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Supporting Information

Modular Two-Step Access to π-Extended Naphthyridine Systems—Potent Building Blocks for Organic Electronics

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1. Experimental Procedures

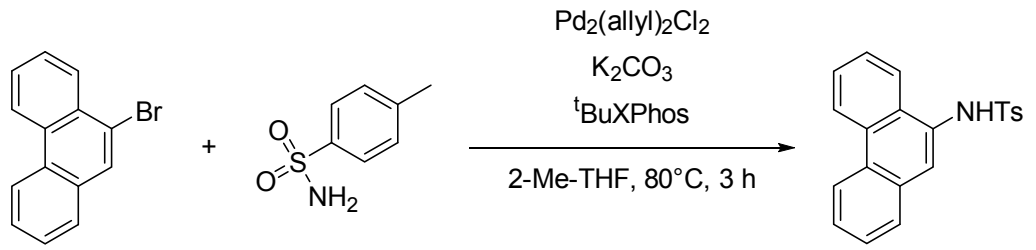
1.1. General Information

All commercially available chemicals were purchased from suppliers (ABCR, Acros, Alfa Aesar, Chempur, Merck and Sigma Aldrich) or obtained from the chemical store of the University of Heidelberg and were used without further purifications. Dry solvents were dispensed from solvent purification system MB SPS-800-Benchtop. Deuterated solvents were supplied from Euriso-Top and used as received. The NMR spectra, if not noted otherwise, were recorded at room temperature on the following spectrometers: Bruker Avance III 300 (300 MHz), Bruker Avance DRX 300 (300 MHz), Bruker Avance III 400 (400 MHz), Bruker Avance III 500 (500 MHz), Bruker Avance III 600 (600 MHz), Bruker Avance III (700 MHz) or Fourier 300 (300 MHz). Chemical shifts δ are quoted in parts per million (ppm) and coupling constants J in Hertz (Hz). ^{1}H and ^{13}C spectra are calibrated in relation to the deuterated solvents, namely $CDCl_3$ (7.26 ppm; 77.16 ppm). ^{19}F spectra were calibrated in relation to the reference measurement of 1,2-difluorobenze (-139 ppm). The following abbreviations were used to indicate the signal multiplicity: for the ^{1}H NMR spectra: s (singlet), d (doublet), t (triplet), q (quartet), quint (quintet), sext (sextet), sept (septet), m (multiplet), as well as their combinations; for the ^{13}C NMR spectra: s (quaternary carbon), d (tertiary carbon (CH)), t (secondary carbon (CH_2)) and q (primary carbon (CH_3)). All the ^{13}C NMR spectra were measured with ^{1}H-decoupling and were interpreted with DEPT135, ^{1}H,^{1}H-COSY and HMBC. All spectra were integrated and processed using TopSpin 3.5 software or MestReNova 14.1.0. Mass spectra (MS and HRMS) were determined at the University of Heidelberg under the direction of Dr. J. Gross. EI+-, ESI+ -, or DART+ -spectra were measured on a Bruker Apex-Qu FT-ICR-MS spectrometer, MALDI on a Bruker Autoflex speed MALDI-TOF instrument. Flash Column Chromatography was accomplished using Silica gel 60 (0.04 – 0.063 mm / 230 – 400 mesh ASTM) purchased from Macherey-Nagel as stationary phase. As eluents the respectively mentioned proportions of petroleum ether (PE), ethyl acetate (EA) and dichloromethane (DCM) were used. Analytical Thin Layer Chromatography (TLC) was carried out on precoated Macherey-Nagel POLYGRAM® SIL G/UV254 or Merck TLC Silical Gel 60 F254 aluminum sheets. Detection was accomplished using UV-light (254 nm). IR spectra were recorded on a Bruker Vector 22, and the absorption maxima were given in wavelength in cm^{-1} units. Melting point was recorded on BÜCHI Melting Point B-540. The cyclic voltammetry (CV) experiments were carried out using PGSTAT101 Potentiostat Galvanostat with a platinum working electrode (Metrohm 6.120.4190, diameter 1 mm), a platinum/titan wire auxiliary electrode (Metrohm 3.109.0790), a silver wire reference electrode (Metrohm 6.1241.060), a 0.1 mol*L^{-1} Bu_4NPF_6 solution in degassed, dry DCM, and ferrocene/ferrocenium as the reference redox system and internal standard (−4.8 eV) for 0.0 V versus Fc^{+}/Fc at room temperature and 0.1 Vs^{-1}. To determine the reduction and oxidation potentials, the half-wave potentials were used.[1] X-ray single-crystal structure analyses were measured on a Bruker Smart APEX-II Quazar Area Detector diffractometer by Dr. F. Rominger (Heidelberg University). Diffraction intensities were corrected for Lorentz and polarization effects. An empirical absorption correction was applied using SADABS based on the Laue symmetry of reciprocal space. Heavy atom diffractions were solved by direct methods and refined against F2 with the full matrix least square algorithm. Hydrogen atoms were either isotropically refined or calculated. The structures were solved and refined using the SHELXTL software package. Absorption spectra were recorded on a Jasco UV-Vis V-670. Fluorescence spectra were recorded on a Jasco FP-6500. Quantum yields were determined by an Ulbricht sphere (6 inch) using a PTI QuantaMaster 40 equipped with a Hamamatsu R928P Photomultiplier. Quantum lifetimes were determined on a Horiba FluoroCube-01-NL lifetime spectrofluorometer with emission monochromator (Seya-Namioka type, 200 nm to 800 nm) and diode excitation (Nano-LED N-375L, 375 ± 10 nm, < 200 ps).

1.2. Synthesis of Ynamides

1.2.1. Synthesis of Ynamides 1a–b

4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 12



12

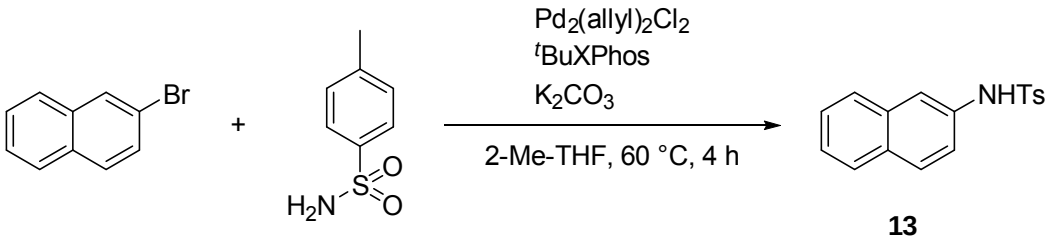
98 %

After Navarro *et al.*[2]

To a suspension of $Pd_2(allyl)_2Cl_2$ (58 mg, 155 µmol, 2 mol % Pd), K_2CO_3 (4.30 g, 31.11 mmol, 2.0 eq), ^{t}BuXPhos (132 mg, 311 µmol, 2 mol %) and Tosylamide (3.20 g, 18.67 mmol, 1,2 eq) in 100 ml dry 2-methyl-THF was added under nitro gen atmosphere 9-bromophenanthrene (4.00 g, 15.56 mmol,1.0 eq). The reaction mixture was stirred at room temperature for 10 minutes and was then heated and stirred in a pre-warmed oil bath at 80°C for 3 hours. After cooling down, 100 ml of ethyl acetate and 100 ml 1M HCl were added and the layers were separated. The aqueous phase was extracted with ethyl acetate (3 x 100 ml) and the combined organic layer was washed with brine, dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure and the crude product was recrystallized from ethyl acetate. The product was isolated as colourless solid (5.298 g, 15.25 mmol, 98 % yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) = 2.32 (s, 3H), 6.85 (s, 1H), 7.14 (d, 2H, J = 8.0 Hz), 7.48-7.71 (m, 7H), 7.80 (dd, 1H, J = 7.5 Hz, J = 1.8 Hz), 7.88 (d, 1H, J = 7.4 Hz), 8.61 (d, 1H, J = 8.0 Hz), 8.67 (d, 1H, J = 8.2 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) = 21.6 (q), 122.1 (d), 122.6 (d), 123.2 (d), 123.3 (d), 127.1 (d), 127,1 (d), 127.2 (d), 127.2 (d), 127.5 (d), 128.2 (s), 128.9 (d), 129.4 (s), 129.7 (d), 129.8 (s), 131.3 (s), 131.4 (s), 136.5 (s), 144.0 (s); FTIR (Neat) ν [cm^{-1}]: 3254, 3064, 2924, 1924, 1738, 1598, 1498, 1453, 1416, 1362, 1321, 1300, 1221, 1187, 1156, 1108, 1089, 1069, 1038, 1022, 951, 908, 888, 864, 818, 797, 762, 747, 723, 707, 670, 615; HRMS-EI+: Calc. for $C_{21}H_{17}NO_2S$: 347.0941, found 347.0975; Mp: 195 °C.

4-methyl-N-(naphthalen-2-yl)benzenesulfonamide 13

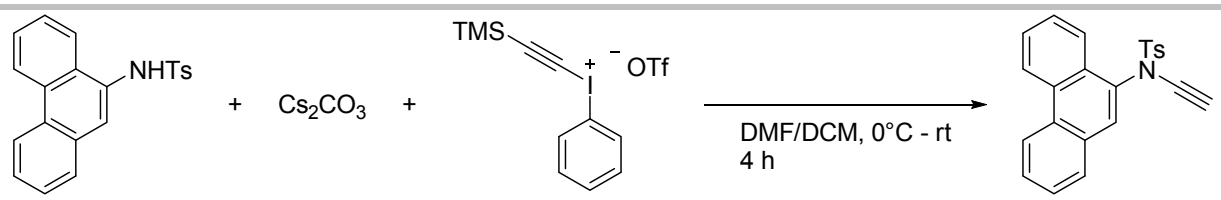


13

$Pd_2(allyl)_2Cl_2$ (35 mg, 97 µmol, 1 mol%) and *tert*-butyl XPhos (82 mg, 193 µmol, 2 mol%) were added under nitrogen atmosphere to a suspension of K_2CO_3 (2.67 g, 19.32 mmol, 2.0 eq) in 30 ml dry 2-Me-THF and stirred for 5 minutes at room temperature. Then Tosylamide (1.98 g, 11.59 mmol, 1.2 eq) and 2-bromonaphthalene (2.00 g, 9.66 mmol, 1.0 eq) were added subsequently and the reaction mixture was stirred at 60 °C for 4 hours. After cooling down to room temperature, water (20 ml) and 1 M HCl (30 ml) were added and the layers were separated. The aqueous phase was extracted with ethyl acetate (2 x 100 ml) and the combined organic layer was washed with brine, dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure and the crude product was purified via recrystallization from ethyl acetate/hexane. The product was isolated as colourless solid (1.993 g, 6.70 mmol, 69 % yield).

Spectral data according to literature[3]

N-ethynyl-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 14

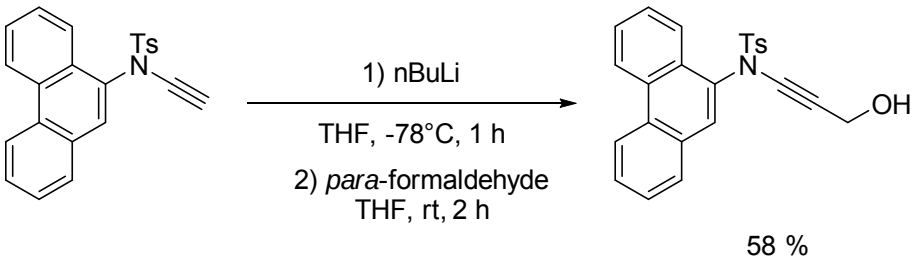


12 **14** 70 %

To a solution of 4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **12** (2.54 g, 7.31 mmol, 1.0 eq) in 40 ml DMF was added Cs_2CO_3 (3.10 g, 9.50 mmol. 1.3 eq) and the reaction mixture was stirred at room temperature for 30 min until the solution was cooled to 0°C and phenyl((trimethylsilyl)ethynyl)iodonium triflate (4.28 g, 9.50 mmol, 1.3 eq) in 15 ml DCM was added dropwise. The ice bath was then removed and the reaction mixture was stirred at room temperature for 4 hours. Then 40 ml water and 50 ml ethyl acetate were added and the layers were separated. The aqueous phase was extracted with ethyl acetate (3 x 50 ml), and the combined organic layer was washed with brine, dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure and the crude product was purified via silica gel flash column chromatography with PE/DCM (2:1) as an eluent. The product was isolated as colourless solid (1.89 g, 5.09 mmol, 70 % yield).

R_f: 0.59 (silica, PE/DCM 2:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) = 2.50 (s, 3H), 2.84 (s, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.47 (s, 1H), 7.55-7.66 (m, 2H), 7.67-7.90 (m, 5H), 8.10 (d, *J* = 8.2 Hz, 1H), 8.69 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) = 21.9 (q), 58.1 (d), 77.4 (s), 122.9 (d), 123.0 (d), 124.3 (d), 127.2 (d), 127.3 (d), 127.5 (d), 127.6 (d), 128.2 (d), 128.7 (d), 129.1 (s), 129.2 (d), 129.9 (d), 130.9 (s), 131.0 (s), 131.6 (s), 133.5 (s), 133.9 (s), 145.4 (s); FTIR (Neat) ν [cm^{-1}]: 3279, 3080, 2128, 1737, 1597, 1492, 1451, 1371, 1308, 1234, 1173, 1118, 1090, 1052, 1034, 948, 903, 882, 855, 831, 808, 766, 742, 722, 702, 677, 664, 630, 605; HRMS-EI+: Calc. for $C_{23}H_{17}NO_2S$: 371.0975, found 371.0977; Mp: 137 °C.

N-(3-hydroxyprop-1-yn-1-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 15



58 %

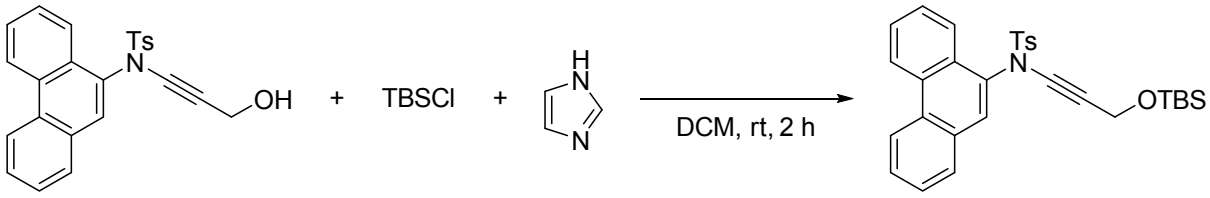
14 **15**

N-ethynyl-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **14** (1.60 g, 4.31 mmol, 1.0 eq) was dissolved under nitrogen atmosphere in 80 ml dry THF. The solution was cooled to -78 °C and *n*-buthylithium (331 mg, 5.17 mmol, 1.2 eq, 2.5 M in hexane, 2.07 ml) was added dropwise and the reaction mixture was stirred at -78°C for 45 min until *para*-formaldehyde (647 mg, 21.54 mmol, 5.0 eq) was added at once and the reaction mixture was slowly warmed up to room temperature and stirred for 16 h. Then the reaction was quenched with 10 ml sat. NH_4Cl solution and was diluted with 50 ml water. THF was removed under reduced pressure and the aqueous phase was extracted with ethyl acetate (3 x 75 ml). The combined organic layer was washed with brine, dried over Na_2SO_4, and filtered. The solvent was removed under reduced pressure and the crude product was purified via silica gel flash column chromatography with DCM (100 %) as an eluent. The product was further purified by washing with methanol (10 ml) and isolated as colourless solid (1.00 g, 2.49 mmol, 58 % yield).

R_f: 0.34 (silica, DCM, 100 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) = 1.52 (t, *J* = 4.5 Hz, 1H), 2.50 (s, 3H), 4.39 (d, *J* = 4.5 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.45 (s, 1H), 7.60 (t, *J* = 7.5 Hz, 2H), 7.64-7.85 (m, 5H), 8.06 (dd, *J* = 8.2 Hz, 1.0 Hz, 1H), 8.69 (t, *J* = 6.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 21.9 (q), 51.5 (t), 68.6 (s), 80.8 (s), 122.9 (d), 123.0 (d), 124.4 (d), 127.3 (d), 127.4 (d), 127.5 (d), 127.6 (d), 128.2 (d), 128.7 (d), 129.2 (d), 129.3 (s), 129.9 (d), 130.9 (s), 131.0 (s), 131.7 (s), 133,9 (s),

134.2 (s), 145.4 (s); FTIR (Neat) ν [cm^{-1}]: 3521, 3069, 2921, 2860, 2242, 1597, 1495, 1452, 1364, 1316, 1216, 1187, 1167, 1088, 1070, 1012, 912, 869, 813, 749, 725, 703, 664, 631, 606; HRMS-ESI: Calc. for $C_{24}H_{19}NNaO_3S$: 424.0978, found: 424,0987; Mp: 149 °C.

N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 1a

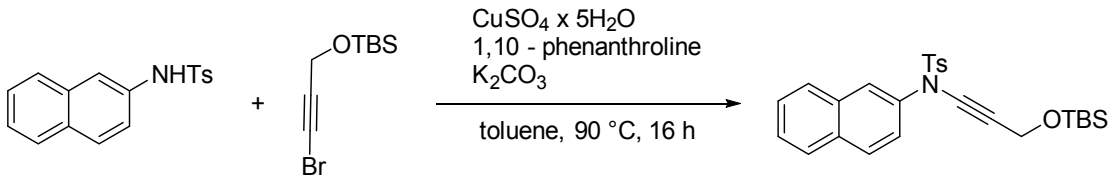


15 **1a** 88 %

N-(3-hydroxyprop-1-yn-1-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **15** (600 mg, 1.49 mmol, 1.0 eq) was dissolved under nitrogen atmosphere in 15 ml dry DCM and TBSCl, (451 mg, 2.99 mmol, 2.0 eq) and 1-H Imidazole (203 mg, 2.99 mmol, 2.0 eq) were added and the reaction mixture was stirred at room temperature for 2 hours. Then water (10 ml) was added and the layers were separated. The aqueous phase was extracted with DCM (2 x 30 ml) and the combined organic layer was washed with brine, dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure und the crude product was purified via silica gel flash column chromatography with PE/EA (10:1) as an eluent. The product was further washed with a small amount of methanol to obtain a colourless solid (680 mg, 1.32 mmol, 88 % yield).

R_f = 0.65 (silica, DCM/PE 2:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) = 0.05 (s, 6H), 0.87 (s, 9H), 2.50 (s, 3H), 4.43 (s, 2H), 7.34 (d, *J* = 8.3 Hz, 2H), 7.44 (s, 1H), 7.56-7.62 (m, 2H), 7.68-7.72 (m, 3H), 7.74 (d, *J* = 7.9 Hz, 1H), 7.79 (d, *J* = 8.3 Hz, 2H), 8.10 (d, *J* = 8.1 Hz, 1H), 8.69 (t, *J* = 8.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): 5.0 (q), 18.4 (s), 21.9 (q), 25.9 (q), 52.1 (t), 69.0 (s), 79.7 (s), 122.9 (d), 123.0 (d), 124.6 (d), 127.2 (d), 127.3 (d), 127.4 (d), 127.5 (d), 128.1 (d), 128.8 (d), 129.2 (d), 129.4 (s), 129.8 (d), 130.9 (s), 131.1 (s), 131.7 (s), 134.1 (s), 134.2 (s), 145.2 (s); FTIR (Neat) ν [cm^{-1}]: 3065, 2954, 2929, 2857, 2242, 1736, 1595, 1496, 1471, 1454, 1389, 1359, 1315, 1294, 1252, 1215, 1171, 1108, 1069, 1057, 1013, 997, 943, 915, 892, 834, 816, 773, 758, 745, 722, 703, 660, 633, 605; HRMS-ESI: Calc. for $C_{30}H_{34}NO_3SSi^+$: 516.2029, found: 516.2023; mp: 140 °C.

N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methyl-N-(naphthalen-2-yl)benzenesulfonamide 1b



13 **1b** 18%

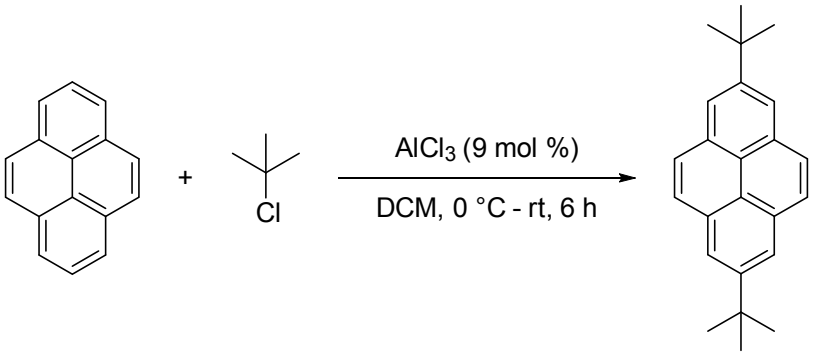
4-methyl-N-(naphthalen-2-yl)benzenesulfonamide **13** (1.00 g, 3.36 mmol, 1.0 eq), bromo-alkyne (1.26 g, 5.04 mmol, 1.5 eq), $CuSO_4$ x $5H_2O$ (126 mg, 0.504 mmol, 15 mol%), phenanthroline (182 mg, 1.01 mmol, 30 mol%) and K_2CO_3 (0.93 g, 6.73 mmol, 2.0 eq) were suspended under nitrogen atmosphere in 5 ml dry toluene and the reaction mixture was stirred at 90 °C for 16 hours. After cooling down to room temperature, water was added, and the layers were separated. The aqueous layer was extracted with ethyl acetate (2x 50 ml) and the combined organic layer was washed with water, brine, dried over Na_2SO_4, and filtered. The solvent was removed under reduced pressure and the crude product was purified via silica gel flash column chromatography with PE/EA (10:1) as an eluent. The product was isolated as colourless oil (280 mg, 0.601 mmol, 18% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) = 0.10 (s, 6H), 0.90 (s, 9H), 2.43 (s, 3H), 4.49 (s, 2H), 7.25 (d, *J* = 8.1 Hz, 2H), 7.35 (dd, *J* = 8.8, 2.2 Hz, 1H), 7.48-7.54 (m, 2H), 7.59 (d, *J* = 8.3 Hz, 2H), 7.59 (d, *J* = 8.3 Hz, 2H), 7.73 (d, *J* = 2.0 Hz, 1H), 7.75-7.80

(m, 2H), 7.81-7.85 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) = -5.0 (q), 18.4 (s), 21.8 (q), 25.9 (q), 52.0 (t), 70.0 (s), 78.8 (s), 124.3 (d), 125.2 (d), 126.8 (d), 126.9 (d), 127.8 (d), 128.3 (d), 128.4 (d), 129.1 (d), 129.7 (d), 132.7 (s), 133.3 (s), 133.4 (s), 136.3 (s), 145.0 (s); IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 3060, 2954, 2929, 2885, 2856, 2243, 1597, 1509, 1464, 1375, 1291, 1255, 1187, 1174, 1151, 1121, 1077, 1006, 969, 928, 902, 834, 813, 778, 747, 704, 667, 648, 631; HRMS-EI+: Calc. for $C_{26}H_{31}NO_3SiS^+$: 465.1788 m/z, found: 465.1741 m/z.

1.2.2. Synthesis of Ynamide 9

2,7-di-tert-butylpyrene 16



6 **16** 85 %

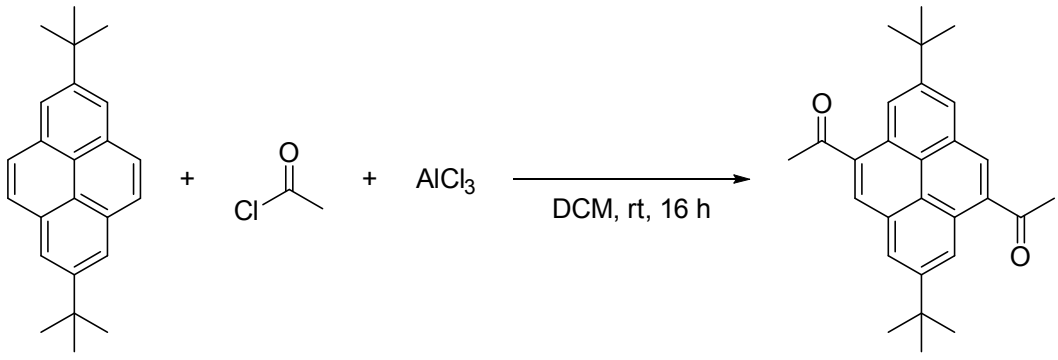
After Zhang *et al*.[4]

Pyrene **6** (6.06 g, 29.96 mmol, 1.0 eq) and $AlCl_3$ (359 mg, 2.70 mmol, 9 mol %) were dissolved in 300 ml dry DCM under nitrogen atmosphere and *tert*-butylchloride (6.10 g, 65.92 mmol, 2.2 eq) in 45 ml dry DCM was added dropwise at 0 °C. The solution was then warmed to room temperature and kept stirring for 6 hours. After this time ice (100 g) and 15 ml conc. HCl solution were added and the layers were separated. The organic solution was washed with water (3 x 150 ml), brine (150 ml), dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure and the product was purified with silica gel flash column chromatography with PE (100 %) as an eluent and recrystallization from PE. The product was isolated as colourless solid (8.02 g, 25.50 mmol, 85 % yield).

R_f (silica, PE) = 0.28; ^{1}H NMR ($CDCl_3$, 300 MHz), δ [ppm] = 1.59 (s, 18 H), 8.03 (s, 4H), 8.19 (s, 4H);

Data are according to literature[4].

1,1'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(ethan-1-one) 17



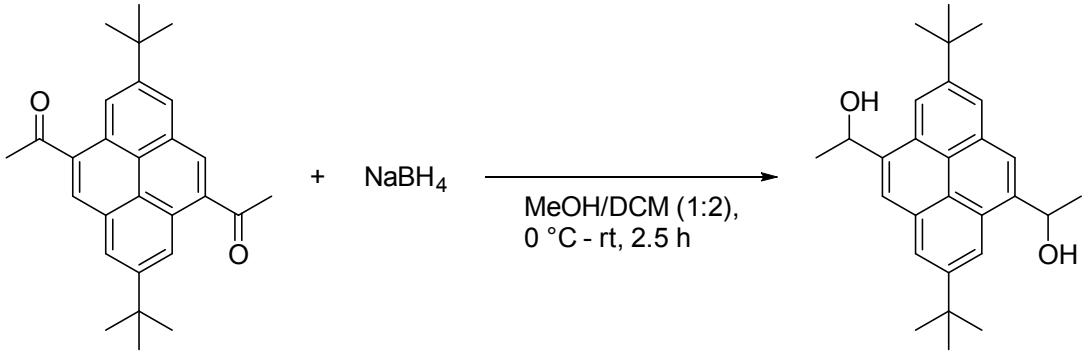
16 **17** 60 %

Under nitrogen atmosphere 2,7-di-tert-butylpyrene **16** (50.0 mg, 159 µmol, 1.0 eq) and acetyl chloride (187 mg, 2.38 mmol, 15 eq) were dissolved in anhydrous DCM (1 ml). At 0 °C aluminium(III)chloride (212 mg, 1.59 mmol, 10 eq) was added in portions. The mixture was stirred for 1 h at room temperature and was quenched with dest. water (10 ml) afterwards. The layers were separated and the aqueous layer was extracted with ethyl acetate (3 x 10 ml). The combined organic layer was washed with KOH-solution and brine (each 10 ml), dried over Na_2SO_4, and filtered. The solvent was removed under reduced pressure and the crude product was purified by recrystallization from ethyl acetate. A yellowish solid was obtained (38.0 mg, 95.4 µmol, 60%).

R_f (silica, PE/EA (5:1)) = 0.12; ^{1}H NMR ($CDCl_3$, 600 MHz), δ [ppm] = 1.60 (s, 18H), 2.95 (s, 6H), 8.33 (d, 2H, *J* = 1.85 Hz), 8.63 (s, 2H), 9.41 (d, 2H, *J* = 1.85 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz) = 29.9 (q), 32.0 (q), 35.7 (s), 124.8 (d), 124.9 (s), 127.4 (s), 129.0 (s), 133.7 (d), 133.8 (s), 150.2 (s), 201.6 (s).

Data according to literature[5]

1,1'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(ethan-1-ol) 7

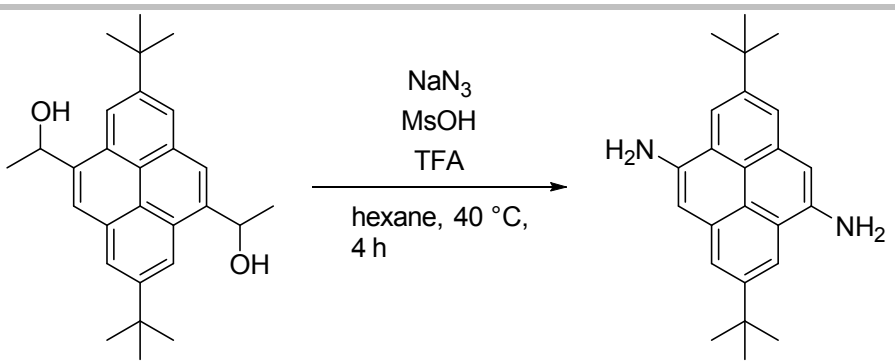


17 **7** Quant.

1,1'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(ethan-1-one) **17** (1.00 g, 2.51 mmol, 1.0 eq) was dissolved in a mixture of DCM an methanol (2:1, 170 ml). Then the solution was cooled to 0 °C and $NaBH_4$ (380 mg, 10.0 mmol, 4.0 eq) was added in portions and the reaction mixture was stirred at room temperature for 2.5 hours. Then 200 ml water was added and the layers were separated. The aqueous phase was extracted with DCM (3 x 50 ml) and the combined organic layer was washed with water, brine, dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure to obtain the product as colourless solid (1.02 g, 2.51 mmol, quant. Yield).

R_f (silica, PE/EA (5:1)) = 0.35; ^{1}H NMR ($CDCl_3$, 600 MHz), δ [ppm] = 1.59 (s, 18 H), 1.84 (dd, 6H, *J* = 6.3 Hz, *J* = 1.8 Hz), 5.89 (dd, 2H, *J* = 12.9 Hz, *J* = 6.7 Hz), 8.23-8.24 (m, 4H), 8.43-8.44 (m, 2H); ^{13}C NMR ($CDCl_3$, 150 MHz) = 24.4 (q), 32.1 (q), 35.5 (s), 67.7 (d), 118.2 (d), 122.7 (d), 123.0 (s), 123.5 (d), 128.4 (s), 130.9 (s), 140.4 (s), 140.5 (s), 148.6 (s); FTIR (Neat) ν [cm^{-1}]: 3295, 2961, 2903, 2866, 1812, 1724, 1601, 1464, 1448, 1393, 1362, 1260, 1231, 1150, 1124, 1072, 1003, 958, 906, 872, 715, 701, 636; HRMS-EI+: Calc. for $C_{28}H_{34}O_2$: 402.2553, found 402.2554; Mp: 251 °C.

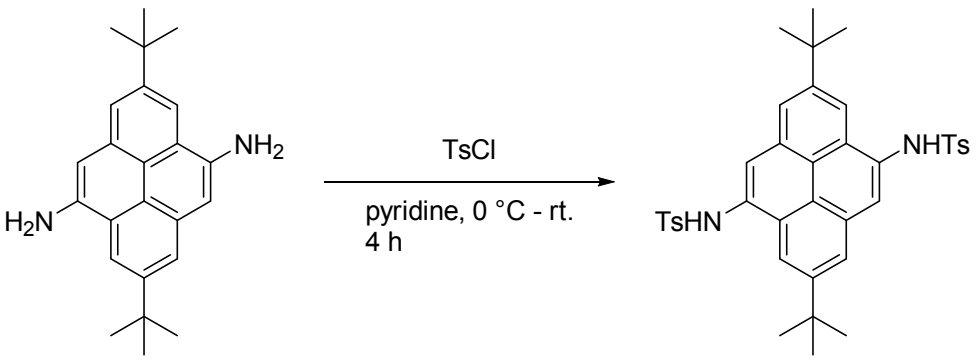
2,7-di-tert-butylpyrene-4,9-diamine 8



7 **8** 88 %

1,1'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(ethan-1-ol) **7** (250 mg, 0.621 mmol, 1.0 eq) was dissolved in a mixture of 6.5 ml hexane, methane sulfonic acid (0.716 g, 7.45 mmol, 12 eq) and trifluoracetic acid (1.70 g, 14.90 mmol, 24 eq) and NaN_3 (202 mg, 3.10 mmol, 5 eq) was added in portions. The reaction mixture was stirred under exclusion of light at 40 °C for 4 hours. Then 10 ml sat. $NaHCO_3$ solution and 10 ml ethyl acetate was added, and the layers were separated. The aqueous layer was extracted with ethyl acetate (3 x 10 ml) and the combined organic layer was washed with brine. The solvent was removed under reduced pressure and the crude product was redissolved in 5 ml THF and the solution was cooled to 0 °C. Then conc. HCl (0.5 ml) was added dropwise under stirring and after 30 min the resulting precipitate was filtered and washed with water, THF and methanol. The solid was then again redissolved in a mixture of a mixture triethylamine and DCM and washed with a diluted solution of K_2CO_3 in water (2 x 20 ml), brine, and dried over Na_2SO_4. The suspension was filtered, and the solvent was removed under reduced pressure to obtain the pure product as yellow solid (188 mg, 545 µmol, 88% yield).
R_f (silica, PE/EA (2:1)) = 0.30; ^{1}H NMR (CD_2Cl_2, 600 MHz), δ [ppm] = 1.55 (s, 18H), 4.41 (bs, 4H), 7.23 (s, 2H), 7.94 (s, 2H), 7.99 (s, 2H); ^{13}C NMR (CD_2Cl_2, 150 MHz) = 31.8 (q), 35.3 (s), 106.6 (d), 112.3 (d), 119.4 (s), 120.4 (d), 124.3 (s), 132.6 (s), 141.5 (s), 148.5 (s); FTIR (Neat) ν [cm^{-1}]: 3380, 2948, 2900, 2863, 1756, 1620, 1603, 1491, 1473, 1389, 1360, 1270, 1256, 1221, 1200, 1170, 912, 877, 830, 734, 687, 631; HRMS-EI+: Calc. for $C_{24}H_{28}N_2$: 344.2247, found 344.2242; Mp: 50 °C (decomp.).

N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(4-methylbenzenesulfonamide) 18



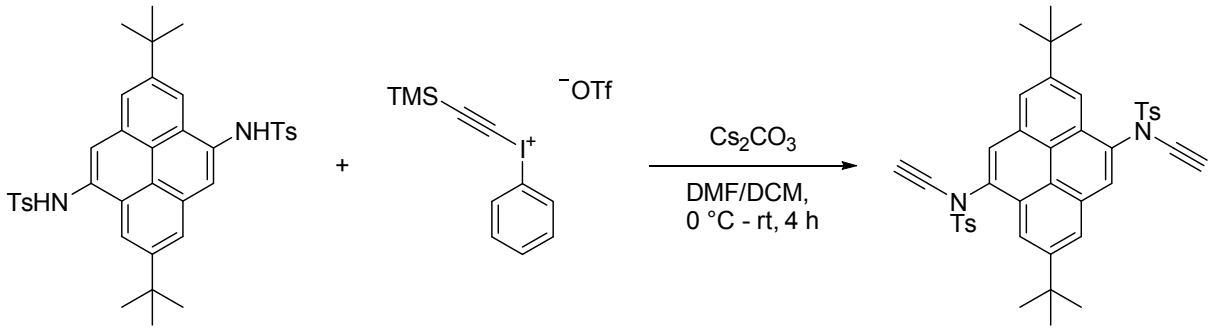
8 **18** 83%

2,7-di-tert-butylpyrene-4,9-diamine **8** (158 mg, 459 µmol, 1.0 eq) was dissolved in 10 ml pyridine and 2 ml DCM and tosyl chloride (262 mg, 1.38 mmol, 3 eq) was added at 0 °C. The ice bath was removed, and the reaction mixture was stirred at room temperature for 4 hours. Then the solvent was removed under reduced pressure and water was added. The resulting

suspension was filtered and washed with water, methanol, DCM and hexane. The product was isolated as colourless solid (248 mg, 380 µmol, 83% yield).

^{1}H NMR (DMSO-d^6, 300 MHz), δ [ppm] = 1.37 (s, 18H), 2.21 (s, 6H), 7.16 (d, 4H, *J* = 8.1 Hz), 7.56 (d, 4H, *J* = 8.1 Hz), 8.06 (s, 2H), 8.12 (s, 2H), 8.21 (s, 2H), 10.52 (s, 2H); ^{13}C NMR (DMSO-d^6, 75 MHz) = 20.8 (q), 31.4 (q), 35.1 (s), 118.2 (d), 121.1 (s), 122.7 (d), 124.3 (d), 126.3 (s), 126.4 (d), 129.6 (d), 130.0 (s), 131.5 (s), 137.9 (s), 142.8 (s), 148.5 (s); FTIR (Neat) ν [cm^{-1}]: 3274, 2957, 2903, 2867, 1599, 1466, 1436, 1378, 1321, 1259, 1217, 1166, 1147, 1131, 1091, 973, 918, 880, 847, 809, 751, 704, 685, 664; HRMS-ESI pos: Calc. for $C_{38}H_{40}N_2NaO_4S_2$: 675,2327, found 675.2326; Mp: >300 °C.

N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-ethynyl-4-methylbenzenesulfonamide) 19

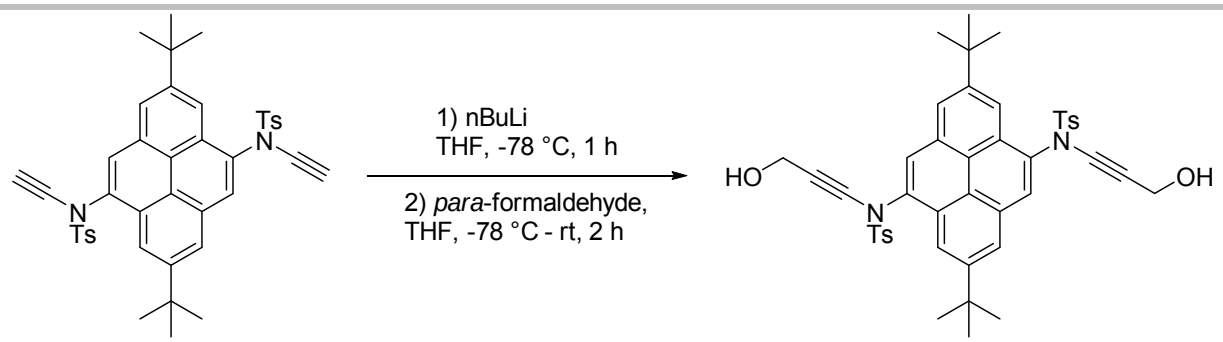


18 **19** 68%

N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(4-methylbenzenesulfonamide) **18** (425 mg, 651 µmol, 1.0 eq) was dissolved in 6.5 ml DMF and Cs_2CO_3 (551 mg, 1.69 mmol, 2.6 eq) was added. The reaction mixture was stirred at room temperature for 30 min and then phenyl((trimethylsilyl)ethynyl)iodonium triflate (879 mg, 1.95 mmol, 3.0 eq) in 2.5 ml DCM was added dropwise at 0 °C. The ice bath was the removed and the reaction mixture was stirred at room temperature for 4 hours. Then 50 ml ethyl acetate and 50 ml water was added and the layers were separated. The aqueous phase was extracted with ethyl acetate (3 x 50 ml) and the combined organic layer was washed with water, brine, dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure and the crude product was purified via silica gel flash column chromatography with DCM/PE (1:1) as an eluent. The product was isolated as colourless solid (309 mg, 441 µmol, 68% yield).

R_f (silica, PE/DCM (1:1)) = 0.58; ^{1}H NMR (CD_2Cl_2, 300 MHz), δ [ppm] = 1.39 (s, 18H), 2.44 (s, 6H), 3.02 (s, 2H), 7.31 (d, 4H, *J* = 8.1 Hz), 7.72 (d, 4H, *J* = 8.1 Hz), 8.06 (s, 2H), 8.17 (d, 2H, *J* = 1,7 Hz), 8.21 (d, 2H, *J* = 1.7 Hz); ^{13}C NMR (CD_2Cl_2, 100 MHz) = 21.8 (q), 31.7 (q), 35.6 (s), 59.3 (d), 77.3 (s), 120.4 (d), 124.0 (s), 124.6 (d), 127.1 (s), 128.7 (d), 129.7 (s), 130.4 (d), 130.5 (s), 133.7, 134.7 (s), 146.1 (s), 150.1 (s). FTIR (Neat) ν [cm^{-1}]: 3282, 2963, 2869, 2131, 1735, 1611, 1596, 1462, 1396, 1362, 1306, 1251, 1215, 1172, 1089, 973, 930, 905, 888, 842, 814, 706, 693, 666, 633; HRMS-ESI pos: Calc. for $C_{42}H_{41}N_2O_4S_2$: 701.2508, found: 701.2510; Mp: 235 °C (decomp.).

N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-hydroxyprop-1-yn-1-yl)-4-methylbenzenesulfonamide) 20

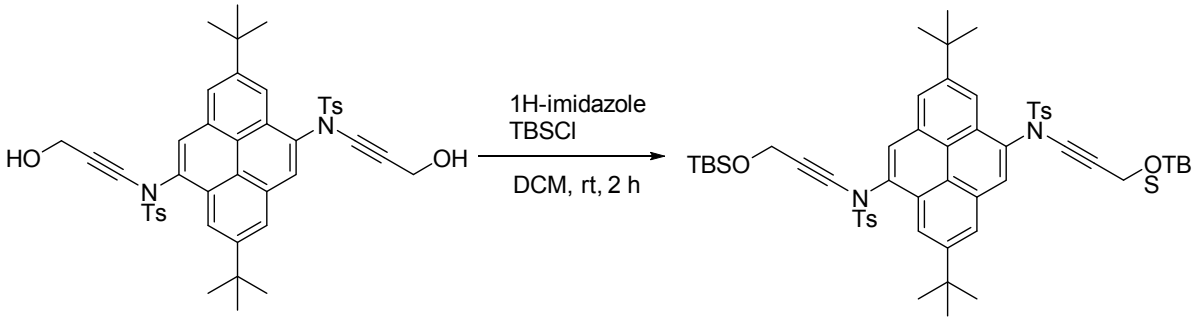


19 **20** 68%

N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-ethynyl-4-methylbenzenesulfonamide) **19** (100 mg, 143 µmol, 1.0 eq) was dissolved under nitrogen atmosphere in 5 ml dry THF and the solution was cooled to -78 °C. Then *n*-BuLi (2.5 M in hexane, 22 mg, 342 µmol, 0.855 ml, 2.4 eq) was added dropwise and the reaction mixture was stirred at -78 °C for 1 hour. Then *para*-formaldehyde (86 mg, 2.85 mmol, 20 eq) was added and the reaction mixture was warmed gradually to room temperature and stirred for 2 hours. Then 15 ml water was added to quench the reaction and THF was removed under reduced pressure. The aqueous phase was extracted with ethyl acetate (3 x 20 ml) and the combined organic layer was washed with brine, dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure and the crude product was purified via silica gel flash column chromatography with DCM/EA (20:1) as an eluent. The product was the further purified by washing with a small amount of methanol (3 ml). The product was isolated as beige solid (74 mg, 97.2 µmol, 68% yield).

R_f (silica, DCM/EA (20:1)) = 0.18; ^{1}H NMR (CD_2Cl_2, 500 MHz), δ [ppm] = 1.36 (s, 18H), 1.66 (t, 2H, *J* = 6.1 Hz), 2.41 (s, 6H), 4.38 (d, 4H, *J* = 6.1 Hz), 7.28 (d, 4H, *J* = 8.0 Hz), 7.69 (d, 4H, *J* = 8.0 Hz), 8.02 (s, 2H), 8.08 (d, 2H, *J* = 1.5 Hz), 8.18 (d, 2H, *J* = 1.5 Hz); ^{13}C NMR (CD_2Cl_2, 125 MHz) = 21.8 (q), 31.7 (q), 35.6 (s), 51.4 (t), 70.2 (d), 80.3 (s), 120.3 (d), 123.4 (s), 124.5 (d), 127.1 (s), 128.6 (d), 129.6 (d), 130.4 (d), 130.5 (s), 134.0 (s), 134.5 (s), 146.0 (s), 150.0 (s); FTIR (Neat) ν [cm^{-1}]: 3559, 2959, 2867, 2242, 1597, 1457, 1369, 1315, 1291, 1262, 1187, 1170, 1123, 1090, 1013, 976, 935, 861, 810, 703, 690, 665; HRMS-ESI pos (DCM/MeOH): calc for $C_{44}H_{45}N_2O_6S_2$: 761.2719, found: 761.2715; Mp: 225 °C.

N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methylbenzenesulfonamide) 9



20 **9** 86%

N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-hydroxyprop-1-yn-1-yl)-4-methylbenzene-sulfonamide) **20** (124 mg, 163 µmol, 1.0 eq) was dissolved in under nitrogen atmosphere in 7 ml DCM and 1H-imidazole (44 mg, 652 µmol, 4.0 eq) and TBS-chloride (98 mg, 652 µmol, 4.0 eq) were added. The reaction mixture was stirred at room temperature for 2 hours. Then 5 ml water was added and the layers were separated. The aqueous layer was extracted with DCM (3 x 10 ml) and the combined organic layer was washed with brine, dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure and the product was purified via silica gel flash column chromatography with DCM (100 %) as an eluent. The product was then

further purified by washing with a small amount of methanol (3 ml). The product was isolated as colourless solid (139 mg, 141 µmol, 86% yield).

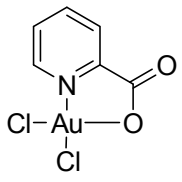
R_f (silica, DCM) = 0.9; ^{1}H NMR ($CDCl_3$, 700 MHz), δ [ppm] = 0.07 (s, 12H), 0.87 (s, 18H), 1.39 (s, 18H), 2.44 (s, 6H), 4.46 (s, 4H), 7.28 (d, 4H, *J* = 6.9 Hz), 7.75 (d, 4H, *J* = 6.9 Hz), 8.01 (s, 2H), 8.13 (d, 2H, *J* = 1.6 Hz), 8.15 (d, 2H, *J* = 1.6 Hz); ^{13}C NMR ($CDCl_3$, 176 MHz) = -5.0 (q), 18.4 (s), 21.8 (q), 26.0 (q), 31.7 (q), 35.4 (s), 52.0 (s), 69.8 (d), 79.2 (s), 120.1 (d), 123.8 (s), 124.1 (d), 127.1 (s), 128.6 (d), 129.3 (d), 130.0 (d), 130.1 (s), 133.9 (s), 134.6 (s), 145.1 (s), 149.5 (s); FTIR (Neat) v [cm^{-1}]: 2956, 2930, 2858, 2235, 1609, 1596, 1471, 1461, 1369, 1318, 1261, 1174, 1069, 930, 913, 894, 832, 814, 777, 705, 689, 665; HRMS-DART pos: calc for $C_{56}H_{73}N_2O_6S_2Si_2$: 989.4449, found: 989.4321; Mp: 217 °C.

1.3. Gold-catalysed synthesis of quinolines

1.3.1. General procedures for gold-catalysed synthesis of quinolines 4a-h and 10a-d

GP.A: $PicAuCl_2$ **3** (5 mol %) was dissolved in DCE and anthranil **2** in DCE (1.5 eq) and Ynamide **1** (1.0 eq) were added (total concentration of ynamide: 0.2 M) and the reaction mixture was stirred at 65 °C for 4 hours. Then the solvent was reduced under reduced pressure and the crude product was purified via silica gel flash column chromatography. The product was further purified by washing with a small amount of methanol.

$PicAuCl_2$ =



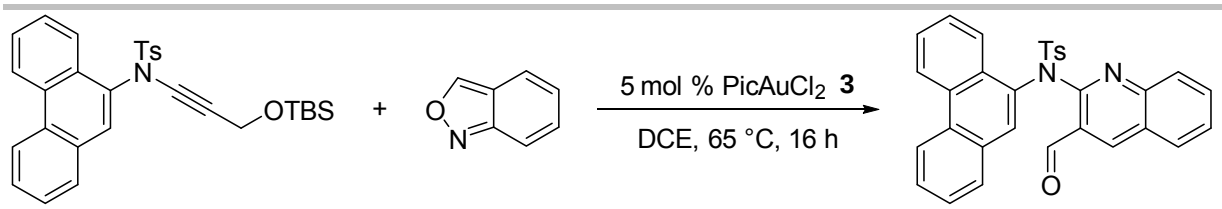
3

GP.B: $PicAuCl_2$ **3** (5 mol %) was dissolved in DCE and anthranil **2** (1.5 eq) and Ynamide **1** (1.0 eq) were added (total concentration of ynamide: 0.2 M) and the reaction mixture was stirred at 65 °C for 4 hours. Then the solvent was reduced under reduced pressure and the crude product was purified via silica gel flash column chromatography. The product was further purified by washing with a small amount of methanol.

GP.C: $PicAuCl_2$ **3** (15 mol %) was dissolved in DCE and anthranil **2a** or **2h-j** (4 eq) and Ynamide **10a-d** (1.0 eq) were added (total concentration of ynamide: 0.1 M) and the reaction mixture was stirred at 65 °C for 4 hours. Then the solvent was reduced under reduced pressure and the crude product was purified via silica gel flash column chromatography. The product was further purified by washing with a small amount of methanol.

1.3.2. Gold-catalysed synthesis of 4a-g

N-(3-formylquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4a



1a **2a** **4a** 75 %

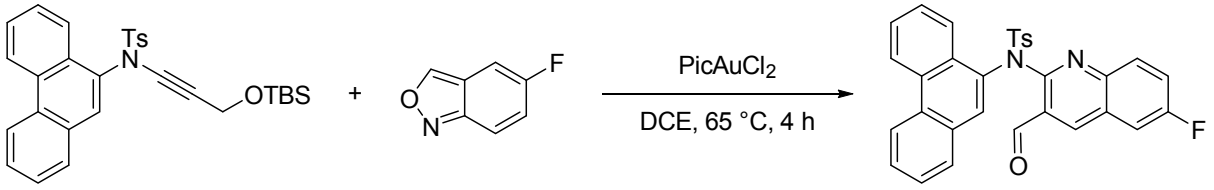
According to **G.P.A**: $PicAuCl_2$ **3** (9.5 mg, 24 µmol, 5 mol %) and anthranil **2a** (87 mg, 727 µmol, 1.5 eq) and N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methyl-N-(phenanthren-9-l)benzenesulfonamide **1a** (250 mg, 485 µmol, 1.0 eq) were stirred at 65 °C for 4 hours in 2.4 ml DCE.

Silica gel flash column chromatography with DCM/PE (2:1) as an eluent.

Colourless solid (181 mg, 360 µmol, 74 % yield).

R_f (silica, DCM/PE 2:1) = 0.28; ^{1}H NMR (500 MHz, CD_2Cl_2) δ (ppm) = 2.49 (s, 3H), 7.25 (d, *J* = 7.0 Hz, 2H), 7.49-7.63 (m, 4H), 7.66-7.73 (m, 4H), 7.77 (s, 1H), 7.78-7.84 (m, 1H), 7.95 (d, *J* = 8.7 Hz, 2H), 8.67 (d, J = 8.3 Hz, 1H), 8.68-8.75 (m, 2H), 8.78 (s, 1H), 11.02 (s, 1H); ^{13}C NMR (150 MHz, CD_2Cl_2): 21.9 (q), 123.0 (d), 123.3 (d), 125.3 (d), 127.0 (s), 127.4 (d), 127.5 (d), 127.6 (d), 127.8 (s), 128.4 (d), 128.5 (d), 129.1 (d), 129.5 (d), 129.6 (d), 129.7 (d), 130.1 (d), 130.8 (s), 131.1 (s), 131.3 (s), 131.8 (s), 132.3 (d), 133.0 (d), 134.4 (s), 135.0 (s), 140.2 (d), 145.3 (s), 148.7 (s), 152.8 (s), 189.1 (s); FTIR (Neat) ν [cm^{-1}]: 3069, 2880, 1691, 1618, 1582, 1492, 1451, 1419, 1369, 1354, 1307, 1256, 1239, 1219, 1190, 1164, 1117, 1102, 1087, 1064, 1037, 1018, 978, 934, 913, 893, 866, 836, 814, 786, 757, 744, 722, 705, 668, 629, 607; HRMS-MALDI: Calc. for $C_{31}H_{23}N_2O_3S^+$: 503.1429, found: 503.1424; Mp: 243 °C (decomp.)

N-(6-fluoro-3-formylquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4b



1a **2b** **4b** 63%

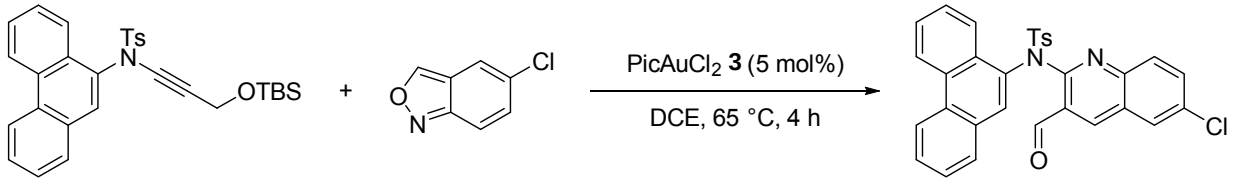
According to **GP.B:** $PicAuCl_2$ **3** (3.8 mg, 9.7 µmol, 5 mol %), anthranil **2b** (40 mg, 291 µmol, 1.5 eq) and N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **1a** (100 mg, 194 µmol, 1.0 eq) were stirred at 65 °C for 4 hours in 1 ml DCE.

Silica gel flash column chromatography with DCM/PE (2:1) as an eluent.

Colourless solid (64 mg, 123 µmol, 63% yield).

R_f (silica, DCM/PE 2:1) = 0.19; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) = 2.49 (s, 3H), 7.25 (d, *J* = 6.7 Hz, 2H), 7.50-7.73 (m, 8H), 7.76 (s, 1H), 7.94 (dd, *J* = 10.1, 5.2 Hz, 1H), 8.62-8.86 (m, 4H), 11.03 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): 21.9 (q), 112.2 (d), 112.5 (d), 122.8 (d), 122.8 (d), 123.1 (d), 123.1 (d), 124.9 (d), 127.1 (d), 127.4 (d), 127.4 (d), 128.2 (d), 129.2 (d), 129.3 (d), 130.0 (d), 130.7 (s), 130.8 (s), 131.0 (s), 131.4 (d), 131.6 (d), 131.6 (s), 131.9 (d), 134.1 (s), 134.9 (s), 139.2 (d), 139.3 (d), 144.7 (s), 145.6 (s), 152.3 (s), 161.2 (d, *J* = 251.3 Hz), 188.8 (d); IR (ATR): ν̃ [cm^{-1}] = 3066, 2890, 1695, 1625, 1592, 1564, 1494, 1449, 1387, 1357, 1342, 1305, 1251, 1232, 1218, 1207, 1185, 1163, 1148, 1128, 1111, 1101, 1088, 1060, 1040, 977, 964, 930, 896, 864, 847, 836, 817, 786, 745, 725, 667, 642, 626, 605; HRMS-DART pos: Calc. for $C_{31}H_{22}FN_2O_3S^+$: 521.1330 m/z, found: 521.1303 m/z; mp: 215 °C (decomp.)

N-(6-chloro-3-formylquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4c



1a **2c** **4c** 65%

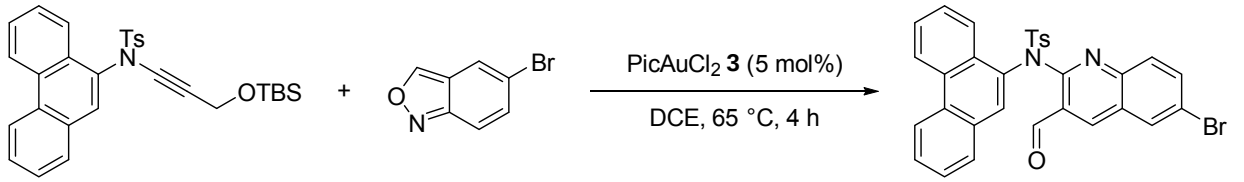
According to **GP.B**: $PicAuCl_2$ **3** (3.8 mg, 9.7 µmol, 5 mol %), anthranil **2c** (45 mg, 291 µmol, 1.5 eq) and N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **1a** (100 mg, 194 µmol, 1.0 eq) were stirred at 65 °C for 4 hours in 1 ml DCE.

Silica gel flash column chromatography with DCM/PE (3:1) as an eluent.

Colourless solid (68 mg, 127 µmol, 65% yield).

R_f (silica, DCM/PE 1:1.5) = 0.39; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) = 2.49 (s, 3H), 7.25 (d, *J* = 8.6 Hz, 2H), 7.52-7.62 (m, 3H), 7.63-7.78 (m, 6H), 7.87 (d, *J* = 9.0 Hz, 1H), 7.92 (d, *J* = 2.3 Hz, 1H), 8.60-8.75 (m, 4H), 10.99 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 21.9 (q), 122.8 (d), 123.1 (d), 124.9 (d), 127.1 (d), 127.4 (d), 127.5 (d), 127.9 (d), 128.2 (d), 128.3 (s), 129.2 (d), 129.3 (d), 130.0 (d), 130.5 (d), 132.0 (d), 133.5 (d), 134.9 (s), 139.0 (d), 144.7 (s), 146.8 (s), 153.0 (s), 188.6 (d); FTIR (Neat) v [cm^{-1}]: 3277, 2963, 2906, 2872, 1594, 1494, 1464, 1444, 1419, 1379, 1337, 1282, 1258, 1189, 1165, 1109, 1085, 977, 892, 844, 834, 786, 752, 719, 696, 660, 631, 619; HRMS-DART: Calc. for $C_{31}H_{22}N_2O_3SCl^+$: 537.1034 m/z, found: 537.1039 m/z; mp: 229 °C (decomp.).

N-(6-bromo-3-formylquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4d



1a **2d** **4d** 51%

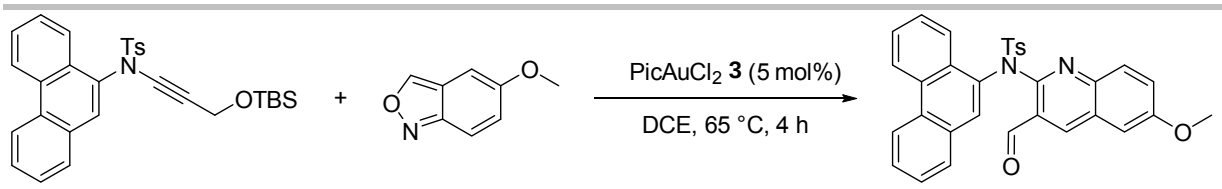
According to **GP.B**: $PicAuCl_2$ **3** (3.8 mg, 9.7 µmol, 5 mol %) and anthranil **2d** (58 mg, 291 µmol, 1.5 eq) in 1 ml DCE and N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **1a** (100 mg, 194 µmol, 1.0 eq) were stirred at 65 °C for 4 hours in 1 ml DCE.

Silica gel flash column chromatography with DCM/PE (3:1) as an eluent.

Colourless solid (58 mg, 100 µmol, 51% yield).

R_f (silica, DCM/PE 1.5:1) = 0.19; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 2.49 (s, 3H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 8.3 Hz, 2H), 7.58 (dt, *J* = 11.0, 4.0 Hz, 1H), 7.64-7-73 (m, 5H), 7.80 (d, *J* = 9.0 Hz, 1H), 7.86 (dd, *J* = 9.0, 2.1 Hz, 1H), 8.10 (d, *J* = 2.1 Hz, 1H), 8.62-8.73 (m, 4H), 10.98 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): 21.9 (q), 122.0 (s), 122.8 (d), 123.1 (d), 124.9 (d), 127.1 (d), 127.4 (d), 127.5 (d), 129.2 (d), 129.3 (d), 130.0 (d), 130.5 (d), 131.3 (d), 134.1 (s), 134.8 (s), 136.0 (d), 138.9 (d), 144.7 (s), 147.0 (s), 153.0 (s), 188.6 (d); FTIR: v [cm^{-1}]: 3061, 2924, 2877, 1695, 1597, 1579, 1483, 1453, 1426, 1406, 1386, 1350, 1307, 1234, 1218, 1183, 1160, 1124, 1106, 1087, 1060, 1039, 1019, 976, 940, 926, 902, 854, 831, 814, 763, 745, 722, 693, 672, 645, 618; HRMS-DART: Calc. for $C_{31}H_{22}N_2O_3SBr^+$: 583.0509 m/z, found: 583.0511 m/z; mp: 227 °C.

N-(3-formyl-6-methoxyquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4e



1a **2e** **4e** 89%

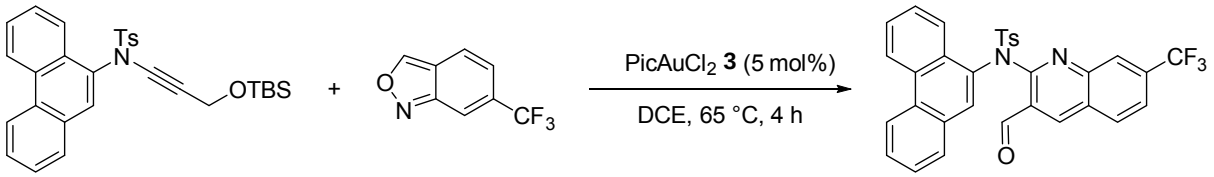
According to **GP.A**: $PicAuCl_2$ **3** (1.9 mg, 4.9 µmol, 5 mol %), anthranil **2e** (29 mg, 194 µmol, 2.0 eq), and N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **1a** (50 mg, 97 µmol, 1.0 eq) were stirred at 65 °C for 4 hours in 1 ml DCE.

Silica gel flash column chromatography with DCM (100%) as an eluent.

Colourless solid (46 mg, 86 µmol, 89% yield).

R_f (silica, DCM/PE 2:1) = 0.29; ^{1}H NMR (700 MHz, $CDCl_3$) δ (ppm) = 2.49 (s, 3H), 3.93 (s, 3H), 7.17 (d, *J* = 2.5 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.44 (dd, *J* = 9.2, 2.6 Hz, 1H), 7.49-7.60 (m, 3H), 7.63-7.74 (m, 3H), 7.80-7.83 (m, 2H), 8.66 (d, *J* = 8.3 Hz, 1H), 7.68-7.72 (m, 2H), 8.73-8.76 (m, 1H), 11.10 (s, 1H); ^{13}C NMR (175 MHz, $CDCl_3$): 21.9 (q), 55.9 (q), 106.1 (d), 122.8 (d) 123.0 (d), 125.1 (d), 125.8 (d), 127.0 (d), 127.3 (d), 127.4 (d), 127.8 (s), 128.1 (d), 129.1 (d), 129.3 (d), 130.0 (d), 130.4 (d), 130.6 (s), 130.9 (s), 131.1 (s), 131.6 (s), 131.7 (s), 134.3 (s), 134.9 (s), 138.2 (d), 144.5 (s), 144.8 (s), 150.8 (s), 159.0 (s), 189.5 (d); IR (ATR): ṽ [cm^{-1}] = 3061, 2968, 2917, 2838, 1682, 1621, 1582, 1497, 1452, 1425, 1375, 1351, 1305, 1249, 1225, 1196, 1163, 1125, 1104, 1088, 1064, 1037, 1021, 968, 937, 897, 843, 818, 785, 760, 745, 717, 672, 621, 609; HRMS-DART pos: Calc. for $C_{32}H_{25}N_2O_4S^+$: 533.1530 m/z, found: 533.1531 m/z; mp: 217 °C (decomp.).

N-(3-formyl-7-(trifluoromethyl)quinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4f



1a **2f** **4f** 59%

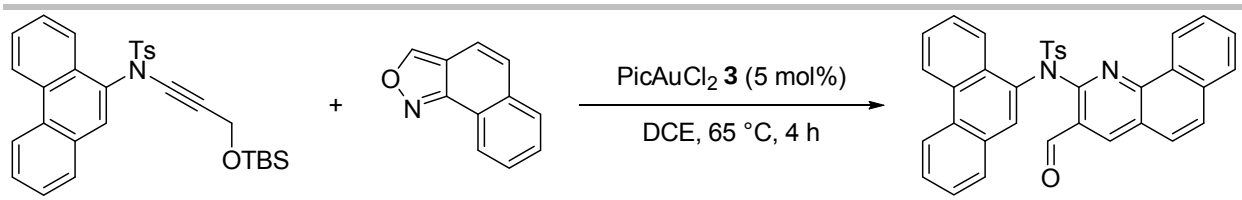
According to **GP.A**: $PicAuCl_2$ **3** (3.8 mg, 9.7 µmol, 5 mol %), anthranil **2f** (54 mg, 291 µmol, 1.5 eq) and N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **1a** (100 mg, 194 µmol, 1.0 eq) were stirred at 65 °C for 4 hours in 1 ml DCE.

Silica gel flash column chromatography with DCM/PE (3:1) as an eluent.

Beige solid (65 mg, 114 µmol, 59% yield).

R_f (silica, DCM/PE 3:1) = 0.33; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) = 2.50 (s, 3H), 7.28 (d, *J* = 8.2 Hz, 2H), 7.57 (d, *J* = 8.3 Hz, 2H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.66-7.75 (m, 5H), 7.77 (dd, *J* = 8.5, 1.2 Hz, 1H), 8.09 (d, *J* = 8.5 Hz, 1H), 8.20 (s, 1H), 8.58-8.65 (m, 1H), 8.68 (d, *J* = 8.3 Hz, 1H), 8.69-8.74 (m, 1H), 8.83 (s, 1H), 11.00 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 21.9 (q), 122.6 (s), 122.8 (d), 123.2 (d), 123.6 (q), 124.7 (d), 126.6 (q), 127.2 (d), 127.5 (d), 127.5 (d), 128.0 (s), 128.4 (d), 129.0 (s), 129.3 (d), 129.4 (d), 130.0 (d), 130.7 (d), 130.7 (s), 130.7 (s), 130.9 (s), 131.7 (s), 132.2 (d), 133.8 (s), 134.1 (s), 134.7 (s), 139.8 (d), 145.0 (s), 147.5 (s), 153.9 (s), 188.3 (d); ^{19}F-NMR (471 MHz, $CDCl_3$): -62.96; IR (ATR): ṽ [cm^{-1}] = 1694, 1590, 1497, 1449, 1421, 1385, 1359, 1345, 1325, 1304, 1285, 1232, 1214, 1186, 1164, 1123, 1088, 1059, 1040, 973, 935, 897, 847, 816, 764, 726, 707, 672, 662, 614; HRMS-DART pos: Calc. for $C_{32}H_{22}F_3N_2O_3S^+$: 571.1298 m/z, found: 571.1277 m/z; mp: 227 °C (decomp.).

N-(3-formylbenzo[h]quinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4g



1a **2g** **4g** 27%

According to **GP.B**: $PicAuCl_2$ **3** (3.8 mg, 9.7 µmol, 5 mol %), anthranil **2g** (66 mg, 388 µmol, 2.0 eq) and N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **1a** (100 mg, 194 µmol, 1.0 eq) were stirred at 65 °C for 4 hours in 1 ml DCE.

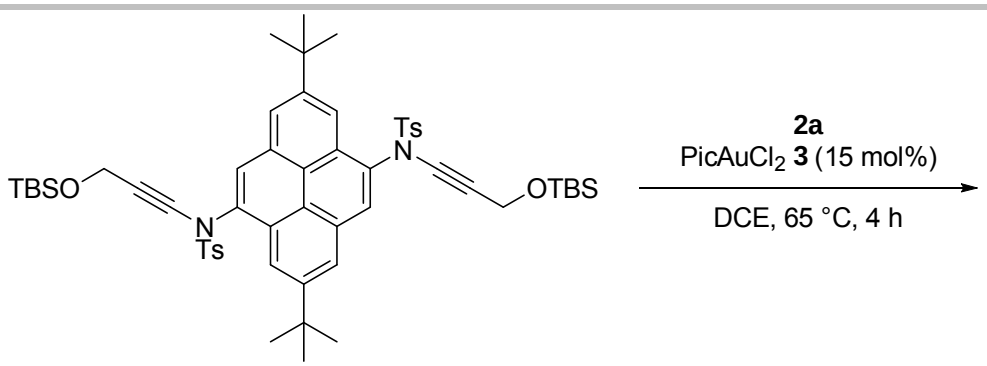
Silica gel flash column chromatography with DCM/PE (3:1) as an eluent.

Pale yellow solid (29 mg, 52 µmol, 27% yield).

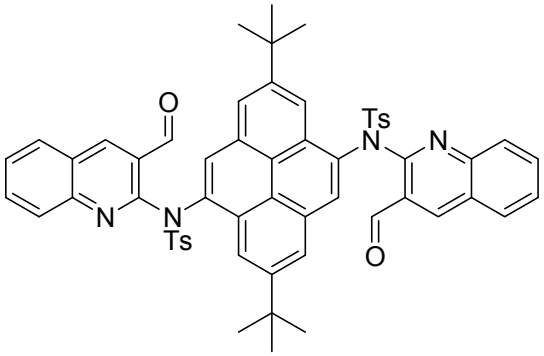
R_f (silica, DCM/PE 3:1) = 0.22; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) = 2.52 (s, 3H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.65-7.81 (m, 7H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 8.14 (s, 1H), 8.63 (d, *J* = 8.1 Hz, 1H), 8.67 (d, *J* = 8.3 Hz, 1H), 8.70 (d, *J* = 8.1 Hz, 1H), 8.80-8.90 (m, 2H), 11.34 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): 21.9 (q), 122.8 (d), 123.0 (d), 125.0 (d), 125.4 (d), 125.4 (d), 125.7 (s), 127.1 (d), 127.3 (d), 127.4 (d), 127.5 (d), 128.1 (d), 128.3 (d), 128.6 (s), 129.3 (d), 129.4 (d), 129.7 (d), 129.8 (d), 129.9 (d), 130.6 (s), 130.7 (s), 130.9 (s), 131.2 (s), 131.8 (d), 134.0 (s), 134.7 (s), 134.9 (s), 138.7 (d), 144.5 (s), 148.0 (s), 152.2 (s), 189.4 (d); IR (ATR): ṽ [cm^{-1}] = 3055, 2888, 1687, 1583, 1483, 1451, 1404, 1357, 1305, 1261, 1226, 1213, 1186, 1161, 1133, 1107, 1086, 1066, 1040, 1020, 998, 961, 922, 896, 873, 836, 816, 801, 754, 730, 701, 665, 643, 617; HRMS-DART pos: Calc. for $C_{35}H_{25}N_2O_3S^+$: 553.1580 m/z, found: 553.1556 m/z; mp: 259 °C (decomp.).

1.3.3. Gold-catalysed synthesis of quinolines 10a-d

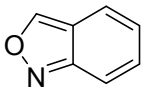
N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-formylquinolin-2-yl)-4-methylbenzenesulfonamide) 10a



9



10a 73%

2a = 

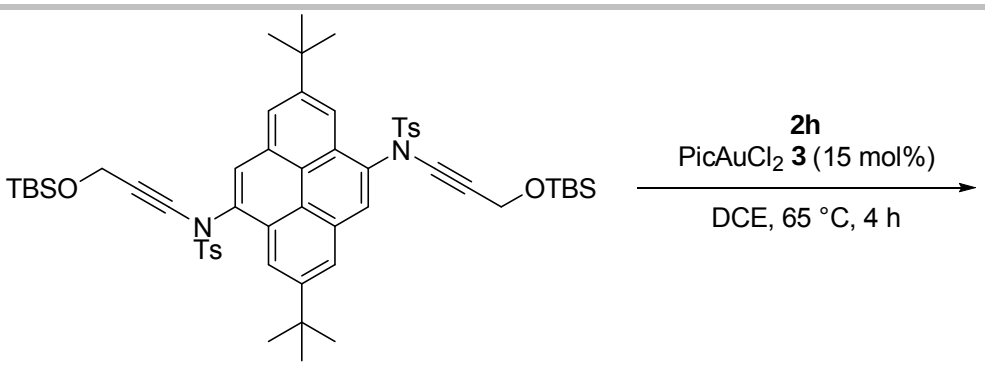
According to **GP.C**: $PicAuCl_2$ **3** (5.9 mg, 15.2 µmol, 15 mol %), anthranil **2a** (48 mg, 404 µmol, 4 eq), and N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methylbenzenesulfonamide) **9** (100 mg, 101 µmol, 1.0 eq) were stirred at 65 °C for 4 hours in 1 ml DCE.

Silica gel flash column chromatography with DCM (100%) as an eluent.

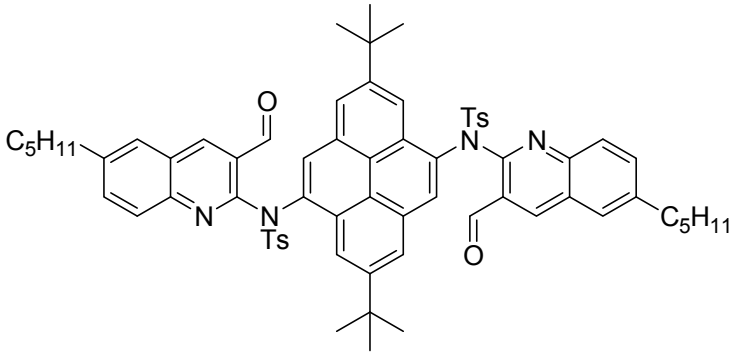
beige solid (71 mg, 73.7 µmol, 73 % yield).

R_f (silica, DCM) = 0.68; ^{1}H NMR (TCE-d^2, 500 MHz, T = 100 °C), δ [ppm] = 1.26 (d, 18H, *J* = 1.3 Hz,), 2.38 (s, 6H), 7.17 (d, 4H, *J* = 7.9 Hz), 7.57 (d, 2H, *J* = 7.2 Hz), 7.70 (d, 4H, *J* = 7.9 Hz), 7.79-7.85 (m, 2H), 7.88 (d, 2H, *J* = 8.0 Hz), 7.98-8.11 (m, 4H), 8.38 (s, 2H), 8.62 (s, 4H), 10.94 (s, 2H); ^{13}C NMR could not be measured due to low solubility; FTIR (Neat) ν [cm^{-1}]: 3103, 2962, 2868, 1916, 1699, 1618, 1585, 1494, 1455, 1421, 1354, 1256, 1161, 1146, 1102, 1086, 1019, 982, 956, 934, 915, 871, 858, 814, 761, 707, 689, 664, 629; HRMS-DART pos (DCM): calc for $C_{58}H_{51}N_4O_6S_2^+$: 963.3245, found: 963.3201; mp: >300 °C.

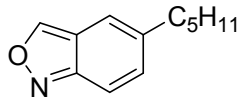
N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-formyl-6-pentylquinolin-2-yl)-4-methylbenzenesulfonamide) 10b



9



10b 52%

2b = 

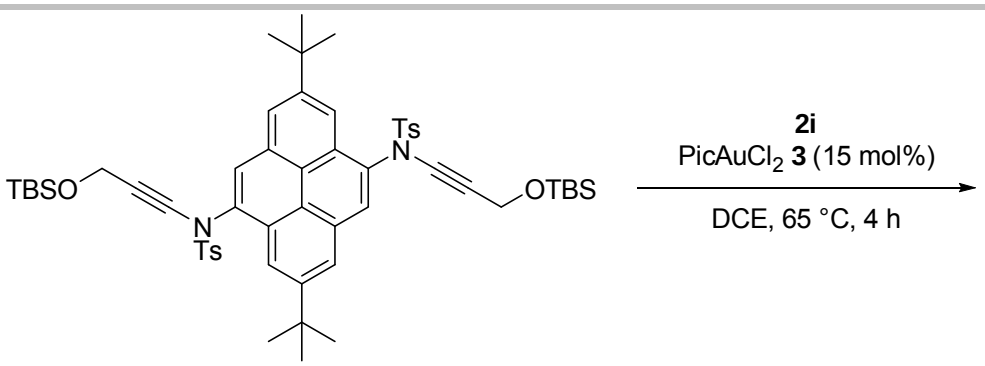
According to **GP.C:** $PicAuCl_2$ **3** (5.9 mg, 15 µmol, 15 mol %), anthranil **2h** (95 mg, 50.5 µmol, 5 eq), and N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methylbenzenesulfonamide) **9** (100 mg, 101 µmol, 1.0 eq) were stirred at 65 °C for 4 hours in 1 ml DCE.

Silica gel flash column chromatography with DCM/PE (3:1) as an eluent.

