid

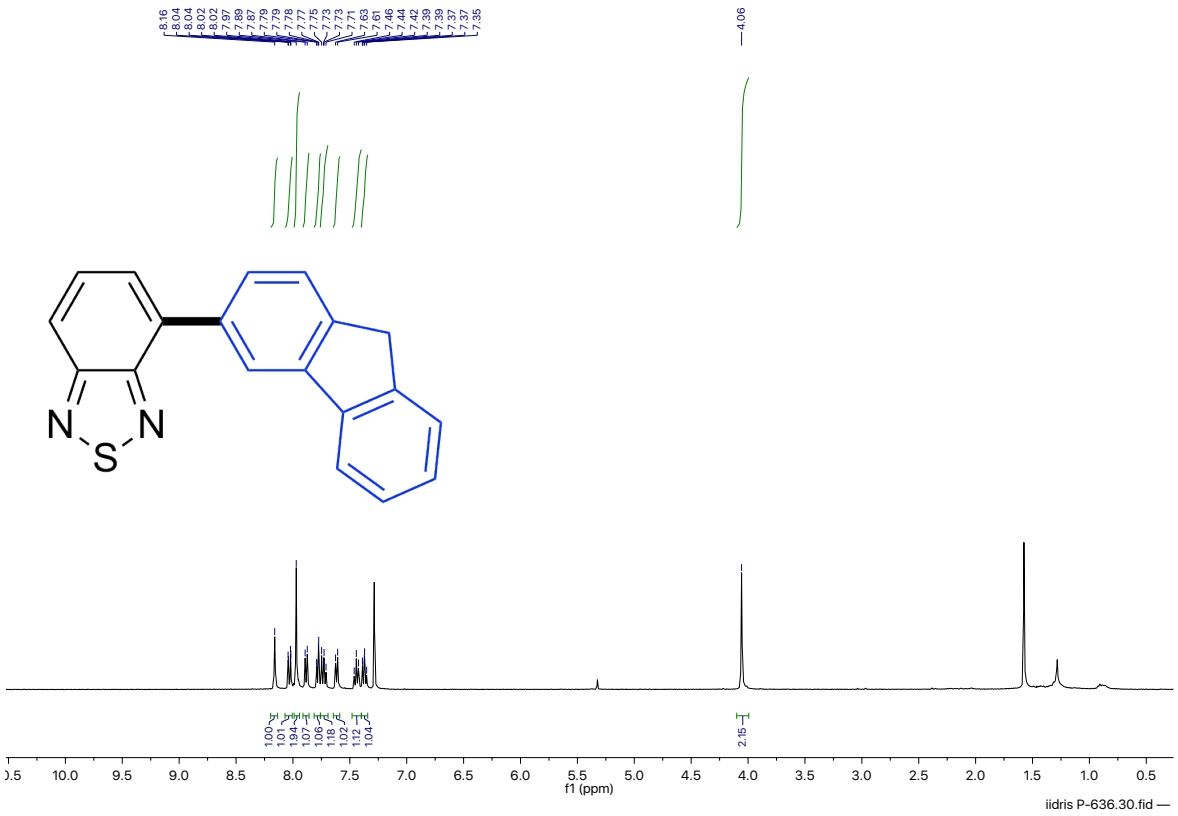

155.60
153.48
147.90
134.19
131.37
129.63
127.18
123.14
120.17
109.74
108.52
101.32
O
O
N
S
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)
iidris P-672.11.fid

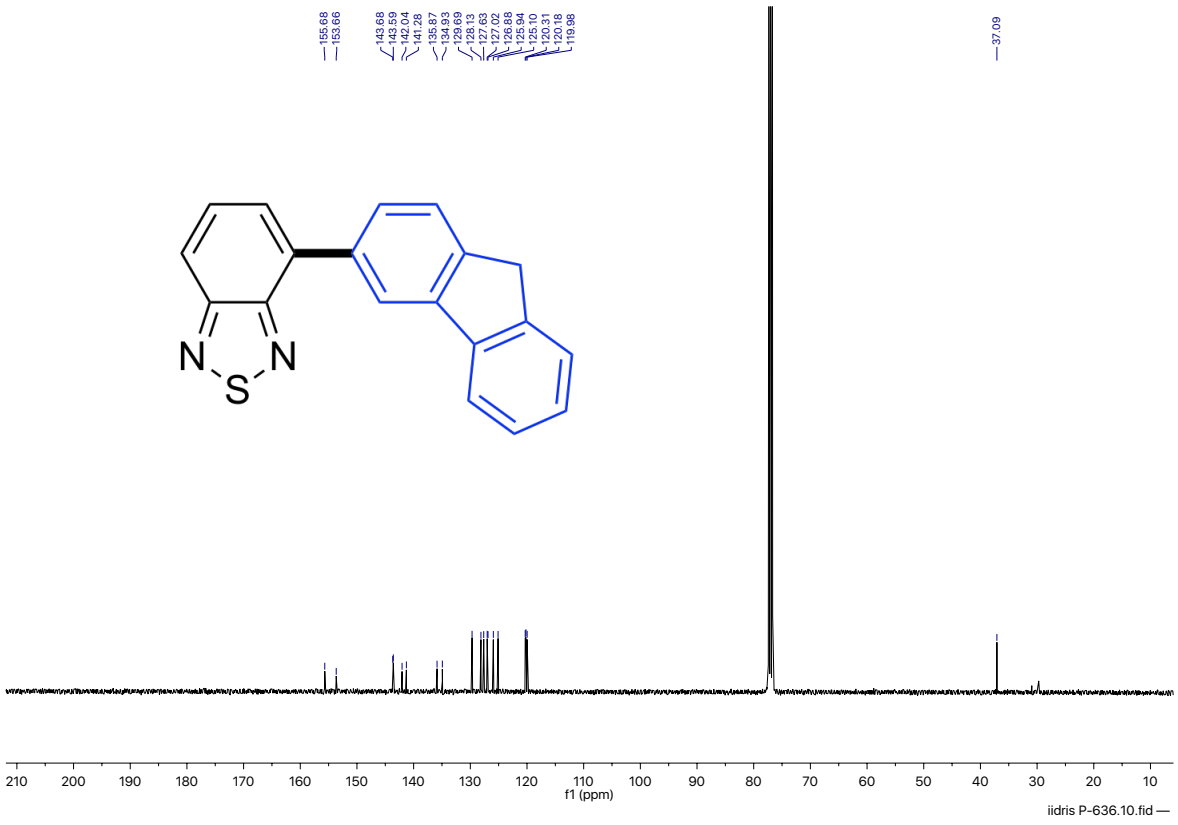
18


8.47
8.46
8.46
8.08
8.08
8.07
8.07
8.06
8.06
8.06
8.05
8.05
8.03
8.01
8.00
7.99
7.99
7.98
7.98
7.95
7.94
7.93
7.92
7.85
7.84
7.83
7.77
7.75
7.75
7.73
7.57
7.57
7.57
7.56
7.56
7.55
N
S
N
1.00
2.02
1.14
0.97
1.01
1.00
1.04
1.97
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
f1 (ppm)
iidris P-610.20.fid

