Supporting Information

Expedient Synthesis of Phenanthro-Imidazo-Pyridine Fused Heteropolynuclear Framework via CDC coupling: A New Class of Luminophores

Biswadip Banerji*[a,b], Satadru Chatterjee[a], K. Chandrasekhar[a], Suvankar Bera[a], Leena Mazumder[a], Chandraday Prodhan[c], Keya Chaudhuri[c]

[a]Organic& Medicinal Chemistry Division, [b]Academy of Scientific and Innovative Research (AcSIR), [c]Department of Chemistry, India ;[c]Molecular Genetics, Indian Institute of Chemical Biology (CSIR-IICB); 4 Raja S. C. Mullick Road, Kolkata, Country. India-700032; Fax: (+) 91 33 24735197, 91 33 24723967; Tel: (+) 91 33 24995709; E-mail: biswadip.banerji@gmail.com,biswadip@iicb.res.in

Table of contents **Page**

General Information:

All the reagents and solvents used in this study, were purchased from Sigma Aldrich, Thermo Fischer Scientific and TCI chemicals respectively. Open capillary was used to measure all the melting points. IR spectrum of the solid sample was recorded in the range 500 to 3500 cm^{-1} in an FT-IR spectrometer in KBr cell. Bruker 600 MHz spectrometer was used to record all ^{1}H and ^{13}C NMR spectra. EI mass spectral analysis was done using JEOL The Mstation JMS-700 instrument. All the UV & Fluorescence data were collected using Jasco & Cary Eclipse spectrophotometer respectively. Bruker Kappa Apex II X-raycrystallography machine was used to solve the crystal structure. Singlet (s), doublet (d), triplet (t) & multiplet (m) were designated as ^{1}H NMR multiplicity patterns. Silica gel (60-120 mesh) and (100-200 mesh) were used for column chromatographic separations.

Synthetic Procedures:

Procedure for the synthesis of 2-(2-iodophenyl)imidazo[1,2-a]pyridine, 3:

To a solution of **1** (1gm, 1.0 eq.) and **2** (2.61gm, 1.0 eq.) in 1,2-DCB (4ml), was added $Cu(OAc)_2.H_2O$ (212 mg, 0.1 eq.), ZnI_2 (340 mg, 0.1 eq.) & 1,10-Phenanthroline (192 mg, 0.1 eq.) and heated in a round bottom flask under ambient air for 24 hours. The reaction was monitored through TLC until the starting material consumed completely. After that, the reaction mixture was diluted with dichloromethane and filtered through celite bed. The organic layer was then concentrated under reduced pressure and subjected to column chromatography (silica gel 60-120 mesh size, ethyl acetate: pet ether) for further purification to get the desired compound, **3** in 85% yield as a yellow solid.

Procedure for the synthesis of 2-([1,1'-biphenyl]-2-yl)imidazo[1,2-a]pyridine, 4:

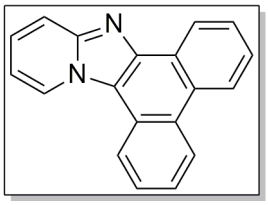
To a solution of Compound **3** in dry DMF (3 ml), different Phenyl boronic acids were used for Suzuki cross coupling reaction in presence of $Pd(PPh_3)_4$ and K_2CO_3 at 130 ^oC in a sealed tube under N_2 atmosphere. The reaction was monitored through TLC until complete consumption of the starting material. After that, the reaction mixture was diluted with ethyl acetate and passed through celite bed and then washed with cold water (2×10 ml) and brine (1×10 ml). The organic layer was then filtered, dried over Na_2SO_4 and concentrated under reduced pressure to get crude solid, which was subjected to column chromatography (silica gel 100-200 mesh size, ethyl acetate: pet ether) for further purification to get the desired compound, **4** in good yield, .

Procedure for the synthesis of phenanthro[9',10':4,5]imidazo[1,2-a]pyridine, 5:

To a solution of Compound **4** (150 mg, 1.0 eq.) in dry DMF (3ml), was added $Pd(OAc)_2$ (6 mg, 0.05 eq.) as catalyst, Ag_2CO_3 (7 mg, 0.05 eq.) as co-oxidant and PivOH (8 μl, 0.15 eq.) as additive at 140 ^oC in a sealed tube under ambient pressure of molecular oxygen for final dehydrogenative cyclisation. After completion of the reaction, monitored by TLC, the reaction mixture was diluted with ethyl acetate, filtered through celite bed and then washed with cold water (4× 10 ml) and brine (2×10 ml). The organic layer was then collected and dried over Na_2SO_4. After that the organic extract was evaporated under reduced pressure to get crude solid.

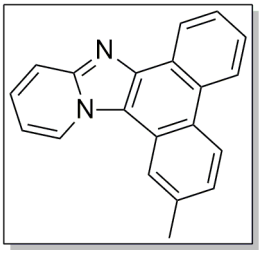
It was then subjected to column chromatography (silica gel 100-200 mesh size, ethyl acetate: pet ether) for further purification to get the desired compound, **5** in 52-85% yield.

phenanthro[9',10':4,5]imidazo[1,2-a]pyridine (5a)



Pale yellow solid; yield 85%; m.p. 98-99^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.19 (d, *J* = 6.0 Hz, 1H), 8.94 (dd, *J* = 6.0, 6.0 Hz, 1H), 8.89 (d, *J* = 6.0 Hz, 1H), 8.76 (d, *J* = 6.0 Hz, 1H), 8.55 (d, *J* = 6.0 Hz, 1H), 7.99 (d, *J* = 6.0 Hz, 1H), 7.74 – 7.80 (m, 3H), 7.68 (t, *J* = 18 Hz, 1H), 7.48 ((t, *J* = 18 Hz, 1H), 7.12 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 147.54, 138.44, 129.76, 129.63, 128.34, 127.47, 127.33, 127.04, 126.51, 126.13, 124.73, 124.59, 123.78, 123.67, 123.20, 120.00, 119.74, 118.29, 112.46; Mass: [EI-HRMS] ($C_{19}H_{12}N_2$) calc. 268.1000 Da, Found: 268.0995Da; FTIR (KBr, ν_{max}, cm^{-1}): 3418.13, 2925.45, 1632.71, 1522.91, 1421.40, 1357.44, 1269.57, 1129.18, 824.21, 748.38, 530.27

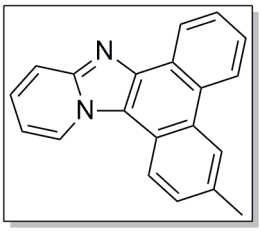
2-methylphenanthro[9',10':4,5]imidazo[1,2-a]pyridine (5b)



Pale yellow solid; yield 83%; m.p. 141-142^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.21 (d, *J* = 6.0 Hz, 1H), 8.91 (d, *J* = 6.0 Hz, 1H), 8.76 (d, *J* = 6.0 Hz, 1H), 8.72 (d, *J* = 6.0 Hz, 1H), 8.31 (s,

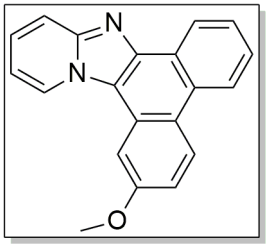
1H), 8.01 (d, *J* = 12.0 Hz, 1H), 7.79 – 7.70 (m, 2H), 7.53 – 7.46 (m, 2H), 7.13 (t, *J* = 12.0 Hz, 3H), 2.71 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 147.44, 137.21, 129.72, 128.38, 127.05, 126.99, 126.57, 126.51, 126.28, 126.13, 126.10, 124.97, 124.47, 123.76, 123.31, 122.98, 119.78, 118.21, 112.41, 22.04; Mass: [EI-HRMS] ($C_{20}H_{14}N_2$) calc. 282.1157 Da, Found: 282.1166Da; FTIR (KBr, ν_{max}, cm^{-1}): 3427.25, 2924.18, 2856.39, 1622.75, 1455.67, 1361.68, 1242.51, 810.54, 725.36

3-methylphenanthro[9',10':4,5]imidazo[1,2-a]pyridine (5c)



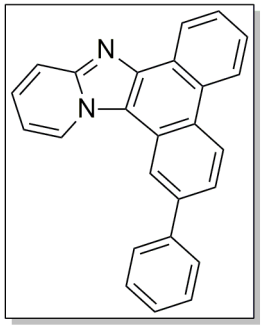
Pale yellow solid; yield 81%; m.p. 140-141^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.11 (t, *J* = 12.0 Hz, 1H), 8.90 (d, *J* = 6.0 Hz, 1H), 8.73 (d, *J* = 6.0 Hz, 1H), 8.65 (s, 1H), 8.38 (t, *J* = 18.0 Hz, 1H), 7.98 (d, *J* = 12.0 Hz, 1H), 7.78 – 7.71 (m, 2H), 7.58 (d, *J* = 6.0 Hz, 1H), 7.46 (t, *J* = 12.0 Hz, 1H), 7.09 (t, *J* = 12.0 Hz, 1H), 2.67 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 147.12, 134.41, 129.42, 128.68, 128.48, 127.35, 126.93, 126.89, 126.42, 125.96, 125.08, 124.62, 123.76, 123.16, 121.27, 119.62, 119.33, 118.12, 112.39, 21.91; Mass: [EI-HRMS] ($C_{20}H_{14}N_2$) calc. 282.1157 Da, Found: 282.1150Da; FTIR (KBr, ν_{max}, cm^{-1}): 3420.66, 2922.33, 1631.70, 1531.35, 1426.16, 1359.92, 1265.92, 1151.49, 764.85, 728.31, 583.18, 533.05

2-methoxyphenanthro[9',10':4,5]imidazo[1,2-a]pyridine (5d)



Pale yellow solid; yield 84%; m.p. 110-111^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.10 (d, *J* = 6.0 Hz, 1H), 8.88 (d, *J* = 6.0 Hz, 1H), 8.78 (d, *J* = 6.0 Hz, 1H), 8.64 (d, *J* = 12.0 Hz, 1H), 7.99 (d, *J* = 6.0 Hz, 1H), 7.91 (s, 1H), 7.74 – 7.69 (m, 2H), 7.48 (t, *J* = 18.0 Hz, 1H), 7.29 (d, *J* = 6.0 Hz, 1H), 7.11 (t, *J* = 12.0 Hz, 1H), 4.08 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 147.57, 141.57, 129.79, 127.10, 126.48, 126.27, 126.16, 126.09, 125.84, 124.79, 123.77, 122.64, 122.34, 118.97, 118.22, 112.45, 112.07, 103.76, 55.61; Mass: [EI-HRMS] ($C_{20}H_{14}N_2O$) calc. 298.1106 Da, Found: 298.1119Da; FTIR (KBr, ν_{max}, cm^{-1}): 3419.82, 2930.69, 1617.08, 1530.07, 1460.03, 1426.44, 1360.23, 1309.93, 1225.38, 1034.91, 816.40, 730.43

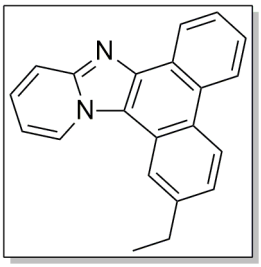
2-phenylphenanthro[9',10':4,5]imidazo[1,2-a]pyridine (5e)



Light yellow solid; yield 82%; m.p. 228-229^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.25 (d, *J* = 6.0 Hz, 1H), 8.94 (d, *J* = 6.0 Hz, 2H), 8.78 (d, *J* = 12.0 Hz, 1H), 8.70 (s, 1H), 8.01 (d, *J* = 6.0 Hz, 1H), 7.91 (d, *J* = 12.0 Hz, 1H), 7.85 (d, *J* = 12.0 Hz, 2H), 7.82 – 7.74 (m, 2H), 7.60 (t, *J* = 12.0 Hz, 2H), 7.51 (t, *J* = 18.0 Hz, 2H), 7.14 (t, *J* = 12.0 Hz, 1H); ^{13}C NMR (150 MHz,DMSO-

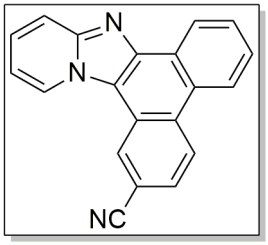
d_6) δ (ppm) 141.50, 141.12, 140.26, 129.49, 129.08, 128.32, 127.79, 127.60, 127.48, 127.14, 127.04, 122.46, 126.53, 126.18, 125.20, 125.07, 124.13, 124.02, 123.83, 123.25, 119.30, 118.37, 118.25, 112.59; Mass: [EI-HRMS] ($C_{25}H_{16}N_2$) calc. 344.1313 Da, Found: 344.1320Da; FTIR (KBr, ν_{max}, cm^{-1}): 3440.88, 3036.96, 1612.30, 1497.30, 1449.63, 1357.89, 1269.80, 1145.92, 824.21, 753.39, 723.79, 689.95

2-ethylphenanthro[9',10':4,5]imidazo[1,2-a]pyridine (5f)



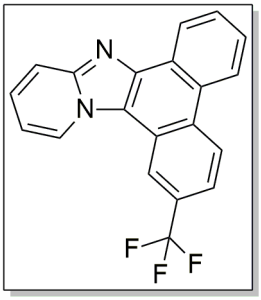
Light yellow solid; yield 80%; m.p. 142-143^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.19 (d, *J* = 12.0 Hz, 1H), 8.91 (d, *J* = 6.0 Hz, 1H), 8.78 (d, *J* = 6.0 Hz, 1H), 8.72 (d, *J* = 6.0 Hz, 1H), 8.31 (s, 1H), 7.98 (d, *J* = 12 Hz, 1H), 7.77 – 7.71(m, 2H), 7.53 (d, *J* = 6.0 Hz, 1H), 7.48 t, *J* = 18.0 Hz, 1H), 7.12 (t, *J* = 18.0 Hz, 1H), 3.00 (q, *J* = 7.6 Hz, 2H), 1.46 (t, *J* = 18.0 Hz, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 147.47, 143.49, 141.16, 129.71, 127.01, 126.94, 126.63, 126.55, 126.33, 125.96, 125.05, 124.57, 123.84, 123.71, 123.00, 119.23, 118.60, 118.24, 112.33, 29.34, 15.87; Mass: [EI-HRMS] ($C_{21}H_{16}N_2$) calc. 296.1313 Da, Found: 296.1317Da; FTIR (KBr, ν_{max}, cm^{-1}): 3430.48, 3042.63, 2961.18, 2923.76, 1622.26, 1519.87, 1453.11, 1422.27, 1359.17, 1242.09, 1150.17, 824.65, 721.61

phenanthro[9',10':4,5]imidazo[1,2-a]pyridine-2-carbonitrile (5g)



Light yellow solid; yield 56%; m.p. 275-276 ^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.13 (d, *J* = 12.0 Hz, 1H), 8.97 (d, *J* = 6.0 Hz, 2H), 8.83 (s, 1H), 8.75 (d, *J* = 6.0 Hz, 1H), 8.03 (d, *J* = 12.0 Hz, 1H), 7.90 – 7.87 (m, 2H), 7.81 (t, *J* = 12.0 Hz, 1H), 7.58 (t, *J* = 18.0 Hz, 1H), 7.24 (t, *J* = 12.0 Hz, 1H);^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 147.92, 138.48, 132.36, 131.09, 130.46, 129.31, 129.14, 128.73, 128.36, 127.69, 127.11, 126.27, 124.09, 124.02, 123.82, 120.02, 118.65, 113.78, 113.31, 111.62; Mass: [EI-MS] ($C_{20}H_{11}N_3$) calc. 293.0953 Da, Found: 293 Da (No HRMS due to matrix peak matching); FTIR (KBr, ν_{max}, cm^{-1}): 3439.70, 2925.00, 2855.20, 2360.99, 2227.19, 1629.55, 1517.10, 1451.47, 1424.55, 1363.11, 1312.44, 1246.50, 828.37, 734.66

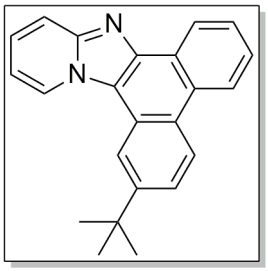
2-(trifluoromethyl)phenanthro[9',10':4,5]imidazo[1,2-a]pyridine (5h)



Pale yellow solid; yield 52%; m.p. 278-279^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.15 (d, *J* = 12.0 Hz, 1H), 8.99 (d, *J* = 6.0 Hz, 1H), 8.96 (d, *J* = 6.0 Hz, 1H), 8.78 (d, *J* = 6.0 Hz, 2H), 8.02 (d, *J* = 12.0 Hz, 1H), 7.90 – 7.84 (m, 2H), 7.80 (t, *J* = 18.0 Hz, 1H), 7.56 (t, *J* = 18.0 Hz, 1H), 7.21