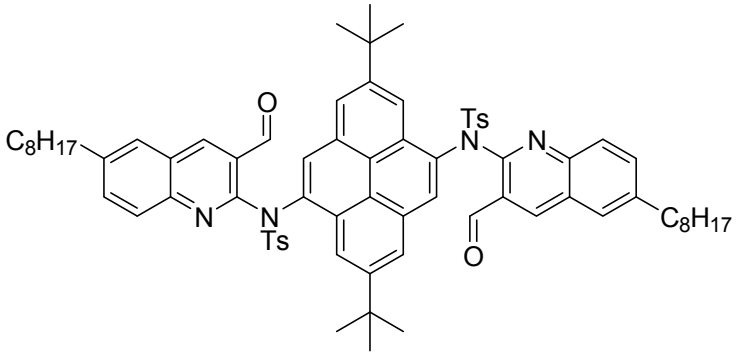
Beige solid (58 mg, 52 µmol, 52 % yield).

R_f (silica, DCM/PE (2:1)) = 0.07; ^{1}H NMR ($CDCl_3$, 500 MHz), δ [ppm] = 0.88 (t, 6H, *J* = 6.7 Hz), 1,23 (s, 18H), 1.29-1.39 (m, 9H), 1.65-1.74 (m, 4H), 2.42 (s, 6H), 2.80 (t, 4H, *J* = 7.4 Hz), 7.20 (s, 4H), 7.66 (s, 2H), 7.71 (d, 2H, *J* = 8.6 Hz), 7.75 (d, 4H, *J* = 7.0 Hz), 8.00 (d, 2H, *J* = 8.7 Hz), 8.05 (s, 2H), 8.40 (s, 2H), 8.59 (s, 4H), 10.99 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) = 14.2 (q), 21.8 (q), 22.6 (t), 30.9 (t), 31.4 (t), 31.7 (q), 35.4 (s), 35.9 (t), 121.6 (d), 123.9 (s), 124.1 (d), 126.8 (s), 127.0 (s), 127.7 (d), 128.7 (d), 129.2 (d), 129.8 (d), 130.1 (s), 133.6 (d), 134.5 (d), 134.8 (s), 136.8 (s), 139.9 (d), 143.2 (s), 144.2 (s), 147.4 (s), 149.3 (s), 152.7 (s), 188.9 (d); FTIR (Neat) ν [cm^{-1}]: 2957, 2928, 2861, 1694, 1584, 1495, 1442, 1360, 1260, 1165, 1114, 1089, 932, 811, 706, 689, 664; HRMS-ESI pos (DCM/MeOH): calc for $C_{68}H_{71}N_4O_6S_2^+$: 1103.4810, found: 1103.4827; Mp: 171 °C (decomp.).

N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-formyl-6-octylquinolin-2-yl)-4-methylbenzenesulfonamide) 10c

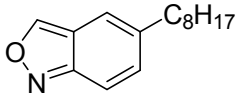


9



10c 81%

2i =



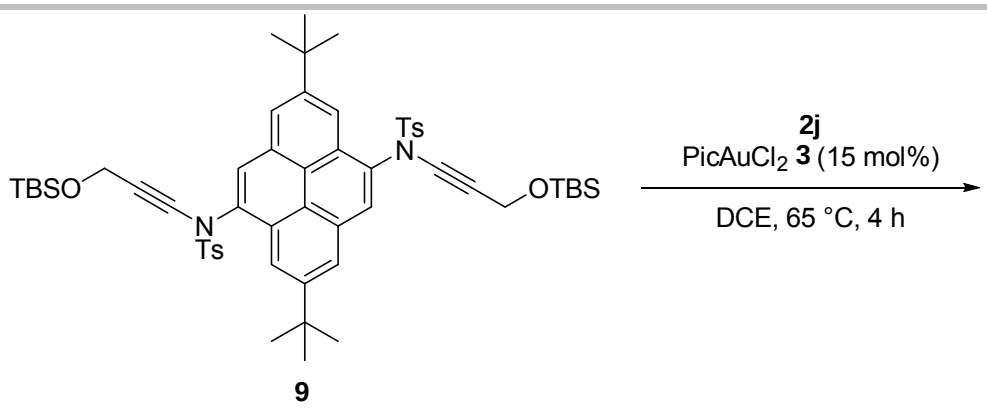
According to **GP.C**: $PicAuCl_2$ **3** (5.9 mg, 15 µmol, 15 mol %), anthranil **2i** (116 mg, 404 µmol, 4.0 eq), and N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methylbenzenesulfonamide) **9** (100 mg, 101 µmol, 1.0 eq) were stirred at 65 °C for 4 hours in 1 ml DCE.

Silica gel flash column chromatography with DCM/PE (3:1) as an eluent.

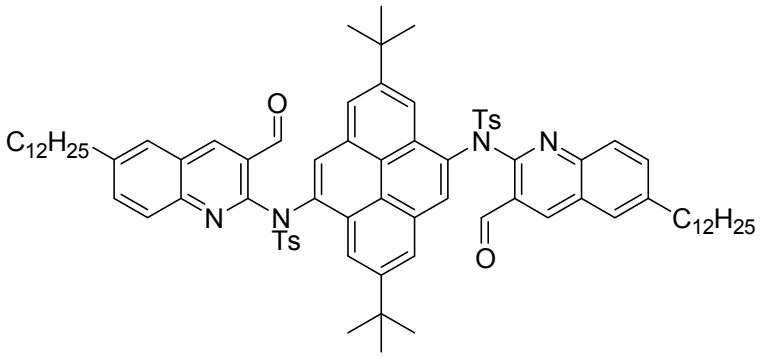
Beige solid (97 mg, 82 µmol, 81% yield).

R_f (silica, DCM) = 0,37; ^{1}H NMR ($CDCl_3$, 300 MHz), δ [ppm] = 0.87 (t, 3H, *J* = 6.5 Hz), 1.15-1.40 (m, 38H), 1.63-1.76 (m, 4H), 2.42 (s, 6H), 2.80 (t, 4H, *J* = 7.5 Hz), 7.20 (d, 4H, *J* = 7.7 Hz), 7.61-7.84 (m, 8H), 7.99 (d, 2H, *J* = 8.6 Hz), 8.05 (d, 2H, *J* = 1.2 Hz), 8.40 (s, 2H), 8.60 (s, 2H), 10.99 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) = 14.2 (q), 21.7 (q), 22.8 (t), 29.3 (t), 29.4 (t), 29.6 (t), 31.2 (t), 31.7 (q), 32.0 (t), 35.4 (s), 36.0 (t), 121.6 (d), 123.9 (s), 124.1 (d), 126.9 (s), 127.2 (s), 127.7 (d), 128.7 (d), 128.7 (s), 129.2 (d), 129.8 (d), 130.2 (s), 133.7 (d), 134.5 (d), 134.8 (s), 136.9 (s), 139.9 (d), 143.2 (s), 144.2 (s), 147.4 (s), 149.3 (s), 152.7 (s), 188.9 (d); FTIR (Neat) ν [cm^{-1}]: 2954, 2925, 2855, 1695, 1584, 1495, 1442, 1360, 1308, 1253, 1165, 1116, 1089, 1043, 964, 897, 836, 812, 706, 689, 664, 638; HRMS-ESI pos (DCM/MeOH): calc for $C_{74}H_{83}N_4O_6S_2^+$: 1187.5749, found: 1187.5768; Mp: 142 °C.

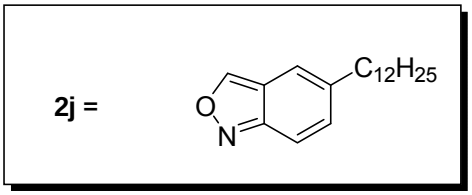
N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(6-dodecyl-3-formylquinolin-2-yl)-4-methylbenzenesulfonamide) 10d



9



10d 76%



According to **GP.C**: $PicAuCl_2$ **3** (3.0 mg, 7.6 µmol, 15 mol %), and anthranil **2j** (58 mg, 202 µmol, 4.0 eq), and N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methylbenzenesulfonamide) **9** (50 mg, 50.5 µmol, 1.0 eq) were stirred at 65 °C for 4 hours in 0.5 ml DCE.

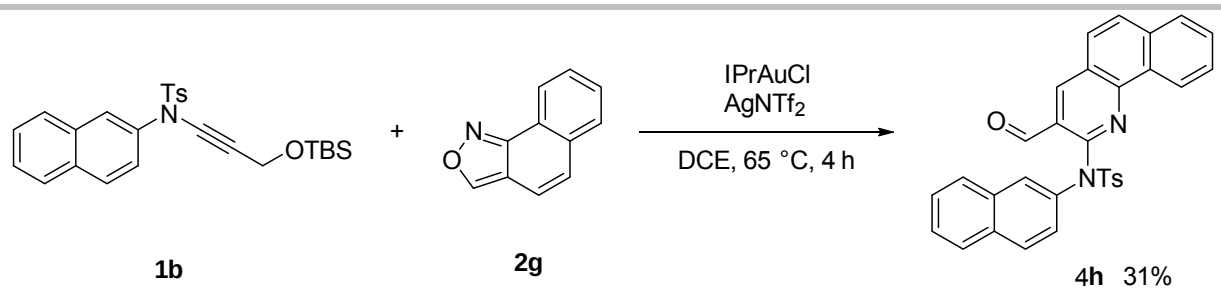
Silica gel flash column chromatography with DCM (100%) as an eluent.

Brownish solid (50 mg, 38.5 µmol, 76% yield).

R_f (silica, DCM) = 0,6; ^{1}H NMR (CD_2Cl_2, 500 MHz), δ [ppm] = 0.86 (t, 6H, *J* = 6.9 Hz), 1.25-1.32 (m, 54H), 1.68-1.71 (m, 4H), 2.42 (s, 6H), 2.80 (t, 4H, *J* = 7.6 Hz), 7.23 (d, 4H, *J* = 6.9 Hz), 7.63-7.84 (m, 8H), 7.99 (d, 2H, *J* = 8.7 Hz), 8.11 (s, 2H), 8.38 (s, 2H), 8.61 (s, 4H), 10.96 (s, 2H); ^{13}C NMR (CD_2Cl_2, 125 MHz) = 14.6 (q), 22.1 (q), 23.4 (t), 29.9 (t), 30.1 (t), 30.2 (t), 30.3 (t), 30.3 (t), 30.4 (t), 31.8 (t), 32.0 (q), 32.6 (t), 35.9 (t), 36.5 (t), 122.1 (d), 124.3 (s), 124.6 (d), 127.4 (s), 128,2 (d), 129.0 (d), 129.4 (s), 129.9 (d), 130.3 (d), 130.7 (s), 134.2 (d), 135.2 (d), 135.4 (s), 137.1 (s), 140.4 (d), 144.0 (s), 145.2 (s), 147.9 (s), 150.1 (s), 153.0 (s), 189.2 (d); FTIR (Neat) ν [cm^{-1}]: 2953, 2924, 2853, 1659, 1584, 1495, 1442, 1360, 1253, 1165, 1089, 962, 812, 706, 689, 663; HRMS-ESI pos (DCM/MeOH): calc for $C_{82}H_{99}N_4O_6S_2$: 1299.0000, found: 1299.0001; Mp: 149 °C.

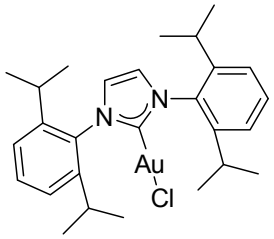
1.3.4. Gold-catalysed synthesis of quinoline 4h

N-(3-formylbenzo[h]quinolin-2-yl)-4-methyl-N-(naphthalen-2-yl)benzenesulfonamide 4h



1b **2g** 4**h** 31%

IPrAuCl =



IPrAuCl (6.7 mg, 10.7 µmol, 5 mol%) and $AgNTf_2$ (4.2 mg, 10.7 µmol, 5 mol%) were stirred in 1.0 ml DCE for 5 min at room temperature until naphtho[1,2-c]isoxazole **2g** (55 mg, 322 µmol, 1.5 eq) in 0.5 ml DCE and N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methyl-N-(naphthalen-2-yl)benzenesulfonamide **1b** (100 mg, 215 µmol, 1.0 eq) in 0.5 ml DCE were added and the reaction mixture was stirred at 65 °C for 4 hours. Then, after cooling down to room temperature, the solvent was removed under reduced pressure and the crude product was purified via silica gel flash column chromatography with DCM (100%) as an eluent. The product was then further purified by washing with a small amount of methanol (1.5 ml). The product was isolated as beige solid (33 mg, 66 µmol, 31% yield).

R_f: 0.41 (silica, DCM (100%)); ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) = 2.52 (s, 3H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.41-7.54 (m, 2H), 7.61 (d, *J* = 8.2 Hz, 2H), 7.68-7.85 (m, 7H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.96 (d, *J* = 7.9 Hz, 1H), 8.08 (s, 1H), 8.71 (d, *J* = 8.1 Hz, 1H), 8.80 (s, 1H), 10.95 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) = 21.9 (q), 125.6 (d), 125.8 (d), 126.0 (s), 126.4 (d), 126.8 (d), 127.1 (d), 127.5 (d), 127.8 (d), 128.0 (s), 128.2 (d), 128.3 (d), 128.5 (d), 129.3 (d), 129.4 (d), 129.8 (d), 130.0 (d), 130.8 (s), 132.7 (s), 133.4 (s), 135.0 (s), 136.3 (s), 137.2 (s), 138.8 (d), 144.1 (s), 148.5 (s), 152.7 (s), 189.6 (d); IR (ATR): ṽ [cm^{-1}] = 3066, 2858, 1688, 1598, 1580, 1508, 1485, 1465, 1444, 1405, 1378, 1344, 1270, 1251, 1231, 1163, 1133, 1123, 1090, 986, 962, 932, 880, 857, 806, 751, 724, 711, 667, 647, 629, 608; HRMS-EI+: Calc. for $C_{31}H_{22}N_2O_3S^+$: 502.1346 m/z, found: 502.1325 m/z; mp.: 201 °C.

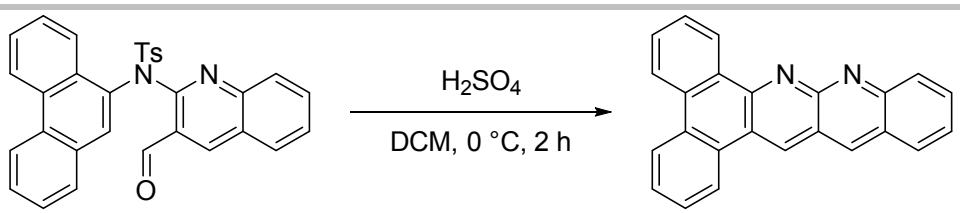
1.4. Synthesis of naphthyridine-based PAHs

1.4.1. General procedure for condensation to phenanthronaphthyridines

GP.D: Qinoline **4a-h** (1.0 eq) was dissolved in DCM (1 ml per mg substance) and the solution as cooled to 0 °C. Then H_2SO_4 (1 vol% of solvent) was added dropwise and the reaction mixture was stirred at 0 °C for 2 hours. Then 1.0 ml of ethylenediamine and 30 ml of a diluted K_2CO_3 solution were added. The layers were separated and the aqueous layer was extracted with DCM (2 x 50 ml). The combined organic layer was washed with water (3 x 30 ml), dried over Na_2SO_4, and filtered. The solvent was removed under reduced pressure and the crude product was purified via recrystallization from $CHCl_3$/hexane.

1.4.2. Synthesis of naphthyridines 5a-h

benzo[b]phenanthro[9,10-g][1,8]naphthyridine 5a



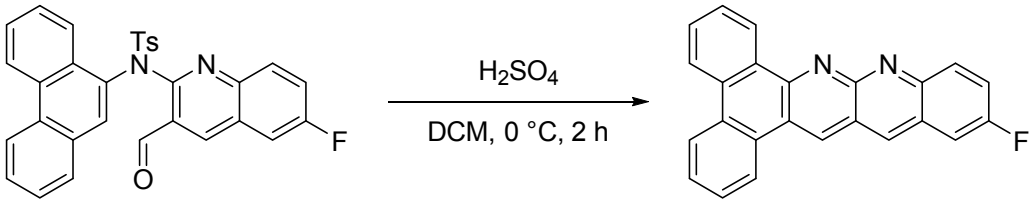
4a **5a** Quant.

According to **GP.D**, N-(3-formylquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 1 (60 mg, 119 µmol, 1.0 eq) and 0.6 ml H_2SO_4 were stirred in 60 ml DCM.

The product was isolated as yellow solid (40 mg, 119 µmol, quant, yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.53-7.57 (m, 1H), 7.66 (pd, 2H, *J* = 7.1, 1.3 Hz), 7.71-7.7 (m, 1H), 7.77-7.82 (m, 1H), 7.82-7.88 (m, 1H), 8.05 (d, *J* = 8.4 Hz, 1H), 8,46 (d, 1H, *J* = 8.8 Hz), 8.49 (d, 1H, *J* = 7.9 Hz), 8.51-8.56 (m, 1H), 8,59-8,64 (m, 1H), 8.99 (s, 1H), 9.40 (s, 1H), 9,77 (dd, 1H, *J* = 8,0 Hz, 1,2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$, 50 °C): 120.4 (s), 122.9 (d), 123.9 (d), 124.1 (d), 124.6 (s), 126.3 (d), 127.2 (s), 128.1 (d), 128.2 (d), 128,2 (s), 128.3 (s), 128.9 (d), 129.0 (s), 130.3 (d), 130.4 (s), 131.0 (d), 131.2 (s), 131.6 (d), 131.8 (d), 133.3 (s), 138.0 (d), 152.1 (s), 153.4 (s), 153.6 (s); FTIR (Neat) ν [cm^{-1}]: 3058, 3024, 2960, 2925, 2852, 1953, 1628, 1598, 1562, 1543, 1509, 1491, 1443, 1403, 1385, 1353, 1336, 1307, 1275, 1170, 1130, 1053, 1040, 962, 924, 854, 805, 774, 755, 744, 718, 694, 669, 612; UV/Vis [nm]: 251, 261, 275, 292, 303, 323, 373, 394, 414, 443; HRMS-DART: Calc. for $C_{24}H_{15}N_2^+$: 331.1230, found: 331.1229; mp: >300°C.

13-fluorobenzo[b]phenanthro[9,10-g][1,8]naphthyridine 5b



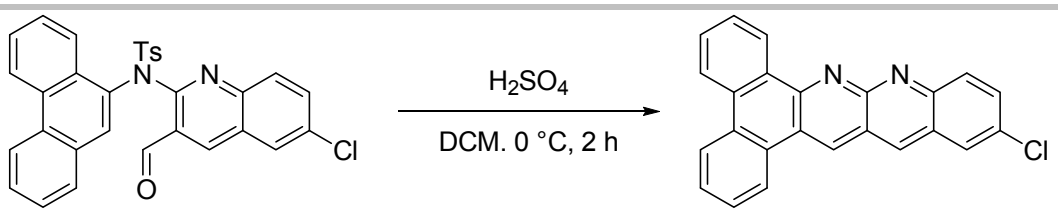
4b **5b** 88%

According to **GP.D**, N-(6-fluoro-3-formylquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **4b** (56 mg, 108 µmol, 1.0 eq) and 0.56 ml H_2SO_4 were stirred in 56 ml DCM.

Yellow solid (32 mg, 91 µmol, 88% Yield).

^{1}H NMR (600 MHz, $CDCl_3$, 50 °C) δ (ppm) = 7.57 (dd, *J* = 8.7, 2.6 Hz, 1H), 7.60-7.69 (m, 3H), 7.71-7.77 (m, 1H), 7.77-7.82 (m, 1H), 8.43 (dd, *J* = 9.5, 5.4 Hz, 1H), 8.48 (d, *J* = 8.0 Hz, 1H), 8.51 (d, *J* = 7.8 Hz, 1H), 8.57 (d, *J* = 7.6 Hz, 1H), 8.87 (s, 1H), 9.31 (s, 1H), 9.73 (dd, *J* = 8.0, 1.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$, 50 °C): 109.5 (d), 109.6 (d), 120.6 (s), 122.9 (d), 123.4 (d), 123.6 (d), 123.9 (d), 124.2 (d), 125.0 (s), 128.1 (d), 128.1 (d), 128.2 (d), 128.7 (s), 129.2 (d), 130.4 (s), 131.2 (d), 131.3 (d), 133.0 (d), 133.1 (d), 133.2 (s), 136.9 (d), 137.0 (d), 149.4 (s), 153.1 (s), 153.3 (s), 160.2 (d, *J* = 251.3 Hz); ^{19}F-NMR (470 MHz, $CDCl_3$, 50 °C): -112.21; IR (ATR): ῡ [cm^{-1}] = 3058, 1915, 1832, 1756, 1638, 1595, 1562, 1545, 1510, 1484, 1463, 1440, 1399, 1377, 1334, 1305, 1288, 1249, 1228, 1193, 1174, 1140, 1129, 1114, 1039, 974, 953, 916, 887, 824, 802, 772, 751, 735, 719, 695, 656, 617; UV/Vis (6.2 µg/ml): λ [nm]: 251, 261, 278, 293, 304, 313, 375, 397, 418; HRMS-EI+: Calc. for $C_{24}H_{13}N_2F^+$: 348.1057 m/z, found: 348.1051 m/z; mp: 287 °C (decomp.).

13-chlorobenzo[b]phenanthro[9,10-g][1,8]naphthyridine 5c



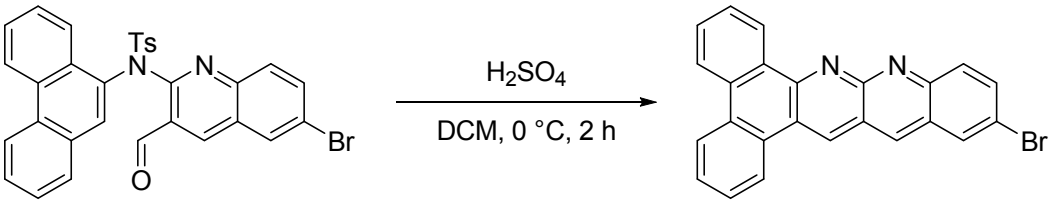
4c **5c** 88%

According to **GP.D**, N-(6-chloro-3-formylquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **4c** (30 mg, 56 µmol, 1.0 eq) and 0.3 ml H_2SO_4 were stirred in 30 ml DCM.

Yellow solid (18 mg, 49 µmol, 88% yield).

^{1}H NMR (600 MHz, $CDCl_3$, 50 °C) δ (ppm) = 7.56-7.70 (m, 3H), 7.73 (t, *J* = 7.5 Hz, 1H), 7.76-7.82 (m, 1H), 7.85 (d, *J* = 1.9 Hz, 1H), 8.29 (d, *J* = 9.2 Hz, 1H), 8.39-8.57 (m, 3H), 8.71 (s, 1H), 9.19 (s, 1H), 9.69 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$, 50 °C): 120.5 (s), 122.9 (d), 123.9 (d), 124.1 (d), 124.8 (s), 126.1 (d), 127.0 (s), 128.1 (d), 128.2 (d), 128.5 (s), 129.2 (d), 130.3 (s), 130.7 (s), 131.4 (d), 131.5 (d), 131.8 (d), 132.1 (s), 132.7 (d), 133.3 (s), 136.8 (d), 150.1 (s), 153.4 (s), 153.5 (s); 0 (d, 1C), 124.7 (s, 1C), 124.0 (d, 1C), 123.7 (d, 1C), 122.8 (d, 1C), 120.4 (s, 1C); FTIR: v [cm^{-1}]: 3428, 3065, 3051, 2983, 2360, 1927, 1790, 1738, 1708, 1622, 1598, 1562, 1543, 1509, 1487, 1446, 1433, 1401, 1380, 1338, 1305, 1280, 1249, 1229, 1163, 1133, 1108, 1067, 1040, 968, 931, 882, 855, 823, 803, 787, 773, 749, 730, 718, 694, 639, 618; UV/Vis (9.0 µg/ml): λ [nm]: 446, 421, 399, 379, 305, 294, 280, 251; HRMS-DART: Calc. for $C_{24}H_{14}N_2Cl^+$: 365.0840 m/z, found: 365.0837 m/z; mp: > 300 °C.

13-bromobenzo[b]phenanthro[9,10-g][1,8]naphthyridine 5d



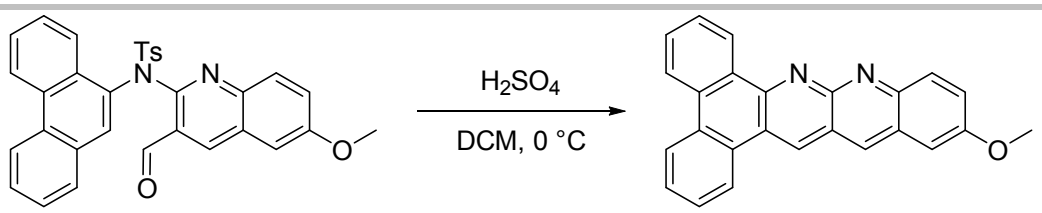
4d **5d** quant.

According to **GP.D**, N-(6-bromo-3-formylquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **4d** (30 mg, 51 µmol, 1.0 eq) and 0.3 ml H_2SO_4 were stirred in 30 ml DCM.

Yellow solid (21 mg, 51 µmol, quant. Yield).

^{1}H NMR (400 MHz, $CDCl_3$, 50 °C) δ (ppm) = 7.56-7.70 (m, 2H), 7.70-7.87 (m, 3H), 8.10 (d, *J* = 2.1 Hz, 1H), 8.25 (d, *J* = 9.3 Hz, 1H), 8.40-8.60 (m, 3H), 8.77 (s, 1H), 9.26 (s, 1H), 9.71 (dd, *J* = 8.0, 1.4 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$, 50 °C): 120.4 (s), 120.5 (s), 123.0 (d), 123.9 (d), 124.2 (d), 125.0 (s), 127.6 (s), 128.1 (d), 128.2 (d), 128.6 (s), 129.2 (d), 129.7 (d), 130.4 (s), 130.8 (s), 131.4 (d), 131.5 (d), 131.8 (d), 133.3 (s), 135.1 (d), 136.8 (d), 150.2 (s), 153.5 (s), 153.7 (s); IR (ATR): ṽ [cm^{-1}] = 3517, 3065, 1663, 1618, 1592, 1562, 1542, 1508, 1484, 1431, 1399, 1383, 1336, 1306, 1269, 1252, 1230, 1163, 1132, 1050, 924, 880, 822, 773, 750, 718, 695, 683, 618; UV/Vis (3.2 µg/ml): λ [nm]: 447, 422, 400, 380, 315, 306, 294, 280, 260, 251; HRMS-DART: Calc. for $C_{24}H_{14}N_2Br^+$: 409.0335 m/z, found: 409.0333 m/z; mp: > 300 °C.

13-methoxybenzo[b]phenanthro[9,10-g][1,8]naphthyridine 5e



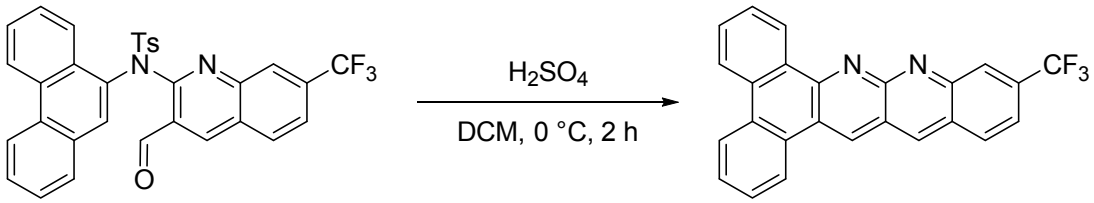
4e **5e** 87%

According to **GP.D**, N-(3-formyl-6-methoxyquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **4e** (36 mg, 68 µmol, 1.0 eq) and 0.36 ml H_2SO_4 were stirred in 36 ml DCM.

Yellow solid (21 mg, 59 µmol, 87% Yield).

^{1}H NMR (400 MHz, $CDCl_3$, 50 °C) δ (ppm) = 3.87 (s, 3H), 6.90 (d, *J* = 2.6 Hz, 1H), 7.37 (dd, *J* = 9.5, 2.7 Hz, 1H), 7.49-7.61 (m, 2H), 7.65-7.78 (m, 2H), 8.21 (d, *J* = 9.5 Hz, 1H), 8.32-8.43 (m, 3H), 8.46 (s, 1H), 8.99 (s, 1H), 9.64-9.73 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$, 50 °C): 55.6 (q), 102.8 (d), 120.3 (s), 122.8 (d), 123.7 (d), 124.0 (d), 124.2 (s), 126.9 (d), 127.8 (d), 127.9 (d), 128.7 (d), 128.8 (s), 130.1 (s), 130.7 (d), 130.8 (d), 131.1 (s), 131.5 (d), 132.9 (s), 134.8 (d), 149.3 (s), 151.9 (s), 152.3 (s), 157.4 (s); IR (ATR): ṽ [cm^{-1}] = 3070, 3033, 3006, 2942, 2915, 2830, 1969, 1837, 1631, 1595, 1561, 1548, 1511, 1484, 1469, 1455, 1437, 1407, 1379, 1306, 1289, 1254, 1231, 1213, 1213, 1192, 1181, 1122, 1040, 1024, 947, 918, 889, 864, 815, 773, 754, 722, 695, 654, 615; HRMS-EI+: Calc. for $C_{25}H_{16}N_2O^+$: 360.1257 m/z, found: 360.1254 m/z; mp: 246 °C (decomp.).

12-(trifluoromethyl)benzo[b]phenanthro[9,10-g][1,8]naphthyridine 5f



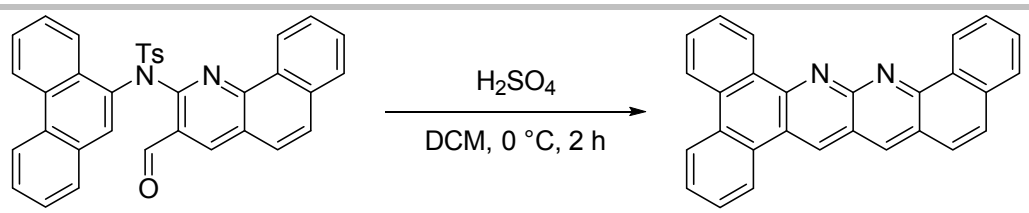
4f **5f** 76%

According to **GP.D**, N-(3-formyl-7-(trifluoromethyl)quinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **4f** (45 mg, 79 µmol, 1.0 eq) and 0.45 ml H_2SO_4 were stirred in 45 ml DCM.

Yellow solid (24 mg, 60 µmol, 76% Yield).

^{1}H NMR (500 MHz, TCE-d^2, 100 °C) δ (ppm) = 7.42-7.98 (m, 5H), 8.07 (d, *J* = 8.6 Hz, 1H), 8.35-8.63 (m, 3H), 8.67 (s, 1H), 8.91 (s, 1H), 9.24 (s, 1H), 9.60 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (125 MHz, TCE-d^2, 100 °C): 121.3 (d), 121.4 (d), 123.1 (d), 124.0 (d), 124.3 (d), 125.2 (s), 125.4 (s), 127.5 (s), 128.3 (d), 128.3 (d), 128.3 (d), 128.6 (s), 129.5 (d), 129.7 (d), 130.5 (s), 130.8 (s), 131.5 (d), 131.7 (d), 132.8 (s), 133.1 (s), 133.5 (s), 138.1 (d), 150.5 (s), 154.0 (s), 154.2 (s); ^{19}F NMR (471 MHz, TCE-d^2, 100 °C): -62.88; IR (ATR): ṽ [cm^{-1}] = 3035, 1644, 1593, 1543, 1509, 1494, 1473, 1453, 1431, 1401, 1385, 1331, 1294, 1271, 1233, 1168, 1142, 1103, 1047, 972, 941, 918, 890, 806, 786, 759, 743, 720, 696, 679, 659, 617; UV/Vis (6.4 µg/ml): λ [nm]: 252, 260, 292, 305, 314, 378, 399, 421; HRMS-EI+: Calc. for $C_{25}H_{13}F_3N_2^+$: 398.1025 m/z, found: 398.1036 m/z; mp: >300 °C.

naphtho[1,2-b]phenanthro[9,10-g][1,8]naphthyridine 5g



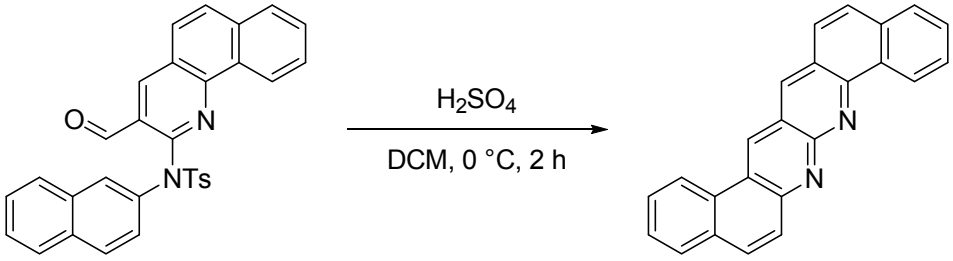
4g **5g** 85%

According to **GP.D**, N-(3-formylbenzo[h]quinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide **4g** (26 mg, 47 µmol, 1.0 eq) and 0.26 ml H_2SO_4 were stirred in 26 ml DCM.

Yellow solid (15 mg, 39.5 µmol, 85% Yield).

^{1}H NMR (500 MHz, TCE-d^2, 100 °C) δ (ppm) = 7.46-8.06 (m, 9H), 8.41-8.59 (m, 2H), 8.59-8.70 (m, 1H), 8.80 (s, 1H), 9.38 (s, 1H), 9.64-9.78 (m, 2H); ^{13}C NMR (125 MHz, TCE-d^2, 100 °C): 120.9 (s), 123.1 (d), 124.0 (d), 124.2 (d), 124.5 (s), 125.5 (d), 126.1 (s), 126.7 (d), 127.8 (d), 127.9 (d), 128.2 (d), 128.2 (d), 128.3 (d), 128.6 (d), 129.0 (d), 129.1 (s), 130.3 (d), 130.4 (s), 130.9 (d), 131.3 (s), 131.5 (d), 133.1 (s), 134.7 (s), 136.5 (d), 151.7 (s), 152.0 (s), 153.3 (s); IR (ATR): ṽ [cm^{-1}] = 3266, 3031, 2926, 2853, 1626, 1595, 1551, 1522, 1491, 1457, 1420, 1397, 1378, 1345, 1301, 1231, 1171, 1132, 1040, 1011, 957, 918, 894, 879, 852, 794, 747, 717, 693, 675, 663, 618, 606; UV/Vis (15 µg/ml): λ [nm]: 252, 274, 306, 318, 412, 436; HRMS-EI+: Calc. for $C_{28}H_{16}N_2^+$: 380.1308 m/z, found: 380.1301 m/z; mp: >300 °C.

dinaphtho[1,2-b:1',2'-g][1,8]naphthyridine 5h



4h **5h** 87%

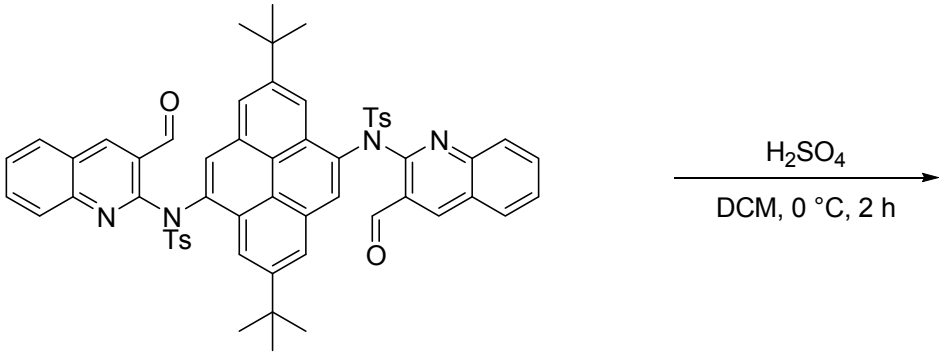
According to **GP.D**, N-(3-formylbenzo[h]quinolin-2-yl)-4-methyl-N-(naphthalen-2-yl)benzenesulfonamide **4h** (33 mg, 66 µmol, 1.0 eq) and 0.33 ml H_2SO_4 were stirred in 33 ml DCM.

Yellow solid (19 mg, 58 µmol, 87% Yield).

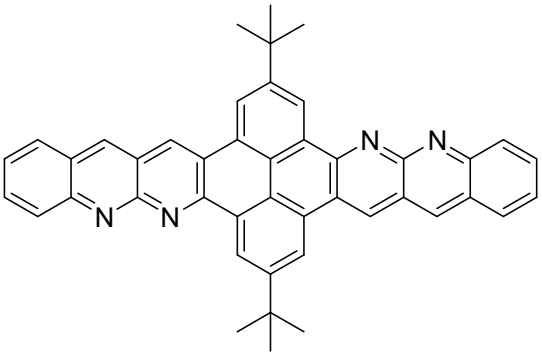
^{1}H NMR (600 MHz, $CDCl_3$, 50 °C) δ (ppm) = 7.52-7.73 (m, 4H), 7.73-7.83 (m, 3H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.99 (d, *J* = 9.3 Hz, 1H), 8.21 (d, *J* = 9.2 Hz, 1H), 8.68 (d, *J* = 8.0 Hz, 1H), 8.79 (s, 1H), 9.49 (s, 1H), 9.76 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 50 °C) = 120.0 (s), 123.3 (d), 124.8 (s), 125.3 (d), 125.9 (s), 126.9 (d), 127.7 (d), 128.0 (d), 128.1 (d), 128.3 (d), 128.6 (d), 129.1 (d), 129.3 (d), 129.9 (s), 130.3 (d), 131.4 (s), 131.8 (d), 134.4 (d), 134.5 (s), 136.5 (d), 152.1 (s), 153.0 (s), 153.3 (s); IR (ATR): ṽ [cm^{-1}] = 3050, 1605, 1592, 1551, 1513, 1493, 1478, 1458, 1428, 1406, 1376, 1338, 1315, 1300, 1273, 1244, 1168, 1147, 1113, 1039, 1016, 984, 923, 896, 875, 861, 829, 803, 774, 738, 720, 701, 627, 607; UV/Vis (DCM, 29.6 µg/ml): λ [nm]: 240, 265, 302, 314, 407, 425, 446; HRMS-EI+: Calc. for $C_{24}H_{14}N_2^+$: 330.1152 m/z, found: 330.1142 m/z; mp.: >300 °C.

1.4.3. Synthesis of Dinaphthyridinopyrenes 11a-d

Compound 11a



10a

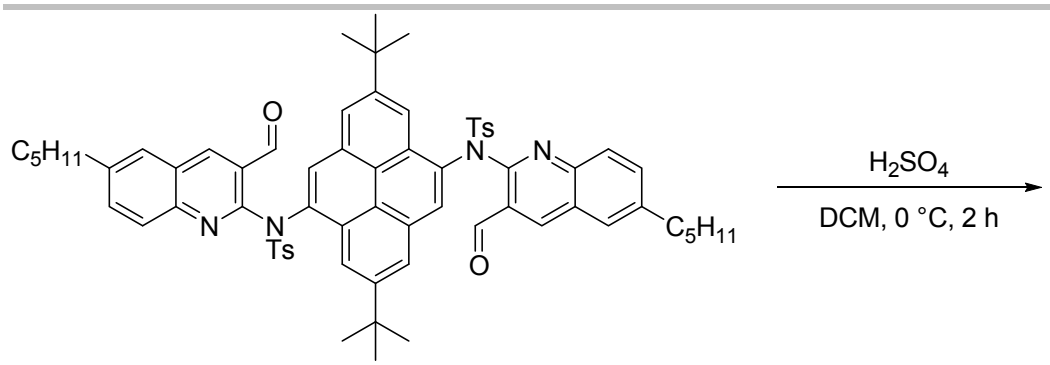


11a 91%

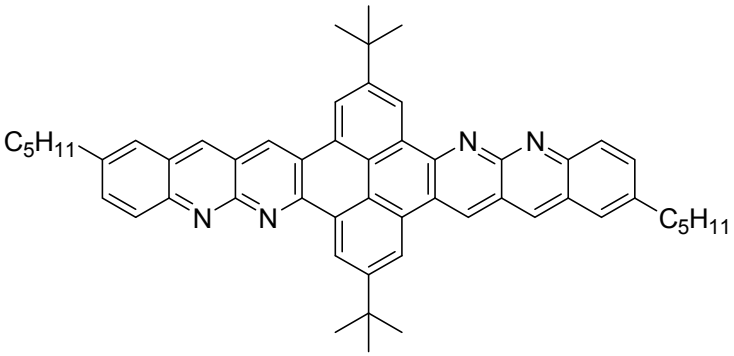
N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-formylquinolin-2-yl)-4-methylbenzenesulfon-amide) **10a** (139 mg, 144 µmol, 1.0 eq) was dissolved in 300 ml DCM and the solution was cooled to 0 °C. Then H_2SO_4 (3.0 ml, 1 vol% of solvent) was added dropwise and the reaction mixture was stirred at 0 °C for 2 hours. Then 5.0 ml ethylenediamine was added dropwise to quench the reaction and 150 ml of a diluted K_2CO_3 solution was added afterwards. Then DCM was removed under reduced pressure and the suspension was filtered. The solid was washed with water, methanol, triethylamine and again methanol. The yellow product was then further purified via recrystallization from $CHCl_3$. The product was isolated as yellow solid (81 mg, 132 µmol, 91% yield).

^{1}H NMR and ^{13}C NMR could not be measured due to low solubility; FTIR (Neat) v [cm^{-1}]: 3051, 2961, 2926, 2867, 1612, 1593, 1538, 1478, 1455, 1428, 1395, 1372, 1318, 1284, 1255, 1232, 1170, 1126, 1001, 913, 880, 869, 849, 800, 788, 746, 737, 644, 617; UV/Vis ($CHCl_3$, 0.0044 mg/ml, [nm]): 260, 287, 324, 339, 424, 443; HRMS-MALDIposPVP: calc for $C_{44}H_{35}N_4^+$: 619.2856, found: 619.2856; mp: > 300 °C.

Compound 11b



10a

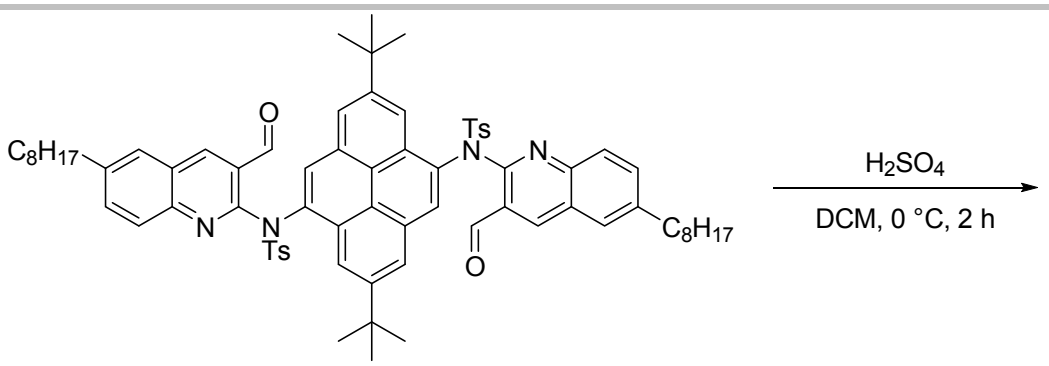


11a 79%

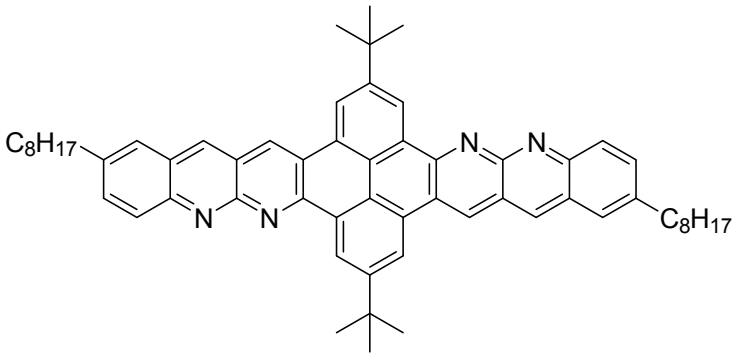
N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-formyl-6-pentylquinolin-2-yl)-4-methylbenzene-sulfonamide) **10b** (50 mg, 45 µmol, 1.0 eq) was dissolved in 50 ml DCM and the solution was cooled to 0 °C. Then H_2SO_4 (0.5 ml, 1 vol% of solvent) was added dropwise and the reaction mixture was stirred at 0 °C for 2 hours. Then 0.5 ml ethylenediamine was added dropwise to quench the reaction and 20 ml of a diluted K_2CO_3 solution was added afterwards. Then DCM was removed under reduced pressure and the suspension was filtered. The solid was washed with water, methanol, triethylamine and again methanol. The yellow product was then further purified via recrystallization from $CHCl_3$. The product was isolated as yellow solid (27 mg, 35.5 µmol, 79% yield).

^1H NMR and ^{13}C NMR could not be measured due to low solubility; FTIR (Neat) ν [cm^{-1}]: 2952, 2927, 2862, 1620, 1592, 1548, 1537, 1470, 1435, 1407, 1367, 1320, 1286, 1251, 1231, 1127, 1008, 969, 914, 881, 867, 841, 809, 786, 764, 751, 738, 726, 716, 659, 644, 621; UV/Vis ($CHCl_3$, 0.01 mg/ml, [nm]): 261, 292, 340, 421, 444; HRMS-MALDIposPVP: calc for $C_{54}H_{55}N_4^+$: 759.4421, found: 759.4423; mp: >300 °C.

Compound 11c



10c

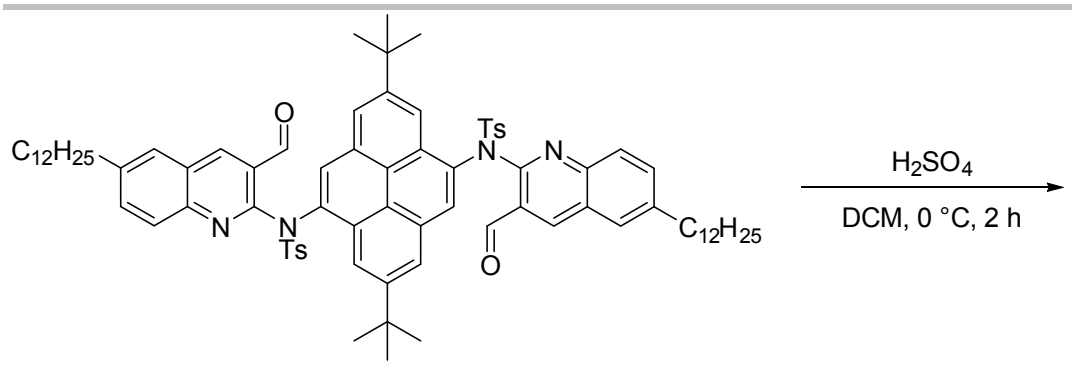


11c 82%

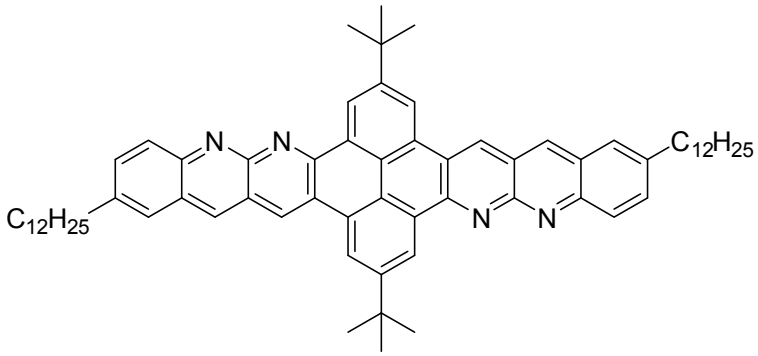
N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-formyl-6-octylquinolin-2-yl)-4-methylbenzene-sulfonamide) **10c** (85 mg, 71 µmol, 1.0 eq) was dissolved in 80 ml DCM and the solution was cooled to 0 °C. Then H_2SO_4 (0.8 ml, 1 vol% of solvent) was added dropwise and the reaction mixture was stirred at 0 °C for 2 hours. Then 1 ml ethylenediamine was added dropwise to quench the reaction and 20 ml of a diluted K_2CO_3 solution was added afterwards. Then DCM was removed under reduced pressure and the suspension was filtered. The solid was washed with water, methanol, triethylamine and again methanol. The yellow product was then further purified via recrystallization from $CHCl_3$. The product was isolated as yellow solid (49 mg, 58 µmol, 82% yield).

^{1}H NMR (TCE-d^2, 600 MHz, 100 °C), δ [ppm] = 0.89 (s, 6H), 1.23-1.51 (m, 22H), 1.78 (s, 20H), 2.85 (t, 4H, *J* = 6.4 Hz), 7.76 (d, 2H, *J* = 8.3 Hz), 7.82 (s, 2H), 8.47 (d, 2H, *J* = 7.9 Hz), 9.05 (s, 2H), 9.09 (s, 2H), 9.56 (s, 2H), 9.99 (s, 2H); ^{13}C NMR could not be measured due to low solubility; FTIR (Neat) v [cm^{-1}]: 2953, 2926, 2850, 1635, 1613, 1591, 1548, 1537, 1494, 1459, 1436, 1406, 1365, 1340, 1322, 1288, 1255, 1233, 1203, 1170, 1133, 1001, 917, 882, 870, 854, 826, 802, 788, 766, 752, 726, 644, 623; UV/Vis ($CHCl_3$, 0.0022 mg/ml, [nm]): 262, 290, 297, 329, 343, 395, 421, 445; HRMS-MALDIposCsI: calc for $C_{60}H_{67}N_4^+$: 843.5360, found: 843.5365; mp: >300 °C.

Compound 11d



10d



11d 62%

N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(6-dodecyl-3-formylquinolin-2-yl)-4-methylben-zenesulfonamide) **10d** (57 mg, 44 µmol, 1.0 eq) was dissolved in 55 ml DCM and the solution was cooled to 0 °C. Then H_2SO_4 (0.55 ml, 1 vol% of solvent) was added dropwise and the reaction mixture was stirred at 0 °C for 2 hours. Then 1 ml ethylenediamine was added dropwise to quench the reaction and 20 ml of a diluted K_2CO_3 solution was added afterwards. Then DCM was removed under reduced pressure and the suspension was filtered. The solid was washed with water, methanol, triethylamine and again methanol. The yellow product was then further purified via recrystallization from $CHCl_3$/hexane. The product was isolated as yellow solid (26 mg, 27 µmol, 62% yield).

^{1}H NMR (TCE-d^2, 600 MHz, 100 °C), δ [ppm] = 0.86 (s, 6H), 1.23-1.32 (m, 28H), 1.35-1.47 (m, 8H), 1.74-1.83 (m, 22H), 2.86 (s, 4H), 7.76 (d, 2H, *J* = 8.4 Hz), 7.82 (s, 2H), 8.38 (s, 2H), 9.05 (s, 2H), 9.57 (s, 2H), 9.98 (s, 2H); ^{13}C NMR could not be measure due to low solubility; FTIR (Neat) v [cm^{-1}]: 2953, 2921, 2851, 1637, 1614, 1592, 1536, 1492, 1466, 1436, 1405, 1367, 1286, 1254, 1235, 1129, 1001, 914, 875, 817, 801, 787, 766, 751, 724, 643, 622; HRMS-MALDIposCsI: calc for $C_{68}H_{84}N_4^{2+}$: 956.6685, found: 956.6685; mp: >300 °C.

2. X-ray crystal structure and –packing of 5c

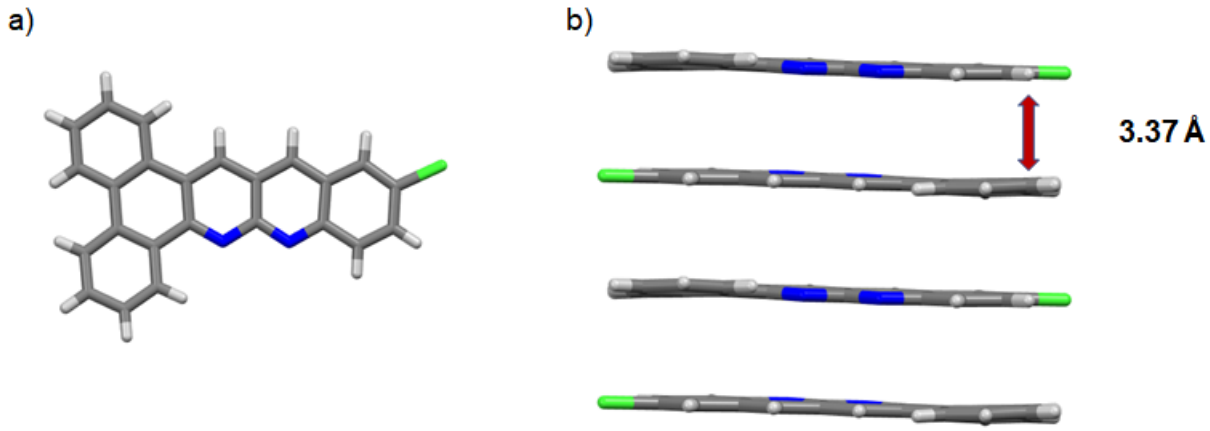


Figure S1: Solid-state structure and packing of 5c

3. Cyclovoltammetry (CV) data of 5a-h

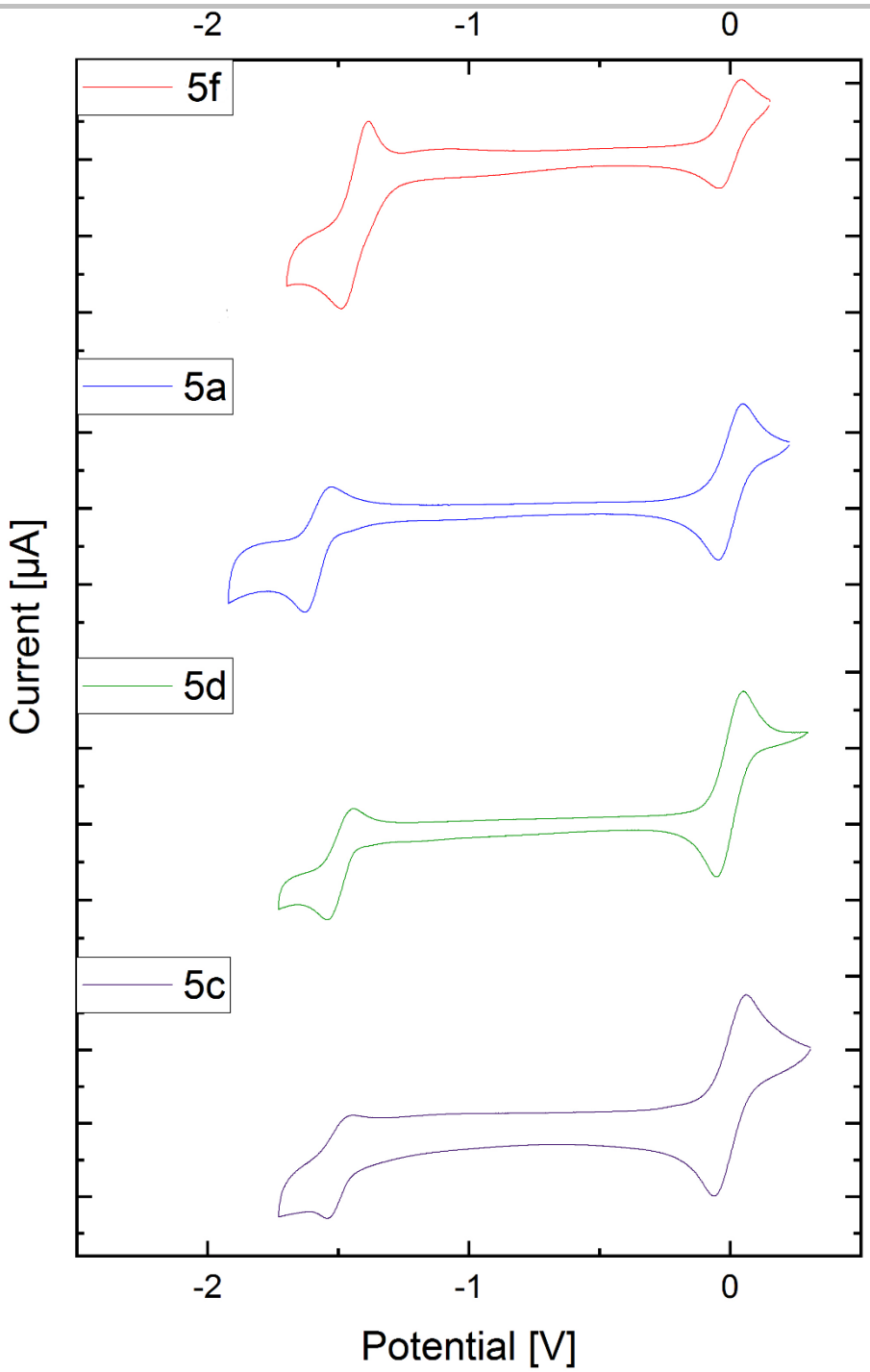


Figure S2: CV spectra of **5a**, **5c**, **5d**, and **5f** in DCM with ferrocene (Fc) as internal standard, scan rate: 0.1 V/s, 0,1 M solution of tetrabutylammonium hexafluorophosphate (Bu_4NPF_6), RE: Ag, WE: Pt, CE: Pt/Ti at room temperature.

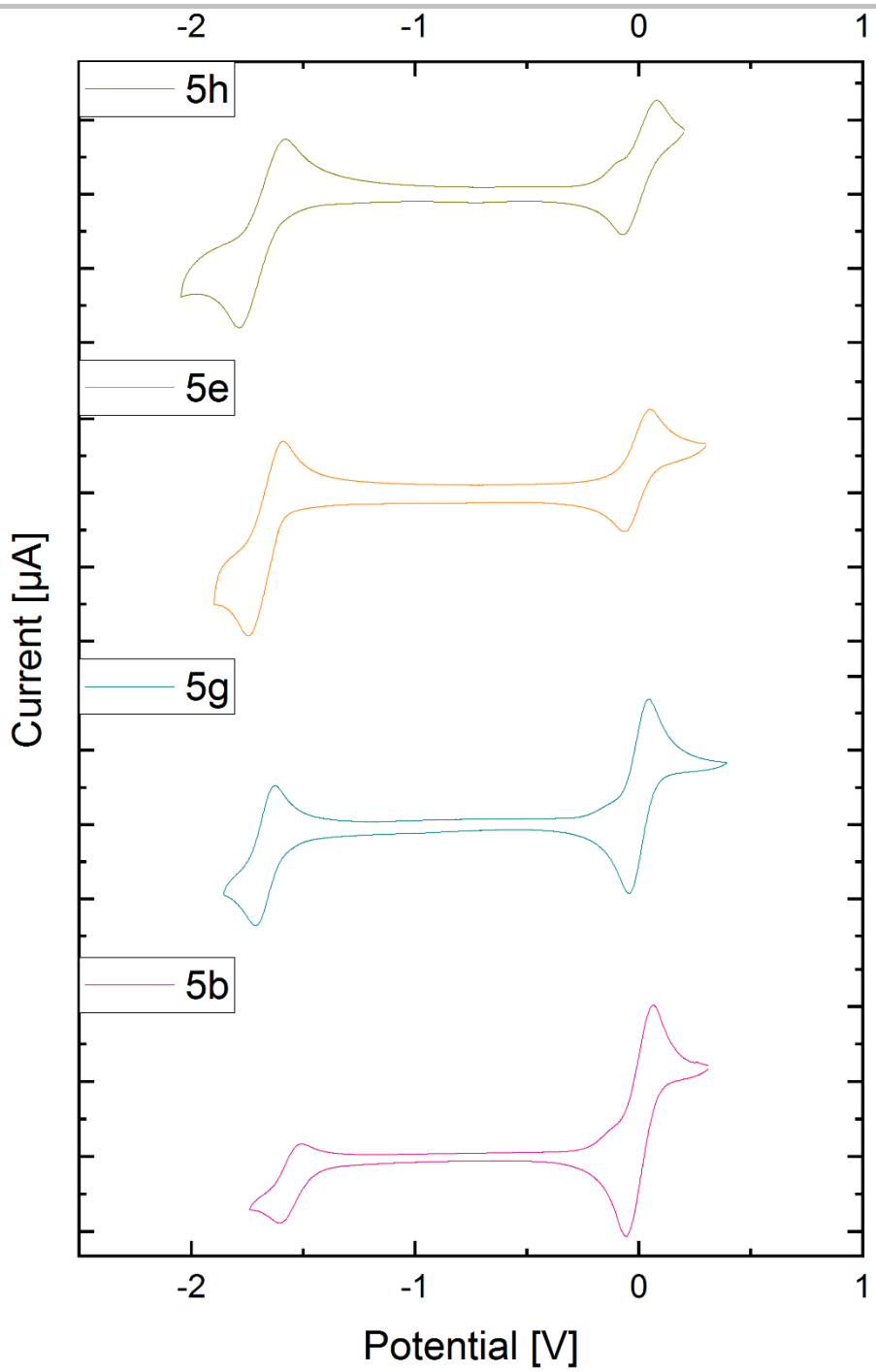


Figure S3: CV spectra of **5b**, **5e**, **5g**, and **5h** in DCM with ferrocene (Fc) as internal standard, scan rate: 0.1 V/s, 0,1 M solution of tetrabutylammonium hexafluorophosphate (Bu_4NPF_6), RE: Ag, WE: Pt, CE: Pt/Ti at room temperature.

4. UV-Vis- and fluorescence spectra of 5a-h and 11a-d

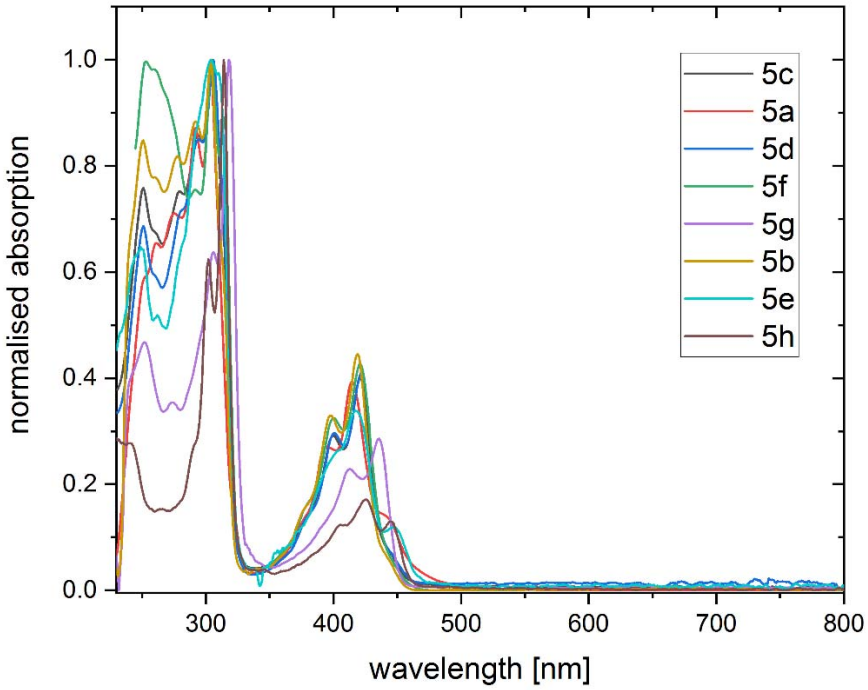


Figure S4: Normalized UV-Vis spectra of **5a**-**h**.

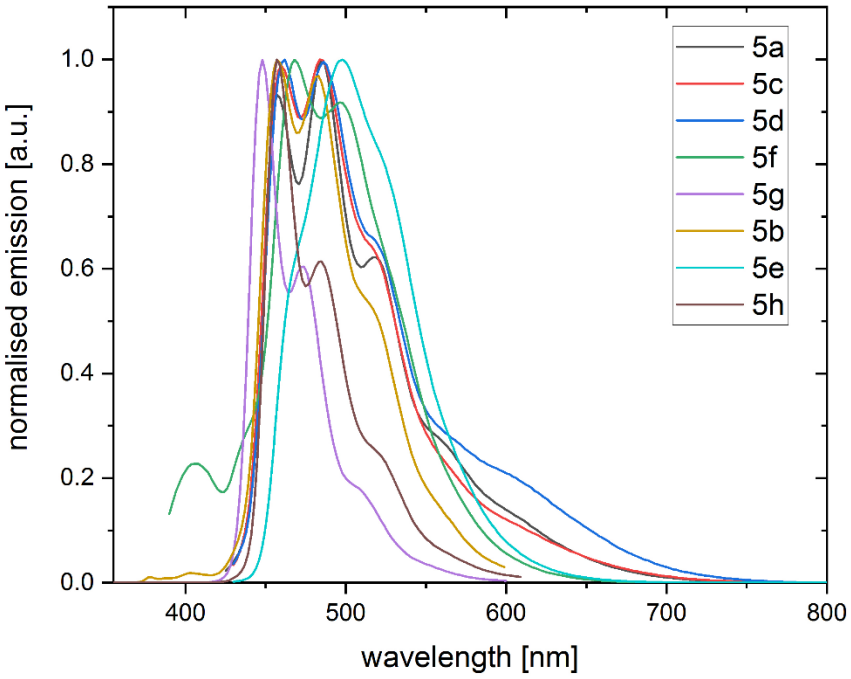


Figure S5: Normalized fluorescence spectra of **5a**-**h**.

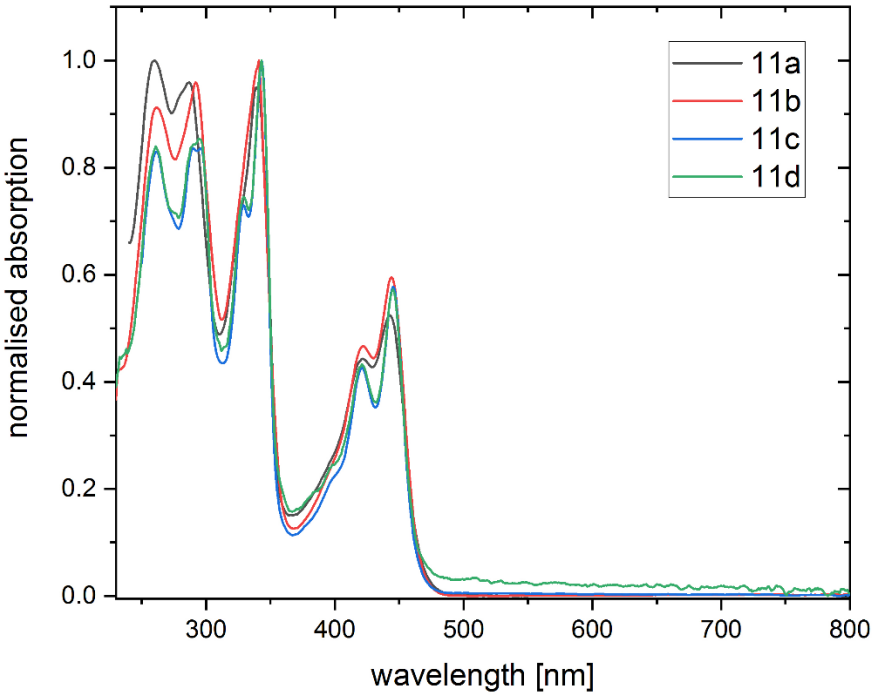


Figure S6: Normalized UV-Vis spectra of **11a-d**.

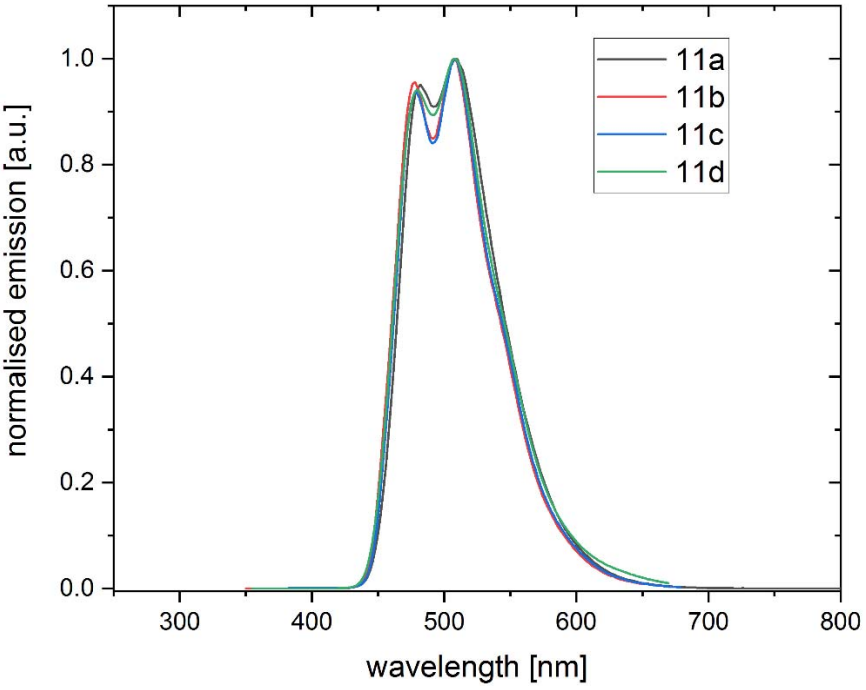


Figure S7: Normalized fluorescence spectra of **11a-d**.

Table S1. Photoluminescence quantum yields (PLQY) of compound **5a-h** and **11a-d**.