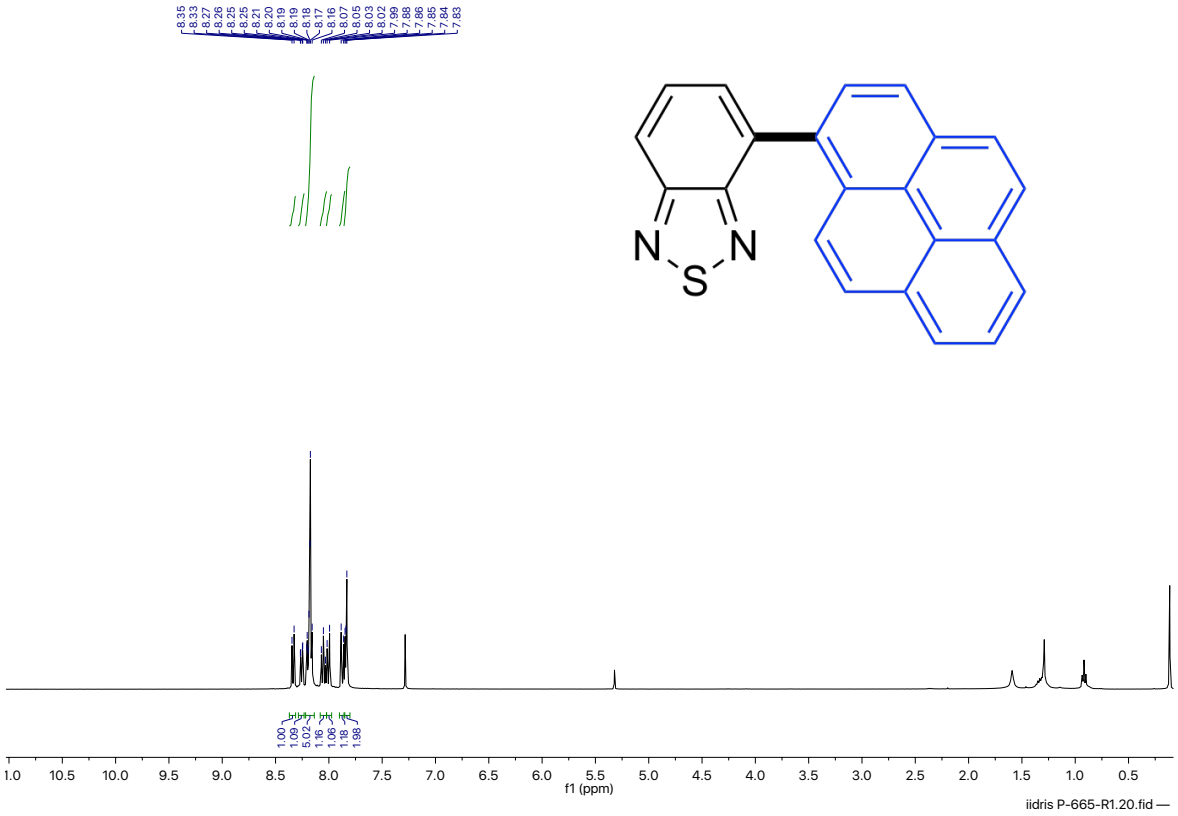

155.67
153.68
134.77
134.54
133.45
133.18
129.67
128.65
128.51
128.14
128.04
127.68
126.84
126.51
126.36
120.60
N
S
N
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
iidris P-610.11.fid

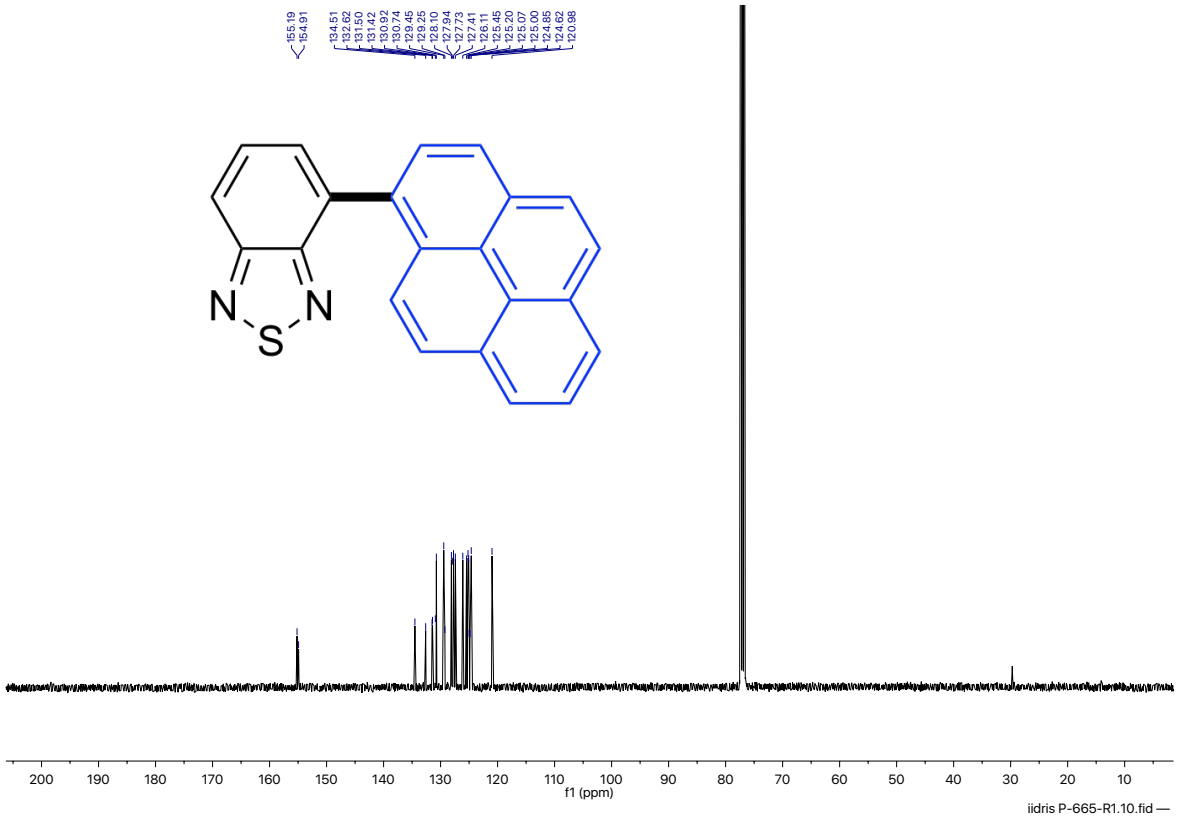
19


8.16
8.04
8.04
8.02
8.02
7.97
7.89
7.87
7.79
7.79
7.78
7.77
7.75
7.73
7.73
7.71
7.63
7.61
7.46
7.44
7.42
7.39
7.39
7.37
7.37
7.35
4.06
N
S
N
1.00
1.01
1.94
1.07
1.06
1.18
1.02
1.12
1.04
2.15
f1 (ppm)
iidris P-636.30.fid

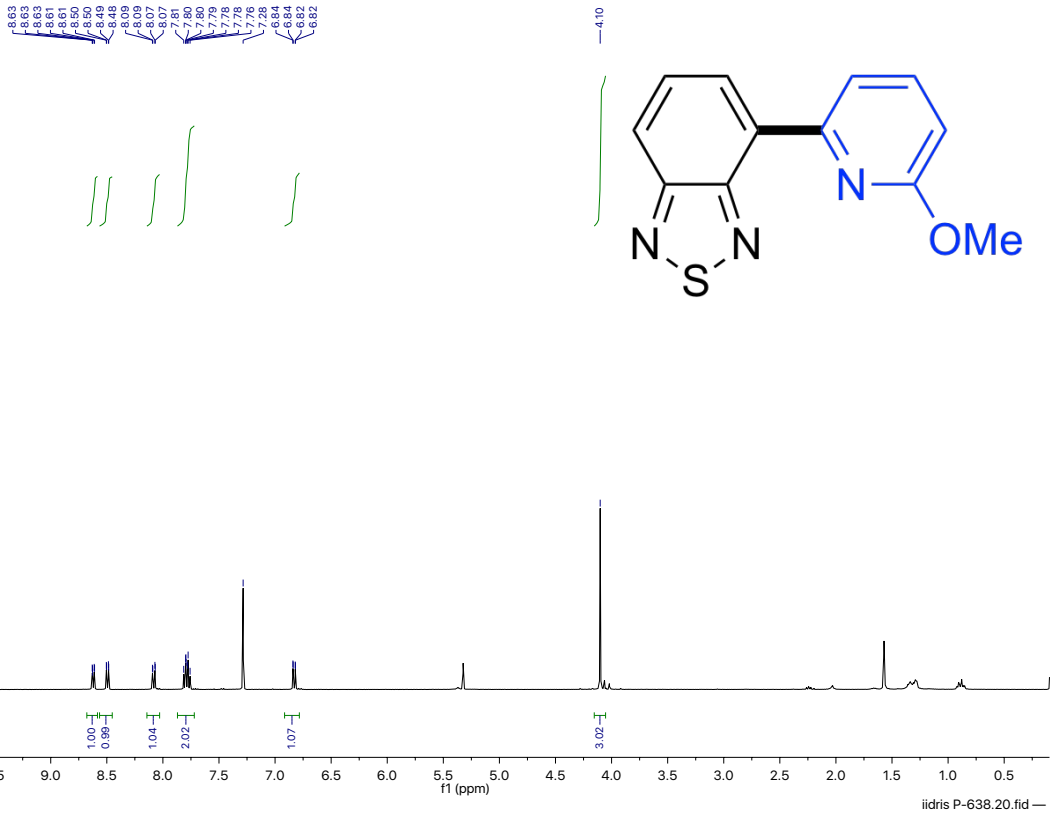

155.68
153.66
143.68
143.59
142.04
141.28
135.87
134.93
129.69
128.13
127.63
127.02
126.88
125.94
125.10
120.31
120.18
119.98
37.09
N
S
N
f1 (ppm)
iidris P-636.10.fid

