Electronic supporting information

An expedient microwave assisted regio and stereoselective synthesis of spiroquinoxaline pyrrolizine derivatives and their AChE inhibitory activity

Adinarayana Murthy Akondi,[a] Sowmya Mekala,[b,c] Mannepalli Lakshmi Kantam,*[a,d] Rajiv Trivedi,*[a] L. Raju Chowhan[e], Amitava Das[b,c]

[a]*Inorganic and Physical Chemistry Division, CSIR-Indian Institute of Chemical Technology, Hyderabad 500007, India,*

[b]*Centre for Chemical Biology, CSIR-Indian Institute of Chemical Technology, Hyderabad 500007, India*

[c]*Academy of Scientific and Innovative Research (AcSIR), 2 Rafi Marg, New Delhi – 110 001, INDIA*

[d]*Institute of Chemical Technology, Matunga, Mumbai,- 400019. India.*

[e]*School of Chemical Sciences, Central University Gujarat, Gandhinagar, 382030, India*

Contents

Experimental section

General remarks

All reagents and solvents were obtained from commercial suppliers and used without further purification. The Thin Layer Chromatography (TLC) was performed on Merck silica gel 60 F254 plates using ethyl acetate and hexane as eluting agents. Thin layer chromatography plates were visualized by exposure to UV-light/iodine and/or by immersion in an acidic staining solution of phosphomolybdic acid followed by heating on a hot plate. All the products were characterized by Mass, ^{1}H and ^{13}C-NMR spectroscopy. The NMR spectra of samples were acquired on a Bruker Avance 400 MHz and 500 MHz spectrometer using TMS as an internal standard in $CDCl_3$. Mass spectra were acquired on a Thermo LCQ fleet ion trap mass spectrometer. High resolution mass spectra were acquired on a Q STAR XL Hybrid LC/MS/MS system, Applied Biosystems, USA. FT-IR data were acquired on a Thermo Nicolet Nexus 670 FT-IR spectrometer with DTGS KBr detector. The single crystal measurements were made on a Rigaku SCX mini diffractometer using graphite monochromated Mo-Ka radiation. The melting points were measured in open capillary tubes and are uncorrected.

General procedure for synthesis of spiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] derivatives

Procedure A: L-Proline (0.2 mmol) and β-nitrostyrene (0.2 mmol) were added to a solution of ninhydrin (0.2 mmol) and 1,2-phenylenediamine (0.2 mmol) in EtOH (2 mL) and the mixture was refluxed for 4-5.5h. The progress of the reaction was monitored by TLC. On completion of the reaction, the reaction mixture was cooled to room temperature a solid mass precipitated out that was filtered off followed by washing with cold ethanol to obtain crude product purified just by recrystallization from EtOH:$CHCl_3$ (9:1) without carrying out column chromatography to give pure **5** (78-93%).

Procedure B: L-Proline (0.2 mmol) and β-nitrostyrene (0.2 mmol) were added to a solution of ninhydrin (0.2 mmol) and 1,2-phenylenediamine (0.2 mmol) in EtOH (2 mL) and the mixture was irradiated under microwave irradiation (150 W power) at 80 ^{o}C for 7-10 minutes. The progress of the reaction was monitored by TLC. On completion of the reaction, the reaction mixture was cooled to room temperature a solid mass precipitated out that was filtered off followed by washing with cold ethanol to obtain crude product purified just by recrystallization from EtOH:$CHCl_3$ (9:1) without carrying out column chromatography to give pure **5** (83-96%).

Biological experimental Procedures:

Ellman's assay (Ellman et al, 1961) is one of the standard methods used to determine the *in vitro* AChE activity which is based on the principle that the substrate is hydrolyzed to form the sulfhydryl compound which reacts with Ellmans reagent, 5'-dithiobis-(2-nitrobenzoic acid) (DTNB) resulting in a mixed disulfide and 2-nitro-5-thiobenzoic acid (TNB). TNB is the yellow coloured compound formed with high molar extinction coefficient

observed in the visible range. Higher is the enzyme activity more will be the yellow colour formed and the efficient inhibitors should be able to reduce the enzyme activity which can also be observed visually through decreased yellow coloured compound TNB.

Enzyme source was mouse brain extracted in the laboratory. Briefly, mouse brain was dissected out from the euthanized mice from in-house animal facility (BIOSAFE, CSIR-IICT, Hyderabad) and homogenized in 30 mM sodium phosphate buffer (NaH_2PO_4/Na_2HPO_4), followed by ultracentrifugation at 100,000 × g. 60 min, at 4°C. The supernatant was collected and used as enzyme source. Chemicals including acetylthiocholine iodide (ATCh) as a substrate and DTNB reagent purchased from Sigma-Aldrich, USA.

The samples were dissolved in DMSO and evaluated for their anti-AChE activity at various concentrations 0.1, 0.3, 1, 3, 10, 30 and 100 µM diluted in 30 mM sodium phosphate buffer wherein commercially available Galanthamine was used as a standard anti-AChE drug. Initially, the small molecules were diluted to their respective concentrations in sodium phosphate buffer followed by pre-incubation of the enzyme source with small molecules for 30 min on ice. Later on, substrate solution of ATCh and DTNB chromogen prepared in 30 mM sodium phosphate buffer were added. ATCh is hydrolysed into thiocholine containing the free sulfhydryl groups, a target of DTNB resulting in formation of yellow colour. The absorbance was measured using a kinetic reaction at 412 nm with 30 s interval for 300 s resulting in increased yellow colour formation which is directly proportional to the AChE enzyme activity, calculated using the following formula:

$$\text{AChE activity } (\mu M\ min^{-1}) = \Delta A_{412} \times vol_{(T)} \times 1000/1.36 \times 10^4 \times \text{lightpath} \times vol_{(s)}$$

Where, ΔA_{412} is the change in absorbance per min

$vol_{(T)}$ is the total assay volume

1.36×10^4 is the molar extinction coefficient of TNB ($m^{-1}cm^{-1}$)

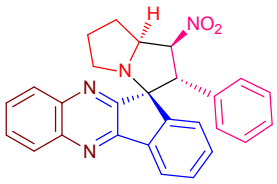
lightpath is the microplate well depth

$vol_{(s)}$ is the sample volume

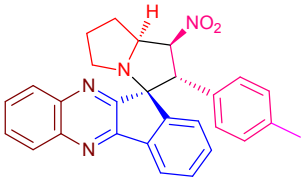
Further, using the AChE activity percent inhibition values were estimated and the IC_{50} values were calculated using Graphpad prism software.

$$\text{Percent inhibition} = \frac{\text{AChE activity of control-AChE activity of sample}}{\text{AChE activity of control}} * 100$$

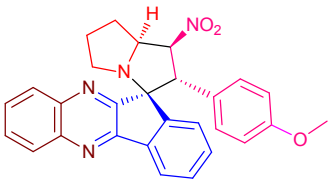
Spectroscopic data of synthesized compounds



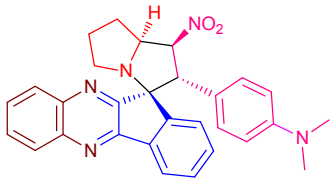
1. 1'-nitro-2'-phenyl-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5a
   Colourless solid, mp 212-214°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 – 8.14 (m, 1H), 8.07 – 8.00 (m, 3H), 7.77 – 7.70 (m, 2H), 7.65 (td, *J* = 7.5, 1.2 Hz, 1H), 7.59 – 7.53 (m, 1H), 6.91 – 6.79 (m, 5H), 6.74 – 6.68 (m, 1H), 5.22 (dd, *J* = 16.8, 8.0 Hz, 1H), 4.93 (d, *J* = 10.3 Hz, 1H), 3.47 (ddd, *J* = 11.0, 8.3, 5.5 Hz, 1H), 2.86 (t, *J* = 7.3 Hz, 1H), 2.30 – 2.21 (m, 1H), 2.11 – 2.03 (m, 1H), 1.91 – 1.79 (m, 1H), 1.69 – 1.63 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.00, 152.88, 143.18, 142.44, 141.10, 138.86, 132.87, 131.23, 130.27, 129.80, 129.67, 129.14, 129.12, 128.36, 128.11, 127.48, 126.58, 122.71, 93.02, 75.43, 64.83, 54.25, 51.30, 27.73, 26.05; HRMS: m/z Calcd. for $C_{27}H_{23}N_4O_2$ $[M+H]^+$: 435.1816; Found, 435.1826 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1530, 1375.



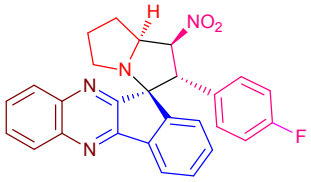
2. 1'-nitro-2'-(p-tolyl)-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5b
   Colourless solid, mp 190-192°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 – 8.14 (m, 1H), 8.08 – 7.98 (m, 3H), 7.77 – 7.69 (m, 2H), 7.65 (td, *J* = 7.6, 1.2 Hz, 1H), 7.56 (td, *J* = 7.5, 0.9 Hz, 1H), 6.75 – 6.65 (m, 3H), 6.62 (d, *J* = 8.0 Hz, 2H), 5.20 (dd, *J* = 16.7, 8.0 Hz, 1H), 4.89 (d, *J* = 10.3 Hz, 1H), 3.47 (ddd, *J* = 11.0, 8.3, 5.5 Hz, 1H), 2.86 (t, *J* = 7.2 Hz, 1H), 2.30 – 2.19 (m, 1H), 2.12 – 2.02 (m, 1H), 2.00 (s, 3H), 1.92 – 1.78 (m, 1H), 1.70 – 1.63 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.15, 152.93, 143.30, 142.43, 141.13, 138.89, 137.13, 131.19, 130.21, 129.77, 129.69, 129.10, 128.85, 128.21, 126.61, 122.68, 93.11, 75.39, 64.75, 53.89, 51.34, 27.74, 26.06, 20.76; HRMS: m/z Calcd. for $C_{28}H_{25}N_4O_2$ $[M+H]^+$: 449.1972; Found, 449.1995 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1530, 1374.



3. 2'-(4-methoxyphenyl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5c
   Colourless solid, mp 189-191°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 – 8.14 (m, 1H), 8.09 – 7.98 (m, 3H), 7.77 – 7.70 (m, 2H), 7.64 (td, *J* = 7.6, 1.2 Hz, 1H), 7.56 (td, *J* = 7.5, 0.8 Hz, 1H), 6.75 (d, *J* = 8.8 Hz, 2H), 6.69 – 6.61 (m, 1H), 6.37 – 6.31 (m, 2H), 5.20 (dd, *J* = 16.8, 8.0 Hz, 1H), 4.87 (d, *J* = 10.4 Hz, 1H), 3.51 (s, 3H), 3.46 (ddd, *J* = 10.9, 6.7, 3.7 Hz, 1H), 2.85 (t, *J* = 7.2 Hz, 1H), 2.29 – 2.19 (m, 1H), 2.11 – 2.02 (m, 1H), 1.91 – 1.78 (m, 1H), 1.70 – 1.65 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.22, 158.71, 152.94, 143.32, 142.44, 141.13, 138.90, 131.21, 130.21, 129.78, 129.67, 129.41, 129.13, 126.56, 124.68, 122.72, 113.56, 93.23, 75.37, 64.71, 54.92, 53.65, 51.31, 27.73, 26.06; HRMS: m/z Calcd. for $C_{28}H_{25}N_4O_3$ $[M+H]^+$: 465.1921; Found, 465.1953 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1540, 1373, 1249, 1033.

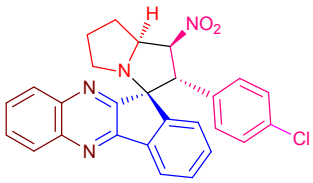


4. N,N-dimethyl-4-(1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizin]-2'-yl)aniline 5d
   Yellow solid, mp 204-205°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 – 8.16 (m, 1H), 8.06 – 7.98 (m, 3H), 7.76 – 7.69 (m, 2H), 7.63 (td, *J* = 7.6, 1.1 Hz, 1H), 7.54 (td, *J* = 7.5, 0.6 Hz, 1H), 6.71 – 6.60 (m, 3H), 6.15 (d, *J* = 8.9 Hz, 2H), 5.19 (dd, *J* = 16.7, 8.1 Hz, 1H), 4.84 (d, *J* = 10.4 Hz, 1H), 3.47 (ddd, *J* = 11.0, 8.3, 5.5 Hz, 1H), 2.85 (t, *J* = 7.2 Hz, 1H), 2.65 (s, 6H), 2.28 – 2.19 (m, 1H), 2.10 – 2.02 (m, 1H), 1.90 – 1.78 (m, 1H), 1.69 – 1.63 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.59, 153.06, 149.51, 143.61, 142.45, 141.20, 138.95, 131.12, 130.06, 129.72, 129.65, 129.07, 129.00, 126.61, 122.66, 119.90, 111.95, 93.39, 75.40, 64.61, 53.63, 51.35, 40.12, 27.72, 26.07; HRMS: m/z Calcd. for $C_{29}H_{28}N_5O_2$ $[M+H]^+$: 478.2238; Found, 478.2202 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1544, 1365, 1194.



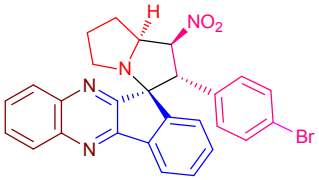
5. 2'-(4-fluorophenyl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5e
   Colourless solid, mp 194-195°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 – 8.13 (m, 1H), 8.08 – 8.02 (m, 2H), 8.01 (d, *J* = 7.7 Hz, 1H), 7.79 – 7.71 (m, 2H), 7.66 (td, *J* = 7.6, 1.2 Hz, 1H), 7.57 (td, *J* = 7.5, 0.8 Hz, 1H), 6.85 – 6.79 (m, 2H), 6.65 (t, *J* = 9.9 Hz, 1H), 6.56 – 6.47 (m, 2H), 5.20 (dd, *J* = 16.9, 7.9 Hz, 1H), 4.90 (d, *J* = 10.3 Hz, 1H), 3.45 (ddd, *J* = 10.9, 8.3, 5.5 Hz, 1H), 2.86 (t, *J* = 7.3 Hz, 1H), 2.30 – 2.21 (m, 1H), 2.11 – 2.04 (m, 1H), 1.91 – 1.79 (m, 1H), 1.69 – 1.62 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.15, 161.82, 160.70, 152.84, 142.97, 142.48, 141.04, 138.88, 131.29,

130.38, 129.97, 129.93, 129.89, 129.61, 129.27, 129.20, 128.69, 126.46, 122.81, 115.25, 115.03, 93.09, 75.33, 64.78, 53.63, 51.28, 27.74, 26.04; HRMS: m/z Calcd. for $C_{27}H_{22}FN_4O_2$ $[M+H]^+$: 453.1721; Found, 453.1739 (Rel. Int.100%); FT-IR (KBr) ν cm^{-1} : 1534, 1375, 1235.



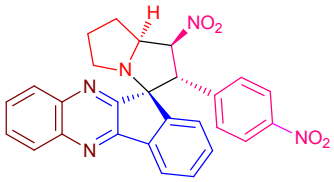
6. 2'-(4-chlorophenyl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5f

Colourless solid, mp 204-206°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 – 8.14 (m, 1H), 8.08 – 8.03 (m, 2H), 8.00 (d, J = 7.7 Hz, 1H), 7.77 – 7.72 (m, 2H), 7.65 (td, J = 7.6, 1.1 Hz, 1H), 7.58 (td, J = 7.5, 0.7 Hz, 1H), 6.82 – 6.76 (m, 4H), 6.66 (t, J = 9.9 Hz, 1H), 5.20 (dd, J = 16.9, 8.0 Hz, 1H), 4.89 (d, J = 10.3 Hz, 1H), 3.45 (ddd, J = 11.0, 8.3, 5.5 Hz, 1H), 2.85 (t, J = 7.3 Hz, 1H), 2.29 – 2.22 (m, 1H), 2.10 – 2.03 (m, 1H), 1.90 – 1.79 (m, 1H), 1.68 – 1.61 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.66, 152.80, 142.83, 142.50, 141.01, 138.88, 133.47, 131.50, 131.30, 130.44, 129.97, 129.64, 129.59, 129.30, 129.22, 128.37, 126.45, 122.87, 92.92, 75.33, 64.79, 53.64, 51.31, 27.76, 26.03; HRMS: m/z Calcd. for $C_{27}H_{22}ClN_4O_2$ $[M+H]^+$: 469.1426; Found, 469.1453 (Rel. Int.100%); FT-IR (KBr) ν cm^{-1} : 1532, 1374, 1100.



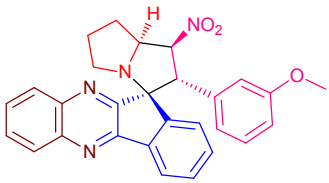
7. 2'-(4-bromophenyl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5g

Colourless solid, mp 210-212°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 – 8.14 (m, 1H), 8.10 – 8.03 (m, 2H), 8.00 (d, J = 7.7 Hz, 1H), 7.78 – 7.71 (m, 2H), 7.65 (td, J = 7.6, 1.2 Hz, 1H), 7.58 (td, J = 7.5, 0.9 Hz, 1H), 6.98 – 6.93 (m, 2H), 6.75 – 6.71 (m, 2H), 6.69 – 6.63 (m, 1H), 5.19 (dd, J = 16.8, 8.0 Hz, 1H), 4.88 (d, J = 10.3 Hz, 1H), 3.44 (ddd, J = 10.9, 8.3, 5.5 Hz, 1H), 2.85 (t, J = 7.3 Hz, 1H), 2.30 – 2.20 (m, 1H), 2.11 – 2.01 (m, 1H), 1.91 – 1.78 (m, 1H), 1.69 – 1.62 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.61, 152.79, 142.80, 142.50, 141.00, 138.88, 132.05, 131.30, 130.44, 129.97, 129.57, 129.29, 129.23, 126.43, 122.88, 121.66, 92.87, 75.27, 64.78, 53.69, 51.29, 27.75, 26.02; HRMS: m/z Calcd. for $C_{27}H_{22}BrN_4O_2$ $[M+H]^+$: 513.0921; Found, 513.0935 (Rel. Int.100%); FT-IR (KBr) ν cm^{-1} : 1533, 1372, 1107.



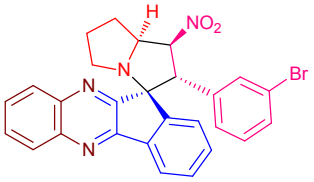
8. 1'-nitro-2'-(4-nitrophenyl)-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5h

   Light brown solid, mp 165-167°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 – 8.13 (m, 1H), 8.10 – 7.99 (m, 3H), 7.79 – 7.73 (m, 2H), 7.71 – 7.65 (m, 3H), 7.59 (td, *J* = 7.5, 0.8 Hz, 1H), 7.08 – 7.00 (m, 2H), 6.73 (t, *J* = 9.8 Hz, 1H), 5.22 (dd, *J* = 16.9, 7.9 Hz, 1H), 5.02 (d, *J* = 10.2 Hz, 1H), 3.45 (ddd, *J* = 11.0, 8.3, 5.5 Hz, 1H), 2.87 (t, *J* = 7.3 Hz, 1H), 2.32 – 2.22 (m, 1H), 2.13 – 2.03 (m, 1H), 1.91 – 1.79 (m, 1H), 1.68 – 1.60 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.04, 152.59, 147.12, 142.56, 142.29, 140.90, 140.75, 138.83, 131.47, 130.74, 130.23, 129.56, 129.53, 129.29, 129.23, 126.39, 123.30, 123.02, 92.63, 75.53, 65.01, 53.93, 51.36, 27.84, 26.01; HRMS: m/z Calcd. for $C_{27}H_{22}N_5O_4$ $[M+H]^+$: 480.1666; Found, 480.1682 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1554, 1369.



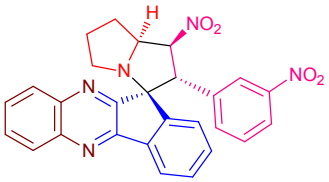
9. 2'-(3-methoxyphenyl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5i

   Pale yellow solid, mp 186-188°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 – 8.13 (m, 1H), 8.08 – 7.99 (m, 3H), 7.76 – 7.68 (m, 2H), 7.65 (td, *J* = 7.6, 1.2 Hz, 1H), 7.56 (td, *J* = 7.5, 0.9 Hz, 1H), 6.71 (dt, *J* = 19.7, 8.9 Hz, 2H), 6.46 – 6.39 (m, 2H), 6.36 – 6.32 (m, 1H), 5.22 (dd, *J* = 16.6, 8.1 Hz, 1H), 4.91 (d, *J* = 10.3 Hz, 1H), 3.47 (ddd, *J* = 10.9, 8.3, 5.5 Hz, 1H), 3.27 (s, 3H), 2.87 (t, *J* = 7.3 Hz, 1H), 2.31 – 2.20 (m, 1H), 2.12 – 2.02 (m, 1H), 1.93 – 1.78 (m, 1H), 1.70 – 1.64 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.05, 159.02, 152.91, 143.28, 142.43, 141.11, 138.89, 134.38, 131.23, 130.27, 129.82, 129.55, 129.18, 129.14, 129.07, 126.58, 122.76, 120.79, 113.77, 113.40, 93.07, 75.42, 64.85, 54.70, 54.24, 51.32, 27.73, 26.05; HRMS: m/z Calcd. for $C_{28}H_{25}N_4O_3$ $[M+H]^+$: 465.1921; Found, 465.1948 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1542, 1372, 1289, 1052.



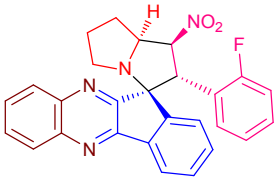
10. 2'-(3-bromophenyl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5j

Colourless solid, mp 176-178°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 – 8.13 (m, 1H), 8.10 – 7.98 (m, 3H), 7.78 – 7.72 (m, 2H), 7.67 (td, *J* = 7.6, 1.0 Hz, 1H), 7.59 (td, *J* = 7.6, 0.6 Hz, 1H), 7.06 – 6.97 (m, 2H), 6.79 – 6.60 (m, 3H), 5.20 (dd, *J* = 16.7, 7.9 Hz, 1H), 4.89 (d, *J* = 10.1 Hz, 1H), 3.44 (ddd, *J* = 10.8, 8.4, 5.6 Hz, 1H), 2.85 (t, *J* = 7.1 Hz, 1H), 2.33 – 2.20 (m, 1H), 2.13 – 2.01 (m, 1H), 1.93 – 1.77 (m, 1H), 1.69 – 1.61 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.54, 152.77, 142.78, 142.47, 140.99, 138.83, 135.38, 131.79, 131.37, 130.65, 130.49, 129.97, 129.58, 129.31, 129.14, 126.77, 126.43, 122.83, 122.10, 92.87, 75.38, 64.93, 53.95, 51.20, 27.72, 26.01; HRMS: m/z Calcd. for $C_{27}H_{22}BrN_4O_2$ $[M+H]^+$: 513.0921; Found, 513.0930 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1536, 1371, 1071.



11. 1'-nitro-2'-(3-nitrophenyl)-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5k

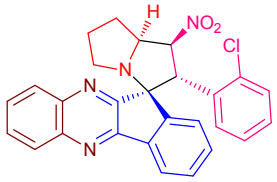
Pale yellow solid, mp 175-177°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 – 8.17 (m, 1H), 8.12 – 7.97 (m, 3H), 7.89 – 7.64 (m, 5H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.19 (d, *J* = 7.8 Hz, 1H), 7.02 (t, *J* = 8.0 Hz, 1H), 6.74 (t, *J* = 9.7 Hz, 1H), 5.23 (dd, *J* = 16.6, 8.0 Hz, 1H), 5.04 (d, *J* = 10.1 Hz, 1H), 3.45 (ddd, *J* = 10.7, 8.4, 5.6 Hz, 1H), 2.87 (t, *J* = 7.2 Hz, 1H), 2.36 – 2.21 (m, 1H), 2.16 – 2.02 (m, 1H), 1.95 – 1.78 (m, 1H), 1.72 – 1.64 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.01, 152.63, 147.74, 142.51, 142.29, 140.93, 138.79, 135.45, 134.23, 131.55, 130.75, 130.22, 129.59, 129.13, 126.37, 123.58, 122.93, 122.62, 92.78, 75.41, 65.00, 53.87, 51.23, 27.80, 26.00; HRMS: m/z Calcd. for $C_{27}H_{22}N_5O_4$ $[M+H]^+$: 480.1666; Found, 480.1685 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1534, 1374.



12. 2'-(2-fluorophenyl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5l

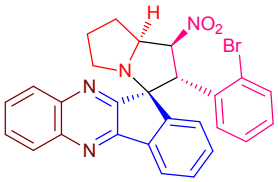
Colourless solid, mp 208-210°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 – 8.17 (m, 1H), 8.05 (ddd, *J* = 15.2, 8.3, 4.5 Hz, 3H), 7.78 – 7.72 (m, 2H), 7.62 (td, *J* = 7.6, 1.2 Hz, 1H), 7.54 (td, *J* = 7.5, 0.9 Hz, 1H), 6.97 (td, *J* = 7.7, 1.6 Hz, 1H), 6.92 – 6.85 (m, 1H), 6.73 – 6.65 (m, 2H), 6.58 – 6.52 (m, 1H), 5.46 (d, *J* = 10.4 Hz, 1H), 5.20 (dd, *J* =

17.0, 7.9 Hz, 1H), 3.50 (ddd, *J* = 11.0, 8.3, 5.4 Hz, 1H), 2.84 (t, *J* = 7.3 Hz, 1H), 2.30 – 2.21 (m, 1H), 2.11 – 2.04 (m, 1H), 1.90 – 1.78 (m, 1H), 1.70 – 1.63 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.90 (d, *J* = 2.5 Hz), 159.95, 153.08, 142.54, 142.35, 140.97, 138.57, 131.12, 130.34, 129.91, 129.66, 129.23 – 129.11 (m), 129.09 – 128.99 (m), 127.34 (d, *J* = 3.3 Hz), 123.78 (d, *J* = 3.6 Hz), 122.31, 120.53, 120.42, 115.60, 115.41, 93.23, 75.21, 64.76, 51.29, 45.09 (d, *J* = 2.1 Hz), 27.88, 26.01; HRMS: m/z Calcd. for $C_{27}H_{22}FN_4O_2$ $[M+H]^+$: 453.1721; Found, 453.1739 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1538, 1371, 1235.



13. 2'-(2-chlorophenyl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5m

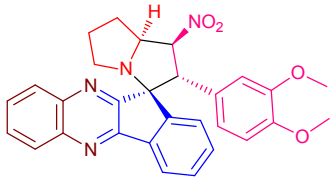
Pale yellow solid, mp 200-202°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.14 (m, 2H), 8.10 – 8.05 (m, 1H), 8.05 – 8.00 (m, 1H), 7.80 – 7.73 (m, 2H), 7.56 (dtd, *J* = 22.8, 7.5, 1.1 Hz, 2H), 7.05 (td, *J* = 8.1, 1.3 Hz, 2H), 6.84 (td, *J* = 7.7, 1.6 Hz, 1H), 6.68 – 6.60 (m, 1H), 6.53 (t, *J* = 9.7 Hz, 1H), 5.83 (d, *J* = 10.2 Hz, 1H), 5.25 (dd, *J* = 16.8, 7.9 Hz, 1H), 3.52 (ddd, *J* = 10.8, 8.3, 5.5 Hz, 1H), 2.85 (t, *J* = 7.2 Hz, 1H), 2.32 – 2.21 (m, 1H), 2.14 – 2.04 (m, 1H), 1.92 – 1.79 (m, 1H), 1.72 – 1.63 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.94, 153.19, 142.53, 142.20, 140.91, 138.45, 135.16, 131.40, 130.85, 130.37, 129.99, 129.66, 129.44, 129.24, 129.20, 128.69, 128.26, 126.46, 122.25, 94.84, 75.57, 64.90, 51.07, 48.79, 27.76, 25.99; HRMS: m/z Calcd. for $C_{27}H_{22}ClN_4O_2$ $[M+H]^+$: 469.1426; Found, 469.1467 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1539, 1370, 1049.



14. 2'-(2-bromophenyl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5n

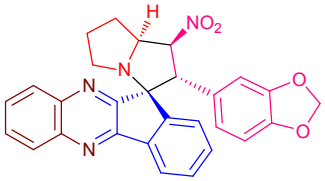
Colourless solid, mp 201-203°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25 (d, *J* = 7.7 Hz, 3H), 8.23 – 8.18 (m, 3H), 8.10 – 8.05 (m, 3H), 8.03 (d, *J* = 7.3 Hz, 3H), 7.80 – 7.73 (m, 6H), 7.59 (td, *J* = 7.6, 1.3 Hz, 3H), 7.53 (td, *J* = 7.5, 0.9 Hz, 3H), 7.28 – 7.25 (m, 4H), 7.02 (dd, *J* = 8.0, 1.6 Hz, 3H), 6.75 (td, *J* = 7.7, 1.7 Hz, 3H), 6.70 – 6.65 (m, 3H), 6.48 (t, *J* = 9.7 Hz, 3H), 5.82 (d, *J* = 10.1 Hz, 3H), 5.26 (dd, *J* = 16.8, 7.9 Hz, 3H), 3.52 (ddd, *J* = 10.7, 8.3, 5.6 Hz, 3H), 2.85 (t, *J* = 7.2 Hz, 3H), 2.30 – 2.22 (m, 3H), 2.13 – 2.06 (m, 3H), 1.91 – 1.80 (m, 3H), 1.71 – 1.64 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.92, 153.24, 142.54, 142.18, 140.90, 138.43, 133.49, 133.23,

130.81, 130.39, 130.01, 129.67, 129.56, 129.25, 129.21, 129.02, 128.66, 127.08, 126.17, 122.24, 95.11, 75.69, 64.94, 51.62, 50.95, 27.69, 25.99; HRMS: m/z Calcd. for $C_{27}H_{22}BrN_4O_2$ $[M+H]^+$: 513.0921; Found, 513.0960 (Rel. Int.100%); FT-IR (KBr) ν cm^{-1} : 1536, 1368, 1046.



