SUPPORTING INFORMATION

An expeditious synthesis of 6,7-Dihydrodibenzo[b,j][4,7] phenanthroline derivatives as fluorescent materials

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1. General remarks

All the reactions were carried out in oven-dried glassware. Progress of reactions was monitored by Thin Layer Chromatography (TLC) while purification of crude compounds was done by column chromatography using Silica gel (Mesh size 100-200). The NMR spectra were recorded on Bruker-400 MHz NMR spectrometer (400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR) with $CDCl_3$or $(CD_3)_2SO$ as the solvent and TMS as an internal reference. Integrals are in accordance with assignments; Coupling constants were reported in Hertz (Hz). All ^{13}C spectra are proton-decoupled.. Multiplicity is indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), br s (broad singlet). FTIR spectra were recorded on a Perkin-Elmer RX-IFT-IR and absorbencies are reported in cm-1. HRMS analyses were recorded using Q-T of Micro mass spectrometer (different mass analyses based on the availability of instruments). Yields refer to quantities obtained after chromatography. Absorption spectra were recorded using JASCO V-670 spectrophotometer. Steady-state fluorescence spectra were recorded on Hitachi F-7000 FL spectrofluorophotometer by excitation at the respective absorption maxima. Quantum yields of compounds were estimated by comparison with the known quantum yields of anthracene in ethanol (Φ = 0.27) at an excitation wavelength of 246 nm using the following equation.

$$\Phi_f = \Phi_{fR} \cdot I/I_R \cdot OD_R/OD \cdot n^2/n^2_R$$

where Φ is the quantum yield, I is the integrated intensity, OD is the optical density, and n is the refractive index. The subscript R refers to anthracene.

The molar extinction coefficient (ε) was calculated using Beer–Lambert's law

$$A = \varepsilon cl$$

The Stoke's Shift was calculated using the following equation.

$$\Delta \bar{\upsilon} = 10^7/\lambda_{max(Absorption)} - 10^7/\lambda_{max(Emission)}$$

Experimental Procedures

Synthesis of 1-(2-Amino-5-bromophenyl)ethanone: [1]

To a stirred solution of 1-(2-aminophenyl)ethanone (0.5 g, 3.7 mmol) in 5.0mL of CH_3CN at 0 ^{0}C was added dropwise *N*-bromosuccinimide (0.66 g, 3.7 mmol) dissolved in 5.0mL CH_3CN. Allowed the mixture to attain room temperature, and continued to stir at room temperature for 3 hours. Removal of the solvent under reduced pressure and purification through a column of silica gel (petroleum ether: ethyl acetate = 5: 1) afforded 1-(2- amino-5-bromophenyl)ethenone as a yellow solids. M. P: 86-88 °C.

Synthesis of 1-(2-Amino-3,5-dibromophenyl)ethanone:[2]

To a stirred solution of 1-(2-aminophenyl)ethanone (0.5 g, 3.7 mmol) in 5.0mL of CH_3CN at 0 ^{0}C was added dropwise *N*-bromosuccinimide (1.32 g, 7.4 mmol) dissolved in 10.0mL CH_3CN. Allowed the mixture to attain room temperature, and continued to stir at room temperature for 3 hours. Removal of the solvent under reduced pressure and purification through a column of silica gel (petroleum ether: ethyl acetate = 5: 1) afforded 1-(2-Amino-3,5-dibromophenyl)ethenone as a brown solids. M. P: 129-131 °C.

General procedure for the synthesis of compound 3 a-d :

2-Aminoarylketone **1** (2.0 mmol) and 1,4 cyclohexanedione **2** (1.0 mmol) were mixed with the given amount of *p*-TsOH and introduced into a test tube (10.0mL). The reaction mixture was kept in a preheated oil-bath for 120 sec at 100 ^{0}C. When the reaction was completed (Initially, the reaction mixture turned to clear liquid at the preheated conditions. Then, immediately the product was precipitated. The completion of the reaction could be monitored by TLC), it was cooled to room temperature, and water (3.0mL) was added to the reaction mixture. The resulting suspension was neutralized by adding sodium bicarbonate to it. Then the mixture was stirred for 5 min and the solid was collected by B¨uchner filtration, washed with H_2O (6.0 mL ×3), and dried in a desiccator to give the desired product.

General procedure for the synthesis of compound 6 a-k :

A mixture of compound **3 b,c** (0.191 mmol), arylboronic acids (0.229 mmol), $Pd(OAc)_2$ (20 mol%) and K_2CO_3 (0.229 mmol) in 3.0 mL of DMF-H_2O (2:1) was stirred at 100 ^{0}C for 3 hours. After completion of the reaction (monitored by TLC), the residue was extracted with EtOAc and washed with saturated brine. The organic layer was dried over anhydrous Na_2SO_4 and purified through a silica gel column

chromatography by gradient elution using EtOAc: hexane to afford the desired compounds in very good yields.

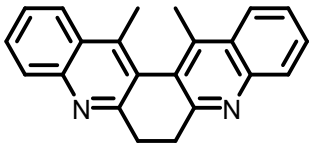
NBS bromination of compound 3a:

Treat a solution of 13,14-dimethyl-6,7-dihydrodibenzo[b,j][4,7] phenanthroline (310 mg, 1.0 mmol) in acetonitrile (10.0mL) with *N*-bromosuccinimide (356 mg, 2.0 mmol). Stir the mixture at 80 ^{0}C for 3 hours. The reaction mixture was cooled to room temperature. Evaporated the solvent under reduced pressure and the compound was extracted with ethyl acetate. The organic phase was washed with water. Purified the compound by passing through column of silica gel (10% EtOAc/Hexane).

General procedure for the synthesis of compound 8 :

A mixture of compound 3 b (0.191 mmol), 2,3-dimethylaniline (0.229 mmol), $Pd(dppf)_2Cl_2$ (10 mol%), SPhos (20 mol%), and NaO*t*-Bu (0.916 mmol) in 4.0mL of 1,4-Dioxane was Stirred at 110 ^{0}C for 12 hours. After the reaction was completed (monitored by TLC), the residue was extracted with EtOAc and washed with saturated brine. The organic layer was dried over anhydrous Na_2SO_4 and purified through a silica gel column chromatography by gradient elution using EtOAc: hexane to afford compounds in very good yields.

Spectral data of Synthesised derivatives



3a

13,14-dimethyl-6,7-dihydrodibenzo[b,j][4,7]phenanthroline **(3a)**

Nature: White powder; **Yield:** 94%; **Rf (50% EtOAc-Hexane):** 0.46, **M. P:** 298-300 ^{0}C.

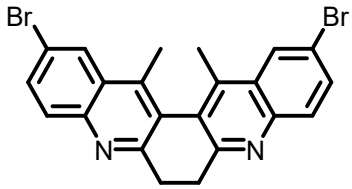
FTIR(KBr)ν_{max}: 827, 906, 1554, 1672, 2937 cm^{-1};

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (t, J = 8.1 Hz, 4H), 7.69 – 7.65 (m, 2H), 7.53 (t, J = 7.6 Hz, 2H), 3.30 (d, J = 10.3 Hz, 2H), 3.13 (d, J = 10.4 Hz, 2H), 2.49 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 161.6, 145.9, 141.9, 129.7, 128.9, 127.8, 126.4, 126.2, 124.5, 34.2, 17.6.

DEPT 135 (101 MHZ, $CDCl_3$): δ 129.7, 128.9, 126.2, 124.5, 34.2 **(↓)**, 17.6 **(↑)**.

HRMS-ESI: Calcd. for $C_{22}H_{18}N_2$ [M+H] + m/z: 311.1548; Found 311.1554



3b

2,11-dibromo-13,14-dimethyl-6,7-dihydrodibenzo[b,j][4,7] phenanthroline **(3b)**

Nature: Green powder; **Yield:** 93 %; **Rf (40% EtOAc-Hexane):** 0.40, **M. P: :** 299-301 ^{0}C.

FTIR(KBr)ν_{max}: 825, 1068, 1309, 1483 cm^{-1};

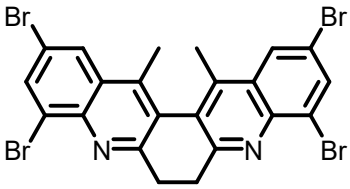
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 (d, J = 2.1 Hz, 2H), 7.95 (d, J = 8.9 Hz, 2H), 7.80 (dd, J = 8.9, 2.1 Hz, 2H), 3.33 (d, J = 10.4 Hz, 2H), 3.16 (d, J = 10.4 Hz, 2H), 2.51 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 162.0, 144.9, 140.9, 133.0, 130.8, 129.0, 127.0, 126.8, 120.2, 34.2, 17.6.

DEPT 135 (101 MHZ, $CDCl_3$): δ 133.2, 130.9, 127.1, 34.3 **(↓)**,17.7 **(↑)**.

HRMS-ESI: Calcd. for $C_{22}H_{16}Br_2N_2$ [M+H] + m/z:

466.9758; Found 466.9750



3c

2,4,9,11-tetrabromo-13,14-dimethyl-6,7-dihydrodibenzo[b,j][4,7] phenanthroline **(3c)**

Nature: Brown powder; **Yield:** 90 %; **Rf (30% EtOAc-Hexane):** 0.46, **M. P: :** 299-301 ^{0}C.

FTIR(KBr)ν_{max}: 704, 835, 1271, 1597 cm^{-1};

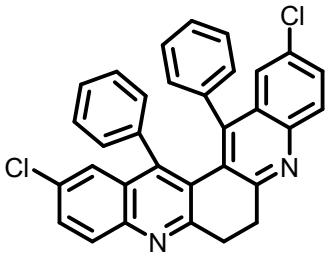
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, *J* = 6.5 Hz, 4H), 3.40 (d, *J* = 10.7 Hz, 2H), 3.12 (d, *J* = 10.6 Hz, 2H), 2.47 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 152.7, 146.7, 140.0, 139.2, 135.1, 130.1, 129.6, 128.5, 128.4, 127.8, 127.6, 127.3, 126.5, 126.0, 123.7, 28.3, 25.5, 14.1.

DEPT 135 (101 MHZ, $CDCl_3$): 132.4, 123.2, 30.6 **(↓)**, 14.1 **(↑)**.

HRMS-ESI: Calcd. for $C_{22}H_{14}Br_4N_2$ [M+H] + m/z: 622.7968; Found: 622.7952

2,11-dichloro-13,14-diphenyl-6,7-dihydrodibenzo[b,j][4,7]phenanthroline **(3d)**



3d

Nature: Brown powder; **Yield: 88**%; **Rf (30% EtOAc-Hexane):** 0.50, **M. P: :** 250-252 ^{0}C.

FTIR(KBr)ν_{max}: 702, 827, 1020, 1076, 1157, 1477 cm^{-1};

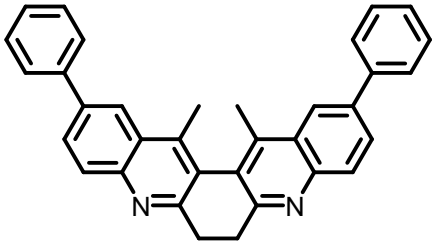
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, J = 8.9 Hz, 2H), 7.58 (d, J = 2.2 Hz, 2H), 7.51 (dd, J = 8.9, 2.3 Hz, 2H), 7.21 – 6.84 (m, 6H), 6.60 – 6.09 (m, 4H), 3.36 (d, J = 10.4 Hz, 2H), 3.22 (d, J = 10.6 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 162.7, 145.8, 145.7, 134.9, 132.0, 130.5, 128.7, 128.1, 126.8, 125.6, 125.0, 34.9.

DEPT 135 (101 MHZ, $CDCl_3$): δ 130.5, 128.7, 128.1, 125.0, 34.9 **(↓)**.

HRMS-ESI: Calcd. for $C_{32}H_{20}Cl_2N_2$ [M+H] + m/z: 503.1078; Found 503.1041

13,14-dimethyl-2,11-diphenyl-6,7-dihydrodibenzo [b,j][4,7] phenanthroline **(6a)**



(6a)

Nature: Yellow powder; **Yield:** 92%; **Rf (40% EtOAc-Hexane):** 0.46, **M. P: :** 269-271 ^{0}C.

FTIR(KBr)ν_{max}: 700, 758, 839, 1487, 3280 cm^{-1};

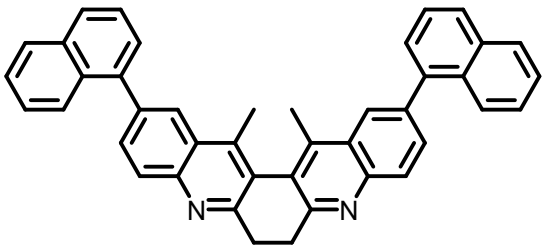
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 1.8 Hz, 2H), 8.09 (d, *J* = 8.6 Hz, 2H), 7.93 (dd, *J* = 8.6, 2.0 Hz, 2H), 7.70 – 7.67 (m, 4H), 7.45 (t, *J* = 7.6 Hz,4H), 7.35 (t, *J* = 7.4 Hz, 2H), 3.31 (d, *J* = 10.3 Hz, 2H), 3.16 (d, *J* = 10.4 Hz, 2H), 2.55 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 161.7, 145.5, 141.8, 141.0, 139.1, 129.5, 129.3, 129.1, 127.9, 127.8, 127.6, 126.8, 122.6, 34.4, 17.7.

DEPT 135 (101 MHZ, $CDCl_3$): 129.5, 129.3, 129.1, 127.8, 127.6, 122.6, 34.4 **(↓)**, 17.7 **(↑).**

HRMS-ESI: Calcd. for $C_{34}H_{26}N_2$ [M+H] + m/z: 463.2174; Found 463.2177

13,14-dimethyl-2,11-di(naphthalen-1-yl)-6,7-dihydrodibenzo [b,j][4,7]phenanthroline **(6b)**



(6b)

Nature: Yellow powder; **Yield:** 87%; **Rf (40% EtOAc-Hexane):** 0.47, **M. P: :** 270-272 ^{0}C.

FTIR(KBr)ν_{max}: 755, 1585, 2922 cm^{-1};

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (d, *J* = 8.5 Hz, 2H), 8.09 (s, 2H), 7.86 – 7.79 (m, 8H), 7.51 – 7.34 (m, 8H), 3.37 (d, *J* = 10.2 Hz, 2H), 3.20 (d, *J* = 10.2 Hz, 2H), 2.49 (s, 6H).

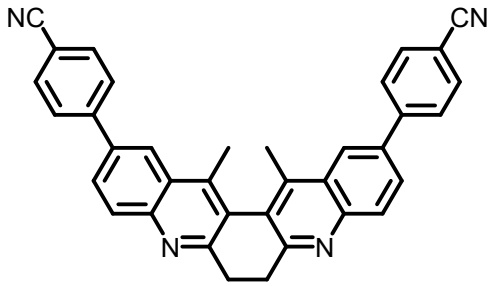
^{13}C NMR (101 MHz, $CDCl_3$): δ 161.8, 145.4, 141.9, 139.9, 138.8, 133.9, 132.1, 131.8, 128.6, 128.5, 128.2, 127.8, 127.4, 126.8, 126.4, 126.0, 125.9, 125.5, 34.3,

17.7.

DEPT 135 (101 MHZ, $CDCl_3$): 132.1, 128.6, 128.5, 128.2, 127.4, 126.4, 126.0, 125.9, 125.5, 34.3 **(↓)**, 17.7 **(↑).**

HRMS-ESI: Calcd. for $C_{42}H_{30}N_2$ [M+H] + m/z: 563.2487; Found 563.2482

4,4'-(13,14-dimethyl-6,7-dihydrodibenzo[b,j][4,7] phenanthroline-2,11-diyl)dibenzonitrile **(6c)**



(6c)

Nature: Yellow powder; **Yield:** 90%; **Rf (40% EtOAc-Hexane):** 0.47, **M. P: :** 225-226 ^{0}C.

FTIR(KBr)ν_{max}: 821, 1020, 1209, 1514, 1602, 2223, 2922, 3305 cm^{-1};

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.25 (d, J = 1.8 Hz, 2H), 8.22 (d, J = 8.6 Hz, 2H), 8.04 – 7.97 (m, 4H), 7.94 (d, J = 7.3 Hz,21H), 7.73 – 7.60 (m, 4H), 3.43 (d, J = 10.4 Hz, 2H), 3.25 (d, J = 10.3 Hz, 2H), 2.66 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 162.1, 142.2, 141.7, 137.7, 131.7, 131.4, 131.0, 129.8, 129.6, 129.1, 127.9, 126.9, 124.5, 124.5, 124.4, 124.4, 122.9, 34.2, 17.8.

DEPT 135 (101 MHZ, $CDCl_3$): 130.2, 130.2, 129.6, 128.9, 127.6, 127.6, 125.7, 122.6, 34.2 **(↓)**, 17.6 **(↑).**

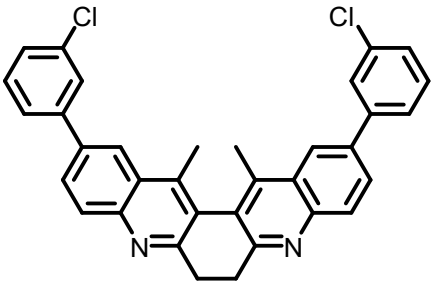
HRMS-ESI: Calcd. for $C_{36}H_{24}N_4$ [M+H] + m/z: 513.2079; Found 513.2074

2,11-bis(3-chlorophenyl)-13,14-dimethyl-6,7-dihydrodibenzo [b,j][4,7]phenanthroline **(6d)**

Nature: Yellow powder; **Yield:** 93%; **Rf (40% EtOAc-Hexane):** 0.44, **M. P: :** 158-160 ^{0}C.

FTIR(KBr)ν_{max}: 779, 837, 1473, 1566, 2962 cm^{-1};

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, *J* = 1.7 Hz, 2H), 8.05 (d, *J* = 8.6 Hz, 2H), 7.83 (dd, *J* = 8.7, 1.8 Hz,



(6d)

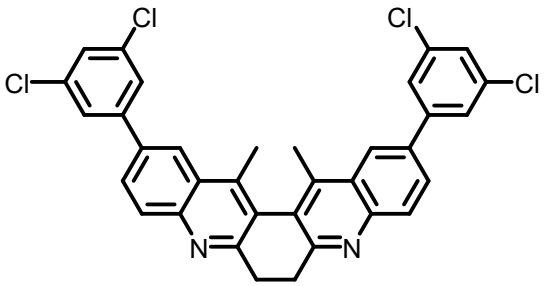
2H), 7.62 (s, 2H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.34 – 7.25 (m, 2H), 3.28 (d, *J* = 10.3 Hz, 2H), 3.12 (d, *J* = 10.4 Hz, 2H), 2.52 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 162.1, 145.8, 142.8, 141.9, 137.6, 135.0, 130.3, 129.7, 129.0, 127.9, 127.8, 127.7, 126.9, 125.8, 122.8, 34.3, 17.7.

DEPT 135 (101 MHZ, $CDCl_3$): 130.3, 129.7, 129.0, 127.8, 127.7, 125.8, 122.8, 34.3 **(↓)**, 17.75 **(↑).**

HRMS-ESI: Calcd. for $C_{34}H_{24}Cl_2N_2$ [M+H] + m/z: 531.1395; Found: 531.1374

2,11-bis(3,5-dichlorophenyl)-13,14-dimethyl-6,7-dihydrodibenzo [b,j][4,7]phenanthroline **(6e)**



(6e)

Nature: Yellow powder; **Yield:** 90%; **Rf (40% EtOAc-Hexane):** 0.42, **M. P: :** 248-250 ^{0}C.

FTIR(KBr)ν_{max}: 734, 804, 1446, 1523, 1597 cm^{-1};

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 – 8.10 (m, 4H), 7.86 (dd, *J* = 8.7, 1.9 Hz, 2H), 7.55 (t, *J* = 2.1 Hz, 4H), 7.34 (t, *J* = 1.7 Hz, 2H), 3.34 (d, *J* = 10.4 Hz, 2H), 3.21 – 3.14 (m, 2H), 2.57 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 152.7, 146.7, 140.0, 139.2, 135.1, 130.1, 129.6, 128.5, 128.4, 127.8, 127.6, 127.3, 126.5, 126.0, 123.7, 28.3, 14.1.

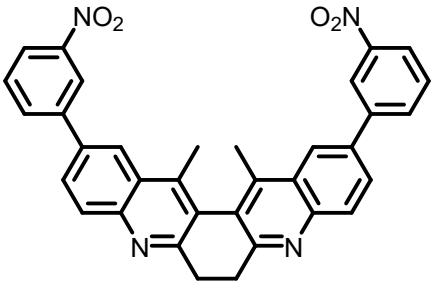
DEPT 135 (101 MHZ, $CDCl_3$): 126.2, 125.1, 124.0, 122.4, 122.2, 120.9, 119.3, 30.5 **(↓)**, 14.1**(↑).**

HRMS-ESI: Calcd. for $C_{34}H_{22}Cl_4N_2$ [M+H] + m/z:599.0615; Found: 599.0614

13,14-dimethyl-2,11-bis(3-nitrophenyl)-6,7-dihydrodibenzo [b,j][4,7]phenanthroline **(6f)**

Nature: Yellow powder; **Yield:** 88%; **Rf (40% EtOAc-Hexane):** 0.47, **M. P: :** 179-181 ^{0}C.

FTIR(KBr)ν_{max}: 686, 754, 1205, 1413, 1597 cm^{-1};



(6f)

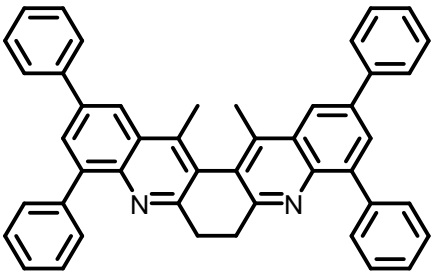
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20 (s, 2H), 8.15 (d, J = 8.6 Hz, 2H), 7.93 (d, J = 8.7 Hz, 2H), 7.72 (s, 2H), 7.61 (d, J = 7.6 Hz, 2H), 7.42 (t, J = 7.8 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 3.38 (d, J = 10.3 Hz, 2H), 3.22 (d, J = 10.3 Hz, 2H), 2.62 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 161.9, 145.6, 142.7, 141.9, 137.5, 134.9, 130.2, 129.6, 128.9, 127.8, 127.7, 127.6, 126.8, 125.7, 122.7, 34.2, 17.6.

DEPT 135 (101 MHZ, $CDCl_3$): 130.3, 129.7, 129.0, 127.8, 127.7, 125.8, 122.7, 34.3 **(↓)**, 17.7 **(↑)**.

HRMS-ESI: Calcd. for $C_{34}H_{24}N_4O_4$ [M+H] + m/z:553.1876; Found: 533.1887

13,14-dimethyl-2,4,9,11-tetraphenyl-6,7-dihydrodibenzo[b,j][4,7] phenanthroline **(6g)**



(6g)

Nature: White powder; **Yield:** 90%; **Rf (40% EtOAc-Hexane):** 0.45, **M. P: :** 182-184 ^{0}C.

FTIR(KBr)ν_{max}: 736, 829, 1220, 1471, 1589 cm^{-1};

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (s, 2H), 7.99 (s, 2H), 7.75- 7.72 (m, 8H), 7.47 (t, *J* = 7.5 Hz, 8H), 7.39 (t, *J* = 7.5 Hz, 4H), 3.33- 3.03 (m, 4H), 2.63 (s, 6H).

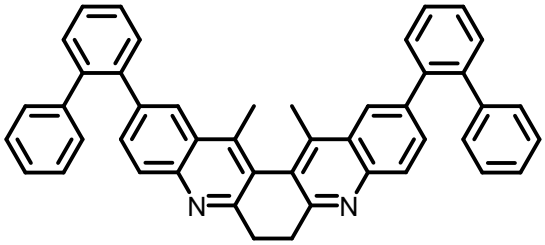
^{13}C NMR (101 MHz, $CDCl_3$): δ 148.1, 142.9, 127.4, 126.9, 120.3, 115.0, 112.3, 31.7, 21.4.

DEPT 135 (101 MHZ, $CDCl_3$): 142.7, 127.3, 126.8, 114.9, 31.0**(↑)**, 21.4 **(↓)**.

HRMS-ESI: Calcd. for $C_{46}H_{34}N_2$ [M+H] + m/z: 615.2800; Found: 615.2809

2,11-di([1,1'-biphenyl]-2-yl)-13,14-dimethyl-6,7-dihydrodibenzo [b,j][4,7]phenanthroline **(6h)**

Nature: Yellow powder; **Yield:** 89%; **Rf (40% EtOAc-Hexane):** 0.46, **M. P: :** 184-186 ^{0}C.



(6h)

FTIR(KBr)ν_{max}: 549, 815, 1118, 1303, 1440, 1552 cm^{-1};

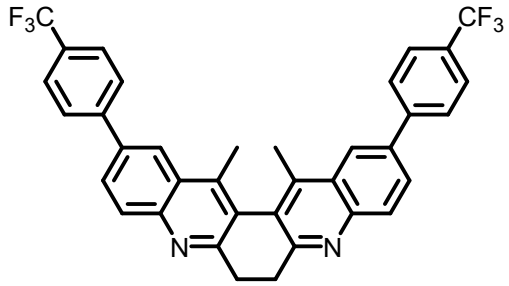
^{1}H NMR (400 MHz, DMSO-d6): δ 8.43 (s, 2H), 8.06 (s, 2H), 7.98 (d, *J* = 7.8 Hz, 4H), 7.81 (d, *J* = 7.7 Hz, 4H), 7.60 – 7.49 (m, 8H), 7.44 (m, 4H), 3.12 – 3.00 (m, 4H), 2.70 (s, 6H).

^{13}C NMR (101 MHz, DMSO-d6): δ 160.8, 158.9, 146.1, 144.9, 144.9, 136.0, 132.8, 130.8, 130.7, 129.3, 129.1, 126.4, 119.0, 116.5, 114.7, 107.3, 34.6, 16.2.

DEPT 135 (101 MHZ, DMSO-d6): 136.0, 132.8, 130.7, 129.3, 126.4, 116.5, 34.6 **(↓)**, 16.2 **(↑)**.

HRMS-ESI: Calcd. for $C_{46}H_{34}N_2$ [M+H] + m/z: 615.2800; Found: 615.2806

13,14-dimethyl-2,11-bis(4-(trifluoromethyl)phenyl)-6,7-dihydrodibenzo[b,j][4,7]phenanthroline **(6i)**



(6g)

Nature: Yellow powder; **Yield:** 90%; **Rf (40% EtOAc-Hexane):** 0.45, **M. P: :** 182-184 ^{0}C.

FTIR(KBr)ν_{max}: 754, 896, 1126, 1207, 1413, 1596 cm^{-1};

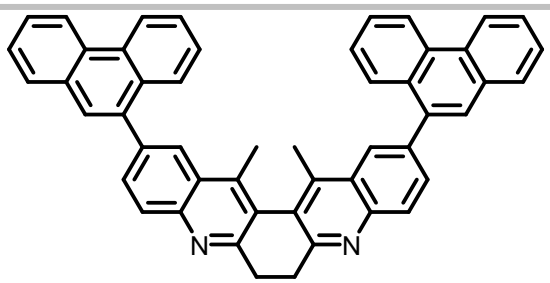
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, J = 6.8 Hz, 4H), 7.94 (d, J = 11.3 Hz, 4H), 7.87 (d, J = 7.2 Hz, 2H), 7.60 (q, J = 7.7 Hz, 4H), 3.40 (d, J = 10.2 Hz, 2H), 3.18 (d, J = 9.8 Hz, 2H), 2.60 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 161.9, 142.6, 141.7, 137.9, 131.7, 131.4, 131.4, 129.6, 129.6, 129.3, 127.9, 126.8, 125.6, 124.5, 124.4, 124.4, 122.9, 33.9, 17.8.

DEPT 135 (101 MHZ, $CDCl_3$): 130.9, 129.6, 129.3, 124.5, 124.4, 124.3, 122.9, 33.9 **(↓)**, 17.8 **(↑)**.

HRMS-ESI: Calcd. for $C_{36}H_{24}F_6N_2$ [M+H] + m/z: 599.1922; Found: 599.1924

13,14-dimethyl-2,11-di(phenanthren-9-yl)-6,7-dihydrodibenzo[b,j] [4,7]phenanthroline **(6j)**



(6h)

Nature: White powder; **Yield:** 88%; **Rf (40% EtOAc-Hexane):** 0.47, **M. P: :** 275-277 ^{0}C.

FTIR(KBr)ν_{max}: 729, 958, 1097, 1226, 1460, 1593 cm^{-1};

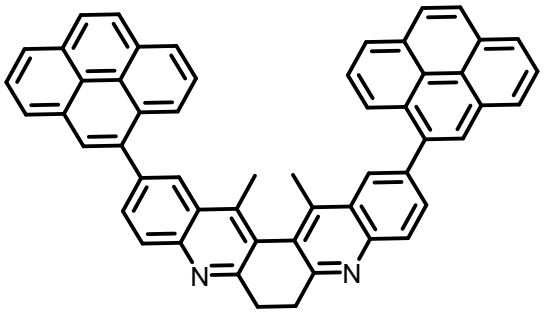
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.74 (d, *J* = 8.1 Hz, 2H), 8.68 (d, *J* = 8.0 Hz, 2H), 8.16 (s, 4H), 7.86 (d, *J* = 8.0 Hz, 6H), 7.74 (s, 2H), 7.60 (m, 6H), 7.48 (t, *J* = 7.3 Hz, 2H), 3.41 (d, *J* = 10.2 Hz, 2H), 3.23 (d, *J* = 10.1 Hz, 2H), 2.53 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 161.9, 145.4, 142.1, 138.9, 138.4, 132.1, 131.5, 131.2, 130.8, 130.2, 128.8, 128.7, 128.2, 127.9, 127.1, 127.0, 126.9, 126.8, 126.8, 125.5, 123.2, 122.7, 34.4, 17.8.

DEPT 135 (101 MHZ, $CDCl_3$): 130.2, 126.0, 128.5, 126.6, 126.2, 124.6, 33.8 **(↓)**, 17.8 **(↑)**.

HRMS-ESI: Calcd. for $C_{50}H_{34}N_2$ [M+H] + m/z: 663.2800; Found: 663.2836

13,14-dimethyl-2,11-di(pyren-4-yl)-6,7-dihydrodibenzo[b,j][4,7] phenanthroline **(6k)**



(6k)

Nature: Yellow powder; **Yield:** 82%; **Rf (40% EtOAc-Hexane):** 0.49, **M. P: :** 280-282 ^{0}C.

FTIR(KBr)ν_{max}:718, 835, 970, 1175, 1584, 2847, 2919, 3039 cm^{-1};

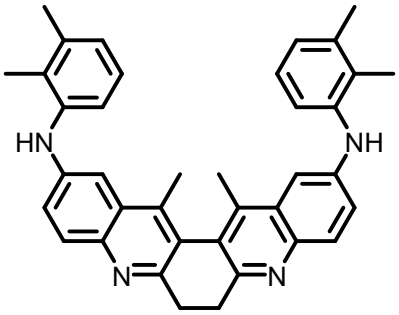
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (d, J = 8.0 Hz, 2H), 8.26 (s, 2H), 8.23 (dd, J = 7.8, 3.6 Hz, 2H), 8.18 (s, 1H), 8.16 (s, 1H), 8.15 (s, 1H), 8.13 (d, J = 5.7 Hz, 3H), 8.08 (d, J = 3.7 Hz, 4H), 8.05 (s, 1H), 8.02 (d, J = 4.7 Hz, 3H), 8.00 (s, 1H), 8.00 – 7.94 (m, 3H), 3.54 (s, 2H), 3.28 (d, J = 10.5 Hz, 2H), 2.60 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 141.4, 139.8, 132.8, 127.1, 125.6, 123.0, 122.8, 120.5, 120.4, 118.7, 108.5, 42.1, 29.2.

DEPT 135 (101 MHZ, $CDCl_3$): 127.01, 125.5, 120.4, 120.3, 118.6, 108.3, 41.9 **(↓)**, 29.1 **(↑)**.

HRMS-ESI: Calcd. for $C_{54}H_{34}N_2$ [M+H] + m/z: 711.2800; Found: 711.2809

N2,N11-bis(2,3-dimethylphenyl)-13,14-dimethyl-6,7-dihydrodibenzo[b,j][4,7]phenanthroline-2,11-diamine **(8)**



(8)

Nature: Red powder; **Yield:** 89%; **Rf (50% EtOAc-Hexane):** 0.50, **M. P: :** 193-195 ^{0}C.

FTIR(KBr)ν_{max}:794, 1004, 1095, 1201, 1463, 1593, 2926, 3275 cm^{-1};

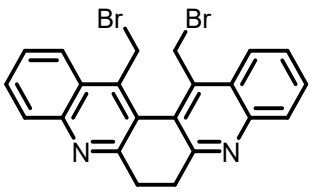
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, *J* = 8.9 Hz, 1H), 7.25 (d, *J* = 9.0 Hz, 1H), 7.20 (s, 1H), 7.15 (d, *J* = 7.9 Hz, 1H), 7.04 (t, *J* = 7.7 Hz, 1H), 6.91 (d, *J* = 7.4 Hz, 1H), 5.63 (s, 1H), 3.18 (d, *J* = 10.1 Hz, 1H), 3.05 (d, *J* = 10.1 Hz, 1H), 2.29 (d, *J* = 2.2 Hz, 6H), 2.16 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 158.6, 143.0, 141.5, 140.4, 139.7, 138.3, 130.0, 129.3, 129.0, 126.9, 126.3, 125.5, 121.9, 119.4, 106.7, 34.2, 20.8, 17.6, 14.0.

DEPT 135 (101 MHZ, $CDCl_3$): 130.0, 126.3, 125.5, 121.9, 119.4, 106.7, 34.2 **(↓)**, 20.8 **(↑)**, 17.6 **(↑)**, 14.0 **(↑)**.

HRMS-ESI: Calcd. for $C_{38}H_{36}N_4$ [M+H] + m/z: 549.3018; Found: 548.2929

13,14-bis(bromomethyl)-6,7-dihydrodibenzo[b,j][4,7]phenanthrolin e **(9a)**



(9a)

Nature: Red powder; **Yield:** 68%; **Rf (40% EtOAc-Hexane):** 0.42, **M. P: :** 359-361 ^{0}C.

FTIR(KBr)ν_{max}: 549, 815, 1120, 1303, 1440, 1552 cm^{-1};

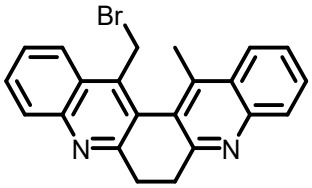
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, J = 8.3 Hz, 2H), 8.09 (d, J = 8.3 Hz, 2H), 7.80 – 7.70 (m, 2H), 7.67 – 7.59 (m, 2H), 4.92 (d, J = 10.7 Hz, 2H), 4.69 (d, J = 10.6 Hz, 2H), 3.34 (d, J = 10.5 Hz, 2H), 3.19 – 3.09 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 161.5, 147.1, 139.5, 130.7, 129.4, 126.9, 125.5, 124.8, 124.0, 34.0, 25.8.

DEPT 135 (101 MHZ, $CDCl_3$): 131.0, 129.3, 127.5, 124.9, 33.9 **(↓)**, 25.8 **(↓)**.

HRMS-ESI: Calcd. for $C_{22}H_{16}Br_2N_2$ [M+H] + m/z: 466.9758; Found: 466.9757

13-(bromomethyl)-14-methyl-6,7-dihydrodibenzo[b,j][4,7] phenanthroline **(9b)**



(9b)

Nature: Brown powder; **Yield: 24**%; **Rf (40% EtOAc-Hexane):** 0.46, **M. P: :** 355-356 ^{0}C.

FTIR(KBr)ν_{max}: 736, 829, 1006, 1074, 1222, 1388, 1471, 1589 cm^{-1};

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 8.3 Hz, 1H), 8.12 (d, *J* = 8.3 Hz, 1H), 8.10 – 8.03 (m, 1H), 8.00 (dd, *J* = 8.4, 0.7 Hz, 1H), 7.72 (m, 2H), 7.66 – 7.53 (m, 2H), 5.00 (d, *J* = 10.6 Hz, 1H), 4.63 (t, *J* = 6.9 Hz, 1H), 3.49 – 3.27 (m, 2H), 3.15 (m, 2H), 2.52 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 161.4, 161.4, 147.0, 139.6, 130.5, 130.2, 129.3, 128.7, 127.6, 126.8, 126.6, 125.6, 125.4, 124.8, 124.6, 33.8, 26.1, 17.3.

DEPT 135 (101 MHZ, $CDCl_3$): 130.5, 130.2, 129.3, 128.7, 126.8, 126.6, 124.8, 124.6, 33.8**(↓)**, 26.1**(↓)**, 17.3 **(↑)**.

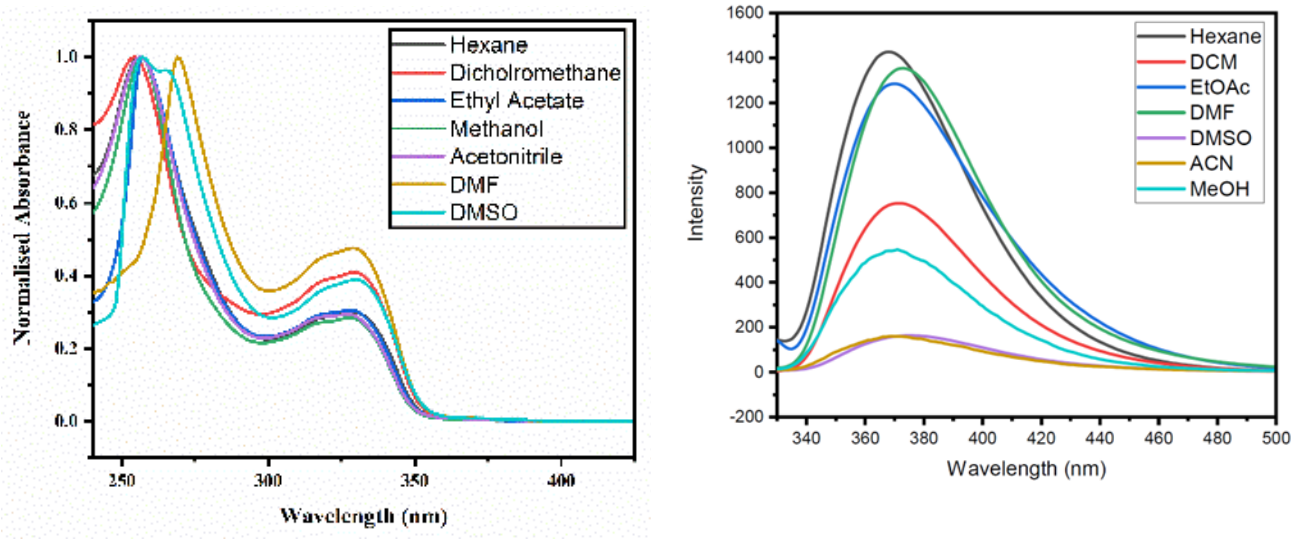
HRMS-ESI: Calcd. for $C_{22}H_{17}BrN_2$ [M+H] + m/z: 389.0653; Found: 389.0666

References

1. H. Xiong, X. Wu, H. Wang, S. Sun, J.-T. Yu and J. Cheng, *Adv. Synth. Catal.*, 2019, **361**, 3538–3542.

2. M. M. Maluleka, and M. J. Mphahlele, *Tetrahedron*, 2013, **69**, 699-704

Absorption and emission spectra of compounds 3a, 6a, 6d, 6f, 8



(a) **(b)**

SI Figure :1

(a) Normalised absorption spectra of compound **3a** recorded at C 2x10-5 M at 298 K

(b) Normalised emission spectra of compound **3a** recorded at C 2x10-5 M at 298 K

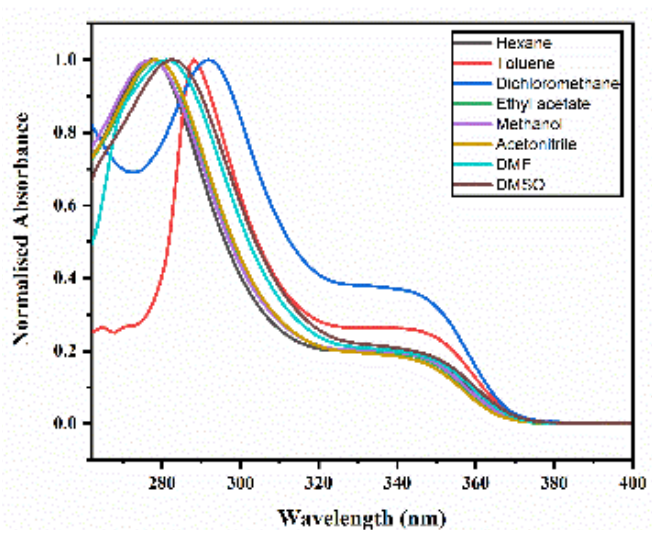
SI Table :1 : Photophysical properties of compound **3a**

Entry	Solvent	Absorption[a] λmax, abs (nm)	Emission[a] λmax, emi (nm)	Molar Extinction Coefficient x 10^4 (ε) π- π *	Stoke's shift $\Delta\ \bar{\upsilon}$ x 10^4 (cm^{-1})[b]	Quantum yield (Φ_f)[c]
1.	Hexane	256, 329	369	5.8975	1.1962	0.4056
2.	CH_2Cl_2	254, 329	372	3.0875	1.2488	0.5997
3.	EtOAc	257, 328	370	4.1235	1.1883	0.5624
4.	Methanol	257, 327	369	4.5657	1.1810	0.1837
5.	CH_3CN	256, 327	371	4.3265	1.2108	0.5367
6.	DMF	269, 329	373	1.3024	1.0365	0.8953
7.	DMSO	257, 330	377	3.3570	1.2385	0.4641

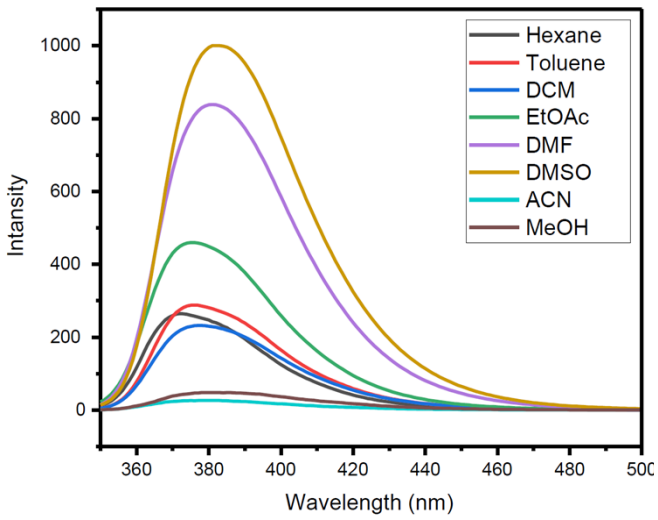
[a]Recorded at 298 K.