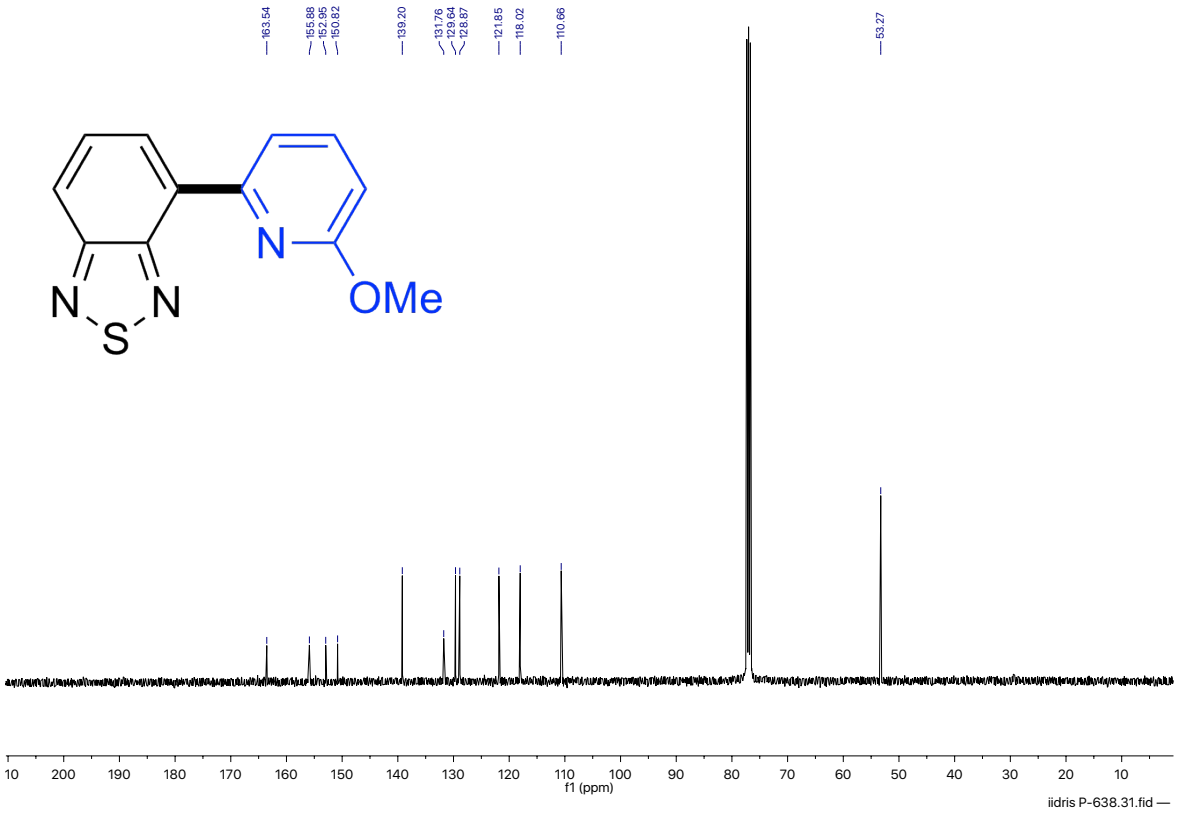
20

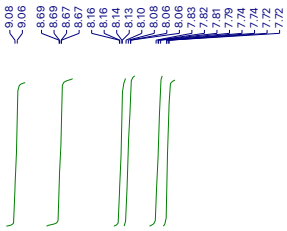

8.35
8.33
8.27
8.26
8.25
8.25
8.21
8.20
8.19
8.19
8.18
8.17
8.16
8.07
8.05
8.03
8.02
7.99
7.88
7.86
7.85
7.84
7.83
N
S
N
1.00
1.09
5.02
1.16
1.06
1.18
1.98
f1 (ppm)
iidris P-665-R1.20.fid

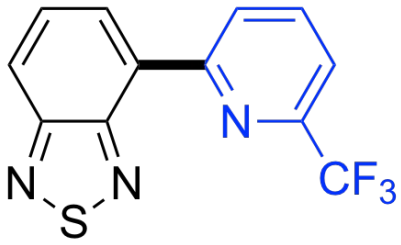

155.19
154.91
134.51
132.62
131.50
131.42
131.32
130.92
130.74
129.45
129.25
128.10
127.94
127.73
127.41
126.11
125.45
125.20
125.07
125.00
124.85
124.62
120.98
N
S
N
f1 (ppm)
iidris P-665-R1.10.fid

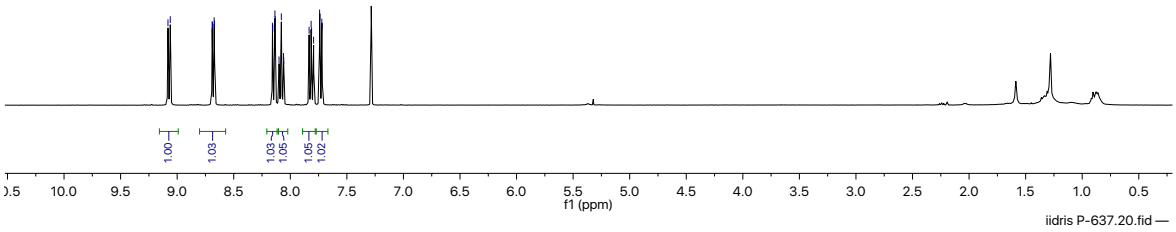
21


8.63
8.63
8.63
8.61
8.61
8.50
8.50
8.49
8.48
8.09
8.09
8.07
8.07
7.81
7.80
7.80
7.79
7.78
7.78
7.76
7.76
7.28
6.84
6.84
6.82
6.82
4.10
N
N
S
N
OMe
1.00
0.99
1.04
2.02
1.07
3.02
f1 (ppm)
iidris P-638.20.fid

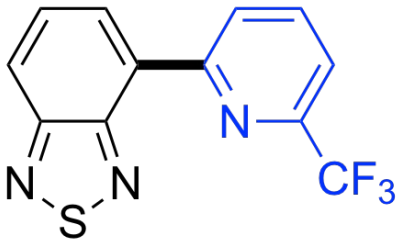

163.54
155.88
152.95
150.82
139.20
131.76
129.64
128.87
121.85
118.02
110.66
53.27
N
N
S
N
OMe
f1 (ppm)
iidris P-638.31.fid


9.08
9.06
8.69
8.69
8.67
8.67
8.16
8.16
8.14
8.13
8.10
8.08
8.06
8.06
7.83
7.82
7.81
7.79
7.74
7.74
7.72
7.72


N
N
S
N
CF3


1.00
1.03
1.03
1.05
1.05
1.02
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
f1 (ppm)
iidris P-637.20.fid