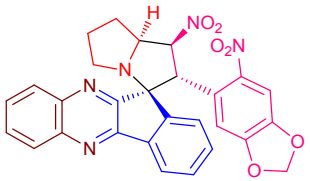
15. 2'-(3,4-dimethoxyphenyl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5o

Pale yellow solid, mp 202-204°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 – 8.11 (m, 1H), 8.09 – 7.98 (m, 3H), 7.76 – 7.69 (m, 2H), 7.65 (td, J = 7.6, 1.3 Hz, 1H), 7.56 (td, J = 7.5, 0.9 Hz, 1H), 6.67 – 6.58 (m, 1H), 6.39 (dd, J = 8.3, 2.1 Hz, 1H), 6.32 (d, J = 8.3 Hz, 1H), 6.25 (d, J = 2.1 Hz, 1H), 5.23 (dd, J = 16.7, 8.0 Hz, 1H), 4.87 (d, J = 10.3 Hz, 1H), 3.58 (s, 3H), 3.49 (ddd, J = 10.9, 8.3, 5.5 Hz, 1H), 3.18 (s, 3H), 2.90 (t, J = 7.2 Hz, 1H), 2.32 – 2.20 (m, 1H), 2.14 – 2.02 (m, 1H), 1.95 – 1.79 (m, 1H), 1.72 – 1.64 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.27, 152.95, 148.16, 143.48, 142.42, 141.10, 138.95, 131.16, 130.20, 129.83, 129.39, 129.24, 129.19, 126.55, 125.07, 122.79, 120.91, 111.01, 110.52, 93.16, 75.48, 64.92, 55.50, 55.12, 54.22, 51.29, 27.74, 26.08; HRMS: m/z Calcd. for $C_{29}H_{27}N_4O_4$ $[M+H]^+$: 495.202721; Found, 495.2055 (Rel. Int.100%); FT-IR (KBr) ν cm^{-1} : 1527, 1372, 1264, 1142, 1025.



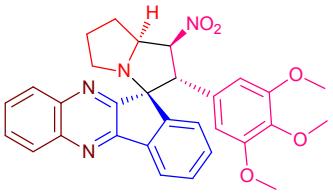
16. 2'-(benzo[d][1,3]dioxol-5-yl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5p

Pale yellow solid, mp 176-178°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 – 8.13 (m, 1H), 8.06 (ddd, J = 9.1, 7.8, 5.3 Hz, 2H), 7.98 (d, J = 7.7 Hz, 1H), 7.77 – 7.70 (m, 2H), 7.64 (td, J = 7.6, 1.2 Hz, 1H), 7.57 (td, J = 7.5, 0.8 Hz, 1H), 6.65 – 6.56 (m, 1H), 6.32 (ddd, J = 30.1, 18.3, 4.9 Hz, 3H), 5.66 (dd, J = 12.7, 1.4 Hz, 2H), 5.17 (dd, J = 16.8, 8.0 Hz, 1H), 4.84 (d, J = 10.4 Hz, 1H), 3.44 (ddd, J = 11.0, 8.3, 5.5 Hz, 1H), 2.83 (t, J = 7.2 Hz, 1H), 2.29 – 2.18 (m, 1H), 2.11 – 2.01 (m, 1H), 1.90 – 1.77 (m, 1H), 1.68 – 1.61 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.05, 152.95, 147.27, 146.87, 143.17, 142.48, 141.10, 138.91, 131.28, 130.31, 129.87, 129.68, 129.23, 129.10, 126.48, 122.76, 122.09, 108.67, 107.94, 100.84, 93.32, 75.26, 64.56, 53.96, 51.29, 27.71, 26.01; HRMS: m/z Calcd. for $C_{28}H_{23}N_4O_4$ $[M+H]^+$: 479.1714; Found, 479.1682 (Rel. Int.100%); FT-IR (KBr) ν cm^{-1} : 1540, 1372, 1251, 1035.



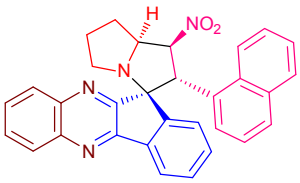
17. 1'-nitro-2'-(6-nitrobenzo[d][1,3]dioxol-5-yl)-1',2',5',6',7',7a' hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5q

Pale green solid, mp 208-210°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.15 (m, 1H), 8.12 – 8.02 (m, 2H), 7.92 (d, *J* = 7.4 Hz, 1H), 7.81 – 7.74 (m, 2H), 7.63 – 7.50 (m, 2H), 6.97 (s, 1H), 6.68 (s, 1H), 6.58 (t, *J* = 9.7 Hz, 1H), 6.29 (d, *J* = 10.2 Hz, 1H), 5.83 – 5.79 (m, 1H), 5.73 – 5.68 (m, 1H), 5.23 (dd, *J* = 16.4, 8.2 Hz, 1H), 3.46 (ddd, *J* = 10.9, 8.3, 5.5 Hz, 1H), 2.83 (t, *J* = 7.2 Hz, 1H), 2.32 – 2.21 (m, 1H), 2.14 – 2.03 (m, 1H), 1.89 – 1.75 (m, 1H), 1.73 – 1.63 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.53, 153.04, 150.54, 146.97, 145.03, 142.59, 141.57, 140.80, 138.42, 131.87, 130.55, 130.22, 129.54, 129.50, 129.17, 127.27, 123.87, 122.45, 108.34, 106.15, 102.74, 94.11, 76.14, 64.84, 51.27, 46.30, 27.80, 25.89; HRMS: m/z Calcd. for $C_{28}H_{22}N_5O_6$ $[M+H]^+$: 524.1565; Found, 524.1585 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1545, 1521, 1336, 1259.



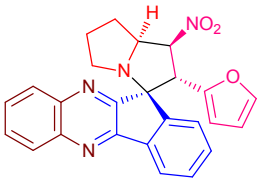
18. 1'-nitro-2'-(3,4,5-trimethoxyphenyl)-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5r

Light orange solid, mp 168-170°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 – 8.11 (m, 1H), 8.09 – 8.00 (m, 3H), 7.75 – 7.69 (m, 2H), 7.65 (td, *J* = 7.6, 1.2 Hz, 1H), 7.57 (td, *J* = 7.5, 0.7 Hz, 1H), 6.60 (t, *J* = 9.8 Hz, 1H), 5.98 (s, 2H), 5.24 (dd, *J* = 16.7, 8.0 Hz, 1H), 4.84 (d, *J* = 10.2 Hz, 1H), 3.56 (s, 3H), 3.49 (ddd, *J* = 10.9, 8.3, 5.6 Hz, 1H), 3.25 (s, 6H), 2.91 (t, *J* = 7.2 Hz, 1H), 2.32 – 2.21 (m, 1H), 2.13 – 2.04 (m, 1H), 1.93 – 1.81 (m, 1H), 1.71 – 1.64 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.21, 152.99, 152.54, 143.49, 142.48, 141.12, 139.08, 137.17, 131.17, 130.33, 129.96, 129.36, 129.34, 129.26, 128.34, 126.55, 122.96, 105.64, 93.20, 75.59, 65.11, 60.64, 55.60, 54.91, 51.33, 27.81, 26.15; HRMS: m/z Calcd. for $C_{30}H_{28}N_4NaO_5$ $[M+Na]^+$: 547.1952; Found, 547.1904 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1587, 1366, 1242, 1125, 1007.



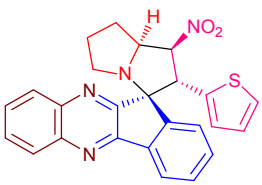
19. 2'-(naphthalen-1-yl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5s

Colourless solid, mp 192-194°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 – 8.21 (m, 1H), 8.20 – 8.15 (m, 2H), 8.05 – 8.00 (m, 1H), 7.86 (d, *J* = 7.5 Hz, 1H), 7.80 – 7.71 (m, 2H), 7.60 – 7.55 (m, 1H), 7.51 (td, *J* = 7.6, 1.2 Hz, 1H), 7.42 – 7.34 (m, 3H), 7.33 – 7.27 (m, 1H), 7.24 (dd, *J* = 7.5, 0.8 Hz, 1H), 6.85 (t, *J* = 7.8 Hz, 1H), 6.60 (t, *J* = 9.1 Hz, 1H), 6.10 (d, *J* = 9.3 Hz, 1H), 5.40 (dd, *J* = 16.6, 7.8 Hz, 1H), 3.56 (ddd, *J* = 9.8, 8.3, 5.9 Hz, 1H), 2.91 – 2.83 (m, 1H), 2.34 – 2.25 (m, 1H), 2.21 – 2.11 (m, 1H), 2.00 – 1.87 (m, 1H), 1.76 – 1.65 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.35, 153.08, 143.39, 142.33, 141.00, 138.41, 133.61, 132.10, 131.03, 130.11, 129.85, 129.69, 129.16, 128.67, 128.15, 126.87, 126.61, 125.85, 125.41, 124.46, 122.87, 122.43, 95.52, 75.40, 65.62, 50.15, 48.96, 27.39, 26.08; HRMS: m/z Calcd. for $C_{31}H_{25}N_4O_2$ $[M+H]^+$: 485.1972; Found, 485.2011 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1537, 1372.



20. 2'-(furan-2-yl)-1'-nitro-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5t

Grey solid, mp 184-186°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 6.9 Hz, 1H), 8.13 – 8.04 (m, 2H), 7.95 (d, *J* = 7.2 Hz, 1H), 7.76 – 7.68 (m, 2H), 7.68 – 7.57 (m, 2H), 6.84 (d, *J* = 0.9 Hz, 1H), 6.59 (t, *J* = 9.7 Hz, 1H), 5.82 (dd, *J* = 3.1, 1.8 Hz, 1H), 5.47 (d, *J* = 3.2 Hz, 1H), 5.17 (dd, *J* = 16.3, 8.4 Hz, 1H), 5.09 (d, *J* = 9.9 Hz, 1H), 3.40 (ddd, *J* = 11.0, 8.3, 5.5 Hz, 1H), 2.85 (t, *J* = 7.2 Hz, 1H), 2.31 – 2.18 (m, 1H), 2.11 – 1.98 (m, 1H), 1.91 – 1.75 (m, 1H), 1.70 – 1.62 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.85, 152.76, 148.26, 143.15, 142.51, 141.97, 141.23, 138.93, 131.40, 130.40, 129.77, 129.09, 126.41, 122.72, 110.08, 107.40, 92.35, 73.83, 64.87, 51.19, 48.00, 27.56, 26.03; HRMS: m/z Calcd. for $C_{25}H_{21}N_4O_3$ $[M+H]^+$: 425.1608; Found, 425.1618 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1537, 1376, 1252.



21. 1'-nitro-2'-(thiophen-2-yl)-1',2',5',6',7',7a'-hexahydrospiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizine] 5u

Colourless solid, mp 209-210°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 – 8.10 (m, 2H), 8.10 – 8.04 (m, 1H), 7.96 (d, *J* = 7.5 Hz, 1H), 7.76 – 7.70 (m, 2H), 7.62 (dtd, *J* = 22.6, 7.4, 1.1 Hz, 2H), 6.74 (dd, *J* = 4.6, 1.6 Hz, 1H), 6.59 (t, *J* = 9.8 Hz, 1H), 6.54 – 6.47 (m, 2H), 5.25 – 5.15 (m, 2H), 3.44 (ddd, *J* = 11.2, 8.3, 5.4 Hz, 1H), 2.89 (t, *J* = 7.2 Hz, 1H), 2.30 – 2.20 (m, 1H), 2.11 – 2.01 (m, 1H), 1.92 – 1.77 (m, 1H), 1.69 – 1.62 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.83, 153.05, 142.88, 142.61, 141.21, 139.28, 135.90, 131.38, 130.50, 129.88, 129.76, 129.19, 129.16, 126.53, 126.40, 124.89, 122.83, 94.78, 74.88, 64.73, 51.44, 49.83, 27.73, 26.06; HRMS: m/z Calcd. for $C_{25}H_{21}N_4O_2S$ $[M+H]^+$: 441.138; Found, 441.1337 (Rel. Int.100%); FT-IR (KBr) *v* cm^{-1} : 1536, 1374, 1244.

Spectra

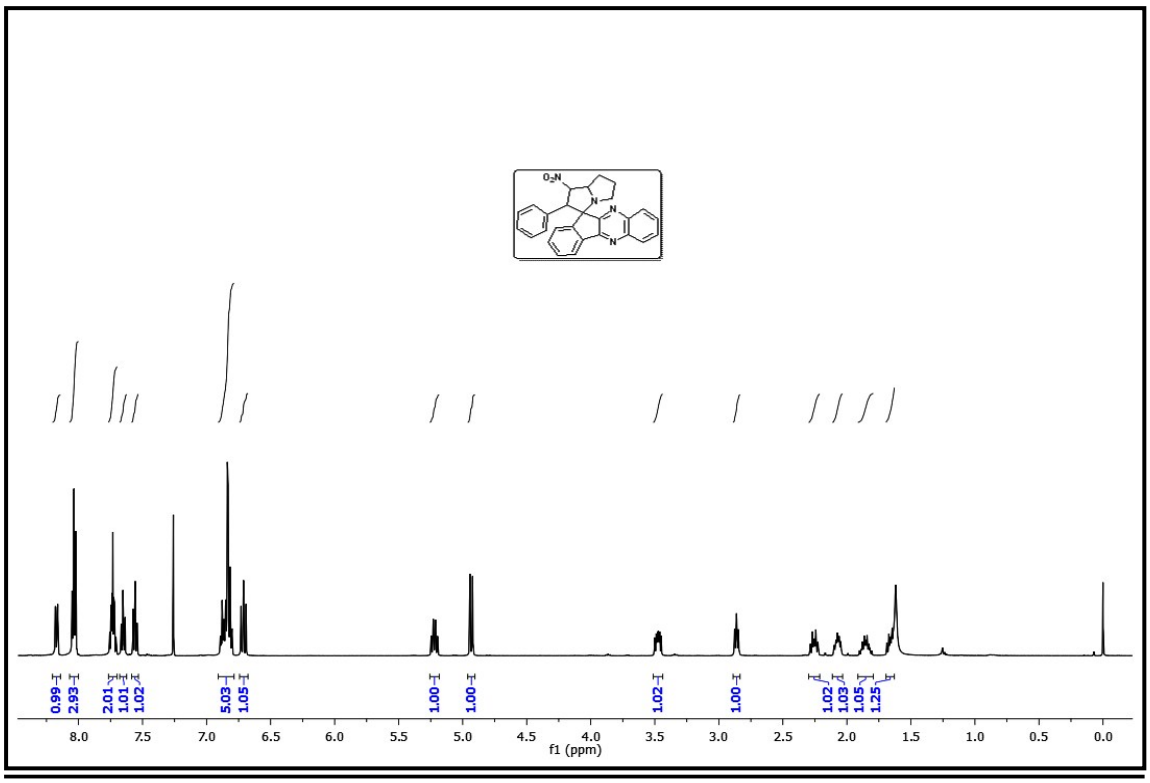


Fig. S1. ^{1}H NMR spectrum of 5a in $CDCl_3$

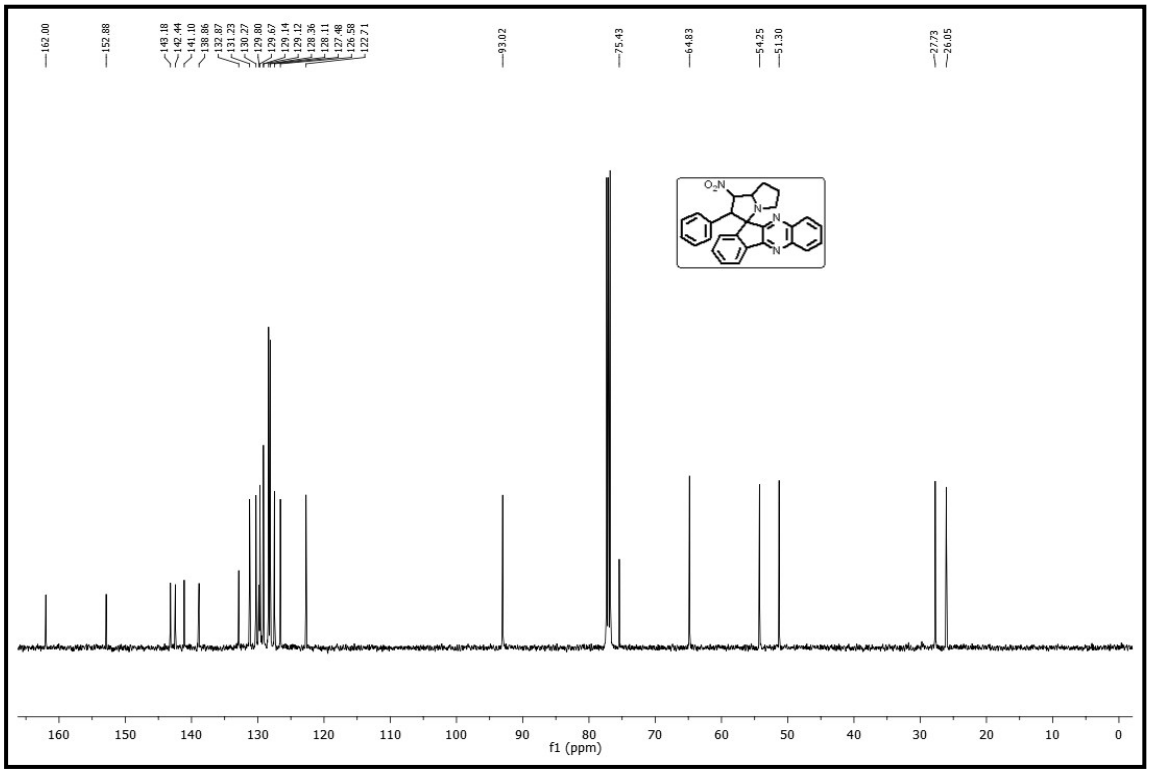


Fig. S2. ^{13}C NMR spectrum of 5a in $CDCl_3$

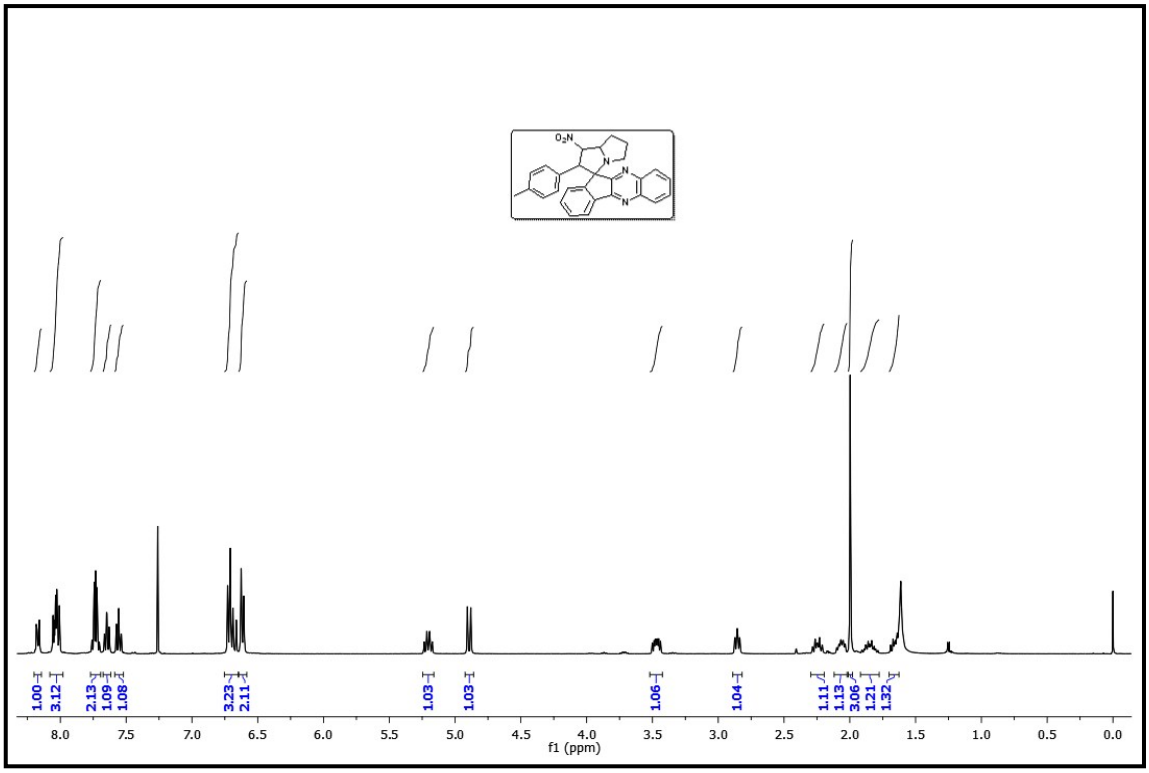


Fig. S3. ^{1}H NMR spectrum of 5b in $CDCl_3$

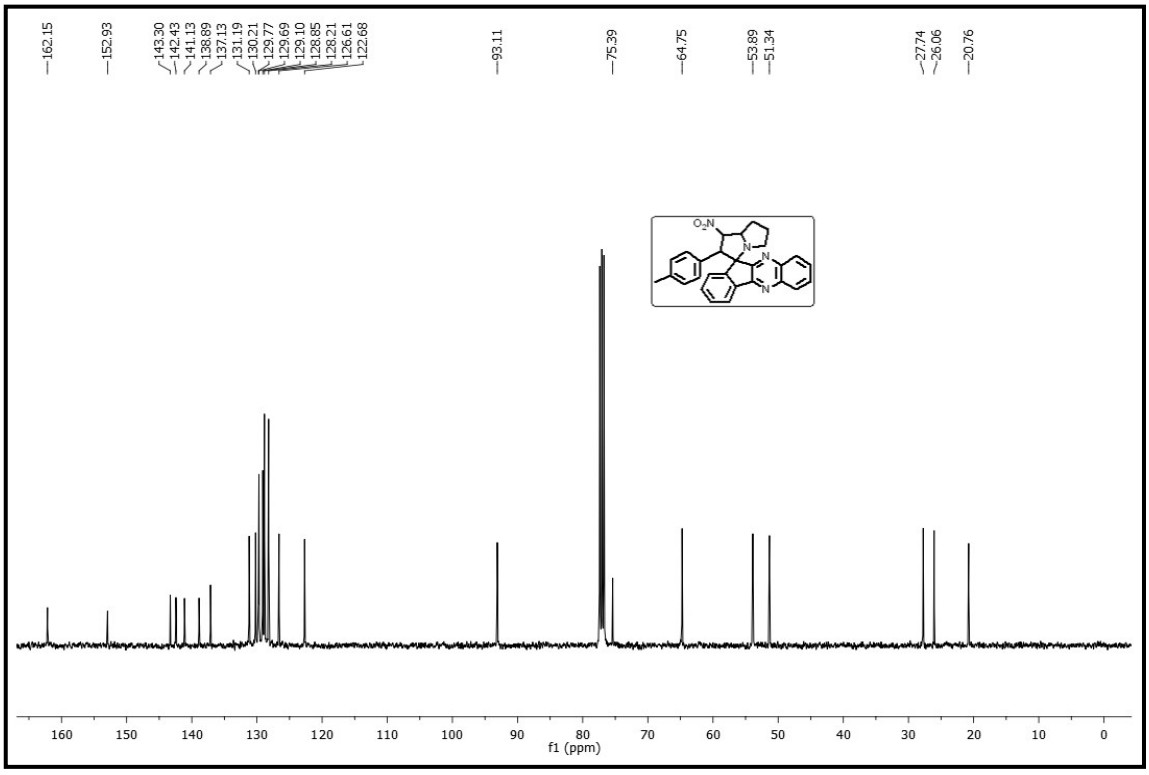


Fig. S4. ^{13}C NMR spectrum of 5b in $CDCl_3$

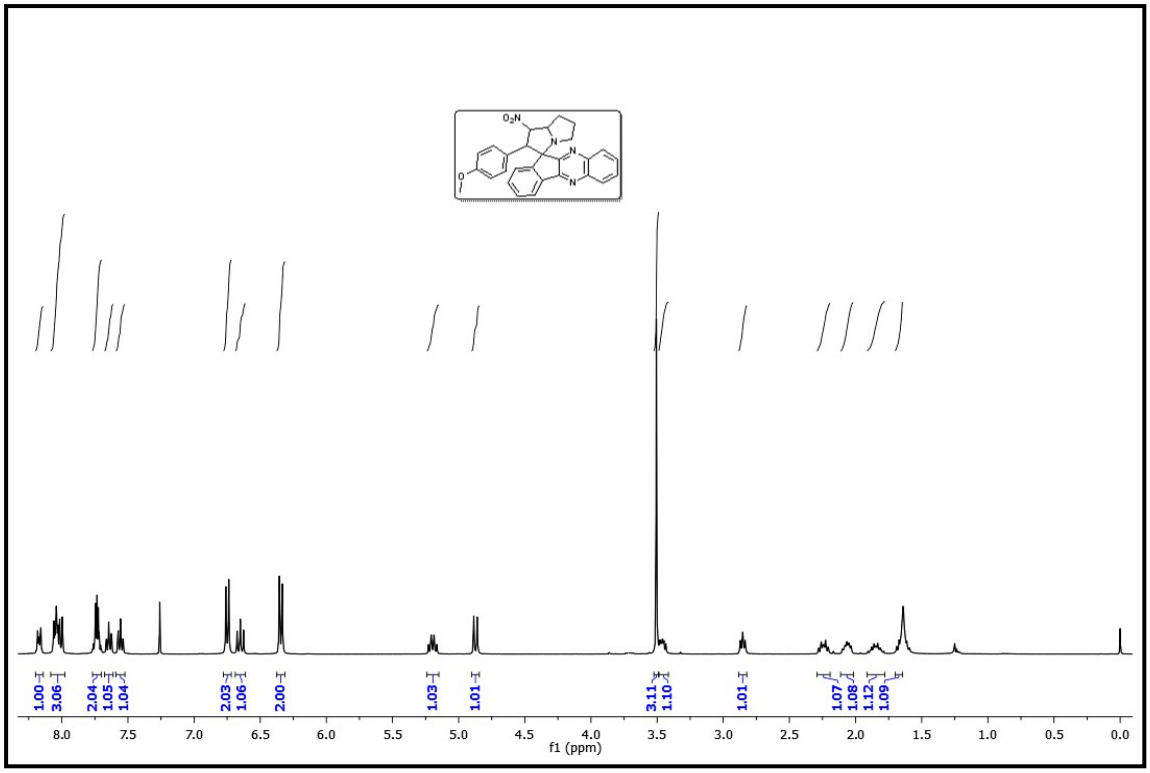


Fig. S5. ^{1}H NMR spectrum of 5c in $CDCl_3$

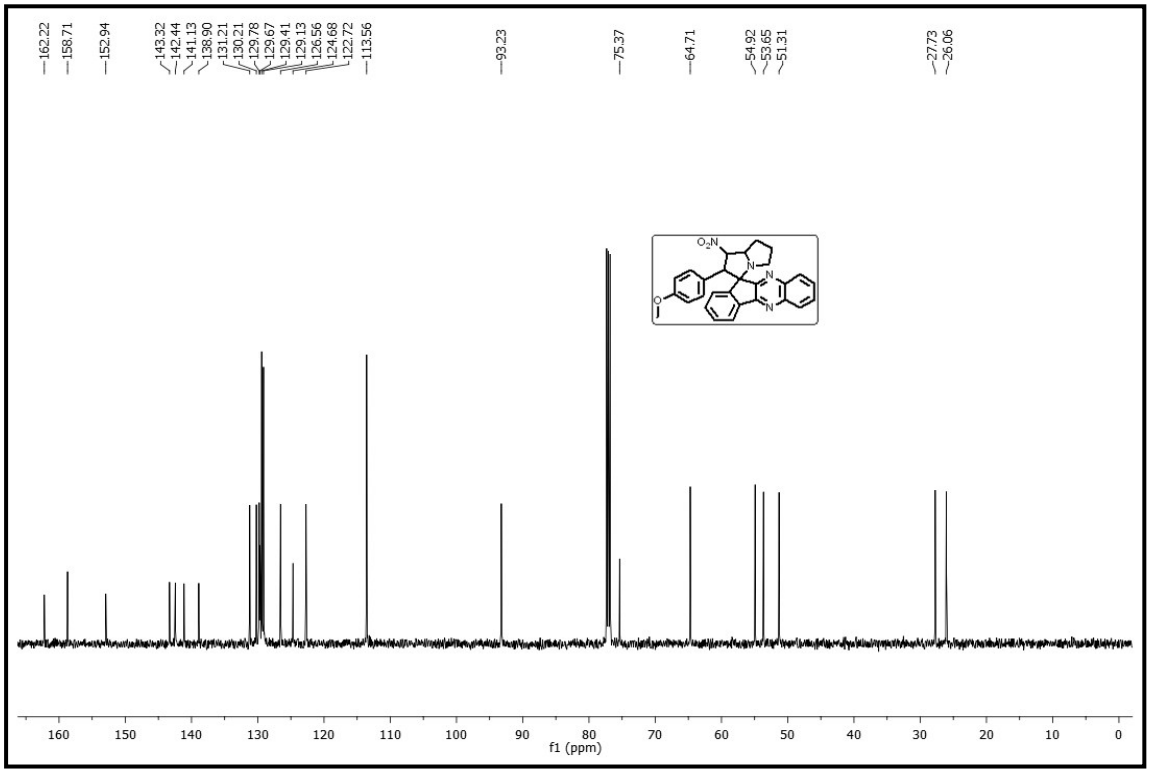


Fig. S6. ^{13}C NMR spectrum of 5c in $CDCl_3$

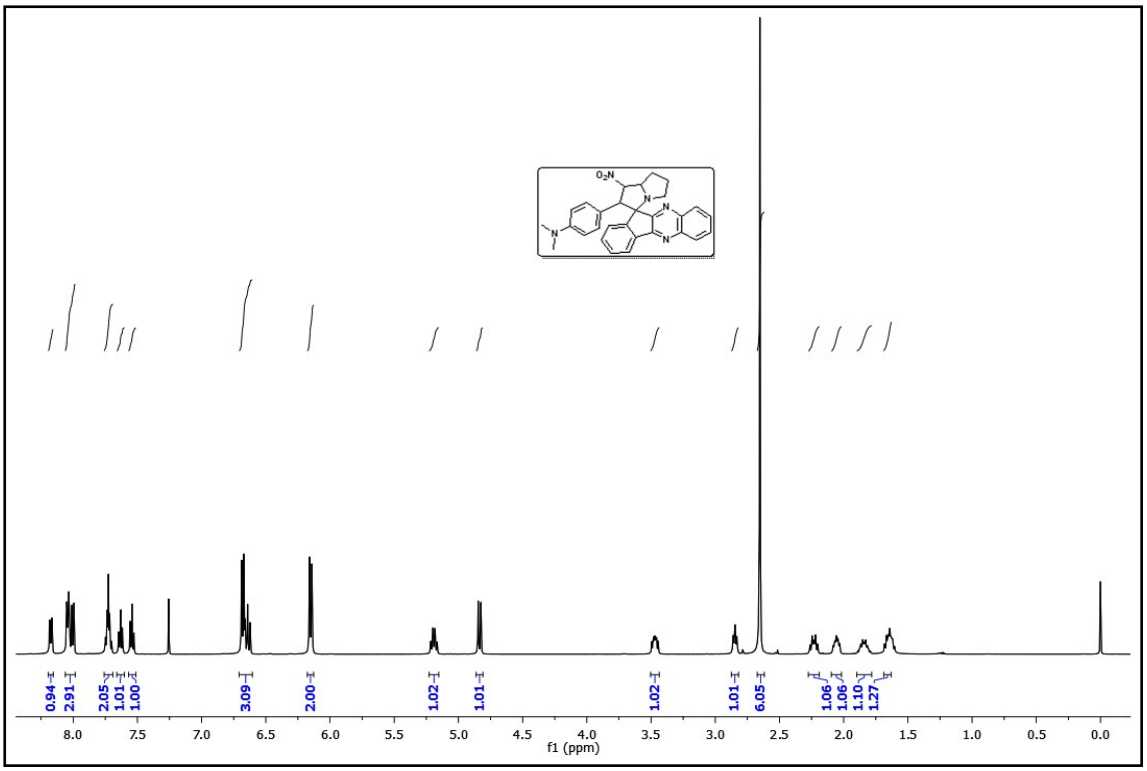


Fig. S7. ^{1}H NMR spectrum of 5d in $CDCl_3$

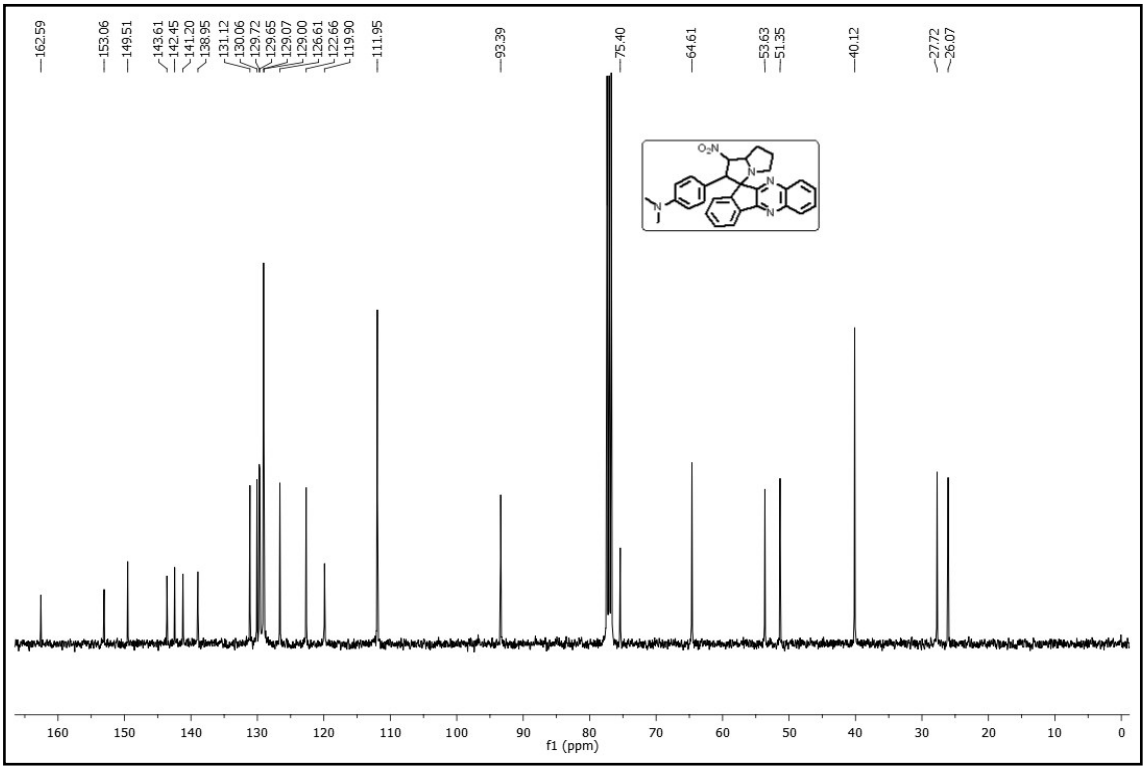


Fig. S8. ^{13}C NMR spectrum of 5d in $CDCl_3$

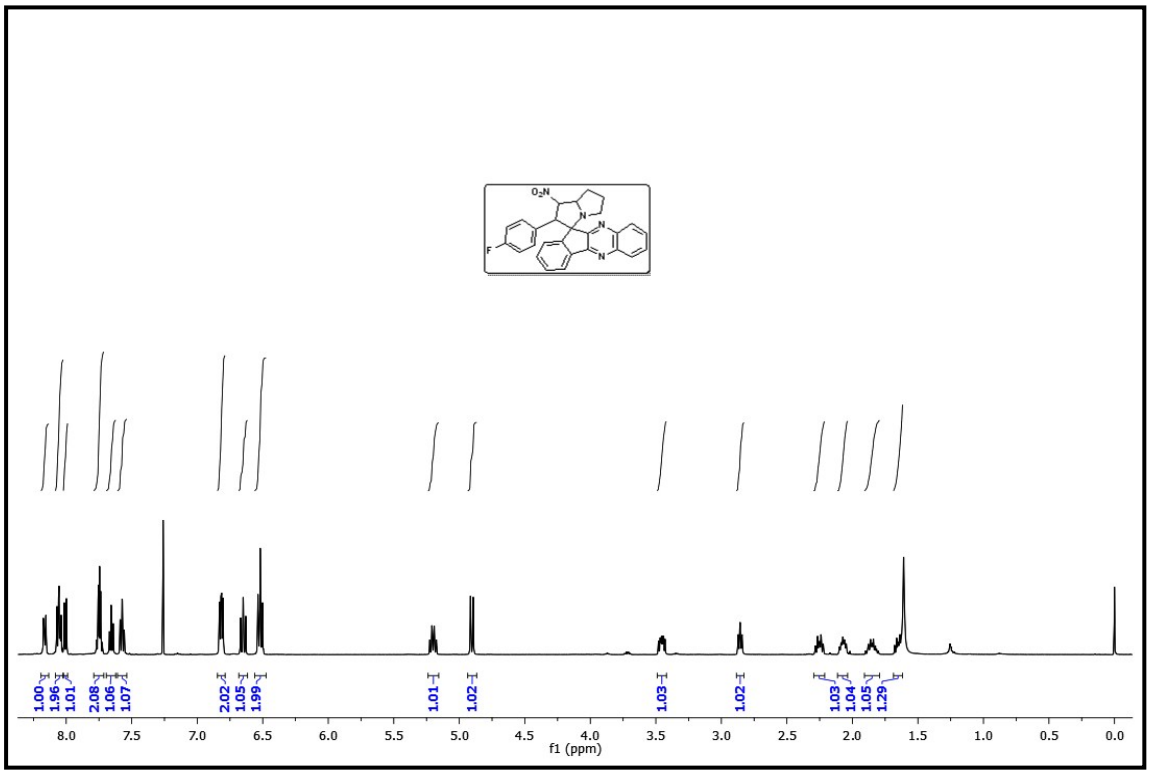


Fig. S9. ^{1}H NMR spectrum of 5e in $CDCl_3$

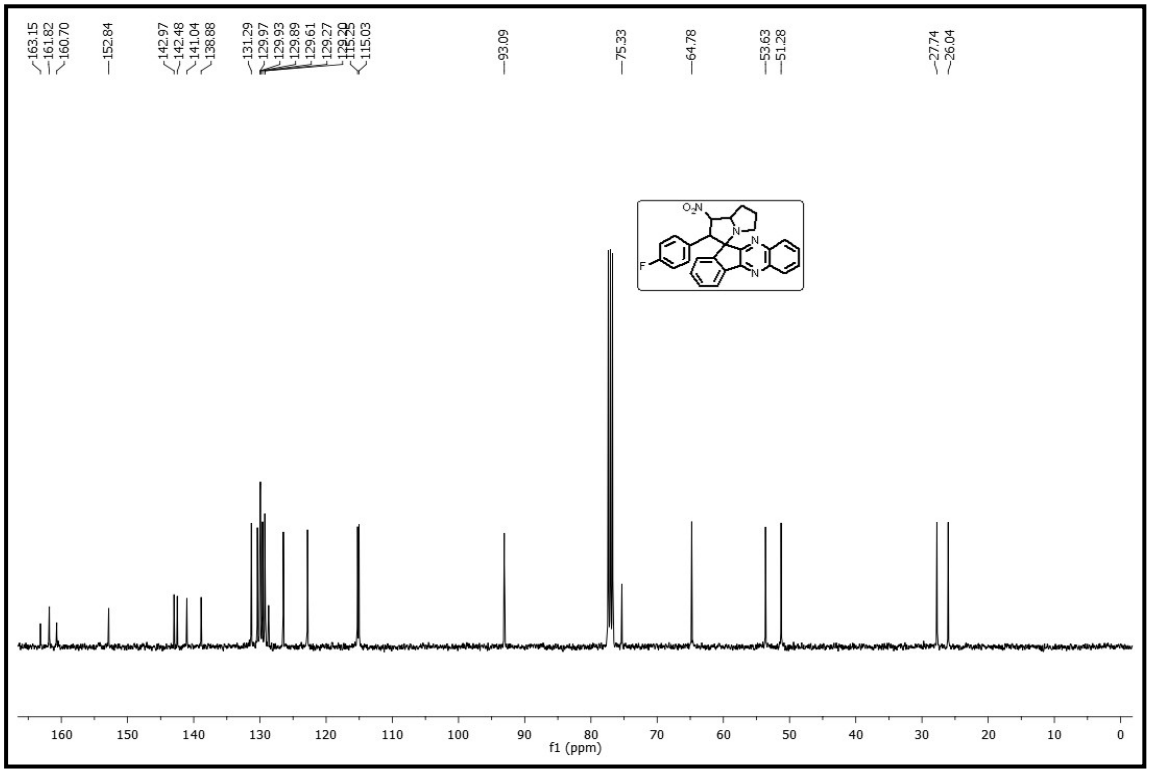


Fig. S10. ^{13}C NMR spectrum of 5e in $CDCl_3$

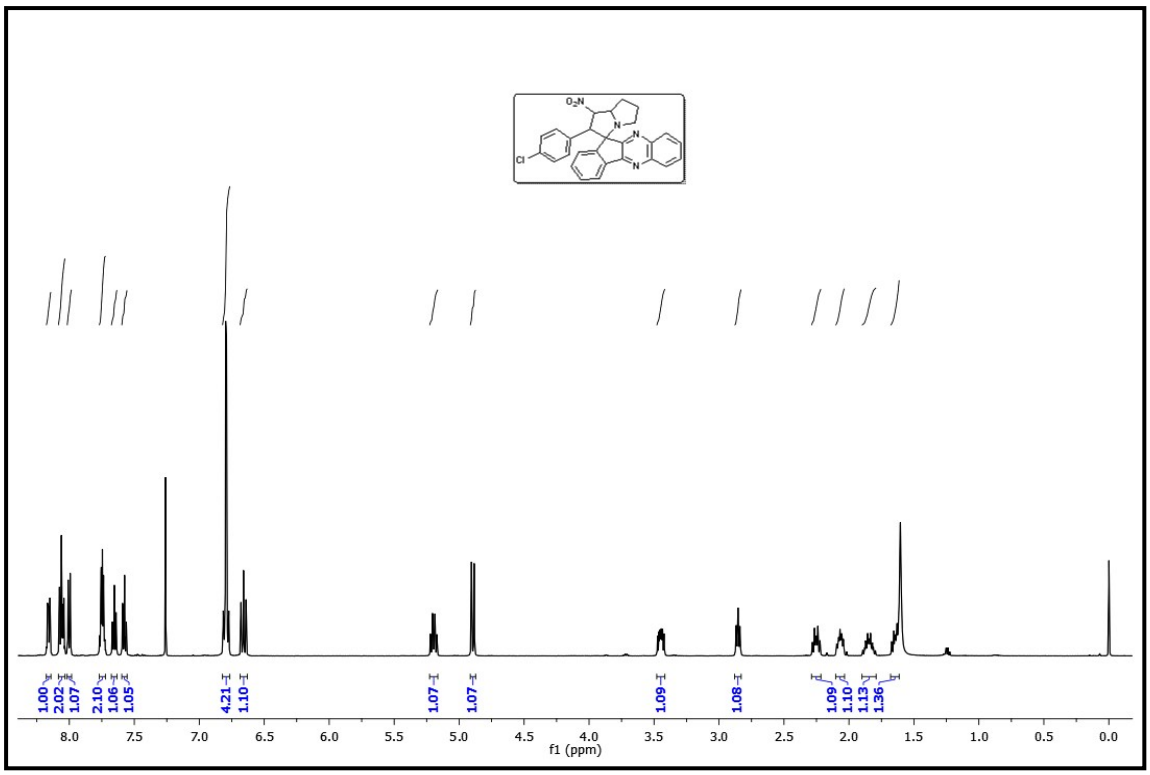


Fig. S11. ^{1}H NMR spectrum of 5f in $CDCl_3$

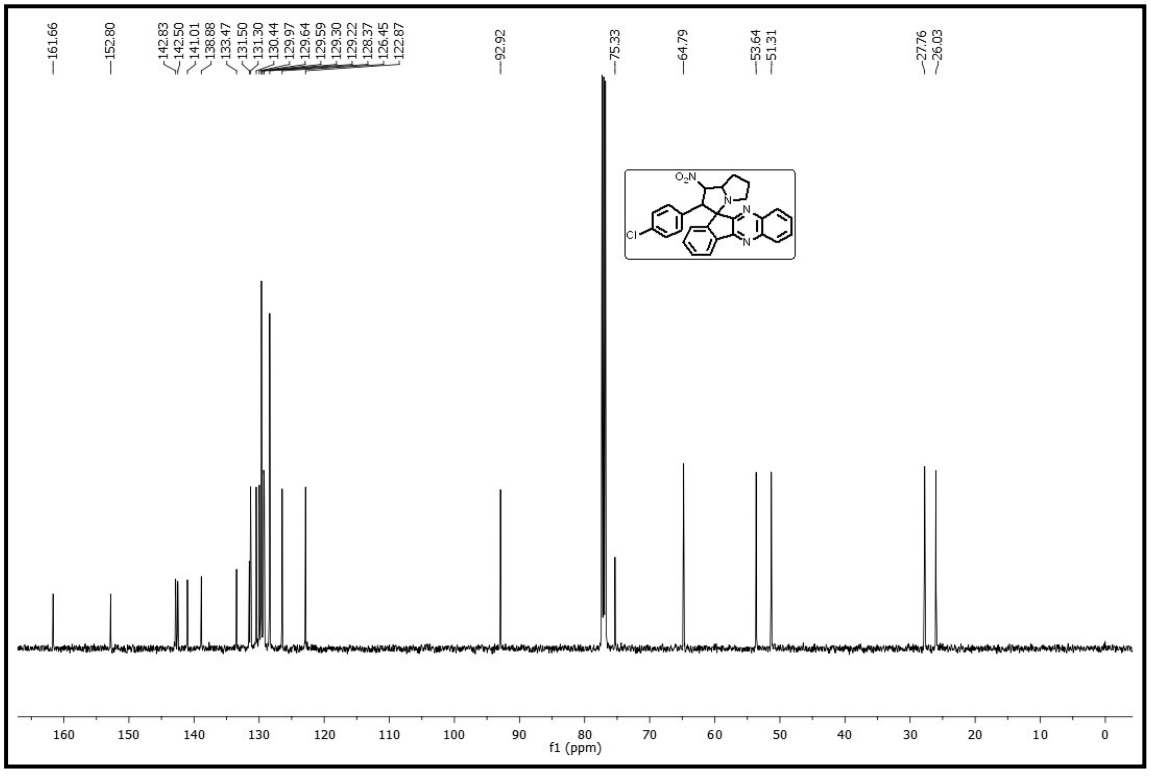


Fig. S12. ^{13}C NMR spectrum of 5f in $CDCl_3$

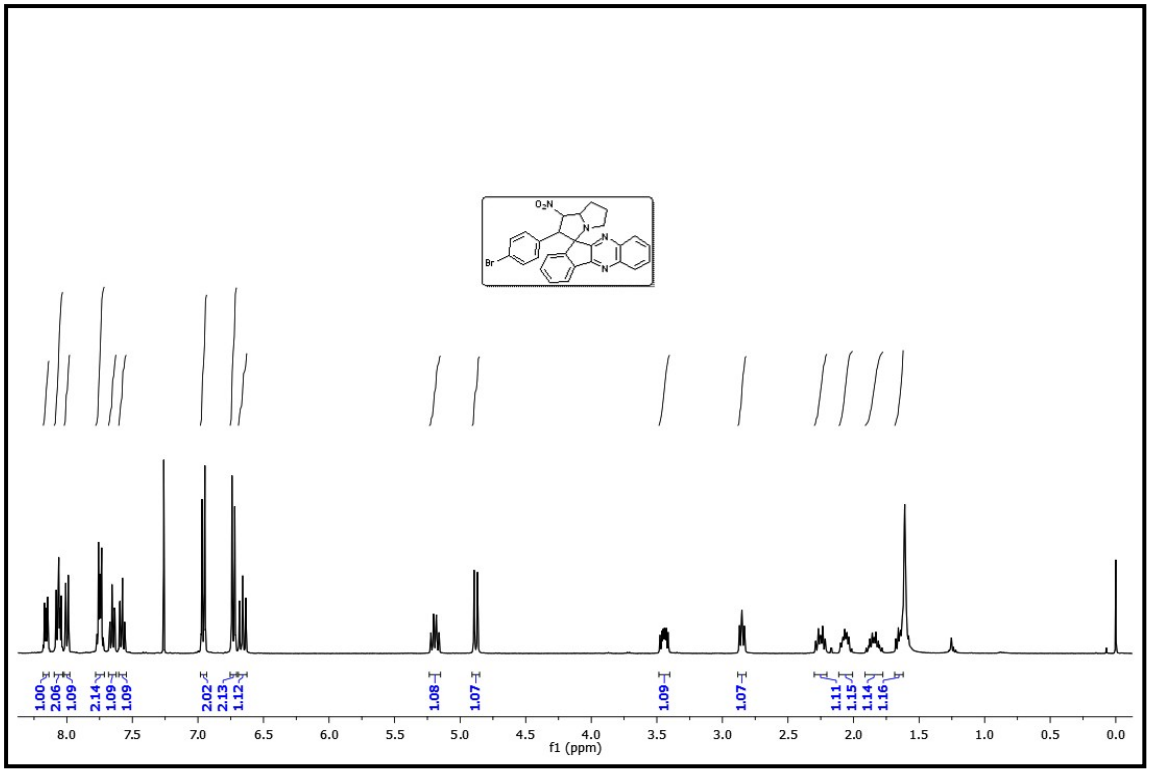


Fig. S13. ^{1}H NMR spectrum of 5g in $CDCl_3$

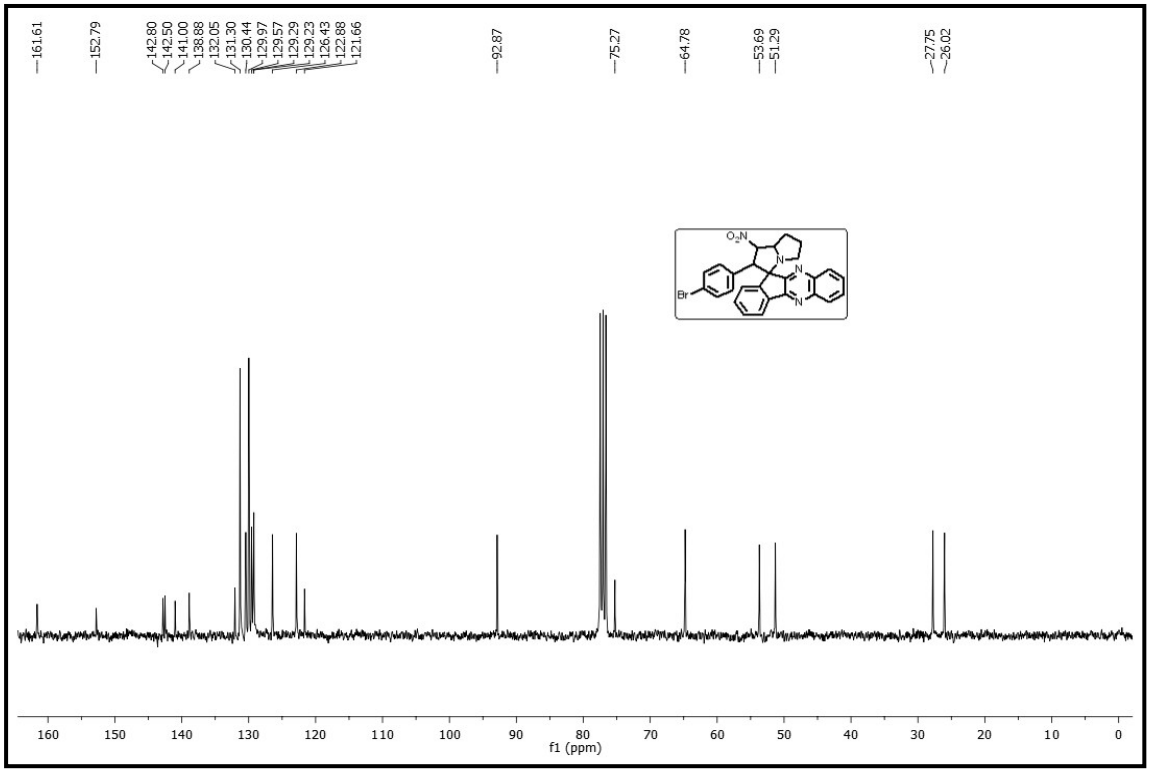


Fig. S14. ^{13}C NMR spectrum of 5g in $CDCl_3$

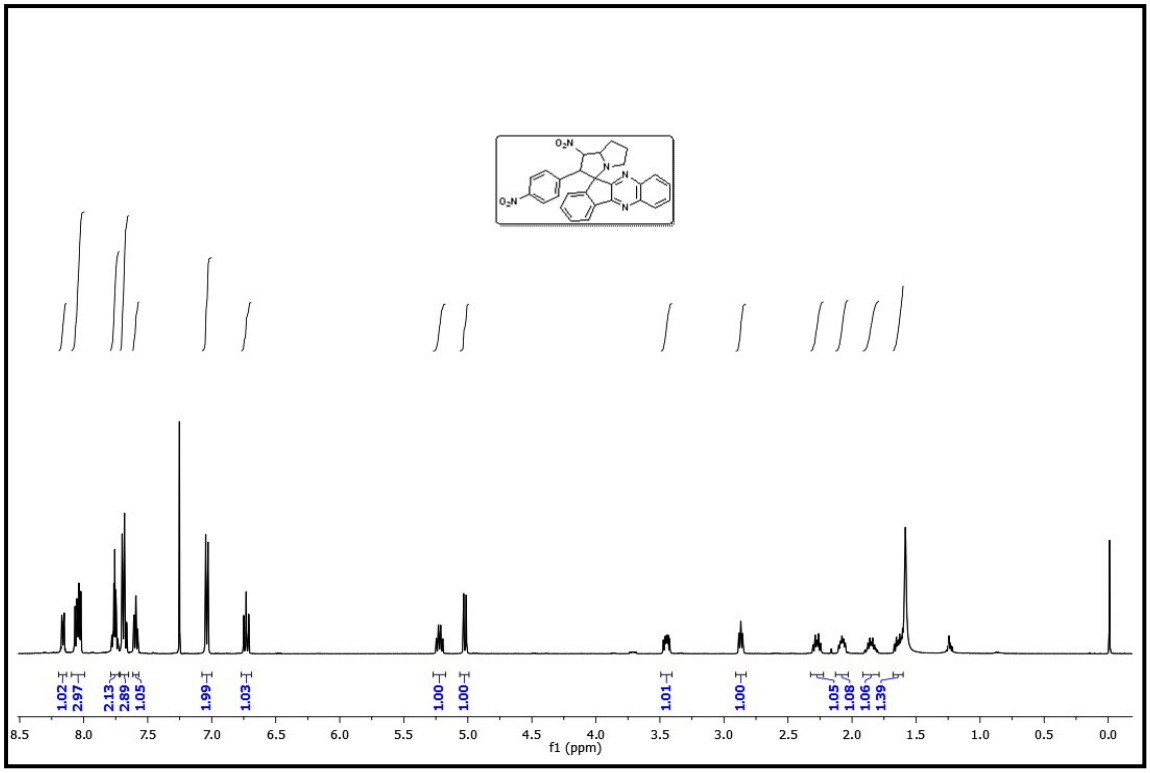


Fig. S15. ^{1}H NMR spectrum of 5h in $CDCl_3$

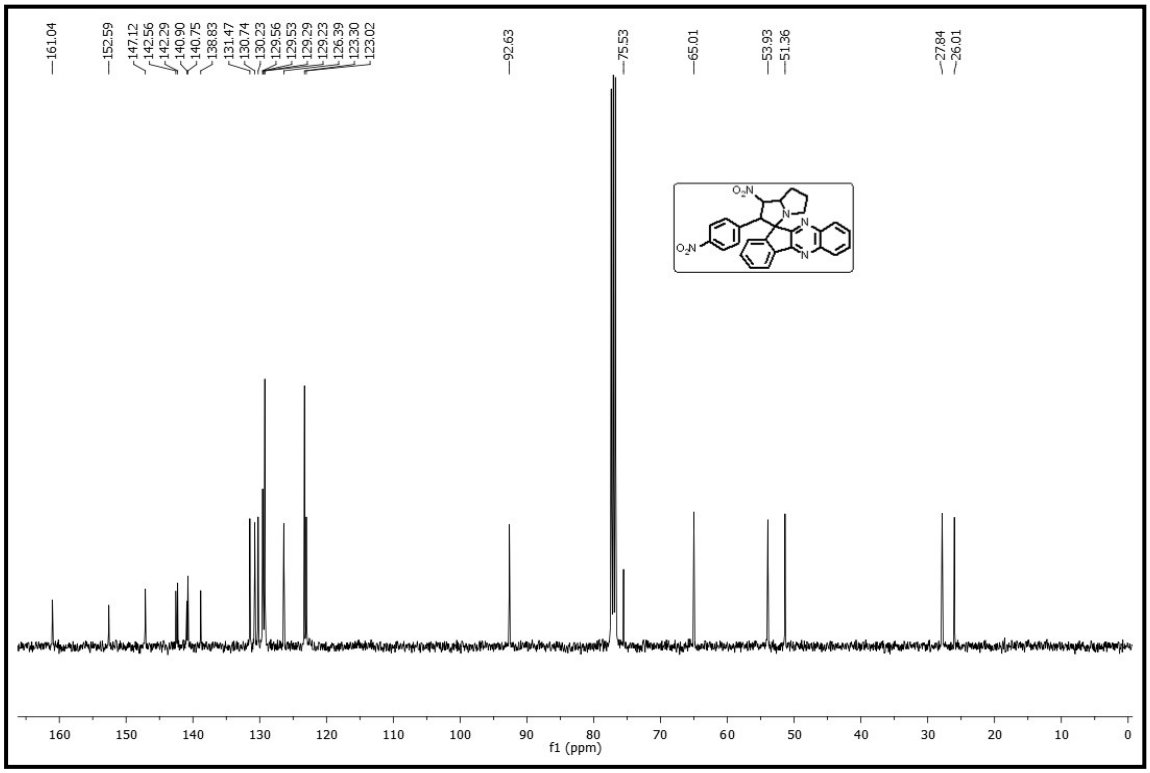


Fig. S16. ^{13}C NMR spectrum of 5h in $CDCl_3$

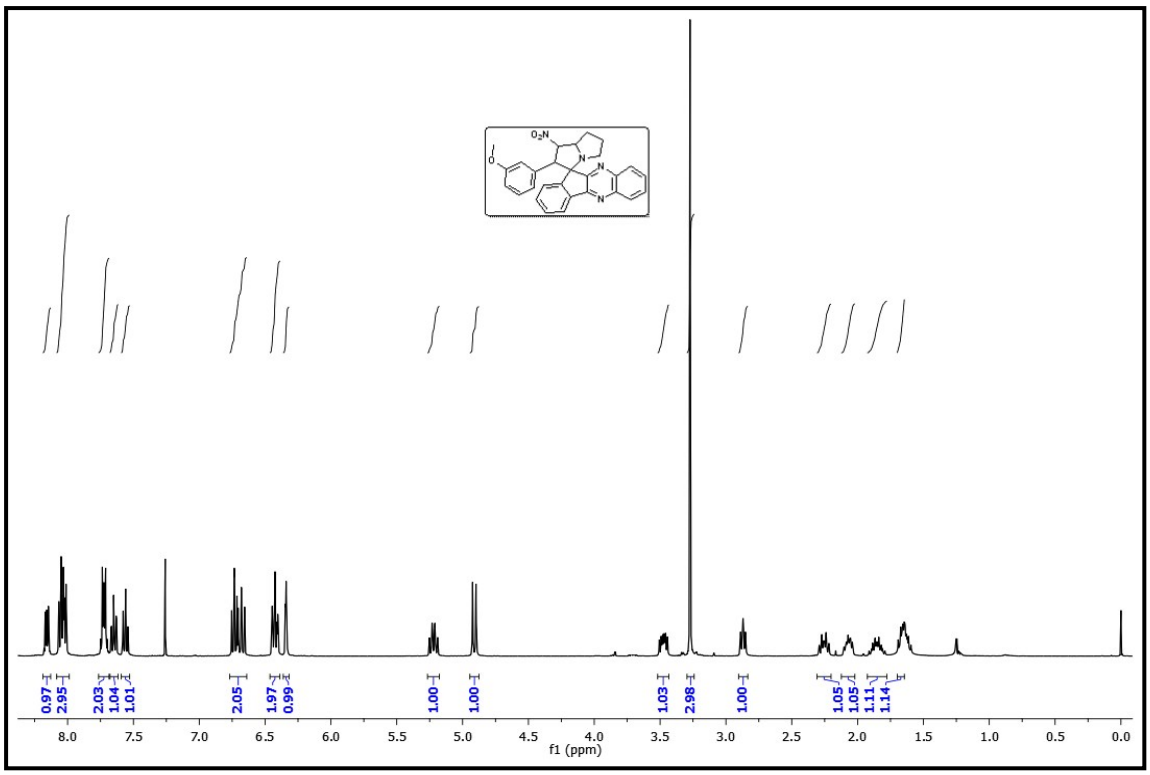


Fig. S17. ^{1}H NMR spectrum of 5i in $CDCl_3$

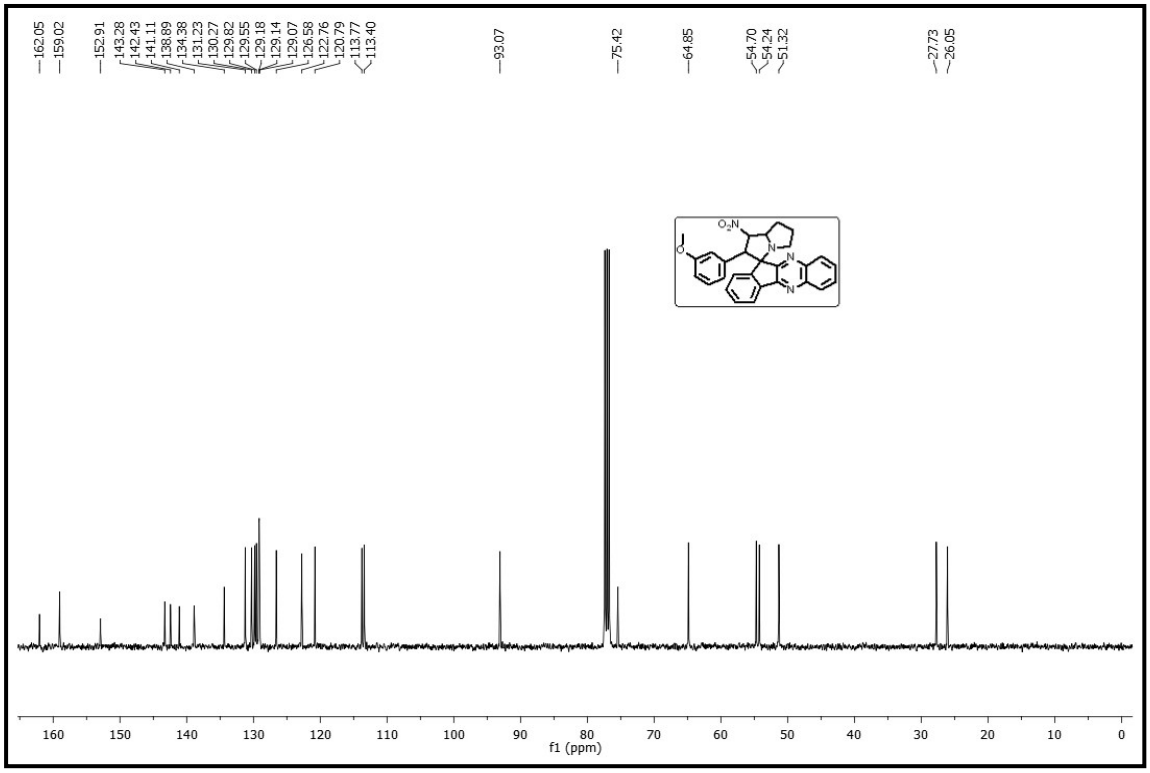


Fig. S18. ^{13}C NMR spectrum of 5i in $CDCl_3$

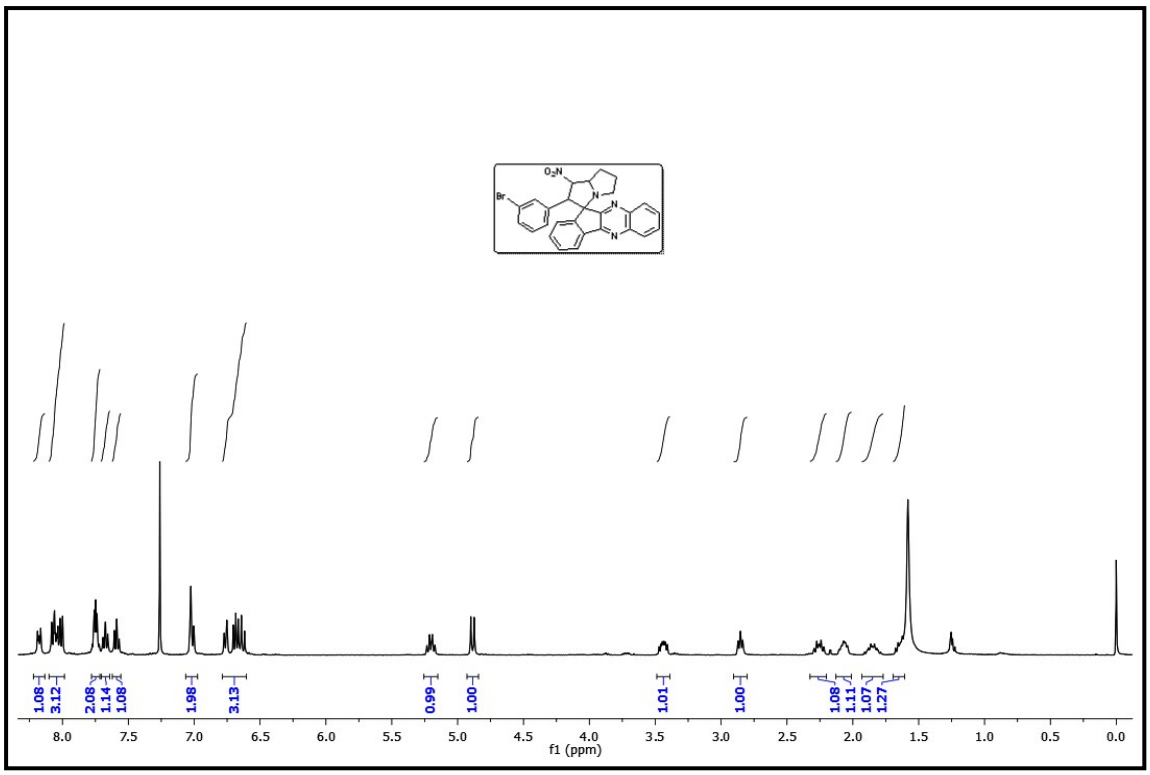


Fig. S19. ^{1}H NMR spectrum of 5j in $CDCl_3$

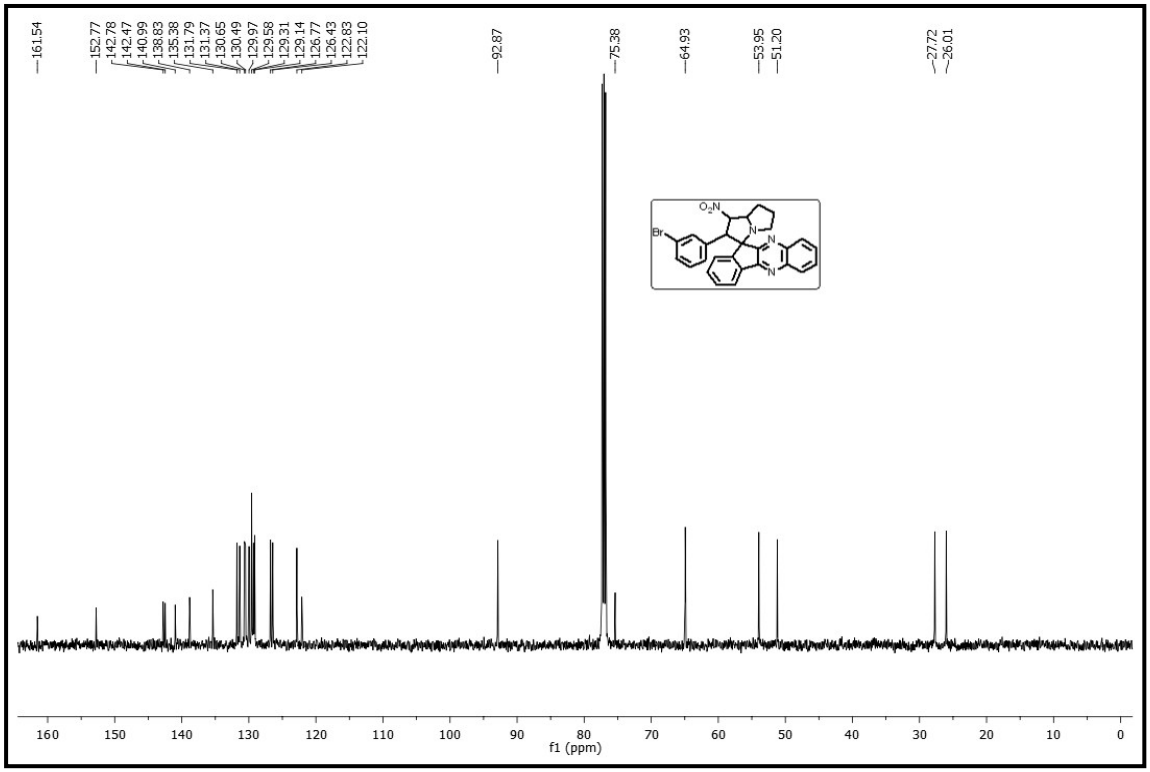


Fig. S20. ^{13}C NMR spectrum of 5j in $CDCl_3$

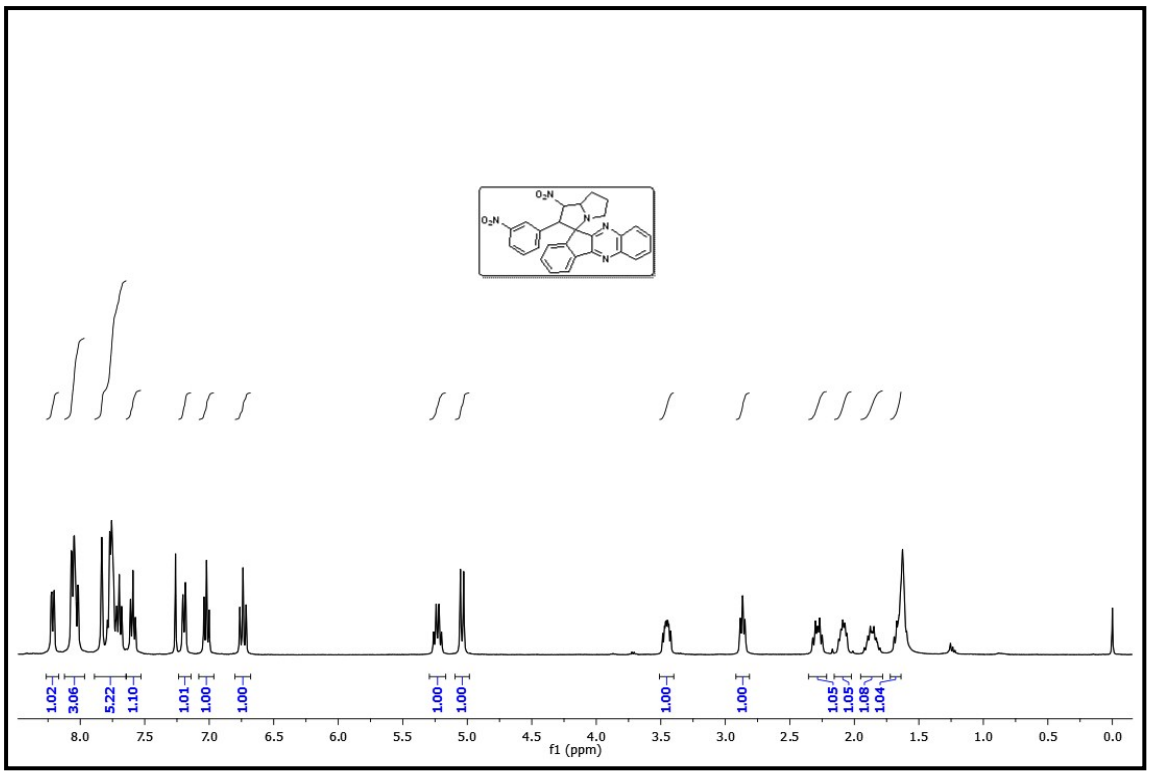


Fig. S21. ^{1}H NMR spectrum of 5k in $CDCl_3$

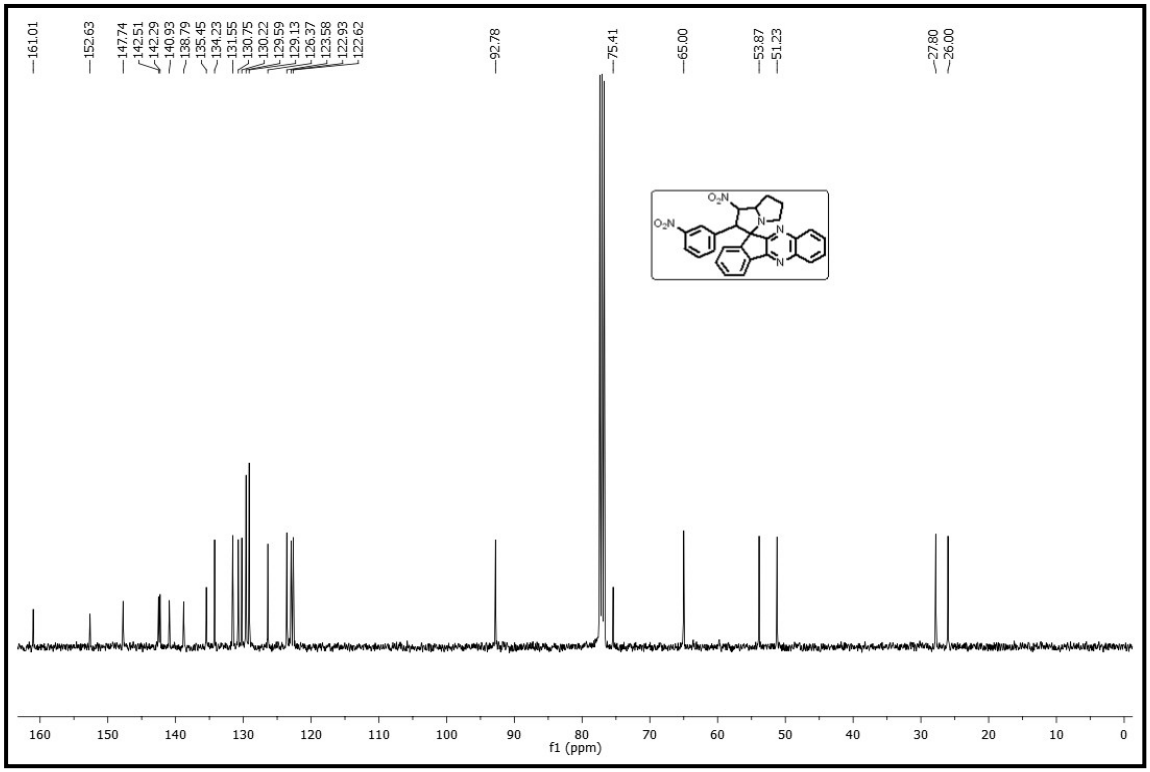


Fig. S22. ^{13}C NMR spectrum of 5k in $CDCl_3$

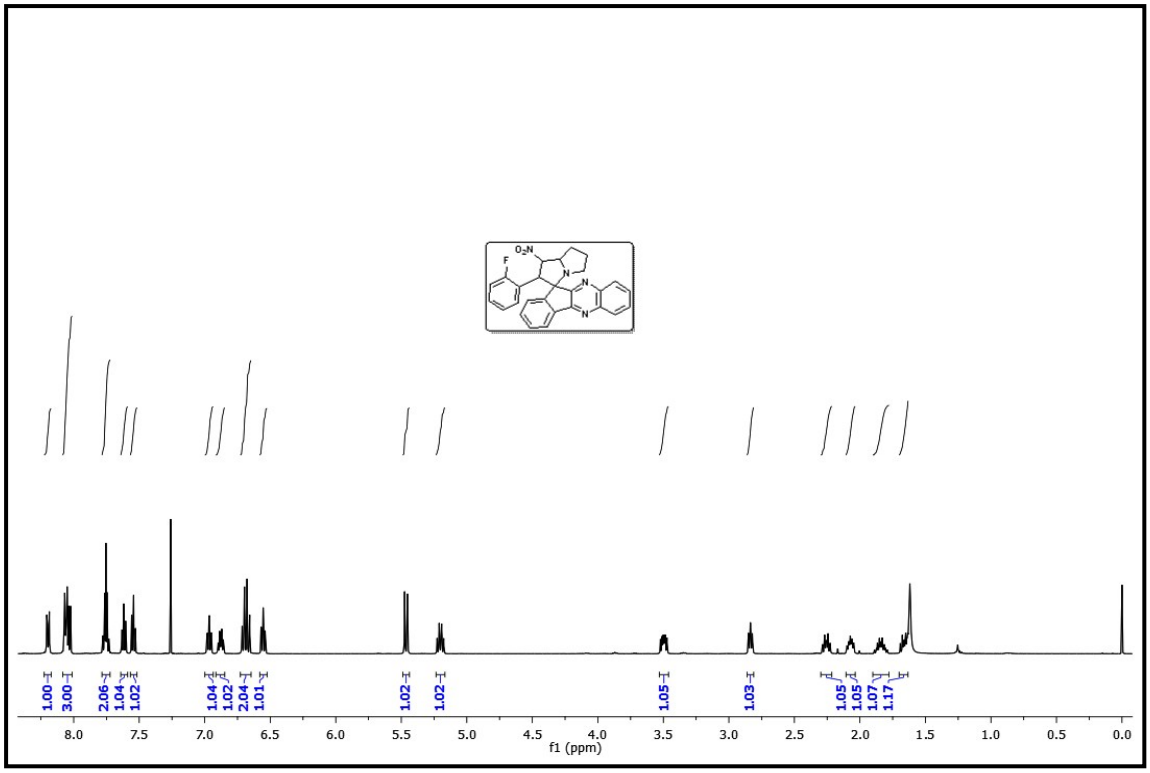


Fig. S23. ^{1}H NMR spectrum of 5l in $CDCl_3$

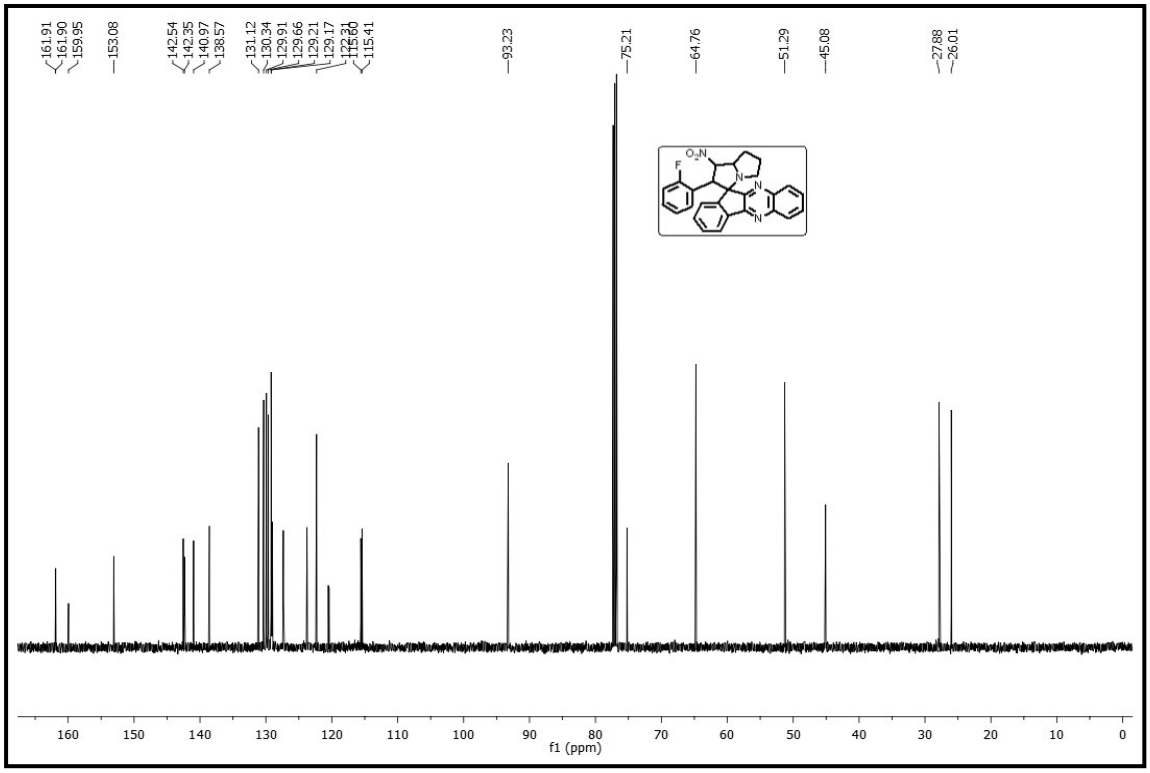


Fig. S24. ^{13}C NMR spectrum of 5l in $CDCl_3$

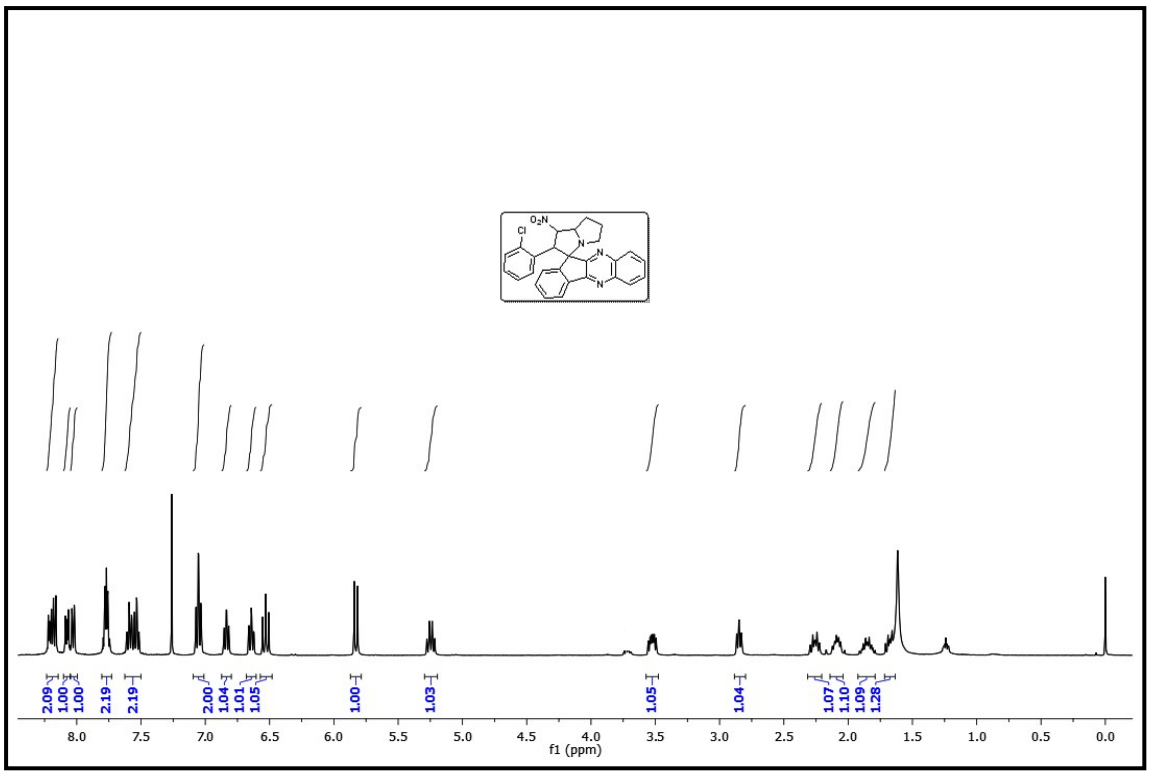


Fig. S25. ^{1}H NMR spectrum of 5m in $CDCl_3$

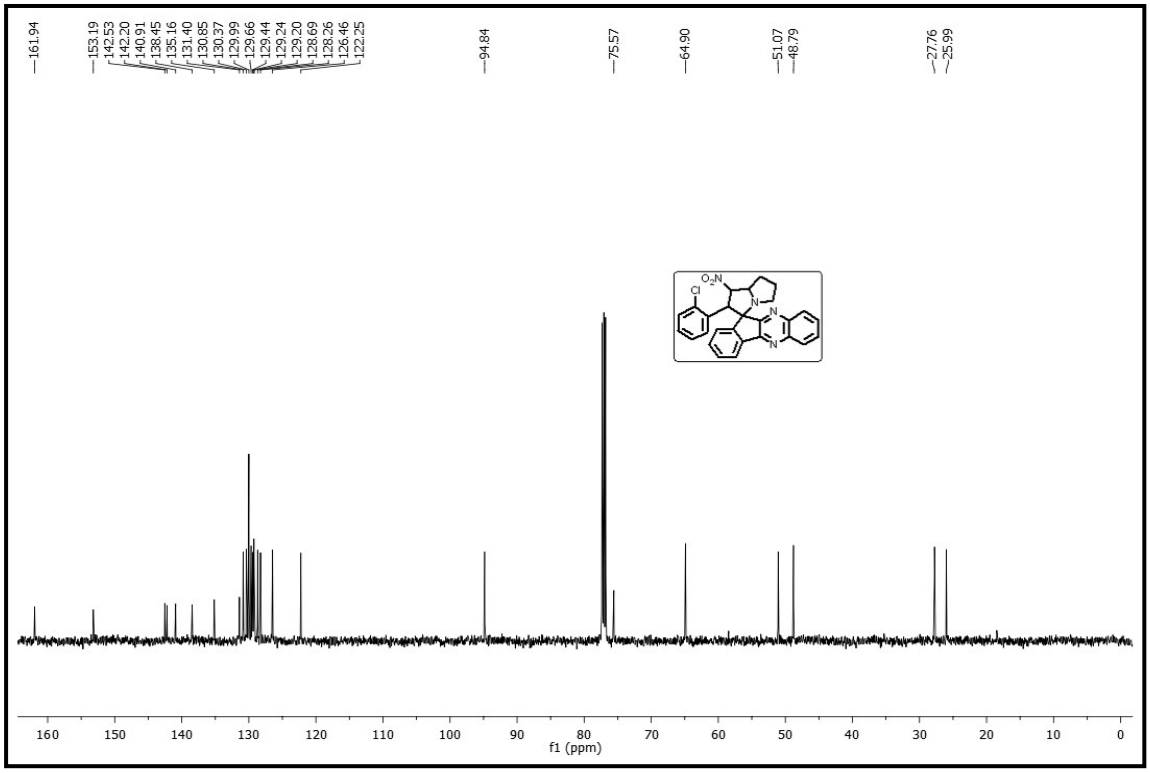


Fig. S26. ^{13}C NMR spectrum of 5m in $CDCl_3$

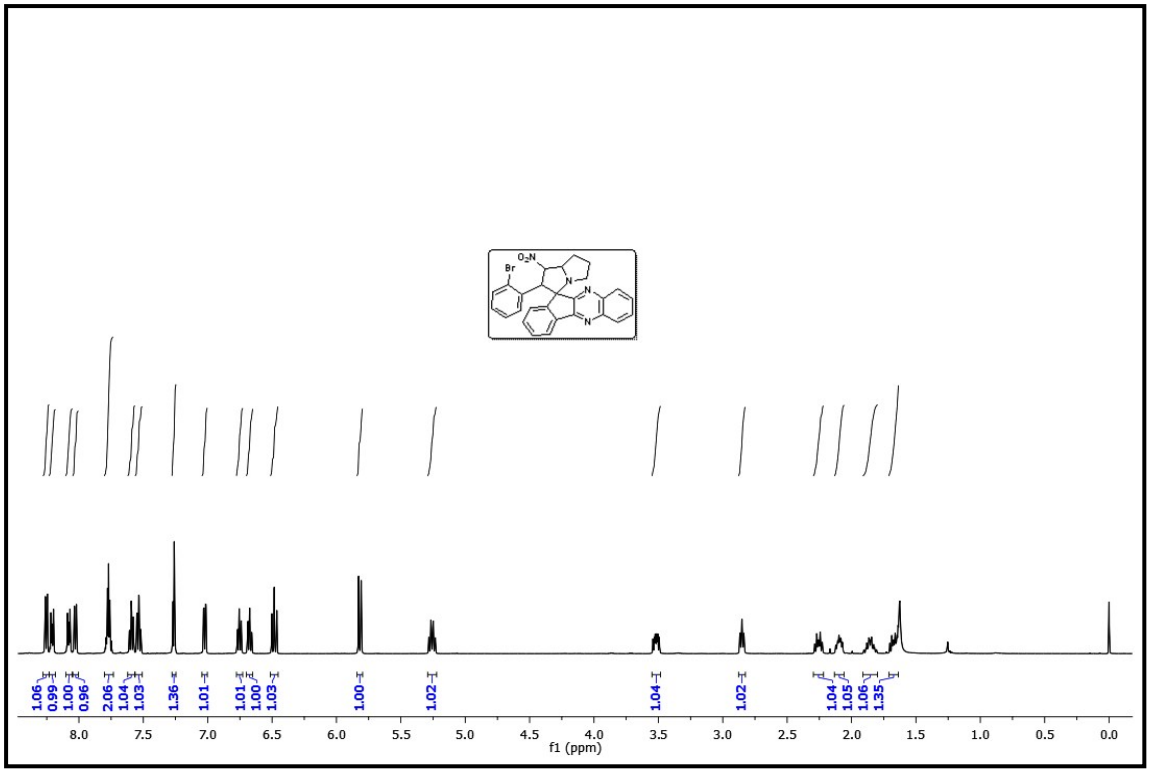


Fig. S27. ^{1}H NMR spectrum of 5n in $CDCl_3$

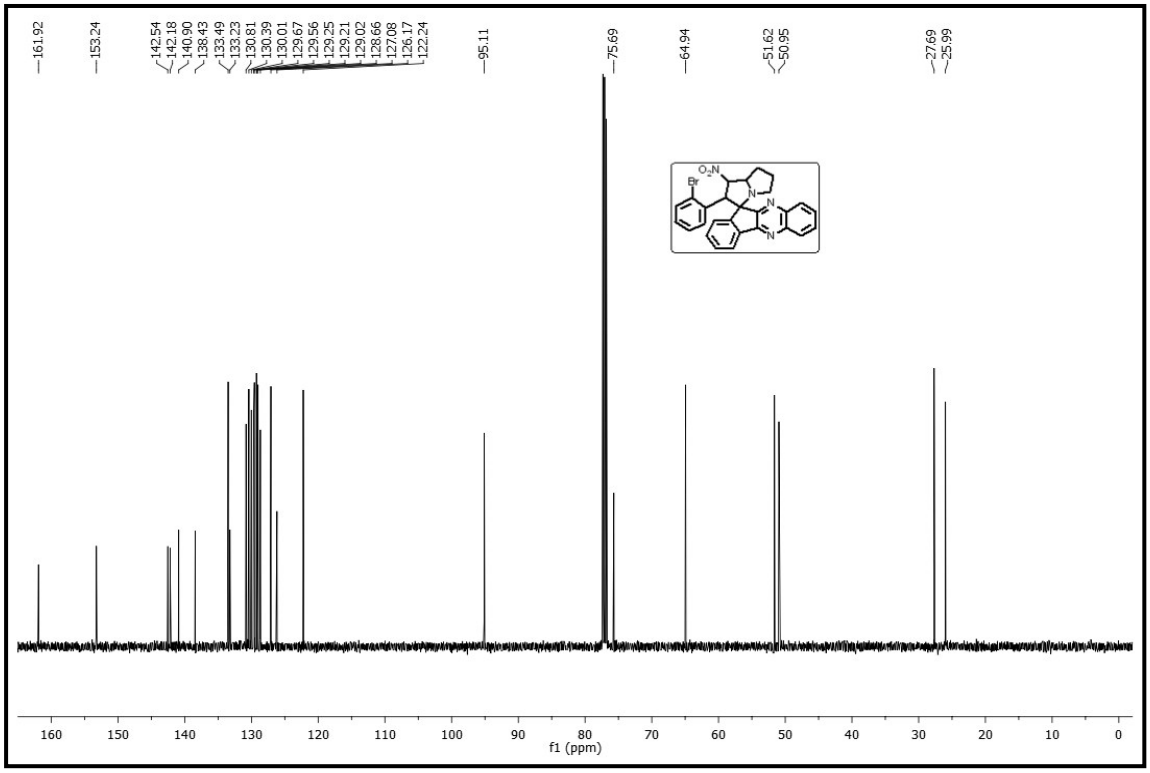


Fig. S28. ^{13}C NMR spectrum of 5n in $CDCl_3$

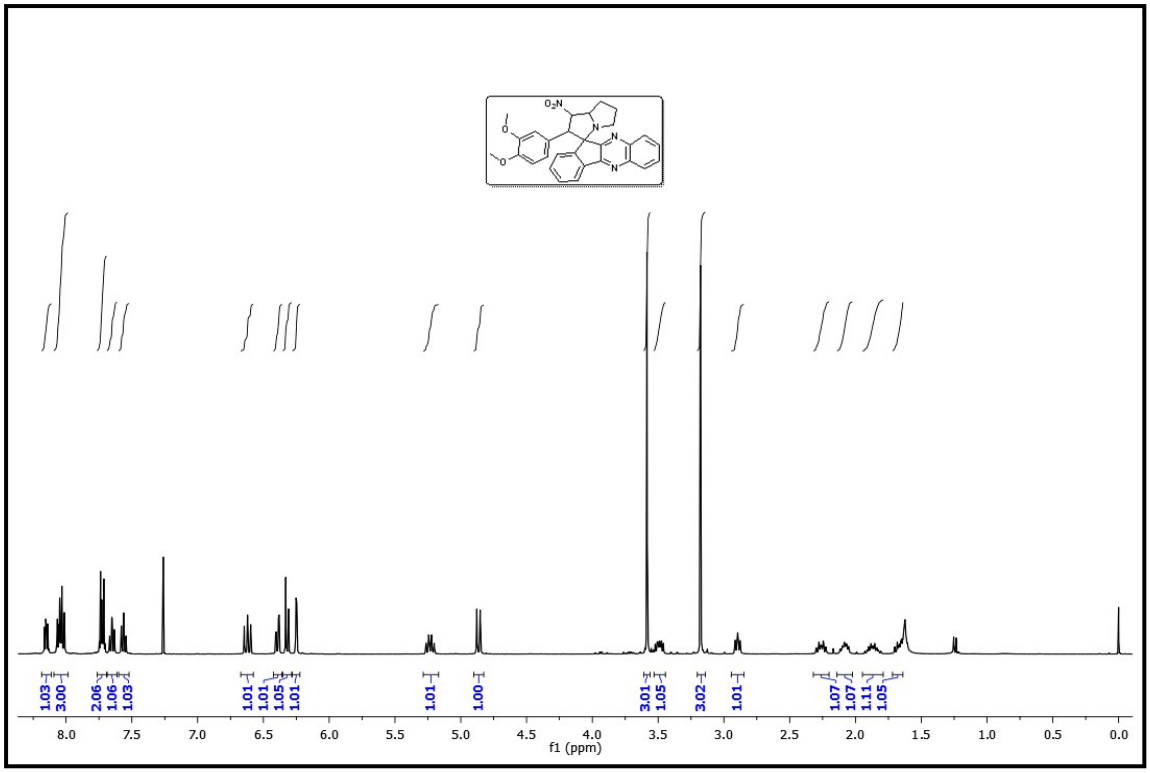


Fig. S29. ^{1}H NMR spectrum of 5o in $CDCl_3$

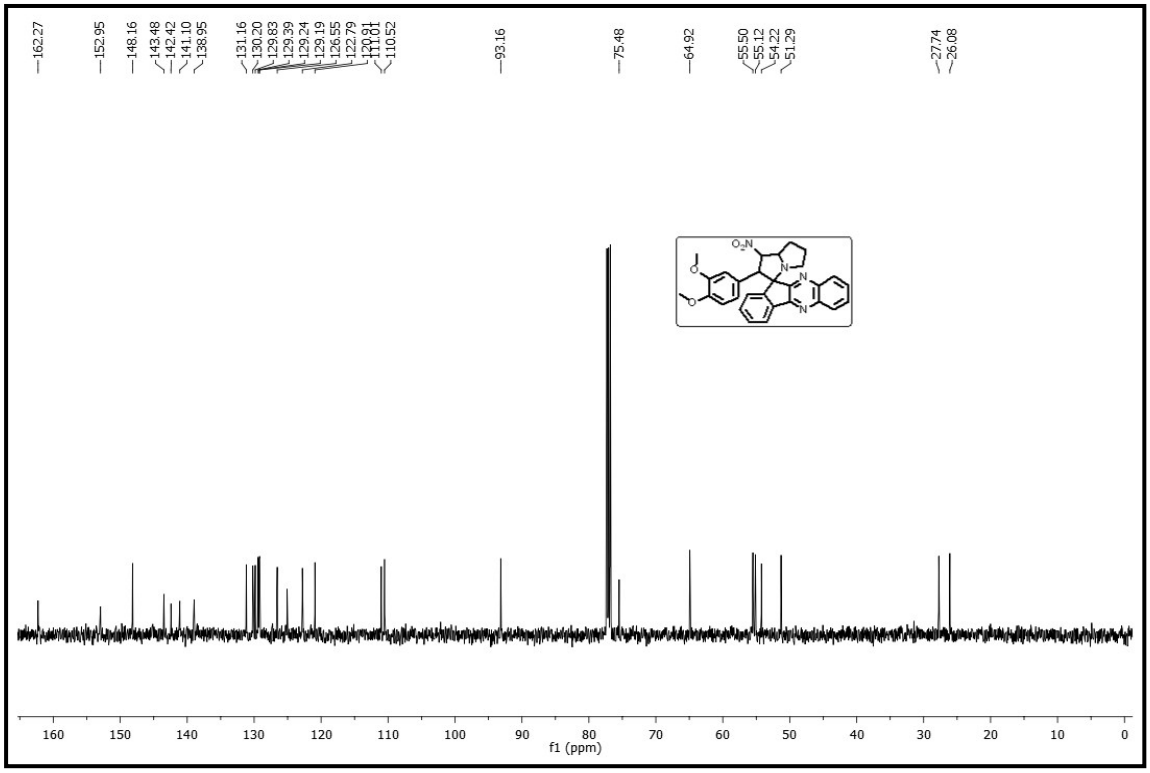


Fig. S30. ^{13}C NMR spectrum of 5o in $CDCl_3$

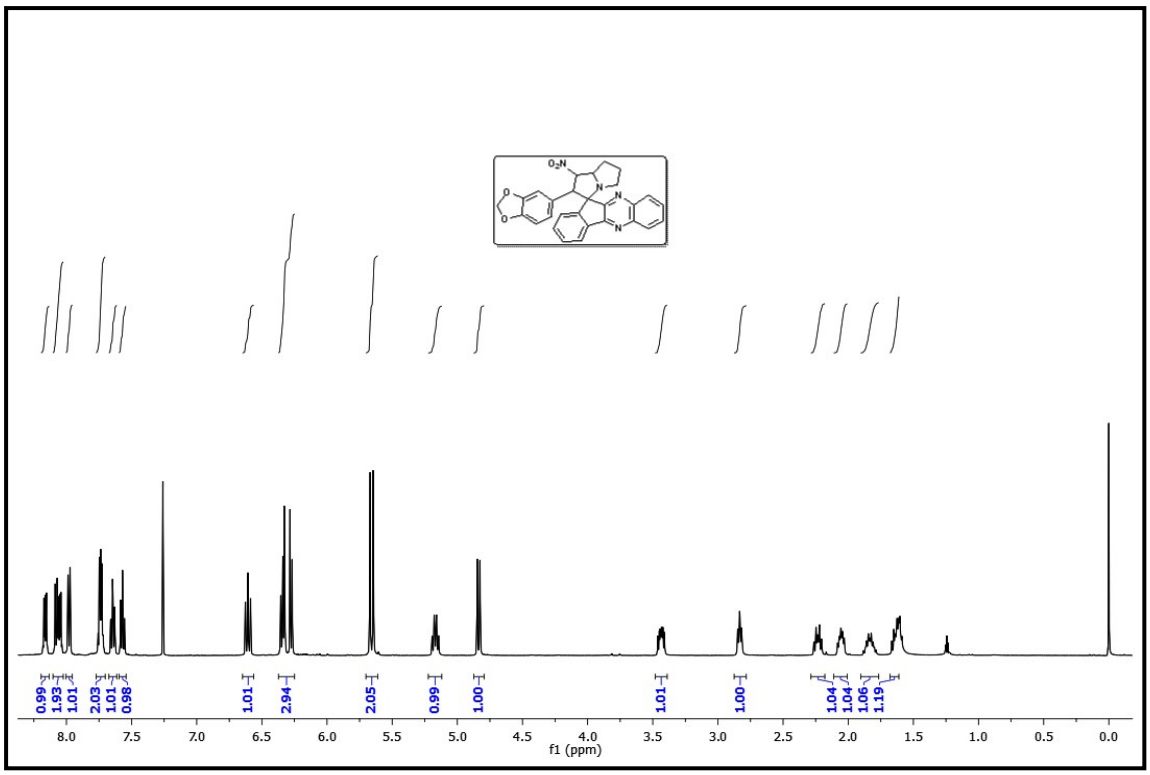


Fig. S31. ^{1}H NMR spectrum of 5p in $CDCl_3$

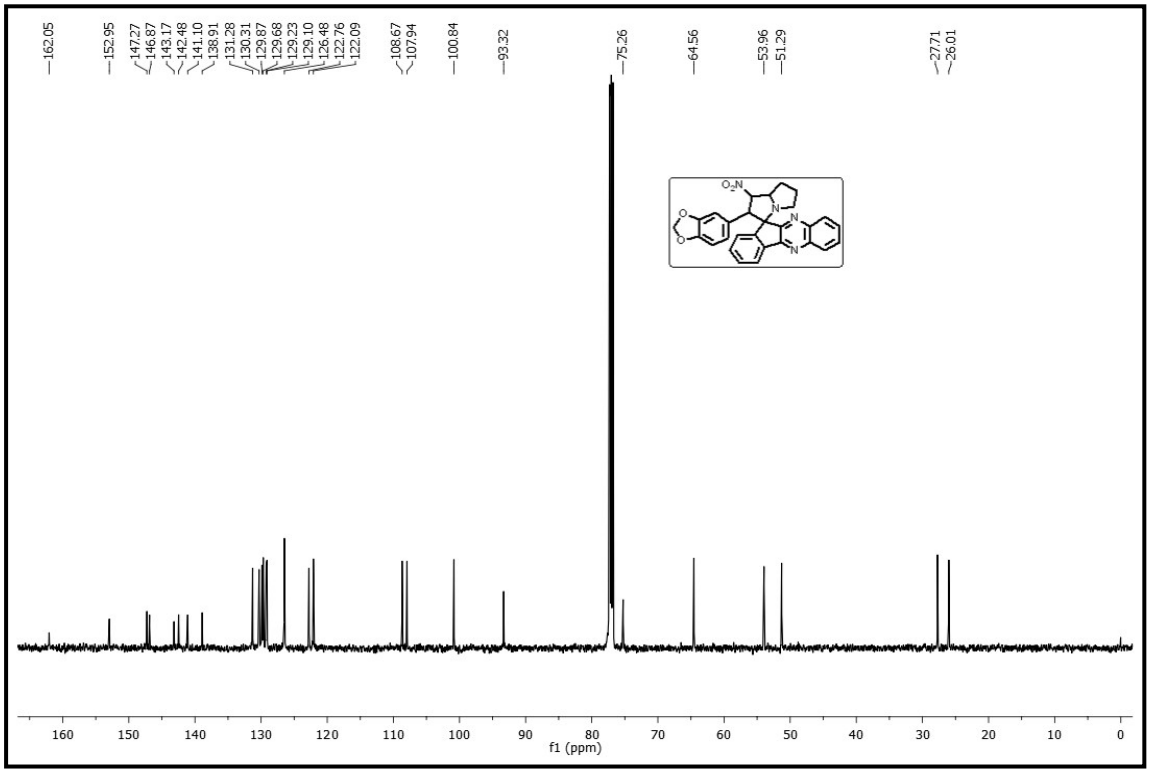


Fig. S32. ^{13}C NMR spectrum of 5p in $CDCl_3$

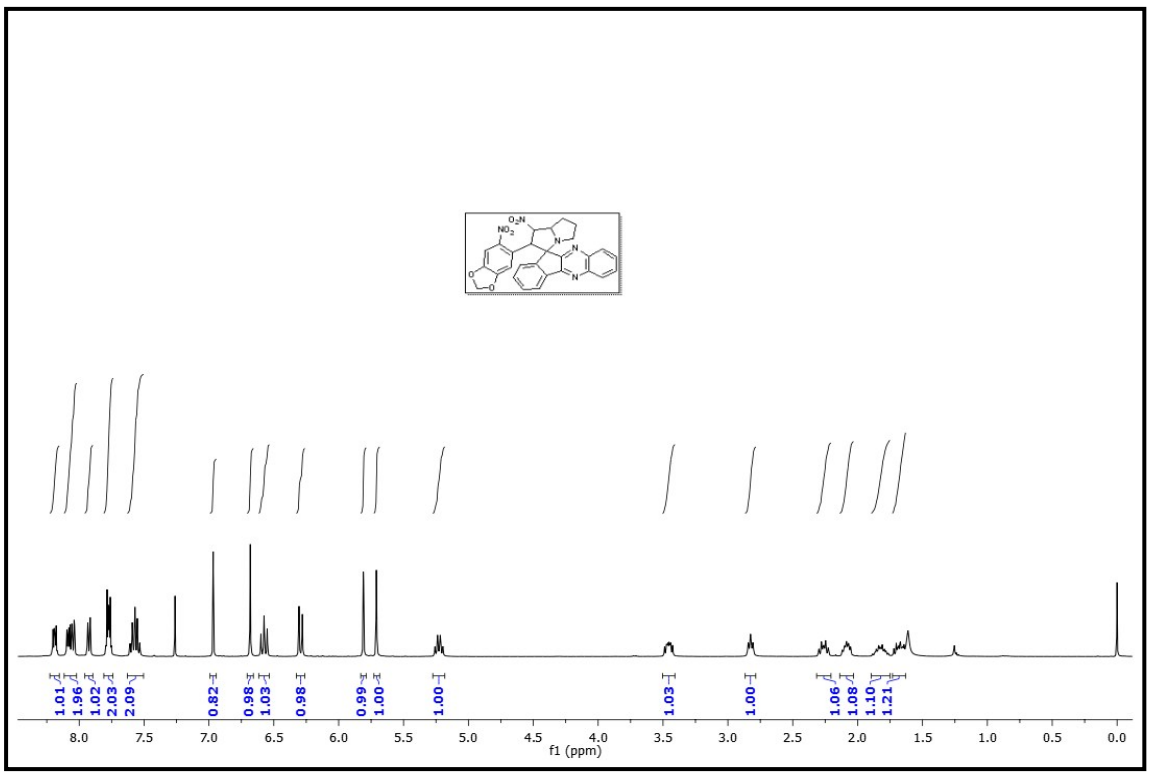


Fig. S33. ^{1}H NMR spectrum of 5q in $CDCl_3$

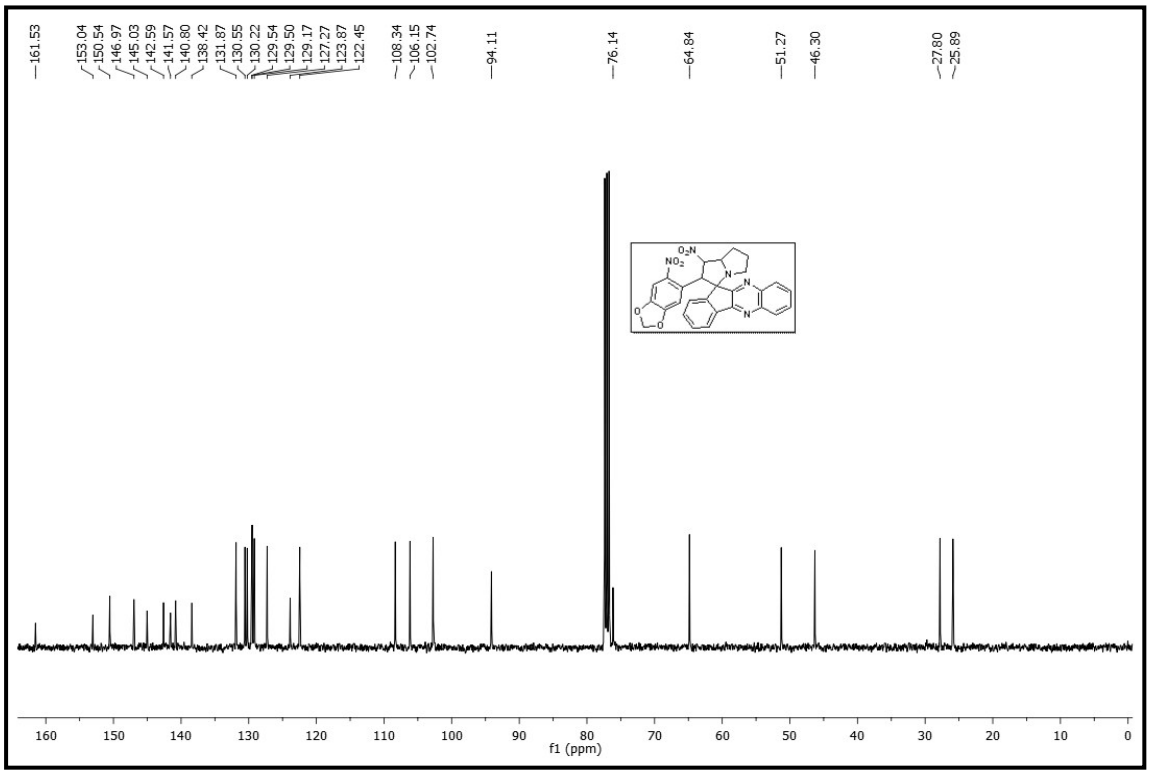


Fig. S34. ^{13}C NMR spectrum of 5q in $CDCl_3$

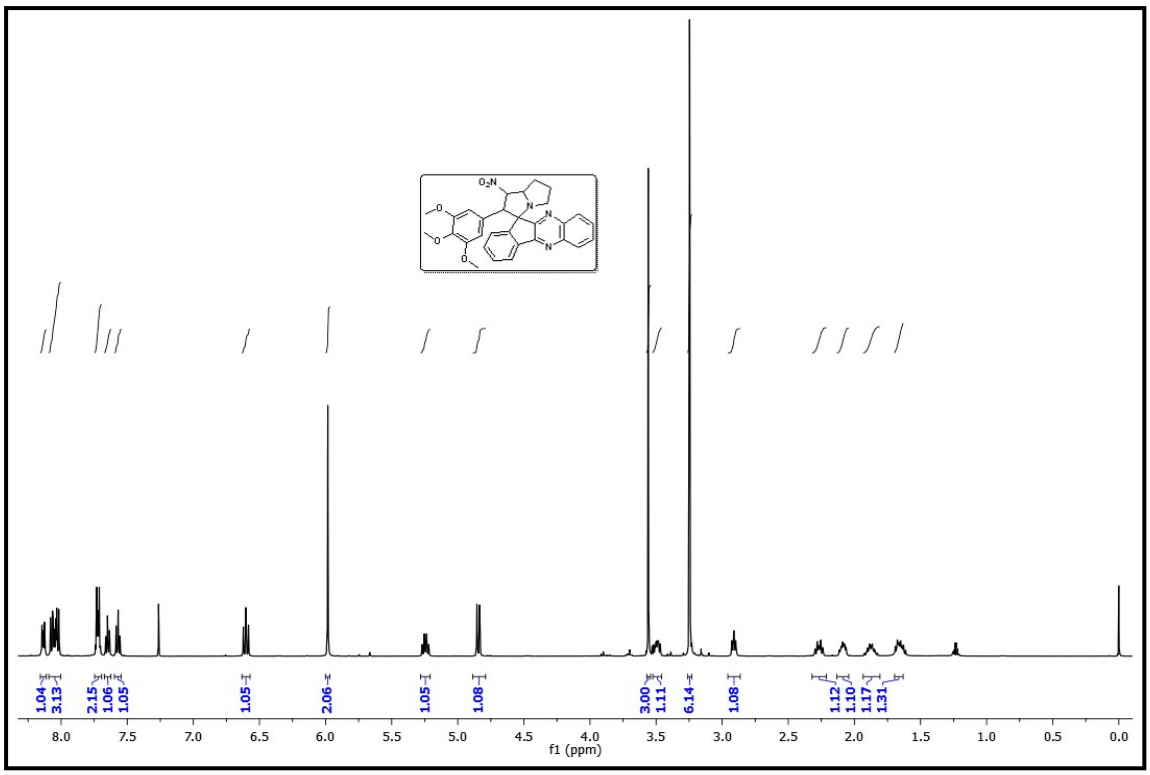


Fig. S35. ^{1}H NMR spectrum of 5r in $CDCl_3$

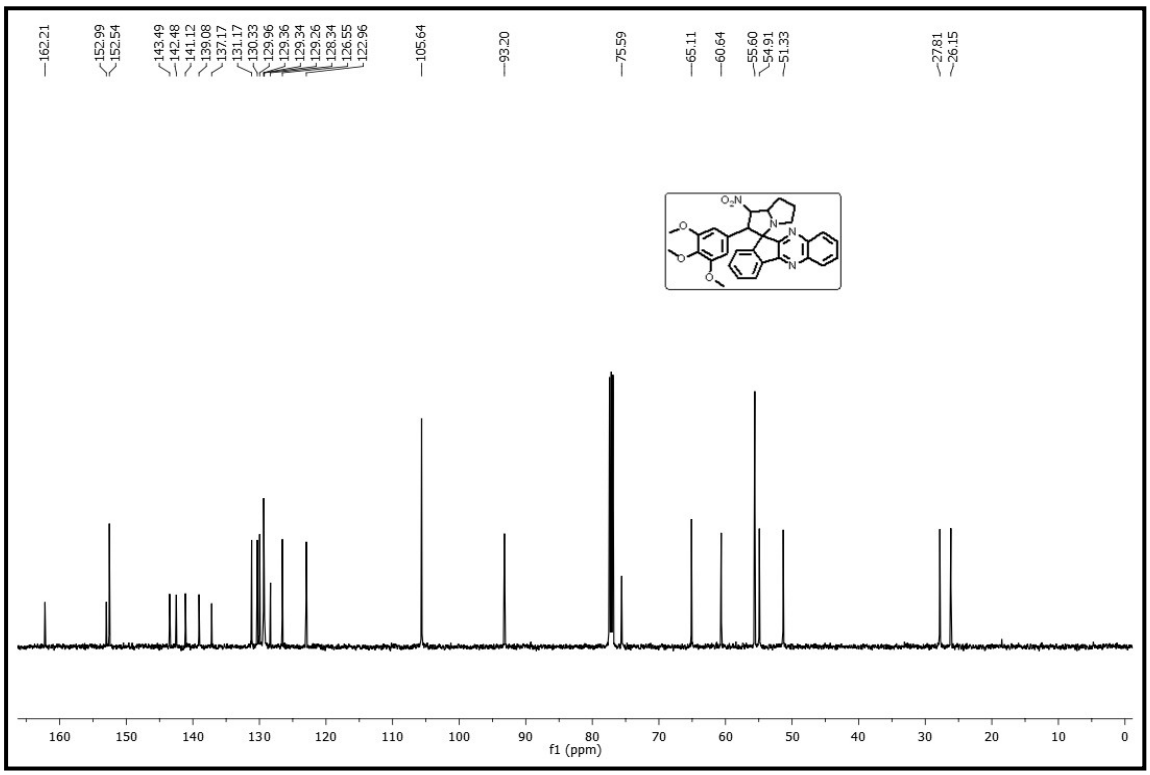


Fig. S36. ^{13}C NMR spectrum of 5r in $CDCl_3$

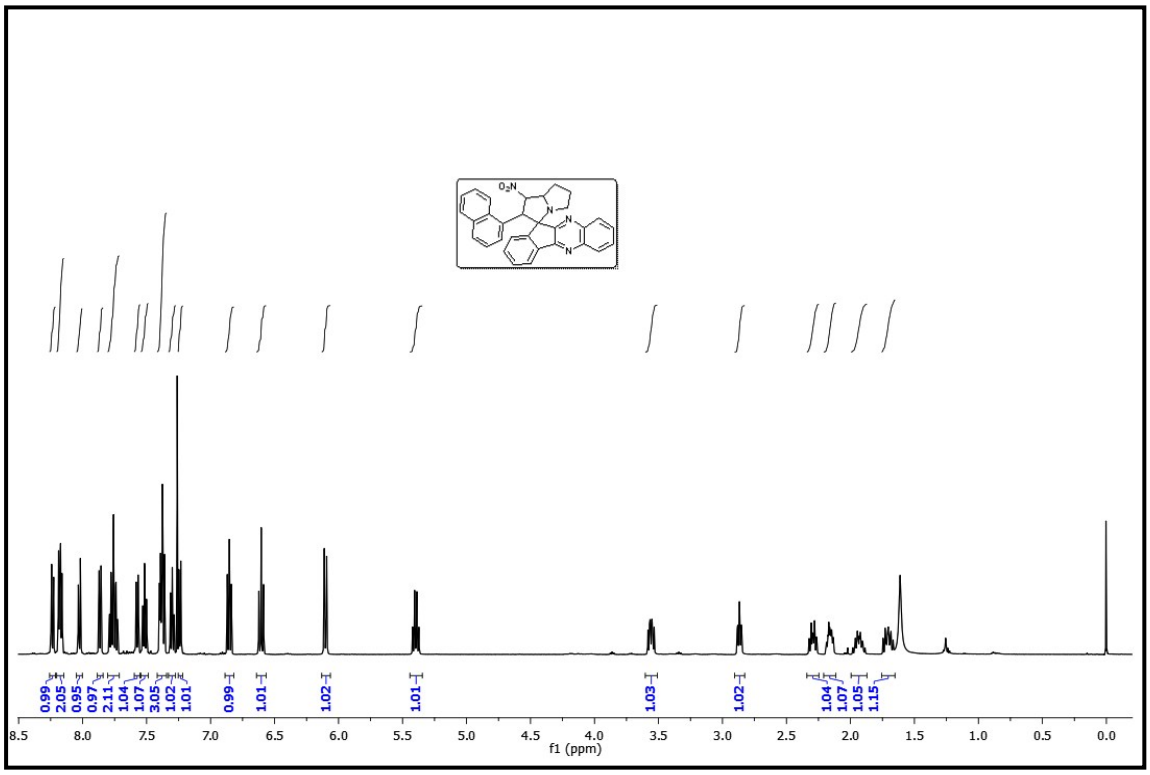


Fig. S37. ^{1}H NMR spectrum of 5s in $CDCl_3$

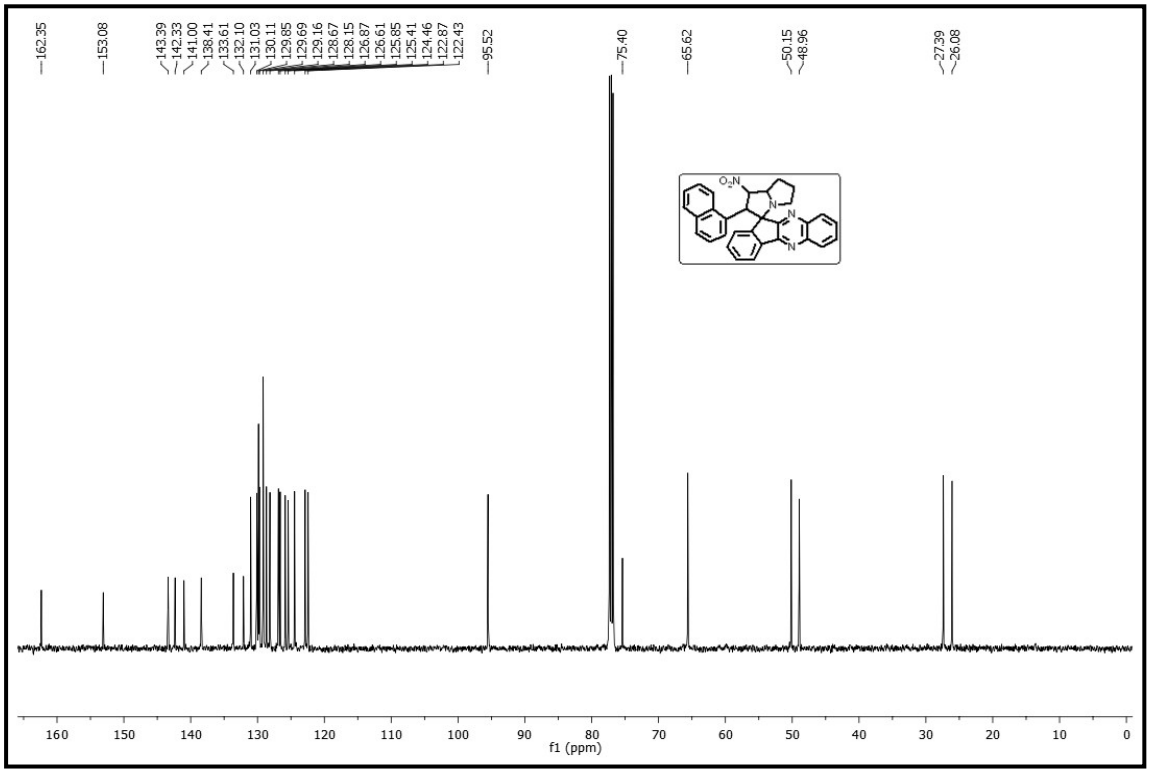


Fig. S38. ^{13}C NMR spectrum of 5s in $CDCl_3$

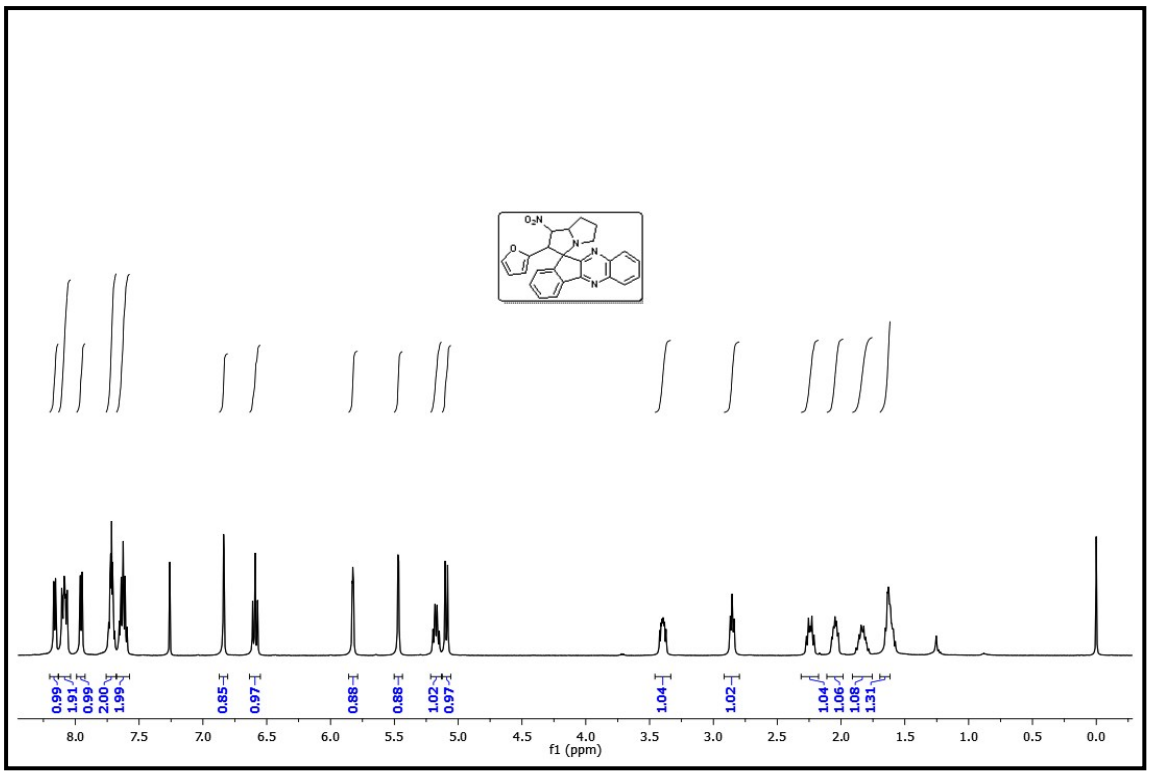


Fig. S39. ^{1}H NMR spectrum of 5t in $CDCl_3$

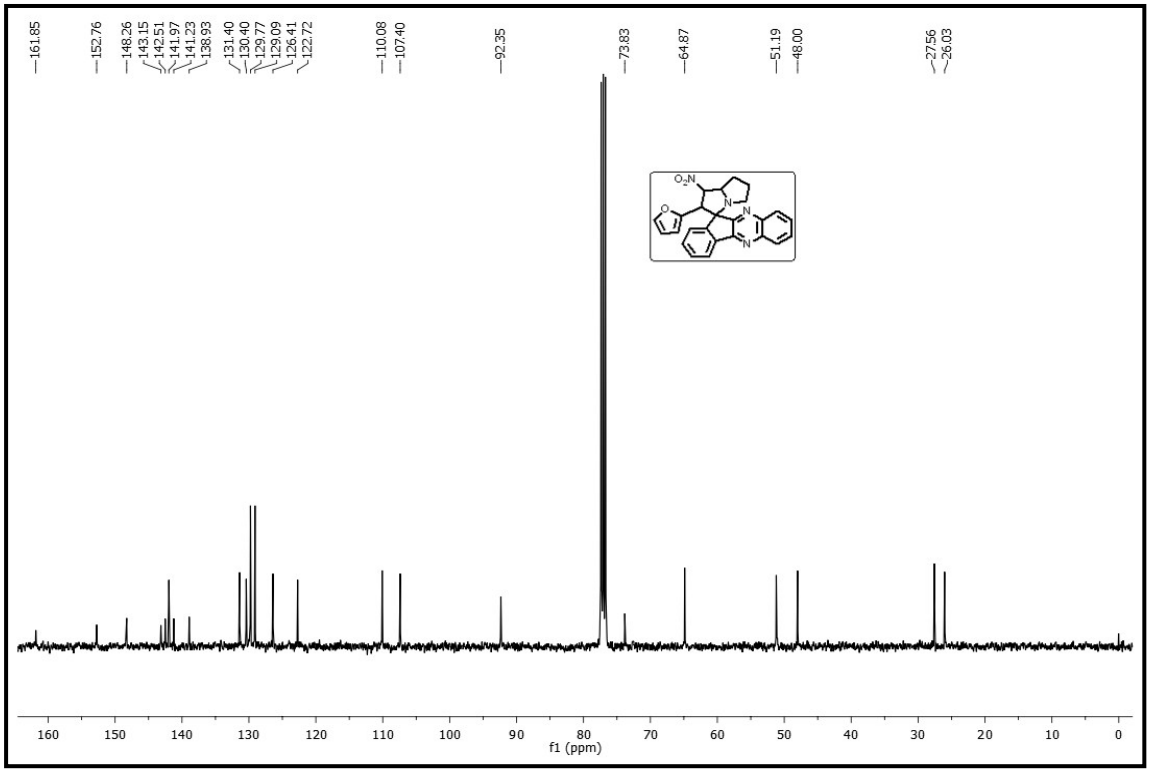


Fig. S40. ^{13}C NMR spectrum of 5t in $CDCl_3$

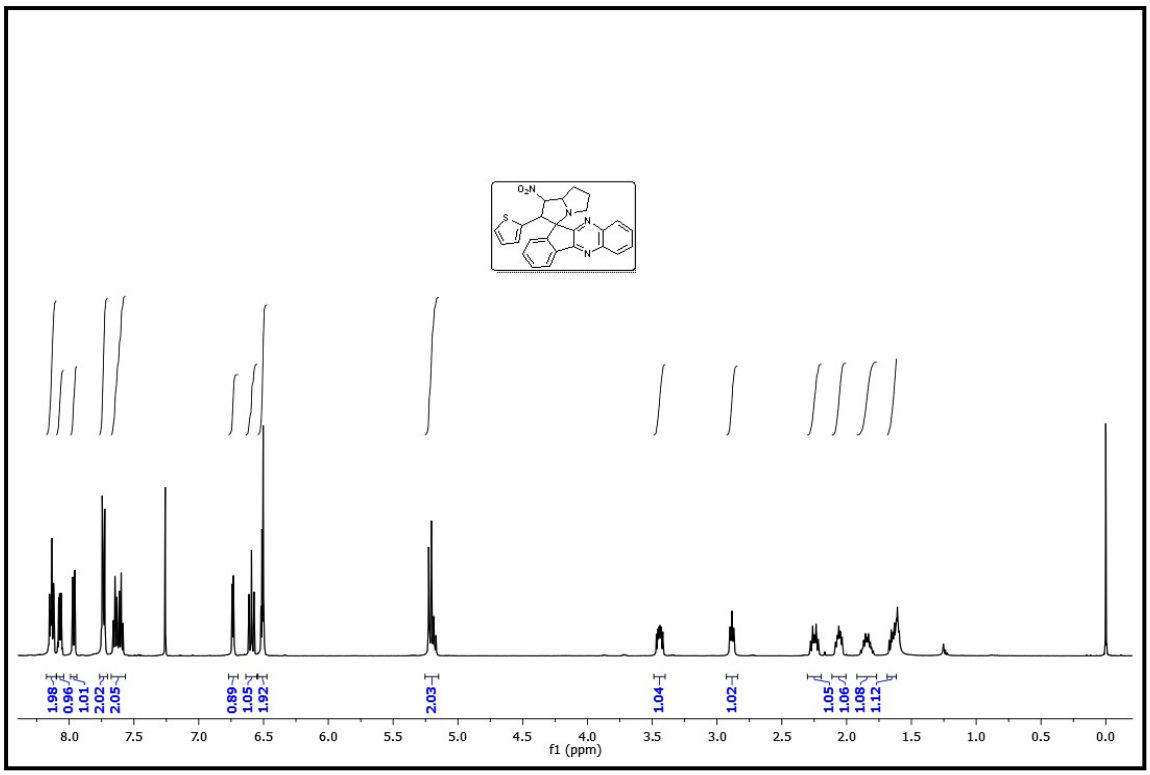


Fig. S41. ^{1}H NMR spectrum of 5u in $CDCl_3$

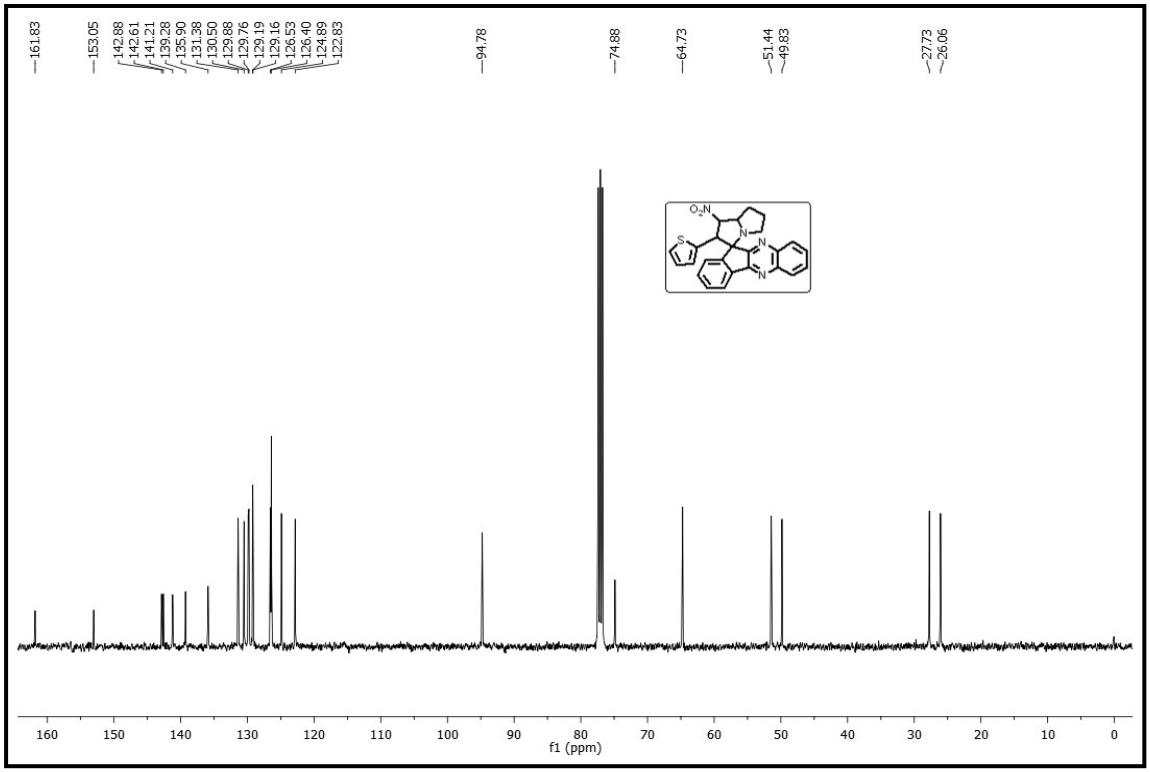
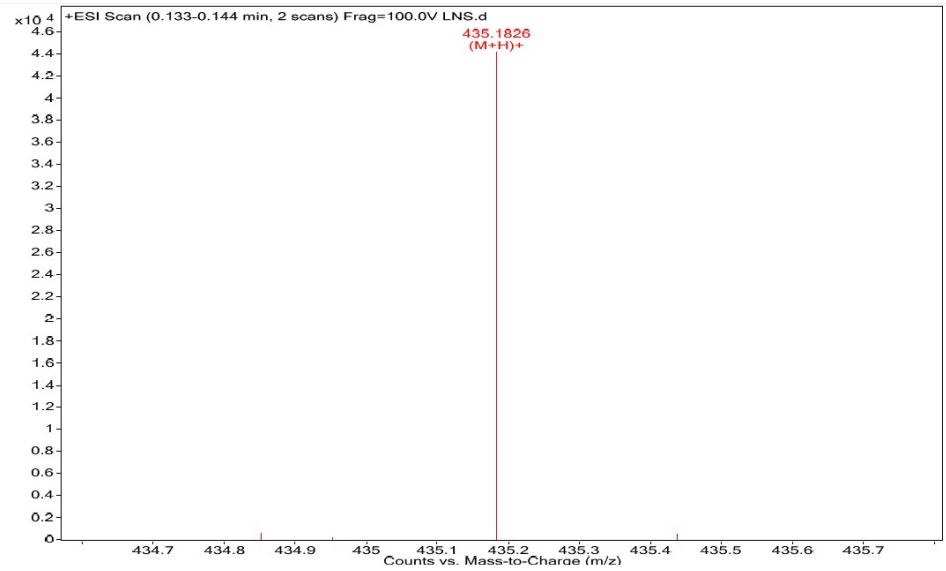


Fig. S42. ^{13}C NMR spectrum of 5u in $CDCl_3$

HRMS spectra

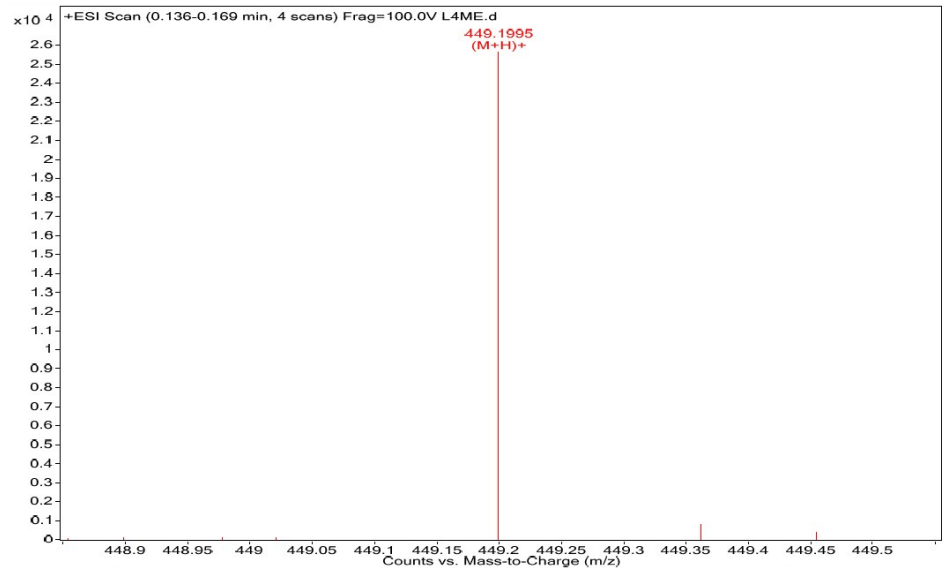
Compound 5a:



m/z	Ion	Formula	Abundance
435.1826	(M+H)+	C27 H23 N4 O2	44178

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C27 H22 N4 O2	C27 H23 N4 O2	435.1816	94.37		434.1754	434.1743	-2.49	2.49	94.82	94.12	94.23	435.1826	19

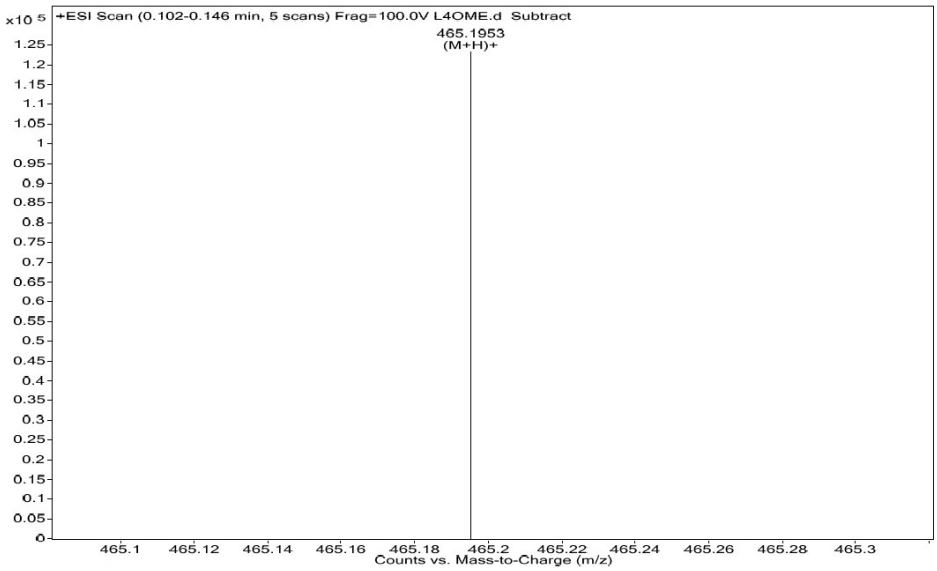
Compound 5b:



m/z	Ion	Formula	Abundance
449.1995	(M+H)+	C28 H25 N4 O2	25645.8

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C28 H24 N4 O2	C28 H25 N4 O2	449.1972	72.79		448.1923	448.1899	-5.33	5.33	96.41	38.95	75.55	449.1995	19

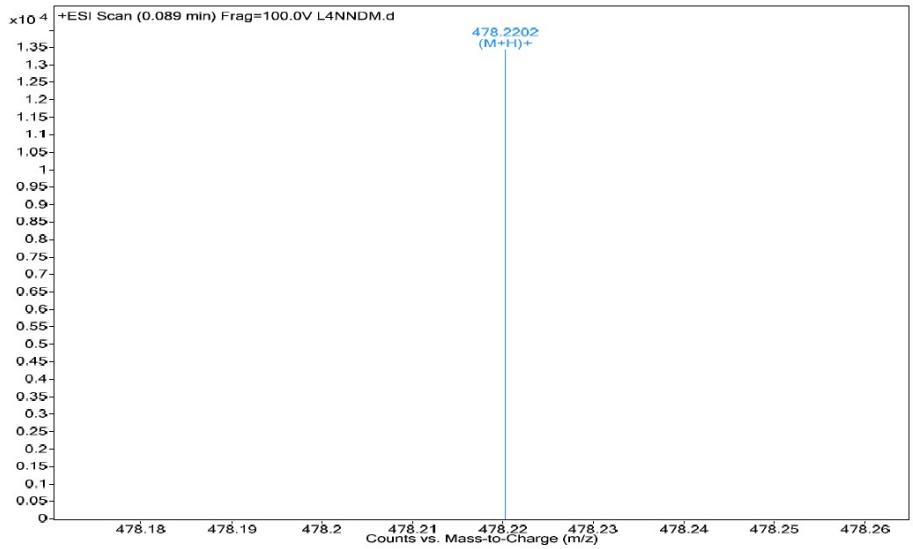
Compound 5c:



m/z	Ion	Formula	Abundance
465.1953	(M+H)+	C28 H25 N4 O3	123303.5

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C28 H24 N4 O3	C28 H25 N4 O3	465.1921	79.42		464.188	464.1848	-6.8	6.8	91.05	99.29	62.52	465.1953	19

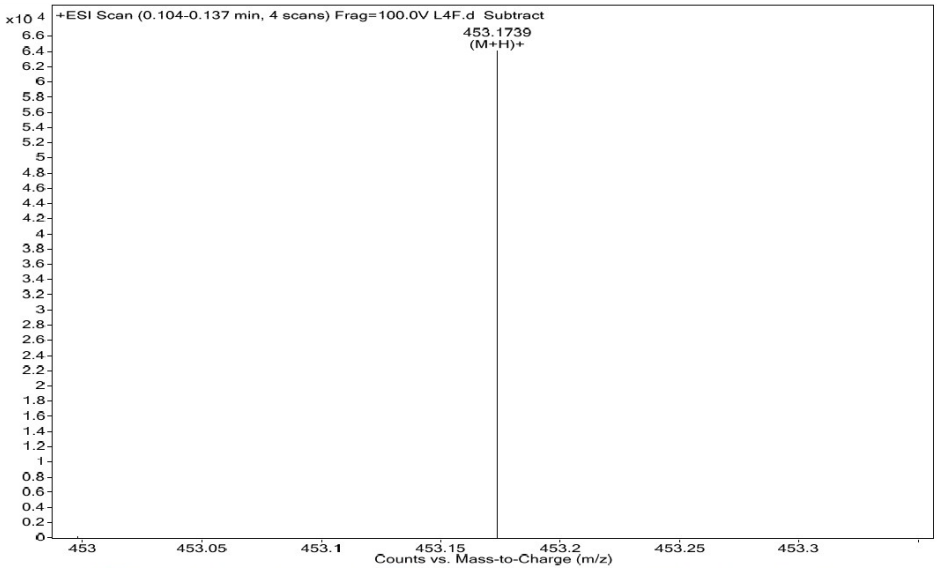
Compound 5d:



m/z	Ion	Formula	Abundance
478.2202	(M+H)+	C29 H28 N5 O2	13422.9

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C29 H27 N5 O2	C29 H28 N5 O2	478.2238	71.44		477.213	477.2165	7.2	7.2	89.32	76.3	58.28	478.2202	19

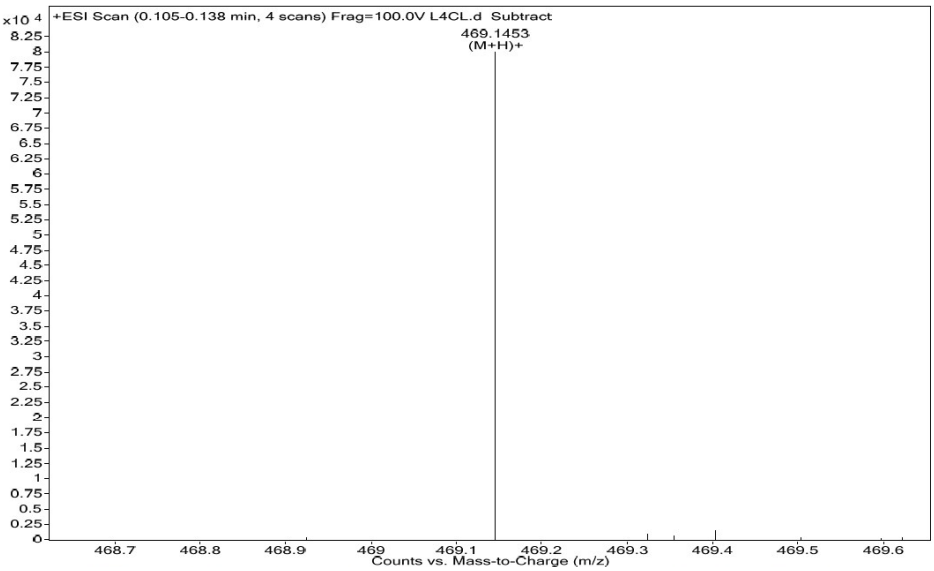
Compound 5e:



m/z	Ion	Formula	Abundance
453.1739	(M+H)+	C27 H22 F N4 O2	64101.5

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
✓	C27 H21 F N4 O2	C27 H22 F N4 O2	453.1721	92.9		452.1666	452.1649	-3.83	3.83	98.28	99.41	86.42	453.1739	19

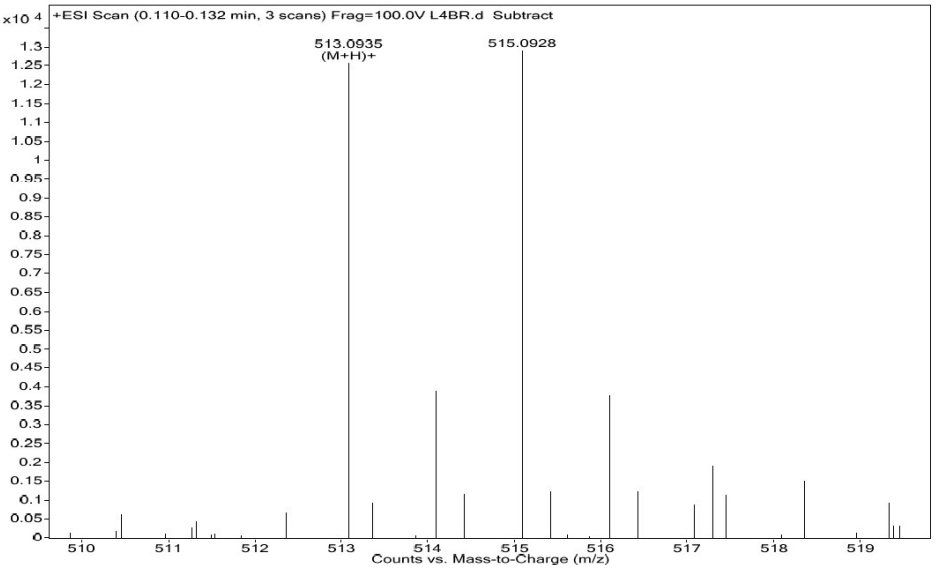
Compound 5f:



m/z	Ion	Formula	Abundance
469.1453	(M+H)+	C27 H22 Cl N4 O2	79989.4

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
✓	C27 H21 Cl N4 O2	C27 H22 Cl N4 O2	469.1426	85.55		468.138	468.1353	-5.81	5.81	98.55	99.42	70.83	469.1453	19

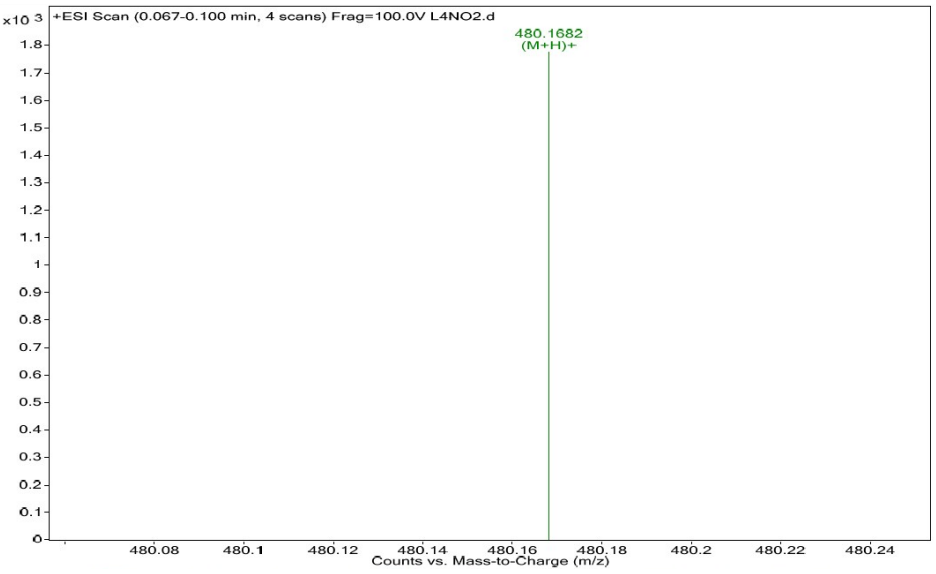
Compound 5g:



m/z	Ion	Formula	Abundance
513.0935	(M+H)+	C27 H22 Br N4 O2	12566.4

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
✓	C27 H21 Br N4 O2	C27 H22 Br N4 O2	513.0921	91.76		512.0867	512.0848	-3.73	3.73	98.86	95.25	85.75	513.0935	19

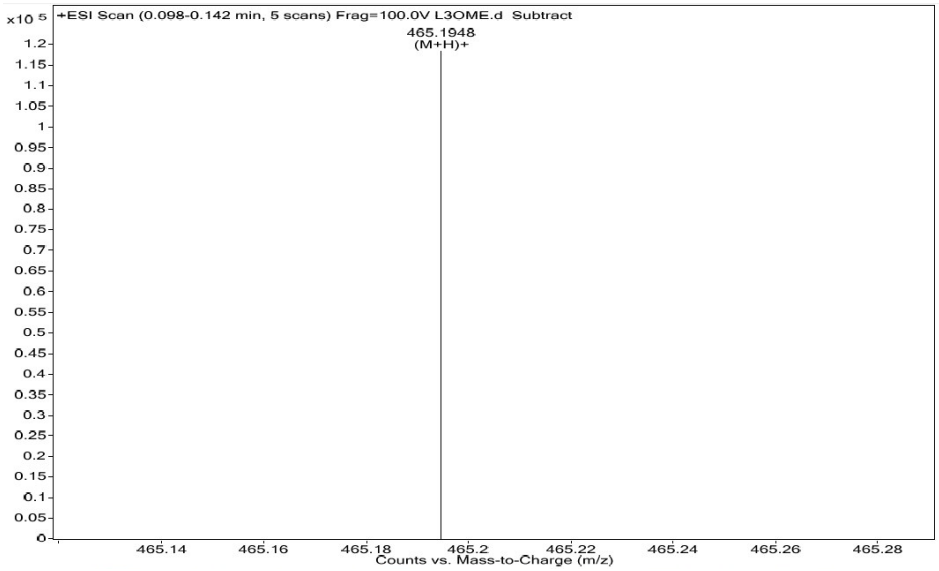
Compound 5h:



m/z	Ion	Formula	Abundance
480.1682	(M+H)+	C27 H22 N5 O4	1777

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
✓	C27 H21 N5 O4	C27 H22 N5 O4	480.1666	42.69		479.1609	479.1594	-3.23	3.23	0	0	89.65	480.1682	20

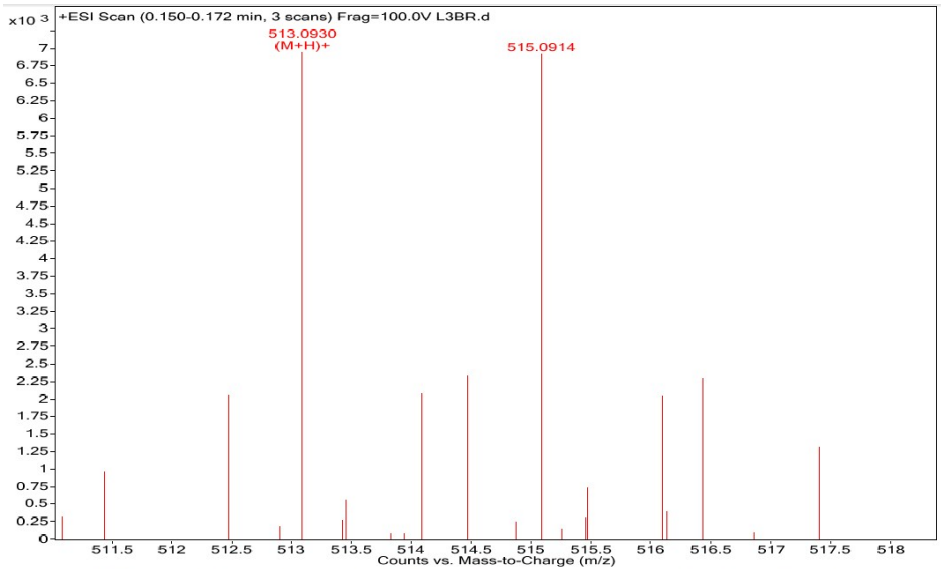
Compound 5i:



m/z	Ion	Formula	Abundance
465.1948	(M+H)+	C28 H25 N4 O3	118423.7

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
✓	C28 H24 N4 O3	C28 H25 N4 O3	465.1921	83.91		464.1875	464.1848	-5.76	5.76	93.43	97.52	71.39	465.1948	19

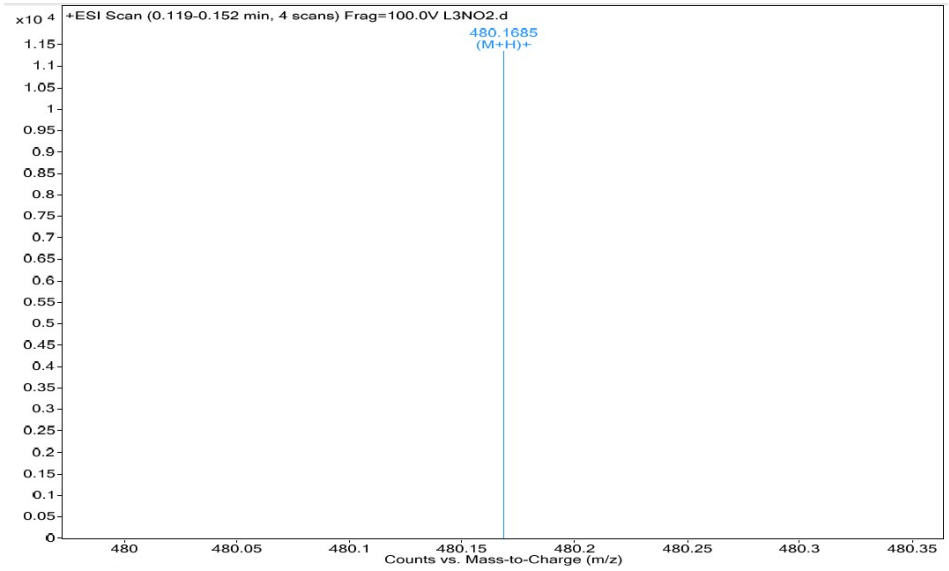
Compound 5j:



m/z	Ion	Formula	Abundance
513.093	(M+H)+	C27 H22 Br N4 O2	6943.2

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
✓	C27 H21 Br N4 O2	C27 H22 Br N4 O2	513.0921	94.05		512.0858	512.0848	-1.88	1.88	90.67	93.85	96.17	513.093	19

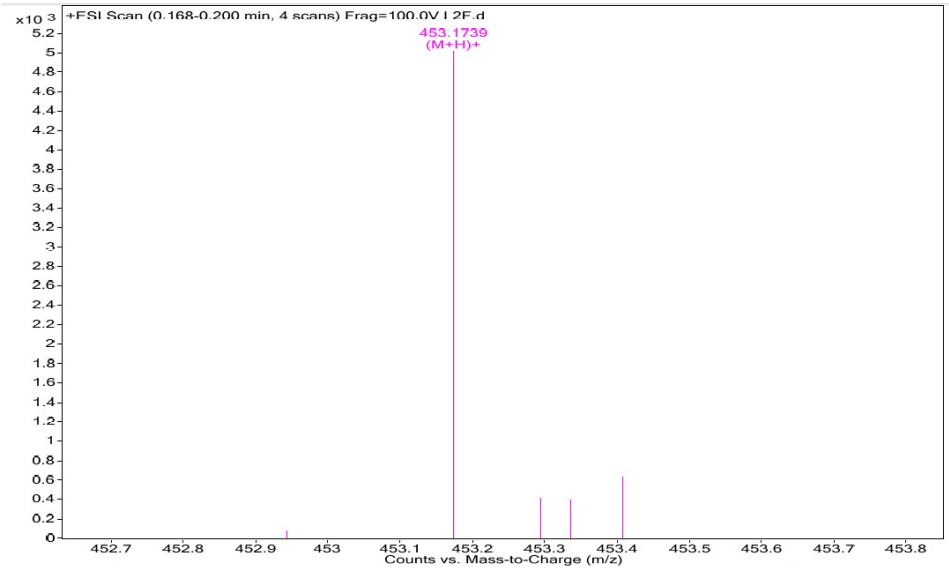
Compound 5k:



m/z	Ion	Formula	Abundance
480.1685	(M+H)+	C27 H22 N5 O4	11349.5

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C27 H21 N5 O4	C27 H22 N5 O4	480.1666	74.51		479.1614	479.1594	-4.26	4.26	90.26	39.12	82.75	480.1685	20

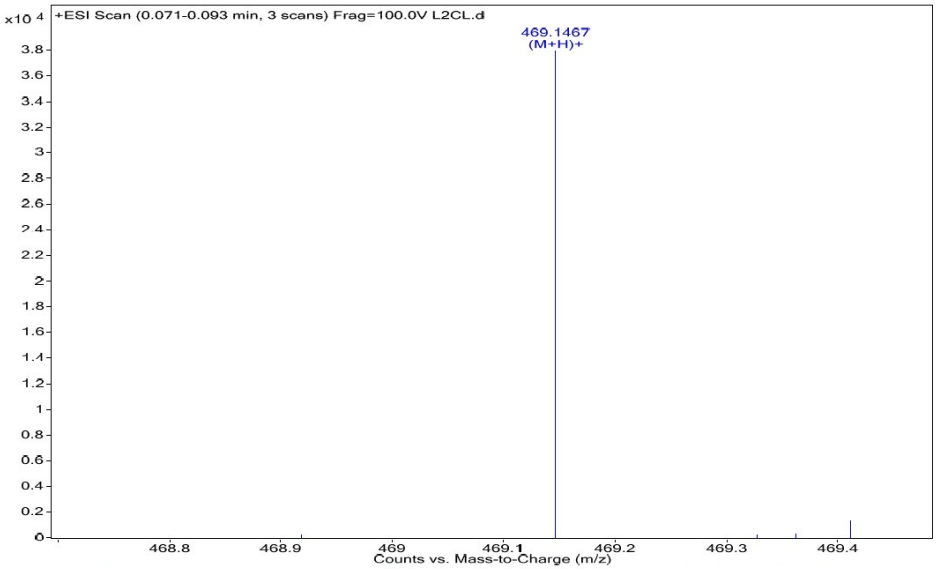
Compound 5l:



m/z	Ion	Formula	Abundance
453.1739	(M+H)+	C27 H22 F N4 O2	5015.8

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C27 H21 F N4 O2	C27 H22 F N4 O2	453.1721	67.45		452.1667	452.1649	-4.04	4.04	74.54	23.81	85.02	453.1739	19

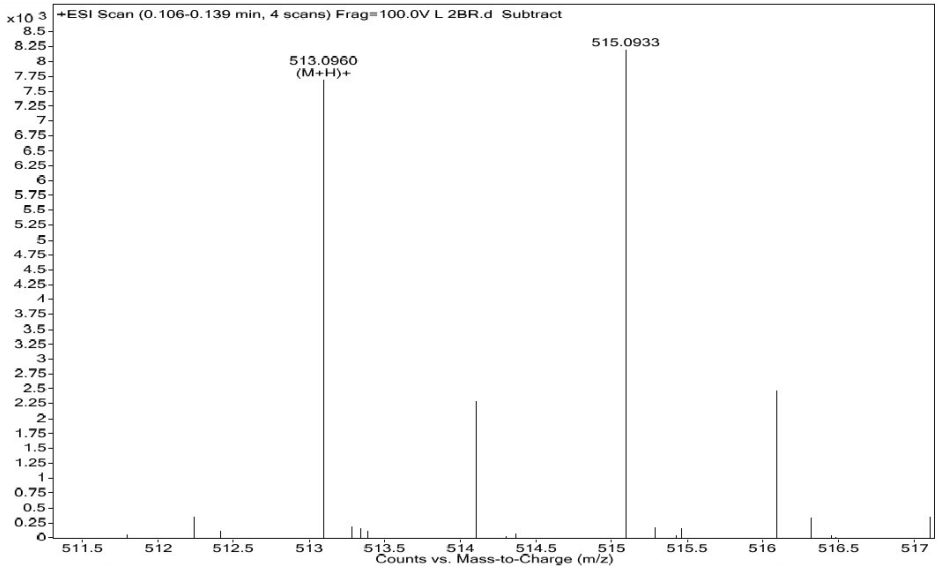
Compound 5m:



m/z	Ion	Formula	Abundance
469.1467	(M+H)+	C27 H22 Cl N4 O2	37946.4

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C27 H21 Cl N4 O2	C27 H22 Cl N4 O2	469.1426	73.59		468.1394	468.1353	-8.71	8.71	97.63	99.92	46	469.1467	19

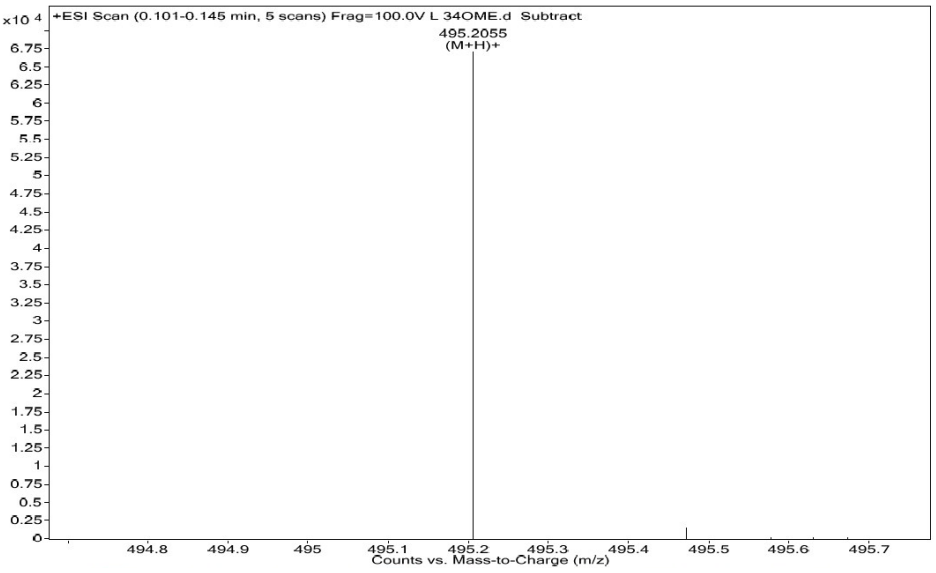
Compound 5n:



m/z	Ion	Formula	Abundance
513.096	(M+H)+	C27 H22 Br N4 O2	7683.9

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C27 H21 Br N4 O2	C27 H22 Br N4 O2	513.0921	77.73		512.0882	512.0848	-6.57	6.57	98.67	83.92	62.07	513.096	19

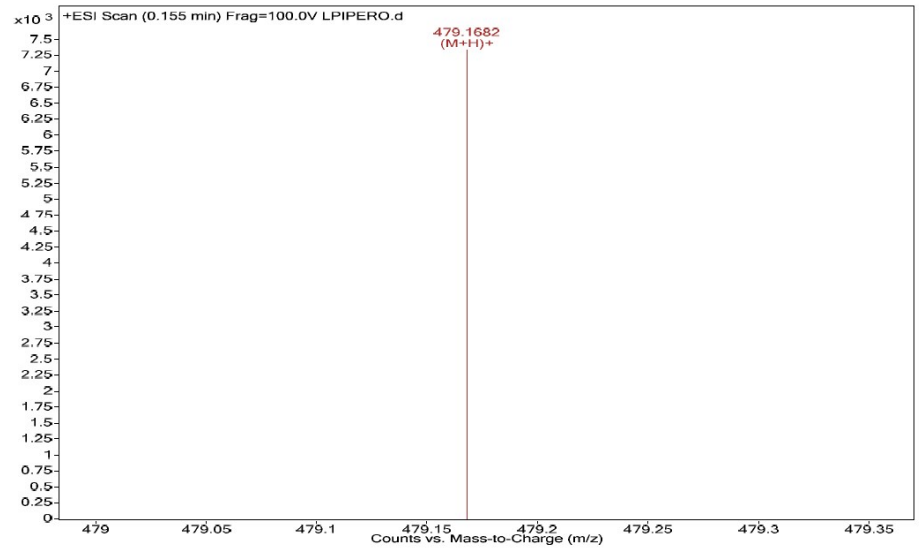
Compound 5o:



m/z	Ion	Formula	Abundance
495.2055	(M+H)+	C29 H27 N4 O4	67079.9

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C29 H26 N4 O4	C29 H27 N4 O4	495.2027	84.35		494.1983	494.1954	-5.77	5.77	95.83	99.34	69.96	495.2055	19

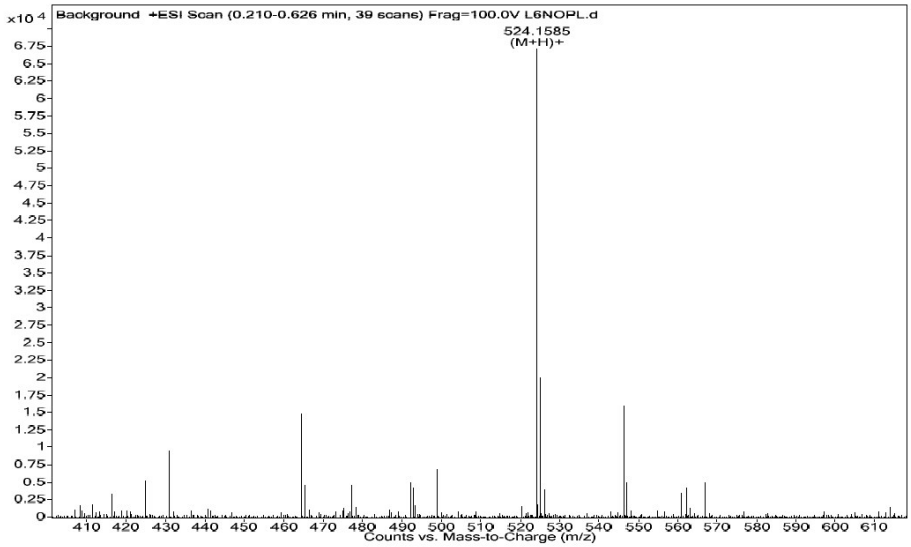
Compound 5p:



m/z	Ion	Formula	Abundance
479.1682	(M+H)+	C28 H23 N4 O4	7329.7

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C28 H22 N4 O4	C28 H23 N4 O4	479.1714	62.12		478.1609	478.1641	6.62	6.62	72.39	47.31	63.36	479.1682	20

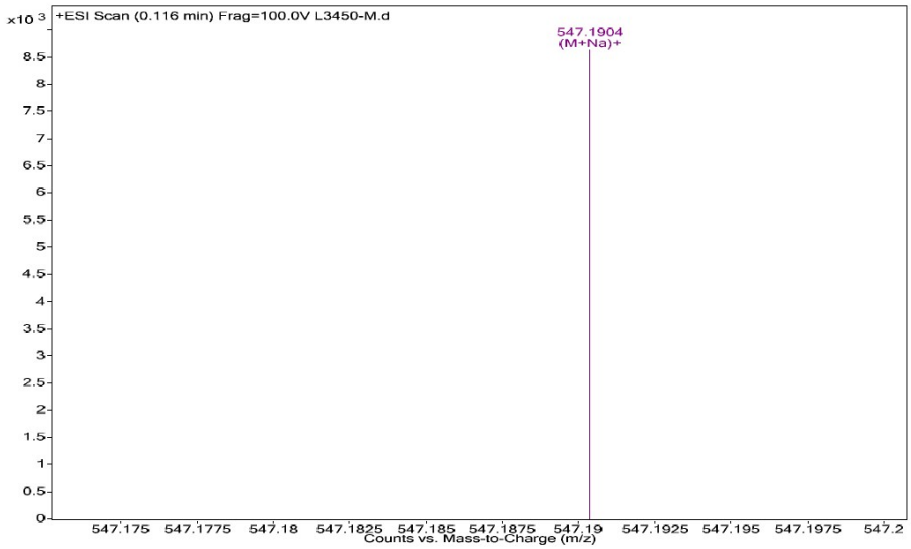
Compound 5q:



m/z	Ion	Formula	Abundance
524.1585	(M+H)+	C28 H22 N5 O6	67097.5

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C28 H21 N5 O6	C28 H22 N5 O6	524.1565	91.44		523.1512	523.1492	-3.86	3.86	96.1	99.56	84.59	524.1585	21

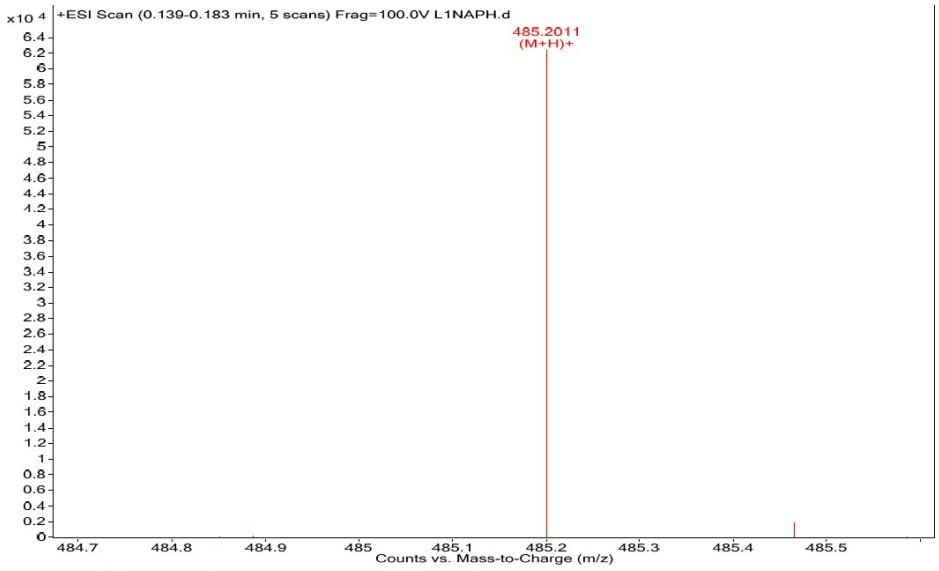
Compound 5r:



m/z	Ion	Formula	Abundance
547.1904	(M+Na)+	C30 H28 N4 Na O5	8626.1

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C30 H28 N4 O5	C30 H28 N4 Na O5	547.1952	42.78		524.2013	524.206	8.85	8.85	66.38	13.56	43.24	547.1904	19

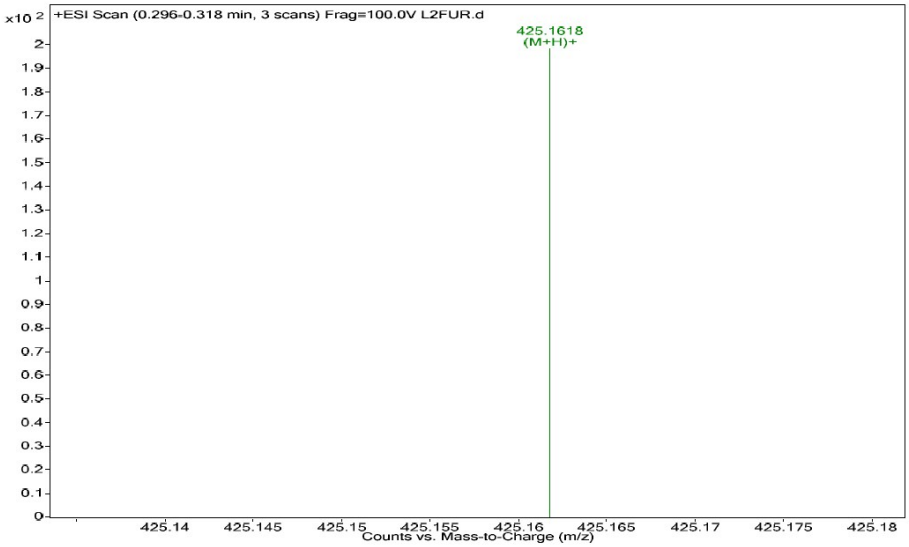
Compound 5s:



m/z	Ion	Formula	Abundance
485.2011	(M+H)+	C31 H25 N4 O2	62370.6

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C31 H24 N4 O2	C31 H25 N4 O2	485.1972	75.76		484.1938	484.1899	-8.05	8.05	98.53	98.87	50.55	485.2011	22

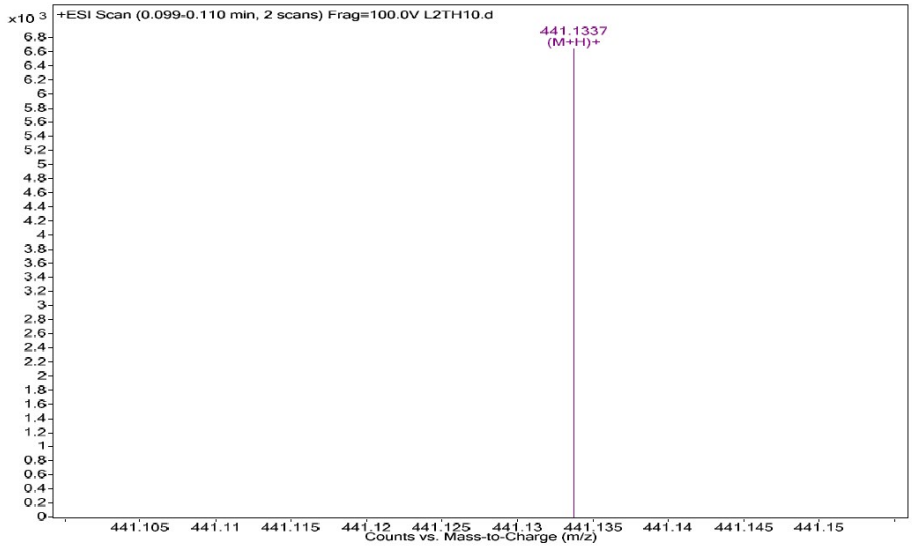
Compound 5t:



m/z	Ion	Formula	Abundance
425.1618	(M+H)+	C25 H21 N4 O3	198.2

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C25 H20 N4 O3	C25 H21 N4 O3	425.1608	45.43		424.1545	424.1535	-2.24	2.24	0	0	95.41	425.1618	18

Compound 5u:



m/z	Ion	Formula	Abundance
441.1337	(M+H)+	C25 H21 N4 O2..	6638.3

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☑	C25 H20 N4 O2 S	C25 H21 N4 O2 S	441.138	57.21		440.1265	440.1307	9.56	9.56	81.61	59.93	41.21	441.1337	18

Crystal data and tables for 5e

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{27}H_{21}FN_4O_2$
Formula Weight	452.49
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.380 X 0.350 X 0.320 mm
Crystal System	triclinic
Lattice Type	Primitive

Lattice Parameters	a = 9.4863(6) Å b = 10.0848(6) Å c = 13.3834(9) Å α = 110.202(3) ^{o} β = 91.710(3) ^{o} γ = 112.977(2) ^{o} V = 1086.0(2) Å^{3}
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.384 g/cm^{3}
F_{000}	472.00
μ(MoKα)	0.954 cm^{-1}

B. Intensity Measurements

Diffractometer	SCX mini
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Voltage, Current	50kV, 30mA
Temperature	20.0^{o}C
Detector Aperture	75 mm (diameter)
Data Images	540 exposures
ω oscillation Range	-120.0 - 60.0^{o}
Exposure Rate	10.0 sec./^{o}
Detector Swing Angle	-30.80^{o}

ω oscillation Range	-120.0 - 60.0^{o}
Exposure Rate	10.0 sec./^{o}
Detector Swing Angle	-30.80^{o}
ω oscillation Range	-120.0 - 60.0^{o}
Exposure Rate	10.0 sec./^{o}
Detector Swing Angle	-30.80^{o}
Detector Position	52.00 mm
Pixel Size	0.146 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 11036 Unique: 4940 (R_{int} = 0.0189)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.789 - 0.970)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	w = 1/ [$\sigma^2(Fo^2)$ + $(0.0679 \cdot P)^2$ + 0.2919 $\cdot$ P] where P = $(Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.0^{o}
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	4940
No. Variables	307
Reflection/Parameter Ratio	16.09

Residuals: R1 (I>2.00σ(I))	0.0453
Residuals: R (All reflections)	0.0525
Residuals: wR2 (All reflections)	0.1289
Goodness of Fit Indicator	0.997
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.25 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.23 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
F1	-0.2406(2)	-0.3203(2)	0.3305(2)	9.53(5)
O1	0.5352(2)	0.4055(2)	0.59710(9)	5.35(3)
O2	0.4712(2)	0.1644(2)	0.56563(9)	6.32(4)
N1	0.5996(2)	0.1866(2)	0.27287(9)	2.82(2)
N2	0.3059(2)	0.2253(2)	0.21070(9)	3.02(2)
N3	0.2303(2)	0.0239(2)	-0.01488(9)	3.09(2)
N4	0.4891(2)	0.2696(2)	0.53571(9)	3.65(3)
C1	0.4376(2)	0.0627(2)	0.23801(9)	2.49(2)
C2	0.3861(2)	0.0597(2)	0.34710(9)	2.49(2)
C3	0.4544(2)	0.2338(2)	0.4169(1)	2.80(3)
C4	0.6047(2)	0.3103(2)	0.3745(1)	3.32(3)
C5	0.7636(2)	0.3669(3)	0.4451(2)	5.39(5)
C6	0.8524(2)	0.2958(2)	0.3683(2)	4.63(4)
C7	0.7245(2)	0.1417(2)	0.2935(2)	3.72(3)
C8	0.4232(2)	-0.0912(2)	0.1532(1)	2.62(2)
C9	0.4693(2)	-0.2004(2)	0.1651(1)	3.28(3)
C10	0.4477(2)	-0.3307(2)	0.0740(2)	3.91(3)
C11	0.3817(2)	-0.3525(2)	-0.0276(2)	3.96(3)
C12	0.3319(2)	-0.2474(2)	-0.0405(1)	3.42(3)
C13	0.3519(2)	-0.1171(2)	0.0506(1)	2.66(2)
C14	0.3031(2)	0.0068(2)	0.0610(1)	2.58(2)
C15	0.3434(2)	0.1090(2)	0.17270(9)	2.51(2)
C16	0.2261(2)	0.2464(2)	0.1334(1)	3.02(3)
C17	0.1786(2)	0.3681(2)	0.1662(2)	4.14(3)
C18	0.1006(2)	0.3917(2)	0.0910(2)	4.69(4)
C19	0.0675(2)	0.2955(2)	-0.0190(2)	4.60(4)
C20	0.1116(2)	0.1765(2)	-0.0532(2)	4.02(3)
C21	0.1916(2)	0.1479(2)	0.0220(1)	3.03(3)
C22	0.2163(2)	-0.0377(2)	0.3422(1)	2.83(3)
C23	0.1043(2)	0.0200(2)	0.3561(2)	3.89(3)
C24	-0.0495(2)	-0.0745(3)	0.3530(2)	5.02(4)
C25	-0.0902(2)	-0.2268(3)	0.3341(2)	5.48(4)
C26	0.0152(3)	-0.2895(3)	0.3189(2)	6.13(5)
C27	0.1683(2)	-0.1940(2)	0.3238(2)	4.47(4)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H2	0.4459	0.0167	0.3765	2.99
H3	0.3799	0.2745	0.4045	3.36
H4	0.6008	0.3967	0.3584	3.98
H5A	0.8174	0.4801	0.4750	6.46
H5B	0.7510	0.3310	0.5041	6.46
H6A	0.9035	0.3603	0.3289	5.56
H6B	0.9296	0.2809	0.4067	5.56
H7A	0.7572	0.0972	0.2269	4.46
H7B	0.6916	0.0674	0.3282	4.46
H9	0.5138	-0.1865	0.2329	3.93
H10	0.4780	-0.4048	0.0812	4.69
H11	0.3710	-0.4394	-0.0878	4.75
H12	0.2859	-0.2630	-0.1085	4.10
H17	0.2001	0.4328	0.2392	4.97
H18	0.0694	0.4725	0.1132	5.63
H19	0.0148	0.3130	-0.0692	5.51
H20	0.0891	0.1135	-0.1266	4.83
H23	0.1329	0.1243	0.3678	4.67
H24	-0.1234	-0.0342	0.3638	6.03
H26	-0.0156	-0.3946	0.3054	7.36
H27	0.2412	-0.2356	0.3145	5.37

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F1	0.0543(8)	0.106(1)	0.191(2)	0.0138(7)	0.0503(9)	0.067(2)
O1	0.0803(9)	0.0582(7)	0.0388(6)	0.0250(7)	0.0042(6)	-0.0047(6)
O2	0.144(2)	0.083(1)	0.0345(6)	0.068(1)	0.0087(7)	0.0252(6)
N1	0.0383(6)	0.0373(6)	0.0329(6)	0.0171(5)	0.0055(5)	0.0140(5)
N2	0.0475(7)	0.0387(6)	0.0338(6)	0.0231(5)	0.0042(5)	0.0151(5)
N3	0.0405(6)	0.0467(7)	0.0314(6)	0.0172(5)	0.0038(5)	0.0183(5)
N4	0.0544(8)	0.0538(8)	0.0298(6)	0.0292(6)	0.0039(5)	0.0090(6)
C1	0.0375(7)	0.0339(6)	0.0273(6)	0.0187(5)	0.0057(5)	0.0128(5)
C2	0.0382(7)	0.0353(6)	0.0260(6)	0.0199(5)	0.0050(5)	0.0128(5)
C3	0.0426(7)	0.0389(7)	0.0274(6)	0.0222(6)	0.0032(5)	0.0105(5)
C4	0.0452(8)	0.0357(7)	0.0398(7)	0.0151(6)	0.0061(6)	0.0112(6)
C5	0.0425(9)	0.071(2)	0.053(1)	0.0094(8)	-0.0033(7)	-0.0003(9)
C6	0.0396(8)	0.062(1)	0.064(1)	0.0147(8)	0.0040(7)	0.0210(9)
C7	0.0382(7)	0.0526(9)	0.0518(9)	0.0212(7)	0.0049(6)	0.0200(7)
C8	0.0372(7)	0.0350(6)	0.0296(6)	0.0173(5)	0.0097(5)	0.0127(5)
C9	0.0515(8)	0.0434(7)	0.0387(7)	0.0275(7)	0.0112(6)	0.0178(6)
C10	0.063(1)	0.0429(8)	0.0515(9)	0.0322(7)	0.0166(7)	0.0171(7)
C11	0.063(1)	0.0401(8)	0.0425(8)	0.0251(7)	0.0144(7)	0.0071(6)
C12	0.0503(8)	0.0431(8)	0.0318(7)	0.0189(6)	0.0081(6)	0.0104(6)
C13	0.0353(6)	0.0354(6)	0.0294(6)	0.0141(5)	0.0077(5)	0.0127(5)
C14	0.0326(6)	0.0363(6)	0.0284(6)	0.0127(5)	0.0059(5)	0.0141(5)
C15	0.0345(6)	0.0343(6)	0.0285(6)	0.0146(5)	0.0054(5)	0.0147(5)
C16	0.0389(7)	0.0403(7)	0.0410(7)	0.0176(6)	0.0051(6)	0.0216(6)
C17	0.061(1)	0.0493(9)	0.0552(9)	0.0318(8)	0.0044(7)	0.0213(7)
C18	0.060(1)	0.058(1)	0.077(2)	0.0342(8)	0.0054(9)	0.0356(9)
C19	0.0523(9)	0.069(1)	0.070(1)	0.0274(8)	0.0015(8)	0.045(1)
C20	0.0489(9)	0.063(1)	0.0466(8)	0.0217(8)	0.0004(7)	0.0316(8)
C21	0.0353(7)	0.0458(7)	0.0389(7)	0.0154(6)	0.0053(5)	0.0243(6)
C22	0.0409(7)	0.0428(7)	0.0285(6)	0.0200(6)	0.0076(5)	0.0168(5)
C23	0.0465(8)	0.0538(9)	0.0574(9)	0.0275(7)	0.0133(7)	0.0254(8)
C24	0.0459(9)	0.080(2)	0.077(2)	0.0328(9)	0.0192(8)	0.036(1)
C25	0.0448(9)	0.073(2)	0.086(2)	0.0151(9)	0.0238(9)	0.037(1)
C26	0.066(2)	0.052(1)	0.114(2)	0.0171(9)	0.036(2)	0.040(2)
C27	0.0524(9)	0.0482(9)	0.078(2)	0.0237(8)	0.0239(8)	0.0307(9)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
F1	C25	1.357(3)	O1	N4	1.2152(17)
O2	N4	1.213(3)	N1	C1	1.4816(14)
N1	C4	1.4785(18)	N1	C7	1.474(3)
N2	C15	1.299(2)	N2	C16	1.385(3)
N3	C14	1.308(3)	N3	C21	1.373(3)
N4	C3	1.4989(19)	C1	C2	1.5597(18)
C1	C8	1.5245(18)	C1	C15	1.530(3)
C2	C3	1.5223(17)	C2	C22	1.5099(17)
C3	C4	1.563(2)	C4	C5	1.537(3)
C5	C6	1.515(3)	C6	C7	1.5070(18)
C8	C9	1.387(3)	C8	C13	1.403(2)
C9	C10	1.387(2)	C10	C11	1.388(3)
C11	C12	1.375(3)	C12	C13	1.3907(18)
C13	C14	1.459(3)	C14	C15	1.4277(16)
C16	C17	1.405(3)	C16	C21	1.4174(18)
C17	C18	1.370(4)	C18	C19	1.398(3)
C19	C20	1.360(3)	C20	C21	1.414(3)
C22	C23	1.386(3)	C22	C27	1.385(3)
C23	C24	1.387(3)	C24	C25	1.354(4)
C25	C26	1.362(4)	C26	C27	1.378(3)

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C2	H2	0.980	C3	H3	0.980
C4	H4	0.980	C5	H5A	0.970
C5	H5B	0.970	C6	H6A	0.970
C6	H6B	0.970	C7	H7A	0.970
C7	H7B	0.970	C9	H9	0.930
C10	H10	0.930	C11	H11	0.930
C12	H12	0.930	C17	H17	0.930
C18	H18	0.930	C19	H19	0.930
C20	H20	0.930	C23	H23	0.930
C24	H24	0.930	C26	H26	0.930
C27	H27	0.930			

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C1	N1	C4	107.11(11)	C1	N1	C7	117.30(12)
C4	N1	C7	107.53(12)	C15	N2	C16	114.66(11)
C14	N3	C21	114.28(12)	O1	N4	O2	123.63(14)
O1	N4	C3	116.88(15)	O2	N4	C3	119.49(12)
N1	C1	C2	103.41(9)	N1	C1	C8	113.16(12)
N1	C1	C15	107.65(12)	C2	C1	C8	117.06(12)
C2	C1	C15	114.59(12)	C8	C1	C15	100.99(10)
C1	C2	C3	100.86(11)	C1	C2	C22	117.26(10)
C3	C2	C22	117.85(12)	N4	C3	C2	113.09(13)
N4	C3	C4	111.80(10)	C2	C3	C4	105.64(11)
N1	C4	C3	105.69(10)	N1	C4	C5	104.97(15)
C3	C4	C5	118.01(15)	C4	C5	C6	104.52(13)
C5	C6	C7	102.15(13)	N1	C7	C6	102.17(15)
C1	C8	C9	129.43(13)	C1	C8	C13	111.02(14)
C9	C8	C13	119.55(12)	C8	C9	C10	118.75(15)
C9	C10	C11	121.13(19)	C10	C11	C12	120.87(14)
C11	C12	C13	118.30(15)	C8	C13	C12	121.34(16)
C8	C13	C14	109.00(11)	C12	C13	C14	129.63(14)
N3	C14	C13	128.24(11)	N3	C14	C15	123.74(15)
C13	C14	C15	107.98(13)	N2	C15	C1	126.14(11)
N2	C15	C14	123.56(15)	C1	C15	C14	110.29(13)
N2	C16	C17	119.18(13)	N2	C16	C21	121.42(16)
C17	C16	C21	119.40(17)	C16	C17	C18	120.13(16)
C17	C18	C19	120.5(2)	C18	C19	C20	120.7(3)
C19	C20	C21	120.44(15)	N3	C21	C16	122.26(16)
N3	C21	C20	118.93(13)	C16	C21	C20	118.79(16)
C2	C22	C23	123.97(14)	C2	C22	C27	118.58(16)
C23	C22	C27	117.45(14)	C22	C23	C24	121.33(19)
C23	C24	C25	118.7(3)	F1	C25	C24	119.1(3)
F1	C25	C26	118.7(3)	C24	C25	C26	122.19(18)
C25	C26	C27	118.7(2)	C22	C27	C26	121.6(2)

Table 7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C1	C2	H2	106.7	C3	C2	H2	106.7
C22	C2	H2	106.7	N4	C3	H3	108.7
C2	C3	H3	108.7	C4	C3	H3	108.7
N1	C4	H4	109.3	C3	C4	H4	109.3
C5	C4	H4	109.3	C4	C5	H5A	110.8
C4	C5	H5B	110.8	C6	C5	H5A	110.8
C6	C5	H5B	110.9	H5A	C5	H5B	108.9
C5	C6	H6A	111.3	C5	C6	H6B	111.3
C7	C6	H6A	111.3	C7	C6	H6B	111.3
H6A	C6	H6B	109.2	N1	C7	H7A	111.3
N1	C7	H7B	111.3	C6	C7	H7A	111.3
C6	C7	H7B	111.3	H7A	C7	H7B	109.2
C8	C9	H9	120.6	C10	C9	H9	120.6
C9	C10	H10	119.4	C11	C10	H10	119.4
C10	C11	H11	119.6	C12	C11	H11	119.6
C11	C12	H12	120.9	C13	C12	H12	120.8
C16	C17	H17	119.9	C18	C17	H17	119.9
C17	C18	H18	119.7	C19	C18	H18	119.7
C18	C19	H19	119.7	C20	C19	H19	119.7
C19	C20	H20	119.8	C21	C20	H20	119.8
C22	C23	H23	119.3	C24	C23	H23	119.3
C23	C24	H24	120.6	C25	C24	H24	120.6
C25	C26	H26	120.6	C27	C26	H26	120.6
C22	C27	H27	119.2	C26	C27	H27	119.2

Table 8. Torsion Angles(°)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C1	N1	C4	C3	16.51(17)	C1	N1	C4	C5	141.96(12)
C4	N1	C1	C2	-36.48(15)	C4	N1	C1	C8	-164.12(12)
C4	N1	C1	C15	85.17(13)	C1	N1	C7	C6	-157.24(10)
C7	N1	C1	C2	84.42(14)	C7	N1	C1	C8	-43.22(16)
C7	N1	C1	C15	-153.94(11)	C4	N1	C7	C6	-36.56(15)
C7	N1	C4	C3	-110.39(13)	C7	N1	C4	C5	15.06(15)
C15	N2	C16	C17	179.30(11)	C15	N2	C16	C21	-0.72(18)
C16	N2	C15	C1	177.10(11)	C16	N2	C15	C14	-1.70(18)
C14	N3	C21	C16	-1.06(17)	C14	N3	C21	C20	-179.63(11)
C21	N3	C14	C13	176.02(11)	C21	N3	C14	C15	-1.37(17)
O1	N4	C3	C2	-175.77(13)	O1	N4	C3	C4	65.14(19)
O2	N4	C3	C2	4.7(2)	O2	N4	C3	C4	-114.43(17)
N1	C1	C2	C3	41.41(14)	N1	C1	C2	C22	170.76(12)
N1	C1	C8	C9	73.03(17)	N1	C1	C8	C13	-106.94(13)
N1	C1	C15	N2	-68.47(15)	N1	C1	C15	C14	110.46(10)
C2	C1	C8	C9	-47.09(18)	C2	C1	C8	C13	132.94(12)
C8	C1	C2	C3	166.57(11)	C8	C1	C2	C22	-64.08(17)
C2	C1	C15	N2	45.94(15)	C2	C1	C15	C14	-135.14(9)
C15	C1	C2	C3	-75.45(10)	C15	C1	C2	C22	53.90(15)
C8	C1	C15	N2	172.70(11)	C8	C1	C15	C14	-8.37(12)
C15	C1	C8	C9	-172.20(12)	C15	C1	C8	C13	7.83(13)
C1	C2	C3	N4	-153.69(11)	C1	C2	C3	C4	-31.11(14)
C1	C2	C22	C23	-92.76(15)	C1	C2	C22	C27	87.94(17)
C3	C2	C22	C23	28.04(19)	C3	C2	C22	C27	-151.26(12)
C22	C2	C3	N4	77.35(16)	C22	C2	C3	C4	-160.07(12)
N4	C3	C4	N1	133.71(13)	N4	C3	C4	C5	16.76(19)
C2	C3	C4	N1	10.31(17)	C2	C3	C4	C5	-106.64(13)
N1	C4	C5	C6	12.25(18)	C3	C4	C5	C6	129.59(14)
C4	C5	C6	C7	-34.1(2)	C5	C6	C7	N1	43.1(2)
C1	C8	C9	C10	-178.01(11)	C1	C8	C13	C12	177.38(10)
C1	C8	C13	C14	-4.66(14)	C9	C8	C13	C12	-2.59(19)
C9	C8	C13	C14	175.37(11)	C13	C8	C9	C10	1.96(19)
C8	C9	C10	C11	0.2(3)	C9	C10	C11	C12	-1.8(3)
C10	C11	C12	C13	1.1(3)	C11	C12	C13	C8	1.0(2)
C11	C12	C13	C14	-176.48(12)	C8	C13	C14	N3	-178.69(11)
C8	C13	C14	C15	-0.97(13)	C12	C13	C14	N3	-1.0(3)
C12	C13	C14	C15	176.77(13)	N3	C14	C15	N2	2.99(19)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
N3	C14	C15	C1	-175.98(11)	C13	C14	C15	N2	-174.86(10)
C13	C14	C15	C1	6.18(13)	N2	C16	C17	C18	179.50(12)
N2	C16	C21	N3	2.2(2)	N2	C16	C21	C20	-179.20(11)
C17	C16	C21	N3	-177.80(12)	C17	C16	C21	C20	0.78(19)
C21	C16	C17	C18	-0.5(3)	C16	C17	C18	C19	-0.0(3)
C17	C18	C19	C20	0.2(3)	C18	C19	C20	C21	0.1(3)
C19	C20	C21	N3	178.01(14)	C19	C20	C21	C16	-0.6(2)
C2	C22	C23	C24	-178.58(12)	C2	C22	C27	C26	179.67(13)
C23	C22	C27	C26	0.3(3)	C27	C22	C23	C24	0.7(3)
C22	C23	C24	C25	-1.1(3)	C23	C24	C25	F1	-179.75(18)
C23	C24	C25	C26	0.5(4)	F1	C25	C26	C27	-179.2(2)
C24	C25	C26	C27	0.5(4)	C25	C26	C27	C22	-0.9(4)

Table 9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
F1	C23	3.600(2)	F1	C27	3.595(3)
O1	C4	2.978(2)	O1	C5	3.059(3)
O2	C2	2.7168(17)	O2	C4	3.413(3)
O2	C5	3.548(3)	O2	C22	3.2338(17)
N1	N2	3.089(2)	N1	C9	3.3288(18)
N1	C13	3.3801(14)	N1	C14	3.3513(16)
N2	N3	2.8729(15)	N2	C2	3.117(3)
N2	C3	3.020(2)	N2	C4	3.164(2)
N2	C13	3.582(2)	N2	C22	3.523(3)
N2	C23	3.413(3)	N3	C12	3.156(3)
N4	C5	2.869(3)	N4	C22	3.2870(14)
C1	C5	3.5863(18)	C1	C23	3.520(3)
C1	C27	3.408(3)	C2	C5	3.5198(19)
C2	C7	3.158(2)	C2	C9	3.279(2)
C3	C7	3.348(3)	C3	C15	3.0484(17)
C3	C23	3.0620(19)	C4	C15	3.0729(17)
C7	C8	2.9335(16)	C7	C9	3.1387(17)
C8	C11	2.7722(19)	C8	C22	3.275(2)
C8	C27	3.485(3)	C9	C12	2.811(3)
C10	C13	2.747(3)	C14	C16	2.668(3)
C14	C20	3.555(3)	C15	C17	3.553(3)
C15	C21	2.666(3)	C15	C22	3.143(2)
C15	C23	3.499(3)	C16	C19	2.786(3)
C17	C20	2.788(3)	C18	C21	2.790(3)
C22	C25	2.759(3)	C23	C26	2.747(3)
C24	C27	2.746(4)			

Table 10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
F1	H24	2.518	F1	H26	2.519
O1	H3	2.542	O1	H4	3.251
O1	H5A	3.153	O1	H5B	2.648
O2	H2	2.401	O2	H3	2.988
O2	H5B	2.854	N1	H2	2.607
N1	H3	2.968	N1	H5A	3.116
N1	H5B	2.958	N1	H6A	2.639
N1	H6B	3.175	N1	H9	3.362
N2	H3	2.489	N2	H4	2.873
N2	H17	2.577	N2	H23	2.921
N3	H12	2.991	N3	H20	2.571
N4	H2	2.567	N4	H4	3.097
N4	H5A	3.323	N4	H5B	2.404
N4	H23	3.467	C1	H3	2.743
C1	H4	2.893	C1	H7A	2.928
C1	H7B	2.639	C1	H9	2.854
C1	H23	3.566	C1	H27	3.382
C2	H4	3.153	C2	H5B	3.476
C2	H7B	2.890	C2	H9	3.132
C2	H23	2.722	C2	H27	2.612
C3	H5A	3.234	C3	H5B	2.665
C3	H7B	3.320	C3	H23	2.775
C4	H2	2.759	C4	H6A	2.805
C4	H6B	3.241	C4	H7A	3.207
C4	H7B	2.762	C5	H2	3.418
C5	H3	3.360	C5	H7A	3.210
C5	H7B	2.665	C6	H4	2.953
C7	H2	2.890	C7	H4	3.101
C7	H5A	3.182	C7	H5B	2.742
C7	H9	2.914	C8	H2	2.774
C8	H7A	2.906	C8	H7B	2.900
C8	H10	3.227	C8	H12	3.276
C8	H27	3.194	C9	H2	2.998
C9	H7A	2.984	C9	H7B	2.777
C9	H11	3.249	C9	H27	2.993
C10	H12	3.245	C11	H9	3.256
C12	H10	3.235	C13	H9	3.256

Table 10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C13	H11	3.217	C14	H12	2.818
C15	H2	3.399	C15	H3	2.904
C15	H4	3.111	C15	H23	3.332
C16	H18	3.245	C16	H20	3.278
C17	H19	3.237	C18	H20	3.235
C19	H17	3.243	C20	H18	3.229
C21	H17	3.278	C21	H19	3.247
C22	H3	2.704	C22	H24	3.256
C22	H26	3.251	C23	H2	3.258
C23	H3	2.712	C23	H27	3.211
C24	H26	3.214	C25	H23	3.195
C25	H27	3.195	C26	H24	3.215
C27	H2	2.536	C27	H9	3.512
C27	H23	3.212	H2	H3	2.810
H2	H5B	3.185	H2	H7B	2.346
H2	H9	2.587	H2	H23	3.548
H2	H27	2.350	H3	H4	2.208
H3	H5B	3.482	H3	H23	2.162
H4	H5A	2.218	H4	H5B	2.782
H4	H6A	3.055	H5A	H6A	2.278
H5A	H6B	2.543	H5A	H7B	3.598
H5B	H6A	2.834	H5B	H6B	2.274
H5B	H7B	2.712	H6A	H7A	2.310
H6A	H7B	2.848	H6B	H7A	2.494
H6B	H7B	2.310	H7A	H9	2.922
H7B	H9	2.296	H9	H10	2.318
H9	H27	2.769	H10	H11	2.304
H11	H12	2.311	H17	H18	2.296
H18	H19	2.319	H19	H20	2.282
H23	H24	2.317	H26	H27	2.306

Table 11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
F1	O1[1]	2.889(3)	F1	O2[1]	3.247(3)
F1	N4[1]	3.095(3)	O1	F1[1]	2.889(3)
O1	N2[2]	3.3946(15)	O1	C4[2]	3.516(3)
O1	C17[2]	3.5029(19)	O2	F1[1]	3.247(3)
O2	O2[3]	3.439(3)	O2	C2[3]	3.525(3)
O2	C9[3]	3.500(2)	O2	C27[3]	3.545(3)
N1	C12[4]	3.405(2)	N2	O1[2]	3.3946(15)
N3	C19[5]	3.541(3)	N3	C20[5]	3.430(2)
N4	F1[1]	3.095(3)	C2	O2[3]	3.525(3)
C4	O1[2]	3.516(3)	C9	O2[3]	3.500(2)
C10	C18[6]	3.466(3)	C12	N1[4]	3.405(2)
C12	C14[4]	3.4509(19)	C13	C13[4]	3.5454(19)
C13	C14[4]	3.5745(19)	C14	C12[4]	3.4509(19)
C14	C13[4]	3.5745(19)	C14	C19[5]	3.507(2)
C17	O1[2]	3.5029(19)	C18	C10[7]	3.466(3)
C19	N3[5]	3.541(3)	C19	C14[5]	3.507(2)
C20	N3[5]	3.430(2)	C20	C21[5]	3.581(3)
C21	C20[5]	3.581(3)	C21	C21[5]	3.5576(17)
C27	O2[3]	3.545(3)			

Symmetry Operators:

(1) -X,-Y,-Z+1
(2) -X+1,-Y+1,-Z+1
(3) -X+1,-Y,-Z+1
(4) -X+1,-Y,-Z
(5) -X,-Y,-Z
(6) X,Y-1,Z
(7) X,Y+1,Z

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
F1	H4[1]	2.822	F1	H5A[1]	3.403
F1	H9[2]	3.527	F1	H11[3]	3.152
O1	H3[4]	3.014	O1	H4[4]	2.690
O1	H17[4]	2.788	O1	H27[5]	3.594
O2	H2[5]	2.573	O2	H7B[5]	3.079
O2	H9[5]	2.622	O2	H24[6]	3.342
O2	H27[5]	2.819	N1	H12[7]	2.697
N3	H7A[7]	2.701	N4	H9[5]	3.474
N4	H27[5]	3.396	C1	H12[7]	3.538
C5	H6B[8]	3.426	C6	H5A[8]	3.182
C6	H12[7]	3.538	C6	H24[9]	3.405
C6	H26[10]	3.294	C7	H12[7]	3.132
C7	H24[9]	3.030	C10	H10[11]	3.107
C10	H11[11]	3.429	C10	H18[12]	3.516
C11	H10[11]	3.109	C12	H7A[7]	3.565
C12	H18[13]	3.478	C12	H19[13]	3.559
C13	H19[13]	3.330	C14	H7A[7]	3.589
C14	H19[13]	3.490	C15	H12[7]	3.515
C17	H6A[2]	3.442	C17	H10[14]	3.395
C17	H27[14]	3.586	C18	H10[14]	3.395
C18	H12[13]	3.425	C18	H26[14]	3.445
C18	H27[14]	3.597	C19	H11[14]	3.484
C21	H7A[7]	3.577	C23	H6B[2]	3.516
C23	H20[13]	3.080	C24	H6B[2]	3.491
C24	H7B[2]	3.348	C24	H20[13]	2.910
C25	H19[13]	3.513	C25	H20[13]	3.346
C26	H5B[5]	3.435	C26	H6A[1]	3.322
C26	H18[12]	3.176	C26	H19[13]	3.262
C27	H5B[5]	3.273	C27	H18[12]	3.312
C27	H19[13]	3.355	H2	O2[5]	2.573
H2	H2[5]	3.596	H3	O1[4]	3.014
H4	F1[10]	2.822	H4	O1[4]	2.690
H4	H12[7]	3.520	H5A	F1[10]	3.403
H5A	C6[8]	3.182	H5A	H5A[8]	3.348
H5A	H6A[8]	3.135	H5A	H6B[8]	2.588
H5A	H26[10]	3.145	H5B	C26[5]	3.435
H5B	C27[5]	3.273	H5B	H6A[8]	3.496

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H5B	H17^{4}	3.329	H5B	H26^{5}	3.231
H5B	H27^{5}	2.911	H6A	C17^{9}	3.442
H6A	C26^{10}	3.322	H6A	H5A^{8}	3.135
H6A	H5B^{8}	3.496	H6A	H12^{7}	3.034
H6A	H17^{9}	3.015	H6A	H26^{10}	2.423
H6B	C5^{8}	3.426	H6B	C23^{9}	3.516
H6B	C24^{9}	3.491	H6B	H5A^{8}	2.588
H6B	H23^{9}	2.890	H6B	H24^{9}	2.855
H6B	H26^{5}	3.585	H7A	N3^{7}	2.701
H7A	C12^{7}	3.565	H7A	C14^{7}	3.589
H7A	C21^{7}	3.577	H7A	H12^{7}	2.793
H7A	H20^{7}	3.002	H7A	H24^{9}	3.020
H7B	O2^{5}	3.079	H7B	C24^{9}	3.348
H7B	H24^{9}	2.459	H9	F1^{9}	3.527
H9	O2^{5}	2.622	H9	N4^{5}	3.474
H9	H24^{9}	3.305	H10	C10^{11}	3.107
H10	C11^{11}	3.109	H10	C17^{12}	3.395
H10	C18^{12}	3.395	H10	H10^{11}	2.526
H10	H11^{11}	2.525	H11	F1^{3}	3.152
H11	C10^{11}	3.429	H11	C19^{12}	3.484
H11	H10^{11}	2.525	H11	H19^{12}	3.407
H12	N1^{7}	2.697	H12	C1^{7}	3.538
H12	C6^{7}	3.538	H12	C7^{7}	3.132
H12	C15^{7}	3.515	H12	C18^{13}	3.425
H12	H4^{7}	3.520	H12	H6A^{7}	3.034
H12	H7A^{7}	2.793	H12	H18^{13}	3.188
H12	H26^{3}	3.442	H17	O1^{4}	2.788
H17	H5B^{4}	3.329	H17	H6A^{2}	3.015
H17	H26^{14}	3.135	H17	H27^{14}	2.997
H18	C10^{14}	3.516	H18	C12^{13}	3.478
H18	C26^{14}	3.176	H18	C27^{14}	3.312
H18	H12^{13}	3.188	H18	H18^{15}	3.566
H18	H19^{15}	2.804	H18	H26^{14}	2.766
H18	H27^{14}	3.016	H19	C12^{13}	3.559
H19	C13^{13}	3.330	H19	C14^{13}	3.490
H19	C25^{13}	3.513	H19	C26^{13}	3.262
H19	C27^{13}	3.355	H19	H11^{14}	3.407

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H19	H18[15]	2.804	H19	H26[13]	3.530
H20	C23[13]	3.080	H20	C24[13]	2.910
H20	C25[13]	3.346	H20	H7A[7]	3.002
H20	H23[13]	3.303	H20	H24[13]	3.054
H23	H6B[2]	2.890	H23	H20[13]	3.303
H24	O2[6]	3.342	H24	C6[2]	3.405
H24	C7[2]	3.030	H24	H6B[2]	2.855
H24	H7A[2]	3.020	H24	H7B[2]	2.459
H24	H9[2]	3.305	H24	H20[13]	3.054
H26	C6[1]	3.294	H26	C18[12]	3.445
H26	H5A[1]	3.145	H26	H5B[5]	3.231
H26	H6A[1]	2.423	H26	H6B[5]	3.585
H26	H12[3]	3.442	H26	H17[12]	3.135
H26	H18[12]	2.766	H26	H19[13]	3.530
H27	O1[5]	3.594	H27	O2[5]	2.819
H27	N4[5]	3.396	H27	C17[12]	3.586
H27	C18[12]	3.597	H27	H5B[5]	2.911
H27	H17[12]	2.997	H27	H18[12]	3.016

Symmetry Operators:

(1) X-1,Y-1,Z
(2) X-1,Y,Z
(3) -X,-Y-1,-Z
(4) -X+1,-Y+1,-Z+1
(5) -X+1,-Y,-Z+1
(6) -X,-Y,-Z+1
(7) -X+1,-Y,-Z
(8) -X+2,-Y+1,-Z+1
(9) X+1,Y,Z
(10) X+1,Y+1,Z
(11) -X+1,-Y-1,-Z
(12) X,Y-1,Z
(13) -X,-Y,-Z
(14) X,Y+1,Z
(15) -X,-Y+1,-Z