[b]Stoke's shift = $\lambda_{max,\ abs} - \lambda_{max,\ emi}$ [cm^{-1}].

[c]Determined with anthracene as a standard Φ_f = 0.27 at excitation wavelength 246 nm.



(a)



(b)

SI Figure:2

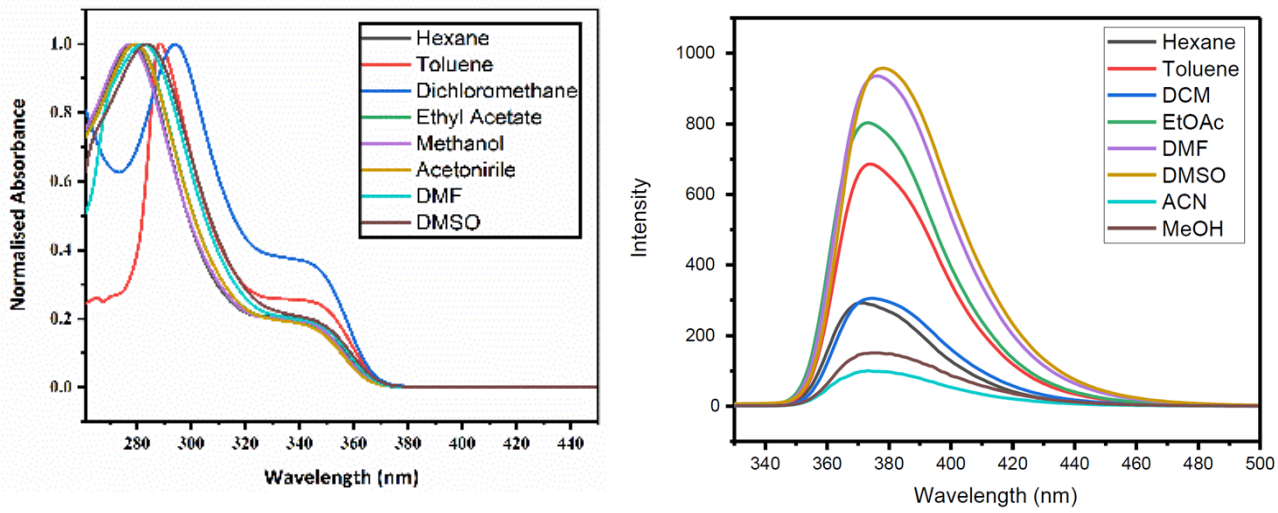
(a) Normalised absorption spectra of compound **6a** recorded at C 2x10-5 M at 298 K

(b) Normalised emission spectra of compound **6a** recorded at C 2x10-5 M at 298 K

SI Table :2 : Photophysical properties of compound **6a**

Entry	Solvent	Absorption[a] λmax, abs (nm)	Emission[a] λmax, emi (nm)	Molar Extinction Coefficient x 10^4 (ε) π- π *	Stoke's shift Δ $\bar{\upsilon}$ x 10^4 (cm^{-1})[b]	Quantum yield (Φ_f)[c]
1.	Hexane	277	372	8.4675	0.9219	0.3641
2.	Toluene	288	376	4.5805	0.8126	0.8974
3.	CH_2Cl_2	292	376	3.2260	0.7650	0.5122
4.	EtOAc	279	376	8.6865	0.9246	0.6615
5.	Methanol	277	380	5.0952	0.9785	0.1213
6.	CH_3CN	278	381	5.7700	0.9724	0.0598
7.	DMF	281	381	3.7900	0.9340	0.7915
8.	DMSO	283	383	5.2665	0.9226	0.7407

[a]Recorded at 298 K.
[b]Stoke's shift = $\lambda_{max,\ abs} - \lambda_{max,\ emi}$ [cm^{-1}].
[c]Determined with anthracene as a standard Φ_f = 0.27 at excitation wavelength 246 nm.



(a) **(b)**

SI Figure :3

(a) Normalised absorption spectra of compound **6d** recorded at C 2x10-5 M at 298 K

(b) Normalised emission spectra of compound **6d** recorded at C 2x10-5 M at 298 K

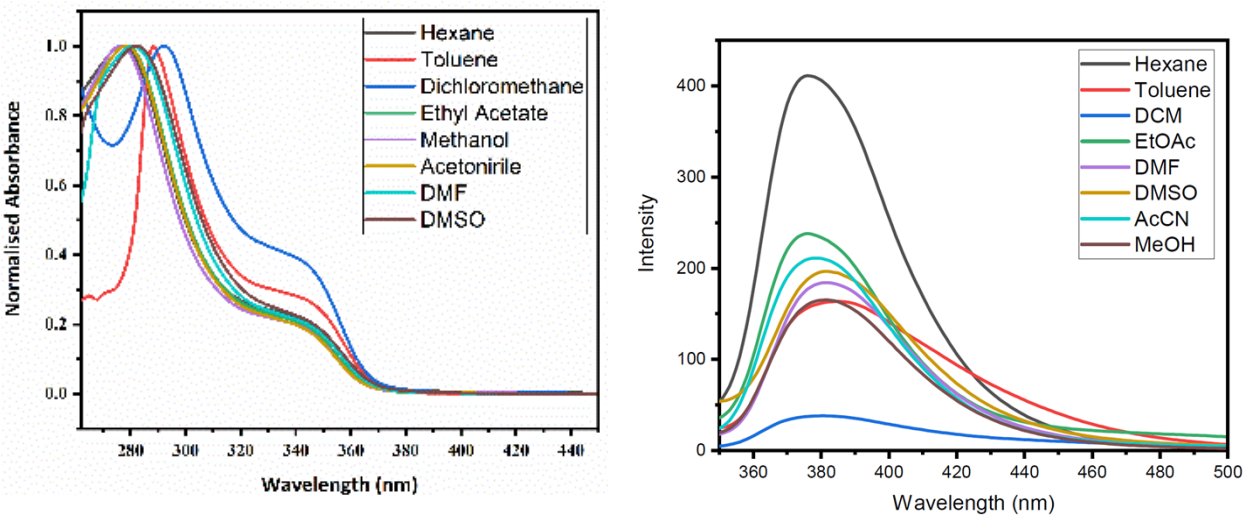
SI Table :3 : Photophysical properties of compound **6d**

Entry	Solvent	Absorption[a] λmax, abs (nm)	Emission[a] λmax, emi (nm)	Molar Extinction Coefficient x 10^4 (ε) π- π *	Stoke's shift $\Delta\ \bar{\upsilon}$ x 10^4 (cm^{-1})[b]	Quantum yield (Φ_f)[c]
1.	Hexane	278	372	7.4475	0.9089	0.4578
2.	Toluene	289	374	5.2830	0.7864	0.9049
3.	CH_2Cl_2	294	374	3.7135	0.7427	0.5281
4.	EtOAc	280	373	7.1560	0.8904	0.6748
5.	Methanol	277	376	7.2067	0.9505	0.2489
6.	CH_3CN	279	373	7.1685	0.9032	0.1697
7.	DMF	282	376	3.1415	0.8865	0.8152
8.	DMSO	284	378	6.3665	0.8756	0.7471

[a]Recorded at 298 K.

[b]Stoke's shift = $\lambda_{max,\ abs} - \lambda_{max,\ emi}$ [cm^{-1}].

[c]Determined with anthracene as a standard $\Phi_f = 0.27$ at excitation wavelength 246 nm.



(a) **(b)**

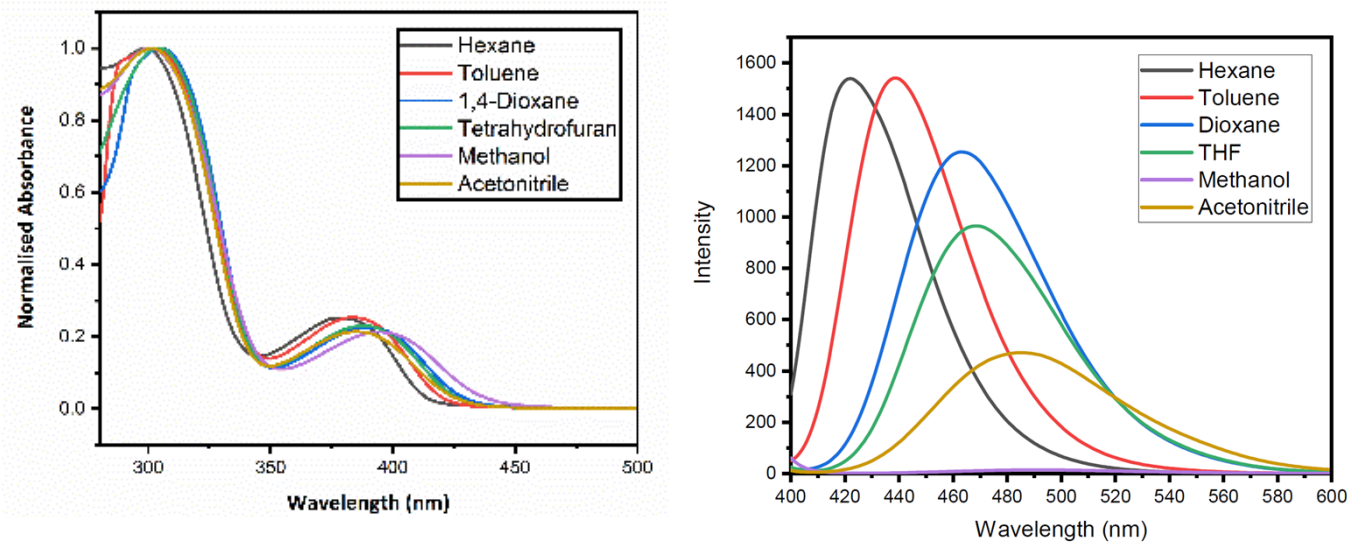
SI Figure :4 :

(a) Normalised absorption spectra of compound **6f** recorded at C 2x10-5 M at 298 K

(b) Normalised emission spectra of compound **6f** recorded at C 2x10-5 M at 298 K

SI Table :4 : Photophysical properties of compound **6f**

Entry	Solvent	Absorption[a] λmax, abs (nm)	Emission[a] λmax, emi (nm)	Molar Extinction Coefficient x 10^4 (ε) π- π *	Stoke's shift $\Delta\ \bar{\upsilon}$ x 10^4 (cm^{-1})[b]	Quantum yield (Φ_f)[c]
1.	Hexane	277	376	8.8975	0.9505	0.0904
2.	Toluene	288	385	4.7150	0.8748	0.0746
3.	CH_2Cl_2	292	380	3.1770	0.7930	0.0242
4.	EtOAc	279	376	6.2330	0.9246	0.0495
5.	Methanol	276	381	6.0666	0.9985	0.0450



(a) **(b)**

SI Figure :5 :

(a) Normalised absorption spectra of compound **8** recorded at C $2x10^{-5}$ M at 298 K

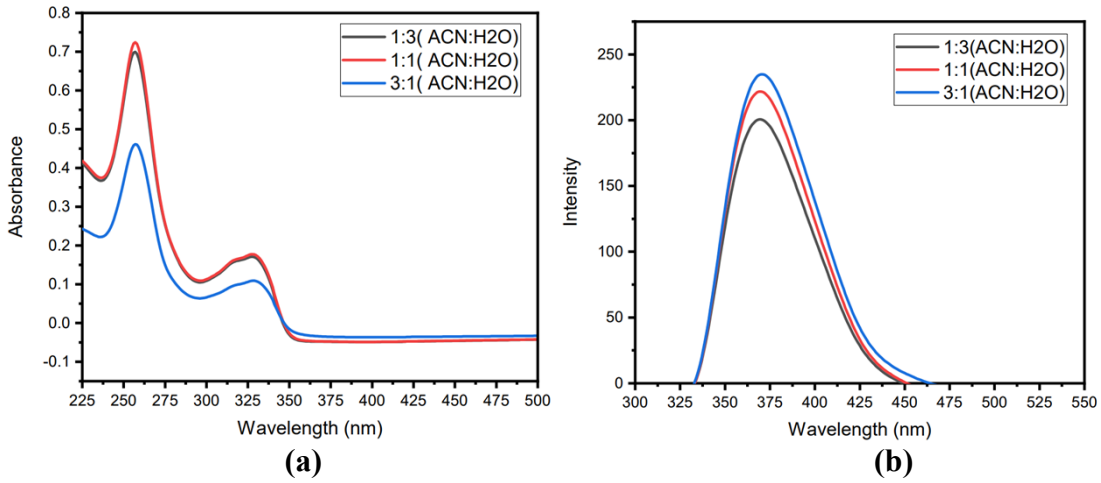
(b) Normalised emission spectra of compound **8** recorded at C $2x10^{-5}$ M at 298 K

SI Table :5 : Photophysical properties of compound **8**

Entry	Solvent	Absorption[a] λmax, abs (nm)	Emission[a] λmax, emi (nm)	Molar Extinction Coefficient x 10^4 (ε) π- π *	Stoke's shift Δ x 10^4 $\bar{\upsilon}$ (cm^{-1})[b]
1.	Hexane	299, 379	421	1.4301	0.9691
2.	Toluene	302, 384	438	2.6726	1.0281
3.	Dioxane	305, 390	468	2.9364	1.1419
4.	THF	304, 388	463	3.1162	1.1296
5.	Methanol	301, 395	492	2.9746	1.2897
6.	CH_3CN	301, 385	484	3.2491	1.2561

[a]Recorded at 298 K.

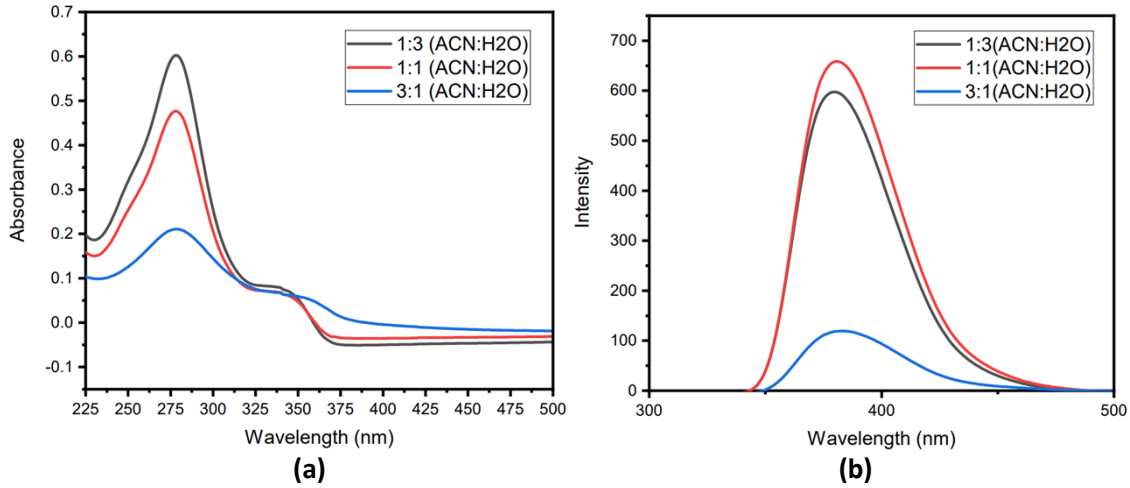
[b]Stoke's shift = $\lambda_{max,\ abs} - \lambda_{max,\ emi}$ [cm^{-1}].



SI Figure :6 :

(a) Absorption spectra of compound **3a** recorded at C $2x10^{-5}$ M at 298 K in acetonitrile:Water (1:3, 1:1, 3:1). (λmax, abs (nm)= 257 nm)

(b) Emission spectra of compound **3a** recorded at C $2x10^{-5}$ M at 298 K in acetonitrile:Water (1:3, 1:1, 3:1). (λmax, abs (nm)=369 nm)

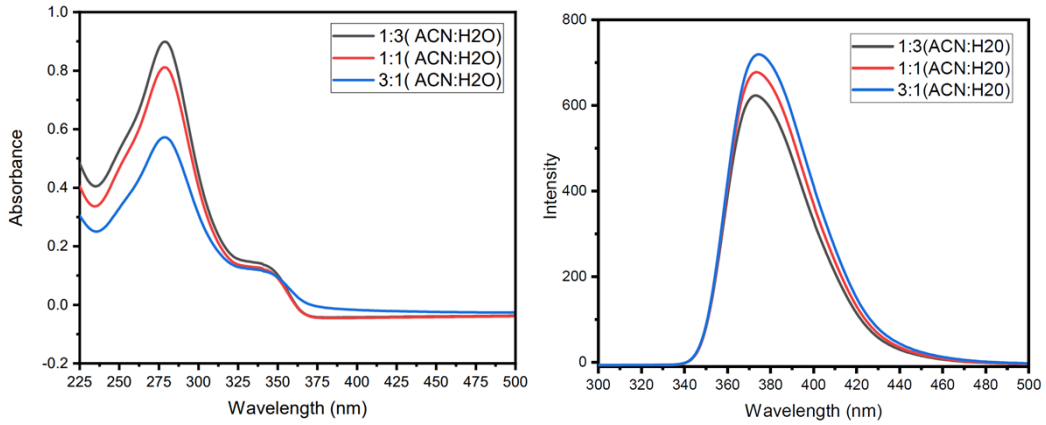


SI Figure :7 :

(a) Absorption spectra of compound **6a** recorded at C $2x10^{-5}$ M at 298 K in acetonitrile:Water (1:3, 1:1, 3:1). (λmax, abs (nm)=278 nm)

(b) Emission spectra of compound **6a** recorded at C $2x10^{-5}$ M at 298 K in

acetonitrile:Water (1:3, 1:1, 3:1). (λmax, abs (nm)= 380nm)

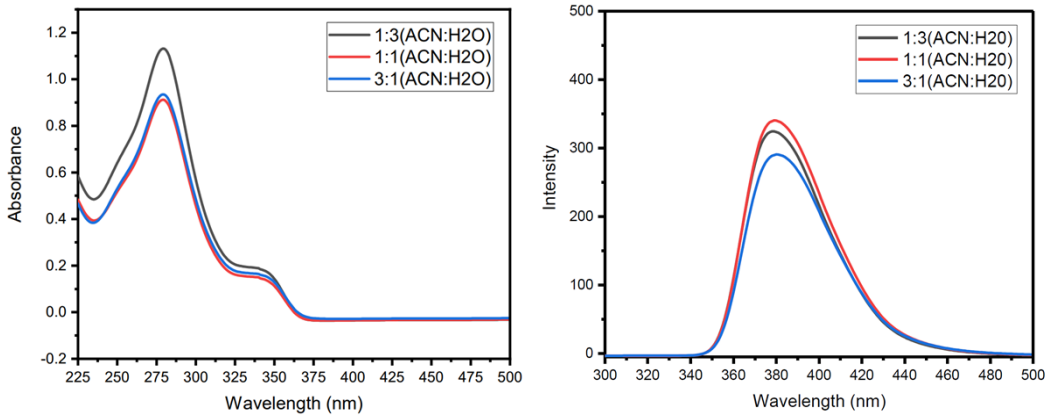


(a) **(b)**

SI Figure :8 :

(a) Absorption spectra of compound **6d** recorded at C 2x10^{-5} M at 298 K in acetonitrile:Water (1:3, 1:1, 3:1). (λmax, abs (nm)=279 nm)

(b) Emission spectra of compound **6d** recorded at C 2x10^{-5} M at 298 K in acetonitrile:Water (1:3, 1:1, 3:1). (λmax, abs (nm)=375 nm)

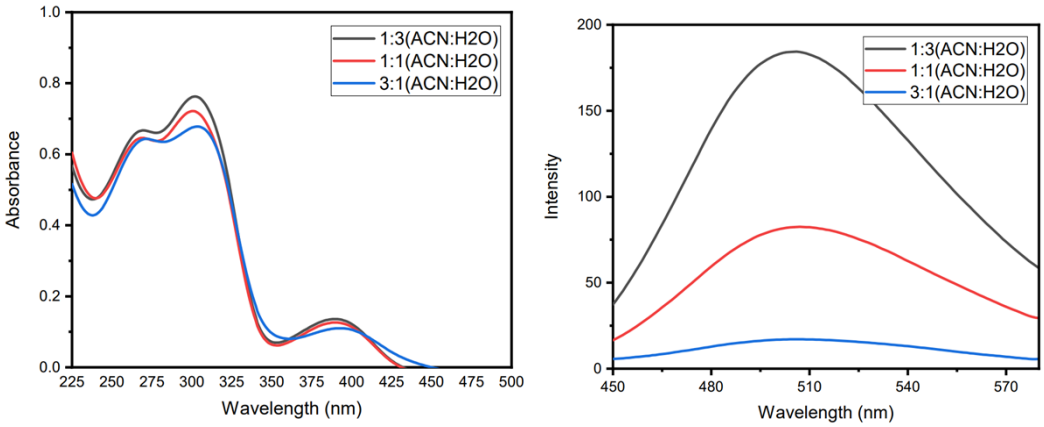


(a) **(b)**

SI Figure :9 :

(a) Absorption spectra of compound **6f** recorded at C 2x10^{-5} M at 298 K in acetonitrile:Water (1:3, 1:1, 3:1). (λmax, abs (nm)=279 nm)

(b) Emission spectra of compound **6f** recorded at C 2x10^{-5} M at 298 K in acetonitrile:Water (1:3, 1:1, 3:1). (λmax, abs (nm)=379 nm)



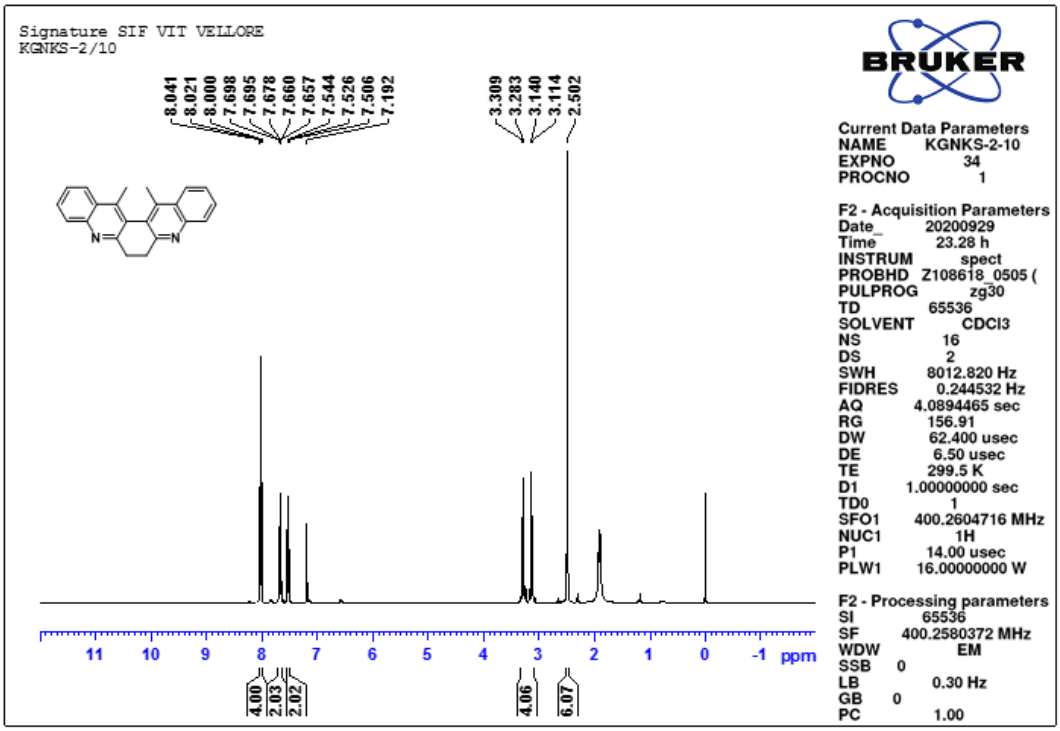
(a) **(b)**

SI Figure :10 :

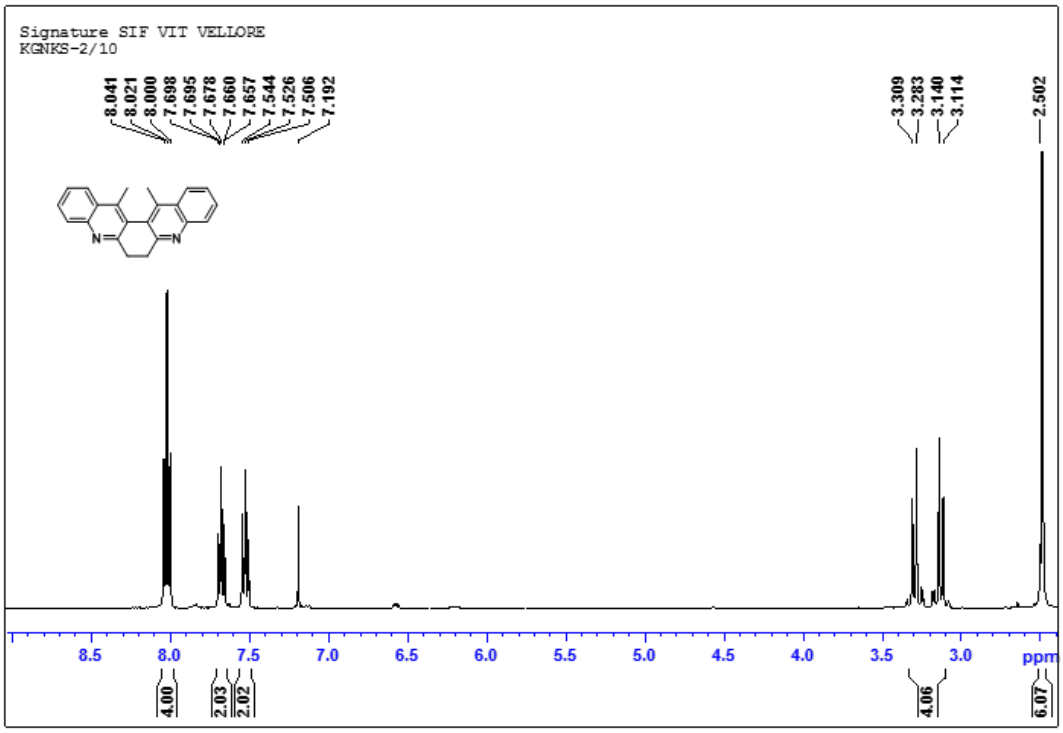
(a) Absorption spectra of compound **8** recorded at C 2x10^{-5} M at 298 K in acetonitrile:Water (1:3, 1:1, 3:1). (λmax, abs (nm)=302 nm)

(b) Emission spectra of compound **8** recorded at C 2x10^{-5} M at 298 K in acetonitrile:Water (1:3, 1:1, 3:1). (λmax, abs (nm)=506 nm)

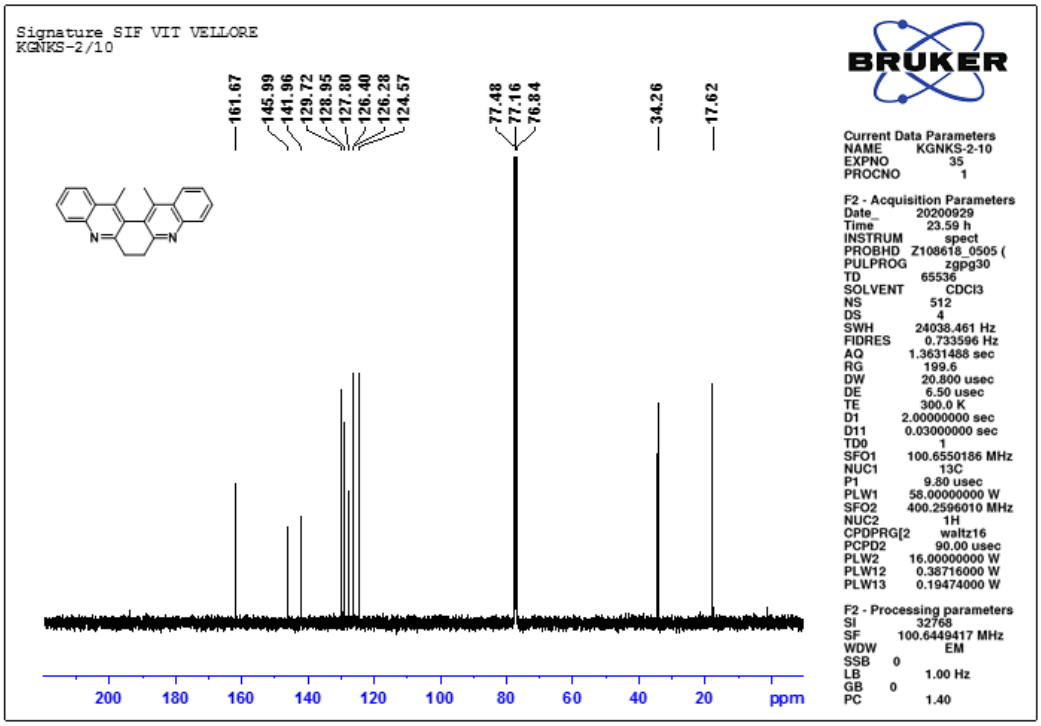
Scanned copies of spectra (^{1}H and ^{13}C NMR, DEPT-135, HRMS, FT-IR)



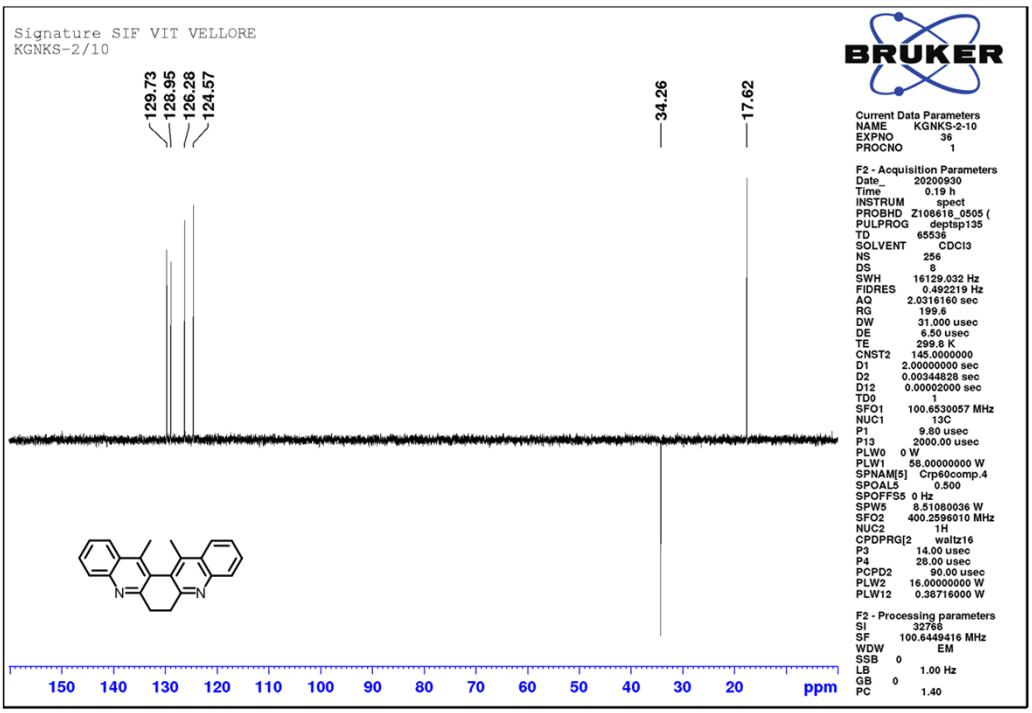
SI Figure. 11: ^{1}H NMR spectrum of compound **3a**



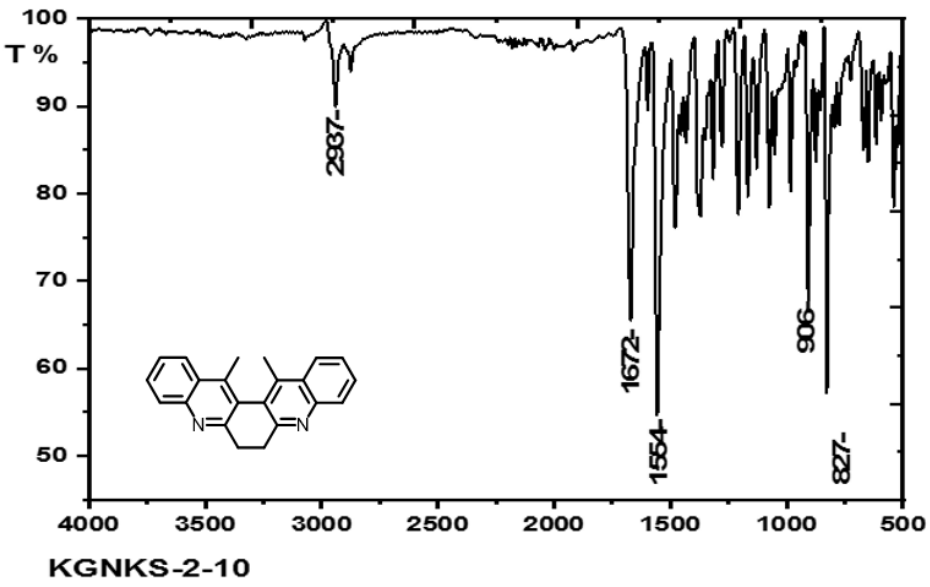
SI Figure. 12: Expansion of ^{1}H NMR spectrum of compound **3a**



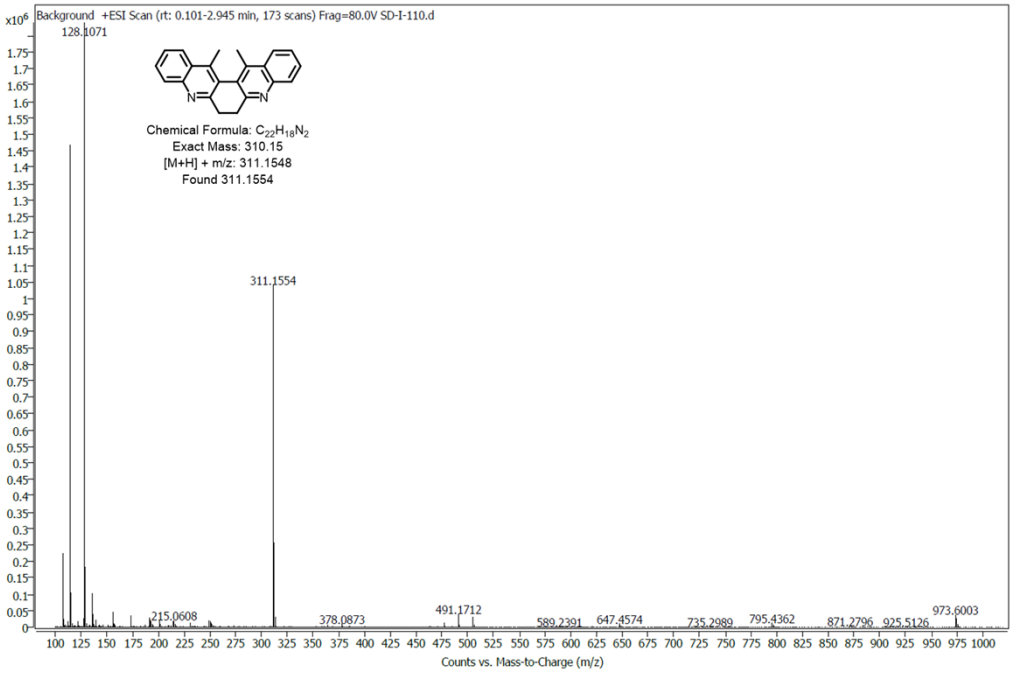
SI Figure. 13: ^{13}C NMR spectrum of compound **3a**



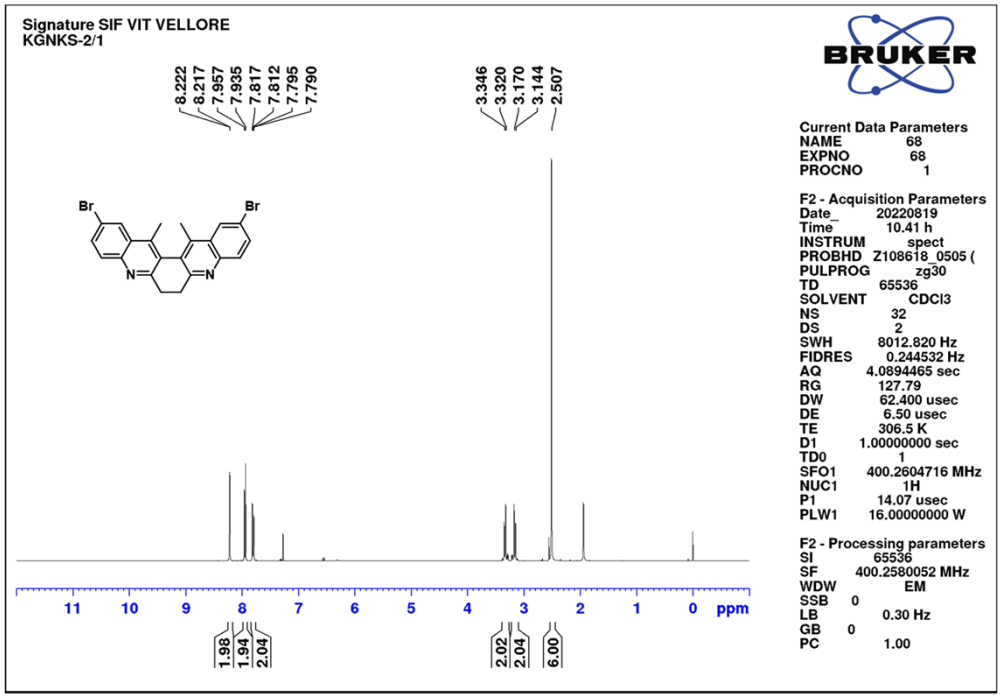
SI Figure. 14: DEPT-135 spectrum of compound **3a**



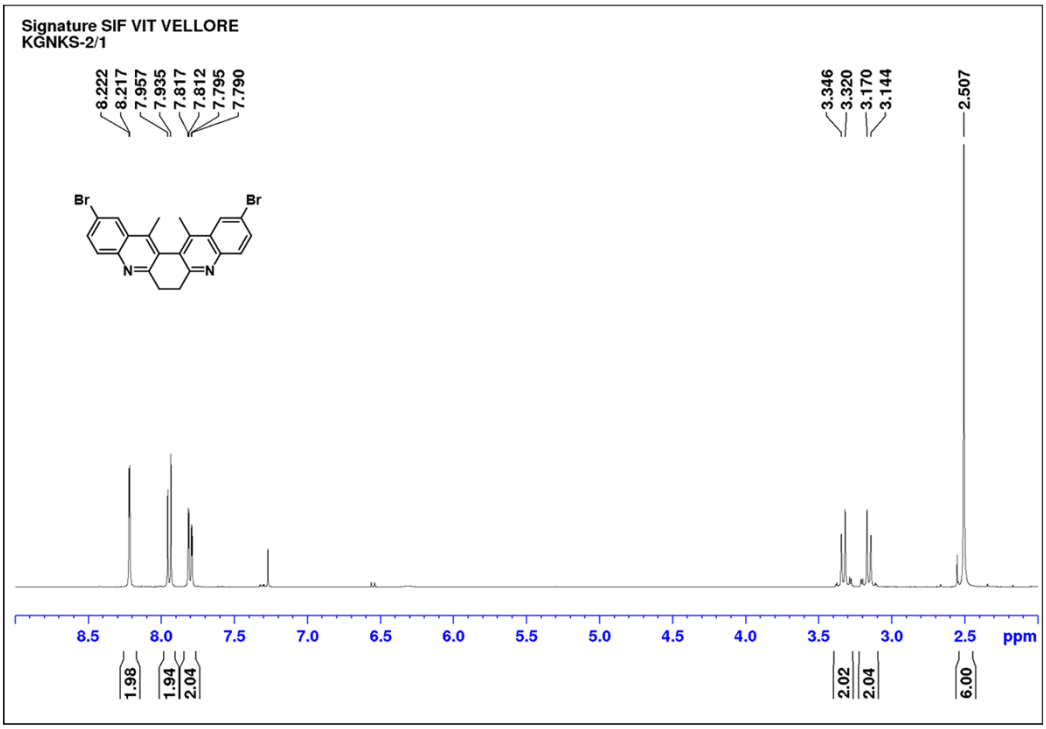
SI Figure. 15: FTIR spectrum of compound **3a**