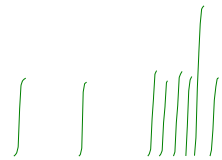

155.76
154.23
152.73
148.31
147.97
138.02
130.29
130.18
130.13
129.75
127.38
122.96
122.90
120.17
119.37
119.34
119.31
119.28

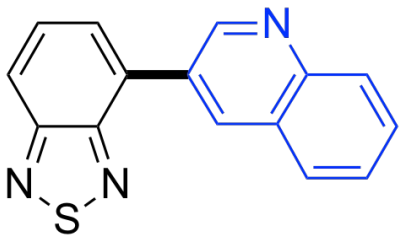

N
N
S
N
CF3

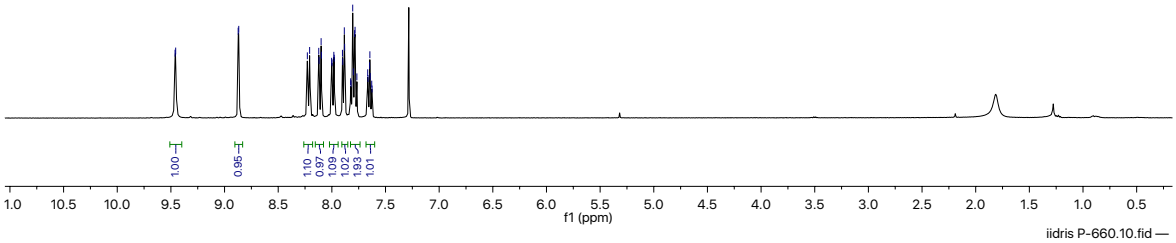
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
iidris P-637.10.fid

23

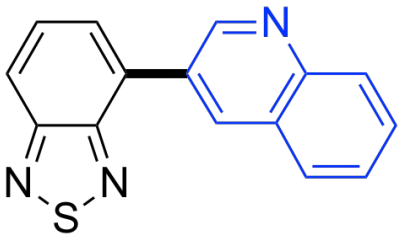

9.46
9.46
8.87
8.87
8.23
8.23
8.21
8.12
8.12
8.10
8.10
8.00
8.00
7.98
7.98
7.90
7.90
7.88
7.88
7.82
7.82
7.81
7.80
7.79
7.78
7.77
7.67
7.66
7.65
7.65
7.64
7.63
7.63




N
N
S
N

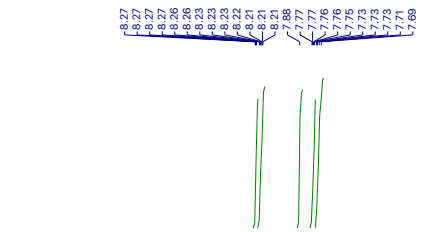

1.00
0.95
1.10
0.97
1.09
1.02
1.93
1.01
1.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
iidris P-660.10.fid —


155.61
155.43
150.58
147.62
136.31
131.13
130.14
130.02
129.62
129.23
128.39
128.14
127.79
127.13
121.47

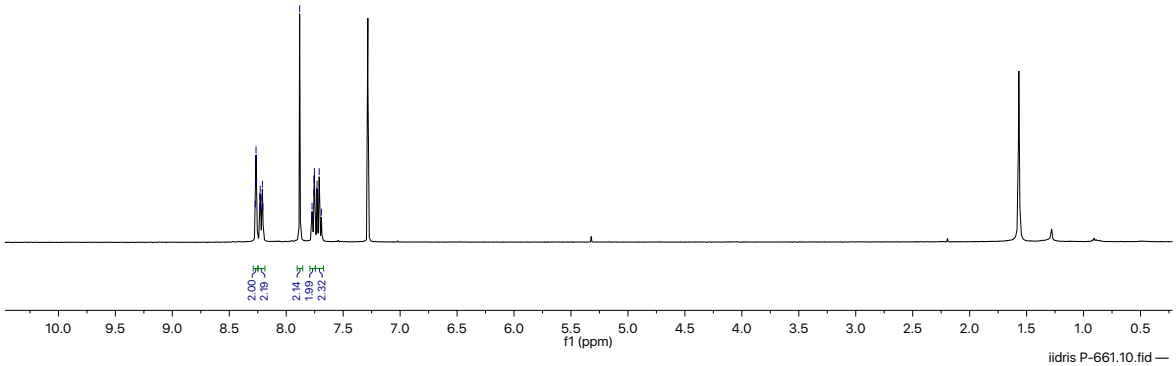

N
N
S
N

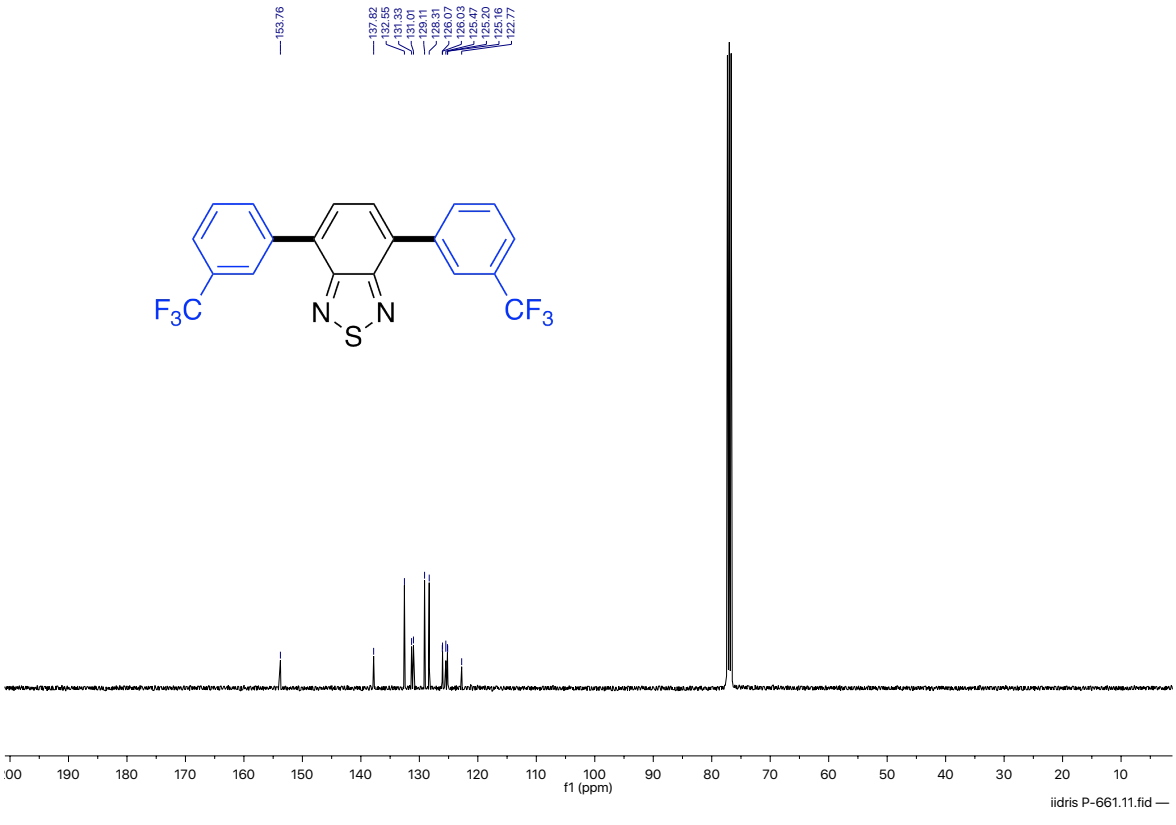
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
iidris P-660.11.fid —