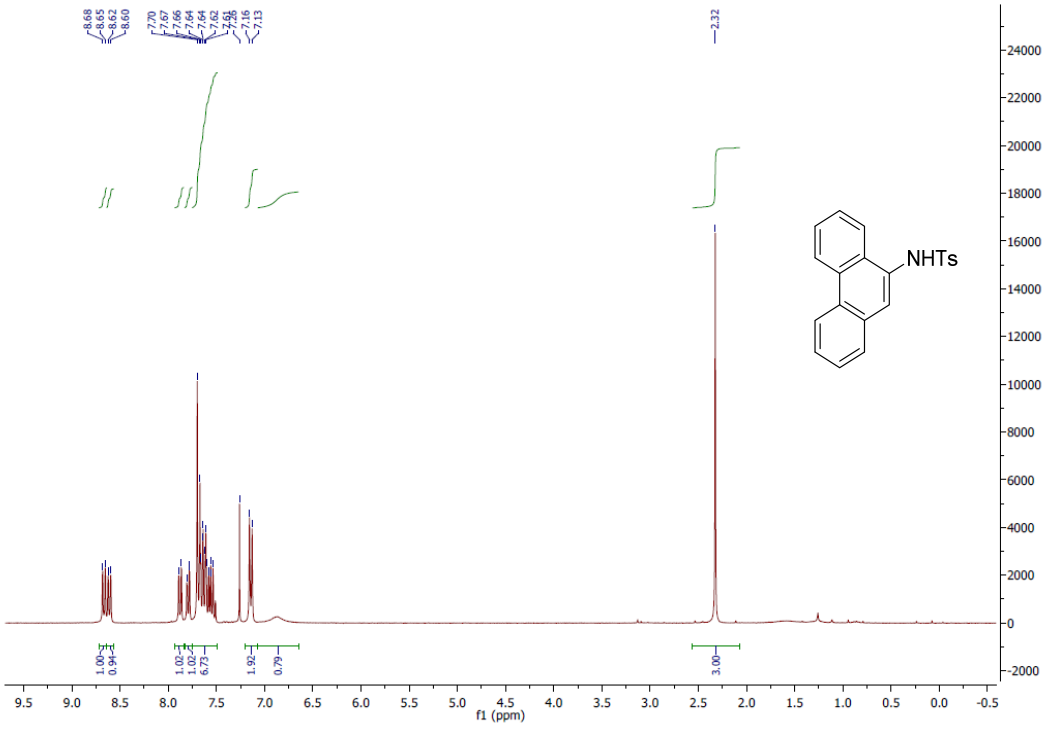
compound	Photoluminescence quantum yield (PLQY)
5a	9 %
5b	8 %
5c	6 %
5d	3 %
5e	23 %
5f	6 %
5g	39 %
5h	30 %
11a	13 %
11b	13 %
11c	13 %
11d	19 %

5. NMR spectra

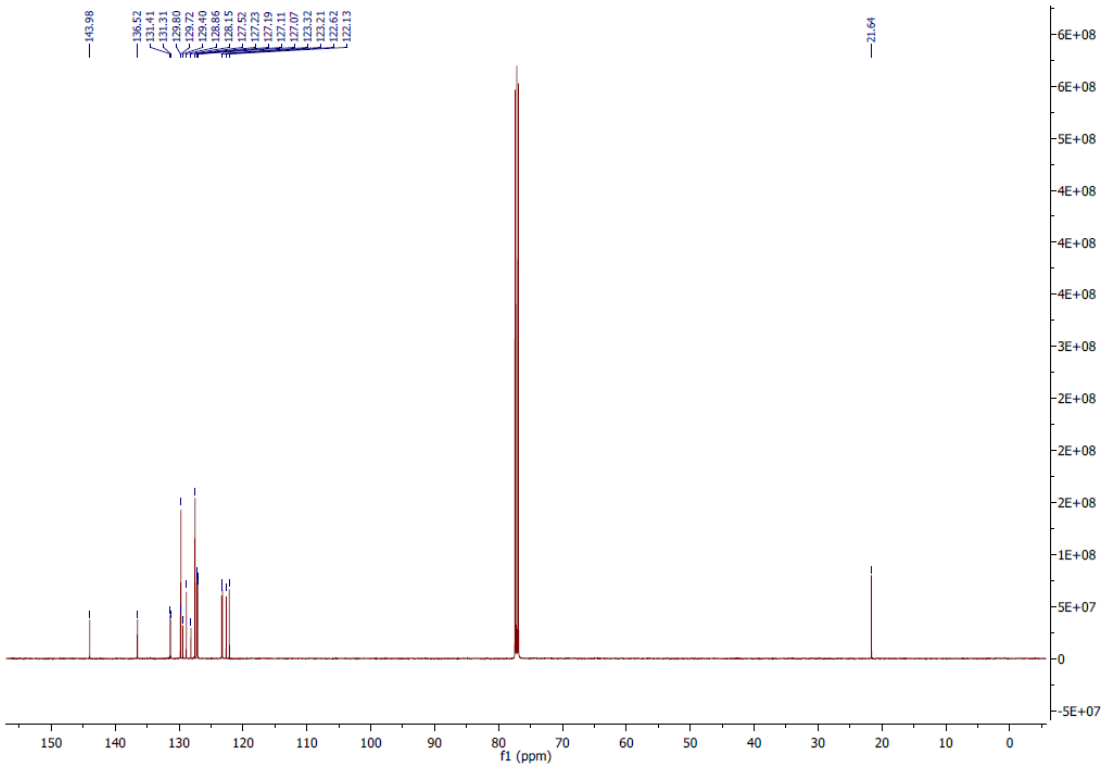
5.1. NMR of ynamides and starting materials

4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 12

^{1}H NMR

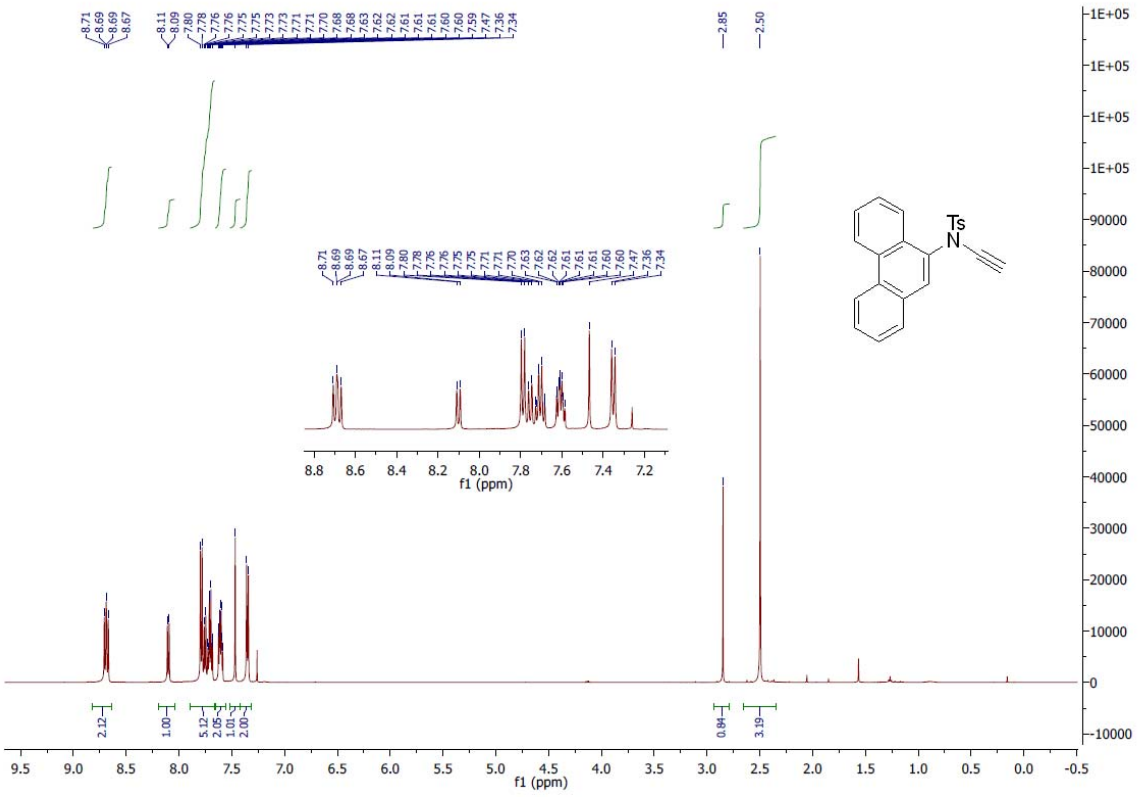


^{13}C NMR:

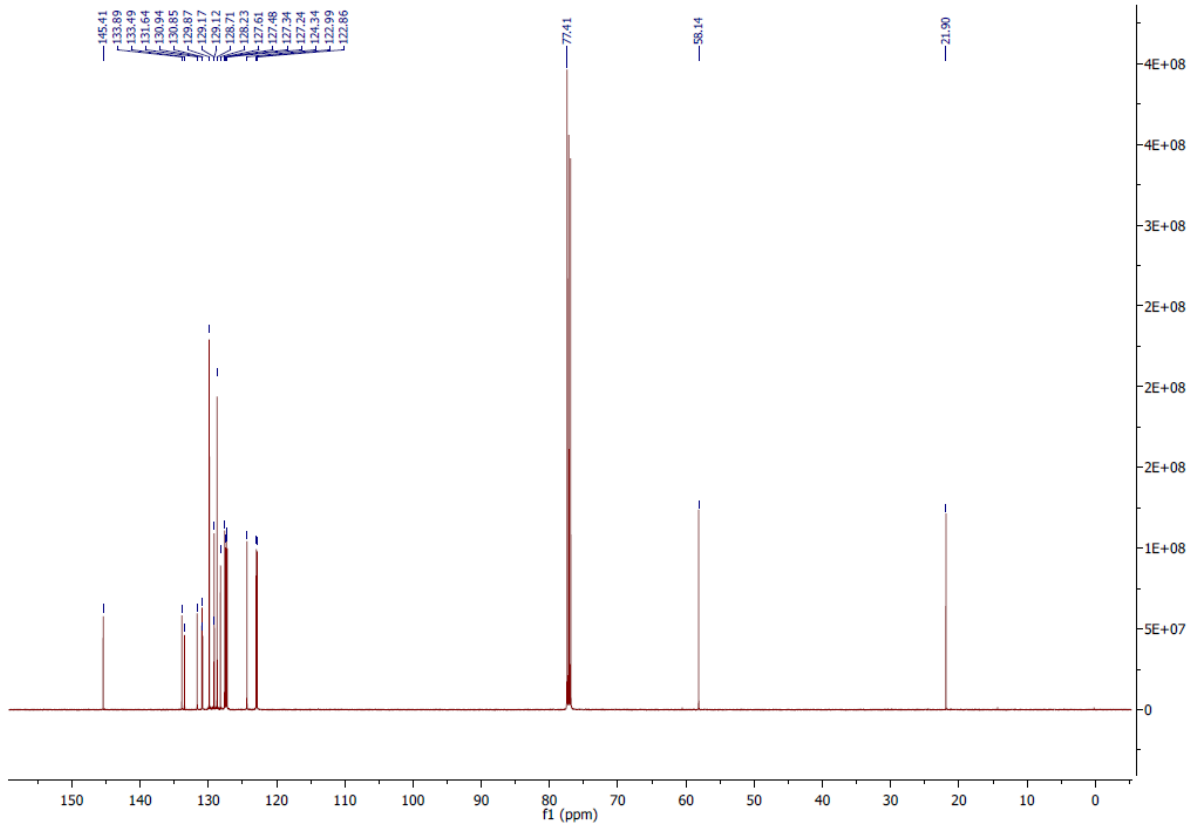


N-ethynyl-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 14

^{1}H NMR:

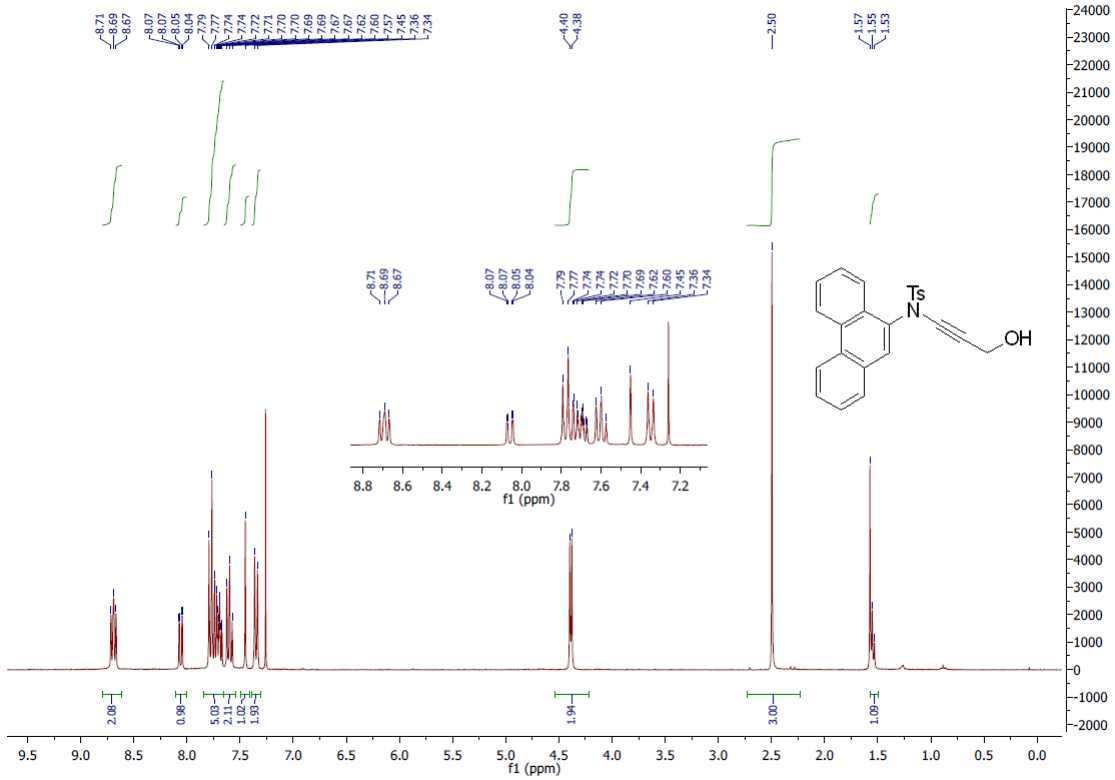


^{13}C NMR:

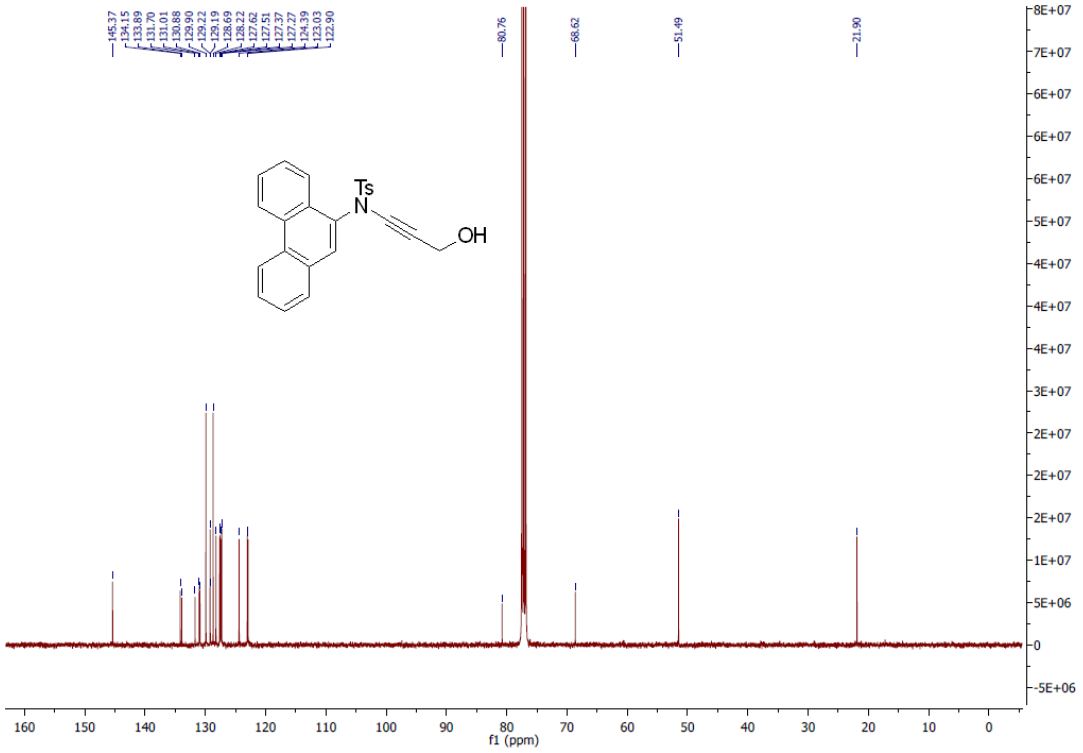


N-(3-hydroxyprop-1-yn-1-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 15

^{1}H NMR:

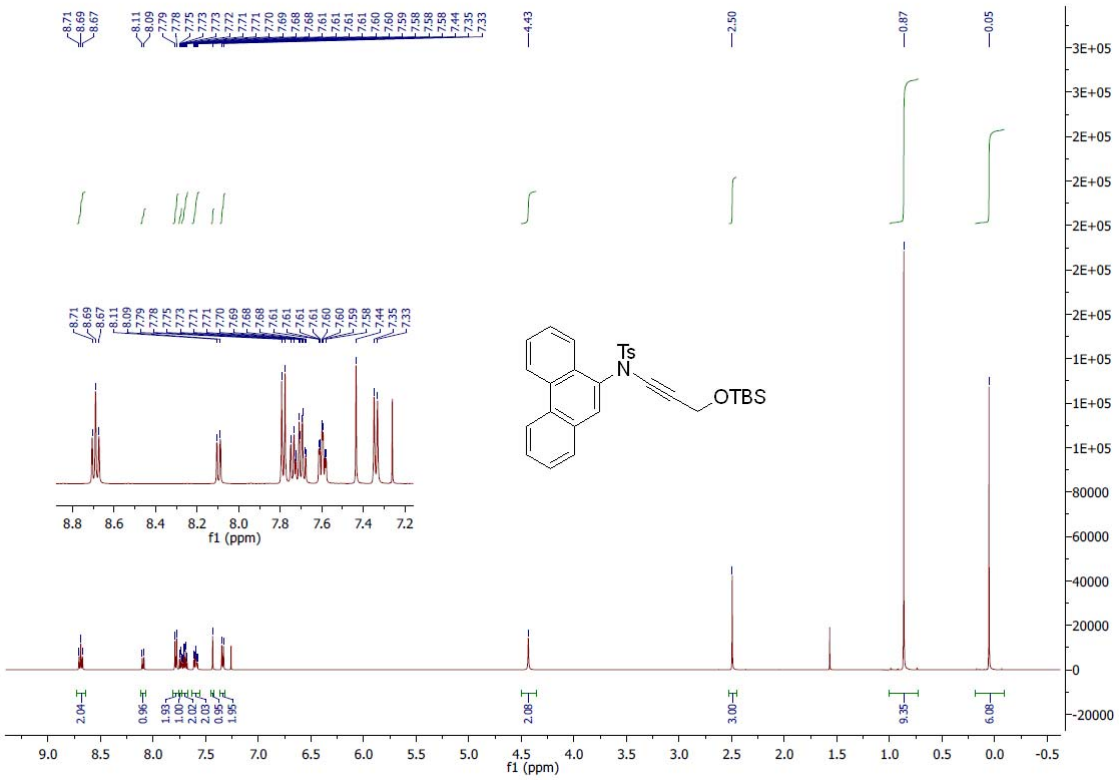


^{13}C NMR:

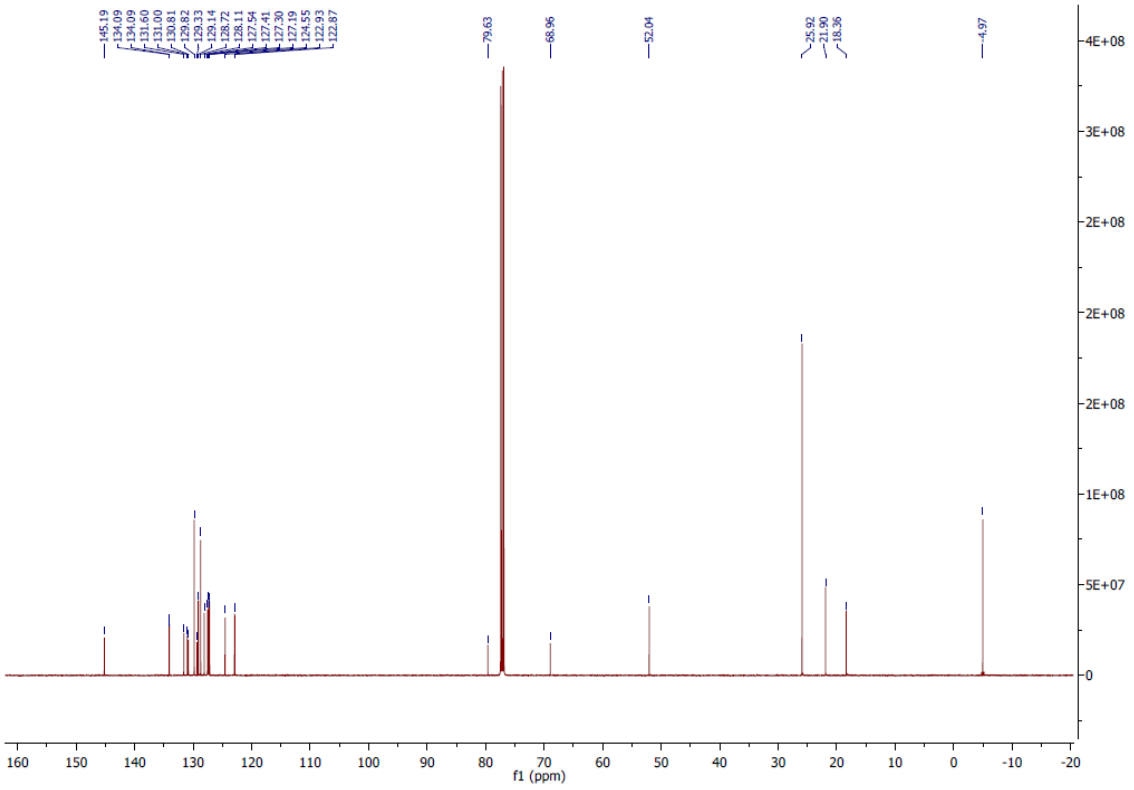


N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 1a

^{1}H NMR:

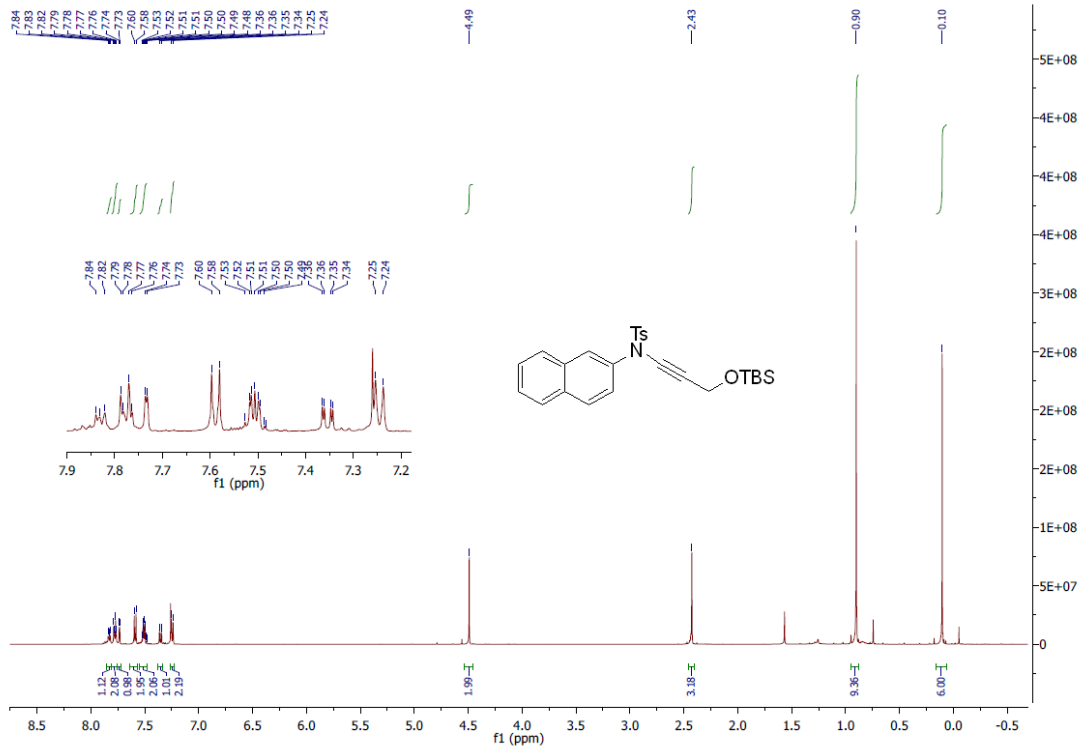


^{13}C NMR:

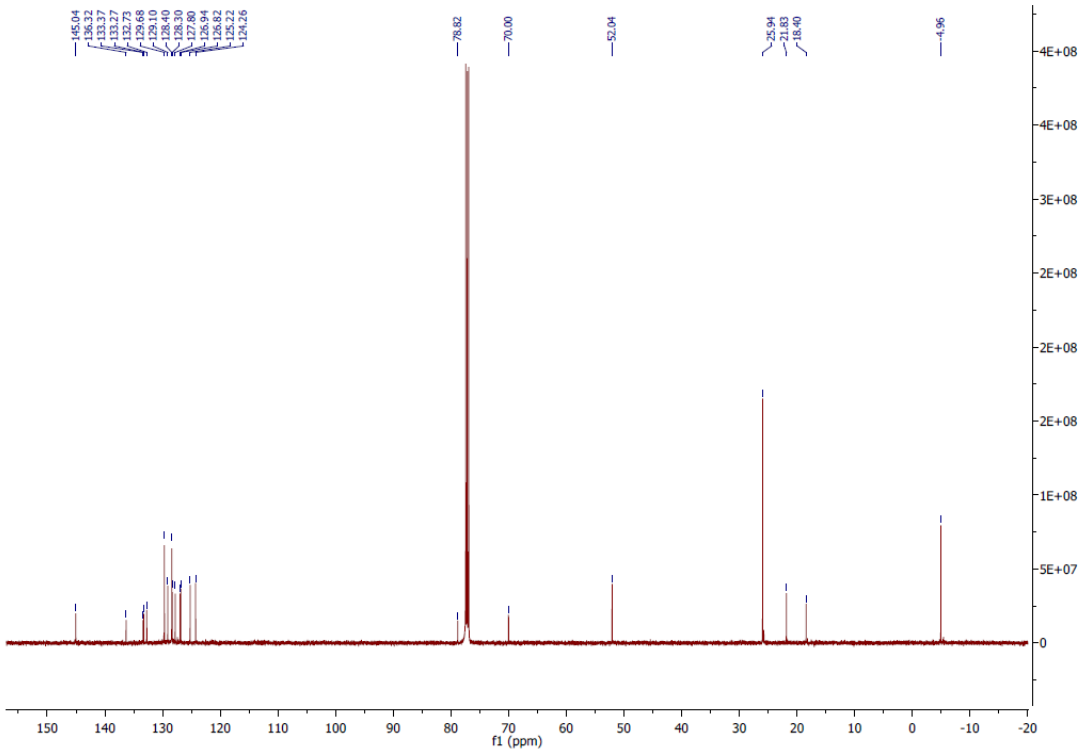


N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methyl-N-(naphthalen-2-yl)benzenesulfonamide 1b

^{1}H NMR:

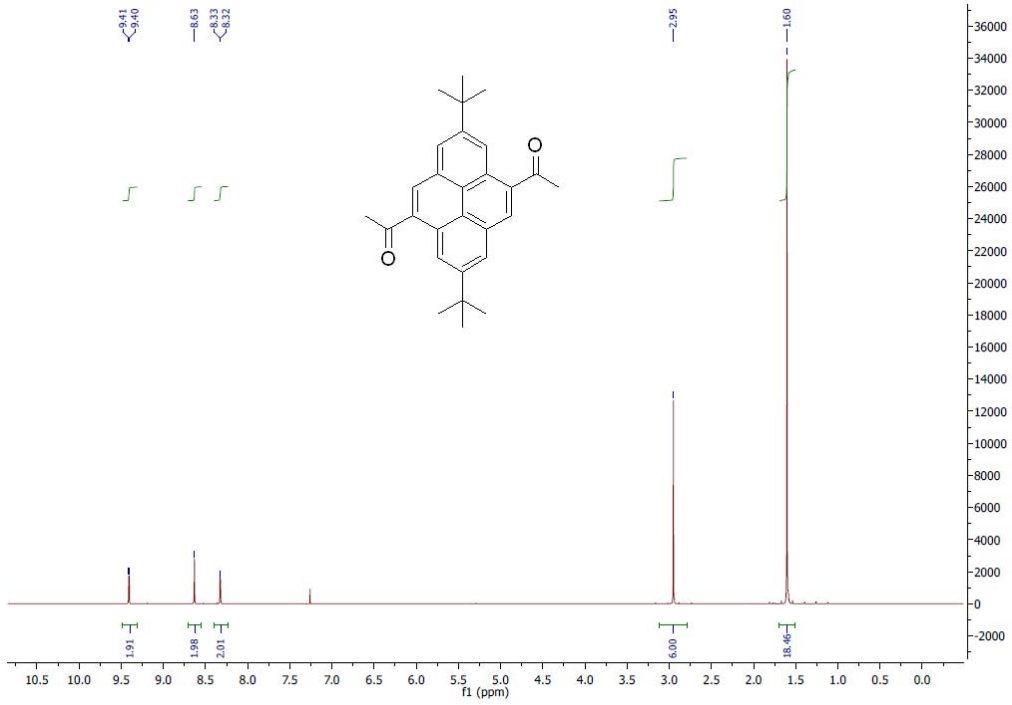


^{13}C NMR:

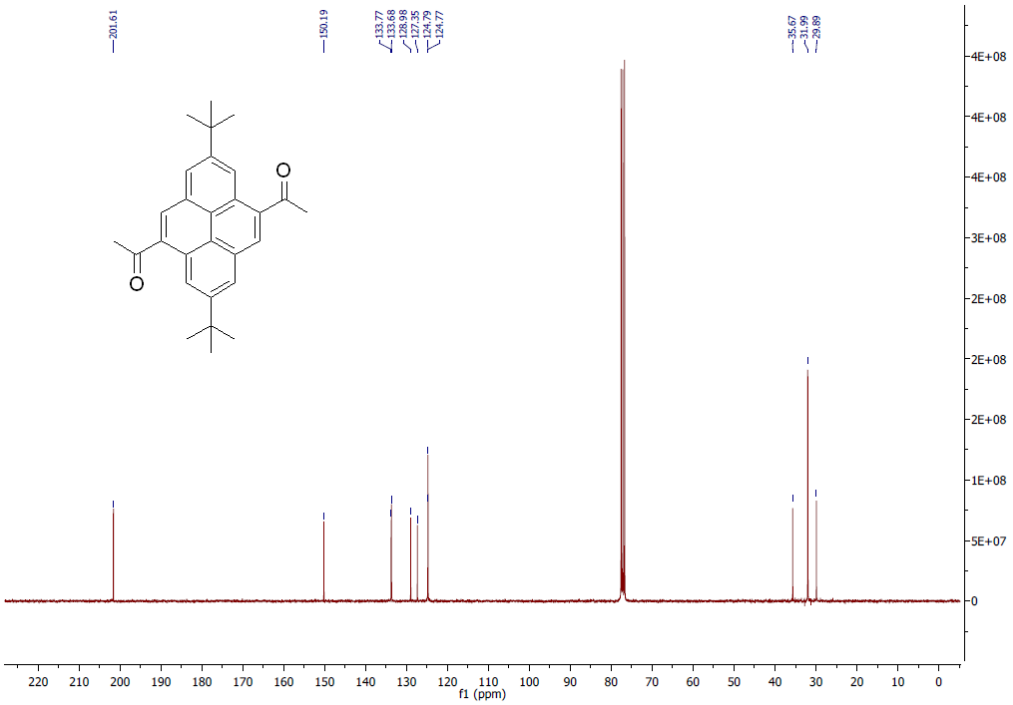


1,1'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(ethan-1-one) 17

^{1}H NMR:

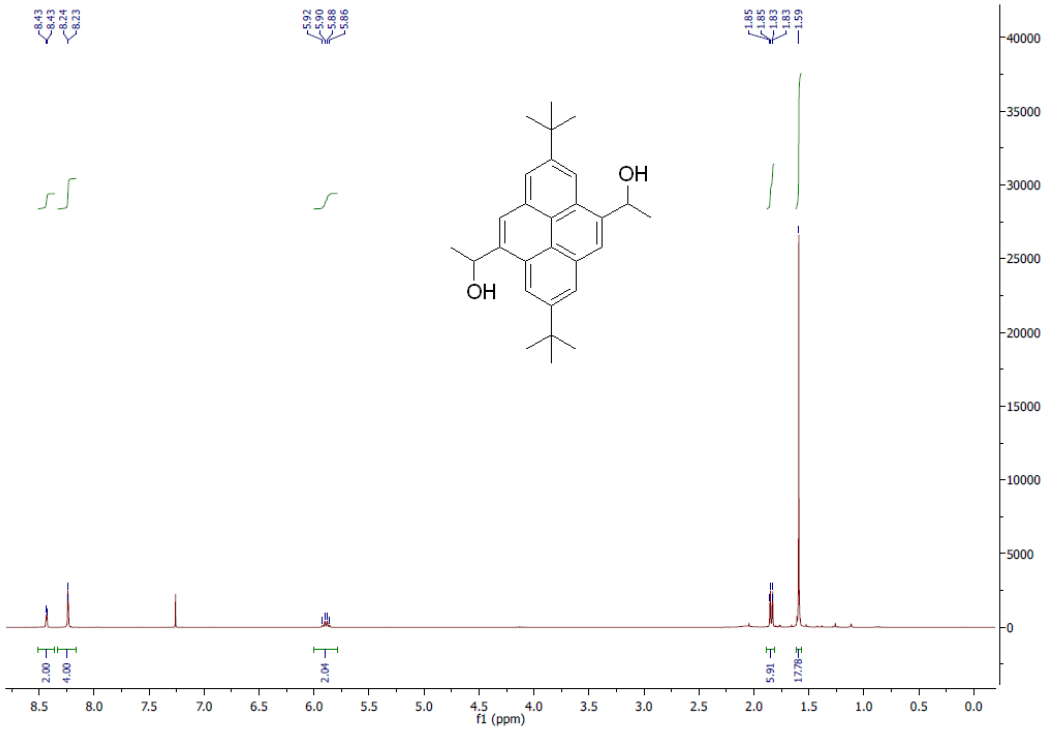


^{13}C NMR:

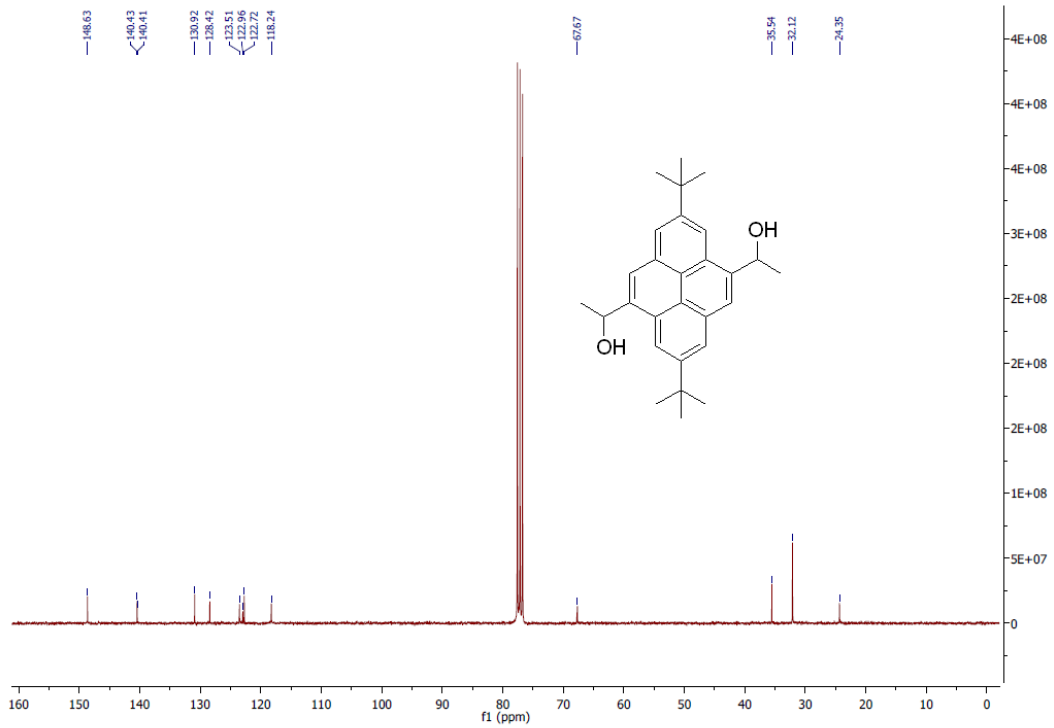


1,1'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(ethan-1-ol) 7

^{1}H NMR:

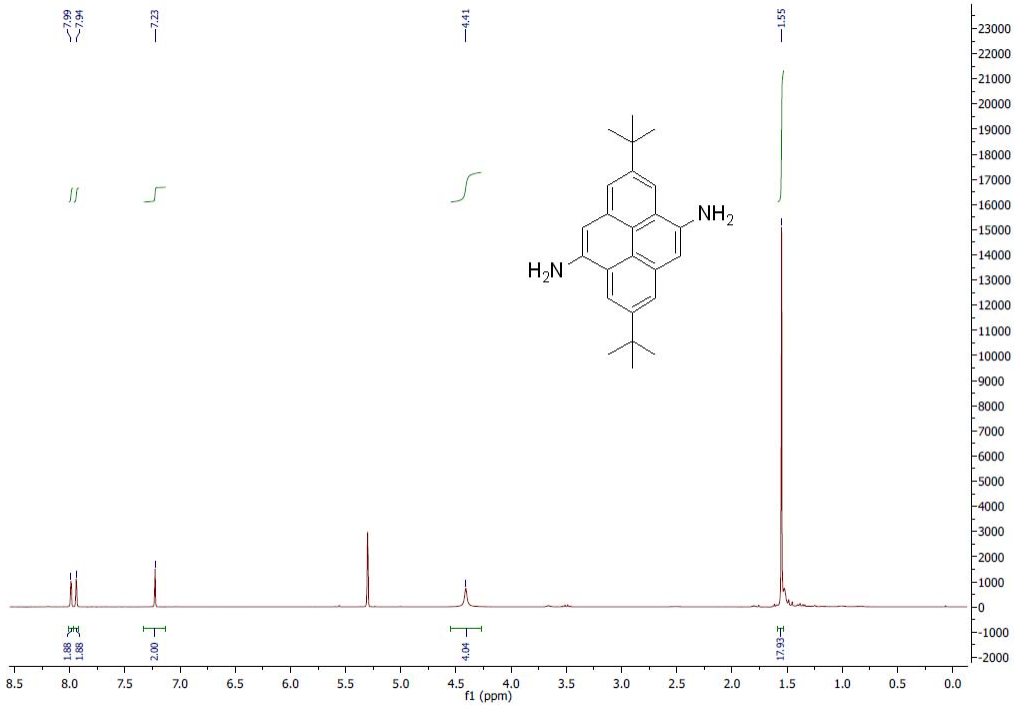


^{13}C NMR:

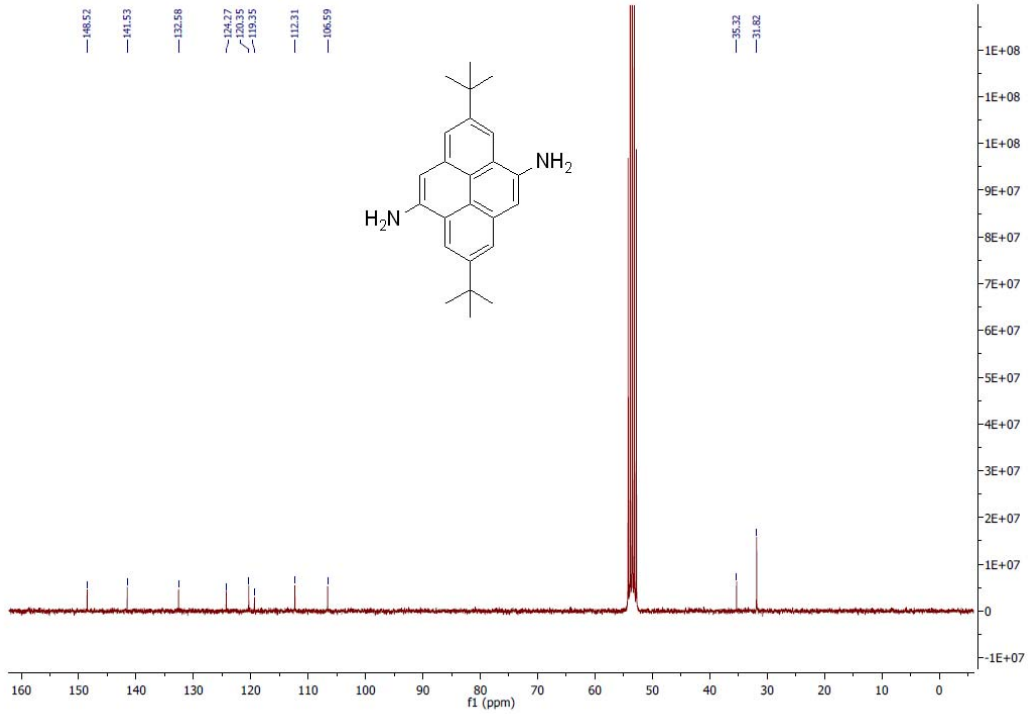


2,7-di-tert-butylpyrene-4,9-diamine 8

^{1}H NMR:

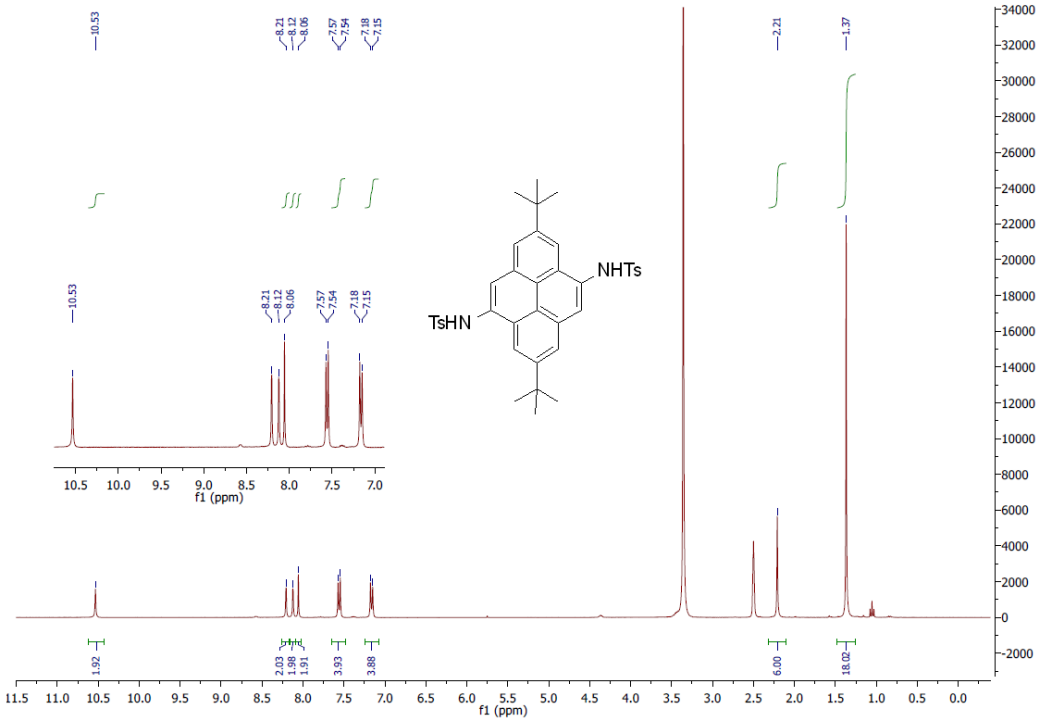


^{13}C NMR:

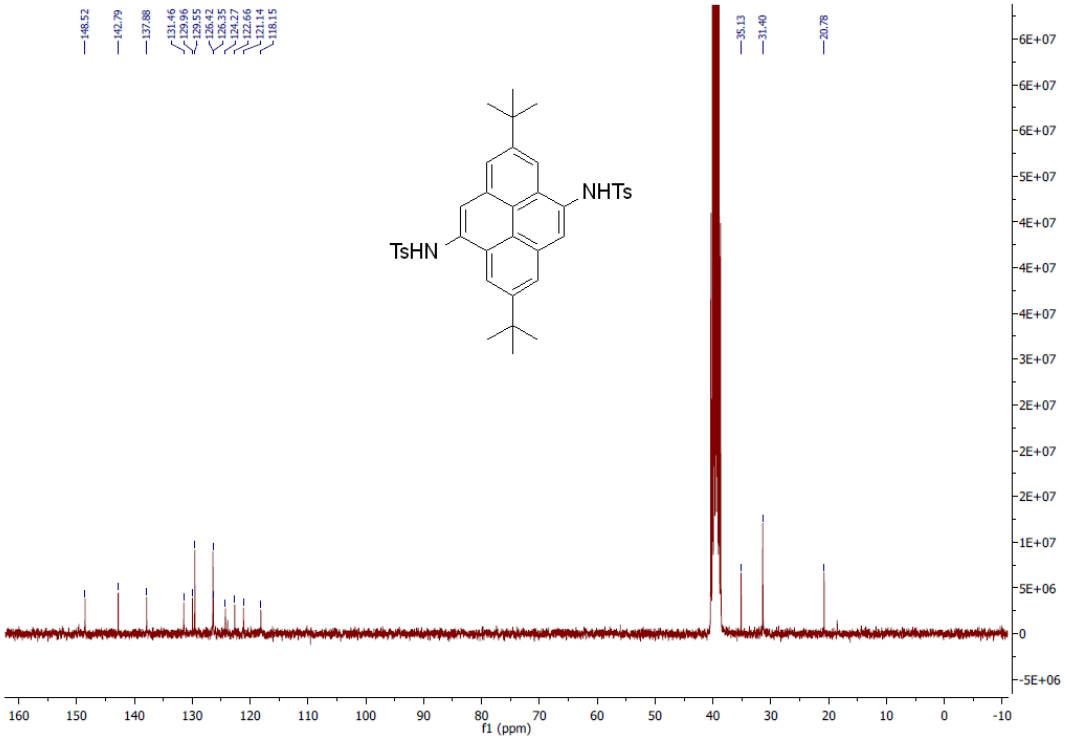


N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(4-methylbenzenesulfonamide) 18

^{1}H NMR:

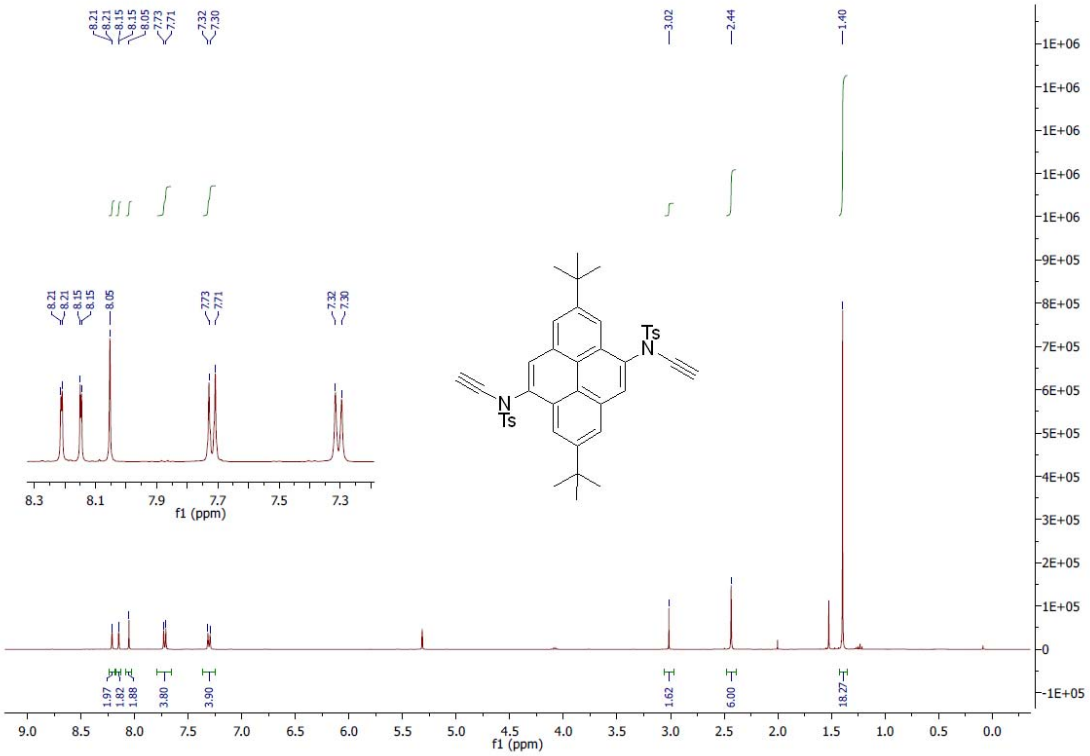


^{13}C NMR:

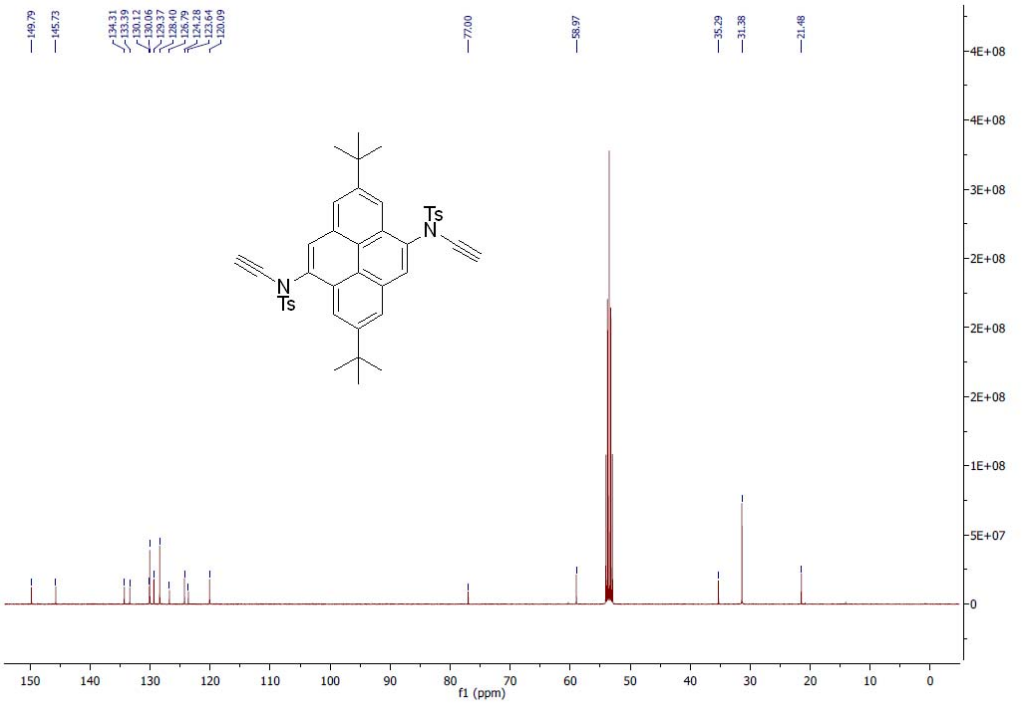


N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-ethynyl-4-methylbenzenesulfonamide) 19

^{1}H NMR:

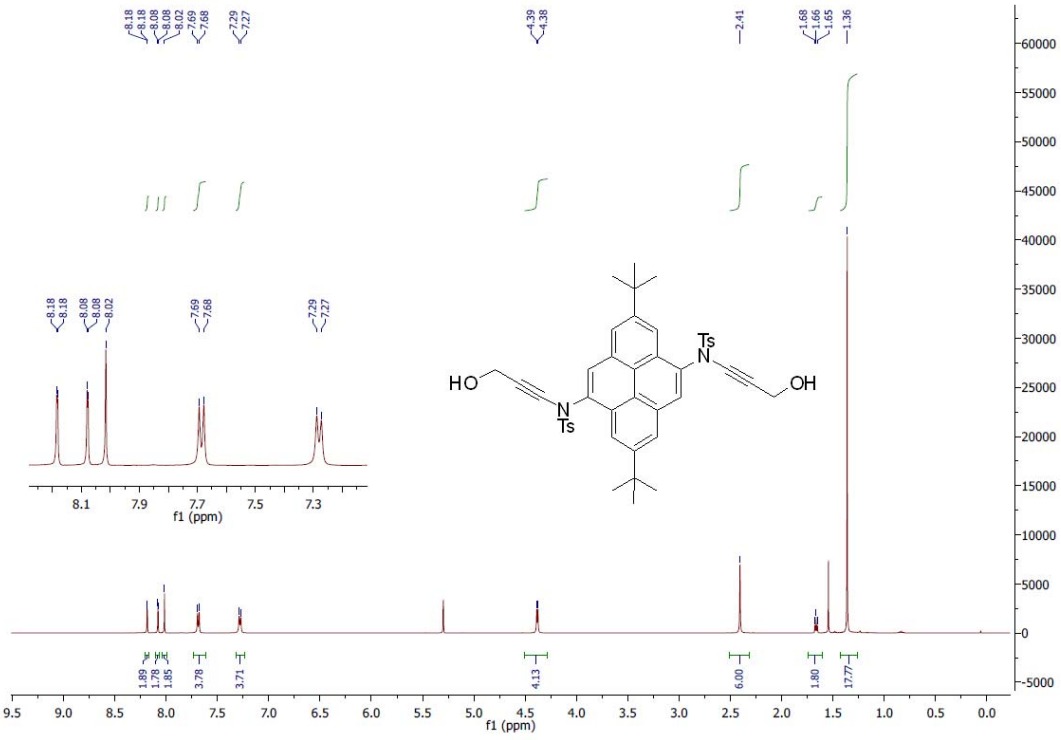


^{13}C NMR:

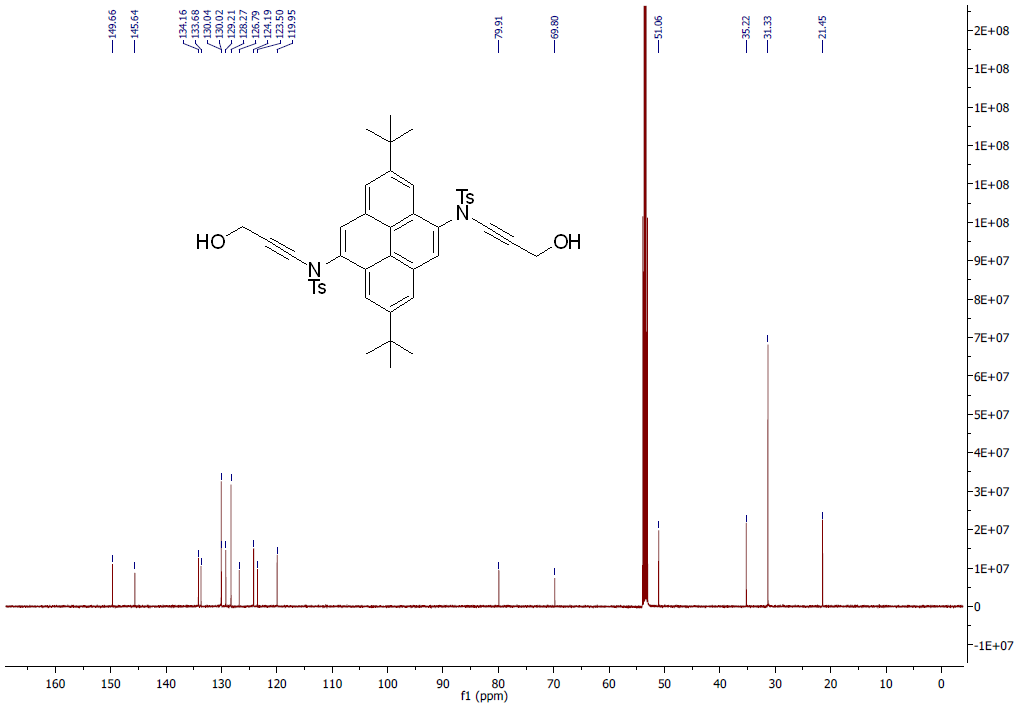


N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-hydroxyprop-1-yn-1-yl)-4-methylbenzenesulfonamide) 20

^{1}H NMR:

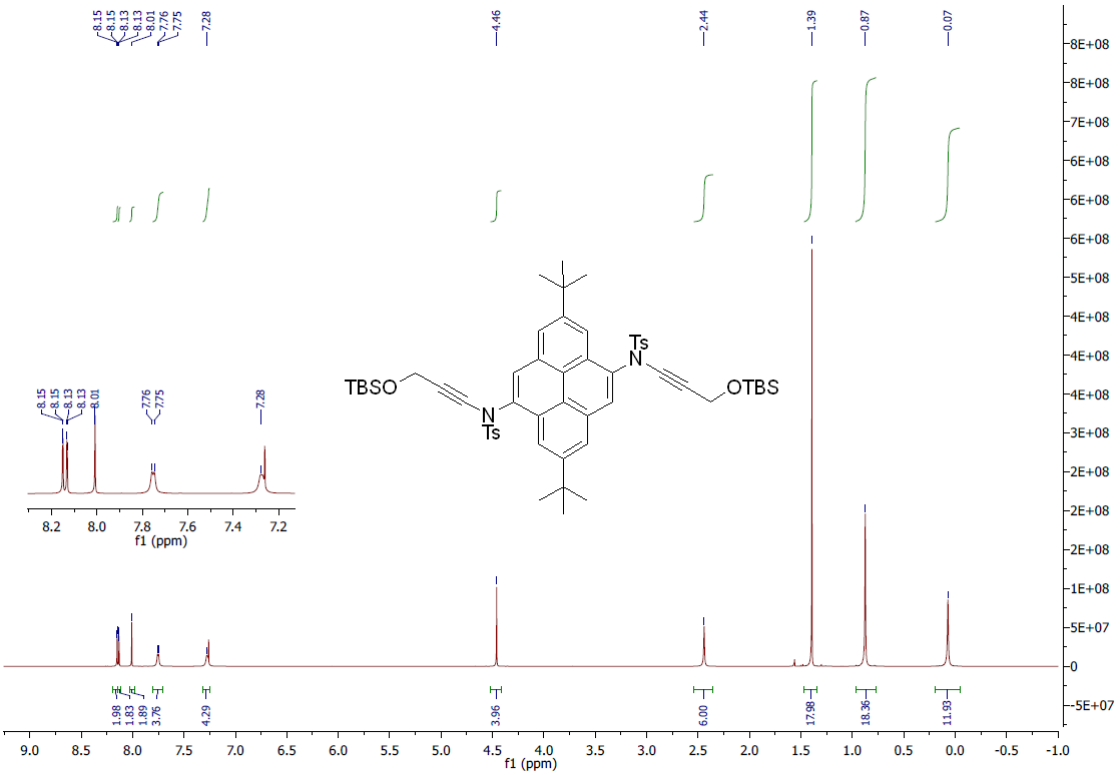


^{13}C NMR:

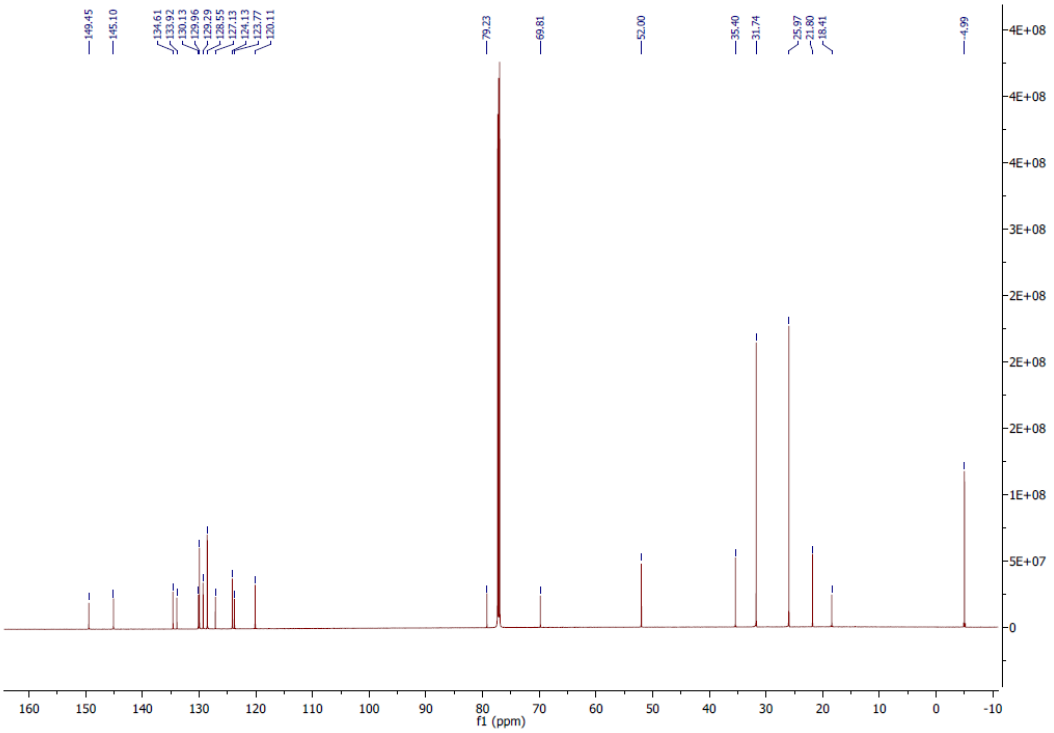


N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-((tert-butyldimethylsilyl)oxy)prop-1-yn-1-yl)-4-methylbenzenesulfonamide) 9

^{1}H NMR:



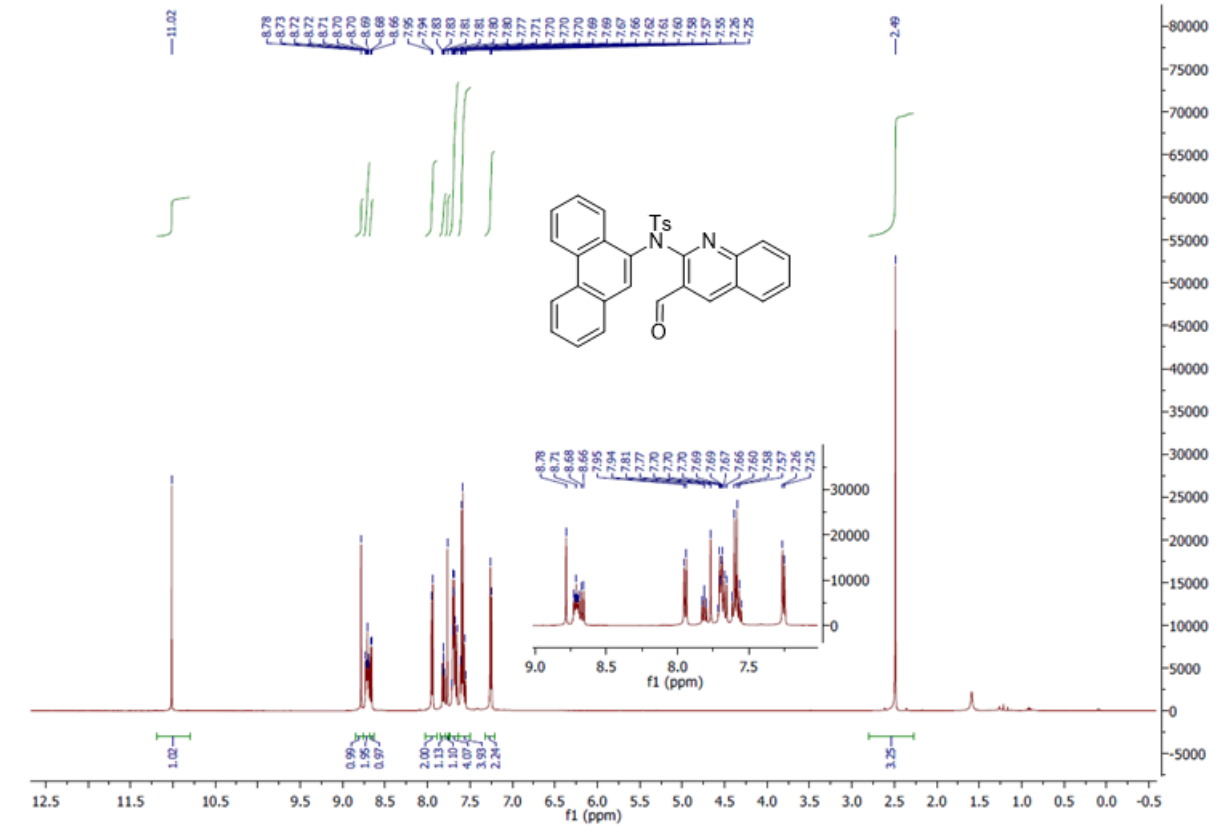
^{13}C NMR:



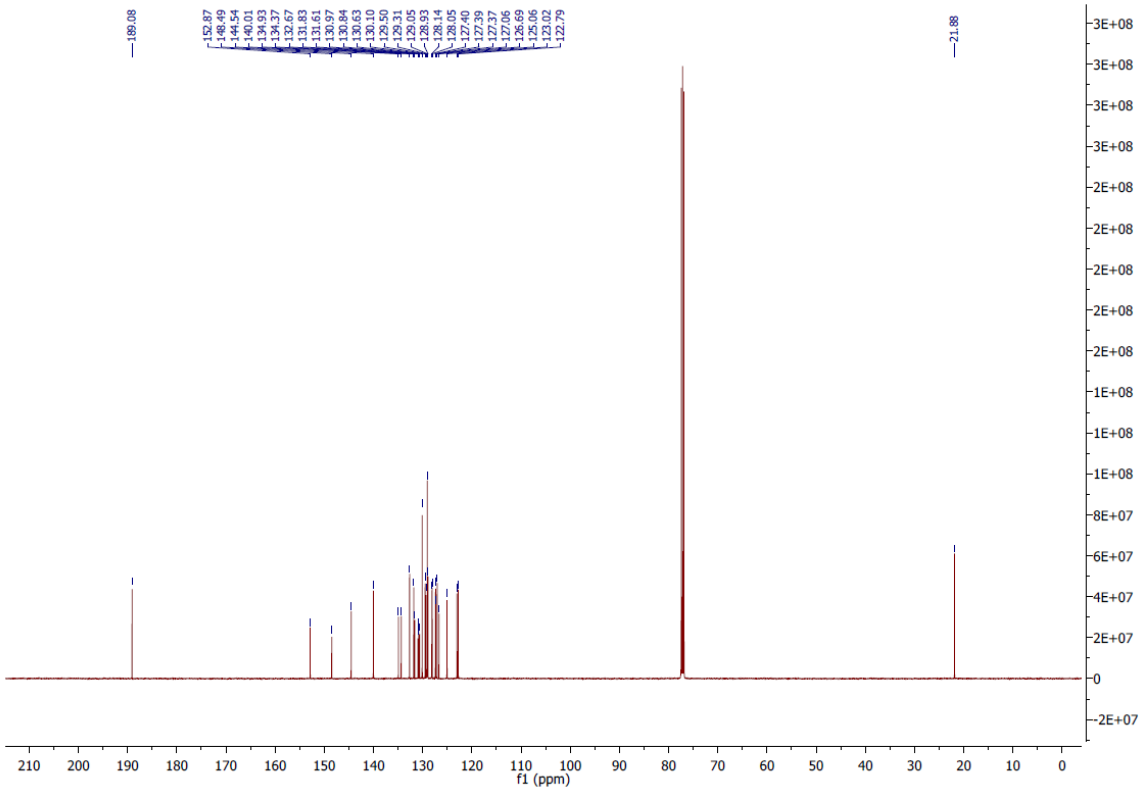
5.2. NMR of Quinolines 4a-h and 10a-d

N-(3-formylquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4a

^{1}H NMR:

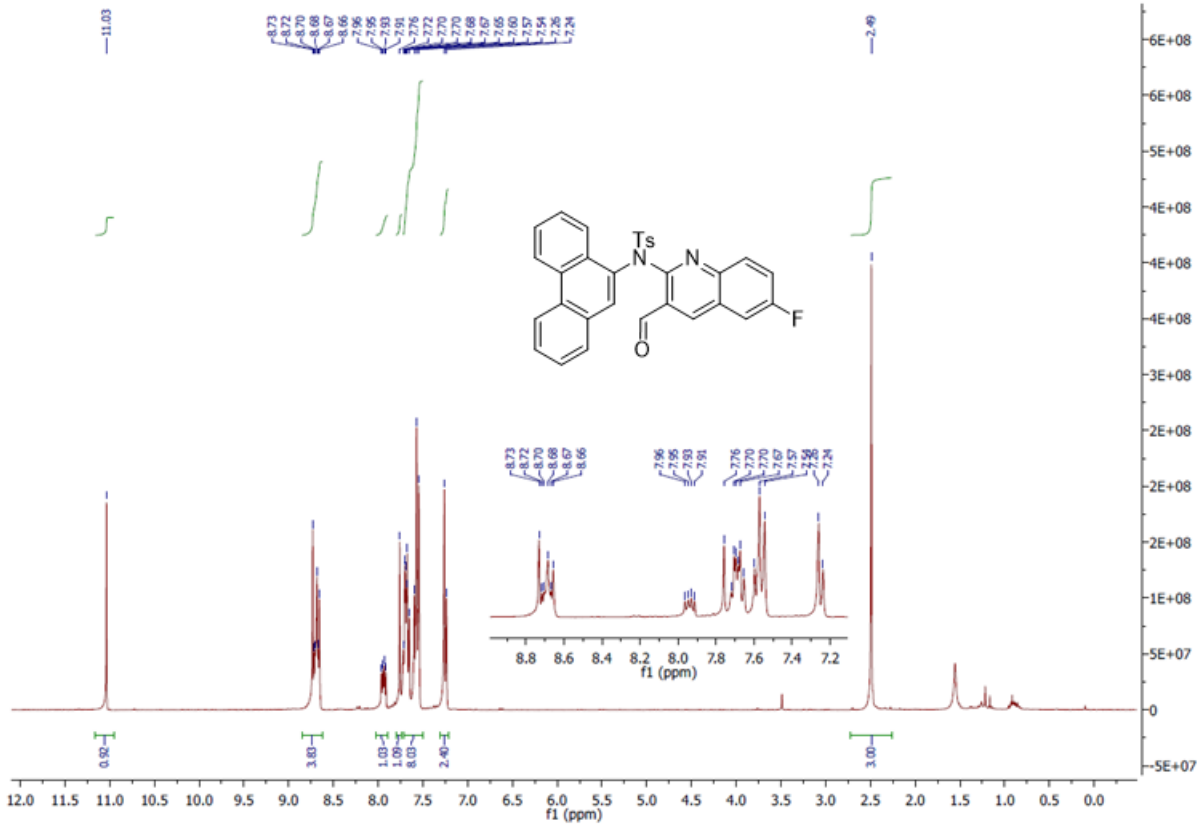


^{13}C NMR:

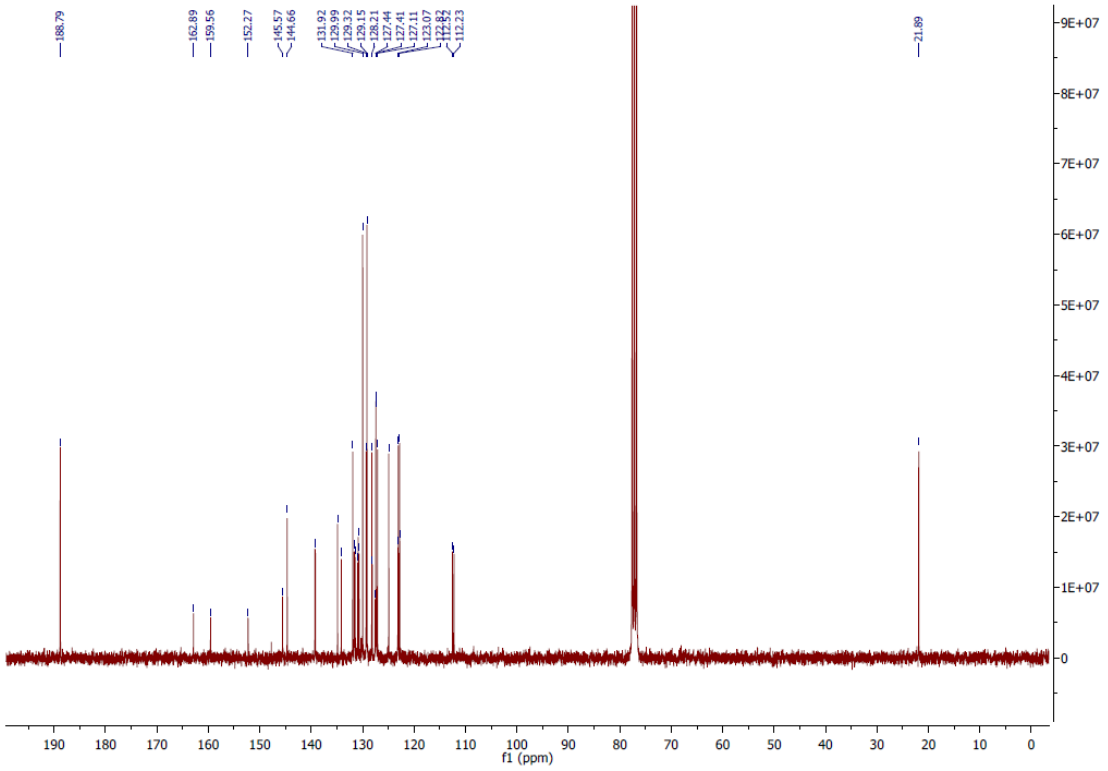


N-(6-fluoro-3-formylquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4b

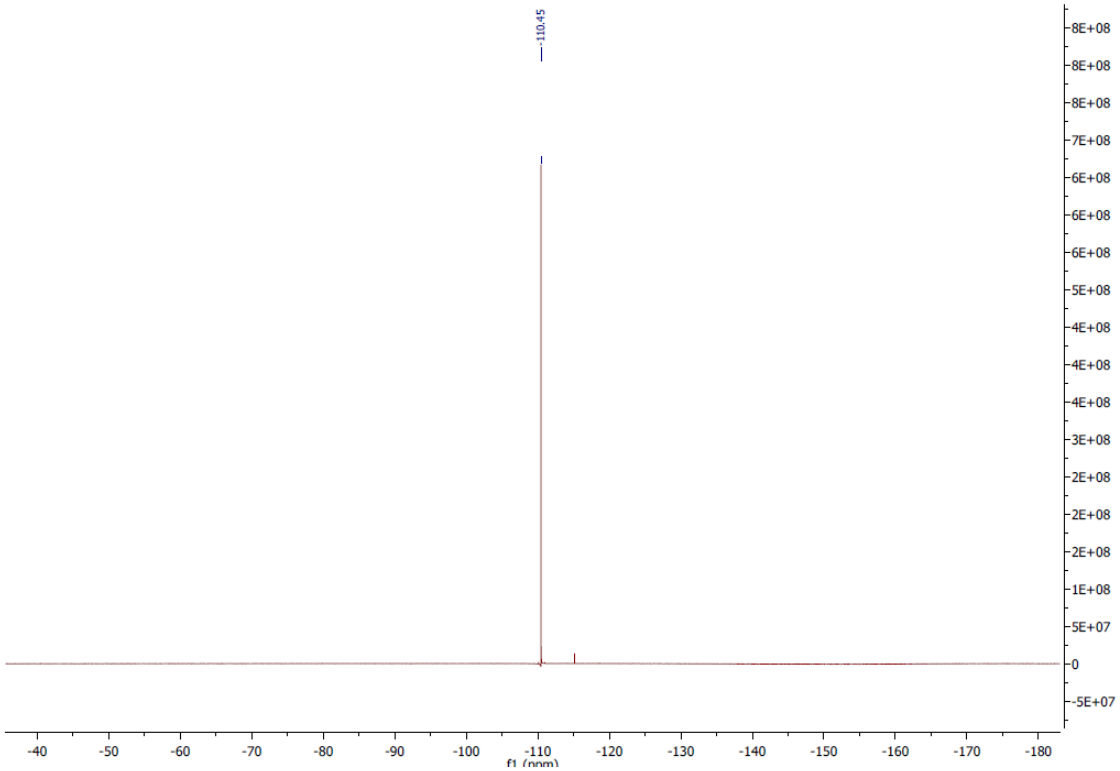
^{1}H NMR:



^{13}C NMR:

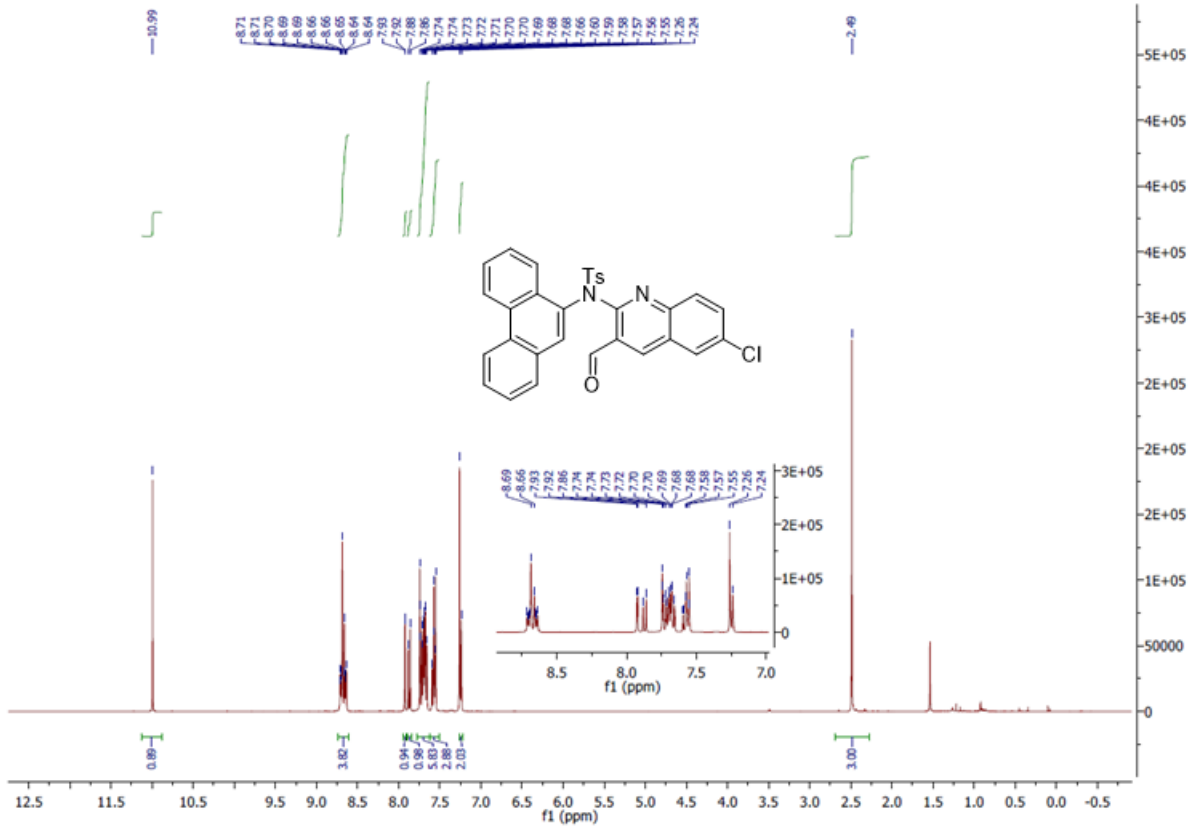


^{19}F NMR:

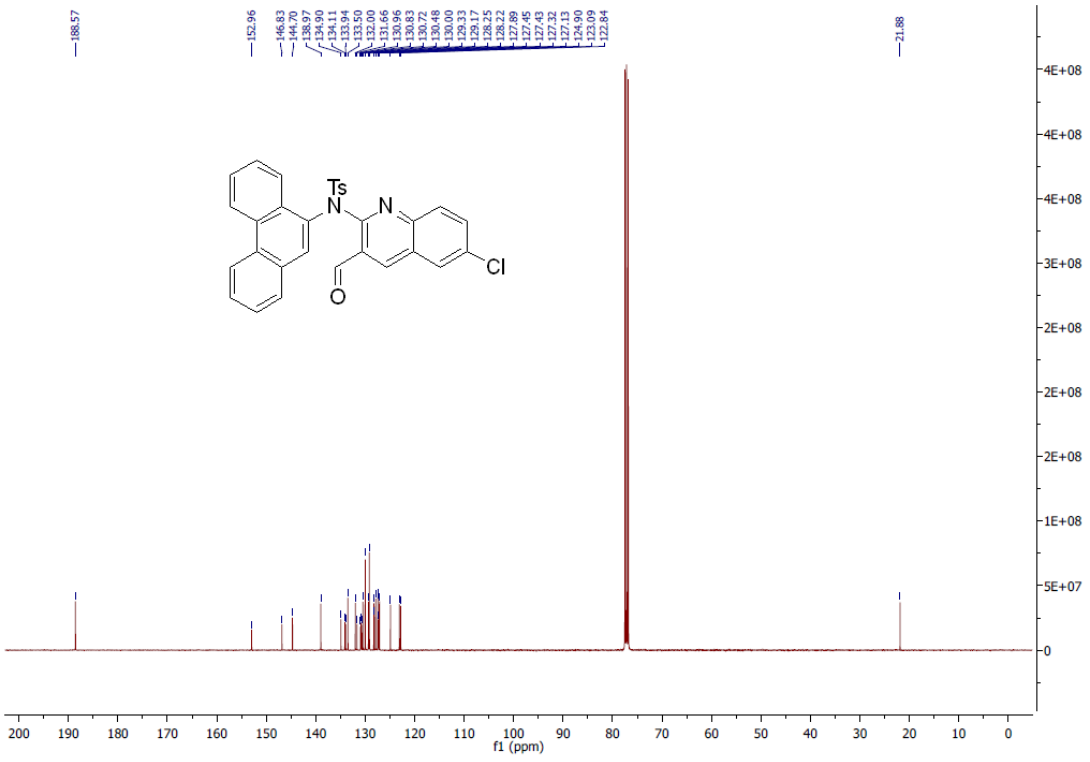


N-(6-chloro-3-formylquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4c

^{1}H NMR:

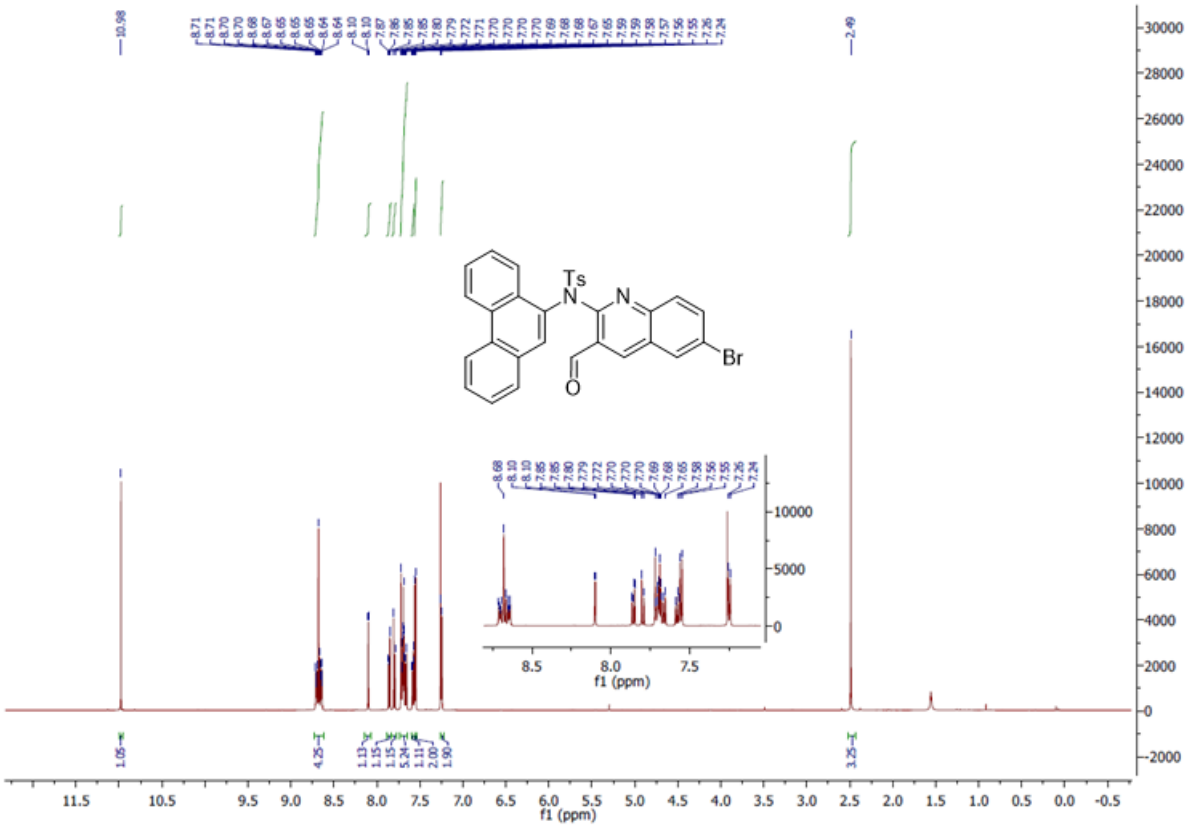


^{13}C NMR:

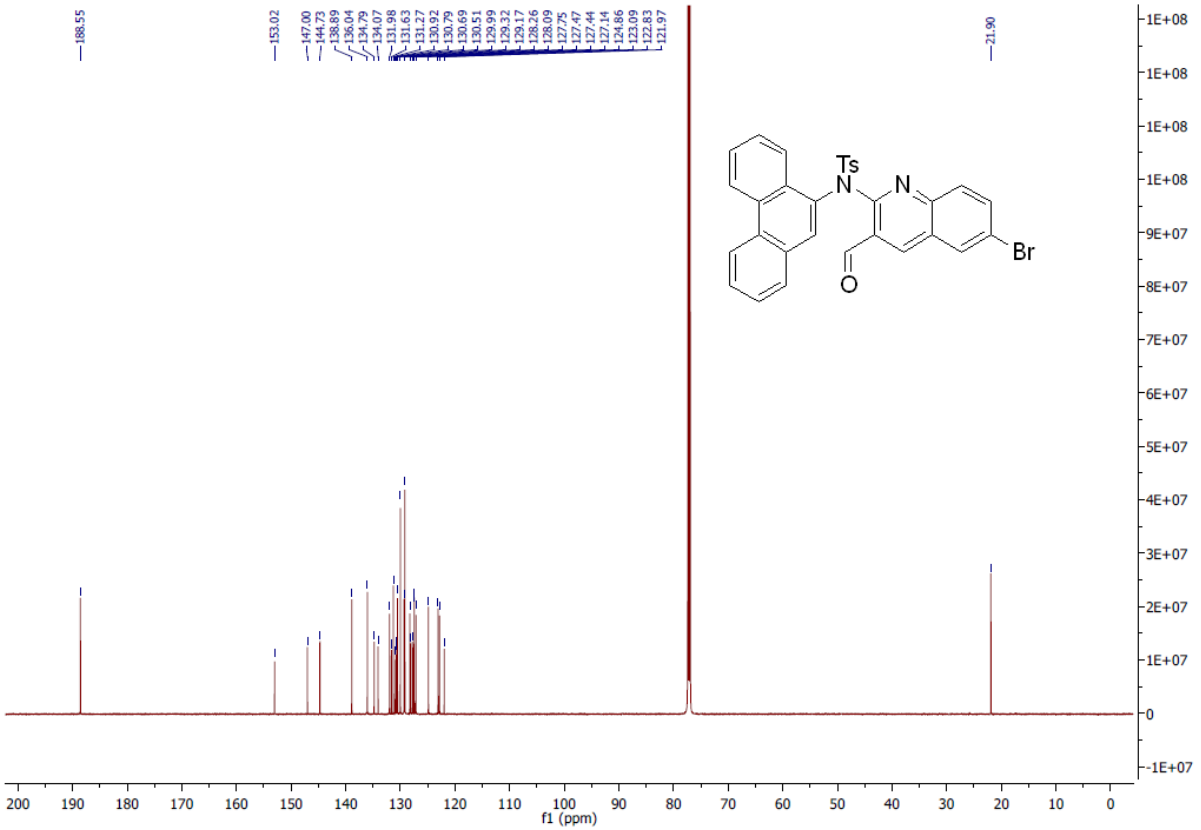


N-(6-bromo-3-formylquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4d

^{1}H NMR:

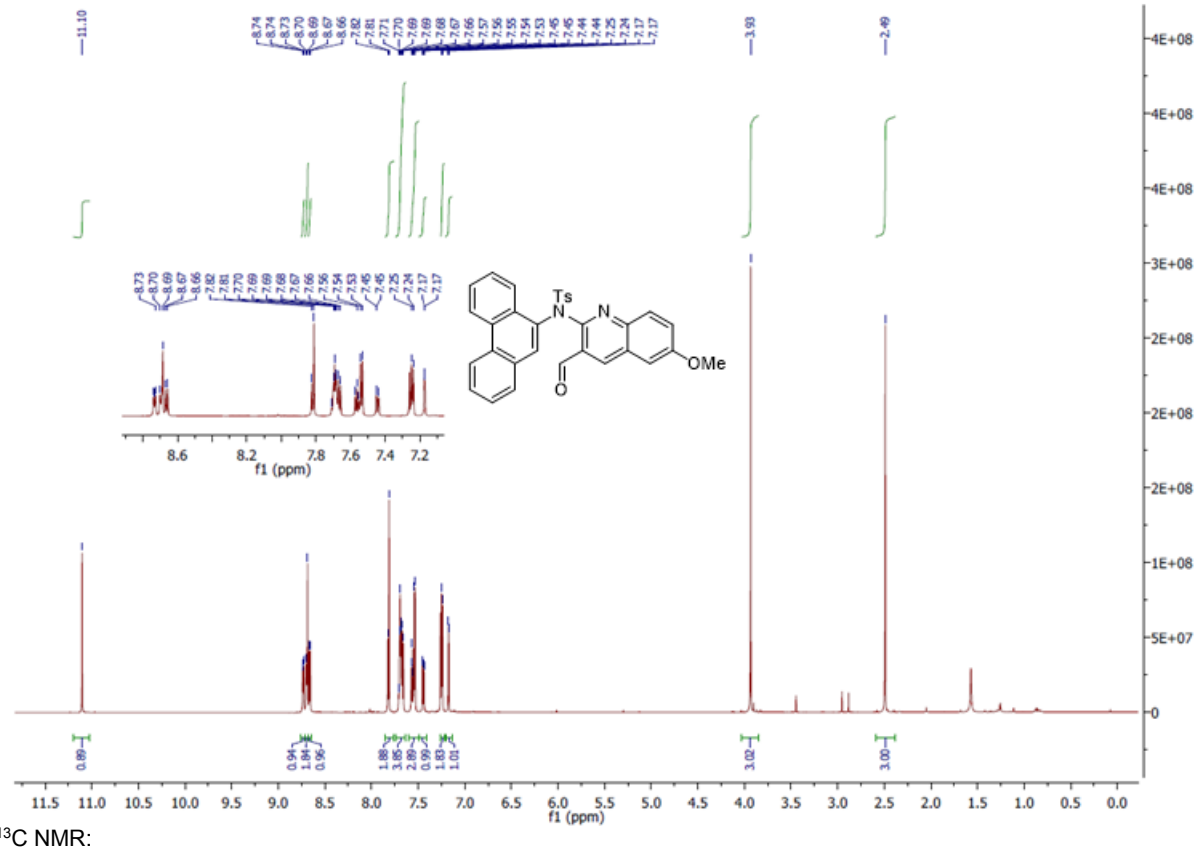


^{13}C NMR:

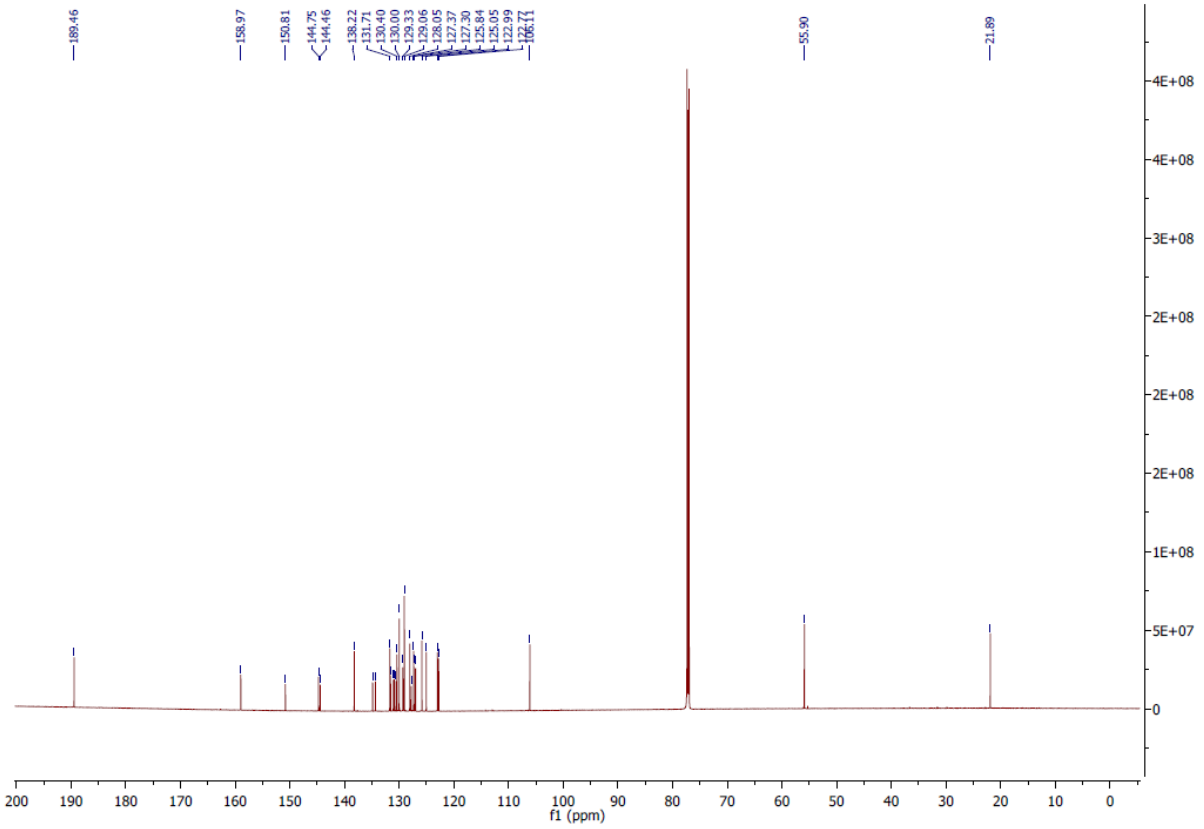


N-(3-formyl-6-methoxyquinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4e

^{1}H NMR:

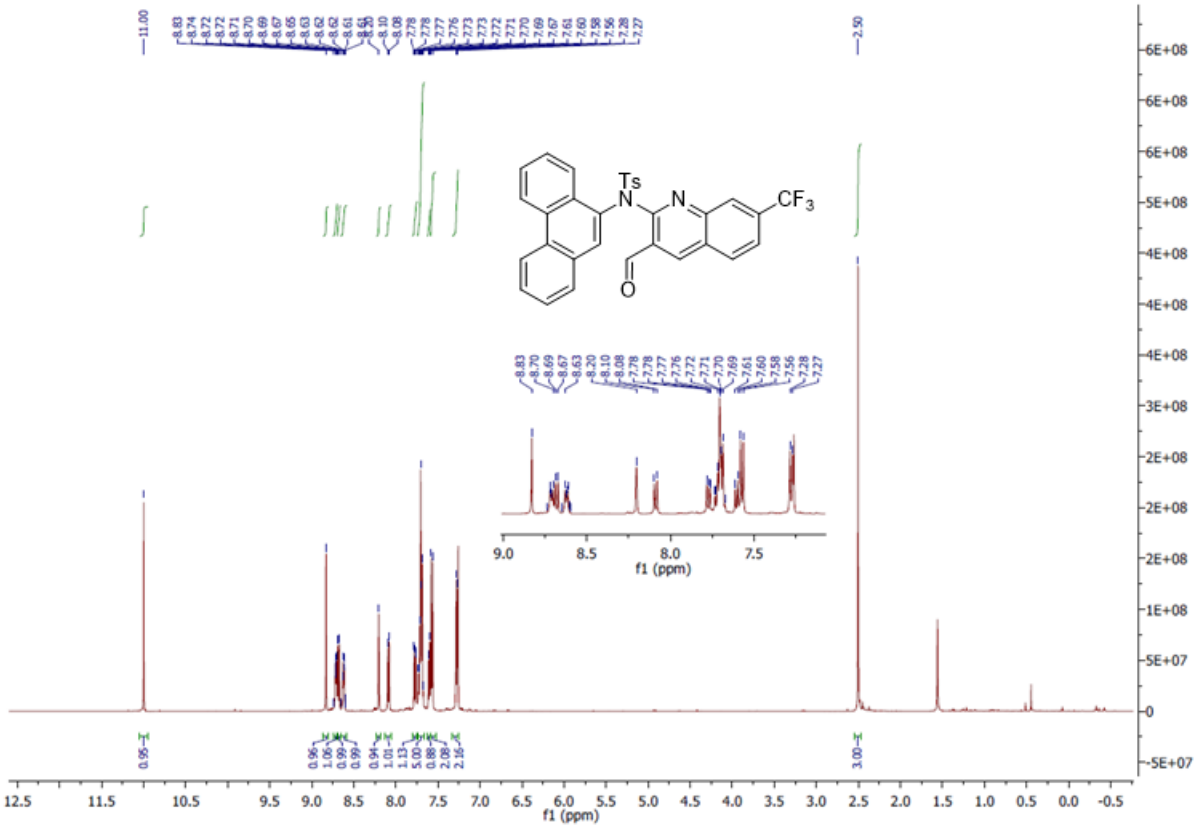


^{13}C NMR:

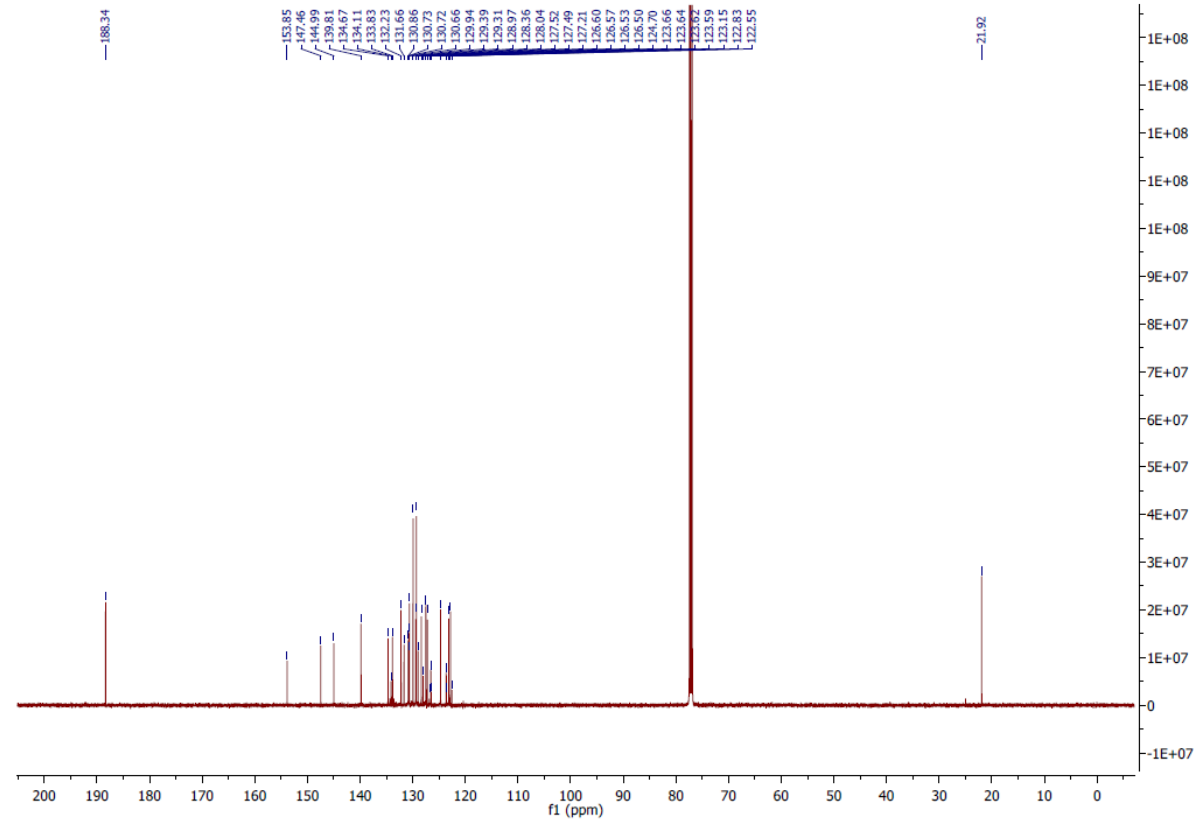


N-(3-formyl-7-(trifluoromethyl)quinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4f

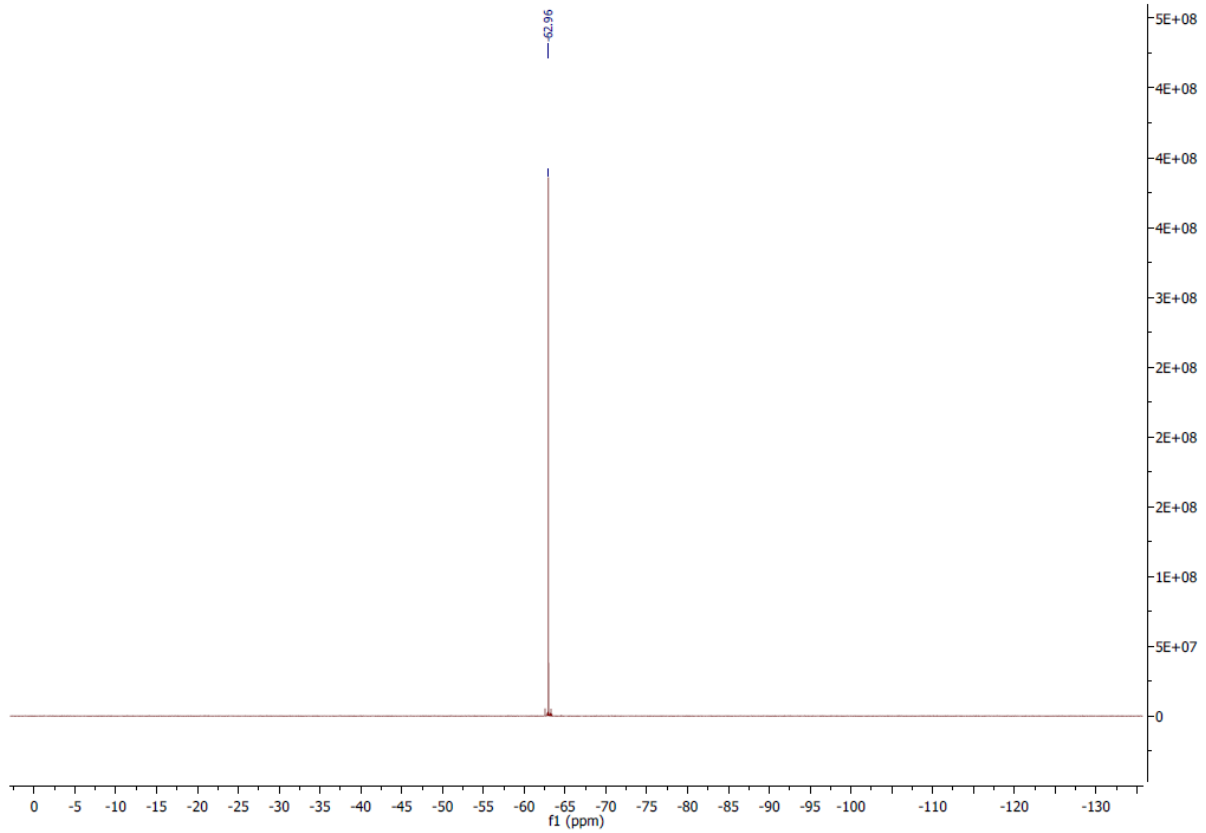
^{1}H NMR:



^{13}C NMR:

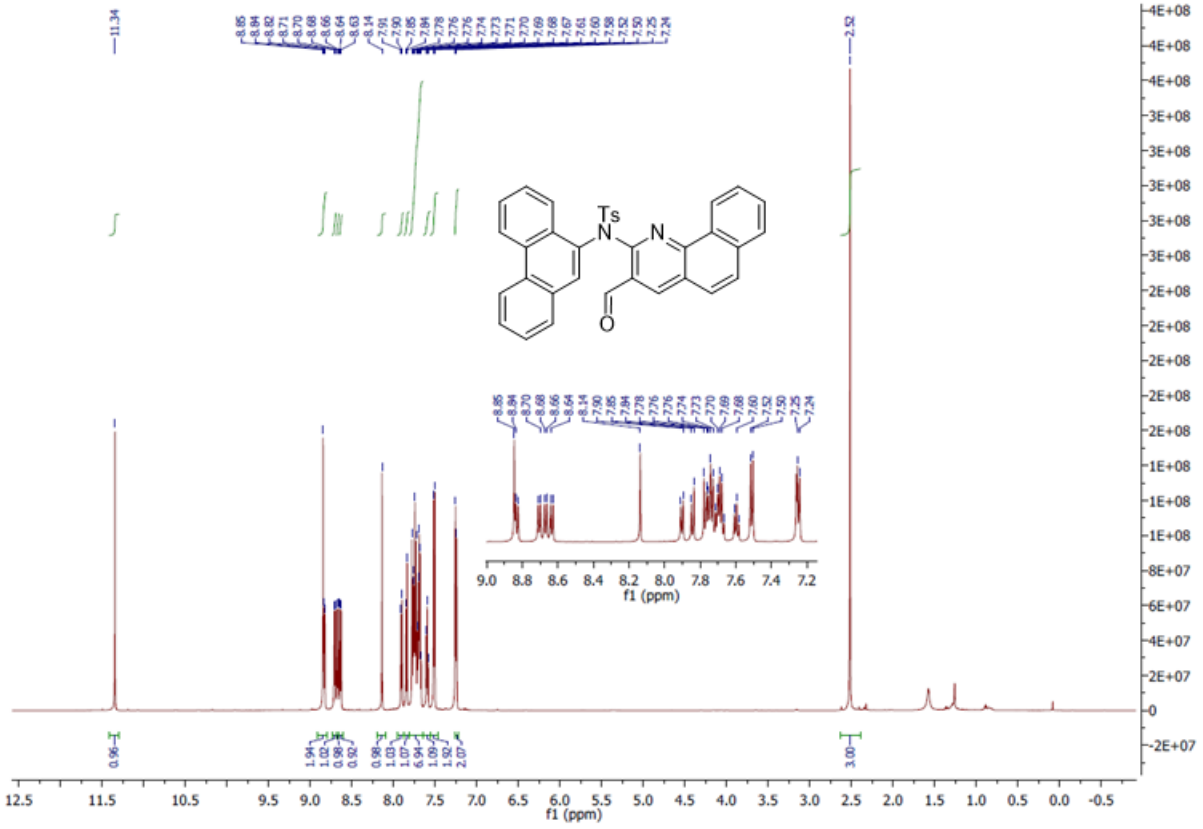


^{19}F NMR:

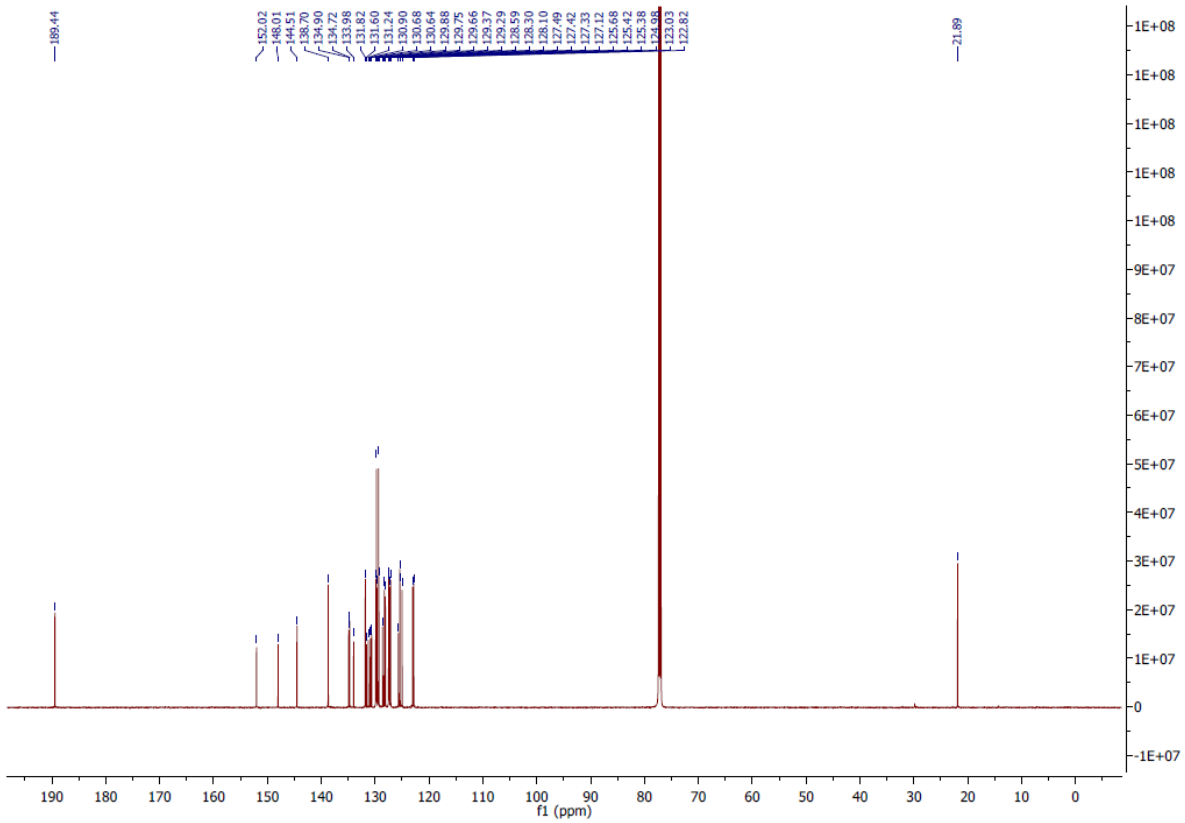


N-(3-formylbenzo[h]quinolin-2-yl)-4-methyl-N-(phenanthren-9-yl)benzenesulfonamide 4g

^{1}H NMR:

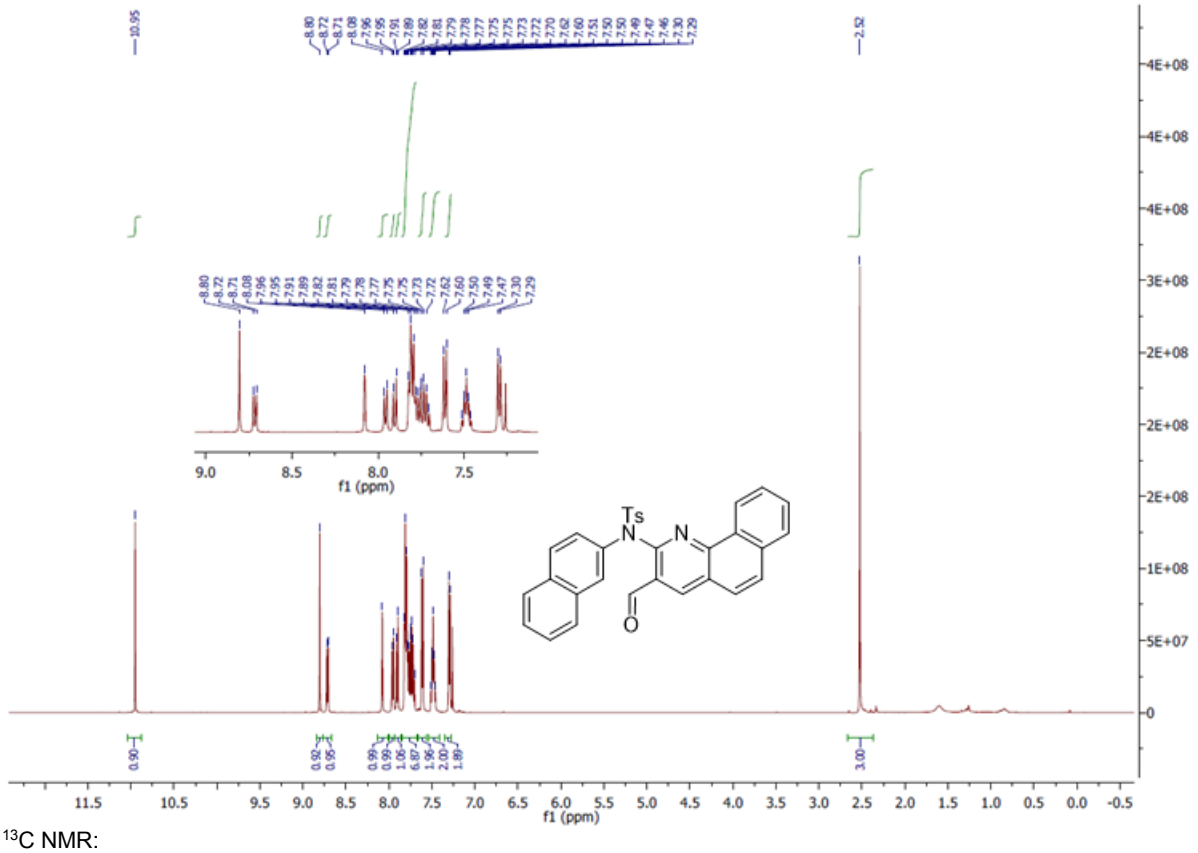


^{13}C NMR:

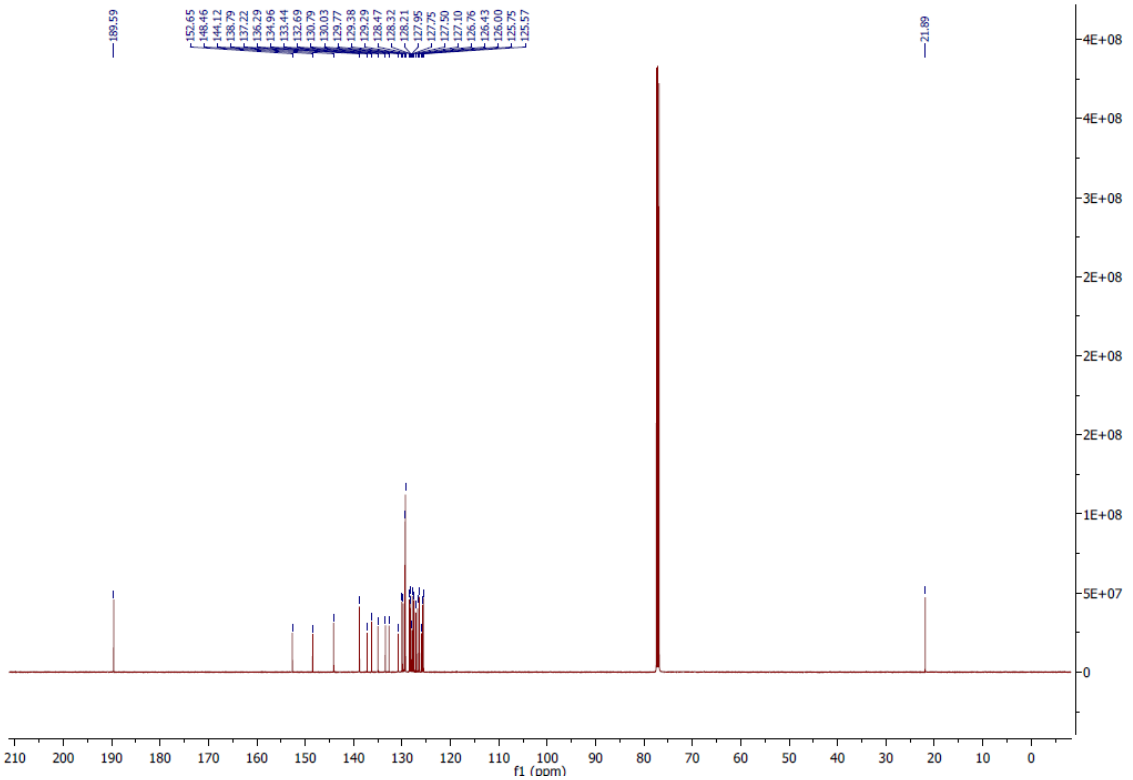


N-(3-formylbenzo[h]quinolin-2-yl)-4-methyl-N-(naphthalen-2-yl)benzenesulfonamide 4h

^{1}H NMR:

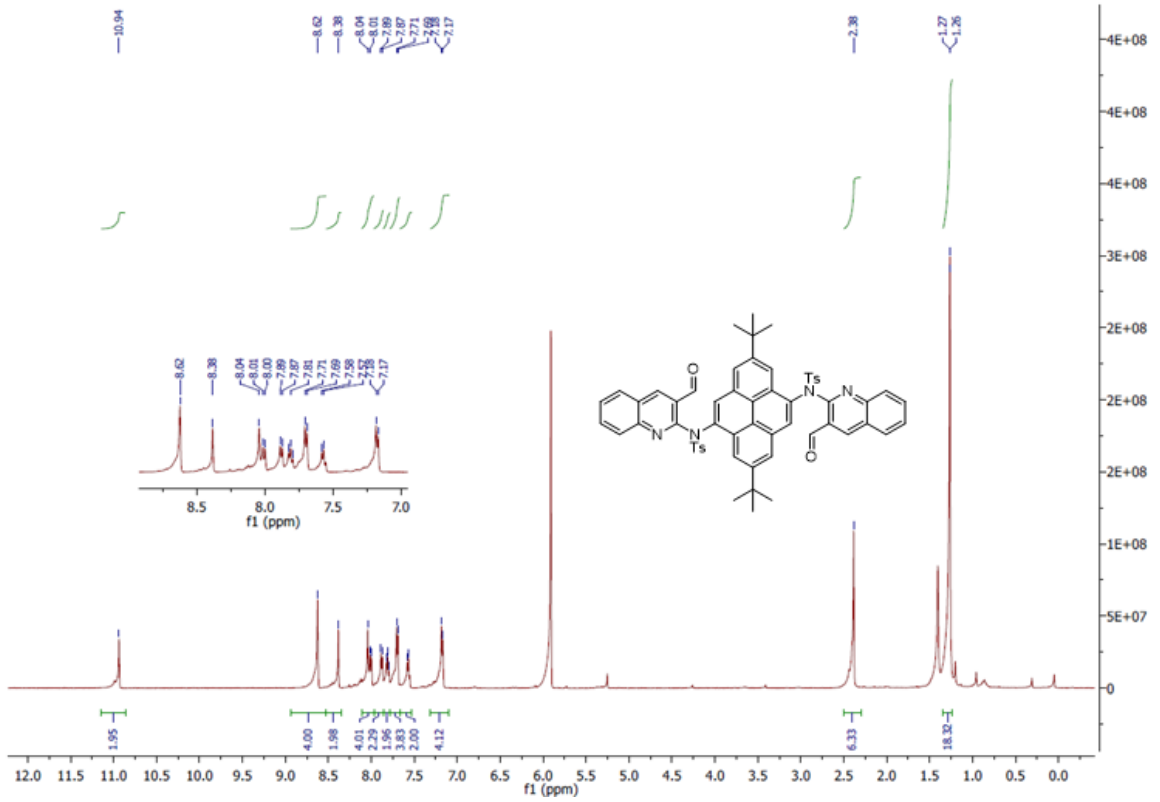


^{13}C NMR:



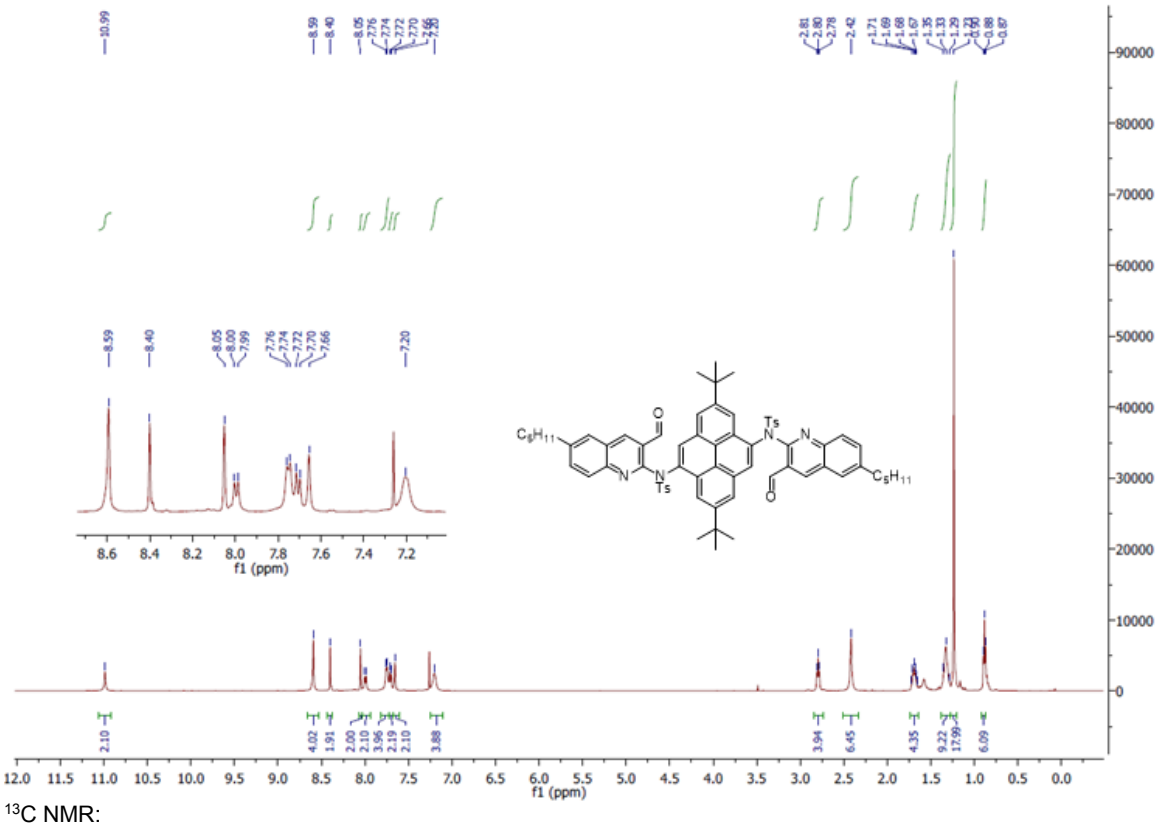
N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-formylquinolin-2-yl)-4-methylbenzenesulfonamide) 10a

^{1}H NMR:

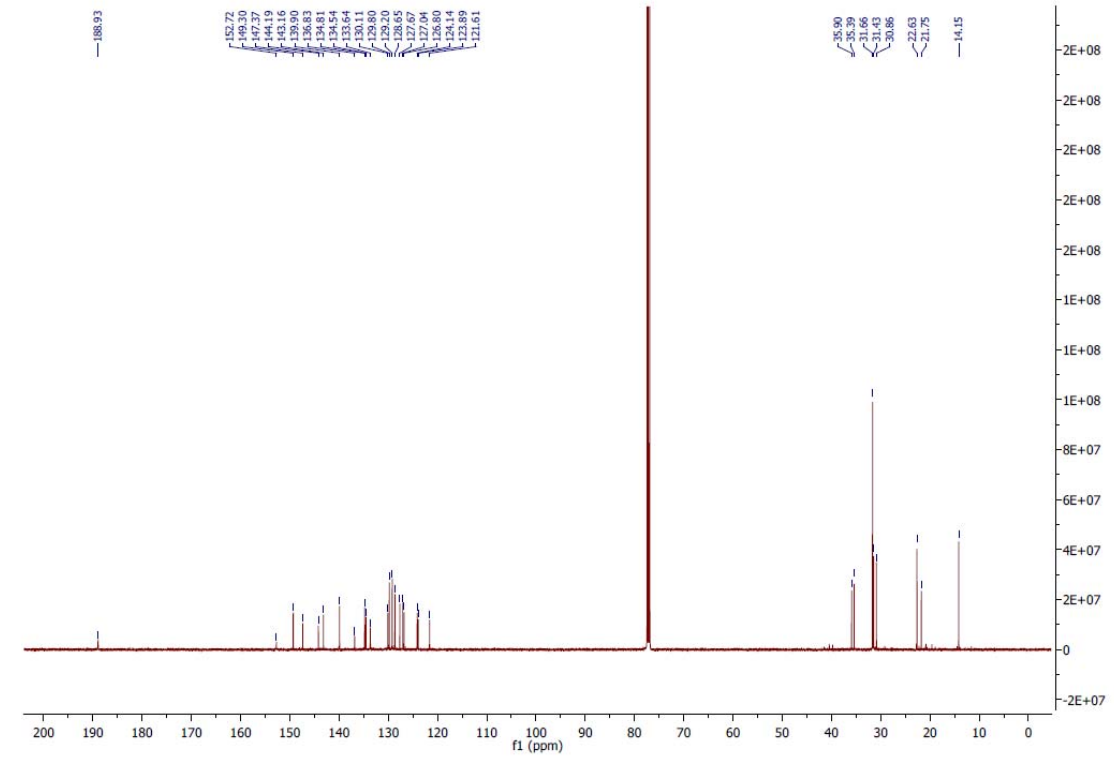


N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-formyl-6-pentylquinolin-2-yl)-4-methylbenzenesulfonamide) 10b

^{1}H NMR:

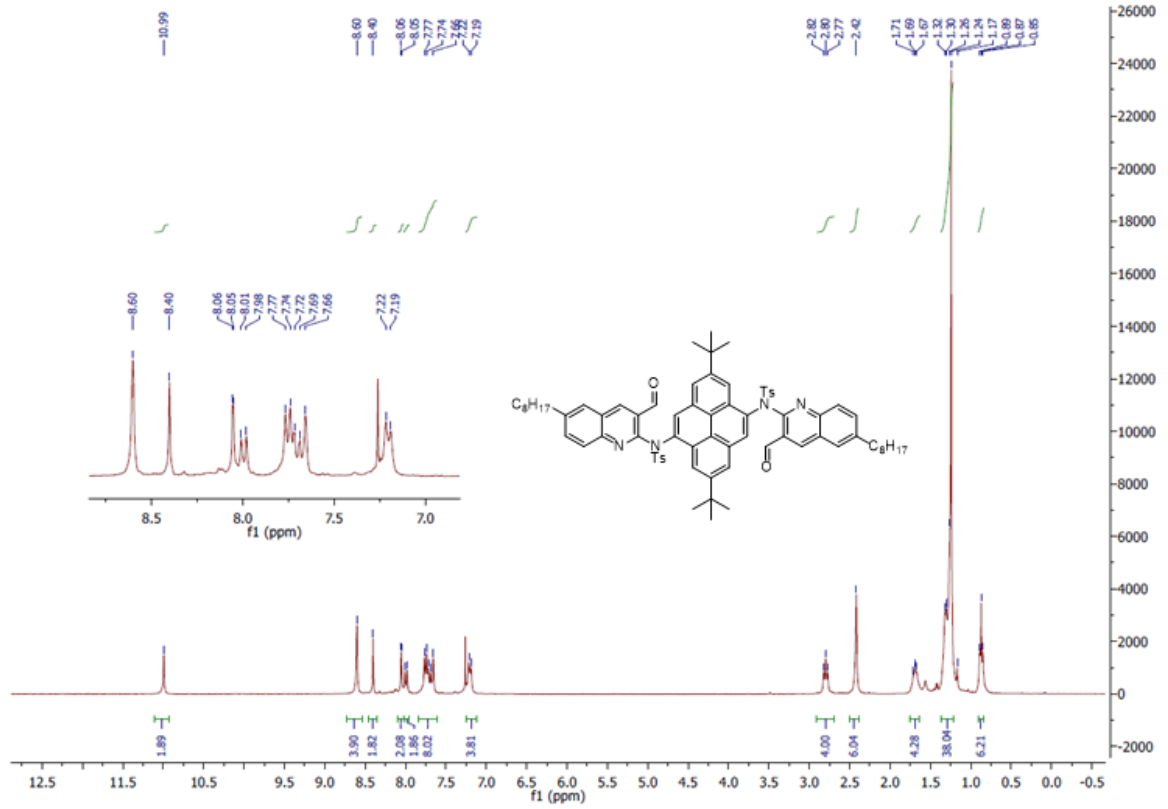


^{13}C NMR:

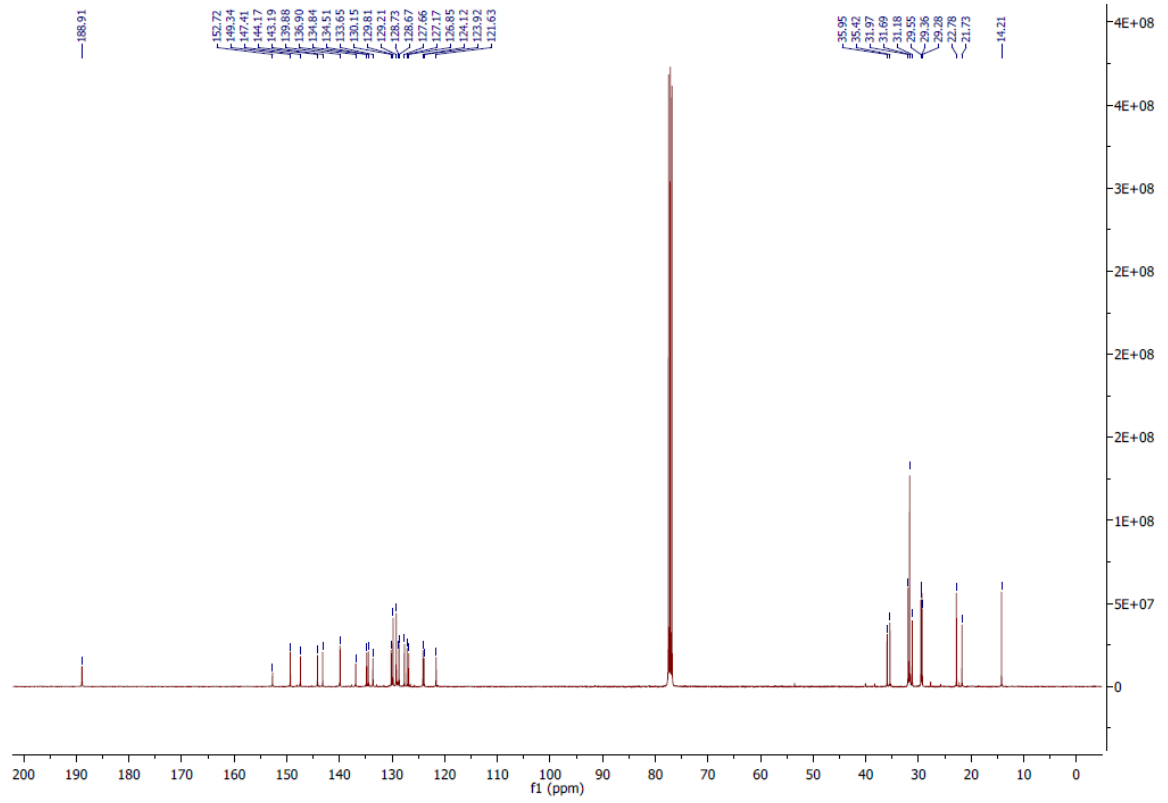


N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(3-formyl-6-octylquinolin-2-yl)-4-methylbenzenesulfonamide) 10c

^{1}H NMR:

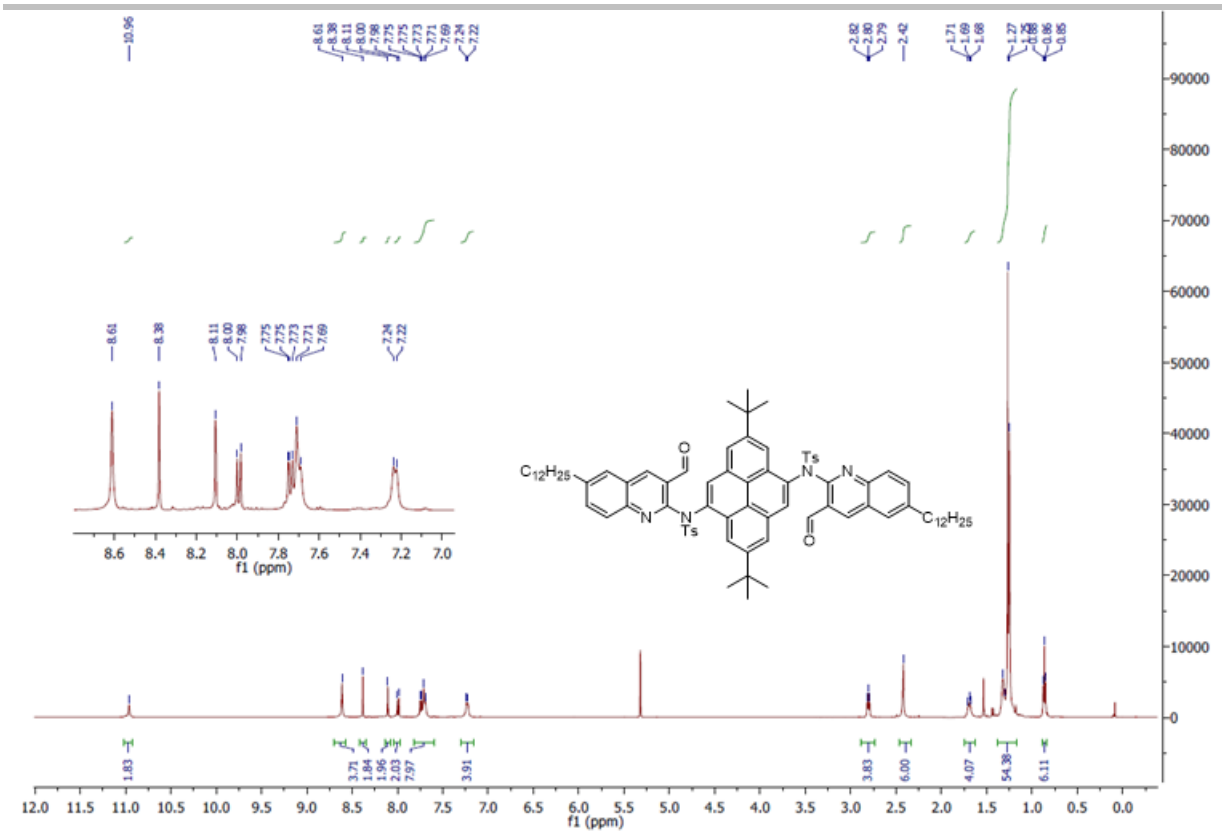


^{13}C NMR:

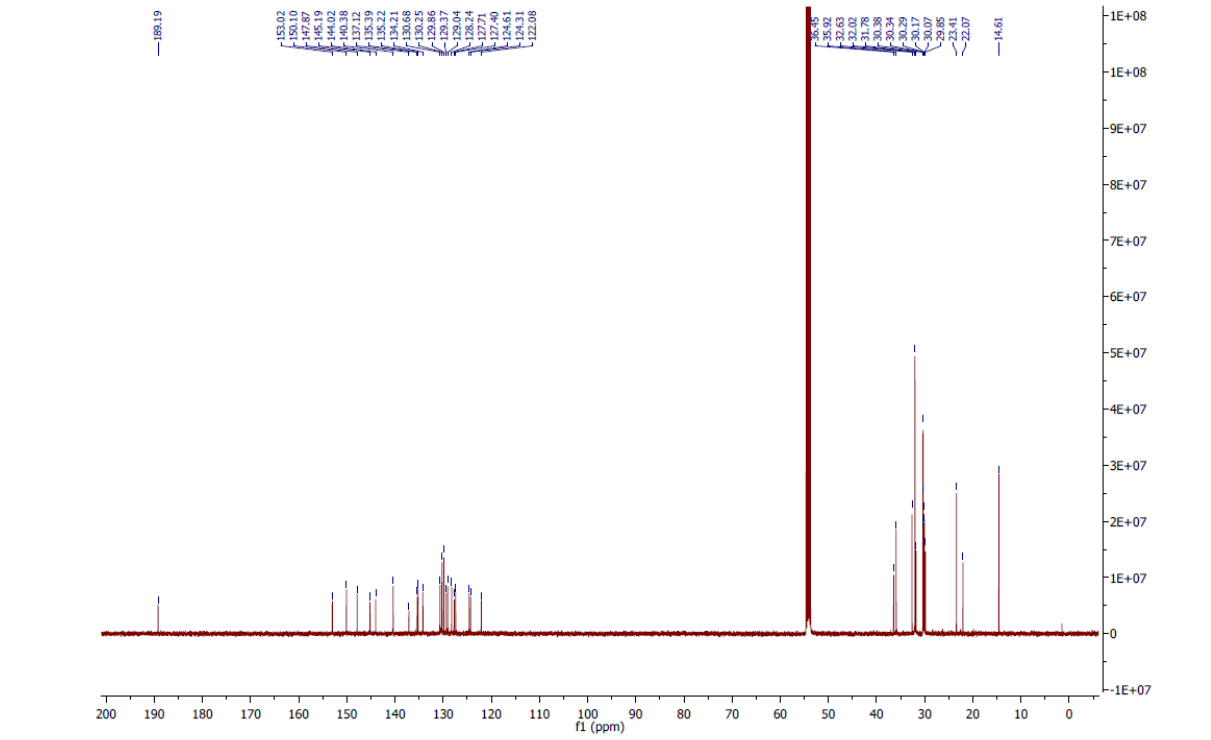


N,N'-(2,7-di-tert-butylpyrene-4,9-diyl)bis(N-(6-dodecyl-3-formylquinolin-2-yl)-4-methylbenzenesulfonamide) 10d

^{1}H NMR:



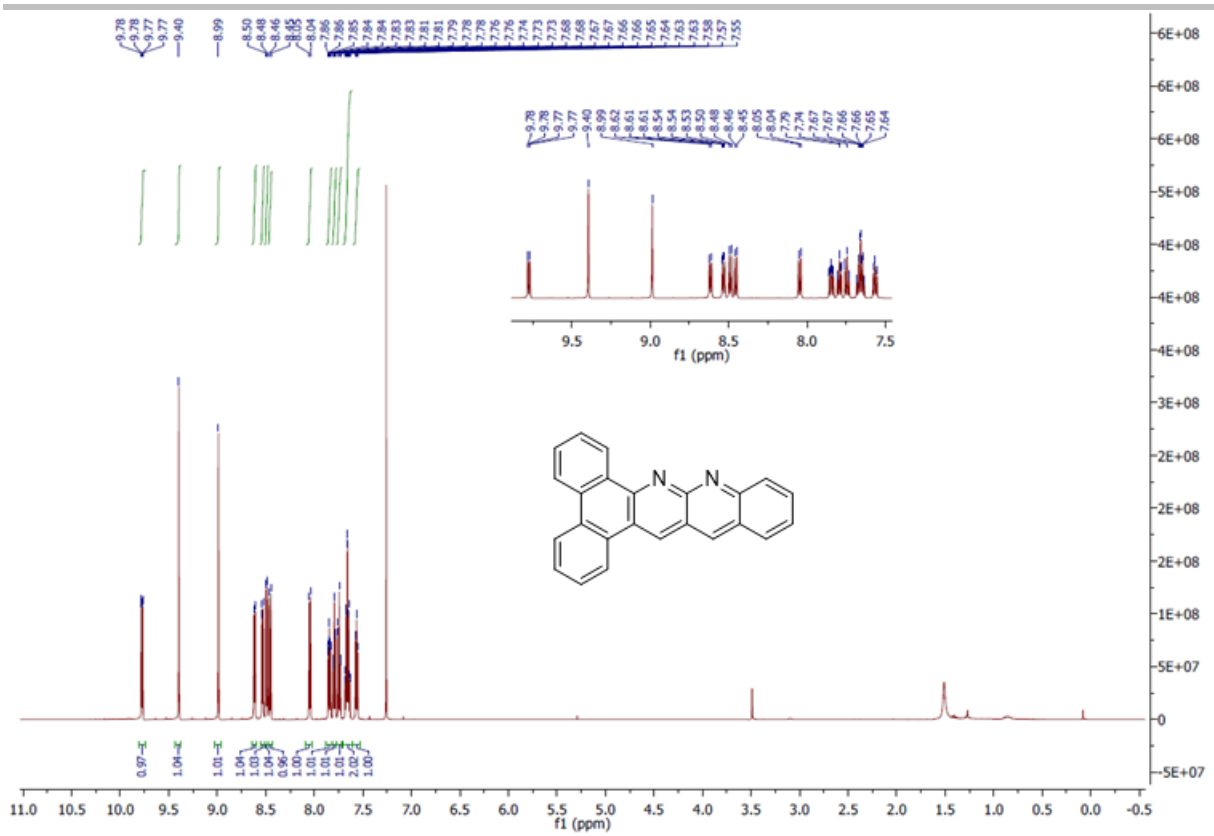
^{13}C NMR:



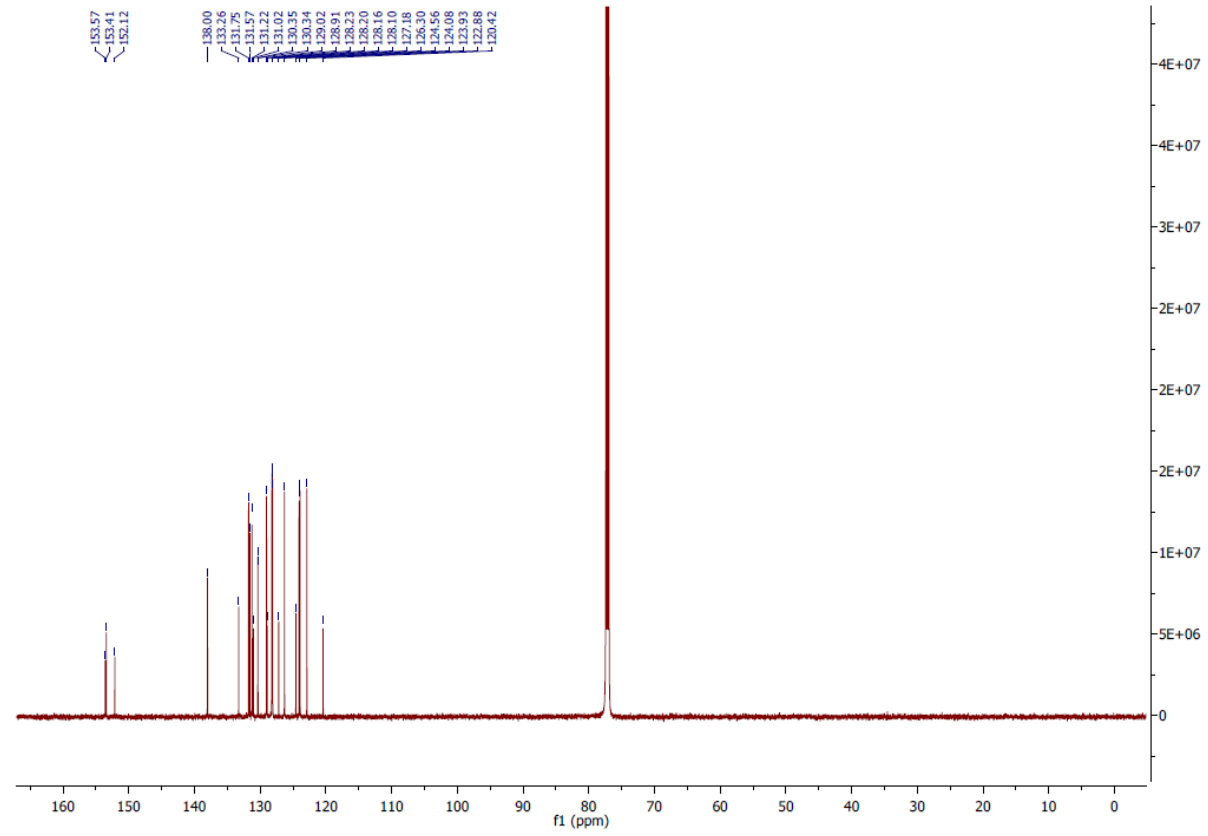
5.3. NMR of Naphthyridines 5a-h and 11c-d

benzo[b]phenanthro[9,10-g][1,8]naphthyridine 5a

^{1}H NMR:

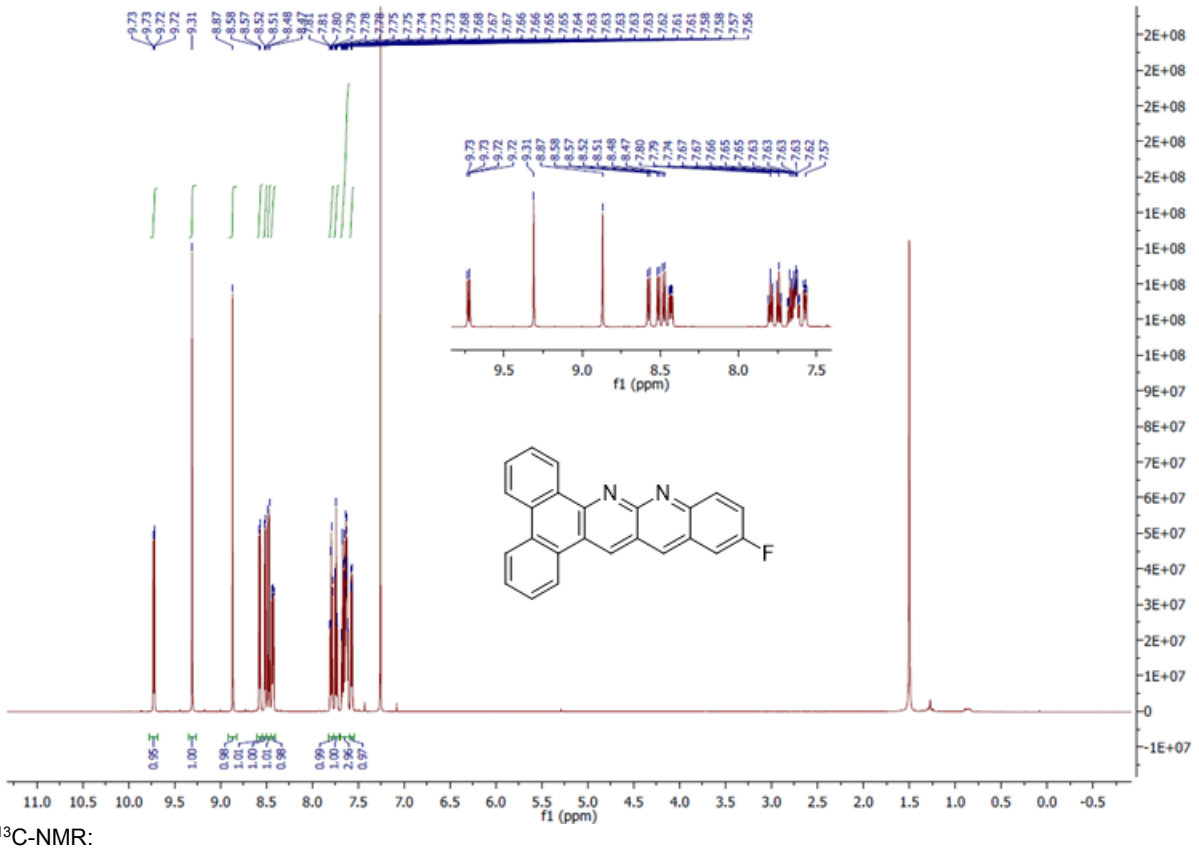


^{13}C NMR:

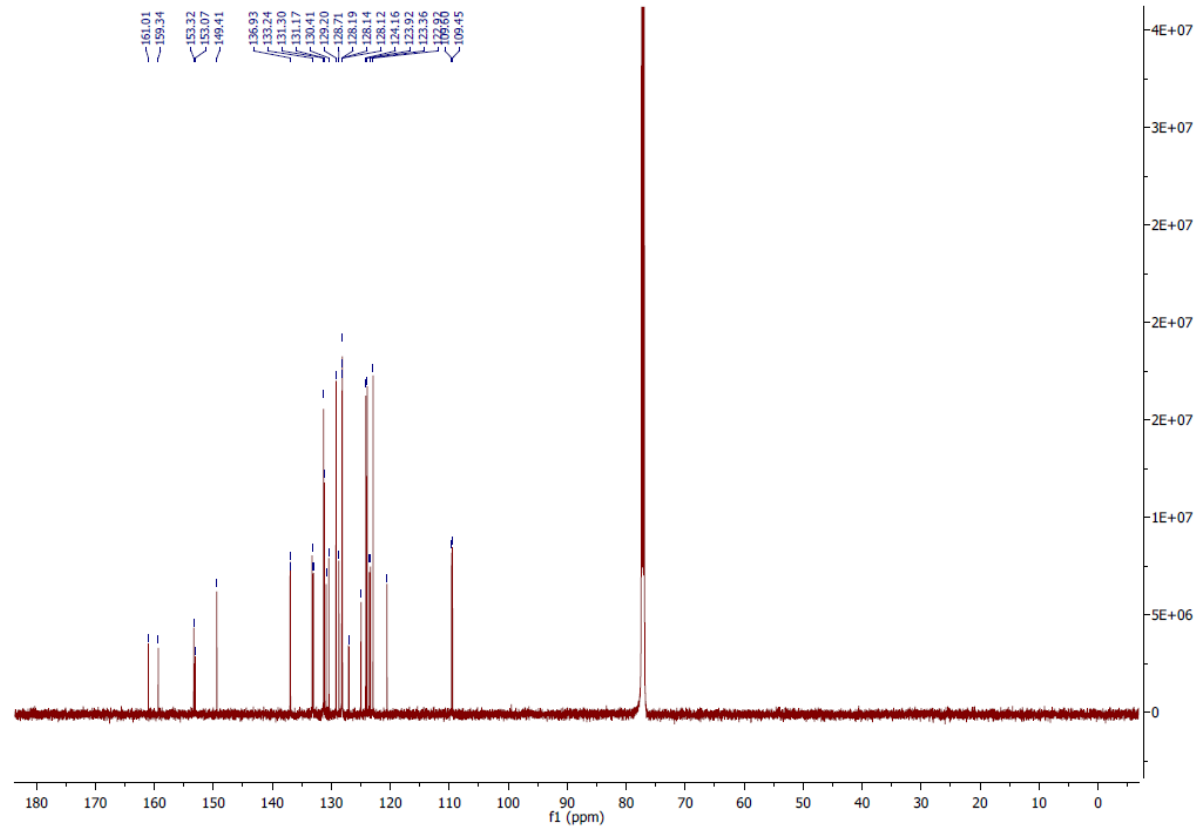


13-fluorobenzo[b]phenanthro[9,10-g][1,8]naphthyridine 5b

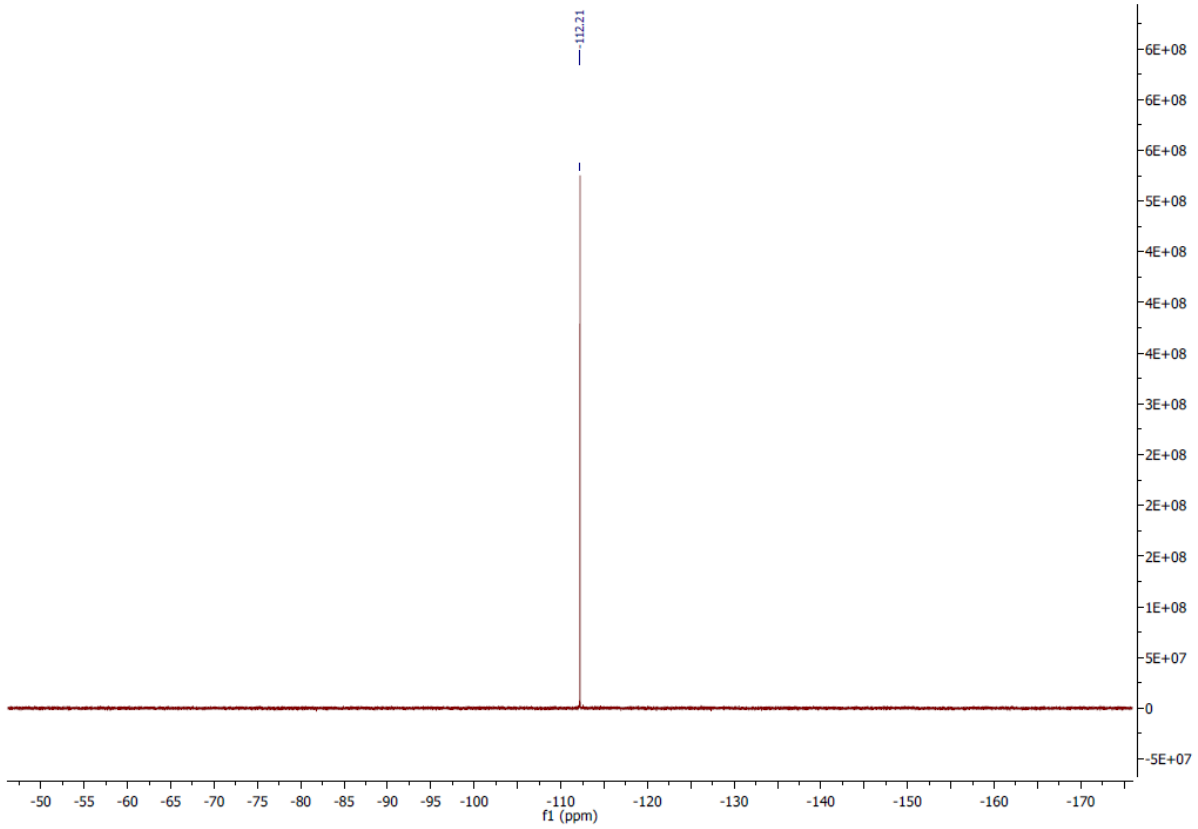
^{1}H NMR:



^{13}C-NMR:

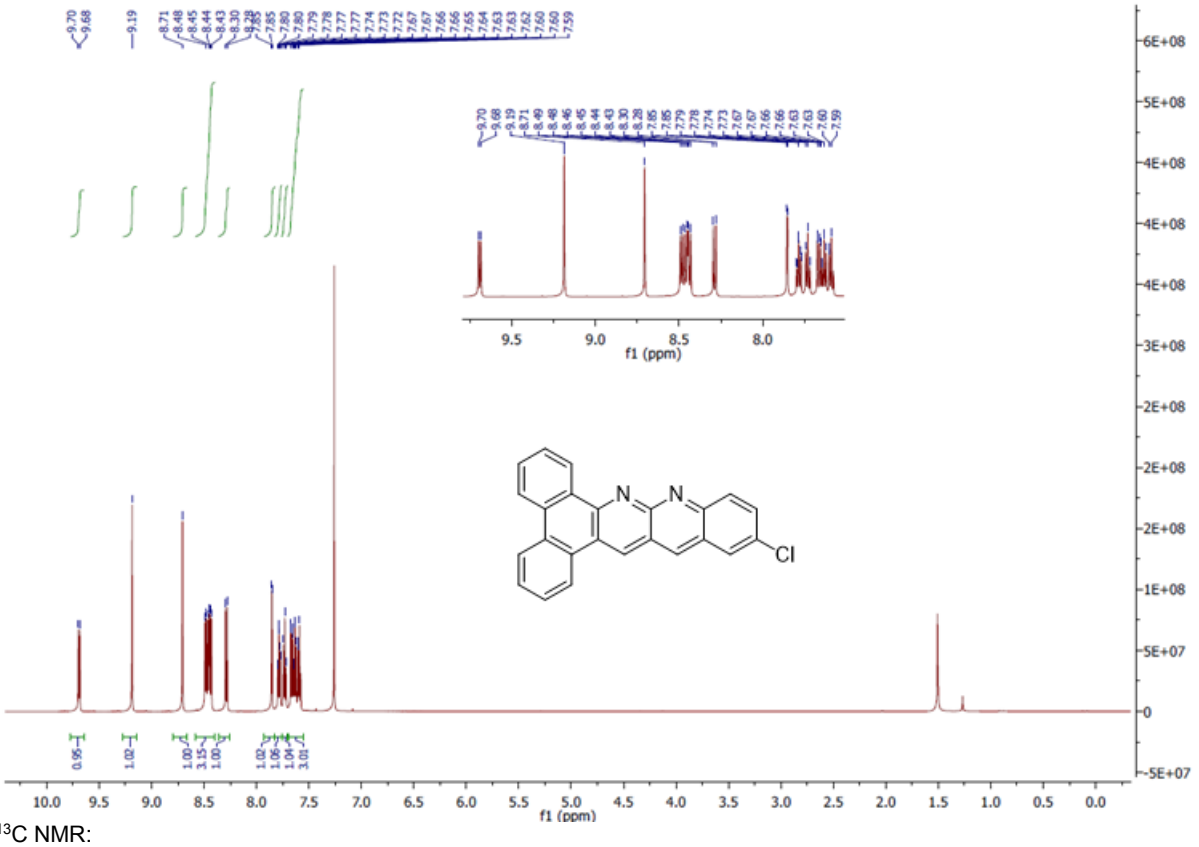


^{19}F NMR:

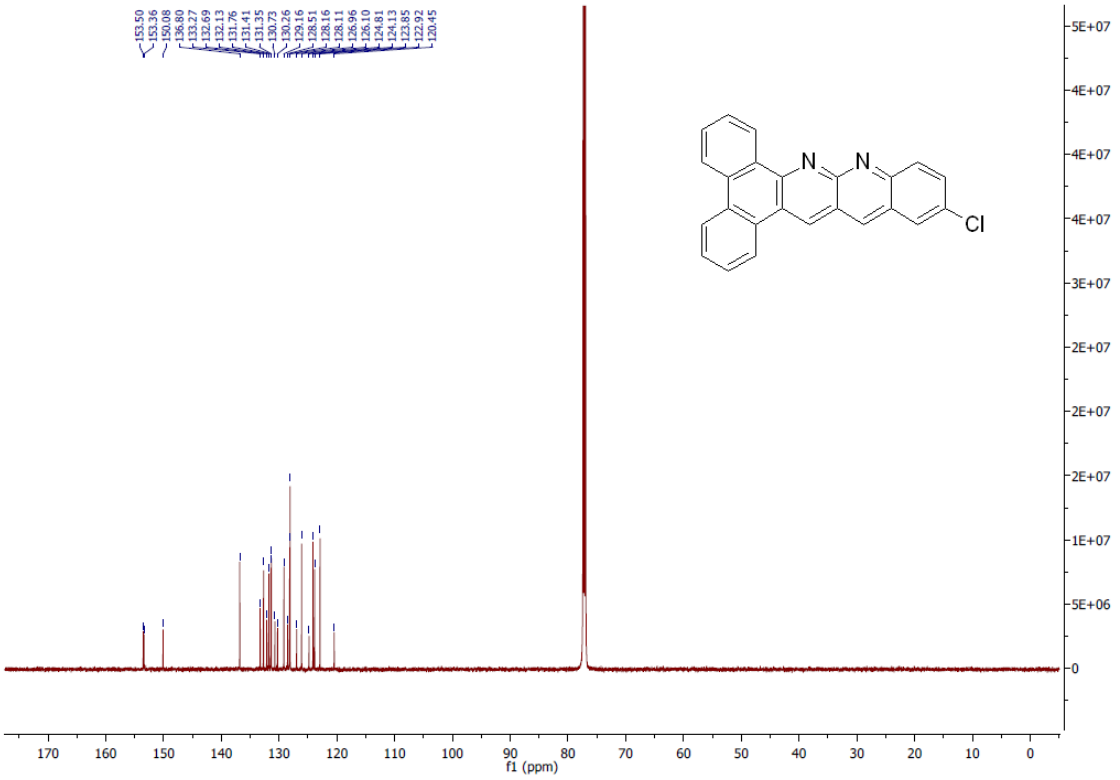


13-chlorobenzo[b]phenanthro[9,10-g][1,8]naphthyridine 5c

^{1}H NMR:

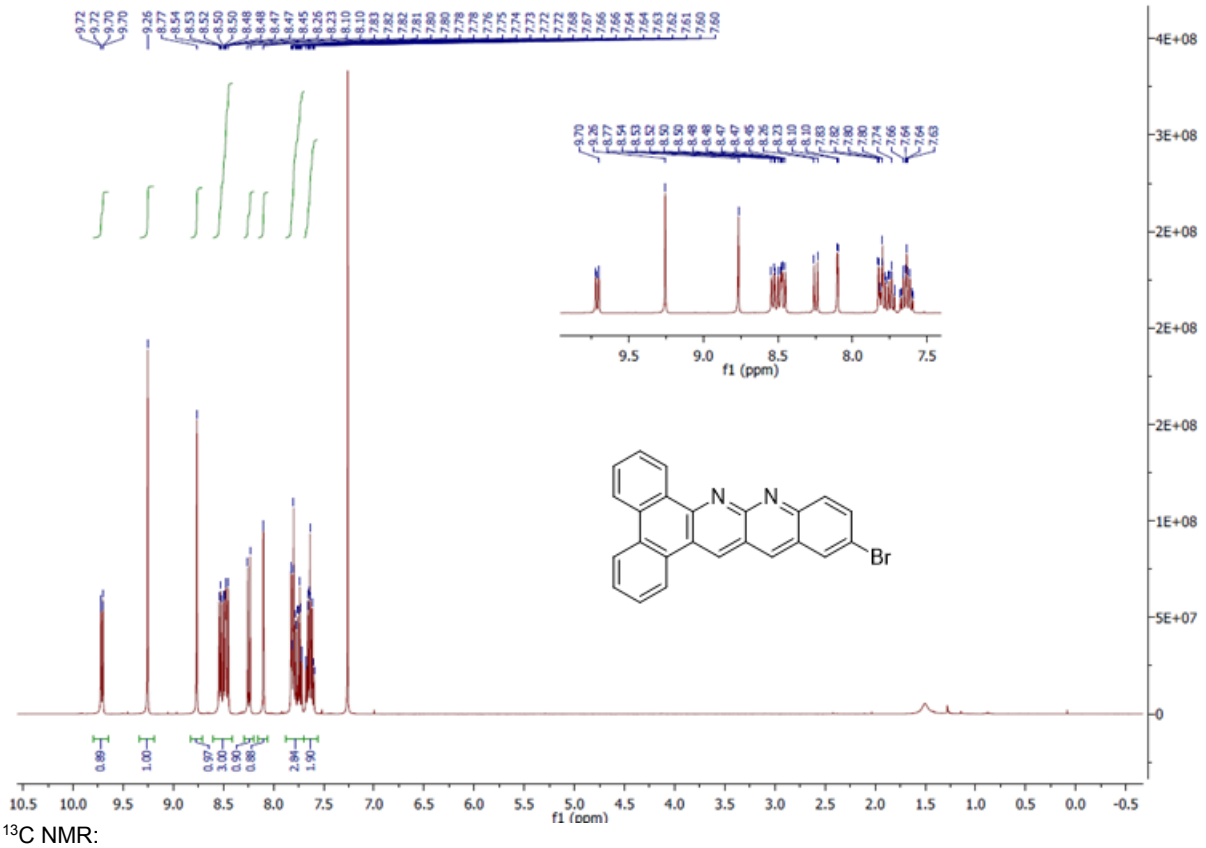


^{13}C NMR:

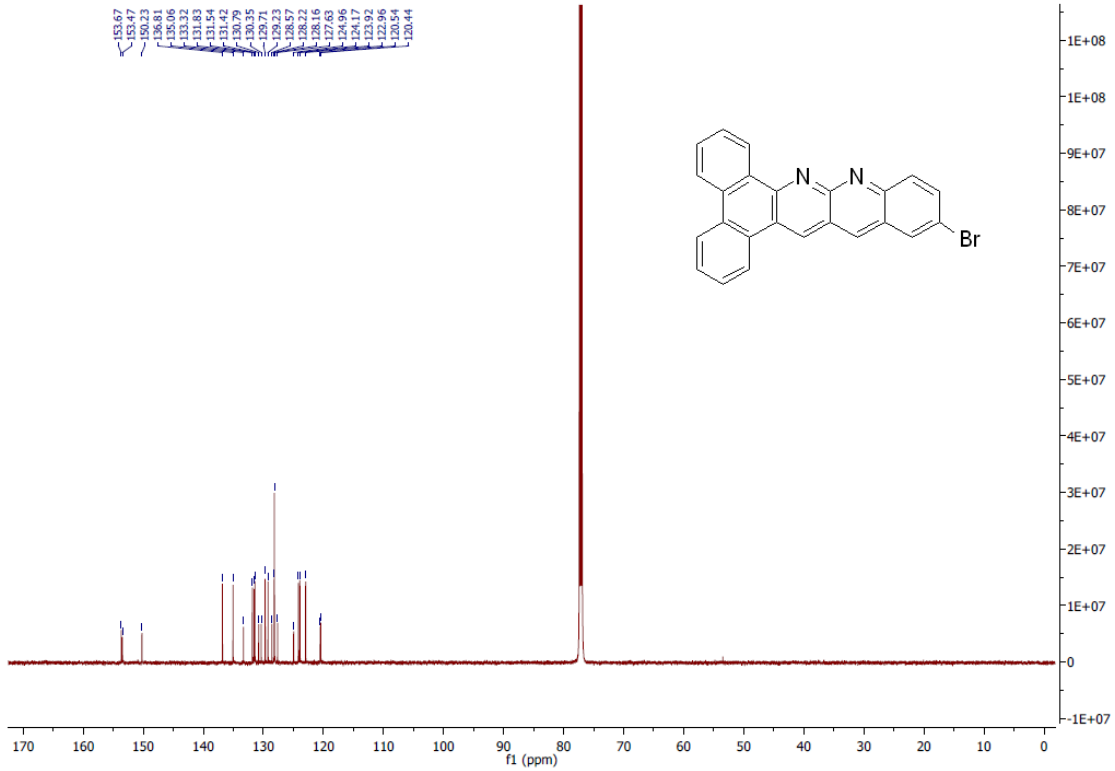


13-bromobenzo[b]phenanthro[9,10-g][1,8]naphthyridine 5d

^{1}H NMR:

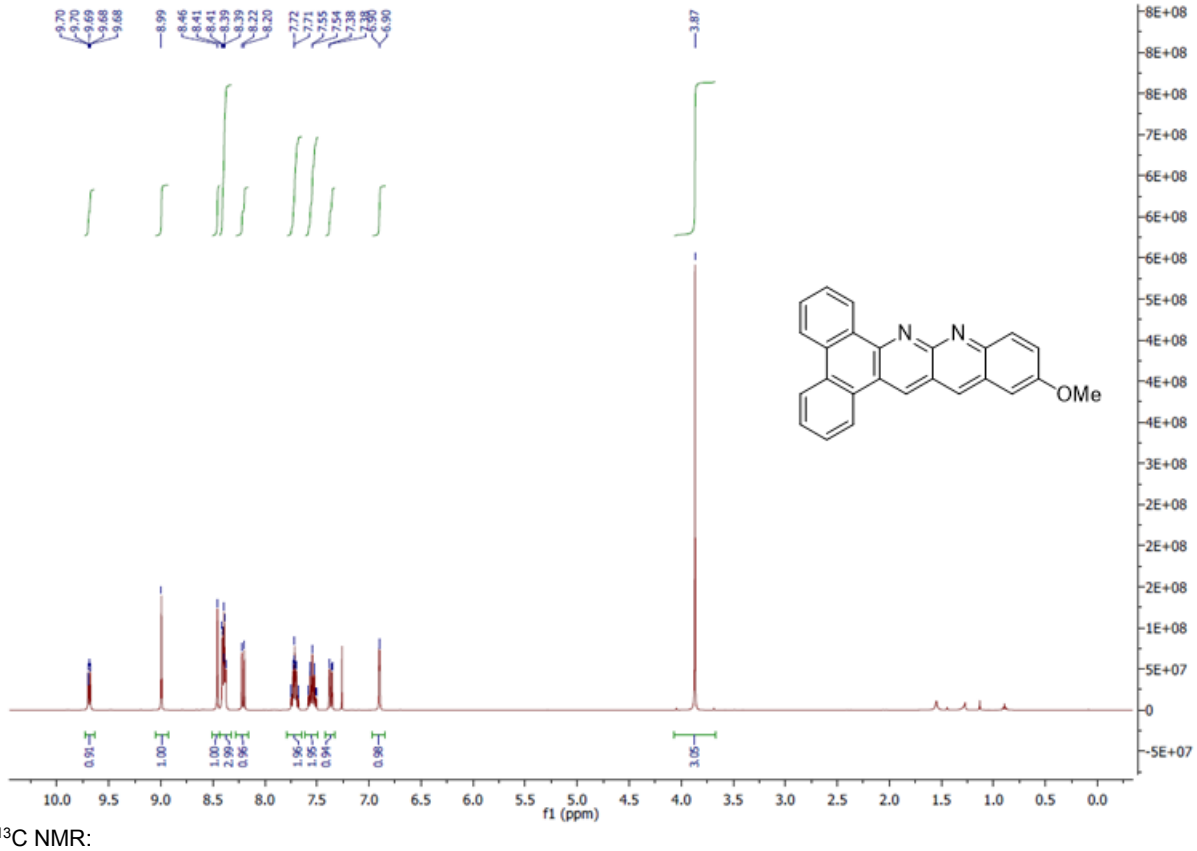


^{13}C NMR:

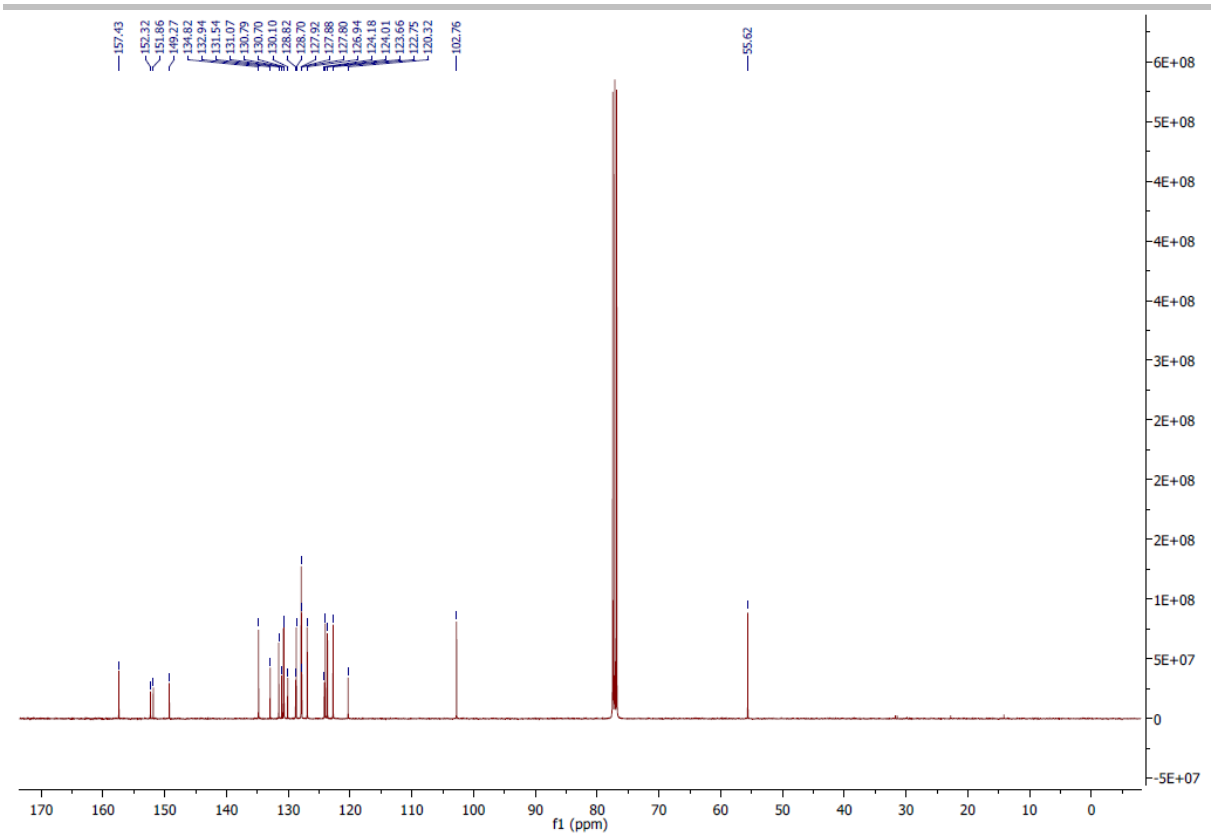


13-methoxybenzo[b]phenanthro[9,10-g][1,8]naphthyridine 5e

^{1}H NMR:

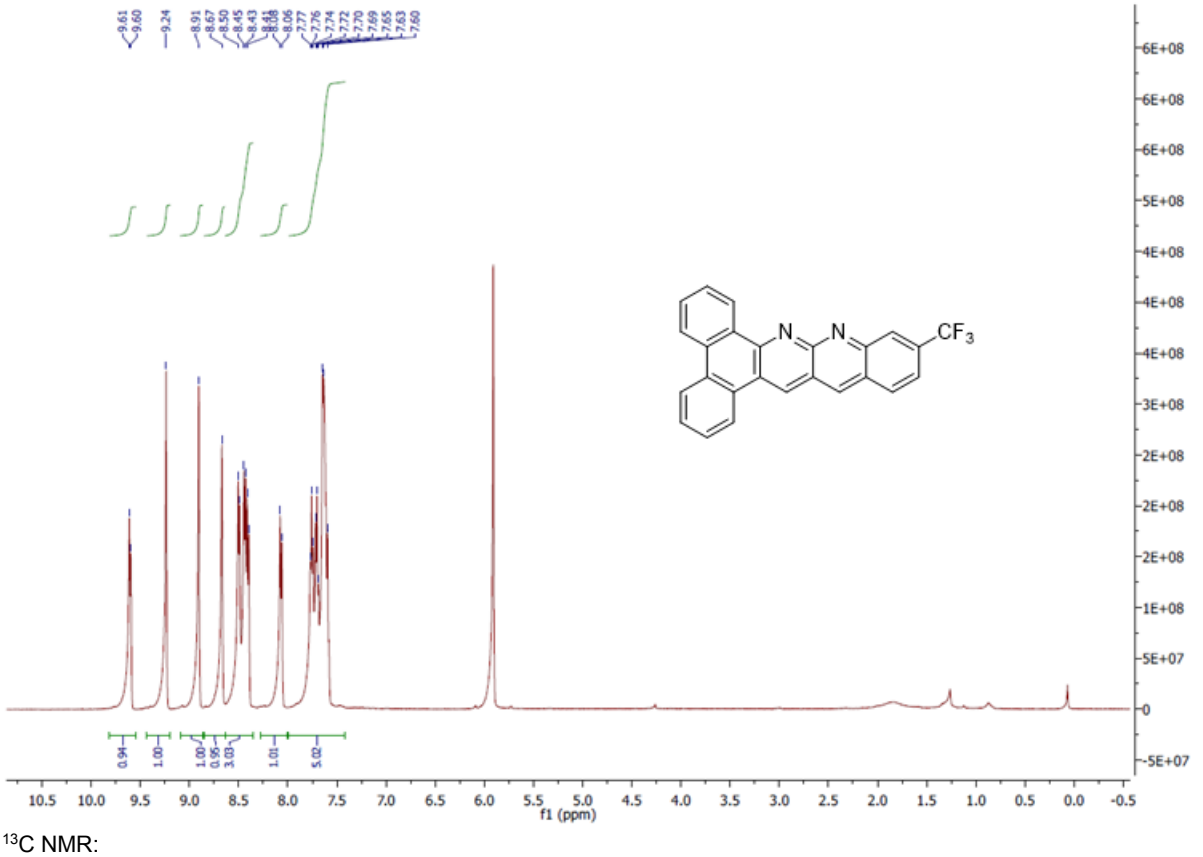


^{13}C NMR:

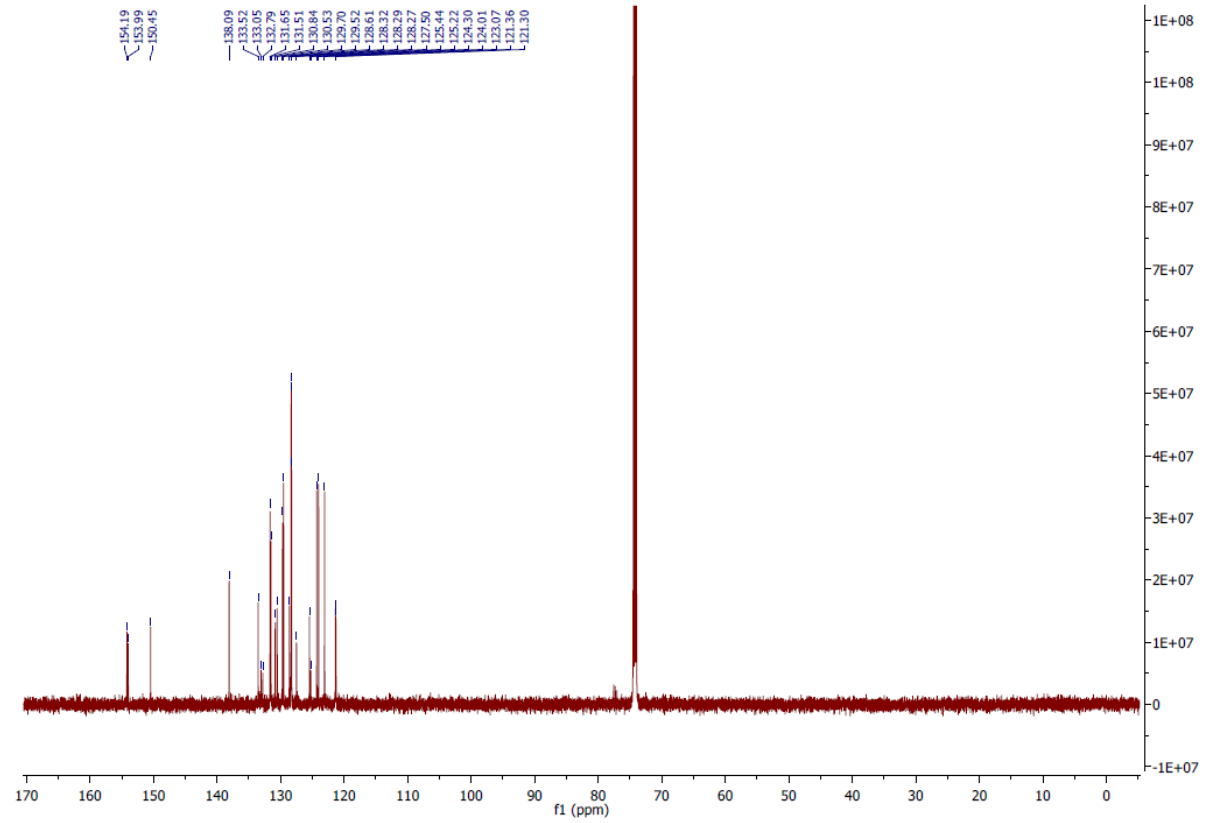


12-(trifluoromethyl)benzo[b]phenanthro[9,10-g][1,8]naphthyridine 5f

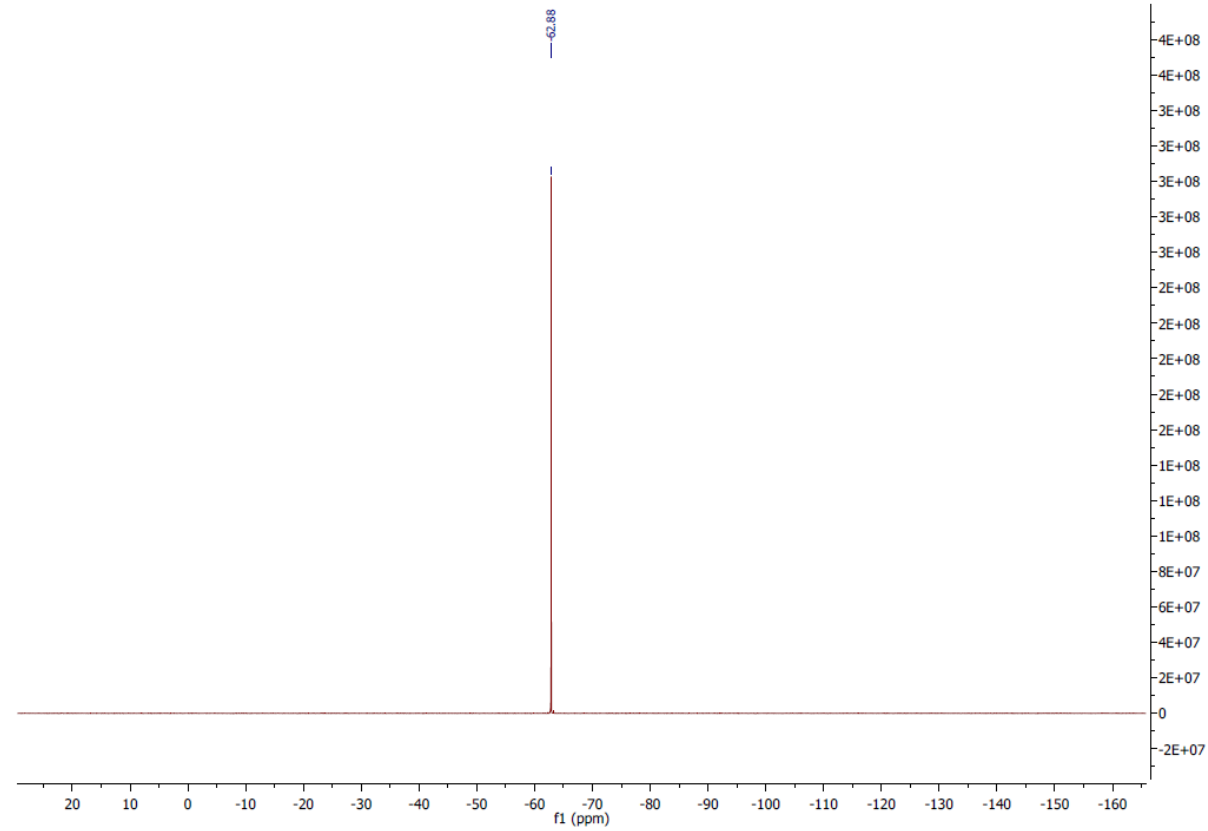
^{1}H NMR:



^{13}C NMR:

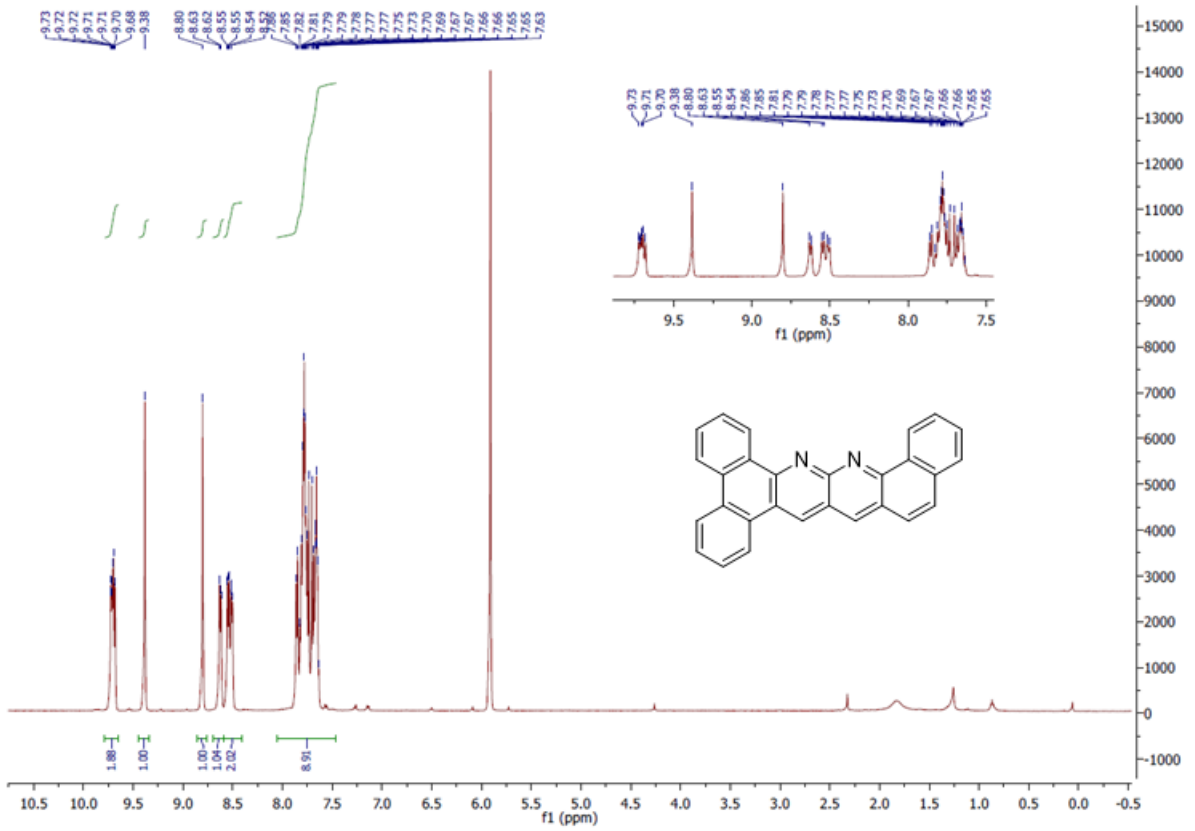


^{19}F NMR:

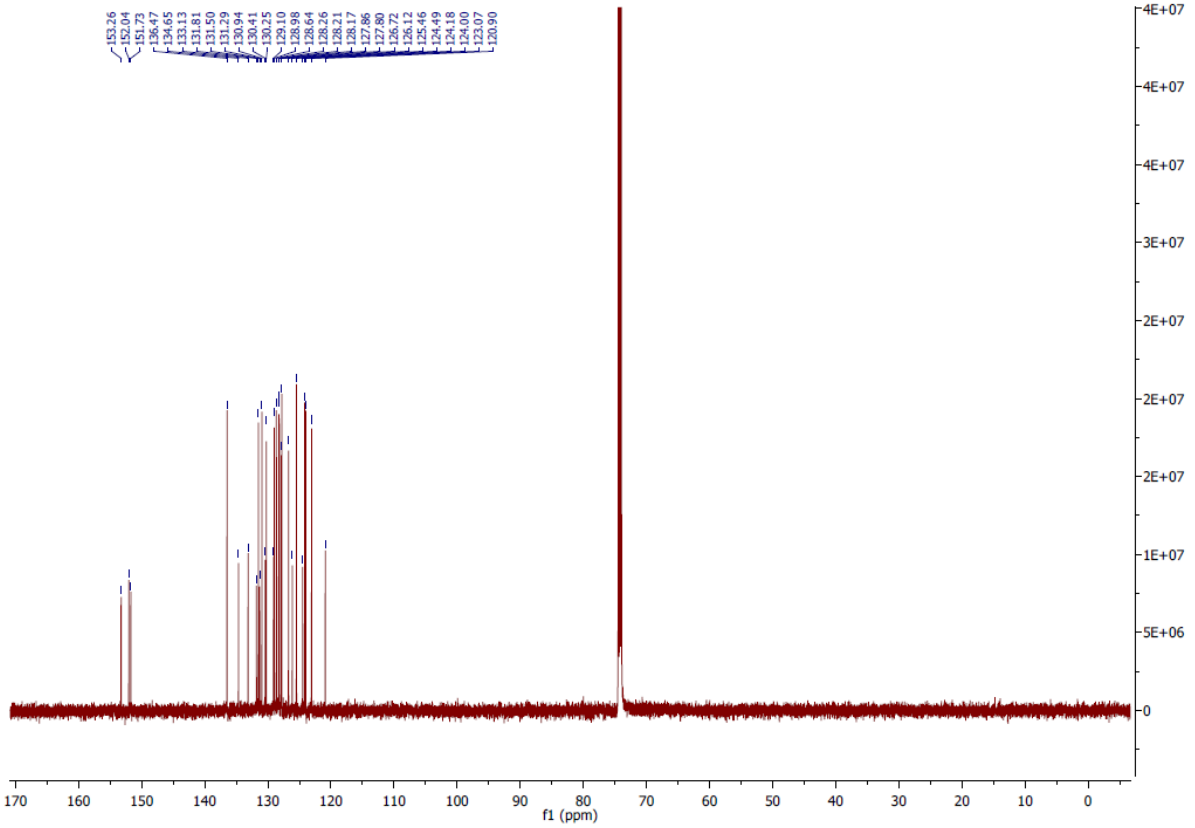


naphtho[1,2-b]phenanthro[9,10-g][1,8]naphthyridine 5g

^{1}H NMR:

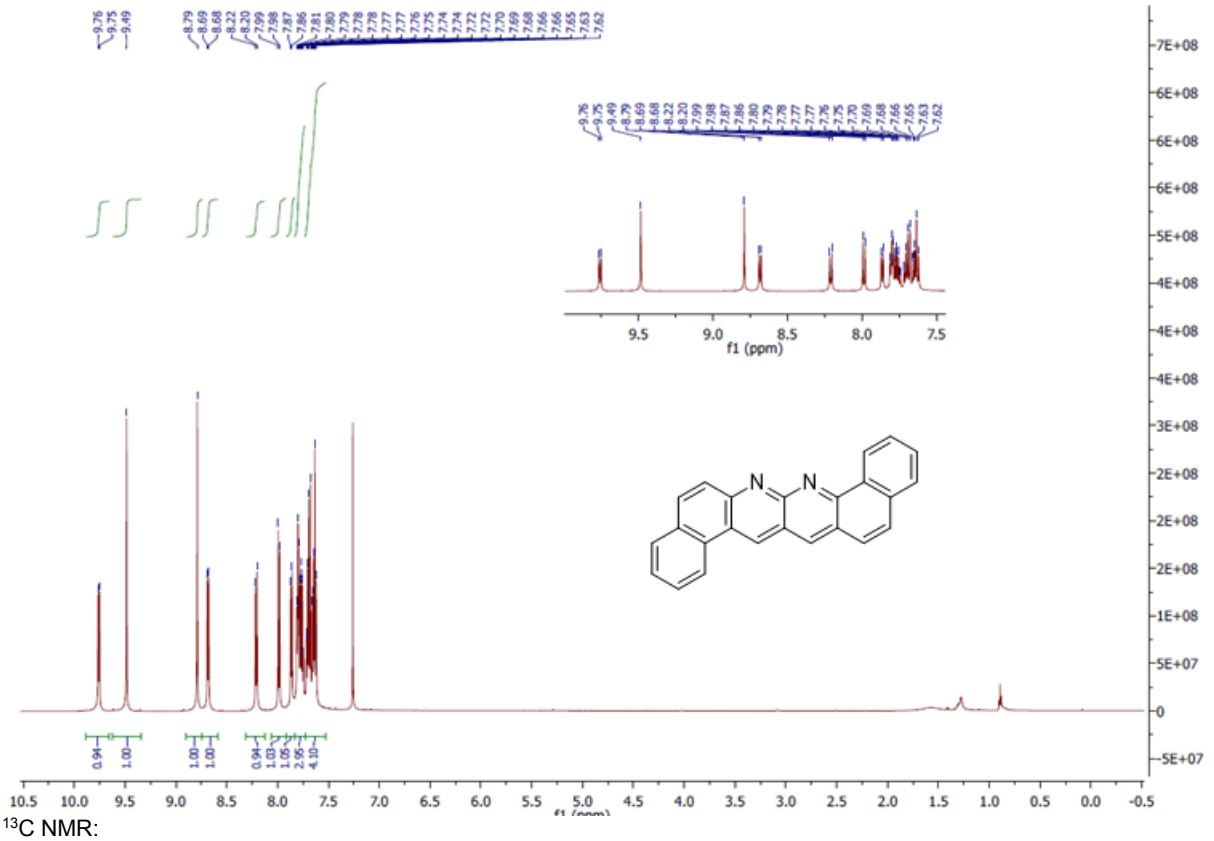


^{13}C NMR:

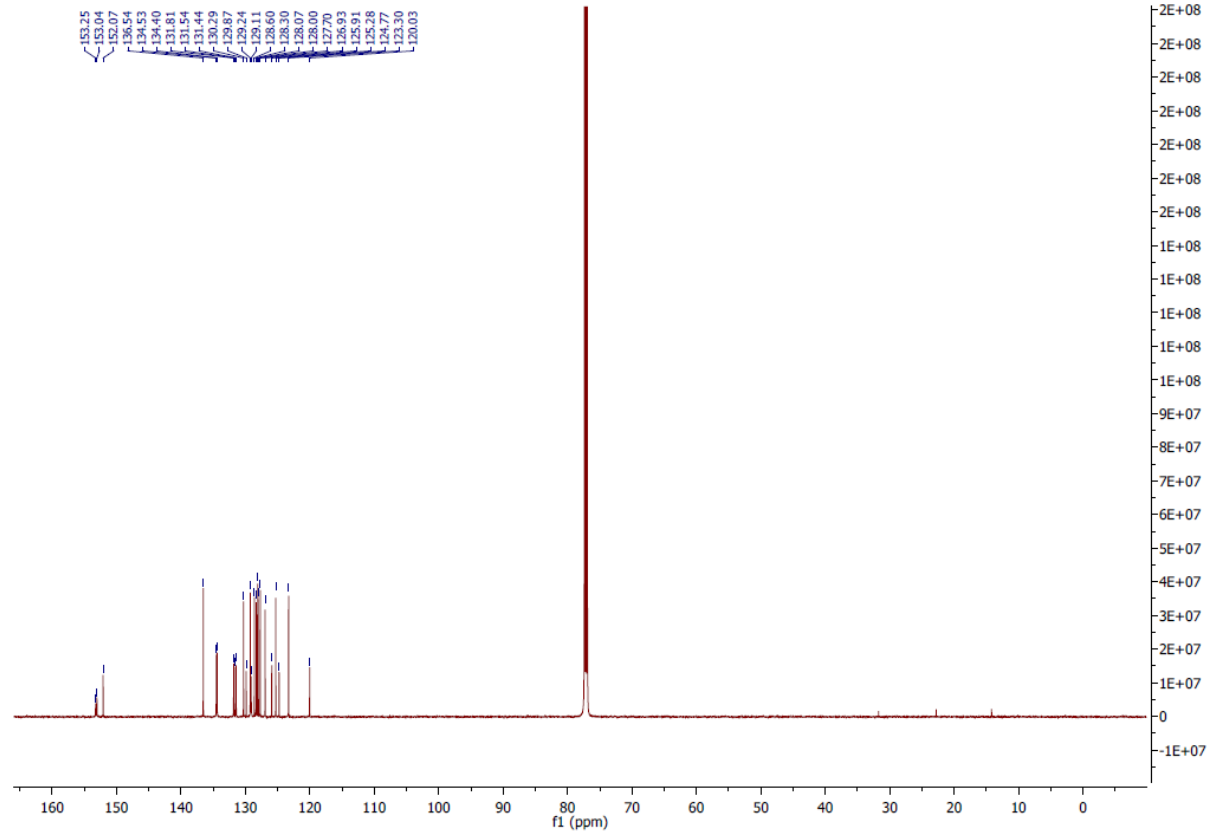


dinaphtho[1,2-b:1',2'-g][1,8]naphthyridine 5h

^{1}H NMR:

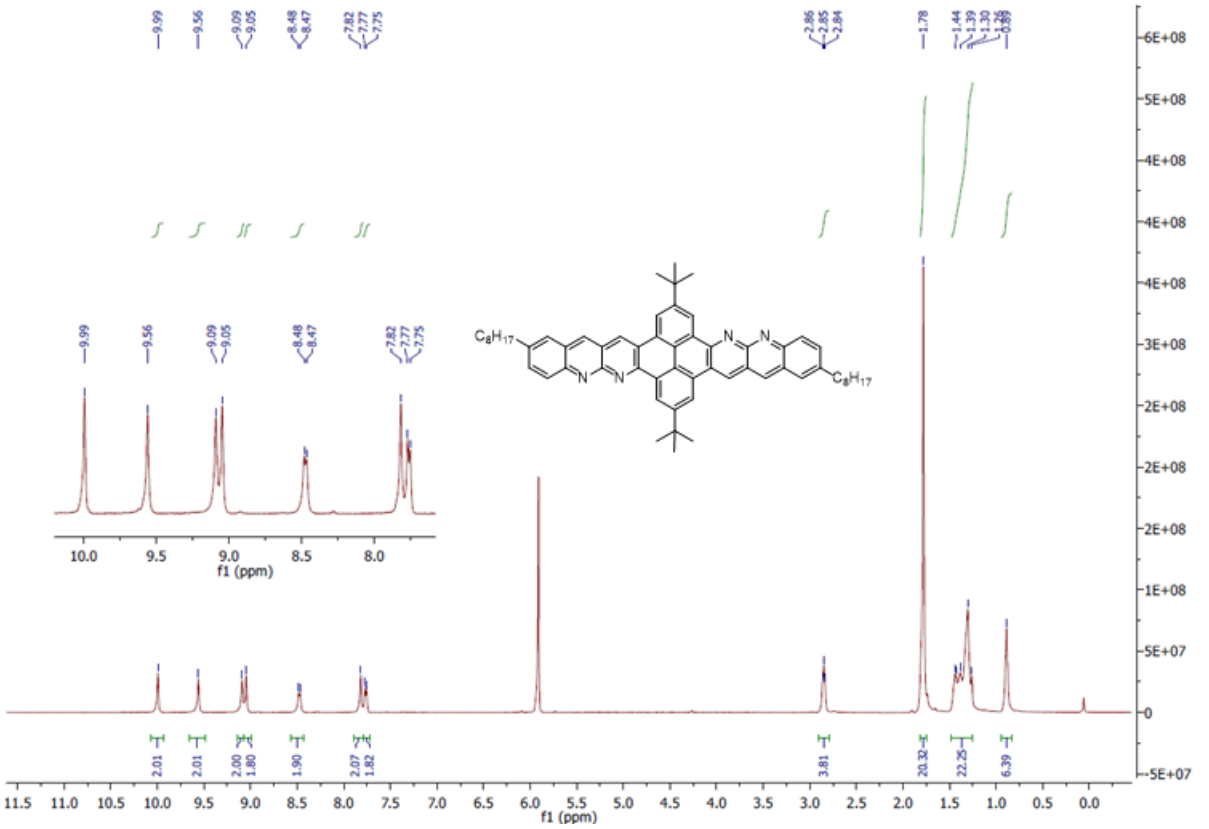


^{13}C NMR:



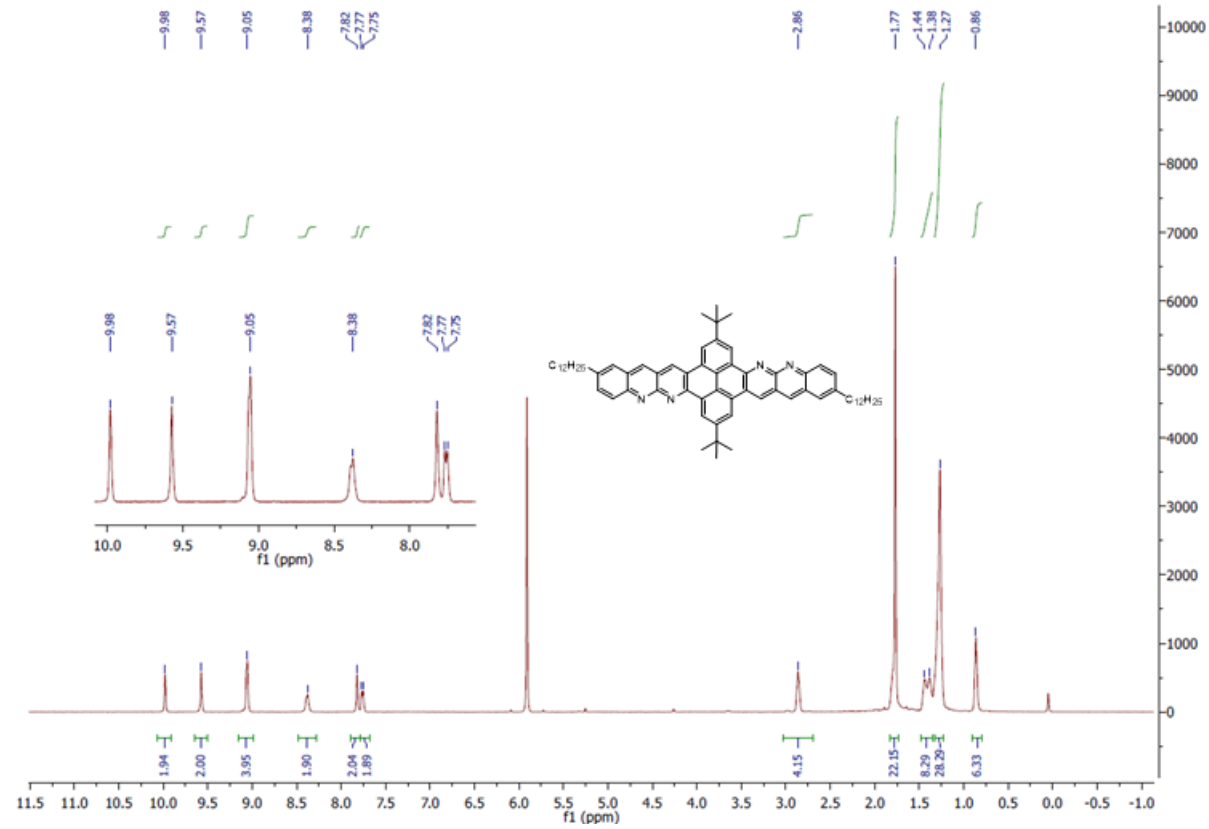
Compound 11c

^{1}H NMR:



Compound 11d

^{1}H NMR:



6. X-ray crystal structures

6.1. Compound 11d

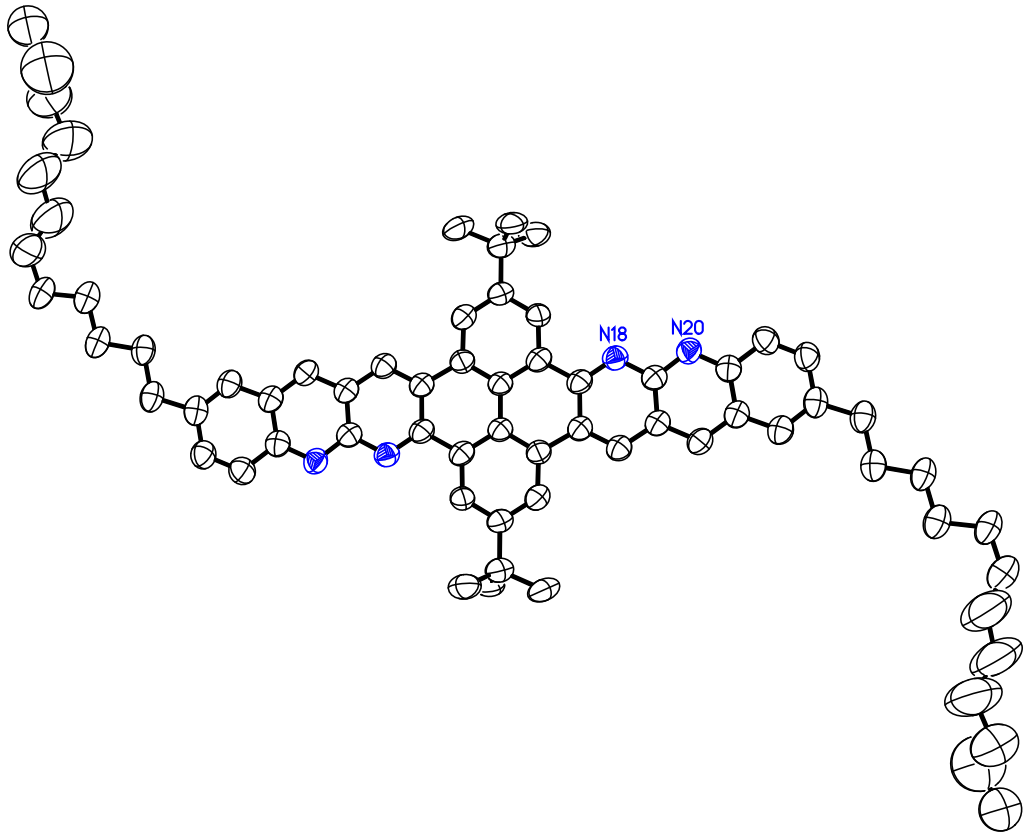


Figure S8: Crystal structure of **11d**.

Table S2: Crystal data and structure refinement for **11d.**

Identification code	stu8	
Empirical formula	$C_{70}H_{84}Cl_6N_4$	
Formula weight	1194.11	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Z	1	
Unit cell dimensions	a = 10.9165(9) Å	α =96.115(9) deg.
	b = 11.0282(10) Å	β = 103.041(9) deg.
	c = 15.7887(18) Å	γ = 117.863(6) deg.
Volume	1586.7(3) $Å^3$	
Density (calculated)	1.25 g/cm^3	
Absorption coefficient	2.80 mm^{-1}	
Crystal shape	plank	
Crystal size	0.200 x 0.042 x 0.029 mm^3	
Crystal colour	orange	
Theta range for data collection	4.7 to 54.2 deg.	
Index ranges	-10≤h≤11, -11≤k≤11, -16≤l≤16	
Reflections collected	10339	
Independent reflections	3844 (R(int) = 0.0525)	

Observed reflections	1895 ($I > 2\sigma(I)$)
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.52 and 0.56
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3844 / 574 / 435
Goodness-of-fit on F^2	1.25
Final R indices (I>2sigma(I))	R1 = 0.123, wR2 = 0.327
Largest diff. peak and hole	0.52 and -0.37 $eÅ^{-3}$

Table S3: Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **11d**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
C11	-0.0175(7)	0.4800(6)	0.4520(4)	0.0562(16)
C12	0.0879(7)	0.5468(6)	0.4098(4)	0.0580(17)
C13	0.0492(7)	0.5065(7)	0.3158(4)	0.0646(18)
H13	0.1213	0.5533	0.2880	0.078
C14	-0.0881(7)	0.4025(7)	0.2623(4)	0.0676(19)
C15	-0.1912(7)	0.3347(7)	0.3043(4)	0.0641(18)
H15	-0.2861	0.2607	0.2689	0.077
C16	-0.1593(7)	0.3721(6)	0.3975(4)	0.0580(16)
C17	-0.2718(7)	0.2995(7)	0.4390(4)	0.0605(17)
N18	-0.4025(6)	0.1984(5)	0.3856(3)	0.0627(15)
C19	-0.5110(7)	0.1318(7)	0.4218(4)	0.0604(17)
N20	-0.6410(6)	0.0323(6)	0.3622(3)	0.0664(16)
C21	-0.7532(7)	-0.0338(6)	0.3934(4)	0.0632(17)
C22	-0.8910(7)	-0.1390(7)	0.3313(5)	0.077(2)
H22	-0.9009	-0.1603	0.2694	0.092
C23	-1.0082(8)	-0.2091(7)	0.3594(5)	0.076(2)
H23	-1.0986	-0.2787	0.3164	0.091
C24	-1.0007(7)	-0.1822(7)	0.4511(5)	0.0675(18)
C25	-0.8695(7)	-0.0841(7)	0.5124(5)	0.0682(18)
H25	-0.8624	-0.0657	0.5740	0.082
C26	-0.7435(7)	-0.0092(6)	0.4864(5)	0.0622(17)
C27	-0.6072(7)	0.0939(7)	0.5467(5)	0.0651(18)
H27	-0.5947	0.1145	0.6091	0.078
C28	-0.4879(7)	0.1672(6)	0.5146(4)	0.0557(16)
C29	-0.3468(7)	0.2738(6)	0.5712(4)	0.0625(17)
H29	-0.3287	0.2984	0.6341	0.075
C30	-0.2375(7)	0.3406(6)	0.5358(4)	0.0583(17)
C31	-1.1385(7)	-0.2635(7)	0.4739(5)	0.076(2)
H31A	-1.1758	-0.3655	0.4509	0.091
H31B	-1.2113	-0.2424	0.4400	0.091
C32	-1.1334(7)	-0.2399(7)	0.5717(4)	0.0714(19)
H32A	-1.0612	-0.2603	0.6072	0.086
H32B	-1.1013	-0.1394	0.5955	0.086
C33	-1.2813(7)	-0.3335(7)	0.5821(5)	0.077(2)
H33A	-1.3521	-0.3110	0.5471	0.092
H33B	-1.3139	-0.4333	0.5559	0.092
C34	-1.2855(8)	-0.3198(8)	0.6767(5)	0.089(2)
H34A	-1.2619	-0.2226	0.7019	0.107
H34B	-1.2104	-0.3357	0.7134	0.107
C35	-1.4352(8)	-0.4258(9)	0.6819(5)	0.099(3)
H35A	-1.5113	-0.4205	0.6373	0.119
H35B	-1.4514	-0.5226	0.6655	0.119
C36	-1.4519(13)	-0.4023(17)	0.7697(7)	0.234(9)
H36A	-1.4724	-0.3238	0.7735	0.281
H36B	-1.5424	-0.4877	0.7683	0.281
C37	-1.3488(17)	-0.372(2)	0.8517(8)	0.237(8)
H37A	-1.2532	-0.3001	0.8484	0.284
H37B	-1.3439	-0.4592	0.8540	0.284
C38	-1.3584(17)	-0.322(2)	0.9407(8)	0.279(10)
H38A	-1.3740	-0.2411	0.9367	0.335
H38B	-1.4480	-0.3989	0.9476	0.335
C39	-1.2392(18)	-0.278(2)	1.0251(9)	0.273(9)
H39A	-1.1595	-0.1826	1.0276	0.328
H39B	-1.2011	-0.3429	1.0206	0.328
C40	-1.270(2)	-0.270(2)	1.1162(9)	0.271(9)
H40A	-1.3700	-0.3465	1.1086	0.326
H40B	-1.2009	-0.2854	1.1602	0.326
H40C	-1.1827	-0.2542	1.1632	0.326
H40D	-1.2796	-0.1860	1.1296	0.326
C41	-1.253(6)	-0.129(3)	1.152(2)	0.299(17)
H41A	-1.3203	-0.1122	1.1078	0.358
H41B	-1.1519	-0.0521	1.1614	0.358
C42	-1.287(3)	-0.128(3)	1.2395(16)	0.178(12)
H42A	-1.2763	-0.0365	1.2628	0.267
H42B	-1.3874	-0.2037	1.2295	0.267
H42C	-1.2194	-0.1437	1.2830	0.267
C41B	-1.402(3)	-0.396(3)	1.1246(15)	0.255(14)

H41C	-1.4879	-0.3932	1.0905	0.306
H41D	-1.4072	-0.4813	1.0921	0.306
C42B	-1.423(2)	-0.423(3)	1.2131(14)	0.204(12)
H42D	-1.5159	-0.5103	1.2025	0.306
H42E	-1.3429	-0.4323	1.2480	0.306
H42F	-1.4243	-0.3434	1.2464	0.306
C43	-0.1272(7)	0.3611(8)	0.1606(5)	0.085(2)
C44	-0.0030(15)	0.4514(19)	0.1257(10)	0.111(6)
H44A	0.0853	0.4517	0.1574	0.166
H44B	-0.0300	0.4122	0.0613	0.166
H44C	0.0154	0.5485	0.1361	0.166
C45	-0.1508(15)	0.2071(13)	0.1373(8)	0.091(5)
H45A	-0.0607	0.2089	0.1674	0.136
H45B	-0.2300	0.1427	0.1579	0.136
H45C	-0.1762	0.1742	0.0723	0.136
C46	-0.2643(14)	0.3570(18)	0.1147(8)	0.087(5)
H46A	-0.2860	0.3301	0.0496	0.131
H46B	-0.3447	0.2876	0.1322	0.131
H46C	-0.2527	0.4507	0.1320	0.131
C44B	-0.2832(18)	0.234(3)	0.1169(14)	0.138(13)
H44D	-0.3516	0.2537	0.1382	0.207
H44E	-0.3094	0.2194	0.0516	0.207
H44F	-0.2881	0.1493	0.1333	0.207
C45B	-0.123(4)	0.494(2)	0.1334(14)	0.154(13)
H45D	-0.1936	0.5108	0.1535	0.231
H45E	-0.0249	0.5763	0.1615	0.231
H45F	-0.1483	0.4783	0.0680	0.231
C46B	-0.020(2)	0.336(3)	0.1299(16)	0.131(12)
H46D	-0.0515	0.3096	0.0642	0.196
H46E	0.0760	0.4221	0.1525	0.196
H46F	-0.0144	0.2588	0.1528	0.196
C51	-0.6758(13)	-0.0777(17)	0.1582(11)	0.112(6)
H51	-0.6385	-0.0043	0.2151	0.135
Cl1	-0.5586(9)	0.0055(8)	0.1034(4)	0.185(4)
Cl2	-0.667(2)	-0.207(2)	0.1942(15)	0.347(10)
Cl3	-0.8391(9)	-0.0971(12)	0.1086(5)	0.259(6)
C51B	-0.5739(16)	-0.0801(19)	0.1815(16)	0.140(10)
H51B	-0.5721	-0.0332	0.2400	0.168
Cl1B	-0.608(3)	0.012(3)	0.112(2)	0.51(2)
Cl2B	-0.7074(14)	-0.2444(10)	0.1629(6)	0.168(5)
Cl3B	-0.4021(13)	-0.0523(11)	0.2037(8)	0.256(6)

Table S4: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **11d**.

Atom	x	y	z	U_{eq}
H13	0.1213	0.5533	0.2880	0.078
H15	-0.2861	0.2607	0.2689	0.077
H22	-0.9009	-0.1603	0.2694	0.092
H23	-1.0986	-0.2787	0.3164	0.091
H25	-0.8624	-0.0657	0.5740	0.082
H27	-0.5947	0.1145	0.6091	0.078
H29	-0.3287	0.2984	0.6341	0.075
H31A	-1.1758	-0.3655	0.4509	0.091
H31B	-1.2113	-0.2424	0.4400	0.091
H32A	-1.0612	-0.2603	0.6072	0.086
H32B	-1.1013	-0.1394	0.5955	0.086
H33A	-1.3521	-0.3110	0.5471	0.092
H33B	-1.3139	-0.4333	0.5559	0.092
H34A	-1.2619	-0.2226	0.7019	0.107
H34B	-1.2104	-0.3357	0.7134	0.107
H35A	-1.5113	-0.4205	0.6373	0.119
H35B	-1.4514	-0.5226	0.6655	0.119
H36A	-1.4724	-0.3238	0.7735	0.281
H36B	-1.5424	-0.4877	0.7683	0.281
H37A	-1.2532	-0.3001	0.8484	0.284
H37B	-1.3439	-0.4592	0.8540	0.284
H38A	-1.3740	-0.2411	0.9367	0.335
H38B	-1.4480	-0.3989	0.9476	0.335
H39A	-1.1595	-0.1826	1.0276	0.328
H39B	-1.2011	-0.3429	1.0206	0.328
H40A	-1.3700	-0.3465	1.1086	0.326
H40B	-1.2009	-0.2854	1.1602	0.326
H40C	-1.1827	-0.2542	1.1632	0.326
H40D	-1.2796	-0.1860	1.1296	0.326
H41A	-1.3203	-0.1122	1.1078	0.358
H41B	-1.1519	-0.0521	1.1614	0.358
H42A	-1.2763	-0.0365	1.2628	0.267
H42B	-1.3874	-0.2037	1.2295	0.267
H42C	-1.2194	-0.1437	1.2830	0.267
H41C	-1.4879	-0.3932	1.0905	0.306

H41D	-1.4072	-0.4813	1.0921	0.306
H42D	-1.5159	-0.5103	1.2025	0.306
H42E	-1.3429	-0.4323	1.2480	0.306
H42F	-1.4243	-0.3434	1.2464	0.306
H44A	0.0853	0.4517	0.1574	0.166
H44B	-0.0300	0.4122	0.0613	0.166
H44C	0.0154	0.5485	0.1361	0.166
H45A	-0.0607	0.2089	0.1674	0.136
H45B	-0.2300	0.1427	0.1579	0.136
H45C	-0.1762	0.1742	0.0723	0.136
H46A	-0.2860	0.3301	0.0496	0.131
H46B	-0.3447	0.2876	0.1322	0.131
H46C	-0.2527	0.4507	0.1320	0.131
H44D	-0.3516	0.2537	0.1382	0.207
H44E	-0.3094	0.2194	0.0516	0.207
H44F	-0.2881	0.1493	0.1333	0.207
H45D	-0.1936	0.5108	0.1535	0.231
H45E	-0.0249	0.5763	0.1615	0.231
H45F	-0.1483	0.4783	0.0680	0.231
H46D	-0.0515	0.3096	0.0642	0.196
H46E	0.0760	0.4221	0.1525	0.196
H46F	-0.0144	0.2588	0.1528	0.196
H51	-0.6385	-0.0043	0.2151	0.135
H51B	-0.5721	-0.0332	0.2400	0.168

Table S5: Anisotropic displacement parameters ($Å^2$) for **11d**. 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	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C11	0.064(4)	0.049(3)	0.060(3)	0.011(3)	0.024(3)	0.030(3)
C12	0.062(4)	0.059(4)	0.058(4)	0.015(3)	0.021(3)	0.033(3)
C13	0.069(4)	0.066(4)	0.068(4)	0.019(3)	0.032(3)	0.036(3)
C14	0.070(4)	0.077(5)	0.057(3)	0.010(3)	0.024(3)	0.038(4)
C15	0.059(4)	0.067(4)	0.060(4)	0.001(3)	0.018(3)	0.031(3)
C16	0.070(4)	0.054(4)	0.066(4)	0.016(3)	0.031(3)	0.039(3)
C17	0.067(4)	0.062(4)	0.064(4)	0.012(3)	0.028(3)	0.039(3)
N18	0.067(3)	0.060(3)	0.061(3)	0.014(3)	0.024(3)	0.032(3)
C19	0.068(4)	0.055(4)	0.064(4)	0.016(3)	0.025(3)	0.033(3)
N20	0.063(3)	0.066(4)	0.072(3)	0.012(3)	0.028(3)	0.033(3)
C21	0.065(4)	0.055(4)	0.075(4)	0.013(3)	0.026(3)	0.034(3)
C22	0.074(4)	0.063(4)	0.082(5)	0.009(3)	0.023(3)	0.028(4)
C23	0.069(4)	0.061(4)	0.088(4)	0.014(4)	0.029(4)	0.025(4)
C24	0.063(4)	0.053(4)	0.095(4)	0.023(3)	0.032(3)	0.031(3)
C25	0.069(4)	0.065(4)	0.084(4)	0.021(3)	0.032(3)	0.040(3)
C26	0.068(4)	0.051(4)	0.078(4)	0.017(3)	0.032(3)	0.034(3)
C27	0.068(4)	0.070(4)	0.071(4)	0.021(3)	0.032(3)	0.040(3)
C28	0.066(4)	0.048(4)	0.068(4)	0.016(3)	0.029(3)	0.036(3)
C29	0.068(4)	0.059(4)	0.067(4)	0.015(3)	0.027(3)	0.035(3)
C30	0.065(4)	0.053(4)	0.063(4)	0.016(3)	0.026(3)	0.031(3)
C31	0.066(4)	0.072(4)	0.103(5)	0.025(4)	0.038(4)	0.039(4)
C32	0.064(4)	0.063(4)	0.099(5)	0.022(4)	0.031(4)	0.038(4)
C33	0.074(5)	0.068(5)	0.108(5)	0.032(4)	0.048(4)	0.040(4)
C34	0.079(5)	0.093(5)	0.111(5)	0.034(5)	0.047(4)	0.046(4)
C35	0.084(5)	0.112(6)	0.112(6)	0.038(5)	0.057(5)	0.045(5)
C36	0.134(10)	0.301(17)	0.124(8)	0.011(10)	0.079(7)	-0.009(11)
C37	0.227(17)	0.38(3)	0.157(9)	0.110(15)	0.113(10)	0.165(18)
C38	0.242(17)	0.47(3)	0.153(9)	0.113(16)	0.125(10)	0.17(2)
C39	0.290(18)	0.41(2)	0.138(10)	0.098(14)	0.088(10)	0.180(17)
C40	0.232(14)	0.35(2)	0.170(10)	0.050(13)	0.091(10)	0.089(13)
C41B	0.19(2)	0.36(3)	0.143(16)	0.046(18)	0.070(15)	0.079(17)
C42B	0.128(17)	0.29(3)	0.150(17)	0.039(17)	0.071(14)	0.060(17)
C43	0.081(5)	0.112(6)	0.060(4)	0.013(4)	0.025(3)	0.046(4)
C44	0.106(10)	0.169(15)	0.060(8)	0.029(11)	0.044(8)	0.065(11)
C45	0.089(12)	0.134(9)	0.056(7)	-0.007(7)	0.020(7)	0.069(9)
C46	0.103(9)	0.116(13)	0.059(7)	0.024(9)	0.025(7)	0.067(10)
C44B	0.099(12)	0.19(2)	0.055(12)	-0.002(15)	0.005(10)	0.039(13)
C45B	0.28(4)	0.191(19)	0.057(12)	0.039(14)	0.057(18)	0.16(2)
C46B	0.110(17)	0.22(4)	0.069(13)	0.00(2)	0.017(13)	0.10(2)
C51	0.092(14)	0.102(14)	0.102(12)	0.024(10)	0.031(11)	0.017(11)
Cl1	0.185(6)	0.150(6)	0.103(4)	-0.003(4)	0.053(4)	-0.002(4)
Cl2	0.251(15)	0.34(2)	0.47(2)	0.212(17)	0.166(16)	0.123(15)
Cl3	0.184(7)	0.430(14)	0.133(5)	0.082(7)	0.067(5)	0.122(8)
C51B	0.14(2)	0.19(2)	0.18(3)	0.13(2)	0.13(2)	0.10(2)
Cl1B	0.46(4)	0.38(3)	0.49(4)	0.19(3)	0.00(3)	0.12(2)
Cl2B	0.209(10)	0.121(6)	0.124(5)	-0.015(4)	0.100(6)	0.032(5)
Cl3B	0.281(12)	0.211(10)	0.280(13)	0.041(8)	0.142(10)	0.109(9)

Table S6: Bond lengths (Å) and angles (deg) for **11d**.

C11-C12	1.402(8)	C43-C44B	1.540(13)
C11-C16	1.419(8)	C43-C45B	1.553(14)
C11-C11#1	1.440(12)	C43-C45	1.582(11)
C12-C13	1.407(8)	C44-H44A	0.9800
C12-C30#1	1.481(8)	C44-H44B	0.9800
C13-C14	1.375(8)	C44-H44C	0.9800
C13-H13	0.9500	C45-H45A	0.9800
C14-C15	1.387(9)	C45-H45B	0.9800
C14-C43	1.524(9)	C45-H45C	0.9800
C15-C16	1.400(8)	C46-H46A	0.9800
C15-H15	0.9500	C46-H46B	0.9800
C16-C17	1.461(8)	C46-H46C	0.9800
C17-N18	1.327(7)	C44B-H44D	0.9800
C17-C30	1.454(9)	C44B-H44E	0.9800
N18-C19	1.361(8)	C44B-H44F	0.9800
C19-N20	1.351(7)	C45B-H45D	0.9800
C19-C28	1.407(9)	C45B-H45E	0.9800
N20-C21	1.338(8)	C45B-H45F	0.9800
C21-C22	1.426(8)	C46B-H46D	0.9800
C21-C26	1.435(9)	C46B-H46E	0.9800
C22-C23	1.355(9)	C46B-H46F	0.9800
C22-H22	0.9500	C51-Cl2	1.630(14)
C23-C24	1.422(9)	C51-Cl1	1.672(12)
C23-H23	0.9500	C51-Cl3	1.678(12)
C24-C25	1.365(9)	C51-H51	1.0000
C24-C31	1.499(9)	C51B-Cl2B	1.649(14)
C25-C26	1.417(9)	C51B-Cl1B	1.672(15)
C25-H25	0.9500	C51B-Cl3B	1.696(13)
C26-C27	1.401(9)	C51B-H51B	1.0000
C27-C28	1.418(8)	C12-C11-C16	118.1(6)
C27-H27	0.9500	C12-C11-C11#1	120.9(7)
C28-C29	1.420(8)	C16-C11-C11#1	121.0(7)
C29-C30	1.359(8)	C11-C12-C13	119.3(6)
C29-H29	0.9500	C11-C12-C30#1	119.9(6)
C31-C32	1.523(8)	C13-C12-C30#1	120.8(6)
C31-H31A	0.9900	C14-C13-C12	123.1(6)
C31-H31B	0.9900	C14-C13-H13	118.4
C32-C33	1.516(7)	C12-C13-H13	118.4
C32-H32A	0.9900	C13-C14-C15	117.5(6)
C32-H32B	0.9900	C13-C14-C43	122.0(6)
C33-C34	1.497(8)	C15-C14-C43	120.5(6)
C33-H33A	0.9900	C14-C15-C16	121.8(6)
C33-H33B	0.9900	C14-C15-H15	119.1
C34-C35	1.530(8)	C16-C15-H15	119.1
C34-H34A	0.9900	C15-C16-C11	120.2(6)
C34-H34B	0.9900	C15-C16-C17	120.1(6)
C35-C36	1.450(10)	C11-C16-C17	119.7(6)
C35-H35A	0.9900	N18-C17-C30	122.8(6)
C35-H35B	0.9900	N18-C17-C16	117.7(6)
C36-C37	1.398(11)	C30-C17-C16	119.5(6)
C36-C42B#2	1.86(3)	C17-N18-C19	119.2(6)
C36-H36A	0.9900	N20-C19-N18	115.0(6)
C36-H36B	0.9900	N20-C19-C28	123.3(6)
C37-C38	1.500(12)	N18-C19-C28	121.6(6)
C37-H37A	0.9900	C21-N20-C19	117.9(6)
C37-H37B	0.9900	N20-C21-C22	118.5(6)
C38-C39	1.480(12)	N20-C21-C26	124.3(6)
C38-H38A	0.9900	C22-C21-C26	117.2(6)
C38-H38B	0.9900	C23-C22-C21	120.8(7)
C39-C40	1.550(11)	C23-C22-H22	119.6
C39-H39A	0.9900	C21-C22-H22	119.6
C39-H39B	0.9900	C22-C23-C24	122.3(7)
C40-C41B	1.510(14)	C22-C23-H23	118.8
C40-C41	1.510(15)	C24-C23-H23	118.8
C40-H40A	0.9900	C25-C24-C23	118.2(7)
C40-H40B	0.9900	C25-C24-C31	124.3(7)
C40-H40C	0.9900	C23-C24-C31	117.5(6)
C40-H40D	0.9900	C24-C25-C26	121.6(7)
C41-C42	1.513(15)	C24-C25-H25	119.2
C41-H41A	0.9900	C26-C25-H25	119.2
C41-H41B	0.9900	C27-C26-C25	123.6(6)
C42-H42A	0.9800	C27-C26-C21	116.5(6)
C42-H42B	0.9800	C25-C26-C21	119.9(6)
C42-H42C	0.9800	C26-C27-C28	119.9(6)
C41B-C42B	1.505(14)	C26-C27-H27	120.1
C41B-H41C	0.9900	C28-C27-H27	120.1
C41B-H41D	0.9900	C19-C28-C27	118.0(6)
C42B-H42D	0.9800	C19-C28-C29	118.7(6)
C42B-H42E	0.9800	C27-C28-C29	123.3(6)
C42B-H42F	0.9800	C30-C29-C28	120.2(6)
C43-C46	1.487(11)	C30-C29-H29	119.9
C43-C46B	1.487(13)	C28-C29-H29	119.9
C43-C44	1.524(11)	C29-C30-C17	117.5(6)

C29-C30-C12#1	123.5(6)
C17-C30-C12#1	119.0(6)
C24-C31-C32	118.9(6)
C24-C31-H31A	107.6
C32-C31-H31A	107.6
C24-C31-H31B	107.6
C32-C31-H31B	107.6
H31A-C31-H31B	107.0
C33-C32-C31	111.5(6)
C33-C32-H32A	109.3
C31-C32-H32A	109.3
C33-C32-H32B	109.3
C31-C32-H32B	109.3
H32A-C32-H32B	108.0
C34-C33-C32	115.1(6)
C34-C33-H33A	108.5
C32-C33-H33A	108.5
C34-C33-H33B	108.5
C32-C33-H33B	108.5
H33A-C33-H33B	107.5
C33-C34-C35	111.7(6)
C33-C34-H34A	109.3
C35-C34-H34A	109.3
C33-C34-H34B	109.3
C35-C34-H34B	109.3
H34A-C34-H34B	107.9
C36-C35-C34	113.7(7)
C36-C35-H35A	108.8
C34-C35-H35A	108.8
C36-C35-H35B	108.8
C34-C35-H35B	108.8
H35A-C35-H35B	107.7
C37-C36-C35	125.7(12)
C37-C36-C42B#2	90.3(14)
C35-C36-C42B#2	108.1(11)
C37-C36-H36A	105.9
C35-C36-H36A	105.9
C42B#2-C36-H36A	122.0
C37-C36-H36B	105.9
C35-C36-H36B	105.9
C42B#2-C36-H36B	19.0
H36A-C36-H36B	106.2
C36-C37-C38	123.5(13)
C36-C37-H37A	106.4
C38-C37-H37A	106.4
C36-C37-H37B	106.4
C38-C37-H37B	106.4
H37A-C37-H37B	106.5
C39-C38-C37	121.6(13)
C39-C38-H38A	106.9
C37-C38-H38A	106.9
C39-C38-H38B	106.9
C37-C38-H38B	106.9
H38A-C38-H38B	106.7
C38-C39-C40	119.9(12)
C38-C39-H39A	107.4
C40-C39-H39A	107.4
C38-C39-H39B	107.4
C40-C39-H39B	107.4
H39A-C39-H39B	106.9
C41B-C40-C39	117.6(14)
C41-C40-C39	111.3(15)
C41-C40-H40A	109.4
C39-C40-H40A	109.4
C41-C40-H40B	109.4
C39-C40-H40B	109.4
H40A-C40-H40B	108.0
C41B-C40-H40C	107.9
C39-C40-H40C	107.9
C41B-C40-H40D	107.9
C39-C40-H40D	107.9
H40C-C40-H40D	107.2
C40-C41-C42	109.2(19)
C40-C41-H41A	109.8
C42-C41-H41A	109.8
C40-C41-H41B	109.8
C42-C41-H41B	109.8
H41A-C41-H41B	108.3
C41-C42-H42A	109.5
C41-C42-H42B	109.5
H42A-C42-H42B	109.5
C41-C42-H42C	109.5
H42A-C42-H42C	109.5
H42B-C42-H42C	109.5
C42B-C41B-C40	123.5(18)
C42B-C41B-H41C	106.5
C40-C41B-H41C	106.5
C42B-C41B-H41D	106.5
C40-C41B-H41D	106.5
H41C-C41B-H41D	106.5
C41B-C42B-H42D	109.5
C36#2-C42B-H42D	23.7
C41B-C42B-H42E	109.5
C36#2-C42B-H42E	86.5
H42D-C42B-H42E	109.5
C41B-C42B-H42F	109.5
C36#2-C42B-H42F	113.7
H42D-C42B-H42F	109.5
H42E-C42B-H42F	109.5
C36#2-C42B-H36B#2	19.2(8)
C46-C43-C14	111.7(7)
C46B-C43-C14	113.6(11)
C46-C43-C44	111.8(9)
C14-C43-C44	113.3(8)
C46B-C43-C44B	111.1(13)
C14-C43-C44B	111.8(9)
C46B-C43-C45B	109.3(14)
C14-C43-C45B	102.4(9)
C44B-C43-C45B	108.2(14)
C46-C43-C45	109.0(8)
C14-C43-C45	105.5(7)
C44-C43-C45	105.0(9)
C43-C44-H44A	109.5
C43-C44-H44B	109.5
H44A-C44-H44B	109.5
C43-C44-H44C	109.5
H44A-C44-H44C	109.5
H44B-C44-H44C	109.5
C43-C45-H45A	109.5
C43-C45-H45B	109.5
H45A-C45-H45B	109.5
C43-C45-H45C	109.5
H45A-C45-H45C	109.5
H45B-C45-H45C	109.5
C43-C46-H46A	109.5
C43-C46-H46B	109.5
H46A-C46-H46B	109.5
C43-C46-H46C	109.5
H46A-C46-H46C	109.5
H46B-C46-H46C	109.5
C43-C44B-H44D	109.5
C43-C44B-H44E	109.5
H44D-C44B-H44E	109.5
C43-C44B-H44F	109.5
H44D-C44B-H44F	109.5
H44E-C44B-H44F	109.5
C43-C45B-H45D	109.5
C43-C45B-H45E	109.5
H45D-C45B-H45E	109.5
C43-C45B-H45F	109.5
H45D-C45B-H45F	109.5
H45E-C45B-H45F	109.5
C43-C46B-H46D	109.5
C43-C46B-H46E	109.5
H46D-C46B-H46E	109.5
C43-C46B-H46F	109.5
H46D-C46B-H46F	109.5
H46E-C46B-H46F	109.5
Cl2-C51-Cl1	116.2(11)
Cl2-C51-Cl3	119.5(11)
Cl1-C51-Cl3	110.3(9)
Cl2-C51-H51	102.6
Cl1-C51-H51	102.6
Cl3-C51-H51	102.6
Cl2B-C51B-Cl1B	114.9(14)
Cl2B-C51B-Cl3B	117.2(12)
Cl1B-C51B-Cl3B	113.3(14)
Cl2B-C51B-H51B	102.9
Cl1B-C51B-H51B	102.9
Cl3B-C51B-H51B	102.9

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1
#2 -x-3,-y-1,-z+2

suggestion for a short experimental part:

11d: orange crystal (plank), dimensions 0.200 x 0.042 x 0.029 mm^3, crystal system triclinic, space group P $\bar{1}$, Z=1, a=10.9165(9) Å, b=11.0282(10) Å, c=15.7887(18) Å, alpha=96.115(9) deg, beta=103.041(9) deg, gamma=117.863(6) deg, V=1586.7(3) $Å^3$, rho=1.250 g/cm^3, T=200(2) K, $Theta_{max}$= 54.221 deg, radiation CuK□, lambda=1.54178 Å, 0.5 deg omega-scans with CCD area detector, covering the asymmetric unit in reciprocal space with a mean redundancy of 2.67 and a completeness of 99.2% to a resolution of 0.95 Å, 10339 reflections measured, 3844 unique (R(int)=0.0525), 1895 observed (I > 2□(I)), intensities were corrected for Lorentz and polarization effects, an empirical scaling and absorption correction was applied using X-Area LANA 1.70.0.0 (STOE, 2017) based on the Laue symmetry of the reciprocal space, mu=2.80mm^{-1}, T_{min}=0.56, T_{max}=1.52, structure solved with SHELXT-2014 (Sheldrick 2014)[2] and refined against F^2 with a Full-matrix least-squares algorithm using the SHELXL-2018/3 (Sheldrick, 2018) software[3], 435 parameters refined, hydrogen atoms were treated using appropriate riding models, goodness of fit 1.25 for observed reflections, final residual values R1(F)=0.123, wR(F^2)=0.327 for observed reflections, residual electron density -0.37 to 0.52 e$Å^{-3}$. CCDC ..... contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Lit. 2: (SHELXT - Integrated space-group and crystal structure determination)
Sheldrick G. M., Acta Cryst. A71 (2015) 3-8.

Lit. 3: (program SHELXL-2018/3 (Sheldrick, 2018) for structure refinement)
Sheldrick G. M., Acta Cryst. (2015). C71, 3-8

Lit. APEX, APEX2, SMART, SAINT, SAINT-Plus:
Bruker (2007). "Program name(s)". Bruker AXS Inc., Madison, Wisconsin, USA.

6.2. Compound 5a

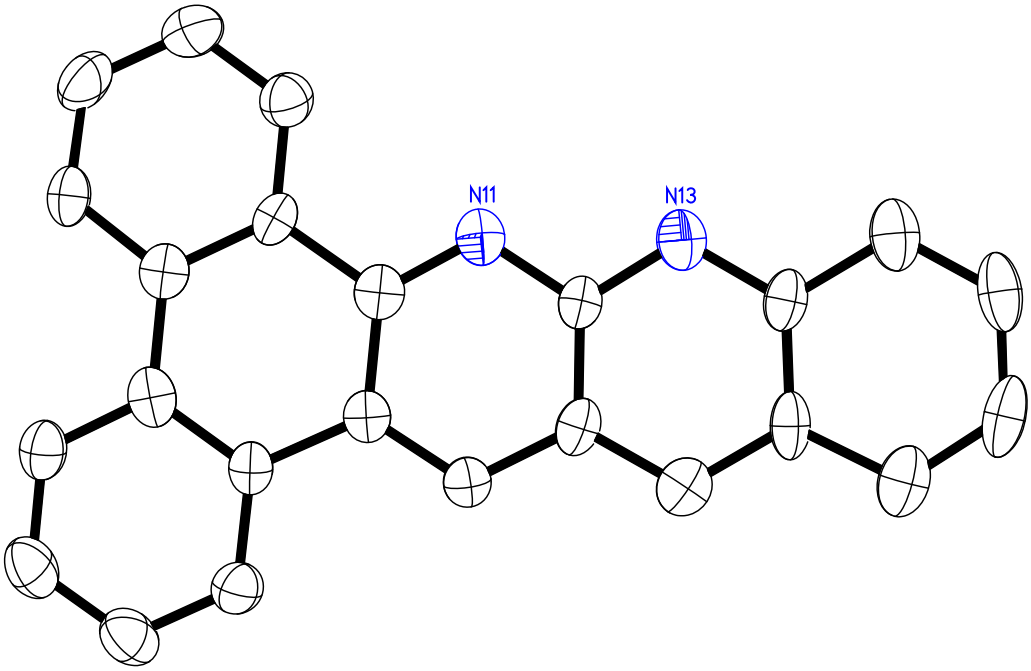


Figure S9: Crystal structure of **5a**.

