Supplementary Material

Multi-component reactions for the synthesis of current spiro-quinoxaline pyrrolizidine carboxylates *via* [3+2] cycloaddition reactions

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General Information:

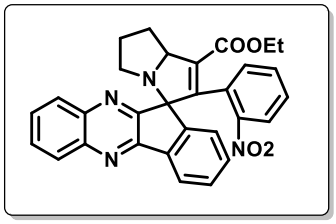
All substrates and reagents were readily and commercially available.TLC analysis was performed using pre-coated glass plates. Column chromatography was conducted using silica gel (60-120 mesh). All ^{1}H and ^{13}C NMR spectra were recorded in deuterated chloroform ($CDCl_3$) on Advance 300 or 400 or Avance 500 spectrometers. Chemical shift (δ) are reported in parts per million (ppm) relative to residual $CHCl_3$ (1H: δ 7.26 (ppm), ^{13}C: δ 77.00 (ppm) as an internal reference. Coupling constant (*j*) is reported in (HZ). Peak multiplicities are indicated as: s-singlet, t-triplet, q-quartet, m-multiplate and dd-doublet of doublet. Mass spectra were recorded by using 70 Ev spectrometer. High resolution mass spectrums (HRMS) were recorded using Applied Bio-sciences HRMS spectrometer at national center for mass spectroscopy.

Spectral data of Synthesized Compounds:

Ethyl 2'-phenyl-5',6',7',7a'-tetrahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine]-1'-carboxylate (5a) :

Compound purified by column chromatography with hexane :ethyl acetate (7:3), white solid **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.28 – 8.24 (m, 1H), 8.05 (d, *J* = 7.6 Hz, 1H), 7.73 – 7.69 (m, 2H), 7.59 – 7.48 (m, 4H), 6.92 (d, *J* = 7.4 Hz, 1H), 6.82 (t, *J* = 7.6 Hz, 2H), 6.52 (d, *J* = 7.3 Hz, 2H), 5.15 (dd, *J* = 9.2, 6.4 Hz, 1H), 4.07 (dt, *J* = 10.9, 3.7 Hz, 2H), 2.84 – 2.70 (m, 2H), 2.53 – 2.44 (m, 1H), 2.09 – 1.97 (m, 2H), 1.91 – 1.84 (m, 1H), 1.02 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 176.05, 153.18, 143.72, 142.70, 142.36, 138.25, 134.84, 133.42, 130.90, 130.12, 130.02, 129.70, 128.97, 128.88, 128.42, 127.86, 127.78, 127.51, 127.15, 122.75, 84.43, 73.03, 60.29, 48.41, 32.92, 27.85, 14.15, 13.79.

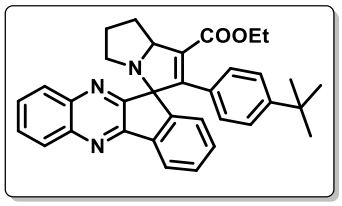
Ethyl 2'-(2-nitrophenyl)-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine]-1'-carboxylate (5b) :



Yield 74% (373 mg), Compound purified by column chromatography with hexane :ethyl acetate (6:4), White solid. mp: 185-187 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.21 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.12 (dd, *J* = 8.1, 1.5 Hz, 1H), 8.07 – 8.04 (m, 1H), 7.83 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.79 – 7.72 (m, 3H), 7.48 – 7.40 (m, 2H), 7.17 – 7.12 (m, 1H), 6.96 (td, *J* = 7.7, 1.1 Hz, 1H), 6.26 (dd, *J* = 7.8, 1.2 Hz, 1H), 5.29 (t, *J* = 7.3 Hz, 1H), 4.14 – 4.03 (m, 2H), 3.32 (td, *J* = 9.7, 5.5 Hz, 1H), 2.78 – 2.73 (m, 1H), 2.48 (dt,

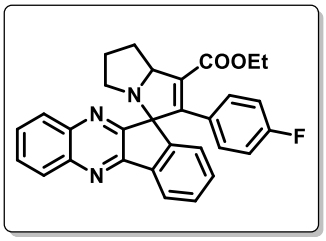
J = 12.5, 7.5 Hz, 1H), 2.09 – 2.00 (m, 2H), 1.91 (ddd, *J* = 17.1, 12.0, 5.1 Hz, 1H), 1.05 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.49, 163.37, 153.09, 148.22, 146.20, 142.98, 142.25, 142.00, 138.47, 138.16, 132.42, 131.27, 130.19, 130.11, 129.97, 129.71, 129.09, 129.09, 128.95, 128.45, 128.41, 124.47, 122.40, 83.55, 71.34, 60.64, 50.47, 31.21, 26.43, 13.73. **HRMS:** (ESI) m/z for $C_{30}H_{24}N_4O_4$ $[M+H]^+$: calcd: 505.1394, found: 505.1385.

Ethyl 2'-(4-(tert-butyl)phenyl)-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine]-1'-carboxylate (5c) :



Yield 90% (464 mg), Compound purified by column chromatography with hexane : ethyl acetate (7:3), White solid. mp: 166-168 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.05 – 8.00 (m, 2H), 7.81 (s, 1H), 7.54 – 7.47 (m, 3H), 6.85 – 6.81 (m, 2H), 6.47 – 6.43 (m, 2H), 5.11 (dd, *J* = 9.3, 6.3 Hz, 1H), 4.10 – 4.00 (m, 2H), 2.72 (ddt, *J* = 13.4, 10.5, 6.5 Hz, 2H), 2.48 (t, 3H), 2.08 – 1.82 (m, 3H), 1.06 (s, 9H), 0.97 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.19, 164.09, 153.32, 152.80, 150.33, 144.01, 142.69, 142.42, 138.29, 134.88, 130.93, 130.30, 130.20, 129.98, 129.67, 128.89, 128.83, 128.36, 127.80, 127.58, 124.90, 124.09, 122.72, 84.30, 72.96, 60.20, 48.41, 34.30, 32.88, 31.07, 29.73, 27.77, 22.72, 13.68. **HRMS:** (ESI) m/z for $C_{34}H_{23}N_3O_2$ $[M+H]^+$: calcd: 516.1237, found: 516.1234.

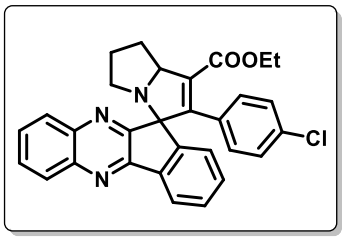
Ethyl 2'-(4-fluorophenyl)-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine]-1'-carboxylate (5d) :



Yield 83% (396 mg), Compound purified by column chromatography with hexane : ethyl acetate (7:3)**,** White solid. mp: 134-136 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.28 – 8.22 (m, 1H), 8.11 – 8.05 (m, 2H), 7.75 – 7.69 (m, 2H), 7.54 (ddd, *J* = 10.1, 7.9, 5.4 Hz, 3H), 6.56 – 6.48 (m, 4H), 4.09 (dddd, *J* = 18.0, 14.2, 7.1, 3.8 Hz, 2H), 3.48 (q, *J* = 7.0 Hz, 1H), 2.84 – 2.78 (m, 1H), 2.72 (ddd, *J* = 10.6, 8.0, 3.0 Hz, 1H), 2.52 – 2.45 (m, 1H), 2.12 – 1.98 (m, 2H), 1.85 (ddd, *J* = 19.0, 6.6, 4.1 Hz, 1H), 1.06 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.68, 163.07, 161.11, 153.09, 152.00, 143.58,

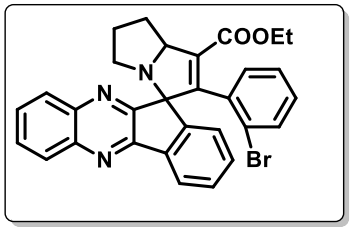
142.74, 142.34, 138.27, 135.25, 130.99, 130.07, 129.83, 129.74, 129.67, 129.03, 128.99, 127.64, 122.86, 114.40, 114.22, 84.41, 73.03, 65.88, 60.41, 48.34, 32.92, 27.87, 15.30, 13.86 . **HRMS:** (ESI) m/z for $C_{30}H_{24}FN_3O_2$ $[M+H]^+$: calcd: 478.2169, found: 478.2160.

Ethyl 2'-(4-chlorophenyl)-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine]-1'-carboxylate (5e) :



Yield 82% (405 mg), Compound purified by column chromatography with hexane : ethyl acetate (7:3) White solid. mp: 174-177 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.27 – 8.23 (m, 1H), 8.10 – 8.04 (m, 2H), 7.75 – 7.70 (m, 2H), 7.60 – 7.50 (m, 3H), 6.84 – 6.79 (m, 2H), 6.49 – 6.44 (m, 2H), 5.13 (dd, *J* = 9.5, 6.3 Hz, 1H), 4.09 (dddd, *J* = 18.0, 10.9, 7.1, 3.7 Hz, 2H), 2.79 (dd, *J* = 9.0, 7.4 Hz, 1H), 2.74 – 2.68 (m, 1H), 2.52 – 2.45 (m, 1H), 2.13 – 1.98 (m, 2H), 1.90 – 1.80 (m, 1H), 1.07 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.58, 153.06, 151.86, 143.43, 142.74, 142.31, 138.23, 135.33, 133.62, 131.88, 131.04, 130.23, 130.07, 129.89, 129.27, 129.04, 127.64, 127.53, 127.61, 127.60, 127.62, 122.92, 122.93, 84.34, 73.08, 60.50, 48.33, 32.94, 27.91, 13.89. **HRMS:** (ESI) m/z for $C_{30}H_{24}ClN_3O_2$ $[M+H]^+$: calcd: 494.1649, found: 494.1640.

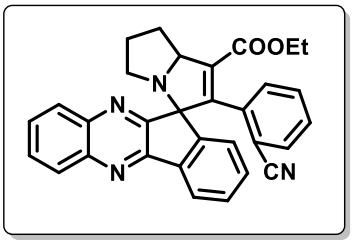
Ethyl 2'-(2-bromophenyl)-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine]-1'-carboxylate (5f) :



Yield 78% (419 mg), Compound purified by column chromatography with hexane : ethyl acetate (7:3) White solid. mp: 189-192 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.28 – 8.22 (m, 1H), 8.07 (ddd, *J* = 10.0, 4.2, 1.8 Hz, 2H), 7.76 – 7.69 (m, 2H), 7.61 – 7.47 (m, 4H), 7.00 – 6.94 (m, 2H), 6.45 – 6.37 (m, 2H), 5.13 (dd, *J* = 9.5, 6.3 Hz, 1H), 4.09 (dddd, *J* = 18.0, 10.9, 7.1, 3.7 Hz, 2H), 2.84 – 2.68 (m, 2H), 2.53 – 2.44 (m, 1H), 2.13 – 1.97 (m, 2H), 1.90 – 1.81 (m, 1H), 1.08 (t, 3H). **^{13}C NMR** (126 MHz,

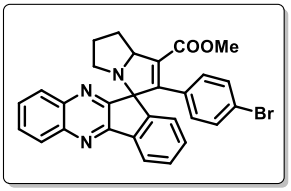
$CDCl_3$) δ 164.04, 163.55, 153.03, 152.16, 143.37, 142.76, 142.31, 138.27, 134.96, 132.18, 131.31, 131.03, 130.54, 130.25, 130.05, 129.88, 129.47, 129.05, 128.82, 127.60, 126.48, 122.94, 122.09, 84.23, 73.01, 51.63, 48.37, 32.87, 29.72, 27.82. **HRMS:** (ESI) m/z for $C_{30}H_{24}BrN_3O_2$ $[M+H]^+$: calcd: 538.1394, found: 538.1385.

Ethyl 2'-(2-cynophenyl)-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine]-1'-carboxylate (5g) :



Yield 75% (363 mg) Compound purified by column chromatography with hexane : ethyl acetate (7:3) White solid. mp: 180-185 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.32 – 8.26 (m, 1H), 8.15 – 8.10 (m, 1H), 8.01 (d, *J* = 7.5 Hz, 1H), 7.83 – 7.74 (m, 3H), 7.54 (t, *J* = 7.3 Hz, 1H), 7.49 – 7.38 (m, 2H), 7.07 (t, *J* = 7.6 Hz, 1H), 6.93 (t, *J* = 7.6 Hz, 1H), 6.22 (d, *J* = 7.8 Hz, 1H), 5.20 (t, *J* = 7.4 Hz, 1H), 4.22 – 4.11 (m, 2H), 3.03 – 2.94 (m, 1H), 2.77 – 2.70 (m, 1H), 2.54 (dt, *J* = 10.3, 7.1 Hz, 1H), 2.14 – 1.96 (m, 3H), 1.10 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.66, 162.86, 153.37, 147.21, 142.98, 142.34, 142.29, 138.90, 137.73, 137.36, 132.22, 131.79, 131.25, 130.25, 130.16, 130.09, 129.16, 129.12, 128.74, 127.96, 126.77, 122.49, 118.41, 113.53, 84.33, 72.68, 60.81, 49.38, 32.69, 27.22, 13.80. **HRMS:** (ESI) m/z for $C_{31}H_{24}N_4O_2$ $[M+H]^+$: calcd: 485.1394, found: 485.1385.

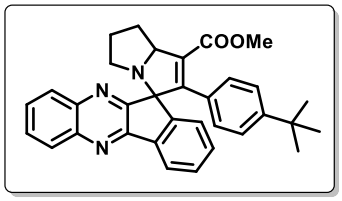
Methyl 2'-(4-bromophenyl)-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine]-1'-carboxylate (5h) :



Yield 82% (429 mg) Compound purified by column chromatography with hexane : ethyl acetate (7:3) White solid. mp: 154-156°C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.26 – 8.21 (m, 1H), 8.10 – 8.05 (m, 2H), 7.75 – 7.69 (m, 2H), 7.61 – 7.47 (m, 4H), 6.99 – 6.96 (m, 2H), 6.42 – 6.39 (m, 2H), 5.13 (dd, *J* = 9.5, 6.3 Hz, 1H), 3.65 (s, 3H), 2.84 – 2.77 (m, 1H), 2.73 – 2.68 (m, 1H), 2.51 – 2.43 (m, 1H), 2.14 – 2.05 (m, 1H), 2.04 – 1.97 (m, 1H), 1.89 – 1.80 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.04,

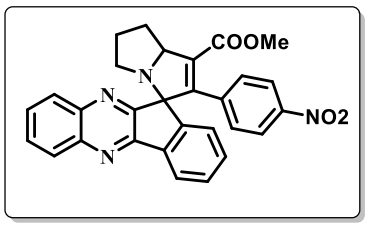
163.55, 153.03, 152.17, 143.36, 142.76, 142.31, 138.27, 134.95, 132.18, 131.04, 130.54, 130.26, 130.05, 129.89, 129.48, 129.06, 127.61, 122.95, 122.10, 84.23, 73.02, 51.64, 48.38, 32.88, 27.82. **HRMS:** (ESI) m/z for $C_{29}H_{22}BrN_3O_2$ $[M+H]^+$: calcd: 524.1494, found: 524.1485.

Methyl 2'-(4-tert-butylphenyl)-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine]-1'-carboxylate (5i) :



Yield 85% (426 mg) Compound purified by column chromatography with hexane : ethyl acetate (7:3) White solid. mp: 170-174 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 – 7.99 (m, 2H), 7.81 (s, 1H), 7.55 – 7.47 (m, 3H), 6.84 – 6.81 (m, 2H), 6.47 – 6.43 (m, 2H), 5.11 (dd, *J* = 9.3, 6.3 Hz, 1H), 4.09 – 4.01 (m, 1H), 2.78 – 2.74 (m, 1H), 2.71 – 2.65 (m, 1H), 2.49 (q, 3H), 2.48 (s, 2H), 2.08 – 1.96 (m, 1H), 1.86 – 1.81 (m, 1H), 1.06 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 164.13, 163.18, 153.11, 152.42, 150.21, 143.74, 141.45, 141.26, 140.01, 139.18, 138.60, 134.70, 130.44, 129.83, 129.46, 128.16, 127.69, 127.57, 127.57, 124.02, 124.02, 122.39, 84.30, 72.93, 60.15, 48.36, 34.28, 32.91, 31.08, 27.78, 20.32, 20.28, 13.68. **HRMS:** (ESI) m/z for $C_{33}H_{32}N_3O_2$ $[M+H]^+$: calcd: 502.1294, found: 502.1285.

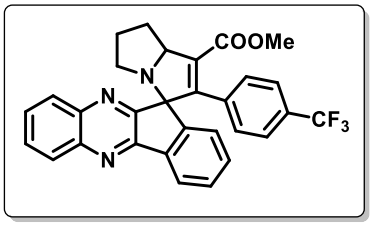
Methyl 2'-(4-nitrophenyl)-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine]-1'-carboxylate (5j) :



Yield 75% (368 mg) Compound purified by column chromatography with hexane : ethyl acetate (6:4) White solid. mp: 203-206 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.28 – 8.23 (m, 1H), 8.10 – 8.04 (m, 2H), 7.76 – 7.70 (m, 4H), 7.63 – 7.52 (m, 3H), 6.75 – 6.70 (m, 2H), 3.65 (d, *J* = 5.0 Hz, 3H), 3.48 (q, *J* = 7.0 Hz, 1H), 2.87 – 2.80 (m, 1H), 2.73 (ddd, *J* = 10.6, 7.9, 3.1 Hz, 1H), 2.50 (ddd, *J* = 8.9, 6.6, 3.4 Hz, 1H), 2.08 (dddd, *J* = 15.7, 10.8, 5.8, 2.6 Hz, 2H), 1.88 (ddd, *J* = 14.8, 10.8, 5.5 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.62, 163.02, 152.80, 151.22, 147.13, 142.83, 142.28, 140.37, 138.24, 135.96, 131.18, 130.54, 130.13, 130.00, 130.10, 129.28, 129.13, 128.97, 128.97, 127.54, 123.09,

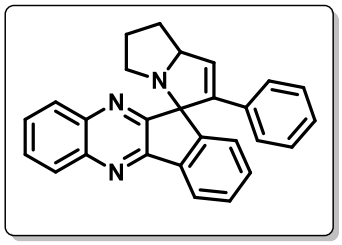
123.09, 122.58, 84.24, 73.12, 51.82, 48.38, 32.85, 27.88. **HRMS:** (ESI) m/z for $C_{29}H_{23}N_4O_4$ $[M+H]^+$: calcd: 491.1260, found: 491.1250.

Methyl 2'-(4-(trifluoromethyl)phenyl)-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine]-1'-carboxylate(5k) :



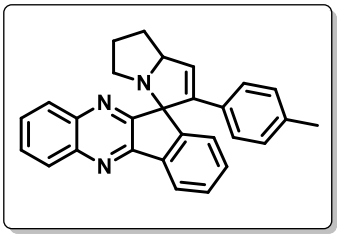
Yield 70% (359 mg) Compound purified by column chromatography with hexane : ethyl acetate (7:3) White solid. mp: 190-194 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.27 – 8.23 (m, 1H), 8.07 (ddd, *J* = 8.7, 5.5, 3.2 Hz, 2H), 7.72 (ddd, *J* = 8.6, 5.0, 2.2 Hz, 2H), 7.60 – 7.52 (m, 3H), 7.11 (d, *J* = 8.3 Hz, 2H), 6.67 (d, *J* = 8.1 Hz, 2H), 5.16 (dd, *J* = 9.5, 6.3 Hz, 1H), 3.64 (s, 3H), 2.84 – 2.78 (m, 1H), 2.72 (ddd, *J* = 10.6, 8.0, 3.0 Hz, 1H), 2.52 – 2.46 (m, 1H), 2.14 – 2.07 (m, 1H), 2.03 – 1.98 (m, 1H), 1.91 – 1.83 (m, 1H). **^{13}C NMR** (101 MHz) δ 163.87, 163.37, 152.98, 151.90, 143.16, 142.79, 142.32, 138.25, 137.08, 135.48, 131.06, 130.35, 130.06, 129.96, 129.78, 129.46, 129.11, 129.08, 128.27, 127.59, 124.29, 124.26, 122.98, 84.27, 73.03, 51.69, 48.37, 32.87, 27.84, 14.22. 130.6 (1C, q, $J^{13}C$-^{19}F =3.9 Hz) **HRMS:** (ESI) m/z for $C_{30}H_{23}O_2N_3F_3$ $[M+H]^+$: calcd: 514.1748, found: 514.1736.

2'-phenyl-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine] (5l) :



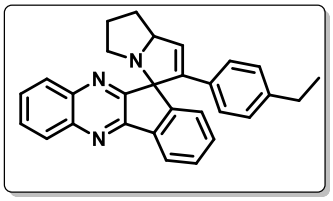
Yield 79% (383 mg) Compound purified by column chromatography with hexane : ethyl acetate (8:2) White solid. mp: 145-150 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 7.3 Hz, 1H), 8.13 (ddd, *J* = 11.5, 8.0, 1.0 Hz, 2H), 7.68 (ddt, *J* = 8.2, 6.9, 5.4 Hz, 2H), 7.55 – 7.45 (m, 2H), 7.36 (d, *J* = 7.5 Hz, 1H), 6.95 – 6.89 (m, 2H), 6.75 (d, *J* = 2.0 Hz, 1H), 6.71 – 6.67 (m, 2H), 4.90 (t, *J* = 7.0 Hz, 1H), 2.72 (dd, *J* = 8.7, 7.0 Hz, 1H), 2.62 – 2.56 (m, 1H), 2.21 (ddd, *J* = 14.4, 7.0, 3.5 Hz, 1H), 1.97 – 1.88 (m, 2H), 1.83 – 1.69 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 165.21, 153.32, 145.38, 142.75, 142.45, 141.56, 138.15, 133.62, 132.84, 131.16, 130.17, 129.81, 129.46, 128.91, 128.74, 128.07, 128.07, 127.58, 127.33, 126.43, 126.43, 122.79, 80.83, 71.62, 49.00, 32.00, 27.49. **HRMS:** (ESI) m/z for $C_{27}H_{21}N_3$ $[M+H]^+$: calcd: 388.1394, found: 388.1385.

2'-(p-tolyl)-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine] (5m) :



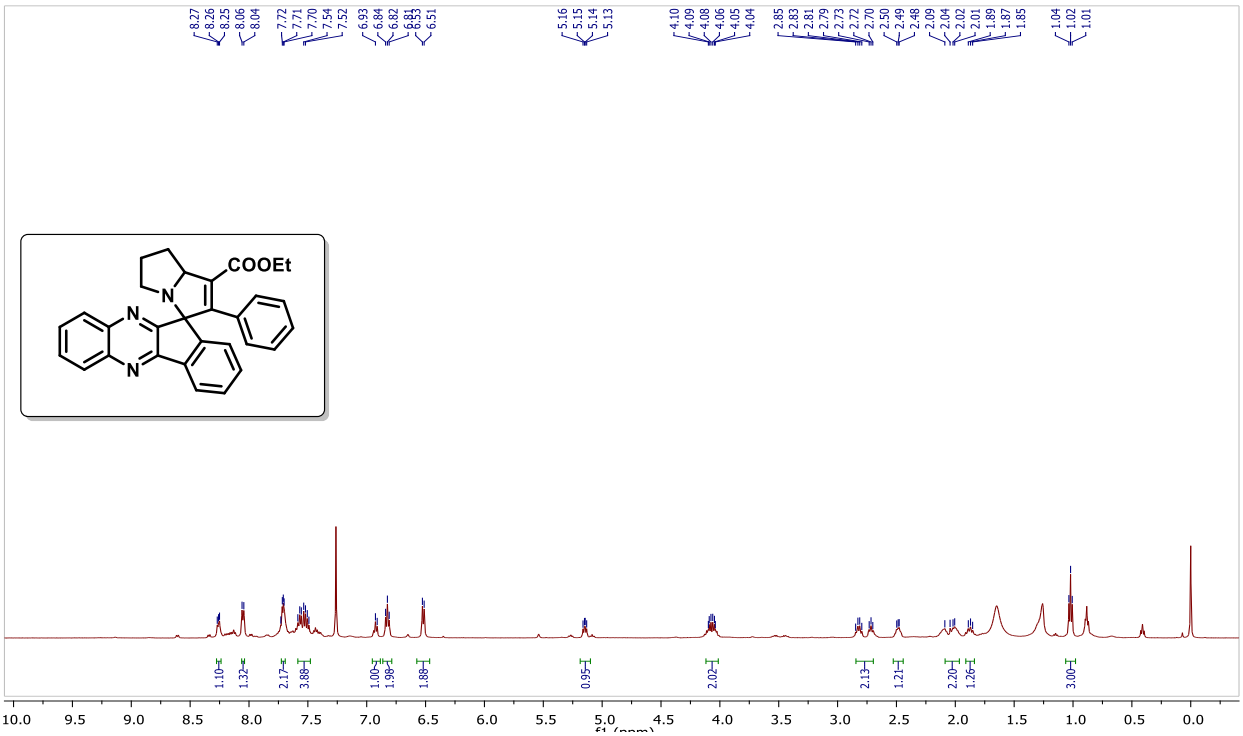
Yield 80% (321 mg) Compound purified by column chromatography with hexane : ethyl acetate (8:2) White solid. mp: 160-164 °C; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.23 (d, *J* = 7.1 Hz, 1H), 8.13 (td, *J* = 8.2, 1.1 Hz, 2H), 7.73 – 7.62 (m, 2H), 7.50 (dtd, *J* = 20.7, 7.3, 1.1 Hz, 2H), 7.36 (d, *J* = 7.3 Hz, 1H), 6.73 – 6.69 (m, 2H), 6.58 (d, *J* = 8.2 Hz, 2H), 4.88 (t, *J* = 6.9 Hz, 1H), 2.71 (dd, *J* = 16.4, 9.3 Hz, 1H), 2.58 (ddd, *J* = 10.5, 7.1, 3.7 Hz, 1H), 2.27 – 2.15 (m, 1H), 2.08 (s, 3H), 1.93 (ddd, *J* = 18.4, 11.0, 6.0 Hz, 2H), 1.70 (dd, *J* = 20.5, 9.2 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 165.35, 153.35, 145.58, 142.74, 142.48, 141.41, 138.14, 137.11, 131.91, 131.17, 130.70, 130.20, 129.77, 129.42, 128.89, 128.80, 128.80, 128.70, 127.58, 126.29, 126.29, 122.76, 80.84, 71.65, 48.95, 32.10, 27.54, 20.95. **HRMS:** (ESI) m/z for $C_{28}H_{23}N_3$ $[M+H]^+$: calcd: 402.1394, found: 402.1385.

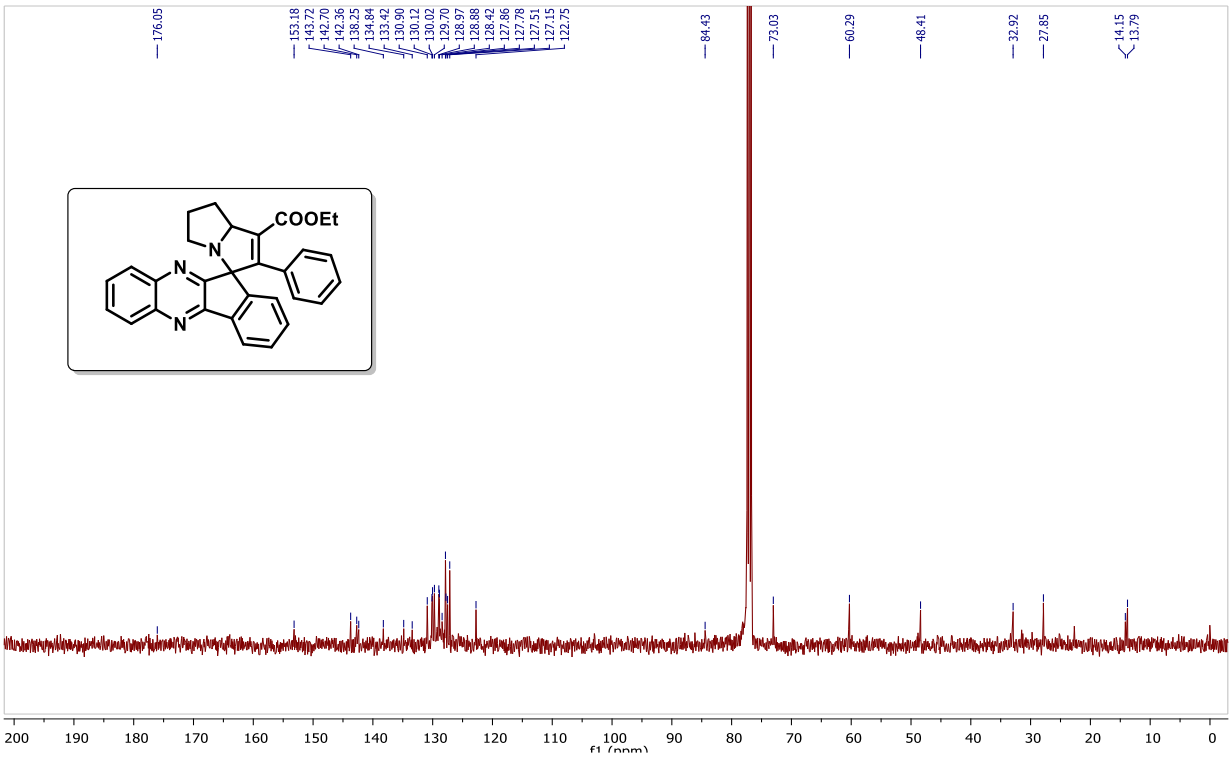
2'-(4-ethylphenyl)-5',6',7',7a'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,3'-pyrrolizine] (5n) :



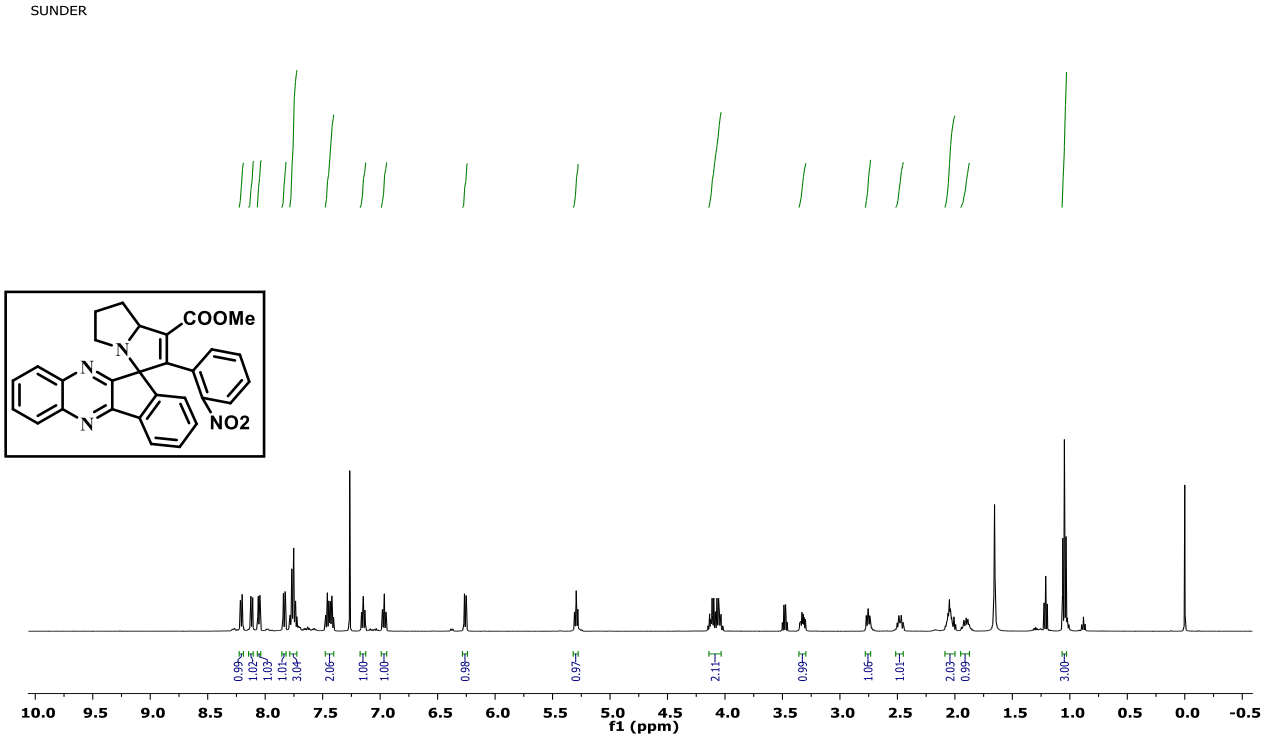
Yield 81% (336 mg) Compound purified by column chromatography with hexane : ethyl acetate (8:2) White solid. mp: 137-140 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 7.5 Hz, 1H), 8.15 – 8.11 (m, 2H), 7.67 (ddd, *J* = 7.8, 7.1, 1.0 Hz, 2H), 7.55 – 7.51 (m, 1H), 7.49 – 7.45 (m, 1H), 7.37 (d, *J* = 7.5 Hz, 1H), 6.72 (d, *J* = 2.1 Hz, 2H), 6.61 (d, *J* = 8.3 Hz, 2H), 4.97 – 4.86 (m, 1H), 2.72 (dd, *J* = 16.5, 9.3 Hz, 1H), 2.63 – 2.56 (m, 1H), 2.41 – 2.34 (m, 2H), 2.20 (ddd, *J* = 14.5, 7.0, 3.5 Hz, 1H), 1.99 – 1.85 (m, 2H), 1.72 (dt, *J* = 17.7, 8.0 Hz, 1H), 1.20 (d, *J* = 7.6 Hz, 1H), 1.02 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.33, 145.55, 144.23, 143.41, 142.74, 142.46, 141.31, 138.17, 136.70, 131.91, 131.19, 130.20, 129.82, 129.45, 128.90, 128.72, 127.60, 127.60, 126.31, 126.31, 122.81, 80.78, 71.59, 48.99, 32.05, 29.73, 28.28, 15.08. **HRMS:** (ESI) m/z for $C_{29}H_{25}N_3$ $[M+H]^+$: calcd: 416.1394, found: 416.1385.

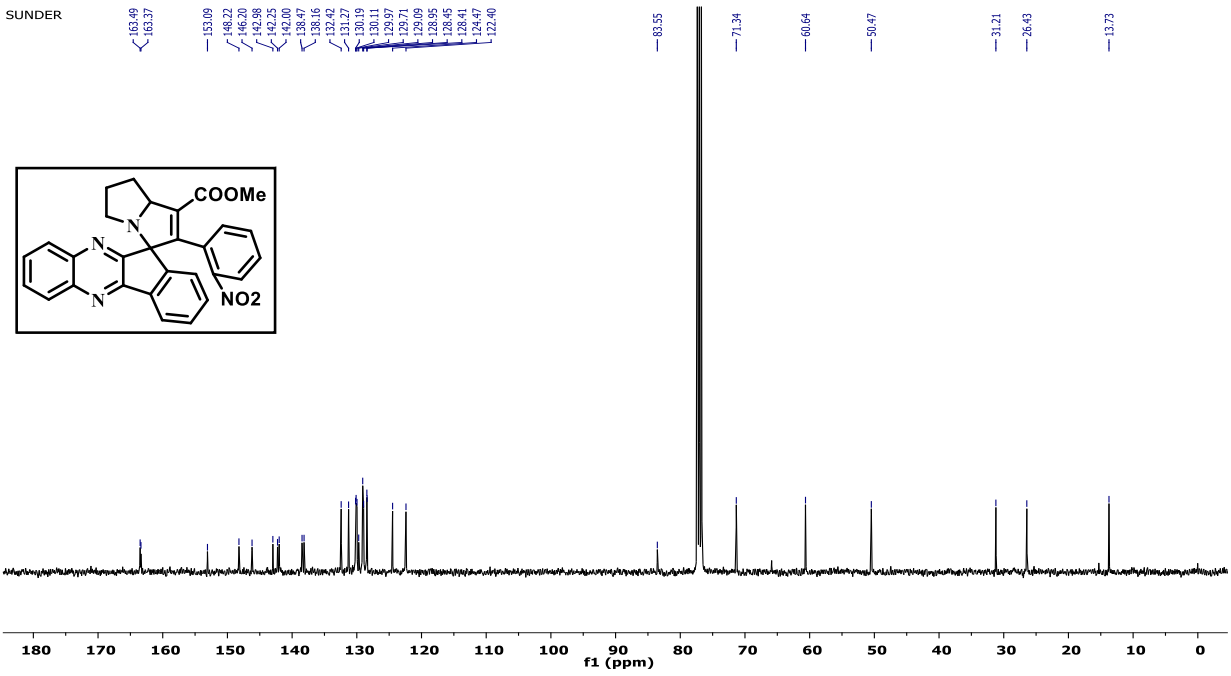
^{1}H NMR and ^{13}C NMR of 5a





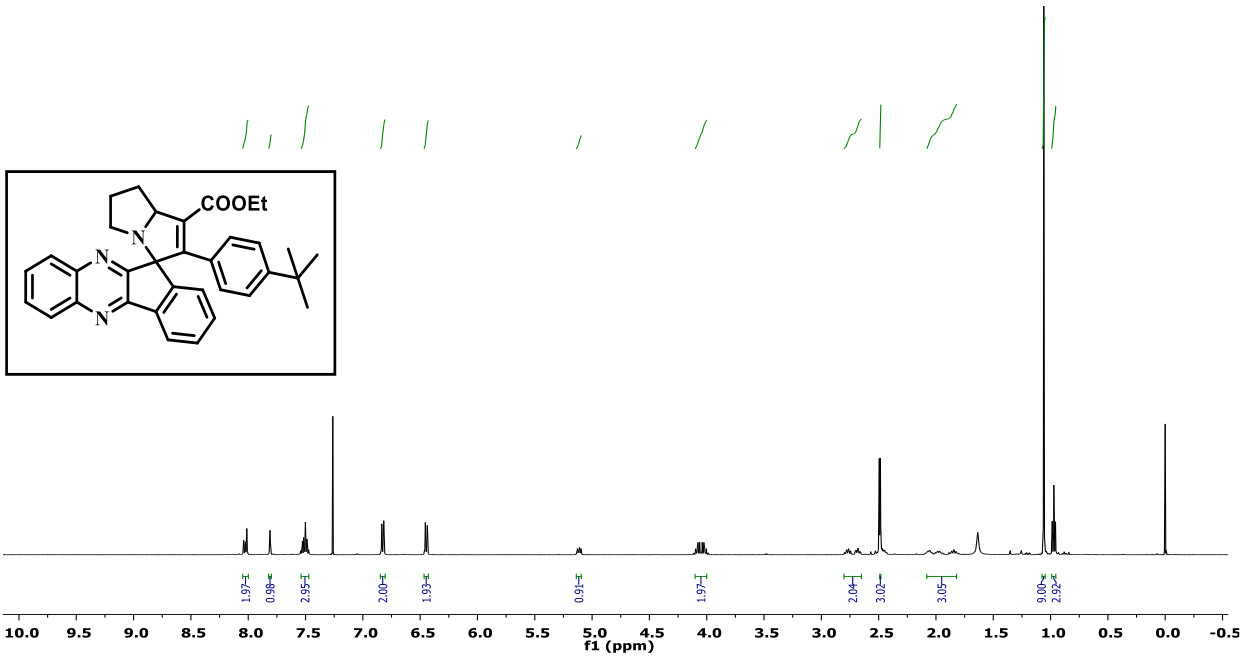
^{1}H NMR and ^{13}C NMR of 5b



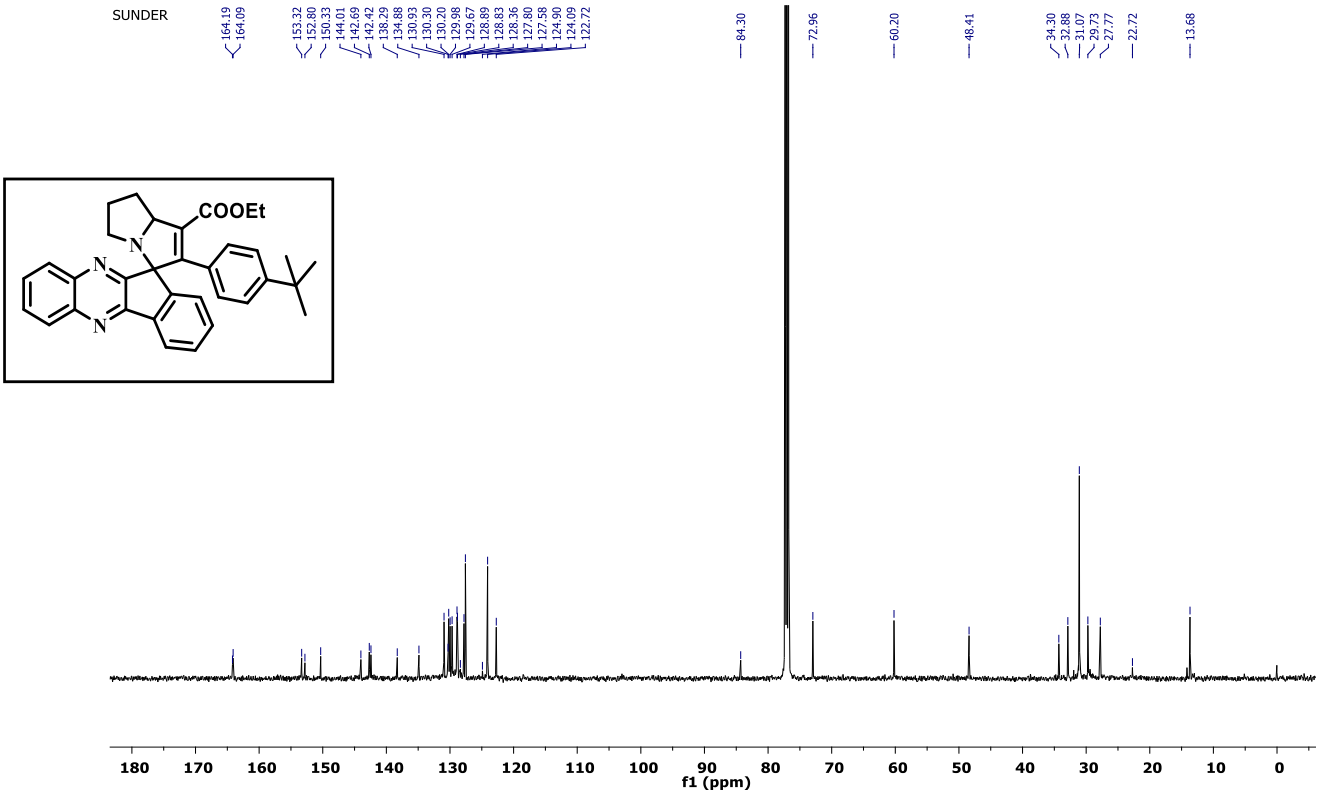


^{1}H NMR and ^{13}C NMR of 5c

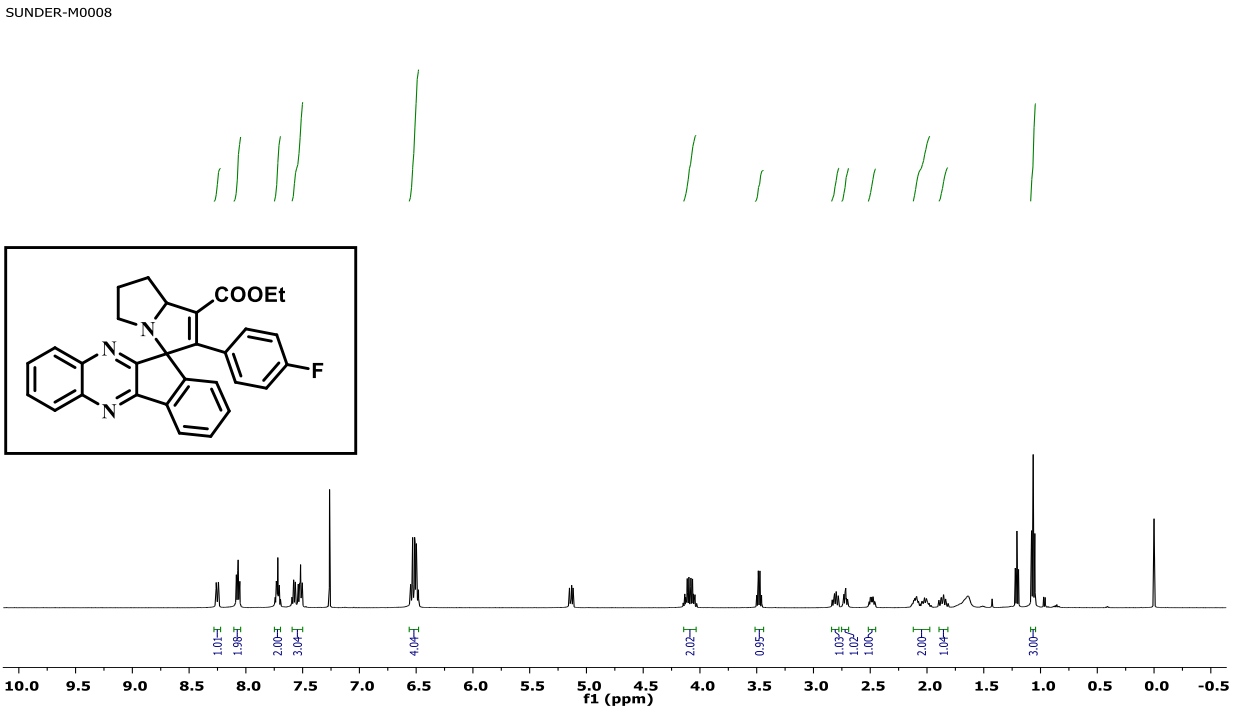
SUNDAR

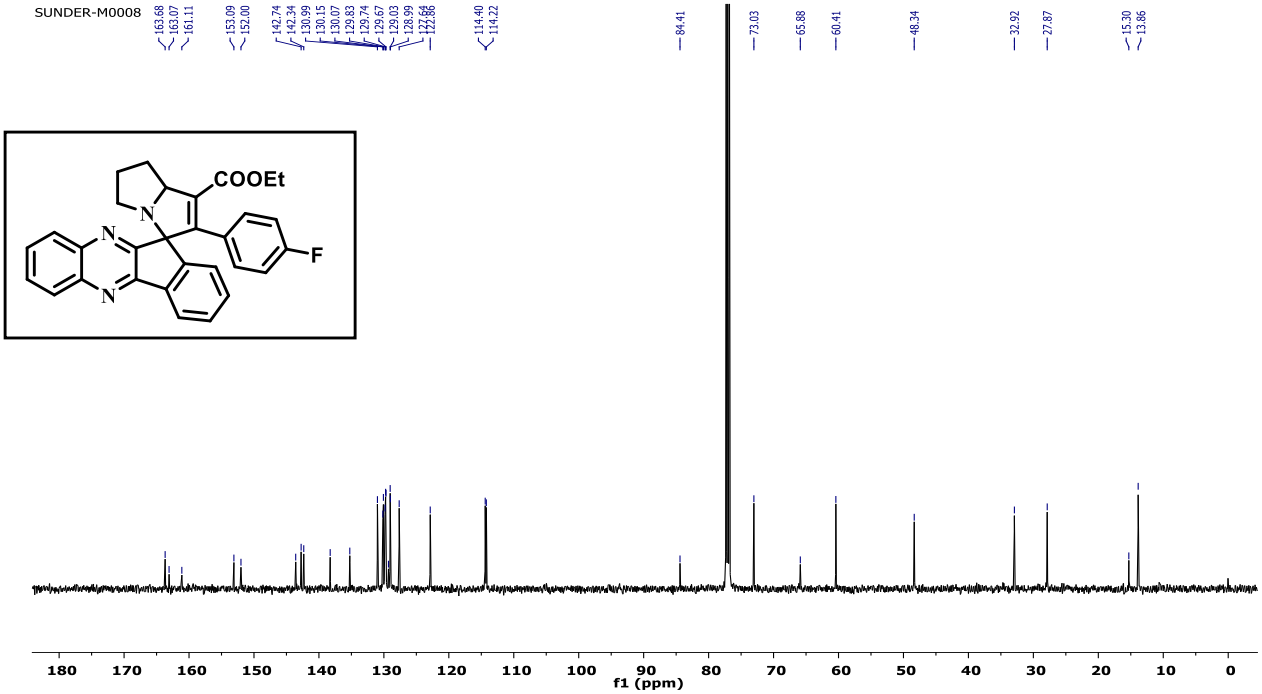


SUNDER

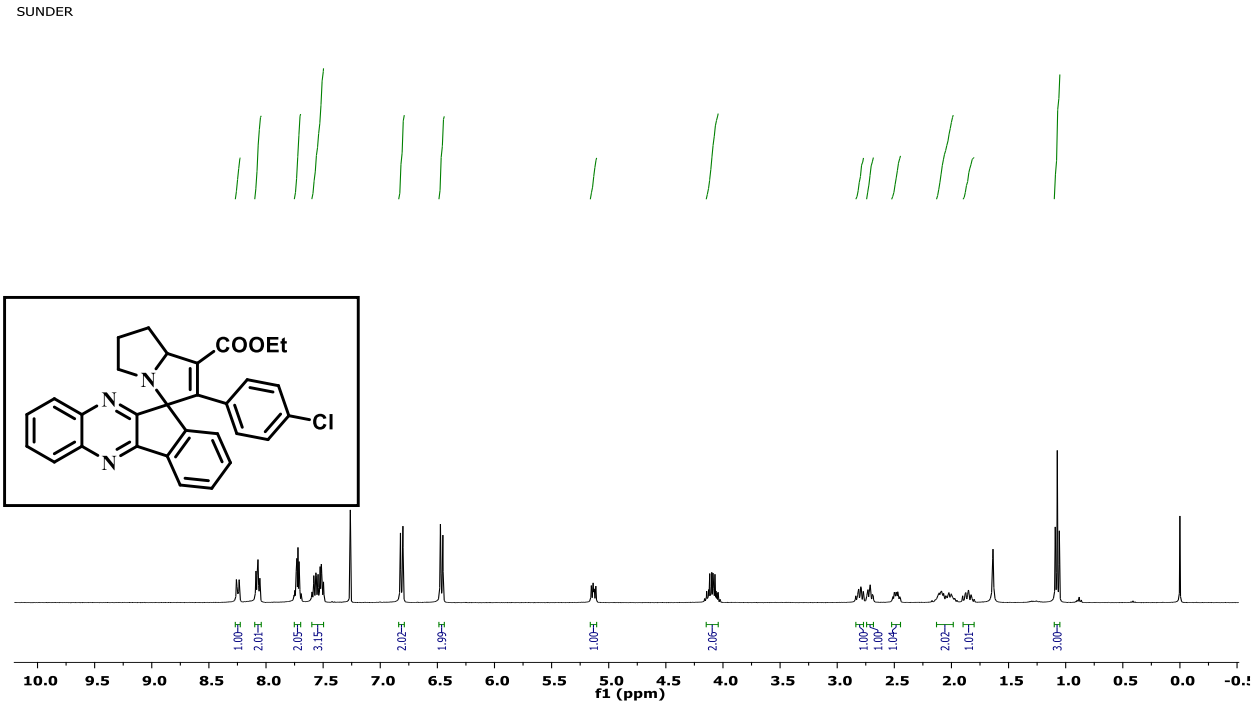


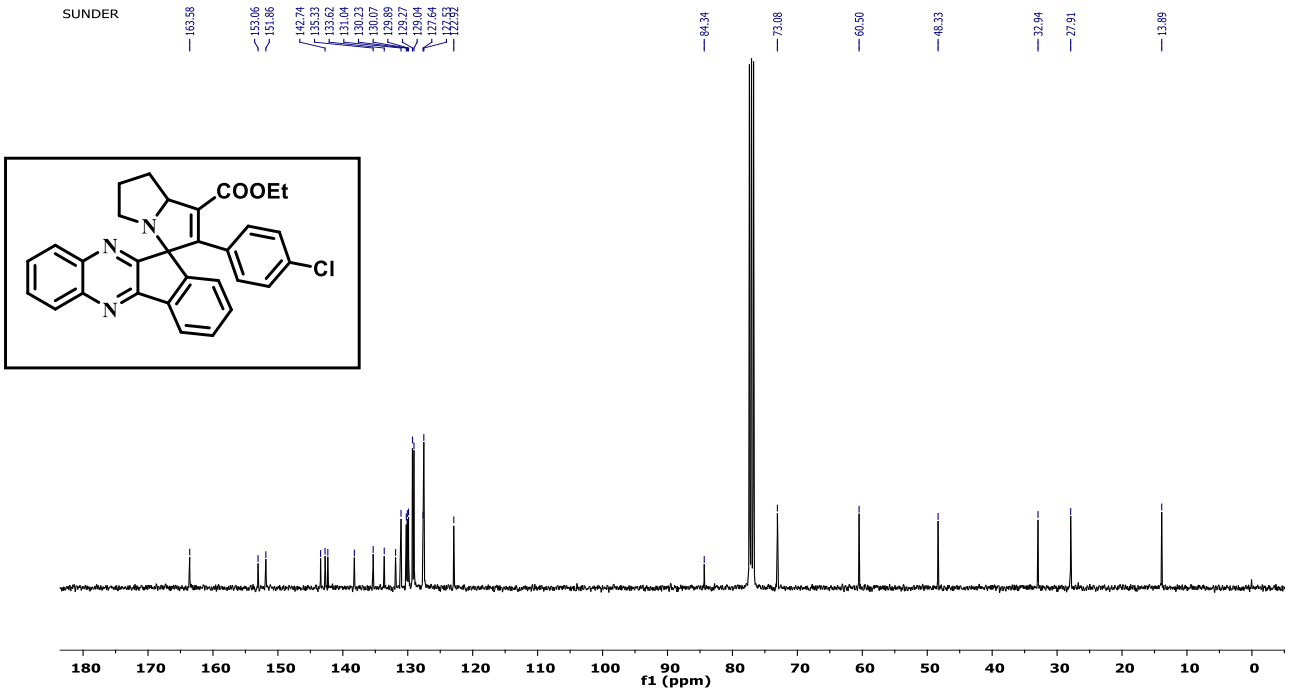
^{1}H NMR and ^{13}C NMR of 5d



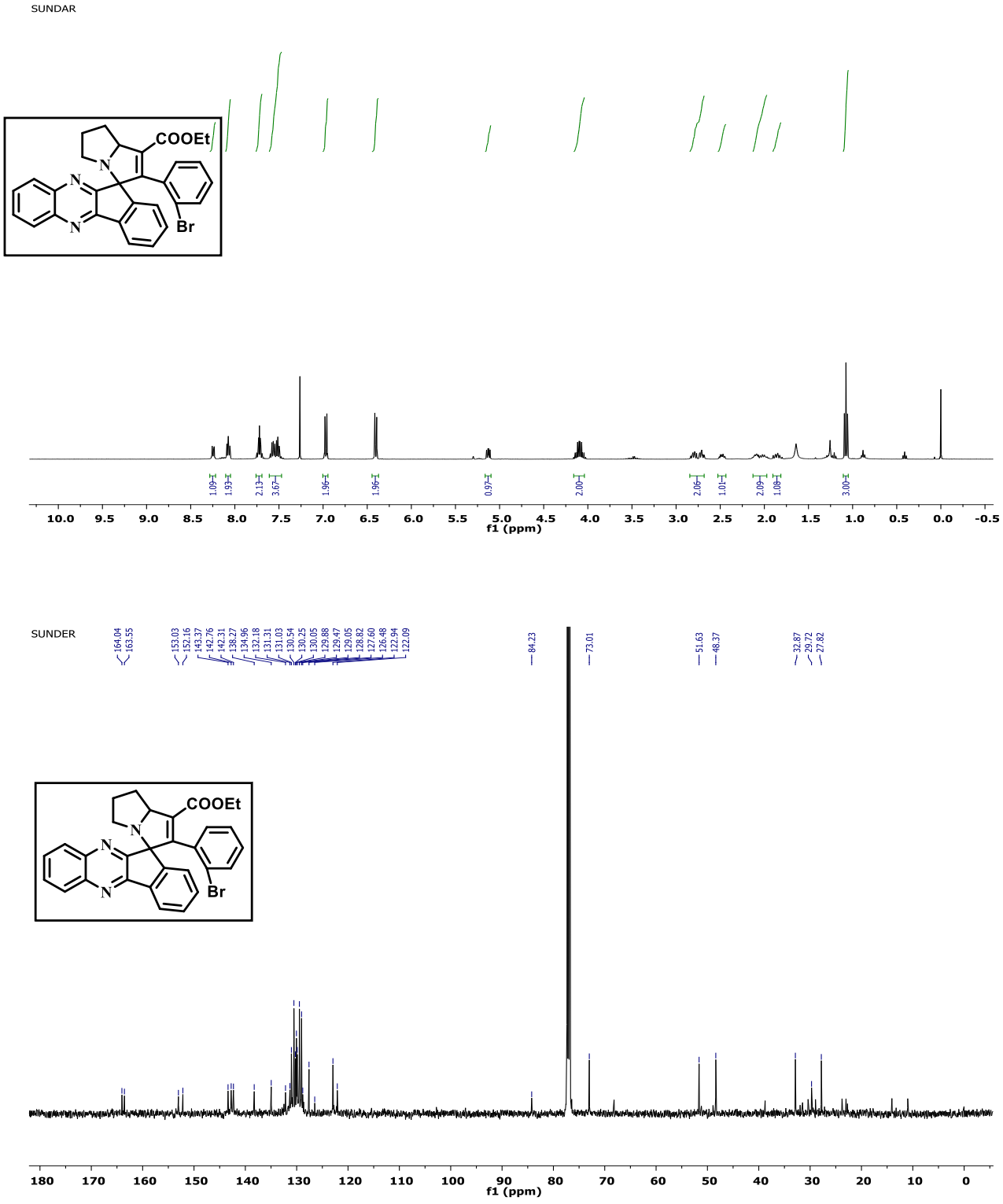


^{1}H NMR and ^{13}C NMR of 5e

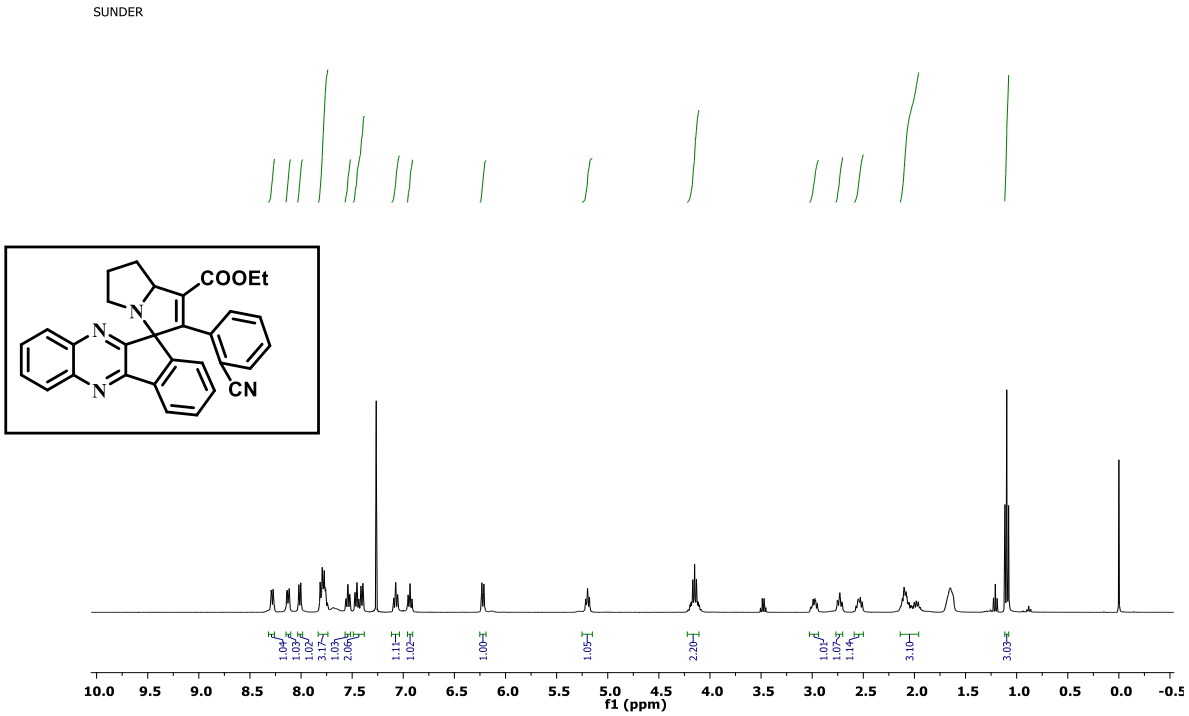


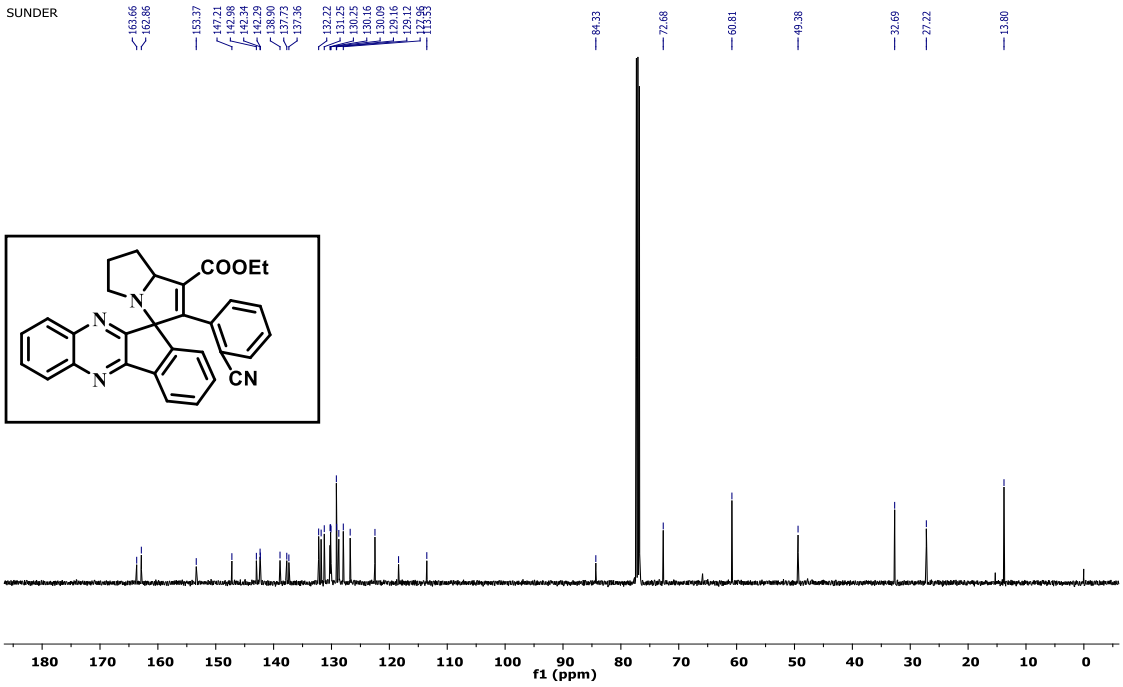


^{1}H NMR and ^{13}C NMR of 5f

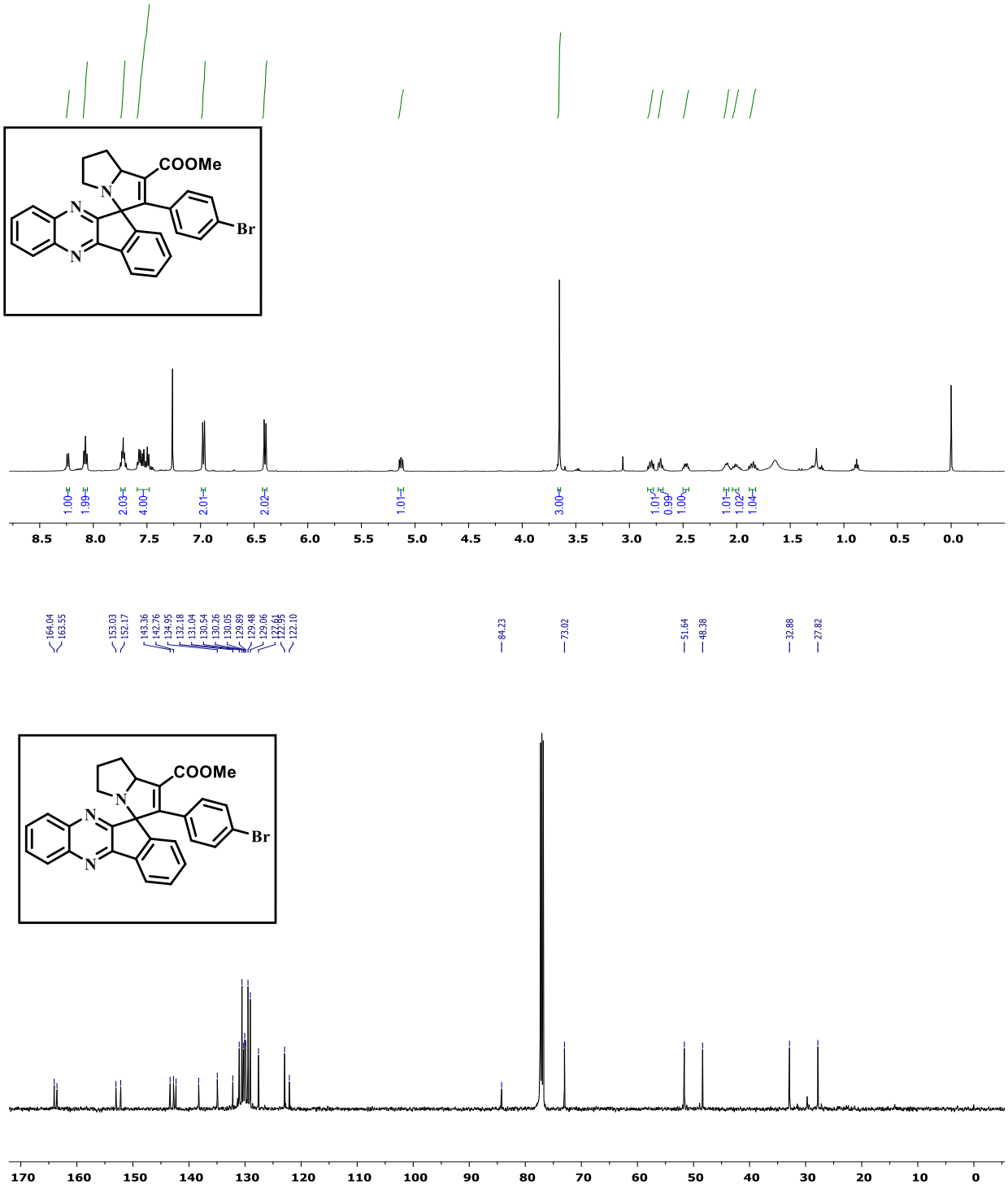


^{1}H NMR and ^{13}C NMR of 5g

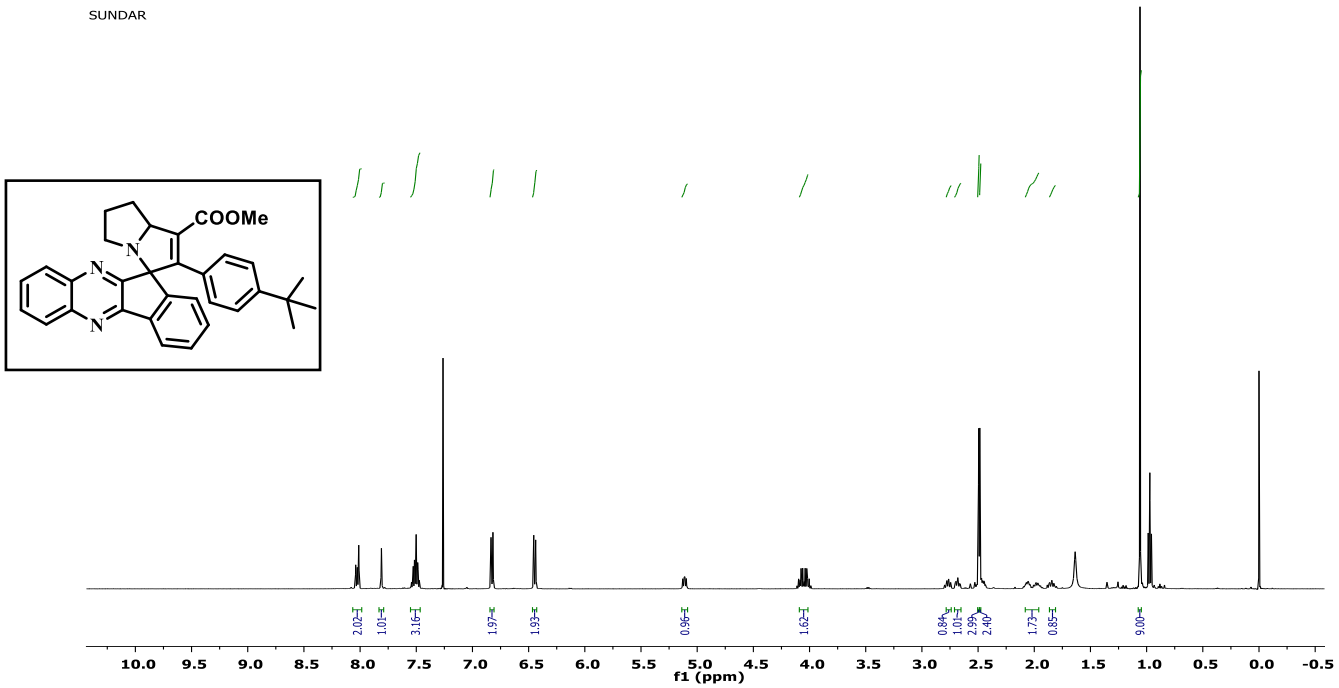


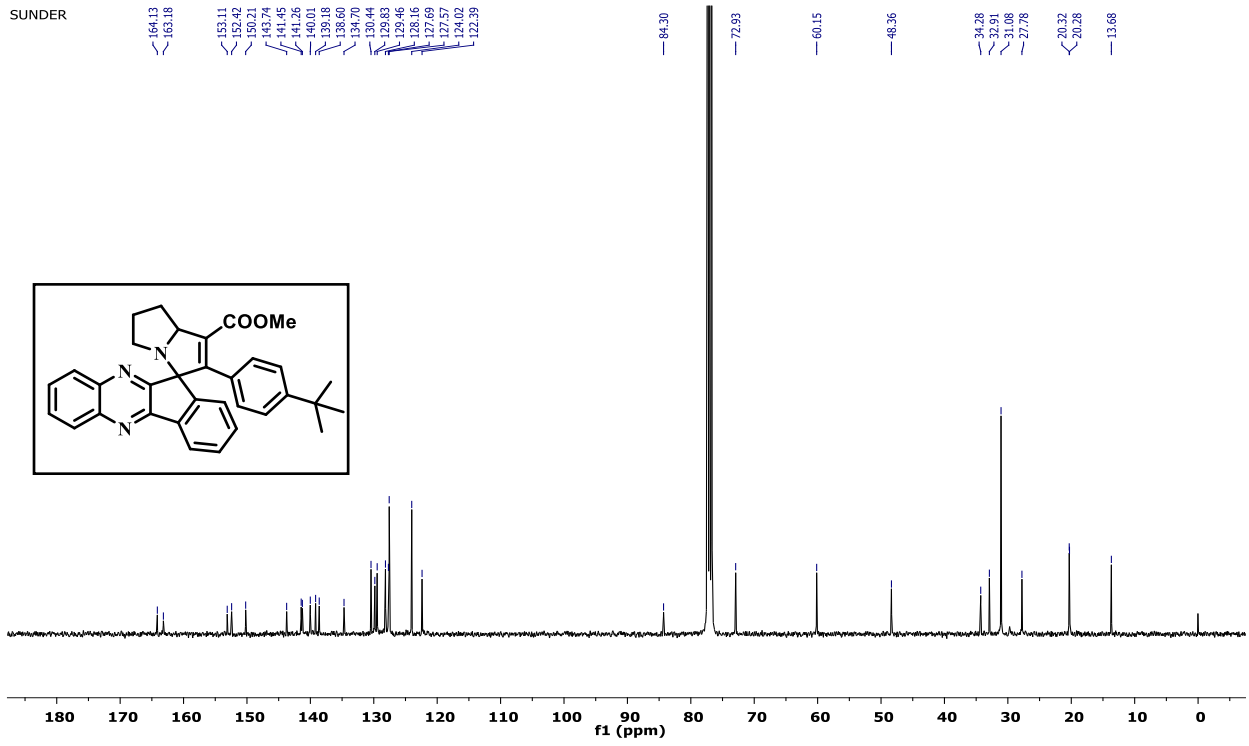


^{1}H NMR and ^{13}C NMR spectra of 5h

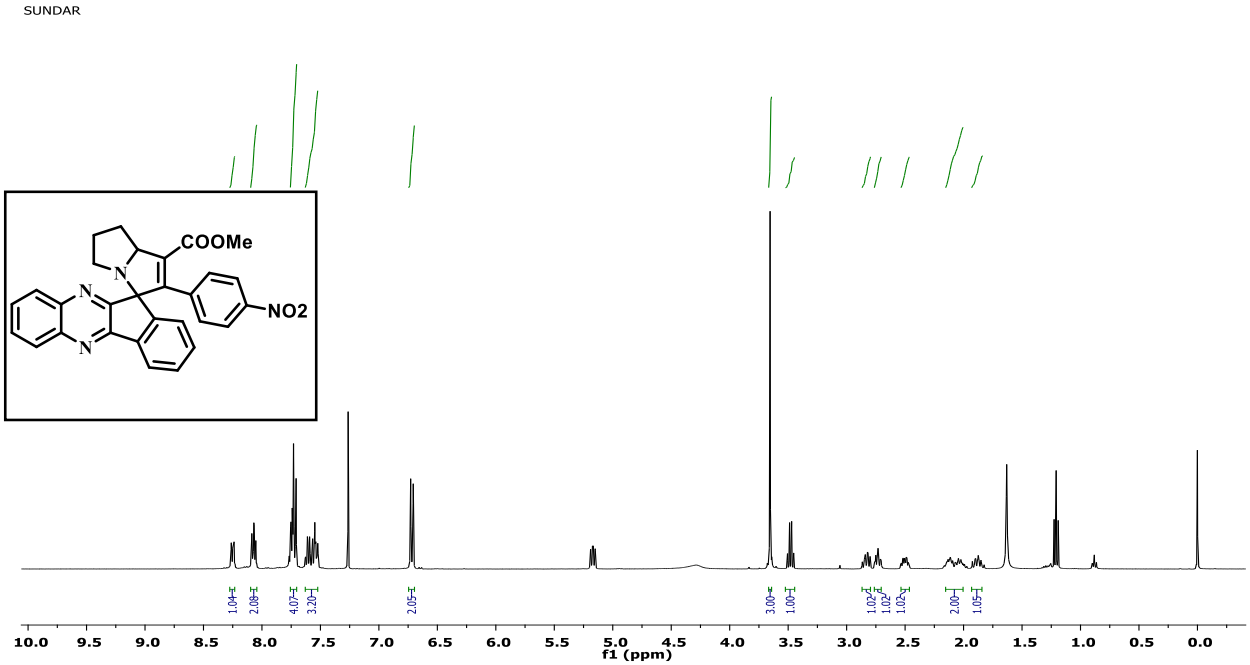


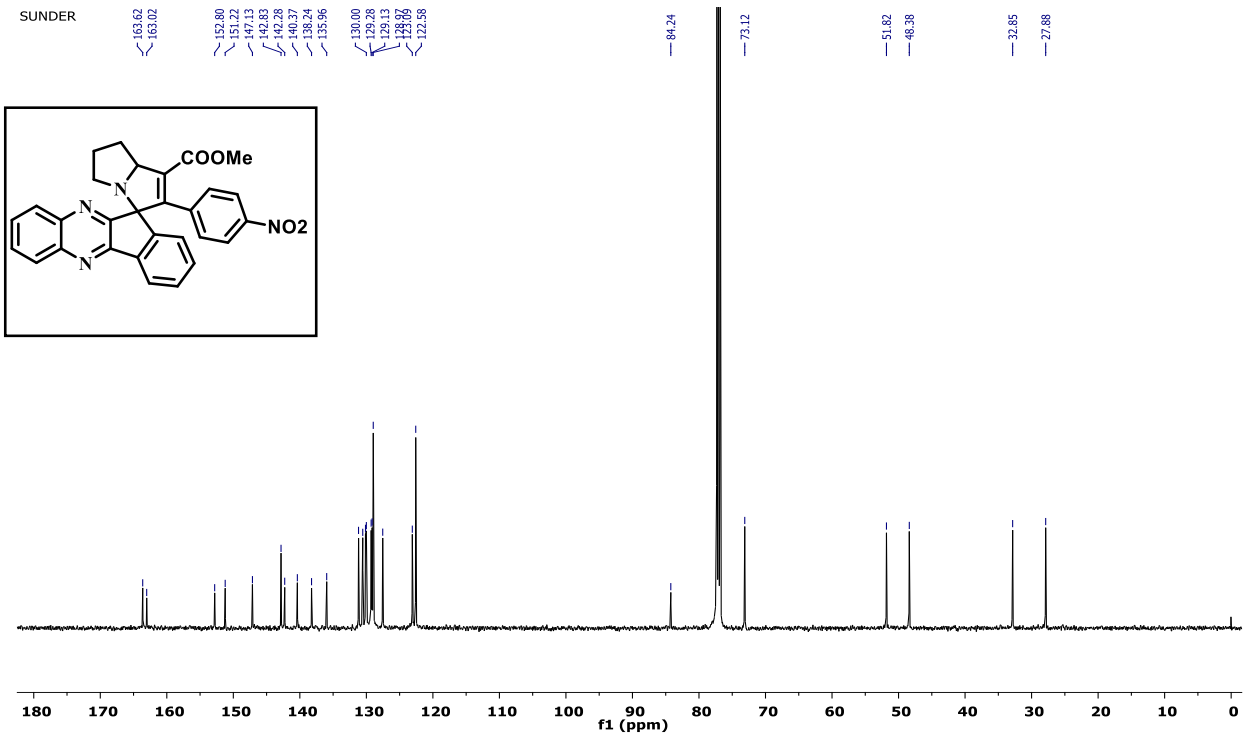
^{1}H NMR and ^{13}C NMR of 5i



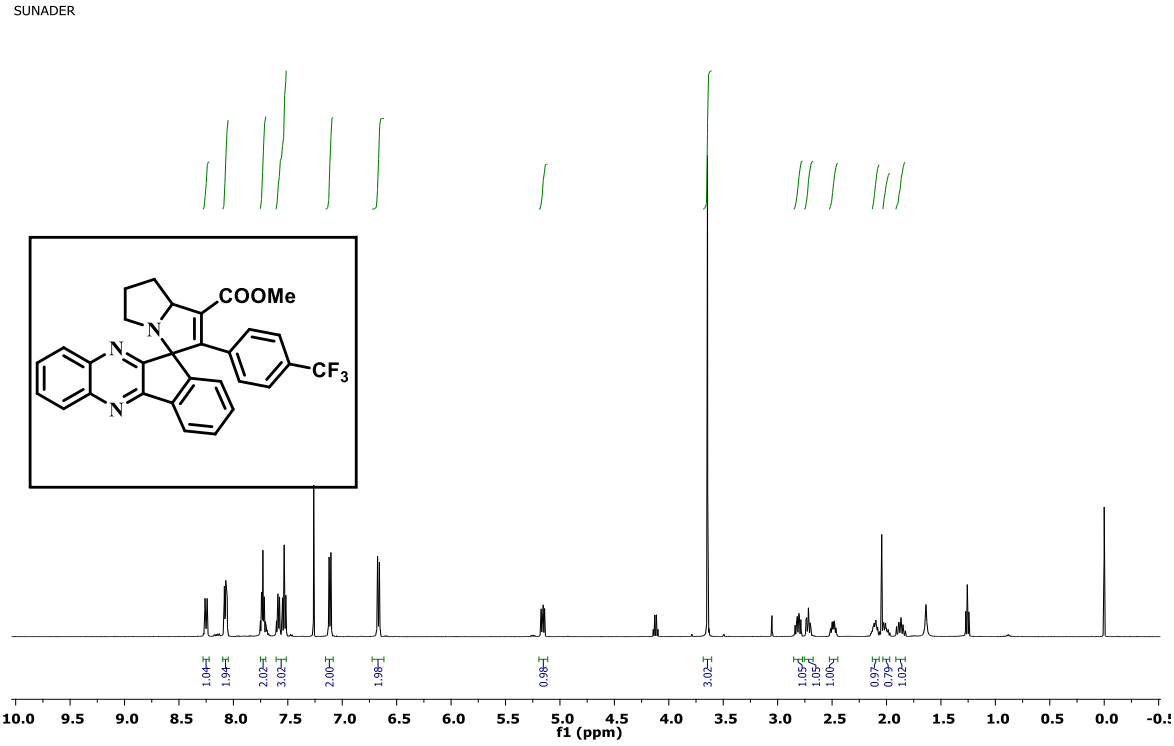


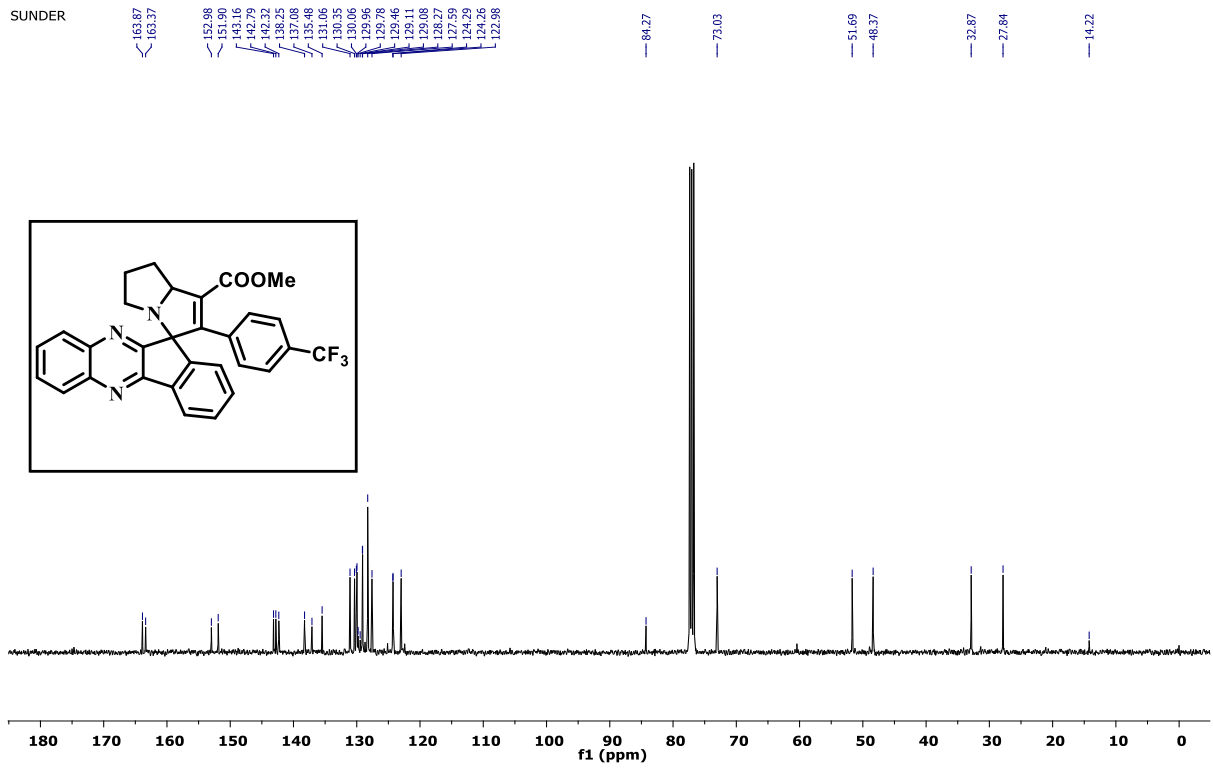
^{1}H NMR and ^{13}C NMR of 5j



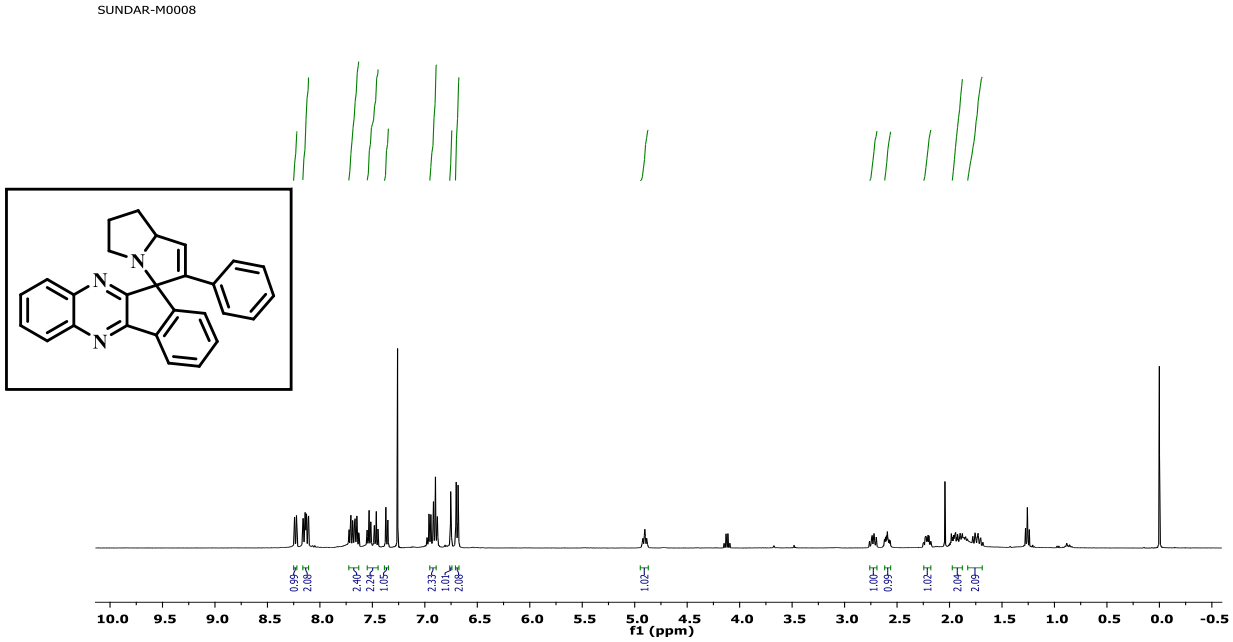


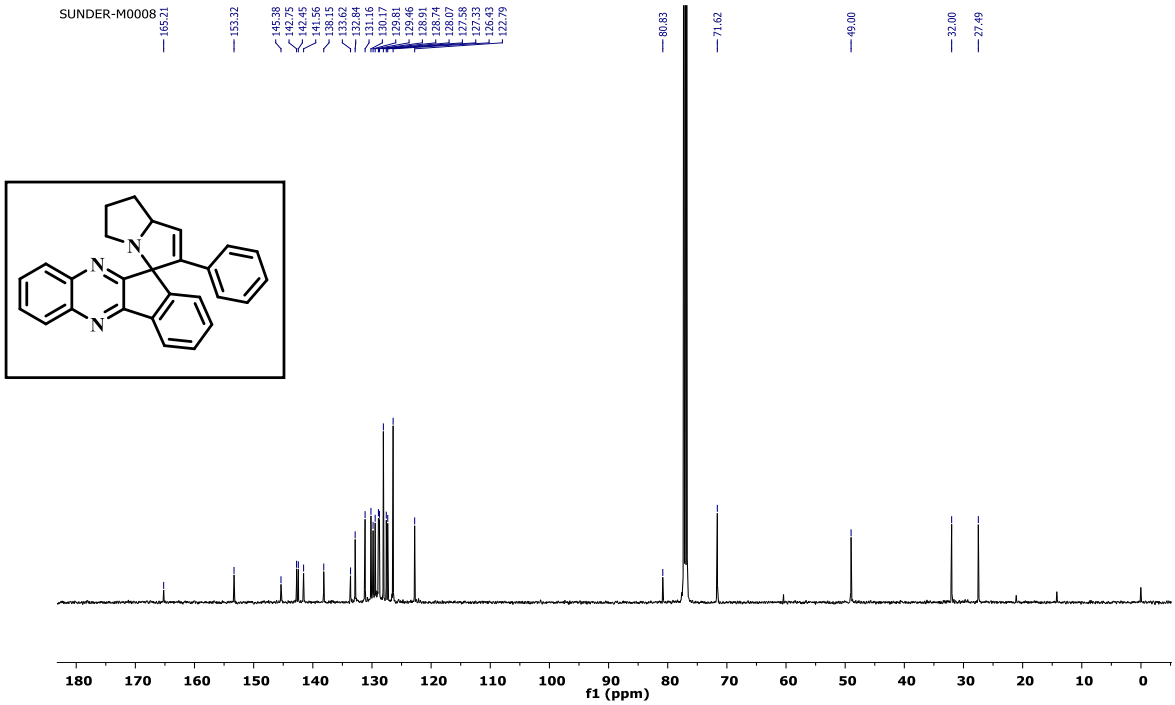
^{1}H NMR and ^{13}C NMR of 5k



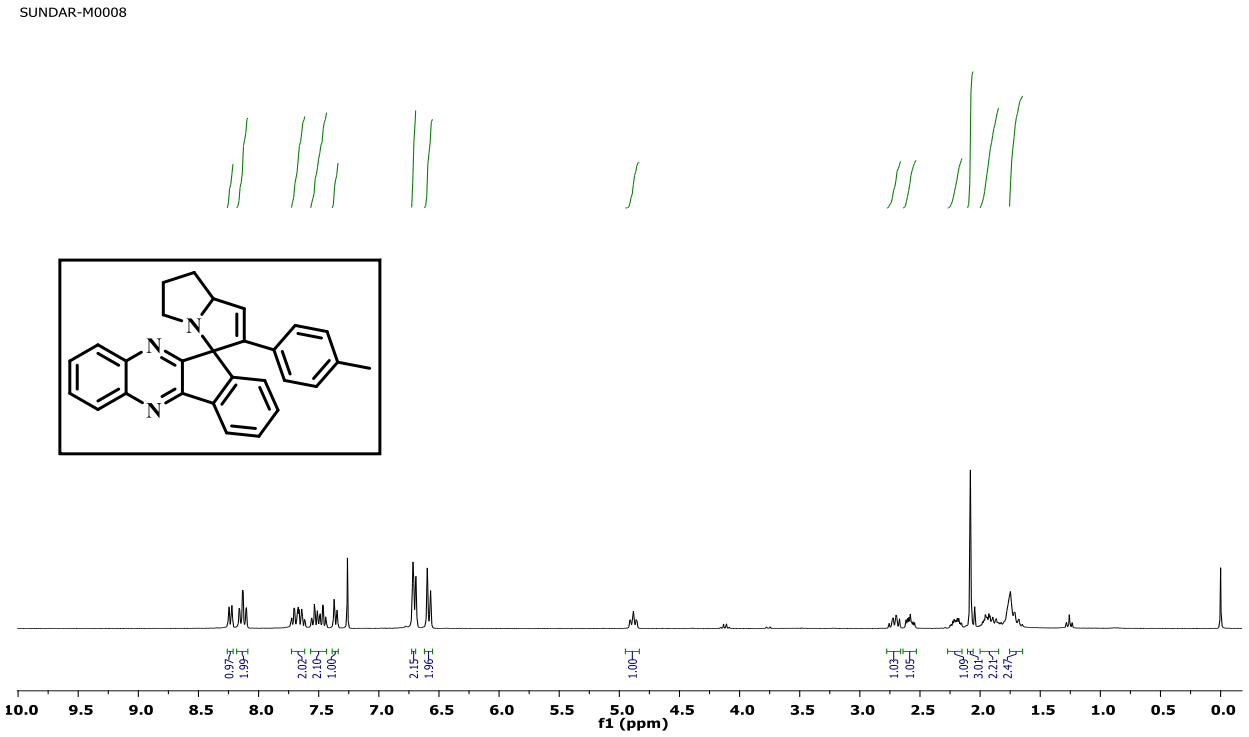


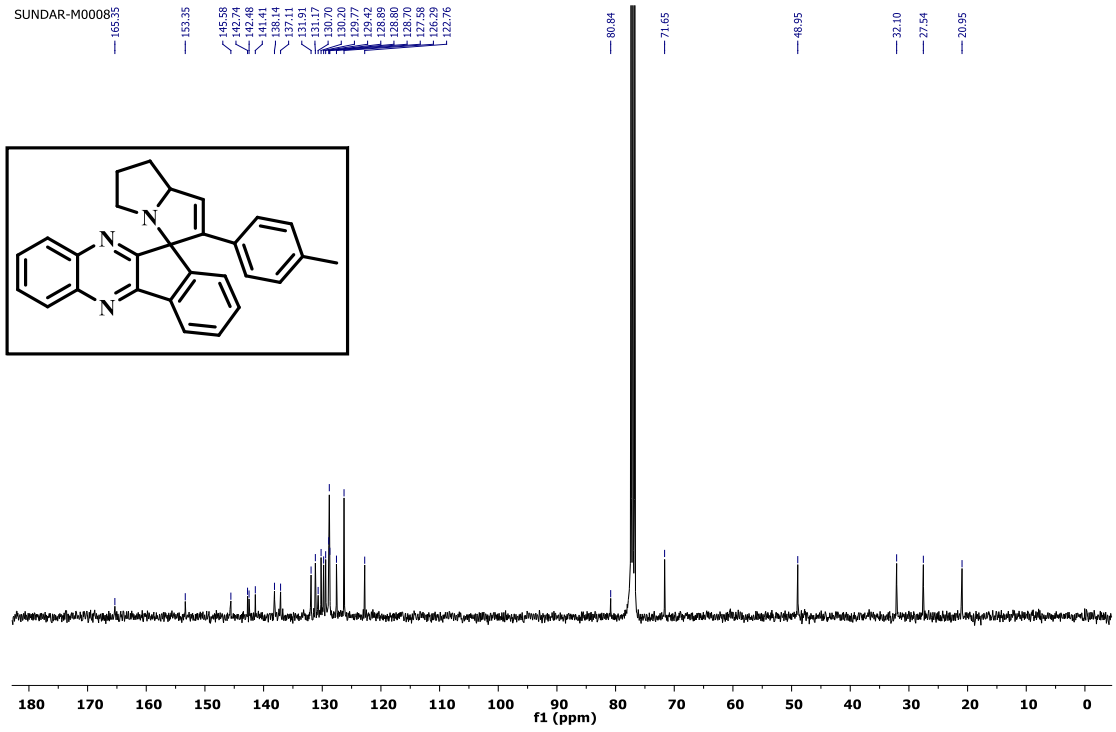
^{1}H NMR and ^{13}C NMR of 5l



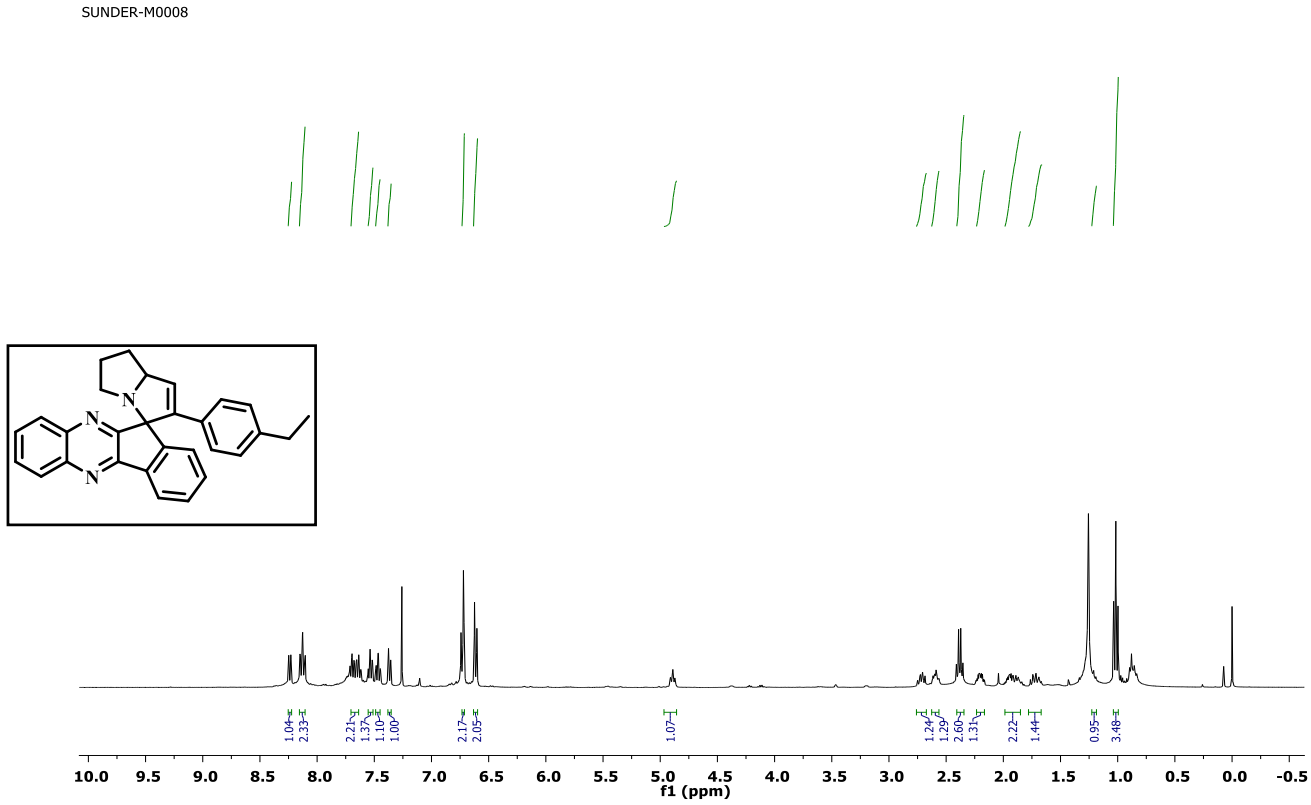


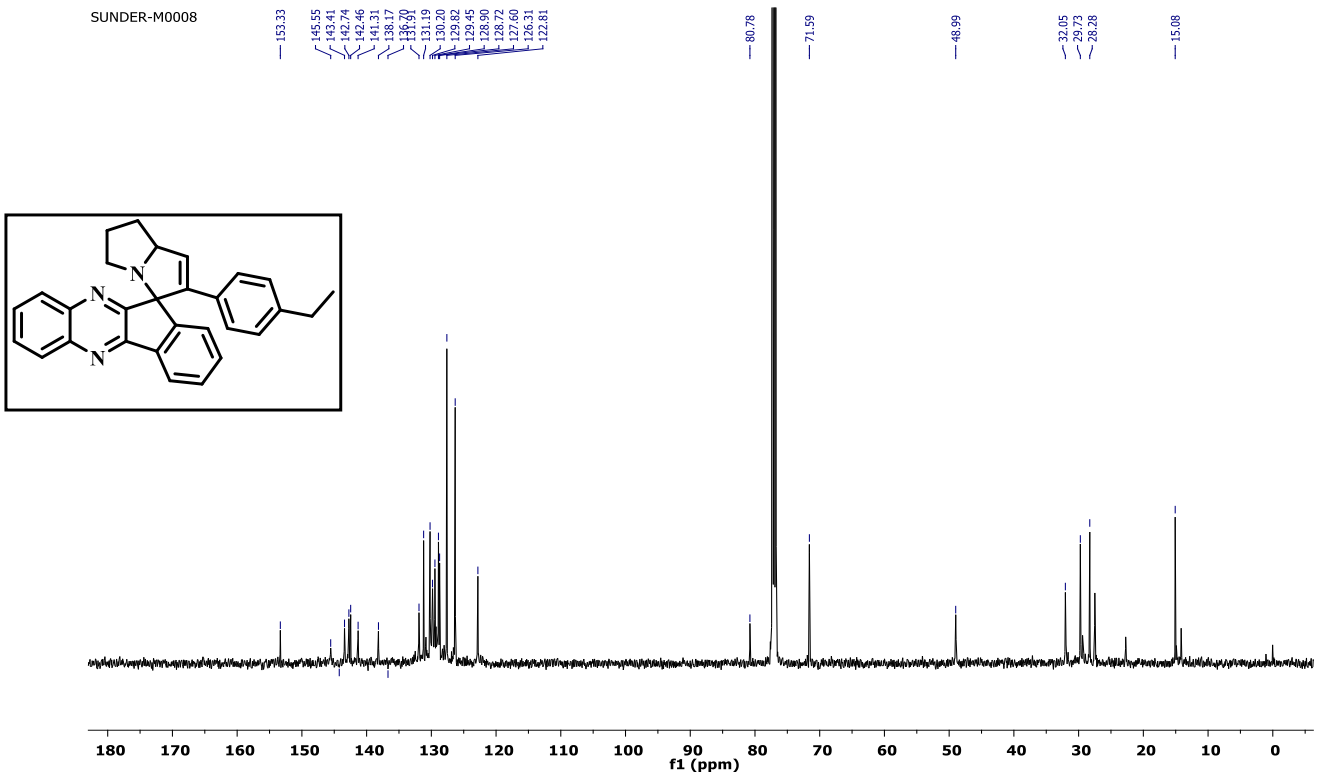
^{1}H NMR and ^{13}C NMR of 5m



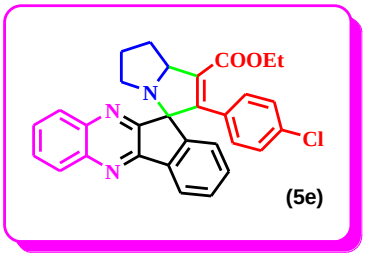


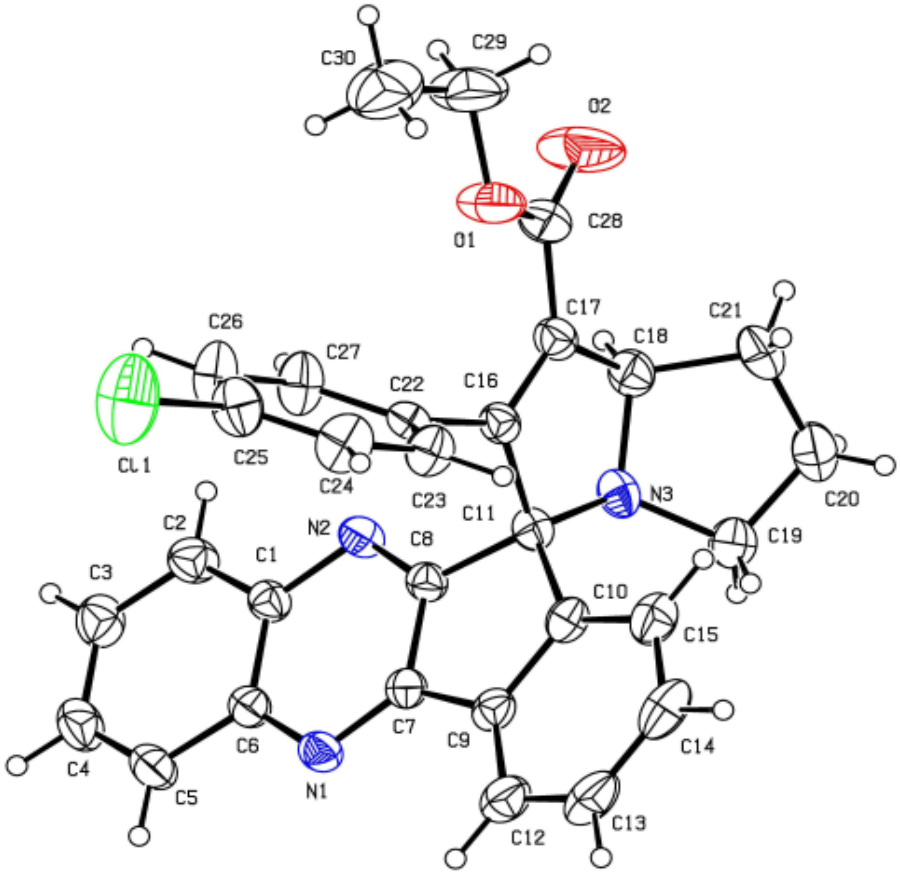
^{1}H NMR and ^{13}C NMR of 5n





X-ray crystallography





The molecular structure of **5e**, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

X-ray crystallography study

X-ray data for the compound was collected at room temperature on a Bruker D8 QUEST instrument with an IμS Mo microsource (λ = 0.7107 A) and a PHOTON-100 detector. The raw data frames of **5h** were reduced and corrected for absorption effects using the Bruker Apex 3 software suite programs [1]. The structure was solved using intrinsic phasing method [2] and further

refined with the SHELXL [2] program and expanded using Fourier techniques. Anisotropic displacement parameters were included for all non-hydrogen atoms. All C bound H atoms of were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 Å, and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H or $1.2U_{eq}(C)$ for other H atoms].

Crystal structure determination of 5e

Crystal Data for $C_{30}H_{24}N_3O_2Cl$ (*M* =493.97 g/mol): monoclinic, space group $P2_1/c$ (no. 14), *a* = 19.6937(15) Å, *b* = 13.4393(9) Å, *c* = 9.6001(7) Å, *β* = 98.102(2)°, *V* = 2515.5(3) Å^3, *Z* = 4, *T* = 294.15 K, μ(MoKα) = 0.185 mm^{-1}, *Dcalc* = 1.304 g/cm^3, 33466 reflections measured (5.162° ≤ 2Θ ≤ 50°), 4432 unique (R_{int} = 0.0678, R_{sigma} = 0.0412) which were used in all calculations. The final R_1 was 0.0604 (I > 2σ(I)) and wR_2 was 0.1693 (all data). CCDC 2049616 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk].

1. SMART & SAINT. Software Reference manuals. Versions 6.28a & 5.625, Bruker Analytical X-ray Systems Inc., Madison, Wisconsin, U.S.A., 2001.
2. Sheldrick, G. M. (2015). Acta Cryst. C71, 3–8.

Figure caption: The molecular structure of KA562, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