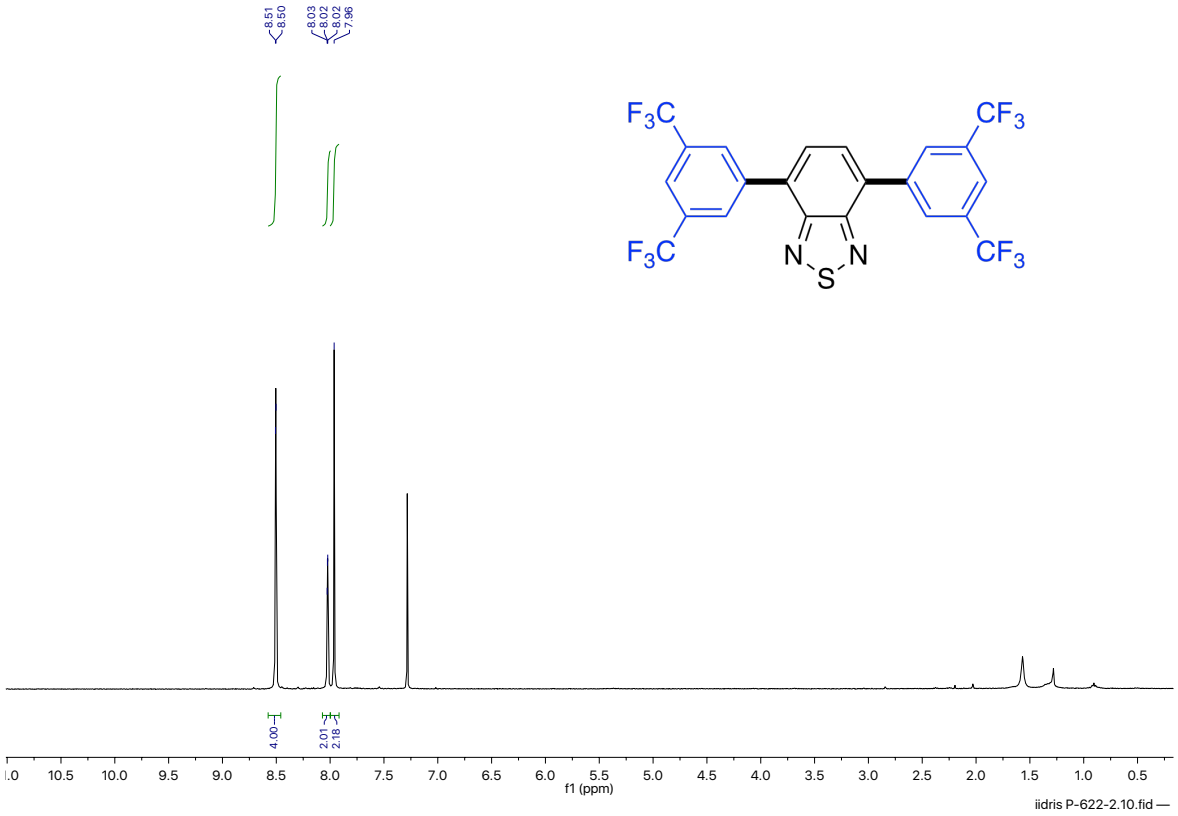
25

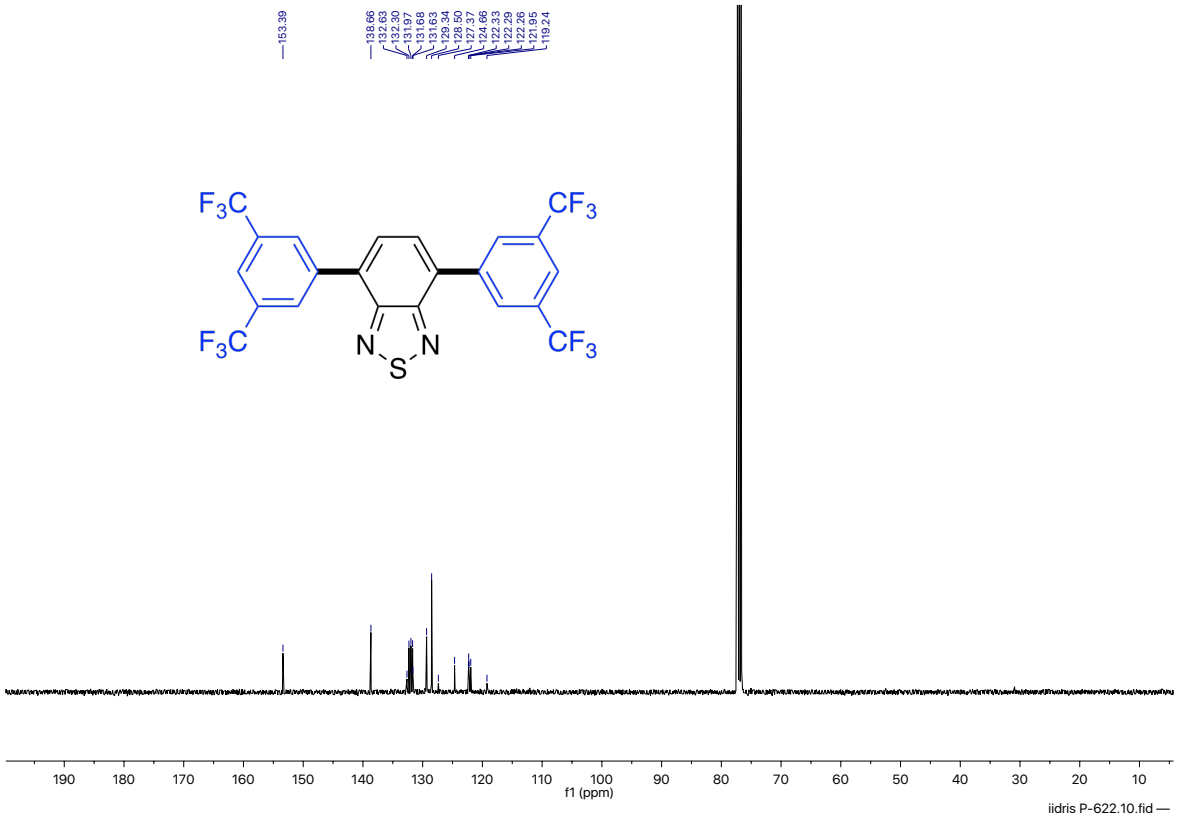

8.27
8.27
8.27
8.27
8.26
8.26
8.23
8.23
8.23
8.22
8.21
8.21
8.21
7.88
7.77
7.77
7.76
7.76
7.75
7.73
7.73
7.71
7.69