Table S7: Crystal data and structure refinement for **5a**.

Identification code	stu5	
Empirical formula	$C_{25}H_{15}Cl_3N_2$	
Formula weight	449.74	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Z	4	
Unit cell dimensions	a = 10.4065(5) Å	α = 90 deg.
	b = 10.1857(5) Å	β =98.493(3) deg.
	c = 19.6197(11) Å	γ = 90 deg.
Volume	2056.83(18) $Å^3$	
Density (calculated)	1.45 g/cm^3	
Absorption coefficient	0.46 mm^{-1}	
Crystal shape	plate	
Crystal size	0.230 x 0.217 x 0.020 mm^3	
Crystal colour	yellow	
Theta range for data collection	2.0 to 21.7 deg.	
Index ranges	-10≤h≤10, -10≤k≤10, -20≤l≤20	
Reflections collected	18967	
Independent reflections	2437 (R(int) = 0.0778)	
Observed reflections	1560 (I > 2σ(I))	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.96 and 0.86	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	2437 / 60 / 308	
Goodness-of-fit on F^2	1.04	
Final R indices (I>2sigma(I))	R1 = 0.060, wR2 = 0.133	
Largest diff. peak and hole	0.28 and -0.30 $eÅ^{-3}$	

Table S8: Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **5a**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}

N11	0.3421(3)	0.6567(4)	0.4443(2)	0.0333(10)
C12	0.4148(4)	0.5737(4)	0.4113(2)	0.0270(11)
N13	0.3459(4)	0.4918(4)	0.3657(2)	0.0372(10)
C14	0.4124(5)	0.4047(4)	0.3319(2)	0.0329(12)
C15	0.3411(5)	0.3174(4)	0.2839(2)	0.0444(13)
H15	0.2490	0.3221	0.2754	0.053
C16	0.4038(6)	0.2285(5)	0.2504(2)	0.0485(14)
H16	0.3550	0.1703	0.2187	0.058
C17	0.5398(6)	0.2196(5)	0.2613(2)	0.0496(14)
H17	0.5817	0.1552	0.2374	0.059
C18	0.6115(5)	0.3016(5)	0.3054(2)	0.0447(13)
H18	0.7036	0.2953	0.3119	0.054
C19	0.5504(5)	0.3978(4)	0.3425(2)	0.0339(12)
C20	0.6187(5)	0.4829(4)	0.3897(2)	0.0378(12)
H20	0.7109	0.4791	0.3984	0.045
C21	0.5525(4)	0.5733(4)	0.4241(2)	0.0299(11)
C22	0.6144(4)	0.6653(4)	0.4725(2)	0.0302(11)
H22	0.7066	0.6681	0.4821	0.036
C23	0.5416(4)	0.7502(4)	0.5054(2)	0.0263(11)
C24	0.6000(4)	0.8481(4)	0.5561(2)	0.0292(11)
C25	0.7349(4)	0.8569(5)	0.5743(2)	0.0407(13)
H25	0.7892	0.7970	0.5548	0.049
C26	0.7903(5)	0.9508(5)	0.6200(2)	0.0485(14)
H26	0.8821	0.9557	0.6315	0.058
C27	0.7122(5)	1.0379(5)	0.6492(2)	0.0466(14)
H27	0.7500	1.1029	0.6806	0.056
C28	0.5799(5)	1.0297(4)	0.6324(2)	0.0393(13)
H28	0.5270	1.0899	0.6527	0.047
C29	0.5203(4)	0.9351(4)	0.5861(2)	0.0325(12)
C30	0.3795(4)	0.9236(4)	0.5713(2)	0.0323(11)
C31	0.2945(5)	1.0042(5)	0.6032(2)	0.0401(13)
H31	0.3297	1.0717	0.6339	0.048
C32	0.1641(5)	0.9866(5)	0.5908(3)	0.0511(14)
H32	0.1099	1.0423	0.6130	0.061
C33	0.1078(5)	0.8904(5)	0.5470(3)	0.0522(14)
H33	0.0163	0.8782	0.5398	0.063
C34	0.1867(5)	0.8125(5)	0.5140(2)	0.0420(13)
H34	0.1487	0.7469	0.4829	0.050
C35	0.3209(4)	0.8273(4)	0.5248(2)	0.0302(11)
C36	0.4029(4)	0.7404(4)	0.4892(2)	0.0299(11)
C41	0.042(2)	0.5291(14)	0.3683(6)	0.082(7)
H41	0.1385	0.5364	0.3699	0.098
Cl1	0.0112(5)	0.4888(5)	0.4504(3)	0.120(2)
Cl2	-0.0273(13)	0.6786(12)	0.3393(8)	0.209(8)
Cl3	-0.0144(9)	0.4094(10)	0.3079(4)	0.154(4)
C41B	0.0551(15)	0.5699(11)	0.3426(6)	0.066(4)
H41B	0.1395	0.5830	0.3735	0.080
Cl1B	0.0806(4)	0.5990(5)	0.2581(2)	0.139(2)
Cl2B	0.0010(6)	0.4104(5)	0.3548(4)	0.141(3)
Cl3B	-0.0567(6)	0.6819(6)	0.3660(4)	0.0950(18)

Table S9: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **5a**.

Atom	x	y	z	U_{eq}
H15	0.2490	0.3221	0.2754	0.053
H16	0.3550	0.1703	0.2187	0.058
H17	0.5817	0.1552	0.2374	0.059
H18	0.7036	0.2953	0.3119	0.054
H20	0.7109	0.4791	0.3984	0.045
H22	0.7066	0.6681	0.4821	0.036
H25	0.7892	0.7970	0.5548	0.049
H26	0.8821	0.9557	0.6315	0.058
H27	0.7500	1.1029	0.6806	0.056
H28	0.5270	1.0899	0.6527	0.047
H31	0.3297	1.0717	0.6339	0.048
H32	0.1099	1.0423	0.6130	0.061
H33	0.0163	0.8782	0.5398	0.063
H34	0.1487	0.7469	0.4829	0.050
H41	0.1385	0.5364	0.3699	0.098
H41B	0.1395	0.5830	0.3735	0.080

Table S10: Anisotropic displacement parameters ($Å^2$) for **5a**. 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	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N11	0.044(2)	0.030(2)	0.025(2)	0.004(2)	0.0029(19)	0.001(2)
C12	0.038(3)	0.023(3)	0.020(2)	0.005(2)	0.005(2)	0.004(2)
N13	0.050(2)	0.034(2)	0.028(2)	0.002(2)	0.007(2)	-0.002(2)
C14	0.052(3)	0.028(3)	0.021(3)	0.003(2)	0.012(2)	0.003(2)
C15	0.070(4)	0.034(3)	0.030(3)	0.002(3)	0.007(3)	-0.001(3)
C16	0.085(4)	0.036(3)	0.023(3)	-0.003(2)	0.004(3)	-0.004(3)
C17	0.090(5)	0.033(3)	0.030(3)	0.000(3)	0.024(3)	0.011(3)
C18	0.068(4)	0.036(3)	0.032(3)	0.007(3)	0.017(3)	0.006(3)
C19	0.064(4)	0.023(3)	0.016(3)	0.003(2)	0.010(2)	0.000(2)
C20	0.046(3)	0.038(3)	0.031(3)	0.009(3)	0.009(2)	0.003(3)
C21	0.045(3)	0.028(3)	0.019(2)	0.006(2)	0.012(2)	0.004(2)
C22	0.035(3)	0.030(3)	0.026(3)	0.003(2)	0.007(2)	-0.001(2)
C23	0.038(3)	0.023(2)	0.019(2)	0.010(2)	0.006(2)	-0.001(2)
C24	0.040(3)	0.025(3)	0.024(3)	0.003(2)	0.009(2)	-0.002(2)
C25	0.038(3)	0.048(3)	0.037(3)	-0.007(3)	0.008(2)	0.000(3)
C26	0.047(3)	0.057(3)	0.040(3)	-0.007(3)	0.004(3)	-0.011(3)
C27	0.055(4)	0.049(3)	0.036(3)	-0.009(3)	0.006(3)	-0.012(3)
C28	0.051(3)	0.034(3)	0.034(3)	-0.003(3)	0.011(2)	0.001(2)
C29	0.051(3)	0.027(3)	0.020(3)	0.008(2)	0.006(2)	-0.003(2)
C30	0.043(3)	0.030(3)	0.025(3)	0.007(2)	0.008(2)	0.000(2)
C31	0.051(4)	0.035(3)	0.035(3)	-0.010(2)	0.010(3)	0.002(3)
C32	0.047(4)	0.050(3)	0.060(4)	-0.010(3)	0.023(3)	0.009(3)
C33	0.038(3)	0.060(4)	0.060(4)	-0.006(3)	0.009(3)	0.005(3)
C34	0.043(3)	0.046(3)	0.038(3)	-0.003(3)	0.005(2)	0.004(3)
C35	0.038(3)	0.027(3)	0.027(3)	0.003(2)	0.010(2)	0.007(2)
C36	0.042(3)	0.028(3)	0.021(3)	0.010(2)	0.008(2)	0.000(2)
C41	0.059(12)	0.104(19)	0.080(15)	-0.011(12)	0.003(11)	-0.007(12)
Cl1	0.100(4)	0.135(5)	0.127(4)	-0.005(4)	0.026(3)	-0.043(3)
Cl2	0.193(12)	0.136(7)	0.264(16)	0.029(8)	-0.077(10)	0.061(7)
Cl3	0.086(4)	0.186(8)	0.178(7)	-0.090(7)	-0.024(5)	-0.013(4)
C41B	0.052(8)	0.073(9)	0.070(10)	-0.011(8)	-0.003(7)	0.008(8)
Cl1B	0.139(3)	0.207(5)	0.064(2)	0.019(3)	-0.010(2)	0.031(3)
Cl2B	0.075(3)	0.062(3)	0.289(10)	0.019(4)	0.034(5)	-0.002(2)
Cl3B	0.054(2)	0.074(3)	0.147(4)	-0.031(3)	-0.015(2)	0.009(2)

Tabelle S11: Bond lengths (Å) and angles (deg) for **5a**.

N11-C36	1.319(5)	C34-H34	0.9500
N11-C12	1.361(5)	C35-C36	1.476(6)
C12-N13	1.349(5)	C41-Cl1	1.738(13)
C12-C21	1.418(6)	C41-Cl3	1.742(13)
N13-C14	1.357(5)	C41-Cl2	1.745(13)
C14-C19	1.422(6)	C41-H41	1.0000
C14-C15	1.422(6)	C41B-Cl3B	1.740(11)
C15-C16	1.342(6)	C41B-Cl1B	1.742(11)
C15-H15	0.9500	C41B-Cl2B	1.748(11)
C16-C17	1.403(7)	C41B-H41B	1.0000
C16-H16	0.9500	C36-N11-C12	118.3(4)
C17-C18	1.346(6)	N13-C12-N11	114.9(4)
C17-H17	0.9500	N13-C12-C21	122.7(4)
C18-C19	1.425(6)	N11-C12-C21	122.4(4)
C18-H18	0.9500	C12-N13-C14	118.0(4)
C19-C20	1.386(6)	N13-C14-C19	122.5(4)
C20-C21	1.384(6)	N13-C14-C15	118.6(4)
C20-H20	0.9500	C19-C14-C15	118.8(4)
C21-C22	1.418(6)	C16-C15-C14	120.1(5)
C22-C23	1.373(6)	C16-C15-H15	119.9
C22-H22	0.9500	C14-C15-H15	119.9
C23-C36	1.435(6)	C15-C16-C17	121.4(5)
C23-C24	1.475(6)	C15-C16-H16	119.3
C24-C25	1.400(6)	C17-C16-H16	119.3
C24-C29	1.401(6)	C18-C17-C16	120.6(5)
C25-C26	1.377(6)	C18-C17-H17	119.7
C25-H25	0.9500	C16-C17-H17	119.7
C26-C27	1.383(6)	C17-C18-C19	120.5(5)
C26-H26	0.9500	C17-C18-H18	119.8
C27-C28	1.370(6)	C19-C18-H18	119.8
C27-H27	0.9500	C20-C19-C14	118.3(4)
C28-C29	1.404(6)	C20-C19-C18	123.2(5)
C28-H28	0.9500	C14-C19-C18	118.5(4)
C29-C30	1.456(6)	C21-C20-C19	120.0(5)
C30-C35	1.415(6)	C21-C20-H20	120.0
C30-C31	1.419(6)	C19-C20-H20	120.0
C31-C32	1.355(6)	C20-C21-C22	123.8(4)
C31-H31	0.9500	C20-C21-C12	118.5(4)
C32-C33	1.376(7)	C22-C21-C12	117.7(4)
C32-H32	0.9500	C23-C22-C21	120.2(4)
C33-C34	1.371(6)	C23-C22-H22	119.9
C33-H33	0.9500	C21-C22-H22	119.9
C34-C35	1.389(6)	C22-C23-C36	117.3(4)

C22-C23-C24	122.9(4)
C36-C23-C24	119.8(4)
C25-C24-C29	119.1(4)
C25-C24-C23	120.9(4)
C29-C24-C23	120.1(4)
C26-C25-C24	121.2(5)
C26-C25-H25	119.4
C24-C25-H25	119.4
C25-C26-C27	120.0(5)
C25-C26-H26	120.0
C27-C26-H26	120.0
C28-C27-C26	119.5(5)
C28-C27-H27	120.2
C26-C27-H27	120.2
C27-C28-C29	122.0(5)
C27-C28-H28	119.0
C29-C28-H28	119.0
C24-C29-C28	118.2(4)
C24-C29-C30	120.4(4)
C28-C29-C30	121.3(4)
C35-C30-C31	116.6(4)
C35-C30-C29	120.7(4)
C31-C30-C29	122.7(4)
C32-C31-C30	121.1(4)
C32-C31-H31	119.4
C30-C31-H31	119.4
C31-C32-C33	122.0(5)
C31-C32-H32	119.0
C33-C32-H32	119.0
C34-C33-C32	118.5(5)
C34-C33-H33	120.7
C32-C33-H33	120.7
C33-C34-C35	121.5(5)
C33-C34-H34	119.2
C35-C34-H34	119.2
C34-C35-C30	120.1(4)
C34-C35-C36	120.1(4)
C30-C35-C36	119.7(4)
N11-C36-C23	124.2(4)
N11-C36-C35	116.7(4)
C23-C36-C35	119.1(4)
Cl1-C41-Cl3	112.0(9)
Cl1-C41-Cl2	112.5(10)
Cl3-C41-Cl2	107.8(11)
Cl1-C41-H41	108.1
Cl3-C41-H41	108.1
Cl2-C41-H41	108.1
Cl3B-C41B-Cl1B	110.0(7)
Cl3B-C41B-Cl2B	109.4(8)
Cl1B-C41B-Cl2B	112.7(7)
Cl3B-C41B-H41B	108.2
Cl1B-C41B-H41B	108.2
Cl2B-C41B-H41B	108.2

6.3. Compound 17

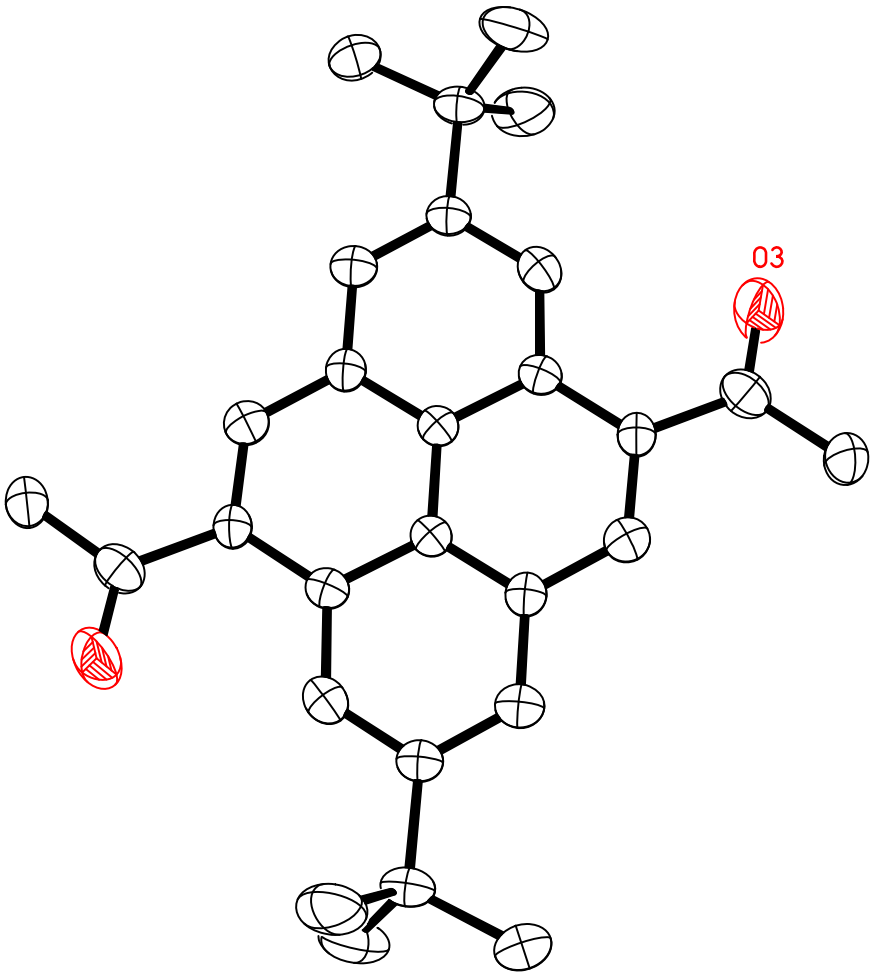


Figure S10: Crystal structure of **17**.

Table S12: Crystal data and structure refinement for **17**.

Identification code	stu6		
Empirical formula	$C_{28}H_{30}O_2$		
Formula weight	398.52		
Temperature	200(2) K		
Wavelength	1.54178 Å		
Crystal system	orthorhombic		
Space group	Pbam		
Z	4		
Unit cell dimensions	a = 12.7159(13) Å	α =	90 deg.
	b = 23.425(2) Å	β =	90 deg.
	c =7.1806(7) Å	γ =	90 deg.
Volume	2138.9(4) $Å^3$		
Density (calculated)	1.24 g/cm^3		

Absorption coefficient	0.59 mm^{-1}
Crystal shape	needle
Crystal size	0.190 x 0.018 x 0.015 mm^3
Crystal colour	pale yellow
Theta range for data collection	3.8 to 56.0 deg.
Index ranges	-13≤h≤11, -24≤k≤25, -7≤l≤5
Reflections collected	6544
Independent reflections	1527 (R(int) = 0.1052)
Observed reflections	734 (I > 2σ(I))
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.67 and 0.78
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	1527 / 200 / 195
Goodness-of-fit on F^2	0.96
Final R indices (I>2sigma(I))	R1 = 0.052, wR2 = 0.098
Largest diff. peak and hole	0.23 and -0.20 $eÅ^{-3}$

Table S13: Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **17**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
C11	-0.0496(4)	0.3966(3)	0.0000	0.0333(13)
H11	-0.0490	0.3560	0.0000	0.040
C21	-0.1445(4)	0.4232(2)	0.0000	0.0307(14)
C31	-0.2412(5)	0.3881(3)	0.029(3)	0.038(4)
O31	-0.3273(4)	0.4084(2)	0.0558(17)	0.077(5)
C41	-0.2346(6)	0.3239(3)	0.020(8)	0.049(6)
H4A1	-0.3024	0.3084	-0.0204	0.073
H4B1	-0.2171	0.3089	0.1435	0.073
H4C1	-0.1798	0.3127	-0.0690	0.073
C111	0.0486(4)	0.4847(2)	0.0000	0.0247(12)
C121	0.0485(4)	0.4252(2)	0.0000	0.0290(13)
C131	0.1436(4)	0.3955(2)	0.0000	0.0311(13)
H131	0.1424	0.3550	0.0000	0.037
C141	0.2393(4)	0.4231(2)	0.0000	0.0301(13)
C151	0.2389(4)	0.4822(2)	0.0000	0.0346(14)
H151	0.3045	0.5016	0.0000	0.042
C161	0.1464(4)	0.5152(2)	0.0000	0.0283(13)
C181	0.3453(4)	0.3921(2)	0.0000	0.0361(14)
C1811	0.3338(4)	0.3265(2)	0.0000	0.0472(16)
H18A1	0.4037	0.3088	0.0000	0.071
H18B1	0.2952	0.3145	0.1114	0.071
H18C1	0.2952	0.3145	-0.1114	0.071
C1821	0.4083(3)	0.4089(2)	0.1744(6)	0.0585(13)
H18D1	0.4761	0.3890	0.1739	0.088
H18E1	0.4202	0.4502	0.1745	0.088
H18F1	0.3686	0.3982	0.2861	0.088
C12	0.8044(4)	0.5117(2)	0.5000	0.0299(13)
H12	0.7346	0.5262	0.5000	0.036
C22	0.8171(4)	0.4534(2)	0.5000	0.0326(14)
C32	0.7210(5)	0.4183(3)	0.527(3)	0.040(4)
O32	0.7257(4)	0.3678(2)	0.5734(9)	0.072(3)
C42	0.6143(4)	0.4433(3)	0.491(7)	0.049(3)
H4A2	0.5604	0.4142	0.5135	0.074
H4B2	0.6101	0.4562	0.3614	0.074
H4C2	0.6028	0.4758	0.5746	0.074
C112	0.9923(4)	0.5307(2)	0.5000	0.0258(12)
C122	0.8878(4)	0.5515(2)	0.5000	0.0264(13)
C132	0.8701(4)	0.6092(2)	0.5000	0.0332(13)
H132	0.7995	0.6225	0.5000	0.040
C142	0.9512(5)	0.6493(2)	0.5000	0.0320(13)
C152	1.0538(4)	0.6274(2)	0.5000	0.0341(14)
H152	1.1106	0.6537	0.5000	0.041
C162	1.0773(4)	0.5692(2)	0.5000	0.0291(13)
C182	0.9328(4)	0.7132(2)	0.5000	0.0349(14)
C1812	0.8160(4)	0.7270(3)	0.5000	0.063(2)
H18A2	0.7830	0.7104	0.6107	0.095
H18B2	0.8064	0.7686	0.5014	0.095
H18C2	0.7833	0.7111	0.3879	0.095
C1822	0.9803(3)	0.7397(2)	0.6731(6)	0.0708(15)
H18D2	0.9490	0.7222	0.7840	0.106
H18E2	1.0564	0.7332	0.6736	0.106
H18F2	0.9663	0.7808	0.6736	0.106

Table S14: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **17**.

Atom	x	y	z	U_{eq}
H11	-0.0490	0.3560	0.0000	0.040
H4A1	-0.3024	0.3084	-0.0204	0.073
H4B1	-0.2171	0.3089	0.1435	0.073
H4C1	-0.1798	0.3127	-0.0690	0.073
H131	0.1424	0.3550	0.0000	0.037
H151	0.3045	0.5016	0.0000	0.042
H18A1	0.4037	0.3088	0.0000	0.071
H18B1	0.2952	0.3145	0.1114	0.071
H18C1	0.2952	0.3145	-0.1114	0.071
H18D1	0.4761	0.3890	0.1739	0.088
H18E1	0.4202	0.4502	0.1745	0.088
H18F1	0.3686	0.3982	0.2861	0.088
H12	0.7346	0.5262	0.5000	0.036
H4A2	0.5604	0.4142	0.5135	0.074
H4B2	0.6101	0.4562	0.3614	0.074
H4C2	0.6028	0.4758	0.5746	0.074
H132	0.7995	0.6225	0.5000	0.040
H152	1.1106	0.6537	0.5000	0.041
H18A2	0.7830	0.7104	0.6107	0.095
H18B2	0.8064	0.7686	0.5014	0.095
H18C2	0.7833	0.7111	0.3879	0.095
H18D2	0.9490	0.7222	0.7840	0.106
H18E2	1.0564	0.7332	0.6736	0.106
H18F2	0.9663	0.7808	0.6736	0.106

Table S15: Anisotropic displacement parameters ($Å^2$) for **17**. 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	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C11	0.034(3)	0.032(3)	0.034(3)	0.000	0.000	0.001(3)
C21	0.029(3)	0.026(3)	0.038(4)	0.000	0.000	-0.003(3)
C31	0.031(3)	0.048(4)	0.036(13)	-0.002(5)	0.004(5)	-0.001(3)
O31	0.033(3)	0.047(3)	0.151(17)	-0.005(4)	0.026(4)	-0.004(3)
C41	0.036(4)	0.035(3)	0.076(17)	0.007(10)	0.005(12)	-0.005(3)
C111	0.026(3)	0.029(3)	0.019(3)	0.000	0.000	-0.001(2)
C121	0.030(3)	0.028(3)	0.029(3)	0.000	0.000	-0.002(3)
C131	0.031(3)	0.036(3)	0.026(3)	0.000	0.000	0.003(3)
C141	0.028(3)	0.032(3)	0.030(3)	0.000	0.000	0.003(3)
C151	0.029(3)	0.039(3)	0.036(3)	0.000	0.000	-0.004(3)
C161	0.026(3)	0.031(3)	0.028(3)	0.000	0.000	0.001(3)
C181	0.026(3)	0.041(3)	0.040(4)	0.000	0.000	0.009(3)
C1811	0.042(4)	0.037(3)	0.062(4)	0.000	0.000	0.010(3)
C1821	0.039(2)	0.070(3)	0.066(3)	-0.014(3)	-0.018(2)	0.017(2)
C12	0.023(3)	0.034(3)	0.032(3)	0.000	0.000	0.003(2)
C22	0.033(3)	0.026(3)	0.039(4)	0.000	0.000	-0.002(3)
C32	0.040(3)	0.027(3)	0.052(13)	0.004(6)	0.005(6)	-0.001(3)
O32	0.044(3)	0.041(3)	0.130(9)	0.017(3)	0.004(3)	-0.008(3)
C42	0.035(3)	0.040(4)	0.073(8)	-0.010(17)	-0.016(14)	-0.008(3)
C112	0.032(3)	0.025(3)	0.021(3)	0.000	0.000	-0.001(2)
C122	0.029(3)	0.022(3)	0.028(3)	0.000	0.000	-0.001(2)
C132	0.039(3)	0.030(3)	0.031(3)	0.000	0.000	0.001(3)
C142	0.040(3)	0.026(3)	0.031(3)	0.000	0.000	0.001(3)
C152	0.039(3)	0.032(3)	0.030(3)	0.000	0.000	-0.004(3)
C162	0.033(3)	0.022(3)	0.032(3)	0.000	0.000	-0.001(2)
C182	0.050(4)	0.023(3)	0.032(3)	0.000	0.000	0.004(3)
C1812	0.059(4)	0.032(4)	0.100(5)	0.000	0.000	0.010(3)
C1822	0.100(4)	0.044(3)	0.069(3)	-0.018(3)	-0.027(3)	0.007(3)

Table S16: Bond lengths (Å) and angles (deg) for **17**.

C11-C21	1.359(7)	C111-C161	1.433(7)
C11-C121	1.416(7)	C121-C131	1.395(7)
C11-H11	0.9500	C131-C141	1.377(7)
C21-C161#1	1.443(7)	C131-H131	0.9500
C21-C31	1.494(8)	C141-C151	1.385(7)
C31-O31	1.210(8)	C141-C181	1.531(7)
C31-C41	1.507(8)	C151-C161	1.407(7)
C41-H4A1	0.9800	C151-H151	0.9500
C41-H4B1	0.9800	C181-C1821	1.538(5)
C41-H4C1	0.9800	C181-C1821#2	1.538(5)
C111-C121	1.395(7)	C181-C1811	1.545(8)
C111-C111#1	1.429(9)	C1811-H18A1	0.9800

C1811-H18B1	0.9800	C141-C181-C1821#2	109.7(3)
C1811-H18C1	0.9800	C1821-C181-C1821#2	109.1(4)
C1821-H18D1	0.9800	C141-C181-C1811	112.8(5)
C1821-H18E1	0.9800	C1821-C181-C1811	107.7(3)
C1821-H18F1	0.9800	C1821#2-C181-C1811	107.7(3)
C12-C22	1.374(7)	C181-C1811-H18A1	109.5
C12-C122	1.412(7)	C181-C1811-H18B1	109.5
C12-H12	0.9500	H18A1-C1811-H18B1	109.5
C22-C162#3	1.443(7)	C181-C1811-H18C1	109.5
C22-C32	1.486(8)	H18A1-C1811-H18C1	109.5
C32-O32	1.230(9)	H18B1-C1811-H18C1	109.5
C32-C42	1.500(10)	C181-C1821-H18D1	109.5
C42-H4A2	0.9800	C181-C1821-H18E1	109.5
C42-H4B2	0.9800	H18D1-C1821-H18E1	109.5
C42-H4C2	0.9800	C181-C1821-H18F1	109.5
C112-C162	1.407(7)	H18D1-C1821-H18F1	109.5
C112-C122	1.416(7)	H18E1-C1821-H18F1	109.5
C112-C112#3	1.452(10)	C22-C12-C122	124.6(5)
C122-C132	1.371(7)	C22-C12-H12	117.7
C132-C142	1.394(7)	C122-C12-H12	117.7
C132-H132	0.9500	C12-C22-C162#3	118.3(5)
C142-C152	1.401(7)	C12-C22-C32	117.0(5)
C142-C182	1.516(7)	C162#3-C22-C32	124.2(5)
C152-C162	1.396(7)	O32-C32-C22	121.8(6)
C152-H152	0.9500	O32-C32-C42	117.8(7)
C182-C1822#4	1.515(5)	C22-C32-C42	120.4(7)
C182-C1822	1.515(5)	C32-C42-H4A2	109.5
C182-C1812	1.520(7)	C32-C42-H4B2	109.5
C1812-H18A2	0.9800	H4A2-C42-H4B2	109.5
C1812-H18B2	0.9800	C32-C42-H4C2	109.5
C1812-H18C2	0.9800	H4A2-C42-H4C2	109.5
C1822-H18D2	0.9800	H4B2-C42-H4C2	109.5
C1822-H18E2	0.9800	C162-C112-C122	120.0(5)
C1822-H18F2	0.9800	C162-C112-C112#3	122.0(6)
C21-C11-C121	124.3(6)	C122-C112-C112#3	117.9(6)
C21-C11-H11	117.8	C132-C122-C12	121.9(5)
C121-C11-H11	117.8	C132-C122-C112	119.6(5)
C11-C21-C161#1	118.3(5)	C12-C122-C112	118.5(5)
C11-C21-C31	118.5(5)	C122-C132-C142	122.8(5)
C161#1-C21-C31	122.5(5)	C122-C132-H132	118.6
O31-C31-C21	123.3(6)	C142-C132-H132	118.6
O31-C31-C41	116.8(7)	C132-C142-C152	116.3(5)
C21-C31-C41	119.9(7)	C132-C142-C182	123.4(5)
C31-C41-H4A1	109.5	C152-C142-C182	120.3(5)
C31-C41-H4B1	109.5	C162-C152-C142	123.8(5)
H4A1-C41-H4B1	109.5	C162-C152-H152	118.1
C31-C41-H4C1	109.5	C142-C152-H152	118.1
H4A1-C41-H4C1	109.5	C152-C162-C112	117.4(5)
H4B1-C41-H4C1	109.5	C152-C162-C22#3	123.9(5)
C121-C111-C111#1	120.0(6)	C112-C162-C22#3	118.7(5)
C121-C111-C161	119.9(5)	C1822#4-C182-C1822	110.2(5)
C111#1-C111-C161	120.1(6)	C1822#4-C182-C142	110.1(3)
C111-C121-C131	119.8(5)	C1822-C182-C142	110.1(3)
C111-C121-C11	118.4(5)	C1822#4-C182-C1812	107.6(3)
C131-C121-C11	121.9(5)	C1822-C182-C1812	107.6(3)
C141-C131-C121	122.2(5)	C142-C182-C1812	111.2(5)
C141-C131-H131	118.9	C182-C1812-H18A2	109.5
C121-C131-H131	118.9	C182-C1812-H18B2	109.5
C131-C141-C151	117.8(5)	H18A2-C1812-H18B2	109.5
C131-C141-C181	123.7(5)	C182-C1812-H18C2	109.5
C151-C141-C181	118.5(5)	H18A2-C1812-H18C2	109.5
C141-C151-C161	123.5(5)	H18B2-C1812-H18C2	109.5
C141-C151-H151	118.3	C182-C1822-H18D2	109.5
C161-C151-H151	118.3	C182-C1822-H18E2	109.5
C151-C161-C111	116.9(5)	H18D2-C1822-H18E2	109.5
C151-C161-C21#1	124.2(5)	C182-C1822-H18F2	109.5
C111-C161-C21#1	118.9(5)	H18D2-C1822-H18F2	109.5
C141-C181-C1821	109.7(3)	H18E2-C1822-H18F2	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z
#2 x,y,-z
#3 -x+2,-y+1,-z+1

#4 x,y,-z+1

6.4. Compound 5c

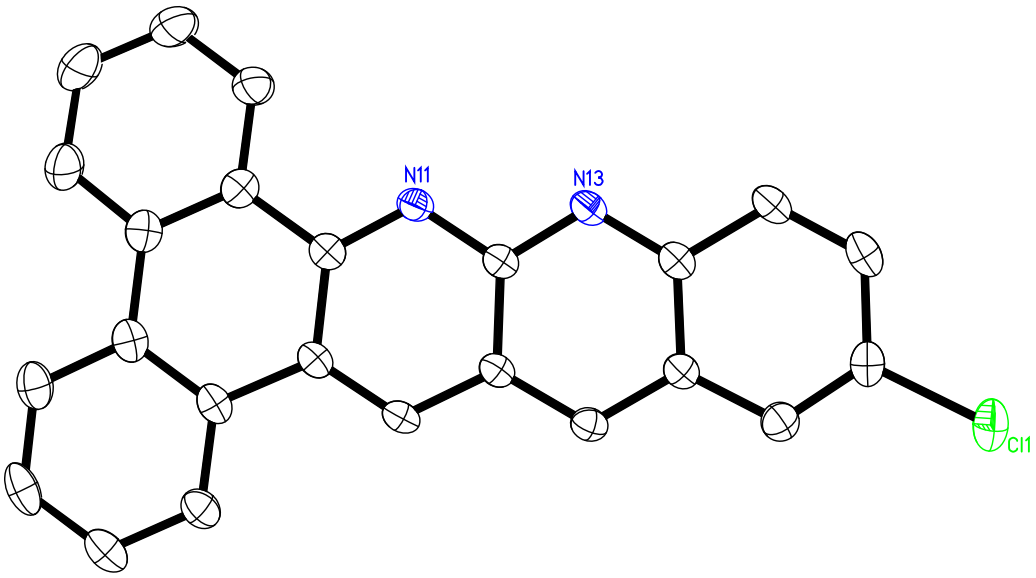


Figure S11: Crystal structure of **5c**.

Table S17: Crystal data and structure refinement for **5c**.

Identification code	stu10	
Empirical formula	$C_{25}H_{14}Cl_4N_2$	
Formula weight	484.18	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Z	2	
Unit cell dimensions	a =6.7171(6) Å	α =74.5286(15) deg.
	b = 12.8506(11) Å	β =86.0490(17) deg.
	c = 13.2342(11) Å	γ =75.8886(15) deg.
Volume	1067.73(16) $Å^3$	
Density (calculated)	1.51 g/cm^3	
Absorption coefficient	0.57 mm^{-1}	
Crystal shape	plank	
Crystal size	0.358 x 0.045 x 0.027 mm^3	
Crystal colour	yellow	
Theta range for data collection	1.6 to 28.7 deg.	
Index ranges	-8≤h≤9, -16≤k≤17, -17≤l≤17	
Reflections collected	21274	
Independent reflections	5428 (R(int) = 0.0478)	
Observed reflections	3643 (I > 2σ(I))	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.96 and 0.72	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	5428 / 60 / 317	
Goodness-of-fit on F^2	1.04	
Final R indices (I>2sigma(I))	R1 = 0.043, wR2 = 0.098	
Largest diff. peak and hole	0.33 and -0.33 $eÅ^{-3}$	

Table S18: Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **5c**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor

Atom	x	y	z	U_{eq}
Cl1	0.3590(1)	0.1748(1)	1.0029(1)	0.0417(2)
N11	0.2886(2)	0.4315(1)	0.3830(1)	0.0229(3)
C12	0.2917(3)	0.4114(2)	0.4892(1)	0.0205(4)

N13	0.3399(2)	0.3032(1)	0.5420(1)	0.0232(3)
C14	0.3423(3)	0.2787(2)	0.6473(1)	0.0217(4)
C15	0.3888(3)	0.1641(2)	0.7042(2)	0.0262(4)
H15	0.4183	0.1081	0.6672	0.031
C16	0.3912(3)	0.1348(2)	0.8103(2)	0.0285(4)
H16	0.4211	0.0586	0.8473	0.034
C17	0.3492(3)	0.2178(2)	0.8664(1)	0.0266(4)
C18	0.3039(3)	0.3274(2)	0.8175(1)	0.0258(4)
H18	0.2763	0.3811	0.8571	0.031
C19	0.2980(3)	0.3615(2)	0.7056(1)	0.0212(4)
C20	0.2511(3)	0.4723(2)	0.6495(1)	0.0224(4)
H20	0.2223	0.5292	0.6855	0.027
C21	0.2462(3)	0.4999(2)	0.5398(1)	0.0203(4)
C22	0.1986(3)	0.6097(2)	0.4762(1)	0.0224(4)
H22	0.1682	0.6699	0.5080	0.027
C23	0.1957(3)	0.6309(2)	0.3691(1)	0.0207(4)
C24	0.1510(3)	0.7435(2)	0.2984(1)	0.0231(4)
C25	0.1027(3)	0.8373(2)	0.3386(2)	0.0283(4)
H25	0.0935	0.8276	0.4124	0.034
C26	0.0683(3)	0.9434(2)	0.2731(2)	0.0332(5)
H26	0.0367	1.0058	0.3019	0.040
C27	0.0798(3)	0.9585(2)	0.1658(2)	0.0356(5)
H27	0.0575	1.0314	0.1207	0.043
C28	0.1237(3)	0.8676(2)	0.1241(2)	0.0324(5)
H28	0.1304	0.8790	0.0501	0.039
C29	0.1588(3)	0.7587(2)	0.1888(1)	0.0256(4)
C30	0.1985(3)	0.6618(2)	0.1447(1)	0.0260(4)
C31	0.1959(3)	0.6727(2)	0.0360(2)	0.0381(5)
H31	0.1755	0.7446	-0.0109	0.046
C32	0.2222(4)	0.5819(2)	-0.0036(2)	0.0473(6)
H32	0.2194	0.5916	-0.0772	0.057
C33	0.2529(4)	0.4760(2)	0.0631(2)	0.0455(6)
H33	0.2698	0.4133	0.0354	0.055
C34	0.2586(3)	0.4621(2)	0.1696(2)	0.0347(5)
H34	0.2798	0.3895	0.2153	0.042
C35	0.2335(3)	0.5536(2)	0.2115(1)	0.0253(4)
C36	0.2407(3)	0.5359(2)	0.3255(1)	0.0218(4)
C41	0.5772(11)	0.1770(7)	0.3644(6)	0.046(3)
H41	0.4930	0.2320	0.4008	0.055
Cl2	0.7085(5)	0.0643(3)	0.4598(2)	0.0440(9)
Cl3	0.4112(7)	0.1398(3)	0.2929(3)	0.0696(10)
Cl4	0.7504(7)	0.2430(3)	0.2793(4)	0.0829(11)
C41B	0.590(2)	0.1884(12)	0.3599(9)	0.058(5)
H41B	0.4924	0.2432	0.3917	0.070
Cl2B	0.7018(12)	0.0693(7)	0.4564(6)	0.089(3)
Cl3B	0.465(3)	0.1456(7)	0.2724(11)	0.136(3)
Cl4B	0.7906(19)	0.2440(6)	0.2957(7)	0.105(3)

Table S19: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **5c**.

Atom	x	y	z	U_{eq}
H15	0.4183	0.1081	0.6672	0.031
H16	0.4211	0.0586	0.8473	0.034
H18	0.2763	0.3811	0.8571	0.031
H20	0.2223	0.5292	0.6855	0.027
H22	0.1682	0.6699	0.5080	0.027
H25	0.0935	0.8276	0.4124	0.034
H26	0.0367	1.0058	0.3019	0.040
H27	0.0575	1.0314	0.1207	0.043
H28	0.1304	0.8790	0.0501	0.039
H31	0.1755	0.7446	-0.0109	0.046
H32	0.2194	0.5916	-0.0772	0.057
H33	0.2698	0.4133	0.0354	0.055
H34	0.2798	0.3895	0.2153	0.042
H41	0.4930	0.2320	0.4008	0.055
H41B	0.4924	0.2432	0.3917	0.070

Table S20: Anisotropic displacement parameters ($Å^2$) for **5c**. 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	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	0.0548(4)	0.0369(3)	0.0253(2)	0.0032(2)	-0.0032(2)	-0.0075(3)
N11	0.0243(8)	0.0194(8)	0.0249(8)	-0.0071(6)	-0.0019(6)	-0.0032(7)

C12	0.0175(9)	0.0192(9)	0.0250(8)	-0.0059(7)	-0.0024(7)	-0.0039(7)
N13	0.0238(8)	0.0179(8)	0.0274(8)	-0.0055(6)	-0.0029(6)	-0.0033(6)
C14	0.0163(9)	0.0203(10)	0.0280(9)	-0.0048(7)	-0.0020(7)	-0.0046(7)
C15	0.0248(10)	0.0181(10)	0.0347(10)	-0.0054(8)	-0.0037(8)	-0.0036(8)
C16	0.0251(10)	0.0206(10)	0.0356(10)	0.0002(8)	-0.0049(8)	-0.0042(8)
C17	0.0242(10)	0.0282(11)	0.0243(9)	0.0001(8)	-0.0025(7)	-0.0074(8)
C18	0.0247(10)	0.0263(11)	0.0268(9)	-0.0063(8)	-0.0024(8)	-0.0065(8)
C19	0.0186(9)	0.0201(9)	0.0254(9)	-0.0054(7)	-0.0025(7)	-0.0049(7)
C20	0.0212(9)	0.0204(10)	0.0257(9)	-0.0075(7)	-0.0014(7)	-0.0032(8)
C21	0.0175(9)	0.0181(9)	0.0253(8)	-0.0056(7)	-0.0025(7)	-0.0035(7)
C22	0.0221(9)	0.0170(9)	0.0288(9)	-0.0075(7)	-0.0019(7)	-0.0036(7)
C23	0.0153(9)	0.0185(9)	0.0269(9)	-0.0040(7)	-0.0020(7)	-0.0030(7)
C24	0.0185(9)	0.0205(10)	0.0286(9)	-0.0018(7)	-0.0044(7)	-0.0052(8)
C25	0.0278(10)	0.0226(10)	0.0326(10)	-0.0051(8)	-0.0031(8)	-0.0035(8)
C26	0.0327(11)	0.0209(11)	0.0441(12)	-0.0044(9)	-0.0047(9)	-0.0060(9)
C27	0.0325(12)	0.0219(11)	0.0434(12)	0.0081(9)	-0.0074(9)	-0.0054(9)
C28	0.0322(11)	0.0297(12)	0.0301(10)	0.0024(8)	-0.0060(8)	-0.0070(9)
C29	0.0194(9)	0.0263(11)	0.0281(9)	-0.0013(8)	-0.0044(7)	-0.0050(8)
C30	0.0200(9)	0.0297(11)	0.0258(9)	-0.0033(8)	-0.0039(7)	-0.0045(8)
C31	0.0450(13)	0.0377(13)	0.0262(10)	-0.0017(9)	-0.0035(9)	-0.0060(11)
C32	0.0651(17)	0.0524(16)	0.0232(10)	-0.0108(10)	-0.0045(10)	-0.0094(13)
C33	0.0628(17)	0.0435(14)	0.0321(11)	-0.0175(10)	-0.0034(11)	-0.0069(12)
C34	0.0451(13)	0.0293(12)	0.0297(10)	-0.0098(9)	-0.0055(9)	-0.0047(10)
C35	0.0209(9)	0.0288(11)	0.0257(9)	-0.0067(8)	-0.0027(7)	-0.0045(8)
C36	0.0170(9)	0.0225(10)	0.0261(9)	-0.0058(7)	-0.0017(7)	-0.0050(7)
C41	0.056(4)	0.032(4)	0.058(5)	-0.030(3)	0.019(4)	-0.010(3)
Cl2	0.0499(15)	0.0541(18)	0.0294(12)	-0.0108(11)	-0.0027(9)	-0.0141(12)
Cl3	0.1033(18)	0.0362(12)	0.0710(12)	-0.0055(12)	-0.0424(12)	-0.0174(13)
Cl4	0.0842(19)	0.0399(15)	0.101(2)	0.0052(14)	0.0397(13)	-0.0080(10)
C41B	0.103(11)	0.028(6)	0.046(7)	-0.009(5)	-0.039(7)	-0.011(6)
Cl2B	0.112(5)	0.075(5)	0.068(4)	-0.010(3)	-0.013(3)	-0.007(4)
Cl3B	0.210(8)	0.064(4)	0.134(5)	-0.062(4)	-0.116(5)	0.040(3)
Cl4B	0.188(7)	0.044(3)	0.097(3)	-0.044(3)	0.040(3)	-0.036(3)

Table S21: Bond lengths (Å) and angles (deg) for **5c**.

Cl1-C17	1.7431(19)	C41-Cl2	1.740(7)
N11-C36	1.327(2)	C41-Cl4	1.769(7)
N11-C12	1.361(2)	C41-H41	1.0000
C12-N13	1.348(2)	C41B-Cl4B	1.741(12)
C12-C21	1.430(2)	C41B-Cl3B	1.749(11)
N13-C14	1.345(2)	C41B-Cl2B	1.750(11)
C14-C15	1.432(3)	C41B-H41B	1.0000
C14-C19	1.438(2)	C36-N11-C12	118.90(15)
C15-C16	1.353(3)	N13-C12-N11	115.30(15)
C15-H15	0.9500	N13-C12-C21	123.17(16)
C16-C17	1.419(3)	N11-C12-C21	121.53(16)
C16-H16	0.9500	C14-N13-C12	117.72(15)
C17-C18	1.351(3)	N13-C14-C15	118.21(16)
C18-C19	1.429(2)	N13-C14-C19	123.39(16)
C18-H18	0.9500	C15-C14-C19	118.40(16)
C19-C20	1.388(3)	C16-C15-C14	120.60(18)
C20-C21	1.400(2)	C16-C15-H15	119.7
C20-H20	0.9500	C14-C15-H15	119.7
C21-C22	1.409(2)	C15-C16-C17	120.17(18)
C22-C23	1.371(2)	C15-C16-H16	119.9
C22-H22	0.9500	C17-C16-H16	119.9
C23-C36	1.444(2)	C18-C17-C16	122.24(17)
C23-C24	1.470(2)	C18-C17-Cl1	119.78(15)
C24-C25	1.404(3)	C16-C17-Cl1	117.98(14)
C24-C29	1.410(3)	C17-C18-C19	119.20(17)
C25-C26	1.381(3)	C17-C18-H18	120.4
C25-H25	0.9500	C19-C18-H18	120.4
C26-C27	1.380(3)	C20-C19-C18	122.72(17)
C26-H26	0.9500	C20-C19-C14	117.88(16)
C27-C28	1.382(3)	C18-C19-C14	119.40(16)
C27-H27	0.9500	C19-C20-C21	119.77(17)
C28-C29	1.405(3)	C19-C20-H20	120.1
C28-H28	0.9500	C21-C20-H20	120.1
C29-C30	1.472(3)	C20-C21-C22	123.97(16)
C30-C35	1.407(3)	C20-C21-C12	118.07(16)
C30-C31	1.409(3)	C22-C21-C12	117.96(16)
C31-C32	1.371(3)	C23-C22-C21	121.00(17)
C31-H31	0.9500	C23-C22-H22	119.5
C32-C33	1.386(3)	C21-C22-H22	119.5
C32-H32	0.9500	C22-C23-C36	116.85(16)
C33-C34	1.374(3)	C22-C23-C24	123.60(16)
C33-H33	0.9500	C36-C23-C24	119.55(16)
C34-C35	1.399(3)	C25-C24-C29	118.96(17)
C34-H34	0.9500	C25-C24-C23	120.74(17)
C35-C36	1.467(2)	C29-C24-C23	120.30(17)
C41-Cl3	1.736(7)	C26-C25-C24	121.28(19)

C26-C25-H25	119.4
C24-C25-H25	119.4
C27-C26-C25	119.89(19)
C27-C26-H26	120.1
C25-C26-H26	120.1
C26-C27-C28	120.01(19)
C26-C27-H27	120.0
C28-C27-H27	120.0
C27-C28-C29	121.40(19)
C27-C28-H28	119.3
C29-C28-H28	119.3
C28-C29-C24	118.44(18)
C28-C29-C30	121.63(17)
C24-C29-C30	119.92(17)
C35-C30-C31	117.45(18)
C35-C30-C29	120.35(17)
C31-C30-C29	122.15(18)
C32-C31-C30	121.5(2)
C32-C31-H31	119.3
C30-C31-H31	119.3
C31-C32-C33	120.5(2)
C31-C32-H32	119.8
C33-C32-H32	119.8
C34-C33-C32	119.6(2)
C34-C33-H33	120.2
C32-C33-H33	120.2
C33-C34-C35	120.8(2)
C33-C34-H34	119.6
C35-C34-H34	119.6
C34-C35-C30	120.15(17)
C34-C35-C36	119.41(18)
C30-C35-C36	120.43(17)
N11-C36-C23	123.74(16)
N11-C36-C35	117.03(16)
C23-C36-C35	119.22(16)
Cl3-C41-Cl2	112.3(5)
Cl3-C41-Cl4	110.3(4)
Cl2-C41-Cl4	110.9(4)
Cl3-C41-H41	107.7
Cl2-C41-H41	107.7
Cl4-C41-H41	107.7
Cl4B-C41B-Cl3B	109.7(8)
Cl4B-C41B-Cl2B	106.7(8)
Cl3B-C41B-Cl2B	107.2(8)
Cl4B-C41B-H41B	111.0
Cl3B-C41B-H41B	111.0
Cl2B-C41B-H41B	111.0

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z
#2 x,y,-z
#3 -x+2,-y+1,-z+1

#4 x,y,-z+1

6.5. Compound 5e

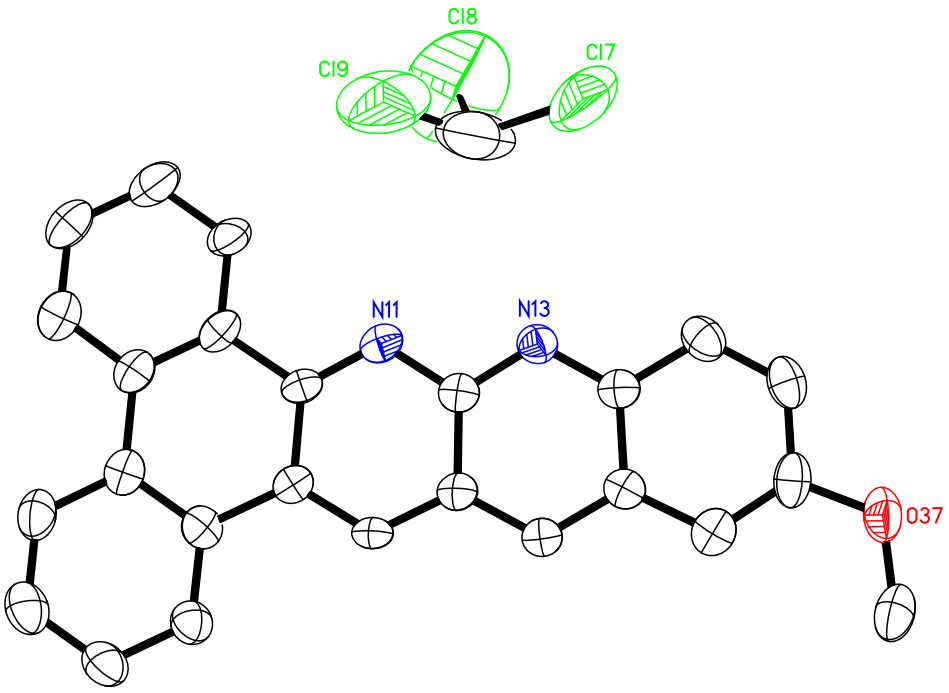


Figure S12: Crystal structure of **5e**.

Table S22: Crystal data and structure refinement for **5e**.

Identification code	stu11	
Empirical formula	$C_{26}H_{17}Cl_3N_2O$	
Formula weight	479.76	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Z	16	
Unit cell dimensions	a = 16.0921(6) Å	α =94.8507(9) deg.
	b = 21.2352(7) Å	β =94.9313(10) deg.
	c = 26.5244(9) Å	γ =92.6591(9) deg.
Volume	8984.8(5) $Å^3$	
Density (calculated)	1.42 g/cm^3	
Absorption coefficient	0.43 mm^{-1}	
Crystal shape	plank	
Crystal size	0.125 x 0.053 x 0.048 mm^3	
Crystal colour	orange	
Theta range for data collection	0.8 to 25.5 deg.	
Index ranges	-19≤h≤19, -25≤k≤25, 0≤l≤32	
Reflections collected	49879	
Independent reflections	49879 (R(int) = ?)	
Observed reflections	16344 (I > 2σ(I))	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.95 and 0.83
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	49879 / 5944 / 2610
Goodness-of-fit on F^2	1.02
Final R indices (I>2sigma(I))	R1 = 0.086, wR2 = 0.200
Largest diff. peak and hole	0.69 and -0.54 eÅ^{-3}

Table S23: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **5e**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
N111	0.8829(3)	0.4230(2)	0.9688(2)	0.0320(14)
C121	0.9278(4)	0.4529(3)	0.9365(2)	0.0281(16)
N131	0.9574(4)	0.4157(2)	0.8994(2)	0.0359(15)
C141	1.0046(4)	0.4422(3)	0.8664(3)	0.0332(17)
C151	1.0366(4)	0.4038(3)	0.8270(3)	0.0423(19)
H151	1.0262	0.3592	0.8248	0.051
C161	1.0814(4)	0.4297(3)	0.7927(3)	0.046(2)
H161	1.1012	0.4030	0.7662	0.055
C171	1.0995(5)	0.4952(4)	0.7952(3)	0.0427(19)
C181	1.0683(4)	0.5343(3)	0.8308(3)	0.0385(18)
H181	1.0791	0.5788	0.8312	0.046
C191	1.0197(4)	0.5100(3)	0.8674(2)	0.0292(16)
C201	0.9887(4)	0.5470(3)	0.9060(2)	0.0287(16)
H201	1.0002	0.5915	0.9088	0.034
C211	0.9408(4)	0.5206(3)	0.9409(3)	0.0296(16)
C221	0.9070(4)	0.5533(3)	0.9806(2)	0.0263(16)
H221	0.9159	0.5981	0.9850	0.032
C231	0.8613(4)	0.5243(3)	1.0139(2)	0.0283(16)
C241	0.8211(4)	0.5589(3)	1.0551(2)	0.0332(17)
C251	0.8296(5)	0.6246(3)	1.0631(3)	0.041(2)
H251	0.8658	0.6472	1.0437	0.049
C261	0.7866(5)	0.6576(3)	1.0987(3)	0.050(2)
H261	0.7929	0.7025	1.1037	0.060
C271	0.7339(5)	0.6242(3)	1.1272(3)	0.051(2)
H271	0.7034	0.6462	1.1515	0.061
C281	0.7262(5)	0.5600(3)	1.1203(3)	0.048(2)
H281	0.6897	0.5378	1.1398	0.057
C291	0.7705(4)	0.5255(3)	1.0850(3)	0.0342(17)
C301	0.7632(4)	0.4551(3)	1.0787(3)	0.0349(17)
C311	0.7182(4)	0.4202(3)	1.1111(3)	0.045(2)
H311	0.6918	0.4419	1.1376	0.054
C321	0.7117(5)	0.3554(3)	1.1050(3)	0.050(2)
H321	0.6797	0.3327	1.1267	0.060
C331	0.7518(5)	0.3224(3)	1.0672(3)	0.057(2)
H331	0.7483	0.2774	1.0634	0.068
C341	0.7966(4)	0.3559(3)	1.0352(3)	0.046(2)
H341	0.8234	0.3338	1.0090	0.056
C351	0.8029(4)	0.4223(3)	1.0411(3)	0.0375(18)
C361	0.8513(4)	0.4563(3)	1.0064(2)	0.0287(16)
O371	1.1494(3)	0.5136(3)	0.7592(2)	0.0519(15)
C371	1.1736(5)	0.5786(3)	0.7600(3)	0.053(2)
H37A1	1.2088	0.5849	0.7323	0.080
H37B1	1.2050	0.5927	0.7926	0.080
H37C1	1.1237	0.6030	0.7556	0.080
N112	0.8537(3)	0.5844(2)	0.8011(2)	0.0311(14)
C122	0.8077(4)	0.5541(3)	0.8338(2)	0.0298(16)
N132	0.7790(4)	0.5918(2)	0.8711(2)	0.0347(15)
C142	0.7331(4)	0.5637(3)	0.9043(2)	0.0301(16)
C152	0.7024(4)	0.6025(3)	0.9441(3)	0.0367(18)
H152	0.7133	0.6470	0.9466	0.044
C162	0.6580(4)	0.5759(3)	0.9782(3)	0.0376(18)
H162	0.6395	0.6022	1.0053	0.045
C172	0.6379(5)	0.5096(3)	0.9750(3)	0.0358(18)
C182	0.6672(4)	0.4716(3)	0.9380(2)	0.0310(17)
H182	0.6554	0.4272	0.9365	0.037
C192	0.7151(4)	0.4967(3)	0.9013(2)	0.0282(16)
C202	0.7462(4)	0.4597(3)	0.8627(2)	0.0304(17)
H202	0.7358	0.4151	0.8599	0.037
C212	0.7927(4)	0.4874(3)	0.8280(2)	0.0250(15)
C222	0.8263(4)	0.4536(3)	0.7872(2)	0.0292(16)
H222	0.8170	0.4089	0.7825	0.035
C232	0.8715(4)	0.4830(3)	0.7545(2)	0.0311(16)
C242	0.9083(4)	0.4494(3)	0.7119(2)	0.0333(17)
C252	0.8988(5)	0.3831(3)	0.7026(3)	0.0424(19)
H252	0.8656	0.3599	0.7233	0.051
C262	0.9357(5)	0.3516(4)	0.6650(3)	0.051(2)
H262	0.9274	0.3069	0.6593	0.061
C272	0.9860(5)	0.3841(3)	0.6344(3)	0.051(2)
H272	1.0130	0.3619	0.6084	0.062

C282	0.9959(5)	0.4490(3)	0.6426(3)	0.048(2)
H282	1.0299	0.4713	0.6217	0.057
C292	0.9574(4)	0.4832(3)	0.6807(2)	0.0373(18)
C302	0.9658(4)	0.5525(3)	0.6876(3)	0.0392(18)
C312	1.0065(5)	0.5876(3)	0.6538(3)	0.048(2)
H312	1.0276	0.5664	0.6250	0.057
C322	1.0164(5)	0.6523(4)	0.6618(3)	0.057(2)
H322	1.0471	0.6750	0.6395	0.069
C332	0.9824(5)	0.6854(4)	0.7019(3)	0.060(2)
H332	0.9880	0.7303	0.7066	0.072
C342	0.9402(5)	0.6511(3)	0.7350(3)	0.050(2)
H342	0.9174	0.6728	0.7629	0.061
C352	0.9308(4)	0.5858(3)	0.7278(3)	0.0386(18)
C362	0.8835(4)	0.5508(3)	0.7628(2)	0.0307(16)
O372	0.5913(3)	0.4900(2)	1.0118(2)	0.0401(13)
C372	0.5646(5)	0.4247(3)	1.0067(3)	0.044(2)
H37A2	0.5272	0.4164	1.0329	0.066
H37B2	0.6133	0.3990	1.0106	0.066
H37C2	0.5348	0.4138	0.9730	0.066
N113	0.6494(3)	0.4218(2)	0.7016(2)	0.0291(14)
C123	0.6944(4)	0.4519(3)	0.6692(2)	0.0240(15)
N133	0.7225(4)	0.4136(2)	0.6318(2)	0.0322(14)
C143	0.7679(4)	0.4398(3)	0.5974(2)	0.0308(17)
C153	0.7976(4)	0.4014(3)	0.5576(2)	0.0332(17)
H153	0.7862	0.3569	0.5554	0.040
C163	0.8419(4)	0.4266(3)	0.5224(3)	0.0365(18)
H163	0.8595	0.3998	0.4953	0.044
C173	0.8627(5)	0.4927(3)	0.5255(3)	0.0339(18)
C183	0.8340(4)	0.5313(3)	0.5622(2)	0.0316(17)
H183	0.8462	0.5756	0.5633	0.038
C193	0.7858(4)	0.5070(3)	0.5994(2)	0.0281(16)
C203	0.7559(4)	0.5454(3)	0.6379(2)	0.0299(17)
H203	0.7672	0.5899	0.6401	0.036
C213	0.7097(4)	0.5188(3)	0.6729(2)	0.0270(16)
C223	0.6754(4)	0.5526(3)	0.7131(2)	0.0253(15)
H223	0.6839	0.5974	0.7170	0.030
C233	0.6306(4)	0.5242(3)	0.7467(2)	0.0277(16)
C243	0.5929(4)	0.5584(3)	0.7885(2)	0.0320(17)
C253	0.6004(4)	0.6247(3)	0.7965(3)	0.0386(18)
H253	0.6326	0.6476	0.7751	0.046
C263	0.5628(5)	0.6570(3)	0.8342(3)	0.049(2)
H263	0.5709	0.7018	0.8395	0.058
C273	0.5129(5)	0.6248(3)	0.8647(3)	0.050(2)
H273	0.4845	0.6472	0.8899	0.060
C283	0.5050(5)	0.5600(3)	0.8579(3)	0.045(2)
H283	0.4719	0.5380	0.8794	0.054
C293	0.5442(4)	0.5252(3)	0.8205(2)	0.0335(17)
C303	0.5385(4)	0.4560(3)	0.8154(2)	0.0348(17)
C313	0.4985(4)	0.4212(3)	0.8502(3)	0.043(2)
H313	0.4752	0.4431	0.8779	0.052
C323	0.4926(5)	0.3564(3)	0.8449(3)	0.054(2)
H323	0.4632	0.3338	0.8679	0.065
C333	0.5296(5)	0.3237(4)	0.8058(3)	0.058(2)
H333	0.5267	0.2787	0.8027	0.069
C343	0.5703(5)	0.3562(3)	0.7715(3)	0.045(2)
H343	0.5952	0.3336	0.7448	0.054
C353	0.5749(4)	0.4221(3)	0.7761(2)	0.0355(17)
C363	0.6198(4)	0.4562(3)	0.7399(2)	0.0276(16)
O373	0.9085(3)	0.5112(2)	0.4879(2)	0.0385(12)
C373	0.9359(5)	0.5761(3)	0.4922(3)	0.0409(19)
H37A3	0.9738	0.5835	0.4660	0.061
H37B3	0.9652	0.5875	0.5259	0.061
H37C3	0.8875	0.6021	0.4876	0.061
N114	0.6193(3)	0.5794(2)	0.5279(2)	0.0328(15)
C124	0.5752(4)	0.5503(3)	0.5612(2)	0.0263(16)
N134	0.5463(4)	0.5885(2)	0.5977(2)	0.0374(15)
C144	0.5001(4)	0.5627(3)	0.6319(3)	0.0338(17)
C154	0.4681(4)	0.6027(3)	0.6709(3)	0.0386(18)
H154	0.4782	0.6473	0.6722	0.046
C164	0.4237(5)	0.5775(3)	0.7055(3)	0.045(2)
H164	0.4040	0.6049	0.7315	0.054
C174	0.4052(4)	0.5120(3)	0.7047(3)	0.0387(18)
C184	0.4376(4)	0.4724(3)	0.6699(3)	0.0356(18)
H184	0.4285	0.4280	0.6710	0.043
C194	0.4846(4)	0.4951(3)	0.6320(2)	0.0304(17)
C204	0.5156(4)	0.4569(3)	0.5941(2)	0.0317(17)
H204	0.5051	0.4123	0.5925	0.038
C214	0.5624(4)	0.4829(3)	0.5583(3)	0.0303(16)
C224	0.5961(4)	0.4485(3)	0.5191(2)	0.0279(16)
H224	0.5880	0.4037	0.5161	0.034
C234	0.6408(4)	0.4766(3)	0.4845(2)	0.0281(16)
C244	0.6805(4)	0.4408(3)	0.4442(2)	0.0340(17)
C254	0.6728(5)	0.3752(3)	0.4373(3)	0.040(2)
H254	0.6382	0.3529	0.4580	0.049
C264	0.7139(5)	0.3416(3)	0.4014(3)	0.050(2)
H264	0.7071	0.2967	0.3969	0.060
C274	0.7656(5)	0.3739(3)	0.3716(3)	0.048(2)

H274	0.7960	0.3511	0.3477	0.057
C284	0.7725(5)	0.4384(3)	0.3770(3)	0.047(2)
H284	0.8070	0.4599	0.3560	0.056
C294	0.7300(4)	0.4738(3)	0.4126(3)	0.0330(17)
C304	0.7372(4)	0.5440(3)	0.4178(2)	0.0338(17)
C314	0.7820(4)	0.5783(3)	0.3849(3)	0.0423(19)
H314	0.8088	0.5559	0.3589	0.051
C324	0.7881(5)	0.6432(3)	0.3893(3)	0.048(2)
H324	0.8204	0.6654	0.3674	0.058
C334	0.7465(5)	0.6762(3)	0.4262(3)	0.051(2)
H334	0.7484	0.7211	0.4286	0.061
C344	0.7025(5)	0.6442(3)	0.4591(3)	0.048(2)
H344	0.6755	0.6673	0.4847	0.057
C354	0.6970(4)	0.5778(3)	0.4552(3)	0.0350(18)
C364	0.6502(4)	0.5448(3)	0.4910(2)	0.0309(16)
O374	0.3564(3)	0.4952(2)	0.7412(2)	0.0507(15)
C374	0.3336(5)	0.4299(3)	0.7425(3)	0.047(2)
H37A4	0.2947	0.4249	0.7685	0.071
H37B4	0.3836	0.4068	0.7505	0.071
H37C4	0.3066	0.4130	0.7092	0.071
N115	0.3776(4)	0.0768(2)	0.9483(2)	0.0323(15)
C125	0.4498(4)	0.0468(3)	0.9434(3)	0.0297(17)
N135	0.5199(4)	0.0857(2)	0.9452(2)	0.0317(15)
C145	0.5919(4)	0.0580(3)	0.9400(2)	0.0276(16)
C155	0.6655(4)	0.0992(3)	0.9412(3)	0.042(2)
H155	0.6621	0.1437	0.9469	0.050
C165	0.7400(4)	0.0739(3)	0.9340(3)	0.041(2)
H165	0.7882	0.1016	0.9342	0.049
C175	0.7486(4)	0.0081(3)	0.9264(3)	0.0353(18)
C185	0.6807(4)	-0.0331(3)	0.9245(3)	0.0331(18)
H185	0.6862	-0.0774	0.9189	0.040
C195	0.6006(4)	-0.0079(3)	0.9312(3)	0.0292(17)
C205	0.5287(4)	-0.0474(3)	0.9300(2)	0.0305(17)
H205	0.5319	-0.0920	0.9257	0.037
C215	0.4507(4)	-0.0202(3)	0.9351(3)	0.0288(17)
C225	0.3749(4)	-0.0568(3)	0.9339(2)	0.0318(17)
H225	0.3744	-0.1016	0.9289	0.038
C235	0.3019(4)	-0.0271(3)	0.9401(3)	0.0326(17)
C245	0.2211(4)	-0.0620(3)	0.9405(3)	0.0326(18)
C255	0.2130(5)	-0.1275(3)	0.9328(3)	0.044(2)
H255	0.2608	-0.1504	0.9262	0.053
C265	0.1376(5)	-0.1600(3)	0.9346(3)	0.049(2)
H265	0.1337	-0.2049	0.9298	0.059
C275	0.0675(5)	-0.1269(4)	0.9436(3)	0.050(2)
H275	0.0153	-0.1490	0.9454	0.061
C285	0.0737(5)	-0.0632(3)	0.9496(3)	0.043(2)
H285	0.0249	-0.0411	0.9554	0.052
C295	0.1486(4)	-0.0282(3)	0.9478(3)	0.0357(18)
C305	0.1533(4)	0.0413(3)	0.9524(3)	0.0314(17)
C315	0.0825(5)	0.0769(3)	0.9579(3)	0.048(2)
H315	0.0297	0.0556	0.9597	0.057
C325	0.0881(5)	0.1413(4)	0.9607(3)	0.057(2)
H325	0.0390	0.1641	0.9630	0.069
C335	0.1631(5)	0.1733(3)	0.9604(3)	0.057(2)
H335	0.1667	0.2183	0.9636	0.069
C345	0.2335(5)	0.1403(3)	0.9553(3)	0.045(2)
H345	0.2856	0.1628	0.9540	0.054
C355	0.2304(4)	0.0746(3)	0.9519(3)	0.0323(17)
C365	0.3075(4)	0.0411(3)	0.9471(3)	0.0287(16)
O375	0.8272(3)	-0.0086(2)	0.9192(2)	0.0487(15)
C375	0.8388(5)	-0.0751(3)	0.9084(3)	0.050(2)
H37A5	0.8969	-0.0811	0.9015	0.075
H37B5	0.8015	-0.0917	0.8787	0.075
H37C5	0.8261	-0.0977	0.9378	0.075
N116	0.4031(3)	-0.0794(2)	0.8013(2)	0.0338(14)
C126	0.3308(4)	-0.0494(3)	0.8071(2)	0.0336(17)
N136	0.2613(3)	-0.0886(2)	0.8038(2)	0.0353(14)
C146	0.1884(4)	-0.0613(3)	0.8086(2)	0.0341(17)
C156	0.1131(4)	-0.1012(3)	0.8061(3)	0.045(2)
H156	0.1158	-0.1458	0.8007	0.054
C166	0.0386(5)	-0.0757(3)	0.8116(3)	0.048(2)
H166	-0.0105	-0.1029	0.8091	0.058
C176	0.0316(4)	-0.0100(3)	0.8209(3)	0.0410(18)
C186	0.1013(4)	0.0305(3)	0.8248(3)	0.0382(18)
H186	0.0964	0.0748	0.8315	0.046
C196	0.1812(4)	0.0056(3)	0.8189(2)	0.0346(17)
C206	0.2545(4)	0.0442(3)	0.8223(2)	0.0331(17)
H206	0.2525	0.0888	0.8282	0.040
C216	0.3303(4)	0.0168(3)	0.8169(2)	0.0288(16)
C226	0.4072(4)	0.0532(3)	0.8190(2)	0.0331(17)
H226	0.4084	0.0980	0.8251	0.040
C236	0.4804(4)	0.0229(3)	0.8120(3)	0.0353(17)
C246	0.5617(4)	0.0583(3)	0.8114(2)	0.0341(17)
C256	0.5679(4)	0.1243(3)	0.8194(3)	0.044(2)
H256	0.5200	0.1466	0.8271	0.052
C266	0.6423(4)	0.1572(3)	0.8164(3)	0.049(2)
H266	0.6460	0.2020	0.8224	0.059

C276	0.7122(4)	0.1252(3)	0.8047(3)	0.054(2)
H276	0.7634	0.1481	0.8016	0.065
C286	0.7070(4)	0.0610(3)	0.7976(3)	0.0468(19)
H286	0.7556	0.0396	0.7902	0.056
C296	0.6325(4)	0.0247(3)	0.8009(3)	0.0398(18)
C306	0.6270(4)	-0.0441(3)	0.7943(2)	0.0365(17)
C316	0.6978(4)	-0.0794(3)	0.7859(2)	0.0476(19)
H316	0.7503	-0.0576	0.7844	0.057
C326	0.6924(5)	-0.1436(3)	0.7800(3)	0.058(2)
H326	0.7410	-0.1661	0.7747	0.070
C336	0.6173(5)	-0.1761(3)	0.7816(3)	0.056(2)
H336	0.6141	-0.2210	0.7769	0.068
C346	0.5462(5)	-0.1442(3)	0.7900(3)	0.045(2)
H346	0.4946	-0.1670	0.7920	0.054
C356	0.5510(4)	-0.0783(3)	0.7955(2)	0.0321(17)
C366	0.4745(4)	-0.0447(3)	0.8030(2)	0.0317(16)
O376	-0.0478(3)	0.0070(2)	0.8265(2)	0.0545(15)
C376	-0.0588(4)	0.0731(3)	0.8377(3)	0.053(2)
H37A6	-0.1169	0.0793	0.8445	0.079
H37B6	-0.0453	0.0960	0.8087	0.079
H37C6	-0.0216	0.0891	0.8677	0.079
N117	0.1630(3)	0.0847(2)	0.7024(2)	0.0353(15)
C127	0.2346(4)	0.0542(3)	0.6967(2)	0.0321(17)
N137	0.3048(3)	0.0917(2)	0.7007(2)	0.0321(14)
C147	0.3769(4)	0.0639(3)	0.6943(2)	0.0319(16)
C157	0.4524(4)	0.1029(3)	0.6970(3)	0.0382(18)
H157	0.4506	0.1476	0.7030	0.046
C167	0.5265(4)	0.0768(3)	0.6911(2)	0.0400(18)
H167	0.5762	0.1033	0.6944	0.048
C177	0.5315(4)	0.0105(3)	0.6800(3)	0.0315(17)
C187	0.4615(4)	-0.0288(3)	0.6764(2)	0.0357(17)
H187	0.4650	-0.0732	0.6694	0.043
C197	0.3826(4)	-0.0026(3)	0.6833(2)	0.0297(16)
C207	0.3096(4)	-0.0408(3)	0.6799(2)	0.0341(17)
H207	0.3111	-0.0854	0.6734	0.041
C217	0.2335(4)	-0.0126(3)	0.6862(2)	0.0305(16)
C227	0.1569(4)	-0.0475(3)	0.6826(2)	0.0341(17)
H227	0.1551	-0.0923	0.6763	0.041
C237	0.0841(4)	-0.0169(3)	0.6883(2)	0.0307(16)
C247	0.0016(4)	-0.0514(3)	0.6850(3)	0.0356(17)
C257	-0.0070(4)	-0.1165(3)	0.6744(3)	0.046(2)
H257	0.0410	-0.1395	0.6684	0.055
C267	-0.0843(5)	-0.1489(3)	0.6722(3)	0.058(2)
H267	-0.0891	-0.1935	0.6646	0.069
C277	-0.1542(5)	-0.1159(3)	0.6812(3)	0.055(2)
H277	-0.2069	-0.1380	0.6812	0.066
C287	-0.1476(5)	-0.0515(3)	0.6902(3)	0.051(2)
H287	-0.1964	-0.0294	0.6958	0.061
C297	-0.0703(4)	-0.0169(3)	0.6914(2)	0.0387(17)
C307	-0.0642(4)	0.0521(3)	0.6997(3)	0.0393(18)
C317	-0.1339(4)	0.0889(3)	0.7035(3)	0.050(2)
H317	-0.1878	0.0681	0.7004	0.060
C327	-0.1279(5)	0.1527(4)	0.7115(3)	0.062(3)
H327	-0.1767	0.1759	0.7141	0.074
C337	-0.0500(5)	0.1839(3)	0.7159(3)	0.062(2)
H337	-0.0448	0.2287	0.7219	0.075
C347	0.0193(4)	0.1504(3)	0.7115(3)	0.052(2)
H347	0.0724	0.1724	0.7140	0.062
C357	0.0143(4)	0.0845(3)	0.7035(2)	0.0375(17)
C367	0.0917(4)	0.0501(3)	0.6984(3)	0.0346(17)
O377	0.6098(3)	-0.0082(2)	0.6738(2)	0.0469(13)
C377	0.6160(4)	-0.0742(3)	0.6583(3)	0.048(2)
H37A7	0.6743	-0.0825	0.6532	0.073
H37B7	0.5810	-0.0854	0.6265	0.073
H37C7	0.5971	-0.0997	0.6847	0.073
N118	0.1200(3)	-0.0803(2)	0.5515(2)	0.0286(14)
C128	0.0471(4)	-0.0503(3)	0.5558(3)	0.0262(16)
N138	-0.0230(3)	-0.0882(2)	0.5502(2)	0.0312(15)
C148	-0.0948(4)	-0.0600(3)	0.5548(2)	0.0259(16)
C158	-0.1714(4)	-0.0999(3)	0.5487(3)	0.0339(18)
H158	-0.1694	-0.1444	0.5412	0.041
C168	-0.2456(4)	-0.0738(3)	0.5538(3)	0.0372(19)
H168	-0.2951	-0.1006	0.5496	0.045
C178	-0.2521(4)	-0.0083(3)	0.5650(3)	0.0323(17)
C188	-0.1822(4)	0.0312(3)	0.5715(3)	0.0319(18)
H188	-0.1865	0.0753	0.5795	0.038
C198	-0.1023(4)	0.0059(3)	0.5663(3)	0.0276(17)
C208	-0.0298(4)	0.0442(3)	0.5713(3)	0.0297(17)
H208	-0.0320	0.0887	0.5777	0.036
C218	0.0474(4)	0.0166(3)	0.5670(3)	0.0263(16)
C228	0.1245(4)	0.0522(3)	0.5712(3)	0.0320(18)
H228	0.1257	0.0969	0.5780	0.038
C238	0.1976(4)	0.0228(3)	0.5655(3)	0.0307(17)
C248	0.2785(4)	0.0572(3)	0.5663(3)	0.0320(17)
C258	0.2873(4)	0.1225(3)	0.5758(3)	0.0369(19)
H258	0.2401	0.1452	0.5840	0.044
C268	0.3620(4)	0.1551(3)	0.5735(3)	0.041(2)

H268	0.3659	0.1999	0.5799	0.049
C278	0.4320(5)	0.1232(3)	0.5618(3)	0.043(2)
H278	0.4835	0.1458	0.5591	0.052
C288	0.4256(4)	0.0591(3)	0.5542(3)	0.039(2)
H288	0.4737	0.0373	0.5463	0.047
C298	0.3507(4)	0.0236(3)	0.5576(3)	0.0339(18)
C308	0.3458(4)	-0.0458(3)	0.5515(3)	0.0307(17)
C318	0.4164(5)	-0.0813(3)	0.5469(3)	0.045(2)
H318	0.4695	-0.0597	0.5466	0.055
C328	0.4112(5)	-0.1453(4)	0.5429(3)	0.053(2)
H328	0.4604	-0.1681	0.5405	0.064
C338	0.3357(5)	-0.1773(3)	0.5422(3)	0.054(2)
H338	0.3325	-0.2223	0.5386	0.065
C348	0.2640(5)	-0.1452(3)	0.5467(3)	0.043(2)
H348	0.2118	-0.1679	0.5468	0.051
C358	0.2680(4)	-0.0795(3)	0.5512(3)	0.0296(17)
C368	0.1917(4)	-0.0449(3)	0.5558(2)	0.0280(16)
O378	-0.3307(3)	0.0107(2)	0.5687(2)	0.0406(14)
C378	-0.3384(5)	0.0764(3)	0.5840(3)	0.047(2)
H37A8	-0.3971	0.0842	0.5882	0.070
H37B8	-0.3186	0.1021	0.5580	0.070
H37C8	-0.3047	0.0879	0.6163	0.070
C41	0.3090(7)	-0.2189(6)	0.7469(5)	0.108(6)
H41	0.3110	-0.1761	0.7661	0.130
Cl1	0.3571(4)	-0.2704(2)	0.7849(2)	0.136(2)
Cl2	0.2061(5)	-0.2447(4)	0.7322(4)	0.283(7)
Cl3	0.3665(4)	-0.2140(2)	0.6948(2)	0.128(2)
C41B	0.2739(18)	-0.2143(15)	0.7559(10)	0.147(16)
H41B	0.2926	-0.1715	0.7728	0.176
Cl31	0.3532(12)	-0.2647(8)	0.7462(8)	0.239(12)
Cl32	0.2143(10)	-0.2138(5)	0.6985(5)	0.088(4)
Cl33	0.2145(15)	-0.2611(6)	0.7918(6)	0.227(10)
C42	1.0339(6)	-0.2220(6)	0.4980(4)	0.070(4)
H42	1.0320	-0.1779	0.5143	0.084
Cl4	0.9315(3)	-0.2501(3)	0.4788(3)	0.165(3)
Cl5	1.0801(4)	-0.2679(2)	0.5429(2)	0.102(2)
Cl6	1.0944(3)	-0.2190(2)	0.4476(1)	0.1063(18)
C42B	1.0056(17)	-0.2260(18)	0.5102(12)	0.120(16)
H42B	1.0225	-0.1827	0.5267	0.143
Cl34	0.9590(14)	-0.2223(6)	0.4489(7)	0.151(9)
Cl35	1.0872(14)	-0.2745(11)	0.5140(11)	0.219(13)
Cl36	0.9264(11)	-0.2606(6)	0.5401(7)	0.137(7)
C43	0.8544(11)	0.2848(12)	0.8964(6)	0.116(9)
H43	0.8774	0.3293	0.9058	0.139
Cl7	0.8678(11)	0.2637(6)	0.8341(4)	0.287(10)
Cl8	0.9019(8)	0.2361(5)	0.9360(5)	0.257(7)
Cl9	0.7500(4)	0.2806(3)	0.9039(3)	0.133(3)
C43B	0.8857(16)	0.2756(14)	0.8926(9)	0.117(10)
H43B	0.9071	0.3185	0.9080	0.140
Cl37	0.8091(9)	0.2849(4)	0.8444(8)	0.267(11)
Cl38	0.8659(8)	0.2301(4)	0.9400(4)	0.150(5)
Cl39	0.9646(8)	0.2406(4)	0.8623(4)	0.156(5)
C44	0.4640(7)	0.2213(6)	0.9969(5)	0.076(5)
H44	0.4647	0.1771	0.9808	0.091
Cl10	0.5668(4)	0.2519(3)	1.0098(4)	0.172(4)
Cl11	0.4104(6)	0.2642(4)	0.9567(4)	0.193(4)
Cl12	0.4108(4)	0.2200(2)	1.0488(2)	0.119(2)
C44B	0.4918(14)	0.2302(17)	0.9775(10)	0.104(13)
H44B	0.4816	0.1852	0.9629	0.125
Cl40	0.5320(11)	0.2261(5)	1.0405(5)	0.144(6)
Cl41	0.4096(8)	0.2698(5)	0.9524(3)	0.051(3)
Cl42	0.5779(7)	0.2589(4)	0.9500(5)	0.103(4)
C45	0.2723(6)	0.2309(5)	0.7438(3)	0.058(3)
H45	0.2512	0.1884	0.7273	0.069
Cl13	0.3219(3)	0.2201(2)	0.8040(2)	0.0819(14)
Cl14	0.3443(3)	0.2621(2)	0.7060(2)	0.1139(17)
Cl15	0.1873(3)	0.2783(2)	0.7478(2)	0.108(2)
C45B	0.2452(14)	0.2187(13)	0.7631(10)	0.050(9)
H45B	0.2461	0.1763	0.7437	0.060
Cl43	0.3467(10)	0.2461(9)	0.7780(9)	0.211(10)
Cl44	0.1759(8)	0.2121(5)	0.8070(4)	0.104(5)
Cl45	0.2109(13)	0.2705(8)	0.7210(7)	0.156(7)
C46	0.6263(8)	0.2818(6)	0.6331(4)	0.088(5)
H46	0.6515	0.3259	0.6407	0.105
Cl16	0.5194(3)	0.2791(2)	0.6378(2)	0.113(2)
Cl17	0.6607(7)	0.2344(4)	0.6769(4)	0.229(5)
Cl18	0.6436(6)	0.2514(3)	0.5731(2)	0.195(5)
C46B	0.653(2)	0.271(2)	0.6367(10)	0.100(14)
H46B	0.6706	0.3161	0.6491	0.120
Cl46	0.5722(13)	0.2773(7)	0.5890(9)	0.194(11)
Cl47	0.6636(6)	0.2304(5)	0.6899(5)	0.049(3)
Cl48	0.7351(10)	0.2430(5)	0.6056(5)	0.110(5)
C47	0.6604(9)	0.7192(8)	0.5983(4)	0.093(6)
H47	0.6351	0.6752	0.5901	0.112
Cl19	0.6421(6)	0.7462(3)	0.6608(2)	0.170(4)
Cl20	0.6156(6)	0.7682(4)	0.5565(4)	0.184(4)
Cl21	0.7663(3)	0.7187(2)	0.5941(2)	0.0970(19)

C47B	0.6247(18)	0.7272(15)	0.6017(9)	0.104(13)
H47B	0.6040	0.6830	0.5894	0.125
Cl49	0.5516(13)	0.7605(6)	0.6398(5)	0.137(7)
Cl50	0.6292(9)	0.7703(4)	0.5499(4)	0.055(4)
Cl51	0.7152(13)	0.7235(6)	0.6418(9)	0.188(11)
C48	0.8567(9)	0.7301(9)	0.8772(6)	0.075(7)
H48	0.8424	0.6879	0.8580	0.091
Cl22	0.9026(5)	0.7796(3)	0.8375(3)	0.109(3)
Cl23	0.9238(8)	0.7199(5)	0.9307(4)	0.098(4)
Cl24	0.7667(4)	0.7617(2)	0.8950(3)	0.107(2)
C48B	0.8983(15)	0.7152(10)	0.8734(8)	0.099(9)
H48B	0.8742	0.6711	0.8639	0.119
Cl52	0.8487(10)	0.7687(6)	0.8363(6)	0.245(8)
Cl53	0.8943(11)	0.7362(6)	0.9370(5)	0.173(7)
Cl54	1.0020(5)	0.7216(3)	0.8621(3)	0.143(4)

Table S24: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **5e**.