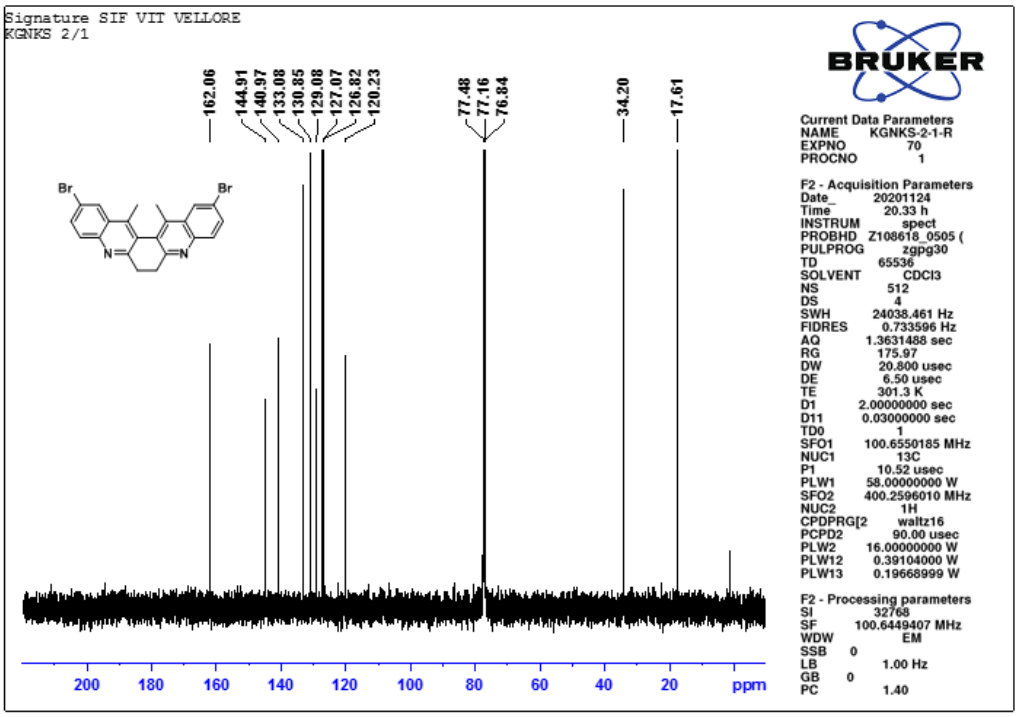
SI Figure. 16: HRMS spectrum of compound **3a**



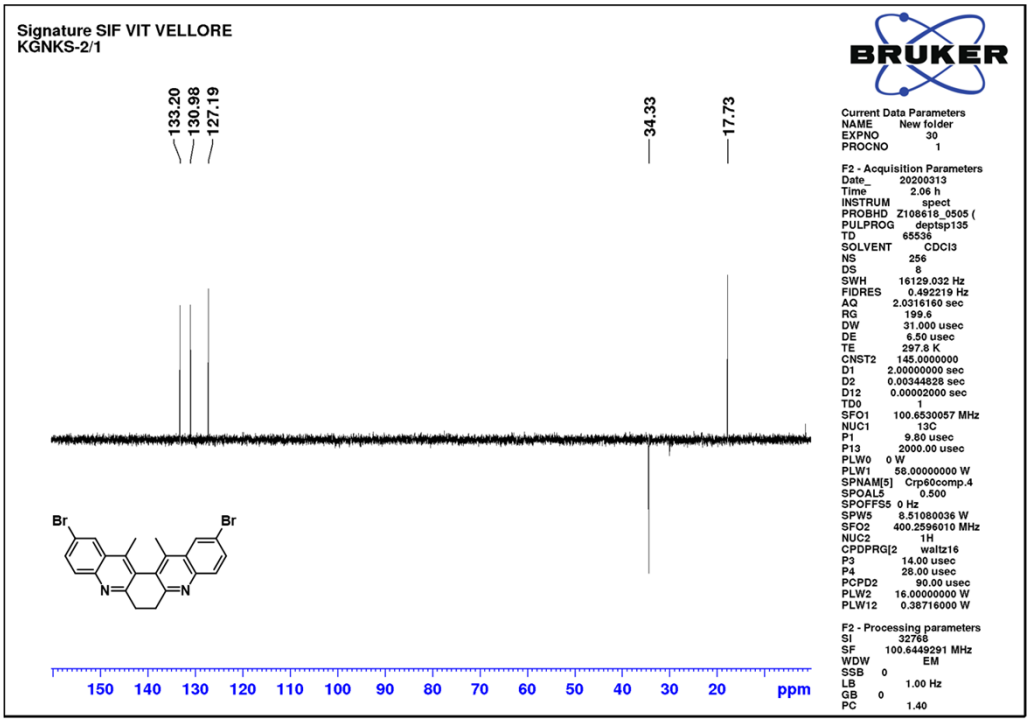
SI Figure. 17: ^{1}H NMR spectrum of compound **3b**



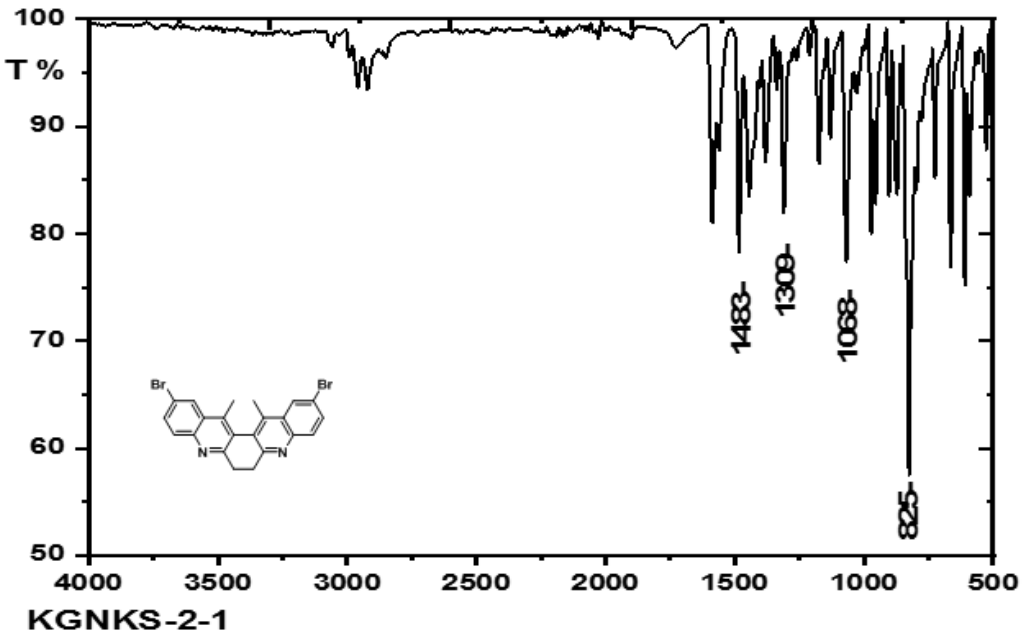
SI Figure. 18: Expansion of ^{1}H NMR spectrum of compound **3b**



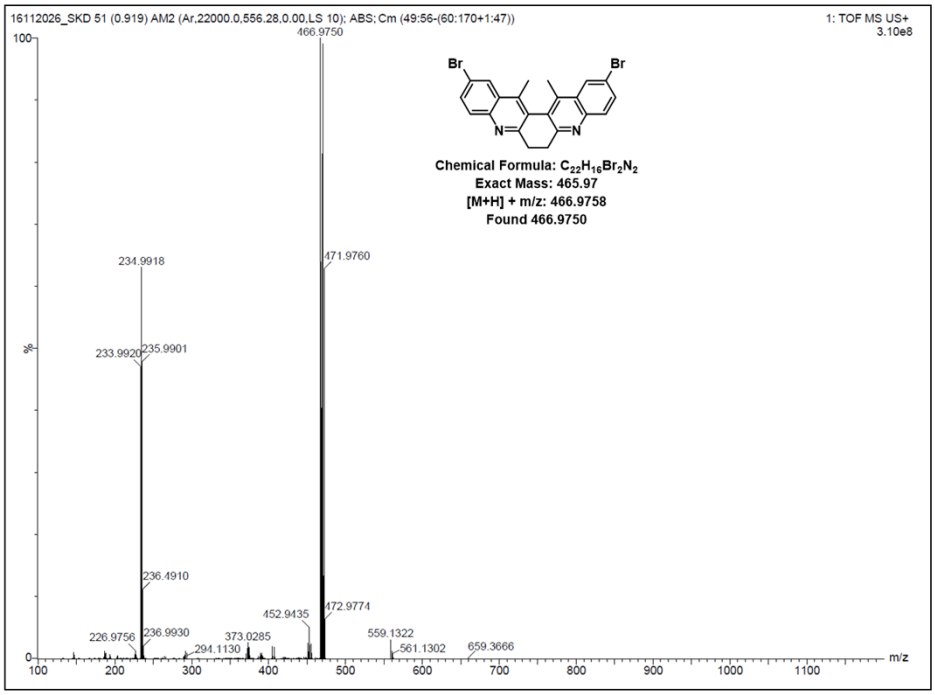
SI Figure. 19: ^{13}C NMR spectrum of compound **3b**



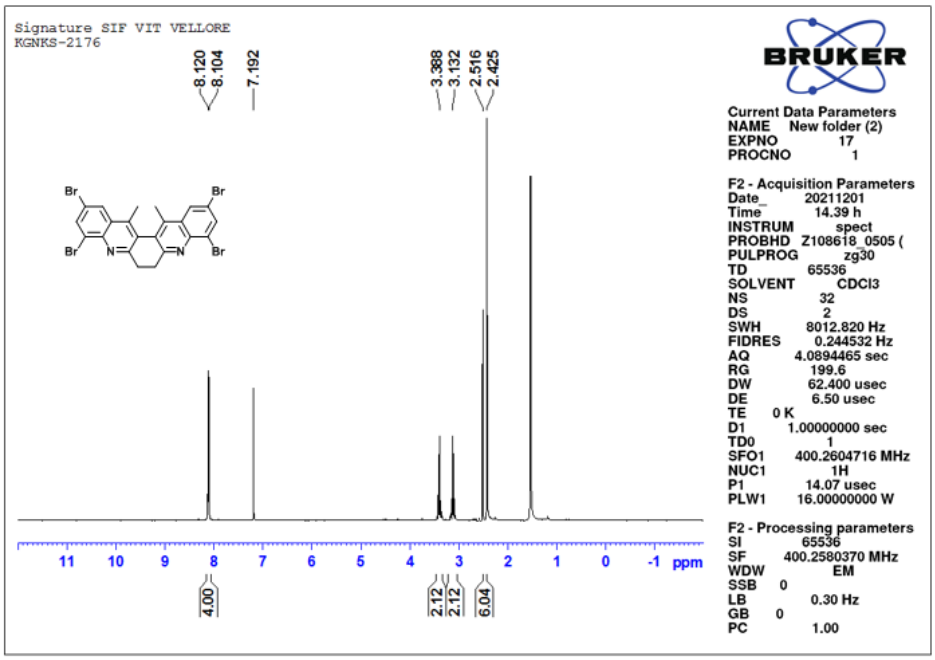
SI Figure. 20: DEPT-135 spectrum of compound **3b**



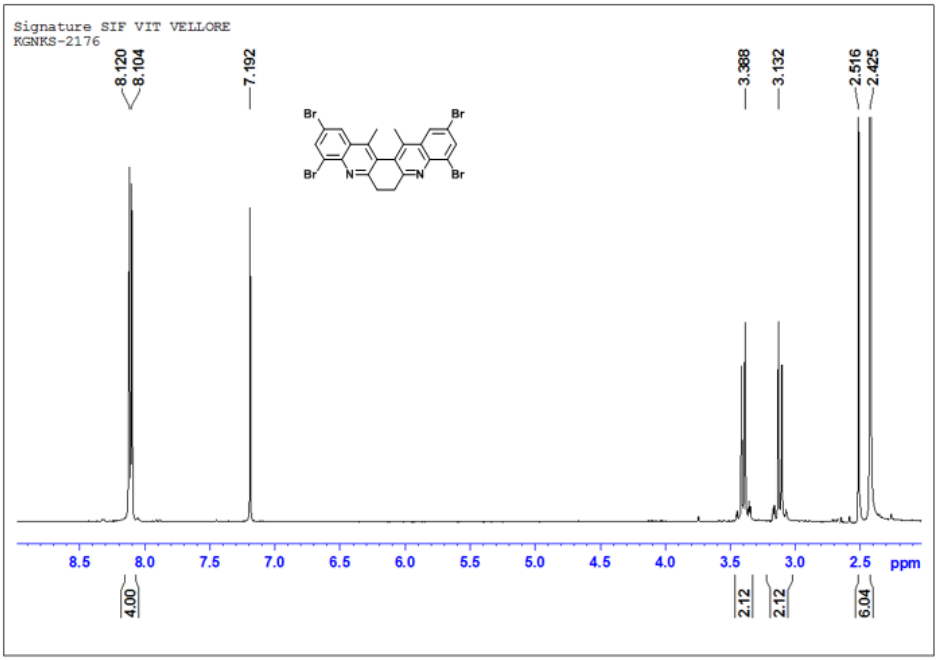
SI Figure. 21: FTIR spectrum of compound **3b**



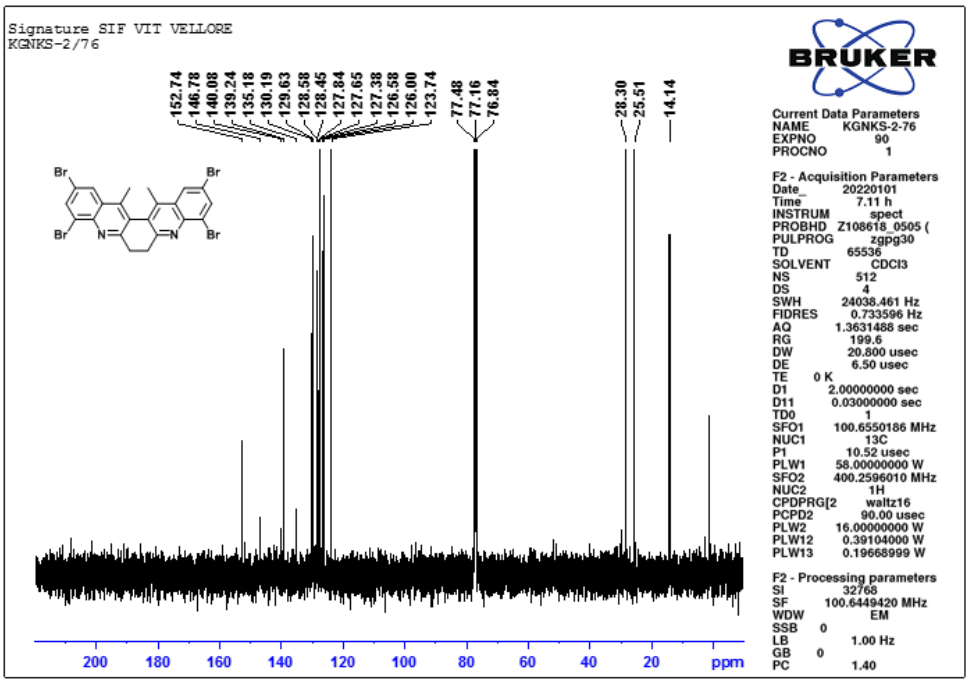
SI Figure. 22: HRMS spectrum of compound **3b**



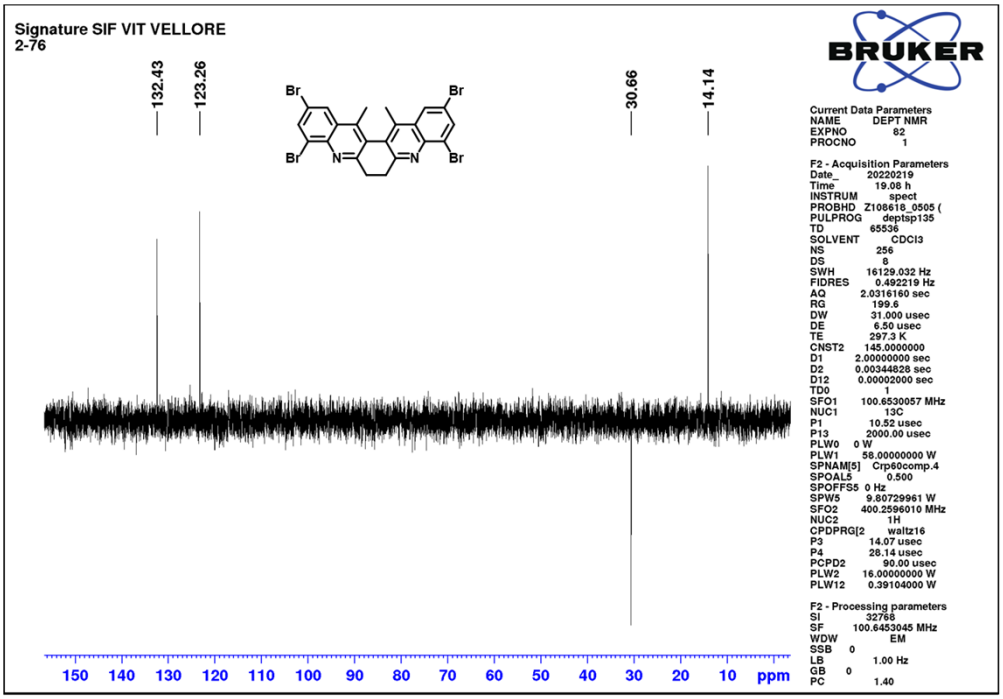
SI Figure. 23: ^{1}H NMR spectrum of compound **3c**



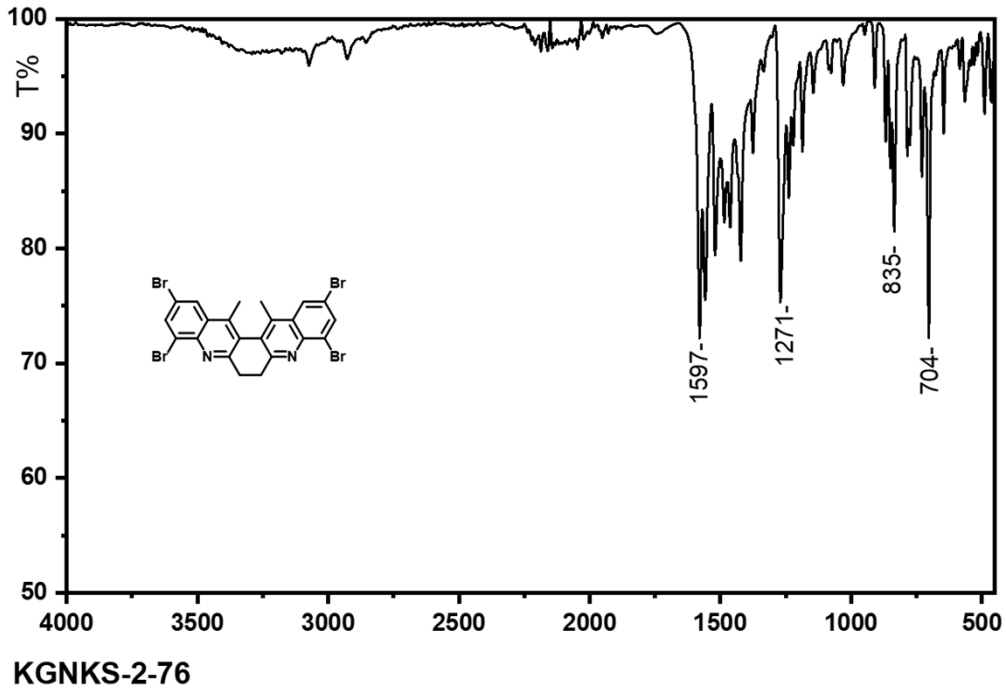
SI Figure. 24: Expansion of ^{1}H NMR spectrum of compound **3c**



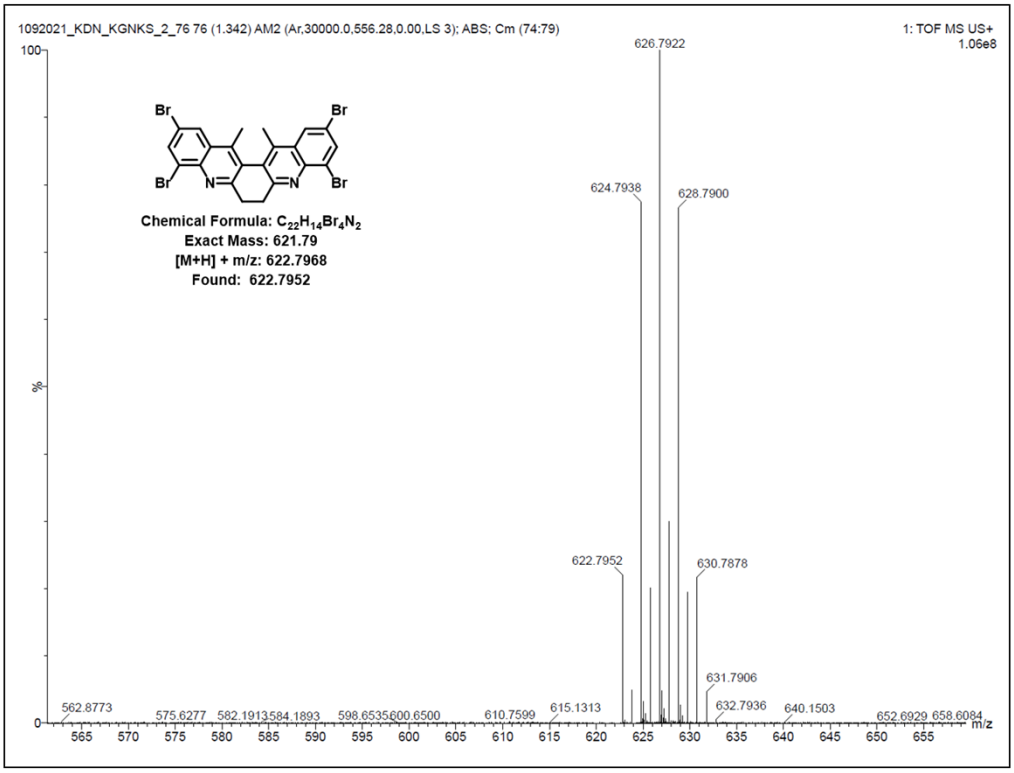
SI Figure. 25: ^{13}C NMR spectrum of compound **3c**



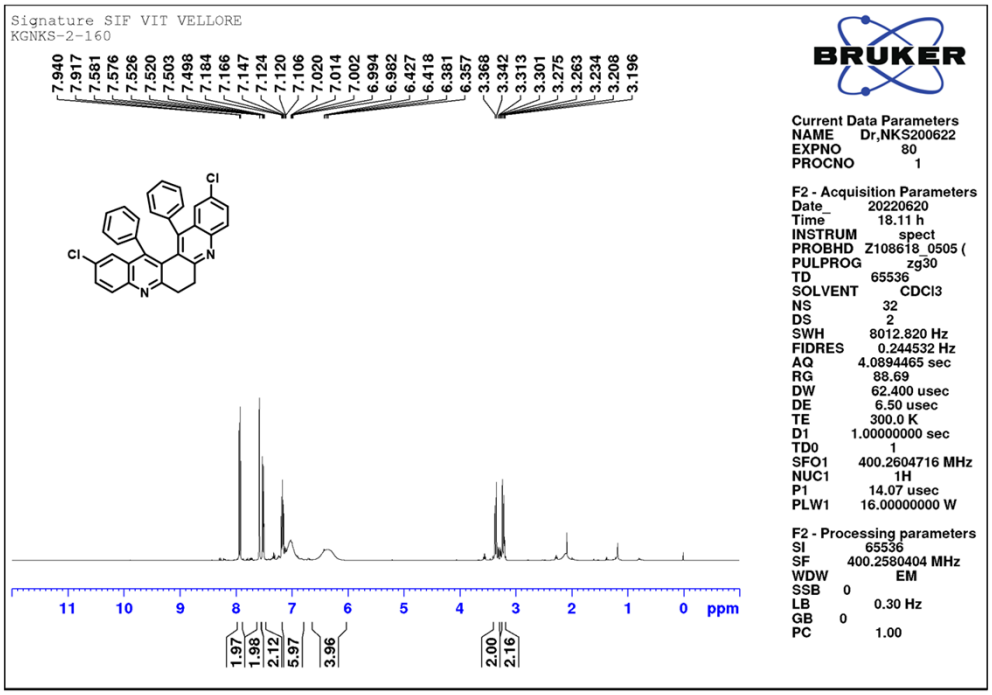
SI Figure. 26: DEPT-135 spectrum of compound **3c**



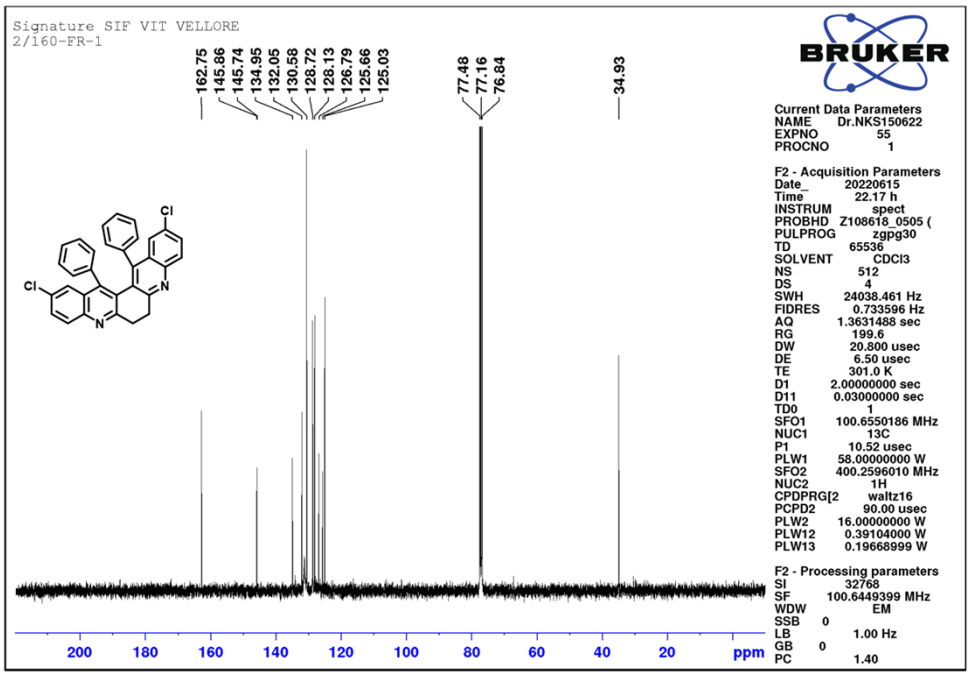
SI Figure. 27: FTIR spectrum of compound **3c**



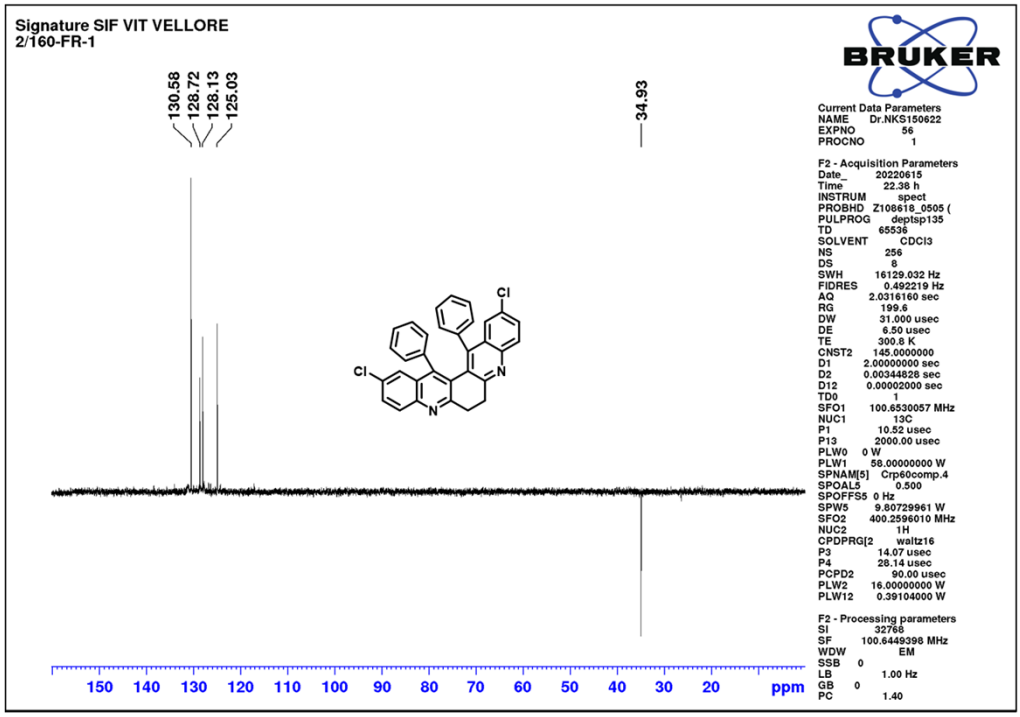
SI Figure. 28: HRMS spectrum of compound **3c**



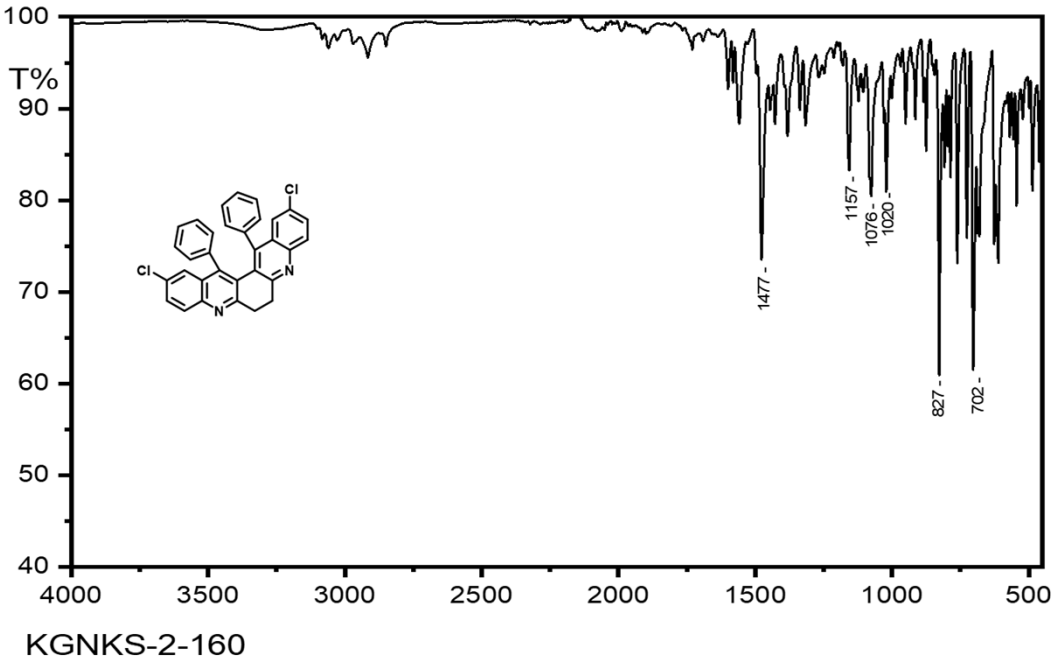
SI Figure. 29: ^{1}H NMR spectrum of compound **3d**



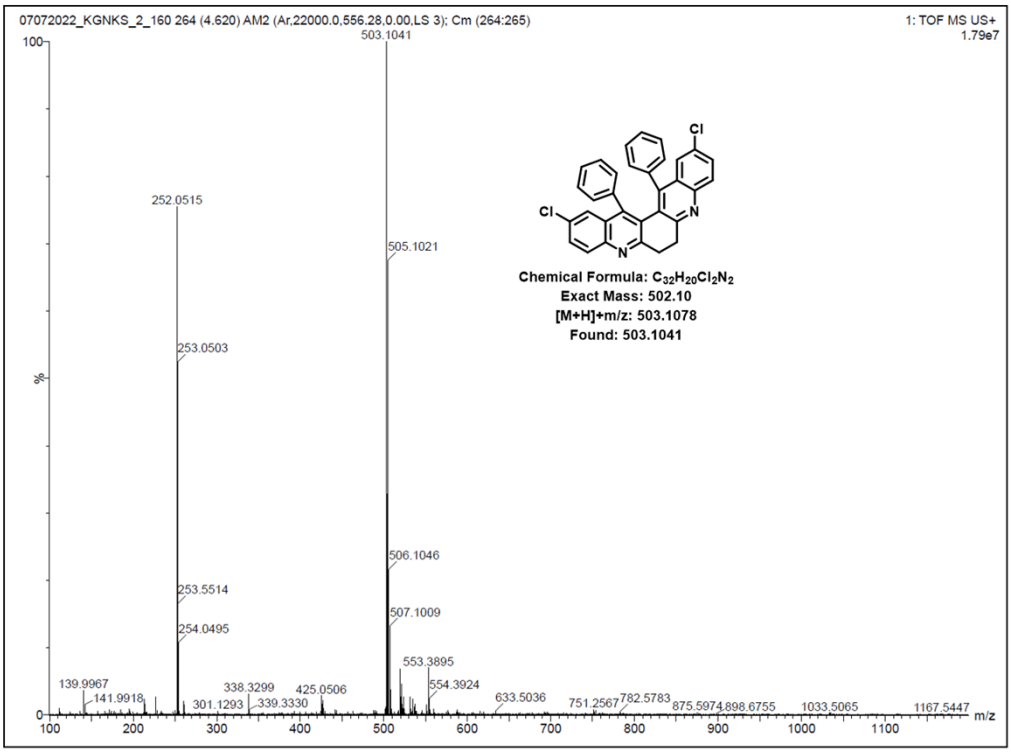
SI Figure. 30: ^{13}C NMR spectrum of compound **3d**



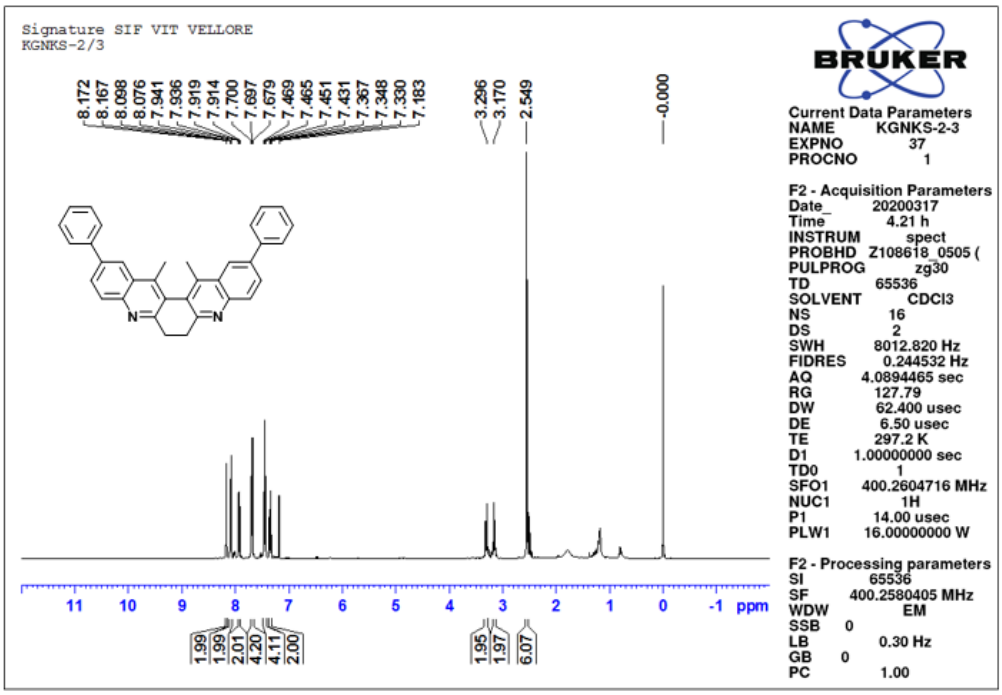
SI Figure. 31: DEPT-135 spectrum of compound **3d**



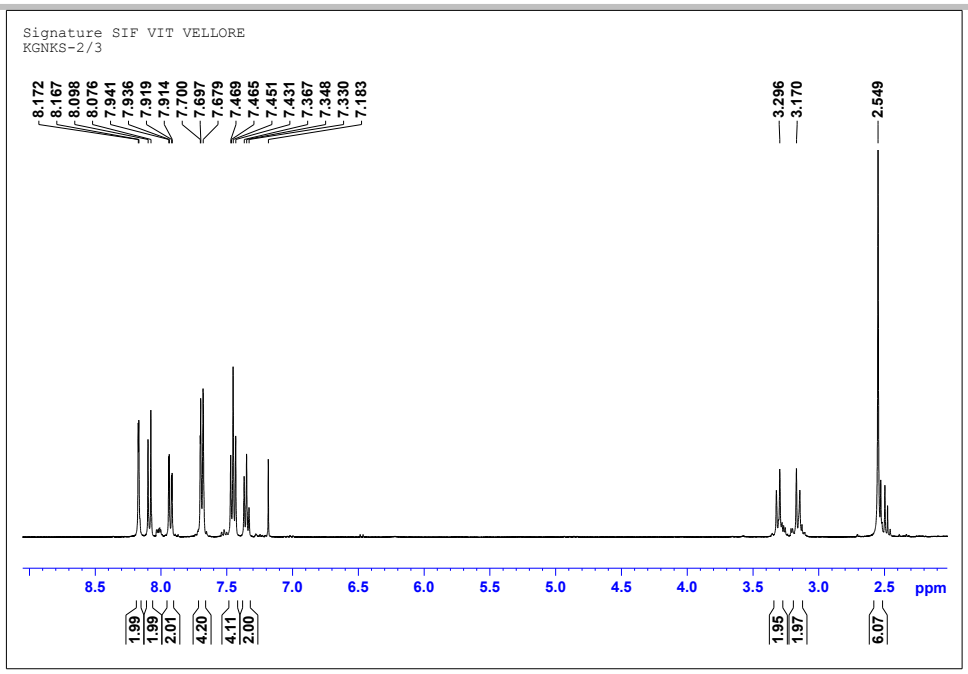
SI Figure. 32: FT-IR spectrum of compound **3d**



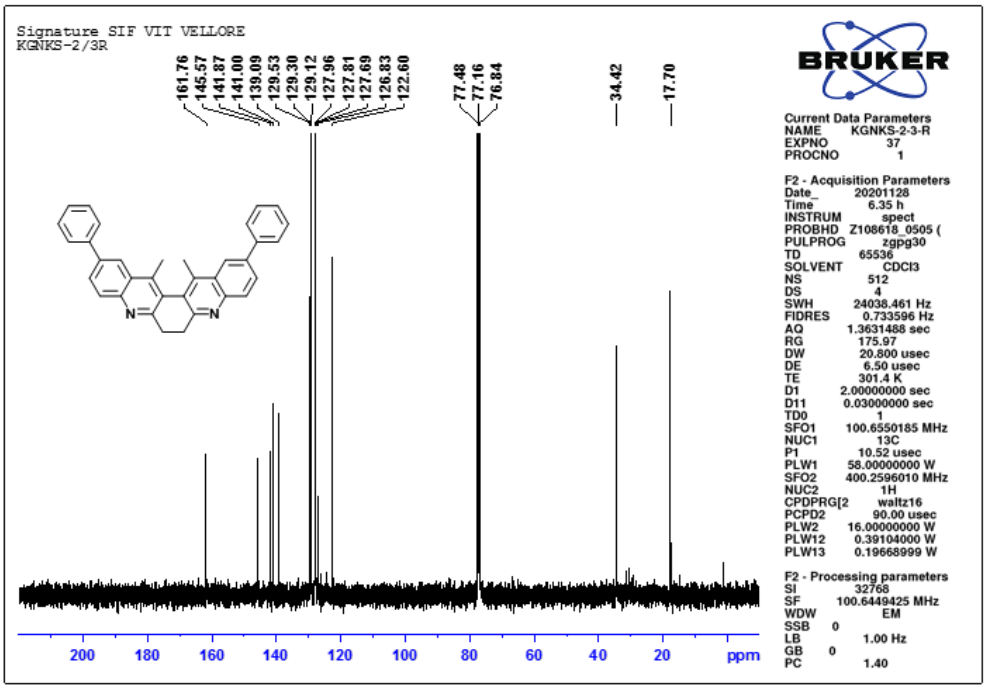
SI Figure. 33: HRMS Spectrum of compound **3d**



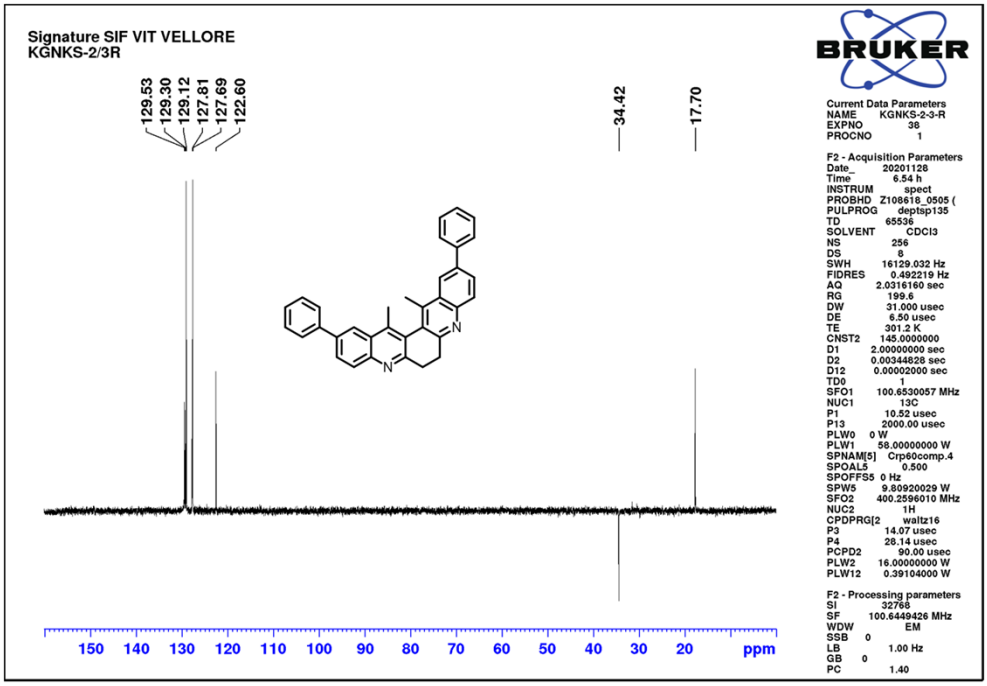
SI Figure. 34: ^{1}H NMR spectrum of compound **6a**