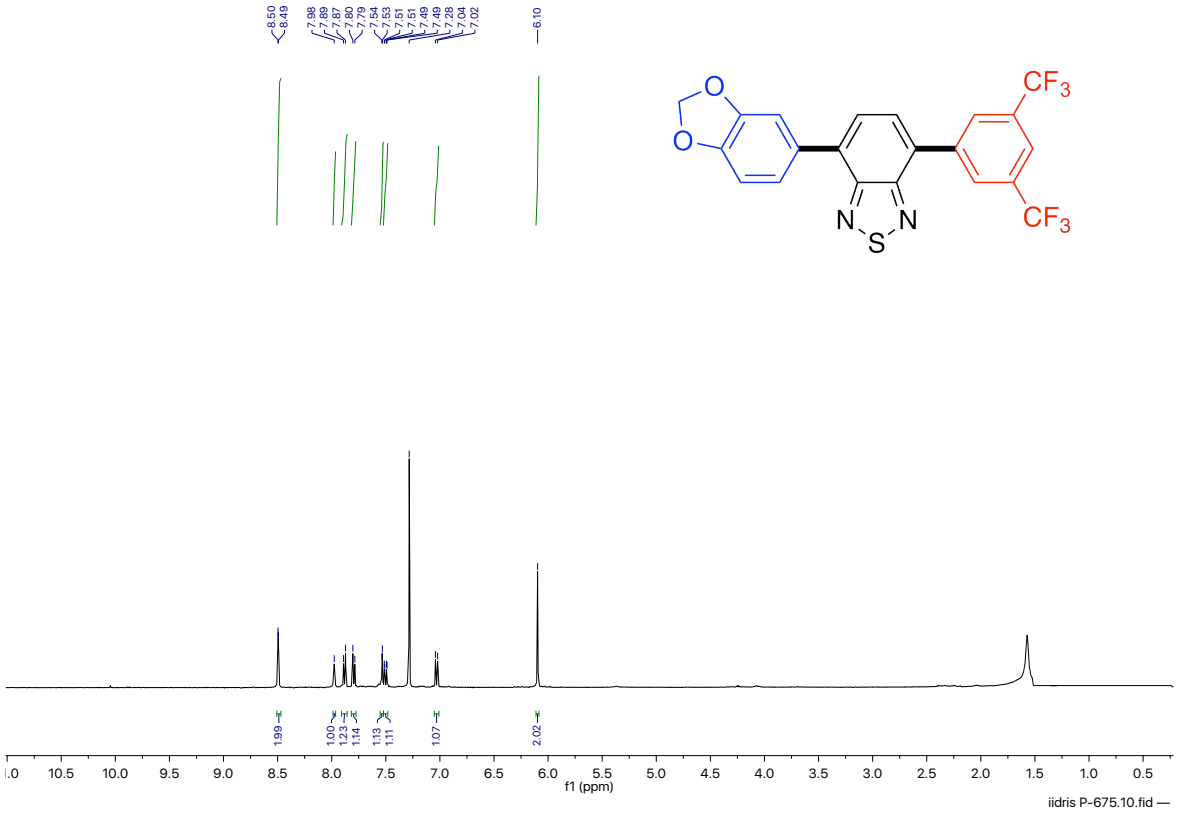

F3C
N
S
N
CF3

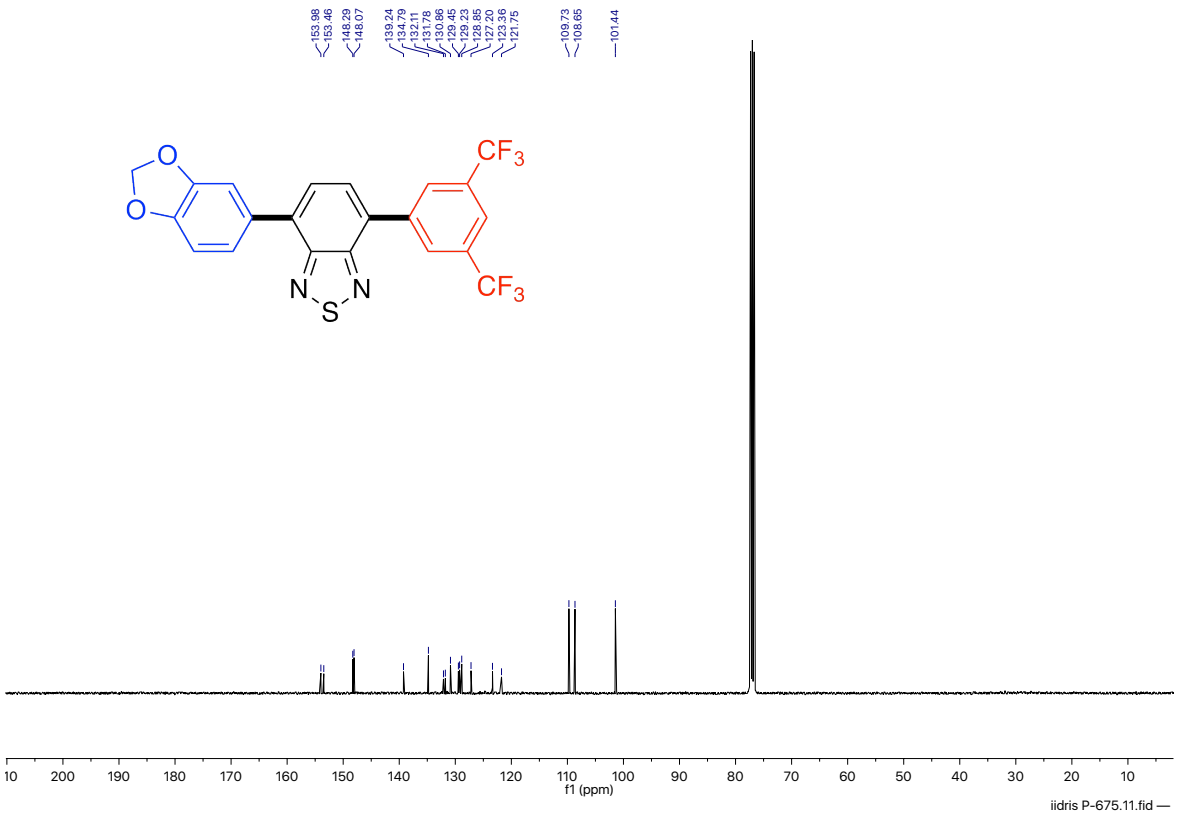

2.00
2.19
2.14
1.99
2.32
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
iidris P-661.10.fid —


153.76
137.82
132.55
131.33
131.01
129.11
128.31
126.07
126.03
125.47
125.20
125.16
122.77
F3C
N
S
N
CF3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
iidris P-661.11.fid —

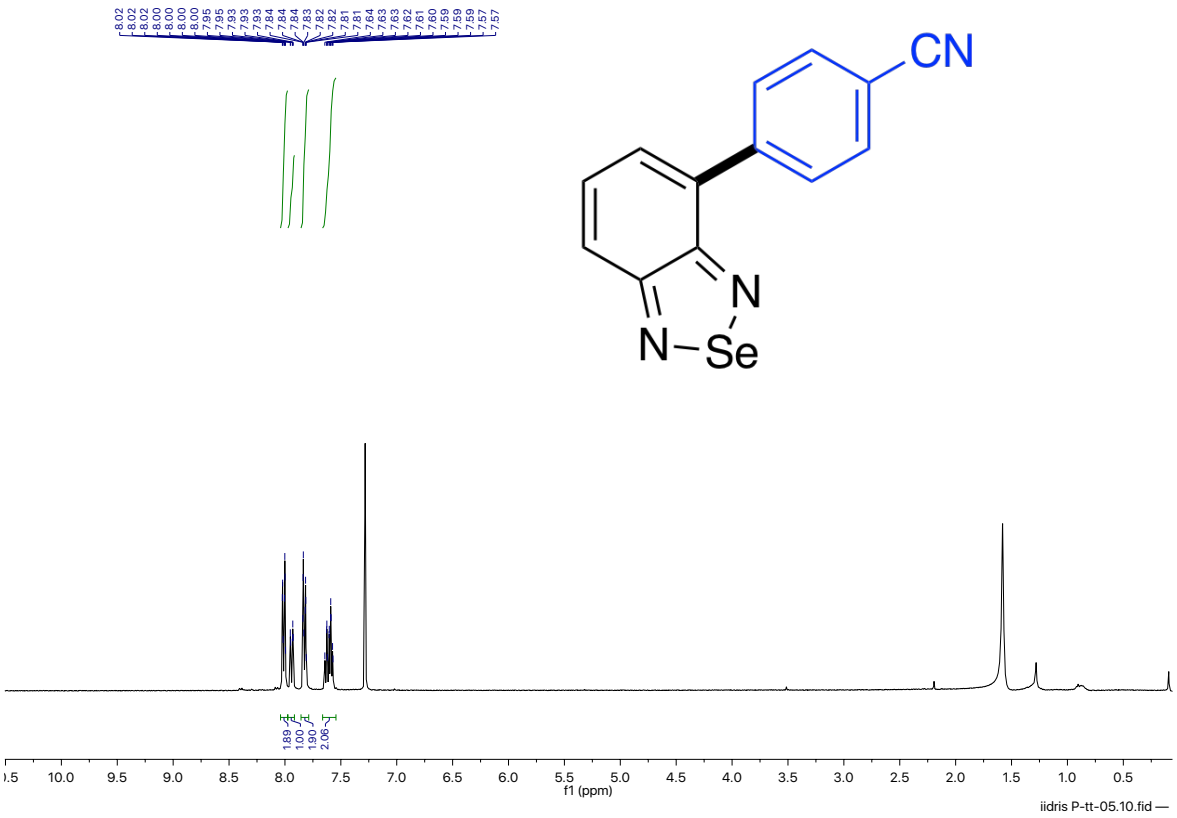

8.51
8.50
8.03
8.02
8.02
7.96
F3C
CF3
F3C
CF3
N
S
N
4.00
2.01
2.18
f1 (ppm)
iidris P-622-2.10.fid