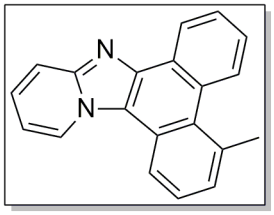
(t, *J* = 12.0 Hz, 1H);^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 148.02, 141.93, 130.46, 128.78, 128.57, 127.75, 127.47, 126.80, 126.33, 125.32, 125.26, 123.97, 123.64, 123.26, 120.62, 118.33, 118.72, 118.53, 116.61, 113.06, 53.40; Mass: [EI-HRMS] ($C_{20}H_{11}F_3N_2$) calc. 336.0874 Da, Found: 336.0879 Da; FTIR (KBr, ν_{max}, cm^{-1}): 2924.32, 2853.80,1739.19, 1624.50, 1460.25, 1324.93, 1292.72, 1262.60, 1166.90, 1110.57, 803.67, 727.58, 594.71

2-(tert-butyl)phenanthro[9',10':4,5]imidazo[1,2-a]pyridine (5i)



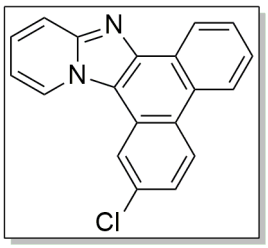
Pale yellow solid; yield 78%; m.p. 154-155^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.17 (d, *J* = 6.0 Hz, 1H), 8.91 (d, *J* = 12.0 Hz, 1H), 8.81 (d, *J* = 12.0 Hz, 1H), 8.73 (d, *J* = 6.0 Hz, 1H), 8.52 (s, 1H), 8.01 (d, *J* = 6.0 Hz, 1H), 7.77 – 7.71 (m, 3H), 7.48 (t, *J* = 12.0 Hz, 1H), 7.14 (t, *J* = 12.0 Hz, 1H), 1.58 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 150.23, 147.49, 141.12, 129.59, 127.06, 126.95, 126.70, 126.39, 126.07, 125.93, 124.33, 123.59, 123.02, 122.87, 119.60, 118.33, 115.79, 114.04, 112.50, 35.16, 31.53;Mass: [EI-HRMS] ($C_{23}H_{20}N_2$) calc. 324.1626 Da, Found: 324.1629Da; FTIR (KBr, ν_{max}, cm^{-1}): 3438.60, 2954.90, 1619.57, 1453.44, 1449.63, 1357.78, 1263.57, 1033.54, 816.45, 769.15, 720.20, 484.13

4-methylphenanthro[9',10':4,5]imidazo[1,2-a]pyridine (5j)



Pale yellow solid; yield 81%; m.p. 141-142^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.18 (d, *J* = 6.0 Hz, 1H), 8.98 (d, *J* = 12.0 Hz, 1H), 8.83 (d, *J* = 6.0 Hz, 1H), 8.45 (d, *J* = 6.0 Hz, 1H), 7.97 (d, *J* = 6.0 Hz, 1H), 7.77 (t, *J* = 12.0 Hz, 1H), 7.71 – 7.64 (m, 2H), 7.53 (d, *J* = 6.0 Hz, 1H), 7.46 (t, *J* = 12.0 Hz, 1H), 7.08 (t, *J* = 12.0 Hz, 1H), 3.20 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 147.89, 141.08, 137.10, 130.67, 129.61, 128.52, 128.38, 128.00, 126.74, 126.54, 126.30, 125.98, 125.56, 125.11, 123.57, 119.78, 118.31, 117.64, 112.31, 27.82;Mass: [EI-HRMS] ($C_{20}H_{14}N_2$) calc. 282.1157 Da, Found: 282.1147 Da; FTIR (KBr, ν_{max}, cm^{-1}): 3425.15, 2924.22, 2855.37, 1730.24, 1633.32, 1460.45, 1349.80, 1270.21, 1210.90, 1142.06, 798.16, 756.46, 716.60

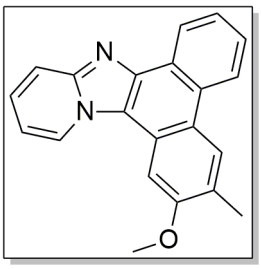
2-chlorophenanthro[9',10':4,5]imidazo[1,2-a]pyridine (5k)



Light yellow solid; yield 75%; m.p. 268-269^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.07 (d, *J* = 6.0 Hz, 1H), 8.90 (d, *J* = 12.0 Hz, 1H), 8.76 (d, *J* = 6.0 Hz, 1H), 8.66 (d, *J* = 6.0 Hz, 1H), 8.43 (s, 1H), 7.98 (d, *J* = 12.0 Hz, 1H), 7.80 – 7.73 (m, 2H), 7.60 (d, *J* = 12.0 Hz, 1H), 7.52 (t, *J* = 18.0 Hz, 1H), 7.16 (t, *J* = 12.0 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 141.89,

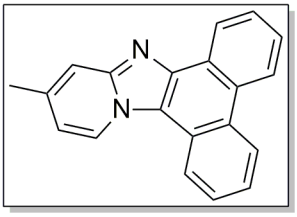
133.36, 129.11, 127.71, 127.32, 126.93, 126.89, 126.59, 126.54, 126.33, 125.98, 124.91, 124.83, 124.57, 123.87, 123.10, 119.22, 118.38, 112.78;Mass: [EI-HRMS] ($C_{19}H_{11}N_2Cl$) calc. 302.0611 Da, Found: 302.0605 Da; FTIR (KBr, ν_{max}, cm^{-1}): 3429.05, 3058.42, 2926.08, 1603.46, 1522.62, 1424.07, 1357.37, 1298.30, 1099.04, 811.52, 759.65, 720.36

2-methoxy-3-methylphenanthro[9',10':4,5]imidazo[1,2-a]pyridine (5l)



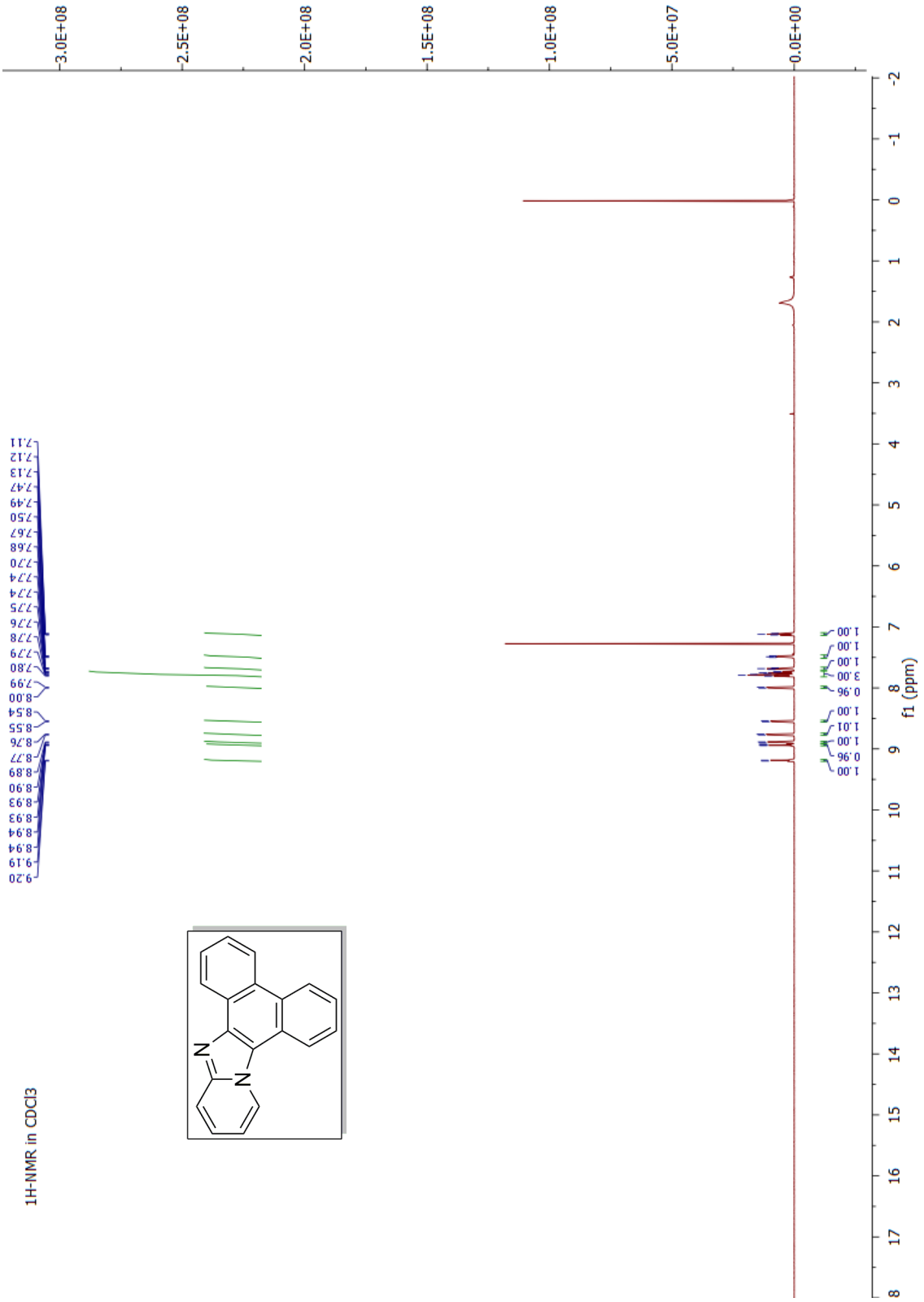
Pale yellow solid; yield 72%; m.p. 137-138^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.85 (t, *J* = 12.0 Hz, 2H), 8.58 (d, *J* = 6.0 Hz, 1H), 8.48 (s, 1H), 7.93 (d, *J* = 12.0 Hz, 1H), 7.70 – 7.67 (m, 2H), 7.54 (s, 1H), 7.41 (t, *J* = 12.0 Hz, 1H), 7.01 (t, *J* = 12.0 Hz, 1H), 4.03 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 157.42, 147.09, 140.62, 129.43, 129.80, 126.25, 126.14, 125.92, 125.76, 125.63, 124.96, 123.65, 122.60, 121.75, 119.20, 118.09, 112.22, 99.39, 55.38, 16.89; Mass: [EI-HRMS] ($C_{21}H_{16}N_2O$) calc. 312.1263 Da, Found: 312.1269 Da; FTIR (KBr, ν_{max}, cm^{-1}): 3420.75, 3061.67, 29.20.71, 2849.71, 1622.66, 1526.41, 1461.86, 1426.10, 1360.93, 1248.58, 1203.10, 1167.81, 1040.93, 800.50, 763.82, 716.70

11-methylphenanthro[9',10':4,5]imidazo[1,2-a]pyridine (5m)

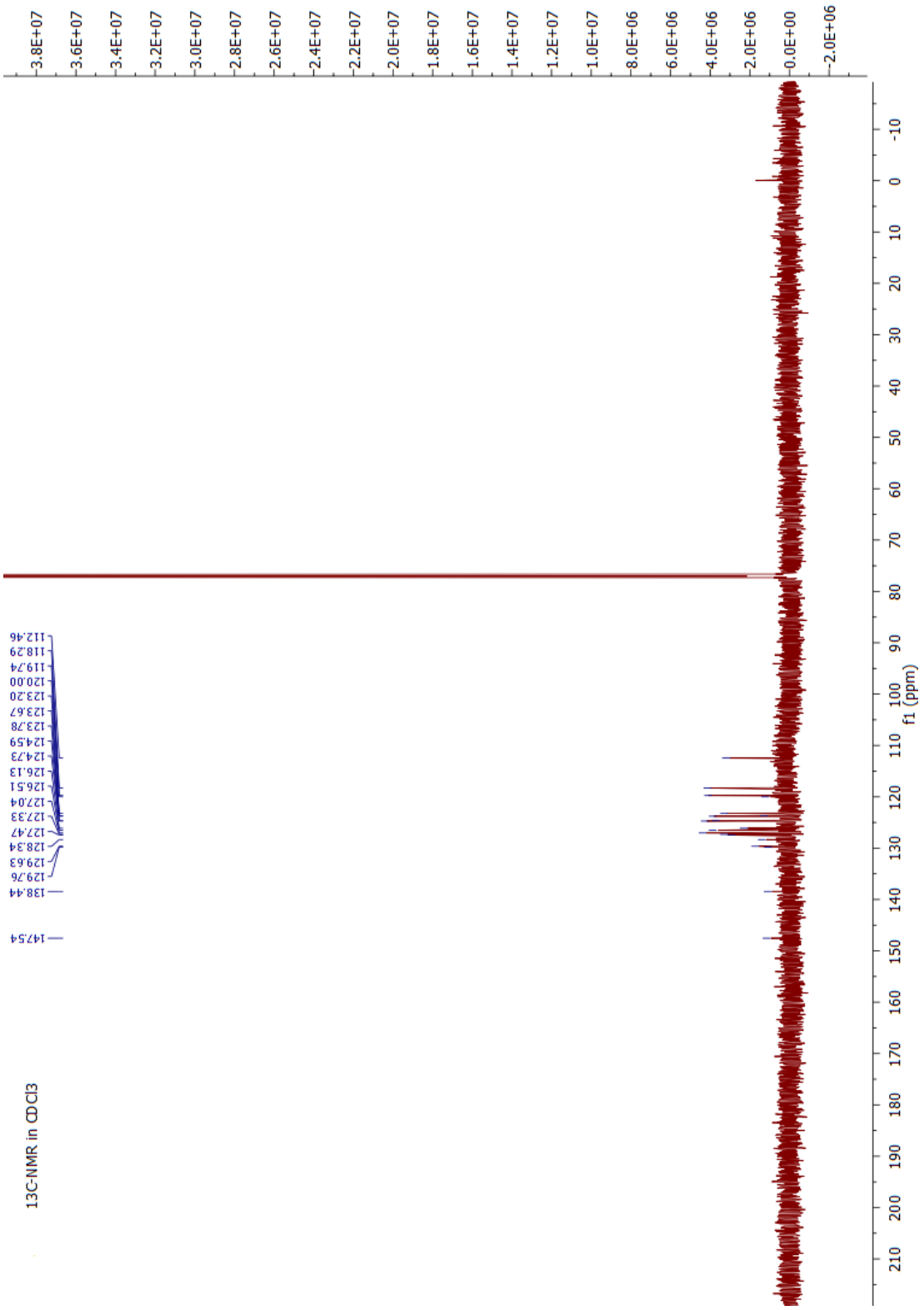


Light yellow solid; yield 83%; m.p. 194-195^{o}C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.02 (d, *J* = 12.0 Hz, 1H), 8.90 (d, *J* = 6.0 Hz, 1H), 8.87 (d, *J* = 6.0 Hz, 1H), 8.75 (d, *J* = 6.0 Hz, 1H), 8.48 (d, *J* = 12.0 Hz, 1H), 7.79 – 7.71 (m, 4H), 7.65 (t, *J* = 12.0 Hz, 1H), 6.91 (d, *J* = 6.0 Hz, 1H), 2.55 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 148.13, 141.11, 137.27, 129.49, 128.04, 127.33, 127.21, 127.11, 126.77, 125.63, 124.51, 124.37, 123.71, 123.69, 123.15, 119.55, 118.95, 116.63, 115.01, 21.51; Mass: [EI-HRMS] ($C_{20}H_{14}N_2$) calc. 282.1157 Da, Found: 282.1148Da; FTIR (KBr, ν_{max}, cm^{-1}): 3429.61, 3043.01, 2917.02, 2851.79, 1644.78, 1606.29, 1521.54, 1490.58, 1447.65, 1418.66, 1361.11, 1298.89, 1237.02, 1206.81, 1166.47, 1037.98, 846.26, 755.08, 715.71, 603.95