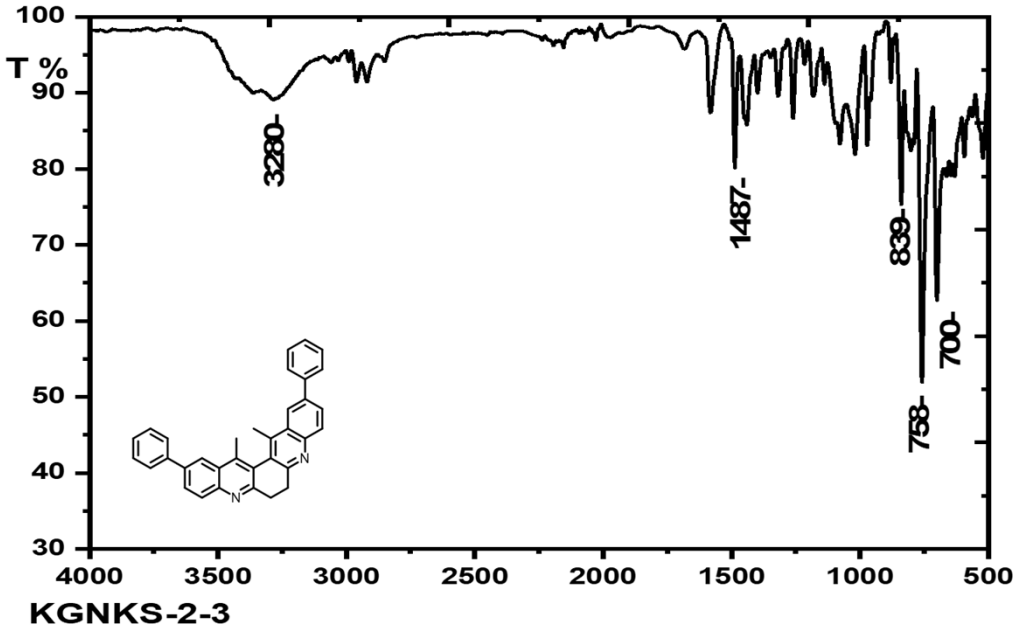
SI Figure. 35: Expansion of ^{1}H NMR spectrum of compound **6a**



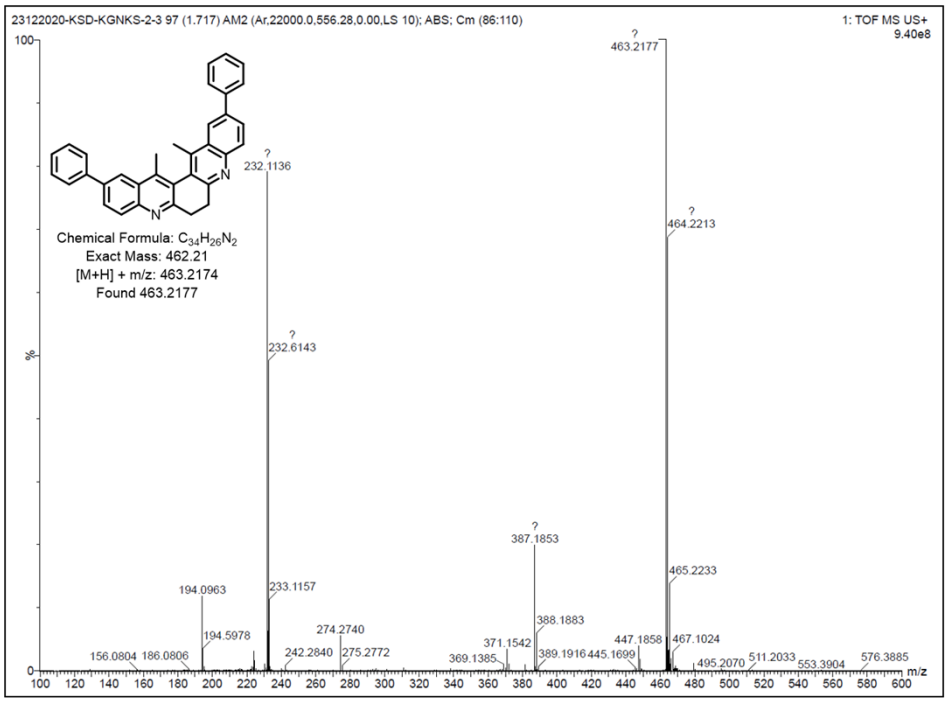
SI Figure. 36: ^{13}C NMR spectrum of compound **6a**



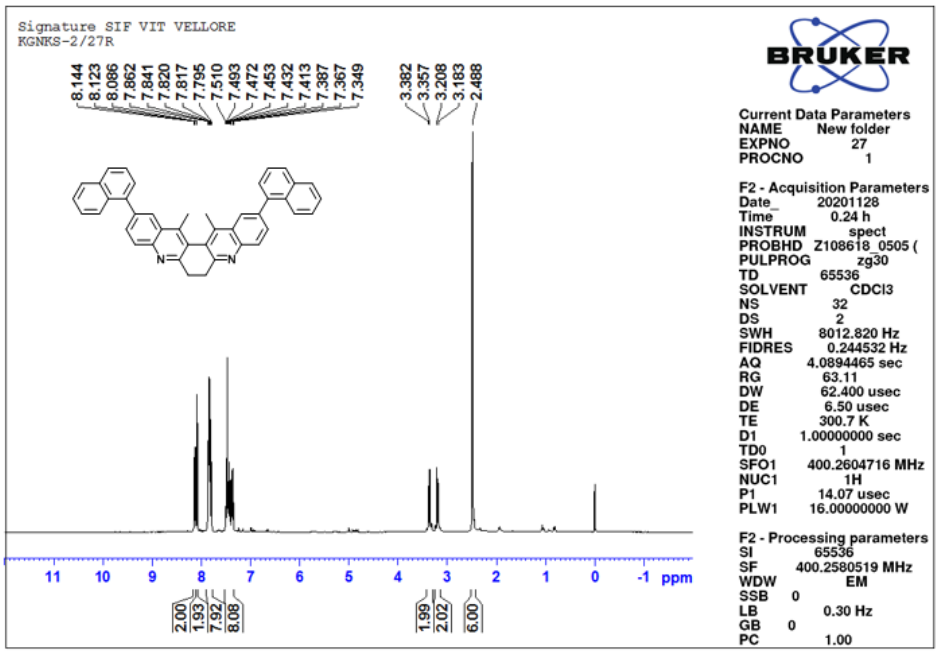
SI Figure. 37: DEPT-135 spectrum of compound **6a**



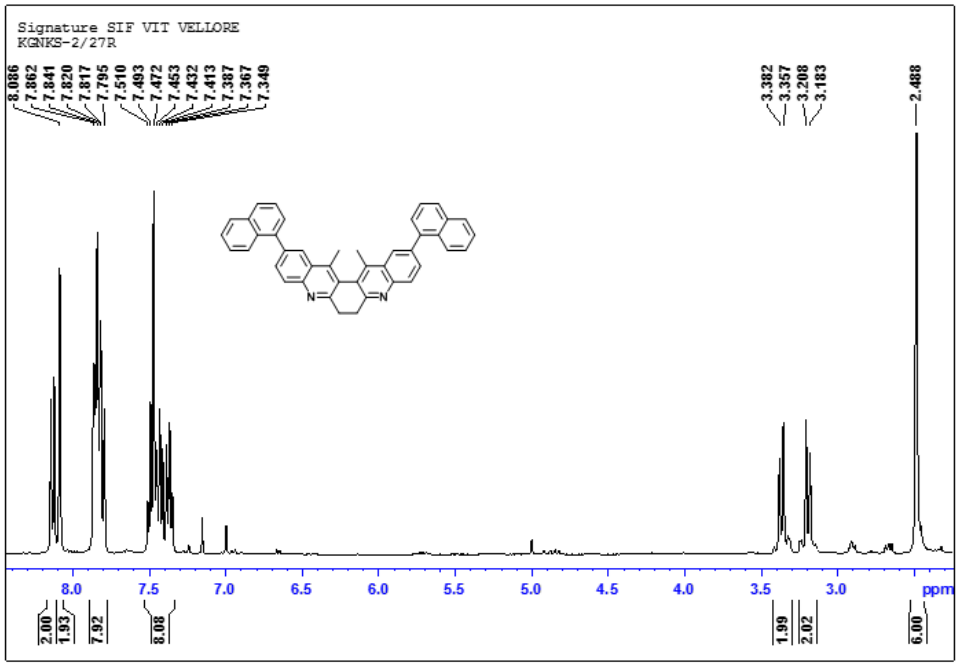
SI Figure. 38: FTIR spectrum of compound **6a**



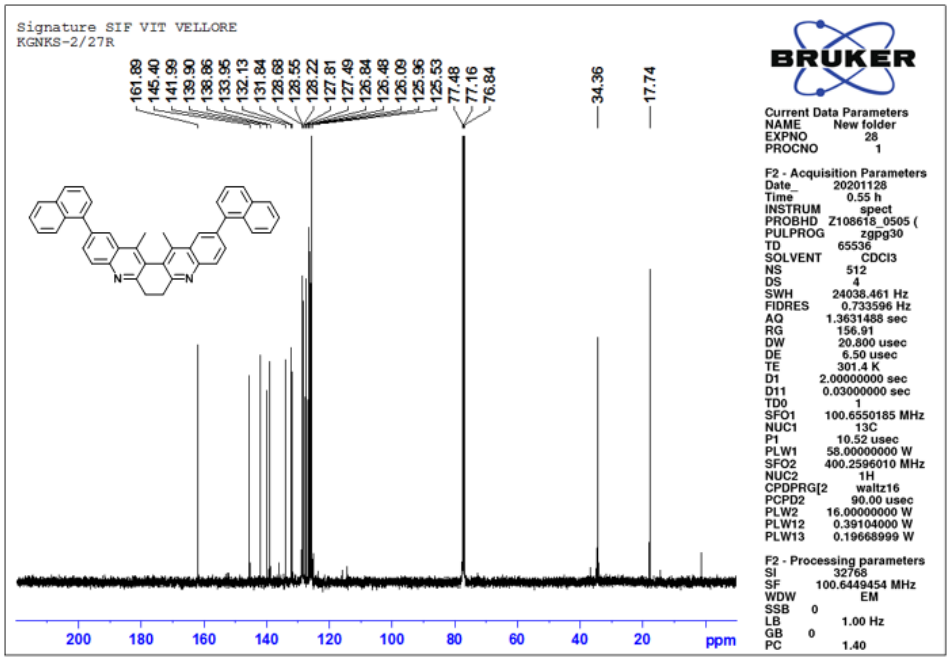
SI Figure. 39: HRMS spectrum of compound **6a**



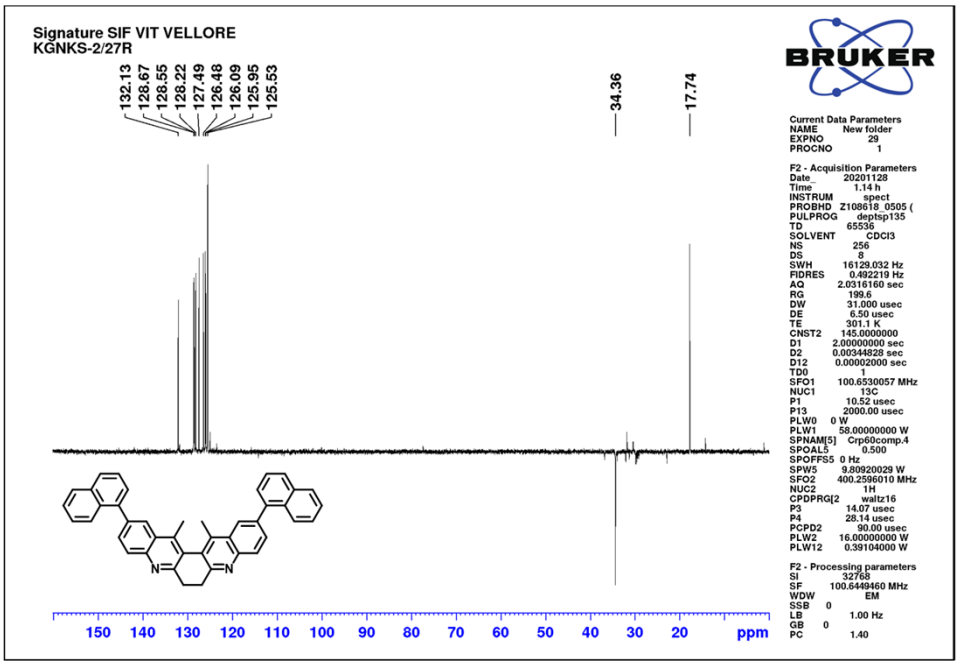
SI Figure. 40: ^{1}H NMR spectrum of compound **6b**



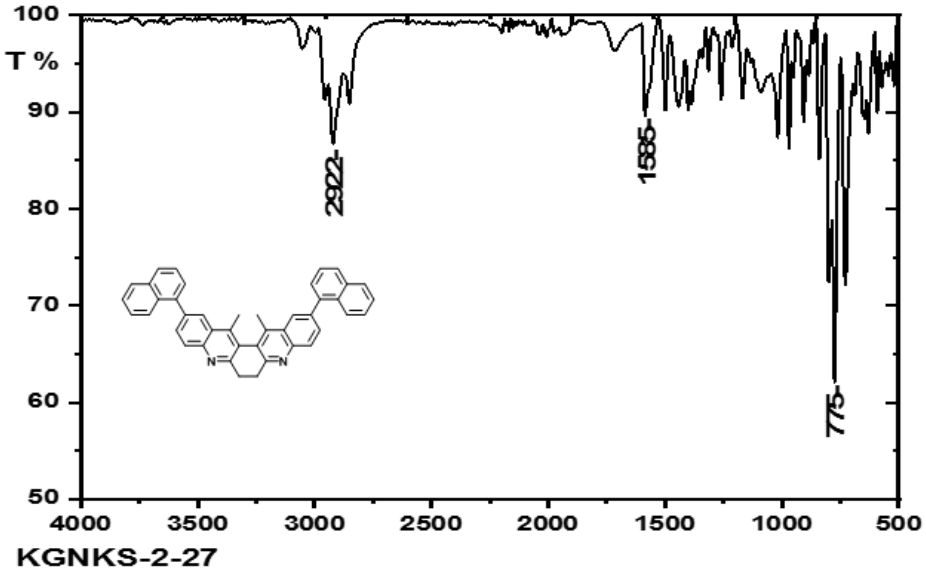
SI Figure. 41: Expansion of ^{1}H NMR spectrum of compound **6b**



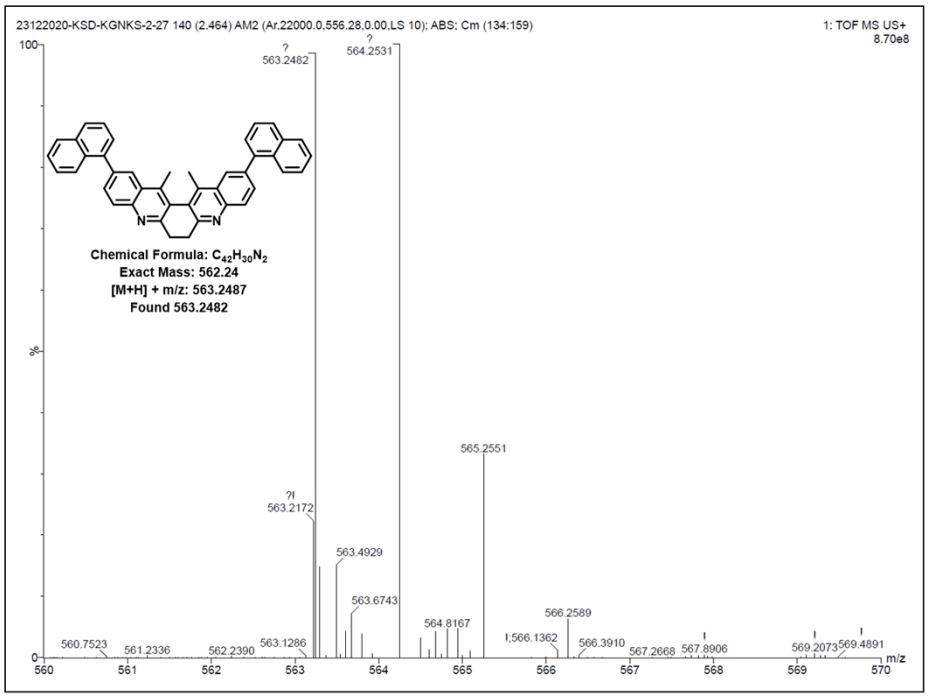
SI Figure. 42: ^{13}C NMR spectrum of compound **6b**



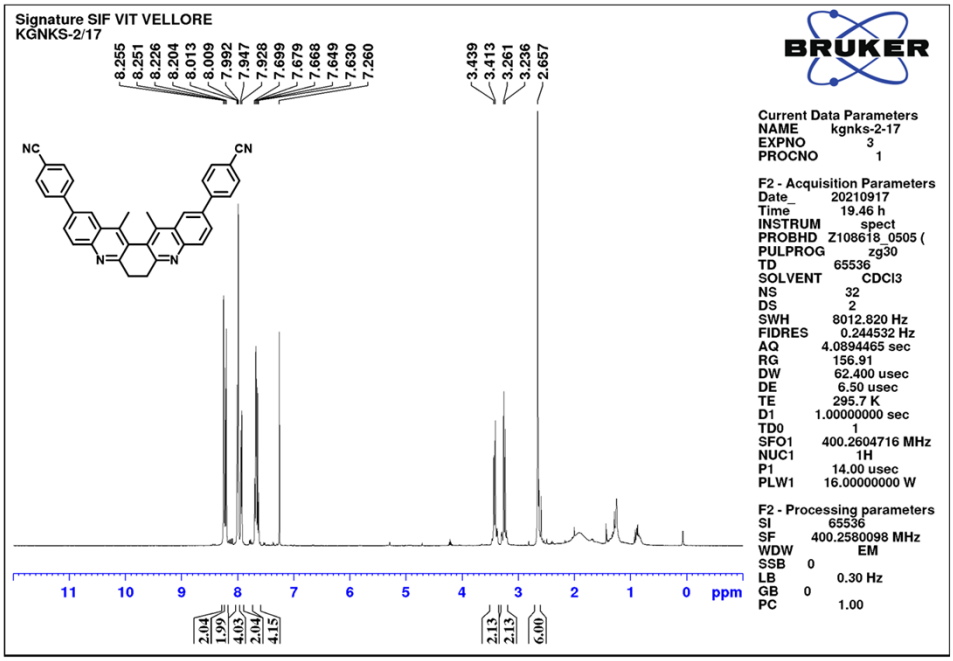
SI Figure. 43: DEPT-135 spectrum of compound **6b**



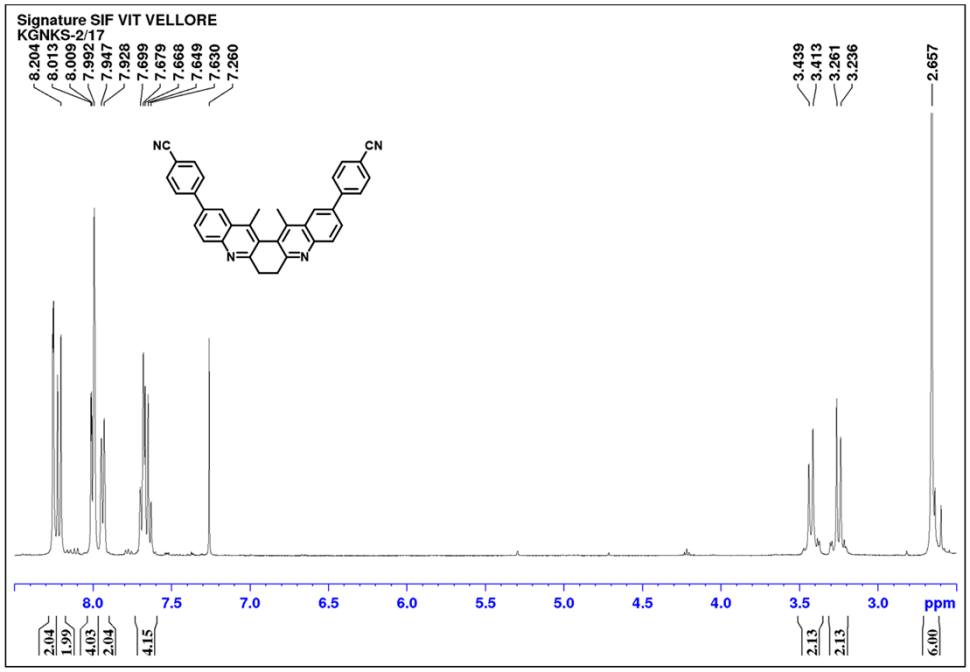
SI Figure. 44: FTIR spectrum of compound **6b**



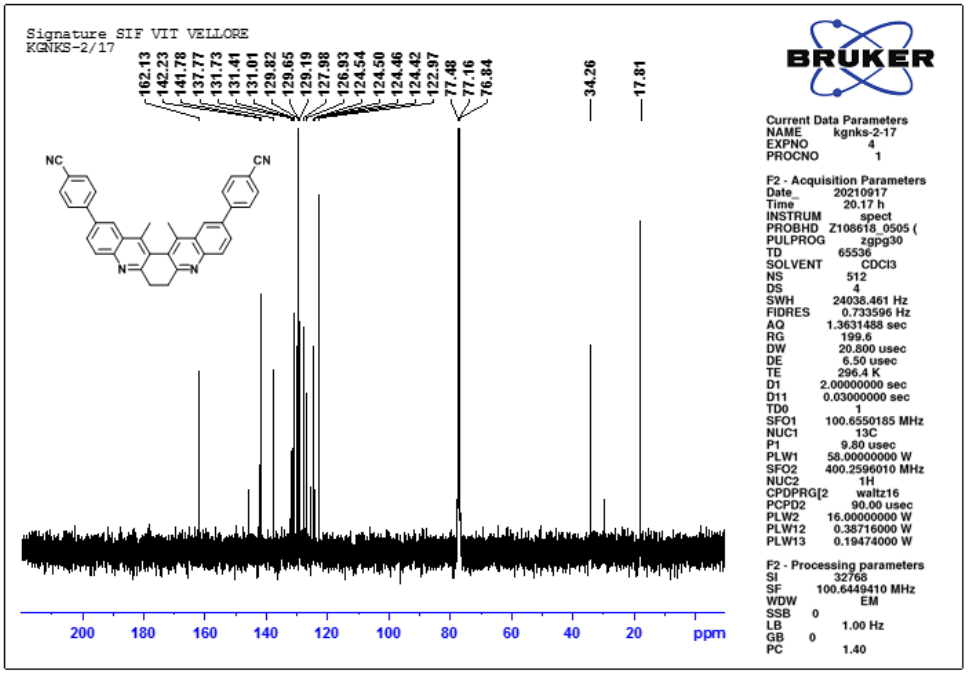
SI Figure. 45: HRMS spectrum of compound **6b**



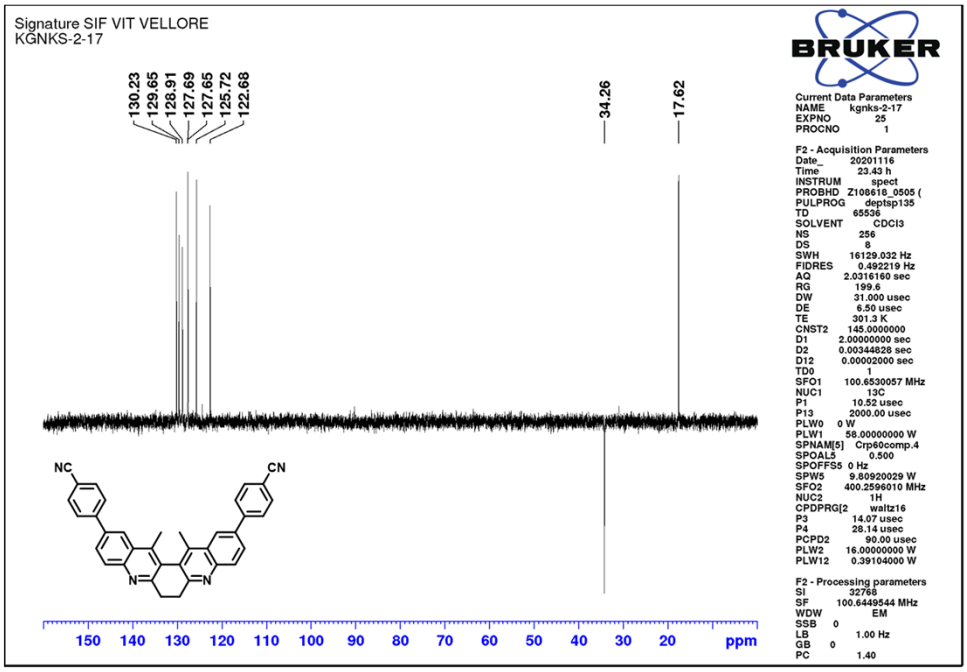
SI Figure. 46: ^{1}H NMR spectrum of compound **6c**



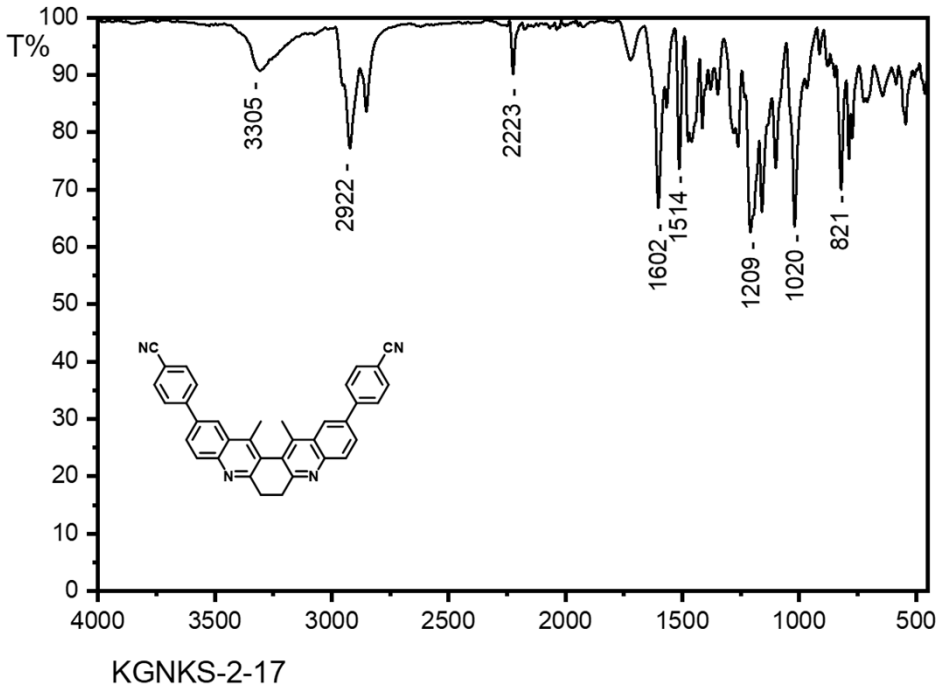
SI Figure. 47: Expansion of ^{1}H NMR spectrum of compound **6c**



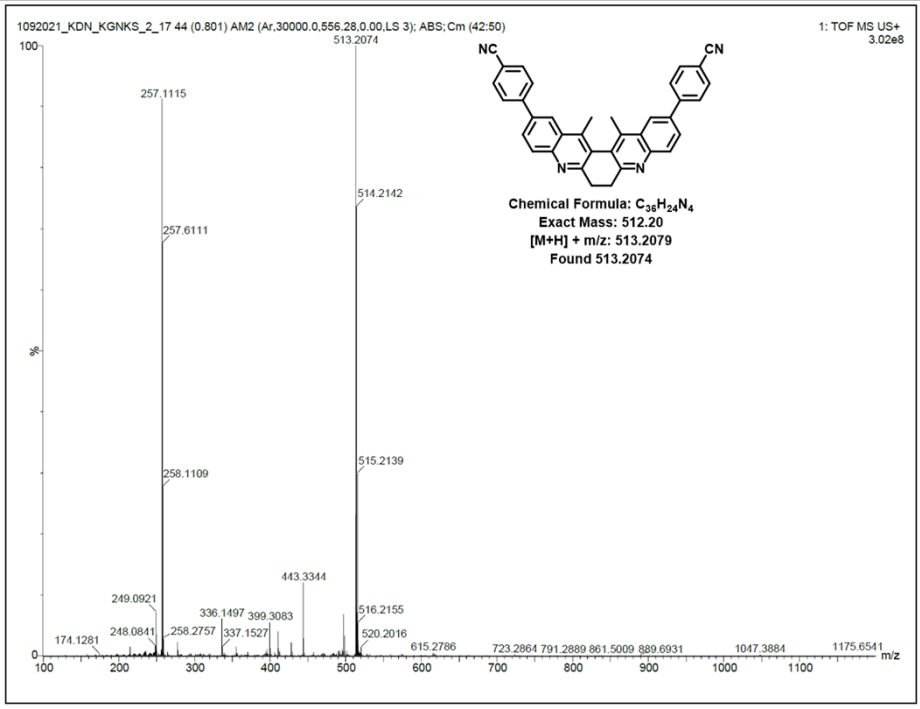
SI Figure. 48: ^{13}C NMR spectrum of compound **6c**



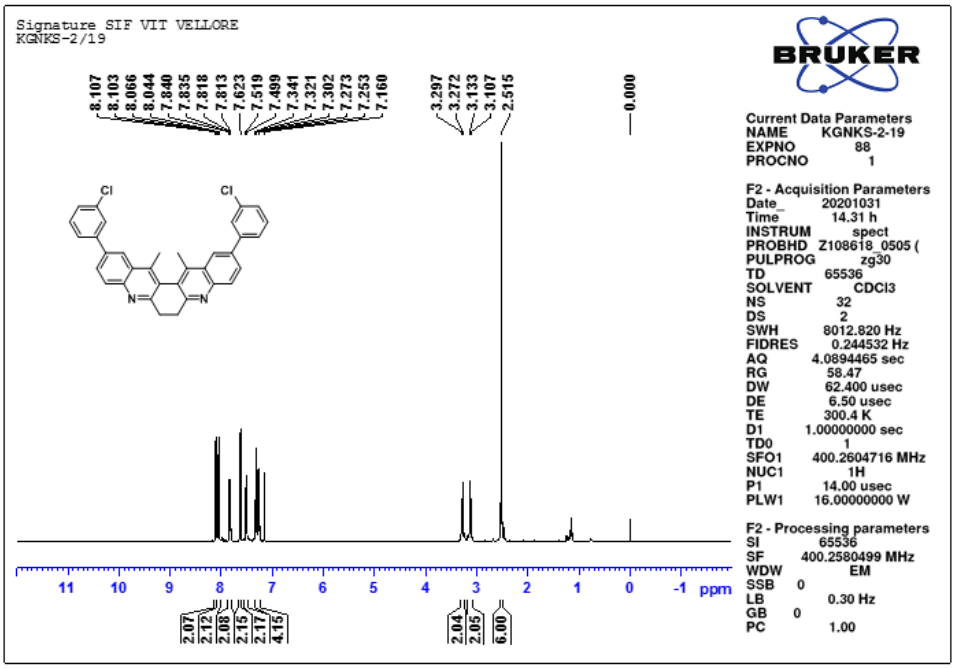
SI Figure. 49: DEPT-135 spectrum of compound **6c**



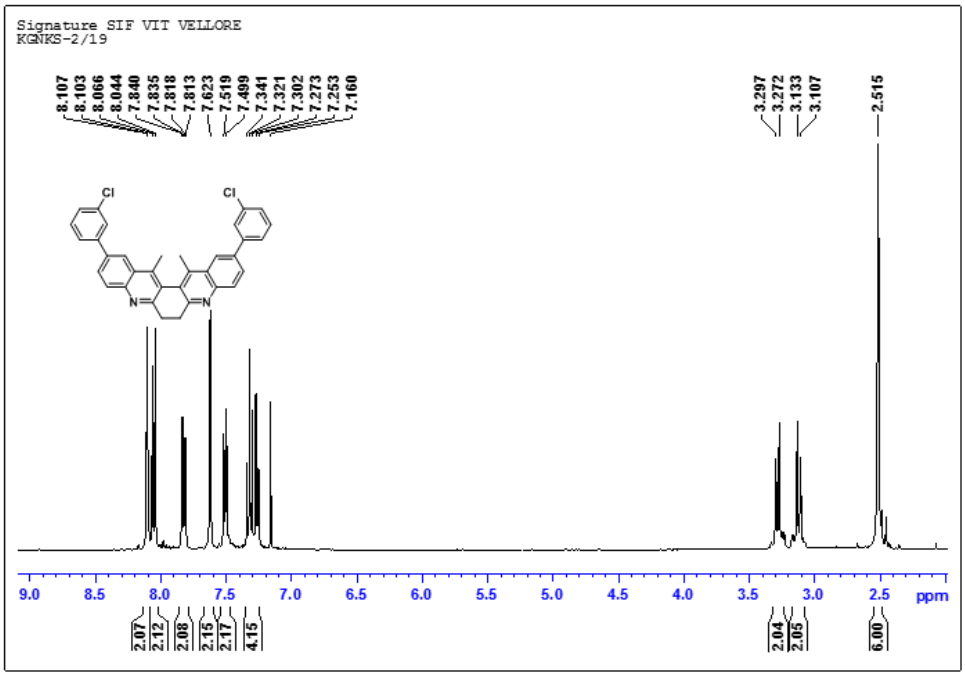
SI Figure. 50: FTIR spectrum of compound **6c**



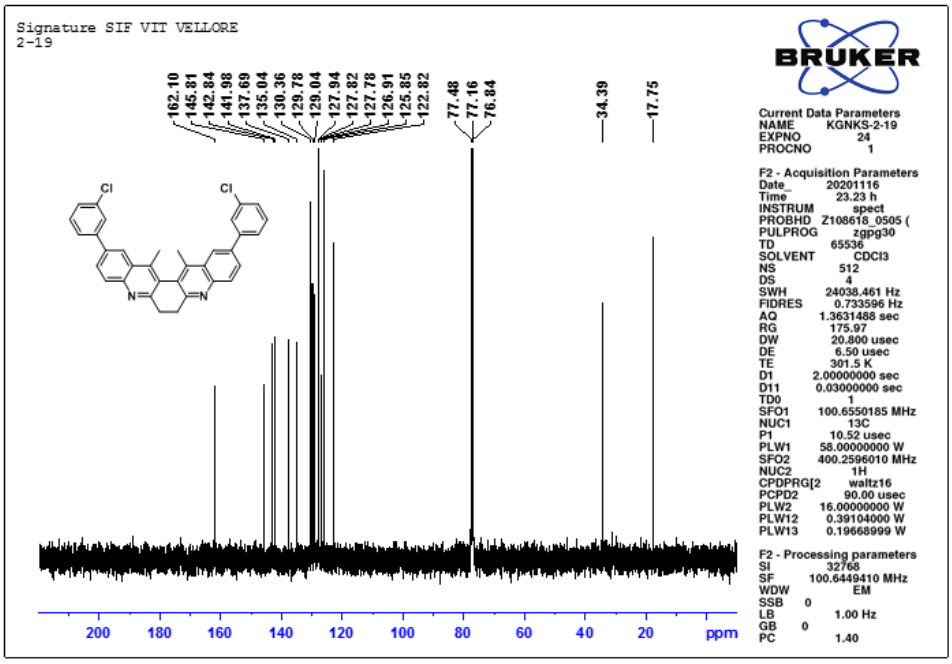
SI Figure. 51: HRMS spectrum of compound **6c**



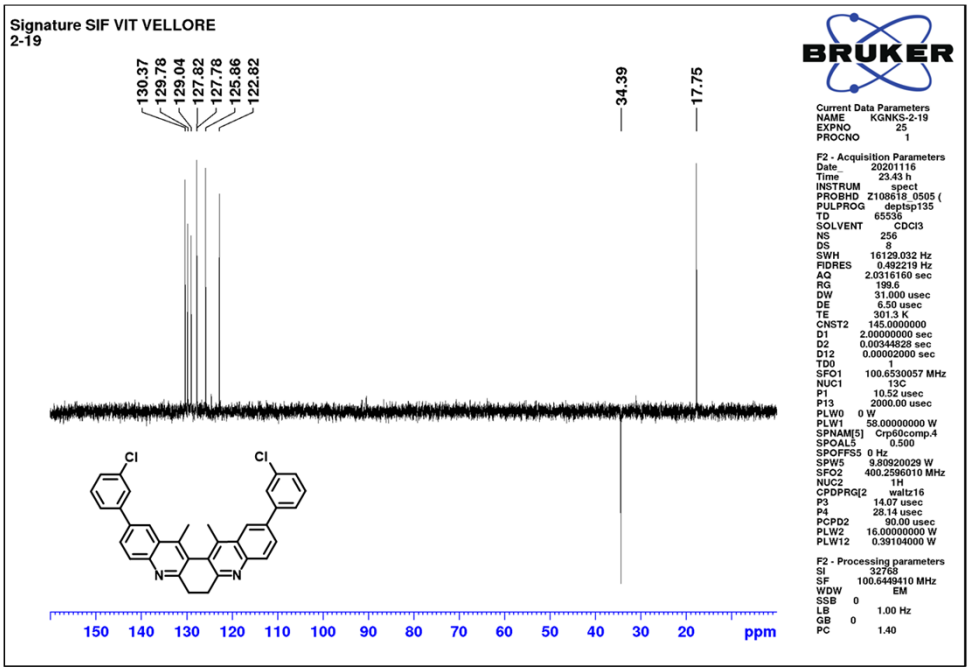
SI Figure. 52: ^{1}H NMR spectrum of compound **6d**



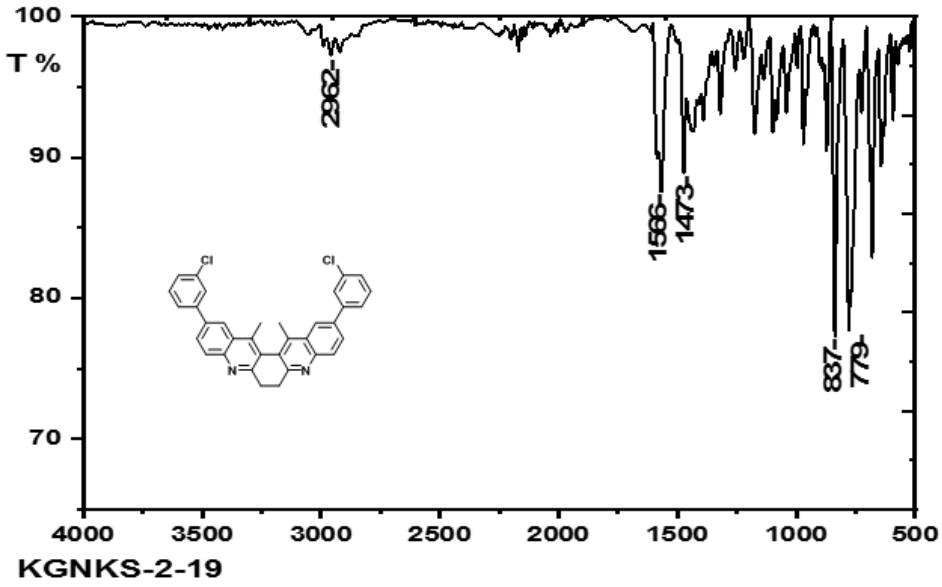
SI Figure. 53: Expansion of ^{1}H NMR spectrum of compound **6d**