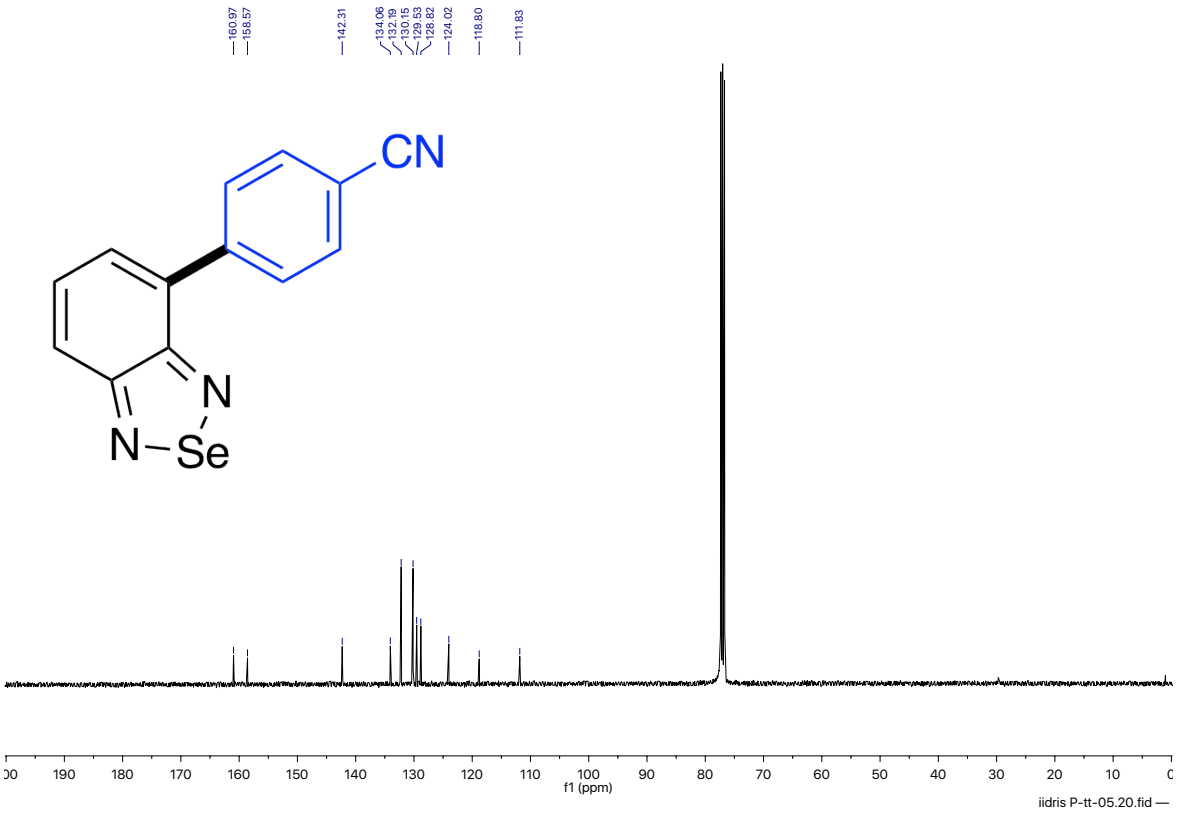

153.39
138.66
132.63
132.30
131.97
131.68
131.63
129.34
128.50
127.37
124.66
122.33
122.29
122.26
121.95
119.24
F3C
CF3
F3C
CF3
N
S
N
f1 (ppm)
iidris P-622.10.fid

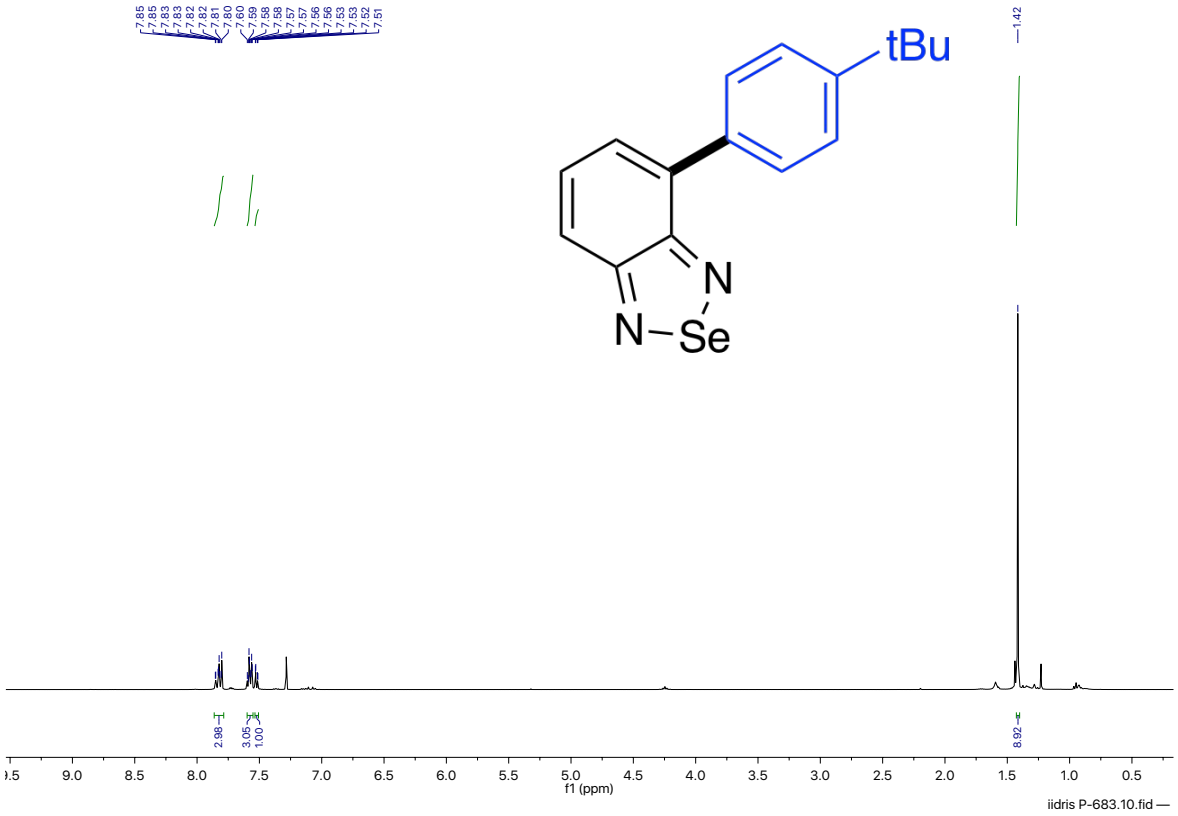

8.50
8.49
7.98
7.89
7.87
7.80
7.79
7.54
7.53
7.51
7.51
7.49
7.49
7.28
7.04
7.02
6.10
O
O
N
S
N
CF3
CF3
1.99
1.00
1.23
1.14
1.13
1.11
1.07
2.02
f1 (ppm)
iidris P-675.10.fid