Atom	x	y	z	U_{eq}
H151	1.0262	0.3592	0.8248	0.051
H161	1.1012	0.4030	0.7662	0.055
H181	1.0791	0.5788	0.8312	0.046
H201	1.0002	0.5915	0.9088	0.034
H221	0.9159	0.5981	0.9850	0.032
H251	0.8658	0.6472	1.0437	0.049
H261	0.7929	0.7025	1.1037	0.060
H271	0.7034	0.6462	1.1515	0.061
H281	0.6897	0.5378	1.1398	0.057
H311	0.6918	0.4419	1.1376	0.054
H321	0.6797	0.3327	1.1267	0.060
H331	0.7483	0.2774	1.0634	0.068
H341	0.8234	0.3338	1.0090	0.056
H37A1	1.2088	0.5849	0.7323	0.080
H37B1	1.2050	0.5927	0.7926	0.080
H37C1	1.1237	0.6030	0.7556	0.080
H152	0.7133	0.6470	0.9466	0.044
H162	0.6395	0.6022	1.0053	0.045
H182	0.6554	0.4272	0.9365	0.037
H202	0.7358	0.4151	0.8599	0.037
H222	0.8170	0.4089	0.7825	0.035
H252	0.8656	0.3599	0.7233	0.051
H262	0.9274	0.3069	0.6593	0.061
H272	1.0130	0.3619	0.6084	0.062
H282	1.0299	0.4713	0.6217	0.057
H312	1.0276	0.5664	0.6250	0.057
H322	1.0471	0.6750	0.6395	0.069
H332	0.9880	0.7303	0.7066	0.072
H342	0.9174	0.6728	0.7629	0.061
H37A2	0.5272	0.4164	1.0329	0.066
H37B2	0.6133	0.3990	1.0106	0.066
H37C2	0.5348	0.4138	0.9730	0.066
H153	0.7862	0.3569	0.5554	0.040
H163	0.8595	0.3998	0.4953	0.044
H183	0.8462	0.5756	0.5633	0.038
H203	0.7672	0.5899	0.6401	0.036
H223	0.6839	0.5974	0.7170	0.030
H253	0.6326	0.6476	0.7751	0.046
H263	0.5709	0.7018	0.8395	0.058
H273	0.4845	0.6472	0.8899	0.060
H283	0.4719	0.5380	0.8794	0.054
H313	0.4752	0.4431	0.8779	0.052
H323	0.4632	0.3338	0.8679	0.065
H333	0.5267	0.2787	0.8027	0.069
H343	0.5952	0.3336	0.7448	0.054
H37A3	0.9738	0.5835	0.4660	0.061
H37B3	0.9652	0.5875	0.5259	0.061
H37C3	0.8875	0.6021	0.4876	0.061
H154	0.4782	0.6473	0.6722	0.046
H164	0.4040	0.6049	0.7315	0.054
H184	0.4285	0.4280	0.6710	0.043
H204	0.5051	0.4123	0.5925	0.038
H224	0.5880	0.4037	0.5161	0.034
H254	0.6382	0.3529	0.4580	0.049
H264	0.7071	0.2967	0.3969	0.060
H274	0.7960	0.3511	0.3477	0.057
H284	0.8070	0.4599	0.3560	0.056
H314	0.8088	0.5559	0.3589	0.051
H324	0.8204	0.6654	0.3674	0.058
H334	0.7484	0.7211	0.4286	0.061
H344	0.6755	0.6673	0.4847	0.057
H37A4	0.2947	0.4249	0.7685	0.071

H37B4	0.3836	0.4068	0.7505	0.071
H37C4	0.3066	0.4130	0.7092	0.071
H155	0.6621	0.1437	0.9469	0.050
H165	0.7882	0.1016	0.9342	0.049
H185	0.6862	-0.0774	0.9189	0.040
H205	0.5319	-0.0920	0.9257	0.037
H225	0.3744	-0.1016	0.9289	0.038
H255	0.2608	-0.1504	0.9262	0.053
H265	0.1337	-0.2049	0.9298	0.059
H275	0.0153	-0.1490	0.9454	0.061
H285	0.0249	-0.0411	0.9554	0.052
H315	0.0297	0.0556	0.9597	0.057
H325	0.0390	0.1641	0.9630	0.069
H335	0.1667	0.2183	0.9636	0.069
H345	0.2856	0.1628	0.9540	0.054
H37A5	0.8969	-0.0811	0.9015	0.075
H37B5	0.8015	-0.0917	0.8787	0.075
H37C5	0.8261	-0.0977	0.9378	0.075
H156	0.1158	-0.1458	0.8007	0.054
H166	-0.0105	-0.1029	0.8091	0.058
H186	0.0964	0.0748	0.8315	0.046
H206	0.2525	0.0888	0.8282	0.040
H226	0.4084	0.0980	0.8251	0.040
H256	0.5200	0.1466	0.8271	0.052
H266	0.6460	0.2020	0.8224	0.059
H276	0.7634	0.1481	0.8016	0.065
H286	0.7556	0.0396	0.7902	0.056
H316	0.7503	-0.0576	0.7844	0.057
H326	0.7410	-0.1661	0.7747	0.070
H336	0.6141	-0.2210	0.7769	0.068
H346	0.4946	-0.1670	0.7920	0.054
H37A6	-0.1169	0.0793	0.8445	0.079
H37B6	-0.0453	0.0960	0.8087	0.079
H37C6	-0.0216	0.0891	0.8677	0.079
H157	0.4506	0.1476	0.7030	0.046
H167	0.5762	0.1033	0.6944	0.048
H187	0.4650	-0.0732	0.6694	0.043
H207	0.3111	-0.0854	0.6734	0.041
H227	0.1551	-0.0923	0.6763	0.041
H257	0.0410	-0.1395	0.6684	0.055
H267	-0.0891	-0.1935	0.6646	0.069
H277	-0.2069	-0.1380	0.6812	0.066
H287	-0.1964	-0.0294	0.6958	0.061
H317	-0.1878	0.0681	0.7004	0.060
H327	-0.1767	0.1759	0.7141	0.074
H337	-0.0448	0.2287	0.7219	0.075
H347	0.0724	0.1724	0.7140	0.062
H37A7	0.6743	-0.0825	0.6532	0.073
H37B7	0.5810	-0.0854	0.6265	0.073
H37C7	0.5971	-0.0997	0.6847	0.073
H158	-0.1694	-0.1444	0.5412	0.041
H168	-0.2951	-0.1006	0.5496	0.045
H188	-0.1865	0.0753	0.5795	0.038
H208	-0.0320	0.0887	0.5777	0.036
H228	0.1257	0.0969	0.5780	0.038
H258	0.2401	0.1452	0.5840	0.044
H268	0.3659	0.1999	0.5799	0.049
H278	0.4835	0.1458	0.5591	0.052
H288	0.4737	0.0373	0.5463	0.047
H318	0.4695	-0.0597	0.5466	0.055
H328	0.4604	-0.1681	0.5405	0.064
H338	0.3325	-0.2223	0.5386	0.065
H348	0.2118	-0.1679	0.5468	0.051
H37A8	-0.3971	0.0842	0.5882	0.070
H37B8	-0.3186	0.1021	0.5580	0.070
H37C8	-0.3047	0.0879	0.6163	0.070
H41	0.3110	-0.1761	0.7661	0.130
H41B	0.2926	-0.1715	0.7728	0.176
H42	1.0320	-0.1779	0.5143	0.084
H42B	1.0225	-0.1827	0.5267	0.143
H43	0.8774	0.3293	0.9058	0.139
H43B	0.9071	0.3185	0.9080	0.140
H44	0.4647	0.1771	0.9808	0.091
H44B	0.4816	0.1852	0.9629	0.125
H45	0.2512	0.1884	0.7273	0.069
H45B	0.2461	0.1763	0.7437	0.060
H46	0.6515	0.3259	0.6407	0.105
H46B	0.6706	0.3161	0.6491	0.120
H47	0.6351	0.6752	0.5901	0.112
H47B	0.6040	0.6830	0.5894	0.125
H48	0.8424	0.6879	0.8580	0.091
H48B	0.8742	0.6711	0.8639	0.119

Table S25: Anisotropic displacement parameters (Å^2) for **5e**. 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	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N111	0.017(3)	0.036(3)	0.041(4)	0.005(3)	-0.006(3)	-0.004(3)
C121	0.017(4)	0.035(4)	0.030(4)	0.002(3)	-0.009(3)	0.000(3)
N131	0.034(4)	0.035(3)	0.038(4)	-0.001(3)	0.003(3)	-0.002(3)
C141	0.026(4)	0.033(4)	0.039(4)	0.004(3)	-0.001(3)	0.002(3)
C151	0.036(5)	0.044(4)	0.046(5)	-0.004(3)	0.003(4)	0.006(4)
C161	0.037(5)	0.058(5)	0.043(5)	-0.002(4)	0.011(4)	0.012(4)
C171	0.031(5)	0.066(5)	0.033(4)	0.008(4)	0.005(3)	0.007(4)
C181	0.027(5)	0.048(5)	0.040(5)	0.010(3)	-0.004(3)	0.004(4)
C191	0.015(4)	0.035(4)	0.035(4)	0.000(3)	-0.007(3)	0.001(3)
C201	0.022(4)	0.032(4)	0.032(4)	0.005(3)	-0.005(3)	0.004(3)
C211	0.019(4)	0.032(4)	0.037(4)	0.002(3)	-0.004(3)	-0.001(3)
C221	0.018(4)	0.022(4)	0.037(4)	0.002(3)	-0.007(3)	0.000(3)
C231	0.024(4)	0.033(4)	0.027(4)	0.007(3)	-0.007(3)	0.000(3)
C241	0.039(5)	0.041(4)	0.018(4)	0.003(3)	-0.006(3)	0.004(3)
C251	0.041(5)	0.042(4)	0.040(5)	-0.002(4)	0.004(4)	0.000(4)
C261	0.062(6)	0.042(5)	0.046(5)	-0.005(4)	0.010(4)	0.007(4)
C271	0.053(6)	0.059(5)	0.038(5)	-0.009(4)	0.006(4)	0.004(4)
C281	0.044(5)	0.060(4)	0.038(5)	-0.005(4)	0.012(4)	-0.008(4)
C291	0.025(4)	0.048(4)	0.029(4)	0.008(3)	-0.007(3)	0.002(3)
C301	0.023(4)	0.045(4)	0.035(4)	0.006(3)	-0.006(3)	-0.004(3)
C311	0.039(5)	0.057(4)	0.039(5)	0.013(4)	0.000(4)	0.001(4)
C321	0.048(5)	0.057(5)	0.047(5)	0.021(4)	0.003(4)	-0.008(4)
C331	0.046(6)	0.049(5)	0.078(7)	0.019(4)	0.009(5)	-0.008(4)
C341	0.033(5)	0.034(4)	0.074(6)	0.008(4)	0.013(4)	-0.003(4)
C351	0.029(5)	0.042(4)	0.042(5)	0.014(3)	0.002(3)	-0.004(3)
C361	0.025(4)	0.028(4)	0.031(4)	0.005(3)	-0.007(3)	-0.004(3)
O371	0.047(4)	0.066(4)	0.044(3)	-0.001(3)	0.018(3)	0.000(3)
C371	0.051(6)	0.073(5)	0.035(5)	0.007(4)	0.006(4)	-0.010(4)
N112	0.030(4)	0.035(3)	0.027(3)	0.005(3)	-0.009(3)	0.001(3)
C122	0.026(4)	0.029(4)	0.032(4)	0.002(3)	-0.009(3)	-0.002(3)
N132	0.037(4)	0.036(3)	0.030(3)	0.004(3)	-0.002(3)	0.000(3)
C142	0.023(4)	0.036(4)	0.031(4)	0.003(3)	-0.001(3)	0.003(3)
C152	0.027(4)	0.042(4)	0.040(4)	-0.003(3)	-0.004(3)	0.010(3)
C162	0.034(5)	0.043(4)	0.033(4)	-0.007(3)	-0.003(3)	0.010(3)
C172	0.027(4)	0.049(4)	0.032(4)	0.003(3)	0.003(3)	0.008(3)
C182	0.024(4)	0.037(4)	0.031(4)	0.005(3)	-0.008(3)	0.001(3)
C192	0.026(4)	0.032(4)	0.024(4)	0.000(3)	-0.007(3)	0.002(3)
C202	0.027(4)	0.027(4)	0.038(4)	0.007(3)	0.002(3)	0.005(3)
C212	0.013(4)	0.030(4)	0.031(4)	-0.001(3)	-0.005(3)	0.001(3)
C222	0.032(4)	0.022(4)	0.032(4)	-0.002(3)	-0.003(3)	0.005(3)
C232	0.032(4)	0.030(4)	0.030(4)	0.005(3)	-0.004(3)	0.002(3)
C242	0.027(4)	0.044(4)	0.029(4)	0.006(3)	-0.003(3)	0.006(3)
C252	0.052(5)	0.045(4)	0.030(4)	0.002(3)	0.003(4)	0.004(4)
C262	0.061(6)	0.053(5)	0.040(5)	0.003(4)	0.006(4)	0.012(4)
C272	0.059(6)	0.065(5)	0.030(5)	-0.002(4)	0.009(4)	0.010(4)
C282	0.046(5)	0.065(5)	0.033(5)	0.009(4)	0.007(4)	0.001(4)
C292	0.037(5)	0.052(4)	0.022(4)	0.007(3)	-0.003(3)	0.000(3)
C302	0.031(5)	0.054(4)	0.030(4)	0.003(3)	-0.008(3)	-0.005(3)
C312	0.039(5)	0.061(5)	0.043(5)	0.012(4)	0.001(4)	0.001(4)
C322	0.055(6)	0.057(5)	0.063(6)	0.027(4)	0.005(4)	-0.002(4)
C332	0.051(6)	0.055(5)	0.077(6)	0.024(4)	0.007(4)	-0.003(4)
C342	0.058(6)	0.041(4)	0.054(5)	0.008(4)	0.011(4)	-0.002(4)
C352	0.035(5)	0.043(4)	0.037(4)	0.005(3)	0.000(3)	-0.003(3)
C362	0.020(4)	0.034(4)	0.036(4)	0.001(3)	-0.008(3)	-0.005(3)
O372	0.033(3)	0.052(3)	0.035(3)	0.001(2)	0.006(2)	0.001(2)
C372	0.041(5)	0.053(4)	0.040(5)	0.008(4)	0.011(4)	-0.001(4)
N113	0.031(4)	0.032(3)	0.024(3)	0.004(2)	-0.003(3)	0.002(3)
C123	0.018(4)	0.024(3)	0.028(4)	0.000(3)	-0.005(3)	0.001(3)
N133	0.035(4)	0.031(3)	0.031(3)	0.004(3)	0.001(3)	0.000(3)
C143	0.028(4)	0.029(4)	0.035(4)	0.000(3)	0.003(3)	0.000(3)
C153	0.031(4)	0.034(4)	0.033(4)	-0.005(3)	0.001(3)	0.004(3)
C163	0.034(5)	0.045(4)	0.031(4)	-0.004(3)	0.004(3)	0.007(3)
C173	0.035(5)	0.042(4)	0.026(4)	0.006(3)	0.002(3)	0.010(3)
C183	0.029(4)	0.033(4)	0.032(4)	0.004(3)	-0.003(3)	-0.003(3)
C193	0.027(4)	0.033(4)	0.020(4)	-0.002(3)	-0.011(3)	-0.003(3)
C203	0.031(4)	0.026(4)	0.034(4)	0.007(3)	0.006(3)	0.002(3)
C213	0.017(4)	0.031(4)	0.032(4)	0.001(3)	-0.001(3)	0.002(3)
C223	0.022(4)	0.020(4)	0.032(4)	-0.004(3)	0.000(3)	0.006(3)
C233	0.022(4)	0.033(4)	0.027(4)	0.002(3)	-0.002(3)	0.001(3)
C243	0.033(4)	0.037(4)	0.025(4)	0.002(3)	0.001(3)	-0.003(3)
C253	0.043(5)	0.043(4)	0.029(4)	0.000(3)	0.002(3)	0.002(3)
C263	0.064(6)	0.039(5)	0.042(5)	-0.003(4)	0.008(4)	0.006(4)
C273	0.056(6)	0.060(5)	0.035(5)	-0.004(4)	0.013(4)	0.008(4)
C283	0.047(5)	0.052(4)	0.036(5)	0.003(4)	0.008(4)	0.002(4)
C293	0.028(4)	0.048(4)	0.024(4)	0.008(3)	-0.003(3)	0.004(3)
C303	0.030(4)	0.045(4)	0.026(4)	0.001(3)	-0.006(3)	-0.009(3)
C313	0.034(5)	0.059(4)	0.035(5)	0.009(4)	0.000(4)	-0.008(4)
C323	0.054(6)	0.061(5)	0.049(5)	0.018(4)	0.007(4)	-0.013(4)
C333	0.059(6)	0.053(5)	0.065(6)	0.018(4)	0.018(5)	-0.010(4)

C343	0.055(5)	0.041(4)	0.039(5)	0.007(3)	0.012(4)	-0.012(4)
C353	0.032(5)	0.043(4)	0.030(4)	0.007(3)	-0.002(3)	-0.004(3)
C363	0.020(4)	0.032(4)	0.028(4)	-0.001(3)	-0.006(3)	-0.005(3)
O373	0.033(3)	0.049(3)	0.034(3)	0.003(2)	0.008(2)	0.000(2)
C373	0.044(5)	0.046(4)	0.035(5)	0.007(4)	0.016(4)	-0.003(4)
N114	0.021(3)	0.033(3)	0.044(4)	0.007(3)	-0.001(3)	0.001(3)
C124	0.018(4)	0.032(4)	0.025(4)	-0.002(3)	-0.013(3)	-0.002(3)
N134	0.038(4)	0.033(3)	0.040(4)	-0.004(3)	0.004(3)	-0.002(3)
C144	0.025(4)	0.037(4)	0.039(4)	-0.001(3)	0.000(3)	0.004(3)
C154	0.035(5)	0.039(4)	0.040(5)	-0.008(3)	0.001(3)	0.003(3)
C164	0.040(5)	0.051(4)	0.042(5)	-0.011(4)	0.007(4)	0.004(4)
C174	0.030(5)	0.052(4)	0.035(4)	0.005(3)	0.005(3)	0.005(4)
C184	0.031(5)	0.039(4)	0.034(4)	0.001(3)	-0.007(3)	0.003(3)
C194	0.024(4)	0.035(4)	0.029(4)	-0.002(3)	-0.009(3)	-0.004(3)
C204	0.032(4)	0.030(4)	0.032(4)	0.002(3)	-0.007(3)	0.006(3)
C214	0.023(4)	0.030(4)	0.035(4)	-0.001(3)	-0.007(3)	-0.001(3)
C224	0.029(4)	0.021(4)	0.032(4)	0.002(3)	-0.006(3)	0.002(3)
C234	0.025(4)	0.030(4)	0.027(4)	0.002(3)	-0.009(3)	0.000(3)
C244	0.040(5)	0.039(4)	0.021(4)	-0.001(3)	-0.005(3)	0.005(3)
C254	0.051(5)	0.036(4)	0.033(5)	-0.001(3)	0.001(4)	0.000(4)
C264	0.072(6)	0.040(5)	0.038(5)	-0.004(4)	0.010(4)	0.008(4)
C274	0.061(6)	0.050(4)	0.031(5)	-0.006(4)	0.005(4)	0.008(4)
C284	0.050(5)	0.050(4)	0.042(5)	0.001(4)	0.016(4)	-0.001(4)
C294	0.029(4)	0.044(4)	0.026(4)	0.004(3)	-0.003(3)	0.005(3)
C304	0.027(4)	0.044(4)	0.030(4)	0.004(3)	-0.004(3)	0.004(3)
C314	0.041(5)	0.057(4)	0.030(4)	0.013(4)	-0.001(3)	0.009(4)
C324	0.041(5)	0.054(4)	0.050(5)	0.018(4)	0.006(4)	-0.002(4)
C334	0.049(6)	0.044(5)	0.061(6)	0.013(4)	0.008(4)	-0.002(4)
C344	0.041(5)	0.037(4)	0.068(6)	0.011(4)	0.016(4)	0.000(4)
C354	0.028(4)	0.041(4)	0.036(4)	0.009(3)	-0.002(3)	0.000(3)
C364	0.027(4)	0.033(4)	0.032(4)	0.004(3)	-0.003(3)	0.000(3)
O374	0.042(4)	0.064(3)	0.047(4)	0.000(3)	0.014(3)	-0.002(3)
C374	0.052(5)	0.063(5)	0.027(4)	0.006(4)	0.008(4)	-0.009(4)
N115	0.038(4)	0.029(3)	0.030(4)	0.001(3)	0.008(3)	0.003(3)
C125	0.037(4)	0.029(4)	0.025(4)	0.010(3)	0.006(3)	0.002(3)
N135	0.045(4)	0.030(3)	0.021(3)	0.001(3)	0.012(3)	-0.005(3)
C145	0.036(4)	0.033(4)	0.013(4)	0.002(3)	0.003(3)	-0.002(3)
C155	0.048(4)	0.033(4)	0.044(5)	0.001(4)	0.013(4)	-0.006(3)
C165	0.045(5)	0.046(4)	0.033(5)	0.003(4)	0.017(4)	-0.012(3)
C175	0.040(4)	0.046(4)	0.021(4)	0.000(3)	0.011(4)	-0.003(3)
C185	0.037(4)	0.030(4)	0.033(5)	0.001(3)	0.013(4)	0.002(3)
C195	0.036(4)	0.034(4)	0.018(4)	0.001(3)	0.008(3)	0.000(3)
C205	0.040(4)	0.032(4)	0.020(4)	0.003(3)	0.002(3)	0.000(3)
C215	0.037(4)	0.026(3)	0.023(4)	0.003(3)	0.000(3)	0.003(3)
C225	0.037(4)	0.033(4)	0.024(4)	0.003(3)	0.001(3)	-0.005(3)
C235	0.040(4)	0.035(4)	0.022(4)	0.003(3)	0.004(4)	-0.003(3)
C245	0.037(4)	0.042(4)	0.019(4)	0.007(3)	0.008(3)	-0.005(3)
C255	0.041(5)	0.042(4)	0.047(5)	0.001(4)	0.005(4)	-0.006(4)
C265	0.046(5)	0.041(5)	0.060(6)	0.004(4)	0.002(4)	-0.009(4)
C275	0.049(5)	0.059(5)	0.043(5)	0.005(4)	0.008(4)	-0.010(4)
C285	0.037(5)	0.053(4)	0.040(5)	0.000(4)	0.003(4)	-0.001(4)
C295	0.043(4)	0.047(4)	0.014(4)	0.000(3)	-0.007(4)	0.001(3)
C305	0.037(4)	0.044(4)	0.015(4)	0.008(3)	0.004(3)	0.008(3)
C315	0.038(5)	0.064(5)	0.042(5)	0.005(4)	0.006(4)	0.011(4)
C325	0.055(5)	0.065(5)	0.056(6)	0.008(5)	0.014(5)	0.025(4)
C335	0.072(6)	0.033(5)	0.071(6)	0.003(4)	0.020(5)	0.014(4)
C345	0.055(5)	0.035(4)	0.049(5)	0.011(4)	0.015(4)	0.008(4)
C355	0.039(4)	0.038(4)	0.020(4)	0.003(3)	0.000(3)	0.008(3)
C365	0.036(4)	0.034(4)	0.018(4)	0.010(3)	0.008(3)	0.000(3)
O375	0.038(3)	0.053(3)	0.056(4)	0.004(3)	0.010(3)	0.001(3)
C375	0.041(5)	0.056(5)	0.053(6)	0.005(4)	0.009(4)	0.009(4)
N116	0.042(3)	0.033(3)	0.025(3)	-0.002(3)	0.001(3)	-0.001(3)
C126	0.048(4)	0.032(4)	0.023(4)	0.006(3)	0.012(4)	0.005(3)
N136	0.043(4)	0.032(3)	0.030(3)	0.000(3)	0.008(3)	-0.006(3)
C146	0.048(4)	0.037(4)	0.016(4)	0.005(3)	0.001(4)	-0.003(3)
C156	0.054(5)	0.039(4)	0.042(5)	-0.003(4)	0.007(4)	-0.008(3)
C166	0.045(5)	0.057(5)	0.042(5)	0.002(4)	0.007(4)	-0.006(4)
C176	0.041(4)	0.052(4)	0.030(4)	0.000(4)	0.002(4)	0.000(3)
C186	0.044(4)	0.044(4)	0.025(4)	-0.003(3)	0.000(4)	0.001(3)
C196	0.044(4)	0.041(4)	0.019(4)	0.011(3)	0.000(3)	0.000(3)
C206	0.045(4)	0.031(4)	0.023(4)	-0.003(3)	0.007(3)	0.004(3)
C216	0.041(4)	0.029(4)	0.016(4)	0.001(3)	0.002(3)	-0.002(3)
C226	0.043(4)	0.030(4)	0.025(4)	0.000(3)	-0.002(3)	-0.004(3)
C236	0.041(4)	0.037(4)	0.026(4)	0.002(3)	-0.005(4)	0.001(3)
C246	0.044(4)	0.036(4)	0.021(4)	0.004(3)	-0.001(3)	-0.002(3)
C256	0.046(5)	0.043(4)	0.040(5)	0.002(4)	-0.006(4)	0.000(4)
C266	0.052(5)	0.038(4)	0.054(5)	-0.002(4)	-0.009(4)	-0.003(3)
C276	0.042(5)	0.053(4)	0.066(6)	0.003(4)	0.000(4)	-0.011(4)
C286	0.038(4)	0.055(4)	0.045(5)	0.000(4)	0.000(4)	0.003(4)
C296	0.036(4)	0.048(4)	0.035(5)	0.005(4)	-0.007(4)	0.006(3)
C306	0.044(4)	0.044(4)	0.021(4)	0.008(3)	-0.005(3)	0.005(3)
C316	0.049(5)	0.060(4)	0.034(5)	0.009(4)	-0.001(4)	0.016(4)
C326	0.067(5)	0.061(5)	0.051(5)	0.010(4)	0.005(5)	0.028(4)
C336	0.078(6)	0.035(5)	0.062(6)	0.014(4)	0.017(5)	0.018(4)
C346	0.060(5)	0.037(4)	0.039(5)	0.007(4)	0.006(4)	0.009(4)
C356	0.045(4)	0.036(4)	0.018(4)	0.007(3)	0.008(3)	0.008(3)
C366	0.045(4)	0.037(4)	0.013(4)	0.003(3)	0.000(3)	0.002(3)

O376	0.043(3)	0.065(4)	0.056(4)	0.005(3)	0.008(3)	0.001(3)
C376	0.047(5)	0.066(5)	0.045(5)	0.003(4)	0.001(4)	0.000(4)
N117	0.046(4)	0.034(3)	0.026(3)	-0.004(3)	0.010(3)	0.003(3)
C127	0.040(4)	0.035(4)	0.021(4)	0.000(3)	0.001(3)	0.006(3)
N137	0.044(4)	0.036(3)	0.016(3)	-0.002(3)	0.005(3)	0.003(3)
C147	0.047(4)	0.036(4)	0.012(4)	-0.002(3)	0.002(3)	0.003(3)
C157	0.050(4)	0.028(4)	0.036(5)	0.002(3)	0.004(4)	-0.006(3)
C167	0.046(4)	0.045(4)	0.029(4)	0.004(3)	0.007(4)	-0.007(3)
C177	0.041(4)	0.038(4)	0.016(4)	0.002(3)	0.006(3)	0.001(3)
C187	0.039(4)	0.039(4)	0.030(4)	0.006(3)	0.003(4)	0.004(3)
C197	0.041(4)	0.029(4)	0.019(4)	0.005(3)	-0.003(3)	0.003(3)
C207	0.047(4)	0.028(4)	0.026(4)	-0.001(3)	-0.006(3)	0.000(3)
C217	0.037(4)	0.035(4)	0.019(4)	0.001(3)	-0.001(3)	0.007(3)
C227	0.043(4)	0.035(4)	0.023(4)	-0.003(3)	0.000(3)	0.007(3)
C237	0.034(4)	0.034(4)	0.024(4)	0.000(3)	0.001(3)	0.007(3)
C247	0.038(4)	0.040(4)	0.026(4)	0.006(3)	-0.010(4)	0.000(3)
C257	0.036(4)	0.042(4)	0.057(5)	0.005(4)	-0.014(4)	0.010(3)
C267	0.046(5)	0.046(5)	0.078(7)	0.009(4)	-0.010(5)	-0.008(4)
C277	0.047(5)	0.065(5)	0.051(5)	0.009(4)	-0.009(4)	-0.004(4)
C287	0.042(5)	0.066(5)	0.044(5)	0.013(4)	-0.004(4)	0.003(4)
C297	0.042(4)	0.053(4)	0.022(4)	0.006(3)	0.001(3)	0.006(3)
C307	0.048(4)	0.053(4)	0.018(4)	0.008(3)	0.004(4)	0.013(3)
C317	0.047(5)	0.064(5)	0.037(5)	0.001(4)	-0.010(4)	0.016(4)
C327	0.054(5)	0.064(5)	0.070(6)	0.012(5)	0.005(5)	0.031(4)
C337	0.068(5)	0.043(5)	0.078(6)	0.015(4)	0.006(5)	0.025(4)
C347	0.058(5)	0.043(4)	0.057(5)	0.006(4)	0.012(4)	0.017(4)
C357	0.041(4)	0.045(4)	0.028(4)	0.007(4)	0.000(4)	0.013(3)
C367	0.041(4)	0.039(4)	0.023(4)	0.004(3)	-0.005(3)	0.007(3)
O377	0.046(3)	0.052(3)	0.040(3)	-0.001(2)	0.003(3)	-0.004(3)
C377	0.046(5)	0.054(4)	0.043(5)	-0.006(4)	0.001(4)	0.009(4)
N118	0.035(3)	0.031(3)	0.020(3)	0.000(3)	0.005(3)	0.005(3)
C128	0.030(4)	0.025(4)	0.025(4)	0.009(3)	0.003(3)	0.000(3)
N138	0.037(3)	0.028(3)	0.029(4)	0.000(3)	0.009(3)	-0.005(3)
C148	0.034(4)	0.033(4)	0.011(4)	0.002(3)	0.002(3)	0.001(3)
C158	0.040(4)	0.034(4)	0.027(4)	-0.005(3)	0.008(4)	-0.007(3)
C168	0.039(4)	0.040(4)	0.032(4)	-0.002(3)	0.010(4)	-0.011(3)
C178	0.034(4)	0.042(4)	0.020(4)	-0.005(3)	0.011(3)	-0.006(3)
C188	0.036(4)	0.027(4)	0.034(5)	0.004(3)	0.011(4)	-0.003(3)
C198	0.032(4)	0.033(4)	0.019(4)	0.006(3)	0.008(3)	-0.003(3)
C208	0.036(4)	0.026(4)	0.026(4)	-0.002(3)	0.003(3)	-0.001(3)
C218	0.033(4)	0.026(3)	0.020(4)	0.004(3)	0.000(3)	0.003(3)
C228	0.034(4)	0.033(4)	0.028(4)	-0.002(3)	0.001(3)	-0.001(3)
C238	0.033(4)	0.037(4)	0.020(4)	-0.002(3)	-0.001(3)	0.001(3)
C248	0.038(4)	0.036(4)	0.022(4)	0.003(3)	0.003(4)	0.001(3)
C258	0.030(4)	0.040(4)	0.041(5)	0.006(4)	0.003(4)	0.003(3)
C268	0.035(4)	0.035(4)	0.049(5)	-0.001(4)	-0.008(4)	-0.004(3)
C278	0.028(4)	0.053(4)	0.047(5)	0.003(4)	0.001(4)	-0.009(4)
C288	0.028(4)	0.049(4)	0.037(5)	-0.005(4)	0.000(4)	-0.002(3)
C298	0.036(4)	0.044(4)	0.020(4)	0.000(3)	-0.004(4)	-0.004(3)
C308	0.030(4)	0.046(4)	0.016(4)	0.004(3)	-0.002(3)	0.010(3)
C318	0.037(5)	0.053(4)	0.046(5)	0.003(4)	0.000(4)	0.014(4)
C328	0.051(5)	0.058(5)	0.055(6)	0.010(5)	0.014(5)	0.019(4)
C338	0.060(5)	0.036(5)	0.071(6)	0.008(4)	0.014(5)	0.015(4)
C348	0.047(5)	0.036(4)	0.047(5)	0.009(4)	0.010(4)	0.008(3)
C358	0.033(4)	0.039(4)	0.016(4)	-0.003(3)	-0.001(3)	0.005(3)
C368	0.039(4)	0.031(4)	0.015(4)	0.005(3)	0.005(3)	0.000(3)
O378	0.033(3)	0.046(3)	0.042(3)	-0.002(3)	0.010(3)	0.001(2)
C378	0.043(5)	0.049(5)	0.050(5)	-0.002(4)	0.010(4)	0.005(4)
C41	0.087(11)	0.030(8)	0.196(16)	-0.061(9)	0.004(11)	0.017(7)
Cl1	0.245(7)	0.058(3)	0.116(4)	0.038(3)	0.054(4)	0.012(3)
Cl2	0.145(6)	0.177(9)	0.474(18)	-0.215(10)	-0.052(9)	0.036(6)
Cl3	0.250(6)	0.058(2)	0.066(3)	-0.0110(19)	-0.009(3)	-0.009(3)
C41B	0.18(3)	0.06(2)	0.20(3)	-0.02(2)	-0.03(3)	0.05(2)
Cl31	0.297(19)	0.119(14)	0.26(2)	-0.110(16)	-0.141(16)	0.103(13)
Cl32	0.149(11)	0.013(5)	0.098(8)	-0.004(5)	-0.017(7)	0.021(5)
Cl33	0.43(3)	0.036(7)	0.203(16)	0.049(9)	-0.064(17)	-0.049(11)
C42	0.053(8)	0.020(6)	0.131(12)	-0.017(7)	0.010(8)	-0.002(6)
Cl4	0.100(4)	0.096(4)	0.278(9)	-0.068(5)	-0.017(5)	-0.008(3)
Cl5	0.171(5)	0.046(3)	0.094(3)	0.029(3)	0.021(3)	-0.010(3)
Cl6	0.174(5)	0.072(3)	0.070(3)	-0.0167(19)	0.017(3)	0.006(3)
C42B	0.11(3)	0.06(2)	0.17(3)	-0.05(2)	-0.02(2)	0.00(3)
Cl34	0.22(2)	0.038(8)	0.166(15)	-0.024(8)	-0.046(13)	-0.057(9)
Cl35	0.156(16)	0.074(12)	0.40(3)	-0.098(19)	-0.038(18)	0.021(11)
Cl36	0.195(16)	0.035(7)	0.178(16)	0.003(9)	0.013(13)	-0.016(8)
C43	0.21(2)	0.052(14)	0.080(15)	-0.005(12)	0.010(16)	-0.018(16)
Cl7	0.49(2)	0.209(12)	0.140(8)	-0.106(7)	0.192(11)	-0.266(13)
Cl8	0.231(11)	0.189(9)	0.403(15)	0.180(10)	0.100(10)	0.150(9)
Cl9	0.139(6)	0.113(5)	0.129(6)	-0.019(4)	-0.024(4)	-0.062(4)
C43B	0.20(2)	0.031(16)	0.12(2)	-0.004(16)	0.025(18)	-0.020(16)
Cl37	0.259(15)	0.050(5)	0.44(2)	0.050(10)	-0.255(16)	-0.025(7)
Cl38	0.254(13)	0.038(4)	0.172(8)	-0.018(5)	0.148(8)	-0.038(6)
Cl39	0.258(12)	0.064(5)	0.162(9)	0.020(5)	0.082(8)	0.041(7)
C44	0.069(9)	0.032(7)	0.118(13)	0.007(8)	-0.024(10)	-0.021(7)
Cl10	0.092(4)	0.090(4)	0.313(12)	-0.065(6)	-0.009(5)	-0.019(3)
Cl11	0.151(7)	0.094(5)	0.347(10)	0.098(6)	0.022(7)	-0.003(5)
Cl12	0.199(6)	0.074(3)	0.077(3)	-0.026(2)	0.010(3)	0.008(3)
C44B	0.106(14)	0.099(14)	0.107(14)	0.007(6)	0.007(6)	0.006(6)

Cl40	0.206(17)	0.059(7)	0.150(11)	-0.022(7)	-0.015(10)	-0.065(8)
Cl41	0.103(8)	0.032(5)	0.021(4)	0.021(3)	0.016(4)	-0.011(5)
Cl42	0.119(8)	0.037(5)	0.160(11)	0.026(6)	0.031(8)	0.007(5)
C45	0.090(10)	0.055(8)	0.029(6)	0.015(6)	0.008(7)	0.002(7)
Cl13	0.117(4)	0.035(2)	0.090(3)	-0.0026(17)	-0.010(2)	0.012(2)
Cl14	0.157(4)	0.058(2)	0.135(4)	0.021(2)	0.045(3)	0.011(2)
Cl15	0.086(3)	0.062(3)	0.166(5)	-0.036(3)	-0.004(3)	0.019(2)
C45B	0.054(10)	0.042(10)	0.054(10)	0.003(6)	0.008(6)	0.002(6)
Cl43	0.120(13)	0.168(18)	0.31(3)	-0.133(17)	-0.011(13)	-0.013(10)
Cl44	0.169(12)	0.073(7)	0.064(7)	-0.020(5)	0.003(7)	0.008(7)
Cl45	0.230(12)	0.072(9)	0.169(11)	0.068(8)	-0.004(9)	-0.018(8)
C46	0.152(15)	0.035(8)	0.073(10)	-0.012(7)	0.032(10)	-0.044(9)
Cl16	0.090(3)	0.095(3)	0.140(5)	-0.028(3)	-0.008(3)	-0.031(3)
Cl17	0.357(12)	0.115(6)	0.227(9)	0.063(6)	0.014(8)	0.079(6)
Cl18	0.347(12)	0.106(4)	0.126(5)	-0.070(4)	0.137(6)	-0.126(6)
C46B	0.104(15)	0.094(15)	0.101(15)	0.010(6)	0.006(6)	0.002(6)
Cl46	0.188(17)	0.079(10)	0.29(2)	-0.061(13)	-0.081(18)	0.026(11)
Cl47	0.041(6)	0.025(5)	0.087(7)	0.012(5)	0.024(5)	0.023(4)
Cl48	0.149(12)	0.048(7)	0.128(11)	0.003(6)	0.014(9)	-0.024(7)
C47	0.134(15)	0.054(10)	0.083(11)	-0.018(9)	-0.020(10)	0.016(10)
Cl19	0.259(10)	0.120(5)	0.122(5)	-0.067(4)	0.099(6)	-0.097(6)
Cl20	0.200(8)	0.121(6)	0.249(9)	0.063(6)	0.042(7)	0.094(6)
Cl21	0.084(3)	0.070(3)	0.130(4)	0.001(3)	-0.011(3)	-0.017(2)
C47B	0.18(3)	0.018(18)	0.11(2)	0.018(18)	0.03(2)	-0.033(19)
Cl49	0.236(18)	0.067(7)	0.119(11)	0.010(7)	0.084(11)	0.007(10)
Cl50	0.100(8)	0.013(5)	0.054(6)	-0.011(4)	0.042(5)	-0.021(5)
Cl51	0.200(17)	0.078(8)	0.26(2)	-0.046(11)	-0.075(18)	0.024(10)
C48	0.114(17)	0.028(12)	0.079(14)	-0.019(10)	0.018(12)	-0.022(11)
Cl22	0.187(8)	0.051(3)	0.093(5)	-0.001(3)	0.055(5)	-0.023(4)
Cl23	0.137(6)	0.039(4)	0.111(8)	0.003(5)	-0.029(6)	-0.001(4)
Cl24	0.098(4)	0.057(3)	0.171(6)	0.032(3)	0.026(4)	0.004(3)
C48B	0.19(2)	0.018(12)	0.094(17)	0.015(11)	0.058(16)	-0.014(14)
Cl52	0.346(19)	0.107(10)	0.278(14)	0.052(9)	-0.079(14)	0.107(11)
Cl53	0.328(19)	0.092(10)	0.087(7)	-0.042(6)	0.074(9)	-0.113(10)
Cl54	0.141(7)	0.117(6)	0.152(7)	-0.041(5)	-0.007(5)	-0.057(5)

Table S26: Bond lengths (Å) and angles (deg) for **5e**.

N111-C361	1.326(7)	C351-C361	1.469(7)
N111-C121	1.348(7)	O371-C371	1.413(7)
C121-N131	1.342(7)	C371-H37A1	0.9800
C121-C211	1.436(7)	C371-H37B1	0.9800
N131-C141	1.349(7)	C371-H37C1	0.9800
C141-C151	1.417(8)	N112-C362	1.327(7)
C141-C191	1.446(7)	N112-C122	1.369(7)
C151-C161	1.345(8)	C122-N132	1.347(7)
C151-H151	0.9500	C122-C212	1.419(7)
C161-C171	1.402(8)	N132-C142	1.355(7)
C161-H161	0.9500	C142-C152	1.420(7)
C171-C181	1.350(8)	C142-C192	1.433(7)
C171-O371	1.371(7)	C152-C162	1.344(8)
C181-C191	1.414(8)	C152-H152	0.9500
C181-H181	0.9500	C162-C172	1.424(8)
C191-C201	1.381(7)	C162-H162	0.9500
C201-C211	1.391(7)	C172-C182	1.349(7)
C201-H201	0.9500	C172-O372	1.361(7)
C211-C221	1.377(7)	C182-C192	1.415(7)
C221-C231	1.364(7)	C182-H182	0.9500
C221-H221	0.9500	C192-C202	1.381(7)
C231-C361	1.440(7)	C202-C212	1.386(7)
C231-C241	1.476(7)	C202-H202	0.9500
C241-C251	1.393(8)	C212-C222	1.409(7)
C241-C291	1.395(8)	C222-C232	1.352(7)
C251-C261	1.381(8)	C222-H222	0.9500
C251-H251	0.9500	C232-C362	1.439(7)
C261-C271	1.392(8)	C232-C242	1.468(7)
C261-H261	0.9500	C242-C252	1.408(7)
C271-C281	1.358(8)	C242-C292	1.409(8)
C271-H271	0.9500	C252-C262	1.349(8)
C281-C291	1.403(8)	C252-H252	0.9500
C281-H281	0.9500	C262-C272	1.395(8)
C291-C301	1.488(7)	C262-H262	0.9500
C301-C351	1.387(8)	C272-C282	1.377(8)
C301-C311	1.405(8)	C272-H272	0.9500
C311-C321	1.370(8)	C282-C292	1.400(8)
C311-H311	0.9500	C282-H282	0.9500
C321-C331	1.396(8)	C292-C302	1.466(8)
C321-H321	0.9500	C302-C312	1.398(8)
C331-C341	1.379(8)	C302-C352	1.402(8)
C331-H331	0.9500	C312-C322	1.372(8)
C341-C351	1.403(7)	C312-H312	0.9500
C341-H341	0.9500	C322-C332	1.390(9)

C322-H322	0.9500	C264-H264	0.9500
C332-C342	1.387(8)	C274-C284	1.363(8)
C332-H332	0.9500	C274-H274	0.9500
C342-C352	1.384(8)	C284-C294	1.401(8)
C342-H342	0.9500	C284-H284	0.9500
C352-C362	1.477(8)	C294-C304	1.483(7)
O372-C372	1.425(6)	C304-C354	1.396(7)
C372-H37A2	0.9800	C304-C314	1.406(8)
C372-H37B2	0.9800	C314-C324	1.373(8)
C372-H37C2	0.9800	C314-H314	0.9500
N113-C363	1.336(7)	C324-C334	1.391(8)
N113-C123	1.352(7)	C324-H324	0.9500
C123-N133	1.351(7)	C334-C344	1.374(8)
C123-C213	1.424(7)	C334-H334	0.9500
N133-C143	1.356(7)	C344-C354	1.404(7)
C143-C153	1.411(7)	C344-H344	0.9500
C143-C193	1.438(7)	C354-C364	1.463(7)
C153-C163	1.352(8)	O374-C374	1.422(7)
C153-H153	0.9500	C374-H37A4	0.9800
C163-C173	1.421(8)	C374-H37B4	0.9800
C163-H163	0.9500	C374-H37C4	0.9800
C173-C183	1.347(7)	N115-C365	1.326(7)
C173-O373	1.362(7)	N115-C125	1.361(7)
C183-C193	1.423(7)	C125-N135	1.363(7)
C183-H183	0.9500	C125-C215	1.423(7)
C193-C203	1.383(7)	N135-C145	1.337(7)
C203-C213	1.380(7)	C145-C195	1.413(7)
C203-H203	0.9500	C145-C155	1.435(8)
C213-C223	1.404(7)	C155-C165	1.358(8)
C223-C233	1.356(7)	C155-H155	0.9500
C223-H223	0.9500	C165-C175	1.409(8)
C233-C363	1.439(7)	C165-H165	0.9500
C233-C243	1.464(7)	C175-O375	1.354(7)
C243-C253	1.402(7)	C175-C185	1.362(8)
C243-C293	1.415(7)	C185-C195	1.438(8)
C253-C263	1.365(8)	C185-H185	0.9500
C253-H253	0.9500	C195-C205	1.393(7)
C263-C273	1.388(8)	C205-C215	1.418(7)
C263-H263	0.9500	C205-H205	0.9500
C273-C283	1.370(8)	C215-C225	1.411(7)
C273-H273	0.9500	C225-C235	1.375(8)
C283-C293	1.397(8)	C225-H225	0.9500
C283-H283	0.9500	C235-C365	1.442(7)
C293-C303	1.463(8)	C235-C245	1.467(8)
C303-C353	1.402(8)	C245-C255	1.386(8)
C303-C313	1.408(8)	C245-C295	1.416(8)
C313-C323	1.369(8)	C255-C265	1.374(8)
C313-H313	0.9500	C255-H255	0.9500
C323-C333	1.392(8)	C265-C275	1.383(8)
C323-H323	0.9500	C265-H265	0.9500
C333-C343	1.378(8)	C275-C285	1.348(8)
C333-H333	0.9500	C275-H275	0.9500
C343-C353	1.394(7)	C285-C295	1.392(8)
C343-H343	0.9500	C285-H285	0.9500
C353-C363	1.469(7)	C295-C305	1.468(7)
O373-C373	1.419(6)	C305-C355	1.401(8)
C373-H37A3	0.9800	C305-C315	1.408(8)
C373-H37B3	0.9800	C315-C325	1.362(8)
C373-H37C3	0.9800	C315-H315	0.9500
N114-C364	1.321(7)	C325-C335	1.359(9)
N114-C124	1.351(7)	C325-H325	0.9500
C124-N134	1.340(7)	C335-C345	1.370(8)
C124-C214	1.430(7)	C335-H335	0.9500
N134-C144	1.356(7)	C345-C355	1.388(7)
C144-C154	1.428(8)	C345-H345	0.9500
C144-C194	1.445(7)	C355-C365	1.470(8)
C154-C164	1.343(8)	O375-C375	1.441(7)
C154-H154	0.9500	C375-H37A5	0.9800
C164-C174	1.407(8)	C375-H37B5	0.9800
C164-H164	0.9500	C375-H37C5	0.9800
C174-C184	1.351(8)	N116-C366	1.331(7)
C174-O374	1.356(7)	N116-C126	1.366(7)
C184-C194	1.414(8)	C126-N136	1.355(7)
C184-H184	0.9500	C126-C216	1.408(7)
C194-C204	1.378(7)	N136-C146	1.343(7)
C204-C214	1.397(8)	C146-C196	1.435(8)
C204-H204	0.9500	C146-C156	1.439(8)
C214-C224	1.383(7)	C156-C166	1.352(8)
C224-C234	1.373(7)	C156-H156	0.9500
C224-H224	0.9500	C166-C176	1.407(8)
C234-C364	1.443(7)	C166-H166	0.9500
C234-C244	1.468(7)	C176-O376	1.361(7)
C244-C254	1.389(7)	C176-C186	1.373(8)
C244-C294	1.411(8)	C186-C196	1.430(8)
C254-C264	1.376(8)	C186-H186	0.9500
C254-H254	0.9500	C196-C206	1.397(7)
C264-C274	1.391(8)	C206-C216	1.388(7)

C206-H206	0.9500	C148-C158	1.452(7)
C216-C226	1.424(7)	C158-C168	1.352(8)
C226-C236	1.386(7)	C158-H158	0.9500
C226-H226	0.9500	C168-C178	1.408(7)
C236-C366	1.433(7)	C168-H168	0.9500
C236-C246	1.480(8)	C178-O378	1.355(7)
C246-C256	1.398(7)	C178-C188	1.361(7)
C246-C296	1.408(8)	C188-C198	1.428(8)
C256-C266	1.370(8)	C188-H188	0.9500
C256-H256	0.9500	C198-C208	1.380(7)
C266-C276	1.385(8)	C208-C218	1.408(7)
C266-H266	0.9500	C208-H208	0.9500
C276-C286	1.359(7)	C218-C228	1.414(7)
C276-H276	0.9500	C228-C238	1.370(7)
C286-C296	1.407(8)	C228-H228	0.9500
C286-H286	0.9500	C238-C368	1.437(7)
C296-C306	1.455(7)	C238-C248	1.461(7)
C306-C356	1.396(7)	C248-C258	1.387(7)
C306-C316	1.416(8)	C248-C298	1.416(8)
C316-C326	1.356(8)	C258-C268	1.368(8)
C316-H316	0.9500	C258-H258	0.9500
C326-C336	1.370(8)	C268-C278	1.385(8)
C326-H326	0.9500	C268-H268	0.9500
C336-C346	1.381(8)	C278-C288	1.358(8)
C336-H336	0.9500	C278-H278	0.9500
C346-C356	1.392(7)	C288-C298	1.405(8)
C346-H346	0.9500	C288-H288	0.9500
C356-C366	1.472(7)	C298-C308	1.466(7)
O376-C376	1.433(7)	C308-C318	1.401(8)
C376-H37A6	0.9800	C308-C358	1.413(8)
C376-H37B6	0.9800	C318-C328	1.354(8)
C376-H37C6	0.9800	C318-H318	0.9500
N117-C367	1.325(7)	C328-C338	1.363(9)
N117-C127	1.360(7)	C328-H328	0.9500
C127-N137	1.344(7)	C338-C348	1.377(8)
C127-C217	1.422(7)	C338-H338	0.9500
N137-C147	1.342(7)	C348-C358	1.388(7)
C147-C197	1.428(7)	C348-H348	0.9500
C147-C157	1.432(8)	C358-C368	1.468(7)
C157-C167	1.354(7)	O378-C378	1.434(7)
C157-H157	0.9500	C378-H37A8	0.9800
C167-C177	1.420(7)	C378-H37B8	0.9800
C167-H167	0.9500	C378-H37C8	0.9800
C177-O377	1.359(7)	C41-Cl1	1.717(12)
C177-C187	1.363(8)	C41-Cl2	1.722(12)
C187-C197	1.428(7)	C41-Cl3	1.735(12)
C187-H187	0.9500	C41-H41	1.0000
C197-C207	1.389(7)	C41B-Cl31	1.72(2)
C207-C217	1.405(7)	C41B-Cl32	1.73(2)
C207-H207	0.9500	C41B-Cl33	1.74(2)
C217-C227	1.400(7)	C41B-H41B	1.0000
C227-C237	1.381(7)	C42-Cl6	1.724(11)
C227-H227	0.9500	C42-Cl5	1.742(11)
C237-C367	1.422(7)	C42-Cl4	1.745(10)
C237-C247	1.477(8)	C42-H42	1.0000
C247-C257	1.387(7)	C42B-Cl35	1.71(2)
C247-C297	1.413(8)	C42B-Cl36	1.73(2)
C257-C267	1.387(8)	C42B-Cl34	1.74(2)
C257-H257	0.9500	C42B-H42B	1.0000
C267-C277	1.379(8)	C43-Cl8	1.696(15)
C267-H267	0.9500	C43-Cl9	1.707(16)
C277-C287	1.366(8)	C43-Cl7	1.711(15)
C277-H277	0.9500	C43-H43	1.0000
C287-C297	1.411(8)	C43B-Cl38	1.69(2)
C287-H287	0.9500	C43B-Cl39	1.72(2)
C297-C307	1.461(8)	C43B-Cl37	1.73(2)
C307-C317	1.402(8)	C43B-H43B	1.0000
C307-C357	1.403(8)	C44-Cl11	1.671(11)
C317-C327	1.350(8)	C44-Cl12	1.685(12)
C317-H317	0.9500	C44-Cl10	1.744(11)
C327-C337	1.382(9)	C44-H44	1.0000
C327-H327	0.9500	C44B-Cl41	1.72(2)
C337-C347	1.357(8)	C44B-Cl42	1.73(2)
C337-H337	0.9500	C44B-Cl40	1.75(2)
C347-C357	1.394(7)	C44B-H44B	1.0000
C347-H347	0.9500	C45-Cl14	1.740(10)
C357-C367	1.483(8)	C45-Cl15	1.741(10)
O377-C377	1.438(6)	C45-Cl13	1.760(10)
C377-H37A7	0.9800	C45-H45	1.0000
C377-H37B7	0.9800	C45B-Cl44	1.69(2)
C377-H37C7	0.9800	C45B-Cl45	1.71(2)
N118-C368	1.339(7)	C45B-Cl43	1.71(2)
N118-C128	1.369(7)	C45B-H45B	1.0000
C128-N138	1.345(7)	C46-Cl17	1.675(12)
C128-C218	1.425(7)	C46-Cl18	1.715(11)
N138-C148	1.337(7)	C46-Cl16	1.735(13)
C148-C198	1.421(7)	C46-H46	1.0000

C46B-Cl47	1.72(2)	C351-C341-H341	119.7
C46B-Cl48	1.73(2)	C301-C351-C341	120.3(6)
C46B-Cl46	1.75(2)	C301-C351-C361	120.7(6)
C46B-H46B	1.0000	C341-C351-C361	119.0(6)
C47-Cl21	1.718(13)	N111-C361-C231	122.6(6)
C47-Cl20	1.720(13)	N111-C361-C351	118.3(6)
C47-Cl19	1.762(12)	C231-C361-C351	119.1(6)
C47-H47	1.0000	C171-O371-C371	118.2(6)
C47B-Cl50	1.72(2)	O371-C371-H37A1	109.5
C47B-Cl51	1.74(2)	O371-C371-H37B1	109.5
C47B-Cl49	1.75(2)	H37A1-C371-H37B1	109.5
C47B-H47B	1.0000	O371-C371-H37C1	109.5
C48-Cl24	1.710(14)	H37A1-C371-H37C1	109.5
C48-Cl22	1.734(14)	H37B1-C371-H37C1	109.5
C48-Cl23	1.743(15)	C362-N112-C122	119.2(5)
C48-H48	1.0000	N132-C122-N112	115.4(6)
C48B-Cl53	1.71(2)	N132-C122-C212	123.4(6)
C48B-Cl54	1.72(2)	N112-C122-C212	121.2(6)
C48B-Cl52	1.74(2)	C122-N132-C142	117.3(6)
C48B-H48B	1.0000	N132-C142-C152	118.4(6)
C361-N111-C121	119.6(6)	N132-C142-C192	123.0(6)
N131-C121-N111	115.8(6)	C152-C142-C192	118.7(6)
N131-C121-C211	122.4(6)	C162-C152-C142	119.8(6)
N111-C121-C211	121.7(6)	C162-C152-H152	120.1
C121-N131-C141	119.2(6)	C142-C152-H152	120.1
N131-C141-C151	120.2(6)	C152-C162-C172	122.1(6)
N131-C141-C191	122.1(6)	C152-C162-H162	118.9
C151-C141-C191	117.6(6)	C172-C162-H162	118.9
C161-C151-C141	120.9(7)	C182-C172-O372	125.5(6)
C161-C151-H151	119.5	C182-C172-C162	119.3(6)
C141-C151-H151	119.5	O372-C172-C162	115.2(6)
C151-C161-C171	121.3(7)	C172-C182-C192	121.1(6)
C151-C161-H161	119.3	C172-C182-H182	119.4
C171-C161-H161	119.3	C192-C182-H182	119.4
C181-C171-O371	125.4(7)	C202-C192-C182	123.2(6)
C181-C171-C161	120.4(6)	C202-C192-C142	117.8(6)
O371-C171-C161	114.2(6)	C182-C192-C142	119.0(6)
C171-C181-C191	120.7(7)	C192-C202-C212	120.3(6)
C171-C181-H181	119.7	C192-C202-H202	119.9
C191-C181-H181	119.7	C212-C202-H202	119.9
C201-C191-C181	123.8(6)	C202-C212-C222	124.3(6)
C201-C191-C141	117.3(6)	C202-C212-C122	118.2(6)
C181-C191-C141	118.9(6)	C222-C212-C122	117.6(6)
C191-C201-C211	121.4(6)	C232-C222-C212	121.8(6)
C191-C201-H201	119.3	C232-C222-H222	119.1
C211-C201-H201	119.3	C212-C222-H222	119.1
C221-C211-C201	125.9(6)	C222-C232-C362	117.1(6)
C221-C211-C121	116.7(6)	C222-C232-C242	123.4(6)
C201-C211-C121	117.4(6)	C362-C232-C242	119.4(6)
C231-C221-C211	122.9(6)	C252-C242-C292	118.6(6)
C231-C221-H221	118.5	C252-C242-C232	121.3(6)
C211-C221-H221	118.5	C292-C242-C232	120.0(6)
C221-C231-C361	116.5(6)	C262-C252-C242	121.7(7)
C221-C231-C241	123.6(6)	C262-C252-H252	119.2
C361-C231-C241	119.9(5)	C242-C252-H252	119.2
C251-C241-C291	119.3(6)	C252-C262-C272	120.6(7)
C251-C241-C231	121.1(6)	C252-C262-H262	119.7
C291-C241-C231	119.6(6)	C272-C262-H262	119.7
C261-C251-C241	121.4(7)	C282-C272-C262	118.9(7)
C261-C251-H251	119.3	C282-C272-H272	120.6
C241-C251-H251	119.3	C262-C272-H272	120.6
C251-C261-C271	119.0(7)	C272-C282-C292	122.0(7)
C251-C261-H261	120.5	C272-C282-H282	119.0
C271-C261-H261	120.5	C292-C282-H282	119.0
C281-C271-C261	120.1(7)	C282-C292-C242	118.3(6)
C281-C271-H271	119.9	C282-C292-C302	121.4(6)
C261-C271-H271	119.9	C242-C292-C302	120.4(6)
C271-C281-C291	121.8(7)	C312-C302-C352	117.8(6)
C271-C281-H281	119.1	C312-C302-C292	121.6(6)
C291-C281-H281	119.1	C352-C302-C292	120.6(6)
C241-C291-C281	118.3(6)	C322-C312-C302	120.8(7)
C241-C291-C301	120.4(6)	C322-C312-H312	119.6
C281-C291-C301	121.3(6)	C302-C312-H312	119.6
C351-C301-C311	118.3(6)	C312-C322-C332	121.3(7)
C351-C301-C291	120.1(6)	C312-C322-H322	119.3
C311-C301-C291	121.5(6)	C332-C322-H322	119.3
C321-C311-C301	121.1(7)	C342-C332-C322	118.3(7)
C321-C311-H311	119.4	C342-C332-H332	120.9
C301-C311-H311	119.4	C322-C332-H332	120.9
C311-C321-C331	120.5(7)	C352-C342-C332	120.9(7)
C311-C321-H321	119.8	C352-C342-H342	119.5
C331-C321-H321	119.8	C332-C342-H342	119.5
C341-C331-C321	119.2(7)	C342-C352-C302	120.6(6)
C341-C331-H331	120.4	C342-C352-C362	119.6(6)
C321-C331-H331	120.4	C302-C352-C362	119.7(6)
C331-C341-C351	120.5(7)	N112-C362-C232	123.0(6)
C331-C341-H341	119.7	N112-C362-C352	117.3(6)

C232-C362-C352	119.7(6)	H37A3-C373-H37C3	109.5
C172-O372-C372	115.9(5)	H37B3-C373-H37C3	109.5
O372-C372-H37A2	109.5	C364-N114-C124	119.1(6)
O372-C372-H37B2	109.5	N134-C124-N114	115.6(6)
H37A2-C372-H37B2	109.5	N134-C124-C214	122.4(6)
O372-C372-H37C2	109.5	N114-C124-C214	122.0(6)
H37A2-C372-H37C2	109.5	C124-N134-C144	118.8(6)
H37B2-C372-H37C2	109.5	N134-C144-C154	119.6(6)
C363-N113-C123	118.4(5)	N134-C144-C194	122.3(6)
N133-C123-N113	114.7(5)	C154-C144-C194	118.0(6)
N133-C123-C213	121.9(5)	C164-C154-C144	120.1(6)
N113-C123-C213	123.4(6)	C164-C154-H154	119.9
C123-N133-C143	118.7(5)	C144-C154-H154	119.9
N133-C143-C153	120.3(6)	C154-C164-C174	122.5(7)
N133-C143-C193	121.8(6)	C154-C164-H164	118.8
C153-C143-C193	117.9(6)	C174-C164-H164	118.8
C163-C153-C143	121.2(6)	C184-C174-O374	126.4(6)
C163-C153-H153	119.4	C184-C174-C164	119.1(6)
C143-C153-H153	119.4	O374-C174-C164	114.5(6)
C153-C163-C173	121.1(6)	C174-C184-C194	121.8(6)
C153-C163-H163	119.5	C174-C184-H184	119.1
C173-C163-H163	119.5	C194-C184-H184	119.1
C183-C173-O373	125.8(6)	C204-C194-C184	124.2(6)
C183-C173-C163	119.6(6)	C204-C194-C144	117.5(6)
O373-C173-C163	114.5(6)	C184-C194-C144	118.3(6)
C173-C183-C193	121.3(6)	C194-C204-C214	120.7(6)
C173-C183-H183	119.4	C194-C204-H204	119.6
C193-C183-H183	119.4	C214-C204-H204	119.6
C203-C193-C183	122.7(6)	C224-C214-C204	124.8(6)
C203-C193-C143	118.5(6)	C224-C214-C124	117.0(6)
C183-C193-C143	118.8(6)	C204-C214-C124	118.1(6)
C213-C203-C193	119.8(6)	C234-C224-C214	122.4(6)
C213-C203-H203	120.1	C234-C224-H224	118.8
C193-C203-H203	120.1	C214-C224-H224	118.8
C203-C213-C223	125.1(6)	C224-C234-C364	116.1(6)
C203-C213-C123	119.3(6)	C224-C234-C244	123.3(6)
C223-C213-C123	115.6(5)	C364-C234-C244	120.6(6)
C233-C223-C213	122.9(6)	C254-C244-C294	119.1(6)
C233-C223-H223	118.6	C254-C244-C234	121.7(6)
C213-C223-H223	118.6	C294-C244-C234	119.1(6)
C223-C233-C363	117.0(5)	C264-C254-C244	121.6(7)
C223-C233-C243	123.9(6)	C264-C254-H254	119.2
C363-C233-C243	119.1(5)	C244-C254-H254	119.2
C253-C243-C293	118.0(6)	C254-C264-C274	119.5(7)
C253-C243-C233	121.6(6)	C254-C264-H264	120.3
C293-C243-C233	120.3(6)	C274-C264-H264	120.3
C263-C253-C243	121.9(6)	C284-C274-C264	119.8(7)
C263-C253-H253	119.0	C284-C274-H274	120.1
C243-C253-H253	119.0	C264-C274-H274	120.1
C253-C263-C273	120.1(7)	C274-C284-C294	121.9(7)
C253-C263-H263	119.9	C274-C284-H284	119.0
C273-C263-H263	119.9	C294-C284-H284	119.0
C283-C273-C263	119.1(7)	C284-C294-C244	118.1(6)
C283-C273-H273	120.5	C284-C294-C304	121.6(6)
C263-C273-H273	120.5	C244-C294-C304	120.4(6)
C273-C283-C293	122.3(7)	C354-C304-C314	118.3(6)
C273-C283-H283	118.9	C354-C304-C294	120.0(6)
C293-C283-H283	118.9	C314-C304-C294	121.7(6)
C283-C293-C243	118.5(6)	C324-C314-C304	121.9(7)
C283-C293-C303	121.6(6)	C324-C314-H314	119.1
C243-C293-C303	119.9(6)	C304-C314-H314	119.1
C353-C303-C313	117.8(6)	C314-C324-C334	119.1(7)
C353-C303-C293	120.6(6)	C314-C324-H324	120.4
C313-C303-C293	121.6(6)	C334-C324-H324	120.4
C323-C313-C303	121.4(7)	C344-C334-C324	120.5(7)
C323-C313-H313	119.3	C344-C334-H334	119.7
C303-C313-H313	119.3	C324-C334-H334	119.7
C313-C323-C333	119.9(7)	C334-C344-C354	120.5(7)
C313-C323-H323	120.1	C334-C344-H344	119.8
C333-C323-H323	120.1	C354-C344-H344	119.8
C343-C333-C323	120.3(7)	C304-C354-C344	119.7(6)
C343-C333-H333	119.8	C304-C354-C364	120.9(6)
C323-C333-H333	119.8	C344-C354-C364	119.4(6)
C333-C343-C353	120.0(7)	N114-C364-C234	123.4(6)
C333-C343-H343	120.0	N114-C364-C354	117.9(6)
C353-C343-H343	120.0	C234-C364-C354	118.8(6)
C343-C353-C303	120.6(6)	C174-O374-C374	118.1(5)
C343-C353-C363	119.4(6)	O374-C374-H37A4	109.5
C303-C353-C363	119.9(6)	O374-C374-H37B4	109.5
N113-C363-C233	122.8(5)	H37A4-C374-H37B4	109.5
N113-C363-C353	117.4(5)	O374-C374-H37C4	109.5
C233-C363-C353	119.8(6)	H37A4-C374-H37C4	109.5
C173-O373-C373	115.8(5)	H37B4-C374-H37C4	109.5
O373-C373-H37A3	109.5	C365-N115-C125	117.5(5)
O373-C373-H37B3	109.5	N115-C125-N135	115.1(6)
H37A3-C373-H37B3	109.5	N115-C125-C215	121.9(6)
O373-C373-H37C3	109.5	N135-C125-C215	122.9(6)