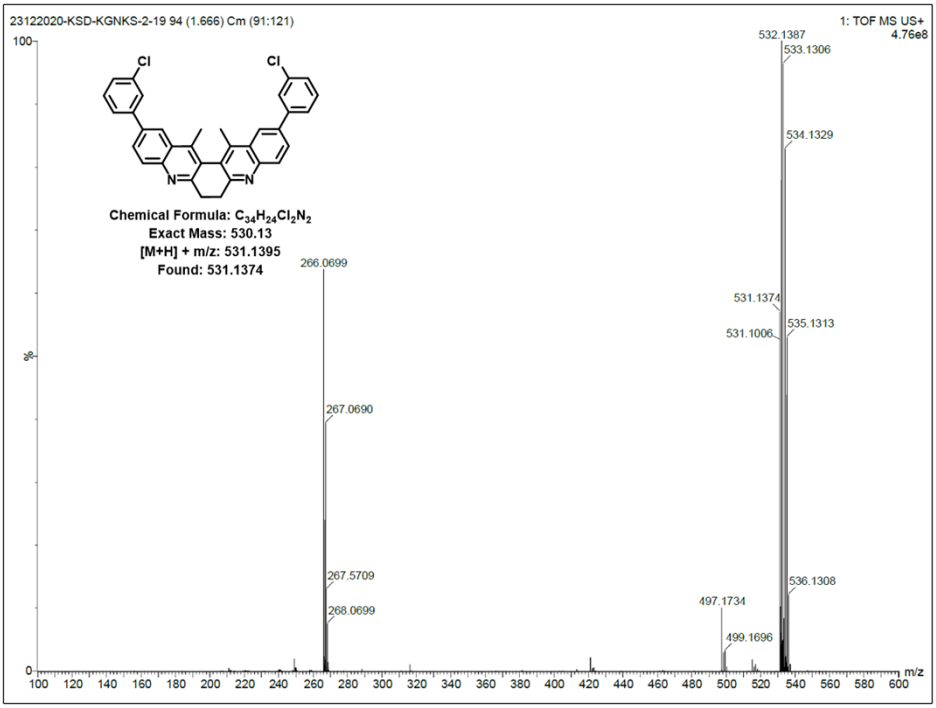
SI Figure. 54: ^{13}C NMR spectrum of compound **6d**



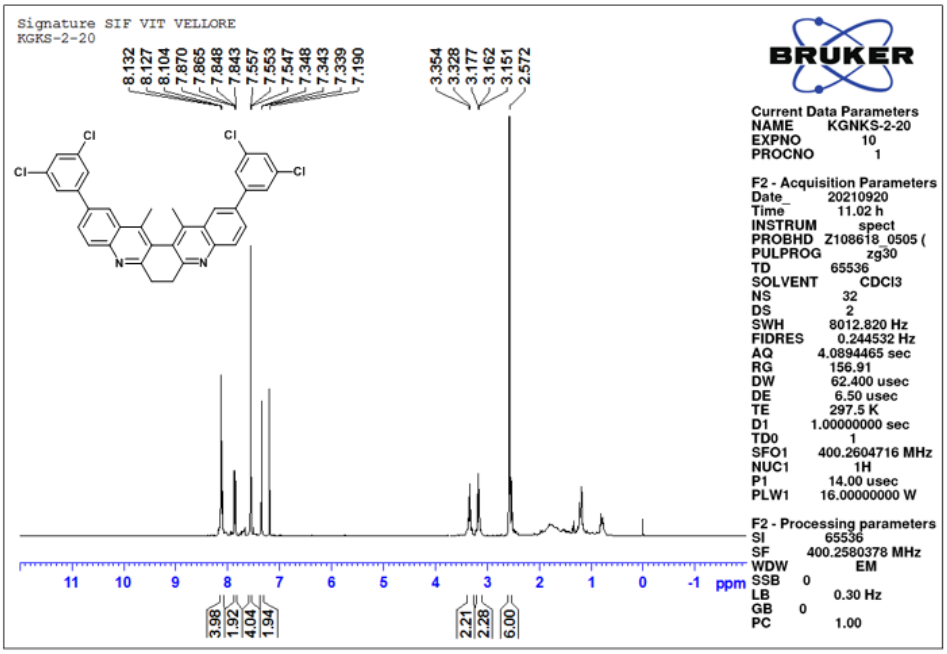
SI Figure. 55: DEPT-135 spectrum of compound **6d**



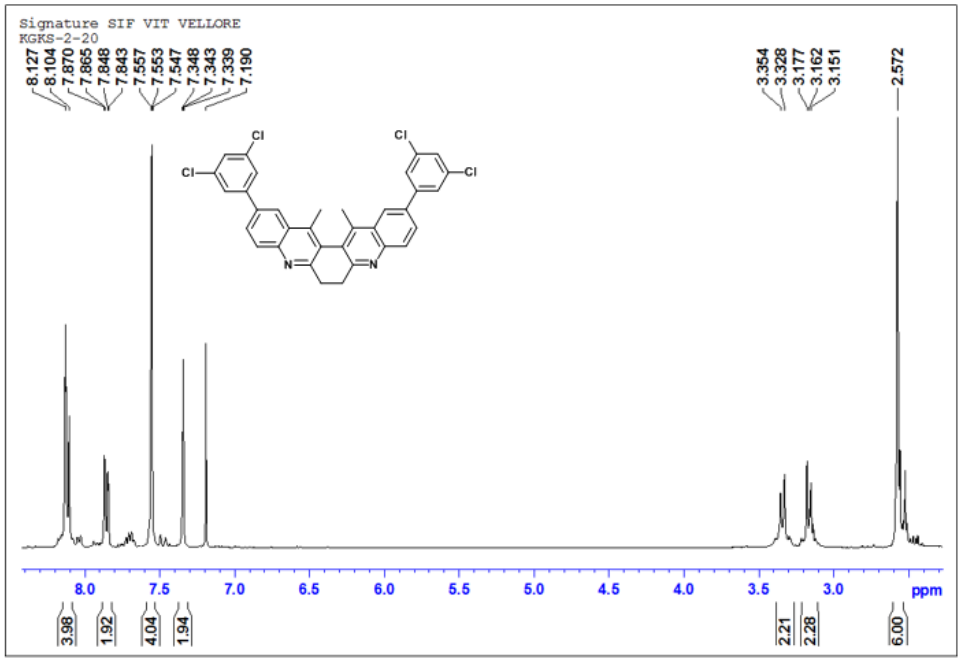
SI Figure. 56: FTIR spectrum of compound **6d**



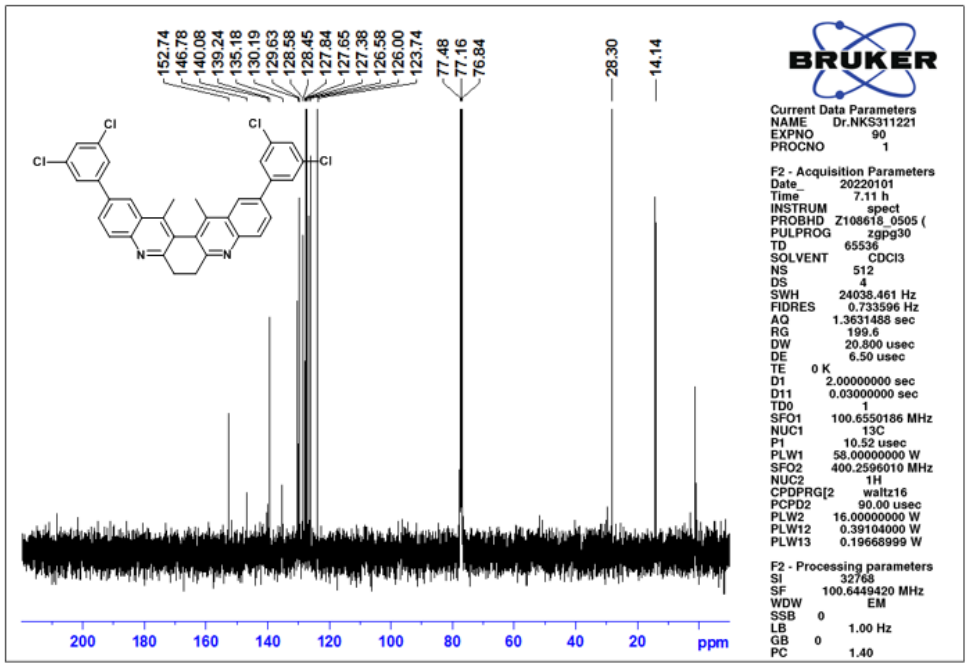
SI Figure. 57: HRMS spectrum of compound **6d**



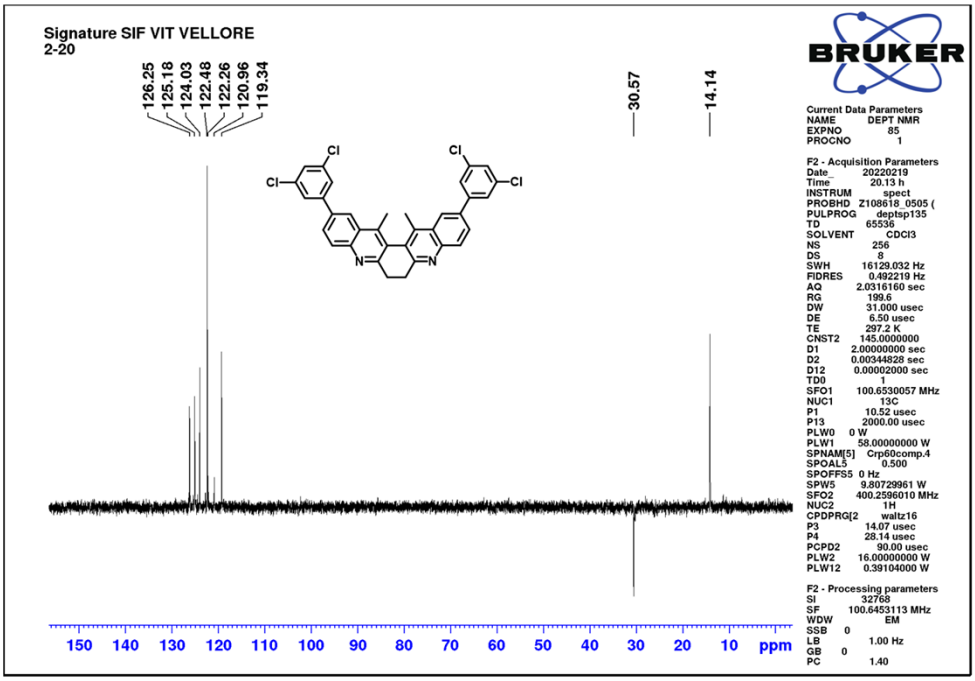
SI Figure. 58: ^{1}H NMR spectrum of compound **6e**



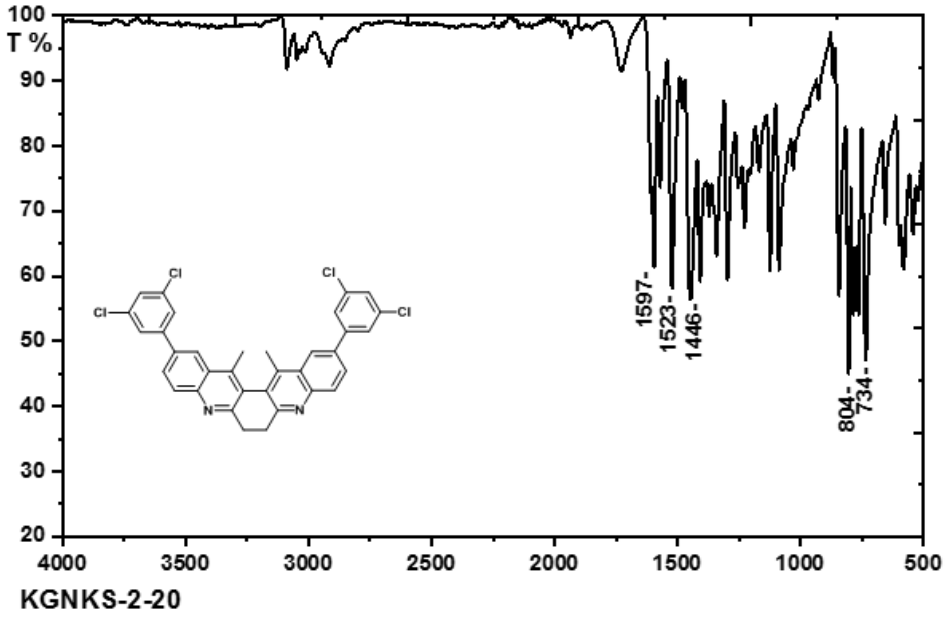
SI Figure. 59: Expansion of ^{1}H NMR spectrum of compound **6e**



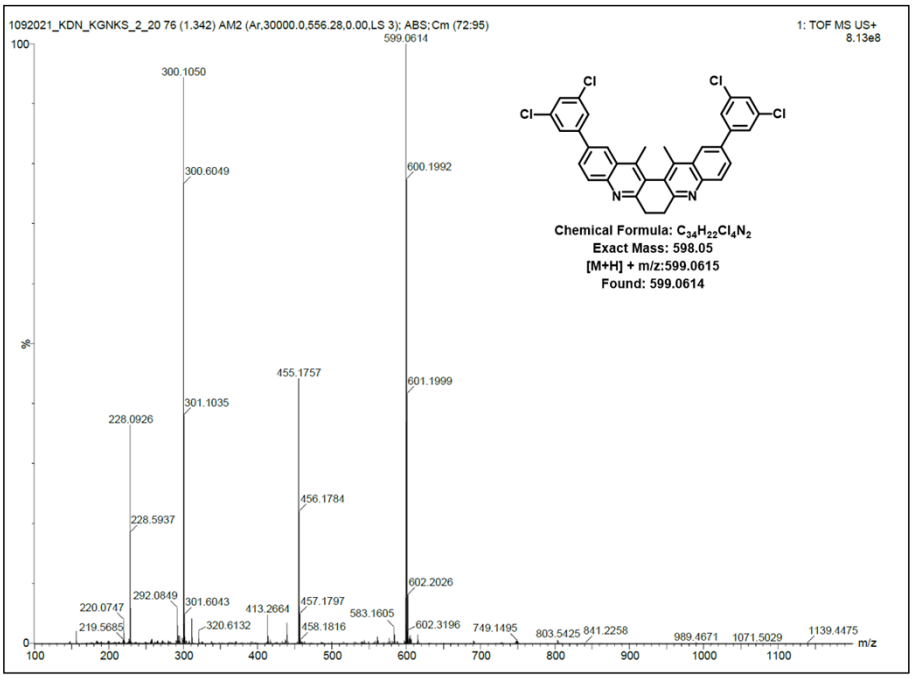
SI Figure. 60: ^{13}C NMR spectrum of compound **6e**



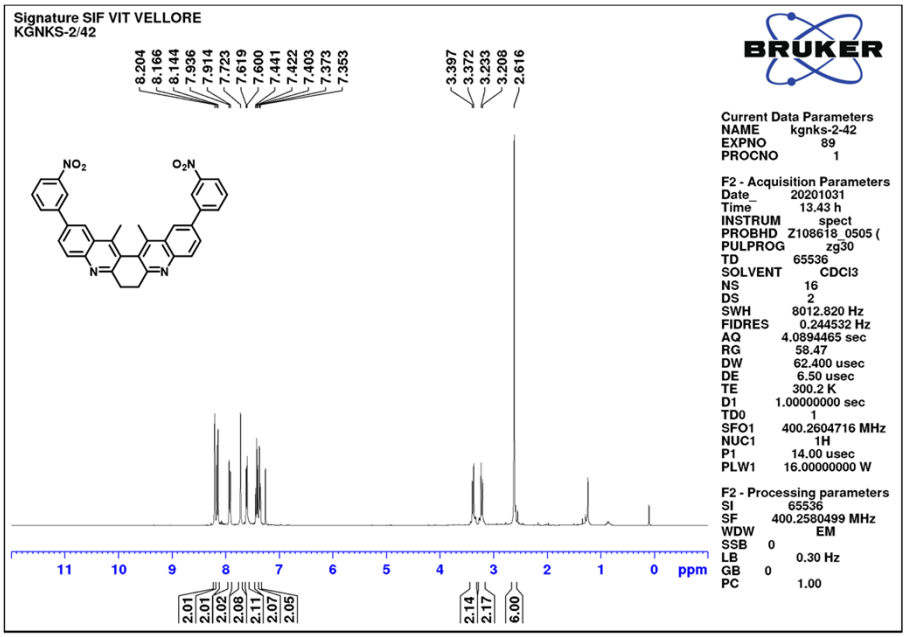
SI Figure. 61: DEPT-135 spectrum of compound **6e**



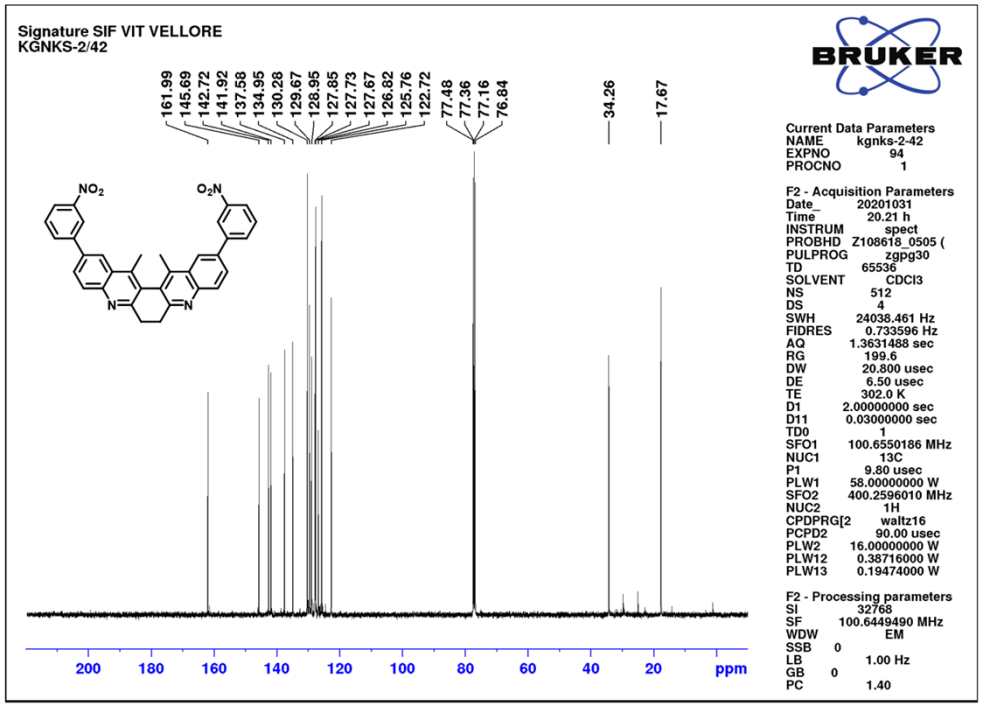
SI Figure. 62: FTIR spectrum of compound **6e**



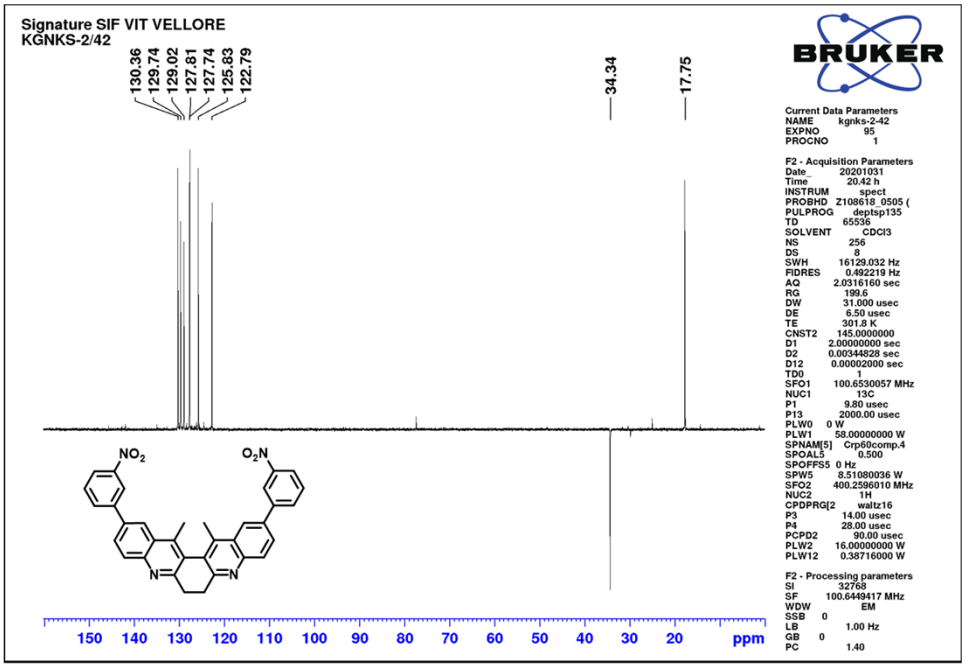
SI Figure. 63: HRMS spectrum of compound **6e**



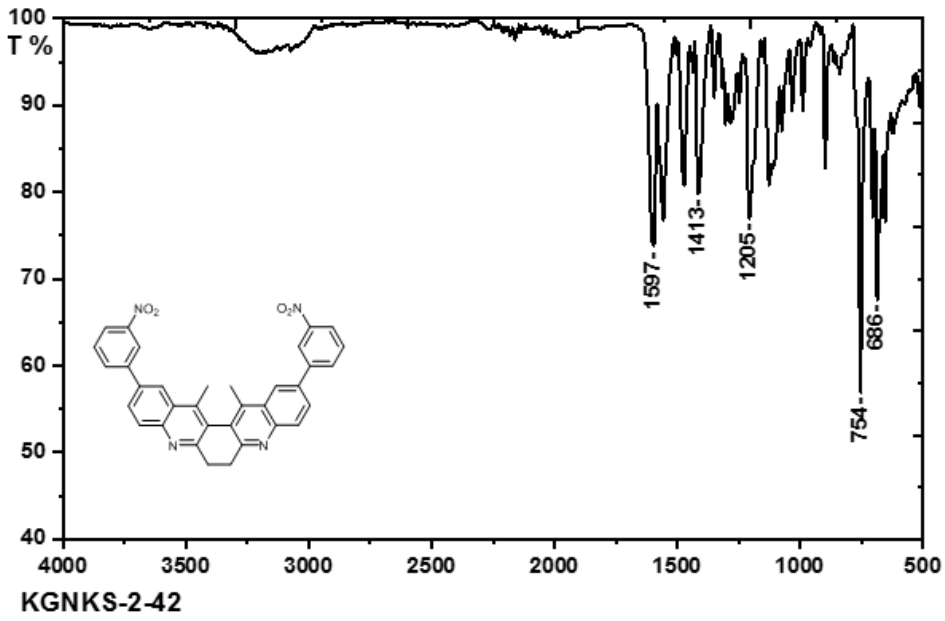
SI Figure. 64: ^{1}H NMR spectrum of compound **6f**



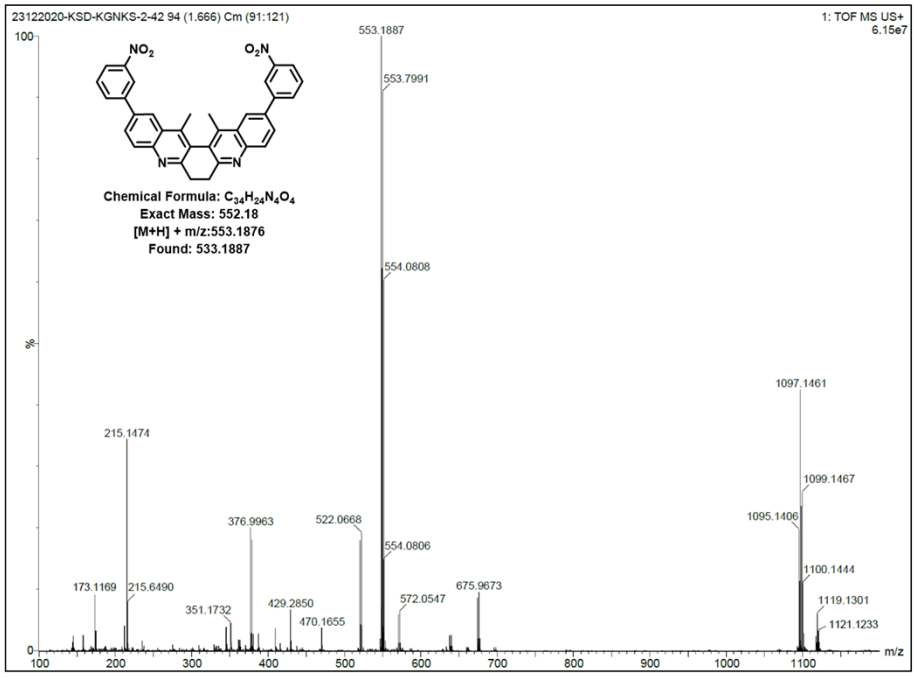
SI Figure. 65: ^{13}C NMR spectrum of compound **6f**



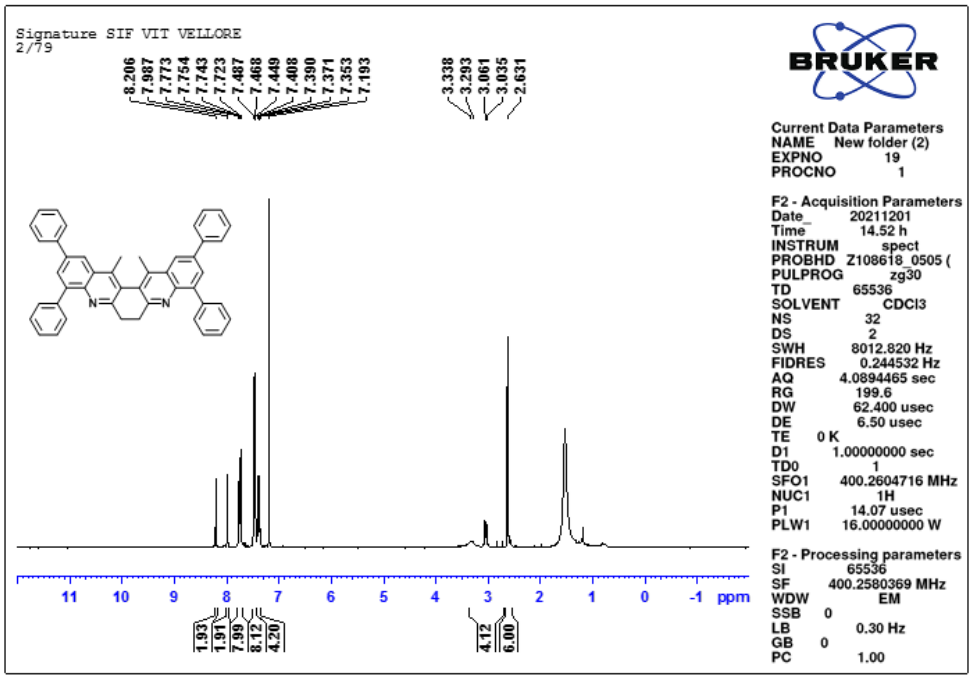
SI Figure. 66: DEPT-135 spectrum of compound **6f**



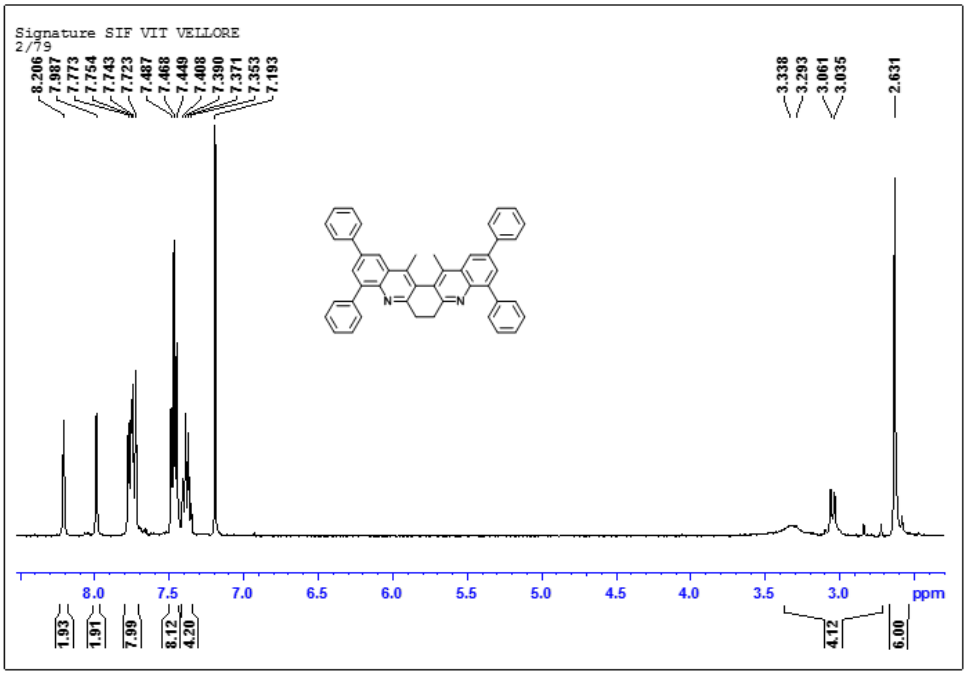
SI Figure. 67: FTIR spectrum of compound **6f**



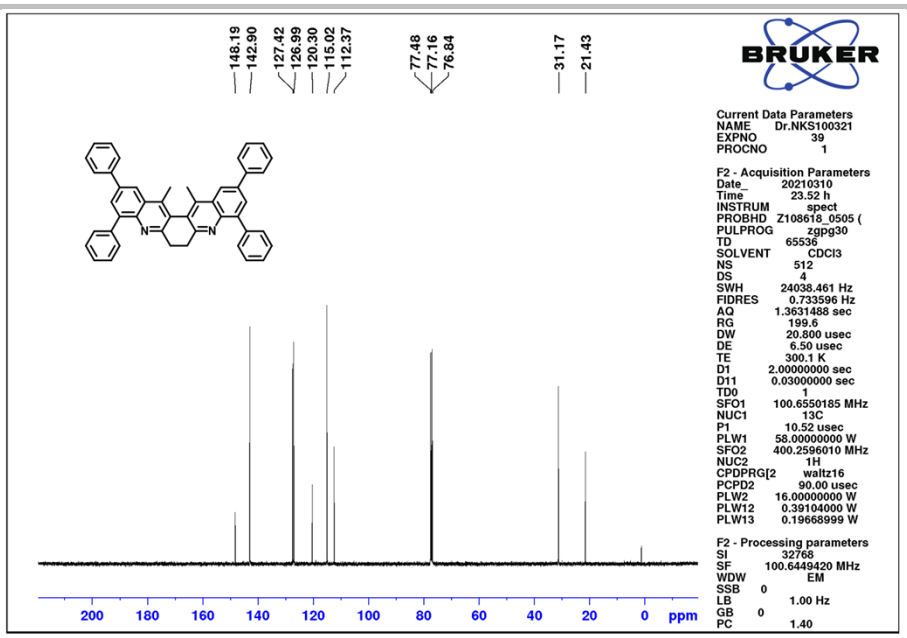
SI Figure. 68: HRMS spectrum of compound **6f**



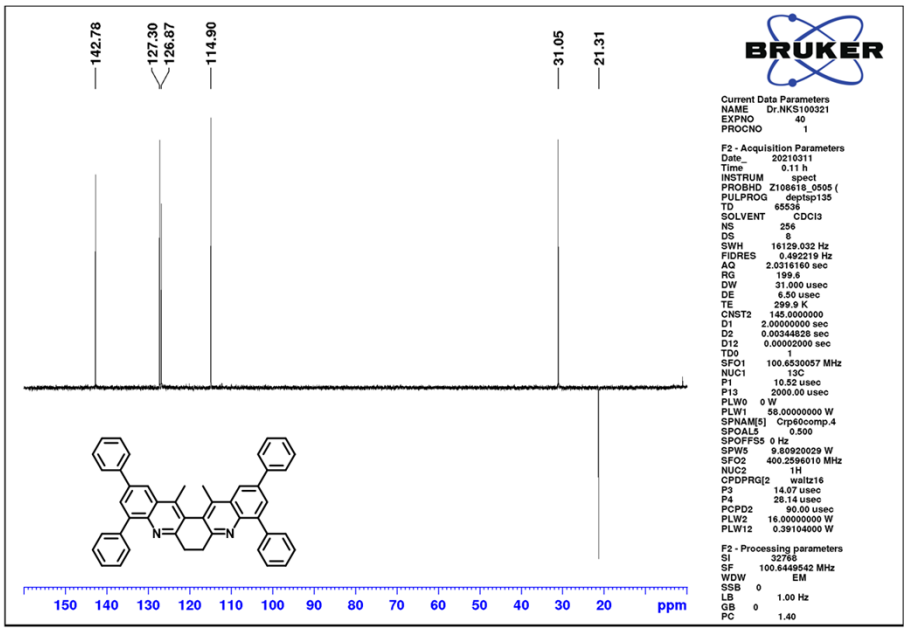
SI Figure. 69: ^{1}H NMR spectrum of compound **6g**



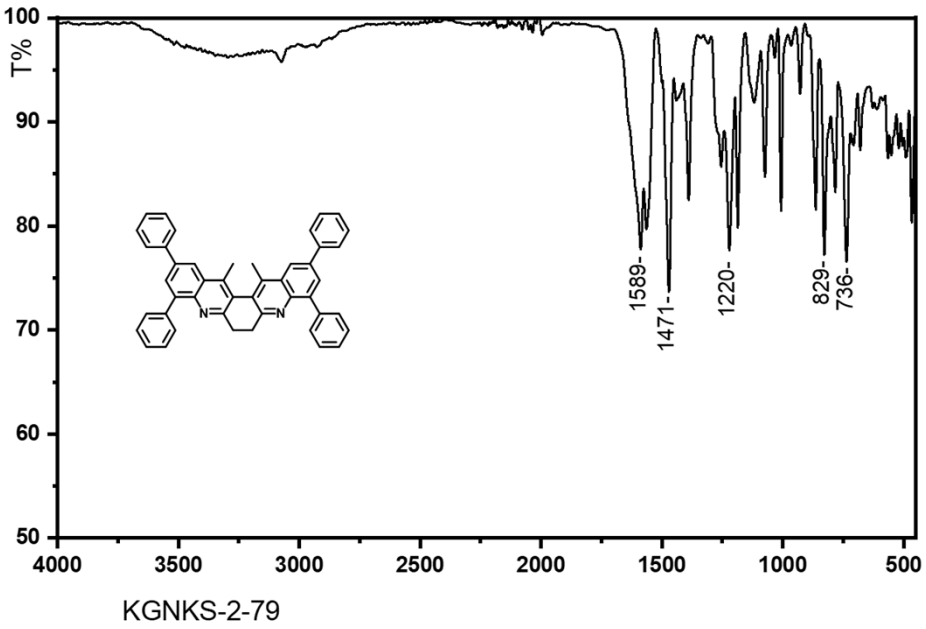
SI Figure. 70: Expansion of ^{1}H NMR spectrum of compound **6g**



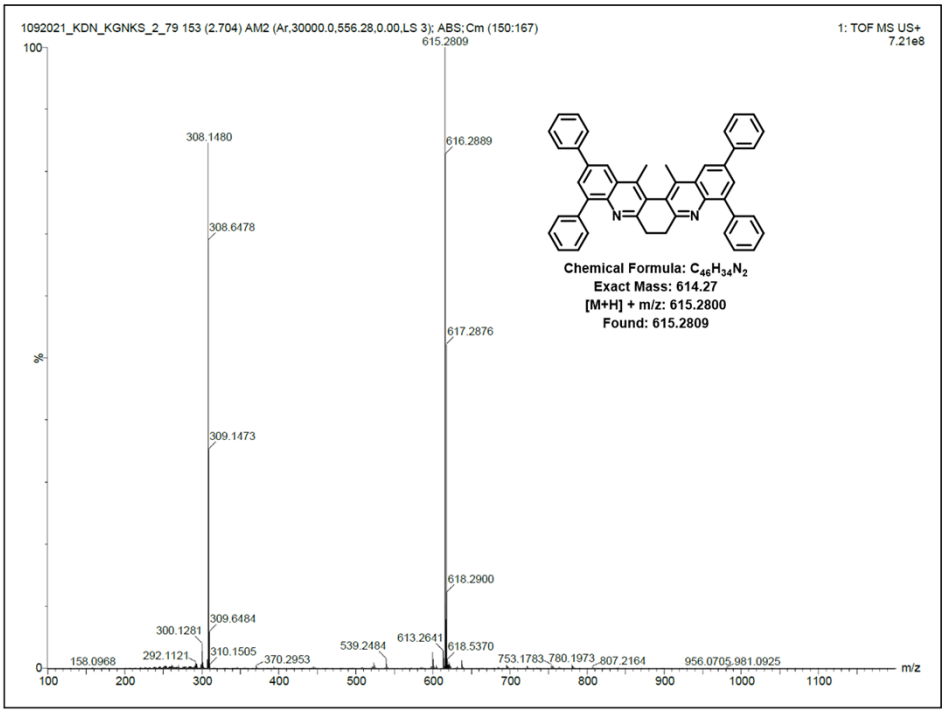
SI Figure. 71: ^{13}C NMR spectrum of compound **6g**



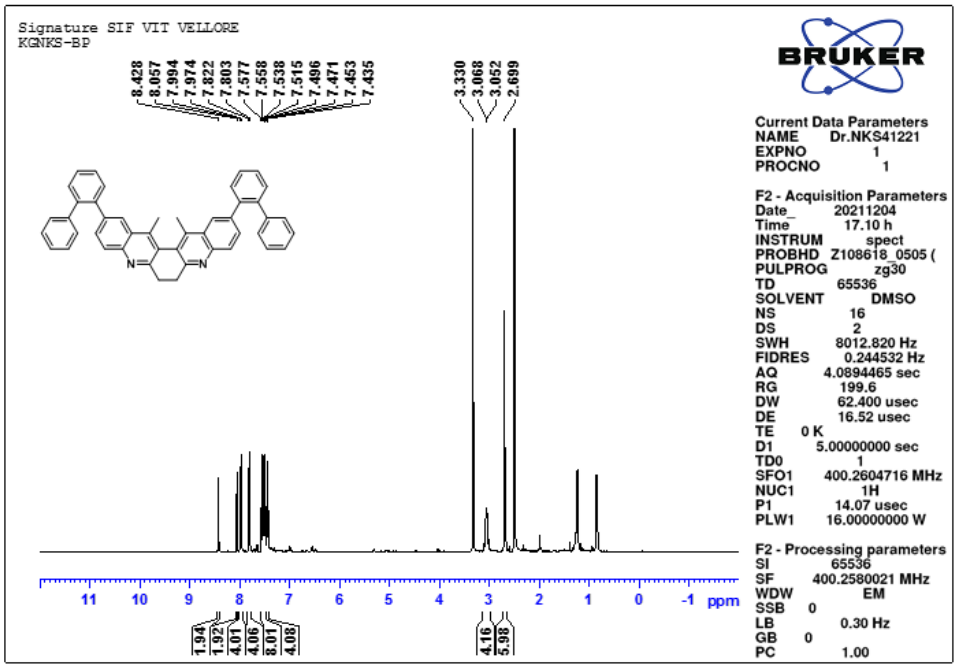
SI Figure. 72: DEPT-135 spectrum of compound **6g**



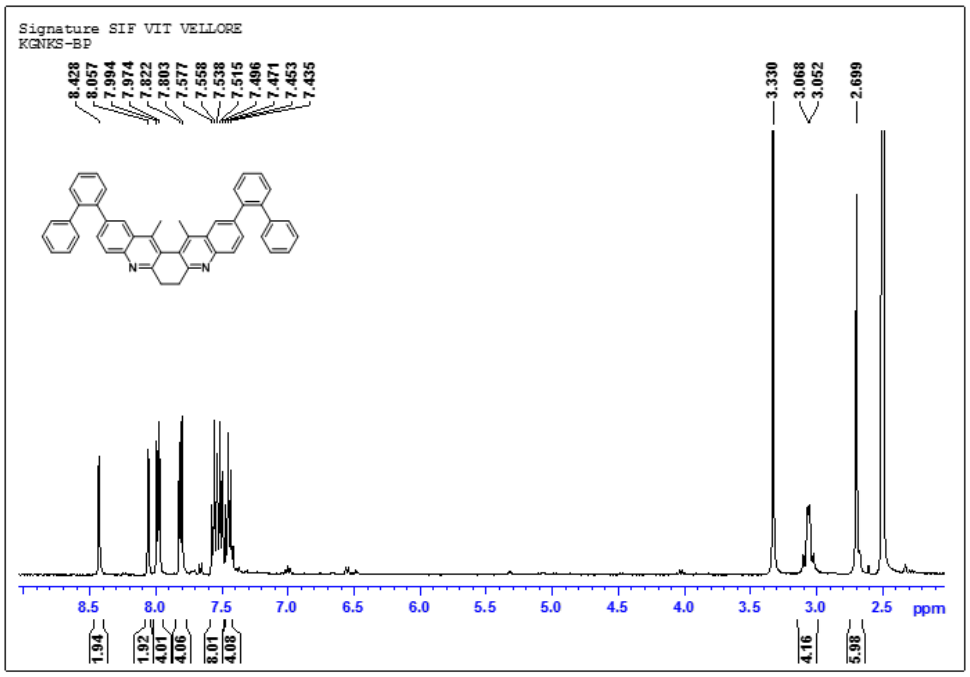
SI Figure. 73: FTIR spectrum of compound **6g**