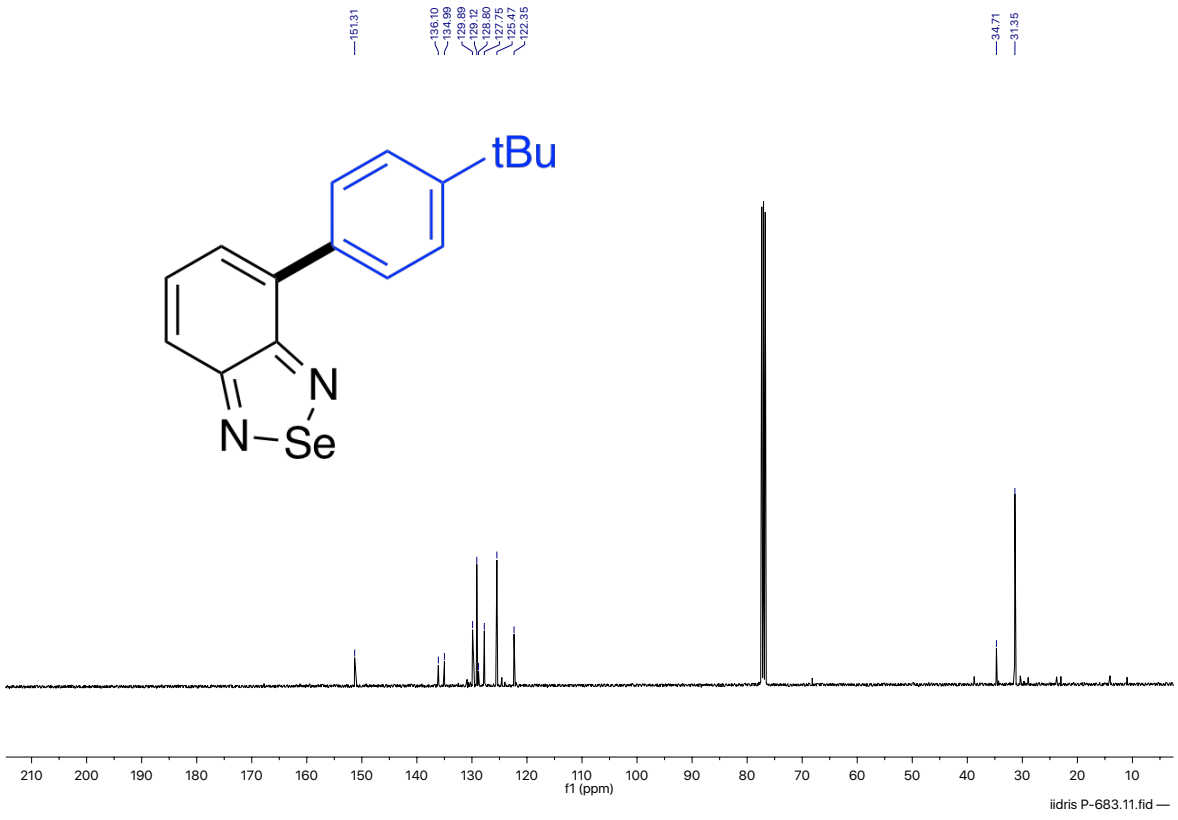

153.98
153.46
148.29
148.07
139.24
134.79
132.11
131.78
130.86
129.45
129.23
128.85
127.20
123.36
121.75
109.73
108.65
101.44
O
O
N
S
N
CF3
CF3
f1 (ppm)
iidris P-675.11.fid

28

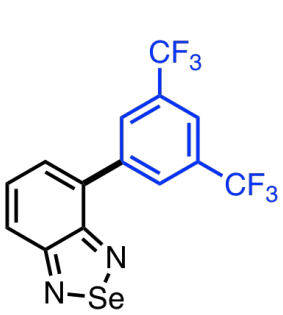

8.02
8.02
8.02
8.00
8.00
8.00
8.00
7.95
7.95
7.93
7.93
7.84
7.84
7.84
7.83
7.82
7.82
7.81
7.81
7.64
7.63
7.62
7.61
7.60
7.59
7.59
7.59
7.57
7.57
CN
N
N
Se
1.89
1.00
1.00
1.90
2.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
iidris P-tt-05.10.fid

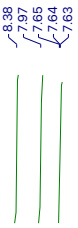

160.97
158.57
142.31
134.06
132.19
130.15
129.53
128.82
124.02
118.80
111.83
CN
N
N
Se
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
iidris P-tt-05.20.fid

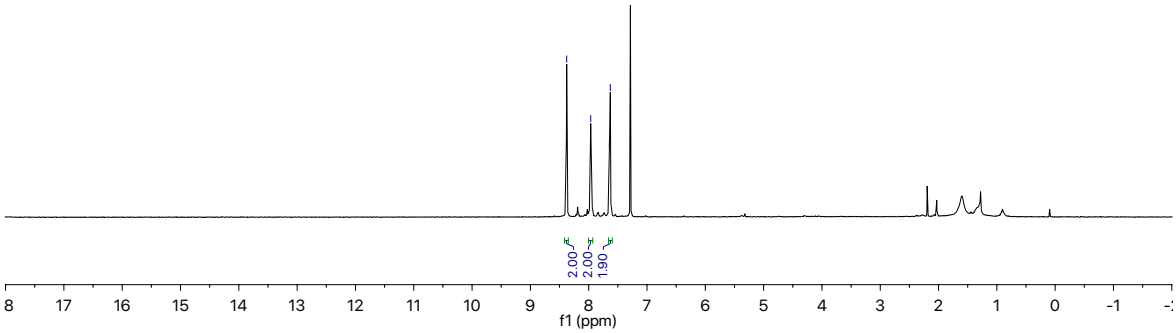

7.85
7.85
7.83
7.83
7.82
7.82
7.81
7.80
7.60
7.59
7.58
7.58
7.57
7.57
7.56
7.56
7.53
7.53
7.52
7.51
1.42
tBu
N
N
Se
2.98
3.05
1.00
8.92
f1 (ppm)
iidris P-683.10.fid


151.31
136.10
134.99
129.89
129.12
128.80
127.75
125.47
122.35
34.71
31.35
tBu
N
N
Se
f1 (ppm)
iidris P-683.11.fid

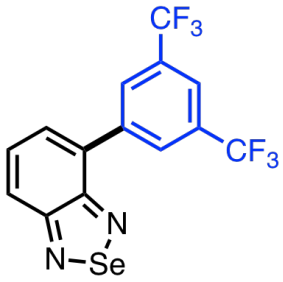
30

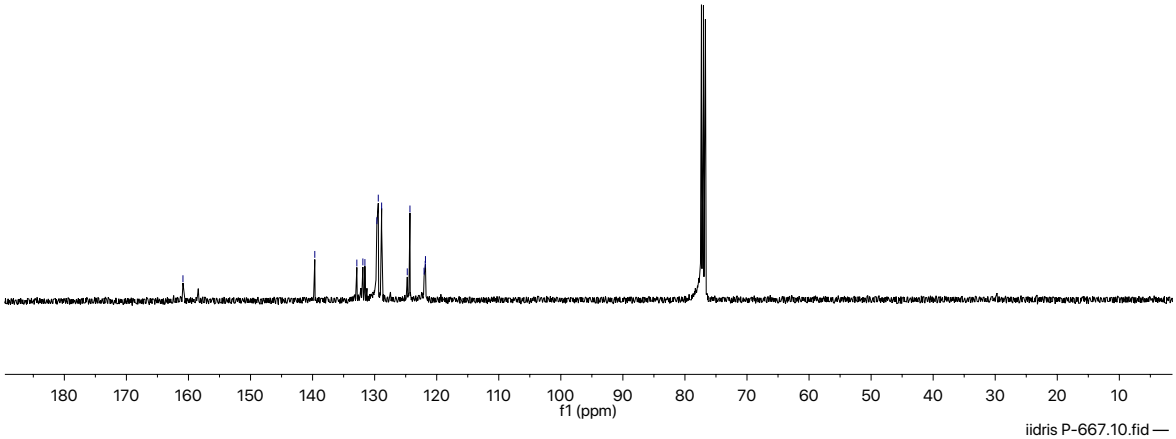

CF3
CF3
N
N–Se


8.38
7.97
7.65
7.64
7.63


2.00
2.00
1.90
8 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)
iidris P-667.20.fid


160.89
139.65
132.87
131.90
131.57
129.64
129.41
128.88
124.74
124.31
122.04
121.85
121.81


CF3
CF3
N
N–Se


180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)
iidris P-667.10.fid

1. Chen, C.-P.; Wu, P.-J.; Liou, S.-Y.; Chan, Y.-H., Ultrabright benzoselenadiazole-based semiconducting polymer dots for specific cellular imaging. *RSC Adv.* **2013,** *3* (38), 17507-17514.
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