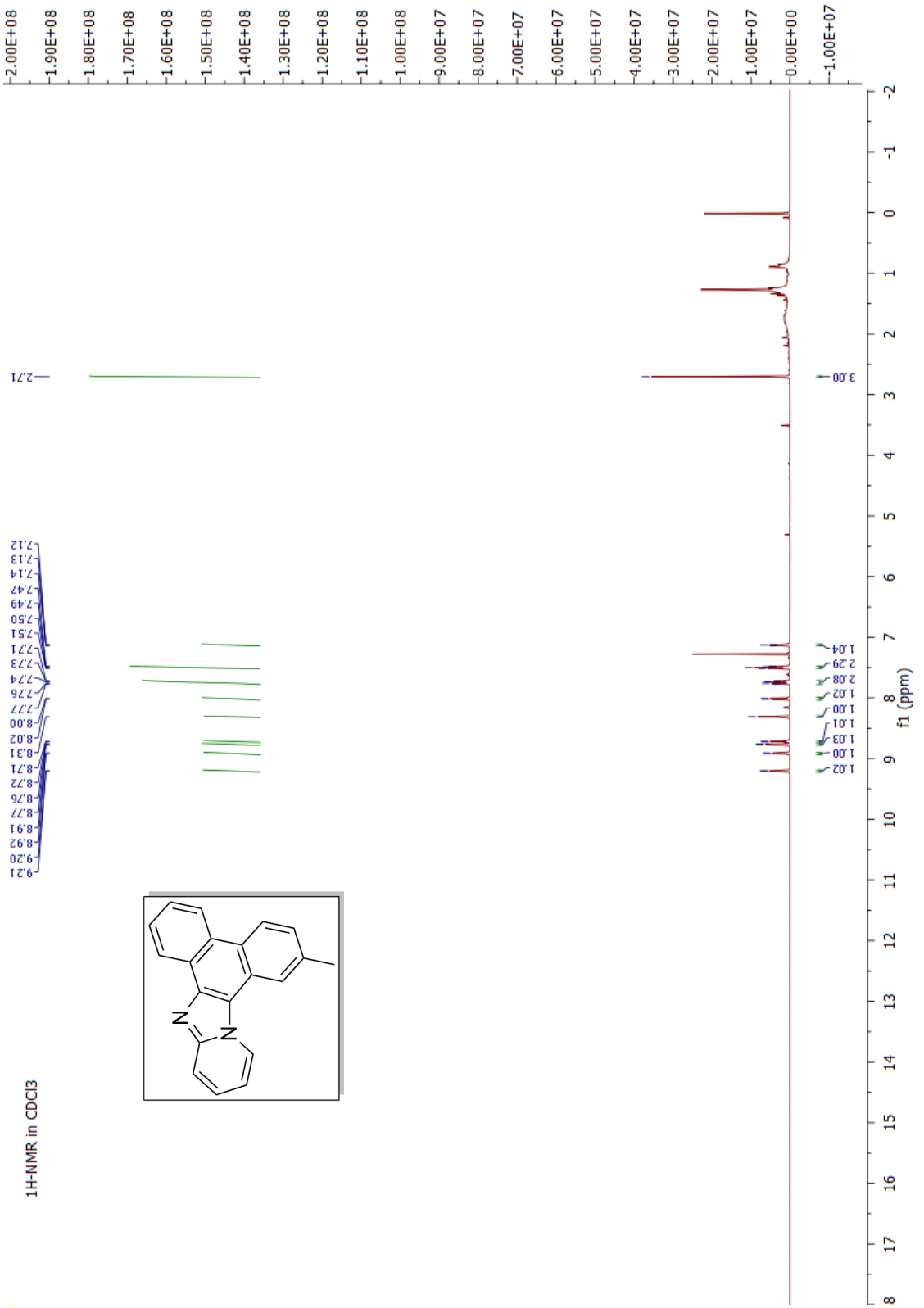
^{1}H NMR spectrum of compound 5a in $CDCl_3$



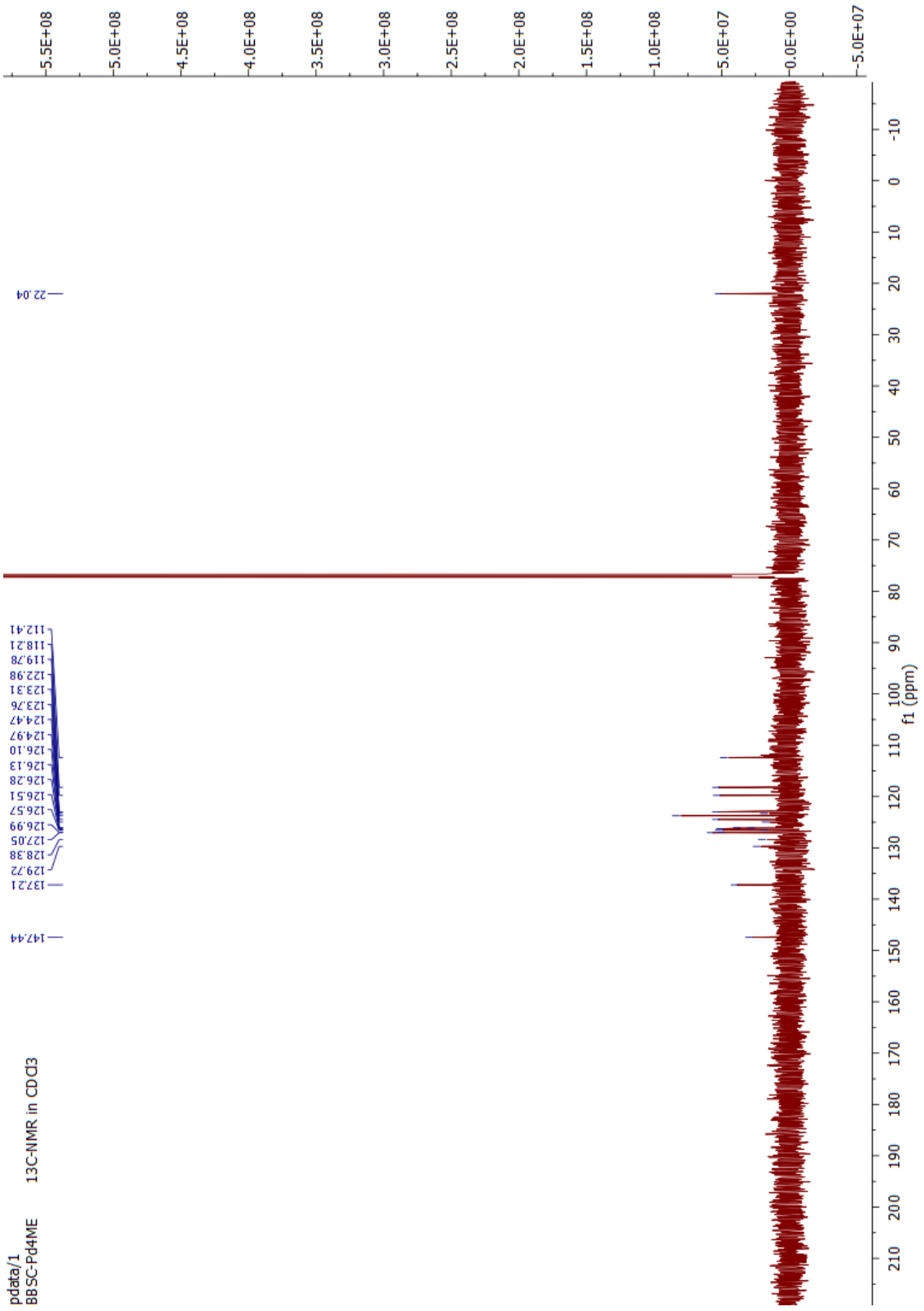
^{13}C NMR spectrum of compound 5a in $CDCl_3$



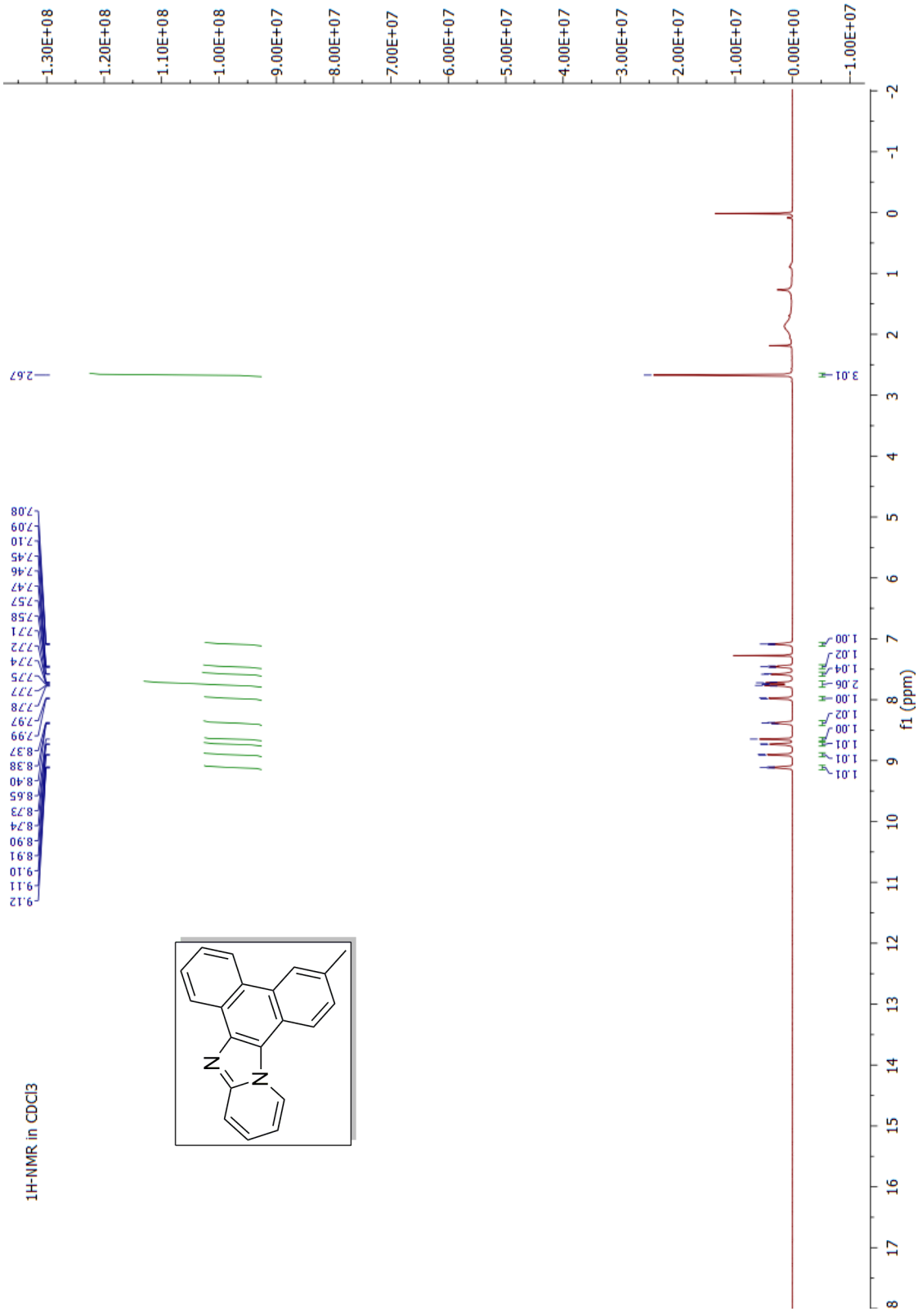
^{1}H NMR spectrum of compound 5b in $CDCl_3$



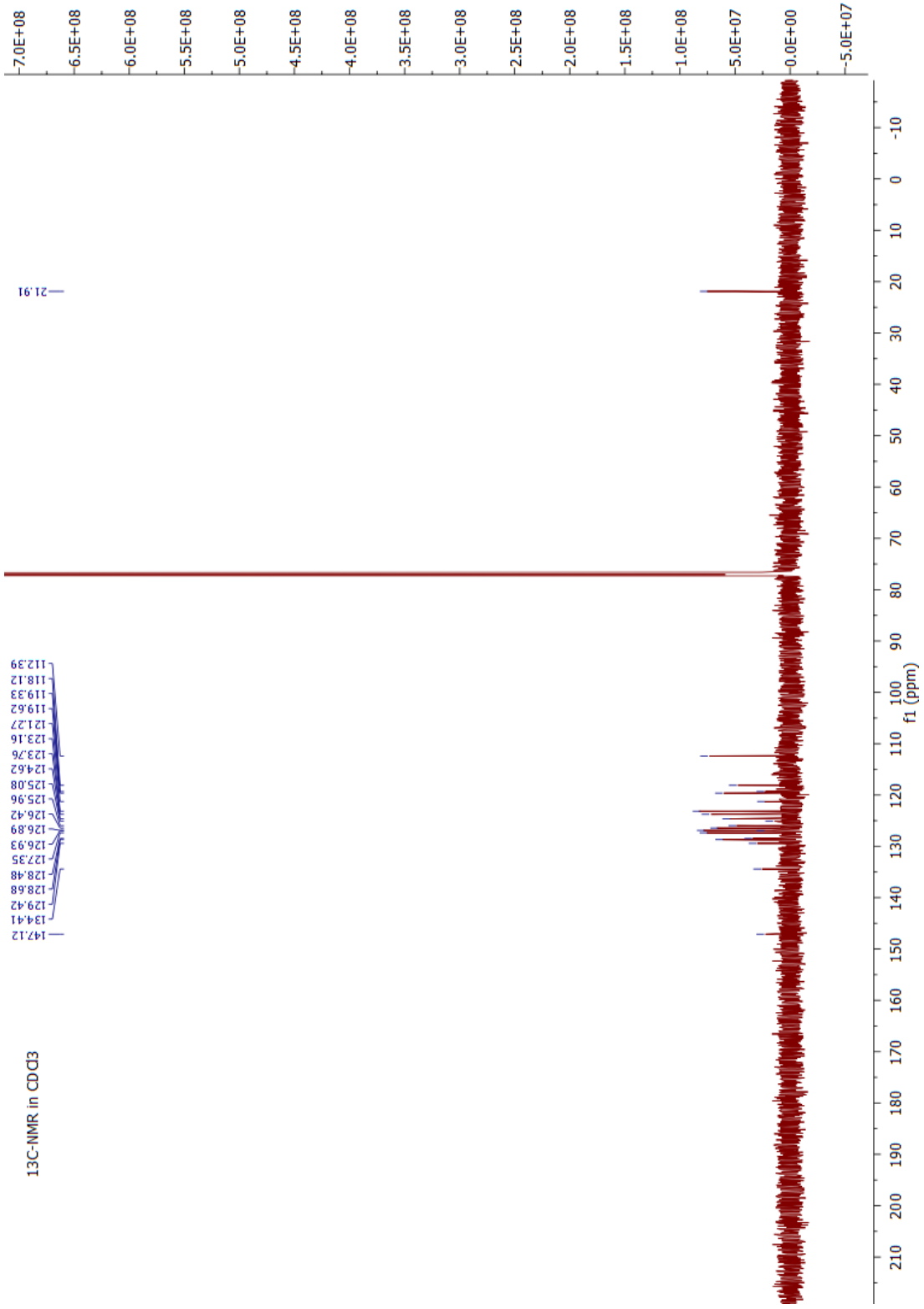
^{13}C NMR spectrum of compound 5b in $CDCl_3$



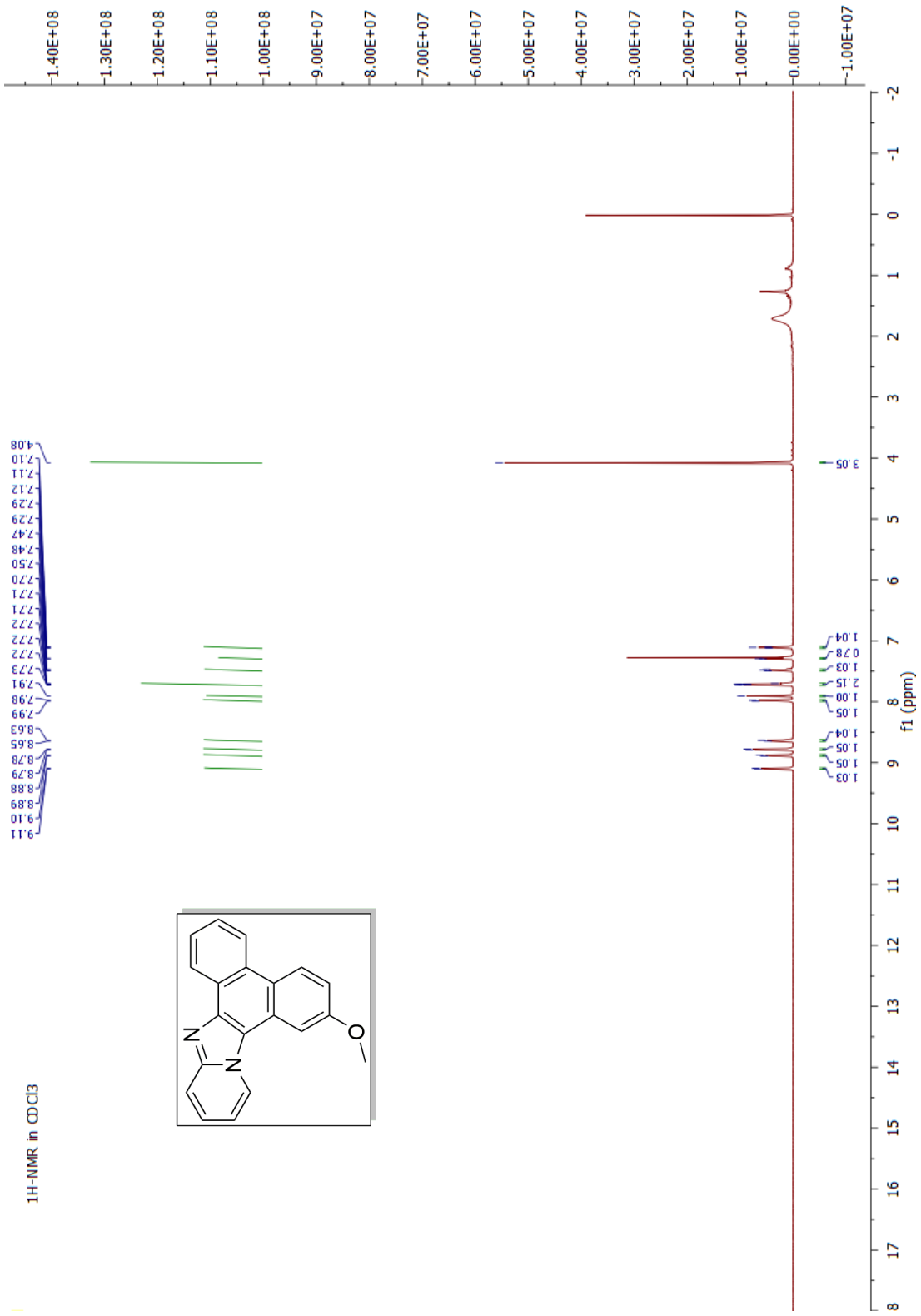
^{1}H NMR spectrum of compound 5c in $CDCl_3$