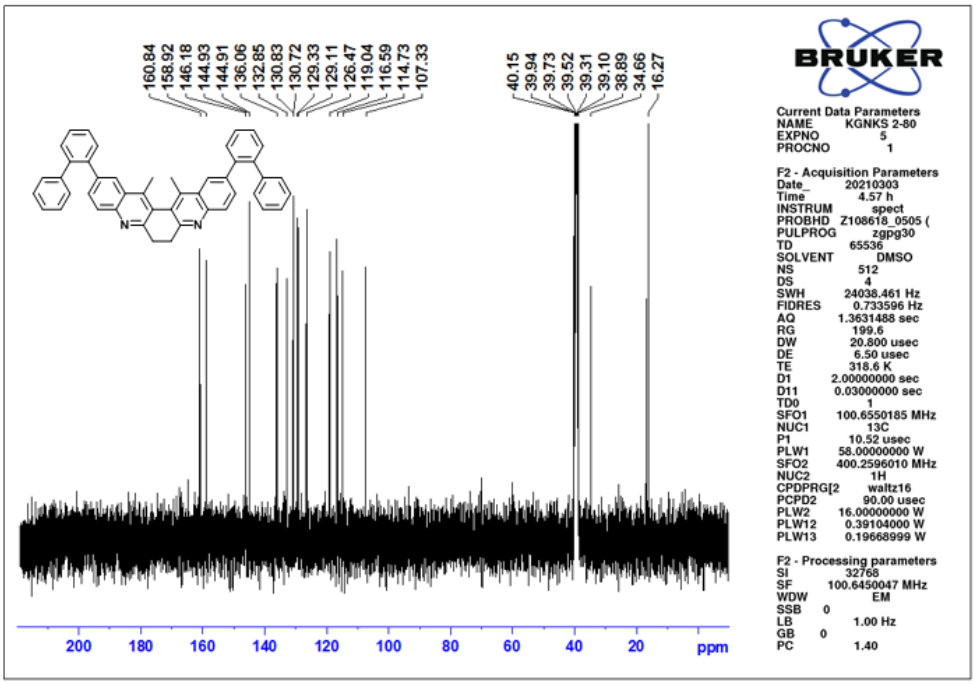
SI Figure. 74: HRMS spectrum of compound **6g**



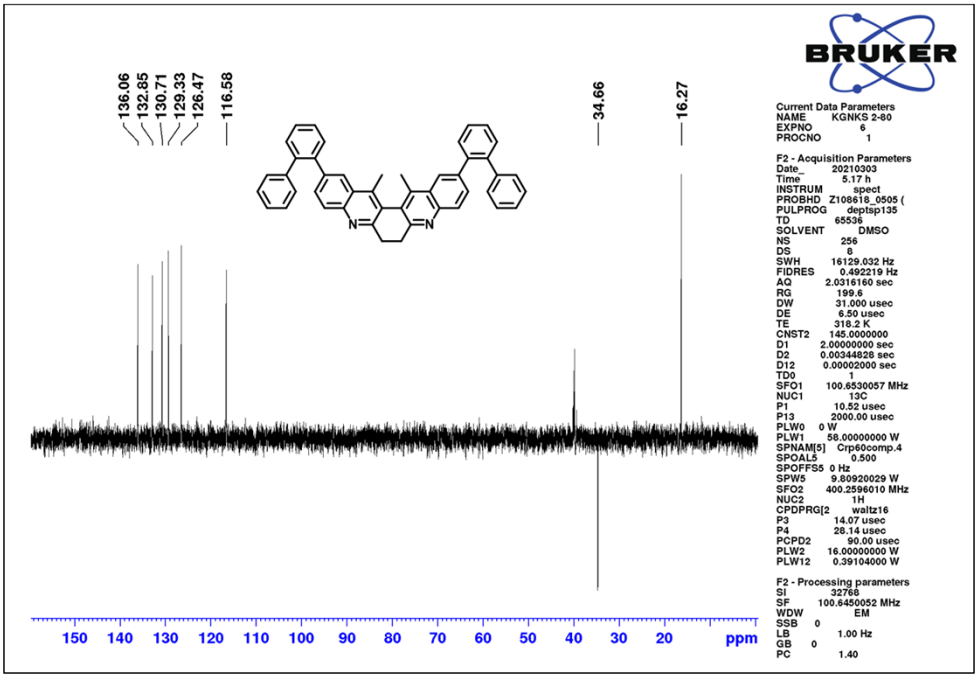
SI Figure. 75: ^{1}H NMR spectrum of compound **6h**



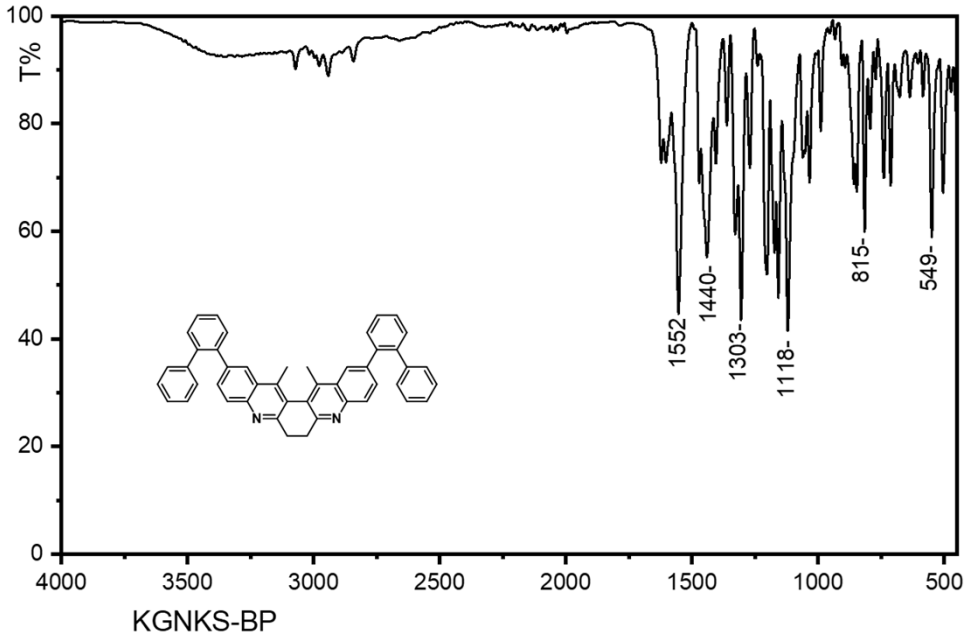
SI Figure. 76: Expansion of ^{1}H NMR spectrum of compound **6h**



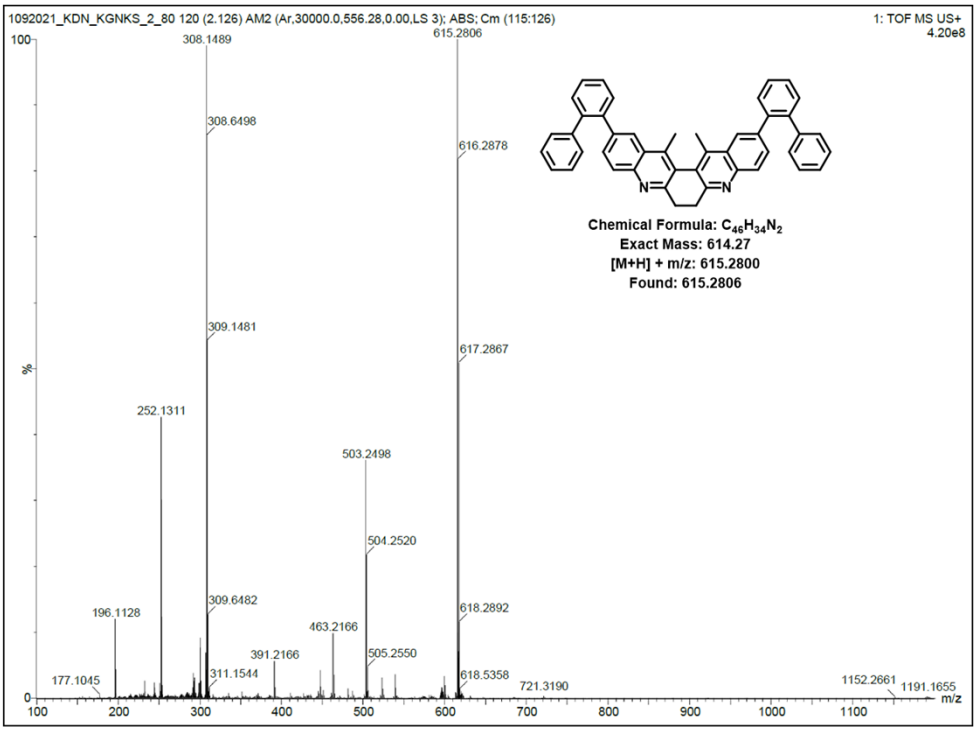
SI Figure. 77: ^{13}C NMR spectrum of compound **6h**



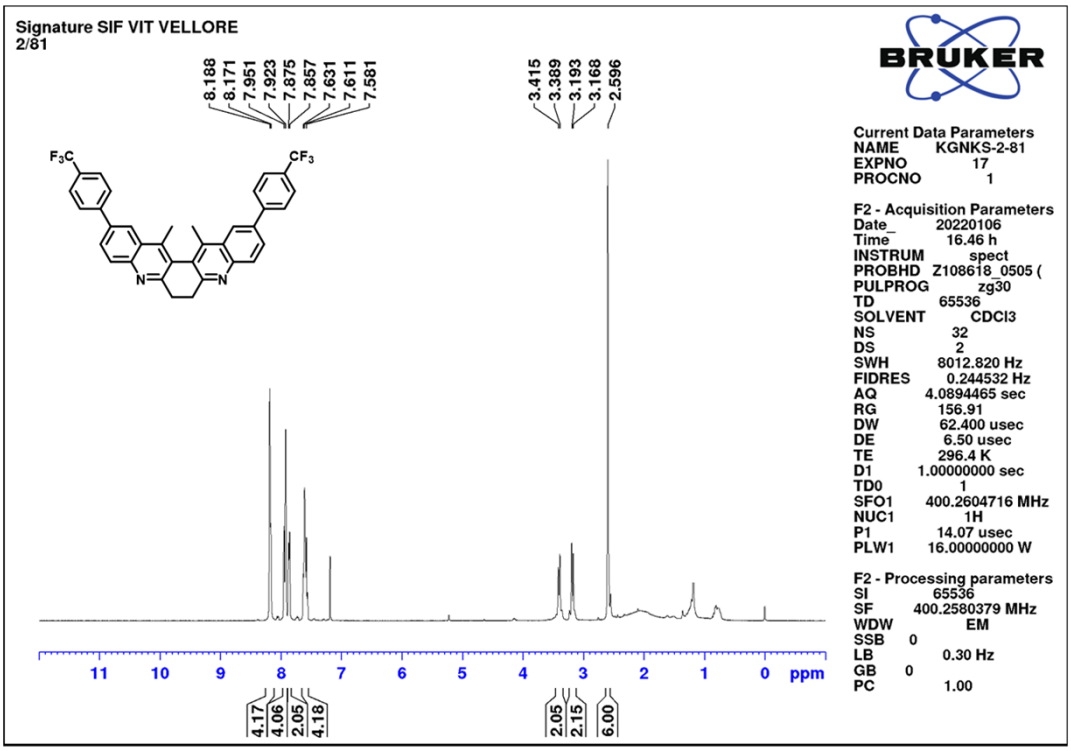
SI Figure. 78: DEPT-135 spectrum of compound **6h**



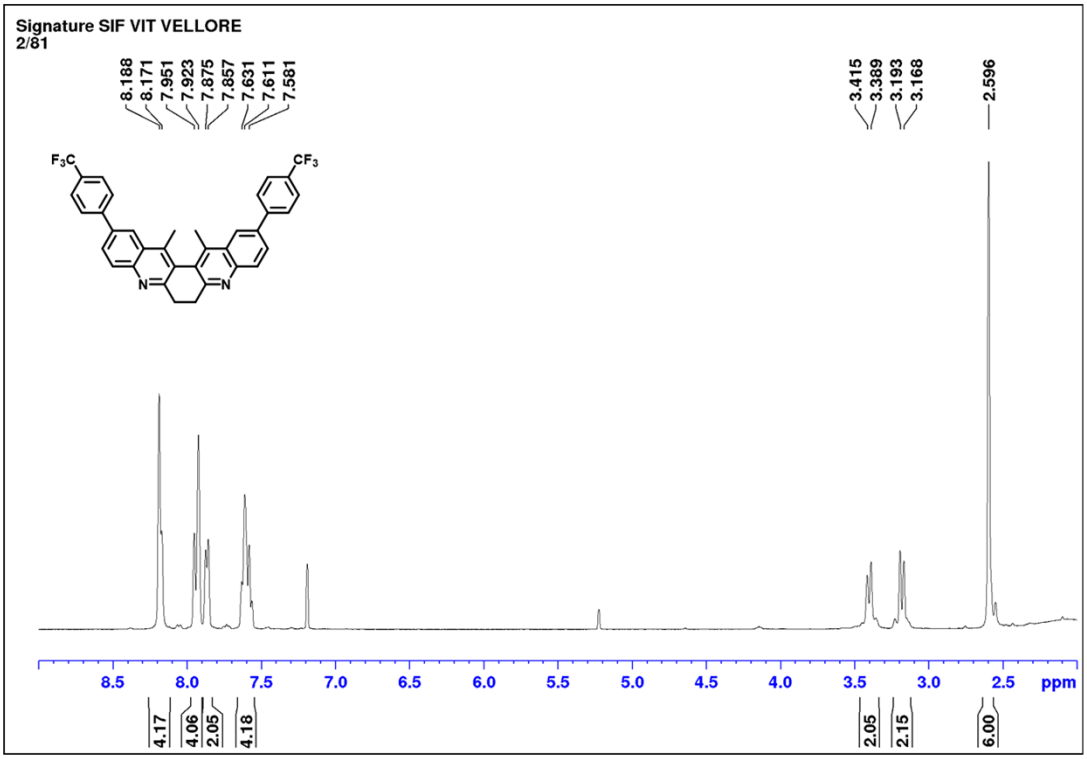
SI Figure. 79: FTIR spectrum of compound **6h**



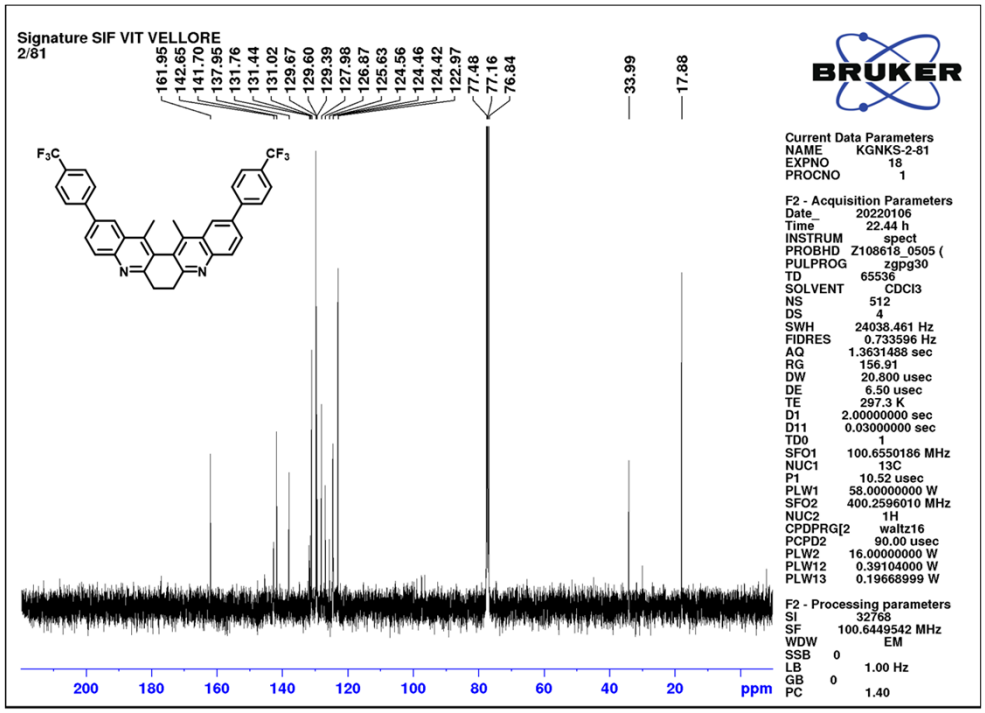
SI Figure. 80: HRMS spectrum of compound **6h**



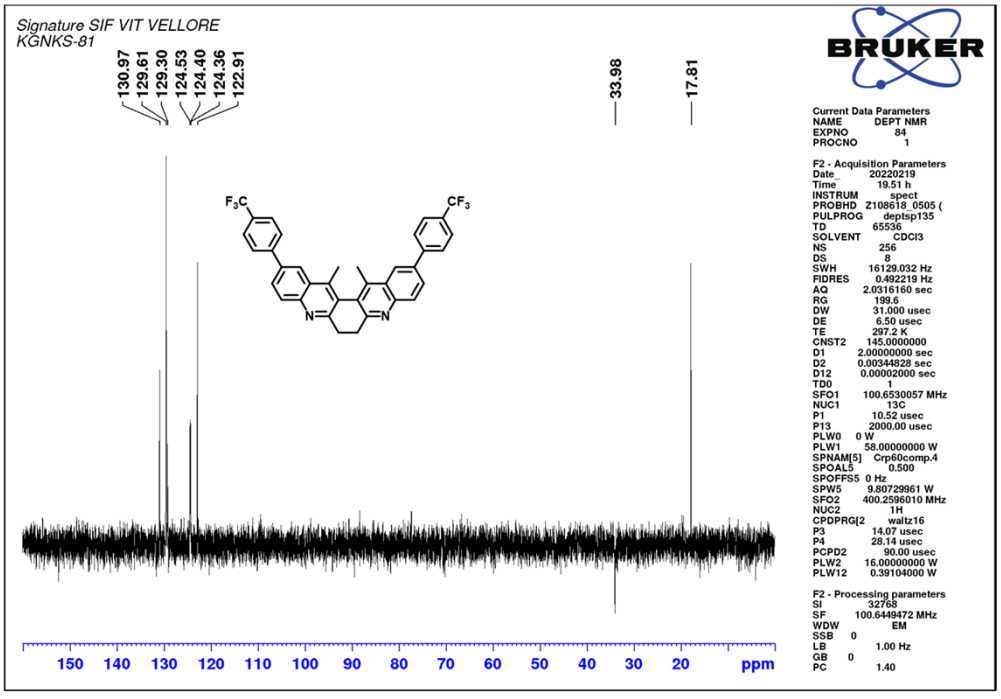
SI Figure. 81: ^{1}H NMR spectrum of compound **6i**



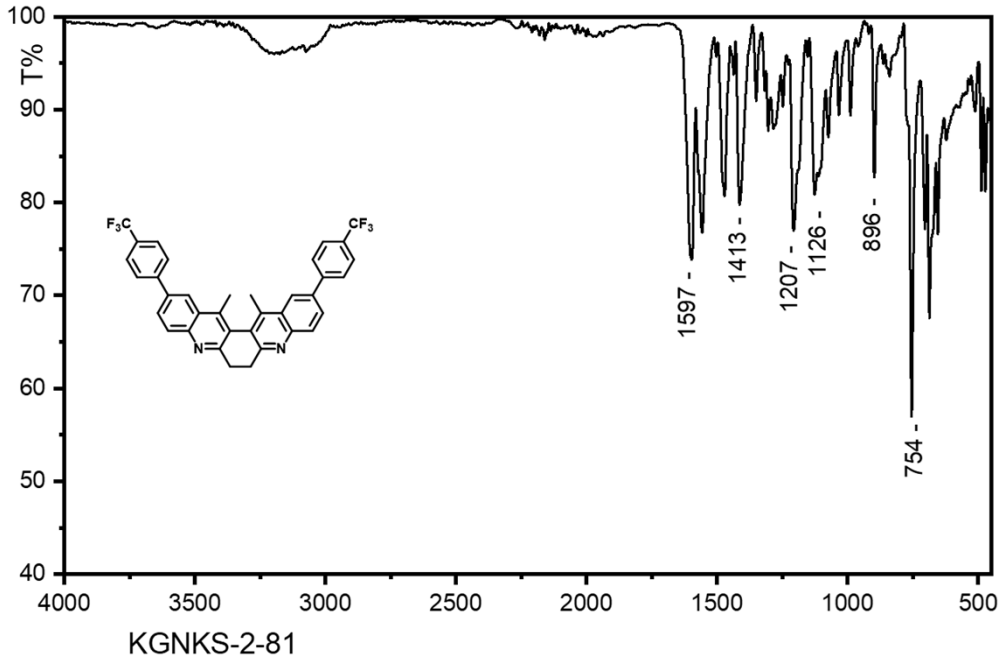
SI Figure. 82: Expansion of ^{1}H NMR spectrum of compound **6i**



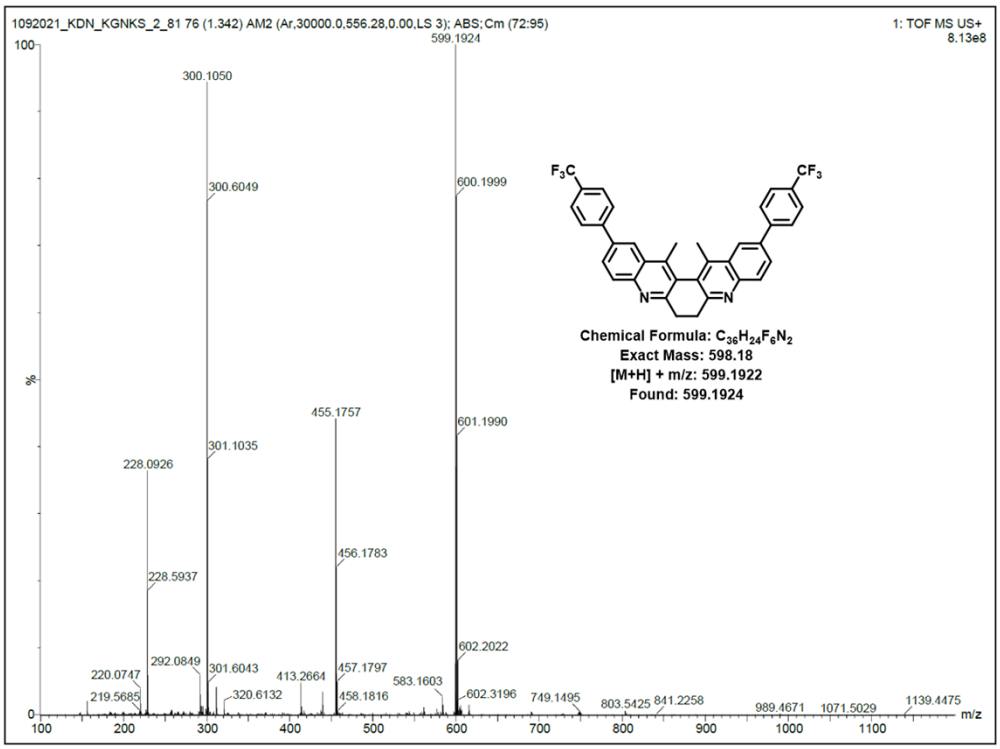
SI Figure. 83: ^{13}C NMR spectrum of compound **6i**



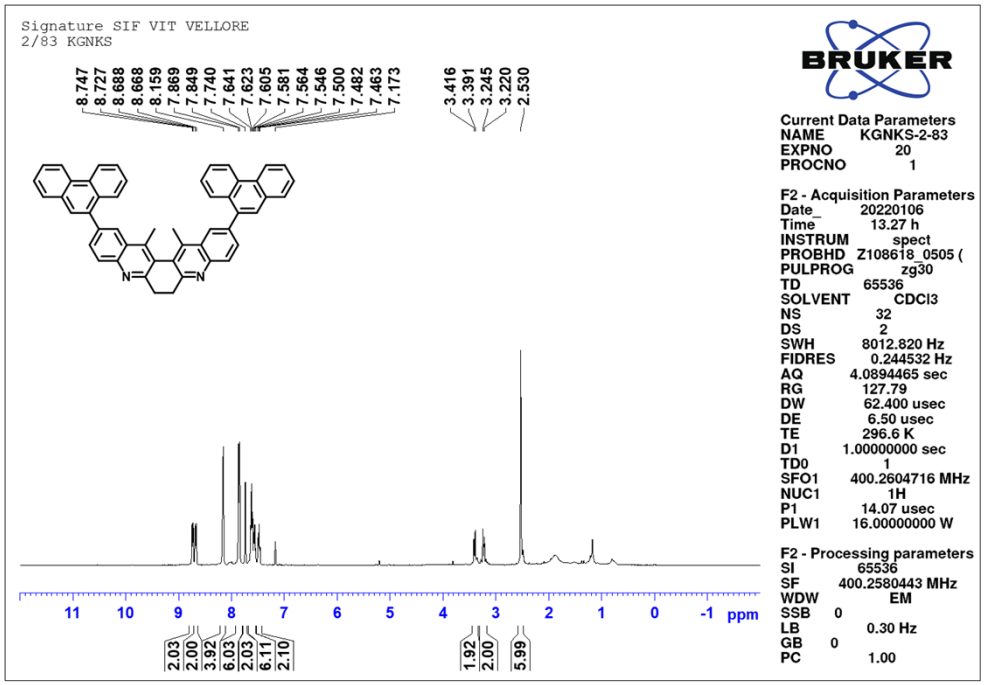
SI Figure. 84: DEPT-135 spectrum of compound **6i**



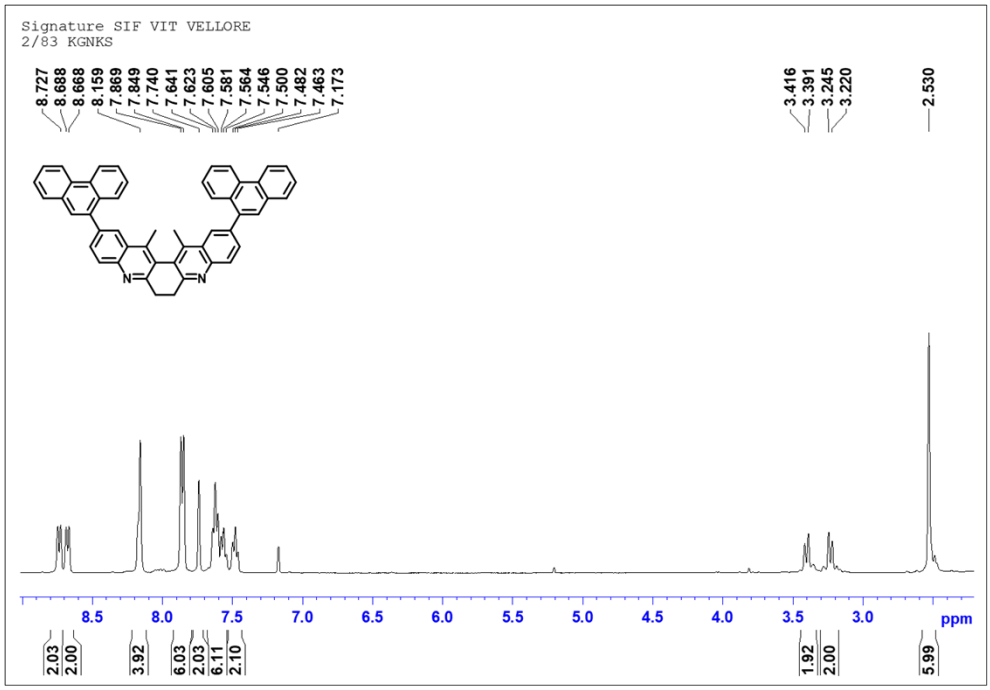
SI Figure. 85: FTIR spectrum of compound **6i**



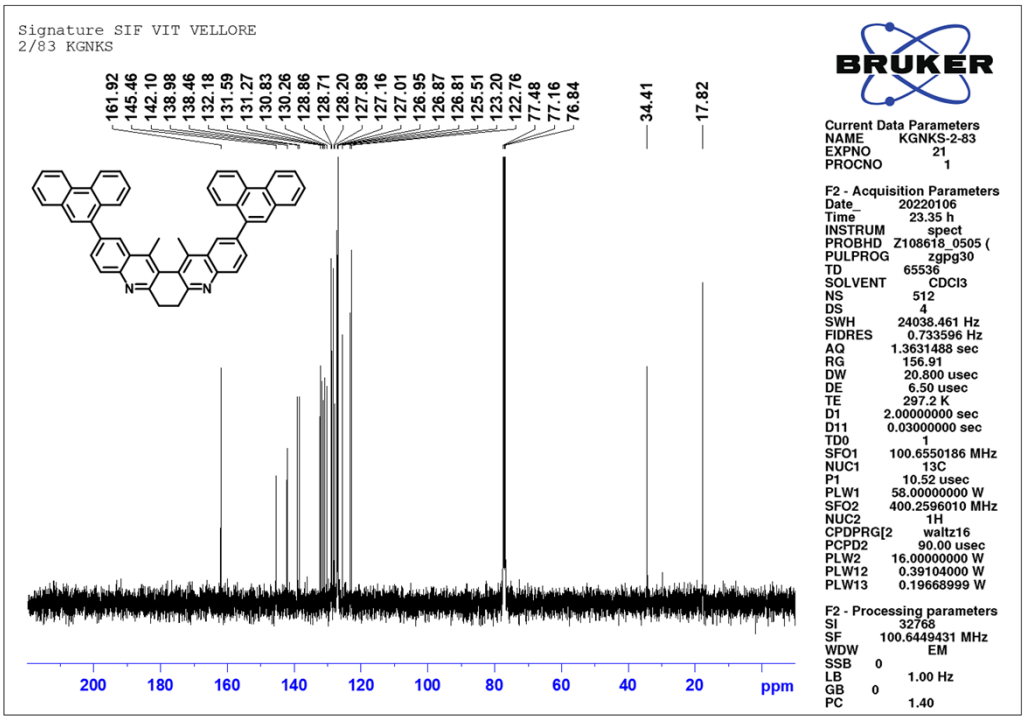
SI Figure. 86: HRMS spectrum of compound **6i**



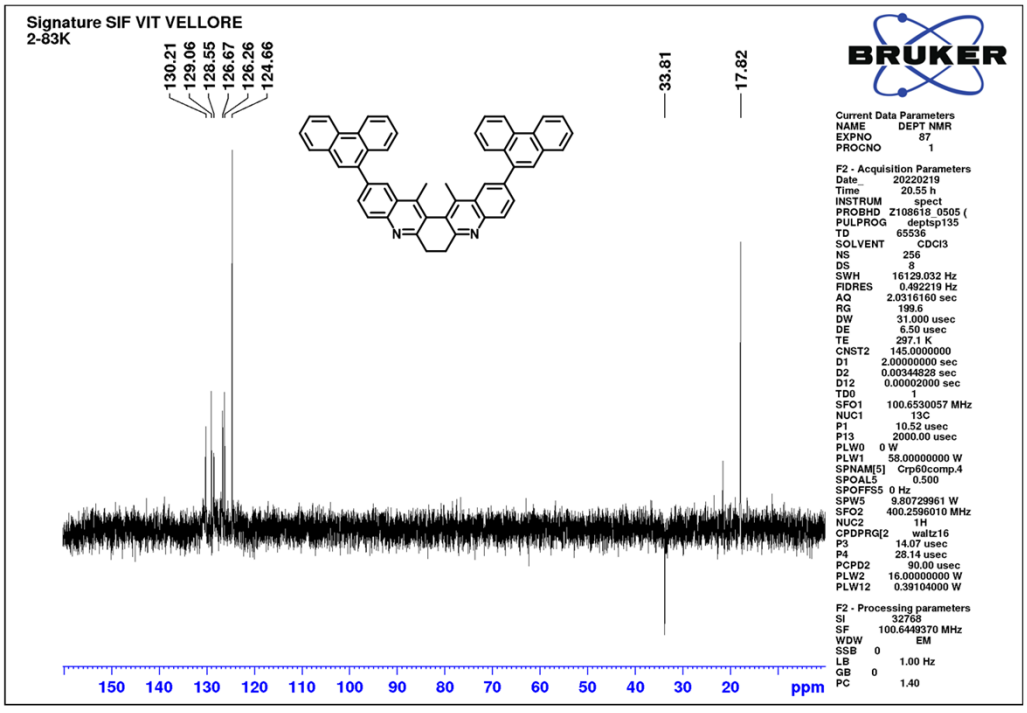
SI Figure. 87: ^{1}H NMR spectrum of compound **6j**



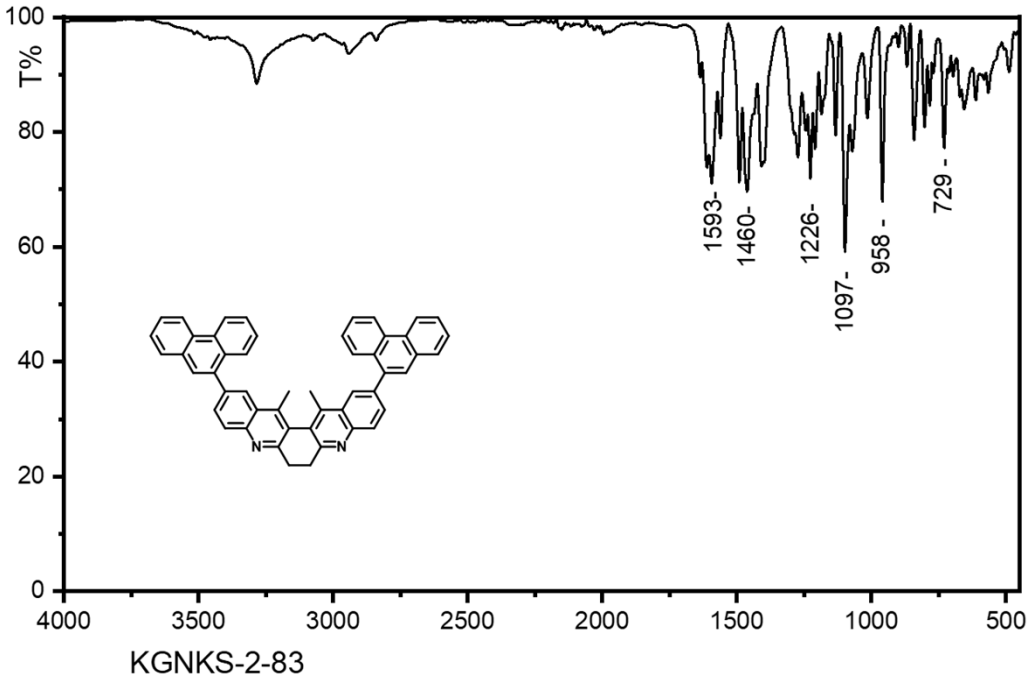
SI Figure. 88: Expansion of ^{1}H NMR spectrum of compound **6j**



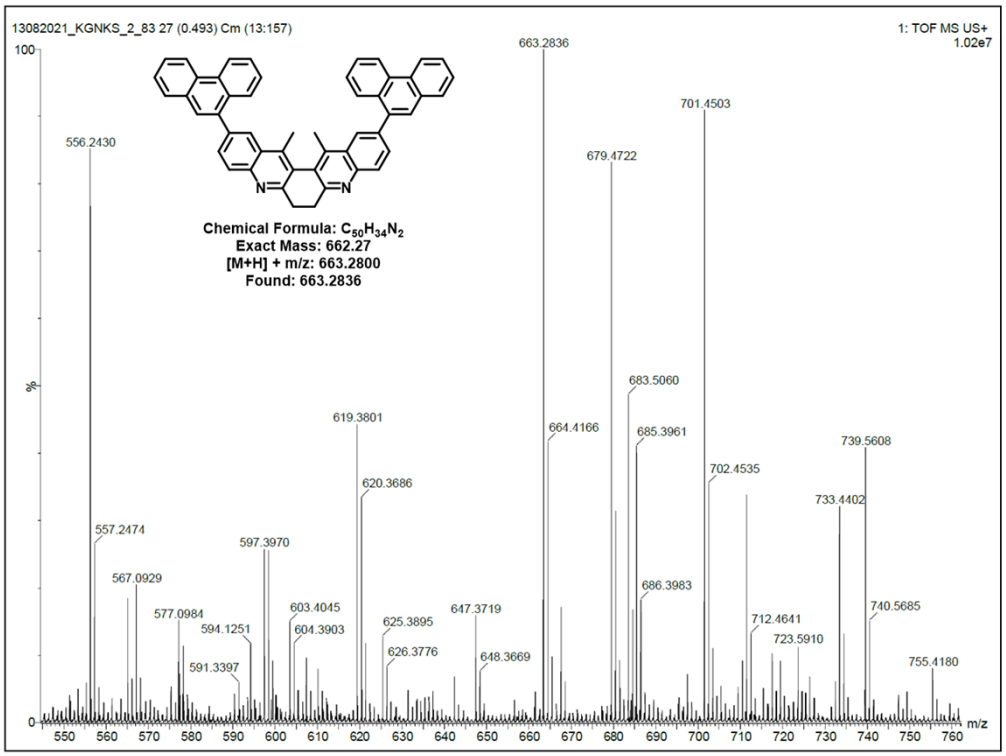
SI Figure. 89: ^{13}C NMR spectrum of compound **6j**



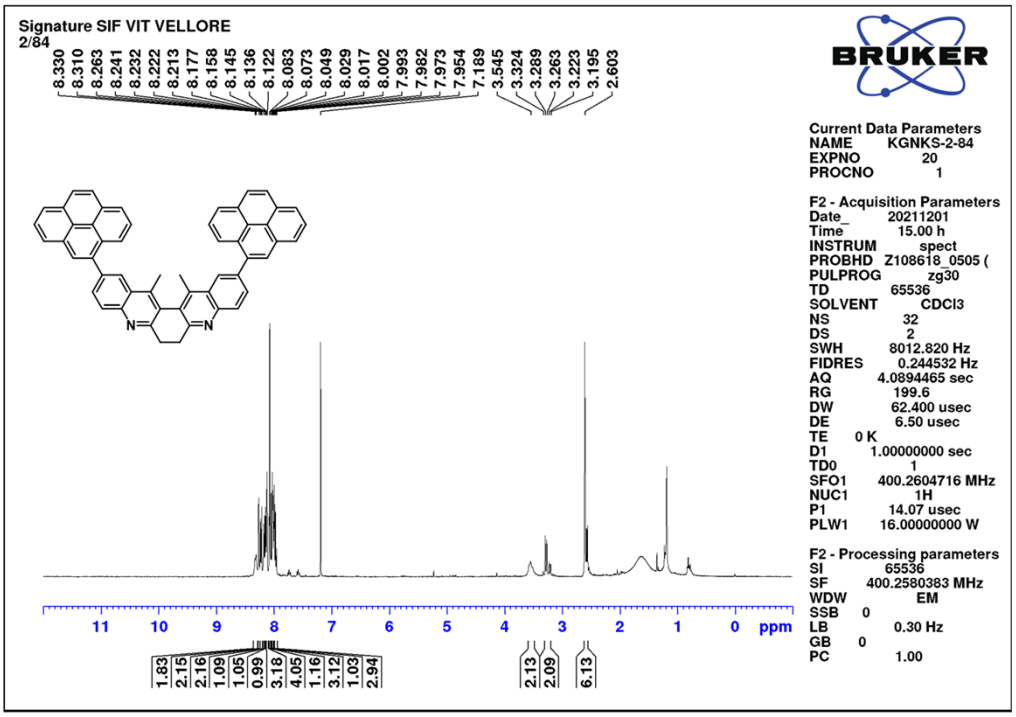
SI Figure. 90: DEPT-135 spectrum of compound **6j**



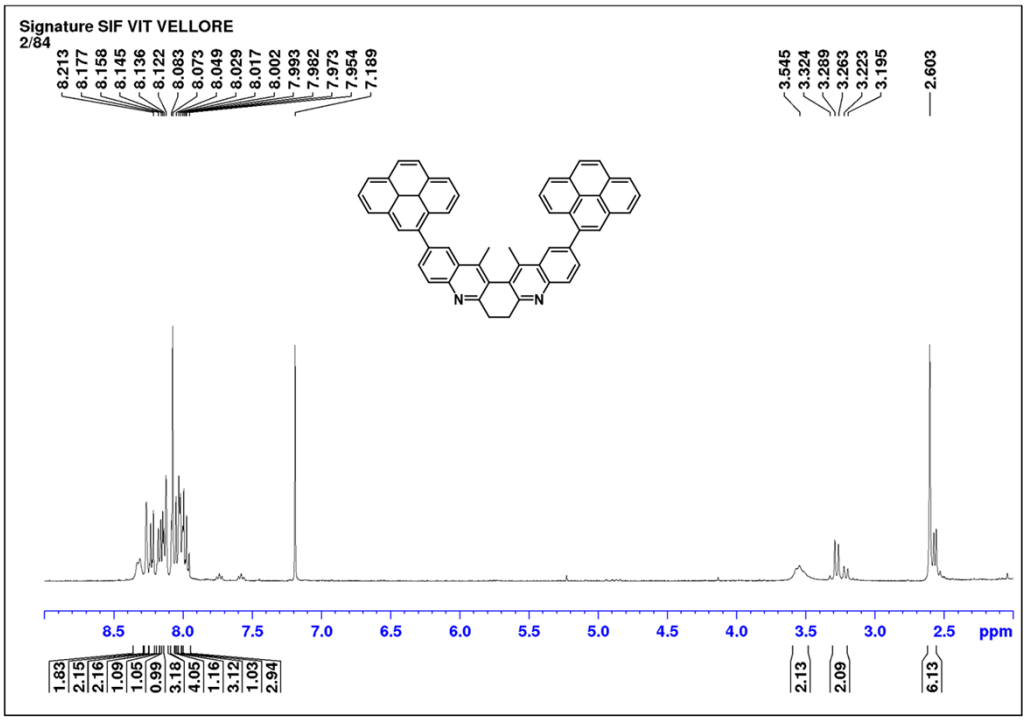
SI Figure. 91: FTIR spectrum of compound **6j**