C145-N135-C125	116.8(5)	C146-C156-H156	119.7
N135-C145-C195	125.4(6)	C156-C166-C176	121.8(7)
N135-C145-C155	116.6(6)	C156-C166-H166	119.1
C195-C145-C155	117.9(6)	C176-C166-H166	119.1
C165-C155-C145	119.4(6)	O376-C176-C186	125.7(6)
C165-C155-H155	120.3	O376-C176-C166	113.7(6)
C145-C155-H155	120.3	C186-C176-C166	120.6(6)
C155-C165-C175	122.4(7)	C176-C186-C196	119.4(6)
C155-C165-H165	118.8	C176-C186-H186	120.3
C175-C165-H165	118.8	C196-C186-H186	120.3
O375-C175-C185	124.9(6)	C206-C196-C186	122.4(6)
O375-C175-C165	114.4(6)	C206-C196-C146	117.4(6)
C185-C175-C165	120.6(6)	C186-C196-C146	120.2(6)
C175-C185-C195	118.4(6)	C216-C206-C196	119.4(6)
C175-C185-H185	120.8	C216-C206-H206	120.3
C195-C185-H185	120.8	C196-C206-H206	120.3
C205-C195-C145	117.4(6)	C206-C216-C126	118.9(6)
C205-C195-C185	121.4(6)	C206-C216-C226	122.5(6)
C145-C195-C185	121.2(6)	C126-C216-C226	118.6(6)
C195-C205-C215	119.4(6)	C236-C226-C216	119.6(6)
C195-C205-H205	120.3	C236-C226-H226	120.2
C215-C205-H205	120.3	C216-C226-H226	120.2
C225-C215-C205	123.0(6)	C226-C236-C366	117.5(6)
C225-C215-C125	119.0(6)	C226-C236-C246	122.2(6)
C205-C215-C125	118.0(6)	C366-C236-C246	120.3(6)
C235-C225-C215	119.6(6)	C256-C246-C296	120.2(6)
C235-C225-H225	120.2	C256-C246-C236	120.7(6)
C215-C225-H225	120.2	C296-C246-C236	119.1(6)
C225-C235-C365	116.9(6)	C266-C256-C246	120.6(7)
C225-C235-C245	122.8(6)	C266-C256-H256	119.7
C365-C235-C245	120.3(6)	C246-C256-H256	119.7
C255-C245-C295	118.6(6)	C256-C266-C276	120.2(7)
C255-C245-C235	121.8(6)	C256-C266-H266	119.9
C295-C245-C235	119.6(6)	C276-C266-H266	119.9
C265-C255-C245	121.6(7)	C286-C276-C266	119.5(7)
C265-C255-H255	119.2	C286-C276-H276	120.3
C245-C255-H255	119.2	C266-C276-H276	120.3
C255-C265-C275	119.6(7)	C276-C286-C296	122.8(7)
C255-C265-H265	120.2	C276-C286-H286	118.6
C275-C265-H265	120.2	C296-C286-H286	118.6
C285-C275-C265	119.6(7)	C286-C296-C246	116.7(6)
C285-C275-H275	120.2	C286-C296-C306	123.0(6)
C265-C275-H275	120.2	C246-C296-C306	120.3(6)
C275-C285-C295	122.8(7)	C356-C306-C316	117.0(6)
C275-C285-H285	118.6	C356-C306-C296	121.3(6)
C295-C285-H285	118.6	C316-C306-C296	121.7(6)
C285-C295-C245	117.7(6)	C326-C316-C306	121.5(7)
C285-C295-C305	121.9(6)	C326-C316-H316	119.2
C245-C295-C305	120.3(6)	C306-C316-H316	119.2
C355-C305-C315	117.5(6)	C316-C326-C336	120.4(7)
C355-C305-C295	120.1(6)	C316-C326-H326	119.8
C315-C305-C295	122.4(6)	C336-C326-H326	119.8
C325-C315-C305	121.3(7)	C326-C336-C346	120.6(7)
C325-C315-H315	119.4	C326-C336-H336	119.7
C305-C315-H315	119.4	C346-C336-H336	119.7
C335-C325-C315	120.9(7)	C336-C346-C356	119.3(7)
C335-C325-H325	119.6	C336-C346-H346	120.3
C315-C325-H325	119.6	C356-C346-H346	120.3
C325-C335-C345	119.5(7)	C346-C356-C306	121.1(6)
C325-C335-H335	120.3	C346-C356-C366	119.0(6)
C345-C335-H335	120.3	C306-C356-C366	119.9(6)
C335-C345-C355	121.4(7)	N116-C366-C236	123.6(6)
C335-C345-H345	119.3	N116-C366-C356	117.5(6)
C355-C345-H345	119.3	C236-C366-C356	118.9(6)
C345-C355-C305	119.4(6)	C176-O376-C376	116.6(6)
C345-C355-C365	119.6(6)	O376-C376-H37A6	109.5
C305-C355-C365	121.0(6)	O376-C376-H37B6	109.5
N115-C365-C235	124.9(6)	H37A6-C376-H37B6	109.5
N115-C365-C355	116.4(6)	O376-C376-H37C6	109.5
C235-C365-C355	118.6(6)	H37A6-C376-H37C6	109.5
C175-O375-C375	116.9(6)	H37B6-C376-H37C6	109.5
O375-C375-H37A5	109.5	C367-N117-C127	118.0(6)
O375-C375-H37B5	109.5	N137-C127-N117	115.3(6)
H37A5-C375-H37B5	109.5	N137-C127-C217	123.2(6)
O375-C375-H37C5	109.5	N117-C127-C217	121.5(6)
H37A5-C375-H37C5	109.5	C147-N137-C127	117.5(5)
H37B5-C375-H37C5	109.5	N137-C147-C197	123.8(6)
C366-N116-C126	118.8(5)	N137-C147-C157	118.7(6)
N136-C126-N116	114.5(6)	C197-C147-C157	117.5(6)
N136-C126-C216	123.6(6)	C167-C157-C147	120.6(6)
N116-C126-C216	121.9(6)	C167-C157-H157	119.7
C146-N136-C126	116.8(6)	C147-C157-H157	119.7
N136-C146-C196	123.8(6)	C157-C167-C177	121.4(6)
N136-C146-C156	118.7(6)	C157-C167-H167	119.3
C196-C146-C156	117.3(6)	C177-C167-H167	119.3
C166-C156-C146	120.6(7)	O377-C177-C187	125.1(6)
C166-C156-H156	119.7	O377-C177-C167	114.3(6)

C187-C177-C167	120.6(6)	C148-C198-C188	120.8(6)
C177-C187-C197	119.2(6)	C198-C208-C218	119.4(6)
C177-C187-H187	120.4	C198-C208-H208	120.3
C197-C187-H187	120.4	C218-C208-H208	120.3
C207-C197-C147	118.0(6)	C208-C218-C228	123.1(6)
C207-C197-C187	121.3(6)	C208-C218-C128	118.1(6)
C147-C197-C187	120.7(6)	C228-C218-C128	118.7(6)
C197-C207-C217	119.1(6)	C238-C228-C218	120.5(6)
C197-C207-H207	120.4	C238-C228-H228	119.8
C217-C207-H207	120.4	C218-C228-H228	119.8
C227-C217-C207	122.8(6)	C228-C238-C368	117.0(6)
C227-C217-C127	118.8(6)	C228-C238-C248	123.2(6)
C207-C217-C127	118.4(6)	C368-C238-C248	119.7(6)
C237-C227-C217	119.9(6)	C258-C248-C298	118.3(6)
C237-C227-H227	120.0	C258-C248-C238	121.8(6)
C217-C227-H227	120.0	C298-C248-C238	119.9(6)
C227-C237-C367	116.9(6)	C268-C258-C248	121.8(7)
C227-C237-C247	122.2(6)	C268-C258-H258	119.1
C367-C237-C247	120.9(6)	C248-C258-H258	119.1
C257-C247-C297	119.2(6)	C258-C268-C278	120.4(7)
C257-C247-C237	121.6(6)	C258-C268-H268	119.8
C297-C247-C237	119.2(6)	C278-C268-H268	119.8
C267-C257-C247	121.4(6)	C288-C278-C268	118.8(7)
C267-C257-H257	119.3	C288-C278-H278	120.6
C247-C257-H257	119.3	C268-C278-H278	120.6
C277-C267-C257	119.7(7)	C278-C288-C298	122.6(7)
C277-C267-H267	120.2	C278-C288-H288	118.7
C257-C267-H267	120.2	C298-C288-H288	118.7
C287-C277-C267	120.0(7)	C288-C298-C248	117.7(6)
C287-C277-H277	120.0	C288-C298-C308	121.9(6)
C267-C277-H277	120.0	C248-C298-C308	120.4(6)
C277-C287-C297	121.8(7)	C318-C308-C358	117.4(6)
C277-C287-H287	119.1	C318-C308-C298	122.6(6)
C297-C287-H287	119.1	C358-C308-C298	120.1(6)
C287-C297-C247	117.7(6)	C328-C318-C308	121.9(7)
C287-C297-C307	121.5(6)	C328-C318-H318	119.1
C247-C297-C307	120.8(6)	C308-C318-H318	119.1
C317-C307-C357	117.0(6)	C318-C328-C338	120.2(7)
C317-C307-C297	123.3(7)	C318-C328-H328	119.9
C357-C307-C297	119.7(6)	C338-C328-H328	119.9
C327-C317-C307	123.1(7)	C328-C338-C348	120.7(7)
C327-C317-H317	118.5	C328-C338-H338	119.7
C307-C317-H317	118.5	C348-C338-H338	119.7
C317-C327-C337	119.2(7)	C338-C348-C358	120.0(7)
C317-C327-H327	120.4	C338-C348-H348	120.0
C337-C327-H327	120.4	C358-C348-H348	120.0
C347-C337-C327	119.9(7)	C348-C358-C308	119.8(6)
C347-C337-H337	120.0	C348-C358-C368	120.3(6)
C327-C337-H337	120.0	C308-C358-C368	119.9(6)
C337-C347-C357	121.7(7)	N118-C368-C238	124.2(6)
C337-C347-H347	119.2	N118-C368-C358	116.0(5)
C357-C347-H347	119.2	C238-C368-C358	119.7(6)
C347-C357-C307	119.1(6)	C178-O378-C378	116.4(6)
C347-C357-C367	119.7(6)	O378-C378-H37A8	109.5
C307-C357-C367	121.2(6)	O378-C378-H37B8	109.5
N117-C367-C237	124.9(6)	H37A8-C378-H37B8	109.5
N117-C367-C357	117.0(6)	O378-C378-H37C8	109.5
C237-C367-C357	118.2(6)	H37A8-C378-H37C8	109.5
C177-O377-C377	115.7(5)	H37B8-C378-H37C8	109.5
O377-C377-H37A7	109.5	Cl1-C41-Cl2	108.9(8)
O377-C377-H37B7	109.5	Cl1-C41-Cl3	107.0(7)
H37A7-C377-H37B7	109.5	Cl2-C41-Cl3	114.7(9)
O377-C377-H37C7	109.5	Cl1-C41-H41	108.7
H37A7-C377-H37C7	109.5	Cl2-C41-H41	108.7
H37B7-C377-H37C7	109.5	Cl3-C41-H41	108.7
C368-N118-C128	118.2(5)	Cl31-C41B-Cl32	107.2(17)
N138-C128-N118	115.5(5)	Cl31-C41B-Cl33	98.7(18)
N138-C128-C218	123.3(6)	Cl32-C41B-Cl33	104.6(17)
N118-C128-C218	121.2(6)	Cl31-C41B-H41B	114.9
C148-N138-C128	116.6(5)	Cl32-C41B-H41B	114.9
N138-C148-C198	125.2(6)	Cl33-C41B-H41B	114.9
N138-C148-C158	117.6(6)	Cl6-C42-Cl5	109.8(6)
C198-C148-C158	117.1(6)	Cl6-C42-Cl4	112.3(7)
C168-C158-C148	119.9(6)	Cl5-C42-Cl4	110.9(7)
C168-C158-H158	120.0	Cl6-C42-H42	107.9
C148-C158-H158	120.0	Cl5-C42-H42	107.9
C158-C168-C178	122.3(6)	Cl4-C42-H42	107.9
C158-C168-H168	118.9	Cl35-C42B-Cl36	107(2)
C178-C168-H168	118.9	Cl35-C42B-Cl34	114(2)
O378-C178-C188	124.4(6)	Cl36-C42B-Cl34	102.4(17)
O378-C178-C168	115.4(6)	Cl35-C42B-H42B	110.9
C188-C178-C168	120.2(6)	Cl36-C42B-H42B	110.9
C178-C188-C198	119.7(6)	Cl34-C42B-H42B	110.9
C178-C188-H188	120.2	Cl8-C43-Cl9	108.1(12)
C198-C188-H188	120.2	Cl8-C43-Cl7	112.2(14)
C208-C198-C148	117.3(6)	Cl9-C43-Cl7	108.6(12)
C208-C198-C188	121.9(6)	Cl8-C43-H43	109.3

Cl9-C43-H43	109.3
Cl7-C43-H43	109.3
Cl38-C43B-Cl39	105.9(14)
Cl38-C43B-Cl37	120.4(19)
Cl39-C43B-Cl37	104.7(14)
Cl38-C43B-H43B	108.4
Cl39-C43B-H43B	108.4
Cl37-C43B-H43B	108.4
Cl11-C44-Cl12	106.7(8)
Cl11-C44-Cl10	110.8(8)
Cl12-C44-Cl10	113.7(8)
Cl11-C44-H44	108.5
Cl12-C44-H44	108.5
Cl10-C44-H44	108.5
Cl41-C44B-Cl42	105.0(15)
Cl41-C44B-Cl40	131(2)
Cl42-C44B-Cl40	102.2(14)
Cl41-C44B-H44B	105.5
Cl42-C44B-H44B	105.5
Cl40-C44B-H44B	105.5
Cl14-C45-Cl15	111.0(6)
Cl14-C45-Cl13	109.8(6)
Cl15-C45-Cl13	112.1(6)
Cl14-C45-H45	107.9
Cl15-C45-H45	107.9
Cl13-C45-H45	107.9
Cl44-C45B-Cl45	109.3(15)
Cl44-C45B-Cl43	123.1(18)
Cl45-C45B-Cl43	101.4(15)
Cl44-C45B-H45B	107.4
Cl45-C45B-H45B	107.4
Cl43-C45B-H45B	107.4
Cl17-C46-Cl18	111.2(9)
Cl17-C46-Cl16	102.9(7)
Cl18-C46-Cl16	108.2(8)
Cl17-C46-H46	111.4
Cl18-C46-H46	111.4
Cl16-C46-H46	111.4
Cl47-C46B-Cl48	99.4(15)
Cl47-C46B-Cl46	135(3)
Cl48-C46B-Cl46	105.2(17)
Cl47-C46B-H46B	104.8
Cl48-C46B-H46B	104.8
Cl46-C46B-H46B	104.8
Cl21-C47-Cl20	110.5(9)
Cl21-C47-Cl19	108.8(8)
Cl20-C47-Cl19	109.5(9)
Cl21-C47-H47	109.3
Cl20-C47-H47	109.3
Cl19-C47-H47	109.3
Cl50-C47B-Cl51	118(2)
Cl50-C47B-Cl49	107.8(15)
Cl51-C47B-Cl49	105.7(16)
Cl50-C47B-H47B	108.2
Cl51-C47B-H47B	108.2
Cl49-C47B-H47B	108.2
Cl24-C48-Cl22	108.8(9)
Cl24-C48-Cl23	110.1(9)
Cl22-C48-Cl23	111.5(11)
Cl24-C48-H48	108.8
Cl22-C48-H48	108.8
Cl23-C48-H48	108.8
Cl53-C48B-Cl54	106.4(15)
Cl53-C48B-Cl52	111.5(14)
Cl54-C48B-Cl52	105.5(12)
Cl53-C48B-H48B	111.1
Cl54-C48B-H48B	111.1
Cl52-C48B-H48B	111.1

6.6. Compound 5h

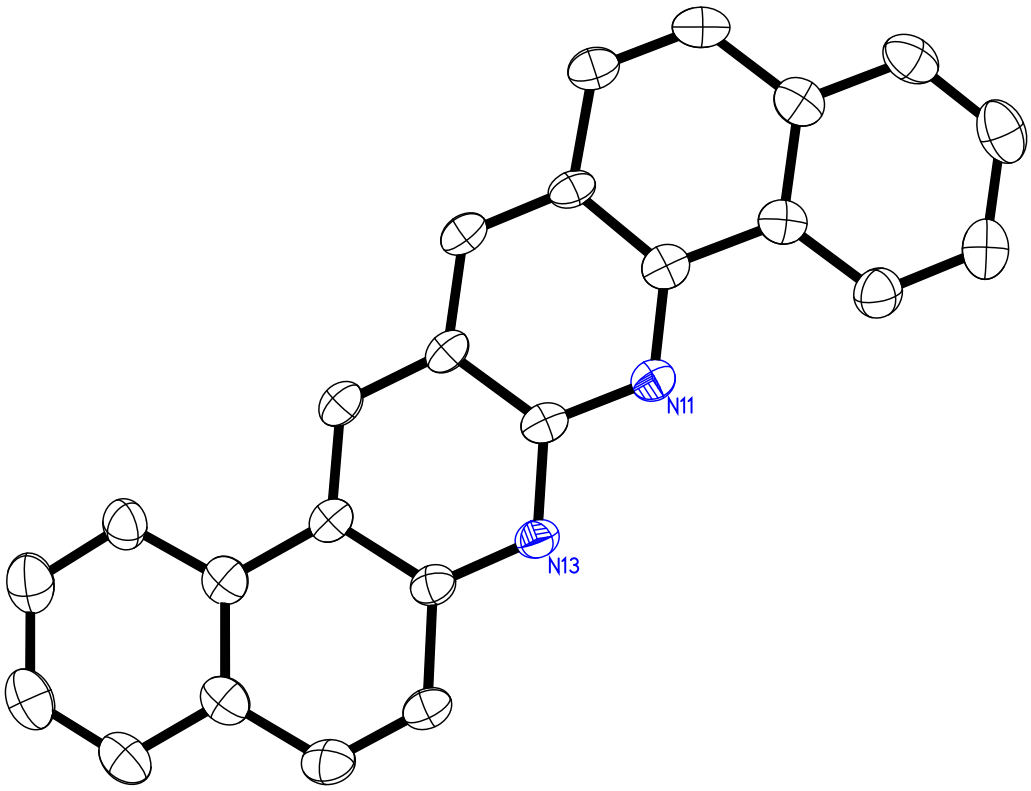


Figure S13: X-ray crystal structure of **5h**.

Table S27: Crystal data and structure refinement for **5h**.

Identification code	stu12	
Empirical formula	$C_{25}H_{15}Cl_3N_2$	
Formula weight	449.74	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	C2/c	
Z	8	
Unit cell dimensions	a = 31.6523(13) Å	α = 90 deg.
	b =7.2389(3) Å	β =127.995(2) deg.
	c = 22.7804(10) Å	γ = 90 deg.
Volume	4113.4(3) $Å^3$	
Density (calculated)	1.45 g/cm^3	
Absorption coefficient	0.46 mm^{-1}	
Crystal shape	plank	
Crystal size	0.295 x 0.071 x 0.030 mm^3	
Crystal colour	yellow	
Theta range for data collection	1.6 to 25.0 deg.	
Index ranges	$-37 \le h \le 37$, $-8 \le k \le 8$, $-27 \le l \le 21$	
Reflections collected	18628	
Independent reflections	3612 (R(int) = 0.0820)	
Observed reflections	2142 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.96 and 0.82	

Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3612 / 0 / 271
Goodness-of-fit on F^2	1.02
Final R indices (I>2sigma(I))	R1 = 0.055, wR2 = 0.119
Largest diff. peak and hole	0.40 and -0.41 eÅ^{-3}

Table S28: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **5h**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
N11	0.6757(1)	0.4994(4)	0.4014(1)	0.0253(7)
C12	0.7201(1)	0.5628(4)	0.4110(2)	0.0250(8)
N13	0.7111(1)	0.6285(4)	0.3486(1)	0.0260(7)
C14	0.7536(1)	0.6886(5)	0.3543(2)	0.0256(8)
C15	0.7430(1)	0.7574(5)	0.2873(2)	0.0300(8)
H15	0.7071	0.7611	0.2426	0.036
C16	0.7829(1)	0.8162(5)	0.2867(2)	0.0337(9)
H16	0.7745	0.8602	0.2414	0.040
C17	0.8378(1)	0.8151(5)	0.3523(2)	0.0312(9)
C18	0.8789(2)	0.8769(5)	0.3499(2)	0.0398(10)
H18	0.8703	0.9204	0.3044	0.048
C19	0.9311(2)	0.8747(5)	0.4130(2)	0.0436(10)
H19	0.9587	0.9162	0.4110	0.052
C20	0.9440(2)	0.8122(5)	0.4799(2)	0.0449(10)
H20	0.9804	0.8108	0.5232	0.054
C21	0.9048(1)	0.7524(5)	0.4841(2)	0.0357(9)
H21	0.9143	0.7113	0.5304	0.043
C22	0.8509(1)	0.7514(4)	0.4206(2)	0.0286(8)
C23	0.8076(1)	0.6868(4)	0.4219(2)	0.0235(8)
C24	0.8155(1)	0.6229(4)	0.4851(2)	0.0265(8)
H24	0.8506	0.6218	0.5313	0.032
C25	0.7720(1)	0.5595(4)	0.4816(2)	0.0236(8)
C26	0.7767(1)	0.4928(4)	0.5431(2)	0.0263(8)
H26	0.8108	0.4900	0.5908	0.032
C27	0.7322(1)	0.4312(4)	0.5344(2)	0.0244(8)
C28	0.7346(1)	0.3649(5)	0.5959(2)	0.0308(8)
H28	0.7679	0.3648	0.6447	0.037
C29	0.6903(1)	0.3031(5)	0.5853(2)	0.0332(9)
H29	0.6928	0.2643	0.6272	0.040
C30	0.6392(1)	0.2938(5)	0.5123(2)	0.0305(9)
C31	0.5941(2)	0.2163(5)	0.5012(2)	0.0373(9)
H31	0.5967	0.1750	0.5428	0.045
C32	0.5465(2)	0.1996(5)	0.4311(2)	0.0425(10)
H32	0.5165	0.1443	0.4244	0.051
C33	0.5419(2)	0.2634(5)	0.3698(2)	0.0400(10)
H33	0.5088	0.2515	0.3212	0.048
C34	0.5851(1)	0.3437(5)	0.3795(2)	0.0356(9)
H34	0.5812	0.3894	0.3373	0.043
C35	0.6344(1)	0.3593(4)	0.4497(2)	0.0274(8)
C36	0.6818(1)	0.4342(4)	0.4612(2)	0.0254(8)
C41	0.5880(2)	0.7898(6)	0.2463(2)	0.0489(11)
H41	0.6213	0.7159	0.2814	0.059
Cl1	0.5950(1)	0.9181(2)	0.1879(1)	0.1018(6)
Cl2	0.5334(1)	0.6399(2)	0.1932(1)	0.0663(4)
Cl3	0.5772(1)	0.9351(2)	0.2977(1)	0.0833(5)

Table S29: Hydrogen coordinates and isotropic displacement parameters (Å^2) for **5h**.

Atom	x	y	z	U_{eq}
H15	0.7071	0.7611	0.2426	0.036
H16	0.7745	0.8602	0.2414	0.040
H18	0.8703	0.9204	0.3044	0.048
H19	0.9587	0.9162	0.4110	0.052
H20	0.9804	0.8108	0.5232	0.054
H21	0.9143	0.7113	0.5304	0.043
H24	0.8506	0.6218	0.5313	0.032
H26	0.8108	0.4900	0.5908	0.032
H28	0.7679	0.3648	0.6447	0.037
H29	0.6928	0.2643	0.6272	0.040
H31	0.5967	0.1750	0.5428	0.045
H32	0.5165	0.1443	0.4244	0.051
H33	0.5088	0.2515	0.3212	0.048
H34	0.5812	0.3894	0.3373	0.043
H41	0.6213	0.7159	0.2814	0.059

Table S30: Anisotropic displacement parameters (Å^2) for **5h**. 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	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N11	0.0269(16)	0.0244(16)	0.0237(15)	-0.0008(13)	0.0150(13)	0.0017(12)
C12	0.029(2)	0.0230(19)	0.0219(18)	-0.0002(15)	0.0148(17)	0.0052(15)
N13	0.0266(16)	0.0291(17)	0.0202(15)	0.0006(13)	0.0133(14)	0.0004(13)
C14	0.030(2)	0.024(2)	0.0218(18)	-0.0028(15)	0.0149(17)	-0.0004(15)
C15	0.032(2)	0.033(2)	0.0210(18)	-0.0013(16)	0.0142(17)	0.0008(16)
C16	0.044(2)	0.032(2)	0.027(2)	-0.0045(17)	0.023(2)	-0.0014(17)
C17	0.040(2)	0.022(2)	0.039(2)	-0.0026(17)	0.028(2)	-0.0005(16)
C18	0.049(3)	0.032(2)	0.049(3)	-0.0008(19)	0.036(2)	-0.0046(18)
C19	0.042(3)	0.039(3)	0.060(3)	-0.004(2)	0.037(2)	-0.0042(19)
C20	0.035(2)	0.040(3)	0.055(3)	0.002(2)	0.025(2)	-0.0017(19)
C21	0.033(2)	0.030(2)	0.039(2)	0.0015(18)	0.020(2)	-0.0035(17)
C22	0.035(2)	0.0151(19)	0.035(2)	-0.0026(15)	0.0209(19)	0.0000(15)
C23	0.0259(19)	0.0178(19)	0.0232(18)	-0.0028(15)	0.0133(17)	0.0033(14)
C24	0.0265(19)	0.023(2)	0.0233(19)	-0.0032(15)	0.0119(16)	0.0019(15)
C25	0.0249(19)	0.0191(19)	0.0201(18)	-0.0033(15)	0.0104(16)	0.0022(14)
C26	0.028(2)	0.022(2)	0.0203(18)	-0.0012(15)	0.0108(16)	0.0030(15)
C27	0.029(2)	0.024(2)	0.0185(18)	-0.0024(15)	0.0138(16)	0.0038(15)
C28	0.036(2)	0.029(2)	0.0256(19)	-0.0007(16)	0.0182(18)	0.0026(16)
C29	0.046(2)	0.030(2)	0.029(2)	0.0033(16)	0.026(2)	0.0056(17)
C30	0.037(2)	0.023(2)	0.038(2)	-0.0006(17)	0.0269(19)	0.0051(16)
C31	0.047(3)	0.032(2)	0.046(2)	0.0071(19)	0.036(2)	0.0087(18)
C32	0.041(3)	0.032(2)	0.064(3)	0.003(2)	0.037(2)	0.0020(18)
C33	0.032(2)	0.038(2)	0.047(2)	-0.004(2)	0.022(2)	-0.0015(18)
C34	0.032(2)	0.039(2)	0.034(2)	0.0019(18)	0.020(2)	0.0057(17)
C35	0.034(2)	0.022(2)	0.031(2)	0.0006(16)	0.0215(18)	0.0051(15)
C36	0.031(2)	0.0171(19)	0.028(2)	-0.0016(15)	0.0178(17)	0.0046(15)
C41	0.037(2)	0.050(3)	0.047(2)	-0.002(2)	0.020(2)	0.004(2)
Cl1	0.0801(10)	0.1002(12)	0.1396(14)	0.0583(10)	0.0749(10)	0.0234(8)
Cl2	0.0575(8)	0.0737(9)	0.0535(7)	-0.0203(6)	0.0270(6)	-0.0175(6)
Cl3	0.0474(7)	0.0927(10)	0.0624(8)	-0.0343(7)	0.0099(6)	0.0142(7)

Table S31: Bond lengths (Å) and angles (deg) for **5h**.

N11-C36	1.337(4)
N11-C12	1.362(4)
C12-N13	1.352(4)
C12-C25	1.427(4)
N13-C14	1.340(4)
C14-C23	1.433(4)
C14-C15	1.437(4)
C15-C16	1.338(5)
C15-H15	0.9500
C16-C17	1.434(5)
C16-H16	0.9500
C17-C18	1.407(5)
C17-C22	1.419(5)
C18-C19	1.369(5)
C18-H18	0.9500
C19-C20	1.387(5)
C19-H19	0.9500
C20-C21	1.372(5)
C20-H20	0.9500
C21-C22	1.401(5)
C21-H21	0.9500
C22-C23	1.464(4)
C23-C24	1.380(4)
C24-C25	1.406(4)
C24-H24	0.9500
C25-C26	1.400(4)
C26-C27	1.374(4)
C26-H26	0.9500
C27-C36	1.432(4)
C27-C28	1.438(4)
C28-C29	1.343(5)
C28-H28	0.9500
C29-C30	1.442(5)
C29-H29	0.9500
C30-C31	1.403(5)
C30-C35	1.418(4)
C31-C32	1.368(5)
C31-H31	0.9500
C32-C33	1.392(5)

C32-H32	0.9500
C33-C34	1.373(5)
C33-H33	0.9500
C34-C35	1.391(5)
C34-H34	0.9500
C35-C36	1.461(5)
C41-Cl1	1.744(4)
C41-Cl2	1.747(4)
C41-Cl3	1.757(4)
C41-H41	1.0000
C36-N11-C12	117.9(3)
N13-C12-N11	115.0(3)
N13-C12-C25	122.7(3)
N11-C12-C25	122.3(3)
C14-N13-C12	117.6(3)
N13-C14-C23	124.3(3)
N13-C14-C15	116.5(3)
C23-C14-C15	119.2(3)
C16-C15-C14	121.0(3)
C16-C15-H15	119.5
C14-C15-H15	119.5
C15-C16-C17	122.3(3)
C15-C16-H16	118.9
C17-C16-H16	118.9
C18-C17-C22	119.5(3)
C18-C17-C16	121.0(3)
C22-C17-C16	119.5(3)
C19-C18-C17	120.2(4)
C19-C18-H18	119.9
C17-C18-H18	119.9
C18-C19-C20	120.4(4)
C18-C19-H19	119.8
C20-C19-H19	119.8
C21-C20-C19	120.8(4)
C21-C20-H20	119.6
C19-C20-H20	119.6
C20-C21-C22	120.6(4)
C20-C21-H21	119.7
C22-C21-H21	119.7
C21-C22-C17	118.5(3)
C21-C22-C23	122.8(3)
C17-C22-C23	118.7(3)
C24-C23-C14	117.0(3)
C24-C23-C22	123.8(3)
C14-C23-C22	119.2(3)
C23-C24-C25	120.5(3)
C23-C24-H24	119.8
C25-C24-H24	119.8
C26-C25-C24	123.9(3)
C26-C25-C12	118.2(3)
C24-C25-C12	117.9(3)
C27-C26-C25	120.1(3)
C27-C26-H26	120.0
C25-C26-H26	120.0
C26-C27-C36	118.0(3)
C26-C27-C28	122.4(3)
C36-C27-C28	119.6(3)
C29-C28-C27	120.8(3)
C29-C28-H28	119.6
C27-C28-H28	119.6
C28-C29-C30	122.0(3)
C28-C29-H29	119.0
C30-C29-H29	119.0
C31-C30-C35	119.0(3)
C31-C30-C29	121.4(3)
C35-C30-C29	119.5(3)
C32-C31-C30	120.9(3)
C32-C31-H31	119.6
C30-C31-H31	119.6
C31-C32-C33	120.1(4)
C31-C32-H32	120.0
C33-C32-H32	120.0
C34-C33-C32	120.1(4)
C34-C33-H33	120.0
C32-C33-H33	120.0
C33-C34-C35	121.3(3)
C33-C34-H34	119.3
C35-C34-H34	119.3
C34-C35-C30	118.6(3)
C34-C35-C36	122.5(3)
C30-C35-C36	118.8(3)
N11-C36-C27	123.5(3)
N11-C36-C35	117.4(3)
C27-C36-C35	119.1(3)
Cl1-C41-Cl2	109.8(2)
Cl1-C41-Cl3	110.9(2)

Cl2-C41-Cl3	108.5(2)
Cl1-C41-H41	109.2
Cl2-C41-H41	109.2
Cl3-C41-H41	109.2

7. Computational Data of 5a-h and 11a and 11b

All geometry optimizations, subsequent frequency analyses, and TD-DFT calculations were performed in with the CPCM model for chloroform using Orca 4.0.1.2[6] on the bwForCluster Justus 2. The B3LYP[7] functional and the 6-311G[8] basis set was employed.

xyz-files

5a

Charge 0, Multiplicity 1

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7	-1.069386000	-0.626509000	0.000000000
6	0.113013000	-1.323642000	0.000000000
6	-1.128235000	-3.451543000	0.000000000
6	0.121032000	-2.777402000	0.000000000
7	1.258245000	-0.586139000	0.000000000
6	2.450795000	-1.247867000	0.000000000
6	2.555790000	-2.702149000	0.000000000
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6	3.653257000	-0.471843000	0.000000000
6	4.888161000	-1.089304000	0.000000000
6	4.991945000	-2.518090000	0.000000000
6	3.856985000	-3.303671000	0.000000000
1	5.798612000	-0.489437000	0.000000000
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1	-1.117832000	-4.542695000	0.000000000
1	-2.364802000	1.351493000	0.000000000
1	-4.425150000	2.800038000	0.000000000
1	-6.683714000	1.710272000	0.000000000
1	-6.882759000	-0.734305000	0.000000000
1	-7.006739000	-2.667374000	0.000000000
1	-7.168587000	-5.119250000	0.000000000
1	-2.878142000	-5.425861000	0.000000000
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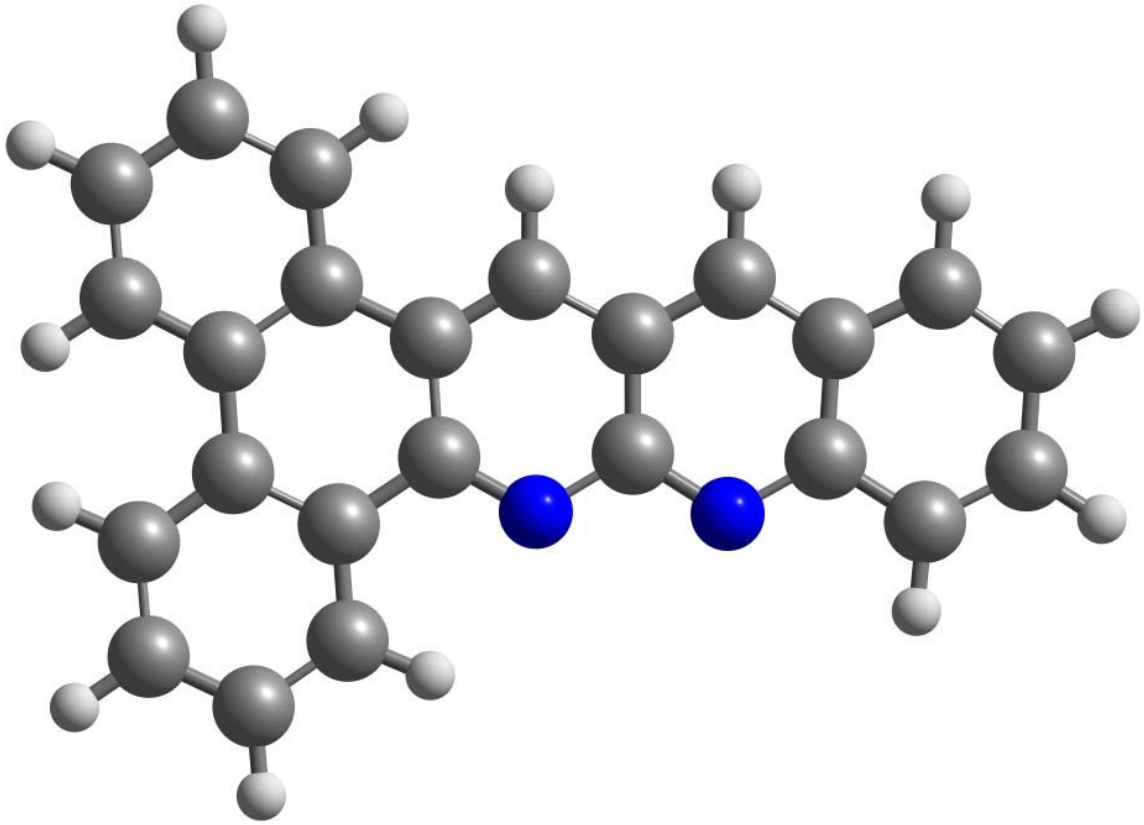

5b

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6	-4.746312000	-1.121150000	0.000000000
6	-3.468397000	-0.488977000	0.000000000
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6	-2.244868000	-1.292554000	0.000000000
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6	-3.652931000	-3.390802000	0.000000000
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6	-6.095054000	-3.252114000	0.000000000
6	-6.192711000	-4.642538000	0.000000000
6	-5.023444000	-5.426625000	0.000000000
7	-1.076017000	-0.625033000	0.000000000
6	0.104936000	-1.322779000	0.000000000
6	-1.134728000	-3.450297000	0.000000000
6	0.114906000	-2.776086000	0.000000000
7	1.251066000	-0.585733000	0.000000000
6	2.441943000	-1.246655000	0.000000000
6	2.548927000	-2.701900000	0.000000000
6	1.355548000	-3.442317000	0.000000000
6	3.642622000	-0.464057000	0.000000000
6	4.881737000	-1.070833000	0.000000000
6	4.950144000	-2.491010000	0.000000000
6	3.847850000	-3.306960000	0.000000000
1	5.806189000	-0.496542000	0.000000000
9	6.234642000	-3.070632000	0.000000000
1	3.527803000	0.618521000	0.000000000
1	3.959835000	-4.390790000	0.000000000
1	1.388440000	-4.535117000	0.000000000
1	-1.124587000	-4.541281000	0.000000000
1	-2.372273000	1.354298000	0.000000000
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1	-6.690897000	1.710811000	0.000000000
1	-6.889255000	-0.733712000	0.000000000
1	-7.012681000	-2.666754000	0.000000000
1	-7.173676000	-5.118488000	0.000000000
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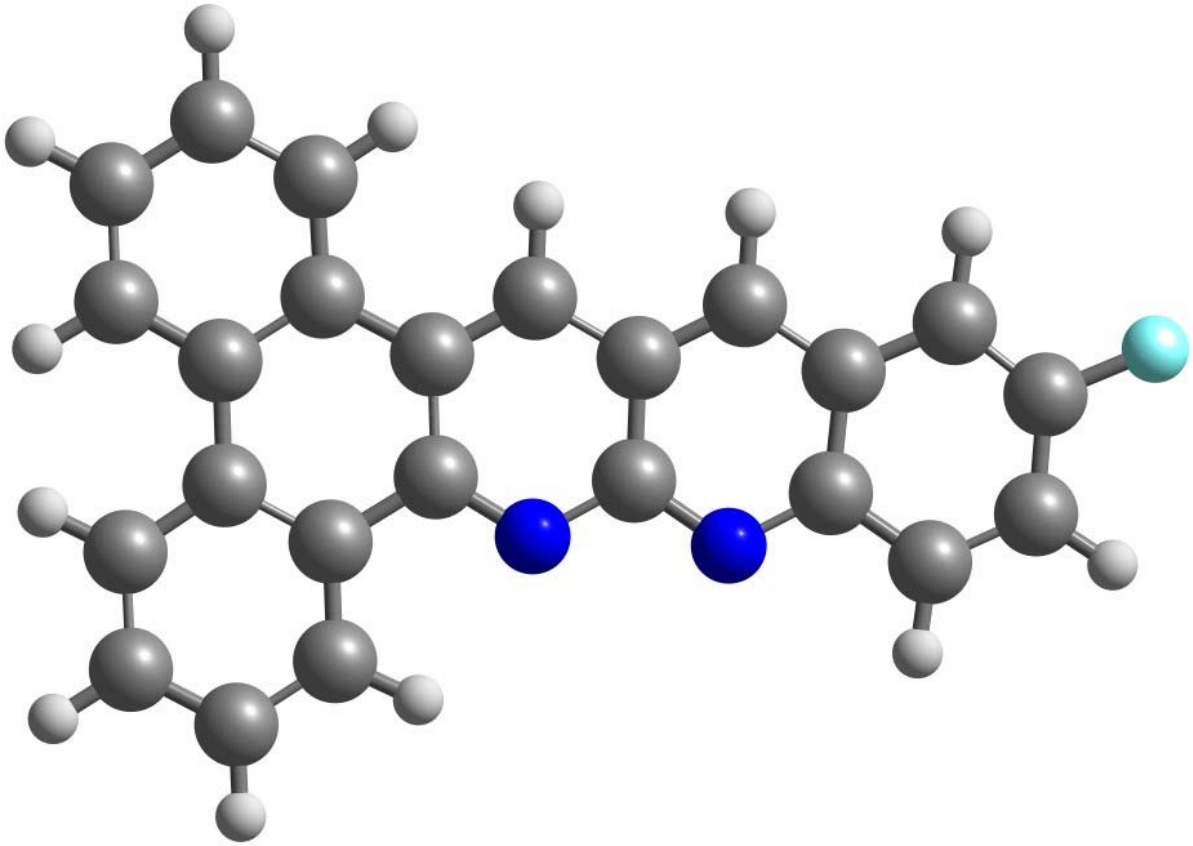

5c

Charge 0; Multiplicity 1

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6	-3.384509000	0.925547000	0.000000000
6	-2.255172000	-1.288452000	0.000000000
6	-2.342216000	-2.739510000	0.000000000
6	-4.849111000	-2.591290000	0.000000000
6	-3.660501000	-3.388681000	0.000000000
6	-3.783219000	-4.800908000	0.000000000
6	-6.102729000	-3.253034000	0.000000000
6	-6.198522000	-4.643598000	0.000000000
6	-5.028271000	-5.426211000	0.000000000
7	-1.087035000	-0.619221000	0.000000000
6	0.094719000	-1.314944000	0.000000000
6	-1.142302000	-3.444683000	0.000000000
6	0.106284000	-2.768572000	0.000000000
7	1.239872000	-0.575659000	0.000000000
6	2.431143000	-1.235610000	0.000000000
6	2.539109000	-2.688899000	0.000000000
6	1.347854000	-3.432899000	0.000000000
6	3.632396000	-0.456320000	0.000000000
6	4.872000000	-1.062452000	0.000000000
6	4.947939000	-2.485548000	0.000000000
6	3.838161000	-3.294656000	0.000000000
1	5.788232000	-0.475892000	0.000000000
17	6.612202000	-3.247134000	-0.000001000
1	3.521426000	0.626920000	0.000000000
1	3.932464000	-4.380186000	0.000000000
1	1.383350000	-4.525651000	0.000000000
1	-1.130556000	-4.535624000	0.000000000
1	-2.385664000	1.358338000	0.000000000
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1	-6.704578000	1.709121000	0.000000000
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1	-7.178850000	-5.120817000	0.000000000
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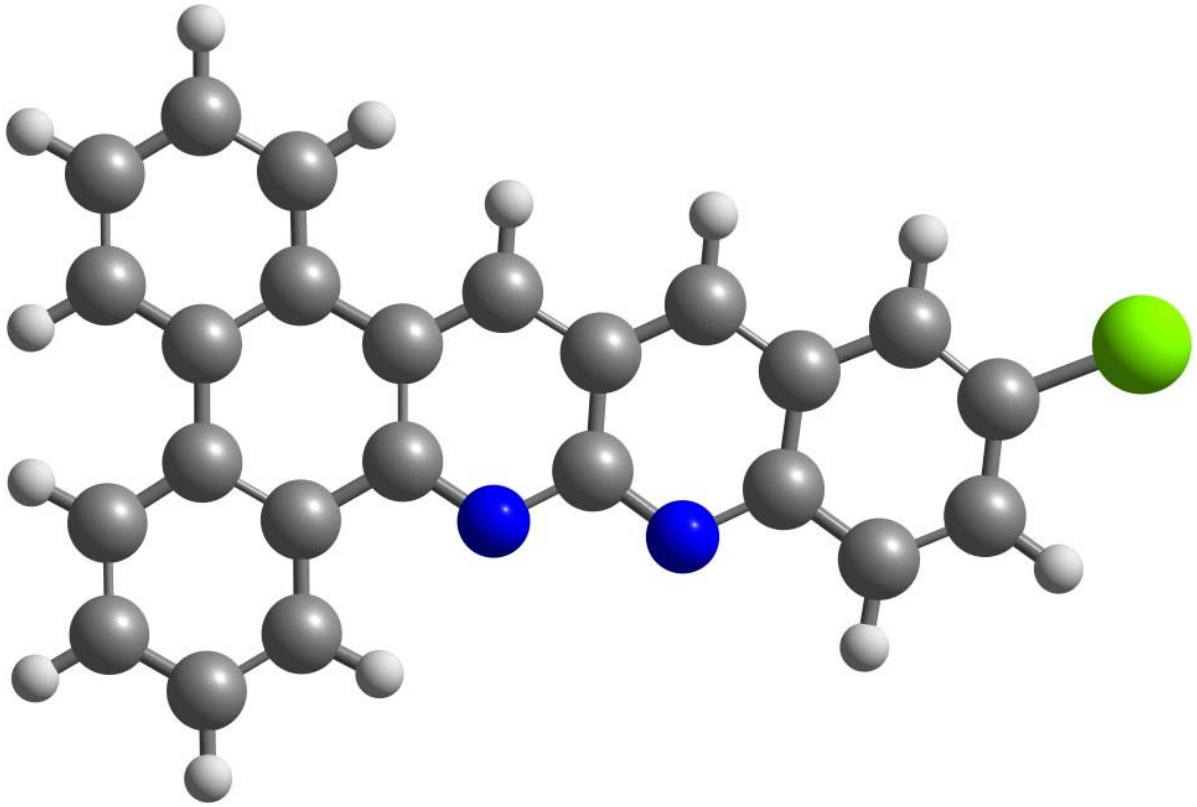

5d

Charge 0; Multiplicity 1

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6	-3.483537000	-0.485512000	0.000000000
6	-3.389472000	0.926613000	0.000000000
6	-2.258632000	-1.286694000	0.000000000
6	-2.344810000	-2.737631000	0.000000000
6	-4.851875000	-2.591074000	0.000000000
6	-3.662711000	-3.387648000	0.000000000
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6	-6.200008000	-4.644274000	0.000000000
6	-5.029214000	-5.426092000	0.000000000
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6	0.091395000	-1.311498000	0.000000000
6	-1.144397000	-3.442035000	0.000000000
6	0.103726000	-2.765216000	0.000000000
7	1.236153000	-0.571360000	0.000000000
6	2.427565000	-1.231091000	0.000000000
6	2.536431000	-2.683788000	0.000000000
6	1.345765000	-3.428667000	0.000000000
6	3.629820000	-0.454389000	0.000000000
6	4.867719000	-1.063414000	0.000000000
6	4.953433000	-2.488504000	0.000000000
6	3.835113000	-3.289110000	0.000000000
1	5.782087000	-0.473622000	-0.000001000
35	6.728717000	-3.302825000	-0.000001000
1	3.521709000	0.629277000	0.000000000
1	3.922809000	-4.375528000	0.000000000
1	1.382252000	-4.521460000	0.000000000
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1	-2.390818000	1.359872000	0.000000000
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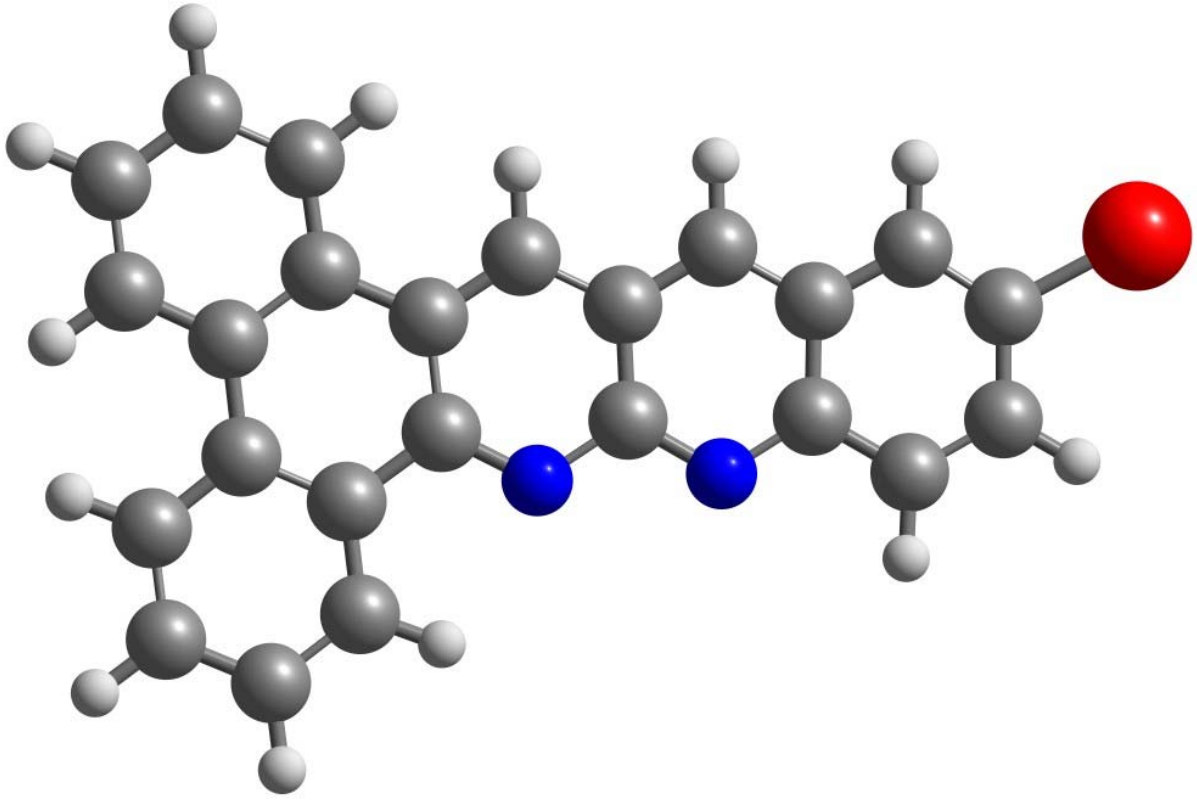
1	-6.903959000	-0.736584000	0.000000000
1	-7.023872000	-2.670140000	0.000000000
1	-7.180035000	-5.122138000	0.000000000
1	-2.889357000	-5.419963000	0.000000000
1	-5.093042000	-6.514728000	0.000000000



5e

Charge 0; Multiplicity 1

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6	-4.762425000	-1.112846000	0.000000000
6	-3.480427000	-0.489599000	0.000000000
6	-3.375017000	0.921427000	0.000000000
6	-2.261262000	-1.301416000	0.000001000
6	-2.359549000	-2.751207000	0.000001000
6	-4.866251000	-2.583278000	0.000000000
6	-3.683732000	-3.389632000	0.000000000
6	-3.818282000	-4.800749000	0.000001000
6	-6.125040000	-3.235186000	-0.000001000
6	-6.232400000	-4.624975000	-0.000001000
6	-5.068278000	-5.416504000	0.000000000
7	-1.088566000	-0.641776000	0.000001000
6	0.088770000	-1.347370000	0.000001000
6	-1.165641000	-3.466139000	0.000001000
6	0.089984000	-2.801757000	0.000001000
7	1.239410000	-0.618582000	0.000002000
6	2.425176000	-1.289826000	0.000001000
6	2.527235000	-2.745585000	0.000001000
6	1.324599000	-3.476527000	0.000001000
6	3.632517000	-0.524205000	0.000001000
6	4.868278000	-1.139472000	0.000000000
6	4.957993000	-2.570475000	0.000000000
6	3.815774000	-3.353784000	0.000000000
1	5.772189000	-0.533531000	0.000000000
8	6.176215000	-3.260371000	-0.000001000
1	3.530440000	0.560249000	0.000001000
1	3.917661000	-4.439291000	0.000000000
1	1.349361000	-4.569696000	0.000001000
1	-1.163455000	-4.557305000	0.000001000
1	-2.372543000	1.345969000	0.000001000
1	-4.423245000	2.807211000	0.000000000
1	-6.689251000	1.731669000	-0.000002000
1	-6.902800000	-0.711890000	-0.000002000
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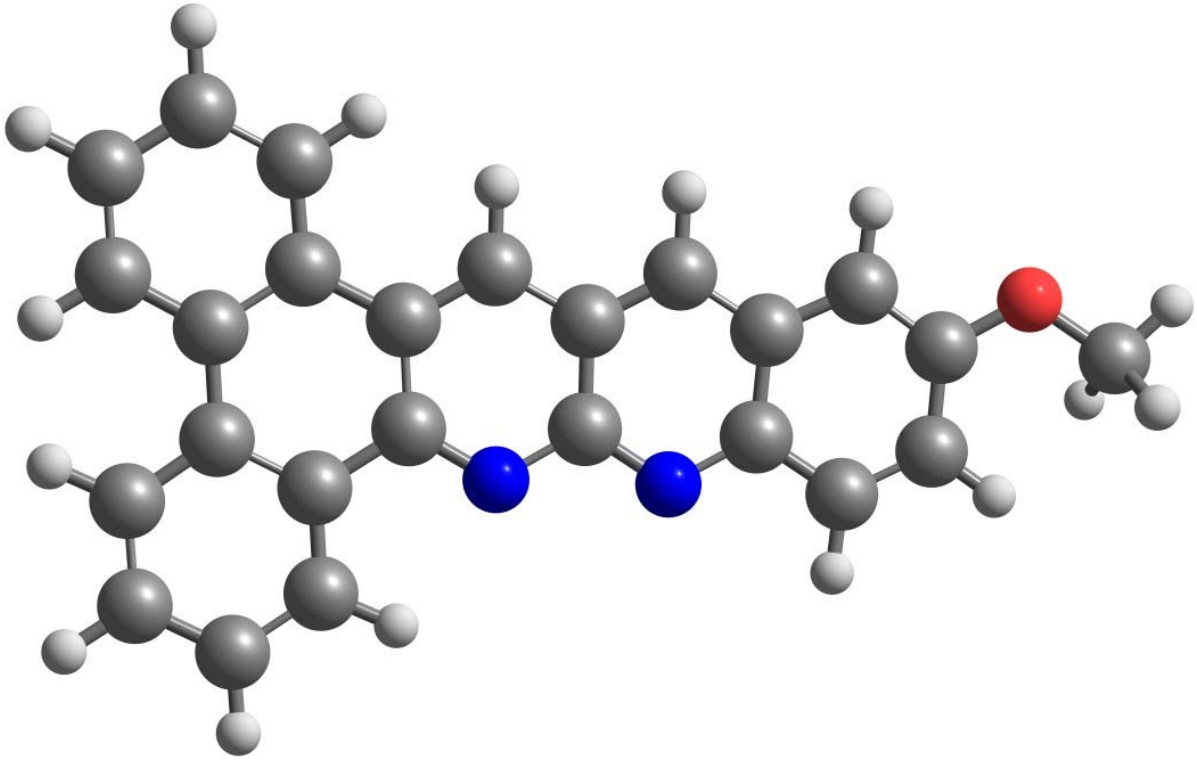
1	-7.216679000	-5.094187000	-0.000001000
1	-2.928237000	-5.428174000	0.000001000
1	-5.140993000	-6.504681000	0.000000000
6	7.416368000	-2.482986000	-0.000002000
1	8.211781000	-3.232502000	-0.000003000
1	7.496522000	-1.857067000	0.902083000
1	7.496520000	-1.857066000	-0.902086000



5f

Charge 0; Multiplicity 1

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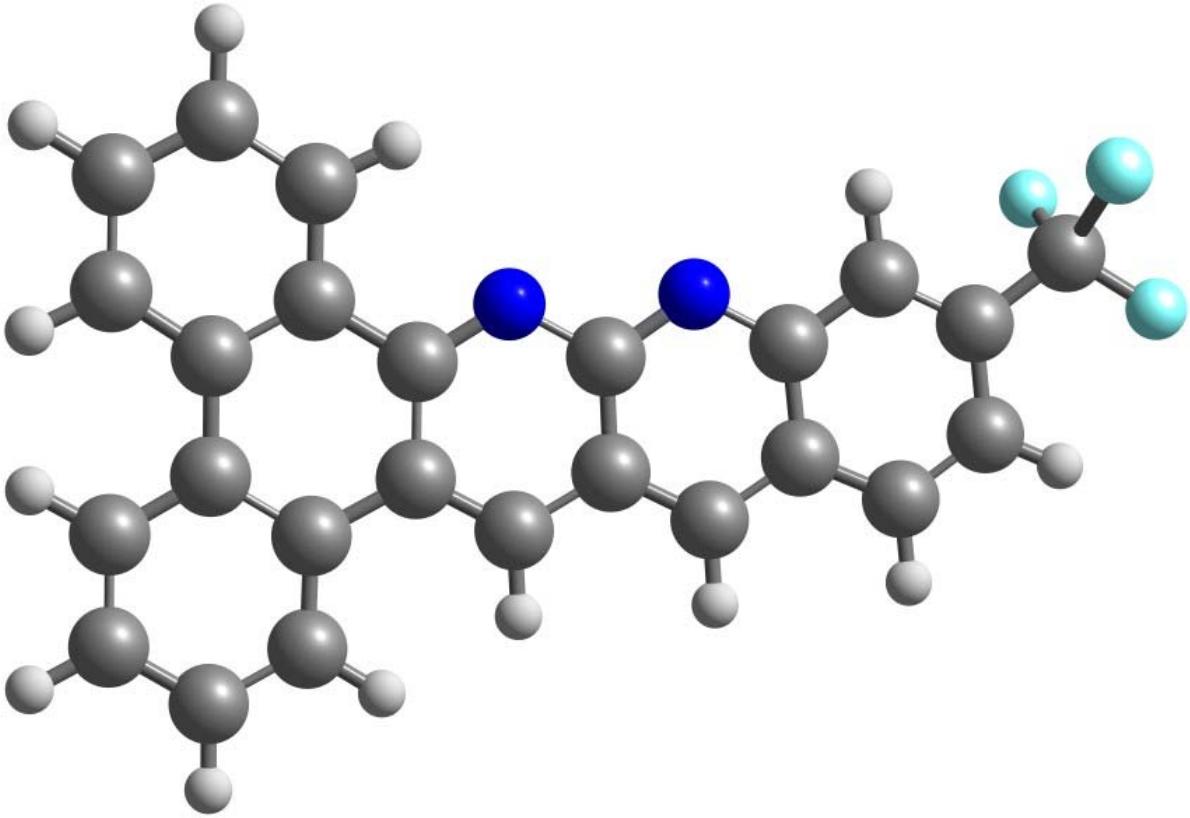
6	-4.579033000	1.728107000	0.027463000
6	-4.825897000	-1.105876000	0.019509000
6	-3.544167000	-0.481644000	0.013713000
6	-3.438047000	0.929520000	0.017706000
6	-2.326037000	-1.292697000	0.003830000
6	-2.424191000	-2.744271000	-0.000134000
6	-4.929605000	-2.576261000	0.014903000
6	-3.747509000	-3.382987000	0.005144000
6	-3.881049000	-4.794159000	0.000624000
6	-6.188137000	-3.228058000	0.019834000
6	-6.294797000	-4.617926000	0.015342000
6	-5.130960000	-5.409770000	0.005588000
7	-1.153553000	-0.632541000	-0.000875000
6	0.023507000	-1.337263000	-0.009652000
6	-1.230134000	-3.458332000	-0.008802000
6	0.024196000	-2.792018000	-0.013711000
7	1.172217000	-0.606296000	-0.014138000
6	2.359124000	-1.277852000	-0.022587000
6	2.458082000	-2.730050000	-0.026904000
6	1.260340000	-3.464543000	-0.022286000
6	3.559259000	-0.505410000	-0.027374000
6	4.792812000	-1.131916000	-0.035810000
6	4.897284000	-2.560658000	-0.040015000
6	3.755985000	-3.334368000	-0.035609000
6	6.026049000	-0.288120000	-0.041132000
1	3.456536000	0.578500000	-0.024030000
1	3.831536000	-4.423418000	-0.038752000
1	1.288414000	-4.557620000	-0.025358000
1	-1.227207000	-4.549260000	-0.011958000
1	-2.436300000	1.355436000	0.012930000
1	-4.486978000	2.814604000	0.030540000
1	-6.751821000	1.738122000	0.041227000
1	-6.965990000	-0.704810000	0.034529000
1	-7.101864000	-2.636797000	0.027255000
1	-7.278878000	-5.087205000	0.019349000
1	-2.991428000	-5.422113000	-0.007079000
1	-5.204002000	-6.497736000	0.001818000
1	5.882801000	-3.020584000	-0.046651000
9	6.093814000	0.565540000	-1.169980000
9	6.103603000	0.565644000	1.086904000
9	7.213281000	-1.052665000	-0.046302000



5g

Charge 0; Multiplicity 1

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6	-4.689550000	1.763017000	0.003758000
6	-4.828804000	-1.077965000	0.009527000
6	-3.571015000	-0.406143000	0.002735000
6	-3.519354000	1.008200000	-0.000087000
6	-2.323626000	-1.171433000	-0.001378000
6	-2.365728000	-2.619924000	0.001517000
6	-4.876026000	-2.550393000	0.012315000
6	-3.662715000	-3.310104000	0.008366000
6	-3.741435000	-4.725643000	0.011136000
6	-6.108437000	-3.251571000	0.018909000
6	-6.160632000	-4.644305000	0.021526000
6	-4.966112000	-5.389699000	0.017602000
7	-1.173282000	-0.465484000	-0.007758000
6	0.024056000	-1.126914000	-0.011752000
6	-1.141674000	-3.289029000	-0.002418000
6	0.081261000	-2.574467000	-0.009116000
7	1.153970000	-0.356926000	-0.018344000
6	2.361128000	-0.966646000	-0.022507000
6	2.514322000	-2.412095000	-0.020197000
6	1.352608000	-3.191286000	-0.013412000
6	3.553508000	-0.126009000	-0.029661000
6	4.846559000	-0.741600000	-0.034321000
6	4.950607000	-2.183670000	-0.031792000
6	3.839160000	-2.982520000	-0.024990000
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1	1.427181000	-4.282460000	-0.011470000
1	-1.096220000	-4.379178000	-0.000431000
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1	-6.983373000	-0.757641000	0.018754000
1	-7.044850000	-2.696885000	0.022086000
1	-7.125553000	-5.152006000	0.026651000
1	-2.827226000	-5.317156000	0.008154000
1	-4.996147000	-6.479834000	0.019613000
1	5.947927000	-2.627699000	-0.035473000
6	5.998766000	0.085839000	-0.041309000
6	3.451036000	1.284850000	-0.032086000
6	5.878790000	1.474820000	-0.043613000
6	4.598944000	2.076228000	-0.038989000
1	2.452218000	1.718619000	-0.028391000
1	4.509723000	3.163334000	-0.040860000
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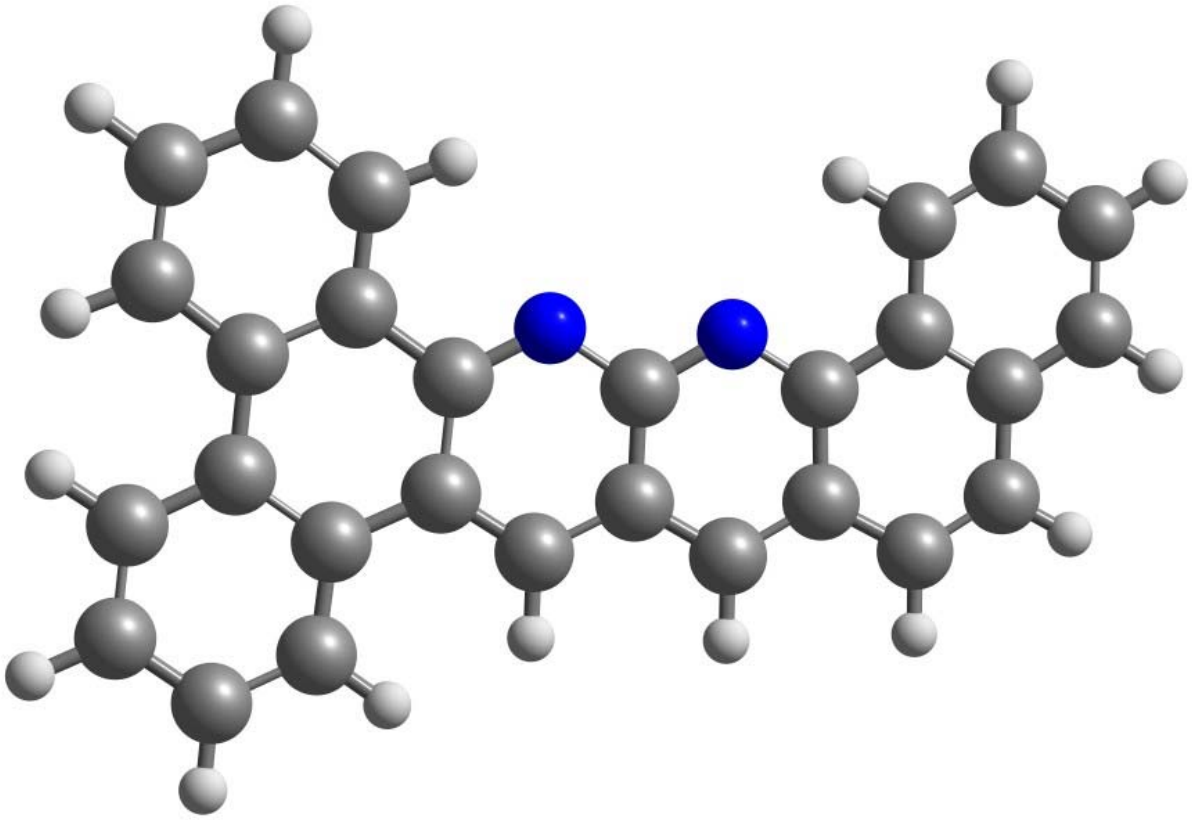
1	6.773372000	2.098395000	-0.049021000



5h

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6	-3.125258000	0.423309000	0.000007000
6	-1.924274000	1.178011000	0.005306000
6	-0.744626000	3.378664000	-0.021219000
6	0.526721000	2.669312000	0.018394000
6	-0.637017000	0.520683000	0.043854000
6	0.531886000	1.229406000	0.050128000
7	1.733519000	3.289041000	0.027836000
6	-0.691197000	4.772996000	-0.050759000
6	1.768997000	4.656134000	-0.001483000
6	0.552301000	5.448750000	-0.041918000
7	3.008490000	5.238561000	0.009119000
6	3.100945000	6.585530000	-0.019301000
6	0.674467000	6.857494000	-0.070987000
6	1.936570000	7.456869000	-0.060635000
6	4.433143000	7.181513000	-0.008057000
6	4.564400000	8.607162000	-0.038636000
6	2.123393000	8.887142000	-0.089757000
6	3.378041000	9.433879000	-0.079323000
6	5.593226000	6.373462000	0.031877000
6	6.860061000	6.956639000	0.041436000
6	5.863845000	9.175857000	-0.028436000
6	6.996401000	8.363531000	0.011101000
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1	-3.058080000	-0.666261000	0.025988000
1	-5.407950000	2.957855000	-0.099681000
1	-3.351160000	4.309987000	-0.091148000
1	-0.620844000	-0.571081000	0.068406000
1	1.508926000	0.749953000	0.079167000
1	-1.604267000	5.369541000	-0.081164000
1	-0.224964000	7.478133000	-0.102154000
1	1.237616000	9.524492000	-0.120875000
1	3.507860000	10.517970000	-0.101950000
1	5.454901000	5.293184000	0.054379000
1	7.748842000	6.325987000	0.072397000
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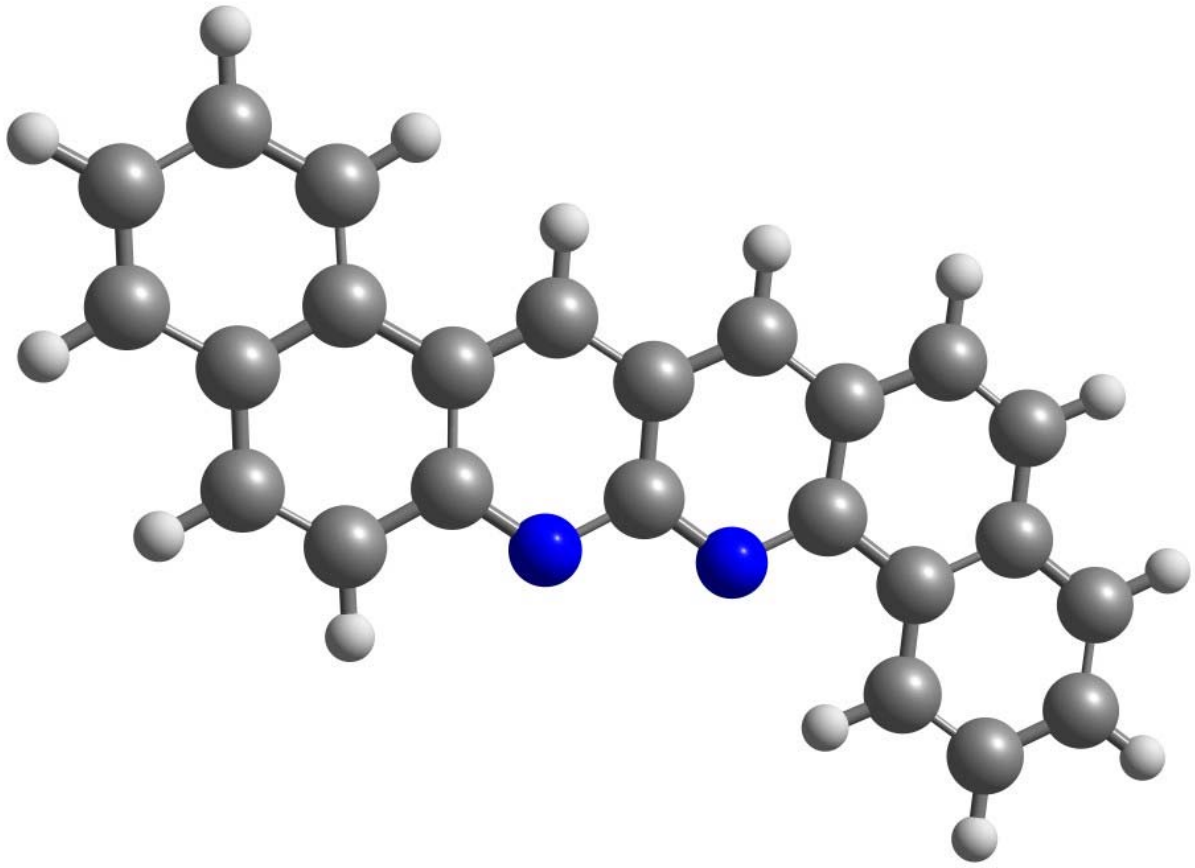
1	7.989591000	8.814267000	0.018584000



11a

Charge 0; Multiplicity 1

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6	3.062987000	0.674184000	-0.034601000
6	1.664684000	-1.384071000	0.071438000
6	2.963710000	-0.778531000	0.038975000
7	4.253324000	1.339547000	-0.065949000
6	5.401000000	0.607225000	-0.026950000
6	4.159495000	-1.513600000	0.074922000
6	5.398861000	-0.845125000	0.041944000
7	6.580837000	1.308828000	-0.052490000
6	7.751305000	0.645805000	-0.016272000
6	7.846647000	-0.803392000	0.044463000
6	6.650674000	-1.514156000	0.074662000
1	-0.287692000	1.419002000	-0.072369000
1	1.967883000	2.527179000	-0.130258000
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1	4.129965000	-2.605595000	0.128863000
1	6.646002000	-2.604234000	0.127168000
6	9.169790000	-1.442155000	0.076373000
6	8.972437000	1.455656000	-0.035312000
6	10.343839000	-0.624700000	0.060638000
6	10.245344000	0.822915000	0.004899000
6	11.419393000	1.640373000	-0.010786000
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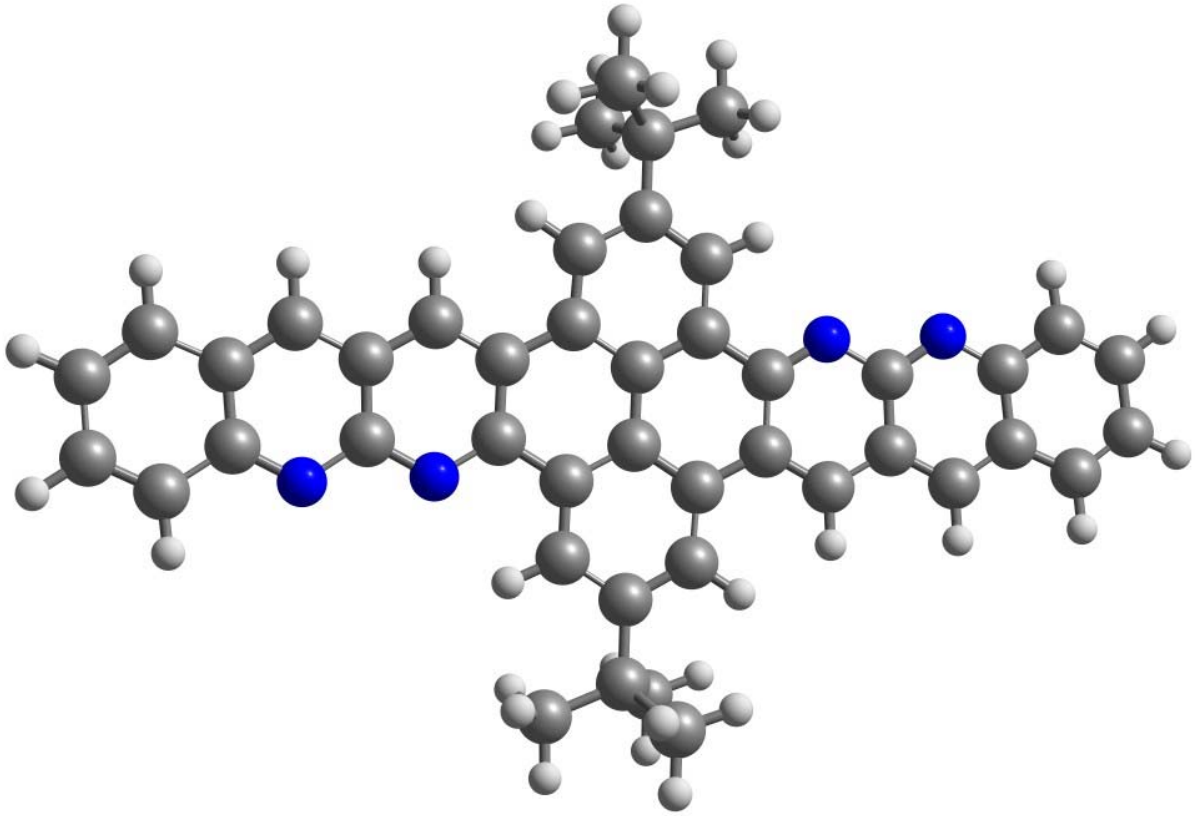

11b

Charge 0; Multiplicity 1

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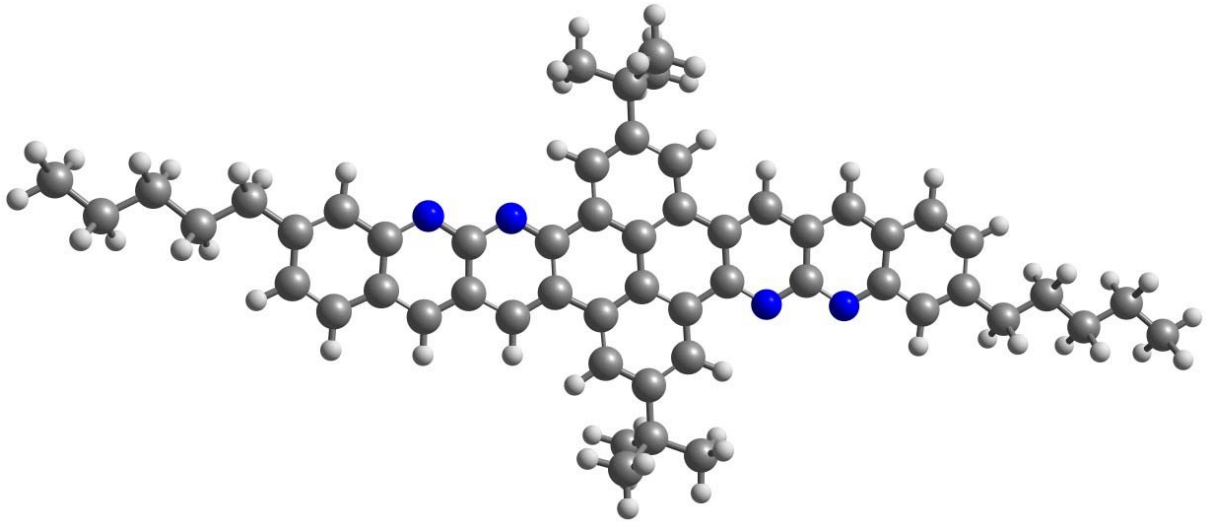

8. References

[1] C. M. Cardona, W. Li, A. E. Kaifer, D. Stockdale, G. C. Bazan, *Adv. Mater.* **2011**, *23*, 2367-2371.

[2] B. R. Rosen, J. C. Ruble, T. J. Beauchamp, A. Navarro, *Org. Lett.* **2011**, *13*, 2564-2567.

[3] T. W. Liwosz, S. R. Chemler, *Chem. Eur. J.* **2013**, *19*, 12771-12777.

[4] Z.-H. Wu, Z.-T. Huang, R.-X. Guo, C.-L. Sun, L.-C. Chen, B. Sun, Z.-F. Shi, X. Shao, H. Li, H.-L. Zhang, *Angew. Chem. Int. Ed.* **2017**, *56*, 13031-13035.

[5] T. Yamato, A. Miyazawa, M. Tashiro, *Chem. Ber.* **1993**, *126*, 2505-2511.

[6] F. Neese, *An Ab Initio, DFT and Semiempirical electronic structure package* **2009**, *3*.

[7] P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* **1994**, *98*, 11623-11627.

[8] R. Krishnan, J. S. Binkley, R. Seeger, J. A. Pople, *J. Chem. Phys.* **1980**, *72*, 650-654.