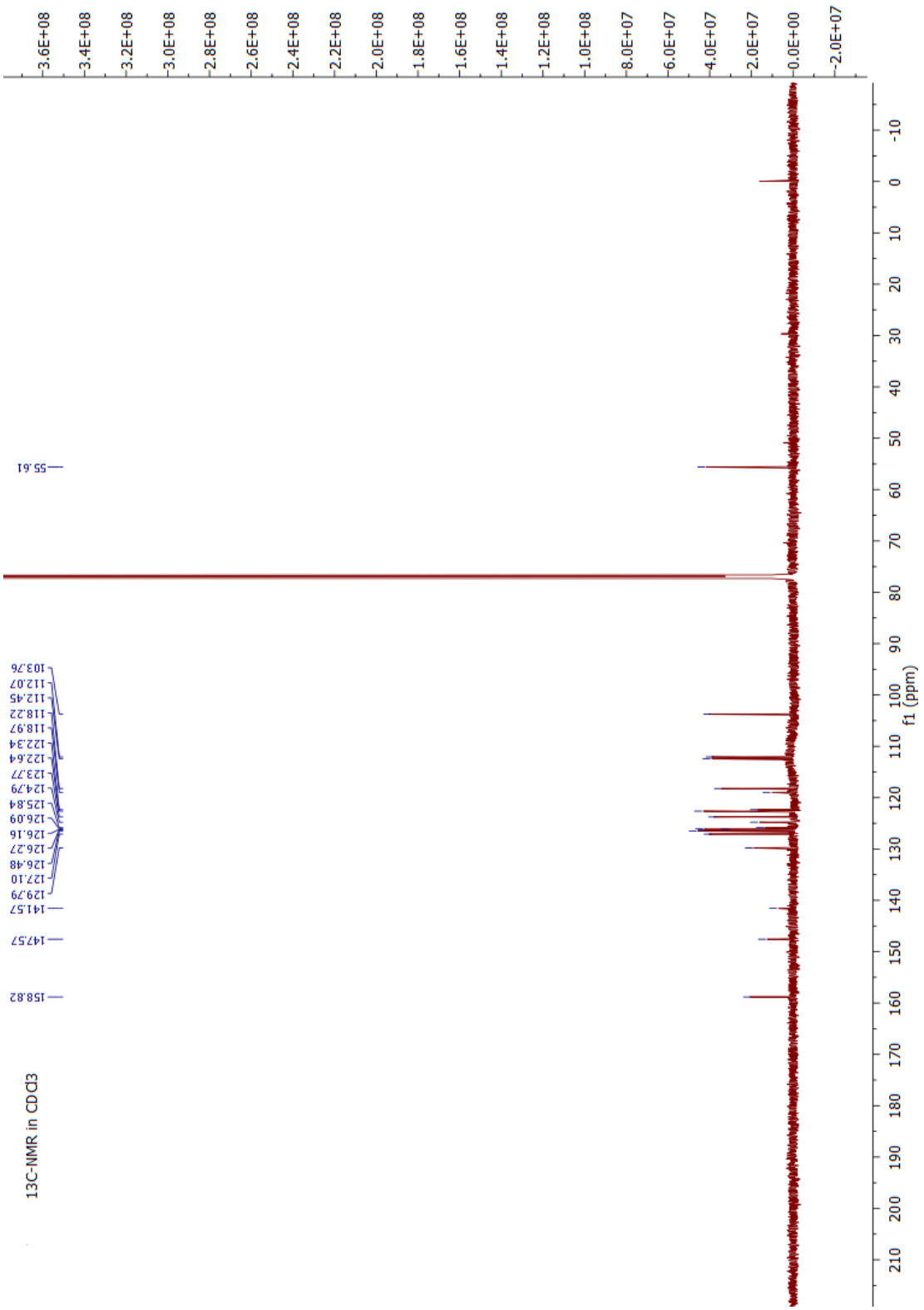
^{13}C NMR spectrum of compound 5c in $CDCl_3$



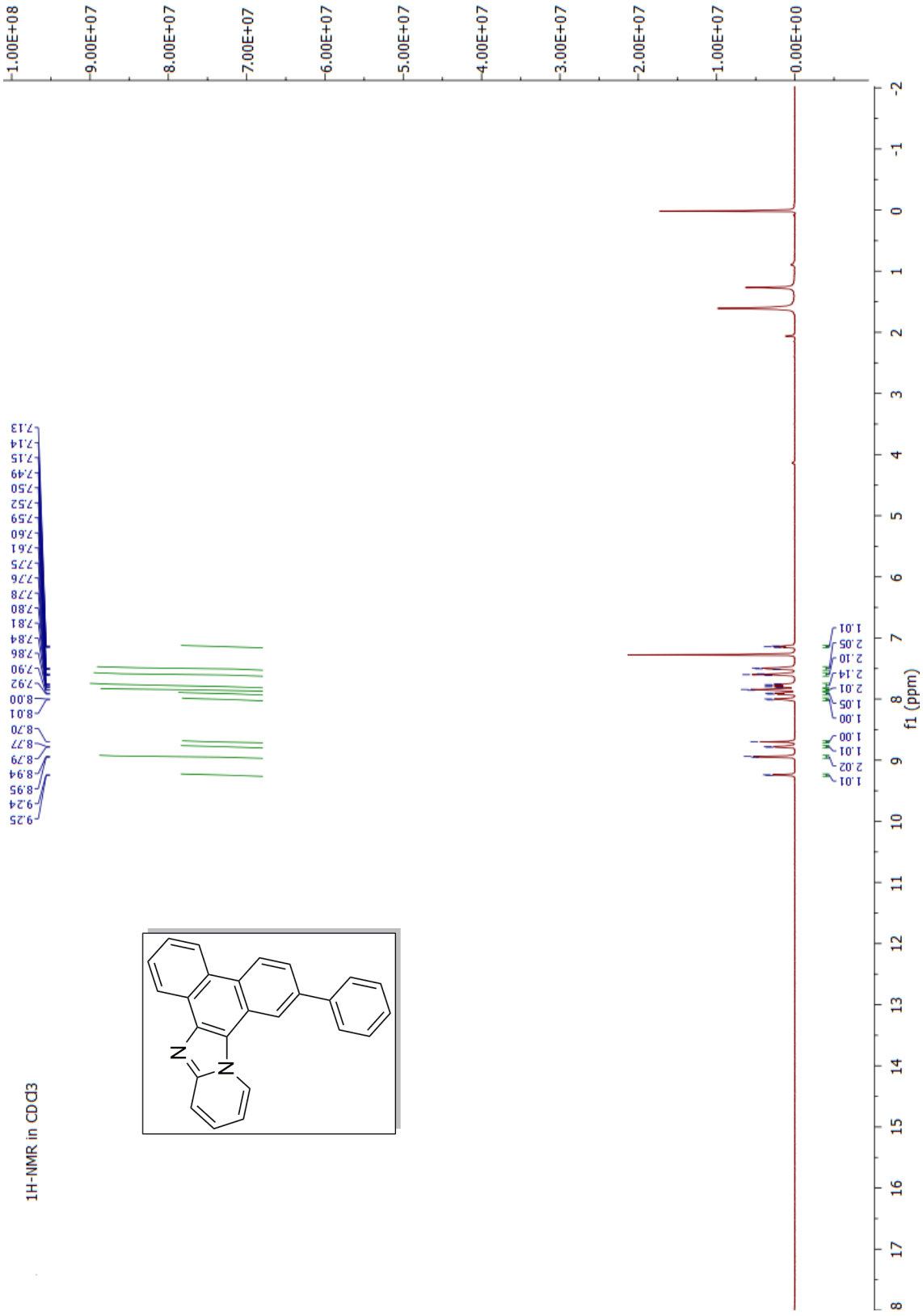
^{1}H NMR spectrum of compound 5d in $CDCl_3$



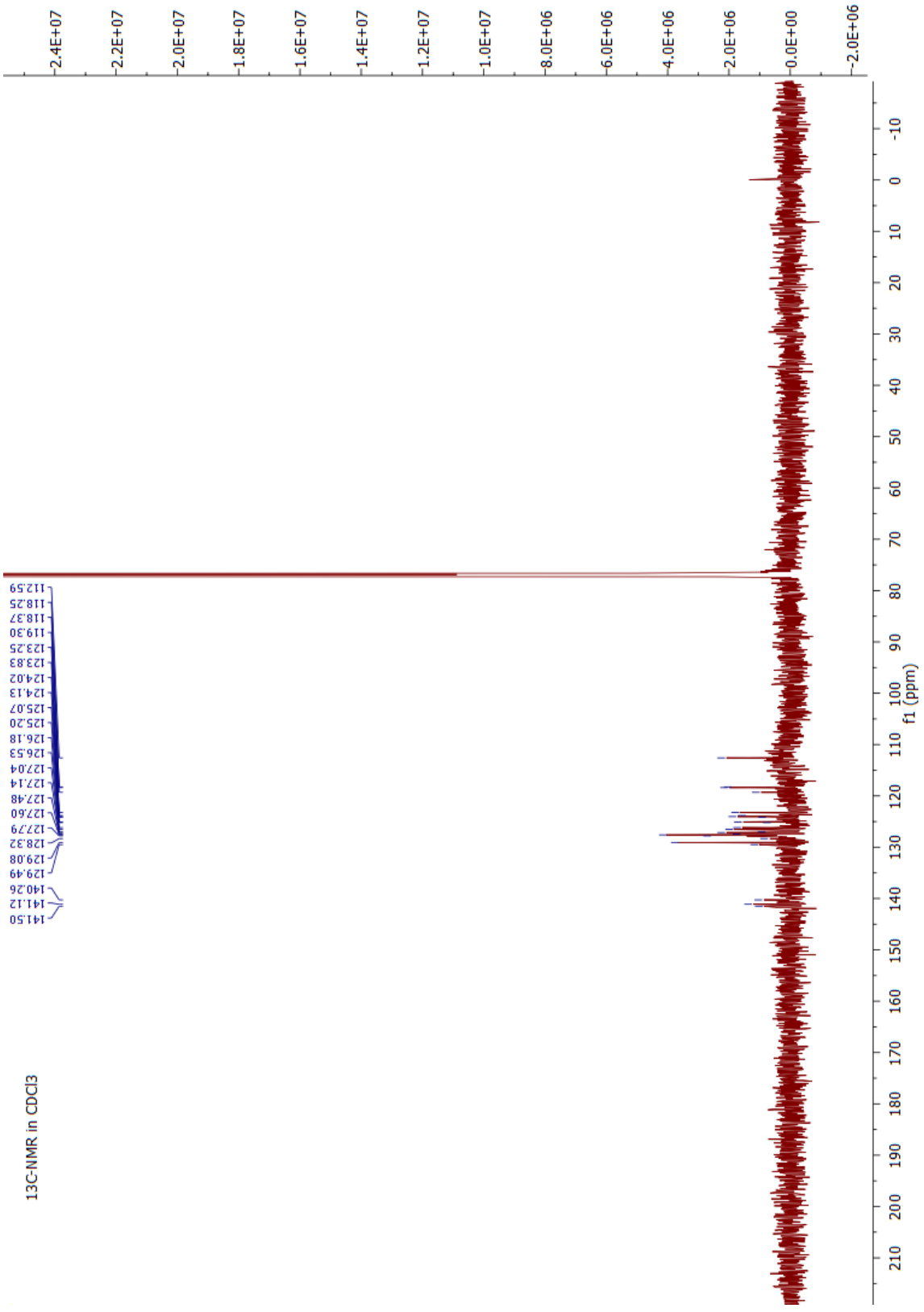
^{13}C NMR spectrum of compound 5d in $CDCl_3$



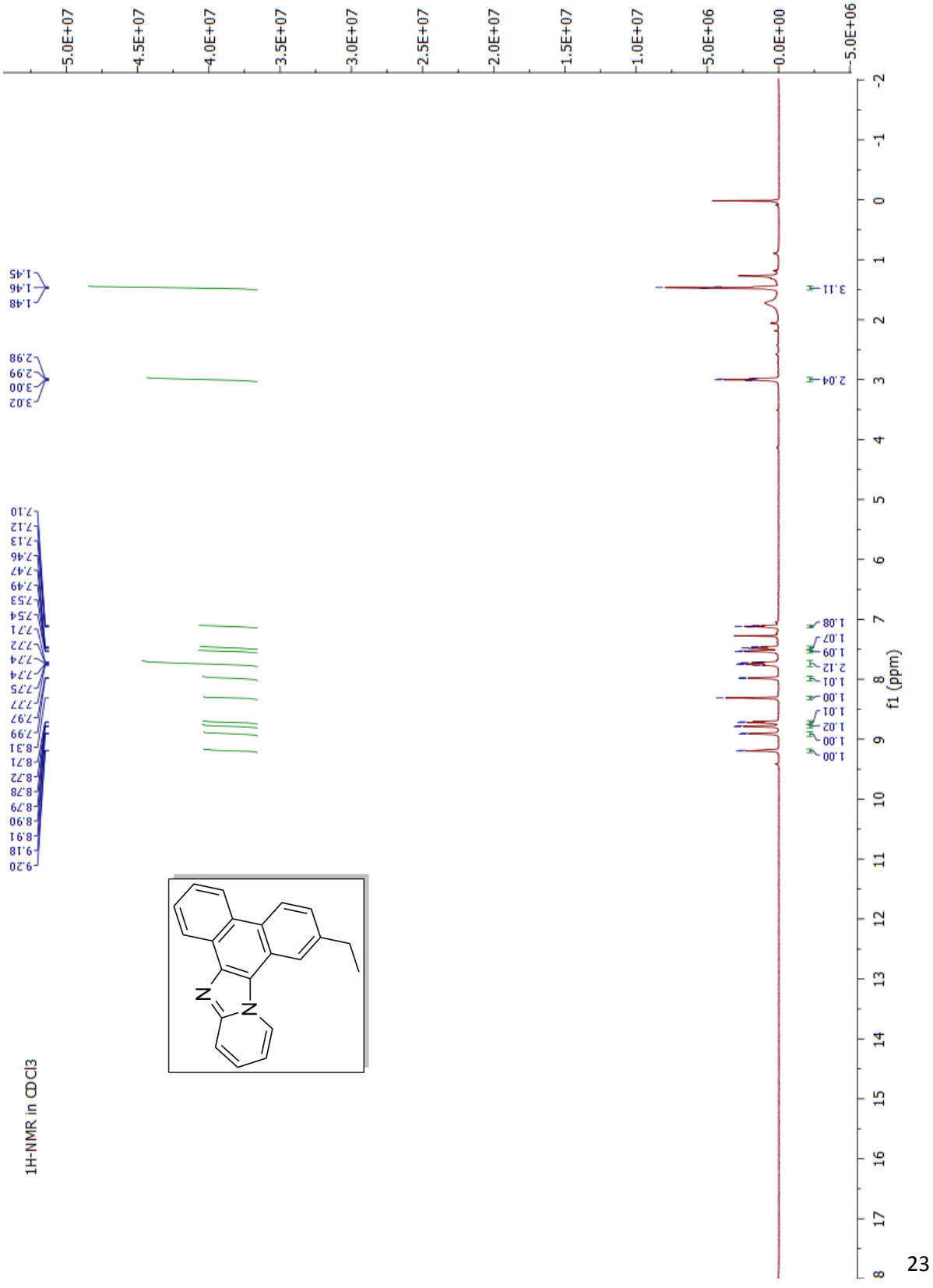
^{1}H NMR spectrum of compound 5e in $CDCl_3$



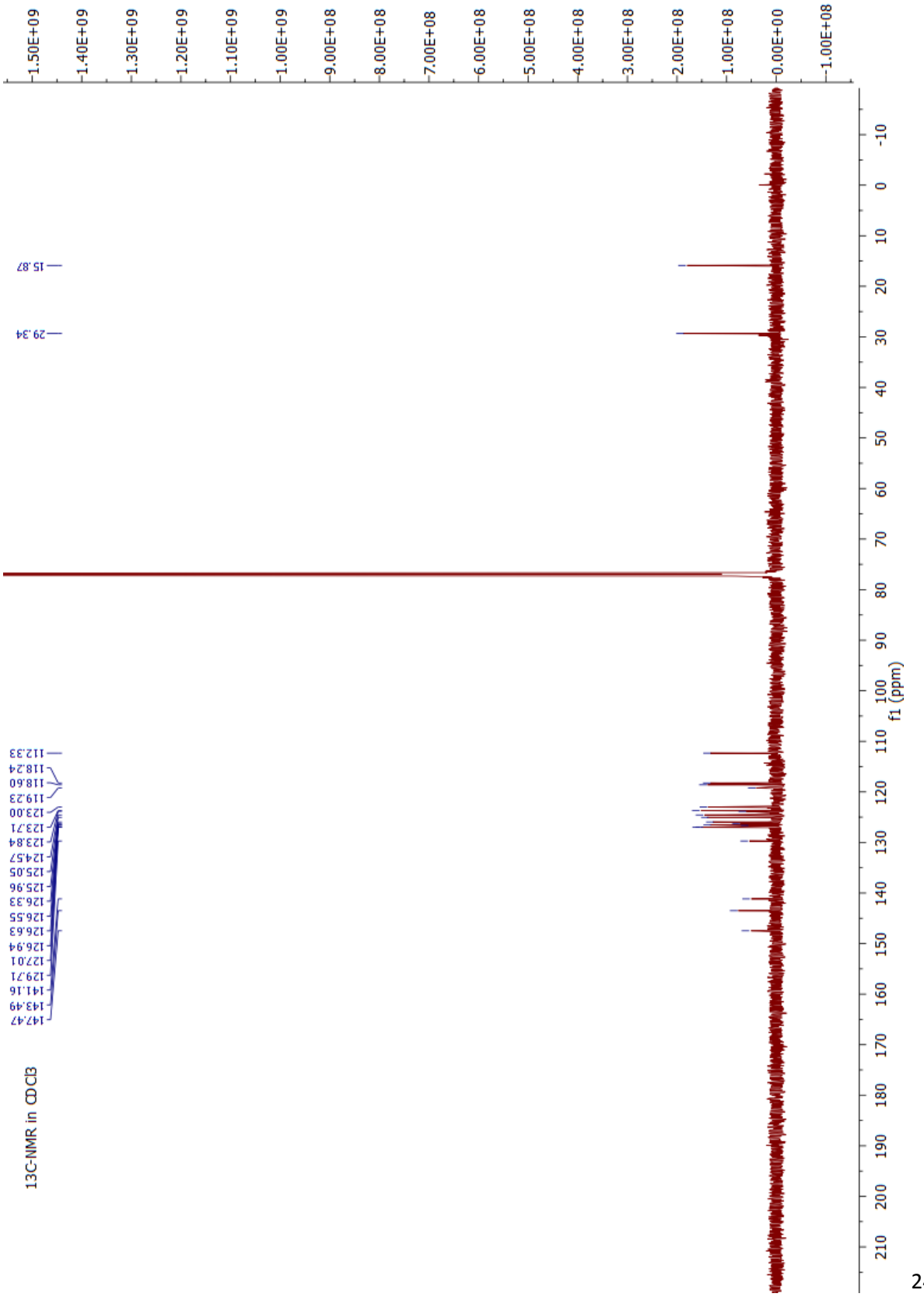
^{13}C NMR spectrum of compound 5e in $CDCl_3$



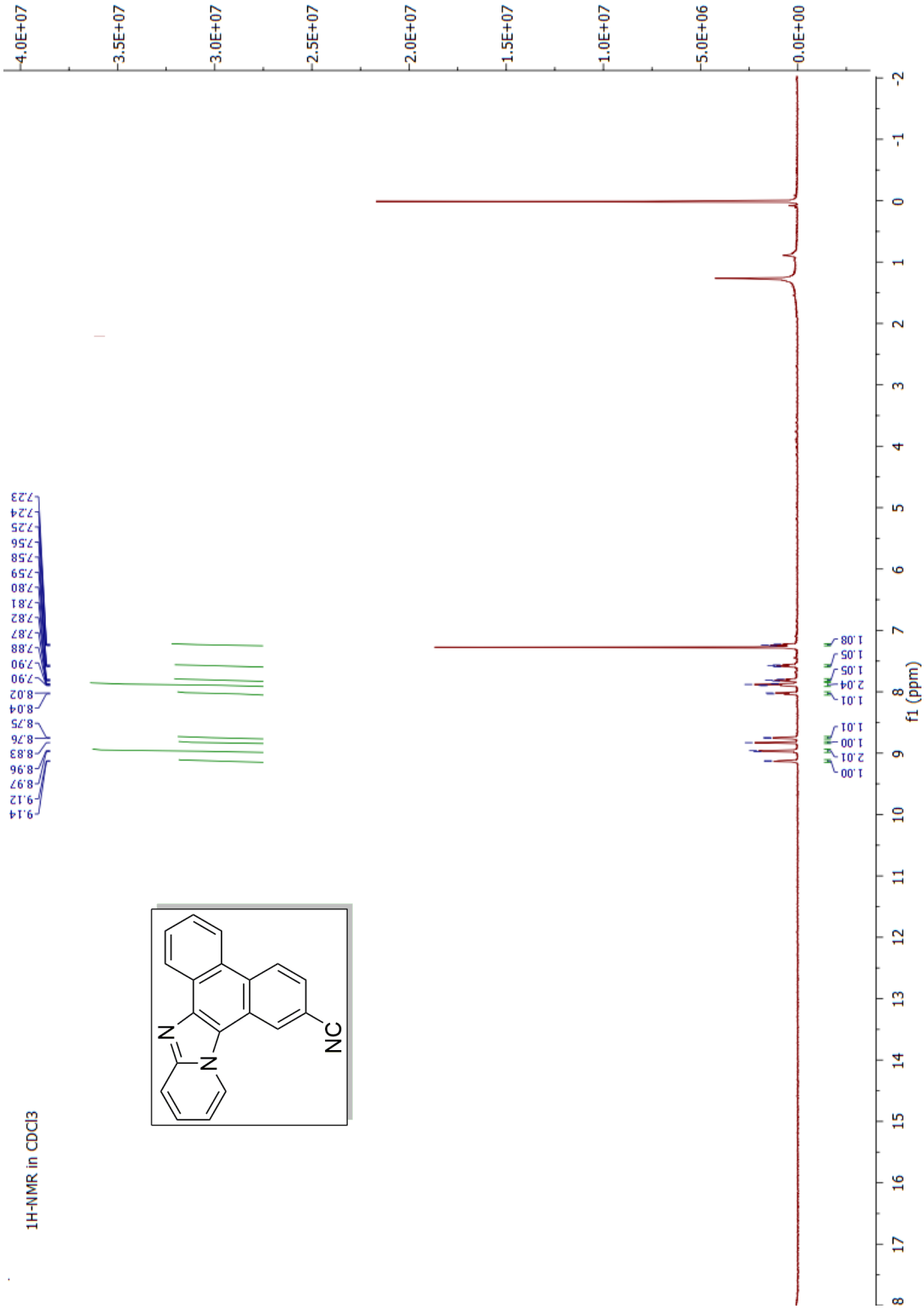
^{1}H NMR spectrum of compound 5f in $CDCl_3$



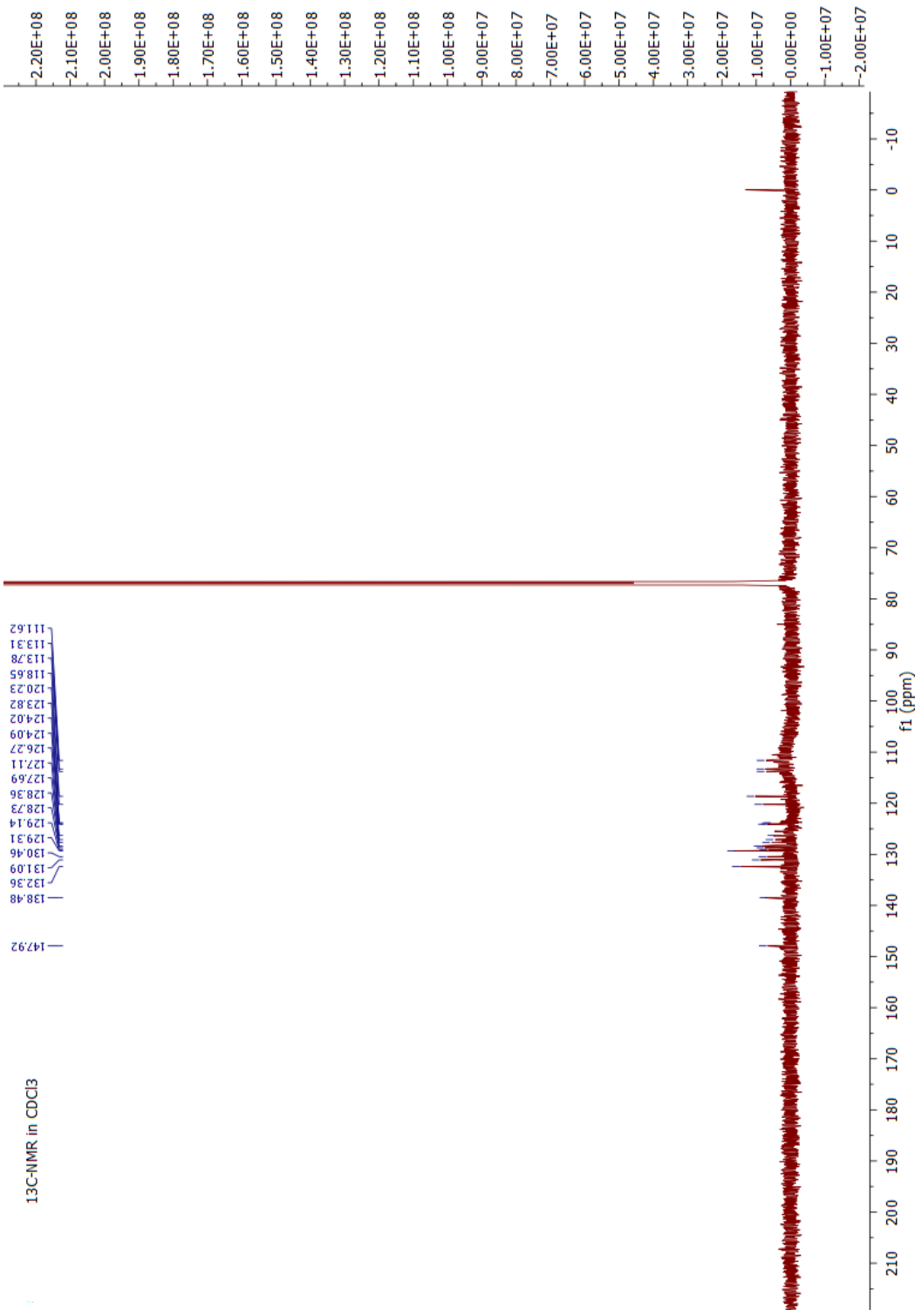
^{13}C NMR spectrum of compound 5f in $CDCl_3$



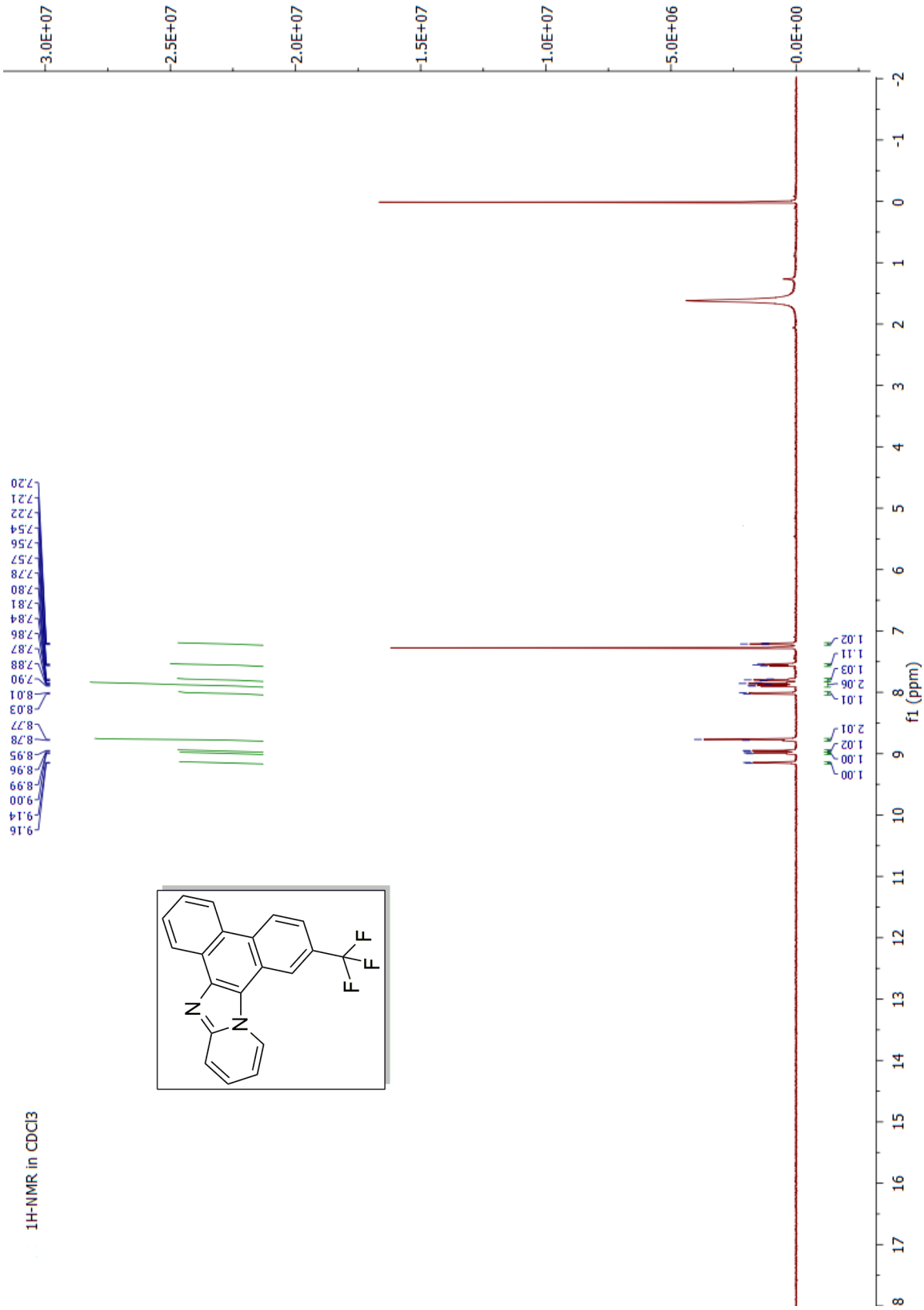
^{1}H NMR spectrum of compound 5g in $CDCl_3$



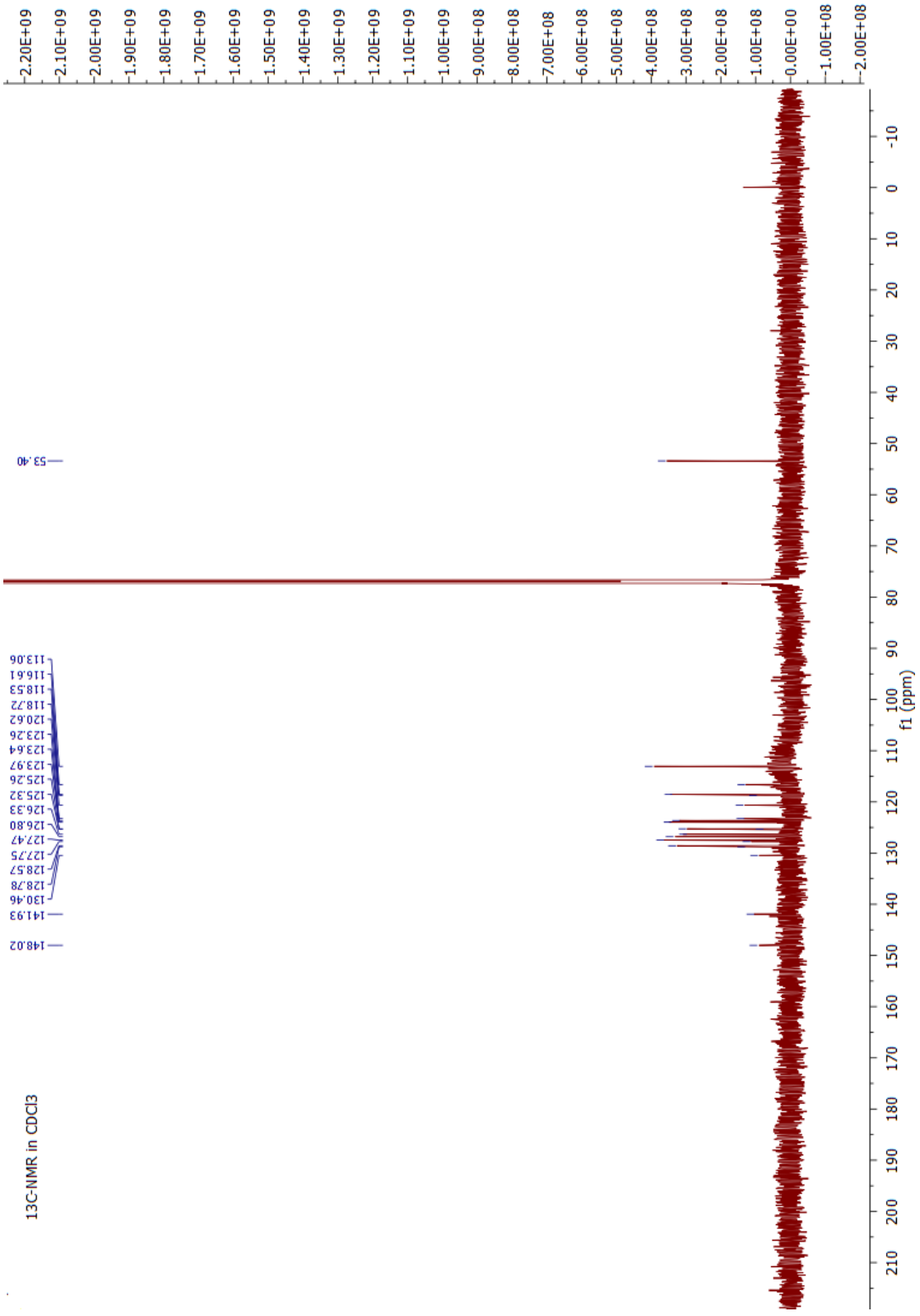
^{13}C NMR spectrum of compound 5g in $CDCl_3$



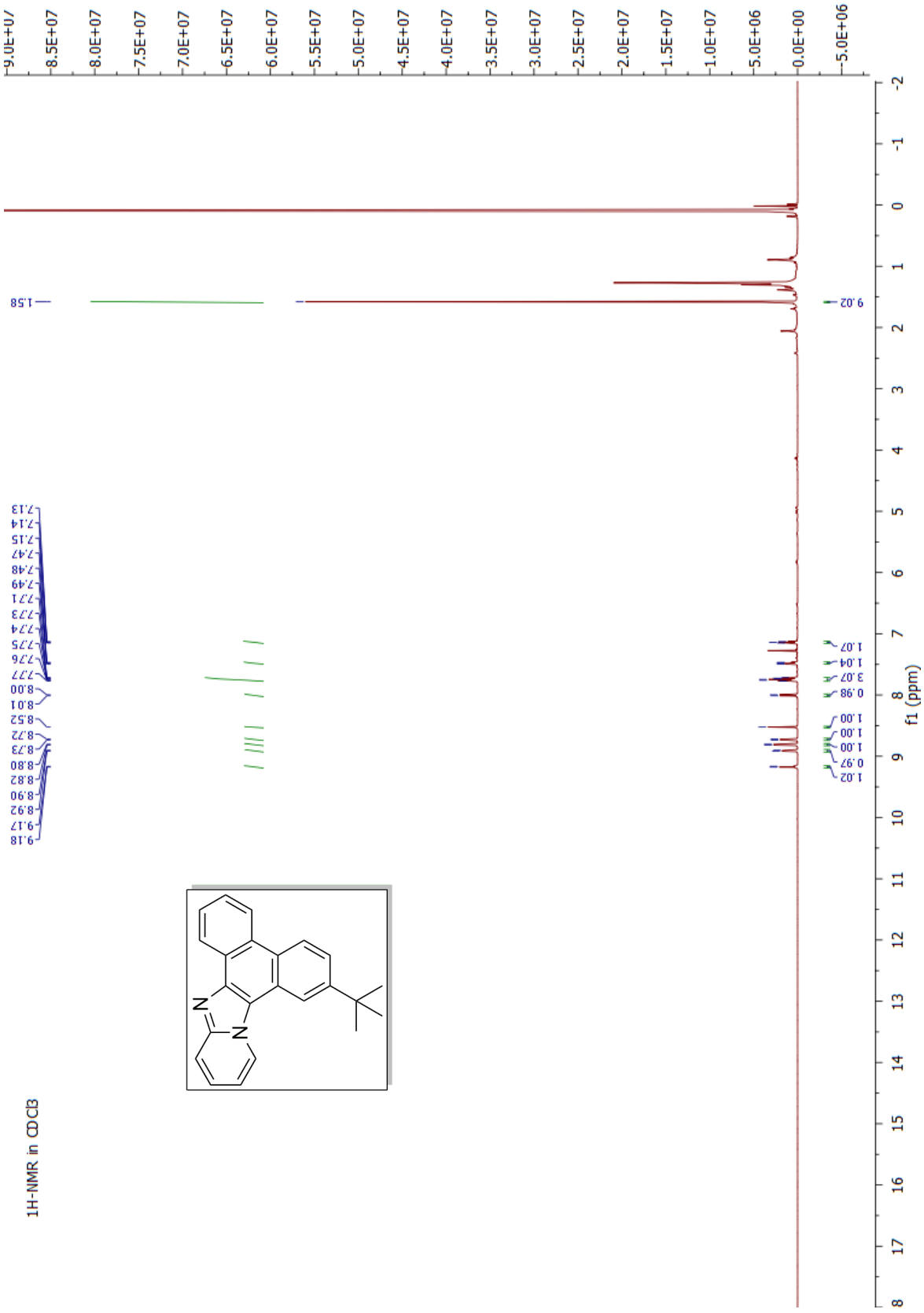
^{1}H NMR spectrum of compound 5h in $CDCl_3$



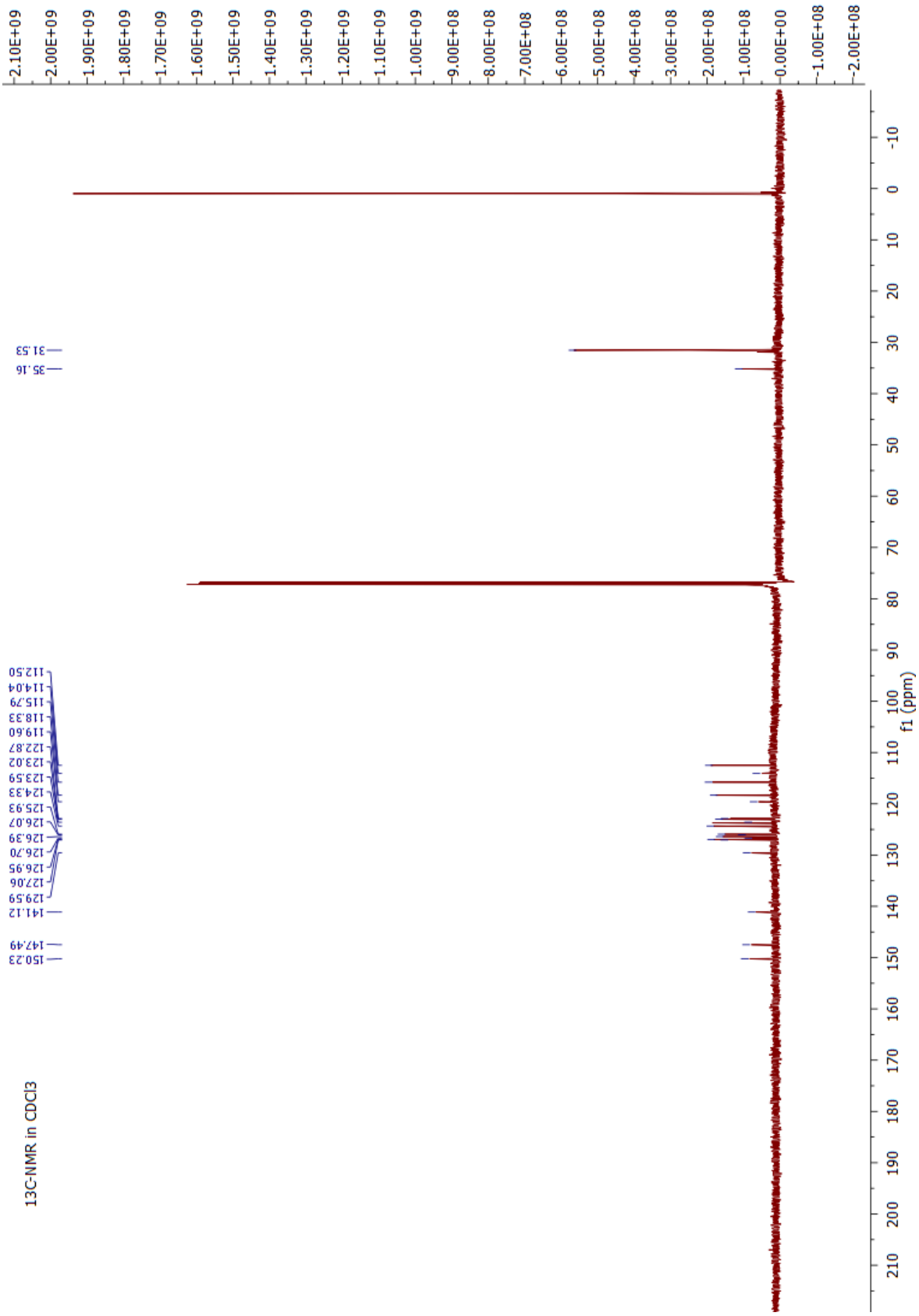
^{13}C NMR spectrum of compound 5h in $CDCl_3$



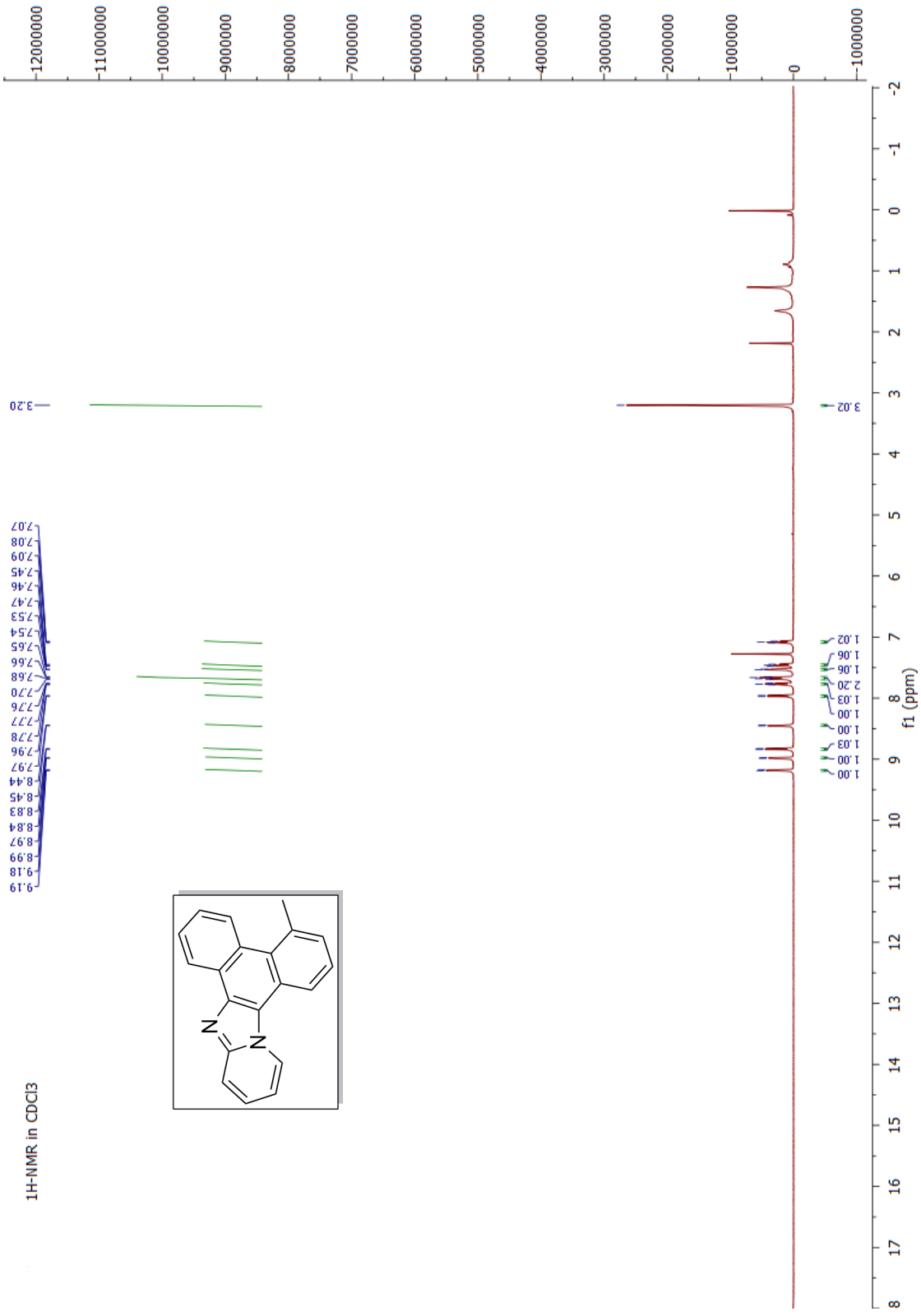
^{1}H NMR spectrum of compound 5i in $CDCl_3$



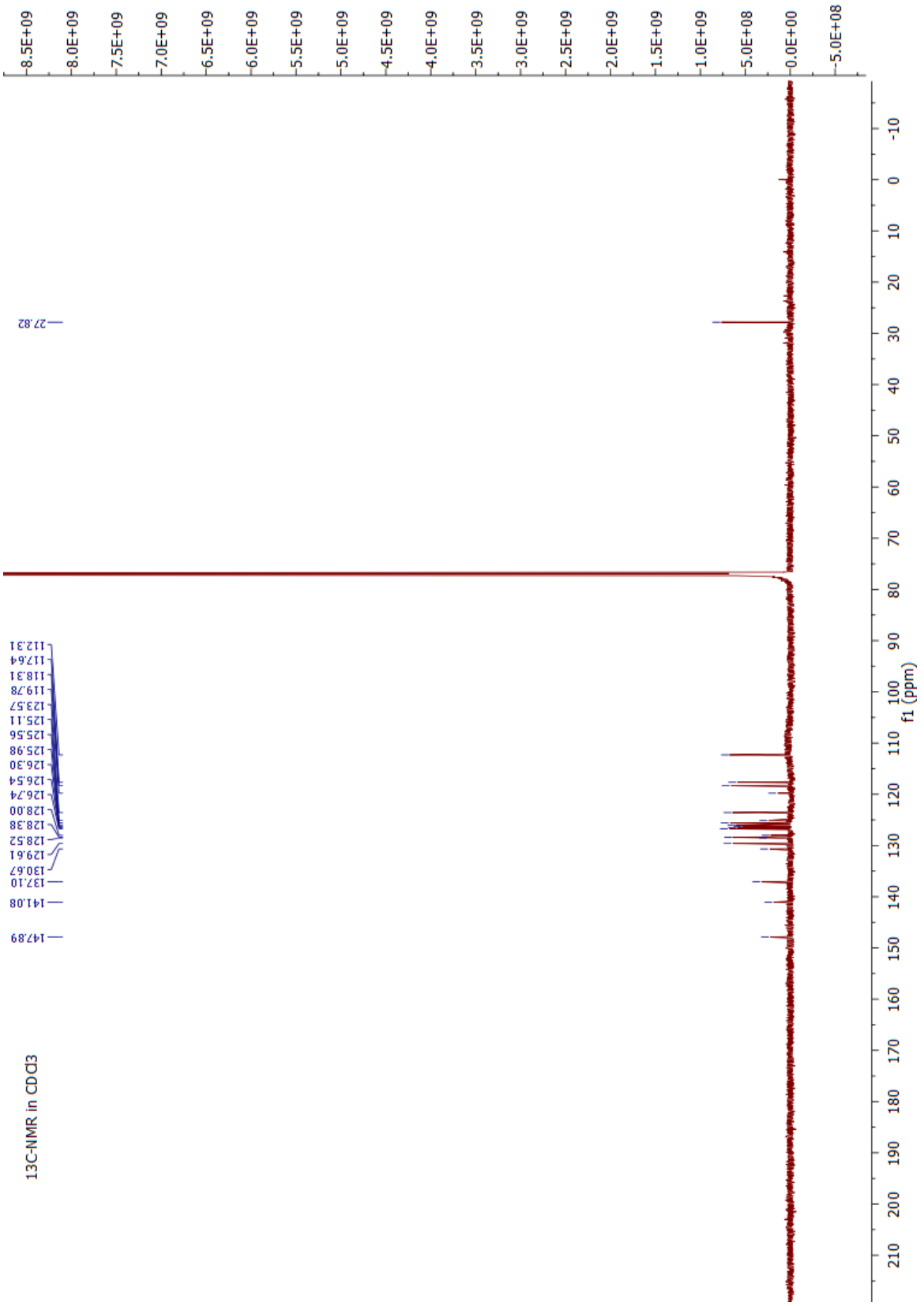
^{13}C NMR spectrum of compound 5i in $CDCl_3$



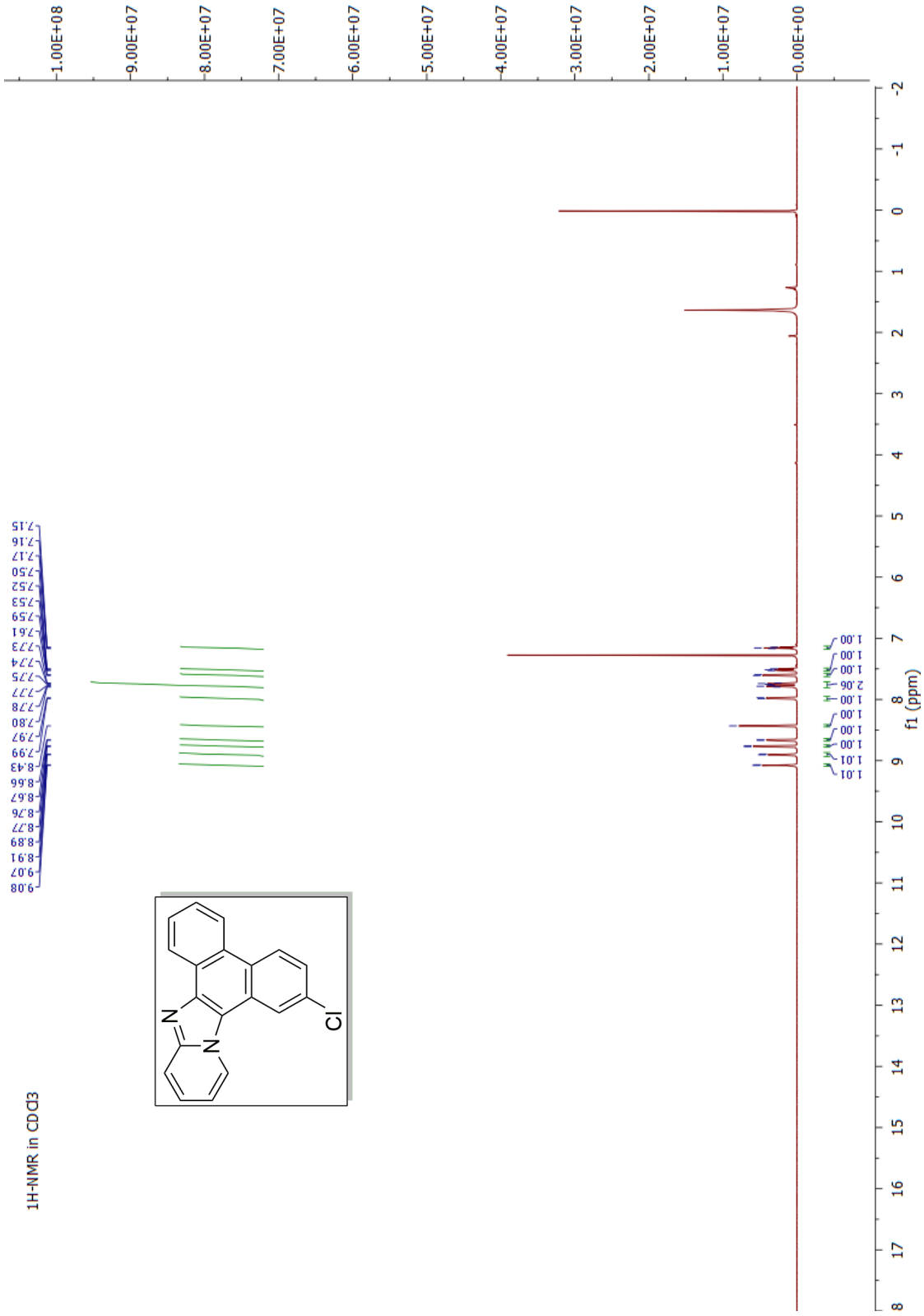
^{1}H NMR spectrum of compound 5j in $CDCl_3$



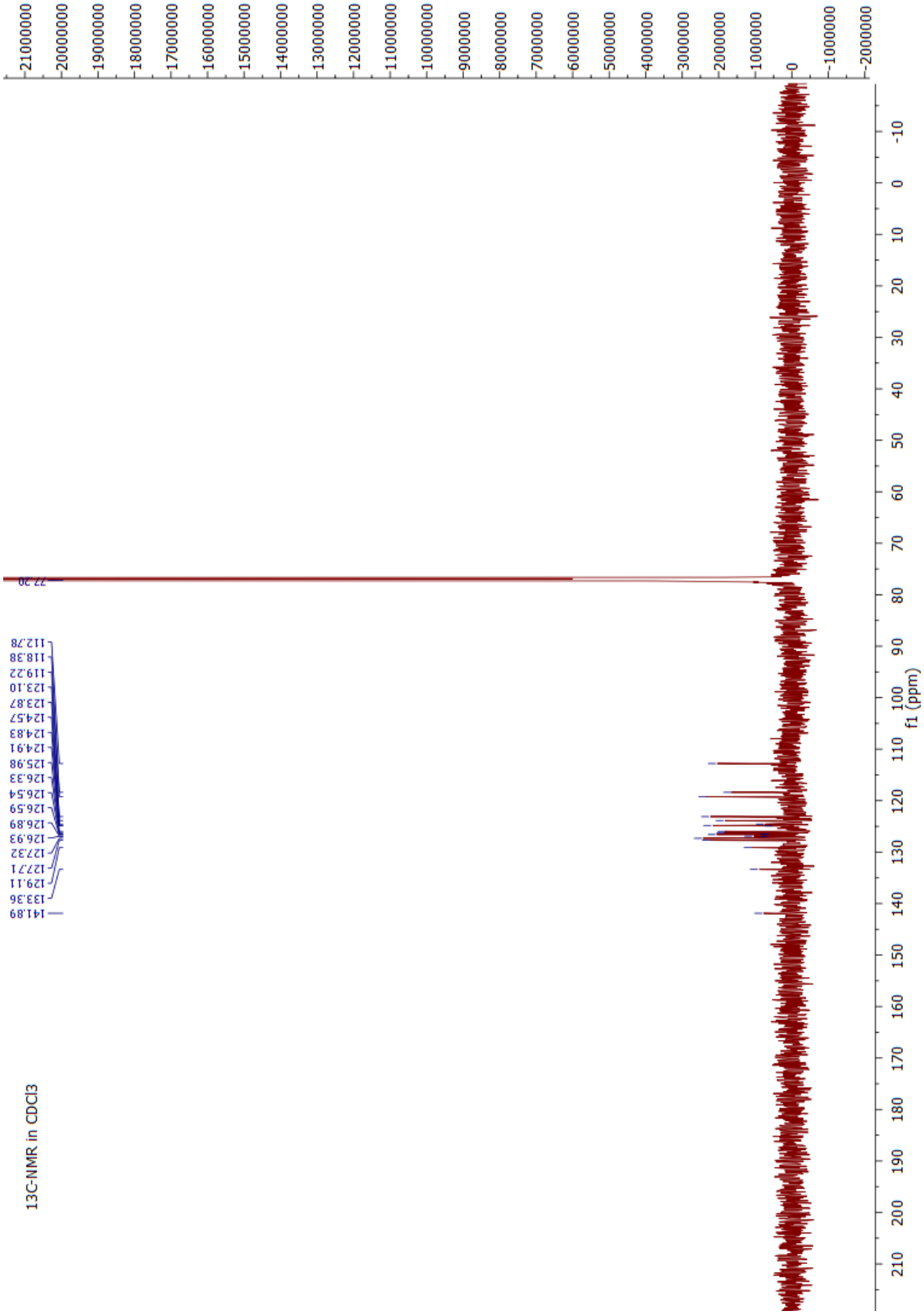
^{13}C NMR spectrum of compound 5j in $CDCl_3$



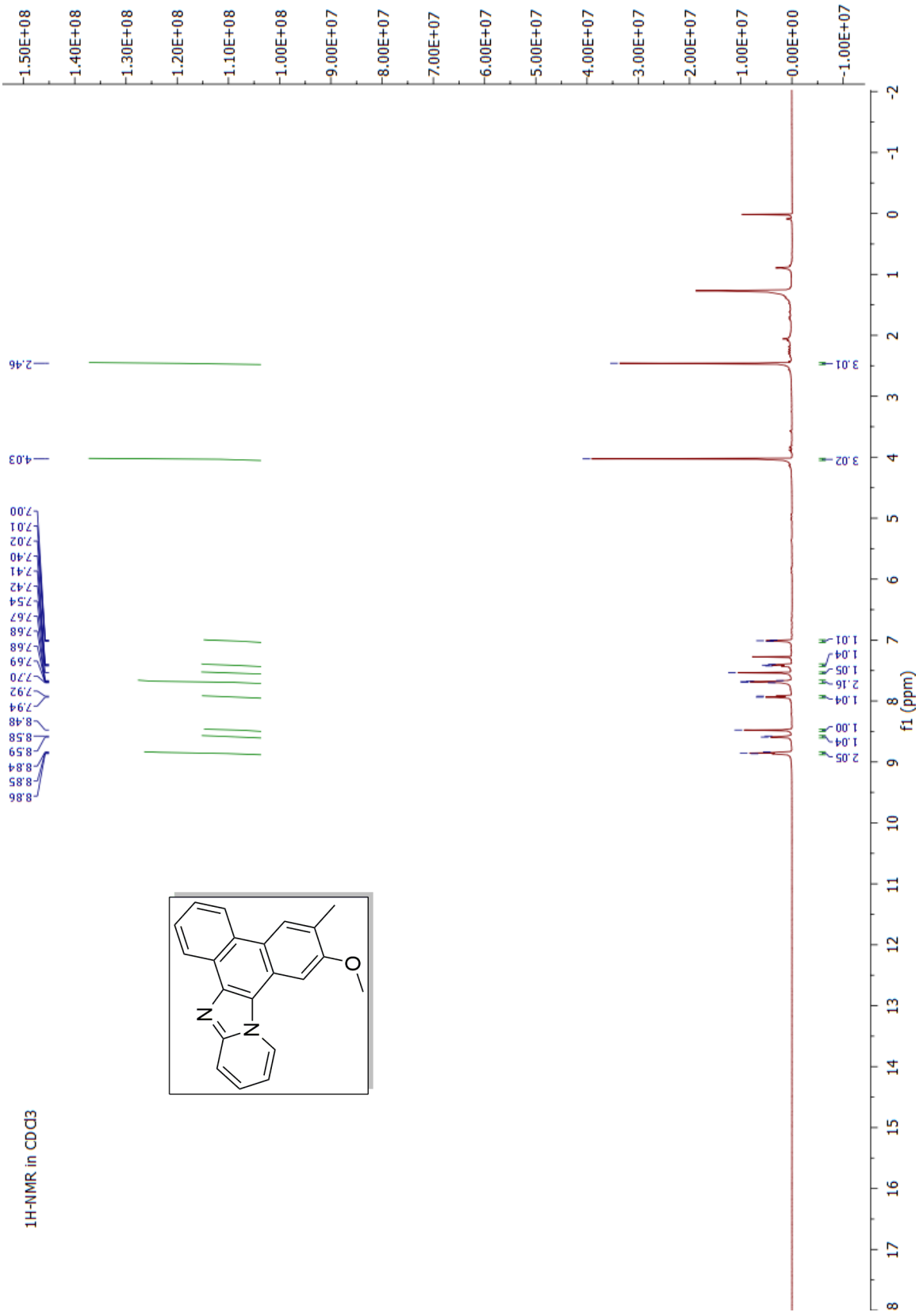
^{1}H NMR spectrum of compound 5k in $CDCl_3$



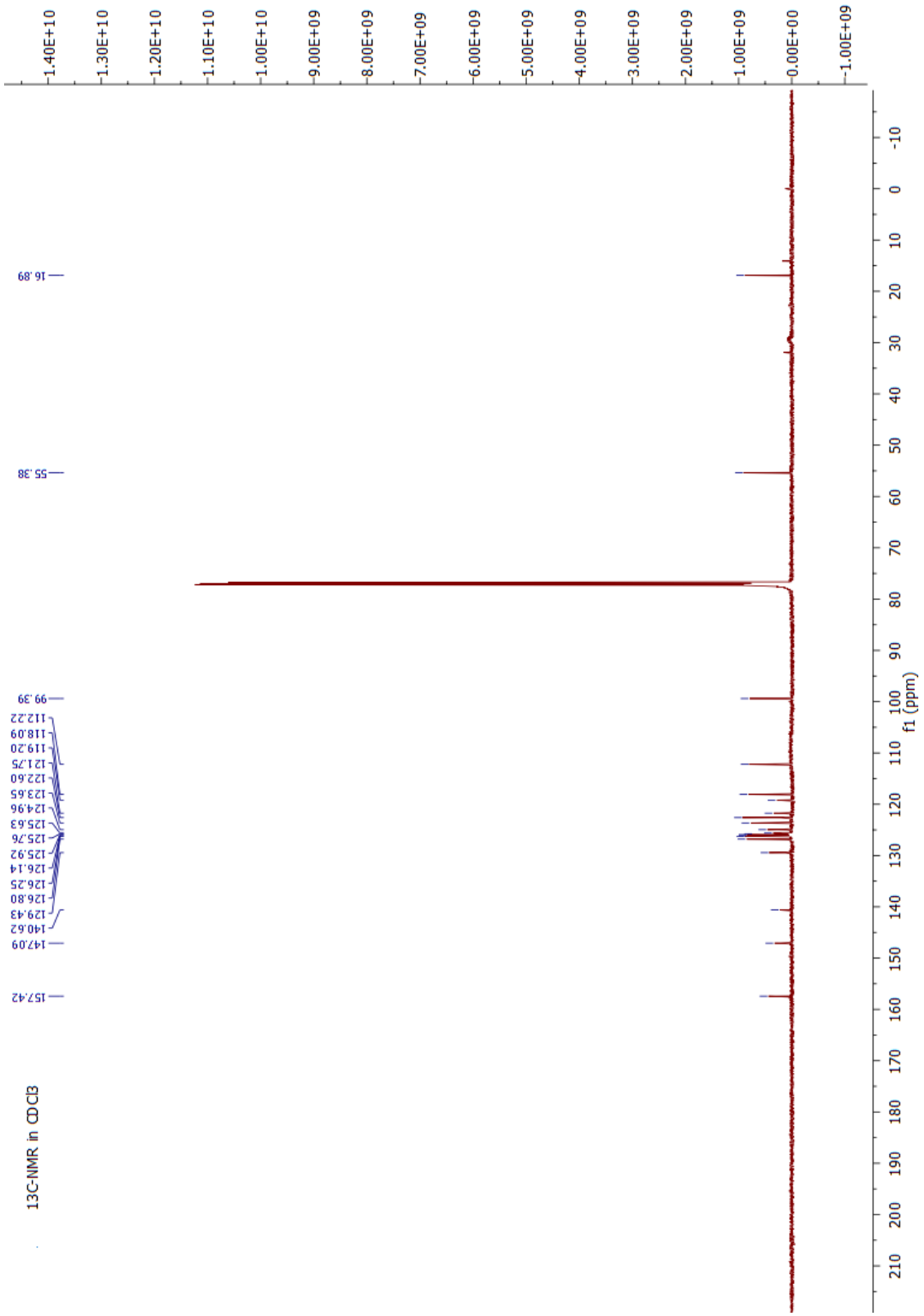
^{13}C NMR spectrum of compound 5k in $CDCl_3$



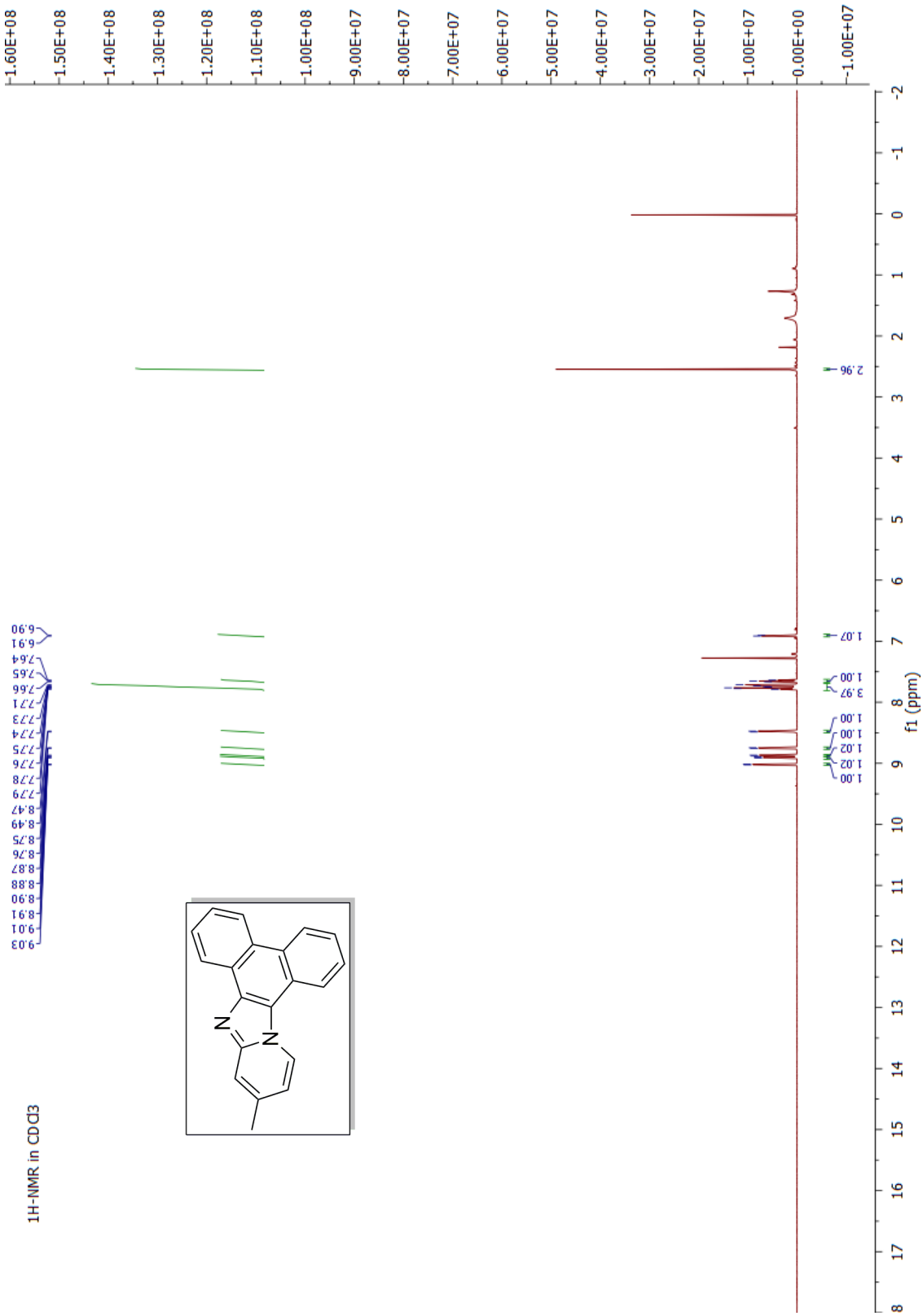
^{1}H NMR spectrum of compound 5l in $CDCl_3$



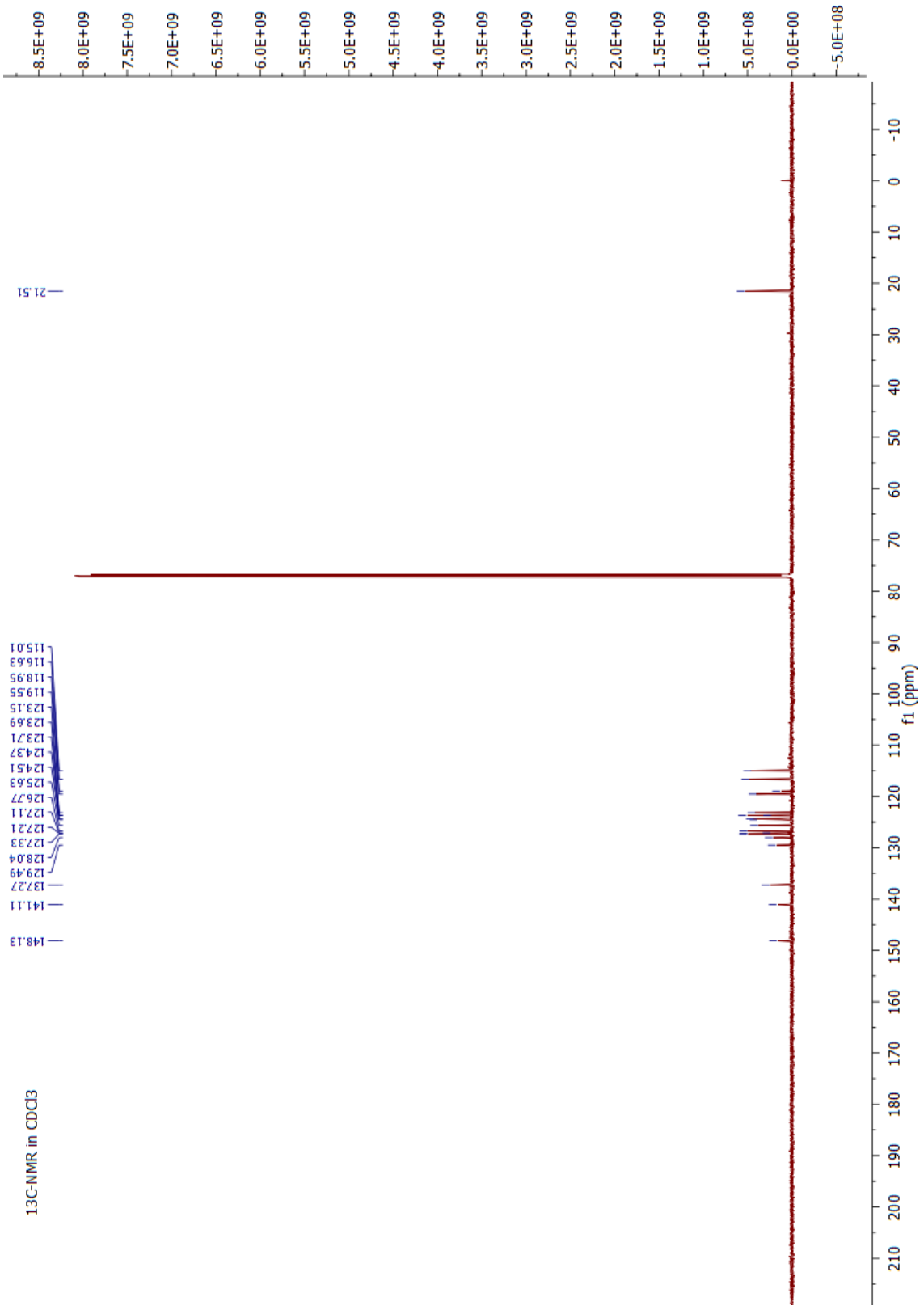
^{13}C NMR spectrum of compound 5l in $CDCl_3$



^{1}H NMR spectrum of compound 5m in $CDCl_3$



^{13}C NMR spectrum of compound 5m in $CDCl_3$



UV/Vis & Fluorescence study

For UV/Vis & Fluorescence study, 5μM of each compound solution was prepared in CH_2Cl_2 and then the respective spectrophotometers were used to record all the data.

Entry	Compound	λ_{max} (nm)	λ_{em} (nm)	Φ_F
1	5d	223	413	0.61
2	5e	224	416	0.44
3	5f	226	410	0.47
4	5j	228	414	0.35
5	5k	227	405	0.22

Table S1: Fluorescence quantum efficiency of the compounds (5 μM in CH_2Cl_2) determined by Phenanthrene (Φ_F = 0.125, λ_{ex} = 255 nm) as a standard.

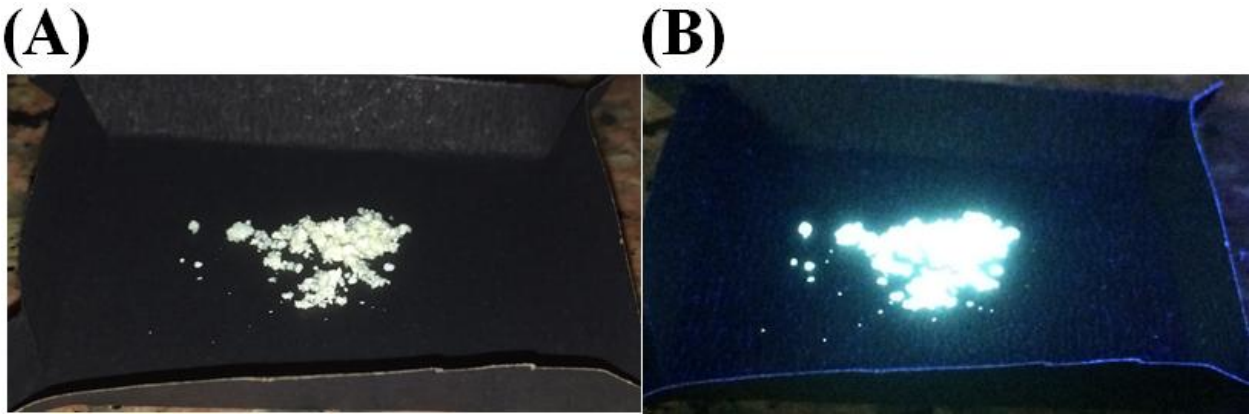


Figure S1: Solid state images of compound **5e** in **(A)** Normal light & **(B)** Under UV (365 nm)

Biological Study

Cell culture

Human hepatocellular liver carcinoma cells (HepG2) cell line (NCCS, Pune, India), were grown in DMEM supplemented with 10% FBS and antibiotics (penicillin-100 µg/ml; streptomycin-50 µg/ml). Cells were cultured at 37 ºC in 95% air, 5% CO_2 incubator.

Cell Cytotoxicity Assay

Cytotoxicity for the compounds **5d** and **5e** was determined using MTT assay. HepG2 cells (1×10^5 cells/well) were cultured in a 96-well plate at incubated at 37 °C, and were exposed to varying concentrations of the two compounds (1, 10, 20, 30, 40, 50, 60, 70, 80, 90 and 100 µM) for 24hrs. After the incubation, 10 µl of MTT solution [5 mg/ml, dissolved in 1X phosphate-buffered saline (PBS)] was added to each well of a 96-well culture plate, and then incubated at 37 ^{o}C for 4 hrs. Media were decanted from wells and 150µl of DMSO was added in each well and absorbance was measured at 550nm (EMax Precision MicroPlate Reader, Molecular Devices, USA). All experiments were performed in triplicate and the relative cell viability (%) was expressed as a percentage relative to the untreated control cells.

Cell Imaging Study

HepG2 Cells were culture in 35 x 10 mm culture dish on coverslip for 24h at 37 ^{o}C. The cells were allowed to incubate with 10µm solutions of the compounds **5d** and **5e,** prepared by dissolving it to the organic solvent DMSO. To characterize the intracellular fluorescence activity of the two compounds, HepG2 cells were preincubated with 10 µM ,20µM and 40µM of **5d** and **5e** for 60 min at 37 ^{o}C followed by washing twice with 1X PBS. Fluorescence images of HepG2

cells were taken by a fluorescence microscope (Leica DM3000, Germany) with an objective lens of 40X magnification.

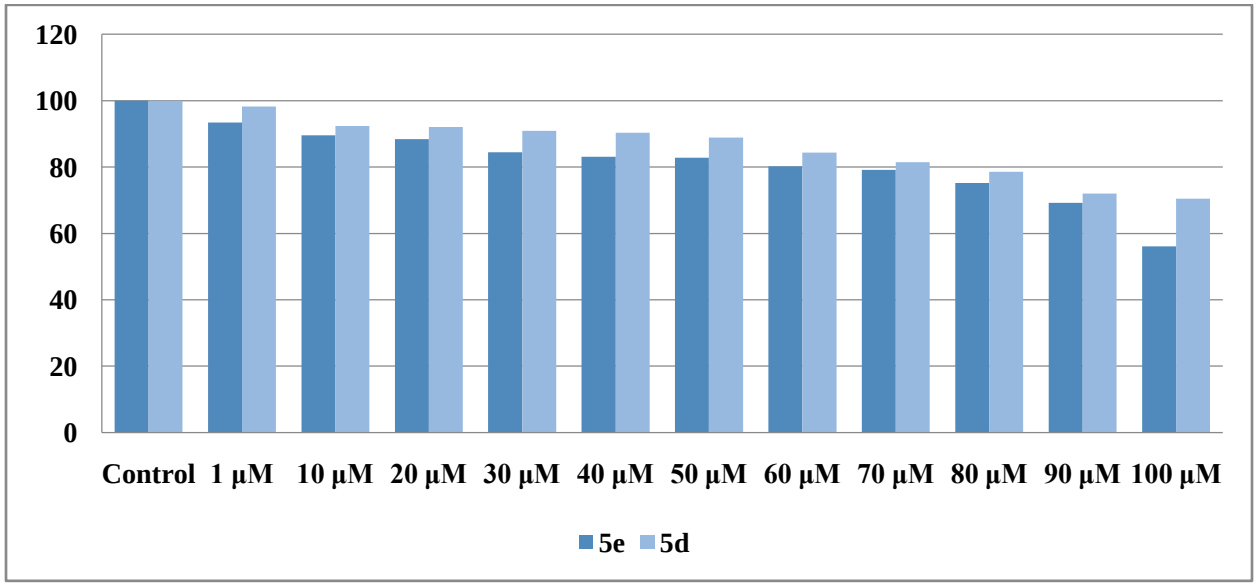


Figure S2: Cell viability curve for compound **5d** and **5e**

Cell imaging picture with compound 5d:

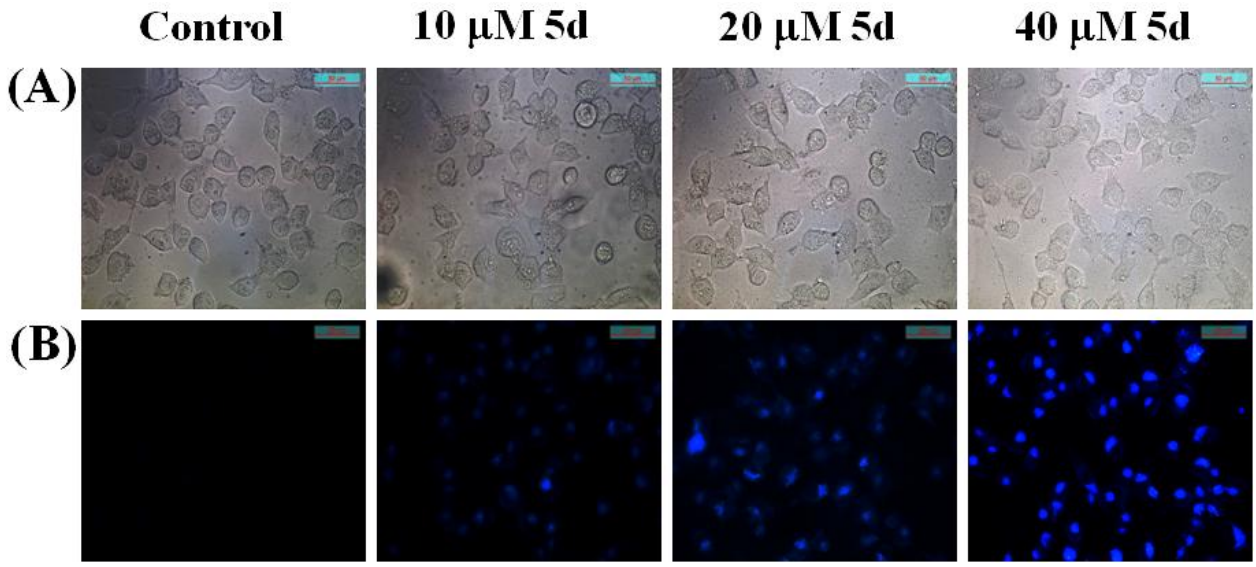


Figure S3: (A) Bright field & **(B)** Fluorescence images of HepG2 cells at 40X magnification after preincubation with 10 µM to 20µM to 40µM of **5d** for 60 min at 37 ^{o}C followed by washing twice with 1X PBS.

Cell imaging picture with compound 5e:

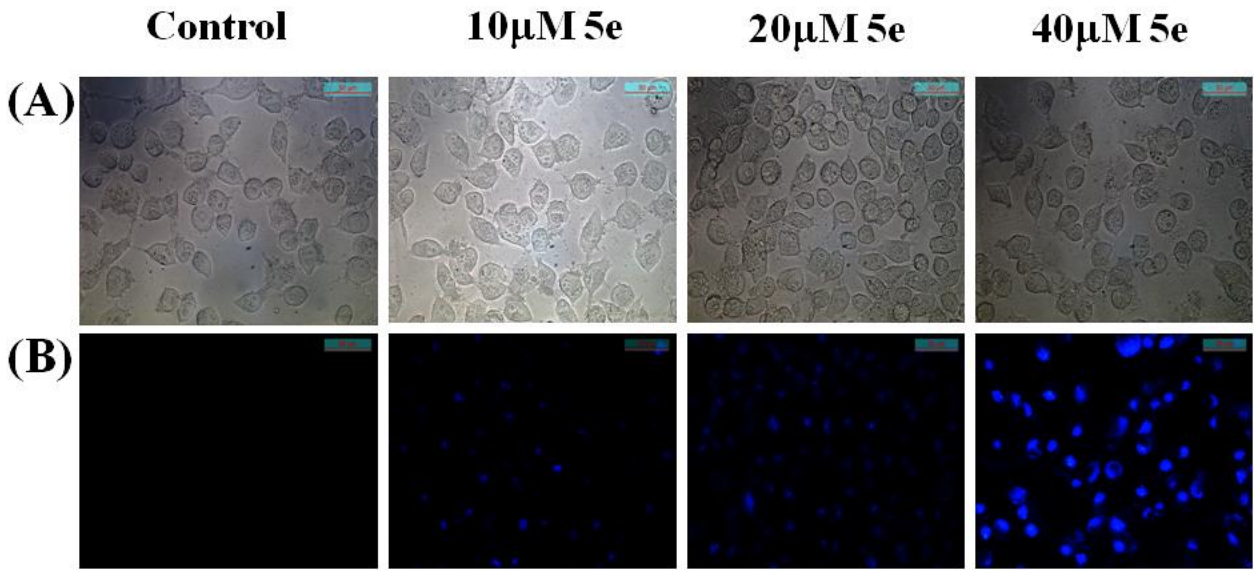


Figure S4: (A) Bright field & **(B)** Fluorescence images of HepG2 cells at 40X magnification after preincubation with 10 µM to 20µM to 40µM of **5e** for 60 min at 37 ^{o}C followed by washing twice with 1X PBS.