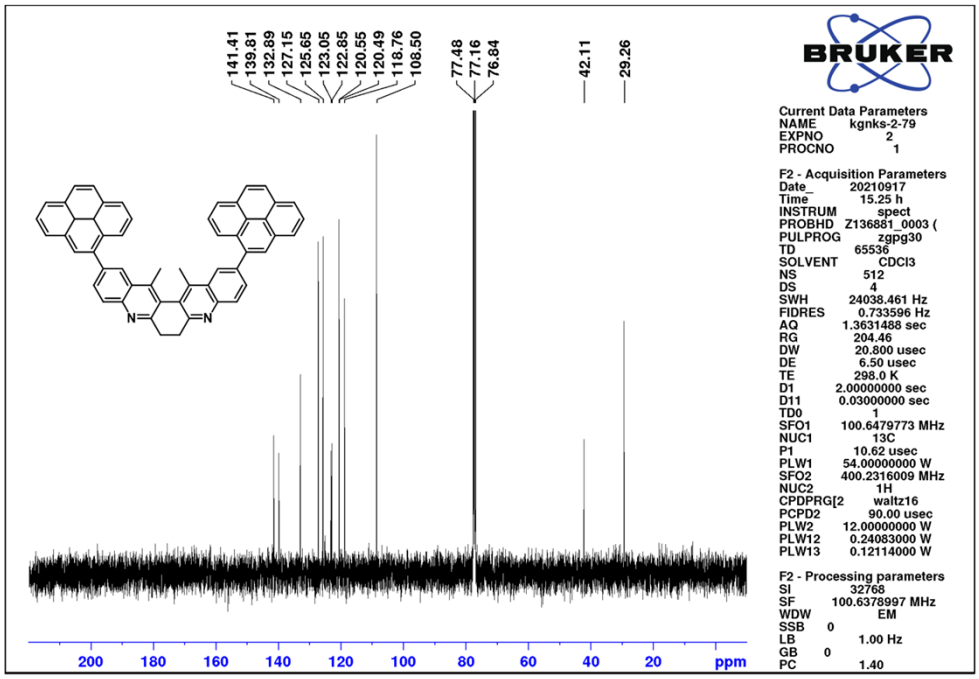
SI Figure. 92: HRMS spectrum of compound **6j**



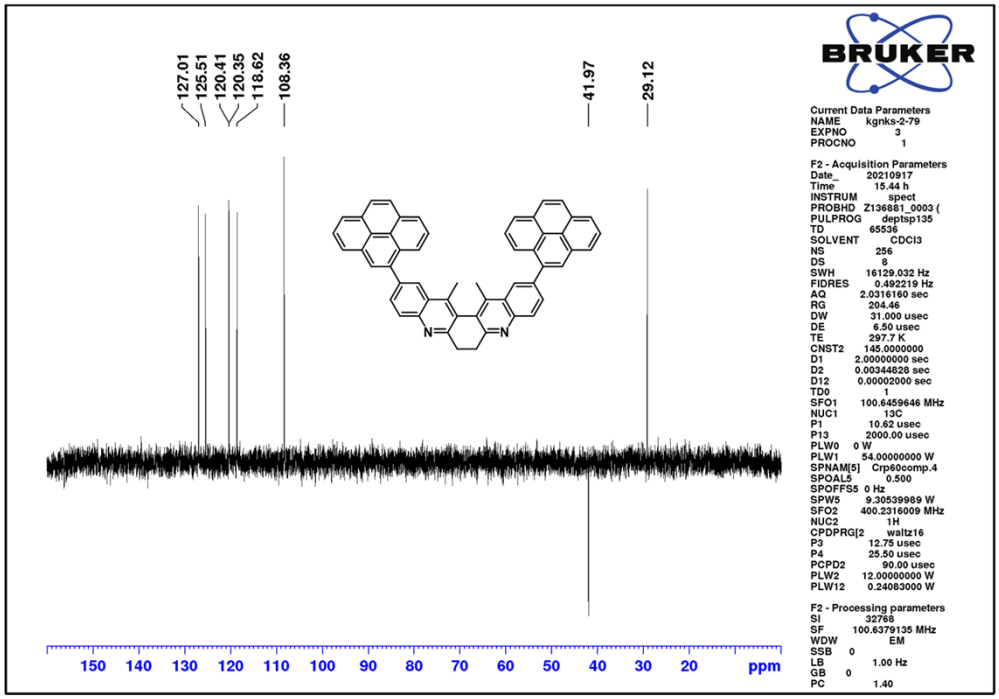
SI Figure. 93: ^{1}H NMR spectrum of compound **6k**



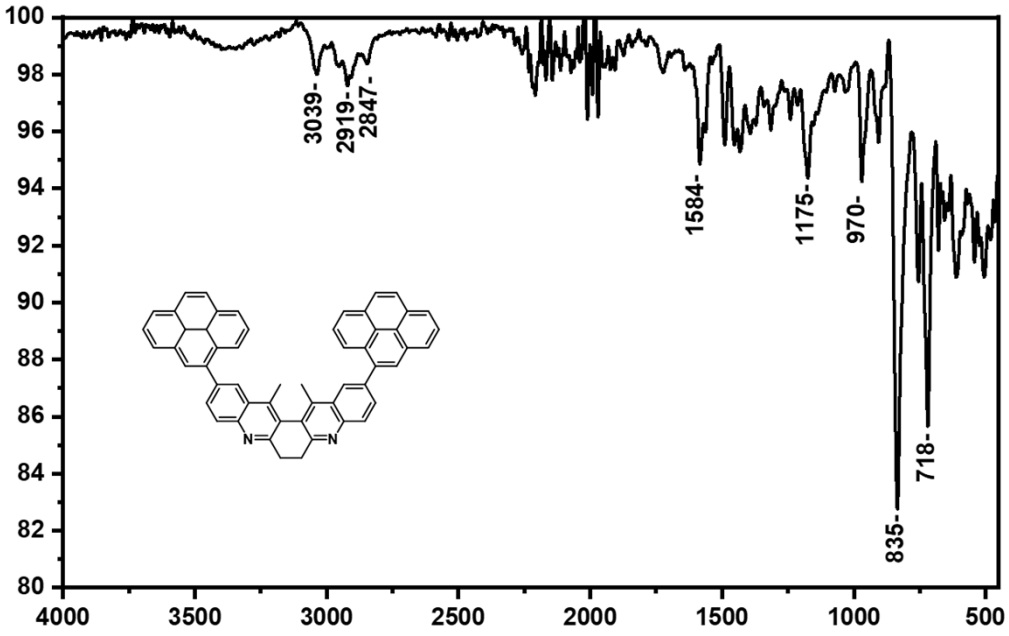
SI Figure. 94: Expansion of ^{1}H NMR spectrum of compound **6k**



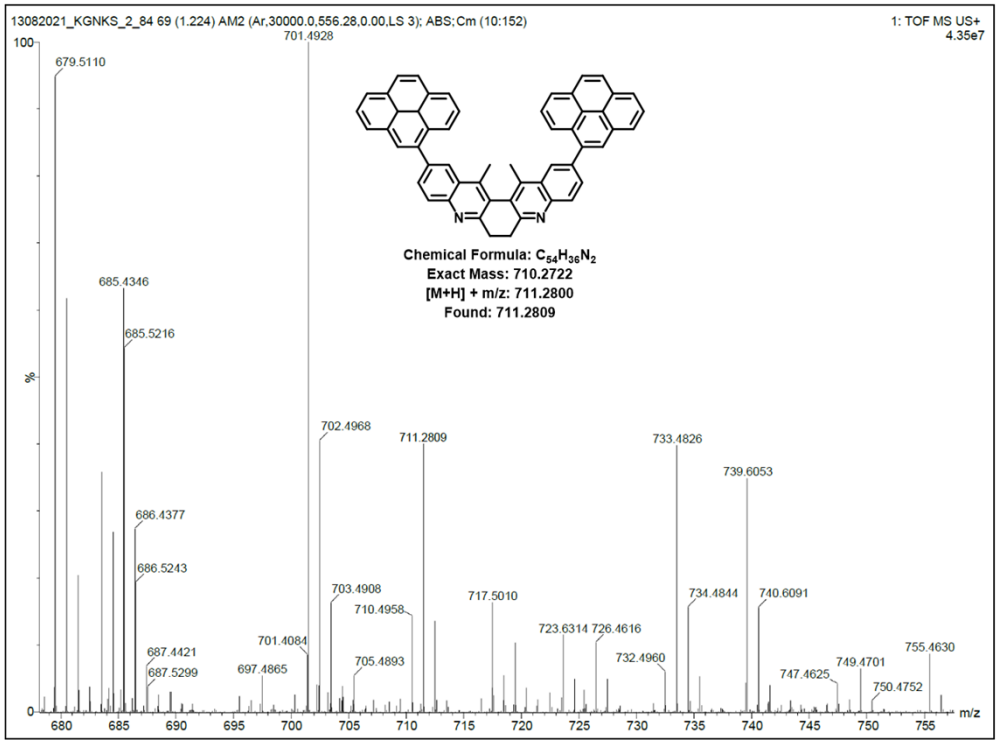
SI Figure. 95: ^{13}C NMR spectrum of compound **6k**



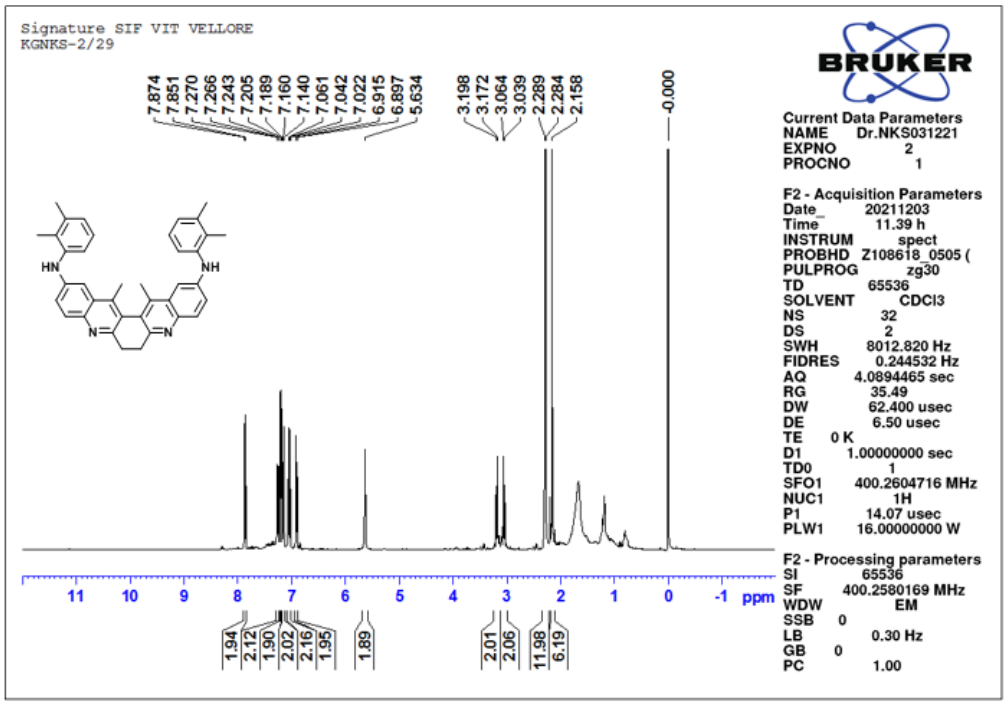
SI Figure. 96: DEPT-135 spectrum of compound **6k**



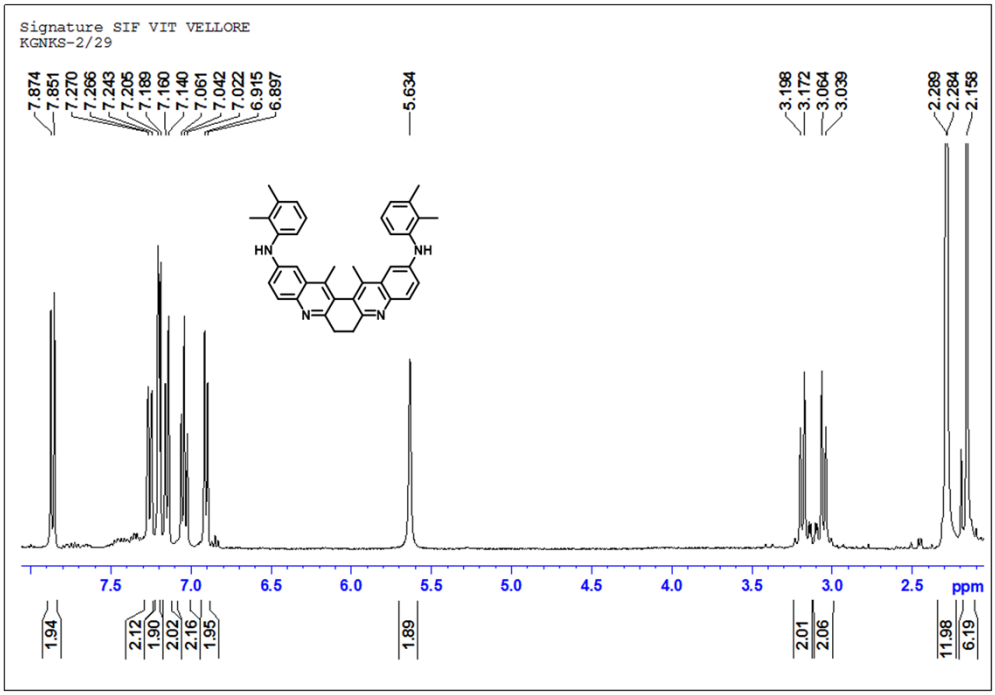
SI Figure. 97: FTIR spectrum of compound **6k**



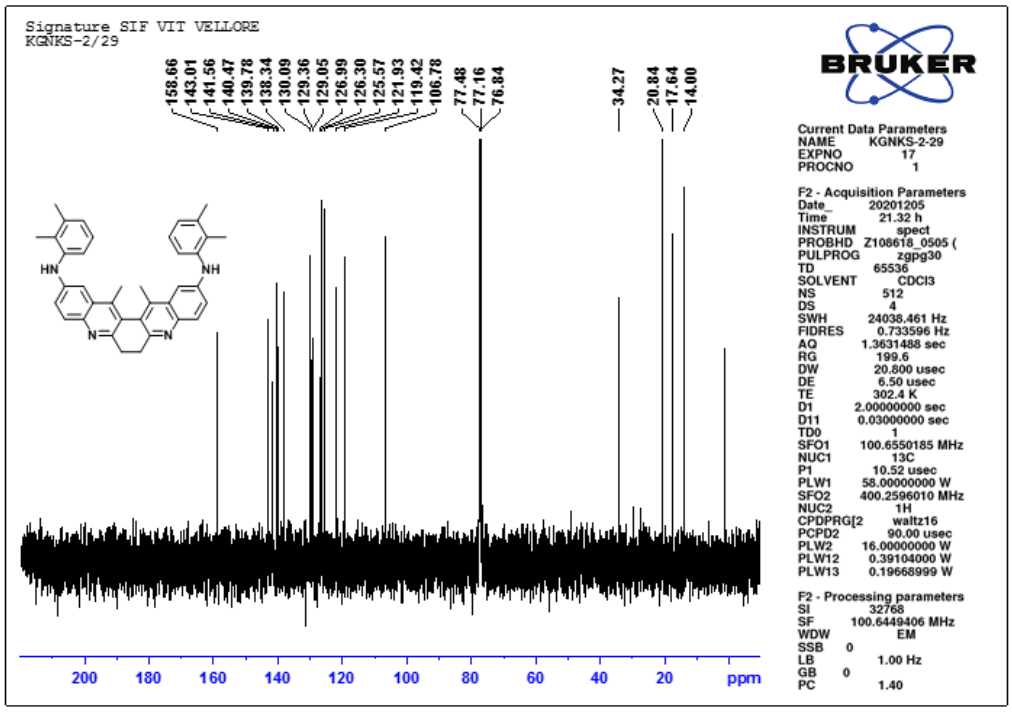
SI Figure. 98: HRMS spectrum of compound **6k**



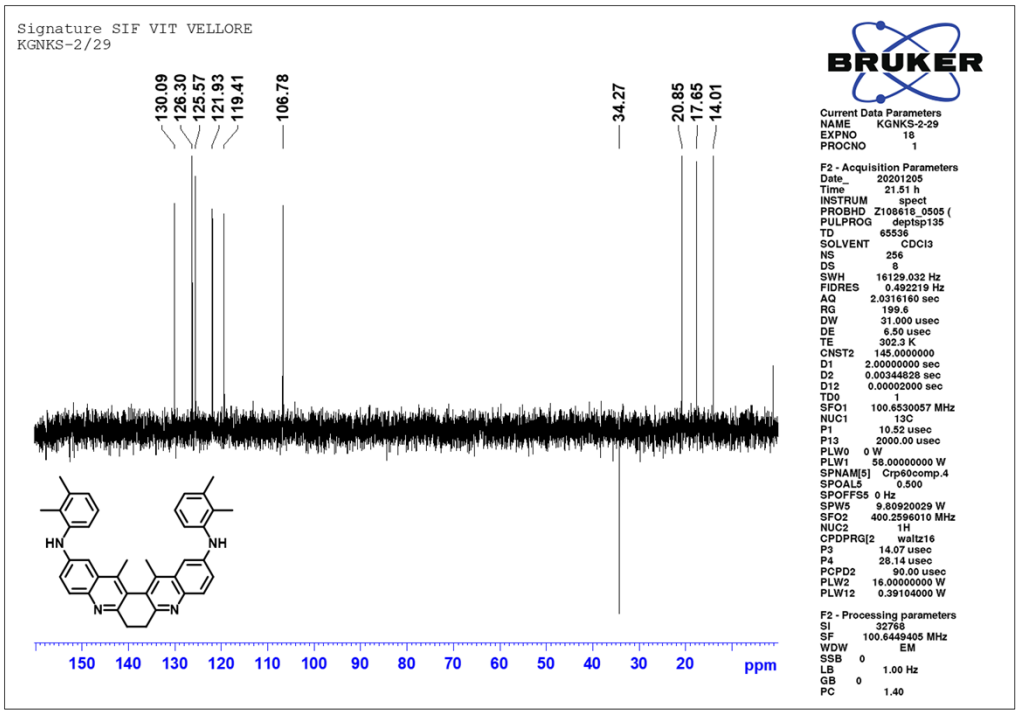
SI Figure. 99: ^{1}H NMR spectrum of compound **8**



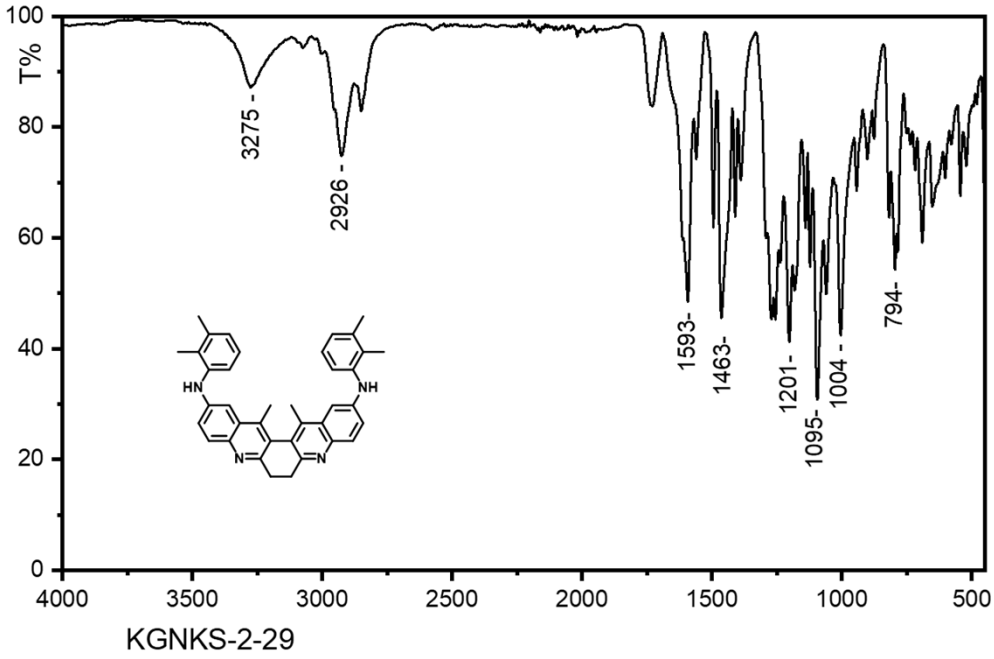
SI Figure. 100: Expansion of ^{1}H NMR spectrum of compound **8**



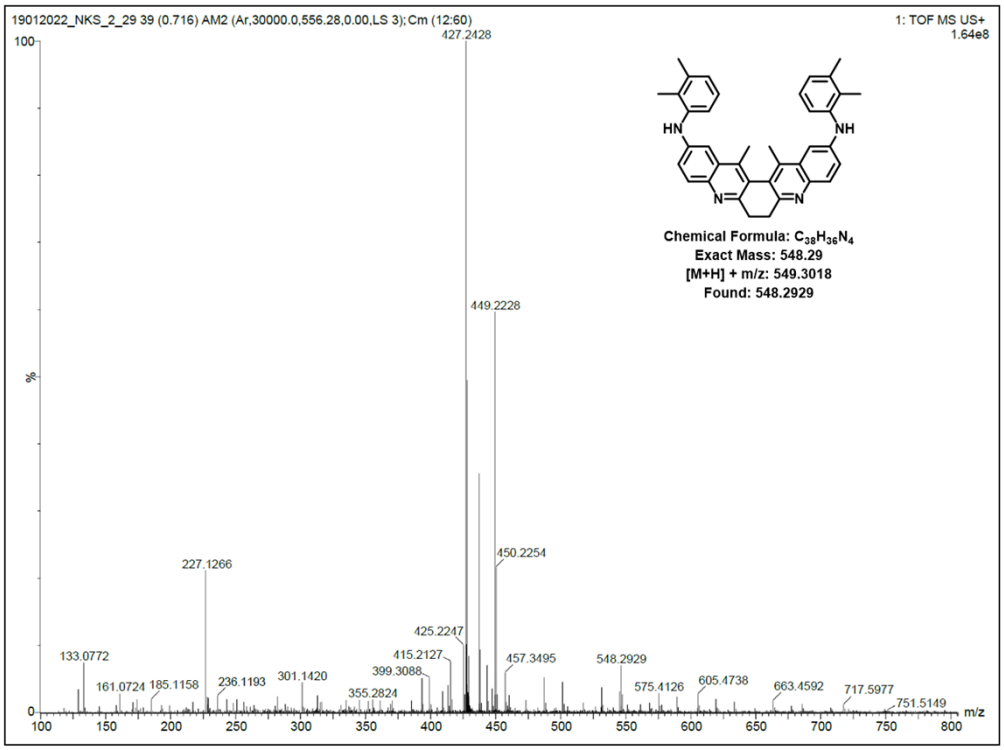
SI Figure. 101: ^{13}C NMR spectrum of compound **8**



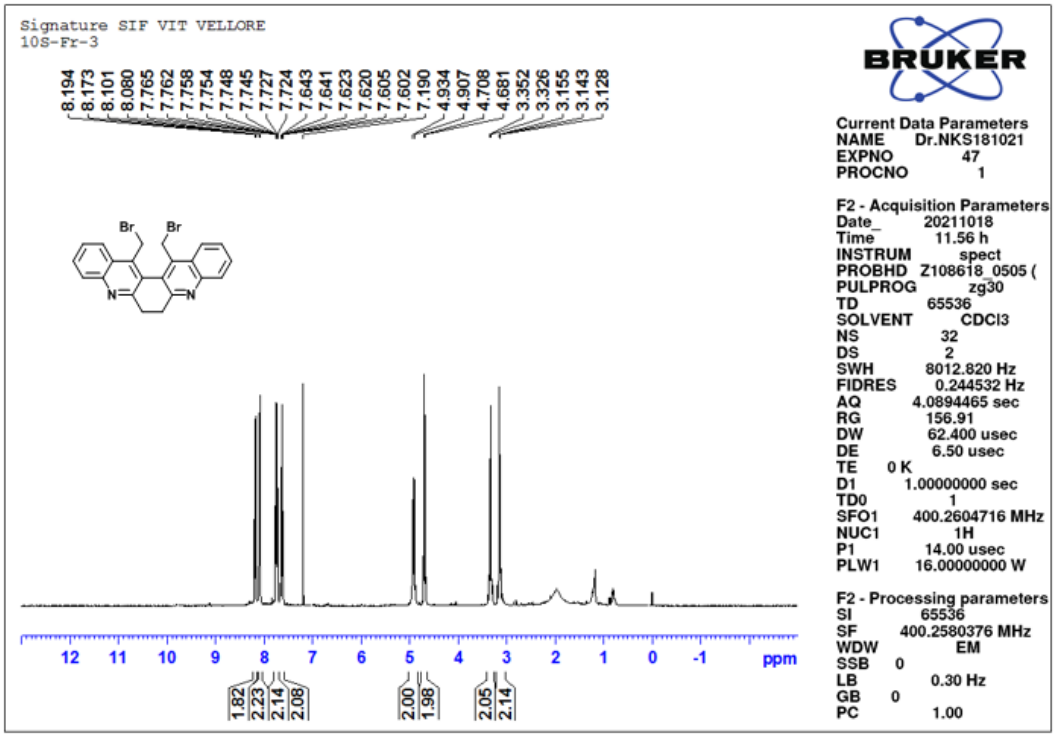
SI Figure. 102: DEPT-135 spectrum of compound **8**



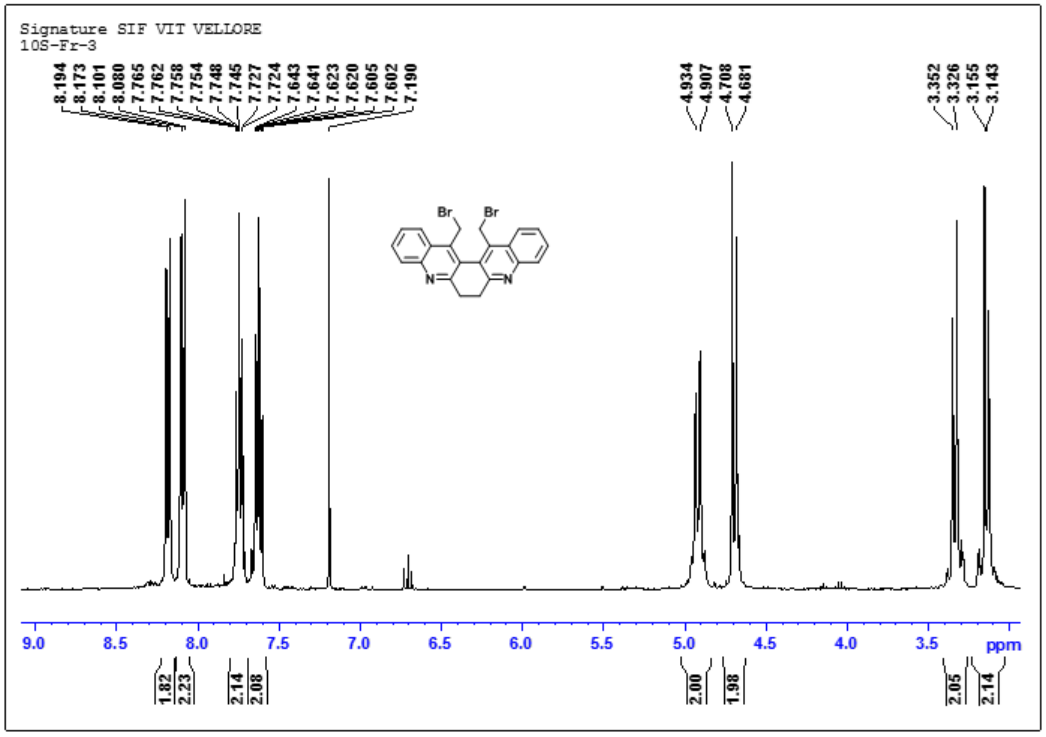
SI Figure. 103: FTIR spectrum of compound **8**



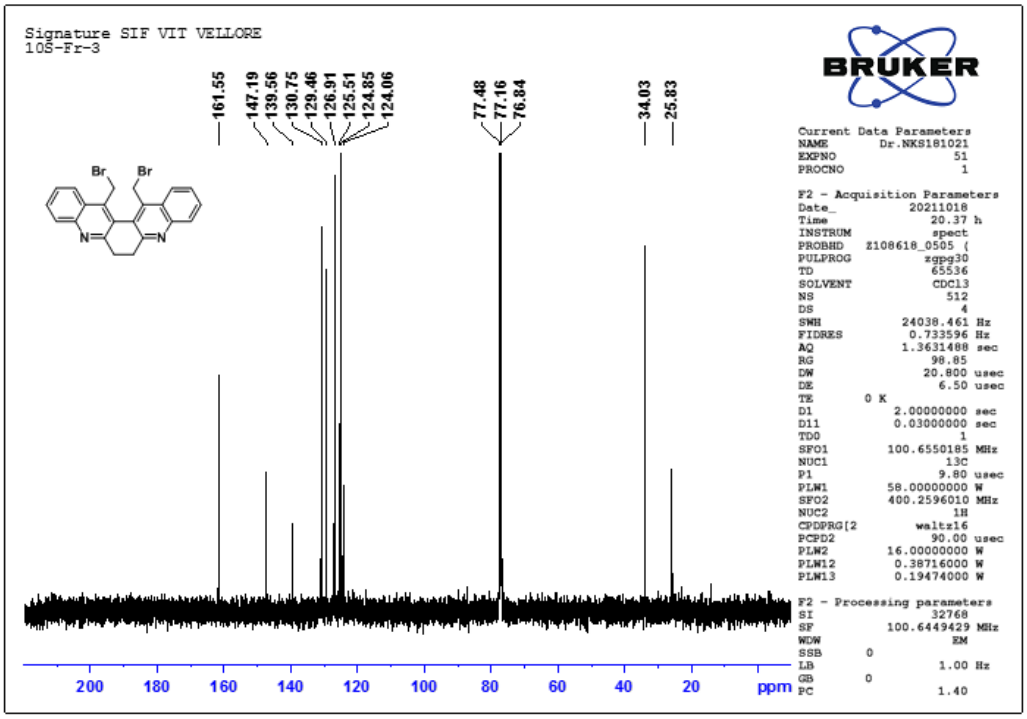
SI Figure. 104 HRMS spectrum of compound **8**



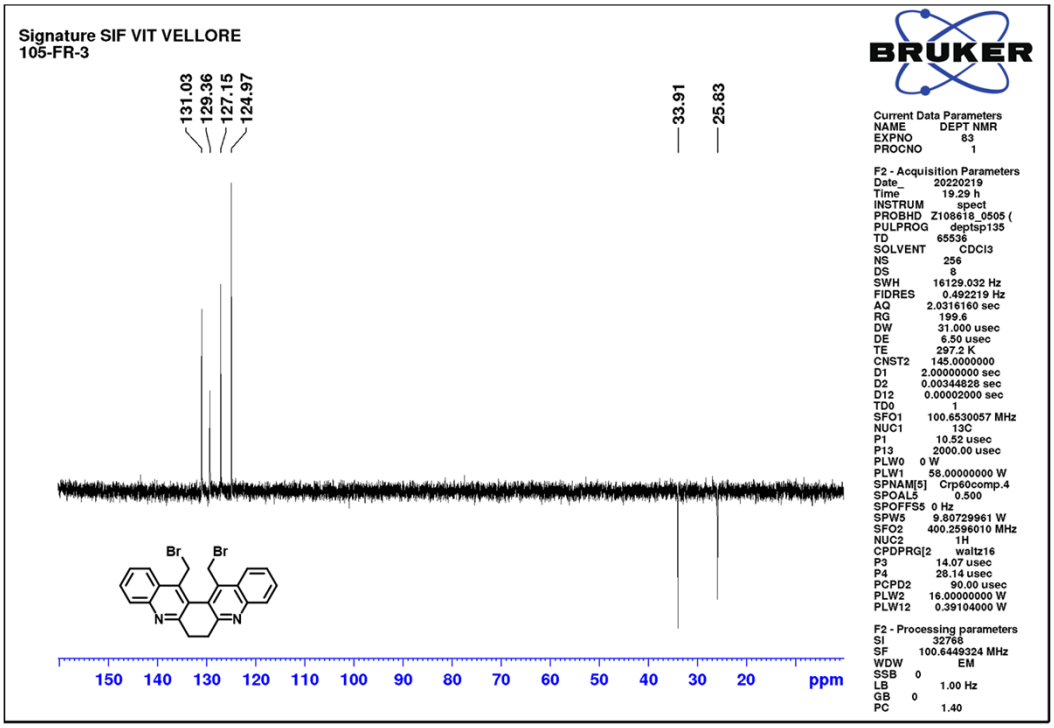
SI Figure. 105: ^{1}H NMR spectrum of compound **9a**



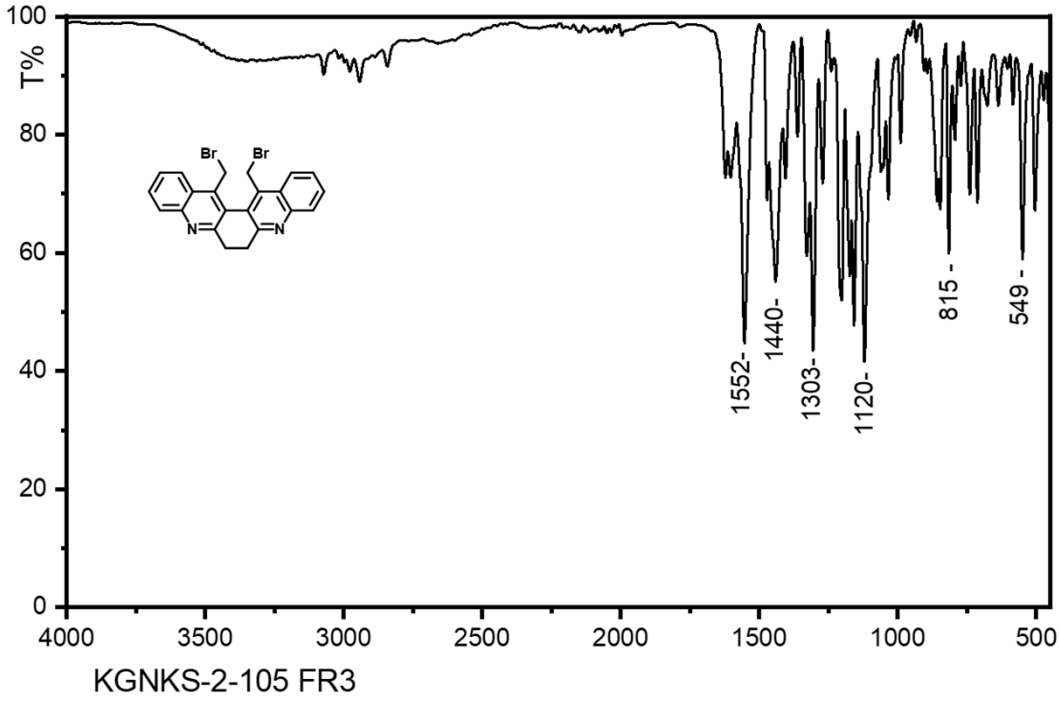
SI Figure. 106: Expansion of ^{1}H NMR spectrum of compound **9a**



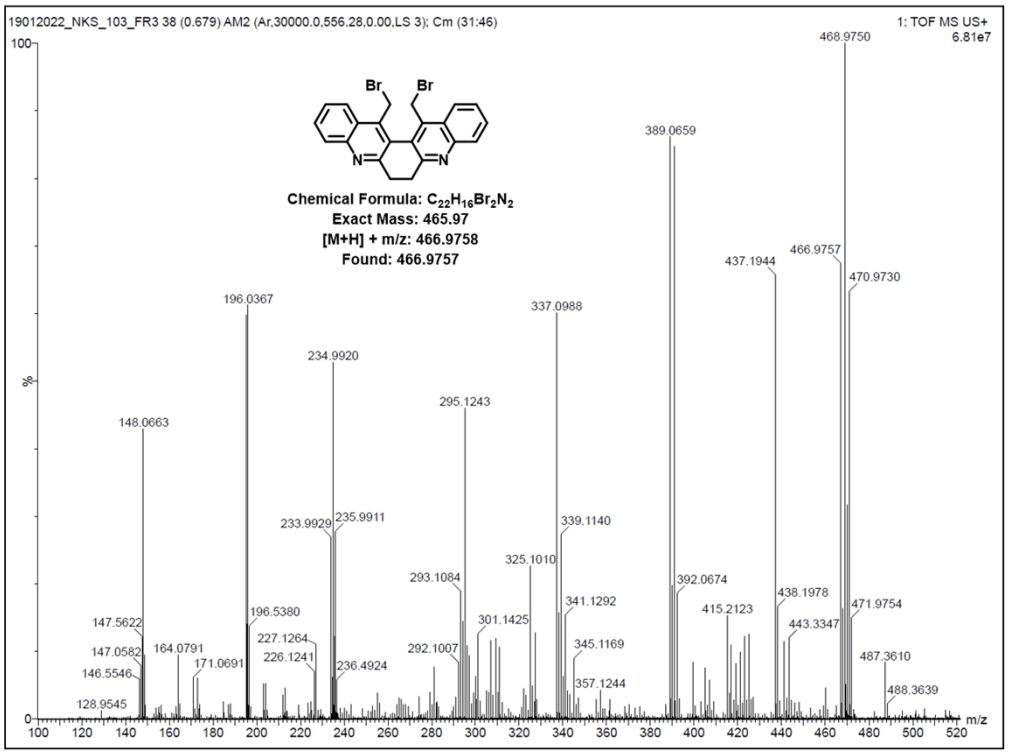
SI Figure. 107: ^{13}C NMR spectrum of compound **9a**



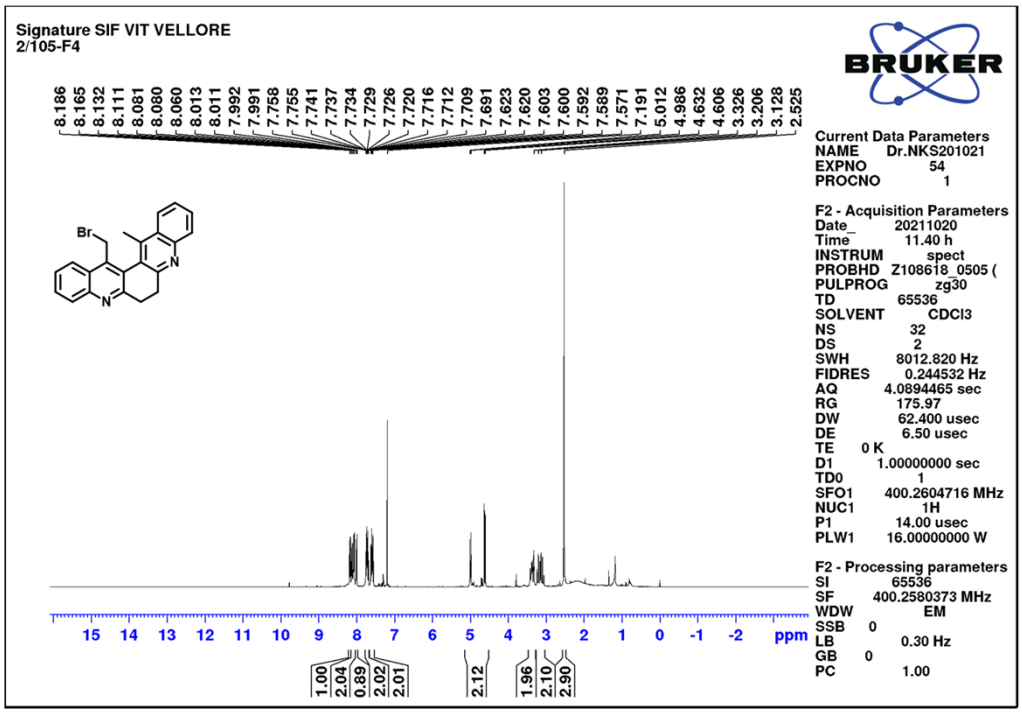
SI Figure. 108: DEPT-135 spectrum of compound **9a**



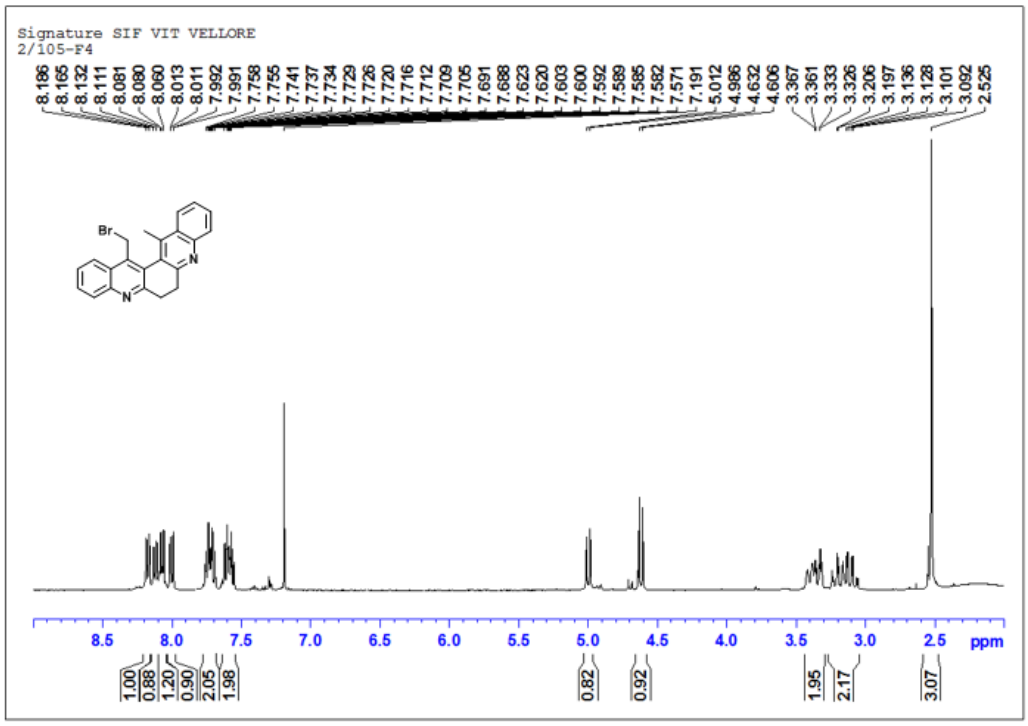
SI Figure. 109: FTIR spectrum of compound **9a**



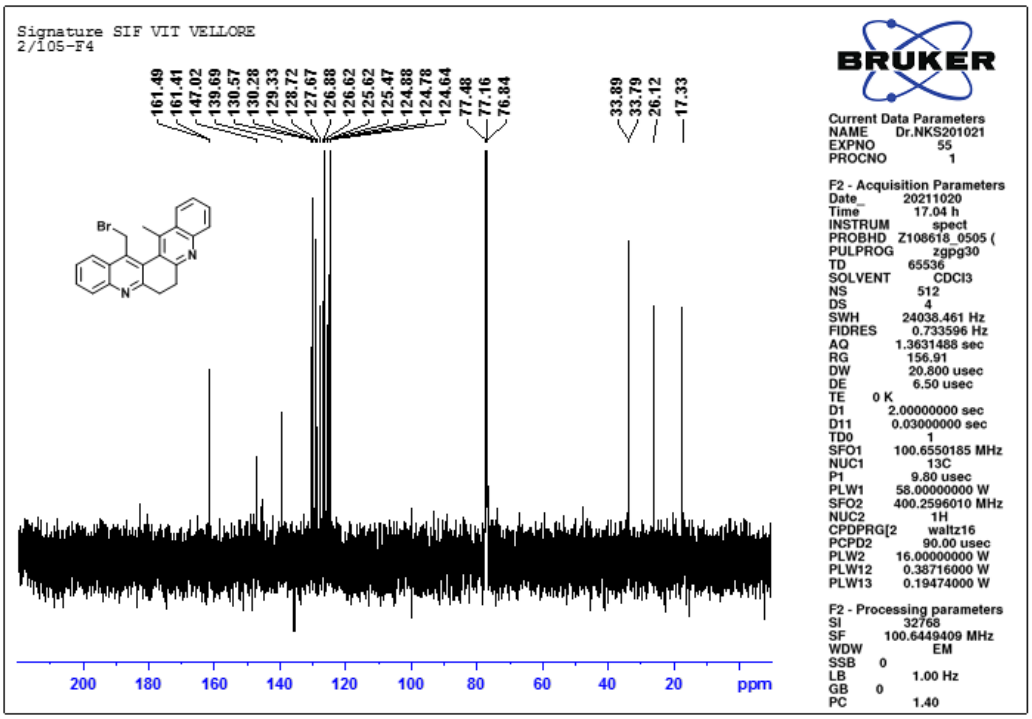
SI Figure. 110: HRMS spectrum of compound **9a**



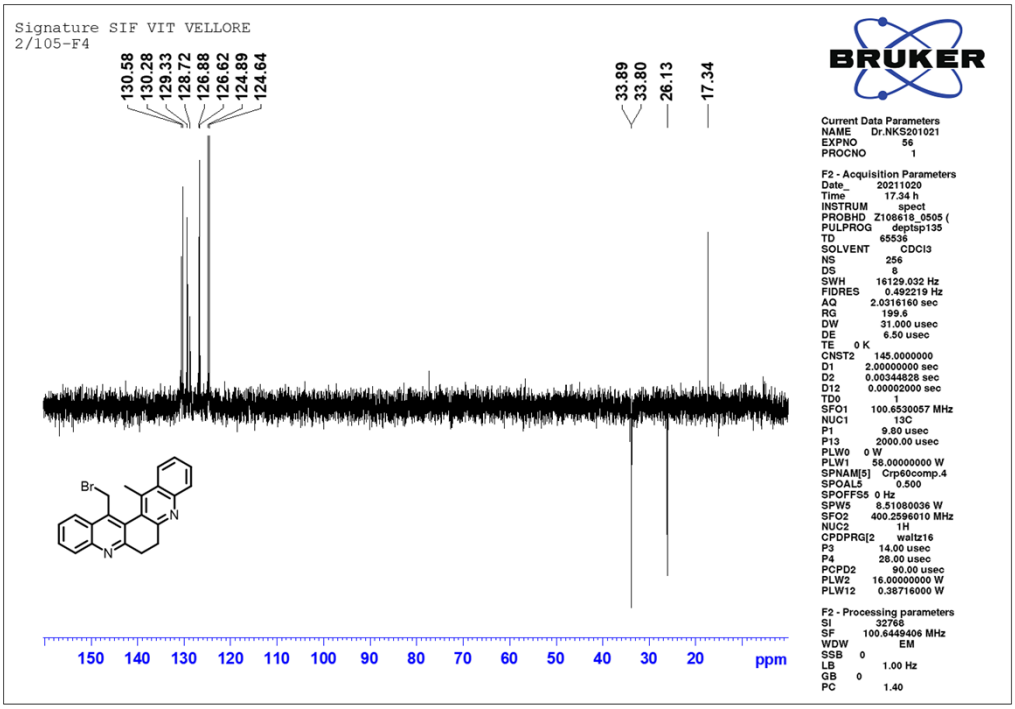
SI Figure. 111: ^{1}H NMR spectrum of compound **9b**



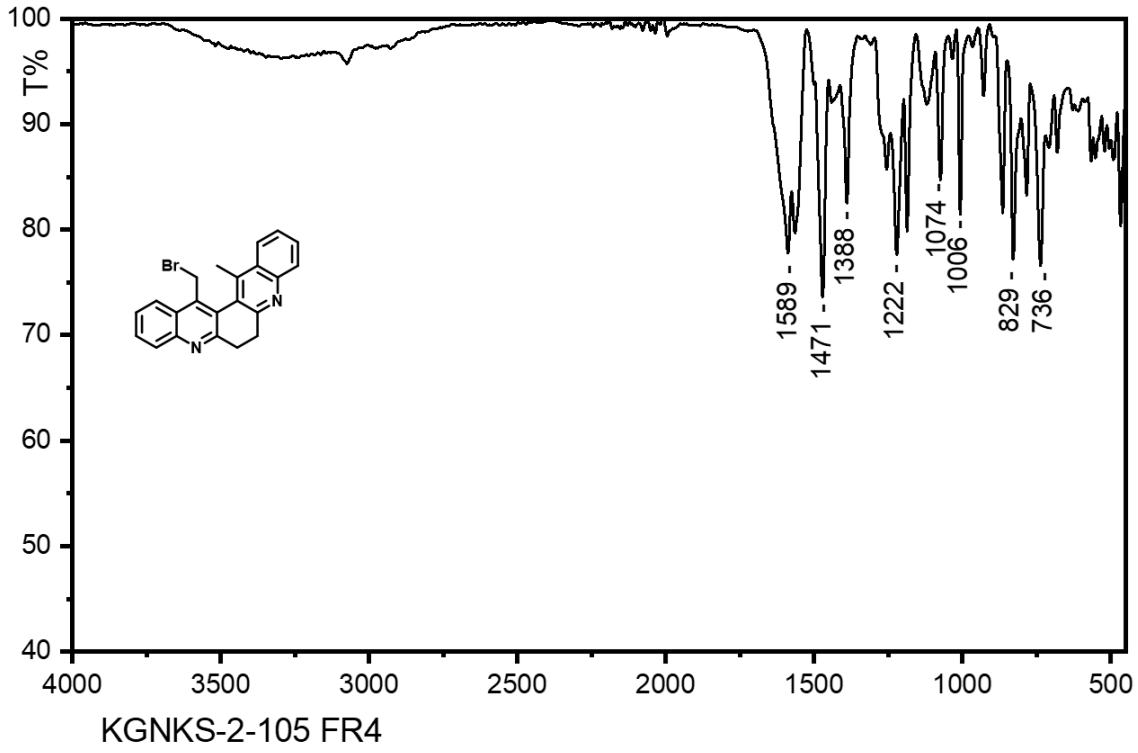
SI Figure. 112: Expansion of ^{1}H NMR spectrum of compound **9b**



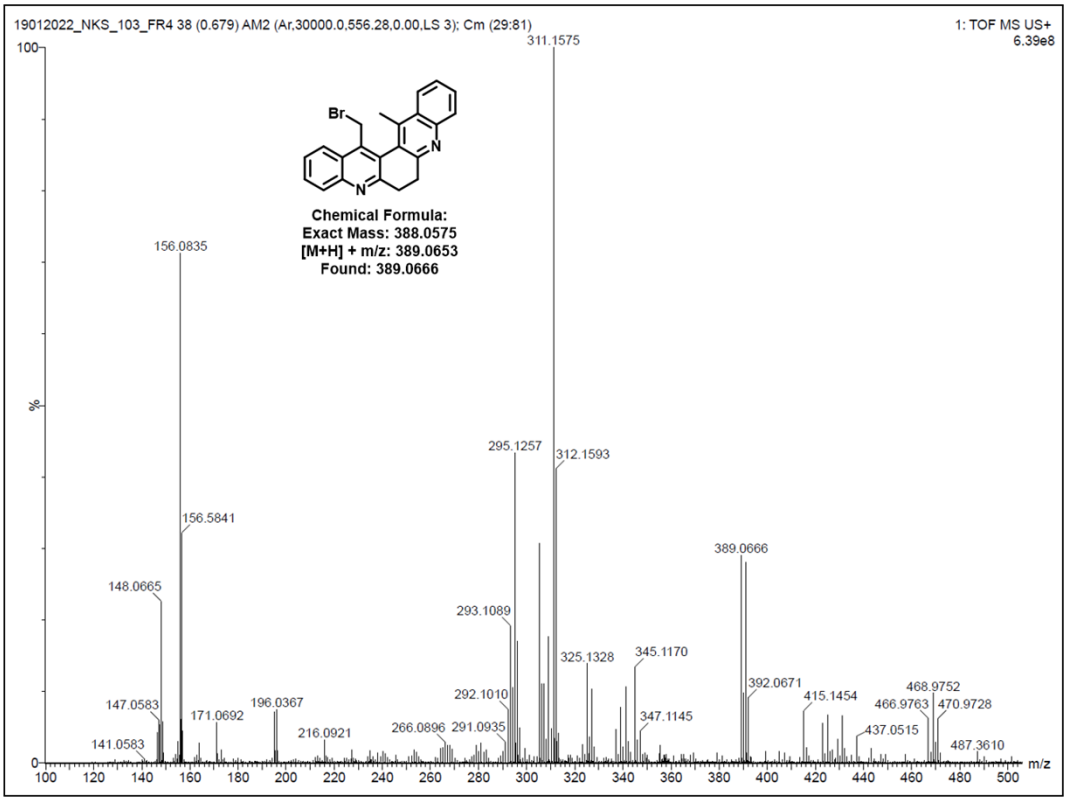
SI Figure. 113: ^{13}C NMR spectrum of compound **9b**



SI Figure. 114: DEPT-135 spectrum of compound **9b**

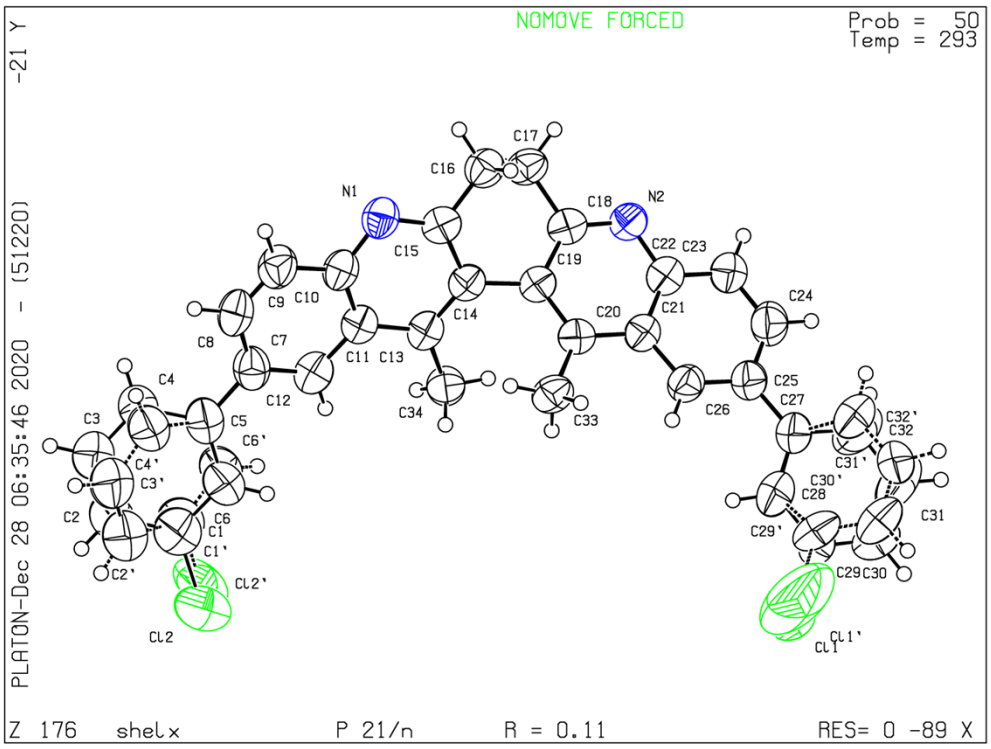


SI Figure. 115: FTIR spectrum of compound **9b**



SI Figure. 116: HRMS spectrum of compound **9b**

Basic crystallographic data of compound 6d



SI Figure. 117: ORTEP diagram of compound **6d**

SI Table 6. Crystal data and structure refinement for kgnks-r1_sq.

Identification code	shelx	
Empirical formula	C34 H24 Cl2 N2	
Formula weight	531.45	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 23.086(6) Å	a= 90°.
	b = 4.9431(7) Å	b= 108.441(14)°.
	c = 26.214(5) Å	g = 90°.
Volume	2837.8(10) Å^3	
Z	4	
Density (calculated)	1.244 Mg/m^3	
Absorption coefficient	0.254 mm^{-1}	
F(000)	1104	
Crystal size	0.400 x 0.150 x 0.100 mm^3	
Theta range for data collection	2.841 to 25.070°.	

Index ranges	-27<=h<=27, -5<=k<=5, -31<=l<=31
Reflections collected	42481
Independent reflections	5003 [R(int) = 0.0819]
Completeness to theta = 25.070°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7452 and 0.3995
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5003 / 357 / 447
Goodness-of-fit on F^2	1.175
Final R indices [I>2sigma(I)]	R1 = 0.1084, wR2 = 0.2958
R indices (all data)	R1 = 0.1681, wR2 = 0.3433
Extinction coefficient	0.077(10)
Largest diff. peak and hole	0.490 and -0.451 e.$Å^{-3}$

SI Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for kgnks-r1_sq. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(5)	6913(2)	10428(10)	6373(2)	84(1)
Cl(2)	6602(3)	9149(19)	4792(1)	200(3)
C(1)	6958(6)	10030(30)	5456(4)	130(3)
C(2)	7541(5)	11240(30)	5618(5)	127(3)
C(3)	7810(5)	11950(20)	6147(4)	121(3)
C(4)	7511(4)	11540(19)	6526(4)	95(3)
C(6)	6637(6)	9710(20)	5832(4)	114(3)
Cl(2')	6856(6)	7020(30)	4993(5)	159(5)
C(4')	7264(10)	12680(40)	6351(9)	104(5)
C(3')	7464(11)	13130(60)	5909(10)	127(5)
C(6')	6792(13)	8590(50)	5950(9)	104(5)
C(2')	7349(13)	11460(60)	5453(12)	130(6)
C(1')	7016(11)	9210(50)	5532(8)	129(6)
C(7)	6603(2)	10039(9)	6788(2)	72(1)
C(8)	6763(2)	11584(9)	7269(2)	80(1)
C(9)	6481(2)	11268(9)	7632(2)	79(1)
C(10)	6004(2)	9378(8)	7562(2)	65(1)
C(11)	5816(2)	7858(8)	7089(2)	60(1)
C(12)	6132(2)	8175(8)	6708(2)	70(1)
C(13)	5291(2)	6133(7)	6994(2)	60(1)

C(14)	4992(2)	6135(7)	7376(2)	59(1)
C(15)	5270(2)	7444(8)	7879(2)	61(1)
C(16)	5029(2)	6824(8)	8331(2)	69(1)
C(17)	4855(2)	3859(8)	8306(2)	67(1)
C(18)	4365(2)	3295(8)	7782(2)	61(1)
C(19)	4406(2)	4707(7)	7319(2)	57(1)
C(20)	3892(2)	4786(8)	6860(2)	58(1)
C(21)	3391(2)	3076(7)	6848(2)	58(1)
C(22)	3429(2)	1470(8)	7307(2)	62(1)
C(23)	2960(2)	-347(9)	7292(2)	70(1)
C(24)	2454(2)	-553(11)	6842(2)	83(1)
C(25)	2387(2)	1118(10)	6385(2)	75(1)
C(26)	2855(2)	2906(9)	6400(2)	67(1)
C(27)	1839(2)	897(15)	5918(2)	107(2)
C(28)	1781(3)	2082(15)	5421(2)	122(2)
Cl(1)	1240(2)	3073(9)	4359(1)	131(2)
C(29)	1276(4)	1730(30)	4958(3)	115(3)
C(30)	850(5)	10(30)	4977(4)	141(4)
C(31)	885(5)	-1480(30)	5433(4)	166(4)
C(32)	1399(5)	-1290(30)	5901(4)	146(4)
Cl(1')	1104(7)	4740(40)	4543(6)	314(9)
C(29')	1206(8)	3070(30)	5094(6)	138(6)
C(30')	654(9)	2510(50)	5146(7)	147(5)
C(31')	711(7)	1500(50)	5622(6)	133(5)
C(32')	1261(6)	1110(60)	6027(7)	135(5)
C(33)	3838(2)	6694(9)	6397(2)	71(1)
C(34)	5115(2)	4285(9)	6510(2)	69(1)
N(1)	5758(2)	9050(7)	7978(1)	69(1)
N(2)	3901(2)	1725(6)	7783(1)	63(1)

SI Table 8. Bond lengths [Å] and angles [°] for kgnks-r1_sq.

C(5)-C(4')	1.386(16)
C(5)-C(6')	1.391(18)
C(5)-C(6)	1.402(10)
C(5)-C(4)	1.420(9)
C(5)-C(7)	1.493(6)
Cl(2)-C(1)	1.731(9)
C(1)-C(2)	1.409(12)

C(1)-C(6)	1.418(11)
C(2)-C(3)	1.373(11)
C(2)-H(2)	0.9300
C(3)-C(4)	1.392(10)
C(3)-H(3)	0.9300
C(4)-H(4)	0.9300
C(6)-H(6)	0.9300
Cl(2')-C(1')	1.725(17)
C(4')-C(3')	1.396(18)
C(4')-H(4')	0.9300
C(3')-C(2')	1.409(19)
C(3')-H(3')	0.9300
C(6')-C(1')	1.386(19)
C(6')-H(6')	0.9300
C(2')-C(1')	1.40(2)
C(2')-H(2')	0.9300
C(7)-C(12)	1.389(6)
C(7)-C(8)	1.419(6)
C(8)-C(9)	1.321(6)
C(8)-H(8)	0.9300
C(9)-C(10)	1.412(6)
C(9)-H(9)	0.9300
C(10)-N(1)	1.389(5)
C(10)-C(11)	1.395(6)
C(11)-C(12)	1.421(6)
C(11)-C(13)	1.438(6)
C(12)-H(12)	0.9300
C(13)-C(14)	1.384(5)
C(13)-C(34)	1.512(6)
C(14)-C(15)	1.425(5)
C(14)-C(19)	1.492(5)
C(15)-N(1)	1.333(5)
C(15)-C(16)	1.493(6)
C(16)-C(17)	1.516(6)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.504(6)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700

C(18)-N(2)	1.324(5)
C(18)-C(19)	1.429(5)
C(19)-C(20)	1.398(5)
C(20)-C(21)	1.425(6)
C(20)-C(33)	1.510(6)
C(21)-C(26)	1.413(6)
C(21)-C(22)	1.420(6)
C(22)-N(2)	1.378(5)
C(22)-C(23)	1.399(6)
C(23)-C(24)	1.375(6)
C(23)-H(23)	0.9300
C(24)-C(25)	1.424(7)
C(24)-H(24)	0.9300
C(25)-C(26)	1.387(6)
C(25)-C(27)	1.461(7)
C(26)-H(26)	0.9300
C(27)-C(28)	1.395(7)
C(27)-C(32')	1.456(15)
C(27)-C(32)	1.473(11)
C(28)-C(29)	1.402(10)
C(28)-C(29')	1.421(15)
C(28)-H(28)	0.9300
Cl(1)-C(29)	1.684(9)
C(29)-C(30)	1.312(11)
C(30)-C(31)	1.385(12)
C(30)-H(30)	0.9300
C(31)-C(32)	1.413(11)
C(31)-H(31)	0.9300
C(32)-H(32)	0.9300
Cl(1')-C(29')	1.613(15)
C(29')-C(30')	1.354(16)
C(30')-C(31')	1.312(16)
C(30')-H(30')	0.9300
C(31')-C(32')	1.386(16)
C(31')-H(31')	0.9300
C(32')-H(32')	0.9300
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600

C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600

C(4')-C(5)-C(6')	117.6(16)
C(6)-C(5)-C(4)	118.3(7)
C(4')-C(5)-C(7)	123.6(11)
C(6')-C(5)-C(7)	118.3(13)
C(6)-C(5)-C(7)	122.3(6)
C(4)-C(5)-C(7)	119.4(6)
C(2)-C(1)-C(6)	119.8(9)
C(2)-C(1)-Cl(2)	121.0(9)
C(6)-C(1)-Cl(2)	119.0(8)
C(3)-C(2)-C(1)	119.7(10)
C(3)-C(2)-H(2)	120.2
C(1)-C(2)-H(2)	120.2
C(2)-C(3)-C(4)	121.1(9)
C(2)-C(3)-H(3)	119.5
C(4)-C(3)-H(3)	119.5
C(3)-C(4)-C(5)	120.7(8)
C(3)-C(4)-H(4)	119.6
C(5)-C(4)-H(4)	119.6
C(5)-C(6)-C(1)	120.2(9)
C(5)-C(6)-H(6)	119.9
C(1)-C(6)-H(6)	119.9
C(5)-C(4')-C(3')	121.0(19)
C(5)-C(4')-H(4')	119.5
C(3')-C(4')-H(4')	119.5
C(4')-C(3')-C(2')	126(2)
C(4')-C(3')-H(3')	117.0
C(2')-C(3')-H(3')	117.0
C(1')-C(6')-C(5)	116.9(19)
C(1')-C(6')-H(6')	121.6
C(5)-C(6')-H(6')	121.6
C(1')-C(2')-C(3')	108(3)
C(1')-C(2')-H(2')	126.2
C(3')-C(2')-H(2')	126.2
C(6')-C(1')-C(2')	131(2)
C(6')-C(1')-Cl(2')	118.0(18)

C(2')-C(1')-Cl(2')	111.1(19)
C(12)-C(7)-C(8)	117.6(4)
C(12)-C(7)-C(5)	120.5(4)
C(8)-C(7)-C(5)	121.9(4)
C(9)-C(8)-C(7)	121.8(4)
C(9)-C(8)-H(8)	119.1
C(7)-C(8)-H(8)	119.1
C(8)-C(9)-C(10)	121.8(4)
C(8)-C(9)-H(9)	119.1
C(10)-C(9)-H(9)	119.1
N(1)-C(10)-C(11)	123.0(4)
N(1)-C(10)-C(9)	118.1(4)
C(11)-C(10)-C(9)	118.8(4)
C(10)-C(11)-C(12)	118.8(4)
C(10)-C(11)-C(13)	118.8(4)
C(12)-C(11)-C(13)	122.4(4)
C(7)-C(12)-C(11)	121.1(4)
C(7)-C(12)-H(12)	119.4
C(11)-C(12)-H(12)	119.4
C(14)-C(13)-C(11)	117.4(4)
C(14)-C(13)-C(34)	123.0(4)
C(11)-C(13)-C(34)	119.5(4)
C(13)-C(14)-C(15)	119.1(4)
C(13)-C(14)-C(19)	124.8(3)
C(15)-C(14)-C(19)	115.9(3)
N(1)-C(15)-C(14)	123.8(4)
N(1)-C(15)-C(16)	118.1(4)
C(14)-C(15)-C(16)	117.9(4)
C(15)-C(16)-C(17)	108.9(3)
C(15)-C(16)-H(16A)	109.9
C(17)-C(16)-H(16A)	109.9
C(15)-C(16)-H(16B)	109.9
C(17)-C(16)-H(16B)	109.9
H(16A)-C(16)-H(16B)	108.3
C(18)-C(17)-C(16)	109.3(3)
C(18)-C(17)-H(17A)	109.8
C(16)-C(17)-H(17A)	109.8
C(18)-C(17)-H(17B)	109.8
C(16)-C(17)-H(17B)	109.8

H(17A)-C(17)-H(17B)	108.3
N(2)-C(18)-C(19)	123.9(4)
N(2)-C(18)-C(17)	118.9(4)
C(19)-C(18)-C(17)	116.9(4)
C(20)-C(19)-C(18)	118.6(4)
C(20)-C(19)-C(14)	124.7(3)
C(18)-C(19)-C(14)	116.5(3)
C(19)-C(20)-C(21)	117.7(3)
C(19)-C(20)-C(33)	122.7(4)
C(21)-C(20)-C(33)	119.5(4)
C(26)-C(21)-C(22)	118.3(4)
C(26)-C(21)-C(20)	123.0(4)
C(22)-C(21)-C(20)	118.7(4)
N(2)-C(22)-C(23)	117.8(4)
N(2)-C(22)-C(21)	122.4(4)
C(23)-C(22)-C(21)	119.7(4)
C(24)-C(23)-C(22)	120.8(4)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(23)-C(24)-C(25)	121.0(4)
C(23)-C(24)-H(24)	119.5
C(25)-C(24)-H(24)	119.5
C(26)-C(25)-C(24)	118.1(4)
C(26)-C(25)-C(27)	122.1(5)
C(24)-C(25)-C(27)	119.8(4)
C(25)-C(26)-C(21)	122.0(4)
C(25)-C(26)-H(26)	119.0
C(21)-C(26)-H(26)	119.0
C(28)-C(27)-C(32')	109.4(9)
C(28)-C(27)-C(25)	123.5(5)
C(32')-C(27)-C(25)	115.7(8)
C(28)-C(27)-C(32)	114.7(6)
C(25)-C(27)-C(32)	119.1(6)
C(27)-C(28)-C(29)	124.3(6)
C(27)-C(28)-C(29')	120.2(9)
C(27)-C(28)-H(28)	117.9
C(29)-C(28)-H(28)	117.9
C(30)-C(29)-C(28)	118.4(8)
C(30)-C(29)-Cl(1)	118.3(7)

C(28)-C(29)-Cl(1)	122.7(7)
C(29)-C(30)-C(31)	122.5(9)
C(29)-C(30)-H(30)	118.8
C(31)-C(30)-H(30)	118.8
C(30)-C(31)-C(32)	121.1(10)
C(30)-C(31)-H(31)	119.4
C(32)-C(31)-H(31)	119.4
C(31)-C(32)-C(27)	117.2(9)
C(31)-C(32)-H(32)	121.4
C(27)-C(32)-H(32)	121.4
C(30')-C(29')-C(28)	126.8(15)
C(30')-C(29')-Cl(1')	108.6(12)
C(28)-C(29')-Cl(1')	124.1(13)
C(31')-C(30')-C(29')	111.1(16)
C(31')-C(30')-H(30')	124.4
C(29')-C(30')-H(30')	124.4
C(30')-C(31')-C(32')	125.0(17)
C(30')-C(31')-H(31')	117.5
C(32')-C(31')-H(31')	117.5
C(31')-C(32')-C(27)	122.2(15)
C(31')-C(32')-H(32')	118.9
C(27)-C(32')-H(32')	118.9
C(20)-C(33)-H(33A)	109.5
C(20)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(20)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(13)-C(34)-H(34A)	109.5
C(13)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(13)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(15)-N(1)-C(10)	116.5(3)
C(18)-N(2)-C(22)	117.4(3)

Symmetry transformations used to generate equivalent atoms:

SI Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for kgnks-r1_sq. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(5)	74(3)	83(3)	99(4)	6(3)	33(3)	-6(2)
Cl(2)	206(4)	301(7)	96(2)	-2(3)	54(2)	-97(4)
C(1)	126(6)	164(7)	104(6)	-12(5)	42(5)	-37(6)
C(2)	120(7)	168(7)	103(7)	-11(6)	50(5)	-40(6)
C(3)	99(6)	155(7)	104(6)	6(5)	24(5)	-40(5)
C(4)	82(5)	114(6)	91(5)	12(4)	29(4)	-15(5)
C(6)	110(7)	150(8)	88(5)	8(5)	38(5)	-42(6)
Cl(2')	197(9)	197(9)	122(7)	-33(6)	107(6)	-56(7)
C(4')	103(10)	118(10)	98(9)	-4(9)	43(8)	-28(9)
C(3')	114(9)	146(10)	117(9)	8(9)	32(8)	-45(9)
C(6')	102(9)	125(11)	98(9)	-5(9)	50(8)	-17(9)
C(2')	118(10)	159(9)	117(10)	-3(9)	41(9)	-40(9)
C(1')	124(9)	164(10)	106(9)	-12(8)	45(8)	-36(9)
C(7)	65(3)	62(3)	90(3)	9(2)	25(2)	-1(2)
C(8)	67(3)	69(3)	99(4)	-8(3)	20(3)	-18(2)
C(9)	79(3)	68(3)	87(3)	-11(2)	23(3)	-16(2)
C(10)	59(3)	57(2)	75(3)	-6(2)	16(2)	-4(2)
C(11)	58(2)	50(2)	68(3)	2(2)	15(2)	4(2)
C(12)	67(3)	59(3)	80(3)	-5(2)	17(2)	2(2)
C(13)	56(2)	49(2)	69(3)	2(2)	12(2)	3(2)
C(14)	59(2)	50(2)	61(2)	4(2)	12(2)	3(2)
C(15)	68(3)	50(2)	62(2)	-1(2)	15(2)	4(2)
C(16)	71(3)	66(3)	69(3)	-9(2)	19(2)	-3(2)
C(17)	74(3)	58(2)	60(2)	5(2)	9(2)	1(2)
C(18)	65(3)	55(2)	59(2)	-1(2)	15(2)	8(2)
C(19)	60(3)	49(2)	59(2)	-1(2)	15(2)	2(2)
C(20)	60(3)	55(2)	58(2)	1(2)	18(2)	7(2)
C(21)	54(2)	55(2)	63(2)	-4(2)	17(2)	5(2)
C(22)	61(3)	55(2)	68(3)	-2(2)	17(2)	5(2)
C(23)	66(3)	70(3)	74(3)	-2(2)	21(2)	-6(2)
C(24)	66(3)	95(3)	90(4)	-10(3)	30(3)	-10(2)
C(25)	58(3)	97(3)	71(3)	-6(2)	23(2)	-6(2)
C(26)	56(3)	79(3)	64(3)	-5(2)	15(2)	2(2)
C(27)	61(3)	185(6)	76(3)	-4(3)	22(3)	-27(3)

C(28)	67(3)	189(6)	93(4)	16(4)	4(3)	-33(4)
Cl(1)	96(2)	204(4)	76(2)	10(2)	4(1)	-32(2)
C(29)	65(5)	211(9)	63(5)	-12(5)	13(4)	-41(5)
C(30)	97(6)	235(10)	74(5)	6(6)	1(5)	-28(7)
C(31)	106(7)	221(10)	133(7)	-11(7)	-17(6)	-70(7)
C(32)	123(7)	171(9)	109(7)	12(7)	-15(6)	-54(7)
Cl(1')	240(12)	345(16)	224(12)	141(11)	-113(9)	-86(11)
C(29')	88(8)	231(11)	69(8)	2(9)	-11(8)	-27(9)
C(30')	78(8)	238(12)	97(9)	5(10)	-13(8)	-29(9)
C(31')	75(8)	238(12)	85(8)	24(9)	24(7)	-43(9)
C(32')	84(8)	213(11)	87(8)	14(9)	-3(7)	-48(9)
C(33)	70(3)	66(3)	66(3)	8(2)	8(2)	7(2)
C(34)	71(3)	68(3)	71(3)	-12(2)	27(2)	-5(2)
N(1)	67(2)	60(2)	77(2)	-10(2)	20(2)	-8(2)
N(2)	65(2)	55(2)	63(2)	3(2)	14(2)	-1(2)

SI Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for kgnks-r1_sq.

	x	y	z	U(eq)
H(2)	7742	11566	5368	152
H(3)	8198	12708	6254	145
H(4)	7704	12002	6883	115
H(6)	6241	9028	5720	137
H(4')	7367	13897	6636	125
H(3')	7693	14687	5916	152
H(6')	6570	7017	5948	125
H(2')	7473	11781	5153	156
H(8)	7075	12854	7330	95
H(9)	6601	12318	7942	94
H(12)	6022	7117	6398	84
H(16A)	4674	7938	8302	83
H(16B)	5338	7217	8672	83
H(17A)	5210	2747	8335	81
H(17B)	4708	3416	8604	81
H(23)	2990	-1428	7589	84
H(24)	2151	-1803	6837	99

H(26)	2815	4028	6106	80
H(28)	2098	3176	5395	146
H(30)	512	-217	4672	170
H(31)	565	-2620	5433	200
H(32)	1458	-2491	6185	175
H(30')	282	2812	4880	177
H(31')	356	996	5693	160
H(32')	1260	979	6381	163
H(33A)	4173	7948	6496	106
H(33B)	3460	7669	6314	106
H(33C)	3848	5678	6088	106
H(34A)	4821	2988	6545	104
H(34B)	5471	3356	6487	104
H(34C)	4942	5337	6190	104

SI Table 11. Torsion angles [°] for kgnks-r1_sq.

C(6)-C(1)-C(2)-C(3)	4(2)
Cl(2)-C(1)-C(2)-C(3)	179.4(10)
C(1)-C(2)-C(3)-C(4)	-1.5(19)
C(2)-C(3)-C(4)-C(5)	-1.1(16)
C(6)-C(5)-C(4)-C(3)	1.0(12)
C(7)-C(5)-C(4)-C(3)	-179.5(7)
C(4)-C(5)-C(6)-C(1)	1.8(14)
C(7)-C(5)-C(6)-C(1)	-177.8(8)
C(2)-C(1)-C(6)-C(5)	-4.4(18)
Cl(2)-C(1)-C(6)-C(5)	-179.6(9)
C(6')-C(5)-C(4')-C(3')	3(3)
C(7)-C(5)-C(4')-C(3')	-169.9(12)
C(5)-C(4')-C(3')-C(2')	-1(2)
C(4')-C(5)-C(6')-C(1')	-2(3)
C(7)-C(5)-C(6')-C(1')	171.1(14)
C(4')-C(3')-C(2')-C(1')	-1.8(18)
C(5)-C(6')-C(1')-C(2')	-1(3)
C(5)-C(6')-C(1')-Cl(2')	-178.2(16)
C(3')-C(2')-C(1')-C(6')	3(3)
C(3')-C(2')-C(1')-Cl(2')	-179.8(10)
C(4')-C(5)-C(7)-C(12)	162.2(13)
C(6')-C(5)-C(7)-C(12)	-10.5(14)

C(6)-C(5)-C(7)-C(12)	21.9(9)
C(4)-C(5)-C(7)-C(12)	-157.6(6)
C(4')-C(5)-C(7)-C(8)	-16.2(14)
C(6')-C(5)-C(7)-C(8)	171.1(14)
C(6)-C(5)-C(7)-C(8)	-156.5(8)
C(4)-C(5)-C(7)-C(8)	24.0(8)
C(12)-C(7)-C(8)-C(9)	0.4(7)
C(5)-C(7)-C(8)-C(9)	178.9(5)
C(7)-C(8)-C(9)-C(10)	-0.1(8)
C(8)-C(9)-C(10)-N(1)	176.0(4)
C(8)-C(9)-C(10)-C(11)	-1.6(7)
N(1)-C(10)-C(11)-C(12)	-174.6(4)
C(9)-C(10)-C(11)-C(12)	2.9(6)
N(1)-C(10)-C(11)-C(13)	8.6(6)
C(9)-C(10)-C(11)-C(13)	-173.9(4)
C(8)-C(7)-C(12)-C(11)	1.0(6)
C(5)-C(7)-C(12)-C(11)	-177.5(4)
C(10)-C(11)-C(12)-C(7)	-2.7(6)
C(13)-C(11)-C(12)-C(7)	174.0(4)
C(10)-C(11)-C(13)-C(14)	1.5(5)
C(12)-C(11)-C(13)-C(14)	-175.2(4)
C(10)-C(11)-C(13)-C(34)	-174.6(4)
C(12)-C(11)-C(13)-C(34)	8.8(6)
C(11)-C(13)-C(14)-C(15)	-10.7(5)
C(34)-C(13)-C(14)-C(15)	165.2(4)
C(11)-C(13)-C(14)-C(19)	173.3(3)
C(34)-C(13)-C(14)-C(19)	-10.8(6)
C(13)-C(14)-C(15)-N(1)	11.2(6)
C(19)-C(14)-C(15)-N(1)	-172.4(3)
C(13)-C(14)-C(15)-C(16)	-164.4(4)
C(19)-C(14)-C(15)-C(16)	12.0(5)
N(1)-C(15)-C(16)-C(17)	-138.7(4)
C(14)-C(15)-C(16)-C(17)	37.1(5)
C(15)-C(16)-C(17)-C(18)	-61.0(5)
C(16)-C(17)-C(18)-N(2)	-137.6(4)
C(16)-C(17)-C(18)-C(19)	36.9(5)
N(2)-C(18)-C(19)-C(20)	10.1(6)
C(17)-C(18)-C(19)-C(20)	-164.1(3)
N(2)-C(18)-C(19)-C(14)	-173.4(3)

C(17)-C(18)-C(19)-C(14)	12.4(5)
C(13)-C(14)-C(19)-C(20)	-46.3(6)
C(15)-C(14)-C(19)-C(20)	137.6(4)
C(13)-C(14)-C(19)-C(18)	137.4(4)
C(15)-C(14)-C(19)-C(18)	-38.7(5)
C(18)-C(19)-C(20)-C(21)	-10.5(5)
C(14)-C(19)-C(20)-C(21)	173.3(3)
C(18)-C(19)-C(20)-C(33)	166.3(4)
C(14)-C(19)-C(20)-C(33)	-9.9(6)
C(19)-C(20)-C(21)-C(26)	-177.8(3)
C(33)-C(20)-C(21)-C(26)	5.3(6)
C(19)-C(20)-C(21)-C(22)	2.3(5)
C(33)-C(20)-C(21)-C(22)	-174.5(3)
C(26)-C(21)-C(22)-N(2)	-172.4(3)
C(20)-C(21)-C(22)-N(2)	7.4(6)
C(26)-C(21)-C(22)-C(23)	4.1(6)
C(20)-C(21)-C(22)-C(23)	-176.1(4)
N(2)-C(22)-C(23)-C(24)	175.1(4)
C(21)-C(22)-C(23)-C(24)	-1.5(6)
C(22)-C(23)-C(24)-C(25)	-1.5(7)
C(23)-C(24)-C(25)-C(26)	1.8(7)
C(23)-C(24)-C(25)-C(27)	-178.6(4)
C(24)-C(25)-C(26)-C(21)	0.9(6)
C(27)-C(25)-C(26)-C(21)	-178.6(4)
C(22)-C(21)-C(26)-C(25)	-3.8(6)
C(20)-C(21)-C(26)-C(25)	176.4(4)
C(26)-C(25)-C(27)-C(28)	11.4(9)
C(24)-C(25)-C(27)-C(28)	-168.1(6)
C(26)-C(25)-C(27)-C(32')	-128.3(13)
C(24)-C(25)-C(27)-C(32')	52.2(14)
C(26)-C(25)-C(27)-C(32)	171.9(8)
C(24)-C(25)-C(27)-C(32)	-7.6(10)
C(25)-C(27)-C(28)-C(29)	175.2(8)
C(32)-C(27)-C(28)-C(29)	13.9(13)
C(32')-C(27)-C(28)-C(29')	-4.4(15)
C(25)-C(27)-C(28)-C(29')	-146.3(9)
C(27)-C(28)-C(29)-C(30)	-5.7(16)
C(27)-C(28)-C(29)-Cl(1)	-176.9(7)
C(28)-C(29)-C(30)-C(31)	-1(2)

Cl(1)-C(29)-C(30)-C(31)	170.9(12)
C(29)-C(30)-C(31)-C(32)	-2(2)
C(30)-C(31)-C(32)-C(27)	11(2)
C(28)-C(27)-C(32)-C(31)	-15.8(16)
C(25)-C(27)-C(32)-C(31)	-178.0(10)
C(27)-C(28)-C(29')-C(30')	-15.4(18)
C(27)-C(28)-C(29')-Cl(1')	173.6(8)
C(28)-C(29')-C(30')-C(31')	17(2)
Cl(1')-C(29')-C(30')-C(31')	-171.2(16)
C(29')-C(30')-C(31')-C(32')	2(3)
C(30')-C(31')-C(32')-C(27)	-22(4)
C(28)-C(27)-C(32')-C(31')	21(3)
C(25)-C(27)-C(32')-C(31')	166.4(19)
C(14)-C(15)-N(1)-C(10)	-1.4(6)
C(16)-C(15)-N(1)-C(10)	174.2(4)
C(11)-C(10)-N(1)-C(15)	-8.6(6)
C(9)-C(10)-N(1)-C(15)	173.9(4)
C(19)-C(18)-N(2)-C(22)	-0.5(6)
C(17)-C(18)-N(2)-C(22)	173.6(3)
C(23)-C(22)-N(2)-C(18)	175.1(4)
C(21)-C(22)-N(2)-C(18)	-8.4(5)

Symmetry transformations used to generate equivalent atoms: